Supporting Information for:

Selectivity in the Electron Transfer Catalyzed Diels-Alder Reaction of (R)-α-Phellandrene and 4-Methoxystyrene

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Supporting Information

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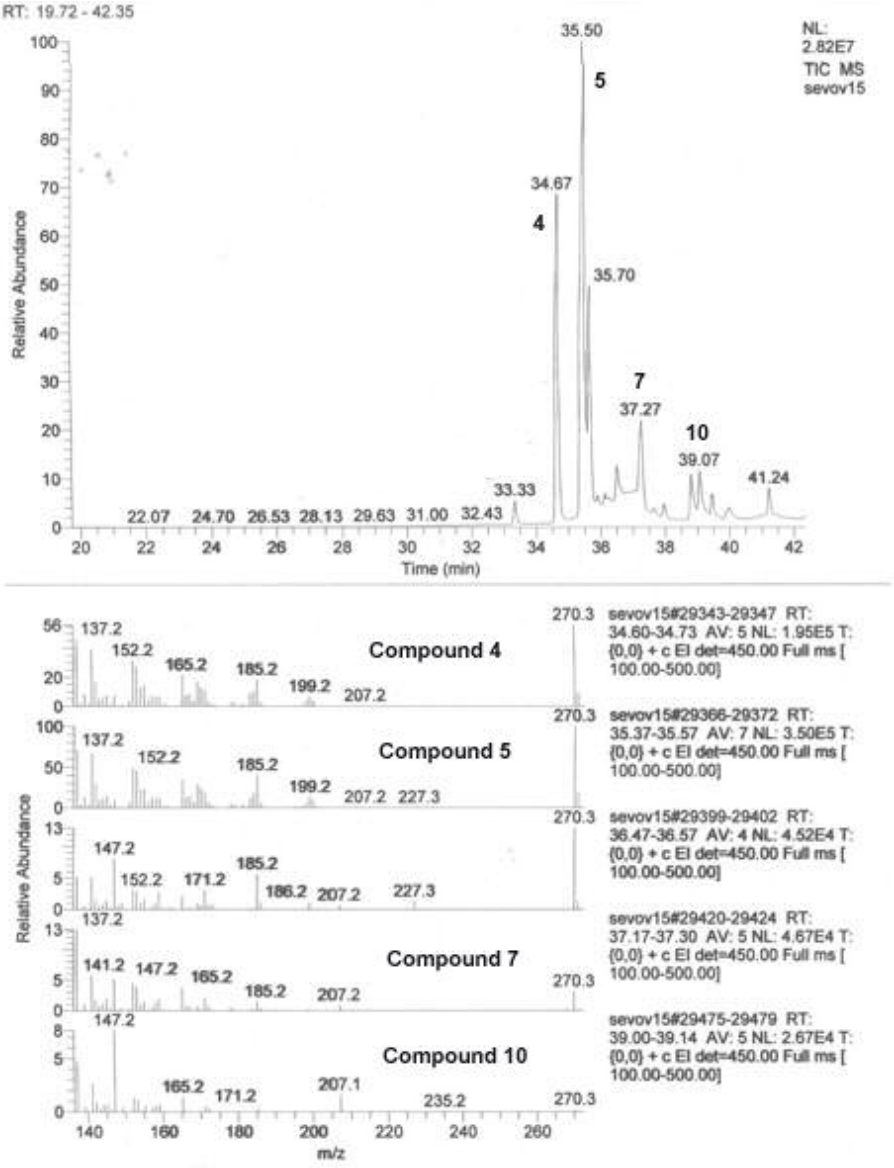
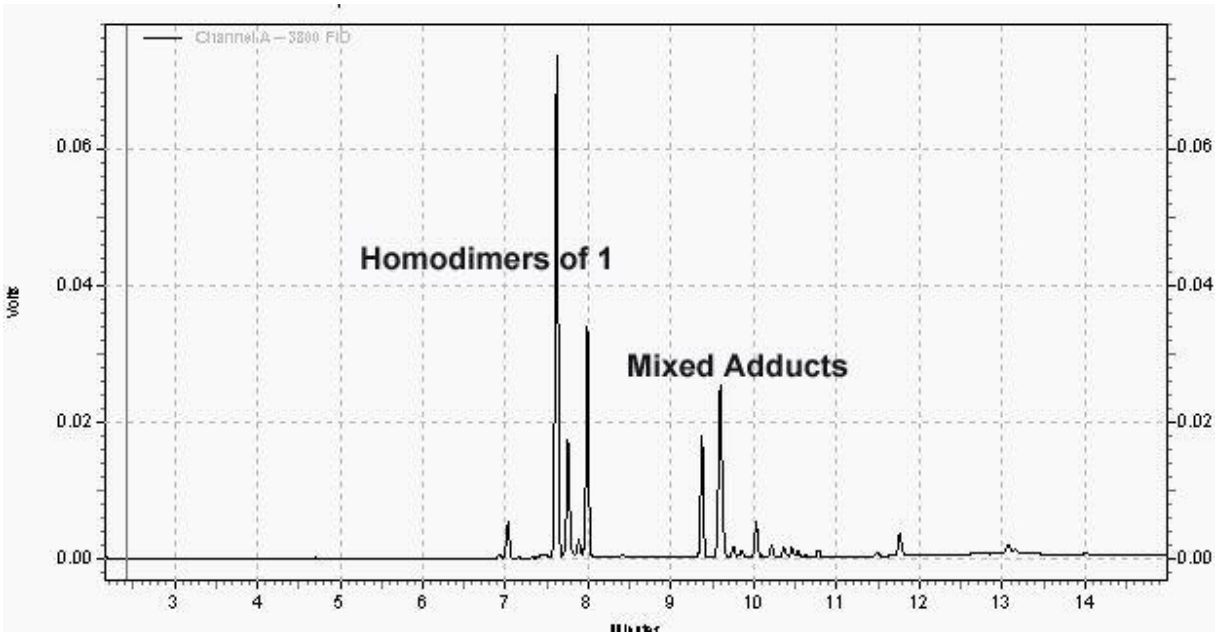
Full citation of reference 20: (a) Gaussian 03, Revision B.05, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Pittsburgh PA,, 2003.

GC/MS spectra of fully characterized compounds **4**, **5**, and **7** and postulated compound **10**.



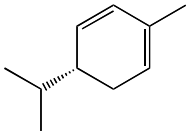
GC trace showing favored formation of homodimers of **1** over mixed adducts.



Reaction Conditions: 1:1 molar ratio (R)-(α)-phellandrene:4-methoxystyrene in a 1.51M solution. 2-mol-% pyrylium salt **3** as electron transfer catalyst. 3 hour irradiation time.

Complete list of Structures

1



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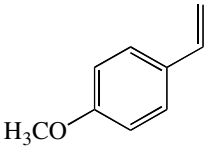

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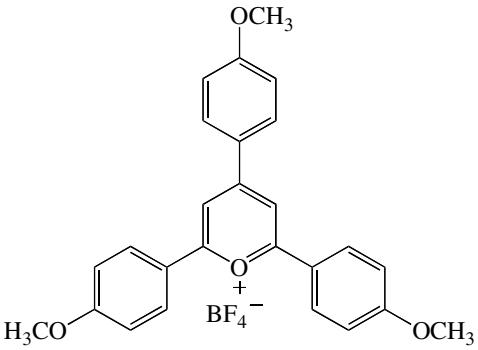

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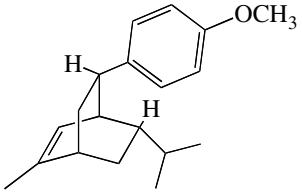

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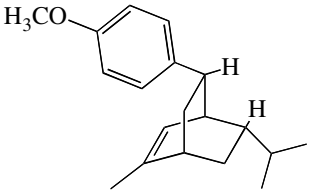
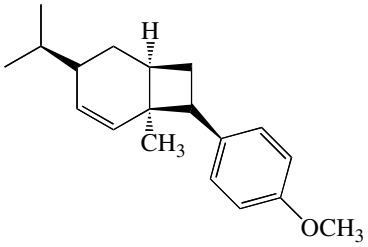


6 Unidentified product isomer observed in GC trace.

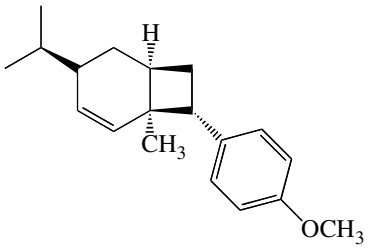
7



8 Unidentified product isomer observed in GC trace.

9 Unidentified product isomer observed in GC trace.

10



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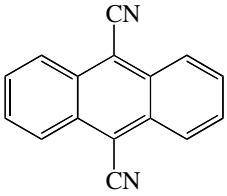
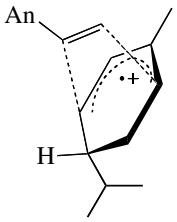
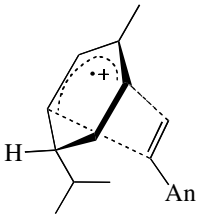


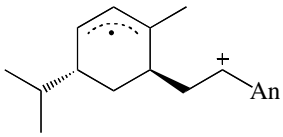
12$^{\bullet+}$



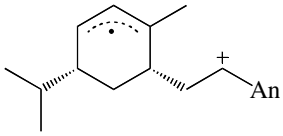
13$^{\bullet+}$



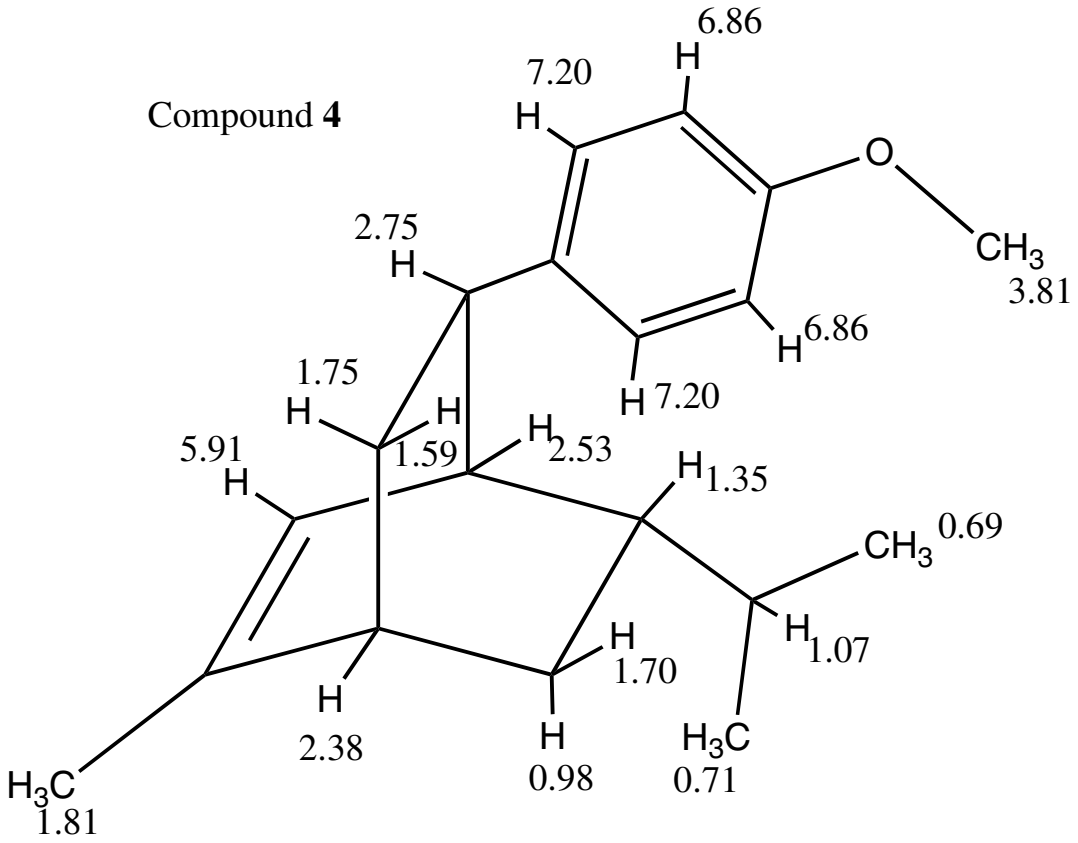
14$^{\bullet+}$



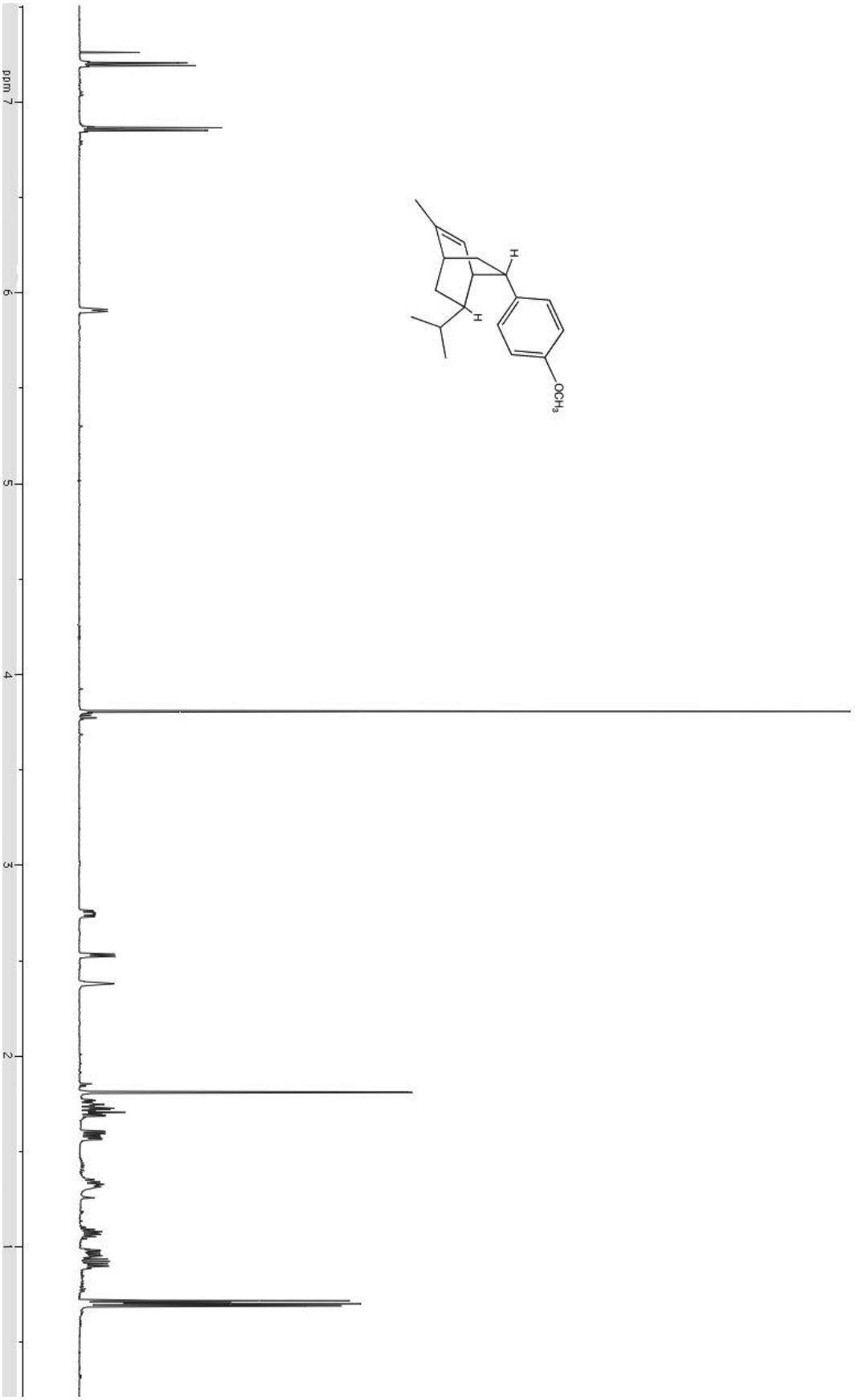
15$^{\bullet+}$



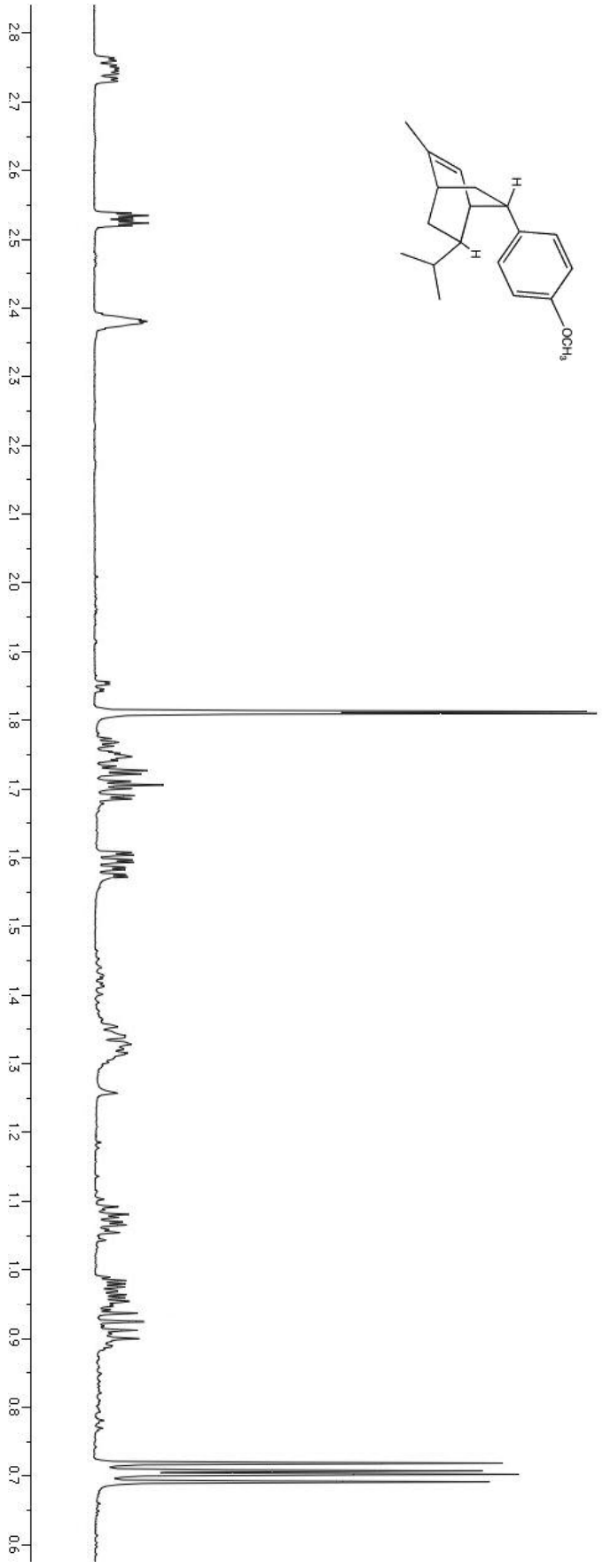
^{1}H NMR assignment for compound **4**



Full ^{1}H NMR for Compound **4**

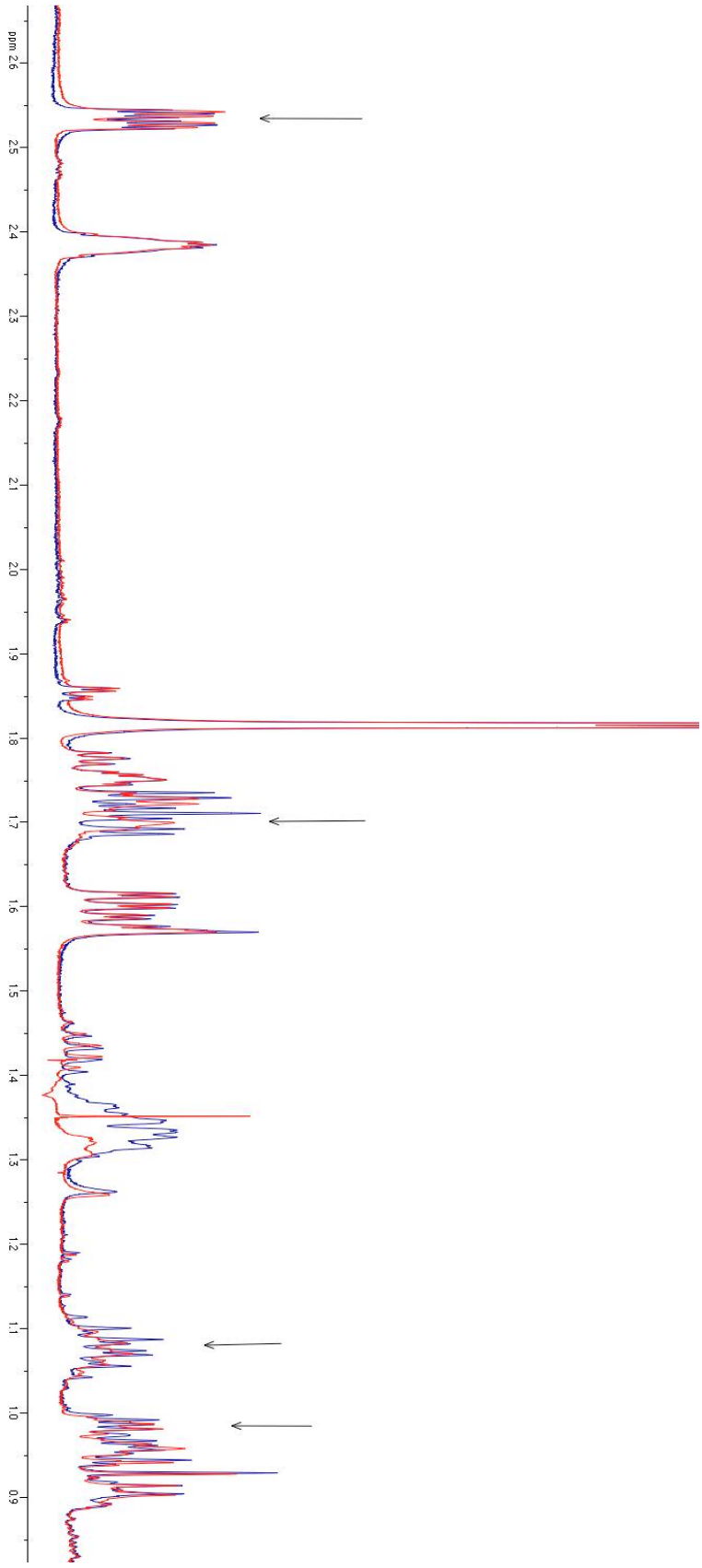


0.6-2.8 ppm range expanded for compound **4**.



