

Supplementary Material

One-pot five-component reaction for synthesis of some novel bis-dihydroquinazolinone derivatives

Ali A. Mohammadi,* Salman Tahery, and Saber Askari

Chemistry & Chemical Engineering Research Center of Iran, P.O. Box 14335-186, Tehran, Iran

E-mail: aliamohammadi@ccerci.ac.ir

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General

Melting points were obtained in open capillary tubes and were measured on an electrothermal 9200 apparatus are uncorrected. Mass spectra were recorded on a Shimadzu QP 1100 BX mass spectrometer. IR spectra were recorded on KBr pellets on a Shimadzu IR-470 spectrophotometer. ^1H and ^{13}C NMR spectra were determined on a Bruker 300 DRX Avance instrument at 300 and 75MHz. Elemental analysis for C, H and N were performed using a Heraeus CHN rapid analyzer. All the reactions are monitored by thin layer chromatography (TLC) with UV light as detecting agent.

General Procedure for the synthesis of bis(1,2-dihydro quinazolinon-4(1H)-one) derivatives (4 a-r)

A mixture of, isatoic anhydride **1** (2 mmol), aldehyde **2** (2 mmol), diamine **3** (1 mmol), 0.15 g (0.3 mmol) alum, and 10 ml EtOH 96% in a 50 ml flask was stirred at reflux for the time period as indicated in table 1. After completion of the reaction (monitored by TLC, ethyl acetate /*n*-hexane, 4:1), the solid products obtained were just filtered off the reaction mixture. Water (25 mL) was added to the resulting solid (for removal of alum), and the resulting solid was separated by filtration. The crude product was washed with hot ethanol to afford the purified product.

Table 1: Synthesis of bisquinazolinone **4a-r** using Alum as catalysts

Products 4	Diamines 3	R	Time (min)	Yield (%) ^a	Mp (°C)	Lit. Yield (Lit. Time)	Lit. Mp (°C)
a	a	H	70	91	297-9	88 (3h) ²⁹	291
b	a	4-Cl	55	93	281-3	74 (3h) ²⁹	255
c	a	4-Me	55	96	295-7	85 (3h) ²⁹	270
d	a	4-NO ₂	55	96	286-8 (dec)	61(3h) ²⁹	275
e	a	2,4-diCl	50	90	310-13 (dec)	-	
f	a	3-EtO,4-OH	70	88	262-4	-	
g	a	3-Cl	55	93	264-6	64 (3h) ²⁹	245
h	a	4-MeO	55	94	250-2	69 (3h) ²⁹	260
i	a	4-CO ₂ H	70	90	308-10	-	
j	a	3-MeO	55	94	237-9	-	
k	a	2,4-diMeO	60	88	247-9	-	
l	b	H	75	90	296-8	-	
m	b	4-Cl	70	91	238-40 (dec)	-	
n	b	4-Me	65	93	281-3	-	
o	b	4-NO ₂	65	92	291-3	-	
p	b	4-MeO	65	90	251-3	-	
q	c	4-Me	75	90	182-4	88 (6h) ²⁸	179-81
r	c	4-Cl	65	85	213-5	79 (6h) ²⁸	212-4

Selected data for new compounds:**3,3'-(ethane-1,2-diyl)bis(2-(2,4-dichlorophenyl)-2,3-dihydroquinazolin-4(1H)-one) (4e):**

White solid; Yield: 88%; mp 310-13 °C (dec); IR (KBr): ν_{\max} = 3248 (NH), 3030, 1629 (C=O), 1521 cm^{-1} ; ^1H NMR (*DMSO-d*₆) δ = 2.86-2.90 (m, 2H, CH₂), 3.89-3.93 (m, 1H, CH₂), 3.96-4.00 (m, 1H, CH₂), 6.20 (d, 1H, J=2.6Hz, CH), 6.31 (d, 1H, J=2.7Hz, CH), 6.65-6.70 (m, 4H, Ar-H), 7.18-7.27 (m, 7H, 2NH, 5Ar-H), 7.35-7.37 (m, 1H, Ar-H), 7.63-7.65 (m, 4H, Ar-H) ppm; ^{13}C NMR (*DMSO-d*₆) δ = 43.09, 68.3, 68.5, 114.9, 115.4, 118.3, 125.3, 128.3, 128.6, 129.2, 130.3, 134.4, 134.9, 143.9, 146.4, 163.1 ppm; MS: *m/z* (%)= 614; Anal. Calcd for C₃₀H₂₂Cl₄N₄O₂: C, 58.84; H, 3.62; N, 9.15; Found: C, 58.76; H, 3.53; N, 9.07%.

3,3'-(ethane-1,2-diyl)bis(2-(3-ethoxy-4-hydroxyphenyl)-2,3-dihydroquinazolin-4(1H)-one) (4f):

White solid; Yield: 81%; mp 262-4 °C; IR (KBr): ν_{\max} = 3397 (OH), 3281 (NH), 2976, 2929, 1634 (C=O), 1514 cm^{-1} ; ^1H NMR (*DMSO-d*₆) δ =1.26 (t, 6H, J=7.0Hz, CH₃), 2.85-2.89 (m, 2H, CH₂), 3.91 (q, 4H, J=7.0Hz, CH₂), 4.02-4.04 (m, 2H, CH₂), 5.69 (s, 2H, CH), 6.61-6.71 (m, 8H, Ar-H), 6.90 (s, 2H, Ar-H), 7.17-7.19 (m, 4H, 2NH, 2Ar-H), 7.61 (d, 2H, J=8.0Hz, Ar-H), 8.99 (s, 2H, OH) ppm; ^{13}C NMR (*DMSO-d*₆) δ = 15.5, 42.8, 64.6, 71.4, 112.8, 115.0, 115.5, 116.0, 117.8, 119.6, 128.2, 132.2, 134.0, 147.4, 147.5, 147.9, 163.3 ppm; MS: *m/z* (%)= 594; Anal. Calcd for C₃₄H₃₄N₄O₆: C, 68.67; H, 5.76; N, 9.42; Found: C, 68.61; H, 5.66; N, 9.35%.

4,4'-(3,3'-(ethane-1,2-diyl)bis(4-oxo-1,2,3,4-tetrahydroquinazolin-3,2-diyl)dibenzoic acid (4i):

White solid; Yield: 80%; mp 308-10 °C; IR (KBr): ν_{\max} = 3414 (OH), 3325 (NH), 2894, 1709 (C=O), 1693 (C=O), 1621 (C=O), 1568 cm^{-1} ; ^1H NMR (*DMSO-d*₆) δ = 2.9-3.00 (m, 2H, CH₂), 4.05-4.18 (m, 2H, CH₂), 5.95(d, 2H, J=2.1Hz, CH), 6.61 (d, 2H, J=8.0Hz, Ar-H), 6.66 (t, 2H, J=7.6Hz, Ar-H), 7.19 (t, 2H, J=7.0Hz, Ar-H), 7.39 (d, 4H, J=8.3Hz, Ar-H), 7.43 (d, 2H, J=2.1Hz, NH), 7.62 (d, 2H, J=6.8Hz, Ar-H), 7.86 (d, 4H, J=8.2Hz, Ar-H), 12.94 (broad, 2H, CO₂H) ppm; ^{13}C NMR (*DMSO-d*₆) δ = 43.4, 70.6, 115.2, 115.5, 118.2, 127.2, 128.3, 130.4, 131.7, 134.2, 146.3, 147.0, 163.3, 167.6 ppm; MS: *m/z* (%)= 562; Anal. Calcd for C₃₂H₂₆N₄O₆: C, 68.32; H, 4.66; N, 9.96; Found: C, 68.23; H, 4.68; N, 9.88%.

3,3'-(ethane-1,2-diyl)bis(2-(3-methoxyphenyl)-2,3-dihydroquinazolin-4(1H)-one) (4j):

White solid; Yield: 94%; mp 237-9 °C; IR (KBr): ν_{\max} = 3240 (NH), 3002, 2930, 2828, 1631 (C=O), 1609 (C=O), 1514 cm^{-1} ; ^1H NMR (*DMSO-d*₆) δ = 2.89-2.94 (m, 1H, CH₂), 2.97-3.03 (m, 1H, CH₂), 3.68 (s, 6H, 2CH₃), 3.99-4.06 (m, 1H, CH₂), 4.10-4.18 (m, 1H, CH₂), 5.84 (d, 1H, J=1.5Hz, CH), 5.89 (d, 1H, J=1.7Hz, CH), 6.64 (t, 2H, J=8.3Hz, Ar-H), 6.69 (s, 2H, Ar-H), 6.85-6.89 (m, 6H, Ar-H), 7.18-7.27 (m, 4H, Ar-H), 7.36 (s, 1H, NH), 7.37 (s, 1H, NH), 7.63-7.65 (m, 2H, Ar-H) ppm; ^{13}C NMR (*DMSO-d*₆) δ = 43.2, 43.4, 55.8, 71.2, 71.5, 113.13, 113.18, 114.3, 114.4, 115.1, 115.4, 115.5, 118.0, 119.0, 128.2, 130.5, 130.6, 134.1, 143.3, 147.3 160.2, 163.3,

163.4 ppm; MS: m/z (%)= 534; Anal. Calcd for $C_{32}H_{30}N_4O_4$: C, 71.89; H, 5.66; N, 10.48; Found: C, 71.81; H, 5.59; N, 10.42%.

3,3'-(ethane-1,2-diyl)bis(2-(2,4-dimethoxyphenyl)-2,3-dihydroquinazolin-4(1H)-one) (4k):

White solid; Yield: 90%; mp 247-9 °C; IR (KBr): ν_{\max} = 3384 (NH), 3067, 2936, 2837, 1649 (C=O), 1610, 1497 cm^{-1} ; 1H NMR ($DMSO-d_6$) δ = 2.78-2.82 (m, 2H, CH_2), 3.68 (s, 3H, OCH_3), 3.81 (s, 3H, OCH_3), 3.96-4.00 (m, 2H, CH_2), 6.02 (d, 2H, $J=1.9Hz$, CH), 6.35 (d, d, 2H, $J=2.3Hz$, $J=8.5Hz$, Ar-H), 6.57 (d, 2H, $J=2.3Hz$, Ar-H), 6.62 (t, 2H, $J=7.1Hz$, Ar-H), 6.65 (d, 2H, $J=8.0Hz$, Ar-H), 6.81 (d, 2H, $J=1.2Hz$, 2NH), 6.92 (d, 2H, $J=8.4Hz$, Ar-H), 7.16 (t, 2H, $J=8.3Hz$, Ar-H), 7.61 (d, 2H, $J=7.7Hz$, Ar-H) ppm; ^{13}C NMR ($DMSO-d_6$) δ = 42.9, 56.0, 56.5, 66.3, 99.6, 105.2, 115.2, 117.6, 120.9, 121.2, 127.7, 128.1, 133.9, 141.6, 158.5, 161.5, 163.7 ppm; MS: m/z (%)= 594; Anal. Calcd for $C_{34}H_{34}N_4O_6$: C, 68.67; H, 5.76; N, 9.42; Found: C, 68.58; H, 5.68; N, 9.34%.

