Electronic Supplementary Material (ESI) for Organic and Biomolecular Chemistry

A facile preparation of trisubstituted amino–furan and –thiophene derivatives

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SUPPORTING INFORMATION

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Part 1: Calculations

Cartesian coordinates and energies for all optimized geometries 1d, 1e, 1g, 2d, 2g, 3dα, 3eα, 3gα, 4d, 4g, and electrophiles at a B3LYP/6-311+G(d,p) level of theory :

Compnd **1d**
Cartesian Coordinates
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.628063	-0.279881	-0.018093
2	6	0	2.622829	-1.584550	0.415473
3	6	0	1.282540	-2.030856	0.441476
4	6	0	0.528869	-0.947761	0.011751
5	8	0	1.316118	0.108181	-0.268461
6	6	0	3.700229	0.651956	-0.230186
7	8	0	3.593876	1.800881	-0.624602
8	7	0	-0.798294	-0.784324	-0.172423
9	6	0	-1.405425	0.446746	-0.659080
10	6	0	-2.802469	-0.029926	-1.116178
11	6	0	-3.121700	-1.181207	-0.148022
12	6	0	-1.761603	-1.859643	0.081279
13	6	0	-1.518258	1.573044	0.376285
14	8	0	-1.870913	2.687756	0.090852
15	8	0	-1.217124	1.185942	1.633796
16	1	0	3.500303	-2.152967	0.684986
17	1	0	0.911586	-2.999607	0.730117
18	1	0	4.692566	0.213849	0.008064
19	1	0	-0.831315	0.869421	-1.486131
20	1	0	-3.535543	0.776007	-1.099276
21	1	0	-2.727521	-0.398546	-2.142220
22	1	0	-3.863283	-1.874182	-0.547335
23	1	0	-3.506756	-0.787509	0.795896
24	1	0	-1.594371	-2.688650	-0.617876
25	1	0	-1.653677	-2.245934	1.099325
26	1	0	-1.298044	1.968758	2.200501

Energy = -743.5337022 hartrees

Compnd **1e**

Cartesian Coordinates

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.288413	-0.881096	-0.201111
2	6	0	-2.065401	-2.174962	0.207254
3	6	0	-0.725807	-2.268212	0.644085
4	6	0	-0.190818	-0.997390	0.481162
5	8	0	-1.110501	-0.165291	-0.040227
6	6	0	-3.454079	-0.213585	-0.708323
7	8	0	-3.532349	0.964338	-1.017427
8	7	0	1.032910	-0.465225	0.774873
9	6	0	1.371779	0.902964	0.344298
10	6	0	1.848385	0.912480	-1.116141
11	6	0	3.046145	-0.042977	-1.270672
12	6	0	0.280473	1.908155	0.738808
13	8	0	-0.188416	1.983661	1.843081
14	8	0	-0.029625	2.745177	-0.267659
15	6	0	2.750719	-1.444523	-0.710887
16	6	0	2.196307	-1.363097	0.719219
17	1	0	-2.799501	-2.966526	0.199683
18	1	0	-0.229746	-3.133894	1.048010
19	1	0	-4.327198	-0.892527	-0.801163
20	1	0	2.218946	1.191452	0.980623
21	1	0	2.131447	1.926404	-1.406409
22	1	0	1.022246	0.613442	-1.767239
23	1	0	3.909787	0.380695	-0.741443
24	1	0	3.333362	-0.112600	-2.323429
25	1	0	-0.748142	3.318654	0.041176
26	1	0	2.013334	-1.950388	-1.344198
27	1	0	3.656173	-2.059655	-0.719407
28	1	0	1.909496	-2.344164	1.096679
29	1	0	2.950801	-0.963948	1.404715

Energy = -782.8 519953 hartrees

Compnd **1g**

Cartesian Coordinates

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.268111	-2.109101	-0.011453
2	6	0	-3.542615	-1.716053	0.328632
3	6	0	-3.557207	-0.306114	0.412095
4	6	0	-2.260611	0.095468	0.114105
5	8	0	-1.480356	-0.972847	-0.147398
6	6	0	-1.651166	-3.386956	-0.207960
7	8	0	-0.472055	-3.570397	-0.480187
8	7	0	-1.654110	1.299767	0.056500
9	6	0	-0.308183	1.467320	-0.526231
10	6	0	-0.274954	2.961305	-0.896497
11	6	0	-1.285067	3.613829	0.063804
12	6	0	-2.392060	2.559810	0.184243
13	6	0	0.767753	1.039594	0.477803
14	8	0	1.998988	0.907892	-0.271282
15	16	0	3.092811	-0.236405	0.201358
16	6	0	2.504145	-1.697151	-0.665289
17	8	0	4.347090	0.196437	-0.382841
18	8	0	2.955525	-0.437415	1.638157
19	1	0	-4.375072	-2.382101	0.499125
20	1	0	-4.388725	0.333714	0.654655
21	1	0	-2.351160	-4.237185	-0.085898
22	1	0	-0.201467	0.830877	-1.408354
23	1	0	0.731507	3.373489	-0.815141
24	1	0	-0.602657	3.090376	-1.931550
25	1	0	-1.663833	4.568812	-0.302588
26	1	0	-0.830084	3.789305	1.042461
27	1	0	-3.131163	2.657829	-0.622656
28	1	0	-2.922015	2.602098	1.139446
29	1	0	0.501033	0.090709	0.941267
30	1	0	0.912585	1.784469	1.264432
31	1	0	2.556738	-1.491587	-1.732724
32	1	0	1.488147	-1.943355	-0.355025
33	1	0	3.184887	-2.504395	-0.395783

Energy = -1257.4424396 hartrees

Compnd **2d**

Cartesian Coordinates

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.818433	-0.318552	0.062536
2	6	0	2.491028	-1.595159	0.468960
3	6	0	1.114318	-1.880878	0.441103
4	6	0	0.360039	-0.797226	-0.001813
5	16	0	1.371651	0.584964	-0.379539
6	6	0	4.127186	0.277002	-0.022489
7	8	0	4.372009	1.413563	-0.392805
8	7	0	-0.988056	-0.744092	-0.156999
9	6	0	-1.712114	0.409161	-0.665186
10	6	0	-3.062165	-0.199645	-1.111226
11	6	0	-3.269293	-1.365329	-0.130378
12	6	0	-1.850888	-1.901086	0.112058
13	6	0	-1.934489	1.541618	0.346559
14	8	0	-2.203472	2.668799	0.021750
15	8	0	-1.848374	1.136060	1.631381
16	1	0	3.244152	-2.309051	0.780844
17	1	0	0.684671	-2.829559	0.727935
18	1	0	4.943558	-0.408290	0.290183
19	1	0	-1.187614	0.866811	-1.508705
20	1	0	-3.870224	0.531951	-1.102112
21	1	0	-2.953555	-0.569608	-2.133704
22	1	0	-3.935046	-2.132548	-0.527893
23	1	0	-3.697494	-1.002274	0.806549
24	1	0	-1.598239	-2.721948	-0.571057
25	1	0	-1.710008	-2.257074	1.136908
26	1	0	-2.003851	1.913987	2.189315

Energy = -1066.5135687 hartrees

Compnd **2g**

Cartesian Coordinates

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.209570	-0.604370	0.148504
2	6	0	-3.375121	0.349435	1.130855
3	6	0	-2.312006	1.263254	1.235352
4	6	0	-1.298672	1.013486	0.310253
5	16	0	-1.674355	-0.383012	-0.684848
6	6	0	-4.092119	-1.690018	-0.190670
7	8	0	-3.888957	-2.533181	-1.050560
8	7	0	-0.160218	1.743368	0.143128
9	6	0	0.769024	1.596649	-0.987922
10	6	0	1.222698	3.044357	-1.257404
11	6	0	1.185392	3.700747	0.132741
12	6	0	-0.034028	3.055145	0.802125
13	6	0	1.970477	0.705911	-0.664880
14	8	0	1.474446	-0.625132	-0.408302
15	16	0	2.515251	-1.682517	0.309357
16	6	0	1.357564	-3.042255	0.446093
17	8	0	3.578781	-2.010621	-0.630213
18	8	0	2.862751	-1.172384	1.629891
19	1	0	-4.253376	0.378227	1.764934
20	1	0	-2.276600	2.067005	1.955879
21	1	0	-5.020671	-1.711760	0.418324
22	1	0	0.239423	1.170956	-1.845620
23	1	0	2.205288	3.095621	-1.730305
24	1	0	0.506152	3.527754	-1.926189
25	1	0	1.092951	4.786453	0.083354
26	1	0	2.096013	3.474183	0.692844
27	1	0	-0.945424	3.641759	0.628811
28	1	0	0.090788	2.938278	1.882214
29	1	0	2.652630	0.674463	-1.519326
30	1	0	2.501170	1.072004	0.218004
31	1	0	1.904741	-3.855537	0.921864
32	1	0	1.036008	-3.320045	-0.555291
33	1	0	0.520092	-2.717972	1.059651

Energy = -1580.4186007 hartrees

Compnd **2-Furancarboxaldehyde**
Cartesian Coordinates
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.255166	0.263755	-0.000019
2	6	0	-0.773425	1.173005	0.000011
3	6	0	-1.980207	0.419720	0.000207
4	6	0	-1.598439	-0.891275	0.000084
5	8	0	-0.253244	-1.004590	-0.000011
6	6	0	1.695965	0.464259	-0.000113
7	8	0	2.532655	-0.412389	-0.000159
8	1	0	-2.149171	-1.817547	0.000115
9	1	0	-0.668626	2.246955	-0.000014
10	1	0	-2.991641	0.792826	0.000346
11	1	0	1.979789	1.536807	-0.000104

Energy = -34 3.4469726 hartrees

Compnd **(*S*)-1-(furan-2-yl)pyrrolidine-2-carboxylic acid**
Cartesian Coordinates
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.965884	-1.075434	-0.330251
2	6	0	-3.506858	0.079314	0.122301
3	6	0	-2.427495	1.008380	0.320500
4	6	0	-1.290661	0.327950	-0.031594
5	8	0	-1.591346	-0.936376	-0.430652
6	1	0	-3.356653	-2.033957	-0.621100
7	7	0	0.033259	0.663906	-0.041057
8	6	0	1.055106	-0.148885	-0.676680
9	6	0	2.200884	0.865033	-0.924898
10	6	0	2.001776	1.922948	0.172892
11	6	0	0.476851	2.008541	0.314131
12	6	0	1.545888	-1.339964	0.152331
13	8	0	2.084295	-2.304297	-0.330621
14	8	0	1.365189	-1.186094	1.482272
15	1	0	-4.555813	0.262055	0.296114
16	1	0	-2.490947	2.024311	0.671854
17	1	0	0.702816	-0.583697	-1.615149
18	1	0	3.184431	0.394230	-0.907747
19	1	0	2.060870	1.309343	-1.913617
20	1	0	2.447922	2.884527	-0.085831
21	1	0	2.445670	1.585735	1.112606
22	1	0	0.046244	2.755335	-0.369512
23	1	0	0.162591	2.264154	1.331007
24	1	0	1.717301	-1.982552	1.908383

Energy = -630.1660786 hartrees

Compnd **(*S*, *S*)-3dα**

Cartesian Coordinates

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.517063	2.760527	-0.429975
2	6	0	1.332141	1.671819	-0.540978
3	6	0	0.624817	0.543494	-0.042655
4	6	0	-0.645540	1.019369	0.315003
5	8	0	-0.699108	2.352206	0.097153
6	1	0	2.339727	1.687627	-0.923558
7	6	0	0.678160	4.168198	-0.708716
8	8	0	1.684325	4.665506	-1.182880
9	1	0	-0.207225	4.785075	-0.453061
10	7	0	-1.781327	0.492373	0.847767
11	6	0	-2.318502	-0.832379	0.555161
12	6	0	-3.446708	-0.959453	1.597305
13	6	0	-4.029016	0.462703	1.659049
14	6	0	-2.836421	1.394854	1.366975
15	1	0	-1.565053	-1.604585	0.683480
16	1	0	-4.178782	-1.719185	1.325170
17	1	0	-2.999901	-1.242545	2.553352
18	1	0	-4.795885	0.590127	0.891800
19	1	0	-4.490107	0.681134	2.623152
20	1	0	-3.092894	2.159935	0.632333
21	1	0	-2.464173	1.897733	2.263929
22	6	0	-2.864182	-0.921227	-0.873368
23	8	0	-2.955115	-0.008673	-1.652541
24	8	0	-3.260485	-2.183098	-1.157169
25	1	0	-3.580520	-2.188854	-2.072190
26	6	0	1.223547	-0.838392	0.141669
27	6	0	2.720318	-0.674149	0.533203
28	8	0	3.602521	-0.361746	-0.215660
29	8	0	2.879235	-0.896850	1.849840
30	6	0	1.163841	-1.683091	-1.166325
31	9	0	-0.112810	-2.013550	-1.451016
32	9	0	1.854662	-2.833344	-1.032182
33	9	0	1.654746	-1.023756	-2.221358
34	6	0	4.220373	-0.730024	2.370319
35	1	0	4.144410	-0.941063	3.433692
36	1	0	4.896403	-1.430154	1.880501
37	1	0	4.558357	0.291384	2.198009
38	8	0	0.531226	-1.605395	1.108574
39	1	0	1.035421	-1.566486	1.931474

Energy = -1423.171946 hartrees

Compnd ***(S, R)*-3dα**

Cartesian Coordinates

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.005758	2.801573	0.014676
2	6	0	-1.652366	1.612924	-0.153566
3	6	0	-0.684018	0.572261	-0.124068
4	6	0	0.556766	1.213613	0.035673
5	8	0	0.356617	2.548255	0.131004
6	1	0	-2.717613	1.499591	-0.276448
7	6	0	-1.432452	4.176300	0.109098
8	8	0	-2.590094	4.546761	0.018883
9	1	0	-0.605926	4.897091	0.275543
10	7	0	1.866463	0.865942	0.115017
11	6	0	2.471561	-0.386652	-0.327767
12	6	0	3.858477	0.065444	-0.840464
13	6	0	4.220901	1.199723	0.126264
14	6	0	2.885793	1.919478	0.345525
15	1	0	1.884996	-0.863489	-1.108717
16	1	0	4.579798	-0.750987	-0.857504
17	1	0	3.748028	0.444245	-1.859900
18	1	0	4.594896	0.792646	1.068946
19	1	0	4.980887	1.872296	-0.273572
20	1	0	2.782503	2.336648	1.349038
21	1	0	2.744907	2.731098	-0.373765
22	6	0	2.633784	-1.392130	0.814177
23	8	0	2.444725	-1.185545	1.985786
24	8	0	3.083056	-2.573278	0.335061
25	1	0	3.182125	-3.176256	1.087039
26	6	0	-1.021661	-0.904702	-0.181570
27	8	0	-0.009362	-1.724308	0.360085
28	1	0	-0.135362	-1.752751	1.318237
29	6	0	-2.365186	-1.119886	0.574765
30	8	0	-3.458584	-0.919774	0.123410
31	8	0	-2.115250	-1.513199	1.833262
32	6	0	-1.194936	-1.407509	-1.644280
33	9	0	-2.036121	-0.640621	-2.347527
34	9	0	-1.650411	-2.672529	-1.677458
35	9	0	-0.004913	-1.392627	-2.288682
36	6	0	-3.266662	-1.682686	2.693233
37	1	0	-3.809981	-0.741529	2.775084
38	1	0	-3.922414	-2.452521	2.287244
39	1	0	-2.863409	-1.983494	3.656558

Energy = -1423.1736943 hartrees

Compnd ***(S, S)*-3eα**

Cartesian Coordinates

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.717687	2.790761	-0.241020
2	6	0	1.540517	1.714215	-0.402591
3	6	0	0.794955	0.546343	-0.082606
4	6	0	-0.499271	0.990261	0.226011
5	8	0	-0.534275	2.339561	0.142612
6	1	0	2.576914	1.760211	-0.694534
7	6	0	0.897638	4.219879	-0.358003
8	8	0	1.934740	4.756486	-0.704307
9	1	0	-0.004471	4.812329	-0.103553
10	7	0	-1.672526	0.410569	0.620439
11	6	0	-2.162046	-0.821356	0.006681
12	6	0	-2.891914	-1.707705	1.053974
13	6	0	-3.490129	-0.872631	2.202074
14	1	0	-1.313704	-1.390285	-0.359406
15	1	0	-3.672174	-2.277498	0.546742
16	1	0	-2.175325	-2.431981	1.445579
17	1	0	-4.338414	-1.402023	2.643667
18	1	0	-2.749099	-0.745412	2.998280
19	6	0	-2.993172	-0.513153	-1.245645
20	8	0	-3.174130	0.577047	-1.723612
21	8	0	-3.477975	-1.648472	-1.803328
22	1	0	-3.941942	-1.395129	-2.615912
23	6	0	1.383516	-0.850099	0.002683
24	8	0	0.553503	-1.744546	0.715242
25	1	0	0.938762	-1.871159	1.591699
26	6	0	-3.913082	0.503746	1.687980
27	1	0	-4.630536	0.388768	0.868641
28	1	0	-4.424242	1.079425	2.463843
29	6	0	-2.692953	1.306644	1.216882
30	1	0	-2.991130	2.078164	0.503352
31	1	0	-2.222452	1.802084	2.070500
32	6	0	1.561737	-1.490498	-1.407939
33	9	0	2.224785	-2.661161	-1.325614
34	9	0	0.356157	-1.748185	-1.958592
35	9	0	2.227044	-0.694856	-2.252949
36	6	0	2.789795	-0.747636	0.660752
37	8	0	3.769765	-0.302177	0.133705
38	8	0	2.741595	-1.198529	1.926870
39	6	0	3.973601	-1.115204	2.683925
40	1	0	3.734172	-1.510660	3.667468
41	1	0	4.745550	-1.712691	2.200020
42	1	0	4.296858	-0.076685	2.748529

Energy = -1462.4908002 hartrees

Compnd ***(S, R)*-3eα**

Cartesian Coordinates

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.103937	2.809437	-0.153349
2	6	0	-1.781857	1.635628	-0.304528
3	6	0	-0.850603	0.569672	-0.165880
4	6	0	0.398583	1.176394	0.037458
5	8	0	0.238086	2.521851	0.051445
6	1	0	-2.843037	1.546983	-0.473477
7	6	0	-1.490711	4.200918	-0.136077
8	8	0	-2.625266	4.602576	-0.323327
9	1	0	-0.654649	4.901241	0.065971
10	7	0	1.686017	0.767855	0.234046
11	6	0	2.233934	-0.413722	-0.437971
12	6	0	3.530886	-0.036811	-1.187950
13	6	0	4.624575	0.488859	-0.236134
14	1	0	1.510545	-0.773913	-1.166176
15	1	0	3.879328	-0.901833	-1.753489
16	1	0	3.259154	0.731628	-1.916901
17	1	0	5.267420	-0.333130	0.091155
18	1	0	5.267721	1.182591	-0.784693
19	6	0	2.468647	-1.580372	0.528553
20	8	0	2.349334	-1.567223	1.727340
21	8	0	2.865409	-2.675642	-0.156628
22	1	0	2.975947	-3.395094	0.482955
23	6	0	-1.243439	-0.895974	-0.121875
24	8	0	-0.230213	-1.728660	0.389202
25	1	0	-0.243084	-1.670050	1.353965
26	6	0	-2.539538	-1.011224	0.732747
27	8	0	-3.653786	-0.801608	0.339716
28	8	0	-2.217554	-1.323977	1.996966
29	6	0	-1.530871	-1.462672	-1.542488
30	9	0	-2.387059	-0.698317	-2.231738
31	9	0	-2.034905	-2.707415	-1.480284
32	9	0	-0.385315	-1.527867	-2.258756
33	6	0	-3.313680	-1.391878	2.938793
34	1	0	-3.818553	-0.427367	2.990990
35	1	0	-4.021038	-2.161143	2.629971
36	1	0	-2.857419	-1.643908	3.892456
37	6	0	4.010520	1.184253	0.998396
38	1	0	3.893215	0.473342	1.818434
39	1	0	4.669743	1.977699	1.359464
40	6	0	2.650707	1.801139	0.686315
41	1	0	2.237066	2.280582	1.574634
42	1	0	2.753667	2.579358	-0.080361

Energy = -1462.4926465 hartrees

Compnd ***(S, S)*-3gα**

Cartesian Coordinates

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.362678	2.299822	-1.154088
2	6	0	2.610679	0.959758	-1.092879
3	6	0	1.682026	0.384868	-0.181098
4	6	0	0.856120	1.437745	0.239650
5	8	0	1.281139	2.590747	-0.337436
6	1	0	3.395641	0.447708	-1.624546
7	6	0	2.996311	3.406802	-1.833797
8	8	0	3.937569	3.296266	-2.598579
9	1	0	2.550076	4.395634	-1.603649
10	7	0	-0.212962	1.588659	1.062630
11	6	0	-1.313940	0.630268	1.258122
12	6	0	-1.987478	1.166128	2.527038
13	6	0	-1.842837	2.692964	2.407126
14	6	0	-0.498742	2.901037	1.687969
15	1	0	-0.926115	-0.373252	1.401210
16	1	0	-3.024207	0.837608	2.606056
17	1	0	-1.446466	0.795260	3.401775
18	1	0	-2.659060	3.108945	1.811763
19	1	0	-1.864163	3.193552	3.376063
20	1	0	-0.548747	3.696499	0.941908
21	1	0	0.310096	3.147870	2.383664
22	6	0	-2.240449	0.635407	0.035820
23	8	0	-3.187527	-0.445754	0.247007
24	6	0	1.714532	-1.057590	0.289808
25	6	0	3.199273	-1.515335	0.393162
26	8	0	3.933267	-1.693892	-0.537399
27	8	0	3.552828	-1.660970	1.682129
28	6	0	1.002231	-2.014700	-0.715370
29	9	0	-0.326357	-1.789010	-0.716336
30	9	0	1.190613	-3.305030	-0.365720
31	9	0	1.439792	-1.858072	-1.970221
32	6	0	4.923509	-2.058862	1.930628
33	1	0	5.014632	-2.115580	3.012039
34	1	0	5.115439	-3.027678	1.470636
35	1	0	5.603796	-1.313586	1.519719
36	8	0	1.042236	-1.230300	1.520668
37	1	0	1.703466	-1.427111	2.196540
38	1	0	-2.778241	1.583053	-0.056182
39	1	0	-1.684684	0.442227	-0.882440
40	16	0	-4.492392	-0.491371	-0.751203
41	6	0	-4.967504	-2.185456	-0.407855
42	1	0	-4.159194	-2.839406	-0.727449
43	1	0	-5.164997	-2.277090	0.658141
44	1	0	-5.872077	-2.367899	-0.987138
45	8	0	-5.508083	0.419501	-0.240464
46	8	0	-4.040316	-0.362293	-2.129952

Energy = -1937.0752051 hartrees

Compnd ***(S, R)*-3gα**

Cartesian Coordinates

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.340361	1.149215	-1.019011
2	6	0	2.929657	-0.090476	-0.628357
3	6	0	1.613863	0.016690	-0.098717
4	6	0	1.284825	1.383508	-0.190403
5	8	0	2.319561	2.053346	-0.749314
6	1	0	3.524196	-0.987010	-0.694882
7	6	0	4.549354	1.673438	-1.604737
8	8	0	5.515978	0.998722	-1.914977
9	1	0	4.537749	2.771881	-1.760082
10	7	0	0.246019	2.203990	0.119376
11	6	0	-1.076228	1.824262	0.640203
12	6	0	-1.547962	3.104729	1.343801
13	6	0	-0.928566	4.232301	0.505506
14	6	0	0.438627	3.673723	0.094829
15	1	0	-1.000602	0.984987	1.323169
16	1	0	-2.636215	3.155560	1.407135
17	1	0	-1.151335	3.123700	2.362472
18	1	0	-1.536921	4.433892	-0.380399
19	1	0	-0.834091	5.169234	1.056011
20	1	0	0.754798	4.010097	-0.893804
21	1	0	1.224045	3.950536	0.806157
22	6	0	-1.983181	1.406731	-0.524643
23	8	0	-3.165281	0.781431	0.056479
24	6	0	0.863000	-1.155995	0.518818
25	8	0	-0.533417	-0.999534	0.518204
26	1	0	-0.940122	-1.515608	-0.196429
27	6	0	1.279753	-2.461981	-0.216930
28	8	0	2.324708	-3.035811	-0.074533
29	8	0	0.309474	-2.834963	-1.060804
30	6	0	1.235107	-1.303914	2.026022
31	9	0	2.556029	-1.342046	2.236949
32	9	0	0.695950	-2.420339	2.554056
33	9	0	0.745983	-0.252740	2.723734
34	6	0	0.558934	-4.016834	-1.856116
35	1	0	1.441758	-3.865654	-2.477058
36	1	0	0.710421	-4.876867	-1.204123
37	1	0	-0.331005	-4.141884	-2.466911
38	1	0	-2.310217	2.259373	-1.124003
39	1	0	-1.466135	0.690301	-1.160603
40	16	0	-3.868811	-0.427905	-0.791837
41	6	0	-4.968790	-0.990495	0.504803
42	1	0	-5.541364	-1.813504	0.078369
43	1	0	-4.363442	-1.326367	1.343922
44	1	0	-5.621869	-0.165116	0.780597
45	8	0	-4.630747	0.122432	-1.901648
46	8	0	-2.864650	-1.457158	-1.069512

