

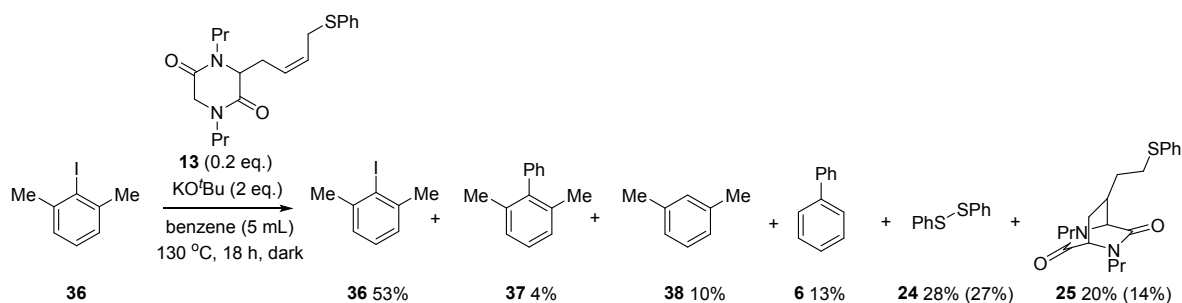
**Evidence of single electron transfer from the enolate anion of an
N,N'-dialkyldiketopiperazine additive in BHAS coupling reactions:**

Katie J. Emery, Tell Tuttle, and John A. Murphy

SUPPORTING INFORMATION

1.1 Experimental supplementary information

Example yield calculation using 1,3,5-trimethoxybenzene as the internal standard ¹H-NMR of the crude mixture (Table 3, entry 3):

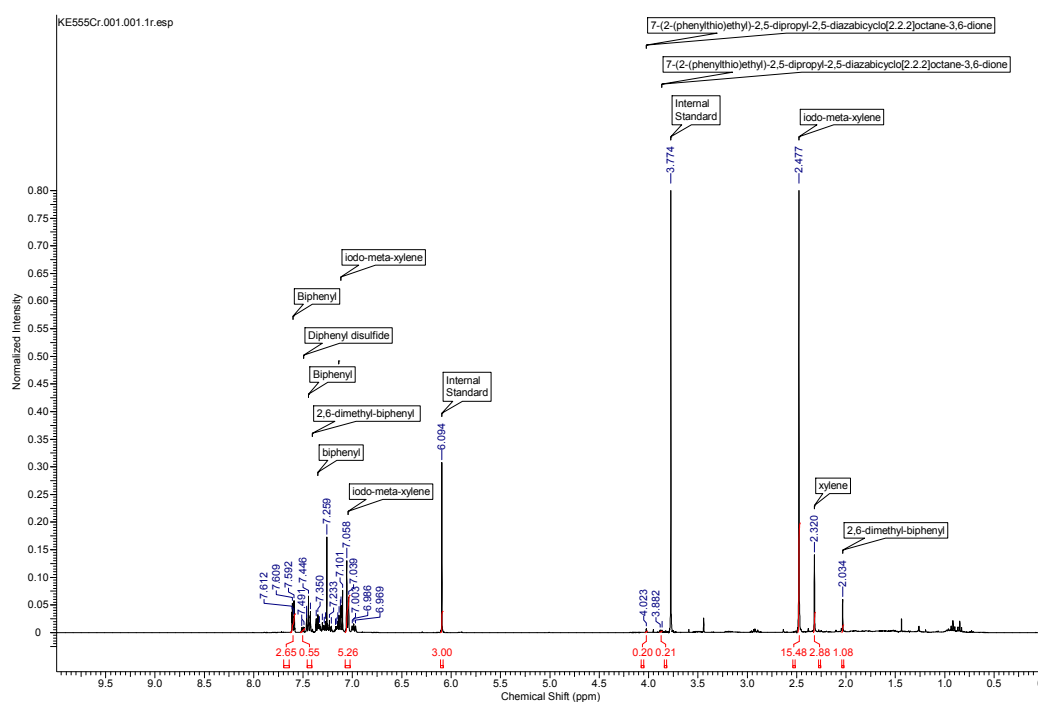


1,3,5-Trimethoxybenzene (16.8 mg, 0.10 mmol) was added to the crude mixture. The integral for the aromatic protons (δ 6.09) is set to 3 units representing 3 protons.

For the coupled product, 2,6-dimethylbiphenyl **37**, the integral of the dimethyl signal (δ 2.03) has 6 H) was measured and the following calculation gave the yield of coupled product:

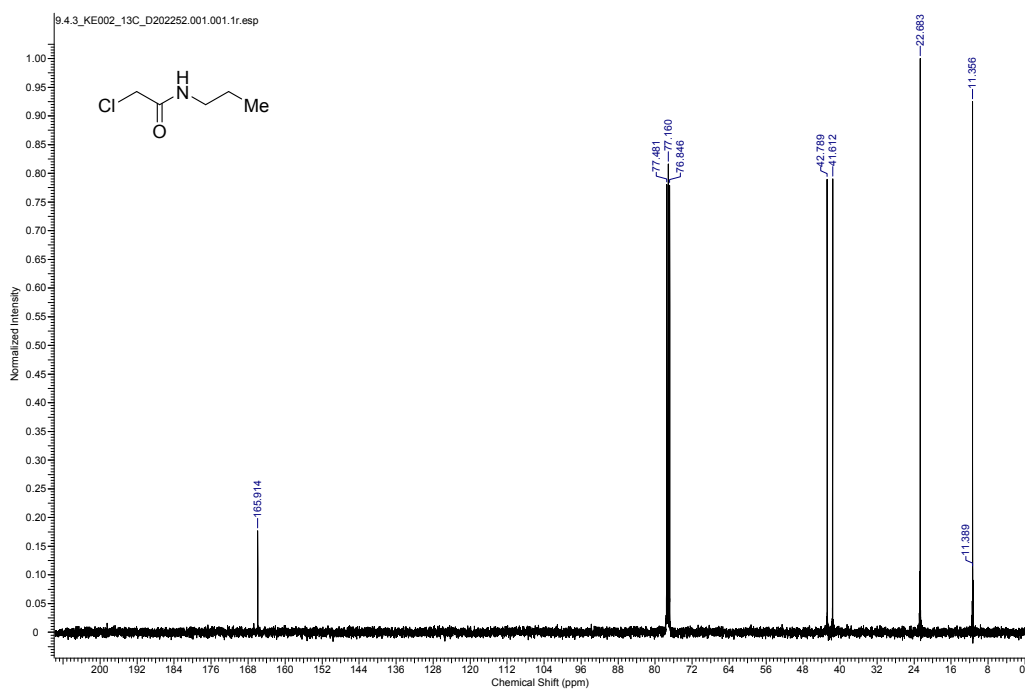
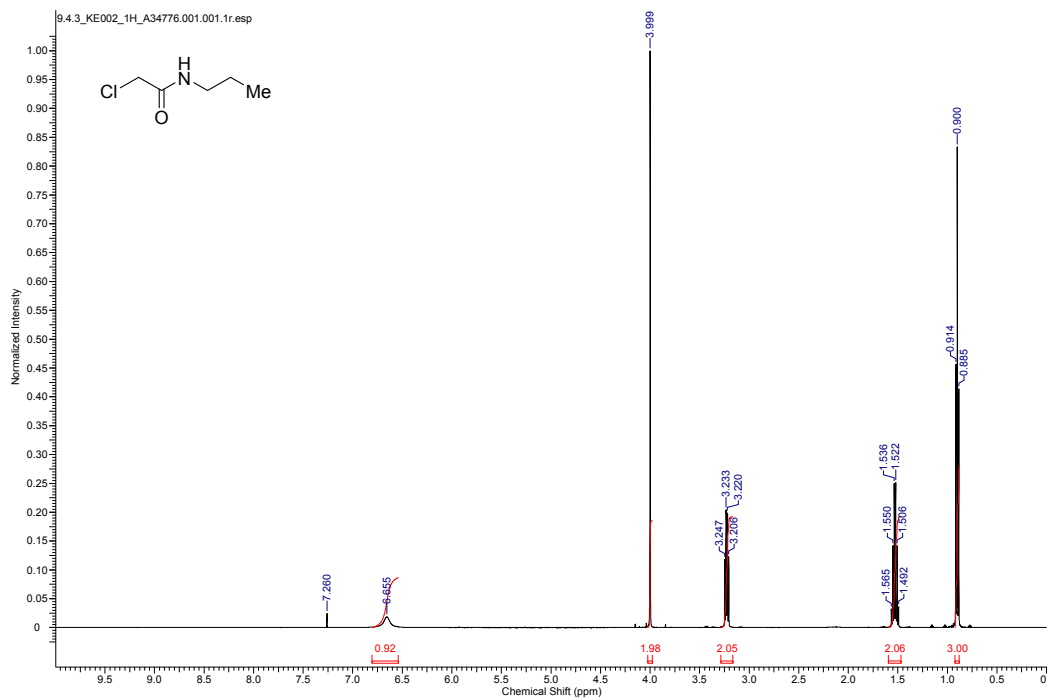
$$(1.08/6) \times 0.1 \text{ mmol} = 0.018 \text{ mmol}$$

$$(0.018 \text{ mmol}/0.5 \text{ mmol}) \times 100 = 3.6\% = 4\%$$

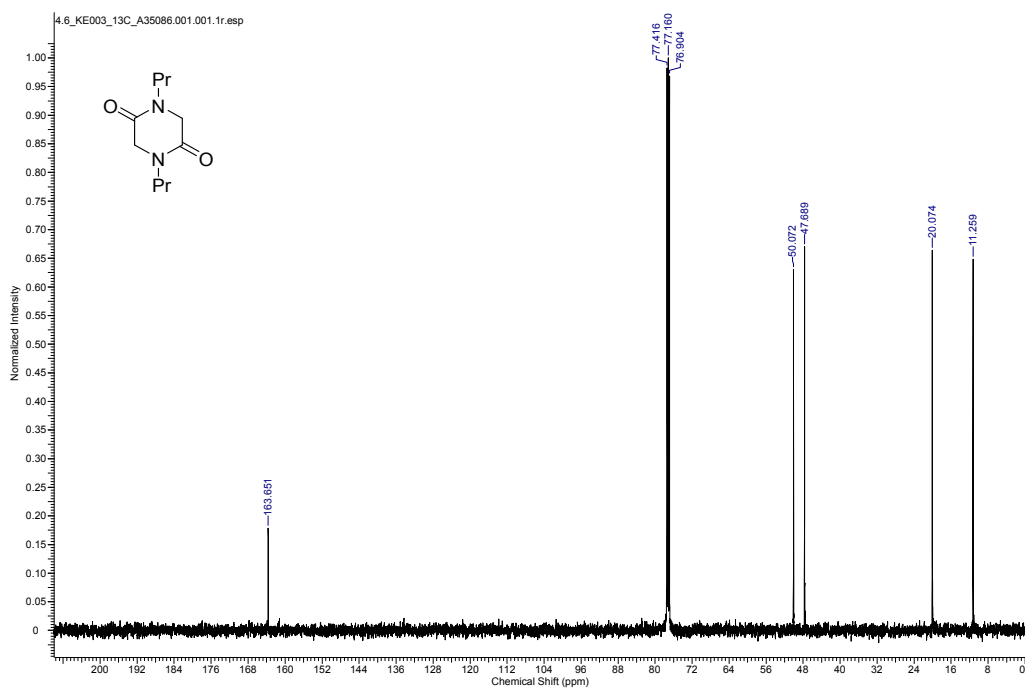
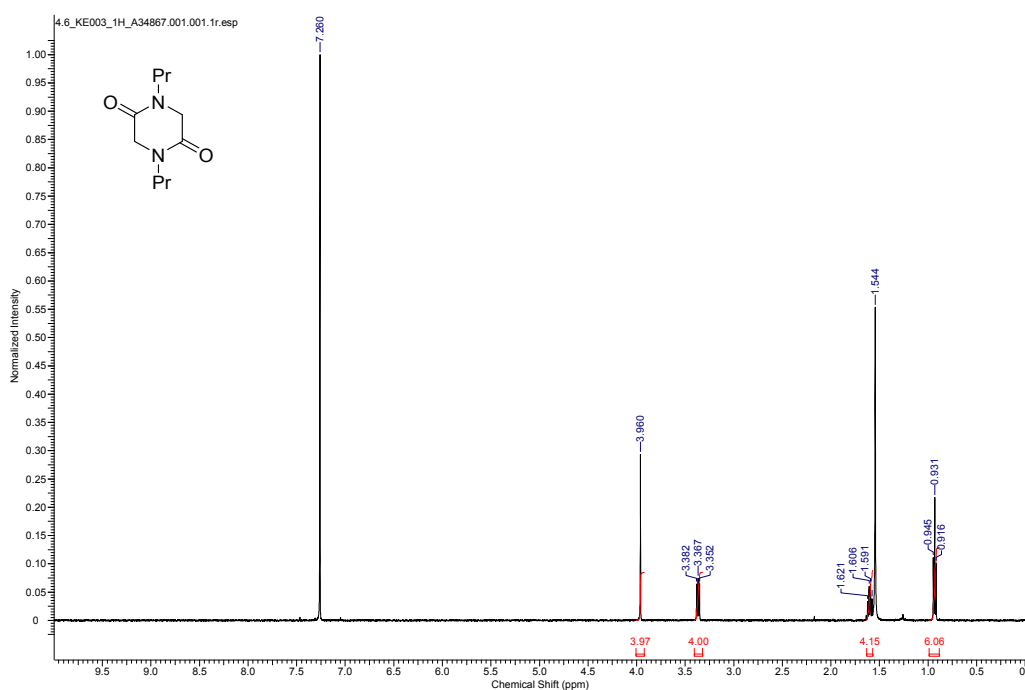


