Electronic Supplementary Material (ESI) for Photochemical & Photobiological Sciences.

Supporting Information for:

The Electronic Transitions of Analogs of Red Wine Pyranoanthocyanin Pigments

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Contents:

Table S1. Optimized Cartesian coordinates (Å) for compound **1** using the MP2/def2-TZVP (a) method in gas phase and by B3-LYP in acetonitrile (b).

(a)

C	-3.2124075	3.2149941	0.0135623
C	-2.0458967	3.9866710	-0.0230383
C	-3.1696923	1.8163535	0.0432492
C	-0.8266044	3.3344509	-0.0286483
C	1.5233240	3.4708166	-0.0804583
O	0.3139255	4.0814060	-0.0581539
C	1.6504170	2.1056787	-0.0711139
C	2.4397720	5.6895333	-0.6866286
C	4.7587249	6.2153288	-0.2663205
C	3.5048130	6.5792203	-0.7550277
C	4.9467415	4.9530962	0.2956610
C	2.6306147	4.4153776	-0.1329068
C	3.8912161	4.0524962	0.3629149
C	-1.9359758	1.1997964	0.0375936
C	0.5044340	1.2791593	-0.0142608
C	-0.7446335	1.9372253	0.0027582
C	0.4997176	-0.1156873	-0.0012849
O	-1.8821659	-0.1623980	0.0721856
C	-0.6974122	-0.8175498	0.0511728
C	-2.0957301	-2.8513030	-0.0655519
C	0.2870519	-3.0811438	0.2517530
C	-0.8324057	-2.2429378	0.0788314
C	0.1565343	-4.4516226	0.2735722
C	-2.2334820	-4.2211322	-0.0494167
C	-1.1103343	-5.0720858	0.1177312
N	-1.2416028	-6.4155461	0.1311814
O	-4.4436951	3.7648034	0.0236987
C	-0.0748622	-7.2624633	0.3149179
C	-2.5548727	-7.0218380	-0.0126275
H	0.3971027	-7.0849512	1.2852228
H	0.6636930	-7.0930755	-0.4727361
H	-0.3861572	-8.3024726	0.2713578
H	-3.2241838	-6.7158041	0.7958552
H	-2.4479808	-8.1023799	0.0230016
H	-3.0113420	-6.7536224	-0.9689593
H	-4.3800065	4.7308669	0.0016803
H	-4.0890672	1.2449252	0.0735776
H	-2.0808353	5.0705164	-0.0418723
H	2.6416157	1.6767465	-0.1363483
H	1.4295896	-0.6647703	-0.0481334
H	1.4682285	5.9695221	-1.0747378
H	5.5848276	6.9149382	-0.3164556
H	3.3570718	7.5593590	-1.1929362
H	5.9157068	4.6742195	0.6925626

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H     4.0365034    3.0875725    0.8352222
H    -2.9765811   -2.2366422   -0.2026268
H    -3.2224909   -4.6413807   -0.1705928
H     1.2752922   -2.6620824    0.3996472
H     1.0435004   -5.0521846    0.4219259
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(b)

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C    -3.2049187    3.2069103   -0.1566286
C    -2.0389177    3.9827957   -0.1598571
C    -3.1645829    1.8075656   -0.1077852
C    -0.8243627    3.3298212   -0.1127126
C     1.5411144    3.4647099   -0.0818270
O     0.3224481    4.0641834   -0.1161844
C     1.6615915    2.1048435   -0.0328680
C     2.3872927    5.7990328   -0.2655354
C     4.7492493    6.2755615   -0.1817657
C     3.4329229    6.7113899   -0.3008589
C     5.0154937    4.9167748   -0.0243502
C     2.6445891    4.4281541   -0.1103920
C     3.9762223    4.0003665    0.0119342
C    -1.9317490    1.1964359   -0.0604247
C     0.5097755    1.2793078   -0.0156150
C    -0.7419886    1.9346401   -0.0608514
C     0.5123787   -0.1166305    0.0339464
O    -1.8670591   -0.1622677   -0.0107838
C    -0.6805135   -0.8227359    0.0369027
C    -2.0948929   -2.8606824   -0.0059069
C     0.2917530   -3.1041089    0.2141078
C    -0.8247752   -2.2501093    0.0818533
C     0.1568751   -4.4689909    0.2558412
C    -2.2457567   -4.2246939    0.0286835
C    -1.1219073   -5.0860777    0.1611965
N    -1.2619282   -6.4305614    0.1963528
O    -4.4301156    3.7686369   -0.2009050
C    -0.0954193   -7.2951848    0.3395797
C    -2.5825405   -7.0420824    0.0911656
H     0.4330381   -7.0963815    1.2757945
H     0.6033342   -7.1594947   -0.4899300
H    -0.4216817   -8.3306153    0.3452845
H    -3.2341132   -6.7243932    0.9095248
H    -2.4770432   -8.1215808    0.1391018
H    -3.0639009   -6.7862013   -0.8565953
H    -4.3702900    4.7339004   -0.2318131
H    -4.0783935    1.2308118   -0.1064631
H    -2.0840521    5.0628997   -0.1985421
H     2.6400476    1.6517714   -0.0144125
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H	1.4482156	-0.6515071	0.0609872
H	1.3705877	6.1509200	-0.3624595
H	5.5635506	6.9886365	-0.2101717
H	3.2181383	7.7653653	-0.4230060
H	6.0364630	4.5704555	0.0722717
H	4.2100745	2.9531443	0.1418856
H	-2.9781843	-2.2464821	-0.1089835
H	-3.2408948	-4.6347276	-0.0473655
H	1.2884598	-2.6931235	0.2947111
H	1.0463660	-5.0704016	0.3638695