Energy = -1937.0800665 hartrees

Compnd **(*S*, *S*)-4d**
Cartesian Coordinates
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.075745	2.650053	-0.422701
2	6	0	1.532742	1.359717	-0.507539
3	6	0	0.632279	0.377282	-0.023651
4	6	0	-0.585622	0.934457	0.401209
5	16	0	-0.546970	2.685971	0.221545
6	1	0	2.522584	1.137805	-0.881903
7	6	0	1.793187	3.876193	-0.742689
8	8	0	2.913974	3.911570	-1.213569
9	1	0	1.242930	4.815114	-0.525245
10	7	0	-1.729615	0.366407	0.909944
11	6	0	-2.421901	-0.779530	0.316135
12	6	0	-3.491639	-1.095462	1.377823
13	6	0	-3.920666	0.294375	1.883478
14	6	0	-2.687448	1.196937	1.669076
15	1	0	-1.749567	-1.618171	0.174153
16	1	0	-4.316449	-1.683692	0.975676
17	1	0	-3.019015	-1.674829	2.174007
18	1	0	-4.761872	0.669943	1.297787
19	1	0	-4.233118	0.272451	2.928272
20	1	0	-2.964580	2.094337	1.104960
21	1	0	-2.221483	1.514093	2.606216
22	6	0	-3.060714	-0.430580	-1.029383
23	8	0	-3.182183	0.676285	-1.488286
24	8	0	-3.508986	-1.544524	-1.652062
25	1	0	-3.903384	-1.269677	-2.493989
26	6	0	1.074094	-1.083780	0.103975
27	6	0	2.541426	-1.101089	0.624346
28	8	0	3.528514	-1.010216	-0.049414
29	8	0	2.538051	-1.197043	1.966324
30	6	0	1.027475	-1.824639	-1.264305
31	9	0	-0.252526	-1.969973	-1.671719
32	9	0	1.559467	-3.056597	-1.171386
33	9	0	1.678335	-1.159265	-2.225650
34	6	0	3.833237	-1.167655	2.611584
35	1	0	3.626411	-1.245860	3.675750
36	1	0	4.437631	-2.007355	2.269455
37	1	0	4.340392	-0.231003	2.381199
38	8	0	0.255131	-1.853998	0.958807
39	1	0	0.581680	-1.735262	1.859566

Energy = -1746.1443231 hartrees

Compnd **(*S*, *R*)-4d**

Cartesian Coordinates

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.922210	2.400946	-0.155301
2	6	0	-1.967908	1.041252	-0.312582
3	6	0	-0.728837	0.371471	-0.147525
4	6	0	0.333482	1.263863	0.097134
5	16	0	-0.284117	2.920941	0.172146
6	1	0	-2.900443	0.531826	-0.514227
7	6	0	-3.026431	3.347317	-0.175371
8	8	0	-4.181450	3.049451	-0.414911
9	1	0	-2.750937	4.398794	0.050086
10	7	0	1.685173	1.106070	0.264830
11	6	0	2.522563	0.118239	-0.429280
12	6	0	3.756254	0.944363	-0.860749
13	6	0	3.942535	1.896121	0.327176
14	6	0	2.502070	2.262606	0.698135
15	1	0	1.999695	-0.319872	-1.274468
16	1	0	4.624479	0.318636	-1.068222
17	1	0	3.510013	1.498926	-1.770252
18	1	0	4.434215	1.383754	1.156675
19	1	0	4.531164	2.780012	0.078002
20	1	0	2.362733	2.452108	1.764915
21	1	0	2.192941	3.159258	0.146461
22	6	0	2.988117	-1.008878	0.493123
23	8	0	2.968148	-1.002873	1.698690
24	8	0	3.530038	-2.010180	-0.232026
25	1	0	3.832099	-2.690920	0.387919
26	6	0	-0.694604	-1.157877	-0.118488
27	8	0	0.494626	-1.684893	0.416916
28	1	0	0.454638	-1.607243	1.379900
29	6	0	-1.912280	-1.650340	0.720050
30	8	0	-3.013780	-1.872303	0.300453
31	8	0	-1.547801	-1.750216	2.008515
32	6	0	-0.788721	-1.773883	-1.544459
33	9	0	-1.828383	-1.294245	-2.238159
34	9	0	-0.897360	-3.112114	-1.493655
35	9	0	0.328795	-1.489760	-2.252906
36	6	0	-2.586207	-2.134470	2.939400
37	1	0	-3.396481	-1.406064	2.912170
38	1	0	-2.969973	-3.121392	2.681783
39	1	0	-2.107149	-2.146561	3.914923

Energy = -1746.1450274 hartrees

Compnd **(*S*, *S*)-4g**

Cartesian Coordinates

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.579201	2.705480	-0.005296
2	6	0	2.208594	1.576261	-0.464100
3	6	0	1.627923	0.368496	0.005954
4	6	0	0.523235	0.586939	0.811351
5	16	0	0.220001	2.309723	1.013689
6	1	0	3.078205	1.626784	-1.105187
7	6	0	1.953953	4.101291	-0.257614
8	8	0	2.883746	4.429823	-0.961729
9	1	0	1.322927	4.861362	0.245575
10	7	0	-0.282901	-0.394488	1.413603
11	6	0	-1.461279	-0.959693	0.694837
12	6	0	-1.988124	-1.960411	1.729280
13	6	0	-1.755096	-1.272348	3.094874
14	6	0	-0.626418	-0.244849	2.852273
15	1	0	-1.119599	-1.450715	-0.216646
16	1	0	-3.034482	-2.209564	1.553983
17	1	0	-1.408318	-2.883332	1.658499
18	1	0	-2.659631	-0.765795	3.436021
19	1	0	-1.482760	-1.994888	3.864808
20	1	0	-0.963521	0.773105	3.079305
21	1	0	0.268202	-0.435077	3.448843
22	6	0	-2.490172	0.106958	0.307980
23	8	0	-3.521697	-0.588920	-0.439650
24	6	0	2.224018	-1.010381	-0.287116
25	6	0	3.766240	-0.913612	-0.083159
26	8	0	4.558859	-0.704984	-0.964001
27	8	0	4.073575	-1.046045	1.207651
28	6	0	1.927818	-1.416604	-1.764733
29	9	0	0.590603	-1.580178	-1.925985
30	9	0	2.511033	-2.581560	-2.079566
31	9	0	2.315211	-0.493928	-2.659090
32	6	0	5.477116	-0.943285	1.530115
33	1	0	5.533473	-1.075819	2.607668
34	1	0	6.038397	-1.723177	1.015107
35	1	0	5.862173	0.034435	1.238278
36	8	0	1.718926	-2.034588	0.521392
37	1	0	0.969726	-1.670480	1.036832
38	1	0	-2.933364	0.577837	1.190741
39	1	0	-2.053901	0.874944	-0.332100
40	16	0	-4.938093	0.226683	-0.646998
41	6	0	-5.677416	-0.922976	-1.805502
42	1	0	-6.665756	-0.524702	-2.033071
43	1	0	-5.056378	-0.958862	-2.697859
44	1	0	-5.752794	-1.895732	-1.324225
45	8	0	-5.672602	0.210431	0.611089
46	8	0	-4.661058	1.498282	-1.299996

Energy = -2260.0484107 hartrees

Compnd ***(S, R)*-4g**

Cartesian Coordinates

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.226481	0.954719	-1.313853
2	6	0	2.653113	-0.139880	-0.722774
3	6	0	1.424774	0.086427	-0.054001
4	6	0	1.026509	1.441610	-0.145152
5	16	0	2.217642	2.361666	-1.070462
6	1	0	3.161894	-1.094061	-0.743900
7	6	0	4.494793	1.032242	-2.017005
8	8	0	5.206849	0.073435	-2.254548
9	1	0	4.794539	2.050179	-2.342472
10	7	0	-0.043858	2.159860	0.311031
11	6	0	-1.380199	1.651505	0.676174
12	6	0	-2.008154	2.836845	1.416203
13	6	0	-1.430393	4.067755	0.703822
14	6	0	-0.009449	3.638082	0.314053
15	1	0	-1.302861	0.777490	1.309471
16	1	0	-3.098498	2.796506	1.395691
17	1	0	-1.690309	2.813514	2.461638
18	1	0	-2.011477	4.304751	-0.191287
19	1	0	-1.426046	4.958790	1.332776
20	1	0	0.269275	4.028657	-0.670455
21	1	0	0.742340	3.981234	1.033311
22	6	0	-2.138638	1.244899	-0.593589
23	8	0	-3.324845	0.511414	-0.169181
24	6	0	0.797769	-1.058245	0.756874
25	8	0	-0.609411	-1.136285	0.717527
26	1	0	-0.903816	-1.544575	-0.113473
27	6	0	1.384588	-2.418546	0.274431
28	8	0	2.305811	-3.009240	0.766529
29	8	0	0.690871	-2.831200	-0.795326
30	6	0	1.132078	-0.887939	2.267930
31	9	0	2.443910	-0.732522	2.481950
32	9	0	0.704999	-1.930932	2.998726
33	9	0	0.514556	0.216424	2.757107
34	6	0	1.100923	-4.084169	-1.387694
35	1	0	2.130550	-4.011239	-1.738437
36	1	0	1.018533	-4.887396	-0.655461
37	1	0	0.418708	-4.243618	-2.218465
38	1	0	-2.468558	2.104556	-1.181069
39	1	0	-1.512713	0.602896	-1.213491
40	16	0	-3.777922	-0.784875	-1.060717
41	6	0	-4.877570	-1.511147	0.151900
42	1	0	-5.293050	-2.404290	-0.313626
43	1	0	-4.293979	-1.762217	1.034937
44	1	0	-5.660858	-0.789605	0.375114
45	8	0	-4.527558	-0.349944	-2.227421
46	8	0	-2.610855	-1.649546	-1.255469

Energy = -2260.0508191 hartrees

Compnd **Methyl trifluoropyruvate**

Cartesian Coordinates

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.021442	-0.328276	-0.480228
2	6	0	1.381455	-0.081419	0.157236
3	8	0	-0.203630	-1.246688	-1.227272
4	6	0	-1.084646	0.751021	-0.193123
5	8	0	-2.303035	0.382729	0.191916
6	8	0	-0.787012	1.893103	-0.411207
7	6	0	-2.614631	-0.993111	0.519799
8	1	0	-2.658132	-1.597650	-0.384698
9	1	0	-1.885142	-1.404309	1.219990
10	1	0	-3.589943	-0.950386	0.997536
11	9	0	1.232870	0.378806	1.415517
12	9	0	2.066549	-1.227697	0.209600
13	9	0	2.091494	0.807770	-0.545387

Energy = -679.6115023 hartrees

Compnd **Hexafluoroacetone**

Cartesian Coordinates

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.719108	0.000002
2	6	0	-1.330414	-0.097291	0.004285
3	8	0	0.000000	1.908668	0.000001
4	6	0	1.330414	-0.097291	-0.004285
5	9	0	1.597100	-0.519384	1.243837
6	9	0	1.236764	-1.169429	-0.806168
7	9	0	2.336624	0.665675	-0.421845
8	9	0	-1.236767	-1.169425	0.806173
9	9	0	-2.336627	0.665676	0.421837
10	9	0	-1.597094	-0.519389	-1.243836

Energy = -788.823093 hartrees

Compnd **Hexafluoroacetone monohydrate**

Cartesian Coordinates

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.015760	-0.027222	0.682746
2	6	0	1.368380	-0.260823	-0.064873
3	6	0	-1.300241	-0.388939	-0.075620
4	9	0	1.477787	-1.581178	-0.333051
5	9	0	2.387048	0.098914	0.710846
6	9	0	1.457458	0.401185	-1.225194
7	8	0	-0.010317	0.268700	1.834606
8	9	0	-1.544238	-1.702747	0.119591
9	9	0	-1.225648	-0.178875	-1.395882
10	9	0	-2.326935	0.302457	0.416660
11	8	0	-0.215141	2.477915	-0.226923
12	1	0	-0.068420	2.903156	-1.077663
13	1	0	-0.660566	3.128016	0.325952

Energy = -865.2884205 hartrees

Compnd **Hexafluoroacetone dihydrate**

Cartesian Coordinates

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.654484	-0.000562	-0.685139
2	6	0	-0.000802	-1.295080	-0.105892
3	8	0	-1.337936	-0.046733	-1.657156
4	6	0	-0.215392	1.367039	-0.068379
5	9	0	-0.370489	1.433659	1.256583
6	9	0	1.106323	1.536903	-0.336125
7	9	0	-0.886408	2.363168	-0.633245
8	9	0	0.212756	-1.241027	1.212094
9	9	0	-0.741564	-2.360285	-0.388354
10	9	0	1.206774	-1.449425	-0.709062
11	8	0	-2.645480	-0.307902	1.042448
12	1	0	-2.766317	-0.219613	1.993232
13	1	0	-3.484704	-0.624128	0.692198
14	8	0	3.968130	0.064959	0.422558
15	1	0	3.396142	0.836144	0.357460
16	1	0	3.454704	-0.650314	0.033737

Energy = -941.7488901 hartrees

Compnd **1,3-Dichloro-1,1,3,3-tetrafluoroacetone**
Cartesian Coordinates
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000001	-0.000006	0.793663
2	6	0	1.244100	-0.483130	-0.010443
3	8	0	0.000002	0.000001	1.983795
4	6	0	-1.244098	0.483127	-0.010443
5	9	0	-1.931321	1.360702	0.727225
6	9	0	-0.885328	1.088692	-1.157511
7	17	0	-2.279883	-0.927102	-0.375348
8	9	0	0.885334	-1.088699	-1.157511
9	17	0	2.279874	0.927107	-0.375351
10	9	0	1.931330	-1.360698	0.727226

Energy = -1509.5069346 hartrees

Compnd **Methyl pyruvate**
Cartesian Coordinates
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.815453	-0.455496	-0.111358
2	6	0	2.144124	-0.209339	0.548211
3	8	0	0.521178	-1.471602	-0.696529
4	6	0	-0.159925	0.751219	-0.105774
5	8	0	-1.472965	0.550927	0.047576
6	8	0	0.280540	1.854403	-0.303105
7	6	0	-2.038714	-0.741988	0.359283
8	1	0	-2.019875	-1.387178	-0.516584
9	1	0	-1.507634	-1.219587	1.184161
10	1	0	-3.062473	-0.529924	0.660012
11	1	0	1.996928	0.041231	1.604038
12	1	0	2.769654	-1.095895	0.455148
13	1	0	2.627744	0.655151	0.087518

Energy = -381.8119555 hartrees

Compnd **1,1,1-Trifluoropropanone**

Cartesian Coordinates

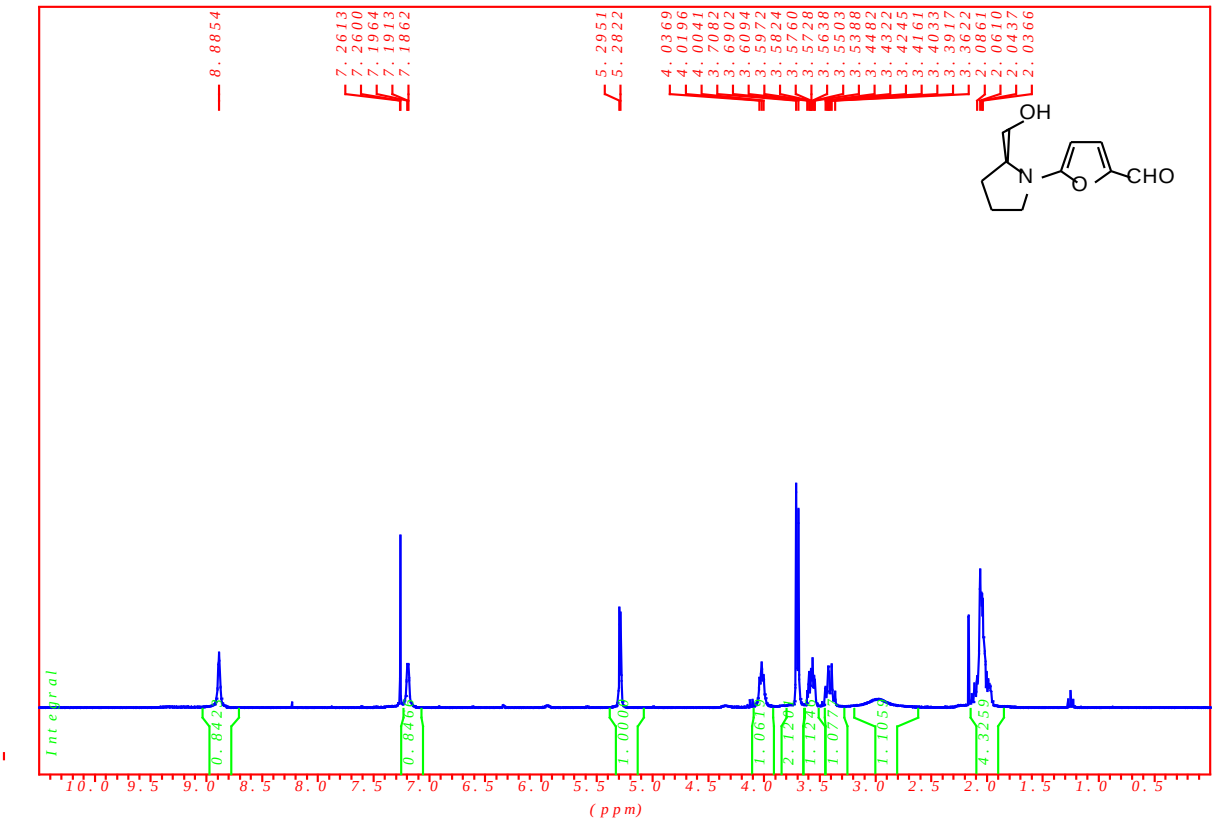
Standard orientation:

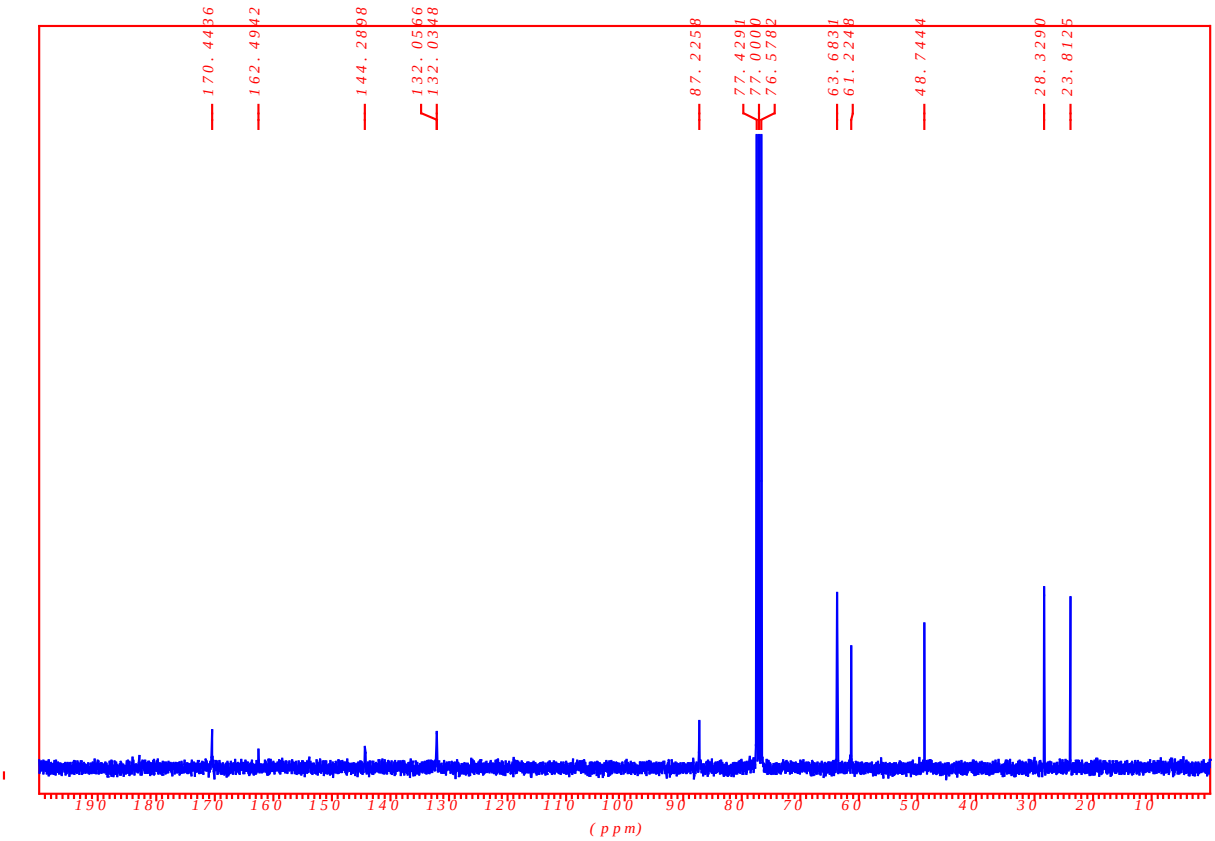
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.912204	0.305938	0.000027
2	6	0	-1.834342	-0.882314	0.000003
3	8	0	-1.252769	1.456462	-0.000002
4	6	0	0.612027	-0.034905	0.000000
5	9	0	1.375641	1.053393	-0.000101
6	9	0	0.922521	-0.773234	1.090652
7	9	0	0.922456	-0.773391	-1.090565
8	1	0	-1.644826	-1.503552	-0.879822
9	1	0	-1.644719	-1.503689	0.879706
10	1	0	-2.866756	-0.537672	0.000086

