Supplementary Material

Acylation of *trans*-2-substituted cyclohexanols: the impact of substituent variation on the pyridine-induced reversal of diastereoselectivity

Sven Hackbusch and Andreas H. Franz*

Department of Chemistry, University of the Pacific, 3601 Pacific Avenue, Stockton, CA 95211, USA
E-mail: afranz@pacific.edu

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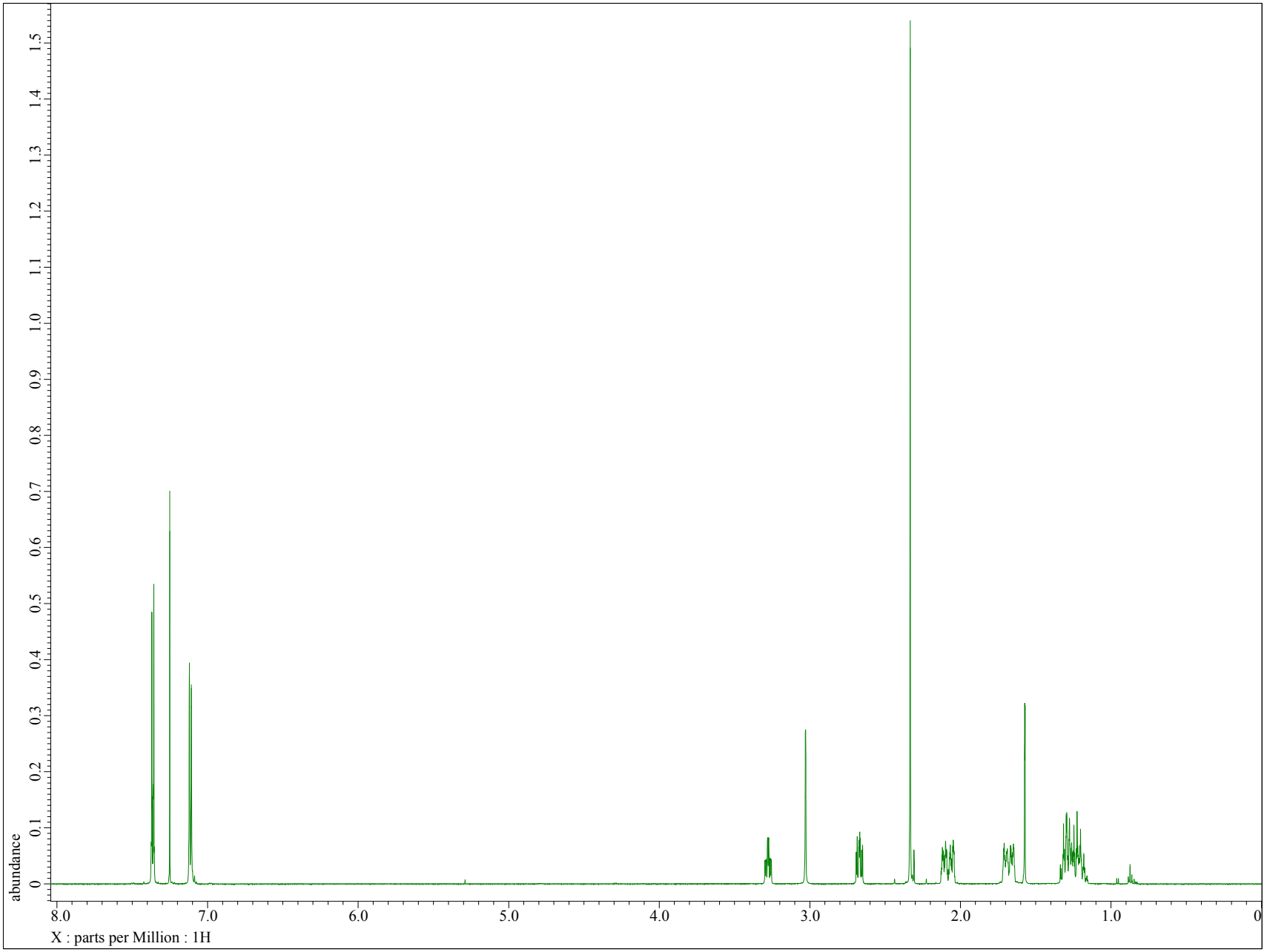
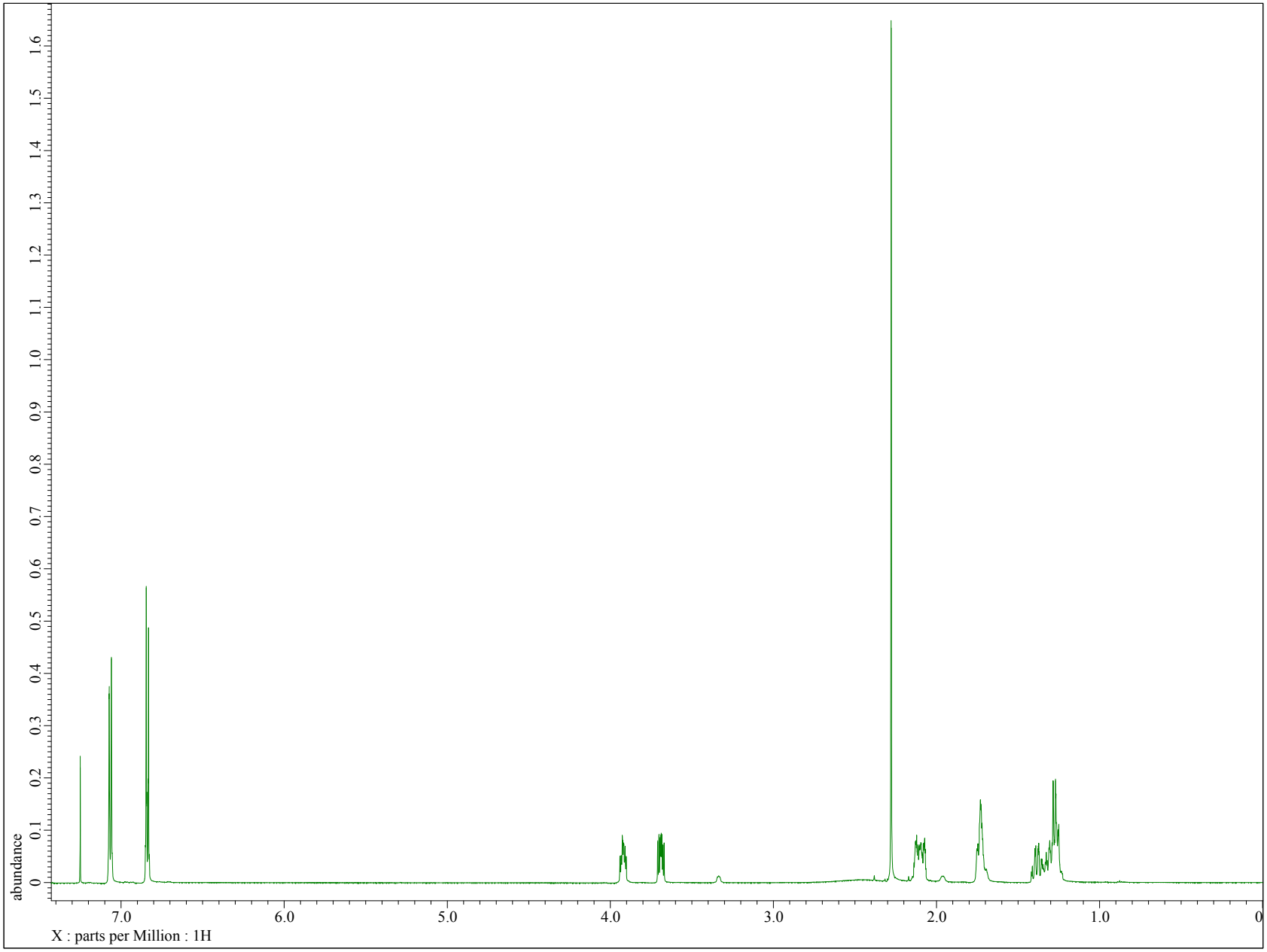
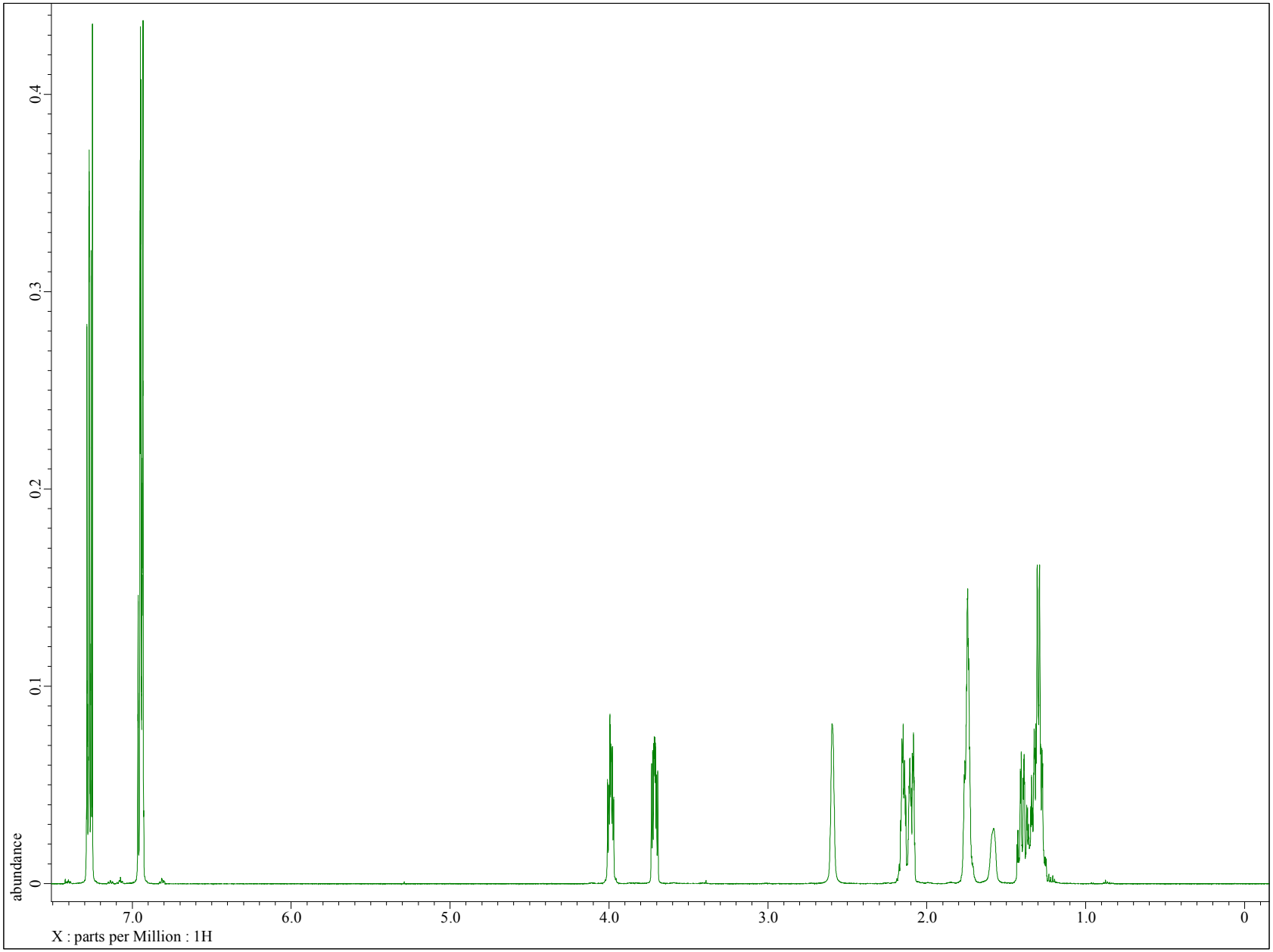


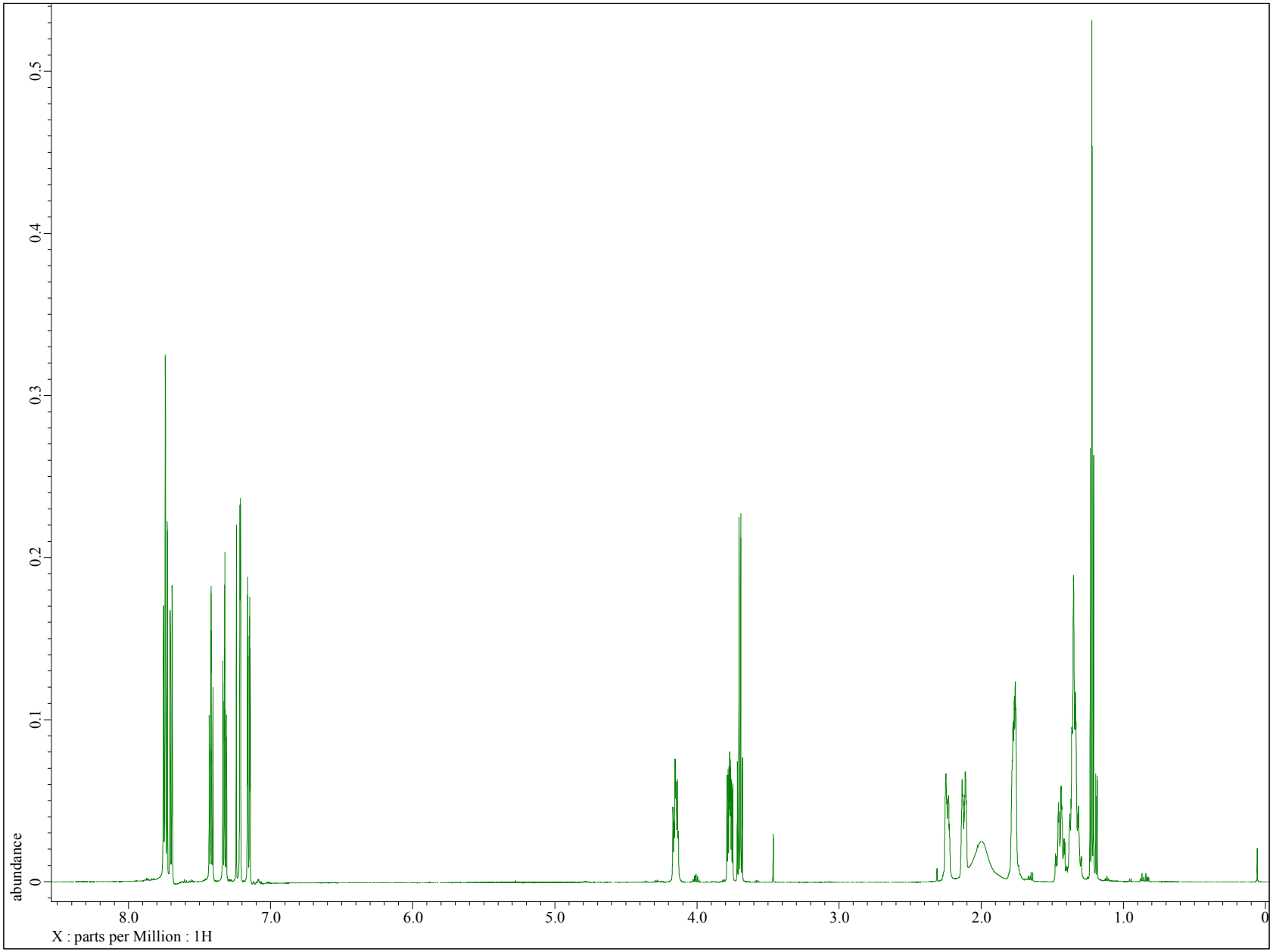
^{1}H NMR of **Compound 1** [(±)-*trans*-2-(*p*-tolylsulfanyl)cyclohexanol]



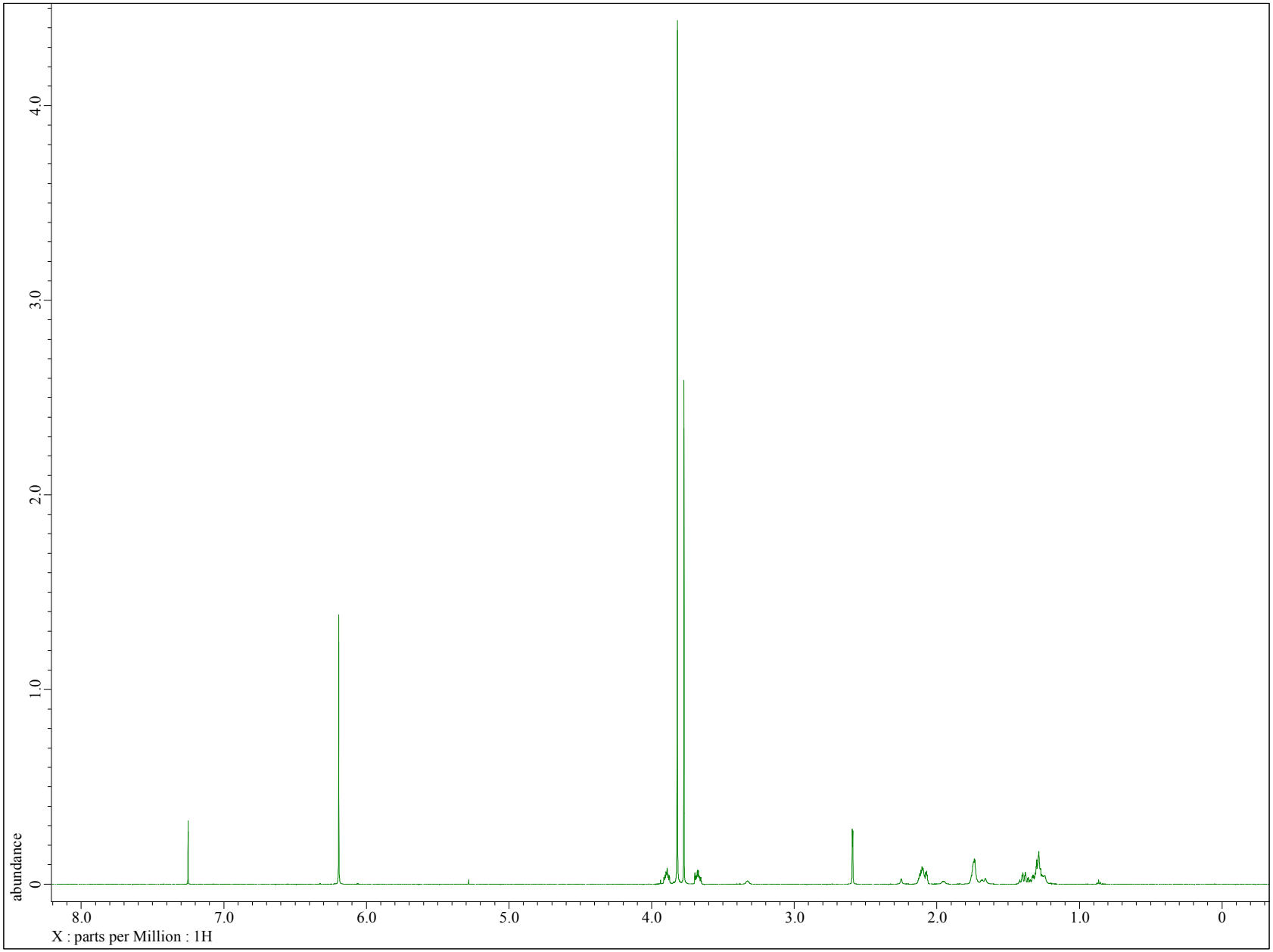
^{1}H NMR of **Compound 2** [(±)-*trans*-2-(*p*-tolyloxy)cyclohexanol]



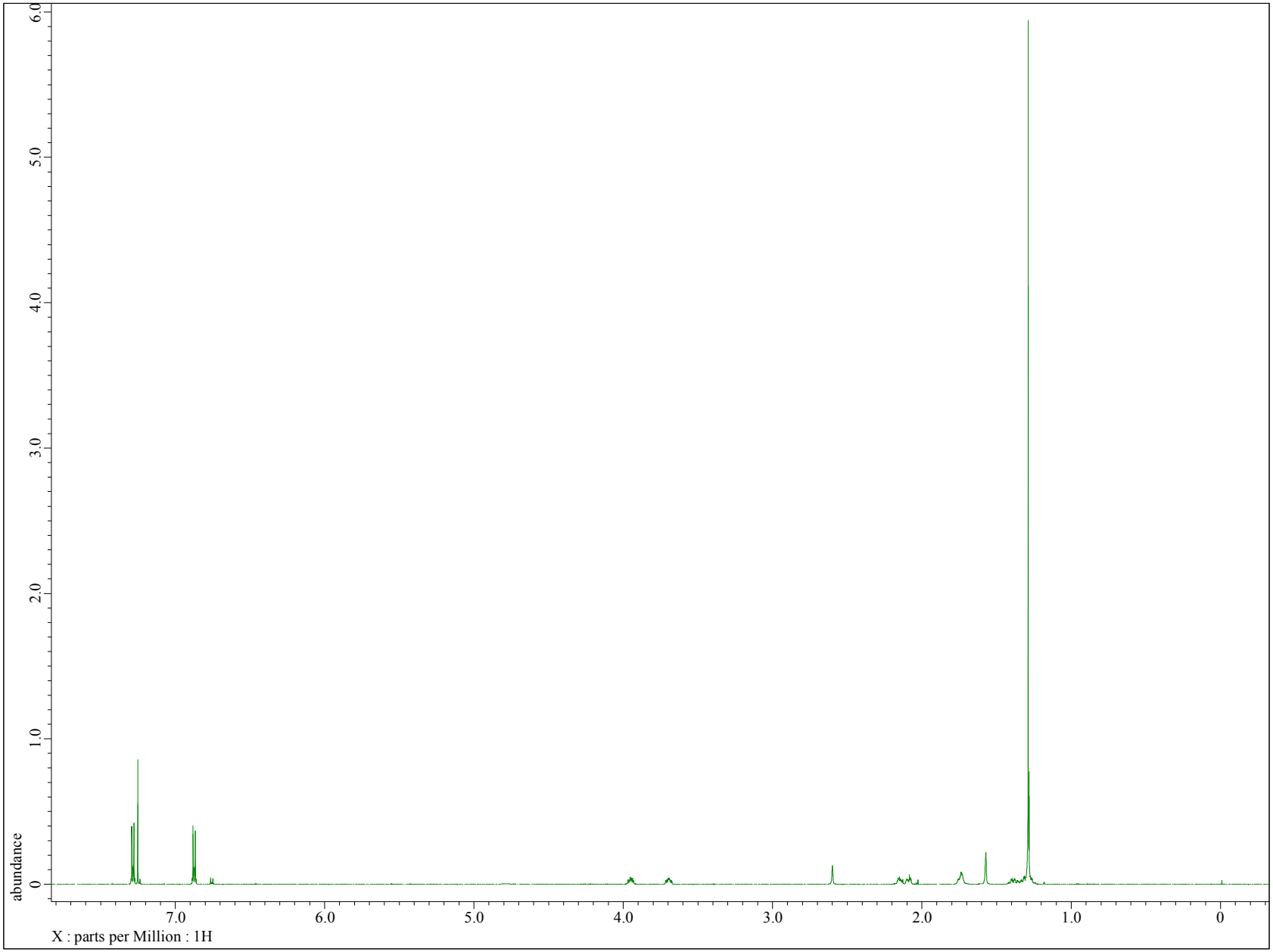
^{1}H NMR of **Compound 3** [(±)-*trans*-2-(phenyloxy)cyclohexanol]



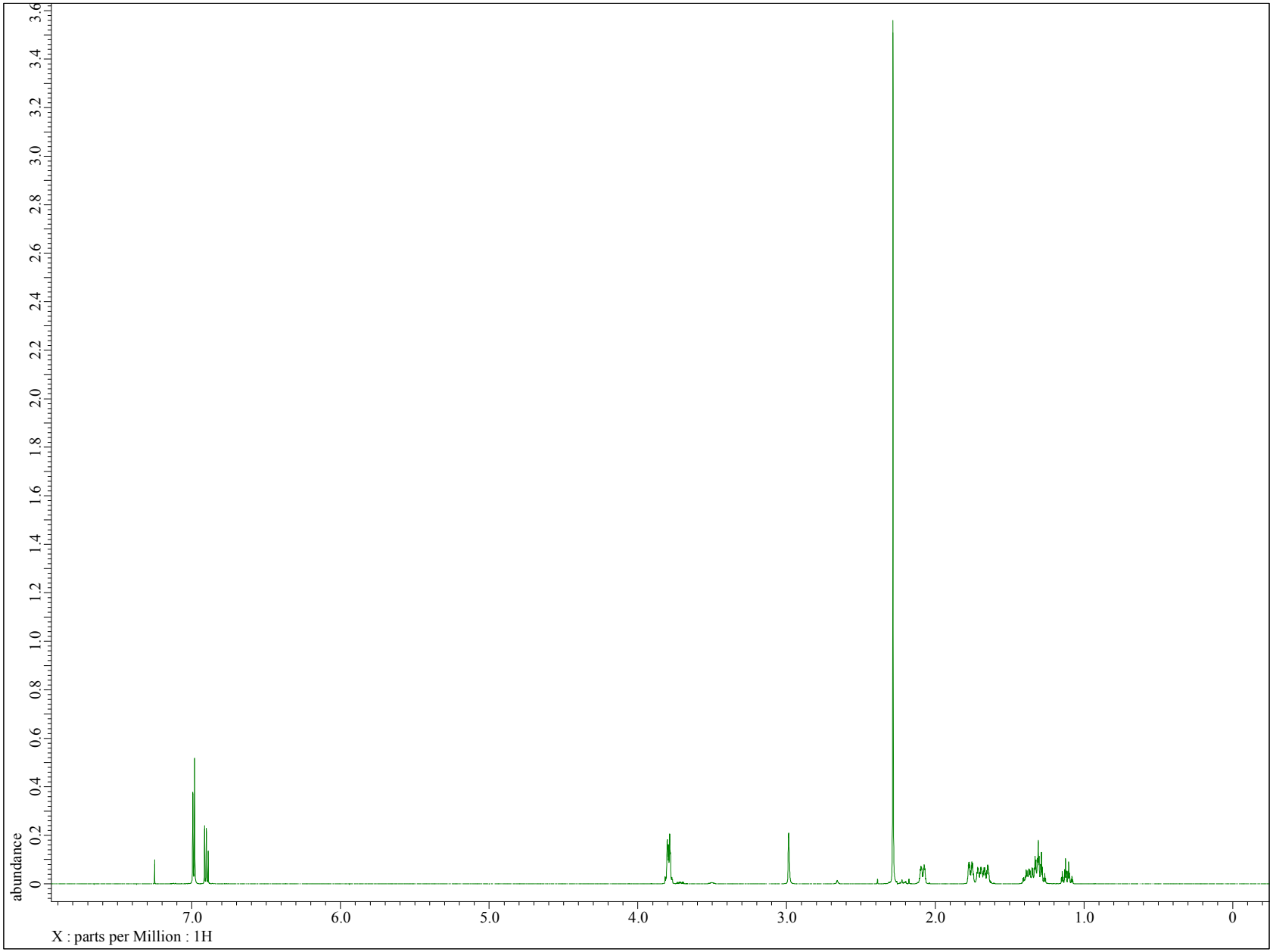
^{1}H NMR of **Compound 4** [(±)-*trans*-2-(napthalen-2-yloxy)cyclohexanol]



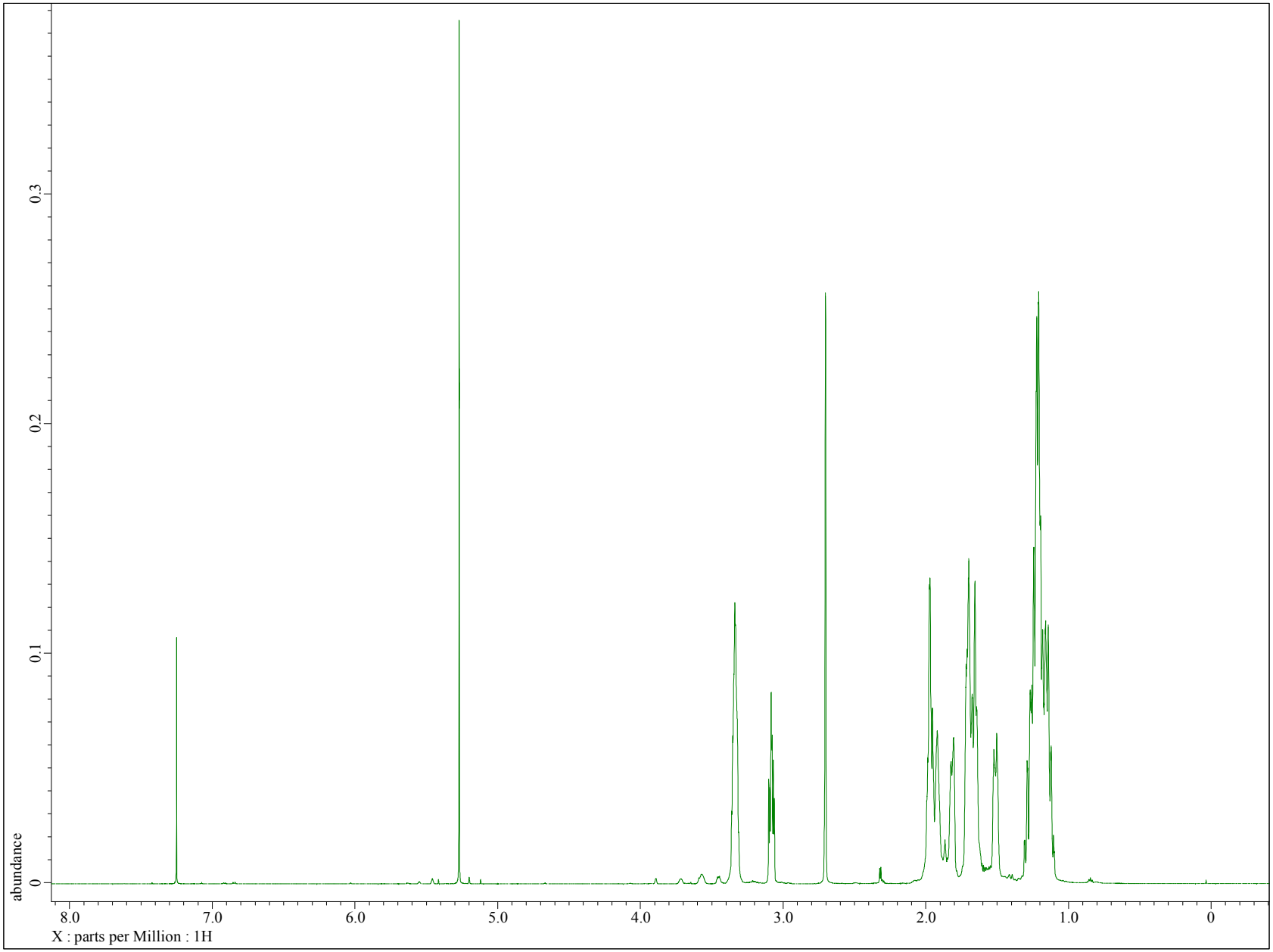
^{1}H NMR of **Compound 5** [(±)-*trans*-2-(3,4,5-trimethylphenyloxy)cyclohexanol]



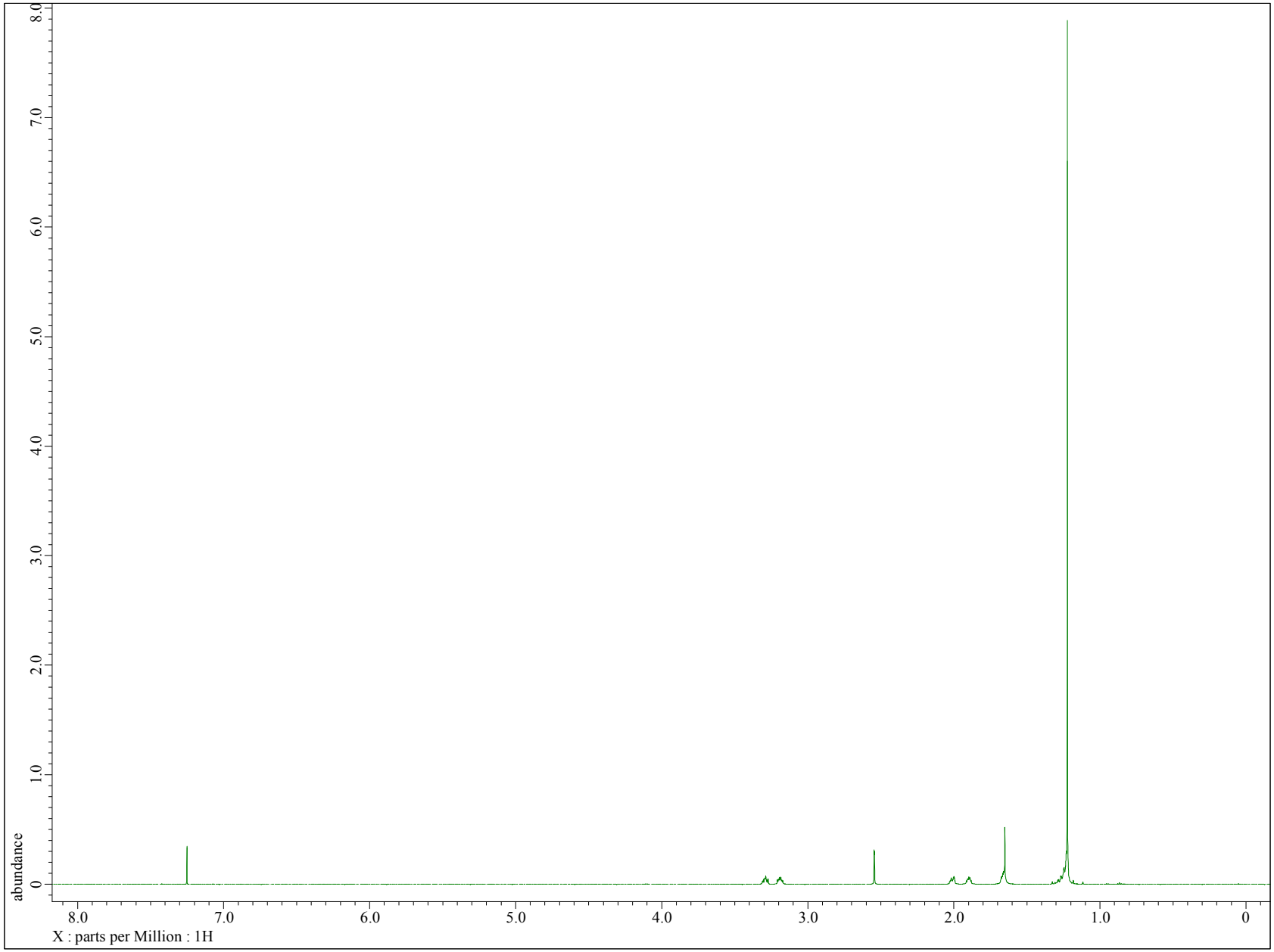
^{1}H NMR of **Compound 6** [(±)-*trans*-2-(*p*-(*tert*-butoxy)phenyloxy)cyclohexanol]



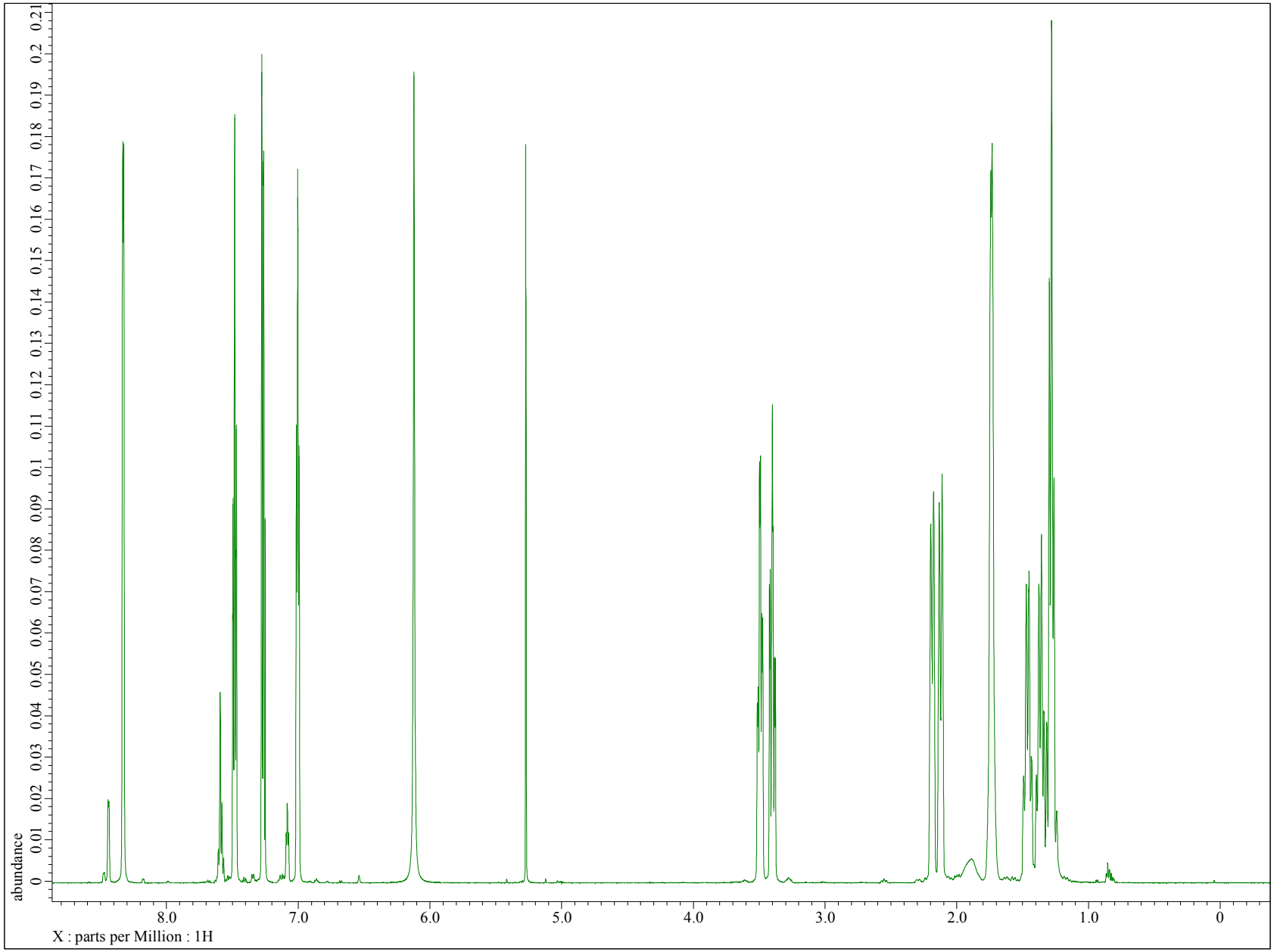
^{1}H NMR of **Compound 7** [(±)-*trans*-2-(2,6-dimethylphenyloxy)cyclohexanol]



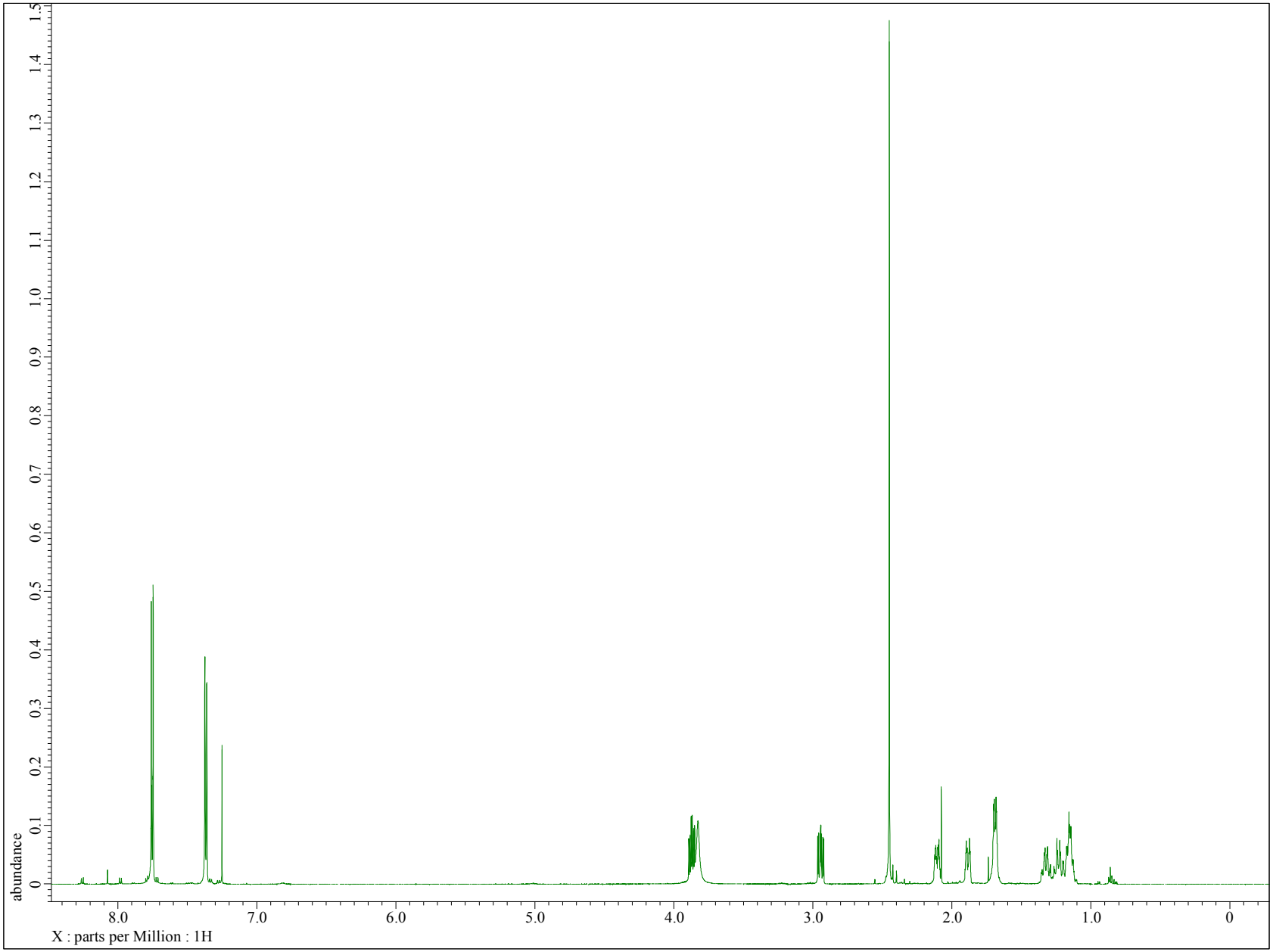
^{1}H NMR of **Compound 8** [(±)-*trans*-2-(cyclohexyloxy)cyclohexanol]



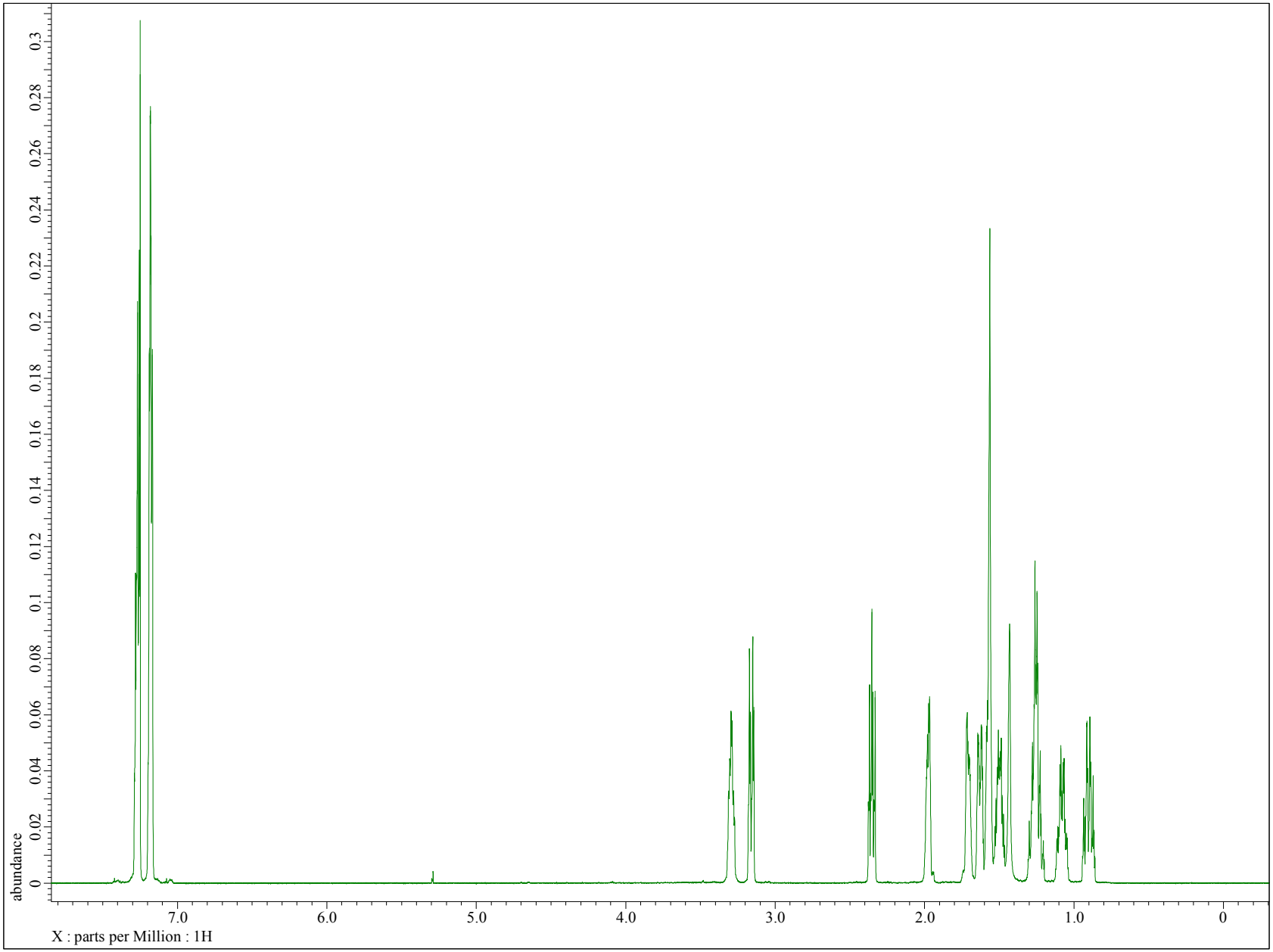
^{1}H NMR of **Compound 9** [(±)-*trans*-2-(*t*-butoxy)cyclohexanol]



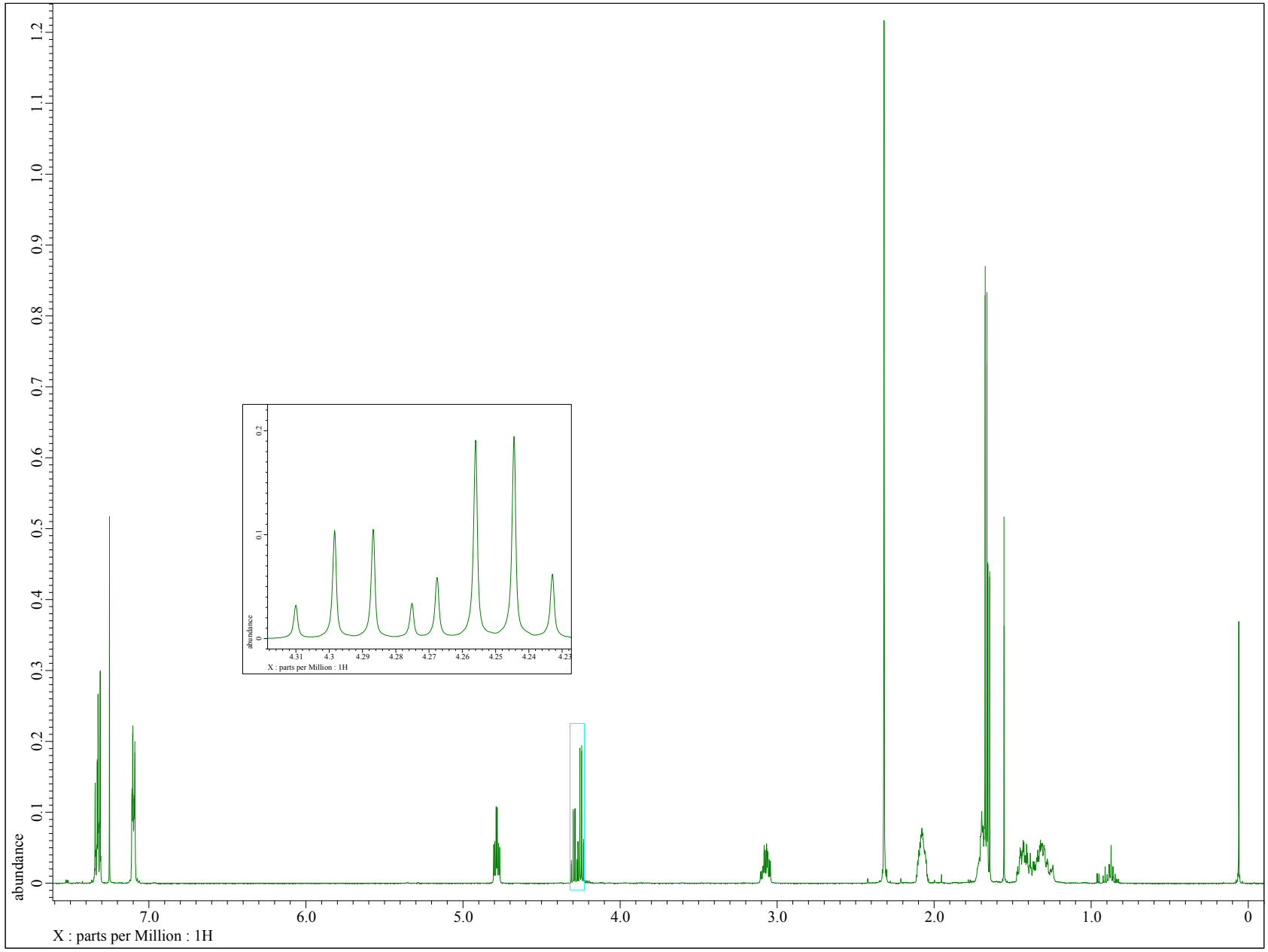
^{1}H NMR of **Compound 10** [(±)-*trans*-2-(pyridine-2-ylthio)cyclohexanol]



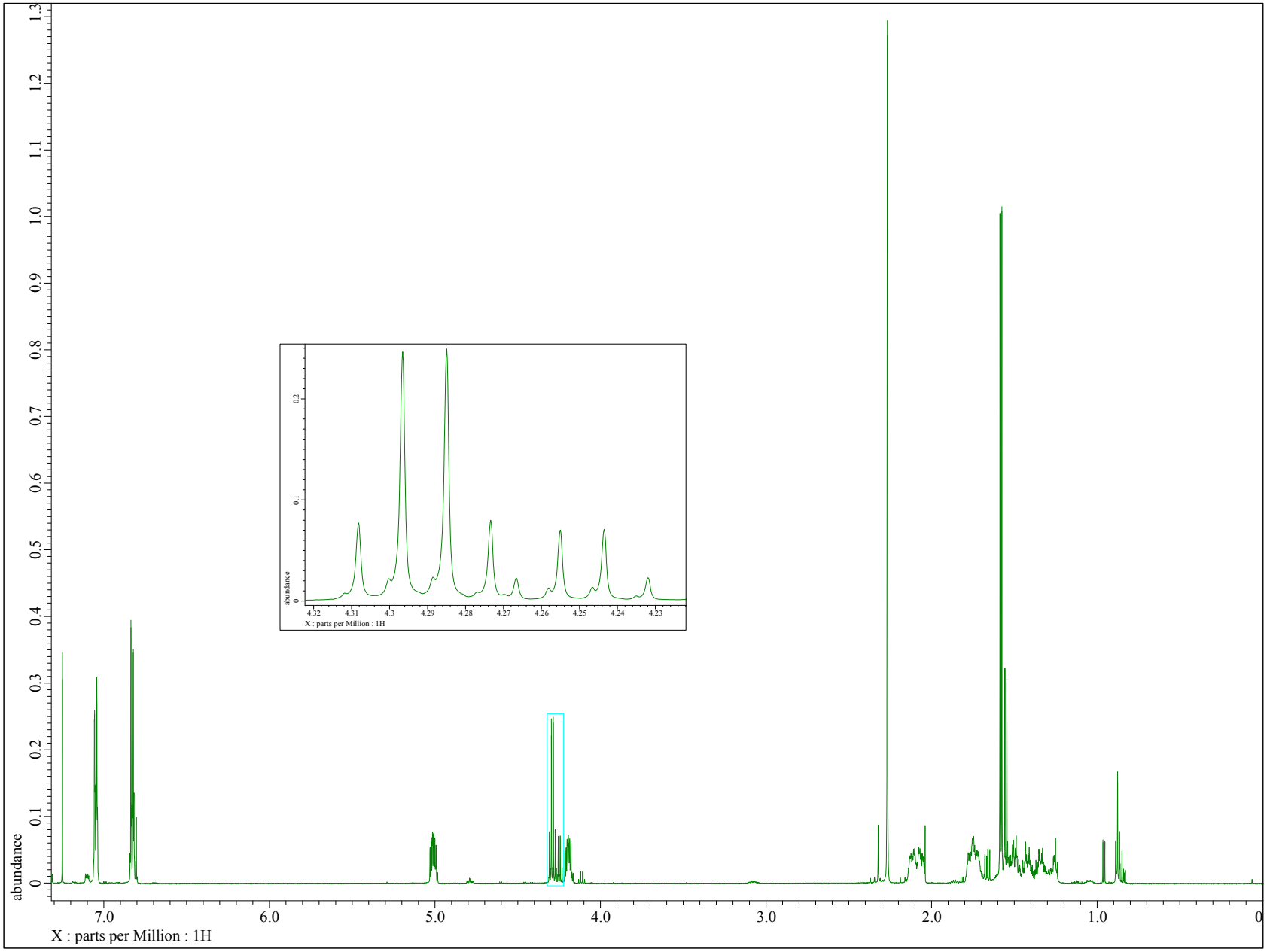
^{1}H NMR of **Compound 11** [(±)-*trans*-2-(*p*-tolylsulfonyl)cyclohexanol]



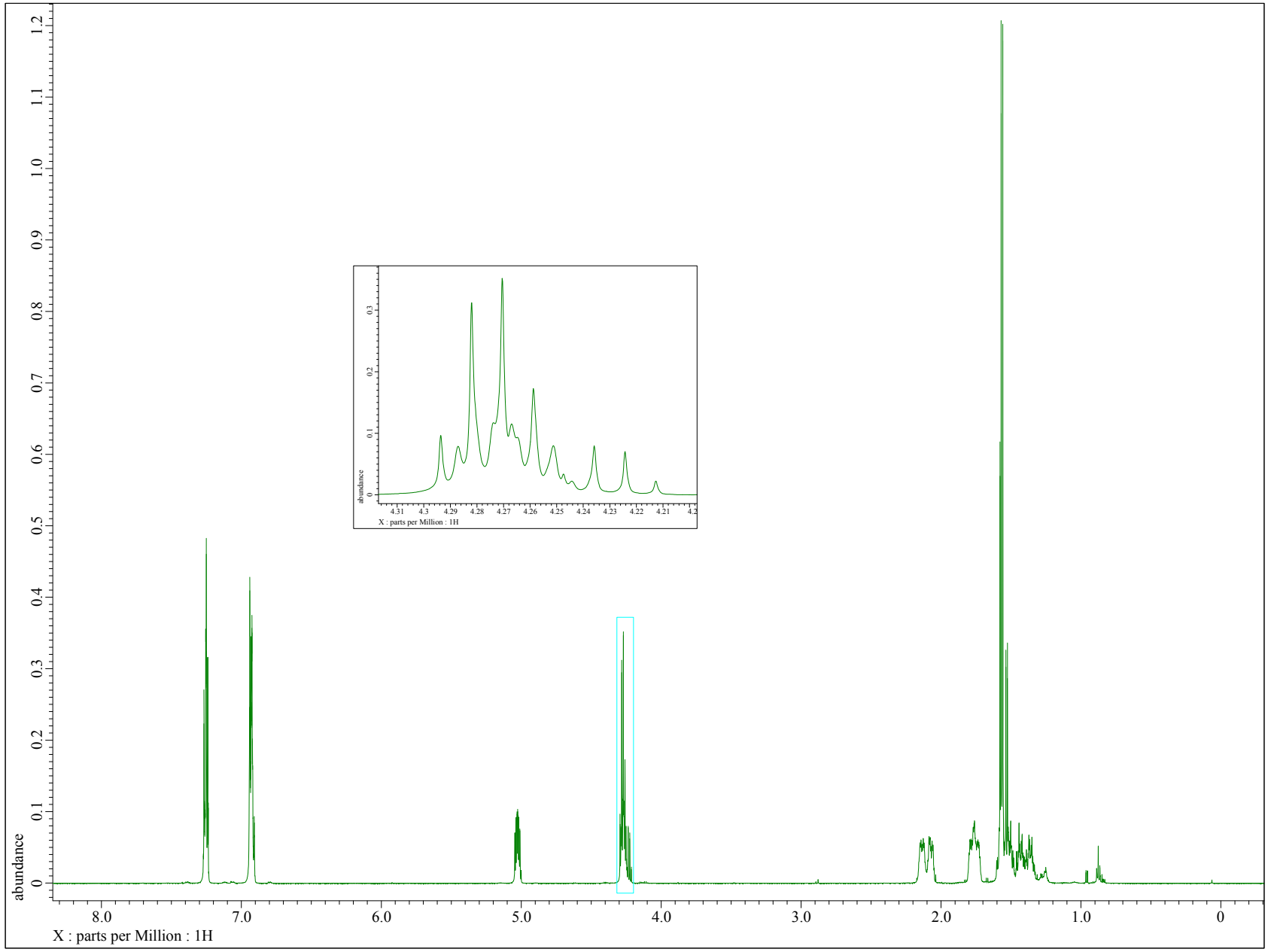
^{1}H NMR of **Compound 12** [(±)-*trans*-2-(benzyl)cyclohexanol]



^{1}H NMR of **Compound 16a+b** [(±)-(trans-2-(p-tolylsulfanyl)cyclohexyl) 2-chloropropanoate]



^{1}H NMR of **Compound 17a+b**[(±)-(*trans*-2-(*p*-tolyloxy)cyclohexyl) 2-chloropropanoate]