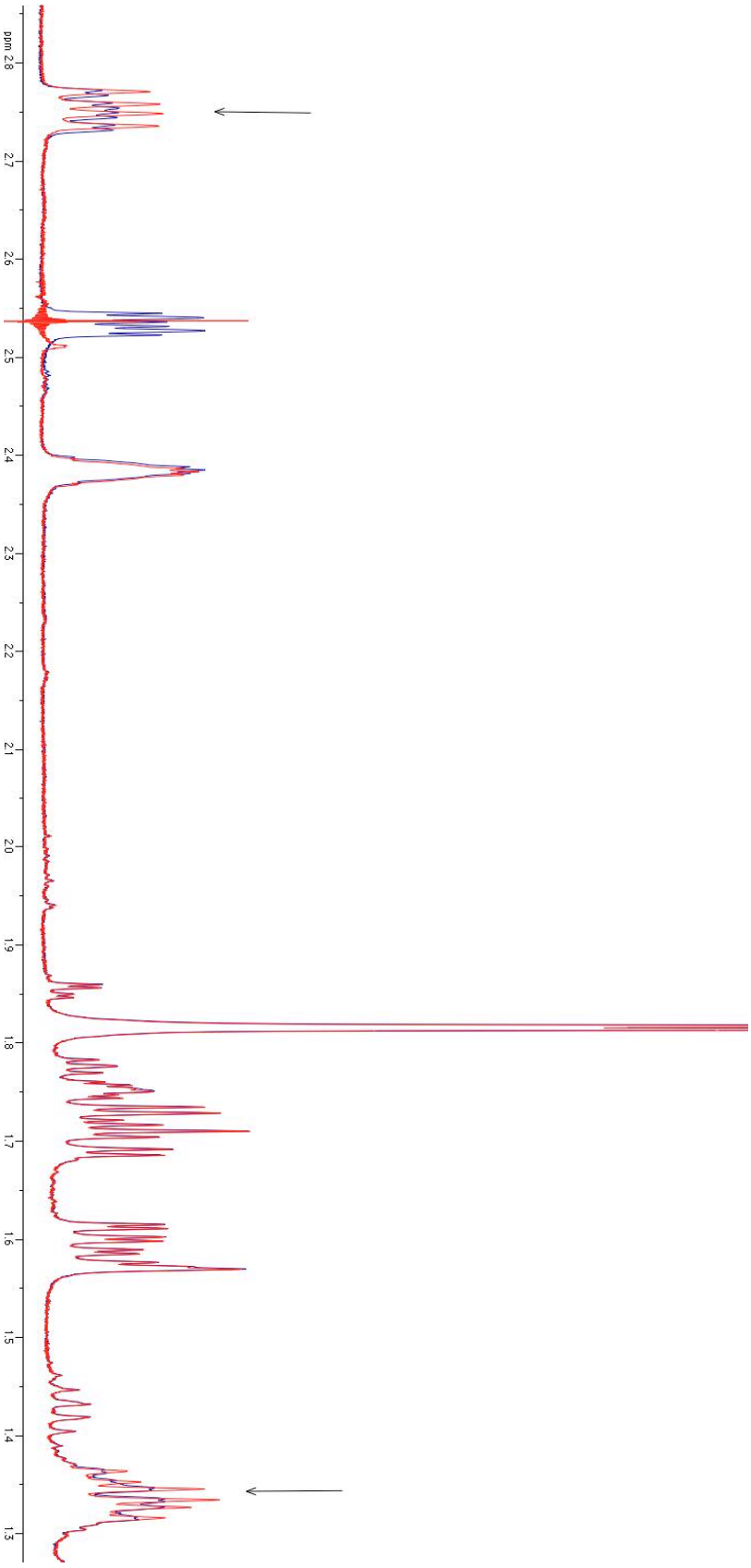
^{1}H Decoupling experiment compound **4**: 1.35 ppm proton

NOTE: Because coupling constants were not successfully extrapolated for each resonance, decoupling experiments were carried out to unambiguously determine ^{3}J couplings.



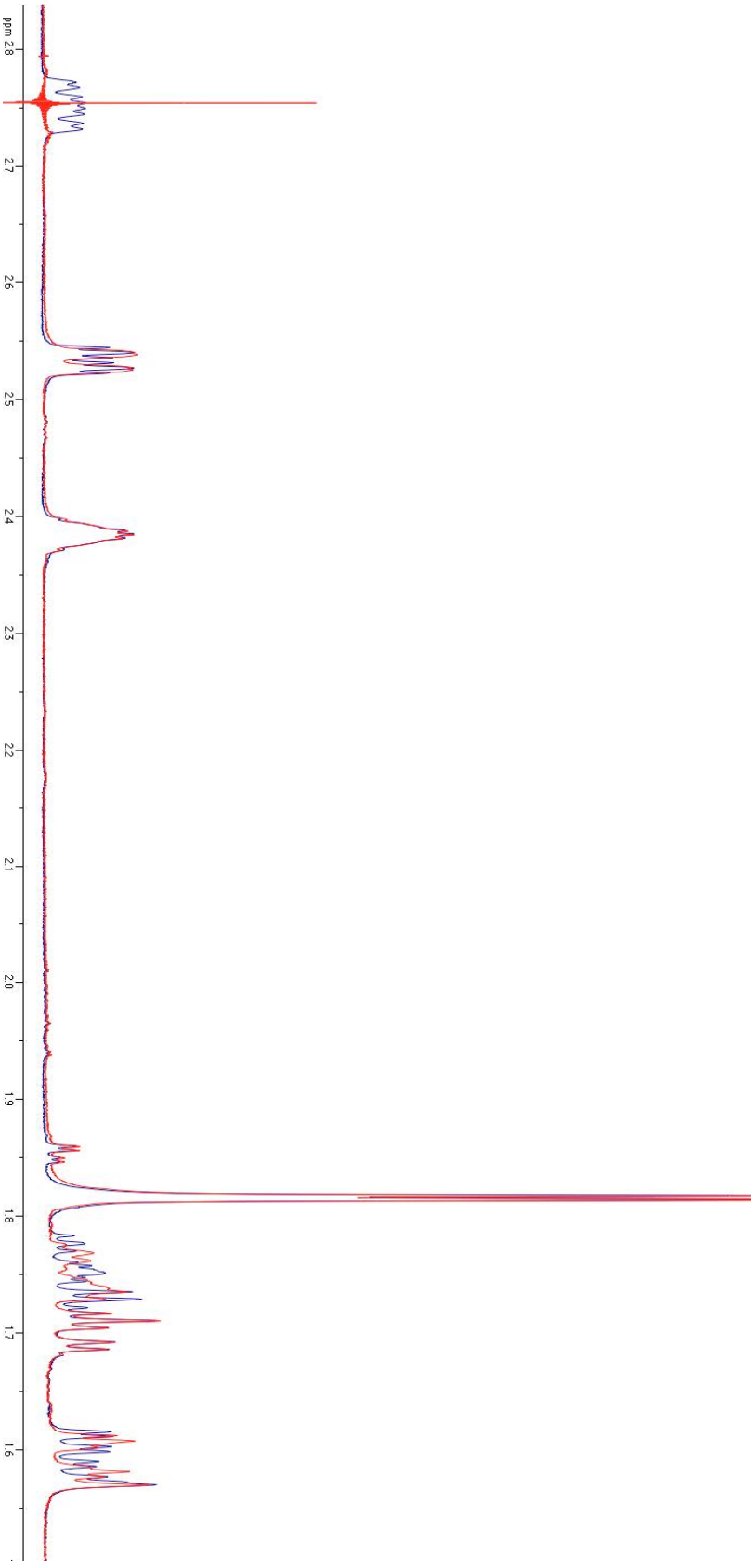
^{1}H Decoupling experiment compound **4**: 2.53 ppm proton

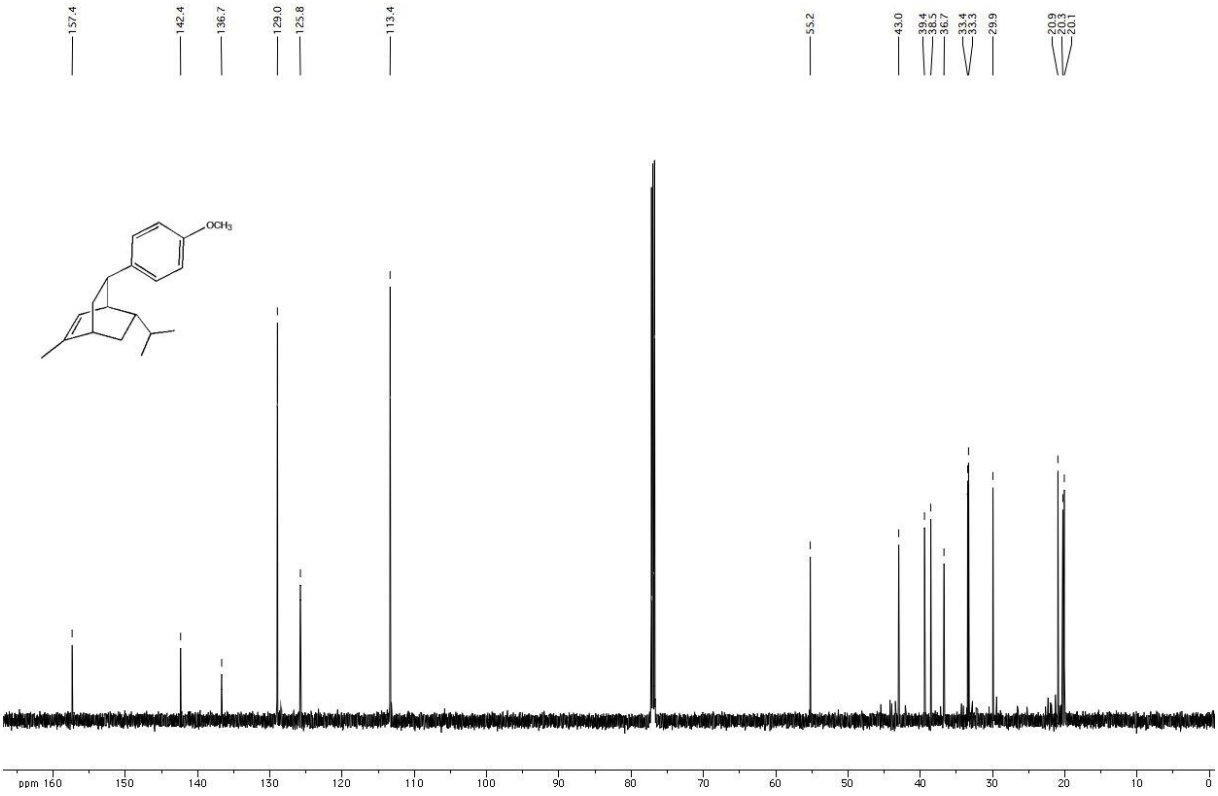
NOTE: Because coupling constants were not successfully extrapolated for each resonance, decoupling experiments were carried out to unambiguously determine ^{3}J couplings.



^{1}H Decoupling experiment compound **4**: 2.75 ppm proton

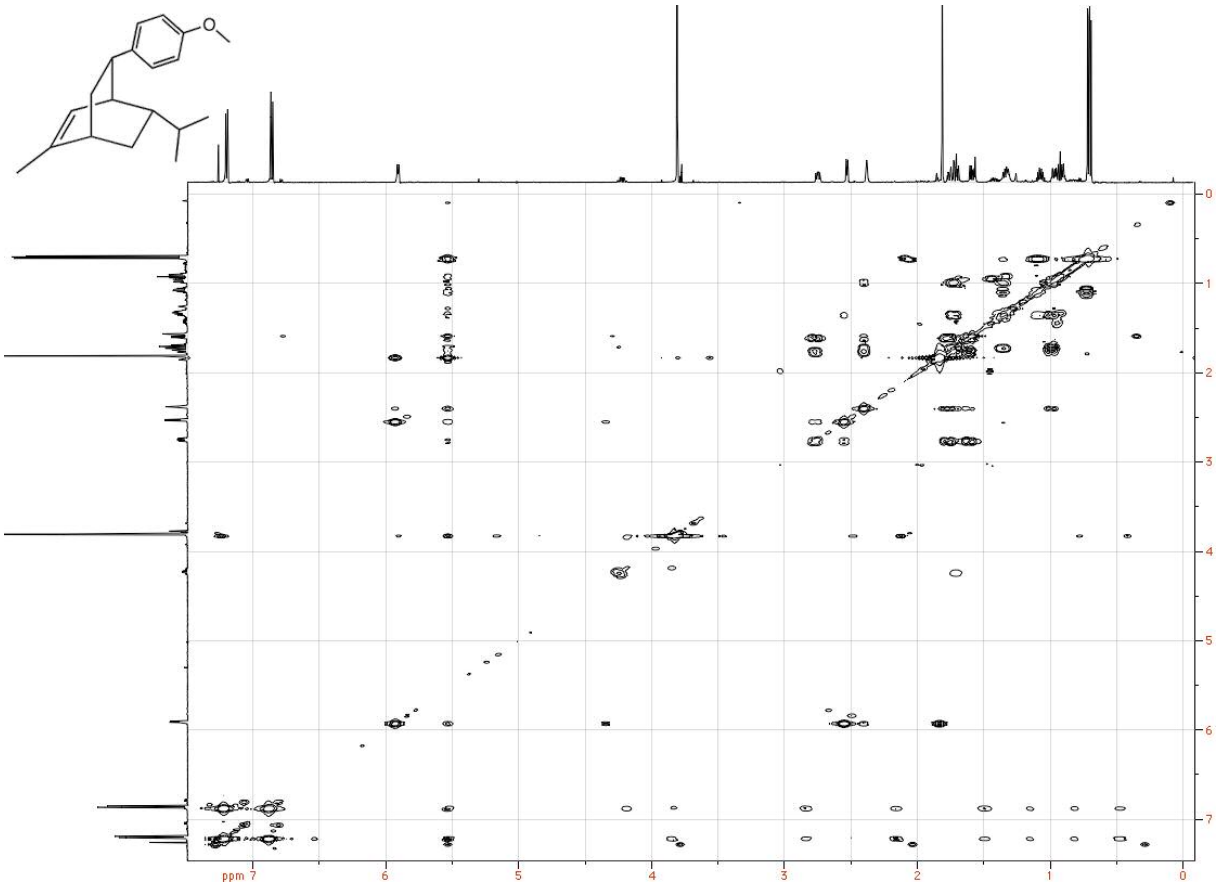
NOTE: Because coupling constants were not successfully extrapolated for each resonance, decoupling experiments were carried out to unambiguously determine ^{3}J couplings.



