SUPPORTING INFORMATION

Progress in modeling complex dye mixtures: a case study for cultural heritage

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Supporting Information

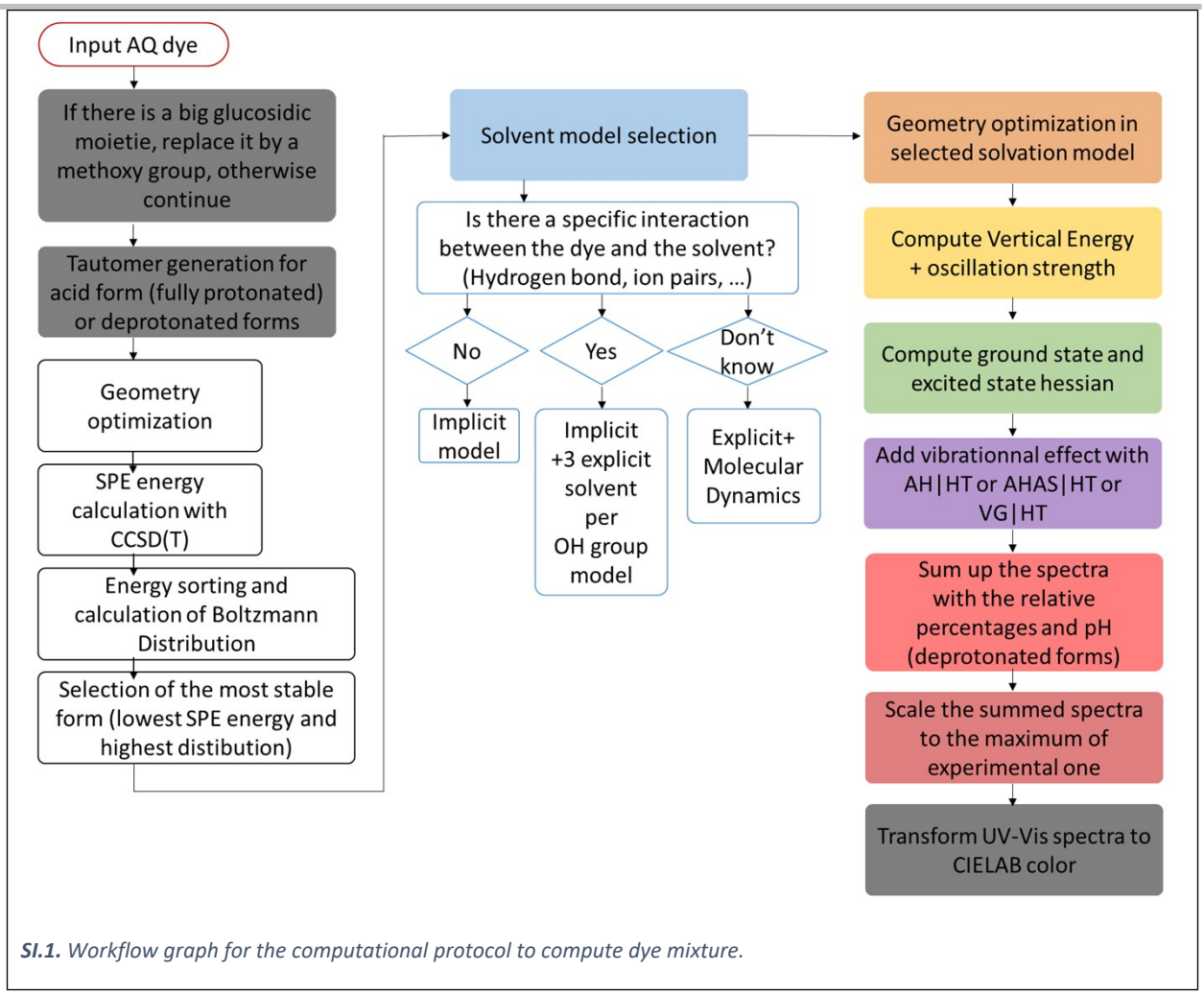
1. Computational method

This computational protocol has been studied by us and compared with available experimental data. We have reported the accuracy of this protocol in a previous article. [1] The computational details can be found in the original article.

UV-Vis Spectrum computation

The relative percentage of madder extract was measured by LC-UV-MS/MS method. Using the measured percentages (Table 1), we computed the absorption spectra and color for all detected molecules. All calculations were carried out using a development version of the ORCA quantum chemistry program package.[2] We first optimized all molecules with the PBE0 functional with the D3(BJ) dispersion correction, along with def2-TZVP basis and matching auxiliary basis. [3–6] The same functional was used for time-dependent DFT (TDDFT) calculations. There is no imaginary frequencies above 10 cm^{-1}. For the neutral form, implicit water solvation was used with the linear response Conductor-like Polarizable Continuum Model (C-PCM). [1] For deprotonated forms, the latest Grimme's open-source Conformer-Rotamer Ensemble Sampling Tool (CREST), which relies on the xTB method was used to generate different deprotonated forms.[7–9] Then, the geometry was reoptimized with PBE0 and the single point energy (SPE) was computed using DLPNO-CCSD(T). [10] The deprotonated form which exhibit lowest SPE was taken into account for further computation. Then, a combined approach involving both implicit and explicit water molecules (3 water molecules per OH group) was used. The water molecules were positioned as to make hydrogen bonds with each hydroxyl group or carboxyl groups. All optimized geometries and other details can be found in the supplementary data. The same protocol was used to compute the vertical absorption energies and excited state (ES) geometries. For madder's molecules, only one bright state (S0→S1) contributes to the visible spectra and was selected accordingly in our calculations. The transition can be described as a combined n->π* and π->π* located on the conjugated rings with the difference densities plotted in SI.7. The SI.6 shows the computed vertical energy compared to experimental data found in the literature.[8] Finally, we have to take into account the pH of the solution of about 6.5 in water. For galiosin, pseudorpurpurin, and munjistin, this leads to the carboxy groups being deprotonated, and for alizarin and purpurin one of their hydroxy groups. The vibrational contributions, including Herzberg–Teller effects, were done using the Excited State Dynamics (ESD) module within ORCA. [11–13]

Three methods were tested: Vertical Gradient (VG), Adiabatic Hessian After-Step (AHAS), and Adiabatic Hessian (AH). For the computed spectra, the linewidth was created using a Gaussian distribution and was set with keyword inlinew 2000 cm^{-1}. AH requires geometry and frequencies at the ES minimum, while VG and AHAS approximate the excited-state structure via a short displacement of the ES potential energy surface. VG approach assumes that the GS is the same as the ES one, while AHAS computes the frequencies at the new position. VG is efficient and reliable for mixture spectra prediction, but AH, though theoretically more accurate, had convergence issues with sugar-containing molecules due to large ES geometry displacements. To address this, sugar moieties were replaced with methoxy groups. AHAS offers a compromise, resolving convergence issues. For full spectra prediction, each computed spectrum (where the oscillator strength "fosc" is proportional to the extinction coefficient) was weighted according to the percentages in Table 1, summed without modifying the oscillator force, and then scaled against experimental data for effective comparison. CIELAB color coordinates were then calculated for the computed and experimental UV-Vis spectra[14–16] The CIELAB represents colors with L* (lightness), a* (green-red), and b* (blue-yellow). ΔE measures color differences, with ΔE_{2000} preferred for accuracy. This work will use ΔE_{2000} to compare computed and experimental madder mixture colors. [46]The experimental pH and pKa of alizarin (pKa_1 =5.2 and pKa_2=11.5) and purpurin (pKa_1= 5.2 and pKa_2=6.8) [17] were taken into account in the percentage following the Henderson-Hasselbach's equation.



