

## Supplementary Information File

# A study of diketopiperazines as electron-donor initiators in transition metal-free haloarene-arene coupling

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**Computational results**  
**NMR spectra**

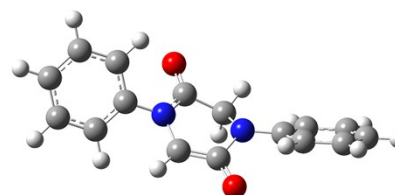
**Pages 1-16**  
**Pages 17-34**

### Computational Results

#### 3,6-dioxo-1,4-diphenylpiperazin-2-ide 20

33

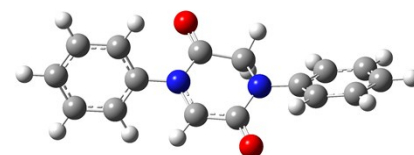
-877.3629690



C	-4.71246	0.80680	1.17685
C	-3.34957	0.87979	0.92357
C	-2.73451	-0.02764	0.03555
C	-3.54210	-1.00055	-0.57811
C	-4.91062	-1.07106	-0.30501
C	-5.51053	-0.17018	0.56924
H	-5.15975	1.51996	1.86964
H	-2.73775	1.64047	1.39840
H	-3.11394	-1.70469	-1.28749
H	-5.50865	-1.83903	-0.79592
H	-6.57808	-0.22413	0.77781
C	-0.68852	1.30270	-0.38257
C	-0.70877	-1.10217	-0.81499
C	0.68027	1.20111	-0.54464
C	0.75370	-1.22259	-0.42659
H	-1.17740	-2.03375	-0.48957
H	-0.76059	-1.04623	-1.92110

H	1.27883	2.09133	-0.66287
C	2.77957	0.01707	-0.00578
C	3.34768	-0.83869	0.94740
C	3.59479	0.94789	-0.66096
C	4.70894	-0.76165	1.23027
H	2.71775	-1.55970	1.45888
C	4.95645	1.01842	-0.36927
H	3.16610	1.60848	-1.41083
C	5.52316	0.16464	0.57574
H	5.13508	-1.43127	1.97683
H	5.57676	1.74582	-0.89198
H	6.58708	0.22073	0.80233
N	-1.35467	0.02784	-0.17874
N	1.39114	-0.03307	-0.29635
O	-1.37609	2.35634	-0.42790
O	1.27539	-2.33320	-0.28744

**3,6-dioxo-1,4-diphenylpiperazin-2-ide 20 after electron transfer**



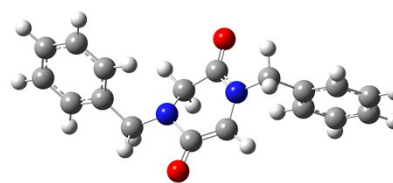
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-877.2553565

C	4.86305	-0.80492	0.99895
C	3.48213	-0.88340	0.85477
C	2.81773	0.01264	0.00625
C	3.55253	0.98425	-0.68115
C	4.93732	1.05717	-0.52309
C	5.60008	0.16342	0.31281
H	5.36799	-1.50556	1.66265
H	2.91490	-1.63681	1.39276
H	3.05930	1.68687	-1.34899
H	5.49515	1.81970	-1.06439
H	6.68057	0.22015	0.43360
C	0.73128	-1.24340	-0.24112
C	0.71903	1.19176	-0.50392
C	-0.70987	-1.16350	-0.29498
C	-0.75812	1.23618	-0.17131
H	1.17825	2.03805	0.01411
H	0.79177	1.37911	-1.58941
H	-1.27479	-2.08712	-0.32533
C	-2.83967	-0.03835	0.01260
C	-3.45348	0.58575	1.09715
C	-3.58723	-0.73168	-0.93713
C	-4.83816	0.50956	1.22729

H	-2.85238	1.12564	1.82470
C	-4.97190	-0.80772	-0.79325
H	-3.08930	-1.20133	-1.78421
C	-5.59847	-0.18682	0.28666
H	-5.32483	0.99490	2.07149
H	-5.56013	-1.34811	-1.53290
H	-6.68033	-0.24405	0.39525
N	1.40230	-0.03356	-0.11776
N	-1.40895	0.00937	-0.12606
O	1.29582	-2.33683	-0.26127
O	-1.33796	2.29212	-0.03197

### 1,4-dibenzyl-3,6-dioxopiperazin-2-ide 21



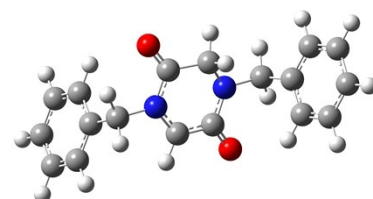
39

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C	-0.76913	-0.15577	0.83674
C	0.39902	-0.94977	0.28871
C	0.95859	1.17007	-0.76421
C	-0.32121	1.69218	-0.68033
H	-0.42128	0.37659	1.74963
H	-1.54353	-0.87149	1.13034
H	1.78874	1.73137	-1.17454
N	1.20643	-0.21938	-0.49706
N	-1.29717	0.77470	-0.14488
C	-2.55752	1.36077	0.25098
H	-2.72796	2.21847	-0.40886
H	-2.50775	1.75948	1.28387
C	2.38414	-0.82406	-1.07595
H	2.25083	-1.91098	-1.03562
H	2.45023	-0.51577	-2.12790
C	3.67163	-0.45364	-0.36186
C	4.89870	-0.73429	-0.97258
C	3.66683	0.13321	0.90517
C	6.09988	-0.44370	-0.32787
H	4.91169	-1.18545	-1.96593
C	4.86822	0.42742	1.55245
H	2.71477	0.37053	1.37783
C	6.08825	0.13929	0.94099
H	7.04717	-0.66908	-0.81705
H	4.84944	0.88836	2.53946
H	7.02479	0.37176	1.44652
C	-3.72501	0.39891	0.16269

C	-4.87701	0.63743	0.92080
C	-3.70258	-0.71210	-0.68615
C	-5.98728	-0.20056	0.82379
H	-4.90157	1.49272	1.59780
C	-4.80967	-1.55620	-0.78285
H	-2.80110	-0.91055	-1.26429
C	-5.95824	-1.30337	-0.03191
H	-6.87529	0.00354	1.42172
H	-4.77319	-2.41964	-1.44674
H	-6.82099	-1.96444	-0.10613
O	-0.69923	2.84729	-1.02933
O	0.57480	-2.14823	0.56706

**1,4-dibenzyl-3,6-dioxopiperazin-2-ide 21 after electron transfer**



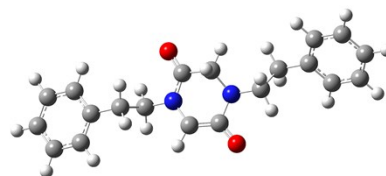
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-955.8606176

C	-0.41981	-1.15318	0.33246
C	0.70495	-0.87413	-0.53174
C	0.43157	1.50995	-0.39348
C	-0.92884	1.24813	0.21605
H	1.28674	-1.70276	-0.91938
H	-1.09135	2.02611	0.97009
H	-1.67346	1.40413	-0.58517
N	1.13948	0.39748	-0.80316
N	-1.08007	-0.05626	0.83318
C	2.41107	0.56685	-1.52267
H	2.46146	1.61622	-1.82151
H	2.36607	-0.06160	-2.41965
C	-2.30416	-0.25173	1.60425
H	-2.21719	-1.22414	2.09657
H	-2.34911	0.53376	2.36938
C	-3.54345	-0.19804	0.73374
C	-4.46068	0.84782	0.84908
C	-3.75998	-1.19480	-0.22676
C	-5.58421	0.90116	0.02015
H	-4.29749	1.62874	1.59275
C	-4.87806	-1.14168	-1.05567
H	-3.04469	-2.01267	-0.31441
C	-5.79396	-0.09349	-0.93325
H	-6.29467	1.72071	0.11976
H	-5.04056	-1.92278	-1.79716
H	-6.66960	-0.05522	-1.57979

C	3.59456	0.18104	-0.66706
C	4.34999	-0.95174	-0.97228
C	3.93399	0.95451	0.44879
C	5.43694	-1.31290	-0.17349
H	4.08895	-1.55736	-1.84061
C	5.01655	0.59459	1.24775
H	3.34599	1.84167	0.68719
C	5.77076	-0.54020	0.93695
H	6.02109	-2.19823	-0.42001
H	5.27828	1.20155	2.11319
H	6.61859	-0.81905	1.56094
O	0.84286	2.64437	-0.56058
O	-0.72642	-2.31442	0.62317

### 3,6-dioxo-1,4-diphenethylpiperazin-2-ide 22



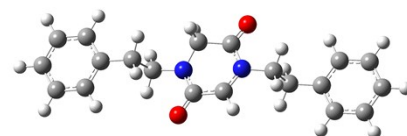
45

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C	-0.67195	-1.04207	-0.04983
C	0.74606	-0.85331	-0.54609
C	0.60591	1.55843	-0.25936
C	-0.76662	1.37172	-0.29869
H	1.31709	-1.73538	-0.24086
H	-1.45509	2.20324	-0.38452
H	0.71181	-0.83168	-1.65855
N	1.35906	0.35240	-0.01792
N	-1.34756	0.10807	0.06387
O	1.22628	2.65294	-0.38930
O	-1.14830	-2.16751	0.19194
C	2.78475	0.42308	-0.26594
H	3.02613	0.05959	-1.28440
H	3.07127	1.47745	-0.21624
C	3.58988	-0.38644	0.76128
H	3.25263	-1.43123	0.76655
H	3.39065	0.03337	1.75491
C	5.06446	-0.33363	0.45675
C	5.85786	0.71215	0.94403
C	5.66417	-1.29403	-0.36623
C	7.21302	0.79391	0.62426
H	5.40305	1.47142	1.58129
C	7.01911	-1.21760	-0.69056
H	5.05853	-2.11354	-0.75557
C	7.79952	-0.17243	-0.19468

H	7.81397	1.61416	1.01602
H	7.46754	-1.97706	-1.33052
H	8.85807	-0.11134	-0.44452
C	-2.74178	0.07287	0.45407
H	-2.89437	-0.78985	1.11085
H	-2.96550	0.99241	1.00873
C	-3.66399	-0.04568	-0.77007
H	-3.46821	0.79914	-1.44222
H	-3.40399	-0.97179	-1.29774
C	-5.11118	-0.06495	-0.35613
C	-5.73034	-1.26555	0.01282
C	-5.85133	1.12003	-0.27271
C	-7.05571	-1.28350	0.44686
H	-5.16240	-2.19514	-0.04378
C	-7.17746	1.10791	0.16082
H	-5.38044	2.06263	-0.55459
C	-7.78492	-0.09550	0.52155
H	-7.52207	-2.22786	0.72611
H	-7.73888	2.04020	0.21515
H	-8.82084	-0.10790	0.85817

**3,6-dioxo-1,4-diphenethylpiperazin-2-ide 22 after electron transfer**



45

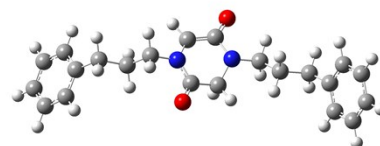
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C	0.79221	1.30013	0.27945
C	-0.71979	1.31611	0.19835
C	-0.74515	-1.13701	0.21270
C	0.64045	-1.07403	0.62225
H	-1.08535	1.65395	1.18450
H	1.14628	-1.98528	0.91935
H	-0.98917	2.08362	-0.53448
N	-1.30790	0.04897	-0.19413
N	1.37557	0.08242	0.56276
O	-1.35970	-2.20880	0.18571
O	1.45214	2.31746	0.15857
C	-2.72162	0.05504	-0.53688
H	-2.90717	0.91408	-1.19374
H	-2.93246	-0.86203	-1.09437
C	-3.63296	0.12354	0.69843
H	-3.44032	1.05295	1.24985
H	-3.38359	-0.72257	1.35022
C	-5.08190	0.06086	0.28898

C	-5.69804	-1.17584	0.06463
C	-5.81961	1.22875	0.07023
C	-7.02296	-1.24392	-0.36437
H	-5.13147	-2.09295	0.23167
C	-7.14582	1.16542	-0.35911
H	-5.35171	2.19874	0.24349
C	-7.75124	-0.07221	-0.57739
H	-7.49011	-2.21394	-0.52983
H	-7.70860	2.08416	-0.51979
H	-8.78706	-0.12415	-0.90962
C	2.83186	0.02950	0.71353
H	3.14996	0.95031	1.20956
H	3.06561	-0.82399	1.35840
C	3.52784	-0.10936	-0.64482
H	3.18190	-1.03120	-1.12949
H	3.23396	0.74101	-1.27150
C	5.02481	-0.13735	-0.46599
C	5.74728	1.05778	-0.37592
C	5.70864	-1.35021	-0.33532
C	7.12527	1.04139	-0.16339
H	5.22350	2.00916	-0.47845
C	7.08755	-1.37097	-0.12335
H	5.15663	-2.28816	-0.40738
C	7.79930	-0.17431	-0.03672
H	7.67554	1.97928	-0.10054
H	7.60772	-2.32339	-0.02967
H	8.87606	-0.18861	0.12546

### 3,6-dioxo-1,4-bis(3-phenylpropyl)piperazin-2-ide 23

51  
-1113.1496574

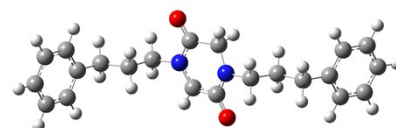


C	0.69508	-0.28580	-0.64361
C	-0.48277	-0.72556	0.20083
C	-0.92680	1.65801	0.28943
C	0.36543	2.04025	-0.03089
H	0.33343	-0.16537	-1.68976
H	1.42496	-1.09991	-0.62693
H	-1.70953	2.38247	0.47714
N	-1.23045	0.29679	0.63339
N	1.29565	0.94317	-0.15426
O	-0.72236	-1.92598	0.43271
O	0.78599	3.22223	-0.19815

