ЖУРНАЛ СТРУКТУРНОЙ ХИМИИ

2019. Том 60, № 2 *Февраль* *DOI: 10.26902/JSC_id39181*

SUPPLEMENTARY MATERIALS TO:

UNRAVELLING THE COMPETENCE OF LEUCOCYANIDIN IN FREE RADICAL SCAVENGING: A THEORETICAL APPROACH BASED ON ELECTRONIC STRUCTURE CALCULATIONS

C. Augustine

Department of Chemistry, St. Berchmans College (Autonomous), Changanacherry, Kottayam, Kerala, India
E-mail: cyril.augustinev@gmail.com

Table S1

Internuclear bond distances calculated for leucocyanidin molecule using various functionals. All the values are in Å units and the basis set used in computational evaluation is 6-31G (*d,p*)

Bond	M05	M052X	M06	M06HF	M062X	M11	X-Ray Crystal Data
C1—C2	1.39001	1.38655	1.38716	1.38555	1.38756	1.38777	1.379
C2—C3	1.39792	1.39530	1.39542	1.39700	1.39675	1.39688	1.383
C3—C4	1.38904	1.38497	1.38583	1.38356	1.38592	1.38590	1.381
C4—C5	1.40185	1.39783	1.39883	1.39836	1.39944	1.39854	1.402
C1—C6	1.39924	1.39603	1.39605	1.39373	1.39728	1.39714	1.389
14C—15C	1.52448	1.52441	1.52031	1.53322	1.52707	1.52916	1.518
5C—16C	1.51280	1.51341	1.50936	1.52157	1.51495	1.51616	1.499
14C—22C	1.50351	1.50312	1.49842	1.51145	1.50450	1.50710	1.507
22C—24C	1.40058	1.39855	1.39826	1.39974	1.39938	1.39896	1.398
24C—25C	1.38406	1.3808	1.38121	1.37997	1.38179	1.38112	1.390
25C—26C	1.40662	1.40221	1.40268	1.40363	1.40417	1.40427	1.385
26C—27C	1.38836	1.38487	1.38565	1.38378	1.38598	1.38548	1.370
27C—28C	1.39304	1.38928	1.39019	1.38789	1.38984	1.38906	1.397
25C—32O	1.36681	1.37302	1.36812	1.37160	1.37098	1.37297	1.371
26C—33O	1.35138	1.35744	1.35286	1.35605	1.35607	1.35676	1.380
15C—16C	1.53131	1.52772	1.52581	1.53554	1.53063	1.53206	1.514
5C—6C	1.40171	1.39663	1.39879	1.39373	1.39764	1.39714	1.396
22C—28C	1.39304	1.38928	1.39019	1.38790	1.38984	1.38904	1.381
C4—O8	1.36868	1.37416	1.36977	1.37325	1.37237	1.37451	1.373
C2—O10	1.35325	1.35918	1.35412	1.35848	1.35778	1.35898	1.369
C6—13O	1.3479	1.35532	1.3504	1.35456	1.35487	1.35464	1.389
13O—14C	1.43238	1.43335	1.43082	1.42308	1.42924	1.43197	1.452
15C—17O	1.39896	1.40708	1.40000	1.40369	1.40393	1.40671	1.419
16C—19O	1.41459	1.42203	1.41526	1.41660	1.41766	1.42136	1.441
25C—32O	1.36681	1.37302	1.36812	1.37160	1.37098	1.37297	1.371
26C—33O	1.35138	1.35744	1.35286	1.35605	1.35607	1.35676	1.380