SI.1. *Workflow graph for the computational protocol to compute dye mixture.*

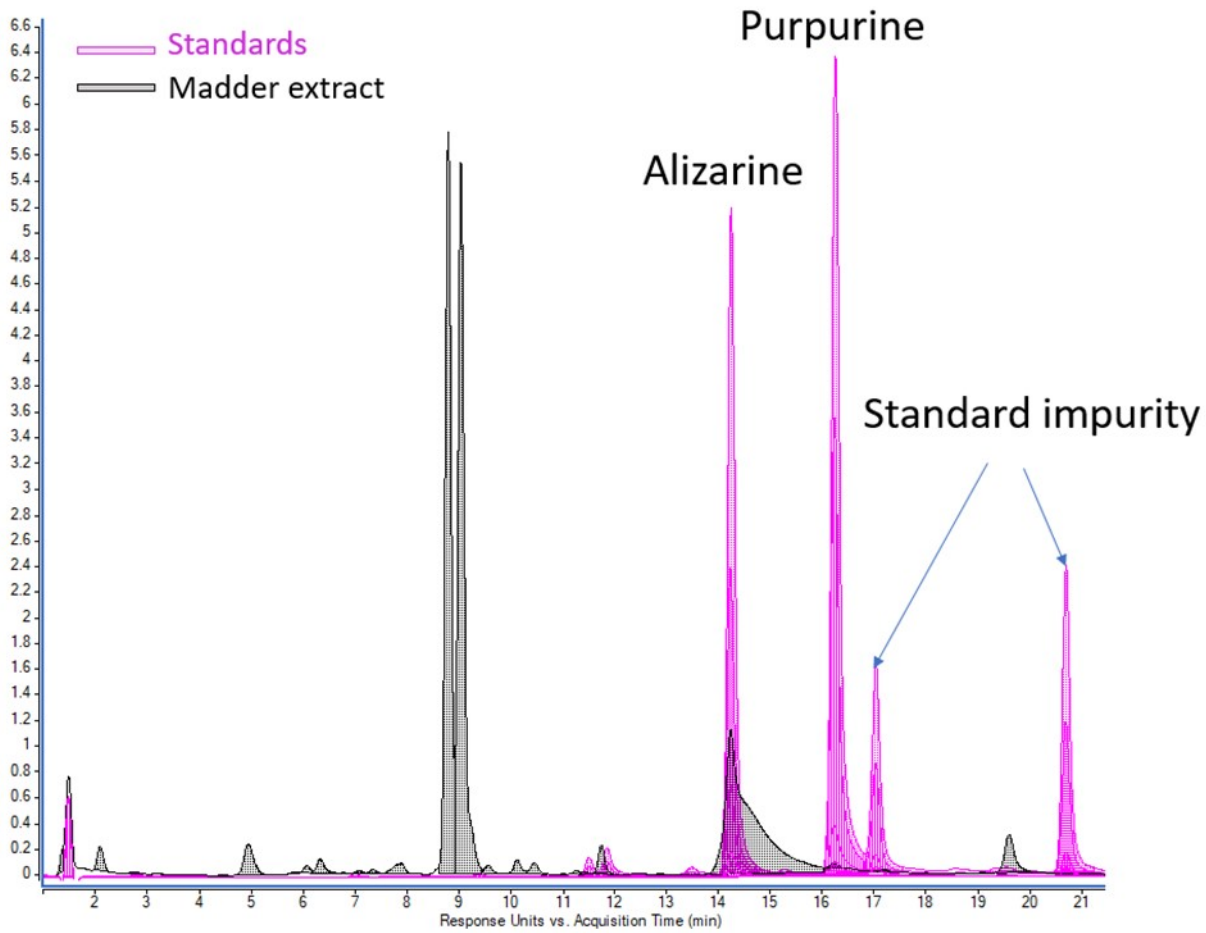
2. Experimental method

Alizarin (97 % purity), purpurin (90%) were purchased from Sigma Aldrich and used without further purification. Madder extract powder (*Rubia tinctorum* L.) is purchased from Ôkhra. Three samples were solubilized in MeOH/H2O 50:50 and sonicated 10 minutes. The Madder extract was diluted at 5 mg/mL, and the standards of Alizarine and Purpurin at 1 and 2 mg/mL respectively. Due to incomplete solubilization, samples were centrifugated and 100 µL of the supernatant was used for LC-UV-MS/MS analysis, 1.5 mL is left for UV-Vis spectra measurement. Relative quantification was performed.

Liquid chromatography-UV-tandem mass spectrometry (LC-UV-MS/MS) experiments were performed on a 1290 Infinity II LC system coupled to a Q-TOF 6540 mass spectrometer equipped with an ESI source operated in the negative and positive ionization mode. The chromatographic separation was carried out on a Zorbax 300SB-C8 (150 × 2.1 mm, 5 µm) column heated at 35 °C at a flow rate of 300 µl/min with water at 0.1% of formic acid as solvent A and acetonitrile as solvent B. Five microliters of samples in MeOH/H2O 50:50 were injected using the following gradient: 0 min (10% B), 25 min (55% B), 30 min (100% B), 35 min (100% B), 36 min (10% B)and 6 min of equilibration time. Ion source conditions were set for negative ion mode: capillary voltage 3.5 kV, Fragmentor voltage 125 V, Skimmer 65 V, Drying gas at 10 l/min, 275 °C, and sheath gas flow at 10 l/min, and 325 °C. UV detection was performed at 232 and 260 nm for quantitation at 260 nm. The TOF was operated in the 50−1700 m/z mass range using a medium isolation window and 20eV of collision energy for MS/MS. Data Acquisition 9.0 and Qualitative Analysis 8.0 software were used to process data.

The UV-Vis spectra of madder extract was measured using an Ocean Optics Flame spectrometer (Model: FLMS00699) with a wavelength range from 300 to 850 nm. The integration time for each measurement ranged from 5 ms to 10 ms. The light source used was a Deuterium-Tungsten Halogen lamp covering the range of 300 nm–850 nm. The blank was done using deionized water. This light source was coupled

to the spectrometer using 400 µm diameter optical fibers and positioned through a 1 cm quartz cuvette holder. The acquisition of spectra was facilitated by the Ocean View software.



