Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

SUPPORTING INFORMATION

Directing Group Wins Over Acidity: Kinetically Controlled Regioselective Lithiation for Functionalization of 2-(2, 4-dihalophenyl)-1, 3-dithiane Derivatives

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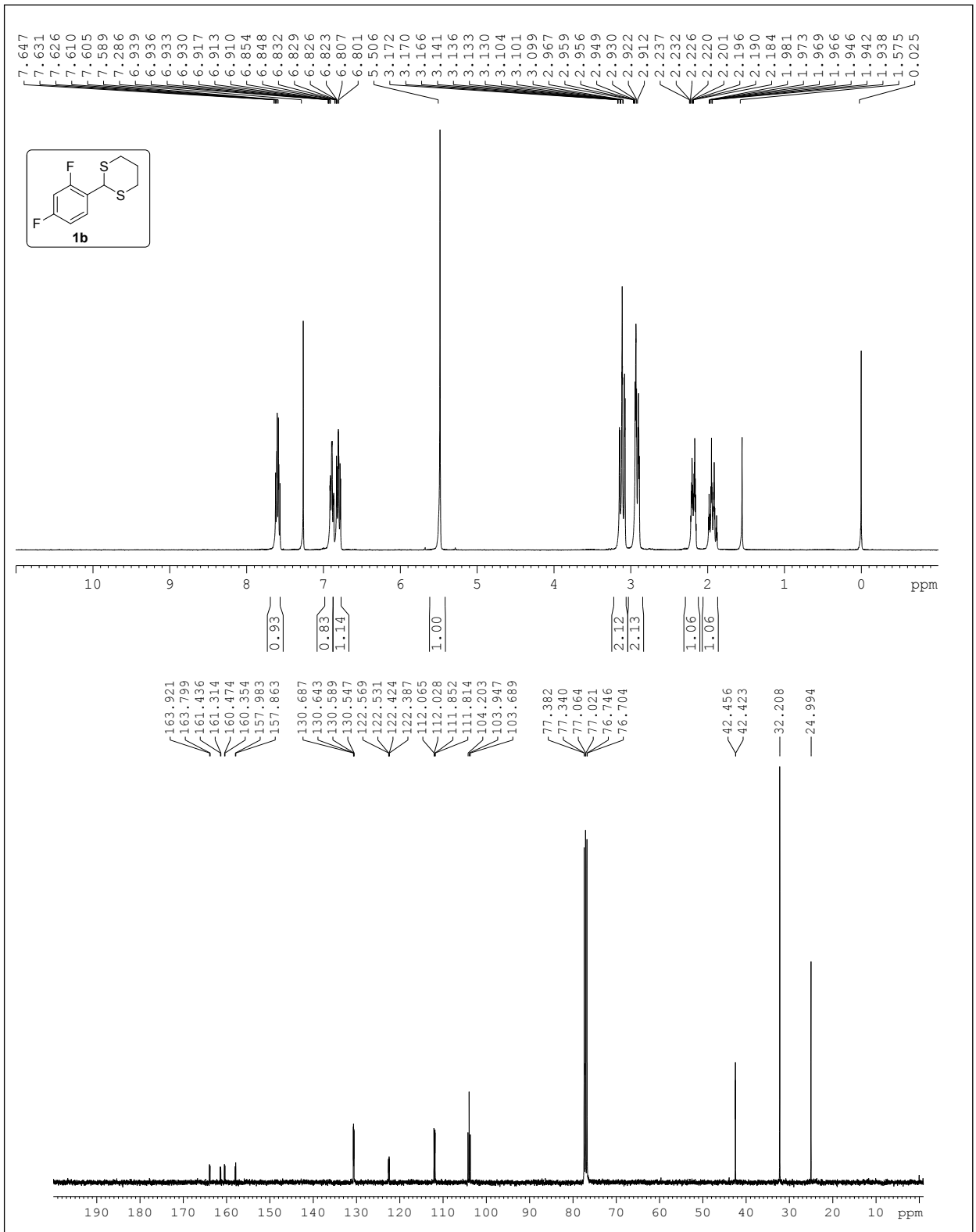