1.2 NMR spectra for the compounds reported

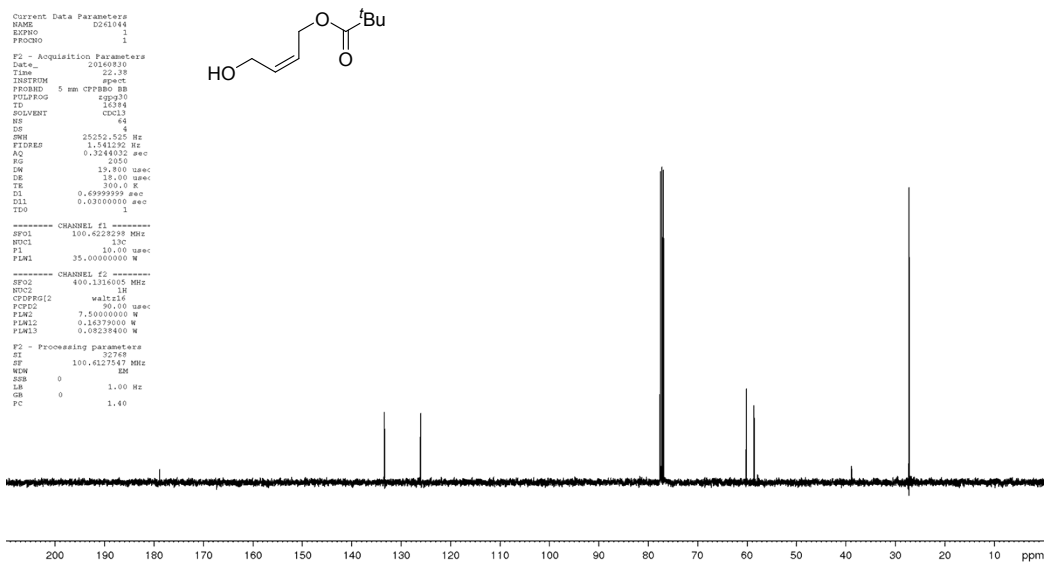
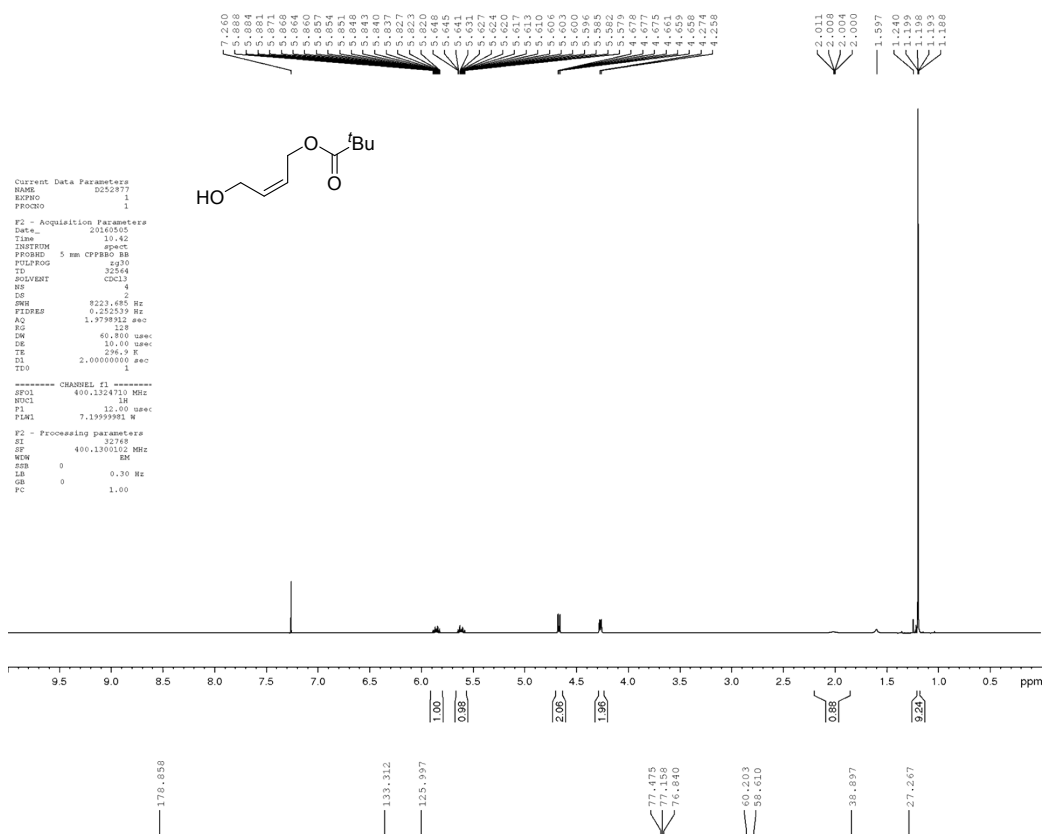
^1H -NMR and ^{13}C -NMR 2-chloro-*N*-propylacetamide



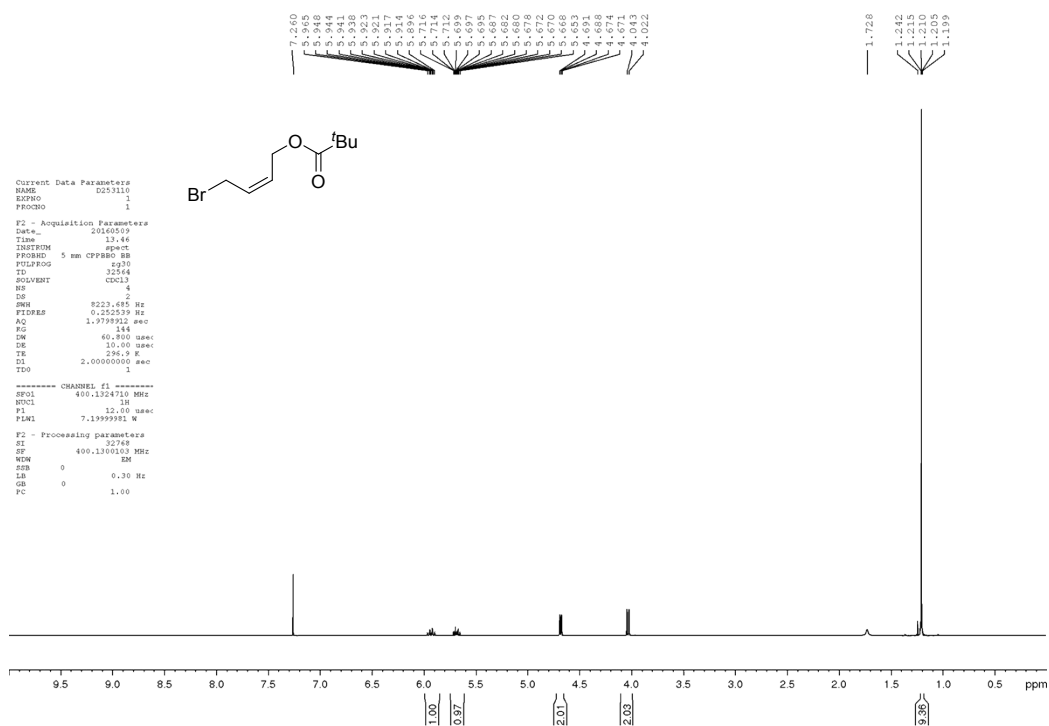
¹H-NMR and ¹³C-NMR 1,4-dipropylpiperazine-2,5-dione 7



¹H-NMR and ¹³C-NMR *cis*-4-hydroxybut-2-en-1-yl pivalate

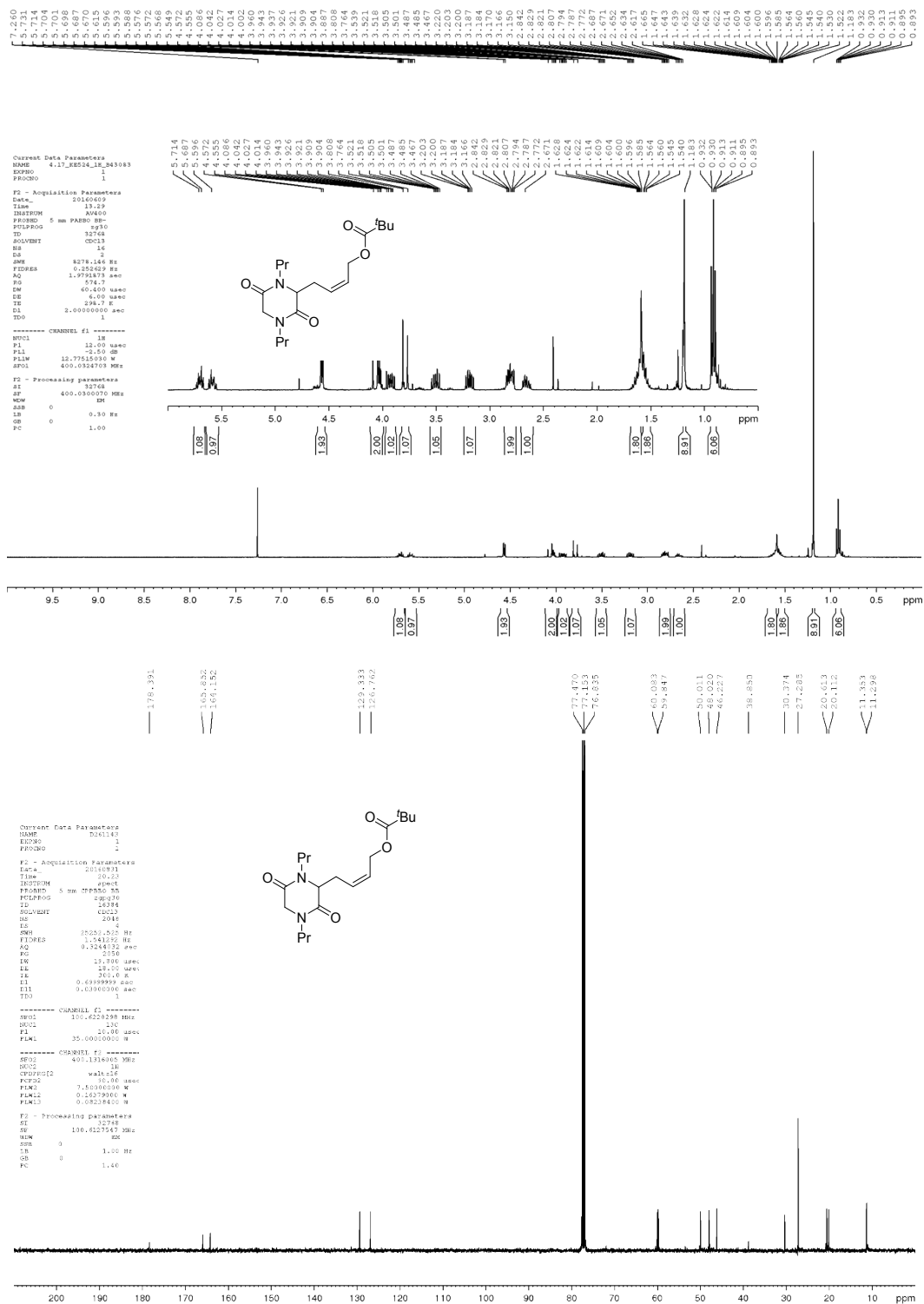


¹H-NMR and ¹³C-NMR *cis*-4-bromobut-2-en-1-yl pivalate 10



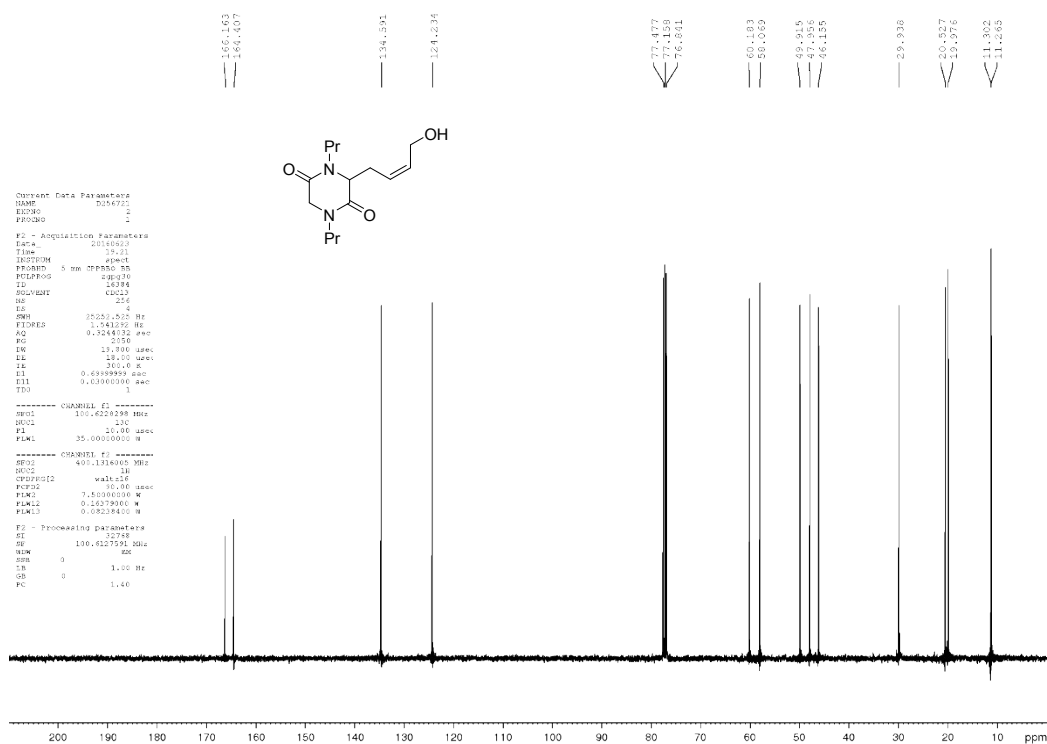
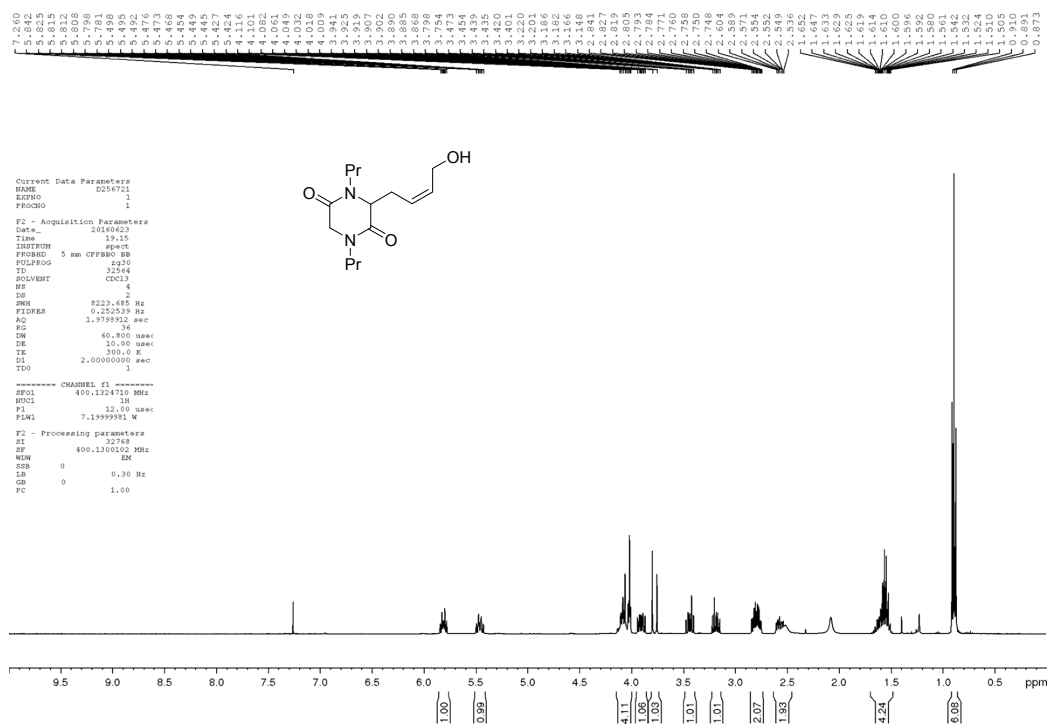
¹H-NMR and ¹³C-NMR *cis*-4-(3,6-dioxo-1,4-dipropylpiperazin-2-yl)but-2-en-1-yl pivalate