© Augustine C., 2019

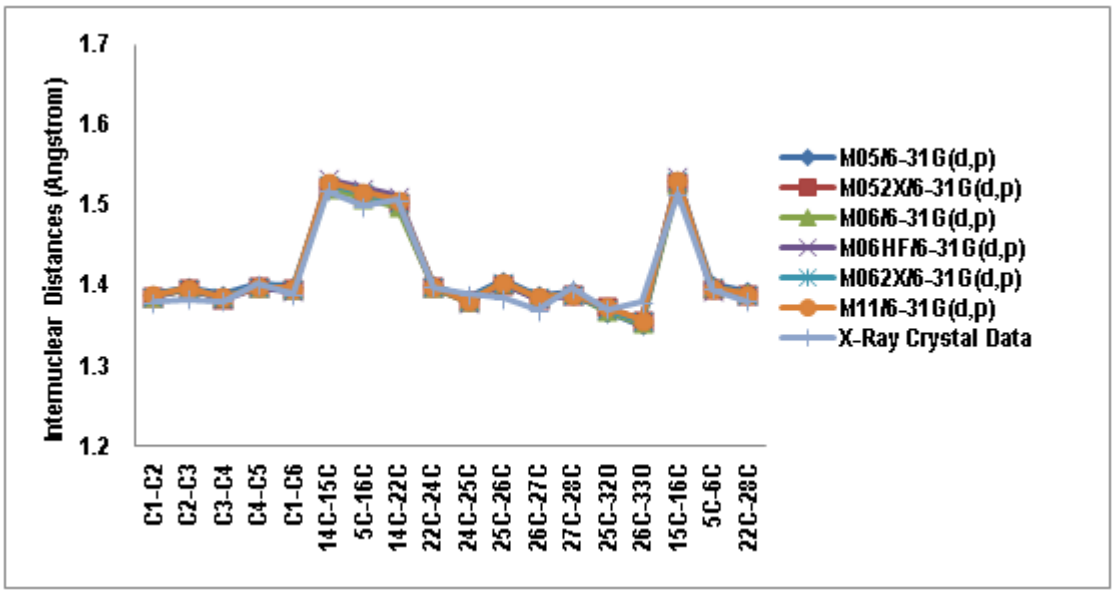

Fig. S2. Various internuclear distances in leucocyanidin calculated using different model chemistries and their comparison with the experimental values from X-ray Crystal data.

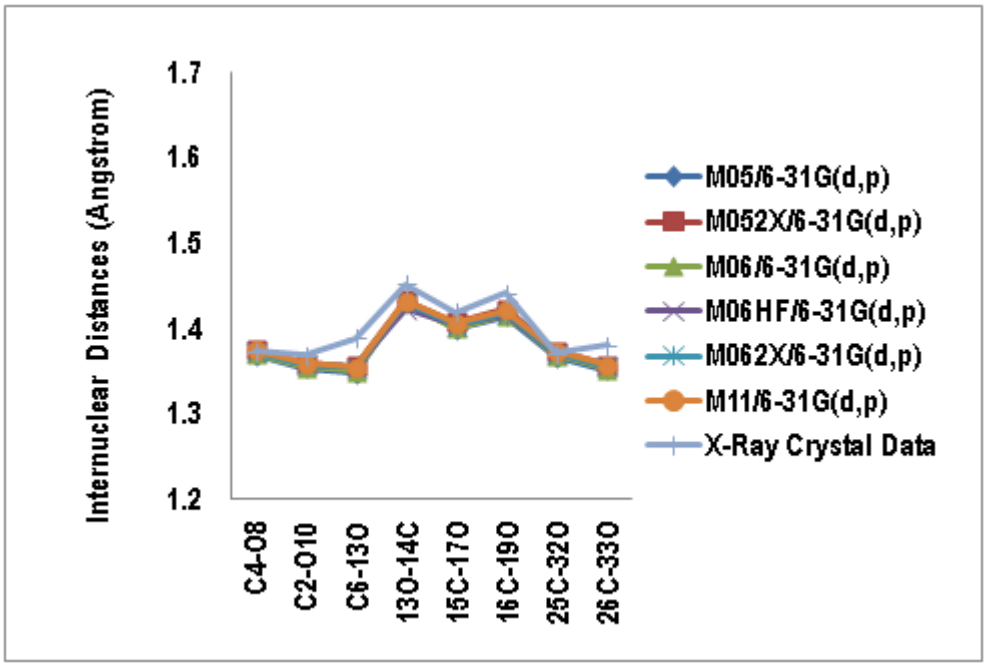

Fig. S3. Various internuclear distances in leucocyanidin calculated using different model chemistries and their comparison with the values from X-ray Crystal data.

