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Supplementary Information

Binding of ellagic acid and urolithin metabolites to CK2 protein, based on the ONIOM method and molecular docking calculations

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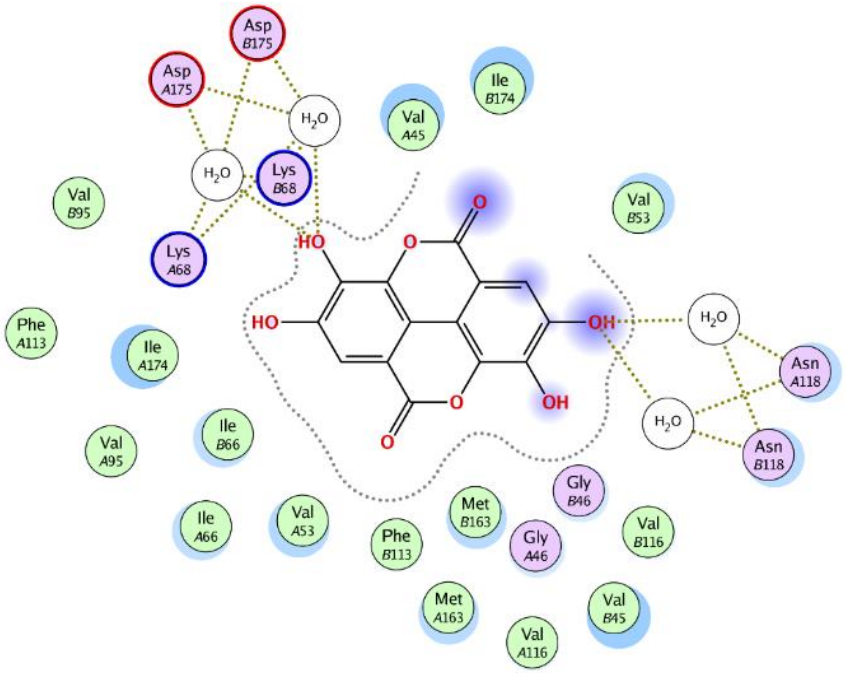
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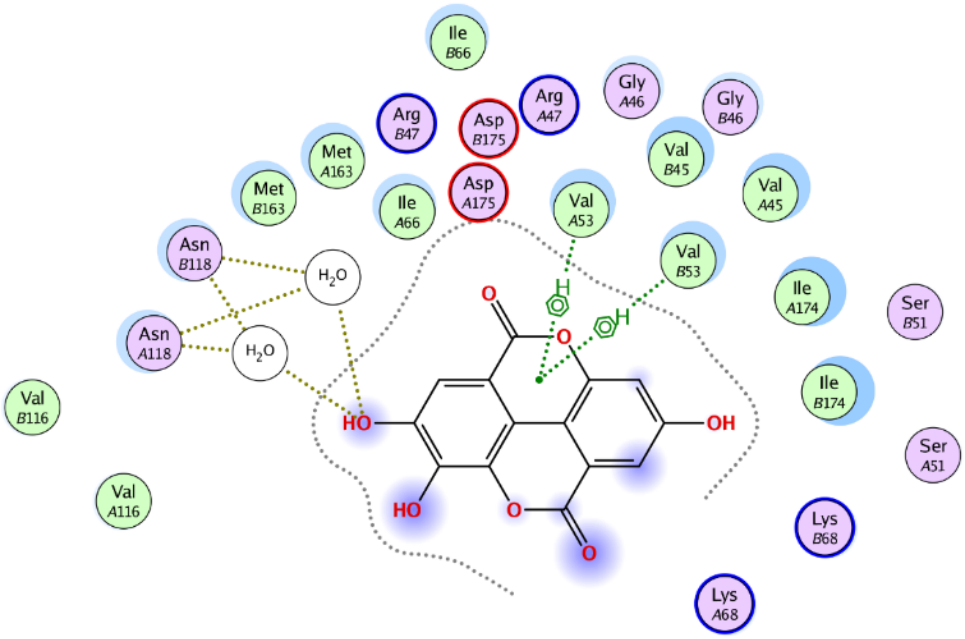
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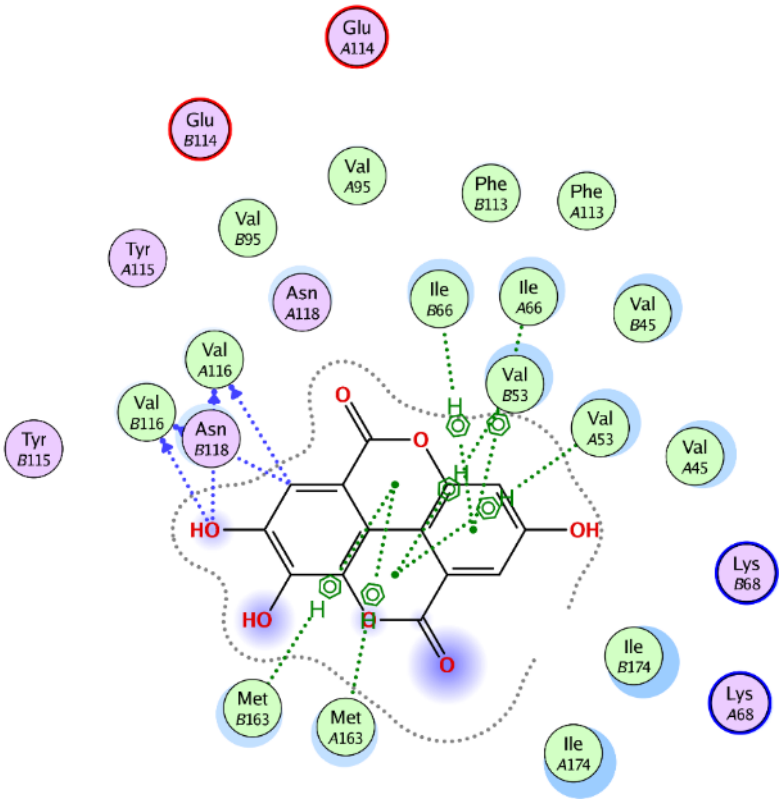
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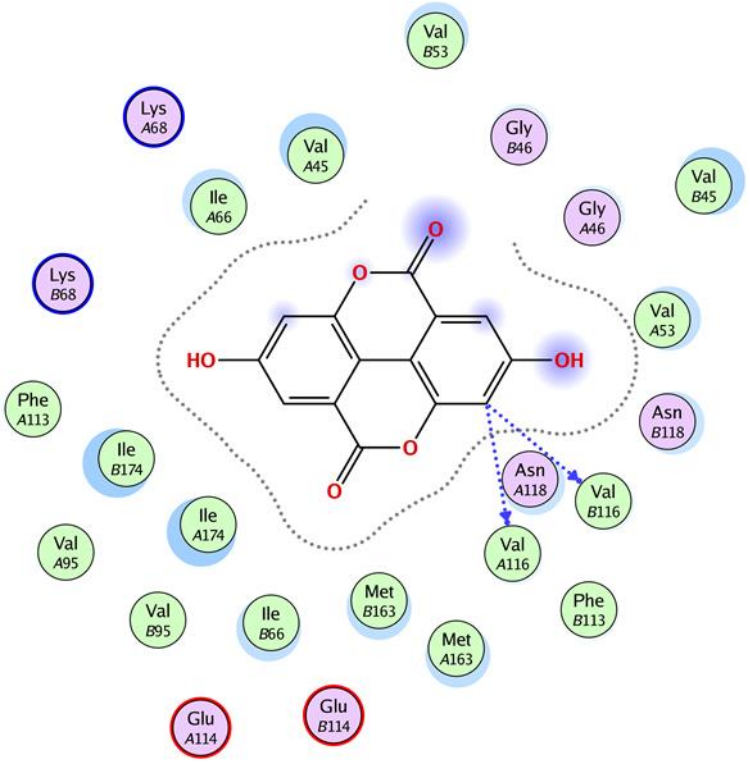
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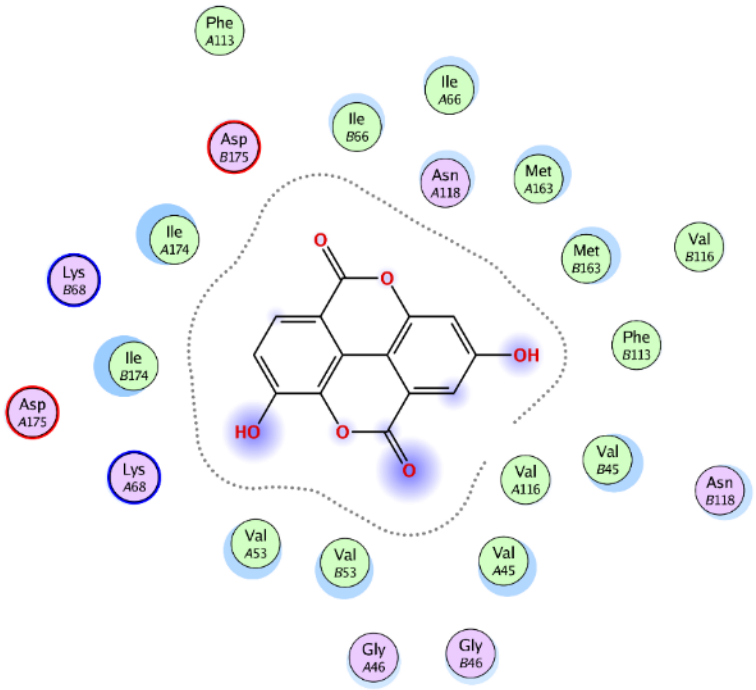
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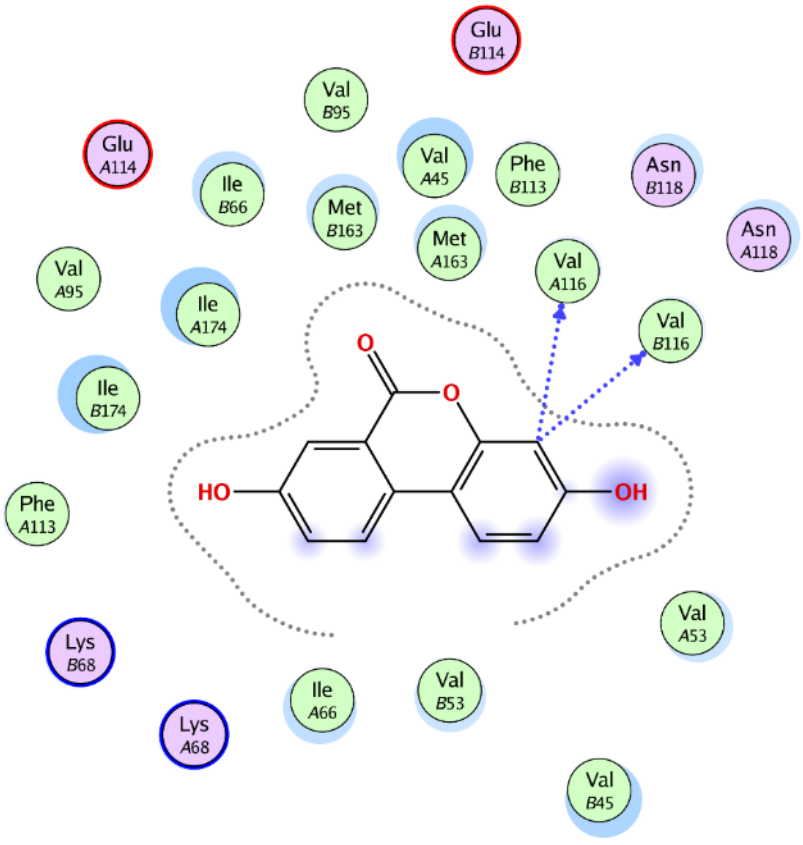
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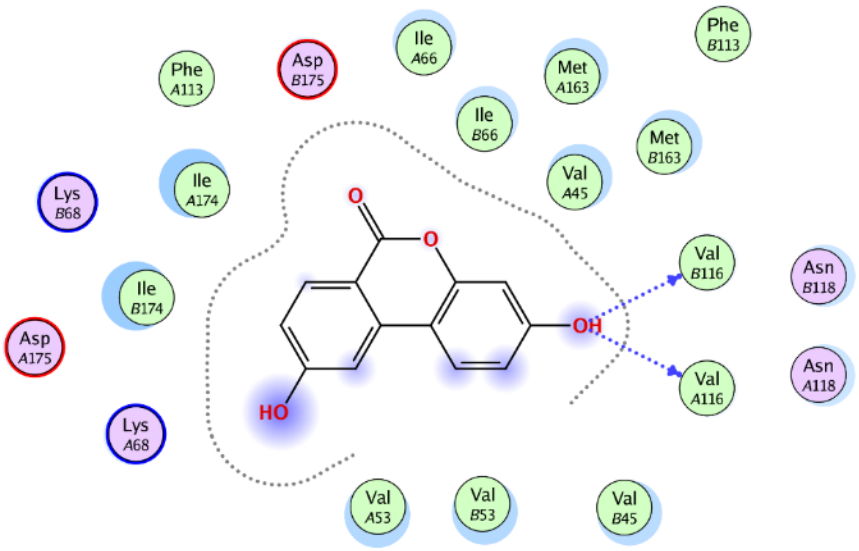
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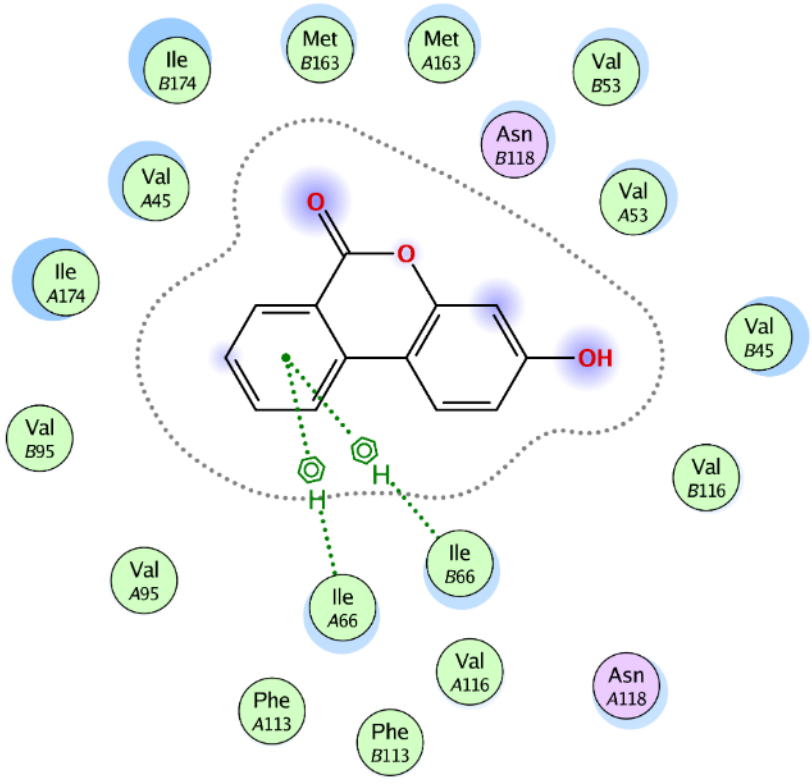