11

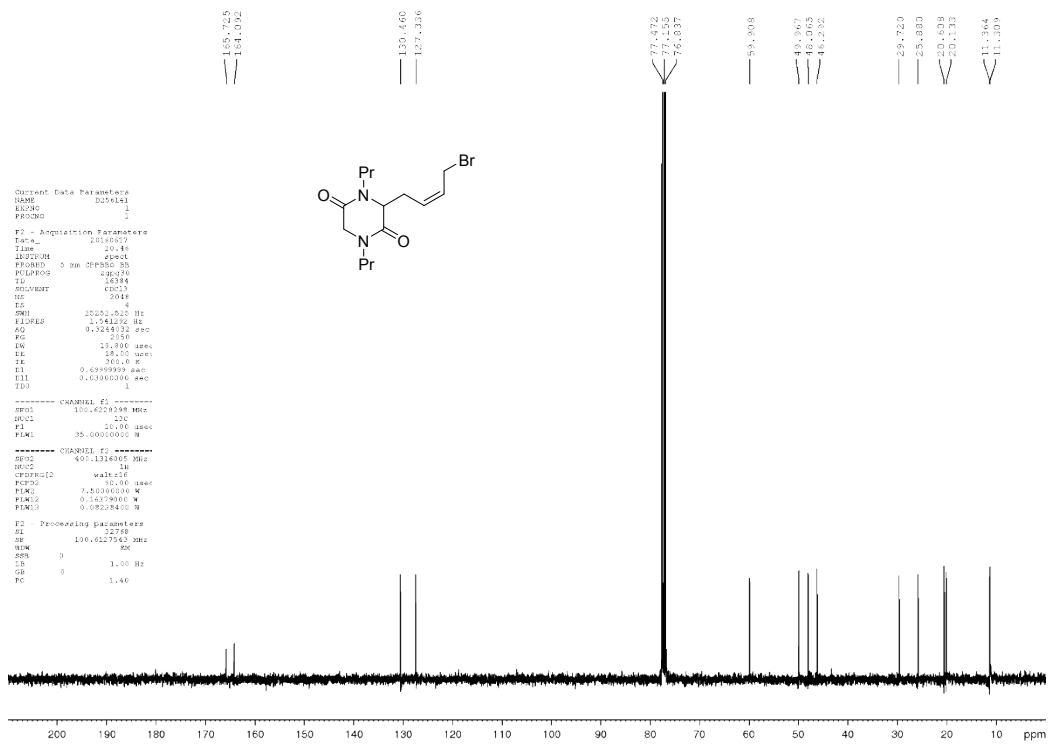
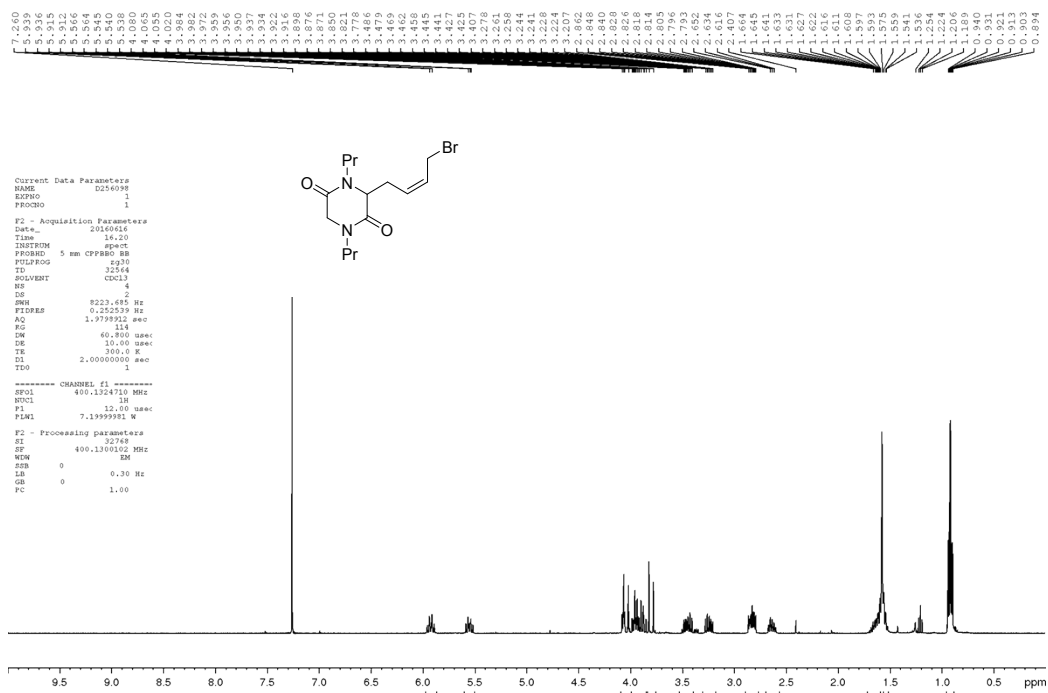


¹H-NMR and ¹³C-NMR *cis*-3-(4-hydroxybut-2-en-1-yl)-1,4-dipropylpiperazine-2,5-dione

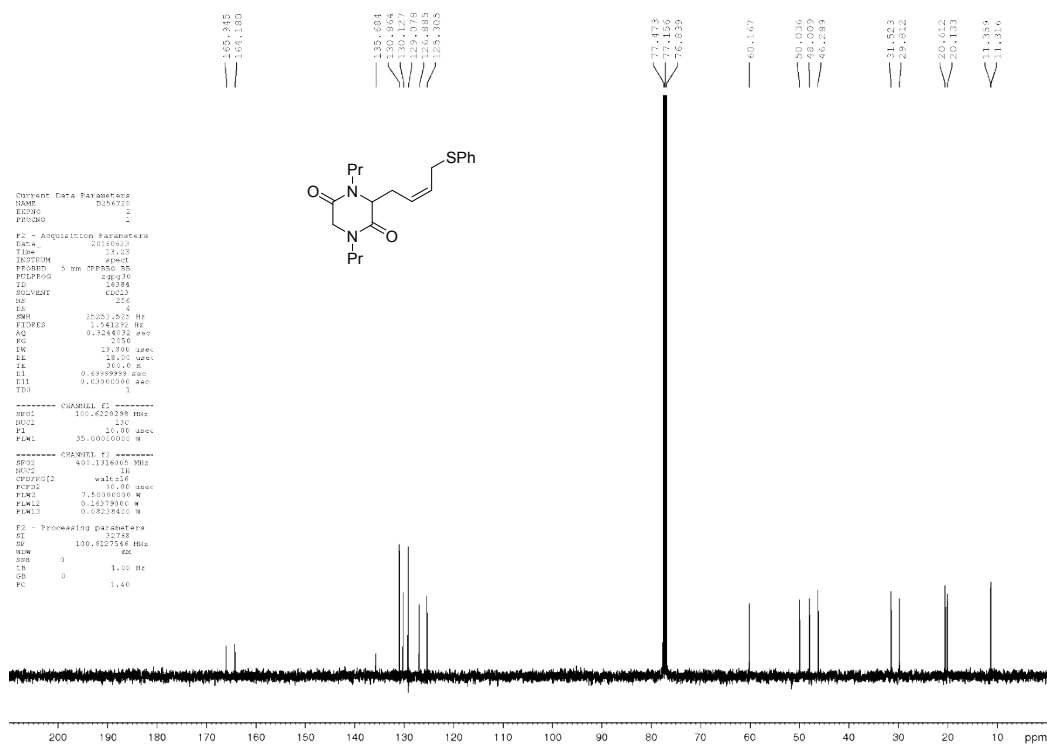
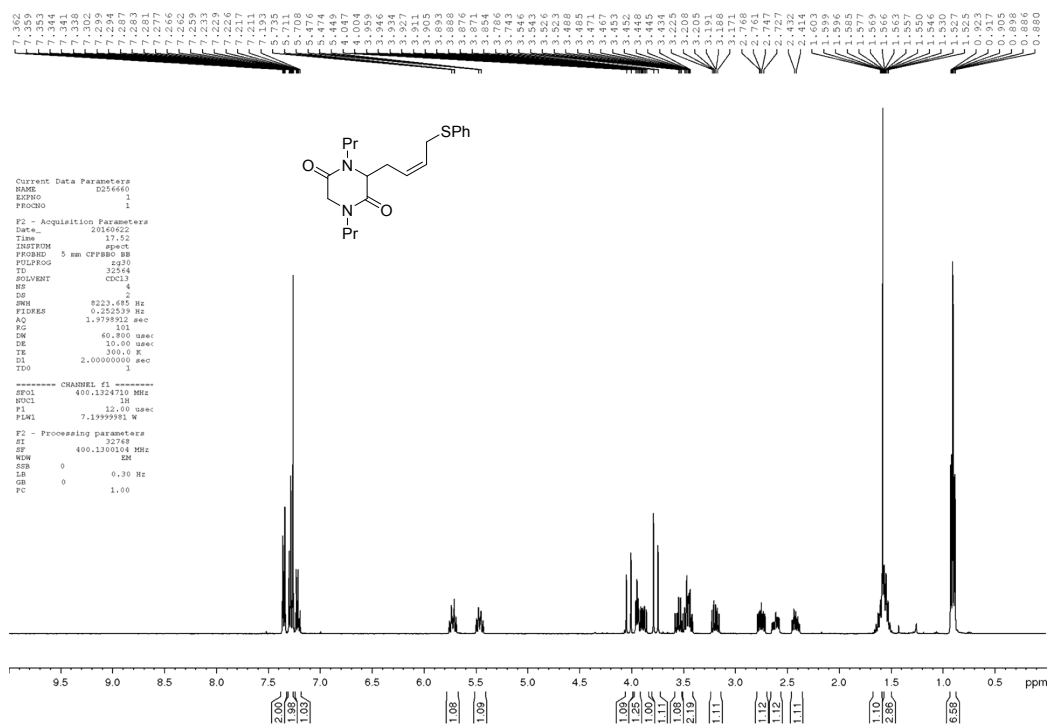
12



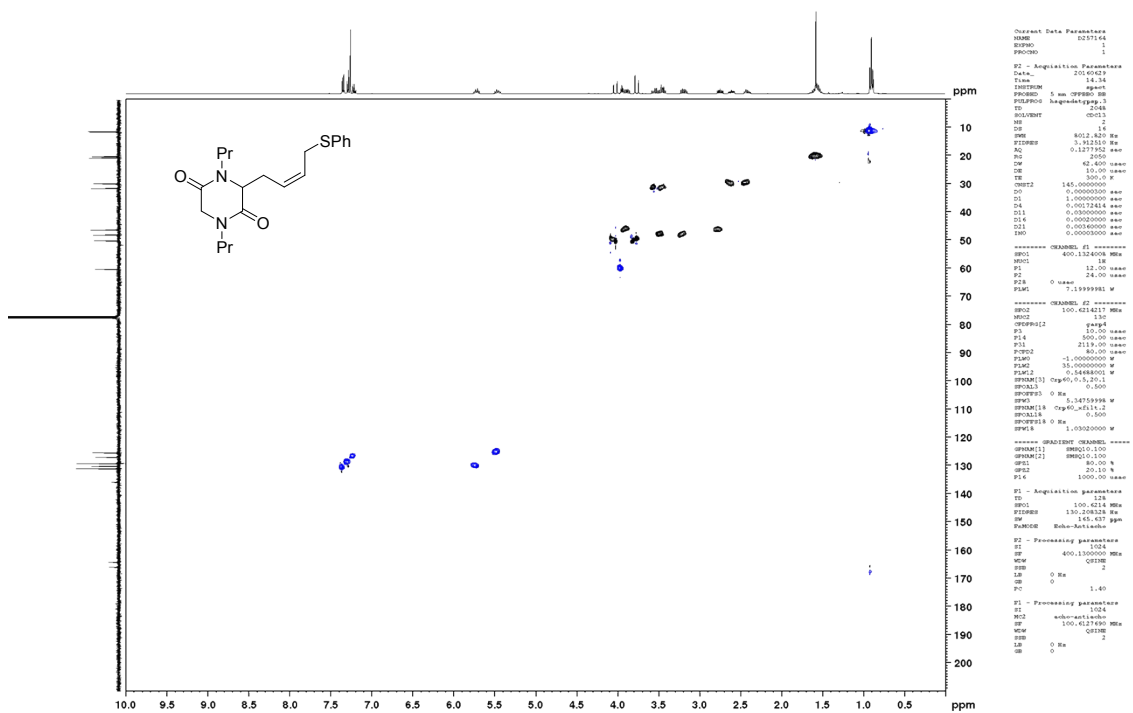
¹H-NMR and ¹³C-NMR *cis*-3-(4-bromobut-2-en-1-yl)-1,4-dipropylpiperazine-2,5-dione



