Supporting Information

Bifunctional Oligofluorenes-Cored Carbazole Dendrimers as Solution Processed Blue Emitters and Hole-Transporters for Electroluminescent Devices

Preecha Moonsin,[1] Narid Prachumrak,[2] Supawadee Namuangruk,[3] Siriporn Jungsuttiwong,[1] Tinnagon Keawin,[1] Taweesak Sudyoadsuk,[1] and Vinich Promarak→,[2,4]

[1]Department of Chemistry, Faculty of Science, Ubon Ratchathani University, Ubon Ratchathani, 34190 Thailand

[2]School of Chemistry and Center of Excellence for Innovation in Chemistry, Institute of Science, Suranaree University of Technology, Muang District, Nakhon Ratchasima, 30000 Thailand

[3]National Nanotechnology Center (NANOTEC), 130 Thailand Science Park, Klong Luang, Pathumthani, 12120 Thailand

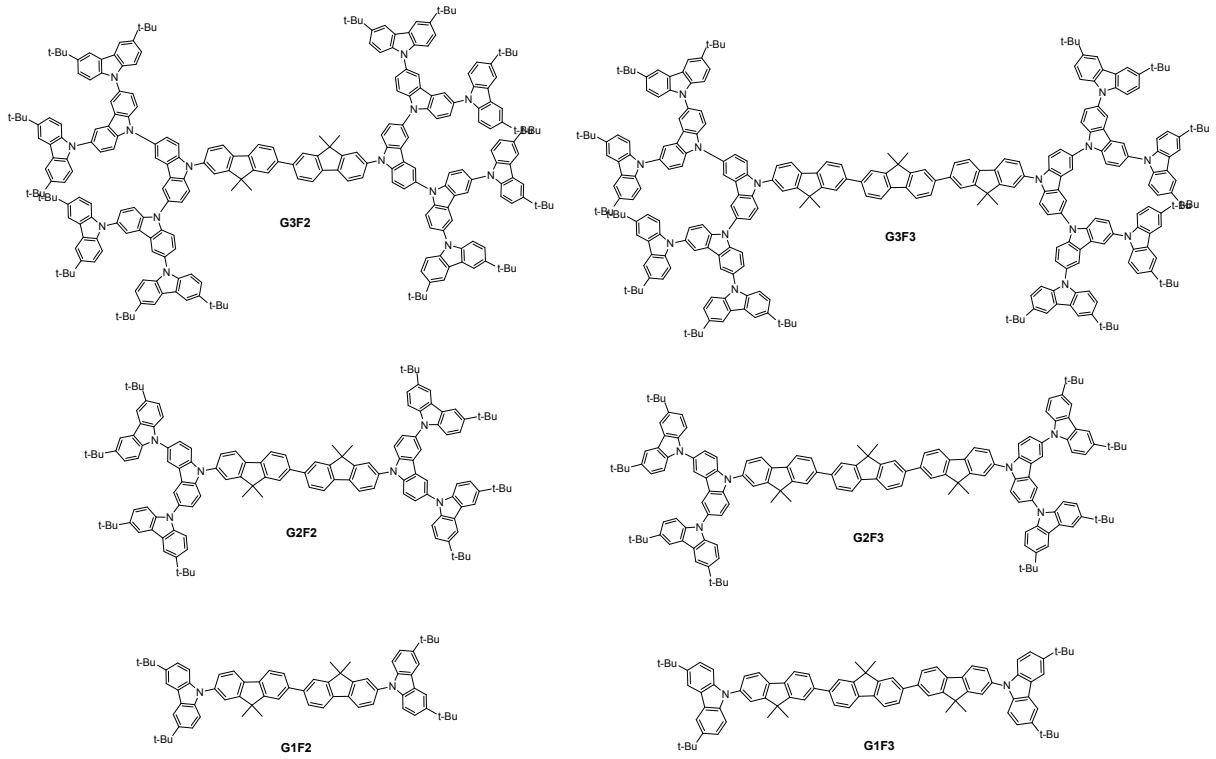
[4]PTT Group Frontier Research Center, PTT Public Company Limited, 555 Vibhavadi Rangsit Road, Chatuchak, Bangkok, 10900 Thailand

→E-mail: pvinich@sut.ac.th

Table of content

Methods of calculation

- tert-Bu and methyl groups are modelled by H atom
- All calculations were performed by Gaussian 09 code
- Geometry optimizations were done by B3LYP/6-31G(d,p) method



Scheme SI_1. Molecular structures of the compounds.

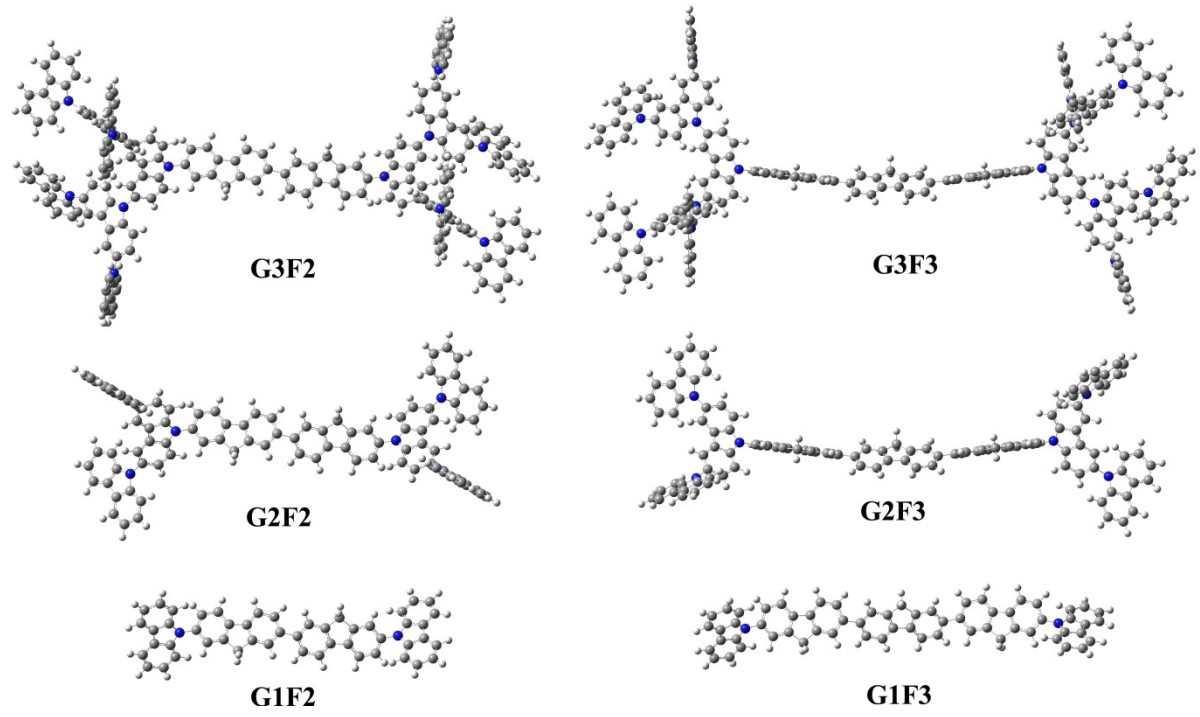


Figure SI-1 The optimized structure of the compounds calculated by B3LYP/6-31G(d,p).

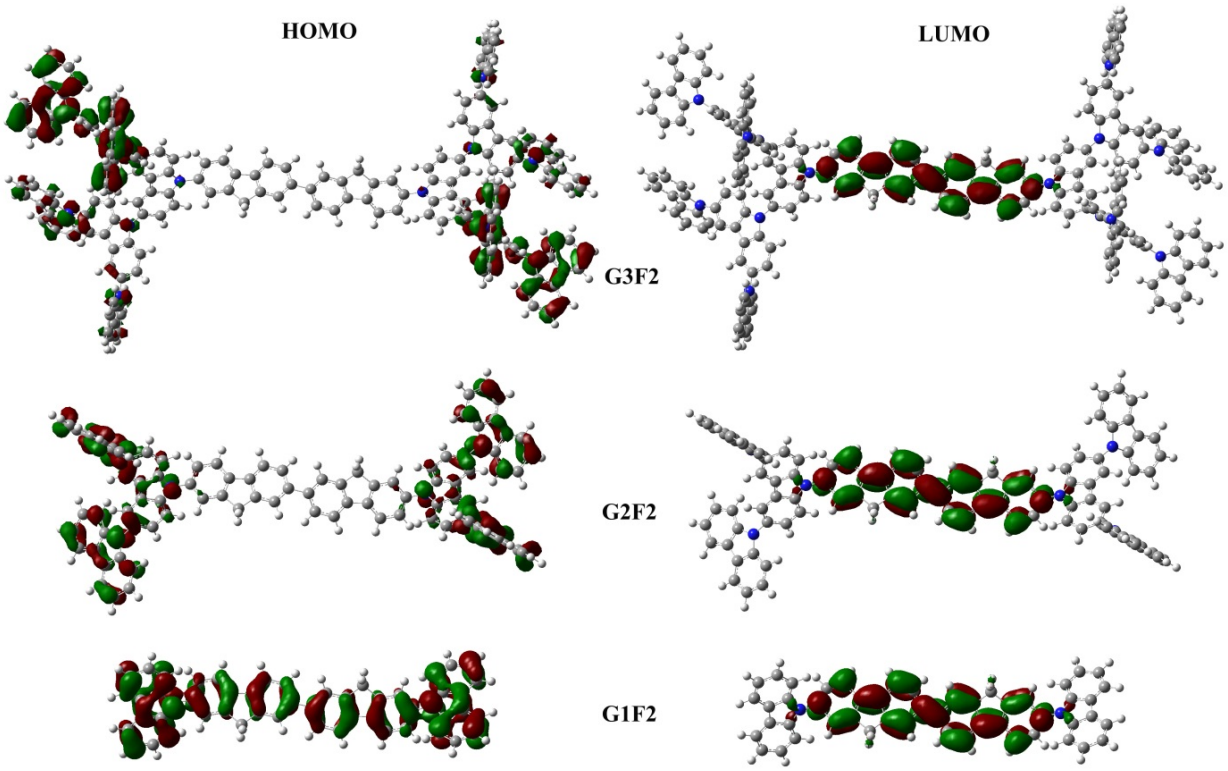


Figure SI_2 HOMO and LUMO of the compounds calculated by B3LYP/6-31G(d,p).

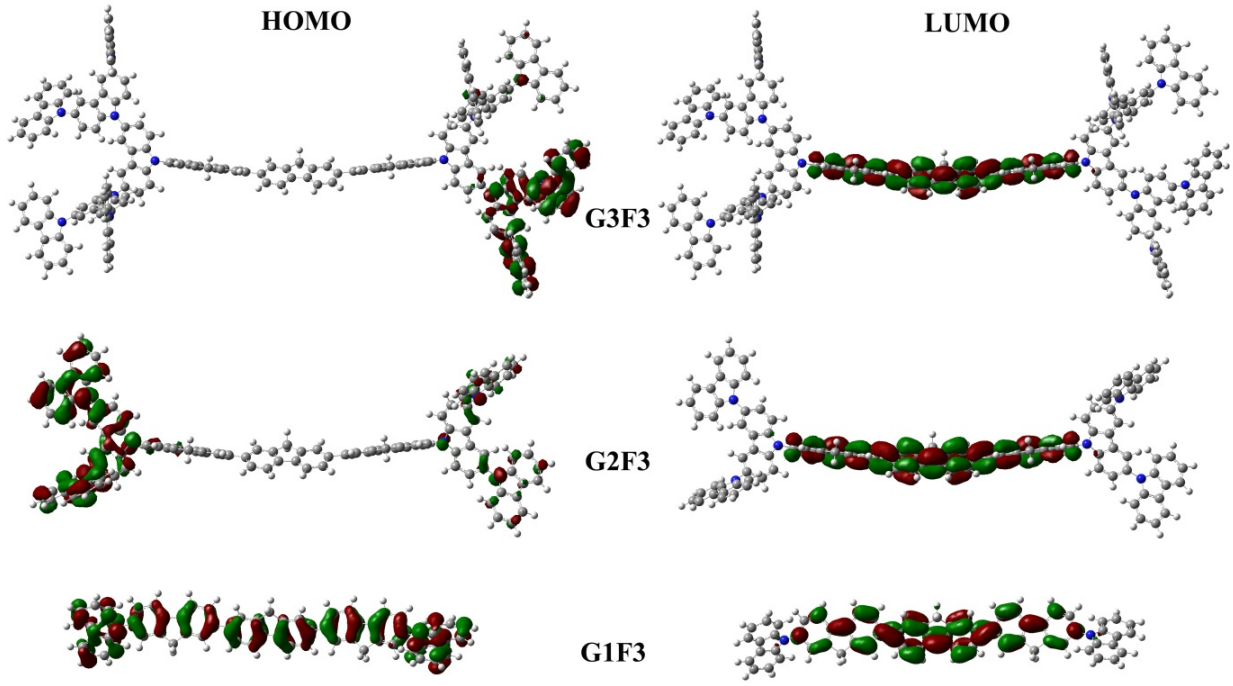


Figure SI_3 HOMO and LUMO of the compounds calculated by B3LYP/6-31G(d,p).

Table SI_1 The calculated HOMO, LUMO and HOMO-LUMO energy gap (Δ_{H-L}) of the studied compounds by TDDFT/B3LYP/6-31G(d,p) in gas (CH_2Cl_2 solvent) phase.

Compound	HOMO	LUMO	Δ_{H-L}
G1F2	-5.21 (-5.31)	-1.51 (-1.51)	3.70 (3.30)
G2F2	-5.19 (-5.29)	-1.78 (-1.58)	3.40 (3.21)
G3F2	-5.20 (-5.26)	-2.04 (-1.61)	3.17 (3.15)
G1F3	-5.18 (-5.27)	-1.56 (-1.59)	3.62 (3.31)
G2F3	-5.16 (-5.27)	-1.76 (-1.64)	3.40 (3.23)
G3F3	-5.18 (-5.26)	-1.95 (-1.68)	3.23 (3.18)

Coordinate for optimized structure of GnFm (n = 1-3, m = 2-3)

Compound G1F2

H	-4.276669	-2.269030	-0.393568
C	-7.206009	1.600166	-0.521461
C	-7.656169	0.350605	-0.067669
C	-6.738377	-0.676389	0.205560
C	-5.385096	-0.438570	0.010684
C	-4.930104	0.820070	-0.437204
C	-5.844820	1.842938	-0.698433
H	-7.934687	2.372614	-0.743485
H	-7.098924	-1.632261	0.573034
H	-5.510536	2.814947	-1.049214
C	-4.208065	-1.367707	0.229661
H	-4.147246	-1.713804	1.269852
C	-3.023629	-0.501661	-0.151062
C	-1.671969	-0.811863	-0.145872
C	-0.724963	0.157297	-0.532581
C	-1.184803	1.432384	-0.917905
C	-2.540724	1.751127	-0.921951
C	-3.467696	0.780276	-0.536863
H	-1.334096	-1.791236	0.181122
H	-0.464138	2.175645	-1.244650
H	-2.864418	2.740804	-1.231667
H	4.147250	1.713648	1.270049
C	1.184799	-1.432272	-0.918083
C	0.724960	-0.157231	-0.532602
C	1.671968	0.811881	-0.145778
C	3.023628	0.501680	-0.151010
C	3.467693	-0.780210	-0.536969
C	2.540719	-1.751015	-0.922172
H	0.464132	-2.175493	-1.244916
H	1.334096	1.791215	0.181336
H	2.864412	-2.740653	-1.232010
C	4.208065	1.367679	0.229815
H	4.276666	2.269078	-0.393304
C	5.385095	0.438569	0.010720
C	6.738377	0.676364	0.205621
C	7.656168	-0.350596	-0.067738
C	7.206006	-1.600101	-0.521682
C	5.844817	-1.842852	-0.698677
C	4.930101	-0.820017	-0.437320
H	7.098924	1.632190	0.573212
H	7.934683	-2.372523	-0.743804
H	5.510532	-2.814819	-1.049576
C	-9.796859	-0.893429	-0.486061
C	-9.899574	0.874902	0.932975
C	-9.394286	-1.868706	-1.402652
C	-11.143460	-0.793015	-0.051691
C	-9.606207	1.966919	1.754467
C	-11.208560	0.334038	0.855023
C	-10.359451	-2.759259	-1.867308
H	-8.367591	-1.927610	-1.746491
C	-12.092861	-1.701395	-0.534263
C	-10.650965	2.525069	2.487566
H	-8.599673	2.364387	1.823363
C	-12.239912	0.914961	1.602132
C	-11.695235	-2.682668	-1.437370
H	-10.070790	-3.526514	-2.579758
H	-13.127839	-1.637137	-0.210566
C	-11.956476	2.010083	2.412596
H	-10.448421	3.375258	3.132329
H	-13.247595	0.512274	1.552184
C	9.796851	0.893503	-0.485970
C	9.899583	-0.875031	0.932812