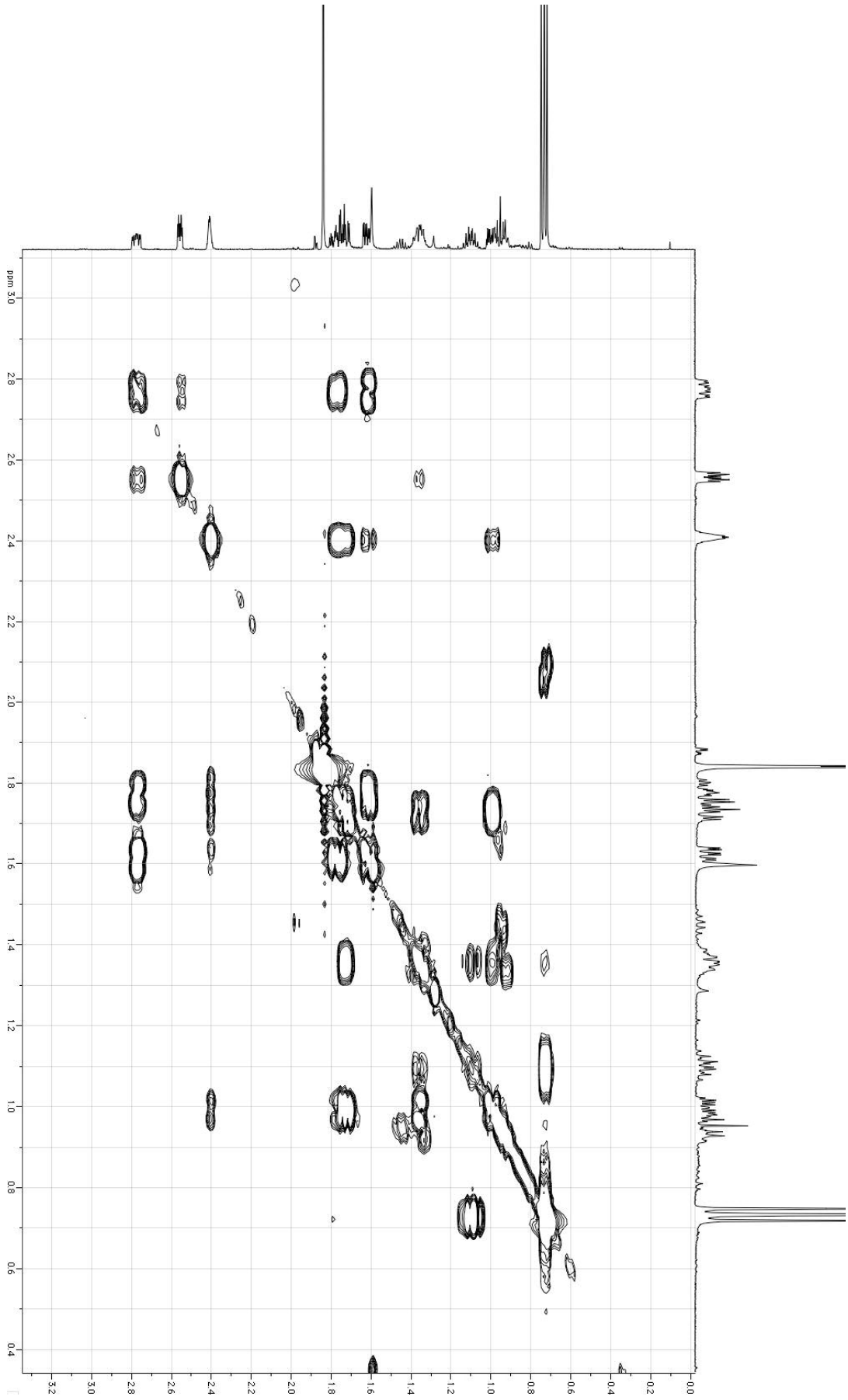


^{13}C NMR for compound **4**

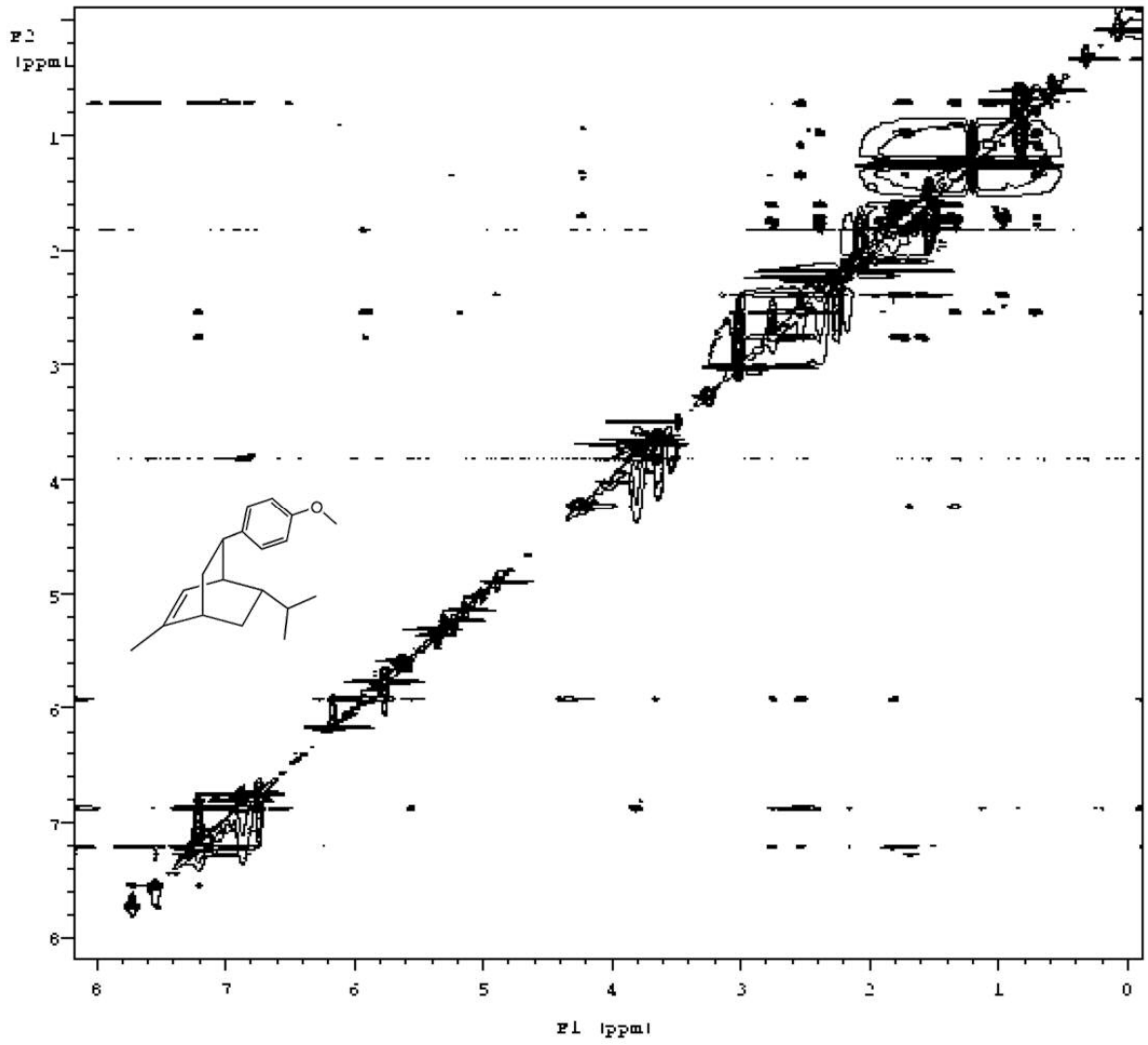
Full COSY NMR of compound **4**.



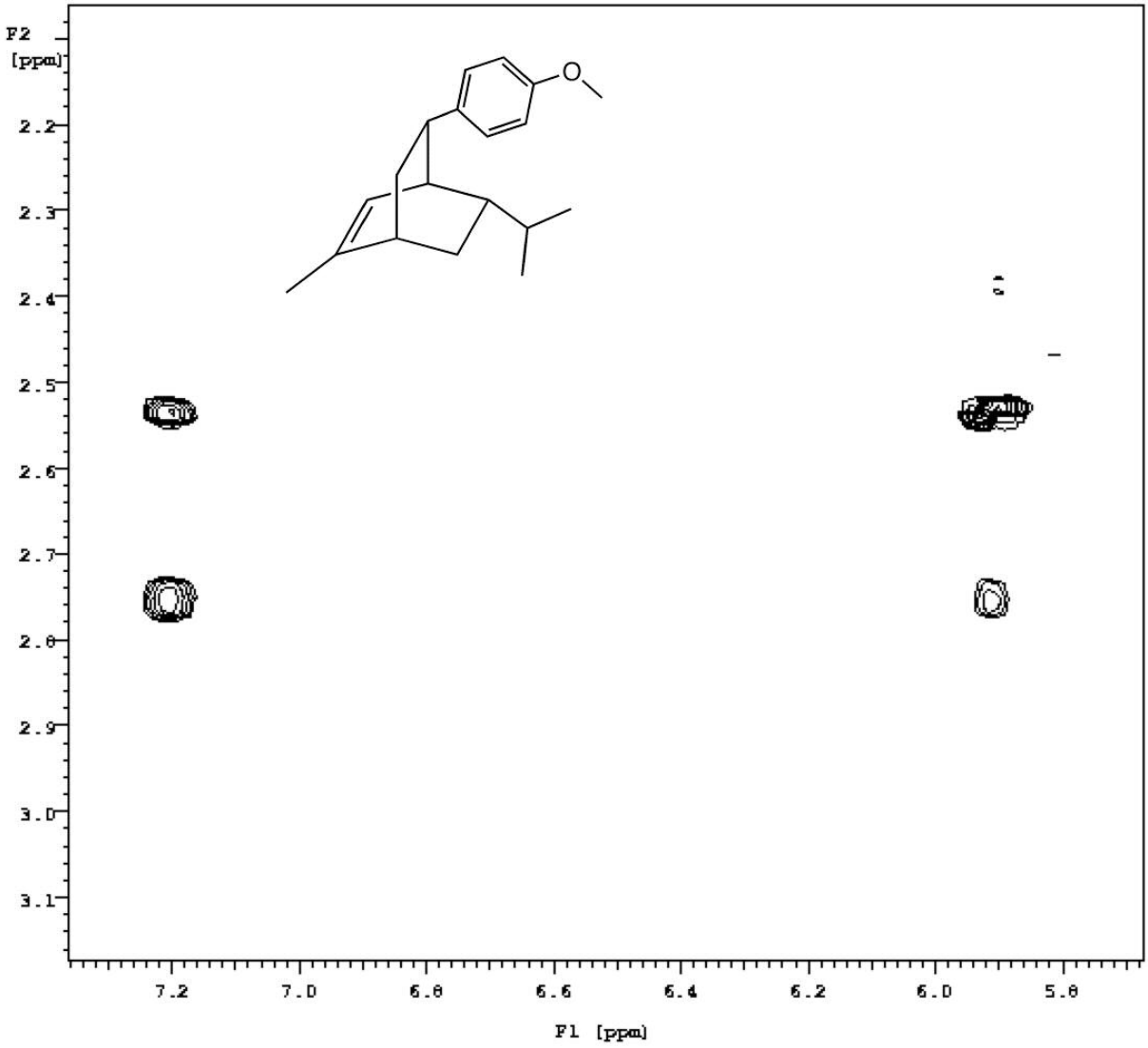
Expanded COSY NMR of compound **4**.



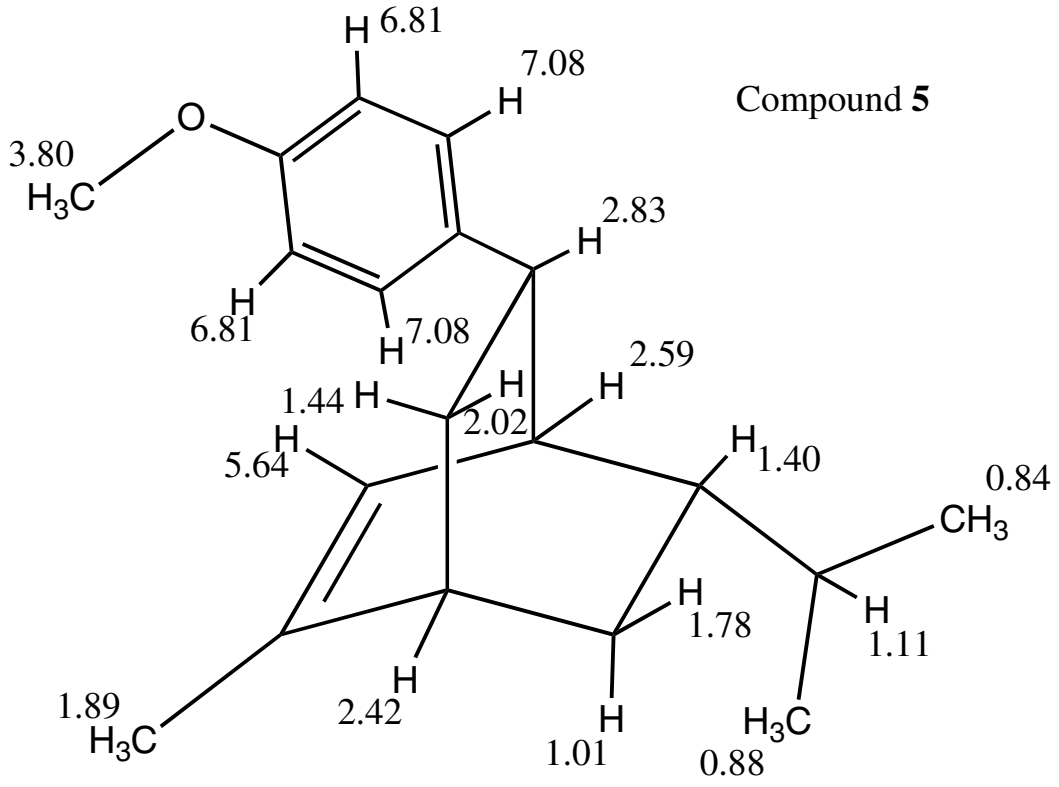
Full ROESY NMR spectrum for compound **4**



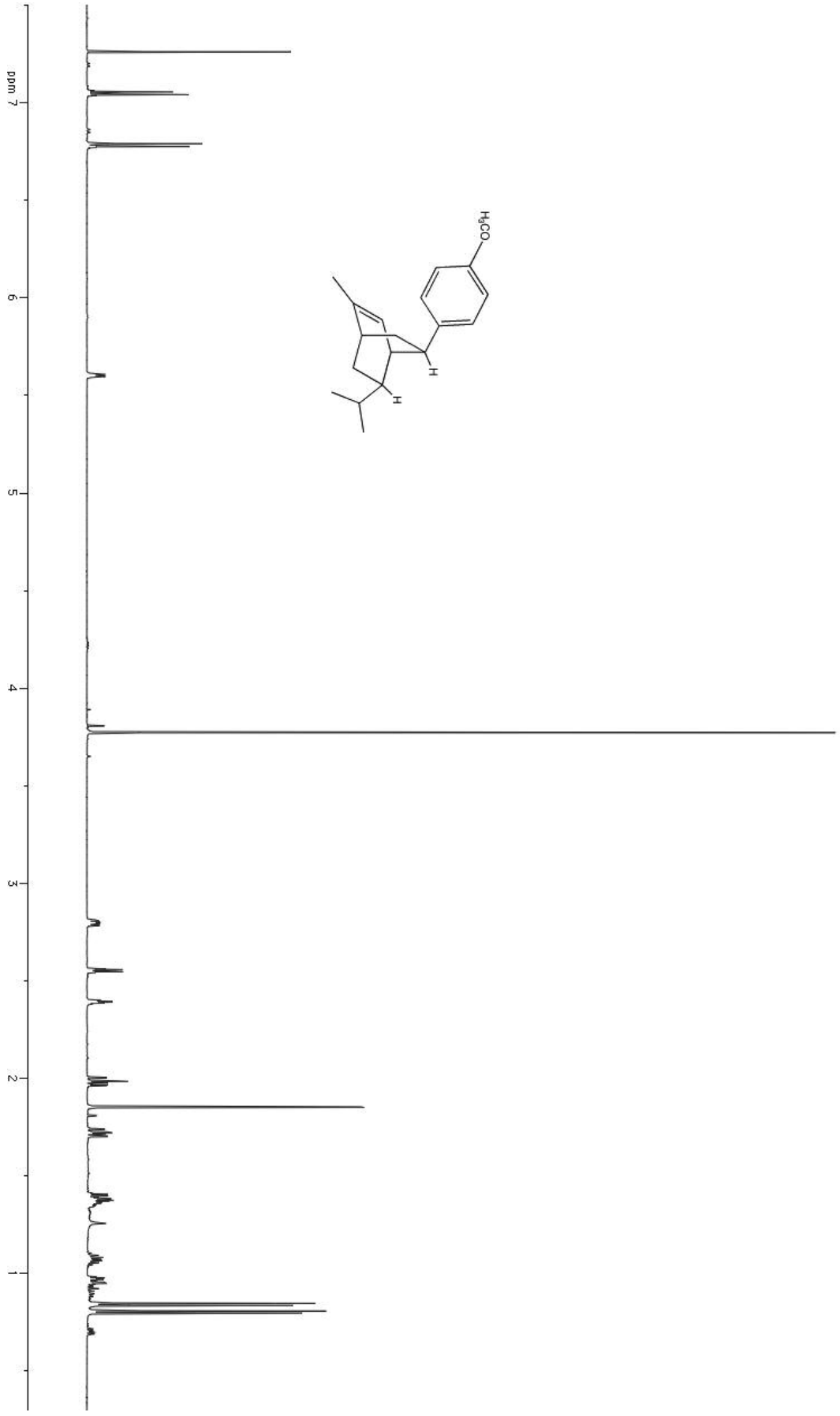
Key ROESY NOE coupling between 5.91 ppm and 2.75 ppm hydrogens indicative of absolute stereochemistry.



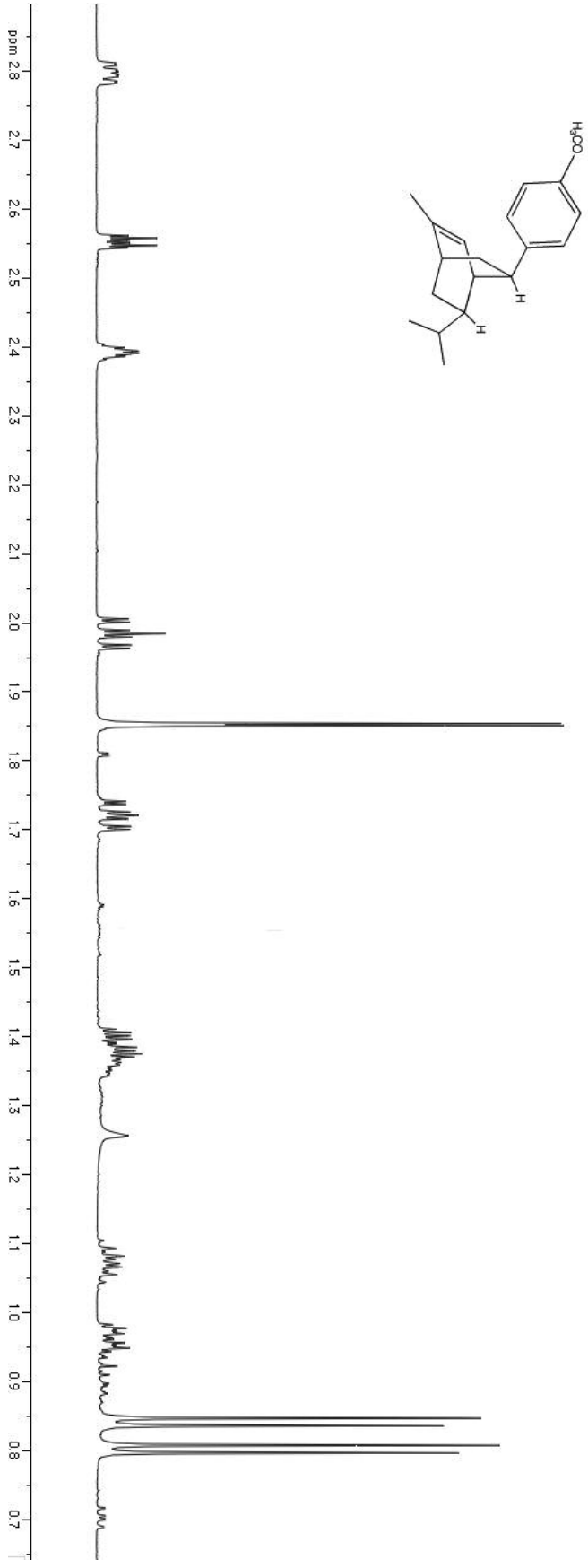
Full ^{1}H NMR assignment for compound **5**



Full ^{1}H NMR for Compound **5**

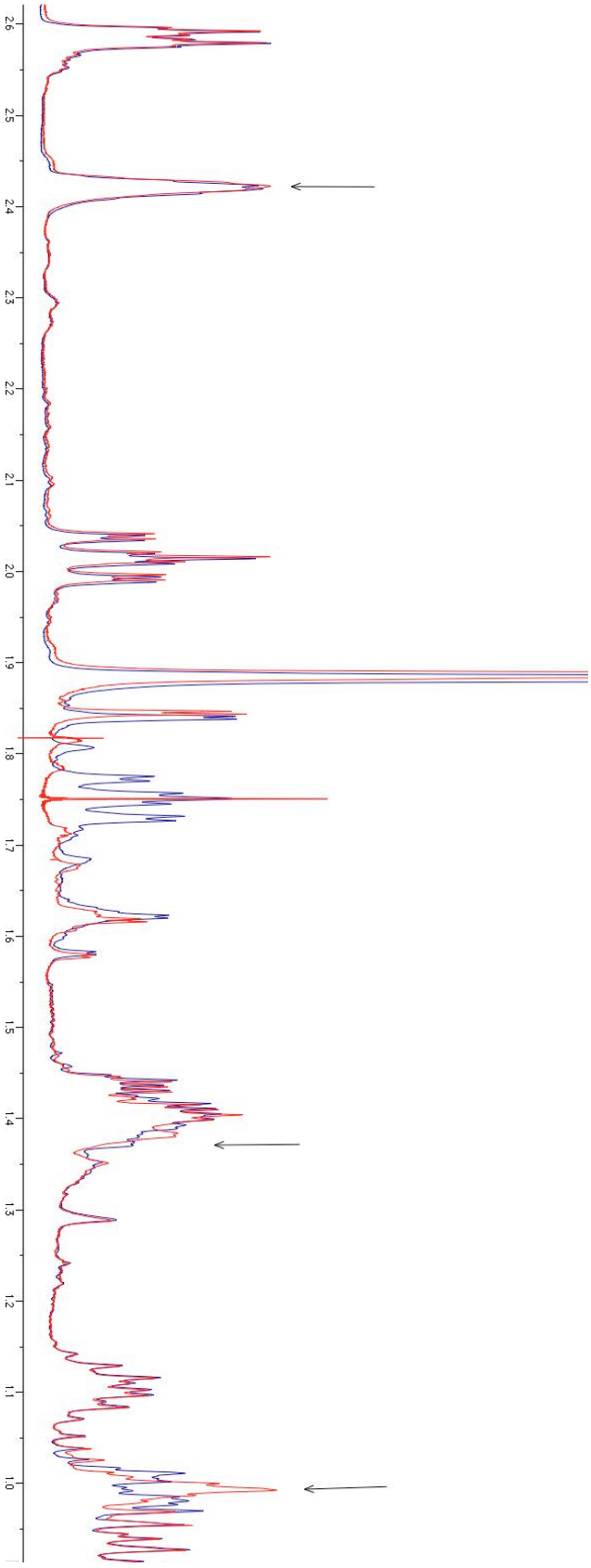


Expanded ^{1}H NMR for Compound **5**



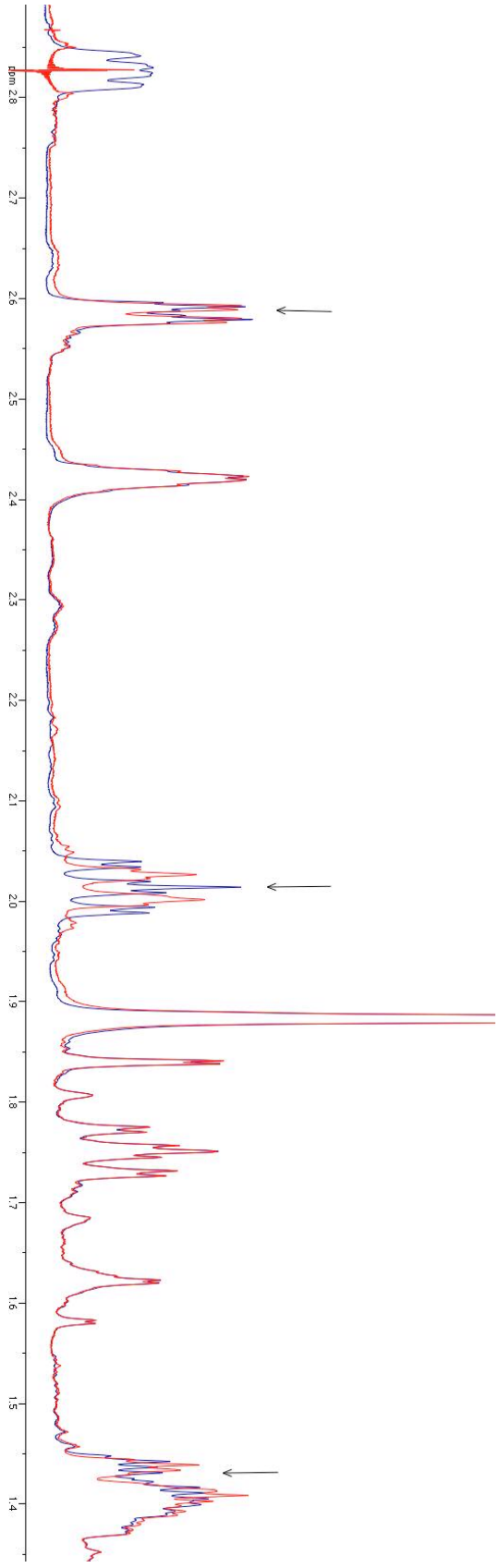
^{1}H Decoupling experiment compound **5**: 1.78 ppm proton

NOTE: Because coupling constants were not successfully extrapolated for each resonance, decoupling experiments were carried out to unambiguously determine ^{3}J couplings.