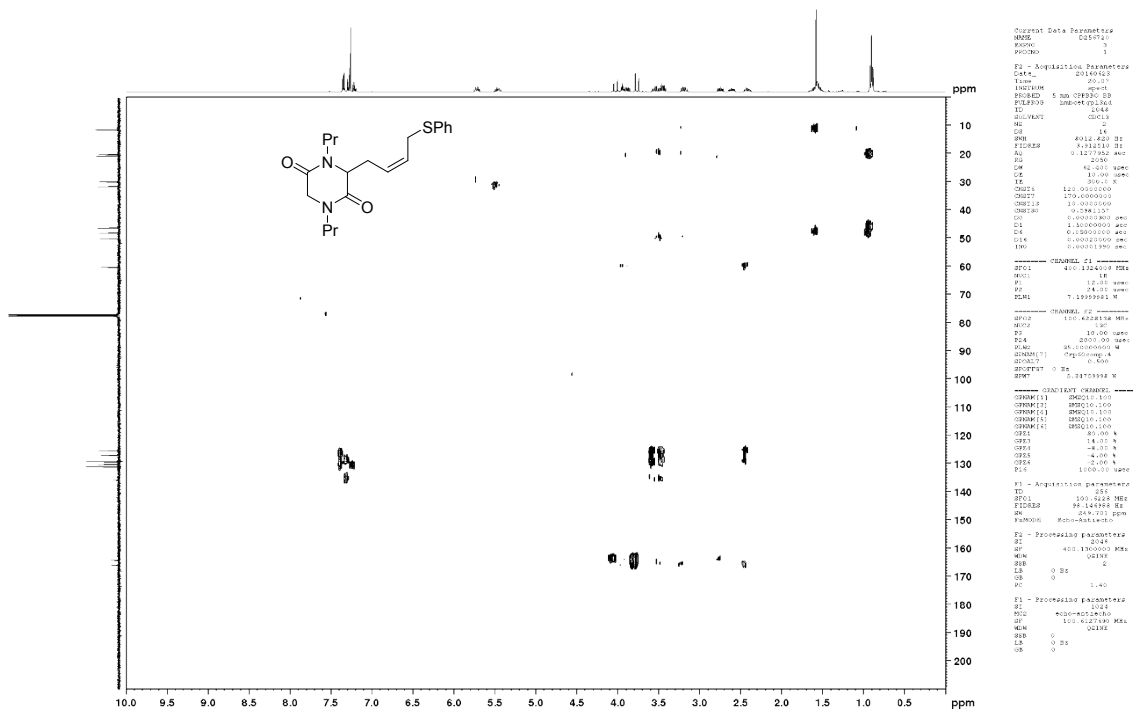
¹H-NMR and ¹³C-NMR *cis*-3-(4-(phenylthio)but-2-en-1-yl)-1,4-dipropylpiperazine-2,5-dione 13



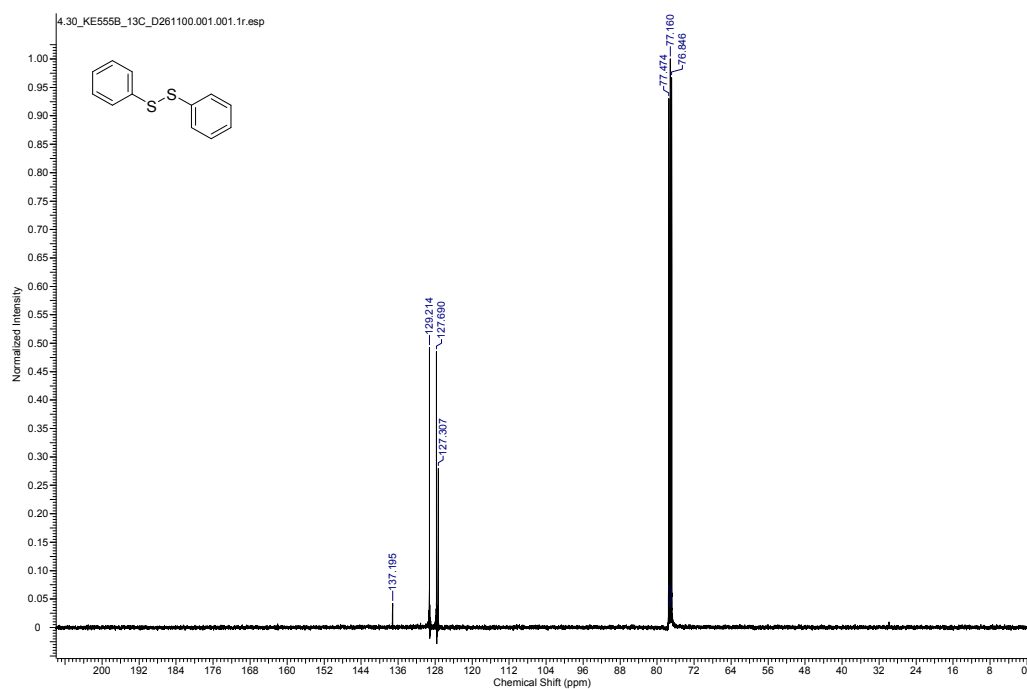
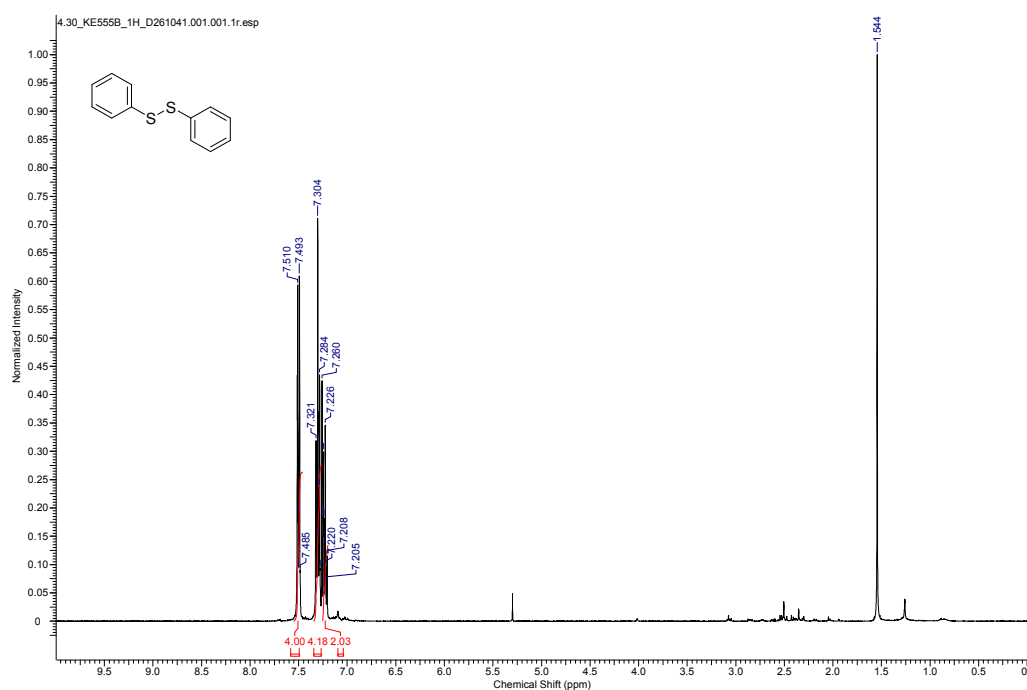
HSQC



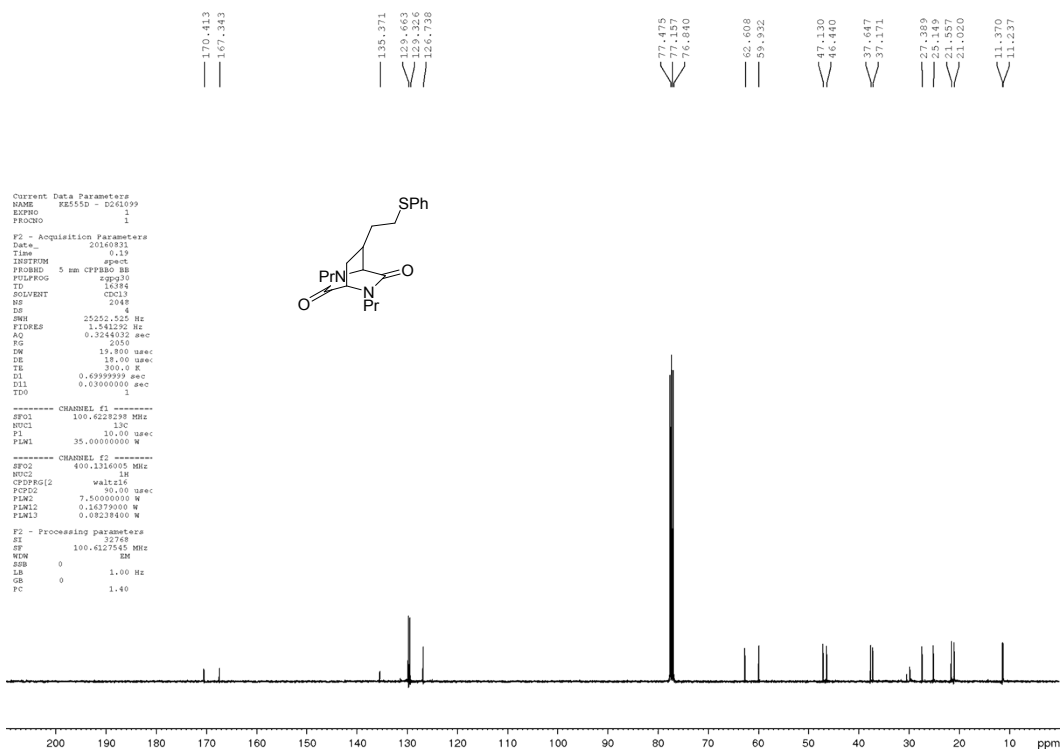
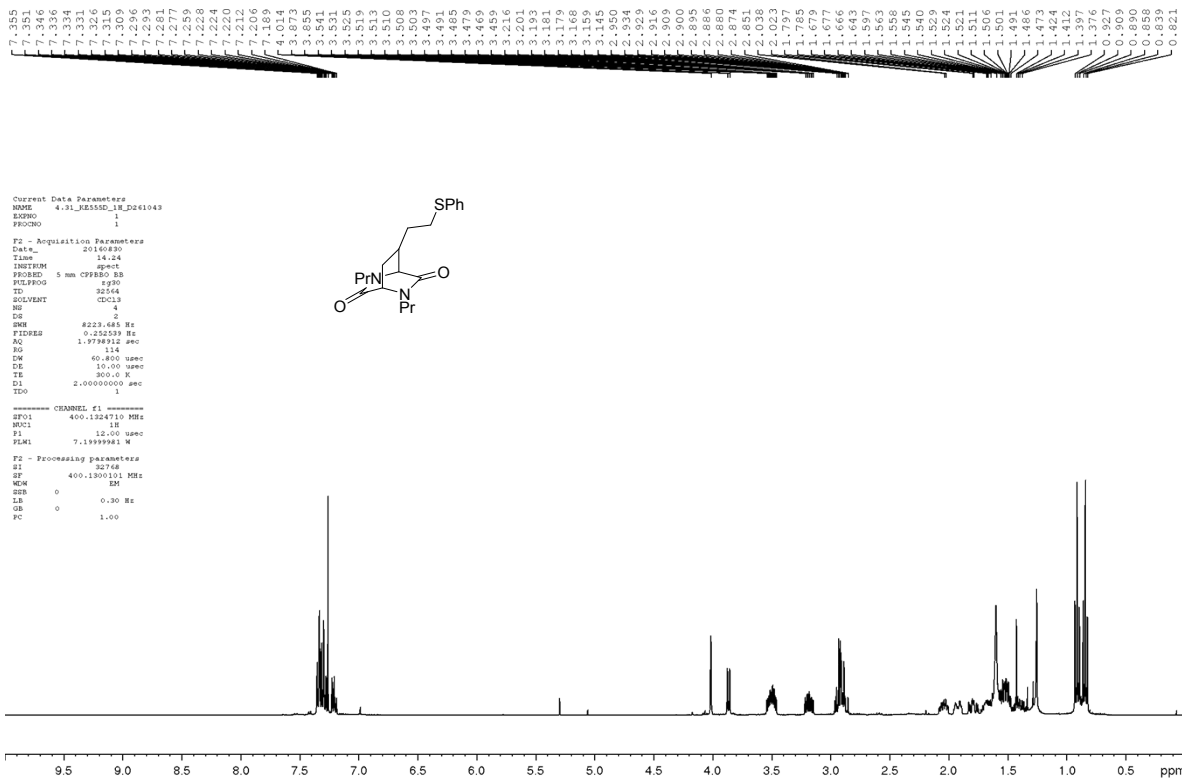
HMBC



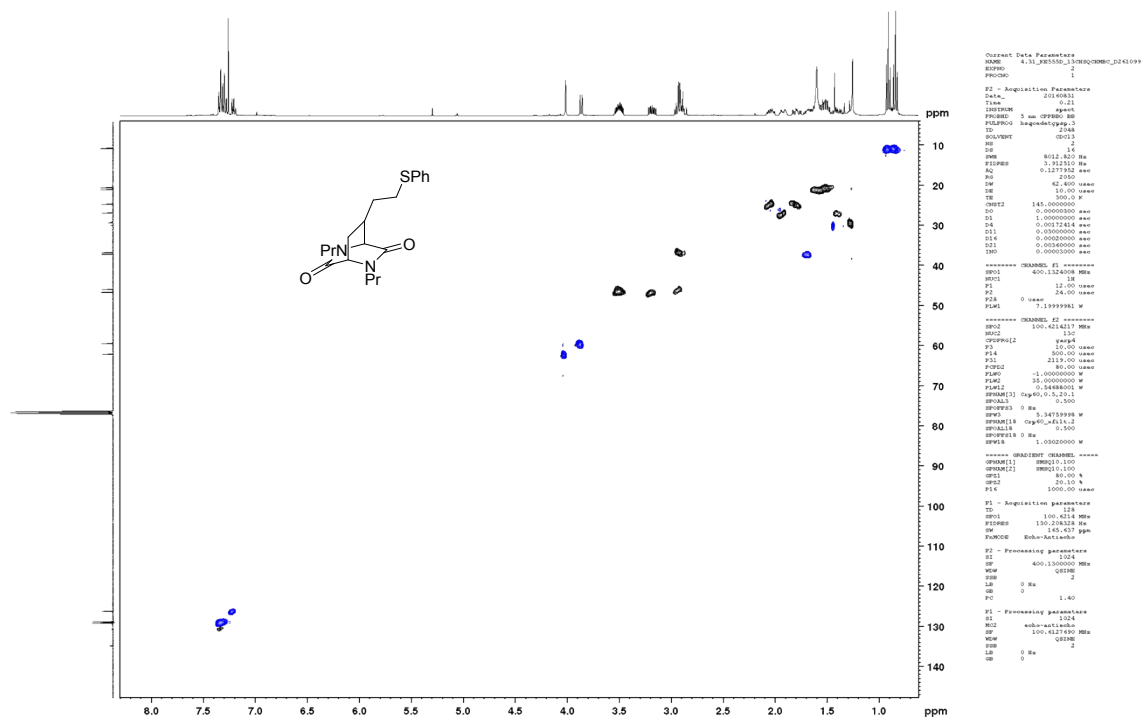
¹H-NMR and ¹³C-NMR diphenyl disulfide 24