Energy = -491.0279214 hartrees

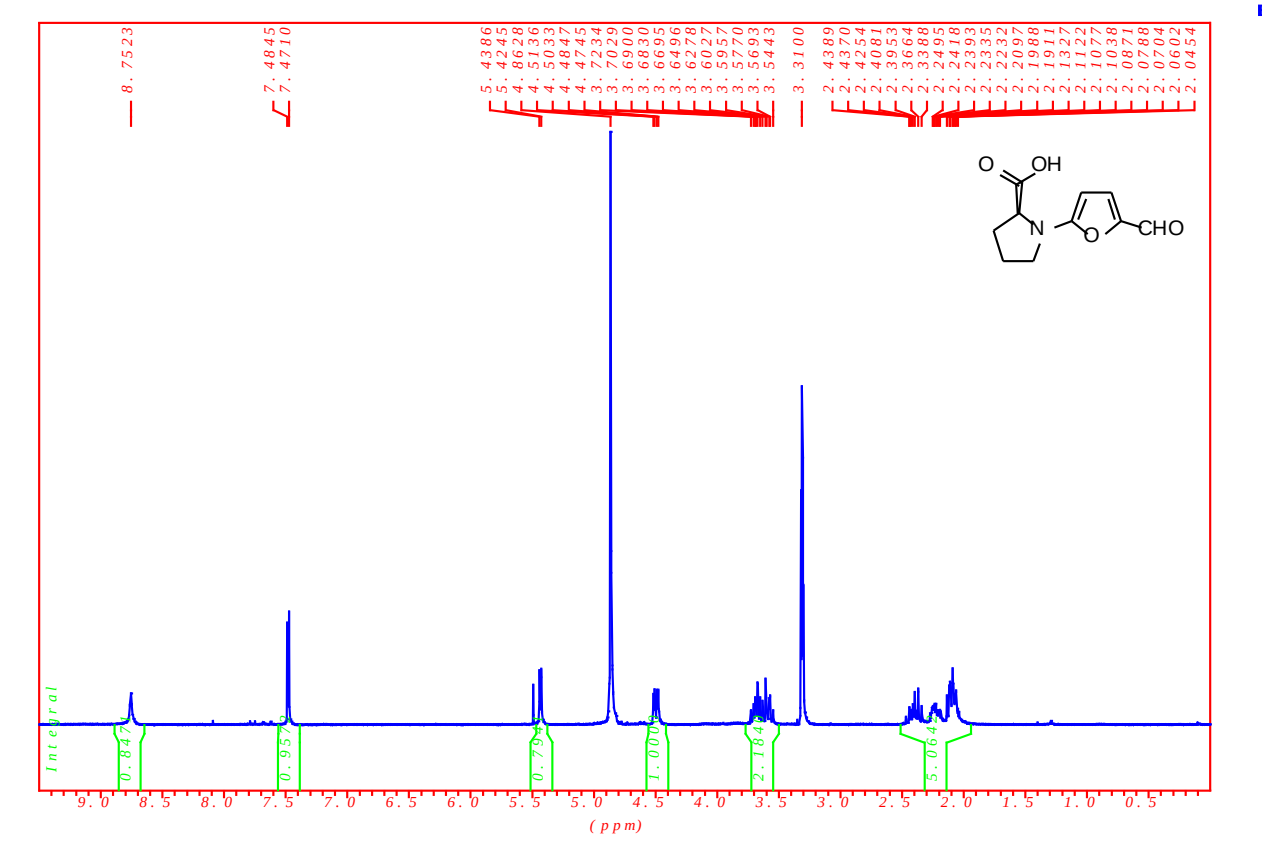
Part 2: NMR spectra

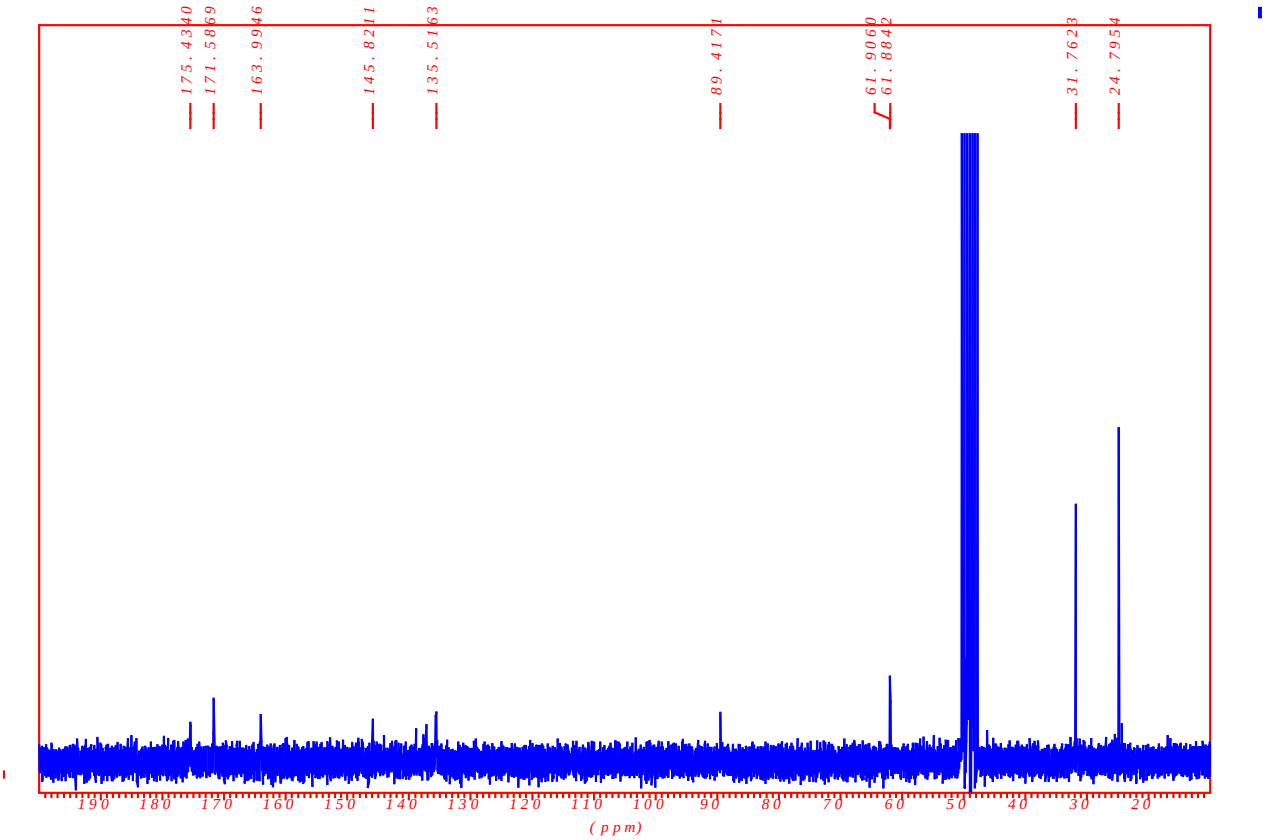
Compnd **1c**



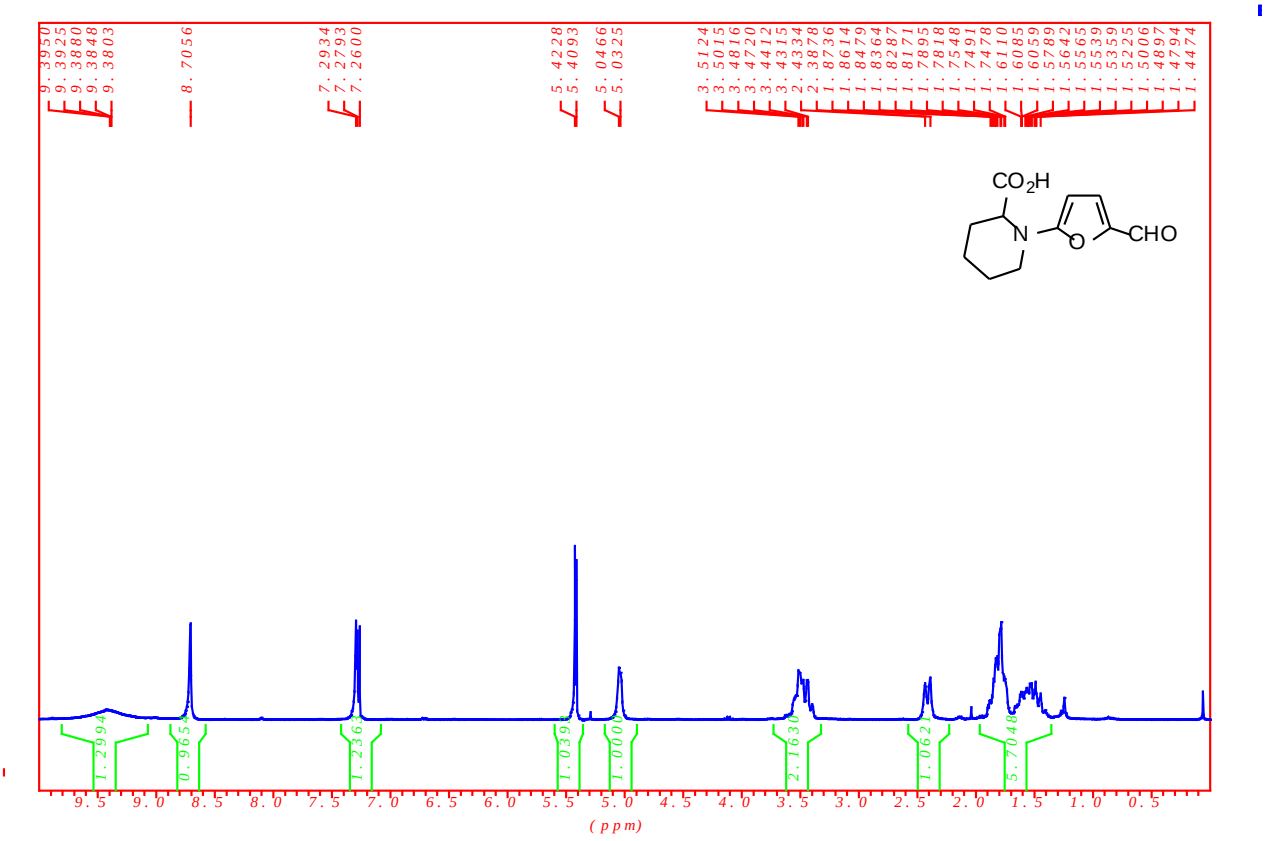


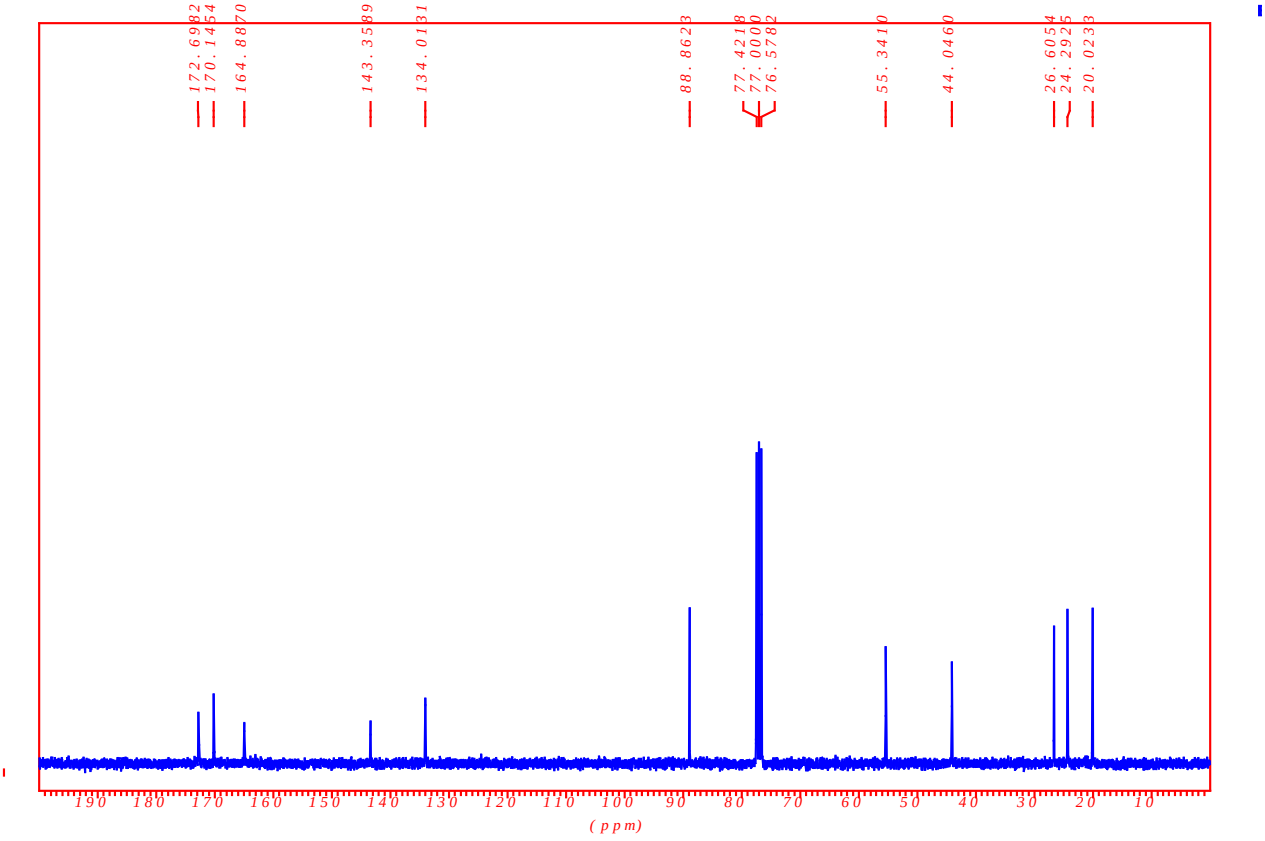
Compnd **1d**


8.7523
7.4845
7.4710
5.4386
5.4245
4.8628
4.5136
4.5033
4.4847
4.4745
3.7234
3.7029
3.6900
3.6830
3.6695
3.6496
3.6278
3.6027
3.5957
3.5770
3.5693
3.5443
3.3100
2.4389
2.4370
2.4254
2.4081
2.3953
2.3664
2.3388
2.2495
2.2418
2.2393
2.2335
2.2232
2.2097
2.1988
2.1911
2.1327
2.1122
2.1077
2.1038
2.0871
2.0788
2.0704
2.0602
2.0454
O
OH
N
O
CHO
Integral
0.847
0.957
0.795
1.000
2.168
5.064
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
(ppm)

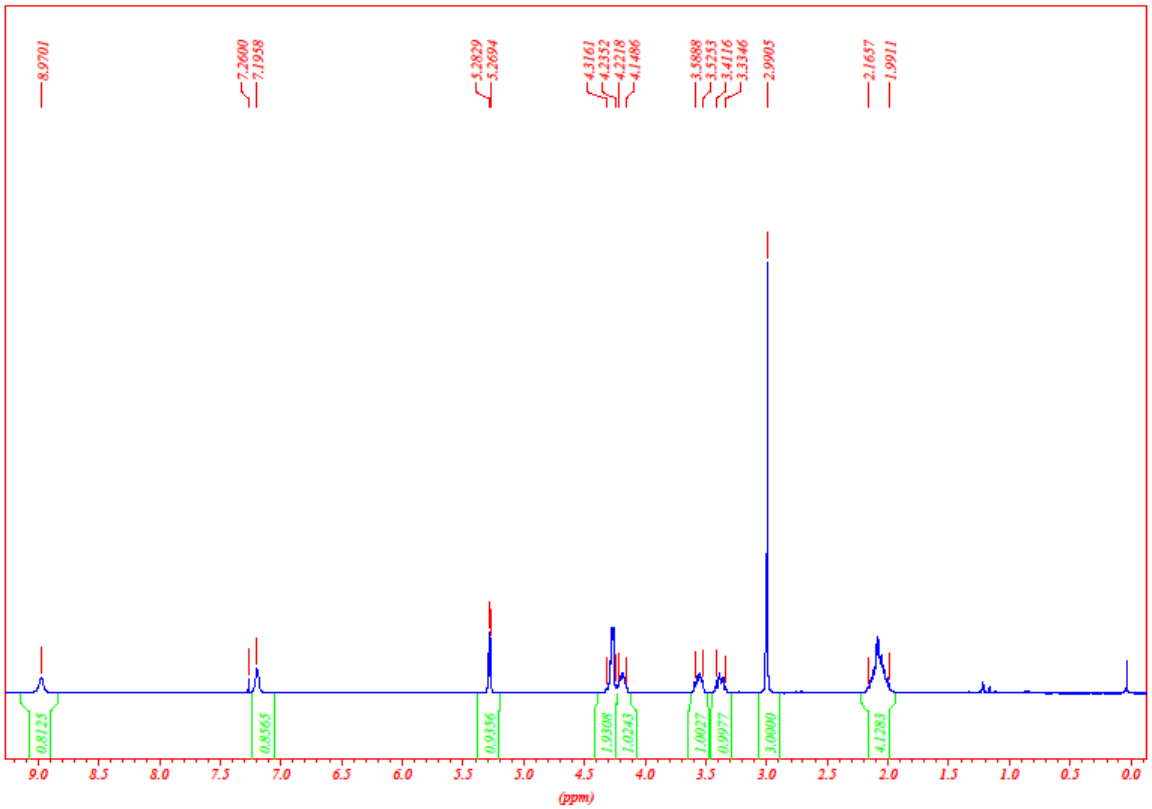

175.4340
171.5869
163.9946
145.8211
135.5163
89.4171
61.9060
61.8842
31.7623
24.7954
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20
(ppm)

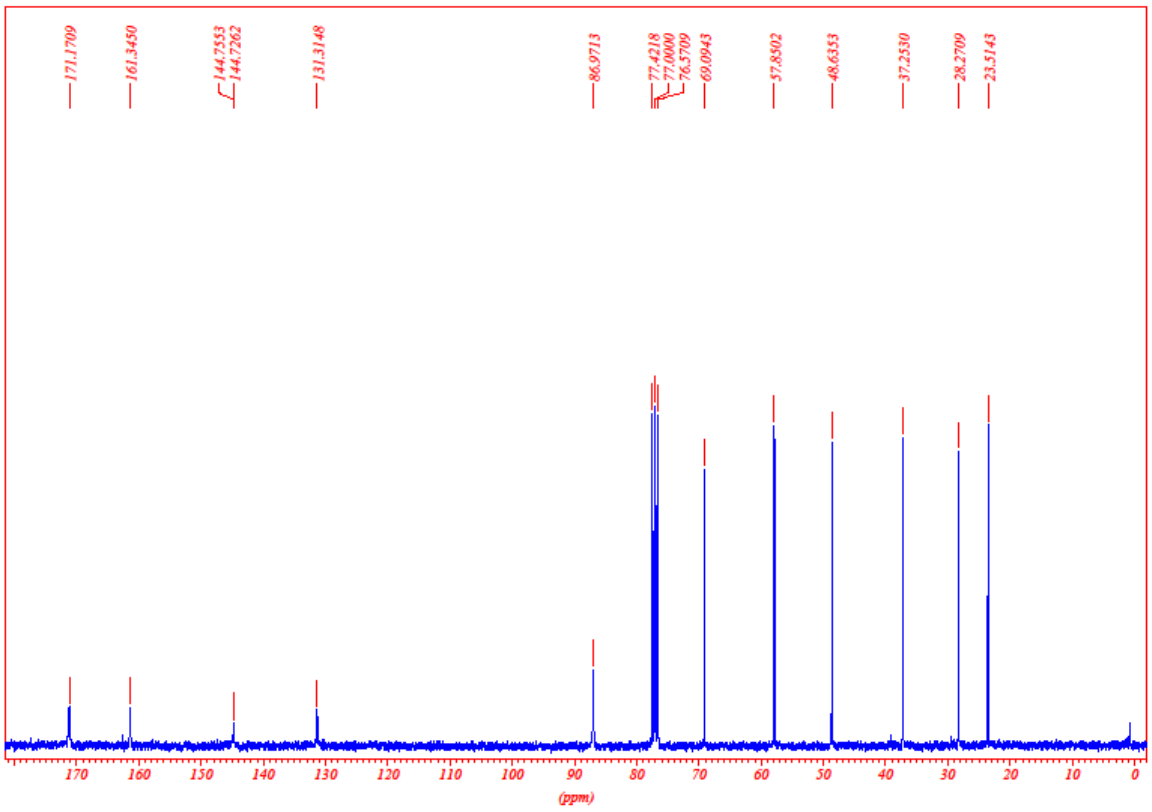
Compnd **1e**


9.3950
9.3925
9.3880
9.3848
9.3803
8.7056
7.2934
7.2793
7.2600
5.4228
5.4093
5.0466
5.0325
3.5124
3.5015
3.4816
3.4720
3.4412
3.4315
3.4334
2.3878
1.8736
1.8614
1.8479
1.8364
1.8287
1.8171
1.7895
1.7818
1.7548
1.7491
1.7478
1.6110
1.6085
1.6059
1.5789
1.5642
1.5565
1.5539
1.5359
1.5225
1.5006
1.4897
1.4794
1.4474
CO2H
N
O
CHO
1.2994
0.9654
1.2366
1.0391
1.0000
2.1630
1.0622
5.7048
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
(ppm)

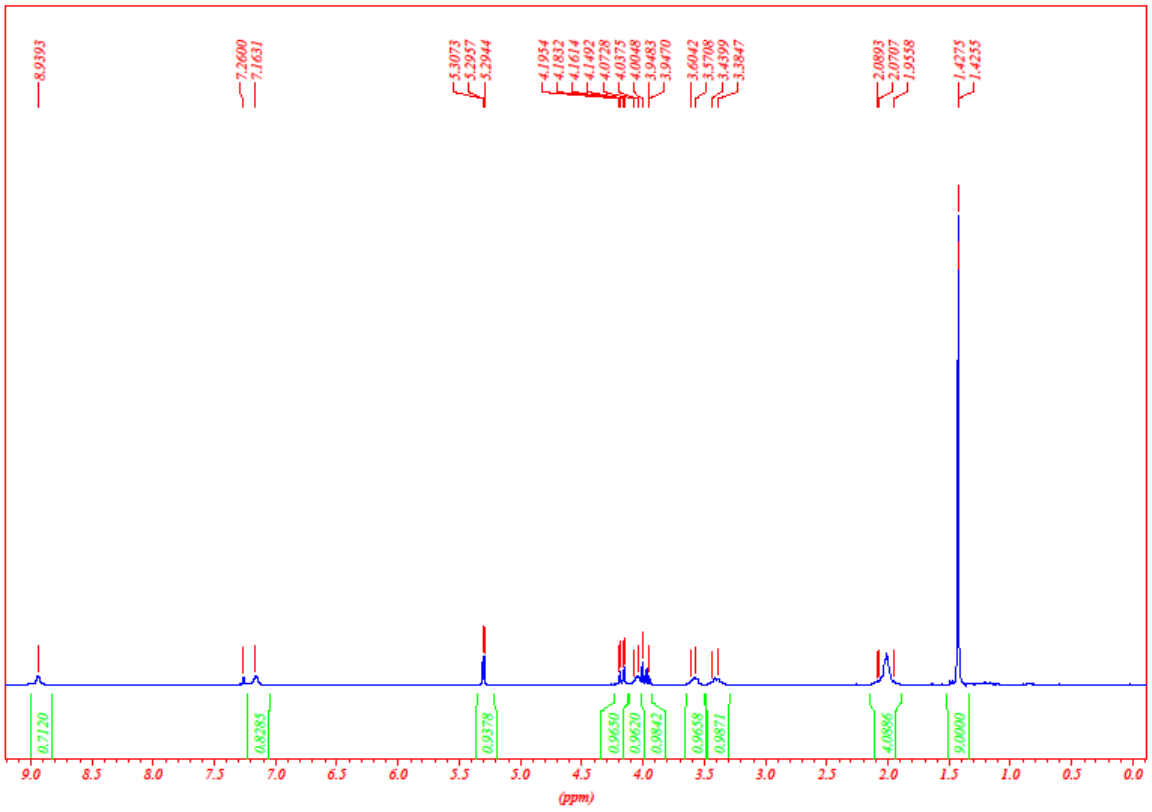

172.6982
170.1454
164.8870
143.3589
134.0131
88.8623
77.4218
77.0000
76.5782
55.3410
44.0460
26.6054
24.2925
20.0233
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
(ppm)

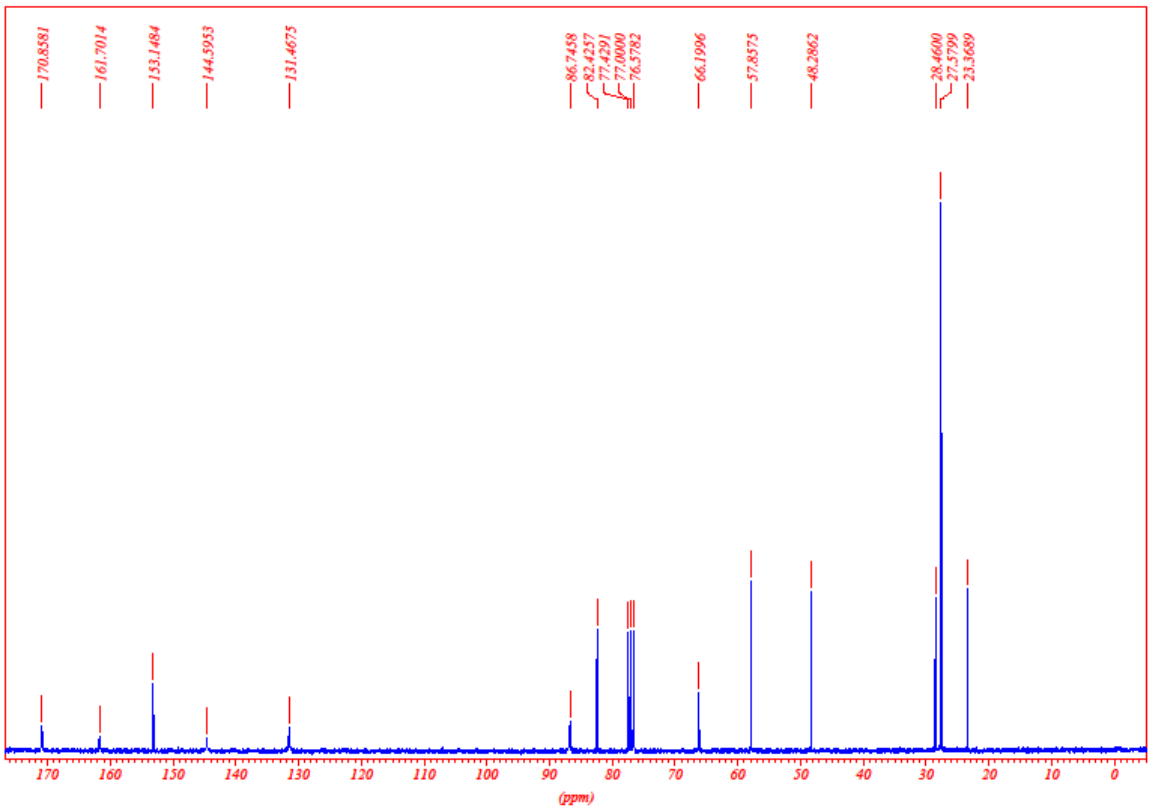
Compnd **1g**



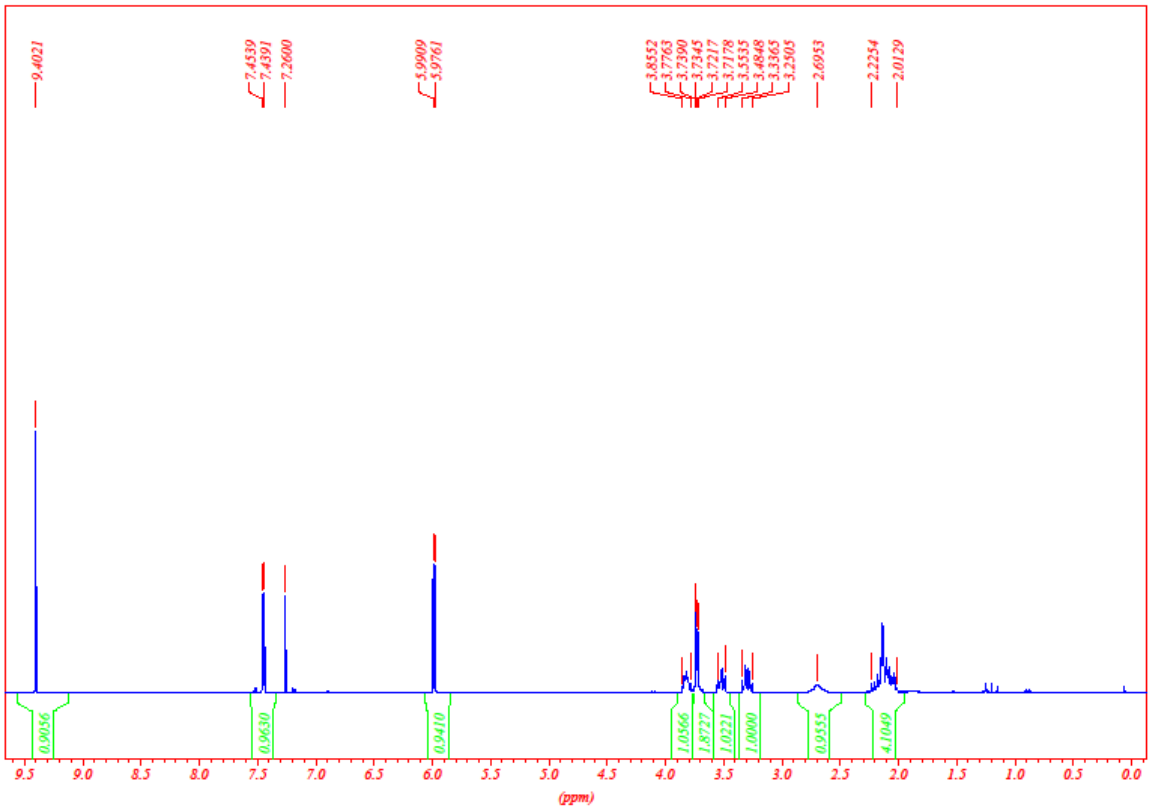


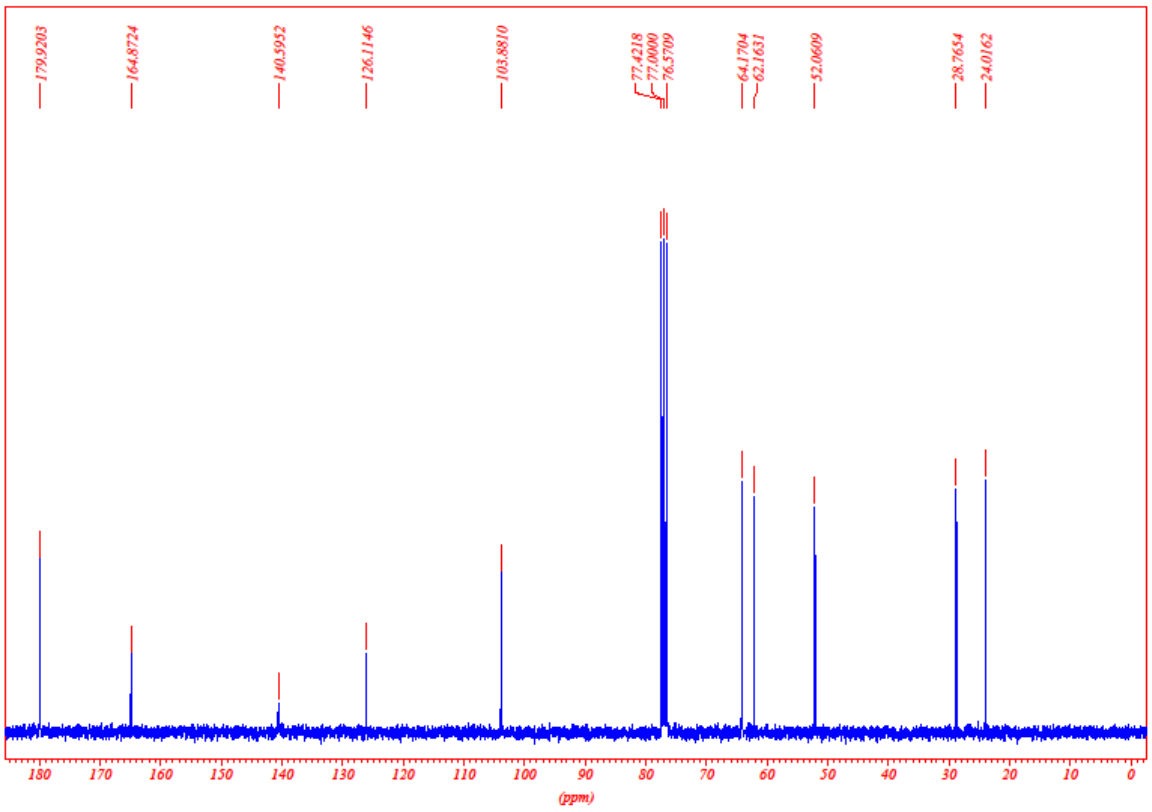
Compnd **1h**


8.9393
7.2600
7.1631
5.3073
5.2957
5.2944
4.1954
4.1832
4.1614
4.1492
4.0728
4.0375
4.0048
3.9483
3.9470
3.6042
3.5708
3.4399
3.3847
2.0893
2.0707
1.9558
1.4275
1.4255
0.7120
0.8285
0.9378
0.9650
0.9620
0.9842
0.9658
0.9871
4.0886
9.0000
(ppm)