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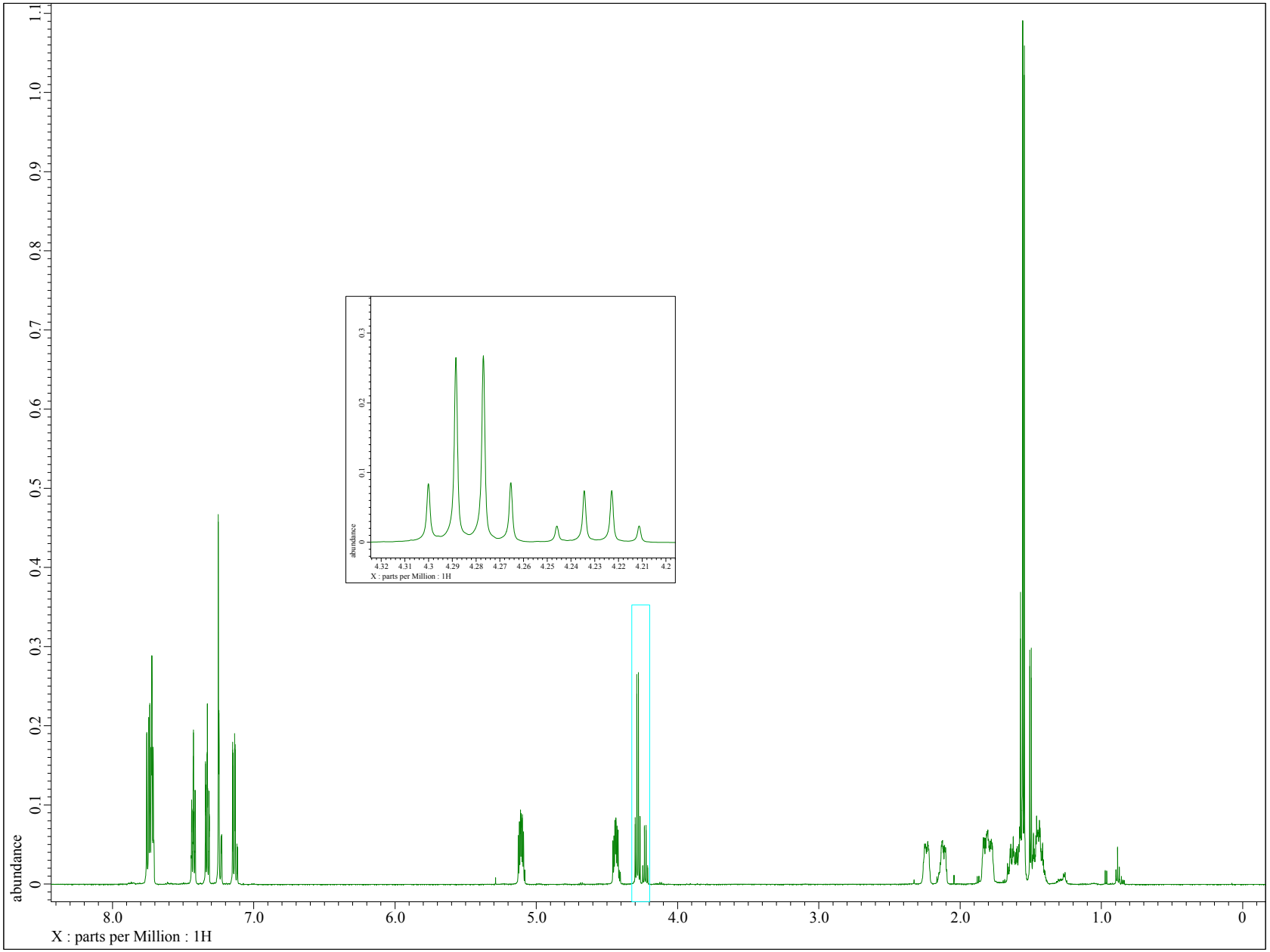
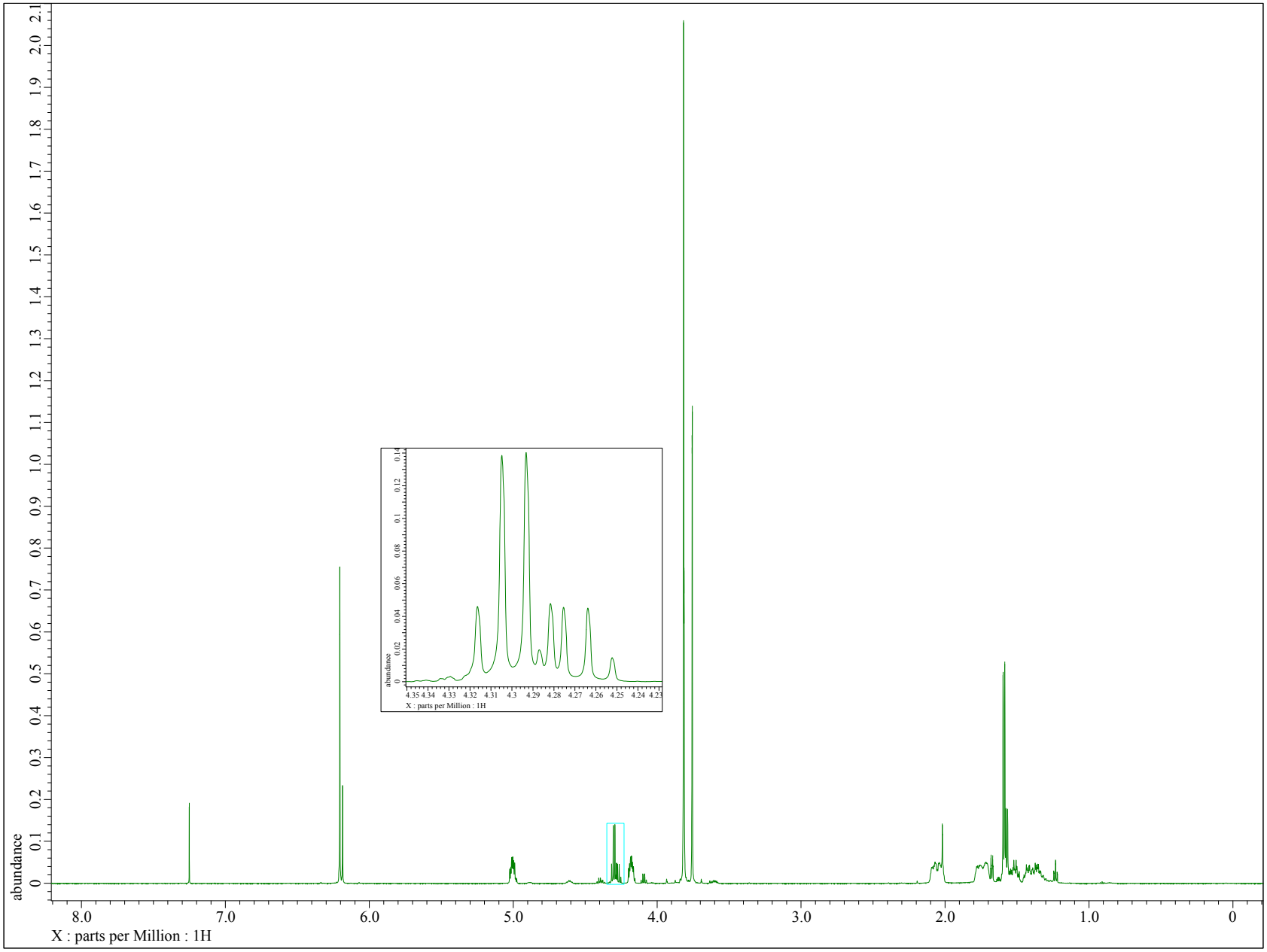


^{1}H NMR of **Compound 19a+b** [(±)-(*trans*-2-(napthalen-2-yloxy)cyclohexyl) 2-chloropropanoate]



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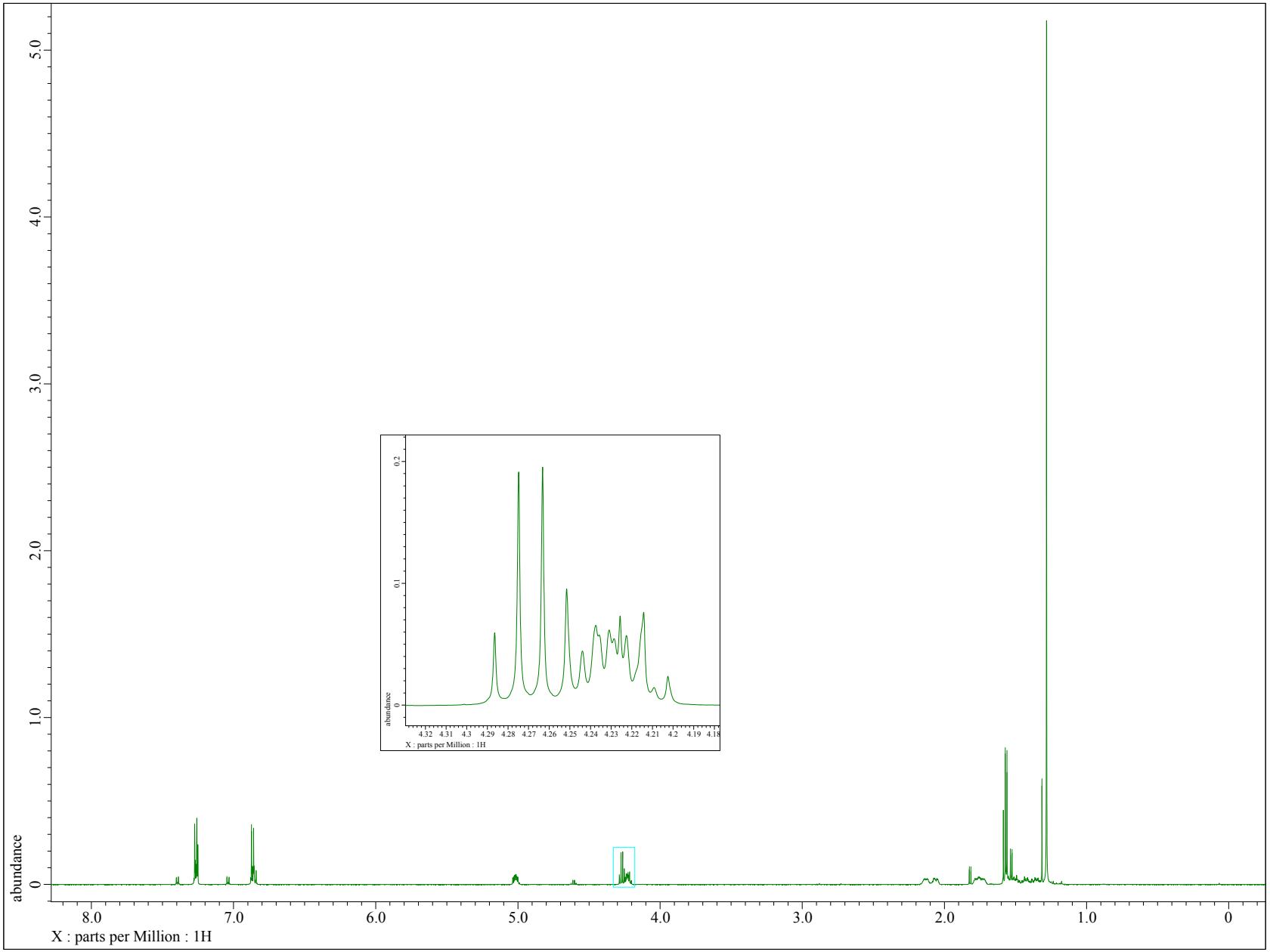

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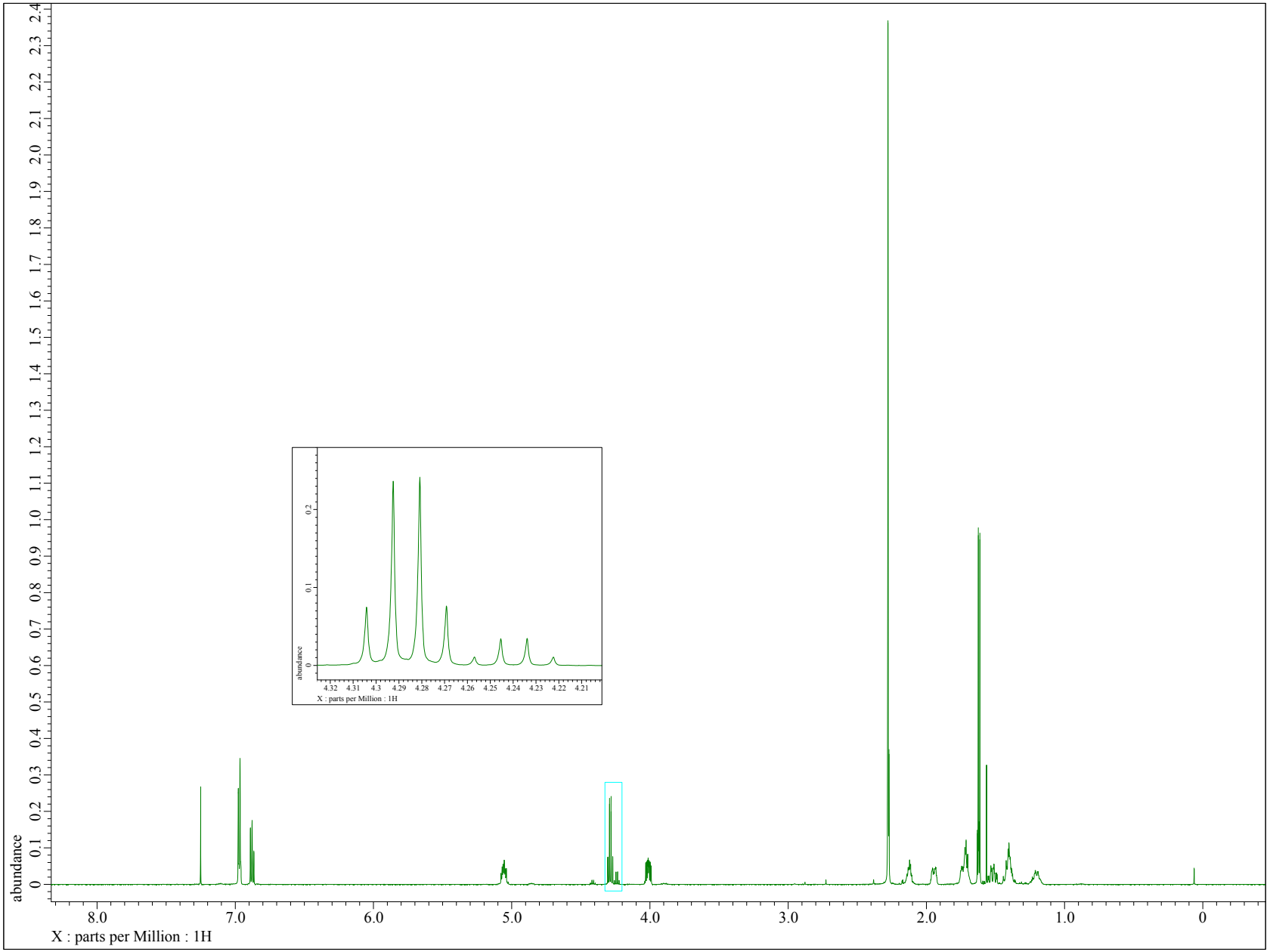
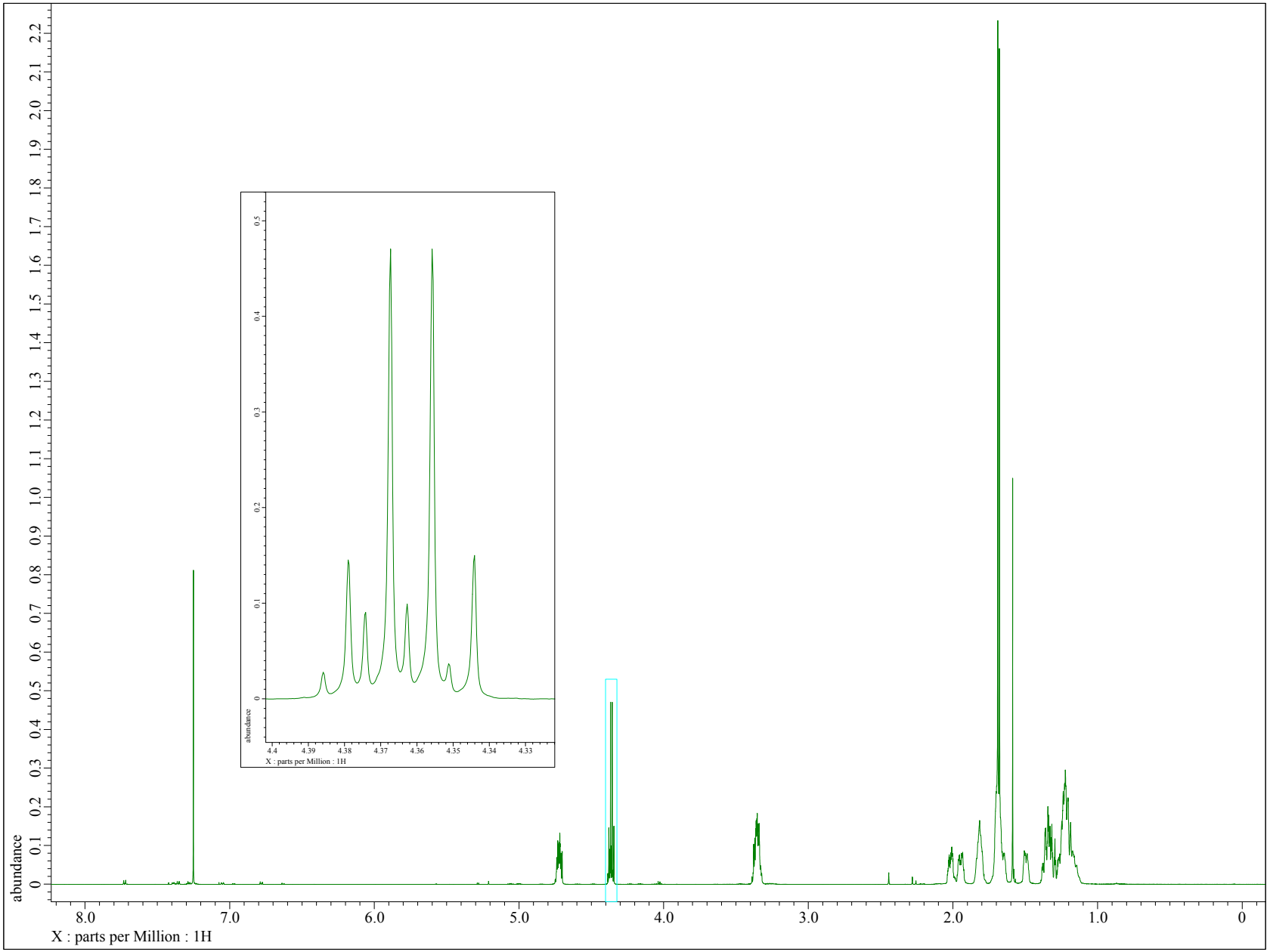
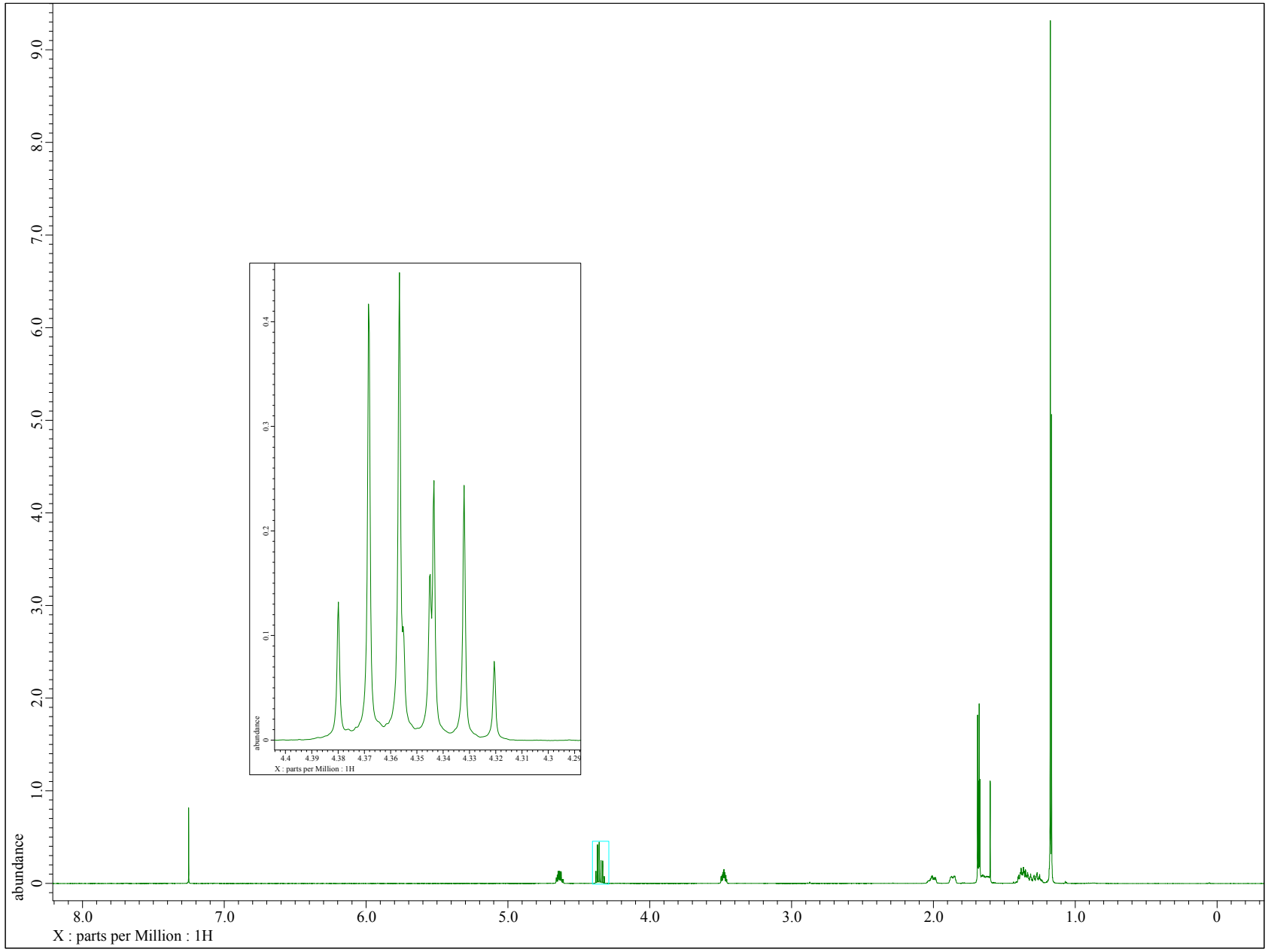


^{1}H NMR of **Compound 22a+b** [(±)-(*trans*-2-(2,6-dimethylphenyloxy)cyclohexyl 2-chloropropanoate]



^{1}H NMR of **Compound 23a+b** [(±)-(*trans*-2-(cyclohexyloxy)cyclohexyl 2-chloropropanoate]



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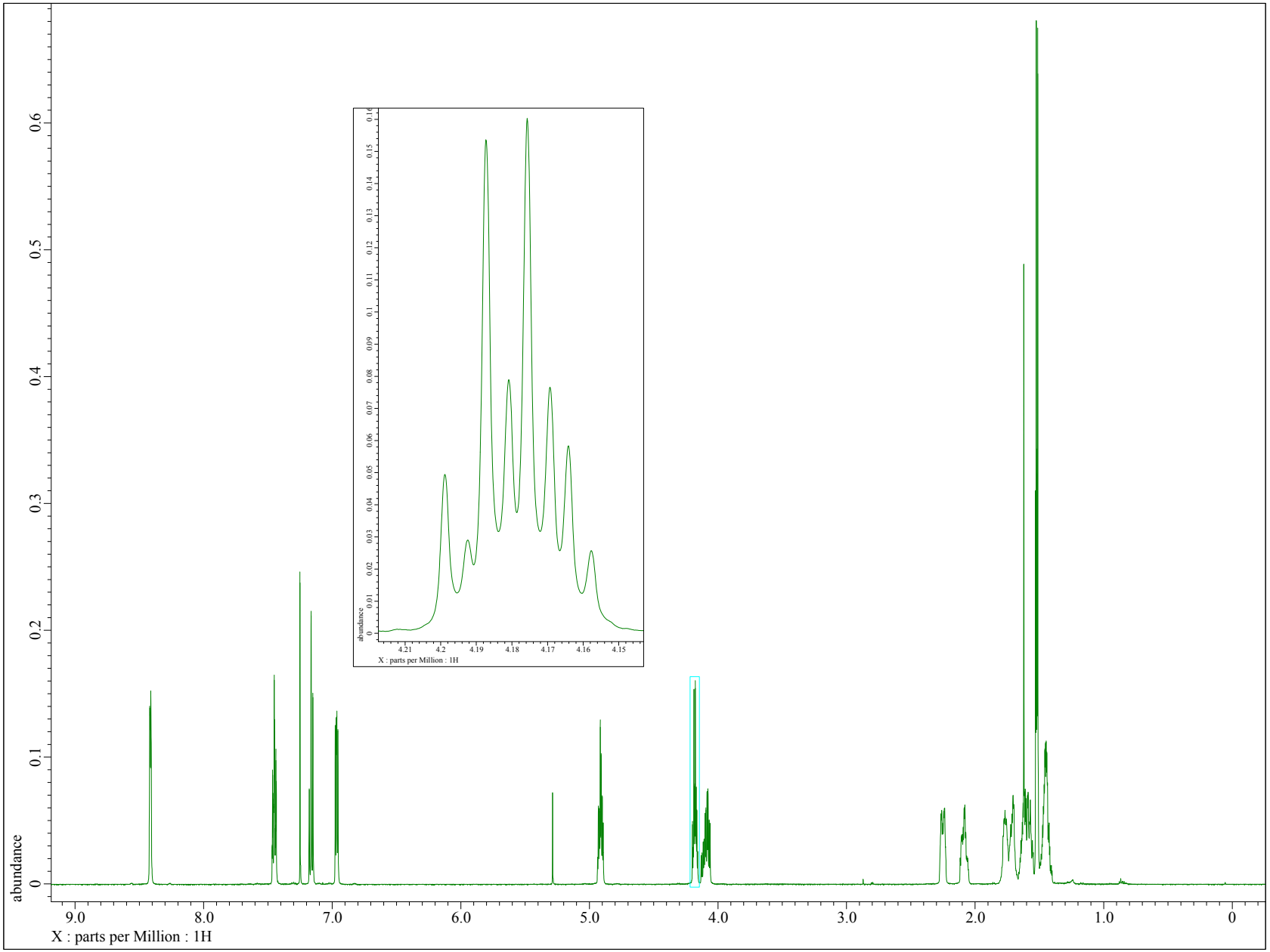

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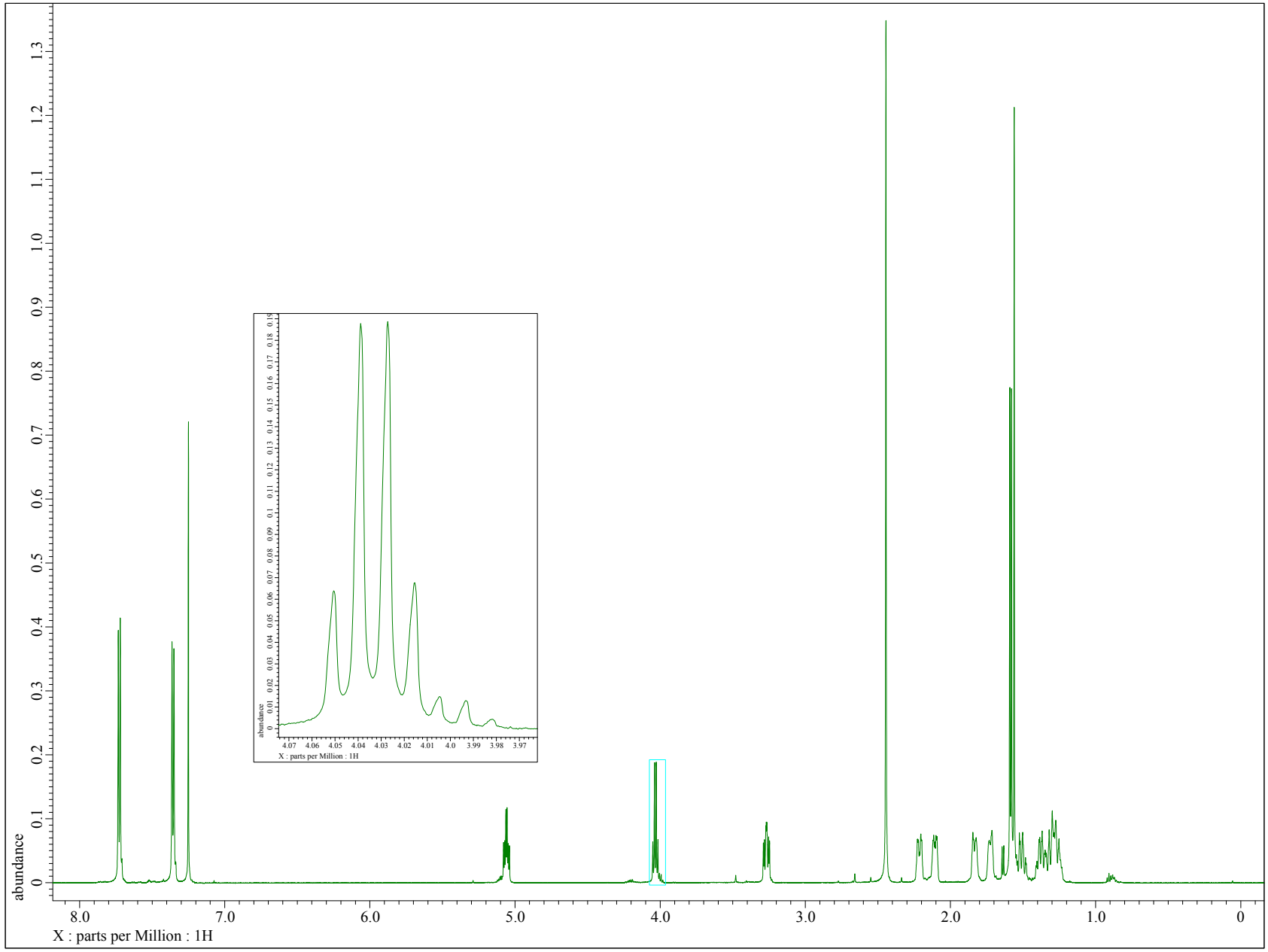
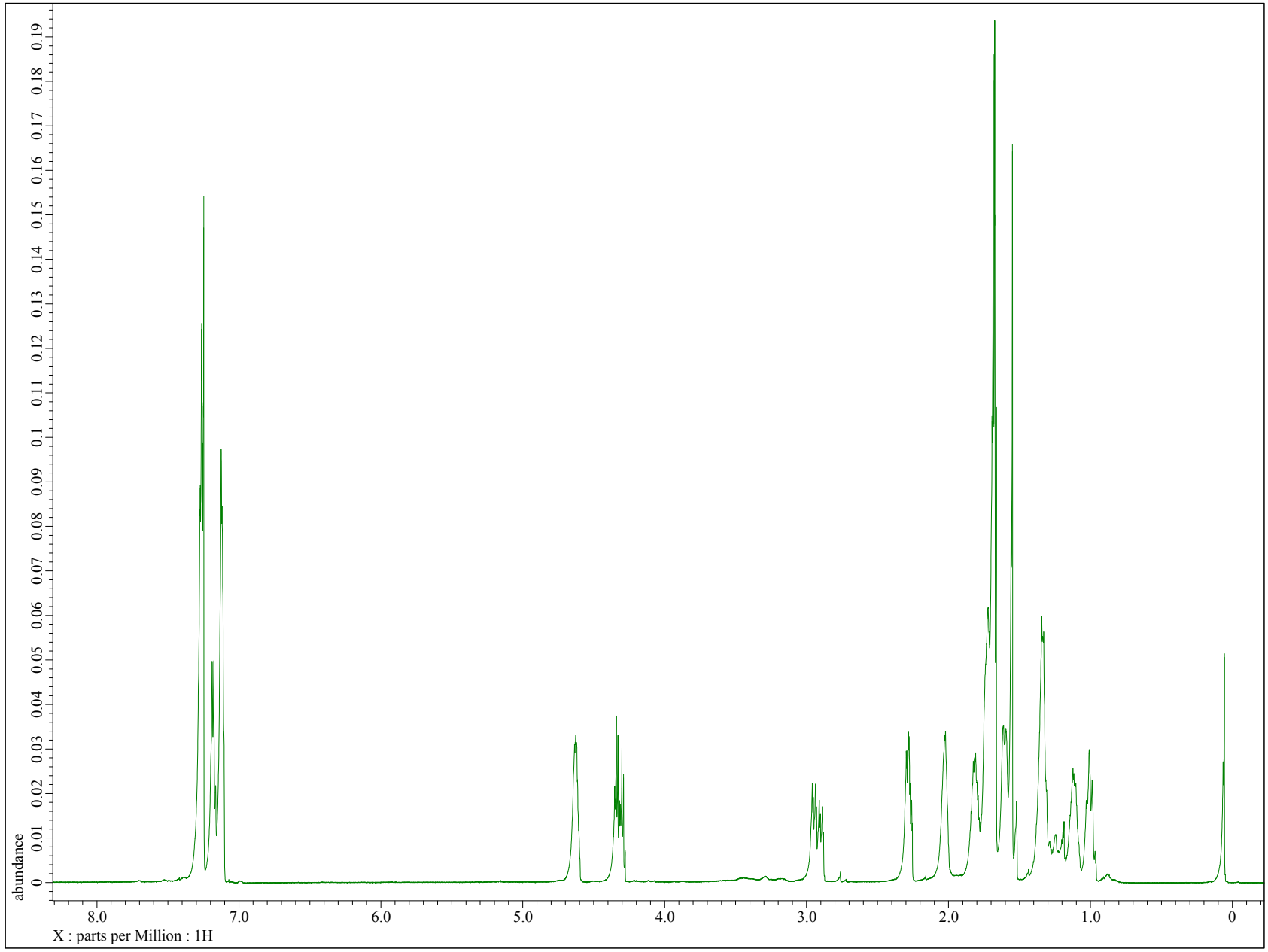
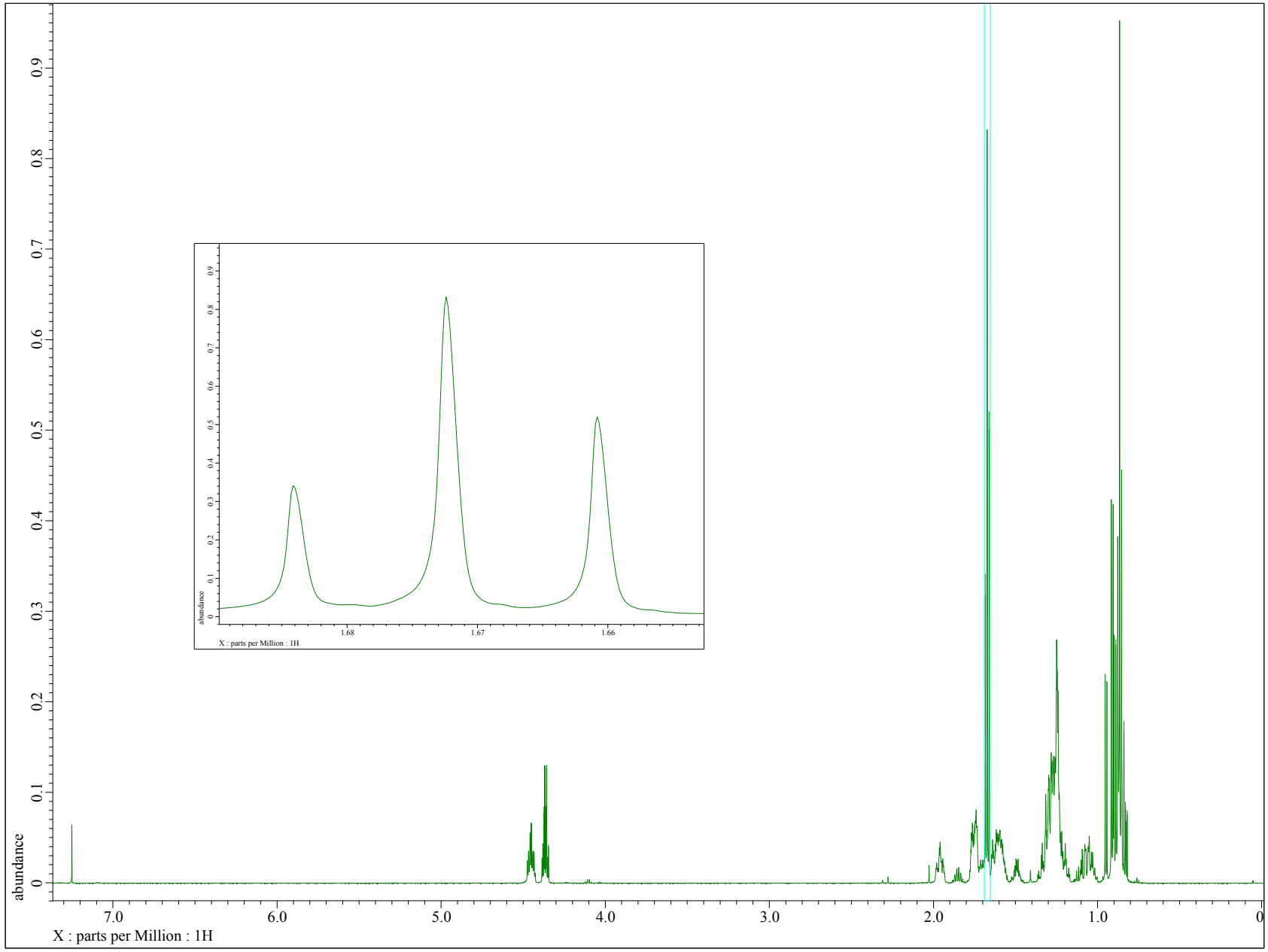


^{1}H NMR of **Compound 26a+b** [(±)-(*trans*-2-(*p*-tolylsulfonyl)cyclohexyl 2-chloropropanoate]



^{1}H NMR of **Compound 27a+b** [(±)-(*trans*-2-benzylcyclohexyl) 2-chloropropanoate]



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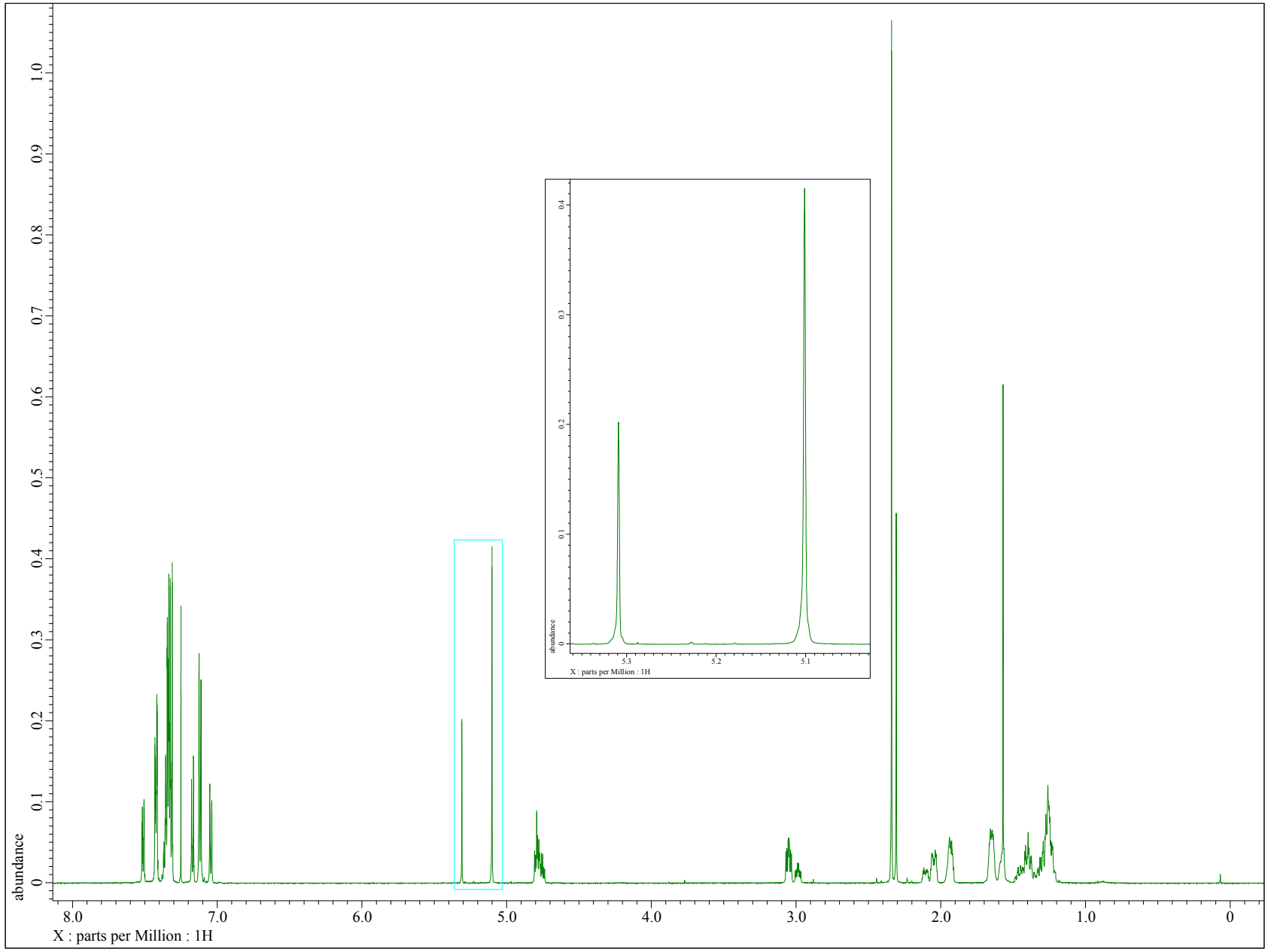
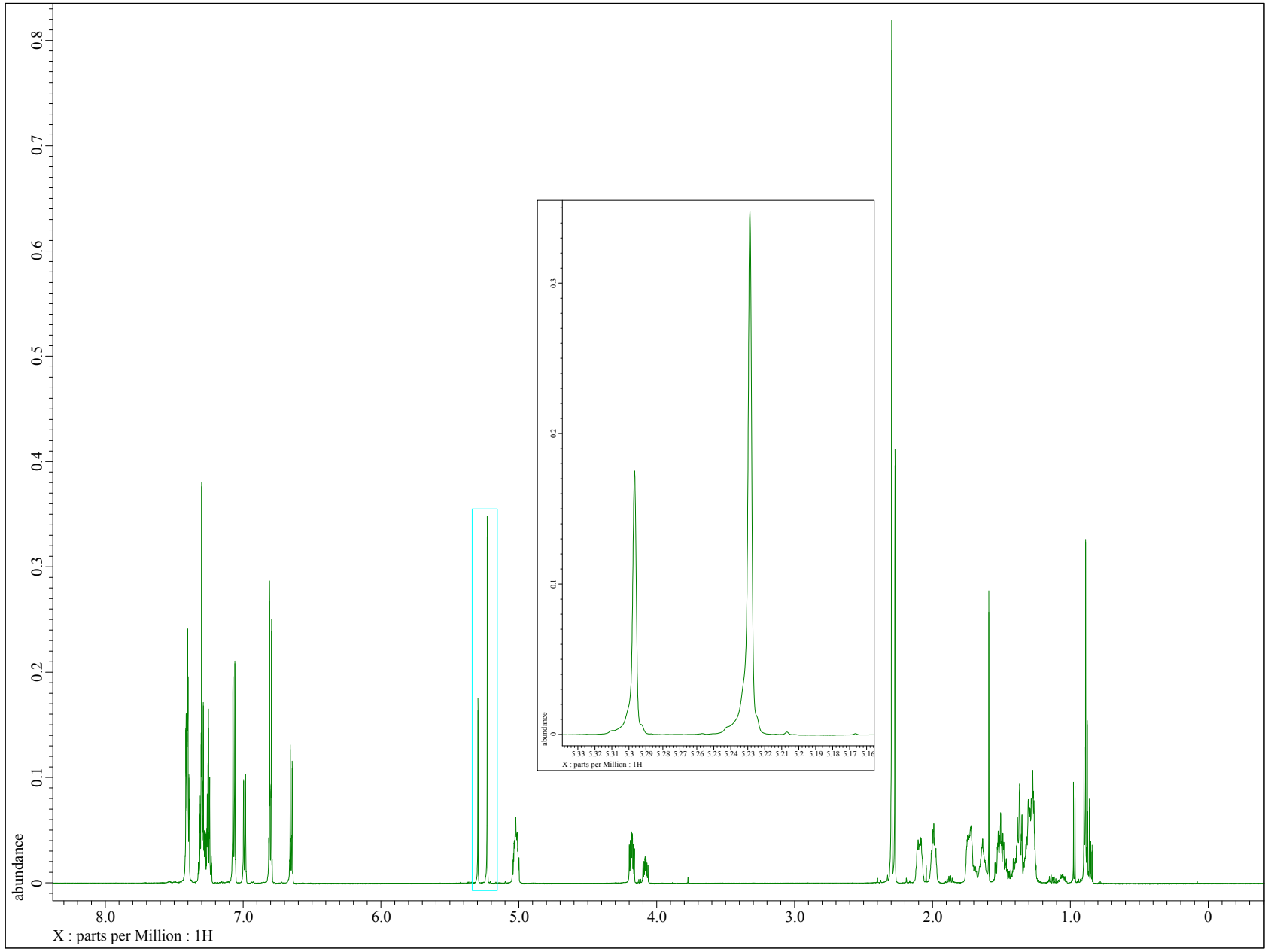
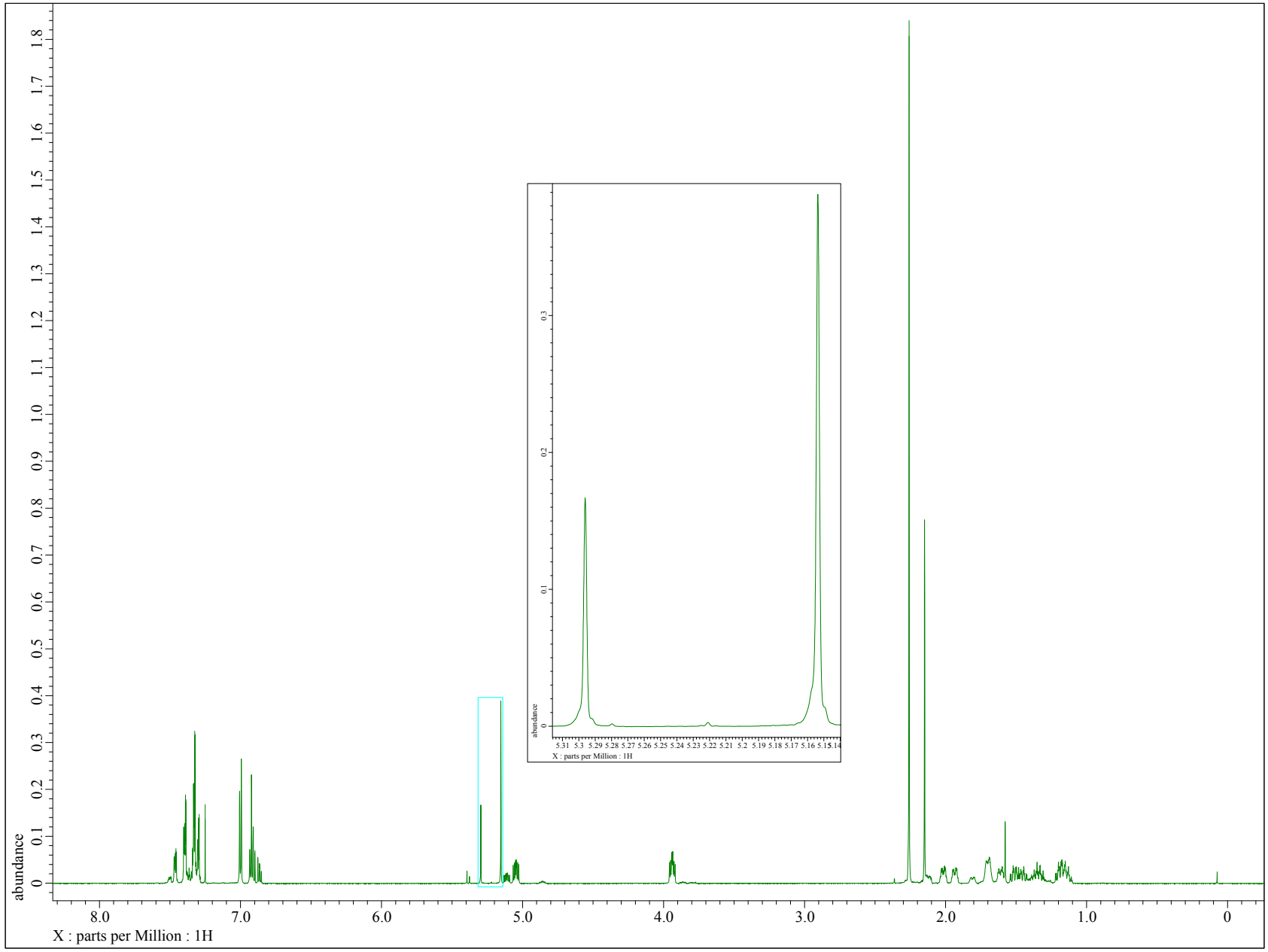


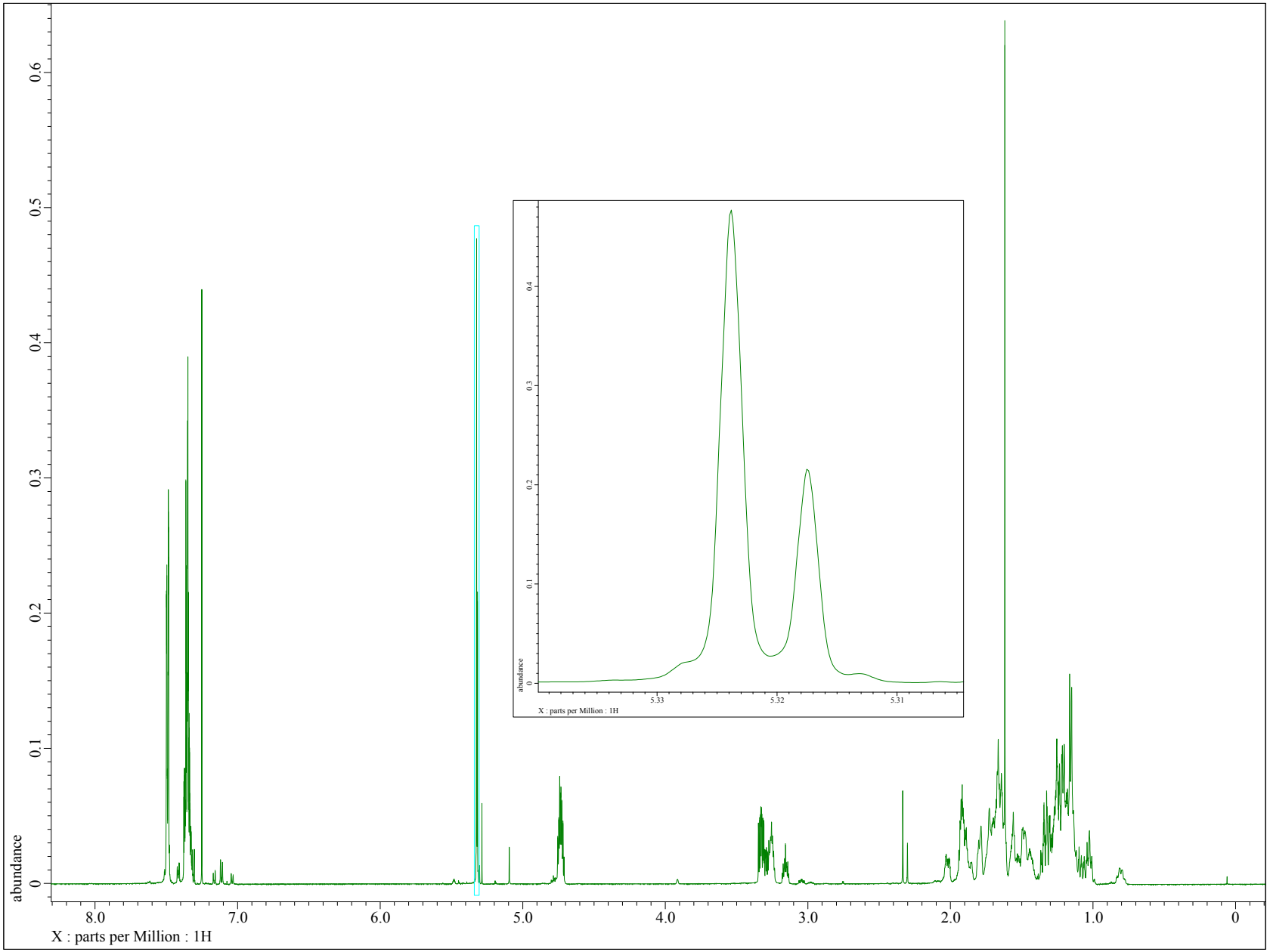
^{1}H NMR of **Compound 29a+b** [(±)-(*trans*-2-(*p*-tolylsulfanyl)cyclohexyl 2-chloro-2-phenylethanoate]



^{1}H NMR of **Compound 30a+b** [(±)-(*trans*-2-(*p*-tolyloxy)cyclohexyl 2-chloro-2-phenylethanoate]



^{1}H NMR of **Compound 31a+b** [(±)-(*trans*-2-(2,6-dimethylphenyloxy)cyclohexyl 2-chloro-2-phenylethanoate]



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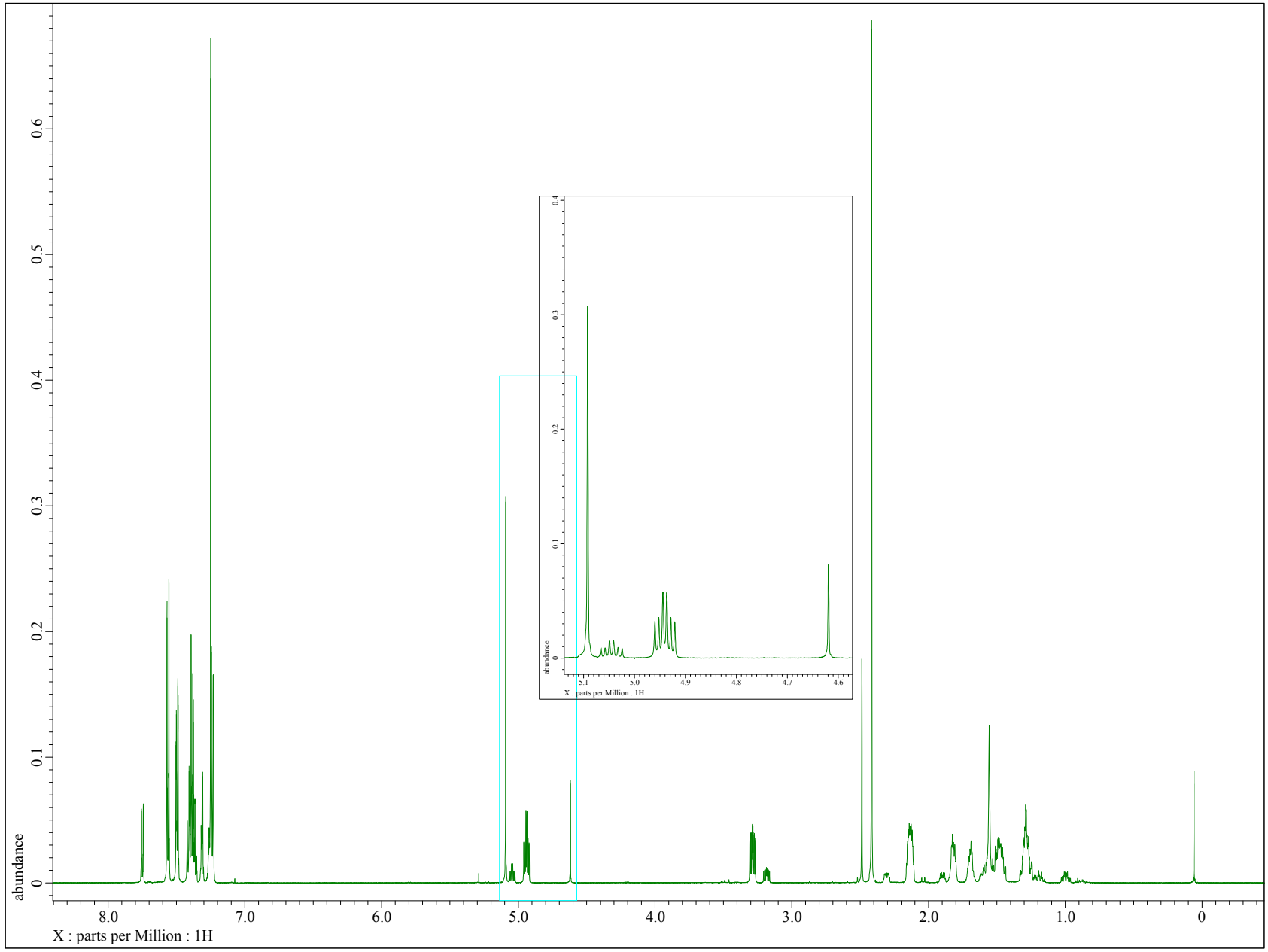
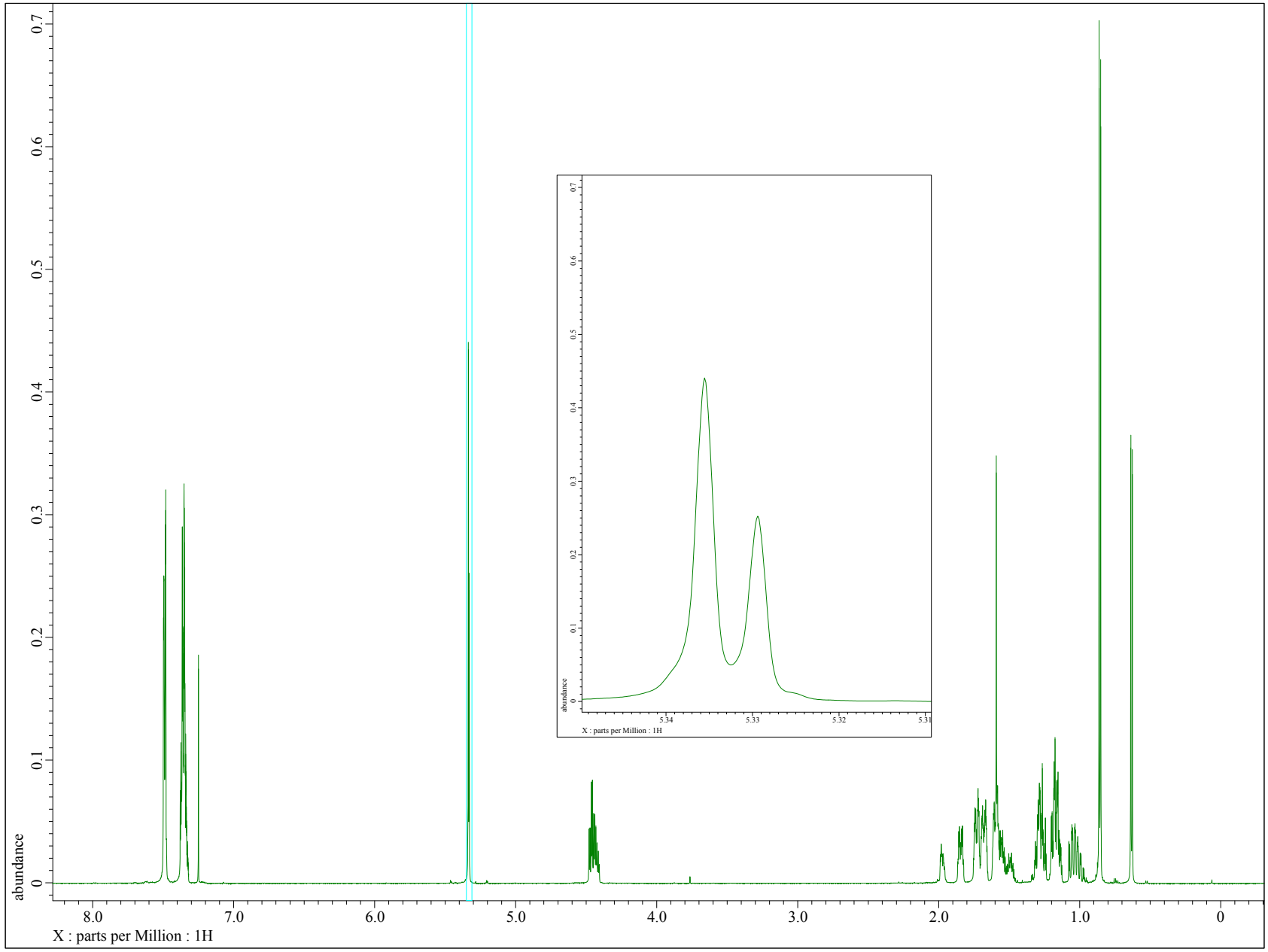
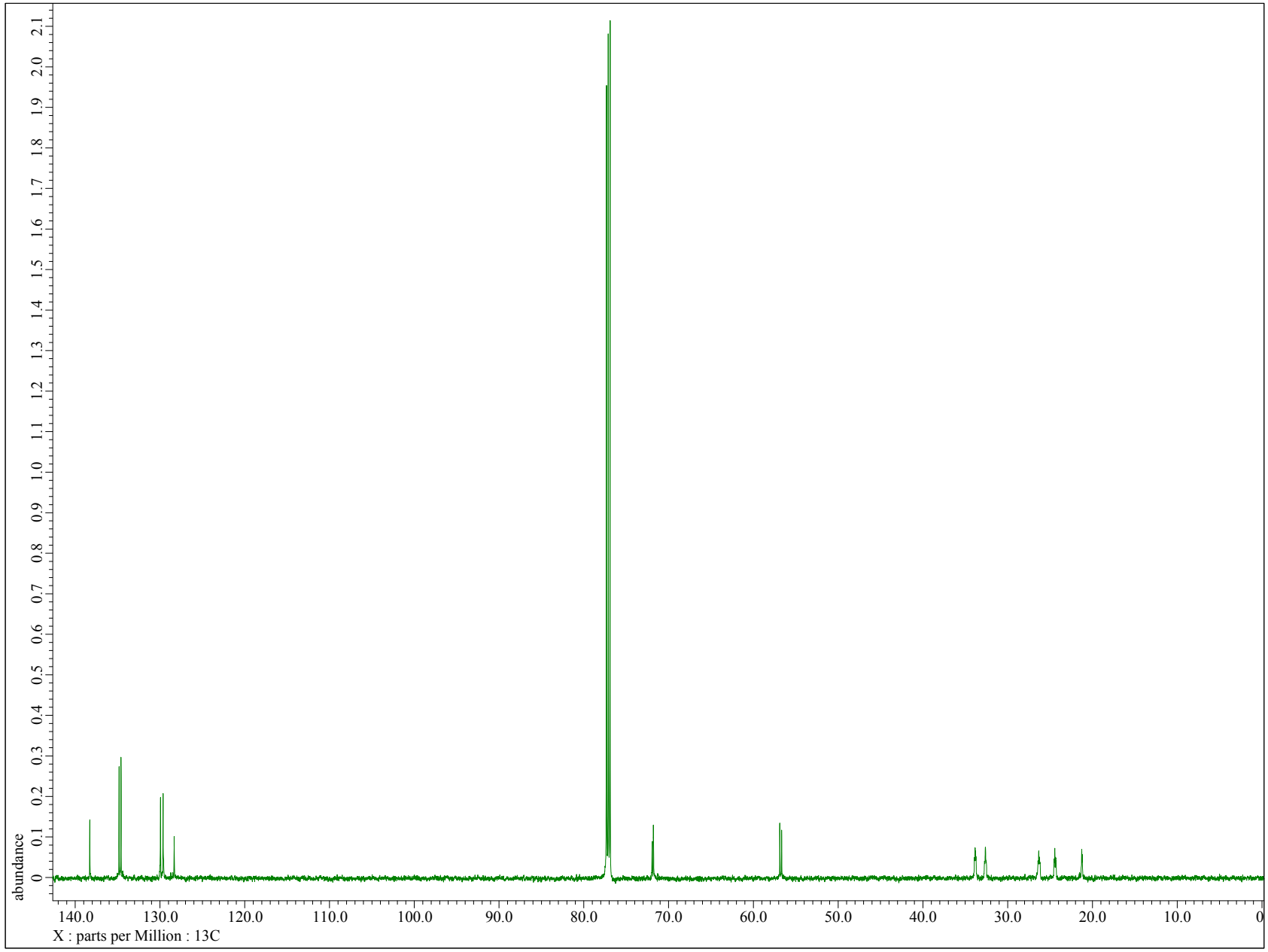


