Supplementary Material

The low K_{Enol} values of β-sulfonyl-substituted amides

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Dedicated to Prof. Michael Orfanopoulos of the University of Crete, Greece on the occasions of his 67th birthday and his retirement

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Table S1. ^{1}H-NMR Spectral Data (in ppm) for R'NHCOCH(SO_2R)Y and Their Enols R'NHC(OH)=C(SO_2R)Y in Several Solvents at Room Temperature[a]

Num.	Y	R	R'	Solvent	Species	Y	R	R'	CH/OH	NH
5a/6a	CO_2Me	Ph	Ph	$CDCl_3$	Amide	3.85	7.57 (2H, t, J = 7.5 Hz), 7.72 (1H, t, J = 7.5 Hz), 7.93 (2H, d, J = 7.3 Hz)	7.17 (IH, t, J = 7.3 Hz), 7.34 (2H, t, J = 8.2 Hz), 7.47 (2H, d, J = 7.7 Hz)	4.96	8.96
				CCl_4	Amide	3.01	6.76 (2H, t, J = 7.6 Hz), 6.87 (1H, t, J = 7.5 Hz), 7.10 (2H, d, J = 7.5 Hz)	6.29 (IH, t, J = 7.5 Hz), 6.49 (2H, t, J = 8.1 Hz), 6.68 (2H, d, J = 7.7 Hz)	3.94	8.06
5b/6b	CO_2Me	Ph	2.4-$(MeO)_2C_6H_3$	$CDCl_3$	Amide	3.87	7.53 (2H, t, J = 7.6 Hz), 7.67 (1H, t, J = 7.5 Hz), 7.92 (2H, d, J = 7.5 Hz)	3.78 (3H, s), 3.82 (3H, s), 6.42 (1H, d, J = 8.6 Hz), 6.47 (1H, s), 8.05 (1H, d, J = 8.6 Hz)	4.97	9.34
					Enol	[b]	[b]	[b]	16.14	10.82
				CCl_4	Amide	2.97	6.73 (2H, t, J = 7.5 Hz), 6.84 (1H, t, J = 8.0 Hz), 7.10 (2H, d, J = 7.6 Hz)	3.09 (3H, s), 3.16 (3H, s), 5.55 (1H, d, J = 8.6 Hz), 5.55 (1H, d, J = 2.8 Hz), 7.21 (1H, d, J = 8.8 Hz)	3.92	8.45
					Enol	[b]	[b]	[b]	15.49	10.20
				C_6D_6	Amide	3.22	6.80 (2H, t, J = 7.6 Hz), 6.88 (1H, t, J = 7.9 Hz), 7.86 (2H, d, J = 7.6 Hz)	3.17 (3H, s), 3.29 (3H, s), 6.42 (1H, dd, J_1 = 8.8 Hz, J_2 = 2.8 Hz), 6.35 (1H, d, J = 2.8	5.06	9.82

								Hz), 8.62 (1H, d, J = 8.8 Hz)		
				DMSO-d_6	Amide	3.85	7.65 (2H, t, J = 7.4 Hz), 7.77 (1H, t, J = 7.2 Hz), 7.94 (2H, d, J = 7.5 Hz)	3.67 (1H, s), 3.82 (1H, s), 6.50 (1H, d, J = 8.6 Hz), 6.47 (1H, s), 7.83 (1H, d, J = 8.8 Hz)	6.08	9.63
5c/6c	CO_2Me	Ph	*i*-Pr	CCl_4[c]	Amide	3.02	6.78 (2H, t, J = 7.3 Hz), 6.89 (1H, t, J = 7.3 Hz), 7.10 (2H, d, J = 7.4 Hz)	0.43 (6H, d, J = 6.5 Hz), 3.16 (1H, oct, J = 6.7 Hz)	3.81	6.08 (d, J 6.6 = Hz)
					Enol	[b]	6.66, [b] , 7.00	0.57 (d, J = 6.6 Hz),[b]	14.98	8.10
				$CDCl_3$	Amide	3.79	7.59 (2H, t, J = 7.5 Hz), 7.72 (1H, t, J = 7.3 Hz), 7.92 (2H, d, J = 7.8 Hz)	1.17 (6H, dd, J_1 J_2 = 6.6 Hz), 3.99 (1H, oct, J = 6.6 Hz)	4.48	6.99 (d, J 6.2 = Hz)
					Enol	[b]	[b]	[b]	15.60	8.02
				DMSO-d_6	Amide	3.64	7.64 (2H, t, J = 7.4 Hz), 7.77 (1H, t, J = 7.4 Hz), 7.87 (2H, d, J = 7.8 Hz)	0.97 (3H, d, J = 6.5 Hz), 1.03 (3H, d, J = 6.6 Hz), 3.74 (1H, oct, J = 6.6 Hz)	5.34	8.19 (d, J 7.4 = Hz)
5d/6d	CO_2Me	Ph	*t*-Bu	$CDCl_3$	Amide	3.80	7.59 (2H, t, J = 7.5 Hz), 7.72 (1H, t, J = 7.4 Hz), 7.93 (2H, d, J = 7.8 Hz)	1.33	4.75	7.00
5e/6e	SO_2Ph	Ph	Ph	$CDCl_3$	Amide	[d]	7.57 (4H, t, J = 7.4 Hz), 7.73 (2H, t, J = 7.1 Hz), 7.95 (4H, d, J = 7.4 Hz)	7.21 (1H, t, J = 7.4 Hz), 7.36 (2H, t, J = 7.9 Hz), 7.43 (2H, d, J = 7.8 Hz)	5.27	8.75

				DMSO-d_6	Amide	[d]	7.66 (4H, t, J = 7.6 Hz), 7.80 (2H, t, J = 7.4 Hz), 7.92 (4H, d, J = 7.6 Hz)	7.12-7.17 (1H, m), 7.30-7.35 (4H, m)	6.35	10.42
5f/6f	SO_2Ph	Ph	2.4-$(MeO)_2C_6H_3$	$CDCl_3$	Amide	[d]	7.57 (4H, t, J = 8.0 Hz), 7.84 (2H, t, J = 8.9 Hz), 7.97 (4H, d, J = 8.1 Hz)	3.80 (3H, s), 3.96 (3H, s), 6.42 (1H, s), 6.53 (1H, d, J = 7.6 Hz), 7.70 (1H, d, J = 7.5 Hz)	5.27	9.20
5g/6g	SO_2Ph	Ph	*i*-Pr	$CDCl_3$	Amide	[d]	7.56 (4H, t, J = 8.0 Hz), 7.80 (2H, t, J = 7.4 Hz), 7.92 (4H, d, J = 7.7 Hz)	1.18 (6H, d, J = 6.6 Hz), 3.95 (1H, oct, J = 6.6 Hz)	5.26	8.19 (d, J 7.4 = Hz)
5h/6h	SO_2Ph	Ph	*t*-Bu	$CDCl_3$	Amide	[d]	7.56 (4H, t, J = 7.8 Hz), 7.70 (2H, t, J = 7.5 Hz), 7.94 (4H, d, J =7.8 Hz)	1.31	5.18	6.77
				DMSO-d_6	Amide	[d]	7.65 (4H, t, J = 7.7 Hz), 7.79 (2H, t, J = 7.6 Hz), 7.87 (4H, d, J = 7.8 Hz)	1.00	6.19	7.89
5i/6i	SO_2Me	Ph	Ph	$CDCl_3$	Amide	3.42	7.58 (2H, t, J = 7.5 Hz), 7.73 (1H, t, J = 7.5 Hz), 7.96 (2H, d, J = 7.7 Hz)	7.19 (1H, t, J = 7.3 Hz), 7.34 (2H, t, J = 8.2 Hz), 7.44 (2H, d, J = 8.1 Hz)	5.27	8.42
				DMSO-d_6	Amide	3.47	7.58 (2H, t, J = 7.5 Hz), 7.72 (1H, t, J = 7.4 Hz), 7.96 (2H, d, J = 7.8 Hz)	7.17 (1H, t, J = 7.3 Hz), 7.34 (2H, t, J = 8.2 Hz), 7.43 (2H, d, J = 8.1 Hz)	6.07	10.62

5j/6j	SO_2 Me	Ph	*i*-Pr	$CDCl_3$	Amide	3.36	7.61 (2H, t, J = 7.4 Hz), 7.74 (1H, t, J = 7.4 Hz), 7.96 (2H, d, J = 7.8 Hz)	1.14 (3H, d, J = 6.6 Hz), 1.18 (3H, d, J = 6.6 Hz), 4.01 (1H, oct, J = 6.7 Hz)	5.05	6.43
				DMSO-d_6	Amide	3.40	7.70 (2H, t, J = 7.7 Hz), 7.83 (1H, t, J = 7.1 Hz), 7.96 (2H, d, J = 8.1 Hz)	0.81 (3H, d, J = 6.5 Hz), 1.18 (3H, d, J = 6.6 Hz), 4.01 (1H, oct, J = 6.7 Hz)	5.82	8.35 (d, J 7.5 = Hz)
5k/6k	CN	Ph	Ph	$CDCl_3$	Amide		7.65 (2H, t, J = 8.0 Hz), 7.81 (1H, t, J = 7.6 Hz), 8.02 (2H, d, J = 7.6 Hz)	7.22 (1H, t, J = 7.6 Hz), 7.38 (2H, t, J = 8.4 Hz), 7.50 (2H, d, J = 8.1 Hz)	5.03	8.26
5l/6l	CN	Ph	*i*-Pr	$CDCl_3$	Amide		7.66 (2H, t, J = 7.8 Hz), 7.81 (1H, t, J = 7.5 Hz), 8.02 (2H, d, J = 8.4 Hz)	1.22 (3H, d, J = 6.4 Hz), 1.25 (3H, d, J = 6.5 Hz), 4.17 (1H, oct, J = 6.6 Hz)	4.74	6.27
				DMSO-d_6	Amide		7.74 (2H, t, J = 7.9 Hz), 7.88 (1H, t, J = 7.6 Hz), 7.91 (2H, d, J = 8.1 Hz)	1.22 (6H, s, br), 3.77 (1H, oct, J = 6.6 Hz)	5.77	8.38
5m/6m	CN	Me	Ph	$CDCl_3$	Amide		3.33	7.24 (1H, t, J = 7.6 Hz), 7.39 (2H, t, J = 8.1 Hz), 7.53 (2H, d, J = 7.6 Hz)	4.88	8.13
				THF-d_8	Amide		3.31	7.11(1H, t, J = 7.5 Hz), 7.30 (2H, t, J = 8.0 Hz), 7.60 (2H, d, J = 8.0 Hz	5.33	10.19
				DMS	Ami		3.40	7.28 (1H, t, J =	5.77	10.85

				O-d_6	de			8.4 Hz), 7.38 (2H, t, J = 8.0 Hz), 7.50 (2H, d, J = 7.6 Hz)		
5n/6n	CN	Me	*i*-Pr	$CDCl_3$	Amide		3.29	1.23 (6H, d, J = 6.6 Hz), 4.08 (1H, oct, J = 6.6 Hz)	4.69	6.53 (d, J = 6 Hz)
				DMSO-d_6	Amide		3.32	1.10 (6H, d, J = 6.6 Hz), 3.87 (1H, oct, J = 6.6 Hz)	5.59	8.59 (d, J = 5.2 Hz)
5o/6o/7o	COMe	C_4F_9	Ph	$CDCl_3$	Enol	2.63		7.22-7.27 (1H, m), 7.36-7.45 (4H, m)	19.08	9.80
				THF-d_8	Enol	2.61		7.21 (1H, t, J = 7.2 Hz), 7.36 (2H, t, J = 8.0 Hz), 7.50 (2H, d, J = 8.0 Hz)	19.05	9.86
				DMSO-d_6	Ion	2.27		6.99 (1H, t, J = 6.4 Hz), 7.26 (2H, t, J = 6.4 Hz), 7.53 (2H, d, J = 6.2 Hz)	10.52	11.21

[a] singlet, [b] Overlaps other signals, [c] Acetone-d_6 was used as external solvent, [d] Y = SO_2R

Table S2. ^{13}C-NMR Spectral Data (in ppm) for R'NHCOCH(SO_2R)Y and Their Enols R'NHC(OH)=C(SO_2R)Y in Several Solvents at Room Temperature[a]

Num.	Y	R	R'	Solvent	Species	Y	R	R'	CH	C=ONH or C_α
5a/6a	CO_2Me	Ph	Ph	$CDCl_3$	Amide	54.01 (q, J = 149 Hz), 163.50 (m, J = 3 Hz)	129.24 (d, J = 164 Hz), 129.33 (d, J = 165 Hz), 135.06 (d, J = 163 Hz), 136.64 (t, J = 9 Hz)	120.14 (d, J = 163 Hz), 125.30 (dt, J_d = 162 Hz, J_t = 8 Hz), 129.00 (d, J = 162 Hz), 136.52 (t, J = 8 Hz)	76.11 (d, J = 145 Hz)	156.26 (d, J = 6 Hz)
5b/6b	CO_2Me	Ph	2.4-$(MeO)_2C_6H_3$	$CDCl_3$	Amide[b]	53.76 (q, J = 149 Hz), 163.32 (m)	129.08 (d, J = 163 Hz), 129.23 (d, J = 164 Hz), 134.75 (d, J = 163 Hz), 136.58 (t, J = 9 Hz)	55.34 (q, J = 144 Hz), 55.85 (q, J = 145 Hz), 98.48 (d, J = 158 Hz), 103.55 (d, J = 162 Hz), 120.16 (t, J = 8 Hz), 120.62 (d, J = 166 Hz), 149.83 (s), 157.08 (s)	76.35 (d, J = 144 Hz)	155.33 (d, J = 5 Hz)
				C_6D_6	Amide	52.78, 163.38	128.67, 129.28, 133.87, 137.60	54.67, 55.14, 99.01, 103.56, 120.64, 121.25, 149.91, 157.22	76.96	155.75
				DMSO-d_6	Amide	53.67 (q, J = 149 Hz), 163.05 (m, J = 3 Hz)	129.44 (d, J = 165 Hz), 130.06 (d, J = 164 Hz), 135.07 (d, J = 164 Hz), 138.10 (t, J = 8 Hz)	55.82 (q, J = 144 Hz), 56.41 (q, J = 146 Hz), 99.37 (d, J = 159 Hz), 104.66 (d, J = 161 Hz), 120.14 (t, J = 7 Hz), 122.42 (d, J = 166 Hz), 149.83 (s), 157.08 (s)	74.51 (d, J = 140 Hz)	157.59 (s)
5c/6c	CO_2Me	Ph	*i*-Pr	$CDCl_3$	Amide[b]	53.76 (q, J = 149 Hz), 163.42 (m, J = 4	129.21 (d, J = 165 Hz), 129.26 (d, J = 165 Hz), 134.88 (d, J =	22.06 (q, J = 127 Hz), 22.11 (q, J = 127 Hz), 42.55 (d, J = 141 Hz)	75.45 (d, J = 144 Hz)	157.42 (d, J = 7 Hz)

						Hz)	163 Hz), 136.89 (t, J = 8 Hz)			
5d/6d	CO_2Me	Ph	*t*-Bu	$CDCl_3$	Amide	53.71 (q, J = 144 Hz), 163.59 (m, J = 4 Hz)	129.16 (d, J = 164 Hz), 129.30 (d, J = 162 Hz), 134.81 (d, J = 162 Hz), 137.04 (t, J = 7 Hz)	28.19 (q, J = 129 Hz), 52.30 (s)	76.24 (d, J = 143 Hz)	157.12 (d, J = 7 Hz)
5e/6e	SO_2Ph	Ph	Ph	$CDCl_3$	Amide	[c]	129.29, 129.55, 135.47, 137.55	120.36, 125.81, 129.19, 136.37	87.60 (	154.11
				DMSO-d_6	Amide	[c]	129.16 (d, J = 162 Hz), 129.56 (d, J = 163 Hz), 135.15 (d, J = 161 Hz), 137.38 (t, J = 7 Hz)	119.45 (d, J = 162 Hz), 124.91 (d, J = 162 Hz), 129.06 (d, J = 161 Hz), 137.27 (t, J = 7 Hz)	85.96 (d, J = 143 Hz)	155.42 (d, J = 4 Hz)
5f/6f	SO_2Ph	Ph	2.4-$(MeO)_2C_6H_3$	$CDCl_3$	Amide	[c]	129.41, 135.23, 137.78	55.54, 56.15, 98.74, 103.79, 120.62, 121.25, 157.64	87.99	157.64
5g/6g	SO_2Ph	Ph	*i*-Pr	$CDCl_3$	Amide	[c]	129.33 (d, J = 164 Hz), 129.60 (d, J = 164 Hz), 135.23 (d, J = 162 Hz), 137.68 (t, J = 7 Hz)	21.93 (q, J = 128 Hz), 43.10 (d, J = 142 Hz)	86.79 (d, J = 143 Hz)	155.44 (m, J = 4 Hz)
5h/6h	SO_2Ph	Ph	*t*-Bu	$CDCl_3$	Amide	[c]	129.27 (d, J = 165 Hz), 129.37 (d, J = 163 Hz), 135.13 (d, J = 162 Hz), 137.80 (t, J = 10 Hz)	28.02 (q, J = 128 Hz), 52.87 (s)	87.45 (d, J = 148 Hz)	155.06 (s)
				DMSO-d_6	Amide	[c]	129.42 (d, J = 164 Hz), 129.98 (d, J = 163 Hz), 135.28 (d, J =	27.96 (q, J = 127 Hz), 51.67 (s)	85.84 (d, J = 144 Hz)	156.44 (m, J = 4 Hz)

							161 Hz), 138.31 (t, J = 9 Hz)			
5i/6i	SO_2Me	Ph	Ph	$CDCl_3$	Amide	40.95 (q, J = 141 Hz)	129.20 (d, J = 163 Hz), 129.41 (d, J = 163 Hz), 135.35 (d, J = 162 Hz), 137.34 (t, J = 7 Hz)	119.52 (d, J = 163 Hz), 125.08 (d, J = 162 Hz), 129.12 (d, J = 161 Hz), 137.22 (t, J = 7 Hz)	85.19 (d, J = 143 Hz)	156.15 (d, J = 6 Hz)
5j/6j	SO_2Me	Ph	*i*-Pr	DMSO-d_6	Amide	41.66 (q, J = 141 Hz)	129.14 (d, J = 163 Hz), 129.23 (d, J = 164 Hz), 135.06 (d, J = 163 Hz), 137.48 (t, J = 8 Hz)	21.45 (q, J = 127 Hz), 21.61 (q, J = 127 Hz), 41.07 (d, J = 144 Hz)	84.36 (d, J = 143 Hz)	156.74 (m, J = 3 Hz)
5k/6k	CN	Ph	Ph	$CDCl_3$	Amide	110.21 (d, J = 10 Hz)	129.47 (d, J = 163 Hz), 129.89 (d, J = 162 Hz), 134.48 (d, J = 163 Hz), 136.23 (t, J = 8 Hz)	120.39 (d, J = 163 Hz), 126.10 (d, J = 164 Hz), 129.31 (d, J = 162 Hz), 136.04 (t, J = 8 Hz)	64.22 (d, J = 147 Hz)	153.67 (m, J = 4 Hz)
5l/6l	CN	Ph	*i*-Pr	$CDCl_3$	Amide	109.63	128.70, 128.75, 133.98, 134.95	21.11, 21.13, 42.57	62.38	153.88
				DMSO-d_6	Amide	112.32	129.83, 130.03, 136.05 (br)	21.87, 22.15, 42.59	63.05	155.76
5m/6m	CN	Me	Ph	THF-d_8	Amide	111.36 (d, J = 9 Hz)	45.94 (q, J = 141 Hz)	119.62 (d, J = 164 Hz), 124.62 (d, J = 160 Hz), 128.61 (d, J = 161 Hz), 137.95 (t, J = 10 Hz)	62.10 (d, J = 146 Hz)	156.21 (m, J = 3 Hz)
				DMSO-d_6	Amide	112.45 (d, J = 9 Hz)	40.61 (q, J = 142 Hz)	120.26 (d, J = 162 Hz), 125.39 (d, J = 164 Hz), 129.52 (d, J = 163 Hz), 138.00 (t, J = 8	62.73 (d, J = 142 Hz)	156.22 (m, J = 4 Hz)

								Hz)		
5n/6n	CN	Me	*i*-Pr	DMSO-d_6	Amide	112.49	40.40	22.14, 42.67	61.31	156.62
5o/6o/7o	COMe	C_4F_9	Ph	$CDCl_3$	Enol	25.58 (q, J = 129 Hz), 198.27 (t, J = 6 Hz)	107.19 (q, J = 32 Hz), 110.76 (t, J = 32 Hz), 115.16 (t, J = 36 Hz), 119.06 (t, J = 32 Hz)	122.39 (d, J = 163 Hz), 126.50 (d, J = 162 Hz), 129.25 (d, J = 162 Hz), 135.10 (t, J = 8 Hz)	95.02 (s)	167.99 (s)
				THF-d_8	Enol	25.58, 198.60	[d]	122.43, 126.12, 128.82, 135.47	94.78 (s)	168.19 (s)

[a] Singlet, [b] Enol signals not observed (low % enol), [c] Y = SO_2Ph, [d] Signals not observed.

Table S3. Cartesian Coordinates of B3LYP/6-31+G* Optimized Enols and Amides

i-PrNHC(OH)=C(CO_2Me)SO_2Ph

C, −0. 0191245142, 0. 3672686599, 1. 6262732675
C, 0. 4483904885, 0. 7265219376, 0. 3244676587
O, −0. 5189003756, 1. 3011083967, 2. 4250443984
H, −0. 4732145632, 2. 1813499673, 1. 92347218
N, −0. 0062140005, −0. 8618465396, 2. 1408751408
H, 0. 4014307868, −1. 581129064, 1. 5417357197
C, −0. 4391952646, −1. 2083038881, 3. 5048447489
H, −1. 2640820446, −0. 5367062679, 3. 7592046179
S, 1. 2187475352, −0. 4477307294, −0. 7683966603
O, 2. 5786997856, −0. 0187091569, −1. 1258048832
O, 1. 037847372, −1. 7908655919, −0. 1483377596
C, 0. 2390418045, −0. 4747948128, −2. 286896358
C, −1. 2293437218, −0. 604207184, −4. 63777765
C, 0. 8033369991, 0. 0049687917, −3. 4681474536
C, −1. 0445564124, −1. 0252189451, −2. 2604250636
C, −1. 7812601958, −1. 083295359, −3. 4444301442
C, 0. 0602906938, −0. 0654629147, −4. 6497531298
H, 1. 8065886076, 0. 4171502789, −3. 4513874817
H, −1. 456231245, −1. 4110624858, −1. 3326856872
H, −2. 7807658992, −1. 5097379142, −3. 4369736815
H, 0. 4910927167, 0. 2995201451, −5. 5783821285
H, −1. 8041747535, −0. 6561615016, −5. 5588044488
C, −0. 9505576941, −2. 6521930598, 3. 4979983055
H, −0. 1541616009, −3. 3533775785, 3. 2173326075
H, −1. 7813022579, −2. 7756294323, 2. 7945620458
H, −1. 3021209452, −2. 929809188, 4. 4974020988
C, 0. 700122127, −0. 9992159396, 4. 5132156909
H, 1. 5496535621, −1. 6530736093, 4. 2818045531
H, 0. 3547674572, −1. 2313443411, 5. 5278255112
H, 1. 0472976879, 0. 0386530448, 4. 4994088412
C, 0. 3744361603, 2. 1129950292, −0. 0661644859
O, −0. 0931081183, 3. 0206733823, 0. 6539119689
O, 0. 8355185892, 2. 3828116738, −1. 2958355695
C, 0. 7902041119, 3. 7581633712, −1. 717535327
H, 1. 2058324369, 3. 7563252326, −2. 7253330307
H, 1. 3949375161, 4. 3793068607, −1. 0522875826
H, −0. 2399228316, 4. 123058332, −1. 7240207289

i-PrNHC(OH)=C(COMe)SO_2Ph

C,0.0051785095,0.6340906971,1.5215568702
C,0.5547967263,1.0805846879,0.2634730693
O,-0.5826411084,1.5134285951,2.3022696842
H,-0.5213009068,2.4324745576,1.7956527429
N,0.036290449,-0.6180804083,1.9779317901
H,0.5563006169,-1.2831518606,1.4047264835
C,-0.4735178455,-1.039553112,3.2938252648
H,-1.3301390394,-0.3992958037,3.5212643596
S,1.3621467294,-0.0445975557,-0.848600501
O,2.6123653617,0.5445006763,-1.3566646108
O,1.4285448258,-1.3752540212,-0.1868411199
C,0.2643143471,-0.2508884206,-2.2743758191
C,-1.3667065787,-0.6871756382,-4.4797788989
C,0.7900901663,-0.0824593685,-3.555900854
C,-1.063245267,-0.6413030291,-2.0776246266
C,-1.8798011759,-0.8552940319,-3.18835685
C,-0.0358011495,-0.304034557,-4.662369969
H,1.8263726404,0.2164934459,-3.6760253767
H,-1.4558059191,-0.7749751554,-1.0735879552
H,-2.9146043562,-1.1549724511,-3.0464977235
H,0.363678283,-0.1755768658,-5.6647070993
H,-2.0063895452,-0.8558558722,-5.341998234
C,-0.9422920139,-2.4941557204,3.1899574332
H,-0.1106295807,-3.1609823103,2.9284018499
H,-1.7242745212,-2.6060344379,2.4308492463
H,-1.3467408804,-2.8273563585,4.1516772535
C,0.593036953,-0.8473363413,4.3820084217
H,1.4760795777,-1.4643230508,4.1757489357
H,0.1922155539,-1.139151917,5.3600569375
H,0.9063953305,0.1997120979,4.4397554892
C,0.449714899,2.4772510536,-0.0745270392

O,-0.1309328386,3.2845988395,0.7093975938
C,1.0115257451,3.0623553939,-1.3491115996
H,2.1034369122,2.9976423323,-1.3545325536
H,0.6984922378,4.1071358692,-1.3997296549
H,0.653844462,2.5315401412,-2.2373229402

i-PrNHCOCH(SO_2Ph)=C(OH)CH_3
N,-0.6716624031,0.136332981,2.20450308
H,-1.0051575912,0.9409795213,1.6766024336
C,-1.2664939031,-0.1586266291,3.5157311974
H,-1.0891500531,-1.2215318298,3.7031645723
S,0.3562349725,1.1475807397,-0.6328769819
O,-0.707265904,1.861808984,0.1149728027
O,1.4350236787,1.9404851082,-1.2453108553
C,-0.4709180018,0.2528355433,-1.9707913913
C,-1.8040367078,-1.0352870881,-4.0380313611
C,-1.4781904796,-0.667888024,-1.6664237867
C,-0.1259487911,0.5448078391,-3.2909971704
C,-0.8018060639,-0.1065784928,-4.3278133001
C,-2.1414576104,-1.3156413389,-2.7085996994
H,-1.7423266308,-0.8758590727,-0.6334798961
H,0.6523710924,1.2730996588,-3.4948497621
H,-0.5431791244,0.1150173892,-5.3596732233
H,-2.923577817,-2.0355925427,-2.483727237
H,-2.3255316747,-1.5409012745,-4.8463625613
C,-0.5855227773,0.6553430504,4.6262427536
H,-0.7247071785,1.7313385027,4.4635731072
H,0.48772031,0.4433295756,4.6567512753
H,-1.0132011507,0.3989507838,5.6031324633
C,-2.7742266649,0.1027634592,3.4455256159
H,-2.9857324857,1.1574292658,3.2258526041

H,-3.2433602277,-0.1370757176,4.405990957
H,-3.2472848626,-0.5104616402,2.6703138423
C,0.438127039,-0.4753786748,1.7546200225
C,1.0528105872,-0.1000780962,0.4488288434
C,2.2082778988,-0.7596811464,0.0346728872
C,2.9680314012,-0.5287034734,-1.2420658211
H,2.3141512997,-0.536796699,-2.1181221991
H,3.7128630312,-1.321517424,-1.3381926268
H,3.46592625,0.4446387411,-1.2215390472
O,2.7628384724,-1.6963123925,0.7791231088
H,2.1725512088,-1.7879371817,1.6156592227
O,0.9753571664,-1.3934884909,2.4367178796

i-PrNHC(OH)=C(SO_2Ph)$_2$
C,-0.8947881786,-0.4567057106,1.4090040716
C,-0.2165117277,0.1074660654,0.2946274621
O,-1.6243017978,0.2716277165,2.2483661176
H,-1.6343997109,1.2208534824,1.9267596723
N,-0.8723946888,-1.760072622,1.7073031139
H,-0.2049114933,-2.3212501917,1.1791166187
C,-1.6007635228,-2.3829453362,2.8262407303
H,-2.5217699969,-1.8100412053,2.9631862066
S,0.5778016085,-0.9059517085,-0.9277317555
O,1.6223865424,-0.1026648074,-1.5774981367
O,0.9504067085,-2.1886657242,-0.2746506341
S,-0.1386476552,1.8622373257,0.0526502343
O,-0.3155161567,2.2025519978,-1.3645356216
O,-1.1026811194,2.4438067685,1.043927329
C,-0.6555514246,-1.3313307793,-2.1797490048
C,-2.5055053055,-2.0104466588,-4.1351152824
C,-1.0584459719,-0.3613731037,-3.1028744324

C,-1.1548324865,-2.6352354687,-2.2243071718
C,-2.0866651843,-2.9707099391,-3.2106203001
C,-1.9906748986,-0.710565126,-4.0807524628
H,-0.6583244589,0.644582553,-3.0448212766
H,-0.8011328283,-3.3750268035,-1.5146293847
H,-2.4767907993,-3.9839059014,-3.2586536446
H,-2.3124771331,0.0351380912,-4.8026191917
H,-3.2292147227,-2.2750850387,-4.9017125261
C,1.4864839923,2.4551642233,0.5591350222
C,3.9759437907,3.3917848721,1.3427568453
C,1.7081788766,2.7575104317,1.9058207855
C,2.4837094958,2.6192561847,-0.4039037476
C,3.7343758996,3.0919024038,-0.0010035157
C,2.964150422,3.2265743241,2.2941667295
H,0.9083325677,2.6491249335,2.6309417372
H,2.282568574,2.3739082998,-1.4396476249
H,4.5195828129,3.223550769,-0.7402950645
H,3.1476145947,3.4707571244,3.3369891871
H,4.9520928564,3.7586520114,1.6491965755
C,-1.9555136262,-3.8206094536,2.433055148
H,-1.0509986865,-4.4157414334,2.2516964846
H,-2.5717079264,-3.8429712016,1.527737137
H,-2.5144823504,-4.3034797976,3.2416595891
C,-0.7787321179,-2.3219391322,4.1220313966
H,0.1623590579,-2.8747034711,4.0127975873
H,-1.3431271489,-2.7681299993,4.9495515714
H,-0.5444152496,-1.2863281319,4.3869828129

i-PrNHC(OH)=C(SO_2Me)$_2$
C,-0.5856656694,-0.136837145,0.8888857902
C,0.0690181781,0.3714318662,-0.2657811747

O,-1.3031205553,0.6363425762,1.6889327747
H,-1.3212895257,1.5636927097,1.3030416226
N,-0.5368629514,-1.4176467739,1.259192234
H,0.0833094918,-2.0105375998,0.7090079762
C,-1.2297821225,-1.9758817609,2.4315751417
H,-2.1617295713,-1.4160095608,2.5467474162
S,0.9287003356,-0.6445607946,-1.4269382264
O,2.1276591361,0.0752578805,-1.8866801212
O,1.0906102845,-1.9920427047,-0.8258699604
S,0.0186037562,2.0845329827,-0.6634960826
O,-0.2858854001,2.271687918,-2.0894357571
O,-0.892589242,2.7240486566,0.340808311
C,-1.5566780391,-3.4437711144,2.146519897
H,-0.6423662767,-4.0300332508,1.9989835246
H,-2.1774757036,-3.5448020005,1.2517935277
H,-2.097546281,-3.8787421919,2.9914382282
C,-0.3899175752,-1.8018190592,3.7038322234
H,0.5626529929,-2.3352410202,3.6170817599
H,-0.926814074,-2.2002589295,4.5707658951
H,-0.181157539,-0.7449674688,3.8873890473
C,1.6565499917,2.7677496616,-0.3587770935
H,2.3644092705,2.2255180802,-0.9848235957
H,1.8869701314,2.6503298136,0.7005699915
H,1.6040775297,3.8239461889,-0.6303667266
C,-0.1646761334,-0.8339000065,-2.848447367
H,0.3838638118,-1.4254125166,-3.5842376115
H,-0.3974711392,0.1606142816,-3.2285738459
H,-1.0647434947,-1.3583133914,-2.5251003825

i-PrNHC(OH)=C($SO_2C_4F_9$)$_2$
C,-0.9125681283,-0.2556560504,1.3305332722

C,-0.2233551502,0.1605564203,0.1326725628
O,-1.6742233864,0.5746145644,2.0239356714
H,-1.7291839967,1.4580022182,1.5633968305
N,-0.8510968325,-1.4820646024,1.8274050897
H,-0.2093623682,-2.1240941667,1.3628775012
C,-1.6073167356,-1.9643991819,3.0043349701
H,-2.5348279778,-1.3872763337,3.039788168
S,0.6252218312,-0.9844207478,-0.899068128
O,1.6784539365,-0.3307680822,-1.6654817354
O,0.8997741787,-2.2068703134,-0.118789895
S,-0.1733902781,1.8558963095,-0.3213086136
O,-0.0202922729,2.0601122247,-1.7524071316
O,-1.264605314,2.5392103306,0.4269457372
C,-1.9368291543,-3.4442540362,2.7892698051
H,-1.0237147911,-4.0488949185,2.7186807481
H,-2.5223078982,-3.5938702277,1.8759736721
H,-2.5199112177,-3.8203231181,3.6362162795
C,-0.8112527637,-1.7180390699,4.2927629456
H,0.1358211271,-2.270398231,4.2789010781
H,-1.3908969446,-2.0560367797,5.1592937912
H,-0.5917526113,-0.6537891182,4.422130132
C,1.4197013911,2.5398512822,0.5121337583
C,-0.7242399984,-1.5258394857,-2.1576513098
C,1.3897701752,4.0908541488,0.71290675
C,2.7999822895,4.7211784425,0.9793553737
C,2.7751520367,6.1819784534,1.5380430256
C,-0.1508733952,-2.2913209752,-3.3926242386
C,-1.2259365383,-3.1043926649,-4.1925340264
C,-0.7751392376,-3.5799428409,-5.6124624874
F,4.0257796666,6.6667024446,1.5317343302
F,2.315746445,6.2080042383,2.7964528147

F,2.0030292418,6.9694335607,0.7741889336
F,3.4960955681,4.7391984605,-0.1785476161
F,3.4636566438,3.9545336135,1.8820019726
F,0.5876019664,4.3710133033,1.7680606707
F,0.8743398957,4.6646579641,-0.3986737704
F,1.5224896799,1.9371955093,1.7198779639
F,2.4690511877,2.1889727031,-0.2462356294
F,-1.3855172154,-0.432525739,-2.5705850713
F,-1.5847357353,-2.3213495778,-1.4748440442
F,0.7976989199,-3.1593060027,-2.9658490165
F,0.4174887854,-1.38855812,-4.2226960007
F,-2.3347480163,-2.3397577535,-4.3543695893
F,-1.5563377337,-4.2069671898,-3.4798702292
F,0.396789943,-4.2298908129,-5.5457060771
F,-0.6546159037,-2.5439761911,-6.4512125824
F,-1.7046148139,-4.4169838608,-6.0989567555

i-PrNHC(OH)=C(COMe)$SO_2C_4F_9$
C,-0.7728727215,0.8689593372,1.7700075117
C,0.0139069163,1.5631840601,0.7633297105
O,-1.7488155161,1.515976915,2.358713511
H,-1.7528173736,2.4783903497,1.9396340322
N,-0.5851147556,-0.3862543866,2.1640070218
H,0.2239535665,-0.8670367739,1.7750811541
C,-1.3818369602,-1.0641842787,3.2054214834
H,-2.388932332,-0.6423560258,3.1524525352
C,-1.4385721431,-2.5582628313,2.8740524675
H,-0.436511238,-3.0061000662,2.886704229
H,-1.8812883509,-2.7303696505,1.8871661835
H,-2.0459860907,-3.0821262292,3.6195202233

C,-0.7980443305,-0.793164921,4.5989617264
H,-0.7721076095,0.2803806728,4.8101168605
H,0.2212974129,-1.1896048251,4.6795450401
H,-1.4146640303,-1.2775706714,5.36495165
C,-0.2975589901,2.951320034,0.4716075608
O,-1.2447907985,3.5145633404,1.085165965
C,0.4641013576,3.8042902074,-0.5147964439
H,0.5356575782,3.3429468981,-1.5021732692
H,1.4887760691,3.970479618,-0.169098111
H,-0.060371046,4.7590560137,-0.5872514519
S,1.2557160602,0.7063572472,-0.1181421506
O,2.2741785968,1.6089831407,-0.6566862086
O,1.6533118524,-0.5068639105,0.6234011715
C,0.3275039945,0.024058173,-1.6585987751
C,1.2597322786,-0.5270359723,-2.7832231224
C,0.5335551222,-1.4465304224,-3.8247107246
C,1.3317677229,-1.7168443127,-5.1420214648
F,-0.4291368778,1.0258573168,-2.1636057271
F,1.7972193156,0.5280394827,-3.4413613699
F,2.2564911504,-1.2460168815,-2.2165669036
F,-0.6468798545,-0.8772488088,-4.1775400382
F,1.4202414838,-0.6082807848,-5.8881780795
F,0.6859314526,-2.6560196974,-5.8508489986
F,2.5677717633,-2.15972581,-4.866614716
F,0.2852090996,-2.6455005249,-3.2478556173
F,-0.5000257746,-0.9557451216,-1.2205669653

i-PrNHCOCH($SO_2C_4F_9$)=C(OH)CH_3
N,0.069352112,-0.4967305351,3.346721022
H,-0.2441119706,0.371262768,2.9214137516
C,-0.5975643441,-0.9637893185,4.5734583347

H,-0.4457877011,-2.0460890995,4.6111022636
S,1.1549755346,0.7659282975,0.6783211977
O,0.2463805156,1.5566482625,1.5259313273
O,2.1670558927,1.4333820029,-0.1428325697
C,0.0399381781,-0.3312324323,5.8187724539
H,-0.0763453514,0.7595579908,5.8066376198
H,1.1071831747,-0.5681035146,5.8702224817
H,-0.4402089305,-0.7156455168,6.7264729385
C,-2.0948098083,-0.6598615491,4.4654538562
H,-2.2768914421,0.4203251634,4.3908994693
H,-2.6161851451,-1.0229479109,5.3576613113
H,-2.5364045514,-1.1447557128,3.5880470776
C,1.167493283,-1.0812700526,2.8472159215
C,1.8368150444,-0.5658549085,1.6109662866
C,3.0131736565,-1.1889507543,1.1632711663
C,3.8538378361,-0.8214282549,-0.0278294908
H,4.5946383415,-1.6117176598,-0.1646600249
H,4.3648995517,0.1302043163,0.14608412
H,3.2638645605,-0.7025429396,-0.9375296643
O,3.5109913487,-2.2034087926,1.8263033669
H,2.865502559,-2.3881655005,2.6166056804
O,1.6663133174,-2.0910320465,3.4191618051
C,-0.0028446309,-0.1265137431,-0.5720631481
C,-0.511219614,0.7853420279,-1.7335864753
C,-1.7525293835,0.211730319,-2.5001536771
C,-2.061937149,0.8995812173,-3.8701319782
F,-3.2411293592,0.4458266451,-4.3220393447
F,-1.119962301,0.6112827916,-4.7774822167
F,-2.1390697262,2.231095686,-3.7262494288
F,-2.848296126,0.3514851224,-1.7188502572
F,-1.5543040162,-1.1081929184,-2.7459767307

F,0.5031348202,0.9496412566,-2.6164138783
F,-0.8535825039,1.9925026284,-1.2273756096
F,-1.0512342995,-0.612718315,0.1312442883
F,0.6829686854,-1.168739798,-1.0961784087

i-PrNHC(OH)=C(SO_2Me)SO_2Ph[a]
C,-0.0773764911,-0.1763105829,1.6750580067
C,-0.5765123998,0.5013347493,0.5291630239
O,-0.8735843544,-0.694117562,2.6032926817
H,-1.8289902007,-0.539756756,2.3399860251
N,1.224695652,-0.3598536087,1.9184465543
H,1.8625077409,0.1491513036,1.3077697867
S,0.4771524675,1.0502845626,-0.7878395852
O,-0.184186097,2.1955155781,-1.4349998443
O,1.8400692907,1.2216119605,-0.2215051119
S,-2.3095181163,0.7795710053,0.3008107083
O,-2.7429516999,0.399654125,-1.050725858
O,-2.9931872568,0.11797963,1.4619899778
C,0.6089315515,-0.2674208483,-2.0145352652
C,0.838540453,-2.2736829316,-3.9187186345
C,-0.3955523387,-0.4121308396,-2.9757258445
C,1.7295093816,-1.1026528501,-1.9955548966
C,1.838176322,-2.1118315655,-2.9552902459
C,-0.2724030575,-1.4241436989,-3.9291098761
H,-1.2560524632,0.2461261144,-2.9673858683
H,2.5123299131,-0.9473544681,-1.2612506185
H,2.7084821621,-2.7626118726,-2.9544944704
H,-1.0468802439,-1.5462809978,-4.6812679377
H,0.9279623125,-3.0581798063,-4.6656764446
C,-2.6131150686,2.547033162,0.4976208447
H,-2.0605926987,3.0749241327,-0.2799737899

H,-2.2873894489,2.8454363564,1.4959686353
H,-3.6926413262,2.6787183069,0.3841294311
C,1.7716630304,-1.067251226,3.0898924937
H,1.0566389974,-1.8530806423,3.3471663299
C,3.1028065871,-1.7109078538,2.6889695066
H,3.8368046626,-0.9512597751,2.390134328
H,2.9694408785,-2.4100524781,1.8563047208
H,3.5225372246,-2.2626115311,3.5368551667
C,1.9224412719,-0.1183238566,4.2876950787
H,0.9585167887,0.3227184103,4.5597613188
H,2.6238728134,0.6927587557,4.0567655512
H,2.3064991946,-0.6647786777,5.157344075

i-PrNHC(OH)=C(SO_2Me)SO_2Ph[b]
C,-0.9940444681,-0.4991192102,0.4368266542
C,-0.3615454613,0.0331918614,-0.7193311068
O,-1.7825508272,0.2400148084,1.2143168745
H,-1.8826352003,1.1486494376,0.8083255423
N,-0.8583436366,-1.7600297528,0.854039468
H,-0.2475195512,-2.3480577066,0.2862525066
S,0.5573292809,-0.9597094725,-1.8698586219
O,1.7848618794,-0.2517243474,-2.2649901028
O,0.6785485171,-2.3262046255,-1.2940314671
S,-0.4117461705,1.7640222553,-1.0829583422
O,-0.4930453693,1.9464311256,-2.5396789702
O,-1.501887771,2.3323007787,-0.2257898144
C,1.106333787,2.5525858004,-0.5172964355
C,3.4292016382,3.7916987836,0.3535980376
C,1.1739724031,3.0296575105,0.7950785209
C,2.176361266,2.6893878791,-1.4040325061
C,3.3418272778,3.3152238179,-0.9577116449

C,2.3469630038,3.6504133534,1.2279463507
H,0.3190887975,2.9385348211,1.456770051
H,2.0970233144,2.3068845024,-2.4142809439
H,4.181782686,3.4279723646,-1.6375008781
H,2.4097687817,4.0312535053,2.2436670203
H,4.3397769065,4.2779363412,0.6938310661
C,-1.6286266985,-2.3768480599,1.9495900993
H,-1.7767488917,-1.6065644771,2.7109715601
C,-2.9998832607,-2.8615464401,1.4570941616
H,-2.8860193818,-3.6324986729,0.6852357236
H,-3.5808467041,-2.0332356821,1.0388710364
H,-3.5708262439,-3.2919248849,2.2884871254
C,-0.7888978163,-3.5122605893,2.542226789
H,0.1736981237,-3.1418219838,2.9108371698
H,-0.5947992118,-4.2927810282,1.7953611236
H,-1.3230577445,-3.9758863533,3.3782977144
C,-0.4730856845,-1.1227629841,-3.3444404529
H,0.0996827827,-1.7379262672,-4.0439007227
H,-0.655632976,-0.1258257712,-3.7469222582
H,-1.4044773765,-1.6194305373,-3.0649003277

i-PrNHC(OH)=C(CN)SO_2Me
C,-0.3503634557,0.3345277306,-0.1438900997
C,0.3756049934,0.9226224415,-1.2016985969
O,-1.0831538365,1.0260325963,0.7169207494
H,-1.0404184902,1.9943481083,0.4648012956
N,-0.3533430088,-0.9922433731,0.0533487012
H,0.2224394954,-1.5464199069,-0.5707425879
S,0.3688021263,2.6593855004,-1.5104037473
O,0.0618533524,2.949434859,-2.9146002799
O,-0.4895125985,3.2565667212,-0.4364810642

C,-1.0850461604,-1.6979351495,1.1229087255
H,-1.9822854459,-1.1070361525,1.3259734919
C,-1.4986728508,-3.0761090992,0.5987186192
H,-0.6200706274,-3.6850472802,0.3474085136
H,-2.1265979576,-2.9891453453,-0.2943948992
H,-2.0643366242,-3.6143318595,1.366262647
C,-0.2433275168,-1.7854666329,2.4034611761
H,0.0360307052,-0.7877179216,2.7565485334
H,0.6730666707,-2.3627846327,2.2298945951
H,-0.8138173678,-2.2811986028,3.1976523095
C,1.1194676692,0.1088726086,-2.0789615383
N,1.7421123752,-0.6077916207,-2.7617647062
C,2.0543938279,3.2318007362,-1.205580922
H,2.7261924253,2.7172076898,-1.8961620035
H,2.3166887002,3.0253401944,-0.1664011983
H,2.0542938994,4.3070884901,-1.4028176143

i-PrNHC(OH)=C(CN)SO_2Ph
C,-1.3010388699,-0.5127794173,-0.015304653
C,-0.5935850516,0.0801721644,-1.0808185272
O,-2.0199405493,0.1754551402,0.8615122407
H,-1.986054149,1.1421183265,0.6039130461
N,-1.3043747137,-1.841482241,0.1739990332
H,-0.7292462422,-2.3912751357,-0.4546305444
S,-0.5427964421,1.8256407039,-1.3446473447
O,-0.7993032075,2.127680257,-2.75632522
O,-1.4254393236,2.4094563229,-0.2840920295
C,1.1339558654,2.3659947307,-0.9792055062
C,3.7332004016,3.1574757242,-0.4268065304
C,1.4672996968,2.7459652163,0.323702008
C,2.0745850532,2.380371501,-2.0124452958

C,3.3826286877,2.7771612519,-1.725532459
C,2.7771410242,3.1453165635,0.5943905684
H,0.7106189303,2.7473341234,1.1014832054
H,1.7829195948,2.0984637602,-3.0187846618
H,4.1239968687,2.7934062256,-2.5194625298
H,3.0481602224,3.4534149054,1.6005199928
H,4.7515613895,3.469157028,-0.2103441868
C,-2.0286013047,-2.5527016632,1.2440658579
H,-2.9234409614,-1.9618306464,1.4580569107
C,-2.4477547964,-3.9277821475,0.7160327945
H,-1.5713445466,-4.5369250692,0.4575141768
H,-3.0799706969,-3.8358096019,-0.1735410526
H,-3.0103230367,-4.4686490431,1.4840662564
C,-1.177100976,-2.6491143631,2.5176807531
H,-0.8916430138,-1.6538408952,2.8727010919
H,-0.2637446811,-3.2279733986,2.333576945
H,-1.7425538671,-3.1472144976,3.3140869637
C,0.1284498733,-0.7327798984,-1.9769674486
N,0.7237360218,-1.454425827,-2.6783935548

t-BuNHC(OH)=C(CO_2Me)SO_2Ph
C,0.1904138892,0.4244693636,1.3369407705
C,0.6590148614,0.7151617028,0.0149630531
O,-0.185128851,1.422590283,2.1242492351
H,-0.0488178722,2.2846080676,1.6047823469
N,0.09866902,-0.7973081559,1.8613882729
H,0.396114722,-1.5421489109,1.2291598723
C,-0.3509873002,-1.184204013,3.2279208516
S,1.2674175954,-0.5434276209,-1.0866312287
O,2.6586476588,-0.2732183054,-1.4777514836
O,0.9507185656,-1.8561341418,-0.4552050411

C,0.2558371541,-0.4680064853,-2.5829218873

C,-1.2707138428,-0.4466661537,-4.9000772206

C,0.8464604655,-0.0731453728,-3.7825450426

C,-1.0834671279,-0.860013343,-2.5215466934

C,-1.8486769574,-0.8423276814,-3.6886379366

C,0.0736273429,-0.0670705274,-4.9469918568

H,1.8919698022,0.215847074,-3.7928760223

H,-1.5175221193,-1.1830069167,-1.5800949341

H,-2.8916756726,-1.1454496175,-3.6539432753

H,0.5238527815,0.232894057,-5.8895776559

H,-1.8685191616,-0.4396501336,-5.8078212162

C,-0.2382933397,-2.718435515,3.2674953189

H,0.7944230867,-3.0453644775,3.0976785504

H,-0.8775472501,-3.183352635,2.5073899755

H,-0.554143566,-3.0888775566,4.2478791844

C,0.574131946,-0.5711382312,4.2964662058

H,1.6151521637,-0.8627587551,4.1172747548

H,0.2829026616,-0.9361505573,5.2883519228

H,0.5137124029,0.5195454415,4.300344428

C,0.7291829428,2.0962303002,-0.3934765299

O,0.3854641575,3.0599108708,0.3246453898

O,1.1839081577,2.3001564115,-1.6381350106

C,1.2803113734,3.6673875947,-2.0771102044

H,1.6625071497,3.6083801741,-3.0963574586

H,1.9707999842,4.2233339199,-1.4381586757

H,0.2979613779,4.1458723932,-2.0588708588

C,-1.8163801286,-0.7684557316,3.4580667322

H,-1.9328163697,0.3173851721,3.4370284197

H,-2.1522956908,-1.1327205596,4.4359982321

H,-2.4662165125,-1.2047420278,2.6907065159

PhNHC(OH)=C(CO_2Me)SO_2Ph

C,-0.2291462771,-1.2976842395,-0.537421387

C,-0.7490894387,0.0049099211,-0.8078349606

O,0.1722965486,-2.0613241997,-1.5375422135

H,0.0097758977,-1.5399039403,-2.3971229329

N,-0.1202858902,-1.8155813156,0.6952305804

H,-0.4522639026,-1.1756160232,1.4233924759

S,-1.373239069,1.0895182612,0.4628860846

O,-2.7691461549,1.4599103883,0.1952110031

O,-1.046561947,0.4465738104,1.7685183684

C,-0.3803297617,2.5968200975,0.3993791133

C,1.1175157864,4.9312178469,0.3907108613

C,-0.9829938557,3.7888389883,-0.0009477857

C,0.9563512638,2.5506221507,0.8026719264

C,1.7070989862,3.7270593473,0.7914151541

C,-0.2240643831,4.9622403129,-0.0002938652

H,-2.0262149808,3.7872499373,-0.2981721057

H,1.3993154626,1.6147128491,1.1295028073

H,2.7475982198,3.7049635397,1.1038041798

H,-0.6830250165,5.899396433,-0.3038142719

H,1.7041600831,5.8461767609,0.3887469673

C,0.3641906809,-3.066186658,1.1507548485

C,1.2698014014,-5.4681887302,2.2997664573

C,0.3061244695,-3.2614116597,2.5429768896

C,0.8800297107,-4.0847812207,0.3337882393

C,1.3265188128,-5.2729542327,0.9187882713

C,0.7547881516,-4.4514592765,3.1097577812

H,-0.0956035983,-2.4754175422,3.1784882321

H,0.931991384,-3.9571829974,-0.7371194373

H,1.7231296427,-6.0541825978,0.2753793949

H,0.6994645845,-4.5819391639,4.1872352513

H,1.619985267,-6.3978730266,2.7394724609
C,-0.8385500169,0.4228769623,-2.1874034483
O,-1.329632307,1.6532536254,-2.3791455549
C,-1.4507330192,2.0979824537,-3.7438370579
H,-2.1178943057,1.4352134616,-4.3000586622
H,-0.4704435673,2.1218696232,-4.2261258671
H,-1.8731685778,3.1004600869,-3.6755990239
O,-0.477750384,-0.2801802334,-3.1554387743

PhNHCOCH(SO_2Ph)=C(OH)OMe
N,-0.1979191444,0.5683803768,1.8433402416
H,-0.5871635151,1.3103556332,1.2578876595
S,-1.4366661687,0.4707861626,-1.1024185964
O,-2.7864284803,0.1156870448,-1.5612272459
O,-1.2455451709,1.7404938848,-0.3508666305
C,-0.3758010626,0.5917529458,-2.5593151288
C,1.227665227,0.8464273757,-4.8089133087
C,-0.8706849868,0.180523365,-3.7968710053
C,0.9044069662,1.1362211859,-2.4265419893
C,1.7087774177,1.2569716545,-3.5604798214
C,-0.0590533702,0.3138914691,-4.9269789023
H,-1.8752443604,-0.2231657958,-3.8645131377
H,1.2607629866,1.4706545302,-1.4569794373
H,2.7055306434,1.6801850844,-3.4708802458
H,-0.4353962368,0.0049823428,-5.8985736249
H,1.8552676539,0.9482572401,-5.6904047514
O,-1.2325653326,-2.3669243382,-1.8120442349
C,-1.2663548035,-3.7306201902,-2.2862314301
H,-1.6888659692,-3.6622402788,-3.2880874524
H,-1.9031873441,-4.3388284124,-1.6401314809
H,-0.2574327531,-4.1479940174,-2.3181165234

C,-0.2201963408,-0.6555886974,1.2739400628
O,0.2141062437,-1.6767293163,1.8944795491
C,-0.7580449351,-0.8299465549,-0.0853321659
C,-0.7741198599,-2.1381817402,-0.5921097146
O,-0.3370162929,-3.1623446644,0.0817419674
H,-0.0082986045,-2.7313303723,1.0084940328
C,0.2670177026,0.964779059,3.1184604425
C,1.1312118916,1.9690486143,5.5987975013
C,0.8282995394,0.0977433547,4.0697517165
C,0.14220646,2.3333426779,3.4195100277
C,0.5706414415,2.8285420396,4.6487056425
C,1.2537162594,0.6110761925,5.2981188055
H,0.9259588218,-0.9554630022,3.8499773131
H,-0.2953744142,3.0066544744,2.6855904545
H,0.4640357535,3.8889021652,4.8623687449
H,1.6860995147,-0.0695781724,6.027301486
H,1.4656543232,2.3532766796,6.5585510805