3,3'-(1,4-phenylene)bis(2-phenyl-2,3-dihydroquinazolin-4(1H)-one) (4l):

Cream solid; Yield: 82 %; mp 296-8 °C; IR (KBr): ν_{\max} = 3305 (NH), 1638 (C=O), 1612, 1512 cm^{-1} ; 1H NMR ($DMSO-d_6$) δ = 6.26 (s, 2H, CH), 6.70-6.75 (m, 4H, Ar-H), 7.24 (s, 4H, Ar-H), 7.29-7.33 (m, 12H, Ar-H), 7.66-7.70 (m, 4H, 2NH, 2Ar-H) ppm; MS: m/z (%)= 522; Anal. Calcd for $C_{34}H_{26}N_4O_2$: C, 78.14; H, 5.01; N, 10.72; Found: C, 78.07; H, 4.92; N, 10.64%. ^{13}C NMR (125 MHz, $DMSO-d_6$) δ : very low soluble in DMSO

3,3'-(1,4-phenylene)bis(2-(4-chlorophenyl)-2,3-dihydroquinazolin-4(1H)-one) (4m):

White solid; Yield: 87%; mp 238-40 °C(dec); IR (KBr): ν_{\max} = 3305 (NH), 1641 (C=O), 1512 cm^{-1} ; 1H NMR ($DMSO-d_6$) δ = 6.29 (d, 2H, $J=2.3Hz$, CH), 6.72 (t, 2H, $J=7.3Hz$, Ar-H), 6.74 (d, 2H, $J=8.1Hz$, Ar-H), 7.22 (s, 4H, Ar-H), 7.23-7.29 (m, 2H, Ar-H), 7.34-7.73 (m, 8H, Ar-H), 7.67 (d, 2H, $J=2.3Hz$, NH), 7.07 (d, 2H, $J=7.0Hz$, Ar-H) ppm; ^{13}C NMR ($DMSO-d_6$) δ = δ 72.5, 115.7, 116.1, 118.6, 127.0, 128.8, 129.2, 129.3, 133.7, 134.8, 139.0, 140.5, 147.1, 162.9 ppm; MS: m/z (%)= 590; Anal. Calcd for $C_{34}H_{24}Cl_2N_4O_2$: C, 69.04; H, 4.09; N, 9.47; Found: C, 68.95; H, 3.99; N, 9.39%.

3,3'-(1,4-phenylene)bis(2-(p-tolyl)-2,3-dihydroquinazolin-4(1H)-one) (4n):

White solid; Yield: 92%; mp 281-3 °C; IR (KBr): ν_{\max} = 3308 (NH), 3022, 2926, 1642 (C=O), 1611, 1512 cm^{-1} ; 1H NMR ($DMSO-d_6$) δ = 2.22 (s, 6H, 2 CH_3), 6.20 (s, 2H, CH), 6.70-6.72 (m, 4H, Ar-H), 7.09-7.23 (m, 10H, Ar-H), 7.54-7.77 (m, 8H, 2NH, 6Ar-H) ppm; MS: m/z (%)= 550; Anal. Calcd for $C_{36}H_{30}Cl_2N_4O_2$: C, 78.52; H, 5.49; N, 10.17; Found: C, 78.44; H, 5.40; N, 10.10%.

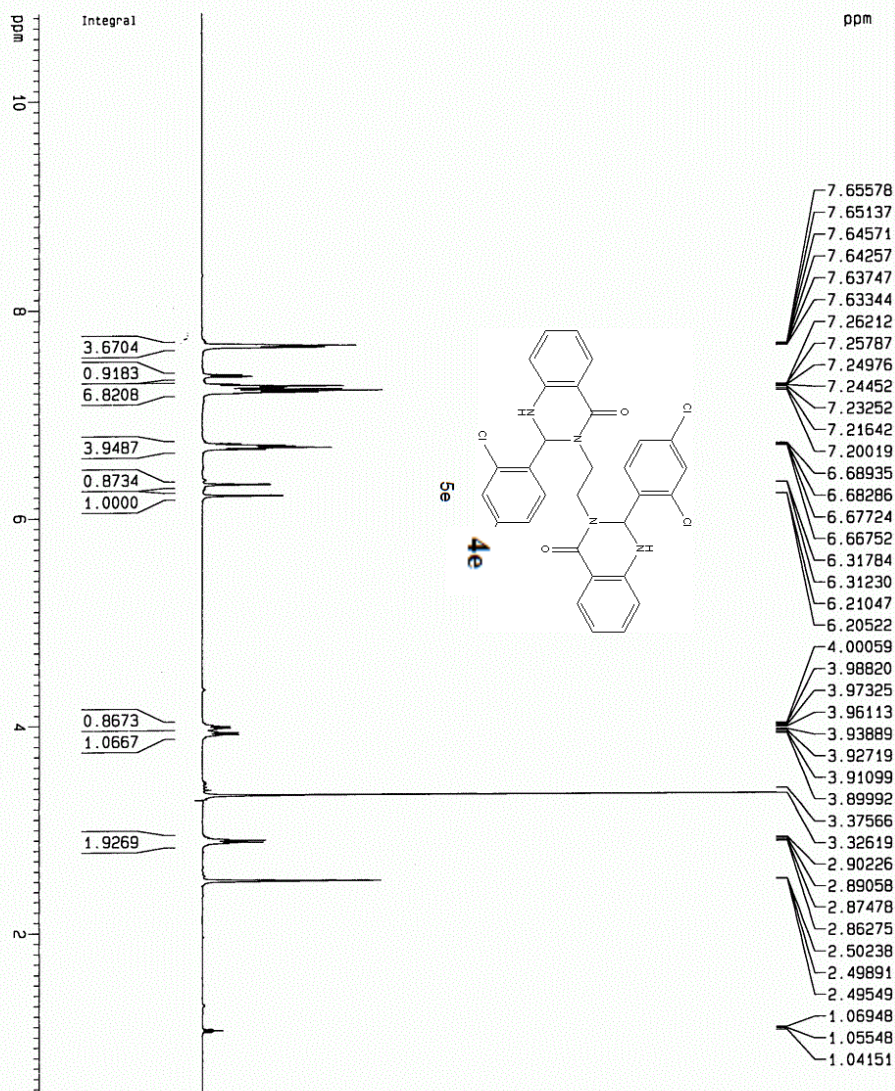
^{13}C NMR (125 MHz, $DMSO-d_6$) δ : very low soluble in DMSO

3,3'-(1,4-phenylene)bis(2-(4-nitrophenyl)-2,3-dihydroquinazolin-4(1H)-one) (4o):

Yellow solid; Yield: 90%; mp 291-3 °C; IR (KBr): ν_{\max} = 3401 (NH), 3102, 3071, 1662 (C=O), 1614, 1513 cm^{-1} ; ^1H NMR (*DMSO-d*₆) δ = 6.48 (d, 2H, J=2.1Hz, CH), 6.73 (t, 2H, J=7.4Hz, Ar-H), 6.76 (d, 2H, J=8.1Hz, Ar-H), 7.28 (t, 2H, J=7.2Hz, Ar-H), 7.33 (s, 4H, Ar-H), 7.62 (d, 4H, J=8.6Hz, Ar-H), 7.73 (d, 2H, J=7.6Hz, Ar-H), 7.82 (d, 2H, J=2.1Hz, 2NH), 8.15 (d, 4H, J=8.6Hz, Ar-H) ppm; ^{13}C NMR (*DMSO-d*₆) δ = 72.3, 115.9, 116.0, 118.9, 124.5, 127.0, 128.6, 128.9, 134.9, 139.0, 146.8, 148.2, 148.8, 162.8 ppm; MS: m/z (%)= 612; Anal. Calcd for $\text{C}_{34}\text{H}_{24}\text{N}_6\text{O}_6$: C, 66.66; H, 3.95; N, 13.72; Found: C, 66.56; H, 3.87; N, 13.63%.

3,3'-(1,4-phenylene)bis(2-(4-methoxyphenyl)-2,3-dihydroquinazolin-4(1H)-one) (4p):

White solid; Yield: 88%; mp 251-3 °C; IR (KBr) : ν_{\max} =3307 (NH), 2948, 2925, 2833, 1638, 1613, 1512 cm^{-1} ; ^1H NMR (*DMSO-d*₆) δ = 3.68 (s, 6H, CH_3), 6.19 (d, 2H, J=2.5Hz, CH), 6.68 (t, 2H, J=7.1Hz, Ar-H), 6.74 (d, 2H, J=8Hz, Ar-H), 6.85 (d, 4H, J=8.7, Ar-H), 7.21 (s, 4H, Ar-H), 7.23-7.27 (m, 6H, Ar-H), 7.58 (d, 2H, J=2.4Hz, 2NH), 7.71 (d, 2H, J=7.0Hz, Ar-H) ppm; ^{13}C NMR (*DMSO-d*₆) δ = 55.9, 72.9, 114.5, 115.6, 116.1, 118.3, 126.9, 128.5, 128.8, 133.5, 134.6, 139.2, 147.4, 159.9, 163.1 ppm; MS: m/z (%)= 582; Anal. Calcd for $\text{C}_{36}\text{H}_{30}\text{N}_4\text{O}_4$: C, 74.21; H, 5.19; N, 9.62; Found: C, 74.14; H, 5.10; N, 9.54%.