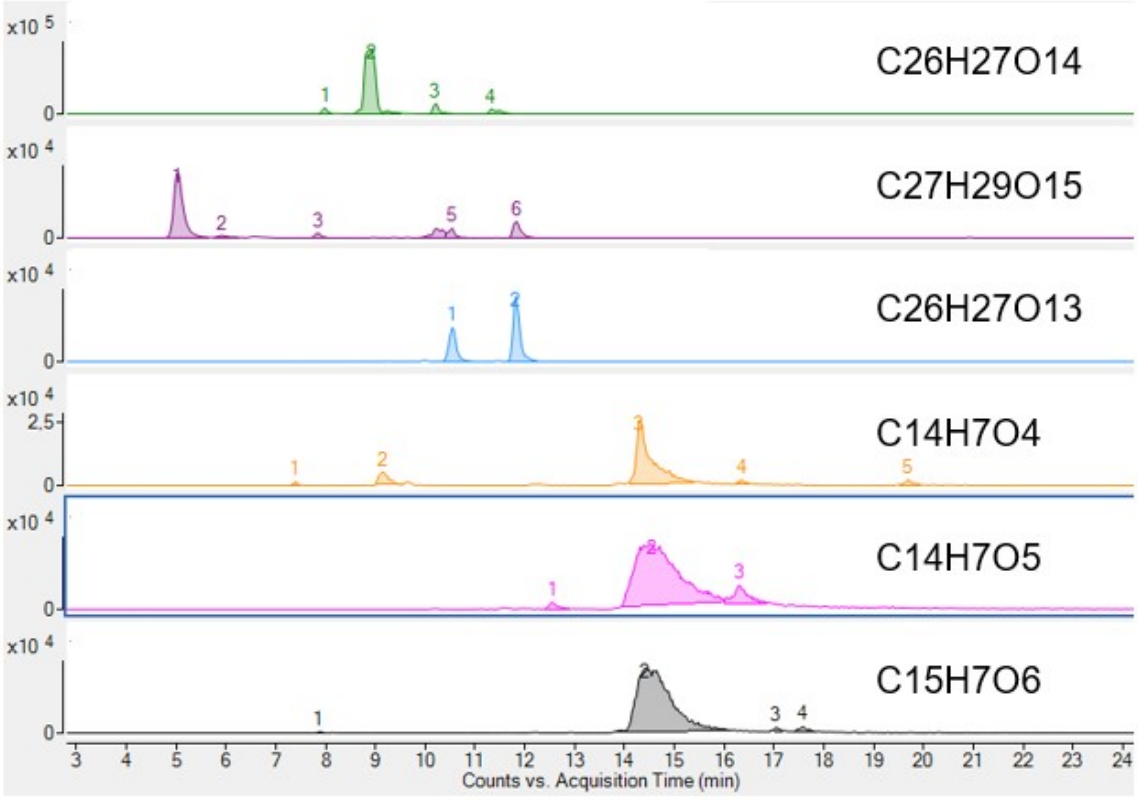
SI.2. Overlay of LC-UV experiments at 260 nm of Madder extract (in black) and Alizarine and Purpurine standard solution at concentrations ranging from 420 µg/mL to 2 ng/mL (in pink).

SI.3. Relative percentage, retention time, mass/z, chemical formula, and attributed molecule for the madder extract (*Rubia Tinctorum* L.) using LC-UV-MS/MS.

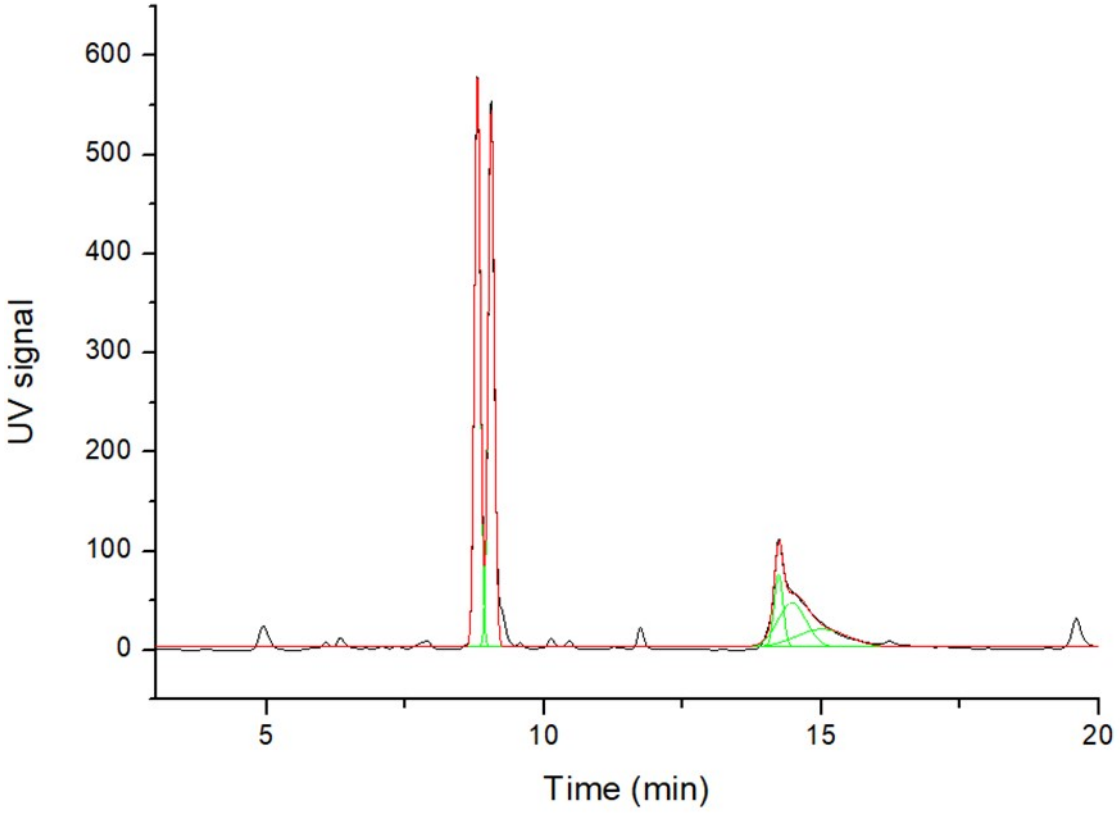
PEAK	RT	AREA SUM %	M/Z $[M-H]^-$	CHEMICAL FORMULAE	MOLECULE ATTRIBUTED
1	1.4	0.4	387.1145	ND	+46
2	1.7	0.05	377.0860	ND	ND
3	2.1	0.97	431.1196	ND	251.0557 + Glc
4	2.7	0.07	459.1142	ND	+46
5	3.2	0.04	387.1140	ND	ND
6	3.9	0.04	729.2606	ND	521.2022+GlcGlc+46
7	4.4	0.03	583.2026	ND	ND
8	**4.9**	**2**	**593.1151**	**C26H25O16**	**Galiosin**
9	5.8	0.04	461.0719	C21H17O12	255.0294+Glc+CO_2
10	6.1	0.33	497.1299	ND	ND
11	6.3	0.74	365.0875	ND	+163
12	6.8	0.02	461.0719	C21H17O12	255.0291+Glc+CO_2

13	7.1	0.11	655.2238	ND	+163
14	7.3	0.14	445.0772	C21H17O11	239.0397+Glc+CO_2
15	7.9	0.77	563.1405- 593.1506- 623.1615	C26H27O14 C27H29O15 C28H31O16	239.0347+Glc-Glc (6-hydroxyrubiadin-3-O-neohesperidoside) 253.0505+Glc-Glc (6-Hydroxyrubiadin-3-O-neohesperidoside) 283.0606+Glc-Glc
16	**8.8**	**30.22**	**563.1411**	**C26H27O14**	**Lucidin primeveroside**
17	**9**	**31.75**	**533.1307**	**C25H25O13**	**Ruberythic acid**
18	9.6	0.4	401.0873	C20H17O9	239.0339+Glc
19	10.1	0.69	563.1402- 593.1505	C26H27O14 C27H29O15	**Lucidin primeveroside** 269.0460+Glc-Glc
20	10.5	0.55	547.1454- 593.1505	C26H27O13 C27H29O15	Rubiadin primeveroside 251.0338+Glc-Glc
21	11	0.01	431.0978	ND	ND
22	11.3	0.13	563.1401	C26H27O14	**Lucidin primeveroside**
23	11.4	0.09	563.1398	C26H27O14	**Lucidin primeveroside**
24	**11.7**	**1.19**	547.1455- 593.1507	C26H27O13 C27H29O15	Rubiadin primeveroside 253.0509+Xyl-Glc+46
25	12.4	0.02	447.1657	ND	+163
26	12.9	0.03	343.0819	ND	ND
27	**14.2**	**6.00**	**239.0346-**	**C14H7O4**	**Alizarin**
27	**14.2**	**11.4**	**255.0300-**	**C14H7O5**	**Purpurin**
27	**14.2**	**8.6**	**283.0245-**	**C15H7O6**	**Munjistin**
27	14.2	0.06	299.0201	C15H7O7	Pseudopurpurin
28	16.2	0.24	255.0298- 299.0196	C14H7O5 C15H7O7	**Purpurin Pseudopurpurin**
29	17.2	0.08	293.1758	ND	
30	17.5	0.02	283.0243	C15H7O6	**Munjistin**
31	18	0.02	255.0297	C14H7O5	**Purpurin**
32	18.3	0.02	299.0195	C15H7O7	**Pseudopurpurin**
33	19.1	0.04	253.0504	C15H9O4	Rubiadin
34	**19.6**	**2.55**	**267.0296**	**C15H7O5**	**Nordamcanthal**
35	20.9	0.01	299.0194	C15H7O7	**Pseudopurpurin**
36	25.8	0.15	299.0192	C15H7O7	**Pseudopurpurin**

SI.4. Extracted ion chromatogram of various isomers in the Madder extract.