C	2.55572	1.25523	-0.80230
H	2.47621	1.10466	-1.89909
H	2.74331	2.31981	-0.63515
C	3.72021	0.42907	-0.26403
H	3.53680	-0.64675	-0.39503
H	3.81574	0.60921	0.81524
C	5.03313	0.79498	-0.96688
H	5.23114	1.86557	-0.81946
H	4.92044	0.62877	-2.04732
C	6.19699	-0.01222	-0.45164
C	6.52445	-1.24562	-1.02700
C	6.94578	0.42828	0.64598
C	7.57083	-2.01831	-0.52293
H	5.94936	-1.60342	-1.88208
C	7.99348	-0.33959	1.15479
H	6.70155	1.38645	1.10638
C	8.31053	-1.56696	0.57101
H	7.81098	-2.97474	-0.98649
H	8.56579	0.02215	2.00857
H	9.12934	-2.16733	0.96552
C	-2.42601	0.02919	1.40904
H	-2.28103	-0.92106	1.93481
H	-2.53531	0.83492	2.14718
C	-3.67067	-0.05475	0.52768
H	-3.77979	0.87682	-0.04445
H	-3.53545	-0.87027	-0.19570
C	-4.93353	-0.30281	1.35874
H	-4.80779	-1.23075	1.93376
H	-5.05649	0.51702	2.08021
C	-6.16431	-0.40544	0.49448
C	-6.89546	0.73755	0.15066
C	-6.57229	-1.63851	-0.02710
C	-8.00468	0.65309	-0.69092
H	-6.58785	1.70601	0.54723
C	-7.68083	-1.72936	-0.86904
H	-6.01022	-2.53737	0.22950
C	-8.40212	-0.58251	-1.20375
H	-8.56154	1.55421	-0.94609
H	-7.98369	-2.69870	-1.26386
H	-9.26885	-0.65125	-1.85986

**3,6-dioxo-1,4-bis(3-phenylpropyl)piperazin-2-ide 23 after electron transfer**

51



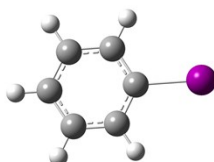


-1113.0537253

C	0.71502	1.26965	0.30894
C	-0.66780	1.45908	-0.27832
C	-0.52770	-0.80965	-1.05662
C	0.61670	-1.12111	-0.22873
H	0.74502	1.84706	1.23881
H	1.42409	1.73782	-0.39670
H	-0.94334	-1.58076	-1.69463
N	-1.17503	0.39808	-0.99876
N	1.06051	-0.11125	0.58963
O	-1.27123	2.51239	-0.16915
O	1.12159	-2.24918	-0.23001
C	2.25966	-0.34251	1.38274
H	2.22078	0.33137	2.24888
H	2.21797	-1.37474	1.74402
C	3.54938	-0.12388	0.59371
H	3.60913	0.91575	0.24195
H	3.53586	-0.77333	-0.29133
C	4.78367	-0.43792	1.44549
H	4.72616	-1.48119	1.78459
H	4.77930	0.19984	2.34023
C	6.06223	-0.22263	0.67497
C	6.72261	1.01002	0.71177
C	6.58567	-1.23840	-0.13304
C	7.87797	1.22553	-0.04014
H	6.32808	1.80983	1.33996
C	7.74025	-1.02850	-0.88654
H	6.08202	-2.20525	-0.17003
C	8.39059	0.20563	-0.84232
H	8.38177	2.19043	0.00381
H	8.13626	-1.83162	-1.50699
H	9.29418	0.37025	-1.42748
C	-2.48295	0.55254	-1.64223
H	-2.56434	1.59054	-1.97722
H	-2.49302	-0.10635	-2.51766
C	-3.62041	0.20746	-0.68731
H	-3.50066	-0.82625	-0.33466
H	-3.56413	0.86586	0.18905
C	-4.98351	0.36805	-1.36787
H	-5.09037	1.40382	-1.71767
H	-5.02769	-0.28446	-2.25066
C	-6.11410	0.02913	-0.42837
C	-6.60478	-1.27805	-0.34304
C	-6.65964	1.00618	0.41143
C	-7.61682	-1.60379	0.56017
H	-6.19063	-2.04933	-0.99379

C	-7.67170	0.68579	1.31612
H	-6.28779	2.03001	0.35398
C	-8.15360	-0.62155	1.39304
H	-7.99019	-2.62588	0.61099
H	-8.08822	1.45944	1.96004
H	-8.94593	-0.87288	2.09658

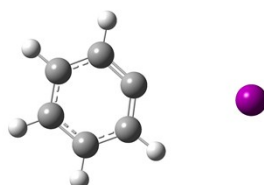
### Iodobenzene neutral



12  
-527.1939762

C	-2.63994	1.20685	0.00000
C	-1.24409	1.21561	0.00000
C	-0.56257	0.00001	-0.00001
C	-1.24409	-1.21561	-0.00000
C	-2.63993	-1.20685	0.00000
C	-3.33876	-0.00000	-0.00000
H	-3.17958	2.15302	-0.00000
H	-0.69853	2.15712	0.00000
H	-0.69851	-2.15710	-0.00000
H	-3.17958	-2.15302	0.00000
H	-4.42747	-0.00002	-0.00000
I	1.55094	0.00000	0.00000

### Iodobenzene radical anion

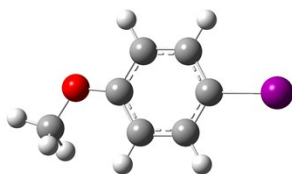


12  
-527.2598495

C	-2.96440	-1.36914	-0.00000
C	-1.64582	-0.89570	0.00017
C	-1.47038	0.47341	0.00018
C	-2.49246	1.40042	0.00007
C	-3.80485	0.90673	-0.00008
C	-4.03561	-0.47090	-0.00013
H	-3.15457	-2.44288	-0.00006
H	-0.78719	-1.56630	0.00027
H	-2.29570	2.47222	0.00009
H	-4.64576	1.60108	-0.00017
H	-5.05823	-0.84711	-0.00027

I 2.15892 0.00970 -0.00002

#### 4-iodoanisole neutral

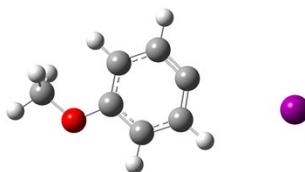


16

-641.6916233

C	1.78395	1.43647	-0.00002
C	0.39921	1.33816	0.00002
C	-0.20132	0.07631	-0.00001
C	0.57542	-1.07517	-0.00002
C	1.97056	-0.97854	-0.00004
C	2.57691	0.28074	-0.00005
H	2.27331	2.40874	-0.00001
H	-0.20783	2.24109	0.00003
H	0.10809	-2.05757	-0.00003
H	2.55967	-1.89119	-0.00005
O	3.91956	0.48372	-0.00002
C	4.75086	-0.66587	0.00006
H	4.57764	-1.27410	-0.89834
H	5.77751	-0.29425	-0.00005
H	4.57778	-1.27390	0.89862
I	-2.30483	-0.07927	0.00001

#### 4-iodoanisole radical anion



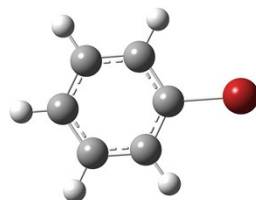
16

-641.7554994

C	-2.08832	-1.14481	-0.00009
C	-0.79259	-0.63033	-0.00016
C	-0.65198	0.74621	-0.00014
C	-1.70533	1.62944	-0.00006
C	-3.01126	1.10631	0.00001
C	-3.19241	-0.27937	-0.00001
H	-2.26808	-2.21937	-0.00010
H	0.08291	-1.27867	-0.00021
H	-1.55144	2.70794	-0.00005
H	-3.85774	1.78823	0.00008
O	-4.41880	-0.88961	0.00006
C	-5.55479	-0.04845	0.00010

H	-5.57690	0.58695	-0.89713
H	-6.42369	-0.71123	0.00012
H	-5.57685	0.58693	0.89735
I	3.06608	-0.04939	0.00003

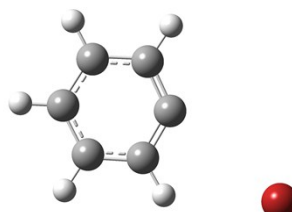
**Bromobenzene neutral**



12  
-2805.7570060

C	2.17326	1.20714	0.00000
C	0.77805	1.21638	-0.00001
C	0.10074	0.00002	-0.00001
C	0.77804	-1.21637	-0.00001
C	2.17322	-1.20717	0.00000
C	2.87199	-0.00001	0.00000
H	2.71309	2.15305	0.00001
H	0.22489	2.15320	-0.00001
H	0.22482	-2.15315	-0.00001
H	2.71308	-2.15305	0.00001
H	3.96060	-0.00004	0.00000
Br	-1.80252	0.00000	0.00000

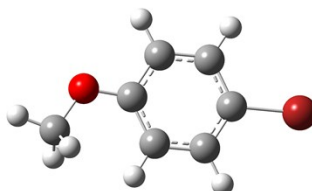
**Bromobenzene radical anion**



12  
-2805.8139944

C	2.23316	-1.38303	0.00050
C	0.97910	-0.75854	0.00428
C	0.97218	0.62133	0.00487
C	2.09562	1.42233	0.00133
C	3.34040	0.77621	-0.00258
C	3.40439	-0.61872	-0.00286
H	2.29482	-2.47177	-0.00004
H	0.04201	-1.31556	0.00622
H	2.02787	2.50992	0.00187
H	4.25728	1.36658	-0.00527
H	4.37446	-1.11530	-0.00601
Br	-2.60416	0.01910	-0.00086

### 4-bromoanisole neutral

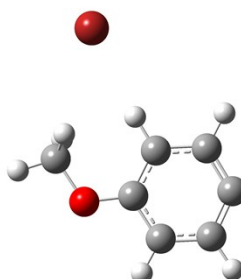


16

-2920.2543669

C	1.23451	1.43018	-0.00001
C	-0.14846	1.31511	0.00003
C	-0.72784	0.04527	0.00000
C	0.05834	-1.09781	-0.00001
C	1.45163	-0.98275	-0.00003
C	2.04190	0.28429	-0.00005
H	1.71190	2.40825	-0.00001
H	-0.77369	2.20532	0.00003
H	-0.40406	-2.08239	-0.00002
H	2.05268	-1.88745	-0.00004
O	3.38213	0.50428	-0.00002
C	4.22760	-0.63484	0.00005
H	4.06199	-1.24520	-0.89837
H	5.24959	-0.25054	-0.00006
H	4.06213	-1.24502	0.89862
Br	-2.62410	-0.11697	0.00001

### 4-bromoanisole radical anion



16

-2920.3172137

C	0.91704	-0.43350	-0.00045
C	1.47455	-1.72246	-0.00030
C	2.84580	-1.83743	0.00000
C	3.71939	-0.76629	0.00039
C	3.16329	0.51427	0.00032
C	1.76941	0.67776	-0.00015
H	-0.16952	-0.32802	-0.00086
H	0.81615	-2.59059	-0.00050
H	4.80078	-0.89932	0.00074
H	3.79553	1.40150	0.00058
O	1.32672	1.96511	-0.00046
C	-0.08580	2.15042	0.00014
H	-0.54543	1.69828	0.88855
H	-0.24498	3.23147	0.00075
H	-0.54609	1.69915	-0.88837
Br	-2.89550	-0.32657	0.00009

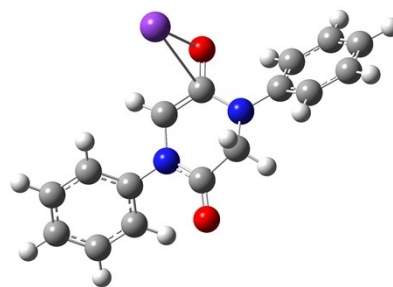
Optimizations of anions **21** and **22** were made including the counterion ( $K^+$ ) to check for any interaction between the phenyl and the benzyl-substituents with the counterion. For both anions, the potassium cation chelated with the C-O bond of the enolate during the optimization and did not interact with the phenyl/benzyl substituents.

### 3,6-dioxo-1,4-diphenylpiperazin-2-ide **20** (with $K^+$ )

34

-1477.1135374

C	-4.66541	-0.55727	1.49192
C	-3.29483	-0.37240	1.36740
C	-2.65402	-0.62256	0.14224
C	-3.42287	-1.06698	-0.94132
C	-4.79880	-1.26144	-0.80170
C	-5.43025	-1.00505	0.41046
H	-5.14113	-0.36289	2.44871
H	-2.70290	-0.03115	2.20763
H	-2.95822	-1.26058	-1.90217
H	-5.37326	-1.61126	-1.65442
H	-6.49940	-1.15708	0.51816
C	-0.62608	0.72277	0.49918
C	-0.57916	-1.13796	-1.06183
C	0.73359	0.82298	0.25559
C	0.89985	-1.35688	-0.79729
H	-1.01595	-2.12455	-1.21576
H	-0.65969	-0.56968	-2.00910
H	1.29560	1.57768	0.78679
C	2.90843	-0.33341	0.08040
C	3.56561	-1.48088	0.53524
C	3.63771	0.83732	-0.14541
C	4.93958	-1.44843	0.75672
H	2.99917	-2.38786	0.70641
C	5.01199	0.86171	0.08422
H	3.12906	1.72283	-0.51229
C	5.66986	-0.28043	0.53570
H	5.44048	-2.34374	1.11201
H	5.56757	1.77653	-0.09825
H	6.74014	-0.26190	0.71421
N	-1.25641	-0.46498	0.03179
N	1.50227	-0.33694	-0.13578
O	-1.32975	1.64173	1.03450