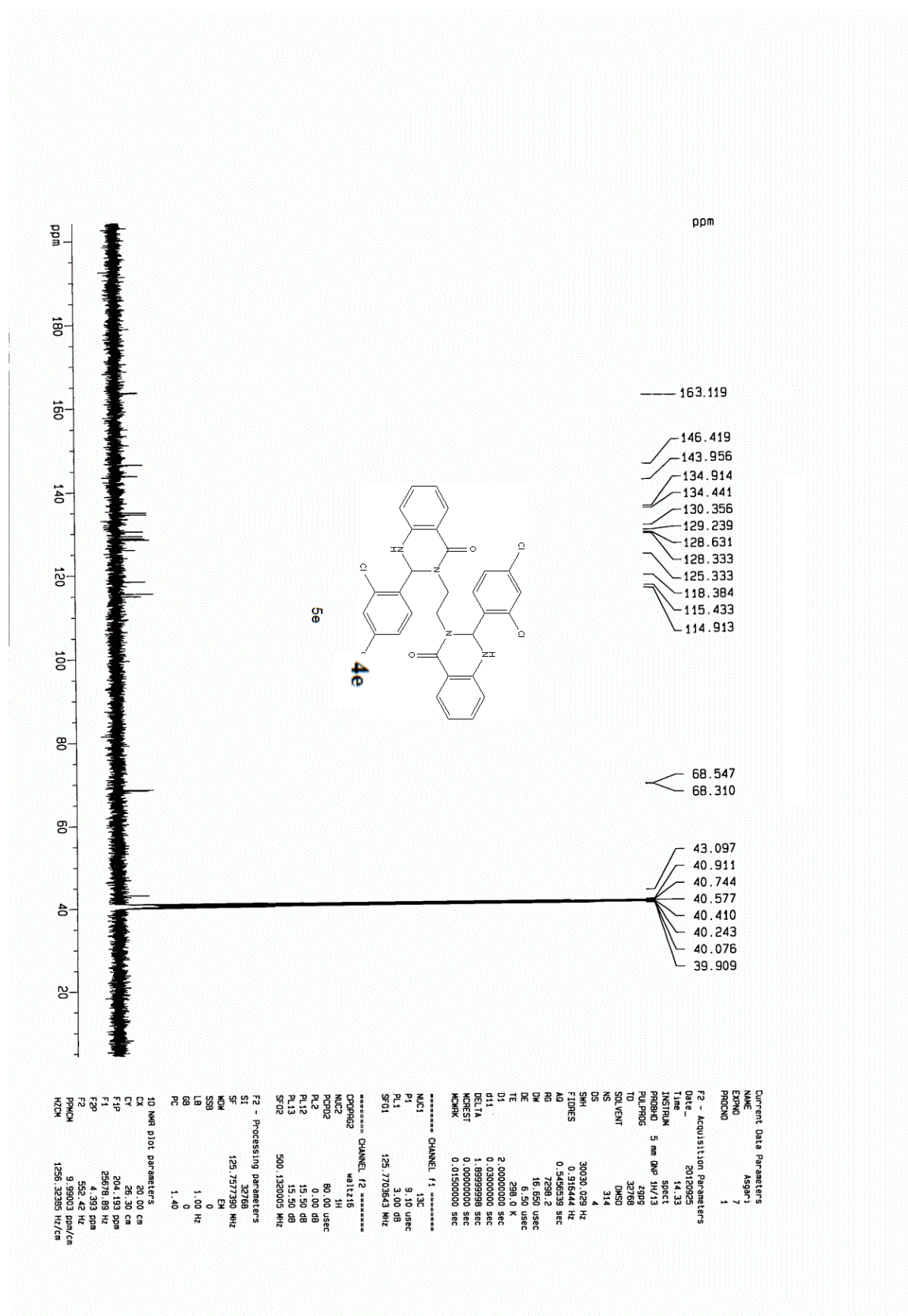
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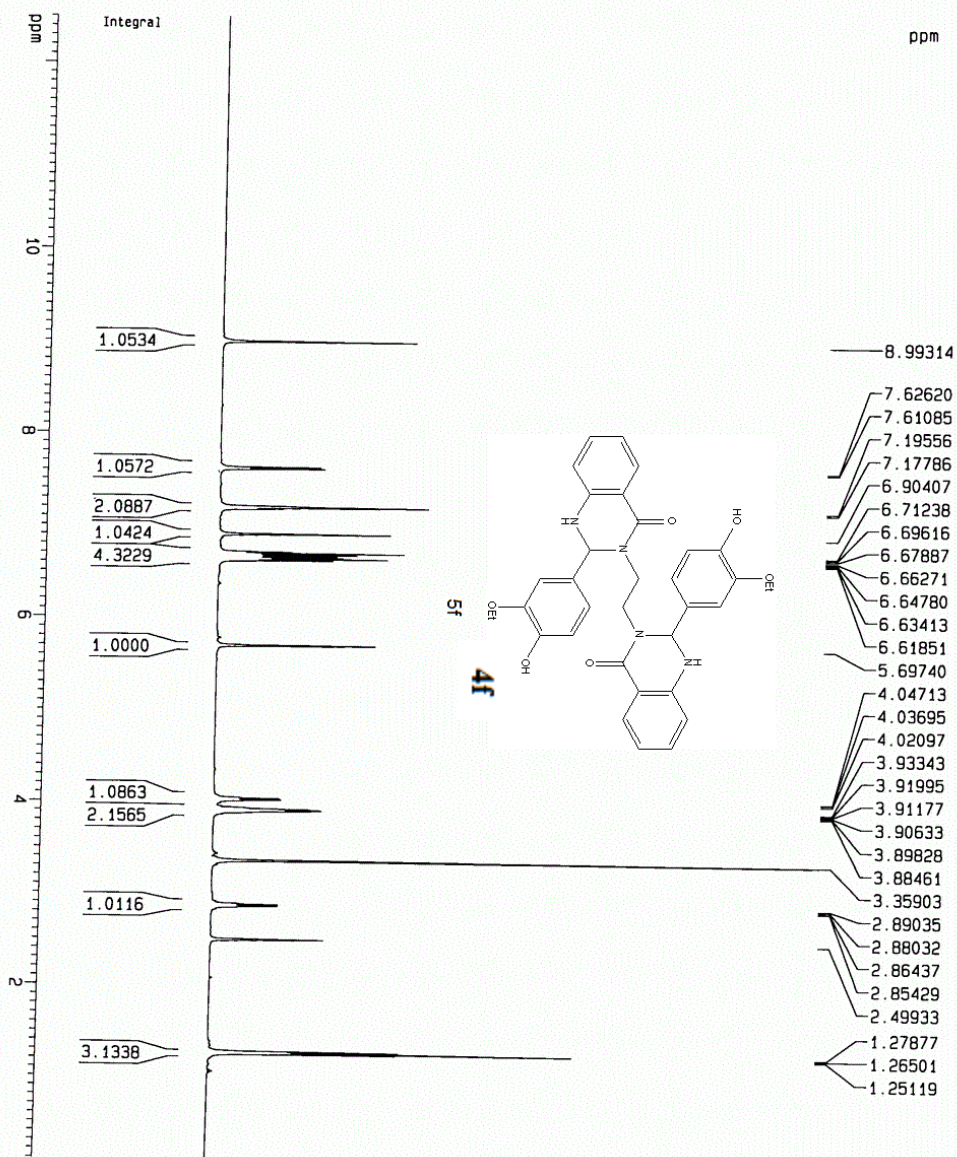
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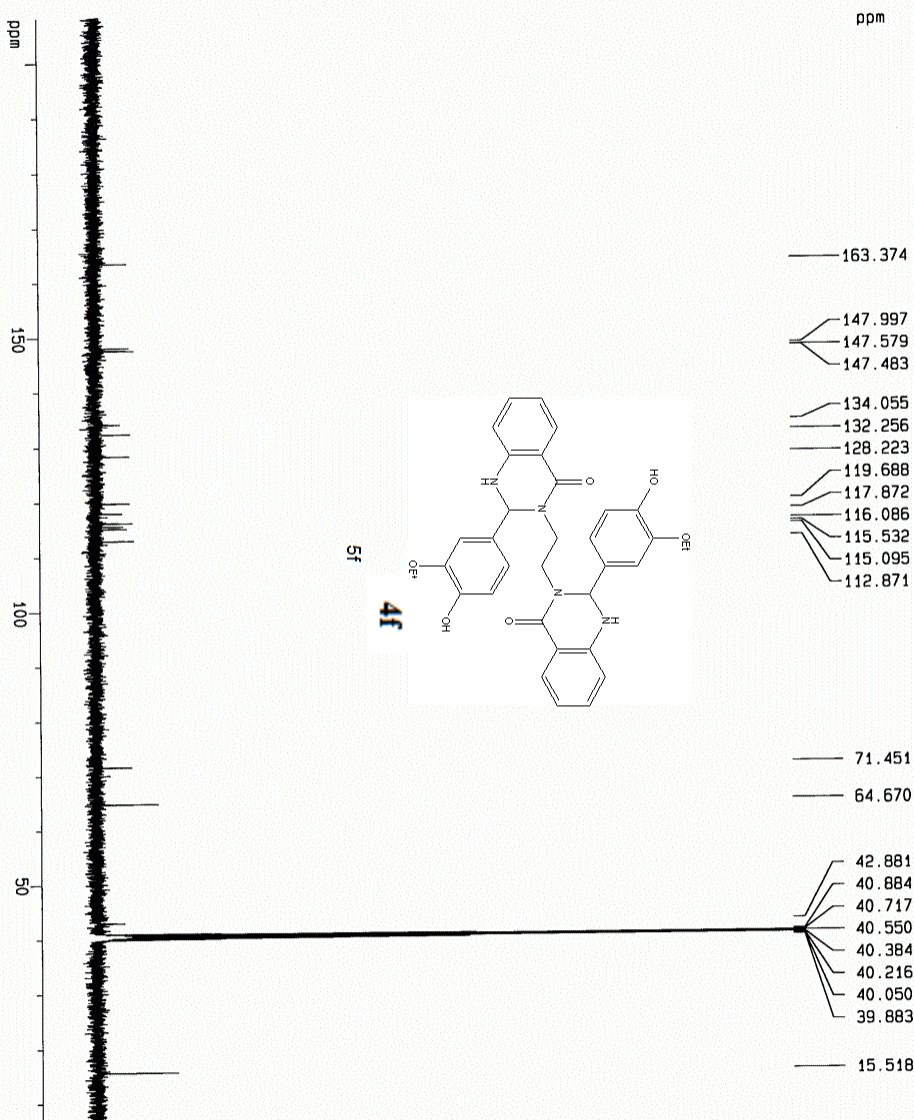
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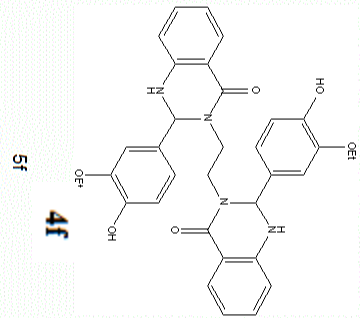
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 F2P: 0.086 ppm
 F2: 43.10 Hz
 PPM/CM: 0.62085 ppm/cm
 HZ/CM: 310.50433 Hz/cm