PhNHC(OH)=C(COMe)SO_2Ph
C,0.2902011029,0.8881259579,1.1471760469
C,0.8689719868,1.1954578405,-0.1414930703
O,-0.2376251836,1.8598909162,1.8419579897
H,-0.0955245997,2.7439828681,1.2501024333
N,0.2690581149,-0.3444484393,1.6780712896
H,0.7439979182,-1.0418635963,1.098766659
S,1.5708904807,-0.0557601883,-1.1928819547
O,2.8368951064,0.4164494806,-1.7750522312
O,1.5778046554,-1.3361472975,-0.4338702241
C,0.4142464998,-0.2938076246,-2.5643014574
C,-1.315566801,-0.7753197206,-4.6819902238
C,0.8979619137,-0.2160783913,-3.8708491946

C,-0.9197128771,-0.6160741312,-2.2982099847
C,-1.7857928336,-0.8526895354,-3.3657833091
C,0.0219428455,-0.4601492713,-4.9331497822
H,1.9409273204,0.0285518754,-4.0440184251
H,-1.2801228759,-0.6818534606,-1.2755135155
H,-2.8254737483,-1.1006280349,-3.1705597007
H,0.3880748057,-0.403103018,-5.9545813151
H,-1.9939171699,-0.9622408642,-5.5101515542
C,0.8569421195,2.5667559699,-0.5771886494
O,0.3383054952,3.4645994783,0.1551528917
C,-0.2482532105,-0.8186550045,2.9092333146
C,-1.1957416996,-1.9929347419,5.2806913817
C,-0.0344977007,-2.185106879,3.1661933299
C,-0.9414265878,-0.0395498388,3.848993872
C,-1.4069271687,-0.6372039494,5.0235595103
C,-0.5044466837,-2.7647735748,4.3418197479
H,0.5045766437,-2.7902389533,2.4406523653
H,-1.111969702,1.0116983377,3.670332679
H,-1.9415336578,-0.0242012092,5.7446147251
H,-0.3273625121,-3.8216496825,4.522464556
H,-1.5628032545,-2.4427067563,6.1989911495
C,1.4420128812,3.0305599741,-1.8889070936
H,2.5271757754,2.8941618733,-1.896963546
H,1.1973137076,4.0882639134,-2.0047215303
H,1.0413990936,2.468685678,-2.7385869797

PhNHCOCH(SO_2Ph)=C(OH)Me
N,-0.2793911342,0.2808312939,1.6769615706
H,-0.7868633528,0.9735896334,1.1245328036
S,-1.6026655309,0.075537199,-1.1995280167
O,-2.8408014594,-0.3997761477,-1.8364659385

O,-1.6606765573,1.3184570766,-0.3893440023
C,-0.4034675631,0.3821690537,-2.5180071451
C,1.3937020936,0.9584798139,-4.5532469595
C,-0.8314545476,0.3132596255,-3.8444425061
C,0.9072156398,0.742585299,-2.1906121587
C,1.8073608681,1.0264565117,-3.2175763456
C,0.078614009,0.605801833,-4.8651419279
H,-1.8587507248,0.0418534376,-4.0651262883
H,1.2228034041,0.8035574212,-1.1529473168
H,2.8291218122,1.3051632103,-2.9752474793
H,-0.2439596784,0.5580206867,-5.9016060659
H,2.0983705346,1.1835241588,-5.3493004443
C,-0.2697199568,-0.967910614,1.1542841433
O,0.2606010598,-1.9312666306,1.7665199861
C,-0.9007493679,-1.2205870259,-0.1734692306
C,-0.9269078622,-2.524291282,-0.6677765182
O,-0.4101555947,-3.52714671,0.0157712494
H,-0.0231402607,-3.1272721339,0.8733894022
C,-1.5141682832,-2.9794248956,-1.9746241456
H,-1.2326858075,-4.023871361,-2.123785243
H,-1.1534969266,-2.3834846672,-2.8173084877
H,-2.6035789397,-2.8884433487,-1.9590098844
C,0.2483996918,0.7434933449,2.9051715916
C,1.2242398031,1.8747942356,5.2868095141
C,0.9604517238,-0.0505046238,3.8187048991
C,0.0299247998,2.1030818844,3.1939098934
C,0.5137380984,2.6613266744,4.3744607895
C,1.4398566942,0.5258241094,4.9984300972
H,1.1290190323,-1.0965202954,3.6079663374
H,-0.5241496713,2.7195828159,2.4892799248
H,0.3325851691,3.7130636594,4.580246944

H,1.9888088503,-0.0981104137,5.6993006066

H,1.6019699352,2.3081571712,6.2088263515

PhNHC(OH)=C(SO_2Me)SO_2Ph[a]

C,0.2767846649,0.7594337254,1.0725463332

C,0.9494123081,1.1937950134,-0.0990456709

O,-0.311507693,1.5949406297,1.9127608527

H,-0.1990654574,2.5341573078,1.5745661166

N,0.2038093441,-0.5406156094,1.4156897122

H,0.7940587732,-1.1463861448,0.842516058

S,1.5814204669,0.0760911043,-1.3298015273

O,2.7101758877,0.7456701274,-1.9951315546

O,1.80391914,-1.2335744953,-0.6620278636

S,1.1335084956,2.9186493551,-0.468545011

O,0.7645378146,3.2076308175,-1.8600084752

O,0.4017642795,3.6549380991,0.6151903576

C,0.2990431678,-0.200419739,-2.5652784765

C,-1.6631128681,-0.6445450959,-4.4742278337

C,0.1895667865,0.6801335842,-3.6447552544

C,-0.5502777345,-1.3021168471,-2.4269676596

C,-1.5375742292,-1.5186997046,-3.3903554744

C,-0.8006355395,0.4488118345,-4.601058746

H,0.858687278,1.5283848914,-3.7254770634

H,-0.425952906,-1.987905505,-1.5959991517

H,-2.2001614961,-2.3747912111,-3.2970777063

H,-0.8958151861,1.1251393231,-5.4459595221

H,-2.4309823291,-0.8185108369,-5.2234702281

C,-0.4790171073,-1.1748141428,2.4866790651

C,-1.7486354044,-2.6459618953,4.5149952309

C,-0.02673925,-2.4616914276,2.8236430604

C,-1.577472514,-0.6278146751,3.1661601108

C,-2.1981094229,-1.3679874497,4.1752268071
C,-0.6588794471,-3.1901509027,3.8296181329
H,0.82468112,-2.8870177046,2.2970056471
H,-1.9426082108,0.3584682438,2.9160385207
H,-3.0474541457,-0.9339186718,4.6963069551
H,-0.2939598608,-4.1831817676,4.0780164351
H,-2.2409275099,-3.2109641056,5.3015238892
C,2.8742800896,3.3395610743,-0.2566356152
H,3.4538496466,2.7648853876,-0.9793377746
H,3.1640905331,3.1063729634,0.7697311571
H,2.9452981154,4.41400475,-0.4470540332

PhNHC(OH)=C(SO_2Me)SO_2Ph[b]
C,-0.8969262926,-0.118899628,0.2028561208
C,-0.2990367797,0.3132478368,-1.0109092548
O,-1.4417393868,0.7330623451,1.0600895714
H,-1.4210056447,1.6532108088,0.6623458746
N,-0.944584644,-1.4114048388,0.5667233399
H,-0.4804769702,-2.0315959737,-0.1022270008
S,0.2874769093,-0.7928346696,-2.275686935
O,1.5736753314,-0.3095577813,-2.7984675208
O,0.2188356151,-2.1770125544,-1.7311971088
S,-0.0592248612,2.0374283542,-1.3504825485
O,-0.2355420124,2.2681994391,-2.7910584179
O,-0.9482435034,2.7686878271,-0.3907505652
C,-1.602113286,-2.0671160921,1.639168042
C,-2.8083293176,-3.6021972032,3.6637439487
C,-1.5605041499,-3.4727526554,1.5942346776
C,-2.2496341686,-1.4319193237,2.7103941969
C,-2.8469348749,-2.2076720282,3.7079309007
C,-2.1573281288,-4.2308938607,2.5981186136

H,-1.0581639142,-3.968656837,0.7667379344
H,-2.2864840411,-0.3546658953,2.7718068244
H,-3.3458893747,-1.7037793757,4.5317246646
H,-2.1130905506,-5.3153359343,2.5435486756
H,-3.27547311,-4.1912414619,4.4479425402
C,-0.9159610573,-0.715375746,-3.6190696678
H,-0.5485145094,-1.3975451906,-4.390683135
H,-0.9558248684,0.3125779541,-3.9807993902
H,-1.8843494561,-1.0459879766,-3.2380553665
C,1.6218288865,2.5129712561,-0.9150451275
C,4.2046395182,3.2615452707,-0.2413233916
C,1.8872436831,2.9499007202,0.3863711403
C,2.6220716136,2.4500068486,-1.8878221909
C,3.9196712928,2.829573692,-1.5400473062
C,3.1903792805,3.3231652538,0.7193944917
H,1.0880658339,3.019024654,1.1166498297
H,2.3876304354,2.1035309078,-2.8868888596
H,4.7074945168,2.7854494008,-2.2867849025
H,3.408865571,3.6699730745,1.725627949
H,5.2174967152,3.5548892831,0.0218892535

PhNHC(OH)=C($SO_2Ph)_2$
C,-0.88866,-0.795344,0.487043
C,0.300334,-0.073669,0.206232
O,-1.016693,-1.573845,1.551207
H,-0.179791,-1.508062,2.101945
N,-1.966328,-0.748383,-0.318307
H,-1.790849,-0.256228,-1.197095
S,0.415602,1.138397,-1.093979
O,1.804871,1.175445,-1.568504
O,-0.674143,0.84815,-2.064455

S,1.775183,-0.333323,1.16201
O,2.474053,0.938399,1.375552
O,1.339244,-1.115384,2.365173
C,0.028762,2.749025,-0.380006
C,-0.566908,5.236724,0.693479
C,1.053053,3.502988,0.198505
C,-1.286183,3.219805,-0.436976
C,-1.579806,4.471934,0.107194
C,0.744803,4.753914,0.735984
H,2.062991,3.112221,0.231528
H,-2.058051,2.628542,-0.917779
H,-2.597231,4.851029,0.064052
H,1.532507,5.350607,1.187588
H,-0.799195,6.212047,1.113126
C,2.877636,-1.427675,0.249839
C,4.592526,-3.119647,-1.122489
C,2.705115,-2.810514,0.361945
C,3.894722,-0.875355,-0.531071
C,4.75503,-1.734551,-1.217615
C,3.570139,-3.656667,-0.333539
H,1.925183,-3.217762,0.996858
H,4.00171,0.200341,-0.600866
H,5.551505,-1.318126,-1.827995
H,3.449979,-4.733358,-0.250754
H,5.265591,-3.782324,-1.660166
C,-3.265659,-1.297206,-0.169604
C,-5.900815,-2.273478,-0.100819
C,-4.052267,-1.315074,-1.334787
C,-3.80828,-1.767884,1.035885
C,-5.118927,-2.251255,1.055952
C,-5.358073,-1.799262,-1.298503

H,-3.633733,-0.950797,-2.270374

H,-3.221553,-1.760239,1.943224

H,-5.528309,-2.613241,1.995558

H,-5.948794,-1.806747,-2.210643

H,-6.918136,-2.653387,-0.070226

PhNHC(OH)=C($SO_2Me)_2$

C,-0.88866,-0.795344,0.487043

C,0.300334,-0.073669,0.206232

O,-1.016693,-1.573845,1.551207

H,-0.179791,-1.508062,2.101945

N,-1.966328,-0.748383,-0.318307

H,-1.790849,-0.256228,-1.197095

S,0.415602,1.138397,-1.093979

O,1.804871,1.175445,-1.568504

O,-0.674143,0.84815,-2.064455

S,1.775183,-0.333323,1.16201

O,2.474053,0.938399,1.375552

O,1.339244,-1.115384,2.365173

C,0.028762,2.749025,-0.380006

C,-0.566908,5.236724,0.693479

C,1.053053,3.502988,0.198505

C,-1.286183,3.219805,-0.436976

C,-1.579806,4.471934,0.107194

C,0.744803,4.753914,0.735984

H,2.062991,3.112221,0.231528

H,-2.058051,2.628542,-0.917779

H,-2.597231,4.851029,0.064052

H,1.532507,5.350607,1.187588

H,-0.799195,6.212047,1.113126

C,2.877636,-1.427675,0.249839

C,4.592526,-3.119647,-1.122489
C,2.705115,-2.810514,0.361945
C,3.894722,-0.875355,-0.531071
C,4.75503,-1.734551,-1.217615
C,3.570139,-3.656667,-0.333539
H,1.925183,-3.217762,0.996858
H,4.00171,0.200341,-0.600866
H,5.551505,-1.318126,-1.827995
H,3.449979,-4.733358,-0.250754
H,5.265591,-3.782324,-1.660166
C,-3.265659,-1.297206,-0.169604
C,-5.900815,-2.273478,-0.100819
C,-4.052267,-1.315074,-1.334787
C,-3.80828,-1.767884,1.035885
C,-5.118927,-2.251255,1.055952
C,-5.358073,-1.799262,-1.298503
H,-3.633733,-0.950797,-2.270374
H,-3.221553,-1.760239,1.943224
H,-5.528309,-2.613241,1.995558
H,-5.948794,-1.806747,-2.210643
H,-6.918136,-2.653387,-0.070226

PhNHC(OH)=C(COMe)$SO_2C_4F_9$
C,-0.0439928202,1.4234029141,2.4509111462
C,0.6874588661,1.9472477423,1.3057148154
O,-0.7131349716,2.2581841058,3.1933042269
H,-0.5423167748,3.2243255624,2.7653744126
N,-0.0507385395,0.1312362741,2.7971504302
H,0.5537354981,-0.4562473253,2.221857772
S,1.4888337948,0.8676351922,0.1857649729
O,2.5500718212,1.5425782393,-0.5578970234

O,1.7439271175,-0.4362739321,0.8358245027
C,-0.7095006813,-0.5438643763,3.8596770478
C,-1.9071905159,-2.0938835904,5.8696932082
C,-0.3949041636,-1.9075475144,3.9906194202
C,-1.6300308486,0.0444976958,4.7396294486
C,-2.2189133135,-0.7398557064,5.7351762523
C,-0.9895627441,-2.6744975324,4.9891961309
H,0.3170976052,-2.3651166378,3.307342155
H,-1.8834430804,1.0906994768,4.6536108256
H,-2.9310450009,-0.276027859,6.412504167
H,-0.7335290516,-3.7268099872,5.0765643206
H,-2.3724728196,-2.6902204875,6.6494237029
C,0.6712453115,3.3792231666,1.0791098243
O,0.0174200323,4.1194301002,1.8690915469
C,1.4111312059,4.0846477897,-0.0311677718
H,2.4924553594,3.9850690746,0.1025463959
H,1.1294515478,5.1383757774,0.0143604235
H,1.1771936,3.6788762719,-1.0178292989
C,0.1212676456,0.4602292831,-1.1015074272
C,0.4594988401,-0.7381951361,-2.0445281269
C,-0.4343927853,-0.8116834211,-3.3301657138
C,-0.3775006754,-2.1717919849,-4.0999847671
F,-0.0945189052,1.5776546566,-1.8342992163
F,-1.0065072962,0.1756302039,-0.4099181939
F,0.2998777227,-1.8870886333,-1.3436578114
F,1.7504207746,-0.638659597,-2.4369179242
F,-0.0427295135,0.1577462518,-4.1882829127
F,-1.729307472,-0.5961892573,-2.9854859723
F,-1.0275439361,-2.033476566,-5.2655881961
F,0.8926872476,-2.5213814948,-4.3534175763
F,-0.9676285939,-3.1478650021,-3.3974182415

$PhNHCOCH(SO_2C_4F_9)=C(OH)CH_3$

N,0.230993922,-0.1388282754,1.9729510281

H,-0.0131142419,0.7516784812,1.5440982984

S,1.192024559,1.1129150377,-0.7366865108

O,0.375812077,1.9220861305,0.1866420546

O,2.1873602481,1.7562432433,-1.5951016603

C,1.2370498275,-0.8133329796,1.3776159495

C,1.8565621622,-0.2818757005,0.1202519183

C,2.9656979603,-0.949384581,-0.4258648638

C,3.754570305,-0.5792042466,-1.6511513404

H,3.1209602892,-0.3997661721,-2.5208080623

H,4.4447937537,-1.3995906616,-1.8572555593

H,4.3229898607,0.339082273,-1.4765330479

O,3.4469536495,-2.0183520451,0.161366489

H,2.8444712661,-2.2126072019,0.9733864356

O,1.6894414505,-1.8834854283,1.859525942

C,-0.0828908585,0.3139866612,-1.9347052113

C,-0.6257596144,1.2885985661,-3.0278751767

C,-1.9371166932,0.7944404073,-3.7299695704

C,-2.3070595043,1.5500410577,-5.0483183156

F,-3.5332447565,1.1660837134,-5.4339520019

F,-1.4417547678,1.2589794872,-6.0284142943

F,-2.313152296,2.8766376003,-4.8491299501

F,-2.9712934356,0.9430525346,-2.8710878151

F,-1.8082267182,-0.5206278372,-4.0392244348

F,0.3361810763,1.4448627946,-3.968777781

F,-0.8822493933,2.48809911,-2.456883035

F,-1.1002192748,-0.1512518283,-1.1757597483

F,0.5207080629,-0.7364412802,-2.5364792154

C,-0.4987863509,-0.4619945539,3.1443830982

C,-2.0688784116,-0.9081953511,5.4291237845
C,-0.325132069,-1.6360229042,3.8932432004
C,-1.4601435154,0.4825896113,3.5450010475
C,-2.2369368621,0.2599678094,4.679131828
C,-1.1146134726,-1.8447732562,5.0276348912
H,0.4126131761,-2.3666160409,3.5950307693
H,-1.5964402425,1.3923222319,2.9640422432
H,-2.9742758942,1.0015881343,4.9745282199
H,-0.9736880485,-2.7567464336,5.602015648
H,-2.6742069246,-1.0841581072,6.3140046491

PhNHC(OH)=C(CN)SO_2Me
C,0.0019182811,0.6570865197,-0.4324674477
C,0.6795150479,1.11785701,-1.5802833533
O,-0.5826432335,1.4577371867,0.4393956641
H,-0.4683506512,2.4050011955,0.1276665164
N,-0.0757494188,-0.6679966418,-0.1812352848
H,0.3821993431,-1.2459973785,-0.8782073754
S,0.8188633712,2.8353367553,-1.9760805338
O,0.4275878985,3.0898434319,-3.3650710176
O,0.1130806082,3.5602508277,-0.8706089185
C,1.2612307991,0.2014811872,-2.4787929965
N,1.7485601533,-0.5998334818,-3.1770584456
C,2.5716160421,3.2419832615,-1.8284052247
H,3.1306137965,2.6368857695,-2.5455885943
H,2.8953229629,3.048308173,-0.8041791571
H,2.6610976543,4.3038836507,-2.0726985927
C,-0.7221879649,-1.4046143409,0.8473339292
C,-1.9167523774,-3.0629112893,2.7742767964
C,-0.6780923895,-2.8027532445,0.711974278
C,-1.3664841691,-0.836314733,1.9560528192

C,-1.9578001032,-1.6739370138,2.9057392505
C,-1.2705301187,-3.6231997729,1.6687223319
H,-0.1802776402,-3.2479986726,-0.1472475235
H,-1.4098509399,0.2355640746,2.079993439
H,-2.4557289402,-1.2231935833,3.7601318913
H,-1.2266010505,-4.7018333867,1.5453713053
H,-2.3805571612,-3.7006354042,3.5212659439

PhNHC(OH)=C(CN)SO_2Ph
C,-0.9022308835,0.0017438122,0.5060342534
C,0.3114905382,0.7108130264,0.592640856
O,-1.0760548051,-1.2091587769,1.0055574286
H,-0.2226956518,-1.488447327,1.4530490025
N,-1.9695038185,0.5590766465,-0.1087363952
H,-1.7871714241,1.4819143656,-0.4891760441
S,1.7721338794,0.0226818733,1.3192987675
O,2.3871074321,1.0033181457,2.217722321
O,1.352694525,-1.3158188505,1.84536202
C,0.4119697891,2.0109218839,0.0584498366
N,0.4403186033,3.0782760722,-0.4177577836
C,-3.3113395359,0.1228751864,-0.266263829
C,-6.0093652725,-0.5316260883,-0.6984861364
C,-4.178811137,1.0398023407,-0.8847064278
C,-3.8006384162,-1.1290281877,0.1356416838
C,-5.1452462669,-1.4398271982,-0.0846640759
C,-5.5154572214,0.713195948,-1.0989761069
H,-3.8040765263,2.0127109846,-1.196794804
H,-3.1506833401,-1.8492706092,0.6099947768
H,-5.5139795898,-2.4119488302,0.2319252728
H,-6.1696315861,1.4363924304,-1.5782198934
H,-7.0517877738,-0.7886010201,-0.8633162712

C,2.9289044926,-0.2831366053,-0.0224822743
C,4.6873167474,-0.7194257672,-2.1203178703
C,2.9155296888,-1.5189470737,-0.6753449471
C,3.8093077279,0.7365653664,-0.3945216448
C,4.6897531357,0.5099296908,-1.4545480174
C,3.805398152,-1.7323913472,-1.7293146459
H,2.2365440495,-2.3006380307,-0.3507669705
H,3.8113382899,1.6791754139,0.142808352
H,5.3800816748,1.2932547297,-1.7544570039
H,3.8133493943,-2.6914491911,-2.2398355922
H,5.3771727901,-0.8909808187,-2.9422730317

PhNHC(OH)=C($SO_2C_4F_9$)$_2$
C,-0.6586518326,0.1209574141,1.1646469822
C,-0.0617175651,0.3026243177,-0.1371169247
O,-1.4684332807,1.0182573738,1.6898960818
H,-1.6081223943,1.7728047441,1.0486400262
N,-0.4255723514,-0.958645548,1.910175799
H,0.2535927018,-1.6016516023,1.4972448181
S,0.8144219393,-0.981098646,-0.9661870081
O,1.7681296516,-0.4421942712,-1.9265260365
O,1.2314322698,-1.9848802761,0.0347045034
C,-0.9916277676,-1.4033660515,3.1393070592
C,-1.9474002129,-2.5024071931,5.5359239967
C,-1.9053064243,-0.6817551398,3.921025471
C,-0.5580683323,-2.6711442404,3.5634926086
C,-1.0328274815,-3.2141814,4.754374229
C,-2.374978609,-1.2433963738,5.1113009168
H,-2.2446550911,0.2971180637,3.6178960288
H,0.149874667,-3.231328134,2.9568896279
H,-0.6876206347,-4.1954517126,5.067584377

H,-3.0833897921,-0.6785974709,5.7111610328

H,-2.3201688561,-2.92415507,6.4649186206

C,-0.5613710716,-1.8690300655,-1.9746079552

C,-0.0037915441,-2.8594297378,-3.0465866038

C,-1.0593170497,-3.8970277744,-3.5623412015

C,-0.6570556519,-4.6571929429,-4.8684268952

F,-1.3198299083,-0.9356872678,-2.5709978048

F,-1.3207597534,-2.5356865375,-1.0717877592

F,1.0315315907,-3.5471284389,-2.507705346

F,0.4453302097,-2.1359413007,-4.0961601034

F,-2.2293939356,-3.2567279815,-3.8093570095

F,-1.2635005196,-4.8241893903,-2.5977119911

F,-1.5479639249,-5.6369123502,-5.0853491294

F,-0.6621304656,-3.8350212506,-5.9245520633

F,0.5620150555,-5.2034840972,-4.7428602762

S,-0.1669930845,1.8591907931,-0.9491394192

O,-0.105105883,1.7529149823,-2.3972503626

O,-1.2704648886,2.6161099663,-0.2947529333

C,1.4102263216,2.8072055662,-0.3865244635

C,1.2705311417,4.3597755241,-0.5141536144

C,2.6394813396,5.1225026603,-0.4786946235

C,2.529795446,6.6641422468,-0.2377957602

F,3.7370177131,7.2163570314,-0.4282424186

F,2.1339781342,6.9283384305,1.0146097702

F,1.6610347386,7.2175907822,-1.0973156908

F,3.2722830136,4.9376942303,-1.658127959

F,3.4048543145,4.6103023576,0.5184995865

F,0.5024907698,4.8058517091,0.5084282813

F,0.6568894535,4.6461703311,-1.6855871869

F,2.4406108114,2.3690259098,-1.1247382652

F,1.6206987232,2.482777731,0.9098768876

2,4-$MeO_2C_6H_3NHC(OH)=C(SO_2Ph)_2$

C,0.1943529976,-0.61511674,-0.623278068

C,-1.1046365488,-0.1183565135,-0.3279455867

O,0.4317777381,-1.4098344109,-1.658161347

H,-0.4288557652,-1.5595711917,-2.1539409695

N,1.2700443793,-0.3155062672,0.1236711543

H,1.0627365357,0.1730688593,0.9991599834

S,-2.5340542604,-0.6817170973,-1.2156200006

O,-3.4119255935,0.4426380739,-1.5622387094

O,-2.0017201228,-1.5296713812,-2.3339274055

C,2.6430708497,-0.6036950123,-0.0793382281

C,5.4266009394,-1.0321884982,-0.2293849228

C,3.5006095791,-0.2193245717,0.9871310577

C,3.2168050375,-1.1942615793,-1.2042906836

C,4.6001041834,-1.4094031926,-1.2874919901

C,4.8706105425,-0.4331233093,0.9131967364

H,2.5908930085,-1.498003043,-2.029935085

H,5.0001673789,-1.8735800227,-2.1808951031

H,5.5350690086,-0.1481966431,1.7198780808

O,6.7829701967,-1.197399221,-0.1961848743

O,2.8698042194,0.3635098943,2.0477438423

C,-3.4680955651,-1.8098372409,-0.1663390466

C,-4.9185105992,-3.5633773147,1.4170795625

C,-3.0644988858,-3.1455045581,-0.0825124402

C,-4.5855891247,-1.3357827482,0.5222870889

C,-5.3118855654,-2.2259514942,1.3161973977

C,-3.7970521741,-4.0226286364,0.7184280169

H,-2.2060752737,-3.4960977114,-0.646195579

H,-4.869873706,-0.293612007,0.4408544496

H,-6.184108368,-1.8702172891,1.8576209414

H,-3.4962271597,-5.064354281,0.7891077189
H,-5.4874772389,-4.250241121,2.0382603346
S,-1.3900501426,1.1333106311,0.900271962
O,-2.7928456023,1.0392182847,1.3272785276
O,-0.3109297899,1.0172141108,1.9124487695
C,-1.1563458409,2.7376333639,0.104108915
C,-0.8002260371,5.2165642699,-1.0917733915
C,-2.18449335,3.2695123285,-0.6798757512
C,0.042634711,3.4263398004,0.3051343752
C,0.2160754533,4.6733899966,-0.3011594214
C,-1.996988157,4.5163549583,-1.2782334828
H,-3.1023087003,2.7110869235,-0.8243242339
H,0.8129634942,3.0014331387,0.9394856052
H,1.1426143741,5.2204843992,-0.1486316901
H,-2.7885578603,4.9403229084,-1.8900929411
H,-0.6619990873,6.1876442897,-1.5602024685
C,3.6290326673,0.7435904339,3.1903317105
H,2.9072957712,1.1569989654,3.8959005769
H,4.3743616656,1.5060639743,2.9317817327
H,4.1272294079,-0.1260527403,3.6361899204
C,7.4180904645,-1.8020114187,-1.3159632612
H,7.0508256136,-2.823783383,-1.4778146603
H,8.4813985386,-1.831917943,-1.0722494968
H,7.2682563192,-1.2087460084,-2.2273864229

2,4-$MeO_2C_6H_3NHC(OH)=C(CO_2Me)SO_2Ph$
C,0.1690406878,-0.4841696868,-1.1351946403
C,-0.5934371759,0.5778177929,-1.7175290946
O,1.1239503508,-1.0593458317,-1.8482675356
H,1.1308720423,-0.6092534921,-2.7616549141
N,-0.0121945577,-0.9580066183,0.1035581749

H,-0.7596960484,-0.4934132933,0.6306575171
C,0.65581882,-1.9971266406,0.7964977726
C,1.803331035,-4.0160846581,2.3971659222
C,0.1952588028,-2.2299440537,2.1215949909
C,1.6919843683,-2.794070909,0.310638893
C,2.268024185,-3.7998629931,1.100260636
C,0.7608204543,-3.225091956,2.9079799368
H,2.0615914823,-2.6410784143,-0.6919496055
H,3.069649077,-4.3946451479,0.6790050068
H,0.4185439203,-3.4142295844,3.9181041907
O,2.2862304213,-4.9653234544,3.2546138506
O,-0.8167235968,-1.4122037629,2.527742087
S,-1.943074857,1.3817799913,-0.8782111582
O,-3.1814695031,1.2820654581,-1.6638230149
O,-1.9401521355,0.8668897613,0.5175128991
C,-1.5144401669,3.1338831641,-0.7578406896
C,-0.9171639406,5.8322111581,-0.5042928683
C,-2.2383543445,4.0639032465,-1.5032724789
C,-0.50285215,3.5296183436,0.1208759267
C,-0.2023573387,4.8874932474,0.2403229114
C,-1.9349558442,5.4214504995,-1.3698480199
H,-3.0253912636,3.7203121189,-2.1658867011
H,0.0319792643,2.7905130386,0.7097042044
H,0.5823113723,5.2075924057,0.9205789374
H,-2.4957101139,6.1565452364,-1.9411788263
H,-0.6835794256,6.8890778727,-0.4045239032
C,-1.3745522229,-1.5792290747,3.826186374
H,-2.1598957088,-0.8264468399,3.904461779
H,-0.618874151,-1.4099008569,4.6034516527
H,-1.8080528314,-2.5803719146,3.9416003266
C,3.3386318404,-5.8086539778,2.8038794969

H,3.0296087998,-6.3987434604,1.9312805092

H,3.558706763,-6.4784826684,3.6368851903

H,4.2359780393,-5.2272743623,2.5548481995

C,-0.2945565022,0.9563384903,-3.0771627589

O,0.5952893613,0.4235518088,-3.7762451691

O,-1.0359182066,1.9594651128,-3.567466138

C,-0.7760342255,2.3513285566,-4.9277721389

H,-0.952062754,1.5118652151,-5.6047770943

H,0.2541176579,2.6998450539,-5.0359038883

H,-1.4802399808,3.159406179,-5.1266067478

Amides

i-PrNHCOCH(CO_2Me)SO_2Ph

S,-0.8587300386,0.5266693435,1.0342555882

O,-0.1341725239,-0.2685417283,2.0362924581

O,-1.4548955818,1.8291168242,1.3792280284

C,0.3228569201,0.8751892148,-0.3972978164

C,1.2609737851,-0.3336662287,-0.6100480198

O,0.8683058854,-1.2518839152,-1.3306117767

N,2.4407751567,-0.2900054245,0.0370889207

C,-2.1439143635,-0.4986337482,0.3050552926

C,-4.1467503468,-2.0630113252,-0.7920039595

C,-2.0061978789,-1.8879607483,0.3280525814

C,-3.2636744077,0.1255260889,-0.2515653593

C,-4.2695620707,-0.6697946778,-0.8034602981

C,-3.0211236493,-2.6696945275,-0.2265369221

H,-1.1279495897,-2.3422020752,0.7727136145

H,-3.3505368981,1.2072498048,-0.2311030586

H,-5.1504799421,-0.2015669847,-1.2338478685

H,-2.9301734404,-3.7521544496,-0.2172200566

H,-4.9329858358,-2.6778846686,-1.2221126859

H,2.6021125866,0.5186221989,0.6304910682
H,-0.3223677704,0.9469547229,-1.2738115548
C,3.4501445749,-1.3676712357,0.0360988605
H,4.2526771529,-0.9783213743,0.6736454124
C,4.0262882314,-1.6038990699,-1.3672668182
H,4.4304272473,-0.6744482164,-1.7843264838
H,3.2577472184,-1.9859434395,-2.0449692348
H,4.8397532433,-2.3372277199,-1.314709521
C,2.9123061975,-2.6555679469,0.6763455777
H,2.5089595681,-2.4549290126,1.6745745511
H,3.7234132074,-3.387416869,0.7713917205
H,2.121319056,-3.0942367671,0.0611563162
C,0.9646675599,2.2243722555,-0.1192747747
O,1.8776332332,2.4110144117,0.6644958711
O,0.3930033083,3.1853258171,-0.8522960883
C,0.864696662,4.5303029835,-0.6140434459
H,0.6811305703,4.8063953686,0.426842393
H,0.286633714,5.1578608523,-1.2915734451
H,1.9329678897,4.5989403247,-0.8332098672

i-PrNHCOCH(COMe)SO_2Ph
S,1.2466979828,1.6625661804,-0.2454524464
O,0.5039912042,2.35928031,0.8148236474
O,2.5817126969,2.126351656,-0.6697029239
C,1.5022114905,-0.1179480361,0.2759431909
C,0.1760108474,-0.8426384967,0.6001836755
O,-0.2920155413,-1.6129640583,-0.2389583898
N,-0.3724278626,-0.5529394181,1.7966872613
C,0.2000698676,1.556112435,-1.7028336187
C,-1.4100102978,1.4065268456,-3.9502270225
C,-1.1831108541,1.6765765518,-1.5546259547

C,0.7956957926,1.3686503523,-2.9529059765
C,-0.0220914508,1.2934338758,-4.0813972867
C,-1.9884049332,1.6008625567,-2.6924680909
H,-1.6117786213,1.8382598578,-0.5713222141
H,1.8758541631,1.305802553,-3.0391143611
H,0.4249352527,1.1532094739,-5.0616115156
H,-3.0663192576,1.6950159868,-2.5953666567
H,-2.0422081768,1.3477867742,-4.832222194
H,0.1803897112,0.0392465582,2.4095043296
H,1.8974404702,-0.5900655773,-0.6260827502
C,-1.5960199723,-1.1713633631,2.3449966086
H,-1.7154868029,-0.6975612173,3.3262576394
C,-1.4252313166,-2.6830704244,2.5579374143
H,-0.5539169347,-2.8911682659,3.1891444152
H,-1.2964913337,-3.1990040366,1.6020299351
H,-2.3127126639,-3.0911338847,3.0560599788
C,-2.8326652482,-0.8350391449,1.5002749868
H,-2.9455509822,0.2497041231,1.3936379925
H,-3.73254665,-1.2242543202,1.9910364917
H,-2.7589883083,-1.2821410907,0.5050115407
C,2.566752642,-0.1103441031,1.391752809
O,2.2602915487,0.1379670318,2.5446355022
C,3.9788220334,-0.4217254478,0.9670495454
H,4.6458405334,-0.3788853674,1.830533425
H,4.2962275057,0.3034563289,0.2076086775
H,4.025033066,-1.4185632987,0.5091826346

i-PrNHCOCH(SO_2Ph)$_2$
S,-0.1306517948,1.7577555686,-0.414822297
S,0.6391008758,-1.2826449401,-1.0095044348
O,-0.7508986378,2.4412936885,0.736077023

O,0.0747727941,-2.5782052304,-0.5948210435
O,1.2832572438,1.995789083,-0.7515720349
O,0.5788988074,-0.8312042344,-2.404443257
C,-0.2244269401,-0.0377334511,0.0929846499
H,0.3733785373,-0.010183364,1.0069484593
C,-1.675718434,-0.4792631252,0.3243847444
O,-2.491802139,-0.3813434907,-0.5867964903
N,-2.0002783066,-0.9660745988,1.5493965528
H,-2.9815171636,-1.2219060319,1.6120239206
C,-1.1948663852,-1.1355134285,2.7687056369
H,-0.1635083302,-1.3339445785,2.4582598413
C,2.3585395494,-1.2519515005,-0.465056247
C,5.008529475,-1.2826630902,0.3453138481
C,2.7573689038,-2.154234727,0.526016594
C,3.2622218923,-0.3744911882,-1.0683718108
C,4.5951306988,-0.3958106674,-0.653332785
C,4.0932775021,-2.1621263781,0.932298141
H,2.0397185971,-2.8516956498,0.9460662148
H,2.9270300379,0.3112097568,-1.8367872837
H,5.3090234454,0.2827713596,-1.1115670029
H,4.4194149415,-2.8622067562,1.6965614206
H,6.0480217974,-1.2932221156,0.6624525551
C,-1.1308836211,2.0835184242,-1.8667273231
C,-2.6411994461,2.7356118392,-4.090635243
C,-2.4453882712,2.5221270737,-1.6879014432
C,-0.5531076303,1.9701380277,-3.13300894
C,-1.3227261896,2.2995513279,-4.2496382997
C,-3.1999470483,2.8499417524,-2.8136587729
H,-2.8602946757,2.6063326095,-0.6902983443
H,0.4695111055,1.631024082,-3.2406885432
H,-0.8898359392,2.2141094214,-5.2423142692

H,-4.2240604671,3.191535696,-2.6925052893
H,-3.2351691377,2.9898370671,-4.9647501747
C,-1.2295871773,0.1240645986,3.6468601212
H,-0.5843693699,-0.0036526109,4.5245699678
H,-2.2504256766,0.3164984201,3.9995512539
H,-0.8958732468,1.0066668362,3.0917050903
C,-1.6953714554,-2.3774732871,3.5156403101
H,-1.0956255624,-2.5433976121,4.4168549995
H,-1.6307248074,-3.2695496318,2.8839992971
H,-2.7389385518,-2.249284844,3.8325310881

i-PrNHCOCH(SO_2Me)$_2$
S,-0.5684932551,-0.9534412593,2.0019867271
S,-1.6147090392,0.6017717165,-0.5310788439
O,-1.0888624245,1.6296131163,-1.4561500697
O,-2.1302991278,-0.6724448758,-1.0536461515
C,-0.1885131426,0.2315291612,0.6131698582
H,-0.003253062,1.1640557731,1.1588643106
C,1.0746501259,-0.1794859882,-0.1960952354
O,1.515494815,-1.3216152171,-0.1325443467
N,1.6427804776,0.8290285403,-0.8952377213
H,1.0637250117,1.6415806483,-1.0882469385
O,0.6037281409,-0.9108026172,2.8840823408
O,-1.883713304,-0.5271759564,2.5227584261
C,-0.7647784237,-2.5963199327,1.2914222804
H,0.2051759051,-2.933425043,0.9311488154
H,-1.4986733661,-2.5357469135,0.48533156
H,-1.1381901614,-3.2079074365,2.1176672338
C,-2.8950197262,1.3997467678,0.4583265294
H,-2.4830979513,2.3081594827,0.9020276834
H,-3.2504125217,0.7078182546,1.2200082097

H,-3.6751267157,1.6500193816,-0.2663320326
C,2.8138249717,0.6148509835,-1.7638546608
H,3.4096879064,-0.1565390911,-1.2676327524
C,2.3924811597,0.1054560567,-3.149396877
H,3.27771286,-0.0861052004,-3.7674774058
H,1.7678974961,0.8444362395,-3.6660167613
H,1.8261888096,-0.8272834485,-3.0649298612
C,3.6200123311,1.9148044613,-1.8360381595
H,4.5187832315,1.7667979374,-2.4445182605
H,3.9299880924,2.2440213618,-0.838333633
H,3.0346392601,2.7195463004,-2.3006262537

i-PrNHCOCH($SO_2C_4F_9$)$_2$
S,0.1813418366,-0.1870917163,1.506198969
S,-1.0198386106,0.7126210776,-1.2539994979
O,-0.58080802,1.3985982529,-2.4798405459
O,-1.6043031983,-0.6224535692,-1.2998076368
C,0.4610395382,0.7461506117,-0.1014255261
H,0.5085897509,1.7745636363,0.2776488482
C,1.8477454339,0.4058959183,-0.7525047989
O,2.6103153644,-0.3058010157,-0.1149143952
N,2.1354935987,1.0144047123,-1.9164621151
H,1.3833796346,1.4714585307,-2.4245225141
O,1.2357281224,0.2233789835,2.4260400674
O,-1.2307978141,0.0137679458,1.8302668872
C,0.318378284,-2.0969280727,1.0848426492
C,-2.3031112332,2.0033688243,-0.4915533028
C,3.4240163525,0.8109302197,-2.6079838294
H,4.1639701102,0.6521743731,-1.8182449453
C,3.374385437,-0.4346332155,-3.5030157505
H,4.3478501246,-0.5948893132,-3.9809568891

H,2.6213080755,-0.3210764256,-4.2924434385

H,3.1323357099,-1.3262055204,-2.9160496002

C,3.7703538132,2.0828907831,-3.3864536196

H,4.7408389916,1.9663080418,-3.8802464222

H,3.8257593571,2.9524173273,-2.7224853896

H,3.0245701956,2.2881037664,-4.1657508329

C,-3.7269475683,1.4024827758,-0.258283654

C,-4.7233985955,2.3872418204,0.4481531034

C,-6.2227457079,1.9413470931,0.4199812617

F,0.620286087,-2.2217939052,-0.2171125996

F,-1.783961444,2.5107981592,0.6423192674

F,-3.643825973,0.2920951899,0.4924331851

F,-4.3526242218,2.5080713955,1.7428487427

F,-6.3605968871,0.6936473092,0.8888375728

F,-6.9296564207,2.776021571,1.1962348409

F,-6.7130479074,1.9976895534,-0.8255996094

F,-4.6550592613,3.607109562,-0.1404910155

F,-4.2163769451,1.0820844665,-1.484360795

F,-2.3762938473,2.9795360622,-1.4054695656

C,1.3508249524,-2.9310839028,1.9264847069

C,0.8839762382,-3.2358349461,3.3916187354

C,2.0260209221,-3.6560839255,4.3716119878

F,1.4755446456,-4.076531814,5.5206049976

F,2.7464084454,-4.6610279637,3.8465490864

F,2.8370377334,-2.6270623096,4.6384400281

F,-0.0192596607,-4.241496156,3.3610111238

F,1.4939250268,-4.1176197104,1.2816634801

F,2.545255932,-2.3126046975,1.9444334915

F,0.2857805714,-2.1316297158,3.9060779805

F,-0.909807569,-2.593309768,1.2956772762

i-PrNHCOCH(COMe)$SO_2C_4F_9$

S,1.1204482613,0.2606555718,0.9848569946

O,0.2570918034,0.6380092578,2.1023467797

O,2.3125414729,1.0344155869,0.6180732243

C,1.6602931326,-1.512502086,1.1481064317

C,0.4966921762,-2.4904515322,1.4704504614

O,0.098819528,-3.2279220019,0.571359585

N,0.0242518423,-2.4390827113,2.7283599259

H,0.5000691597,-1.8124248019,3.369317796

H,2.0243238208,-1.7758072447,0.1537033441

C,-1.0908632207,-3.2571307122,3.2525687631

H,-1.1866949503,-2.9330399058,4.2951727127

C,-0.7526186451,-4.754509345,3.2416749

H,0.1775123047,-4.9492949989,3.7874876561

H,-0.6423963845,-5.1220706208,2.2176007613

H,-1.5575661683,-5.3181822637,3.7275980667

C,-2.4075015548,-2.9430888933,2.5287415855

H,-2.6275196743,-1.8708511884,2.5689495823

H,-3.230933587,-3.4812470773,3.0125568749

H,-2.3617763229,-3.2520697259,1.4805536165

C,2.8285196459,-1.4982764752,2.169347966

O,2.6009390495,-1.3798989543,3.3578857065

C,4.2116674448,-1.6442559786,1.5941256979

H,4.9516672884,-1.6370054882,2.3968015572

H,4.4045224896,-0.8183782065,0.8976580202

H,4.2880017056,-2.5782544753,1.022263725

C,0.0104459727,0.1971758924,-0.5912934814

C,-0.2082047545,1.6131133904,-1.2190284571

C,-1.4241130054,1.6853950183,-2.2057653686

C,-1.4576506471,2.9537957261,-3.1202663533

F,-2.6325066853,2.9864911087,-3.7664115003

F,-1.3375082907,4.0700709179,-2.3857361723
F,-0.4733479361,2.9188205017,-4.0276484721
F,0.9153521176,1.9597325892,-1.887763451
F,-0.4193569806,2.501037634,-0.2191788228
F,-1.3986248888,0.5990608254,-3.0180184782
F,-2.569003159,1.6702805091,-1.4868324502
F,-1.1680055115,-0.3405425079,-0.2302067787
F,0.6173036837,-0.6050299456,-1.4887805791

i-PrNHCOCH(SO_2Me)SO_2Ph
C,-1.5128385657,-0.2051096803,-0.8583611368
C,-0.4599760993,-1.0583867507,-0.1248855159
O,-0.5063496563,-1.2435223025,1.0886906475
N,0.4643711425,-1.6131256802,-0.9476205564
H,0.5490315284,-1.2238096001,-1.8825772295
H,-1.7805163647,-0.6475461908,-1.8235106733
S,-3.1617331533,-0.0372309665,0.0183968759
O,-3.0657279642,1.0141688279,1.0407564965
O,-4.1556478277,0.0507777216,-1.0615295095
S,-0.814866777,1.4442904983,-1.4281979735
O,0.2591079605,1.0104917582,-2.3488912403
O,-1.9335399102,2.2574894613,-1.9075835793
C,-0.0462268569,2.2585617656,-0.0255095394
C,1.1704825427,3.5971295687,2.0685962862
C,1.3308329774,2.111565223,0.1649685883
C,-0.8267163011,3.0716311935,0.8008916731
C,-0.2039602363,3.7405913689,1.8553159083
C,1.9372382286,2.7880319457,1.2245860399
H,1.9124488722,1.501050851,-0.5164839336
H,-1.8913745507,3.1689631605,0.6266588067
H,-0.7958302503,4.3743216044,2.5094740916

H,3.0073484074,2.6888159413,1.3841003869
H,1.6470931664,4.1227801689,2.8918866363
C,-3.4254316525,-1.6197623442,0.8525245205
H,-2.7049876928,-1.7277400574,1.6605864296
H,-3.3459569304,-2.4285471595,0.1225080147
H,-4.4518915286,-1.5520400589,1.2242385627
C,1.566996744,-2.4522536459,-0.4502460389
H,1.1613705654,-2.9859213975,0.4146018554
C,1.9525190209,-3.4591165608,-1.538119842
H,2.7446950469,-4.1224294965,-1.1745091328
H,2.3321122616,-2.9498034123,-2.4338140762
H,1.0950340154,-4.0753065555,-1.8297291671
C,2.7606900289,-1.6052773343,0.0125187387
H,3.5482764983,-2.2516742755,0.4175925537
H,2.4575959126,-0.905047706,0.7969397284
H,3.1863270981,-1.0370096834,-0.8242636962

i-PrNHCOCH(CN)SO_2Me
S,0.9380883575,1.4561616628,-1.1053321403
O,0.0642533367,2.2036978691,-0.1910211861
O,2.3041433422,1.9094856101,-1.3951663027
C,1.1060590046,-0.2992154161,-0.4041742024
C,-0.2928024667,-0.8534721837,-0.0246161623
O,-1.049705727,-1.1728507156,-0.9394126159
N,-0.5711270271,-0.9224546443,1.2898948084
H,0.1346271506,-0.5974380411,1.939200762
H,1.48770303,-0.9003642914,-1.2353836693
C,-1.864654756,-1.3626601627,1.8641127738
H,-1.7134299448,-1.2735075569,2.9459556183
C,-2.152851555,-2.8340064772,1.5378889128
H,-1.3275118617,-3.476489122,1.8642825027

H,-2.3038036858,-2.9750801334,0.4640972988
H,-3.0617925396,-3.1537208044,2.0602750929
C,-3.0110748951,-0.4265951232,1.4582418188
H,-2.7731301045,0.6140370475,1.7029294029
H,-3.9219925006,-0.7080611825,1.9991322641
H,-3.211497947,-0.4958296549,0.385477719
C,0.0711290501,1.1987019523,-2.6681918925
H,0.7193341472,0.6322572229,-3.3395143344
H,-0.103729128,2.2038291923,-3.0615747712
H,-0.8643494398,0.6726084569,-2.4765620261
C,2.0854827914,-0.2642434765,0.6711573561
N,2.8186853772,-0.2653374305,1.5722891341

i-PrNHCOCH(CN)SO_2Ph
S,1.4568459827,0.8790817497,-0.1801836408
O,0.9506810641,1.758413791,0.8904308805
O,2.8395876943,0.975630767,-0.6623491815
C,1.2384181036,-0.8913114506,0.4261185172
C,-0.2138700045,-1.2480740471,0.8755237916
O,-0.8002096317,-2.1540719262,0.2957659052
N,-0.6823130397,-0.5270474055,1.9147523495
H,-0.1261542157,0.2671178777,2.2147442288
H,1.4630479647,-1.5184883858,-0.4409899738
C,-1.9919874807,-0.7346747693,2.572388165
H,-2.0004240336,0.0051409628,3.3810635984
C,-2.0880422733,-2.1318476042,3.1998905005
H,-1.2494890265,-2.3112697561,3.8813769212
H,-2.0864534486,-2.9092376941,2.4307463634
H,-3.0187450095,-2.2135175542,3.7730361326
C,-3.1631791091,-0.4311504859,1.6273825927
H,-3.0912374831,0.5871884655,1.22877747

H,-4.1100626636,-0.514563576,2.1734295624
H,-3.1824479112,-1.1354943537,0.7908834809
C,2.2154148562,-1.128402665,1.4813163436
N,2.9703434949,-1.3296451358,2.3407314818
C,0.3474757282,0.9767579105,-1.5879960616
C,-1.3499725366,1.1271179977,-3.7692849065
C,-0.93235531,1.508954814,-1.4150966224
C,0.800716283,0.5278326808,-2.8324246564
C,-0.0621574494,0.6038224676,-3.9263745346
C,-1.7824232082,1.5823625762,-2.5203077934
H,-1.2430385075,1.8710480328,-0.4409729026
H,1.8119615642,0.1489192383,-2.9431082707
H,0.2741805182,0.2624221942,-4.9011799992
H,-2.7792980676,1.9982787792,-2.4052227079
H,-2.0162871989,1.1858899603,-4.6256253173

t-BuNHCOCH(CO_2Me)SO_2Ph
S,0.9749619597,1.5714586133,-0.7645689421
O,-0.1083489071,2.2528921583,-0.0406895265
O,2.3413698096,2.1225259417,-0.7865444154
C,1.1415653687,-0.1739228776,-0.0591722451
C,-0.2477790111,-0.6997610404,0.3669204589
O,-0.9437975544,-1.2440876436,-0.4913526086
N,-0.5900074096,-0.4933438197,1.6525267875
C,0.4536564681,1.3081579353,-2.4658672893
C,-0.331750056,0.9321503705,-5.0933596214
C,-0.9088786614,1.2198807602,-2.7585281272
C,1.4321871218,1.2150420171,-3.459245269
C,1.028611208,1.0256906738,-4.782360885
C,-1.296538587,1.0308096492,-4.0861129888
H,-1.6437329574,1.2988206415,-1.9655772421

H,2.481724791,1.3098468516,-3.1994803584
H,1.7756668188,0.9588978237,-5.5684457689
H,-2.3523789808,0.9594379534,-4.331474998
H,-0.64097884,0.7850037462,-6.1248537772
H,0.087087622,0.0083365313,2.2215564299
H,1.4733068861,-0.7787528689,-0.9041014062
C,-1.8996291804,-0.8245271046,2.270788214
C,-2.1353243258,-2.3453081976,2.2168743858
H,-1.3336854237,-2.8794108538,2.7404587342
H,-2.1743140501,-2.6985208678,1.1832770841
H,-3.0858758467,-2.5913367657,2.7051089538
C,-3.0309751553,-0.0690745919,1.5482732105
H,-2.8463769599,1.0106592761,1.5668400718
H,-3.9870706264,-0.2670330879,2.0474410972
H,-3.1108544473,-0.391858555,0.5070420777
C,2.2350199344,-0.120417622,0.9942013514
O,2.0903368759,0.3039260887,2.126178322
O,3.3852630513,-0.6027365132,0.5120969604
C,4.5262764082,-0.5235303836,1.3952164864
H,4.7261728266,0.5206168224,1.6466158198
H,5.3527080912,-0.9534821121,0.8302193971
H,4.3373379723,-1.0949843476,2.3072157793
C,-1.8063206152,-0.3574079089,3.7324378356
H,-0.9926000686,-0.8687926592,4.2614847333
H,-2.7415659215,-0.5801383673,4.2564492395
H,-1.6344693277,0.724274234,3.792511939

PhNHCOCH(CO_2Me)SO_2Ph
C,-0.4236525712,0.926437219,-0.3832889864
C,0.6613751302,-0.0553757341,0.1442849101
O,0.3853810405,-0.9523284755,0.9255318744

N,1.8916102905,0.1707213019,-0.4036376093
H,1.9548356449,0.9542308471,-1.0479594455
C,3.0960901597,-0.5492476698,-0.2071081195
C,5.5638912368,-1.8589815256,0.0653342325
C,3.2121062234,-1.6466116821,0.6595739318
C,4.2173515754,-0.112409023,-0.9324008457
C,5.4412219189,-0.7640278031,-0.7956351233
C,4.4469928997,-2.2890231521,0.7847277379
H,2.3520464202,-1.9850539361,1.220558285
H,4.1281790229,0.7397146155,-1.6035777732
H,6.2987514326,-0.4134076896,-1.3638663708
H,4.5290106477,-3.1382846835,1.4582395895
H,6.5175391978,-2.3682059746,0.1733283319
H,-0.6546842442,0.6443194223,-1.4162646387
C,0.0811570968,2.3675026418,-0.444152827
O,0.8031140882,2.7438950057,-1.3528565867
O,-0.2841033919,3.1042905396,0.593848697
S,-2.0741038326,0.7991325727,0.4833251329
O,-1.9061396938,0.8707524249,1.9374305756
O,-2.8987929692,1.7827860484,-0.245194226
C,-2.6890823168,-0.8375718289,0.0431975643
C,-3.7272729032,-3.3212690572,-0.60895446
C,-3.3810880379,-0.9902803937,-1.161916898
C,-2.5171254528,-1.8982846968,0.9350506458
C,-3.0451588608,-3.1462677958,0.5995998568
C,-3.8958267496,-2.2469556669,-1.4881522127
H,-3.5331311807,-0.1362587826,-1.8145720365
H,-1.9782255665,-1.7413203256,1.8619059989
H,-2.9226653731,-3.9818572671,1.2831870304
H,-4.4384836191,-2.3816045673,-2.4198292138
H,-4.1344021809,-4.2964325475,-0.8635184998