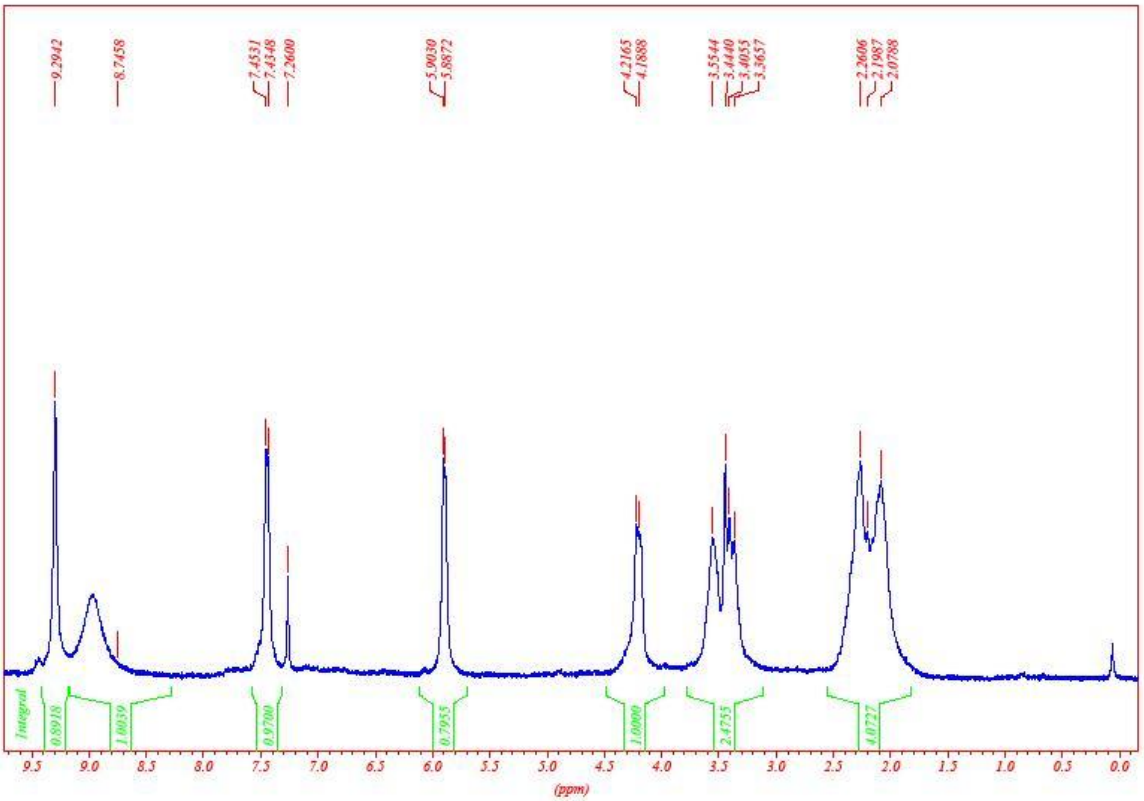

170.8581
161.7014
153.1484
144.5953
131.4675
86.7458
82.4257
77.4291
77.0000
76.5782
66.1996
57.8575
48.2862
28.4600
27.5799
23.3689
(ppm)

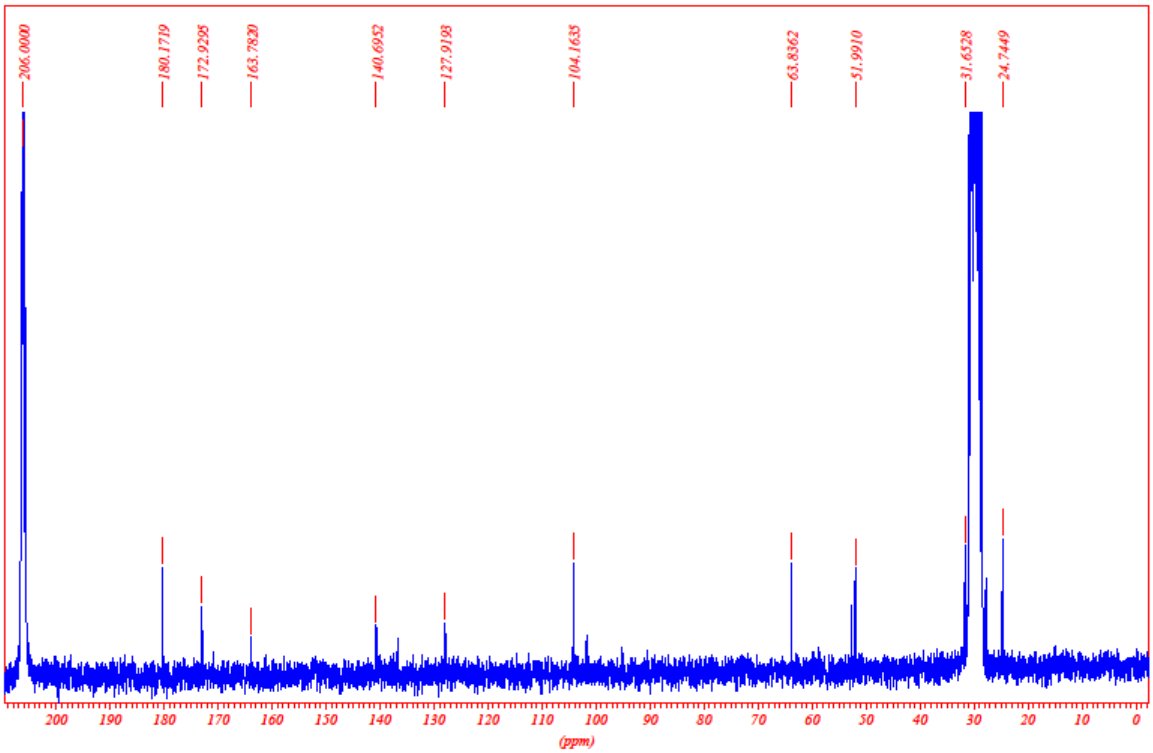
Compnd **2c**


9.4021
7.4539
7.4391
7.2600
5.9909
5.9761
3.8552
3.7763
3.7390
3.7345
3.7217
3.7178
3.5535
3.4848
3.3365
3.2503
2.6933
2.2254
2.0129
0.9956
0.9630
0.9410
1.0566
1.8727
1.0221
1.0000
0.9555
4.1049
(ppm)

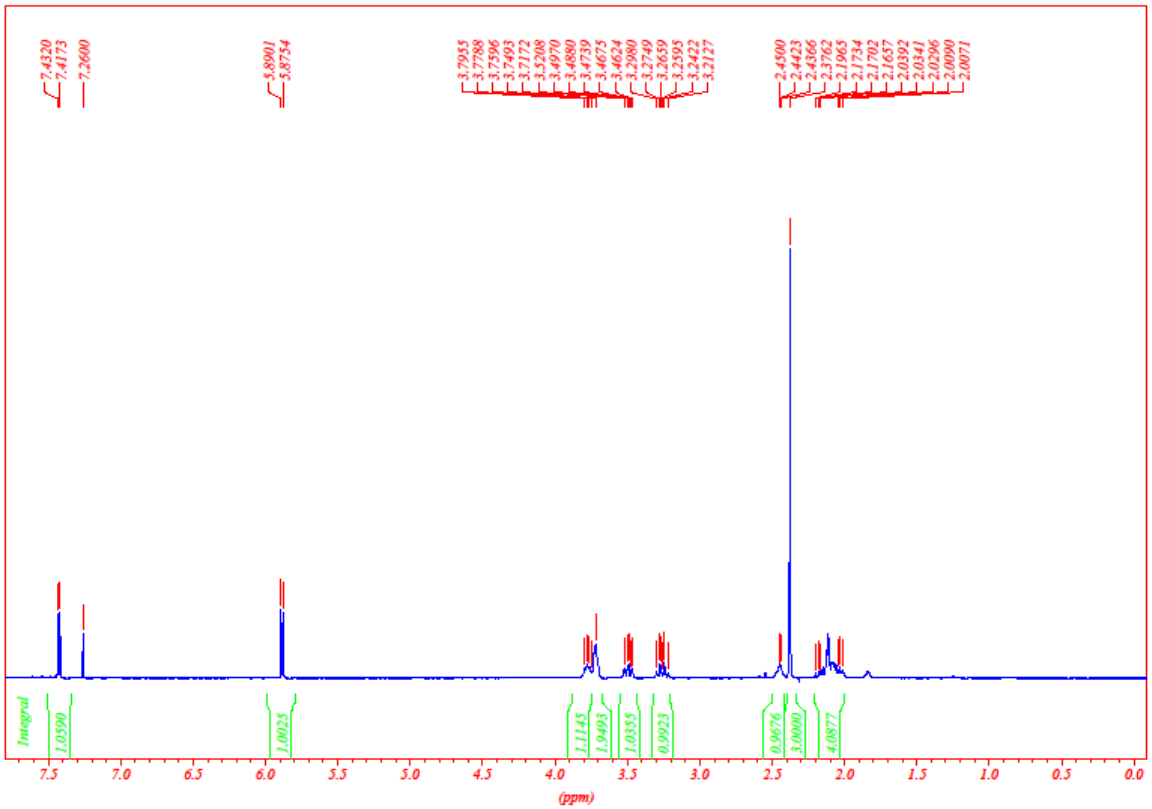

179.9203
164.8724
140.5952
126.1146
103.8810
77.4218
77.0000
76.5709
64.1704
62.1631
52.0609
28.7654
24.0162
(ppm)

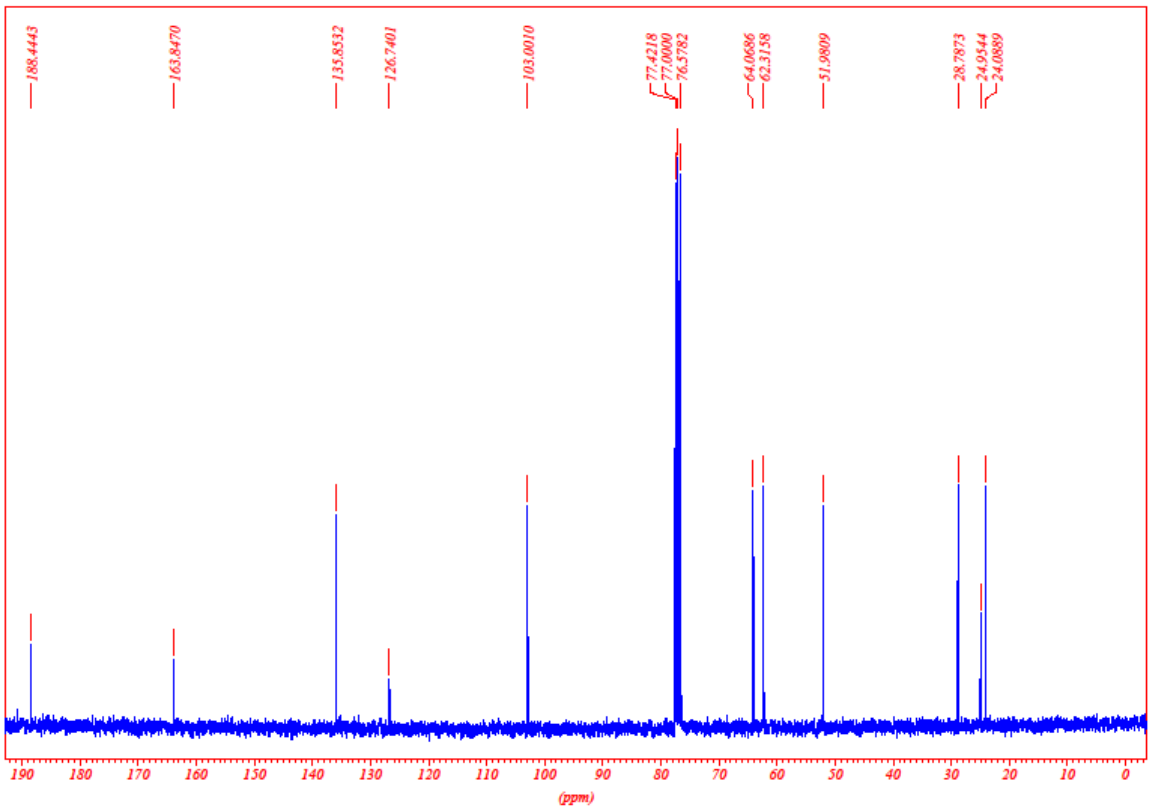
Compnd **2d**


9.2942
8.7458
7.4531
7.4348
7.2600
5.9039
5.8872
4.2165
4.1898
3.5544
3.4440
3.4055
3.3657
2.3606
2.1987
2.0788
Integral
0.8918
1.0039
0.9700
0.7955
1.0000
2.4755
4.0727
(ppm)

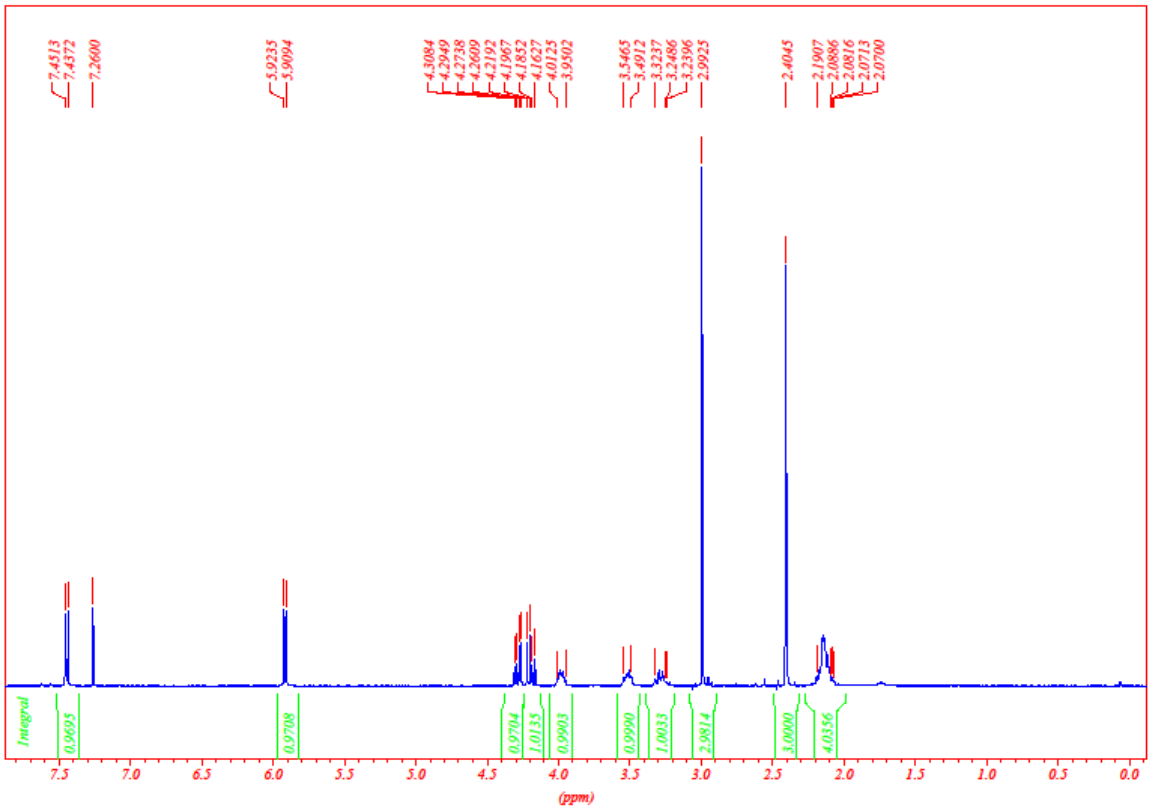

206.0000
180.1719
172.9295
163.7820
140.6952
127.9198
104.1635
63.8362
51.9910
31.6528
24.7449
(ppm)

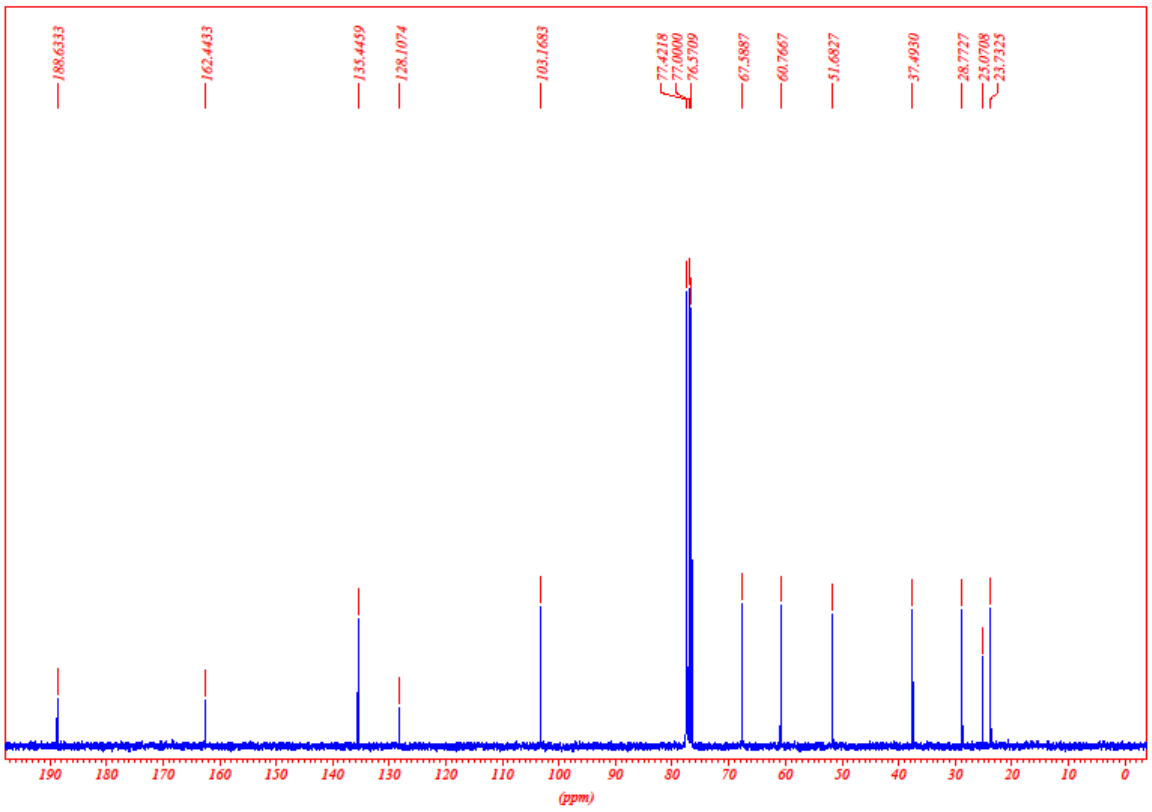
Compnd **2e**


7.4320
7.4173
7.2600
5.8901
5.8734
3.7955
3.7788
3.7596
3.7493
3.7172
3.5208
3.4970
3.4880
3.4739
3.4675
3.4624
3.3980
3.2749
3.2659
3.2595
3.2422
3.2127
2.4500
2.4423
2.4366
2.3762
2.1965
2.1734
2.1702
2.1657
2.0392
2.0341
2.0296
2.0090
2.0071
Integral
1.0590
1.0025
1.1145
1.9493
1.0355
0.9923
0.9676
3.0000
4.0877
(ppm)

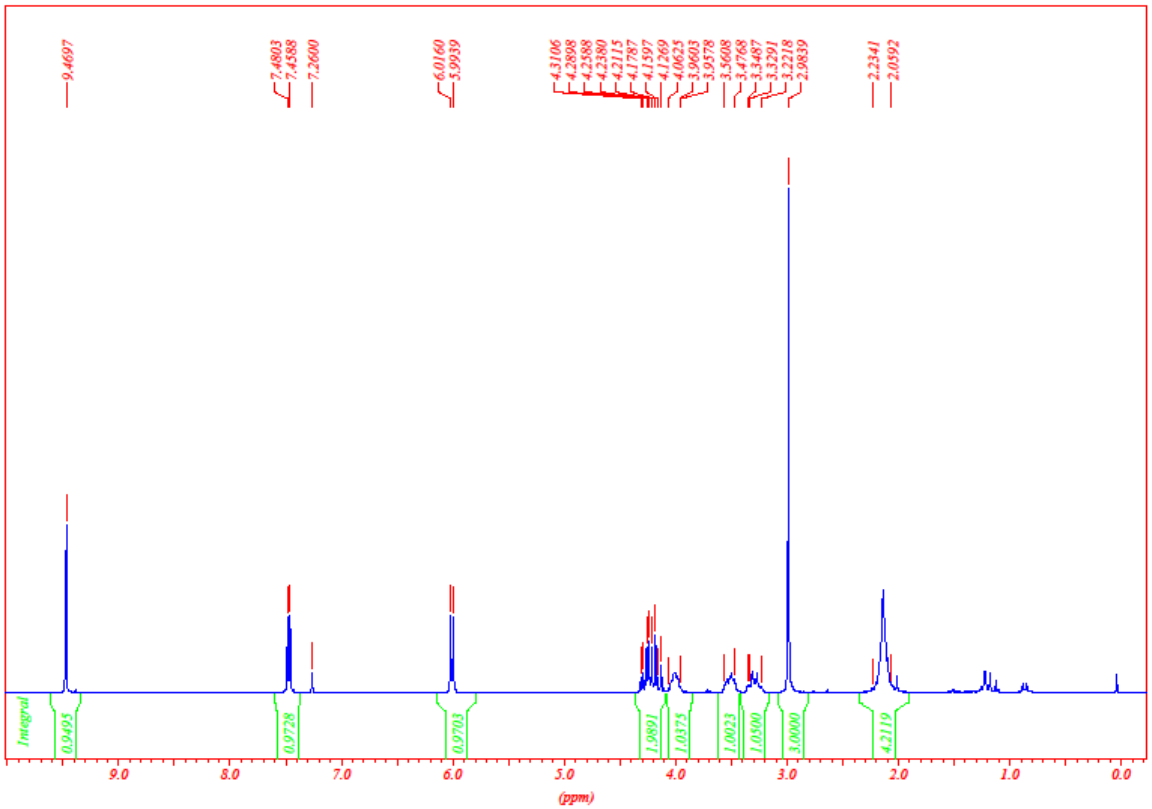

188.4443
163.8470
135.8532
126.7401
103.0010
77.4218
77.0000
76.5782
64.0686
62.3158
51.9809
28.7873
24.9544
24.0869
(ppm)

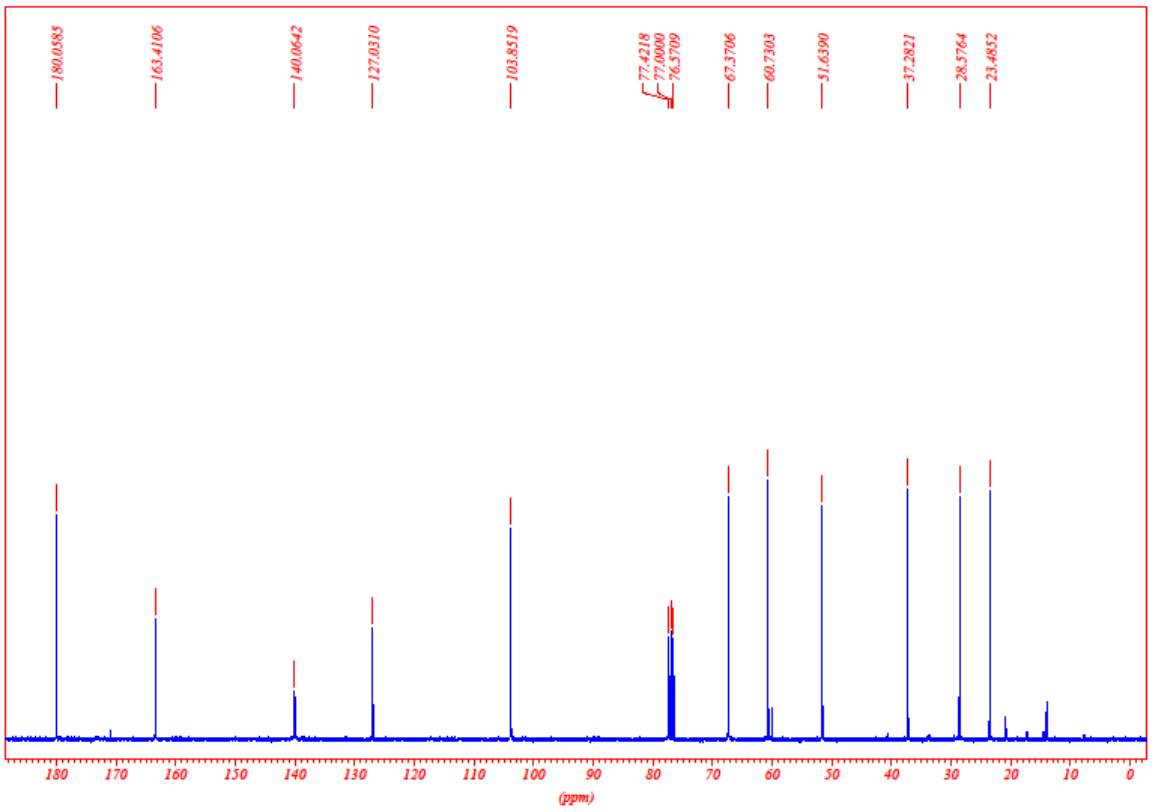
Compnd **2f**


7.4513
7.4372
7.2600
5.9235
5.9094
4.3084
4.2949
4.2738
4.2609
4.2192
4.1967
4.1852
4.1627
4.0125
3.9502
3.5465
3.4912
3.3237
3.2486
3.2396
2.9925
2.4045
2.1907
2.0886
2.0816
2.0713
2.0700
Integral
0.9695
0.9708
0.9704
1.0135
0.9903
0.9990
1.0033
2.9814
3.0000
4.0356
(ppm)