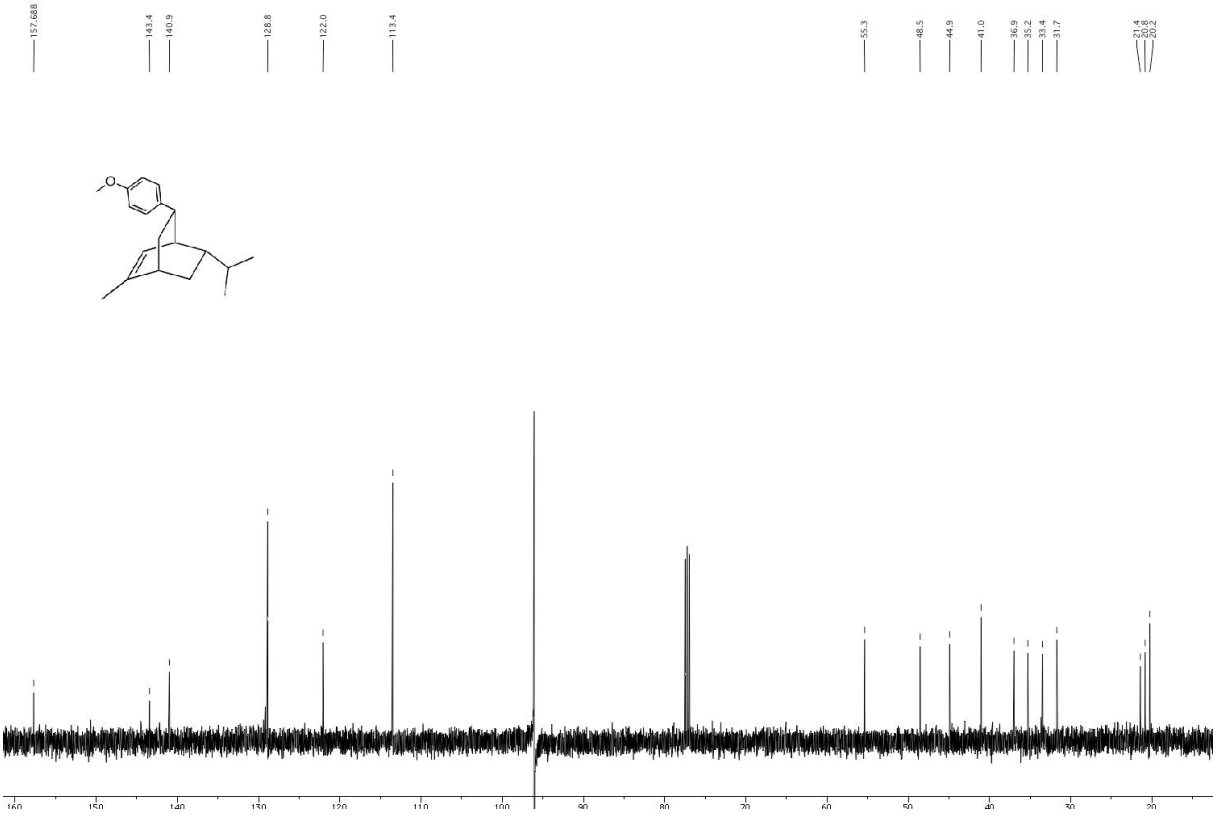


^{1}H Decoupling experiment compound **5**: 2.83 ppm proton

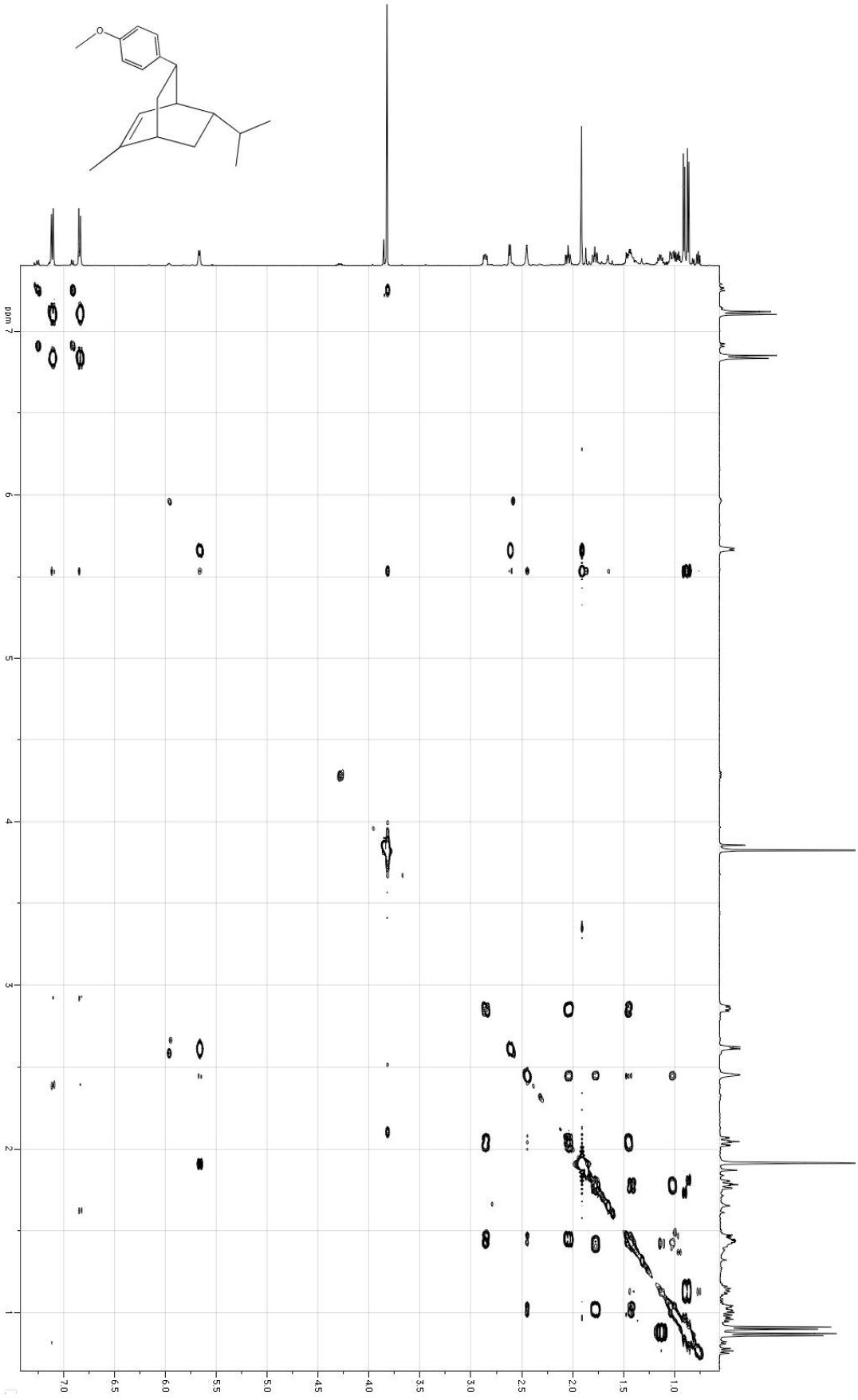
NOTE: Because coupling constants were not successfully extrapolated for each resonance, decoupling experiments were carried out to unambiguously determine ^{3}J couplings.



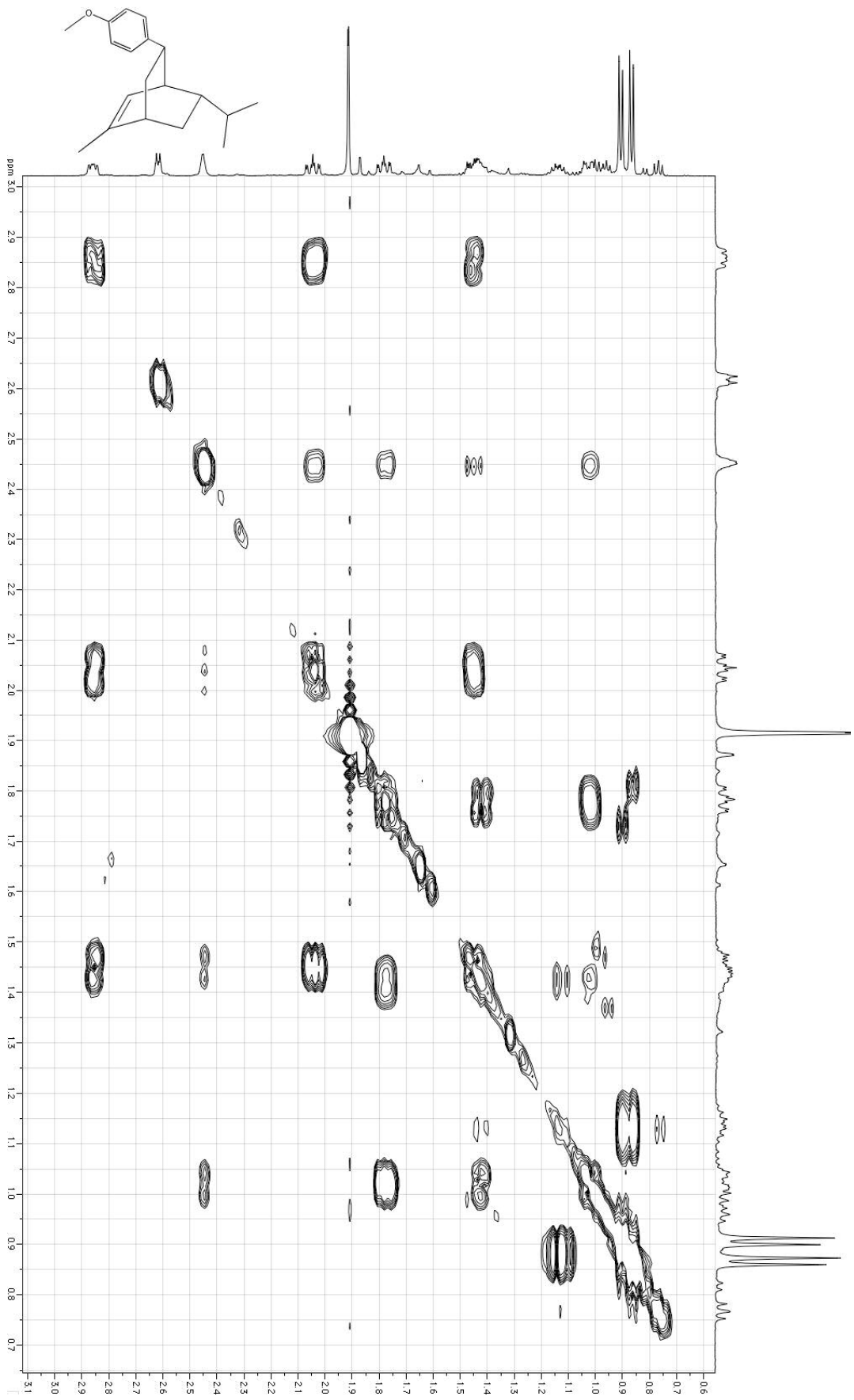
^{13}C NMR spectrum of **5**. Peak at 96 ppm is phasing issue.