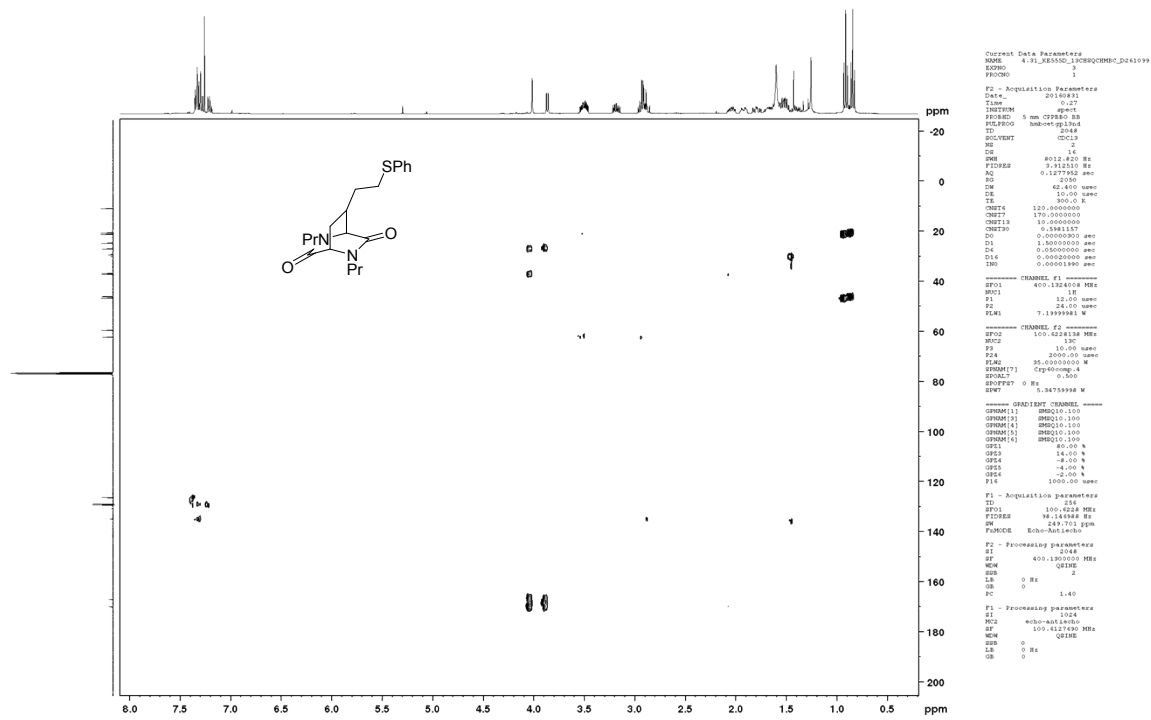
¹H-NMR and ¹³C-NMR 7-(2-(phenylthio)ethyl)-2,5-dipropyl-2,5-diazabicyclo[2.2.2]octane-3,6-dione 25



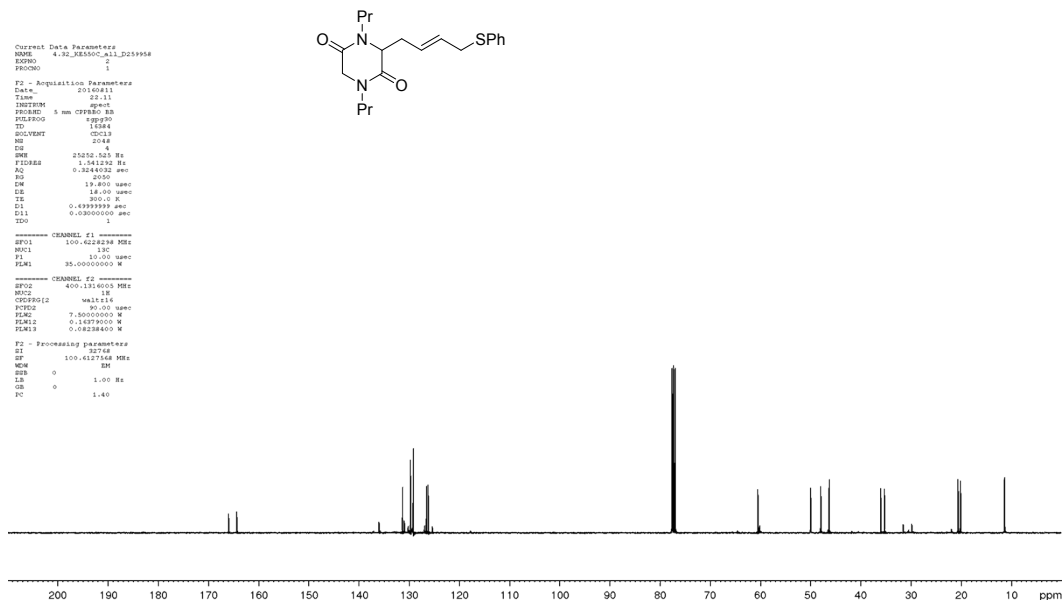
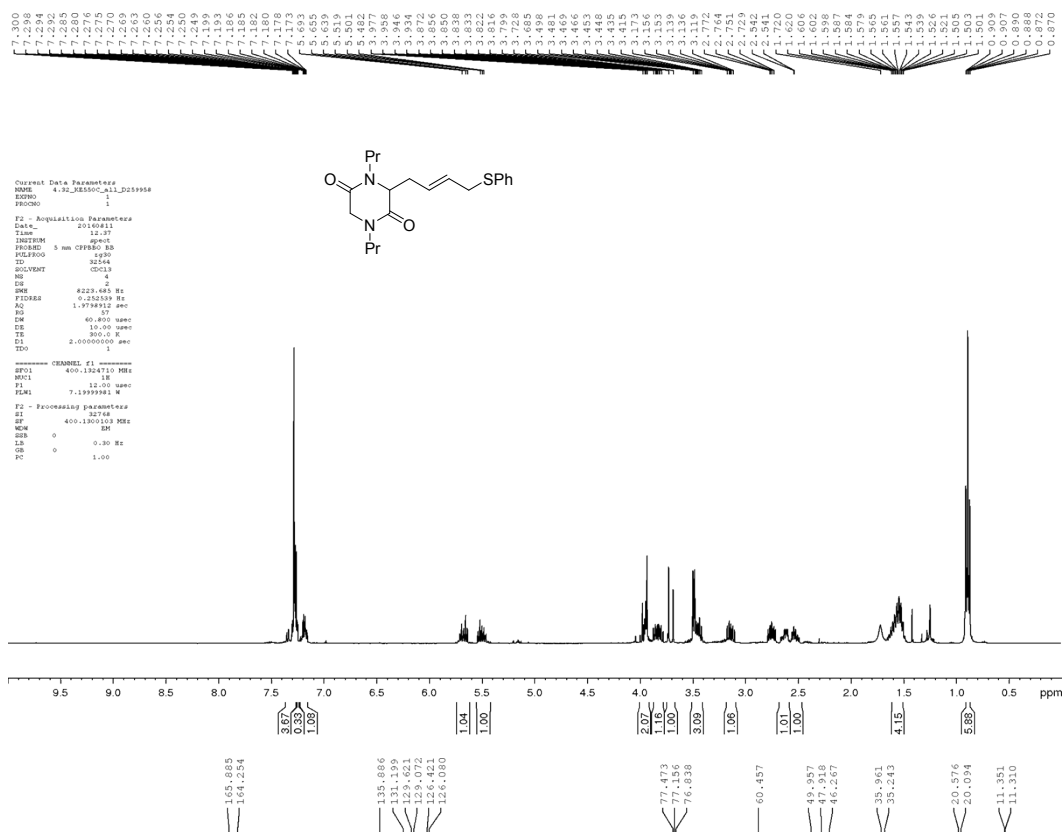
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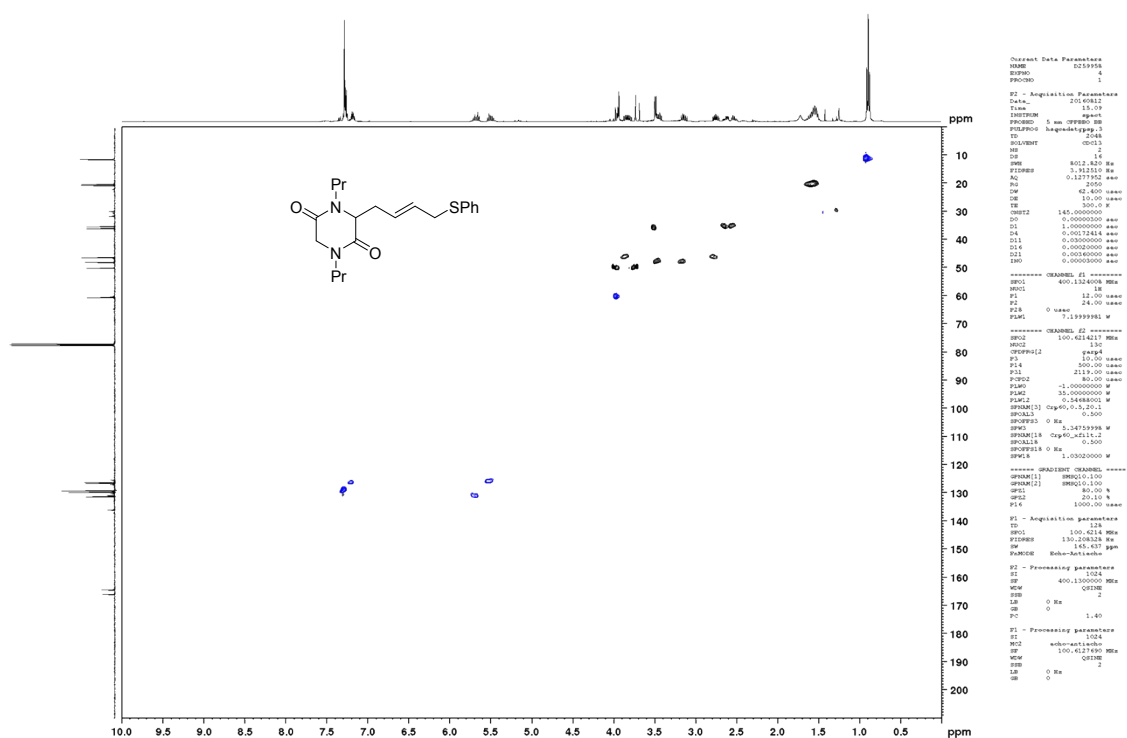
HMBC



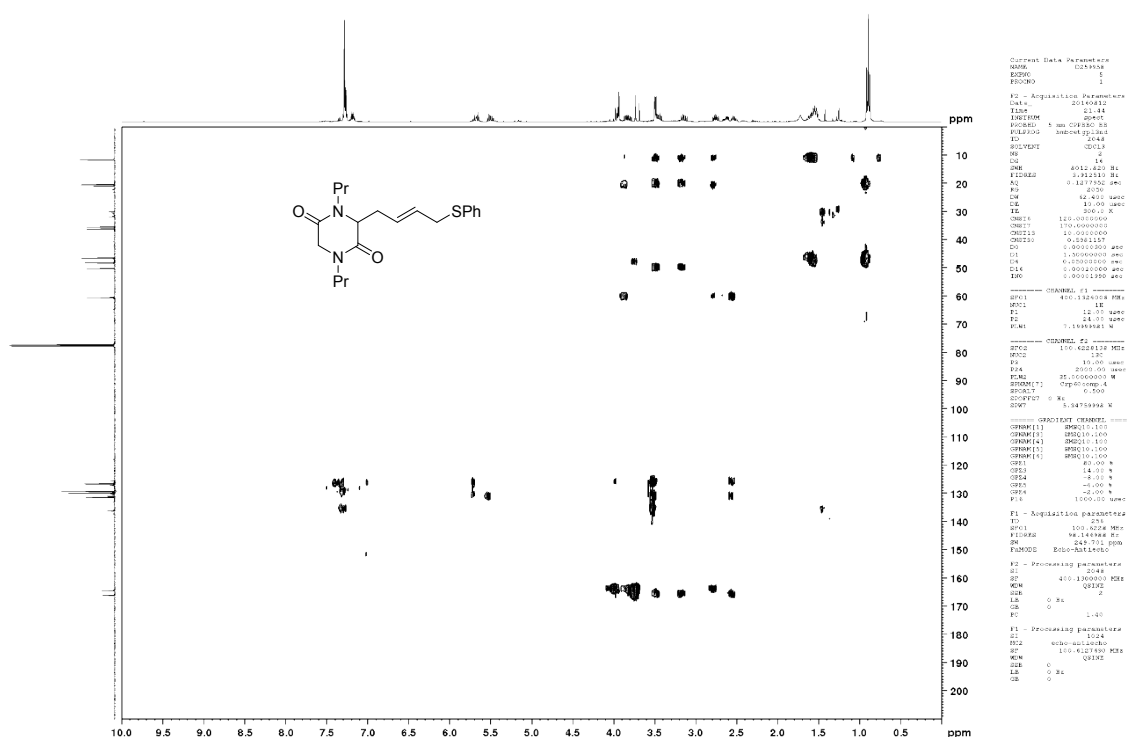
¹H-NMR and ¹³C-NMR (E)-3-(4-(phenylthio)but-2-en-1-yl)-1,4-dipropylpiperazine-2,5-dione 26