SI.5. Deconvolution LC-UV experiments at 260 nm of Madder extract and fit of the peak at retention time RT=14.2min**.**



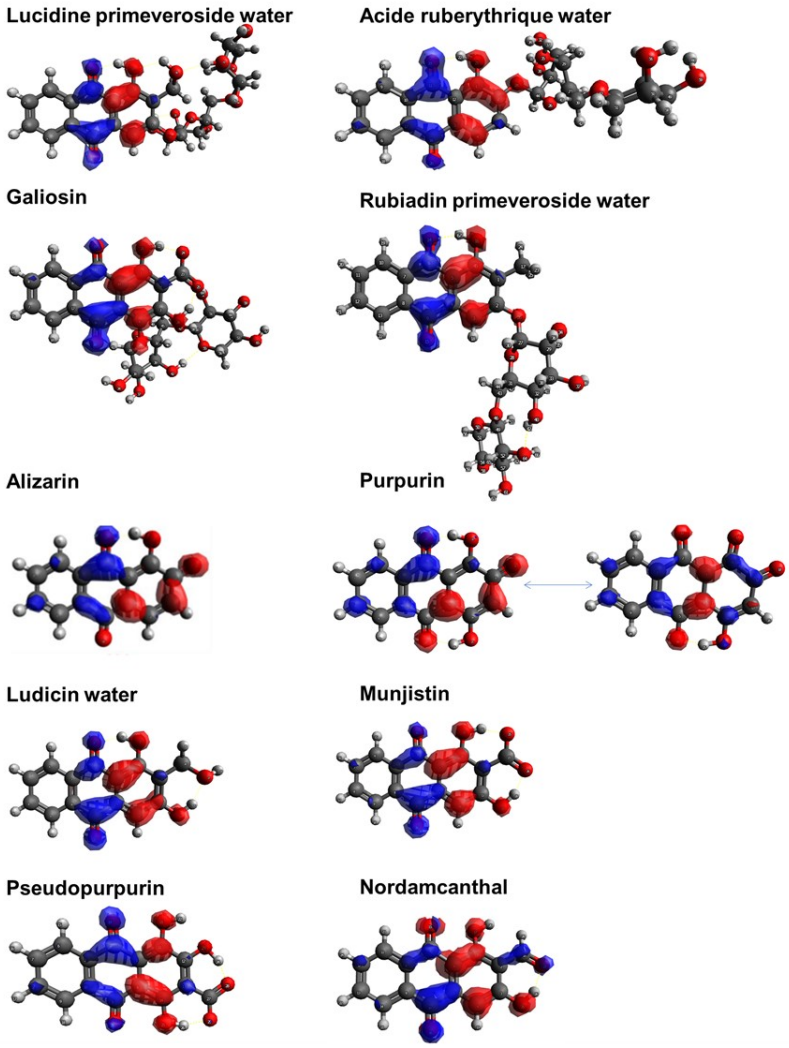
SI.6. Benchmark of functional (B3LYP, B2PLYP and PBE0) for TD-DFT computation of Vertical energy (VE). The table represents the absolute error deviation (calc.-exp.) for computed VE of different deprotonated forms of alizarin.

	Absolute error deviation (eV)		
	B3LYP	B2PLYP	PBE0
Alizarin neutral	0.06	0.06	0.05
Alizarin monoanionic	0.30	0.27	0.21
Alizarin dianionic	0.01	0.04	0.05

SI.7. Experimental and computed maximum absorption energies of some madder molecules and their respective error deviation (in eV) which are less than 0.10 eV. The experimental data is extracted from the literature. [18]

Molecules	Calc. VE (eV)	Exp. (eV)	Abs. Calc.-Exp (eV)
Lucidin primeveroside	3.03	3.05	0.02
Ruberythric acid	2.91	2.97	0.06
Galiosin	2.82	2.86	0.04
Rubiadin primeveroside	3.08	3.01	0.07
Anthragallol	3.10	3.00	0.10
Lucidin	3.02	3.00	0.02
Alizarin	2.93	2.90	0.03
Purpurin	2.59	2.58	0.01
Xanthopurpurin	3.05	2.98	0.07
Rubiadin	3.05	3.02	0.03

SI.8. Difference in electronic densities for the first transition $S_0 \rightarrow S_1$ of madder molecules. The red represents an increase in electronic density and the blue a decrease. The isovalue is 0.002 a.u.



SI.9. Total computation time for each method (VG, AHAS and AH) for alizarin and lucidin primeveroside.

Calculation time	Alizarin	Lucidin primeveroside
VG	23 h	164 h
AHAS	21 h	164 h
AH	29 h	26 h

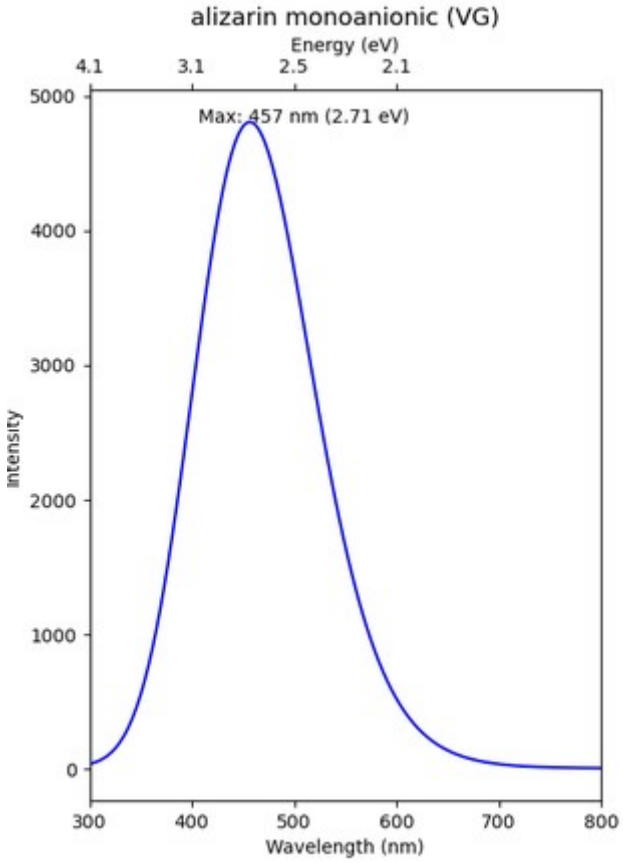
SI.10. ΔE_{2000} formula for color difference between two L*, a*, b* coordinates of two samples. [19,20]