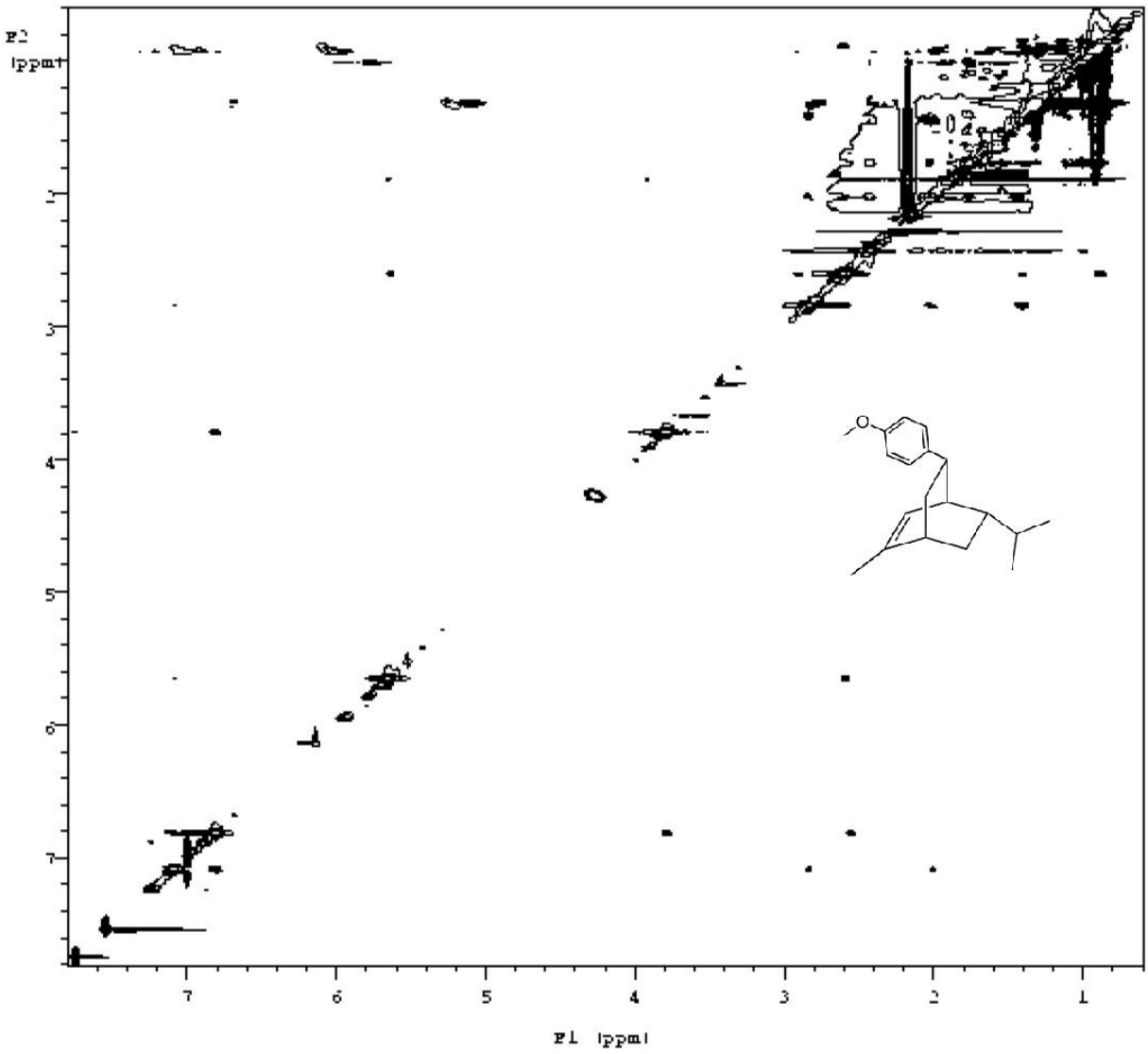
Full COSY NMR for **5**



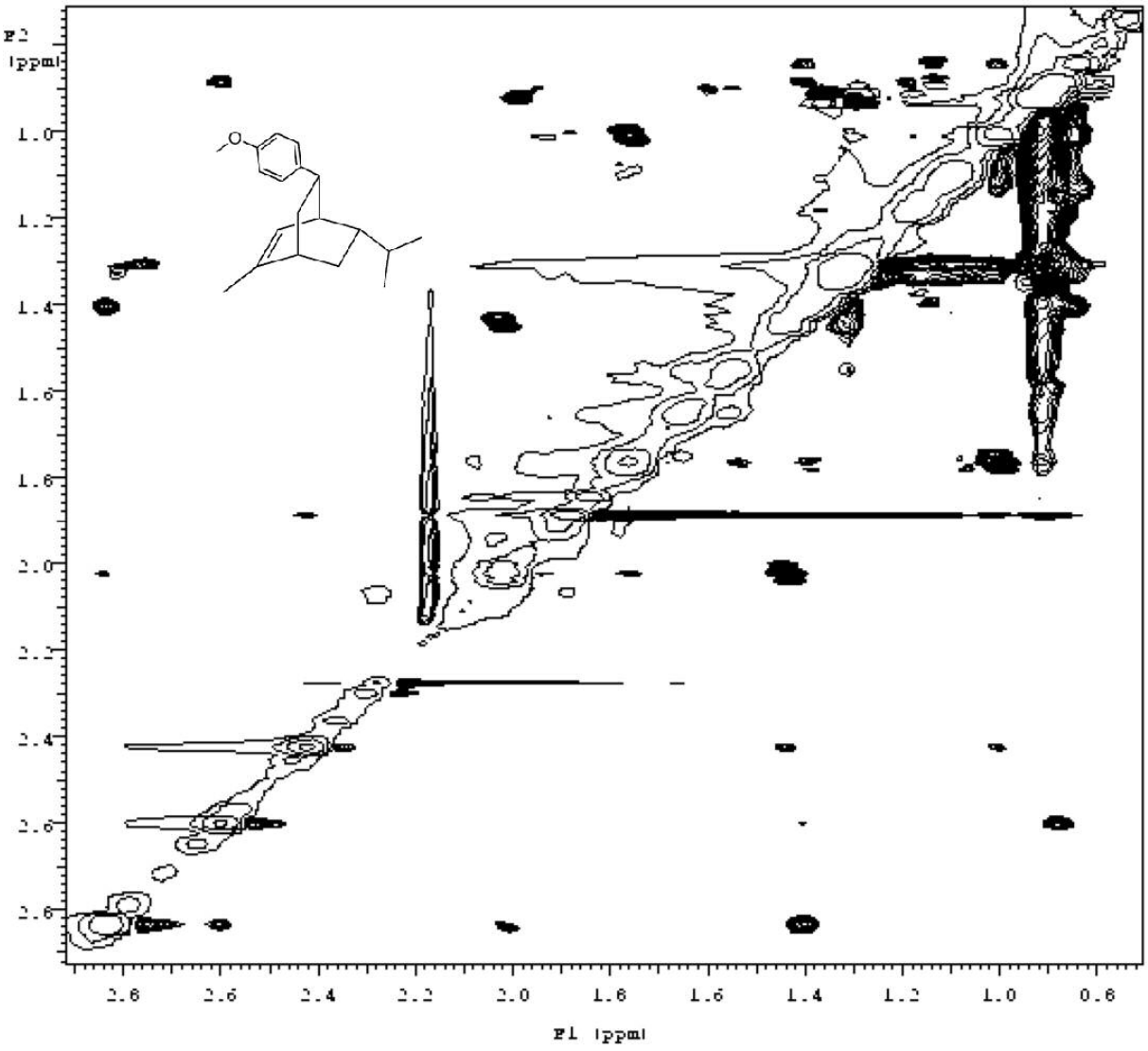
Expanded COSY for **5**



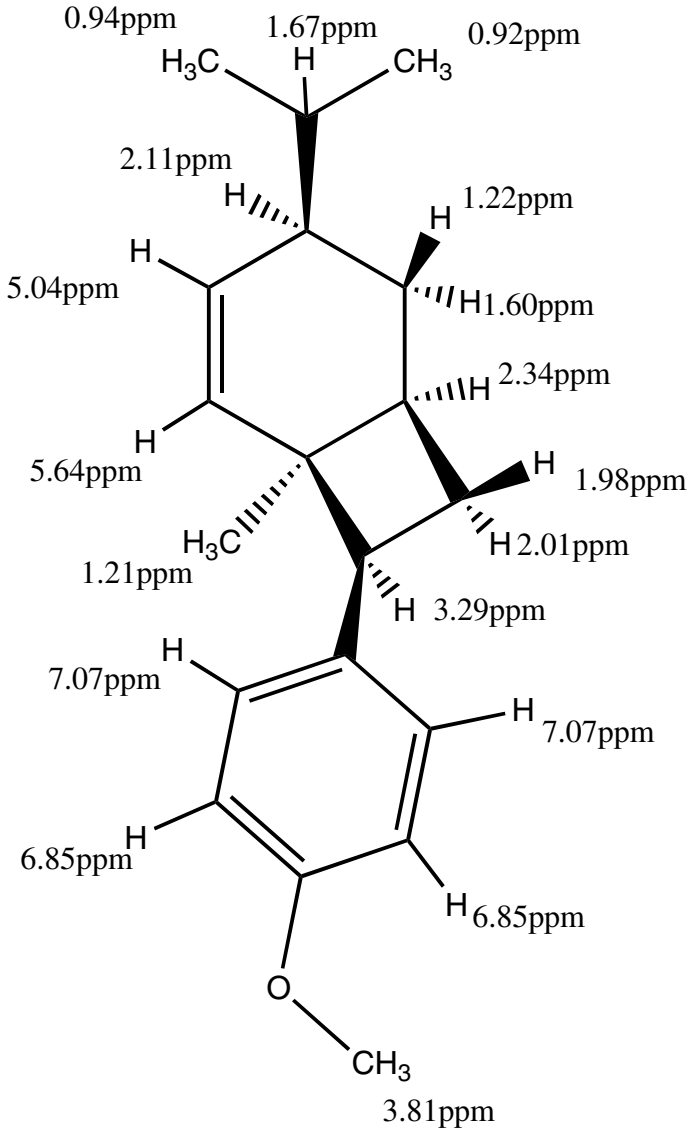
Full ROESY for compound **5**



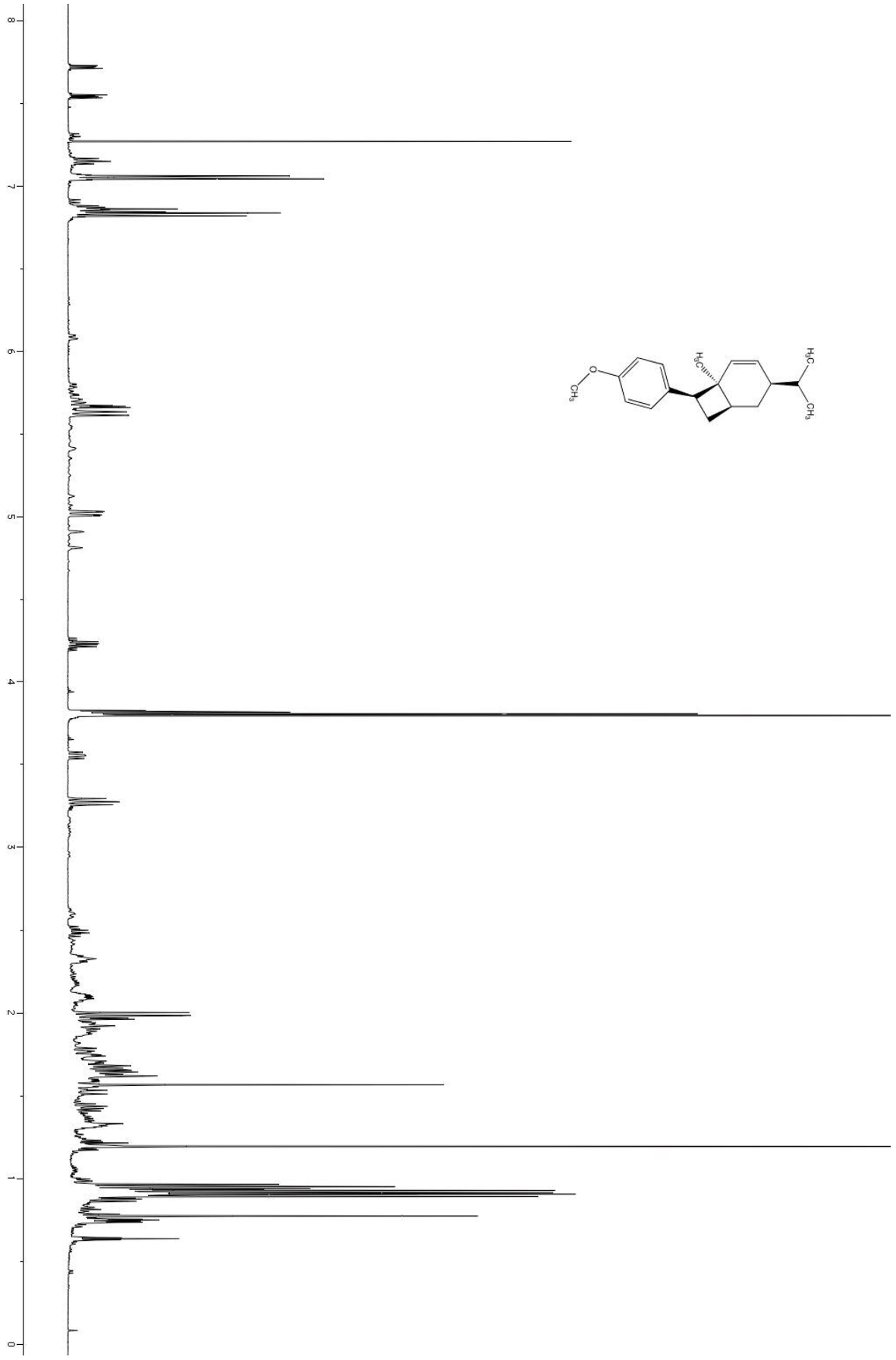
Key NOE at of **5** observed at 1.4 ppm and 2.83 ppm crosspeak between *exo* and benzylic protons for overall *endo* stereochemistry.



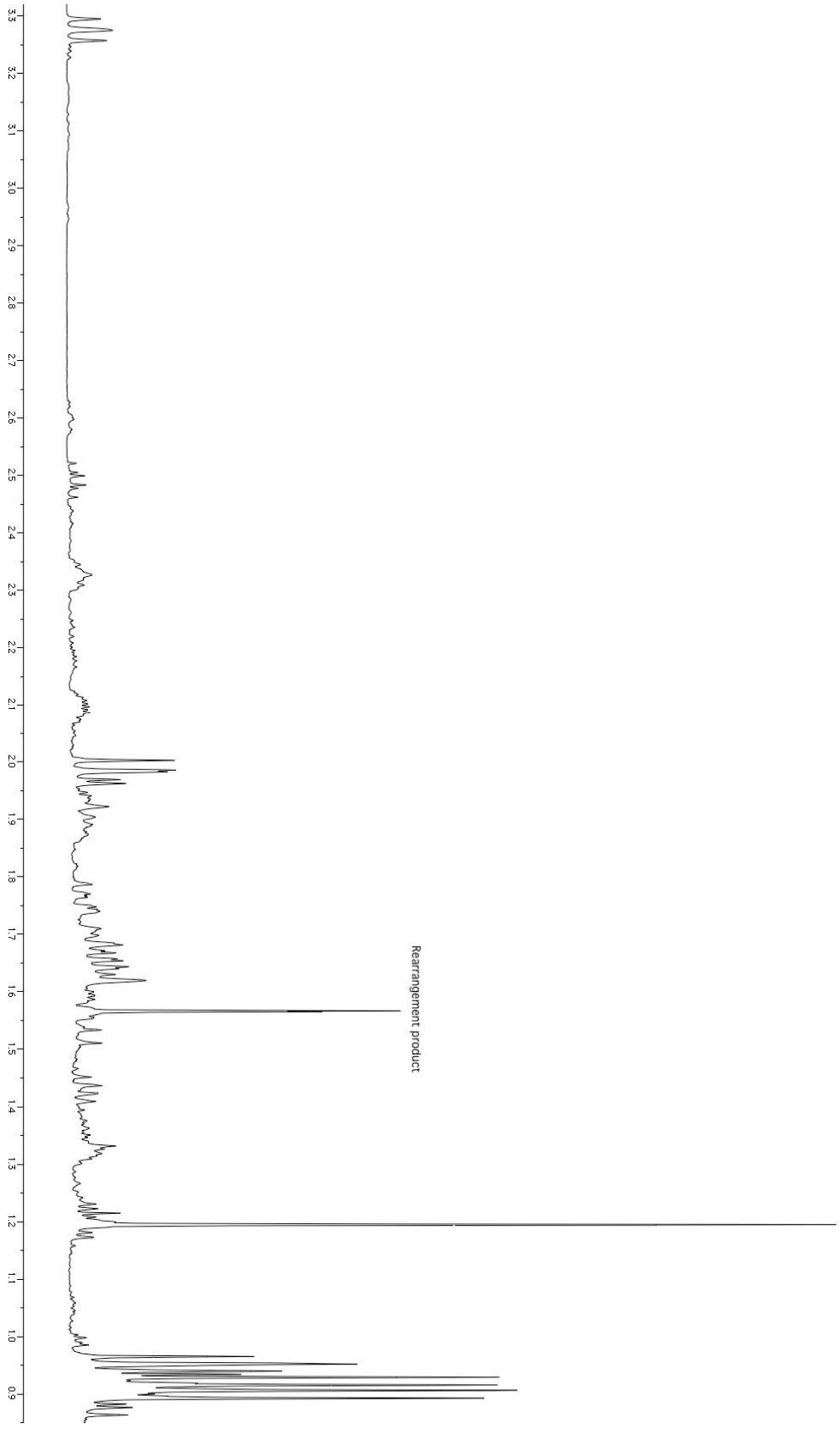
^{1}H NMR assignment of compound **7**



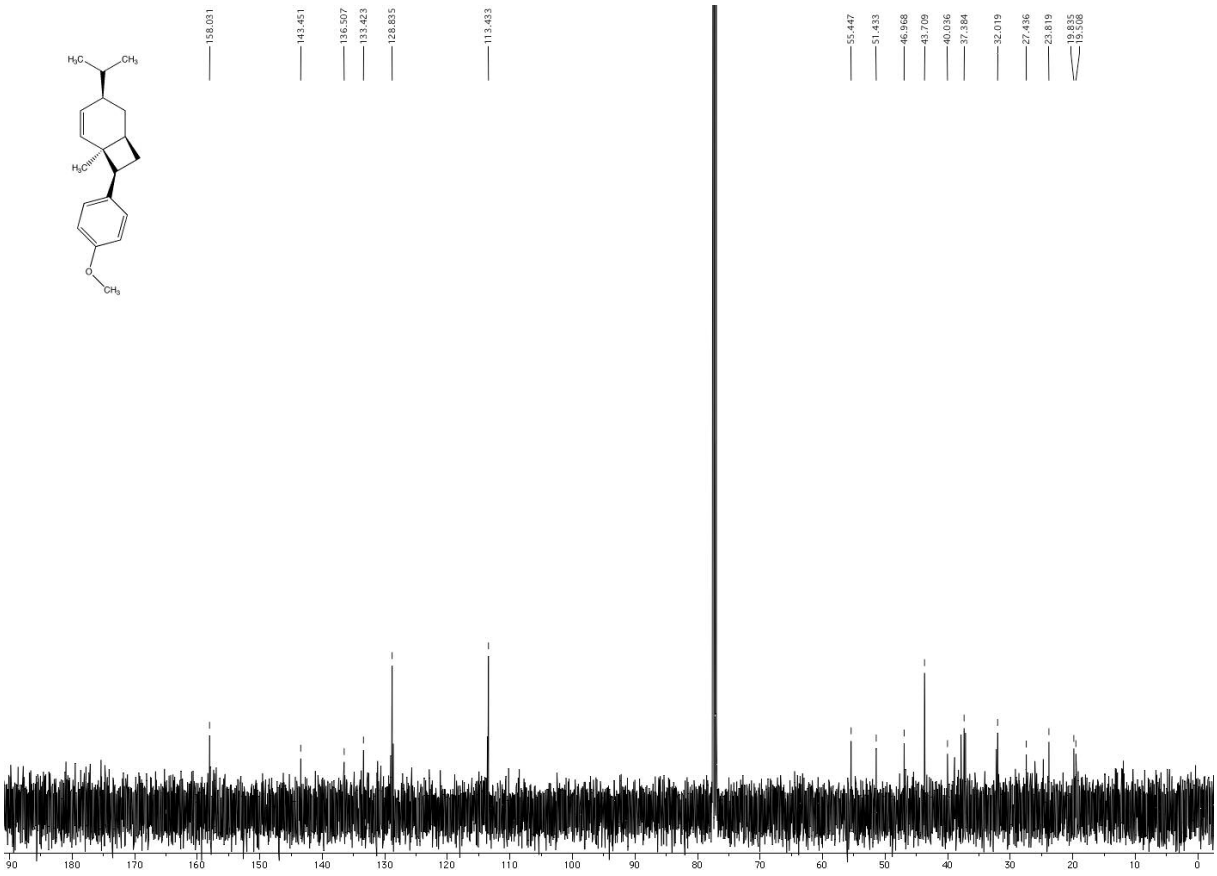
Full ^{1}H NMR spectrum of **7**



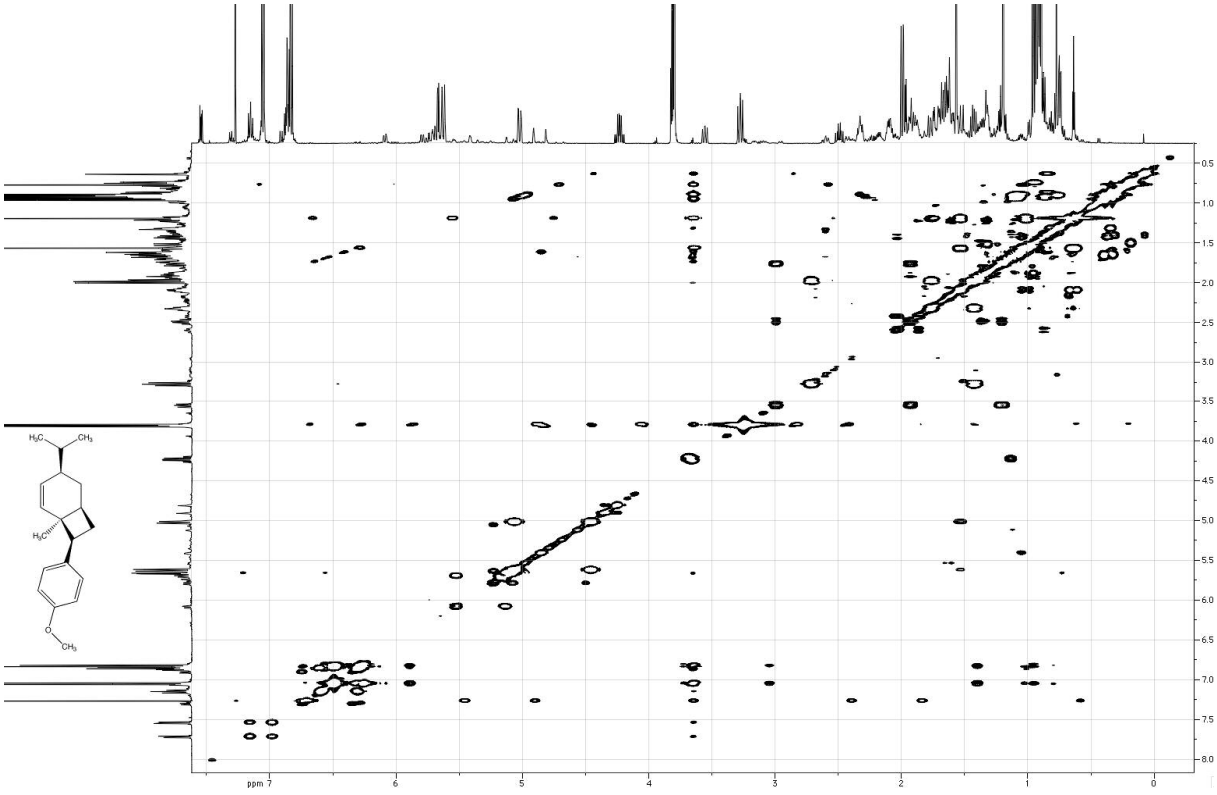
Expanded ^{1}H NMR spectrum of **7**



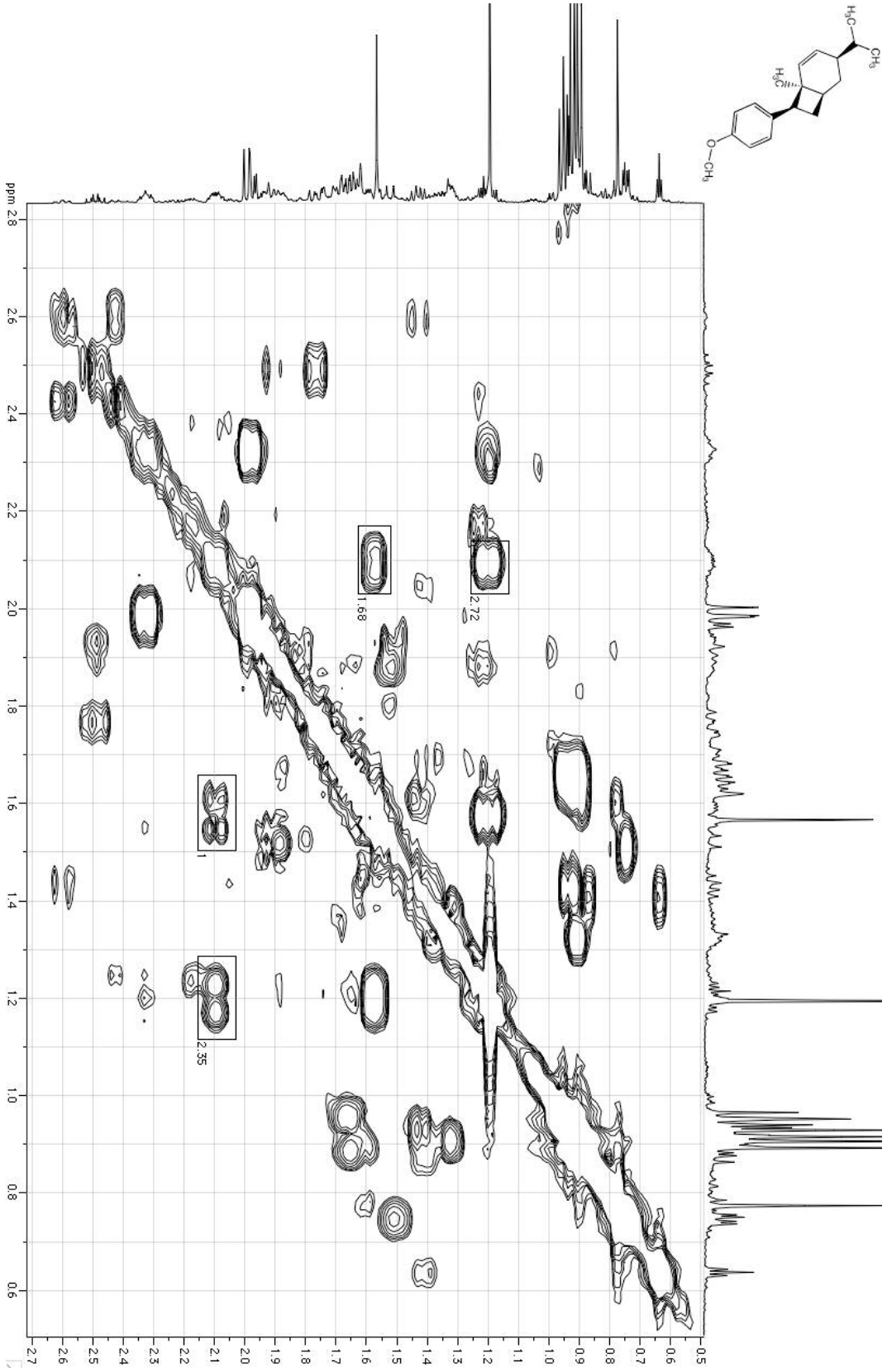
^{13}C NMR spectrum of **7**.