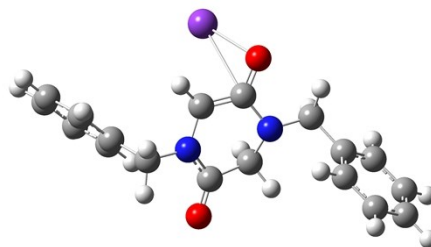


O	1.46802	-2.36294	-1.22038
K	-0.79052	3.39422	-0.70295

**1,4-dibenzyl-3,6-dioxopiperazin-2-ide 21 (with K<sup>+</sup>)**

40  
-1555.7093143

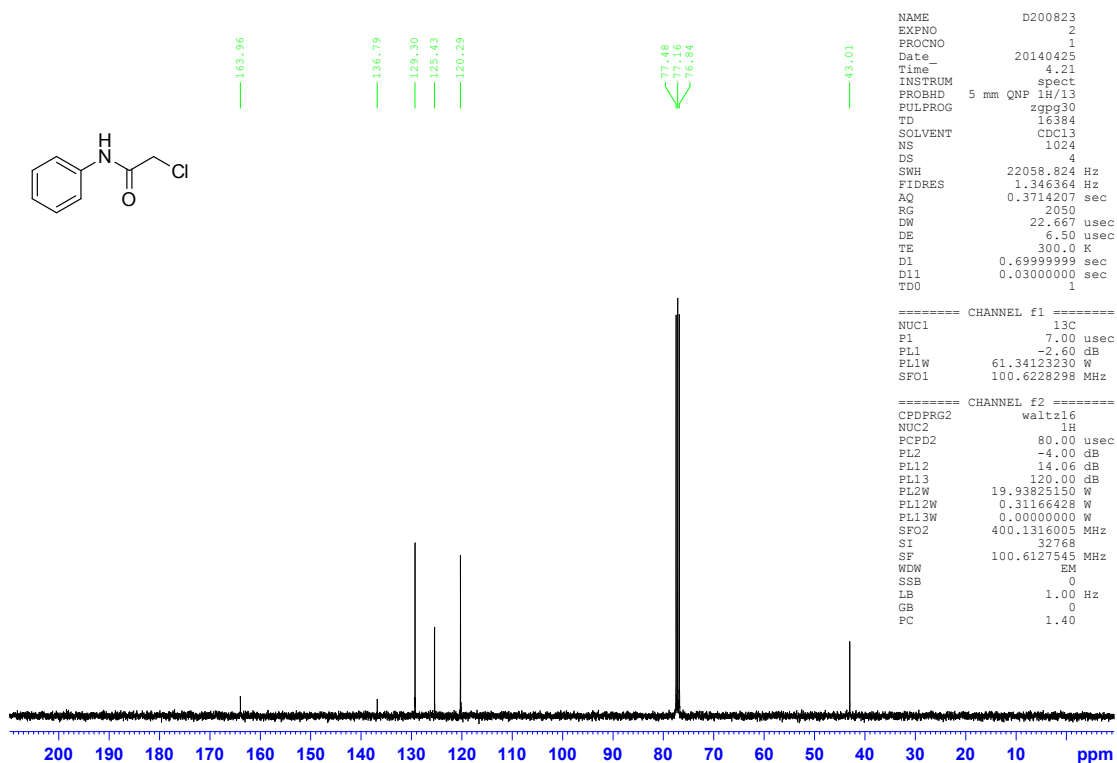
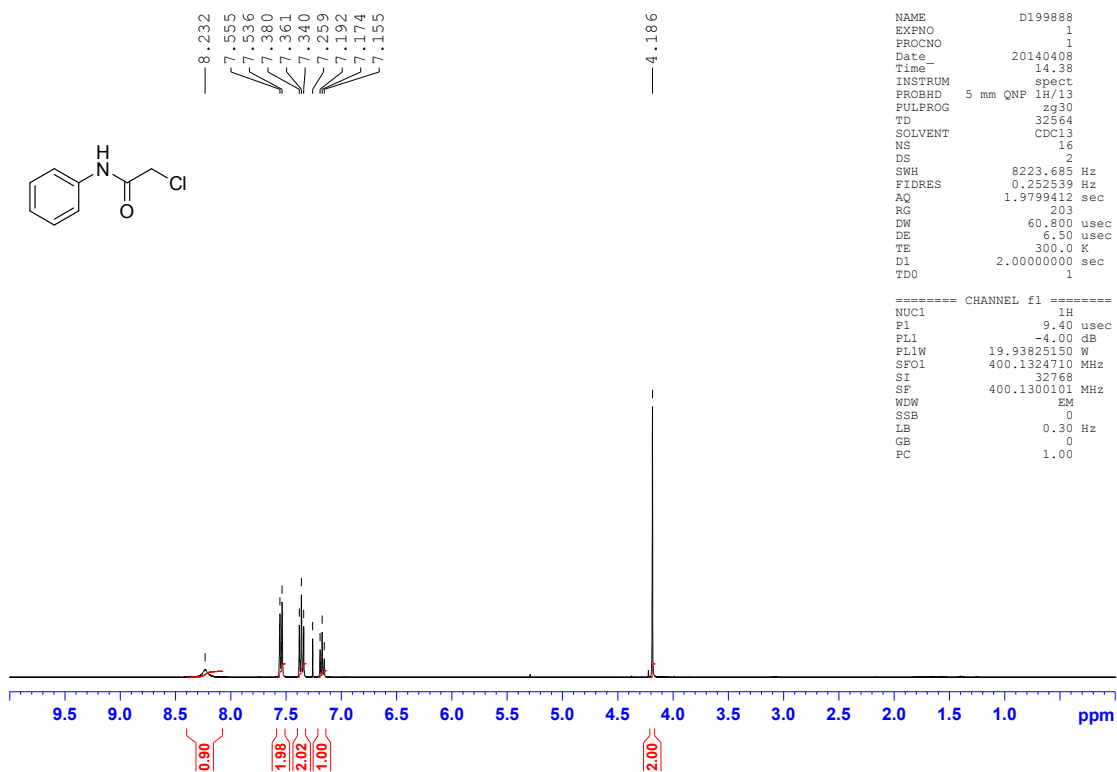
C	-1.00860	-0.62257	0.71430
C	0.08826	-1.53374	0.19816
C	0.91363	0.49974	-0.83992
C	-0.29989	1.16378	-0.76378
H	-0.65114	-0.18664	1.67150
H	-1.87673	-1.24676	0.93579
H	1.70741	0.88319	-1.46925
N	0.98802	-0.91143	-0.58420
N	-1.37891	0.42121	-0.22627
C	-2.55602	1.17179	0.17222
H	-2.63767	2.01976	-0.51156
H	-2.43325	1.58647	1.18979
C	2.15557	-1.62202	-1.07431
H	1.98192	-2.68494	-0.89108
H	2.24191	-1.46016	-2.15498
C	3.42362	-1.16636	-0.38092
C	4.54712	-0.78060	-1.11190
C	3.47794	-1.13228	1.01709
C	5.71397	-0.37255	-0.46107
H	4.51037	-0.79874	-2.19865
C	4.63832	-0.72498	1.66935
H	2.60193	-1.43166	1.58850
C	5.76185	-0.34363	0.93060
H	6.58216	-0.07749	-1.04272
H	4.67157	-0.71030	2.75472
H	6.66802	-0.02969	1.43971
C	-3.81911	0.33768	0.13090
C	-4.79724	0.49180	1.11549
C	-4.04103	-0.57732	-0.90315
C	-5.98309	-0.24194	1.06536
H	-4.62809	1.19041	1.93176
C	-5.22128	-1.31585	-0.95338
H	-3.27253	-0.71253	-1.65918
C	-6.19799	-1.14957	0.03018
H	-6.73299	-0.11077	1.83962
H	-5.37797	-2.02700	-1.75890

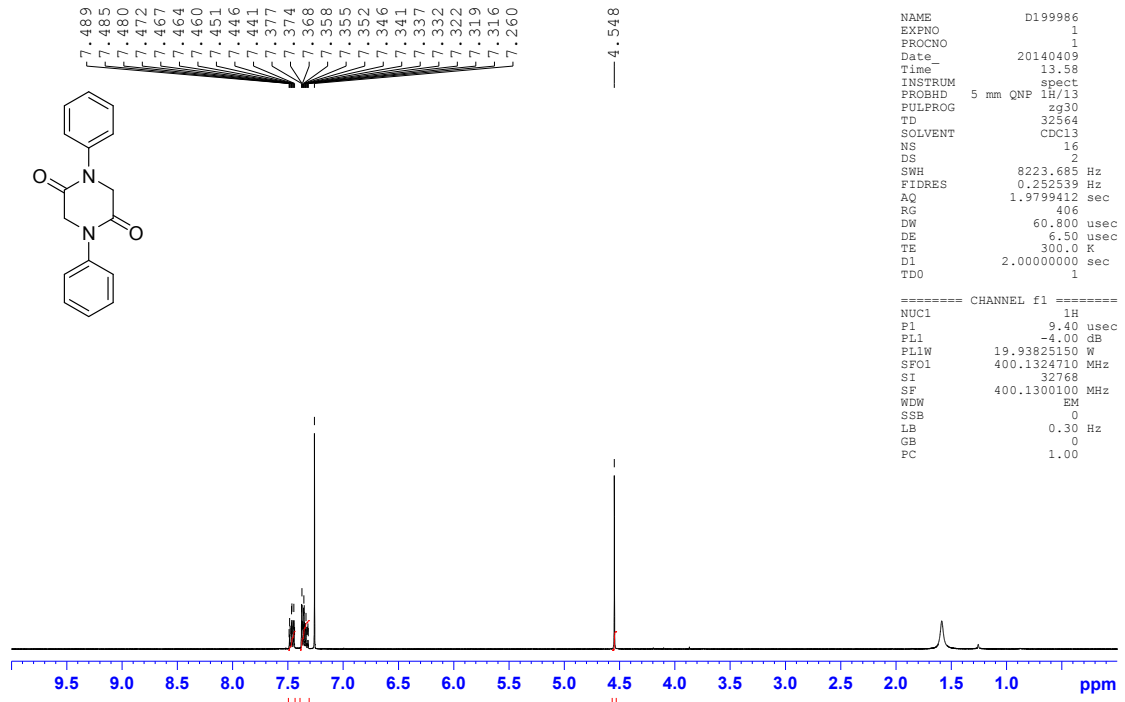


H	-7.11542	-1.72873	-0.00736
O	-0.48137	2.38445	-1.10249
O	0.14680	-2.72395	0.53132
K	1.49458	3.22026	0.27651



# NMR Spectra



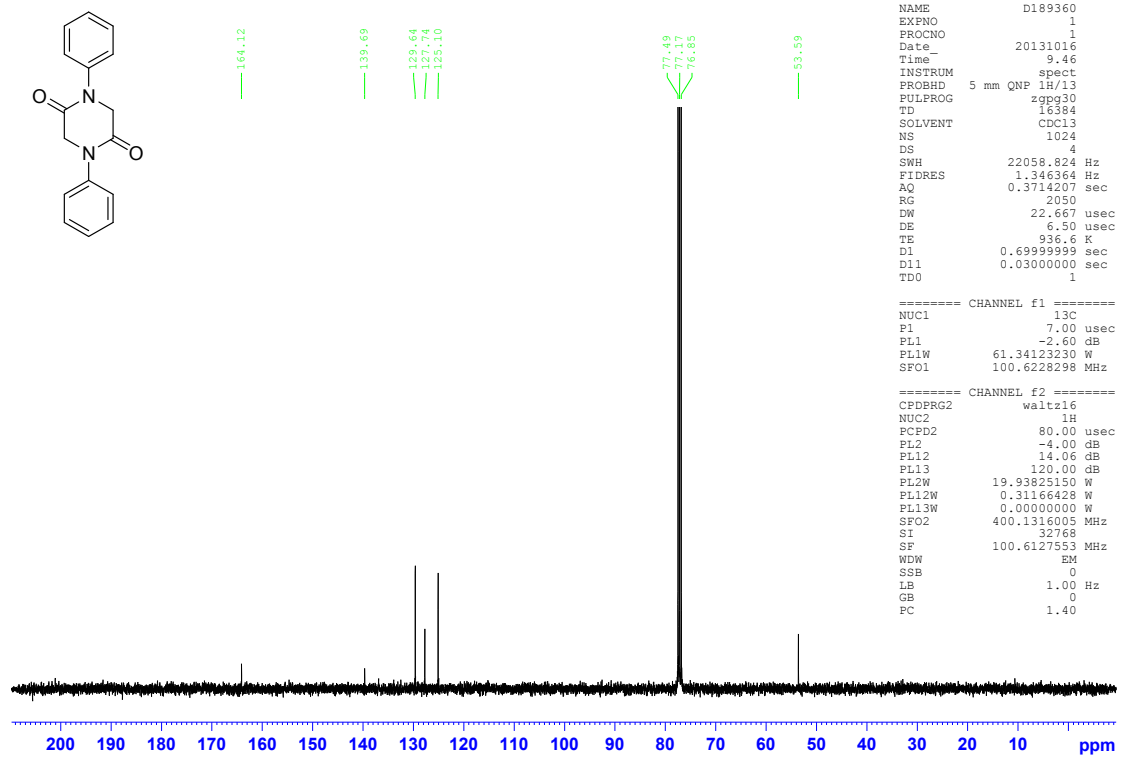


```

NAME          D199986
EXPNO         1
PROCNO        1
Date_         20140409
Time_         13.58
INSTRUM       spect
PROBHD        5 mm QNP 1H/13
PULPROG       zg30
TD            32564
SOLVENT       CDCl3
NS            16
DS            2
SWH           8223.685 Hz
FIDRES        0.252539 Hz
AQ            1.9799412 sec
RG            406
DW            60.800 usec
DE            6.50 usec
TE            300.0 K
D1            2.00000000 sec
D11           1
TD0           1
  
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            9.40 usec
PL1          -4.00 dB
PL1W         19.93825150 W
SFO1         400.1324710 MHz
SI           32768
SF           400.1300100 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```