Table S2. Optimized Cartesian coordinates (Å) for compound **2** using the MP2/def2-TZVP(a) method in gas phase and by B3-LYP in acetonitrile (b).

(a)

C	-1.9549352	4.1597652	-0.3930560
C	-0.7203481	3.5519239	-0.2630579
C	-0.6002257	2.1638659	-0.1152909
C	-1.7692071	1.3892573	-0.1063773
C	-3.0170307	1.9619381	-0.2342018
C	-3.0981083	3.3522670	-0.3762212
O	0.3981427	4.3305755	-0.2695169
C	1.6221658	3.7655117	-0.1503517
C	1.7860566	2.4089856	-0.0175127
C	0.6634346	1.5539422	0.0159317
O	-4.3416944	3.8567332	-0.4944024
C	3.5634494	6.8755750	-0.9208258
C	4.7868127	6.5887182	-0.3166950
C	4.9659888	5.3791698	0.3537072
C	2.5192571	5.9612514	-0.8597131
C	2.7029192	4.7386399	-0.1971905
C	3.9327398	4.4530545	0.4139881
C	0.6974644	0.1620159	0.1508385
O	-1.6758677	0.0360770	0.0297041
C	-0.4757365	-0.5732075	0.1571325
C	-0.5723623	-2.0062827	0.2941854
C	0.5829354	-2.7792549	0.4623997
C	0.4970519	-4.1597015	0.6002061
C	-1.8338280	-2.6295584	0.2580136
C	-1.9268688	-4.0066239	0.4140279
C	-0.7615168	-4.7954045	0.5826987
O	-0.8032277	-6.1148698	0.8369615
C	-1.6014527	-6.9543983	-0.0214176
O	1.6601690	-4.8146869	0.8086615
O	-3.0907043	-4.6884323	0.4696933
H	-2.0209481	5.2371422	-0.4991634
H	-3.9198101	1.3639779	-0.2245880

H	2.7901499	2.0090629	0.0308018
H	-4.3078280	4.8202618	-0.5871994
H	3.4238046	7.8149714	-1.4425773
H	5.5962022	7.3078529	-0.3625217
H	5.9098536	5.1619392	0.8394916
H	1.5723438	6.1804746	-1.3375263
H	4.0687860	3.5312513	0.9679963
H	1.6421429	-0.3528530	0.2510919
H	1.5769576	-2.3519444	0.4885838
H	-2.7237921	-2.0301147	0.1425401
H	-2.6066916	-7.0631520	0.3760354
H	-1.0944602	-7.9169769	-0.0374773
H	-1.6409758	-6.5397020	-1.0296229
C	1.8707851	-6.0591101	0.1200437
C	-4.2922913	-3.9297039	0.3573120
H	1.4991727	-6.8958649	0.7057049
H	2.9480413	-6.1381642	-0.0075586
H	1.3873191	-6.0416661	-0.8589031
H	-5.1008033	-4.6511160	0.4336989
H	-4.3437755	-3.4203187	-0.6078166
H	-4.3696559	-3.2030937	1.1693354

(b)

C	-1.9444367	4.1531910	-0.4687347
C	-0.7193105	3.5450874	-0.3030106
C	-0.6020084	2.1587451	-0.1352568
C	-1.7720461	1.3855724	-0.1423018
C	-3.0143463	1.9525204	-0.3055626
C	-3.0881711	3.3428237	-0.4675897
O	0.4073408	4.3083813	-0.2958885
C	1.6331321	3.7533028	-0.1439700
C	1.7873334	2.4023707	0.0188212
C	0.6583879	1.5545747	0.0335919
O	-4.3206625	3.8604448	-0.6221701
C	3.5088267	6.9509084	-0.7610043
C	4.7817042	6.6151136	-0.3075254
C	5.0216719	5.3430921	0.2081498
C	2.4787139	6.0234287	-0.7015169
C	2.7130243	4.7377140	-0.1907020
C	3.9985946	4.4097513	0.2667301
C	0.6924145	0.1565930	0.1956292
O	-1.6703733	0.0376896	0.0156159
C	-0.4730031	-0.5698300	0.1840689
C	-0.5868580	-2.0147396	0.3448347
C	0.5550314	-2.8040995	0.4924744
C	0.4465468	-4.1807147	0.6469857