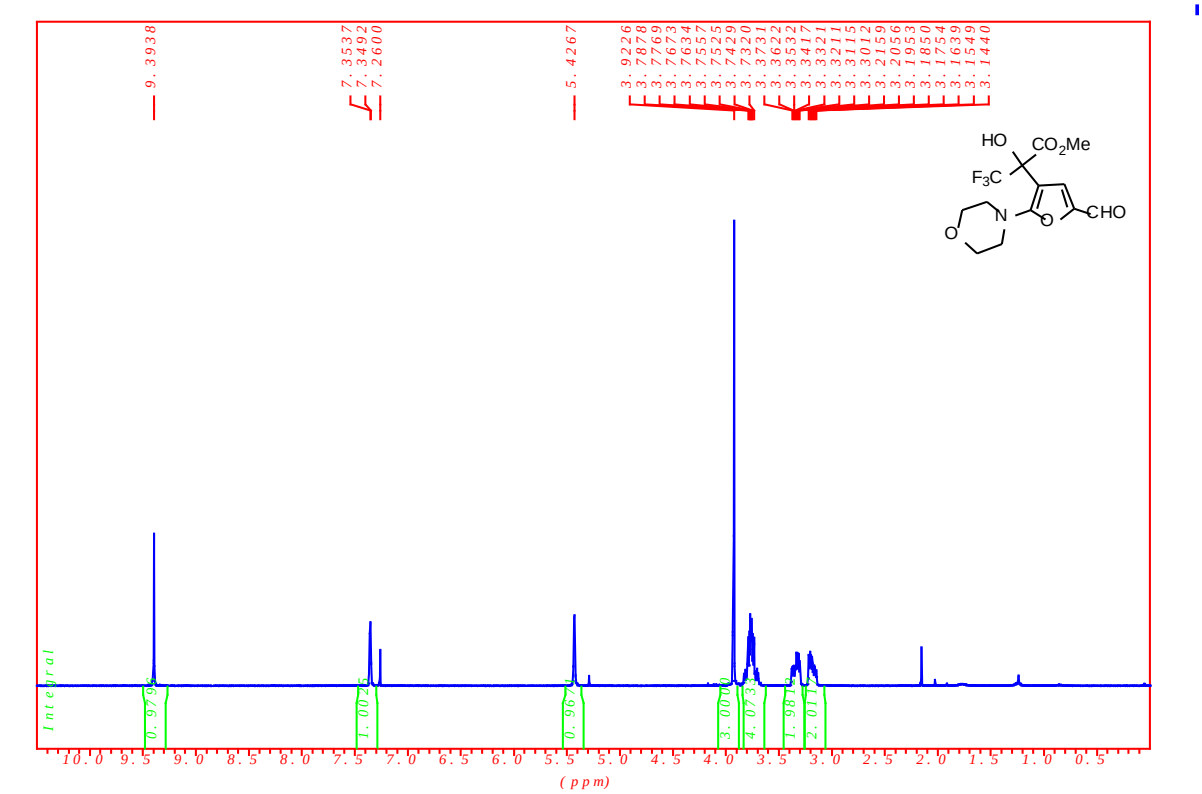

188.6333
162.4433
135.4459
128.1074
103.1683
77.4218
77.0000
76.5709
67.5887
60.7667
51.6827
37.4930
28.7727
25.0708
23.7325
(ppm)

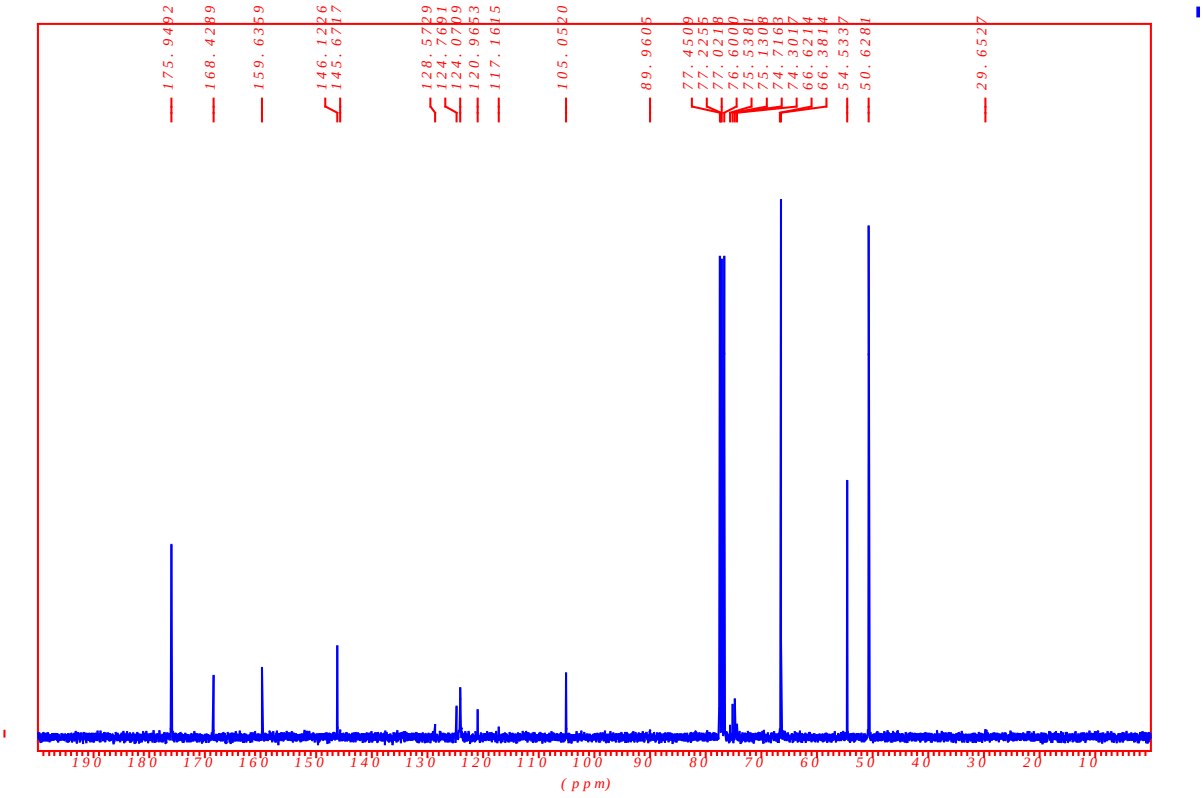
Compnd **2g**


9.4697
7.4803
7.4588
7.2600
6.0160
5.9939
4.3106
4.2898
4.2588
4.2380
4.2115
4.1787
4.1597
4.1269
4.0625
3.9603
3.9578
3.5608
3.4768
3.3487
3.3291
3.2218
2.9839
2.2341
2.0592
Integral
0.9495
0.9728
0.9703
1.9891
1.0375
1.0923
1.0500
3.0000
4.2119
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
(ppm)

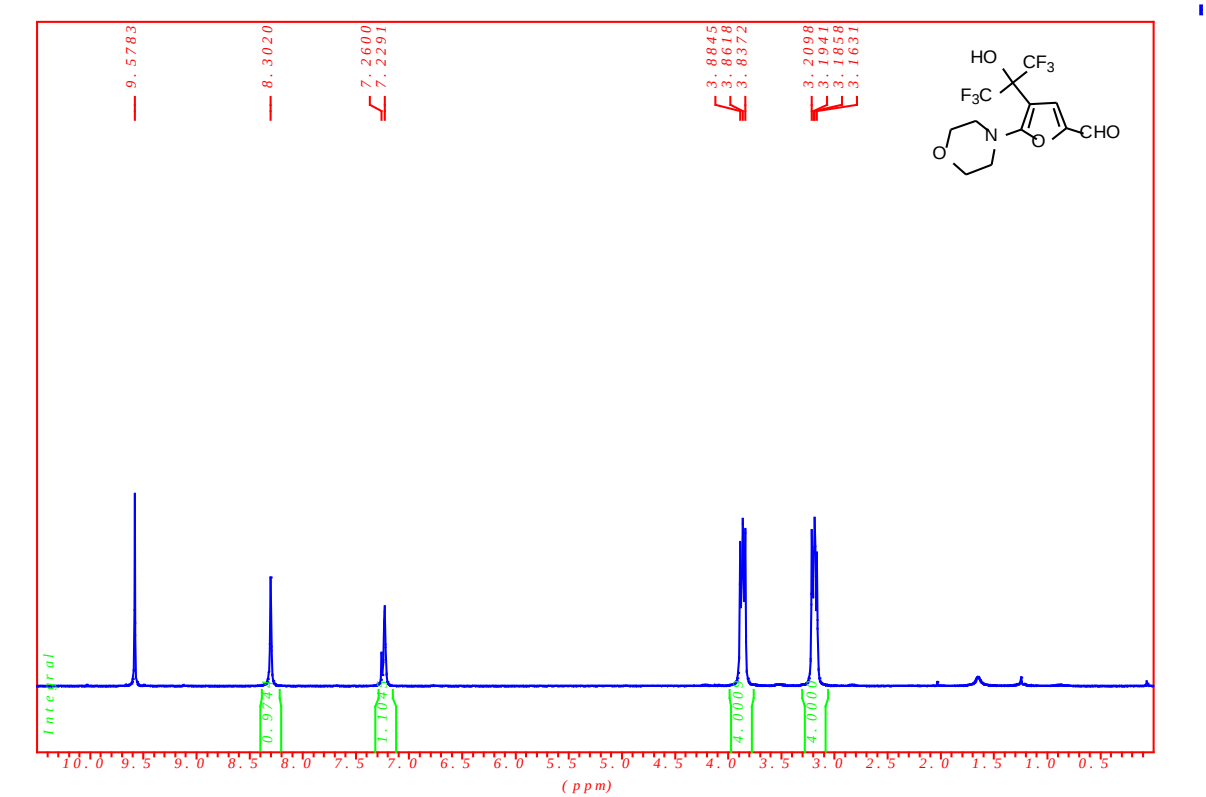

180.0585
163.4106
140.0642
127.0310
103.8519
77.4218
77.0000
76.5709
67.3706
60.7303
51.6390
37.2821
28.5764
23.4852
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)

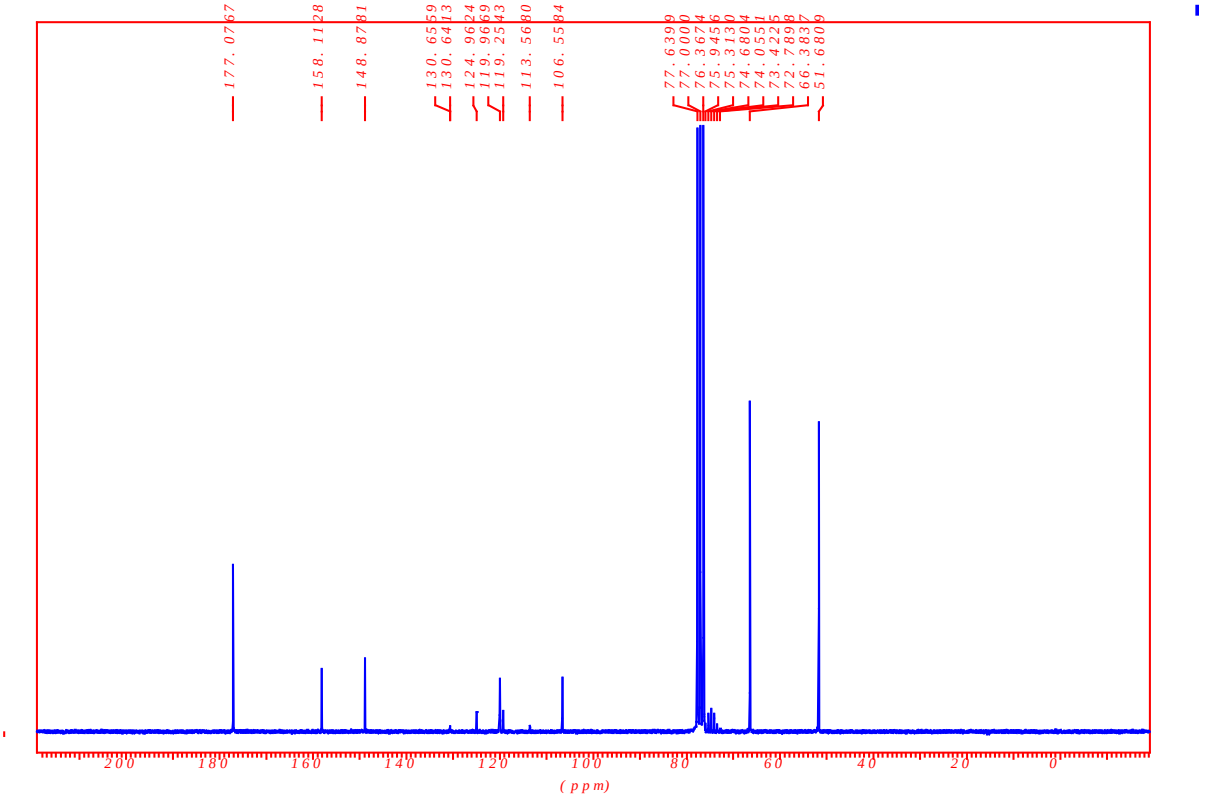
Compnd **3aα**


9.3938
7.3537
7.3492
7.2600
5.4267
3.9226
3.7878
3.7769
3.7673
3.7634
3.7557
3.7525
3.7429
3.7320
3.3731
3.3622
3.3532
3.3417
3.3321
3.3211
3.3115
3.3012
3.2159
3.2056
3.1953
3.1850
3.1754
3.1639
3.1549
3.1440
HO
CO2Me
F3C
N
O
O
CHO
Integral
0.9793
1.0025
0.9627
3.0000
4.0734
1.9814
2.0117
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
(ppm)

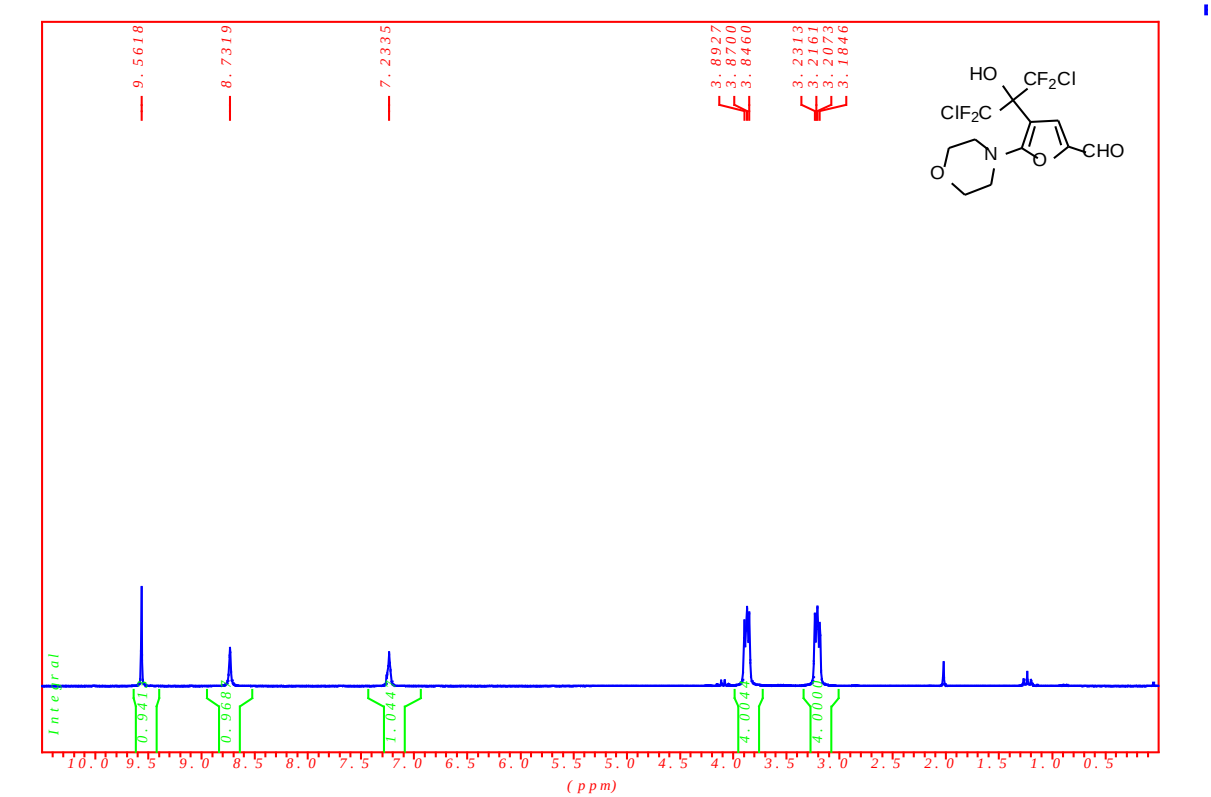

175.9492
168.4289
159.6359
146.1226
145.6717
128.5729
124.7691
124.0709
120.9653
117.1615
105.0520
89.9605
77.4509
77.2255
77.0218
76.6000
75.5381
75.1308
74.7163
74.3017
66.6214
66.3814
54.5337
50.6281
29.6527
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
(ppm)

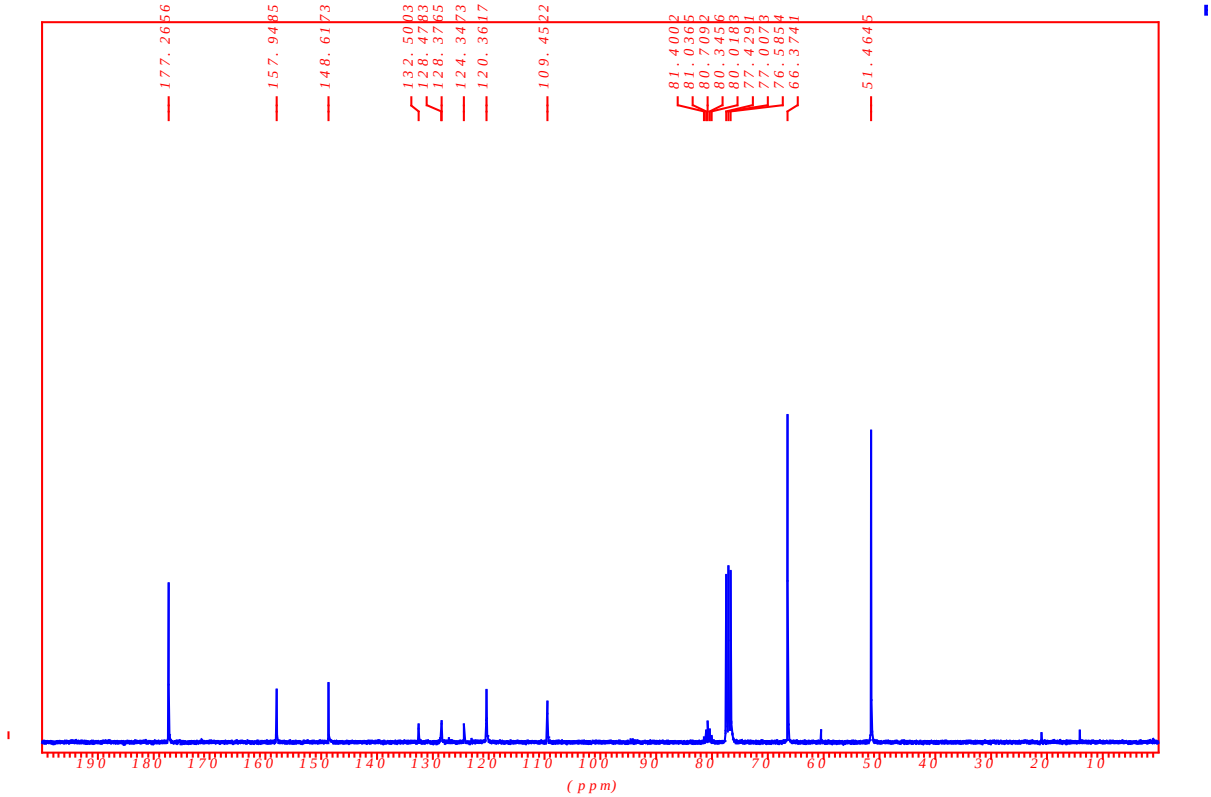
Compnd **3aβ**


9.5783
8.3020
7.2600
7.2291
3.8845
3.8618
3.8372
3.2098
3.1941
3.1858
3.1631
HO
CF3
F3C
N
O
O
CHO
Integral
0.974
1.104
4.000
4.000
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
(ppm)

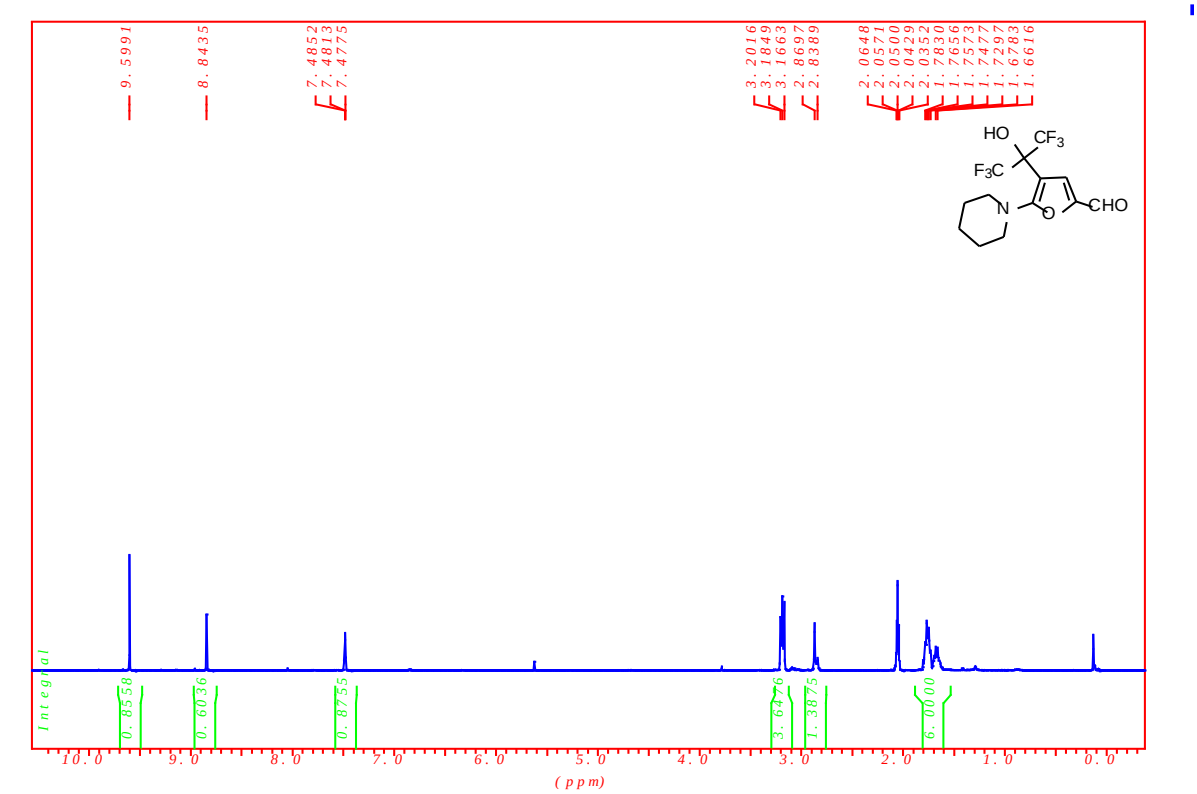

177.0767
158.1128
148.8781
130.6559
130.6413
124.9624
119.9669
119.2543
113.5680
106.5584
77.6399
77.0000
76.3674
75.9456
75.3130
74.6004
74.0551
73.4225
72.7898
66.3837
51.6809
200 180 160 140 120 100 80 60 40 20 0
(ppm)

