

Supplementary Information

Novel (*E*)-1-(pyrrole-2-yl)-3-(aryl)-2-(propen-1-one) derivatives as efficient singlet oxygen quenchers: Kinetics and quantum chemical calculations

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1. Experimental data

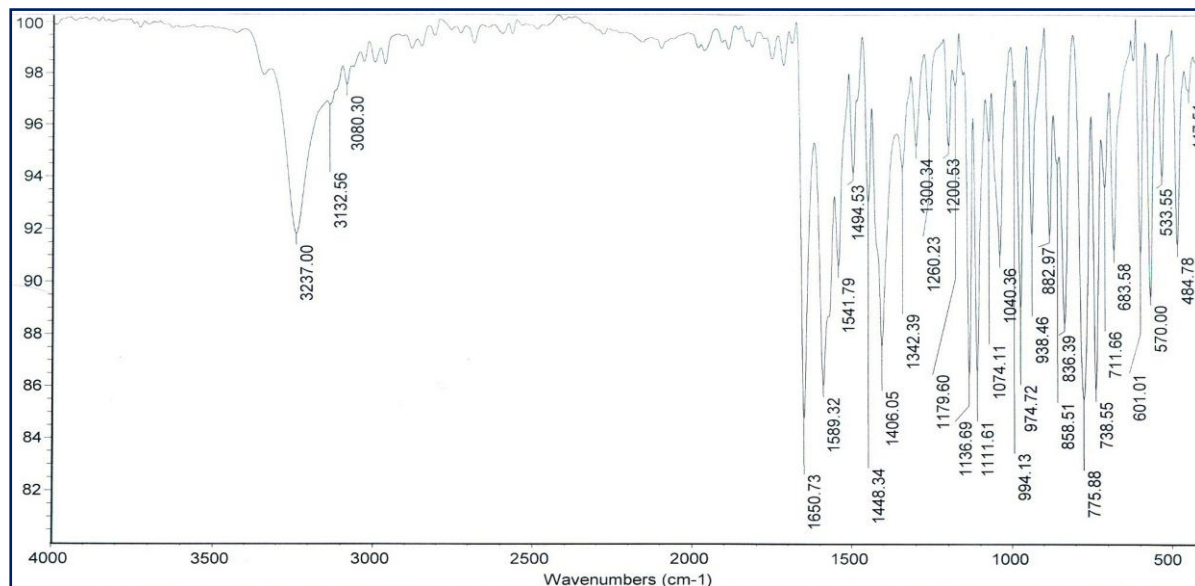


Fig. S1 IR spectra for (E)-3-phenyl-1-(1H-pyrrol-2-yl)prop-2-en-1-one (3a)

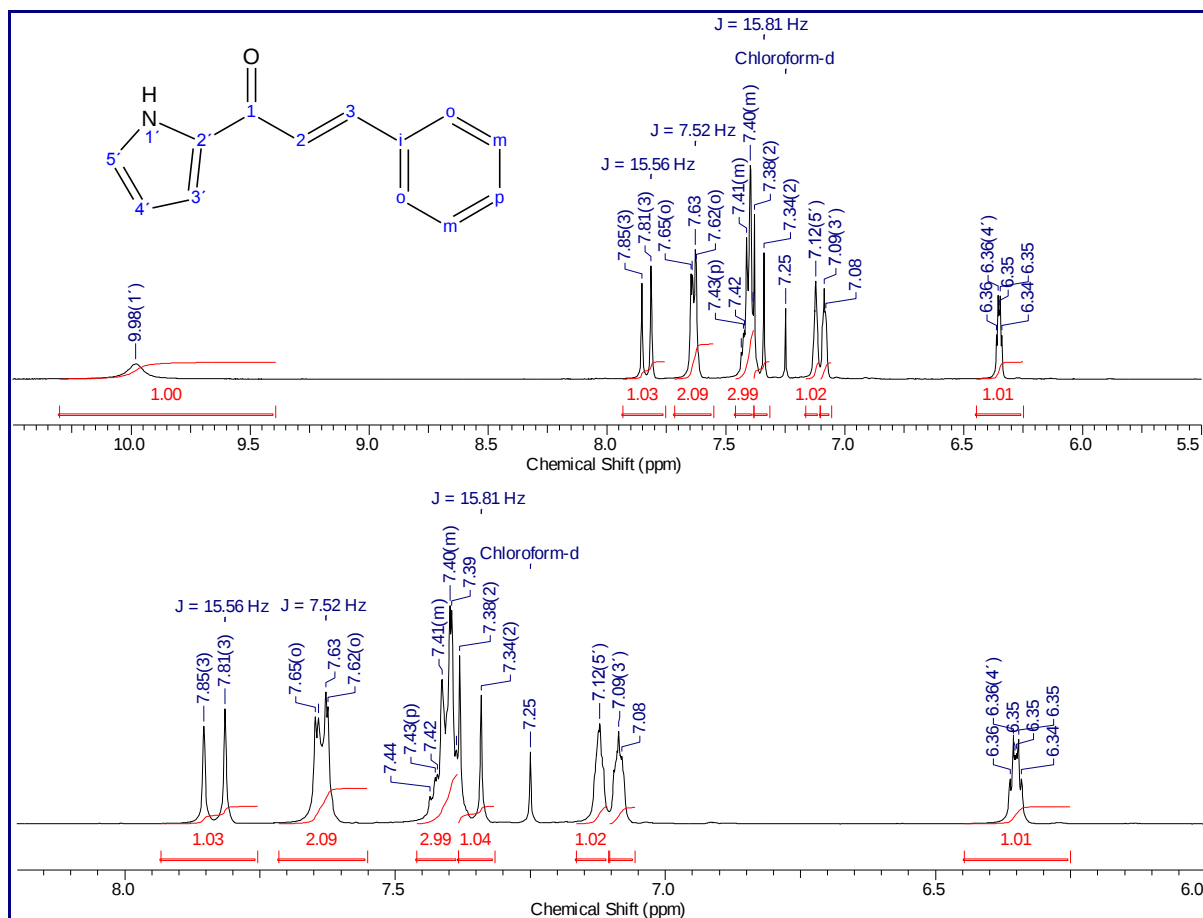


Fig. S2 ¹H-NMR spectra for (E)-3-phenyl-1-(1H-pyrrol-2-yl)prop-2-en-1-one (3a)

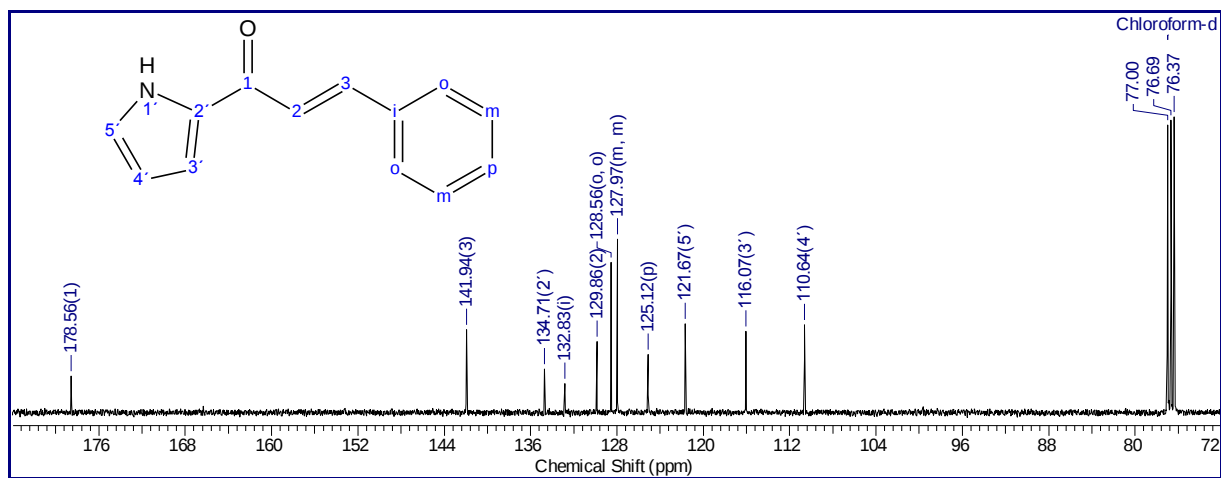


Fig. S3 ^{13}C -NMR spectra for (E)-3-phenyl-1-(1H-pyrrol-2-yl)prop-2-en-1-one (3a)