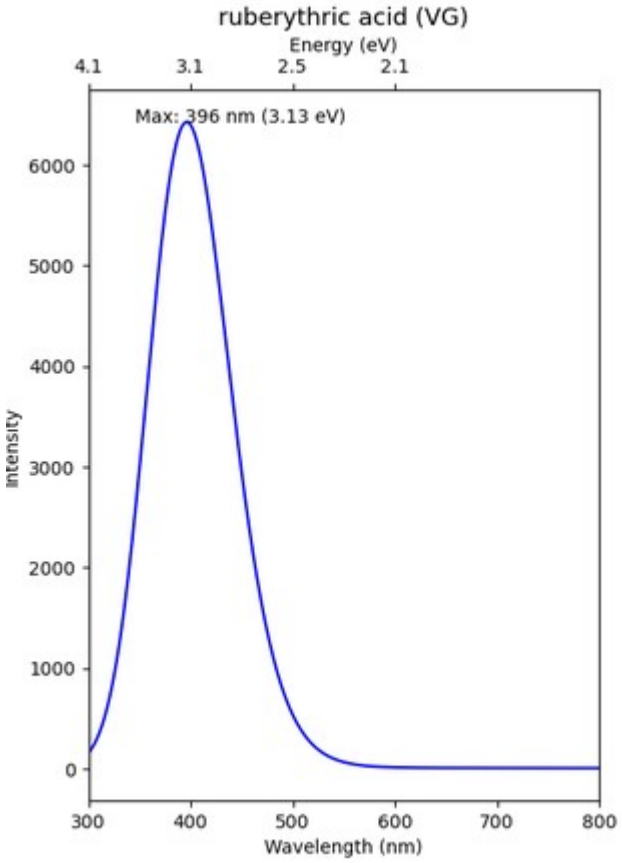
$$\Delta E_{2000} = \sqrt{(\frac{\Delta L'}{K_L S_L})^2 + (\frac{\Delta C'}{K_C S_C})^2 + (\frac{\Delta H'}{K_H S_H})^2}$$

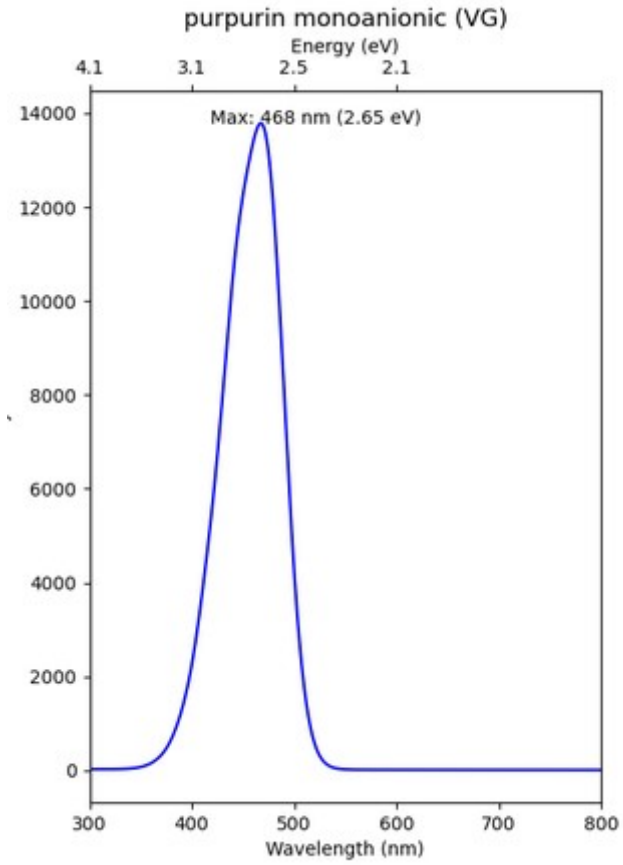
where:

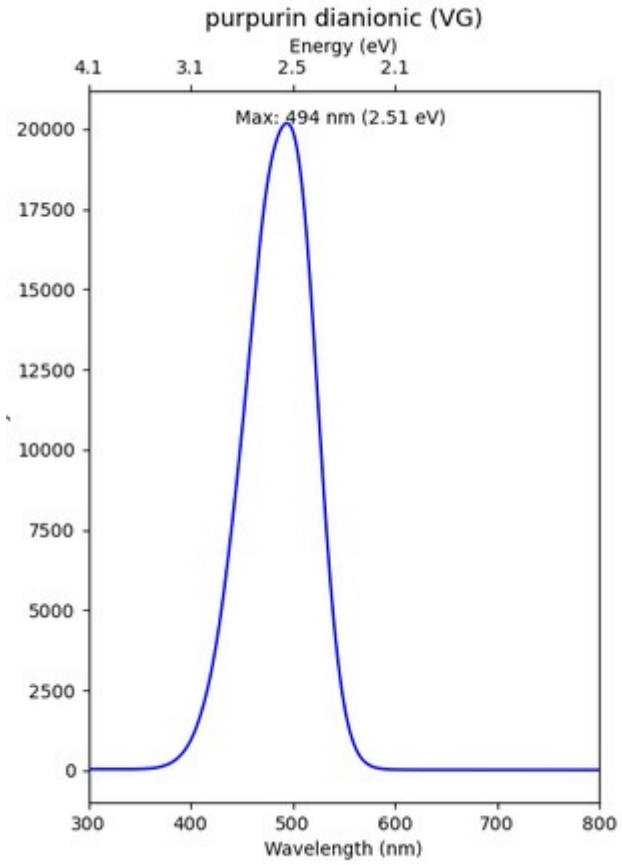
$\overline{L'} = (L_1 + L_2)/2,$
$\Delta L' = L_2 - L_1,$
$C_1 = \sqrt{a_1^2 + b_1^2},$
$C_2 = \sqrt{a_2^2 + b_2^2},$
$\overline{C} = (C_1 + C_2)/2,$
$G = (1 - \sqrt{\frac{\overline{C^7}}{\overline{C^7} + 25^7}})/2,$
$a_1' = a_1(1 + G),$
$a_2' = a_2(1 + G),$
$C_1' = \sqrt{a_1'^2 + b_1^2},$
$C_2' = \sqrt{a_2'^2 + b_2^2},$
$\overline{C'} = (C_1' + C_2')/2,$
$\Delta C' = C_2' - C_1',$
$\Delta H' = 2\sqrt{C_1' C_2'}\sin(\Delta h'/2),$
$S_L = 1 + \frac{0.015(\overline{L}' - 50)^2}{\sqrt{20 + (\overline{L}' - 50)^2}},$
$S_C = 1 + 0.045\overline{C}',$
$S_H = 1 + 0.015\overline{C}'T,$
$\Delta\theta = 30\exp\{-(\frac{\overline{H'} - 275^o}{25})\},$
$R_C = \sqrt{\frac{\overline{C^7}}{\overline{C^7} + 25^7}}),$
$R_T = -2R_C\sin(2\Delta\theta),$
$K_L = 1 - default,$
$K_C = 1 - default,$
$K_H = 1 - default.$