Figure 1 ^{1}H and ^{13}C NMR spectrum of compound **1b**

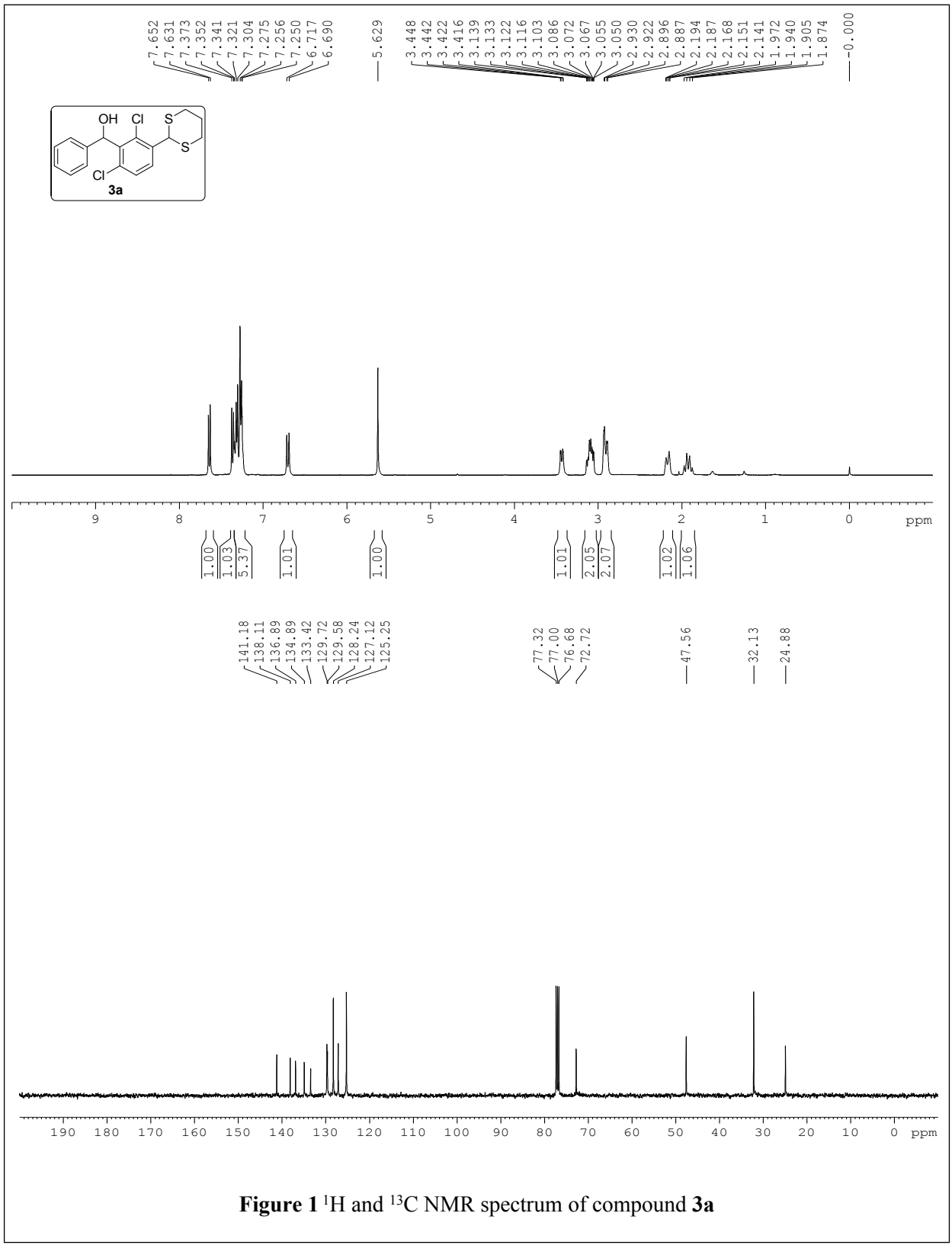


Figure 1 ^{1}H and ^{13}C NMR spectrum of compound **3a**

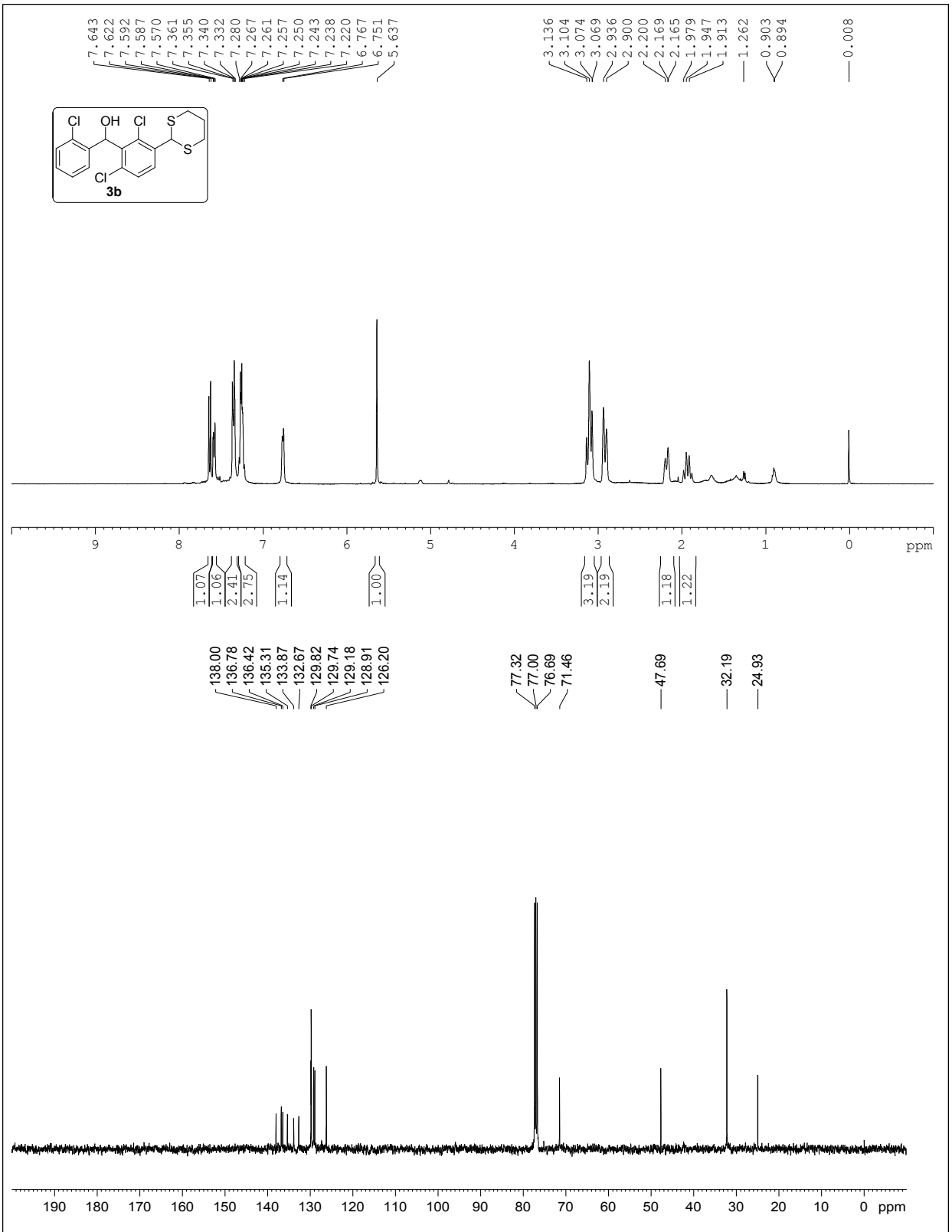


Figure 2. ^{1}H and ^{13}C NMR spectrum of compound **3b**

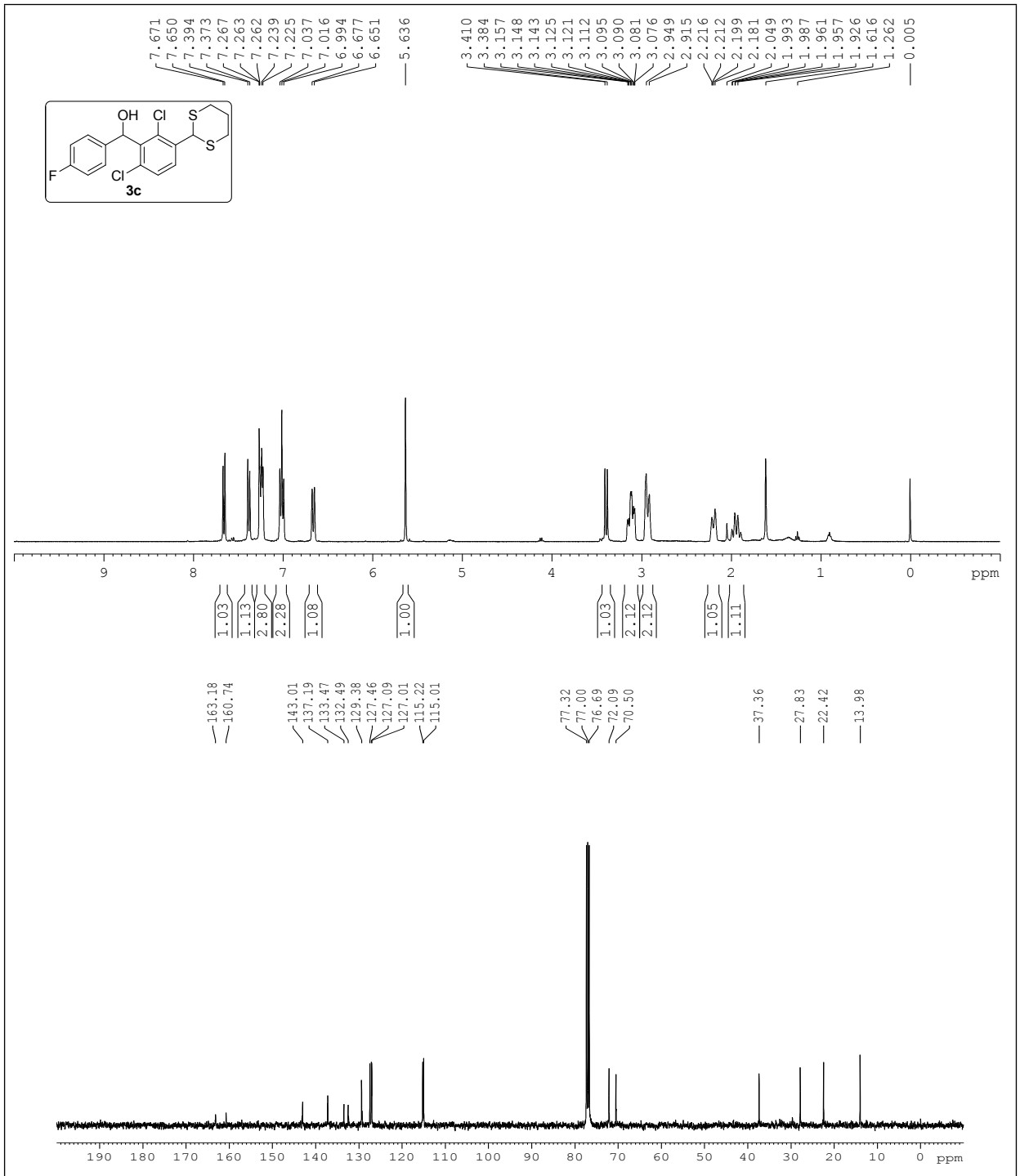


Figure 3. ^{1}H and ^{13}C NMR spectrum of compound **3c**

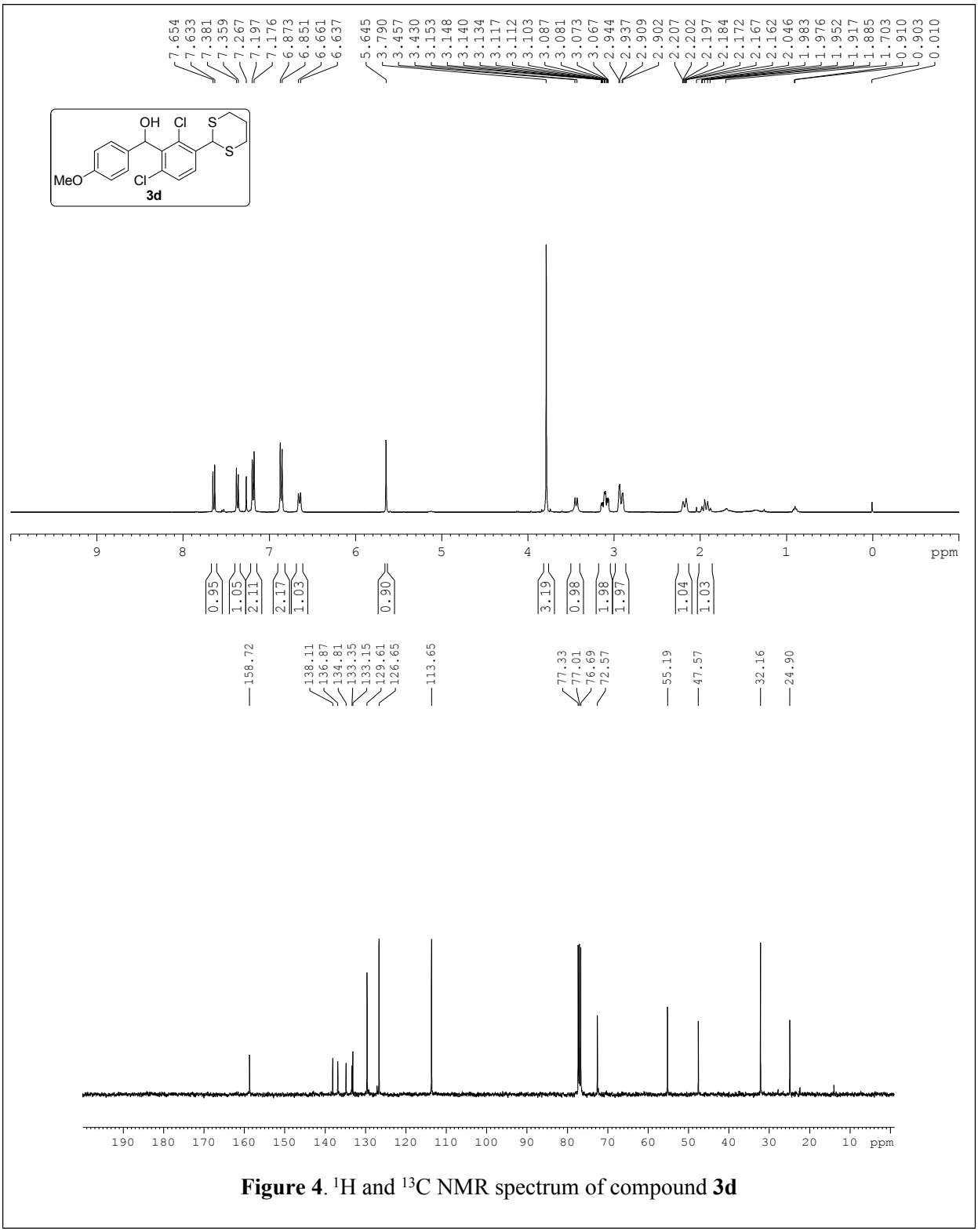


Figure 4. ^{1}H and ^{13}C NMR spectrum of compound **3d**

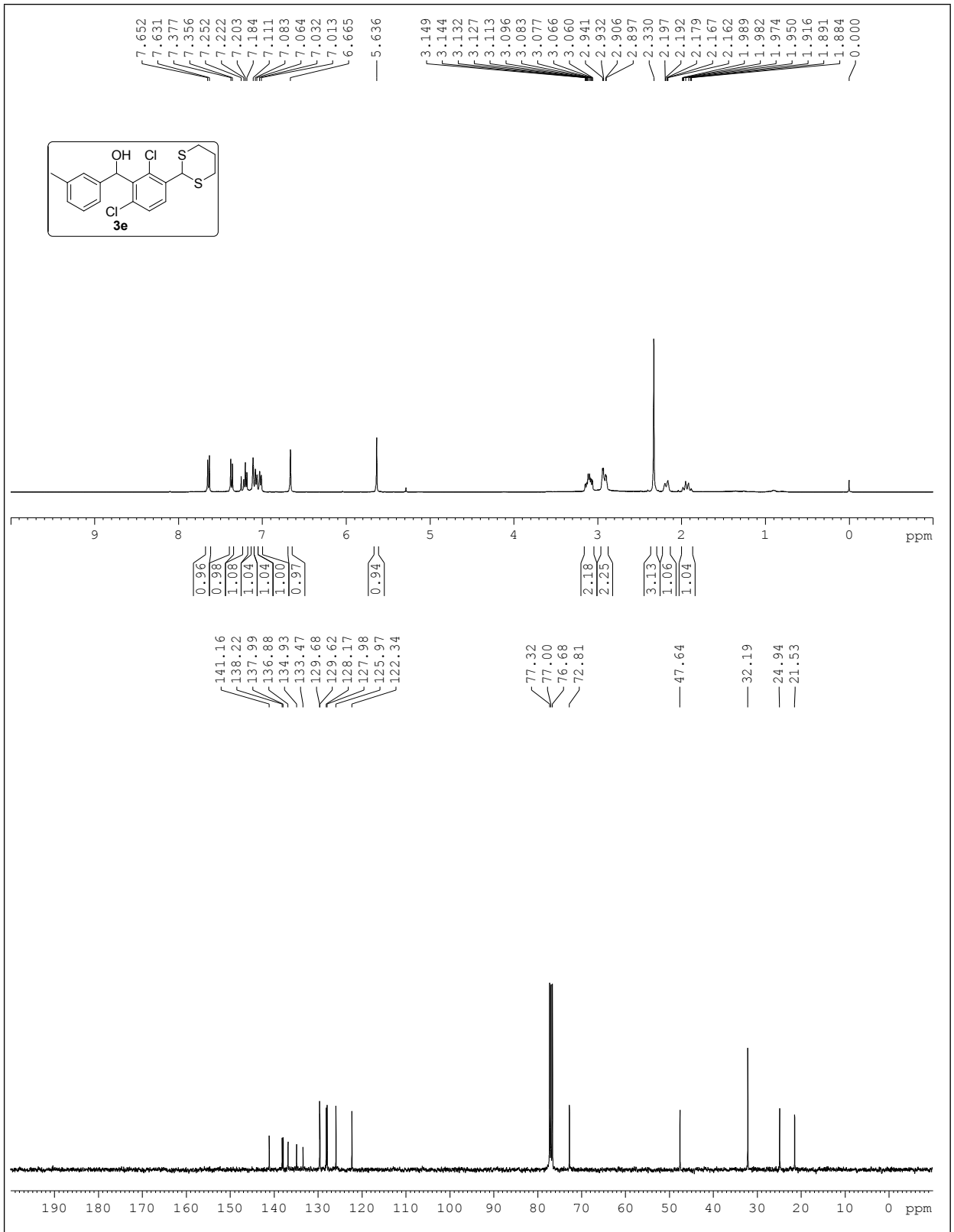


Figure 5. ^{1}H and ^{13}C NMR spectrum of compound **3e**

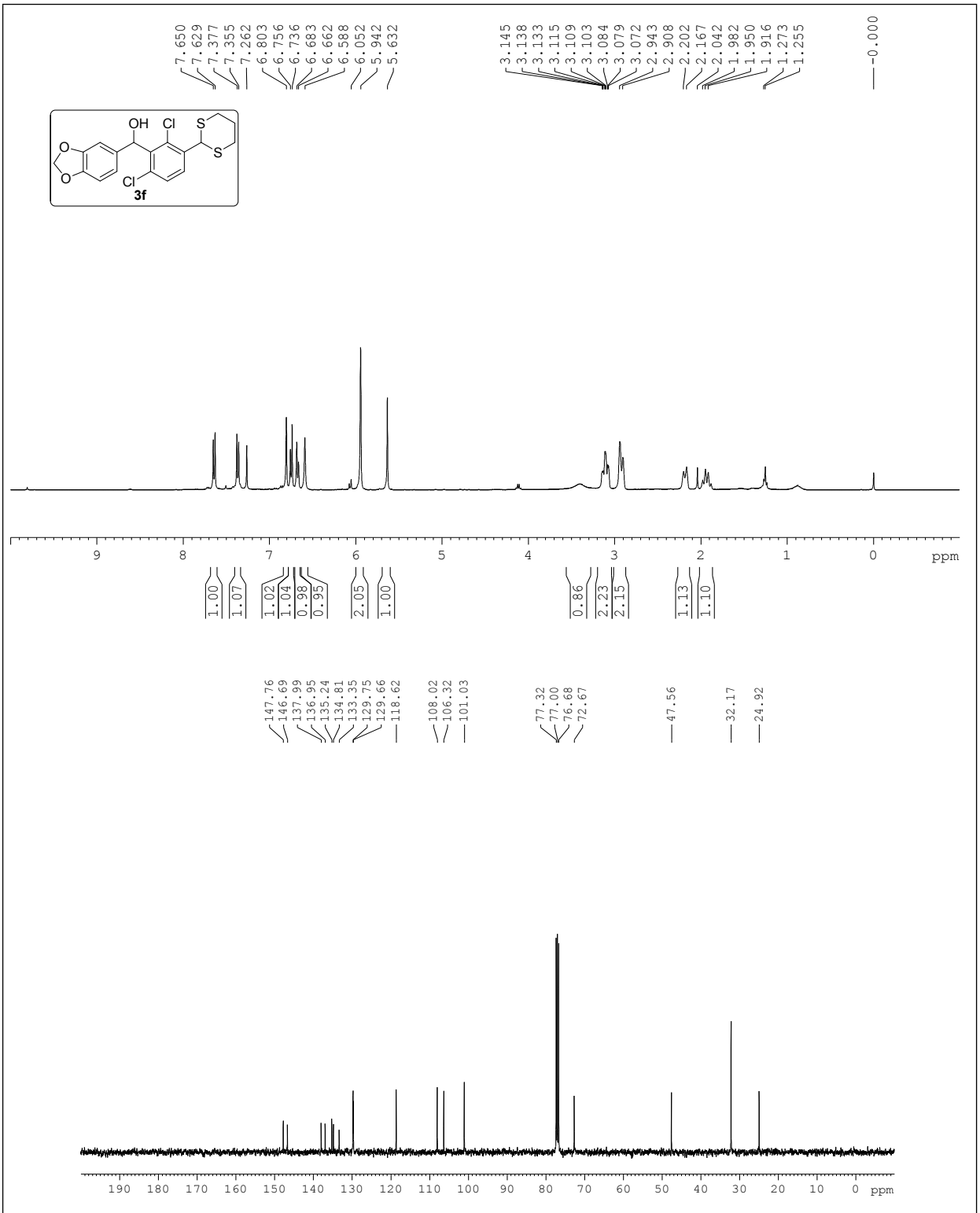


Figure 6. ^{1}H and ^{13}C NMR spectrum of compound **3f**