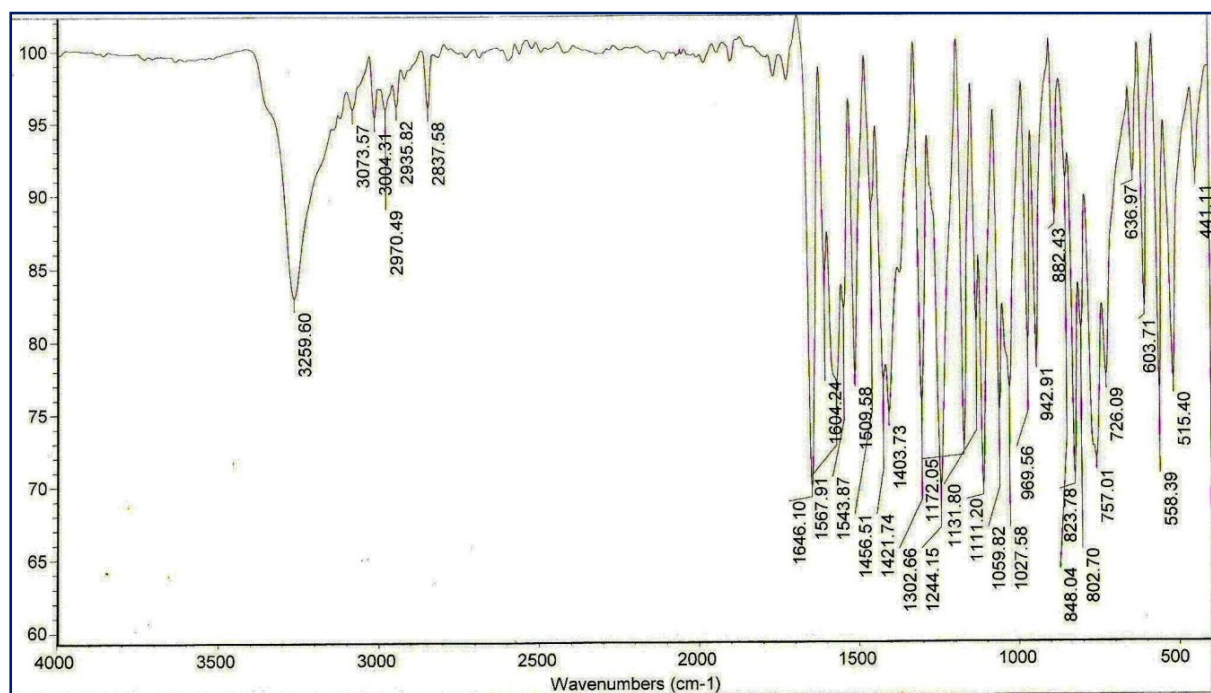


Fig. S4 IR spectra for (E)-3-(4-methoxyphenyl)-1-(1H-pyrrol-2-yl)prop-2-en-1-one (3b)

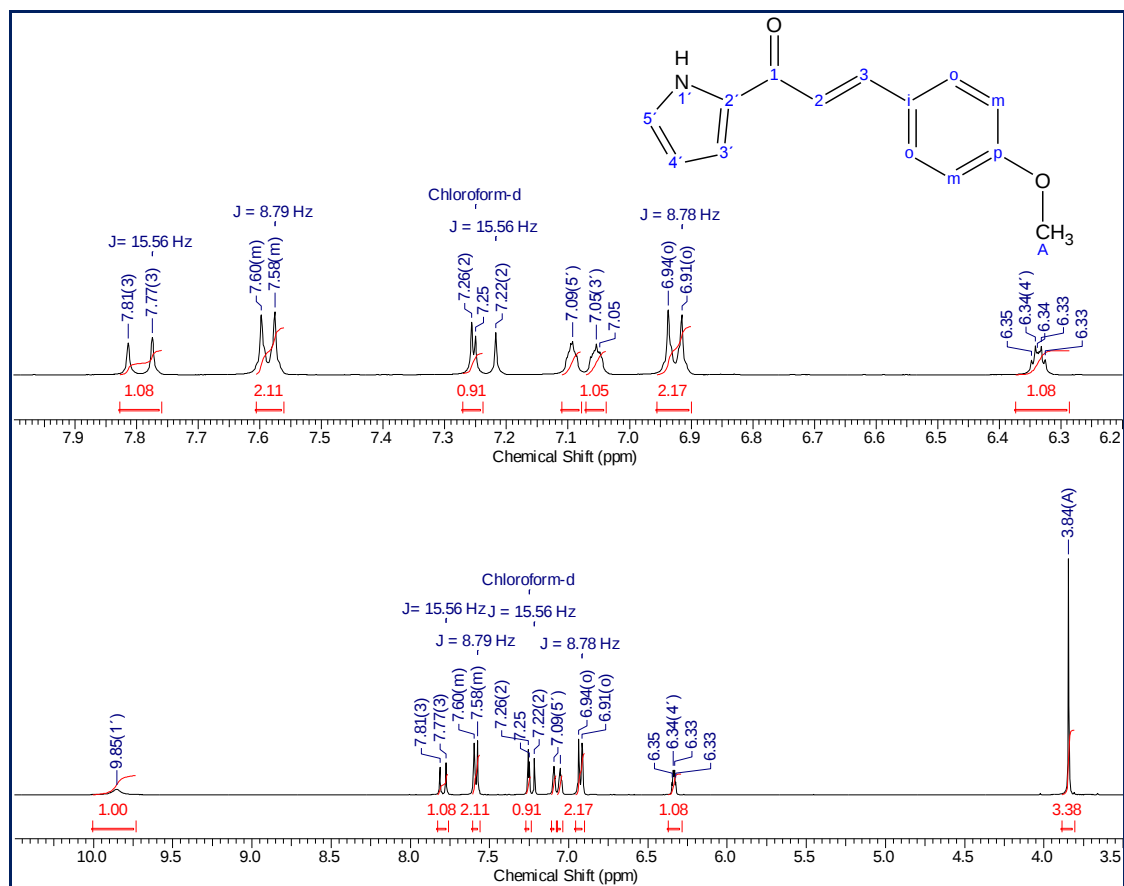


Fig. S5 ^1H -NMR spectra for *(E)*-3-(4-methoxyphenyl)-1-(1H-pyrrol-2-yl)prop-2-en-1-one (**3b**)

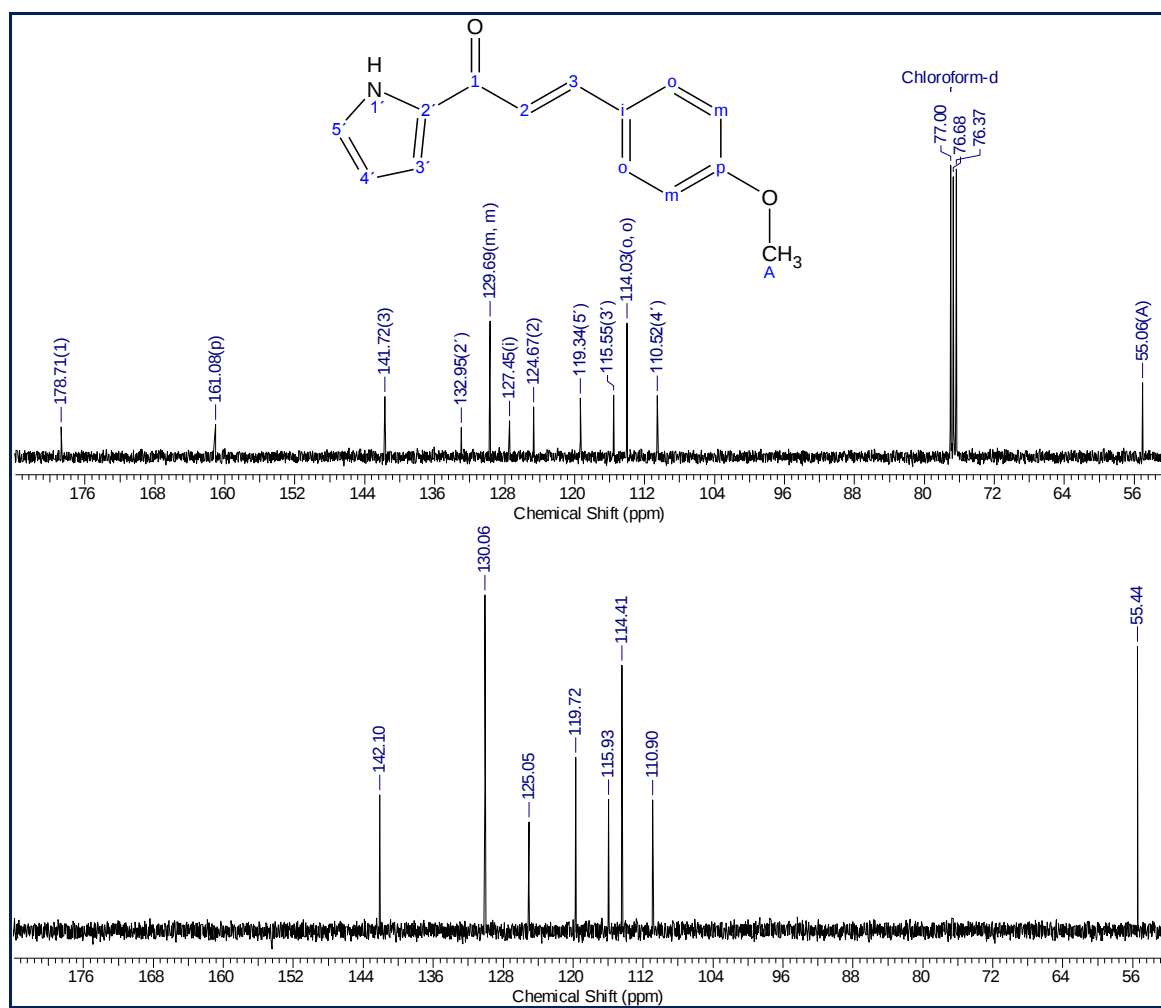


Fig. S6 ¹³C-NMR spectra for (*E*)-3-(4-methoxyphenyl)-1-(1H-pyrrol-2-yl)prop-2-en-1-one (**3b**)