Table S4

Chemical shifts (in ppm) *from various* ^{1}H *and* ^{13}C *resonances in leucocyanidin, theoretical prediction from the optimized molecular structures using various functionals in connection with* 6-31+G(*d*, *p*) *basis set*

Atom	M05	M052X	M06	M06HF	M062X	M11	Mean (ppm)
C1	96.88235	106.419275	91.0703	130.263125	104.103975	105.043125	105.6303583
C2	160.01335	170.606175	153.6073	192.508525	167.665175	166.922125	168.553775
C3	92.95115	103.938375	84.7909	126.548525	99.276075	101.613825	101.5198083
C4	158.10485	168.781975	150.5585	189.385325	165.214275	164.267025	166.0519917
C5	104.27095	114.321375	97.7316	139.554625	112.607775	112.031425	113.419625
C6	161.34545	173.224175	154.6273	194.303225	169.457475	169.355125	170.3854583
C14	81.83325	84.008875	76.7363	81.698625	81.805475	82.129125	81.36860833
C15	70.00965	72.678675	66.0868	68.386825	69.757375	70.590625	69.58499167
C16	67.81125	70.877275	62.69	68.617525	68.050175	69.270025	67.88604167
C22	132.96445	144.767175	125.4426	173.378425	142.905475	142.938025	143.7326917
C24	115.38925	131.300675	107.1993	162.487525	127.802375	128.848225	128.8378917
C25	143.90605	152.723275	137.9423	173.960825	151.573875	148.175725	151.3803417
C26	145.93115	158.497375	140.4195	184.222925	156.979175	154.256825	156.717825
C27	117.37835	127.717675	110.5421	156.884725	125.185075	125.521325	127.204875
C28	123.14435	136.594775	116.0537	163.077125	132.712475	134.006425	134.2648083
H7	6.085691667	6.286041667	6.220308333	7.332183333	6.760825	6.525508333	6.535093056
H9	5.809591667	6.369441667	5.604508333	7.175583333	6.183925	6.490608333	6.272276389
H11	4.034491667	4.263641667	3.968108333	5.057283333	4.421325	4.163408333	4.318043056
H12	4.094491667	4.234141667	3.920208333	4.981383333	4.325325	4.106908333	4.277076389
H18	3.950891667	3.828341667	3.927808333	3.777683333	3.921325	4.010308333	3.902726389
H20	5.098791667	4.784341667	5.126908333	4.209983333	4.905125	4.976408333	4.850259722
H21	3.681791667	4.096341667	4.060908333	4.112883333	4.052625	4.271108333	4.045943056
H23	4.334991667	4.661841667	4.294408333	4.765283333	4.481525	4.859208333	4.566209722
H29	8.216891667	7.844441667	8.088108333	8.839883333	8.176525	8.055508333	8.203559722
H30	7.178791667	7.316041667	7.095008333	7.241483333	7.462325	7.785208333	7.346476389
H31	7.343291667	7.152041667	7.061508333	8.069383333	7.357325	7.306008333	7.381593056
H34	3.846091667	4.396841667	3.951208333	5.520283333	4.569025	4.364908333	4.441393056
H35	5.319791667	6.043841667	5.011608333	8.327583333	5.938325	5.877908333	6.086509722
H36	2.675591667	2.855141667	2.989908333	2.895583333	2.799525	3.246908333	2.910443056