Full COSY NMR of **7**

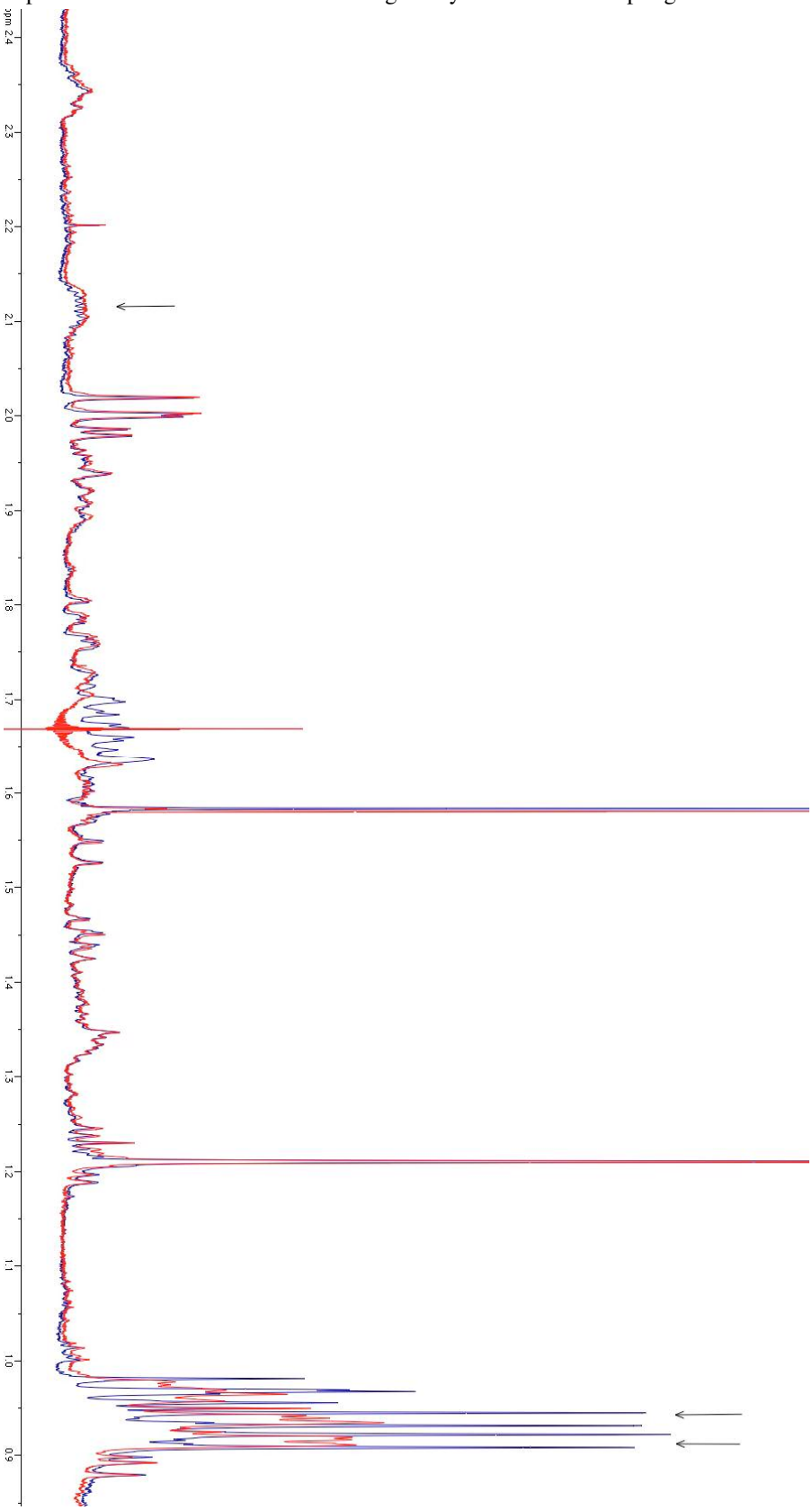


Expanded COSY NMR of **7**. Coupling intensities between 2.11 ppm and 1.22 ppm hydrogens are stronger than couplings between 2.11 ppm and 1.60 ppm indicating *trans* and *cis* respectively. This will be shown explicitly with decoupling data on the next page. This was the key coupling because ROESY data will show the stereochemistry of the rest of the molecule relative to half.

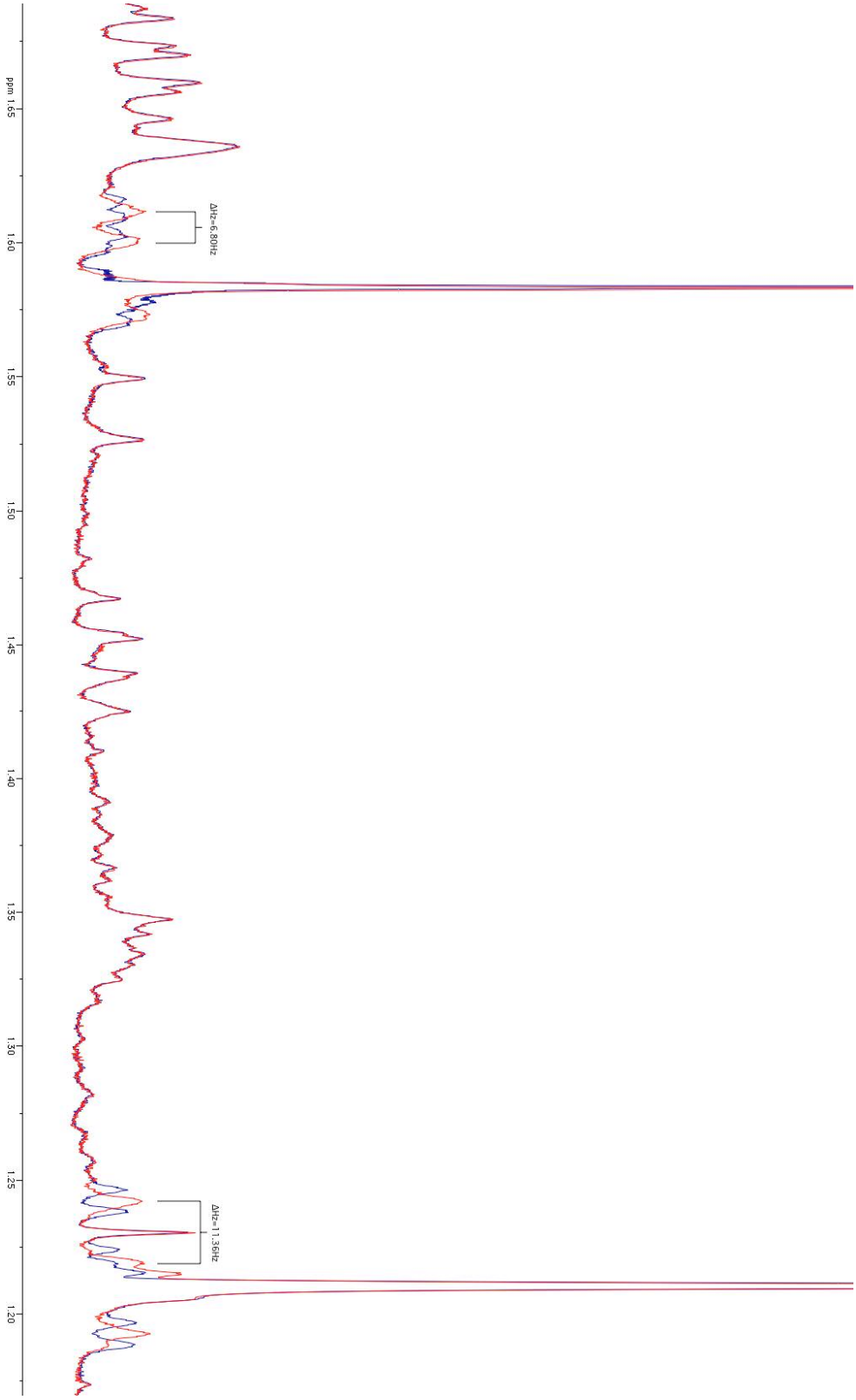


^{1}H Decoupling experiment compound **7**: 1.67 ppm proton

NOTE: Because coupling constants were not successfully extrapolated for each resonance, decoupling experiments were carried out to unambiguously determine ^{3}J couplings.

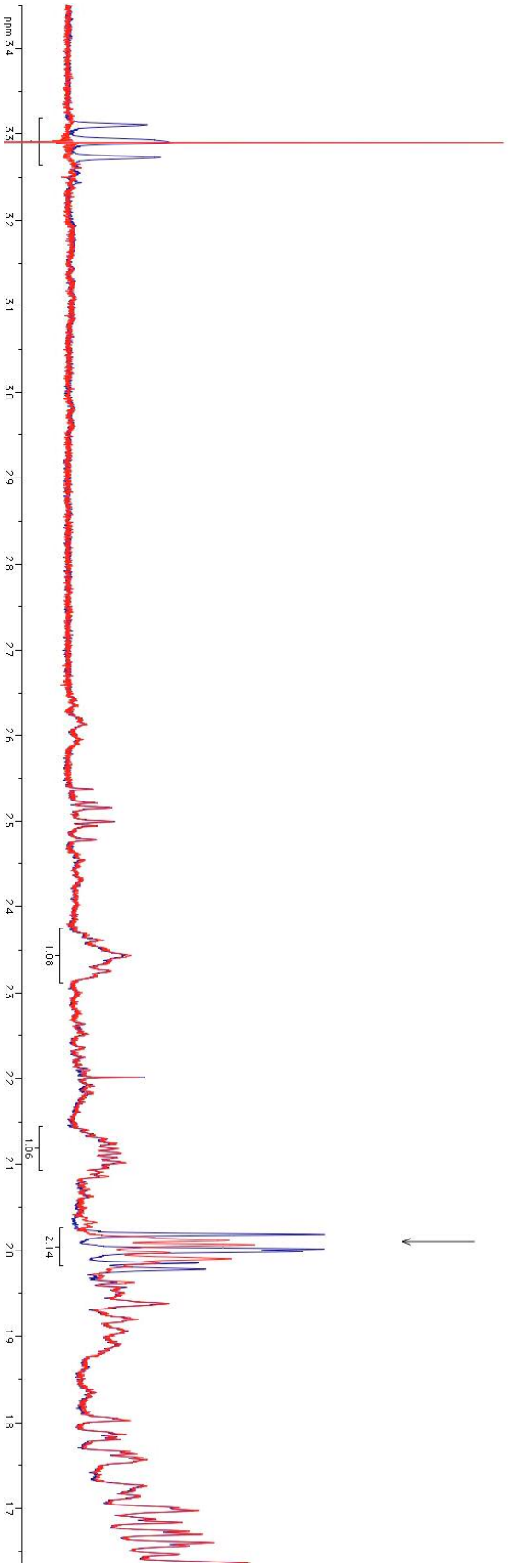


Decoupling the 2.34 ppm proton leaves only geminal coupling and vicinal coupling to the 2.11 ppm hydrogen. The red spectrum is the decoupled data overlayed on the blue unaltered ^{1}H NMR spectrum. One can see that a weaker *cis* coupling remains between the 2.11 ppm and 1.60 ppm proton while a stronger *trans* coupling is left for the 1.22 ppm proton.

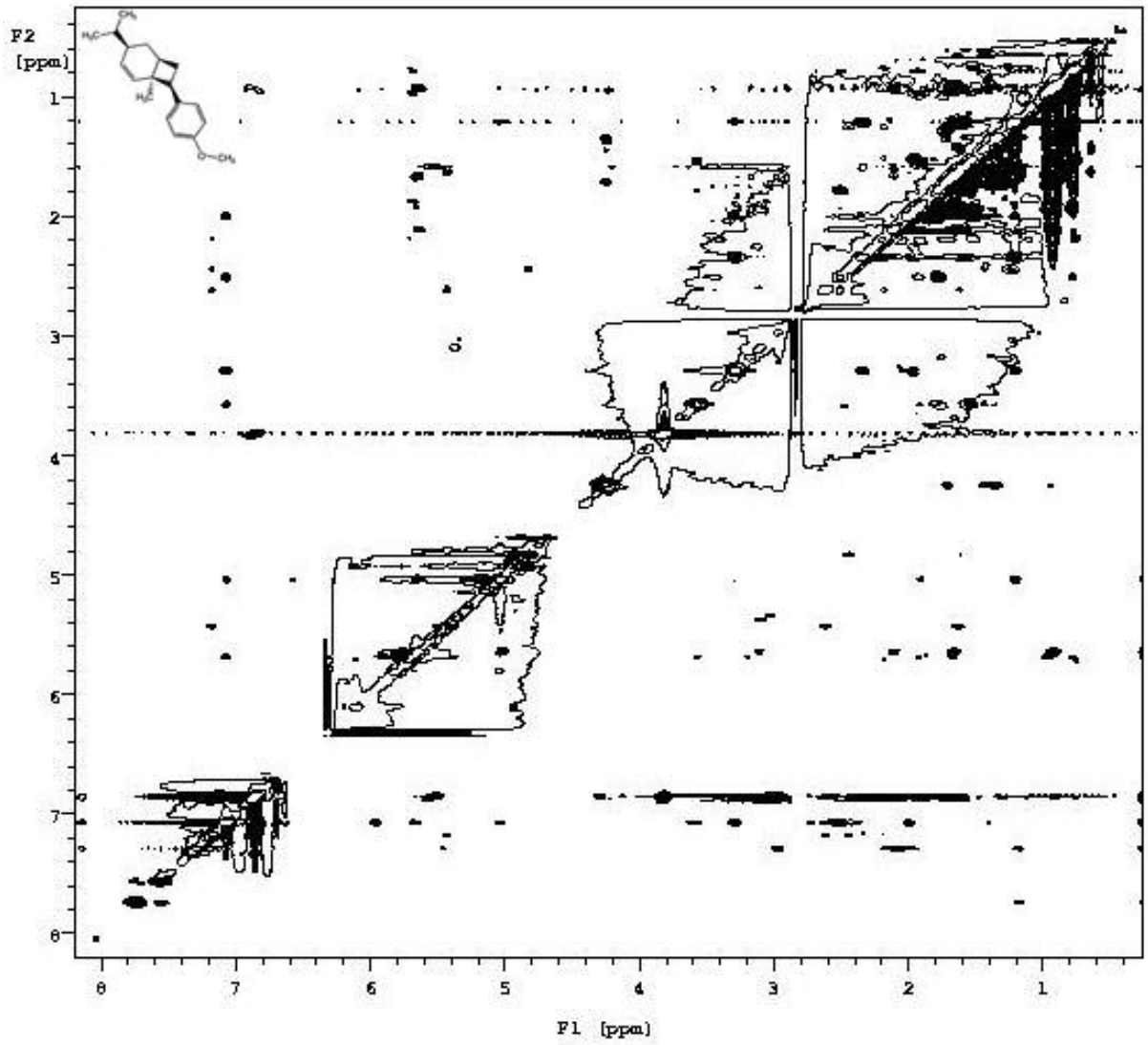


^{1}H Decoupling experiment compound **7**: 3.29 ppm proton

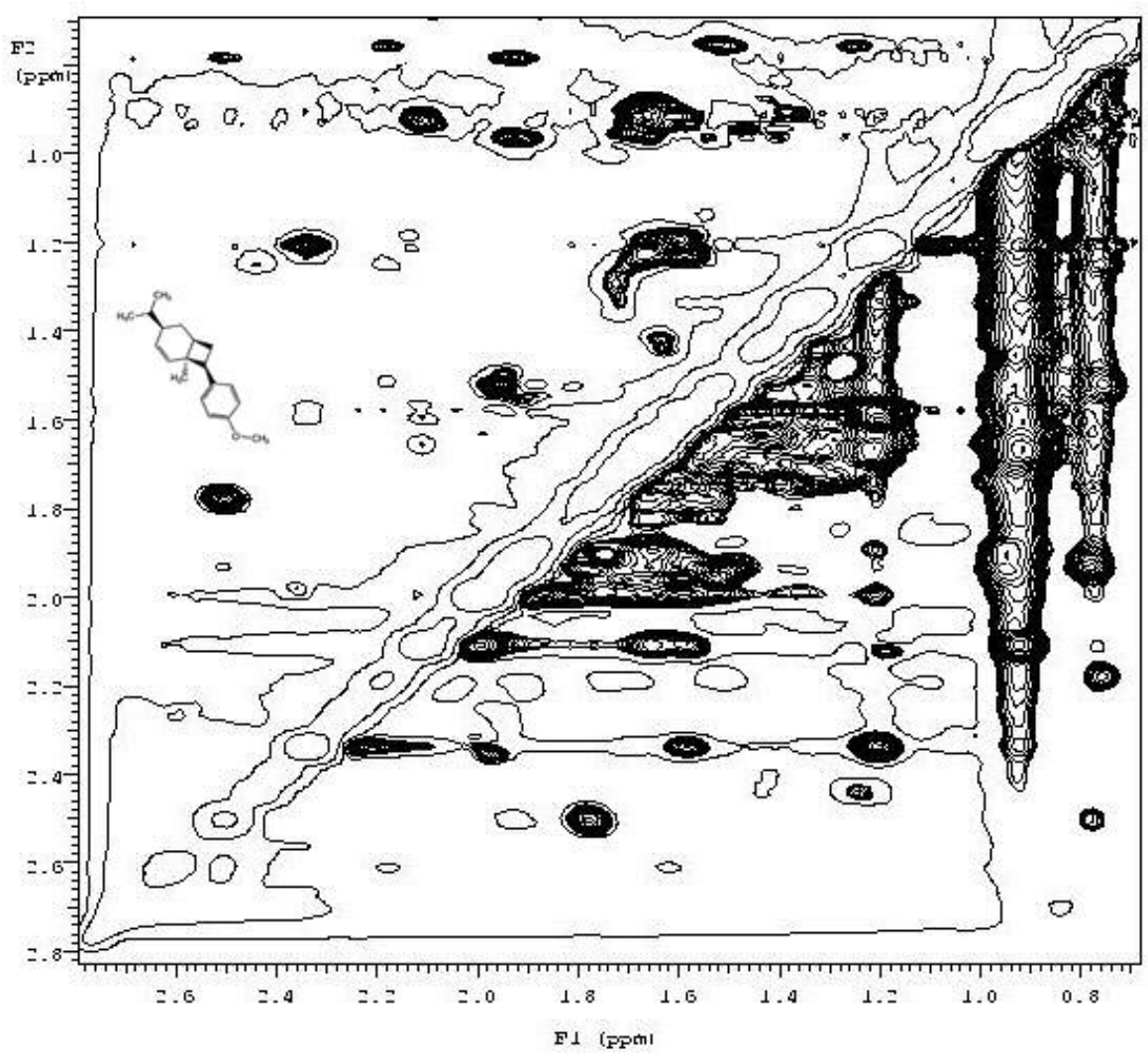
NOTE: Because coupling constants were not successfully extrapolated for each resonance, decoupling experiments were carried out to unambiguously determine ^{3}J couplings.