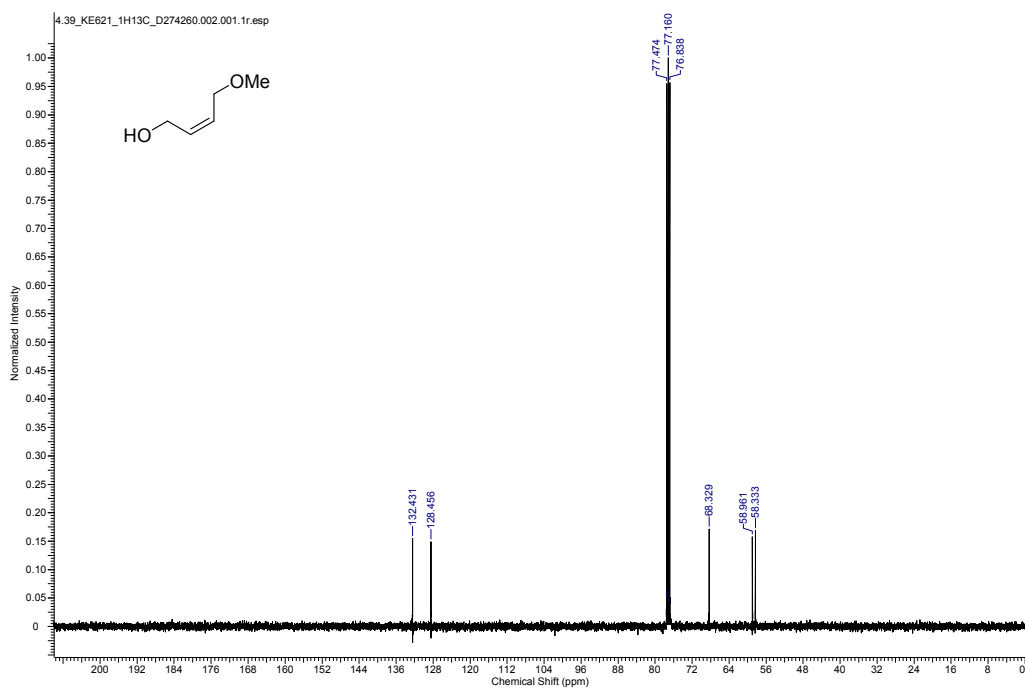
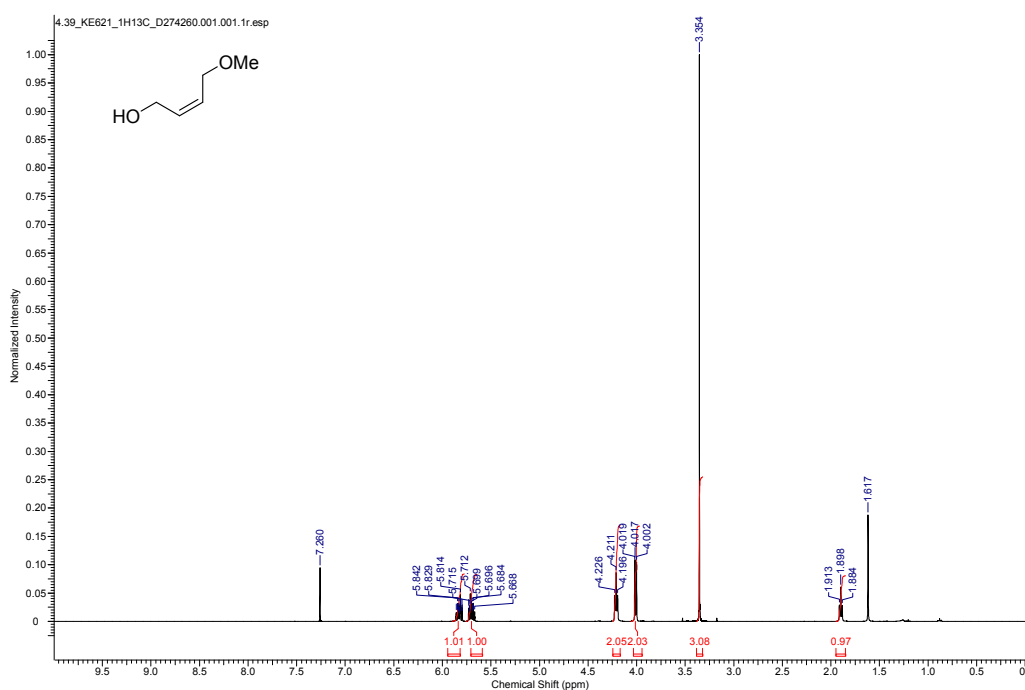
HSQC



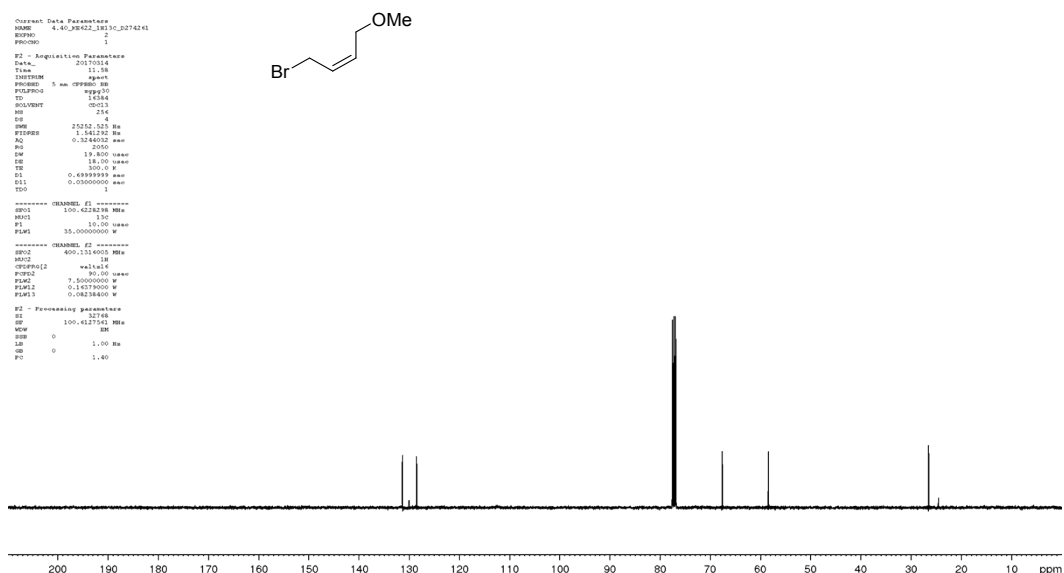
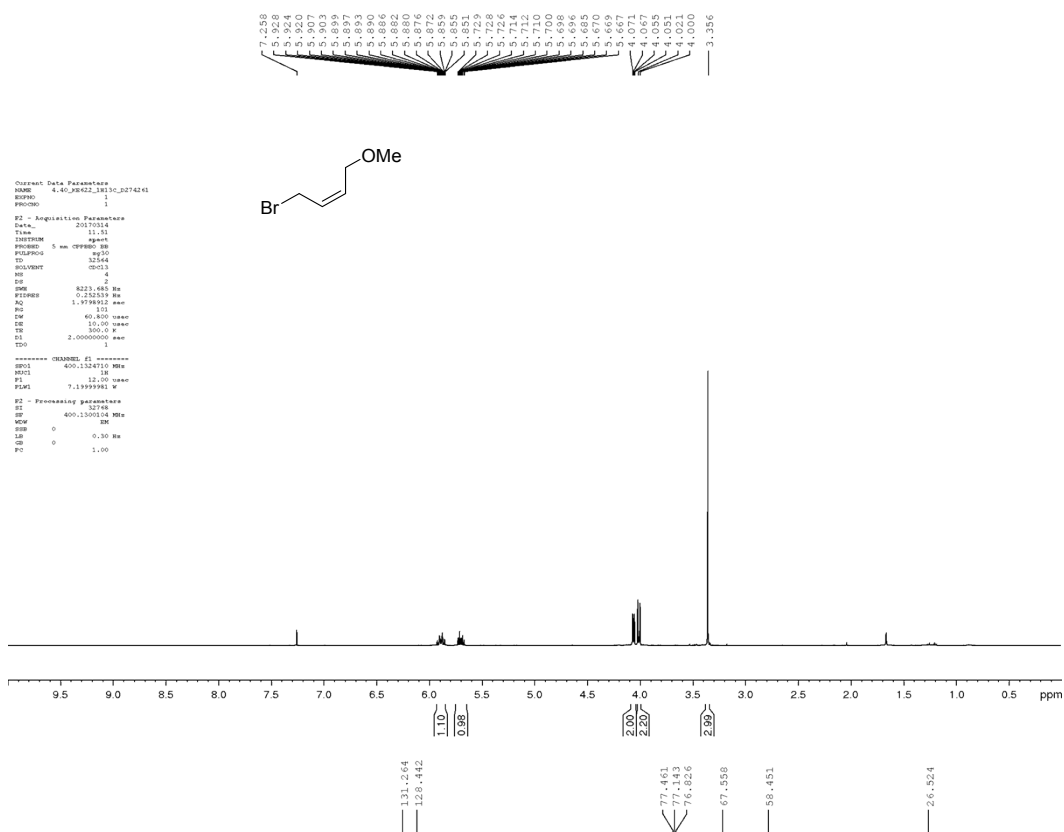
HMBC



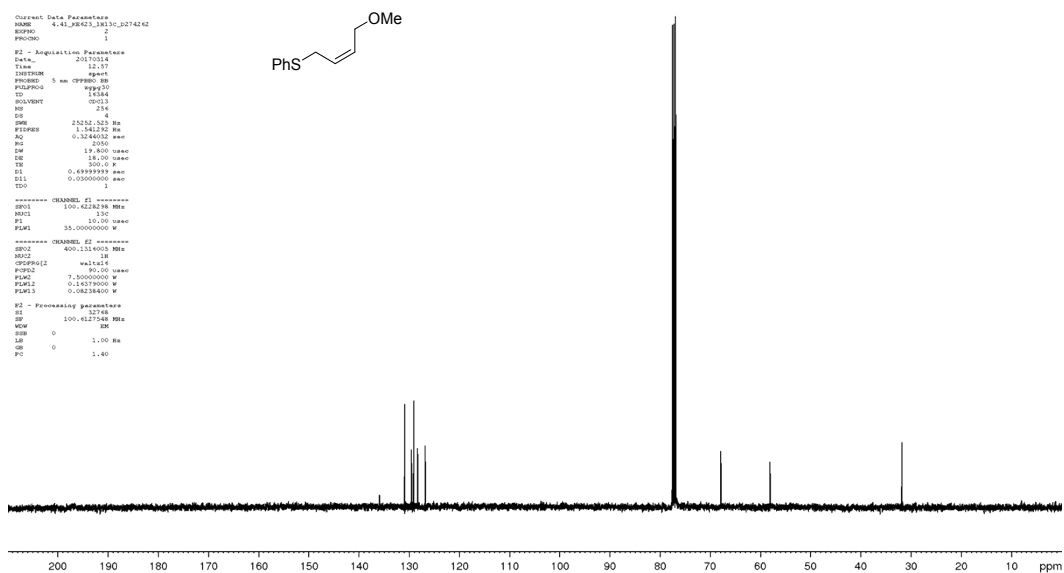
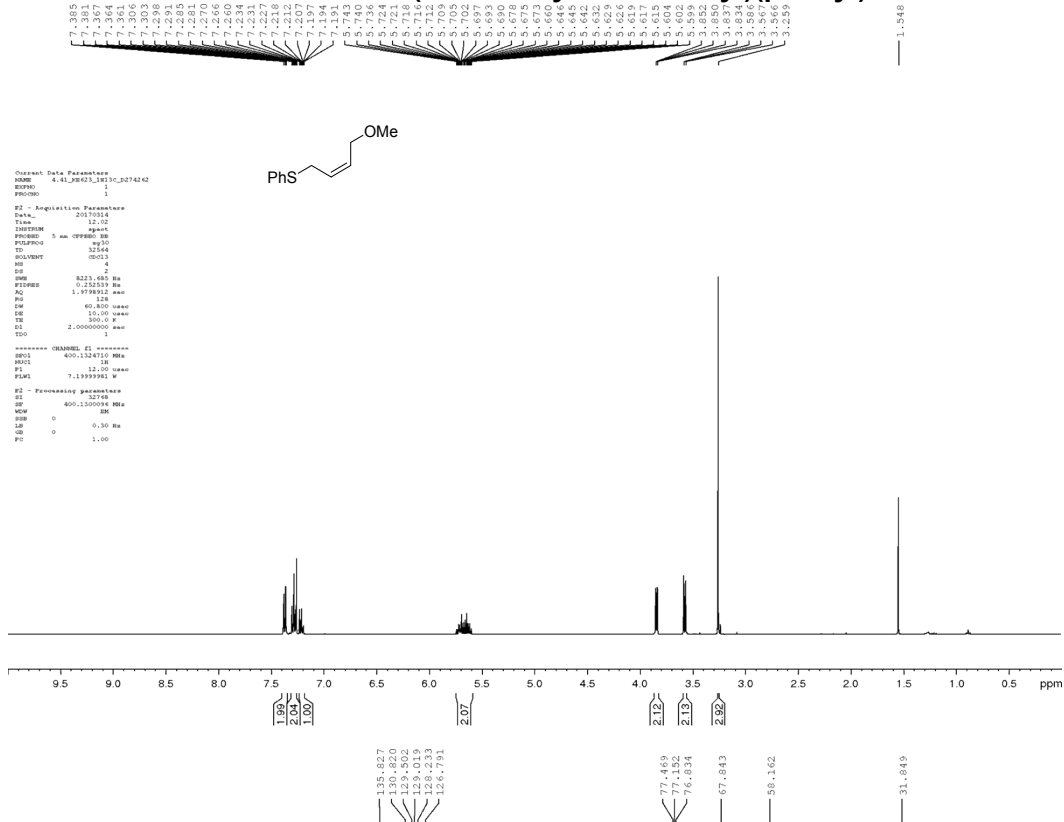
¹H-NMR and ¹³C-NMR *cis*-4-methoxybut-2-en-1-ol 32