C,0.1473867698,4.4836845391,0.6021756324
H,-0.2635187113,4.8992473658,1.5210498287
H,-0.2509012673,5.0009127694,-0.2736085319
H,1.238738593,4.5340390563,0.6010976068

PhNHCOCH(COMe)SO_2Ph
S,-1.5290202815,-1.7291986169,-0.4541998547
O,-0.745546425,-2.3349178918,0.6324324905
O,-2.8499347368,-2.2649415611,-0.8329221666
C,-1.8480626593,0.0674444397,-0.007433015
C,-0.539508412,0.8514210276,0.208098827
O,-0.1377280278,1.589906584,-0.6876982279
N,0.0758450868,0.6239602351,1.3976701723
C,-0.503389401,-1.6499739733,-1.9264059453
C,1.0755476268,-1.5252933585,-4.1960534361
C,0.8859764178,-1.6877496091,-1.7874173342
C,-1.1202515345,-1.5569306744,-3.1768454574
C,-0.3176042479,-1.4946793619,-4.3168675376
C,1.6752355708,-1.6249646107,-2.9371570658
H,1.3342044441,-1.7758970992,-0.8031773111
H,-2.2029906186,-1.5546508956,-3.2529430511
H,-0.7802422519,-1.4275123229,-5.2975376765
H,2.7573884839,-1.654823096,-2.8473940251
H,1.6956064893,-1.475649428,-5.0871557914
H,-0.445143799,0.0335149012,2.0433001042
H,-2.3079877824,0.4776766638,-0.9087033431
C,-2.8520554428,0.0624006181,1.162585833
O,-2.4704826272,-0.1092251584,2.3073300092
C,-4.2992591415,0.2710442052,0.8010948171
H,-4.9177976765,0.2262482769,1.6997569359
H,-4.609540113,-0.5029225957,0.0882534855

H,-4.4290354202,1.243216098,0.3076285539
C,1.2887689516,1.1606833921,1.885370536
C,3.677019344,2.1257148767,3.0022715432
C,2.0959458569,2.0456587062,1.1527481297
C,1.6826869174,0.7636491652,3.1748998283
C,2.8678810285,1.2444419647,3.7267506941
C,3.282288394,2.5175866698,1.7212308509
H,1.7924174571,2.3558368162,0.162171199
H,1.0578906086,0.0759054965,3.7405830952
H,3.1582269526,0.9279661971,4.7251535098
H,3.9011109702,3.2037141916,1.1483789502
H,4.6015296985,2.5013399277,3.432201474

PhNHCOCH(SO_2Me)SO_2Ph
C,1.0251945846,-0.9591772818,0.5630225048
C,-0.3316185256,-1.0478454418,-0.1639930391
O,-0.403103554,-1.1927828418,-1.3789134921
N,-1.3952790769,-0.9788792892,0.687290846
H,-1.170365475,-0.7096622307,1.6422721728
C,-2.7784644397,-1.0010320548,0.3791878722
C,-5.5524420488,-1.0397333543,-0.0443059437
C,-3.2848360553,-1.2397540484,-0.907724423
C,-3.6641106767,-0.7829557082,1.448346745
C,-5.0408538244,-0.8021871558,1.2352331304
C,-4.6685932991,-1.2566623428,-1.1034334868
H,-2.6074132885,-1.4028971983,-1.7343017318
H,-3.2716459947,-0.6000877212,2.4466695923
H,-5.7124925502,-0.631741808,2.0723687496
H,-5.0535374901,-1.4421949095,-2.1028456784
H,-6.6257692349,-1.0559534318,-0.2116186749

H,1.0517044894,-1.607272458,1.4456887879
S,2.5103921165,-1.5037426855,-0.4431095085
O,2.8740559066,-0.4281564434,-1.3757379669
O,3.47269503,-2.0015272873,0.5500887144
S,1.2808798453,0.7294623759,1.36076103
O,0.1984601116,0.7440834222,2.3719567648
O,2.6822966285,0.8415946254,1.7635737832
C,0.9084225851,1.9761013251,0.1259577013
C,0.3502958264,3.9494389458,-1.7305085939
C,-0.3910296081,2.4873477871,0.0498570147
C,1.9377951466,2.437083873,-0.6996105292
C,1.6460074955,3.4328268921,-1.6324629324
C,-0.6651172143,3.4805701987,-0.8915067039
H,-1.1621494227,2.1306265294,0.7237712113
H,2.9345955031,2.0207810375,-0.6168303334
H,2.4331974193,3.8023852204,-2.2832556438
H,-1.6687732892,3.8899795688,-0.9630480977
H,0.1318074725,4.7240500322,-2.4608891453
C,1.9575518778,-2.9352351366,-1.4003414961
H,1.243908579,-2.6149027484,-2.156009477
H,1.5306970753,-3.6781945392,-0.7226405051
H,2.8795445898,-3.3224639166,-1.8438207958

PhNHCOCH(SO_2Ph)$_2$
S,0.6469430697,1.6309337992,-0.0895371362
S,1.4462064958,-1.4017805956,-0.719014594
O,0.0586931637,2.2673350688,1.1070846851
O,0.9199930592,-2.7166698201,-0.3247052639
O,2.0506462834,1.8727850664,-0.4515078079
O,1.4580342678,-0.9527593929,-2.116401549
C,0.4745224261,-0.1840197225,0.3220682708

H,0.9503185311,-0.2220435064,1.3075622911
C,-1.0079287202,-0.5942486018,0.3721872736
O,-1.5898978013,-0.9891324296,-0.6243571225
N,-1.561725458,-0.4451580962,1.6165096694
C,3.1217850108,-1.2890895766,-0.06308896
C,5.7132769901,-1.2083138329,0.9134136378
C,3.4628688978,-2.0929189123,1.0293960124
C,4.0540526416,-0.4554746797,-0.6835030084
C,5.3581489571,-0.4210777926,-0.1859232645
C,4.769198007,-2.0439076301,1.5192443449
H,2.7267010172,-2.7612270967,1.4649970891
H,3.761199919,0.1514651742,-1.5315338013
H,6.0946626301,0.2229533025,-0.658051171
H,5.0510137499,-2.6665984651,2.3638388568
H,6.7301989444,-1.1759309132,1.2955725972
C,-0.4016835348,1.9984058342,-1.4960177521
C,-2.0123111425,2.6374442561,-3.6518901879
C,-1.6905527858,2.4843777034,-1.258255608
C,0.1013566702,1.8288700232,-2.7884019616
C,-0.7188238974,2.1531920615,-3.8695646388
C,-2.4965751331,2.8050351491,-2.3510681069
H,-2.0449465834,2.6192167632,-0.2419668284
H,1.102189801,1.4442307744,-2.9416604702
H,-0.3459979637,2.0236632135,-4.8815364549
H,-3.5004208683,3.1853163579,-2.1845188868
H,-2.6451943046,2.8863875361,-4.4996669511
H,-0.9996763255,0.0525324521,2.2967595818
C,-2.9059013668,-0.6643948779,2.0055445858
C,-5.5193032817,-1.0681654122,2.9422096516
C,-3.8233676356,-1.383096806,1.2240240737
C,-3.3008812113,-0.152077665,3.2522765479

C,-4.5990330663,-0.3548676182,3.7162936352

C,-5.1216184245,-1.5756422202,1.7031286865

H,-3.523049684,-1.7775557087,0.2628770347

H,-2.5897228626,0.4076632558,3.8570825147

H,-4.8896073884,0.0479643139,4.6829319143

H,-5.8270165946,-2.1340705664,1.0932145059

H,-6.5320950455,-1.2269574906,3.3020152478

PhNHCOCH(SO_2Me)$_2$

S,-0.8702990111,-2.6587349348,-0.220682656

S,-2.2253622909,0.180398447,-0.1138254838

O,-1.9881312056,1.4645878529,0.5873449418

O,-2.3475717315,0.1491406828,-1.5783359118

C,-0.7702198617,-0.8873597572,0.3685670995

H,-0.8444449988,-1.0084596434,1.4561611003

C,0.5905990407,-0.2193949851,0.0037184796

O,1.387874604,-0.8030136597,-0.7173853276

N,0.7925203479,0.9847923372,0.6005600273

H,-0.0338270452,1.4179973594,1.0076177726

C,1.9283691965,1.8291178285,0.4990059747

C,4.0921438106,3.6118944525,0.4347751889

C,3.1661773939,1.4046354994,-0.0059174856

C,1.7783380274,3.1439359358,0.9692971227

C,2.8550812106,4.0275991765,0.93663154

C,4.2358779394,2.3034492049,-0.0316555644

H,3.2853265915,0.3946048993,-0.3731449353

H,0.8161236417,3.4728355938,1.3560515024

H,2.7237131066,5.0425702053,1.3021060092

H,5.192651657,1.968286509,-0.4235380241

H,4.9323882919,4.300159086,0.4082704349

O,0.1849755874,-3.377991522,0.5000693775

O,-2.2803981128,-3.0492448649,-0.0184438899

C,-0.5523440611,-2.6647893958,-1.9937808115

H,0.4951782071,-2.4212056375,-2.1598004988

H,-1.2209411575,-1.9410180443,-2.4646471599

H,-0.7952555616,-3.683020969,-2.3105750233

C,-3.7035683732,-0.5357968588,0.6303553743

H,-3.5578630868,-0.6030368652,1.7101367216

H,-3.8945835301,-1.5126919585,0.1909754484

H,-4.4922467895,0.1852423915,0.3966216689

PhNHCOCH(COMe)$SO_2C_4F_9$

S,1.9099885395,-0.3989765558,-0.9925308475

O,1.6630708932,-1.2793235066,-2.1288800935

O,3.1189728271,-0.5019029614,-0.1666347858

C,1.8212217436,1.3785305395,-1.6060005019

C,0.4408987874,1.7423173842,-2.220149647

O,0.2237419217,1.4285440361,-3.3825423419

N,-0.4103601174,2.3892812504,-1.3823667411

C,2.4595951572,2.3472937699,-0.5852459569

O,1.7791324188,2.9122321218,0.2539732825

C,3.9412254943,2.5753265429,-0.7213695261

C,0.4175467471,-0.6229570396,0.205226169

C,0.5865520323,-1.8805999835,1.1218986847

C,-0.7514951632,-2.3594093222,1.7841293905

C,-0.5773618501,-3.3635951895,2.9707167844

F,-1.7838338209,-3.8401237801,3.3106759465

F,-0.6891459553,-0.7390466475,-0.5493212298

F,0.326659658,0.4826772367,0.9711962385

F,1.0791659878,-2.8971822193,0.3776356932

F,1.4714556666,-1.5763490939,2.0984738178

F,-1.509082681,-2.9651207719,0.8433913943

F,-1.4201664754,-1.2785827004,2.2603532189
F,0.2068706437,-4.3901878662,2.6094594826
F,-0.0419620048,-2.7575363975,4.0382501162
C,-1.7201765059,2.8569856874,-1.648870666
C,-4.3229073063,3.840146327,-2.0024018326
C,-2.3294759895,3.6294947082,-0.6458618737
C,-2.4169984431,2.574756658,-2.8336497157
C,-3.7130349539,3.0715188929,-2.996148212
C,-3.6224565693,4.1164440462,-0.8239633473
H,2.4855451695,1.2587950234,-2.4692218705
H,-0.0158452446,2.648869515,-0.4795508654
H,4.1647792737,2.9966530585,-1.7107045475
H,4.4742884335,1.6204393527,-0.6437804866
H,4.2827928206,3.2609833442,0.0564235469
H,-5.3310350252,4.2201993873,-2.1426445173
H,-1.7879245856,3.8468706021,0.2724838223
H,-1.9490233054,1.9827485306,-3.6083527347
H,-4.2475653733,2.8494605847,-3.9160993479
H,-4.0811007105,4.712791258,-0.0397113406

PhNHCOCH(CN)SO_2Me
S,2.6474858315,-0.7970773639,0.2107977449
O,1.8452202508,-1.7838991508,-0.5235650802
O,4.0093714145,-0.4502194662,-0.2125322036
C,1.6653565873,0.8311783837,0.1943583525
C,0.205488749,0.5781855001,0.6412185904
O,-0.0086259077,0.4075468983,1.8372812704
N,-0.7141794451,0.5415154225,-0.3536690153
H,-0.3667419132,0.6775544742,-1.2967212527
H,2.1402495725,1.4562839367,0.9566815369
C,2.683795503,-1.2487556307,1.9587487131

H,3.2433212073,-0.4887529289,2.5072243349
H,3.2089437714,-2.2074660492,1.9883967944
H,1.6635904548,-1.3406931018,2.3314687554
C,1.829249224,1.4365303719,-1.118366688
N,1.8890000801,1.9150307131,-2.1752653926
C,-2.1090569292,0.2976566376,-0.2654568426
C,-4.8742409289,-0.1569882187,-0.2711969346
C,-2.7859436878,0.1144216912,0.9490287236
C,-2.8168827991,0.2533423417,-1.4771297322
C,-4.1912212779,0.0265543755,-1.4773751665
C,-4.1649495561,-0.1110886322,0.9306899605
H,-2.2428071622,0.1474915594,1.8833678882
H,-2.2899823939,0.3932781924,-2.418937759
H,-4.7261632142,-0.0072847153,-2.4225152989
H,-4.6851526728,-0.2525061982,1.874376869
H,-5.946070766,-0.3341374655,-0.2701506815

PhNHCOCH(CN)SO_2Ph
S,2.3703599316,1.1943272745,-0.4970308818
O,1.7839920149,1.9135778542,0.6503194912
O,3.7197283195,1.4991657536,-0.9847570504
C,2.381241362,-0.6315648429,-0.0192613324
C,0.9767958002,-1.1973049847,0.3419619247
O,0.5352127553,-2.1371765471,-0.3028543412
N,0.3762697889,-0.5722159755,1.3889554559
H,0.8506128202,0.2551578468,1.7428582467
H,2.7124131603,-1.1621204762,-0.916039962
C,3.3486311288,-0.8086037427,1.056231511
N,4.0983491473,-0.9601885266,1.9302234576
C,-0.8866647341,-0.8389862038,1.9733537641
C,-3.3525041572,-1.2361709433,3.2479584039

C,-1.7072935754,-1.9085238908,1.5845286044
C,-1.3024882719,0.0265850409,2.9986442816
C,-2.5282837162,-0.1731320715,3.6300943238
C,-2.9333989299,-2.0942649569,2.2289359369
H,-1.3887396152,-2.5765677979,0.7959134803
H,-0.6621006744,0.852102728,3.3026829735
H,-2.8362308465,0.5030767756,4.4230556844
H,-3.5641844899,-2.9255415357,1.92488361
H,-4.3077770729,-1.3937647426,3.7408806912
C,1.2237410143,1.2558703398,-1.8751931988
C,-0.5311420032,1.3300843154,-4.0137441808
C,-0.1239209794,1.538422657,-1.6356787038
C,1.71396599,1.0179333672,-3.163136428
C,0.8224488323,1.0561713465,-4.2359949515
C,-1.0023472462,1.5738599383,-2.7202484099
H,-0.4712811786,1.7398400299,-0.6279173001
H,2.7712263924,0.8283026943,-3.3196437199
H,1.1863748383,0.8781104938,-5.2438243838
H,-2.0525664336,1.7948013716,-2.5529027897
H,-1.2204394716,1.3587375109,-4.8532542076

PhNHCOCH($SO_2C_4F_9$)$_2$
S,0.200200746,1.6740420718,0.7193588101
C,-0.469842222,-0.052633513,1.034249047
H,0.0258670204,-0.3826761269,1.9530879265
C,-2.0096234549,0.0470094891,1.2294720868
O,-2.6559812215,0.8955146838,0.6404715931
N,-2.4877508375,-0.8890406541,2.095563504
H,-1.8356997216,-1.6073217943,2.3910956622
C,-3.840274781,-1.1338058731,2.4554037356
C,-6.4473043251,-1.7404897861,3.2777659934

C,-4.1018691174,-2.3219383021,3.1554428004

C,-4.8839784343,-0.2435876184,2.1654057291

C,-6.1796452318,-0.5597473477,2.5818642645

C,-5.3997594032,-2.6211571861,3.5639406098

H,-3.2902442626,-3.012544907,3.376443633

H,-4.6850212089,0.6716415191,1.6249580994

H,-6.9859223981,0.1327112367,2.3554547653

H,-5.590228256,-3.5447020551,4.1036931543

H,-7.459904868,-1.9729536533,3.5951058239

S,0.0397459279,-1.4371902496,-0.1106127937

O,1.3950926658,-1.1952552295,-0.5965108376

O,-0.3257611419,-2.6435454881,0.6414815985

C,-1.1587036137,-1.338296536,-1.6252139162

C,-0.6212345338,-2.1884486826,-2.8242776382

C,-1.7127542225,-2.5163253637,-3.9004818465

C,-1.1536289894,-3.0338524238,-5.2666343494

F,-1.2796178556,-0.0576323471,-1.9826260567

F,-2.3460862533,-1.8138458378,-1.2059234785

F,-0.136167162,-3.3560957874,-2.3372541817

F,0.3823919337,-1.5014780578,-3.4111080459

F,-2.4349046321,-1.3967029556,-4.1504748017

F,-2.5351137682,-3.4689526108,-3.4062048989

F,-0.5206470852,-2.0568745348,-5.9266406734

F,-2.1800436899,-3.4622683914,-6.0152219662

F,-0.3040869811,-4.0542558728,-5.0716792773

O,0.1267594601,2.0389202186,-0.6871629954

C,2.0906064884,1.4714225969,1.1311714741

C,2.665748721,2.7600005025,1.8051016835

C,4.2331255567,2.8171802791,1.8228066828

C,4.8416338949,3.8960591938,2.7782893607

F,4.2986357309,5.0988888104,2.5389340448

F,6.1626497272,3.966402907,2.5594708622

F,4.7149508449,1.6099271676,2.2128724624

F,2.2254830533,0.4198747266,1.9744414533

F,2.7429706316,1.2265483292,-0.0087951268

F,4.674388928,3.0831536467,0.5737855728

F,2.2123852169,3.83425667,1.1174839368

F,4.6389335762,3.5715795669,4.0619462865

F,2.2178349635,2.8183497879,3.0797777327

O,-0.3556509907,2.4735267752,1.8092695462

2,4-$MeO_2C_6H_3NHCOCH(SO_2Ph)_2$

S,0.8028261855,1.9574714628,-1.6564737599

O,-0.5442833157,2.4503182966,-1.9812443544

O,1.5457329914,2.4748667971,-0.4975256059

C,0.5465837578,0.119248018,-1.3941499289

C,-0.688766788,-0.126348326,-0.5019945364

O,-1.6298927724,-0.7658645807,-0.9630958813

N,-0.6070093188,0.3984596439,0.7448898864

H,0.259350099,0.8634087567,1.0097079216

H,0.3147949481,-0.2946210495,-2.3776574946

C,1.8133605299,2.1318132639,-3.1317653865

C,3.3355342679,2.4890143503,-5.4145537058

C,1.1806759529,2.1113980851,-4.3782629845

C,3.1883112128,2.3349783732,-3.0015706671

C,3.9481687905,2.5178672304,-4.1578838558

C,1.955886776,2.2867027603,-5.5259069484

H,0.1043301519,1.9856859232,-4.4429552554

H,3.6467948221,2.3483994303,-2.0194054006

H,5.0192307583,2.6793544927,-4.0751443137

H,1.4806969319,2.2776321418,-6.5029281225

H,3.9342963435,2.6300567079,-6.3106370777

C,-1.5854901334,0.3621586637,1.7631293692
C,-3.3996711789,0.4177346012,3.9089445166
C,-1.2378563824,0.9891543415,2.9878696818
C,-2.8435354632,-0.225257001,1.6434380911
C,-3.7539033314,-0.2017466301,2.7101679268
C,-2.1352796977,1.0162430202,4.0473304764
H,-3.1154804043,-0.7001952298,0.7106452661
H,-4.7237787337,-0.6664017639,2.5781232539
H,-1.8910391212,1.4912551039,4.9898180765
O,0.0102170133,1.5397189884,3.0152009664
O,-4.2027459585,0.501916045,5.0137085023
C,0.4357980376,2.243303941,4.1766760161
H,-0.2267356005,3.0926054042,4.3844705141
H,1.4389461737,2.6054725085,3.9484114769
H,0.4722756411,1.5779716194,5.0483583454
C,-5.5027317153,-0.0691297554,4.9474158485
H,-6.1071868418,0.4059105738,4.1637075512
H,-5.9582949918,0.1174730126,5.9215344067
H,-5.4542019373,-1.1511919148,4.7676510527
S,2.0737557406,-0.7812534585,-0.8117104756
O,3.1252412171,-0.5119480038,-1.8066672941
O,2.2768800077,-0.4809045196,0.6127561769
C,1.5844162063,-2.5045538262,-0.9656156058
C,0.8302939338,-5.1575365081,-1.2079161641
C,1.7982429618,-3.1627221025,-2.1800991114
C,1.0065172737,-3.147965964,0.1316158204
C,0.6291733077,-4.4856859079,0.0015372147
C,1.4159569504,-4.5000631413,-2.2948456708
H,2.2721021032,-2.6413920728,-3.0059845599
H,0.8684701287,-2.6143531111,1.0663231486
H,0.1793315008,-5.0011427931,0.8453558174

H,1.5800326973,-5.0286042123,-3.2297778685
H,0.5336643719,-6.1987117852,-1.3030156952

2,4-$MeO_2C_6H_3NHCOCH(CO_2Me)SO_2Ph$
S,2.5384504355,0.6964339531,-1.6278537176
O,2.2141593338,1.4646922095,-0.4130153705
O,3.9296340229,0.5614652521,-2.0911938526
C,1.9033786437,-1.0494561483,-1.4260959221
C,0.4439211288,-1.1346631596,-0.9193836919
O,-0.4051492973,-1.6399750602,-1.648908236
N,0.2278871416,-0.642229571,0.3271502022
H,1.0123046644,-0.1937311684,0.793329214
H,1.8979979399,-1.4621049381,-2.4351924892
C,1.544852796,1.3373337077,-2.9832821854
C,0.0147246825,2.3100776535,-5.075916479
C,0.3585285066,2.0169795911,-2.696699759
C,1.9851208289,1.139339689,-4.2948878873
C,1.2085276922,1.6325104198,-5.34470155
C,-0.4077770625,2.5041376434,-3.7574322321
H,0.0531516438,2.1705597337,-1.6668302077
H,2.9231880585,0.6263625089,-4.4830086571
H,1.5383943519,1.4915307628,-6.3701983659
H,-1.3325423305,3.0360086304,-3.5521305063
H,-0.5861207212,2.6915313484,-5.8972448474
C,-0.9918507605,-0.5875458098,1.0376487281
C,-3.3167096416,-0.3764252687,2.60748984
C,-0.94942453,0.0267900917,2.3160907615
C,-2.208435433,-1.0895223179,0.5778269072
C,-3.3715297645,-0.9881226786,1.3551362716
C,-2.0980914281,0.1324942693,3.0893939217
H,-2.2480760045,-1.5605322715,-0.394940684

H,-4.2972665964,-1.3907925799,0.9616344944

H,-2.0868346363,0.5981471243,4.0674243406

O,0.2825828918,0.4818987055,2.6972956817

O,-4.3831953893,-0.2179505577,3.4498445417

C,0.4071995492,1.1891157847,3.9261552746

H,-0.2299841429,2.0820139305,3.9314293958

H,1.4548792098,1.4864658964,3.9899024348

H,0.1521489107,0.5468666505,4.7784666258

C,-5.6505757629,-0.7086651675,3.0322253812

H,-5.9873052252,-0.2106254387,2.113564786

H,-6.3405326935,-0.4771430598,3.8455453906

H,-5.6245105788,-1.7944365508,2.8722719438

C,2.9101917962,-1.8681373356,-0.6184608791

O,3.4347490844,-2.8730040476,-1.0411001832

O,3.1158439127,-1.3477103708,0.6013631817

C,4.0715857187,-2.0368773742,1.435977156

H,5.046365299,-2.0589883224,0.9432649411

H,3.7318330183,-3.0570649399,1.630678083

H,4.1143069373,-1.4570511192,2.3573683043

Table S4. Cartesian Coordinates of B3LYP/6-31G** Optimized Enols and Amides

i- PrNHC(OH)=C(CO_2Me)SO_2Ph

C,-0.0039189377,0.3601423479,1.6124466652

C,0.4707370837,0.7056101443,0.3089645904

O,-0.4944598467,1.3037052254,2.3944887366

H,-0.4271359733,2.1767776649,1.8656344546

N,0.0002652842,-0.8683587178,2.126883452

H,0.4126594008,-1.5860012959,1.5300230001

C,-0.4525405287,-1.2001711307,3.4853086562

H,-1.2901127671,-0.5350057175,3.7136354985
S,1.2240596106,-0.4748008498,-0.7774474996
O,2.5836322149,-0.0599762188,-1.146008251
O,1.0277268791,-1.8123055568,-0.1538795972
C,0.2331528122,-0.4912819226,-2.2842058153
C,-1.2577710217,-0.5939748751,-4.617815701
C,0.7613164213,0.053852547,-3.4530207574
C,-1.0243005186,-1.097568611,-2.2643798326
C,-1.7721274248,-1.1420568794,-3.4396930497
C,0.0062574373,-0.0016936291,-4.6253253898
H,1.7478903197,0.5016329461,-3.4301580936
H,-1.401576065,-1.5374567424,-1.3474776155
H,-2.7513694436,-1.6109616863,-3.4384220025
H,0.4073382534,0.4149528448,-5.5443111749
H,-1.8420462382,-0.6345625154,-5.5323582322
C,-0.9455189738,-2.6490869862,3.492657937
H,-0.1340890296,-3.3428894166,3.2443903021
H,-1.7549648627,-2.7958023265,2.7717829673
H,-1.3174706883,-2.914507169,4.4861376858
C,0.6610579405,-0.9572330937,4.5129969069
H,1.5261848805,-1.5967310048,4.3082348708
H,0.3016567221,-1.1801043962,5.5229380283
H,0.9865157277,0.0856582584,4.4879046204
C,0.4121418668,2.092135627,-0.0696925379
O,-0.052964146,2.9964118449,0.6571935999
O,0.8781420853,2.373793141,-1.2947868633
C,0.8250259024,3.753604566,-1.6926088239
H,1.2294705913,3.7750466241,-2.7038673828
H,1.431001999,4.3693827846,-1.024624049
H,-0.203866967,4.1198237754,-1.6815392029

i-PrNHC(OH)=C(COMe)SO_2Ph

C,0.0267730703,0.6357293012,1.494969917

C,0.6133402905,1.0713801702,0.244648461

O,-0.5553190743,1.5234196056,2.2498303442

H,-0.4424581963,2.4641390998,1.7037014624

N,0.0313721972,-0.6235031712,1.9367027821

H,0.5780821161,-1.2817561021,1.3826668323

C,-0.5173950294,-1.0326041019,3.2378855204

H,-1.3948928449,-0.4058255789,3.4189823182

S,1.4038786133,-0.0606090677,-0.8640134144

O,2.6361370692,0.5319117132,-1.4065544969

O,1.4866499053,-1.3786491156,-0.1851532546

C,0.2725303881,-0.2827344438,-2.2548598912

C,-1.4287573408,-0.6982982303,-4.4056448952

C,0.7125394664,0.0242202874,-3.5418088259

C,-1.0034641229,-0.8048443351,-2.0272613917

C,-1.8551286653,-1.0080804599,-3.1104119014

C,-0.1490843441,-0.186616839,-4.6208160129

H,1.7147678608,0.4134387915,-3.6823655513

H,-1.3237672643,-1.0497895597,-1.0196603818

H,-2.8498726352,-1.4105376272,-2.9457520828

H,0.1827260857,0.048219694,-5.627501461

H,-2.0964006307,-0.8590494583,-5.2467347121

C,-0.9519158967,-2.4971416089,3.1457081033

H,-0.0964369604,-3.1510713285,2.9404193854

H,-1.6919960523,-2.6418043539,2.3532328976

H,-1.3953709013,-2.8181999668,4.092349886

C,0.4963138639,-0.7933605411,4.3649727507

H,1.4028904777,-1.387152275,4.2067995434

H,0.0652845027,-1.0779901638,5.3303640696

H,0.7751160609,0.2621003269,4.4125443376

C,0.5324745753,2.4656987972,-0.0705600922
O,-0.0511841271,3.2694383046,0.7224627756
C,1.1115442564,3.0720524744,-1.3246525048
H,2.1969136769,2.9544807675,-1.3439656403
H,0.842516772,4.1284847963,-1.3373773011
H,0.7215904373,2.5849042989,-2.2231475753

i-PrNHCOCH(SO_2Ph)=C(OH)CH_3
N,-0.6788831894,0.1307335443,2.1538984467
H,-0.9935254401,0.9556872566,1.6477110463
C,-1.2761938753,-0.195849557,3.4548116759
H,-1.1121738469,-1.2662257257,3.6076419852
S,0.3748801659,1.1825176963,-0.6441848851
O,-0.6637798111,1.9127738011,0.1196658421
O,1.4479917863,1.953448753,-1.2899767738
C,-0.4853984578,0.2763503314,-1.9468902913
C,-1.8418577391,-1.0626336205,-3.9603610013
C,-1.5548290114,-0.5588483109,-1.6120207277
C,-0.0921163553,0.4595591381,-3.2721106477
C,-0.7793984314,-0.2179841915,-4.2818849522
C,-2.2295634174,-1.2321292029,-2.6275297412
H,-1.8539994193,-0.6777062293,-0.5755277172
H,0.7297777473,1.1305539359,-3.4957664504
H,-0.4842541417,-0.0819189177,-5.3177327693
H,-3.0603596534,-1.8859135455,-2.3808011342
H,-2.3728051536,-1.5887849799,-4.747925116
C,-0.5830350626,0.5679262168,4.5915286793
H,-0.6994774753,1.6497098629,4.4639816673
H,0.4835283601,0.3315462631,4.6130023821
H,-1.0157325314,0.2897641389,5.5582513248
C,-2.7791043602,0.0862317739,3.3945343166

H,-2.9761638458,1.1497596248,3.2153582109
H,-3.2523086957,-0.1828642045,4.3432301775
H,-3.2583944697,-0.4894748703,2.597080653
C,0.4504713246,-0.4535736558,1.7163450503
C,1.0758476127,-0.057272042,0.4295009542
C,2.2444259178,-0.7144647591,0.0394589448
C,3.0212316917,-0.4770830013,-1.2255497754
H,2.3841193392,-0.5605159973,-2.1097379667
H,3.8144369526,-1.2234062302,-1.2777781941
H,3.4466816462,0.5278662141,-1.233601795
O,2.7740907798,-1.6438946162,0.7958324765
H,2.1382463049,-1.7210858869,1.6205760882
O,0.9891710597,-1.3713950928,2.4000917658

i-PrNHC(OH)=C(SO_2Ph)$_2$
C,-0.8808908526,-0.449042137,1.3931178969
C,-0.1930347939,0.1148794032,0.2844600446
O,-1.6070080674,0.2787578913,2.227119218
H,-1.5998097471,1.2285378149,1.8965108665
N,-0.8617796219,-1.7545638622,1.6772951517
H,-0.1853857692,-2.3075433194,1.1532851115
C,-1.6144659674,-2.3810926854,2.7749226736
H,-2.5463637963,-1.8193396139,2.8804984479
S,0.5932503699,-0.8969618023,-0.9370485005
O,1.624811991,-0.0924224986,-1.6033160025
O,0.9803509513,-2.1726010955,-0.2816638211
S,-0.1138962378,1.8650812451,0.061663419
O,-0.3000990805,2.2253772231,-1.3484441001
O,-1.0716956979,2.4321713044,1.068096071
C,-0.6575407097,-1.3329111693,-2.1633164038
C,-2.5399762157,-2.03635512,-4.0725086043

C,-1.1339285679,-0.3551956433,-3.0414106587
C,-1.0991784973,-2.6550153562,-2.231639476
C,-2.0479553744,-3.0026832434,-3.1945638135
C,-2.082600433,-0.7179839585,-3.995724164
H,-0.7772562681,0.6654118712,-2.9648087224
H,-0.6883912328,-3.3936982507,-1.5535868713
H,-2.3961087138,-4.0290429113,-3.2603980142
H,-2.4631843544,0.0315010837,-4.6827855877
H,-3.2781692944,-2.3101888989,-4.8205293281
C,1.5090275801,2.4533348359,0.5673822962
C,3.9923868494,3.3909976244,1.3539268394
C,1.715443113,2.7943300436,1.9060399461
C,2.5189949477,2.5802814395,-0.3873504571
C,3.7667536655,3.0525722594,0.0182125485
C,2.9687255258,3.2642147687,2.2955508568
H,0.9032744495,2.7121917733,2.6191946442
H,2.32672958,2.3041790922,-1.4160234272
H,4.5625752938,3.156192748,-0.7126676412
H,3.1419138332,3.5379903863,3.3317140611
H,4.9668433321,3.7585220668,1.6616196359
C,-1.9379335222,-3.8235233381,2.3769308284
H,-1.0208238735,-4.4073380221,2.2356601442
H,-2.5143978424,-3.8570873414,1.4481018347
H,-2.5224544786,-4.3090437169,3.1632605453
C,-0.8381129451,-2.3014616151,4.0962013119
H,0.1145681195,-2.8365879884,4.0208870684
H,-1.4199277528,-2.7529149726,4.9063778749
H,-0.6325704615,-1.2613554823,4.3603356441

i-PrNHC(OH)=C(SO_2Me)$_2$
C,-0.5856656694,-0.136837145,0.8888857902

C,0.0690181781,0.3714318662,-0.2657811747
O,-1.3031205553,0.6363425762,1.6889327747
H,-1.3212895257,1.5636927097,1.3030416226
N,-0.5368629514,-1.4176467739,1.259192234
H,0.0833094918,-2.0105375998,0.7090079762
C,-1.2297821225,-1.9758817609,2.4315751417
H,-2.1617295713,-1.4160095608,2.5467474162
S,0.9287003356,-0.6445607946,-1.4269382264
O,2.1276591361,0.0752578805,-1.8866801212
O,1.0906102845,-1.9920427047,-0.8258699604
S,0.0186037562,2.0845329827,-0.6634960826
O,-0.2858854001,2.271687918,-2.0894357571
O,-0.892589242,2.7240486566,0.340808311
C,-1.5566780391,-3.4437711144,2.146519897
H,-0.6423662767,-4.0300332508,1.9989835246
H,-2.1774757036,-3.5448020005,1.2517935277
H,-2.097546281,-3.8787421919,2.9914382282
C,-0.3899175752,-1.8018190592,3.7038322234
H,0.5626529929,-2.3352410202,3.6170817599
H,-0.926814074,-2.2002589295,4.5707658951
H,-0.181157539,-0.7449674688,3.8873890473
C,1.6565499917,2.7677496616,-0.3587770935
H,2.3644092705,2.2255180802,-0.9848235957
H,1.8869701314,2.6503298136,0.7005699915
H,1.6040775297,3.8239461889,-0.6303667266
C,-0.1646761334,-0.8339000065,-2.848447367
H,0.3838638118,-1.4254125166,-3.5842376115
H,-0.3974711392,0.1606142816,-3.2285738459
H,-1.0647434947,-1.3583133914,-2.5251003825

i-PrNHC(OH)=C(COMe)$SO_2C_4F_9$

C,-0.7631737302,0.8498432454,1.7714213848

C,0.0294242741,1.5237107701,0.7547843341

O,-1.7205693553,1.5164324701,2.3487051775

H,-1.6911205107,2.4953214641,1.8921157549

N,-0.5819082166,-0.4074904545,2.1658597398

H,0.2256788092,-0.8909361642,1.7802239384

C,-1.3850253219,-1.0632710804,3.2121913022

H,-2.3932514341,-0.6476685295,3.1364822708

C,-1.4311931592,-2.5642078212,2.9179844892

H,-0.4290453671,-3.0063306612,2.9618508904

H,-1.8510760114,-2.7611679429,1.9275382451

H,-2.050727235,-3.072661858,3.6617325393

C,-0.8256657542,-0.7534049958,4.6064737907

H,-0.8141496917,0.3243199883,4.7866753461

H,0.1950259154,-1.1361524594,4.7115673749

H,-1.447141878,-1.2225883679,5.3757492461

C,-0.2882380809,2.8993117378,0.455966272

O,-1.2306695539,3.4692394821,1.0780823783

C,0.4502759141,3.7421355888,-0.5537859506

H,0.4855789731,3.2660332156,-1.5347896846

H,1.4854379148,3.8958404266,-0.2410234142

H,-0.0678587508,4.6990298536,-0.6197933906

S,1.2640529927,0.6586971764,-0.1269093357

O,2.2947741355,1.5564244288,-0.6516251894

O,1.6472538035,-0.5574441741,0.6178882262

C,0.3342507148,0.0071108269,-1.6544190253

C,1.2636786548,-0.518091138,-2.7798555032

C,0.5283434349,-1.4019202067,-3.8289042257

C,1.3259838392,-1.6439323239,-5.1384251923

F,-0.4184201486,1.0165882485,-2.1442321448

F,1.7992817495,0.5497310581,-3.41375837

F,2.2527306584,-1.2564129473,-2.2298618998

F,-0.6427947413,-0.8077775285,-4.1648446013

F,1.3995378432,-0.5213477662,-5.8604693765

F,0.6986952438,-2.580425467,-5.8610732009

F,2.56448495,-2.0698653293,-4.8577966961

F,0.2720257348,-2.6068801815,-3.2734162583

F,-0.4844906151,-0.9797926839,-1.2283093415

i-PrNHCOCH($SO_2C_4F_9$)=C(OH)CH_3

N,0.0530244094,-0.4874325162,3.3409504906

H,-0.2670013395,0.3792011299,2.9200570835

C,-0.5929906935,-0.9688070953,4.5709208545

H,-0.4492271117,-2.0526481654,4.5873249808

S,1.1191027699,0.7867497659,0.6762292734

O,0.203953595,1.566258797,1.5289915741

O,2.1301113926,1.467906034,-0.1355387255

C,0.0737958236,-0.3678692034,5.8150643811

H,-0.025446042,0.7229932898,5.8235632574

H,1.1361831386,-0.6223491479,5.8394143549

H,-0.3936006739,-0.7599602451,6.7241370146

C,-2.0882994915,-0.6526657346,4.4957960537

H,-2.2622930593,0.4290224989,4.452294406

H,-2.5988525709,-1.034266,5.3844185761

H,-2.5455289609,-1.1093773502,3.6133335467

C,1.1596898237,-1.0517421668,2.8401872292

C,1.8110053424,-0.5360918102,1.6049951823

C,2.977308552,-1.1784128362,1.1525947186

C,3.7923242579,-0.8266048952,-0.0603675409

H,4.5434803507,-1.6057649877,-0.1918081865

H,4.2807336475,0.1406129488,0.0768963125

H,3.1757920561,-0.744409151,-0.9554282668

O,3.4636290658,-2.1829310336,1.8231160233
H,2.7975991104,-2.3305698582,2.6319168301
O,1.6754260608,-2.0531155827,3.4176427645
C,-0.0106441512,-0.1127103768,-0.5639985115
C,-0.4998361201,0.7884639266,-1.7283567665
C,-1.7134244375,0.1957246587,-2.5016914714
C,-1.9993905217,0.8756269427,-3.8676314746
F,-3.1755744771,0.4364433724,-4.3322480692
F,-1.0460642595,0.5720730533,-4.7542218235
F,-2.0591810011,2.2057008729,-3.7222032013
F,-2.8182057298,0.3277307072,-1.7352762475
F,-1.4874096873,-1.120073173,-2.7360797376
F,0.5275621987,0.9499314378,-2.5929504812
F,-0.8639958919,1.9919045415,-1.2339510648
F,-1.0640629508,-0.5908644137,0.1314357822
F,0.684407634,-1.1515730118,-1.076914284

i-PrNHC(OH)=C($SO_2C_4F_9$)$_2$
C,-0.9207119378,-0.2637034935,1.3482824301
C,-0.2331363794,0.151075396,0.1541925848
O,-1.6817834205,0.5644196808,2.0371889877
H,-1.726579232,1.4445925674,1.5638288863
N,-0.8534587583,-1.4923678209,1.8408621824
H,-0.2033518035,-2.1250865369,1.3769677182
C,-1.6195499604,-1.9756198621,3.0069870722
H,-2.5595976016,-1.4181933239,3.0181206416
S,0.6185082966,-0.9867514533,-0.8773571116
O,1.6797987903,-0.3226633111,-1.6255290449
O,0.8939974357,-2.210722434,-0.0981849371
S,-0.1982547296,1.8434355378,-0.3002385086
O,-0.1058325287,2.0486382167,-1.737684726

O,-1.2719936163,2.5187311418,0.4846918385
C,-1.9143085803,-3.4633543944,2.8034994564
H,-0.9881507161,-4.0482744751,2.7673983887
H,-2.467081847,-3.6349761396,1.8757088875
H,-2.5134409726,-3.8413598192,3.6361498304
C,-0.8592273008,-1.6963918539,4.3089297542
H,0.101790518,-2.2210081315,4.3200841322
H,-1.4456159029,-2.0402919896,5.166557059
H,-0.6729497028,-0.6263411608,4.4283735717
C,1.4077488113,2.5155640966,0.4754723544
C,-0.7141434585,-1.5114809884,-2.1333556716
C,1.3808345804,4.0569277156,0.6772853772
C,2.7936097764,4.6663160466,0.9134764545
C,2.7793396169,6.1131821397,1.4770305258
C,-0.1292952374,-2.2519052064,-3.3656989162
C,-1.1994003859,-3.0418892063,-4.1735894736
C,-0.7356409773,-3.4893570487,-5.5858360271
F,4.0194178782,6.613090736,1.4220944893
F,2.368776565,6.1188378031,2.7497581256
F,1.9653263557,6.8882697722,0.7484920425
F,3.4584326213,4.6852278344,-0.2604411925
F,3.464072848,3.8868363265,1.7971625236
F,0.6079929113,4.3317069552,1.7524911529
F,0.8475769073,4.6361613445,-0.4205280514
F,1.539699893,1.9155827922,1.6768991144
F,2.4295429793,2.1695110372,-0.317766787
F,-1.3734037703,-0.4171493633,-2.5385055109
F,-1.5664559377,-2.3216087181,-1.4645738414
F,0.8113639706,-3.1285580181,-2.9456261013
F,0.4397859475,-1.3350949864,-4.1761475652
F,-2.2992288741,-2.2656732848,-4.3270603811

F,-1.5325764055,-4.15113068,-3.4767296015

F,0.4502463852,-4.1082039138,-5.5120611387

F,-0.6339157033,-2.4378102176,-6.4036725765

F,-1.6387788474,-4.3411393085,-6.0873985181

i-PrNHC(OH)=C(SO_2Me)SO_2Ph[a]

C,-0.1258189475,-0.1521430768,1.6391166707

C,-0.6119476758,0.566372753,0.5132975411

O,-0.9267087664,-0.6751053198,2.5520053961

H,-1.8765081392,-0.4597509976,2.2981232534

N,1.1751290908,-0.3651851357,1.8591050512

H,1.8130560396,0.1645379326,1.2681759505

S,0.4529546676,1.093389363,-0.7947878336

O,-0.218926549,2.2022969367,-1.4897182172

O,1.8013835173,1.3117423254,-0.2124791882

S,-2.3334053324,0.9013673606,0.3257901397

O,-2.8308155041,0.5142790342,-1.0007193027

O,-2.9994506826,0.2840154934,1.5203842802

C,0.6332496836,-0.2697607842,-1.9625995989

C,0.9546389937,-2.3319912202,-3.7859525168

C,-0.450768421,-0.6464977813,-2.7607346195

C,1.8743295965,-0.8996531492,-2.0685104242

C,2.029427387,-1.9378022462,-2.9883417941

C,-0.2798920047,-1.6871111142,-3.671959791

H,-1.4059067862,-0.1452418917,-2.6563611624

H,2.7011569757,-0.5644297085,-1.4536549488

H,2.9912692186,-2.432458017,-3.0834111745

H,-1.1138616631,-1.9924116043,-4.2962942191

H,1.0787982443,-3.1403270575,-4.5005045745

C,-2.555443547,2.6794081736,0.5003032078

H,-1.9870725107,3.1648114263,-0.2919708981
H,-2.2023242199,2.9749718361,1.4885834512
H,-3.6267173859,2.8641142413,0.3984217297
C,1.7147463519,-1.1319442953,2.993184855
H,0.9953147099,-1.9263141259,3.2080380743
C,3.0431145705,-1.7596147015,2.5629459925
H,3.7812079279,-0.9880274987,2.3142821912
H,2.9105086432,-2.4037732287,1.6890926573
H,3.4556364805,-2.3626665403,3.3765283837
C,1.862899439,-0.2491798074,4.2394707935
H,0.8979900426,0.1737660637,4.5293093262
H,2.5623347799,0.5730289467,4.0536662041
H,2.2450672096,-0.8384888609,5.0792450676

i-PrNHC(OH)=C(SO_2Me)SO_2Ph[b]
C,-0.981303539,-0.5070696907,0.4291213013
C,-0.3424323548,0.0222038968,-0.7246324739
O,-1.7708664188,0.2322597027,1.1962875038
H,-1.8667820127,1.1355260162,0.7708184684
N,-0.8408162329,-1.7674922158,0.8427095364
H,-0.2238459302,-2.3479168381,0.2749698697
S,0.5716564409,-0.9687035368,-1.8714133835
O,1.7910431794,-0.2562886372,-2.2779445632
O,0.7011428207,-2.3298781788,-1.2915171532
S,-0.4068059421,1.7462936996,-1.084012271
O,-0.4930616058,1.9368945418,-2.5383333122
O,-1.4994554483,2.3006087665,-0.2198924586
C,1.1007881683,2.5457565098,-0.5156958695
C,3.405650614,3.8019954021,0.3651948882
C,1.1456574131,3.0530395744,0.7849973021
C,2.1853260826,2.6614092194,-1.3868439409

C,3.3418085563,3.2952450216,-0.9343634868
C,2.3098357669,3.6828277308,1.2226287002
H,0.2782031717,2.9737409301,1.4300071476
H,2.1211247814,2.2539257122,-2.3874202987
H,4.1934389656,3.3927429962,-1.600255023
H,2.3565630067,4.0865431682,2.2292805185
H,4.3099462187,4.2949005961,0.7095585738
C,-1.602181027,-2.374614138,1.9469086968
H,-1.704331241,-1.6121443963,2.7237951285
C,-3.0025709602,-2.8017906789,1.4876943467
H,-2.9391402258,-3.5580546678,0.6980420668
H,-3.5623465474,-1.9445173712,1.1051473618
H,-3.5637338926,-3.2287714975,2.3251961036
C,-0.7879234598,-3.5462484154,2.4999268993
H,0.1970810651,-3.2167553807,2.8422835879
H,-0.6458843377,-4.3213966844,1.7380862797
H,-1.3116934269,-4.001697831,3.3447803261
C,-0.4768404601,-1.1309488117,-3.3302902646
H,0.0914913414,-1.7200525176,-4.0529841668
H,-0.6869367632,-0.1308255677,-3.7080752611
H,-1.3918057665,-1.6507463289,-3.0437606804

i-PrNHC(OH)=C(CN)SO_2Me
S,0.9012450865,1.4565404153,-1.090438819
O,-0.0424168047,2.138735364,-0.1978263012
O,2.2499465328,1.9810210883,-1.322101161
C,1.1174618301,-0.2990835068,-0.4163319687
C,-0.2730842836,-0.8680680321,-0.0291581841
O,-1.0419275523,-1.1779135922,-0.9352733287
N,-0.530750635,-0.9495174826,1.2881454249
H,0.1781483871,-0.6206415045,1.928837722

H,1.4953861338,-0.8894624959,-1.2557483273
C,-1.8320458745,-1.3603835043,1.8606021153
H,-1.6817346417,-1.2887112681,2.9434269258
C,-2.1595964745,-2.8176270004,1.5139432836
H,-1.3577084529,-3.486440821,1.8402890296
H,-2.2975969254,-2.9349980804,0.4372388779
H,-3.0827804387,-3.1183271878,2.018721984
C,-2.948627743,-0.3883842689,1.4593147189
H,-2.6838606616,0.639339404,1.7229423676
H,-3.8741928232,-0.6528493022,1.9799935069
H,-3.128842435,-0.4351352619,0.3833921832
C,0.1011956141,1.1644419668,-2.6809761144
H,0.828565262,0.7170113832,-3.3591395816
H,-0.202895489,2.1500838037,-3.0383272013
H,-0.7559976987,0.5103574929,-2.521019069
C,2.1039967444,-0.2626006406,0.6503517998
N,2.8397466514,-0.256109056,1.5492181624

i-PrNHC(OH)=C(CN)SO_2Ph
C,-1.2613048548,-1.0328263048,0.4421168221
C,-0.5462144108,-0.4299278755,-0.6124260515
O,-1.977739704,-0.3531306142,1.3202645504
H,-1.9201320486,0.6167355774,1.0684763682
N,-1.2697946539,-2.3638822587,0.6081224414
H,-0.6864325405,-2.9020766985,-0.0195097972
S,-0.5068164743,1.315289836,-0.8425228147
O,-0.8061267053,1.6540594579,-2.2360463416
O,-1.3580758393,1.8728235038,0.2583625381
C,1.1751601598,1.848467376,-0.5099290331
C,3.7815300507,2.634700189,-0.0063677874
C,1.5230510183,2.2651247552,0.7764187805

C,2.105172795,1.8256108609,-1.5517872468
C,3.4169283177,2.2190535098,-1.2887169814
C,2.8366823946,2.6623772967,1.0220719962
H,0.7710316104,2.2936333289,1.5567470378
H,1.8004995744,1.5193084063,-2.5461121296
H,4.1511821823,2.2064416321,-2.0879514355
H,3.1202404063,2.9982575671,2.0147006799
H,4.8034905493,2.9440208917,0.1910148939
C,-2.000913402,-3.0802673182,1.6666024257
H,-2.9143410059,-2.5088549003,1.8530112545
C,-2.3742386844,-4.4691834885,1.1440853257
H,-1.4775795916,-5.0591671065,0.9191084566
H,-2.9804090183,-4.401993175,0.2364398466
H,-2.9455159062,-5.0140349359,1.9003766621
C,-1.1825887811,-3.1416062086,2.962729291
H,-0.935512314,-2.1355714611,3.3108291685
H,-0.2504189349,-3.6959950208,2.809850642
H,-1.7540317361,-3.6451430988,3.7490463341
C,0.178544997,-1.2280943526,-1.5193391006
N,0.7771764756,-1.9348017126,-2.2322738078

t-BuNHC(OH)=C(CO_2Me)SO_2Ph
C,0.2016760914,0.4182385885,1.3291808669
C,0.6729783016,0.6953864085,0.0044596454
O,-0.1674157963,1.4255842771,2.097436494
H,-0.0148710726,2.2780260652,1.5479345948
N,0.1084964474,-0.8020620506,1.8543008476
H,0.4094971532,-1.544749223,1.2216046284
C,-0.3532834174,-1.1758746146,3.2169897758
S,1.2699935264,-0.5659172215,-1.0888340223
O,2.6591077226,-0.3060668323,-1.4881638105

O,0.941173878,-1.8720827753,-0.4536186858
C,0.2515364738,-0.4823371726,-2.5751518878
C,-1.2888393875,-0.4396300827,-4.878459241
C,0.8165785768,-0.0210911293,-3.7626041555
C,-1.0682664693,-0.9344817842,-2.5219005307
C,-1.8402575901,-0.9057051297,-3.681963648
C,0.0363601485,-0.0028525935,-4.9195034075
H,1.8496281397,0.3063463638,-3.765701108
H,-1.4767498842,-1.3136481737,-1.591327322
H,-2.8681009321,-1.2543727772,-3.6544483262
H,0.4652587966,0.3497292598,-5.8526261228
H,-1.8926016721,-0.4231149327,-5.7810113239
C,-0.249221069,-2.709217865,3.2723728476
H,0.782223068,-3.0408831218,3.1146655836
H,-0.8822739611,-3.1756330376,2.5103153756
H,-0.5755809546,-3.0698231443,4.2512861261
C,0.5645519887,-0.5555688333,4.2865887583
H,1.6024200508,-0.8629603211,4.126079671
H,0.2570637528,-0.8967477819,5.2803169982
H,0.5168042736,0.5340122373,4.2654475614
C,0.7532248173,2.0745910463,-0.3939913983
O,0.4082528591,3.034229345,0.330202493
O,1.2128340607,2.2902841062,-1.634652955
C,1.2962364321,3.6627316593,-2.0520616273
H,1.6668354583,3.6276690588,-3.0758377414
H,1.9873861318,4.2168349676,-1.413385065
H,0.314101684,4.1388801556,-2.0141439344
C,-1.817338085,-0.7484415709,3.4293946839
H,-1.9236094563,0.3362563982,3.385840428
H,-2.1634665202,-1.0917563743,4.4095276373
H,-2.4623440649,-1.1937819939,2.6654410966

PhNHC(OH)=C(CO_2Me)SO_2Ph

C,-0.235660761,-1.2900704685,-0.5311611308

C,-0.7555184173,0.0169102637,-0.7863271297

O,0.1524384633,-2.0355357229,-1.5416260554

H,-0.0285790713,-1.4836526881,-2.3912549911

N,-0.1232304988,-1.8080828138,0.7005320791

H,-0.455456407,-1.1654590694,1.4263789696

S,-1.367599247,1.0922402791,0.4880837351

O,-2.7637936084,1.4657958448,0.2346162813

O,-1.0226442448,0.4475637409,1.78671153

C,-0.3733854962,2.5934935705,0.4130558558

C,1.130424142,4.9195889153,0.3771294959

C,-0.9535040591,3.7701530596,-0.0578357719

C,0.9428070202,2.5614284698,0.8777054022

C,1.6963419806,3.7336258605,0.8526287258

C,-0.1910699964,4.9387154939,-0.0724204682

H,-1.9834543232,3.7567939849,-0.3945506074

H,1.3623609804,1.6387660294,1.2638600554

H,2.720850424,3.7233188099,1.211573916

H,-0.6311085565,5.8639545878,-0.4318212843

H,1.7198913338,5.8315184998,0.3633257962

C,0.3636586289,-3.0587150039,1.1464788708

C,1.277418769,-5.4635296367,2.2727810427

C,0.3060609982,-3.2661843779,2.5353548354

C,0.8840333119,-4.0669184701,0.3210500955

C,1.3339328393,-5.2563360529,0.8952637346

C,0.7590349495,-4.4579190619,3.090612673

H,-0.0985929788,-2.4867906201,3.175534913

H,0.9350943775,-3.9261302047,-0.7475343219

H,1.7342647698,-6.0299786562,0.2465385783

H,0.7046793441,-4.5984977655,4.1659284802
H,1.6311131729,-6.3947481234,2.7038868612
C,-0.8579517435,0.4246146006,-2.1633325998
O,-1.353738749,1.6511348811,-2.3664387467
C,-1.4648429811,2.073845877,-3.7366238189
H,-2.1341421488,1.4107650132,-4.2885256803
H,-0.4853063774,2.0779696064,-4.2193998041
H,-1.8759949665,3.0814465067,-3.6917689267
O,-0.4988309733,-0.2850953586,-3.1284105898