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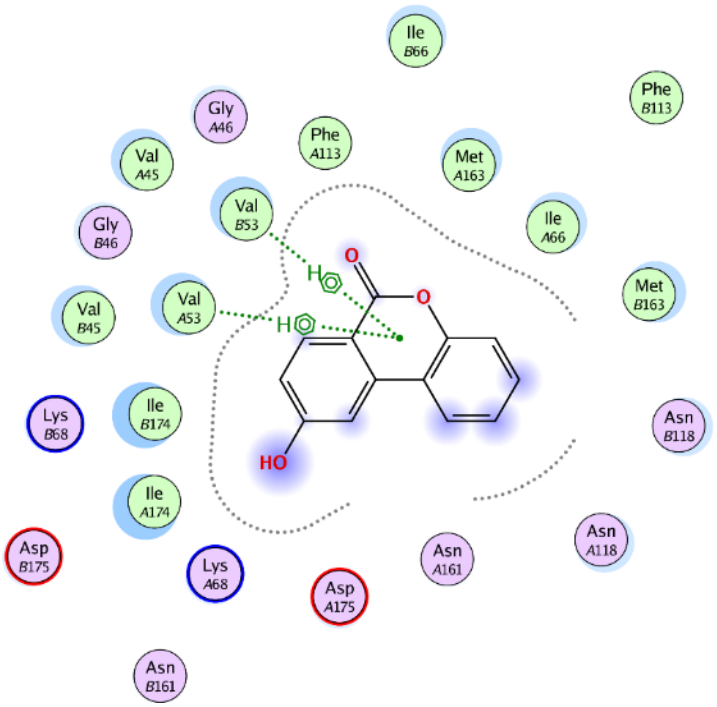
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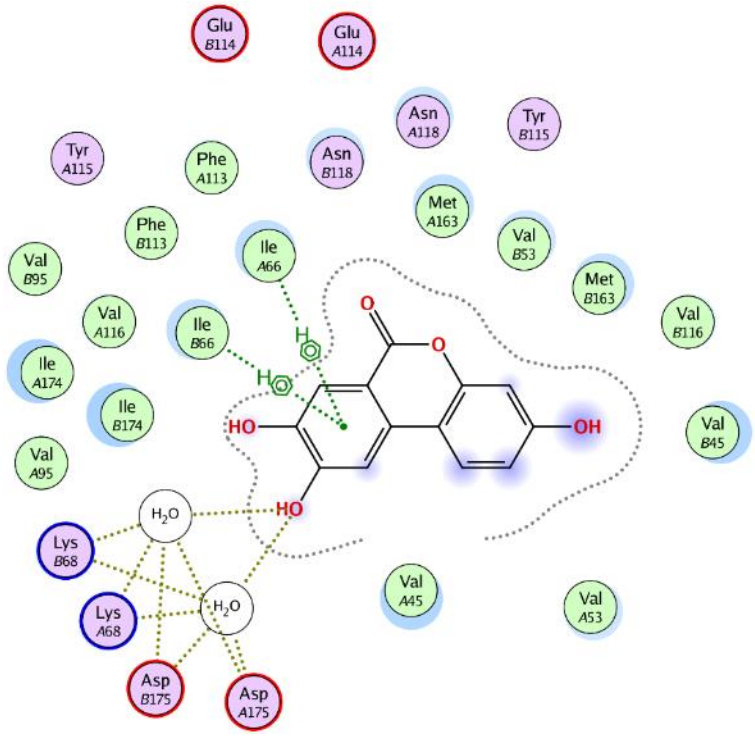
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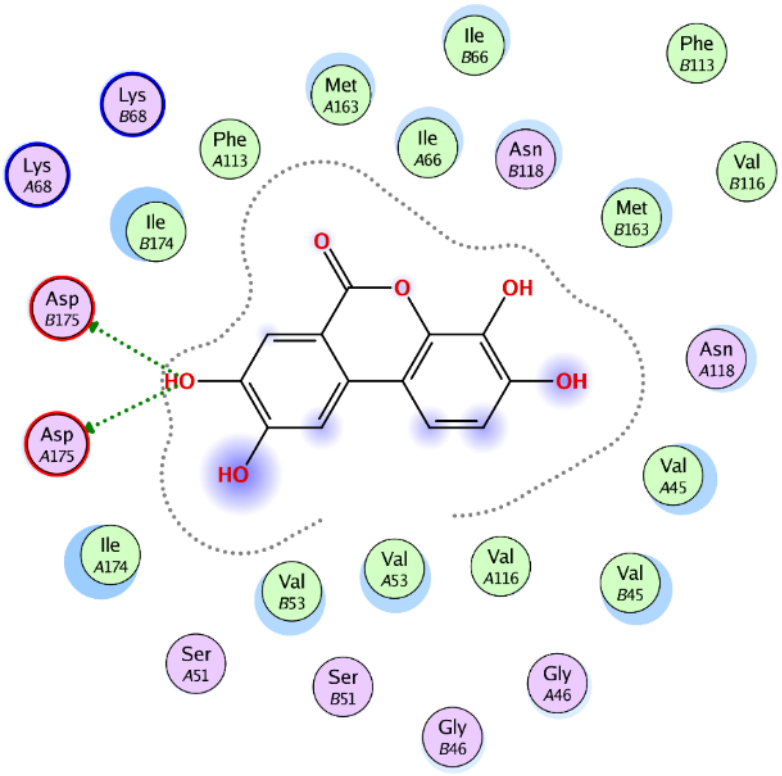
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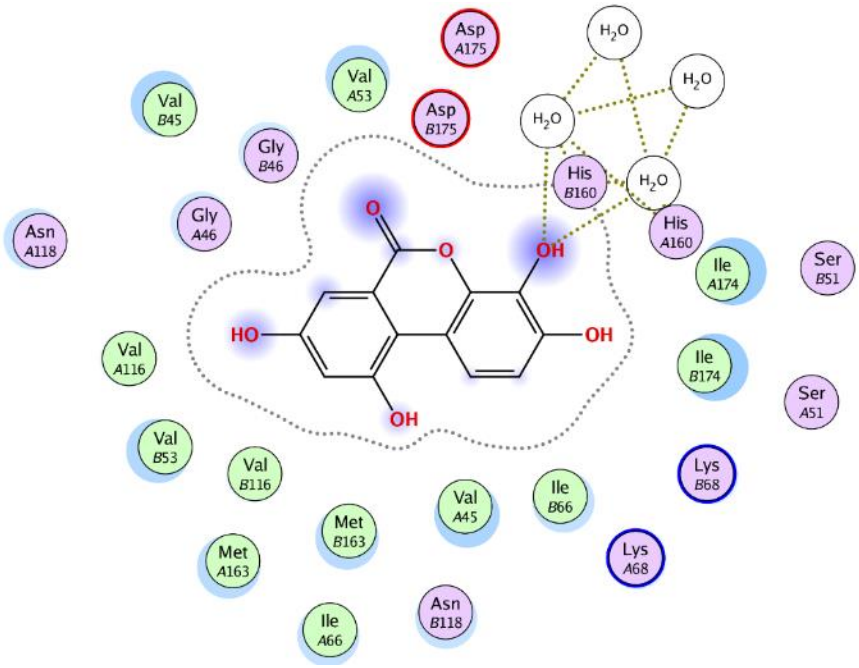
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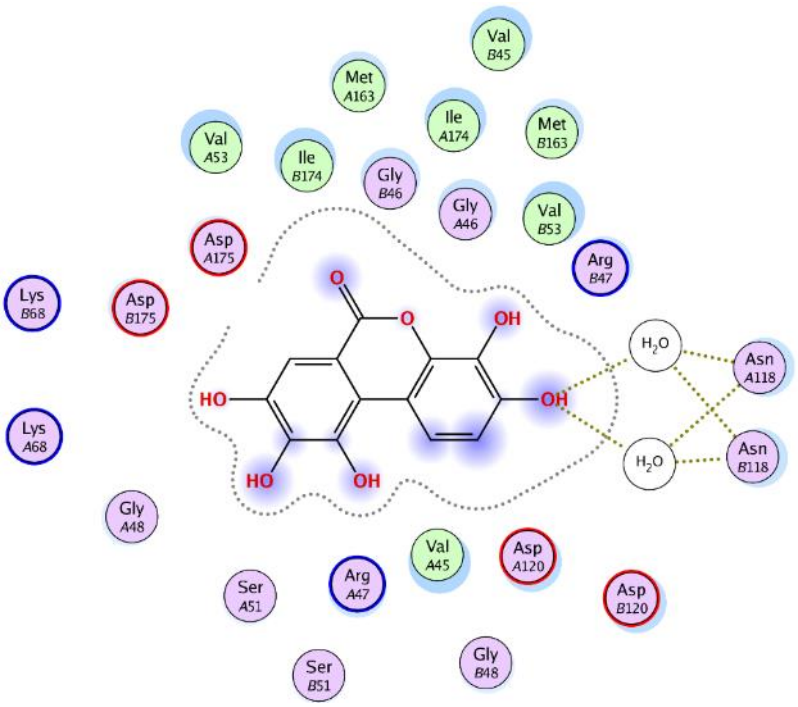
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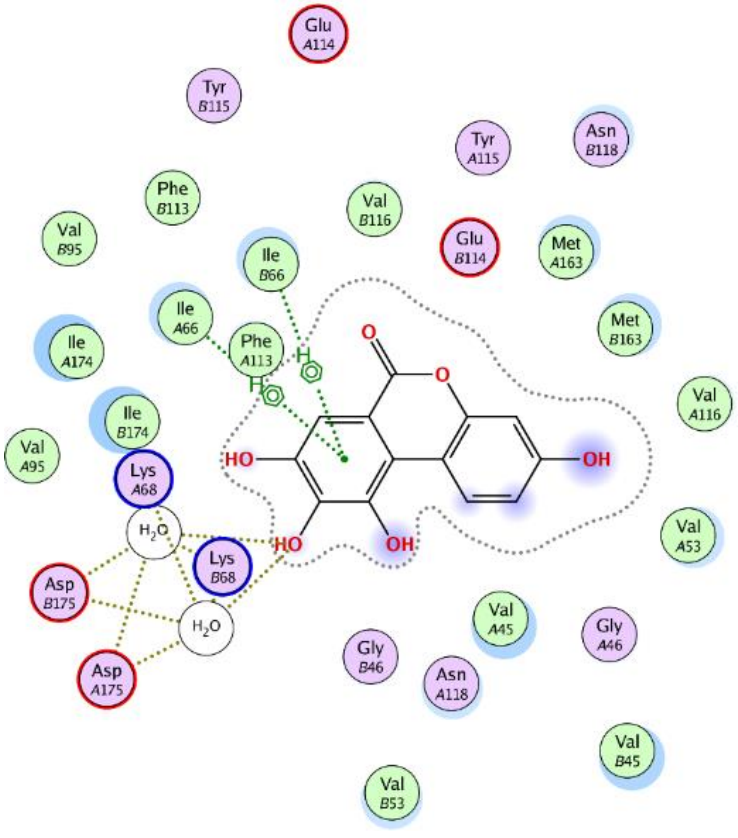
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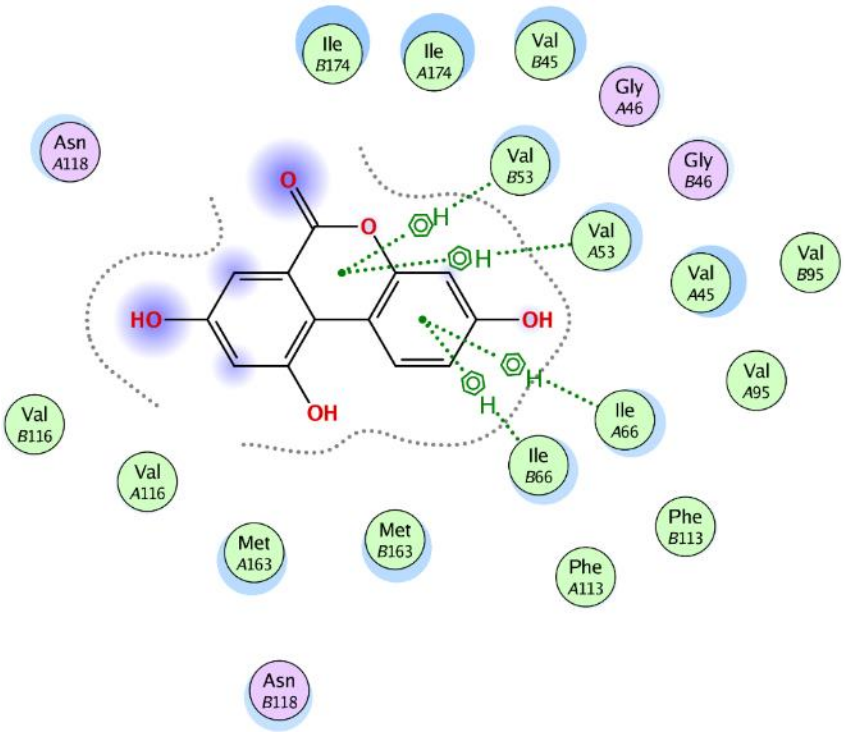
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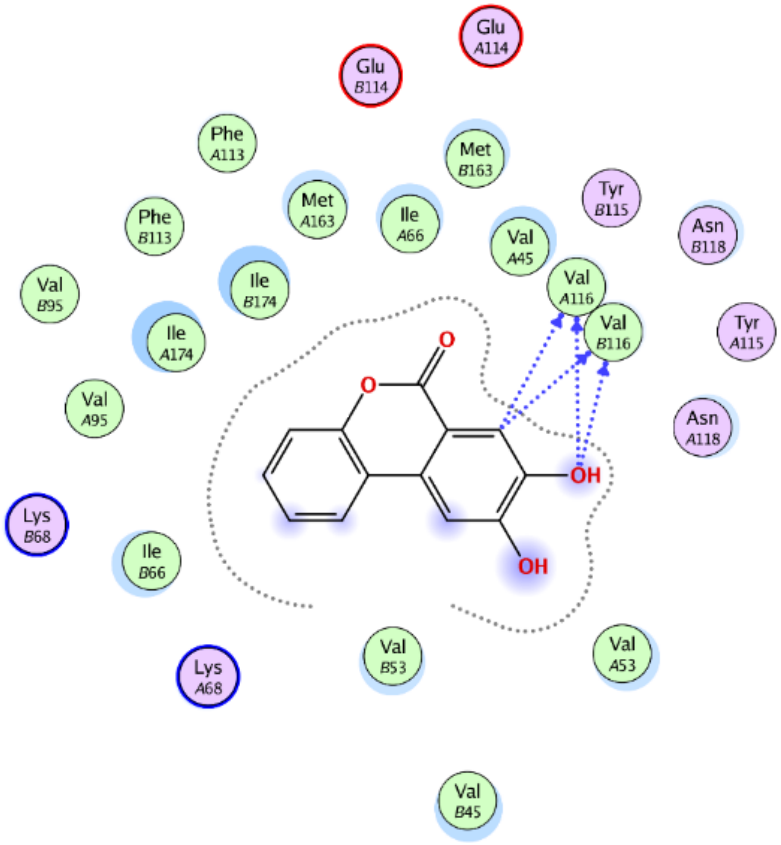
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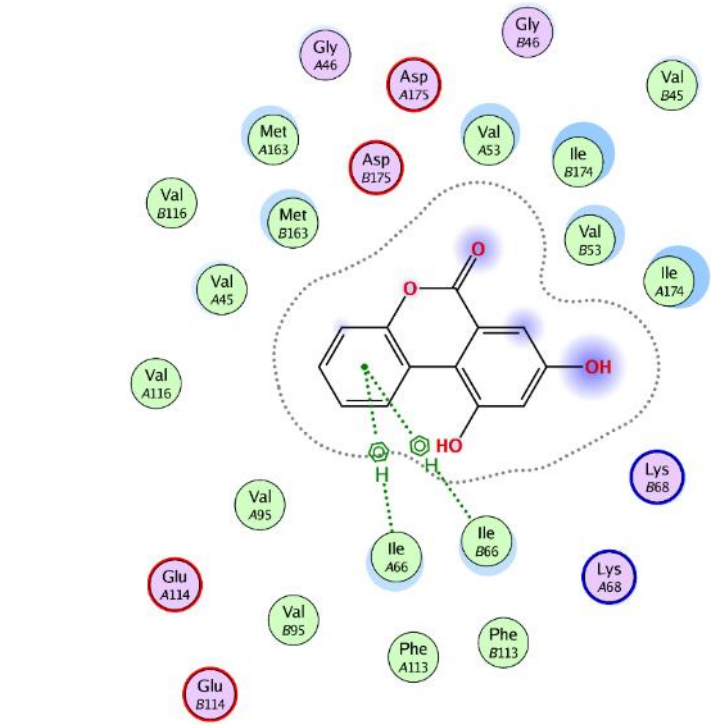