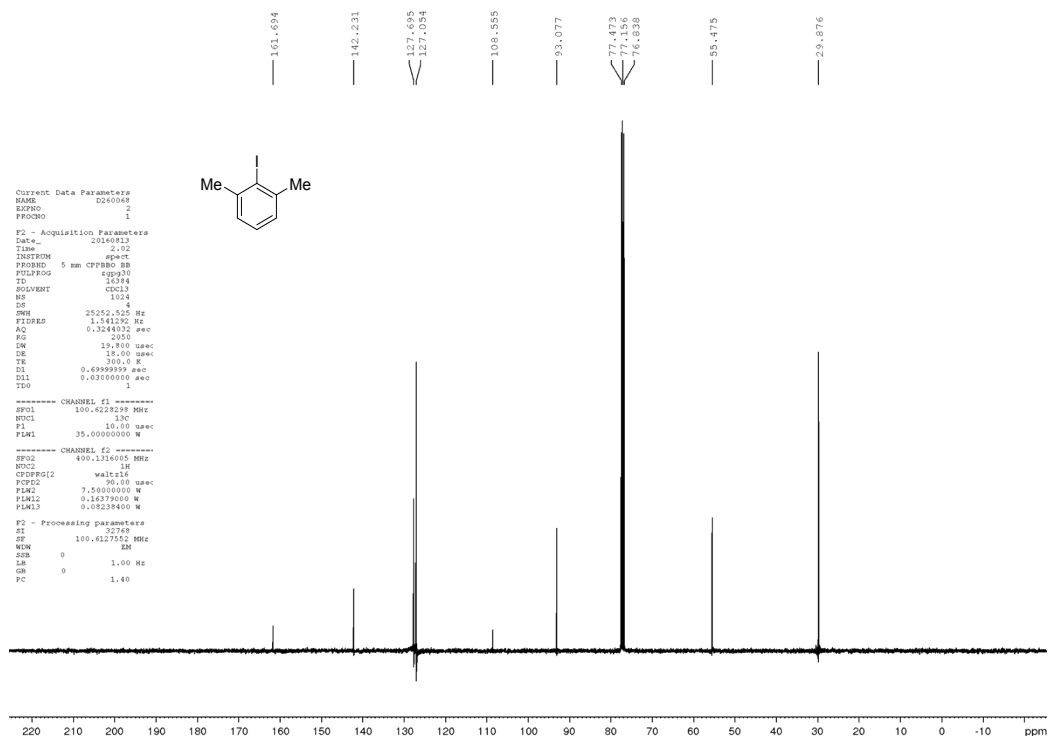
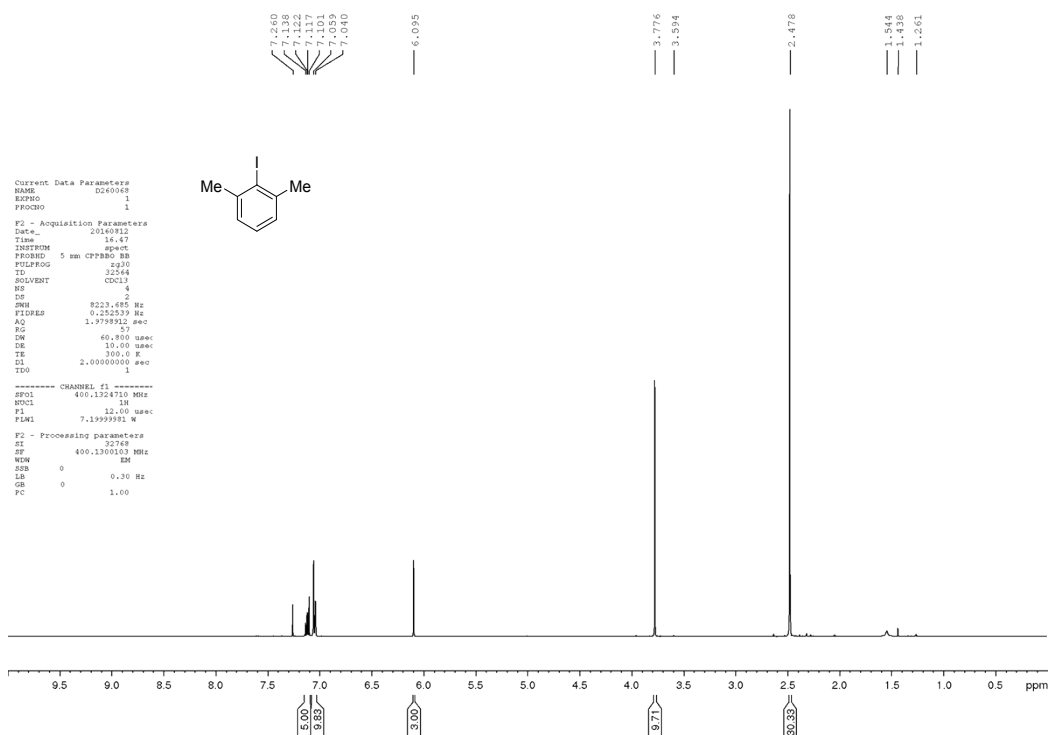
¹H-NMR and ¹³C-NMR *cis*-1-bromo-4-methoxybut-2-ene 33



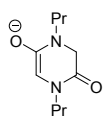
¹H-NMR and ¹³C-NMR *cis*-(4-methoxybut-2-en-1-yl)(phenyl)sulfane 34



¹H-NMR and ¹³C-NMR Iodo-*m*-xylene 36



1.3 XYZ coordinates for computational optimisations

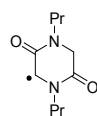


Enolate anion 8 in benzene

31

-651.2494131

C	1.09766	-1.31030	-1.01114
C	-0.25598	-1.54171	-0.85917
C	-0.39270	-0.68684	1.41033
C	1.06343	-1.12076	1.42370
H	-0.85494	-1.98727	-1.63940
H	1.56546	-0.62359	2.25541
H	1.07917	-2.20401	1.60368
N	-0.99541	-1.01576	0.26032
N	1.76928	-0.85118	0.18249
O	-0.93836	-0.08052	2.34605
O	1.79364	-1.46834	-2.05196
C	-2.35834	-0.56934	0.02229
H	-2.83142	-1.28472	-0.65784
H	-2.89450	-0.59066	0.97303
C	-2.40342	0.83585	-0.57339
H	-1.93962	1.52310	0.14088
H	-1.79068	0.84585	-1.47992
C	-3.83166	1.27220	-0.88615
H	-3.85914	2.28033	-1.30489
H	-4.29547	0.59608	-1.61023
H	-4.44853	1.26754	0.01701
C	2.40137	0.45497	0.06179
H	3.11381	0.57947	0.88715
H	2.97722	0.44055	-0.86702
C	1.42443	1.63540	0.04331
H	0.86835	1.66706	0.98711
H	0.68986	1.46070	-0.75085
C	2.14639	2.96162	-0.18039
H	1.45195	3.80468	-0.18617
H	2.88324	3.14111	0.60845
H	2.67871	2.95665	-1.13573

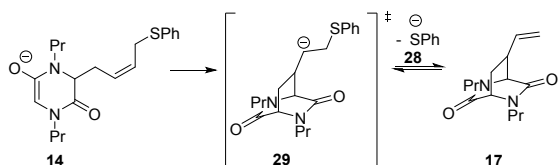


Radical 9 in benzene

31

-651.1544696

C	0.82862	1.18260	-0.36753
C	-0.61407	1.21798	-0.28654
C	-0.84757	-1.17041	-0.37225
C	0.64396	-1.24926	-0.12831
H	-1.11187	2.17357	-0.22355
H	0.76806	-1.48490	0.93938
H	1.01085	-2.10663	-0.69508
N	-1.39088	0.09556	-0.42397
N	1.38802	-0.06302	-0.50808
O	-1.52852	-2.17137	-0.45516
O	1.49443	2.21741	-0.36392
C	-2.85157	0.22859	-0.49793
H	-3.06657	1.17187	-1.00344
H	-3.22301	-0.58789	-1.11716
C	-3.49171	0.18724	0.88566
H	-3.23177	-0.76214	1.36156
H	-3.06628	0.98764	1.49874
C	-5.00726	0.33700	0.79433
H	-5.46295	0.30522	1.78483
H	-5.28051	1.28724	0.32856
H	-5.44285	-0.46843	0.19810
C	2.84221	-0.17387	-0.52473
H	3.09811	-1.08768	-1.06986
H	3.22702	0.67608	-1.08959
C	3.46396	-0.19278	0.87104
H	3.07282	-1.04347	1.43815
H	3.16029	0.71724	1.39592
C	4.98569	-0.27907	0.79488
H	5.43083	-0.29916	1.79079
H	5.30070	-1.18380	0.26798
H	5.39616	0.58097	0.26001



Ionic cyclisation of 14 – starting species 14 in benzene

52

-1436.4472934

C	-1.61570	-1.02625	-0.06472
C	-0.45075	-0.10265	-0.39184
C	-1.99927	1.57283	-1.28609
C	-2.86753	0.51127	-1.47847
N	-0.91635	1.26932	-0.41098
N	-2.74427	-0.69537	-0.70827
O	-2.07780	2.72837	-1.79187
O	-1.50762	-1.98191	0.72210
C	-0.00333	2.31429	0.00664
H	1.02691	1.94353	-0.05934
H	-0.10260	3.15164	-0.68990
C	-0.26475	2.79462	1.43455
H	-1.28248	3.19309	1.48771
H	-0.22498	1.93101	2.10797
C	0.74773	3.85307	1.86370
H	0.58600	4.17882	2.89390
H	1.76939	3.46635	1.78830
H	0.68436	4.73414	1.21877
C	-3.95717	-1.44800	-0.42900
H	-4.58212	-1.41932	-1.32713
H	-3.67794	-2.48554	-0.23564
C	-4.72139	-0.88104	0.76508
H	-4.91968	0.17806	0.57624
H	-4.07193	-0.93958	1.64350
C	-6.02303	-1.63713	1.01351
H	-6.56450	-1.22901	1.86954
H	-6.68149	-1.57876	0.14194
H	-5.82796	-2.69460	1.21331
H	0.27785	-0.20818	0.41258
C	0.19842	-0.58449	-1.71860
H	0.58679	-1.59252	-1.55304
H	-0.59959	-0.64255	-2.46791
C	1.24796	0.36175	-2.21301
H	0.87724	1.35759	-2.44994
C	2.55179	0.13314	-2.38767
H	3.17998	0.94870	-2.73727
C	3.27116	-1.14734	-2.11773
H	3.93645	-1.40874	-2.94373
S	4.40798	-1.02042	-0.67278
C	3.21951	-0.87235	0.65240
C	2.43720	-1.96892	1.02227
C	3.10183	0.32834	1.35133
C	1.54292	-1.86369	2.08093
H	2.52906	-2.90196	0.47706
C	2.22144	0.42252	2.42740
H	3.69628	1.18317	1.04947
C	1.44244	-0.67038	2.79229
H	0.91036	-2.70412	2.33682
H	2.13275	1.35843	2.96742
H	0.73992	-0.58774	3.61318
H	2.59959	-1.98652	-1.94526
H	-3.69449	0.55436	-2.16911

Ionic cyclisation of 14 – transition state 29 in benzene

52

-1436.4179170

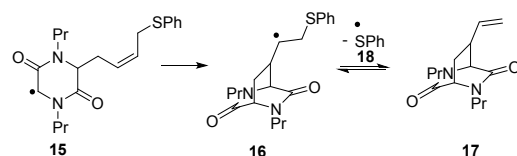
C	1.36917	1.16214	1.33077
C	2.27016	-0.05661	1.19765
C	1.81131	-0.27293	-1.13717
C	0.52222	0.11560	-0.63627
N	2.79736	-0.11880	-0.16457
N	0.47589	1.17942	0.32683
O	2.02453	-0.81405	-2.22862
O	1.45674	1.99417	2.23613
C	4.12300	-0.67722	-0.35625
H	4.27564	-1.51743	0.33639
H	4.15938	-1.08046	-1.36989
C	5.22585	0.36034	-0.15573
H	5.08760	1.15674	-0.89253
H	5.11655	0.82167	0.83146
C	6.61447	-0.25821	-0.29307
H	7.39946	0.48953	-0.16342
H	6.76907	-1.04046	0.45532
H	6.74157	-0.71248	-1.27960
C	-0.59486	2.15831	0.25325
H	-1.52652	1.61831	0.04756
H	-0.68169	2.62751	1.23522
C	-0.34923	3.21156	-0.82337
H	-0.16751	2.70655	-1.77729
H	0.56274	3.76213	-0.57334
C	-1.53482	4.16449	-0.94812
H	-1.35404	4.93168	-1.70379
H	-2.43902	3.61766	-1.22885
H	-1.73233	4.66791	0.00263
H	3.09645	0.05298	1.89926
C	1.44190	-1.32835	1.50236
H	2.09745	-2.19247	1.35216
H	1.14933	-1.30783	2.55695
C	0.21668	-1.47515	0.61459
H	-0.65158	-0.92012	0.98161
H	-0.29623	0.13415	-1.34506
C	-0.04892	-2.70692	0.01728
H	0.70322	-3.48730	-0.00523
C	-1.25767	-2.87330	-0.78178
H	-1.30519	-3.82747	-1.30504
S	-2.93637	-2.83664	0.20548
C	-3.40148	-1.12837	0.08396
C	-3.54970	-0.49131	-1.15525
C	-3.68526	-0.40155	1.24748
C	-3.97851	0.83129	-1.22546
H	-3.35622	-1.04379	-2.06747
C	-4.13541	0.91210	1.17204
H	-3.55011	-0.87907	2.21140
C	-4.28641	1.53582	-0.06456
H	-4.08817	1.30557	-2.19485
H	-4.35769	1.45385	2.08458
H	-4.63158	2.56163	-0.12124
H	-1.43645	-2.06827	-1.50456