PhNHC(OH)=C(COMe)SO_2Ph
C,0.2735560769,0.9340576767,1.1649131931
C,0.9176750884,1.2205755748,-0.1440956831
O,-0.2632458181,1.88214642,1.7973318998
H,0.0207801031,3.0427068997,0.9681611001
N,0.2766177441,-0.3281096783,1.6520934549
H,0.8046431062,-0.996833917,1.0900490664
S,1.6251284151,-0.0424515755,-1.1942112269
O,2.8567148669,0.455393626,-1.8234794812
O,1.688100656,-1.3013292307,-0.4119036095
C,0.4236517107,-0.3211233562,-2.5110583463
C,-1.3880841632,-0.8248061155,-4.5476160344
C,0.8134985358,-0.1194119792,-3.8347558108
C,-0.855574455,-0.7824775355,-2.1886778309
C,-1.7628590775,-1.0295239784,-3.2161075533
C,-0.104389356,-0.3746378167,-4.8561447065
H,1.8208961049,0.2200991469,-4.0483626026
H,-1.1368680264,-0.9488730529,-1.1537918658
H,-2.760348667,-1.3858819399,-2.9788327795
H,0.1873490152,-0.2234717748,-5.8908007145
H,-2.0990984808,-1.0207224484,-5.3444629223

C,0.9434194182,2.5452017524,-0.586204465
O,0.413195809,3.5065986083,0.1308698882
C,-0.2647927694,-0.8226303157,2.8602845949
C,-1.2690682201,-2.014947103,5.1950860581
C,-0.0553303768,-2.1892356107,3.1122373591
C,-0.9837120981,-0.0523472382,3.7872066172
C,-1.4764277598,-0.6592217804,4.9430508208
C,-0.5532924007,-2.7774006635,4.2700478197
H,0.5018392642,-2.7863306947,2.3948631433
H,-1.1455236735,0.9985832864,3.6014272557
H,-2.030560539,-0.0544145566,5.6551279377
H,-0.3796315495,-3.8345296955,4.44782214
H,-1.6582362999,-2.4720678342,6.0995226469
C,1.5435209854,3.0452412303,-1.8702005772
H,2.6238119586,2.8908708053,-1.8761188726
H,1.312846659,4.1072342459,-1.9574116789
H,1.1397984132,2.5140706189,-2.7358580348

PhNHCOCH(SO_2Ph)=C(OH)Me
N,-0.2845373146,0.2776330391,1.6597384526
H,-0.8085636515,0.9646648278,1.1163895301
S,-1.6204575576,0.082928309,-1.2001917268
O,-2.8496086625,-0.3924620037,-1.8511689456
O,-1.6850182243,1.3170936991,-0.3796338436
C,-0.4112893797,0.399478144,-2.5013200394
C,1.4127427576,0.9613645476,-4.5115181615
C,-0.793910368,0.2384748691,-3.8326798245
C,0.866788346,0.8487649911,-2.1579687951
C,1.7802582073,1.1251951034,-3.1723438743
C,0.1301455894,0.5228688503,-4.8407184262
H,-1.800643183,-0.0926032168,-4.0620864978

H,1.1424218201,0.9834399023,-1.1169637761
H,2.776911132,1.4725959727,-2.9188224914
H,-0.1559488477,0.4035177739,-5.881094677
H,2.1285647045,1.1800499583,-5.2980727493
C,-0.282427311,-0.9689467671,1.133952641
O,0.2492748602,-1.937393554,1.7393822805
C,-0.921382624,-1.2135722593,-0.1859537253
C,-0.9482589736,-2.5241001554,-0.6684296566
O,-0.4236297829,-3.5080897309,0.021446432
H,-0.0337697485,-3.0703807048,0.8744780746
C,-1.5436057361,-2.9831918759,-1.9698293779
H,-1.31548933,-4.0427256936,-2.0881148831
H,-1.1342169608,-2.4271891463,-2.8170440171
H,-2.6234059245,-2.8254643581,-1.9761769975
C,0.2533205783,0.7335241316,2.8846074284
C,1.2514164056,1.851216427,5.2586403677
C,0.9652882671,-0.0670160425,3.7910312605
C,0.0476384771,2.092690298,3.1767172347
C,0.5425148905,2.6438501983,4.3538970729
C,1.4550266187,0.5029323858,4.9667683508
H,1.1241474039,-1.1124624266,3.5743325791
H,-0.5041373876,2.7132036832,2.4752205882
H,0.3718664173,3.6957856908,4.5626927758
H,2.0037875799,-0.1251087521,5.6627103222
H,1.6381869125,2.2794338849,6.178127095

PhNHC(OH)=C(SO_2Me)SO_2Ph[a]
C,0.2798616633,0.7625239622,1.065078162
C,0.9582932563,1.1939686135,-0.1045989487
O,-0.3028128917,1.6015637092,1.8973982682
H,-0.1730591072,2.5375768597,1.5444470211

N,0.2062258992,-0.5387374577,1.4007586613
H,0.8045519972,-1.1385791105,0.8306109033
S,1.5843588088,0.0806118002,-1.3335979044
O,2.7047412814,0.7533440141,-2.0076363725
O,1.8131171426,-1.2267608366,-0.6660488712
S,1.1480345742,2.9156733625,-0.4543808838
O,0.7707764063,3.229349361,-1.8370142769
O,0.428008059,3.6383420986,0.6460030225
C,0.2955555304,-0.2003338285,-2.5575651124
C,-1.6766186821,-0.6586923487,-4.4470720186
C,0.1341180311,0.7100665247,-3.6048257893
C,-0.5049769096,-1.3391340608,-2.4447353885
C,-1.4974850505,-1.5628929534,-3.398607322
C,-0.8621366255,0.4713699278,-4.5501680582
H,0.7681080545,1.5855070631,-3.6661590076
H,-0.3350011481,-2.0435127263,-1.6391019476
H,-2.1235809747,-2.4467091251,-3.3254320006
H,-0.9995946486,1.169620065,-5.369793815
H,-2.44947691,-0.8375438191,-5.1886634441
C,-0.4818351962,-1.1689935941,2.468310959
C,-1.7599054734,-2.6234308578,4.4974340117
C,-0.0250100987,-2.4475790367,2.8234001155
C,-1.5911977617,-0.6229084134,3.1286983093
C,-2.2146825633,-1.3543346159,4.139171967
C,-0.6618873072,-3.1676590608,3.8298465918
H,0.8342507427,-2.8709003297,2.3100157927
H,-1.9599016481,0.3562554869,2.8599321343
H,-3.0719742225,-0.9216905389,4.6463218024
H,-0.2941741355,-4.15489131,4.092692917
H,-2.2554013123,-3.1820042154,5.2851718824
C,2.8914779803,3.313549331,-0.2453964654

H,3.4585244765,2.7193338616,-0.9606707658

H,3.1756479842,3.0858572126,0.7823774506

H,2.9850603788,4.3827752856,-0.4462017796

PhNHC(OH)=C(SO_2Me)SO_2Ph[b]

C,-0.8857598252,-0.126243612,0.2009049422

C,-0.2837630654,0.2985970754,-1.0135497453

O,-1.4411849268,0.729365569,1.0397130382

H,-1.422021167,1.6418066025,0.6156880535

N,-0.9168297776,-1.4170896874,0.5688773861

H,-0.4421822255,-2.0302690623,-0.0990589376

S,0.3008110051,-0.808679392,-2.270001035

O,1.5827705255,-0.3240159036,-2.7981234952

O,0.2343757646,-2.1887918212,-1.7207021831

S,-0.0590619885,2.0176409024,-1.3523378119

O,-0.2373483681,2.2537135186,-2.7907982874

O,-0.9545764079,2.7370302666,-0.3882264114

C,-1.5827267756,-2.0698588774,1.6357584678

C,-2.8136970081,-3.5911497455,3.6484982018

C,-1.6242646994,-3.4716780464,1.5482601948

C,-2.1566380277,-1.4314026955,2.7448104984

C,-2.7693503567,-2.2003933123,3.734958418

C,-2.2328934632,-4.2232003841,2.5476942499

H,-1.1794425731,-3.966659288,0.6891340482

H,-2.1229906421,-0.3568012254,2.8364111368

H,-3.212152892,-1.6956720818,4.5885762847

H,-2.2544009492,-5.30533498,2.4615645982

H,-3.2913462849,-4.1753806714,4.4286045912

C,-0.9115085017,-0.7275995611,-3.6019668895

H,-0.5468346406,-1.3907566715,-4.389109136

H,-0.9660311475,0.3054810396,-3.9435278715

H,-1.8715230559,-1.0748244921,-3.2183671949
C,1.6129919965,2.5094097413,-0.9132310492
C,4.1803202402,3.2854709813,-0.2286650944
C,1.8592678906,2.9846624908,0.3771582543
C,2.6253335042,2.4220611911,-1.8707411682
C,3.915190962,2.8148127063,-1.5163719113
C,3.1549433311,3.3722755689,0.7153252975
H,1.0482030657,3.0680708698,1.091187065
H,2.4032642585,2.0449823324,-2.8605760573
H,4.7131743553,2.7526801682,-2.2494701375
H,3.3600114541,3.7482566557,1.7127904111
H,5.1878707161,3.5894837314,0.038909179

PhNHC(OH)=C(SO_2Ph)$_2$
C,-0.8826250124,-0.7796444681,0.4749406737
C,0.3091409684,-0.0616941182,0.1952099477
O,-1.0036724664,-1.5686548932,1.5257106095
H,-0.1571412776,-1.4963388344,2.0676977725
N,-1.9600232862,-0.7112875685,-0.3280693367
H,-1.7768820346,-0.2232756563,-1.207059021
S,0.4262974576,1.1580620535,-1.0897731644
O,1.817897473,1.2072785344,-1.553264385
O,-0.6556709773,0.8705561,-2.0676586899
S,1.7732119136,-0.3462782245,1.1486677793
O,2.4861190012,0.912378847,1.3856354126
O,1.3201147607,-1.1414459882,2.3377423564
C,0.0254753632,2.7559269422,-0.3619646046
C,-0.5990898548,5.2225198688,0.733844443
C,1.0249460522,3.4827334239,0.2893164402
C,-1.2766810042,3.2458317908,-0.4827125775
C,-1.5848360765,4.4874918108,0.072910907

C,0.7008769908,4.7222272181,0.838824779

H,2.0254418947,3.0768187888,0.369650743

H,-2.0230618932,2.6728328697,-1.020215604

H,-2.5923219386,4.8816301575,-0.0178667108

H,1.4672019421,5.2981838715,1.3481256746

H,-0.8429193087,6.1894389309,1.1638526842

C,2.8650896209,-1.4421338537,0.2323268464

C,4.5625699336,-3.1410713756,-1.1444895657

C,2.709408872,-2.8230058911,0.3753669457

C,3.8582486132,-0.8947347419,-0.5813761993

C,4.7085850597,-1.7582341741,-1.2709983196

C,3.5663121249,-3.6725166619,-0.3225241264

H,1.946876408,-3.2203308643,1.0354227429

H,3.9495023397,0.1797739761,-0.6735649151

H,5.4861893379,-1.3477297699,-1.9073841574

H,3.4599221702,-4.7476995723,-0.2173433162

H,5.2290907456,-3.8068296656,-1.6846116495

C,-3.2523835844,-1.2725328611,-0.175156839

C,-5.8658896561,-2.2875891054,-0.0839965538

C,-4.0106927601,-1.3940567531,-1.3500593063

C,-3.8137157054,-1.6530842713,1.0519209922

C,-5.1122699038,-2.1605031963,1.082942857

C,-5.3073672054,-1.8971924341,-1.3018643358

H,-3.5754501816,-1.0975648623,-2.300632425

H,-3.2459301625,-1.557229116,1.9658511567

H,-5.5371544182,-2.4546221569,2.0381220479

H,-5.8786450706,-1.9860746083,-2.2209382681

H,-6.8756248339,-2.6838354636,-0.0450320892

PhNHC(OH)=C(SO_2Me)$_2$

C,-0.1172608022,0.6042175588,0.0945690058

C,0.5805197551,0.9990009206,-1.0786724688
O,-0.8000510116,1.4639356052,0.8246053756
H,-0.7536940088,2.3676153622,0.3813726246
N,-0.1087688616,-0.6657297886,0.5314675396
H,0.500443983,-1.2743311149,-0.0199811598
S,1.4011420199,-0.1235588389,-2.1741519634
O,2.6440246833,0.5049495629,-2.6478404373
O,1.4812400625,-1.4440052576,-1.4984159229
S,0.6311075445,2.6890068681,-1.5789039032
O,0.3557508102,2.8042727632,-3.0176576416
O,-0.2589257881,3.4345336279,-0.6299707709
C,-0.7800914181,-1.2869787947,1.6143692114
C,-1.9929326445,-2.7437453332,3.6852259812
C,-0.3984397038,-2.6138644651,1.8738165764
C,-1.7796803287,-0.6919714264,2.3977505225
C,-2.3725184865,-1.4278910167,3.4242570015
C,-1.0007393802,-3.3334774546,2.9004076309
H,0.3746732725,-3.076831924,1.2662858416
H,-2.0893480038,0.3250412765,2.2128075904
H,-3.1449787248,-0.9567727497,4.0248991766
H,-0.6907802053,-4.3574749845,3.0853599683
H,-2.4631988608,-3.3026631898,4.4879878483
C,2.2986620508,3.2989787374,-1.2826135381
H,2.9865032543,2.6874202382,-1.8654876626
H,2.505216956,3.2282197902,-0.2142303891
H,2.3057000835,4.3400131075,-1.611830884
C,0.3161681105,-0.3290702452,-3.5985343484
H,0.8406933761,-0.9882167514,-4.293253007
H,0.1442488973,0.6553685036,-4.0332452634
H,-0.6146866308,-0.7859902872,-3.2603925339

PhNHC(OH)=C(COMe)$SO_2C_4F_9$

C,-0.087067778,1.4352128445,2.4780466807

C,0.6800308012,1.9465784161,1.3056880424

O,-0.7427585051,2.2584874252,3.1698001028

H,-0.4273995748,3.5166089165,2.5733055581

N,-0.0549791377,0.1216539945,2.7844621083

H,0.5692882081,-0.4426461539,2.2127441658

S,1.5009493435,0.8707817672,0.1746928457

O,2.5631525051,1.563822083,-0.5531547134

O,1.7720228875,-0.4259395468,0.8266109989

C,-0.7094255143,-0.5695103259,3.83279355

C,-1.9129495637,-2.1335049784,5.8259077937

C,-0.4165717904,-1.9390523265,3.9384277658

C,-1.6120303687,0.0172202458,4.7317959282

C,-2.2026782652,-0.7738480533,5.7178423984

C,-1.0140693884,-2.7122891083,4.9282079391

H,0.2817765439,-2.3943539359,3.2408297611

H,-1.8404427715,1.0695770019,4.6583835165

H,-2.900117918,-0.311553689,6.4102277648

H,-0.7750363982,-3.7692966008,4.9955028266

H,-2.3802042805,-2.7352861438,6.5990416073

C,0.6806753832,3.3316304219,1.0653594354

O,0.0334318876,4.1318492014,1.867025499

C,1.3826931875,4.0661777316,-0.0427154686

H,2.4655795878,4.005441205,0.0856989996

H,1.0628650078,5.10754013,-0.0010720258

H,1.157073232,3.642686188,-1.0212344334

C,0.1381285518,0.4831496124,-1.0943528524

C,0.4634575407,-0.7298207665,-2.0066724886

C,-0.4332515949,-0.8059292097,-3.2765837155

C,-0.3904927024,-2.1731311056,-4.010761416

F,-0.0443137615,1.5910854643,-1.8468268985
F,-0.989943324,0.2287218882,-0.4018284242
F,0.2855235778,-1.8583048779,-1.2834082216
F,1.7522898351,-0.6489665233,-2.4038306918
F,-0.0284803,0.1442816377,-4.1468889013
F,-1.719362087,-0.5677835721,-2.921411116
F,-1.0130398372,-2.0518301761,-5.1893655132
F,0.8782013246,-2.5454814152,-4.2253247633
F,-1.0096550567,-3.1139639289,-3.2905826697

$PhNHCOCH(SO_2C_4F_9)=C(OH)CH_3$
N,0.402404372,-0.4488683028,2.8825778187
H,0.1438222118,0.4359469512,2.451351821
S,1.3247295154,0.8164834938,0.1689311366
O,0.4891042694,1.6020105385,1.0971467968
O,2.3249994306,1.4866910577,-0.6634035207
C,1.4097124837,-1.1091650838,2.2757228437
C,2.0002660259,-0.5748869331,1.0142814186
C,3.0935349446,-1.2570107837,0.4515043154
C,3.8487128542,-0.8932045157,-0.7962664052
H,3.1849522258,-0.7312540893,-1.6452773392
H,4.5403790576,-1.7078740542,-1.0118072957
H,4.4049737071,0.0348610637,-0.6471660166
O,3.5698195528,-2.3202884342,1.0370569543
H,2.9624135969,-2.4817024827,1.8716720672
O,1.8862684138,-2.1726442884,2.7546302803
C,0.090863115,0.0173489913,-1.0418501825
C,-0.4090146364,0.9869170683,-2.1453229795
C,-1.6874945545,0.4843727046,-2.8763924144
C,-2.0071826826,1.2332043205,-4.1981863429
F,-3.2285382303,0.8765377774,-4.6132388659

F,-1.119235634,0.9153193475,-5.1458256905
F,-1.9850432336,2.5575759685,-3.9997617284
F,-2.7434201,0.6361964362,-2.0482044646
F,-1.5372005902,-0.8296486313,-3.1728573931
F,0.5819932285,1.1322471317,-3.0540301504
F,-0.6863694332,2.1852863248,-1.5866908766
F,-0.9461414878,-0.4335329586,-0.3074309705
F,0.7054045651,-1.0341515655,-1.6261165257
C,-0.300291854,-0.7766491993,4.0671359253
C,-1.8199547077,-1.2341088396,6.3792097023
C,-0.0947151255,-1.9427525722,4.8187972482
C,-1.2686082241,0.1534219916,4.4794066422
C,-2.0204833581,-0.0753079176,5.6269119925
C,-0.8588393978,-2.1562585773,5.966674737
H,0.6491648624,-2.6609647269,4.509060273
H,-1.4284926655,1.0562750387,3.8954322602
H,-2.764119233,0.6549479424,5.9312934787
H,-0.6935020144,-3.0614137571,6.5436432666
H,-2.4056989878,-1.414623054,7.2750614682

PhNHC(OH)=C(CN)SO_2Me
C,0.0021721435,0.6563111178,-0.4281977334
C,0.6891216385,1.1142359922,-1.5717708884
O,-0.589406433,1.4605061949,0.4283852459
H,-0.4564772342,2.4049056761,0.1021797139
N,-0.0697657322,-0.6688128812,-0.1779219091
H,0.3933408644,-1.2415746445,-0.8733636449
S,0.80933879,2.8295133737,-1.9578822213
O,0.38702147,3.1018191191,-3.3325996588
O,0.1237130112,3.5384282011,-0.8292070007
C,1.2824239653,0.2020903464,-2.4663494429

N,1.7804838777,-0.5927015958,-3.1639543798
C,2.561529494,3.2359100924,-1.8386179694
H,3.1071400023,2.6212447857,-2.556173408
H,2.9001469308,3.0508011689,-0.8190576563
H,2.6540153282,4.2930448142,-2.0951261964
C,-0.7187687423,-1.4042682465,0.8465710671
C,-1.9211405244,-3.0576405971,2.7674116933
C,-0.6786134128,-2.8010341304,0.7109774153
C,-1.3630960475,-0.8348790597,1.9537392688
C,-1.958387844,-1.6702803301,2.8994896472
C,-1.2749130766,-3.6187988922,1.6650581564
H,-0.1802899715,-3.2455593453,-0.1471800631
H,-1.4011184711,0.2365942941,2.0763616783
H,-2.4564588988,-1.2196193796,3.7526951594
H,-1.233752651,-4.6966441785,1.5421301709
H,-2.3882586764,-3.6935917953,3.5124026559

PhNHC(OH)=C(CN)SO_2Ph
C,-0.9175225903,0.017002934,0.4705330657
C,0.305177025,0.7144364322,0.5147226568
O,-1.0958946555,-1.1654776799,1.0215479207
H,-0.2293220468,-1.4261660021,1.4623543204
N,-1.9815287976,0.5675515654,-0.1553550632
H,-1.7963176244,1.4829015117,-0.5476789799
S,1.7428371801,0.0389090518,1.2842636528
O,2.3405417886,1.0211813845,2.1908120223
O,1.3071585272,-1.2951316735,1.8115175053
C,0.4210989153,1.9909587476,-0.0700933101
N,0.4650671978,3.0393086548,-0.58482382
C,-3.3256235346,0.1341985692,-0.2817832012
C,-6.0264370577,-0.5273849354,-0.6492377614

C,-4.2339973892,1.0892338819,-0.7648032005
C,-3.7742011478,-1.1610578619,0.0122153502
C,-5.1212821215,-1.4740494677,-0.1712648569
C,-5.5725880762,0.7581252753,-0.9481081145
H,-3.8883553442,2.0947389659,-0.9922320124
H,-3.087451144,-1.9099226899,0.3762728211
H,-5.459768996,-2.4792643635,0.061513913
H,-6.2602214739,1.5102650906,-1.3223182704
H,-7.07088829,-0.7870700074,-0.7885789177
C,2.9275792322,-0.2840083884,-0.023867003
C,4.7383806992,-0.7511215922,-2.0641379536
C,2.955576149,-1.5403876074,-0.6326997284
C,3.7940232307,0.7410898417,-0.4107652491
C,4.7005110837,0.4986498452,-1.4422368479
C,3.8723331282,-1.7690312689,-1.6577218018
H,2.2857902845,-2.3222799707,-0.2931921158
H,3.7645658314,1.6987670833,0.0964071434
H,5.3804253702,1.2848927122,-1.7544357706
H,3.9130810062,-2.7431356113,-2.135014061
H,5.4489913016,-0.9347702326,-2.8642875272

PhNHC(OH)=C($SO_2C_4F_9$)$_2$
C,-0.9258843638,-0.2102902053,1.9697474867
C,-0.3464328372,-0.0413478824,0.6638167997
O,-1.7436174949,0.6810151877,2.4839496255
H,-1.8971765591,1.413465411,1.8168915664
N,-0.6638517558,-1.2741725569,2.7299447487
H,0.0027166681,-1.9252243974,2.3103263746
S,0.5427924312,-1.3159411533,-0.1589485147
O,1.5205518075,-0.7585747752,-1.0858982862
O,0.9422621912,-2.3267867303,0.8434677366

C,-1.2443360142,-1.693722734,3.9607086293

C,-2.2532310781,-2.7238437606,6.3582594584

C,-1.846761864,-0.8337719483,4.8875521051

C,-1.1375306305,-3.063612557,4.2424630292

C,-1.6388412996,-3.572845757,5.4362892867

C,-2.351363555,-1.3617319735,6.0762007749

H,-1.9162182617,0.225673367,4.6911864226

H,-0.6679101971,-3.7255253338,3.5200623706

H,-1.5511322752,-4.6350816406,5.641642929

H,-2.8191559059,-0.6913460185,6.7906620085

H,-2.6475575341,-3.1198901548,7.2885969065

C,-0.7986094813,-2.1858788327,-1.1975242307

C,-0.2056555276,-3.1186920353,-2.2876833375

C,-1.2367204936,-4.1407359848,-2.8486938916

C,-0.7989401518,-4.8352851502,-4.1661527291

F,-1.5670092614,-1.2516240639,-1.7734187118

F,-1.544082889,-2.9005138676,-0.3261329467

F,0.8273593918,-3.8117433882,-1.7561752858

F,0.2424798869,-2.3487986896,-3.3010590964

F,-2.4067898219,-3.5009352378,-3.0873726111

F,-1.437133034,-5.1022061619,-1.9204036354

F,-1.6454836922,-5.8389211307,-4.427668973

F,-0.8251104821,-3.9716955017,-5.1852598021

F,0.4385189704,-5.3328328501,-4.0400827418

S,-0.4820145562,1.5039213871,-0.1592806313

O,-0.4624887111,1.3827228724,-1.6086948539

O,-1.5836357674,2.2504244049,0.5149243437

C,1.0877855958,2.4549670636,0.357661502

C,0.932399002,3.9954045702,0.2175013699

C,2.2936020843,4.7503283066,0.2361452491

C,2.171983358,6.2810143209,0.4673346963

F,3.3602927253,6.8508021938,0.236221476
F,1.807926022,6.5393107003,1.7278733714
F,1.2672025622,6.8066024146,-0.3689392595
F,2.9110705847,4.557201553,-0.9478307359
F,3.0610438646,4.2424186898,1.231484031
F,0.1772496677,4.441184095,1.2467565241
F,0.3101028477,4.2698940187,-0.9497719179
F,2.1026365368,2.0186370151,-0.398453337
F,1.3172369754,2.1486993897,1.6512268523

2,4-$MeO_2C_6H_3NHC(OH)=C(SO_2Ph)_2$
C,0.2092533489,-0.6380659837,-0.543134864
C,-1.0822235606,-0.1315545002,-0.2344238013
O,0.4426899992,-1.349741894,-1.6317877892
H,-0.4129209772,-1.3966423031,-2.1622312674
N,1.2717852785,-0.4302598403,0.2506595592
H,1.0648355277,0.0677643882,1.1200537144
S,-2.4879839426,-0.5798284315,-1.2061721253
O,-3.3447880999,0.5864140637,-1.4429557582
O,-1.9340559557,-1.3089722058,-2.3959907626
C,2.6429566873,-0.6981968714,0.0175033859
C,5.4195488826,-1.1030192514,-0.2029747418
C,3.5517934719,0.0446776205,0.8151898409
C,3.1589064612,-1.6413617465,-0.8683374552
C,4.5384446172,-1.8425070982,-0.9910524285
C,4.9202630075,-0.1580633798,0.7075981812
H,2.4840746317,-2.2301350731,-1.4710705988
H,4.8975113194,-2.5824359413,-1.6947437824
H,5.62806032,0.400696842,1.3058871175
O,6.7792854271,-1.2153937446,-0.2304873287
O,2.9716021097,0.9403263374,1.6681427793

C,-3.4535670144,-1.8072115746,-0.3135734834
C,-4.9525837098,-3.7109088749,1.026525902
C,-3.1192316788,-3.1566093537,-0.4488093404
C,-4.5279157374,-1.3926590717,0.4745809035
C,-5.2774178366,-2.3582628536,1.1456859907
C,-3.8766437202,-4.1096185848,0.2301702562
H,-2.2955502742,-3.4510988858,-1.0890442819
H,-4.7572503055,-0.3385535865,0.5618687439
H,-6.1162806596,-2.051036902,1.7623088723
H,-3.6306528189,-5.1623068129,0.1306122574
H,-5.5410537572,-4.4568867285,1.5523985463
S,-1.3712413689,1.045668448,1.058755622
O,-2.7629202052,0.9102104155,1.5070250647
O,-0.2712160929,0.8968732275,2.0421268563
C,-1.1788045141,2.6844539338,0.3362569068
C,-0.870668257,5.2035206022,-0.7736952429
C,-2.2918961682,3.3277015581,-0.2078519673
C,0.0849215757,3.2803182355,0.3399486837
C,0.2324631106,4.54764992,-0.2231647671
C,-2.1280404465,4.5959686355,-0.7637750325
H,-3.2564888317,2.8358226933,-0.1999576463
H,0.9286528341,2.764132927,0.7844209625
H,1.2080707465,5.0242485239,-0.2262675947
H,-2.984831849,5.1089048117,-1.1896197816
H,-0.750663656,6.1911827982,-1.2091201014
C,3.7885993723,1.6028613435,2.6254386593
H,3.1065835849,2.1872798902,3.2431152432
H,4.5090999898,2.2724608125,2.140493416
H,4.3274884579,0.8829507249,3.2522012177
C,7.3533911695,-2.1542744179,-1.1275666603
H,7.0309299869,-3.1785074763,-0.9016488095

H,8.4330000971,-2.0792460092,-0.9909847035
H,7.1037439788,-1.9214143411,-2.1703653675

2,4-$MeO_2C_6H_3NHC(OH)=C(CO_2Me)SO_2Ph$
C,0.1764661681,-0.4799755033,-1.1397550506
C,-0.5933183193,0.5798748379,-1.7188701251
O,1.1500322475,-1.0172493427,-1.8450240732
H,1.1488490187,-0.5337740759,-2.7529454475
N,-0.031858559,-0.9710791362,0.0869940581
H,-0.7920731918,-0.5130240827,0.6004808695
C,0.6419411527,-2.0021769336,0.7826573878
C,1.7983170219,-4.011715926,2.3822060934
C,0.2343153836,-2.1856164372,2.1312782379
C,1.6270358968,-2.844866296,0.271083669
C,2.2081728563,-3.8443227926,1.0605951251
C,0.804728799,-3.1766253741,2.9173658397
H,1.9489934179,-2.728132376,-0.752042001
H,2.9702390686,-4.4759851517,0.6224839461
H,0.5056897892,-3.3295267315,3.9460360516
O,2.2908352362,-4.9499552671,3.2436816486
O,-0.7337391582,-1.3263067872,2.5578173489
S,-1.9648377934,1.3513567363,-0.8996588978
O,-3.1862695588,1.2484014648,-1.7079044645
O,-1.9766488795,0.8253973847,0.4907755926
C,-1.5535153415,3.1018148134,-0.7558366377
C,-0.977692186,5.7982436457,-0.4718321921
C,-2.219097772,4.0278653666,-1.5573325907
C,-0.6137752787,3.5026747337,0.1960415649
C,-0.3241942646,4.8595193239,0.3308879463
C,-1.9254099843,5.3839838443,-1.4094594796
H,-2.9553958519,3.6784776781,-2.2715035734

H,-0.1309239917,2.7653184886,0.8283522293
H,0.4043969851,5.1843899089,1.0673878281
H,-2.439753133,6.1164041495,-2.0243607764
H,-0.7518412004,6.854723706,-0.3608403539
C,-1.2546534738,-1.469255602,3.8713029289
H,-2.0216498231,-0.7010888541,3.9703213515
H,-0.476831884,-1.3111975563,4.6282755634
H,-1.7051130822,-2.4585331512,4.0158400317
C,3.2946575493,-5.8315282762,2.7648072462
H,2.9337433737,-6.436346437,1.9232786658
H,3.5416454238,-6.4887288557,3.5997573415
H,4.1958360708,-5.2877957107,2.4540330469
C,-0.2697081267,0.9651406086,-3.0663626456
O,0.649107059,0.4491609176,-3.7414966566
O,-1.0124921841,1.9559919259,-3.5789871345
C,-0.7018438877,2.351331238,-4.9251336457
H,-0.8427327517,1.5150476732,-5.6131218113
H,0.3295640146,2.7035302989,-4.9966307709
H,-1.3991971552,3.1561580124,-5.1546432848

i-PrNHCOCH(CO_2Me)SO_2Ph
S,-0.79330166,0.4460627159,0.9953748901
O,-0.0775102351,-0.4174312834,1.9441636567
O,-1.3279269247,1.752540633,1.4119419269
C,0.3681970242,0.7937503632,-0.4507371847
C,1.3396679429,-0.3948765318,-0.6095055192
O,0.9650754298,-1.3676203979,-1.2630968068
N,2.5204644857,-0.2759531564,0.023690591
C,-2.1403692463,-0.4894874557,0.2590805929
C,-4.252112336,-1.9102127443,-0.8190329809
C,-1.9674173486,-1.8467444428,-0.0224334706

C,-3.3457311312,0.1704136757,0.0143670164
C,-4.4076158365,-0.5535747266,-0.5277139637
C,-3.0375651642,-2.553658913,-0.5684245866
H,-1.017033143,-2.3286786998,0.1690389832
H,-3.4417702944,1.2216690075,0.2610160297
H,-5.3549618129,-0.0587660067,-0.7177414948
H,-2.9219851869,-3.6084060866,-0.7968112369
H,-5.0812820888,-2.469616912,-1.2419563224
H,2.6605649618,0.5722864029,0.5624252437
H,-0.2758974767,0.8131624484,-1.3296689567
C,3.5290086709,-1.3482226283,0.1090360946
H,4.3287554609,-0.9190827725,0.7232228353
C,4.1096435787,-1.6839591015,-1.2708204011
H,4.5326233532,-0.7920056968,-1.7430107252
H,3.3326685386,-2.0890042731,-1.9225142172
H,4.9058619658,-2.4285509849,-1.1703480621
C,2.9769005217,-2.5842251841,0.83177663
H,2.5556250321,-2.308001844,1.8021693236
H,3.7788677531,-3.3121321979,0.9919111965
H,2.1929382846,-3.0546423571,0.2348523164
C,0.9562946446,2.1716869002,-0.2102920118
O,1.891257,2.411329281,0.530698826
O,0.2985772534,3.0975264106,-0.9143070007
C,0.7093240596,4.4611714542,-0.6837829015
H,0.5446059692,4.7270852698,0.36217812
H,0.0848778014,5.0657370044,-1.3396416017
H,1.7659587842,4.587310889,-0.9286656291

i-PrNHCOCH(COMe)SO_2Ph
S,1.0288712123,1.6306076663,-0.2028227207
O,0.1087321357,2.2045984591,0.7875077888

O,2.349841264,2.233242846,-0.4580074022
C,1.3809652345,-0.1433737551,0.2880135474
C,0.0689139922,-0.8451166169,0.7055853571
O,-0.5875007682,-1.4214019295,-0.1603480693
N,-0.2642412478,-0.7296825148,2.0044315589
C,0.1718951478,1.5018922856,-1.77628475
C,-1.1339362055,1.3432823442,-4.2081440379
C,-1.2164563887,1.3593265436,-1.7908542759
C,0.9194400741,1.573895158,-2.9531859049
C,0.2542591209,1.4928556582,-4.1759550943
C,-1.8669455945,1.2799941025,-3.020988203
H,-1.7693652617,1.3225754575,-0.8602024668
H,1.9936334308,1.7129692818,-2.9035111752
H,0.8186644964,1.5539484513,-5.1011670723
H,-2.9461813315,1.1695306836,-3.0515997644
H,-1.6475885479,1.2808273316,-5.1628098204
H,0.3811339582,-0.2082845703,2.5887214761
H,1.7022887477,-0.6141081329,-0.6429722488
C,-1.5103787849,-1.248318545,2.5949824238
H,-1.4440545206,-0.9738510928,3.6537997482
C,-1.5885928597,-2.777771864,2.4985931152
H,-0.716639129,-3.2414733201,2.9697991136
H,-1.6297184966,-3.0923471461,1.4537591961
H,-2.4866803844,-3.1391810871,3.0097662956
C,-2.7438532271,-0.5587238011,1.9964516092
H,-2.6640375162,0.5276086513,2.0972801939
H,-3.6485026938,-0.8892133748,2.5169796326
H,-2.8418861465,-0.8085894326,0.9374199174
C,2.5345405845,-0.1008673181,1.3038062846
O,2.3276415235,0.132390721,2.4819057782
C,3.9166234774,-0.3415449672,0.7549906655

H,4.6474062217,-0.2996562777,1.5631124983
H,4.1362511762,0.4290633029,0.0081353523
H,3.9654569068,-1.3151032982,0.2538117528

i-PrNHCOCH(SO_2Ph)$_2$
S,0.2084876996,1.8145564804,0.043384302
S,0.6856107652,-1.2961027988,-0.4208996574
O,-0.4096308245,2.6087665461,1.1158533638
O,-0.0569489971,-2.5060102271,-0.0300523774
O,1.6538931459,1.9053553288,-0.2224603169
O,0.7522126925,-0.8618099252,-1.820426337
C,-0.0716323673,0.063921618,0.6140701169
H,0.4949541703,0.0661799008,1.5501994008
C,-1.5602720331,-0.2444001382,0.8365631596
O,-2.3941112338,0.0175787347,-0.0189158287
N,-1.843952702,-0.8027823766,2.0397694993
C,2.3610351778,-1.4780932493,0.2147946633
C,4.9320234884,-1.837414502,1.1739940677
C,2.6031099276,-2.4851150671,1.1524689009
C,3.3832839726,-0.6555695812,-0.2632379801
C,4.6745738331,-0.8418844968,0.2289774662
C,3.9007208247,-2.6596359465,1.6325432218
H,1.791754721,-3.1281661641,1.4745983148
H,3.1669017563,0.1179502154,-0.988321379
H,5.479806258,-0.2081865957,-0.1287628828
H,4.1060903678,-3.4415894788,2.3569825099
H,5.9410276112,-1.9762466099,1.5506011845
C,-0.6646614513,2.1534541893,-1.4841098203
C,-1.9515728566,2.8601679093,-3.8248593378
C,-1.9581122387,2.674941994,-1.4145780127
C,0.0020531936,1.9871396291,-2.698724136

C,-0.6558373394,2.3432483462,-3.8750477804
C,-2.5996770055,3.0287881896,-2.5988945325
H,-2.4403653571,2.8002586904,-0.453660437
H,1.0071608822,1.587615274,-2.7167956189
H,-0.1536050523,2.2180534201,-4.8290103344
H,-3.6053634062,3.4354320418,-2.5638333465
H,-2.457937121,3.1366954087,-4.7450007622
H,-1.0777594937,-1.1225725354,2.6156550993
C,-3.1826413013,-1.319778181,2.355166463
H,-3.8715180989,-0.6876153552,1.7885108305
C,-3.4515250868,-1.1561066495,3.8522655146
H,-2.7497196936,-1.7526987551,4.4484545094
H,-4.4609334823,-1.5006632178,4.0949684938
H,-3.3601630203,-0.1103129335,4.1586074089
C,-3.3355704723,-2.7697926804,1.8780961917
H,-2.6527584504,-3.4348322814,2.4191538405
H,-3.1126465641,-2.8469509476,0.8115428172
H,-4.3579404066,-3.1224043075,2.0490525165

i-PrNHCOCH(SO_2Me)$_2$
S,-0.6016477929,-0.998885005,1.9716950143
S,-1.5795528333,0.6549454491,-0.5117364765
O,-1.0453907498,1.7140766293,-1.3938606638
O,-2.0854917515,-0.5997659558,-1.0854752712
C,-0.1823533101,0.2333171481,0.6409845211
H,0.0095701368,1.142107333,1.2213075553
C,1.0981708474,-0.1619130527,-0.1513017778
O,1.5891736581,-1.2776171601,-0.0372923873
N,1.6274018237,0.8392065358,-0.8894630406
H,1.0145315709,1.6150221855,-1.1211804432
O,0.5382240862,-0.9923656618,2.8915570967

O,-1.9343661799,-0.6008921443,2.4638234645
C,-0.7691921961,-2.6013345111,1.1724267741
H,0.212876786,-2.9110519632,0.8243387863
H,-1.4777618519,-2.4961454601,0.3498992815
H,-1.1644571565,-3.2587610323,1.9495147181
C,-2.8697574623,1.421660988,0.4855368064
H,-2.4618273686,2.3168111573,0.9561696244
H,-3.2259941903,0.7086301328,1.2253348828
H,-3.6435782069,1.6921058179,-0.2361606273
C,2.8035447908,0.6184645189,-1.746532854
H,3.4367111743,-0.0854603077,-1.199278739
C,2.4036797148,-0.0147822751,-3.0854549992
H,3.290770663,-0.2006150765,-3.6995584368
H,1.7323825332,0.6451911503,-3.6455262085
H,1.8952526501,-0.9681014482,-2.9212719465
C,3.5460347719,1.9447182152,-1.9209127404
H,4.4493420692,1.7953374492,-2.5192153526
H,3.8390239727,2.3639326148,-0.9541677585
H,2.9225990294,2.6813127477,-2.4417929501

i-PrNHCOCH($SO_2C_4F_9$)$_2$
S,0.1682530864,-0.1663365157,1.5320891328
S,-1.0278072505,0.6967686435,-1.221313996
O,-0.6058319419,1.3540371026,-2.4690099159
O,-1.6000798668,-0.645455605,-1.2332615486
C,0.4434839679,0.7650418362,-0.0696664982
H,0.4730878438,1.7966167307,0.2979046944
C,1.8342928178,0.4324871764,-0.7090610386
O,2.6093675835,-0.2641366659,-0.0723112805
N,2.1099590427,1.0315775292,-1.8816951829
H,1.3482892944,1.4588317688,-2.3985614114

O,1.2190194177,0.253003169,2.4520211763
O,-1.2457605412,0.0116617229,1.8632620072
C,0.3306536555,-2.0466472006,1.0720906881
C,-2.2871167073,1.9839647626,-0.4627473299
C,3.3923865897,0.8073464137,-2.572958949
H,4.1377632171,0.6864551266,-1.7820009802
C,3.3475527022,-0.4774555122,-3.4092594754
H,4.3155002071,-0.6524020371,-3.8895027803
H,2.5853099138,-0.4084511217,-4.1928947776
H,3.1197605821,-1.339032878,-2.7765361324
C,3.7279024761,2.0443644419,-3.4076968155
H,4.6959868089,1.9136929226,-3.8991203059
H,3.7780437238,2.9417830473,-2.7844831446
H,2.9789749126,2.2093206864,-4.1915082699
C,-3.7065954183,1.3914958536,-0.2516192624
C,-4.6935332883,2.3833217237,0.4336996371
C,-6.1820477401,1.9432401181,0.3822617327
F,0.6313667569,-2.1414370447,-0.2320025336
F,-1.7771058322,2.4688174161,0.6829523871
F,-3.6413049274,0.2855444412,0.5049795467
F,-4.3341485582,2.5026669029,1.7295992514
F,-6.3174227582,0.6876685306,0.8240963171
F,-6.8982374648,2.7600608039,1.1634434174
F,-6.6474309558,2.0222878409,-0.8690493541
F,-4.605355558,3.5956342725,-0.163886856
F,-4.1780416053,1.0774058212,-1.4840899683
F,-2.3457282081,2.967819243,-1.3663085917
C,1.3728881832,-2.8689972854,1.8951858306
C,0.8939041332,-3.2133273613,3.3344083331
C,2.0257593123,-3.6680568475,4.292462738
F,1.4778602404,-4.1438478443,5.4171467128

F,2.7489498486,-4.6401965506,3.7171919962

F,2.8262754169,-2.6455724701,4.6003494476

F,-0.012618312,-4.2112260656,3.2619908407

F,1.5487464045,-4.034767282,1.2262633423

F,2.549366691,-2.2216802902,1.9507595531

F,0.3025515559,-2.1194415664,3.8770302867

F,-0.8870900519,-2.5644476039,1.2793573293

i-PrNHCOCH(COMe)$SO_2C_4F_9$

S,1.1260576884,0.2477995239,1.0011394405

O,0.2924924712,0.6132809722,2.1456480491

O,2.295252732,1.0388042303,0.5992877278

C,1.6916674043,-1.5136414408,1.1581048144

C,0.5061630659,-2.4693254927,1.4566976531

O,0.0308749419,-3.109587979,0.5240302143

N,0.086559837,-2.4828554068,2.734088966

H,0.6157335875,-1.9212293611,3.3916599484

H,2.0543826917,-1.7674912336,0.1616188443

C,-1.0755237454,-3.2519261309,3.2205249945

H,-1.1309612609,-3.0110710431,4.2878454102

C,-0.8530491211,-4.7630692836,3.0757514667

H,0.0593488748,-5.0745815768,3.5933549102

H,-0.7689902773,-5.037352278,2.0220609527

H,-1.6963809977,-5.3073805958,3.5123787858

C,-2.3721490785,-2.7798461374,2.5501587774

H,-2.5064783872,-1.7028556558,2.6853234795

H,-3.2299271242,-3.2945020058,2.9943442485

H,-2.3512632934,-2.997407836,1.4801834504

C,2.8491308208,-1.4882375928,2.1819416339

O,2.6162343472,-1.4322648067,3.3741702012

C,4.2403840862,-1.5194142617,1.6092954973

H,4.9736508218,-1.5068280511,2.4159798561
H,4.3763819593,-0.6463636622,0.960763912
H,4.3773349712,-2.4126750196,0.9891765485
C,-0.0209667023,0.1472835989,-0.5265288813
C,-0.2158917897,1.5403513254,-1.1880527284
C,-1.4317641418,1.591732156,-2.1582701289
C,-1.4494285373,2.8282096576,-3.0971542107
F,-2.6317361926,2.8810186364,-3.7213923762
F,-1.2814505744,3.9517629201,-2.3872800216
F,-0.4808225439,2.7377641165,-4.0139705847
F,0.9051073219,1.8404527027,-1.8785105924
F,-0.4075479232,2.4595608167,-0.2153284625
F,-1.4171158291,0.4818634639,-2.9352687994
F,-2.5660849187,1.6105399786,-1.4265667415
F,-1.2009503201,-0.3416087216,-0.1151283027
F,0.5459956685,-0.6921711375,-1.4114465829

i-PrNHCOCH(SO_2Me)SO_2Ph
C,-1.5776972417,-0.2316703915,-0.8492936812
C,-0.5247091289,-1.0757980107,-0.1014991339
O,-0.6343868003,-1.3460726928,1.0899027845
N,0.4746256549,-1.527488227,-0.8977191966
H,0.5864666001,-1.0856641643,-1.8049350281
H,-1.8414246516,-0.6955403111,-1.8045067368
S,-3.2153522675,-0.0308742866,0.0267740846
O,-3.064883778,0.9531548735,1.1065635323
O,-4.2008635441,0.1646563399,-1.0421321695
S,-0.8804120391,1.4033948901,-1.4486240029
O,0.1425436359,0.9611961345,-2.4205943031
O,-1.9961964588,2.2504969516,-1.8678596235
C,-0.0313726672,2.1833486451,-0.0729879952

C,1.3132047725,3.4795029766,1.9648803506
C,1.3603190116,2.0827633442,-0.0069342652
C,-0.7647416093,2.9353594994,0.8481077207
C,-0.0769514157,3.580016722,1.8747928513
C,2.0313575757,2.7372402544,1.0253139978
H,1.8981828659,1.5224063084,-0.7618545151
H,-1.8423846719,2.9982495308,0.7689235285
H,-0.630150478,4.1641477876,2.6030955642
H,3.1130318811,2.673399071,1.0892755888
H,1.8398896538,3.9876853451,2.767102865
C,-3.5473558578,-1.6433199386,0.7690383496
H,-2.8118956676,-1.8383122562,1.5448848612
H,-3.5302910178,-2.4052177027,-0.0119434309
H,-4.5581119755,-1.5467572164,1.1714396258
C,1.5717506705,-2.3560413735,-0.3778527477
H,1.1375662066,-2.9232454694,0.4503793487
C,2.0340909542,-3.3193635151,-1.4737438289
H,2.821238295,-3.9763090892,-1.0926742044
H,2.4451600779,-2.7738947746,-2.3316410997
H,1.2076748805,-3.9420482953,-1.8278577187
C,2.719464412,-1.4984485896,0.1699016715
H,3.4960219403,-2.1357086017,0.6052403533
H,2.3561424447,-0.8209600909,0.9465482747
H,3.1804494379,-0.9042834769,-0.6275116713

i-PrNHCOCH(CN)SO_2Me
S,0.9012450865,1.4565404153,-1.090438819
O,-0.0424168047,2.138735364,-0.1978263012
O,2.2499465328,1.9810210883,-1.322101161
C,1.1174618301,-0.2990835068,-0.4163319687
C,-0.2730842836,-0.8680680321,-0.0291581841

O,-1.0419275523,-1.1779135922,-0.9352733287
N,-0.530750635,-0.9495174826,1.2881454249
H,0.1781483871,-0.6206415045,1.928837722
H,1.4953861338,-0.8894624959,-1.2557483273
C,-1.8320458745,-1.3603835043,1.8606021153
H,-1.6817346417,-1.2887112681,2.9434269258
C,-2.1595964745,-2.8176270004,1.5139432836
H,-1.3577084529,-3.486440821,1.8402890296
H,-2.2975969254,-2.9349980804,0.4372388779
H,-3.0827804387,-3.1183271878,2.018721984
C,-2.948627743,-0.3883842689,1.4593147189
H,-2.6838606616,0.639339404,1.7229423676
H,-3.8741928232,-0.6528493022,1.9799935069
H,-3.128842435,-0.4351352619,0.3833921832
C,0.1011956141,1.1644419668,-2.6809761144
H,0.828565262,0.7170113832,-3.3591395816
H,-0.202895489,2.1500838037,-3.0383272013
H,-0.7559976987,0.5103574929,-2.521019069
C,2.1039967444,-0.2626006406,0.6503517998
N,2.8397466514,-0.256109056,1.5492181624

i-PrNHCOCH(CN)SO_2Ph
S,1.474114101,0.8627801213,-0.1778530355
O,0.9872661669,1.7388320231,0.903469054
O,2.8466301878,0.9602713792,-0.6834310729
C,1.2515442202,-0.9023101537,0.419987724
C,-0.2022423898,-1.259833408,0.8674285608
O,-0.7721215752,-2.1933592715,0.3218255061
N,-0.6841109792,-0.5004702071,1.8735174909
H,-0.1389992912,0.3098436293,2.1441884654
H,1.4746262553,-1.5342364781,-0.4429521798

C,-2.003200679,-0.7010642735,2.5088842636
H,-2.0492911115,0.071552431,3.2842251346
C,-2.0873973717,-2.0729566494,3.1892856744
H,-1.2731555953,-2.2001941805,3.9082793122
H,-2.0287280095,-2.8734213713,2.4488760321
H,-3.0370938906,-2.1627011873,3.7256461231
C,-3.1527164424,-0.4664194563,1.5199578419
H,-3.0971093138,0.5363052667,1.0849693593
H,-4.1133260114,-0.5595143798,2.0361508238
H,-3.1178344612,-1.2008454543,0.7125364125
C,2.2200086312,-1.1379053819,1.4818022675
N,2.968178089,-1.3297679668,2.3487610008
C,0.341676858,0.9736383592,-1.5635005928
C,-1.3929736016,1.1462176016,-3.7087650949
C,-0.9253316504,1.5254973693,-1.3668531821
C,0.7648341064,0.5197255902,-2.8153562388
C,-0.117192681,0.6063230161,-3.8908813238
C,-1.7945635199,1.6091783332,-2.4541163936
H,-1.2079435306,1.8930062084,-0.3872921867
H,1.7685087057,0.1288564291,-2.9430293726
H,0.1940245896,0.2602502026,-4.8712616073
H,-2.7821323033,2.0392749333,-2.3216664313
H,-2.0747125322,1.2125105005,-4.5511196953

t-BuNHCOCH(CO_2Me)SO_2Ph
S,0.8996621964,1.5226171533,-0.7601349916
O,-0.2284151285,2.1712088795,-0.078368411
O,2.2503783137,2.1057710117,-0.7162682087
C,1.0631930534,-0.2236762516,-0.0653693789
C,-0.3256658216,-0.7122007157,0.4006584747
O,-1.0741811016,-1.2062647788,-0.4419050502

N,-0.6081062041,-0.5189197278,1.7012950452
C,0.4674284716,1.2664488369,-2.4862248486
C,-0.1732248562,0.9274655595,-5.1540436223
C,-0.8503332036,0.9567657947,-2.8305522415
C,1.4692492606,1.4121462062,-3.447290804
C,1.1381088638,1.2414671035,-4.7914305907
C,-1.1628303385,0.7855454773,-4.178215231
H,-1.6045045997,0.8430759128,-2.0621708181
H,2.4764208172,1.668739674,-3.1389662509
H,1.9027459395,1.3581340743,-5.5530944407
H,-2.1808155272,0.5419596425,-4.4652626098
H,-0.4261132044,0.7944080558,-6.2017354064
H,0.1070309104,-0.0517387457,2.2502131703
H,1.3572768112,-0.8371637238,-0.9167814678
C,-1.9152443004,-0.795713412,2.3450532382
C,-2.238649484,-2.2971451649,2.2448335094
H,-1.4619876002,-2.8929327006,2.7351212815
H,-2.3085922494,-2.60483956,1.2001482549
H,-3.1935096452,-2.5071392863,2.7377561666
C,-3.0159160909,0.0459647513,1.673792774
H,-2.7648469815,1.1097571753,1.7167603714
H,-3.9713432514,-0.1091706118,2.1857778204
H,-3.1306786735,-0.241154703,0.6271708438
C,2.1889118931,-0.1769565401,0.9509300055
O,2.0766779519,0.211563457,2.0984943934
O,3.3335817762,-0.6066321977,0.4115210484
C,4.4962921112,-0.5029710971,1.259232737
H,4.6760626909,0.5426873636,1.5166030432
H,5.3199220837,-0.9035189815,0.6703518184
H,4.3542136898,-1.0828211449,2.173497837
C,-1.7601669248,-0.3853353432,3.8172415075

H,-0.963790824,-0.9574641271,4.3054747028
H,-2.6915633311,-0.5729863857,4.3583302805
H,-1.5266771926,0.6810189701,3.9075559478