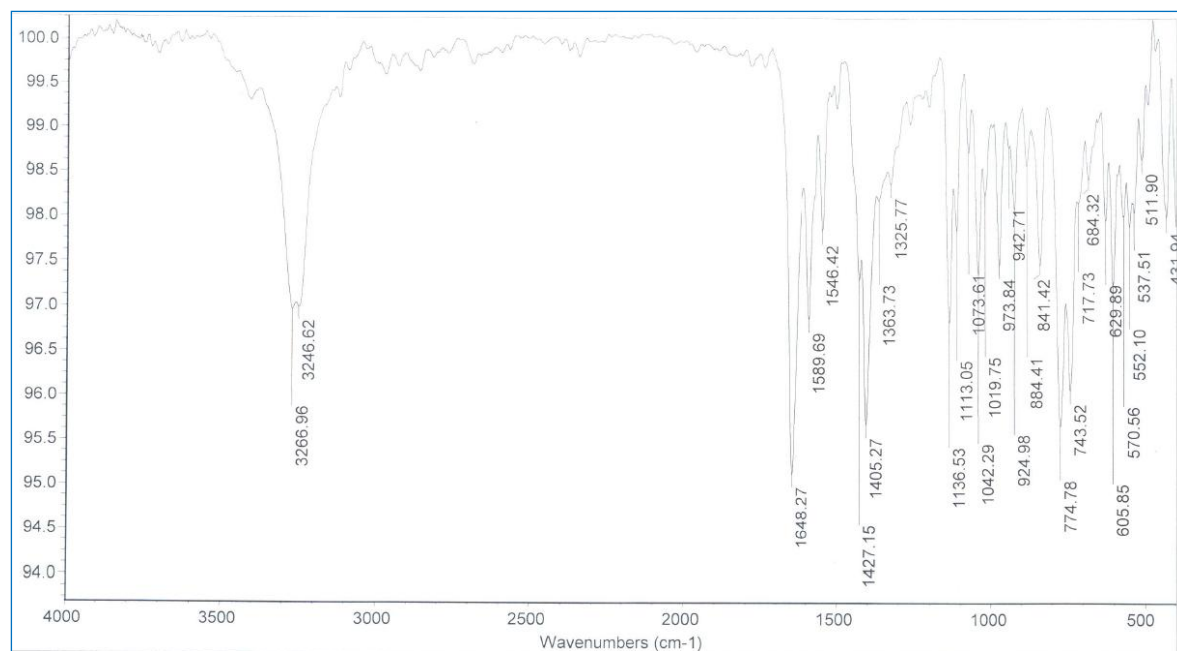


Fig. S7 IR spectra for (*E*)-3-(4-fluorophenyl)-1-(1H-pyrrol-2-yl)prop-2-en-1-one (**3c**)

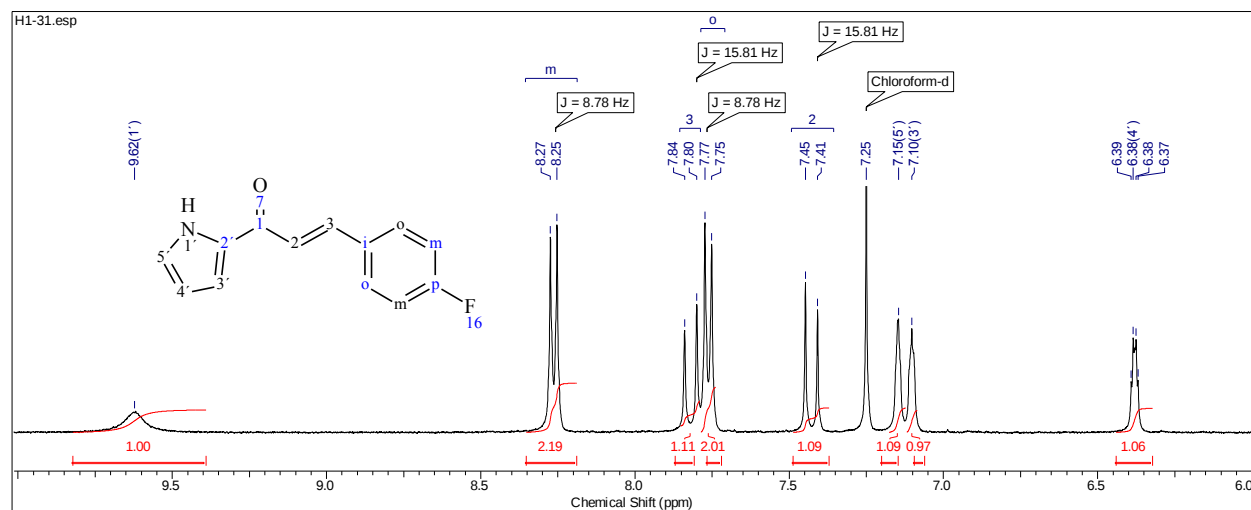


Fig. S8 ¹H-NMR spectra for (*E*)-3-(4-fluorophenyl)-1-(1H-pyrrol-2-yl)prop-2-en-1-one (**3c**)

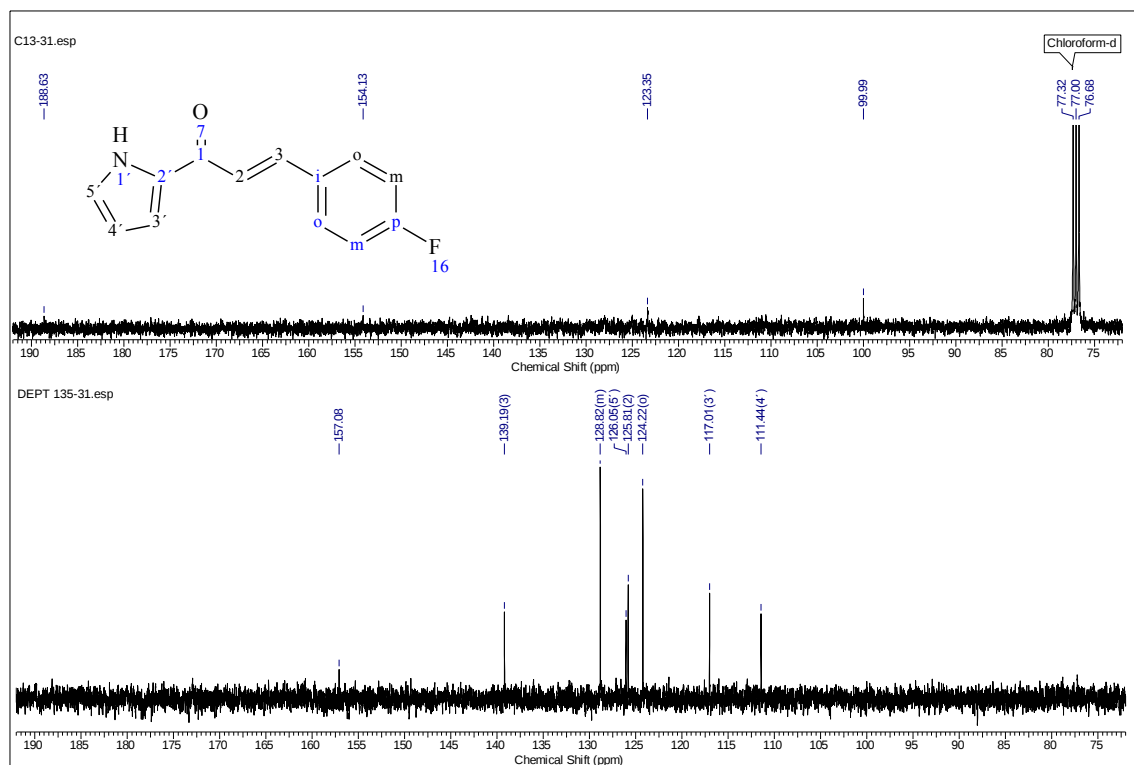


Fig. S9 ^{13}C -NMR spectra for (E)-3-(4-fluorophenyl)-1-(1H-pyrrol-2-yl)prop-2-en-1-one (3c)

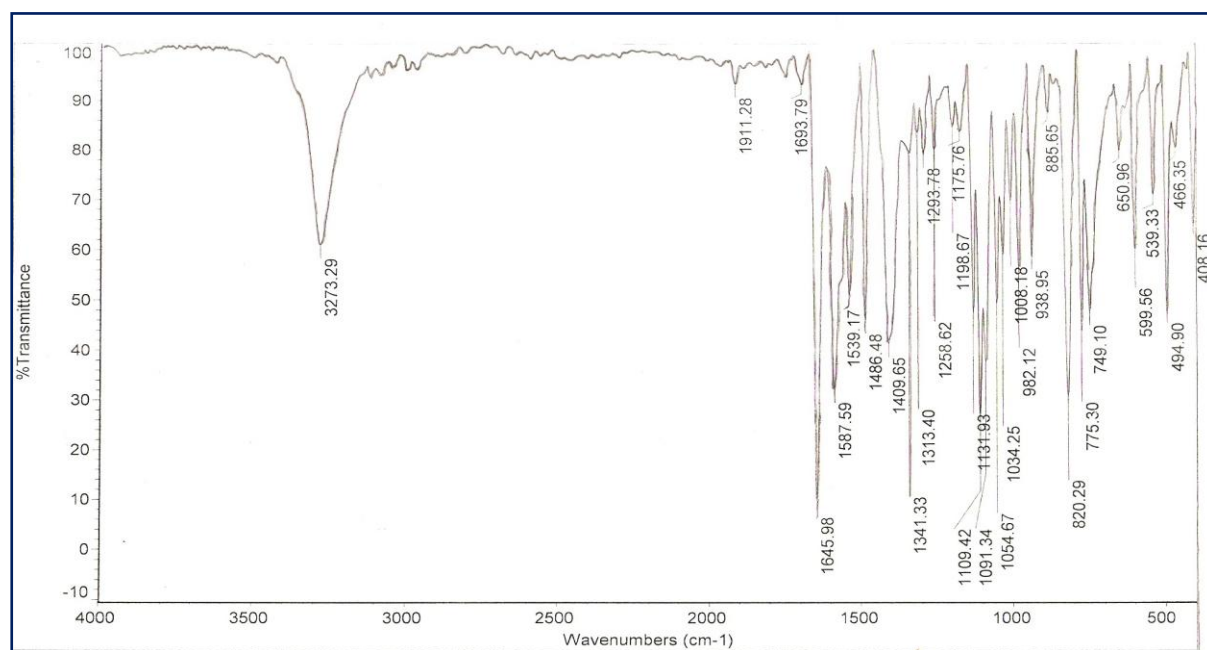


Fig. S10 IR spectra for (E)-3-(4-chlorophenyl)-1-(1H-pyrrol-2-yl)prop-2-en-1-one (3d)