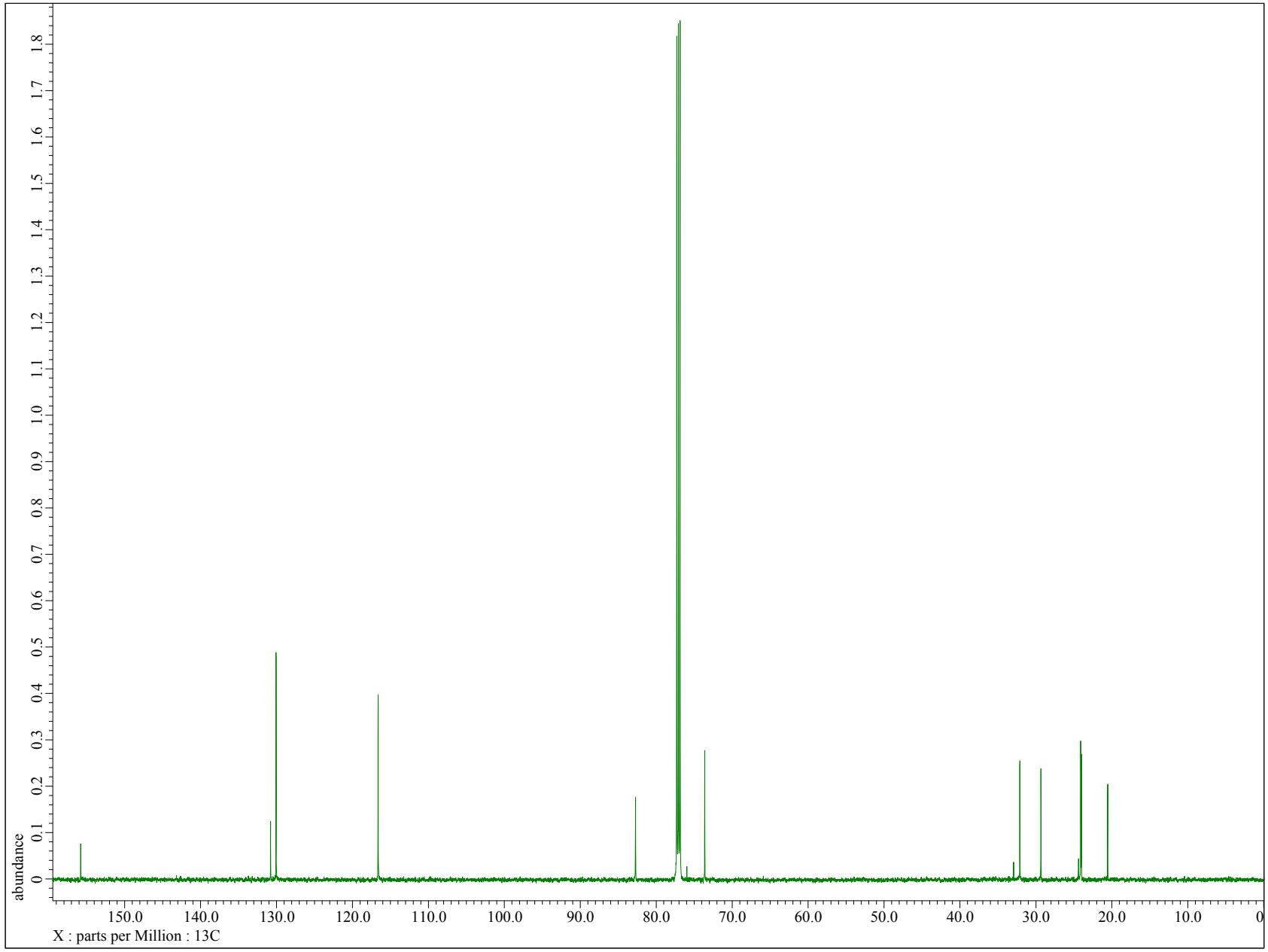
^{1}H NMR of **Compound 33a+b** [(±)-(*trans*-2-(*p*-tolylsulfonyl)cyclohexyl 2-chloro-2-phenylethanoate]



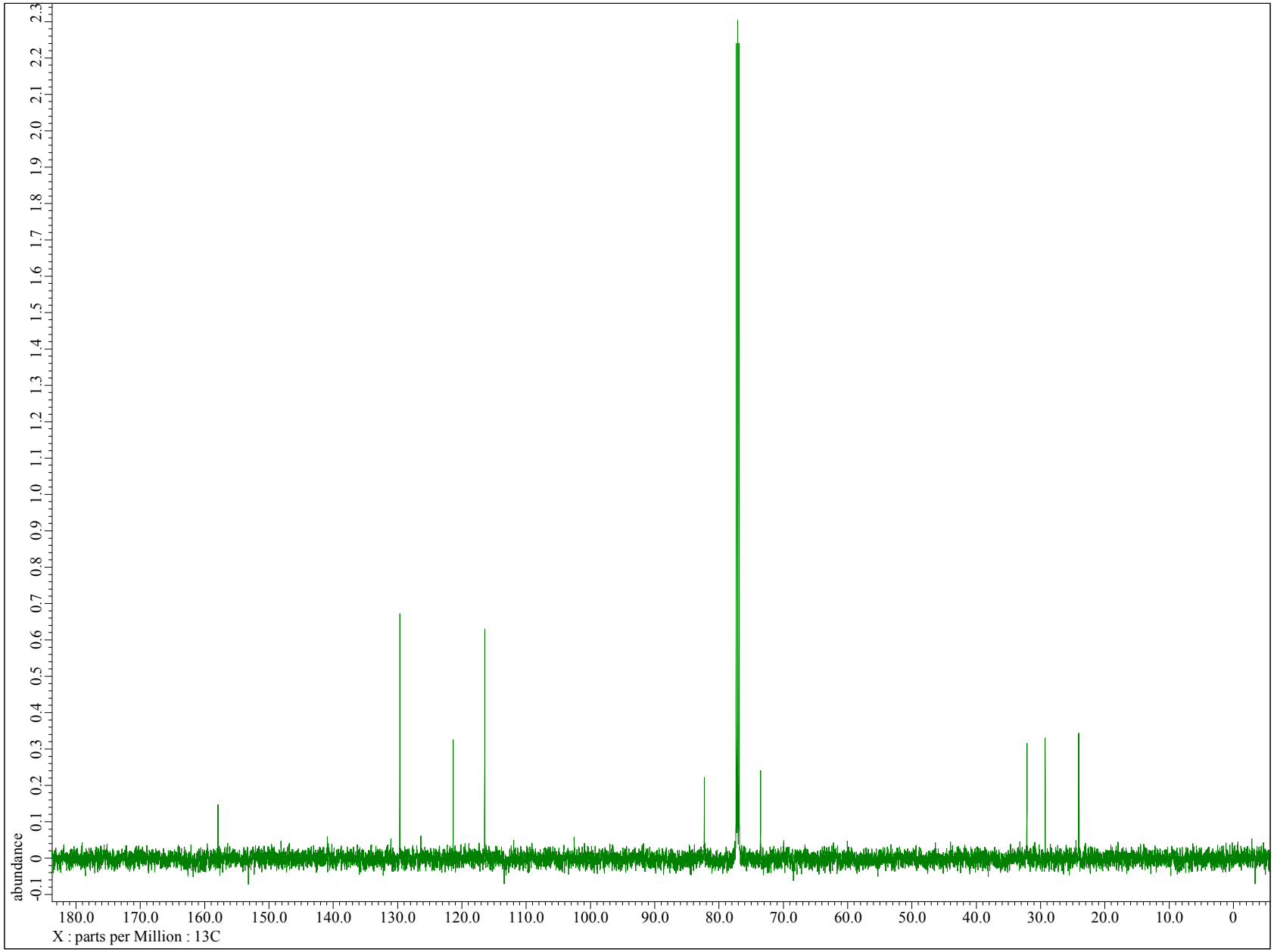
^{1}H NMR of **Compound 34a+b** [(±)-*trans*-2-(methyl)cyclohexyl 2-chloro-2-phenylethanoate]



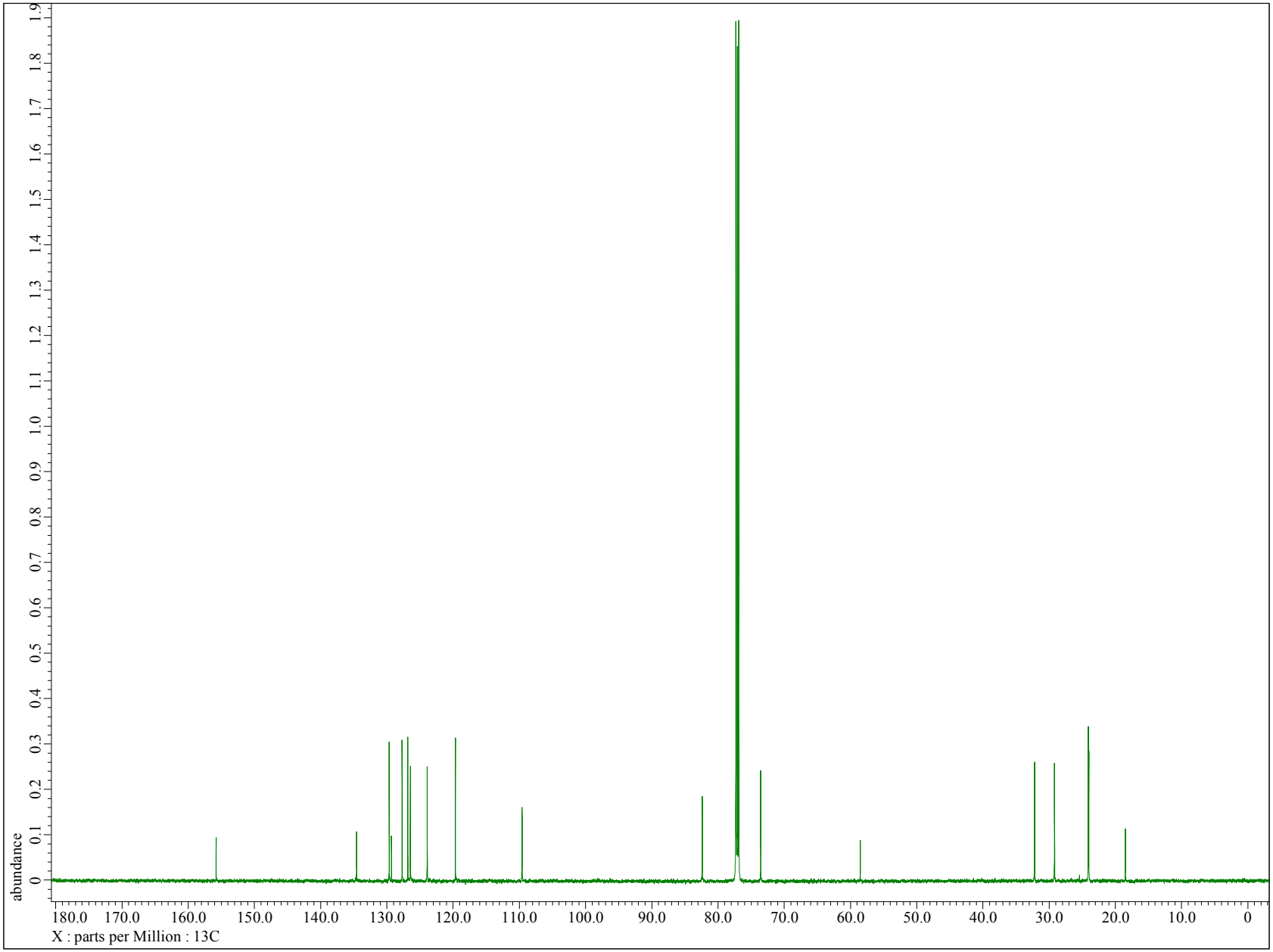
^{13}C NMR of **Compound 1** [(±)-*trans*-2-(*p*-tolylsulfanyl)cyclohexanol]



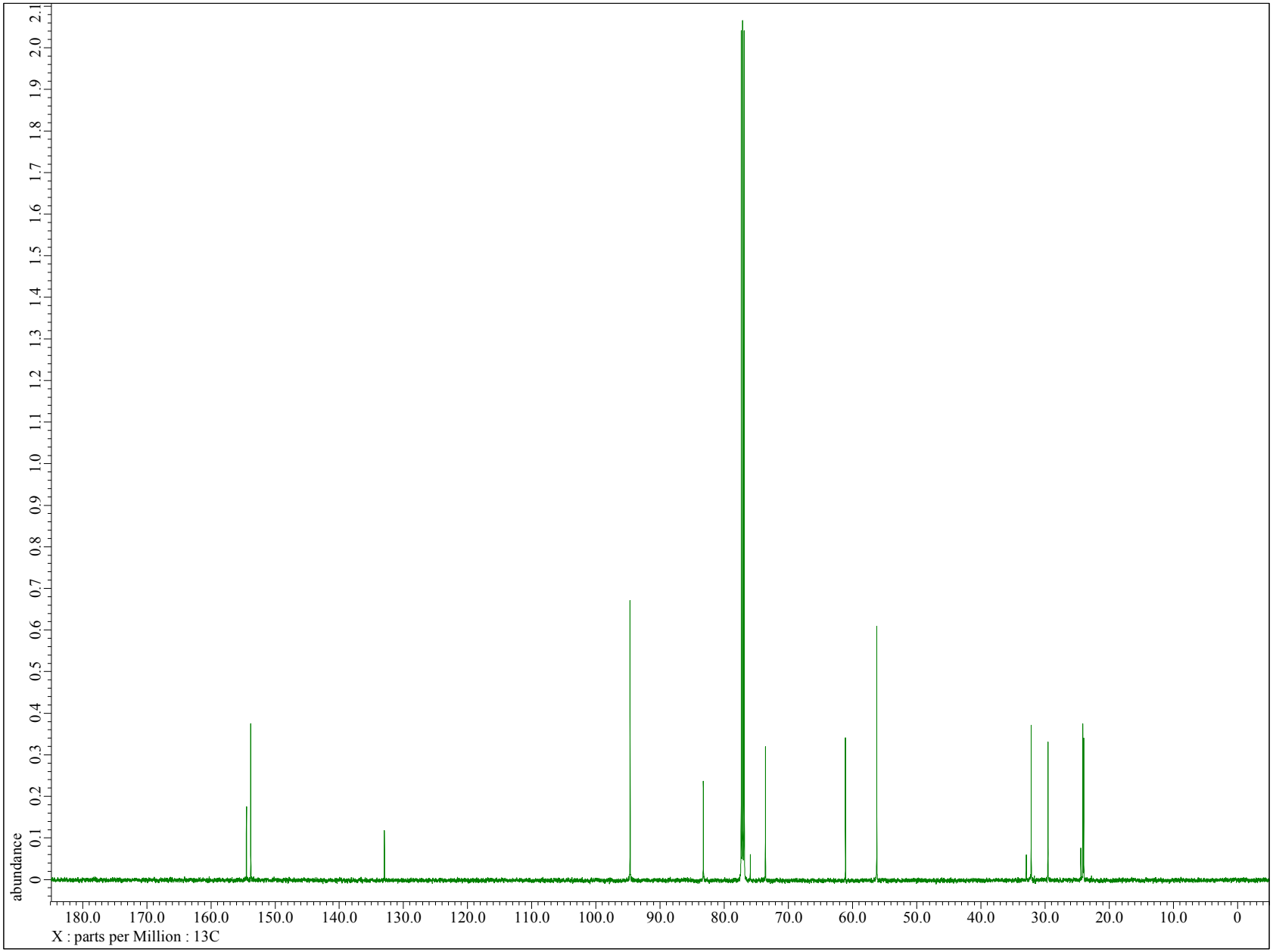
^{13}C NMR of **Compound 2** [(±)-*trans*-2-(*p*-tolyloxy)cyclohexanol]



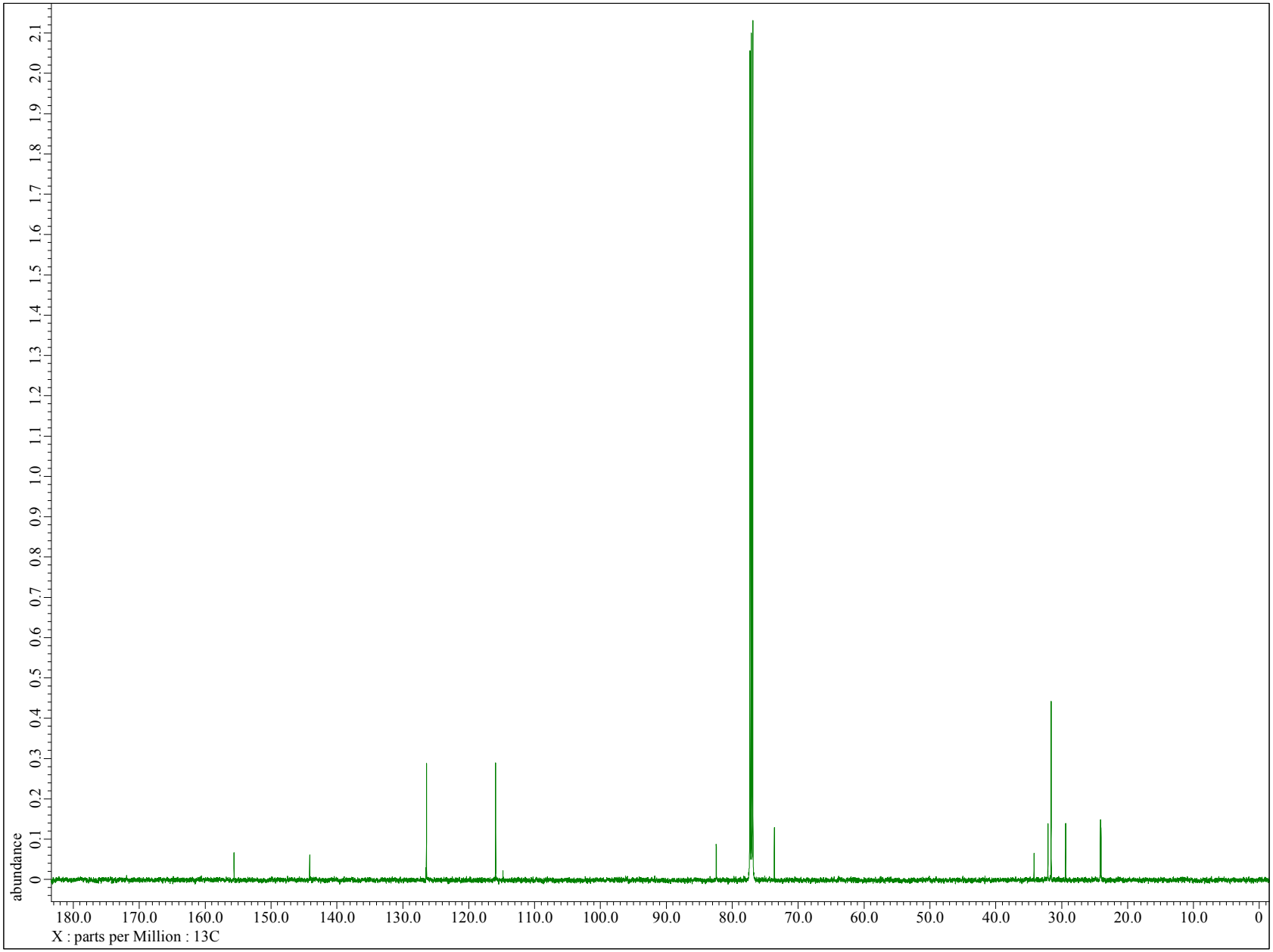
^{13}C NMR of **Compound 3** [(±)-*trans*-2-(phenyloxy)cyclohexanol]



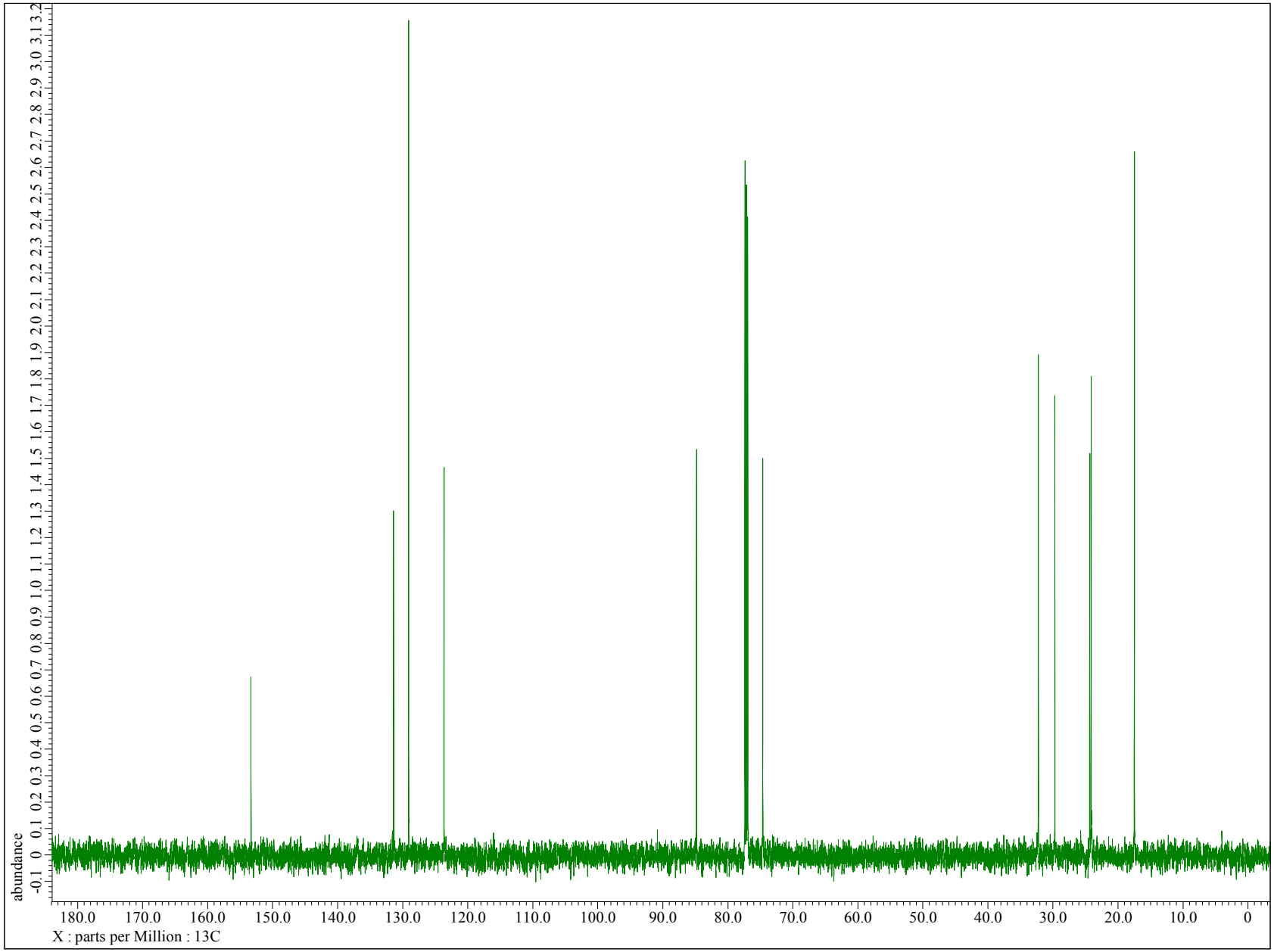
^{13}C NMR of **Compound 4** [(±)-*trans*-2-(napthalen-2-yloxy)cyclohexanol]



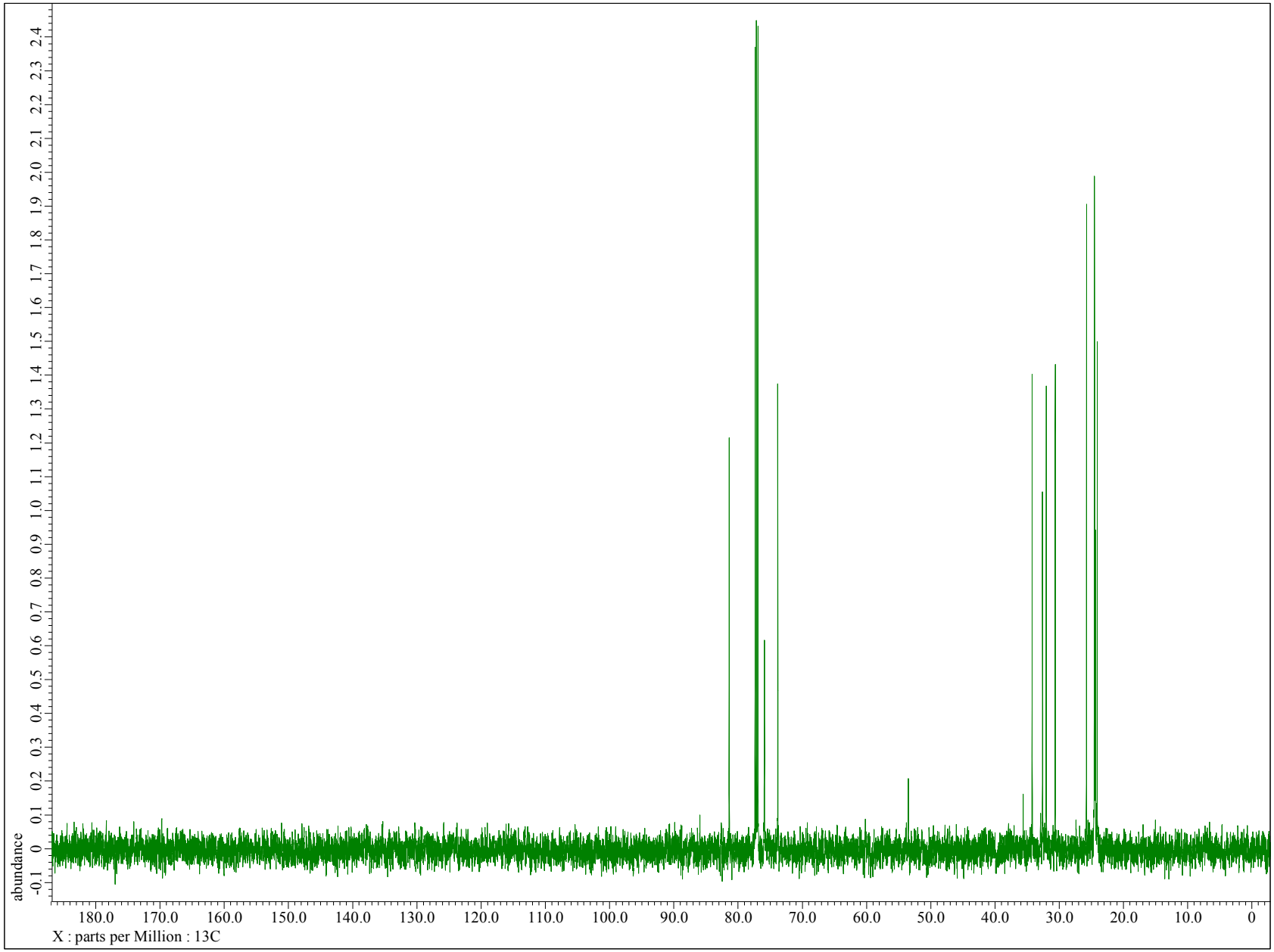
^{13}C NMR of **Compound 5** [(±)-*trans*-2-(3,4,5-trimethylphenyloxy)cyclohexanol]



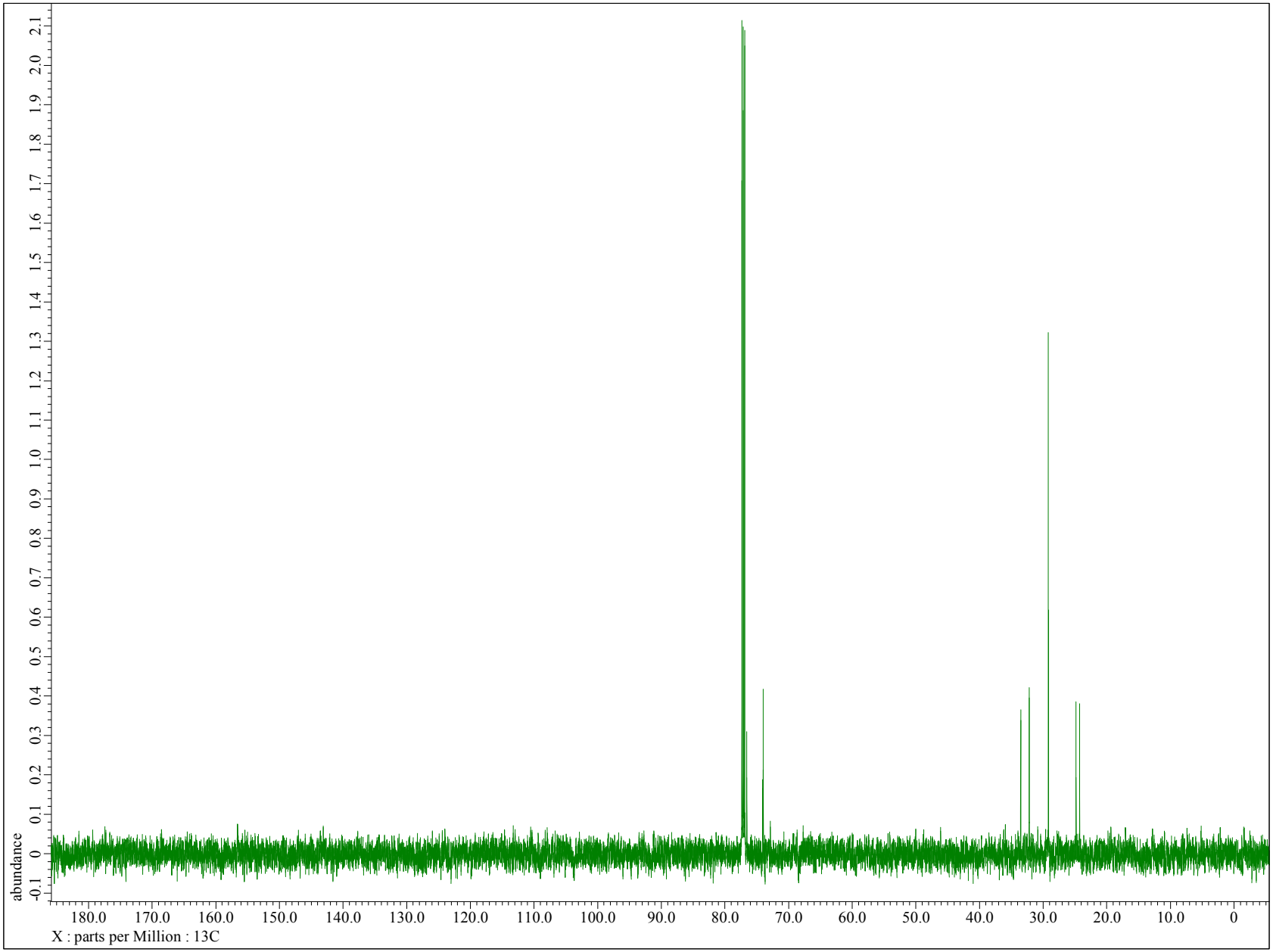
^{13}C NMR of **Compound 6** [(±)-*trans*-2-(*p*-(*tert*-butoxy)phenyloxy)cyclohexanol]



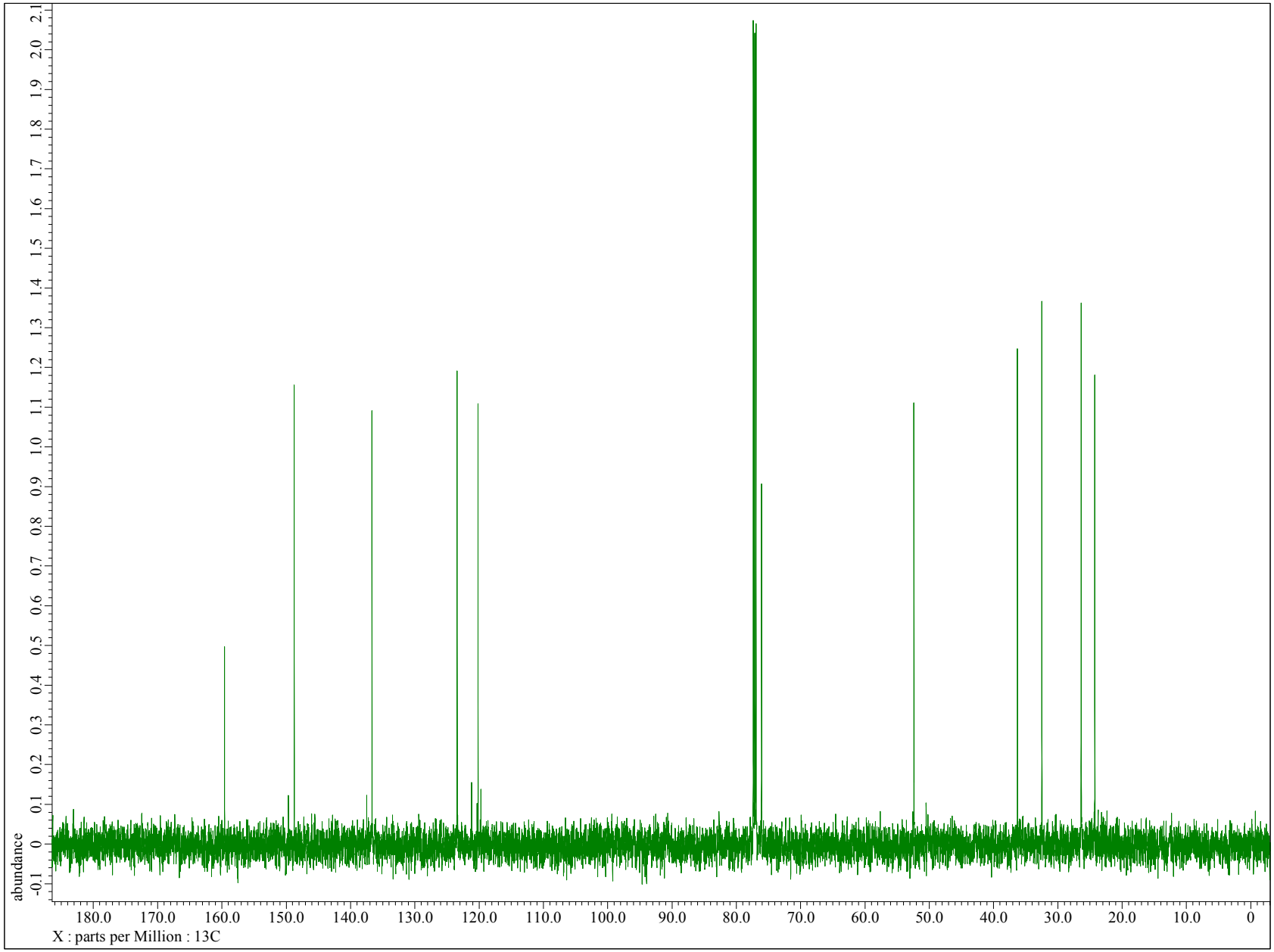
^{13}C NMR of **Compound 7** [(±)-*trans*-2-(2,6-dimethylphenyloxy)cyclohexanol]



^{13}C NMR of **Compound 8** [(±)-*trans*-2-(cyclohexyloxy)cyclohexanol]



^{13}C NMR of **Compound 9** [(±)-*trans*-2-(*t*-butoxy)cyclohexanol]



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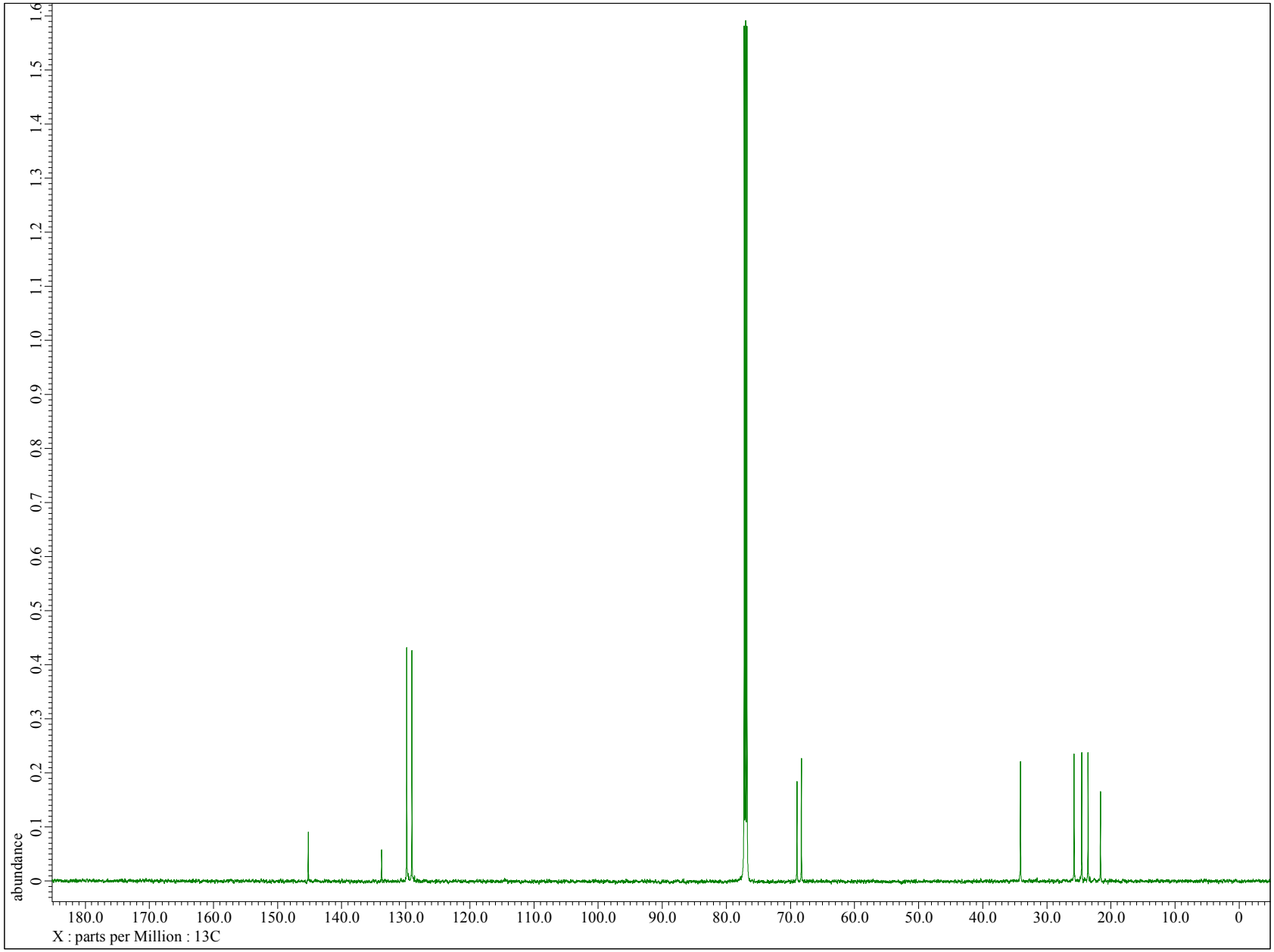
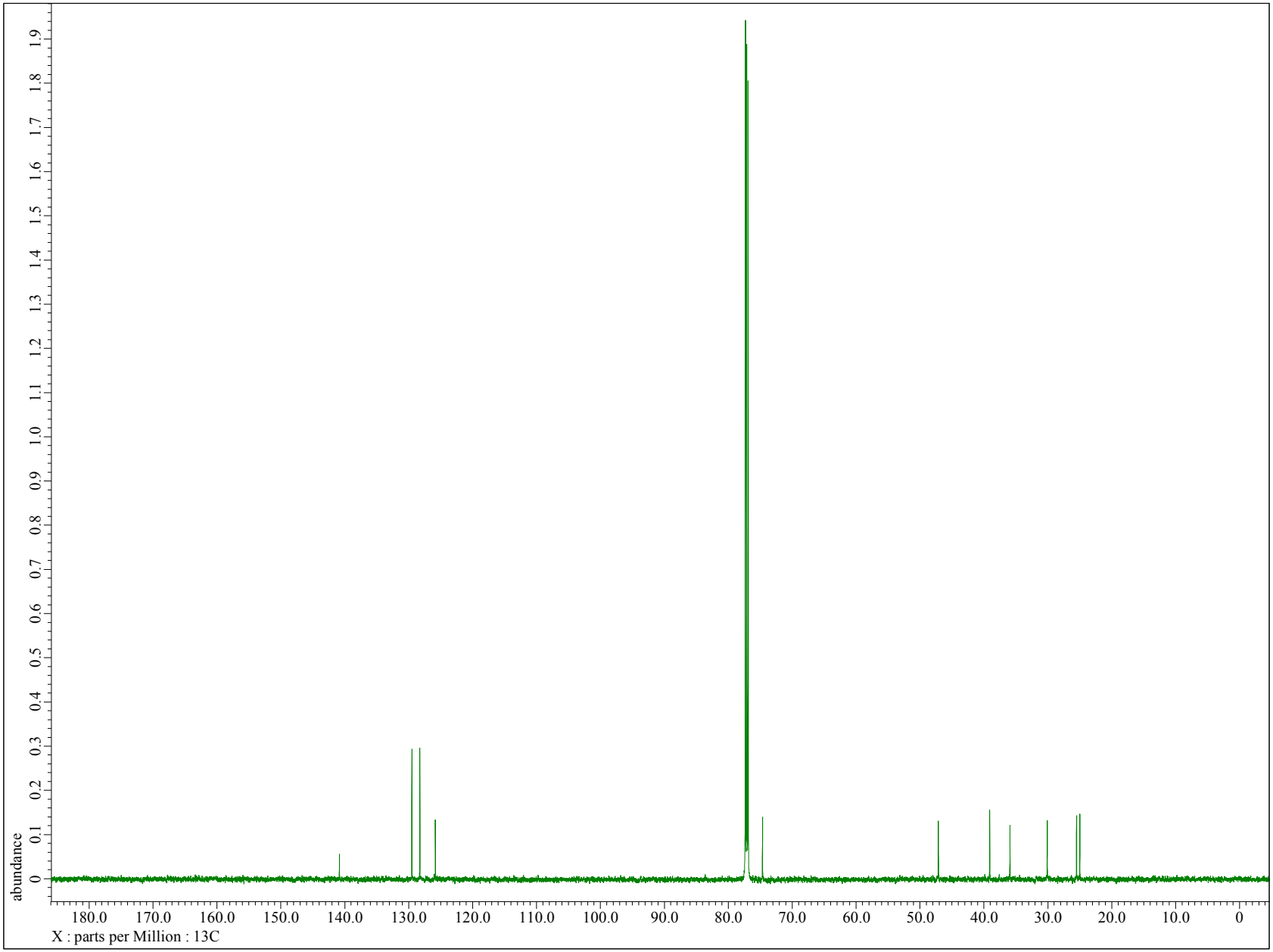


^{13}C NMR of **Compound 11** [(±)-*trans*-2-(*p*-tolylsulfonyl)cyclohexanol]



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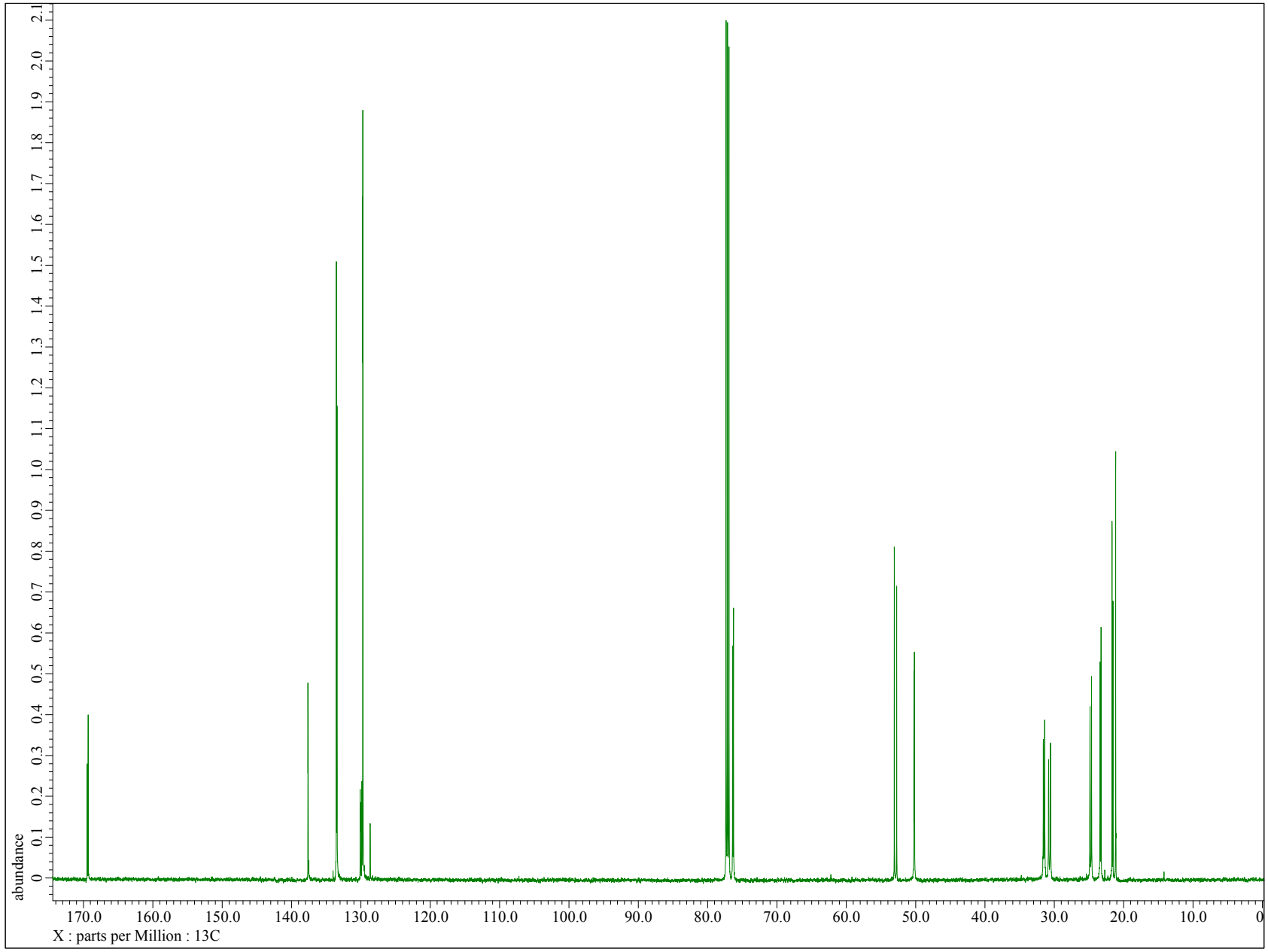
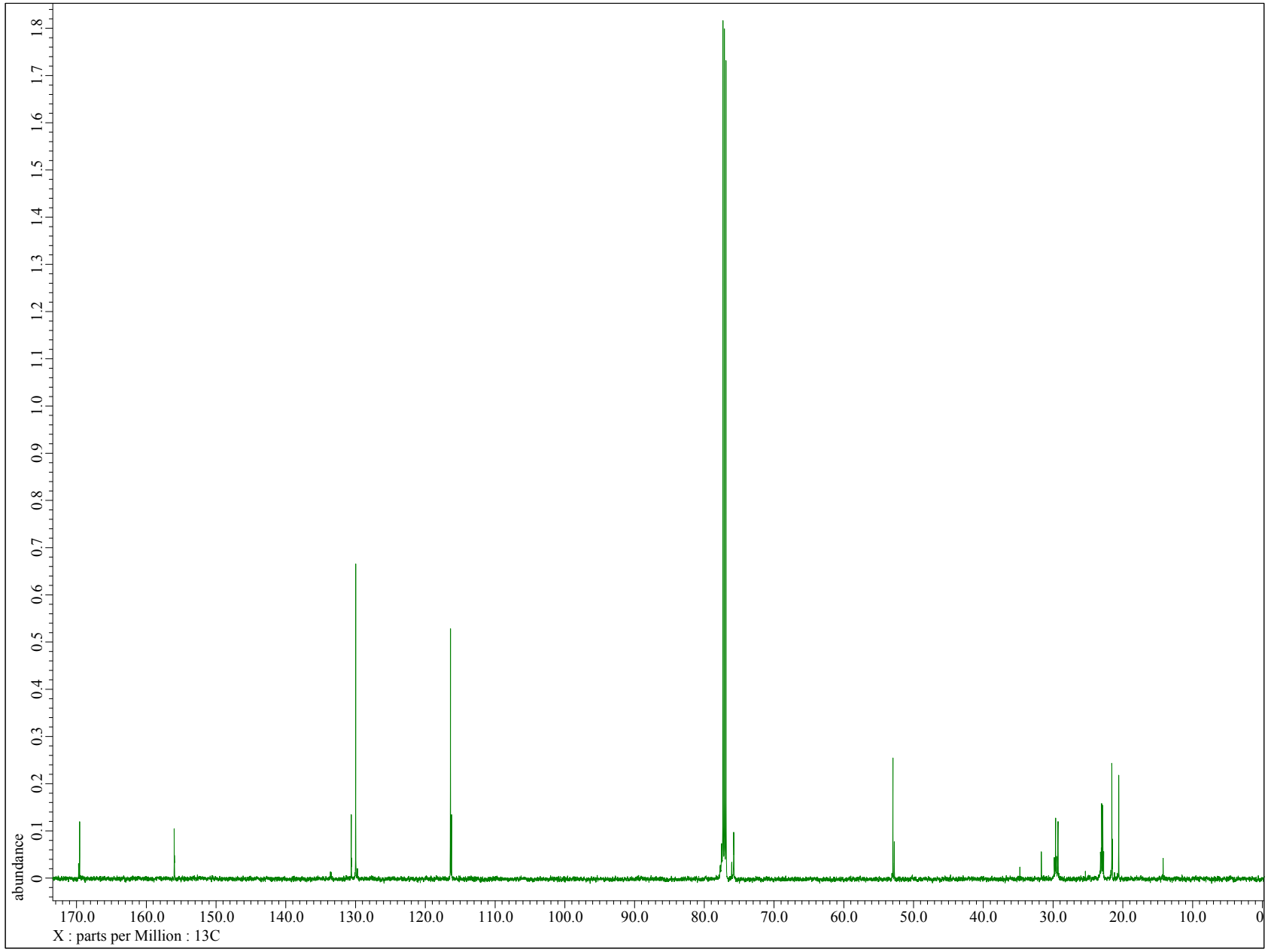


^{13}C NMR of **Compound 16a+b** [(±)-(*trans*-2-(*p*-tolylsulfanyl)cyclohexyl) 2-chloropropanoate]



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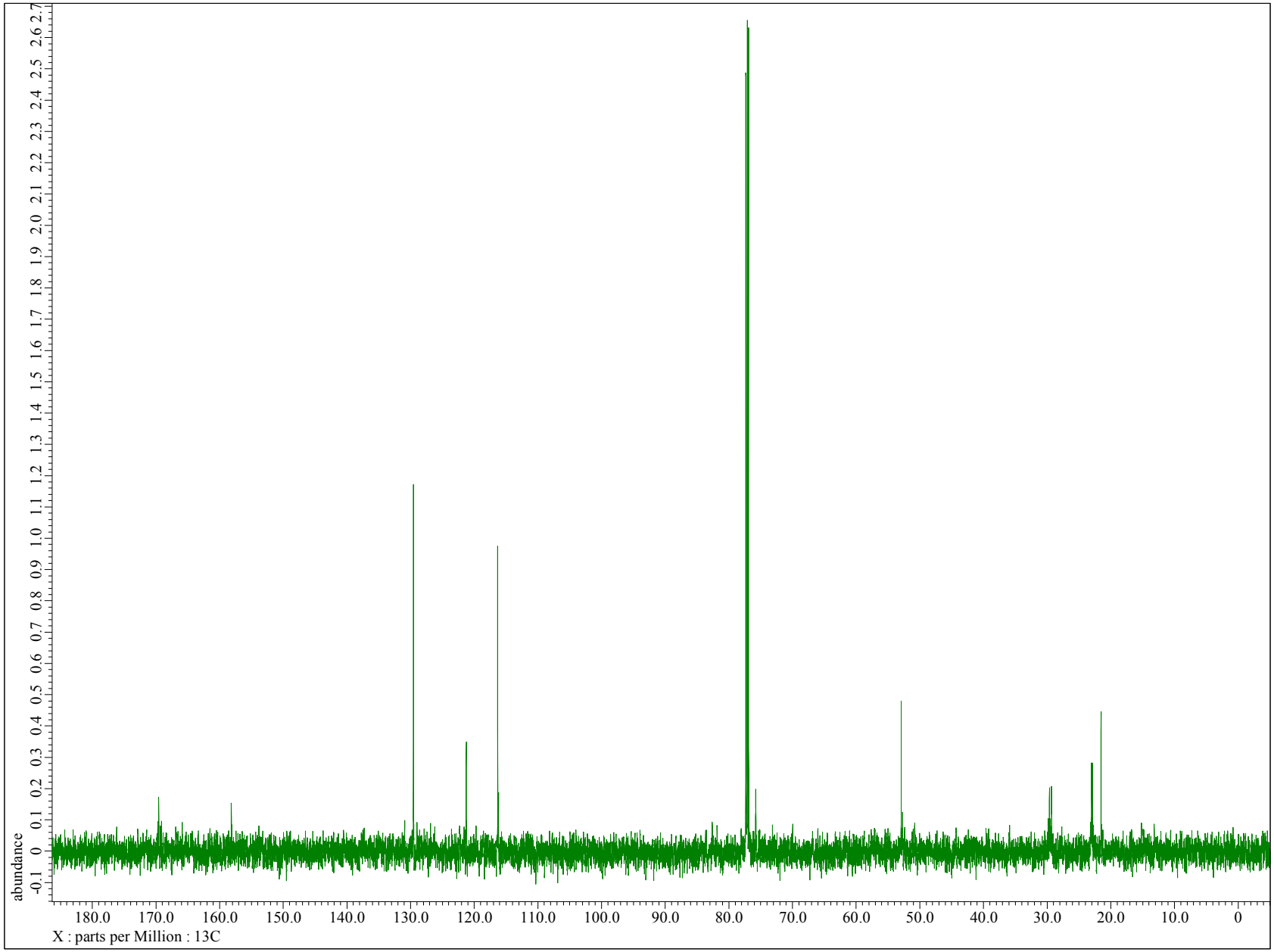
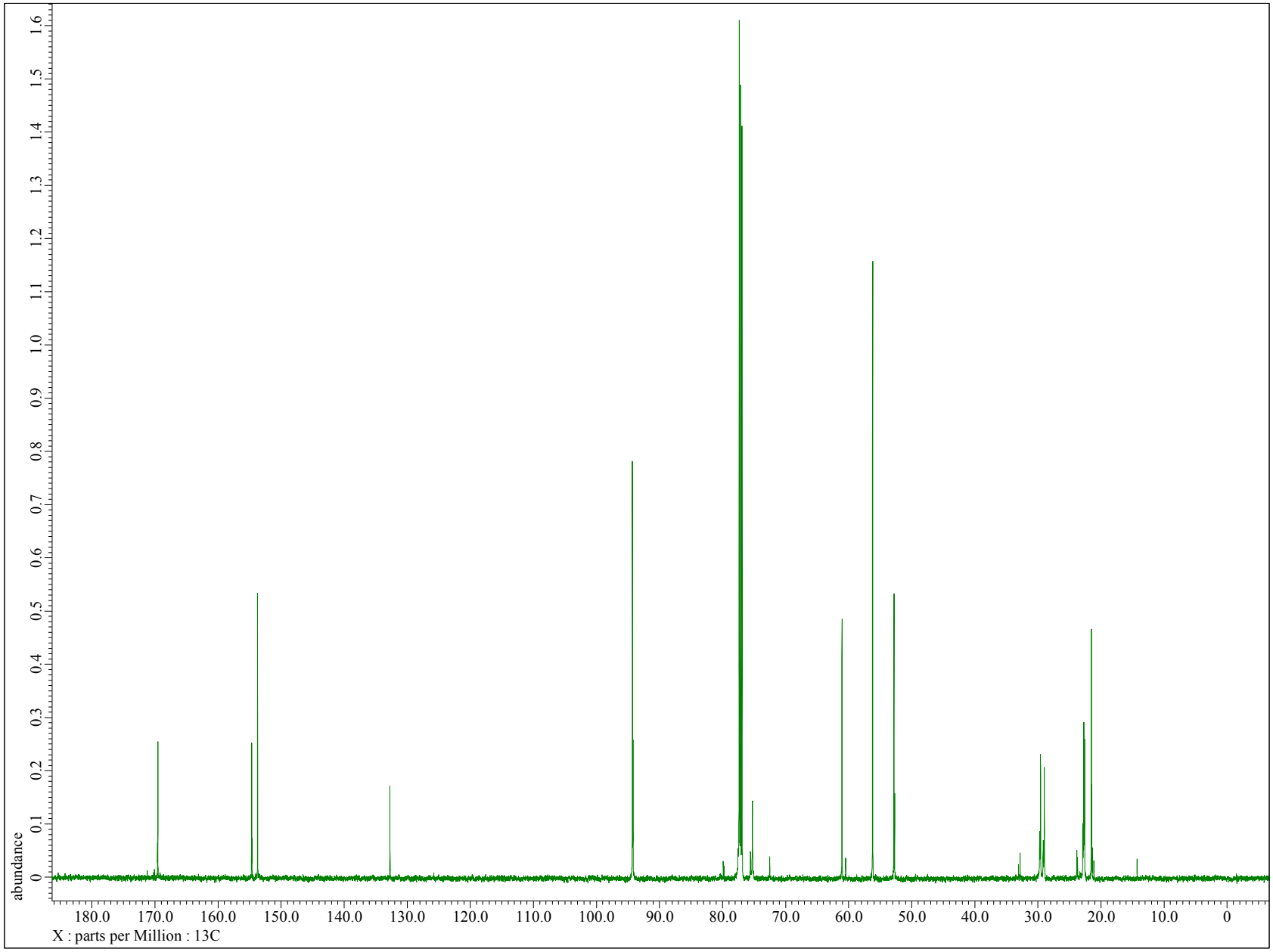