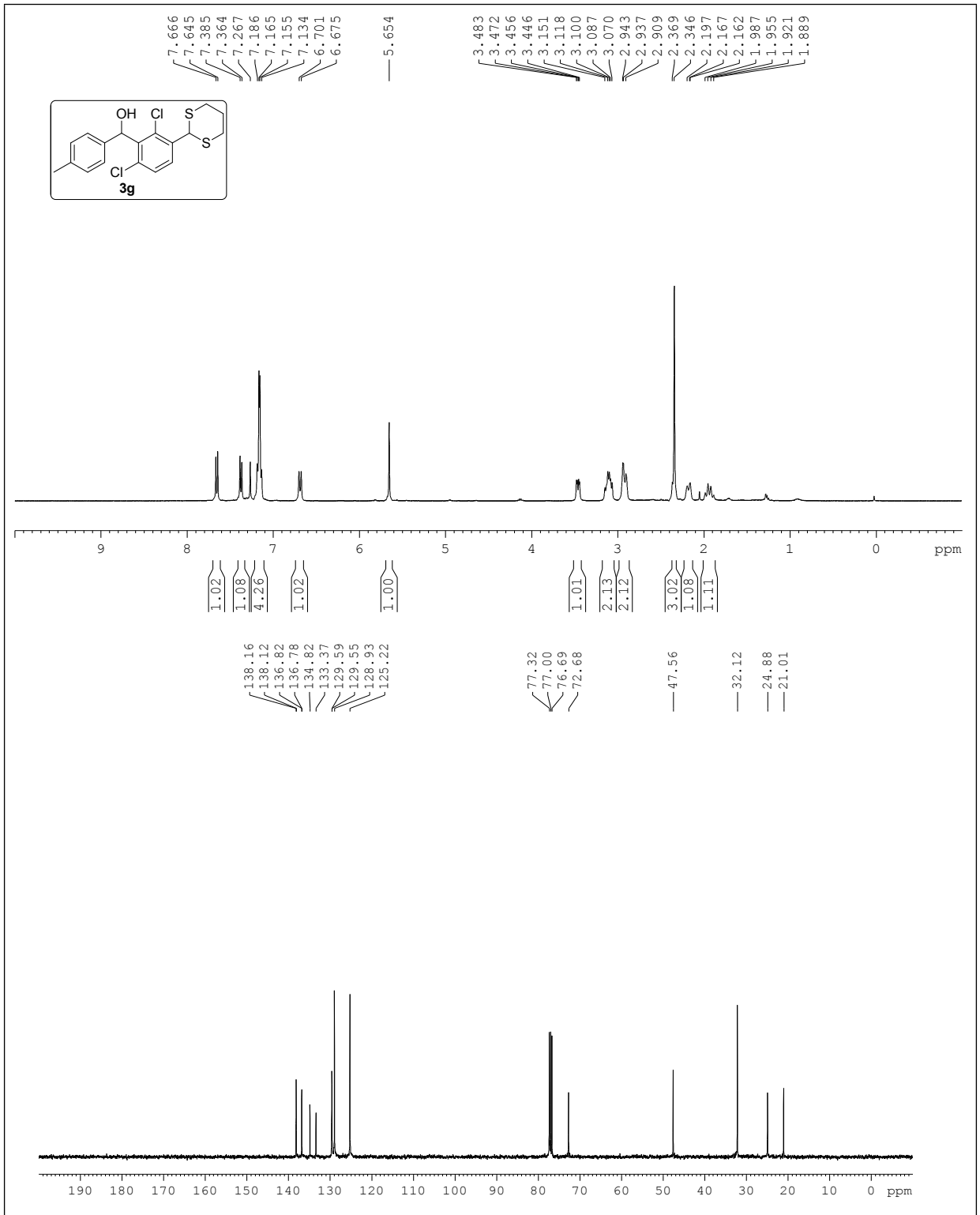


Figure 7. ^{1}H and ^{13}C NMR spectrum of compound **3g**

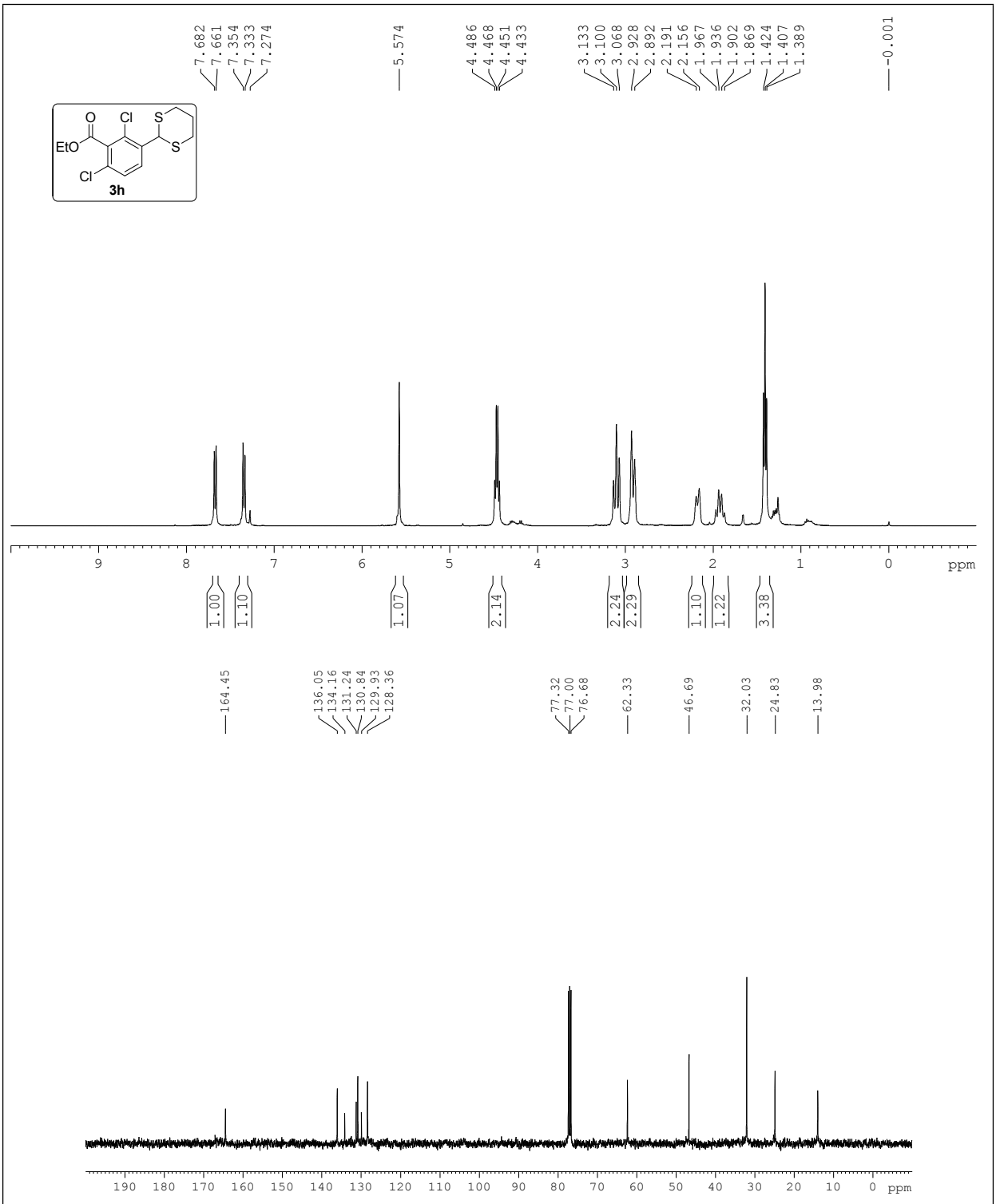


Figure 8. ^{1}H and ^{13}C NMR spectrum of compound **3h**

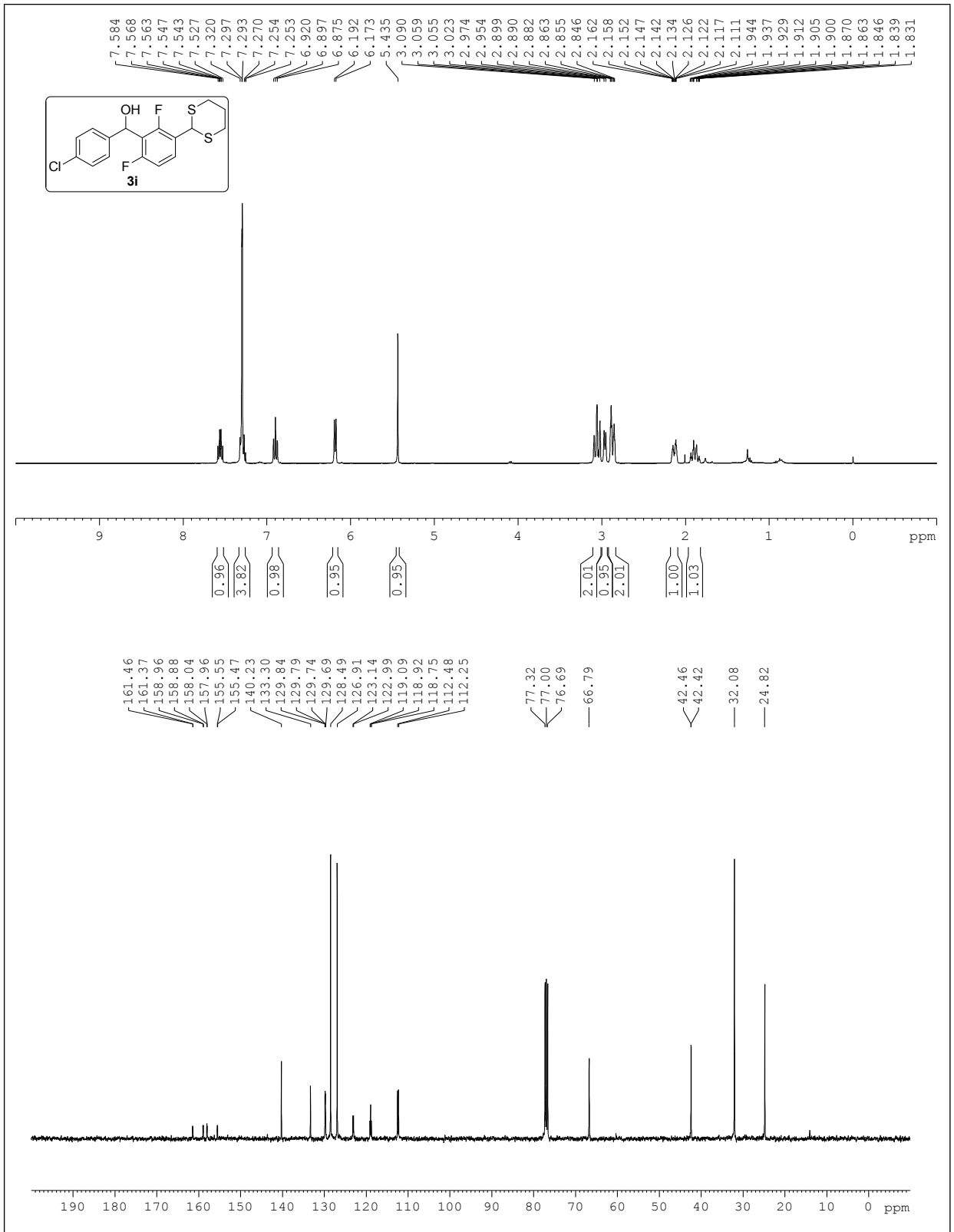


Figure 9. ^{1}H and ^{13}C NMR spectrum of compound **3i**

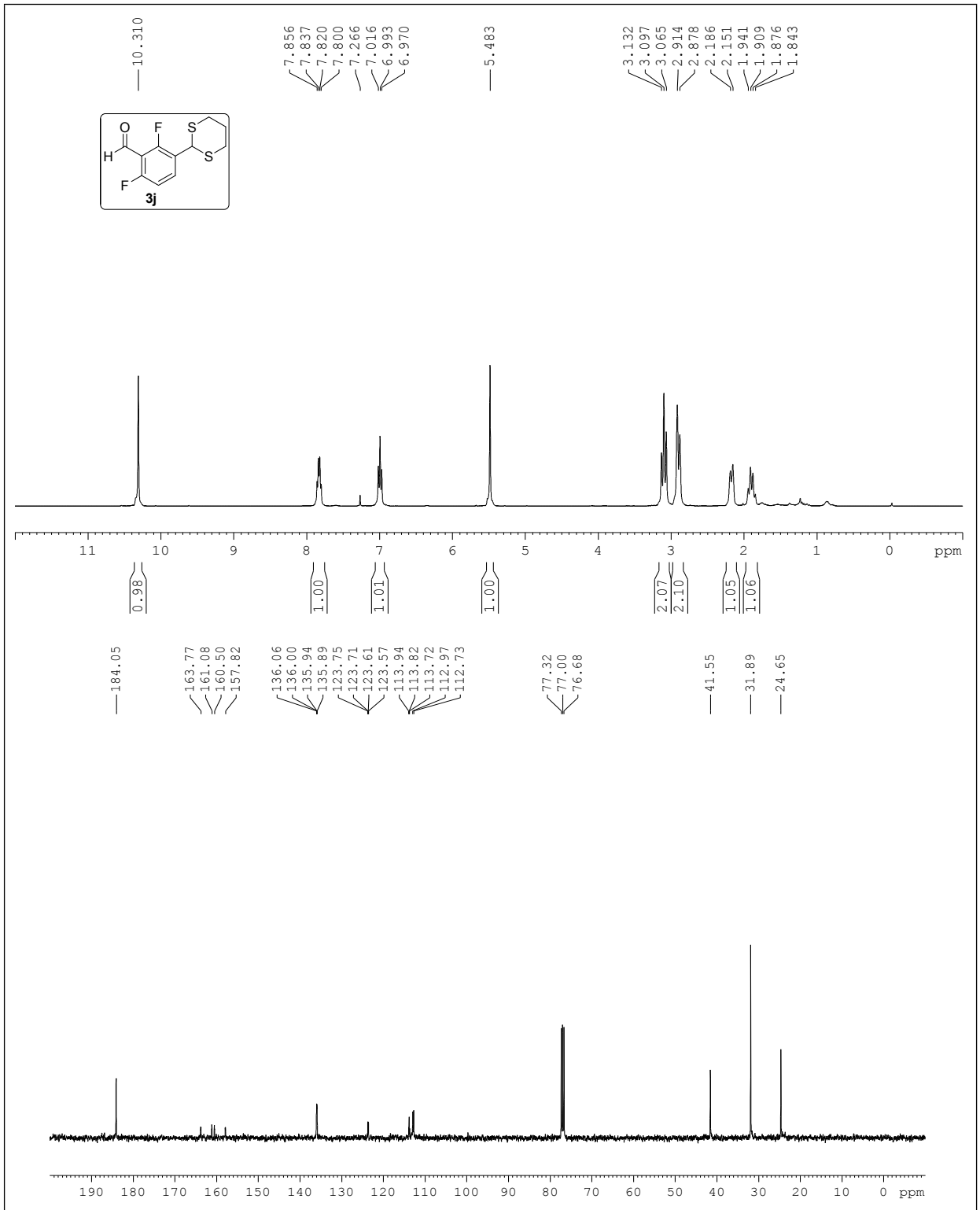


Figure 10. ^{1}H and ^{13}C NMR spectrum of compound **3j**

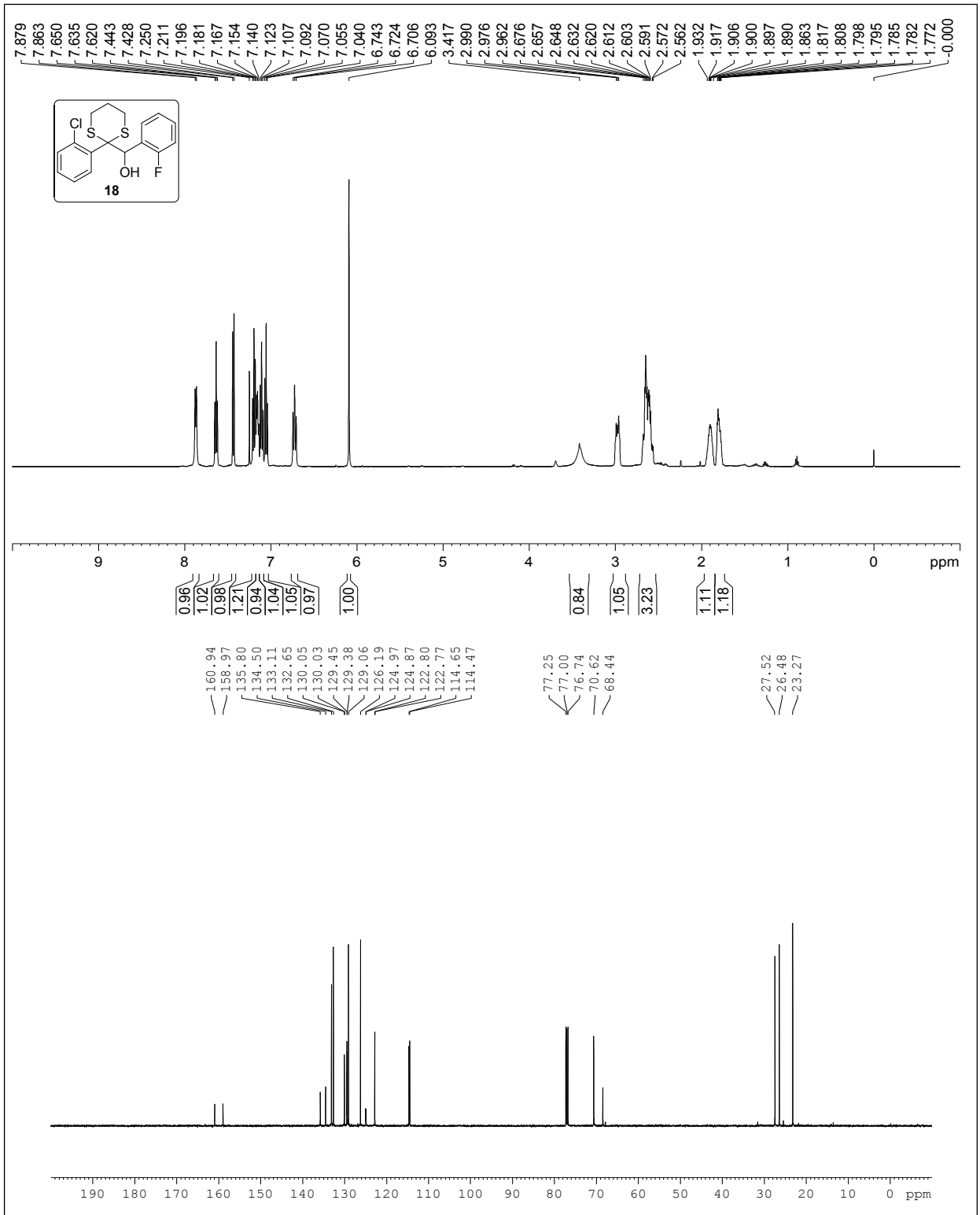


Figure 11. ^{1}H and ^{13}C NMR spectrum of compound **18**

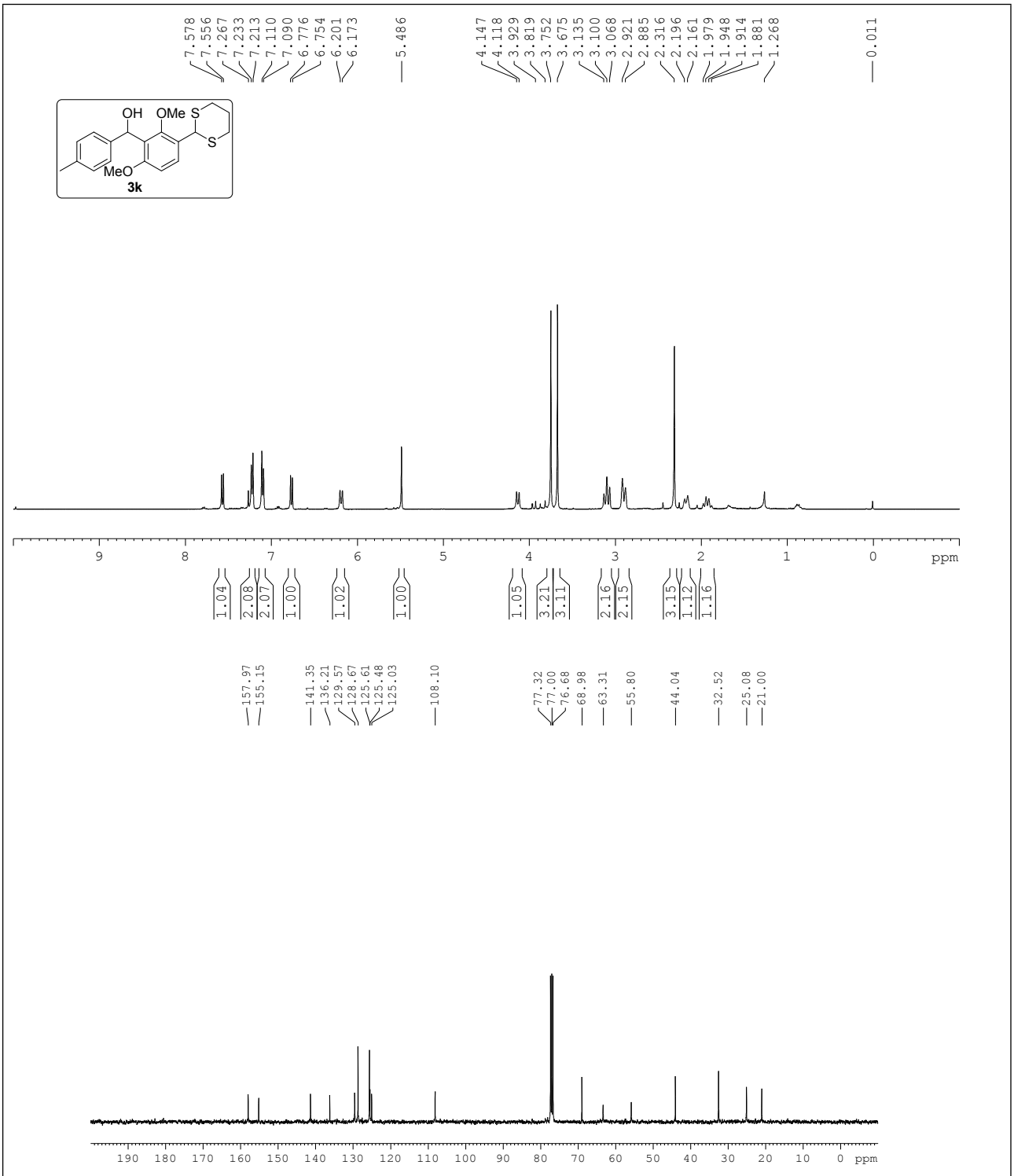


Figure 12. ^{1}H and ^{13}C NMR spectrum of compound **3k**

Figure 13. ^{1}H and ^{13}C NMR spectrum of compound **16**

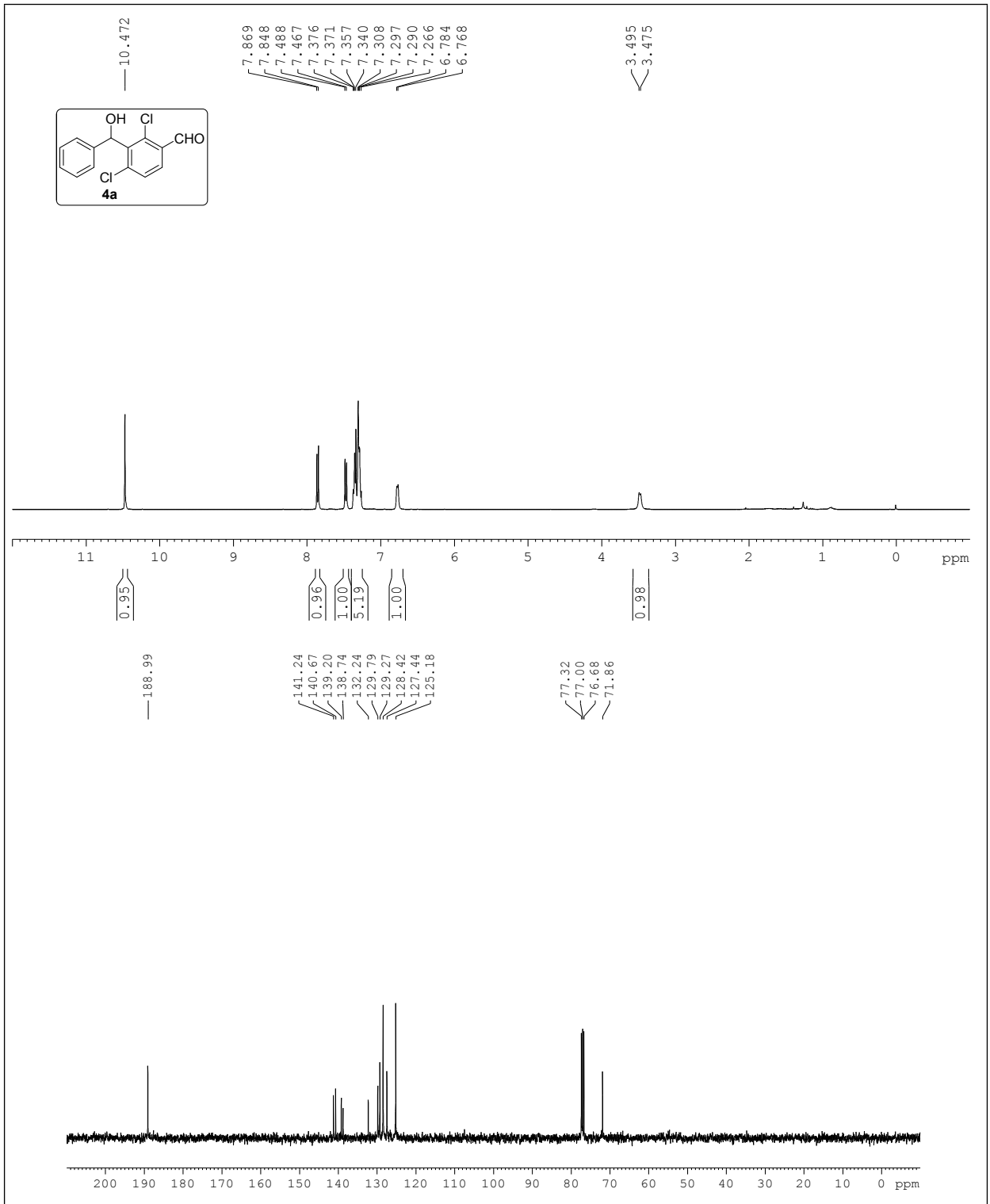