C	-1.8533066	-2.6204352	0.3523891
C	-1.9701058	-3.9921284	0.5208297
C	-0.8150529	-4.7939667	0.6664311
O	-0.9004782	-6.1250977	0.9274151
C	-1.4630896	-6.9736816	-0.0975170
O	1.6085803	-4.8675508	0.8371402
O	-3.1502117	-4.6492754	0.6001633
H	-2.0169411	5.2251740	-0.5941293
H	-3.9117219	1.3508417	-0.3092913
H	2.7763289	1.9834001	0.1155892
H	-4.2866585	4.8217147	-0.7297839
H	3.3180971	7.9372948	-1.1639505
H	5.5830744	7.3417454	-0.3524115
H	6.0069615	5.0801605	0.5708284
H	1.4958136	6.2908199	-1.0624515
H	4.2000382	3.4346015	0.6878936
H	1.6374266	-0.3437454	0.3323836
H	1.5503505	-2.3857585	0.4804074
H	-2.7364381	-2.0131099	0.2492578
H	-2.5233326	-6.7708538	-0.2347863
H	-1.3173144	-7.9932198	0.2510890
H	-0.9294234	-6.8272698	-1.0391561
C	1.8450244	-6.0596283	0.0629749
C	-4.3659409	-3.9063700	0.4634967
H	1.3856373	-6.9283509	0.5301485
H	2.9258261	-6.1823435	0.0302196
H	1.4619639	-5.9386862	-0.9524087
H	-5.1663163	-4.6359851	0.5530406
H	-4.4198682	-3.4201518	-0.5134373
H	-4.4604293	-3.1600647	1.2559573

Table S3. Optimized Cartesian coordinates (Å) for compound **3** using the MP2/def2-TZVP (a) method in gas phase and by B3-LYP in acetonitrile (b).

(a)

C	-2.1141525	3.4459062	0.2353355
C	-0.9357717	2.7405579	0.0825906
C	-0.9104597	1.3395023	0.1181249
C	-2.1207111	0.6555726	0.3096878
C	-3.3145960	1.3264899	0.4656595
C	-3.2995065	2.7260517	0.4275072
O	0.2244109	3.4324160	-0.0983940
C	1.3929880	2.7732902	-0.2669010
C	1.4594208	1.4010275	-0.2611044
C	0.2957282	0.6322449	-0.0517130
O	-4.4929933	3.3280697	0.5874615
C	3.4073606	5.7897386	-1.2011404

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C     4.6963579    5.3657766   -0.8805563
C     4.8985818    4.0939814   -0.3454570
C     2.3205728    4.9502130   -0.9920909
C     2.5243288    3.6658922   -0.4660563
C     3.8210590    3.2422460   -0.1392434
C     0.2286579   -0.7681158   -0.0301662
O    -2.1209674   -0.7074350    0.3506502
C    -0.9778990   -1.4064960    0.1805423
C    -1.1743615   -2.8367554    0.2268554
C    -0.0902930   -3.7021814    0.4325254
C    -0.2711119   -5.0766712    0.4634998
C    -2.4609688   -3.3848930    0.0609839
C    -2.6428034   -4.7515777    0.0844867
C    -1.5529020   -5.6142302    0.2816022
O    -1.8407828   -6.9234202    0.2845704
C    -0.7589962   -7.8388449    0.4675116
H    -2.1051469    4.5301589    0.2097658
H    -4.2464730    0.7964893    0.6190242
H     2.4133688    0.9260591   -0.4475180
H    -4.3942765    4.2909660    0.5508488
H     3.2491323    6.7774960   -1.6176312
H     5.5401856    6.0264176   -1.0413567
H     5.8975682    3.7692987   -0.0795833
H     1.3208755    5.2758943   -1.2518141
H     3.9830864    2.2699695    0.3120288
H     1.1135740   -1.3644244   -0.2045316
H     0.9038668   -3.3082820    0.6090421
H     0.5831850   -5.7161136    0.6386765
H    -3.3107277   -2.7345560   -0.1035625
H    -3.6250078   -5.1883583   -0.0533938
H    -0.0223401   -7.7313108   -0.3311741
H    -1.2053689   -8.8276683    0.4243475
H    -0.2856918   -7.6903918    1.4400594
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(b)