C	9.394269	1.868911	-1.402418
C	11.143457	0.793030	-0.051627
C	9.606226	-1.967164	1.754153
C	11.208568	-0.334153	0.854924
C	10.359428	2.759532	-1.866956
H	8.367571	1.927863	-1.746240
C	12.092852	1.701480	-0.534078
C	10.650993	-2.525416	2.487162
H	8.599694	-2.364643	1.823004
C	12.239928	-0.915180	1.601940
C	11.695217	2.682882	-1.437041
H	10.070760	3.526888	-2.579293
H	13.127833	1.637177	-0.210400
C	11.956503	-2.010418	2.412251
H	10.448457	-3.375696	3.131808
H	13.247610	-0.512484	1.552039
N	-9.047023	0.123498	0.115873
N	9.047023	-0.123512	0.115825
H	12.422293	3.393769	-1.817253
H	12.748344	-2.470397	2.995327
H	-12.422316	-3.393500	-1.817678
H	-12.748311	2.469981	2.995745

Compound G2F2

H	-4.336341	-2.149350	-0.698022
C	-7.156475	1.801863	-0.833266
C	-7.641897	0.562918	-0.389254
C	-6.757250	-0.491119	-0.112780
C	-5.396275	-0.289966	-0.296268
C	-4.904442	0.957612	-0.736916
C	-5.787746	2.007271	-0.999976
H	-7.862173	2.595296	-1.056172
H	-7.147560	-1.438194	0.247378
H	-5.423809	2.970878	-1.343866
C	-4.246505	-1.251345	-0.072843
H	-4.201327	-1.600400	0.967123
C	-3.037054	-0.417085	-0.445633
C	-1.694562	-0.765198	-0.437109
C	-0.720242	0.177885	-0.819988
C	-1.142842	1.466325	-1.203926
C	-2.488967	1.823312	-1.210301
C	-3.443310	0.877563	-0.829766
H	-1.385531	-1.754460	-0.111635
H	-0.401130	2.189413	-1.528471
H	-2.783794	2.822161	-1.519168
H	4.201372	1.600414	0.967228
C	1.142842	-1.466052	-1.204119
C	0.720253	-0.177656	-0.820023
C	1.694584	0.765382	-0.437059
C	3.037074	0.417265	-0.445651
C	3.443319	-0.877341	-0.829941
C	2.488966	-1.823043	-1.210566
H	0.401123	-2.189103	-1.528731
H	1.385563	1.754609	-0.111470
H	2.783782	-2.821855	-1.519560
C	4.246536	1.251474	-0.072778
H	4.336369	2.149547	-0.697859
C	5.396298	0.290112	-0.296320
C	6.757272	0.491222	-0.112794
C	7.641907	-0.562800	-0.389381
C	7.156472	-1.801682	-0.833544
C	5.787739	-2.007051	-1.000288
C	4.904451	-0.957411	-0.737112
H	7.147598	1.438250	0.247470
H	7.862157	-2.595101	-1.056540
H	5.423791	-2.970611	-1.344300
C	-9.824270	-0.581396	-0.874578
C	-9.874392	1.121133	0.617866
C	-9.450095	-1.535438	-1.824952
C	-11.172713	-0.444619	-0.455904
C	-9.550478	2.163396	1.490864
C	-11.204422	0.642550	0.499365
C	-10.442158	-2.357389	-2.348296
H	-8.423017	-1.623585	-2.160596
C	-12.151981	-1.295628	-0.977299
C	-10.579747	2.739569	2.227236
H	-8.531802	2.521873	1.586830
C	-12.221753	1.220214	1.264969
C	-11.783318	-2.249209	-1.926405
H	-10.191775	-3.094500	-3.103869
H	-13.186324	-1.226162	-0.656508
C	-11.907217	2.275259	2.121804
H	-10.368691	3.566443	2.896980
H	-13.242701	0.856735	1.209482
C	9.824306	0.581554	-0.874512
C	9.874376	-1.121185	0.617695
C	9.450159	1.535742	-1.824750
C	11.172739	0.444696	-0.455838
C	9.550431	-2.163560	1.490548
C	11.204416	-0.642602	0.499285
C	10.442240	2.357753	-2.347962
H	8.423086	1.623951	-2.160393
C	12.152031	1.295760	-0.977101
C	10.579678	-2.739844	2.226864
H	8.531748	-2.522035	1.586442
C	12.221722	-1.220377	1.264838
C	11.783395	2.249483	-1.926075
H	10.191881	3.094972	-3.103438
H	13.186366	1.226233	-0.656301
C	11.907154	-2.275532	2.121526
H	10.368599	-3.566805	2.896493

H	13.242676	-0.856901	1.209426
N	-9.042930	0.373129	-0.219128
N	9.042941	-0.373056	-0.219212
C	-12.972179	2.952831	4.293232
C	-14.057832	3.545240	2.392104
C	-12.080800	2.423108	5.230283
C	-14.140946	3.652787	4.689695
C	-14.435323	3.762578	1.064251
C	-14.834015	4.031057	3.475852
C	-12.368888	2.617309	6.579242
H	-11.197726	1.876223	4.918229
C	-14.405645	3.833342	6.052352
C	-15.615526	4.465521	0.833413
H	-13.829067	3.399025	0.241733
C	-16.016517	4.733328	3.214810
C	-13.516639	3.316858	6.990335
H	-11.691781	2.215812	7.327574
H	-15.295947	4.367089	6.372700
C	-16.402582	4.945050	1.894656
H	-15.931362	4.646584	-0.189862
H	-16.622792	5.110966	4.033338
C	-13.880505	-2.719266	-3.227983
C	-12.774015	-4.510607	-2.385864
C	-14.280996	-1.434944	-3.605947
C	-14.613441	-3.871569	-3.612749
C	-11.881301	-5.357067	-1.722866
C	-13.906913	-5.015554	-3.074991
C	-15.440642	-1.316899	-4.368438
H	-13.707409	-0.560642	-3.318047
C	-15.775921	-3.723475	-4.378526
C	-12.131080	-6.726636	-1.770500
H	-11.025979	-4.960926	-1.186299
C	-14.133262	-6.396571	-3.107100
C	-16.184977	-2.446405	-4.750605
H	-15.773920	-0.329458	-4.674237
H	-16.349132	-4.595541	-4.680310
C	-13.242602	-7.245559	-2.456731
H	-11.452176	-7.405893	-1.263122
H	-14.995824	-6.799319	-3.630509
C	12.774073	4.510930	-2.385348
C	13.880670	2.719654	-3.227470
C	11.881303	5.357339	-1.722359
C	13.907006	5.015937	-3.074377
C	14.281232	1.435362	-3.605463
C	14.613595	3.871996	-3.612141
C	12.131046	6.726916	-1.769919
H	11.025969	4.961148	-1.185847
C	14.133313	6.396962	-3.106419
C	15.440944	1.317388	-4.367867
H	13.707647	0.561028	-3.317661
C	15.776149	3.723973	-4.377821
C	13.242590	7.245899	-2.456069
H	11.452098	7.406134	-1.262547
H	14.995894	6.799760	-3.629757
C	16.185278	2.446932	-4.749919
H	15.774276	0.329971	-4.673684
H	16.349357	4.596070	-4.679517
C	14.057736	-3.545597	2.391683
C	12.972045	-2.953468	4.292878
C	14.435257	-3.762727	1.063805
C	14.833867	-4.031625	3.475373
C	12.080651	-2.423883	5.229993
C	14.140774	-3.653536	4.689257
C	15.615439	-4.465676	0.832884
H	13.829034	-3.399018	0.241332
C	16.016351	-4.733897	3.214247
C	12.368687	-2.618333	6.578928
H	11.197602	-1.876918	4.918007
C	14.405422	-3.834340	6.051892
C	16.402447	-4.945411	1.894071
H	15.931297	-4.646582	-0.190413
H	16.622588	-5.111693	4.032730
C	13.516402	-3.317992	6.989935
H	11.691567	-2.216948	7.327308
H	15.295696	-4.368172	6.372176
N	12.765414	3.116773	-2.483385
N	12.929328	-2.892251	2.896868
N	-12.929410	2.891861	2.897212
N	-12.765310	-3.116447	-2.483843
H	-17.085671	-2.318946	-5.343161
H	-13.711094	3.451335	8.049943
H	-17.318370	5.487193	1.680075
H	-13.407700	-8.318422	-2.475340
H	13.710818	-3.452661	8.049526
H	17.318222	-5.487551	1.679426
H	13.407659	8.318767	-2.474628
H	17.086027	2.319525	-5.342403

Compound G3F2

H	4.344476	2.132695	-1.021593
C	7.147757	-1.831539	-1.155467
C	7.636624	-0.594998	-0.710231
C	6.757806	0.463644	-0.434522
C	5.396057	0.268779	-0.619521
C	4.899715	-0.976682	-1.061748
C	5.778227	-2.030465	-1.324612
H	7.850353	-2.628285	-1.376761
H	7.152516	1.408955	-0.074279
H	5.410181	-2.992134	-1.669262
C	4.250152	1.234753	-0.397031
H	4.205383	1.583335	0.643078

C	3.037937	0.405508	-0.771667
C	1.696803	0.759087	-0.764113
C	0.719504	-0.180236	-1.148172
C	1.137060	-1.470210	-1.532743
C	2.481642	-1.832500	-1.538404
C	3.439025	-0.890484	-1.156237
H	1.391424	1.749323	-0.438310
H	0.392797	-2.190184	-1.858206
H	2.772699	-2.832272	-1.847707
H	-4.205613	-1.582630	0.643229
C	-1.137260	1.470553	-1.533084
C	-0.719698	0.180666	-1.148226
C	-1.696998	-0.758592	-0.764015
C	-3.038137	-0.405032	-0.771693
C	-3.439231	0.890872	-1.156545
C	-2.481846	1.832823	-1.538869
H	-0.392997	2.190470	-1.858674
H	-1.391620	-1.748758	-0.438000
H	-2.772904	2.832529	-1.848387
C	-4.250352	-1.234226	-0.396940
H	-4.344641	-2.132275	-1.021353
C	-5.396263	-0.268313	-0.619659
C	-6.758018	-0.463160	-0.434680
C	-7.636834	0.595410	-0.710659
C	-7.147980	1.831861	-1.156143
C	-5.778444	2.030776	-1.325271
C	-4.899929	0.977064	-1.062133
H	-7.152738	-1.408404	-0.074273
H	-7.850589	2.628543	-1.377628
H	-5.410395	2.992376	-1.670113
C	9.832873	0.513549	-1.216900
C	9.857539	-1.136227	0.331407
C	9.469776	1.439973	-2.198563
C	11.177642	0.381607	-0.783107
C	9.515173	-2.146293	1.234901
C	11.193170	-0.672833	0.208275
C	10.469950	2.239906	-2.739508
H	8.444824	1.524264	-2.541480
C	12.165739	1.209465	-1.324761
C	10.531743	-2.704849	2.001320
H	8.492323	-2.492293	1.331478
C	12.198169	-1.233856	1.002126
C	11.806954	2.134627	-2.304688
H	10.229218	2.956359	-3.517854
H	13.197749	1.145064	-0.995156
C	11.863407	-2.254735	1.891337
H	10.307176	-3.505594	2.698039
H	13.223548	-0.883039	0.944451
C	-9.833093	-0.513085	-1.217406
C	-9.857730	1.136498	0.331098
C	-9.469991	-1.439434	-2.199134
C	-11.177844	-0.381252	-0.783519
C	-9.515338	2.146489	1.234667
C	-11.193354	0.673067	0.207990
C	-10.470144	-2.239403	-2.740067
H	-8.445048	-1.523642	-2.542100
C	-12.165916	-1.209150	-1.325158
C	-10.531877	2.704921	2.001218
H	-8.492490	2.492510	1.331199
C	-12.198320	1.233985	1.001957
C	-11.807130	-2.134238	-2.305158
H	-10.229404	-2.955793	-3.518468
H	-13.197906	-1.144852	-0.995471
C	-11.863529	2.254771	1.891261
H	-10.307299	3.505583	2.698029
H	-13.223699	0.883162	0.944306
N	9.040209	-0.411746	-0.536966
N	-9.040435	0.412167	-0.537416
C	12.926880	-2.814859	4.096039
C	13.964846	-3.588710	2.239365
C	12.069232	-2.182004	4.999828
C	14.065558	-3.537473	4.536625
C	14.324363	-3.914739	0.929023
C	14.729827	-4.031677	3.349003
C	12.351633	-2.300161	6.356226
H	11.203944	-1.624871	4.658310
C	14.344654	-3.625810	5.903859
C	15.463286	-4.689926	0.740300
H	13.727653	-3.588752	0.084329
C	15.885875	-4.789034	3.136984
C	13.480159	-3.013050	6.811447
H	11.694992	-1.842319	7.088381
H	15.220687	-4.153802	6.266391
C	16.247455	-5.120280	1.830753
H	15.760130	-4.981365	-0.261569
H	16.502308	-5.118317	3.967142
C	13.882549	2.562948	-3.655813
C	12.838567	4.372806	-2.785762
C	14.250508	1.271558	-4.042218
C	14.628241	3.698931	-4.063515
C	11.982196	5.238974	-2.100800
C	13.960140	4.856808	-3.507559
C	15.378538	1.128528	-4.842550
H	13.668024	0.407328	-3.742818
C	15.773601	3.532057	-4.848037
C	12.248720	6.602227	-2.164263
H	11.129934	4.863940	-1.545090
C	14.223397	6.229613	-3.541085
C	16.143629	2.245005	-5.239358
H	15.681508	0.143204	-5.180396
H	16.375757	4.382090	-5.152011
C	13.360279	7.100221	-2.875102