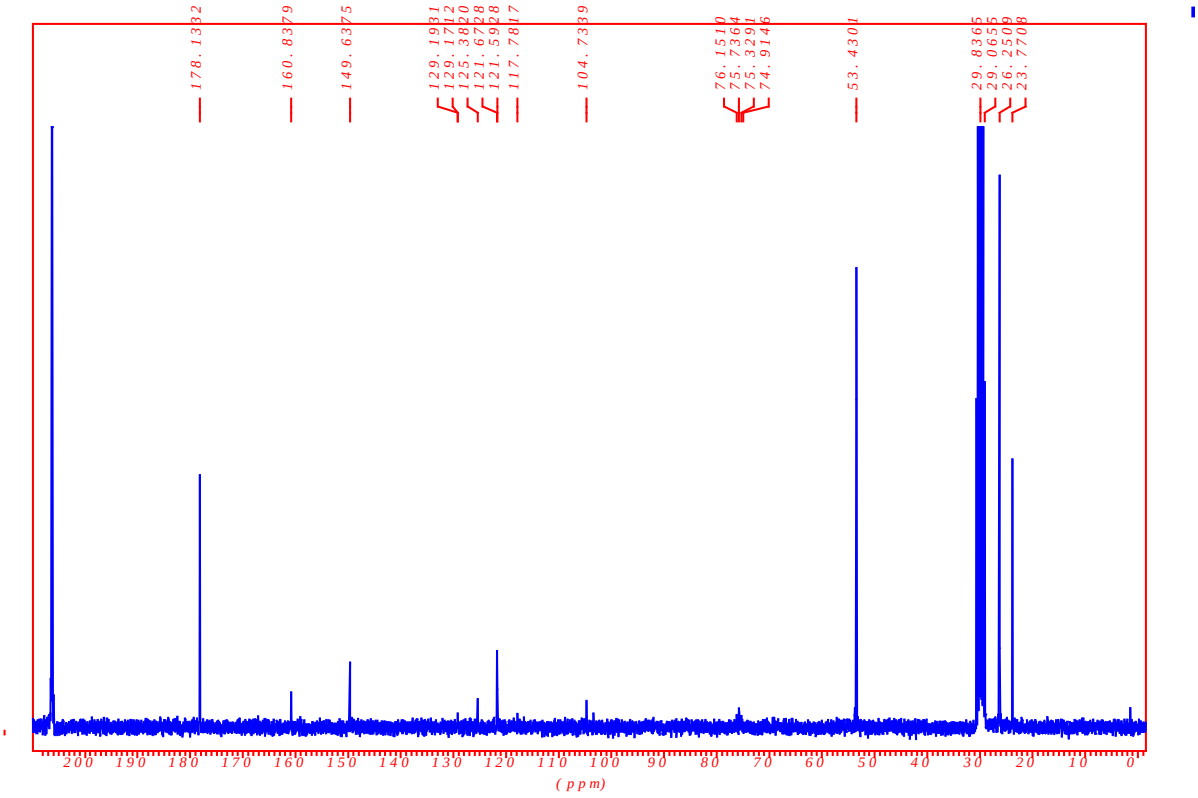
Compnd **3aγ**



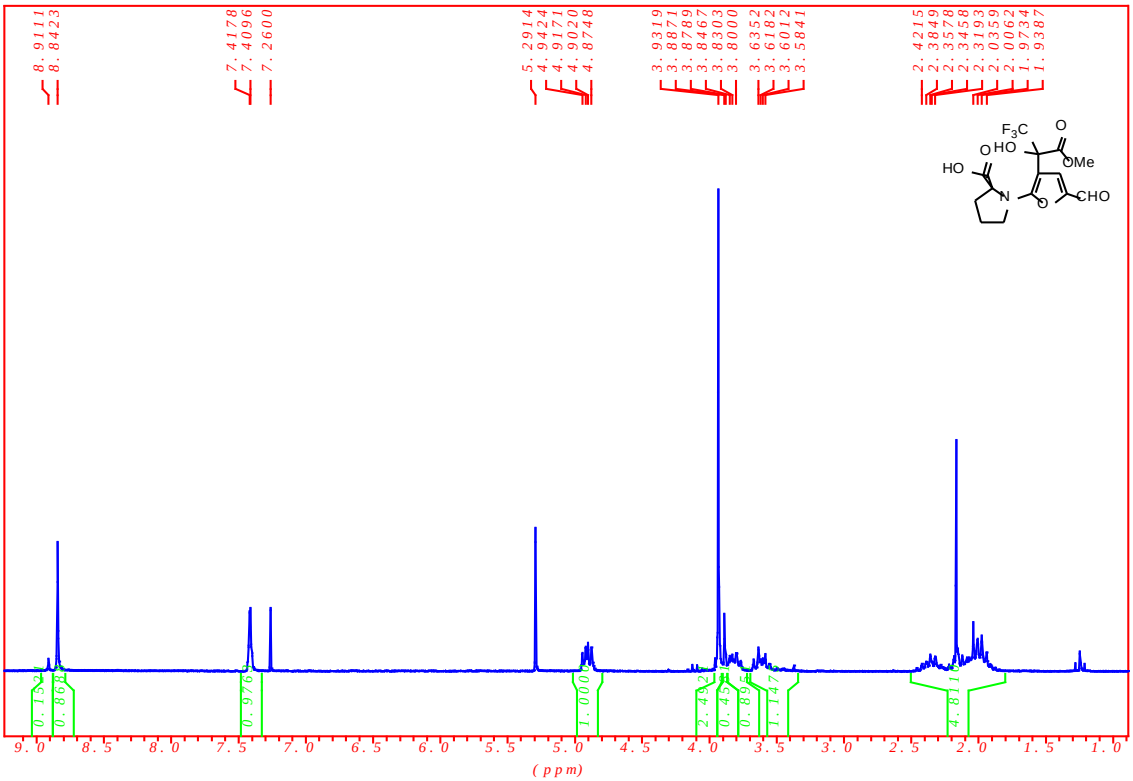


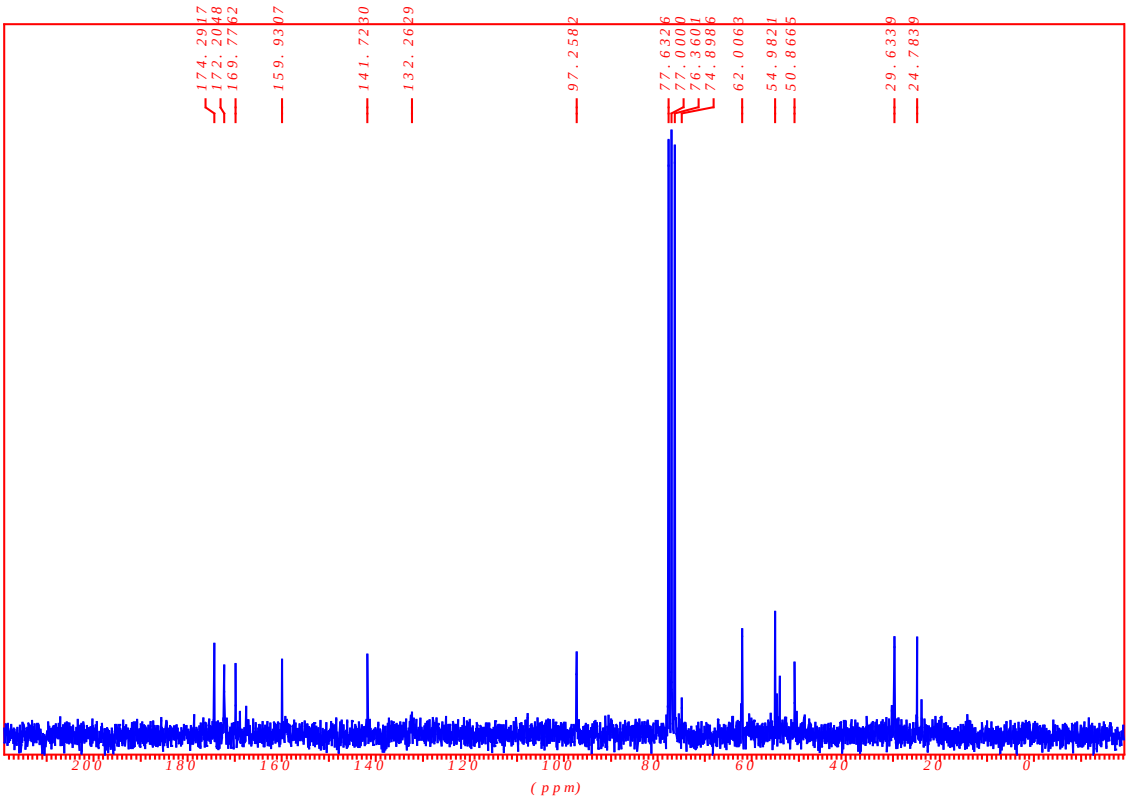
Compnd **3bβ**


9.5991
8.8435
7.4852
7.4813
7.4775
3.2016
3.1849
3.1663
2.8697
2.8389
2.0648
2.0571
2.0500
2.0429
2.0352
1.7830
1.7656
1.7573
1.7477
1.7297
1.6783
1.6616
HO
CF3
F3C
N
O
CHO
Integral
0.8558
0.6036
0.8755
3.6476
1.3875
6.0000
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
(ppm)

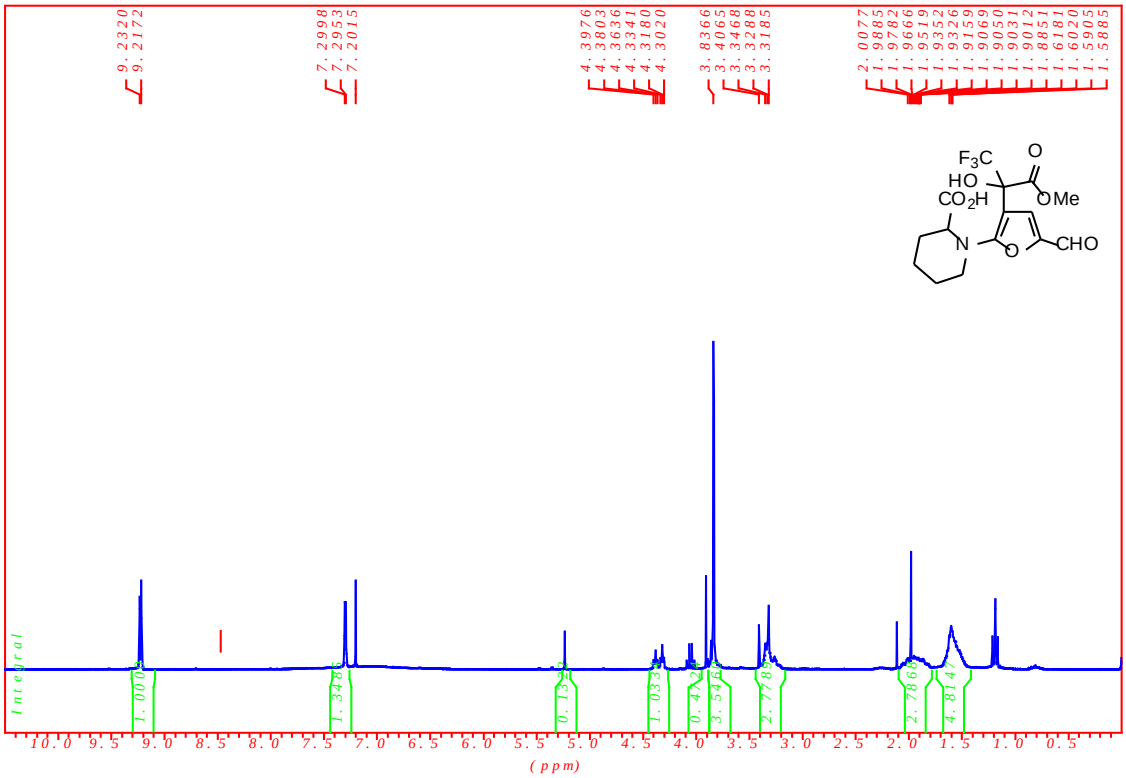

178.1382
160.8379
149.6375
129.1931
129.1712
125.3820
121.6728
121.5928
117.7817
104.7339
76.1510
75.7364
75.3291
74.9146
53.4301
29.8365
29.0655
26.2509
23.7708
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)

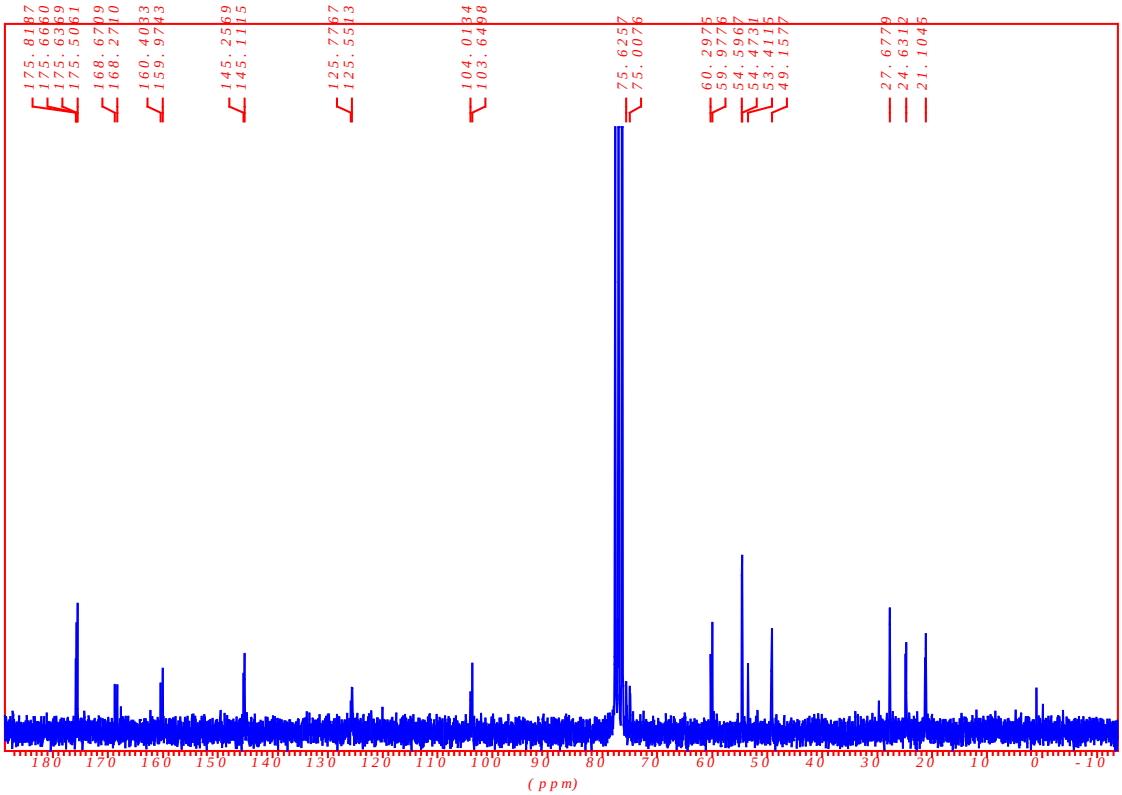
Compnd **3dα**



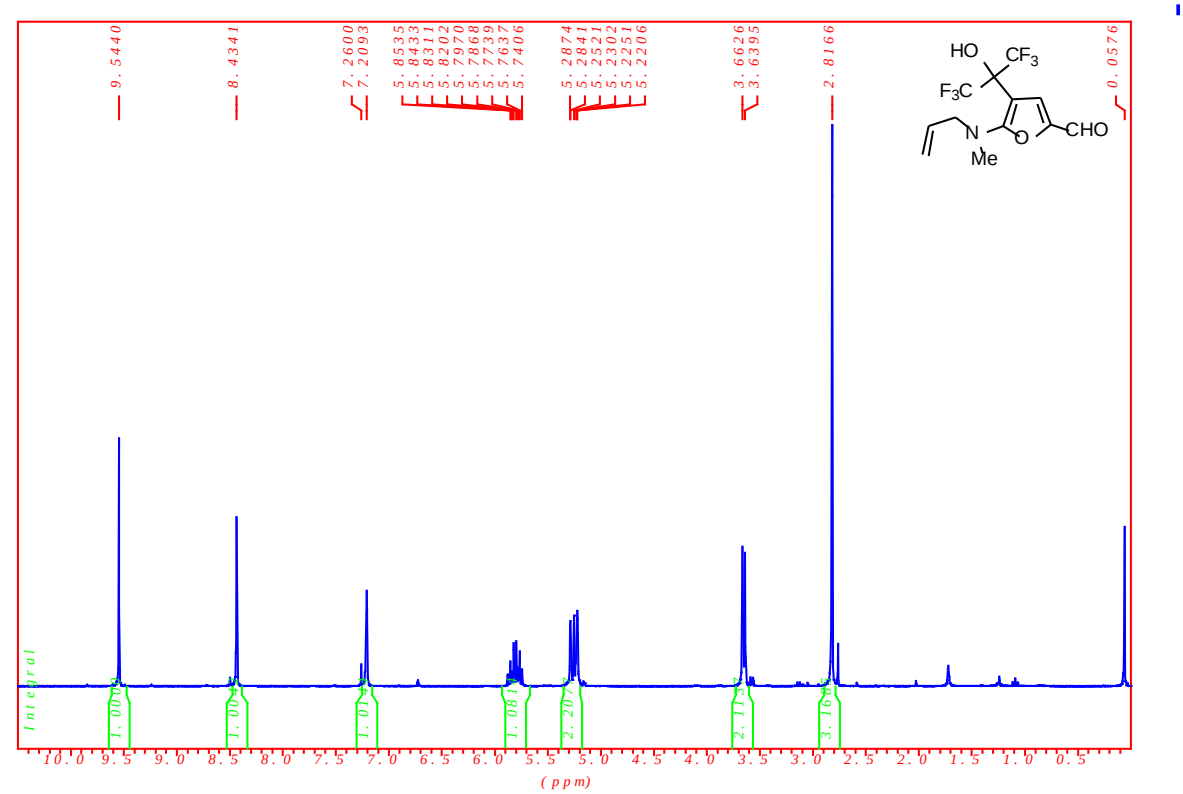


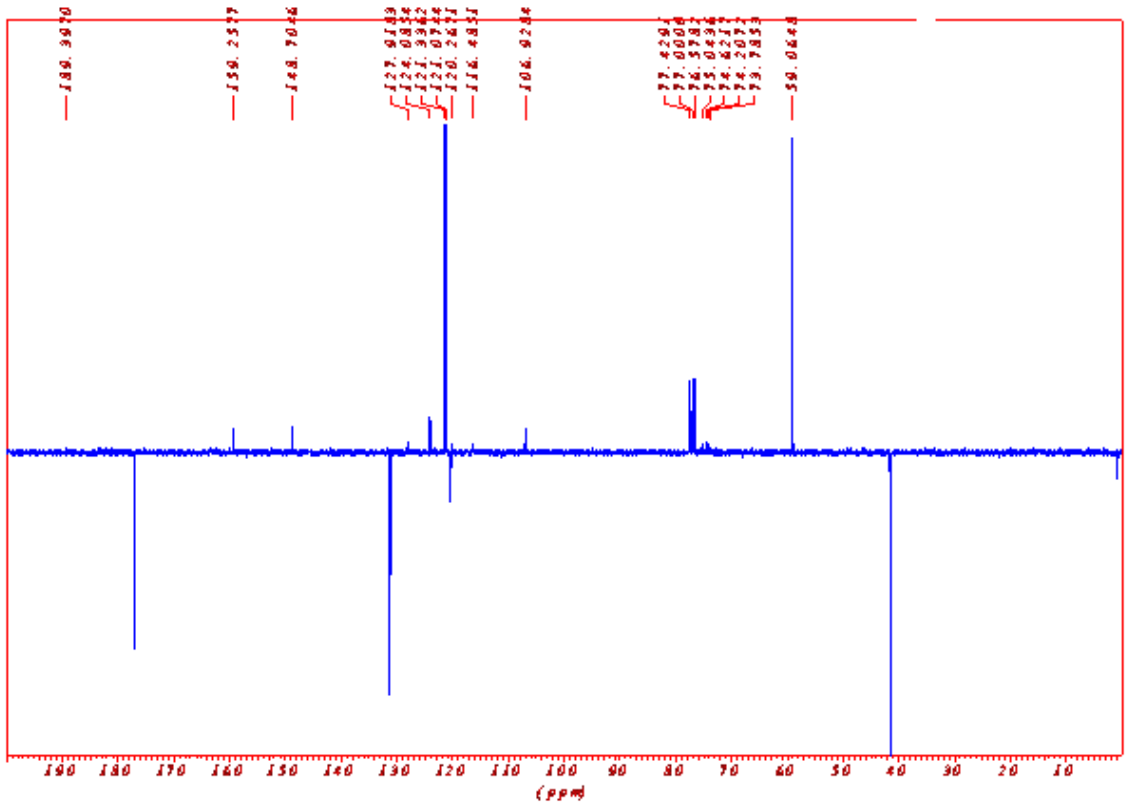
Compnd **3eα**



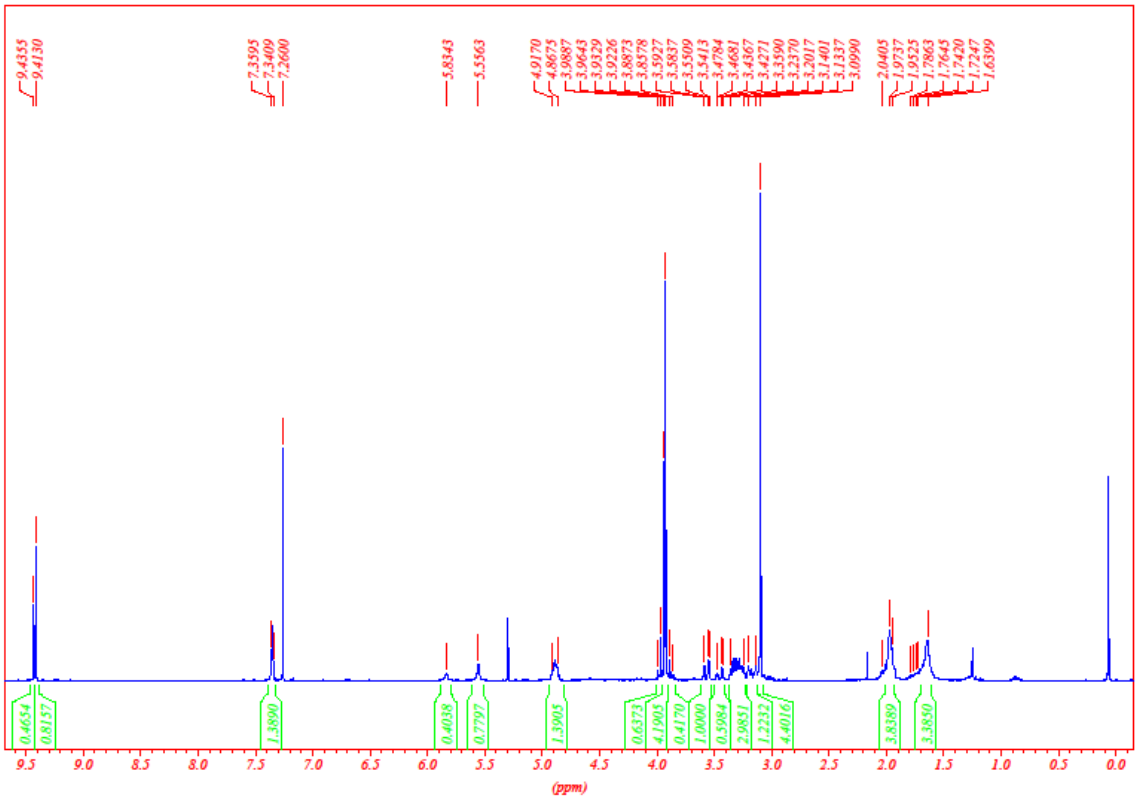


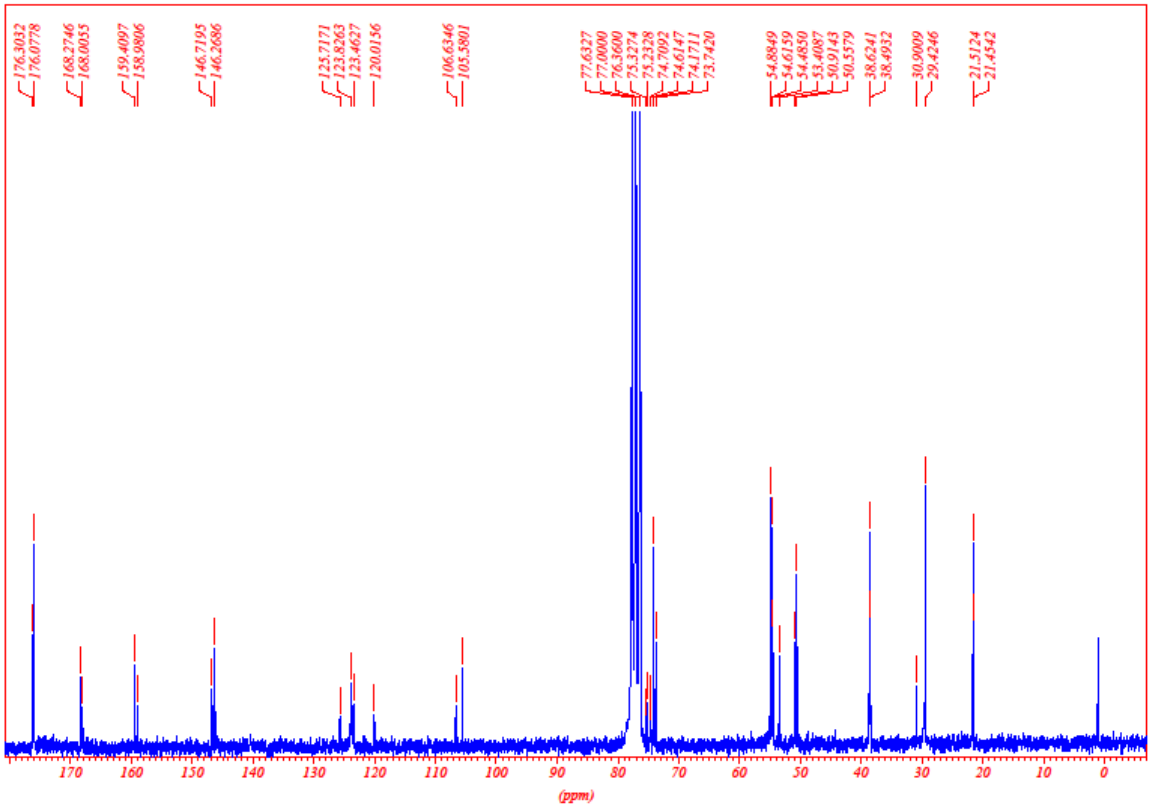
Compnd **3fβ**


9.5440
8.4341
7.2600
7.2093
5.8535
5.8433
5.8311
5.8202
5.7970
5.7868
5.7739
5.7637
5.7406
5.2874
5.2841
5.2521
5.2302
5.2251
5.2206
3.6626
3.6395
2.8166
0.0576
HO
CF3
F3C
N
Me
O
CHO
Integral
1.00
1.00
1.01
1.08
2.20
2.17
3.16
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
(ppm)