PhNHCOCH(CO_2Me)SO_2Ph
C,-0.4219766329,0.9460078462,-0.3608653627
C,0.6586593579,-0.0332551012,0.1802048542
O,0.3906843714,-0.8954255515,1.0007714461
N,1.875057999,0.1594068089,-0.4080103145
H,1.9326082808,0.9389859599,-1.0558715591
C,3.0743957169,-0.5650224793,-0.2112558564
C,5.5274152953,-1.8948318831,0.0550085795
C,3.1876631628,-1.6503223531,0.6695795753
C,4.1911849784,-0.1511931801,-0.9535618606
C,5.4077514112,-0.8131906898,-0.8193936835
C,4.415044464,-2.3022898995,0.7912095934
H,2.3281655812,-1.9669787798,1.2422997077
H,4.102398191,0.691066872,-1.6355607177
H,6.2625677471,-0.4808017326,-1.4007534617
H,4.4960732889,-3.1417393699,1.4756227422
H,6.4758559496,-2.4120913052,0.1606691839
H,-0.6345561966,0.6688528806,-1.3982249702
C,0.0904364506,2.3841173465,-0.4116145559
O,0.8702529263,2.7480678512,-1.2738840762
O,-0.3429316097,3.138411535,0.5886344752
S,-2.078195512,0.8133064394,0.4801294899
O,-1.9291465821,0.8897200737,1.9346849506
O,-2.9057355972,1.7793543897,-0.2632354206
C,-2.6645466997,-0.8308525607,0.03712635
C,-3.6651373269,-3.3240226699,-0.6228700922
C,-3.3779508249,-0.9836296847,-1.154035148

C,-2.455084666,-1.8972864876,0.9128596505
C,-2.9630836846,-3.1502637226,0.5723108387
C,-3.8743831055,-2.2445330443,-1.4838730486
H,-3.5571920647,-0.123822521,-1.7902378847
H,-1.9012591516,-1.7377237111,1.829104645
H,-2.811272658,-3.9910992879,1.2418707861
H,-4.4325862466,-2.3803189206,-2.4050076122
H,-4.0568484559,-4.3035045506,-0.8811062883
C,0.1082360103,4.5093505829,0.5968834282
H,-0.3462485874,4.9531099118,1.4803764672
H,-0.225645202,5.0183494624,-0.3092326241
H,1.1977500875,4.5466976167,0.6562008312

PhNHCOCH(COMe)SO_2Ph
S,-1.5141509367,-1.7089786555,-0.462105786
O,-0.7144388051,-2.3131443631,0.6112896202
O,-2.8395335021,-2.2428867095,-0.8223446864
C,-1.8165359367,0.0842636237,-0.0120078752
C,-0.4935743903,0.8420701244,0.2094379012
O,-0.0479883703,1.5284111214,-0.7033868621
N,0.0811149032,0.639636801,1.4242375162
C,-0.5149378573,-1.6347792605,-1.9499918838
C,1.0194533593,-1.5365488339,-4.2463331517
C,0.8761521846,-1.624943826,-1.8339818999
C,-1.1544878103,-1.6065024568,-3.1907384347
C,-0.3738071827,-1.556271196,-4.3445157141
C,1.6426861541,-1.5743800218,-2.9971805861
H,1.34079269,-1.668937825,-0.8554860015
H,-2.2369261327,-1.6440992839,-3.2434166263
H,-0.8527068573,-1.5388306853,-5.3184219871
H,2.7256402557,-1.5666510996,-2.9268512545

H,1.6224929186,-1.4967236181,-5.1484195508
H,-0.4719392961,0.0804213135,2.0695201345
H,-2.2645883002,0.5085028874,-0.9119088384
C,-2.8222505028,0.0697927446,1.1529259359
O,-2.4457561096,-0.1062451171,2.2980494545
C,-4.2707014762,0.2527091542,0.7858839842
H,-4.8879836688,0.2142624959,1.6837899055
H,-4.5594793337,-0.543439246,0.0905975005
H,-4.4155453672,1.2092166669,0.2706964825
C,1.2928219426,1.1665118849,1.92079285
C,3.6713112499,2.1240443412,3.0552110388
C,2.1255827534,2.020475153,1.1817507826
C,1.6576135565,0.7964882241,3.2250083082
C,2.8382271853,1.2738149423,3.7851765337
C,3.3059282598,2.4888261055,1.7594124852
H,1.840507076,2.3055094655,0.1792387767
H,1.0129245529,0.1322913667,3.7946938623
H,3.1063939935,0.9784561235,4.7951930824
H,3.9450633324,3.1508950055,1.1822020026
H,4.5926151681,2.4967628529,3.4919827811

PhNHCOCH(SO_2Me)SO_2Ph
C,1.0411985911,-0.9831568546,0.5470198712
C,-0.3149153663,-1.0757673237,-0.1831324711
O,-0.3849177333,-1.2670847789,-1.3904046649
N,-1.3769669016,-0.9591160168,0.6639751445
H,-1.1474350798,-0.663869322,1.6091526292
C,-2.757755383,-0.9719840569,0.350341267
C,-5.5253528511,-0.9807494443,-0.0873498542
C,-3.2604470836,-1.2519614832,-0.9284832951
C,-3.6439615877,-0.6977786854,1.403736508

C,-5.0179187341,-0.7024158229,1.1830462826
C,-4.6408255143,-1.2527504055,-1.1309743085
H,-2.5782196032,-1.4563262386,-1.7406055804
H,-3.2526290597,-0.4831487034,2.3951626529
H,-5.6909023558,-0.4886426811,2.0078666608
H,-5.0241154736,-1.4696078141,-2.1237141112
H,-6.5968959274,-0.9855850251,-0.260295885
H,1.0645855134,-1.6388284242,1.4230026352
S,2.5296515823,-1.4996267228,-0.4583362165
O,2.8317270559,-0.4416499516,-1.4305094823
O,3.5247912086,-1.9295516306,0.5295152274
S,1.2878847509,0.6952479351,1.3589620467
O,0.2228529578,0.6914594153,2.3869606278
O,2.6928576583,0.826789032,1.7396839232
C,0.8797238561,1.9455416171,0.1404334793
C,0.2682295999,3.9382293093,-1.6720916771
C,-0.4089918582,2.4855210558,0.1368429915
C,1.8744913186,2.3899238978,-0.7340249869
C,1.5542315271,3.3937330229,-1.646157627
C,-0.7101045504,3.4886564755,-0.7830810244
H,-1.1479160866,2.1380555953,0.8489177165
H,2.8628920533,1.9494326151,-0.7060811724
H,2.3120864619,3.7502787287,-2.336155707
H,-1.7055638446,3.9206541271,-0.7999519631
H,0.0283619059,4.720235074,-2.3862993598
C,2.0048122164,-2.9741742567,-1.3592804537
H,1.2382948583,-2.7008132798,-2.0790276381
H,1.6506821806,-3.7207680769,-0.6466782119
H,2.9183869126,-3.3271111015,-1.8428455513

$PhNHCOCH(SO_2Ph)_2$

S,0.6790544679,1.5037033619,0.0269329836

S,1.5459153705,-1.4702496295,-0.7349249897

O,0.1690216968,2.0756249844,1.2908556372

O,1.1163598738,-2.8214643145,-0.3583619826

O,2.0443742555,1.7954409007,-0.4244948444

O,1.5059678635,-0.9917724904,-2.1220034117

C,0.5313446208,-0.3284100782,0.3407770234

H,0.972502025,-0.4143365273,1.3383209847

C,-0.953015843,-0.7535216134,0.3407926281

O,-1.4484689839,-1.338979588,-0.6047902417

N,-1.5980361455,-0.3791149622,1.4898953475

C,3.2216405934,-1.2668859071,-0.1080597408

C,5.8190065078,-1.0557151364,0.8210282148

C,3.620928851,-2.0485512667,0.9793130325

C,4.1012826598,-0.394734168,-0.7497378134

C,5.4086320497,-0.294367171,-0.2751249936

C,4.9292303634,-1.9323477149,1.4464974969

H,2.9251371408,-2.749243367,1.4278858167

H,3.7613087619,0.1911507792,-1.5937412697

H,6.1056030838,0.380011079,-0.7623754591

H,5.2558124735,-2.5337108469,2.2891146163

H,6.838309795,-0.9707516107,1.1857668621

C,-0.4781831944,1.9144785049,-1.278524541

C,-2.2540964079,2.6269827518,-3.2710707806

C,-1.6872937877,2.5170929263,-0.9241481702

C,-0.1339116745,1.6651582433,-2.6095504825

C,-1.0390355097,2.0247983197,-3.6061722937

C,-2.5773812265,2.8746597634,-1.9357301893

H,-1.9118111649,2.7079127961,0.1185615434

H,0.8052252293,1.1845149126,-2.8522398877

H,-0.7936646038,1.8322110374,-4.6455717699

H,-3.5207374987,3.3460703371,-1.6793233704
H,-2.9524603231,2.9042176155,-4.0550083767
H,-1.0879727961,0.2587368371,2.08986339
C,-2.9683847492,-0.535041769,1.8061966541
C,-5.648218468,-0.7739869195,2.5871324399
C,-3.8357176313,-1.3606516607,1.0763567077
C,-3.4465184278,0.1642335856,2.9248064397
C,-4.7782895536,0.0437858977,3.3103992067
C,-5.16756316,-1.4685203748,1.4768453282
H,-3.4676600058,-1.8958191404,0.2128347724
H,-2.7716945301,0.8028621378,3.4900303074
H,-5.1339576433,0.5913381897,4.1780732941
H,-5.8348118204,-2.1091275012,0.9077333426
H,-6.6871662388,-0.869024925,2.8868816127

PhNHCOCH(SO_2Me)$_2$
S,-0.8788306275,-2.6528217329,-0.2422435136
S,-2.2138800907,0.1818803662,-0.0897389021
O,-1.9834176652,1.4608701369,0.6202300351
O,-2.3303322379,0.1600941461,-1.5538512042
C,-0.7703646954,-0.896660727,0.3808374206
H,-0.8413603157,-1.0339301949,1.4657447697
C,0.6021490094,-0.2399998177,0.0350461774
O,1.4275786347,-0.8583193012,-0.6210111792
N,0.7775136222,0.991857643,0.5782544183
H,-0.0607899198,1.4333523392,0.9490255892
C,1.9174519274,1.8287342127,0.4830329999
C,4.0812130531,3.6054746909,0.4164642047
C,3.1619802755,1.3928210871,0.0074406722
C,1.7620693139,3.1516527447,0.9236289787
C,2.8388728064,4.0321653418,0.8891575753

C,4.2305626685,2.2893377114,-0.0202645083
H,3.2812596731,0.3757607819,-0.3365259067
H,0.7942845508,3.4873461603,1.2874112507
H,2.7036497373,5.0536304822,1.2316132489
H,5.192470672,1.946470782,-0.3898202975
H,4.9218371878,4.291651342,0.3887272064
O,0.1562906596,-3.3997729236,0.4738949973
O,-2.2939552881,-3.0338726079,-0.0761863502
C,-0.5342568665,-2.599666861,-2.007361613
H,0.5167871004,-2.3595416057,-2.1455453449
H,-1.1884570814,-1.8512217747,-2.4569080567
H,-0.7817508362,-3.6002380862,-2.3677761011
C,-3.6906388427,-0.53785311,0.6487477061
H,-3.5492525051,-0.5933552863,1.7285724005
H,-3.868353259,-1.5197261251,0.2177193099
H,-4.4830935923,0.1738323128,0.4067115822

PhNHCOCH(COMe)$SO_2C_4F_9$
S,1.9328843018,-0.4145899574,-0.9866196967
O,1.7091243916,-1.2957895675,-2.1274768513
O,3.1258276765,-0.5176991243,-0.1376462283
C,1.8388619752,1.3573151767,-1.5949449569
C,0.4472497888,1.6985589453,-2.1954754555
O,0.2105706506,1.3500818408,-3.3417127374
N,-0.3901424685,2.3587264607,-1.3532098269
C,2.4720590947,2.3222440304,-0.5717615674
O,1.7901958569,2.897361376,0.2584703361
C,3.9594063261,2.5225501899,-0.6811666295
C,0.4320919133,-0.6103763962,0.1748482736
C,0.5765562642,-1.8556501038,1.0957162215
C,-0.7704283956,-2.291974057,1.7426893505

C,-0.6174766219,-3.2807385753,2.9300876544
F,-1.824082054,-3.7585987869,3.2545122729
F,-0.6632205304,-0.7190493326,-0.5932771561
F,0.3512951732,0.4982782672,0.9351567077
F,1.0523872874,-2.8866987186,0.3638662163
F,1.4547525686,-1.5534242062,2.075649772
F,-1.5275650085,-2.8885747929,0.7986142396
F,-1.4110280441,-1.1889697924,2.2011165156
F,0.1765282681,-4.3018583562,2.5823723025
F,-0.0978330203,-2.6603124407,3.9939882351
C,-1.7084454105,2.803302289,-1.6043548007
C,-4.3266983995,3.7437127441,-1.9324685748
C,-2.3217083668,3.5611839697,-0.5948299934
C,-2.4097496569,2.5154822178,-2.7842394177
C,-3.7128989395,2.9905209966,-2.9333090756
C,-3.6224341957,4.0264938967,-0.7605839637
H,2.4946181513,1.2492696605,-2.4644622276
H,0.0192248421,2.6267134404,-0.4608060072
H,4.2113611811,2.9255634706,-1.6693211786
H,4.4661084392,1.5572243708,-0.579868803
H,4.2957095575,3.2094966171,0.0956610805
H,-5.3413675785,4.1067147877,-2.0627216219
H,-1.7756668446,3.7831492167,0.3186439546
H,-1.9344927437,1.9339601506,-3.5611218188
H,-4.2513697376,2.7642534162,-3.8489084308
H,-4.0844494363,4.6114942533,0.0289784963

PhNHCOCH(CN)SO_2Me
S,2.6464348547,-0.807473635,0.241655362
O,1.8047508967,-1.8337634287,-0.3810931143
O,3.9819763203,-0.4932384564,-0.2726457557

C,1.6628197943,0.8133348152,0.1795099784
C,0.2033439766,0.552085892,0.6246722071
O,-0.0066747013,0.3427792747,1.8135470794
N,-0.7167227312,0.5557938977,-0.3701364356
H,-0.3708560064,0.7303490197,-1.3054400576
H,2.1232571819,1.4606105958,0.9311713712
C,2.7608910253,-1.1316809253,2.0129025011
H,3.4208390987,-0.3883997088,2.461334045
H,3.1947891036,-2.1301147919,2.0948683038
H,1.76014173,-1.0917278209,2.4421970339
C,1.8276523207,1.3923737025,-1.1433698942
N,1.8821860737,1.8451645868,-2.2117294279
C,-2.1111196454,0.317440906,-0.2838330421
C,-4.8749089885,-0.1203231396,-0.2879862035
C,-2.7723301779,0.0412678977,0.9205650321
C,-2.8340693887,0.3729933588,-1.4841860482
C,-4.208054433,0.1541249676,-1.4832496448
C,-4.1504464315,-0.1742354858,0.9026462974
H,-2.2125550201,-0.0031593128,1.8434243721
H,-2.3182227944,0.5857345621,-2.4174406574
H,-4.75562747,0.1984733561,-2.4196056708
H,-4.6592805706,-0.3883855483,1.8377542221
H,-5.9467747605,-0.291022634,-0.286180486

PhNHCOCH(CN)SO_2Ph
S,2.3705029473,1.1779616138,-0.4938837958
O,1.7844290338,1.8924072197,0.6554818898
O,3.7156193109,1.4890069403,-0.9850646235
C,2.3790679875,-0.6435711243,-0.0259026058
C,0.9760050749,-1.2114933326,0.3428170931
O,0.5358659451,-2.1562717004,-0.2904643024

N,0.3821905898,-0.5752488014,1.3882579219
H,0.8564450255,0.2565423114,1.727222223
H,2.7020847315,-1.1773532388,-0.9227038052
C,3.3473809841,-0.8221199118,1.0470345831
N,4.0963882819,-0.9681483201,1.9221363115
C,-0.8809730338,-0.8368044132,1.9711733551
C,-3.3501254693,-1.2226054057,3.2337461061
C,-1.6911769059,-1.9188742235,1.5990635166
C,-1.3096151554,0.046865149,2.9731294413
C,-2.5372865344,-0.1478007565,3.5986604595
C,-2.9187284745,-2.098126651,2.2371858923
H,-1.3593311002,-2.5963563394,0.8254437644
H,-0.6774396714,0.8830872628,3.2613447734
H,-2.8560903028,0.5426885924,4.3735397437
H,-3.5423988845,-2.9383563559,1.9465259353
H,-4.3073948348,-1.375751193,3.721967395
C,1.2217797061,1.2460975975,-1.8672786115
C,-0.5348064312,1.3393979509,-3.9984428108
C,-0.1267969513,1.5130965064,-1.6209672003
C,1.7122023118,1.0368151709,-3.1587850056
C,0.8194056128,1.0838624593,-4.2279258319
C,-1.0062307741,1.5570960163,-2.7020597988
H,-0.4709343769,1.6947024782,-0.6093930694
H,2.7708239374,0.8621220843,-3.3167384131
H,1.1819215967,0.9273363722,-5.2387664304
H,-2.0574267177,1.7651265428,-2.5308991031
H,-1.2253575586,1.3746695995,-4.8354549974

PhNHCOCH($SO_2C_4F_9$)$_2$
S,0.2017621539,1.7078192436,0.6727392885
C,-0.459778414,-0.0076404181,1.0273153408

H,0.0316380447,-0.3047600367,1.9577768912
C,-2.0004937096,0.0778988763,1.2113285186
O,-2.6459596337,0.9404289055,0.6443523805
N,-2.4764939532,-0.8870268599,2.0468087336
H,-1.8217778152,-1.6124868266,2.312898937
C,-3.8272455412,-1.1441006479,2.3966349525
C,-6.4324775328,-1.7763868904,3.1945594828
C,-4.0822090089,-2.3297494776,3.1002671056
C,-4.8777859287,-0.2681568291,2.0920802181
C,-6.1717547271,-0.5978022801,2.4957173542
C,-5.3792947562,-2.6416886423,3.4957300723
H,-3.264413765,-3.007214255,3.3341628721
H,-4.6799797242,0.6443667149,1.5485565331
H,-6.9836085688,0.0826779584,2.257421133
H,-5.5642876955,-3.563315626,4.0388293147
H,-7.444654209,-2.0188984631,3.5022335597
S,0.0632822307,-1.4097400318,-0.0757715569
O,1.404667361,-1.1593965951,-0.5959980167
O,-0.2639024489,-2.6052392755,0.7116548871
C,-1.1584804685,-1.3420511191,-1.5493536134
C,-0.6205559355,-2.1658087079,-2.7531135123
C,-1.7180150129,-2.4931342773,-3.8069808437
C,-1.162947389,-2.9929903708,-5.1684857645
F,-1.3195782013,-0.0639505608,-1.8958637788
F,-2.3212171933,-1.8543619406,-1.1099426463
F,-0.1164339791,-3.3299912707,-2.2819909269
F,0.3596887863,-1.4537417993,-3.3438239951
F,-2.4470020269,-1.3756866878,-4.0365112656
F,-2.5207594043,-3.4554934069,-3.3048840003
F,-0.5677319101,-1.9955082417,-5.8279004428
F,-2.1780947197,-3.4568398824,-5.905475493

F,-0.2798317498,-3.9812029673,-4.9709959047
O,0.1036797794,2.0496349021,-0.7394218535
C,2.081249251,1.485083204,1.0489862489
C,2.6621393539,2.7424126781,1.7533287754
C,4.2195404655,2.7714836119,1.7671475972
C,4.8278737379,3.8057288256,2.7530800011
F,4.2617902605,5.0060373838,2.5731095125
F,6.1415737871,3.904603617,2.5209114028
F,4.6779609548,1.5455517776,2.1182335932
F,2.2218036349,0.4120493538,1.8600647451
F,2.715309069,1.2795007067,-0.1064153519
F,4.6565120498,3.072719863,0.5266815582
F,2.2254074852,3.8394351964,1.0960926763
F,4.6408286235,3.4153699676,4.0180428851
F,2.2180159226,2.7617721857,3.0285094148
O,-0.334851002,2.5306466013,1.754280912

2,4-$MeO_2C_6H_3NHCOCH(SO_2Ph)_2$
S,2.5368517776,0.6829905113,-1.6255447292
O,2.2139535999,1.4451587386,-0.4079905177
O,3.9243835532,0.5555925136,-2.0964227265
C,1.9052574109,-1.0567664848,-1.4300674761
C,0.4450508325,-1.1439692519,-0.9252348775
O,-0.4036866412,-1.6441272496,-1.653922831
N,0.2374203768,-0.6519281394,0.3235365935
H,1.0232784787,-0.2064944036,0.7866269872
H,1.9005518505,-1.4744611794,-2.4362046005
C,1.5361035394,1.3266092112,-2.9713731043
C,-0.0032476382,2.3048607329,-5.0496037938
C,0.3382990029,1.9805081416,-2.6774030776

C,1.9845177829,1.1609867021,-4.2833567977
C,1.2027630054,1.6562915044,-5.3259523366
C,-0.4331284149,2.4694448274,-3.7311886452
H,0.0308623994,2.1117673281,-1.6460761613
H,2.9329040966,0.6701078704,-4.4730038941
H,1.5373507096,1.5402028574,-6.3520085516
H,-1.3671776561,2.9809498447,-3.5215159219
H,-0.6084844343,2.6878852168,-5.8657283632
C,-0.9819573146,-0.5903550318,1.0313016094
C,-3.304991924,-0.3661177171,2.5959707742
C,-0.9381683075,0.0292283602,2.305863354
C,-2.1983662365,-1.0902322632,0.5718190767
C,-3.3597286728,-0.9820156656,1.3464821396
C,-2.0865281796,0.1417014405,3.0765504231
H,-2.2319319355,-1.5623734525,-0.399680644
H,-4.2867970017,-1.3820572837,0.9560551731
H,-2.0766541215,0.6115694018,4.051385039
O,0.2951571046,0.482960411,2.682347719
O,-4.369624435,-0.2006195415,3.4369386296
C,0.4154707616,1.1916969763,3.9073227289
H,-0.2203247871,2.0849849133,3.9147095391
H,1.4615437028,1.4908607893,3.9789508396
H,0.1569700819,0.5570120287,4.7637752937
C,-5.632266279,-0.691647413,3.0152226907
H,-5.9693586829,-0.2018809488,2.0927257421
H,-6.3303920764,-0.4595934244,3.8208208773
H,-5.612000235,-1.7772960427,2.856243517
C,2.9110610774,-1.8685996595,-0.6168764637
O,3.4518050998,-2.866488267,-1.0279964036
O,3.0974869201,-1.3420145765,0.6063117079
C,4.0479903681,-2.0325726181,1.4415339985

H,5.0278696521,-2.0486042383,0.9605233354
H,3.7174196063,-3.057374541,1.6236580298
H,4.0824883831,-1.4657806282,2.3704761986

2,4-$MeO_2C_6H_3NHCOCH(CO_2Me)SO_2Ph$
S,0.8124393096,1.951459344,-1.651014153
O,-0.5307935454,2.460895463,-1.9588675938
O,1.5778752554,2.4555004472,-0.5019261369
C,0.5521282957,0.1195165879,-1.3898481274
C,-0.6927807377,-0.1186456903,-0.507326292
O,-1.6356225274,-0.746078609,-0.97305248
N,-0.6052099383,0.4030544166,0.7415082303
H,0.2654837326,0.8545220105,1.0094353512
H,0.3255700426,-0.3027072915,-2.3700943451
C,1.8025389697,2.1214746805,-3.1390218216
C,3.2893459324,2.4822164737,-5.4400733932
C,1.1454633624,2.1593880184,-4.3710538839
C,3.1855462219,2.2714997102,-3.0320880527
C,3.9274557184,2.4546745121,-4.1979642718
C,1.9028790121,2.3363033918,-5.5281101363
H,0.0649358882,2.0764118924,-4.4122879614
H,3.6605275083,2.2426529179,-2.059364489
H,5.0042370571,2.5750073236,-4.1348772678
H,1.4096596411,2.3713044891,-6.4944477272
H,3.8746119679,2.6241631651,-6.3437785163
C,-1.5859144572,0.3693581711,1.7563331621
C,-3.3999659346,0.4217726721,3.8978033167
C,-1.2344761243,0.984242734,2.9846871597
C,-2.8469343801,-0.2076780128,1.6299885863
C,-3.7564955102,-0.1855225559,2.6943363943
C,-2.1321356806,1.0091710987,4.0424719045

H,-3.1144406858,-0.6732355629,0.6921668721
H,-4.7291059733,-0.6417158984,2.5605147385
H,-1.8869815489,1.4738896985,4.9886204515
O,0.0183915698,1.5224805394,3.0155011739
O,-4.2012430369,0.5036834554,5.0021303276
C,0.4467032955,2.1990501073,4.188587366
H,-0.2044601532,3.0515854725,4.4155854219
H,1.4541929894,2.5563354744,3.9751668208
H,0.4734010232,1.5227160382,5.0515495971
C,-5.501128823,-0.058897147,4.9235811592
H,-6.10347263,0.4211820528,4.1419088073
H,-5.965616726,0.1184385795,5.8947312203
H,-5.4641990919,-1.1391698658,4.7330089819
S,2.0707376831,-0.7675026504,-0.7822064037
O,3.1403651092,-0.4982270519,-1.7557023931
O,2.2442608242,-0.4676335863,0.6451529184
C,1.5923101926,-2.4911801469,-0.9433662556
C,0.8602717273,-5.1452289632,-1.1943743273
C,1.8613581719,-3.1581635248,-2.1404369713
C,0.9742042852,-3.1278992399,0.1344943989
C,0.6066981682,-4.4660144041,-0.0008306525
C,1.4888120203,-4.4960749099,-2.259865664
H,2.3682194918,-2.6392756074,-2.9467386213
H,0.7998079499,-2.5860572544,1.0571905534
H,0.1252570522,-4.9774441636,0.826543289
H,1.6939647428,-5.0323675871,-3.181018245
H,0.5713293927,-6.1872313146,-1.2932624194

Table S5. Cartesian Coordinates of Transition Structure of **7o** <->**6o** Calculated at the B3LYP/6-31+G*

N,0.2765670673,-0.088460498,1.8632833036
H,0.0791673321,0.7945487154,1.3923166601
S,1.3956730667,0.982884505,-0.854372028
O,0.6044435998,1.8860640146,0.0080126509
O,2.4532515209,1.5136725396,-1.7118411679
C,1.2609187615,-0.8037475341,1.3036298631
C,1.940891612,-0.3977061337,0.0722065692
C,3.0321715776,-1.2138937453,-0.3906578489
C,3.878338207,-0.939878179,-1.6072242095
H,3.2819151204,-0.7948270035,-2.5103988554
H,4.5473542779,-1.7929955103,-1.7351883071
H,4.4664642284,-0.0278500467,-1.4676070536
O,3.3513012813,-2.2504179773,0.2780442659
H,2.5050683935,-2.2669155289,1.2397220833
O,1.6503459092,-1.8940669312,1.8786922502
C,0.0820386721,0.2343789287,-2.0401969529
C,-0.8077743879,1.293177098,-2.7662473094
C,-1.5761553357,0.7347427222,-4.0132634371
C,-2.7357779816,1.6430673094,-4.5385035198
F,-3.1749635822,1.1475313657,-5.7054730267
F,-2.3034117839,2.8973050095,-4.7379036768
F,-3.7589654177,1.6656014464,-3.6741890447
F,-2.1163939463,-0.4704030449,-3.7006452835
F,-0.6969902367,0.5703507899,-5.0279878874
F,-0.0249351977,2.3162393186,-3.1797047965
F,-1.7153917925,1.764828647,-1.8773647416
F,-0.708093893,-0.5774765393,-1.3006966404
F,0.7396990662,-0.5196678074,-2.9519311361
C,-0.4934979993,-0.3331516542,3.0313015938
C,-2.1376090085,-0.6065052159,5.2893154694
C,-0.4127703415,-1.4923204887,3.8172438094
C,-1.3989697033,0.6835775295,3.3805494043

C,-2.2131161729,0.5462548478,4.5019109675

C,-1.2382973344,-1.6148605673,4.9382629146

H,0.2788790059,-2.2816615801,3.5624265927

H,-1.4633275339,1.5819520074,2.7705835359

H,-2.9065544253,1.3426475549,4.757860855

H,-1.1695096756,-2.5161362345,5.5416492305

H,-2.7719826495,-0.715882129,6.1643848039

Table S6. Electronic Energies, Enthalpies, Free Energies, and Entropies of Amides and Enols Calculated at B3LYP/6-31+G* in Hartrees (S in e.u.)

Amide	E	H	G	S
i-PrNHCOCH(SO2Ph)2	-1886.421353	-1886.054500	-1886.138113	175.98
i-PrNHCOCH(SO2Me)2	-1502.950568	-1502.695938	-1502.762640	140.39
i-PrNHCOCH(SO2C4F9)2	-3525.111999	-3524.811238	-3524.929786	249.51
i-PrNHCOCH(CO2Me)SO2Ph	-1334.678637	-1334.362678	-1334.436784	155.97
i-PrNHCOCH(CO2Me)SO2Ph	-1334.678637	-1334.362678	-1334.436784	155.97
i-PrNHCOCH(COMe)SO2Ph	-1259.445476	-1259.136261	-1259.207745	150.45
i-PrNHCOCH(COMe)SO2Ph	-1259.445476	-1259.136261	-1259.207745	150.45
i-PrNHCOCH(COMe)SO2Ph	-1259.443291	-1259.134397	-1259.206246	151.22
i-PrNHCOCH(COMe)SO2C4F9	-2078.797011	-2078.520877	-2078.611242	190.19
i-PrNHCOCH(COMe)SO2C4F9	-2078.797011	-2078.520877	-2078.611242	190.19
i-PrNHCOCH(SO2Me)SO2Ph	-1694.681108	-1694.370258	-1694.444781	156.85
i-PrNHCOCH(CN)SO2Me	-1007.292856	-1007.080564	-1007.139900	124.88
i-PrNHCOCH(CN)SO2Me	-1007.292856	-1007.080564	-1007.139900	124.88
i-PrNHCOCH(CN)SO2Ph	-1199.031138	-1198.762700	-1198.830634	142.98
t-BuNHCOCH(CO2Me)SO2Ph	-1373.995237	-1373.650285	-1373.726864	161.17
PhNHCOCH(SO2Ph)2	-1999.532213	-1999.168766	-1999.253813	179.00
PhNHCOCH(SO2Me)2	-1616.060946	-1615.809748	-1615.876954	141.45
PhNHCOCH(SO2C4F9)2	-3638.226632	-3637.929279	-3638.051011	256.21
PhNHCOCH(CO2Me)SO2Ph	-1447.784829	-1447.472591	-1447.548243	159.22
PhNHCOCH(CO2Me)SO2Ph	-1447.784829	-1447.472591	-1447.548243	159.22
PhNHCOCH(COMe)SO2Ph	-1372.561655	-1372.256093	-1372.329115	153.69
PhNHCOCH(COMe)SO2Ph	-1372.561655	-1372.256093	-1372.329115	153.69
PhNHCOCH(COMe)SO2C4F9	-2191.906983	-2191.634464	-2191.725420	191.43
PhNHCOCH(COMe)SO2C4F9	-2191.906983	-2191.634464	-2191.725420	191.43
PhNHCOCH(SO2Me)SO2Ph	-1807.793238	-1807.485805	-1807.561080	158.43
PhNHCOCH(SO2Me)SO2Ph	-1807.793238	-1807.485805	-1807.561080	158.43
PhNHCOCH(CN)SO2Me	-1120.406135	-1120.197417	-1120.258654	128.88
PhNHCOCH(CN)SO2Me	-1120.406135	-1120.197417	-1120.258654	128.88
PhNHCOCH(CN)SO2Ph	-1312.146307	-1311.881384	-1311.950647	145.78
2,4-(MeO)2PhNHCOCH(SO2Ph)2	-2228.591327	-2228.157181	-2228.253963	203.70
2,4-(MeO)2PhNHCOCH(CO2Me)SO2Ph	-1676.844855	-1676.461991	-1676.550141	185.53
MeSO2CH(CONH2)2	-965.826717	-965.673499	-965.724536	107.42
MeSO2CH(CONH2)2	-965.826717	-965.673499	-965.724536	107.42
i-PrNHCOCH(CO2Me)2	-782.929507	-782.665171	-782.732332	141.35
i-PrNHCOCH(CO2Me)CO2CH2CF3	-1119.986202	-1119.713606	-1119.790279	161.37
i-PrNHCOCH(CO2CH2CF3)2	-1457.041842	-1456.761237	-1456.847648	181.87

i-PrNHCOCH(CN)CO2Me	-647.285286	-647.068163	-647.128013	125.97
i-PrNHCOCH(CN)CO2CH2CF3	-984.339491	-984.114239	-984.184164	147.17
i-PrNHCOCH(CN)CO2CH(CF3)2	-1321.384555	-1321.151771	-1321.231223	167.22
i-PrNHCOCH(CN)2	-511.634806	-511.465209	-511.518005	111.12
PhNHCOCH(CO2Me)2	-896.042129	-895.781124	-895.848959	142.77
PhNHCOCH(CO2Me)CO2CH2CF3	-1233.098506	-1232.829418	-1232.907254	163.82
PhNHCOCH(CO2CH2CF3)2	-1570.153467	-1569.876189	-1569.963952	184.71
PhNHCOCH(CN)CO2Me	-760.396562	-760.182812	-760.243760	128.28
PhNHCOCH(CN)CO2CH2CF3	-1097.450369	-1097.228470	-1097.298805	148.03
PhNHCOCH(CN)CO2CH(CF3)2	-1434.494669	-1434.265309	-1434.345408	168.58
PhNHCOCH(CN)2	-624.744480	-624.578311	-624.632566	114.19
i-PrNHCOMe	-327.172070	-327.003171	-327.047202	92.67
t-BuNHCOMe	-366.489899	-366.292073	-366.338406	97.52
PhNHCOCH3	-440.281036	-440.115437	-440.162059	98.13
24MeO2PhNHCOMe	-669.337045	-669.100703	-669.157858	120.29
H2NCOCH3	-209.178468	-209.147192	-209.181749	72.73
H2NCOCH2SO2Ph	-988.835113	-988.682599	-988.735358	111.04
H2NCOCH2SO2Me	-797.096262	-796.997988	-797.042316	93.30
H2NCOCH2SO2C4F9	-1808.196074	-1808.067576	-1808.139655	151.71
H2NCOCH2CO2Me	-437.095581	-436.970673	-437.015264	93.85
H2NCOCH2CO2CH2CF3	-774.154877	-774.016857	-774.071547	115.10
H2NCOCH2CN	-301.434697	-301.385952	-301.423583	79.20
Enol				
i-PrNHC(OH)=C(SO2Ph)2	-1886.416371	-1886.049075	-1886.130155	170.65
i-PrNHC(OH)=C(SO2Me)2	-1502.944223	-1502.689076	-1502.752951	134.44
i-PrNHC(OH)=C(SO2C4F9)2	-3525.127131	-3524.825490	-3524.943899	249.21
i-PrNHC(OH)=C(CO2Me)SO2Ph	-1334.677255	-1334.361661	-1334.433895	152.03
i-PrNHCOCH(SO2Ph)=C(OH)OMe	-1334.677255	-1334.361662	-1334.433877	151.99
i-PrNHC(OH)=C(COMe)SO2Ph	-1259.448128	-1259.139976	-1259.210000	147.38
i-PrNHCOCH(SO2Ph)=C(OH)Me	-1259.450468	-1259.141367	-1259.211337	147.26
i-PrNHCOCH(SO2Ph)=C(OH)Me	-1259.450468	-1259.141367	-1259.211337	147.26
i-PrNHC(OH)=C(COMe)SO2C4F9	-2078.808853	-2078.533293	-2078.620070	182.64
i-PrNHCOCH(SO2C4F9)=C(OH)Me	-2078.810007	-2078.533907	-2078.621046	183.40
i-PrNHC(OH)=C(SO2Me)SO2Ph[a]	-1694.680378	-1694.369206	-1694.441806	152.80
i-PrNHC(OH)=C(SO2Me)SO2Ph[b]	-1694.680282	-1694.368995	-1694.441295	152.2
i-PrNHC(OH)=C(CN)SO2Me	-1007.290577	-1007.078135	-1007.136912	123.71
i-PrNHCOC(CN)=S(OH)OMe	-1007.290578	-1007.078135	-1007.136906	123.69
i-PrNHC(OH)=C(CN)SO2Ph	-1199.029537	-1198.760889	-1198.828209	141.69
t-BuNHC(OH)=C(CO2Me)SO2Ph	-1373.989606	-1373.644953	-1373.719048	155.95

PhNHC(OH)=C(SO2Ph)2	-1999.526128	-1999.162463	-1999.245588	174.95
PhNHC(OH)=C(SO2Me)2	-1616.053358	-1615.801725	-1615.867199	137.80
PhNHC(OH)=C(SO2C4F9)2	-3638.234392	-3637.936292	-3638.056741	253.51
PhNHC(OH)=C(CO2Me)SO2Ph	-1447.787093	-1447.475100	-1447.549073	155.69
PhNHCOCH(SO2Ph)=C(OH)OMe	-1447.782272	-1447.471912	-1447.545416	154.70
PhNHC(OH)=C(COMe)SO2Ph	-1372.558141	-1372.254119	-1372.325011	149.21
PhNHCOCH(SO2Ph)=C(OH)Me	-1372.562090	-1372.256191	-1372.326920	148.86
PhNHC(OH)=C(COMe)SO2C4F9	-2191.917154	-2191.645796	-2191.735086	187.93
PhNHCOCH(SO2C4F9)=C(OH)Me	-2191.920156	-2191.647245	-2191.736182	187.18
PhNHC(OH)=C(SO2Me)SO2Ph[a]	-1807.789730	-1807.482173	-1807.556310	156.04
PhNHC(OH)=C(SO2Me)SO2Ph[b]	-1807.789605	-1807.481860	-1807.555683	155.37
PhNHC(OH)=C(CN)SO2Me	-1120.399164	-1120.190071	-1120.250199	126.55
PhNHCOC(CN)=S(OH)OMe	-1120.399164	-1120.190071	-1120.250198	126.55
PhNHC(OH)=C(CN)SO2Ph	-1312.138273	-1311.873027	-1311.942606	146.44
2,4-(MeO)2PhNHC(OH)C(SO2Ph)2	-2228.578915	-2228.144540	-2228.239841	200.58
2,4-(MeO2)PhNHC(OH)= C(CO2Me)SO2Ph	-1676.839393	-1676.456875	-1676.542755	180.75
MeSO2CH(CONH2)2/CO	-965.829371	-965.676686	-965.725804	103.38
MeSO2CH(CONH2)2/SO	-965.825257	-965.671961	-965.721024	103.26
i-PrNHC(OH)=C(CO2Me)2	-782.933353	-782.669513	-782.732399	132.36
i-PrNHC(OH)=C(CO2Me)CO2CH2CF3	-1119.992974	-1119.720911	-1119.793755	153.31
i-PrNHC(OH)=C(CO2CH2CF3)2	-1457.050024	-1456.769519	-1456.851684	172.93
i-PrNHC(OH)=C(CN)CO2Me	-647.292305	-647.075229	-647.132258	120.03
i-PrNHC(OH)=C(CN)CO2CH2CF3	-984.349221	-984.123819	-984.190767	140.90
i-PrNHC(OH)=C(CN)CO2CH(CF3)2	-1321.396150	-1321.163030	-1321.238207	158.22
i-PrNHC(OH)=C(CN)2	-511.631022	-511.460900	-511.512540	108.69
PhNHC(OH)=C(CO2Me)2	-896.043857	-895.783628	-895.848703	136.96
PhNHC(OH)=C(CO2Me)CO2CH2CF3	-1233.102860	-1232.834395	-1232.908865	156.74
PhNHC(OH)=C(CO2CH2CF3)2	-1570.159431	-1569.882556	-1569.965709	175.01
PhNHC(OH)=C(CN)CO2Me-2	-760.401393	-760.187775	-760.246414	123.42
PhNHC(OH)=C(CN)CO2CH2CF3	-1097.457766	-1097.235708	-1097.304721	145.25
PhNHC(OH)=C(CN)CO2CH(CF3)2	-1434.504406	-1434.274732	-1434.351599	161.78
PhNHC(OH)=C(CN)2	-624.739261	-624.572655	-624.626725	113.80
i-PrNHC(OH)=CH2	-327.121534	-326.953439	-326.996185	89.97
t-BuNHC(OH)=CH2	-366.433815	-366.235891	-366.280925	94.78
PhNHC(OH)=CH2	-440.234398	-440.069955	-440.115032	94.87
2,4-(MeO)2PhNHCOH=CH2	-669.285776	-669.050665	-669.107287	119.17
H2NC(OH)=CH2	-209.226954	-209.099106	-209.131052	67.24
H2NC(OH)=CHSO2Ph	-988.861875	-988.656272	-988.708646	110.23
H2NC(OH)=CHSO2Me	-797.120967	-796.973588	-797.016944	91.25
H2NC(OH)=CHSO2C4F9	-1808.213821	-1808.050183	-1808.121123	149.31

H2NC(OH)=CHCO2Me	-437.098164	-436.968231	-437.010529	89.02
H2NC(OH)=CHCO2CH2CF3	-774.152777	-774.019341	-774.071877	110.57
H2NC(OH)=CHCN	-301.466318	-301.354437	-301.390928	76.80
TS of Enol 7o Enol 6o				
	-2191.917068	-2191.648072	-2191.736637	186.40

[a] hydrogen-bonding with an oxygen atom of the SO_2Me group.

[b] hydrogen-bonding with an oxygen atom of the SO_2Ph group.

Table S7. Electronic Energies, Enthalpies, Free Energies, and Entropies of Amides and Enols Calculated at B3LYP/6-31G** in Hartrees (S in e.u.)

Amide	E	H	G	S
i-PrNHCOCH(SO2Ph)2	-1886.408798	-1886.041714	-1886.124734	174.73
i-PrNHCOCH(SO2Me)2	-1502.943700	-1502.688917	-1502.754668	138.38
i-PrNHCOCH(SO2C4F9)2	-3524.983982	-3524.681250	-3524.798443	246.65
i-PrNHCOCH(CO2Me)SO2Ph	-1334.669048	-1334.352898	-1334.425920	153.69
i-PrNHCOCH(COMe)SO2Ph	-1259.438885	-1259.129563	-1259.200396	149.08
i-PrNHCOCH(COMe)SO2C4F9	-2078.731240	-2078.454037	-2078.543478	188.25
i-PrNHCOCH(SO2Me)SO2Ph	-1694.671789	-1694.360876	-1694.436186	158.50
i-PrNHCOCH(CN)SO2Me	-1007.286144	-1007.073842	-1007.132702	123.88
i-PrNHCOCH(CN)SO2Ph	-1199.022079	-1198.753468	-1198.820741	141.59
t-BuNHCOCH(CO2Me)SO2Ph	-1373.987501	-1373.642515	-1373.718466	159.85
PhNHCOCH(SO2Ph)2	-1999.514055	-1999.150298	-1999.234195	176.57
PhNHCOCH(SO2Me)2	-1616.048377	-1615.796987	-1615.863849	140.72
PhNHCOCH(SO2C4F9)2	-3638.091381	-3637.791875	-3637.911846	252.50
PhNHCOCH(CO2Me)SO2Ph	-1447.769248	-1447.456882	-1447.532275	158.68
PhNHCOCH(COMe)SO2Ph	-1372.548442	-1372.242645	-1372.315330	152.98
PhNHCOCH(COMe)SO2C4F9	-2191.835437	-2191.561848	-2191.651597	188.89
PhNHCOCH(SO2Me)SO2Ph	-1807.777788	-1807.470133	-1807.545136	157.86
PhNHCOCH(CN)SO2Me	-1120.393000	-1120.184160	-1120.245024	128.10
2,4MeO2PhNHCOCH(SO2Ph)2	-2228.569349	-2228.135049	-2228.231637	203.29
2,4MeO2PhNHCOCH(CO2Me)SO2Ph	-1676.824691	-1676.441780	-1676.529851	185.36
MeSO2CH(CONH2)2	-965.816882	-965.663302	-965.713843	106.37
i-PrNHCOCH(CO2Me)2	-782.919797	-782.655565	-782.723203	142.36
i-PrNHCOCH(CO2Me)CO2CH2CF3	-1119.952406	-1119.679517	-1119.756454	161.93
i-PrNHCOCH(CO2CH2CF3)2	-1456.984352	-1456.703065	-1456.787765	178.27
i-PrNHCOCH(CN)CO2Me	-647.277458	-647.060373	-647.120148	125.81
i-PrNHCOCH(CN)CO2CH2CF3	-984.307843	-984.082189	-984.151553	145.99

i-PrNHCOCH(CN)CO2CH(CF3)2	-1321.333445	-1321.099845	-1321.179912	168.51
i-PrNHCOCH(CN)2	-511.628349	-511.458794	-511.511701	111.35
PhNHCOCH(CO2Me)2	-896.027288	-895.766298	-895.834421	143.38
PhNHCOCH(CO2Me)CO2CH2CF3	-1233.059308	-1232.789908	-1232.866363	160.91
PhNHCOCH(CO2CH2CF3)2	-1570.090539	-1569.812320	-1569.898481	181.34
PhNHCOCH(CN)CO2Me	-760.383401	-760.169567	-760.230122	127.45
PhNHCOCH(CN)CO2CH2CF3	-1097.413431	-1097.191038	-1097.260865	146.96
PhNHCOCH(CN)CO2CH(CF3)2	-1434.437894	-1434.207780	-1434.287059	166.86
PhNHCOCH(CN)2	-624.732773	-624.566516	-624.620681	114.00
i-PrNHCOMe	-327.173930	-327.005129	-327.049544	93.48
t-BuNHCOMe	-366.489899	-366.292781	-366.336758	92.56
PhNHCOCH3	-440.283079	-440.118687	-440.164084	98.13
2,4-(MeO)2PhNHCOMe	-669.330850	-669.094678	-669.152105	120.87
H2NCOCH3	-209.223224	-209.143455	-209.178516	73.79
H2NCOCH2SO2Ph	-988.850764	-988.671344	-988.724044	110.92
H2NCOCH2SO2Me	-797.112076	-796.988987	-797.033141	92.93
H2NCOCH2SO2C4F9	-1808.142516	-1807.995238	-1808.066802	150.62
H2NCOCH2CO2Me	-437.088804	-436.961283	-437.005386	92.82
H2NCOCH2CO2CH2CF3	-774.119428	-773.982965	-774.036171	111.98
H2NCOCH2CN	-301.458601	-301.378193	-301.415864	79.29
Enol				
i-PrNHC(OH)=C(SO2Ph)2	-1886.410206	-1886.042784	-1886.123485	169.85
i-PrNHC(OH)=C(SO2Me)2	-1502.942433	-1502.687262	-1502.750943	134.03
i-PrNHC(OH)=C(SO2C4F9)2	-3524.998750	-3524.695268	-3524.812879	247.53
i-PrNHC(OH)=C(CO2Me)SO2Ph	-1334.673003	-1334.357541	-1334.429180	150.78
i-PrNHC(OH)=C(COMe)SO2Ph/CO	-1259.447836	-1259.140620	-1259.209630	145.24
i-PrNHCOCH(COH=CH2)SO2Ph	-1259.449506	-1259.140707	-1259.209486	144.76
i-PrNHC(OH)=C(COMe)SO2C4F9	-2078.747069	-2078.471291	-2078.557905	182.30
i-PrNHCOCH(COH=CH2)SO2C4F9	-2078.747764	-2078.471265	-2078.558255	183.09
i-PrNHC(OH)=C(SO2Me)SO2Ph[a]	-1694.676470	-1694.365102	-1694.437364	152.09
i-PrNHC(OH)=C(SO2Me)SO2Ph[b]	-1694.675930	-1694.364580	-1694.436686	151.76
i-PrNHC(OH)=C(CN)SO2Me	-1007.288298	-1007.075856	-1007.134543	123.52
i-PrNHCOC(CN)=S(OH)OMe	-1007.288298	-1007.075855	-1007.134532	123.50
i-PrNHC(OH)=C(CN)SO2Ph	-1199.024996	-1198.756255	-1198.823184	140.86
t-BuNHC(OH)=C(CO2Me)SO2Ph	-1373.987869	-1373.643475	-1373.717218	155.21
PhNHC(OH)=C(SO2Ph)2	-1999.513578	-1999.149758	-1999.232748	174.67
PhNHC(OH)=C(SO2Me)2	-1616.045561	-1615.793921	-1615.859641	138.32
PhNHC(OH)=C(SO2C4F9)2	-3638.100111	-3637.800131	-3637.919156	250.51
PhNHC(OH)=C(CO2Me)SO2Ph	-1447.777017	-1447.465198	-1447.538813	154.94

PhNHCOCH(SO2Ph)=C(OH)OMe[c]	-1447.777017	-1447.465201	-1447.538796	154.89
PhNHC(OH)=C(COMe)SO2Ph	-1372.554805	-1372.249168	-1372.319886	148.84
PhNHCOCH(SO2Ph)=C(OH)OMe[c]	-1372.554805	-1372.249178	-1372.319878	148.80
PhNHC(OH)=C(COMe)SO2C4F9	-2191.851887	-2191.578485	-2191.667288	186.90
PhNHCOCH(COH=CH2)SO2C4F9	-2191.851906	-2191.578459	-2191.667066	186.49
PhNHC(OH)=C(SO2Me)SO2Ph	-1807.779736	-1807.472010	-1807.545723	155.14
PhNHC(OH)=C(SO2Me)SO2Ph	-1807.779385	-1807.471519	-1807.545475	155.65
PhNHC(OH)=C(CN)SO2Me	-1120.391063	-1120.181968	-1120.242737	127.90
PhNHCOC(CN)=S(OH)OMe	-1120.391062	-1120.181974	-1120.243421	129.33
PhNHC(OH)=C(CN)SO2Ph	-1312.127978	-1311.862634	-1311.931334	144.59
2,4-(MeO)2PhNHC(OH)C(SO2Ph)2	-2228.564226	-2228.129864	-2228.223393	196.85
2,4-(MeO)2PhNHC(OH)=C(CO2Me)SO2Ph	-1676.826562	-1676.444342	-1676.530286	180.89
MeSO2CH(CONH2)2/CO	-965.825077	-965.672569	-965.721570	103.13
MeSO2CH(CONH2)2/SO	-965.820186	-965.666633	-965.715450	102.74
i-PrNHC(OH)=C(CO2Me)2	-782.931002	-782.667604	-782.730176	131.70
i-PrNHC(OH)=C(CO2Me)CO2CH2CF3	-1119.964960	-1119.692982	-1119.766264	154.23
i-PrNHC(OH)=C(CO2CH2CF3)2	-1456.998146	-1456.717228	-1456.798732	171.54
i-PrNHC(OH)=C(CN)CO2Me	-647.289826	-647.072990	-647.130142	120.29
i-PrNHC(OH)=C(CN)CO2CH2CF3	-984.322408	-984.096785	-984.163152	139.68
i-PrNHC(OH)=C(CN)CO2CH(CF3)2	-1321.349346	-1321.115626	-1321.191030	158.70
i-PrNHC(OH)=C(CN)2	-511.628957	-511.458621	-511.510272	108.71
PhNHC(OH)=C(CO2Me)2	-896.035867	-895.776120	-895.841127	136.82
PhNHC(OH)=C(CO2Me)CO2CH2CF3	-1233.069331	-1232.800974	-1232.876298	158.53
PhNHC(OH)=C(CO2CH2CF3)2	-1570.101607	-1569.824516	-1569.908980	177.77
PhNHC(OH)=C(CN)CO2Me	-760.393479	-760.180106	-760.238898	123.74
PhNHC(OH)=C(CN)CO2CH2CF3	-1097.424491	-1097.202451	-1097.271472	145.27
PhNHC(OH)=C(CN)CO2CH(CF3)2	-1434.452098	-1434.221783	-1434.298844	162.19
PhNHC(OH)=C(CN)2	-624.731543	-624.564624	-624.618132	112.62
i-PrNHC(OH)=CH2	-327.125768	-326.957297	-326.999507	88.84
t-BuNHC(OH)=CH2	-366.440103	-366.243595	-366.288250	93.98
PhNHC(OH)=CH2	-440.233716	-440.068885	-440.113690	94.30
24MeO2PhNHCOH=CH2	-669.284158	-669.046667	-669.103136	118.85
H2NC(OH)=CH2	-209.178191	-209.098541	-209.130446	67.15
H2NC(OH)=CHSO2Ph	-988.829087	-988.650010	-988.702402	110.27
H2NC(OH)=CHSO2Me	-797.092392	-796.969508	-797.012729	90.97
H2NC(OH)=CHSO2C4F9	-1808.127984	-1807.980905	-1808.051512	148.61
H2NC(OH)=CHCO2Me	-437.091139	-436.963835	-437.006115	88.99
H2NC(OH)=CHCO2CH2CF3	-774.124981	-773.989067	-774.041909	111.22
H2NC(OH)=CHCN	-301.430938	-301.350331	-301.386760	76.67

[a] hydrogen-bonding with an oxygen atom of the SO_2Me group.

[b] hydrogen-bonding with an oxygen atom of the SO_2Ph group.

[c] No stable structure, converged to the enol on the amide.