H	11.592931	7.306703	-1.663697
H	15.086437	6.624528	-4.067273
C	-12.838406	-4.372502	-2.786523
C	-13.882956	-2.562651	-3.655913
C	-11.981748	-5.238665	-2.101912
C	-13.960016	-4.856566	-3.508218
C	-14.251267	-1.271253	-4.041961
C	-14.628482	-3.698694	-4.063744
C	-12.248017	-6.601953	-2.165638
H	-11.129453	-4.863602	-1.546274
C	-14.223027	-6.229412	-3.541995
C	-15.379483	-1.128280	-4.842040
H	-13.668905	-0.406964	-3.742497
C	-15.774031	-3.531887	-4.848003
C	-13.359619	-7.100008	-2.876372
H	-11.591985	-7.306412	-1.665368
H	-15.086106	-6.624365	-4.068091
C	-16.144417	-2.244827	-5.238960
H	-15.682710	-0.142943	-5.179616
H	-16.376056	-4.381988	-5.152048
C	-13.964752	3.589002	2.239590
C	-12.927103	2.814286	4.096073
C	-14.324101	3.915527	0.929328
C	-14.729734	4.031746	3.349318
C	-12.069639	2.180957	4.999704
C	-14.065669	3.536980	4.536823
C	-15.462852	4.691005	0.740768
H	-13.727385	3.589694	0.084578
C	-15.885616	4.789401	3.137454
C	-12.352129	2.298681	6.356121
H	-11.204420	1.623798	4.658051
C	-14.344861	3.624874	5.904066
C	-16.247023	5.121151	1.831302
H	-15.759549	4.982838	-0.261030
H	-16.502073	5.118510	3.967662
C	-13.480560	3.011615	6.811504
H	-11.695632	1.840457	7.088166
H	-15.220821	4.152902	6.266722
N	-12.799141	-2.981010	-2.881721
N	-12.873418	2.851329	2.701990
N	12.873309	-2.851438	2.701929
N	12.798982	2.981352	-2.881302
C	13.850500	9.319107	-1.805235
C	13.602562	9.302656	-4.059238
C	13.964445	8.970640	-0.456674
C	14.021166	10.656964	-2.245935
C	13.376430	8.941872	-5.390201
C	13.862873	10.646465	-3.685387
C	14.239038	9.988458	0.453836
H	13.848459	7.942737	-0.130543
C	14.296117	11.659934	-1.308869
C	13.427491	9.948845	-6.351303
H	13.166761	7.913775	-5.664837
C	13.909748	11.638092	-4.672428
C	14.401005	11.320979	0.036889
H	14.332688	9.743698	1.507875
H	14.429406	12.689213	-1.629751
C	13.693864	11.283773	-6.000839
H	13.256730	9.694340	-7.393288
H	14.109712	12.671474	-4.403515
H	14.613635	12.090450	0.772647
H	13.729471	12.043919	-6.775145
C	17.498047	2.579960	-7.329241
C	18.422016	1.296623	-5.703468
C	16.648027	3.374806	-8.102996
C	18.765864	2.160531	-7.808627
C	18.692011	0.601918	-4.521240
C	19.355786	1.341018	-6.770729
C	17.092414	3.759411	-9.365912
H	15.674448	3.678886	-7.734349
C	19.187544	2.562484	-9.081454
C	19.911261	-0.064981	-4.426337
H	17.979119	0.586261	-3.704022
C	20.573371	0.661281	-6.648341
C	18.349658	3.362245	-9.852834
H	16.450676	4.378318	-9.986218
H	20.155959	2.251177	-9.462800
C	20.843882	-0.040781	-5.477549
H	20.144975	-0.612725	-3.517985
H	21.299038	0.684803	-7.456400
H	18.666878	3.681485	-10.840801
H	21.784414	-0.572529	-5.371643
C	17.641091	-7.197307	2.068937
C	18.521743	-5.507988	0.838280
C	16.813624	-8.015492	2.842799
C	18.912529	-7.637514	1.618834
C	18.763226	-4.296095	0.185399
C	19.474768	-6.559041	0.832991
C	17.284624	-9.283444	3.175462
H	15.837007	-7.676254	3.170345
C	19.361216	-8.916513	1.968575
C	19.973327	-4.154539	-0.489880
H	18.035909	-3.491842	0.207241
C	20.682663	-6.389517	0.146124
C	18.546030	-9.732172	2.747608
H	16.660896	-9.937962	3.777303
H	20.332818	-9.268119	1.633153
C	20.924767	-5.188737	-0.514425
H	20.184917	-3.222391	-1.005719
H	21.422616	-7.184761	0.132363
H	18.884382	-10.725324	3.026525
H	21.857430	-5.046009	-1.051394

C	13.968997	-2.033213	9.072141
C	13.773841	-4.289547	8.955051
C	14.047521	-0.667809	8.784714
C	14.164816	-2.530279	10.386581
C	13.574911	-5.607882	8.536452
C	14.040165	-3.971054	10.311817
C	14.311556	0.201619	9.840519
H	13.912888	-0.298229	7.773971
C	14.428660	-1.633709	11.428740
C	13.659678	-6.612102	9.498026
H	13.360118	-5.840905	7.499200
C	14.120925	-5.000495	11.257040
C	14.497964	-0.271772	11.150799
H	14.377569	1.267701	9.643588
H	14.580757	-1.997911	12.440859
C	13.932502	-6.316317	10.844798
H	13.510397	-7.645240	9.198013
H	14.325526	-4.773653	12.299565
H	14.701468	0.433039	11.951102
H	13.994549	-7.123191	11.568497
C	-13.969823	2.031022	9.071774
C	-13.774150	4.287356	8.955572
C	-14.048644	0.665747	8.783810
C	-14.165637	2.527620	10.386391
C	-13.574890	5.605807	8.537499
C	-14.040653	3.968398	10.312195
C	-14.312981	-0.204029	9.839253
H	-13.913994	0.296527	7.772937
C	-14.429785	1.630706	11.428178
C	-13.659504	6.609675	9.499454
H	-13.359959	5.839181	7.500354
C	-14.121264	4.997493	11.257807
C	-14.499392	0.268895	11.149702
H	-14.379228	-1.270018	9.641900
H	-14.581882	1.994551	12.440425
C	-13.932508	6.313431	10.846090
H	-13.509964	7.642894	9.199851
H	-14.326004	4.770295	12.300227
H	-14.703137	-0.436180	11.949710
H	-13.994435	7.120039	11.570097
C	-17.640374	7.198294	2.070221
C	-18.521066	5.509691	0.838606
C	-16.812931	8.015998	2.844619
C	-18.911658	7.638911	1.620083
C	-18.762629	4.298140	0.185119
C	-19.473924	6.560895	0.833632
C	-17.283799	9.283871	3.177772
H	-15.836429	7.676464	3.172204
C	-19.360216	8.917818	1.970324
C	-19.972628	4.157092	-0.490449
H	-18.035452	3.493756	0.206727
C	-20.681720	6.391886	0.146465
C	-18.545052	9.732995	2.749885
H	-16.660084	9.938013	3.780034
H	-20.331699	9.269728	1.634877
C	-20.923897	5.191454	-0.514689
H	-20.184269	3.225219	-1.006764
H	-21.421544	7.187253	0.132940
H	-18.883300	10.726072	3.029196
H	-21.856483	5.049127	-1.051898
C	-17.499140	-2.579650	-7.328659
C	-18.423023	-1.296692	-5.702533
C	-16.649141	-3.374252	-8.102686
C	-18.767073	-2.160287	-7.807789
C	-18.692946	-0.602223	-4.520148
C	-19.356941	-1.341020	-6.769666
C	-17.093668	-3.758684	-9.365605
H	-15.675467	-3.678282	-7.734250
C	-19.188899	-2.562063	-9.080624
C	-19.912262	0.064514	-4.424966
H	-17.979954	-0.586625	-3.703016
C	-20.574591	-0.661452	-6.646998
C	-18.351032	-3.361586	-9.852272
H	-16.451944	-4.377400	-9.986115
H	-20.157406	-2.250792	-9.461766
C	-20.845026	0.040383	-5.476053
H	-20.145918	0.612065	-3.516483
H	-21.300366	-0.684935	-7.454961
H	-18.668357	-3.680690	-10.840248
H	-21.785608	0.571999	-5.369927
C	-13.601943	-9.302194	-4.060965
C	-13.848720	-9.319297	-1.806835
C	-13.376613	-8.941014	-5.391959
C	-13.861606	-10.646184	-3.687318
C	-13.962099	-8.971222	-0.458122
C	-14.019158	-10.657100	-2.247790
C	-13.427822	-9.947772	-6.353279
H	-13.167426	-7.912784	-5.666462
C	-13.908649	-11.637588	-4.674573
C	-14.235868	-9.989372	0.452261
H	-13.846306	-7.943364	-0.131785
C	-14.293279	-11.660411	-1.310847
C	-13.693564	-11.282876	-6.003008
H	-13.257677	-9.692953	-7.395288
H	-14.108121	-12.671101	-4.405799
C	-14.397586	-11.321842	0.035052
H	-14.329064	-9.744919	1.506412
H	-14.426385	-12.689651	-1.631930
H	-13.729306	-12.042845	-6.777481
H	-14.609571	-12.091576	0.770723
N	13.596637	8.503860	-2.911794
N	17.297114	2.050647	-6.050577

N	17.411468	-5.903568	1.590252
N	13.732025	-3.107367	8.209597
N	-13.732544	3.105456	8.209665
N	-17.410867	5.904741	1.590969
N	-17.298086	-2.050541	-6.049925
N	-13.595712	-8.503680	-2.913323

Compound G1F3

H	8.174859	1.145026	1.808840
C	11.438853	-0.119749	-1.551743
C	11.825453	0.229996	-0.248527
C	10.865018	0.336116	0.770492
C	9.532096	0.098174	0.466075
C	9.143435	-0.265548	-0.841006
C	10.102151	-0.378346	-1.850530
H	12.195272	-0.176737	-2.327257
H	11.179620	0.590244	1.778018
H	9.817614	-0.650355	-2.862789
C	8.318646	0.147691	1.372731
H	8.408310	-0.549661	2.216011
C	7.187266	-0.231832	0.437841
C	5.831148	-0.349719	0.703413
C	4.939480	-0.708566	-0.327117
C	5.458993	-0.940714	-1.616408
C	6.819621	-0.822254	-1.889911
C	7.691025	-0.465833	-0.858550
H	5.445455	-0.140295	1.697215
H	4.783094	-1.245446	-2.409378
H	7.190493	-1.016064	-2.892518
H	-8.186474	1.088881	1.792754
C	-5.457540	-1.000860	-1.619134
C	-4.939641	-0.755718	-0.331629
C	-5.833554	-0.396103	0.696584
C	-7.190673	-0.291130	0.430800
C	-7.693066	-0.538368	-0.863679
C	-6.819161	-0.894707	-1.892985
H	-4.779244	-1.305390	-2.410166
H	-5.448877	-0.176043	1.688495
H	-7.188732	-1.097431	-2.894310
C	-8.324205	0.087928	1.363120
H	-8.409687	-0.604486	2.210936
C	-9.537466	0.023141	0.457334
C	-10.868052	0.283442	0.753255
C	-11.828872	0.155614	-0.262665
C	-11.443423	-0.221242	-1.558484
C	-10.103691	-0.462865	-1.858445
C	-9.146636	-0.345489	-0.847778
H	-11.178294	0.592670	1.746639
H	-12.205751	-0.331790	-2.322381
H	-9.819071	-0.751889	-2.865952
C	13.715486	1.643003	0.611960
C	14.252967	-0.410945	-0.190580
C	13.057670	2.817979	0.986624
C	15.120637	1.503557	0.747518
C	14.226700	-1.706675	-0.713933
C	15.463315	0.192843	0.236515
C	13.826784	3.849780	1.519899
H	11.986112	2.926952	0.861585
C	15.869306	2.555989	1.286956
C	15.437756	-2.386353	-0.822801
H	13.296006	-2.170489	-1.021084
C	16.666185	-0.512806	0.115646
C	15.217909	3.723154	1.674171
H	13.337956	4.772265	1.819352
H	16.946008	2.463071	1.397181
C	16.647944	-1.798161	-0.417214
H	15.442989	-3.394036	-1.227917
H	17.600978	-0.062883	0.437877
C	-13.958954	-0.221059	1.013137
C	-14.010761	1.344320	-0.629227
C	-13.594859	-1.241203	1.896440
C	-15.273118	0.312735	0.995832
C	-13.691084	2.231654	-1.660706
C	-15.305714	1.312569	-0.051039
C	-14.564335	-1.709925	2.780141
H	-12.594171	-1.658919	1.891286
C	-16.227527	-0.176238	1.895465
C	-14.696163	3.079446	-2.120622
H	-12.694295	2.263674	-2.086410
C	-16.297049	2.175388	-0.532922
C	-15.867268	-1.183175	2.785883
H	-14.305399	-2.501937	3.476754
H	-17.237796	0.223060	1.894419
C	-15.988091	3.052666	-1.567981
H	-14.472580	3.777133	-2.922381
H	-17.293571	2.162030	-0.100652
N	13.194866	0.475932	0.040968
N	-13.197843	0.409981	0.022763
H	-0.007463	0.888461	-1.870856
C	-3.016558	-1.398228	1.155139
C	-3.484815	-0.872148	-0.065266
C	-2.541421	-0.457021	-1.026321
C	-1.185008	-0.570587	-0.761319
C	-0.731713	-1.098878	0.465888
C	-1.655406	-1.514065	1.427733
H	-3.736493	-1.746457	1.889388
H	-2.884395	-0.022598	-1.961243
H	-1.325217	-1.932019	2.374590
C	-0.002123	-0.181959	-1.626034
H	0.001269	-0.719169	-2.583674
C	1.183527	-0.558585	-0.759791

C	2.539021	-0.431294	-1.023109
C	3.485603	-0.838364	-0.061671
C	3.021064	-1.370157	1.157725
C	1.660816	-1.498830	1.429062
C	0.734067	-1.091797	0.466667
H	2.878426	0.007454	-1.957290
H	1.333791	-1.920662	2.375301
H	3.743354	-1.712744	1.892298
H	17.574599	-2.354817	-0.517446
H	15.787622	4.545854	2.095105
H	-16.598547	-1.569767	3.489018
H	-16.748920	3.725763	-1.950991

Compound G2F3

H	8.169509	0.316830	1.404543
C	11.454011	-0.233253	-2.128377
C	11.830199	-0.157523	-0.779357
C	10.866490	-0.260349	0.235859
C	9.535280	-0.429747	-0.117782
C	9.154384	-0.515357	-1.474534
C	10.118262	-0.420949	-2.481189
H	12.216155	-0.134603	-2.894394
H	11.176655	-0.216730	1.275588
H	9.839177	-0.480013	-3.528990
C	8.317211	-0.568833	0.772666
H	8.403560	-1.425310	1.454069
C	7.191864	-0.747390	-0.227021
C	5.834708	-0.919895	0.001236
C	4.949483	-1.056838	-1.086337
C	5.475222	-1.013434	-2.393258
C	6.836895	-0.839961	-2.629019
C	7.702047	-0.706426	-1.541012
H	5.443491	-0.923239	1.014681
H	4.803437	-1.146647	-3.235412
H	7.213064	-0.820700	-3.648003
H	-8.183127	0.187974	1.377887
C	-5.447040	-1.051831	-2.422112
C	-4.928915	-1.106978	-1.112518
C	-5.822984	-0.995324	-0.029191
C	-7.180725	-0.837263	-0.263991
C	-7.682786	-0.781969	-1.580580
C	-6.808884	-0.889412	-2.664486
H	-4.768861	-1.166404	-3.261850
H	-5.438683	-1.007442	0.986802
H	-7.178442	-0.859084	-3.685622
C	-8.314850	-0.689136	0.730767
H	-8.394349	-1.557682	1.397616
C	-9.528855	-0.552423	-0.165633
C	-10.861333	-0.380403	0.181737
C	-11.820871	-0.279314	-0.837901
C	-11.436075	-0.341524	-2.185346
C	-10.094417	-0.494682	-2.532159
C	-9.137293	-0.606304	-1.520905
H	-11.172521	-0.312369	1.219761
H	-12.198401	-0.279571	-2.954892
H	-9.808802	-0.539771	-3.578904
C	13.725416	1.086370	0.302092
C	14.248837	-0.836242	-0.773406
C	13.076368	2.203644	0.834933
C	15.126273	0.909830	0.439756
C	14.215814	-2.043815	-1.476269
C	15.460742	-0.319617	-0.247225
C	13.845932	3.140865	1.515132
H	12.009335	2.348230	0.708720
C	15.879039	1.851341	1.148307
C	15.416596	-2.718132	-1.668319
H	13.286785	-2.440815	-1.869533
C	16.654445	-1.023568	-0.432228
C	15.235469	2.967857	1.682517
H	13.379132	4.031234	1.922790
H	16.947694	1.726073	1.289340
C	16.629939	-2.218985	-1.151062
H	15.432216	-3.646615	-2.229140
H	17.590774	-0.661524	-0.020115
C	-13.954577	-0.974013	0.290966
C	-14.010543	0.950112	-0.901943
C	-13.588930	-2.180188	0.895158
C	-15.273566	-0.463573	0.400536
C	-13.696207	2.070799	-1.675645
C	-15.309126	0.766600	-0.361466
C	-14.557795	-2.866901	1.618448
H	-12.587351	-2.581529	0.790291
C	-16.227289	-1.156739	1.152143
C	-14.705869	2.993516	-1.925965
H	-12.700532	2.215100	-2.079454
C	-16.304576	1.717690	-0.604593
C	-15.866512	-2.360457	1.758021
H	-14.314612	-3.817266	2.081589
H	-17.235699	-0.774115	1.271329
C	-16.002125	2.825884	-1.396287
H	-14.503728	3.861761	-2.544047
H	-17.298758	1.611020	-0.183049
N	13.200900	0.023473	-0.436398
N	-13.194351	-0.110869	-0.501676
C	18.092395	-4.248634	-0.932284
C	18.960942	-2.478586	-2.052838
C	17.280600	-5.110041	-0.189164
C	19.397290	-4.624346	-1.343582
C	19.166811	-1.249281	-2.684791
C	19.951699	-3.494244	-2.059366
C	17.790135	-6.367223	0.127134