Figure 14. ^{1}H and ^{13}C NMR spectrum of compound **4a**

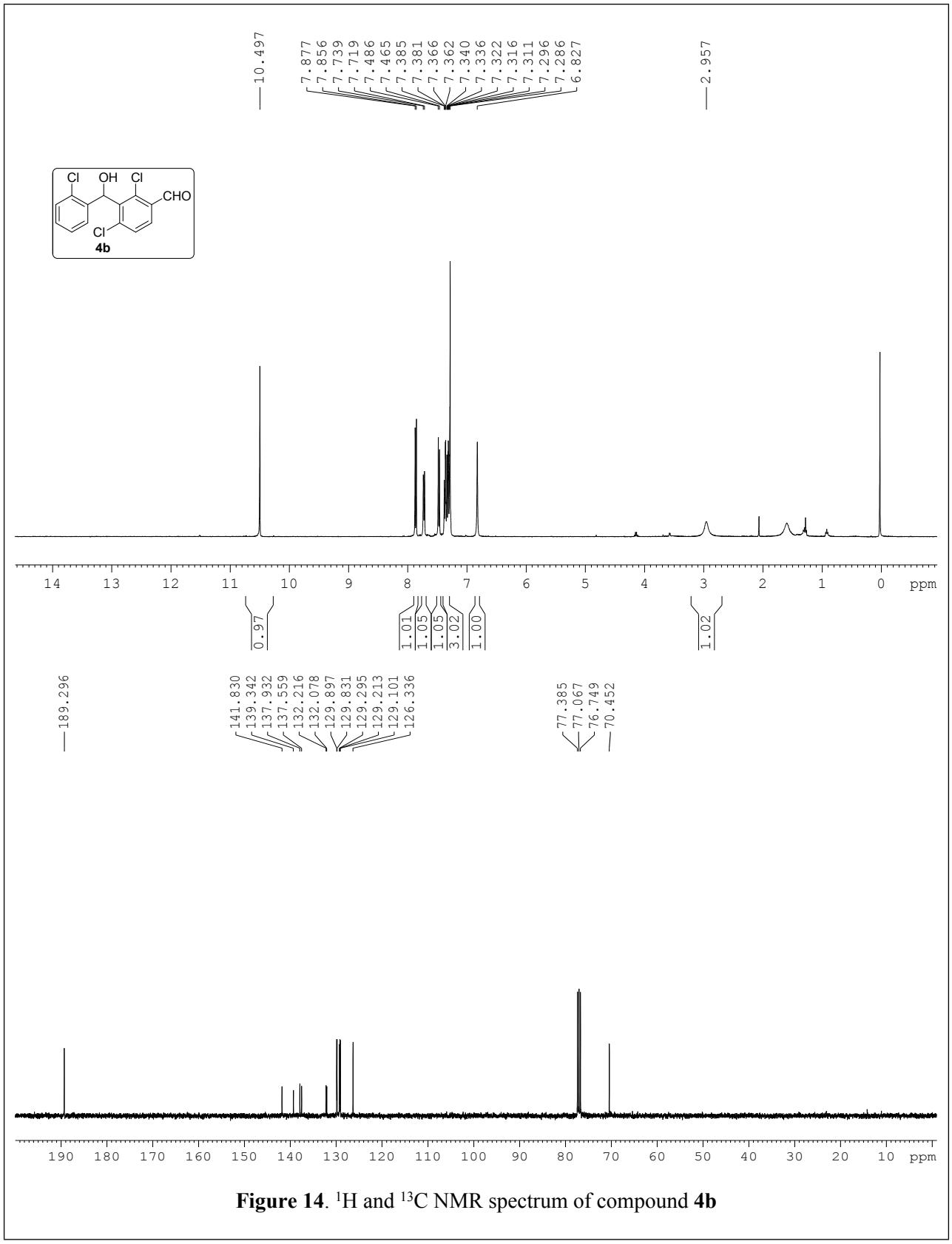


Figure 14. ^{1}H and ^{13}C NMR spectrum of compound **4b**

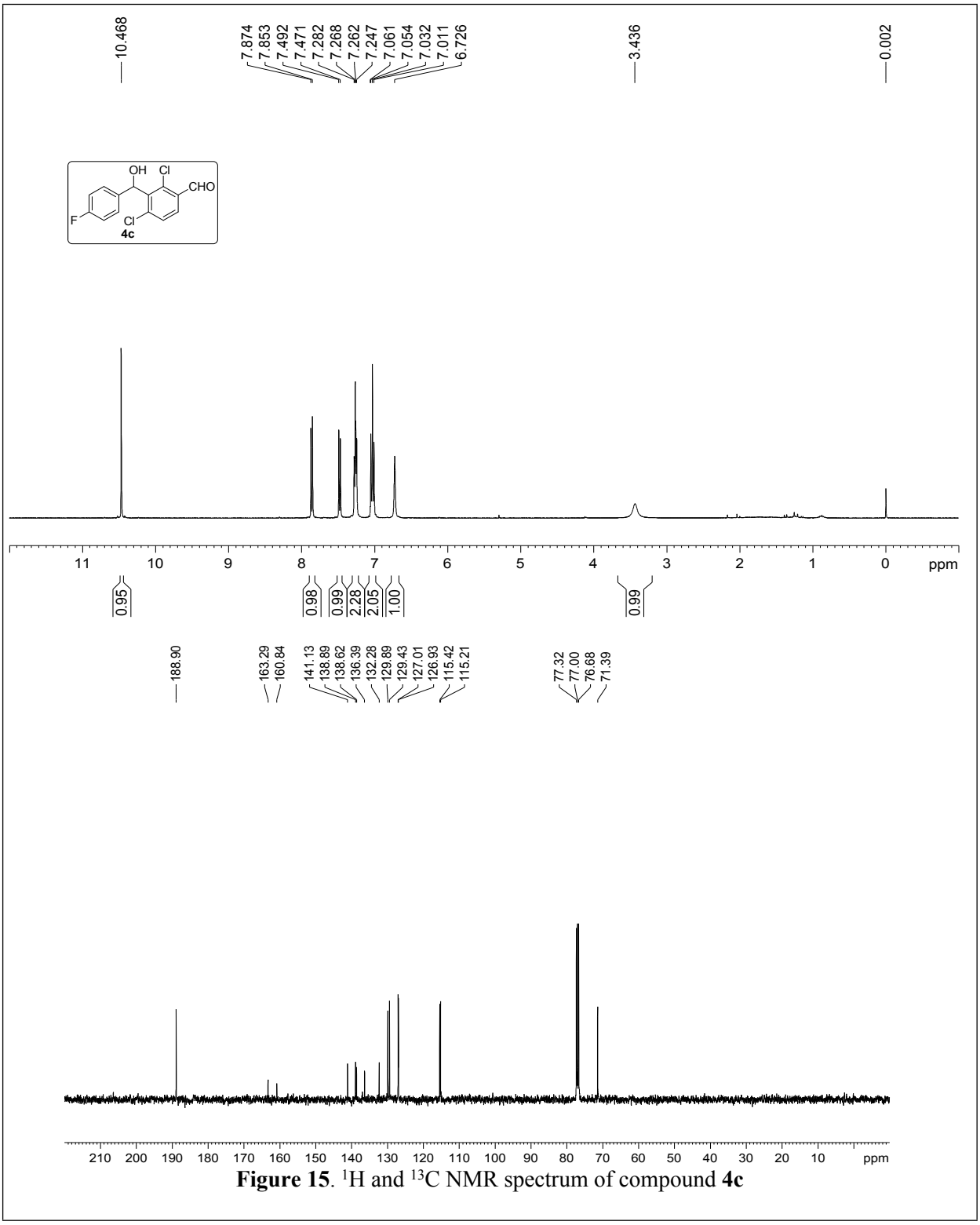


Figure 15. ^{1}H and ^{13}C NMR spectrum of compound **4c**

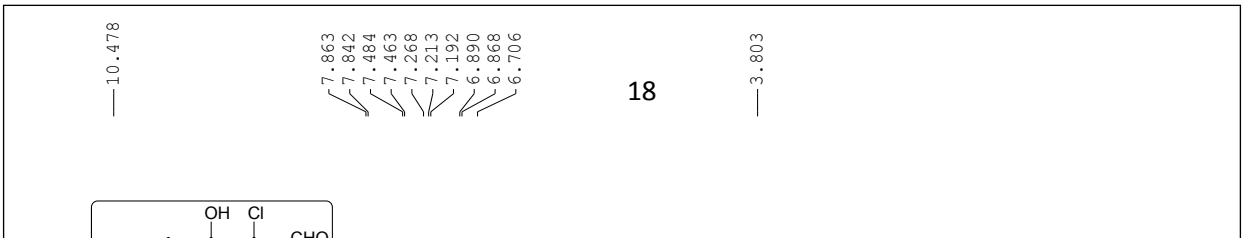


Figure 16. ^{1}H and ^{13}C NMR spectrum of compound **4d**

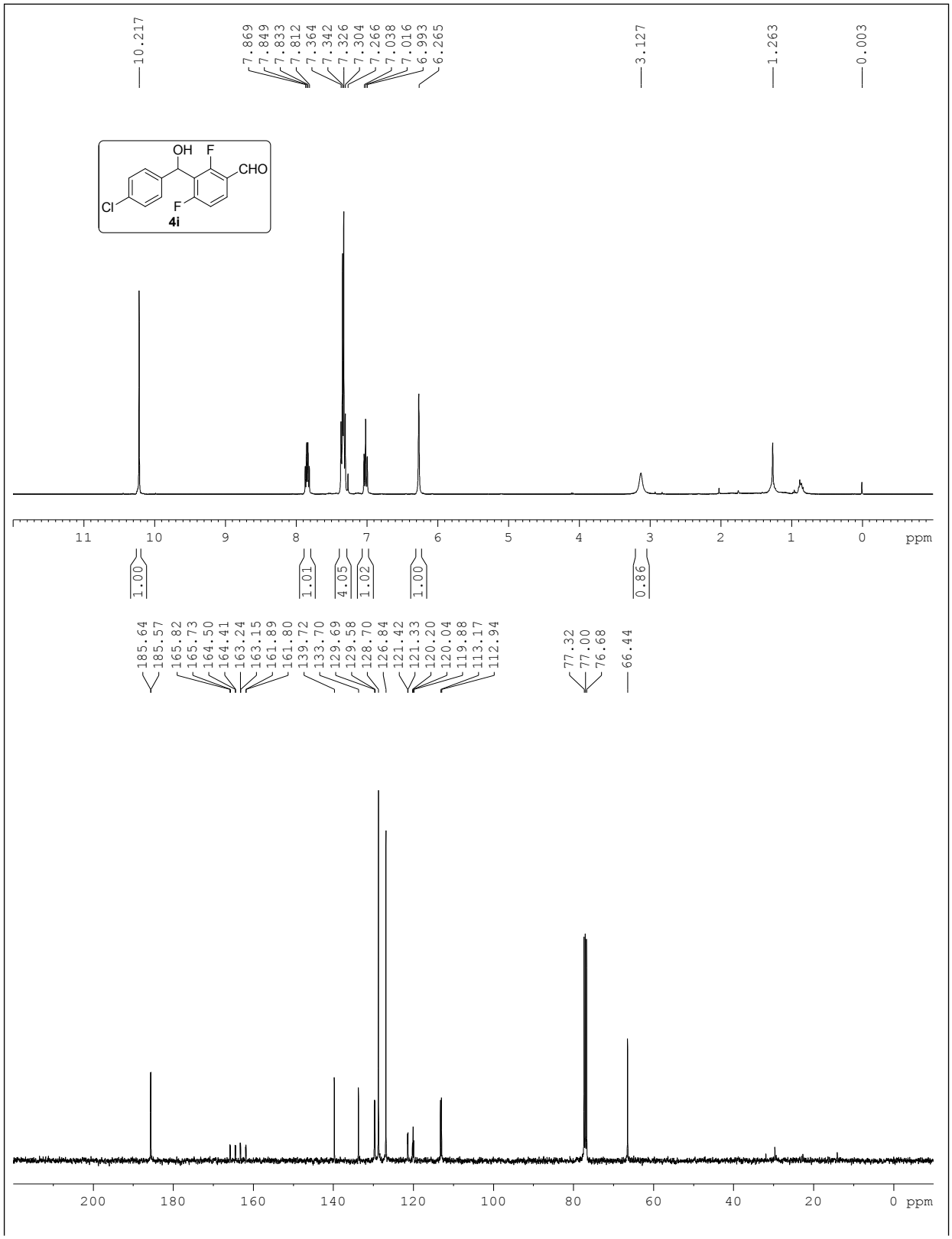


Figure 17. ^{1}H and ^{13}C NMR spectrum of compound **4i**

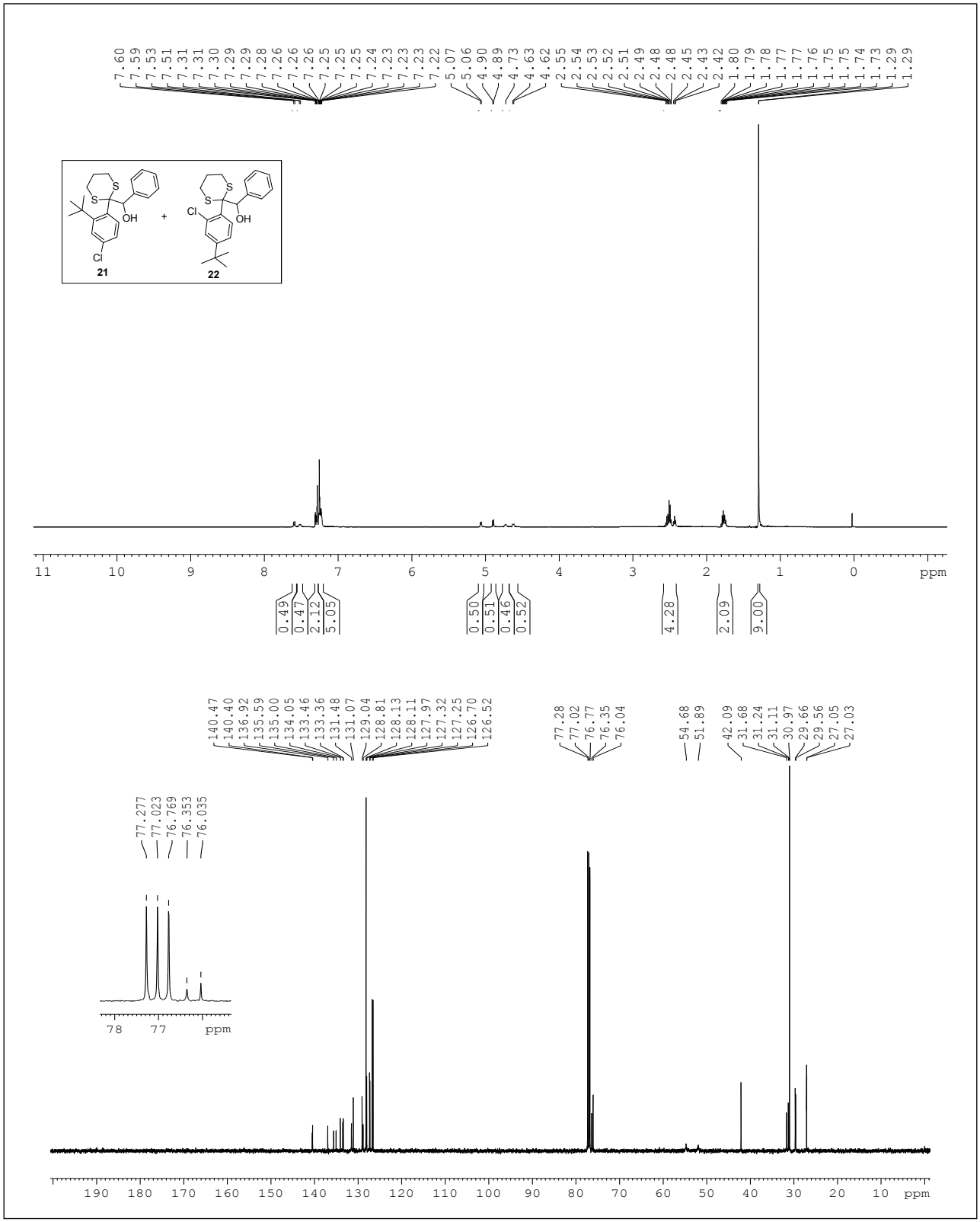


Figure 18. ^{1}H and ^{13}C NMR spectrum of compound **21** and **22**

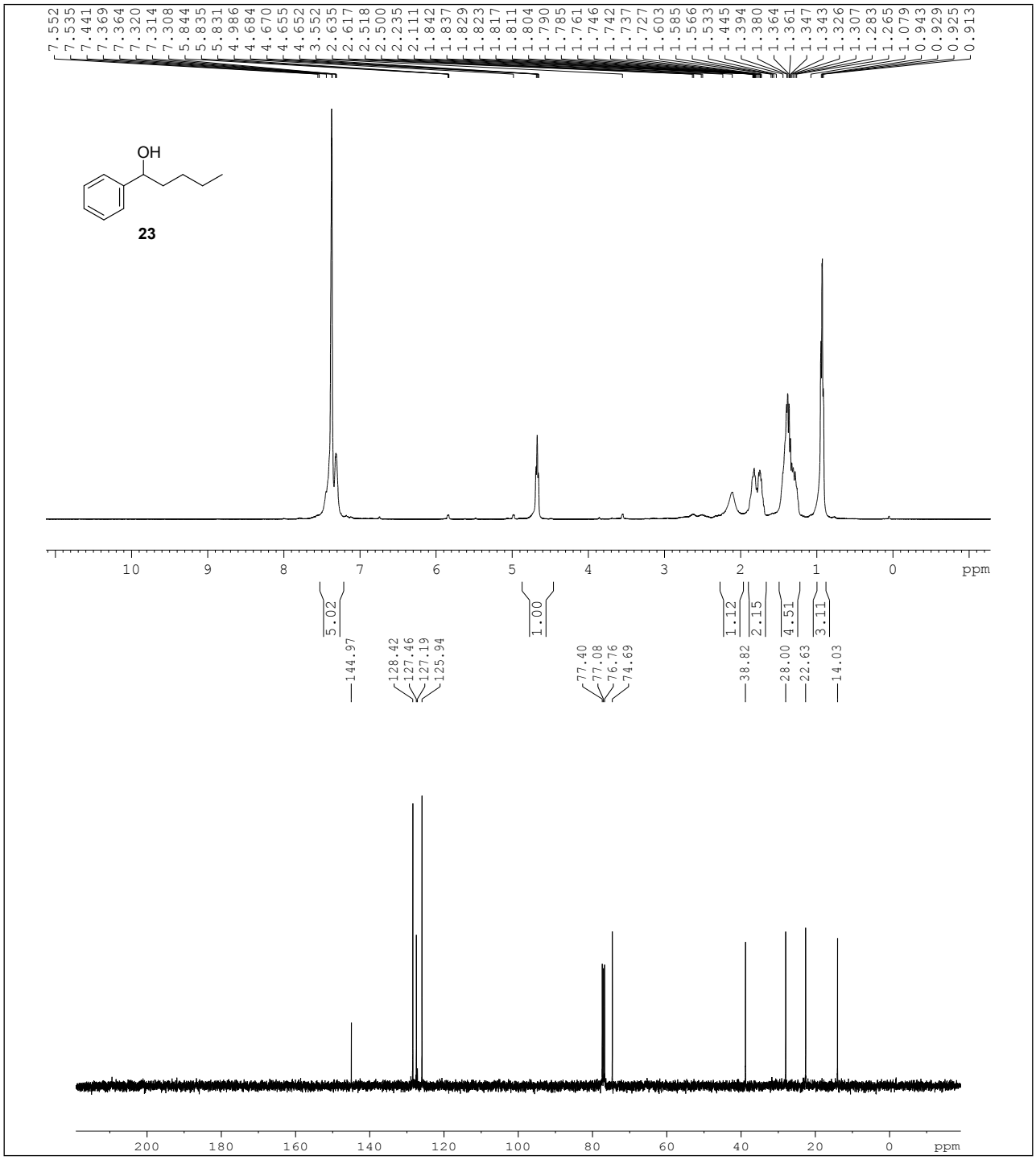
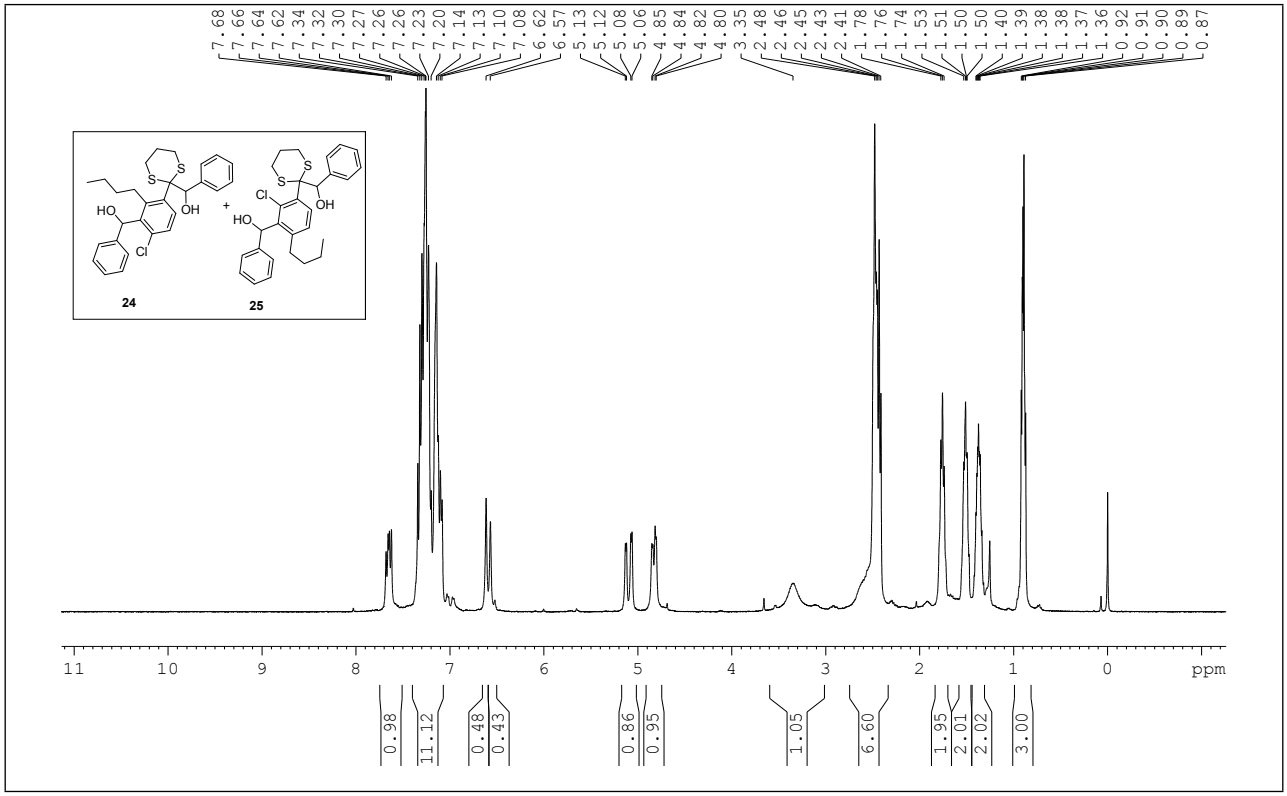