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C    -2.0871343    3.4141893    0.1832451
C    -0.9177290    2.7173367    0.0482939
C    -0.8904925    1.3277928    0.0790039
C    -2.0869422    0.6382446    0.2506791
C    -3.2776482    1.2898763    0.3893571
C    -3.2620729    2.6840405    0.3532929
O     0.2322771    3.3803467   -0.1124860
C     1.3941272    2.7494566   -0.2637710
C     1.4844843    1.4014399   -0.2602867
C     0.3141410    0.6299423   -0.0741008
O    -4.4332681    3.2874299    0.4904724
C     3.3628152    5.8209508   -1.1146169
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C	4.6501963	5.4121186	-0.8168543
C	4.8763838	4.1370193	-0.3275320
C	2.3012695	4.9594352	-0.9234953
C	2.5239009	3.6741332	-0.4433984
C	3.8200705	3.2701466	-0.1431362
C	0.2654367	-0.7709977	-0.0453806
O	-2.0552457	-0.6993293	0.2813880
C	-0.9322365	-1.3926478	0.1410864
C	-1.1459950	-2.8346538	0.2080057
C	-0.0774353	-3.7191194	0.2823825
C	-0.2732013	-5.0808418	0.3503565
C	-2.4407761	-3.3626545	0.2040321
C	-2.6489873	-4.7136381	0.2664449
C	-1.5664771	-5.5890391	0.3422895
O	-1.8638371	-6.8822442	0.4054630
C	-0.8388464	-7.8504897	0.4902438
H	-2.0962378	4.4857978	0.1594186
H	-4.1973391	0.7578889	0.5218401
H	2.4262414	0.9226419	-0.4160491
H	-4.3608679	4.2302931	0.4573954
H	3.1843064	6.8084234	-1.4945788
H	5.4741273	6.0849955	-0.9609001
H	5.8723234	3.8204018	-0.0845623
H	1.3073859	5.2831299	-1.1581841
H	4.0095714	2.2928640	0.2539134
H	1.1582996	-1.3403313	-0.1772452
H	0.9316164	-3.3603746	0.3025930
H	0.5780511	-5.7254633	0.4134110
H	-3.2887175	-2.7115834	0.1462753
H	-3.6428826	-5.1164974	0.2595231
H	-0.1951338	-7.8096240	-0.3793943
H	-1.3356165	-8.8062632	0.5255899
H	-0.2519055	-7.7145428	1.3899753

Table S4. Optimized Cartesian coordinates (Å) for compound **4** using the MP2/def2-TZVP (a) method in gas phase and by B3-LYP in acetonitrile (b).

(a)

C	-1.9899491	3.2951711	0.2564348
C	-0.8267359	2.5735693	0.0969460
C	-0.8204483	1.1696361	0.1318462
C	-2.0375222	0.5020588	0.3312711
C	-3.2221100	1.1936582	0.4948616
C	-3.1850551	2.5931276	0.4569492
O	0.3457463	3.2450598	-0.0895638
C	1.5021366	2.5709212	-0.2641955
C	1.5474960	1.1959739	-0.2602040

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C     0.3745498    0.4482138   -0.0449684
O    -4.2872794    3.3495067    0.6105044
C     3.5645671    5.5630863   -1.1685946
C     4.8490997    5.1039231   -0.8797177
C     5.0326683    3.8162849   -0.3767116
C     2.4628221    4.7435485   -0.9591433
C     2.6476435    3.4431759   -0.4656154
C     3.9405971    2.9837213   -0.1714130
C     0.2867425   -0.9545400   -0.0196127
O    -2.0593463   -0.8596470    0.3746907
C    -0.9243650   -1.5718626    0.2010851
C    -1.1331142   -3.0062583    0.2568659
C    -0.0612860   -3.8674300    0.5400450
C    -0.2662275   -5.2380471    0.5794400
C    -2.4064261   -3.5472967    0.0252896
C    -2.5890518   -4.9226543    0.0596984
C    -1.5281841   -5.7924507    0.3333274
C    -1.7258367   -7.2781151    0.3450077
H    -1.9918832    4.3780260    0.2351947
H    -4.1492622    0.6536367    0.6528753
H     2.4918876    0.7042944   -0.4504639
H    -5.0662659    2.7913701    0.7521386
H     3.4216460    6.5633360   -1.5598855
H     5.7045618    5.7494438   -1.0401156
H     6.0285295    3.4645030   -0.1347324
H     1.4661852    5.0976420   -1.1920893
H     4.0907125    1.9981303    0.2540482
H     1.1601145   -1.5672653   -0.1969430
H     0.9198243   -3.4690345    0.7716686
H     0.5657975   -5.8931183    0.8168217
H    -3.2412122   -2.8939325   -0.1966867
H    -3.5760251   -5.3321028   -0.1285842
H    -2.7753712   -7.5378117    0.4814868
H    -1.1463424   -7.7458475    1.1420237
H    -1.3940280   -7.7136042   -0.6012802
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(b)