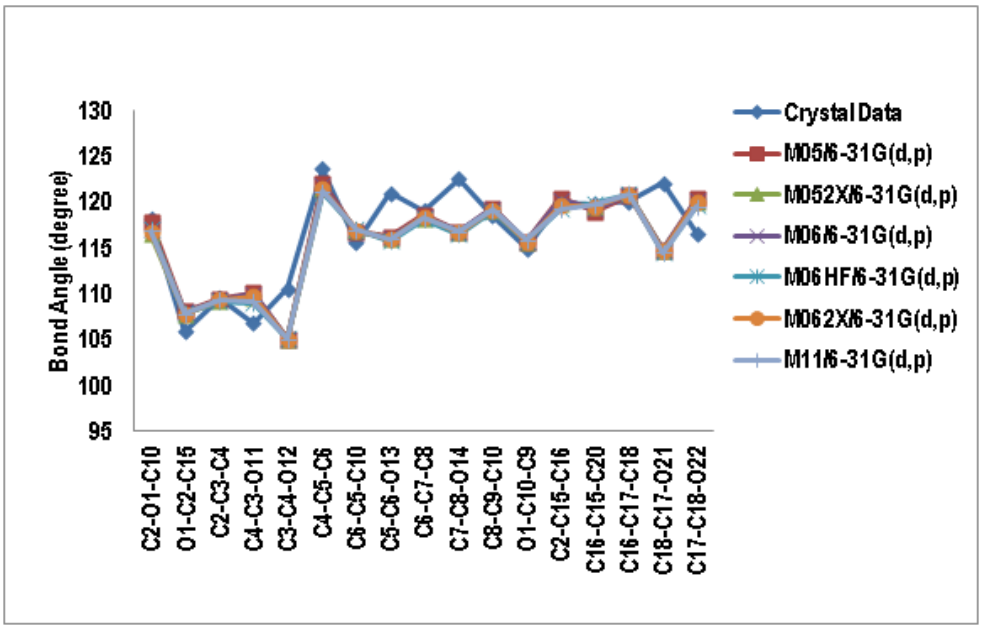

Fig. S5. Comparison of calculated bond angles in leucocyanidin with the experimental data.