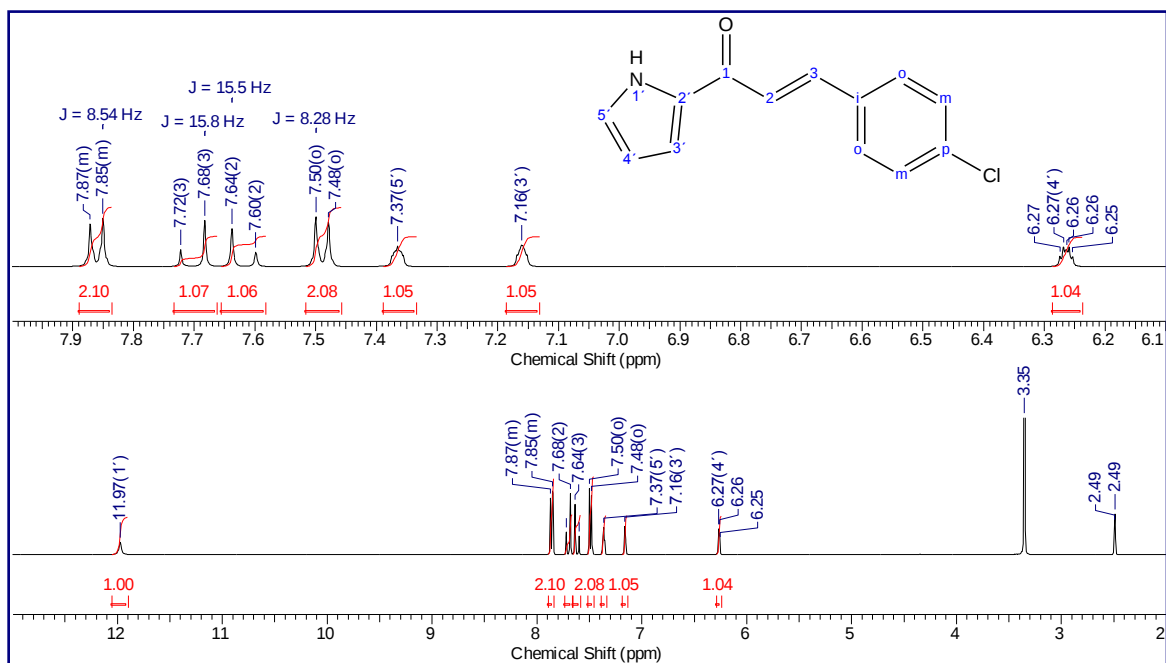


Fig. S11 ¹H-NMR spectra for (*E*)-3-(4-chlorophenyl)-1-(1H-pyrrol-2-yl)prop-2-en-1-one (**3d**)

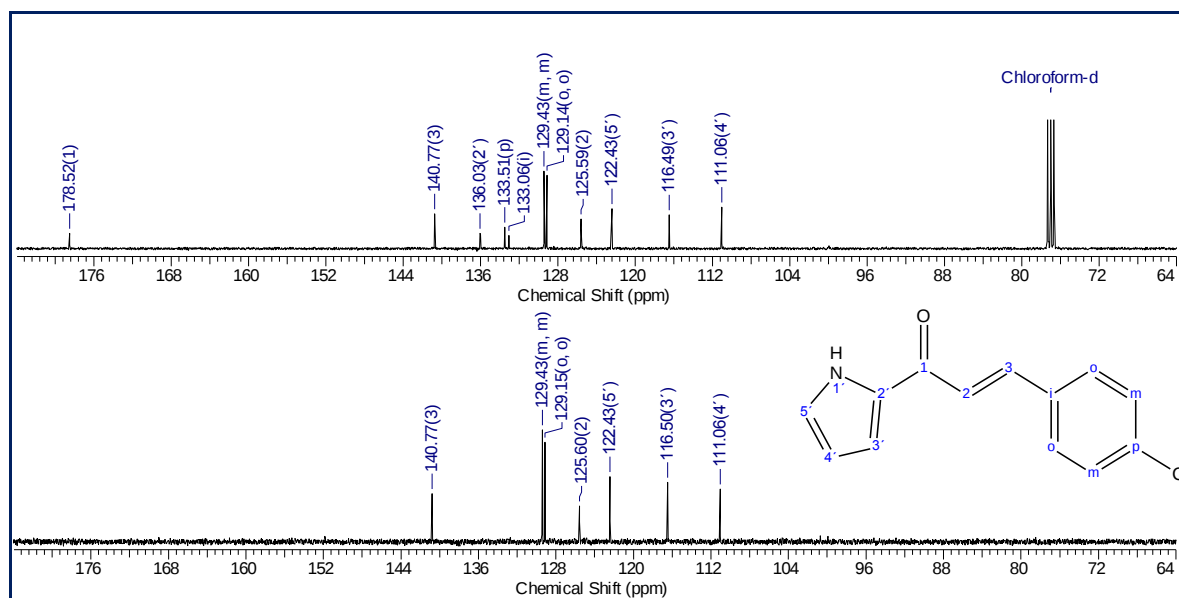


Fig. S12 ¹³C-NMR spectra for (*E*)-3-(4-chlorophenyl)-1-(1H-pyrrol-2-yl)prop-2-en-1-one (**3d**)

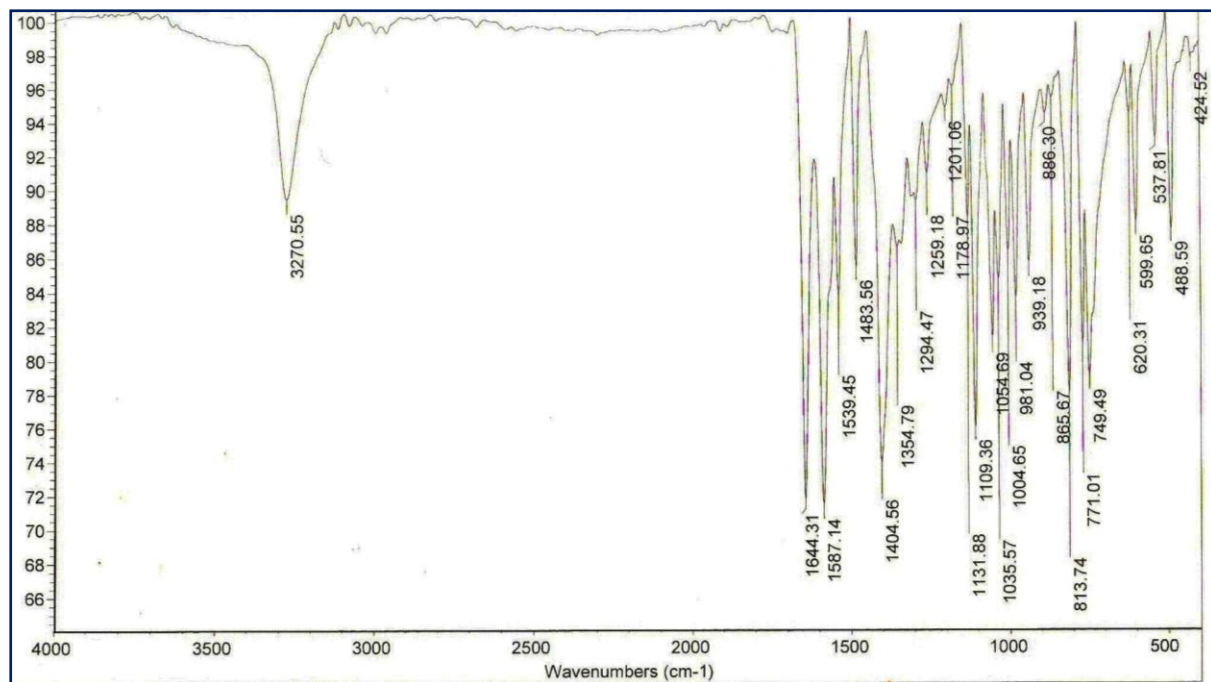


Fig. S13 IR spectra for (E)-3-(4-chlorophenyl)-1-(1H-pyrrol-2-yl)prop-2-en-1-one (**3d**)