^{13}C NMR of **Compound 18a+b** [(±)-(*trans*-2-(phenyloxy)cyclohexyl 2-chloropropanoate]

^{13}C NMR of **Compound 19a+b** [(±)-(*trans*-2-(napthalen-2-yloxy)cyclohexyl) 2-chloropropanoate]



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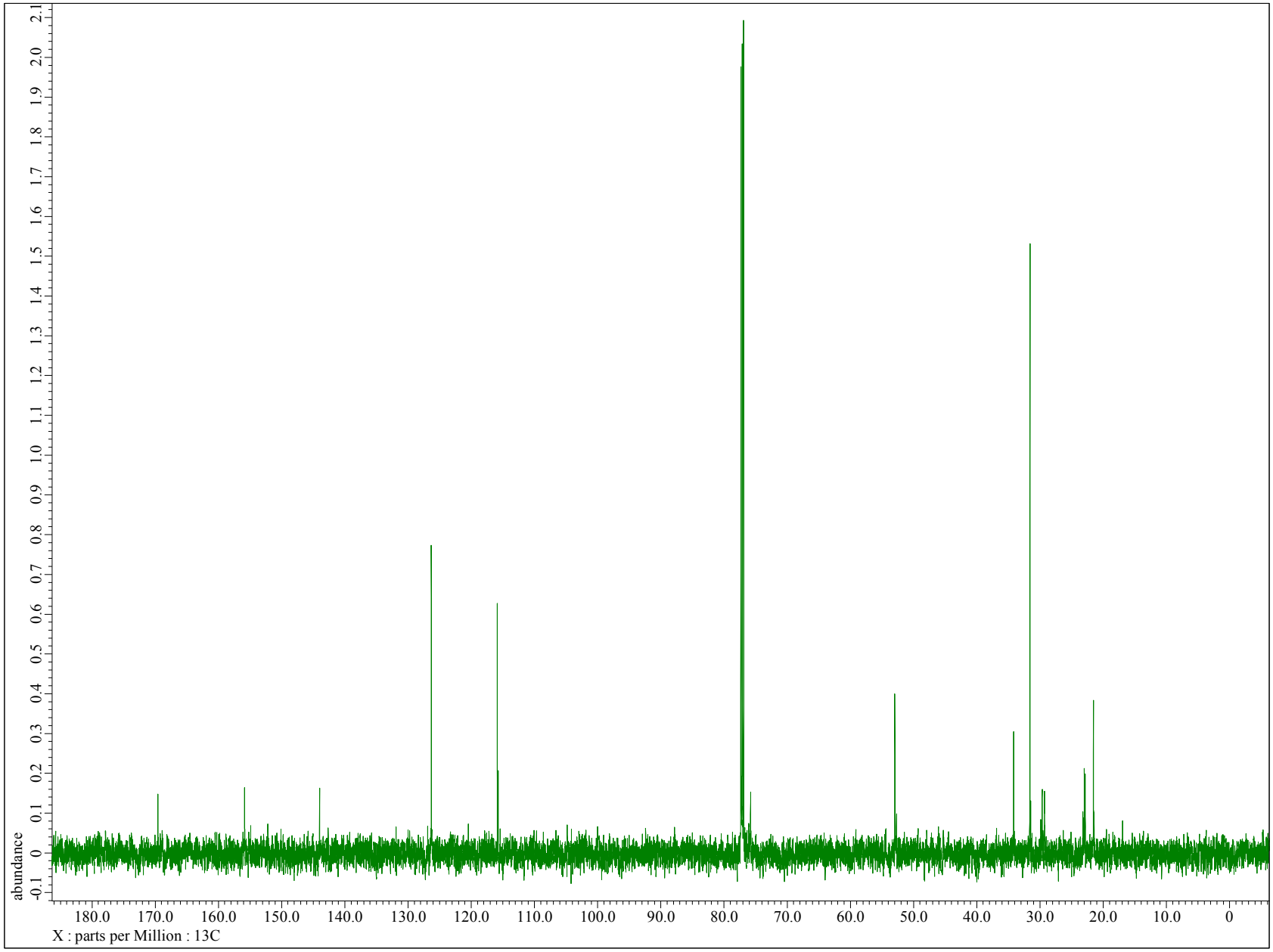
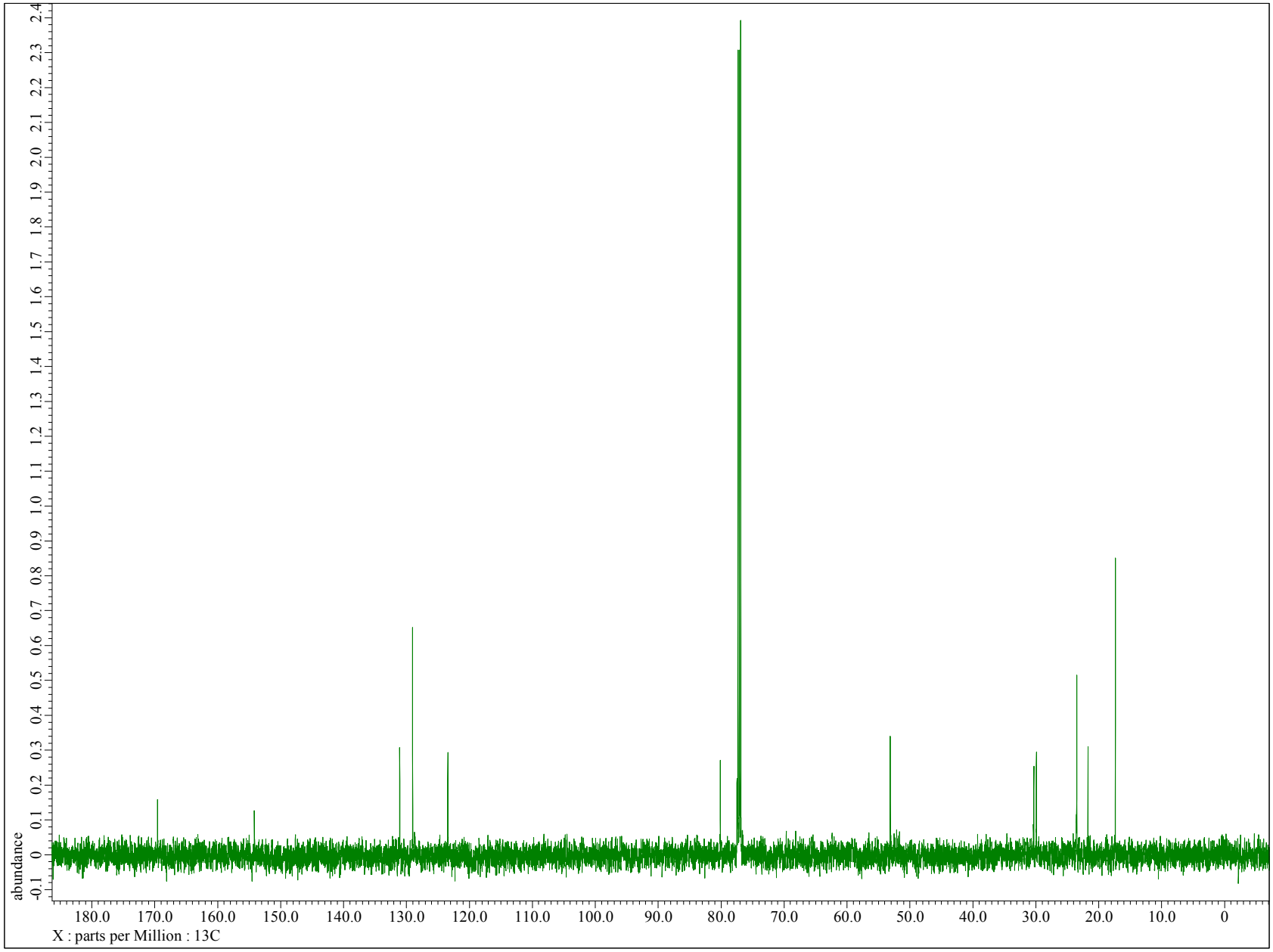
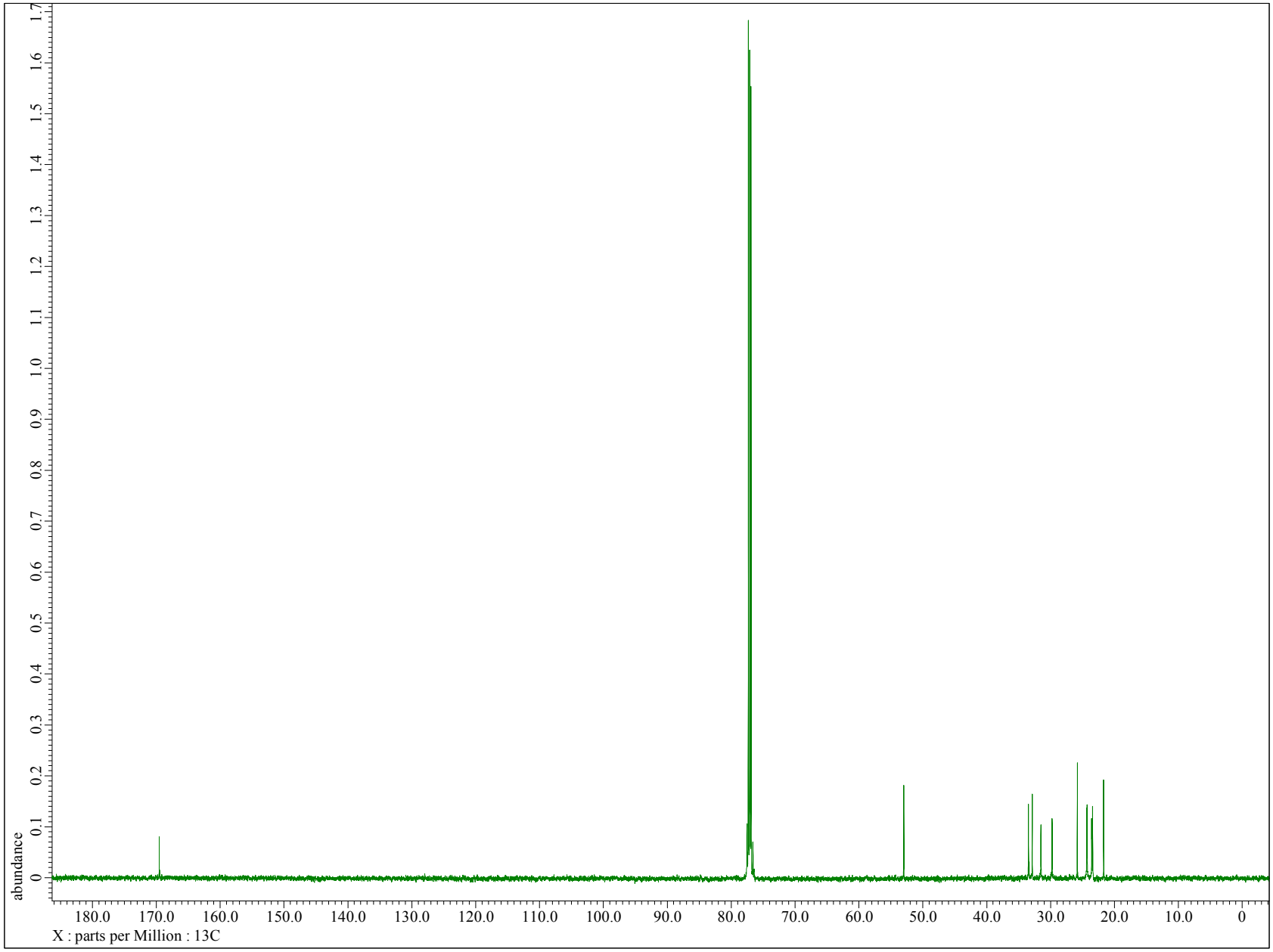


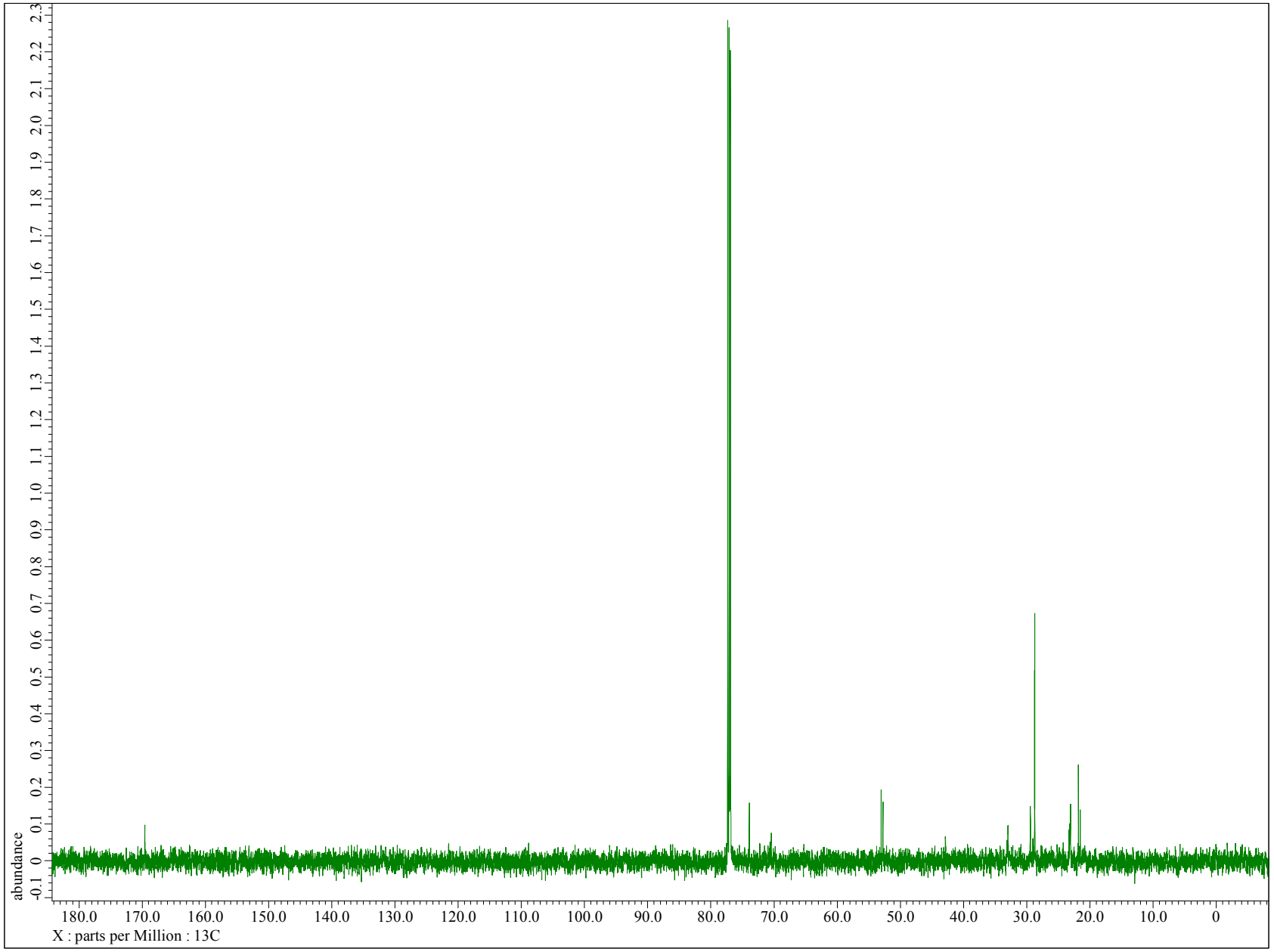
^{13}C NMR of **Compound 21a+b** [(±)-(*trans*-2-(*p-tert*-butyl-phenyloxy)cyclohexyl 2-chloropropanoate]



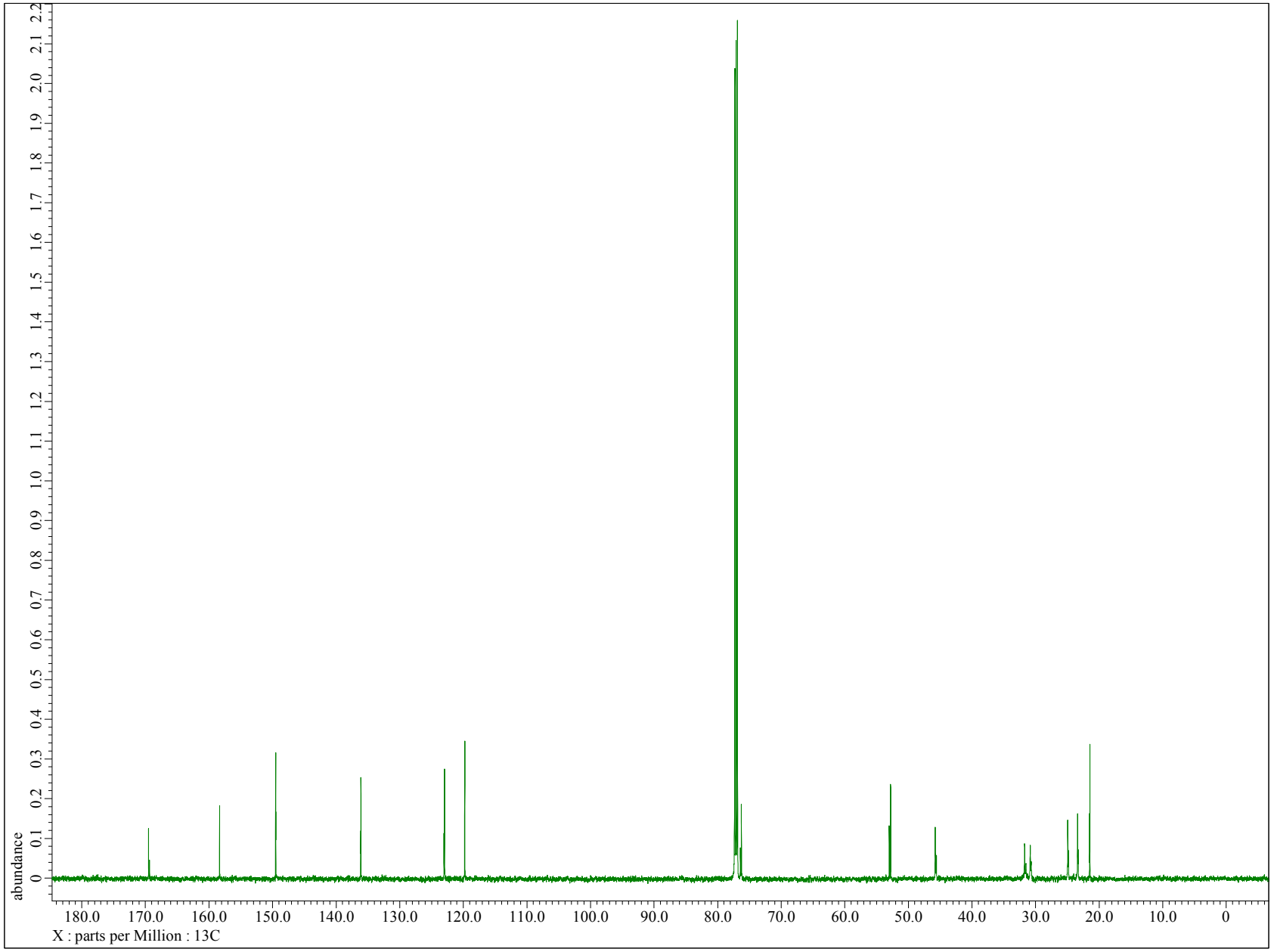
^{13}C NMR of **Compound 22a+b** [(±)-(*trans*-2-(2,6-dimethylphenyloxy)cyclohexyl 2-chloropropanoate]



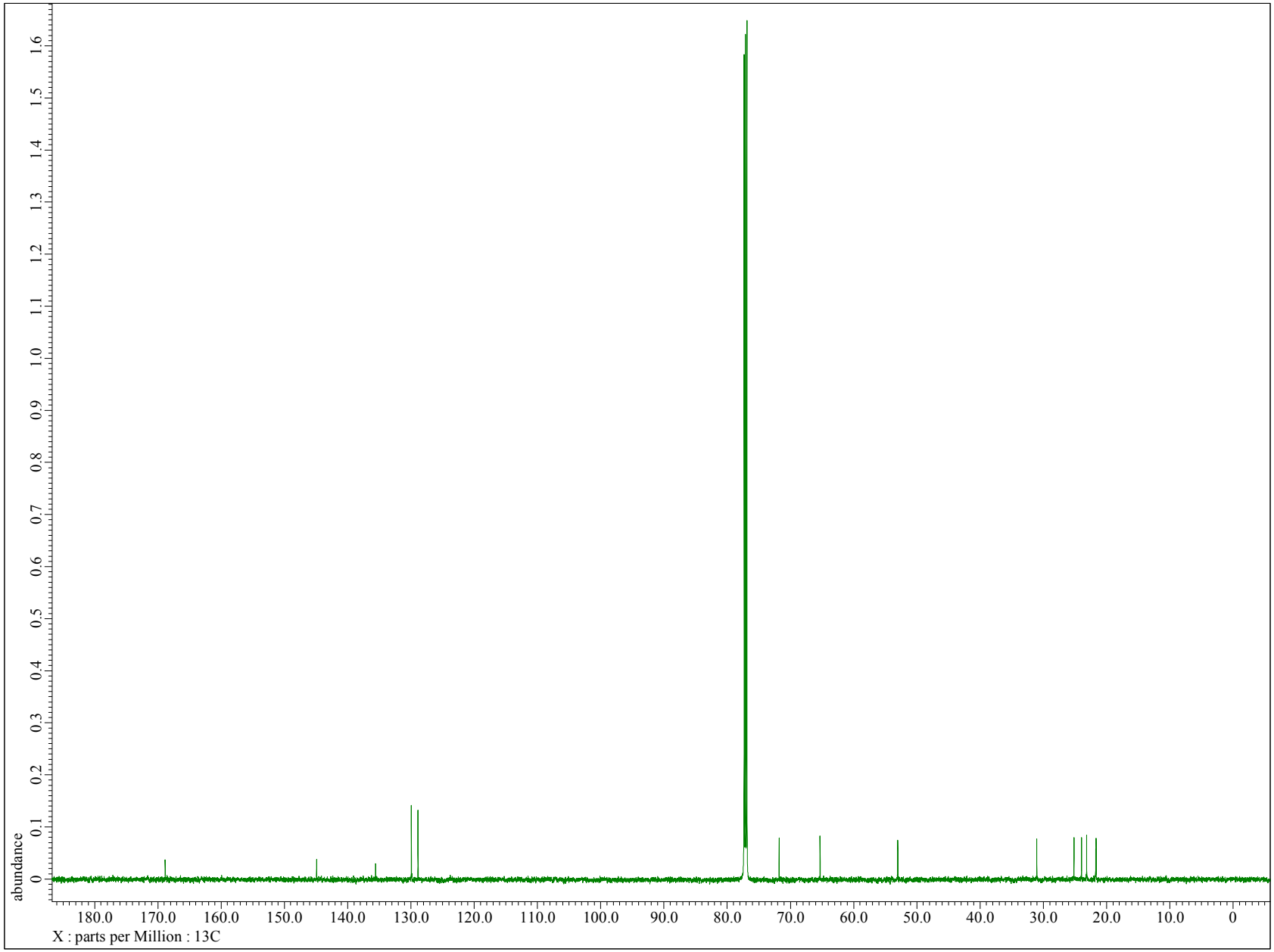
^{13}C NMR of **Compound 23a+b** [(±)-(*trans*-2-(cyclohexyloxy)cyclohexyl 2-chloropropanoate]



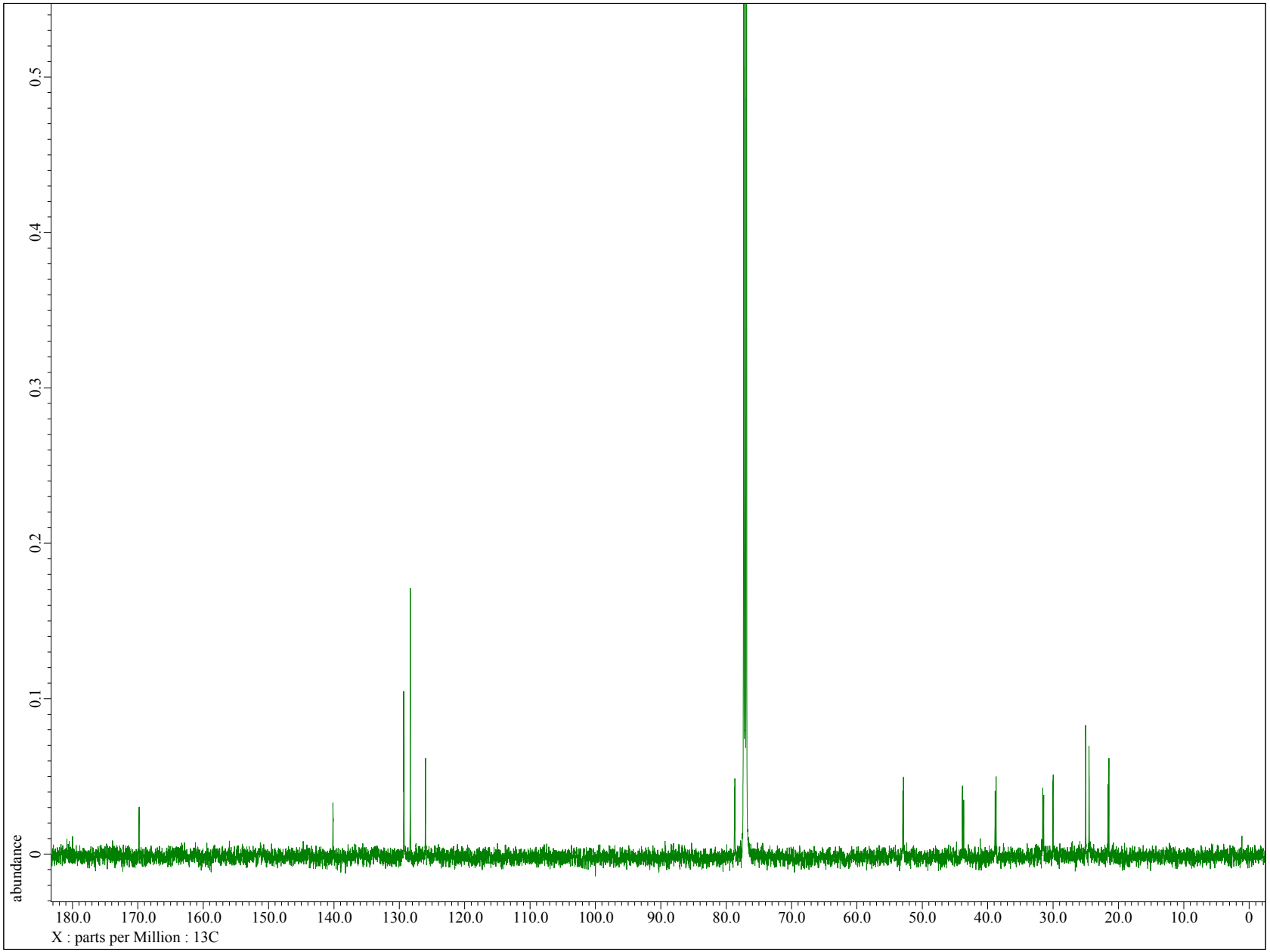
^{13}C NMR of **Compound 24a+b** [(±)-(*trans*-2-(*tert*-butoxy)cyclohexyl 2-chloropropanoate]



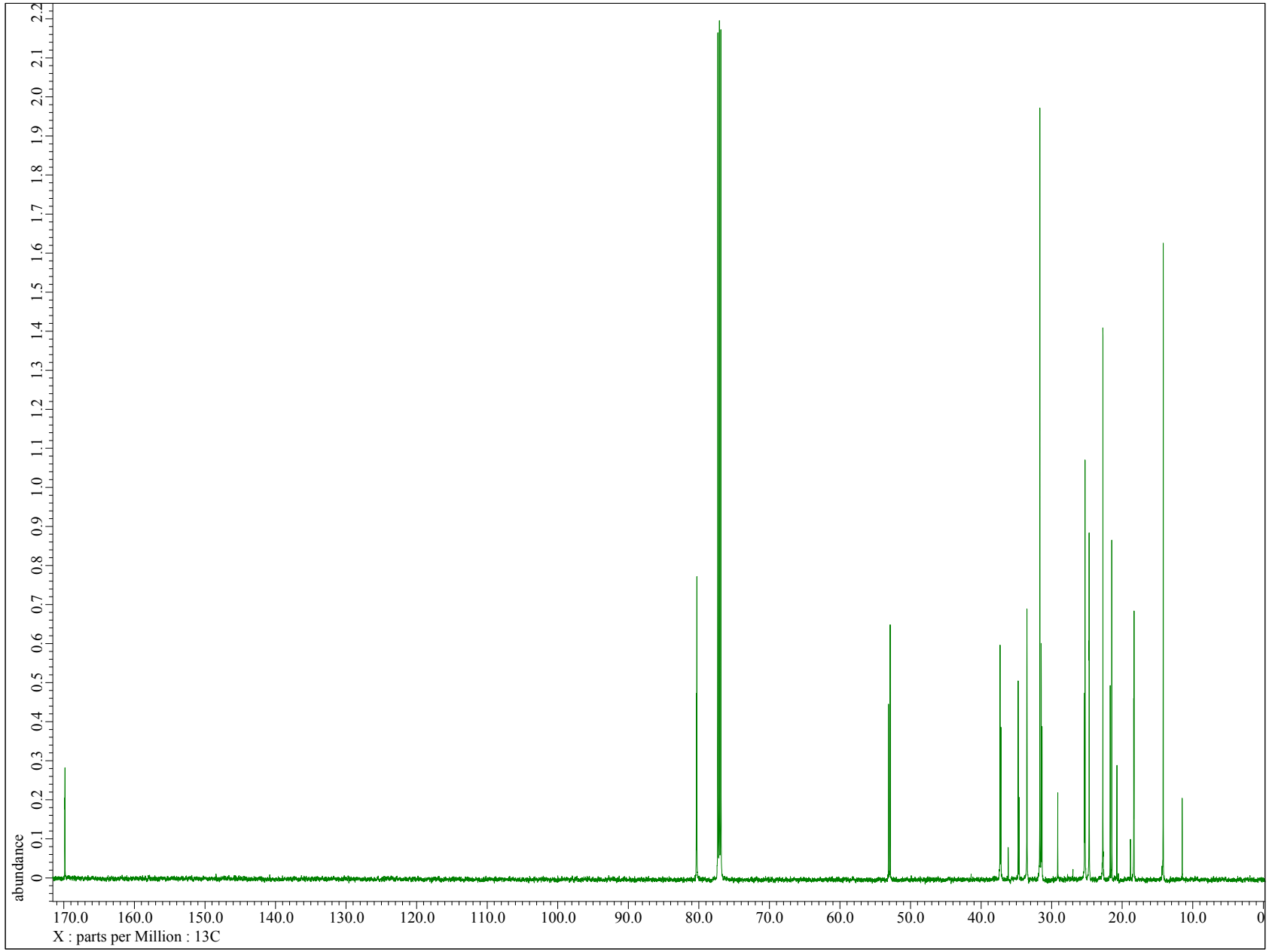
^{13}C NMR of **Compound 25a+b** [(±)-*trans*-2-(pyridin-2-ylthio)cyclohexyl 2-chloropropanoate]



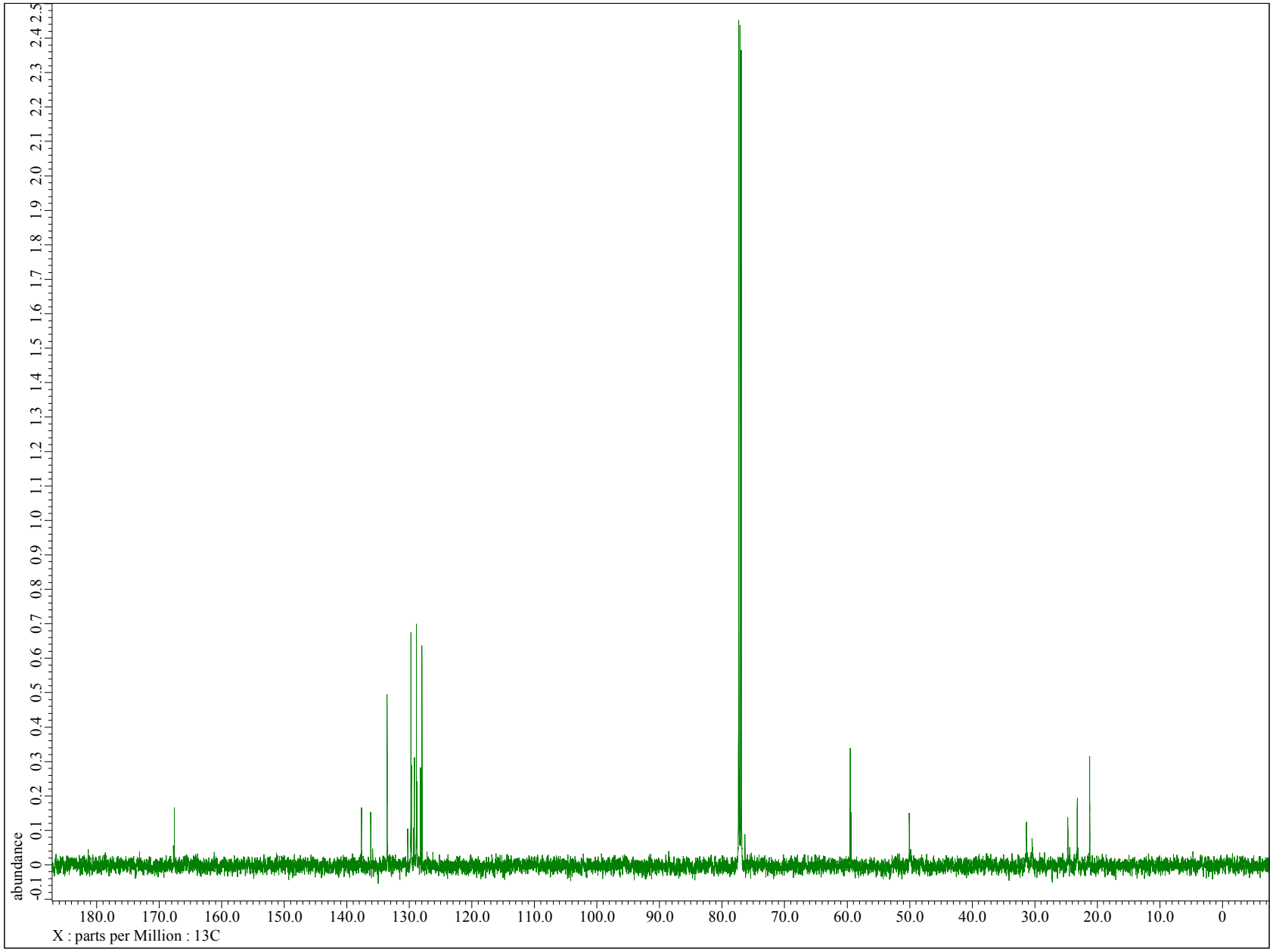
^{13}C NMR of **Compound 26a+b** [(±)-(*trans*-2-(*p*-tolylsulfonyl)cyclohexyl 2-chloropropanoate]



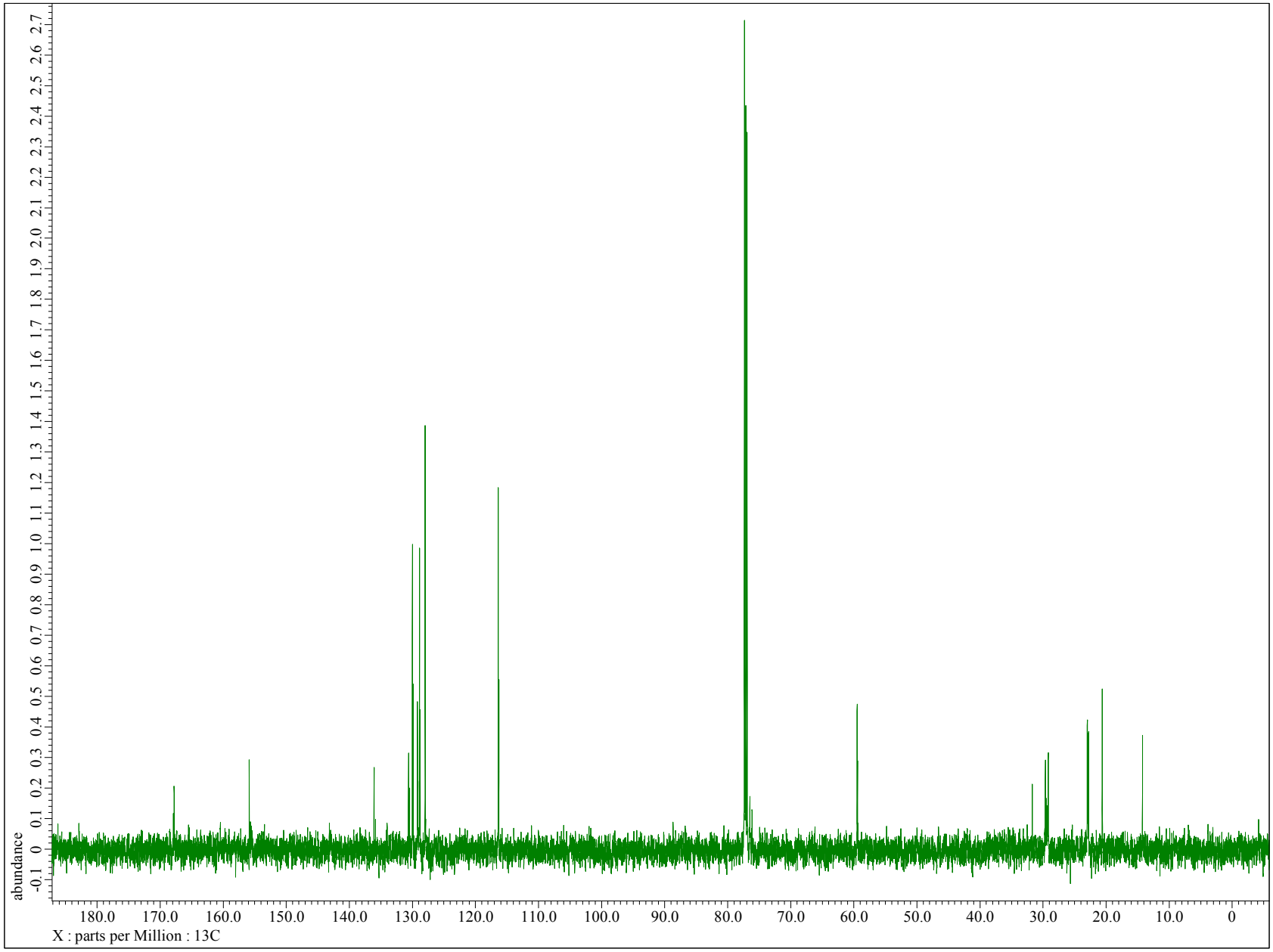
^{13}C NMR of **Compound 27a+b** [(±)-(*trans*-2-benzylcyclohexyl) 2-chloropropanoate]



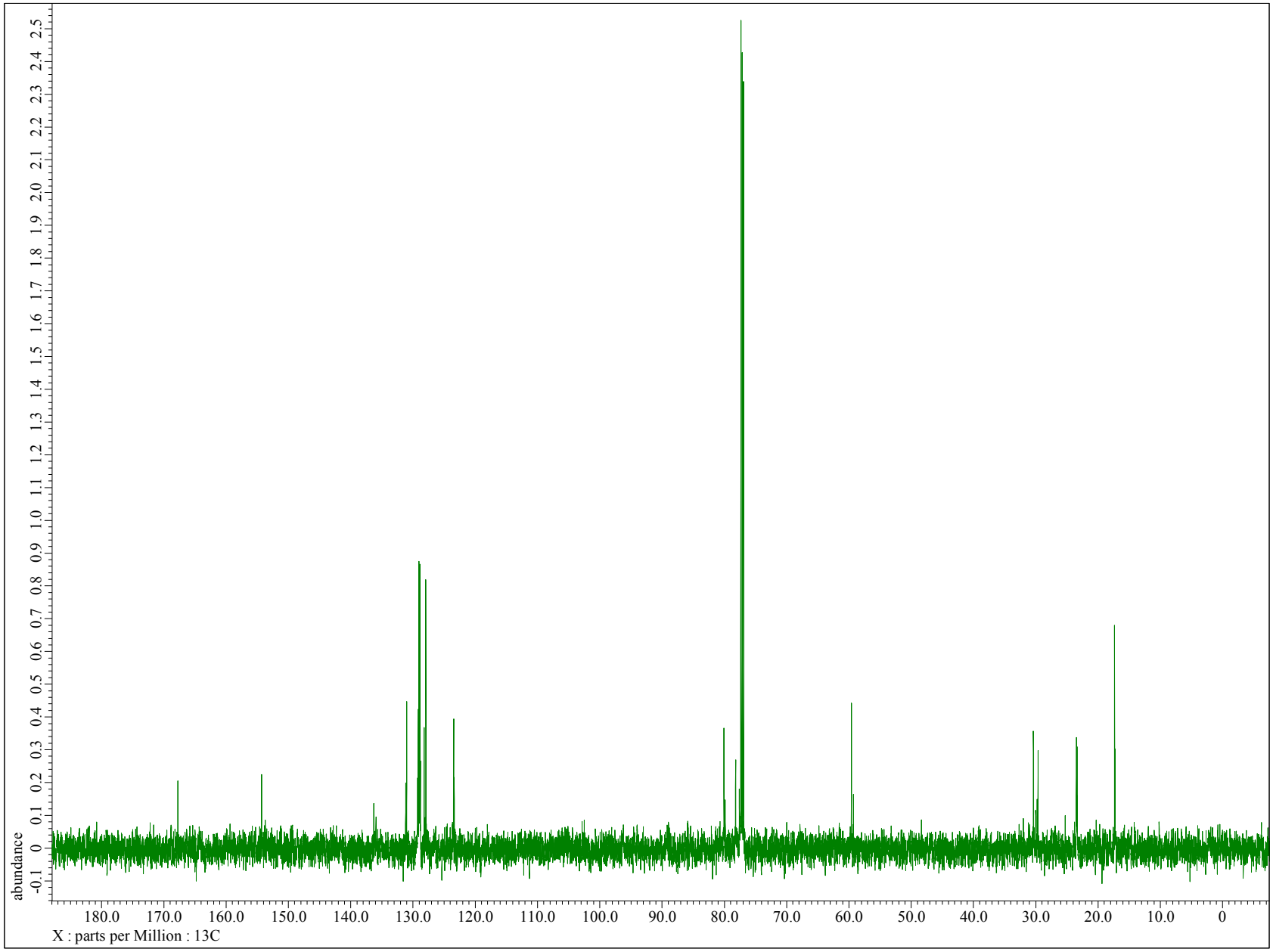
^{13}C NMR of **Compound 28a+b** [(±)-(*trans*-2-methylcyclohexyl) 2-chloropropanoate]



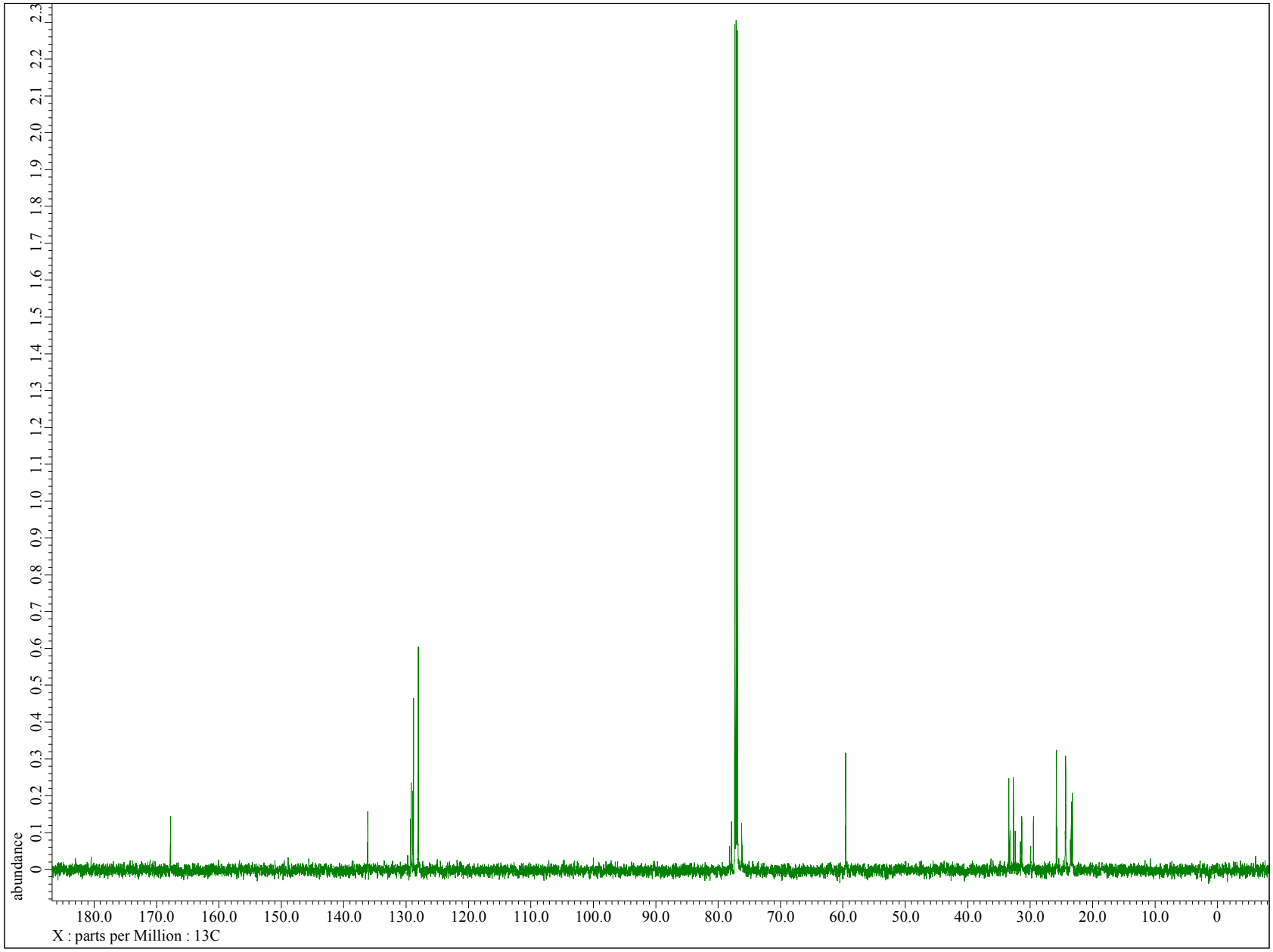
^{13}C NMR of **Compound 29a+b** [(±)-(*trans*-2-(*p*-tolylsulfanyl)cyclohexyl 2-chloro-2-phenylethanoate]



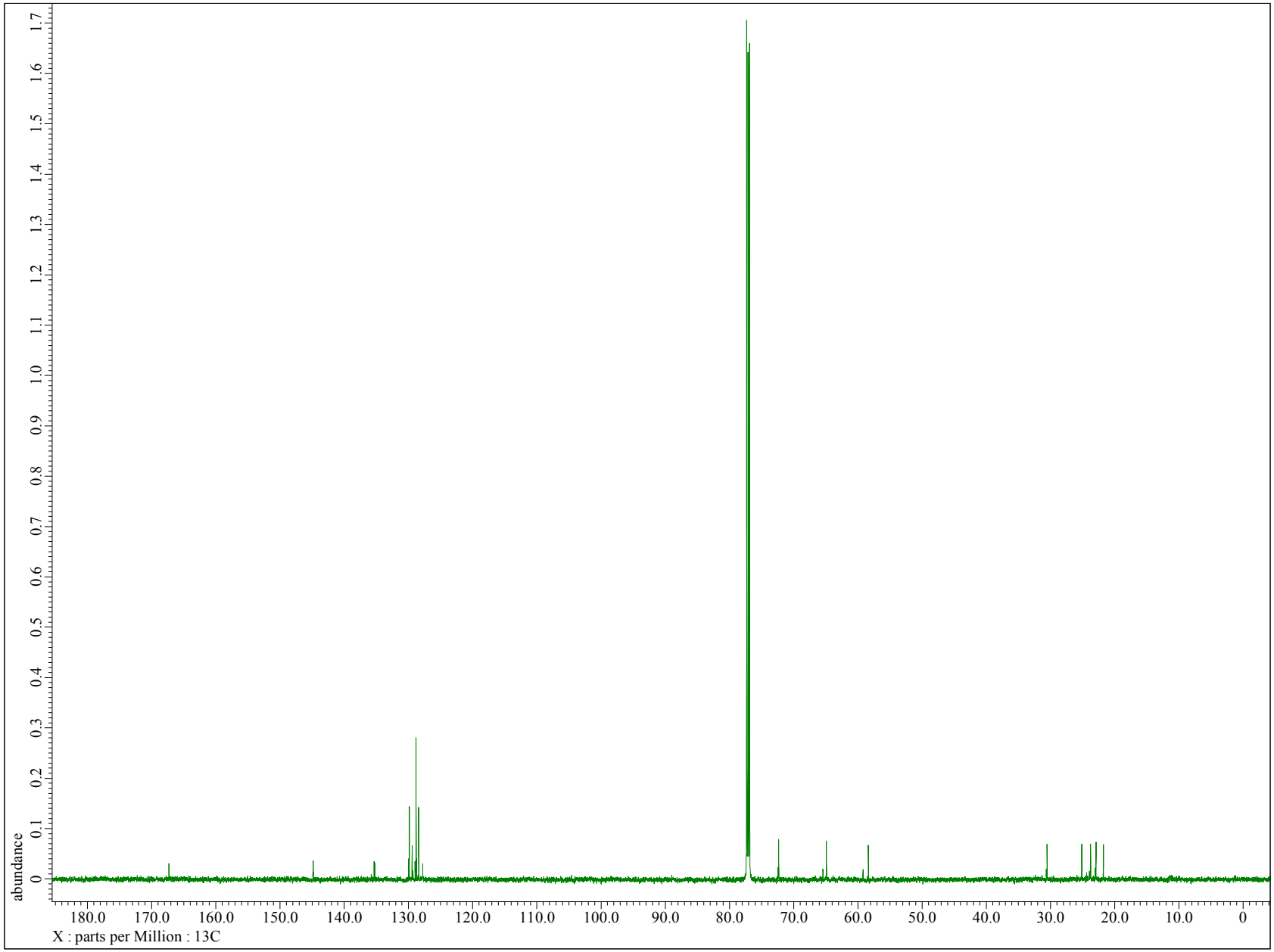
^{13}C NMR of **Compound 30a+b** [(±)-(*trans*-2-(*p*-tolyloxy)cyclohexyl 2-chloro-2-phenylethanoate]



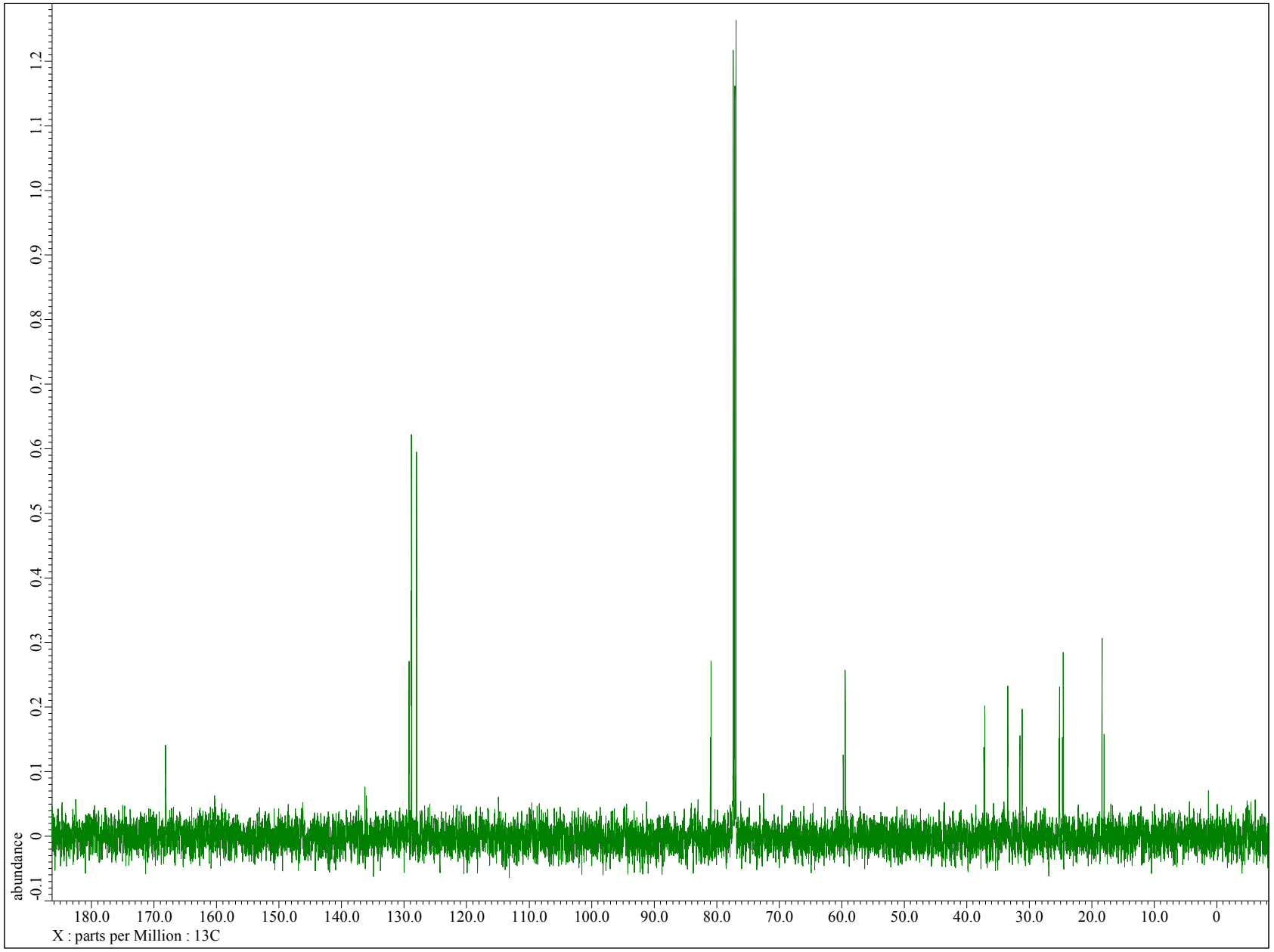
^{13}C NMR of **Compound 31a+b** [(±)-(*trans*-2-(2,6-dimethylphenyloxy)cyclohexyl 2-chloro-2-phenylethanoate]



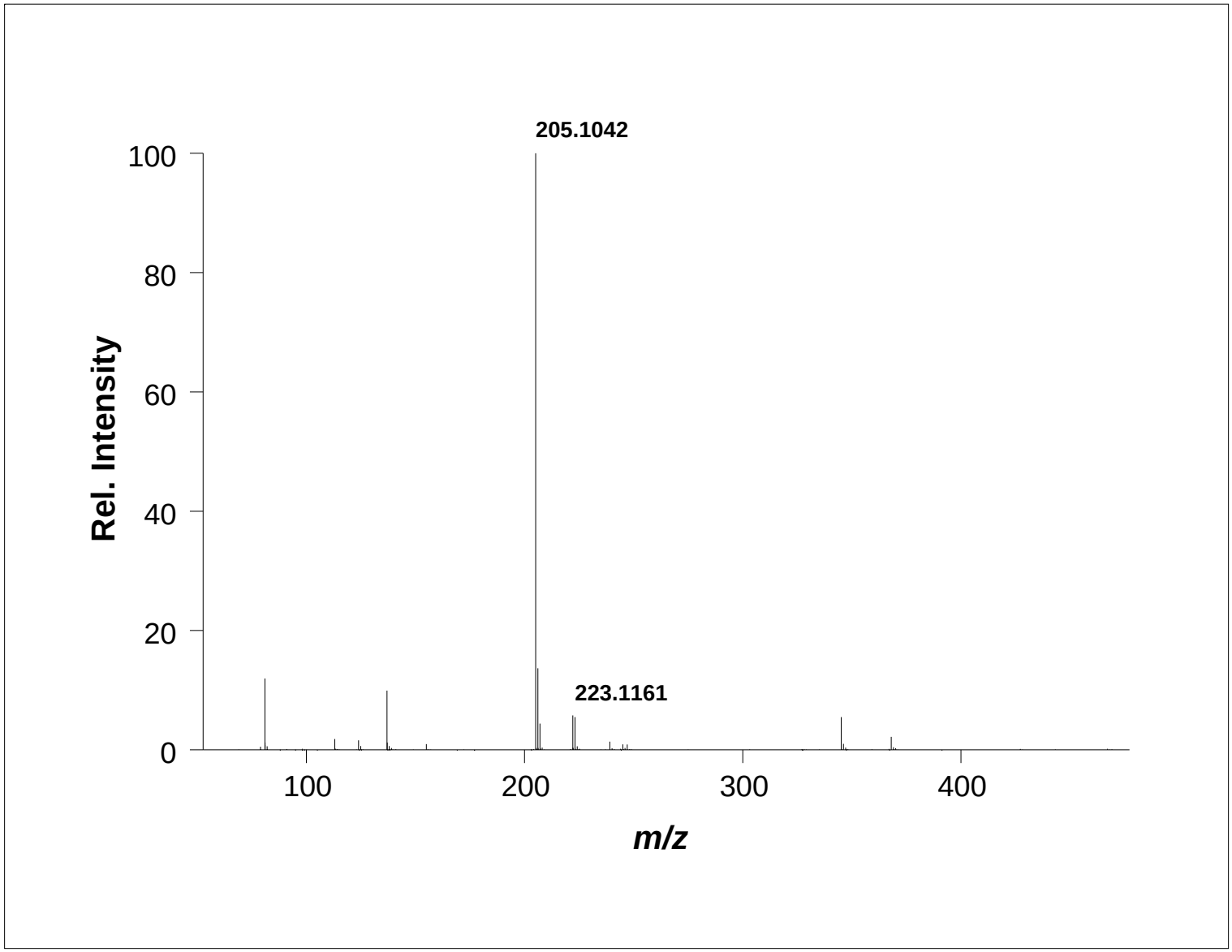
^{13}C NMR of **Compound 32a+b** [(±)-(*trans*-2-(cyclohexyloxy)cyclohexyl 2-chloro-2-phenylethanoate]