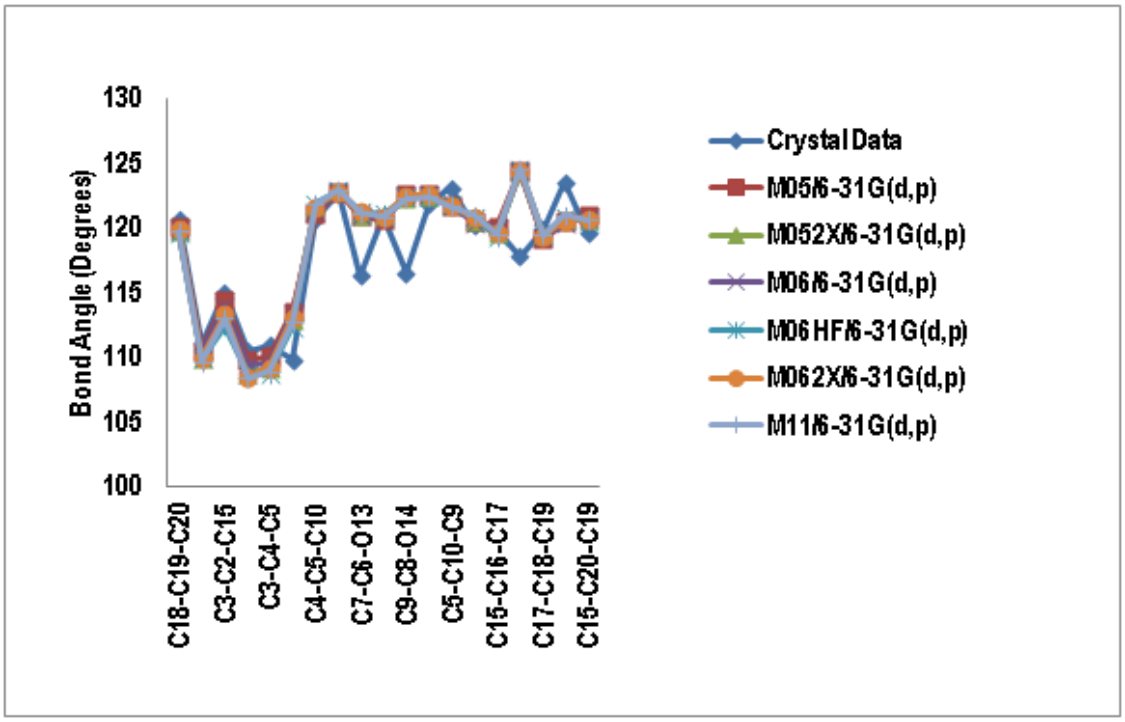

Fig. S6. Calculated bond angles in leucocyanidin using various model chemistries and their comparison with the experimental values.

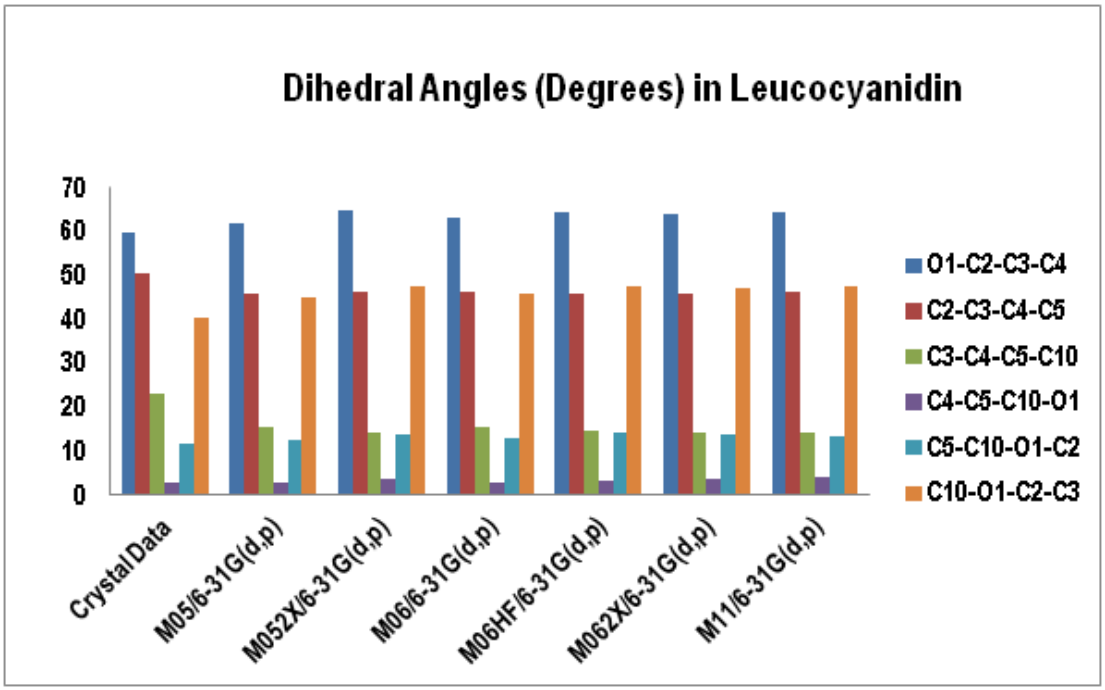

Fig. S7. Comparison of certain dihedral angles (calculated) in leucocyanidin with the experimental values from X-ray Crystal data.

Table S 8

Bond angles calculated for leucocyanidin molecule using various functionals. All the values are in degrees and the basis set used in computational evaluation is 6-31G (*d*, *p*).