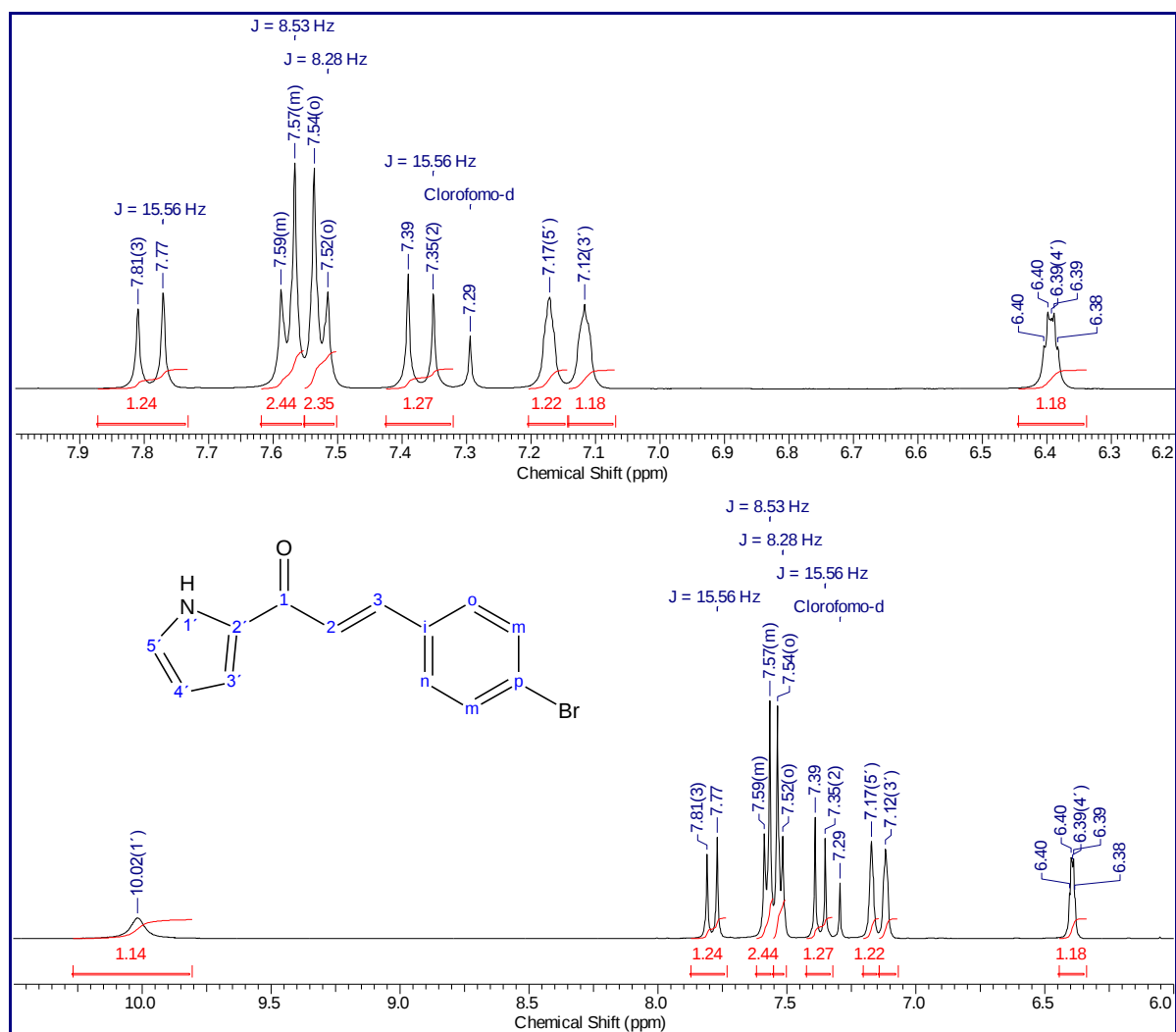


Fig. S14 ^1H -NMR spectra for (E) -3-(4-bromophenyl)-1-(1H-pyrrol-2-yl)prop-2-en-1-one (**3e**)

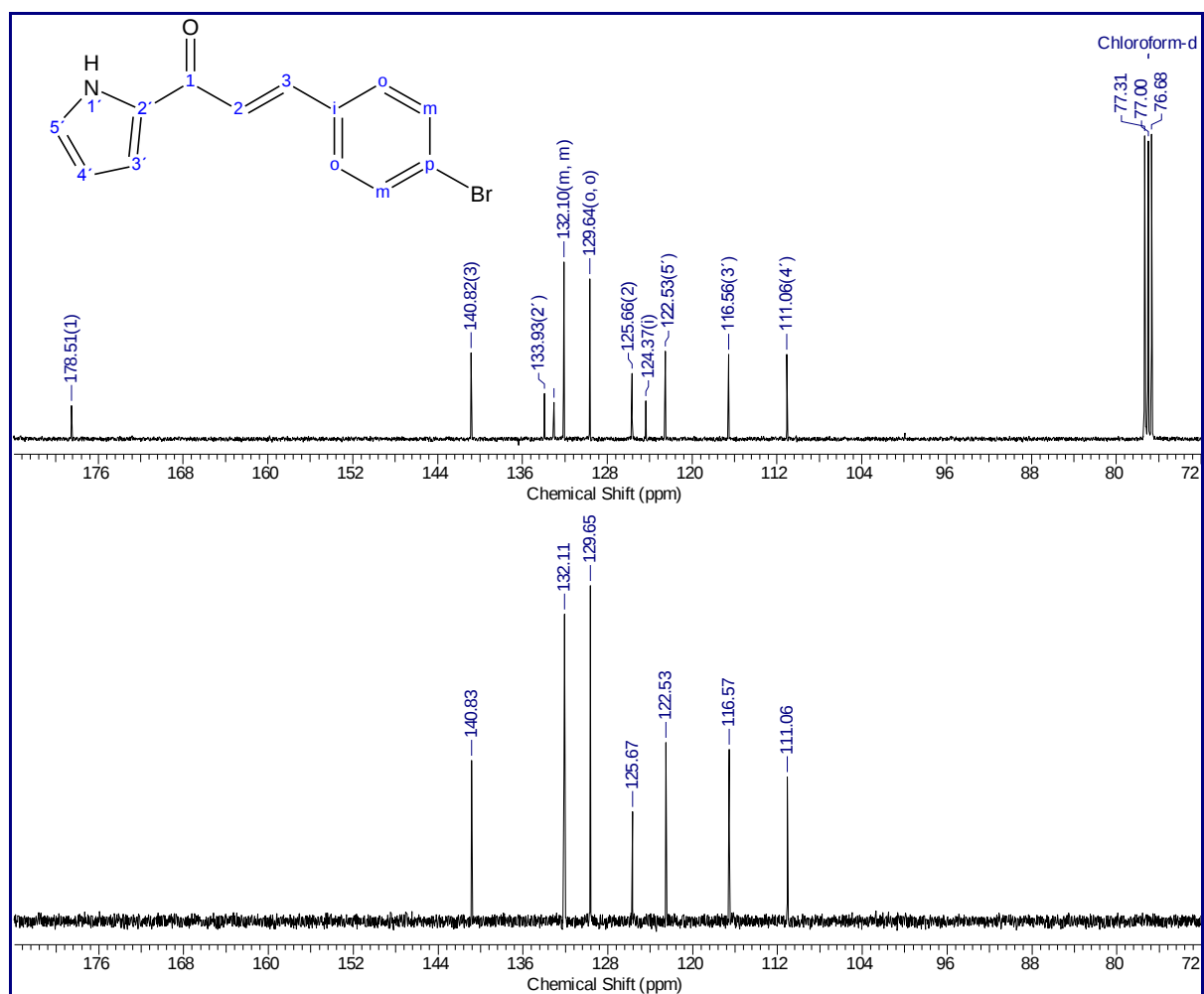


Fig. S15 ^{13}C -NMR spectra for (E)-3-(4-bromophenyl)-1-(1H-pyrrol-2-yl)prop-2-en-1-one (**3e**)

2. HOMO and LUMO molecular orbitals calculated at the $T_1(\pi_H\pi_L^*)$ state minima

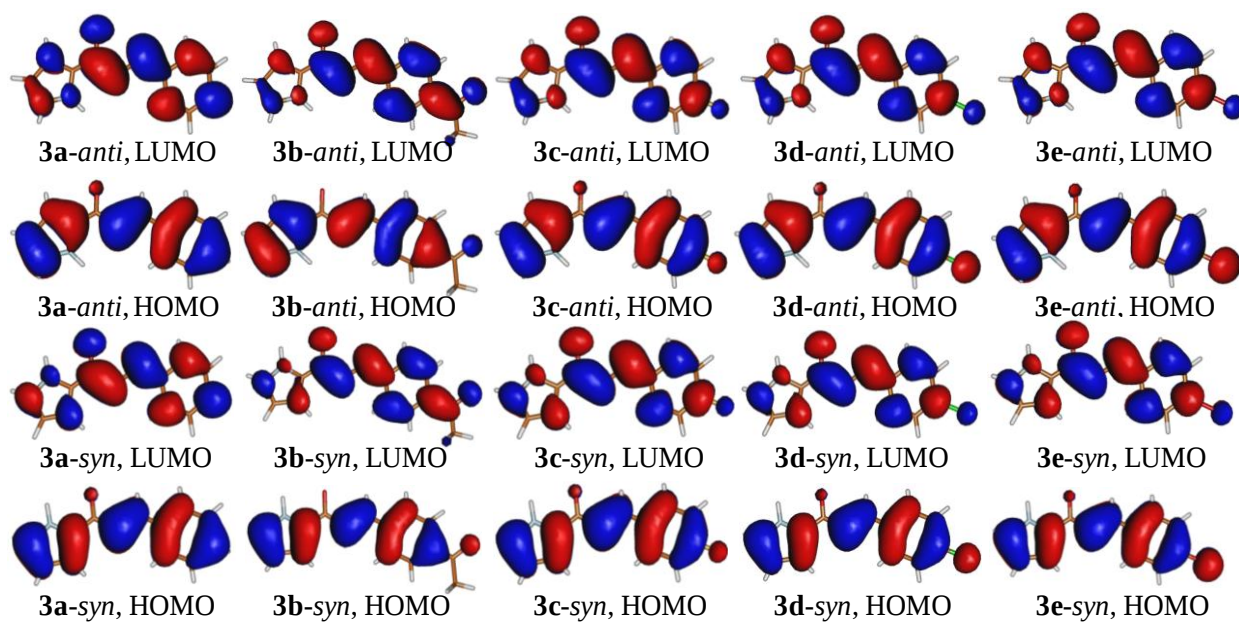


Fig. S16 B3LYP Frontier MOs for the UB3LYP-D3/TZVP + COSMO ($\epsilon = 24.852$) $T_1(\pi_H\pi_L^*)$ state minima of all the PAPs compounds.