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C    -1.9835581    3.2891191    0.2271953
C    -0.8200711    2.5684632    0.0920431
C    -0.8094810    1.1662051    0.1395251
C    -2.0287296    0.4983313    0.3203098
C    -3.2164851    1.1823007    0.4594713
C    -3.1797121    2.5827838    0.4131713
O     0.3559059    3.2308209   -0.0880767
C     1.5236076    2.5629023   -0.2344735
C     1.5737812    1.1950478   -0.1985030
C     0.3924025    0.4467265   -0.0022448
```

O	-4.2950865	3.3237819	0.5452392
C	3.5424325	5.5958837	-1.1461592
C	4.8371657	5.1505230	-0.8918312
C	5.0465701	3.8596731	-0.4109846
C	2.4594969	4.7584571	-0.9215168
C	2.6627159	3.4535367	-0.4483294
C	3.9698141	3.0137994	-0.1924438
C	0.3150060	-0.9591602	0.0389752
O	-2.0354321	-0.8616166	0.3628442
C	-0.8961106	-1.5788307	0.2205605
C	-1.1202955	-3.0179863	0.2657394
C	-0.0532961	-3.9078587	0.4716250
C	-0.2747200	-5.2722927	0.5042704
C	-2.4088410	-3.5453193	0.0979981
C	-2.6163720	-4.9153335	0.1248861
C	-1.5580831	-5.8046759	0.3281248
C	-1.7774528	-7.2905282	0.3469675
H	-1.9831192	4.3691041	0.1944031
H	-4.1474564	0.6501656	0.6015137
H	2.5154384	0.6906334	-0.3480368
H	-5.0752717	2.7649000	0.6708925
H	3.3762233	6.5973288	-1.5220024
H	5.6801884	5.8077027	-1.0642999
H	6.0503545	3.5140406	-0.2000761
H	1.4578075	5.1082905	-1.1278916
H	4.1467917	2.0221002	0.2012220
H	1.2051421	-1.5526835	-0.0964419
H	0.9490545	-3.5358406	0.6324100
H	0.5606670	-5.9402911	0.6770703
H	-3.2468940	-2.8829706	-0.0664153
H	-3.6190902	-5.3007793	-0.0142484
H	-2.8364300	-7.5381216	0.4159845
H	-1.2555856	-7.7524945	1.1876743
H	-1.3829922	-7.7458380	-0.5661411

Table S5. Optimized Cartesian coordinates (Å) for compound **5** using the MP2/def2-TZVP (a) method in gas phase and by B3-LYP in acetonitrile (b).

(a)

C	-2.0063420	2.5102157	-1.2794434
C	-0.8815391	1.8667630	-0.8108031
C	-0.9262173	0.5356403	-0.3644900
C	-2.1545705	-0.1403594	-0.4077870
C	-3.3017573	0.4740037	-0.8705345
C	-3.2151761	1.8032494	-1.3031069
O	0.3047098	2.5389274	-0.7944246
C	1.4266672	1.9430822	-0.3398801
C	1.4214340	0.6464650	0.1223019

C	0.2314720	-0.1038681	0.1141896
O	-4.2790678	2.4828917	-1.7672282
C	3.5443158	5.0304058	-0.4065753
C	4.8253934	4.4804486	-0.4377402
C	4.9893384	3.0954703	-0.4470763
C	2.4270666	4.2055927	-0.3847863
C	2.5912024	2.8118847	-0.3823975
C	3.8809637	2.2595967	-0.4163962
C	0.0967653	-1.4394137	0.5381367
O	-2.2285959	-1.4300385	0.0254623
C	-1.1277431	-2.0639586	0.4836911
C	-1.3819517	-3.4415562	0.8716218
C	-0.5491866	-4.0741862	1.8069289
C	-0.7839778	-5.3976451	2.1557836
C	-2.4529755	-4.1445519	0.2995365
C	-2.6708003	-5.4709443	0.6493715
C	-1.8390626	-6.1004143	1.5746125
H	-1.9698910	3.5357464	-1.6258056
H	-4.2395437	-0.0705330	-0.8886231
H	2.3381023	0.2284234	0.5154821
H	-5.0737593	1.9292359	-1.7446406
H	3.4157199	6.1062851	-0.3973196
H	5.6936395	5.1286557	-0.4607226
H	5.9835974	2.6665757	-0.4871358
H	1.4330086	4.6340015	-0.3510223
H	4.0191286	1.1853772	-0.4594579
H	0.2511339	-3.5251352	2.2897407
H	-0.1486702	-5.8801396	2.8889768
H	-3.0922855	-3.6593273	-0.4276030
H	-3.4902559	-6.0174741	0.1977876
H	-2.0153134	-7.1345719	1.8459433
H	0.9550238	-2.0048207	0.8754332

(b)

C	-2.0034866	2.5234680	-1.2290866
C	-0.8810842	1.8721890	-0.7744481
C	-0.9236449	0.5362146	-0.3483419
C	-2.1511411	-0.1390647	-0.3956017
C	-3.2987235	0.4759603	-0.8450304
C	-3.2108989	1.8122719	-1.2601908
O	0.3060017	2.5361042	-0.7393285
C	1.4394513	1.9403396	-0.3029602
C	1.4343538	0.6369957	0.1237052
C	0.2384135	-0.1105553	0.1101095
O	-4.2857672	2.4831670	-1.7119030
C	3.5521170	5.0151990	-0.7711042
C	4.8166249	4.5350931	-0.4416270

C	4.9756977	3.2027205	-0.0658656
C	2.4510201	4.1726630	-0.7266501
C	2.6002690	2.8285423	-0.3483771