```

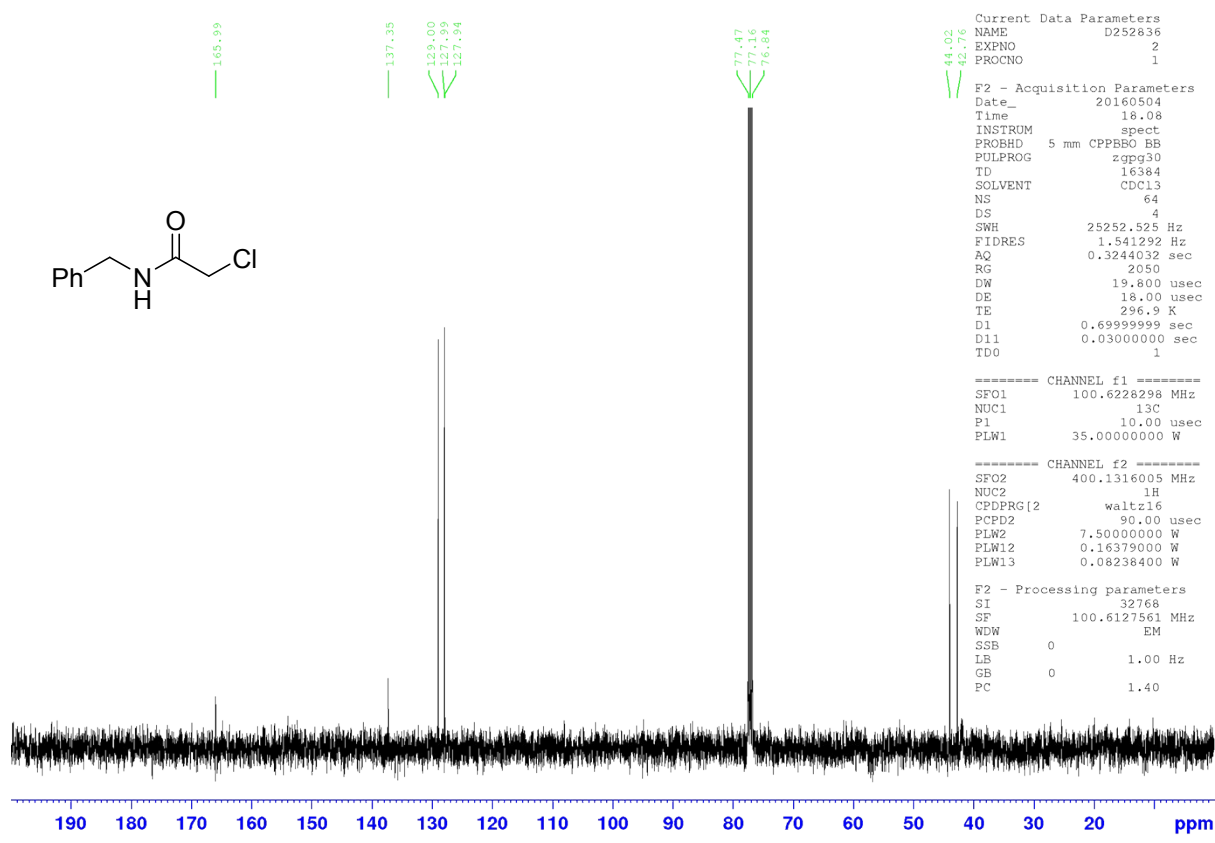
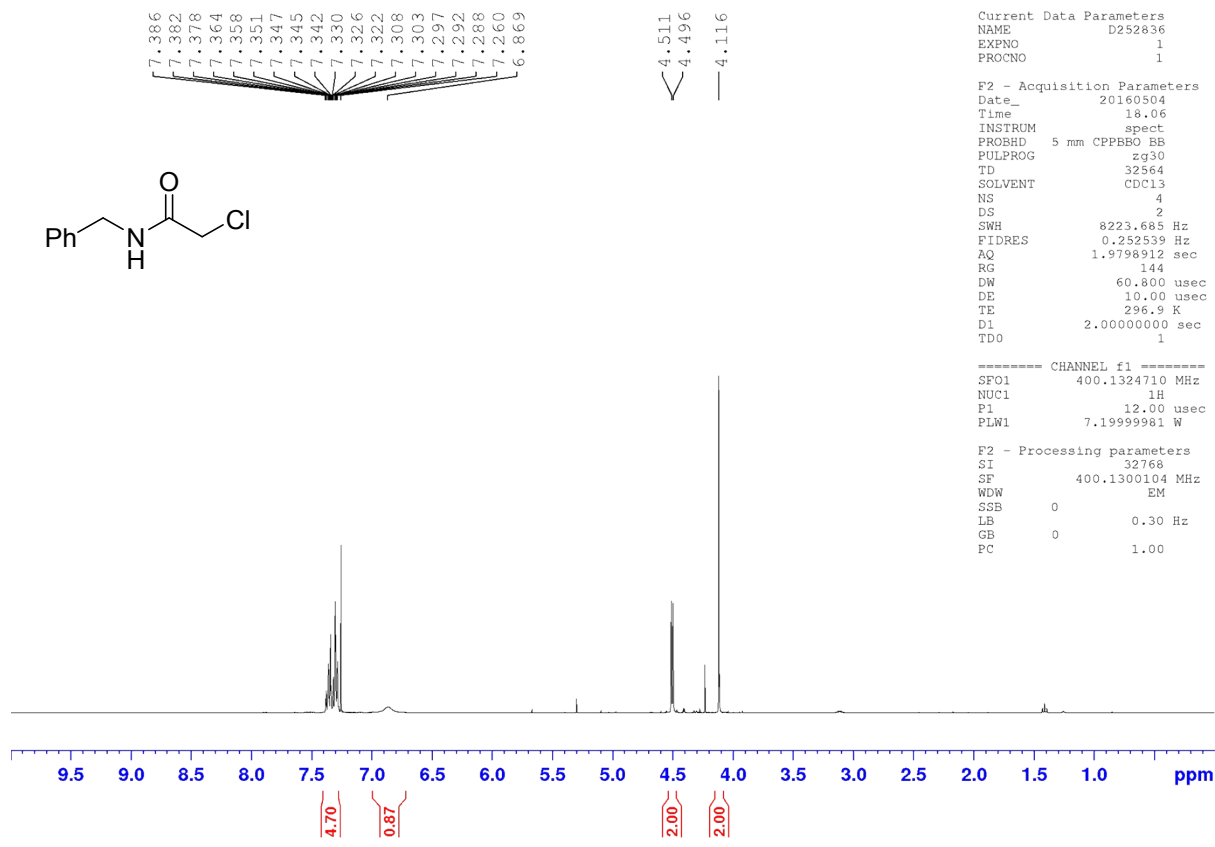
NAME          D189360
EXPNO         1
PROCNO        1
Date_         20131016
Time_         9.46
INSTRUM       spect
PROBHD        5 mm QNP 1H/13
PULPROG       zgpg30
TD            16384
SOLVENT       CDCl3
NS            1024
DS            4
SWH           22058.824 Hz
FIDRES        1.346364 Hz
AQ            0.3714207 sec
RG            2050
DW            22.667 usec
DE            6.50 usec
TE            936.6 K
D1            0.699999999 sec
D11           0.030000000 sec
TD0           1
  
```

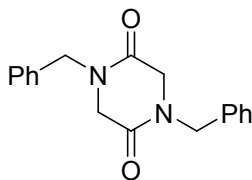
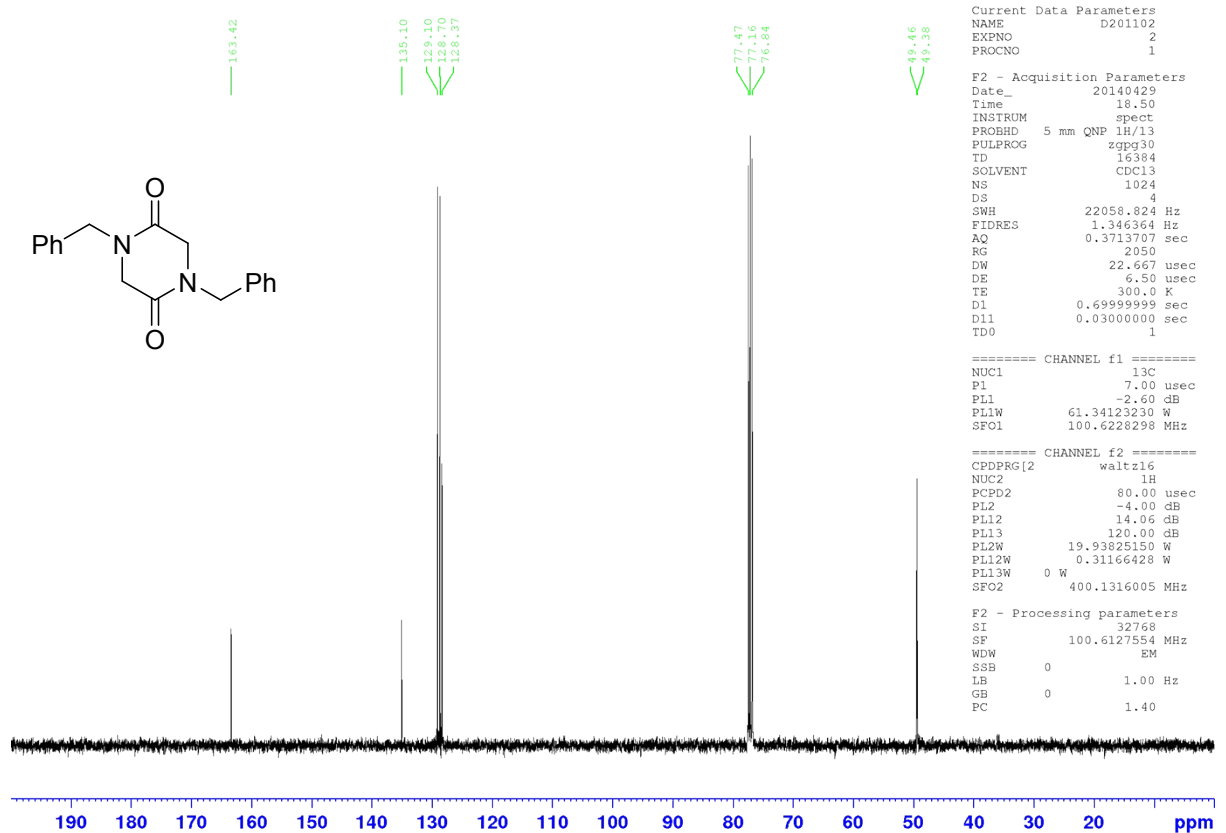
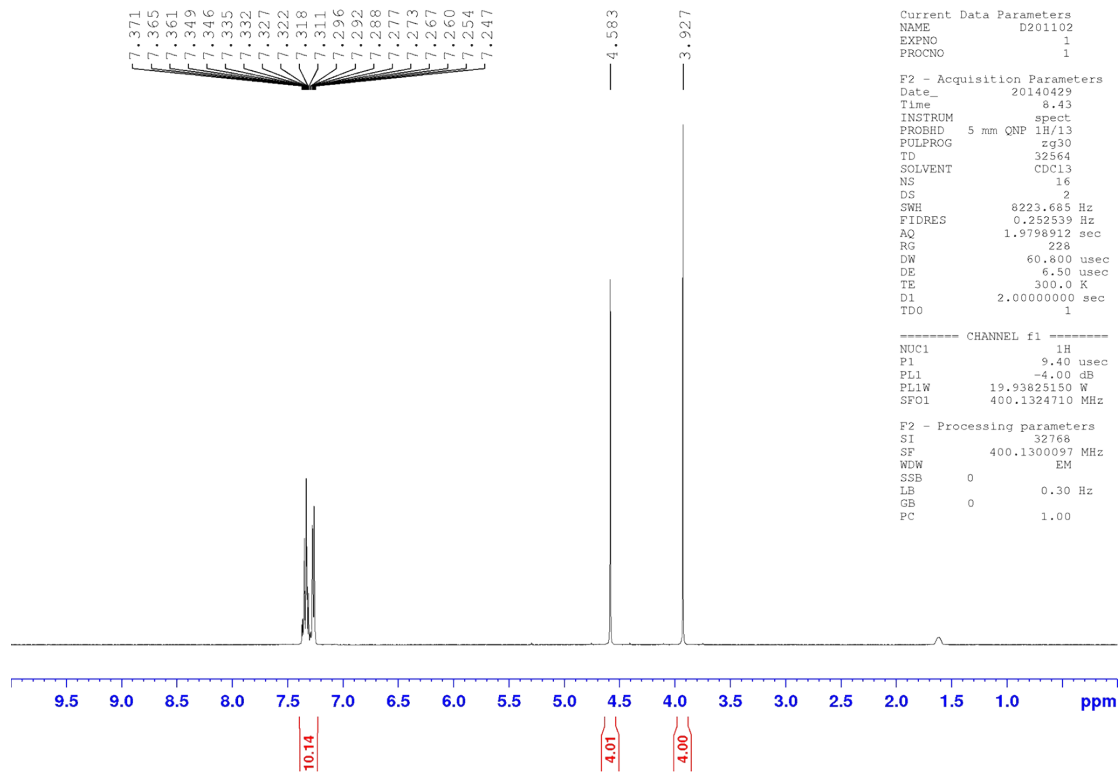
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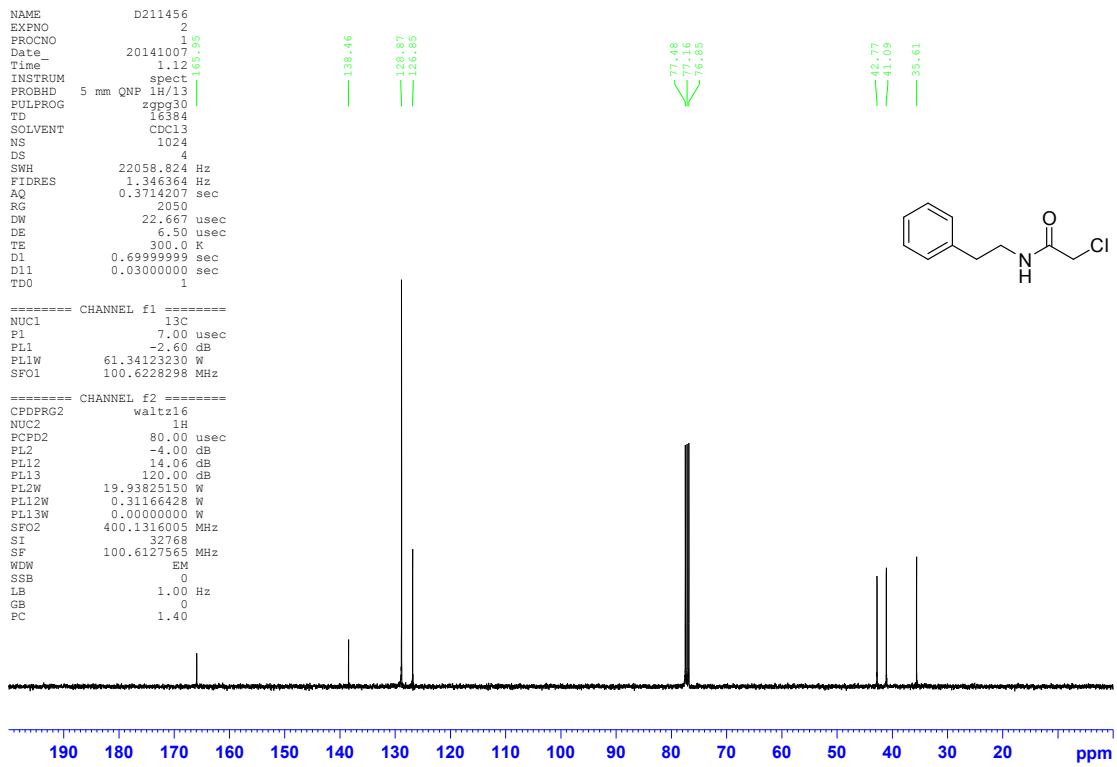
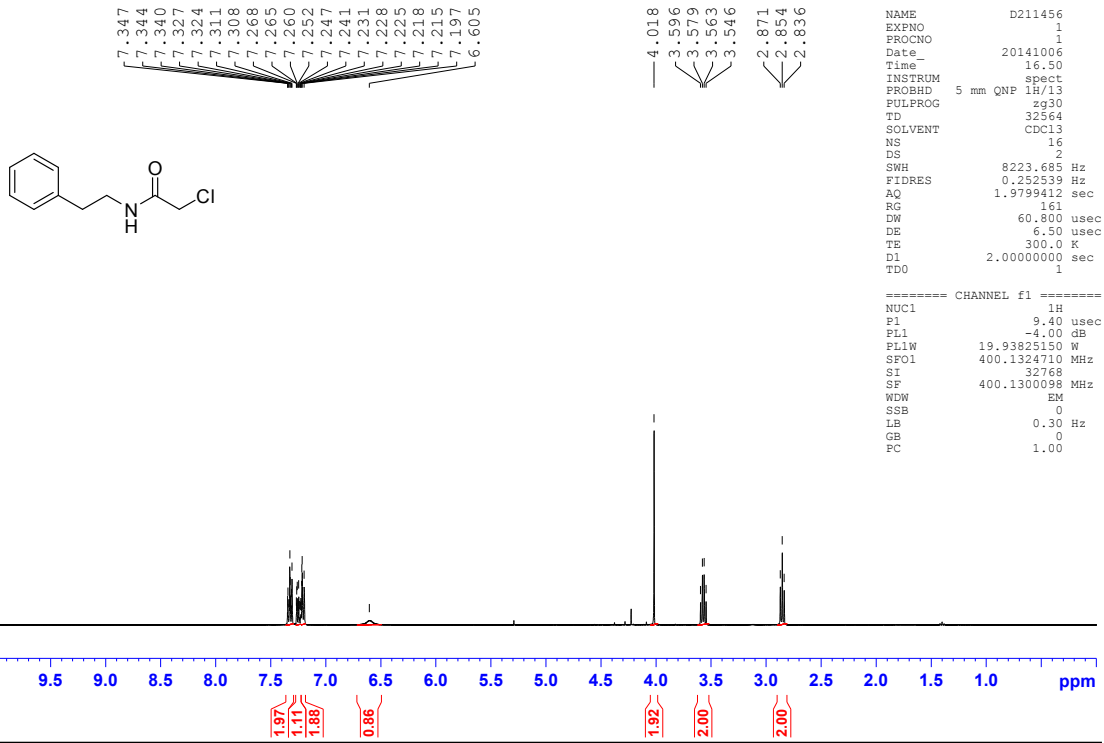
===== CHANNEL f1 =====
NUC1          13C
P1            7.00 usec
PL1          -2.60 dB
PL1W         61.34123230 W
SFO1         100.6228298 MHz
  