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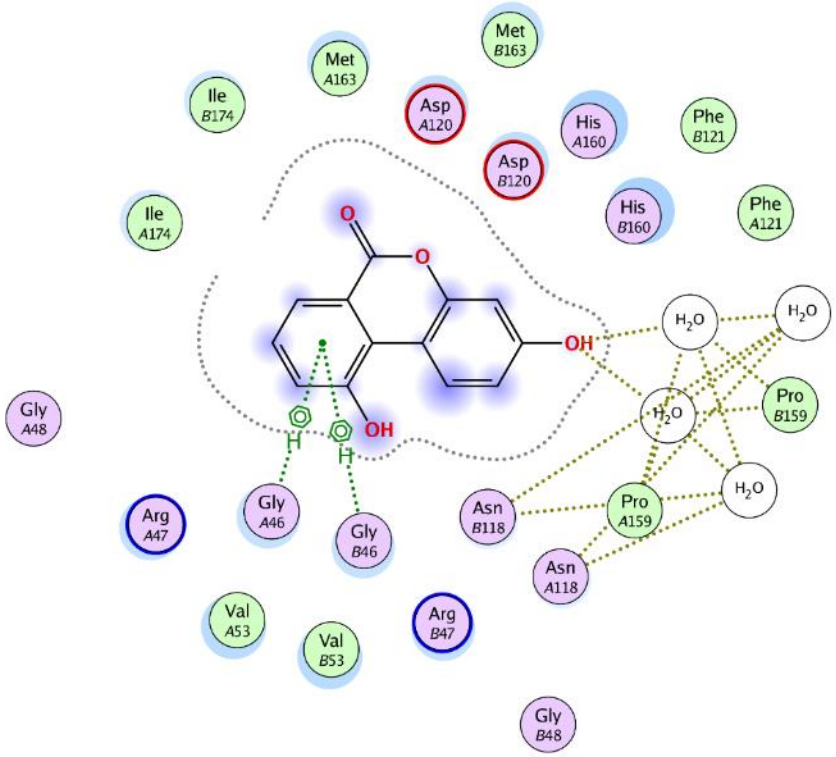
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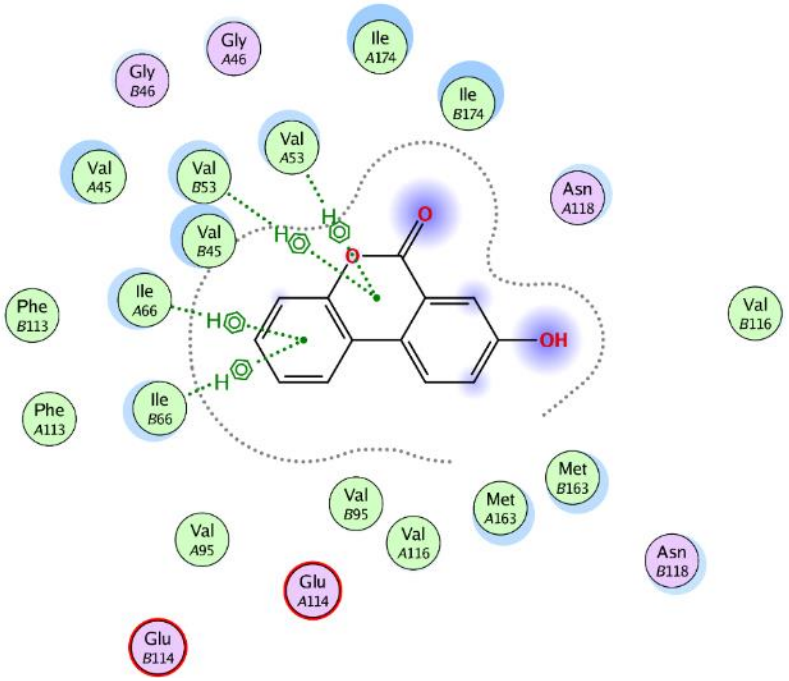
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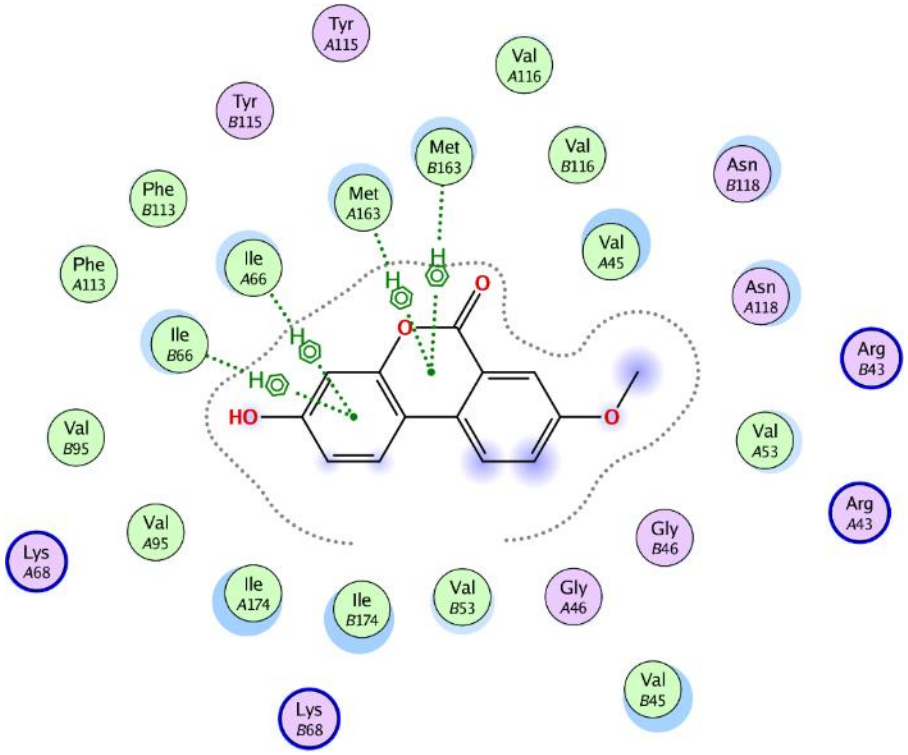
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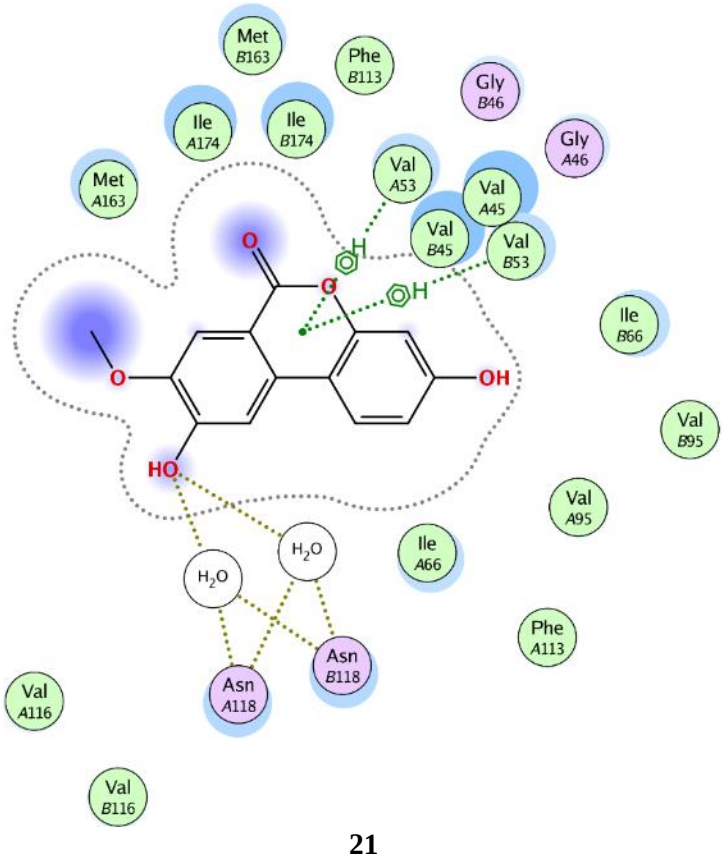
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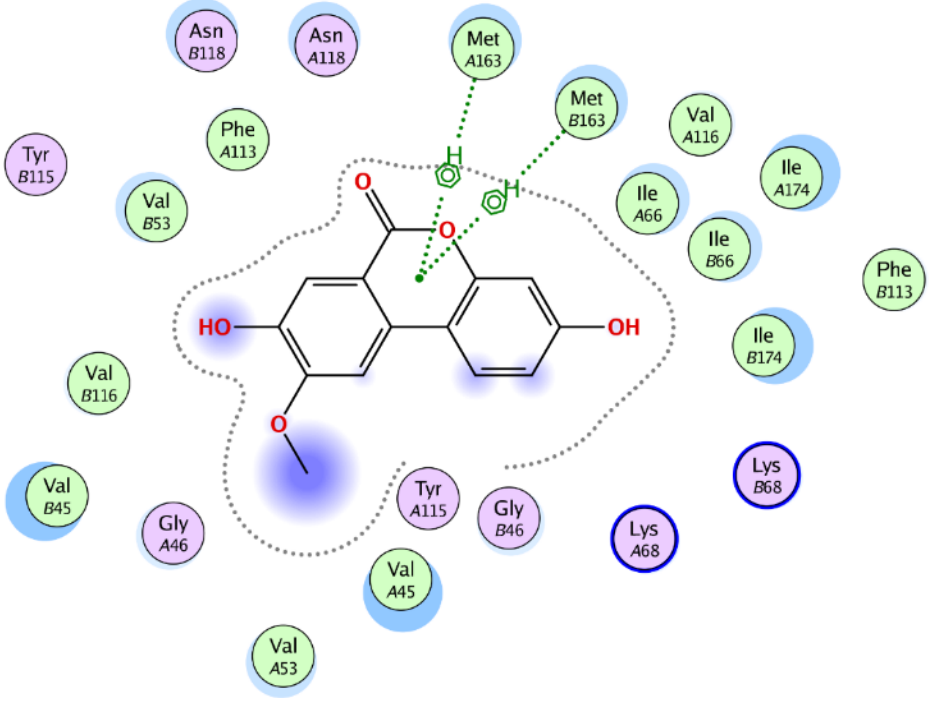
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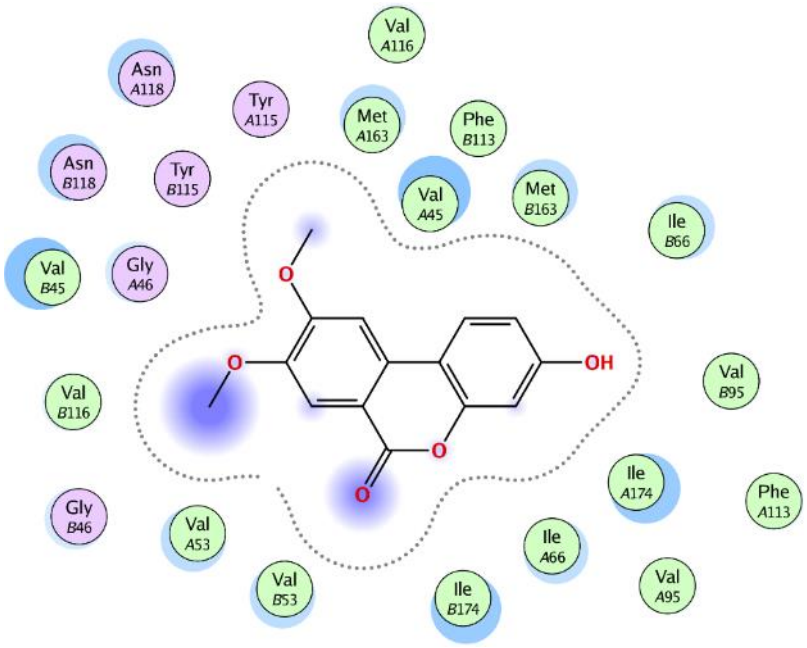
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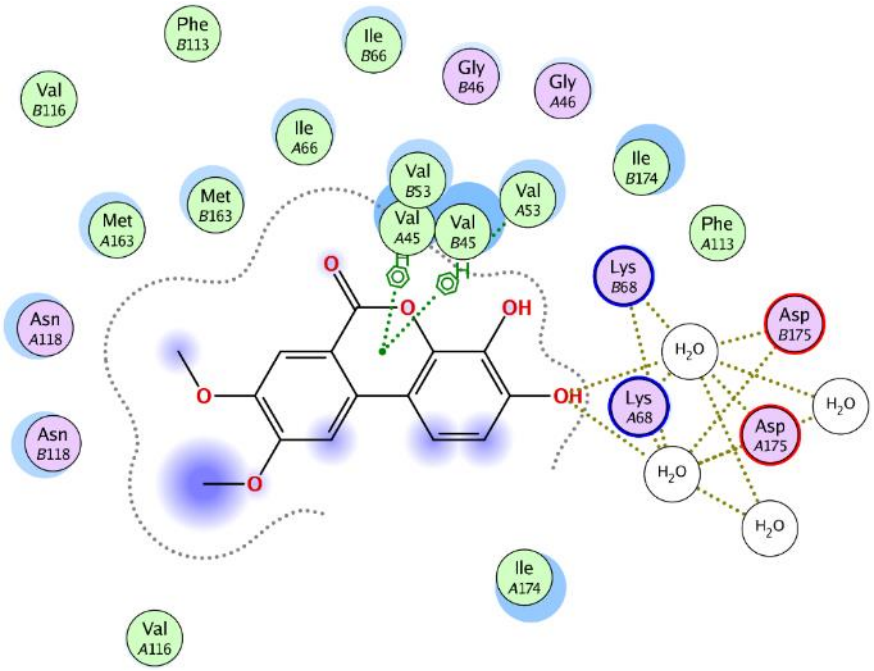
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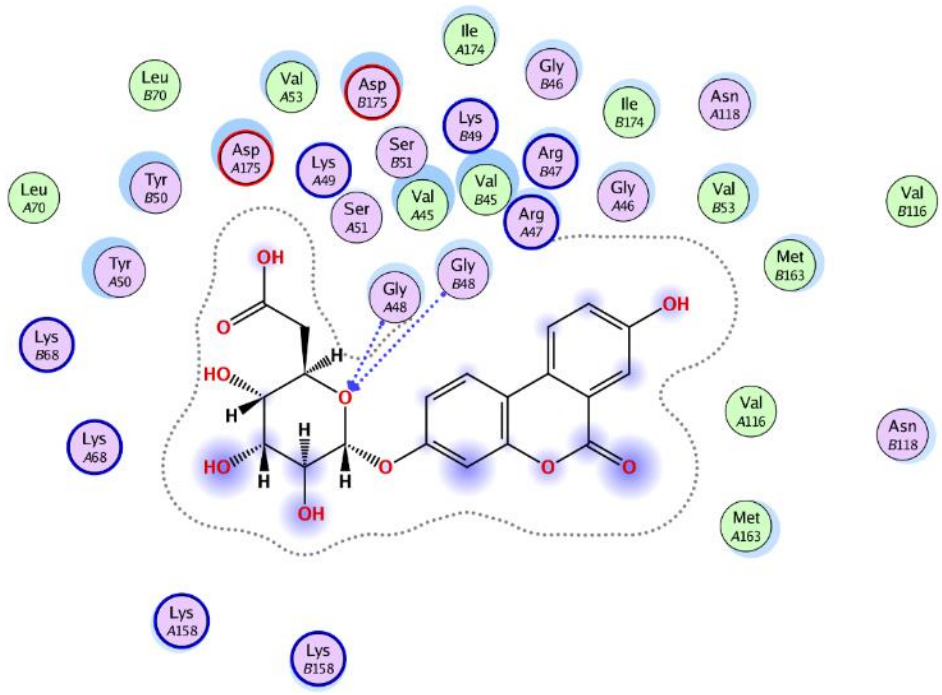
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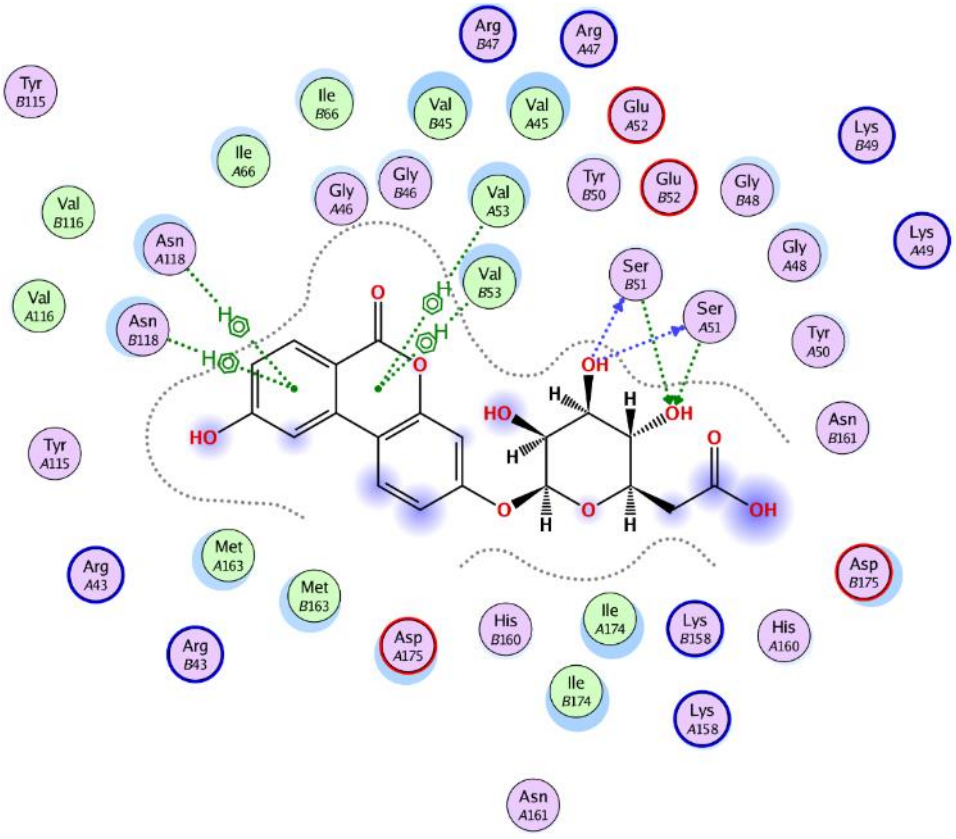
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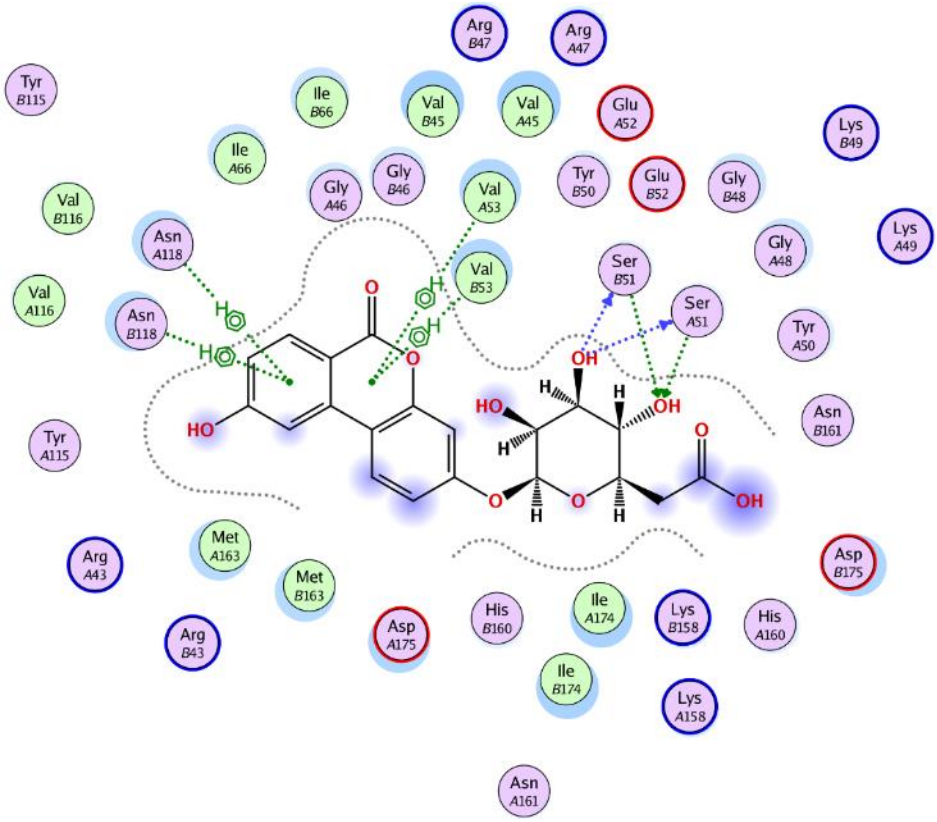