C	3.8804506	2.3549154	-0.0186134
C	0.1141335	-1.4573014	0.5114030
O	-2.2068369	-1.4339759	0.0180091
C	-1.1036800	-2.0837590	0.4569566
C	-1.3714843	-3.4712468	0.8315958
C	-0.4196652	-4.2156136	1.5463626
C	-0.6751256	-5.5340289	1.8892795
C	-2.5848091	-4.0808397	0.4762118
C	-2.8321052	-5.4016981	0.8206809
C	-1.8800491	-6.1324435	1.5264764
H	-1.9633058	3.5525039	-1.5562865
H	-4.2379090	-0.0597730	-0.8742122
H	2.3460247	0.1808172	0.4743708
H	-5.0760022	1.9243910	-1.7054912
H	3.4227234	6.0492428	-1.0636576
H	5.6746428	5.1943605	-0.4780291
H	5.9567826	2.8232207	0.1885736
H	1.4750563	4.5585261	-0.9825811
H	4.0319192	1.3241966	0.2692472
H	0.5148010	-3.7666537	1.8527919
H	0.0649235	-6.0953584	2.4448781
H	-3.3276686	-3.5248399	-0.0774171
H	-3.7693295	-5.8622336	0.5359086
H	-2.0761989	-7.1628753	1.7948847
H	0.9835092	-2.0008416	0.8453583

Table S6. Optimized Cartesian coordinates (Å) for compound **6** using the MP2/def2-TZVP (a) method in gas phase and by B3-LYP in acetonitrile (b).

(a)

C	-2.1256475	2.7191734	0.2518354
C	-0.9608097	2.0009381	0.1175043
C	-0.9485103	0.5983081	0.1603547
C	-2.1671762	-0.0722575	0.3371596
C	-3.3562033	0.6091452	0.4740517
C	-3.3213880	2.0100728	0.4309859
O	0.2150686	2.6646765	-0.0585061
C	1.3834720	1.9994958	-0.2075436
C	1.4346217	0.6308230	-0.1759085
C	0.2543809	-0.1175770	0.0168021
O	-4.4382078	2.7486188	0.5597325
C	3.4021810	5.0382623	-1.0993609
C	4.6984095	4.5830363	-0.8718769
C	4.9087352	3.2843937	-0.4128882
C	2.3186736	4.2026252	-0.8711649

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C     2.5224322    2.8897571   -0.4204880
C     3.8314559    2.4407015   -0.1899230
C     0.1792921   -1.5250805    0.0536242
O    -2.1706969   -1.4327963    0.3786988
C    -1.0290517   -2.1450580    0.2374186
C    -1.2483646   -3.5871462    0.2911080
C    -0.1735161   -4.4649057    0.5026196
C    -0.3758746   -5.8335287    0.5466175
C    -2.5383031   -4.1161259    0.1280398
C    -2.7511862   -5.4846100    0.1646814
C    -1.6634897   -6.3157668    0.3740939
F    -1.8651453   -7.6486323    0.4160426
H    -2.1271552    3.7992203    0.2220108
H    -4.2867562    0.0753646    0.6125570
H     2.3761614    0.1266960   -0.3265296
H    -5.2186486    2.1883013    0.6771790
H     3.2350188    6.0457887   -1.4580018
H     5.5419858    5.2383592   -1.0483010
H     5.9139340    2.9310018   -0.2228184
H     1.3158247    4.5600326   -1.0575241
H     4.0105836    1.4426348    0.1860565
H     1.0709794   -2.1155303   -0.0844953
H     0.8264803   -4.0857563    0.6566352
H     0.4422786   -6.5193401    0.7185355
H    -3.3776116   -3.4573722   -0.0410767
H    -3.7382265   -5.9059433    0.0320624
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(b)

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C    -2.1218974    2.7185246    0.2909147
C    -0.9572247    2.0005103    0.1268386
C    -0.9461662    0.5964149    0.1575197
C    -2.1614593   -0.0745887    0.3575176
C    -3.3474386    0.6128342    0.5256486
C    -3.3147350    2.0128189    0.4912535
O     0.2125888    2.6752702   -0.0602295
C     1.3707435    2.0070299   -0.2395745
C     1.4209075    0.6312519   -0.2381991
C     0.2510939   -0.1198790   -0.0227770
O    -4.4182478    2.7652382    0.6485818
C     3.4077948    5.0137312   -1.1473297
C     4.6973622    4.5618449   -0.8691980
C     4.8929638    3.2739277   -0.3711509
C     2.3131507    4.1865207   -0.9323363
C     2.5100705    2.8855043   -0.4446106
C     3.8079533    2.4332108   -0.1611544
C     0.1670300   -1.5248301   -0.0001974
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O	-2.1790057	-1.4368788	0.3984545
C	-1.0413839	-2.1440175	0.2224559
C	-1.2504550	-3.5798961	0.2815768
C	-0.1832652	-4.4377243	0.5908643