3. Cartesian coordinates of the calculated minima

Ground state minimum: 3a-*anti*

C	-4.3020536	-1.4904037	-0.2718491
C	-5.1064632	-0.3864317	-0.0249172
C	-4.2521152	0.7062175	0.2064876
C	-2.9388936	0.2551202	0.0971024
N	-3.0066635	-1.0967256	-0.1987997
H	-2.2221200	-1.7141357	-0.3293692
H	-4.5612608	-2.5133810	-0.4902785
H	-6.1846743	-0.3834729	-0.0167061
H	-4.5319930	1.7231114	0.4284227
C	-1.7121332	1.0252941	0.2537587
O	-1.7716274	2.2267894	0.5463283
C	-0.4188963	0.3357863	0.0551664
C	0.7457933	0.9808502	0.2377895
H	-0.4269978	-0.7051304	-0.2416763
H	0.6843866	2.0234148	0.5379870
C	2.0954116	0.4476866	0.0826547
C	3.1845519	1.2936692	0.3489158
C	2.3608632	-0.8728280	-0.3210803
C	4.4925451	0.8399367	0.2199029
H	2.9977169	2.3151740	0.6603109
C	3.6659513	-1.3244612	-0.4497945
H	1.5447199	-1.5507339	-0.5370982
C	4.7377083	-0.4708629	-0.1798345
H	5.3183153	1.5084820	0.4308460
H	3.8527601	-2.3448041	-0.7622462
H	5.7551683	-0.8281615	-0.2820232

Ground state minimum: 3a-*syn*

C	-5.1167772	-0.1873660	0.0259865
C	-4.4966398	-1.3961886	-0.2638304
C	-3.1077587	-1.1686816	-0.2358459
C	-2.9069401	0.1787702	0.0717746
N	-4.1541715	0.7446047	0.2241364
H	-4.3009748	1.7173406	0.4515645
H	-6.1623946	0.0638396	0.1019547
H	-4.9979548	-2.3284529	-0.4704035
H	-2.3367971	-1.8998857	-0.4180117
C	-1.7139593	0.9905148	0.2411618
O	-1.8139971	2.1946881	0.5261228
C	-0.4134973	0.3211998	0.0617655
C	0.7433642	0.9853654	0.2256277
H	-0.4258139	-0.7276257	-0.2038447
H	0.6742933	2.0351557	0.4983352
C	2.0971051	0.4585803	0.0821864
C	3.1813943	1.3157969	0.3322648
C	2.3699341	-0.8681850	-0.2960988
C	4.4921154	0.8666935	0.2123357
H	2.9889804	2.3423437	0.6237852
C	3.6777503	-1.3148251	-0.4164661
H	1.5574664	-1.5546647	-0.4993829
C	4.7447966	-0.4501915	-0.1626863
H	5.3144120	1.5436481	0.4108437
H	3.8705339	-2.3399085	-0.7100766
H	5.7644542	-0.8037228	-0.2583202

Ground state minimum: 3b-*anti*

C	-5.3928029	-1.0485050	-0.1528477
C	-6.1790720	0.0544885	0.1529212
C	-5.3075093	1.1241473	0.4198080
C	-4.0015840	0.6608651	0.2728679
N	-4.0917920	-0.6762234	-0.0805154
H	-3.3182931	-1.2983510	-0.2493938
H	-5.6692883	-2.0572897	-0.4122199
H	-7.2569035	0.0709098	0.1759623
H	-5.5705288	2.1338897	0.6898815
C	-2.7644164	1.4064079	0.4471385
O	-2.7984222	2.5946543	0.7897724
C	-1.4804841	0.7064622	0.2054550
C	-0.3064379	1.3240575	0.4131564
H	-1.5064297	-0.3185730	-0.1411927
H	-0.3461685	2.3499380	0.7679489
C	1.0309916	0.7712922	0.2214116
C	2.1408499	1.5676142	0.5532433
C	1.2672209	-0.5191890	-0.2805047
C	3.4319789	1.0933198	0.3963337
H	1.9797123	2.5674072	0.9391206
C	2.5586159	-0.9926943	-0.4389235
H	0.4386069	-1.1595015	-0.5533184
C	3.6614390	-0.1942962	-0.1020086
H	4.2788585	1.7145001	0.6569512
H	2.7015845	-1.9912737	-0.8288917
C	5.0700732	-0.6724190	-0.2584007
O	6.0076786	0.0472818	0.0567863
C	5.3134791	-2.0555697	-0.8115441
H	4.8449393	-2.8118733	-0.1771570
H	4.8794975	-2.1528514	-1.8095987
H	6.3846067	-2.2386254	-0.8622417

Ground state minimum: 3b-*syn*

C	-6.1844894	0.2509945	0.2066424
C	-5.5825695	-0.9516741	-0.1432660
C	-4.1915207	-0.7431615	-0.1186675
C	-3.9705939	0.5872075	0.2473673
N	-5.2090984	1.1610611	0.4374188
H	-5.3423614	2.1242043	0.7097628
H	-7.2261916	0.5110703	0.3036808
H	-6.0978576	-1.8672616	-0.3864827
H	-3.4316697	-1.4748218	-0.3409411
C	-2.7663415	1.3727172	0.4405537
O	-2.8398448	2.5629789	0.7820408
C	-1.4756945	0.6916515	0.2140905
C	-0.3084178	1.3304504	0.3953173
H	-1.5070189	-0.3436086	-0.0989768
H	-0.3537582	2.3660320	0.7204929
C	1.0318404	0.7815935	0.2108363
C	2.1397346	1.5875205	0.5260431
C	1.2711255	-0.5170681	-0.2686020
C	3.4321635	1.1137112	0.3769389
H	1.9765613	2.5941628	0.8933580
C	2.5636749	-0.9895512	-0.4205703
H	0.4437995	-1.1642953	-0.5291893
C	3.6647292	-0.1822831	-0.0985494 ... cont

H	4.2766226	1.7430693	0.6262394
H	2.7086231	-1.9945002	-0.7934852
C	5.0730150	-0.6611577	-0.2472597
O	6.0105836	0.0623244	0.0628253
C	5.3182813	-2.0491366	-0.7859857
H	4.8501758	-2.7991107	-0.1435240
H	4.8837102	-2.1569393	-1.7828833
H	6.3897235	-2.2318593	-0.8347856

Ground state minimum: 3c-anti

C	-4.2324423	-1.6993928	-0.2809414
C	-5.0905023	-0.6346923	-0.0423510
C	-4.2911530	0.4988443	0.1886831
C	-2.9571246	0.1115275	0.0872504
N	-2.9579518	-1.2432215	-0.2034562
H	-2.1439911	-1.8226628	-0.3276053
H	-4.4407591	-2.7345783	-0.4963939
H	-6.1676295	-0.6837618	-0.0392863
H	-4.6209804	1.5018002	0.4052622
C	-1.7701510	0.9413959	0.2448066
O	-1.8892576	2.1399282	0.5314953
C	-0.4439943	0.3152866	0.0541965
C	0.6862855	1.0196075	0.2345621
H	-0.3997879	-0.7268872	-0.2351068
H	0.5716416	2.0602499	0.5254347
C	2.0606930	0.5547043	0.0877623
C	3.1055422	1.4590314	0.3399716
C	2.3938006	-0.7573766	-0.2938700
C	4.4367673	1.0793124	0.2216290
H	2.8706839	2.4748763	0.6344494
C	3.7163830	-1.1525776	-0.4164425
H	1.6162832	-1.4816405	-0.4984061
C	4.7125779	-0.2228060	-0.1547312
H	5.2447876	1.7722204	0.4154935
H	3.9818964	-2.1598214	-0.7092977
F	6.0083828	-0.6093660	-0.2731081

Ground state minimum: 3c-syn

C	-5.1094752	-0.4414619	0.0297025
C	-4.4300209	-1.6208216	-0.2481916
C	-3.0544061	-1.3230961	-0.2290537
C	-2.9209500	0.0365433	0.0610626
N	-4.1945741	0.5403751	0.2123208
H	-4.3895504	1.5071682	0.4285370
H	-6.1661849	-0.2426401	0.1075431
H	-4.8842732	-2.5797827	-0.4409407
H	-2.2481209	-2.0166314	-0.4052861
C	-1.7704630	0.9095536	0.2175949
O	-1.9305408	2.1100008	0.4908409
C	-0.4381232	0.3049840	0.0426553
C	0.6832497	1.0273043	0.2071915
H	-0.3977246	-0.7448483	-0.2163753
H	0.5607807	2.0733427	0.4750927
C	2.0615551	0.5684415	0.0750019
C	3.1008174	1.4752187	0.3411977
C	2.4024249	-0.7427138	-0.3035908
C	4.4345791	1.0975605	0.2431099
H	2.8602085	2.4910021	0.6320254
C	3.7276531	-1.1355180	-0.4071784
H	1.6293304	-1.4681293	-0.5214849 ... cont

C	4.7177683	-0.2041031	-0.1292221
H	5.2381967	1.7923268	0.4496452
H	3.9986242	-2.1421555	-0.6981785
F	6.0167529	-0.5885942	-0.2277721

Ground state minimum: 3d-anti

C	-4.1783639	-1.8503067	-0.3209132
C	-5.0775185	-0.8205425	-0.0792744
C	-4.3229304	0.3378926	0.1759436
C	-2.9743875	0.0006027	0.0859726
N	-2.9224343	-1.3495972	-0.2218298
H	-2.0867350	-1.8975759	-0.3446939
H	-4.3463795	-2.8893627	-0.5523336
H	-6.1520930	-0.9087126	-0.0900525
H	-4.6915746	1.3253380	0.4010435
C	-1.8213322	0.8716025	0.2658038
O	-1.9865361	2.0620396	0.5619849
C	-0.4698444	0.2971468	0.0824112
C	0.6305478	1.0481917	0.2557146
H	-0.3833339	-0.7444383	-0.1995273
H	0.4756645	2.0864709	0.5358944
C	2.0220294	0.6354281	0.1083415
C	3.0314109	1.5868933	0.3223904
C	2.4067334	-0.6705808	-0.2405053
C	4.3753905	1.2595491	0.1945879
H	2.7602815	2.6005281	0.5928468
C	3.7430522	-1.0126798	-0.3711454
H	1.6598977	-1.4345199	-0.4131342
C	4.7156833	-0.0407015	-0.1520965
H	5.1430567	2.0028487	0.3615685
H	4.0294099	-2.0205219	-0.6396077
Cl	6.4203057	-0.4749923	-0.3193899