Figure 19. ^{1}H and ^{13}C NMR spectrum of compound **23**



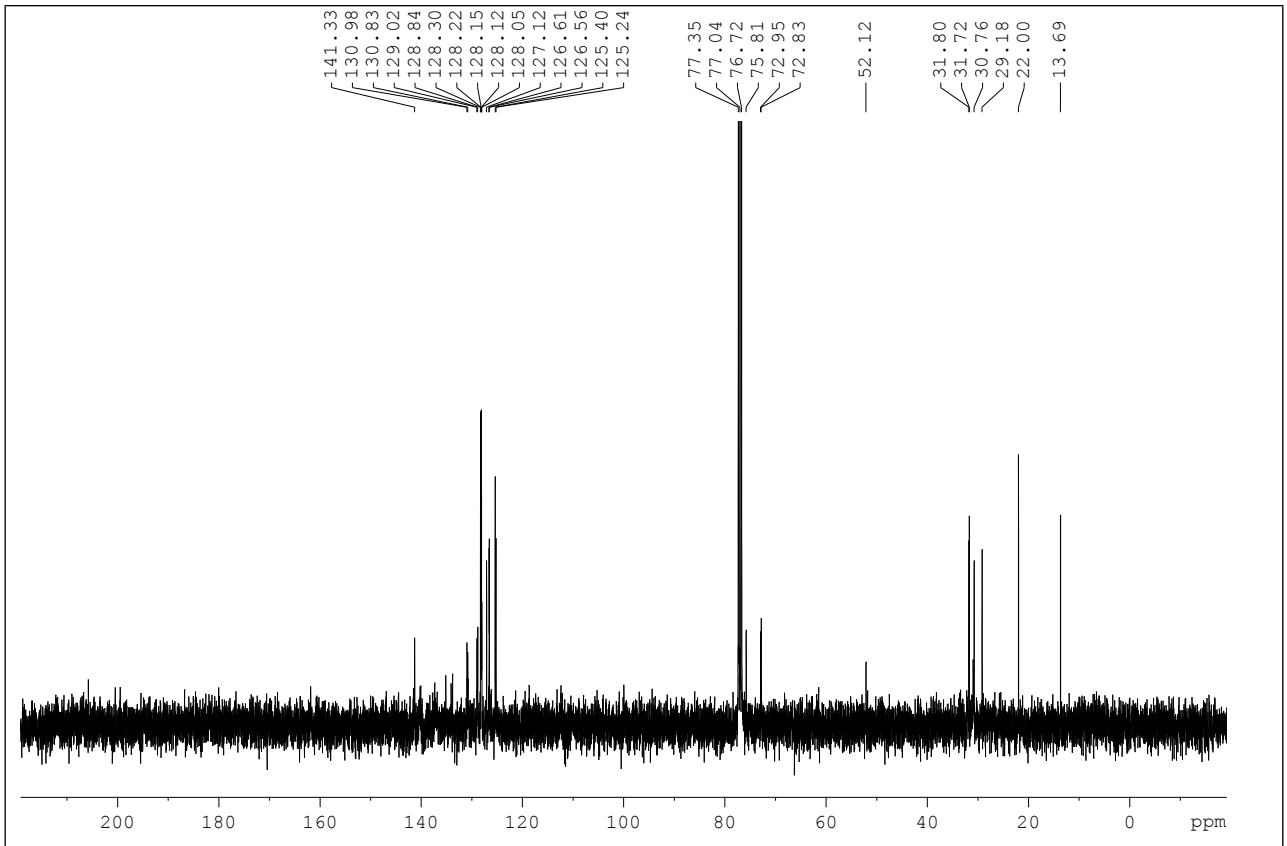


Figure 20. ^{1}H and ^{13}C NMR spectrum of compound **24** and **25**

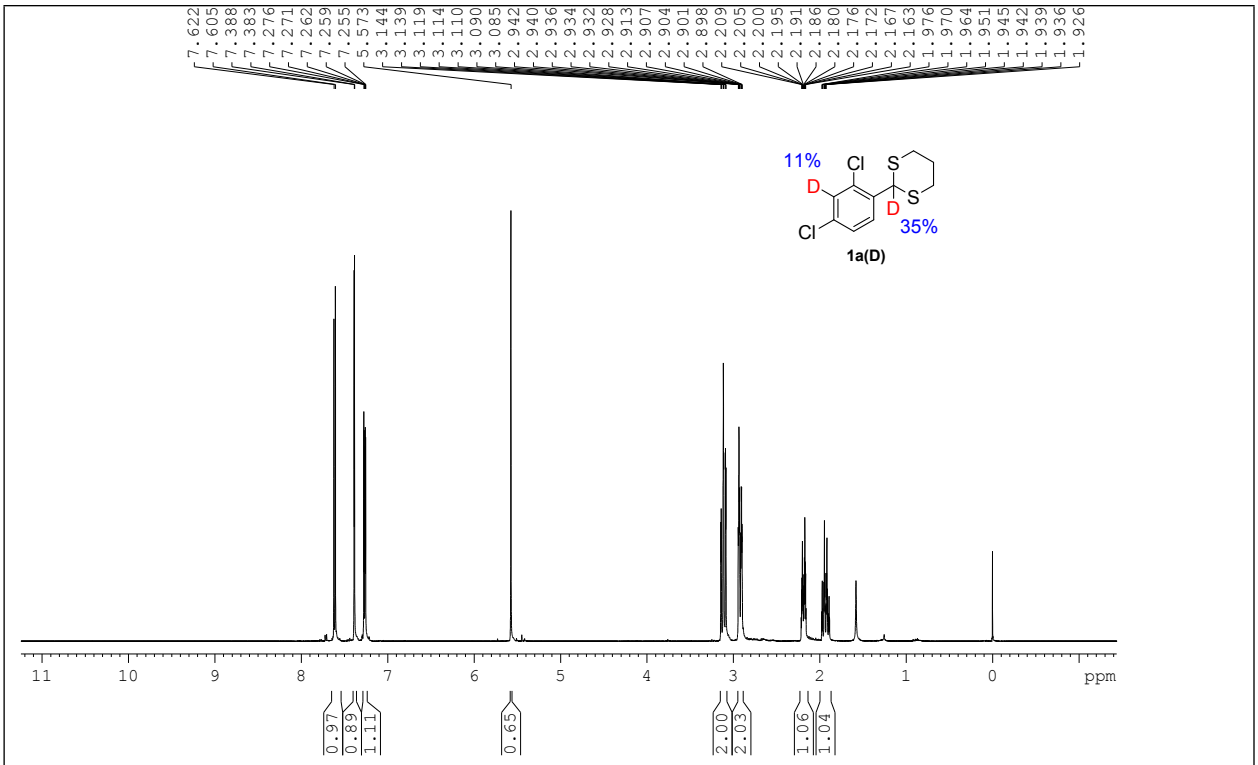
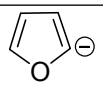
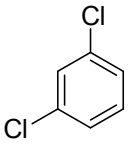
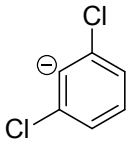
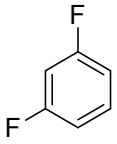
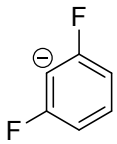
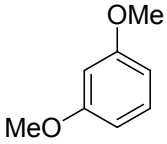
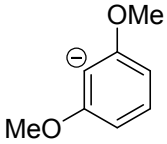
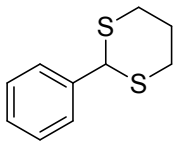


Figure 21. ^{1}H NMR spectrum of compound **1a(D)**

pKa calculations

Table 1 –Gases State Gibbs Free Energies and Change in Solvation Free Energies.