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- 147.579
- 147.483
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- 132.256
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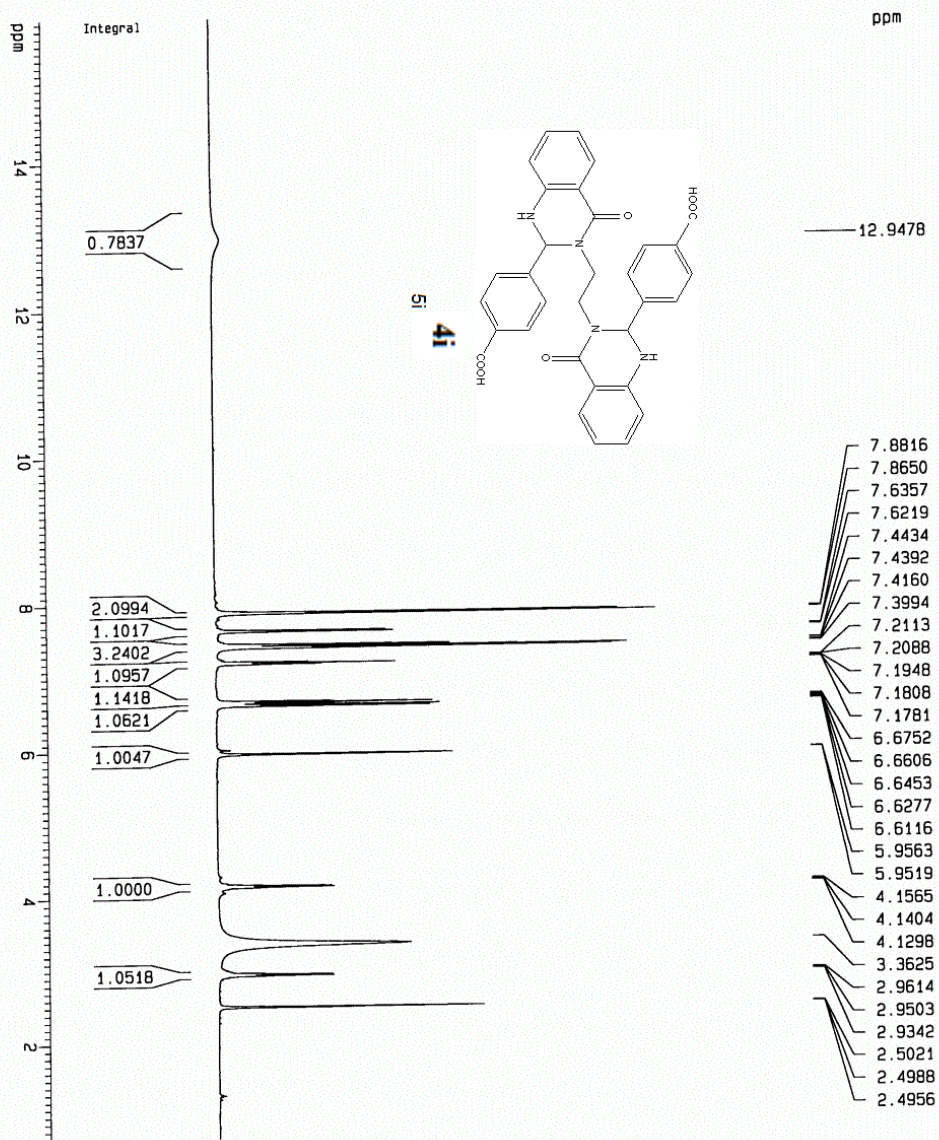
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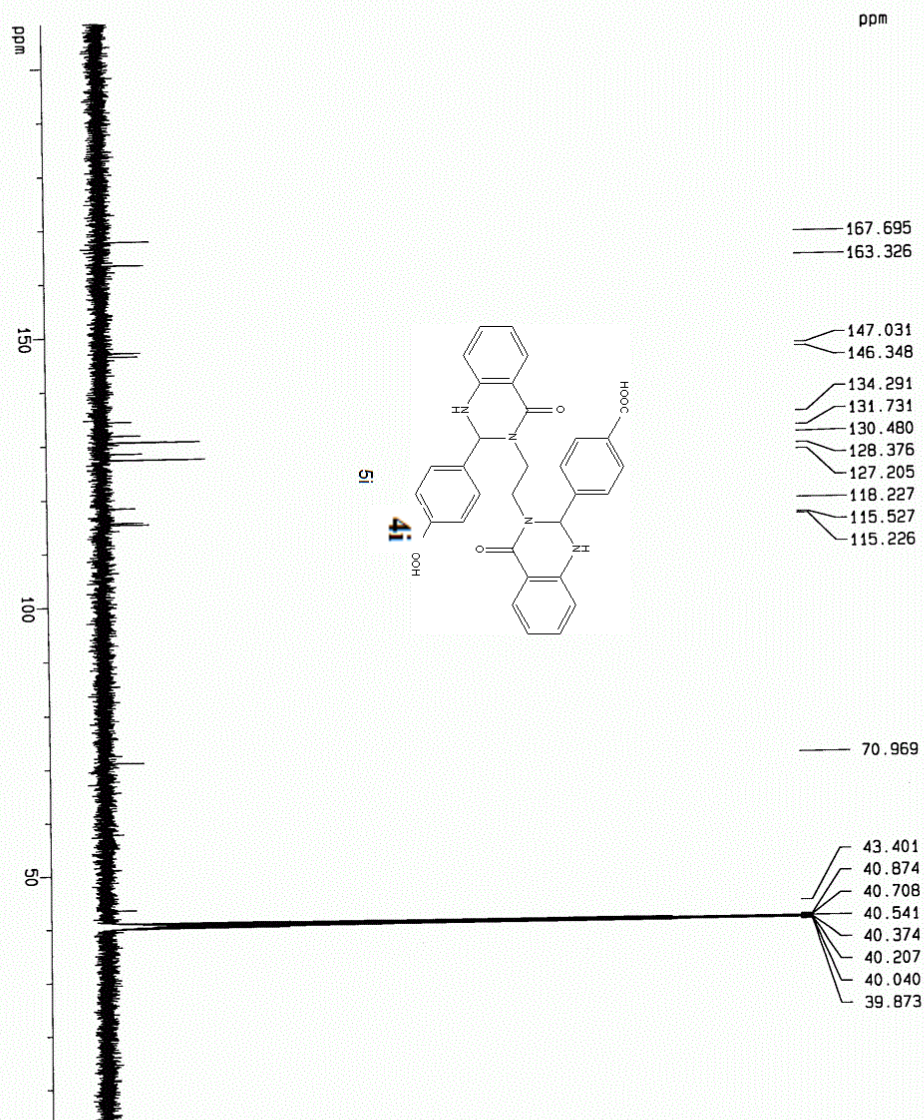
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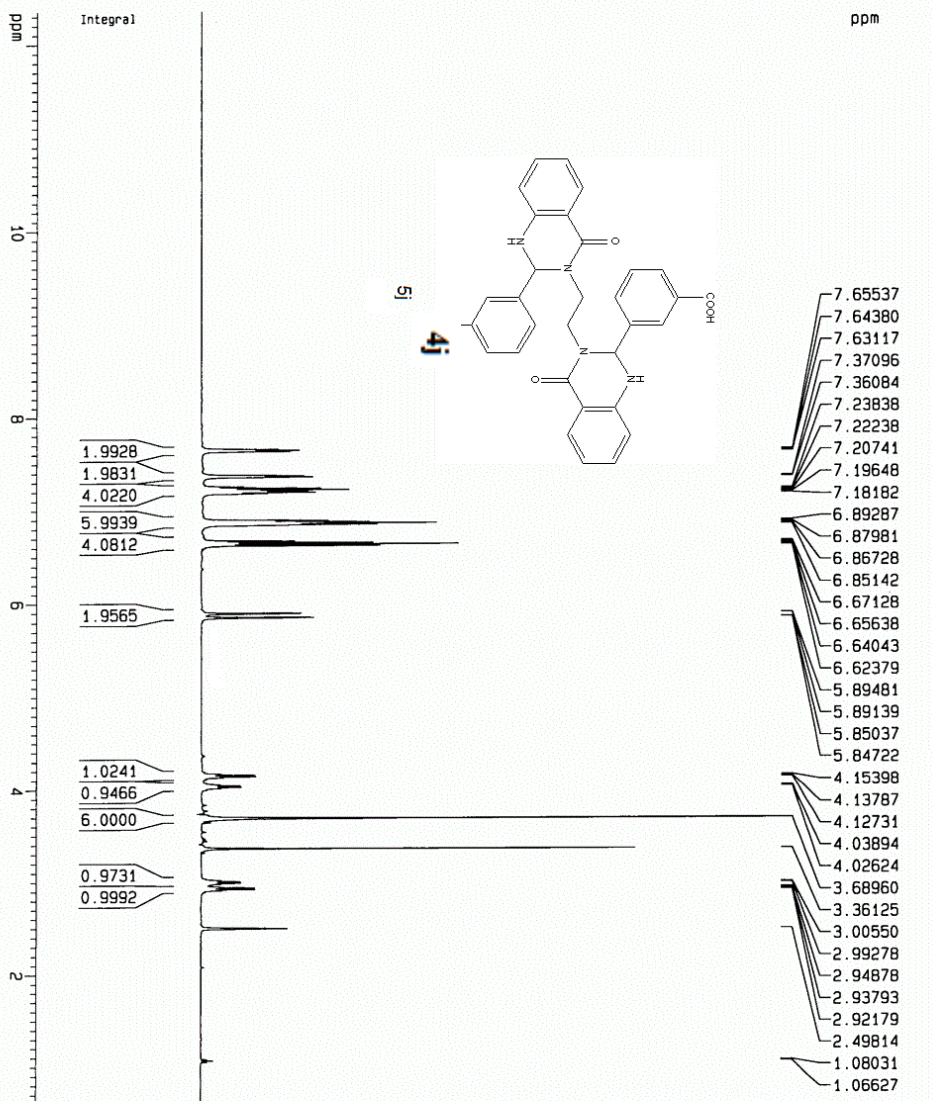
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 RG 14566.5
 DM 16.660 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 WPREST 0.00000000 sec
 KEKMK 0.01500000 sec

***** CHANNEL f1 *****
 NUC1 13C
 P1 9.10 usec
 PL1 3.00 dB
 SF01 125.7705643 MHz

***** CHANNEL f2 *****
 CDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 1.00 dB
 PL3 15.50 dB
 SF02 500.132005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577360 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

10 NMR plot parameters
 CX 20.00 cm
 CY 24.11 cm
 F1P 208.227 Dpm
 F1 26186.16 Hz
 F2P 3.586 Dpm
 F2 450.97 Hz
 PPMCN 10.23205 Dpm/Ca
 HZCN 1286.75954 Hz/Ca



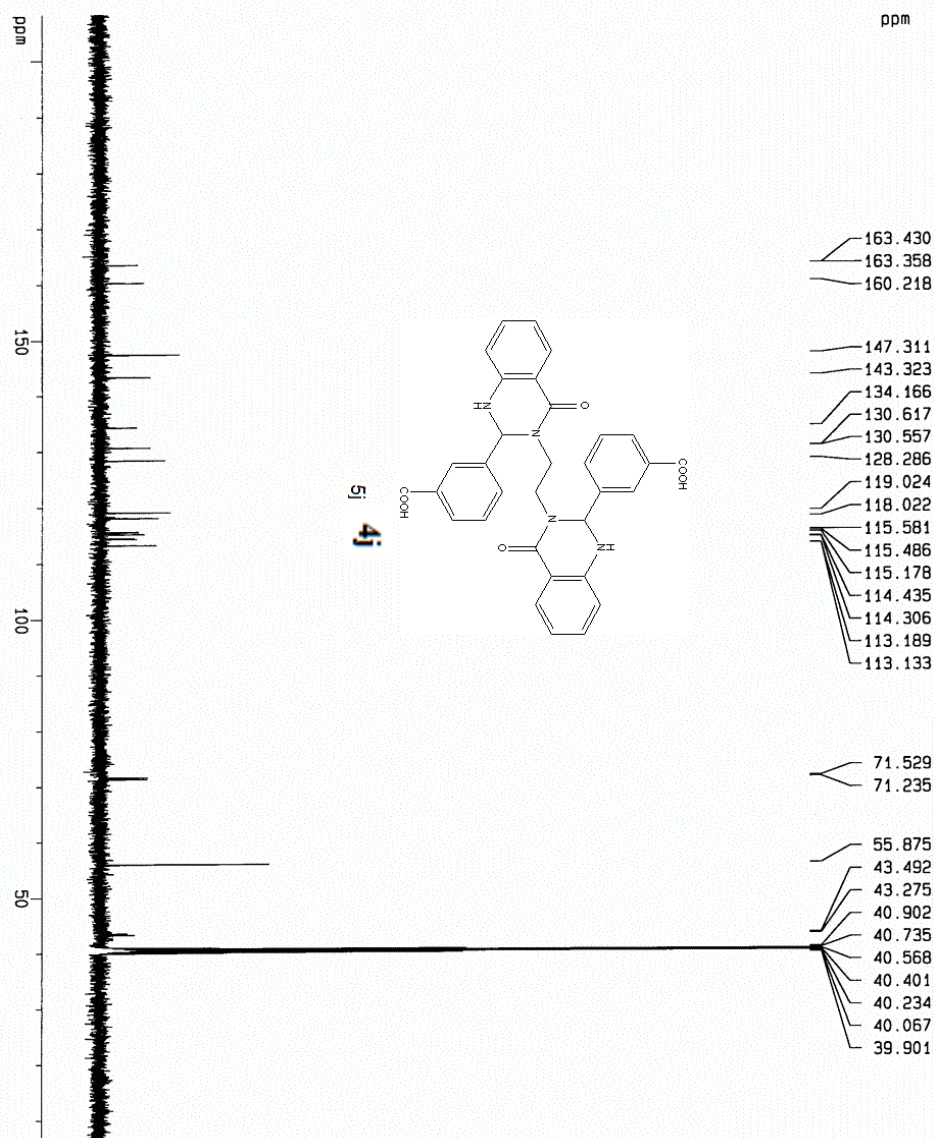
Current Data Parameters
 NAME Asger1
 EXPNO 21
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20121007
 Time 15.13
 INSTRUM spect
 PROBRD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 8
 DS 0
 SMH 10330.578 Hz
 FIDRES 0.315264 Hz
 AQ 1.5860596 sec
 RG 101.6
 DM 48.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 5.00000000 sec
 MICREST 0.00000000 sec
 MCKMK 0.01500000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 10.50 usec
 PL1 -3.00 dB
 SF01 500.1330895 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300049 MHz
 MCM EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 16.34 cm
 F1P 12.353 ppm
 F1 6178.10 Hz
 F2P 0.608 ppm
 F2 303.17 Hz
 PPKCW 0.58734 ppm/cm
 HZCW 293.74673 Hz/cm



- 163.430
- 163.358
- 160.218
- 147.311
- 143.323
- 134.166
- 130.617
- 130.557
- 128.286
- 119.024
- 118.022
- 115.581
- 115.486
- 115.178
- 114.435
- 114.306
- 113.189
- 113.133
- 71.529
- 71.235
- 55.875
- 43.492
- 43.275
- 40.902
- 40.735
- 40.568
- 40.401
- 40.234
- 40.067
- 39.901