Ground state minimum: 3d-syn

C	-5.1035440	-0.6317203	-0.0046195
C	-4.3763537	-1.7827278	-0.2810026
C	-3.0135681	-1.4341373	-0.2392165
C	-2.9353463	-0.0727342	0.0632762
N	-4.2291198	0.3820733	0.1991193
H	-4.4636198	1.3392940	0.4185111
H	-6.1680307	-0.4732504	0.0583545
H	-4.7914894	-2.7564617	-0.4872950
H	-2.1794228	-2.0958081	-0.4079573
C	-1.8205073	0.8401311	0.2428044
O	-2.0264437	2.0306978	0.5266971
C	-0.4639082	0.2874689	0.0732204
C	0.6273808	1.0540174	0.2364749
H	-0.3817586	-0.7596270	-0.1871457
H	0.4650030	2.0956674	0.4998465
C	2.0222981	0.6477547	0.1004960
C	3.0267282	1.6025375	0.3231130
C	2.4139464	-0.6572978	-0.2449133
C	4.3731217	1.2786550	0.2093301
H	2.7505438	2.6158748	0.5904507
C	3.7526803	-0.9957825	-0.3624674
H	1.6710151	-1.4235369	-0.4253584
C	4.7199744	-0.0209043	-0.1333489
H	5.1366135	2.0248849	0.3837183
H	4.0437196	-2.0031026	-0.6289020
Cl	6.4283971	-0.4509190	-0.2830357

Ground state minimum: 3e-anti

C	-4.1005800	-2.0214861	-0.3205227
C	-5.0428409	-1.0326703	-0.0718285
C	-4.3386812	0.1582618	0.1777311
C	-2.9771375	-0.1186029	0.0767817
N	-2.8674240	-1.4653958	-0.2312785
H	-2.0092100	-1.9760254	-0.3603553
H	-4.2238231	-3.0670508	-0.5509669
H	-6.1124738	-1.1688732	-0.0738394
H	-4.7491465	1.1282512	0.4063961
C	-1.8626393	0.8018193	0.2519207
O	-2.0776609	1.9823086	0.5552669
C	-0.4883287	0.2876306	0.0584337
C	0.5804106	1.0754427	0.2628981
H	-0.3594497	-0.7407397	-0.2541700
H	0.3835837	2.0984069	0.5716266
C	1.9876723	0.7197642	0.1149720
C	2.9584887	1.7061693	0.3471460
C	2.4240564	-0.5649123	-0.2510856
C	4.3150737	1.4336044	0.2182661
H	2.6477743	2.7043509	0.6323568
C	3.7733523	-0.8531010	-0.3827687
H	1.7083934	-1.3553966	-0.4355651
C	4.7075161	0.1526732	-0.1467831
H	5.0486254	2.2071405	0.3998679
H	4.0941541	-1.8466812	-0.6646603
Br	6.5802945	-0.2448883	-0.3298397

Ground state minimum: 3e-syn

C	-5.0798750	-0.8350938	-0.0266191
C	-4.3066337	-1.9543120	-0.3084558
C	-2.9590420	-1.5516904	-0.2615557
C	-2.9360793	-0.1900215	0.0490752
N	-4.2472642	0.2117341	0.1847428
H	-4.5204850	1.1575162	0.4089208
H	-6.1499492	-0.7199029	0.0354504
H	-4.6819804	-2.9426358	-0.5214450
H	-2.0987317	-2.1783903	-0.4323393
C	-1.8593601	0.7658840	0.2355439
O	-2.1135047	1.9466077	0.5213307
C	-0.4807972	0.2683458	0.0710229
C	0.5774598	1.0792043	0.2369176
H	-0.3552559	-0.7748632	-0.1878495
H	0.3717105	2.1138874	0.4974438
C	1.9884551	0.7301764	0.1064329
C	2.9514184	1.7283514	0.3205995
C	2.4349841	-0.5605853	-0.2251835
C	4.3108245	1.4605704	0.2104804
H	2.6327620	2.7319071	0.5775351
C	3.7872652	-0.8437807	-0.3392160
H	1.7253294	-1.3595324	-0.3976363
C	4.7130775	0.1733326	-0.1197943
H	5.0379108	2.2433435	0.3792529
H	4.1156456	-1.8421112	-0.5951709
Br	6.5906149	-0.2169412	-0.2787064

Triplet state minimum: 3a-anti

C	-4.3012383	-1.5183228	-0.2953863
C	-5.1023914	-0.4107829	-0.0646883
C	-4.2448309	0.6807235	0.1811132
C	-2.9336658	0.2233756	0.0961084
N	-3.0020256	-1.1277513	-0.1990965
H	-2.2187237	-1.7500756	-0.3115865
H	-4.5597188	-2.5409025	-0.5160996
H	-6.1807043	-0.4017567	-0.0756418
H	-4.5233505	1.6993842	0.3961286
C	-1.7033609	0.9923701	0.2739136
O	-1.7641958	2.2131281	0.5764256
C	-0.4376764	0.3454438	0.0965701
C	0.8128453	1.0623609	0.2855936
H	-0.4057237	-0.6980538	-0.1839907
H	0.7254215	2.0978465	0.5893362
C	2.0761538	0.5202307	0.1115841
C	3.2423552	1.3401109	0.3473781
C	2.3145240	-0.8448211	-0.2983113
C	4.5080965	0.8395263	0.1921587
H	3.0934385	2.3686202	0.6545403
C	3.5953798	-1.3240807	-0.4483571
H	1.4780880	-1.5019089	-0.4920204
C	4.7064168	-0.4997495	-0.2077924
H	5.3660517	1.4745561	0.3772052
H	3.7494118	-2.3513170	-0.7566247
H	5.7094232	-0.8881542	-0.3284601

Triplet state minimum: 3a-syn

C	-5.1084222	-0.2135406	-0.0261176
C	-4.4846879	-1.4263816	-0.2847275
C	-3.0953282	-1.2038326	-0.2258306
C	-2.8968869	0.1500369	0.0701796
N	-4.1408441	0.7198892	0.1848131
H	-4.2853461	1.6966449	0.3959250
H	-6.1538825	0.0443292	0.0211009
H	-4.9836632	-2.3599828	-0.4915012
H	-2.3219161	-1.9395009	-0.3778939
C	-1.7061182	0.9708879	0.2568140
O	-1.8175858	2.1984284	0.5286715
C	-0.4362757	0.3339261	0.1203972
C	0.8075122	1.0622113	0.2995392
H	-0.4123034	-0.7200527	-0.1177945
H	0.7158417	2.1020159	0.5886855
C	2.0751492	0.5271517	0.1251025
C	3.2369456	1.3571949	0.3421828
C	2.3185102	-0.8405406	-0.2706162
C	4.5052186	0.8638759	0.1784207
H	3.0843477	2.3882871	0.6394794
C	3.6014679	-1.3126266	-0.4294523
H	1.4843586	-1.5054866	-0.4476090
C	4.7090168	-0.4780216	-0.2089154
H	5.3606491	1.5070684	0.3476392
H	3.7594066	-2.3423350	-0.7281462
H	5.7137603	-0.8608029	-0.3354676

Triplet state minimum: 3b-anti

C	-5.3797233	-1.0776929	-0.1840677
C	-6.1639656	0.0291540	0.1110171
C	-5.2899087	1.0960210	0.3899526
C	-3.9853379	0.6267069	0.2601415
N	-4.0761997	-0.7094086	-0.0946150
H	-3.3036727	-1.3362846	-0.2496654
H	-5.6565508	-2.0855333	-0.4464294
H	-7.2419815	0.0505687	0.1207138
H	-5.5513004	2.1071651	0.6559485
C	-2.7445979	1.3702480	0.4546541
O	-2.7796726	2.5730270	0.8061520
C	-1.4877295	0.7012178	0.2362156
C	-0.2335127	1.3800285	0.4683967
H	-1.4778559	-0.3244224	-0.1040203
H	-0.3086917	2.3945952	0.8409633
C	1.0184000	0.8443048	0.2653001
C	2.1965201	1.6336676	0.5657629
C	1.2480393	-0.4951042	-0.2415931
C	3.4484109	1.1359068	0.3861893
H	2.0560249	2.6394815	0.9435977
C	2.5152751	-0.9765388	-0.4173499
H	0.4063523	-1.1268543	-0.4882484
C	3.6535818	-0.1874927	-0.1107751
H	4.3182060	1.7361443	0.6177759
H	2.6414279	-1.9809911	-0.7982106
C	5.0306825	-0.6834277	-0.2868858
O	5.9923412	0.0313033	0.0009689
C	5.2490997	-2.0791438	-0.8245557
H	4.7883897	-2.8246571	-0.1716890
H	4.8001444	-2.1899876	-1.8146929
H	6.3178049	-2.2720014	-0.8909517