```

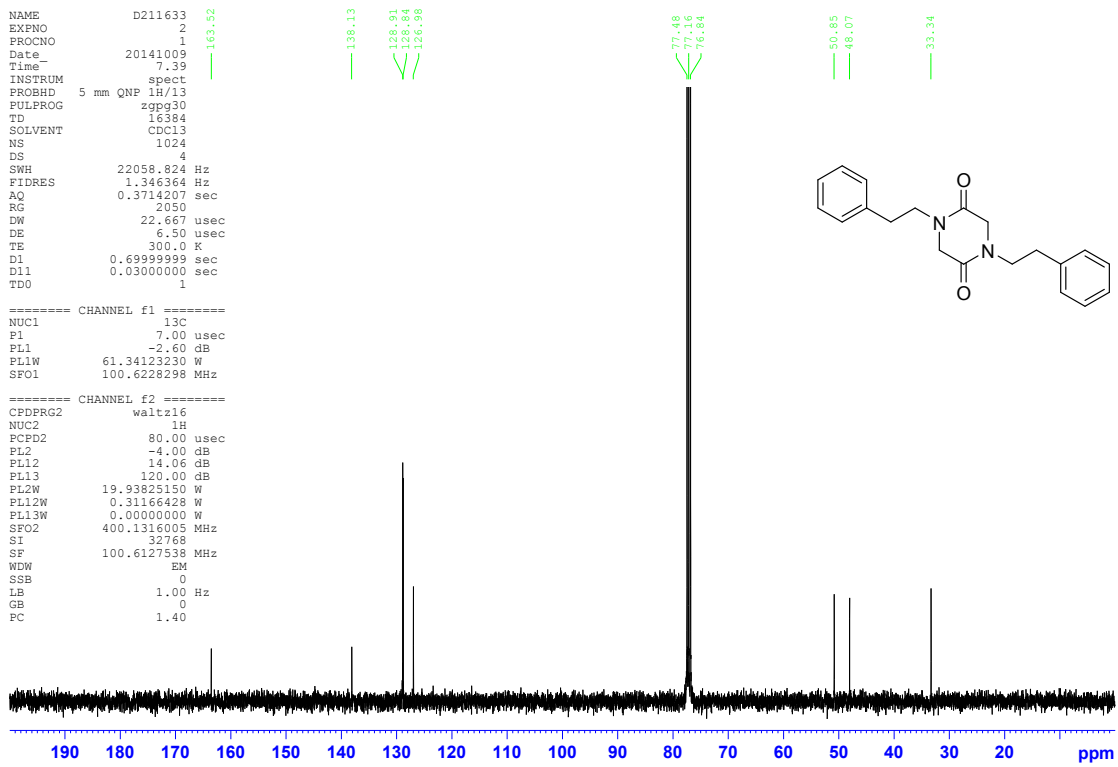
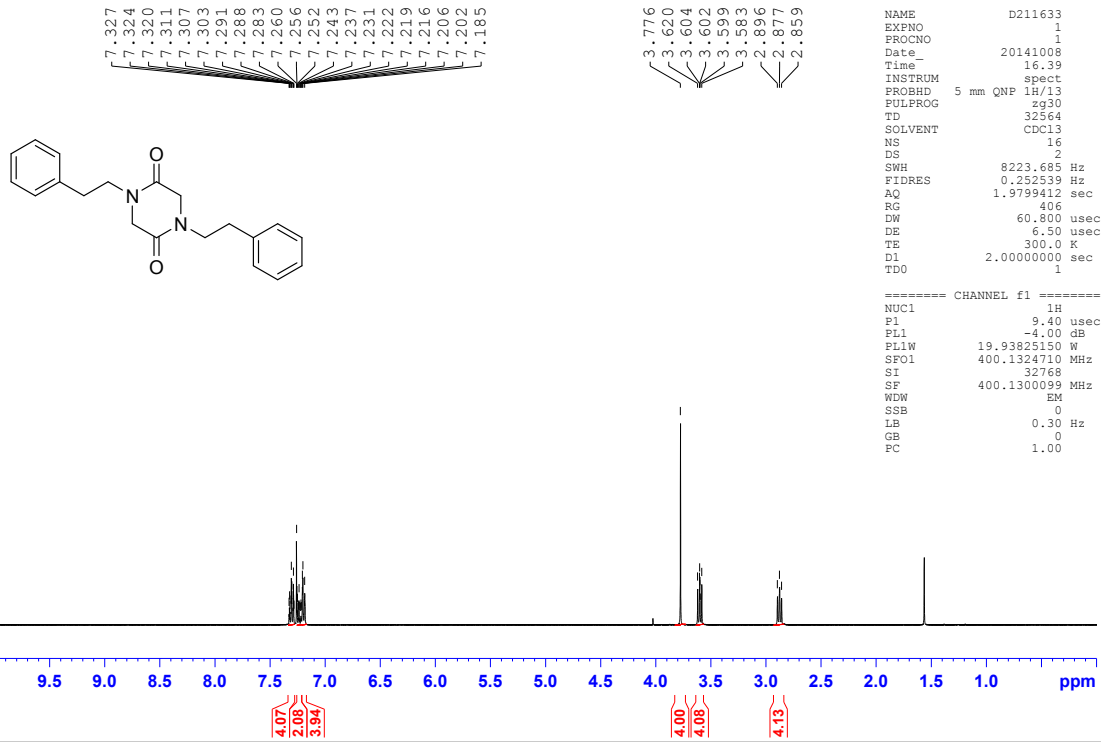
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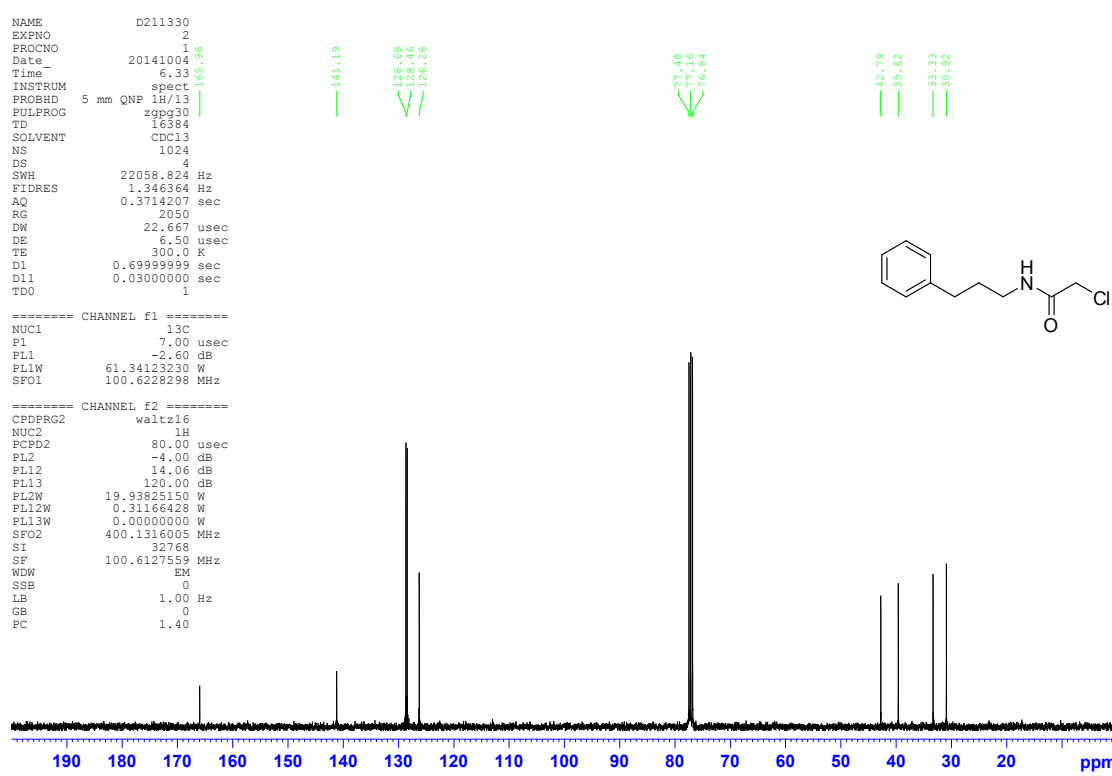
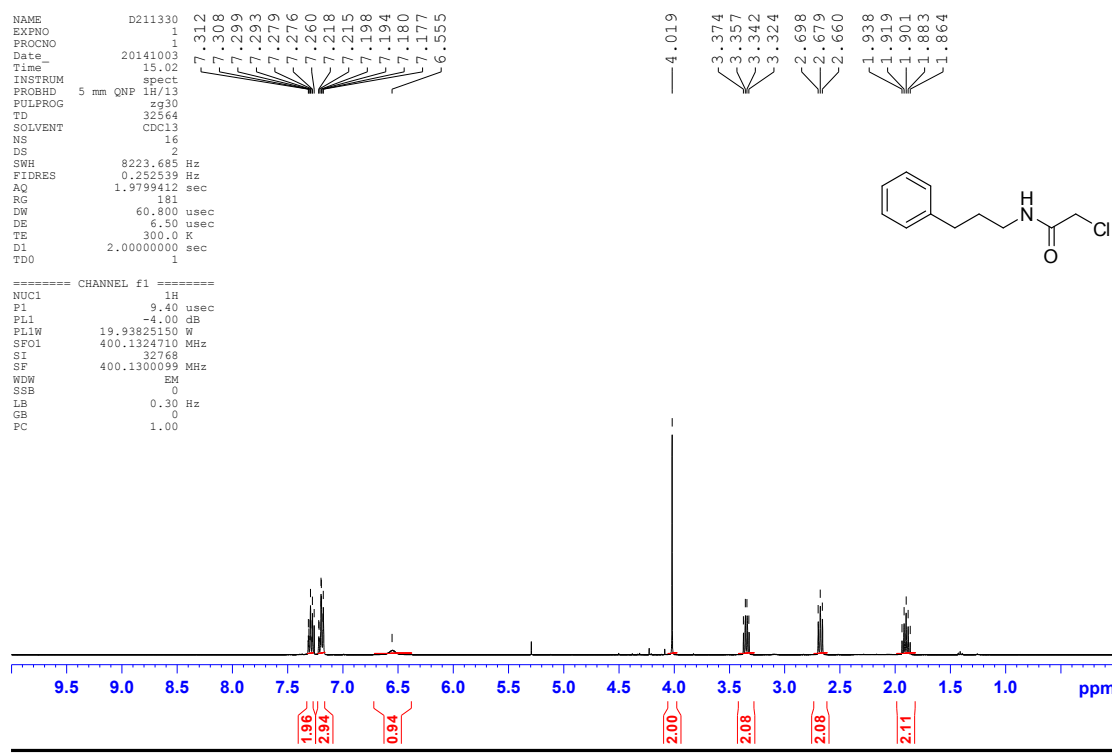
===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2          -4.00 dB
PL12         14.06 dB
PL13         120.00 dB
PL2W         19.93825150 W
PL12W        0.31166428 W
PL13W        0.00000000 W
SFO2         400.1316005 MHz
SI           32768
SF           100.6127553 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```











```

NAME          D211524
EXPNO         1
PROCNO        1
Date_         20141007
Time_         15.48
INSTRUM       spect
PROBHD        5 mm QNP 1H/13
PULPROG       zg30
TD            32564
SOLVENT       CDCl3
NS            16
DS            2
SWH           8223.685 Hz
FIDRES        0.252539 Hz
AQ            1.9799412 sec
RG            228
DW            60.800 usec
DE            6.50 usec
TE            300.0 K
D1            2.00000000 sec
TD0           1

```

```

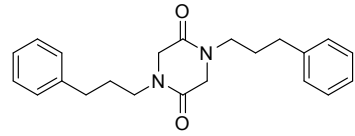
7.300
7.295
7.284
7.280
7.268
7.260
7.252
7.200
7.186

```

```

3.851
3.441
3.422
3.404
2.662
2.643
2.624
1.934
1.919
1.915
1.901
1.897
1.881
1.877
1.859

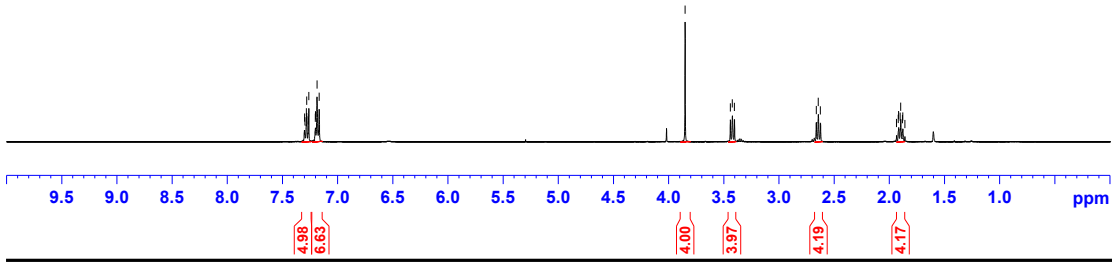
```



```

===== CHANNEL f1 =====
NUC1          1H
P1            9.40 usec
PL1          -4.00 dB
PL1W         19.93825150 W
SFO1         400.1324710 MHz
SI           32768
SF           400.1300099 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