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Figure S1. The 2D interactions of ligands in the ATP binding site of CK2 using MOE program.

Table S1. Total Energies for twenty-eight ligand-protein complexes

Cpd. No.	$E_{complex)}$/a.u.	$E_{protein)}$/a.u.	$E_{(L,HQ)}$/a.u.	$E_{(L^*,HQ))}$/a.u.	$E_{(L^*,HQ^{sp}))}$/a.u.
1	-1144.78	-6.19	-1138.54147	-1138.55597	-1138.53718
2	-1069.44	-6.06	-1063.34518	-1063.35355	-1063.34083
3	-1069.56	-6.19	-1063.33946	-1063.34925	-1063.33592
4	-994.34	-6.16	-988.14325	-988.14938	-988.13965
5	-994.38	-6.20	-988.14039	-988.15008	-988.14469
6	-807.02	-6.15	-800.82884	-800.83453	-800.82276
7	-807.04	-6.18	-800.83023	-800.83692	-800.82867
8	-731.82	-6.16	-725.63142	-725.63689	-725.63015
9	-731.82	-6.16	-725.63285	-725.63905	-725.63127
10	-882.25	-6.18	-876.03060	-876.03589	-876.02694
11	-957.37	-6.10	-951.23140	-951.23310	-951.22869
12	-957.34	-6.08	-951.22197	-951.22643	-951.21872
13	-1032.65	-6.19	-1026.41773	-1026.42985	-1026.42570
14	-957.46	-6.19	-951.21633	-951.23248	-951.22376
15	-882.10	-6.03	-876.01981	-876.03012	-876.02080
16	-807.04	-6.18	-800.83282	-800.83767	-800.83111
17	-806.96	-6.10	-800.82668	-800.83017	-800.82454
18	-807.00	-6.14	-800.82245	-800.82891	-800.82174
19	-731.75	-6.11	-725.62943	-725.63831	-725.62976
20	-846.18	-6.03	-840.11107	-840.12303	-840.10970
21	-921.42	-6.09	-915.31590	-915.33448	-915.31189
22	-921.50	-6.15	-915.30758	-915.31886	-915.30330
23	-960.68	-6.05	-954.59202	-954.60160	-954.58782
24	-1035.91	-6.09	-1029.79308	-1029.80877	-1029.78789
25	-1530.78	-6.02	-1524.68469	-1524.71326	-1524.65795
26	-1530.76	-5.97	-1524.68826	-1524.71955	-1524.65157
27	-1530.74	-5.98	-1524.67409	-1524.68800	-1524.65784
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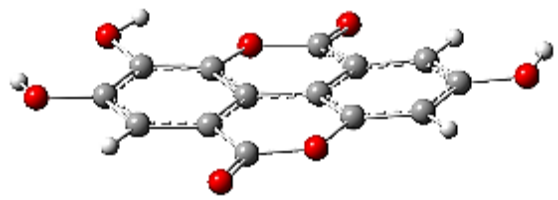
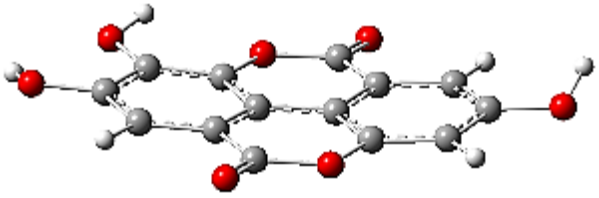

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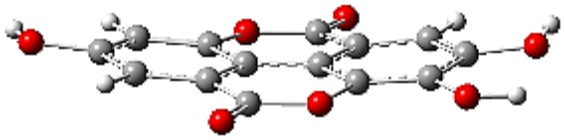
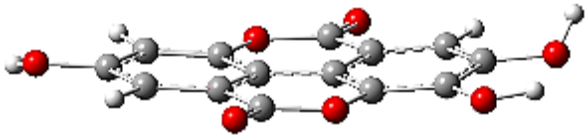

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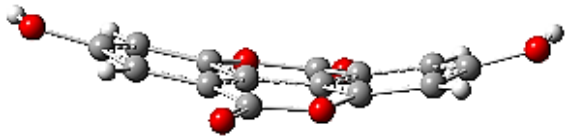


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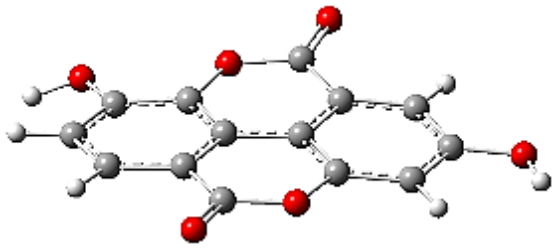
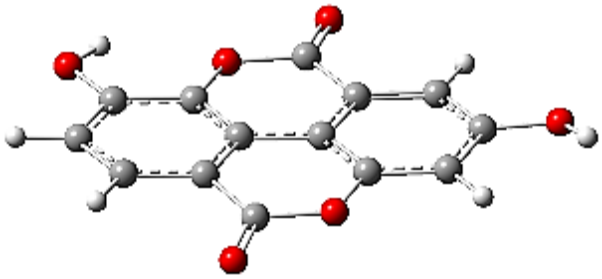

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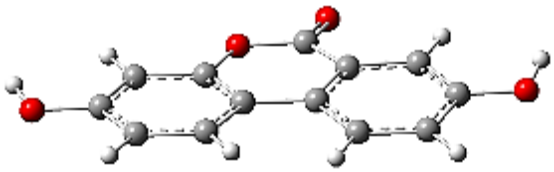
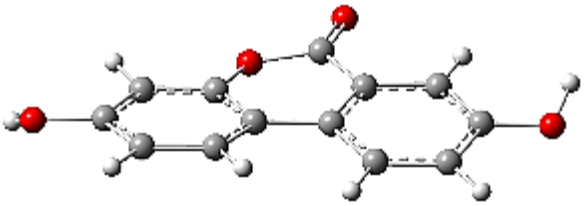

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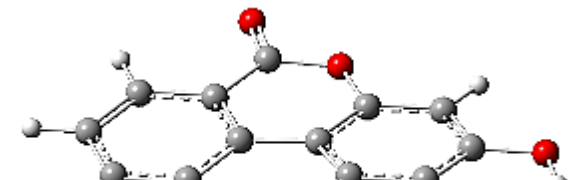
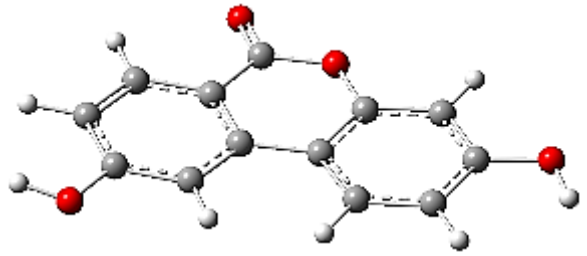

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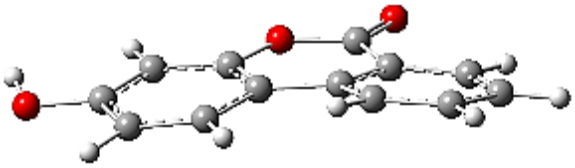
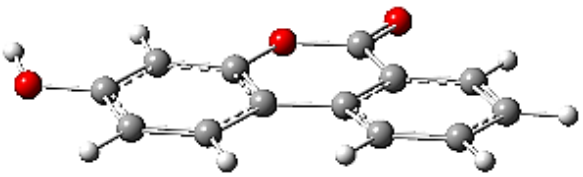

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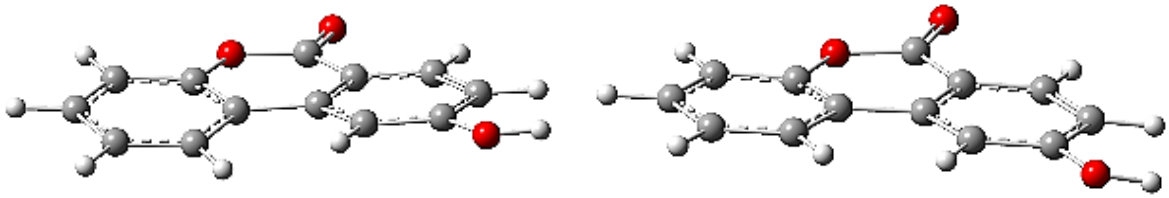

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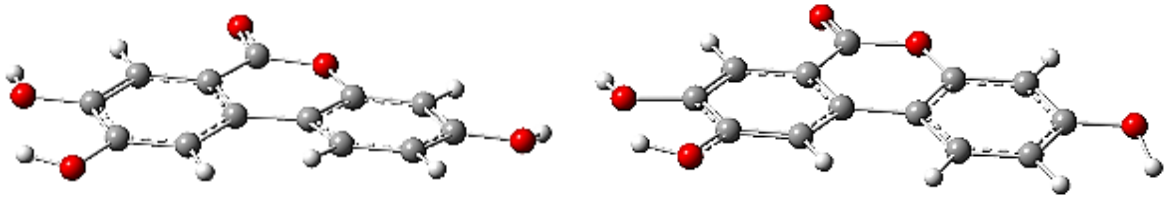

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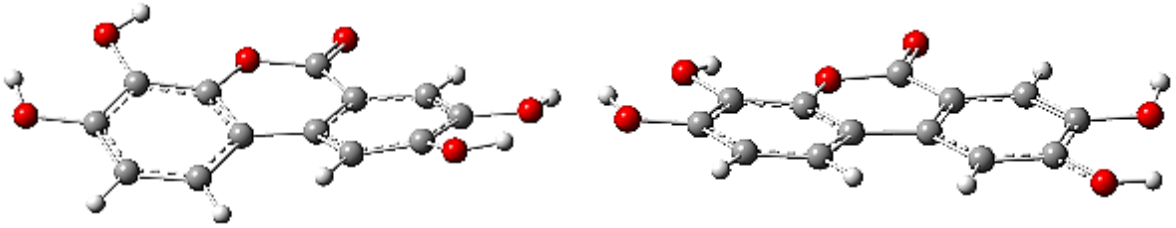

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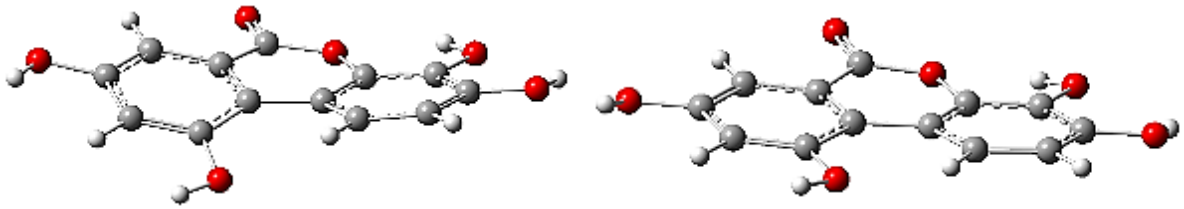

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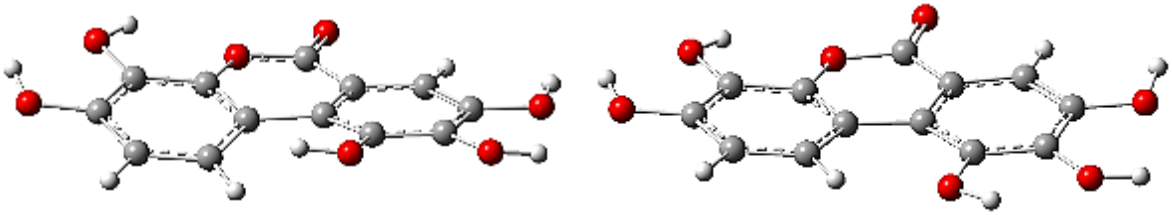

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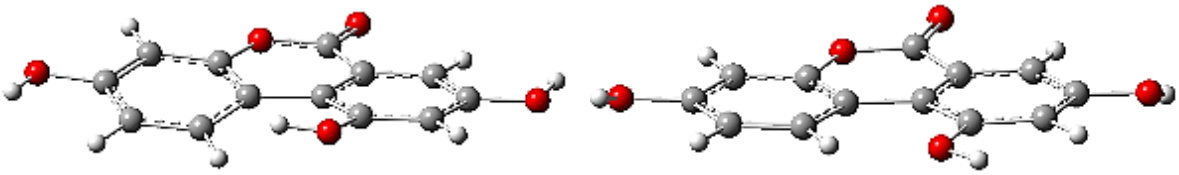

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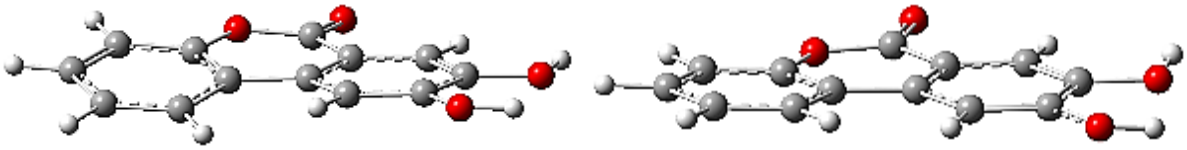

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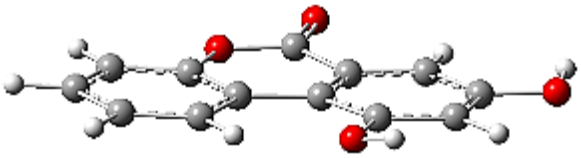

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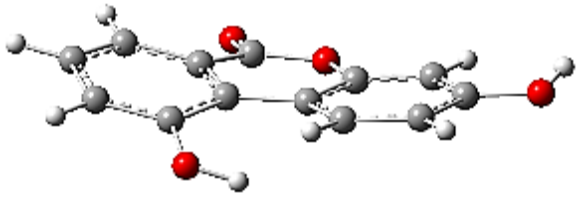


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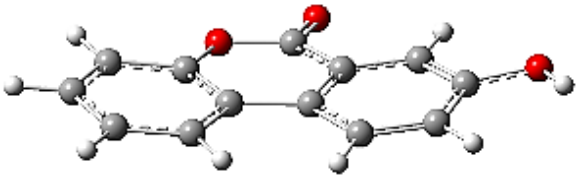


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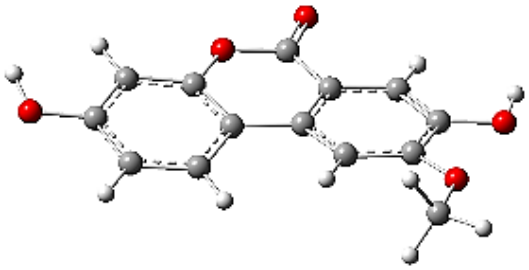
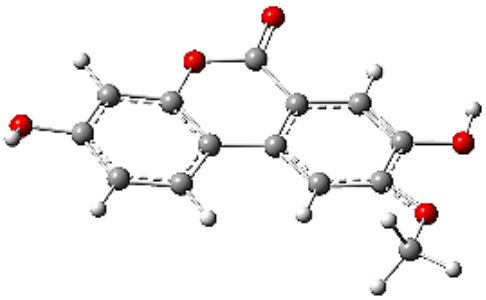

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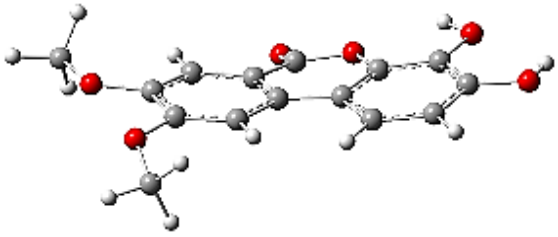
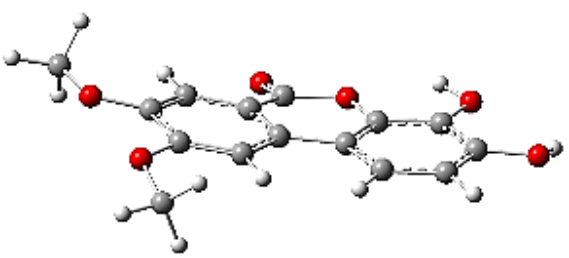

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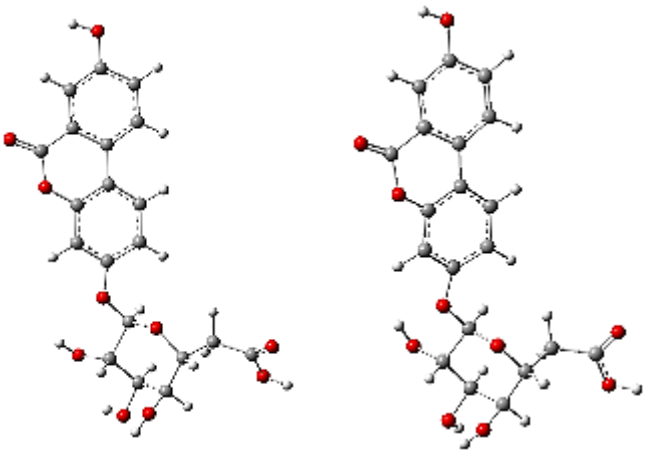

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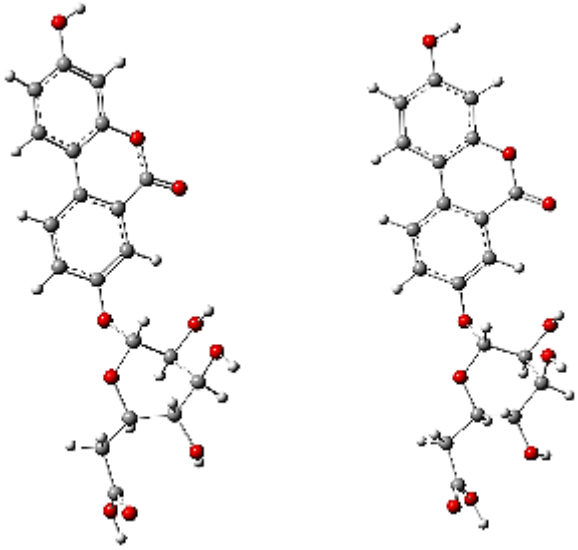

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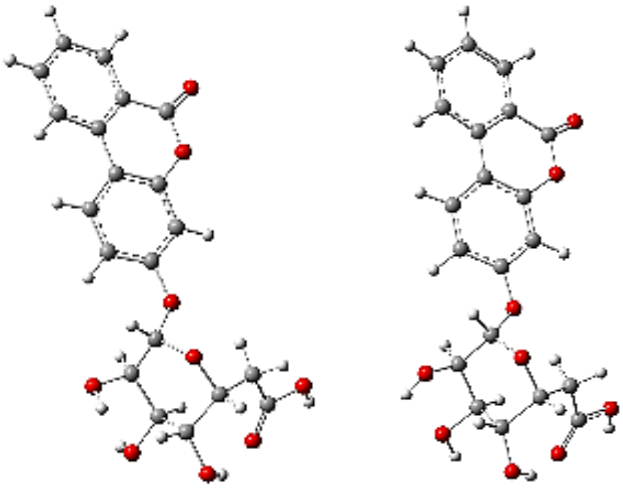
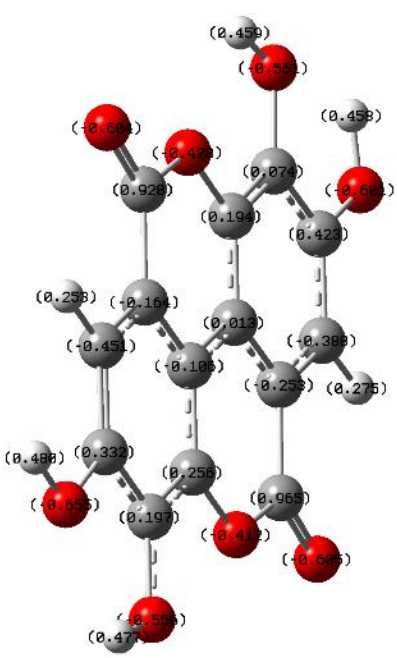
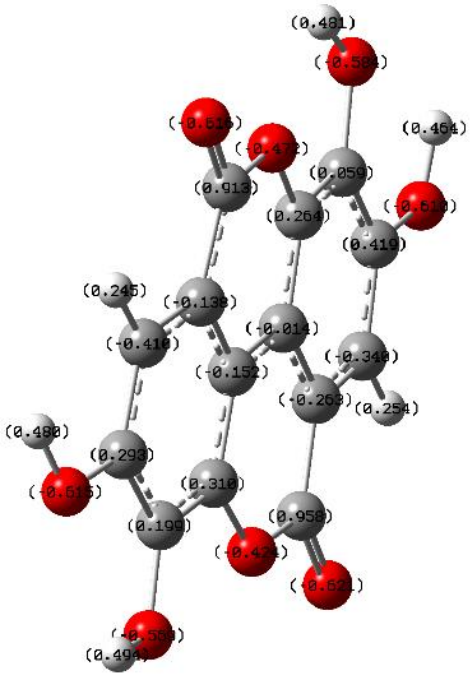


28

Figure S2. The docked (left panel) and the ONIOM optimized structures (right panel) of ligands.