Current Data Parameters
 NAME: Asper1
 EXPNO: 22
 PROCNO: 1

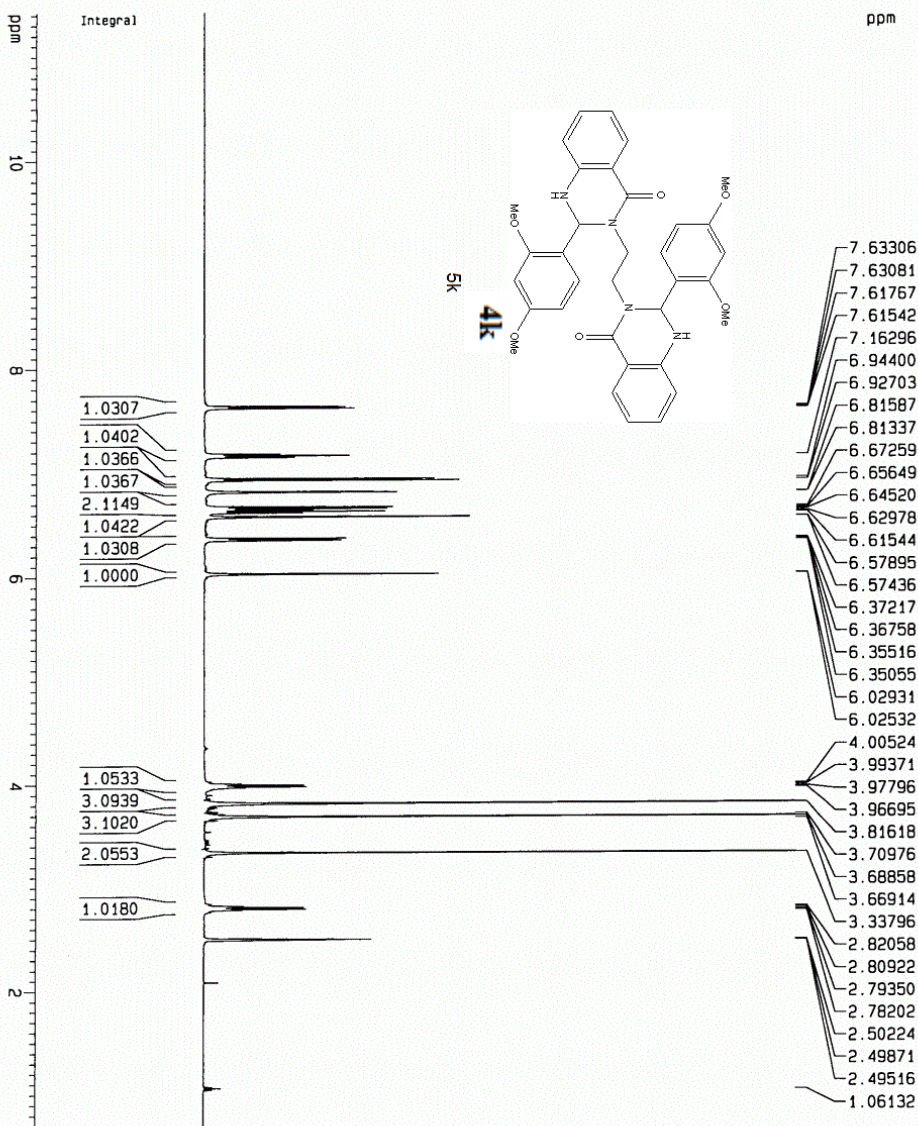
F2 - Acquisition Parameters
 Date_ Time: 20121007 15.15
 INSTRUM: spect
 PROBD0: 5 mm QNP 1H/13
 PULPROG: zgpg
 TD: 2098
 SOLVENT: DMSO
 NS: 186
 DS: 4
 SMH: 30030.029 Hz
 FIDRES: 0.91644 Hz
 AQ: 0.546539 sec
 RG: 1290.2
 DM: 16.650 usec
 DE: 6.50 usec
 TE: 298.0 K
 D1: 2.0000000 sec
 D11: 0.0300000 sec
 DELTA: 1.8999999 sec
 MCREST: 0.0000000 sec
 MCRNK: 0.0150000 sec

***** CHANNEL f1 *****
 NUC1: 13C
 P1: 9.10 usec
 PL1: 3.00 dB
 SF01: 125.7703643 MHz

***** CHANNEL f2 *****
 CDPRG2: waltz16
 NUC2: 1H
 PCPD2: 80.00 usec
 PL2: 0.00 dB
 PL12: 15.50 dB
 PL13: 15.50 dB
 SF02: 500.1350005 MHz

F2 - Processing parameters
 SI: 32768
 SF: 125.7577390 MHz
 MCM: EM
 SSB: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.40

1D NMR plot parameters
 CX: 20.00 cm
 CY: 15.39 cm
 F1P: 208.267 ppm
 F1: 26186.16 Hz
 F2P: 856.78 Hz
 F2: 6.813 ppm
 PPMCN: 10.07071 ppm/cm
 HZCN: 1266.46912 Hz/cm



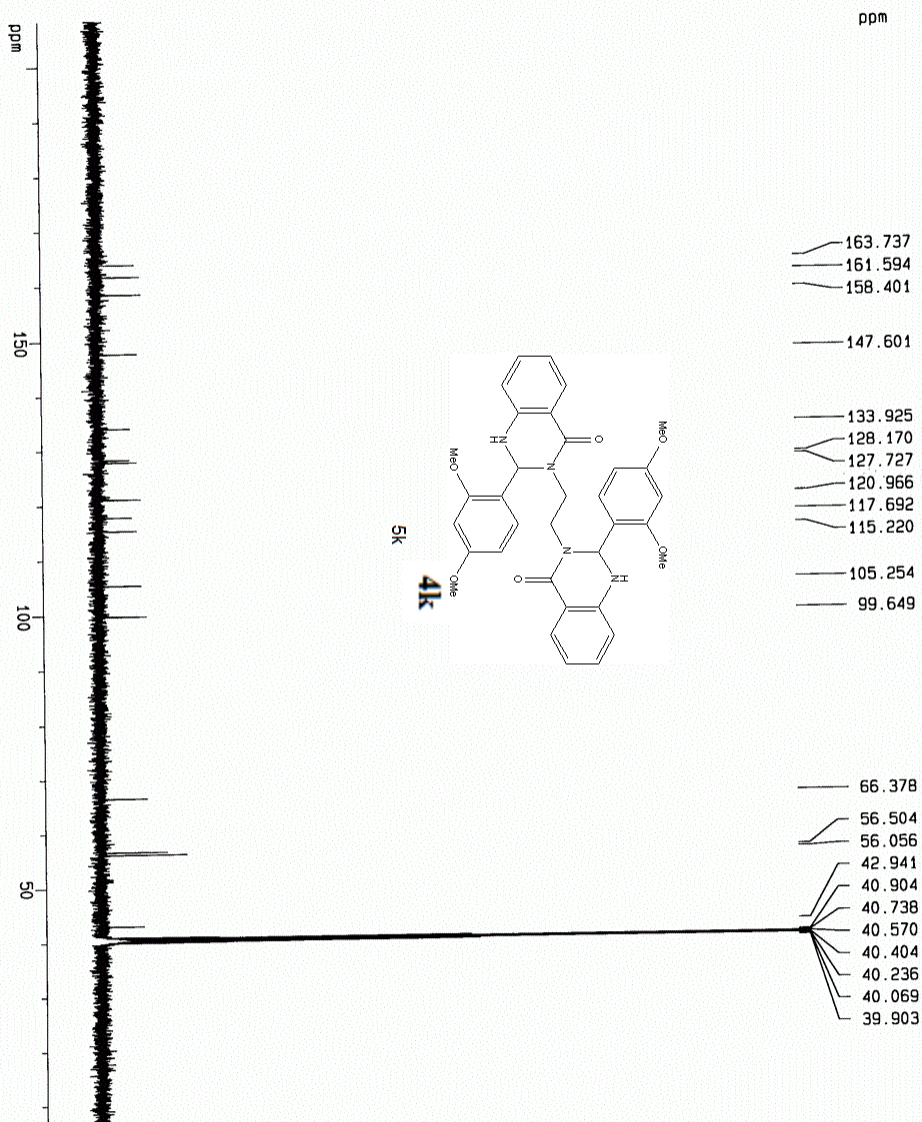
Current Data Parameters
 NAME Asgar1
 EXPNO 26
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20121008
 Time 10:46
 INSTRUM spect
 PROBRD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 8
 DS 0
 SMH 10330.578 Hz
 FIDRES 0.315264 Hz
 AQ 1.5860596 sec
 RG 128
 DW 48.400 usec
 DE 6.30 usec
 TE 298.0 K
 D1 5.00000000 sec
 MCRCST 0.00000000 sec
 MCKMK 0.01500000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 10.50 usec
 PL1 -3.00 dB
 SF01 500.1330885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300049 MHz
 NQM EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

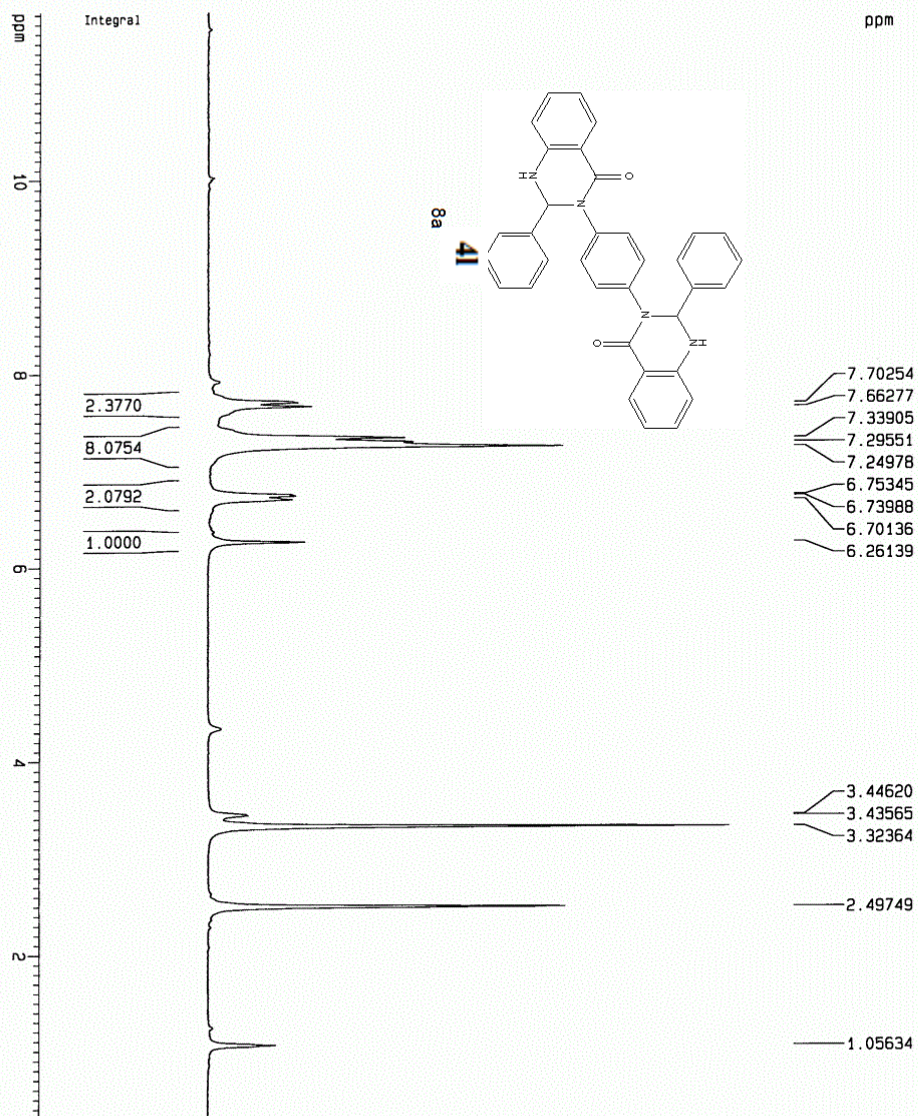
10 NMR plot parameters.
 CX 20.00 cm
 CY 27.10 cm
 FIP 11.423 ppm
 F1 5712.76 Hz
 F2P 0.699 ppm
 F2 349.70 Hz
 PPMCM 0.53617 ppm/cm
 HZCM 268.15295 Hz/cm