```



```

NAME          D211524
EXPNO         2
PROCNO        1
Date_         20141008
Time_         6.39
INSTRUM       spect
PROBHD        5 mm QNP 1H/13
PULPROG       zgpg30
TD            16384
SOLVENT       CDCl3
NS            1024
DS            4
SWH           22058.824 Hz
FIDRES        1.346364 Hz
AQ            0.3714207 sec
RG            2050
DW            22.667 usec
DE            6.50 usec
TE            300.0 K
D1            0.69999999 sec
D11           0.03000000 sec
TD0           1

```

```

143.42
141.02
128.63
128.35
128.29

```

```

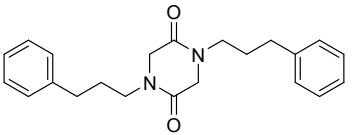
77.48
77.16
76.84

```

```

50.06
48.90
39.19
28.12

```

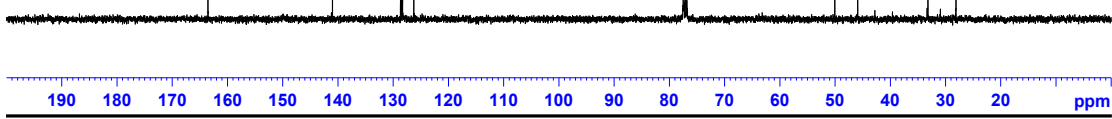


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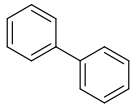
===== CHANNEL f1 =====
NUC1          13C
P1            7.00 usec
PL1          -2.60 dB
PL1W         61.34123230 W
SFO1         100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2          1H
PCPD2        80.00 usec
PL2          -4.00 dB
PL12         14.06 dB
PL13         120.00 dB
PL2W         19.93825150 W
PL12W        0.31166428 W
PL13W        0.00000000 W
SFO2         400.1316005 MHz
SI           32768
SF           100.6127547 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

```



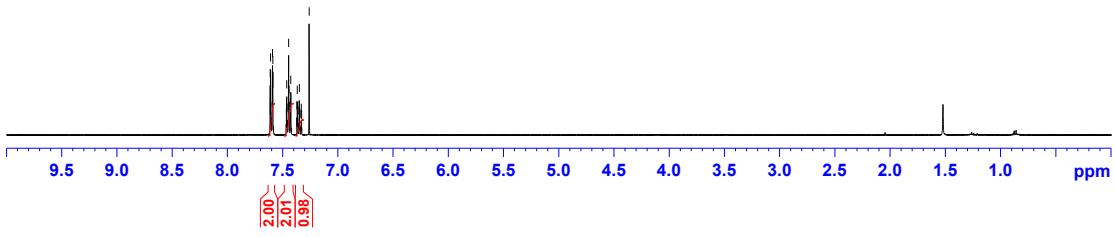




7.612  
7.609  
7.591  
7.588  
7.463  
7.459  
7.445  
7.442  
7.430  
7.426  
7.370  
7.367  
7.364  
7.354  
7.349  
7.344  
7.334  
7.330  
7.327  
7.260

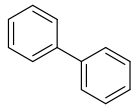
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NAME          D196557
EXPNO         1
PROCNO        1
Date_         20140220
Time         16.50
INSTRUM       spect
PROBHD        5 mm QNP 1H/13
PULPROG       zg30
TD            32768
SOLVENT       CDCl3
NS            16
DS            2
SWH           8223.695 Hz
FIDRES        0.252539 Hz
AQ            1.9799412 sec
RG            406
DW            60.800 usec
DE            6.50 usec
TE            300.0 K
D1            2.00000000 sec
TD0           1
  
```



```

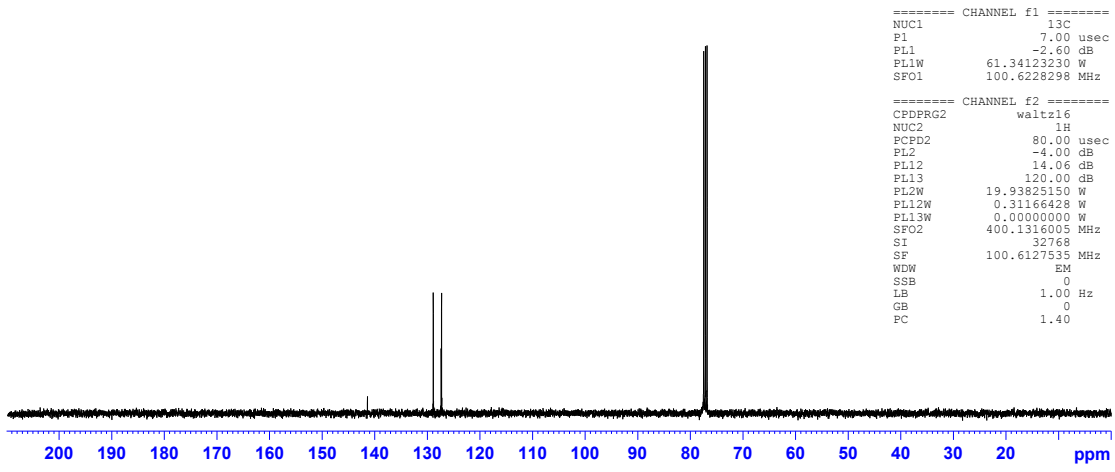
===== CHANNEL f1 =====
NUC1          1H
P1            9.40 usec
PL1          -4.00 dB
PL1W         19.93825150 W
SFO1         400.1324710 MHz
SI           32768
SF           400.1300099 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00
  
```



141.41  
128.90  
127.39  
127.32  
77.48  
77.36  
76.84

```

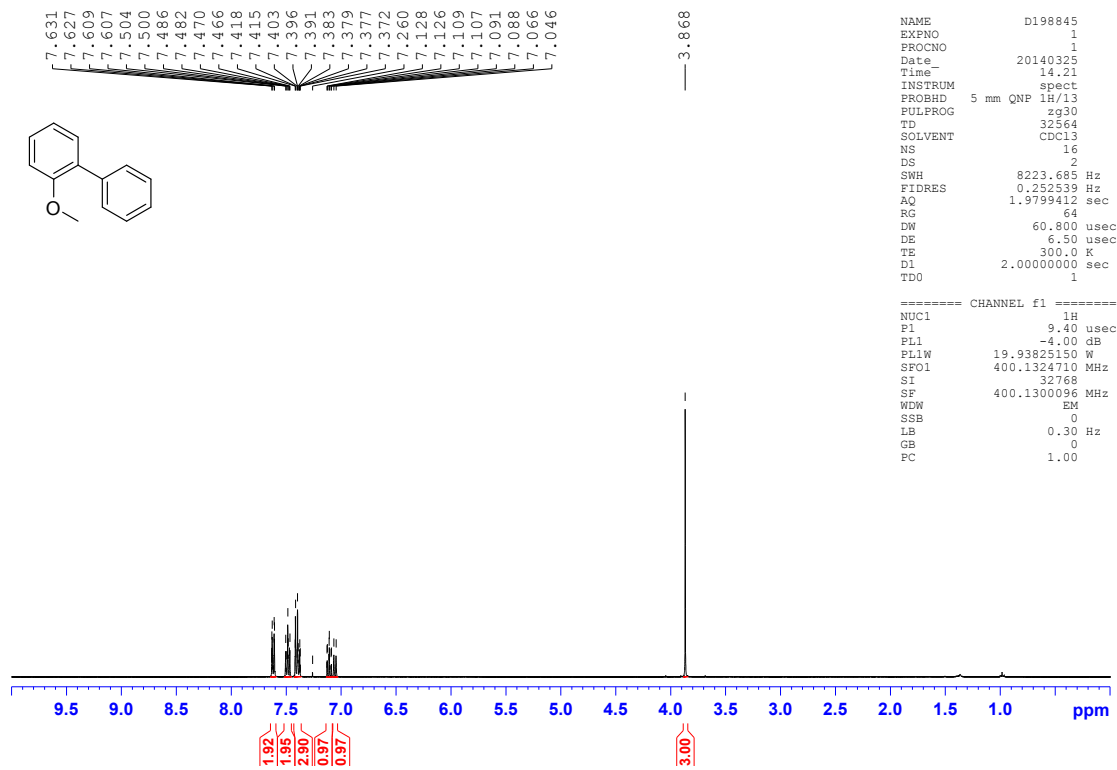
NAME          D198321
EXPNO         1
PROCNO        1
Date_         20140318
Time         18.53
INSTRUM       spect
PROBHD        5 mm QNP 1H/13
PULPROG       zgpg30
TD            16384
SOLVENT       CDCl3
NS            1024
DS            4
SWH           22058.824 Hz
FIDRES        1.346364 Hz
AQ            0.3714207 sec
RG            2050
DW            22.667 usec
DE            6.50 usec
TE            300.0 K
D1            0.69999999 sec
D11           0.03000000 sec
TD0           1
  
```



```

===== CHANNEL f1 =====
NUC1          13C
P1            7.00 usec
PL1          -2.60 dB
PL1W         61.34123230 W
SFO1         100.6228298 MHz

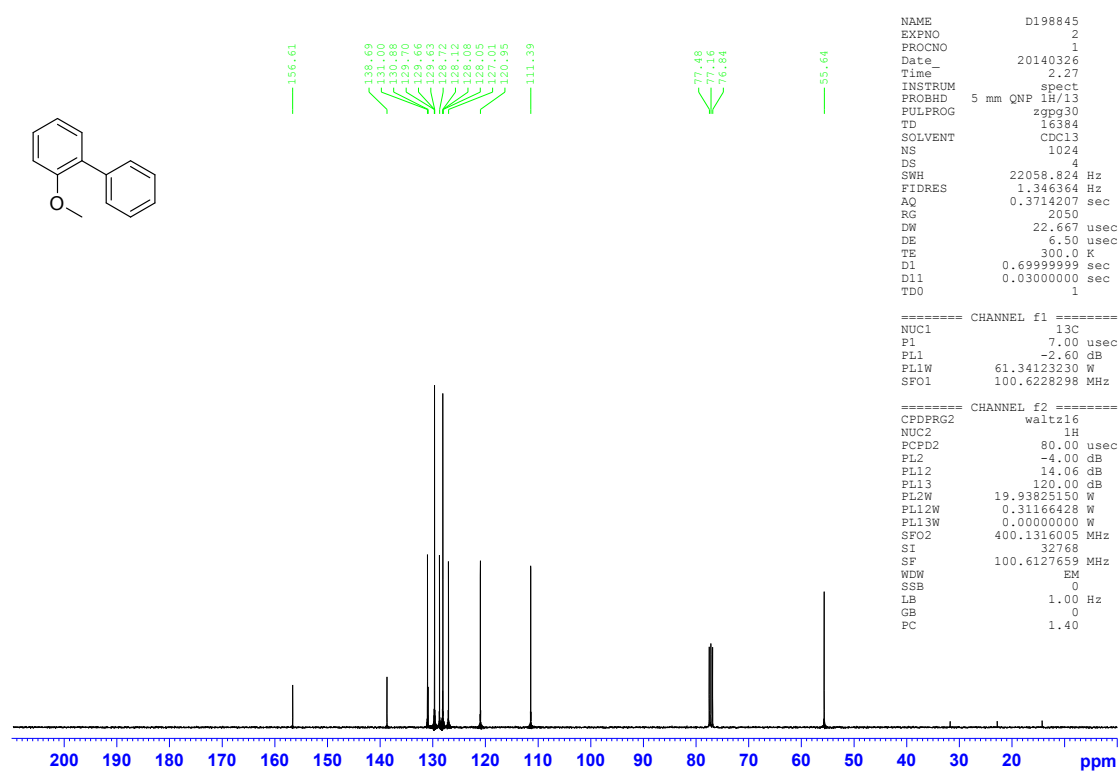
===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2          -4.00 dB
PL12         14.06 dB
PL13         120.00 dB
PL2W         19.93825150 W
PL12W        0.31166428 W
PL13W        0.00000000 W
SFO2         400.1316005 MHz
SI           32768
SF           100.6127535 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
  
```



```

NAME          D198845
EXPNO         1
PROCNO        1
Date_         20140325
Time_         14.21
INSTRUM       spect
PROBHD        5 mm QNP 1H/13
PULPROG       zg30
TD            32564
SOLVENT       CDCl3
NS            16
DS            2
SWH           8223.685 Hz
FIDRES        0.252539 Hz
AQ            1.9799412 sec
RG            64
DW            60.800 usec
DE            6.50 usec
TE            300.0 K
D1            2.00000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          1H
P1            9.40 usec
PL1          -4.00 dB
PL1W         19.93825150 W
SFO1         400.1324710 MHz
SI           32768
SF           400.1300096 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00
  