Triplet state minimum: 3b-syn

C	-6.1642612	0.2160240	0.1797794
C	-5.5597770	-0.9714206	-0.2158141
C	-4.1698537	-0.7641939	-0.1801513
C	-3.9503329	0.5548618	0.2394941
N	-5.1849316	1.1184768	0.4483680
H	-5.3156747	2.0705964	0.7585799
H	-7.2057454	0.4728185	0.2856321
H	-6.0741351	-1.8769777	-0.4958040
H	-3.4081692	-1.4852563	-0.4293996
C	-2.7465201	1.3419186	0.4693336
O	-2.8308906	2.5341073	0.8572169
C	-1.4871670	0.6962137	0.2358397
C	-0.2382810	1.3884643	0.4475202
H	-1.4871146	-0.3298060	-0.1024017
H	-0.3156972	2.4133115	0.7917770
C	1.0169914	0.8541149	0.2533718
C	2.1920587	1.6601193	0.5150018
C	1.2492986	-0.5007452	-0.2064415
C	3.4459715	1.1638115	0.3397240
H	2.0499194	2.6780900	0.8587863
C	2.5179521	-0.9811960	-0.3778155
H	0.4087919	-1.1465795	-0.4192303
C	3.6544755	-0.1745808	-0.1127312
H	4.3130729	1.7789393	0.5411356
H	2.6456426	-1.9986269	-0.7223841
C	5.0315545	-0.6690848	-0.2874810
O	5.9936728	0.0610501	-0.0379612 ... cont

C	5.2517436	-2.0819529	-0.7766322
H	4.8046267	-2.8054185	-0.0900713
H	4.7889779	-2.2315566	-1.7554513
H	6.3207373	-2.2712020	-0.8513505

Triplet state minimum: 3c-anti

C	-4.2255205	-1.7287477	-0.3057819
C	-5.0825263	-0.6644867	-0.0723028
C	-4.2822227	0.4695159	0.1742479
C	-2.9492580	0.0807916	0.0871850
N	-2.9480581	-1.2717230	-0.2101418
H	-2.1339275	-1.8528234	-0.3240501
H	-4.4310293	-2.7629289	-0.5282175
H	-6.1598801	-0.7111604	-0.0819488
H	-4.6127191	1.4720868	0.3911425
C	-1.7602690	0.9123139	0.2642454
O	-1.8836888	2.1280371	0.5683543
C	-0.4632435	0.3318219	0.0835804
C	0.7482480	1.1118383	0.2689698
H	-0.3791924	-0.7082604	-0.1994862
H	0.6095079	2.1461751	0.5566320
C	2.0374575	0.6285537	0.1104140
C	3.1611157	1.5093043	0.3366350
C	2.3433568	-0.7311646	-0.2731668
C	4.4525671	1.0765141	0.1995537
H	2.9640572	2.5347183	0.6238559
C	3.6432861	-1.1582777	-0.4087725
H	1.5435359	-1.4335559	-0.4584421
C	4.6802415	-0.2564198	-0.1720660
H	5.2946515	1.7346497	0.3698422
H	3.8766114	-2.1756007	-0.6953336
F	5.9568989	-0.6811714	-0.3049480

Triplet state minimum: 3c-syn

C	-5.0989570	-0.4699151	-0.0240115
C	-4.4137735	-1.6539391	-0.2594195
C	-3.0377443	-1.3588984	-0.2084445
C	-2.9089899	0.0092650	0.0590957
N	-4.1805519	0.5163903	0.1652684
H	-4.3751237	1.4884004	0.3570266
H	-6.1562934	-0.2653974	0.0202663
H	-4.8641230	-2.6163603	-0.4445860
H	-2.2275678	-2.0565290	-0.3473626
C	-1.7619389	0.8929702	0.2308888
O	-1.9358745	2.1164180	0.4883889
C	-0.4612170	0.3209628	0.0973258
C	0.7429545	1.1108036	0.2791012
H	-0.3841272	-0.7318329	-0.1356671
H	0.5997132	2.1438393	0.5710582
C	2.0363593	0.6370569	0.1155590
C	3.1551126	1.5189232	0.3560437
C	2.3474856	-0.7151135	-0.2871277
C	4.4492875	1.0923999	0.2171871
H	2.9541648	2.5398512	0.6570882
C	3.6497006	-1.1356210	-0.4271196
H	1.5503332	-1.4168520	-0.4871328
C	4.6822263	-0.2338748	-0.1725483
H	5.2882660	1.7514455	0.4004870
H	3.8863850	-2.1480143	-0.7289725
F	5.9618271	-0.6530530	-0.3061457

Triplet state minimum: 3d-anti

C	-4.1723020	-1.8833433	-0.3183572
C	-5.0689629	-0.8475287	-0.1047469
C	-4.3119613	0.3144005	0.1460762
C	-2.9651567	-0.0288199	0.0811523
N	-2.9131128	-1.3824255	-0.2072564
H	-2.0779442	-1.9360638	-0.3050082
H	-4.3391262	-2.9253289	-0.5367253
H	-6.1438041	-0.9312188	-0.1304376
H	-4.6797170	1.3063957	0.3513660
C	-1.8087662	0.8452066	0.2672780
O	-1.9787284	2.0560237	0.5634953
C	-0.4892031	0.3090587	0.1019040
C	0.6891746	1.1351190	0.2849760
H	-0.3653071	-0.7302270	-0.1693322
H	0.5088851	2.1654488	0.5648077
C	1.9948702	0.7062788	0.1282236
C	3.0828855	1.6343181	0.3412743
C	2.3599242	-0.6425172	-0.2447262
C	4.3889507	1.2578268	0.1970293
H	2.8456004	2.6531264	0.6224496
C	3.6739773	-1.0127732	-0.3871496
H	1.5915542	-1.3826944	-0.4171584
C	4.6899443	-0.0706895	-0.1689448
H	5.1906801	1.9657460	0.3599130
H	3.9314761	-2.0257710	-0.6668601
Cl	6.3661692	-0.5495481	-0.3532423

Triplet state minimum: 3e-anti

C	-4.0976239	-2.0525162	-0.3180274
C	-5.0357172	-1.0506176	-0.1211760
C	-4.3267481	0.1416393	0.1278511
C	-2.9671358	-0.1495590	0.0779978
N	-2.8598289	-1.5020924	-0.2006090
H	-2.0029532	-2.0249876	-0.2788547
H	-4.2218953	-3.1019654	-0.5288412
H	-6.1062272	-1.1759858	-0.1567294
H	-4.7347384	1.1201486	0.3216568
C	-1.8472677	0.7695531	0.2694705
O	-2.0664357	1.9716602	0.5682294
C	-0.5067278	0.2875467	0.1045352
C	0.6365507	1.1575623	0.3020068
H	-0.3408759	-0.7430293	-0.1773866
H	0.4140106	2.1743545	0.6003943
C	1.9586477	0.7868264	0.1363656
C	3.0073131	1.7546897	0.3680563
C	2.3793765	-0.5377272	-0.2635920
C	4.3281783	1.4353688	0.2195611
H	2.7279268	2.7575612	0.6675823
C	3.7077997	-0.8514315	-0.4096672
H	1.6423947	-1.3051531	-0.4536080
C	4.6855056	0.1267377	-0.1704195
H	5.0960374	2.1760927	0.3981793
H	4.0018767	-1.8487251	-0.7086125
Br	6.5285572	-0.3159509	-0.3743631

Triplet state minimum: 3d-syn

C	-5.0920272	-0.6620584	-0.0237007
C	-4.3628859	-1.8119932	-0.2947456
C	-2.9994905	-1.4645191	-0.2456831
C	-2.9224047	-0.0996854	0.0567098
N	-4.2119675	0.3543199	0.1843186
H	-4.4431275	1.3128867	0.4014638
H	-6.1562024	-0.5009364	0.0340768
H	-4.7768065	-2.7860717	-0.5024078
H	-2.1637185	-2.1256546	-0.4090407
C	-1.8095224	0.8238445	0.2419137
O	-2.0292487	2.0337971	0.5215788
C	-0.4875138	0.3027283	0.0955247
C	0.6832705	1.1392540	0.2712839
H	-0.3708487	-0.7434351	-0.1503197
H	0.4977077	2.1727636	0.5373471
C	1.9932768	0.7161297	0.1246271
C	3.0754133	1.6509504	0.3325026
C	2.3648782	-0.6344846	-0.2320621
C	4.3845523	1.2778860	0.2001345
H	2.8331342	2.6722803	0.6008753
C	3.6816189	-1.0014834	-0.3636440
H	1.5999635	-1.3794092	-0.4007372
C	4.6919594	-0.0528603	-0.1497386
H	5.1821578	1.9914301	0.3601684
H	3.9436845	-2.0168303	-0.6312072
Cl	6.3724571	-0.5278022	-0.3190883

Triplet state minimum: 3e-syn

C	-5.0673999	-0.8637223	-0.0486544
C	-4.2917618	-1.9912979	-0.2819700
C	-2.9433957	-1.5897439	-0.2315977
C	-2.9221253	-0.2151632	0.0336113
N	-4.2294135	0.1915704	0.1377680
H	-4.4992612	1.1455893	0.3286778
H	-6.1374909	-0.7427327	-0.0040088
H	-4.6656513	-2.9861492	-0.4655994
H	-2.0811833	-2.2222218	-0.3686386
C	-1.8476593	0.7547642	0.2083757
O	-2.1169133	1.9611393	0.4578105
C	-0.5046670	0.2816644	0.0907103
C	0.6299467	1.1633441	0.2786911
H	-0.3445970	-0.7628302	-0.1373197
H	0.4010793	2.1854528	0.5549533
C	1.9566603	0.7969300	0.1314637
C	2.9986174	1.7712561	0.3608750
C	2.3849476	-0.5308603	-0.2463387
C	4.3227915	1.4546850	0.2292740
H	2.7136308	2.7771700	0.6453662
C	3.7161928	-0.8415964	-0.3778765
H	1.6519489	-1.3031356	-0.4332843
C	4.6874729	0.1433490	-0.1420395
H	5.0858530	2.2007627	0.4074267
H	4.0156354	-1.8418481	-0.6619574
Br	6.5352423	-0.2953757	-0.3249414