Bond	Crystal Data	M05	M052X	M06	M06HF	M062X	M11
C2—O1—C10	118.2	117.93	116.556	117.117	117.143	116.852	116.946
O1—C2—C15	105.9	108.065	107.8	108.141	107.949	107.803	107.8
C2—C3—C4	109.6	109.471	109.224	109.373	109.227	109.4	109.391
C4—C3—O11	106.8	110.122	109.547	110.013	109.034	109.74	109.191
C3—C4—O12	110.6	105.112	105.103	105.115	105.204	105.106	105.059
C4—C5—C6	123.7	122.107	121.45	121.811	121.055	121.455	121.183
C6—C5—C10	115.6	116.834	116.88	116.859	117.057	116.971	117
C5—C6—O13	121	116.294	116.042	116.183	115.825	115.975	115.954
C6—C7—C8	119.1	118.606	118.292	118.508	118.227	118.433	118.309
C7—C8—O14	122.6	116.819	116.77	116.849	116.538	116.7	116.856
C8—C9—C10	118.6	119.361	119.149	119.348	119.017	119.227	119.238
O1—C10—C9	115	115.704	115.696	115.691	115.815	115.682	115.892
C2—C15—C16	120	120.461	119.81	120.308	119.278	119.686	119.252
C16—C15—C20	119.8	119.023	119.609	119.297	119.898	119.555	119.741
C16—C17—C18	120.1	120.774	120.928	120.832	120.94	120.844	120.91
C18—C17—O21	122.1	114.783	114.765	114.829	114.544	114.693	114.533
C17—C18—O22	116.6	120.376	119.996	120.298	119.643	120.11	119.599
C18—C19—C20	120.7	120.017	119.799	119.909	119.687	119.844	119.748
O1—C2—C3	111	110.546	109.86	110.485	109.877	109.969	109.628
C3—C2—C15	115	114.46	113.478	113.98	112.415	113.316	112.971
C2—C3—O11	110.5	109.793	108.74	109.424	108.651	108.471	108.386
C3—C4—C5	110.9	110.036	109.161	109.608	108.76	109.193	108.902
C5—C4—O12	109.8	113.545	112.852	113.356	112.314	113.046	112.685
C4—C5—C10	120.7	121.054	121.656	121.323	121.866	121.558	121.791
C5—C6—C7	122.7	122.805	122.945	122.852	122.855	122.808	122.91
C7—C6—O13	116.3	120.901	121.013	120.964	121.319	121.217	121.135
C7—C8—C9	120.9	120.636	120.933	120.706	121.055	120.822	120.867
C9—C8—O14	116.5	122.542	122.293	122.441	122.405	122.475	122.273
O1—C10—C5	121.9	122.556	122.523	122.602	122.404	122.597	122.447
C5—C10—C9	123.1	121.739	121.779	121.705	121.779	121.718	121.657
C2—C15—C20	120.2	120.513	120.568	120.379	120.807	120.74	120.988
C15—C16—C17	119.8	120.104	119.574	119.857	119.354	119.679	119.51
C16—C17—O21	117.8	124.443	124.307	124.339	124.516	124.463	124.557
C17—C18—C19	119.9	119.116	119.407	119.277	119.559	119.374	119.439
C19—C18—O22	123.5	120.508	120.597	120.425	120.799	120.515	120.962
C15—C20—C19	119.6	120.964	120.682	120.827	120.56	120.702	120.652

Table S 9

Comparison of the dihedral angles calculated for leucocyanidin molecule with the available experimental data. All the values are in degrees and the basis set used in computational evaluation is 6-31G (*d*, *p*)

Bonds	Crystal Data	M05	M052X	M06	M06HF	M062X	M11
O1—C2—C3—C4	59.7	61.619	64.576	62.964	64.23	63.99	64.443
C2—C3—C4—C5	50.2	45.598	46.111	46.044	45.82	45.758	46.059
C3—C4—C5—C10	23	15.388	14.283	15.255	14.478	14.236	14.01
C4—C5—C10—O1	2.6	2.763	3.519	2.924	3.24	3.478	4.012
C5—C10—O1—C2	11.5	12.618	13.885	12.94	14.113	13.768	13.494
C10—O1—C2—C3	40.1	44.892	47.624	45.803	47.551	47.193	47.316