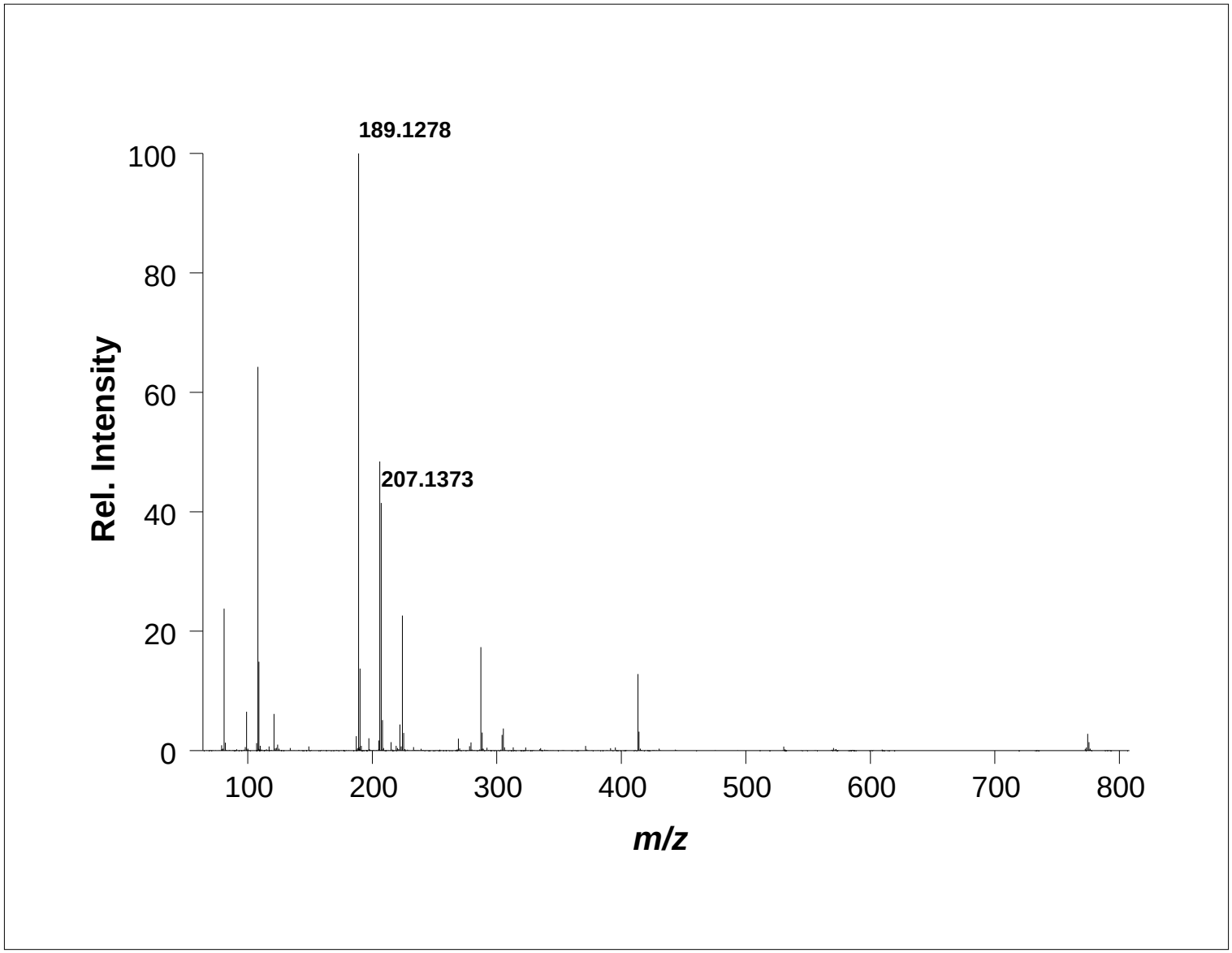
^{13}C NMR of **Compound 33a+b** [(±)-(*trans*-2-(*p*-tolylsulfonyl)cyclohexyl 2-chloro-2-phenylethanoate]



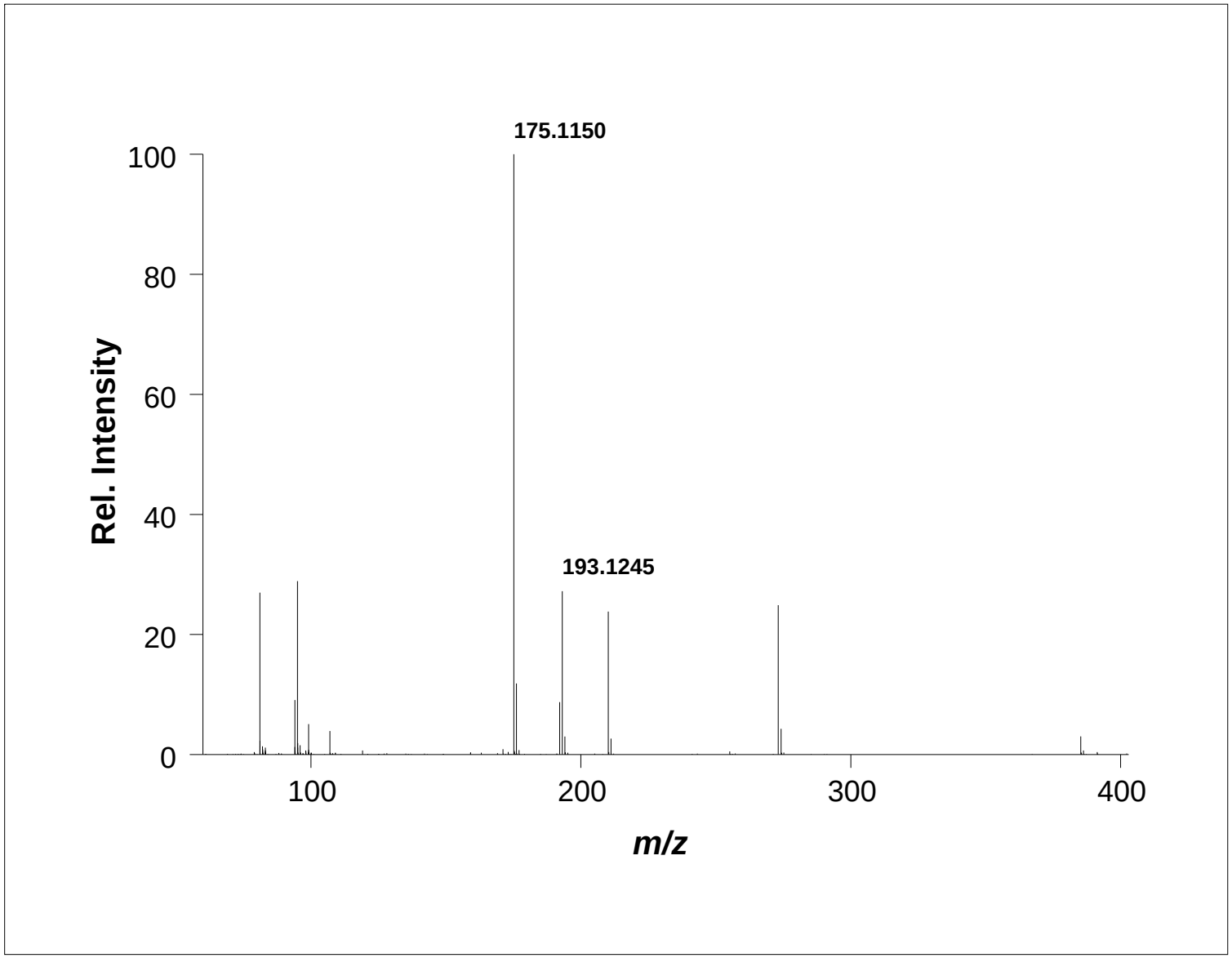
^{13}C NMR of **Compound 34a+b** [(±)-*trans*-2-(methyl)cyclohexyl 2-chloro-2-phenylethanoate]



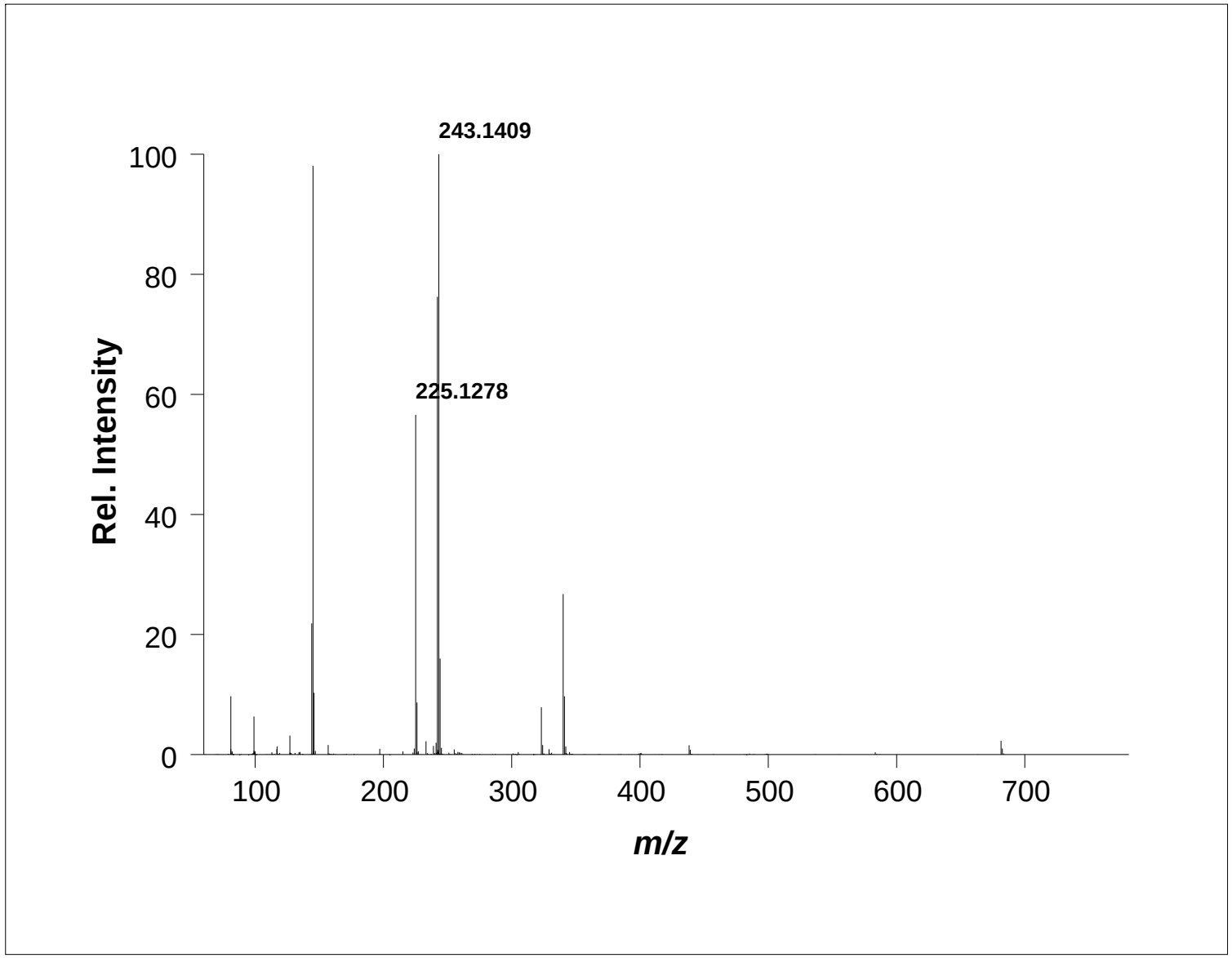
HRMS of **Compound 1** [(±)-*trans*-2-(*p*-tolylsulfanyl)cyclohexanol]



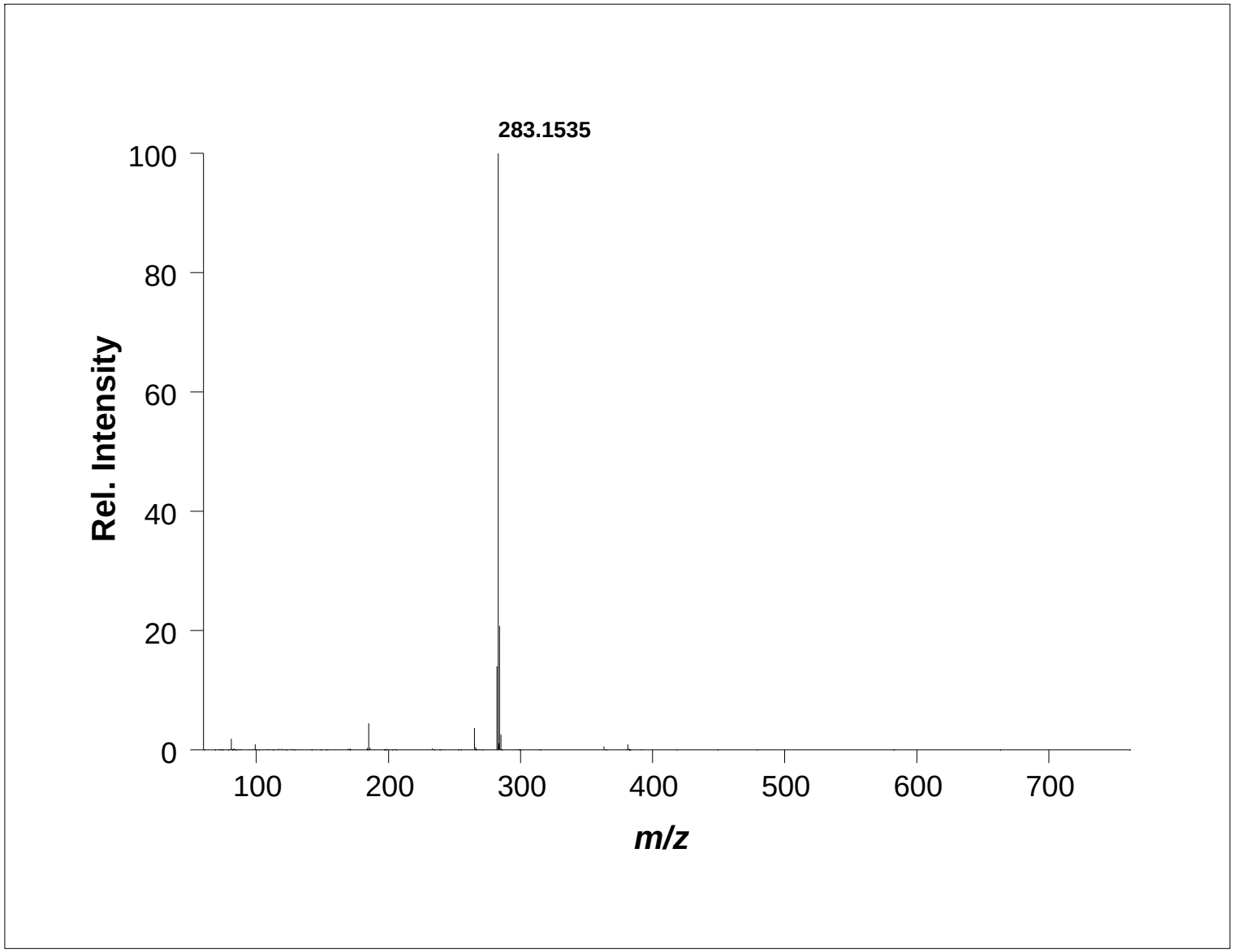
HRMS of **Compound 2** [(±)-*trans*-2-(*p*-tolyloxy)cyclohexanol]



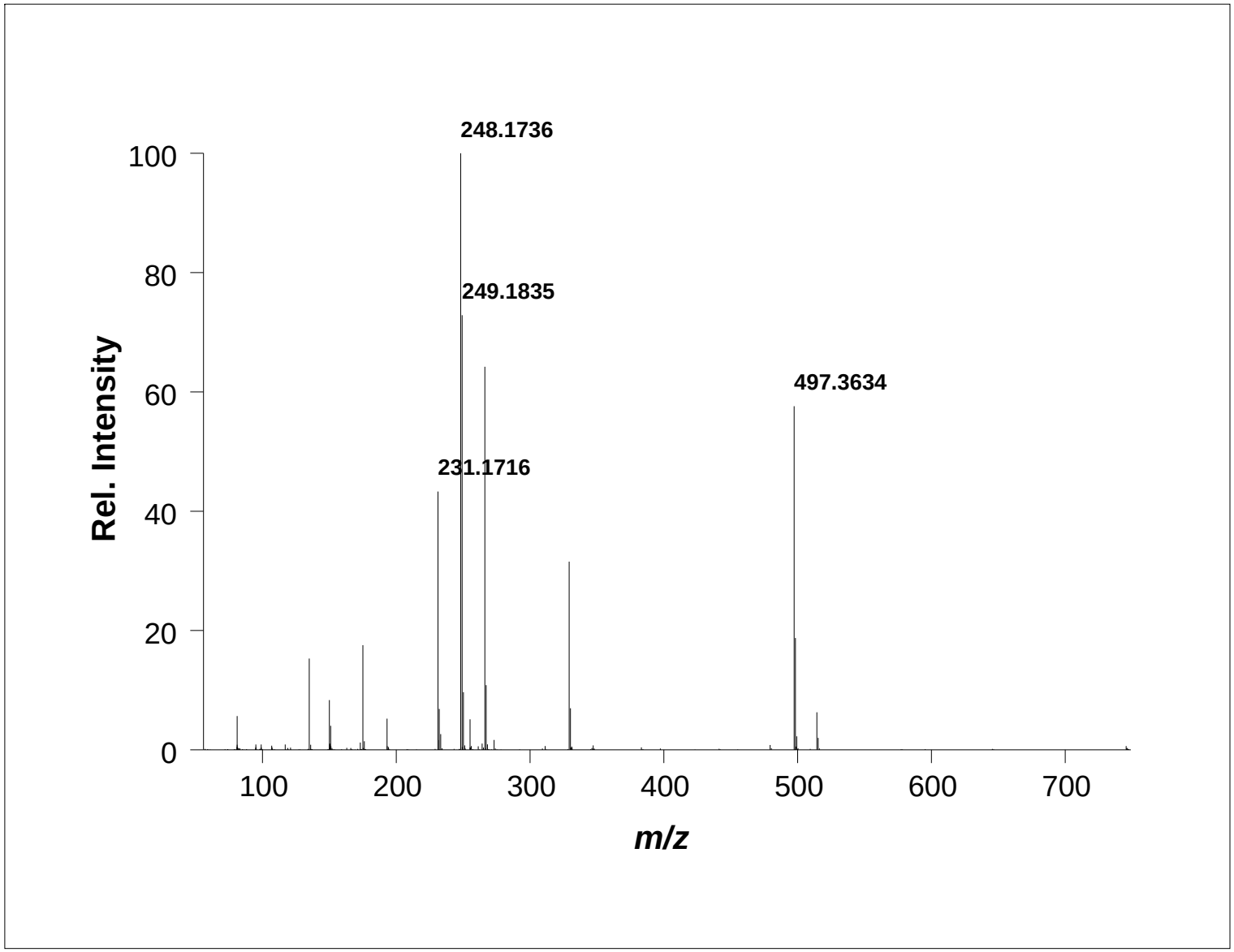
HRMS of **Compound 3** [(±)-*trans*-2-(phenyloxy)cyclohexanol]



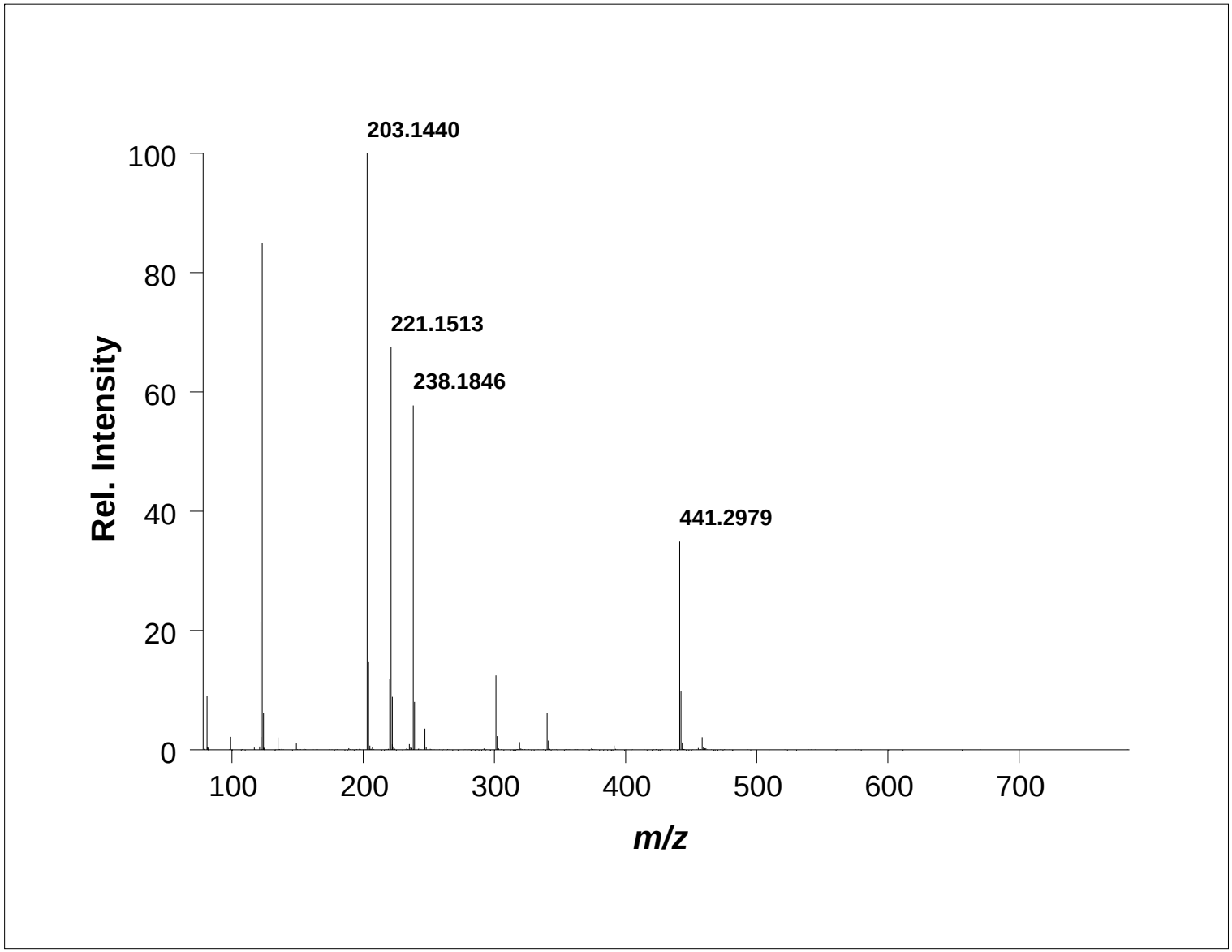
HRMS of **Compound 4** [(±)-*trans*-2-(napthalen-2-yloxy)cyclohexanol]



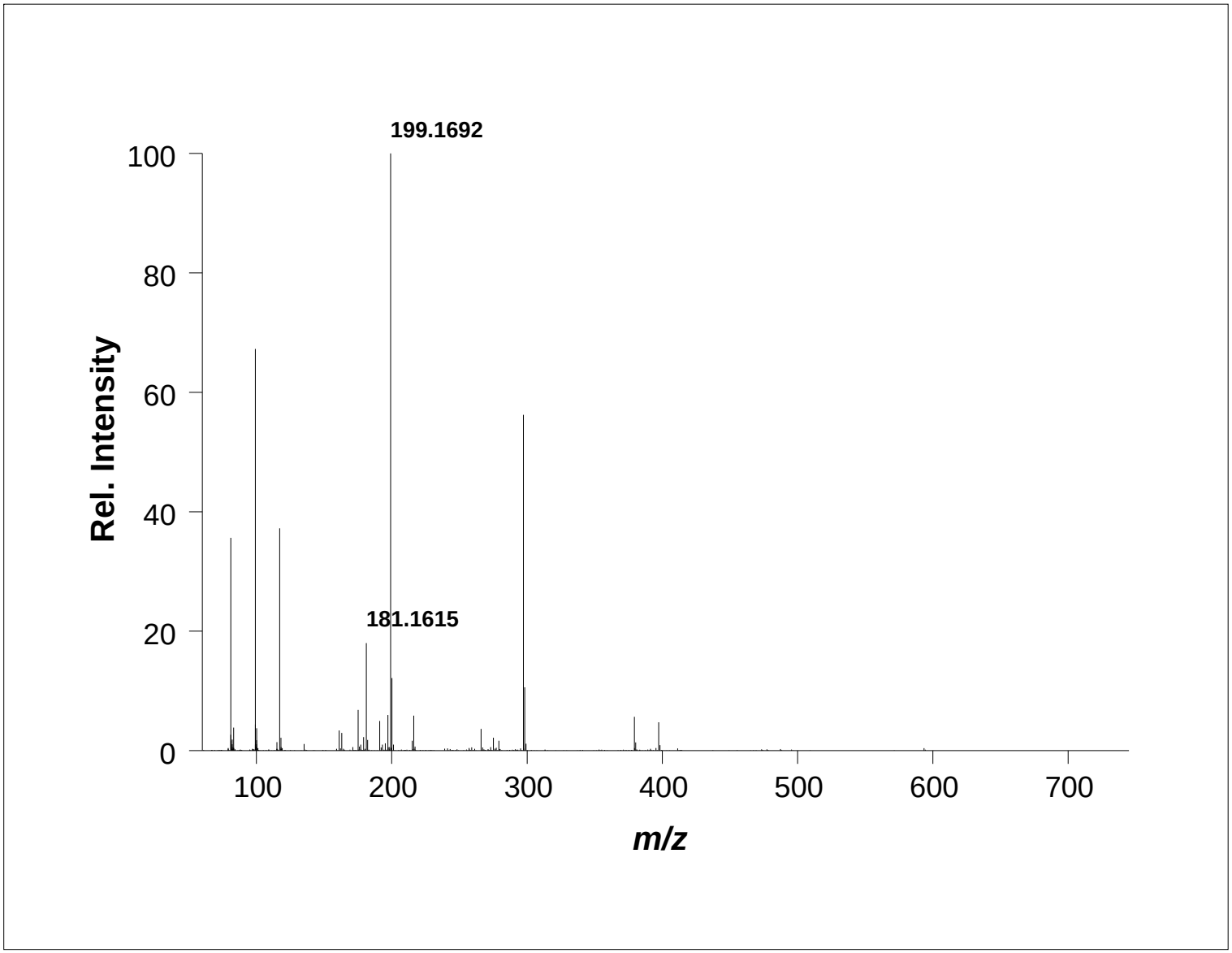
HRMS of **Compound 5** [(±)-*trans*-2-(3,4,5-trimethylphenyloxy)cyclohexanol]



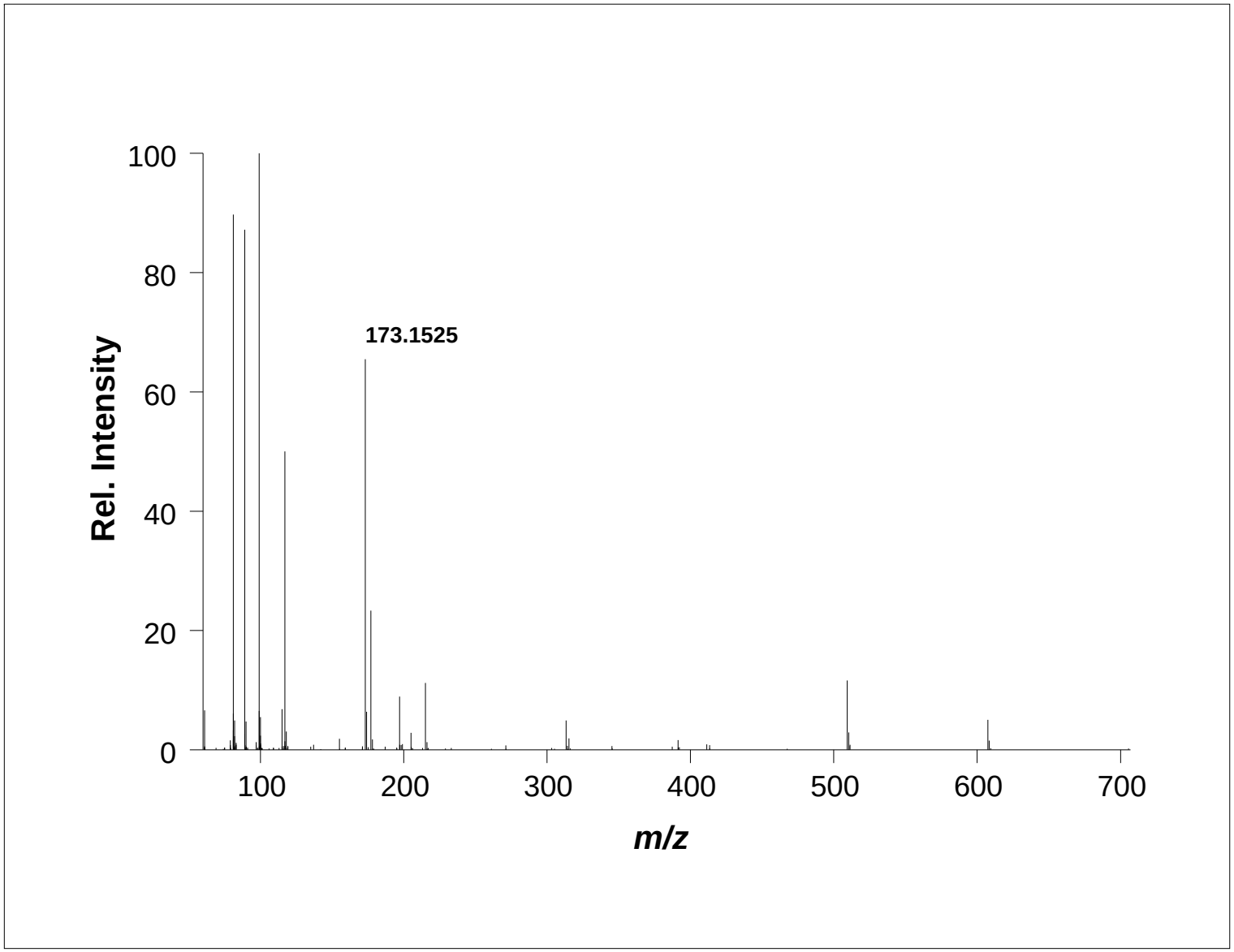
HRMS of **Compound 6** [(±)-*trans*-2-(*p*-(*tert*-butoxy)phenyloxy)cyclohexanol]



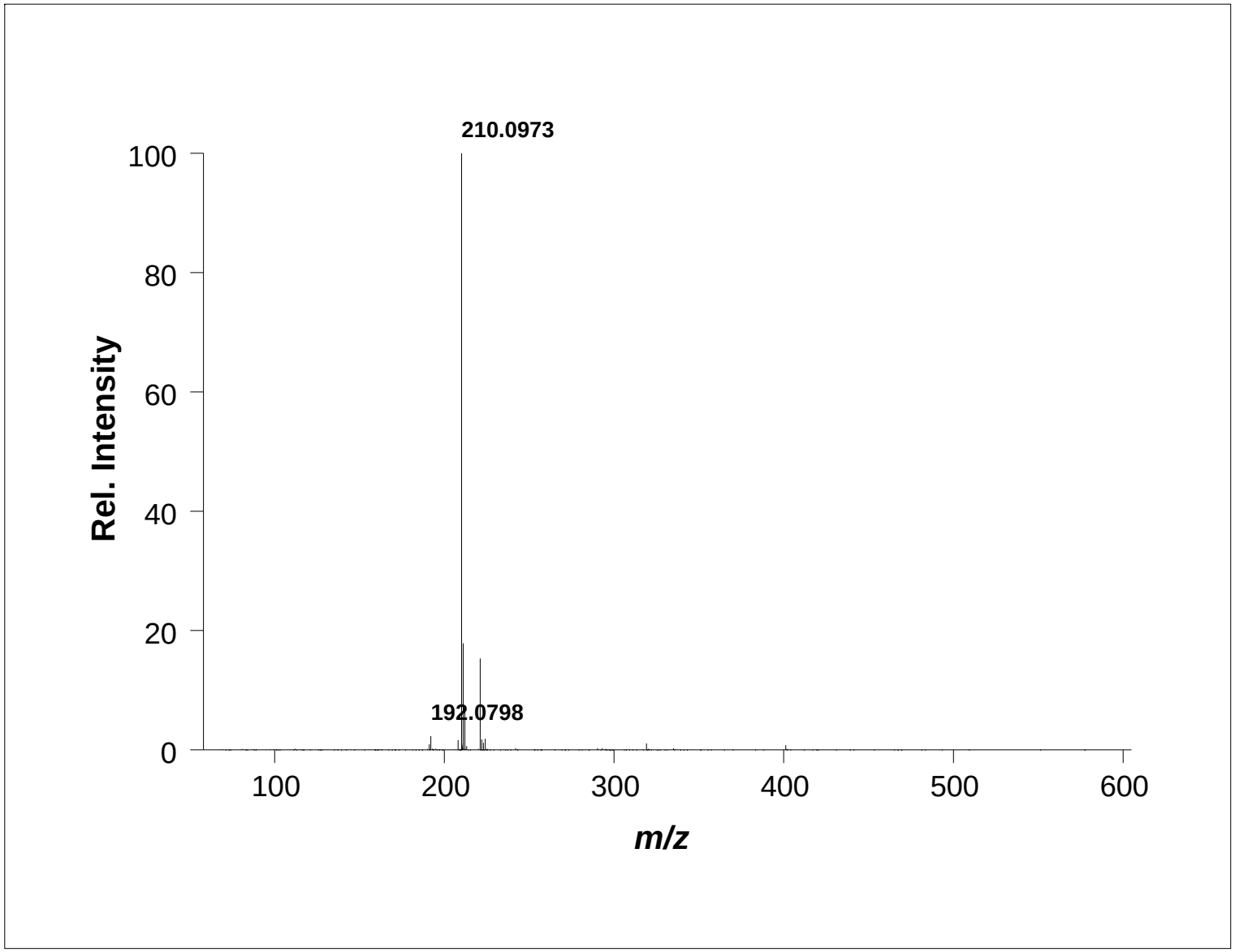
HRMS of **Compound 7** [(±)-*trans*-2-(2,6-dimethylphenyloxy)cyclohexanol]



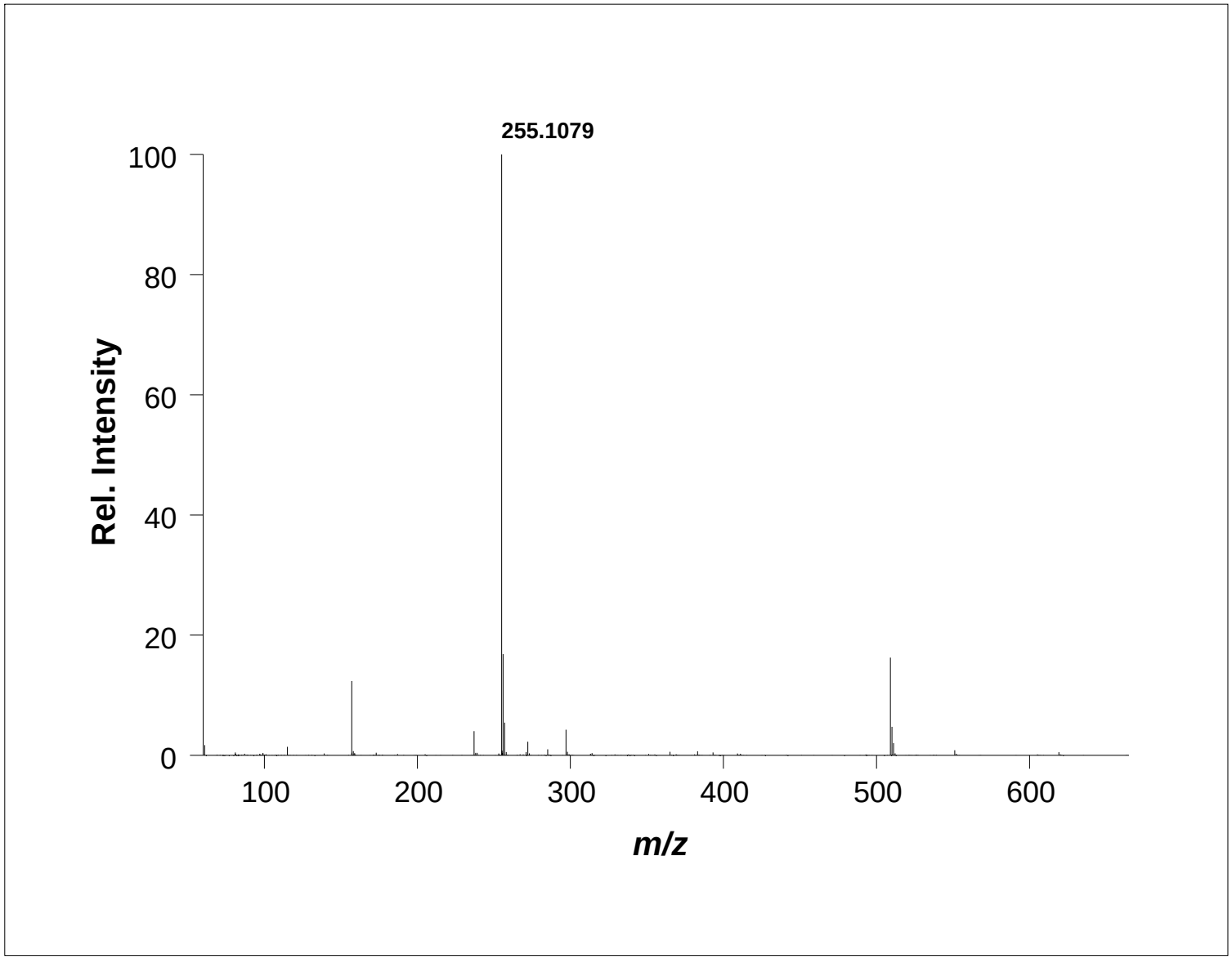
HRMS of **Compound 8** [(±)-*trans*-2-(cyclohexyloxy)cyclohexanol]



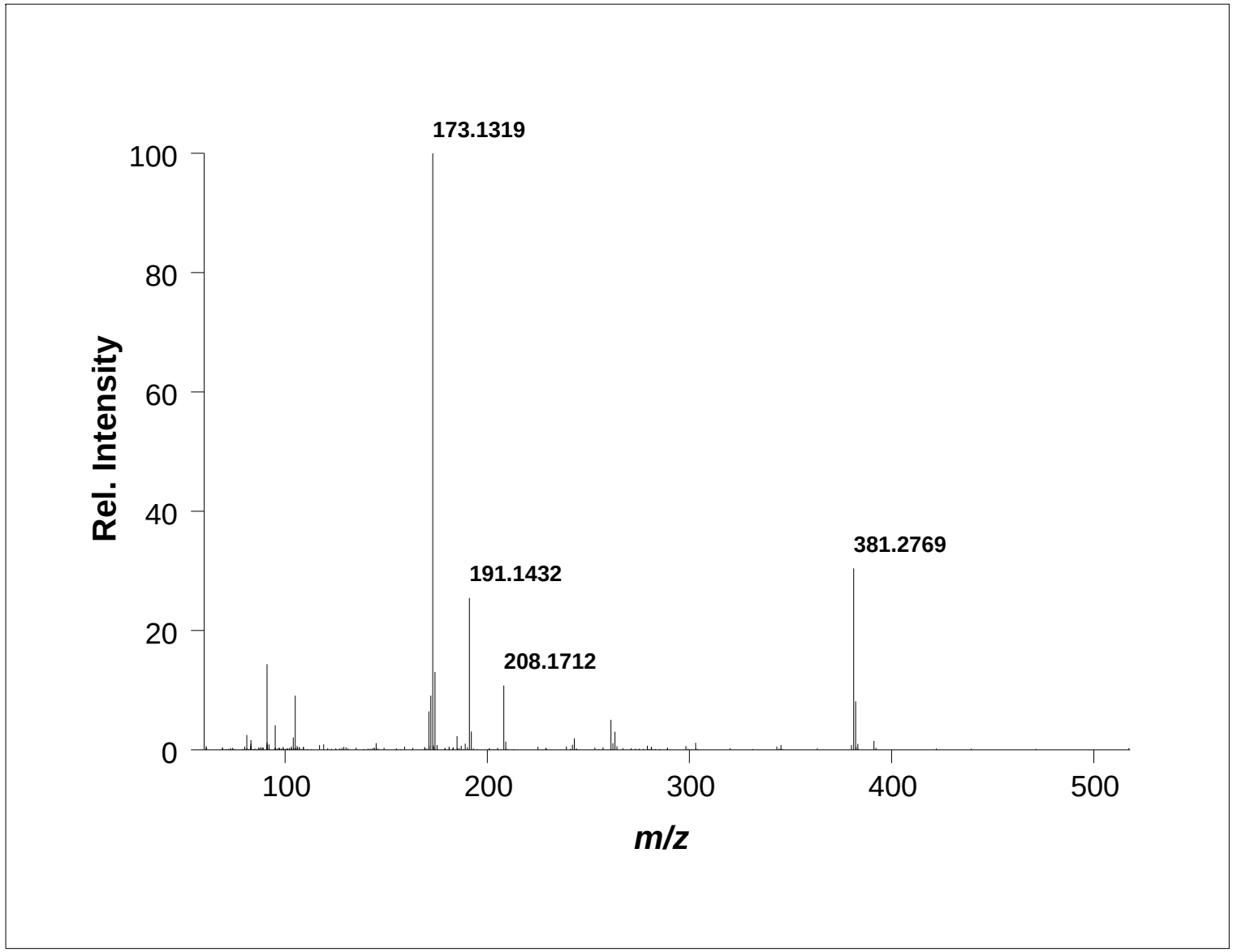
HRMS of **Compound 9** [(±)-*trans*-2-(*t*-butoxy)cyclohexanol]



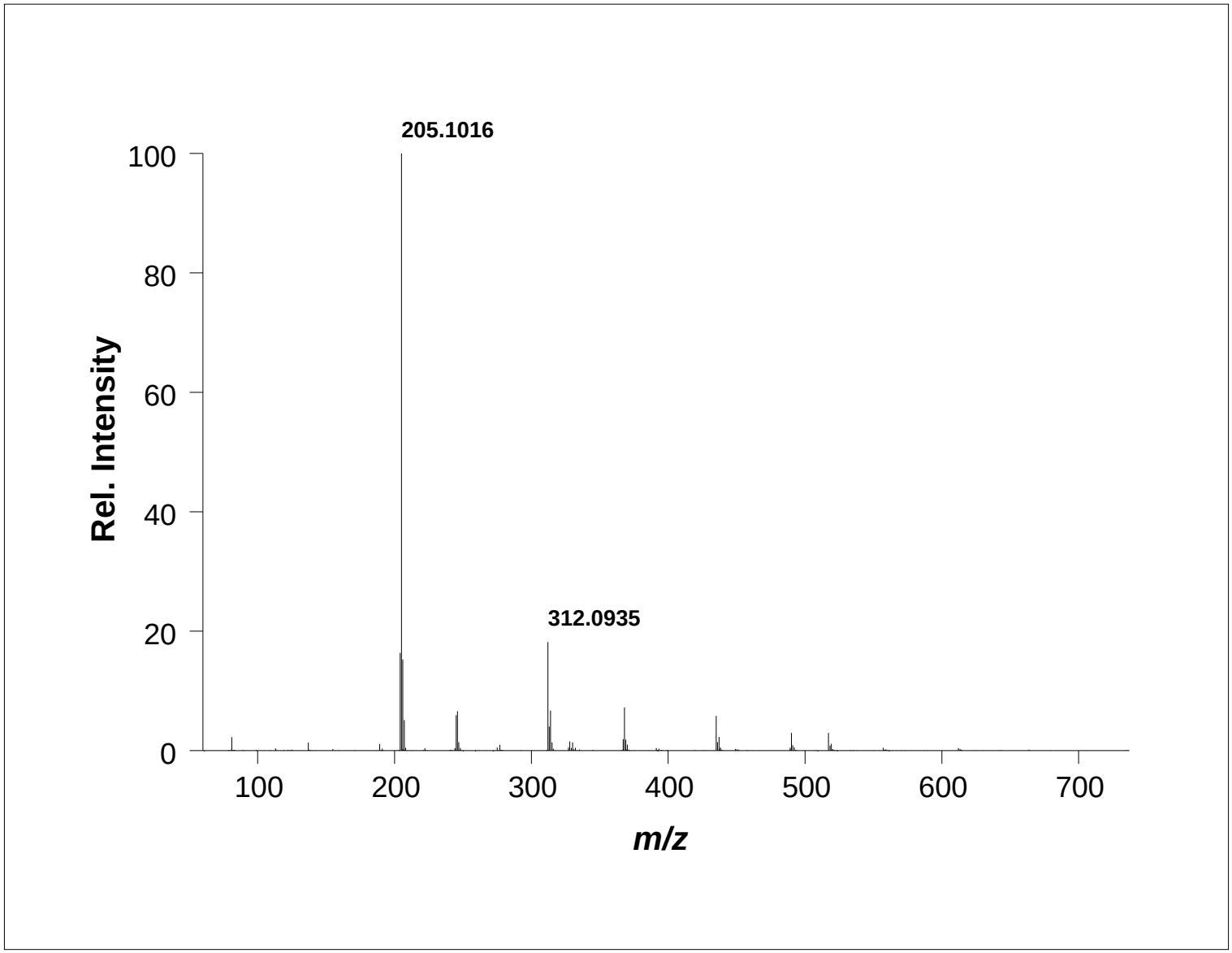
HRMS of **Compound 10** [(±)-*trans*-2-(pyridine-2-ylthio)cyclohexanol]



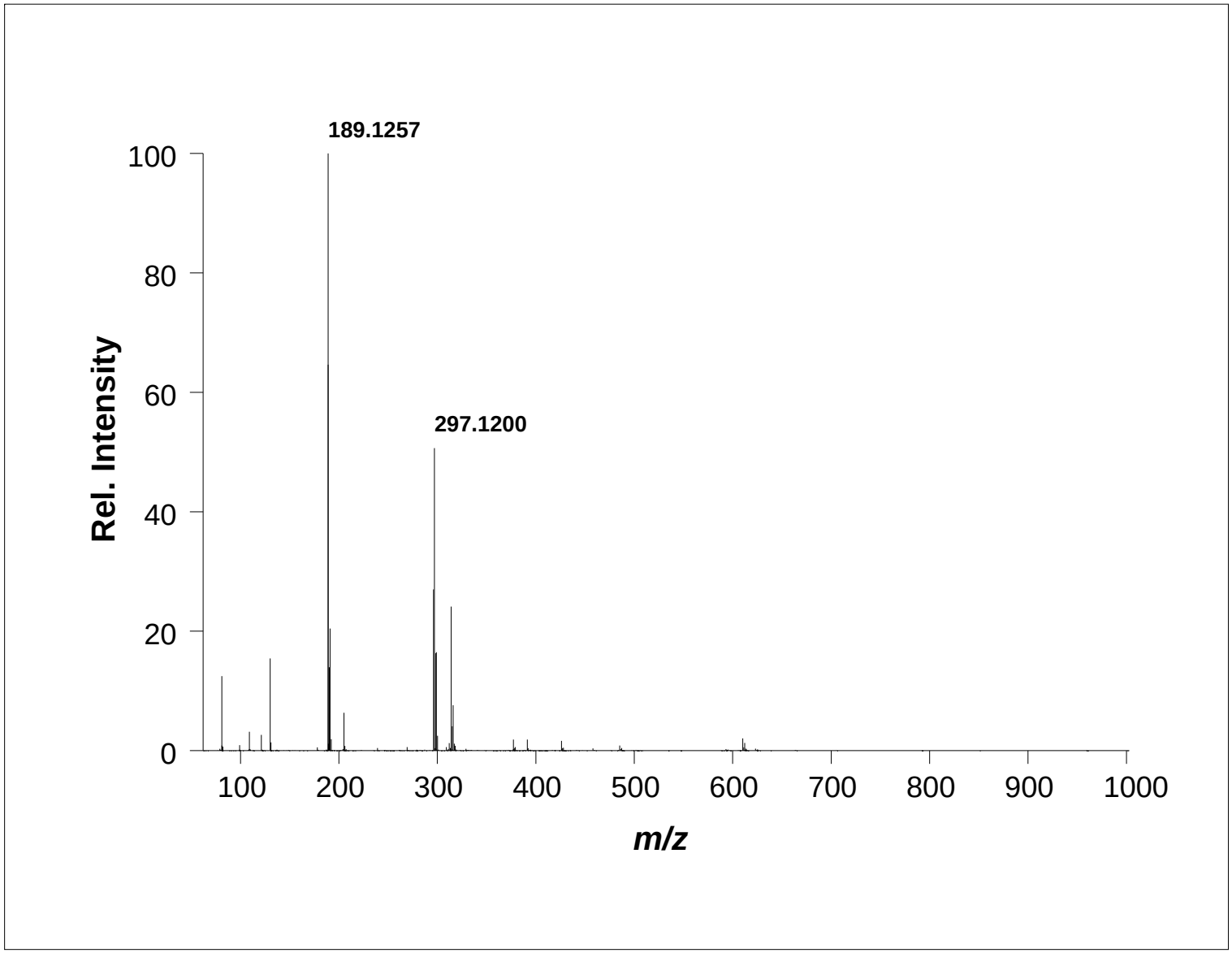
HRMS of **Compound 11** [(±)-*trans*-2-(*p*-tolylsulfonyl)cyclohexanol]



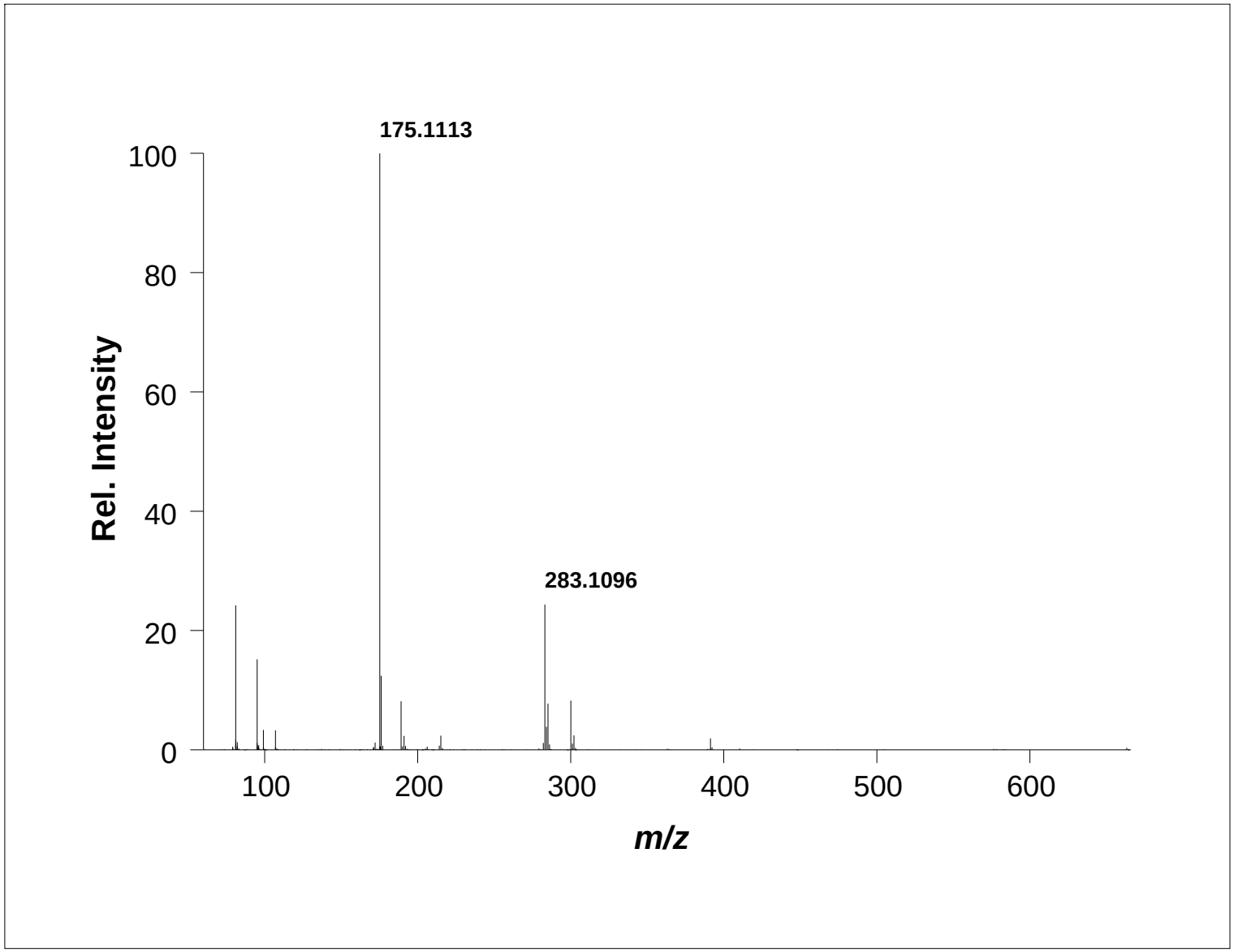
HRMS of **Compound 12** [(±)-*trans*-2-(benzyl)cyclohexanol]



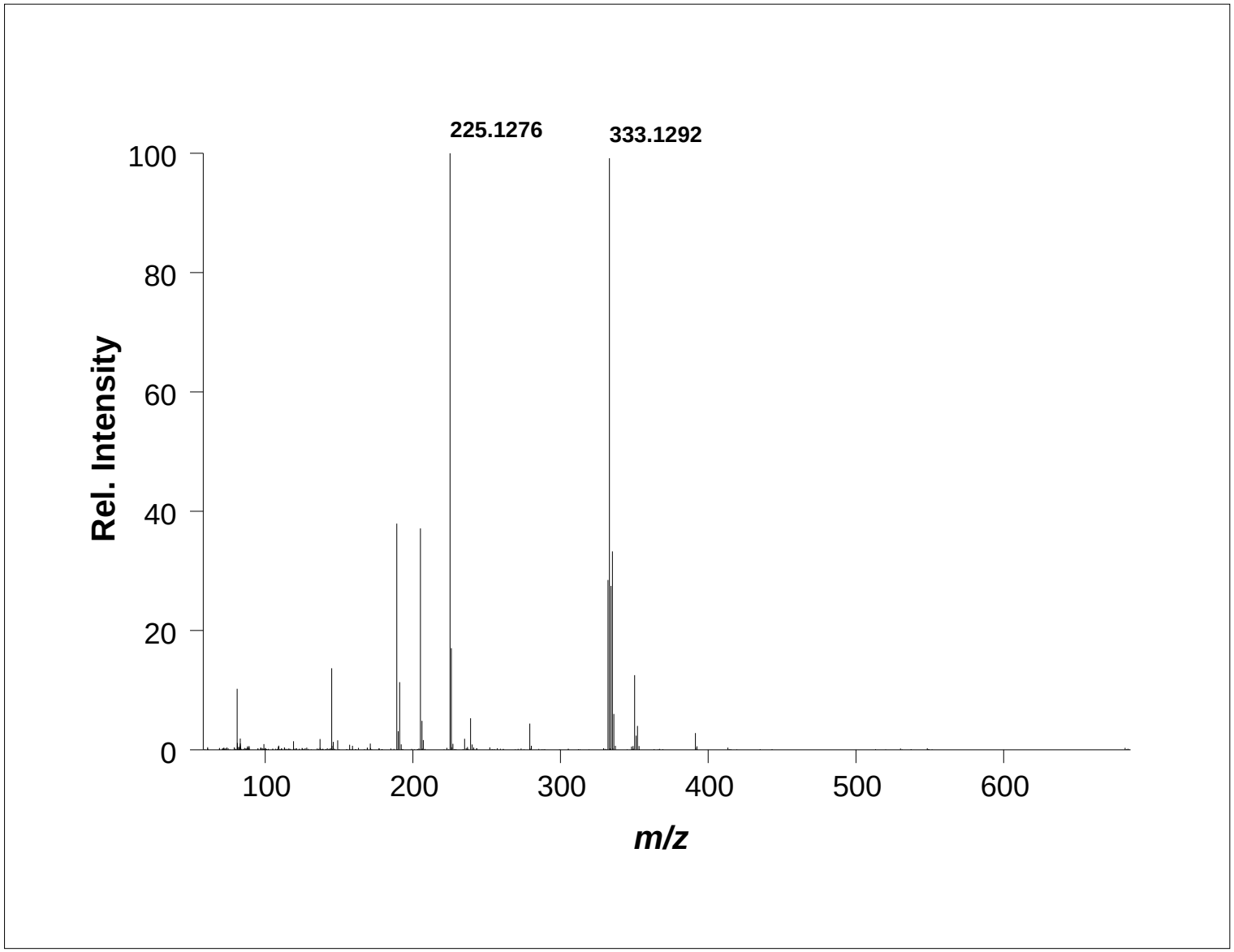
HRMS of **Compound 16a+b** [(±)-(*trans*-2-(*p*-tolylsulfanyl)cyclohexyl) 2-chloropropanoate]



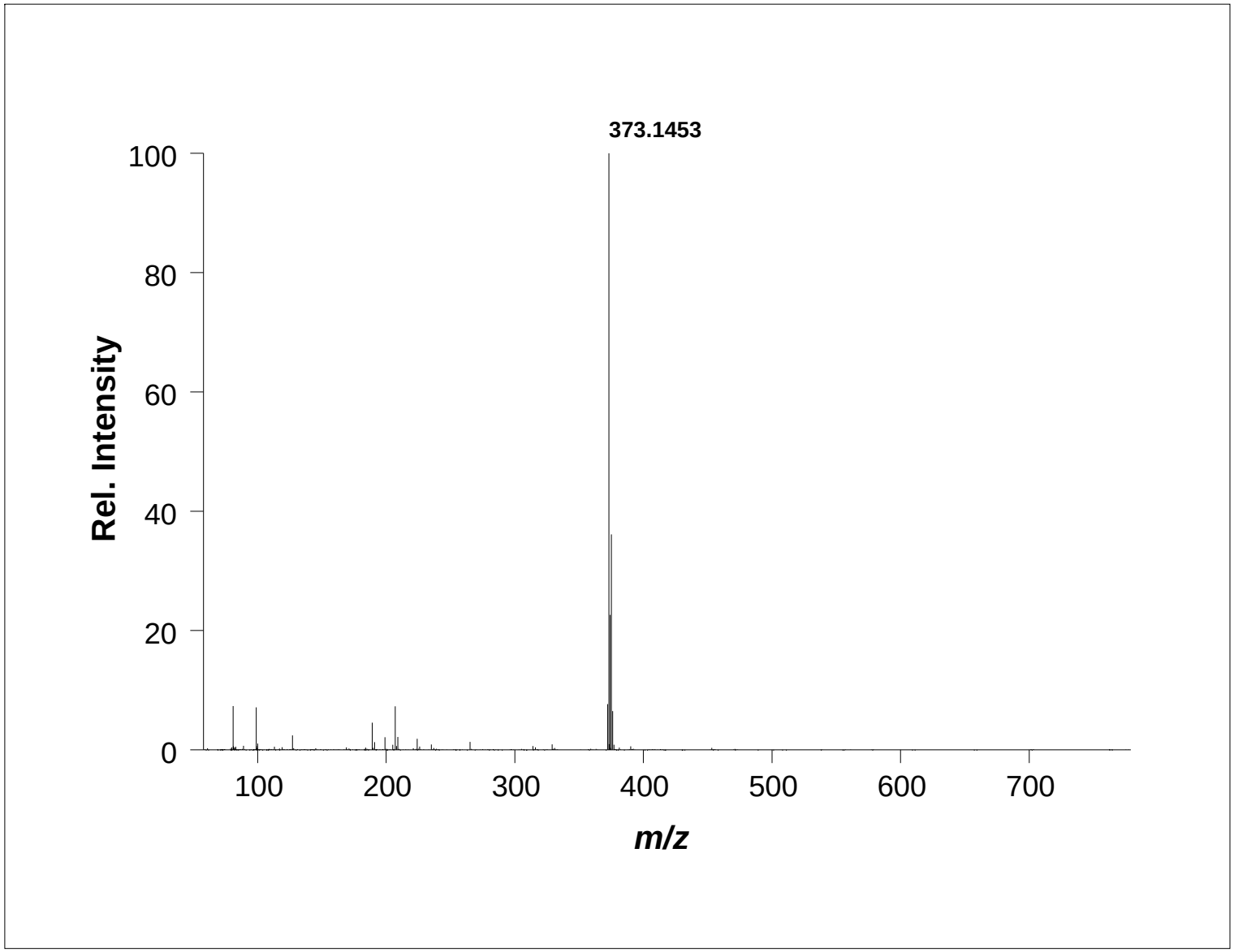
HRMS of **Compound 17a+b** [(±)-(*trans*-2-(*p*-tolyloxy)cyclohexyl) 2-chloropropanoate]