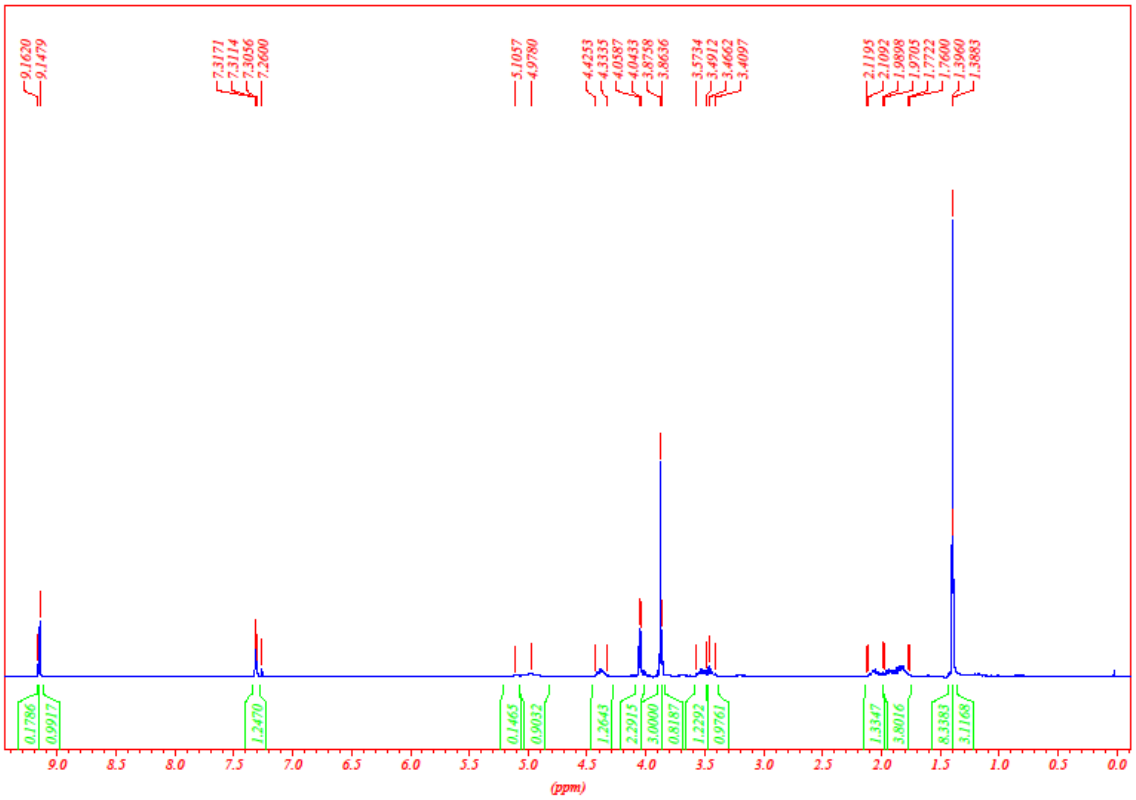

189.3970
159.2577
148.7046
127.9169
124.0834
121.3962
121.0724
120.2671
116.4851
106.9284
77.4291
77.0004
76.5718
75.0496
74.4217
74.2072
73.7853
59.0648
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
(ppm)

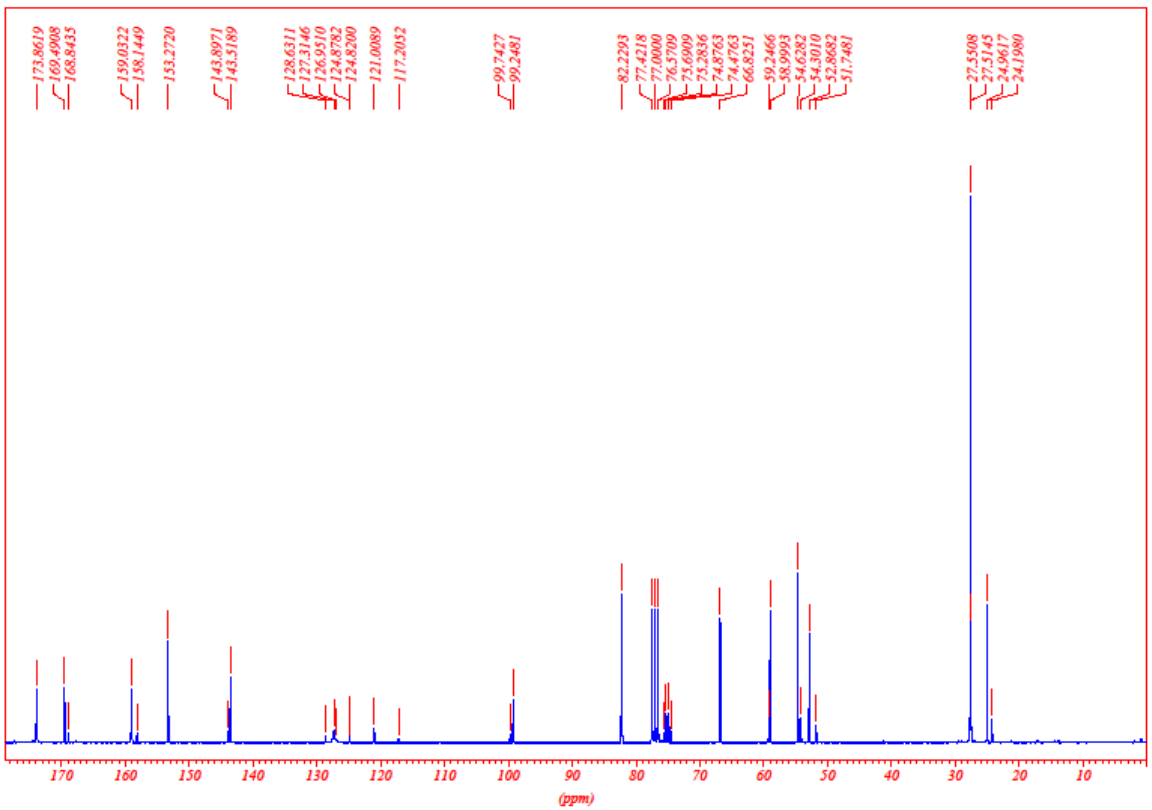
Compnd **3gα**



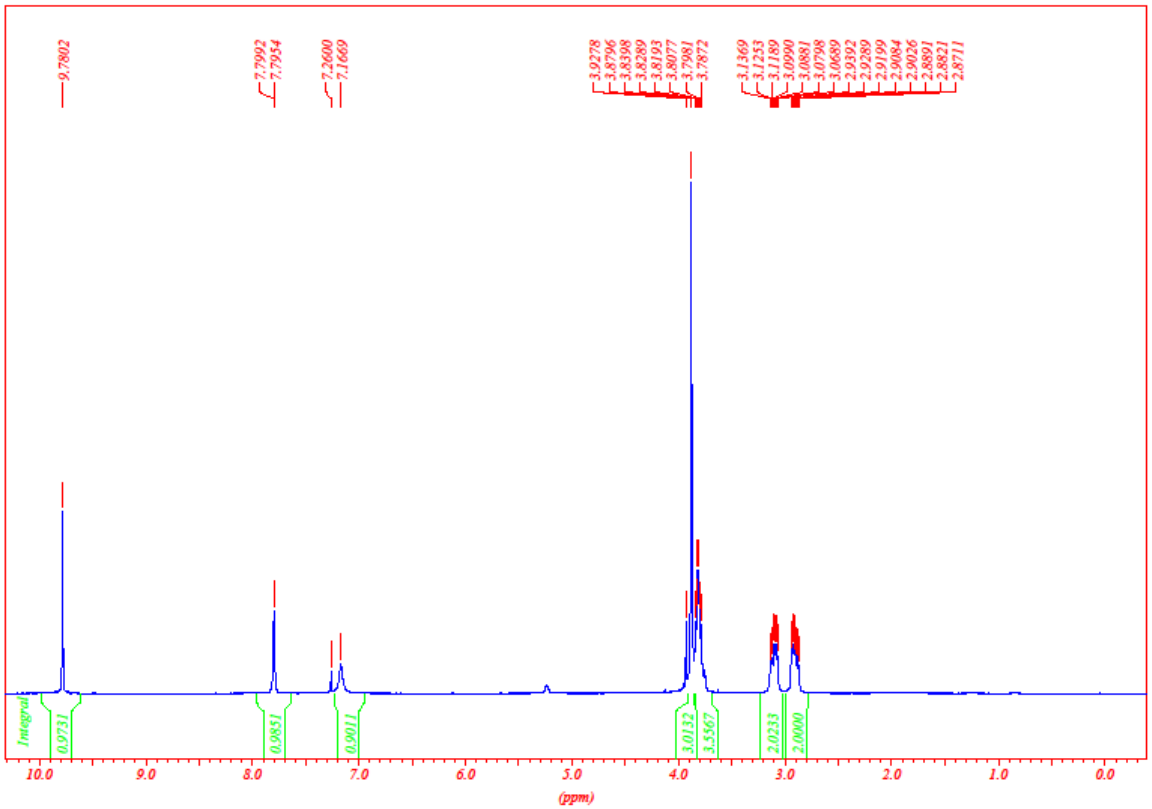


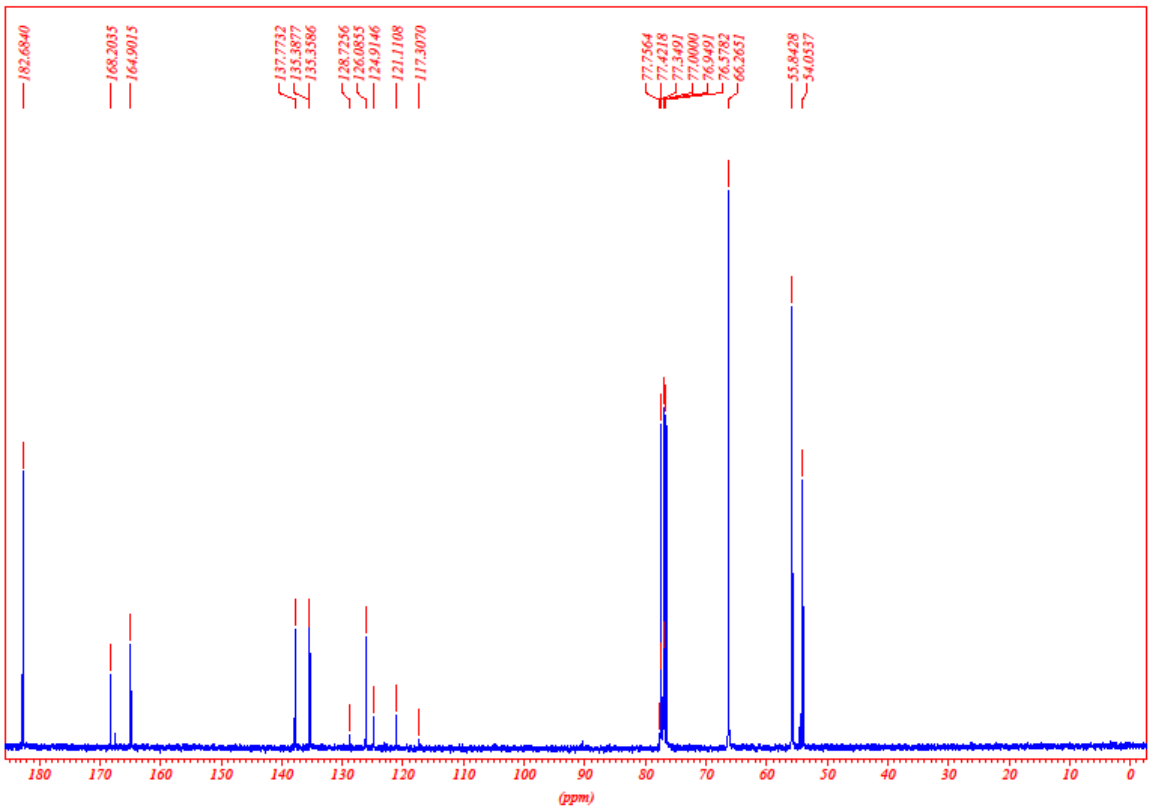
Compnd **3hα**


9.1620
9.1479
7.3171
7.3114
7.3056
7.2600
5.1057
4.9780
4.4253
4.3335
4.0587
4.0433
3.8758
3.8636
3.5734
3.4912
3.4662
3.4097
2.1195
2.1092
1.9898
1.9705
1.7722
1.7600
1.3960
1.3883
0.1786
0.9917
1.2470
0.1465
0.0932
1.2643
2.2915
3.0000
0.8187
1.2292
0.9761
1.3347
3.8016
8.3383
3.1168
(ppm)

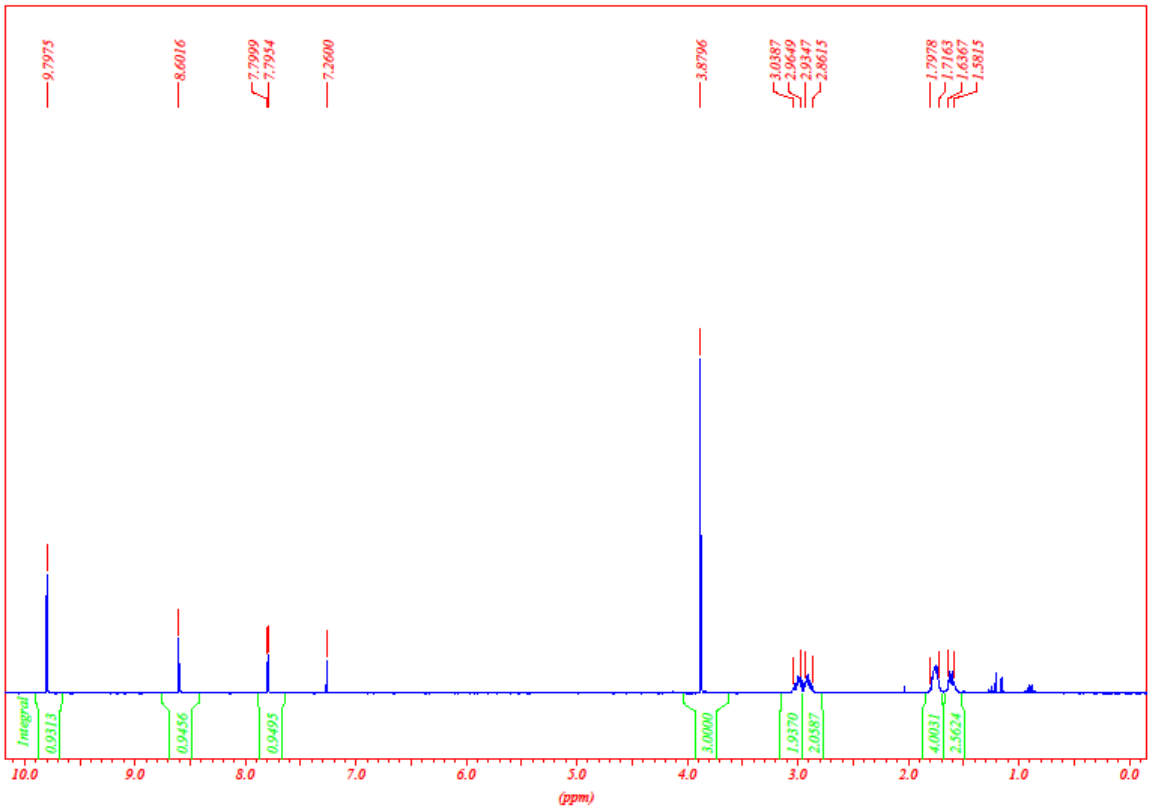

173.8619
169.4908
168.8435
159.0322
158.1449
153.2720
143.8971
143.5189
128.6311
127.3146
126.9510
124.8782
124.8200
121.0089
117.2052
99.7427
99.2481
82.2293
77.4218
77.0000
76.5709
75.6909
75.2836
74.8763
74.4763
66.8251
59.2466
58.9993
54.6282
54.3010
52.8682
51.7481
27.5508
27.5143
24.9617
24.1980
(ppm)

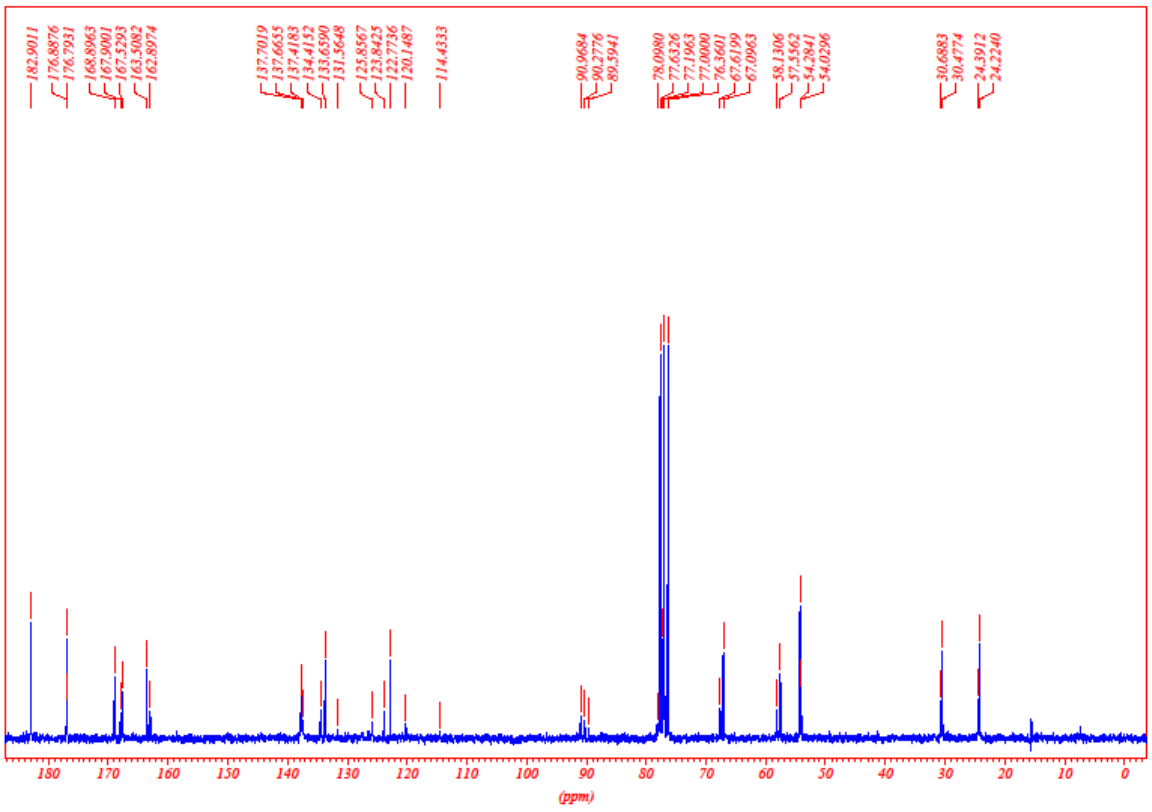
Compnd **4a**


9.7802
7.7992
7.7954
7.2600
7.1669
3.9278
3.8796
3.8398
3.8289
3.8193
3.8077
3.7981
3.7872
3.1369
3.1253
3.1189
3.0990
3.0881
3.0798
3.0689
2.9392
2.9289
2.9199
2.9084
2.9026
2.8891
2.8821
2.8711
Integral
0.9731
0.9851
0.9911
3.0132
3.5567
2.0233
2.0000
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
(ppm)

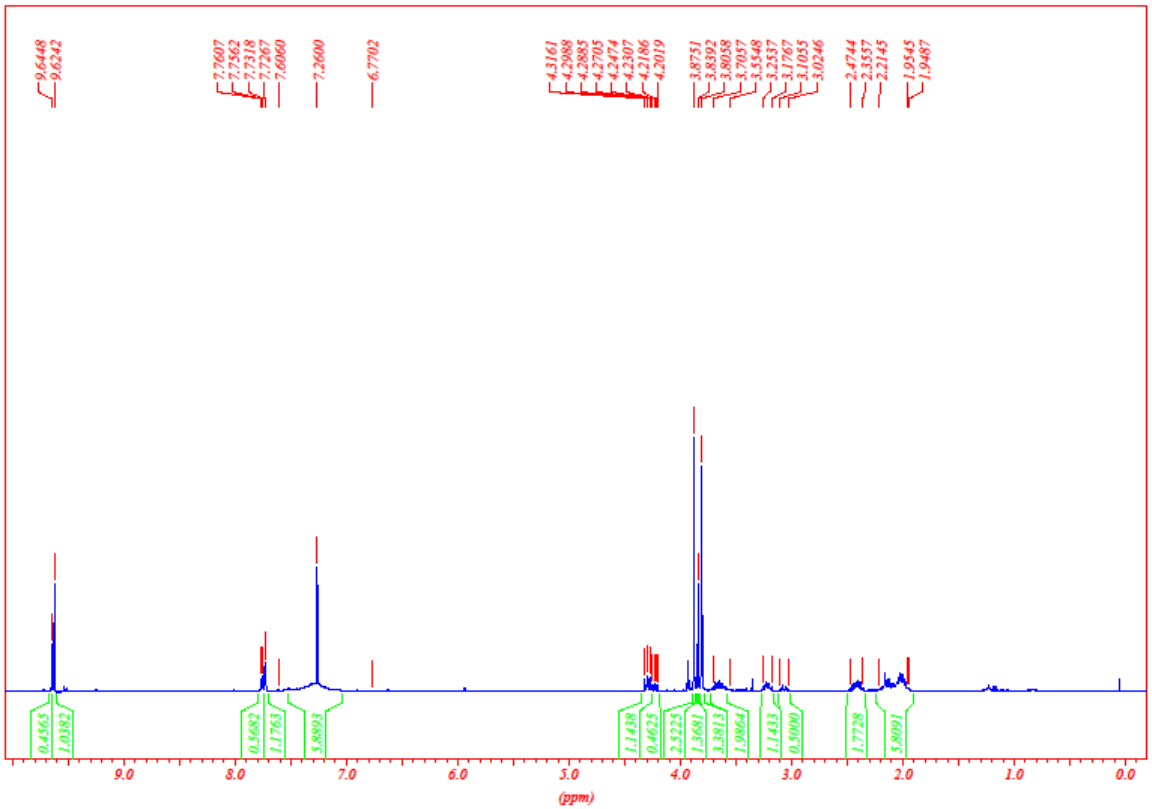

182.6840
168.2035
164.9015
137.7732
135.3877
133.5386
128.7236
126.0835
124.9146
121.1108
117.3070
77.7564
77.4218
77.3491
77.0000
76.9491
76.5782
66.2651
55.8428
54.0537
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)

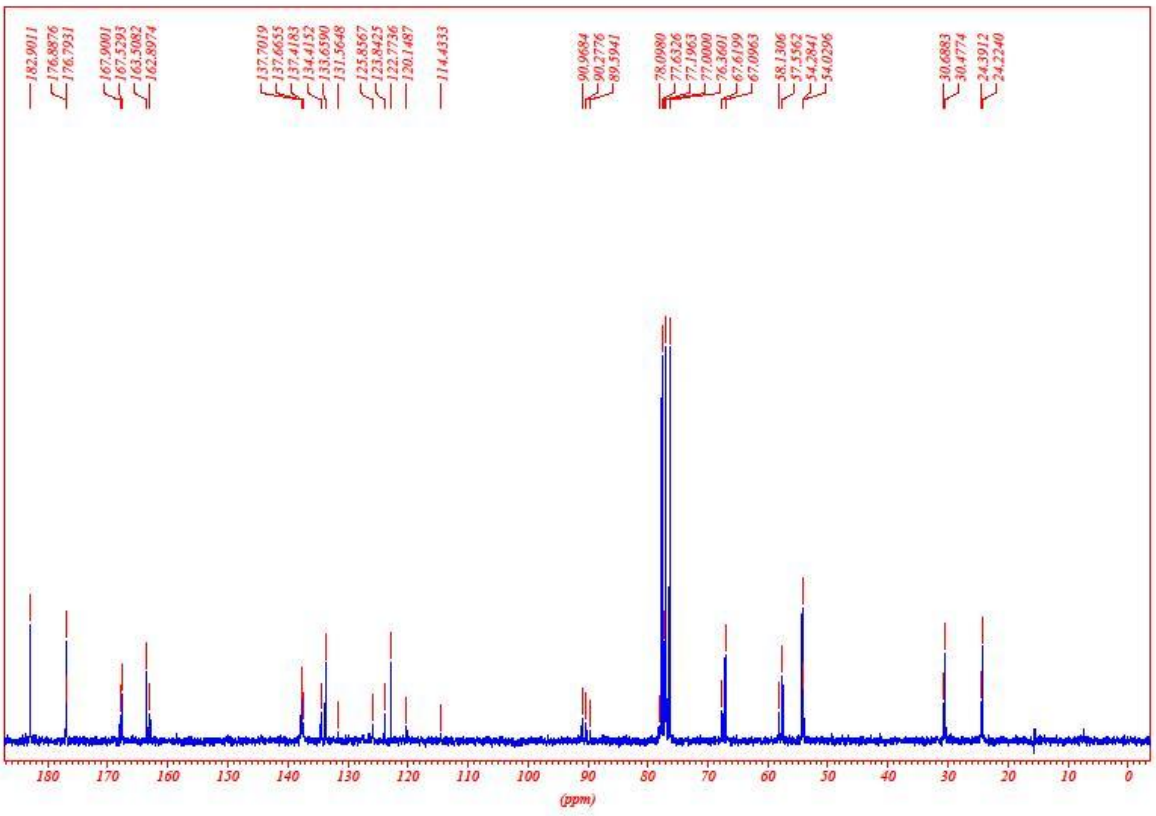
Compnd **4b**


9.7975
8.6016
7.7999
7.7934
7.2600
3.8796
3.0387
2.9649
2.9347
2.8615
1.7978
1.7163
1.6367
1.5815
Integral
0.9313
0.9456
0.9495
3.0000
1.9370
2.0587
4.0031
2.5624
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
(ppm)