- 163.737
- 161.594
- 158.401
- 147.601
- 133.925
- 128.170
- 127.727
- 120.966
- 117.692
- 115.220
- 105.254
- 99.649
- 66.378
- 56.504
- 56.056
- 42.941
- 40.904
- 40.738
- 40.570
- 40.404
- 40.236
- 40.069
- 39.903

```

Current Data Parameters
NAME          Aspar1
EXPNO        24
PROCNO       1
F2 - Acquisition Parameters
Date_        20121008
Time         10.40
INSTRUM     spect
PROBHD      5 mm QNP 1H/13
PULPROG     zgpg30
TD           32768
SOLVENT     DMSO
NS           186
DS           4
SMH          30030.029 Hz
FIDRES      0.316444 Hz
AQ          0.345659 sec
RG          7.5912
DM          10.450 usec
TE          299.0 K
DELT1       2.0000000 sec
DELT2       0.0300000 sec
DELT3       1.8699999 sec
SFO1         125.7703643 MHz
===== CHANNEL f1 =====
NUC1         13C
P1           9.10 usec
PL1         3.00 dB
SFO2         125.7703643 MHz
===== CHANNEL f2 =====
CPDPRG2     waltz16
NUC2         1H
PCPD2       80.00 usec
PL2         0.00 dB
PL12        15.50 dB
PL13        15.50 dB
SFO2         500.1326005 MHz
F2 - Processing parameters
SI           32768
SF           125.7517350 MHz
SM           EM
MM           0
SSB          0
GB           0
PC           1.40
=====
1D NMR Plot parameters
CX           20.00 cm
CY           15.59 cm
F1P         208.227 ppm
F1          26166.16 Hz
F2P         6.813 ppm
F2          856.78 Hz
PNUCK       10.07071 ppm/cm
HZCM        1266.46912 Hz/cm
    
```



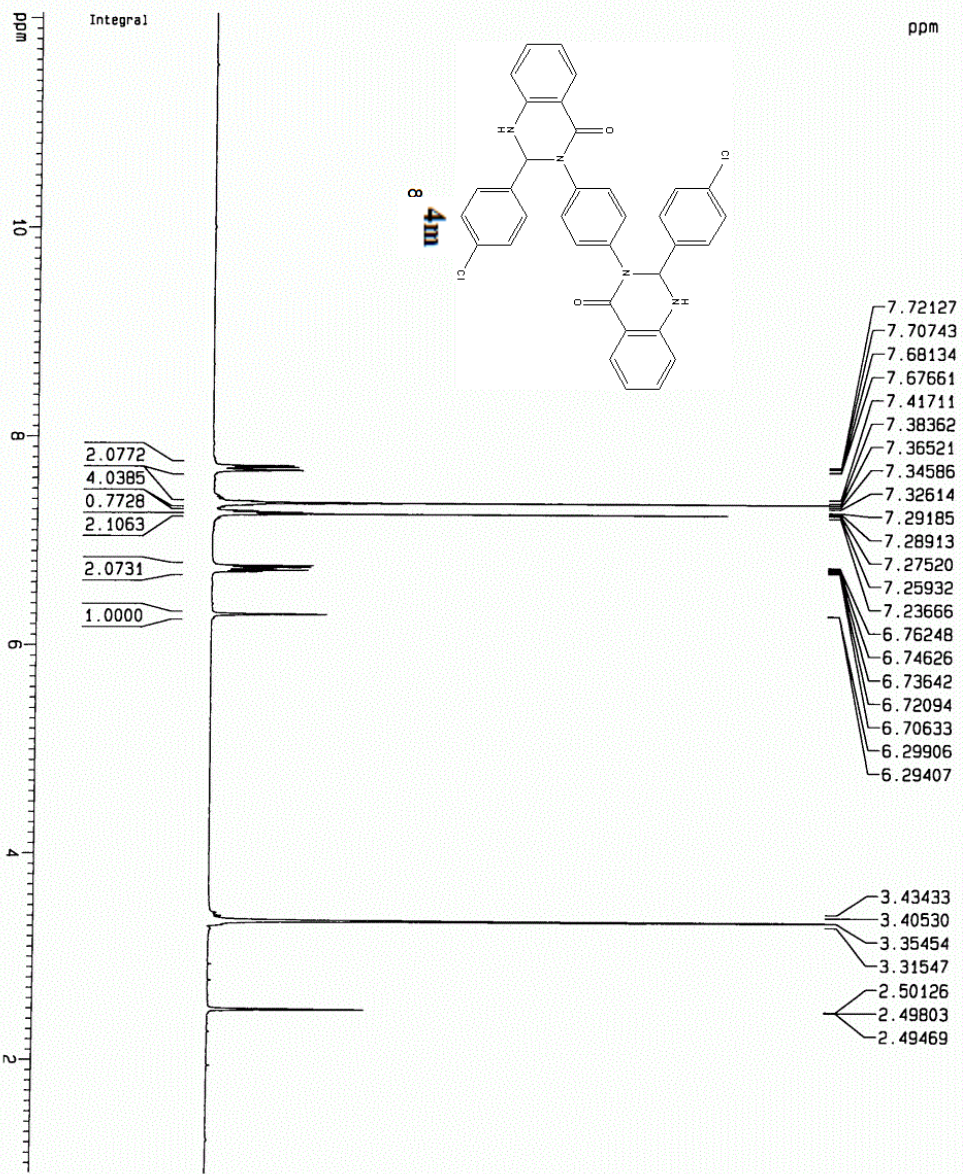
Current Data Parameters
 NAME Asgar1
 EXPNO 6
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120925
 Time 14.20
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 2030
 FIDRES 0.32768
 SOLVENT DMSO
 NS 8
 DS 0
 SMH 10330.578 Hz
 FIDRES 0.315264 Hz
 AQ 1.5860696 sec
 RG 228.1
 DM 48.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 5.00000000 sec
 MCREST 0.00000000 sec
 MCHNK 0.01500000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 10.50 usec
 PL1 -9.00 dB
 SF01 500.1330895 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300049 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 9.36 cm
 F1P 11.725 ppm
 F1 5864.00 Hz
 F2P 0.304 ppm
 F2 131.93 Hz
 PPMCN 0.57106 ppm/c
 HZCN 285.60327 Hz/cm



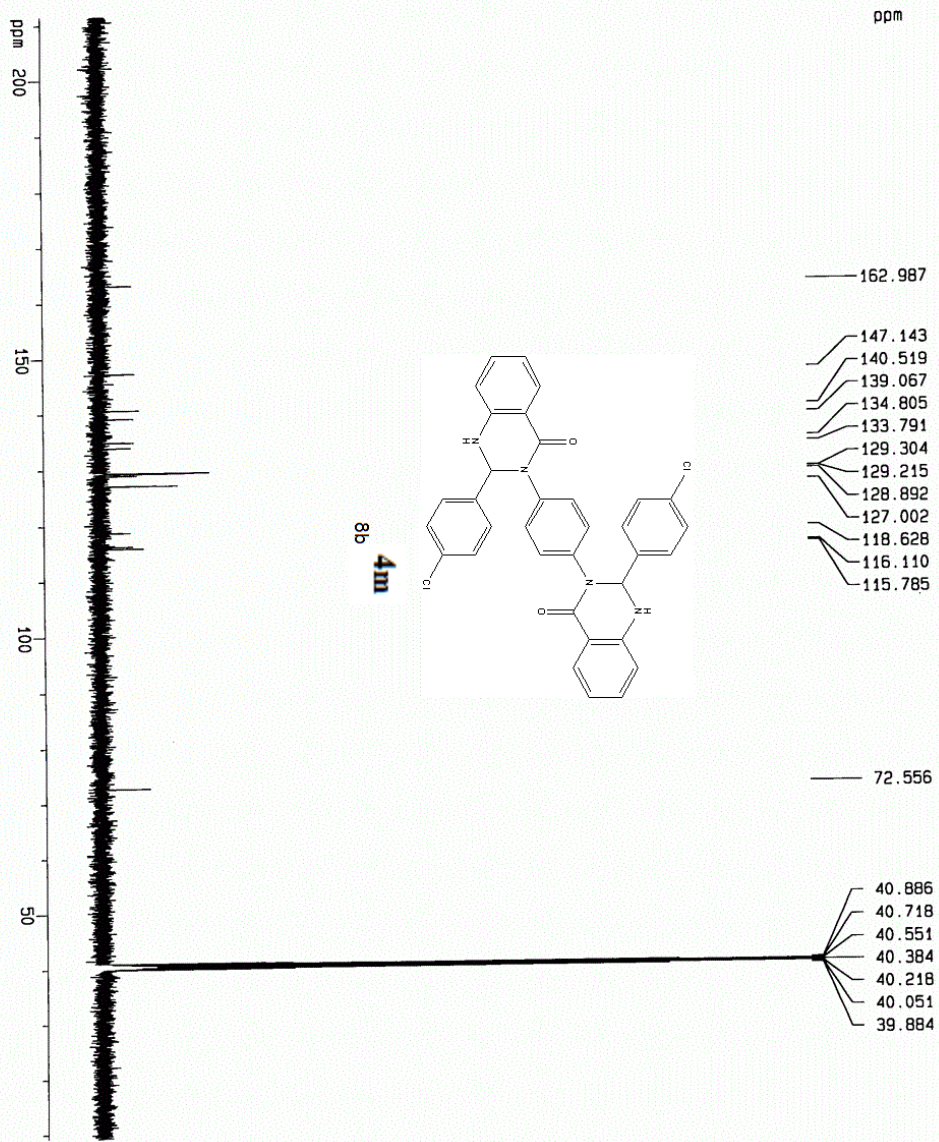
Current Data Parameters
 NAME Asger1
 EXPNO 20
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20121001
 Time 14.58
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 16
 DS 0
 SMH 10330.578 Hz
 FIDRES 0.315264 Hz
 AQ 1.5860696 sec
 RG 181
 DM 48.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 5.00000000 sec
 MCHEST 0.00000000 sec
 MCHKR 0.01500000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 10.50 usec
 PL1 -3.00 dB
 SFO1 500.1330885 MHz

F2 - Processing parameters
 S1 32768
 SF 500.1300049 MHz
 MDM EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

10 NMR plot parameters
 CX 20.00 cm
 CY 33.83 cm
 F1P 12.051 ppm
 F1 6026.86 Hz
 F2P 0.909 ppm
 F2 454.40 Hz
 PPMCM 0.55710 ppm/c
 HZCM 278.62314 Hz/cm