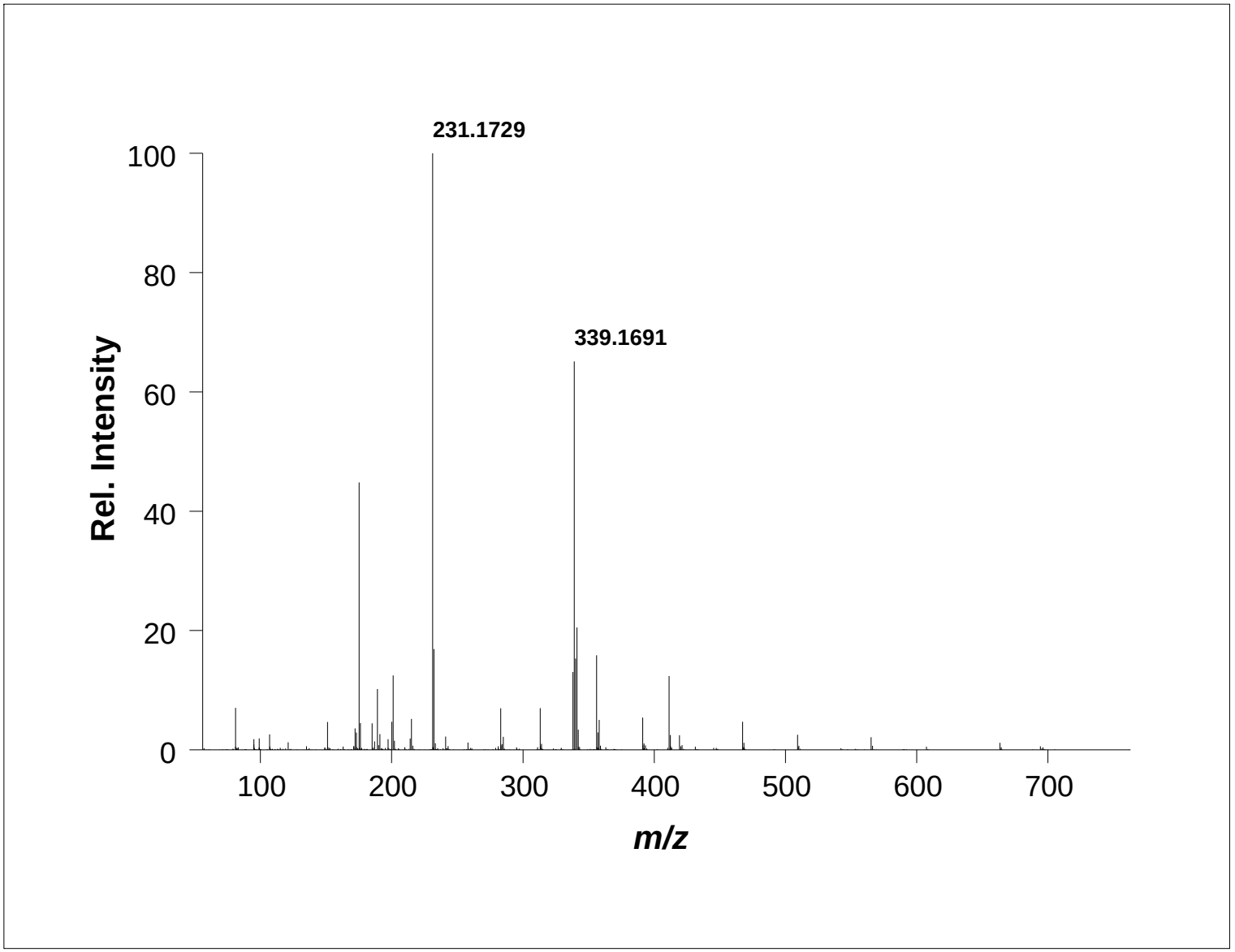
HRMS NMR of **Compound 18a+b** [(±)-(*trans*-2-(phenyloxy)cyclohexyl 2-chloropropanoate]



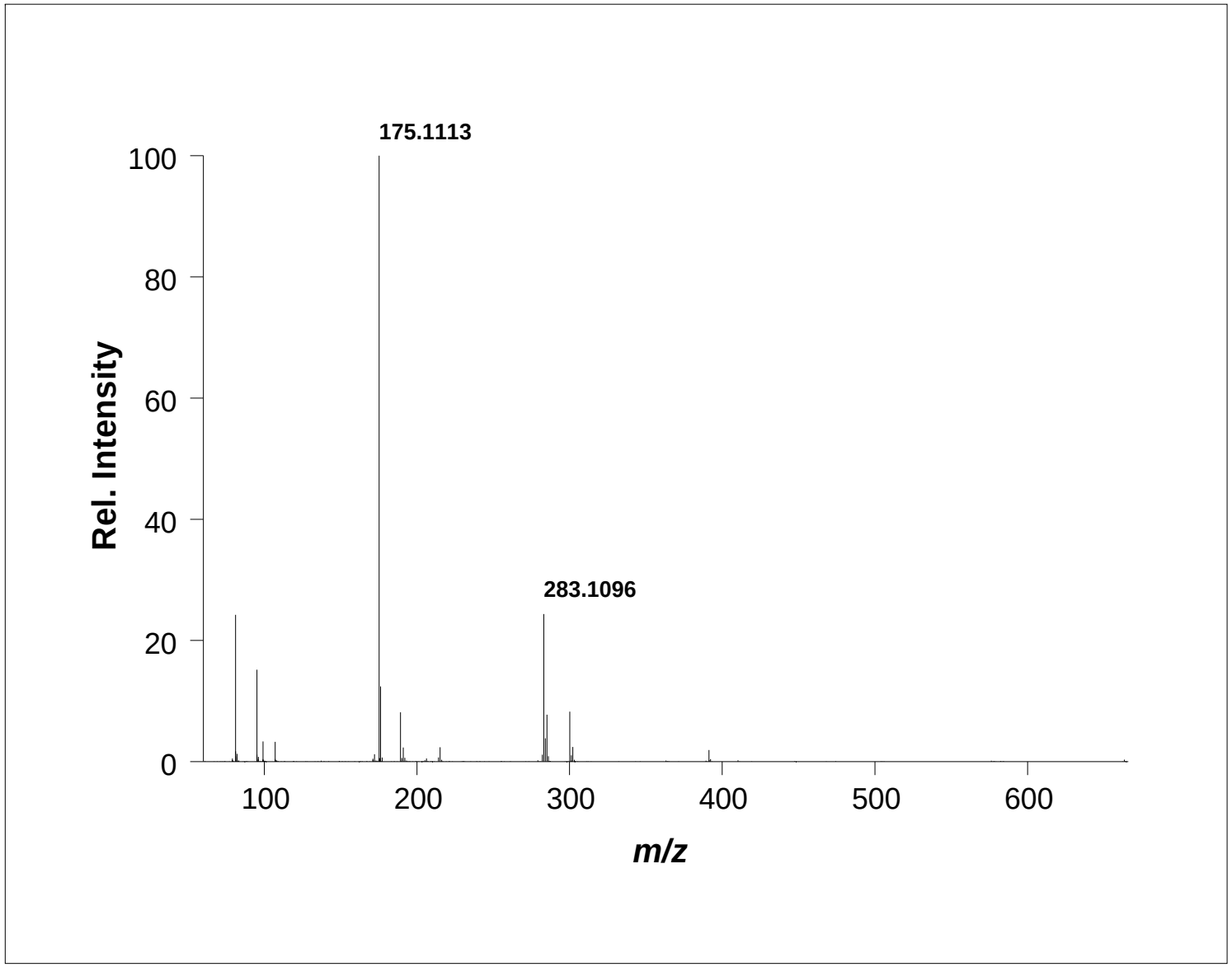
HRMS of **Compound 19a+b** [(±)-(*trans*-2-(napthalen-2-yloxy)cyclohexyl) 2-chloropropanoate]



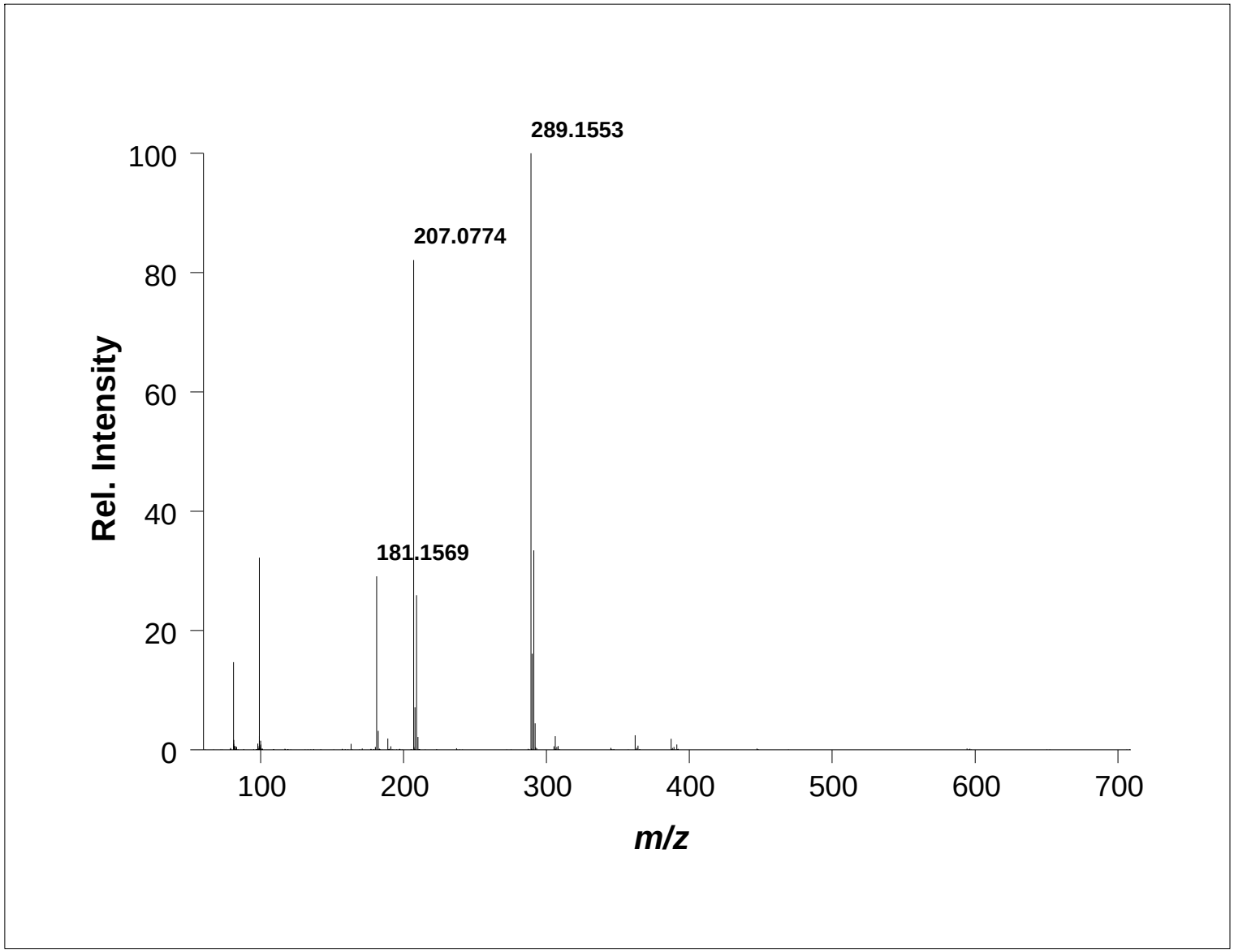
HRMS of **Compound 20a+b** [(±)-(*trans*-2-(3,4,5-trimethoxyphenyloxy)cyclohexanol]



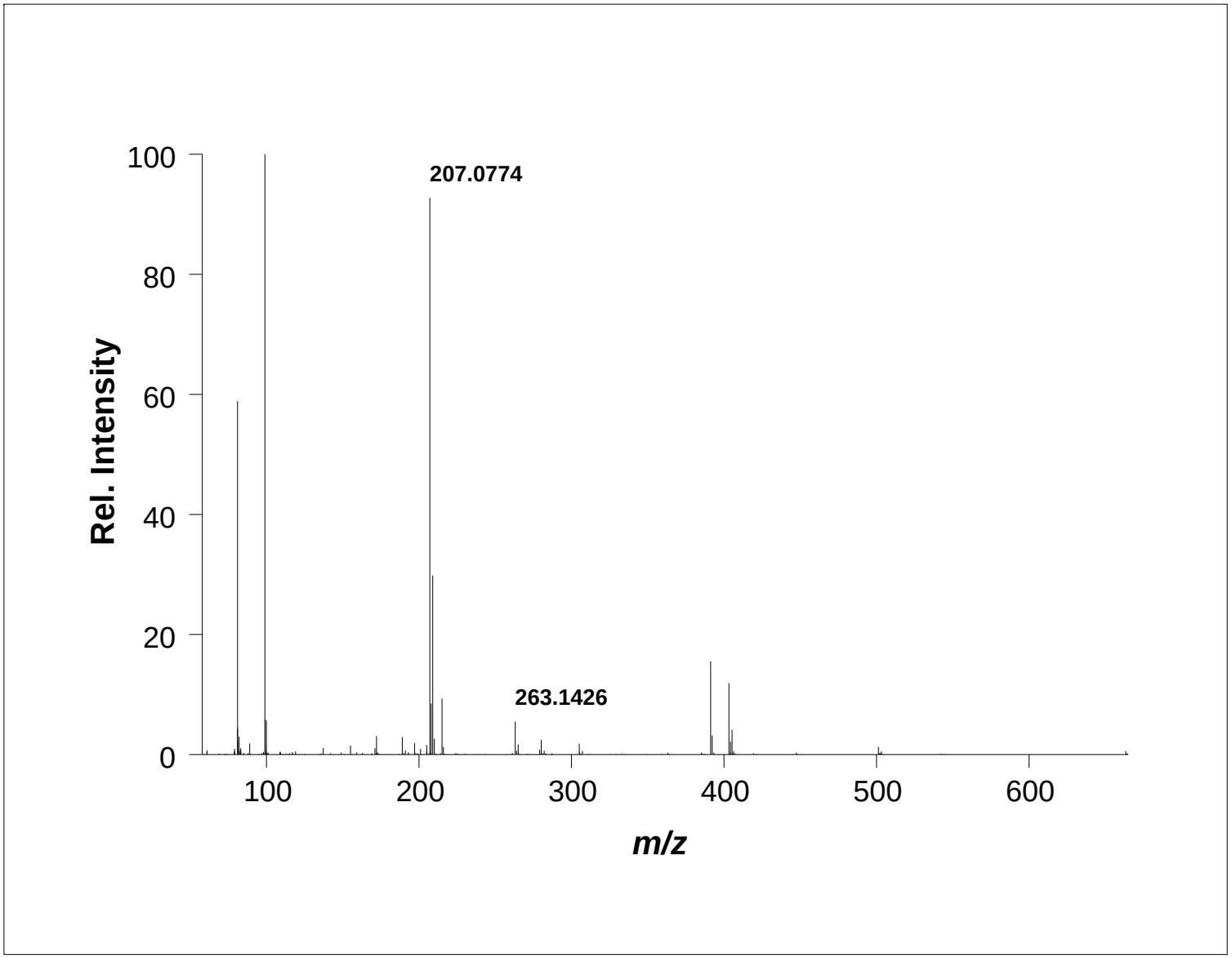
HRMS of **Compound 21a+b** [(±)-(*trans*-2-(*p*-*tert*-butyl-phenyloxy)cyclohexyl 2-chloropropanoate]



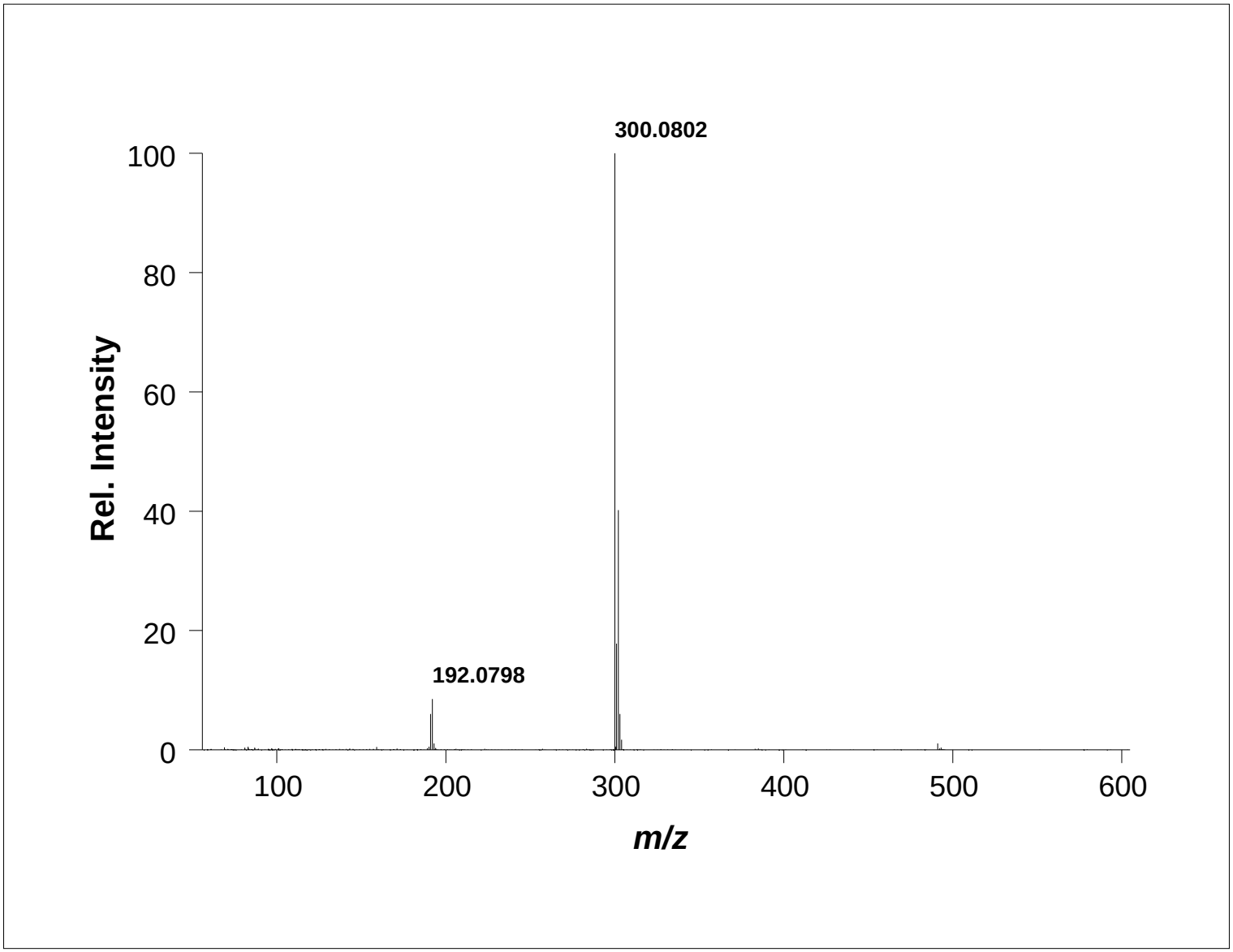
HRMS of **Compound 22a+b** [(±)-(*trans*-2-(2,6-dimethylphenyloxy)cyclohexyl 2-chloropropanoate]



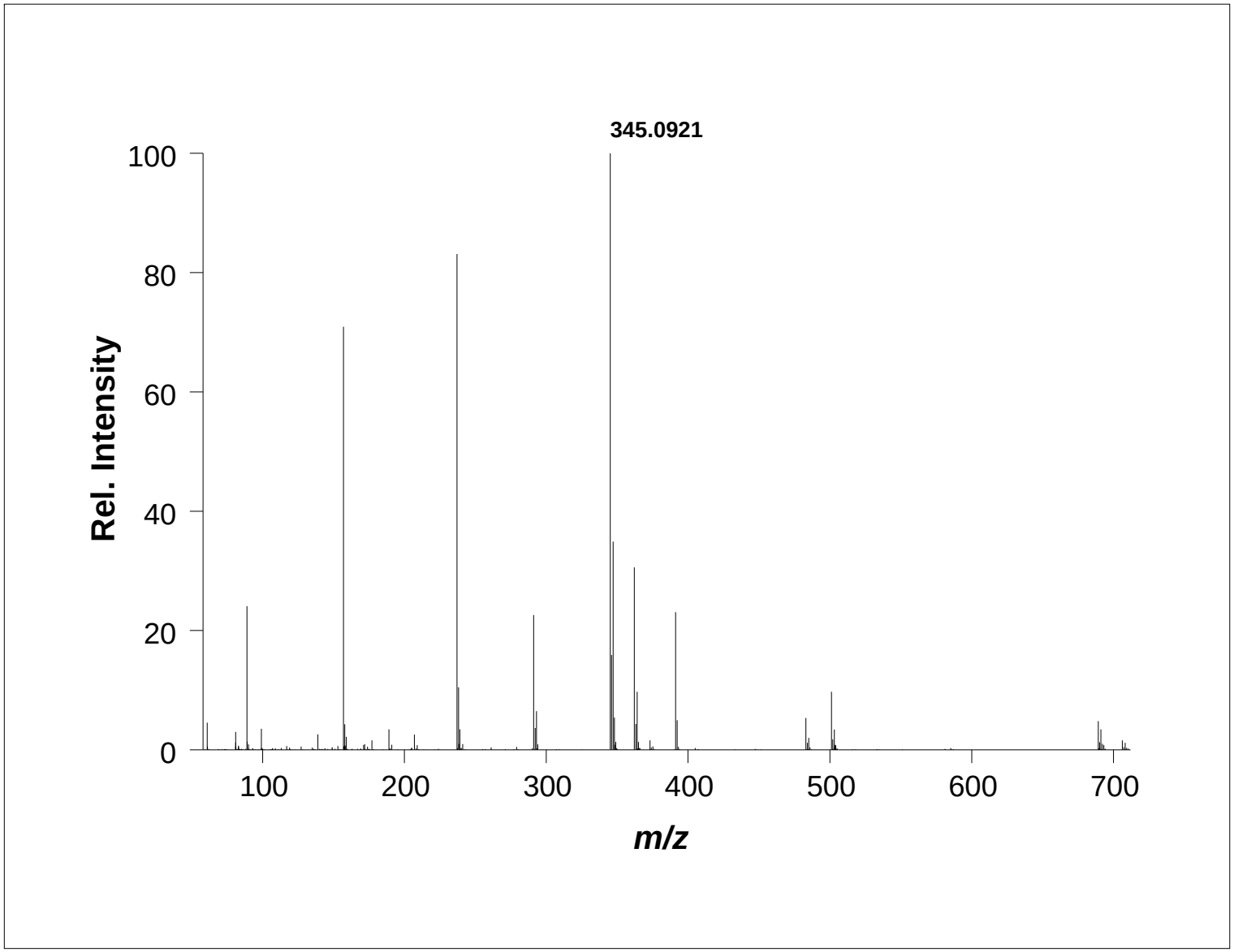
HRMS of **Compound 23a+b** [(±)-(*trans*-2-(cyclohexyloxy)cyclohexyl 2-chloropropanoate]



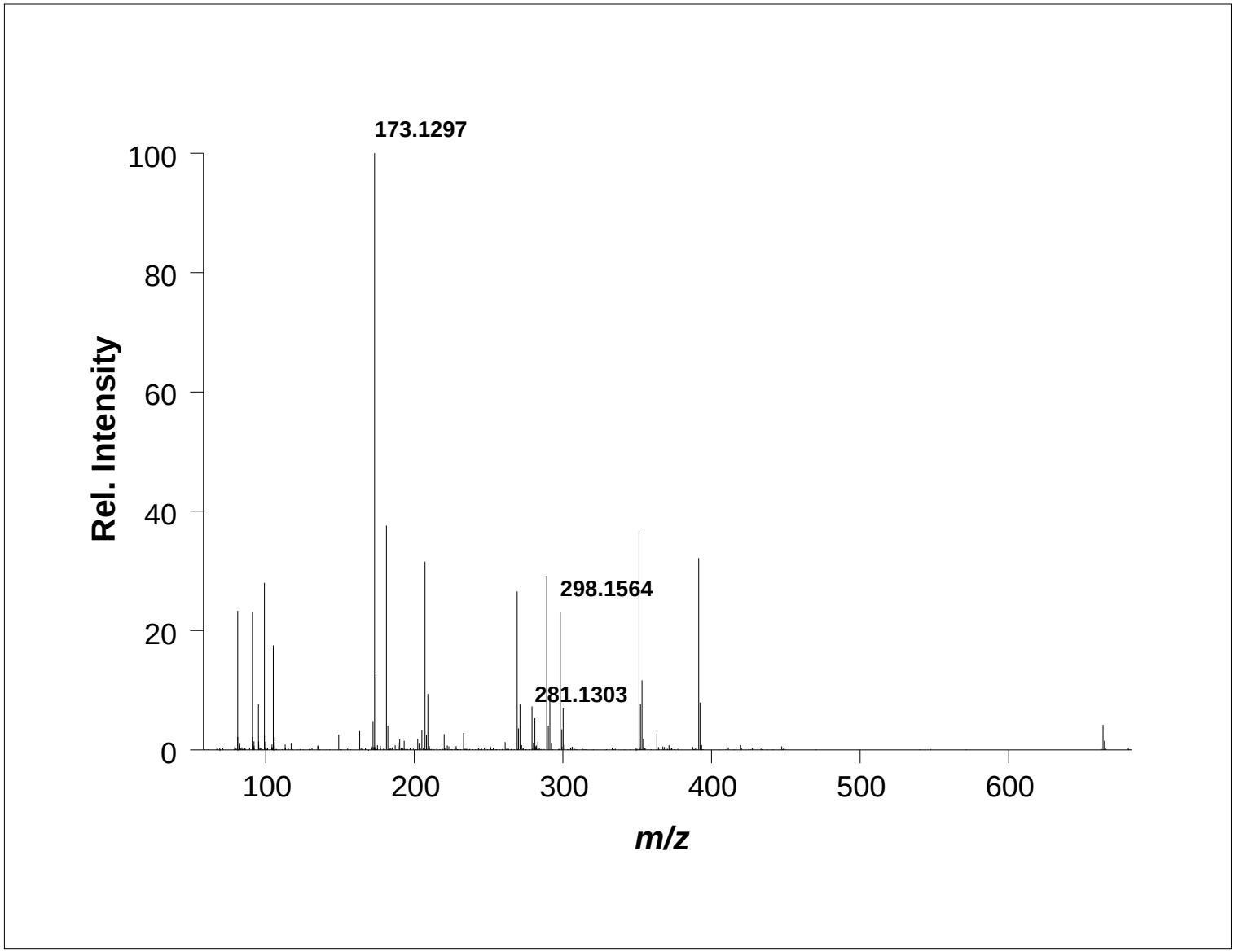
HRMS of **Compound 24a+b** [(±)-(*trans*-2-(*tert*-butoxy)cyclohexyl 2-chloropropanoate]



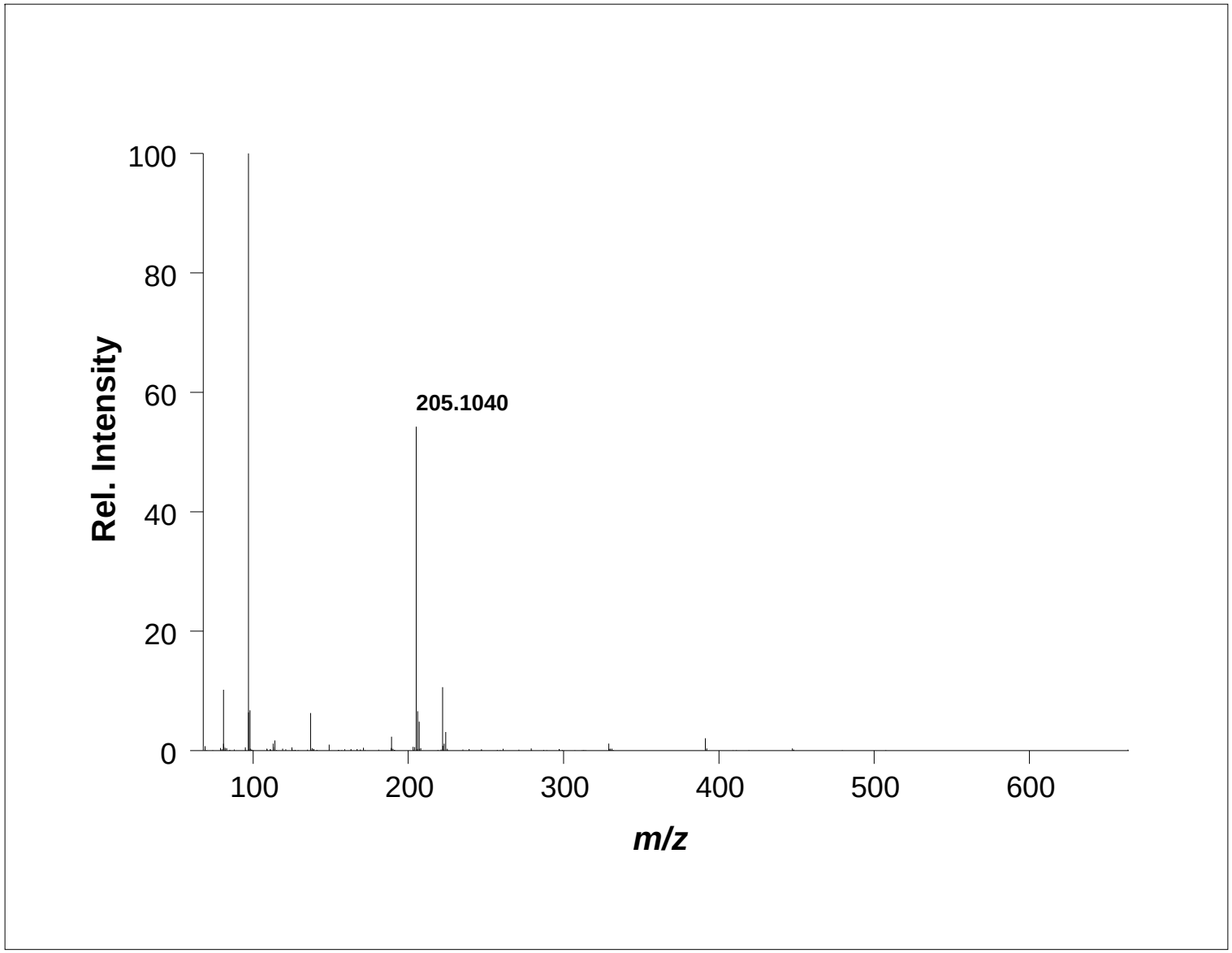
HRMS of **Compound 25a+b** [(±)-*trans*-2-(pyridin-2-ylthio)cyclohexyl 2-chloropropanoate]



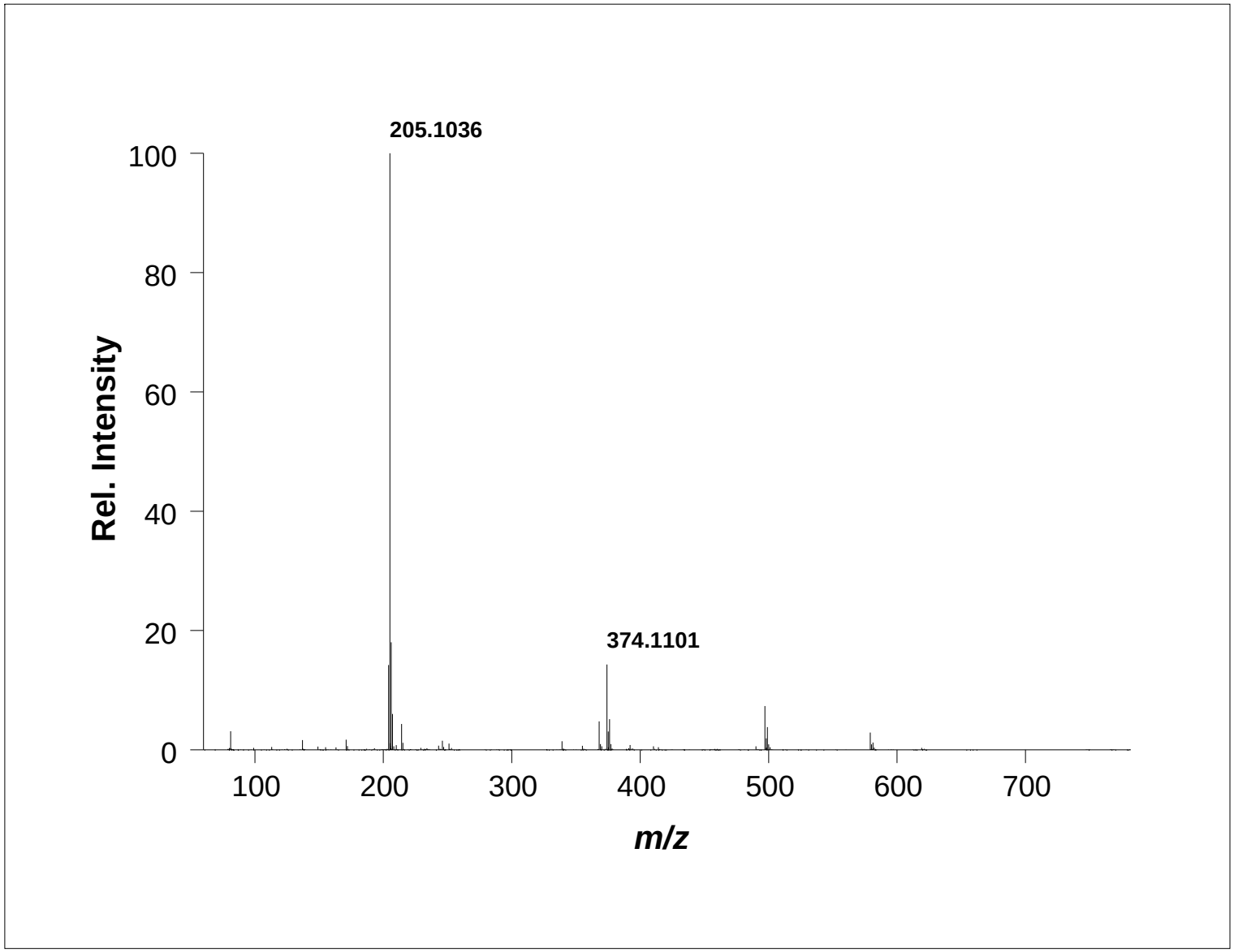
HRMS of **Compound 26a+b** [(±)-(*trans*-2-(*p*-tolylsulfonyl)cyclohexyl 2-chloropropanoate]



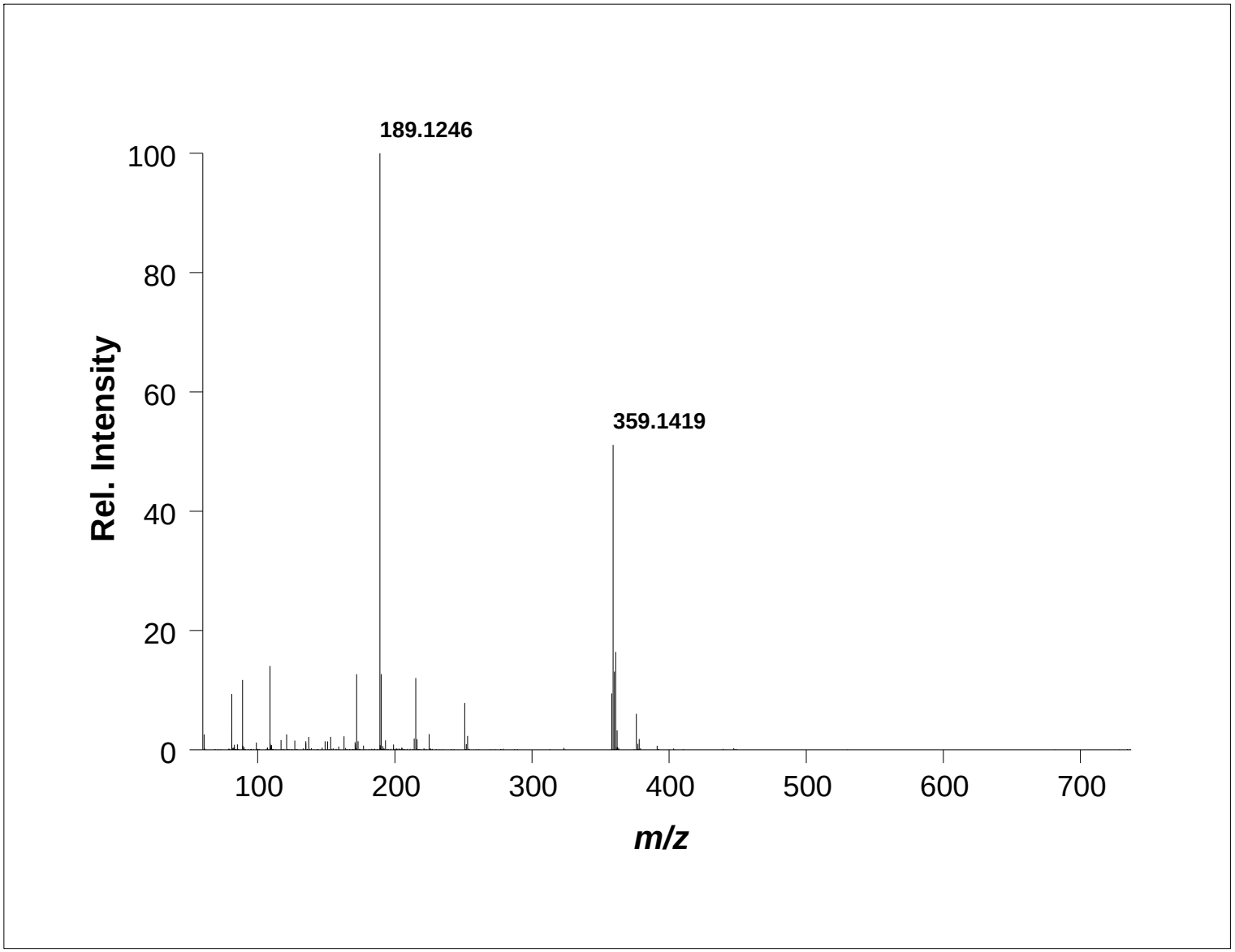
HRMS of **Compound 27a+b** [(±)-(*trans*-2-benzylcyclohexyl) 2-chloropropanoate]



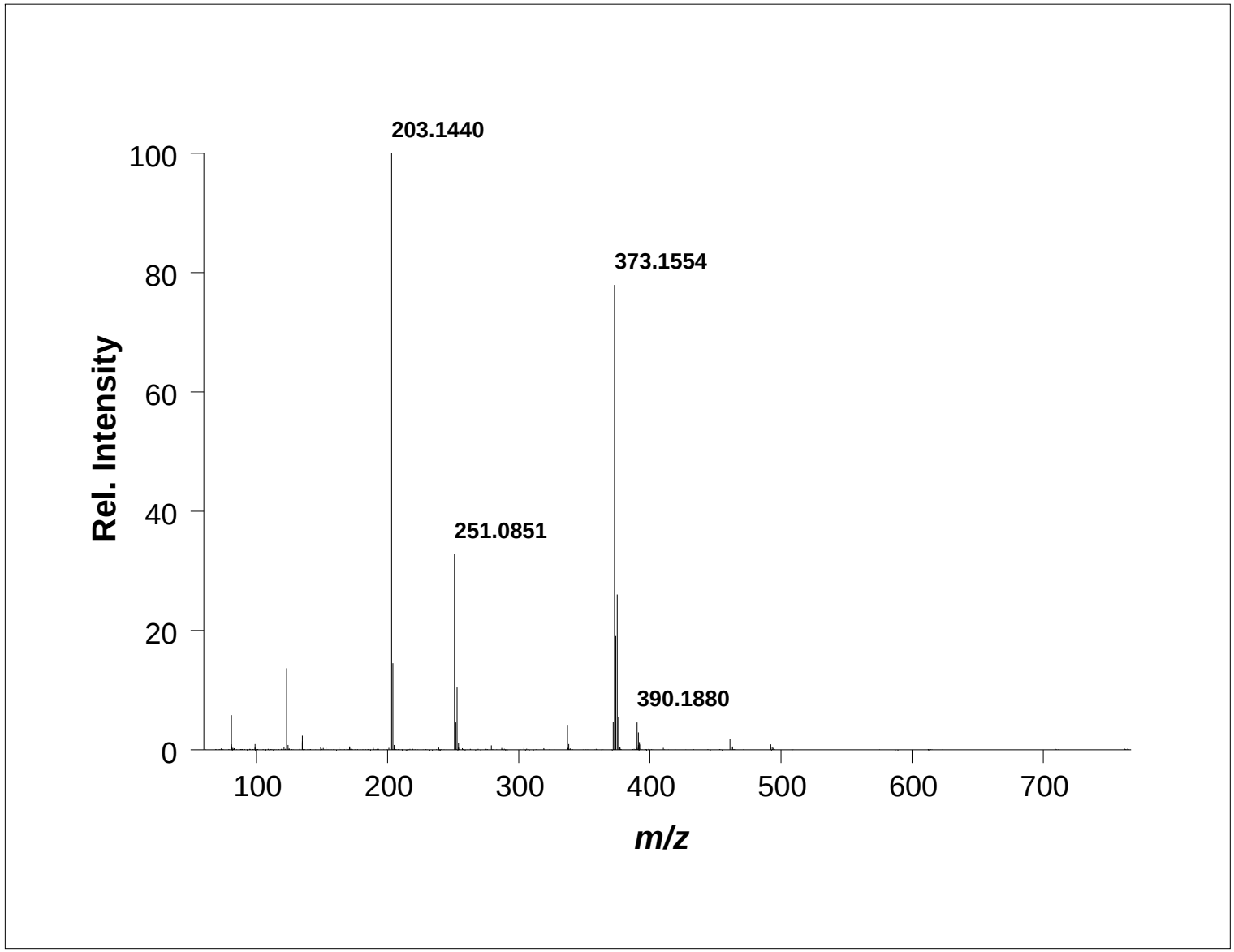
HRMS of **Compound 28a+b** [(±)-(*trans*-2-methylcyclohexyl) 2-chloropropanoate]



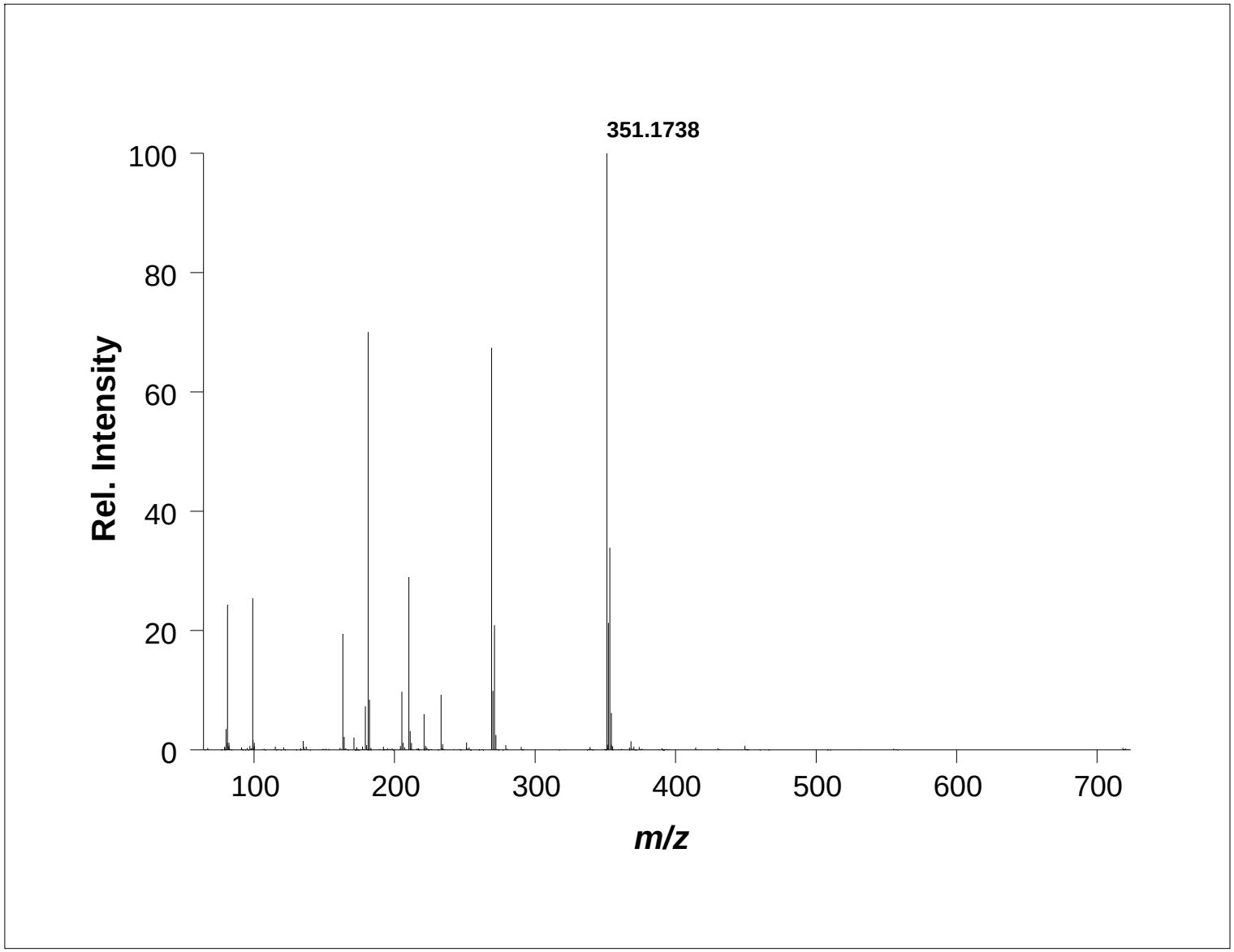
HRMS of **Compound 29a+b** [(±)-(*trans*-2-(*p*-tolylsulfanyl)cyclohexyl 2-chloro-2-phenylethanoate]



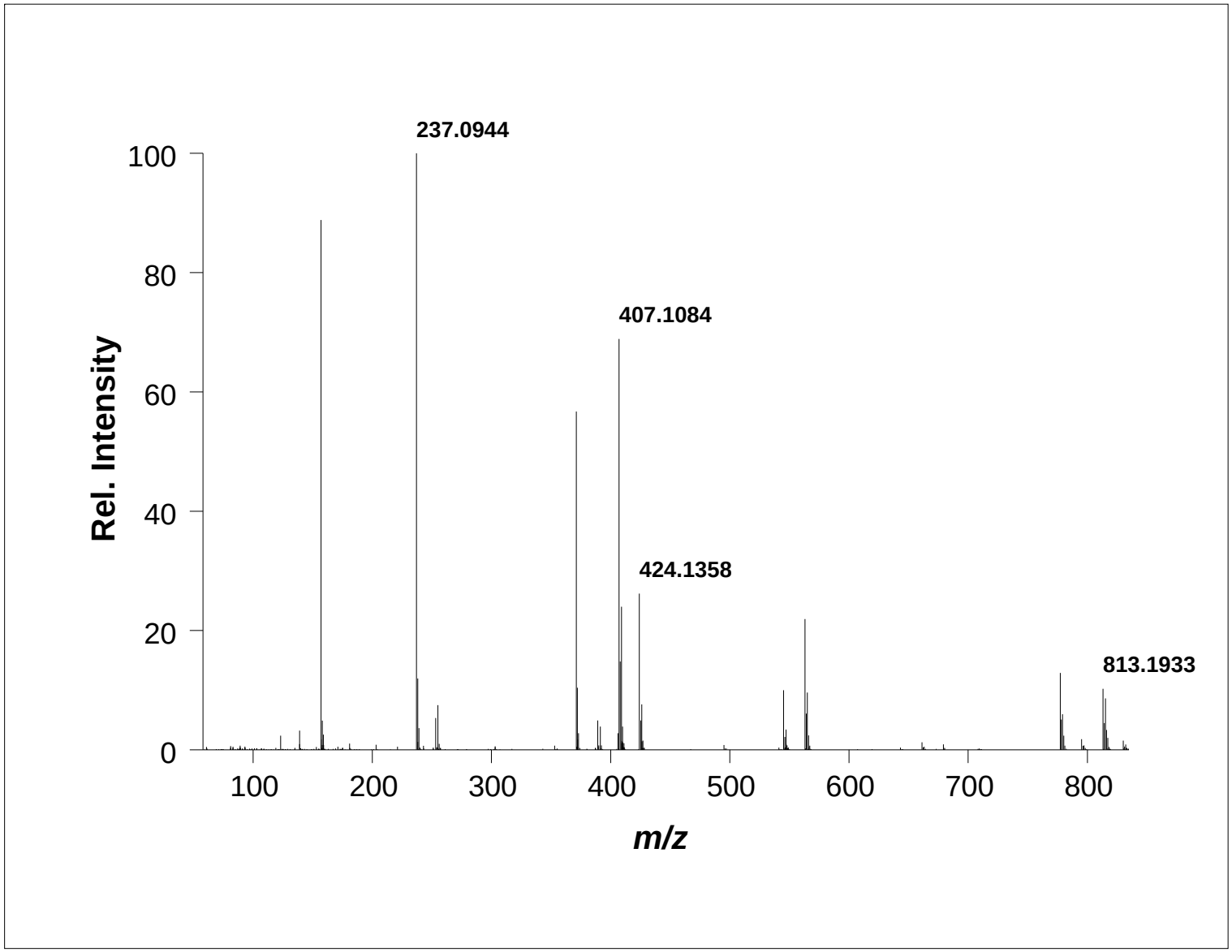
HRMS of **Compound 30a+b** [(±)-(*trans*-2-(*p*-tolyloxy)cyclohexyl 2-chloro-2-phenylethanoate]



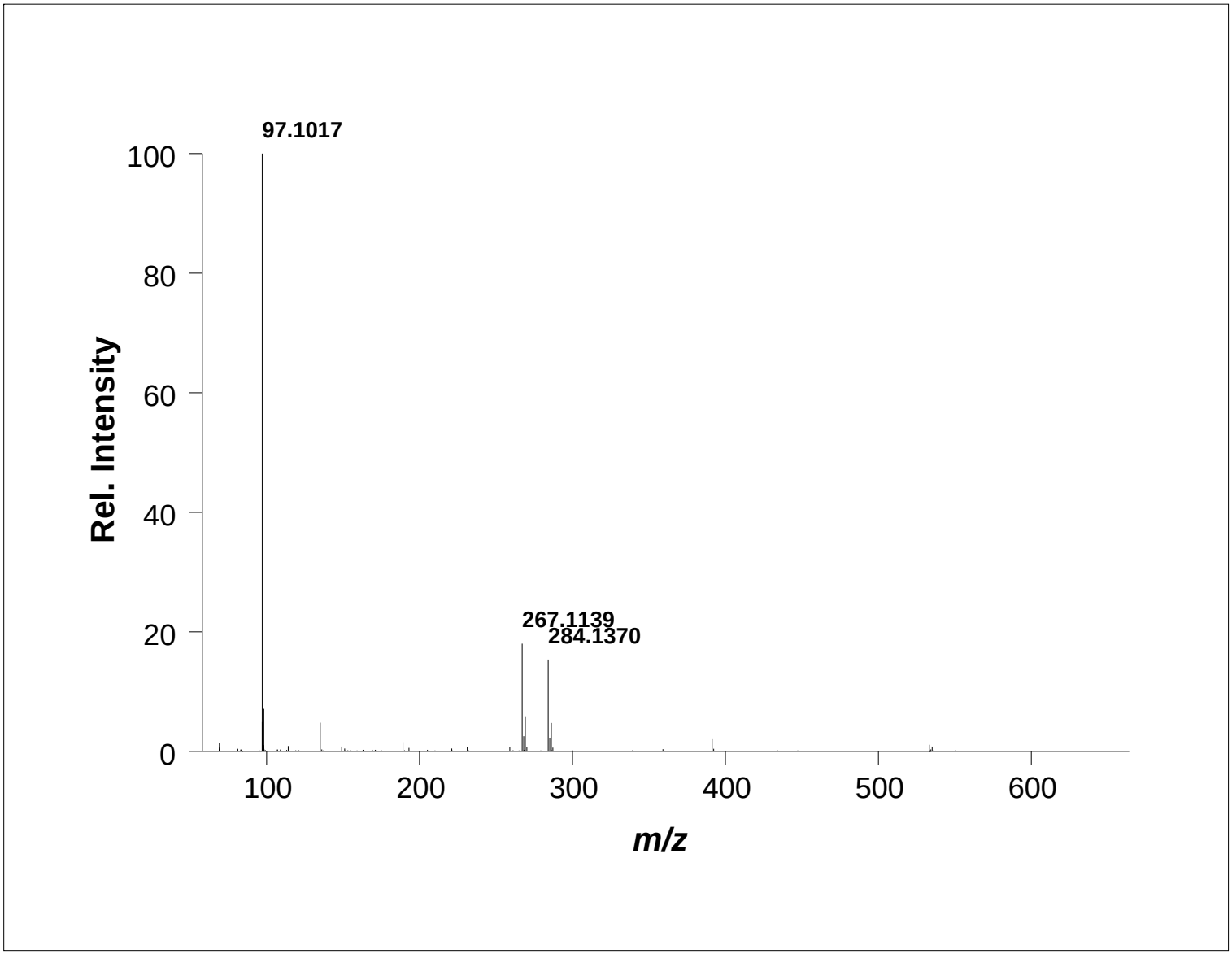
HRMS of **Compound 31a+b** [(±)-(*trans*-2-(2,6-dimethylphenyloxy)cyclohexyl 2-chloro-2-phenylethanoate]



HRMS of **Compound 32a+b** [(±)-(*trans*-2-(cyclohexyloxy)cyclohexyl 2-chloro-2-phenylethanoate]



HRMS of **Compound 33a+b** [(±)-(*trans*-2-(*p*-tolylsulfonyl)cyclohexyl 2-chloro-2-phenylethanoate]



HRMS of **Compound 34a+b** [(±)-*trans*-2-(methyl)cyclohexyl 2-chloro-2-phenylethanoate]

Summary of Molecular Modeling results – computed energies:

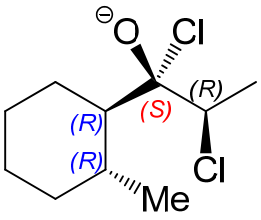
Absolute energies of transition states:

R = ΔE_{B3LYP}/kcal/mol	**Methyl**		**Tolyloxy**		**Tolylsulfanyl**	
without pyridine	*R*,*R*,*R*,*R*	*R*,*R*,*R*,*S*	*R*,*R*,*R*,*R*	*R*,*R*,*R*,*S*	*R*,*R*,*R*,*R*	*R*,*R*,*R*,*S*
(e,e)	-917238.2163	-917240.2189	-1109293.7038	-1109298.5906	-1311939.2743	-1311942.9114
(a,a)	-917236.5461	-917238.2685	-1109306.7131	-1109309.1628	-1311953.5759	-1311955.942
	R,*R*,*S*,*R*	*R*,*R*,*S*,*S*	*R*,*R*,*S*,*R*	*R*,*R*,*S*,*S*	*R*,*R*,*S*,*R*	*R*,*R*,*S*,*S*
(e,e)	-917240.6841	-917239.3685	-1109298.7502	-1109297.7596	-1311948.2415	-1311947.7902
(a,a)	-917239.2913	-917237.5212	-1109304.6038	-1109302.6917	-1311953.8853	-1311952.2611
with pyridine	*R*,*R*,*R*,*R*	*R*,*R*,*R*,*S*	*R*,*R*,*R*,*R*	*R*,*R*,*R*,*S*	*R*,*R*,*R*,*R*	*R*,*R*,*R*,*S*
(e,e)	-784131.576	-784127.7715	-976177.6536	-976175.2147	-1178830.9975	-1178827.5322
(a,a)	-784133.0195	-784129.2173	-976184.6173	-976182.1331	-1178847.5079	-1178843.6702
	R,*R*,*S*,*R*	*R*,*R*,*S*,*S*	*R*,*R*,*S*,*R*	*R*,*R*,*S*,*S*	*R*,*R*,*S*,*R*	*R*,*R*,*S*,*S*
(e,e)	-784127.1259	-784131.24	-976190.7173	-976193.8837	-1178845.9168	-1178850.8146
(a,a)	-784128.8834	-784132.1068	-976190.6056	-976188.696	-1178843.0616	-1178846.8201

Relative energies (lowest respective diastereomeric transition state in bold) **of transition states:**

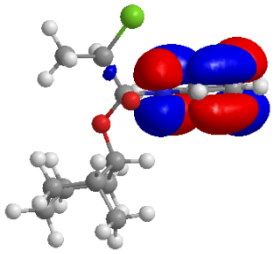
R = ΔE_{B3LYP}/kcal	**Methyl**		**Tolyloxy**		**Tolylsulfanyl**	
without pyridine	*R*,*R*,*R*,*R*	*R*,*R*,*R*,*S*	*R*,*R*,*R*,*R*	*R*,*R*,*R*,*S*	*R*,*R*,*R*,*R*	*R*,*R*,*R*,*S*
(e,e)	2.47	**0.47**	15.46	10.57	16.67	13.03
(a,a)	4.14	2.42	**2.45**	**0.00**	2.37	**0.00**
	R,*R*,*S*,*R*	*R*,*R*,*S*,*S*	*R*,*R*,*S*,*R*	*R*,*R*,*S*,*S*	*R*,*R*,*S*,*R*	*R*,*R*,*S*,*S*
(e,e)	**0.00**	1.32	10.41	11.40	7.70	8.15
(a,a)	1.39	3.16	4.56	6.47	**2.06**	3.68
with pyridine	*R*,*R*,*R*,*R*	*R*,*R*,*R*,*S*	*R*,*R*,*R*,*R*	*R*,*R*,*R*,*S*	*R*,*R*,*R*,*R*	*R*,*R*,*R*,*S*
(e,e)	1.44	5.25	16.23	18.67	19.82	23.28
(a,a)	**0.00**	3.80	9.27	11.75	**3.31**	7.14
	R,*R*,*S*,*R*	*R*,*R*,*S*,*S*	*R*,*R*,*S*,*R*	*R*,*R*,*S*,*S*	*R*,*R*,*S*,*R*	*R*,*R*,*S*,*S*
(e,e)	5.89	1.78	**3.17**	**0.00**	4.90	**0.00**
(a,a)	4.14	**0.91**	3.28	5.19	7.75	3.99

Nomenclature examples:



2-Methyl (*R*,*R*,*S*,*R*)

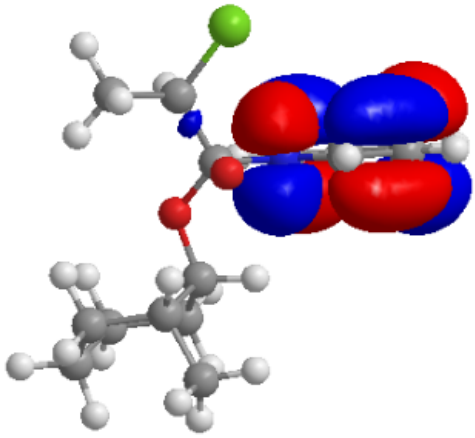
(1*S*,2*R*)-1,2-dichloro-1-((1*R*,2*R*)-2-methylcyclohexyl)propan-1-olate



2-Methyl (*R*,*R*,***R***,*R*)-(a,a)

LUMO representation and Cartesian coordinates of pyridinium transition state structures (catalyzed reaction)**:**

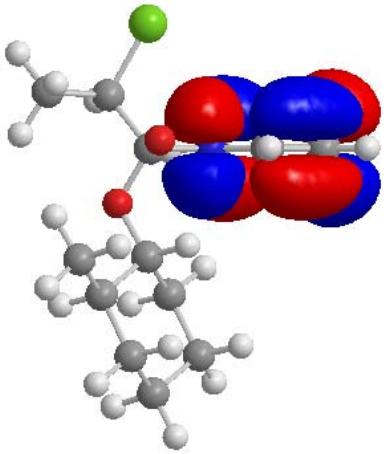
2-Methyl (*R*,*R*,*R*,*R*)-(a,a)



C(1)	-7.2879	-5.6833	-7.6697
C(2)	-8.1287	-5.3072	-8.7186
C(3)	-8.5039	-3.9676	-8.8318
C(4)	-8.0287	-3.0448	-7.8971
N(5)	-7.1936	-3.3733	-6.8436
C(6)	-6.8498	-4.7114	-6.7676
C(7)	-6.695	-2.3503	-5.8188
O(8)	-7.036	-1.0381	-6.1974
O(9)	-5.3026	-2.4698	-5.6295
C(10)	-7.3602	-2.6053	-4.4633
C(11)	-4.5188	-2.143	-6.7488
C(12)	-6.9559	-1.5986	-3.3833
Cl(13)	-9.1393	-2.6552	-4.6156
H(14)	-6.9774	-6.7339	-7.5541
H(15)	-8.4923	-6.0542	-9.4418
H(16)	-9.1703	-3.6437	-9.6474
H(17)	-8.3416	-1.9942	-7.9997
H(18)	-6.1898	-5.0191	-5.941
H(19)	-7.0813	-3.6214	-4.1067
C(20)	-3.3705	-3.1566	-6.836
H(21)	-5.131	-2.2344	-7.6761
C(22)	-3.9789	-0.7076	-6.62
H(23)	-7.4271	-1.8418	-2.4031
H(24)	-5.8551	-1.5974	-3.2161
H(25)	-7.2552	-0.5599	-3.6503
C(26)	-2.9805	-0.587	-5.4531
H(27)	-4.8332	-0.021	-6.3918
C(28)	-3.3849	-0.1912	-7.943
C(29)	-2.4075	-3.0381	-5.6463
H(30)	-2.8031	-3.0115	-7.7846
H(31)	-3.7826	-4.1931	-6.8815
H(32)	-3.5223	-0.7382	-4.4886
H(33)	-2.5575	0.4447	-5.4162
C(34)	-1.8447	-1.6151	-5.5394
H(35)	-1.571	-3.7688	-5.7588
H(36)	-3.0601	0.8703	-7.8488
H(37)	-2.9419	-3.2994	-4.7022
H(38)	-1.2003	-1.3989	-6.4231
H(39)	-4.1376	-0.2334	-8.7631
H(40)	-1.1899	-1.5333	-4.6388