Molecule	Ggas (Hartree)	ΔG_{solv} (kcal/mole)
	-229.438940	-54.43138568
	-230.059837	-2.111567785
	-1151.530430	-2.003636237
	-1150.937778	-44.2952328
	-430.819479	-2.388299254
	-430.223152	-48.85032063
	-461.325356	-3.975269515
	-460.708539	-49.64913959



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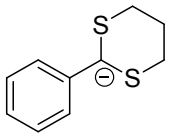

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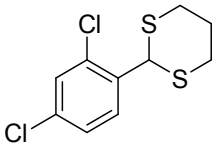

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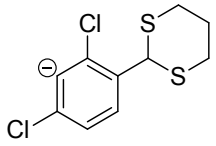

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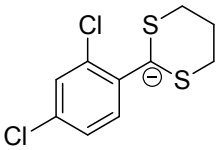

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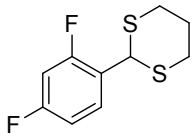

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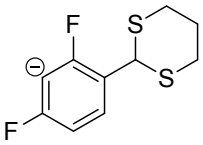

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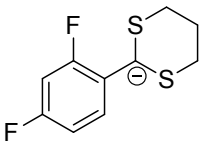

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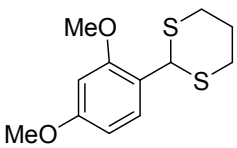

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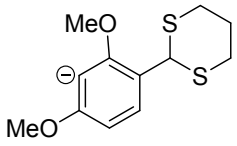
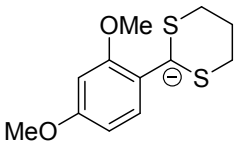
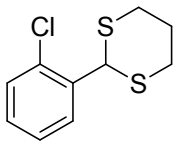
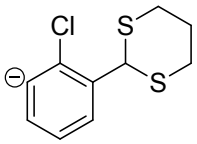
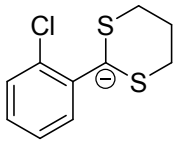
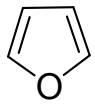
	-1413.159221	-51.36914176
	-1413.184273	-43.31443623
	-1644.333479	-5.464348372
	-1643.722371	-49.55062068
	-1643.765536	-39.9723233

Table 2- Cartesian Coordinates of the optimized structures in gas phase



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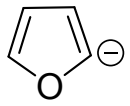
3	6	0	-0.716284	0.955355	-0.000037
4	6	0	-1.093062	-0.346051	-0.000072
5	8	0	0.000067	-1.156464	0.000158
6	1	0	2.047172	-0.840310	-0.000268
7	1	0	1.370128	1.809923	0.000191
8	1	0	-1.370341	1.809769	-0.000061
9	1	0	-2.047074	-0.840540	-0.000108



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2	6	0	-1.190938	0.063144	-0.000426
3	6	0	-0.231756	1.132383	0.000252
4	6	0	0.984411	0.527392	-0.000126
5	8	0	0.830048	-0.826933	-0.000205
6	1	0	-2.265482	0.185359	-0.000693
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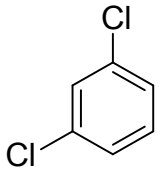

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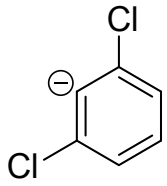
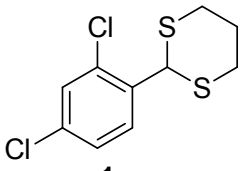
3	6	0	-1.191949	-0.001247	-0.000058
4	6	0	-0.000003	-0.713032	0.000016
5	6	0	1.191947	-0.001232	0.000082
6	6	0	1.209100	1.386721	0.000051
7	1	0	-0.000014	3.152708	-0.000032
8	1	0	-2.149346	1.917196	-0.000020
9	1	0	0.000010	-1.791763	0.000032
10	1	0	2.149322	1.917219	0.000037
11	17	0	-2.701920	-0.881500	0.000012
12	17	0	2.701933	-0.881492	-0.000027



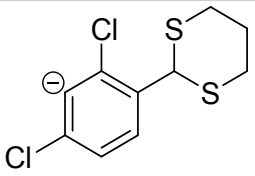
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	2.042179	-0.000009
2	6	0	-1.204413	1.341084	-0.000001
3	6	0	-1.130905	-0.047691	0.000079
4	6	0	0.000000	-0.813000	0.000002
5	6	0	1.130905	-0.047691	-0.000082
6	6	0	1.204413	1.341084	-0.000013
7	1	0	0.000000	3.125766	-0.000012
8	1	0	-2.152443	1.863169	-0.000026
9	1	0	2.152443	1.863168	0.000009
10	17	0	-2.799129	-0.874938	-0.000069
11	17	0	2.799129	-0.874938	0.000079



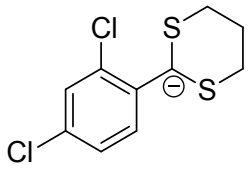
1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.471639	0.815814	0.000008
2	6	0	1.081674	0.760629	-0.000050
3	6	0	0.397972	-0.461990	-0.000119
4	6	0	1.180894	-1.621460	-0.000140
5	6	0	2.565567	-1.591699	-0.000130
6	6	0	3.202472	-0.360041	-0.000075
7	1	0	2.970036	1.772469	0.000105
8	17	0	0.247120	2.291913	0.000127
9	1	0	0.681601	-2.581163	-0.000163
10	1	0	3.139317	-2.506191	-0.000137
11	17	0	4.947427	-0.282615	0.000048
12	6	0	-1.099788	-0.633968	-0.000086
13	16	0	-1.862010	0.012562	1.546137
14	16	0	-1.862111	0.012834	-1.546128
15	1	0	-1.299705	-1.703961	-0.000164
16	6	0	-3.565528	-0.595873	1.277577
17	6	0	-3.565606	-0.595658	-1.277555
18	6	0	-4.228516	-0.087220	0.000075
19	1	0	-4.113049	-0.257483	2.156295
20	1	0	-3.558925	-1.688232	1.299743
21	1	0	-4.113181	-0.257121	-2.156182
22	1	0	-3.558997	-1.688013	-1.299905
23	1	0	-5.268770	-0.429148	0.000078

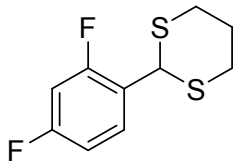
24	1	0	-4.244377	1.003239	0.000165



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.540657	0.918004	0.000124
2	6	0	1.175824	0.803414	0.000287
3	6	0	0.440571	-0.393243	0.000140
4	6	0	1.198765	-1.574109	-0.000075
5	6	0	2.585442	-1.537677	-0.000162
6	6	0	3.183390	-0.283066	-0.000145
7	17	0	0.199213	2.362188	0.000324
8	1	0	0.690283	-2.531227	-0.000174
9	1	0	3.162520	-2.453578	-0.000277
10	17	0	5.032809	-0.337936	-0.000113
11	6	0	-1.057682	-0.566091	0.000085
12	16	0	-1.867447	0.055668	1.537355
13	16	0	-1.867177	0.056164	-1.537309
14	1	0	-1.254563	-1.637314	-0.000126
15	6	0	-3.519017	-0.686724	1.276965
16	6	0	-3.519035	-0.685840	-1.277468
17	6	0	-4.225259	-0.233337	-0.000087
18	1	0	-4.095819	-0.398092	2.155969
19	1	0	-3.430129	-1.777201	1.290822
20	1	0	-4.095691	-0.396152	-2.156224
21	1	0	-3.430590	-1.776337	-1.292315
22	1	0	-5.238708	-0.653322	-0.000263
23	1	0	-4.319640	0.853645	0.000307



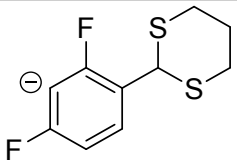
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.509527	0.739826	-0.099199
2	6	0	1.162745	0.948426	0.157583
3	6	0	0.209671	-0.107948	0.326055
4	6	0	0.827763	-1.402147	0.296423
5	6	0	2.166654	-1.625150	0.058726
6	6	0	3.016962	-0.546495	-0.163647
7	1	0	3.161874	1.592342	-0.214996
8	17	0	0.721616	2.645393	0.396417
9	1	0	0.183122	-2.252511	0.461920
10	1	0	2.549169	-2.636753	0.030462
11	17	0	4.735645	-0.807008	-0.491301
12	6	0	-1.188818	0.038588	0.563072
13	16	0	-2.142803	-1.310750	1.169356
14	16	0	-2.171451	1.361710	-0.066523
15	6	0	-3.087108	-1.828452	-0.331993
16	6	0	-3.081697	0.493661	-1.414064
17	6	0	-3.919324	-0.693338	-0.931695
18	1	0	-3.732963	-2.649252	-0.010436
19	1	0	-2.383670	-2.219047	-1.071558
20	1	0	-3.725907	1.254095	-1.863224
21	1	0	-2.361428	0.171435	-2.170294
22	1	0	-4.497479	-1.087588	-1.777510
23	1	0	-4.636337	-0.342473	-0.184240



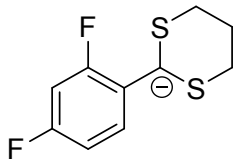
1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.774167	0.171933	-0.998096
2	6	0	1.397576	0.150310	-0.854168
3	6	0	0.765502	-0.057746	0.371774
4	6	0	1.596987	-0.249910	1.477968
5	6	0	2.980945	-0.236496	1.378504
6	6	0	3.543064	-0.024019	0.133169
7	1	0	3.224656	0.336690	-1.965093
8	9	0	0.661248	0.340344	-1.959892
9	1	0	1.141949	-0.415042	2.445245
10	1	0	3.613427	-0.386309	2.240684
11	9	0	4.883562	-0.006215	0.011000
12	6	0	-0.728769	-0.084926	0.543055
13	16	0	-1.467065	1.543805	0.109853
14	16	0	-1.460721	-1.505939	-0.368423
15	1	0	-0.942185	-0.250805	1.597988
16	6	0	-3.204106	1.199201	0.564157
17	6	0	-3.199830	-1.323106	0.166409
18	6	0	-3.833023	0.022534	-0.177194
19	1	0	-3.730223	2.124946	0.334567
20	1	0	-3.264604	1.050930	1.644897
21	1	0	-3.722599	-2.134841	-0.337924
22	1	0	-3.261340	-1.514973	1.240224
23	1	0	-4.892393	-0.022620	0.096228

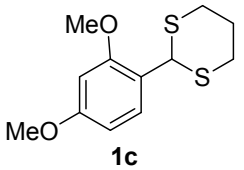
24	1	0	-3.780481	0.192349	-1.253140



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.847665	0.168937	-1.094845
2	6	0	-1.491748	0.142162	-0.892632
3	6	0	-0.814845	-0.041736	0.322952
4	6	0	-1.616409	-0.218627	1.457872
5	6	0	-2.999296	-0.206174	1.345351
6	6	0	-3.536471	-0.013009	0.074669
7	9	0	-0.657690	0.313125	-1.991715
8	1	0	-1.150264	-0.366320	2.425296
9	1	0	-3.634015	-0.341878	2.213191
10	9	0	-4.932659	-0.013303	0.045059
11	6	0	0.677474	-0.065827	0.489114
12	16	0	1.449759	-1.497593	-0.383539
13	16	0	1.459614	1.543366	0.035507
14	1	0	0.900937	-0.211837	1.546085
15	6	0	3.160635	-1.328459	0.239151
16	6	0	3.166480	1.199492	0.593040
17	6	0	3.830543	0.004770	-0.089647
18	1	0	3.707574	-2.153654	-0.217964
19	1	0	3.168093	-1.495319	1.320531
20	1	0	3.719301	2.115519	0.382528
21	1	0	3.170092	1.061483	1.678523
22	1	0	4.875777	-0.044182	0.240349
23	1	0	3.833495	0.156245	-1.170279



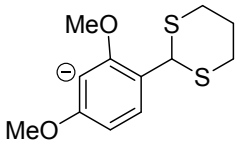
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.876119	-0.882297	0.105271
2	6	0	1.532969	-1.011417	-0.189188
3	6	0	0.613075	0.067964	-0.297233
4	6	0	1.245968	1.333008	-0.105906
5	6	0	2.594782	1.497278	0.179620
6	6	0	3.401739	0.383361	0.295438
7	1	0	3.497261	-1.765219	0.159749
8	9	0	1.114871	-2.283361	-0.441402
9	1	0	0.624256	2.211327	-0.197261
10	1	0	3.011184	2.486197	0.321751
11	9	0	4.737699	0.519834	0.591322
12	6	0	-0.774236	-0.069140	-0.633887
13	16	0	-1.749894	1.346898	-0.996787
14	16	0	-1.727697	-1.508154	-0.292413
15	6	0	-2.730273	1.544696	0.557314
16	6	0	-2.702928	-0.947555	1.172576
17	6	0	-3.551551	0.298541	0.901779
18	1	0	-3.388545	2.402084	0.393667
19	1	0	-2.048323	1.790462	1.375228
20	1	0	-3.344584	-1.791434	1.440778
21	1	0	-2.014405	-0.767698	2.002322
22	1	0	-4.162627	0.512468	1.788579
23	1	0	-4.239886	0.087024	0.078410



1c

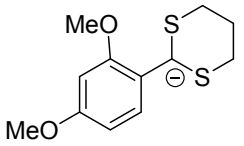
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.353122	0.934561	-0.000338
2	6	0	-0.970001	0.813862	-0.000243
3	6	0	-0.360940	-0.460869	-0.000258
4	6	0	-1.198625	-1.567370	-0.000466
5	6	0	-2.587499	-1.468634	-0.000628
6	6	0	-3.162857	-0.203338	-0.000552
7	1	0	-2.836254	1.898424	-0.000282
8	8	0	-0.134794	1.879077	-0.000238
9	1	0	-0.752083	-2.553437	-0.000555
10	1	0	-3.186718	-2.364989	-0.001035
11	8	0	-4.502471	0.037348	-0.000920
12	6	0	1.128607	-0.670629	-0.000064
13	16	0	1.913495	-0.032620	-1.540744
14	16	0	1.913047	-0.032424	1.540756
15	1	0	1.308183	-1.744862	0.000008
16	6	0	3.604251	-0.676765	-1.276894
17	6	0	3.603913	-0.676533	1.277539
18	6	0	4.279636	-0.183154	0.000369
19	1	0	4.159880	-0.351550	-2.155765
20	1	0	3.575674	-1.769051	-1.297383
21	1	0	4.159248	-0.351089	2.156511
22	1	0	3.575410	-1.768816	1.298245
23	1	0	5.312995	-0.546414	0.000538
24	1	0	4.316696	0.907000	0.000269

25	6	0	-0.673423	3.189774	0.000166
26	6	0	-5.390015	-1.068950	0.001549
27	1	0	-1.277903	3.371851	0.891878
28	1	0	0.181311	3.859697	0.000826
29	1	0	-1.277147	3.372673	-0.891870
30	1	0	-6.391829	-0.648985	0.003056
31	1	0	-5.258460	-1.687136	-0.889602
32	1	0	-5.255113	-1.685733	0.893142



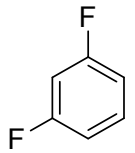
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.410022	1.034680	-0.000135
2	6	0	-1.042952	0.837145	-0.000117
3	6	0	-0.396418	-0.423623	-0.000089
4	6	0	-1.218805	-1.548136	-0.000114
5	6	0	-2.604694	-1.426258	-0.000139
6	6	0	-3.154841	-0.135123	-0.000122
7	8	0	-0.153772	1.909160	-0.000118
8	1	0	-0.771461	-2.536495	-0.000120
9	1	0	-3.203519	-2.328449	-0.000208
10	8	0	-4.547831	0.036111	-0.000163
11	6	0	1.088940	-0.635512	-0.000042
12	16	0	1.907943	-0.003119	-1.533823
13	16	0	1.907856	-0.003073	1.533764
14	1	0	1.277435	-1.709521	-0.000021
15	6	0	3.575087	-0.708826	-1.276368
16	6	0	3.575014	-0.708788	1.276426
17	6	0	4.273388	-0.241519	0.000042
18	1	0	4.146867	-0.409529	-2.155577
19	1	0	3.510909	-1.801296	-1.288881
20	1	0	4.146744	-0.409465	2.155659
21	1	0	3.510836	-1.801258	1.288968
22	1	0	5.296364	-0.638978	0.000077
23	1	0	4.342958	0.847632	0.000027
24	6	0	-0.711013	3.207175	-0.000098

25	6	0	-5.364871	-1.103074	0.000811
26	1	0	-1.338018	3.376373	0.877869
27	1	0	0.141220	3.889347	0.000102
28	1	0	-1.337706	3.376539	-0.878260
29	1	0	-6.396089	-0.747850	0.001262
30	1	0	-5.210237	-1.729897	-0.887034
31	1	0	-5.209141	-1.729105	0.889011



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.408971	0.863103	0.062734
2	6	0	-1.057835	1.029658	-0.199259
3	6	0	-0.158458	-0.079895	-0.353492
4	6	0	-0.797948	-1.336182	-0.282334
5	6	0	-2.162563	-1.516186	-0.044662
6	6	0	-2.973723	-0.411922	0.149470
7	1	0	-3.065730	1.712777	0.175125
8	8	0	-0.514439	2.274770	-0.388047
9	1	0	-0.183592	-2.212975	-0.428390
10	1	0	-2.554823	-2.522732	-0.000151
11	8	0	-4.339415	-0.451009	0.419109
12	6	0	1.248770	0.077097	-0.646006
13	16	0	2.185344	-1.284993	-1.232760
14	16	0	2.242501	1.333097	0.089018
15	6	0	3.040479	-1.890736	0.295607
16	6	0	3.074809	0.399102	1.450279
17	6	0	3.888877	-0.803712	0.962084
18	1	0	3.669158	-2.728443	-0.019145
19	1	0	2.291150	-2.271282	0.994777
20	1	0	3.728563	1.121939	1.947453
21	1	0	2.316831	0.077726	2.169975
22	1	0	4.425187	-1.242194	1.814226
23	1	0	4.643071	-0.454951	0.250047
24	6	0	-1.317675	3.408990	-0.208452

25	6	0	-4.939927	-1.717145	0.494694
26	1	0	-1.726337	3.464951	0.807045
27	1	0	-0.670581	4.267896	-0.378364
28	1	0	-2.151924	3.443025	-0.919955
29	1	0	-5.996125	-1.549436	0.702310
30	1	0	-4.843988	-2.272241	-0.445949
31	1	0	-4.510570	-2.326849	1.298391