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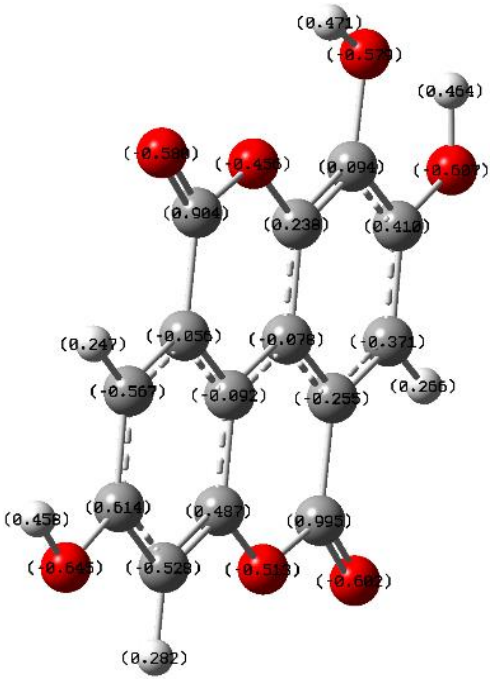

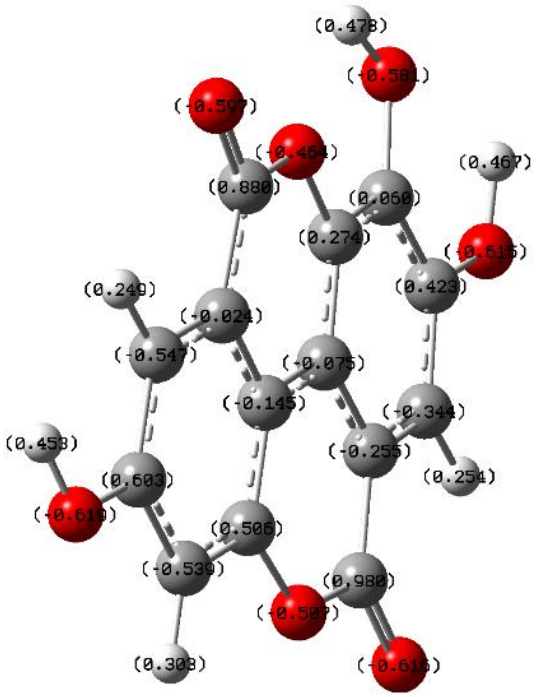

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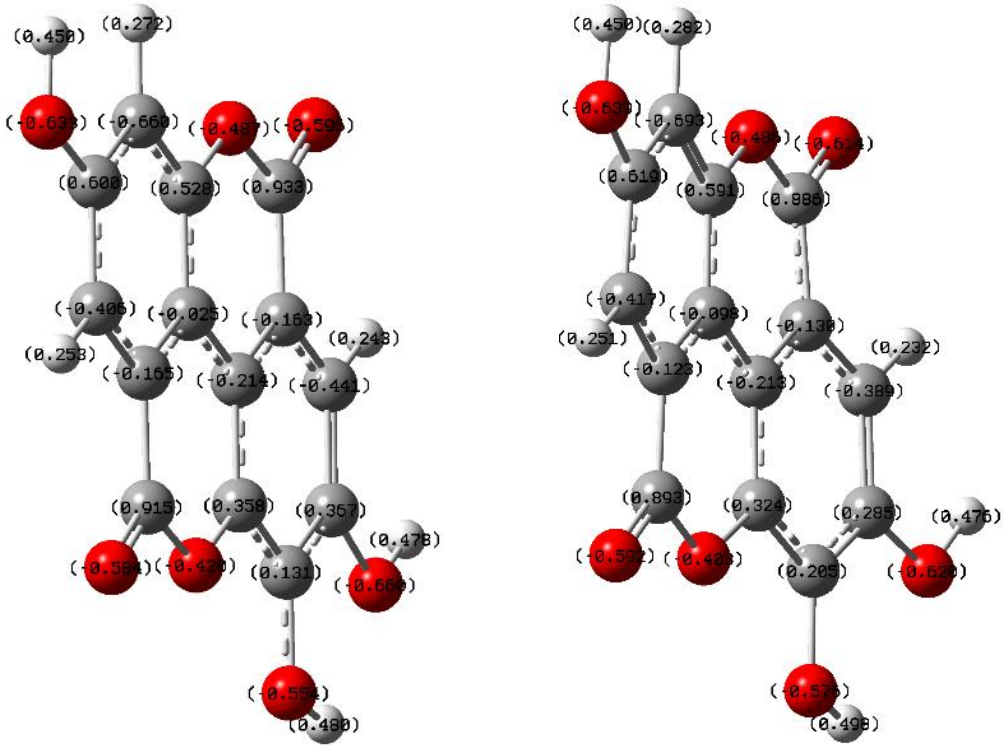

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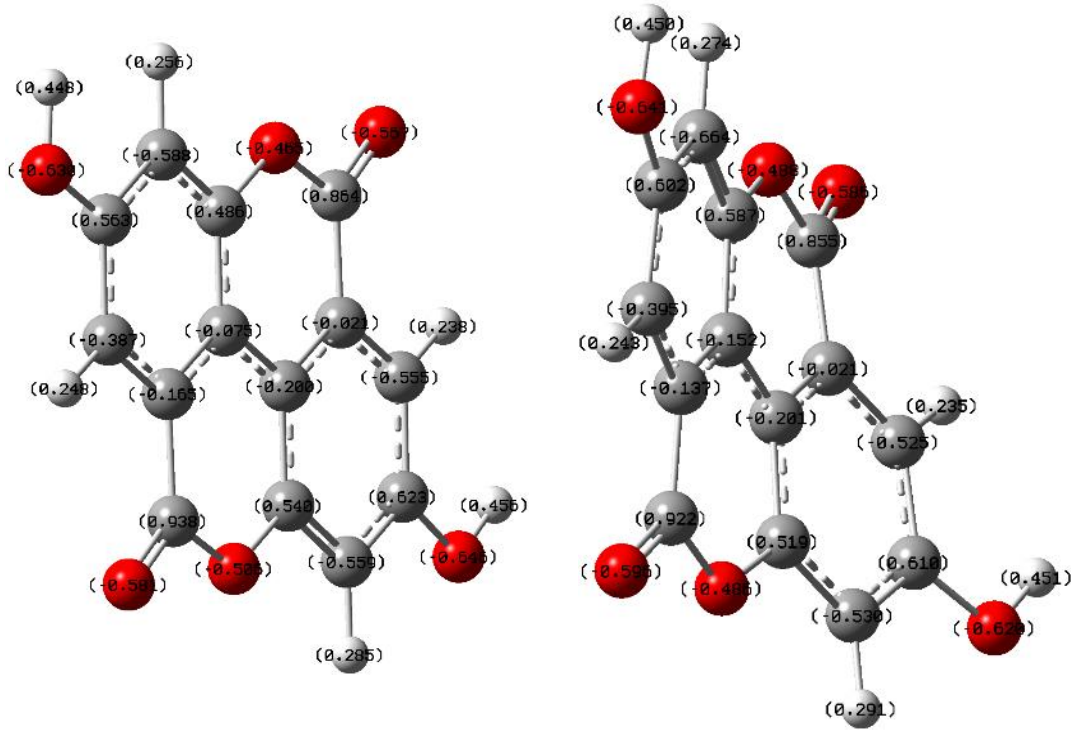

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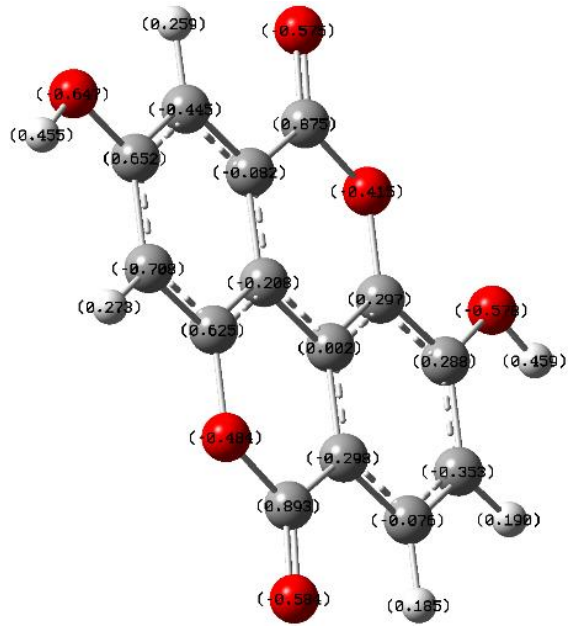

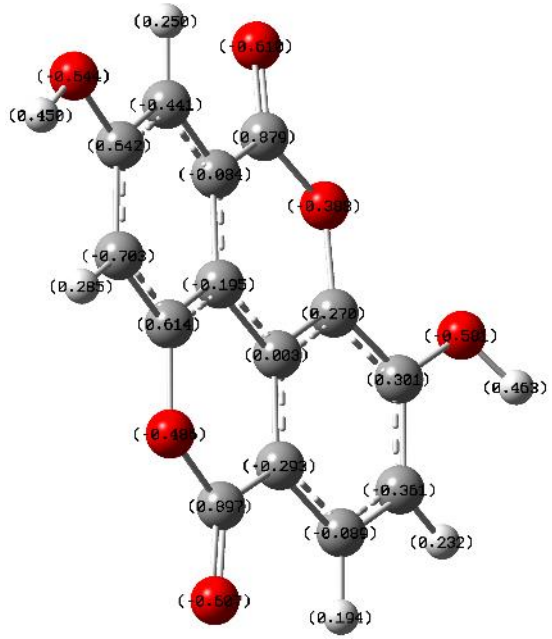

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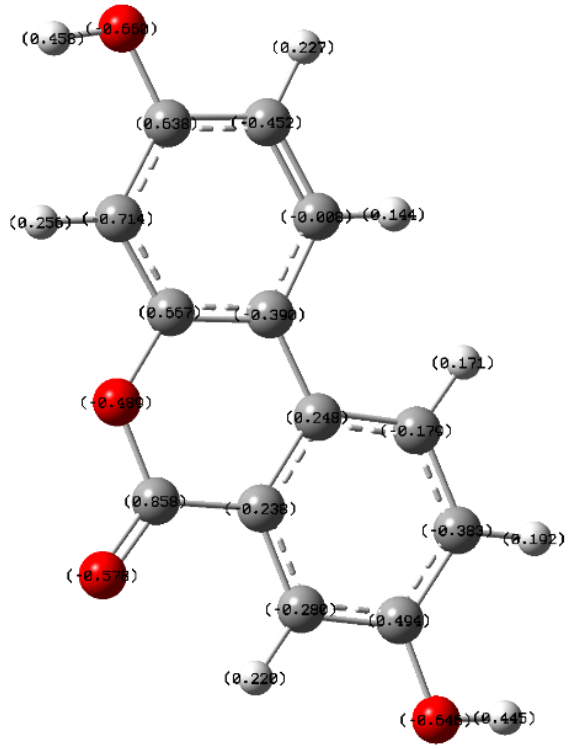

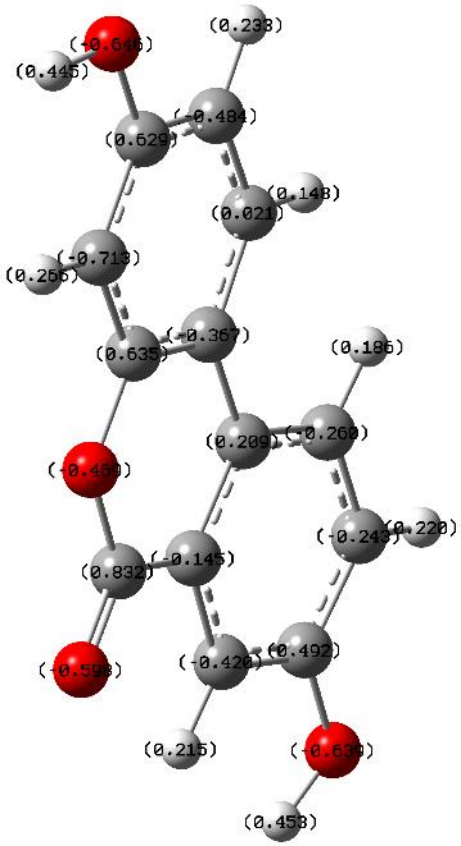

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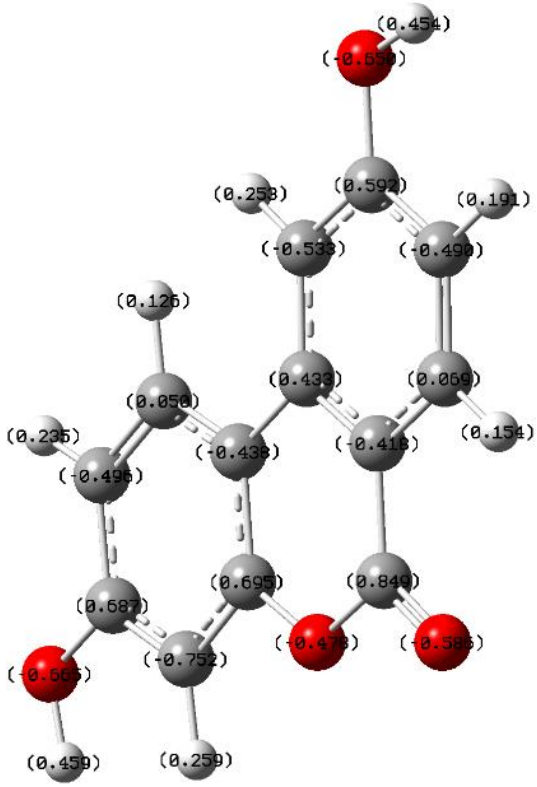
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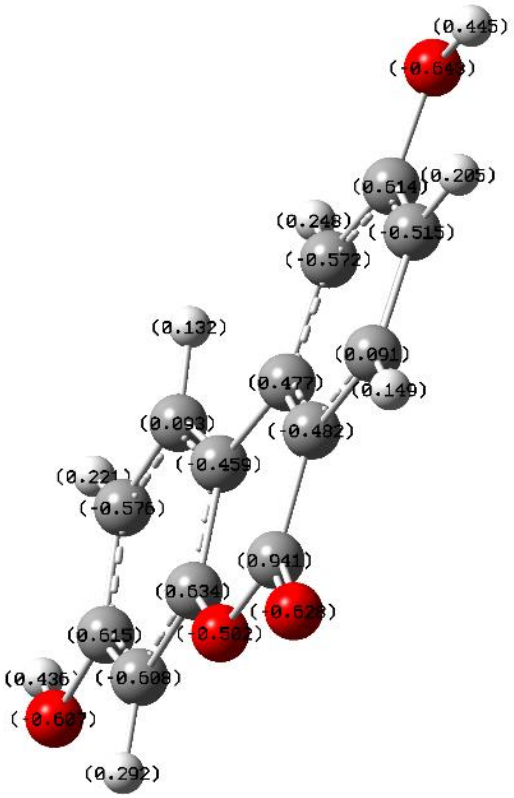
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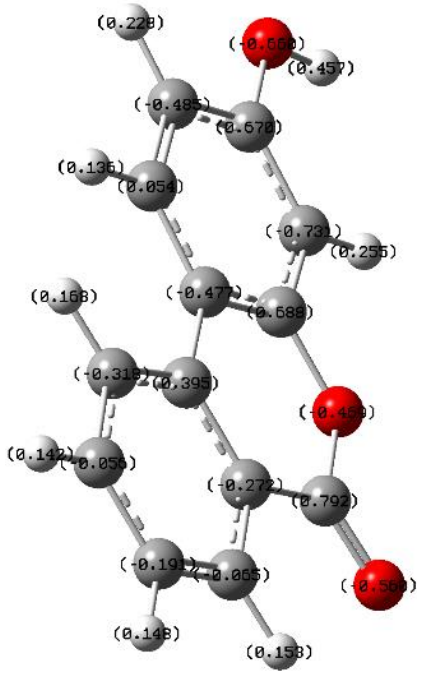
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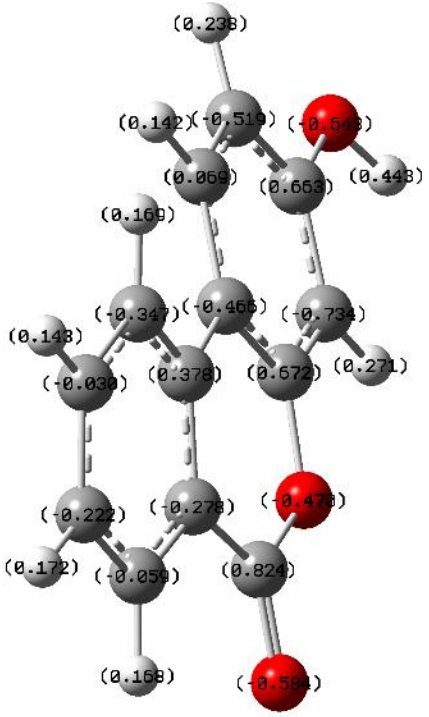
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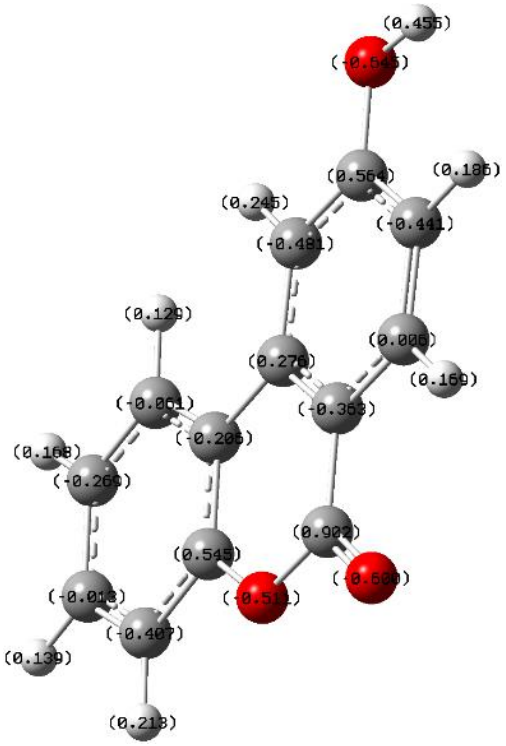