Table S8. Energies for Isodesmic Reactions of β-Sulfonyl-substituted Amides at B3LYP/6-31+G* in kcal/mol

							ΔE	ΔH	ΔG
i-PrNHC(OH)=C(SO2Ph)2	+	CH4	=	i-PrNHC(OH)=CH2	+	H2C(SO2Ph)2	22.9	22.8	19.5
i-PrNHCOCH(SO2Ph)2	+	CH4	=	i-PrNHCOCH3	+	H2C(SO2Ph)2	-5.7	-5.0	-7.5
i-PrNHC(OH)=C(SO2Me)2	+	CH4	=	i-PrNHC(OH)=CH2	+	H2C(SO2Me)2	30.4	30.1	25.8
i-PrNHCOCH(SO2Me)2	+	CH4	=	i-PrNHCOCH3	+	H2C(SO2Me)2	2.6	3.2	-0.2
i-PrNHC(OH)=C($SO_2C_4F_9$)$_2$	+	CH4	=	i-PrNHC(OH)=CH2	+	H2C($SO_2C_4F_9$)$_2$	33.1	32.8	29.3
i-PrNHCOCH($SO_2C_4F_9$)$_2$	+	CH4	=	i-PrNHCOCH3	+	H2C($SO_2C_4F_9$)$_2$	-8.1	-7.4	-11.6
i-PrNHC(OH)=C(SO2Me)SO2Ph	+	CH4	=	i-PrNHC(OH)=CH2	+	CH2(SO2Me)SO2Ph	28.4	28.1	24.5
i-PrNHCOCH(SO2Me)SO2Ph	+	CH4	=	i-PrNHCOCH3	+	CH2(SO2Me)SO2Ph	-2.8	-2.3	-5.3
i-PrNHC(OH)=C(CO2Me)SO2Ph	+	CH4	=	i-PrNHC(OH)=CH2	+	CH2(CO2Me)SO2Ph	35.8	35.8	32.7
i-PrNHCOCH(CO2Me)SO2Ph	+	CH4	=	i-PrNHCOCH3	+	CH2(CO2Me)SO2Ph	4.9	5.3	2.5
i-PrNHC(OH)=C(COMe)SO2Ph	+	CH4	=	i-PrNHC(OH)=CH2	+	CH2(COMe)SO2Ph	31.0	31.5	27.9
i-PrNHCOCH(COMe)SO2Ph	+	CH4	=	i-PrNHCOCH3	+	CH2(COMe)SO2Ph	-2.4	-2.0	-5.5
i-PrNHC(OH)=C(COMe)SO2C4F9	+	CH4	=	i-PrNHC(OH)=CH2	+	CH2(COMe)SO2C4F9	36.4	36.7	31.8
i-PrNHCOCH(COMe)SO2C4F9	+	CH4	=	i-PrNHCOCH3	+	CH2(COMe)SO2C4F9	-2.7	-2.3	-5.7
i-PrNHC(OH)=C(CN)SO2Me	+	CH4	=	i-PrNHC(OH)=CH2	+	CH2(CN)SO2Me	29.9	29.7	27.0
i-PrNHCOCH(CN)SO2Me	+	CH4	=	i-PrNHCOCH3	+	CH2(CN)SO2Me	-0.4	0.1	-3.2
i-PrNHC(OH)=C(CN)SO2Ph	+	CH4	=	i-PrNHC(OH)=CH2	+	CH2(CN)SO2Ph	28.1	28.0	25.3
i-PrNHCOCH(CN)SO2Ph	+	CH4	=	i-PrNHCOCH3	+	CH2(CN)SO2Ph	-2.6	-2.1	-5.2
PhNHC(OH)=C(SO2Ph)2	+	CH4		PhNHC(OH)=CH2	+	H2C(SO2Ph)2	20.9	20.8	17.4
PhNHCOCH(SO2Ph)2	+	CH4	=	PhNHCOCH3	+	H2C(SO2Ph)2	-6.3	-6.2	-7.3
PhNHC(OH)=C(SO2Me)2	+	CH4	=	PhNHC(OH)=CH2	+	H2C(SO2Me)2	28.0	27.7	22.9
PhNHCOCH(SO2Me)2	+	CH4	=	PhNHCOCH3	+	H2C(SO2Me)2	1.7	1.7	-0.9

PPhNHC(OH)=C(SO2C4F9)2	+	CH4	=	PhNHC(OH)=CH2	+	CH2(SO2C4F9)2	24.7	24.8	22.0
PhNHCOCH(SO2C4F9)2	+	CH4		PhNHCOCH3	+	CH2(SO2C4F9)2	-11.9	-11.6	-14.0
hNHC(OH)=C(SO2Me)SO2Ph	+	CH4	=	PhNHC(OH)=CH2	+	H2C(SO2Me)SO2Ph	26.2	26.0	22.1
PhNHCOCH(SO2Me)SO2Ph	+	CH4	=	PhNHCOCH3	+	H2C(SO2Me)SO2Ph	-2.6	-2.7	-4.7
PhNHC(OH)C=(CO2Me)SO2Ph	+	CH4	=	PhNHC(OH)=CH2	+	H2C(CO2Me)SO2Ph	33.8	33.9	30.4
PhNHCOCH(CO2Me)SO2Ph	+	CH4	=	PhNHCOCH3	+	H2C(CO2Me)SO2Ph	1.4	1.3	0.0
PhNHC(OH)=C(COMe)SO2Ph	+	CH4		PhNHC(OH)=CH2	+	CH2(COMe)SO2Ph	29.2	30.0	25.5
PhNHCOCH(COMe)SO2Ph	+	CH4	=	PhNHCOCH3	+	CH2(COMe)SO2Ph	0.3	0.3	-1.7
PhNHC(OH)=C(COMe)SO2C4F9	+	CH4	=	PhNHC(OH)=CH2	+	CH2(COMe)SO2C4F9	33.5	34.2	29.4
PhNHCOCH(COMe)SO2C4F9	+	CH4	=	PhNHCOCH3	+	CH2(COMe)SO2C4F9	-3.9	-3.9	-6.5
PhNHCOCH(CN)SO2Me	+	CH4	=	PhNHC(OH)=CH2	+	CH2(CN)SO2Me	0.5	0.5	-1.1
PhNHC(OH)=C(CN)SO2Me	+	CH4	=	PhNHCOCH3	+	CH2(CN)SO2Me	27.2	26.9	23.5
PhNHCOCH(CN)SO2Ph	+	CH4	=	PhNHC(OH)=CH2	+	CH2(CN)SO2Ph	-0.5	-0.5	-2.3
PhNHC(OH)=C(CN)SO2Ph	+	CH4	=	PhNHCOCH3	+	CH2(CN)SO2Ph	25.5	25.3	22.5
2,4-$MeO_2C_6H_3$NHC(OH)=C(CO_2Me)SO_2Ph	+	CH_4	=	2,4-$MeO_2C_6H_3$NHC(OH)=CH_2	+	CH_2(CO_2Me)SO_2Ph	34.4	34.6	31.3
2,4-$MeO_2C_6H_3$NHCOCH(CO_2Me)SO_2Ph	+	CH_4	=	2,4-$MeO_2C_6H_3$NHCOCH$_3$	+	CH_2(CO_2Me)SO_2Ph	5.7	6.4	4.2
2,4-$MeO_2C_6H_3$NHC(OH)C($SO_2Ph)_2$	+	CH_4	=	2,4-$MeO_2C_6H_3$NHC(OH)=CH_2	+	$H_2C(SO_2Ph)_2$	21.8	21.7	18.6
2,4-$MeO_2C_6H_3$NHCOCH($SO_2Ph)_2$	+	CH_4	=	2,4-$MeO_2C_6H_3$NHCOCH$_2$	+	$H_2C(SO_2Ph)_2$	-2.6	-1.8	-4.3
i-PrNHC(OH)=C(SO2Ph)2	+	H2C=CH2	=	i-PrNHC(OH)=CH2	+	H2C=C(SO2Ph)2	19.3	18.8	16.6
i-PrNHCOCH(SO2Ph)2	+	H2C=CH2	=	i-PrNHCOCH3	+	H2C=C(SO2Ph)2	-9.3	-9.0	-10.5
i-PrNHC(OH)=C(SO2Me)2	+	H2C=CH2	=	i-PrNHC(OH)=CH2	+	H2C=C(SO2Me)2	20.8	20.3	18.0
i-PrNHCOCH(SO2Me)2	+	H2C=CH2	=	i-PrNHCOCH3	+	H2C=C(SO2Me)2	-6.9	-6.6	-8.0
i-PrNHC(OH)=C($SO_2C_4F_9)_2$	+	H2C=CH2	=	i-PrNHC(OH)=CH2	+	H2C($SO_2C_4F_9)_2$	26.2	25.5	23.7
i-PrNHCOCH($SO_2C_4F_9)_2$	+	H2C=CH2	=	i-PrNHCOCH3	+	H2C($SO_2C_4F_9)_2$	-15.1	-14.4	-17.2
i-PrNHC(OH)=C(SO2Me)SO2Ph	+	H2C=CH2	=	i-PrNHC(OH)=CH2	+	H2C=C(SO2Me)SO2Ph	19.9	19.4	17.1

i-PrNHCOCH(SO2Me)SO2Ph	+	H2C=CH2	=	i-PrNHCOCH3	+	H2C=C(SO2Me)SO2Ph	-11.3	-11.0	-12.8
i-PrNHC(OH)=C(CO2Me)SO2Ph	+	H2C=CH2	=	i-PrNHC(OH)=CH2	+	H2C=C(CO2Me)SO2Ph	24.6	24.2	21.8
i-PrNHCOCH(CO2Me)SO2Ph	+	H2C=CH2	=	i-PrNHCOCH3	+	H2C=C(CO2Me)SO2Ph	-6.3	-6.3	-8.4
i-PrNHC(OH)=C(COMe)SO2Ph	+	H2C=CH2	=	i-PrNHC(OH)=CH2	+	H2C=C(COMe)SO2Ph	27.8	28.0	25.6
i-PrNHCOCH(COMe)SO2Ph	+	H2C=CH2	=	i-PrNHCOCH3	+	H2C=C(COMe)SO2Ph	-5.6	-5.5	-7.8
i-PrNHC(OH)=C(COMe)SO2C4F9	+	H2C=CH2	=	i-PrNHC(OH)=CH2	+	CH2=C(COMe)SO2C4F9	31.6	31.6	27.8
i-PrNHCOCH(COMe)SO2C4F9	+	H2C=CH2	=	i-PrNHCOCH3	+	CH2=C(COMe)SO2C4F9	-7.5	-7.4	-9.7
i-PrNHC(OH)=C(CN)SO2Me	+	H2C=CH2	=	i-PrNHC(OH)=CH2	+	H2C=C(CN)SO2Me	21.5	21.0	19.5
i-PrNHCOCH(CN)SO2Me	+	H2C=CH2	=	i-PrNHCOCH3	+	H2C=C(CN)SO2Me	-8.8	-8.7	-10.6
i-PrNHC(OH)=C(CN)SO2Ph	+	H2C=CH2	=	i-PrNHC(OH)=CH2	+	H2C=C(CN)SO2Ph	20.5	20.1	18.7
i-PrNHCOCH(CN)SO2Ph	+	H2C=CH2	=	i-PrNHCOCH3	+	H2C=C(CN)SO2Ph	-10.2	-10.0	-11.8
PhNHC(OH)=C(SO2Ph)2	+	H2C=CH2	=	PhNHC(OH)=CH2	+	H2C=C(SO2Ph)2	17.3	16.9	14.4
PhNHCOCH(SO2Ph)2	+	H2C=CH2	=	PhNHCOCH3	+	H2C=C(SO2Ph)2	-9.9	-10.2	-10.2
PhNHC(OH)=C(SO2Me)2	+	H2C=CH2	=	PhNHC(OH)=CH2	+	H2C=C(SO2Me)2	18.4	17.9	15.1
PhNHCOCH(SO2Me)2	+	H2C=CH2	=	PhNHCOCH3	+	H2C=C(SO2Me)2	-7.8	-8.1	-8.6
PhNHC(OH)=C(SO2C4F9)2	+	H2C=CH2	=	PhNHC(OH)=CH2	+	CH2=C(SO2C4F9)2	22.6	21.9	19.9
PhNHCOCH(SO2C4F9)2	+	H2C=CH2		PhNHCOCH3	+	CH2=C(SO2C4F9)2	-18.9	-18.8	-19.6
PhNHC(OH)=C(SO2Me)SO2Ph	+	H2C=CH2	=	PhNHC(OH)=CH2	+	H2C=C(SO2Me)SO2Ph	17.8	17.3	14.7
PhNHCOCH(SO2Me)SO2Ph	+	H2C=CH2	=	PhNHCOCH3	+	H2C=C(SO2Me)SO2Ph	-11.1	-11.4	-12.2
PhNHC(OH)C=(CO2Me)SO2Ph	+	H2C=CH2	=	PhNHC(OH)=CH2	+	H2C=C(CO2Me)SO2Ph	22.7	22.3	19.5
PhNHCOCH(CO2Me)SO2Ph	+	H2C=CH2	=	PhNHCOCH3	+	H2C=C(CO2Me)SO2Ph	-9.8	-10.3	-10.8
PhNHC(OH)=C(COMe)SO2Ph	+	H2C=CH2		PhNHC(OH)=CH2	+	H2C=C(COMe)SO2Ph	26.0	26.5	23.2
PhNHCOCH(COMe)SO2Ph	+	H2C=CH2	=	PhNHCOCH3	+	H2C=C(COMe)SO2Ph	-2.9	-3.2	-4.1
PhNHC(OH)=C(COMe)SO2C4F9	+	H2C=CH2	=	PhNHC(OH)=CH2	+	CH2=C(COMe)SO2C4F9	28.8	29.1	25.4
PhNHCOCH(COMe)SO2C4F9	+	H2C=CH2	=	PhNHCOCH3	+	CH2=C(COMe)SO2C4F9	-8.7	-9.0	-10.5

PhNHCOCH(CN)SO2Me	+	H2C=CH2		PhNHC(OH)=CH2	+	H2C=C(CN)SO2Me	23.2	22.8	21.3
PhNHC(OH)=C(CN)SO2Me	+	H2C=CH2	=	PhNHCOCH3	+	H2C=C(CN)SO2Me	-12.2	-12.9	-13.8
PhNHCOCH(CN)SO2Ph	+	H2C=CH2	=	PhNHC(OH)=CH2	+	H2C=C(CN)SO2Ph	22.9	22.6	20.9
PhNHC(OH)=C(CN)SO2Ph	+	H2C=CH2	=	PhNHCOCH3	+	H2C=C(CN)SO2Ph	-13.1	-13.7	-14.0
2,4MeO2PhNHC(OH)=C(CO2Me)SO2Ph	+	H2C=CH2	=	24MeO2PhNHC(OH)=CH2	+	H2C=C(CO2Me)SO2Ph	26.7	26.2	25.1
2,4MeO2PhNHCOCH(CO2Me)SO2Ph	+	H2C=CH2	=	24MeO2PhNHCOCH3	+	H2C=C(CO2Me)SO2Ph	-5.5	-8.4	-11.3
2,4MeO2PhNHC(OH)C(SO2Ph)2	+	H2C=CH2	=	24MeO2PhNHC(OH)=CH2	+	H2C=C(SO2Ph)2	18.2	17.7	15.7
2,4MeO2PhNHCOCH(SO2Ph)2	+	H2C=CH2	=	24MeO2PhNHCOCH3	+	H2C=C(SO2Ph)2	-6.2	-5.8	-7.2

Table S9. Energies for Isodesmic Reactions of β-Sulfonyl-substituted Amides at B3LYP/6-31G** in kcal/mol

							ΔE	ΔH	ΔG
i-PrNHC(OH)=C(SO2Ph)2	+	CH4	=	i-PrNHC(OH)=CH2	+	H2C(SO2Ph)2	24.6	24.9	22.8
i-PrNHCOCH(SO2Ph)2	+	CH4	=	i-PrNHCOCH3	+	H2C(SO2Ph)2	-3.0	-2.4	-5.3
i-PrNHC(OH)=C(SO2Me)2	+	CH4	=	i-PrNHC(OH)=CH2	+	H2C(SO2Me)2	35.8	35.7	31.7
i-PrNHCOCH(SO2Me)2	+	CH4	=	i-PrNHCOCH3	+	H2C(SO2Me)2	6.3	6.7	2.7
i-PrNHC(OH)=C($SO_2C_4F_9$)$_2$	+	CH4	=	i-PrNHC(OH)=CH2	+	H2C($SO_2C_4F_9$)$_2$	35.4	35.4	33.0
i-PrNHCOCH($SO_2C_4F_9$)$_2$	+	CH4	=	i-PrNHCOCH3	+	H2C($SO_2C_4F_9$)$_2$	-4.1	-3.4	-7.5
i-PrNHC(OH)=C(SO2Me)SO2Ph	+	CH4	=	i-PrNHC(OH)=CH2	+	CH2(SO2Me)SO2Ph	33.5	33.5	30.1
i-PrNHCOCH(SO2Me)SO2Ph	+	CH4	=	i-PrNHCOCH3	+	CH2(SO2Me)SO2Ph	0.7	1.1	-1.6
i-PrNHC(OH)=C(CO2Me)SO2Ph	+	CH4	=	i-PrNHC(OH)=CH2	+	CH2(CO2Me)SO2Ph	40.9	41.2	38.0
i-PrNHCOCH(CO2Me)SO2Ph	+	CH4	=	i-PrNHCOCH3	+	CH2(CO2Me)SO2Ph	8.2	8.3	4.6
i-PrNHC(OH)=C(COMe)SO2Ph	+	CH4	=	i-PrNHC(OH)=CH2	+	CH2(COMe)SO2Ph	36.9	38.2	34.5
i-PrNHCOCH(COMe)SO2Ph	+	CH4	=	i-PrNHCOCH3	+	CH2(COMe)SO2Ph	1.0	1.3	-2.7
i-PrNHC(OH)=C(COMe)SO2C4F9	+	CH4	=	i-PrNHC(OH)=CH2	+	CH2(COMe)SO2C4F9	41.1	42.0	37.7
i-PrNHCOCH(COMe)SO2C4F9	+	CH4	=	i-PrNHCOCH3	+	CH2(COMe)SO2C4F9	0.9	1.2	-2.8
i-PrNHC(OH)=C(CN)SO2Me	+	CH4	=	i-PrNHC(OH)=CH2	+	CH2(CN)SO2Me	33.9	34.0	31.5
i-PrNHCOCH(CN)SO2Me	+	CH4	=	i-PrNHCOCH3	+	CH2(CN)SO2Me	2.4	2.7	-1.1
i-PrNHC(OH)=C(CN)SO2Ph	+	CH4	=	i-PrNHC(OH)=CH2	+	CH2(CN)SO2Ph	32.0	32.0	29.4
i-PrNHCOCH(CN)SO2Ph	+	CH4	=	i-PrNHCOCH3	+	CH2(CN)SO2Ph	-0.1	0.3	-3.5
PhNHC(OH)=C(SO2Ph)2	+	CH4		PhNHC(OH)=CH2	+	H2C(SO2Ph)2	25.3	25.4	22.2
PhNHCOCH(SO2Ph)2	+	CH4	=	PhNHCOCH3	+	H2C(SO2Ph)2	-4.0	-4.1	-5.6
PhNHC(OH)=C(SO2Me)2	+	CH4	=	PhNHC(OH)=CH2	+	H2C(SO2Me)2	32.7	32.6	28.3
PhNHCOCH(SO2Me)2	+	CH4	=	PhNHCOCH3	+	H2C(SO2Me)2	4.9	4.8	2.2
PhNHC(OH)=C(SO2C4F9)2	+	CH4	=	PhNHC(OH)=CH2	+	CH2(SO2C4F9)2	31.3	31.2	28.0

PhNHCOCH(SO2C4F9)2	+	CH4	=	PhNHCOCH3	+	CH2(SO2C4F9)2	-9.2	-8.9	-10.7
PhNHC(OH)=C(SO2Me)SO2Ph	+	CH4	=	PhNHC(OH)=CH2	+	CH2(SO2Me)SO2Ph	30.9	30.9	26.9
PhNHCOCH(SO2Me)SO2Ph	+	CH4	=	PhNHCOCH3	+	CH2(SO2Me)SO2Ph	0.1	-0.1	-2.2
PhNHC(OH)C=(CO2Me)SO2Ph	+	CH4	=	PhNHC(OH)=CH2	+	CH2(CO2Me)SO2Ph	38.4	38.8	35.2
PhNHCOCH(CO2Me)SO2Ph	+	CH4	=	PhNHCOCH3	+	CH2(CO2Me)SO2Ph	4.0	3.8	2.4
PhNHC(OH)=C(COMe)SO2Ph	+	CH4		PhNHC(OH)=CH2	+	CH2(COMe)SO2Ph	36.3	36.3	32.0
PhNHCOCH(COMe)SO2Ph	+	CH4	=	PhNHCOCH3	+	CH2(COMe)SO2Ph	2.7	2.5	0.5
PhNHC(OH)=C(COMe)SO2C4F9	+	CH4	=	PhNHC(OH)=CH2	+	CH2(COMe)SO2C4F9	39.1	39.3	34.6
PhNHCOCH(COMe)SO2C4F9	+	CH4	=	PhNHCOCH3	+	CH2(COMe)SO2C4F9	-0.8	-0.9	-3.9
PhNHCOCH(CN)SO2Me	+	CH4	=	PhNHC(OH)=CH2	+	CH2(CN)SO2Me	31.9	31.9	29.2
PhNHC(OH)=C(CN)SO2Me	+	CH4	=	PhNHCOCH3	+	CH2(CN)SO2Me	1.1	0.8	-1.0
PhNHCOCH(CN)SO2Ph	+	CH4	=	PhNHC(OH)=CH2	+	CH2(CN)SO2Ph	30.5	30.6	27.6
PhNHC(OH)=C(CN)SO2Ph	+	CH4	=	PhNHCOCH3	+	CH2(CN)SO2Ph	-0.7	-1.0	-3.1
2,4MeO2PhNHC(OH)=C(CO2Me)SO2Ph	+	CH4	=	24MeO2PhNHC(OH)=CH2	+	CH2(CO2Me)SO2Ph	38.0	38.0	36.2
2,4MeO2PhNHCOCH(CO2Me)SO2Ph	+	CH4	=	24MeO2PhNHCOCH3	+	CH2(CO2Me)SO2Ph	8.5	9.5	5.7
2,4MeO2PhNHC(OH)C(SO2Ph)2	+	CH4	=	24MeO2PhNHC(OH)=CH2	+	H2C(SO2Ph)2	26.7	26.8	22.9
2,4MeO2PhNHCOCH(SO2Ph)2	+	CH4	=	24MeO2PhNHCOCH3	+	H2C(SO2Ph)2	-0.7	-0.1	-2.6
i-PrNHC(OH)=C(SO2Ph)2	+	H2C=CH2	=	i-PrNHC(OH)=CH2	+	H2C=C(SO2Ph)2	19.1	19.1	18.1
i-PrNHCOCH(SO2Ph)2	+	H2C=CH2	=	i-PrNHCOCH3	+	H2C=C(SO2Ph)2	-8.5	-8.2	-10.0
i-PrNHC(OH)=C(SO2Me)2	+	H2C=CH2	=	i-PrNHC(OH)=CH2	+	H2C=C(SO2Me)2	23.9	23.7	21.8
i-PrNHCOCH(SO2Me)2	+	H2C=CH2	=	i-PrNHCOCH3	+	H2C=C(SO2Me)2	-5.5	-5.3	-7.3
i-PrNHC(OH)=C($SO_2C_4F_9$)$_2$	+	H2C=CH2	=	i-PrNHC(OH)=CH2	+	H2C($SO_2C_4F_9$)$_2$	27.5	27.2	26.1
i-PrNHCOCH($SO_2C_4F_9$)$_2$	+	H2C=CH2	=	i-PrNHCOCH3	+	H2C($SO_2C_4F_9$)$_2$	-12.0	-11.6	-14.3
i-PrNHC(OH)=C(SO2Me)SO2Ph	+	H2C=CH2	=	i-PrNHC(OH)=CH2	+	H2C=C(SO2Me)SO2Ph	23.0	22.8	20.8
i-PrNHCOCH(SO2Me)SO2Ph	+	H2C=CH2	=	i-PrNHCOCH3	+	H2C=C(SO2Me)SO2Ph	-9.9	-9.6	-10.9

i-PrNHC(OH)=C(CO2Me)SO2Ph	+	H2C=CH2	=	i-PrNHC(OH)=CH2	+	H2C=C(CO2Me)SO2Ph	27.7	27.7	25.4
i-PrNHCOCH(CO2Me)SO2Ph	+	H2C=CH2	=	i-PrNHCOCH3	+	H2C=C(CO2Me)SO2Ph	-5.0	-5.2	-8.1
i-PrNHC(OH)=C(COMe)SO2Ph/CO	+	H2C=CH2	=	i-PrNHC(OH)=CH2	+	H2C=C(COMe)SO2Ph	31.5	32.6	30.2
i-PrNHCOCH(COMe)SO2Ph	+	H2C=CH2	=	i-PrNHCOCH3	+	H2C=C(COMe)SO2Ph	-4.3	-4.4	-7.0
i-PrNHC(OH)=C(COMe)SO2C4F9	+	H2C=CH2	=	i-PrNHC(OH)=CH2	+	CH2=C(COMe)SO2C4F9	34.7	35.4	32.3
i-PrNHCOCH(COMe)SO2C4F9	+	H2C=CH2	=	i-PrNHCOCH3	+	CH2=C(COMe)SO2C4F9	-5.5	-5.5	-8.1
i-PrNHC(OH)=C(CN)SO2Me	+	H2C=CH2	=	i-PrNHC(OH)=CH2	+	H2C=C(CN)SO2Me	23.7	23.5	22.4
i-PrNHCOCH(CN)SO2Me	+	H2C=CH2		i-PrNHCOCH3	+	H2C=C(CN)SO2Me	-7.8	-7.7	-10.2
i-PrNHC(OH)=C(CN)SO2Ph	+	H2C=CH2	=	i-PrNHC(OH)=CH2	+	H2C=C(CN)SO2Ph	22.7	22.5	21.2
i-PrNHCOCH(CN)SO2Ph	+	H2C=CH2	=	i-PrNHCOCH3	+	H2C=C(CN)SO2Ph	-9.3	-9.3	-11.8
PhNHC(OH)=C(SO2Ph)2	+	H2C=CH2	=	PhNHC(OH)=CH2	+	H2C=C(SO2Ph)2	19.8	19.6	17.6
PhNHCOCH(SO2Ph)2	+	H2C=CH2	=	PhNHCOCH3	+	H2C=C(SO2Ph)2	-9.5	-9.8	-10.2
PhNHC(OH)=C(SO2Me)2	+	H2C=CH2	=	PhNHC(OH)=CH2	+	H2C=C(SO2Me)2	20.9	20.6	18.3
PhNHCOCH(SO2Me)2	+	H2C=CH2	=	PhNHCOCH3	+	H2C=C(SO2Me)2	-6.9	-7.2	-7.7
PhNHC(OH)=C(SO2C4F9)2	+	H2C=CH2	=	PhNHC(OH)=CH2	+	CH2=C(SO2C4F9)2	23.4	23.0	21.2
PhNHCOCH(SO2C4F9)2	+	H2C=CH2	=	PhNHCOCH3	+	CH2=C(SO2C4F9)2	-17.1	-17.2	-17.5
PhNHC(OH)=C(SO2Me)SO2Ph	+	H2C=CH2	=	PhNHC(OH)=CH2	+	H2C=C(SO2Me)SO2Ph	20.4	20.1	17.5
PhNHCOCH(SO2Me)SO2Ph	+	H2C=CH2		PhNHCOCH3	+	H2C=C(SO2Me)SO2Ph	-10.4	-10.8	-11.5
PhNHC(OH)C=(CO2Me)SO2Ph	+	H2C=CH2	=	PhNHC(OH)=CH2	+	H2C=C(CO2Me)SO2Ph	25.2	25.2	22.5
PhNHCOCH(CO2Me)SO2Ph	+	H2C=CH2	=	PhNHCOCH3	+	H2C=C(CO2Me)SO2Ph	-9.2	-9.8	-10.3
PhNHC(OH)=C(COMe)SO2Ph	+	H2C=CH2	=	PhNHC(OH)=CH2	+	H2C=C(COMe)SO2Ph	30.9	30.7	27.8
PhNHCOCH(COMe)SO2Ph	+	H2C=CH2	=	PhNHCOCH3	+	H2C=C(COMe)SO2Ph	-2.7	-3.2	-3.8
PhNHC(OH)=C(COMe)SO2C4F9	+	H2C=CH2		PhNHC(OH)=CH2	+	CH2=C(COMe)SO2C4F9	32.7	32.6	29.3
PhNHCOCH(COMe)SO2C4F9	+	H2C=CH2	=	PhNHCOCH3	+	CH2=C(COMe)SO2C4F9	-7.2	-7.6	-9.2
PhNHCOCH(CN)SO2Me	+	H2C=CH2		PhNHC(OH)=CH2	+	H2C=C(CN)SO2Me	21.7	21.5	20.1

PhNHC(OH)=C(CN)SO2Me	+	H2C=CH2	=	PhNHCOCH3	+	H2C=C(CN)SO2Me	-9.1	-9.7	-10.1
PhNHCOCH(CN)SO2Ph	+	H2C=CH2	=	PhNHC(OH)=CH2	+	H2C=C(CN)SO2Ph	21.3	21.0	19.4
PhNHC(OH)=C(CN)SO2Ph	+	H2C=CH2	=	PhNHCOCH3	+	H2C=C(CN)SO2Ph	-10.0	-10.5	-11.3
2,4MeO2PhNHC(OH)=C(CO2Me)SO2Ph	+	H2C=CH2	=	24MeO2PhNHC(OH)=CH2	+	H2C=C(CO2Me)SO2Ph	24.8	24.5	23.5
2,4MeO2PhNHCOCH(CO2Me)SO2Ph	+	H2C=CH2		24MeO2PhNHCOCH3	+	H2C=C(CO2Me)SO2Ph	-4.7	-4.0	-6.9
2,4MeO2PhNHC(OH)C(SO2Ph)2	+	H2C=CH2		24MeO2PhNHC(OH)=CH2	+	H2C=C(SO2Ph)2	21.2	21.0	18.3
2,4MeO2PhNHCOCH(SO2Ph)2	+	H2C=CH2		24MeO2PhNHCOCH3	+	H2C=C(SO2Ph)2	-6.2	-5.8	-7.2

Table S10. Energies for Isodesmic Reactions of β-Carbonyl-substituted Amides at B3LYP/6-31+G* in kcal/mol

							ΔE	ΔH	ΔG
i-PrNHC(OH)=C(CO_2Me)$_2$	+	CH_4	=	i-PrNHC(OH)=CH_2	+	$CH_2(CO_2Me)_2$	33.4	33.7	29.0
i-PrNHCOCH(CO_2Me)$_2$	+	CH_4	=	i-PrNHCOCH_3	+	$CH_2(CO_2Me)_2$	-0.7	-0.3	-3.1
i-PrNHC(OH)=C(COMe)CO_2Me	+	CH_4	=	i-PrNHC(OH)=CH_2	+	CH_2(COMe)CO_2Me	39.1	39.2	34.7
i-PrNHCOCH(COMe)CO_2Me	+	CH_4	=	i-PrNHCOCH_3	+	CH_2(COMe)CO_2Me	-2.4	-2.0	-5.8
i-PrNHC(OH)=C(COMe)$_2$	+	CH_4	=	i-PrNHC(OH)=CH_2	+	$CH_2(COMe)_2$	36.1	36.1	31.6
i-PrNHCOCH(COMe)$_2$	+	CH_4	=	i-PrNHCOCH_3	+	$CH_2(COMe)_2$	-1.5	-1.1	-4.7
i-PrNHC(OH)=C(CN)CO_2Me	+	CH_4	=	i-PrNHC(OH)=CH_2	+	CH_2(CN)CO_2Me	34.8	34.8	30.5
i-PrNHCOCH(CN)CO_2Me	+	CH_4	=	i-PrNHCOCH_3	+	CH_2(CN)CO_2Me	-1.3	-0.9	-4.2
i-PrNHC(OH)=C(CN)COMe	+	CH_4	=	i-PrNHC(OH)=CH_2	+	CH_2(CN)COMe	38.4	38.6	35.2
i-PrNHCOCH(CN)COMe	+	CH_4	=	i-PrNHCOCH_3	+	CH_2(CN)COMe	-2.8	-2.4	-5.8
PhNHC(OH)=C(CO_2Me)$_2$	+	CH_4	=	PhNHC(OH)=CH_2	+	CH_2(CO2Me)$_2$	32.0	32.2	27.4

PhNHCOCH(CO_2Me)$_2$	+	CH_4	=	$PhNHCOCH_3$	+	$CH_2(CO2Me)_2$	-0.2	-0.4	-2.3
PhNHC(OH)=C(COMe)CO_2Me	+	CH_4	=	PhNHC(OH)=CH_2	+	CH_2(COMe)CO_2Me	36.8	37.7	32.3
PhNHCOCH(COMe)CO_2Me	+	CH_4	=	$PhNHCOCH_3$	+	CH_2(COMe)CO_2Me	-7.3	-6.9	-8.1
PhNHC(OH)=C(COMe)$_2$	+	CH_4	=	PhNHC(OH)=CH_2	+	CH_2(COMe)$_2$	35.6	35.2	29.6
PhNHCOCH(COMe)$_2$	+	CH_4	=	$PhNHCOCH_3$	+	CH_2(COMe)$_2$	0.8	0.7	-1.3
PhNHC(OH)=C(CN)CO_2Me	+	CH_4	=	PhNHC(OH)=CH_2	+	CH_2(CN)CO_2Me	32.5	32.3	27.5
PhNHCOCH(CN)CO_2Me	+	CH_4	=	$PhNHCOCH_3$	+	CH_2(CN)CO_2Me	-1.6	-1.8	-4.0
PhNHC(OH)=C(CN)COMe	+	CH_4	=	PhNHC(OH)=CH_2	+	CH_2(CN)COMe	36.1	36.2	32.6
PhNHCOCH(CN)COMe	+	CH_4	=	$PhNHCOCH_3$	+	CH_2(CN)COMe	-5.2	-5.2	-7.2
i-PrNHC(OH)=C(CO_2Me)$_2$	+	H_2C=CH_2	=	i-PrNHC(OH)=CH_2	+	CH_2=C(CO_2Me)$_2$	28.2	28.0	25.1
i-PrNHCOCH(CO_2Me)$_2$	+	H_2C=CH_2	=	$i\text{-PrNHCOCH}_3$	+	CH_2=C(CO_2Me)$_2$	-5.9	-5.9	-7.0
i-PrNHC(OH)=C(COMe)CO_2Me	+	H_2C=CH_2	=	i-PrNHC(OH)=CH_2	+	CH_2=C(COMe)CO_2Me	32.4	31.6	30.0
i-PrNHCOCH(COMe)CO_2Me	+	H_2C=CH_2	=	$i\text{-PrNHCOCH}_3$	+	CH_2=C(COMe)CO_2Me	-9.1	-9.6	-10.5
i-PrNHC(OH)=C(COMe)$_2$	+	H_2C=CH_2	=	i-PrNHC(OH)=CH_2	+	CH_2=C(COMe)$_2$	30.7	29.9	28.0
i-PrNHCOCH(COMe)$_2$	+	H_2C=CH_2	=	$i\text{-PrNHCOCH}_3$	+	CH_2=C(COMe)$_2$	-6.9	-7.3	-8.3
i-PrNHC(OH)=C(CN)CO_2Me	+	H_2C=CH_2	=	i-PrNHC(OH)=CH_2	+	CH_2=C(CN)CO_2Me	27.2	26.9	24.6
i-PrNHCOCH(CN)CO_2Me	+	H_2C=CH_2	=	$i\text{-PrNHCOCH}_3$	+	CH_2=C(CN)CO_2Me	-8.9	-8.8	-10.0
i-PrNHC(OH)=C(CN)COMe	+	H_2C=CH_2	=	i-PrNHC(OH)=CH_2	+	CH_2=C(CN)COMe	31.7	31.7	29.9
i-PrNHCOCH(CN)COMe	+	H_2C=CH_2	=	$i\text{-PrNHCOCH}_3$	+	CH_2=C(CN)COMe	-9.5	-9.3	-11.1
PhNHC(OH)=C(CO_2Me)$_2$	+	H_2C=CH_2	=	PhNHC(OH)=CH_2	+	CH_2=C(CO_2Me)$_2$	26.7	26.5	23.5
PhNHCOCH(CO_2Me)$_2$	+	H_2C=CH_2	=	$PhNHCOCH_3$	+	CH_2=C(CO_2Me)$_2$	-5.4	-6.0	-6.2
PhNHC(OH)=C(COMe)CO_2Me	+	H_2C=CH_2	=	PhNHC(OH)=CH_2	+	CH_2=C(COMe)CO_2Me	30.1	30.1	27.7
PhNHCOCH(COMe)CO_2Me	+	H_2C=CH_2	=	$PhNHCOCH_3$	+	CH_2=C(COMe)CO_2Me	-14.0	-14.5	-12.8
PhNHC(OH)=C(COMe)$_2$	+	H_2C=CH_2	=	PhNHC(OH)=CH_2	+	CH_2=C(COMe)$_2$	30.1	29.0	26.0
PhNHCOCH(COMe)$_2$	+	H_2C=CH_2	=	$PhNHCOCH_3$	+	CH_2=C(COMe)$_2$	-4.6	-5.5	-4.8

$PhNHC(OH)=C(CN)CO_2Me$	+	$H_2C=CH_2$	=	$PhNHC(OH)=CH_2$	+	$CH_2=C(CN)CO_2Me$	24.9	24.4	21.7
$PhNHCOCH(CN)CO_2Me$	+	$H_2C=CH_2$	=	$PhNHCOCH_3$	+	$CH_2=C(CN)CO_2Me$	-9.2	-9.8	-9.8
$PhNHC(OH)=C(CN)COMe$	+	$H_2C=CH_2$	=	$PhNHC(OH)=CH_2$	+	$CH_2=C(CN)COMe$	29.4	29.4	27.3
$PhNHCOCH(CN)COMe$	+	$H_2C=CH_2$	=	$PhNHCOCH_3$	+	$CH_2=C(CN)COMe$	-11.9	-12.1	-12.5

Table S11. Energies for Isodesmic Reactions of β-Carbonyl-substituted Amides at B3LYP/6-31G** in kcal/mol

							ΔE	ΔH	ΔG
i-PrNHC(OH)=C(CO_2Me)$_2$	+	CH_4	=	i-PrNHC(OH)=CH_2	+	$CH_2(CO_2Me)_2$	39.1	39.7	35.0
i-PrNHCOCH(CO_2Me)$_2$	+	CH_4	=	i-PrNHCOCH_3	+	$CH_2(CO_2Me)_2$	1.8	2.1	-0.8
i-PrNHC(OH)=C(COMe)CO_2Me	+	CH_4	=	i-PrNHC(OH)=CH_2	+	CH_2(COMe)CO_2Me	44.6	45.3	40.9
i-PrNHCOCH(COMe)CO_2Me	+	CH_4	=	i-PrNHCOCH_3	+	CH_2(COMe)CO_2Me	0.5	0.7	-3.5
i-PrNHC(OH)=C(COMe)$_2$	+	CH_4	=	i-PrNHC(OH)=CH_2	+	$CH_2(COMe)_2$	41.6	42.6	39.0
i-PrNHCOCH(COMe)$_2$	+	CH_4	=	i-PrNHCOCH_3	+	$CH_2(COMe)_2$	2.1	2.4	-1.7
i-PrNHC(OH)=C(CN)CO_2Me	+	CH_4	=	i-PrNHC(OH)=CH_2	+	CH_2(CN)CO_2Me	38.8	39.0	35.0
i-PrNHCOCH(CN)CO_2Me	+	CH_4	=	i-PrNHCOCH_3	+	CH_2(CN)CO_2Me	0.8	1.1	-2.7
i-PrNHC(OH)=C(CN)COMe	+	CH_4	=	i-PrNHC(OH)=CH_2	+	CH_2(CN)COMe	45.6	45.4	42.1
i-PrNHCOCH(CN)COMe	+	CH_4	=	i-PrNHCOCH_3	+	CH_2(CN)COMe	-0.1	0.1	-3.9
PhNHC(OH)=C(CO_2Me)$_2$	+	CH_4	=	PhNHC(OH)=CH_2	+	CH_2(CO2Me)$_2$	37.2	37.8	33.0
PhNHCOCH(CO_2Me)$_2$	+	CH_4	=	PhNHCOCH_3	+	CH_2(CO2Me)$_2$	2.2	1.9	0.1
PhNHC(OH)=C(COMe)CO_2Me	+	CH_4	=	PhNHC(OH)=CH_2	+	CH_2(COMe)CO_2Me	43.5	43.8	38.5
PhNHCOCH(COMe)CO_2Me	+	CH_4	=	PhNHCOCH_3	+	CH_2(COMe)CO_2Me	-6.1	-6.0	-7.4
PhNHC(OH)=C(COMe)$_2$	+	CH_4	=	PhNHC(OH)=CH_2	+	$CH_2(COMe)_2$	40.5	40.8	36.0
PhNHCOCH(COMe)$_2$	+	CH_4	=	PhNHCOCH_3	+	$CH_2(COMe)_2$	3.6	3.4	1.4
PhNHC(OH)=C(CN)CO_2Me	+	CH_4	=	PhNHC(OH)=CH_2	+	CH_2(CN)CO_2Me	36.1	36.2	31.6
PhNHCOCH(CN)CO_2Me	+	CH_4	=	PhNHCOCH_3	+	CH_2(CN)CO_2Me	0.2	-0.1	-2.6
PhNHC(OH)=C(CN)COMe	+	CH_4	=	PhNHC(OH)=CH_2	+	CH_2(CN)COMe	43.8	43.3	39.1
PhNHCOCH(CN)COMe	+	CH_4	=	PhNHCOCH_3	+	CH_2(CN)COMe	-3.3	-3.5	-6.1
i-PrNHC(OH)=C(CO_2Me)$_2$	+	$H_2C=CH_2$	=	i-PrNHC(OH)=CH_2	+	CH_2=C(CO_2Me)$_2$	32.0	32.3	29.5
i-PrNHCOCH(CO_2Me)$_2$	+	$H_2C=CH_2$	=	i-PrNHCOCH_3	+	CH_2=C(CO_2Me)$_2$	-5.2	-5.3	-6.3
i-PrNHC(OH)=C(COMe)CO_2Me	+	$H_2C=CH_2$	=	i-PrNHC(OH)=CH_2	+	CH_2=C(COMe)CO_2Me	35.8	35.6	34.4

i-PrNHCOCH(COMe)CO_2Me	+	$H_2C=CH_2$	=	i-PrNHCOCH_3	+	$CH_2=C(COMe)CO_2Me$	-8.3	-9.0	-10.0
i-PrNHC(OH)=$C(COMe)_2$	+	$H_2C=CH_2$	=	i-PrNHC(OH)=CH_2	+	$CH_2=C(COMe)_2$	33.9	34.1	33.4
i-PrNHCOCH$(COMe)_2$	+	$H_2C=CH_2$	=	i-PrNHCOCH_3	+	$CH_2=C(COMe)_2$	-5.6	-6.1	-7.3
i-PrNHC(OH)=C(CN)CO_2Me	+	$H_2C=CH_2$	=	i-PrNHC(OH)=CH_2	+	$CH_2=C(CN)CO_2Me$	29.7	29.7	27.8
i-PrNHCOCH(CN)CO_2Me	+	$H_2C=CH_2$	=	i-PrNHCOCH_3	+	$CH_2=C(CN)CO_2Me$	-8.3	-8.3	-9.9
i-PrNHC(OH)=C(CN)COMe	+	$H_2C=CH_2$	=	i-PrNHC(OH)=CH_2	+	CH_2=C(CN)COMe	37.2	37.0	35.2
*i*i-PrNHCOCH(CN)COMe	+	$H_2C=CH_2$	=	i-PrNHCOCH_3	+	CH_2=C(CN)COMe	-8.4	-8.3	-10.7
PhNHC(OH)=$C(CO_2Me)_2$	+	$H_2C=CH_2$	=	PhNHC(OH)=CH_2	+	$CH_2=C(CO_2Me)_2$	30.1	30.4	27.4
PhNHCOCH$(CO_2Me)_2$	+	$H_2C=CH_2$	=	PhNHCOCH_3	+	$CH_2=C(CO_2Me)_2$	-4.9	-5.5	-5.5
PhNHC(OH)=C(COMe)CO_2Me	+	$H_2C=CH_2$	=	PhNHC(OH)=CH_2	+	$CH_2=C(COMe)CO_2Me$	34.7	34.1	31.9
PhNHCOCH(COMe)CO_2Me	+	$H_2C=CH_2$	=	PhNHCOCH_3	+	$CH_2=C(COMe)CO_2Me$	-14.9	-15.7	-13.9
PhNHC(OH)=$C(COMe)_2$	+	$H_2C=CH_2$	=	PhNHC(OH)=CH_2	+	$CH_2=C(COMe)_2$	32.7	32.3	30.4
PhNHCOCH$(COMe)_2$	+	$H_2C=CH_2$	=	PhNHCOCH_3	+	$CH_2=C(COMe)_2$	-4.2	-5.1	-4.2
PhNHC(OH)=C(CN)CO_2Me	+	$H_2C=CH_2$	=	PhNHC(OH)=CH_2	+	$CH_2=C(CN)CO_2Me$	27.0	26.9	24.4
PhNHCOCH(CN)CO_2Me	+	$H_2C=CH_2$	=	PhNHCOCH_3	+	$CH_2=C(CN)CO_2Me$	-8.9	-9.5	-9.8
PhNHC(OH)=C(CN)COMe	+	$H_2C=CH_2$	=	PhNHC(OH)=CH_2	+	CH_2=C(CN)COMe	35.5	34.9	32.3
PhNHCOCH(CN)COMe	+	$H_2C=CH_2$	=	PhNHCOCH_3	+	CH_2=C(CN)COMe	-11.6	-12.0	-12.9

Table S12. Analytical data, mps and yields of the formal amides R'NHCOCH(SO_2R)Y

Compound					Calculated %			Found %		
No.	R	Formula	mp, ˚C	yield, %	C	H	N	C	H	N
5a/6a	Ph	$C_{12}H_{13}NO_5S$	205-206	88	57.66	4.50	4.20	57.88	4.72	3.90
5b/6b	2.4-$(MeO)_2C_6H_3$	$C_{18}H_{19}NO_7S$	211-212	92	54.96	4.83	3.56	54.93	4.92	3.81
5c/6c	*i*-Pr	$C_{13}H_{17}NO_5S$	182-183	76	52.12	5.69	4.68	52.36	5.87	4.66
5d/6d	*t*-Bu	$C_{14}H_{19}NO_5S$	196-197	77	53.67	6.07	4.47	53.77	6.20	4.48
5e/6e	Ph	$C_{20}H_{17}NO_5S_2$	216-217[a]	90	57.83	4.10	3.37	57.82	4.39	3.30
5f/6f	2.4-$(MeO)_2C_6H_3$	$C_{22}H_{21}NO_7S_2$	202-203	42	55.67	4.45	2.95	55.46	4.26	2.80
5g/6g	*i*-Pr	$C_{17}H_{19}NO_5S_2$	205-206	87	53.54	4.99	3.67	53.77	5.07	3.81
5h/6h	*t*-Bu	$C_{18}H_{21}NO_5S_2$	199-200	47	54.66	5.35	3.54	54.75	5.16	3.24
5i/6i	Ph	$C_{15}H_{15}NO_4S_2$	208-210	89	50.99	4.25	3.97	50.66	4.53	3.87
5j/6j	*i*-Pr	$C_{12}H_{17}NO_5S_2$	201-202	82	45.14	5.33	4.39	45.08	5.30	4.40
5k/6k	Ph	$C_{15}H_{12}N_2O_3S$	220-221	93	59.99	4.03	9.33	59.70	3.75	9.16
5l/6l	*i*-Pr	$C_{12}H_{14}N_2O_3S$	209-210	86	54.12	5.30	10.52	54.13	5.17	10.39
5m/6m	Ph	$C_{10}H_{10}N_2O_3S$	214-215	87	50.41	4.23	11.76	50.11	4.06	11.49
5n/6n	*i*-Pr	$C_7H_{12}N_2O_3S$	204-205	82	41.37	5.46	13.78	41.67	5.19	14.01
5o/6o/7o	Ph	$C_{14}H_{10}F_9NO_4S$	177-178	92	36.60	2.18	3.05	36.77	2.37	2.83

[a] (lit. Dubenko, R.G.; Neplyuev, V.M.; Pel'kis, P.S., *Zhur. Organ. Khim.*, **1968**, 4, 453; *Chem. Abstr.*, **1968**, 104664) mp 215-216 ˚C.

Figure S1. ORTEP structure of compound **7o**

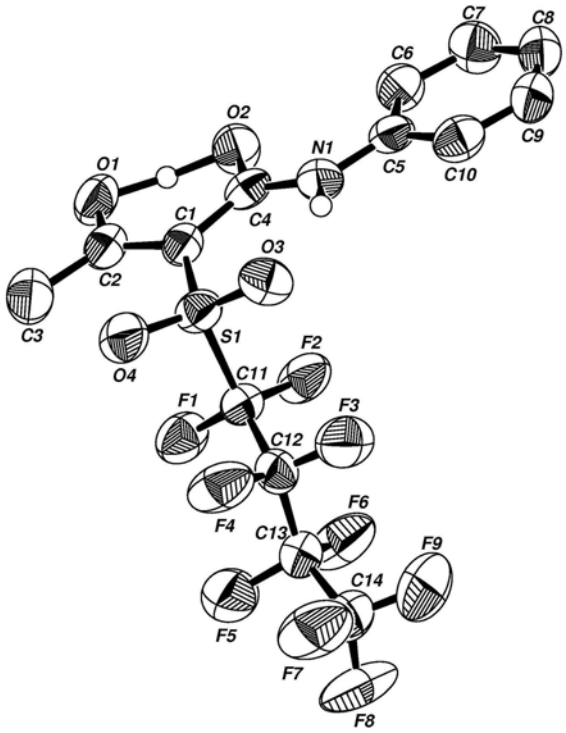
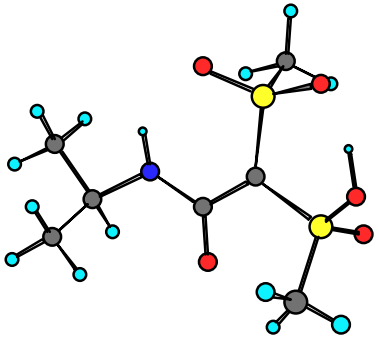


Figure S2. Calculated Structures

i-PrNHCOC=(SMe(=O) OH)SO_2Me



i-PrNHCOC=(S(Ph)(=O)OH)SO_2Ph

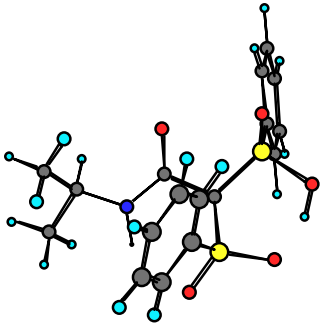
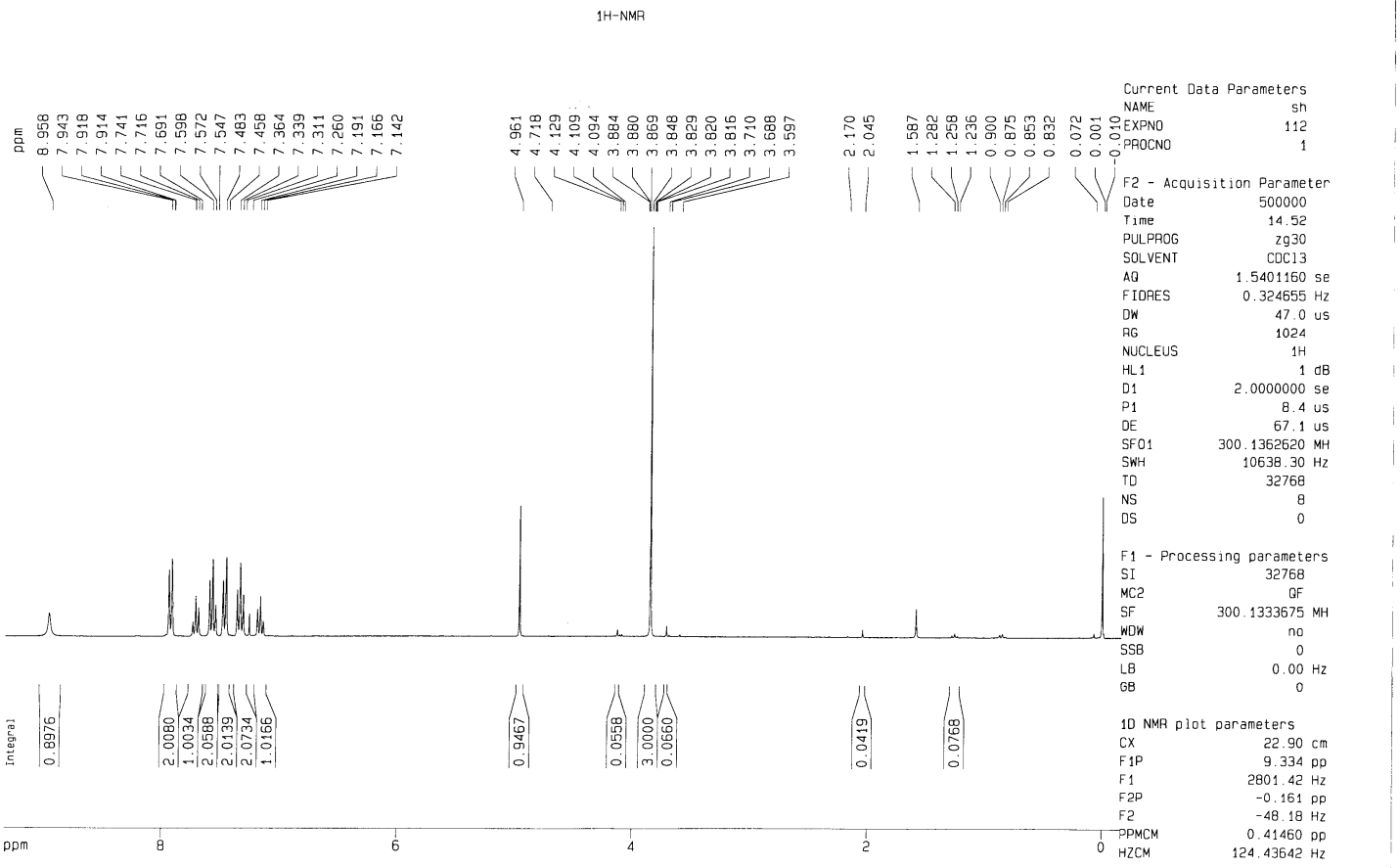


Figure S3. ^{1}H and ^{13}C NMR spectra of the compounds **5a-n** and **7o**.