H	16.290129	-4.808621	0.133956
C	19.883861	-5.894276	-1.011970
C	20.390950	-1.043254	-3.316736
H	18.399088	-0.483233	-2.685652
C	21.173475	-3.259671	-2.701205
C	19.076673	-6.760366	-0.280352
H	17.179025	-7.055683	0.703541
H	20.880654	-6.197605	-1.319452
C	21.387803	-2.034203	-3.324924
H	20.576045	-0.095706	-3.814282
H	21.942717	-4.026686	-2.714221
C	17.029198	4.717151	1.879273
C	15.783892	4.312843	3.730781
C	17.570026	4.725445	0.590735
C	17.509312	5.585121	2.893771
C	14.870910	3.807664	4.660538
C	16.714095	5.327076	4.076064
C	18.614302	5.610348	0.332720
H	17.187879	4.068147	-0.182667
C	18.560569	6.463884	2.606932
C	14.891177	4.344977	5.945552
H	14.173372	3.021763	4.391896
C	16.712170	5.849128	5.374889
C	19.109601	6.470303	1.328201
H	19.052577	5.635300	-0.660723
H	18.940239	7.133945	3.373107
C	15.798634	5.357283	6.302535
H	14.191325	3.969822	6.686636
H	17.417794	6.626177	5.655017
C	-16.713890	-3.421310	3.870546
C	-18.030082	-3.608419	2.033204
C	-15.700649	-3.104697	4.779562
C	-17.861782	-4.157761	4.261955
C	-18.563340	-3.554066	0.742626
C	-18.702244	-4.276961	3.088805
C	-15.844951	-3.550795	6.091239
H	-14.834053	-2.527899	4.475324
C	-17.980790	-4.593684	5.586815
C	-19.793675	-4.169566	0.524115
H	-18.036329	-3.052834	-0.061874
C	-19.937931	-4.886438	2.841141
C	-16.970151	-4.290462	6.494297
H	-15.071123	-3.318007	6.816999
H	-18.853253	-5.158762	5.902494
C	-20.478787	-4.827310	1.560306
H	-20.230033	-4.140415	-0.470052
H	-20.465589	-5.401437	3.638960
C	-18.215960	3.552066	-2.335072
C	-16.945617	5.153702	-1.352710
C	-18.710737	2.358441	-2.867471
C	-18.940512	4.767853	-2.433966
C	-15.948396	5.858755	-0.673078
C	-18.129723	5.790320	-1.806386
C	-19.955106	2.394743	-3.492362
H	-18.144433	1.436060	-2.799164
C	-20.189195	4.775326	-3.066749
C	-16.146521	7.221815	-0.465081
H	-15.053274	5.361428	-0.315757
C	-18.302498	7.161486	-1.583901
C	-20.691439	3.587989	-3.590761
H	-20.362130	1.479849	-3.912986
H	-20.756821	5.697857	-3.149697
C	-17.308539	7.871061	-0.916548
H	-15.386126	7.792227	0.060379
H	-19.203341	7.663739	-1.925109
N	-16.823653	-3.092127	2.516488
N	-17.005839	3.795211	-1.677551
N	17.835329	-2.945134	-1.367009
N	15.981715	3.948316	2.395984
H	0.003867	0.845048	-2.242812
C	-3.005662	-2.065603	0.191537
C	-3.473819	-1.278362	-0.879176
C	-2.530768	-0.656428	-1.721811
C	-1.174234	-0.825403	-1.488269
C	-0.721412	-1.615125	-0.410485
C	-1.644653	-2.237669	0.432483
H	-3.725175	-2.572054	0.827401
H	-2.873404	-0.023504	-2.535728
H	-1.314392	-2.857564	1.261225
C	0.009185	-0.252972	-2.243414
H	0.013257	-0.562502	-3.296901
C	1.194420	-0.813635	-1.482327
C	2.550420	-0.631605	-1.709249
C	3.494952	-1.242303	-0.860203
C	3.029498	-2.032011	0.209742
C	1.669015	-2.218579	0.442977
C	0.744065	-1.607221	-0.406306
H	2.891406	0.002992	-2.522598
H	1.340579	-2.840595	1.270850
H	3.751138	-2.528898	0.850771
H	22.331846	-1.840212	-3.824725
H	19.443245	-7.748022	-0.017968
H	19.926358	7.146223	1.094388
H	15.787289	5.755084	7.312632
H	-17.431135	8.935038	-0.738815
H	-21.437248	-5.294706	1.356502
H	-17.051096	-4.624102	7.524248
H	-21.659468	3.581281	-4.082203

Compound G3F3

H	8.155801	-0.131070	0.812729

C	11.459195	-0.591993	-2.716762	H	13.258483	-2.867389	-2.399093
C	11.827048	-0.551964	-1.364512	C	16.638758	-1.467735	-0.969320
C	10.859484	-0.679326	-0.356246	C	15.245178	2.571954	1.075625
C	9.529806	-0.838584	-0.720587	H	13.398327	3.661135	1.279695
C	9.156238	-0.888169	-2.081417	H	16.948695	1.305202	0.722921
C	10.124816	-0.768260	-3.080916	C	16.600063	-2.673287	-1.669299
H	12.225810	-0.475939	-3.475989	H	15.391550	-4.107811	-2.726791
H	11.164974	-0.662137	0.685750	H	17.579236	-1.110344	-0.562261
H	9.850617	-0.800150	-4.131093	C	-13.977234	-1.402838	-0.490508
C	8.306927	-1.000268	0.159194	C	-13.974619	0.625423	-1.492373
H	8.389764	-1.873887	0.818874	C	-13.640623	-2.667041	0.001922
C	7.187324	-1.152847	-0.851106	C	-15.285443	-0.872827	-0.341466
C	5.829014	-1.332417	-0.634946	C	-13.621710	1.804363	-2.154996
C	4.950373	-1.441548	-1.730820	C	-15.282921	0.426029	-0.980014
C	5.483092	-1.362949	-3.033461	C	-14.630097	-3.396224	0.651271
C	6.845680	-1.182158	-3.257000	H	-12.645305	-3.075494	-0.131205
C	7.704313	-1.077109	-2.160697	C	-16.261231	-1.613494	0.332555
H	5.431925	-1.363211	0.375689	C	-14.601286	2.777419	-2.316583
H	4.816001	-1.474396	-3.882413	H	-12.619487	1.955037	-2.539747
H	7.227537	-1.135570	-4.272955	C	-16.248004	1.426219	-1.132686
H	-8.186971	-0.285468	0.718252	C	-15.929066	-2.875699	0.823816
C	-5.440273	-1.397231	-3.114223	H	-14.411725	-4.389741	1.028477
C	-4.926953	-1.497780	-1.805179	H	-17.263320	-1.223642	0.479799
C	-5.824622	-1.422203	-0.721838	C	-15.904082	2.596972	-1.808144
C	-7.181260	-1.253778	-0.955994	H	-14.369539	3.696247	-2.844734
C	-7.677950	-1.151163	-2.271600	H	-17.247868	1.310525	-0.726917
C	-6.800679	-1.223376	-3.355737	N	13.198635	-0.382371	-1.009995
H	-4.759376	-1.484223	-3.954995	N	-13.190642	-0.488728	-1.191198
H	-5.443977	-1.469753	0.294406	C	18.068874	-4.686399	-1.359288
H	-7.166405	-1.156855	-4.376511	C	18.891430	-3.014541	-2.643589
C	-8.318463	-1.138216	0.039364	C	17.287660	-5.486808	-0.521601
H	-8.403232	-2.030038	0.674058	C	19.348973	-5.106437	-1.804233
C	-9.528409	-0.965196	-0.855929	C	19.077214	-1.835308	-3.369844
C	-10.861778	-0.800060	-0.508392	C	19.874935	-4.037005	-2.626314
C	-11.814620	-0.655905	-1.528506	C	17.794572	-6.726711	-0.148699
C	-11.426223	-0.669950	-2.875524	H	16.312027	-5.158930	-0.180309
C	-10.083819	-0.818921	-3.222172	C	19.850891	-6.346869	-1.398753
C	-9.132051	-0.972125	-2.211167	C	20.262283	-1.690071	-4.082568
H	-11.178328	-0.769674	0.529958	H	18.315932	-1.063482	-3.392942
H	-12.185136	-0.572521	-3.644986	C	21.070655	-3.861221	-3.329807
H	-9.793373	-0.826615	-4.268436	C	19.066995	-7.158221	-0.577809
C	13.729298	0.686563	-0.287802	H	17.206486	-7.385009	0.481926
C	14.236953	-1.259324	-1.323322	H	20.836516	-6.682401	-1.704587
C	13.086618	1.818952	0.220262	C	21.258457	-2.688380	-4.061764
C	15.127248	0.496462	-0.134400	H	20.430914	-0.798623	-4.677337
C	14.191154	-2.477266	-2.007747	H	21.848746	-4.617527	-3.314823
C	15.452352	-0.747930	-0.798089	C	17.052144	4.309068	1.268800
C	13.859558	2.759007	0.891978	C	15.779695	3.948934	3.106006
H	12.022173	1.971085	0.081998	C	17.617626	4.288242	-0.009116
C	15.883306	1.440747	0.567011	C	17.521161	5.197160	2.270953
C	15.384075	-3.169186	-2.182706	C	14.853156	3.467830	4.035207

C	16.706969	4.967454	3.445534	N	17.800227	-3.416925	-1.872015
C	18.664329	5.165034	-0.272115	N	15.994986	3.555984	1.783838
H	17.244514	3.622039	-0.778861	C	15.910057	4.890840	8.160686
C	18.588815	6.056244	1.993203	C	15.474643	6.938551	7.288620
C	14.848453	4.036381	5.304111	C	16.206883	3.538062	8.348069
H	14.151340	2.683240	3.775444	C	15.777189	5.782856	9.255999
C	16.701792	5.510251	4.734101	C	15.207597	8.015955	6.439684
C	19.156367	6.039143	0.719090	C	15.498955	7.090310	8.699104
H	19.115049	5.190465	-1.258636	C	16.355081	3.083169	9.656313
H	18.981854	6.728282	2.749214	H	16.322678	2.866481	7.504315
C	15.764300	5.048602	5.658481	C	15.931216	5.298450	10.560318
H	14.127596	3.704564	6.043761	C	14.975999	9.258915	7.024236
H	17.415885	6.273648	5.025531	H	15.179530	7.888362	5.363024
C	-16.853211	-4.057052	2.837589	C	15.263726	8.351315	9.259601
C	-18.075016	-4.179526	0.936578	C	16.216664	3.950157	10.753985
C	-15.891939	-3.766244	3.809291	H	16.585916	2.035979	9.828917
C	-17.993934	-4.846115	3.136388	H	15.832506	5.968318	11.409834
C	-18.553317	-4.067622	-0.371554	C	15.005454	9.429971	8.419064
C	-18.775275	-4.924733	1.920042	H	14.767582	10.112582	6.385907
C	-16.074453	-4.293083	5.083094	H	15.280176	8.484529	10.337633
H	-15.024543	-3.158074	3.577816	H	16.337859	3.562947	11.760984
C	-18.170717	-5.347636	4.429542	H	14.823344	10.413029	8.842223
C	-19.744798	-4.711966	-0.685862	C	20.189446	8.309428	0.413746
H	-18.006722	-3.510774	-1.124525	C	21.527755	6.516260	0.046077
C	-19.984219	-5.545195	1.590423	C	19.113890	9.156965	0.691979
C	-17.204491	-5.075622	5.398482	C	21.463151	8.816766	0.048059
H	-15.337315	-4.107131	5.857071	C	22.057570	5.228446	-0.070108
H	-19.045541	-5.934049	4.691171	C	22.318055	7.671527	-0.186270
C	-20.463773	-5.440668	0.284390	C	19.334177	10.529964	0.610750
H	-20.134634	-4.666431	-1.697194	H	18.140896	8.759226	0.959307
H	-20.551103	-6.101033	2.330198	C	21.656385	10.201330	-0.025119
C	-18.065415	3.518451	-2.702827	C	23.396069	5.110385	-0.437241
C	-16.781156	4.926474	-1.481359	H	21.448830	4.351868	0.123525
C	-18.585100	2.424196	-3.399694	C	23.660315	7.523170	-0.555042
C	-18.747378	4.762071	-2.662564	C	20.591334	11.050993	0.258717
C	-15.787117	5.500568	-0.684232	H	18.514768	11.210432	0.823354
C	-17.926116	5.662464	-1.881253	H	22.625362	10.606485	-0.302755
C	-19.800435	2.587965	-4.055338	C	24.191912	6.243109	-0.680754
H	-18.052927	1.480488	-3.443043	H	23.832781	4.120528	-0.533517
C	-19.978790	4.900041	-3.310412	H	24.279640	8.396950	-0.736973
C	-15.941146	6.830642	-0.309290	H	20.729871	12.126517	0.206691
H	-14.916862	4.933070	-0.373918	H	25.231594	6.115847	-0.966204
C	-18.073792	6.992051	-1.474615	C	22.902855	-3.305209	-5.857350
C	-20.500613	3.811201	-4.009062	C	23.372181	-1.455775	-4.631379
H	-20.224599	1.766940	-4.623657	C	22.312439	-4.443773	-6.412192
H	-20.531689	5.833190	-3.275710	C	24.119184	-2.776828	-6.361677
C	-17.074643	7.575814	-0.695256	C	23.364121	-0.417460	-3.695864
H	-15.177855	7.316135	0.289473	C	24.418920	-1.596011	-5.578894
H	-18.951363	7.569295	-1.747008	C	22.966566	-5.058831	-7.477155
N	-16.910782	-3.656799	1.502364	H	21.375583	-4.833401	-6.029160
N	-16.872907	3.627887	-1.985296	C	24.755765	-3.415836	-7.432142