```

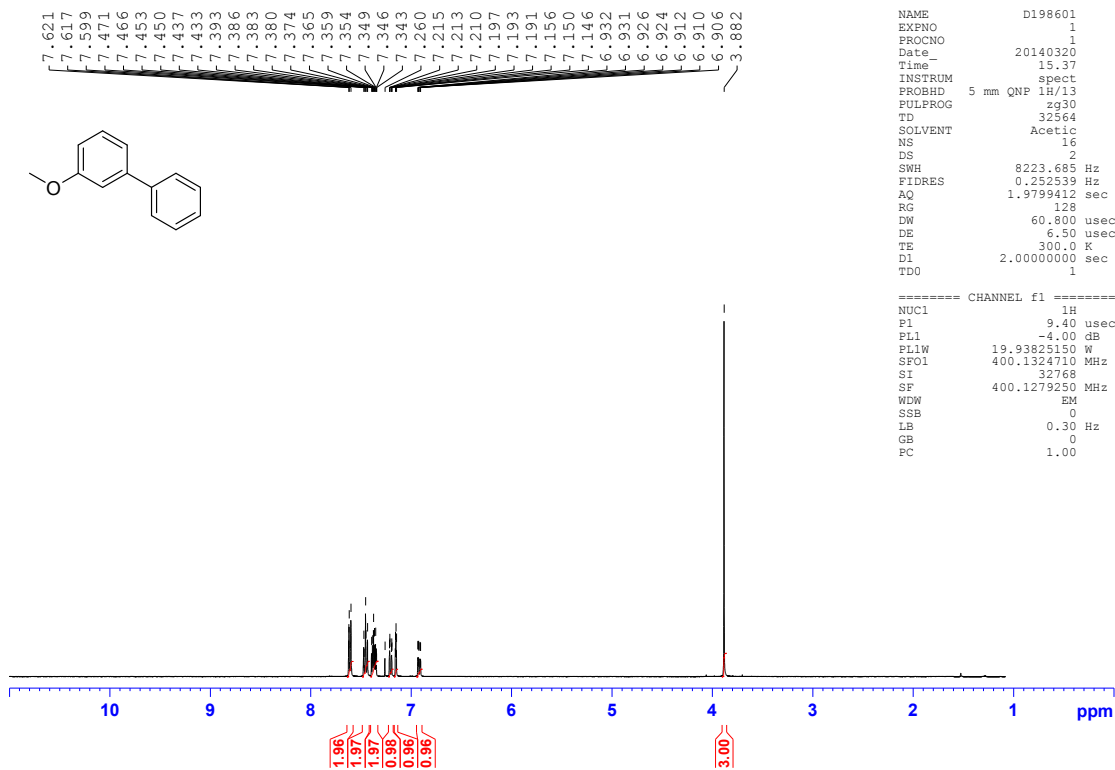
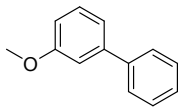


```

NAME          D198845
EXPNO         2
PROCNO        1
Date_         20140326
Time_         2.27
INSTRUM       spect
PROBHD        5 mm QNP 1H/13
PULPROG       zgpg30
TD            16384
SOLVENT       CDCl3
NS            1024
DS            4
SWH           22058.824 Hz
FIDRES        1.346364 Hz
AQ            0.3714207 sec
RG            2050
DW            22.667 usec
DE            6.50 usec
TE            300.0 K
D1            0.6999999 sec
D11           0.03000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          13C
P1            7.00 usec
PL1          -2.60 dB
PL1W         61.34123230 W
SFO1         100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2          -4.00 dB
PL12         14.06 dB
PL13         120.00 dB
PL2W         19.93825150 W
PL12W        0.31166428 W
PL13W        0.00000000 W
SFO2         400.1316005 MHz
SI           32768
SF           100.6127659 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
  
```

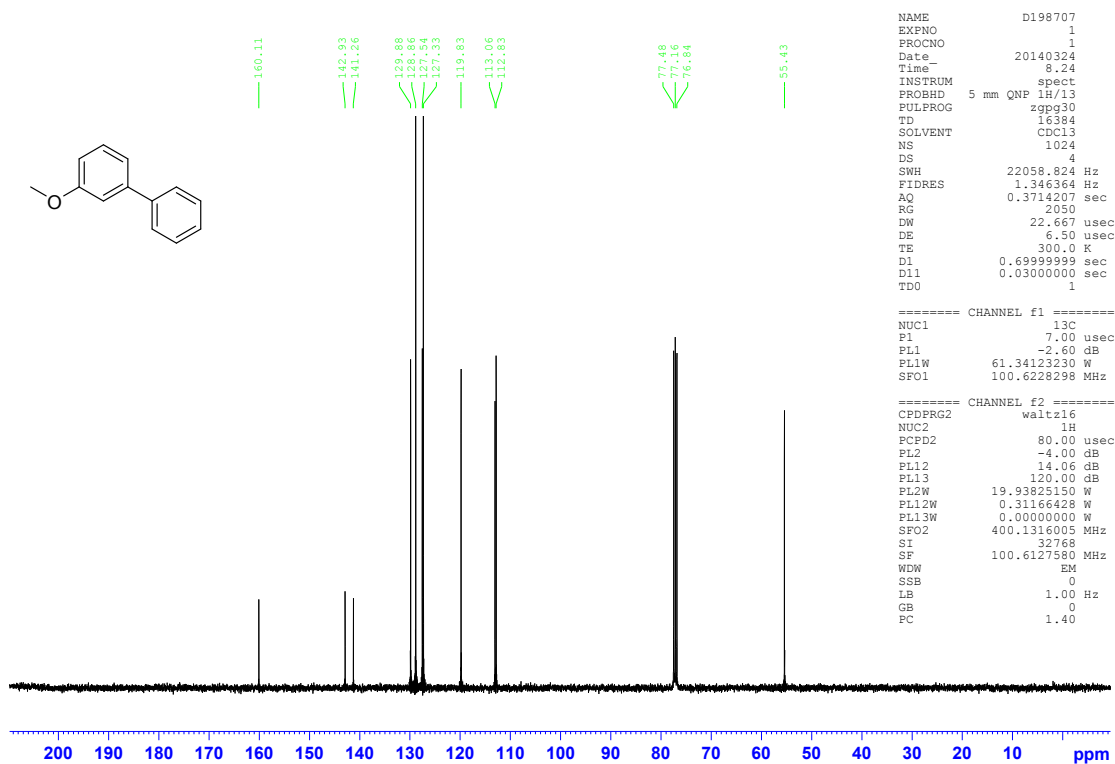
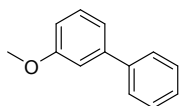


```

NAME          D198601
EXPNO         1
PROCNO       1
Date_        20140320
Time_        15.37
INSTRUM     spect
PROBHD       5 mm QNP 1H/13
PULPROG     zg30
TD           32768
SOLVENT     Acetic
NS           16
DS           2
SWH          8223.685 Hz
FIDRES       0.252539 Hz
AQ           1.9799412 sec
RG           128
DW           60.800 usec
DE           6.50 usec
TE           300.0 K
D1           2.00000000 sec
TD0          1
  
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            9.40 usec
PL1          -4.00 dB
PL1W         19.93825150 W
SFO1         400.1324711 MHz
SI            32768
SF           400.1279250 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00
  
```



```

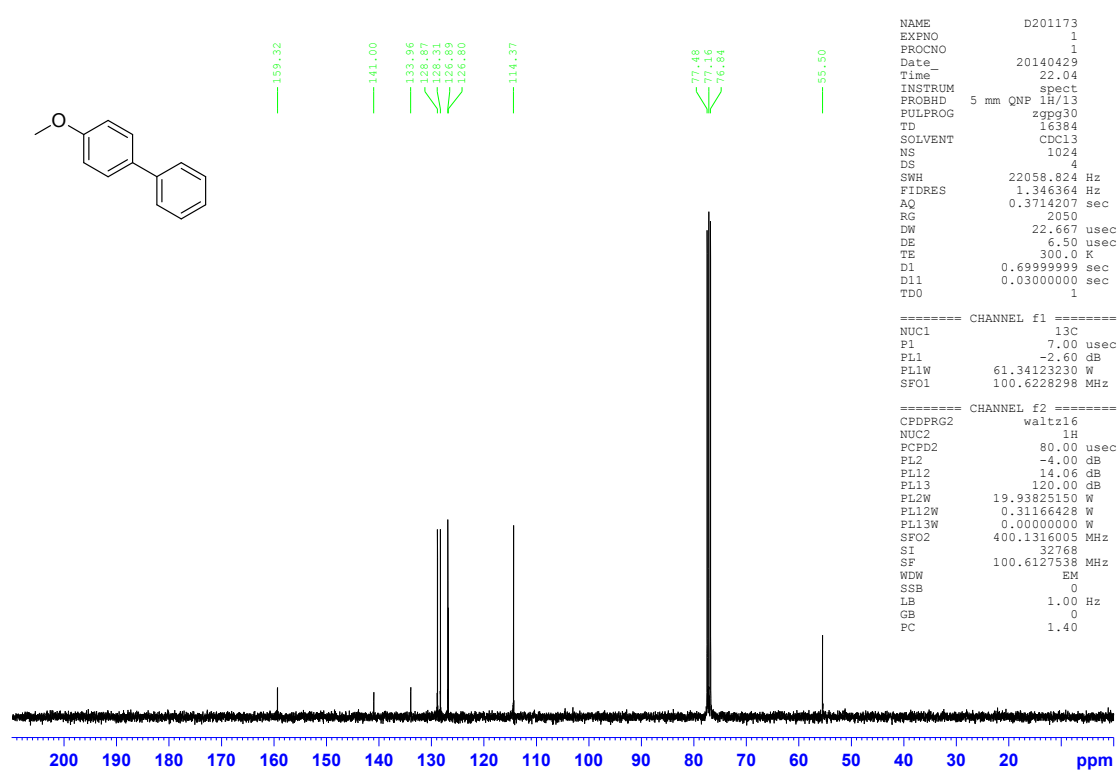
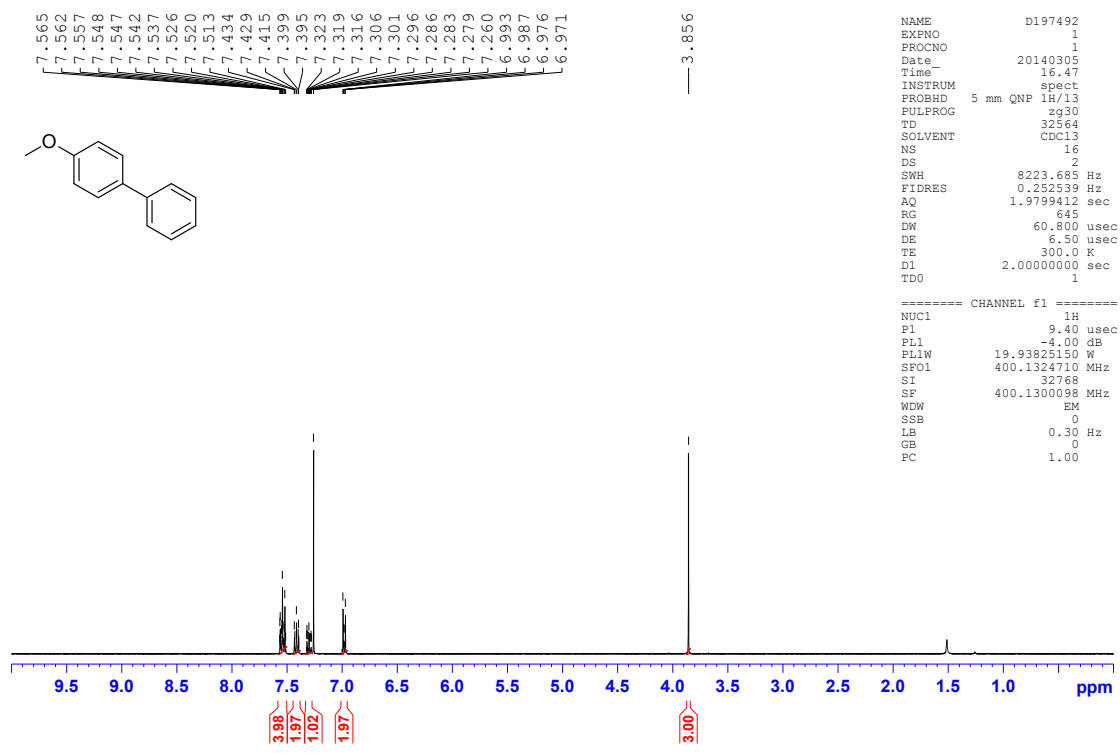
NAME          D198707
EXPNO         1
PROCNO       1
Date_        20140324
Time_        8.24
INSTRUM     spect
PROBHD       5 mm QNP 1H/13
PULPROG     zgpg30
TD           16384
SOLVENT     CDCl3
NS           1024
DS           4
SWH          22058.824 Hz
FIDRES       1.346364 Hz
AQ           0.3714207 sec
RG           2050
DW           22.667 usec
DE           6.50 usec
TE           300.0 K
D1           0.69999999 sec
D11          0.03000000 sec
TD0          1
  
```

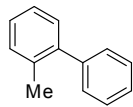
```

===== CHANNEL f1 =====
NUC1          13C
P1            7.00 usec
PL1          -2.60 dB
PL1W         61.34123230 W
SFO1         100.6228298 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2     waltz16
NUC2          1H
PCPD2       80.00 usec
PL2          -4.00 dB
PL12         14.06 dB
PL13         120.00 dB
PL2W         19.93825150 W
PL12W        0.31166428 W
PL13W        0.00000000 W
SFO2         400.1316005 MHz
SI            32768
SF           100.6127580 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
  
```





7.657  
7.638  
7.459  
7.441  
7.401  
7.383  
7.367  
7.314  
7.291

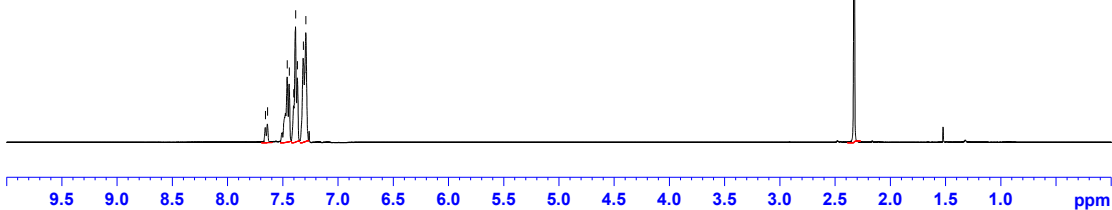
2.330

```

NAME          D205946
EXPNO         1
PROCNO       1
Date_         20140709
Time_        10.38
INSTRUM      spect
PROBHD       5 mm QNP 1H/13
PULPROG      zgpg30
TD           32564
SOLVENT      CDCl3
NS           16
DS           4
SWH          8223.685 Hz
FIDRES       0.252539 Hz
AQ           1.9799412 sec
RG           101
DW           60.800 usec
DE           6.50 usec
TE           300.0 K
D1           2.00000000 sec
TDO          1
  
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            9.40 usec
PL1          -4.00 dB
PL1W         19.93825150 W
SFO1         400.1324710 MHz
SI           32768
SF           400.1300098 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00
  
```



0.49  
2.49  
3.13  
3.87

3.00

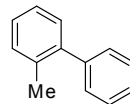
```

NAME          D205946
EXPNO         2
PROCNO       1
Date_         20140710
Time_         4.27
INSTRUM      spect
PROBHD       5 mm QNP 1H/13
PULPROG      zgpg30
TD           16384
SOLVENT      CDCl3
NS           1024
DS           4
SWH          22058.824 Hz
FIDRES       1.346364 Hz
AQ           0.3714207 sec
RG           2050
DW           22.667 usec
DE           6.50 usec
TE           300.0 K
D1           0.69999999 sec
D11          0.03000000 sec
TDO          1
  
```

142.13  
142.09  
135.47  
135.43  
135.39  
135.35  
135.31  
135.27  
135.23  
135.19  
135.15  
135.11  
135.07  
135.03