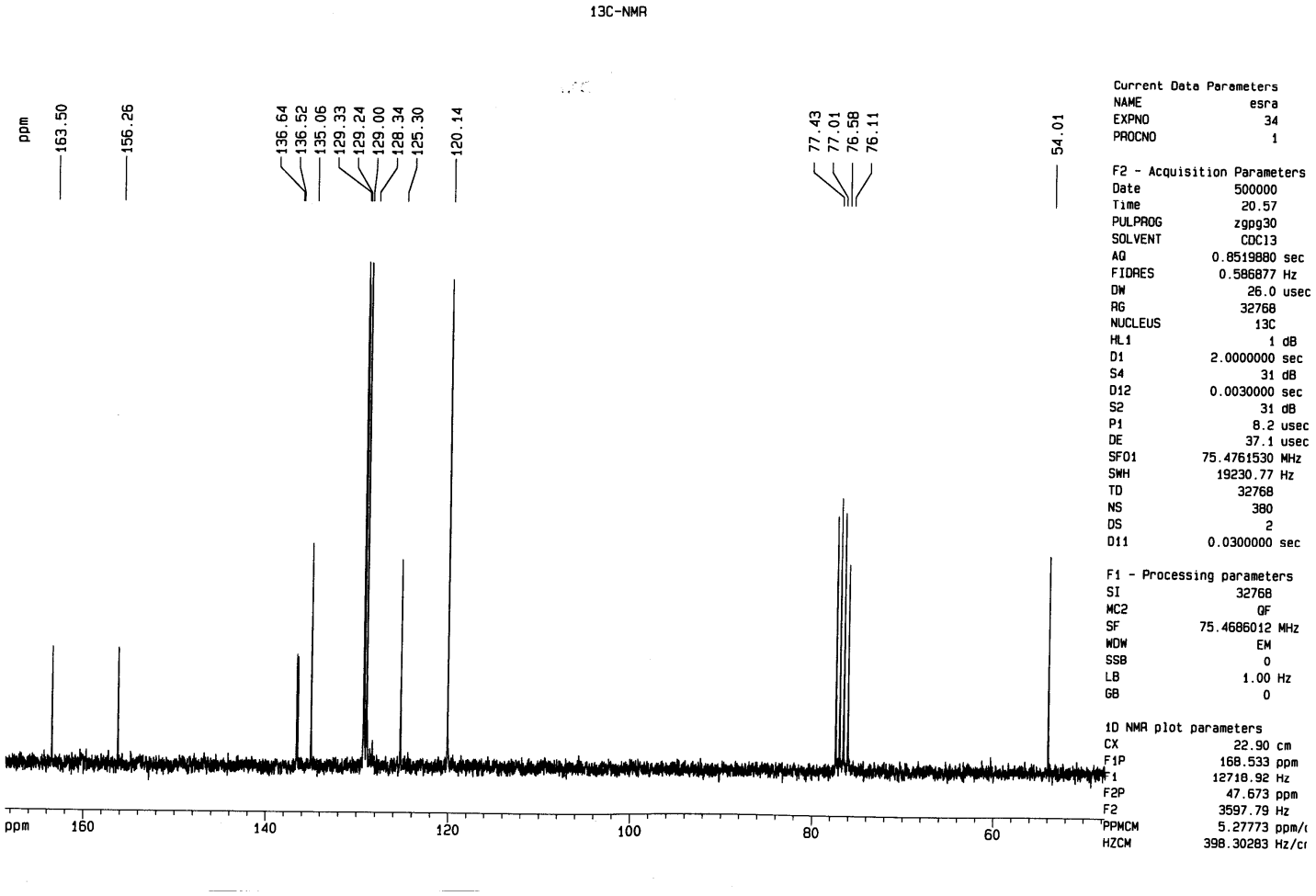
^{1}H NMR spectrum of **5a**.

PhNHCOCH(CO_2Me)SO_2Ph in $CDCl_3$



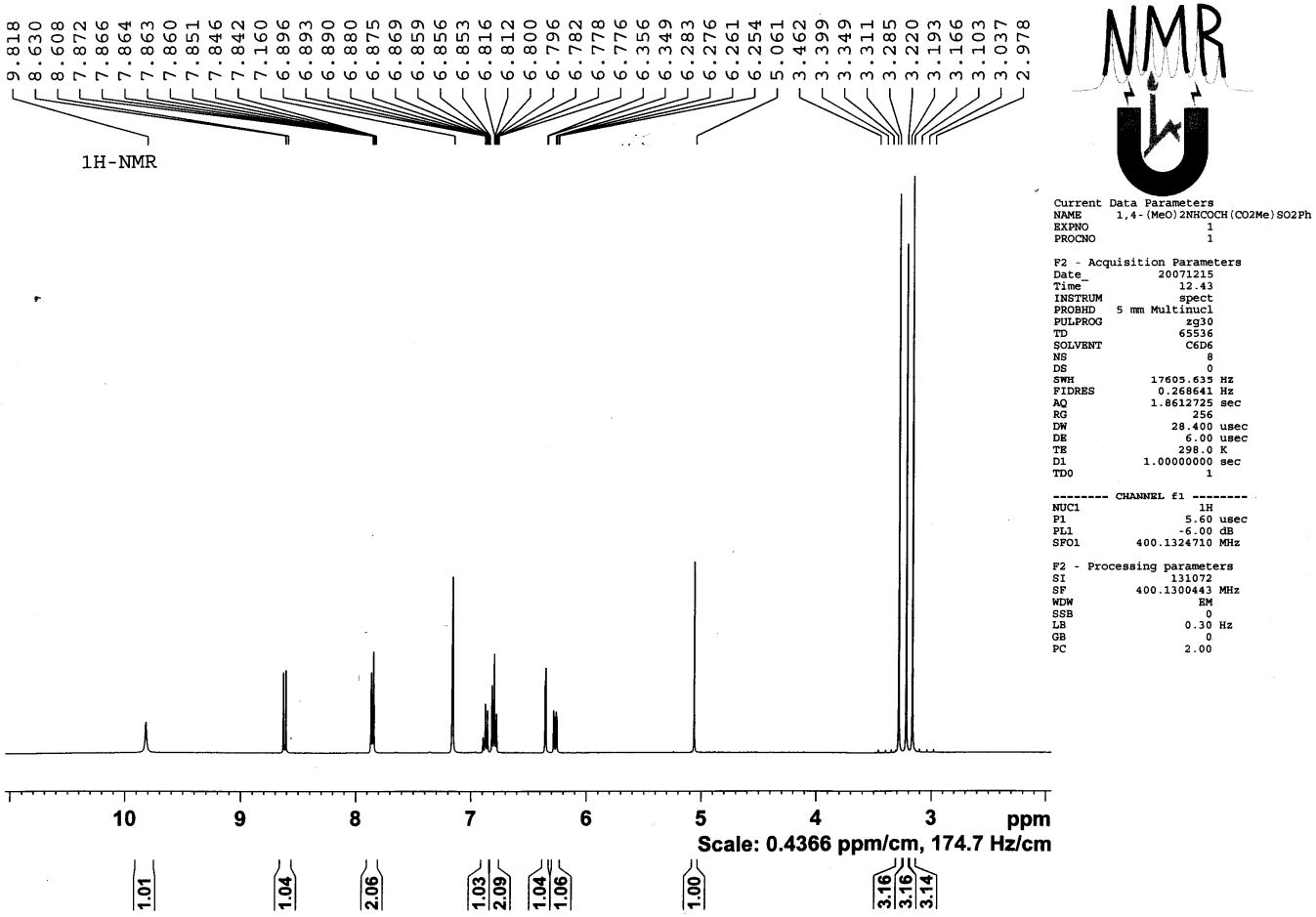
^{13}C NMR spectrum of **5a**.

PhNHCOCH(CO_2Me)SO_2Ph in $CDCl_3$



^{1}H NMR spectrum of **5b**.

2,4-$(MeO)_2NHCOCH(CO_2Me)SO_2Ph$ in C_6D_6

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Current Data Parameters
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EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
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Time              12.43
INSTRUM           spect
PROBHD   5 mm Multinucl
PULPROG           zg30
TD               65536
SOLVENT           C6D6
NS                   8
DS                   0
SWH          17605.635 Hz
FIDRES        0.268641 Hz
AQ            1.8612725 sec
RG                 256
DW              28.400 usec
DE               6.00 usec
TE              298.0 K
D1           1.00000000 sec
TD0                  1

-------- CHANNEL f1 --------
NUC1                 1H
P1                5.60 usec
PL1              -6.00 dB
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 131072
SF          400.1300443 MHz
WDW                  EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                2.00
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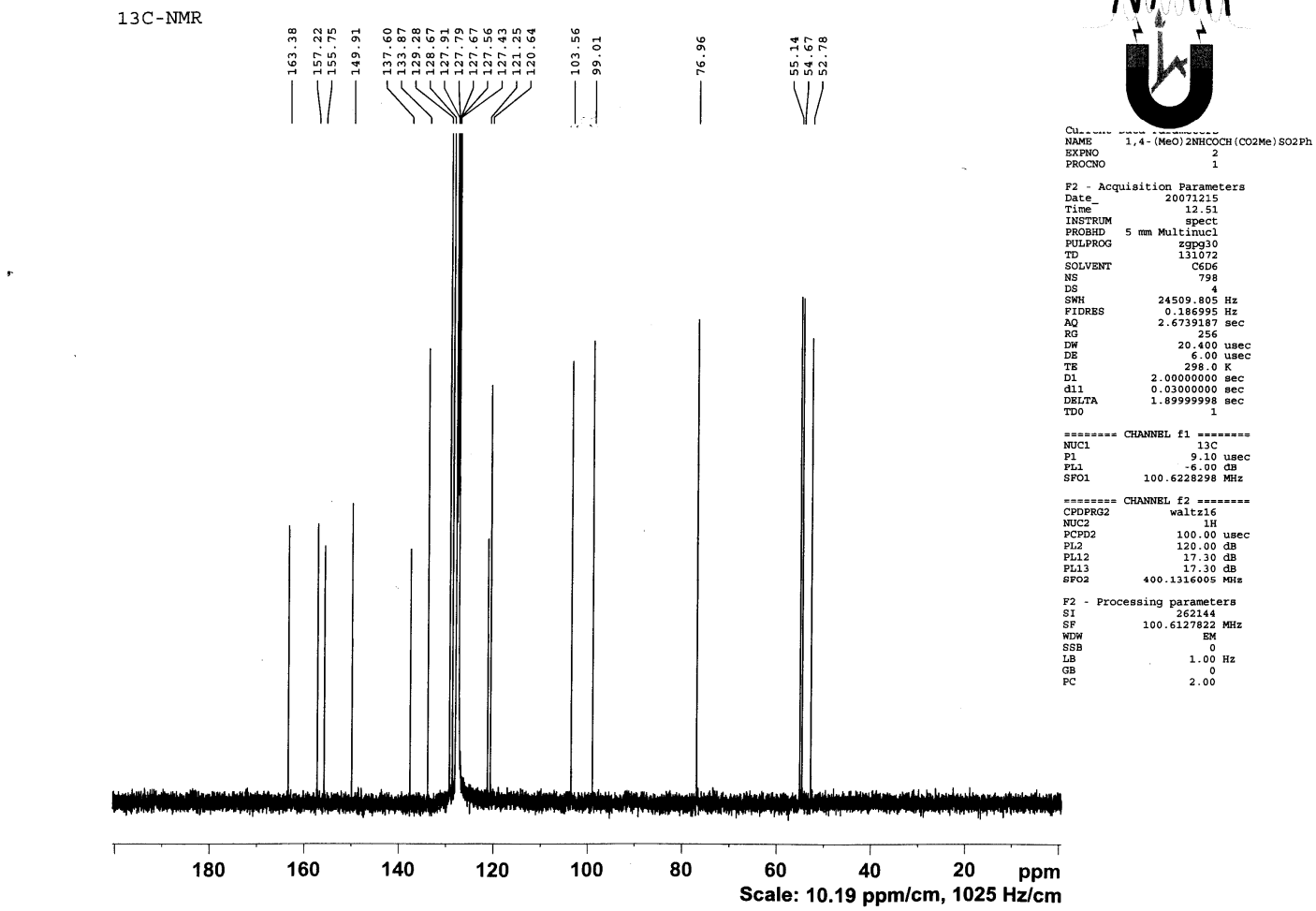
^{13}C NMR spectrum of **5b**.

2,4-$(MeO)_2NHCOCH(CO_2Me)SO_2Ph$ in C_6D_6



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PROCNO	1
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PULPROG	zgpg30
TD	131072
SOLVENT	C6D6
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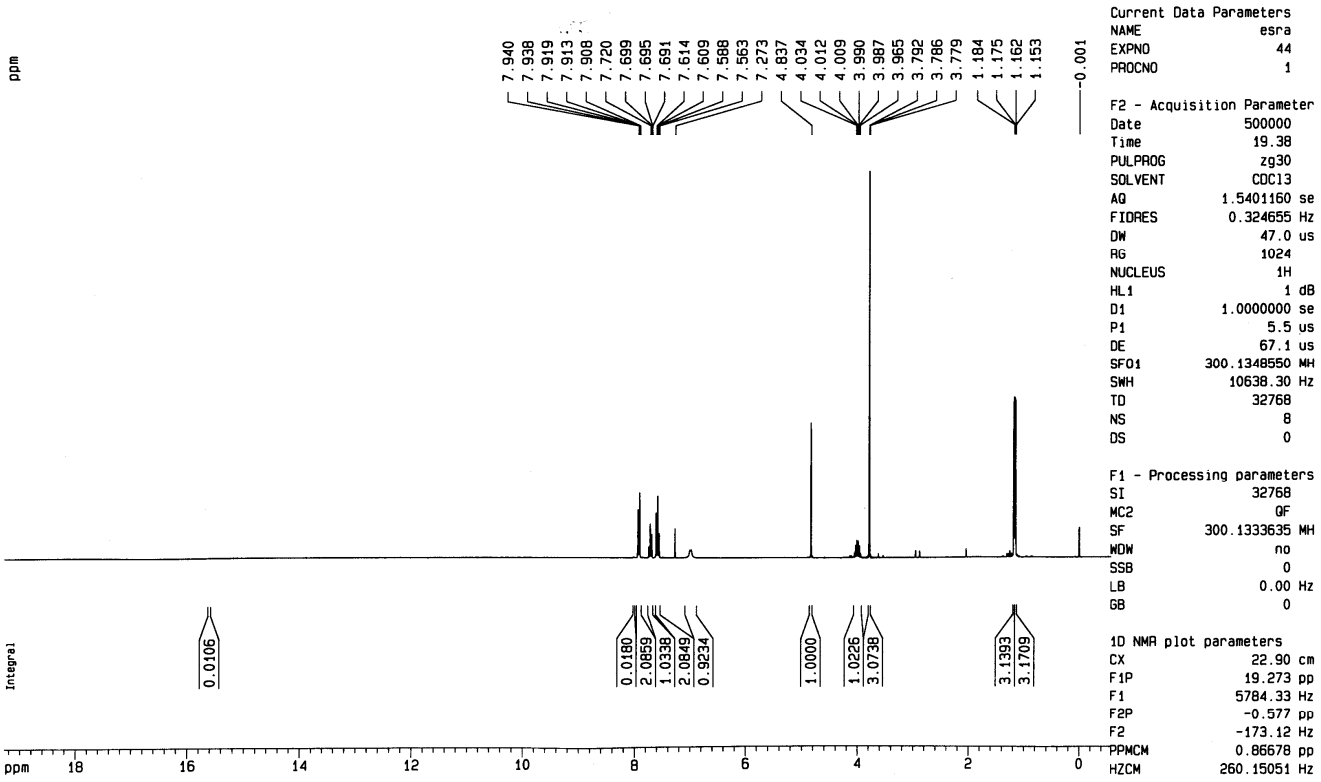
DS	4
SWH	24509.805 Hz
FIDRES	0.186995 Hz
AQ	2.6739187 sec
RG	256
DW	20.400 usec
DE	6.00 usec
TE	298.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.10 usec
PL1	-6.00 dB
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	100.00 usec
PL2	120.00 dB
PL12	17.30 dB
PL13	17.30 dB
SFO2	400.1316005 MHz
F2 - Processing parameters	
SI	262144
SF	100.6127822 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	2.00

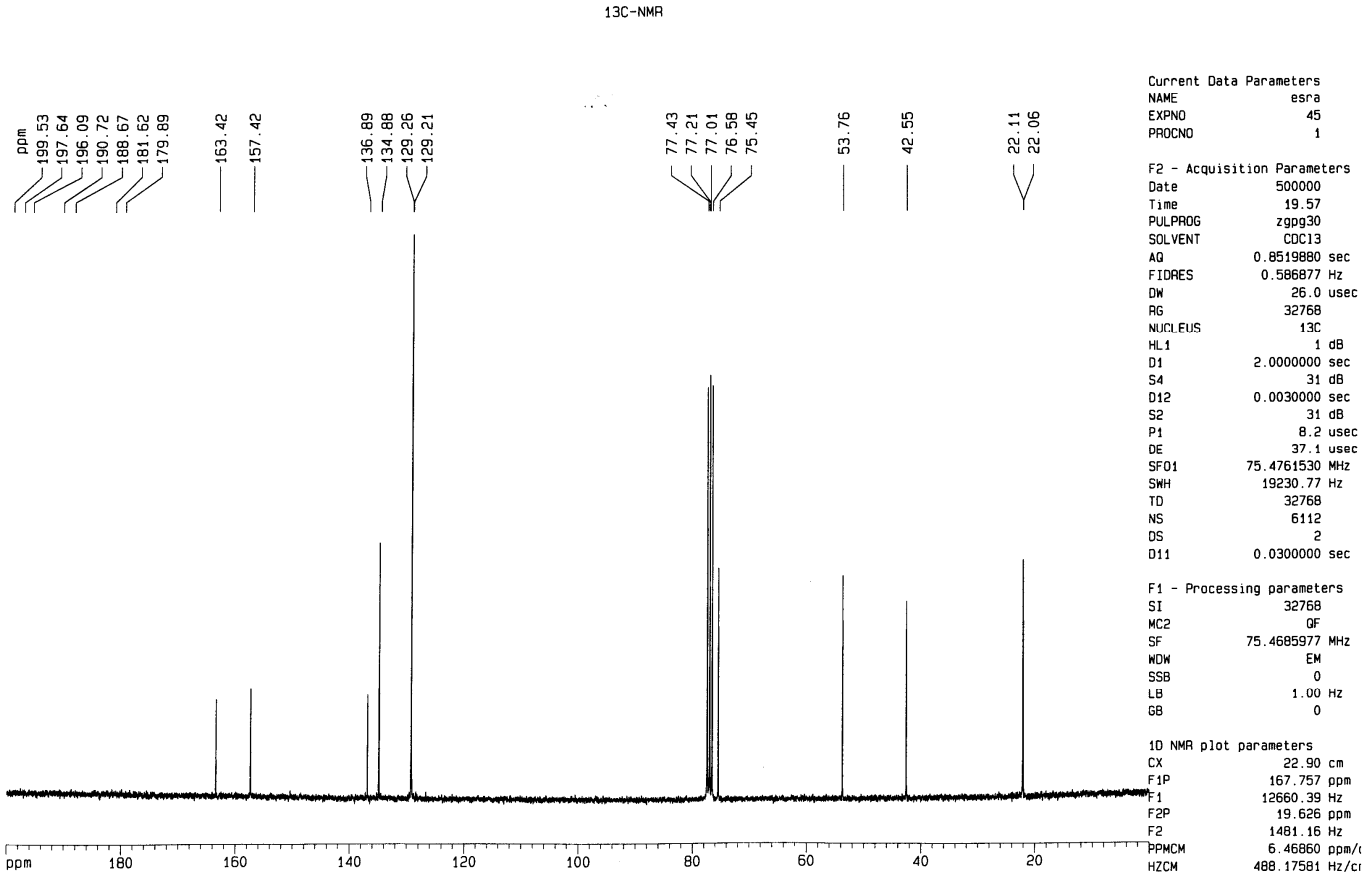
^{1}H NMR spectrum of **5c**.

i-PrNHCOCH(CO_2Me)SO_2Ph in $CDCl_3$



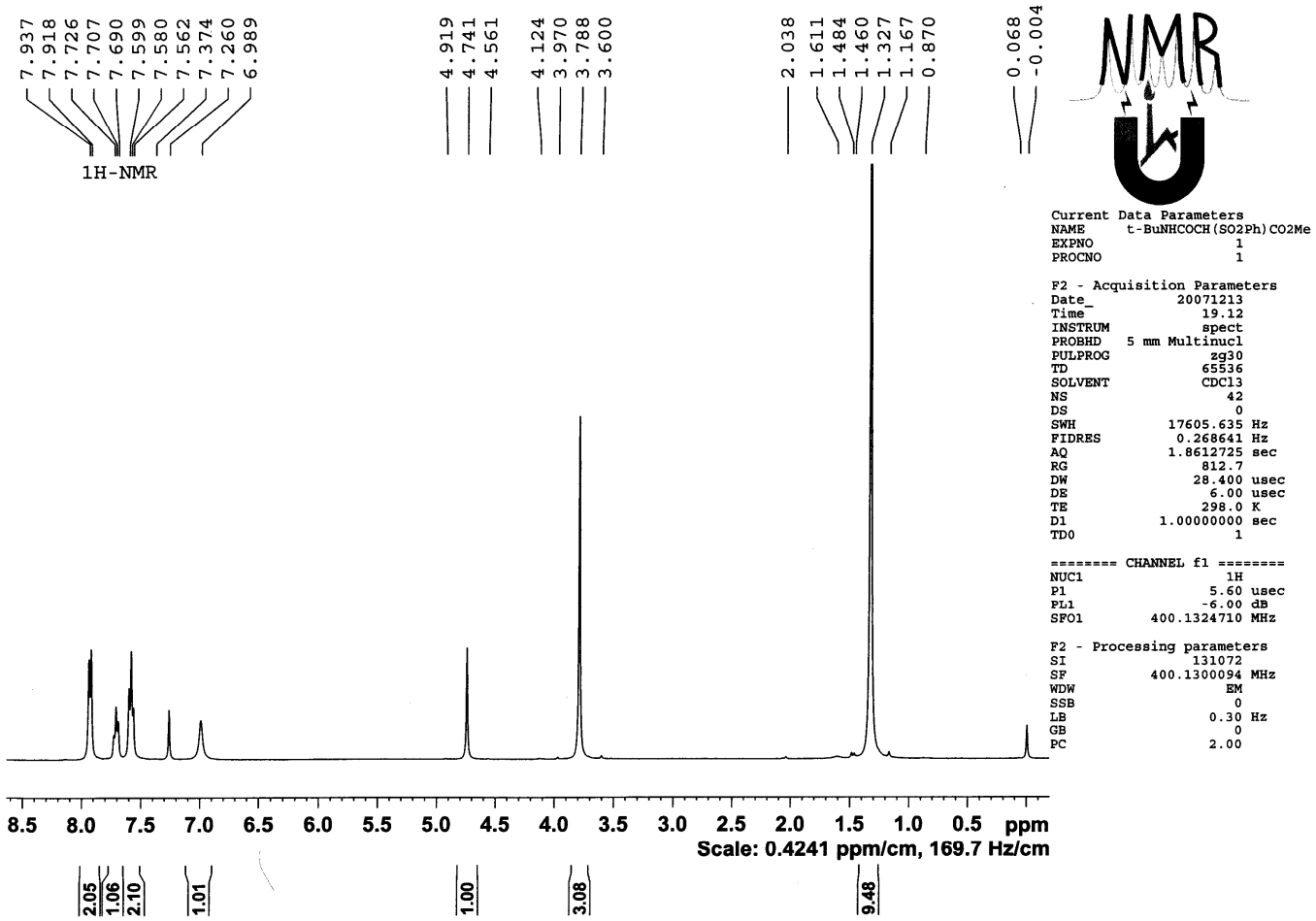
^{13}C NMR spectrum of **5c**.

i-PrNHCOCH(CO_2Me)SO_2Ph in $CDCl_3$



^{1}H NMR spectrum of **5d**.

t-BuNHCOCH(CO_2Me)SO_2Ph in $CDCl_3$

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PROCNO                         1

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Time                       19.12
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PULPROG                    zg30
TD                        65536
SOLVENT                   CDCl3
NS                           42
DS                            0
SWH                   17605.635 Hz
FIDRES                 0.268641 Hz
AQ                     1.8612725 sec
RG                         812.7
DW                        28.400 usec
DE                         6.00 usec
TE                        298.0 K
D1                    1.00000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                          1H
P1                         5.60 usec
PL1                       -6.00 dB
SFO1                400.1324710 MHz

F2 - Processing parameters
SI                        131072
SF                  400.1300094 MHz
WDW                           EM
SSB                            0
LB                          0.30 Hz
GB                             0
PC                          2.00
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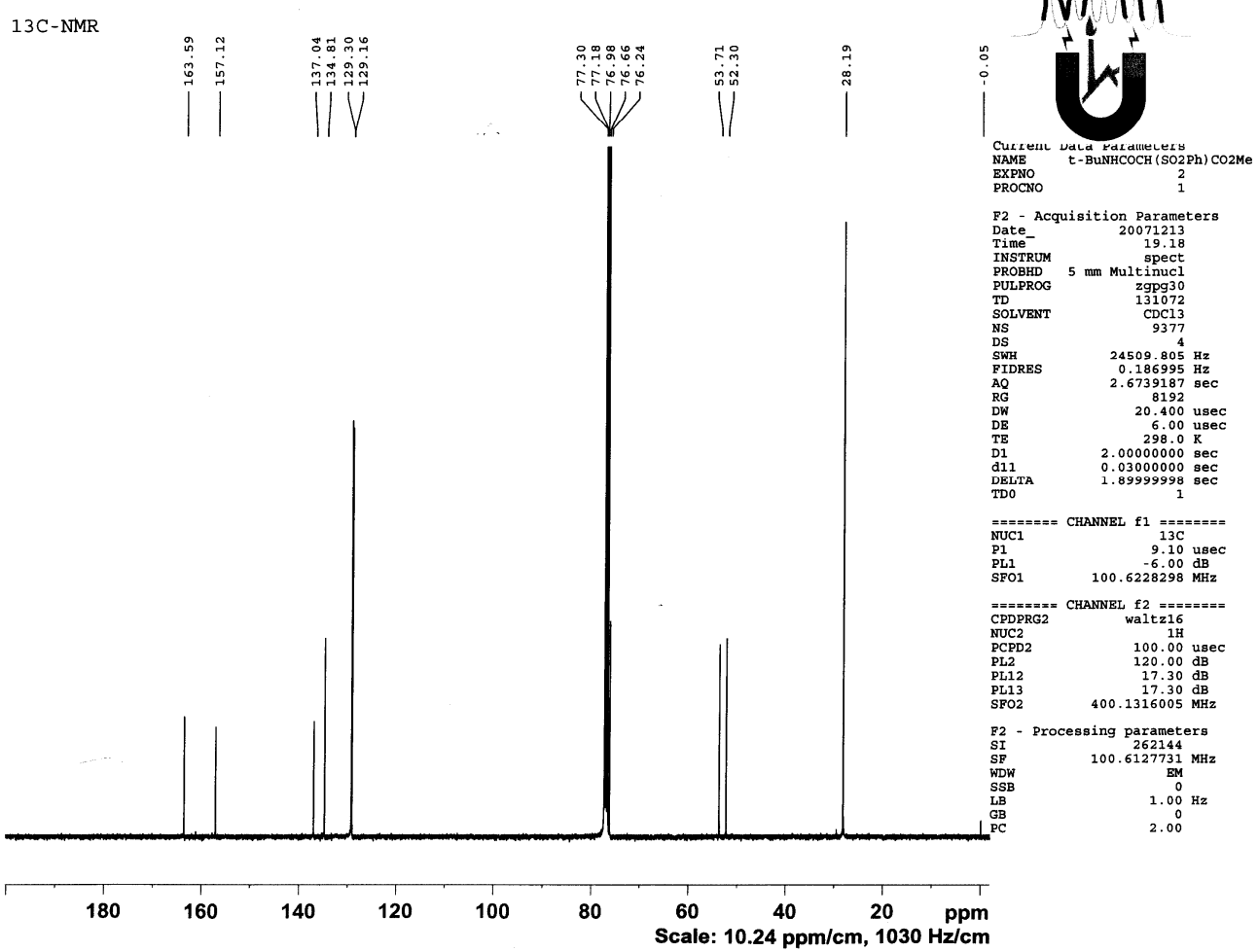
^{13}C NMR spectrum of **5d**.

t-BuNHCOCH(CO_2Me)SO_2Ph in $CDCl_3$



Current Data Parameters
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EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
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Time 19.18
INSTRUM spect
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PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 9377
DS 4
SWH 24509.805 Hz
FIDRES 0.186995 Hz
AQ 2.6739187 sec
RG 8192
DW 20.400 usec
DE 6.00 usec
TE 298.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

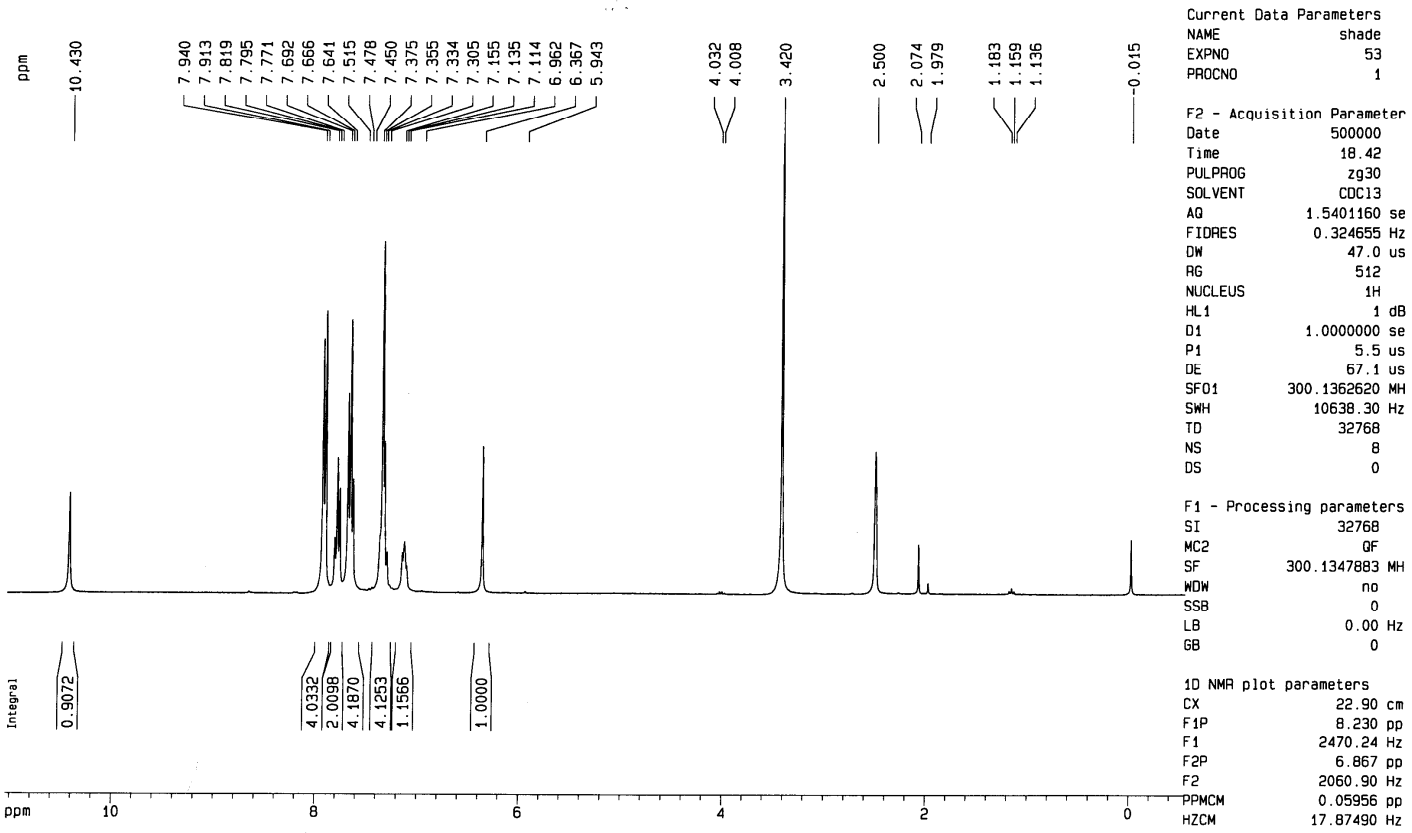
======== CHANNEL f1 ========
NUC1 13C
P1 9.10 usec
PL1 -6.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 17.30 dB
PL13 17.30 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 262144
SF 100.6127731 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00

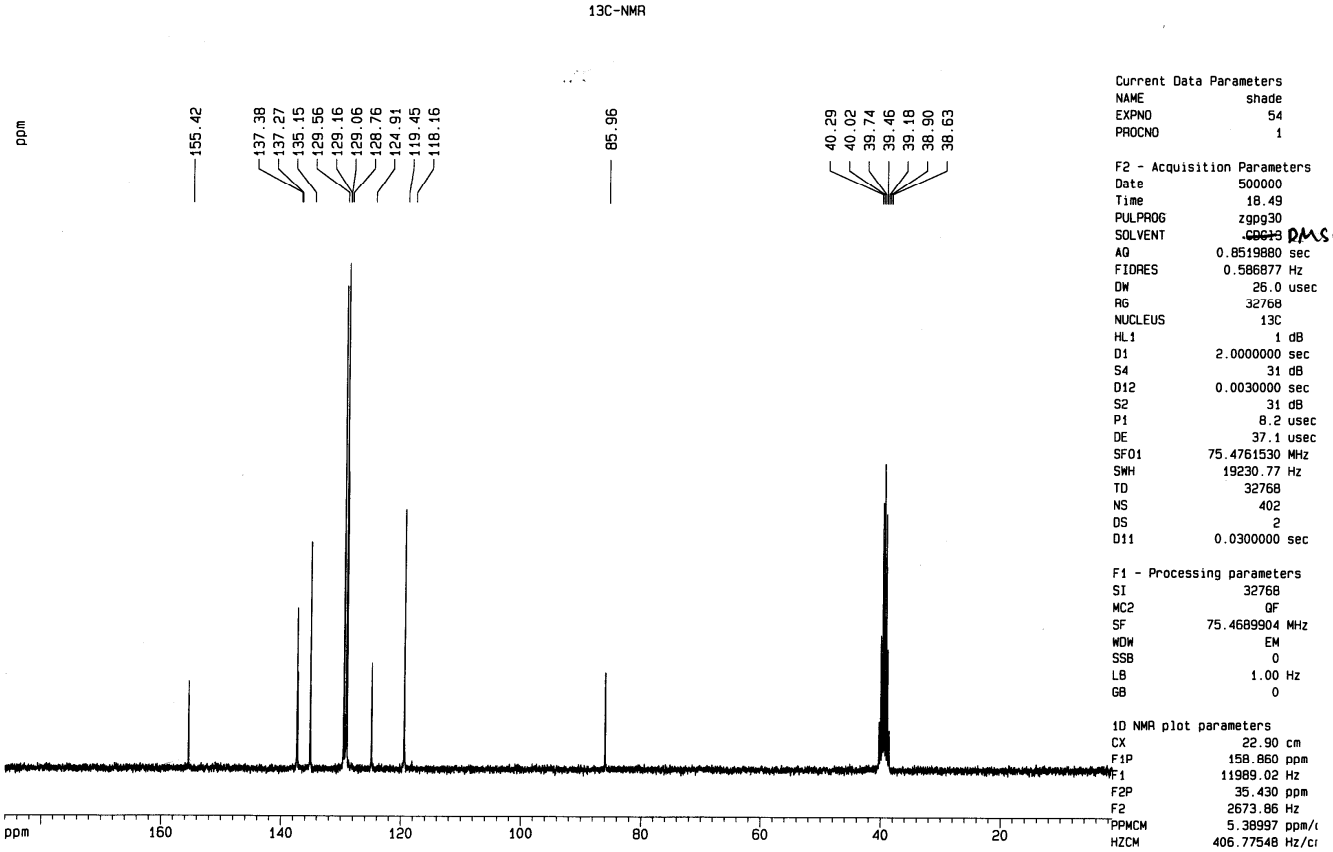
^{1}H NMR spectrum of **5e**.

PhNHCOCH(SO_2Ph)$_2$ in DMSO-d_6



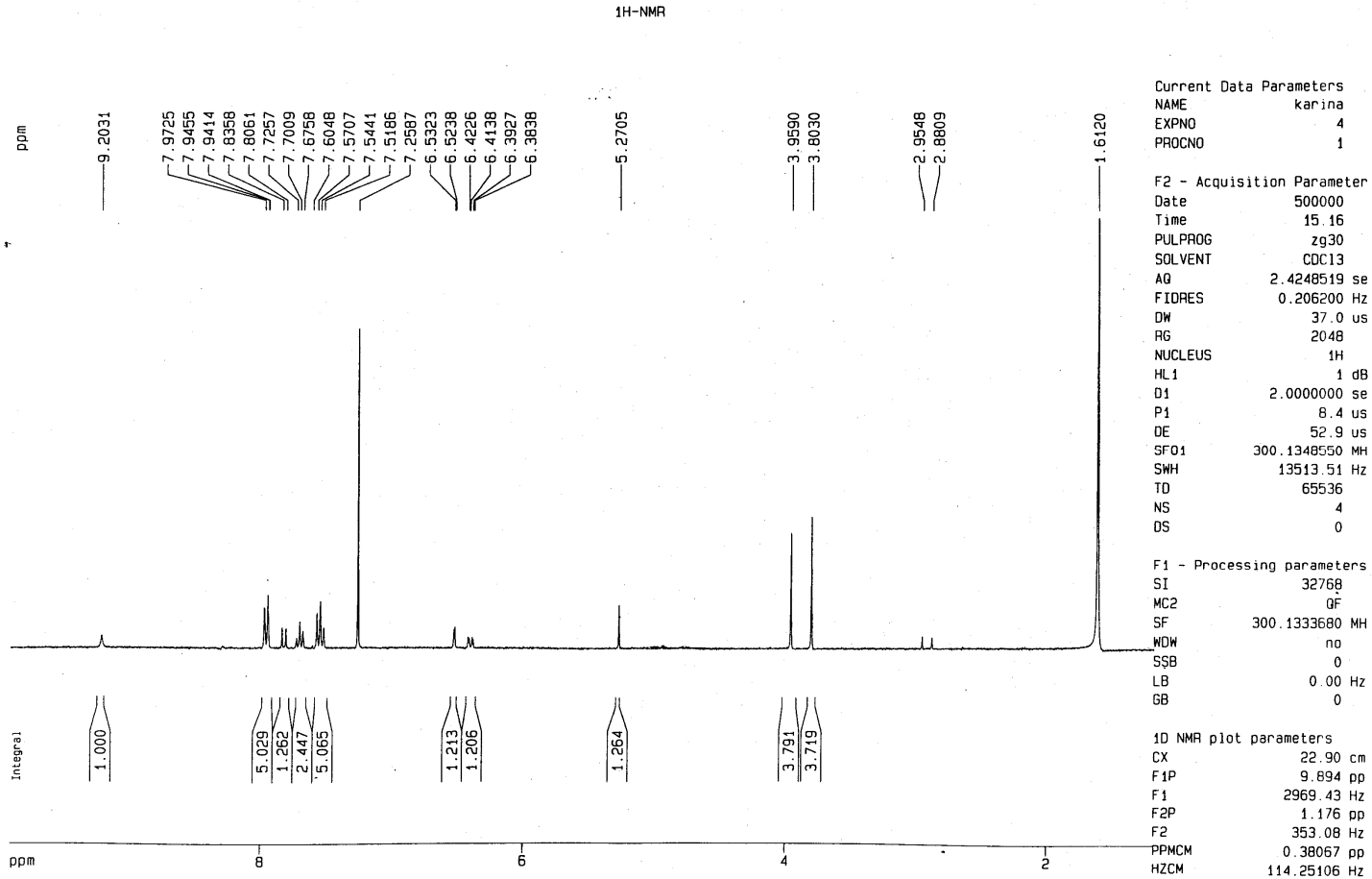
^{13}C NMR spectrum of **5e**.

PhNHCOCH(SO_2Ph)$_2$ in DMSO-d_6



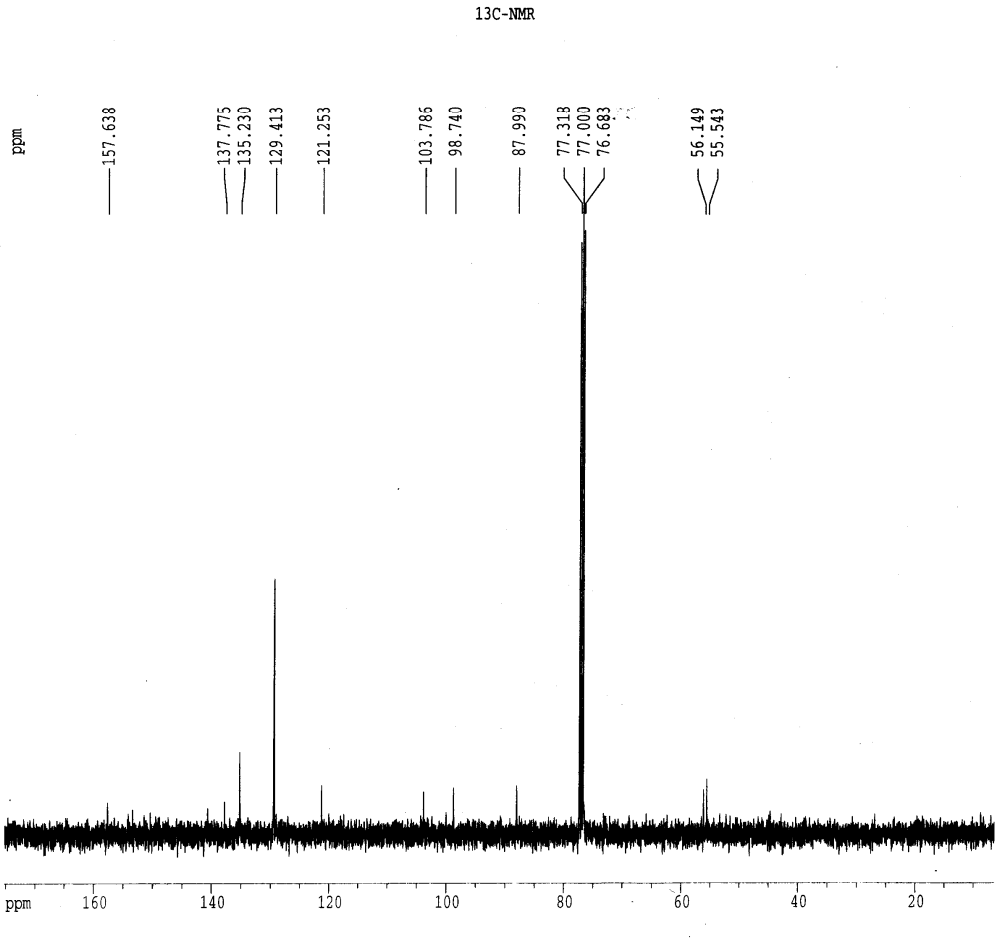
^{1}H NMR spectrum of **5f**.

2,4-$(MeO)_2C_6H_3NHCOCH(SO_2Ph)_2$ in $CDCl_3$



^{13}C NMR spectrum of **5f**.

2,4-$(MeO)_2C_6H_3NHCOCH(SO_2Ph)_2$ in $CDCl_3$

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Current Data Parameters
NAME                  karina
EXPNO                      5
PROCNO                     1

F2 - Acquisition Parameters
Date_              20051128
Time                  14.17
INSTRUM             drx400
PROBHD     5 mm Multinu
PULPROG             zgpg30
TD                    65536
SOLVENT               cdcl3
NS                      200
DS                        4
SWH               24271.844 Hz
FIDRES             0.370359 Hz
AQ                 1.3500916 sec
RG                     8192
DW                    20.600 usec
DE                    30.00 usec
TE                    300.0 K
D1                 1.00000000 sec
D11                0.03000000 sec
D12                0.00002000 sec

============ CHANNEL f1 =============
NUC1                     13C
P1                      8.98 usec
PL1                    -6.00 dB
SFO1             100.6247019 MHz

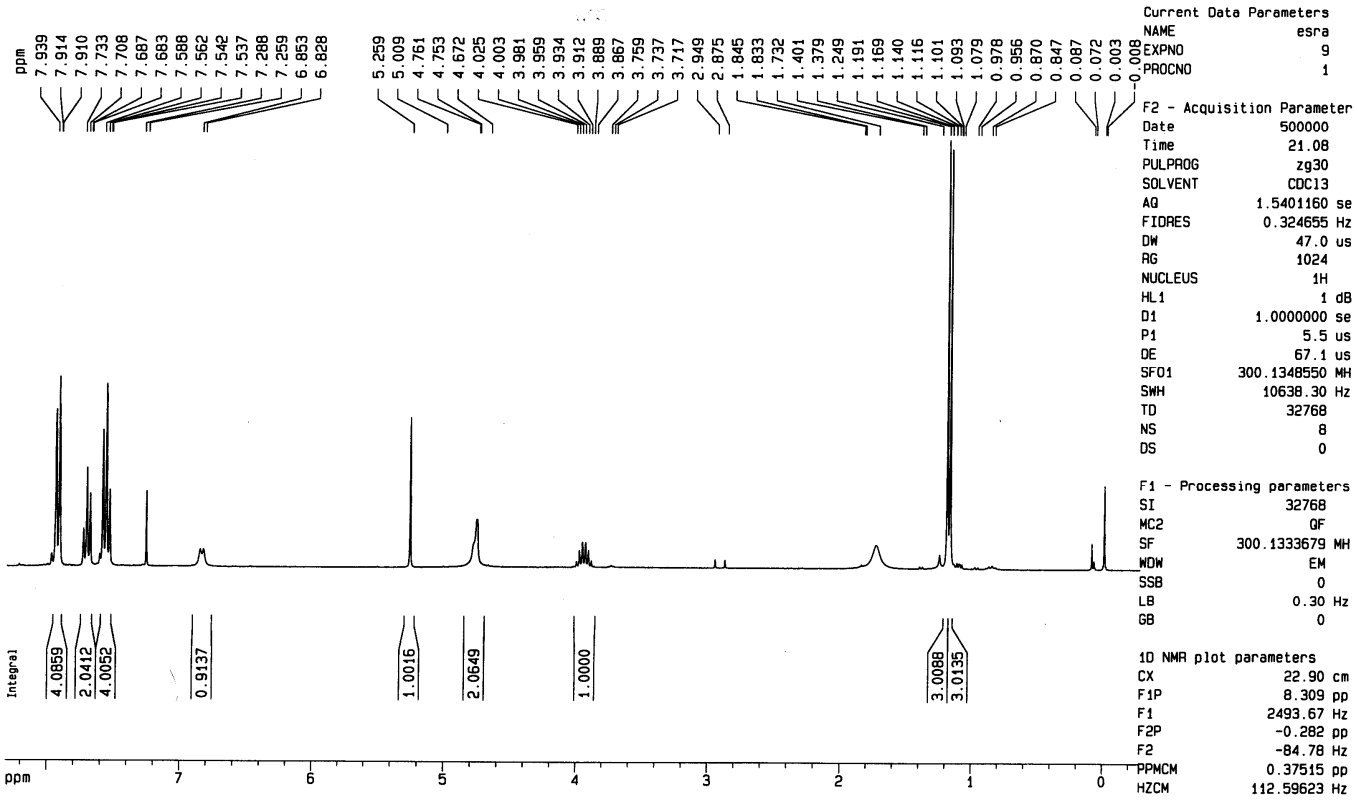
============ CHANNEL f2 =============
CPDPRG2              waltz16
NUC2                     1H
PCPD2                100.00 usec
PL2                  120.00 dB
PL12                  18.20 dB
PL13                  18.20 dB
SFO2             400.1316005 MHz

F2 - Processing parameters
SI                       32768
SF               100.6127719 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40

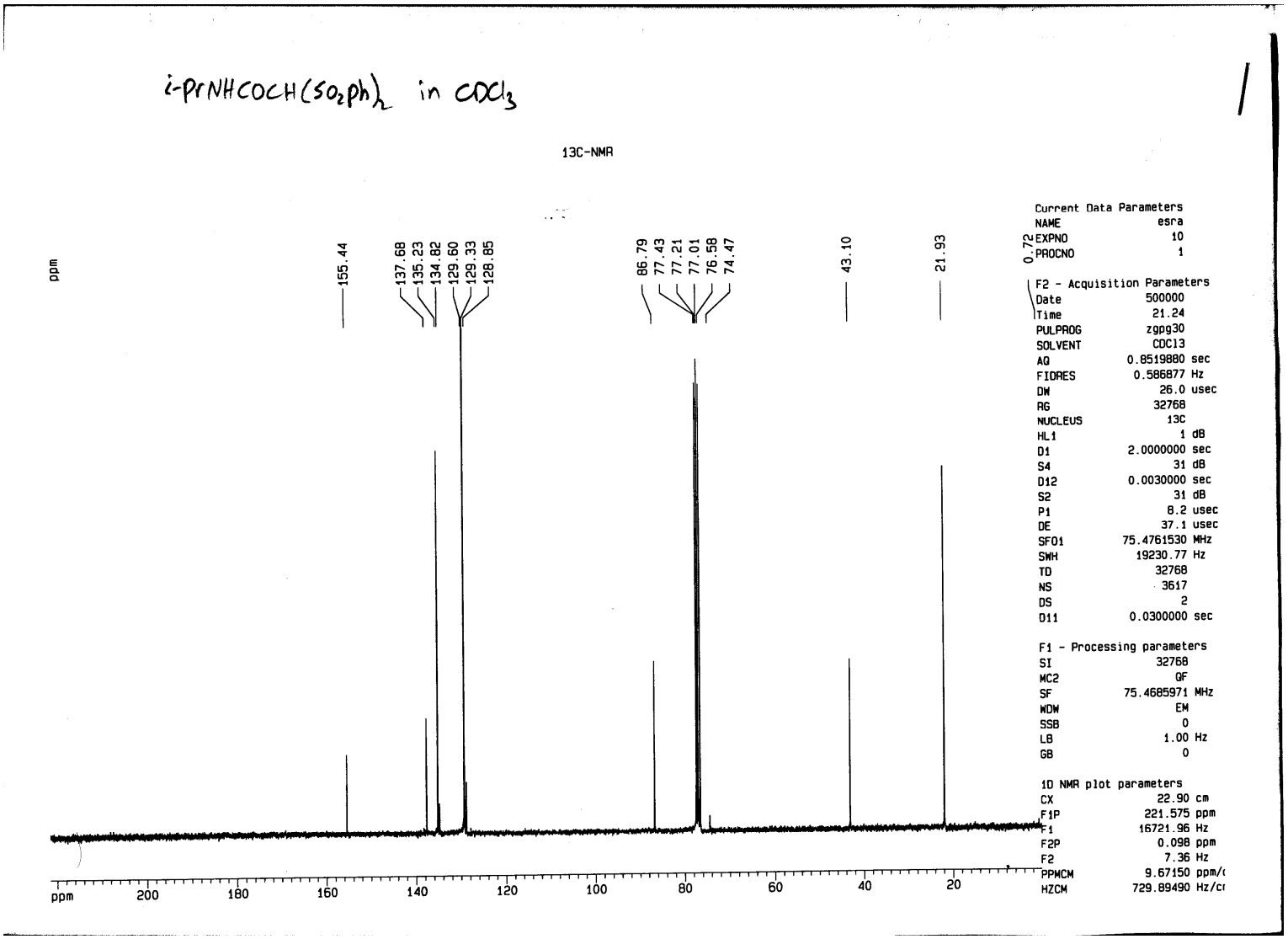
1D NMR plot parameters
CX                       20.00 cm
F1P                     175.231 ppm
F1                    17630.47 Hz
F2P                       6.395 ppm
F2                     643.45 Hz
PPMCM                 8.44178 ppm/cm
HZCM                849.35120 Hz/cm
```

^{1}H NMR spectrum of **5g**.

i-PrNHCOCH(SO_2Ph)$_2$ in $CDCl_3$

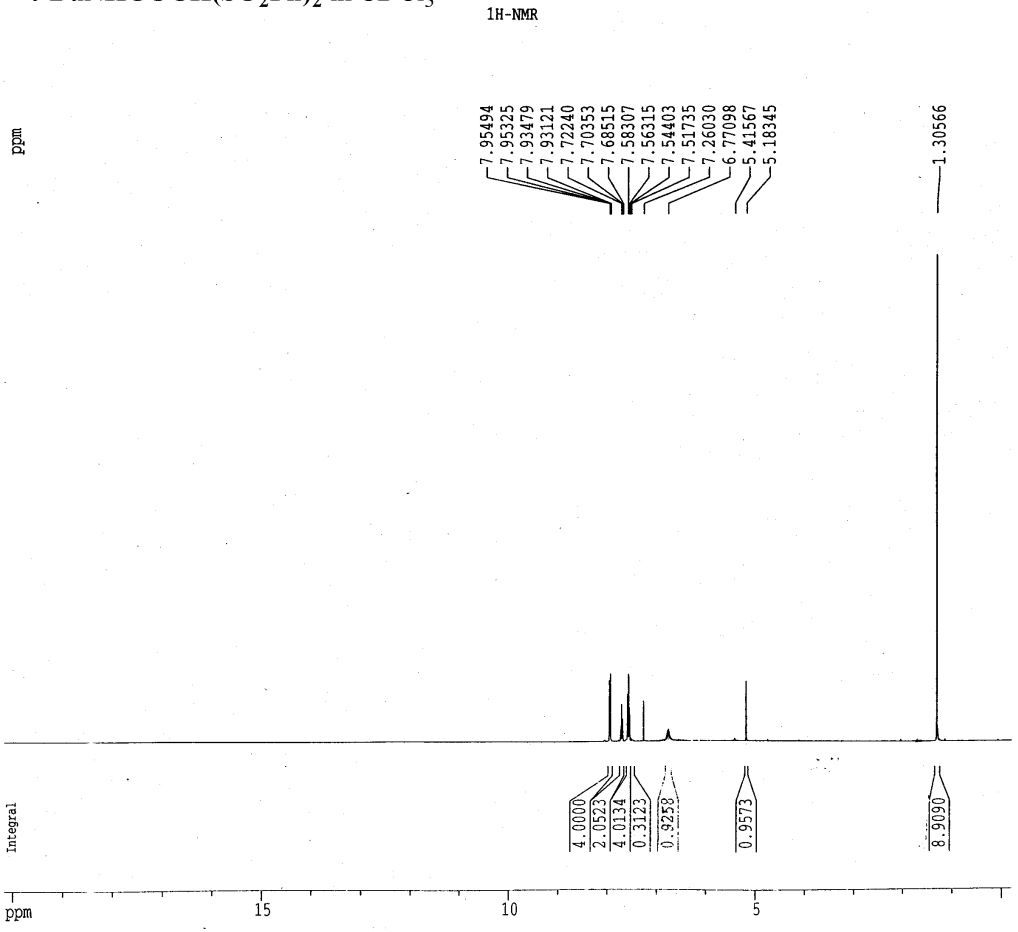


^{13}C NMR spectrum of **5g**.



^{1}H NMR spectrum of **5h**.

_t_-BuNHCOCH(SO$_2$Ph)$_2$ in $CDCl_3$

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Current Data Parameters
NAME
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PROCNO                 1

F2 - Acquisition Parameters
Date_           20051121
Time               14.14
INSTRUM          drx400
PROBHD     5 mm Multinu
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    0
SWH           17985.611 Hz
FIDRES         0.274439 Hz
AQ             1.8219508 sec
RG                  362
DW                27.800 usec
DE                10.00 usec
TE                300.0 K
D1             2.00000000 sec

============ CHANNEL f1 =============
NUC1                1H
P1                5.59 usec
PL1              -6.00 dB
SFO1        400.1320007 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300090 MHz
WDW                   no
SSB                    0
LB                 0.00 Hz
GB                     0
PC                 1.00

1D NMR plot parameters
CX                20.00 cm
F1P               20.174 ppm
F1              8072.24 Hz
F2P               -0.205 ppm
F2              -81.86 Hz
PPMCM           1.01893 ppm/cm
HZCM          407.70490 Hz/cm
```
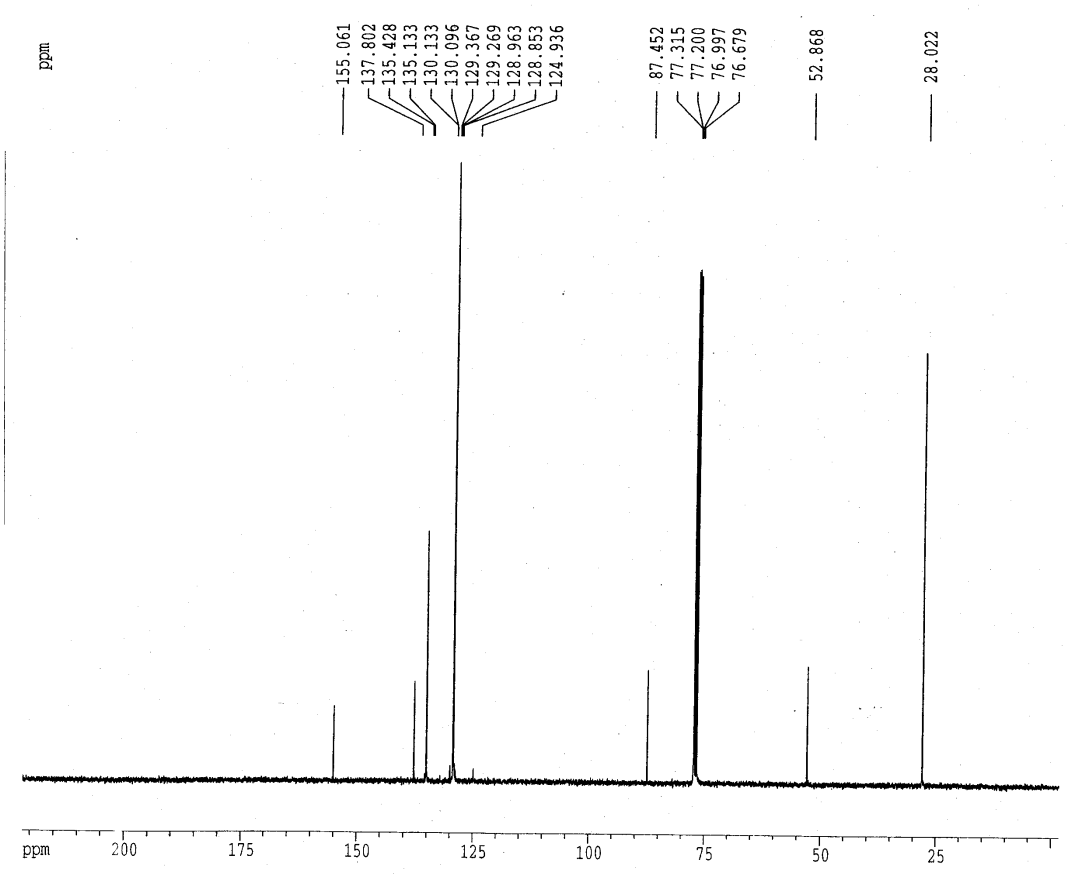


^{13}C NMR spectrum of **5h**.