C	24.417074	0.493806	-3.731127
H	22.567234	-0.326414	-2.965813
C	25.464957	-0.665954	-5.591429
C	24.177316	-4.555268	-7.983291
H	22.528409	-5.945938	-7.925203
H	25.688049	-3.024190	-7.829078
C	25.457283	0.376194	-4.669060
H	24.433087	1.311131	-3.016006
H	26.273749	-0.758786	-6.310725
H	24.662610	-5.060276	-8.812810
H	26.262293	1.104571	-4.670165
C	19.769035	-8.838709	1.151856
C	19.876949	-9.495909	-1.015896
C	19.606262	-8.117897	2.338055
C	20.243097	-10.176013	1.152150
C	19.799572	-9.573613	-2.409074
C	20.311737	-10.595747	-0.232008
C	19.912648	-8.762436	3.534336
H	19.258180	-7.090761	2.327391
C	20.543474	-10.799196	2.369095
C	20.178513	-10.770317	-3.012858
H	19.453789	-8.732231	-2.999647
C	20.687588	-11.786266	-0.865274
C	20.374167	-10.089916	3.554498
H	19.794719	-8.223959	4.470186
H	20.907288	-11.822674	2.386600
C	20.621201	-11.866850	-2.253014
H	20.128799	-10.855554	-4.094496
H	21.023989	-12.637068	-0.279485
H	20.603375	-10.563005	4.504399
H	20.911706	-12.784397	-2.755366
C	-17.236608	9.386281	1.037632
C	-17.273505	10.042022	-1.133149
C	-17.211763	8.651583	2.226304
C	-17.345655	10.800893	1.038618
C	-17.245773	10.092517	-2.529392
C	-17.368983	11.219575	-0.347397
C	-17.282595	9.357576	3.425016
H	-17.144619	7.569150	2.216010
C	-17.414955	11.484780	2.258045
C	-17.328869	11.344811	-3.133712
H	-17.159997	9.188343	-3.122086
C	-17.451886	12.465006	-0.981149
C	-17.380324	10.759639	3.445404
H	-17.265093	8.809942	4.362816
H	-17.498446	12.567760	2.276023
C	-17.433752	12.521157	-2.371536
H	-17.310945	11.410817	-4.217675
H	-17.526494	13.375788	-0.393702
H	-17.432994	11.279150	4.397242
H	-17.499368	13.481133	-2.874311
C	-22.016537	4.797350	-5.753033
C	-22.901209	3.195079	-4.414553
C	-21.169603	5.707188	-6.391405
C	-23.361622	4.614960	-6.166271
C	-23.120602	2.228345	-3.429594
C	-23.926698	3.591720	-5.311371
C	-21.693621	6.446916	-7.448975
H	-20.139233	5.830980	-6.076079
C	-23.862431	5.372993	-7.231339
C	-24.385532	1.648930	-3.362329
H	-22.334583	1.942598	-2.738966
C	-25.188524	2.992318	-5.221218
C	-23.026345	6.286680	-7.866110
H	-21.056031	7.161539	-7.961284
H	-24.890337	5.246703	-7.559401
C	-25.410764	2.021962	-4.248580
H	-24.582348	0.894934	-2.605668
H	-25.984566	3.283861	-5.900529
H	-23.404205	6.880868	-8.692425
H	-26.385149	1.549787	-4.169571
C	-21.939287	-7.452006	-0.016227
C	-22.825443	-5.439128	-0.569993
C	-21.097403	-8.492740	0.385031
C	-23.261144	-7.696711	-0.469973
C	-23.054496	-4.077234	-0.784670
C	-23.826996	-6.411556	-0.823441
C	-21.603767	-9.789585	0.339107
H	-20.083816	-8.297881	0.718085
C	-23.744626	-9.009960	-0.504813
C	-24.303043	-3.700038	-1.273644
H	-22.288281	-3.339075	-0.574141
C	-25.072929	-6.004202	-1.314551
C	-22.914080	-10.049790	-0.097809
H	-20.969546	-10.615858	0.646823
H	-24.754850	-9.213992	-0.848284
C	-25.303777	-4.650392	-1.539860
H	-24.505854	-2.647708	-1.450202
H	-25.850482	-6.736173	-1.514022
H	-23.278638	-11.072185	-0.119068
H	-26.265727	-4.322692	-1.921777
C	-17.402508	-6.942798	7.068084
C	-17.474121	-4.827948	7.883059
C	-17.302360	-8.072929	6.252247
C	-17.554331	-7.050572	8.474766
C	-17.504393	-3.438803	8.032503
C	-17.599992	-5.699986	8.995251
C	-17.369870	-9.321908	6.865301
H	-17.174754	-7.980586	5.179150
C	-17.620128	-8.318613	9.064196
C	-17.649360	-2.929632	9.320938
H	-17.423161	-2.780120	7.174659

C	-17.743847	-5.160723	10.279060	C	-3.472851	-1.677527	-1.572066
C	-17.529914	-9.448039	8.256076	C	-2.526538	-1.030917	-2.392090
H	-17.296218	-10.216013	6.253078	C	-1.171015	-1.206350	-2.157634
H	-17.737667	-8.418740	10.139532	C	-0.722664	-2.027102	-1.101380
C	-17.765312	-3.778016	10.435671	C	-1.649240	-2.674917	-0.281429
H	-17.676208	-1.853312	9.464107	H	-3.731004	-3.021710	0.094389
H	-17.841373	-5.814299	11.141311	H	-2.865458	-0.373812	-3.188147
H	-17.581599	-10.436603	8.701862	H	-1.322495	-3.318820	0.530168
H	-17.876309	-3.348408	11.426518	C	0.015326	-0.611353	-2.890283
N	15.725048	5.600122	6.970374	H	0.024740	-0.890582	-3.952150
N	20.237505	6.912390	0.408717	C	1.197355	-1.192567	-2.139834
N	22.456804	-2.497641	-4.806353	C	2.554202	-1.002303	-2.354515
N	19.549258	-8.433640	-0.167874	C	3.494955	-1.635307	-1.517829
N	-17.193161	8.933663	-0.284359	C	3.025447	-2.455588	-0.472976
N	-21.745753	3.931546	-4.689409	C	1.664103	-2.651221	-0.252741
N	-21.682872	-6.078819	-0.080382	C	0.742763	-2.017509	-1.089474
N	-17.354132	-5.590284	6.717718	H	2.898242	-0.344277	-3.147685
H	0.008911	0.486172	-2.858158	H	1.332450	-3.296924	0.555429
C	-3.009205	-2.496296	-0.523239	H	3.744440	-2.968993	0.157963

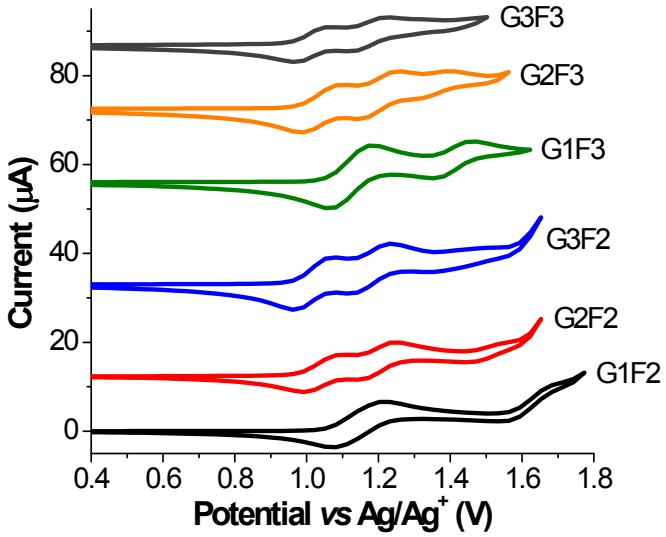


Figure SI_4 CV curves of **GnFm** measured in CH_2Cl_2/n-Bu_4NPF_6 at a scan rate of 50 mV s^{-1}.

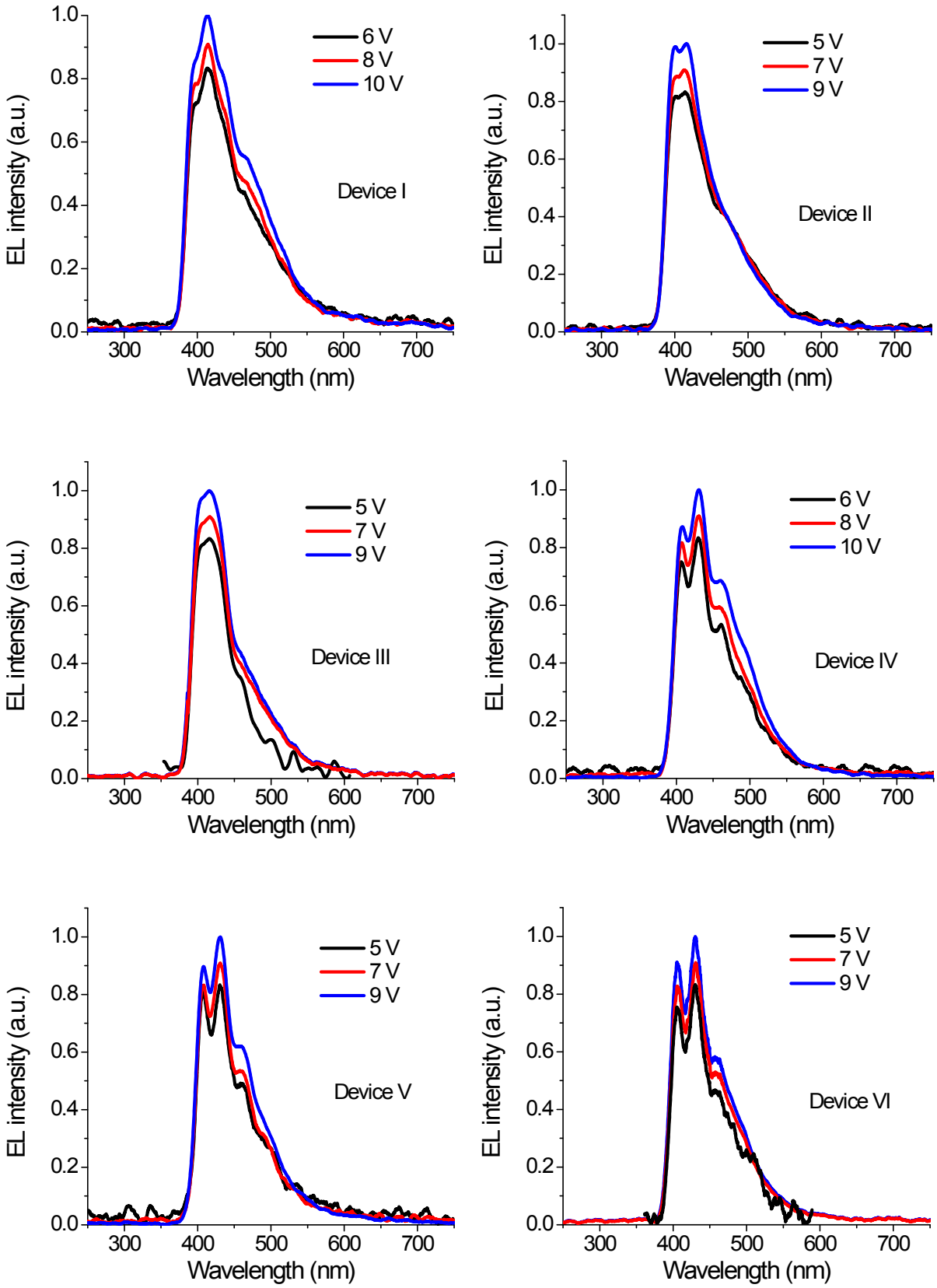


Figure SI_5. Plots of EL spectra at different applied voltages of the blue OLEDs (device I-VI).

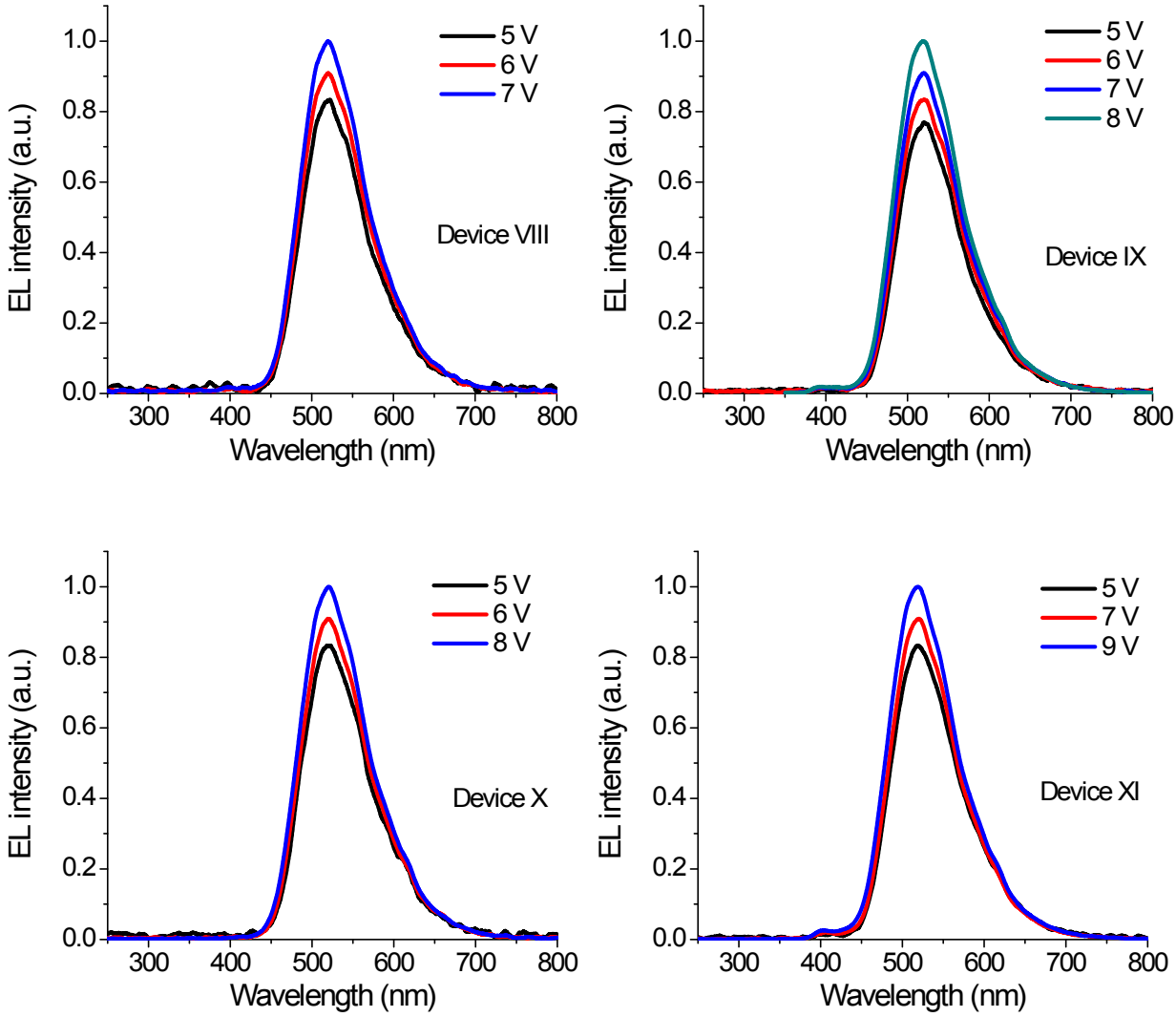
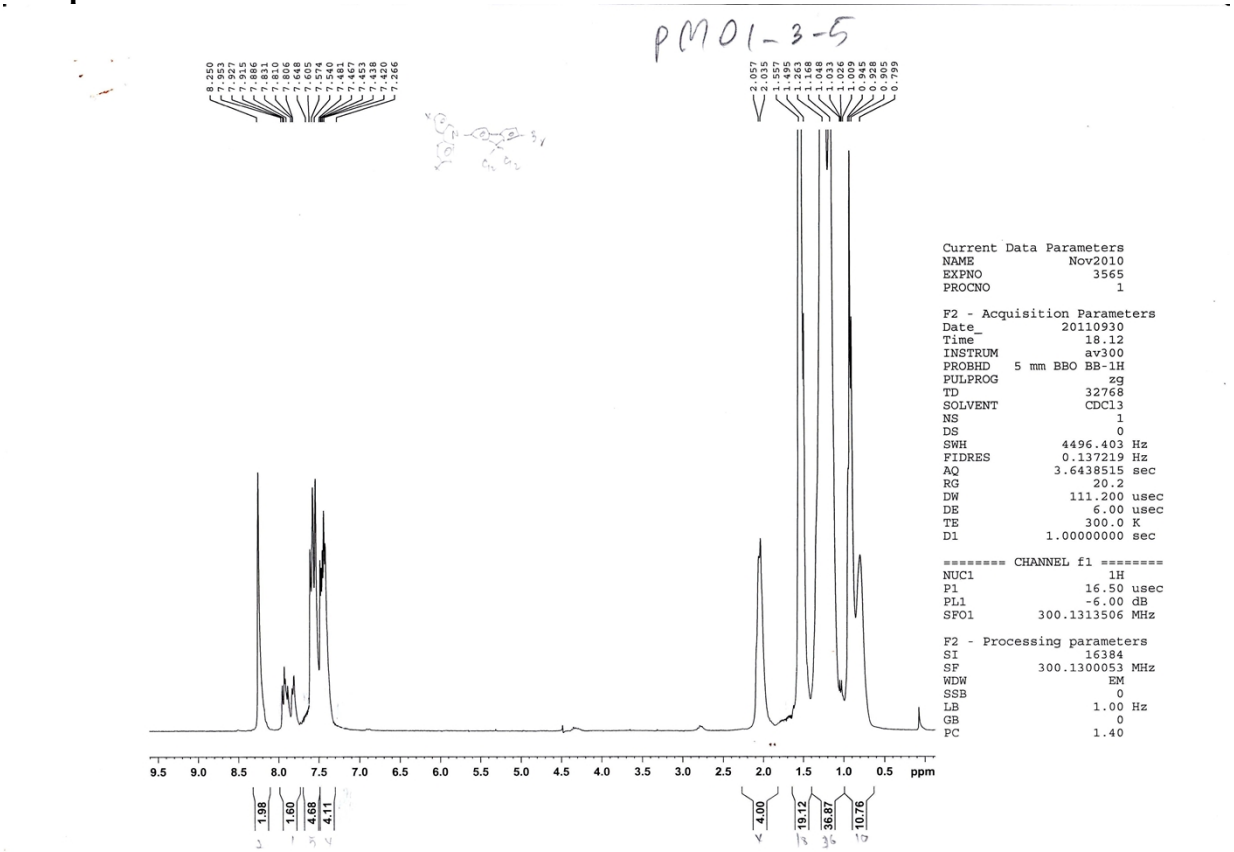
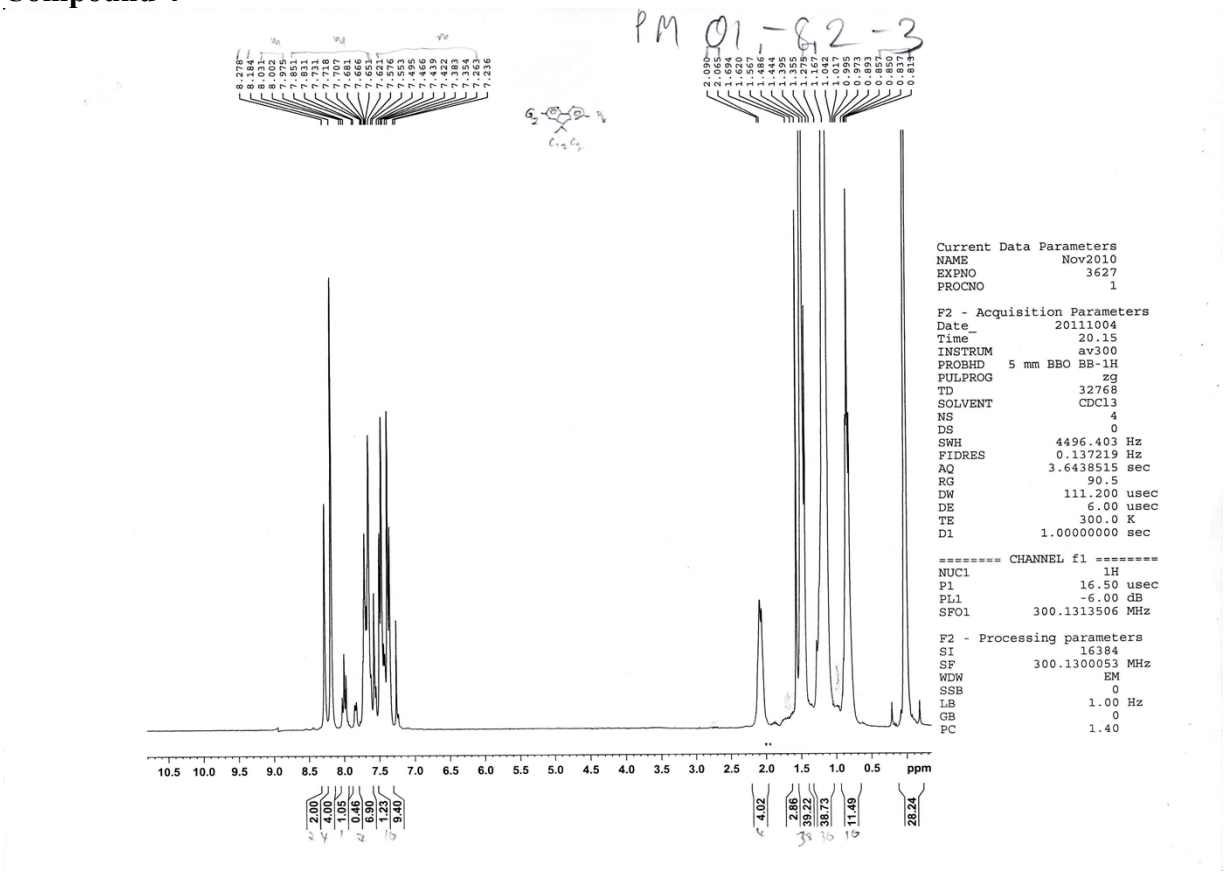