Current Data Parameters
 NAME: Assent1
 EXPNO: 18
 PROCNO: 1

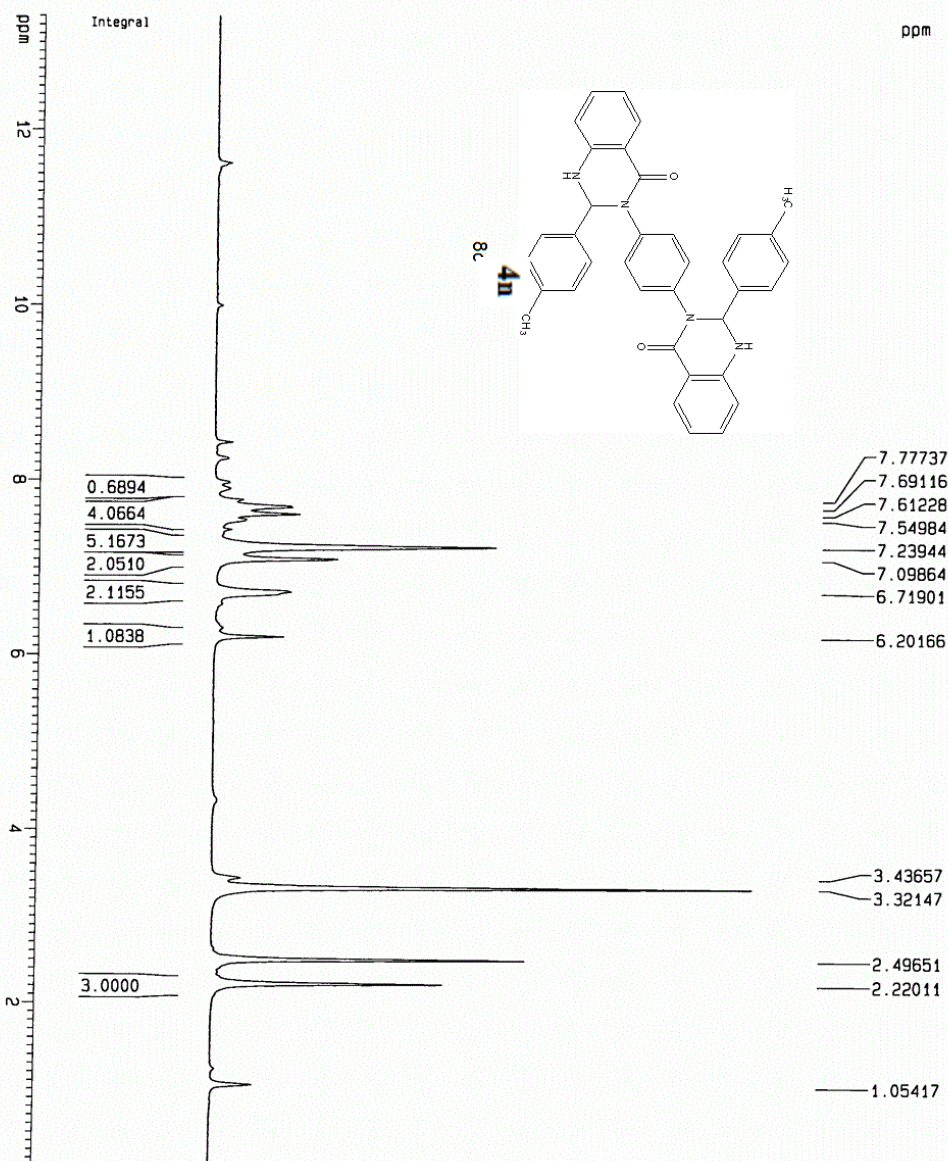
F2 - Acquisition Parameters
 Date_ : 20121001
 Time : 14.47
 INSTRUM: spect
 PROBNM: 5 mm QNP 1H/13
 PULPROG: zgpg30
 TD: 32768
 SO: VENT
 NS: 300
 DS: 4
 SM: 300.30, 029 Hz
 FIDRES: 0.916444 Hz
 AQ: 0.546539 sec
 RG: 9195.2
 DE: 16.650 usec
 TE: 298.0 K
 D1: 2.00000000 sec
 D11: 0.03000000 sec
 DELTA: 1.89999998 sec
 ACQRES: 0.00000000 sec
 MCNMR: 0.01500000 sec

***** CHANNEL f1 *****
 NUC1: 13C
 P1: 9.10 usec
 PL1: 3.00 dB
 SF01: 125.7703643 MHz

***** CHANNEL f2 *****
 CPDPRG2: waltz16
 NUC2: 1H
 PCPD2: 80.00 usec
 PL2: 0.00 dB
 PL12: 15.50 dB
 PL13: 15.50 dB
 SF02: 500.1320005 MHz

F2 - Processing parameters
 SI: 32768
 SF: 125.7577390 MHz
 NDM: EM
 SSB: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.40

10 MHz pilot parameters
 CX: 24.00 ca
 CY: 24.11 ca
 F1P: 214.654 ppm
 F1: 26591.97 Hz
 F2P: 9.233 ppm
 F2: 1161.14 Hz
 PPRCK: 10.11104 ppm/ca
 HZCK: 1271.54175 Hz/cm



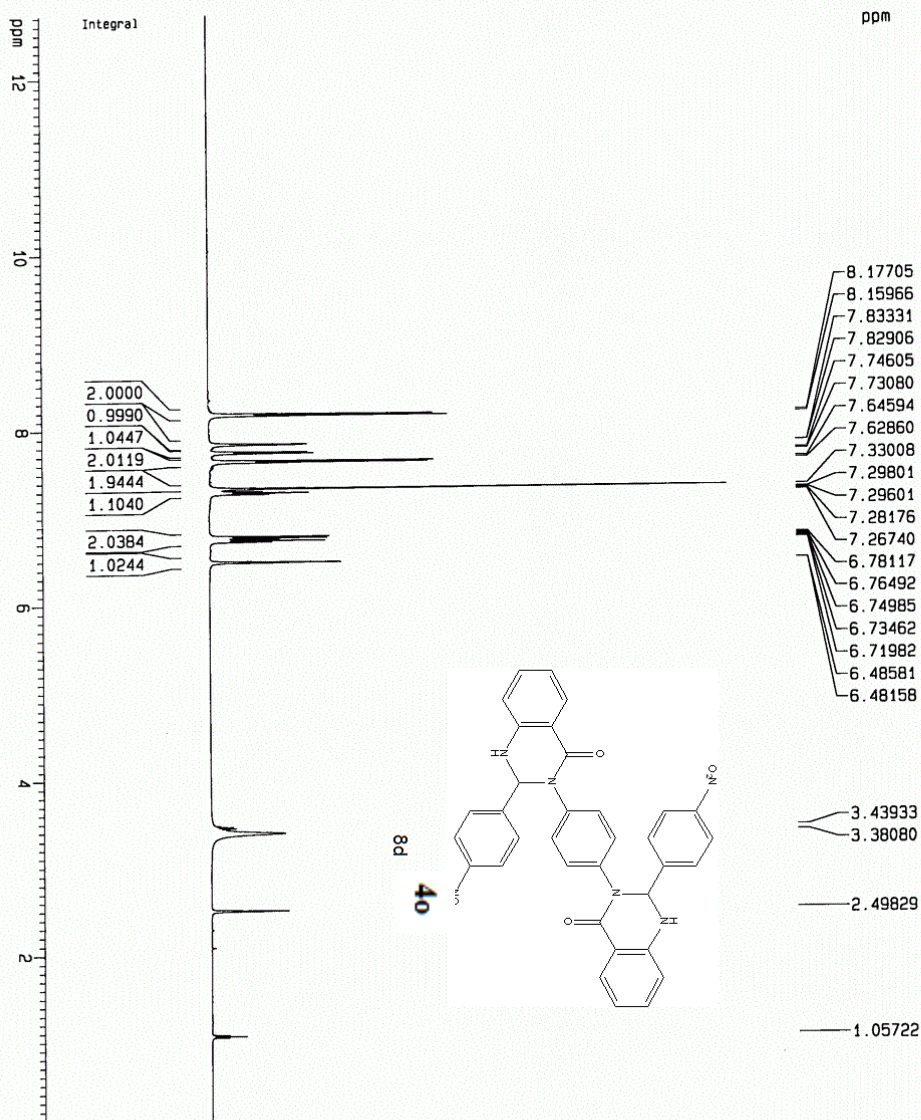
Current Data Parameters
 NAME Aspar1
 EXPNO 9
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120925
 Time 17.05
 INSTNUM spect
 PROBNM 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 16
 DS 0
 SH1 10330.578 Hz
 FIDRES 0.315264 Hz
 AQ 1.5860696 sec
 RG 228.1
 DW 48.400 usec
 DE 6.50 usec
 TE 298.0 K
 O1 5.00000000 sec
 MCHRES 0.00000000 sec
 MCHRK 0.01500000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 10.50 usec
 PL1 -3.00 dB
 SFO1 500.1330885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1330049 MHz
 WDM EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

10 MHz plot parameters
 CX 20.00 cm
 CY 9.36 cm
 F1P 13.307 ppm
 F1 6655.07 Hz
 F2P 0.141 ppm
 F2 70.49 Hz
 PPMCM 0.65829 ppm/cm
 HZCM 329.22900 Hz/cm



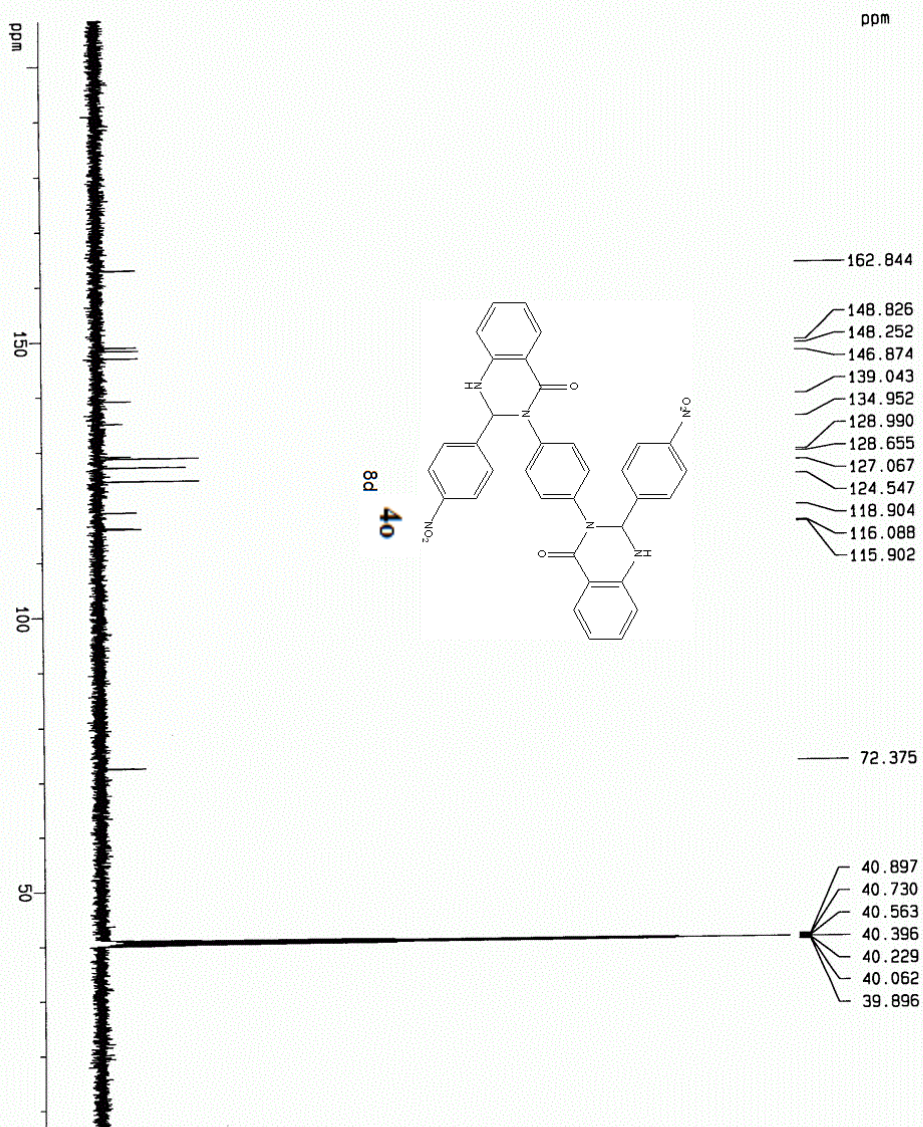
Current Data Parameters
 NAME: Aspar1
 EXPNO: 25
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20121008
 Time: 10.11
 INSTRUM: spect
 PROBRD: 5 mm QNP 1H/13
 PULPROG: zgpg30
 TD: 32768
 SOLVENT: DMSO
 NS: 8
 DS: 0
 SMH: 10330.578 Hz
 FIDRES: 0.315264 Hz
 AQ: 1.5860596 sec
 RG: 128
 DE: 48.400 usec
 TE: 6.50 usec
 D1: 297.9 K
 MCHEST: 5.00000000 sec
 MCMRK: 0.00000000 sec
 0.01500000 sec