C	-0.3786812	-5.8094366	0.6368957
C	-2.5218665	-4.1175266	0.0263842
C	-2.7203077	-5.4892874	0.0638871
C	-1.6447805	-6.3140287	0.3677034
F	-1.8343305	-7.6319942	0.4093165
H	-2.1269389	3.8014061	0.2732635
H	-4.2727024	0.0701354	0.6855817
H	2.3667844	0.1437242	-0.4319519
H	-5.1964525	2.2049554	0.7865083
H	3.2553049	6.0140922	-1.5347231
H	5.5473431	5.2133403	-1.0348783
H	5.8929017	2.9279626	-0.1376859
H	1.3127316	4.5346992	-1.1575947
H	3.9673022	1.4473276	0.2602238
H	1.0416373	-2.1346019	-0.1822641
H	0.7935117	-4.0372354	0.8351663
H	0.4261467	-6.4892368	0.8880200
H	-3.3487827	-3.4629886	-0.2185567
H	-3.6892010	-5.9281248	-0.1401646

Table S7. Optimized Cartesian coordinates (Å) for compound **7** using the MP2/def2-TZVP (a) method in gas phase and by B3-LYP in acetonitrile (b).

(a)

C	-2.1091035	2.9150348	0.2653257
C	-0.9363200	2.2087738	0.1091929
C	-0.9102370	0.8046214	0.1489026
C	-2.1192925	0.1211592	0.3501751
C	-3.3124122	0.7967679	0.5110244
C	-3.2947646	2.1972848	0.4673723
O	0.2273849	2.8937943	-0.0793821
C	1.3932054	2.2391760	-0.2515726
C	1.4572292	0.8626499	-0.2404417
C	0.2956554	0.1029487	-0.0241374
O	-4.4059817	2.9381681	0.6159268
C	3.4064024	5.2612352	-1.1597354
C	4.7002870	4.8144815	-0.8931954
C	4.9061596	3.5249204	-0.4034946
C	2.3173580	4.4279916	-0.9403815
C	2.5245257	3.1254599	-0.4602102
C	3.8271810	2.6780726	-0.1889842
C	0.2268639	-1.3051429	0.0068718
O	-2.1224321	-1.2415481	0.3963055
C	-0.9749946	-1.9339192	0.2269135

C	-1.1674179	-3.3755775	0.2860834
C	-0.0920201	-4.2192005	0.6060671
C	-0.2704995	-5.5925258	0.6466576
C	-2.4294287	-3.9284414	0.0176233
C	-2.6091709	-5.3022003	0.0524095
C	-1.5298605	-6.1387565	0.3654102
C	-1.7139924	-7.5553166	0.4042104
N	-1.8636644	-8.7185402	0.4356660
H	-2.1269271	3.9976973	0.2398691
H	-4.2324777	0.2452728	0.6711161
H	2.4078429	0.3821987	-0.4276762
H	-5.1794388	2.3720603	0.7576045
H	3.2465896	6.2626373	-1.5413279
H	5.5457659	5.4713205	-1.0608914
H	5.9095202	3.1823921	-0.1802461
H	1.3137358	4.7729096	-1.1561073
H	3.9958947	1.6912673	0.2263435
H	1.1088244	-1.9069648	-0.1667956
H	0.8767047	-3.8050790	0.8598798
H	0.5530310	-6.2479117	0.9043096
H	-3.2615170	-3.2825772	-0.2334165
H	-3.5782086	-5.7365943	-0.1632645

(b)

C	-2.1022169	2.9089130	0.2385304
C	-0.9317492	2.2021037	0.0989707
C	-0.9035746	0.7990628	0.1497345
C	-2.1153915	0.1170943	0.3388948
C	-3.3091536	0.7870145	0.4830669
C	-3.2890313	2.1883979	0.4335487
O	0.2360691	2.8754986	-0.0882661
C	1.4108282	2.2249190	-0.2359619
C	1.4774463	0.8552591	-0.1952123
C	0.3065048	0.0988832	0.0049870
O	-4.4108084	2.9156768	0.5708957
C	3.3872640	5.2869901	-1.1342908
C	4.6887007	4.8531946	-0.8937838
C	4.9168567	3.5589004	-0.4310157
C	2.3159053	4.4350774	-0.9114877
C	2.5376962	3.1272233	-0.4539807
C	3.8519086	2.6980805	-0.2148320
C	0.2450595	-1.3140106	0.0505319
O	-2.1049700	-1.2431101	0.3846865
C	-0.9546505	-1.9389365	0.2400231
C	-1.1607166	-3.3886993	0.2915198
C	-0.0891049	-4.2503478	0.5632466
C	-0.2824915	-5.6185901	0.6036681

C	-2.4353490	-3.9260471	0.0649435
C	-2.6355327	-5.2944236	0.0977473
C	-1.5581452	-6.1449720	0.3682637
C	-1.7614051	-7.5585813	0.4077962
N	-1.9257391	-8.6992731	0.4389549
H	-2.1151665	3.9887320	0.2033639
H	-4.2328384	0.2442478	0.6318098
H	2.4241684	0.3604508	-0.3439491
H	-5.1840182	2.3490927	0.7061527
H	3.2069167	6.2906798	-1.4972627
H	5.5227053	5.5224785	-1.0629447
H	5.9261270	3.2226898	-0.2318685
H	1.3087202	4.7755103	-1.1060730
H	4.0438760	1.7036955	0.1645206
H	1.1409623	-1.8983673	-0.0879107
H	0.8968298	-3.8581132	0.7669403
H	0.5456695	-6.2780847	0.8228548
H	-3.2692093	-3.2741078	-0.1503926
H	-3.6189521	-5.7042019	-0.0864201

Table S8. Optimized Cartesian coordinates (Å) for compound **8** using the MP2/def2-TZVP (a) method in gas phase and by B3-LYP in acetonitrile (b).