-

***t*-BuNHCOCH(SO$_2$Ph)$_2$** in $CDCl_3$ 13C-NMR

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Current Data Parameters
NAME
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
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Time                14.27
INSTRUM            drx400
PROBHD     5 mm Multinu
PULPROG            zgpg30
TD                  65536
SOLVENT             cdcl3
NS                   3954
DS                      4
SWH           24271.844 Hz
FIDRES         0.370359 Hz
AQ            1.3500916 sec
RG                   8192
DW              20.600 usec
DE              30.00 usec
TE                300.0 K
D1           1.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec

============ CHANNEL f1 =============
NUC1                13C
P1                 8.98 usec
PL1               -6.00 dB
SFO1        100.6247019 MHz

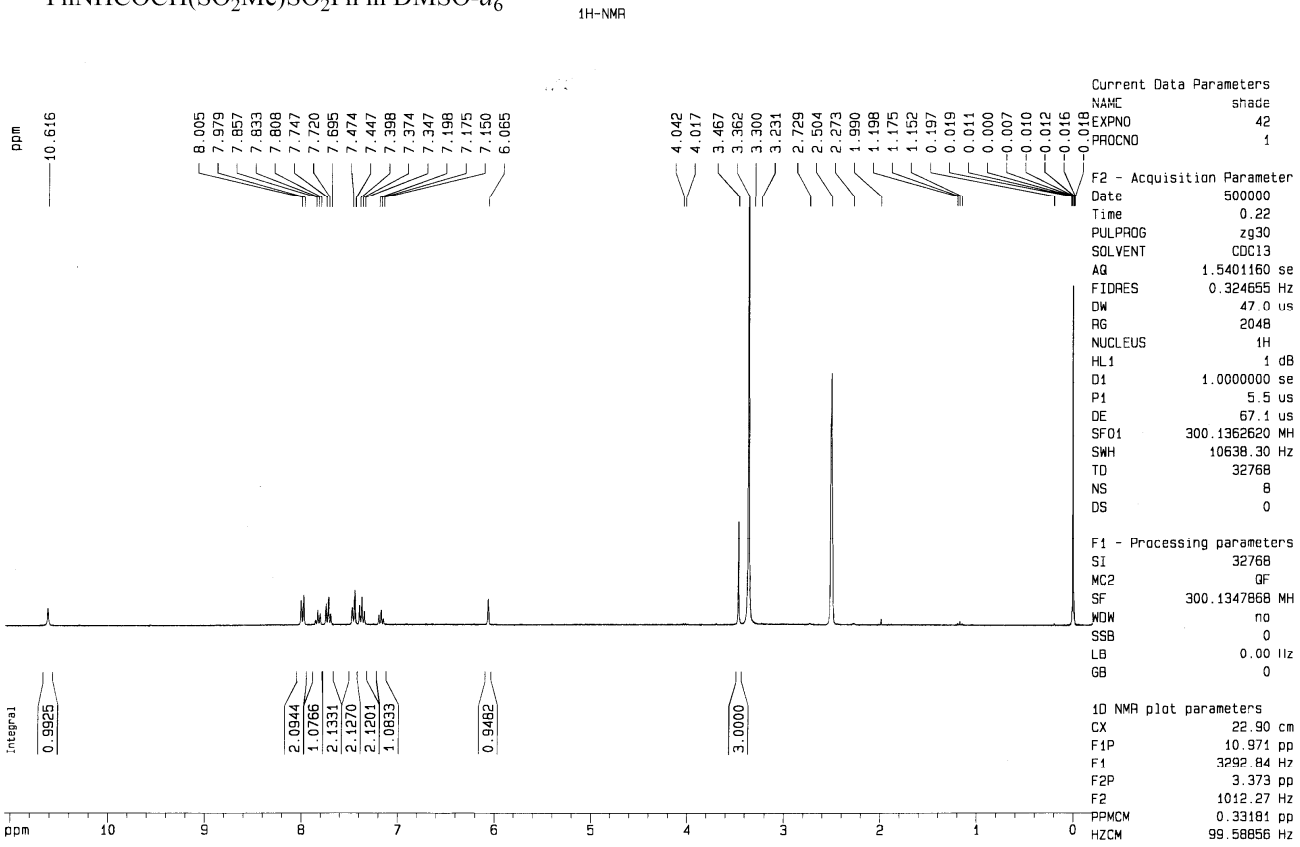
============ CHANNEL f2 =============
CPDPRG2         waltz16
NUC2                1H
PCPD2           100.00 usec
PL2             120.00 dB
PL12             18.20 dB
PL13             18.20 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                  32768
SF          100.6127734 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40

1D NMR plot parameters
CX                 20.00 cm
F1P              221.680 ppm
F1             22303.81 Hz
F2P               -1.749 ppm
F2              -175.94 Hz
PPMCM          11.17142 ppm/cm
HZCM         1123.98767 Hz/cm
```

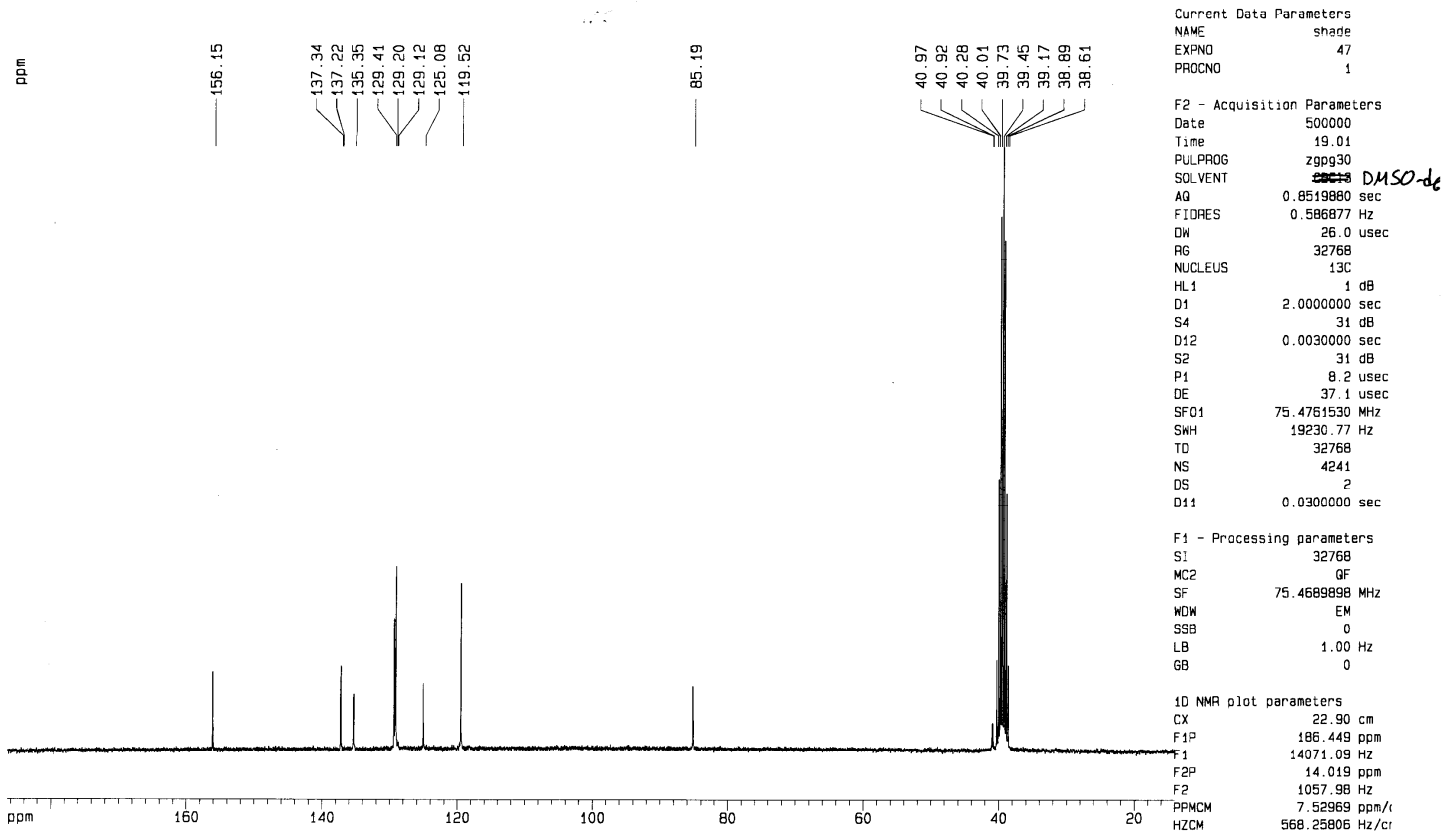

^{1}H NMR spectrum of **5i**.

PhNHCOCH(SO_2Me)SO_2Ph in DMSO-d_6



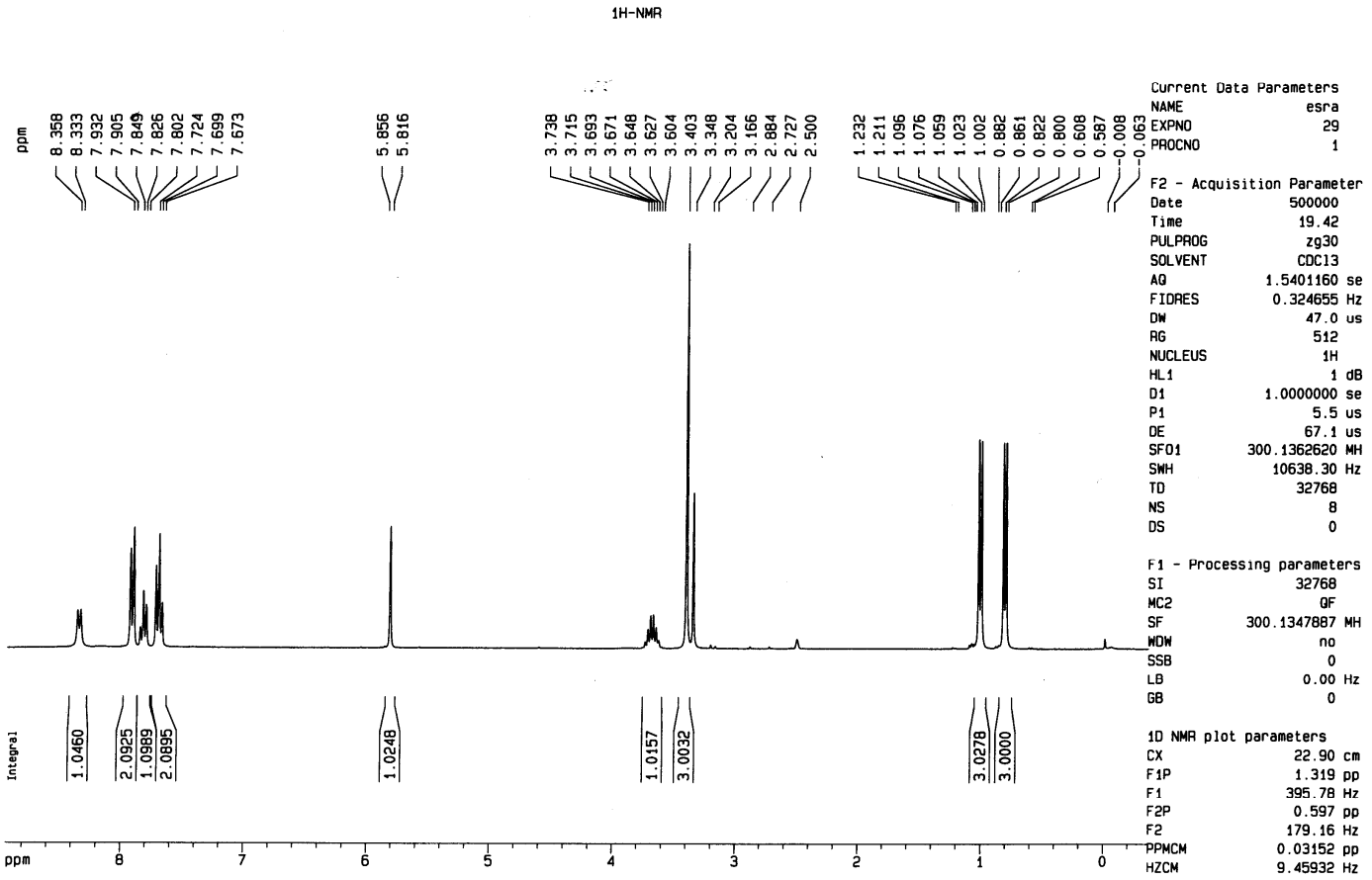
^{13}C NMR spectrum of **5i**.

PhNHCOCH(SO_2Me)SO_2Ph in DMSO-d_6



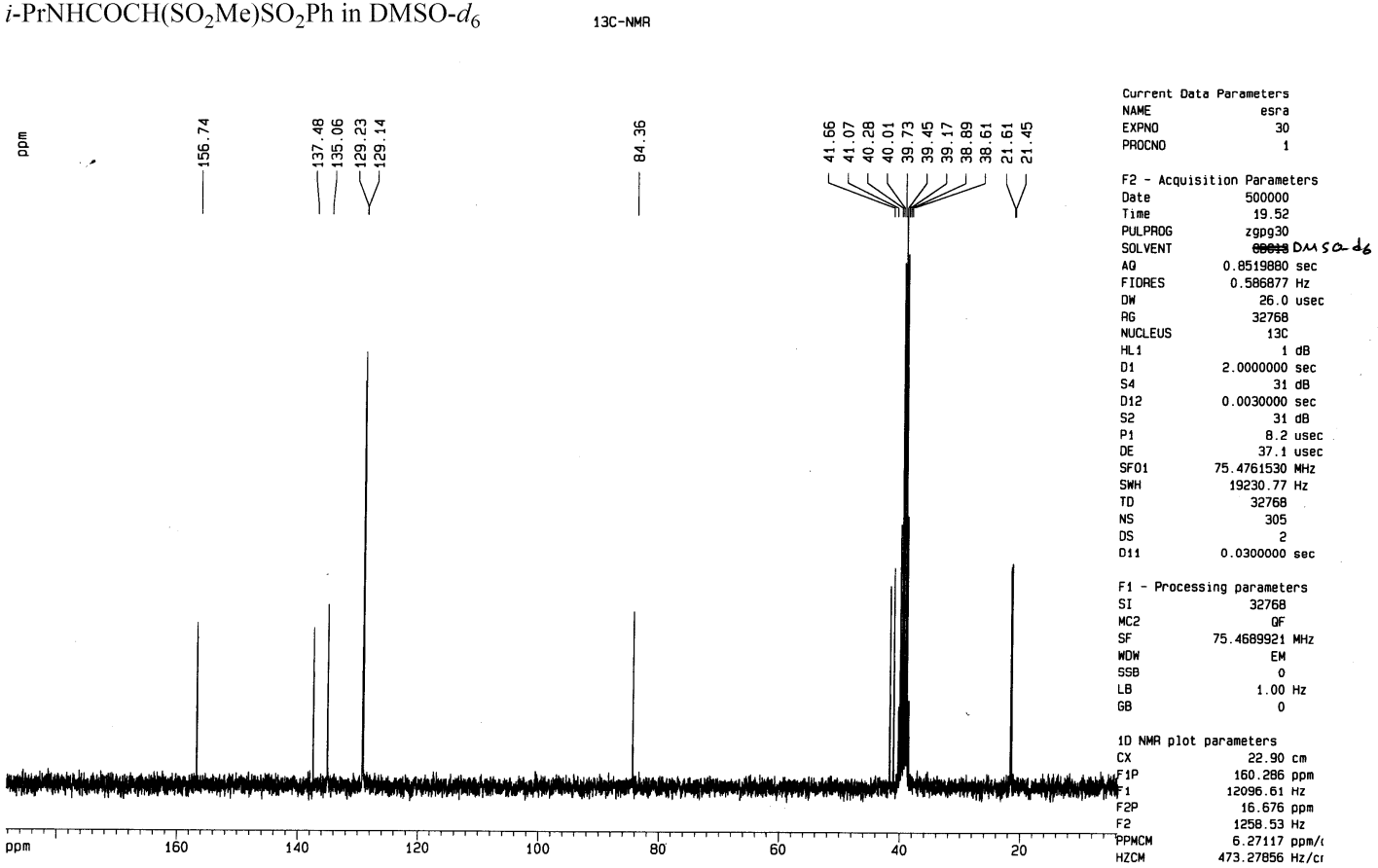
^{1}H NMR spectrum of **5j**.

i-PrNHCOCH(SO_2Me)SO_2Ph in DMSO-d_6

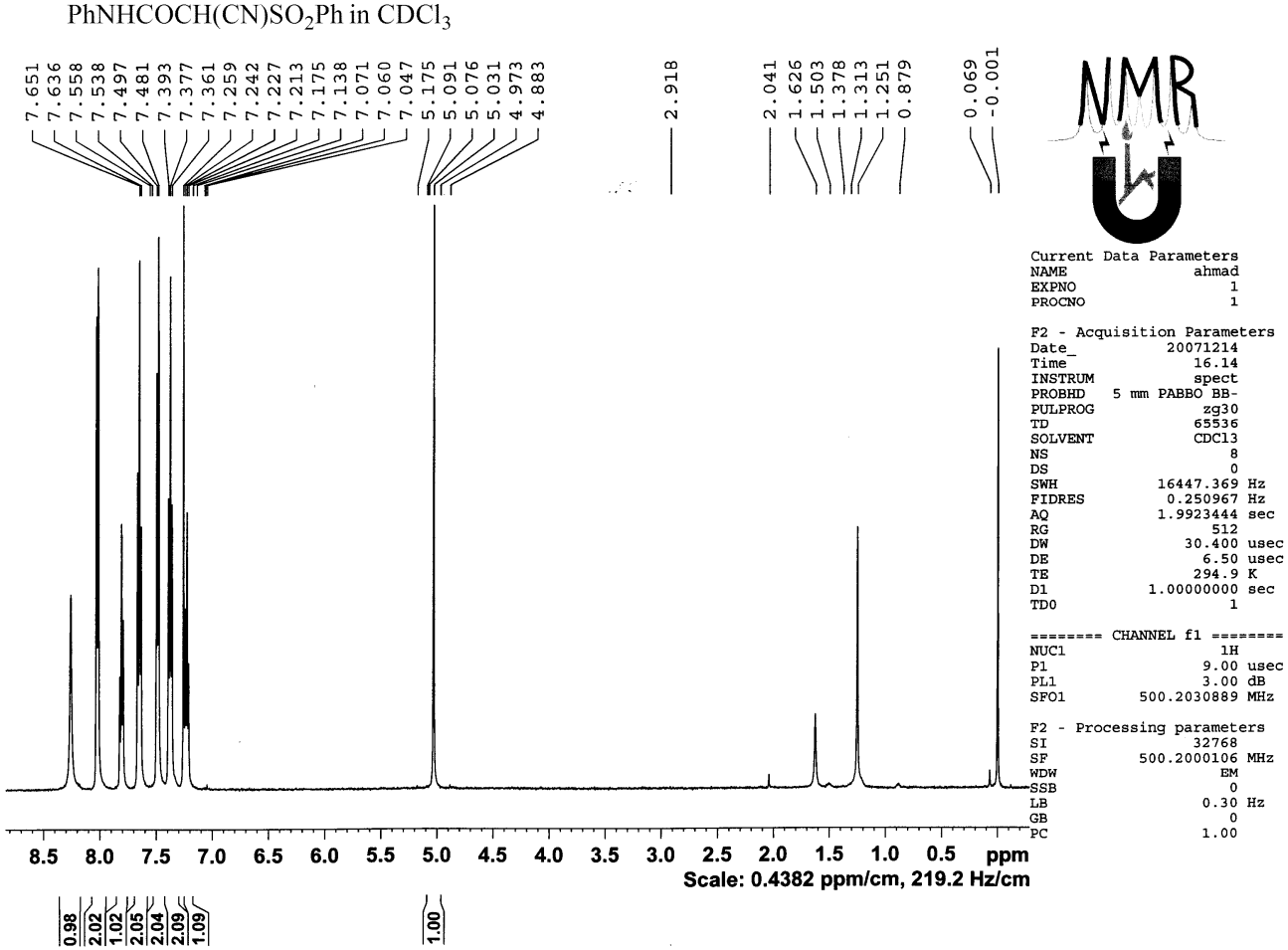


^{13}C NMR spectrum of **5j**.

i-PrNHCOCH(SO_2Me)SO_2Ph in DMSO-d_6



^{1}H NMR spectrum of **5k**.

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Current Data Parameters
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EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
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PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       8
DS                       0
SWH              16447.369 Hz
FIDRES           0.250967 Hz
AQ               1.9923444 sec
RG                     512
DW                  30.400 usec
DE                   6.50 usec
TE                  294.9 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   9.00 usec
PL1                  3.00 dB
SFO1          500.2030889 MHz

F2 - Processing parameters
SI                   32768
SF            500.2000106 MHz
WDW                     EM
SSB                      0
LB                   0.30 Hz
GB                       0
PC                   1.00
```
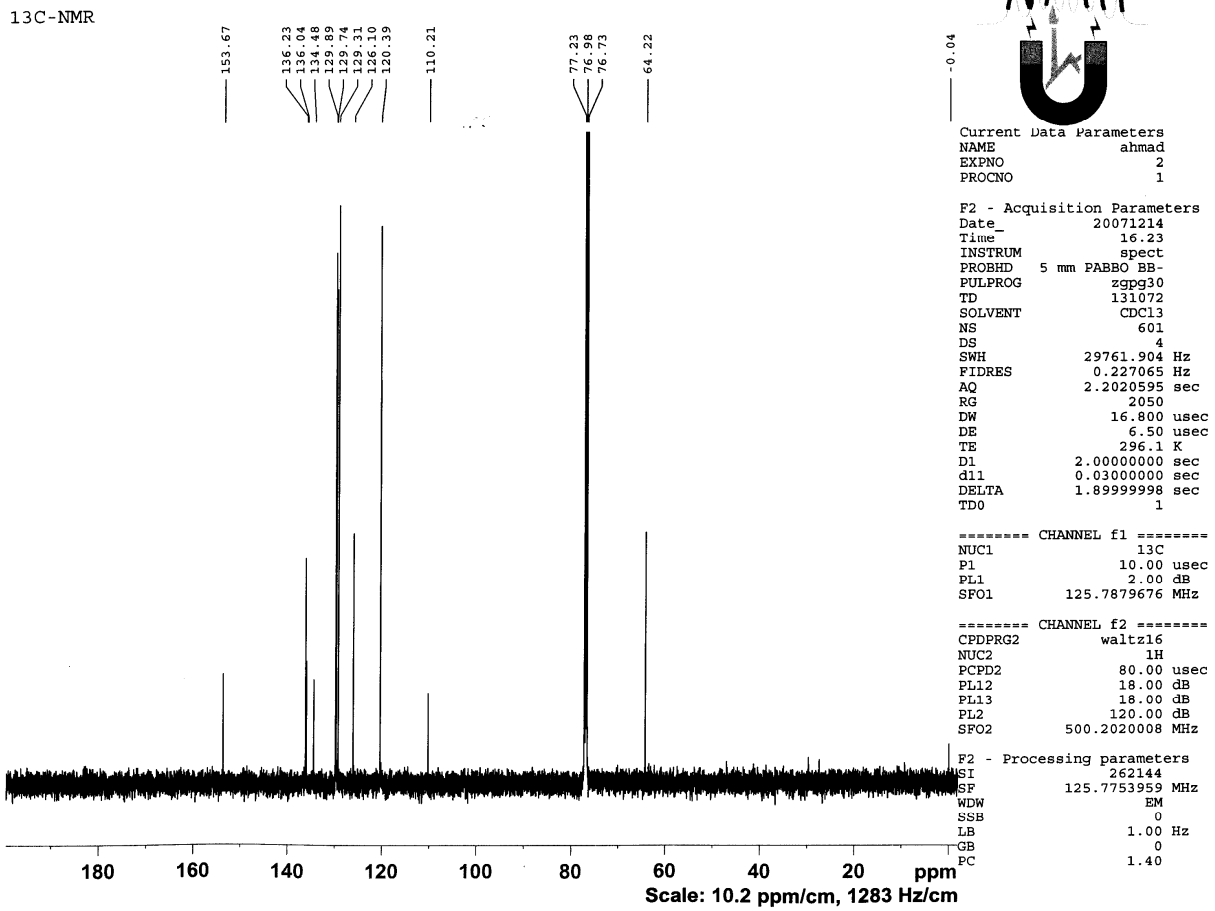
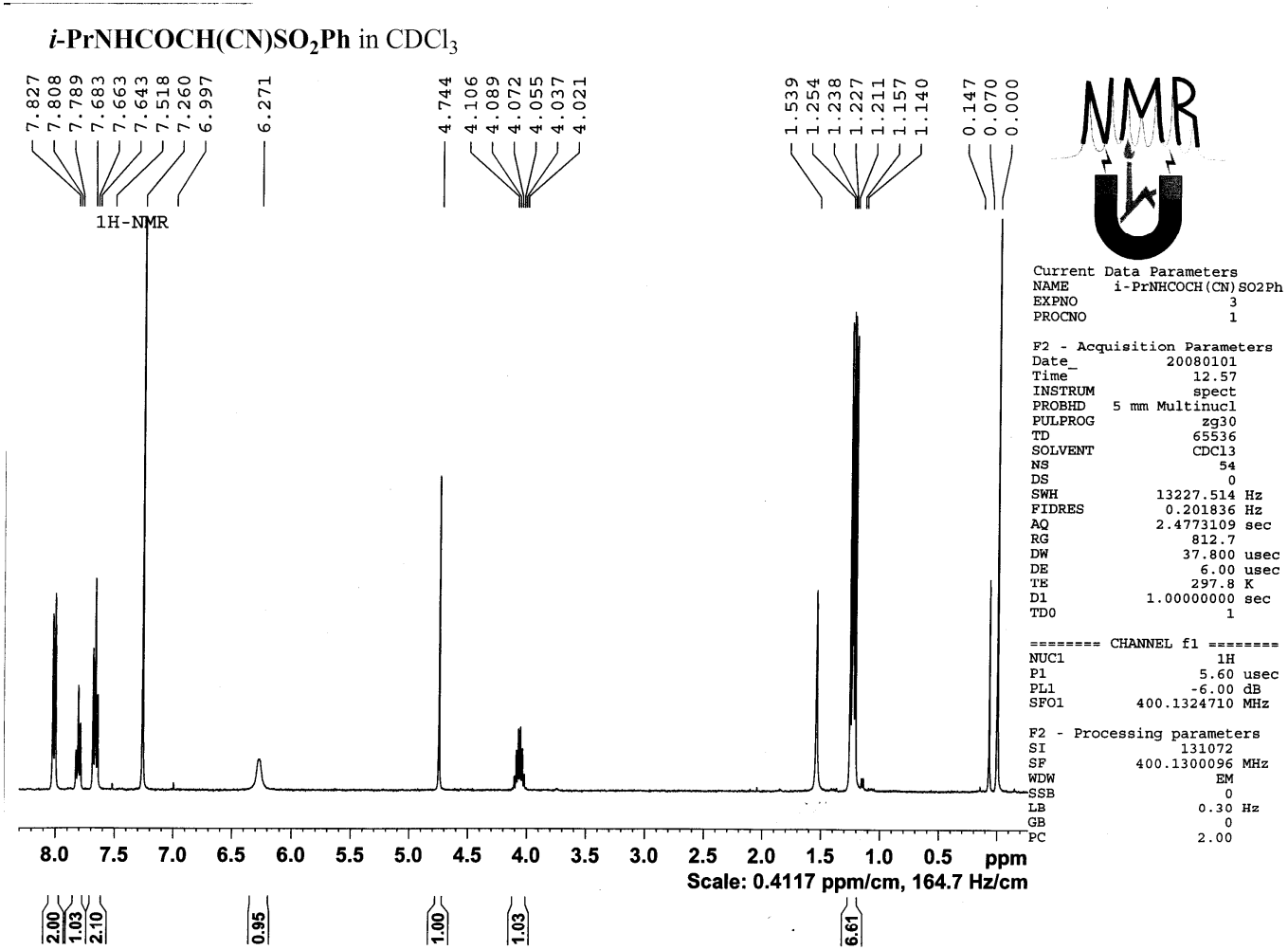


^{13}C NMR spectrum of **5k**.

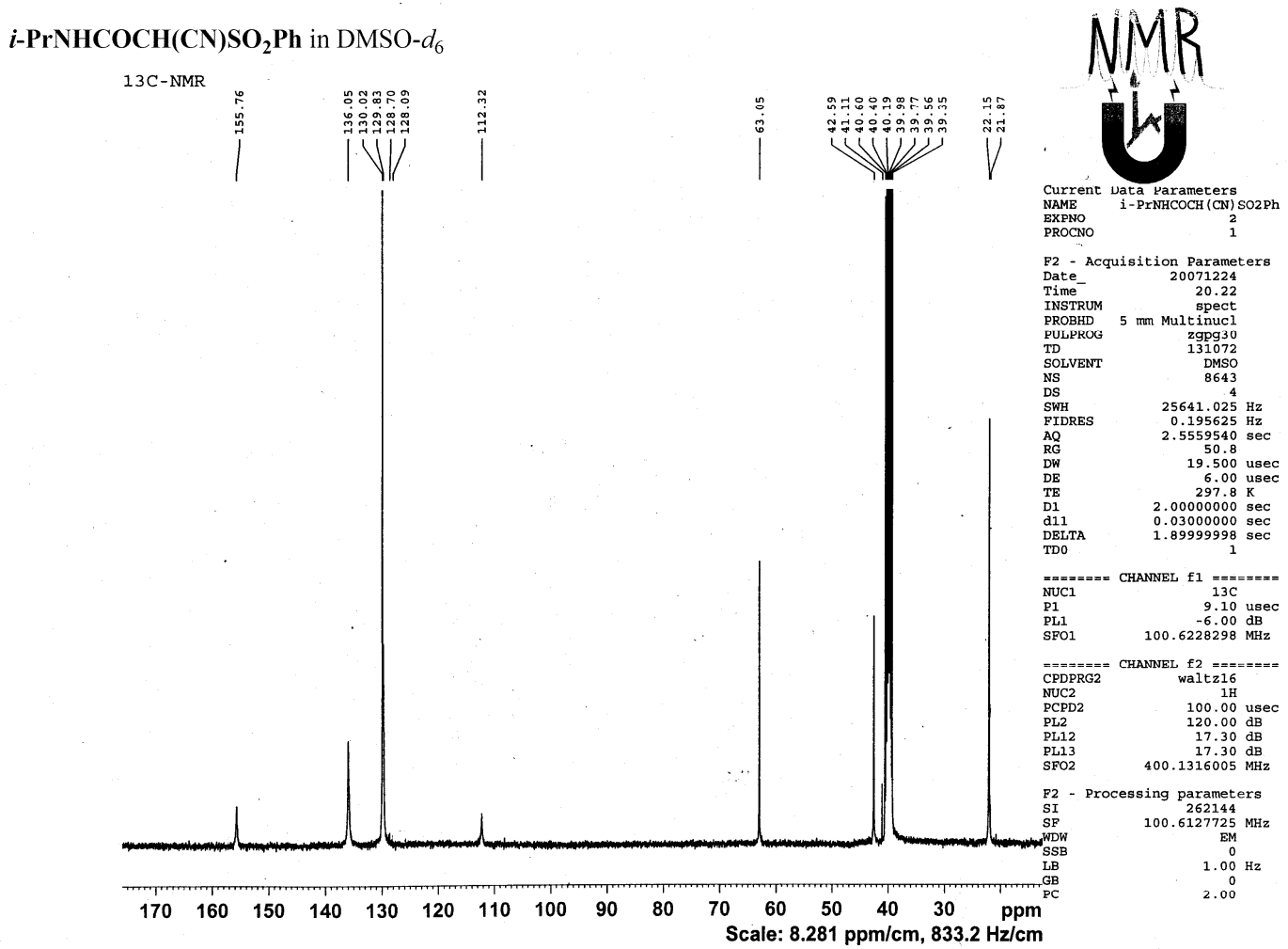
PhNHCOCH(CN)SO_2Ph in $CDCl_3$



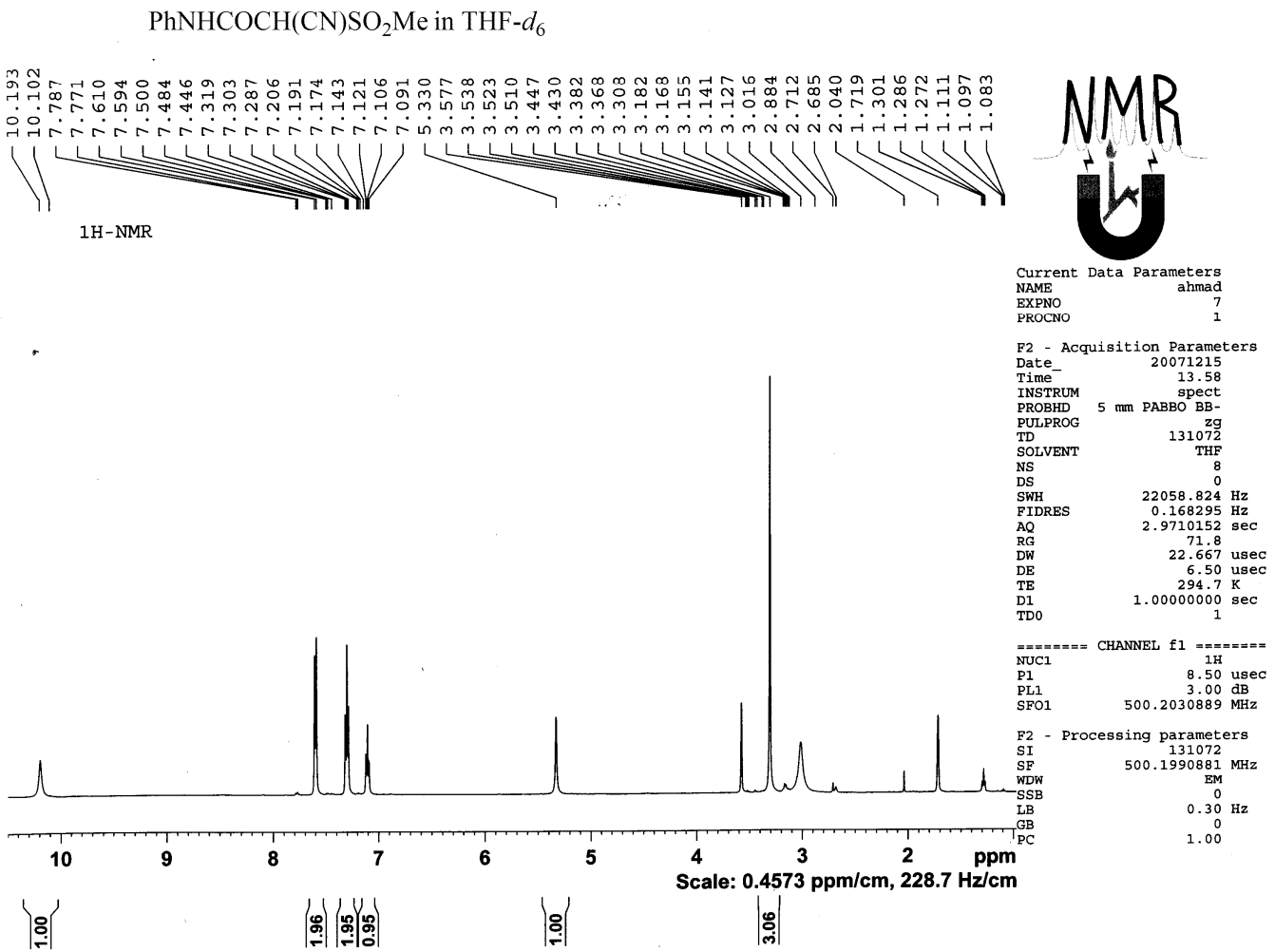
^{1}H NMR spectrum of **51**.



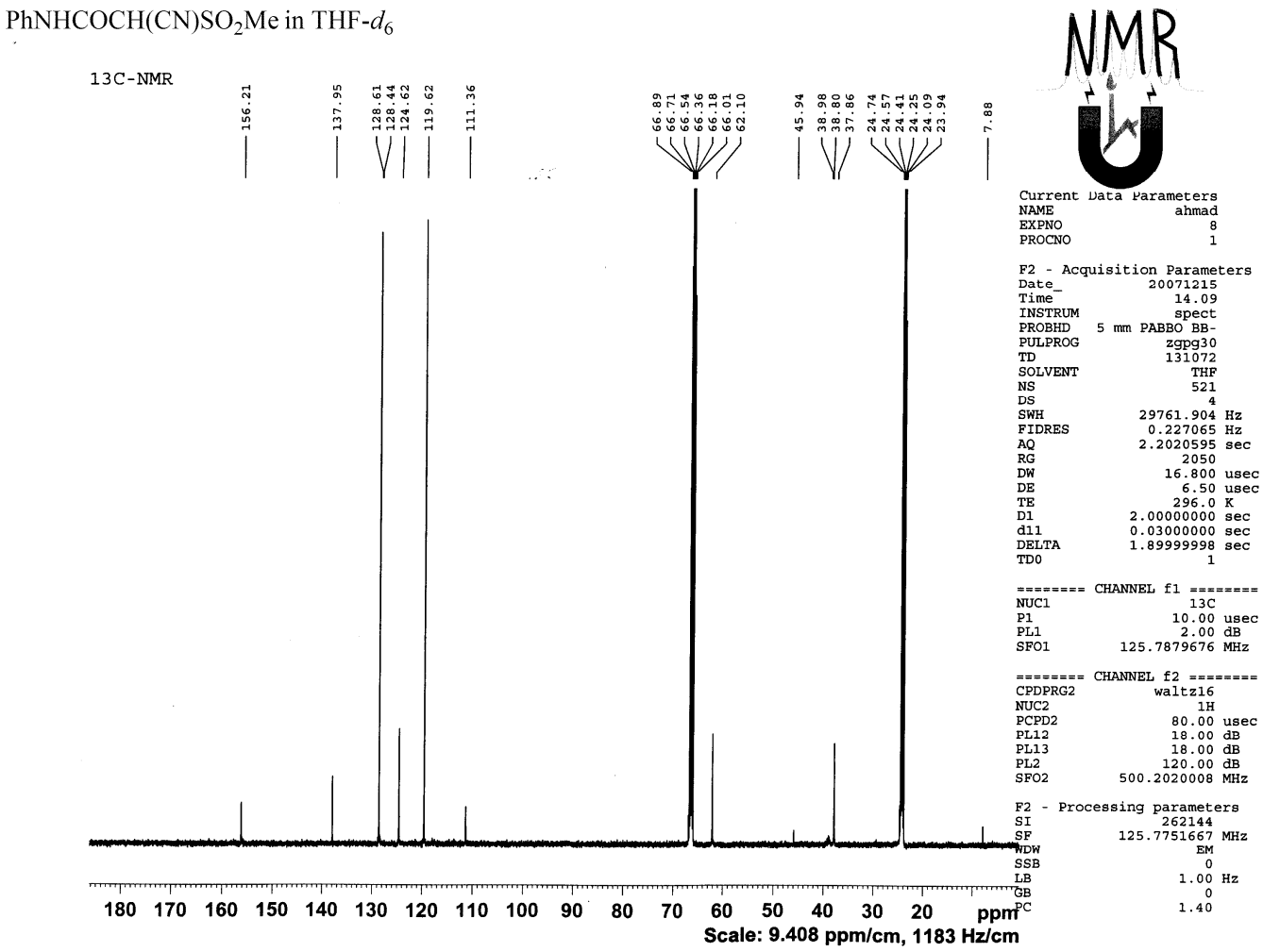
^{13}C NMR spectrum of **51**.



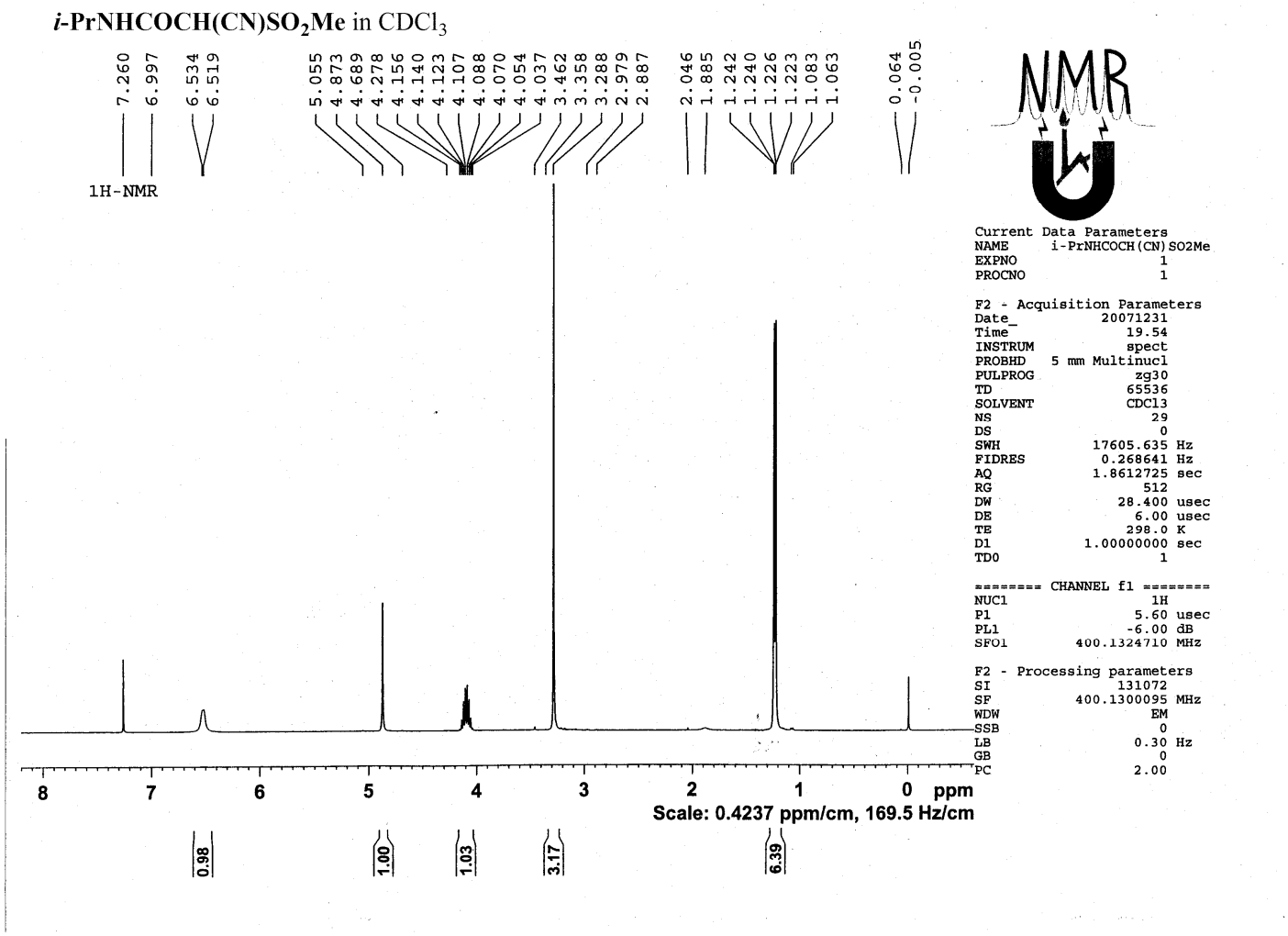
^{1}H NMR spectrum of **5m**.



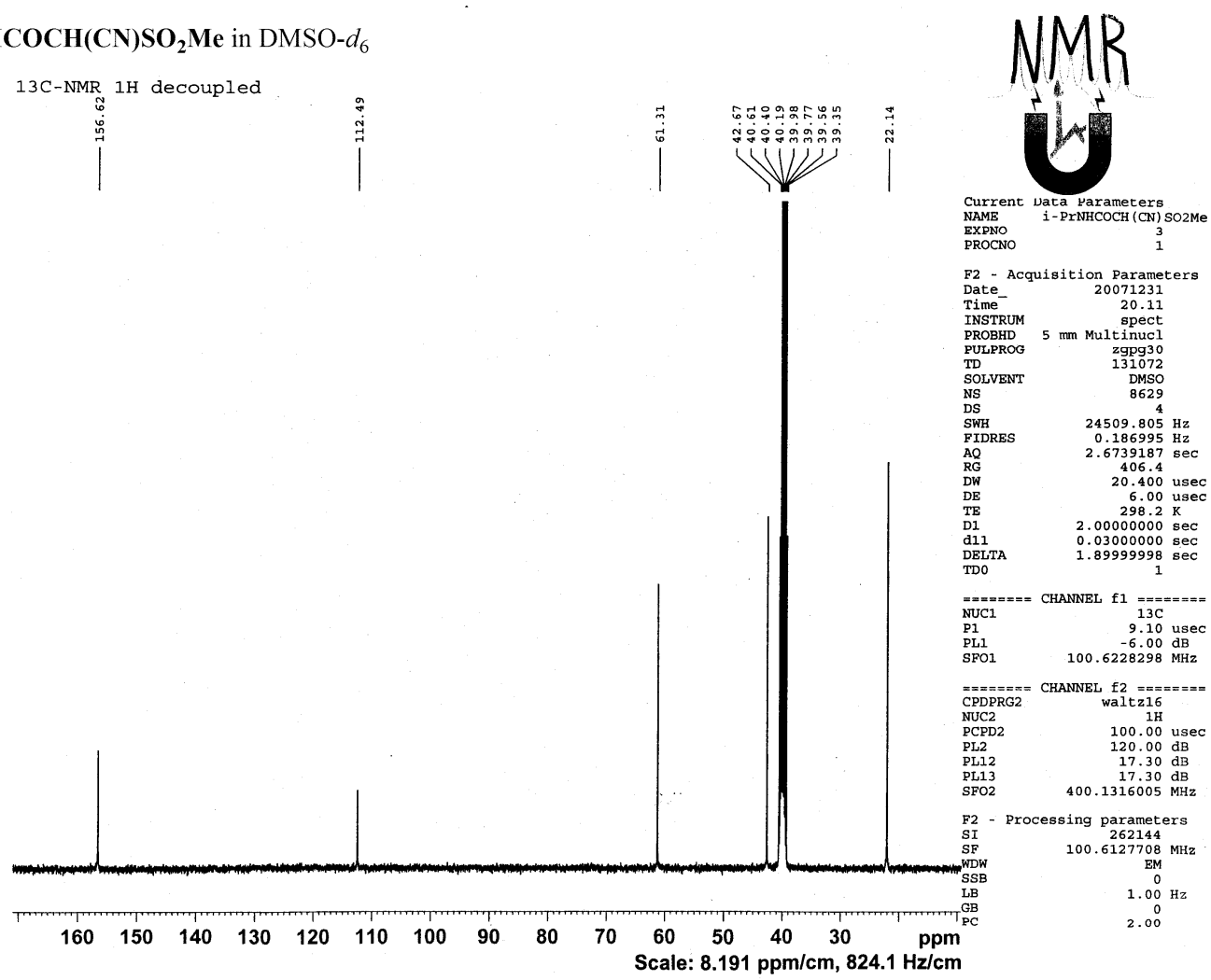
^{13}C NMR spectrum of **5m**.



^{1}H NMR spectrum of **5n**.

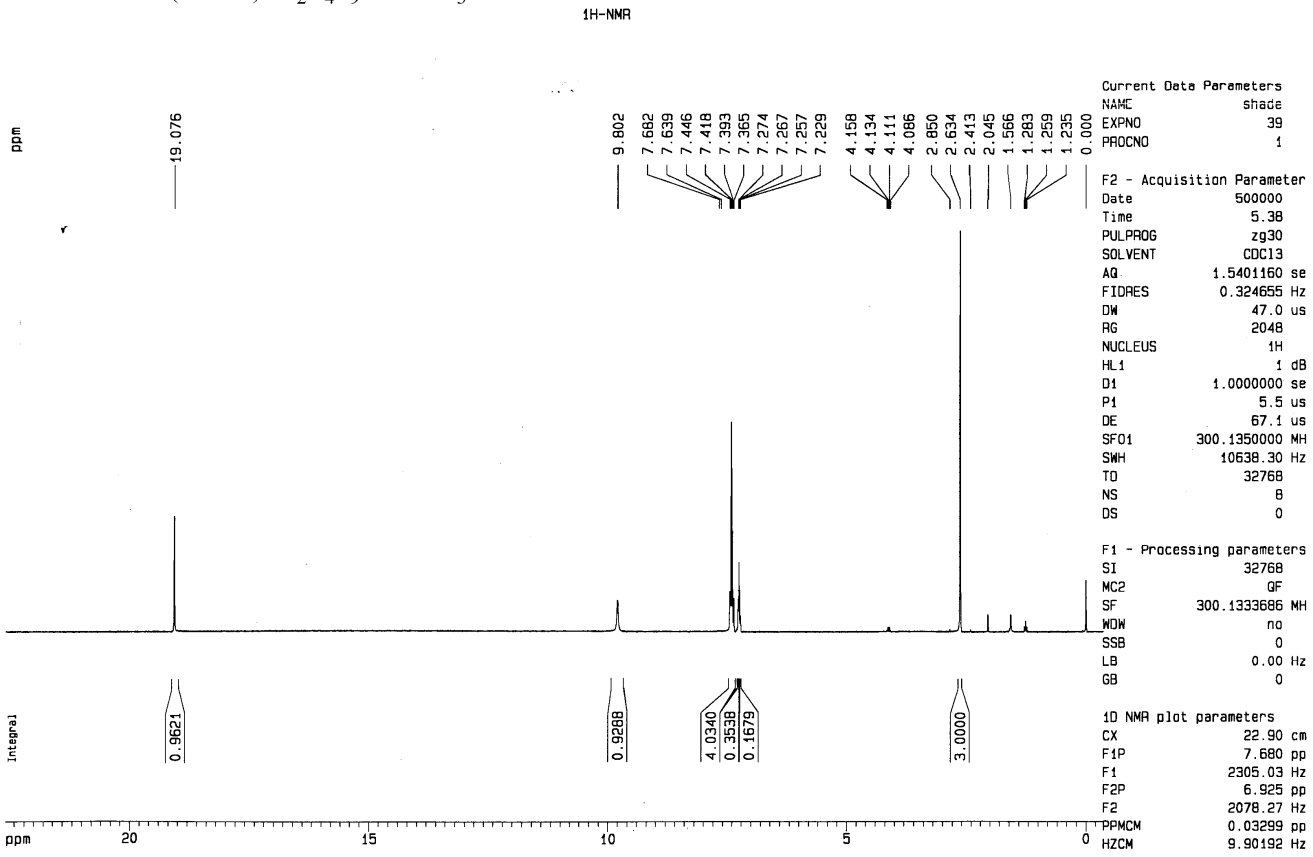


^{13}C NMR spectrum of **5n**.



^{1}H NMR spectrum of **7o**.

PhNHCOCH(COMe)$SO_2C_4F_9$ in $CDCl_3$



^{13}C NMR spectrum of **7o**.