***** CHANNEL f1 *****
 NUC1: 1H
 P1: 10.50 usec
 PL1: -3.00 dB
 SF01: 500.1330885 MHz

F2 - Processing parameters
 SI: 32768
 SF: 500.1300049 MHz
 RQM: CM
 SSB: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00

10 NMR plot parameters
 CX: 20.00 cm
 CY: 9.36 cm
 F1P: 12.725 ppm
 F1: 6384.24 Hz
 F2P: 0.071 ppm
 F2: 35.59 Hz
 PPM/CM: 0.53270 ppm/cm
 HZ/CM: 316.43213 Hz/cm



- ppm
- 162.844
 - 148.826
 - 148.252
 - 146.874
 - 139.043
 - 134.952
 - 128.990
 - 128.655
 - 127.067
 - 124.547
 - 118.904
 - 116.088
 - 115.902
 - 72.375
 - 40.897
 - 40.730
 - 40.563
 - 40.396
 - 40.229
 - 40.062
 - 39.896

```

Current Data Parameters
NAME      Asp1
EXPNO    23
PROCNO   1

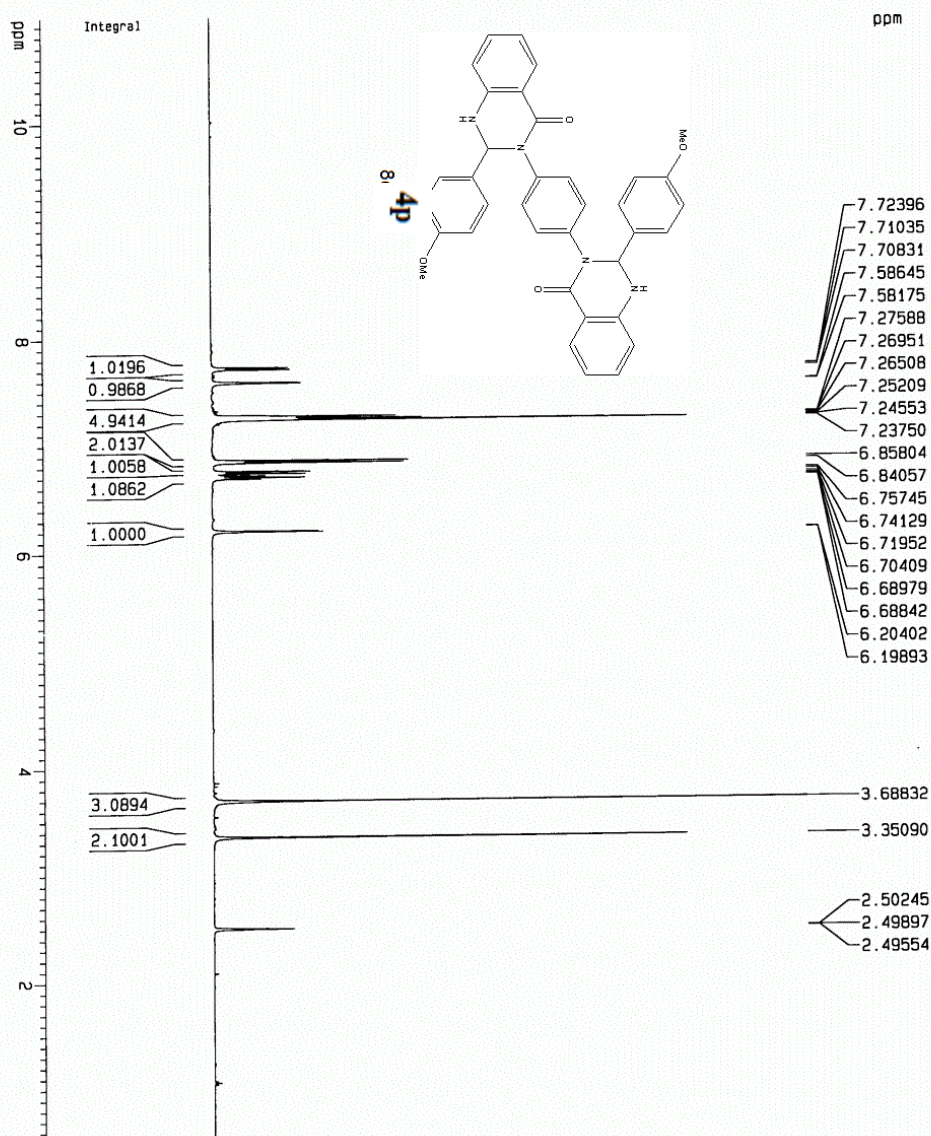
F2 - Acquisition Parameters
Date_    20121008
Time     10.06
INSTRUM spect
PROBHD   5 mm QNP 1H/13
PULPROG zgpg
TO       32768
SOLVENT DMSO
NS       188
DS       4
SMH      30030.029 Hz
FIDRES   0.916444 Hz
AQ        0.546539 sec
RG        2560.3
DM        16.650 usec
DE        6.50 usec
TE        298.0 K
D1        2.0000000 sec
d11       0.0300000 sec
DELTA    1.8899998 sec
ACQST    0.0000000 sec
MKMK     0.0150000 sec

***** CHANNEL f1 *****
NUC1      13C
P1        9.10 usec
PL1       3.00 dB
SFO1     125.7703643 MHz

***** CHANNEL f2 *****
CPDPRG2  waltz16
NUC2      1H
PCPD2    80.00 usec
PL2      0.00 dB
PL12     15.50 dB
PL13     15.50 dB
SFO2     500.1320005 MHz

F2 - Processing parameters
SI        32768
SF        125.7577390 MHz
KMCW      EM
SSB       0
LB         1.00 Hz
GB         0
PC         1.40

10 NMR plot parameters
CX        20.00 cm
CY        12.50 cm
F1P       208.267 ppm
F1        26186.16 Hz
F2P       656.78 Hz
F2        8113 ppm
PCKMCH   10.00071 ppm/cm
HCKMCH   1286.46912 Hz/cm
    
```



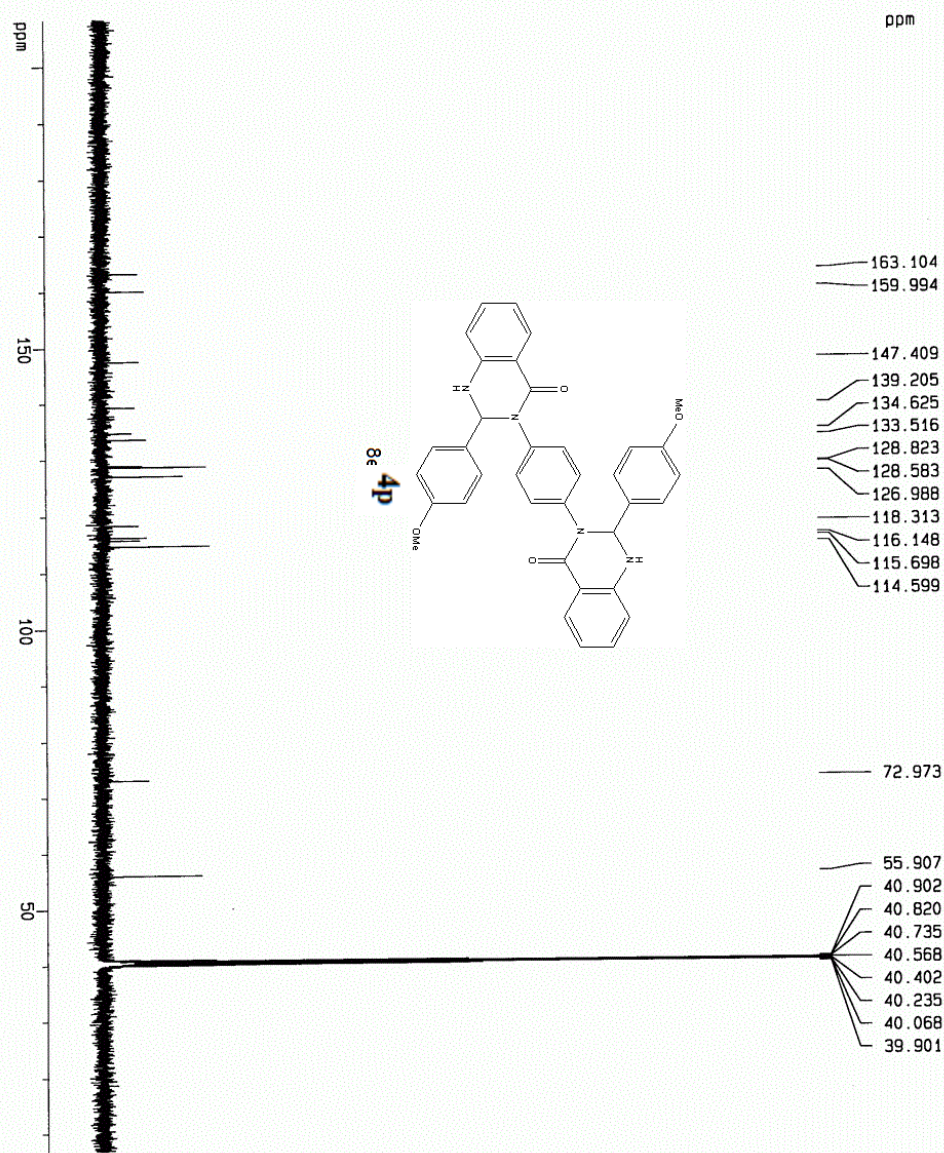
Current Data Parameters
 NAME Aspar1
 EXPNO 28
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20121008
 Time 13.26
 INSTRUM spect
 PROBD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 32768
 SOLVENT DMSO
 NS 8
 DS 0
 SMH 10330.578 Hz
 FIDRES 0.315264 Hz
 AQ 1.5860596 sec
 RG 128
 DM 48.400 usec
 DE 6.30 usec
 TE 298.0 K
 D1 5.00000000 sec
 MCREST 0.00000000 sec
 MCMRK 0.01500000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 10.50 usec
 PL1 -3.00 dB
 SF01 500.1330885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1330049 MHz
 MDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 14.53 cm
 F1P 10.381 ppm
 F1 5491.72 Hz
 F2P 0.560 ppm
 F2 279.90 Hz
 PPM/CM 0.52105 ppm/cm
 HZ/CM 260.59116 Hz/cm



- 163.104
- 159.994
- 147.409
- 139.205
- 134.625
- 133.516
- 128.823
- 128.583
- 126.988
- 118.313
- 116.148
- 115.698
- 114.599
- 72.973
- 55.907
- 40.902
- 40.820
- 40.735
- 40.568
- 40.402
- 40.235
- 40.068
- 39.901

Current Data Parameters
 NAME Aspart1
 EXPNO 27
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20121008
 Time 13.21
 INSTRUM spect
 PROBNM 5 mm QNP 1H/13
 PULPROG zgpg
 TO 32768
 SOLVENT DMSO
 NS 166
 DS 4
 SMH 30030.029 Hz
 FIDRES 0.316444 Hz
 AQ 0.546539 sec
 RG 2896.3
 DM 16.650 USEC
 DE 6.50 USEC
 TE 298.0 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.8899999 sec
 ACQST 0.0000000 sec
 MCNMR 0.0150000 sec

***** CHANNEL f1 *****
 NUC1 13C
 P1 9.10 USEC
 PL1 3.00 DB
 SFO1 125.7708413 MHz

***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 USEC
 PL2 0.00 DB
 PL12 13.50 DB
 PL13 13.50 DB
 SFO2 500.1350005 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577350 MHz
 NDM 599
 EN 0
 SSF 1.00 HZ
 LB 08
 GB 0
 PC 1.40

1D NMR plot parameters
 CV 90.00 cm
 CY 15.59 cm
 F1P 208.227 ppm
 F2P 26186.16 Hz
 F3P 6.813 ppm
 F3 666.78 Hz
 PPMCK 10.07071 ppm/Hz
 HZCK 1286.46912 Hz/cm