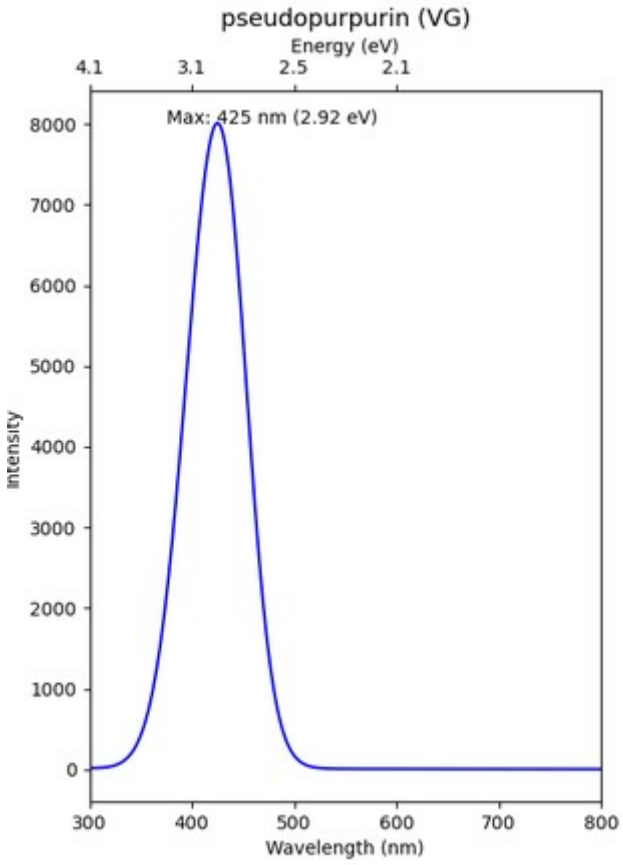
SI.11. Computed individual spectra using Vertical Gradient (VG) method.

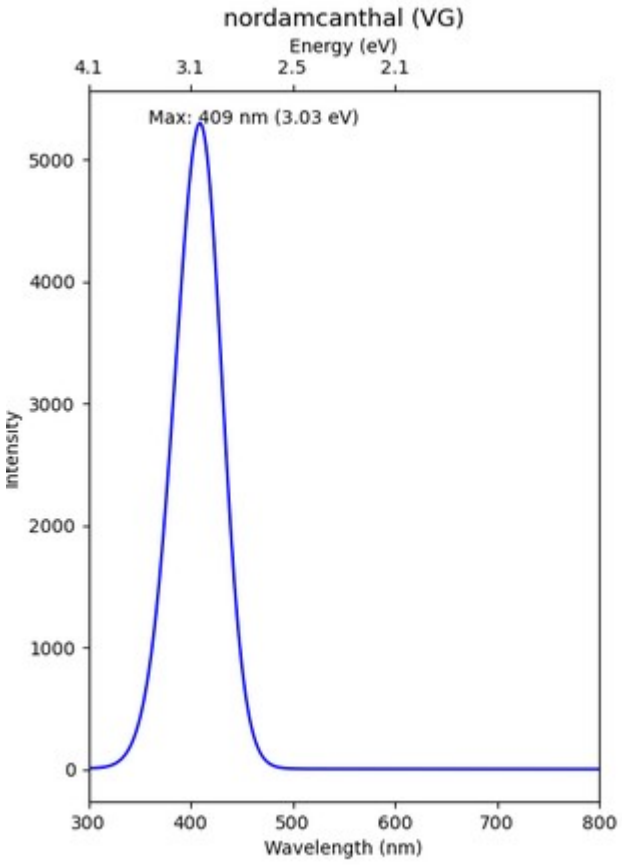


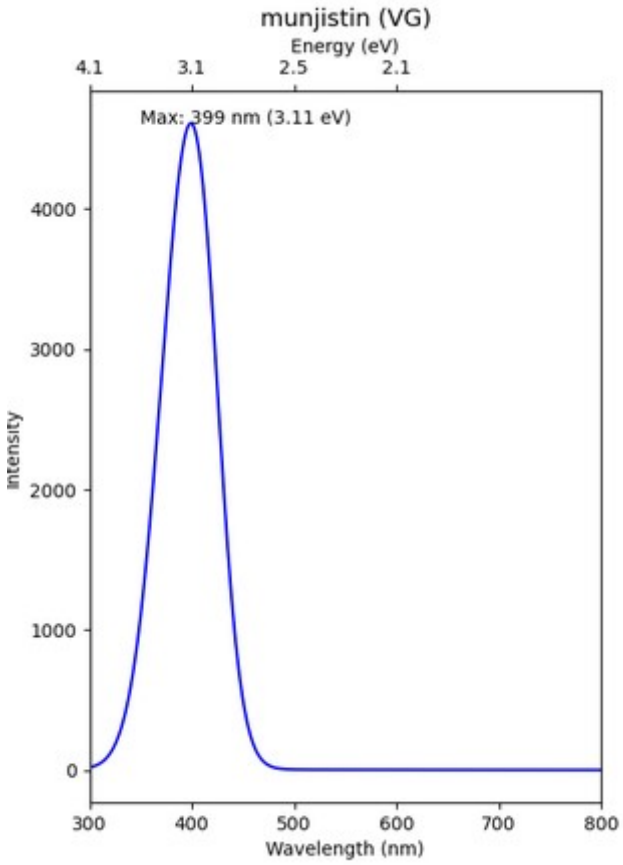


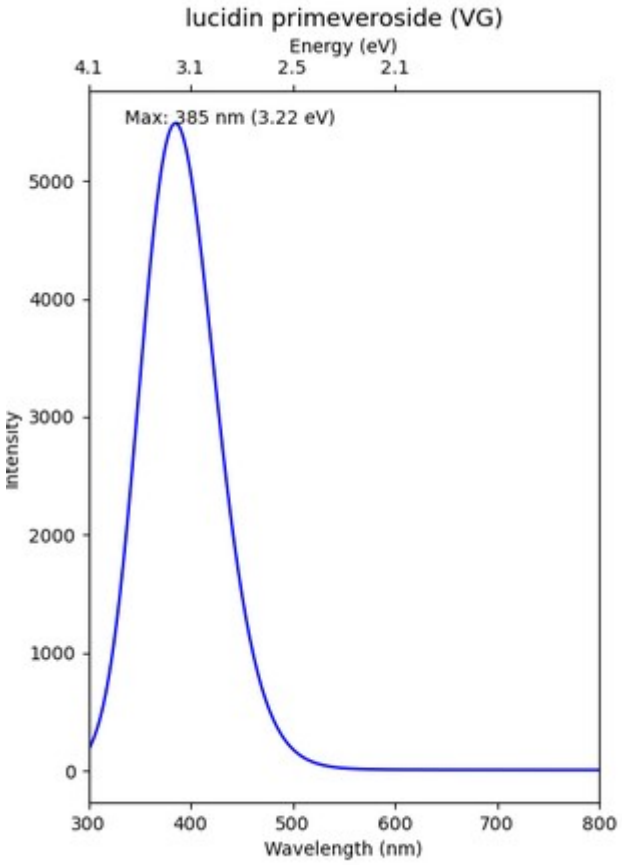

purpurin monoanionic (VG)
Energy (eV)
4.1
3.1
2.5
2.1
Max: 468 nm (2.65 eV)
14000
12000
10000
8000
6000
4000
2000
0
300
400
500
600
700
800
Wavelength (nm)