Full ROESY NMR of **7.**



Expanded ROESY NMR spectrum of **7**. Strong NOE coupling shows methyl group at 1.21 ppm is *cis* to 2.34 ppm bridgehead proton. NOE coupling oupling between that same methyl group at 1.21 ppm and 3.29 ppm benzylic proton (seen in full ROESY) indicates *trans* relationship between anisole ring and methyl group. 1.60 ppm proton has NOE with 2.34 ppm proton and with the decoupling data presented previously, the two halves of the molecule are connected for an absolute determination of stereochemistry.



Effect of Varying Catalyst Concentration

Conditions	**0.8-mol-%**	**3.3-mol-%**	**6.0-mol-%**	**11.1-mol-%**
Diene Dimers	1.00	1.00	1.00	1.00
D.A. Products	1.63	2.47	2.46	2.50
DIenophile Dimer	0.12	0.22	0.22	0.21
----	**----**	**----**	**----**	**----**
A	32.8%	36.6%	36.6%	36.4%
B	57.0%	62.4%	61.8%	61.9%
C	1.5%	0.8%	1.2%	1.3%
D	4.7%	0.2%	0.4%	0.4%
E	1.4%	0.0%	0.0%	0.0%
F	1.6%	0.0%	0.0%	0.0%
G	0.9%	0.0%	0.0%	0.0%

Time Variation Effects on Product Ratios

Reaction Time (Hr)	**0.8**	**2.5**	**6.0**
Diene Dimers	1	1	1
D.A. Products	2.55	2.63	2.59
Dienophile Dimer	0.42	0.46	0.43
----	**----**	**----**	**----**
4	38.0%	36.2%	36.4%
5	57.4%	57.7%	56.5%
6	2.5%	2.3%	2.1%
7	1.2%	2.0%	2.0%
8	0.0%	0.4%	0.9%
9	0.0%	0.4%	1.0%
10	0.9%	0.9%	1.0%

Diene radical cation 1$^{\bullet+}$

1	6	0	-0.672728	0.013035	0.344617
2	6	0	0.144291	-1.209344	0.150213
3	6	0	1.514753	-1.217602	-0.017049
4	6	0	2.281555	-0.018106	-0.025941
5	6	0	1.590993	1.193988	0.027982
6	6	0	0.114575	1.305689	0.039672
7	6	0	-2.076671	-0.034918	-0.367292
8	6	0	3.775874	-0.077258	-0.101881
9	6	0	-2.863002	-1.311817	-0.035970
10	6	0	-2.901584	1.206985	0.007168
11	1	0	-0.909239	0.001267	1.428660
12	1	0	-0.366680	-2.166886	0.199092
13	1	0	2.031790	-2.168978	-0.113898
14	1	0	2.162331	2.120066	0.000284
15	1	0	-0.182432	2.125787	0.705411
16	1	0	-0.162164	1.678776	-0.966560
17	1	0	-1.882937	-0.013659	-1.449096
18	1	0	4.229535	0.915975	-0.097137
19	1	0	4.090908	-0.600595	-1.014137
20	1	0	4.180872	-0.650317	0.742091
21	1	0	-3.860474	-1.252001	-0.481619
22	1	0	-2.996450	-1.432610	1.046320
23	1	0	-2.398137	-2.221128	-0.430576
24	1	0	-3.865954	1.178361	-0.508958
25	1	0	-2.415546	2.146524	-0.274142
26	1	0	-3.103757	1.235506	1.085143

E(B3LYP/6-31G*)= -390.4098673 h

ChelpG charges			Mulliken Spin densities		
1	C	0.001296	1	C	-0.012484
2	C	0.063840	2	C	0.317567
3	C	-0.171562	3	C	0.078203
4	C	0.278169	4	C	0.080504
5	C	-0.083214	5	C	0.459140
6	C	0.089011	6	C	-0.025789
7	C	0.275053	7	C	0.015506
8	C	-0.344512	8	C	-0.008867
9	C	-0.337001	9	C	-0.000600
10	C	-0.268076	10	C	0.001098
11	H	0.061703	11	H	0.042292
12	H	0.116445	12	H	-0.014764
13	H	0.162562	13	H	-0.005193
14	H	0.143435	14	H	-0.020758
15	H	0.055283	15	H	0.018352
16	H	0.059689	16	H	0.051000
17	H	-0.028211	17	H	0.002432
18	H	0.126821	18	H	-0.000157
19	H	0.140181	19	H	0.010172
20	H	0.141519	20	H	0.010469
21	H	0.119183	21	H	0.000289
22	H	0.088543	22	H	0.000186
23	H	0.079701	23	H	0.000345
24	H	0.100031	24	H	0.001019
25	H	0.056184	25	H	0.000008
26	H	0.073927	26	H	0.000030

12$^{\bullet+}$ (Ion-molecule complex for trans attack leading to Intermediate **14**$^{\bullet+}$)

1	6	0	3.233619	0.564021	0.489798
2	6	0	2.595746	-0.716264	-0.091180
3	6	0	1.833019	-0.428449	-1.352150
4	6	0	1.362164	0.804909	-1.672832
5	6	0	1.584028	1.947159	-0.814243
6	6	0	2.428338	1.806161	0.262400
7	6	0	0.917838	3.250770	-1.150473
8	6	0	0.261951	1.612580	2.130902
9	6	0	-0.401591	0.435750	1.950918
10	6	0	-1.609255	0.216672	1.196559
11	6	0	-2.308649	1.251189	0.513382
12	6	0	-3.472857	0.991514	-0.169417
13	6	0	-4.003606	-0.323205	-0.202574
14	6	0	-3.329199	-1.367902	0.465345
15	6	0	-2.158080	-1.089314	1.146682
16	8	0	-5.141314	-0.463478	-0.886588
17	6	0	-5.783959	-1.744902	-0.959559
18	6	0	3.583314	-1.908097	-0.261519
19	1	0	4.214799	0.739234	0.014849
20	1	0	3.450380	0.437562	1.555176
21	1	0	1.832055	-1.053430	0.636111
22	1	0	1.608829	-1.270140	-2.005247
23	1	0	0.779284	0.946275	-2.579672
24	1	0	2.659252	2.678487	0.869701
25	1	0	1.130888	4.026001	-0.409807
26	1	0	-0.169874	3.129512	-1.232103
27	1	0	1.262535	3.612839	-2.127994
28	1	0	-0.105189	2.558145	1.746564
29	1	0	1.119381	1.661077	2.792777
30	1	0	0.006322	-0.447760	2.440505
31	1	0	-1.933034	2.268825	0.542696
32	1	0	-4.018538	1.775362	-0.683960
33	1	0	-3.720527	-2.378011	0.454762
34	1	0	-1.646097	-1.894624	1.666883
35	1	0	-6.683573	-1.582483	-1.551712
36	1	0	-6.055858	-2.098684	0.040175
37	1	0	-5.137905	-2.474765	-1.458430
38	1	0	2.970260	-2.745208	-0.627306
39	6	0	4.672506	-1.642126	-1.312755
40	1	0	5.366543	-0.854614	-0.995666
41	1	0	5.267545	-2.546549	-1.475147
42	1	0	4.248332	-1.345337	-2.279125
43	6	0	4.195715	-2.338096	1.079231
44	1	0	3.423965	-2.548868	1.829636
45	1	0	4.790089	-3.248585	0.951384
46	1	0	4.864396	-1.570642	1.486544

E(B3LYP/6-31G*)= -814.609404712 h, ZPE = 0.403608 h
S**2 before annihilation 0.7564, after 0.7500

TS$_{12,14}$ (from ion-molecule complex to Intermediate 14$^{\bullet+}$)

1	6	0	2.953921	0.459468	0.619104
2	6	0	2.389264	-0.800441	-0.072887
3	6	0	1.612456	-0.453211	-1.310860
4	6	0	1.184948	0.803106	-1.619913
5	6	0	1.426051	1.920208	-0.756195
6	6	0	2.120910	1.707469	0.444310
7	6	0	0.926819	3.281011	-1.145014
8	6	0	0.525614	1.646679	1.946405
9	6	0	-0.206027	0.465654	1.865245
10	6	0	-1.420222	0.239660	1.154956
11	6	0	-2.115684	1.256399	0.436983
12	6	0	-3.295809	0.986859	-0.213580

13	6	0	-3.851073	-0.316636	-0.177145
14	6	0	-3.187003	-1.341782	0.530276
15	6	0	-1.999557	-1.057421	1.177593
16	8	0	-5.002335	-0.467051	-0.836763
17	6	0	-5.666975	-1.738857	-0.839146
18	6	0	3.457956	-1.903267	-0.355763
19	1	0	3.936862	0.701687	0.185754
20	1	0	3.142024	0.265671	1.679296
21	1	0	1.662237	-1.271221	0.611474
22	1	0	1.360700	-1.274132	-1.980440
23	1	0	0.627618	0.971957	-2.538177
24	1	0	2.492548	2.594010	0.954568
25	1	0	1.018467	4.005286	-0.330804
26	1	0	-0.117611	3.249174	-1.477767
27	1	0	1.509827	3.664264	-1.994078
28	1	0	0.077596	2.590691	1.653363
29	1	0	1.274976	1.720622	2.728030
30	1	0	0.199069	-0.398709	2.389694
31	1	0	-1.724320	2.268163	0.415706
32	1	0	-3.836721	1.756646	-0.753767
33	1	0	-3.599355	-2.342539	0.574740
34	1	0	-1.494931	-1.848086	1.726878
35	1	0	-6.573052	-1.589281	-1.424924
36	1	0	-5.929667	-2.040988	0.179882
37	1	0	-5.041730	-2.503151	-1.312516
38	1	0	2.897154	-2.749495	-0.779076
39	6	0	4.506742	-1.481810	-1.396628
40	1	0	5.151780	-0.674071	-1.030611
41	1	0	5.159474	-2.327674	-1.635724
42	1	0	4.044982	-1.144288	-2.331797
43	6	0	4.119741	-2.392203	0.940499
44	1	0	3.375220	-2.708092	1.681520
45	1	0	4.768627	-3.249995	0.736649
46	1	0	4.744458	-1.615340	1.396786

E(B3LYP/6-31G*)= -814.606635224 h, ZPE = 0.404618 h, ν_{imag}=-244.1748 cm^{-1}
S**2 before annihilation 0.7683, after 0.7502

14$^{\bullet+}$ (*Trans*-Intermediate extended conformation)

1	6	0	-2.420857	-0.652240	-0.408209
2	6	0	-3.629564	-0.247645	0.459649
3	6	0	-3.902649	1.220104	0.319001
4	6	0	-2.984874	2.119546	-0.176420
5	6	0	-1.679844	1.740871	-0.534087
6	6	0	-1.240197	0.338775	-0.329675
7	6	0	-0.681723	2.732471	-1.013395
8	6	0	-0.464060	0.170451	1.091564
9	6	0	0.861734	0.808186	1.183762
10	6	0	2.072946	0.287392	0.715415
11	6	0	2.189916	-0.984594	0.061390
12	6	0	3.401173	-1.442793	-0.387106
13	6	0	4.575466	-0.665494	-0.202307
14	6	0	4.496503	0.590261	0.445618
15	6	0	3.274438	1.046252	0.886667
16	8	0	5.696758	-1.208853	-0.669491
17	6	0	6.951017	-0.522198	-0.523531
18	6	0	-4.916026	-1.097562	0.215055
19	1	0	-2.735762	-0.694766	-1.457626
20	1	0	-2.078863	-1.657510	-0.141758
21	1	0	-3.372382	-0.413774	1.521739
22	1	0	-4.873917	1.586020	0.647026
23	1	0	-3.264563	3.166211	-0.271780
24	1	0	-0.493353	0.068640	-1.086130
25	1	0	0.206210	2.720176	-0.354951

26	1	0	-1.076829	3.750770	-1.049380
27	1	0	-0.302039	2.465123	-2.009544
28	1	0	-0.376155	-0.913411	1.214593
29	1	0	-1.122473	0.548033	1.877379
30	1	0	0.912205	1.780317	1.671192
31	1	0	1.309539	-1.603622	-0.077072
32	1	0	3.499830	-2.403830	-0.880510
33	1	0	5.384356	1.192225	0.596558
34	1	0	3.214663	2.011704	1.381976
35	1	0	7.691418	-1.178830	-0.978145
36	1	0	7.187077	-0.371103	0.534504
37	1	0	6.930016	0.436502	-1.051323
38	1	0	-5.666144	-0.693773	0.910892
39	6	0	-5.481145	-0.950522	-1.206484
40	1	0	-4.820811	-1.396311	-1.959556
41	1	0	-6.446069	-1.462206	-1.282053
42	1	0	-5.641024	0.099533	-1.478647
43	6	0	-4.701289	-2.573381	0.580126
44	1	0	-4.310215	-2.686494	1.598468
45	1	0	-5.649065	-3.118990	0.526580
46	1	0	-4.005505	-3.067088	-0.108694

E(B3LYP/6-31G*)= -814.620667328 h, ZPE = 0.406585 h
S**2 before annihilation 0.7700, after 0.7503

14$^{\bullet+}$ (*Trans*-Intermediate reactive conformation)

1	6	0	2.953787	0.424386	0.827737
2	6	0	2.564244	-0.855357	0.054671
3	6	0	1.605551	-0.553358	-1.056334
4	6	0	1.197089	0.717681	-1.418556
5	6	0	1.401515	1.815554	-0.577942
6	6	0	1.887609	1.537732	0.799090
7	6	0	1.052381	3.211839	-0.977698
8	6	0	0.634982	1.241788	1.775662
9	6	0	-0.173398	0.035926	1.513541
10	6	0	-1.452501	-0.012248	0.951172
11	6	0	-2.141950	1.139869	0.446098
12	6	0	-3.396421	1.034059	-0.097912
13	6	0	-4.048315	-0.224831	-0.158695
14	6	0	-3.398716	-1.381419	0.337678
15	6	0	-2.135302	-1.268337	0.871261
16	8	0	-5.266140	-0.210802	-0.695067
17	6	0	-6.033844	-1.422314	-0.786465
18	6	0	3.795380	-1.669162	-0.486447
19	1	0	3.861795	0.849589	0.385541
20	1	0	3.204040	0.182006	1.866328
21	1	0	2.064644	-1.558408	0.738983
22	1	0	1.304114	-1.393446	-1.680884
23	1	0	0.665932	0.858789	-2.357677
24	1	0	2.319705	2.447165	1.231323
25	1	0	0.464109	3.723218	-0.202913
26	1	0	0.501715	3.249061	-1.921766
27	1	0	1.967331	3.810966	-1.099640
28	1	0	0.019810	2.145295	1.791305
29	1	0	1.093821	1.139849	2.766544
30	1	0	0.234360	-0.909567	1.863914
31	1	0	-1.672534	2.115946	0.495820
32	1	0	-3.926045	1.899933	-0.480793
33	1	0	-3.886196	-2.348116	0.302383
34	1	0	-1.638015	-2.156570	1.251801
35	1	0	-6.977131	-1.129427	-1.245255
36	1	0	-6.217985	-1.838698	0.208892
37	1	0	-5.524463	-2.155722	-1.419549
38	1	0	3.369478	-2.573220	-0.945350

39	6	0	4.595055	-0.934492	-1.571828
40	1	0	5.092539	-0.037882	-1.183911
41	1	0	5.379209	-1.590382	-1.964012
42	1	0	3.964034	-0.630878	-2.414519
43	6	0	4.700387	-2.119560	0.669508
44	1	0	4.137779	-2.667448	1.434975
45	1	0	5.488067	-2.782950	0.297458
46	1	0	5.193815	-1.269214	1.154282

E(B3LYP/6-31G*)= -814.618989495 h, ZPE = 0.407044 h
S**2 before annihilation 0.7674, after 0.7502

$TS_{14,5}$ (from $14^{\bullet+}$ to *endo* [4+2] product 5)

1	6	0	-2.998207	0.276998	-1.025878
2	6	0	-2.429984	-0.954976	-0.272370
3	6	0	-1.270272	-0.546250	0.600576
4	6	0	-1.238046	0.729309	1.207306
5	6	0	-1.723305	1.801046	0.492867
6	6	0	-2.054859	1.495839	-0.938688
7	6	0	-1.774259	3.201254	1.006170
8	6	0	-0.695790	1.228006	-1.698915
9	6	0	0.068070	0.011816	-1.259266
10	6	0	1.400862	0.010704	-0.770736
11	6	0	2.065871	1.175187	-0.279233
12	6	0	3.358804	1.114883	0.179094
13	6	0	4.067002	-0.114504	0.170185
14	6	0	3.434190	-1.285836	-0.305417
15	6	0	2.132598	-1.213705	-0.755929
16	8	0	5.316967	-0.056565	0.628584
17	6	0	6.132458	-1.238789	0.656531
18	6	0	-3.494823	-1.753462	0.570382
19	1	0	-3.966783	0.567594	-0.607614
20	1	0	-3.176648	0.031997	-2.078686
21	1	0	-2.069997	-1.691892	-1.000770
22	1	0	-0.695670	-1.351234	1.055948
23	1	0	-0.741563	0.870442	2.165224
24	1	0	-2.523303	2.357935	-1.423876
25	1	0	-1.217606	3.885486	0.350330
26	1	0	-1.379406	3.286798	2.022173
27	1	0	-2.810949	3.566982	1.009270
28	1	0	-0.077669	2.127641	-1.635821
29	1	0	-0.949273	1.094246	-2.758807
30	1	0	-0.250133	-0.926817	-1.704349
31	1	0	1.548440	2.128132	-0.263012
32	1	0	3.872425	1.995566	0.549917
33	1	0	3.960339	-2.232584	-0.323788
34	1	0	1.650910	-2.115589	-1.125028
35	1	0	7.090016	-0.917290	1.063831
36	1	0	6.272823	-1.635415	-0.354064
37	1	0	5.688806	-1.999574	1.306769
38	1	0	-2.948340	-2.594368	1.020802
39	6	0	-4.145453	-0.958693	1.710181
40	1	0	-4.726316	-0.105612	1.340545
41	1	0	-4.839721	-1.605176	2.257103
42	1	0	-3.411994	-0.580099	2.429261
43	6	0	-4.556592	-2.345490	-0.371086
44	1	0	-4.102976	-2.955896	-1.160524
45	1	0	-5.243923	-2.985750	0.191574
46	1	0	-5.156814	-1.563023	-0.849736

E(B3LYP/6-31G*)= -814.617573235 h, ZPE = 0.407672 h, ν_{imag}= -98.7138 cm^{-1}
S**2 before annihilation 0.7683, after 0.7501

$13^{\bullet+}$ (Ion-molecule complex for cis attack leading to Intermediate $15^{\bullet+}$)

1	6	0	1.802001	0.456752	1.021827

2	6	0	2.529160	1.652972	0.361200
3	6	0	3.320587	1.215498	-0.838081
4	6	0	3.790902	-0.049799	-0.988107
5	6	0	3.528804	-1.072054	0.002236
6	6	0	2.580458	-0.823502	0.968563
7	6	0	4.321682	-2.347064	-0.045309
8	6	0	1.622582	2.879483	0.058358
9	1	0	0.831686	0.286791	0.522452
10	1	0	1.553222	0.691407	2.061623
11	1	0	3.284475	2.008320	1.086972
12	1	0	3.587767	1.973881	-1.571930
13	1	0	4.429466	-0.297752	-1.832541
14	1	0	4.044896	-3.034375	0.758379
15	1	0	5.394548	-2.134089	0.042624
16	1	0	4.185605	-2.859451	-1.006694
17	1	0	2.299620	3.648340	-0.342012
18	6	0	0.561515	2.599636	-1.017268
19	1	0	-0.187688	1.875437	-0.675519
20	1	0	0.027465	3.521898	-1.269164
21	1	0	1.006934	2.212788	-1.941853
22	6	0	0.987207	3.449828	1.334391
23	1	0	1.740910	3.660255	2.102237
24	1	0	0.467704	4.388381	1.114833
25	1	0	0.248277	2.762710	1.764150
26	6	0	0.839848	-2.794000	-0.384345
27	6	0	-0.266000	-2.602990	0.383832
28	1	0	0.985787	-2.298676	-1.338746
29	1	0	-0.336523	-3.166658	1.313250
30	6	0	-1.381542	-1.729943	0.109042
31	6	0	-2.429292	-1.638389	1.060214
32	6	0	-1.511822	-0.972655	-1.089822
33	6	0	-3.543068	-0.846059	0.850604
34	1	0	-2.355616	-2.213468	1.979328
35	6	0	-2.613168	-0.180454	-1.313959
36	1	0	-0.743509	-1.031180	-1.853760
37	6	0	-3.647873	-0.105192	-0.347012
38	1	0	-4.324660	-0.805083	1.599628
39	1	0	-2.726990	0.389926	-2.229680
40	8	0	-4.673436	0.686765	-0.666749
41	6	0	-5.790565	0.814864	0.225961
42	1	0	-6.478100	1.498678	-0.270029
43	1	0	-6.275991	-0.154335	0.379010
44	1	0	-5.473746	1.237225	1.185160
45	1	0	2.414807	-1.559243	1.750333
46	1	0	1.578649	-3.537445	-0.108009