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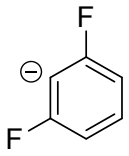
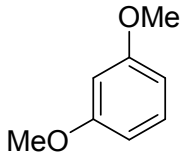
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000002	1.764284	-0.000001
2	6	0	-1.210733	1.080144	0.000010
3	6	0	-1.180376	-0.303523	-0.000004
4	6	0	0.000001	-1.026484	-0.000004
5	6	0	1.180370	-0.303523	-0.000006
6	6	0	1.210725	1.080147	-0.000008
7	1	0	-0.000007	2.845121	0.000008
8	1	0	-2.158247	1.597350	0.000005
9	1	0	-0.000008	-2.105611	-0.000013
10	1	0	2.158244	1.597346	-0.000011
11	9	0	-2.343718	-0.982253	0.000001
12	9	0	2.343730	-0.982245	0.000009

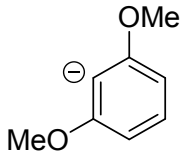


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000010	1.740796	-0.000002
2	6	0	-1.202239	1.035636	0.000025
3	6	0	-1.130108	-0.355232	0.000030
4	6	0	0.000002	-1.134049	0.000006
5	6	0	1.130104	-0.355220	-0.000020
6	6	0	1.202230	1.035642	-0.000019
7	1	0	-0.000009	2.824455	0.000000
8	1	0	-2.157087	1.548731	0.000008
9	1	0	2.157068	1.548755	-0.000036
10	9	0	-2.382267	-0.984859	-0.000023
11	9	0	2.382284	-0.984849	0.000012

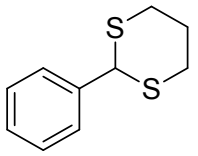


15

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.026984	1.652784	0.000236
2	6	0	0.289092	2.068516	0.000363
3	6	0	1.346221	1.155408	-0.000098
4	6	0	1.051960	-0.203461	-0.000652
5	6	0	-0.275934	-0.646188	-0.000897
6	6	0	-1.309063	0.280686	-0.000448
7	1	0	-1.846136	2.356904	0.000602
8	1	0	0.510686	3.127556	0.000815
9	1	0	2.363847	1.512104	-0.000078
10	8	0	1.987802	-1.194839	-0.001272
11	1	0	-0.454225	-1.709795	-0.001510
12	8	0	-2.629015	-0.052928	-0.000784
13	6	0	3.358101	-0.833051	0.001204
14	6	0	-2.984558	-1.425097	0.001236
15	1	0	3.914593	-1.766101	0.004019
16	1	0	3.620700	-0.258439	-0.890338
17	1	0	3.616708	-0.255473	0.891985
18	1	0	-2.608651	-1.933256	0.892593
19	1	0	-4.070504	-1.453445	0.002242
20	1	0	-2.610319	-1.935500	-0.889548

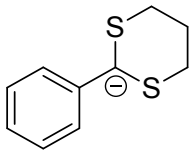


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.024216	1.629444	0.000059
2	6	0	0.294759	2.051559	-0.000056
3	6	0	1.331585	1.112296	-0.000132
4	6	0	0.991325	-0.247493	0.000005
5	6	0	-0.308580	-0.741226	0.000131
6	6	0	-1.274183	0.247019	0.000120
7	1	0	-1.843007	2.341718	0.000126
8	1	0	0.529121	3.110642	-0.000139
9	1	0	2.355231	1.467039	-0.000350
10	8	0	2.004610	-1.227692	0.000014
11	8	0	-2.646779	-0.059749	0.000118
12	6	0	3.340210	-0.808899	0.000031
13	6	0	-2.983834	-1.429730	-0.000168
14	1	0	3.952855	-1.711999	0.000029
15	1	0	3.594240	-0.213527	-0.887559
16	1	0	3.594204	-0.213521	0.887617
17	1	0	-2.585663	-1.946321	0.876866
18	1	0	-4.076286	-1.466373	-0.000130
19	1	0	-2.585736	-1.945945	-0.877460



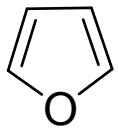
1e

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.083389	-0.000037	1.295060
2	6	0	1.711660	-0.000034	1.077380
3	6	0	1.202321	0.000007	-0.223024
4	6	0	2.092323	0.000036	-1.296783
5	6	0	3.465000	0.000033	-1.078819
6	6	0	3.964036	-0.000003	0.218366
7	1	0	3.465005	-0.000067	2.307283
8	1	0	1.029529	-0.000061	1.916502
9	1	0	1.708418	0.000064	-2.308982
10	1	0	4.142698	0.000058	-1.922020
11	1	0	5.032095	-0.000006	0.389573
12	6	0	-0.281999	0.000007	-0.476246
13	16	0	-1.021489	-1.538006	0.207872
14	16	0	-1.021499	1.538003	0.207927
15	1	0	-0.467836	0.000030	-1.549397
16	6	0	-2.768179	-1.276317	-0.267054
17	6	0	-2.768179	1.276319	-0.267025
18	6	0	-3.395454	-0.000005	0.286522
19	1	0	-3.286085	-2.156527	0.111954
20	1	0	-2.843232	-1.300481	-1.356665
21	1	0	-3.286094	2.156521	0.111990
22	1	0	-2.843219	1.300502	-1.356636
23	1	0	-4.457025	-0.000003	0.017726
24	1	0	-3.335967	-0.000018	1.375637

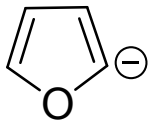


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.180397	1.192633	-0.278330
2	6	0	1.838145	1.201993	0.055900
3	6	0	1.086855	-0.000044	0.238405
4	6	0	1.838035	-1.202079	0.055601
5	6	0	3.180313	-1.192735	-0.278626
6	6	0	3.887327	-0.000073	-0.454983
7	1	0	3.690769	2.142456	-0.405901
8	1	0	1.330666	2.148151	0.181529
9	1	0	1.330529	-2.148253	0.180989
10	1	0	3.690576	-2.142589	-0.406431
11	1	0	4.937774	-0.000062	-0.716013
12	6	0	-0.291733	-0.000005	0.608033
13	16	0	-1.247101	-1.471429	0.700364
14	16	0	-1.247027	1.471377	0.700525
15	6	0	-2.308775	-1.287401	-0.798872
16	6	0	-2.307949	1.287488	-0.799545
17	6	0	-3.140531	0.000344	-0.791789
18	1	0	-2.966229	-2.161128	-0.816951
19	1	0	-1.667251	-1.323718	-1.682572
20	1	0	-2.964566	2.161802	-0.818878
21	1	0	-1.665500	1.322462	-1.682605
22	1	0	-3.795786	0.000181	-1.672653
23	1	0	-3.787444	0.000818	0.090491

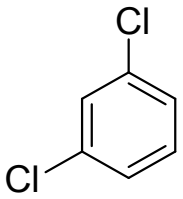
Cartesian coordinates of the optimized structures in solution phase



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.095986	-0.345528	-0.000270
2	6	0	0.716950	0.955275	0.000183
3	6	0	-0.716977	0.955257	-0.000126
4	6	0	-1.095974	-0.345558	-0.000159
5	8	0	0.000015	-1.157215	0.000345
6	1	0	2.050431	-0.839991	-0.000400
7	1	0	1.370418	1.810556	0.000328
8	1	0	-1.370469	1.810521	-0.000217
9	1	0	-2.050409	-0.840042	-0.000234

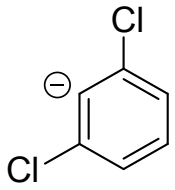


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.554611	-1.166831	-0.000275
2	6	0	-1.191567	0.059978	0.000153
3	6	0	-0.231142	1.130714	-0.000086
4	6	0	0.983690	0.530112	0.000395
5	8	0	0.830990	-0.827181	-0.000242
6	1	0	-2.264980	0.187460	0.000247
7	1	0	-0.413144	2.194674	-0.000099
8	1	0	1.991989	0.911484	0.000666

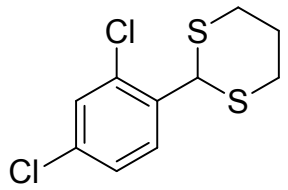


13

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000013	2.072546	0.000040
2	6	0	-1.209632	1.387421	-0.000117
3	6	0	-1.189983	-0.000247	-0.000147
4	6	0	0.000000	-0.715426	-0.000024
5	6	0	1.189978	-0.000229	0.000121
6	6	0	1.209620	1.387432	0.000160
7	1	0	-0.000015	3.153565	0.000070
8	1	0	-2.148223	1.920753	-0.000207
9	1	0	0.000012	-1.794194	-0.000043
10	1	0	2.148201	1.920782	0.000281
11	17	0	-2.704231	-0.882059	-0.000309
12	17	0	2.704243	-0.882053	0.000292



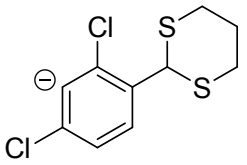
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	2.046877	0.000043
2	6	0	-1.204045	1.346817	-0.000108
3	6	0	-1.134055	-0.042389	-0.000130
4	6	0	0.000000	-0.817173	-0.000015
5	6	0	1.134055	-0.042389	0.000134
6	6	0	1.204045	1.346818	0.000167
7	1	0	0.000000	3.129038	0.000063
8	1	0	-2.149084	1.872444	-0.000203
9	1	0	2.149084	1.872444	0.000282
10	17	0	-2.775873	-0.879567	-0.000328
11	17	0	2.775873	-0.879567	0.000287



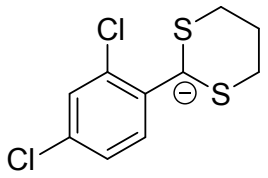
1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.479414	0.814708	-0.000151
2	6	0	1.089921	0.761276	-0.000161
3	6	0	0.399417	-0.457053	0.000046
4	6	0	1.177720	-1.620504	0.000260
5	6	0	2.563050	-1.595677	0.000240
6	6	0	3.202676	-0.365878	0.000020
7	1	0	2.982075	1.769198	-0.000286
8	17	0	0.261418	2.302166	-0.000371
9	1	0	0.675852	-2.578425	0.000442
10	1	0	3.130800	-2.513894	0.000413
11	17	0	4.951475	-0.294494	0.000077
12	6	0	-1.098542	-0.627527	0.000123
13	16	0	-1.869501	0.020945	1.542190
14	16	0	-1.869559	0.020125	-1.542281
15	1	0	-1.301244	-1.695866	0.000403
16	6	0	-3.571562	-0.602122	1.278347
17	6	0	-3.571628	-0.602757	-1.278026
18	6	0	-4.237119	-0.101143	0.000054
19	1	0	-4.119101	-0.264763	2.156892
20	1	0	-3.549674	-1.692950	1.300868
21	1	0	-4.119191	-0.265785	-2.156705

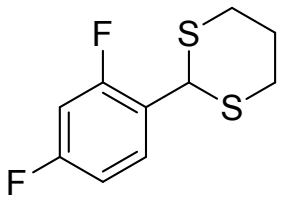
22	1	0	-3.549787	-1.693600	-1.300039
23	1	0	-5.270680	-0.460262	0.000168
24	1	0	-4.273314	0.988860	-0.000211



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.540990	0.917353	0.000217
2	6	0	1.169924	0.793083	0.000219
3	6	0	0.437126	-0.404698	-0.000405
4	6	0	1.199978	-1.581753	-0.000904
5	6	0	2.586660	-1.544733	-0.000895
6	6	0	3.184939	-0.290964	-0.000430
7	17	0	0.215860	2.357040	0.001146
8	1	0	0.694373	-2.538931	-0.001186
9	1	0	3.161152	-2.461170	-0.001190
10	17	0	5.021136	-0.324362	0.000049
11	6	0	-1.062035	-0.580772	-0.000394
12	16	0	-1.862794	0.043883	1.537833
13	16	0	-1.862929	0.046290	-1.537518
14	1	0	-1.259352	-1.650530	-0.001148
15	6	0	-3.530320	-0.667829	1.278954
16	6	0	-3.530426	-0.665855	-1.279686
17	6	0	-4.223254	-0.204521	0.000015
18	1	0	-4.097709	-0.360295	2.156186
19	1	0	-3.452908	-1.756710	1.301123
20	1	0	-4.097913	-0.357062	-2.156405
21	1	0	-3.452954	-1.754691	-1.303477
22	1	0	-5.237185	-0.617073	-0.000257
23	1	0	-4.316364	0.882300	0.000852



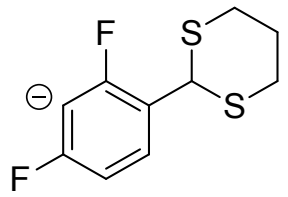
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.507794	0.729635	-0.094027
2	6	0	1.166265	0.959838	0.172504
3	6	0	0.198705	-0.076185	0.350982
4	6	0	0.780897	-1.381609	0.311783
5	6	0	2.115670	-1.632431	0.065473
6	6	0	2.983916	-0.569385	-0.160086
7	1	0	3.178932	1.566822	-0.215272
8	17	0	0.740823	2.658858	0.422721
9	1	0	0.120904	-2.221358	0.471708
10	1	0	2.476118	-2.651419	0.029048
11	17	0	4.691081	-0.864606	-0.501170
12	6	0	-1.196057	0.126297	0.613112
13	16	0	-2.180087	-1.175887	1.271061
14	16	0	-2.149094	1.362424	-0.219211
15	6	0	-3.051000	-1.846226	-0.216065
16	6	0	-2.990842	0.360111	-1.521055
17	6	0	-3.848132	-0.779708	-0.968360
18	1	0	-3.712758	-2.630225	0.155480
19	1	0	-2.313062	-2.308749	-0.874291
20	1	0	-3.610796	1.069798	-2.072016
21	1	0	-2.232027	-0.026600	-2.204161
22	1	0	-4.370155	-1.259759	-1.803496
23	1	0	-4.615948	-0.367411	-0.308531



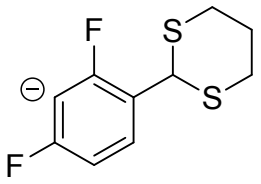
1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.785685	-0.100759	-1.004674
2	6	0	1.409601	-0.087610	-0.863073
3	6	0	0.768497	0.034120	0.368797
4	6	0	1.593257	0.147865	1.491923
5	6	0	2.978201	0.140136	1.398536
6	6	0	3.544773	0.014739	0.144032
7	1	0	3.241850	-0.197988	-1.978385
8	9	0	0.675595	-0.200002	-1.988494
9	1	0	1.133958	0.245490	2.465990
10	1	0	3.603931	0.229069	2.274098
11	9	0	4.890155	0.004127	0.027623
12	6	0	-0.726126	0.049332	0.536067
13	16	0	-1.469069	1.519519	-0.285809
14	16	0	-1.471922	-1.545256	-0.002437
15	1	0	-0.945513	0.147664	1.597006
16	6	0	-3.204460	1.309960	0.260028
17	6	0	-3.206225	-1.235484	0.496851
18	6	0	-3.843426	-0.011883	-0.154452
19	1	0	-3.730322	2.150692	-0.189541
20	1	0	-3.243656	1.436660	1.343233
21	1	0	-3.733866	-2.143943	0.210868
22	1	0	-3.244461	-1.159540	1.584760

23	1	0	-4.894658	0.017048	0.147765
24	1	0	-3.821817	-0.112987	-1.240230

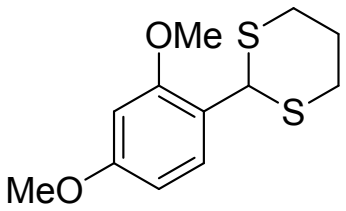


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.846499	-0.239043	-1.076530
2	6	0	-1.488624	-0.204806	-0.872792
3	6	0	-0.810827	0.054670	0.325529
4	6	0	-1.615604	0.304459	1.443280
5	6	0	-3.000047	0.290906	1.334186
6	6	0	-3.535237	0.021595	0.080481
7	9	0	-0.669088	-0.454106	-1.971504
8	1	0	-1.150980	0.510658	2.399078
9	1	0	-3.632111	0.483308	2.191504
10	9	0	-4.933462	0.025264	0.034423
11	6	0	0.684197	0.091652	0.488309
12	16	0	1.466034	-1.536226	0.125509
13	16	0	1.441293	1.469569	-0.472310
14	1	0	0.908043	0.300581	1.533038
15	6	0	3.176269	-1.157746	0.658599
16	6	0	3.157750	1.350173	0.154778
17	6	0	3.830178	0.001524	-0.089020
18	1	0	3.727021	-2.082269	0.491219
19	1	0	3.171436	-0.967313	1.733715
20	1	0	3.694742	2.145739	-0.359808
21	1	0	3.154981	1.590439	1.219795
22	1	0	4.867774	0.077728	0.251443
23	1	0	3.855482	-0.213089	-1.158349