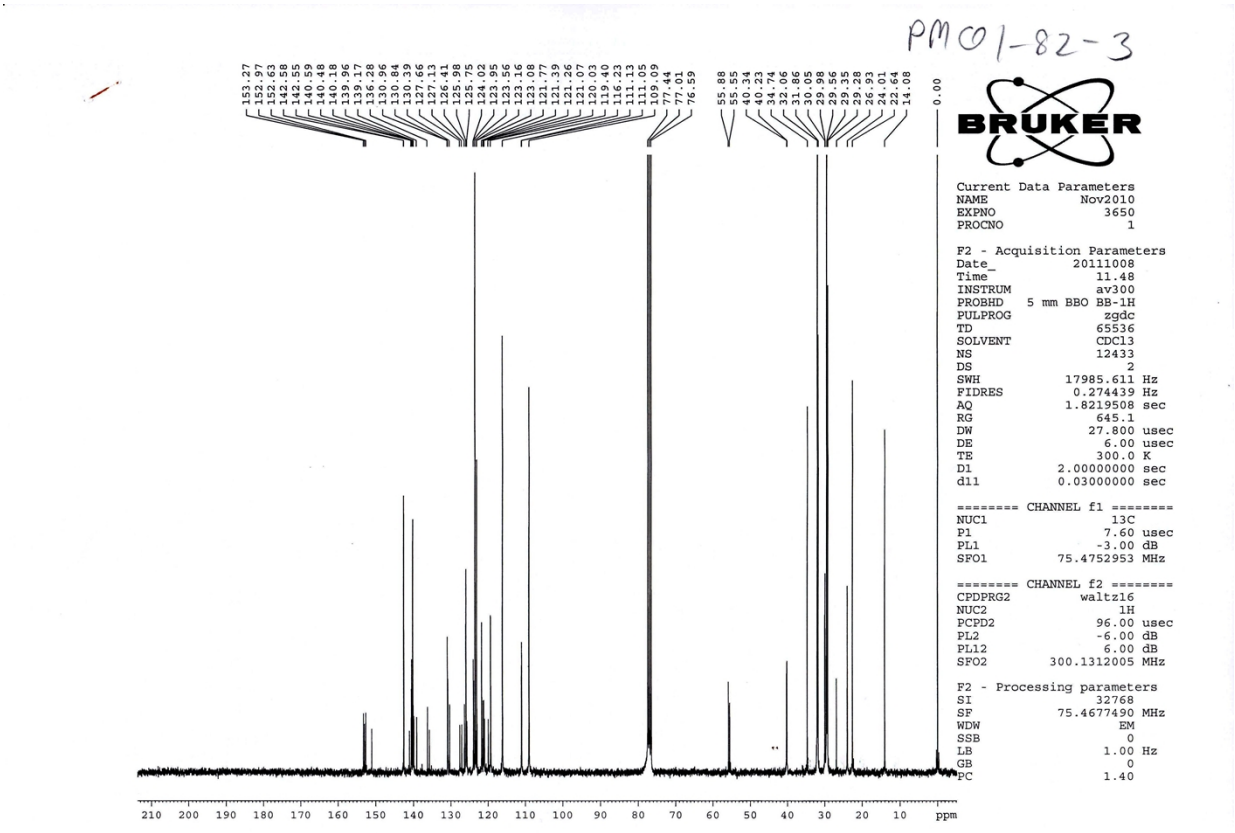
Figure SI_6. Plots of EL spectra at different applied voltages of the blue OLEDs (device I-VI).

Figure SI_6. ^{1}H-NMR and ^{13}C NMR spectra
Compound 3

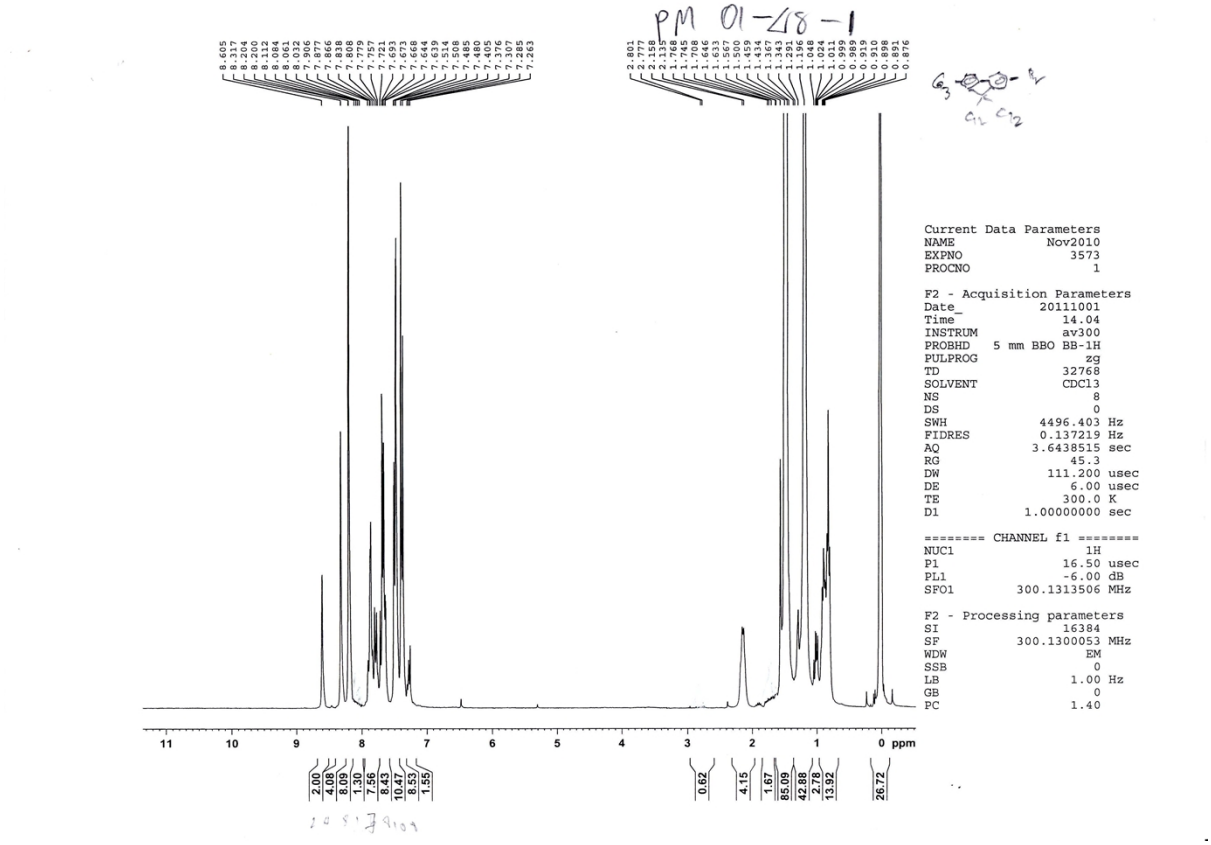


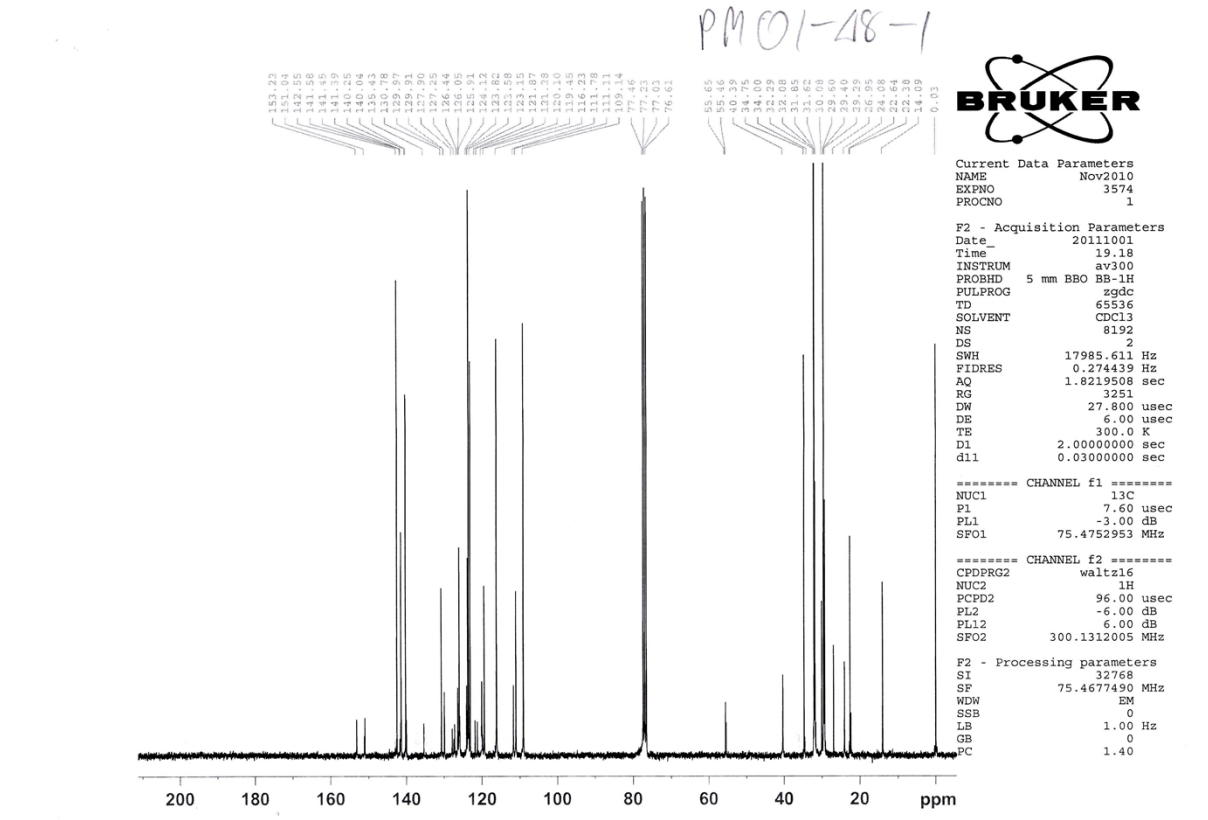
Compound 4


PM 01-82-3
Current Data Parameters
NAME Nov2010
EXPNO 3627
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111004
Time 20.15
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 90.5
DW 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 16.50 usec
PL1 -6.00 dB
SFO1 300.1313506 MHz
F2 - Processing parameters
SI 16384
SF 300.1300053 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
ppm