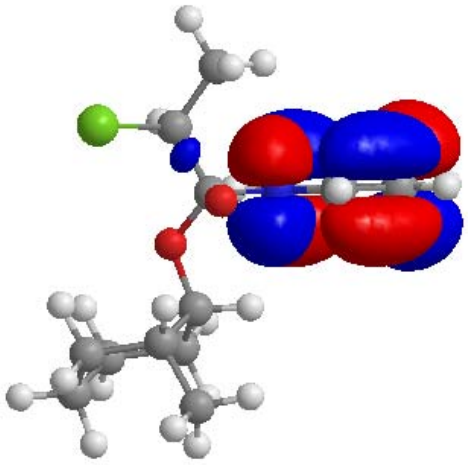
H(41) -2.5006 -0.7773 -8.2735

2-Methyl (*R*,*R*,***R***,*R*)-(e,e)



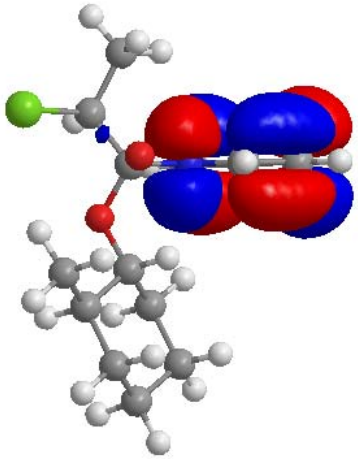
C(1)	-9.2181	-4.7466	-7.6664
C(2)	-9.2248	-4.728	-9.062
C(3)	-8.4767	-3.7531	-9.7233
C(4)	-7.7504	-2.8244	-8.974
N(5)	-7.7184	-2.8017	-7.5905
C(6)	-8.4674	-3.7915	-6.9778
C(7)	-6.9074	-1.7801	-6.7891
O(8)	-6.3652	-0.7842	-7.6265
O(9)	-5.88	-2.4187	-6.0647
C(10)	-7.7867	-1.038	-5.777
C(11)	-4.905	-3.0544	-6.8523
C(12)	-7.0418	0.0404	-4.985
Cl(13)	-9.218	-0.3308	-6.5784
H(14)	-9.7899	-5.5112	-7.1167
H(15)	-9.8032	-5.4737	-9.6301
H(16)	-8.4577	-3.7197	-10.8245
H(17)	-7.1625	-2.068	-9.5166
H(18)	-8.4517	-3.8346	-5.8777
H(19)	-8.2026	-1.7586	-5.0401
C(20)	-5.051	-4.5747	-6.7191
H(21)	-5.0139	-2.7758	-7.9251
C(22)	-3.5097	-2.6097	-6.3802
H(23)	-7.7065	0.5272	-4.2346
H(24)	-6.185	-0.3887	-4.4179
H(25)	-6.6396	0.8421	-5.6447
C(26)	-2.4077	-3.3638	-7.1476
H(27)	-3.4104	-2.8608	-5.294
C(28)	-3.3018	-1.092	-6.536
C(29)	-3.9566	-5.3179	-7.497
H(30)	-6.0454	-4.9058	-7.0986
H(31)	-5.0011	-4.8635	-5.6424
H(32)	-1.4027	-3.0642	-6.7653
H(33)	-2.4459	-3.0813	-8.2263
C(34)	-2.5671	-4.8838	-7.0156
H(35)	-4.0762	-6.4202	-7.3672
H(36)	-2.283	-0.7896	-6.2027
H(37)	-4.0605	-5.1017	-8.587
H(38)	-1.7775	-5.4041	-7.6088
H(39)	-4.0252	-0.5065	-5.9258
H(40)	-2.4295	-5.1835	-5.9495
H(41)	-3.4181	-0.7772	-7.5977

2-Methyl (*R*,*R*,***R***,*S*)-(a,a)



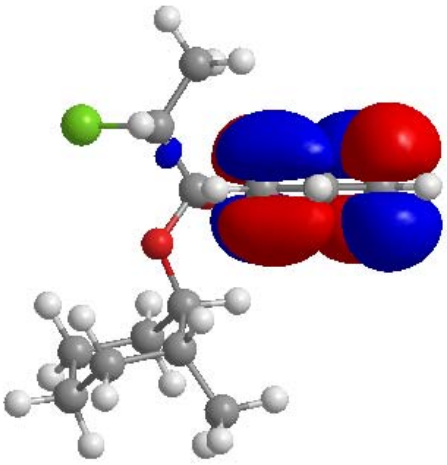
C(1)	-7.1361	-5.9605	-7.4022
C(2)	-7.8963	-5.7144	-8.5468
C(3)	-8.2364	-4.3969	-8.8573
C(4)	-7.8069	-3.3654	-8.0186
N(5)	-7.0493	-3.5635	-6.8776
C(6)	-6.7386	-4.8843	-6.6062
C(7)	-6.5885	-2.4216	-5.9666
O(8)	-6.921	-1.169	-6.5154
O(9)	-5.204	-2.5234	-5.7165
C(10)	-7.3154	-2.5279	-4.6218
C(11)	-4.3814	-2.3619	-6.844
C(12)	-8.8387	-2.5785	-4.7613
Cl(13)	-6.863	-1.1881	-3.5258
H(14)	-6.8545	-6.9906	-7.1313
H(15)	-8.2237	-6.545	-9.192
H(16)	-8.8382	-4.1742	-9.7529
H(17)	-8.0898	-2.3338	-8.2785
H(18)	-6.1385	-5.089	-5.7053
H(19)	-6.983	-3.4482	-4.0931
C(20)	-3.25	-3.394	-6.7522
H(21)	-4.9651	-2.5708	-7.7705
C(22)	-3.8227	-0.9293	-6.8983
H(23)	-9.3355	-2.6853	-3.7695
H(24)	-9.2398	-1.6588	-5.2443
H(25)	-9.1674	-3.4491	-5.3722
C(26)	-2.8556	-0.6608	-5.7298
H(27)	-4.6731	-0.2084	-6.7941
C(28)	-3.1807	-0.6096	-8.2607
C(29)	-2.3195	-3.1215	-5.562
H(30)	-2.6538	-3.3944	-7.6941
H(31)	-3.6804	-4.4202	-6.6623
H(32)	-3.4268	-0.6703	-4.7704
H(33)	-2.4167	0.3606	-5.8229
C(34)	-1.7352	-1.7054	-5.6403
H(35)	-1.4935	-3.8722	-5.5445
H(36)	-2.8252	0.4455	-8.2986
H(37)	-2.8849	-3.2387	-4.6071
H(38)	-1.0654	-1.6244	-6.5279
H(39)	-3.9138	-0.7397	-9.0894
H(40)	-1.1019	-1.5064	-4.7428
H(41)	-2.3073	-1.2587	-8.4858

2-Methyl (*R*,*R*,***R***,*S*)-(e,e)



C(1)	-9.2126	-4.7545	-7.6468
C(2)	-9.2303	-4.7368	-9.0426
C(3)	-8.4903	-3.7606	-9.7105
C(4)	-7.7603	-2.8295	-8.9669
N(5)	-7.7172	-2.8061	-7.5843
C(6)	-8.4594	-3.7973	-6.9645
C(7)	-6.908	-1.7788	-6.7887
O(8)	-6.3838	-0.7838	-7.6382
O(9)	-5.8798	-2.4184	-6.0644
C(10)	-7.8067	-1.0473	-5.7839
C(11)	-4.9095	-3.0617	-6.8524
C(12)	-9.0685	-0.4616	-6.4231
Cl(13)	-6.9204	0.2545	-4.9336
H(14)	-9.7801	-5.5191	-7.0924
H(15)	-9.8126	-5.4833	-9.6059
H(16)	-8.4808	-3.7268	-10.8118
H(17)	-7.1803	-2.0713	-9.5156
H(18)	-8.4381	-3.8342	-5.8643
H(19)	-8.1139	-1.743	-4.973
C(20)	-5.0543	-4.5802	-6.6958
H(21)	-5.0297	-2.797	-7.9275
C(22)	-3.5085	-2.6132	-6.4011
H(23)	-9.6995	0.0668	-5.6716
H(24)	-8.8229	0.2647	-7.2306
H(25)	-9.7105	-1.2535	-6.8698
C(26)	-2.4169	-3.3795	-7.1718
H(27)	-3.3968	-2.8505	-5.313
C(28)	-3.298	-1.0986	-6.5788
C(29)	-3.9702	-5.3372	-7.4743
H(30)	-6.0532	-4.9159	-7.059
H(31)	-4.9925	-4.8529	-5.6155
H(32)	-1.4066	-3.0754	-6.8075
H(33)	-2.4693	-3.1128	-8.2539
C(34)	-2.575	-4.8973	-7.0155
H(35)	-4.0899	-6.437	-7.3252
H(36)	-2.2732	-0.7952	-6.2654
H(37)	-4.0866	-5.1384	-8.5664
H(38)	-1.7928	-5.4271	-7.6101
H(39)	-4.0097	-0.5044	-5.9634
H(40)	-2.4252	-5.1812	-5.9467
H(41)	-3.4305	-0.7959	-7.6421

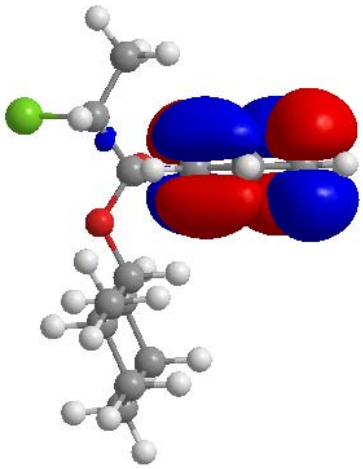
2-Methyl (*R*,*R*,***S***,*R*)-(a,a)



C(1)	-8.2112	-5.4162	-7.9623
C(2)	-7.6241	-5.3728	-9.228
C(3)	-6.7217	-4.3476	-9.5155
C(4)	-6.4311	-3.4026	-8.5295
N(5)	-6.9848	-3.4102	-7.2611
C(6)	-7.8776	-4.4393	-7.0211
C(7)	-6.6116	-2.3584	-6.212
O(8)	-7.2438	-2.6142	-4.98
O(9)	-5.2098	-2.3154	-6.0656
C(10)	-7.0837	-0.9772	-6.6765
C(11)	-4.6411	-3.4844	-5.5309
C(12)	-8.574	-0.9429	-7.0232
Cl(13)	-6.7256	0.2803	-5.4553
H(14)	-8.9271	-6.2145	-7.7094
H(15)	-7.8685	-6.1341	-9.9856
H(16)	-6.2424	-4.2874	-10.5057
H(17)	-5.7116	-2.6022	-8.7643
H(18)	-8.349	-4.4925	-6.0276
H(19)	-6.5075	-0.6665	-7.5753
C(20)	-4.2661	-3.2474	-4.0631
H(21)	-5.3696	-4.3259	-5.5919
C(22)	-3.4087	-3.8594	-6.3705
H(23)	-8.8928	0.07	-7.3612
H(24)	-8.8176	-1.6435	-7.8533
H(25)	-9.2067	-1.2238	-6.1509
C(26)	-2.2923	-2.8119	-6.2067
H(27)	-3.714	-3.8631	-7.4496
C(28)	-2.9131	-5.287	-6.0785
C(29)	-3.1557	-2.1977	-3.9124
H(30)	-3.9306	-4.2048	-3.6007
H(31)	-5.1619	-2.9255	-3.4817
H(32)	-2.6321	-1.8425	-6.6445
H(33)	-1.39	-3.1208	-6.7854
C(34)	-1.919	-2.5791	-4.7365
H(35)	-2.8759	-2.0929	-2.8367
H(36)	-2.058	-5.5561	-6.7398
H(37)	-3.5315	-1.2017	-4.2465
H(38)	-1.4534	-3.4984	-4.311
H(39)	-3.7177	-6.036	-6.2597

H(40)	-1.1524	-1.7707	-4.6639
H(41)	-2.5713	-5.4158	-5.029

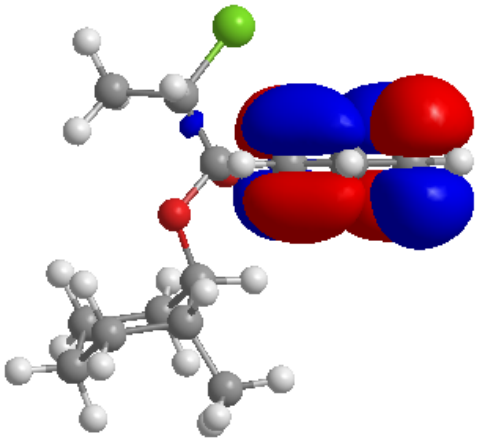
2-Methyl (*R*,*R*,***S***,*R*)-(e,e)



C(1)	-9.2423	-4.4506	-8.6347
C(2)	-8.4684	-4.9281	-9.6939
C(3)	-7.2028	-4.3781	-9.902
C(4)	-6.7509	-3.3718	-9.0464
N(5)	-7.4824	-2.8685	-7.9845
C(6)	-8.7305	-3.4415	-7.8154
C(7)	-6.9217	-1.7867	-7.0572
O(8)	-7.8714	-1.4063	-6.0917
O(9)	-5.7142	-2.2122	-6.4624
C(10)	-6.6189	-0.5193	-7.8673
C(11)	-5.7713	-3.4135	-5.7352
C(12)	-7.8224	-0.0239	-8.6735
Cl(13)	-6.0235	0.8029	-6.8188
H(14)	-10.2429	-4.8709	-8.4446
H(15)	-8.8474	-5.7274	-10.3501
H(16)	-6.5666	-4.7382	-10.7262
H(17)	-5.7458	-2.9543	-9.2125
H(18)	-9.3534	-3.0869	-6.9797
H(19)	-5.7805	-0.7113	-8.5716
C(20)	-6.2621	-3.1704	-4.3026
H(21)	-6.4441	-4.1425	-6.2399
C(22)	-4.3589	-4.0273	-5.712
H(23)	-7.5748	0.8928	-9.2568
H(24)	-8.1638	-0.7847	-9.4109
H(25)	-8.6886	0.2178	-8.0167
C(26)	-4.3294	-5.3118	-4.8629
H(27)	-3.6629	-3.2864	-5.2435
C(28)	-3.8351	-4.3362	-7.1268
C(29)	-6.2313	-4.4554	-3.4631
H(30)	-7.3088	-2.7899	-4.2941
H(31)	-5.626	-2.3933	-3.8165
H(32)	-3.2925	-5.7233	-4.8259
H(33)	-4.9739	-6.0882	-5.3389
C(34)	-4.8189	-5.0491	-3.4337
H(35)	-6.574	-4.2413	-2.4223
H(36)	-2.8267	-4.8075	-7.0884

H(37)	-6.9409	-5.2006	-3.8958
H(38)	-4.815	-5.9982	-2.8461
H(39)	-3.7322	-3.4152	-7.7431
H(40)	-4.1244	-4.341	-2.9223
H(41)	-4.515	-5.0356	-7.664

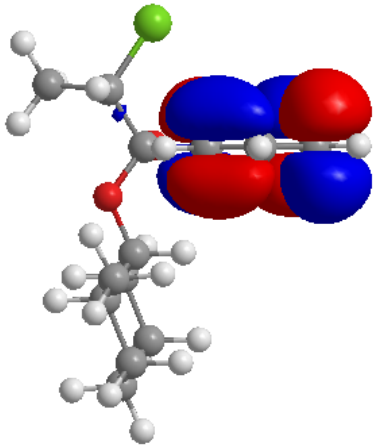
2-Methyl (*R*,*R*,***S***,*S*)-(a,a)



C(1)	-8.3266	-5.3306	-7.9954
C(2)	-7.7135	-5.3139	-9.2493
C(3)	-6.7476	-4.3415	-9.5141
C(4)	-6.4254	-3.4169	-8.5184
N(5)	-7.0047	-3.3969	-7.2617
C(6)	-7.9574	-4.3769	-7.0436
C(7)	-6.6182	-2.3513	-6.2106
O(8)	-7.2248	-2.6163	-4.9678
O(9)	-5.2169	-2.276	-6.0655
C(10)	-7.1098	-0.9707	-6.6549
C(11)	-4.6101	-3.4461	-5.5772
C(12)	-6.7597	0.1499	-5.6732
Cl(13)	-8.8694	-0.9855	-6.966
H(14)	-9.0932	-6.0869	-7.7607
H(15)	-7.9893	-6.0523	-10.0187
H(16)	-6.2481	-4.3036	-10.4956
H(17)	-5.6617	-2.6535	-8.7364
H(18)	-8.4556	-4.4029	-6.0622
H(19)	-6.6539	-0.7177	-7.6374
C(20)	-4.3248	-3.3026	-4.0767
H(21)	-5.287	-4.3164	-5.7415
C(22)	-3.3152	-3.6955	-6.3703
H(23)	-7.1015	1.1417	-6.0492
H(24)	-7.226	-0.0119	-4.6753
H(25)	-5.6598	0.2301	-5.5197
C(26)	-2.2487	-2.6312	-6.0526
H(27)	-3.5577	-3.6133	-7.4621
C(28)	-2.7768	-5.1245	-6.1767
C(29)	-3.2689	-2.2276	-3.7817
H(30)	-3.9751	-4.2788	-3.6668
H(31)	-5.2597	-3.0612	-3.5198
H(32)	-2.595	-1.641	-6.4347
H(33)	-1.3017	-2.8641	-6.5945
C(34)	-1.9704	-2.5071	-4.5487
H(35)	-3.0592	-2.1918	-2.6857
H(36)	-1.8625	-5.2959	-6.7899

H(37)	-3.6628	-1.2239	-4.0683
H(38)	-1.5025	-3.4444	-4.1668
H(39)	-3.5297	-5.883	-6.491
H(40)	-1.2373	-1.685	-4.3653
H(41)	-2.5107	-5.3396	-5.1195

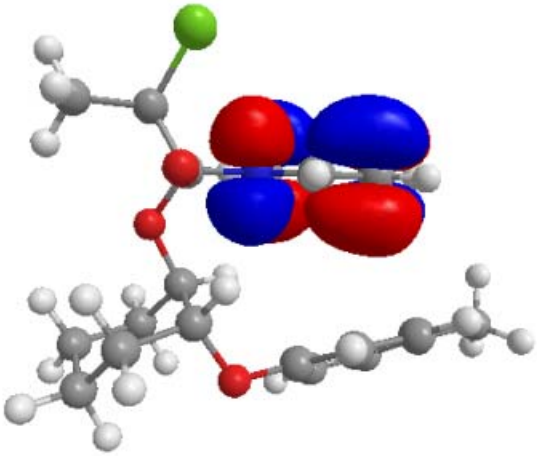
2-Methyl (*R*,*R*,***S***,*S*)-(e,e)



C(1)	-9.1639	-4.4263	-8.8309
C(2)	-8.3604	-4.8671	-9.8833
C(3)	-7.0825	-4.3233	-10.0257
C(4)	-6.6516	-3.3553	-9.1172
N(5)	-7.4139	-2.886	-8.0616
C(6)	-8.6706	-3.4558	-7.9551
C(7)	-6.8905	-1.82	-7.0941
O(8)	-7.8541	-1.4974	-6.121
O(9)	-5.6775	-2.2147	-6.4895
C(10)	-6.6135	-0.5163	-7.8517
C(11)	-5.7127	-3.4235	-5.7746
C(12)	-6.1427	0.629	-6.9516
Cl(13)	-8.0429	-0.0055	-8.7944
H(14)	-10.1755	-4.8403	-8.6932
H(15)	-8.7267	-5.6311	-10.5873
H(16)	-6.4237	-4.6547	-10.8443
H(17)	-5.6406	-2.9359	-9.2375
H(18)	-9.3203	-3.1243	-7.1306
H(19)	-5.8233	-0.691	-8.6142
C(20)	-6.1739	-3.1955	-4.329
H(21)	-6.3927	-4.148	-6.2764
C(22)	-4.2982	-4.0333	-5.7703
H(23)	-5.9183	1.5462	-7.5434
H(24)	-6.9068	0.902	-6.1892
H(25)	-5.2077	0.3621	-6.4091
Lp(26)	-5.319	-2.3261	-6.9559
Lp(27)	-5.5846	-1.8017	-6.0644
C(28)	-4.2804	-5.3465	-4.9654
H(29)	-3.6039	-3.31	-5.2728
C(30)	-3.7605	-4.2929	-7.1891
C(31)	-6.156	-4.4978	-3.5161
H(32)	-7.2101	-2.7898	-4.2918
H(33)	-5.5122	-2.4419	-3.8398
H(34)	-3.2492	-5.7731	-4.9482

H(35)	-4.9376	-6.0972	-5.4648
C(36)	-4.7584	-5.1268	-3.5248
H(37)	-6.4734	-4.2967	-2.4647
H(38)	-2.7544	-4.7699	-7.1563
H(39)	-6.8919	-5.2163	-3.9497
H(40)	-4.7736	-6.0977	-2.974
H(41)	-3.6446	-3.3498	-7.7688

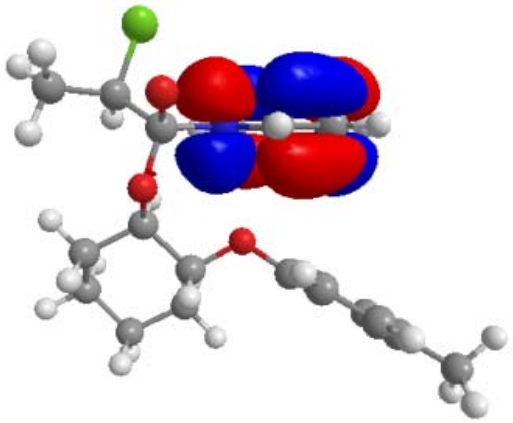
2-OTol (*R*,*R*,***R***,*R*)-(a,a)



C(1)	-10.4885	2.1198	-5.8188
C(2)	-11.4643	1.3239	-6.4198
C(3)	-11.0592	0.2369	-7.1958
C(4)	-9.6956	-0.0191	-7.3484
N(5)	-8.693	0.7448	-6.775
C(6)	-9.1398	1.8109	-6.0151
C(7)	-7.2087	0.4333	-6.9907
O(8)	-6.3861	1.3167	-6.2649
O(9)	-6.8123	0.4574	-8.3449
C(10)	-6.8773	-0.9643	-6.4526
C(11)	-7.3281	1.4939	-9.1395
C(12)	-5.4036	-1.3504	-6.6046
Cl(13)	-7.3844	-1.1293	-4.7473
H(14)	-10.7795	2.9866	-5.2046
H(15)	-12.5336	1.5526	-6.288
H(16)	-11.8075	-0.4053	-7.6874
H(17)	-9.3865	-0.8675	-7.9793
H(18)	-8.388	2.4606	-5.5414
H(19)	-7.4775	-1.7246	-6.9984
C(20)	-6.982	1.164	-10.5987
H(21)	-8.4385	1.4694	-9.0628
C(22)	-6.7907	2.8773	-8.7577
H(23)	-5.2136	-2.3849	-6.2361
H(24)	-4.7317	-0.6653	-6.0402
H(25)	-5.0848	-1.3292	-7.6715
C(26)	-5.2923	3.0015	-9.0484
H(27)	-6.9465	3.0827	-7.6741
O(28)	-7.4705	3.8861	-9.457
C(29)	-5.4747	1.2682	-10.8691
H(30)	-7.3385	0.1365	-10.8509
H(31)	-7.5217	1.8583	-11.2852
H(32)	-4.9426	4.0341	-8.8084

H(33)	-4.7246	2.3104	-8.3808
C(34)	-4.9621	2.6684	-10.5093
H(35)	-5.2637	1.0511	-11.9435
C(36)	-8.7739	4.0584	-9.0681
H(37)	-4.928	0.5028	-10.2687
H(38)	-3.8595	2.7247	-10.6738
C(39)	-9.839	3.7059	-9.9077
H(40)	-5.4318	3.4234	-11.1833
C(41)	-11.1696	3.9082	-9.5376

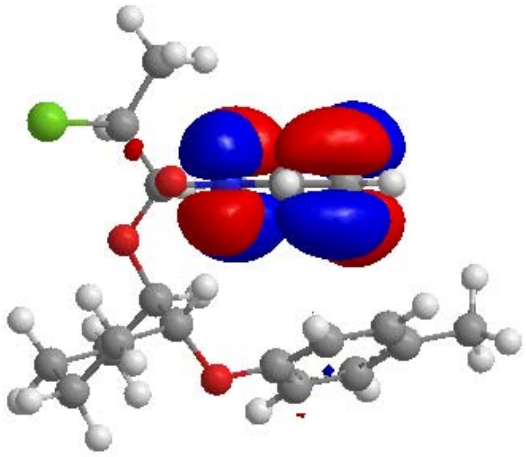
2-OTol (*R*,*R*,***R***,*R*)-(e,e)



C(1)	-10.2922	-3.4244	-7.6843
C(2)	-10.0539	-4.2178	-8.8071
C(3)	-8.7509	-4.3078	-9.2979
C(4)	-7.729	-3.6031	-8.6572
N(5)	-7.9168	-2.7965	-7.5469
C(6)	-9.2255	-2.7428	-7.0938
C(7)	-6.7884	-2.0166	-6.8565
O(8)	-7.1376	-1.9087	-5.491
O(9)	-6.7183	-0.6744	-7.2926
C(10)	-5.4072	-2.6795	-6.8489
C(11)	-6.4711	-0.4649	-8.6617
C(12)	-4.3713	-1.9558	-5.9815
Cl(13)	-5.5242	-4.3816	-6.3104
H(14)	-11.3115	-3.3272	-7.2779
H(15)	-10.8785	-4.7578	-9.2985
H(16)	-8.5333	-4.9235	-10.1853
H(17)	-6.7137	-3.6837	-9.0732
H(18)	-9.4424	-2.1007	-6.2256
H(19)	-4.9963	-2.7418	-7.8781
C(20)	-5.2991	0.5162	-8.7905
H(21)	-6.1822	-1.41	-9.1701
C(22)	-7.72	0.1054	-9.3417
H(23)	-3.3678	-2.4339	-6.0625
H(24)	-4.6516	-1.9546	-4.904
H(25)	-4.2411	-0.8941	-6.2847
C(26)	-7.4395	0.5063	-10.7939
H(27)	-8.0689	0.9957	-8.7658
O(28)	-8.7119	-0.8779	-9.3059
C(29)	-5.0143	0.8829	-10.2522
H(30)	-5.5228	1.4447	-8.2132

H(31)	-4.3768	0.0692	-8.3499
H(32)	-7.2063	-0.4059	-11.3933
H(33)	-8.3412	0.98	-11.2498
C(34)	-6.2659	1.4884	-10.8962
H(35)	-4.168	1.6087	-10.3073
C(36)	-9.9657	-0.4817	-9.679
H(37)	-4.7039	-0.0294	-10.8152
H(38)	-6.0633	1.7343	-11.966
C(39)	-10.5167	-0.8839	-10.9024
H(40)	-6.5292	2.4429	-10.3815
C(41)	-11.8257	-0.5599	-11.2622

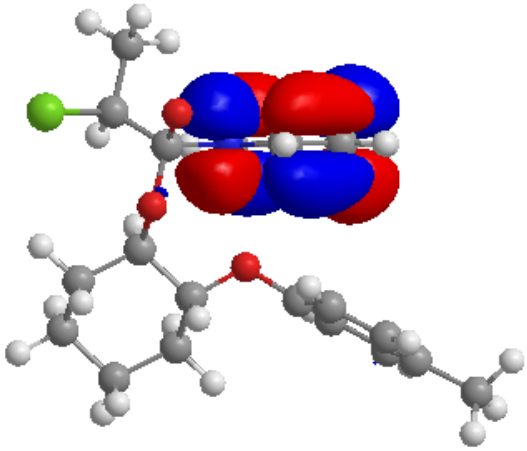
2-OTol (*R*,*R*,***R***,*S*)-(a,a)



C(1)	-10.6181	2.01	-5.9534
C(2)	-11.5424	1.1577	-6.5582
C(3)	-11.0706	0.0683	-7.2927
C(4)	-9.6931	-0.1341	-7.4003
N(5)	-8.741	0.6861	-6.8193
C(6)	-9.253	1.7538	-6.1033
C(7)	-7.2391	0.436	-6.9903
O(8)	-6.4826	1.3711	-6.2587
O(9)	-6.8315	0.4378	-8.3426
C(10)	-6.8794	-0.9344	-6.4006
C(11)	-7.3469	1.4622	-9.1535
C(12)	-7.3468	-1.1047	-4.9526
Cl(13)	-5.1205	-1.25	-6.4977
H(14)	-10.962	2.8805	-5.3722
H(15)	-12.6237	1.3445	-6.4626
H(16)	-11.7772	-0.617	-7.7873
H(17)	-9.3299	-0.9846	-7.9985
H(18)	-8.5423	2.4484	-5.6299
H(19)	-7.3391	-1.7404	-7.013
C(20)	-7.0719	1.076	-10.6137
H(21)	-8.4535	1.4771	-9.0366
C(22)	-6.7522	2.8386	-8.8365
H(23)	-7.0931	-2.1154	-4.5576
H(24)	-8.4512	-0.9993	-4.8613
H(25)	-6.8823	-0.3512	-4.2768
C(26)	-5.2652	2.9079	-9.1952
H(27)	-6.8515	3.0792	-7.7535
O(28)	-7.4365	3.8472	-9.5318

C(29)	-5.5753	1.1248	-10.9492
H(30)	-7.4701	0.0531	-10.8178
H(31)	-7.6183	1.7655	-11.2997
H(32)	-4.8743	3.9358	-9.0035
H(33)	-4.6911	2.2199	-8.5296
C(34)	-5.0077	2.5194	-10.657
H(35)	-5.4172	0.8672	-12.0238
C(36)	-8.7166	4.056	-9.0872
H(37)	-5.0273	0.3624	-10.3466
H(38)	-3.9119	2.5369	-10.8692
C(39)	-9.8271	3.6872	-9.8586
H(40)	-5.4837	3.2671	-11.3347
C(41)	-11.1345	3.9172	-9.4281

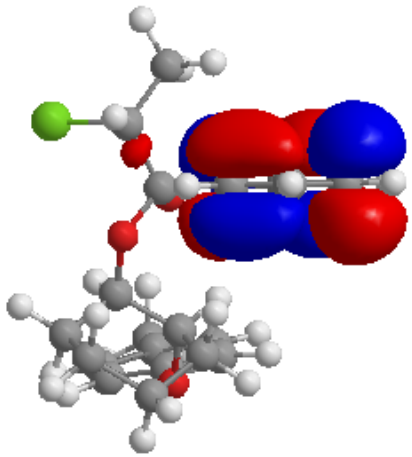
2-OTol (*R*,*R*,***R***,*S*)-(e,e)



C(1)	-10.1128	-3.5835	-8.0496
C(2)	-9.6656	-4.4425	-9.0541
C(3)	-8.2985	-4.4971	-9.3284
C(4)	-7.4218	-3.6933	-8.5957
N(5)	-7.8175	-2.8238	-7.593
C(6)	-9.183	-2.8054	-7.3561
C(7)	-6.8509	-1.9238	-6.8102
O(8)	-7.4006	-1.7595	-5.5186
O(9)	-6.8209	-0.6166	-7.3502
C(10)	-5.4519	-2.5041	-6.5661
C(11)	-6.3166	-0.4795	-8.6557
C(12)	-5.4884	-3.8867	-5.9047
Cl(13)	-4.4456	-1.4228	-5.5539
H(14)	-11.1876	-3.5085	-7.8193
H(15)	-10.3788	-5.0569	-9.6261
H(16)	-7.9178	-5.1583	-10.1232
H(17)	-6.3516	-3.7398	-8.8467
H(18)	-9.5613	-2.1107	-6.5896
H(19)	-4.8806	-2.5988	-7.5121
C(20)	-5.2511	0.6235	-8.6423
H(21)	-5.8419	-1.4207	-9.0063
C(22)	-7.4372	-0.1041	-9.6299
H(23)	-4.4631	-4.3061	-5.7812
H(24)	-6.0578	-4.6267	-6.5086
H(25)	-5.9613	-3.855	-4.8972
C(26)	-6.8801	0.1553	-11.0339

H(27)	-7.9568	0.8077	-9.2505
O(28)	-8.3456	-1.1637	-9.6708
C(29)	-4.6757	0.8689	-10.0428
H(30)	-5.696	1.5699	-8.2525
H(31)	-4.4198	0.3456	-7.9521
H(32)	-6.4463	-0.7888	-11.4418
H(33)	-7.6962	0.4687	-11.7273
C(34)	-5.797	1.2419	-11.0196
H(35)	-3.9145	1.6845	-10.0065
C(36)	-9.5316	-0.9206	-10.3045
H(37)	-4.1559	-0.0519	-10.3996
H(38)	-5.3778	1.3787	-12.0452
C(39)	-9.8363	-1.5328	-11.5268
H(40)	-6.2498	2.2154	-10.7152
C(41)	-11.077	-1.3673	-12.1446

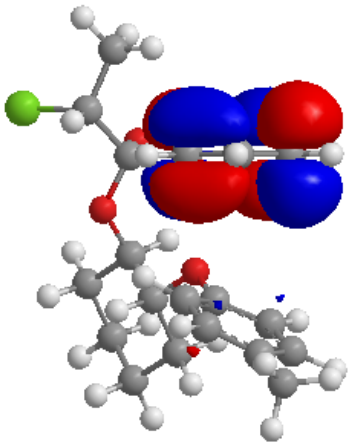
2-OTol (*R*,*R*,***S***,*R*)-(a,a)



C(1)	-3.0522	3.3203	0.6698
C(2)	-3.9013	2.5461	1.4619
C(3)	-3.3644	1.4673	2.1664
C(4)	-2.001	1.187	2.0512
N(5)	-1.1252	1.9198	1.2691
C(6)	-1.6972	2.9889	0.6014
C(7)	0.3691	1.5922	1.1406
O(8)	0.6663	0.3813	1.7957
O(9)	0.721	1.6112	-0.2291
C(10)	1.169	2.6894	1.8529
C(11)	0.8986	0.3617	-0.8429
C(12)	0.7377	2.9047	3.3058
Cl(13)	2.923	2.3382	1.8019
H(14)	-3.447	4.1794	0.1044
H(15)	-4.9743	2.7845	1.533
H(16)	-4.0105	0.844	2.8052
H(17)	-1.5984	0.3323	2.6163
H(18)	-1.0371	3.6041	-0.0308
H(19)	1.0545	3.6516	1.3071
C(20)	1.4828	0.6127	-2.24
H(21)	1.6719	-0.1965	-0.2637
C(22)	-0.4091	-0.429	-0.9357
H(23)	1.3429	3.7001	3.7985
H(24)	0.8444	1.9757	3.9105

H(25)	-0.3245	3.2305	3.3751
C(26)	-1.4108	0.2498	-1.877
H(27)	-0.8971	-0.5185	0.0629
O(28)	-0.1871	-1.7307	-1.4058
C(29)	0.4776	1.3102	-3.1671
H(30)	2.4096	1.23	-2.1591
H(31)	1.7906	-0.3548	-2.7024
H(32)	-2.3345	-0.371	-1.9623
H(33)	-1.7319	1.2272	-1.4484
C(34)	-0.8163	0.4928	-3.2703
H(35)	0.9237	1.4441	-4.1815
C(36)	0.4492	-2.5662	-0.5272
H(37)	0.2464	2.3293	-2.7762
H(38)	-1.5556	1.0295	-3.9118
C(39)	1.7707	-2.98	-0.7395
H(40)	-0.6036	-0.4843	-3.7649
C(41)	2.4039	-3.8931	0.1059

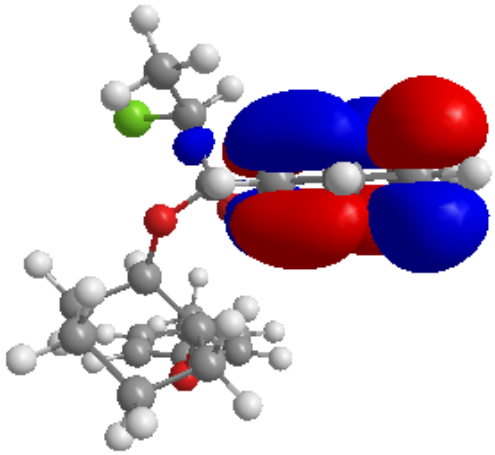
2-OTol (*R*,*R*,***S***,*R*)-(e,e)



C(1)	-10.2541	-3.3967	-7.8802
C(2)	-9.8851	-4.3701	-8.8094
C(3)	-8.5288	-4.5633	-9.0762
C(4)	-7.5838	-3.7742	-8.4164
N(5)	-7.9031	-2.7896	-7.4976
C(6)	-9.259	-2.6408	-7.2565
C(7)	-6.8432	-1.9158	-6.8122
O(8)	-5.5494	-2.4505	-6.9832
O(9)	-6.9264	-0.5976	-7.3078
C(10)	-7.0709	-1.8595	-5.2962
C(11)	-6.4964	-0.4284	-8.6366
C(12)	-7.1726	-3.2469	-4.6573
Cl(13)	-5.7828	-0.9265	-4.4742
H(14)	-11.3173	-3.2133	-7.6574
H(15)	-10.6502	-4.9694	-9.3276
H(16)	-8.2092	-5.3235	-9.8068
H(17)	-6.5202	-3.9335	-8.6524
H(18)	-9.5703	-1.8519	-6.555
H(19)	-7.9994	-1.293	-5.069
C(20)	-5.3867	0.629	-8.6421
H(21)	-6.0824	-1.3748	-9.0531
C(22)	-7.6691	0.0131	-9.5139

H(23)	-7.3536	-3.1789	-3.5598
H(24)	-6.2434	-3.8409	-4.8117
H(25)	-8.0171	-3.8361	-5.0793
C(26)	-7.2077	0.3603	-10.9326
H(27)	-8.15	0.9055	-9.0464
O(28)	-8.5934	-1.0348	-9.5497
C(29)	-4.92	0.9562	-10.0662
H(30)	-5.7582	1.562	-8.1551
H(31)	-4.5191	0.2676	-8.0391
H(32)	-6.8236	-0.5585	-11.4362
H(33)	-8.0635	0.7376	-11.5415
C(34)	-6.1055	1.4277	-10.9168
H(35)	-4.1327	1.7471	-10.0381
C(36)	-9.7934	-0.7507	-10.1396
H(37)	-4.4618	0.0502	-10.5292
H(38)	-5.7665	1.6442	-11.958
C(39)	-10.1463	-1.3157	-11.3717
H(40)	-6.5126	2.3789	-10.4983
C(41)	-11.3981	-1.0971	-11.9493

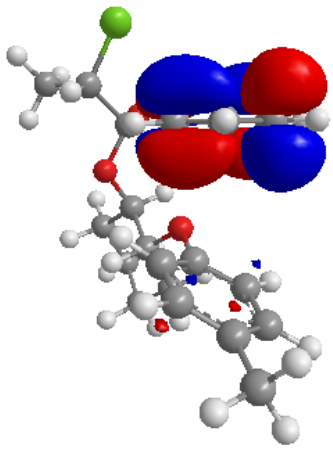
2-OTol (*R*,*R*,***S***,*S*)-(a,a)



C(1)	-3.2166	2.891	0.4993
C(2)	-3.9364	2.3231	1.5513
C(3)	-3.2576	1.5252	2.4735
C(4)	-1.8856	1.3139	2.3151
N(5)	-1.1339	1.8422	1.2802
C(6)	-1.8475	2.6363	0.3974
C(7)	0.3741	1.5818	1.1348
O(8)	0.6838	0.3741	1.7947
O(9)	0.7341	1.6047	-0.2309
C(10)	1.1425	2.6846	1.8714
C(11)	1.1763	0.3932	-0.7819
C(12)	0.9447	4.0934	1.3108
Cl(13)	2.8893	2.3027	1.9406
H(14)	-3.7215	3.5338	-0.2394
H(15)	-5.0173	2.5083	1.6555
H(16)	-3.7994	1.0711	3.3186
H(17)	-1.3679	0.6899	3.0603
H(18)	-1.2988	3.1008	-0.4373
H(19)	0.818	2.6895	2.9363
C(20)	1.7571	0.7043	-2.1683

H(21)	2.0193	0.0225	-0.1517
C(22)	0.0498	-0.6418	-0.8853
H(23)	1.5421	4.8446	1.8772
H(24)	-0.1155	4.4211	1.3895
H(25)	1.2473	4.1622	0.2415
C(26)	-1.02	-0.2184	-1.898
H(27)	-0.4713	-0.7804	0.091
O(28)	0.5454	-1.8953	-1.271
C(29)	0.6744	1.1547	-3.1588
H(30)	2.5401	1.4956	-2.083
H(31)	2.2675	-0.199	-2.5774
H(32)	-1.7934	-1.0177	-1.992
H(33)	-1.5521	0.6877	-1.5258
C(34)	-0.4212	0.088	-3.2765
H(35)	1.129	1.3438	-4.1606
C(36)	1.3545	-2.5079	-0.3513
H(37)	0.2251	2.1174	-2.8179
H(38)	-1.2222	0.4386	-3.9705
C(39)	2.7285	-2.662	-0.5789
H(40)	0.0078	-0.843	-3.717
C(41)	3.556	-3.3374	0.3197

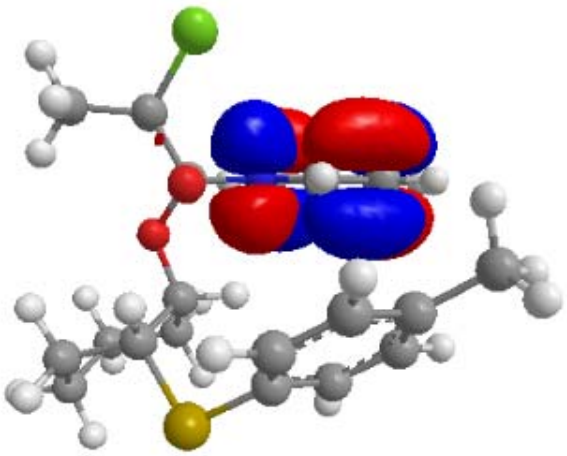
2-OTol (*R*,*R*,***S***,*S*)-(e,e)



C(1)	-10.2648	-3.3422	-7.3717
C(2)	-10.1004	-4.2473	-8.4208
C(3)	-8.8226	-4.4365	-8.9492
C(4)	-7.7519	-3.7093	-8.4239
N(5)	-7.8688	-2.7925	-7.3935
C(6)	-9.1515	-2.6489	-6.8911
C(7)	-6.6732	-1.9944	-6.8538
O(8)	-5.4479	-2.5228	-7.3113
O(9)	-6.7847	-0.6364	-7.2184
C(10)	-6.5986	-2.0541	-5.3238
C(11)	-6.6466	-0.3746	-8.5943
C(12)	-5.3617	-1.3681	-4.7363
Cl(13)	-6.6853	-3.7431	-4.7469
H(14)	-11.2631	-3.1628	-6.9417
H(15)	-10.9632	-4.7982	-8.8271
H(16)	-8.6628	-5.1462	-9.7766
H(17)	-6.7546	-3.866	-8.8633
H(18)	-9.308	-1.9115	-6.0892

H(19)	-7.4883	-1.5552	-4.8827
C(20)	-5.505	0.6324	-8.774
H(21)	-6.3885	-1.2999	-9.1581
C(22)	-7.9529	0.1872	-9.1581
H(23)	-5.3741	-1.3924	-3.6221
H(24)	-5.3103	-0.2958	-5.0322
H(25)	-4.4158	-1.8532	-5.0674
C(26)	-7.7917	0.6194	-10.6188
H(27)	-8.2635	1.0616	-8.5374
O(28)	-8.9261	-0.8108	-9.0586
C(29)	-5.3372	1.0386	-10.2439
H(30)	-5.7096	1.5432	-8.1622
H(31)	-4.5502	0.1925	-8.3978
H(32)	-7.5868	-0.2762	-11.2526
H(33)	-8.7344	1.0822	-10.9962
C(34)	-6.6465	1.627	-10.7832
H(35)	-4.5141	1.7859	-10.3434
C(36)	-10.2134	-0.4086	-9.2832
H(37)	-5.0484	0.1467	-10.8493
H(38)	-6.528	1.8997	-11.8592
C(39)	-10.8871	-0.7535	-10.4619
H(40)	-6.8921	2.5648	-10.2304
C(41)	-12.2264	-0.4189	-10.6679

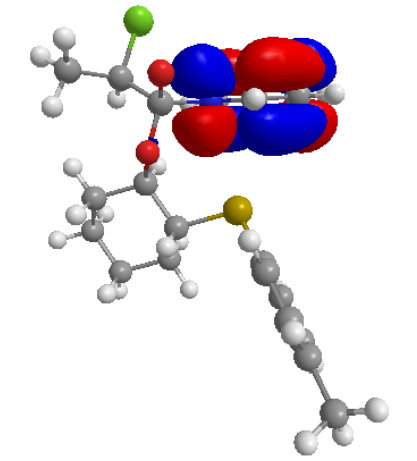
2-STol (*R*,*R*,***R***,*R*)-(a,a)



C(1)	-9.8785	-1.5281	-5.1213
C(2)	-9.4644	-2.7899	-5.55
C(3)	-8.2164	-2.9165	-6.1629
C(4)	-7.4241	-1.7794	-6.3335
N(5)	-7.7948	-0.5103	-5.9253
C(6)	-9.0359	-0.4315	-5.3187
C(7)	-6.9051	0.713	-6.1742
O(8)	-7.542	1.8992	-5.7629
O(9)	-6.5466	0.8032	-7.5359
C(10)	-5.6094	0.6033	-5.3669
C(11)	-7.6281	0.9731	-8.4167
C(12)	-4.6723	1.8003	-5.5462
Cl(13)	-5.9566	0.3483	-3.6336
H(14)	-10.8604	-1.3976	-4.6386
H(15)	-10.1124	-3.6698	-5.4112
H(16)	-7.8658	-3.8996	-6.5155

H(17)	-6.4485	-1.8857	-6.8336
H(18)	-9.3837	0.5564	-4.9797
H(19)	-5.0583	-0.3104	-5.6805
C(20)	-7.3521	0.1408	-9.6754
H(21)	-8.5438	0.5545	-7.943
C(22)	-7.819	2.465	-8.7475
H(23)	-3.7264	1.6678	-4.9721
H(24)	-5.1416	2.7506	-5.2051
H(25)	-4.3811	1.9341	-6.6127
C(26)	-6.6762	3.0063	-9.6262
H(27)	-7.8229	3.0761	-7.8134
S(28)	-9.4244	2.7401	-9.5864
C(29)	-6.1625	0.6858	-10.4759
H(30)	-7.1585	-0.9211	-9.3901
H(31)	-8.2565	0.1246	-10.3282
H(32)	-6.8746	4.0632	-9.9245
H(33)	-5.7407	3.0299	-9.0159
C(34)	-6.4081	2.1475	-10.87
H(35)	-6.0035	0.0667	-11.3912
C(36)	-10.4862	2.301	-8.1743
H(37)	-5.2312	0.612	-9.8659
H(38)	-5.5225	2.5456	-11.421
C(39)	-10.5843	3.1428	-7.0647
H(40)	-7.2736	2.2053	-11.5708
C(41)	-11.3811	2.7695	-5.9804

2-STol (*R*,*R*,***R***,*R*)-(e,e)

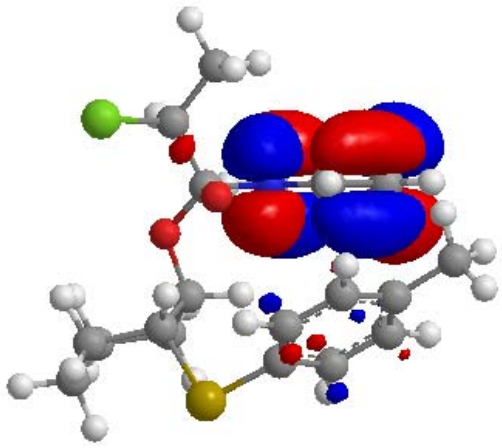


C(1)	-9.9207	-4.295	-7.3325
C(2)	-9.5654	-5.1058	-8.4109
C(3)	-8.3123	-4.9271	-8.9987
C(4)	-7.451	-3.9535	-8.4873
N(5)	-7.7527	-3.1341	-7.4127
C(6)	-9.0114	-3.3407	-6.8707
C(7)	-6.7868	-2.0903	-6.8332
O(8)	-7.063	-2.0089	-5.4492
O(9)	-7.0751	-0.793	-7.313
C(10)	-5.2936	-2.4197	-6.9067
C(11)	-6.8971	-0.5646	-8.6912
C(12)	-4.4089	-1.4869	-6.0717
Cl(13)	-4.9754	-4.1036	-6.3906
H(14)	-10.9081	-4.4023	-6.8558

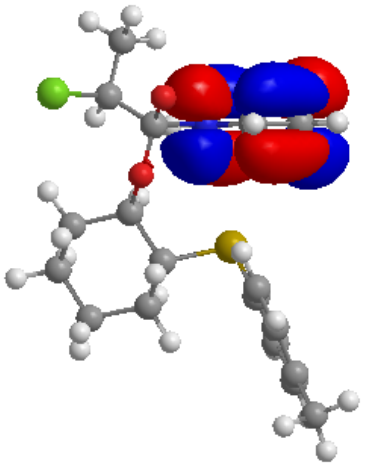
H(15)	-10.2632	-5.8661	-8.7954
H(16)	-8.0078	-5.5477	-9.8566
H(17)	-6.4715	-3.8302	-8.9733
H(18)	-9.3192	-2.6995	-6.0298
H(19)	-4.9451	-2.3842	-7.9597
C(20)	-5.7283	0.4134	-8.8841
H(21)	-6.6624	-1.5063	-9.2332
C(22)	-8.1826	0.0496	-9.2786
H(23)	-3.3272	-1.6844	-6.2531
H(24)	-4.5866	-1.6055	-4.9788
H(25)	-4.5858	-0.4153	-6.3081
C(26)	-7.9971	0.4835	-10.744
H(27)	-8.4448	0.9456	-8.6653
S(28)	-9.5259	-1.1935	-9.2318
C(29)	-5.5437	0.8322	-10.3481
H(30)	-5.8989	1.3254	-8.2634
H(31)	-4.7745	-0.0456	-8.5356
H(32)	-7.7974	-0.407	-11.3868
H(33)	-8.9227	0.9726	-11.1312
C(34)	-6.8292	1.4663	-10.8887
H(35)	-4.6997	1.5582	-10.434
C(36)	-10.9029	-0.0093	-9.2362
H(37)	-5.2748	-0.06	-10.9622
H(38)	-6.695	1.749	-11.9602
C(39)	-11.6086	0.2325	-10.4159
H(40)	-7.0541	2.4031	-10.3256
C(41)	-12.6614	1.1498	-10.4188

2-STol (*R*,*R*,***R***,*S*)-(a,a)

C(1)	-9.8986	-1.5993	-5.2035
C(2)	-9.4354	-2.8159	-5.7064
C(3)	-8.1794	-2.8586	-6.3142
C(4)	-7.4278	-1.6851	-6.4063
N(5)	-7.8526	-0.457	-5.9328
C(6)	-9.0986	-0.4618	-5.3295
C(7)	-6.9998	0.8084	-6.0752
O(8)	-7.7408	1.9468	-5.7062
O(9)	-6.4986	0.9341	-7.3898
C(10)	-5.8066	0.7175	-5.1197
C(11)	-7.4868	1.0914	-8.376
C(12)	-6.2154	0.4049	-3.6782

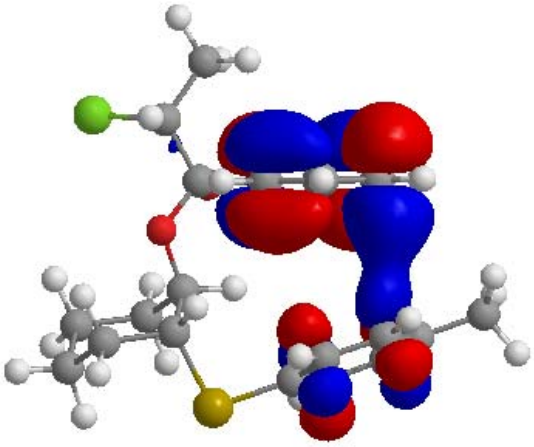


Cl(13)	-4.8339	2.2185	-5.1528
H(14)	-10.8831	-1.5378	-4.7131
H(15)	-10.0487	-3.7269	-5.6206
H(16)	-7.7872	-3.8063	-6.7163
H(17)	-6.4377	-1.7271	-6.8877
H(18)	-9.4802	0.4872	-4.9231
H(19)	-5.1134	-0.0794	-5.4679
C(20)	-7.0473	0.3186	-9.6263
H(21)	-8.4239	0.6126	-8.0136
C(22)	-7.7141	2.585	-8.6755
H(23)	-5.3304	0.3497	-3.0035
H(24)	-6.7277	-0.5806	-3.6016
H(25)	-6.9073	1.1759	-3.2695
C(26)	-6.5324	3.2105	-9.4386
H(27)	-7.8177	3.1632	-7.7268
S(28)	-9.2649	2.8188	-9.6246
C(29)	-5.8212	0.9507	-10.2967
H(30)	-6.8228	-0.7417	-9.3587
H(31)	-7.8855	0.2797	-10.3617
H(32)	-6.7599	4.2653	-9.7231
H(33)	-5.654	3.2602	-8.7498
C(34)	-6.1155	2.4066	-10.6774
H(35)	-5.5424	0.3691	-11.2077
C(36)	-10.3916	2.3262	-8.2805
H(37)	-4.9483	0.9109	-9.603
H(38)	-5.2111	2.8672	-11.1425
C(39)	-10.5872	3.1545	-7.1731
H(40)	-6.9234	2.438	-11.4454
C(41)	-11.4163	2.7343	-6.1316



2-STol (*R*,*R*,***R***,*S*)-(e,e)

C(1)	-9.9683	-4.2726	-7.1671
C(2)	-9.6243	-5.0939	-8.2413
C(3)	-8.3771	-4.9204	-8.8425
C(4)	-7.5136	-3.939	-8.3505
N(5)	-7.8062	-3.1037	-7.2853
C(6)	-9.0568	-3.3102	-6.7254
C(7)	-6.8416	-2.0337	-6.7488
O(8)	-7.1016	-1.9114	-5.365
O(9)	-7.148	-0.7597	-7.28
C(10)	-5.3522	-2.3816	-6.8344



C(11)	-6.9969	-0.5852	-8.6685
C(12)	-5.0195	-3.741	-6.2076
Cl(13)	-4.3273	-1.1486	-6.0326
H(14)	-10.9505	-4.3785	-6.6795
H(15)	-10.3252	-5.8594	-8.6107
H(16)	-8.0785	-5.5505	-9.6957
H(17)	-6.537	-3.824	-8.8443
H(18)	-9.3574	-2.6624	-5.8868
H(19)	-5.0132	-2.3933	-7.8909
C(20)	-5.8132	0.3569	-8.9319
H(21)	-6.7983	-1.5505	-9.1814
C(22)	-8.2845	0.0372	-9.2418
H(23)	-3.9434	-3.9978	-6.3438
H(24)	-5.5991	-4.5727	-6.6633
H(25)	-5.2329	-3.7589	-5.1148
C(26)	-8.1363	0.4194	-10.7259
H(27)	-8.507	0.9595	-8.6521
S(28)	-9.6499	-1.1774	-9.1134
C(29)	-5.6615	0.6993	-10.4194
H(30)	-5.9468	1.299	-8.3487
H(31)	-4.8599	-0.1051	-8.5879
H(32)	-7.9896	-0.4966	-11.3472
H(33)	-9.0593	0.9272	-11.0951
C(34)	-6.9418	1.3558	-10.9452
H(35)	-4.7944	1.387	-10.5668
C(36)	-10.997	0.0398	-9.0601
H(37)	-5.4476	-0.2303	-10.9985
H(38)	-6.8324	1.5923	-12.0304
C(39)	-11.7494	0.2992	-10.2069
H(40)	-7.117	2.3202	-10.4118
C(41)	-12.776	1.2451	-10.1636

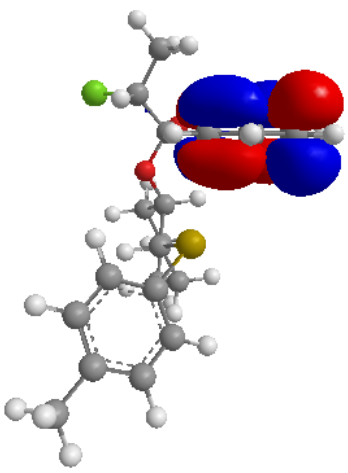
2-STol (*R*,*R*,***S***,*R*)-(a,a)

C(1)	-9.7928	-1.7191	-6.3864
C(2)	-9.3682	-2.8113	-5.6276
C(3)	-8.1215	-2.7526	-5.004
C(4)	-7.3402	-1.6033	-5.1474
N(5)	-7.7253	-0.4949	-5.8795
C(6)	-8.9642	-0.6001	-6.4889
C(7)	-6.8642	0.7641	-6.0188
O(8)	-5.6194	0.5964	-5.3846

O(9)	-6.7098	1.0971	-7.3804
C(10)	-7.5644	1.9383	-5.3267
C(11)	-5.9477	0.1862	-8.1323
C(12)	-7.9624	1.6329	-3.8809
Cl(13)	-6.5554	3.4152	-5.3696
H(14)	-10.7687	-1.741	-6.8968
H(15)	-10.0025	-3.7066	-5.5305
H(16)	-7.758	-3.6039	-4.4067
H(17)	-6.3605	-1.5772	-4.6456
H(18)	-9.3078	0.2567	-7.0887
H(19)	-8.483	2.2098	-5.8916
C(20)	-4.5213	0.7236	-8.3074
H(21)	-5.9146	-0.7887	-7.5953
C(22)	-6.6475	-0.0017	-9.4901
H(23)	-8.4736	2.5016	-3.4055
H(24)	-7.078	1.3747	-3.2556
H(25)	-8.6753	0.7798	-3.823
C(26)	-6.5845	1.2862	-10.332
H(27)	-7.7259	-0.2414	-9.3108
S(28)	-5.9332	-1.3865	-10.449
C(29)	-4.4873	2.0219	-9.1265
H(30)	-4.0445	0.9012	-7.3155
H(31)	-3.8908	-0.0443	-8.8143
H(32)	-7.0519	1.1276	-11.3328
H(33)	-7.1968	2.0731	-9.8285
C(34)	-5.1552	1.8245	-10.4933
H(35)	-3.4312	2.3557	-9.266
C(36)	-6.3681	-2.7429	-9.321
H(37)	-5.0106	2.8348	-8.5698
H(38)	-5.175	2.7932	-11.048
C(39)	-7.6864	-3.1923	-9.2297
H(40)	-4.5464	1.1193	-11.1061
C(41)	-8.0039	-4.2388	-8.3607

2-STol (*R*,*R*,***S***,*R*)-(e,e)

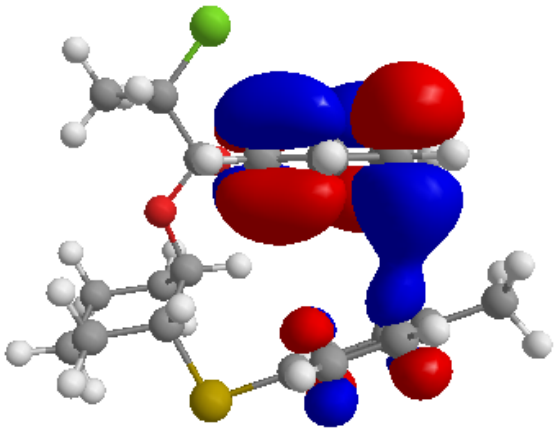
C(1)	-9.8478	-4.3386	-7.1187
C(2)	-9.4796	-5.3096	-8.0508
C(3)	-8.2111	-5.2379	-8.6286
C(4)	-7.3518	-4.1996	-8.2619
N(5)	-7.6749	-3.2139	-7.3453
C(6)	-8.9403	-3.3271	-6.796