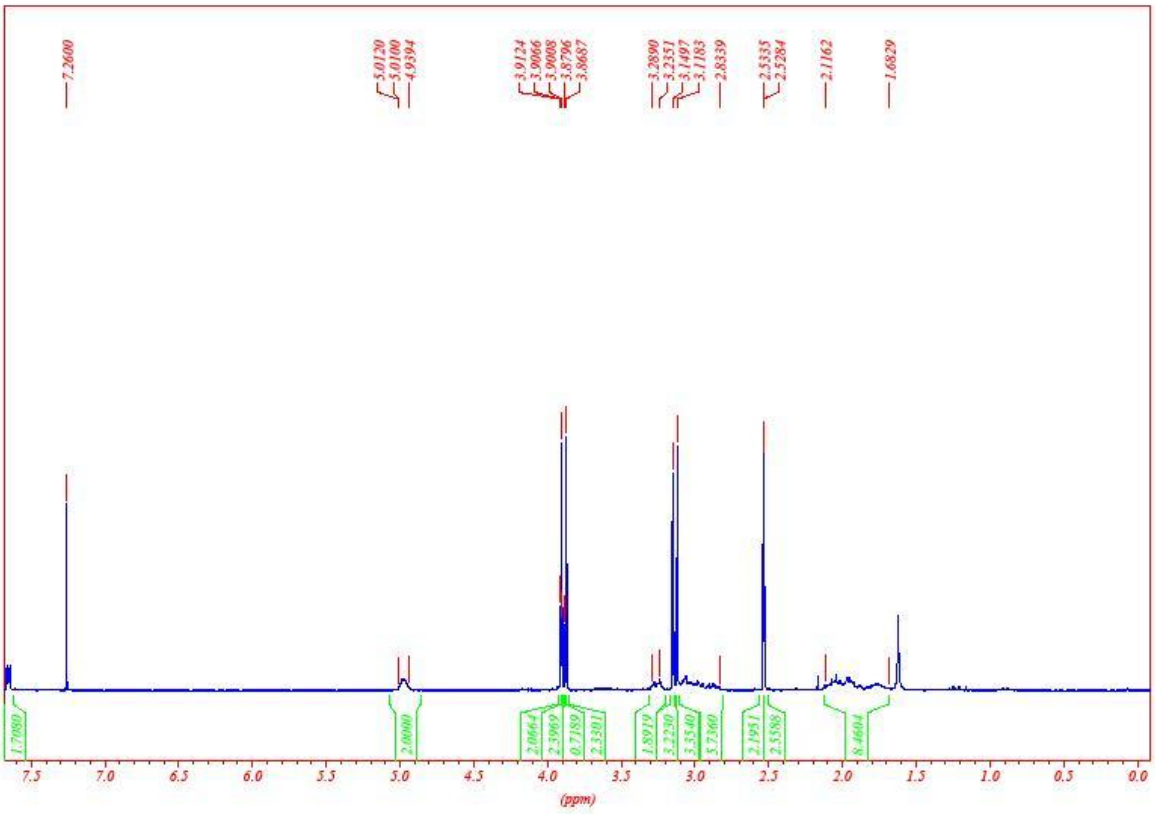

182.9011
176.8876
176.7931
168.8963
167.9001
167.5293
163.5082
162.8974
137.7019
137.6655
137.4183
134.4152
133.6590
131.5648
125.8567
123.8425
122.7736
120.1487
114.4333
90.9684
90.2776
89.5941
78.0980
77.6326
77.1963
77.0000
76.3601
67.6199
67.0963
58.1306
57.5562
54.2841
54.0296
30.6883
30.4774
24.3912
24.2240
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)

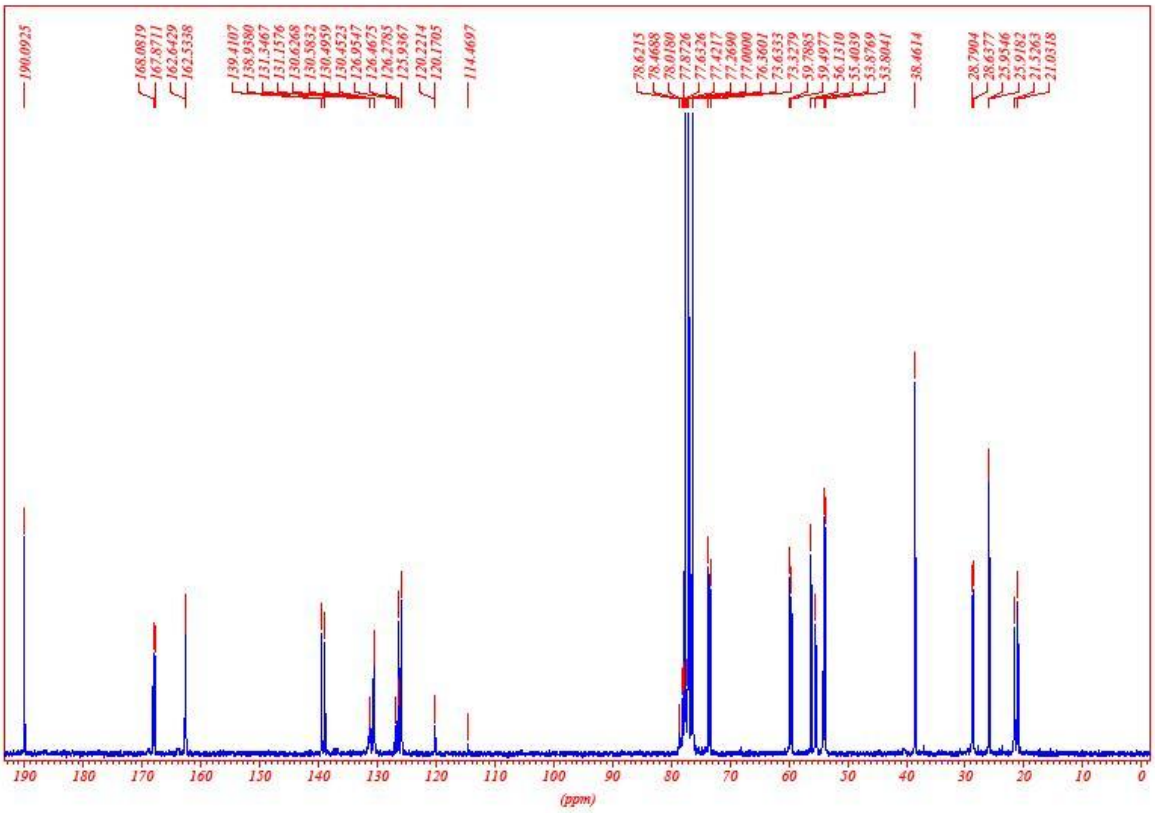
Compnd **4d**



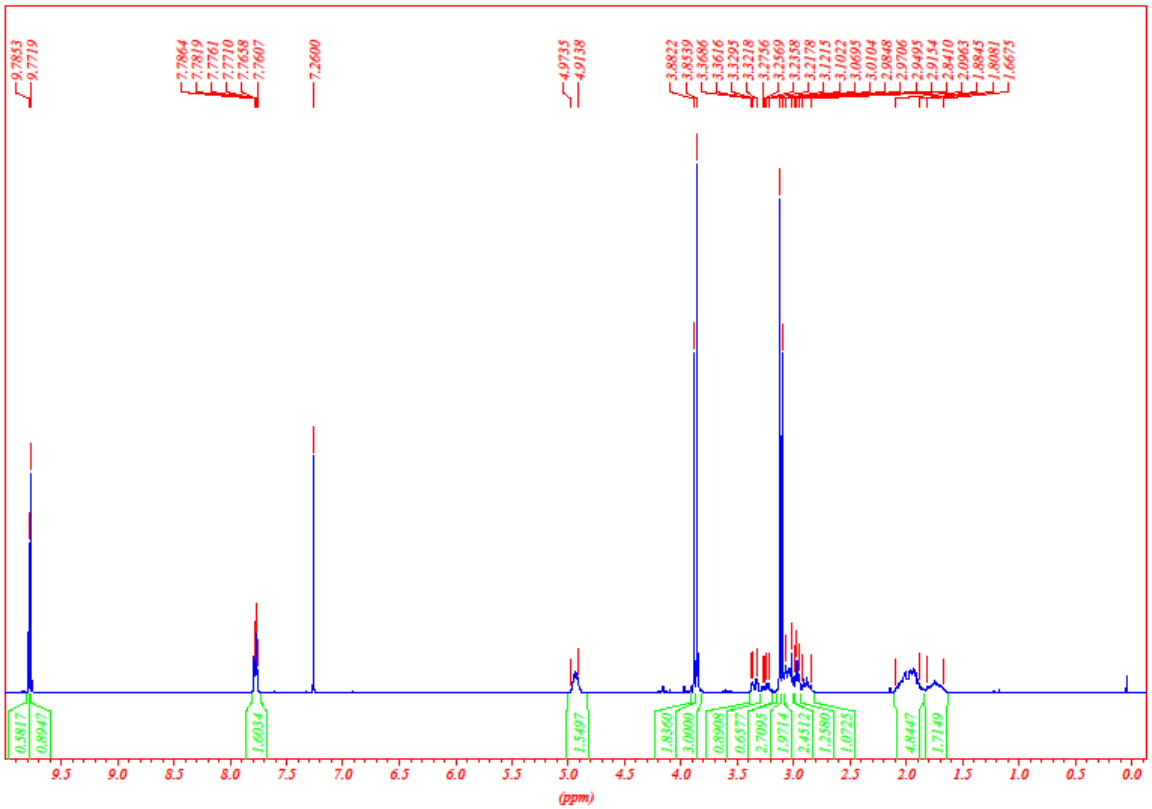


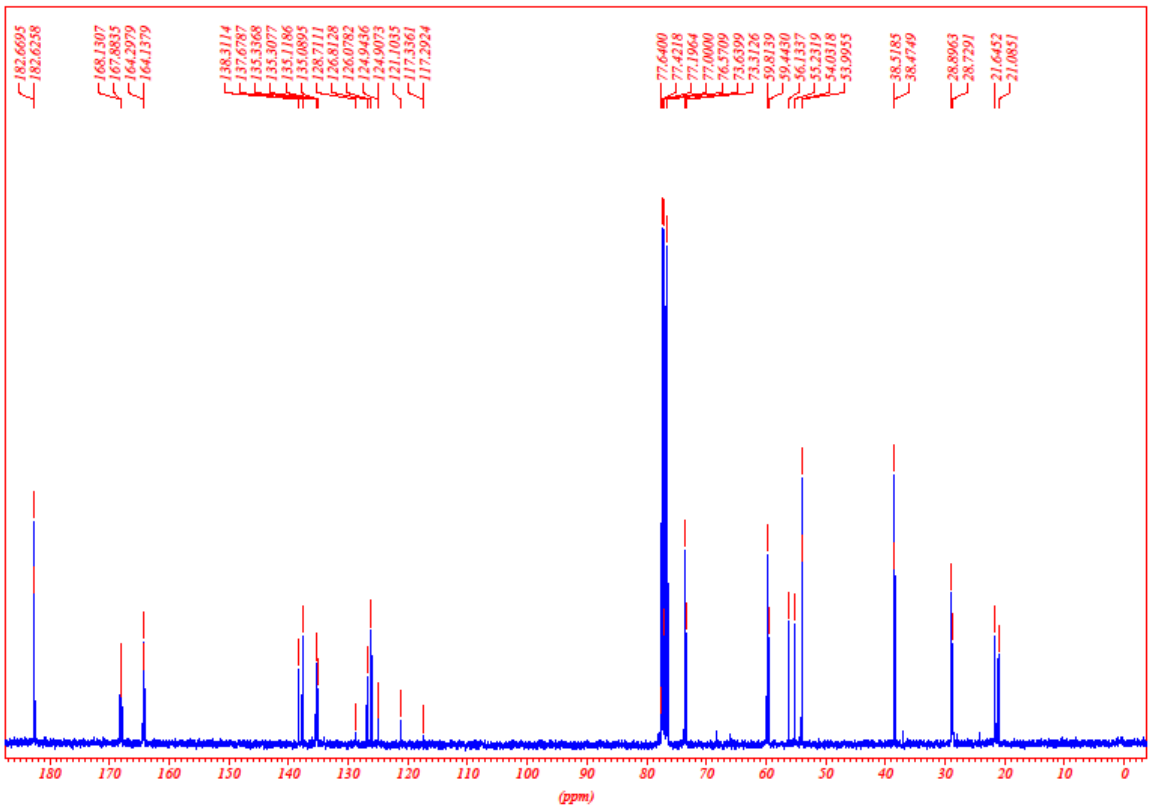
Compnd **4f**



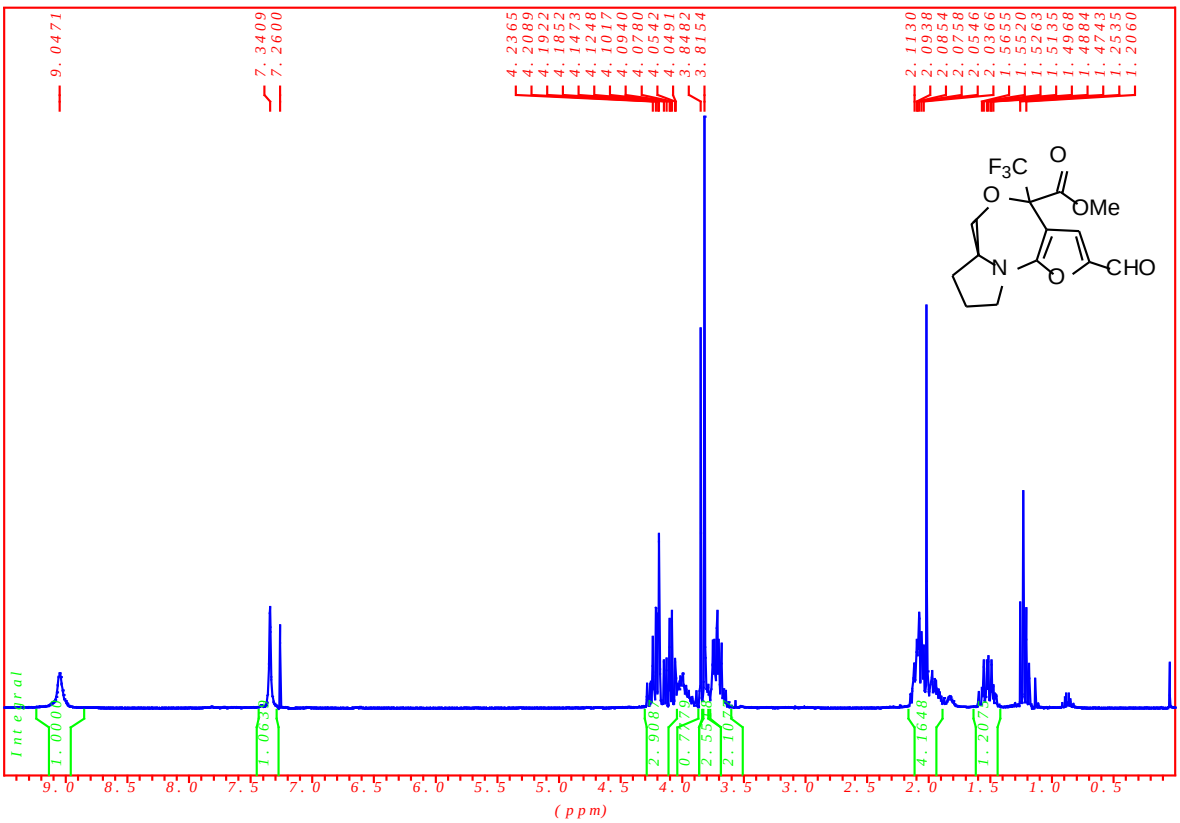


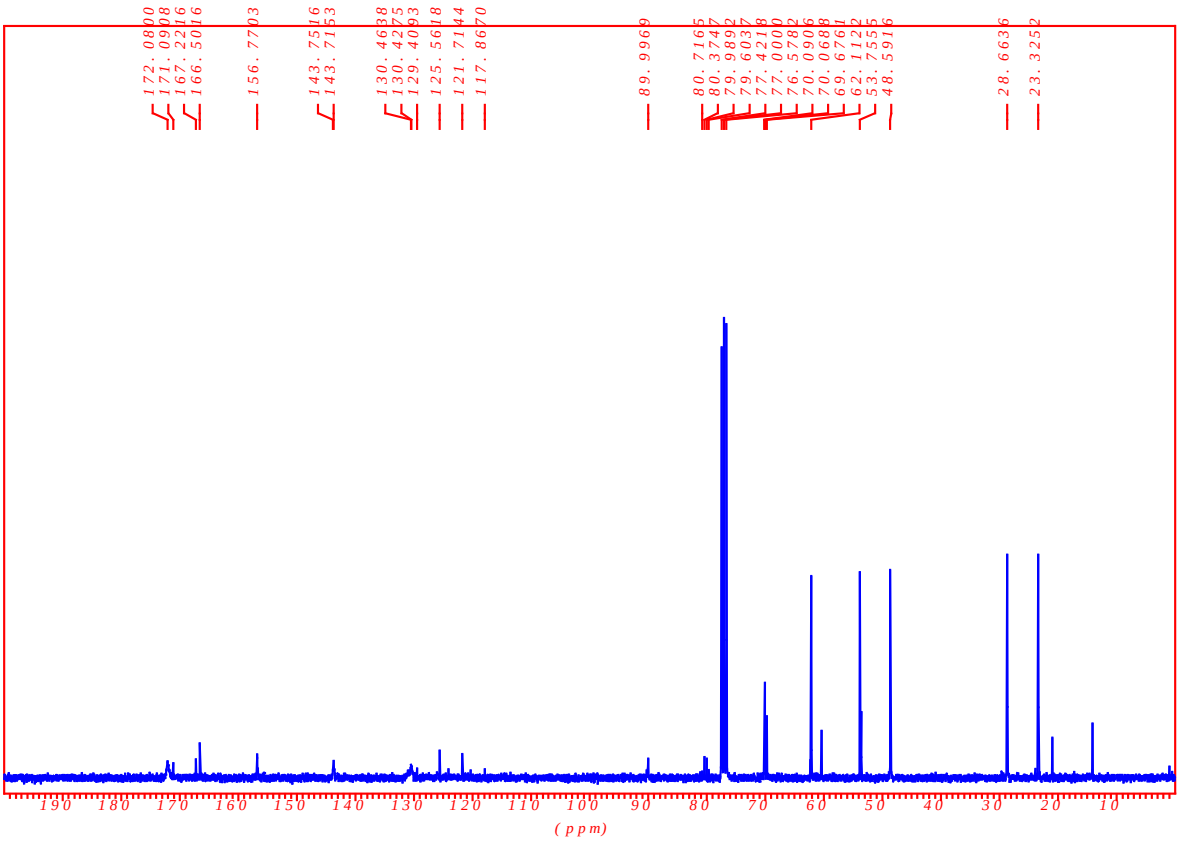
Compnd **4g**



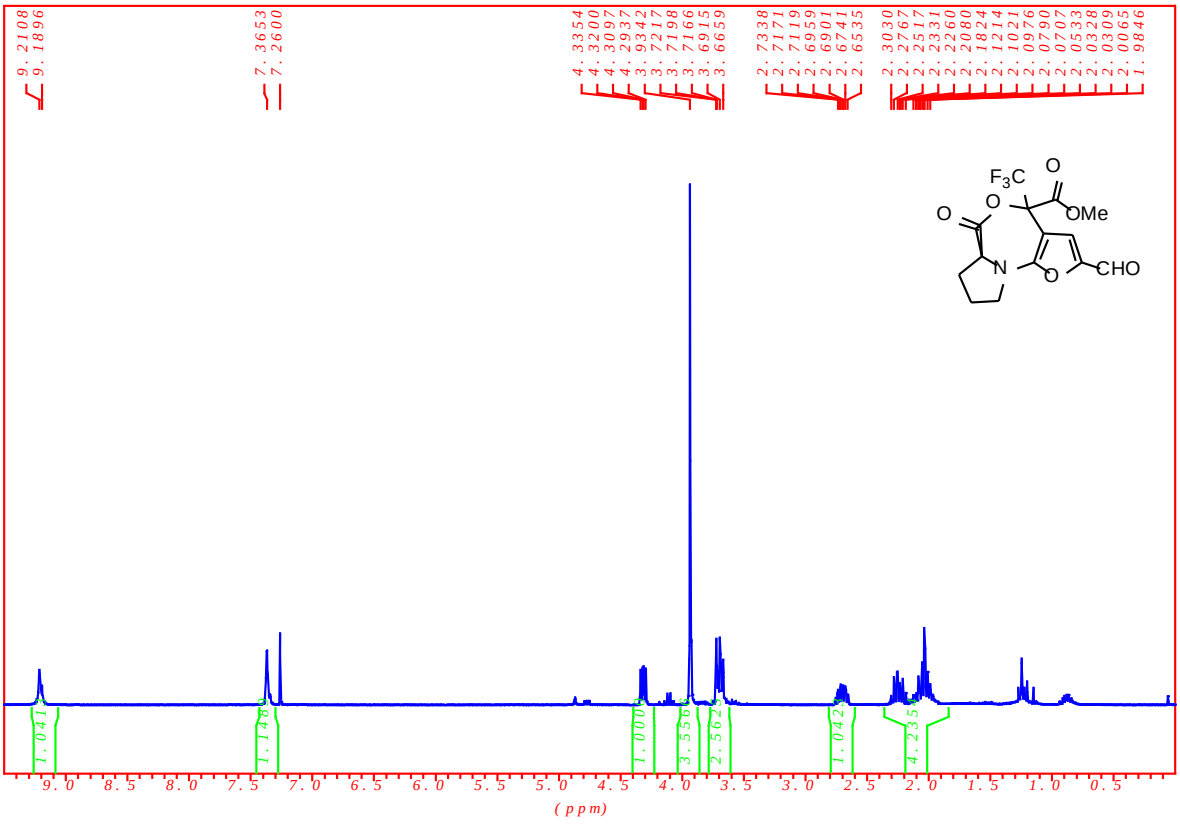


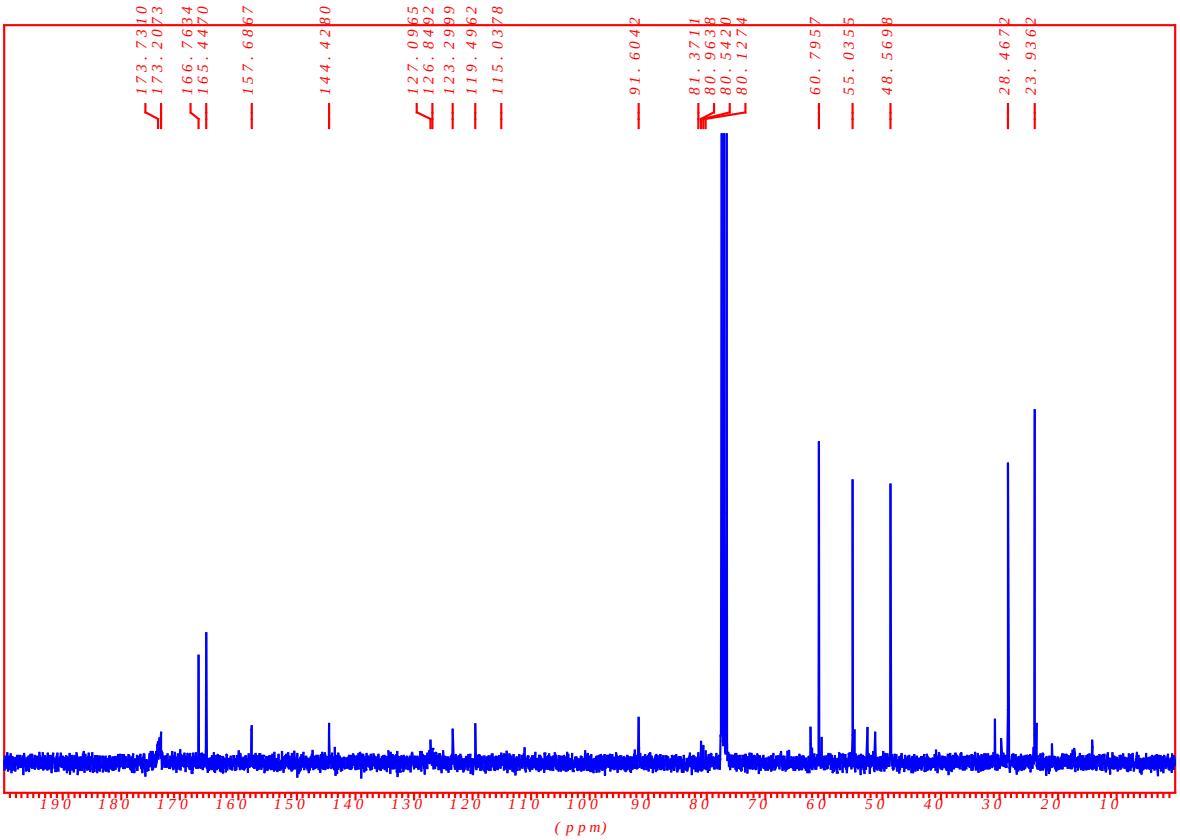
Compnd **5**





Compnd **6**


9.2108
9.1896
7.3653
7.2600
4.3354
4.3200
4.3097
4.2937
3.9342
3.7217
3.7198
3.7166
3.6915
3.6659
2.7338
2.7171
2.7119
2.6959
2.6901
2.6741
2.6535
2.3030
2.2767
2.2517
2.2331
2.2260
2.2080
2.1824
2.1214
2.1021
2.0976
2.0790
2.0707
2.0533
2.0328
2.0309
2.0065
1.9846
F3C
O
O
O
OMe
N
O
CHO
1.041
1.148
1.000
3.556
2.562
1.042
4.235
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
(ppm)


173.7310
173.2073
166.7634
165.4470
157.6867
144.4280
127.0965
126.8492
123.2999
119.4962
115.0378
91.6042
81.3711
80.9638
80.5420
80.1274
60.7957
55.0355
48.5698
28.4672
23.9362
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
(ppm)