E(B3LYP/6-31G*)= -814.609246098 h, ZPE = 0.403596 h,
S**2 before annihilation 0.7566, after 0.7500

$TS_{13,15}$ (from ion-molecule complex to Intermediate $15^{\bullet+}$)

1	6	0	1.640177	0.314088	0.793041
2	6	0	2.554351	1.494277	0.390792
3	6	0	3.384308	1.118910	-0.806319
4	6	0	3.794507	-0.158952	-1.031790
5	6	0	3.446801	-1.209150	-0.117544
6	6	0	2.349993	-1.030019	0.747562
7	6	0	4.238768	-2.482726	-0.130020
8	6	0	1.810824	2.845895	0.197562
9	1	0	0.778338	0.295618	0.115026
10	1	0	1.232235	0.474904	1.794711
11	1	0	3.276939	1.657687	1.210596
12	1	0	3.735626	1.916163	-1.458881
13	1	0	4.486570	-0.377090	-1.841826
14	1	0	4.001355	-3.128054	0.720221

15	1	0	5.314269	-2.272113	-0.113216
16	1	0	4.048867	-3.048225	-1.054202
17	1	0	2.595930	3.569180	-0.068196
18	6	0	0.796927	2.828842	-0.957460
19	1	0	-0.061341	2.180623	-0.742983
20	1	0	0.403592	3.836411	-1.127754
21	1	0	1.249221	2.489173	-1.897150
22	6	0	1.163566	3.337092	1.500529
23	1	0	1.885464	3.362607	2.325246
24	1	0	0.771163	4.351196	1.372082
25	1	0	0.323566	2.701055	1.805128
26	6	0	0.989741	-2.422334	-0.185046
27	6	0	-0.204572	-2.317477	0.529099
28	1	0	1.052119	-2.032039	-1.196153
29	1	0	-0.257931	-2.854879	1.475435
30	6	0	-1.356269	-1.550987	0.192812
31	6	0	-2.441904	-1.505804	1.109642
32	6	0	-1.509338	-0.847622	-1.040319
33	6	0	-3.600712	-0.803261	0.840243
34	1	0	-2.355188	-2.041577	2.051179
35	6	0	-2.655747	-0.143891	-1.319365
36	1	0	-0.720084	-0.879011	-1.784467
37	6	0	-3.720340	-0.109280	-0.383316
38	1	0	-4.405674	-0.793458	1.565138
39	1	0	-2.784154	0.384490	-2.258078
40	8	0	-4.787882	0.598797	-0.757761
41	6	0	-5.933573	0.680989	0.103021
42	1	0	-6.651823	1.300583	-0.432377
43	1	0	-6.358642	-0.312603	0.278309
44	1	0	-5.670946	1.155151	1.054378
45	1	0	2.344037	-1.629879	1.653769
46	1	0	1.619062	-3.283334	0.012911

E(B3LYP/6-31G*)= -814.604397855 h, ZPE = 0.404632 h, ν_{imag}= -262.5617 cm^{-1}
S**2 before annihilation 0.7698, after 0.7503

15$^{\bullet+}$ (*Cis*-Intermediate extended conformation)

1	6	0	1.798786	0.296332	0.355269
2	6	0	3.127564	1.074747	0.350133
3	6	0	4.079676	0.397874	-0.586731
4	6	0	4.042610	-0.963136	-0.811834
5	6	0	3.120727	-1.804638	-0.174769
6	6	0	1.980807	-1.216528	0.603861
7	6	0	3.291336	-3.289690	-0.225219
8	6	0	2.998023	2.598601	0.065645
9	1	0	1.308679	0.428135	-0.618132
10	1	0	1.119476	0.708032	1.108978
11	1	0	3.571306	0.987226	1.359969
12	1	0	4.859147	0.992587	-1.058682
13	1	0	4.809134	-1.416835	-1.436141
14	1	0	3.347838	-3.716145	0.786642
15	1	0	4.198754	-3.573834	-0.763624
16	1	0	2.439552	-3.783631	-0.716626
17	1	0	4.029656	2.980191	0.055847
18	6	0	2.380369	2.908642	-1.307083
19	1	0	1.319269	2.635221	-1.348411
20	1	0	2.445217	3.981061	-1.518200
21	1	0	2.895786	2.380578	-2.118298
22	6	0	2.253831	3.333989	1.189468
23	1	0	2.701938	3.133433	2.169879
24	1	0	2.287795	4.416008	1.024806
25	1	0	1.196041	3.047425	1.234582
26	6	0	0.633036	-1.988137	0.275164
27	6	0	-0.515867	-1.420919	1.006307

28	1	0	0.477451	-1.989831	-0.807805
29	1	0	-0.400224	-1.374045	2.089997
30	6	0	-1.720215	-0.939550	0.496608
31	6	0	-2.704892	-0.433936	1.408311
32	6	0	-2.056283	-0.931519	-0.900569
33	6	0	-3.923705	0.039074	0.979898
34	1	0	-2.476989	-0.431090	2.470770
35	6	0	-3.264942	-0.456979	-1.334692
36	1	0	-1.347154	-1.309632	-1.628608
37	6	0	-4.220599	0.035031	-0.404621
38	1	0	-4.643832	0.409039	1.699534
39	1	0	-3.528573	-0.447549	-2.386907
40	8	0	-5.360000	0.466684	-0.935928
41	6	0	-6.407118	0.979416	-0.094306
42	1	0	-7.210956	1.256243	-0.774819
43	1	0	-6.755436	0.208192	0.599741
44	1	0	-6.063070	1.861616	0.454524
45	1	0	2.171237	-1.394963	1.675502
46	1	0	0.769086	-3.032938	0.587873

E(B3LYP/6-31G*)= -814.619229378 h, ZPE = 0.406433 h
S**2 before annihilation 0.7695, after 0.7503

ChelpG charges			Mulliken Spin densities		
1	C	0.037396	1	C	0.011909
2	C	0.066115	2	C	-0.028535
3	C	-0.026614	3	C	0.402008
4	C	-0.267587	4	C	-0.170856
5	C	0.132842	5	C	0.406611
6	C	0.138062	6	C	-0.023648
7	C	-0.192114	7	C	-0.035086
8	C	0.298857	8	C	0.002627
9	H	-0.030583	9	H	-0.000843
10	H	-0.024808	10	H	-0.000801
11	H	-0.003783	11	H	0.018249
12	H	0.107120	12	H	-0.019541
13	H	0.155051	13	H	0.007296
14	H	0.078314	14	H	0.018639
15	H	0.088306	15	H	0.000829
16	H	0.068791	16	H	0.018457
17	H	-0.047928	17	H	-0.000200
18	C	-0.219271	18	C	0.002389
19	H	0.038826	19	H	0.000047
20	H	0.069970	20	H	-0.000131
21	H	0.034697	21	H	0.000056
22	C	-0.274293	22	C	0.000059
23	H	0.063500	23	H	0.000041
24	H	0.078972	24	H	-0.000040
25	H	0.048928	25	H	0.000045
26	C	0.104026	26	C	-0.018130
27	C	-0.135583	27	C	0.265939
28	H	-0.008074	28	H	0.001764
29	H	0.117652	29	H	-0.012247
30	C	0.086464	30	C	-0.069267
31	C	-0.071234	31	C	0.097967
32	C	-0.064184	32	C	0.081263
33	C	-0.257873	33	C	-0.045440
34	H	0.130732	34	H	-0.004454
35	C	-0.264447	35	C	-0.043709
36	H	0.142149	36	H	-0.003706
37	C	0.505131	37	C	0.089340
38	H	0.154191	38	H	0.001572
39	H	0.159037	39	H	0.001539
40	O	-0.324207	40	O	0.021488
41	C	0.077865	41	C	-0.001997

42 H 0.101217	42 H -0.000044
43 H 0.052609	43 H 0.001739
44 H 0.052642	44 H 0.001717
45 H -0.003475	45 H 0.014594
46 H 0.026596	46 H 0.010493

TS for closure of *Cis*-Intermediate 15$^{\bullet+}$ to hypothetical *endo* [4+2] product

1	6	0	-3.188640	0.305626	0.571935
2	6	0	-2.735721	-0.542366	-0.651617
3	6	0	-1.377920	-0.077542	-1.136132
4	6	0	-1.219556	1.309267	-1.363918
5	6	0	-1.822068	2.180696	-0.486401
6	6	0	-2.293544	1.549067	0.795533
7	6	0	-1.826562	3.665342	-0.643047
8	6	0	-2.977482	-2.074975	-0.570723
9	1	0	-3.169009	-0.300664	1.485864
10	1	0	-4.225568	0.622085	0.434012
11	1	0	-3.381565	-0.225360	-1.487122
12	1	0	-0.760240	-0.780530	-1.692130
13	1	0	-0.579837	1.667986	-2.168009
14	1	0	-2.859514	4.036872	-0.700216
15	1	0	-1.299264	3.989071	-1.544581
16	1	0	-1.376768	4.161314	0.228495
17	1	0	-2.697638	-2.466510	-1.559860
18	6	0	-2.151591	-2.850033	0.466334
19	1	0	-2.312612	-2.485251	1.488505
20	1	0	-2.445017	-3.904903	0.458694
21	1	0	-1.077938	-2.821188	0.247439
22	6	0	-4.477886	-2.359609	-0.379887
23	1	0	-5.086234	-1.841610	-1.130348
24	1	0	-4.677570	-3.431724	-0.474235
25	1	0	-4.828406	-2.048513	0.611569
26	6	0	-0.986607	1.140346	1.581453
27	6	0	-0.220973	0.003067	0.979357
28	1	0	-0.359700	2.024953	1.720024
29	1	0	-0.634756	-0.982100	1.160846
30	6	0	1.154895	0.024721	0.635702
31	6	0	1.841441	-1.209885	0.434739
32	6	0	1.913000	1.225546	0.477298
33	6	0	3.181616	-1.261394	0.113432
34	1	0	1.292642	-2.140073	0.554674
35	6	0	3.245731	1.187610	0.149815
36	1	0	1.434735	2.189482	0.611593
37	6	0	3.904216	-0.055346	-0.035343
38	1	0	3.669150	-2.219872	-0.017261
39	1	0	3.827710	2.095142	0.028953
40	8	0	5.197478	0.024108	-0.345897
41	6	0	5.966955	-1.171590	-0.550854
42	1	0	6.972917	-0.828199	-0.788092
43	1	0	5.986849	-1.779426	0.359371
44	1	0	5.565031	-1.751318	-1.387989
45	1	0	-2.823047	2.275842	1.418810
46	1	0	-1.310000	0.820332	2.582125

E(B3LYP/6-31G*)= -814.609655316 h, ZPE = 0.407258 h, ν_{imag}= -119.2984 cm^{-1}
S**2 before annihilation 0.7645, after 0.7501

4$^{\bullet+}$ (*exo* [4+2] product)

1	6	0	3.115616	-1.354360	0.036869
2	6	0	2.328643	-1.038407	1.285873
3	6	0	2.140700	0.501307	1.341030
4	6	0	2.505138	-0.906894	-1.100682
5	6	0	1.348318	0.985903	0.092610

6	6	0	1.215883	-0.208512	-0.900199
7	6	0	0.927560	-1.707481	1.175118
8	6	0	0.259641	-1.350494	-0.181677
9	6	0	1.886891	2.281958	-0.575795
10	6	0	3.305317	2.192167	-1.156037
11	6	0	1.780463	3.460951	0.409539
12	6	0	-1.167483	-0.929181	-0.162777
13	6	0	-1.758655	-0.179990	0.890955
14	6	0	-3.089303	0.188280	0.867294
15	6	0	-3.890157	-0.168341	-0.246128
16	6	0	-3.318068	-0.903170	-1.321725
17	6	0	-1.994004	-1.264299	-1.272404
18	8	0	-5.176352	0.129765	-0.381843
19	6	0	-5.875931	0.866260	0.639592
20	6	0	4.414759	-2.083142	0.090683
21	1	0	2.839215	-1.396820	2.184791
22	1	0	3.124063	0.979057	1.393058
23	1	0	1.615934	0.769182	2.265486
24	1	0	2.895080	-1.114073	-2.094263
25	1	0	0.327191	1.235497	0.404912
26	1	0	0.746807	0.100622	-1.837376
27	1	0	0.323266	-1.385369	2.029472
28	1	0	1.010864	-2.796498	1.254759
29	1	0	0.329678	-2.205987	-0.857045
30	1	0	1.204537	2.494998	-1.412383
31	1	0	3.579025	3.148244	-1.615276
32	1	0	3.391363	1.423245	-1.931159
33	1	0	4.055601	1.978505	-0.385781
34	1	0	2.053171	4.398714	-0.085634
35	1	0	2.454796	3.334408	1.264720
36	1	0	0.760963	3.572768	0.797559
37	1	0	-1.164800	0.094190	1.755852
38	1	0	-3.511946	0.740284	1.698205
39	1	0	-3.955659	-1.168820	-2.158190
40	1	0	-1.566702	-1.833133	-2.093562
41	1	0	-6.895343	0.965832	0.270670
42	1	0	-5.426381	1.854749	0.772575
43	1	0	-5.870062	0.309522	1.581396
44	1	0	5.140849	-1.533523	0.706068
45	1	0	4.846857	-2.236755	-0.901867
46	1	0	4.290476	-3.062288	0.574907

E(B3LYP/6-31G*)= -814.627854917 h, ZPE = 0.409869 h
S**2 before annihilation 0.7549, after 0.7500

5$^{\bullet+}$ (*endo* [4+2] product)

1	6	0	-1.663432	1.857959	-0.092919
2	6	0	-1.929801	1.316885	1.290472
3	6	0	-2.983904	0.182357	1.170143
4	6	0	-1.197397	0.907261	-0.948850
5	6	0	-2.472894	-0.931517	0.210227
6	6	0	-1.098878	-0.463035	-0.394665
7	6	0	-0.594491	0.728578	1.830495
8	6	0	-0.112789	-0.437114	0.916860
9	6	0	-3.486752	-1.412044	-0.865817
10	6	0	-3.978162	-0.346613	-1.854660
11	6	0	-4.681452	-2.097092	-0.173379
12	6	0	1.322461	-0.436294	0.532159
13	6	0	2.078382	-1.637290	0.638244
14	6	0	3.417425	-1.673497	0.333010
15	6	0	4.068861	-0.493817	-0.121847
16	6	0	3.328742	0.709657	-0.275103
17	6	0	1.986573	0.720149	0.038513

18	8	0	5.360782	-0.624930	-0.389506
19	6	0	6.144977	0.497406	-0.840575
20	6	0	-1.888784	3.294947	-0.428738
21	1	0	-2.286001	2.099513	1.967566
22	1	0	-3.924686	0.609187	0.808462
23	1	0	-3.189703	-0.225599	2.165602
24	1	0	-0.892488	1.134732	-1.967601
25	1	0	-2.250162	-1.825218	0.806220
26	1	0	-0.720068	-1.193801	-1.113060
27	1	0	-0.733028	0.359113	2.852484
28	1	0	0.157579	1.521947	1.884934
29	1	0	-0.312222	-1.391256	1.411931
30	1	0	-2.964527	-2.185543	-1.448620
31	1	0	-4.679504	-0.798554	-2.564627
32	1	0	-3.162589	0.091634	-2.439225
33	1	0	-4.509298	0.470750	-1.352793
34	1	0	-5.349048	-2.540358	-0.919655
35	1	0	-5.272590	-1.383803	0.413116
36	1	0	-4.353873	-2.897727	0.499611
37	1	0	1.588575	-2.538429	0.995955
38	1	0	4.006894	-2.578298	0.435616
39	1	0	3.807828	1.607977	-0.645987
40	1	0	1.421243	1.635765	-0.101981
41	1	0	7.156706	0.110728	-0.949872
42	1	0	6.126062	1.298142	-0.095696
43	1	0	5.774145	0.856570	-1.805037
44	1	0	-2.944612	3.563325	-0.283800
45	1	0	-1.615691	3.526667	-1.462172
46	1	0	-1.317314	3.950658	0.243245

E(B3LYP/6-31G*)= -814.627689679 h, ZPE = 0.409536 h
S**2 before annihilation 0.7547, after 0.7500

Cartesian coordinates of **1-1**$^{\bullet+}$

1	6	0	1.964005	-0.980349	0.274360
2	6	0	2.990451	0.026894	-0.290977
3	6	0	3.068603	1.263759	0.558093
4	6	0	2.067239	1.662426	1.384903
5	6	0	0.847756	0.895084	1.526826
6	6	0	0.780260	-0.346329	0.940439
7	6	0	-0.271274	1.459428	2.354198
8	6	0	-0.983833	0.234744	-1.480334
9	6	0	-1.377157	1.532713	-1.254398
10	6	0	-2.776265	1.789736	-0.996542
11	6	0	-3.675206	0.784458	-0.824322
12	6	0	4.396889	-0.577900	-0.577982
13	1	0	2.450005	-1.611711	1.038621
14	1	0	1.639965	-1.678287	-0.504812
15	1	0	2.608639	0.371868	-1.272029
16	1	0	3.953153	1.889298	0.452040
17	1	0	2.160158	2.590542	1.943558
18	1	0	-0.097276	-0.964368	1.111776
19	1	0	-1.138615	0.795498	2.383016
20	1	0	-0.593566	2.437169	1.973466
21	1	0	0.066412	1.625122	3.385557
22	1	0	0.038593	0.039251	-1.792477
23	1	0	4.980971	0.243268	-1.018761
24	6	0	5.129543	-1.031502	0.694317
25	1	0	4.640216	-1.891015	1.168241
26	1	0	6.151084	-1.340111	0.450040
27	1	0	5.194166	-0.229834	1.439308
28	6	0	4.331807	-1.704316	-1.619332
29	1	0	3.819061	-1.381960	-2.533867

30	1	0	5.341354	-2.020398	-1.900862
31	1	0	3.813346	-2.589389	-1.231821
32	6	0	-1.960747	-0.898410	-1.556400
33	1	0	-1.485910	-1.829481	-1.230519
34	6	0	-3.305157	-0.669829	-0.820178
35	1	0	-4.091929	-1.211152	-1.364165
36	6	0	-0.429003	2.692472	-1.348589
37	1	0	-0.749588	3.380355	-2.141728
38	1	0	-0.419387	3.275697	-0.418735
39	1	0	0.592572	2.372453	-1.566001
40	1	0	-3.107854	2.824183	-0.949288
41	1	0	-4.715445	1.038995	-0.641638
42	1	0	-2.160196	-1.053783	-2.631362
43	6	0	-3.328405	-1.259083	0.640963
44	1	0	-2.444406	-0.858065	1.158987
45	6	0	-4.575956	-0.826018	1.428049
46	1	0	-4.591645	-1.316867	2.406469
47	1	0	-4.609363	0.254127	1.603041
48	1	0	-5.495487	-1.115418	0.903784
49	6	0	-3.238815	-2.792819	0.618781
50	1	0	-4.120459	-3.224688	0.129858
51	1	0	-2.352413	-3.169112	0.097581
52	1	0	-3.204550	-3.183135	1.641479

E(B3LYP/6-31G*)= -781.110868698 h, ZPE = 0.472158 h
S**2 before annihilation 0.7572, after 0.7500