Ionic cyclisation of 14 – products 17 and 30 in benzene

52

-1436.4979773

C	-1.27020	0.34615	-1.53844
C	-2.07929	-0.91338	-1.21155
C	-1.79431	-0.40127	1.09894
C	-0.37308	-0.42513	0.53416
N	-2.67403	-0.74421	0.12224
N	-0.34821	0.54223	-0.57182
O	-2.09436	-0.08943	2.23997
O	-1.44535	1.04394	-2.52612
C	-4.09901	-0.49070	0.26753
H	-4.64291	-1.24474	-0.30960
H	-4.34645	-0.62882	1.32154
C	-4.48154	0.91612	-0.18984
H	-3.91338	1.63704	0.40651
H	-4.17323	1.05214	-1.23171
C	-5.97938	1.16519	-0.04256
H	-6.24621	2.17380	-0.36233
H	-6.55446	0.45851	-0.64709
H	-6.29237	1.04776	0.99824
C	0.55659	1.68280	-0.55351
H	1.54489	1.32968	-0.24816
H	0.62873	2.04854	-1.57964
C	0.06649	2.78844	0.37804
H	-0.01213	2.39013	1.39577
H	-0.94162	3.08604	0.07078
C	1.01069	3.98710	0.35595
H	0.66745	4.77527	1.02895
H	2.01571	3.68709	0.66258
H	1.07900	4.40776	-0.65095
H	-2.86954	-1.04140	-1.94861
C	-1.10390	-2.10222	-1.15914
H	-1.67394	-3.00686	-0.93800
H	-0.61873	-2.22621	-2.12924
C	-0.05376	-1.81524	-0.04838
H	0.93183	-1.73820	-0.52543
H	0.34036	-0.11518	1.29555
C	0.02173	-2.91587	0.96868
H	0.21042	-3.90053	0.54377
C	-0.08626	-2.79445	2.28925
H	0.00967	-3.66170	2.93247
S	3.29876	-1.83730	-1.68363
C	3.50419	-0.58635	-0.47277
C	3.06394	-0.75278	0.85815
C	4.10850	0.65341	-0.77865
C	3.18966	0.25856	1.80583
H	2.61252	-1.69795	1.14248
C	4.24356	1.65825	0.17097
H	4.46619	0.81358	-1.78979
C	3.77754	1.47829	1.47472
H	2.82621	0.08797	2.81513
H	4.71083	2.59679	-0.11144
H	3.87667	2.26540	2.21338
H	-0.27535	-1.84273	2.77478



Radical cyclisation of 15 – starting species 15 in benzene

52

-1436.3403354

C	2.51442	-0.98285	-0.49034
C	1.44924	0.08518	-0.31860
C	2.93266	1.29333	1.21241
C	3.61359	0.02605	1.38662
N	1.98769	1.32363	0.22346
N	3.48950	-1.00043	0.48482
O	3.23665	2.28202	1.88020
O	2.45915	-1.81623	-1.37192
C	1.37857	2.60296	-0.13548
H	0.42450	2.39308	-0.62358
H	1.16843	3.15902	0.78214
C	2.27629	3.42756	-1.05453
H	3.23304	3.58879	-0.55122
H	2.47867	2.84998	-1.96217
C	1.62963	4.76359	-1.40772
H	2.27247	5.35313	-2.06322
H	0.67460	4.61460	-1.91876
H	1.43894	5.35235	-0.50684
C	4.49553	-2.06925	0.46340
H	4.80246	-2.24574	1.49686
H	4.01106	-2.96955	0.08586
C	5.69226	-1.69615	-0.40572
H	6.12177	-0.76113	-0.03307
H	5.33760	-1.51030	-1.42306
C	6.74216	-2.80276	-0.40193
H	7.59577	-2.53297	-1.02516
H	7.11128	-2.98966	0.60976
H	6.32629	-3.73688	-0.78726
H	1.05719	0.28890	-1.31687
C	0.32259	-0.52078	0.55813
H	0.02959	-1.47822	0.12225
H	0.74371	-0.72776	1.54787
C	-0.85474	0.40167	0.70039
H	-0.75157	1.19848	1.43254
C	-1.99141	0.32599	0.00690
H	-2.77773	1.04631	0.21679
C	-2.31309	-0.68948	-1.04262
H	-1.43290	-1.22153	-1.40325
S	-3.43828	-2.01145	-0.42478
C	-4.87096	-1.00997	-0.05024
C	-5.69299	-0.55189	-1.08102
C	-5.17541	-0.69197	1.27306
C	-6.80528	0.23025	-0.78911
H	-5.46133	-0.81514	-2.10716
C	-6.29617	0.08240	1.56177
H	-4.53143	-1.04859	2.06818
C	-7.10936	0.54634	0.53287
H	-7.44020	0.58351	-1.59305
H	-6.52975	0.32545	2.59181
H	-7.98015	1.14981	0.76042
H	-2.79828	-0.22199	-1.90082
H	4.35641	-0.07081	2.16378

**Radical cyclisation of 15 – transition state
cyclisation to 16 in benzene**

52

-1436.3236327

C	1.60080	1.02777	1.17158
C	1.62562	-0.49111	1.17274
C	1.87491	-0.55144	-1.20390
C	0.91811	0.56430	-1.04486
N	2.34549	-0.97870	0.00216
N	1.16381	1.50128	-0.03242
O	2.14895	-1.04971	-2.28775
O	1.87450	1.72650	2.12976
C	3.22804	-2.13064	0.12622
H	2.74649	-2.88022	0.76653
H	3.32942	-2.56140	-0.87101
C	4.59675	-1.75573	0.68709
H	5.07309	-1.05608	-0.00534
H	4.46966	-1.22681	1.63723
C	5.47323	-2.98854	0.88604
H	6.46466	-2.71241	1.24774
H	5.02894	-3.67396	1.61254
H	5.59842	-3.53216	-0.05392
C	0.95103	2.93018	-0.25171
H	0.07789	3.03883	-0.90182
H	0.71775	3.37698	0.71608
C	2.17418	3.60044	-0.87065
H	2.42939	3.08200	-1.80023
H	3.01953	3.47559	-0.18795
C	1.91835	5.08006	-1.13886
H	2.79876	5.55943	-1.56904
H	1.08937	5.21232	-1.83919
H	1.66623	5.60640	-0.21497
H	2.13471	-0.82113	2.07632
C	0.16489	-1.01745	1.14043
H	0.21600	-2.10842	1.18987
H	-0.35823	-0.66912	2.03534
C	-0.60426	-0.60552	-0.10037
H	-1.17856	0.31662	-0.02513
H	0.49759	0.96456	-1.95844
C	-1.07186	-1.55829	-0.99189
H	-0.70020	-2.57705	-0.93639
C	-2.07023	-1.23872	-2.03872
H	-1.90987	-1.80534	-2.95668
S	-3.79182	-1.71271	-1.51548
C	-3.91176	-0.66498	-0.07571
C	-4.20469	0.69188	-0.21982
C	-3.66091	-1.18830	1.19224
C	-4.23147	1.52153	0.89693
H	-4.40501	1.09323	-1.20700
C	-3.69753	-0.35766	2.30902
H	-3.42714	-2.24136	1.29563
C	-3.97618	0.99806	2.16215
H	-4.45566	2.57515	0.77909
H	-3.50248	-0.77002	3.29223
H	-3.99796	1.64420	3.03173
H	-2.08847	-0.17397	-2.27760

**Radical cyclisation of 15 – intermediate 16 in
benzene**

52

-1436.3557025

C	-1.92479	0.72265	-1.58262
C	-2.43863	-0.68051	-1.25656
C	-1.17314	-0.62616	0.76244
C	-0.16129	-0.29188	-0.33353
N	-2.37976	-0.87720	0.19664
N	-0.67103	0.85664	-1.08783
O	-0.91899	-0.65961	1.95456
O	-2.54346	1.56235	-2.21306
C	-3.59729	-0.96662	0.99107
H	-4.26377	-1.69503	0.51969
H	-3.31286	-1.35381	1.97104
C	-4.29025	0.38724	1.13127
H	-3.58711	1.08767	1.59305
H	-4.52310	0.77936	0.13550
C	-5.56227	0.28033	1.96661
H	-6.05203	1.25032	2.06388
H	-6.27444	-0.41119	1.50874
H	-5.33812	-0.08584	2.97161
C	0.08011	2.10036	-1.17544
H	1.10149	1.86623	-1.49278
H	-0.39300	2.69638	-1.95800
C	0.10192	2.86764	0.14329
H	0.58237	2.25342	0.91258
H	-0.92969	3.04065	0.46565
C	0.84192	4.19319	-0.01002
H	0.92334	4.71498	0.94503
H	1.85316	4.03157	-0.39306
H	0.32066	4.85009	-0.71093
H	-3.46636	-0.78352	-1.59798
C	-1.47861	-1.67700	-1.93495
H	-1.85615	-2.68930	-1.78278
H	-1.45355	-1.47823	-3.00748
C	-0.07351	-1.51205	-1.28832
H	0.65812	-1.24083	-2.06354
H	0.79447	-0.02949	0.11587
C	0.36775	-2.76527	-0.60110
H	0.15016	-3.69893	-1.10857
C	1.36876	-2.79307	0.48134
H	1.43666	-3.78193	0.93133
S	3.10212	-2.42636	-0.13910
C	3.26061	-0.70120	0.28274
C	3.11378	-0.27721	1.60628
C	3.55287	0.23132	-0.71275
C	3.23213	1.07030	1.92341
H	2.90779	-1.00191	2.38586
C	3.69557	1.57815	-0.38480
H	3.65856	-0.09919	-1.73972
C	3.52778	2.00114	0.92965
H	3.10506	1.39247	2.95015
H	3.92354	2.29735	-1.16369
H	3.62564	3.05068	1.18101
H	1.16979	-2.06622	1.27128

Radical cyclisation of 15 – transition state C-S cleavage in benzene (16 $\rightarrow$ 17+18)

52

-1436.3453638

C	-2.00798	0.54352	-1.59482
C	-2.40760	-0.88262	-1.21133
C	-1.06731	-0.66397	0.74596
C	-0.12014	-0.31194	-0.40362
N	-2.27298	-1.03198	0.24296
N	-0.74674	0.78071	-1.15946
O	-0.77887	-0.59773	1.92788
O	-2.71307	1.32196	-2.21236
C	-3.45618	-1.10205	1.09173
H	-4.12926	-1.85936	0.67979
H	-3.12716	-1.44091	2.07529
C	-4.16179	0.24848	1.19850
H	-3.44953	0.97768	1.59794
H	-4.44144	0.59040	0.19633
C	-5.39624	0.16471	2.09098
H	-5.89476	1.13224	2.16525
H	-6.11713	-0.55483	1.69402
H	-5.12552	-0.15297	3.10095
C	-0.11167	2.08524	-1.27431
H	0.93059	1.93440	-1.57203
H	-0.62375	2.61547	-2.07935
C	-0.18218	2.88528	0.02316
H	0.32300	2.32802	0.81932
H	-1.23235	2.98476	0.31548
C	0.45691	4.25994	-0.14863
H	0.46854	4.81338	0.79179
H	1.48874	4.16791	-0.49917
H	-0.09176	4.85400	-0.88376
H	-3.43949	-1.06606	-1.50307
C	-1.41582	-1.83715	-1.89885
H	-1.70249	-2.86411	-1.66641
H	-1.46794	-1.70226	-2.98009
C	0.01252	-1.52488	-1.35369
H	0.64642	-1.19856	-2.18745
H	0.83465	0.02735	-0.00338
C	0.63383	-2.74393	-0.74490
H	0.64290	-3.61975	-1.38884
C	1.25320	-2.82941	0.47002
H	1.53486	-3.80435	0.84717
S	3.48797	-2.25650	-0.03497
C	3.37416	-0.54376	0.33663
C	3.11723	-0.11788	1.64882
C	3.52623	0.41729	-0.67351
C	3.00394	1.23461	1.93984
H	3.00211	-0.85752	2.43295
C	3.43519	1.77185	-0.37163
H	3.71842	0.09050	-1.68894
C	3.16805	2.18373	0.93202
H	2.79250	1.54989	2.95479
H	3.56659	2.50744	-1.15766
H	3.08639	3.23933	1.16361
H	1.14682	-2.04524	1.21202

Radical cyclisation of 15 – products 17 in benzene

40

-806.5874061

C	0.29707	0.44476	1.51284
C	-0.08337	-1.02144	1.29426
C	-0.26338	-0.55455	-1.03796
C	-1.17098	0.47968	-0.36717
N	0.25811	-1.37623	-0.09002
N	-0.36453	1.21556	0.61246
O	-0.04430	-0.61706	-2.23413
O	1.07341	0.84554	2.36156
C	1.39065	-2.24704	-0.37750
H	1.30945	-3.13646	0.25414
H	1.29899	-2.56178	-1.41837
C	2.72542	-1.54081	-0.14662
H	2.76134	-0.65608	-0.79042
H	2.77034	-1.18460	0.88811
C	3.90518	-2.46181	-0.44089
H	4.85462	-1.95041	-0.27621
H	3.88350	-3.34416	0.20411
H	3.88271	-2.80399	-1.47862
C	-0.02544	2.61609	0.39921
H	-0.94291	3.15777	0.15060
H	0.34922	3.00284	1.34842
C	1.01923	2.79272	-0.70087
H	0.64297	2.35220	-1.63024
H	1.91423	2.22887	-0.41943
C	1.36083	4.26404	-0.91482
H	2.10812	4.38507	-1.70033
H	0.47358	4.83294	-1.20497
H	1.75972	4.70779	0.00084
H	0.47822	-1.65085	1.98127
C	-1.60673	-1.15377	1.46333
H	-1.88324	-2.20164	1.33359
H	-1.89637	-0.84970	2.47022
C	-2.29958	-0.26507	0.39059
H	-2.91374	0.49797	0.87409
H	-1.56108	1.16669	-1.11554
C	-3.15423	-1.06210	-0.55307
H	-2.65182	-1.86583	-1.09095
C	-4.44910	-0.84507	-0.75247
H	-5.02406	-1.44934	-1.44391
H	-4.97510	-0.05434	-0.22616

Radical cyclisation of 15 – products 18 in benzene

12

-629.7431433

C	-2.23859	0.00003	0.00000
C	-1.53711	1.20175	-0.00001
C	-0.14683	1.21039	0.00001
C	0.55154	-0.00006	-0.00001
C	-0.14689	-1.21043	-0.00001
C	-1.53720	-1.20169	0.00002
H	-3.32135	0.00009	0.00000
H	-2.07227	2.14410	-0.00001
H	0.39209	2.15074	0.00002
H	0.39193	-2.15083	-0.00002
H	-2.07238	-2.14404	0.00002
S	2.31327	-0.00000	0.00000