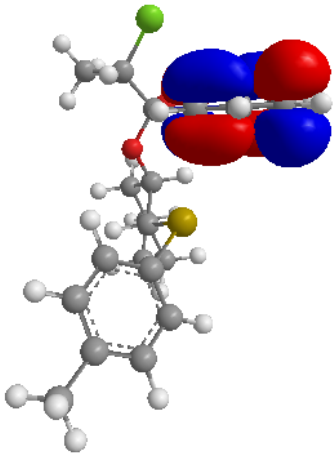
C(7)	-6.7119	-2.0804	-6.963
O(8)	-5.429	-2.3066	-7.5
O(9)	-7.2598	-0.8525	-7.3903
C(10)	-6.5309	-2.0195	-5.442
C(11)	-7.2034	-0.6381	-8.7786
C(12)	-6.1042	-3.3612	-4.8411
Cl(13)	-5.3499	-0.7588	-4.9751
H(14)	-10.8448	-4.3646	-6.651
H(15)	-10.1775	-6.1154	-8.3278
H(16)	-7.8936	-5.9908	-9.3677
H(17)	-6.3584	-4.16	-8.7348
H(18)	-9.2524	-2.5577	-6.0726
H(19)	-7.4777	-1.6996	-4.9562
C(20)	-6.0188	0.2826	-9.1011
H(21)	-7.0776	-1.6024	-9.3226
C(22)	-8.5087	0.0229	-9.2509
H(23)	-5.9961	-3.2978	-3.7339
H(24)	-5.1316	-3.7099	-5.2568
H(25)	-6.8557	-4.158	-5.0394
C(26)	-8.4521	0.3475	-10.7543
H(27)	-8.639	0.9697	-8.6727
S(28)	-9.9127	-1.1175	-8.9605
C(29)	-5.948	0.6042	-10.6002
H(30)	-6.1171	1.2343	-8.5263
H(31)	-5.0575	-0.1855	-8.7845
H(32)	-8.3624	-0.5948	-11.346
H(33)	-9.3878	0.8592	-11.0837
C(34)	-7.2543	1.2503	-11.0784
H(35)	-5.0911	1.2906	-10.8025
C(36)	-11.1828	0.1736	-8.805
H(37)	-5.7613	-0.3352	-11.1734
H(38)	-7.2051	1.4414	-12.1773
C(39)	-12.0307	0.4562	-9.8771
H(40)	-7.3881	2.2389	-10.5784
C(41)	-12.9975	1.4564	-9.7515

2-STol (*R*,*R*,*S*,*S*)-(a,a)

C(1)	-9.8002	-1.7306	-6.3742
C(2)	-9.3562	-2.8338	-5.6445
C(3)	-8.0961	-2.7806	-5.0461
C(4)	-7.3235	-1.6255	-5.1838



N(5)	-7.7302	-0.5036	-5.8862
C(6)	-8.9776	-0.6061	-6.4739
C(7)	-6.8749	0.7609	-6.0187
O(8)	-5.6309	0.6044	-5.3804
O(9)	-6.7042	1.099	-7.3765
C(10)	-7.5673	1.9472	-5.3413
C(11)	-5.9274	0.1967	-8.1235
C(12)	-6.7394	3.2348	-5.3642
Cl(13)	-8.0327	1.5473	-3.6639
H(14)	-10.786	-1.7481	-6.8655
H(15)	-9.9837	-3.7342	-5.5505
H(16)	-7.7158	-3.6416	-4.4735
H(17)	-6.3329	-1.605	-4.7052
H(18)	-9.3361	0.2578	-7.0567
H(19)	-8.5303	2.1543	-5.8576
C(20)	-4.49	0.7198	-8.2456
H(21)	-5.9239	-0.7886	-7.6053
C(22)	-6.5842	0.0459	-9.5074
H(23)	-7.296	4.0854	-4.9077
H(24)	-6.4874	3.5408	-6.4047
H(25)	-5.7818	3.1243	-4.8069
C(26)	-6.4845	1.3531	-10.3159
H(27)	-7.6691	-0.1912	-9.3676
S(28)	-5.8473	-1.3196	-10.4775
C(29)	-4.4179	2.0382	-9.029
H(30)	-4.0348	0.8649	-7.2388
H(31)	-3.8553	-0.0426	-8.7554
H(32)	-6.9207	1.2224	-11.3346
H(33)	-7.1065	2.1329	-9.8133
C(34)	-5.0467	1.8834	-10.4196
H(35)	-3.3546	2.3636	-9.1282
C(36)	-6.2612	-2.6906	-9.3598
H(37)	-4.9487	2.8425	-8.4671
H(38)	-5.0419	2.8668	-10.9481
C(39)	-7.5746	-3.1551	-9.267
H(40)	-4.4251	1.1898	-11.0328
C(41)	-7.8768	-4.21	-8.4036

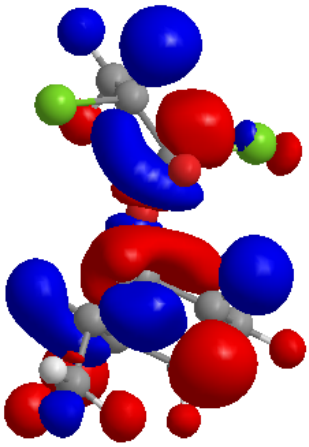


2-STol (*R*,*R*,***S***,*S*)-(e,e)

C(1)	-9.7696	-4.393	-7.3466
C(2)	-9.3063	-5.3638	-8.2385

C(3)	-7.9941	-5.2736	-8.7088
C(4)	-7.1917	-4.2115	-8.2884
N(5)	-7.608	-3.2281	-7.4103
C(6)	-8.9101	-3.3615	-6.9618
C(7)	-6.6783	-2.0928	-6.9563
O(8)	-5.3702	-2.2859	-7.4443
O(9)	-7.2112	-0.8562	-7.3878
C(10)	-6.5697	-2.0495	-5.4299
C(11)	-7.0339	-0.5836	-8.7577
C(12)	-5.5952	-0.9776	-4.9085
Cl(13)	-6.1192	-3.6444	-4.7708
H(14)	-10.7941	-4.4505	-6.9593
H(15)	-9.978	-6.1757	-8.5512
H(16)	-7.6041	-6.0215	-9.4106
H(17)	-6.1704	-4.1562	-8.6793
H(18)	-9.2897	-2.5805	-6.2741
H(19)	-7.5746	-1.8344	-5.0071
C(20)	-5.8472	0.3752	-8.9181
H(21)	-6.8303	-1.5169	-9.3161
C(22)	-8.3092	0.0849	-9.3081
H(23)	-5.5555	-0.9598	-3.797
H(24)	-5.8898	0.0323	-5.2493
H(25)	-4.5571	-1.1702	-5.2576
C(26)	-8.1253	0.5309	-10.7684
H(27)	-8.5365	0.9716	-8.6805
S(28)	-9.6792	-1.1339	-9.2369
C(29)	-5.6383	0.8032	-10.3766
H(30)	-6.0366	1.2699	-8.2858
H(31)	-4.8946	-0.0855	-8.5363
H(32)	-7.9891	-0.3721	-11.4132
H(33)	-9.0312	1.0653	-11.1413
C(34)	-6.9072	1.4542	-10.9396
H(35)	-4.764	1.5038	-10.4444
C(36)	-11.0175	0.0902	-9.199
H(37)	-5.3903	-0.0965	-10.9853
H(38)	-6.7537	1.6905	-12.0148
C(39)	-11.7414	0.3785	-10.3616
H(40)	-7.1108	2.4121	-10.4011
C(41)	-12.7765	1.3174	-10.309

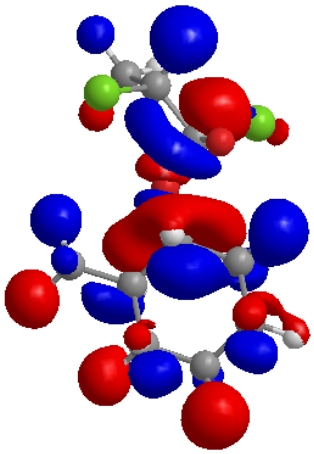
LUMO representation and Cartesian coordinates of chloride transition state structures (uncatalyzed reaction)**:**



2-Methyl (*R*,*R*,***R***,*R*)-(a,a)

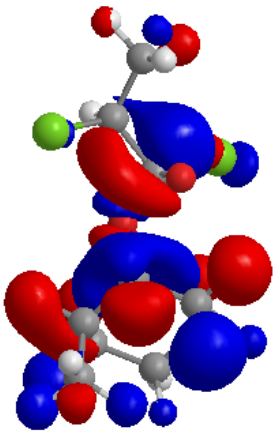
Cl(1)	-3.8543	-2.4417	2.6622
C(2)	-2.798	-2.173	1.2173
O(3)	-1.5487	-1.7898	1.7407
O(4)	-3.3977	-1.2657	0.312
C(5)	-2.609	-3.5088	0.495
C(6)	-2.9283	0.0559	0.3291
C(7)	-3.882	-4.0512	-0.1618
Cl(8)	-1.3159	-3.3783	-0.7374
C(9)	-3.3691	0.8107	1.5873
C(10)	-3.4579	0.7446	-0.9422
C(11)	-4.9843	0.9368	-0.8703
C(12)	-2.7227	2.0607	-1.2542
C(13)	-4.8922	0.9945	1.6534
C(14)	-5.4201	1.6917	0.3928
H(15)	-2.2262	-4.2692	1.2123
H(16)	-1.8153	0.0364	0.2532
H(17)	-3.7012	-5.04	-0.6432
H(18)	-4.6979	-4.2039	0.5795
H(19)	-4.2708	-3.3645	-0.9477
H(20)	-3.0055	0.3016	2.5084
H(21)	-2.8862	1.8158	1.6029
H(22)	-3.2455	0.0689	-1.8124
H(23)	-5.3461	1.4737	-1.7789
H(24)	-5.4815	-0.0632	-0.8757
H(25)	-1.6263	1.8929	-1.36
H(26)	-3.0818	2.5012	-2.2125
H(27)	-2.8661	2.8296	-0.4648
H(28)	-5.1644	1.59	2.5574
H(29)	-5.3913	0.0032	1.7602
H(30)	-6.5343	1.753	0.4326
H(31)	-5.0447	2.7408	0.3595

2-Methyl (*R*,*R*,***R***,*R*)-(e,e)



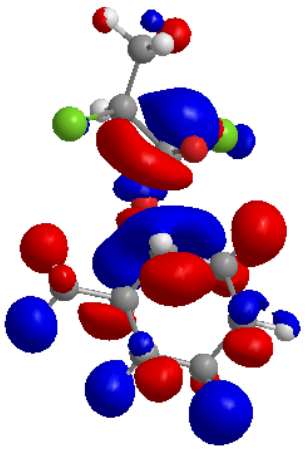
Cl(1)	-1.1401	-1.3749	2.745
C(2)	-0.906	-0.6137	1.1197
O(3)	-0.4132	0.6802	1.3738
O(4)	-2.0953	-0.6789	0.3561
C(5)	0.1865	-1.3807	0.372
C(6)	-2.8941	0.4731	0.332
C(7)	-0.1892	-2.819	0.0056
Cl(8)	0.6719	-0.4999	-1.1105
C(9)	-3.5352	0.7543	1.6948
C(10)	-3.9817	0.2674	-0.7377
C(11)	-4.9349	1.4754	-0.79
C(12)	-3.3794	0.0184	-2.1329
C(13)	-4.4875	1.9569	1.6385
C(14)	-5.5736	1.7426	0.5785
H(15)	1.1119	-1.4029	0.9904
H(16)	-2.2744	1.3424	0.009
H(17)	0.6541	-3.3416	-0.502
H(18)	-0.4386	-3.4256	0.9044
H(19)	-1.0674	-2.8586	-0.6776
H(20)	-4.0981	-0.147	2.0351
H(21)	-2.7588	0.9723	2.4639
H(22)	-4.5817	-0.6352	-0.4579
H(23)	-4.3722	2.3807	-1.1194
H(24)	-5.7389	1.2964	-1.5433
H(25)	-2.7484	0.8765	-2.4579
H(26)	-4.1788	-0.1233	-2.8955
H(27)	-2.7472	-0.8976	-2.157
H(28)	-4.9604	2.1172	2.637
H(29)	-3.9084	2.8802	1.3977
H(30)	-6.2349	2.6401	0.5229
H(31)	-6.2154	0.877	0.8681

2-Methyl (*R*,*R*,***R***,*S*)-(a,a)



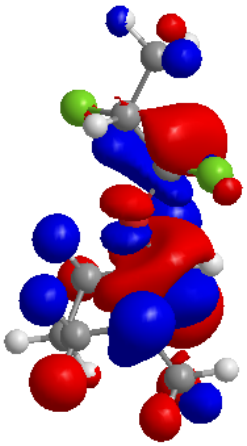
Cl(1)	-3.8581	-2.3459	2.646
C(2)	-2.7788	-2.1562	1.2045
O(3)	-1.5194	-1.7649	1.6944
O(4)	-3.3852	-1.2708	0.2756
C(5)	-2.6069	-3.5178	0.5247
C(6)	-2.8859	0.0414	0.2404
C(7)	-2.0556	-4.6243	1.4314
Cl(8)	-1.5291	-3.3738	-0.9011
C(9)	-3.2594	0.8395	1.4942
C(10)	-3.4339	0.7199	-1.029
C(11)	-4.9448	0.9946	-0.9108
C(12)	-2.6477	1.9906	-1.4013
C(13)	-4.7712	1.0843	1.6025
C(14)	-5.3004	1.7938	0.3501
H(15)	-3.5857	-3.8504	0.1132
H(16)	-1.7768	-0.0111	0.1274
H(17)	-1.9229	-5.5801	0.874
H(18)	-1.0679	-4.3505	1.8669
H(19)	-2.7408	-4.8591	2.2759
H(20)	-2.8871	0.3408	2.4171
H(21)	-2.7384	1.8252	1.4721
H(22)	-3.287	0.0132	-1.888
H(23)	-5.3086	1.5341	-1.817
H(24)	-5.4925	0.0221	-0.8808
H(25)	-1.5666	1.7659	-1.549
H(26)	-3.024	2.4299	-2.3533
H(27)	-2.7181	2.7813	-0.6238
H(28)	-4.9943	1.696	2.5091
H(29)	-5.3073	0.1148	1.7281
H(30)	-6.4077	1.9163	0.4232
H(31)	-4.8697	2.8202	0.2891

2-Methyl (*R*,*R*,***R***,*S*)-(e,e)



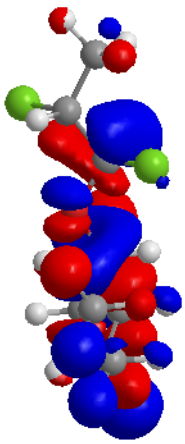
Cl(1)	-2.8749	-2.9473	-0.7534
C(2)	-2.616	-1.9669	0.7467
O(3)	-3.813	-2.017	1.4834
O(4)	-2.1706	-0.6705	0.3853
C(5)	-1.5219	-2.6228	1.5948
C(6)	-3.1331	0.3503	0.3822
C(7)	-1.8019	-4.0754	1.9957
Cl(8)	-1.2338	-1.6795	3.0927
C(9)	-4.1398	0.181	-0.7606
C(10)	-2.3907	1.6927	0.2539
C(11)	-3.3825	2.8675	0.1726
C(12)	-1.4109	1.9213	1.4201
C(13)	-5.1222	1.3587	-0.8348
C(14)	-4.3694	2.6853	-0.9869
H(15)	-0.5567	-2.5858	1.042
H(16)	-3.6622	0.3617	1.3638
H(17)	-0.9751	-4.4926	2.616
H(18)	-2.7426	-4.1684	2.5845
H(19)	-1.89	-4.7485	1.1145
H(20)	-3.5931	0.0972	-1.7297
H(21)	-4.7349	-0.7528	-0.6316
H(22)	-1.7975	1.675	-0.695
H(23)	-3.9474	2.9462	1.1314
H(24)	-2.8285	3.827	0.0378
H(25)	-1.9407	1.9078	2.3995
H(26)	-0.8961	2.9045	1.3264
H(27)	-0.6145	1.1444	1.4532
H(28)	-5.8215	1.22	-1.694
H(29)	-5.7427	1.3862	0.0926
H(30)	-5.0927	3.5352	-1.0113
H(31)	-3.8167	2.6948	-1.9563

2-Methyl (*R*,*R*,***S***,*R*)-(a,a)



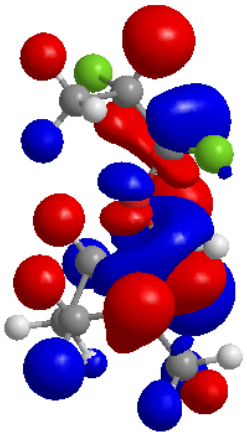
Cl(1)	-0.8274	-2.1319	1.3305
C(2)	-2.6262	-2.1722	1.1335
O(3)	-3.1901	-2.1501	2.4208
O(4)	-3.0221	-1.1048	0.2902
C(5)	-3.0379	-3.4841	0.4621
C(6)	-3.1235	0.1509	0.9101
C(7)	-2.5966	-4.7497	1.2052
Cl(8)	-4.8163	-3.5522	0.2461
C(9)	-4.5616	0.392	1.3875
C(10)	-2.69	1.2237	-0.1048
C(11)	-3.6994	1.3357	-1.2625
C(12)	-2.4211	2.5856	0.5605
C(13)	-5.556	0.4897	0.2217
C(14)	-5.1324	1.5794	-0.7708
H(15)	-2.623	-3.5145	-0.57
H(16)	-2.4208	0.1964	1.7748
H(17)	-2.9631	-5.6706	0.6956
H(18)	-1.4892	-4.8469	1.2501
H(19)	-2.9792	-4.7705	2.2508
H(20)	-4.8917	-0.4157	2.0806
H(21)	-4.604	1.3343	1.982
H(22)	-1.7078	0.9044	-0.5429
H(23)	-3.3933	2.1508	-1.9601
H(24)	-3.6837	0.3896	-1.8552
H(25)	-1.6439	2.4986	1.3538
H(26)	-2.0501	3.3278	-0.1829
H(27)	-3.3291	3.018	1.0332
H(28)	-6.5789	0.7086	0.6113
H(29)	-5.617	-0.4904	-0.3074
H(30)	-5.8348	1.5948	-1.6384
H(31)	-5.2056	2.5795	-0.2837

2-Methyl (*R*,*R*,***S***,*R*)-(e,e)



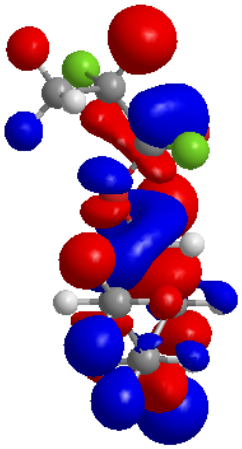
Cl(1)	-0.0363	1.2528	0.221
C(2)	-0.6922	-0.3476	0.7559
O(3)	-0.7687	-0.3251	2.1596
O(4)	-1.9261	-0.5903	0.1021
C(5)	0.2836	-1.4558	0.3552
C(6)	-3.0311	0.0827	0.6444
C(7)	1.7102	-1.278	0.8862
Cl(8)	-0.3245	-3.0534	0.8945
C(9)	-3.7757	-0.8416	1.6159
C(10)	-3.9748	0.5101	-0.4924
C(11)	-5.2184	1.2102	0.0875
C(12)	-3.2836	1.4356	-1.5096
C(13)	-5.013	-0.1494	2.2043
C(14)	-5.9578	0.312	1.0877
H(15)	0.3245	-1.525	-0.7547
H(16)	-2.7017	1.005	1.1753
H(17)	2.3634	-2.1321	0.5937
H(18)	2.202	-0.3679	0.4766
H(19)	1.7323	-1.2019	1.9971
H(20)	-4.0909	-1.7696	1.0823
H(21)	-3.1089	-1.1644	2.4488
H(22)	-4.3106	-0.4064	-1.0393
H(23)	-4.9091	2.1528	0.5979
H(24)	-5.9148	1.4981	-0.7356
H(25)	-2.8938	2.355	-1.0176
H(26)	-3.9909	1.7532	-2.309
H(27)	-2.4314	0.9322	-2.0188
H(28)	-5.5505	-0.8449	2.8925
H(29)	-4.6926	0.731	2.8105
H(30)	-6.8248	0.862	1.5258
H(31)	-6.3689	-0.5784	0.5553

2-Methyl (*R*,*R*,***S***,*S*)-(a,a)



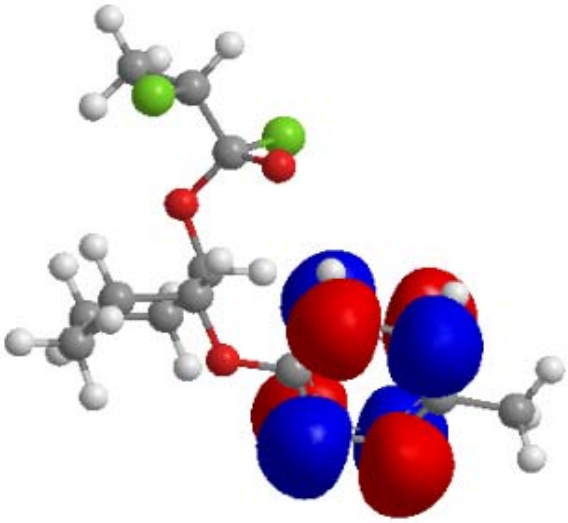
Cl(1)	-0.9199	-2.1305	1.53
C(2)	-2.6591	-2.2145	1.0374
O(3)	-3.3971	-2.348	2.2279
O(4)	-3.0038	-1.096	0.2462
C(5)	-2.8823	-3.4763	0.204
C(6)	-3.2582	0.0897	0.9526
C(7)	-2.1808	-3.4591	-1.1571
Cl(8)	-4.6316	-3.7749	-0.0378
C(9)	-4.7657	0.2427	1.1908
C(10)	-2.7	1.2634	0.1295
C(11)	-3.4971	1.4538	-1.1741
C(12)	-2.6071	2.5634	0.948
C(13)	-5.5459	0.4248	-0.1194
C(14)	-5.0023	1.6136	-0.9221
H(15)	-2.5298	-4.3636	0.7761
H(16)	-2.7172	0.0689	1.9274
H(17)	-2.334	-4.4174	-1.705
H(18)	-2.5574	-2.6379	-1.8083
H(19)	-1.0807	-3.3257	-1.0558
H(20)	-5.1695	-0.641	1.7374
H(21)	-4.9529	1.1206	1.8522
H(22)	-1.6442	1.0113	-0.1543
H(23)	-3.1084	2.3361	-1.7353
H(24)	-3.3403	0.5658	-1.8329
H(25)	-1.9711	2.4238	1.8519
H(26)	-2.1488	3.3818	0.3471
H(27)	-3.5999	2.9234	1.2939
H(28)	-6.6292	0.5804	0.101
H(29)	-5.473	-0.5031	-0.7346
H(30)	-5.5438	1.6929	-1.8951
H(31)	-5.1993	2.5616	-0.3696

2-Methyl (*R*,*R*,***S***,*S*)-(e,e)



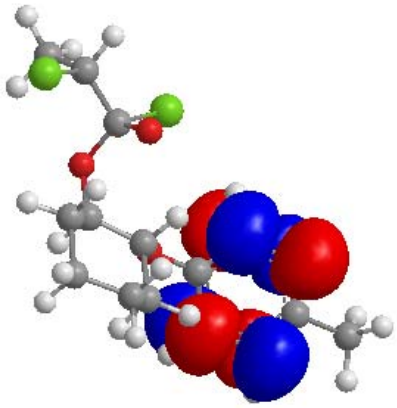
Cl(1)	-0.0836	1.1894	0.1238
C(2)	-0.7283	-0.4157	0.6561
O(3)	-0.6865	-0.4013	2.0625
O(4)	-2.0064	-0.6537	0.1017
C(5)	0.2169	-1.5153	0.1716
C(6)	-3.0701	0.0037	0.7378
C(7)	0.2521	-1.6873	-1.3498
Cl(8)	-0.191	-3.0828	0.9355
C(9)	-3.7163	-0.9289	1.7696
C(10)	-4.1102	0.412	-0.3198
C(11)	-5.3198	1.0865	0.3548
C(12)	-3.5185	1.3536	-1.3844
C(13)	-4.9185	-0.2594	2.4501
C(14)	-5.9581	0.1716	1.4082
H(15)	1.2492	-1.2991	0.5276
H(16)	-2.7086	0.9322	1.236
H(17)	0.9879	-2.4678	-1.6526
H(18)	-0.7395	-1.9876	-1.758
H(19)	0.5553	-0.7497	-1.8669
H(20)	-4.0506	-1.8674	1.2669
H(21)	-2.9797	-1.2315	2.5493
H(22)	-4.4709	-0.5107	-0.8406
H(23)	-4.9918	2.0368	0.839
H(24)	-6.0857	1.3567	-0.4107
H(25)	-3.1138	2.2815	-0.9207
H(26)	-4.2923	1.6546	-2.127
H(27)	-2.6953	0.8707	-1.9574
H(28)	-5.385	-0.9617	3.1816
H(29)	-4.5727	0.6327	3.0246
H(30)	-6.8047	0.6996	1.9088
H(31)	-6.3825	-0.7321	0.9094

2-OTol (*R*,*R*,***R***,*R*)-(a,a)



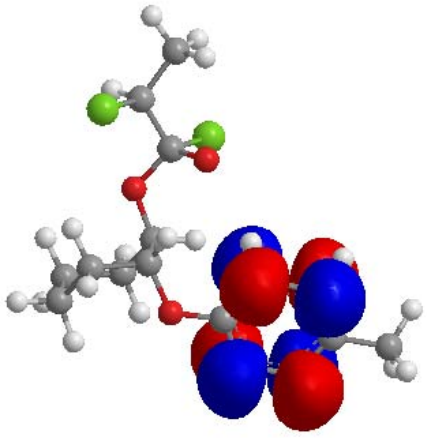
Cl(1)	-2.4148	-1.6477	1.9824
C(2)	-2.4975	-0.5552	0.5429
O(3)	-2.0784	-1.3342	-0.5494
O(4)	-1.7424	0.6162	0.7711
C(5)	-3.9501	-0.1505	0.2949
C(6)	-0.3667	0.5129	0.5171
C(7)	-4.5384	0.7574	1.3779
Cl(8)	-4.1188	0.6463	-1.3003
C(9)	0.3565	1.4602	1.4846
C(10)	-0.0552	0.8894	-0.937
C(11)	-0.3973	2.3621	-1.2066
O(12)	1.3052	0.714	-1.2197
C(13)	0.0007	2.93	1.2197
C(14)	0.3163	3.3098	-0.2323
C(15)	1.8519	-0.5434	-1.1659
C(16)	3.1753	-0.6891	-0.7257
C(17)	3.7954	-1.9337	-0.6052
C(18)	3.1013	-3.1091	-0.9019
C(19)	1.7723	-2.9891	-1.3164
C(20)	1.1654	-1.737	-1.4343
C(21)	3.7728	-4.4524	-0.7708
H(22)	-4.5802	-1.0641	0.2116
H(23)	-0.0299	-0.5235	0.7513
H(24)	-5.609	0.9904	1.1745
H(25)	-3.9934	1.726	1.449
H(26)	-4.5024	0.2797	2.3823
H(27)	0.0956	1.1968	2.5378
H(28)	1.4605	1.3263	1.3943
H(29)	-0.6503	0.2921	-1.6639
H(30)	-0.1234	2.6296	-2.2554
H(31)	-1.4989	2.5178	-1.1224

2-OTol (*R*,*R*,***R***,*R*)-(e,e)



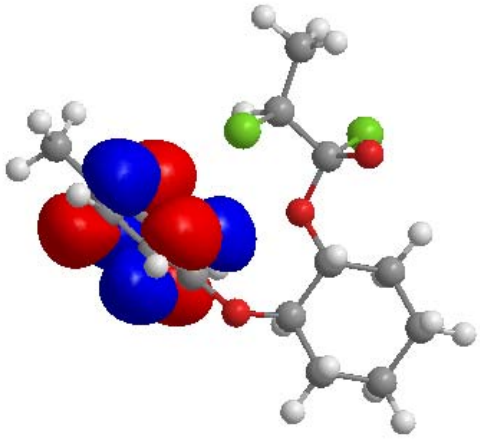
Cl(1)	-7.3254	-8.6774	-5.9067
C(2)	-6.4141	-7.624	-7.061
O(3)	-5.6878	-8.5338	-7.8497
O(4)	-5.6806	-6.6383	-6.3567
C(5)	-7.4334	-6.9308	-7.9694
C(6)	-4.2922	-6.8021	-6.2168
C(7)	-8.3248	-5.9111	-7.2547
Cl(8)	-6.6267	-6.142	-9.3586
C(9)	-3.5578	-6.5426	-7.5379
C(10)	-3.8656	-8.0679	-5.4672
C(11)	-2.333	-8.1673	-5.4052
O(12)	-4.3868	-8.0147	-4.1641
C(13)	-2.0362	-6.626	-7.3681
C(14)	-1.6659	-7.9898	-6.775
C(15)	-4.1528	-9.1219	-3.3894
C(16)	-5.0807	-10.1682	-3.3023
C(17)	-4.9005	-11.2549	-2.4451
C(18)	-3.8063	-11.3091	-1.5779
C(19)	-2.9327	-10.218	-1.5677
C(20)	-3.1339	-9.135	-2.4255
C(21)	-3.6281	-12.4811	-0.6466
H(22)	-8.0873	-7.6978	-8.4429
H(23)	-3.9825	-5.9517	-5.5535
H(24)	-9.071	-5.4646	-7.9517
H(25)	-7.7331	-5.075	-6.8182
H(26)	-8.9065	-6.3752	-6.4274
H(27)	-3.843	-7.279	-8.3204
H(28)	-3.83	-5.5343	-7.9331
H(29)	-4.256	-8.9779	-5.9755
H(30)	-1.935	-7.3828	-4.7178
H(31)	-2.0231	-9.157	-4.9922

2-OTol (*R*,*R*,***R***,*S*)-(a,a)

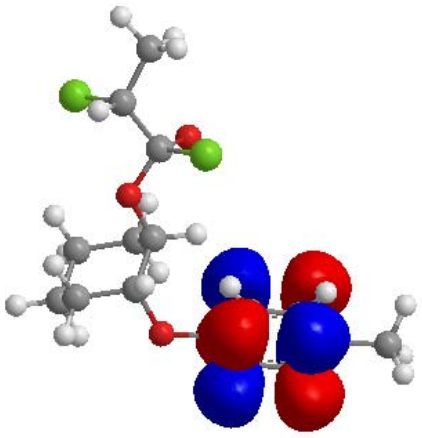


Cl(1)	-2.4043	-1.6677	2.0443
C(2)	-2.4975	-0.6323	0.5629
O(3)	-2.0115	-1.3907	-0.5141
O(4)	-1.7981	0.5761	0.7955
C(5)	-3.9589	-0.2881	0.2685
C(6)	-0.4013	0.5024	0.6728
C(7)	-4.8742	-1.5019	0.0742
Cl(8)	-4.083	0.744	-1.192
C(9)	0.2068	1.5036	1.6649
C(10)	0.0394	0.8282	-0.7599
C(11)	-0.302	2.2816	-1.1202
O(12)	1.4236	0.6743	-0.9074
C(13)	-0.1515	2.9528	1.3075
C(14)	0.2968	3.2823	-0.1217
C(15)	1.9957	-0.5645	-0.7609
C(16)	3.2986	-0.6492	-0.2486
C(17)	3.9476	-1.8662	-0.0361
C(18)	3.3052	-3.0756	-0.3131
C(19)	1.9906	-3.0162	-0.7826
C(20)	1.3544	-1.7905	-0.9918
C(21)	3.9993	-4.3933	-0.0784
H(22)	-4.363	0.3362	1.096
H(23)	-0.0602	-0.5141	0.976
H(24)	-5.9205	-1.1908	-0.1504
H(25)	-4.9339	-2.1357	0.9865
H(26)	-4.5297	-2.1507	-0.7629
H(27)	-0.1478	1.2747	2.6986
H(28)	1.3169	1.393	1.685
H(29)	-0.4705	0.1889	-1.5156
H(30)	0.0664	2.5148	-2.1481
H(31)	-1.409	2.4162	-1.1478

2-OTol (*R*,*R*,***R***,*S*)-(e,e)



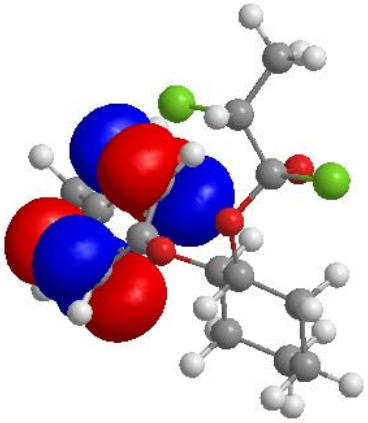
Cl(1)	-3.4061	-3.3701	1.1362
C(2)	-2.5469	-2.6855	-0.3034
O(3)	-1.8353	-3.7367	-0.9075
O(4)	-1.7663	-1.5797	0.1156
C(5)	-3.5803	-2.1864	-1.3175
C(6)	-0.3935	-1.7957	0.2947
C(7)	-4.598	-3.2398	-1.7695
Cl(8)	-2.7624	-1.5458	-2.7783
C(9)	-0.1154	-2.7954	1.4259
C(10)	0.2732	-0.4531	0.6286
C(11)	1.7812	-0.6529	0.8367
O(12)	0.1383	0.4901	-0.3998
C(13)	1.3888	-2.9889	1.6637
C(14)	2.0645	-1.648	1.9681
C(15)	-1.0724	1.0848	-0.6538
C(16)	-1.3484	1.5099	-1.9611
C(17)	-2.5659	2.0852	-2.3279
C(18)	-3.5875	2.249	-1.3896
C(19)	-3.3444	1.8092	-0.0858
C(20)	-2.1197	1.2387	0.2683
C(21)	-4.9202	2.8401	-1.7729
H(22)	-4.1297	-1.3182	-0.8903
H(23)	0.0382	-2.1644	-0.6659
H(24)	-5.2955	-2.8305	-2.5363
H(25)	-5.2412	-3.5924	-0.9332
H(26)	-4.1007	-4.1332	-2.2111
H(27)	-0.5934	-2.4337	2.367
H(28)	-0.5473	-3.7977	1.2021
H(29)	-0.1262	-0.0342	1.5801
H(30)	2.244	-1.0244	-0.1086
H(31)	2.2686	0.3232	1.0745



2-OTol (*R*,*R*,***S***,*R*)-(a,a)

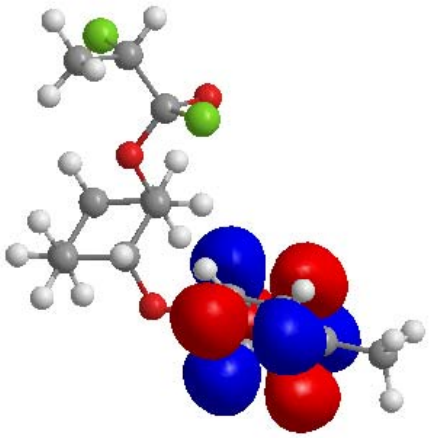
Cl(1)	-2.4844	-2.0669	-0.7309
C(2)	-2.6069	-0.6999	0.4493
O(3)	-2.2095	-1.1882	1.7056
O(4)	-1.8399	0.3891	-0.0296
C(5)	-4.063	-0.2431	0.5589
C(6)	-0.4585	0.3075	0.2071
C(7)	-5.046	-1.3363	0.9908
Cl(8)	-4.2116	1.1272	1.7053
C(9)	-0.0891	1.0594	1.4919
C(10)	0.2613	0.9097	-1.0046
C(11)	-0.0419	2.4102	-1.1158
O(12)	1.6511	0.7626	-0.9177
C(13)	-0.3669	2.5654	1.3845
C(14)	0.3411	3.1672	0.1643
C(15)	2.1981	-0.4935	-0.8459
C(16)	3.3852	-0.6689	-0.1208
C(17)	3.986	-1.9167	0.0508
C(18)	3.4046	-3.0666	-0.4888
C(19)	2.2055	-2.9184	-1.1912
C(20)	1.6153	-1.6635	-1.3567
C(21)	4.0199	-4.4278	-0.286
H(22)	-4.3933	0.167	-0.4214
H(23)	-0.1685	-0.7619	0.3134
H(24)	-6.0852	-0.9412	1.0689
H(25)	-4.7758	-1.7678	1.9813
H(26)	-5.0919	-2.1744	0.2606
H(27)	-0.6415	0.6442	2.3665
H(28)	0.9942	0.904	1.7103
H(29)	-0.0873	0.431	-1.9511
H(30)	0.5057	2.845	-1.986
H(31)	-1.129	2.5618	-1.3179

2-OTol (*R*,*R*,***S***,*R*)-(e,e)



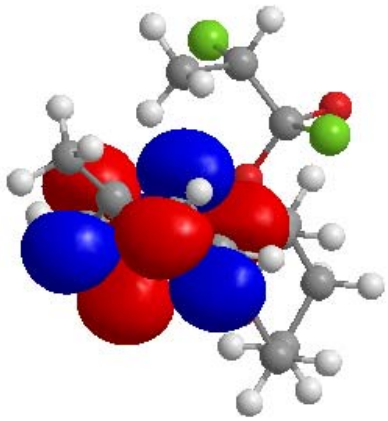
Cl(1)	-5.1143	-8.1603	-8.1619
C(2)	-6.3927	-7.5718	-7.0201
O(3)	-6.8797	-8.6917	-6.3268
O(4)	-5.8787	-6.521	-6.2193
C(5)	-7.5441	-7.0051	-7.8617
C(6)	-5.2622	-6.8363	-4.9954
C(7)	-8.1758	-7.9995	-8.8437
Cl(8)	-8.8553	-6.3554	-6.8286
C(9)	-4.1302	-7.8605	-5.1081
C(10)	-6.2527	-7.1704	-3.8768
C(11)	-5.508	-7.3729	-2.5485
O(12)	-7.1754	-6.1235	-3.7402
C(13)	-3.4014	-8.0313	-3.7671
C(14)	-4.3971	-8.4246	-2.6692
C(15)	-8.2132	-6.3844	-2.8844
C(16)	-9.2818	-7.2165	-3.2443
C(17)	-10.3639	-7.4386	-2.3912
C(18)	-10.4435	-6.7961	-1.1523
C(19)	-9.4189	-5.9092	-0.8097
C(20)	-8.3449	-5.6902	-1.6745
C(21)	-11.6077	-7.0491	-0.2286
H(22)	-7.178	-6.1243	-8.4354
H(23)	-4.7761	-5.8748	-4.6848
H(24)	-9.0216	-7.538	-9.4039
H(25)	-8.5723	-8.9004	-8.3227
H(26)	-7.4571	-8.3483	-9.6176
H(27)	-4.5293	-8.8577	-5.4045
H(28)	-3.3915	-7.5377	-5.88
H(29)	-6.7978	-8.1106	-4.112
H(30)	-5.0593	-6.4055	-2.2189
H(31)	-6.2146	-7.6938	-1.7463

2-OTol (*R*,*R*,***S***,*S*)-(a,a)



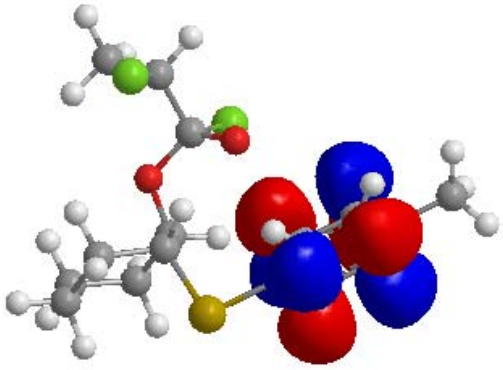
Cl(1)	-2.4873	-2.1263	-0.6531
C(2)	-2.6457	-0.6291	0.3504
O(3)	-2.3815	-1.0249	1.6735
O(4)	-1.8051	0.3899	-0.1489
C(5)	-4.0887	-0.1286	0.2897
C(6)	-0.4562	0.3073	0.2263
C(7)	-4.519	0.3692	-1.0929
Cl(8)	-4.3589	1.1682	1.4953
C(9)	-0.1997	1.109	1.5089
C(10)	0.3788	0.8593	-0.9343
C(11)	0.1139	2.3584	-1.1279
O(12)	1.7506	0.6869	-0.7149
C(13)	-0.4577	2.6101	1.3173
C(14)	0.3767	3.1603	0.1543
C(15)	2.2677	-0.581	-0.6198
C(16)	3.394	-0.7893	0.189
C(17)	3.9636	-2.0495	0.3761
C(18)	3.4092	-3.18	-0.2286
C(19)	2.2682	-3.0002	-1.0151
C(20)	1.7064	-1.7337	-1.1913
C(21)	4.0261	-4.5402	-0.0241
H(22)	-4.7773	-0.9436	0.6063
H(23)	-0.1899	-0.7608	0.3951
H(24)	-5.5819	0.704	-1.0922
H(25)	-4.4407	-0.4302	-1.8632
H(26)	-3.8987	1.2273	-1.4379
H(27)	-0.8282	0.7341	2.3489
H(28)	0.8585	0.9596	1.8302
H(29)	0.1057	0.36	-1.8945
H(30)	0.7521	2.7535	-1.9543
H(31)	-0.9453	2.5146	-1.4437

2-OTol (*R*,*R*,***S***,*S*)-(e,e)



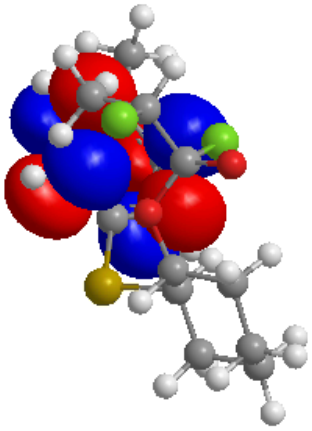
Cl(1)	-0.409	-2.4932	-1.6442
C(2)	-1.5603	-1.634	-0.5455
O(3)	-2.18	-2.654	0.1975
O(4)	-0.8968	-0.641	0.2132
C(5)	-2.641	-0.9574	-1.3887
C(6)	-0.2031	-1.0968	1.3437
C(7)	-2.1291	0.1904	-2.2618
Cl(8)	-3.9716	-0.3624	-0.3484
C(9)	-1.1525	-1.1614	2.5503
C(10)	0.9351	-0.1194	1.6662
C(11)	1.6817	-0.5615	2.9313
O(12)	1.8877	-0.0534	0.6386
C(13)	-0.4224	-1.604	3.8256
C(14)	0.7391	-0.6542	4.1371
C(15)	1.5818	0.6444	-0.5012
C(16)	1.862	0.0849	-1.7553
C(17)	1.5462	0.7317	-2.9507
C(18)	0.9393	1.9902	-2.9415
C(19)	0.6758	2.5765	-1.7008
C(20)	0.985	1.914	-0.5118
C(21)	0.5806	2.7054	-4.2183
H(22)	-3.1255	-1.714	-2.0459
H(23)	0.241	-2.0978	1.138
H(24)	-2.9443	0.626	-2.8839
H(25)	-1.339	-0.1466	-2.969
H(26)	-1.7034	1.0149	-1.6475
H(27)	-1.6123	-0.1582	2.7163
H(28)	-1.997	-1.8651	2.3757
H(29)	0.5195	0.8924	1.8728
H(30)	2.1603	-1.5542	2.7556
H(31)	2.5024	0.1602	3.1613

2-STol (*R*,*R*,***R***,*R*)-(a,a)

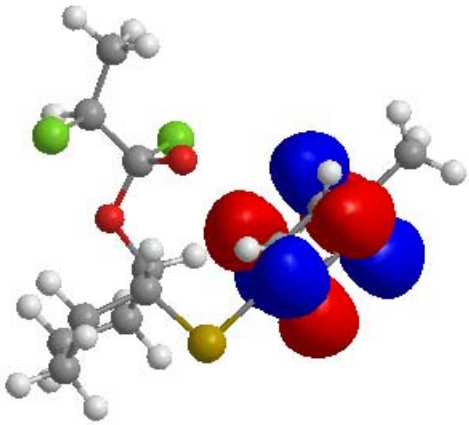


Cl(1)	-2.4251	0.3559	1.8738
C(2)	-1.8881	0.6425	0.1701
O(3)	-1.5849	-0.6348	-0.3392
O(4)	-0.8239	1.5742	0.1455
C(5)	-3.0509	1.2063	-0.6446
C(6)	0.4532	1.0182	0.3137
C(7)	-3.499	2.606	-0.2167
Cl(8)	-2.6466	1.2192	-2.3892
C(9)	1.3328	2.0491	1.0328
C(10)	1.0355	0.6298	-1.0578
C(11)	1.3913	1.8678	-1.903
S(12)	2.52	-0.4263	-0.8631
C(13)	1.5983	3.2885	0.1689
C(14)	2.2617	2.8855	-1.1535
C(15)	1.6116	-1.9094	-0.3224
C(16)	1.6004	-2.2617	1.0287
C(17)	0.8977	-3.3937	1.4456
C(18)	0.2157	-4.1969	0.5242
C(19)	0.2425	-3.835	-0.8276
C(20)	0.9387	-2.7024	-1.2543
C(21)	-0.5551	-5.4095	0.9828
H(22)	-3.9209	0.5158	-0.5717
H(23)	0.3643	0.1391	0.9927
H(24)	-4.3623	2.9592	-0.8268
H(25)	-2.6824	3.3553	-0.3254
H(26)	-3.8336	2.6266	0.8445
H(27)	0.8478	2.3567	1.9904
H(28)	2.3074	1.5843	1.3142
H(29)	0.289	0.0509	-1.6529
H(30)	1.8866	1.5667	-2.8567
H(31)	0.4445	2.381	-2.2001

2-STol (*R*,*R*,***R***,*R*)-(e,e)



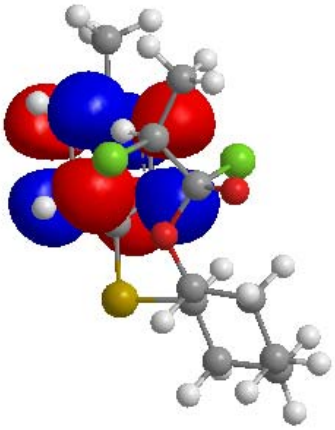
Cl(1)	-6.2005	-9.6377	-6.9442
C(2)	-6.2959	-8.0717	-7.8366
O(3)	-5.8223	-8.3264	-9.1354
O(4)	-5.6743	-7.0004	-7.1504
C(5)	-7.7762	-7.7081	-8.0168
C(6)	-4.2723	-6.9595	-7.0129
C(7)	-8.5298	-7.4047	-6.7212
Cl(8)	-7.9646	-6.3253	-9.1416
C(9)	-3.4674	-7.4356	-8.225
C(10)	-3.7592	-7.5859	-5.7046
C(11)	-2.2364	-7.3817	-5.5508
S(12)	-4.5185	-6.799	-4.2334
C(13)	-1.9645	-7.1747	-8.0433
C(14)	-1.4578	-7.8762	-6.7772
C(15)	-5.6848	-8.1085	-3.768
C(16)	-7.041	-7.797	-3.6486
C(17)	-7.9545	-8.7901	-3.2898
C(18)	-7.5313	-10.0997	-3.0375
C(19)	-6.1653	-10.3908	-3.1282
C(20)	-5.2439	-9.4038	-3.4829
C(21)	-8.5363	-11.1578	-2.6575
H(22)	-8.3002	-8.5448	-8.5324
H(23)	-4.0459	-5.8646	-6.9231
H(24)	-9.6009	-7.1669	-6.9157
H(25)	-8.087	-6.5372	-6.1824
H(26)	-8.5288	-8.2785	-6.0329
H(27)	-3.5895	-8.5358	-8.3621
H(28)	-3.8047	-6.9094	-9.1502
H(29)	-3.9295	-8.6852	-5.738
H(30)	-2.002	-6.2994	-5.407
H(31)	-1.8654	-7.9227	-4.6463



2-STol (*R*,*R*,***R***,*S*)-(a,a)

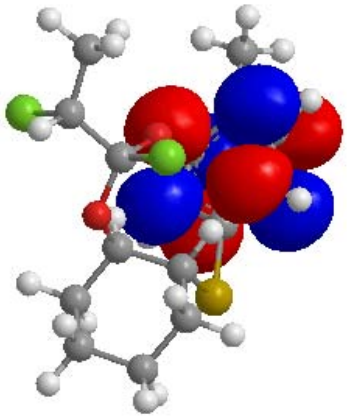
Cl(1)	-2.3952	0.3619	1.8671
C(2)	-1.889	0.6198	0.1484
O(3)	-1.5744	-0.6454	-0.3791
O(4)	-0.8299	1.561	0.1188
C(5)	-3.0585	1.1917	-0.6543
C(6)	0.4471	1.0246	0.3468
C(7)	-4.3213	0.3239	-0.6567
Cl(8)	-2.5742	1.4754	-2.3569
C(9)	1.2833	2.0841	1.0758
C(10)	1.0884	0.6103	-0.9908
C(11)	1.4822	1.8289	-1.8474
S(12)	2.5643	-0.4397	-0.7114
C(13)	1.5741	3.3034	0.1916
C(14)	2.31	2.8696	-1.0816
C(15)	1.6372	-1.9082	-0.1624
C(16)	1.5999	-2.2344	1.1948
C(17)	0.88	-3.3525	1.6208
C(18)	0.2036	-4.1645	0.7038
C(19)	0.2609	-3.8324	-0.6546
C(20)	0.9771	-2.7156	-1.091
C(21)	-0.5918	-5.3564	1.1751
H(22)	-3.3171	2.1985	-0.2572
H(23)	0.3443	0.1583	1.0399
H(24)	-5.1338	0.7925	-1.259
H(25)	-4.7401	0.1828	0.3641
H(26)	-4.128	-0.6868	-1.0828
H(27)	0.7531	2.4119	2.0023
H(28)	2.2492	1.6383	1.412
H(29)	0.3677	0.0179	-1.6045
H(30)	2.0254	1.5073	-2.7678
H(31)	0.5493	2.3296	-2.2035

2-STol (*R*,*R*,***R***,*S*)-(e,e)



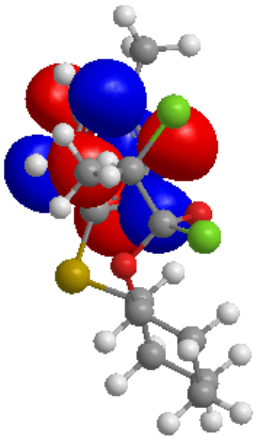
Cl(1)	-5.8931	-9.7963	-7.025
C(2)	-6.2971	-8.1527	-7.6536
O(3)	-6.0078	-8.1116	-9.027
O(4)	-5.6875	-7.1267	-6.8891
C(5)	-7.816	-7.9554	-7.5435
C(6)	-4.2851	-6.9976	-6.8595
C(7)	-8.66	-8.9846	-8.3054
Cl(8)	-8.2992	-6.321	-8.1015
C(9)	-3.5369	-7.4344	-8.1231
C(10)	-3.6589	-7.5892	-5.5836
C(11)	-2.1464	-7.2909	-5.5255
S(12)	-4.3789	-6.8725	-4.0572
C(13)	-2.0313	-7.1416	-8.0306
C(14)	-1.4282	-7.7974	-6.7829
C(15)	-5.7759	-8.0161	-3.86
C(16)	-7.0835	-7.5316	-3.9376
C(17)	-8.1596	-8.4091	-3.7889
C(18)	-7.9483	-9.7744	-3.5654
C(19)	-6.6329	-10.2412	-3.4672
C(20)	-5.5501	-9.3707	-3.6011
C(21)	-9.1022	-10.7372	-3.444
H(22)	-8.116	-7.9841	-6.4742
H(23)	-4.1143	-5.8916	-6.7839
H(24)	-9.7501	-8.781	-8.1919
H(25)	-8.5042	-10.0205	-7.9309
H(26)	-8.4321	-8.9833	-9.3957
H(27)	-3.6483	-8.5319	-8.2826
H(28)	-3.9326	-6.8963	-9.0175
H(29)	-3.763	-8.6982	-5.5995
H(30)	-1.9688	-6.1924	-5.434
H(31)	-1.6878	-7.7747	-4.6292

2-STol (*R*,*R*,*S*,*R*)-(a,a)



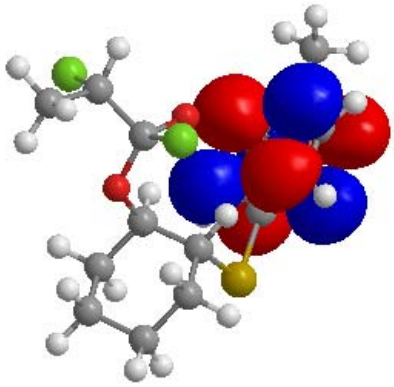
Cl(1)	-1.7685	-0.3684	-1.4719
C(2)	-1.8726	0.5868	0.0628
O(3)	-1.8639	-0.3577	1.1063
O(4)	-0.8199	1.5386	0.0732
C(5)	-3.2043	1.3371	0.1227
C(6)	0.1919	1.3275	1.022
C(7)	-4.4485	0.4493	0.0137
Cl(8)	-3.3175	2.2753	1.6465
C(9)	1.0025	2.627	1.1247
C(10)	1.0822	0.132	0.643
C(11)	1.9541	0.4333	-0.5902
S(12)	2.1608	-0.3456	2.0466
C(13)	1.8028	2.9126	-0.1529
C(14)	2.7436	1.744	-0.47
C(15)	0.8359	-1.0906	3.0497
C(16)	0.3468	-0.4169	4.1695
C(17)	-0.6743	-0.9884	4.9339
C(18)	-1.2098	-2.2361	4.5988
C(19)	-0.701	-2.9045	3.478
C(20)	0.3189	-2.3436	2.7093
C(21)	-2.3247	-2.8535	5.4053
H(22)	-3.2369	2.0976	-0.6889
H(23)	-0.3022	1.1815	2.0116
H(24)	-5.3841	1.0503	0.0878
H(25)	-4.4802	-0.3207	0.8176
H(26)	-4.5025	-0.0813	-0.9626
H(27)	0.318	3.484	1.3351
H(28)	1.7036	2.5717	1.9906
H(29)	0.4624	-0.7594	0.3859
H(30)	2.6476	-0.4156	-0.8
H(31)	1.2906	0.5137	-1.4849

2-STol (*R*,*R*,*S*,*R*)-(e,e)

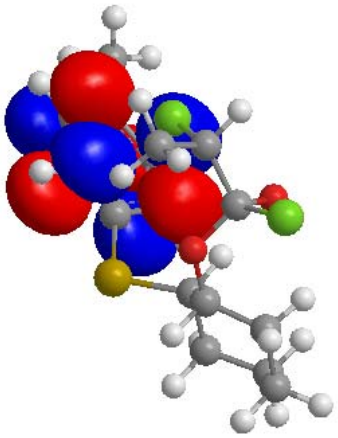


Cl(1)	-6.2914	-8.4697	-9.278
C(2)	-6.269	-8.0303	-7.5234
O(3)	-5.881	-9.17	-6.7972
O(4)	-5.4693	-6.8883	-7.2723
C(5)	-7.6918	-7.68	-7.0725
C(6)	-4.0958	-7.0592	-7.0255
C(7)	-8.2884	-6.449	-7.7598
Cl(8)	-8.8221	-9.0623	-7.1874
C(9)	-3.3595	-7.87	-8.0952
C(10)	-3.7705	-7.5352	-5.5996
C(11)	-2.2445	-7.5609	-5.3743
S(12)	-4.4744	-6.4021	-4.3435
C(13)	-1.844	-7.8747	-7.8449
C(14)	-1.5353	-8.4086	-6.4402
C(15)	-5.598	-7.5783	-3.5314
C(16)	-6.9545	-7.2596	-3.4247
C(17)	-7.8331	-8.142	-2.7931
C(18)	-7.373	-9.3456	-2.2476
C(19)	-6.0106	-9.6489	-2.3516
C(20)	-5.1242	-8.7728	-2.9802
C(21)	-8.3106	-10.3036	-1.5561
H(22)	-7.6549	-7.4627	-5.9825
H(23)	-3.6784	-6.0209	-7.1006
H(24)	-9.2715	-6.1725	-7.3141
H(25)	-8.4532	-6.6132	-8.848
H(26)	-7.6281	-5.5593	-7.6521
H(27)	-3.7043	-8.9295	-8.0929
H(28)	-3.5559	-7.4422	-9.1071
H(29)	-4.1223	-8.5816	-5.4651
H(30)	-1.828	-6.5258	-5.4131
H(31)	-2.0077	-7.9745	-4.3638

2-STol (*R*,*R*,*S*,*S*)-(a,a)



Cl(1)	-1.8041	-0.3878	-1.462
C(2)	-1.8692	0.5922	0.0587
O(3)	-1.8635	-0.3581	1.0986
O(4)	-0.822	1.5449	0.0855
C(5)	-3.2041	1.3363	0.1127
C(6)	0.2528	1.2627	0.9421
C(7)	-3.3676	2.41	-0.967
Cl(8)	-3.4433	2.0713	1.7282
C(9)	1.072	2.5527	1.088
C(10)	1.1142	0.1046	0.4123
C(11)	1.8917	0.5029	-0.8563
S(12)	2.2944	-0.4702	1.6925
C(13)	1.7794	2.9407	-0.2172
C(14)	2.6909	1.8032	-0.6936
C(15)	1.0469	-1.3063	2.722
C(16)	0.6378	-0.7319	3.9268
C(17)	-0.3277	-1.3703	4.7081
C(18)	-0.8876	-2.5885	4.3058
C(19)	-0.4562	-3.1588	3.1026
C(20)	0.5091	-2.5294	2.3151
C(21)	-1.9488	-3.2729	5.1301
H(22)	-4.04	0.6073	0.0182
H(23)	-0.1698	1.0399	1.9501
H(24)	-4.364	2.9046	-0.9012
H(25)	-3.2961	1.9812	-1.9914
H(26)	-2.5933	3.206	-0.8846
H(27)	0.4071	3.3885	1.4141
H(28)	1.834	2.4316	1.8937
H(29)	0.4759	-0.7692	0.1425
H(30)	2.5654	-0.325	-1.1822
H(31)	1.1637	0.6505	-1.6903



2-STol (*R*,*R*,*S*,*S*)-(e,e)

Cl(1)	-6.0957	-7.908	-9.7189
C(2)	-6.24	-7.9122	-7.9119
O(3)	-5.8048	-9.1769	-7.4762
O(4)	-5.5738	-6.7984	-7.3468
C(5)	-7.7323	-7.8076	-7.5812
C(6)	-4.2186	-6.9327	-6.9927
C(7)	-8.3479	-6.4374	-7.8769
Cl(8)	-8.0525	-8.2474	-5.8783
C(9)	-3.3387	-7.567	-8.0761
C(10)	-4.0354	-7.552	-5.5942
C(11)	-2.5387	-7.6708	-5.2355
S(12)	-4.775	-6.4578	-4.3252
C(13)	-1.8652	-7.6302	-7.6507
C(14)	-1.7405	-8.3944	-6.3272
C(15)	-5.7368	-7.6424	-3.3401
C(16)	-6.997	-7.2341	-2.8872
C(17)	-7.7815	-8.095	-2.1183
C(18)	-7.3277	-9.3755	-1.7839
C(19)	-6.0661	-9.7752	-2.2388
C(20)	-5.2713	-8.9184	-3.0042
C(21)	-8.1926	-10.2904	-0.954
H(22)	-8.2935	-8.5796	-8.1548
H(23)	-3.8452	-5.8784	-6.9104
H(24)	-9.4447	-6.433	-7.6797
H(25)	-8.2149	-6.1458	-8.9424
H(26)	-7.8937	-5.636	-7.2516
H(27)	-3.6519	-8.6121	-8.2964
H(28)	-3.4141	-6.9813	-9.0235
H(29)	-4.4831	-8.5705	-5.5947
H(30)	-2.0895	-6.6569	-5.1021
H(31)	-2.4061	-8.2117	-4.2684