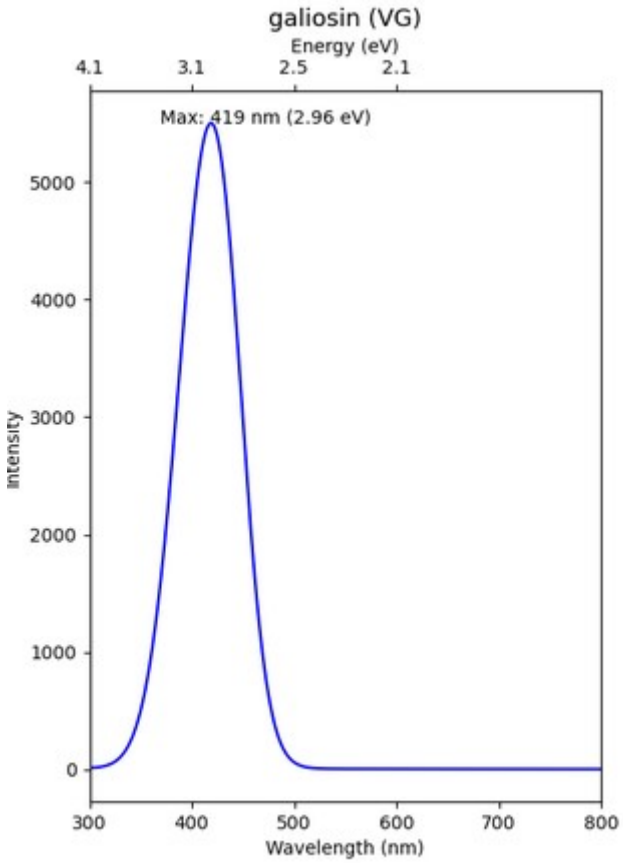

purpurin dianionic (VG)
Energy (eV)
4.1
3.1
2.5
2.1
Max: 494 nm (2.51 eV)
20000
17500
15000
12500
10000
7500
5000
2500
0
300
400
500
600
700
800
Wavelength (nm)


pseudopurpurin (VG)
Energy (eV)
4.1
3.1
2.5
2.1
Max: 425 nm (2.92 eV)
8000
7000
6000
5000
4000
3000
2000
1000
0
Intensity
300
400
500
600
700
800
Wavelength (nm)

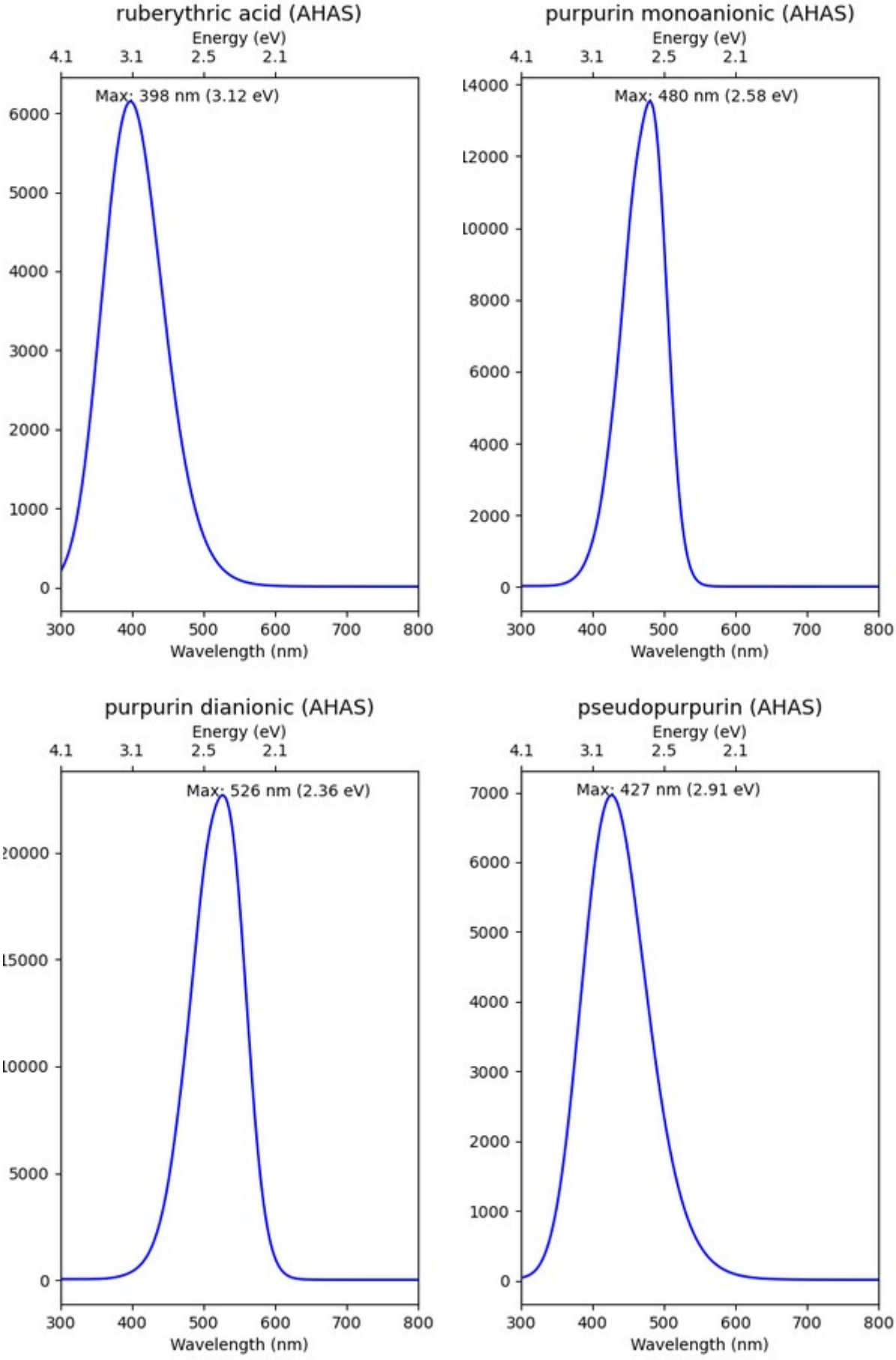

nordamcanthal (VG)
Energy (eV)
4.1
3.1
2.5
2.1
Max: 409 nm (3.03 eV)
5000
4000
3000
2000
1000
0
Intensity
300
400
500
600
700
800
Wavelength (nm)

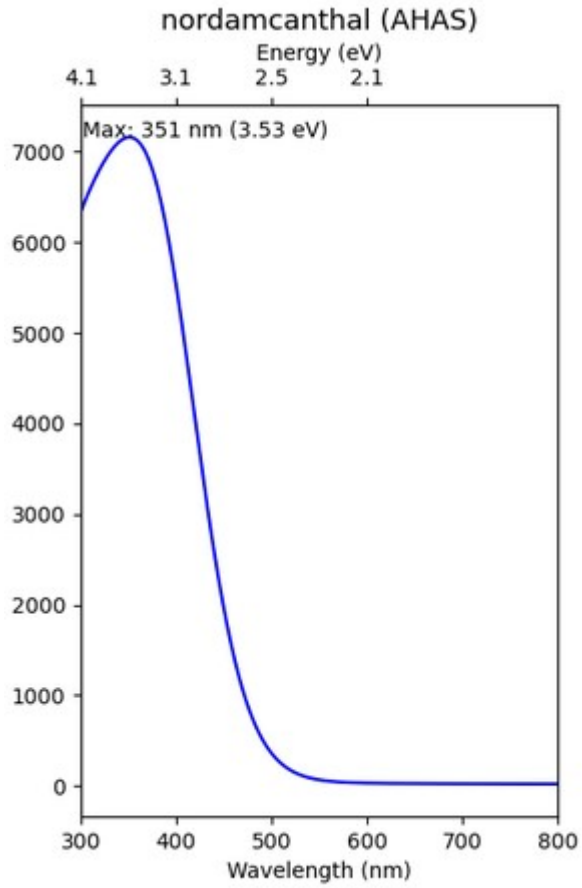

munjistin (VG)
Energy (eV)
4.1
3.1
2.5
2.1
Max: 399 nm (3.11 eV)
4000
3000
2000
1000
0
Intensity
300
400
500
600
700
800
Wavelength (nm)