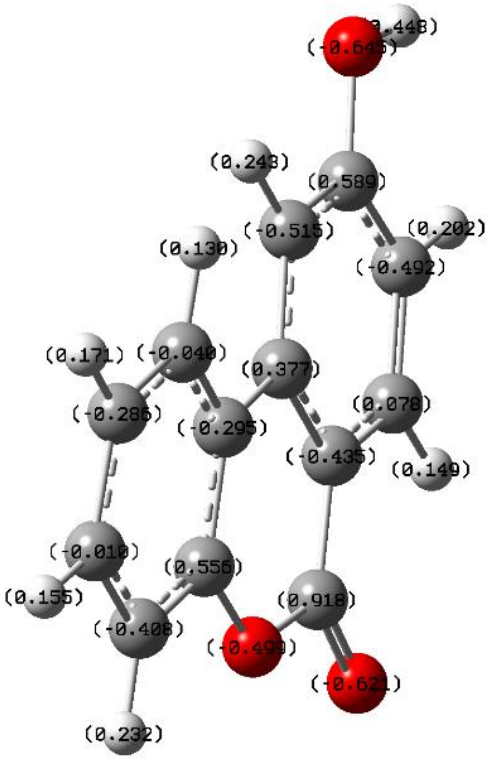

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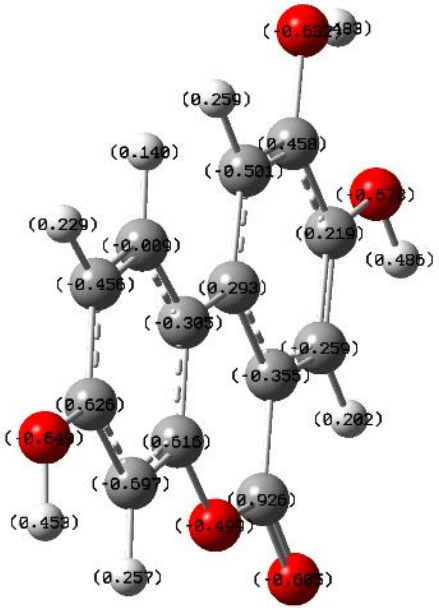

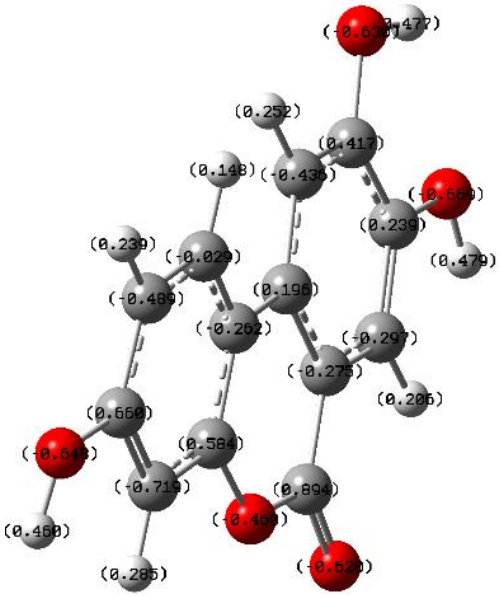

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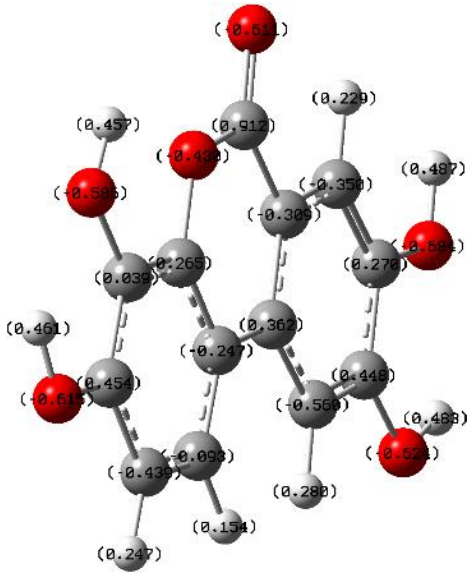

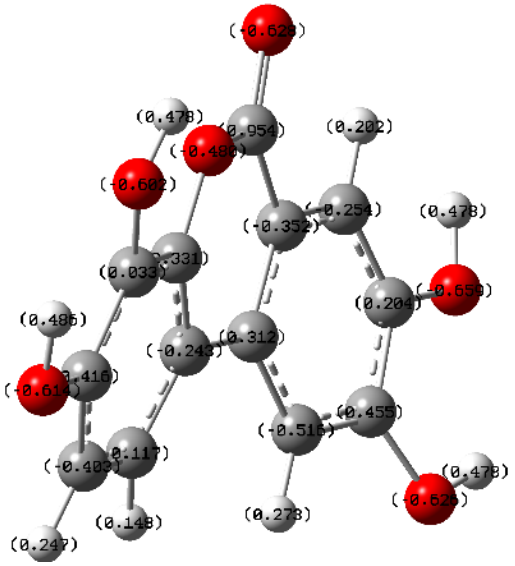

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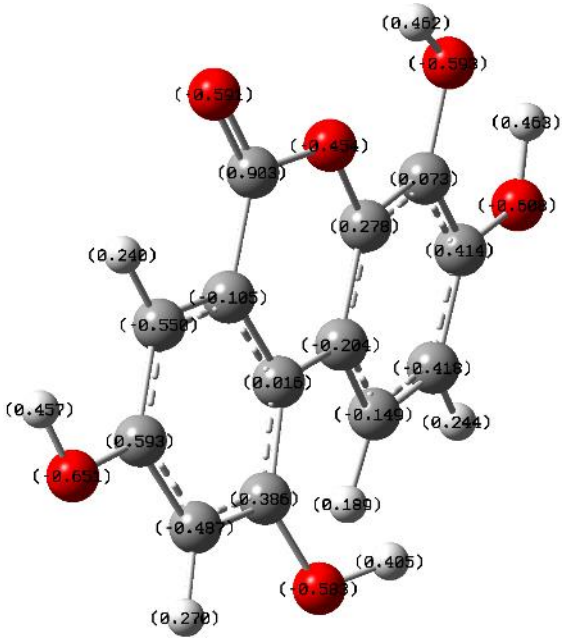

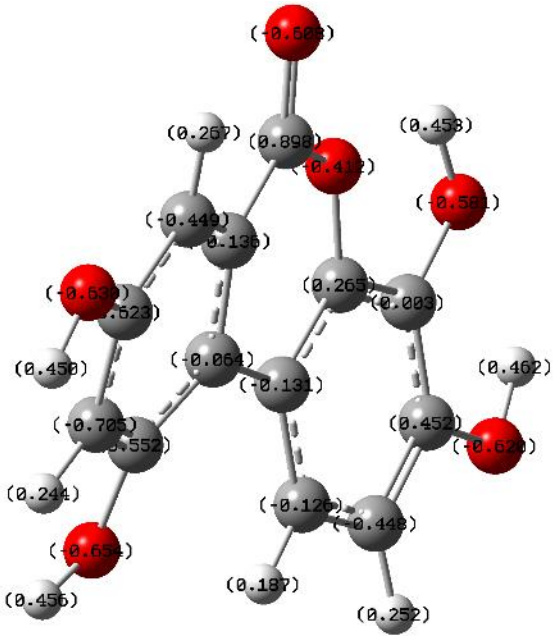

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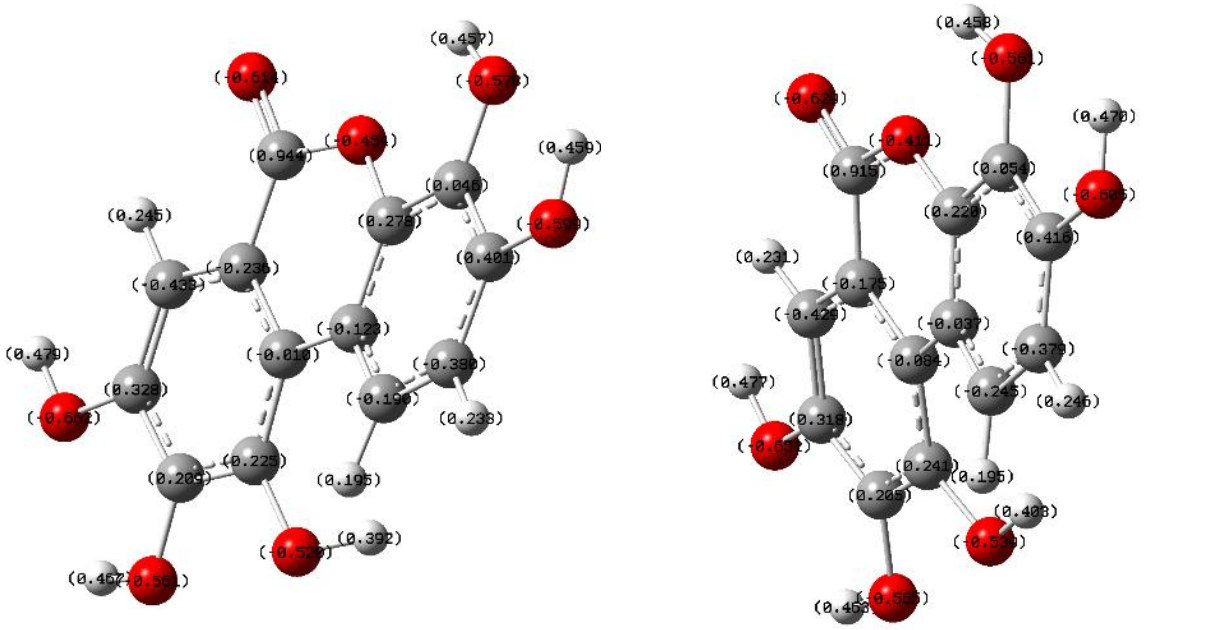

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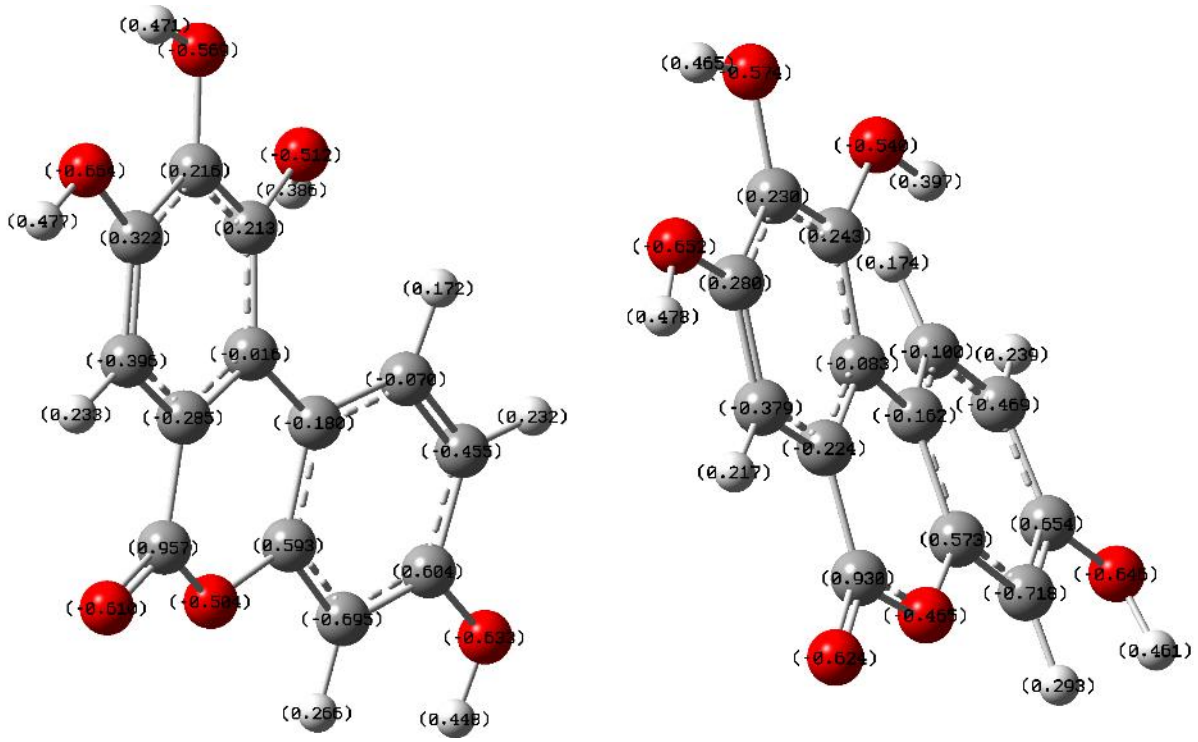

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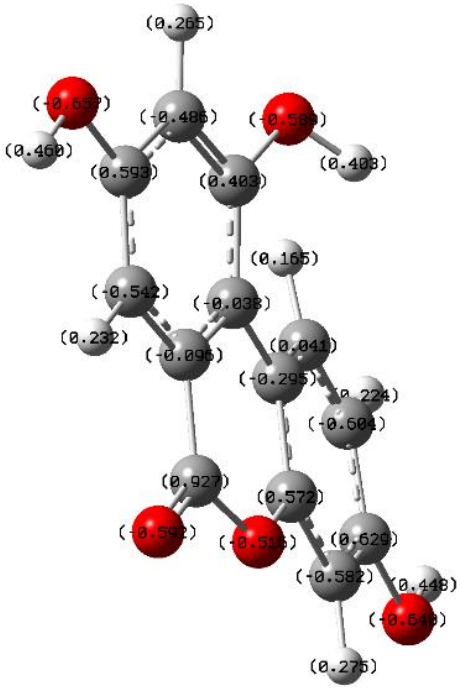
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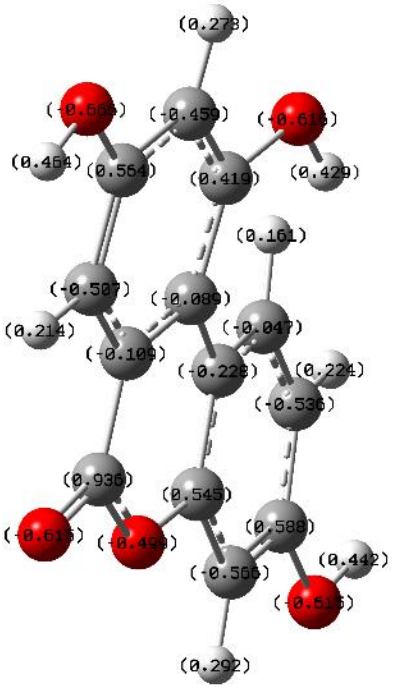
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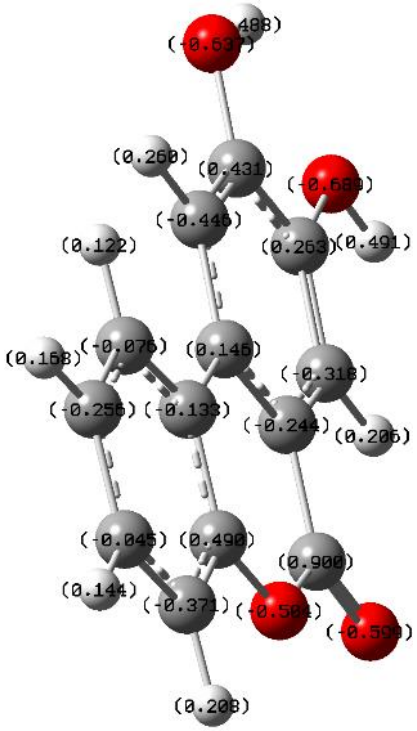
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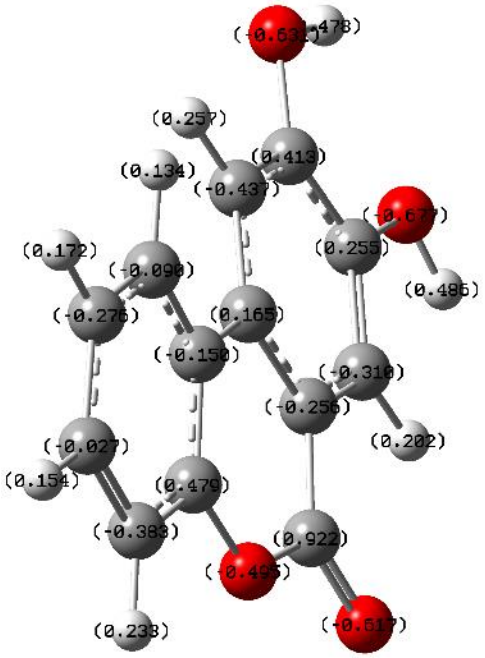
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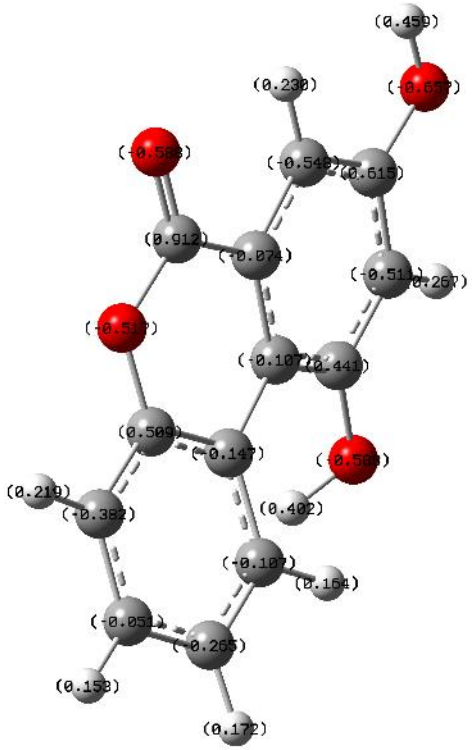