77.46  
77.46  
77.46

20.38



```

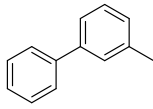
===== CHANNEL f1 =====
NUC1          13C
P1            7.00 usec
PL1          -2.60 dB
PL1W         61.34123230 W
SFO1         100.6228298 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2          1H
PCPD2        80.00 usec
PL2          -4.00 dB
PL12         14.06 dB
PL13         120.00 dB
PL2W         19.93825150 W
PL12W        0.31166428 W
PL13W        0.00000000 W
SFO2         400.1316005 MHz
SI           32768
SF           100.6127603 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
  
```



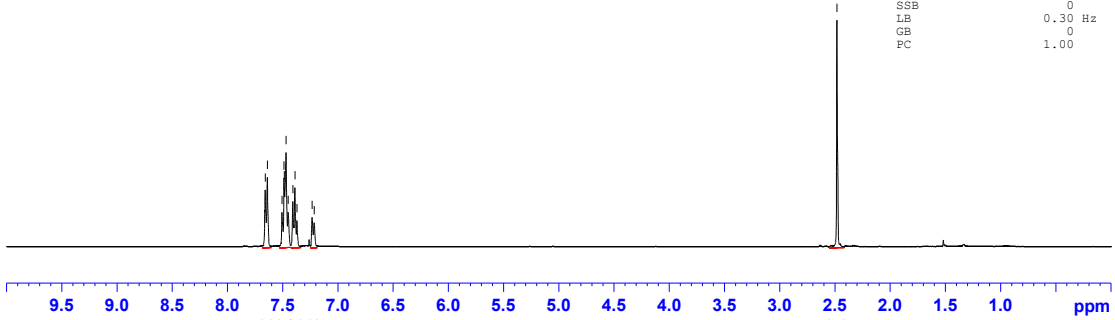
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm



7.658  
7.638  
7.506  
7.488  
7.485  
7.469  
7.450  
7.408  
7.389  
7.371  
7.293  
7.215

```

NAME      D209687
EXPNO     1
PROCNO    1
Date_     20140911
Time      11.31
INSTRUM   spect
PROBHD    5 mm QNP 1H/13
PULPROG   zg30
TD         32768
SOLVENT   CDCl3
NS         16
DS         2
SWH        8223.695 Hz
FIDRES     0.252539 Hz
AQ         1.9799412 sec
RG          80.6
DW         60.800 usec
DE         6.50 usec
TE         300.0 K
D1         2.00000000 sec
TDO        1
  
```



2.04  
3.98  
1.99  
0.97

3.00

```

===== CHANNEL f1 =====
NUC1      1H
P1         9.40 usec
PL1       -4.00 dB
PL1W      19.93825150 W
SFO1      400.1324710 MHz
SI         32768
SF         400.1300096 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```

```

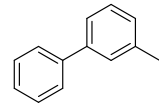
NAME      D209687
EXPNO     2
PROCNO    1
Date_     20140912
Time      1.26
INSTRUM   spect
PROBHD    5 mm QNP 1H/13
PULPROG   zgpg30
TD         16384
SOLVENT   CDCl3
NS         1024
DS         4
SWH        22058.824 Hz
FIDRES     1.346364 Hz
AQ         0.3714207 sec
RG          2050
DW         22.667 usec
DE         6.50 usec
TE         300.0 K
D1         0.69999999 sec
D11        0.03000000 sec
TDO        1
  
```

141.40  
141.40  
138.45  
138.45

138.83  
138.80  
138.13  
138.13  
134.42  
134.42

77.46  
77.46  
76.84  
76.84

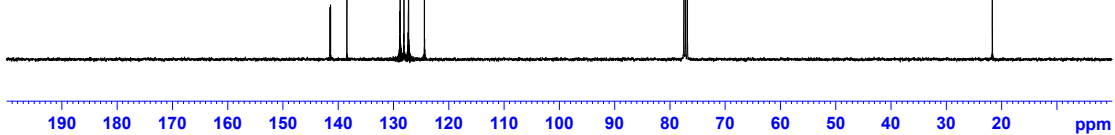
21.67

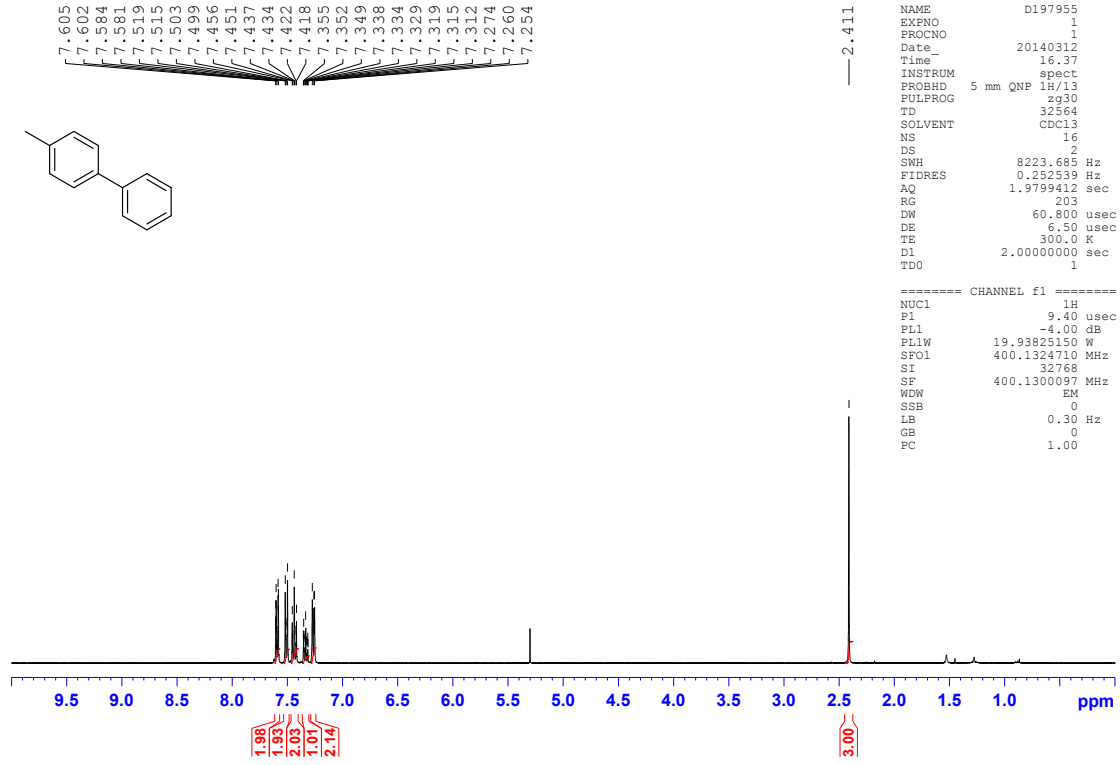


```

===== CHANNEL f1 =====
NUC1      13C
P1         7.00 usec
PL1       -2.60 dB
PL1W      61.34123230 W
SFO1      100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2     80.00 usec
PL2       -4.00 dB
PL12      14.06 dB
PL13      120.00 dB
PL2W      19.93825150 W
PL12W     0.31166428 W
PL13W     0.00000000 W
SFO2      400.1316005 MHz
SI         32768
SF         100.6127606 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```



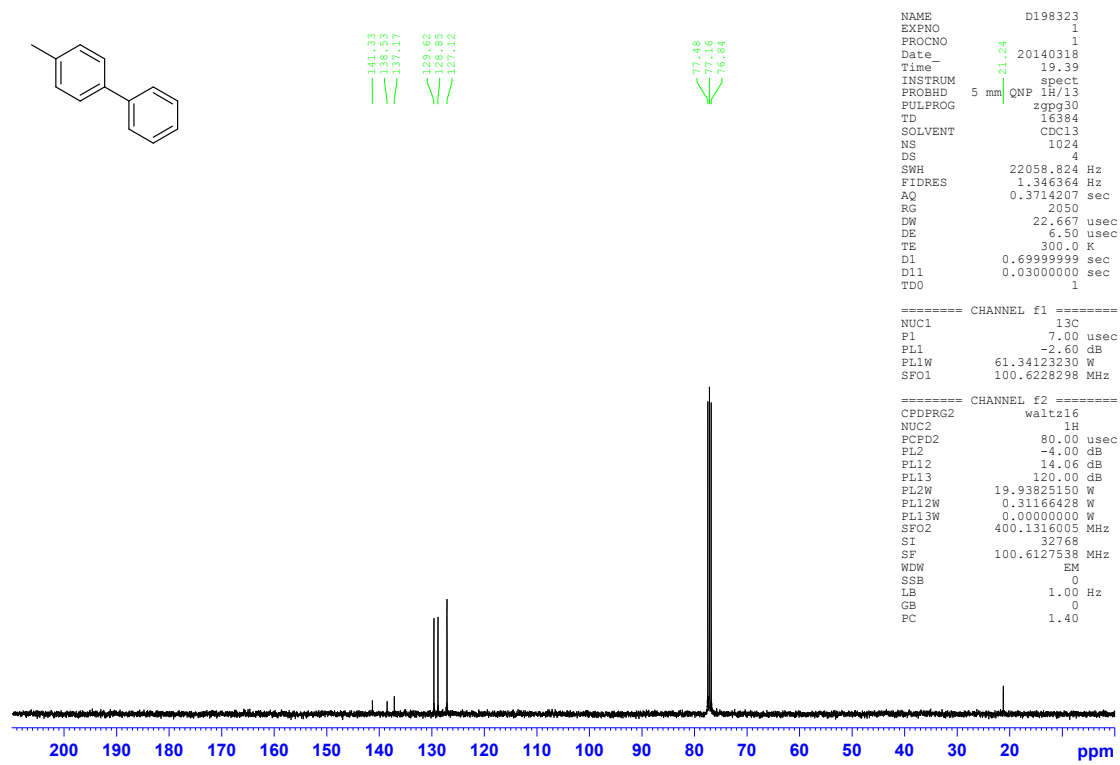


```

NAME          D197955
EXPNO         1
PROCNO        1
Date_         20140312
Time_         16.37
INSTRUM       spect
PROBHD        5 mm QNP 1H/13
PULPROG       zg30
TD            32564
SOLVENT       CDCl3
NS            16
DS            2
SWH           8223.685 Hz
FIDRES        0.252539 Hz
AQ            1.9799412 sec
RG            203
DW            60.800 usec
DE            6.50 usec
TE            300.0 K
D1            2.00000000 sec
TDO           1
  
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            9.40 usec
PL1           -4.00 dB
PL1W          19.93825150 W
SFO1          400.1324710 MHz
SI            32768
SF            400.1300097 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```



```

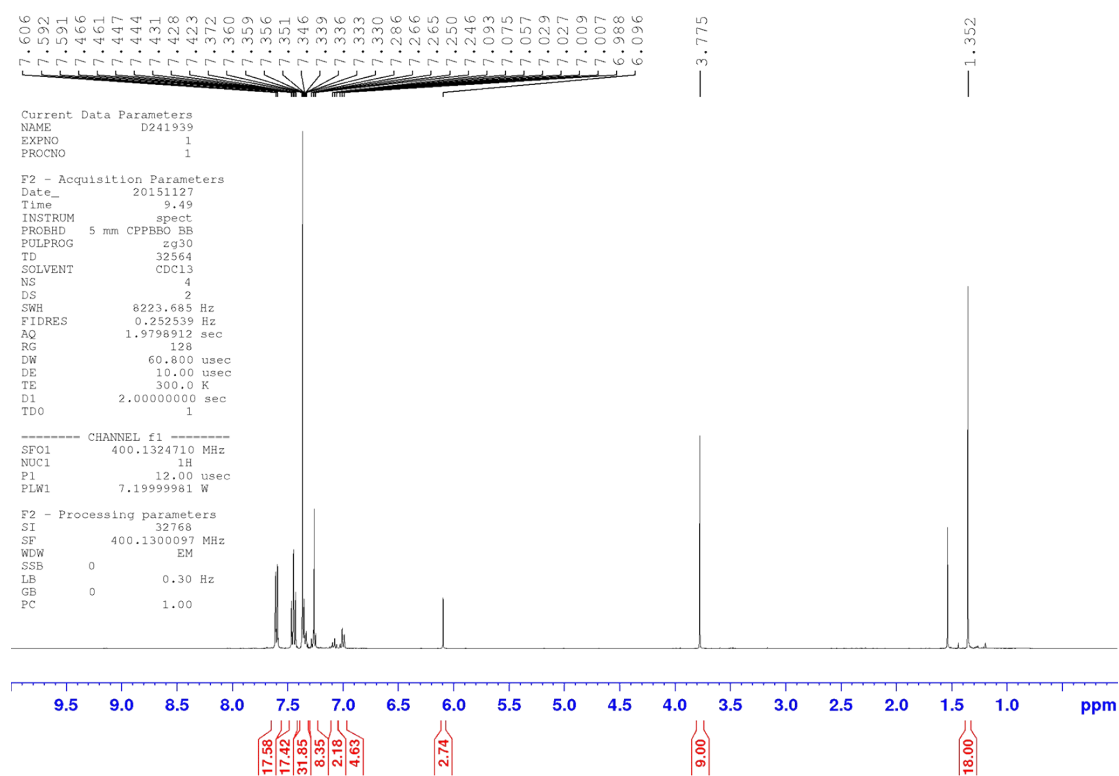
NAME          D198323
EXPNO         1
PROCNO        1
Date_         20140318
Time_         19.39
INSTRUM       spect
PROBHD        5 mm QNP 1H/13
PULPROG       zgpg30
TD            16384
SOLVENT       CDCl3
NS            1024
DS            4
SWH           22058.824 Hz
FIDRES        1.346364 Hz
AQ            0.3714207 sec
RG            2050
DW            22.667 usec
DE            6.50 usec
TE            300.0 K
D1            0.699999999 sec
D11           0.030000000 sec
TDO           1
  
```

```

===== CHANNEL f1 =====
NUC1          13C
P1            7.00 usec
PL1           -2.60 dB
PL1W          61.34123230 W
SFO1          100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           -4.00 dB
PL12          14.06 dB
PL13          120.00 dB
PL2W          19.93825150 W
PL12W         0.31166428 W
PL13W         0.00000000 W
SFO2          400.1316005 MHz
SI            32768
SF            100.6127538 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```

Example of crude NMR containing biphenyl **37** and *tert*-butoxybenzene **48**



Example of crude NMR containing 4-methoxy-1,1'-biphenyl **40**, 1-(*tert*-butoxy)-3-methoxybenzene **44** and 1-(*tert*-butoxy)-4-methoxybenzene **46**