(a)

C	-1.9499346	2.8576331	-1.3480573
C	-0.8149738	2.2167458	-0.8910751
C	-0.8497606	0.8840255	-0.4530144
C	-2.0783179	0.2022919	-0.4880912
C	-3.2296212	0.8108425	-0.9363896
C	-3.1541718	2.1425298	-1.3662006
O	0.3657829	2.8959205	-0.8808838
C	1.4971757	2.3053756	-0.4428565
C	1.5029297	1.0041107	0.0084193
C	0.3170068	0.2497145	0.0079867
O	-4.3082204	2.6810115	-1.7945044
C	3.6002053	5.4019775	-0.4891440
C	4.8823862	4.8570947	-0.5501065
C	5.0513193	3.4732136	-0.5857954
C	2.4861648	4.5731156	-0.4642257
C	2.6556625	3.1802534	-0.4887177
C	3.9465660	2.6329485	-0.5520436
C	0.1933182	-1.0900763	0.4286557
O	-2.1388886	-1.0917812	-0.0593945
C	-1.0293990	-1.7170454	0.3858160
C	-1.2742642	-3.0974889	0.7773121
C	-0.4251862	-3.7317878	1.6976532
C	-0.6423085	-5.0542956	2.0534504

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C    -2.3563838   -3.8014491    0.2256865
C    -2.5779110   -5.1258047    0.5739664
C    -1.7135307   -5.7287116    1.4795842
N    -1.9430886   -7.1363703    1.8499412
H    -1.8947961    3.8865648   -1.6865834
H    -4.1767129    0.2857481   -0.9589950
H     2.4258586    0.5879445    0.3890923
H    -4.1755756    3.5992817   -2.0739628
H     3.4690727    6.4770434   -0.4587286
H     5.7478242    5.5088669   -0.5749909
H     6.0461544    3.0486418   -0.6484027
H     1.4914150    4.9971272   -0.4045584
H     4.0872622    1.5602241   -0.6169834
H     0.3846717   -3.1851292    2.1666694
H    -0.0082963   -5.5621996    2.7682111
H    -3.0109354   -3.3161889   -0.4875485
H    -3.3985637   -5.6936824    0.1555218
H     1.0581272   -1.6518741    0.7552965
O    -2.9266376   -7.6859316    1.3655041
O    -1.1314249   -7.6504304    2.6124872
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(b)

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C    -1.9488075    2.8635092   -1.3058704
C    -0.8163239    2.2178948   -0.8639956
C    -0.8481791    0.8839580   -0.4306066
C    -2.0770245    0.2043141   -0.4576335
C    -3.2300471    0.8122091   -0.8913369
C    -3.1538194    2.1470013   -1.3144192
O     0.3687076    2.8846583   -0.8508124
C     1.5085893    2.2987286   -0.4233201
C     1.5135953    0.9969541    0.0138539
C     0.3219941    0.2488915    0.0169855
O    -4.3033805    2.7039836   -1.7313475
C     3.5911413    5.4063209   -0.7668004
C     4.8741604    4.8992002   -0.5786038
C     5.0556792    3.5379840   -0.3431907
C     2.4927104    4.5609740   -0.7208917
C     2.6649489    3.1887380   -0.4795116
C     3.9629293    2.6872298   -0.2926657
C     0.2057824   -1.1002872    0.4325305
O    -2.1219014   -1.0900354   -0.0371622
C    -1.0076573   -1.7237790    0.3916949
C    -1.2611856   -3.1181917    0.7675120
C    -0.3645020   -3.8063831    1.5960563
C    -0.5969225   -5.1266694    1.9372509
C    -2.4044199   -3.7749656    0.2923329
C    -2.6432542   -5.0969966    0.6252419
```

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C    -1.7337293   -5.7539749    1.4429067
N    -1.9826859   -7.1592743    1.7986474
H    -1.9052360    3.8921349   -1.6374223
H    -4.1727541    0.2844917   -0.9086166
H     2.4294853    0.5510912    0.3667901
H    -4.1709227    3.6227803   -2.0063312
H     3.4456008    6.4633925   -0.9489444
H     5.7301769    5.5610263   -0.6172952
H     6.0517229    3.1382897   -0.2031222
H     1.5007998    4.9650597   -0.8630740
H     4.1285087    1.6324716   -0.1235969
H     0.5083543   -3.3121454    1.9975840
H     0.0867667   -5.6593495    2.5805574
H    -3.1017790   -3.2573444   -0.3495947
H    -3.5174215   -5.6102618    0.2543711
H     1.0799632   -1.6423651    0.7572256
O    -2.9985095   -7.6910833    1.3718793
O    -1.1611538   -7.7301807    2.5027453
```