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.869393	0.863484	0.099236
2	6	0	1.535123	1.010817	-0.222896
3	6	0	0.598524	-0.048221	-0.339968
4	6	0	1.193503	-1.323330	-0.121005
5	6	0	2.533867	-1.514339	0.191938
6	6	0	3.357749	-0.413615	0.311038
7	1	0	3.511034	1.731357	0.157043
8	9	0	1.139652	2.287432	-0.504944
9	1	0	0.556827	-2.190756	-0.212194
10	1	0	2.926273	-2.509405	0.353899
11	9	0	4.680626	-0.575330	0.635057
12	6	0	-0.780397	0.133215	-0.724647
13	16	0	-1.722226	1.533798	-0.201951
14	16	0	-1.785241	-1.265510	-1.088737
15	6	0	-2.608732	0.875414	1.280739
16	6	0	-2.671548	-1.571780	0.506050
17	6	0	-3.468098	-0.355514	0.983418
18	1	0	-3.232415	1.697836	1.636403
19	1	0	-1.872301	0.651409	2.055283
20	1	0	-3.336815	-2.417051	0.321664
21	1	0	-1.942048	-1.873493	1.260286
22	1	0	-4.012539	-0.630084	1.893885

23	1	0	-4.217345	-0.098137	0.230291



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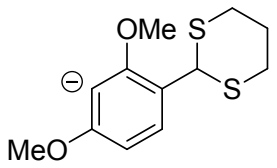
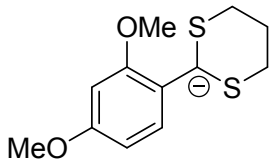
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.462451	0.499025	-0.005950
2	6	0	1.065647	0.551403	-0.005195
3	6	0	0.299885	-0.628156	0.008659
4	6	0	0.991009	-1.841630	0.020770
5	6	0	2.372837	-1.914957	0.019672
6	6	0	3.113573	-0.733805	0.006289
7	1	0	3.030348	1.412885	-0.016060
8	1	0	0.420253	-2.761384	0.031587
9	1	0	2.884514	-2.866480	0.029413
10	6	0	-1.203538	-0.656446	0.010933
11	16	0	-1.921265	0.098983	1.531702
12	16	0	-1.921833	0.038969	-1.538121
13	1	0	-1.511424	-1.699784	0.031467
14	6	0	-3.671525	-0.379795	1.284479
15	6	0	-3.673380	-0.426056	-1.272556
16	6	0	-4.296095	0.149510	-0.003570
17	1	0	-4.189045	0.018863	2.155683
18	1	0	-3.743199	-1.468051	1.327556
19	1	0	-4.190258	-0.056452	-2.156878
20	1	0	-3.748221	-1.515000	-1.277808
21	1	0	-5.355973	-0.123310	0.001944

22	1	0	-4.243130	1.238944	-0.023241
23	8	0	0.382827	1.722792	-0.017419
24	6	0	1.097291	2.954336	-0.027625
25	1	0	1.718591	3.043762	-0.920336
26	1	0	1.717743	3.059039	0.864039
27	1	0	0.341097	3.733214	-0.034677
28	8	0	4.466539	-0.871761	0.006225
29	6	0	5.282144	0.297166	-0.003228
30	1	0	5.106759	0.893500	-0.900157
31	1	0	6.308483	-0.056766	-0.000140
32	1	0	5.106302	0.907979	0.883796



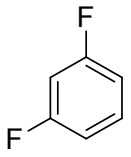
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.525030	0.579424	-0.001057
2	6	0	1.134478	0.560543	-0.002009
3	6	0	0.335610	-0.606753	0.000037
4	6	0	1.011313	-1.832071	0.002046
5	6	0	2.395327	-1.887939	0.002438
6	6	0	3.106546	-0.679331	0.001298
7	1	0	0.437956	-2.751989	0.003299
8	1	0	2.912916	-2.840289	0.003619
9	6	0	-1.167613	-0.639815	0.000670
10	16	0	-1.906512	0.083743	1.530248
11	16	0	-1.907715	0.077624	-1.531162
12	1	0	-1.478282	-1.683456	0.002884
13	6	0	-3.649384	-0.421018	1.279939
14	6	0	-3.650423	-0.426014	-1.277538
15	6	0	-4.286049	0.115888	0.000406
16	1	0	-4.175509	-0.045820	2.156841
17	1	0	-3.704813	-1.511302	1.305276
18	1	0	-4.177234	-0.054226	-2.155481
19	1	0	-3.705923	-1.516384	-1.298563
20	1	0	-5.341540	-0.175315	0.001401
21	1	0	-4.251686	1.206550	-0.001716
22	8	0	0.395495	1.738696	-0.005509

23	6	0	1.093791	2.971532	-0.000313
24	1	0	1.731869	3.078517	-0.878930
25	1	0	1.724861	3.074866	0.883829
26	1	0	0.325117	3.743351	-0.001728
27	8	0	4.492103	-0.862997	0.002780
28	6	0	5.317150	0.290257	-0.001803
29	1	0	5.145594	0.906967	-0.885549
30	1	0	6.341787	-0.080103	-0.001375
31	1	0	5.147072	0.912955	0.877978



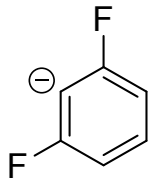
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.458917	0.354042	-0.017234
2	6	0	1.153176	0.756033	0.269170
3	6	0	0.080277	-0.172189	0.412636
4	6	0	0.468054	-1.522295	0.289396
5	6	0	1.768329	-1.941205	0.029979
6	6	0	2.772823	-1.000430	-0.141786
7	1	0	3.232174	1.096632	-0.117419
8	1	0	-0.296734	-2.275353	0.415396
9	1	0	2.001519	-2.994750	-0.056232
10	6	0	-1.284055	0.245583	0.748979
11	16	0	-2.438588	-0.961547	1.305266
12	16	0	-2.071832	1.503316	-0.220187
13	6	0	-3.219756	-1.618562	-0.244772
14	6	0	-2.863527	0.539146	-1.587238
15	6	0	-3.857052	-0.518309	-1.096720
16	1	0	-3.974102	-2.337135	0.081366
17	1	0	-2.466047	-2.159211	-0.821092
18	1	0	-3.370406	1.276114	-2.213788
19	1	0	-2.076814	0.074306	-2.185928
20	1	0	-4.338307	-0.980419	-1.966351
21	1	0	-4.647518	-0.028467	-0.520863
22	8	0	0.847294	2.075256	0.479235

23	6	0	1.861836	3.053892	0.351750
24	1	0	2.670638	2.898198	1.071023
25	1	0	1.384864	4.009213	0.555325
26	1	0	2.280769	3.071334	-0.657920
27	8	0	4.037569	-1.476311	-0.426550
28	6	0	5.087978	-0.538990	-0.590247
29	1	0	4.891700	0.144290	-1.420795
30	1	0	5.981313	-1.118369	-0.808918
31	1	0	5.252794	0.043465	0.319970

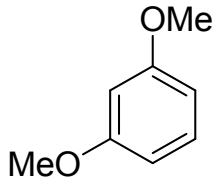


14

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000005	1.765405	-0.000014
2	6	0	-1.211264	1.081058	0.000426
3	6	0	-1.177829	-0.302064	0.000151
4	6	0	-0.000006	-1.029060	0.000150
5	6	0	1.177829	-0.302061	0.000003
6	6	0	1.211280	1.081054	-0.000359
7	1	0	0.000016	2.846523	-0.000158
8	1	0	-2.158347	1.599859	0.000382
9	1	0	0.000023	-2.108519	0.000046
10	1	0	2.158345	1.599888	-0.000583
11	9	0	-2.345824	-0.983533	-0.000310
12	9	0	2.345810	-0.983550	0.000108

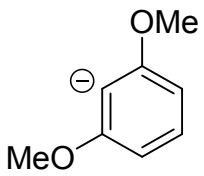


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000001	1.741237	0.000083
2	6	0	-1.203395	1.038790	-0.000159
3	6	0	-1.130498	-0.349768	-0.000334
4	6	0	0.000002	-1.129883	-0.000077
5	6	0	1.130486	-0.349766	0.000258
6	6	0	1.203389	1.038798	0.000241
7	1	0	-0.000008	2.823390	0.000150
8	1	0	-2.155485	1.553734	-0.000226
9	1	0	2.155484	1.553733	0.000382
10	9	0	-2.376887	-0.992630	-0.000260
11	9	0	2.376900	-0.992626	0.000218

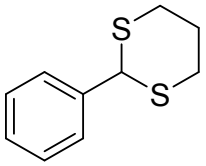


15

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.024722	1.655657	0.000194
2	6	0	0.293949	2.068747	0.000212
3	6	0	1.349126	1.153239	-0.000195
4	6	0	1.051005	-0.206031	-0.000565
5	6	0	-0.278696	-0.646293	-0.000647
6	6	0	-1.310492	0.283538	-0.000256
7	1	0	-1.839639	2.365366	0.000496
8	1	0	0.518075	3.127307	0.000498
9	1	0	2.367756	1.506867	-0.000256
10	8	0	1.986374	-1.197268	-0.001154
11	1	0	-0.464487	-1.708872	-0.001042
12	8	0	-2.630985	-0.048875	-0.000340
13	6	0	3.363935	-0.834108	0.001105
14	6	0	-2.990478	-1.427573	0.000790
15	1	0	3.918395	-1.767707	0.003684
16	1	0	3.622157	-0.260214	-0.890564
17	1	0	3.618540	-0.257465	0.892019
18	1	0	-2.613901	-1.932740	0.891989
19	1	0	-4.075951	-1.452777	0.001984
20	1	0	-2.615820	-1.933687	-0.890686



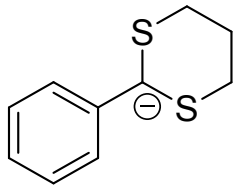
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.017008	1.622708	0.001877
2	6	0	0.300709	2.045992	-0.007127
3	6	0	1.339052	1.109587	-0.008439
4	6	0	1.003039	-0.250106	-0.000524
5	6	0	-0.302294	-0.749021	0.006788
6	6	0	-1.272521	0.239365	0.008784
7	1	0	-1.833645	2.335649	0.002365
8	1	0	0.532359	3.104458	-0.014307
9	1	0	2.362041	1.459604	-0.016396
10	8	0	2.009090	-1.225187	0.000362
11	8	0	-2.643328	-0.051453	0.020213
12	6	0	3.361491	-0.811504	0.003367
13	6	0	-3.032542	-1.412739	-0.016250
14	1	0	3.961667	-1.719264	0.012369
15	1	0	3.613472	-0.228821	-0.888148
16	1	0	3.605347	-0.216426	0.888874
17	1	0	-2.630414	-1.972543	0.829438
18	1	0	-4.121543	-1.411483	0.021546
19	1	0	-2.694941	-1.903753	-0.931201



1e

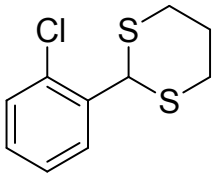
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.100025	0.001570	1.288070
2	6	0	1.725826	0.001360	1.080049
3	6	0	1.206095	-0.000254	-0.217083
4	6	0	2.088361	-0.001546	-1.298556
5	6	0	3.463480	-0.001355	-1.090291
6	6	0	3.972893	0.000191	0.203914
7	1	0	3.489040	0.002814	2.297478
8	1	0	1.053180	0.002464	1.927035
9	1	0	1.696840	-0.002744	-2.307736
10	1	0	4.134671	-0.002412	-1.938695
11	1	0	5.042213	0.000354	0.367060
12	6	0	-0.279068	-0.000391	-0.464511
13	16	0	-1.027418	-1.533738	0.222484
14	16	0	-1.027275	1.533967	0.220399
15	1	0	-0.471370	-0.001114	-1.535485
16	6	0	-2.771193	-1.277537	-0.275181
17	6	0	-2.771073	1.277258	-0.276911
18	6	0	-3.403396	0.000260	0.267305
19	1	0	-3.291579	-2.156668	0.101511
20	1	0	-2.825796	-1.303022	-1.364755
21	1	0	-3.291379	2.156950	0.098577
22	1	0	-2.825680	1.301259	-1.366515

23	1	0	-4.458414	0.000113	-0.022990
24	1	0	-3.368336	0.001000	1.357554



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.168258	-1.193580	-0.289236
2	6	0	1.830913	-1.201894	0.070556
3	6	0	1.082530	-0.000119	0.267155
4	6	0	1.831103	1.201631	0.071259
5	6	0	3.168471	1.193355	-0.288529
6	6	0	3.870093	-0.000094	-0.479655
7	1	0	3.675922	-2.142511	-0.425939
8	1	0	1.330706	-2.150152	0.208557
9	1	0	1.331131	2.149934	0.209741
10	1	0	3.676179	2.142368	-0.424511
11	1	0	4.914453	-0.000197	-0.761395
12	6	0	-0.289982	0.000058	0.670729
13	16	0	-1.258673	-1.469391	0.710182
14	16	0	-1.258312	1.469985	0.709107
15	6	0	-2.279311	-1.286299	-0.819267
16	6	0	-2.279422	1.285929	-0.819450
17	6	0	-3.109627	-0.000265	-0.837143
18	1	0	-2.931871	-2.160720	-0.850940
19	1	0	-1.613875	-1.327016	-1.683767
20	1	0	-2.932339	2.160098	-0.850972
21	1	0	-1.614546	1.326799	-1.684391

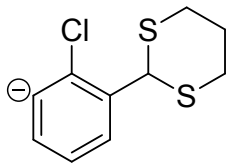
22	1	0	-3.729855	-0.000175	-1.740375
23	1	0	-3.792302	-0.000278	0.016868



1d

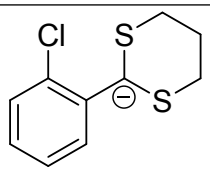
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.177993	0.595744	-0.000069
2	6	0	1.787155	0.625649	-0.000020
3	6	0	1.035330	-0.555970	0.000178
4	6	0	1.747112	-1.761464	0.000232
5	6	0	3.132299	-1.802997	0.000166
6	6	0	3.852488	-0.615427	0.000048
7	1	0	3.720931	1.529367	-0.000227
8	17	0	1.035073	2.204043	-0.000234
9	1	0	1.188133	-2.687978	0.000301
10	1	0	3.643484	-2.755638	0.000206
11	1	0	4.933771	-0.626434	-0.000026
12	6	0	-0.470476	-0.641106	0.000129
13	16	0	-1.198035	0.046983	1.545045
14	16	0	-1.197918	0.046472	-1.545048
15	1	0	-0.730974	-1.697935	0.000300
16	6	0	-2.929600	-0.477083	1.277856
17	6	0	-2.929512	-0.477490	-1.277830
18	6	0	-3.567511	0.062203	-0.000095
19	1	0	-3.460126	-0.111343	2.156072
20	1	0	-2.977127	-1.568475	1.300841
21	1	0	-3.459970	-0.112018	-2.156199

22	1	0	-2.977049	-1.568887	-1.300480
23	1	0	-4.623135	-0.229203	-0.000086
24	1	0	-3.530597	1.152184	-0.000266



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.284884	0.656974	0.000031
2	6	0	1.915444	0.623054	0.000083
3	6	0	1.091964	-0.513777	0.000014
4	6	0	1.757049	-1.749477	-0.000059
5	6	0	3.143862	-1.804729	-0.000095
6	6	0	3.877661	-0.617409	-0.000081
7	17	0	1.032602	2.254324	0.000123
8	1	0	1.174067	-2.663781	-0.000104
9	1	0	3.641629	-2.771477	-0.000140
10	1	0	4.965273	-0.704498	-0.000098
11	6	0	-0.415592	-0.579044	-0.000029
12	16	0	-1.184743	0.096873	1.536617
13	16	0	-1.184670	0.097141	-1.536568
14	1	0	-0.686624	-1.634226	-0.000119
15	6	0	-2.879660	-0.538288	1.277536
16	6	0	-2.879594	-0.538078	-1.277676
17	6	0	-3.556181	-0.042076	-0.000046
18	1	0	-3.438053	-0.212294	2.155626
19	1	0	-2.862641	-1.632435	1.292352
20	1	0	-3.437946	-0.211951	-2.155741

21	1	0	-2.862563	-1.632223	-1.292665
22	1	0	-4.594632	-0.396571	-0.000100
23	1	0	-3.581166	1.048834	0.000045



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.183995	-0.036291	-0.416411
2	6	0	1.942780	0.433816	-0.017416
3	6	0	0.800103	-0.405759	0.174611
4	6	0	1.112977	-1.794229	-0.001394
5	6	0	2.350973	-2.266267	-0.381409
6	6	0	3.415288	-1.392364	-0.619522
7	1	0	3.986759	0.678757	-0.538554
8	17	0	1.897025	2.164633	0.371070
9	1	0	0.310403	-2.496718	0.169325
10	1	0	2.487216	-3.334996	-0.507682
11	1	0	4.389764	-1.748282	-0.925859
12	6	0	-0.510573	0.017773	0.558274
13	16	0	-1.687833	-1.141216	1.164814
14	16	0	-1.234687	1.550517	0.070424
15	6	0	-2.814142	-1.356874	-0.283800
16	6	0	-2.388389	0.978300	-1.249806
17	6	0	-3.425135	-0.038544	-0.764186
18	1	0	-3.597930	-2.044365	0.044817
19	1	0	-2.258820	-1.837320	-1.093424
20	1	0	-2.885148	1.881791	-1.613716
21	1	0	-1.799074	0.561516	-2.070569

22	1	0	-4.126904	-0.250837	-1.581563
23	1	0	-4.002622	0.405507	0.051575