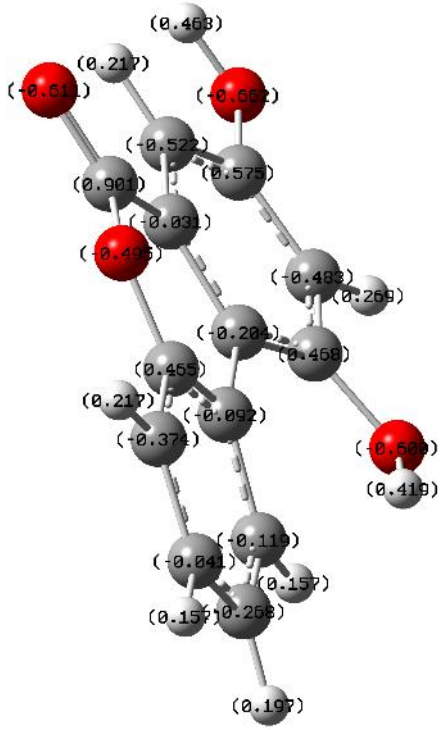

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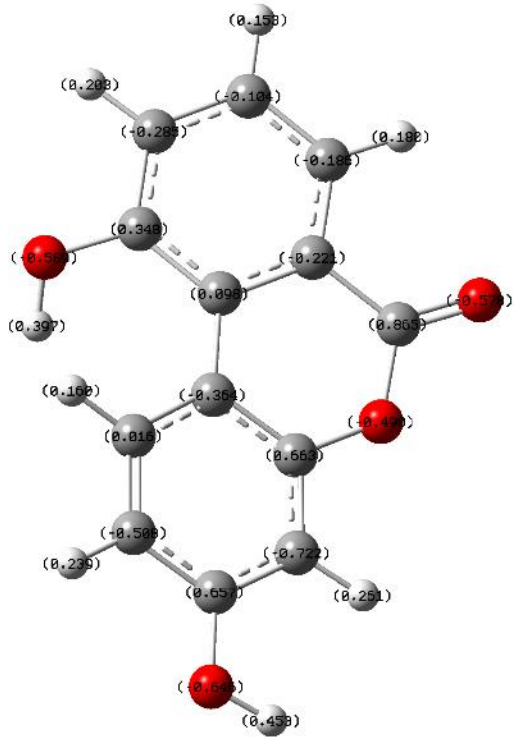

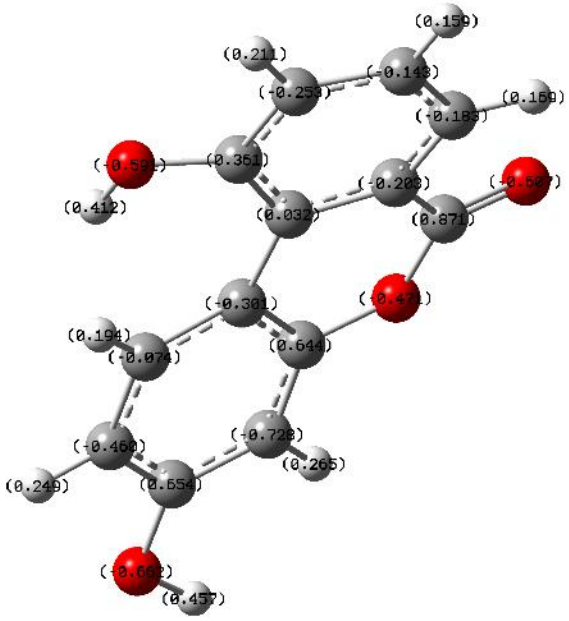

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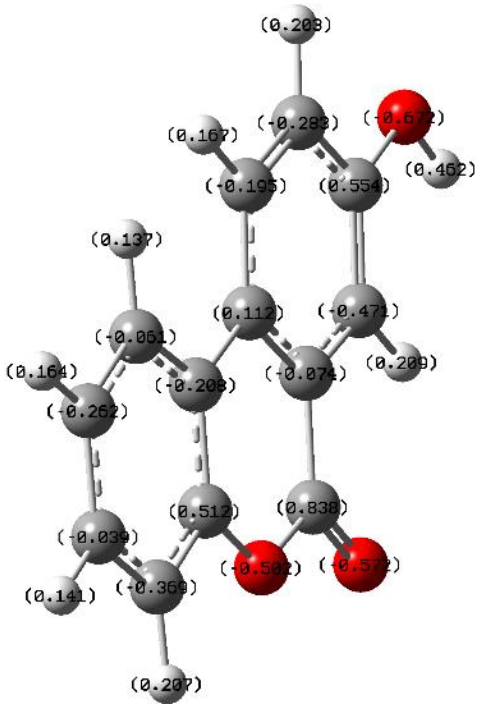

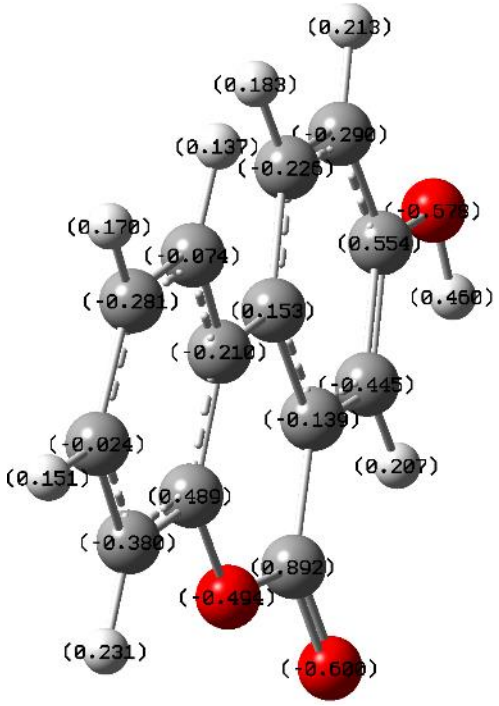

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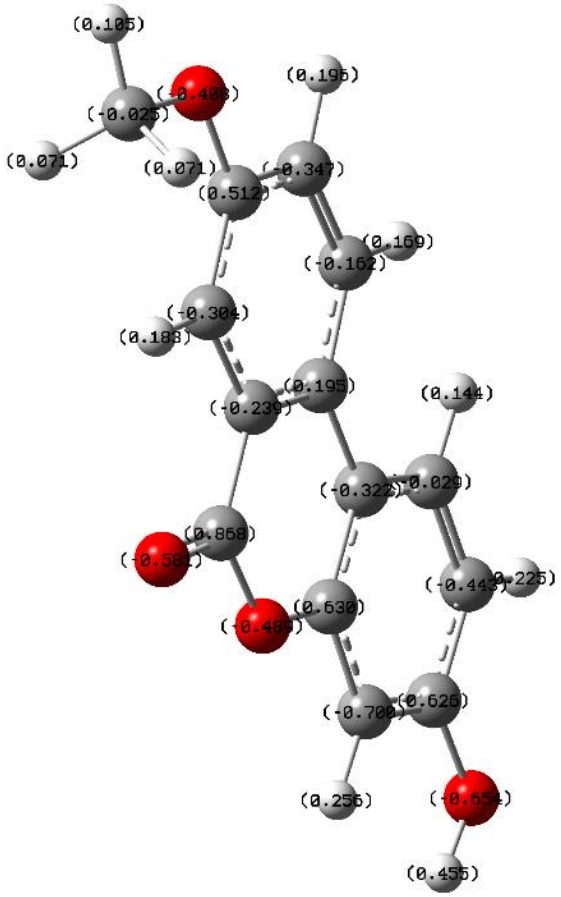

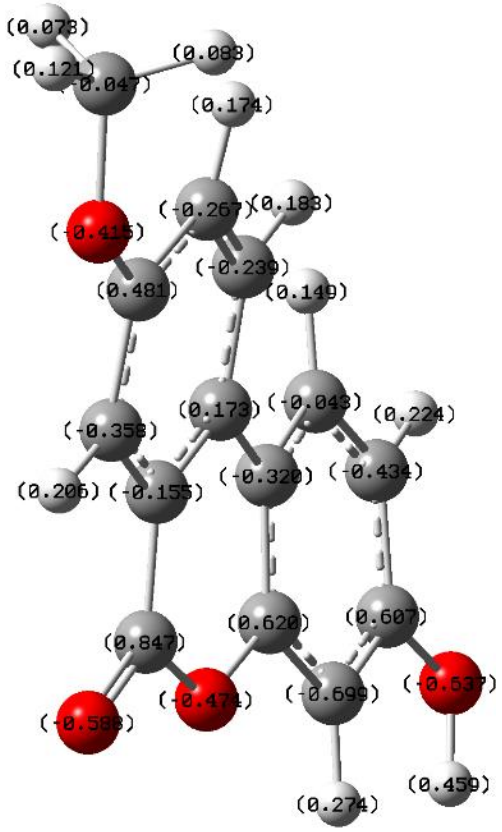

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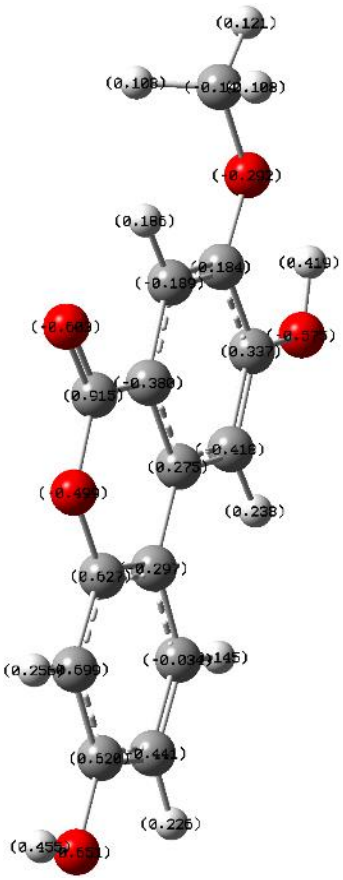

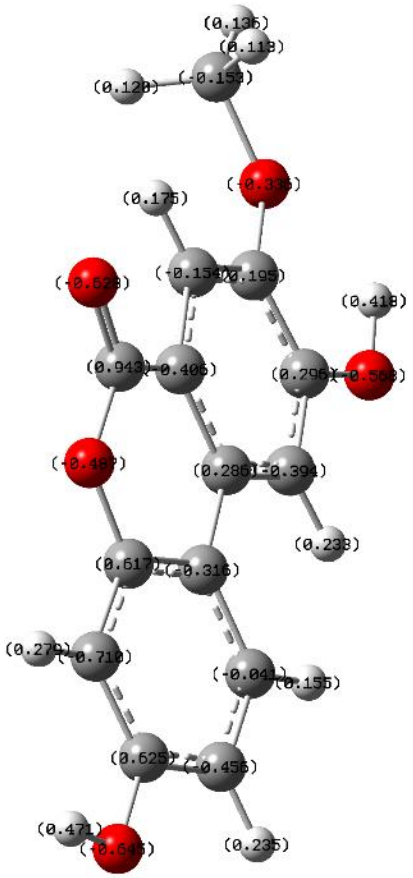

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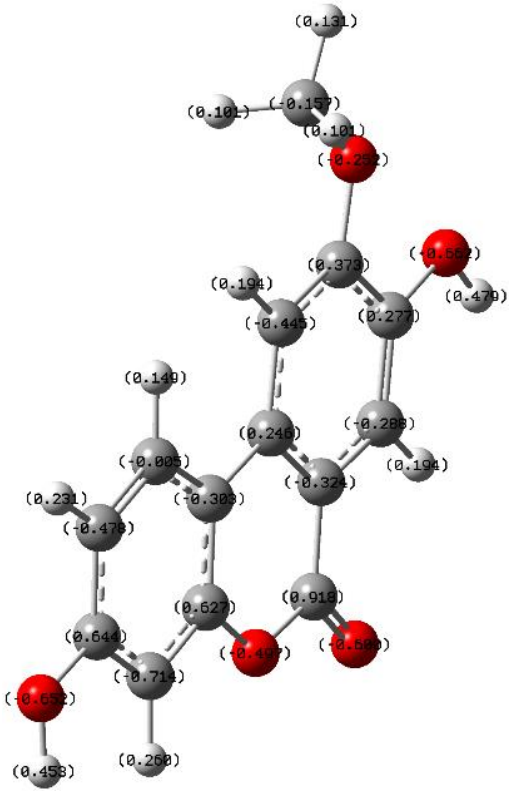

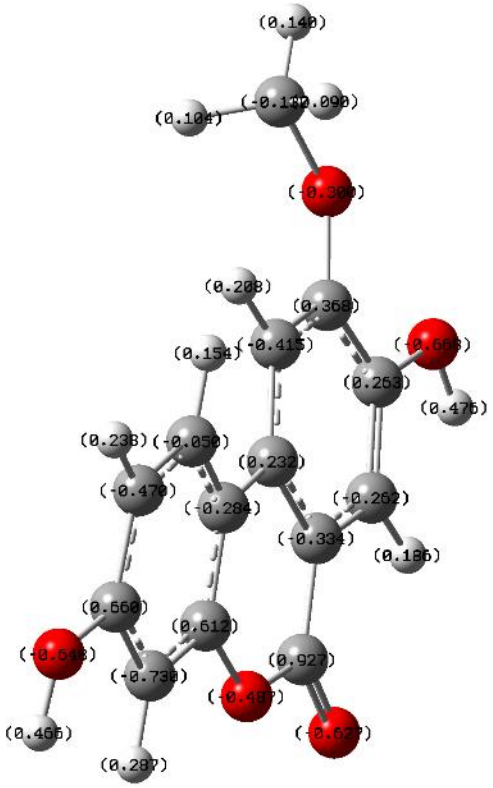

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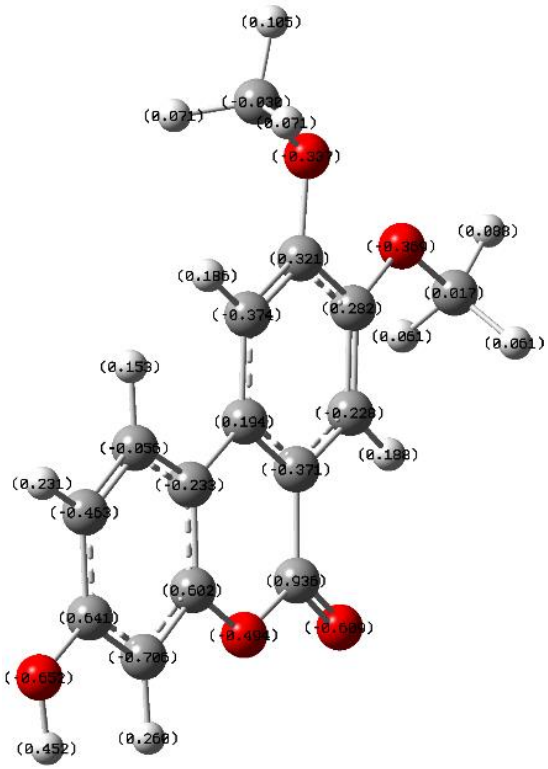