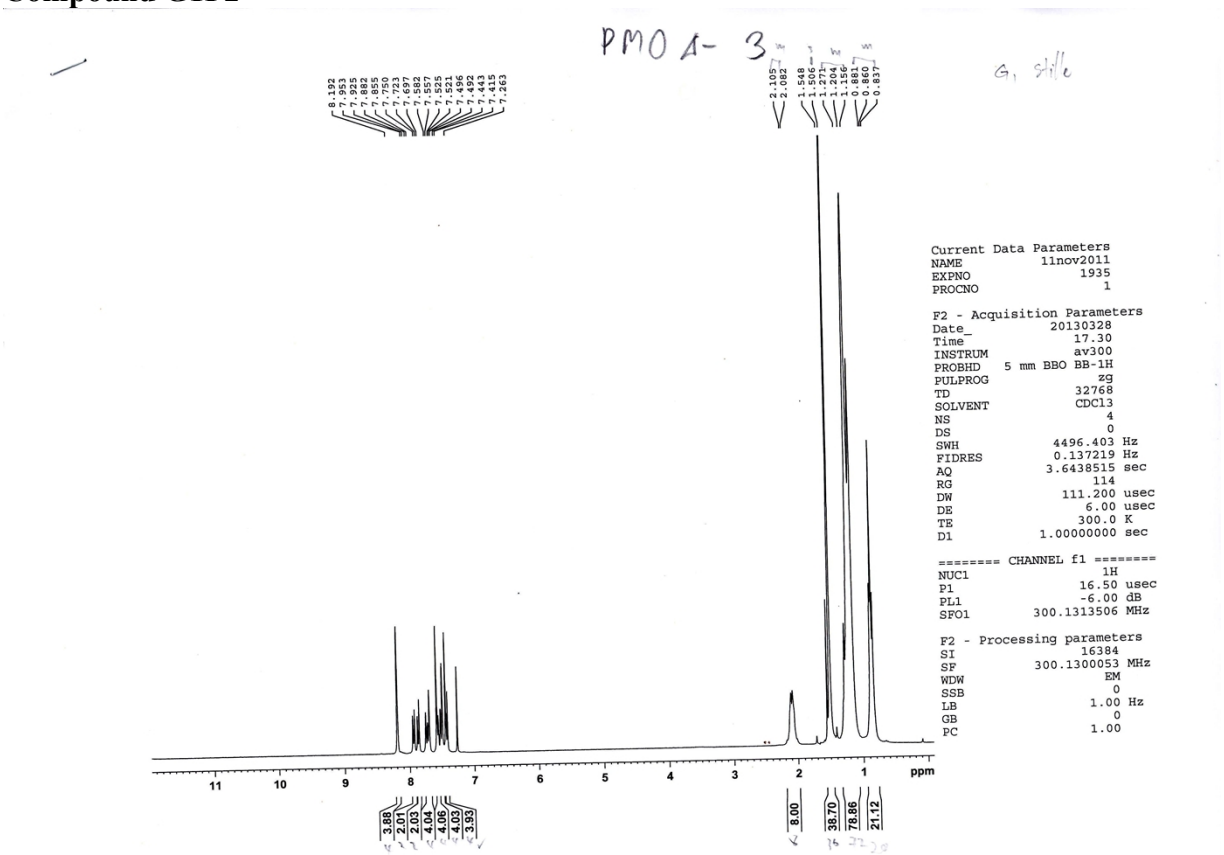

PM01-82-3
BRUKER
Current Data Parameters
NAME Nov2010
EXPNO 3650
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111008
Time 11.48
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 12433
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 645.1
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 7.60 usec
PL1 -3.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 96.00 usec
PL2 -6.00 dB
PL12 6.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
ppm

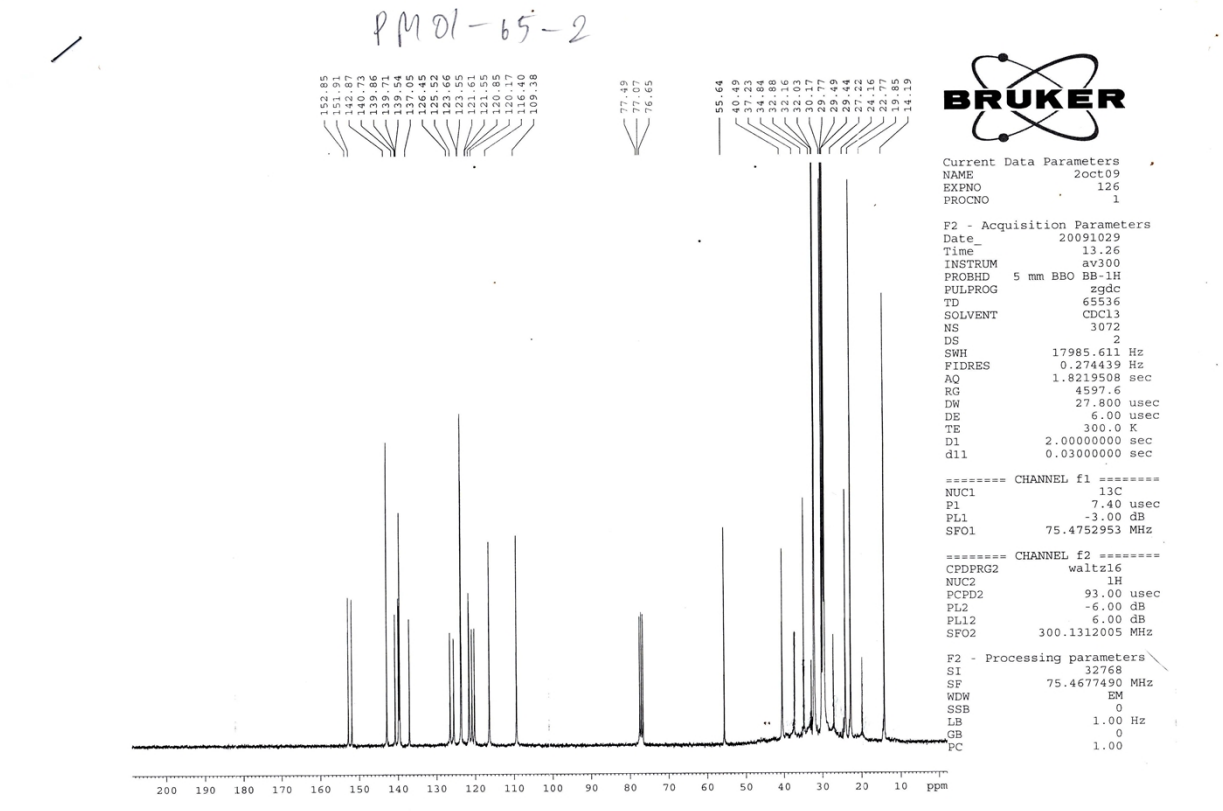
Compound 5


PM 01-18-1
Current Data Parameters
NAME Nov2010
EXPNO 3573
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111001
Time 14.04
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 45.3
DW 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 16.50 usec
PL1 -6.00 dB
SFO1 300.1313506 MHz
F2 - Processing parameters
SI 16384
SF 300.1300053 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.00 4.08 8.09 1.30 7.56 8.43 10.47 8.53 1.55
0.62 4.15 1.67 85.09 42.88 2.78 13.92 26.72

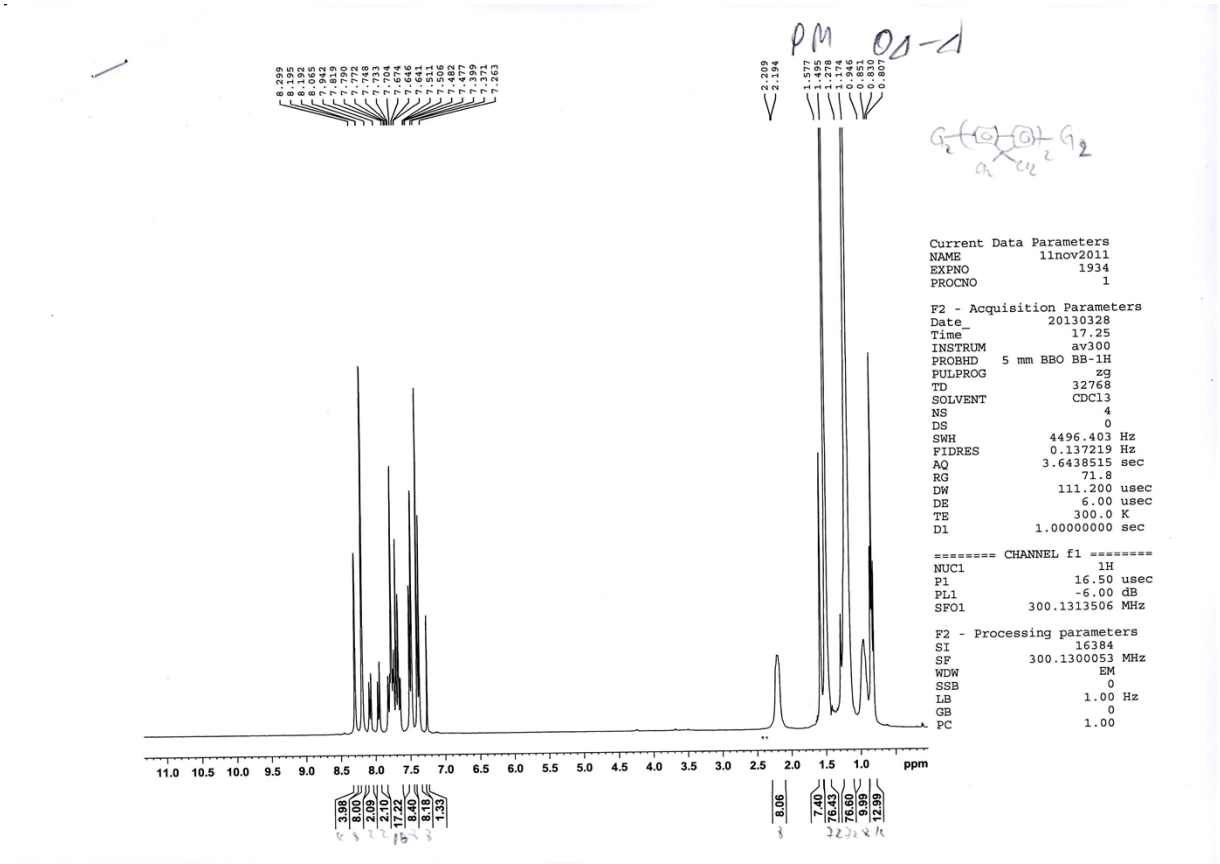

PM01-18-1
BRUKER
Current Data Parameters
NAME Nov2010
EXPNO 3574
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111001
Time 19.18
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 8192
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 3251
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 7.60 usec
PL1 -3.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 96.00 usec
PL2 -6.00 dB
PL12 6.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 ppm