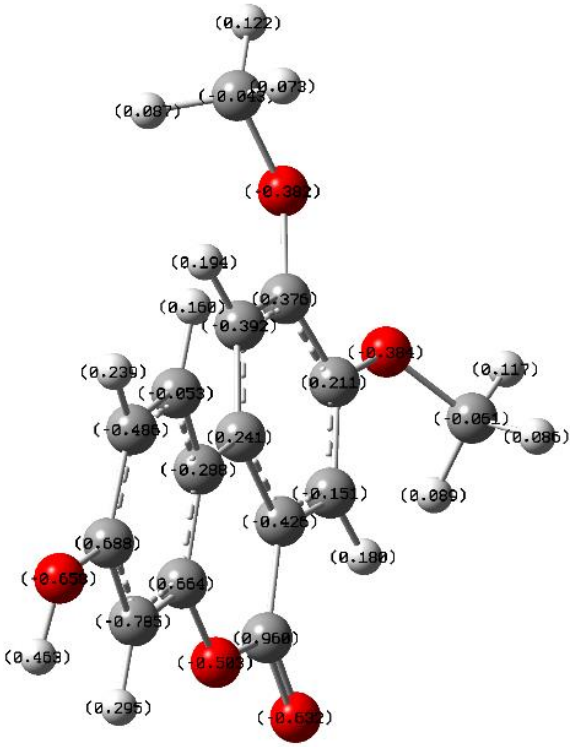

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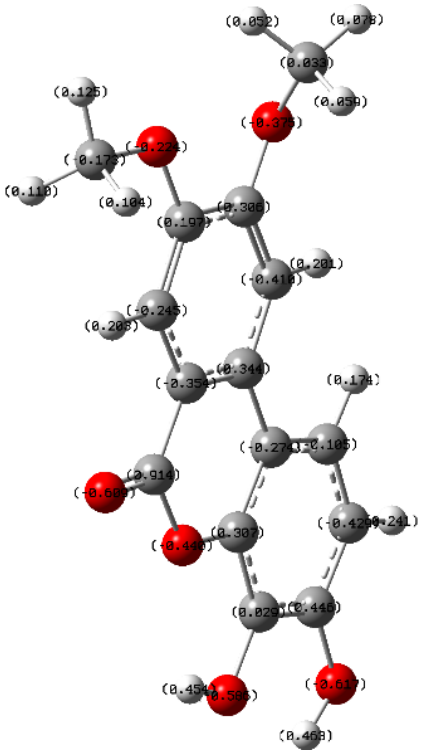

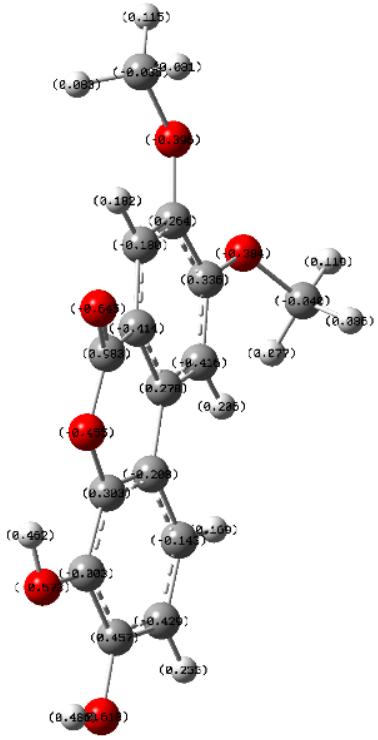

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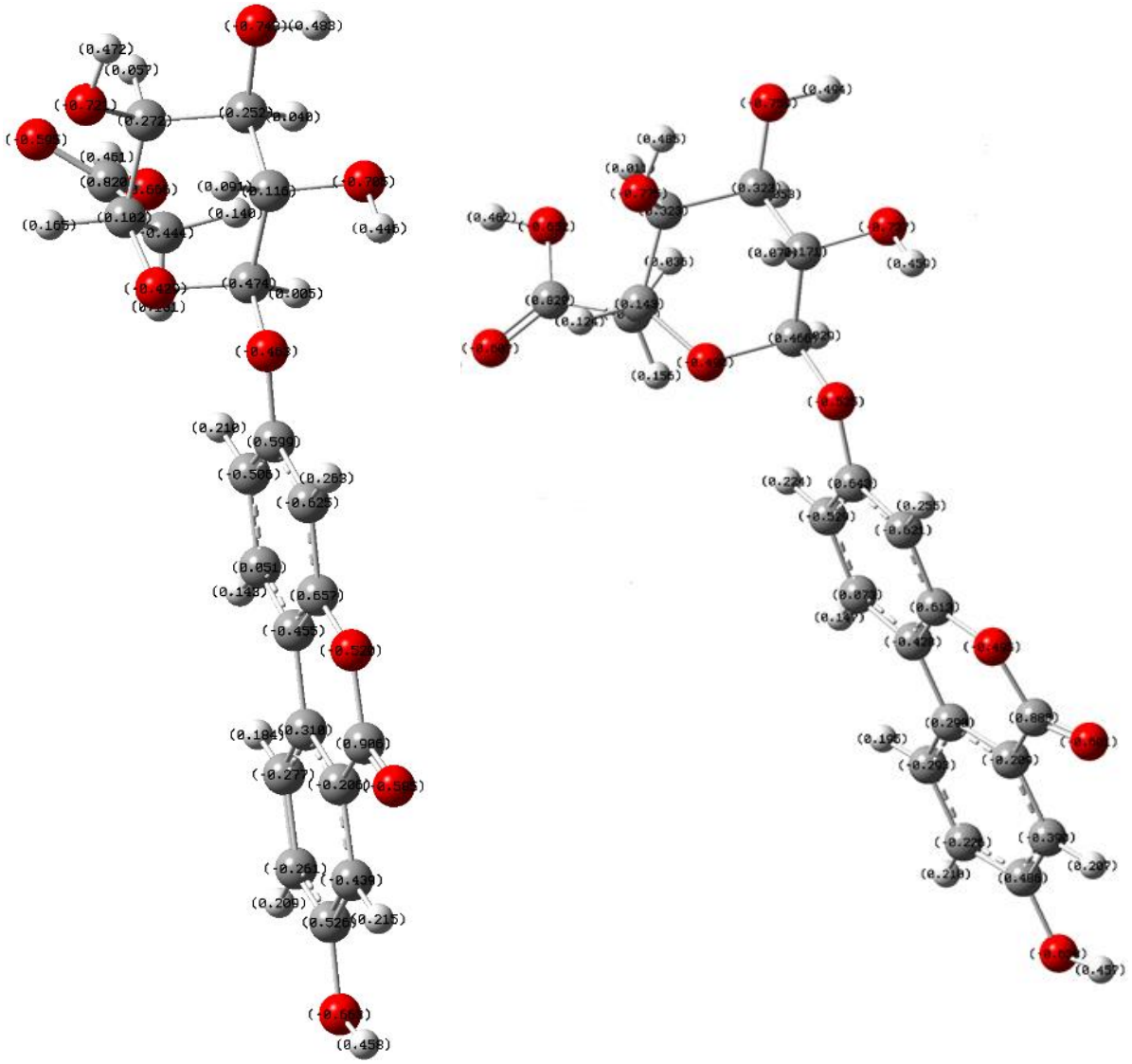

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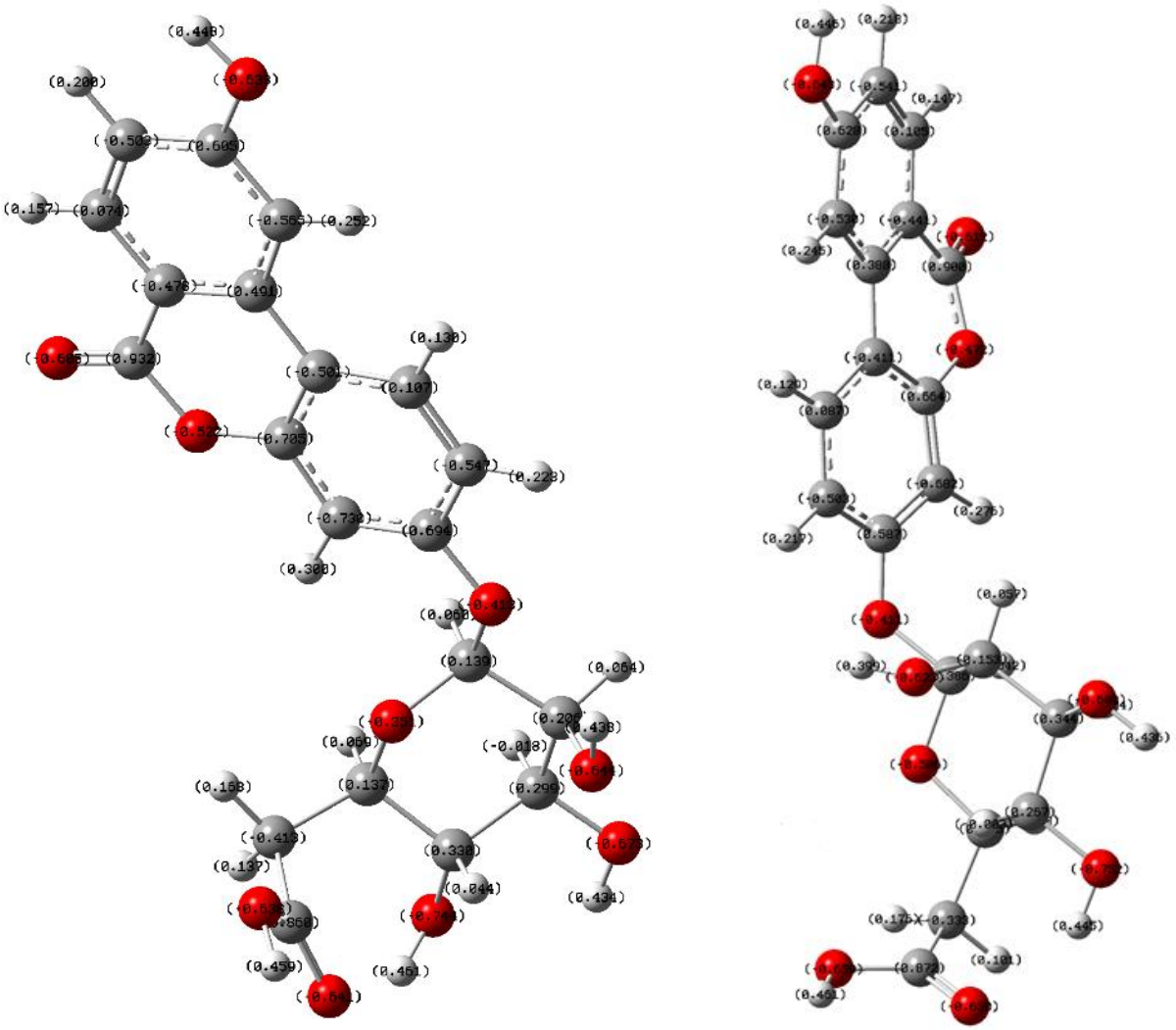

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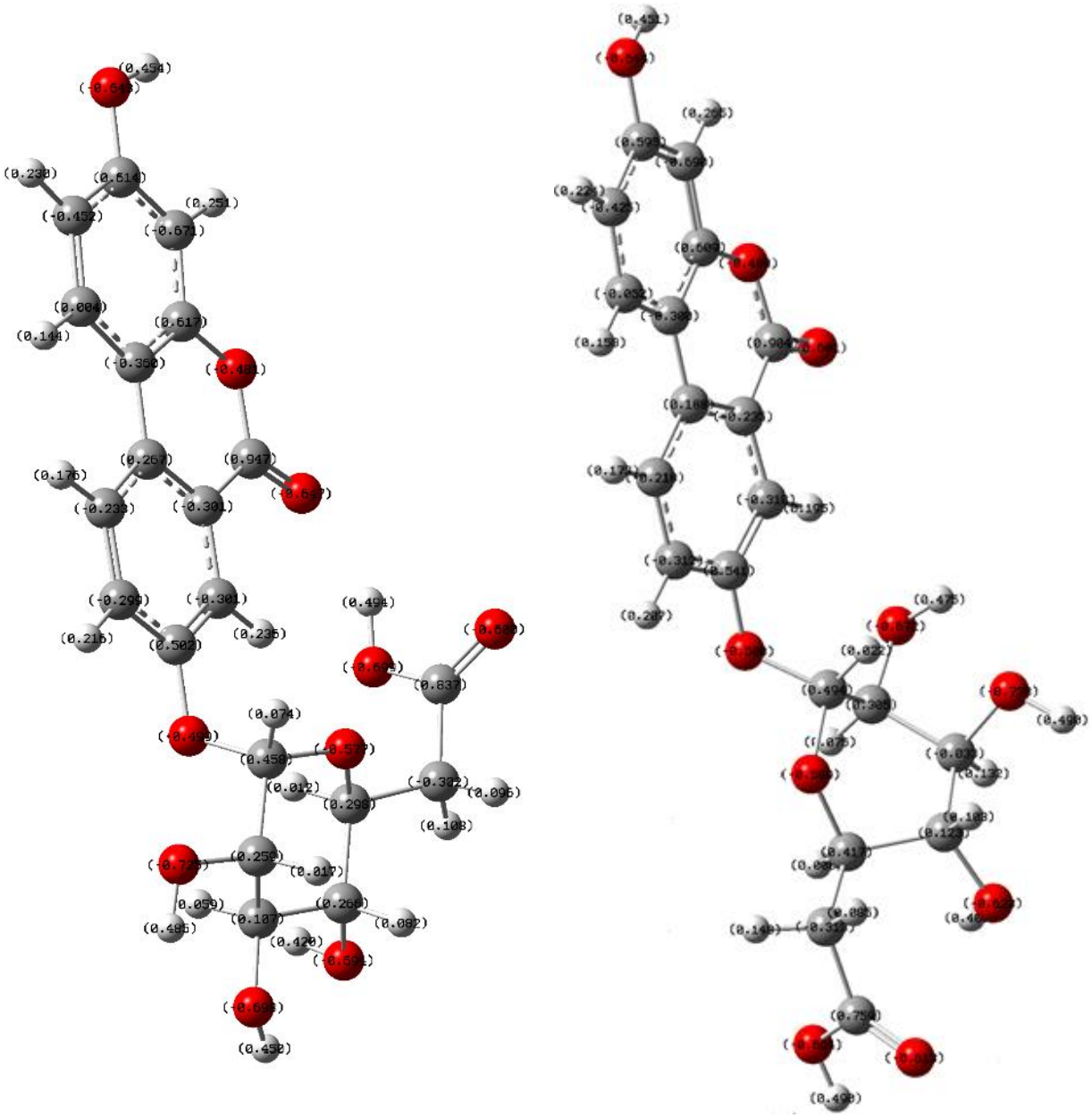

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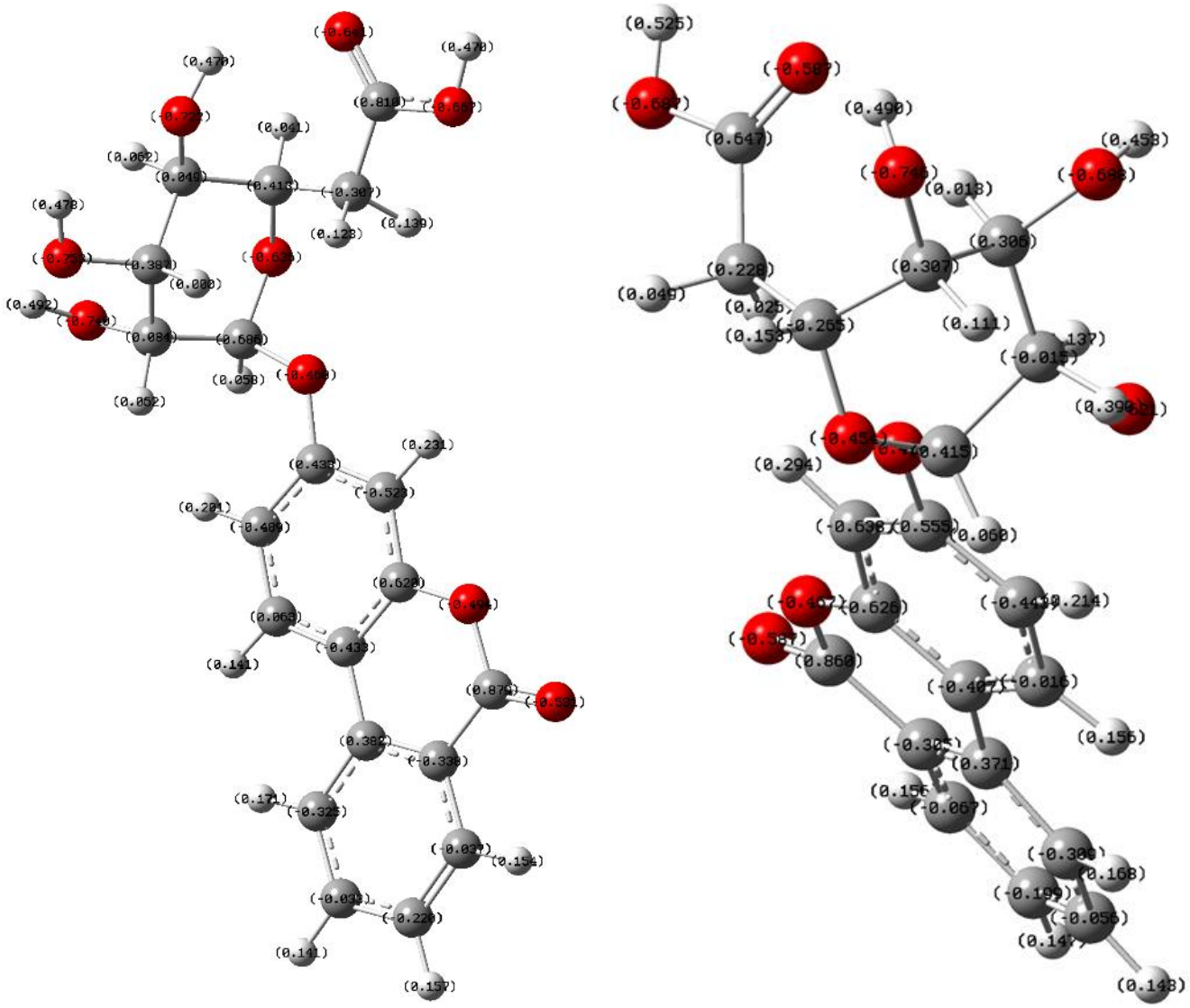

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Figure S3. The charge distributions of the optimized free ligands (left panel) and those placed in the binding site of CK2 (right panel).