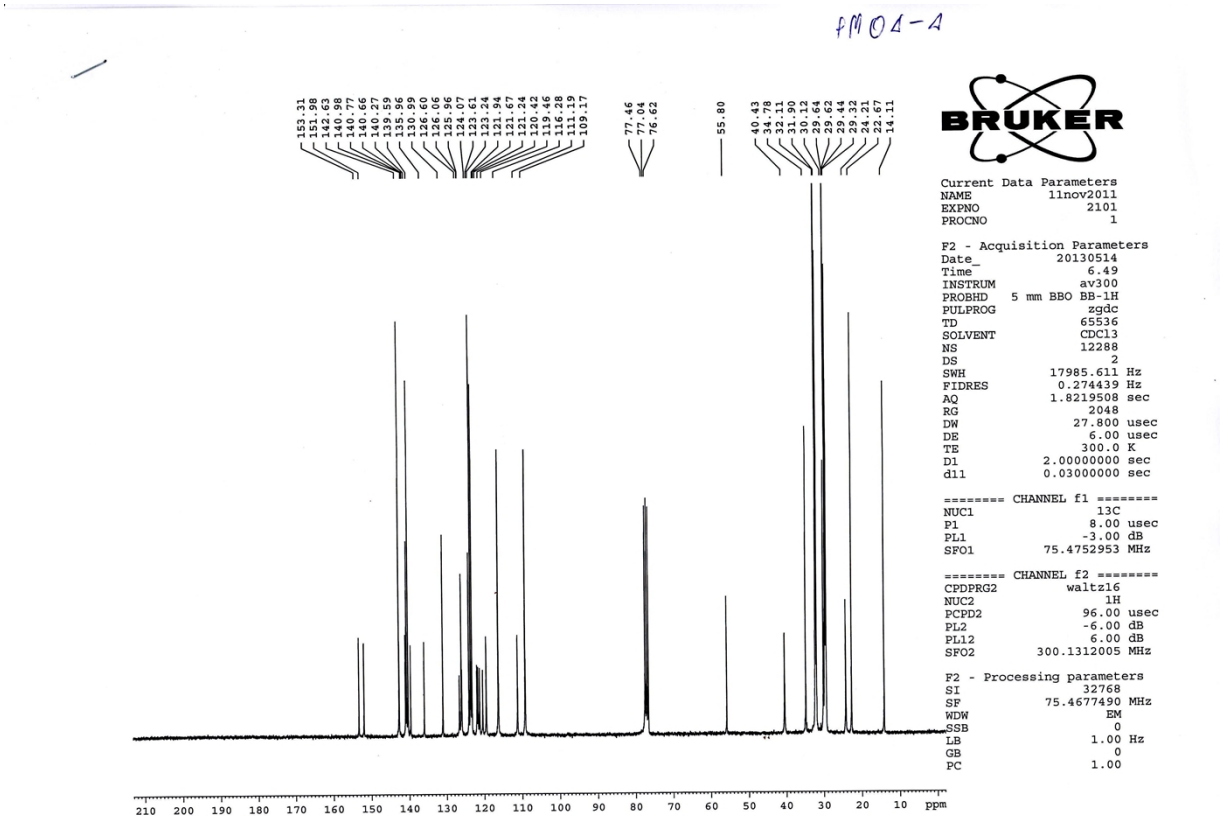
Compound G1F2



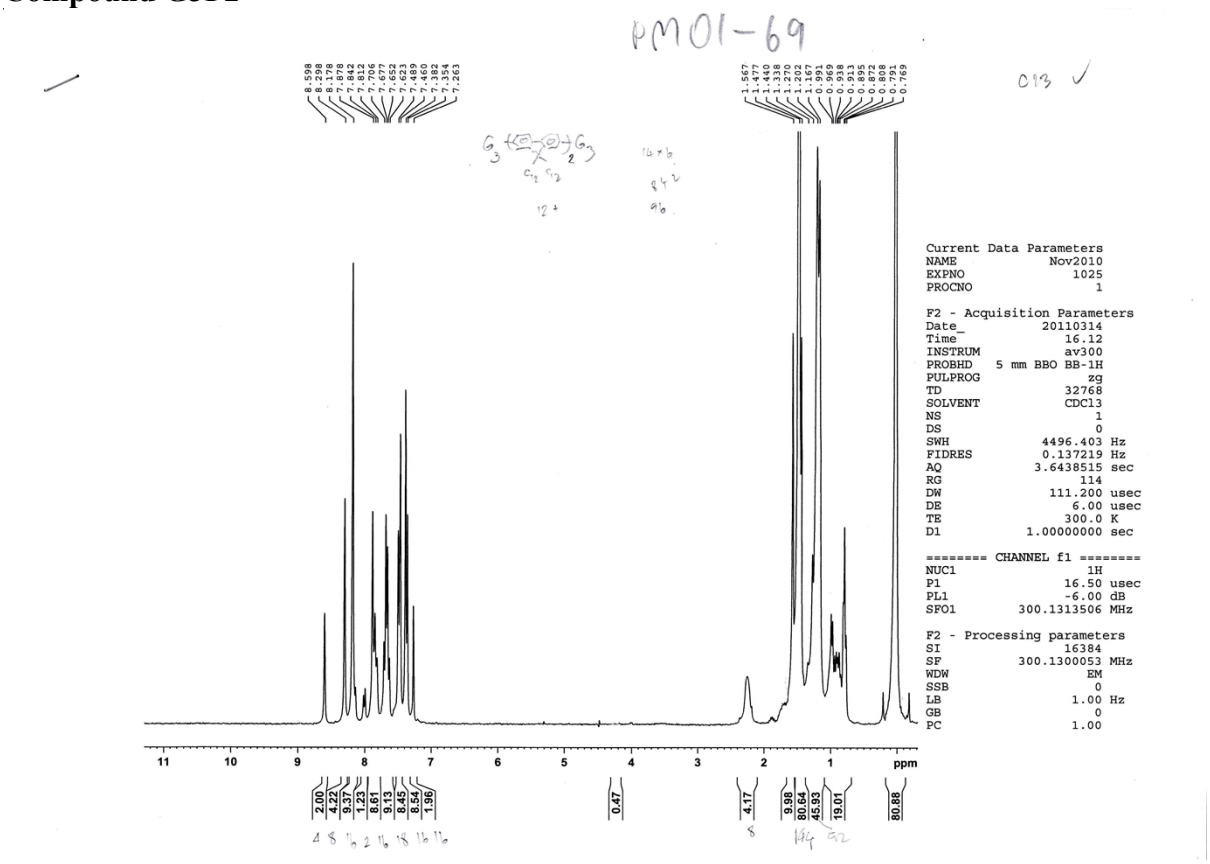


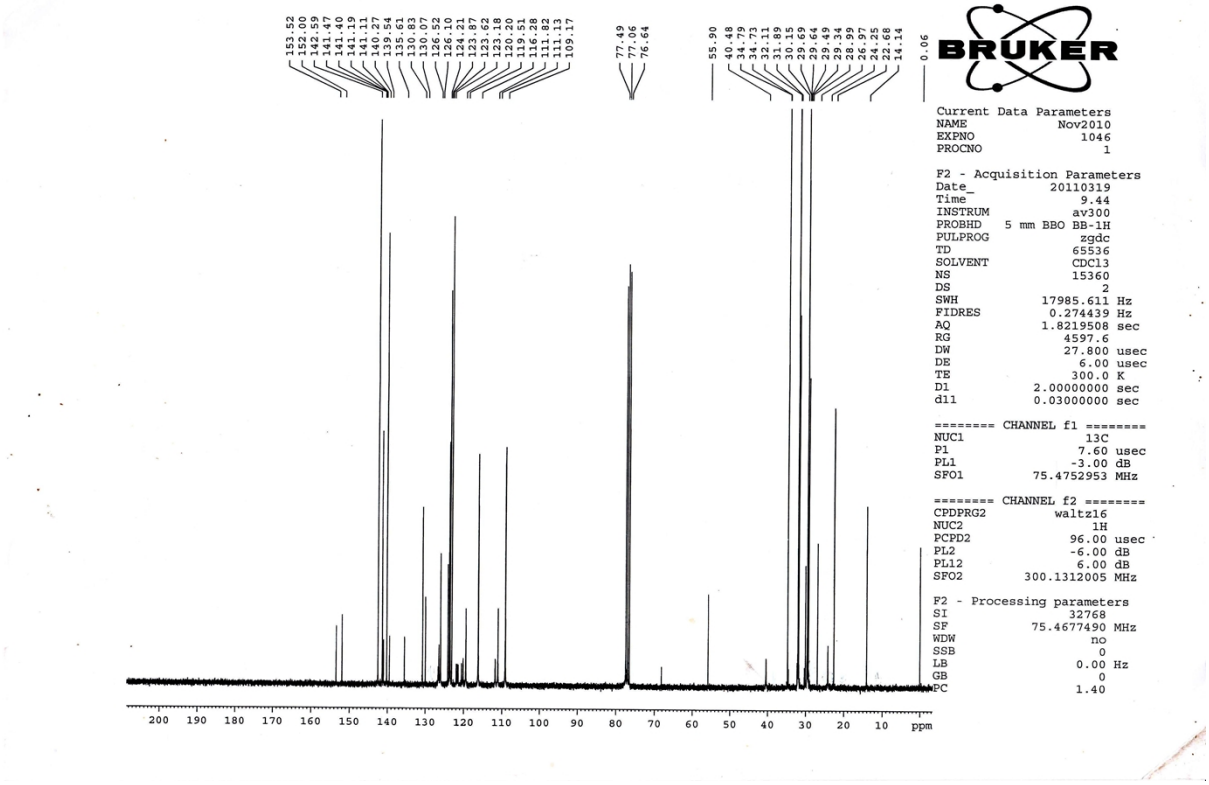
Compound G2F2



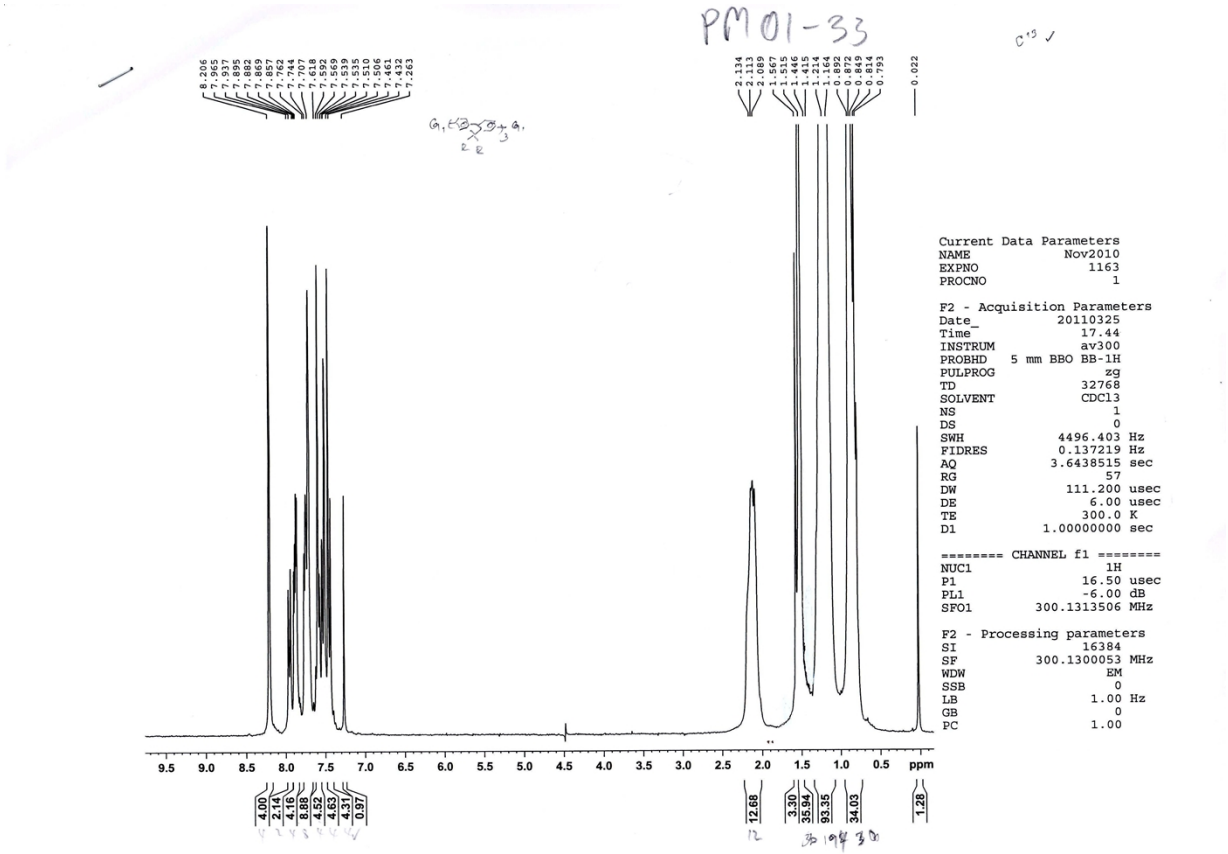


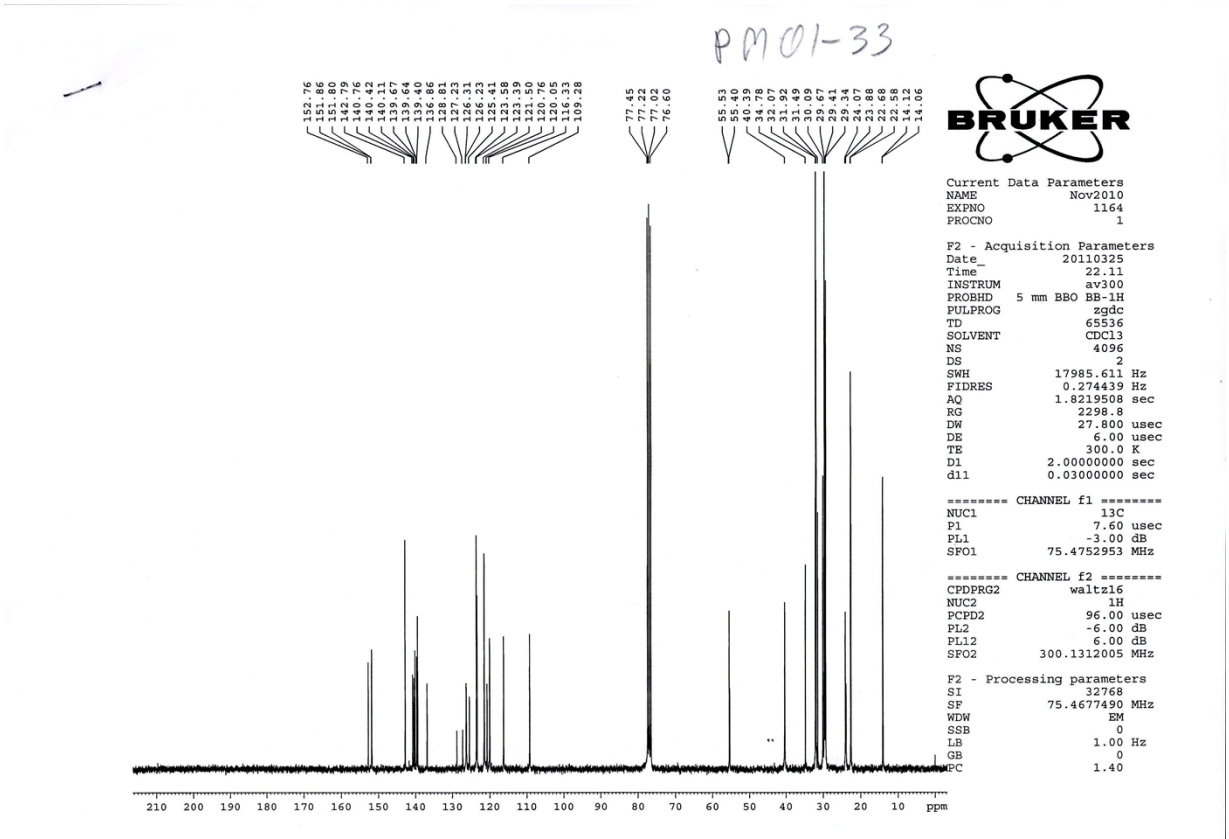
Compound G3F2



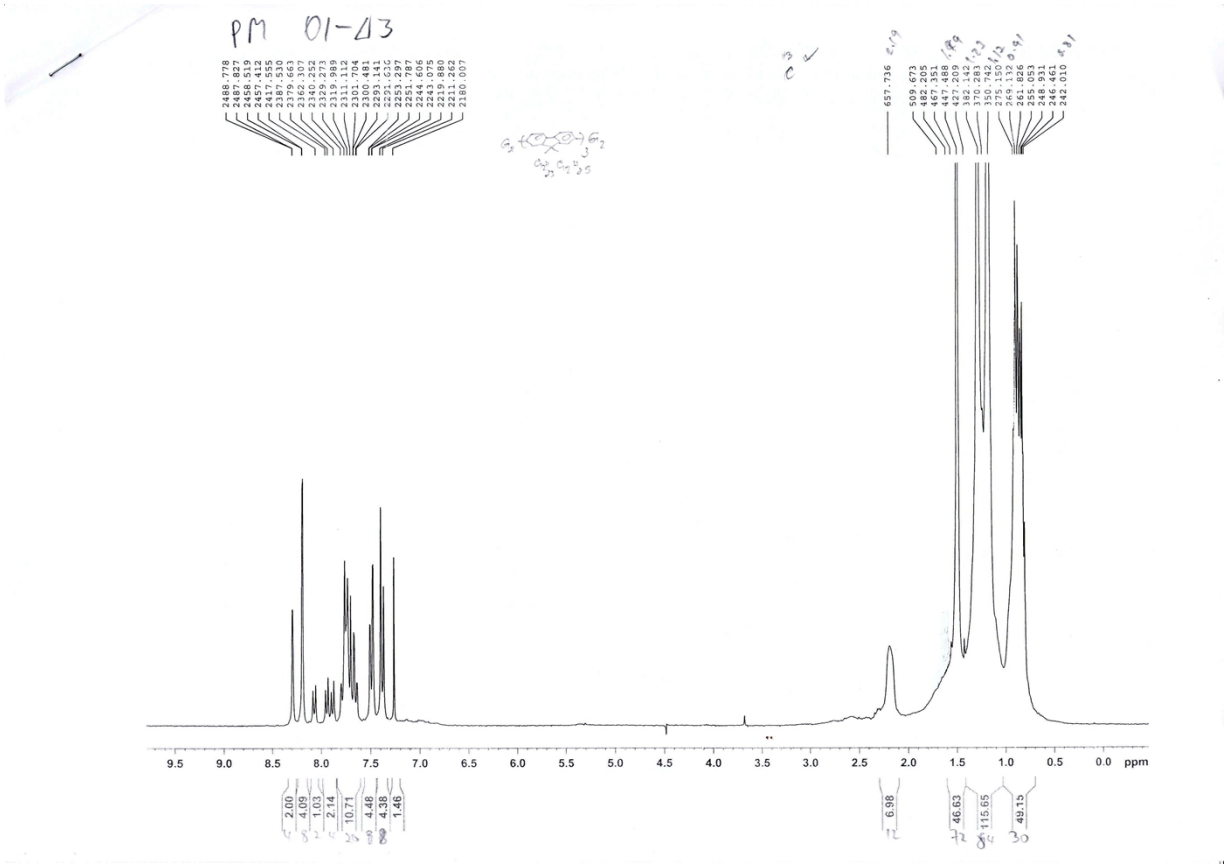


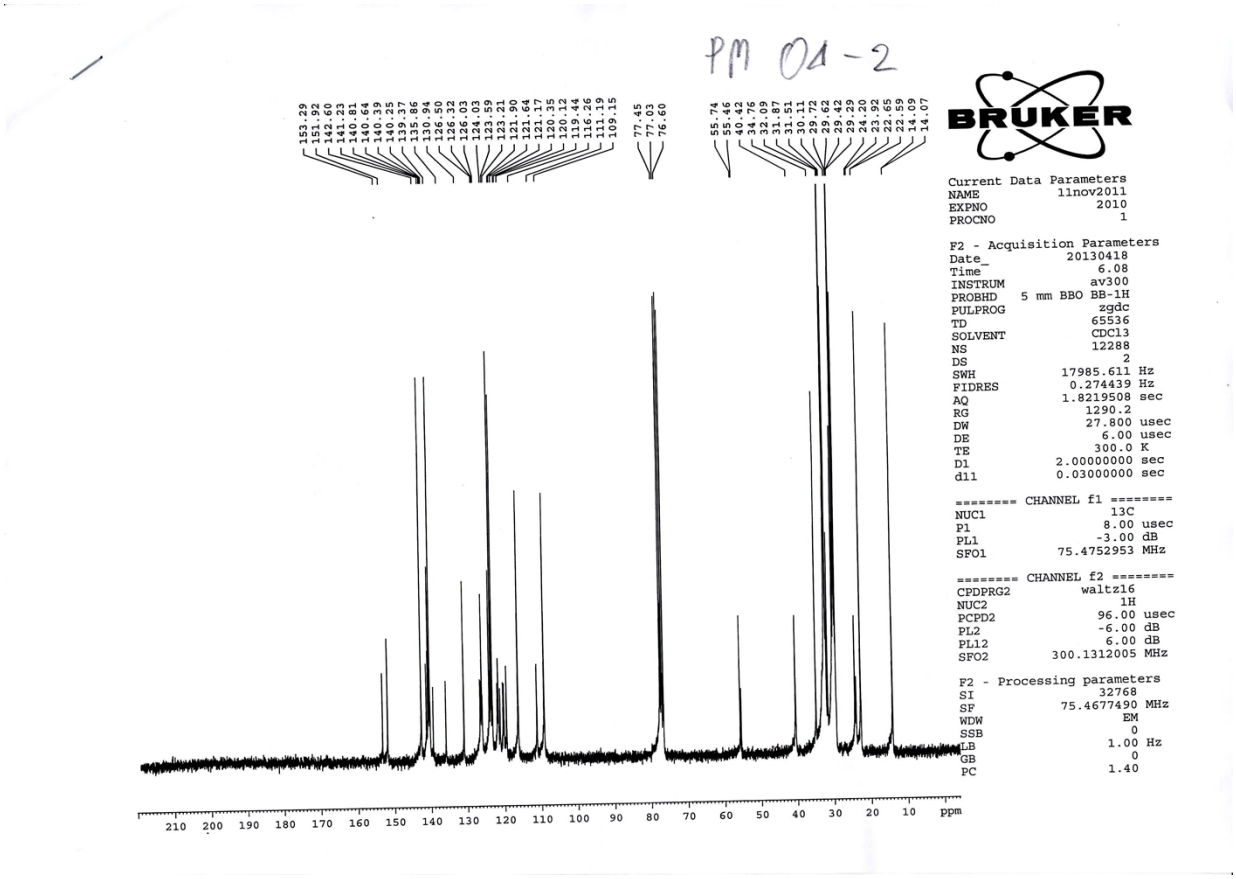
Compound G1F3





Compound G2F3





Compound G3F3