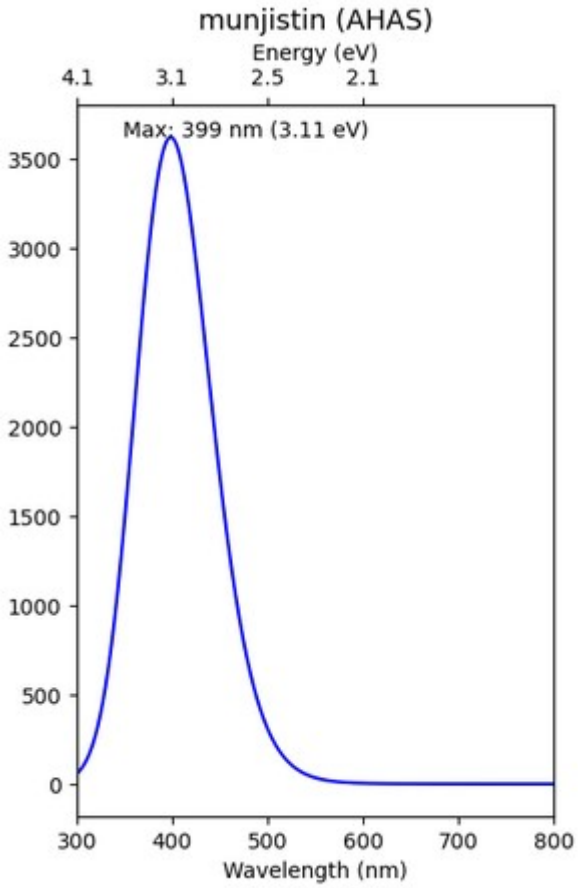

lucidin primeveroside (VG)
Energy (eV)
4.1
3.1
2.5
2.1
Max: 385 nm (3.22 eV)
5000
4000
3000
2000
1000
0
Intensity
300
400
500
600
700
800
Wavelength (nm)

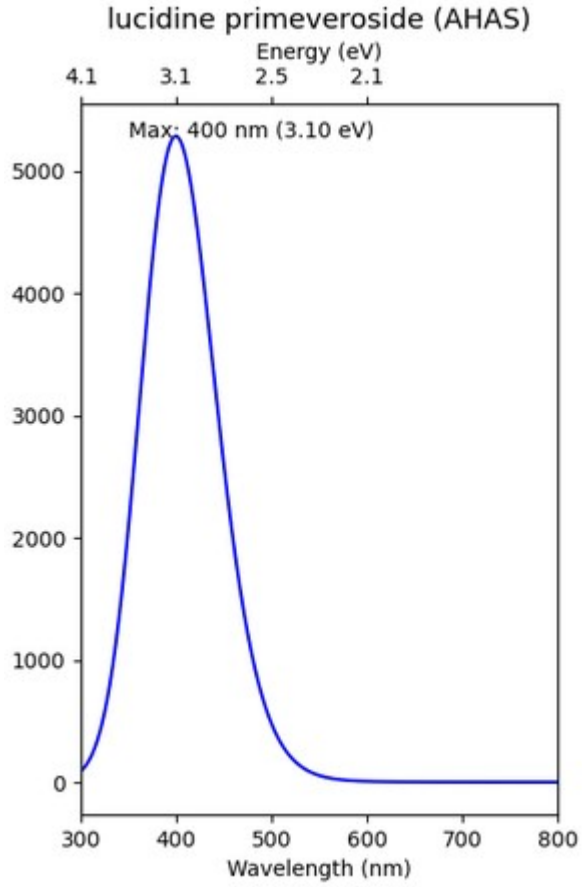

galiosin (VG)
Energy (eV)
4.1
3.1
2.5
2.1
Max: 419 nm (2.96 eV)
5000
4000
3000
2000
1000
0
Intensity
300
400
500
600
700
800
Wavelength (nm)

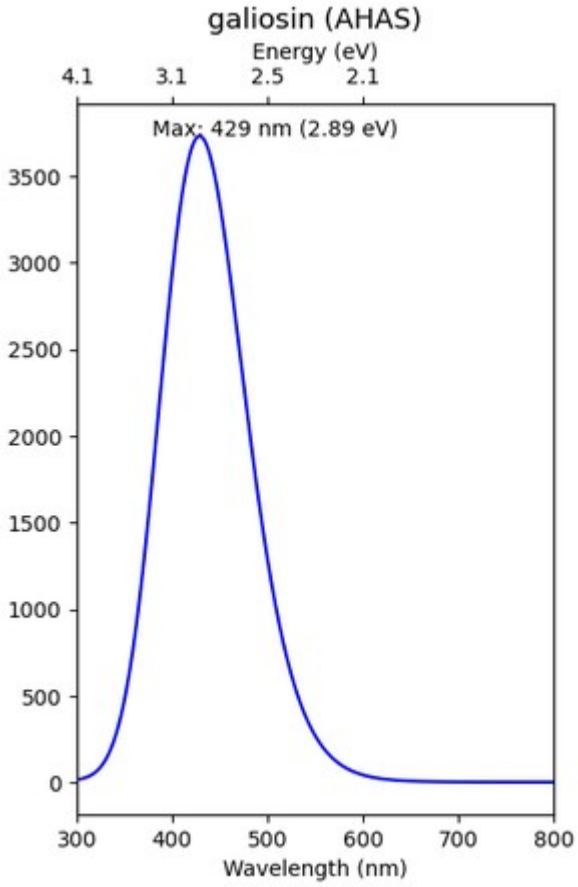
SI.12. Computed individual spectra using Adiabatic Hessian After Step (AHAS) method.

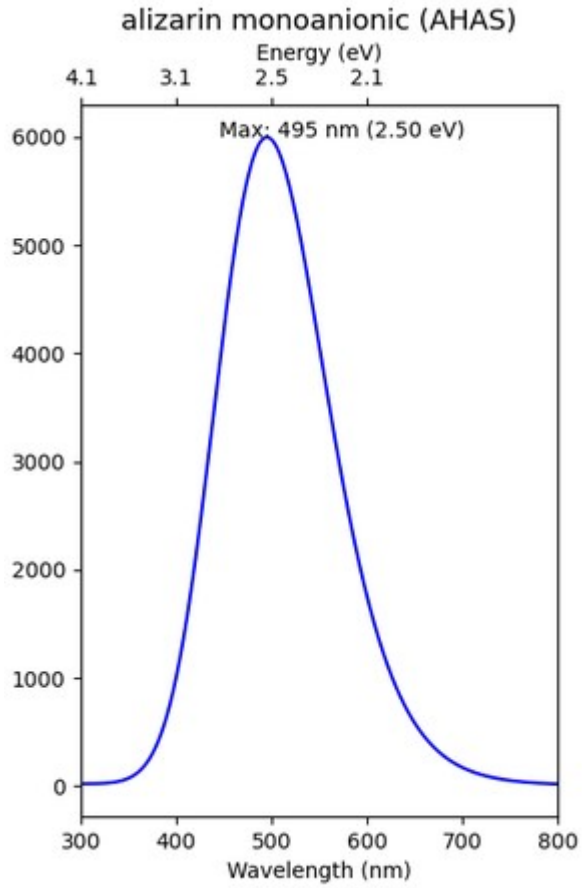



nordamcanthal (AHAS)
Energy (eV)
4.1
3.1
2.5
2.1
Max: 351 nm (3.53 eV)
7000
6000
5000
4000
3000
2000
1000
0
300
400
500
600
700
800
Wavelength (nm)

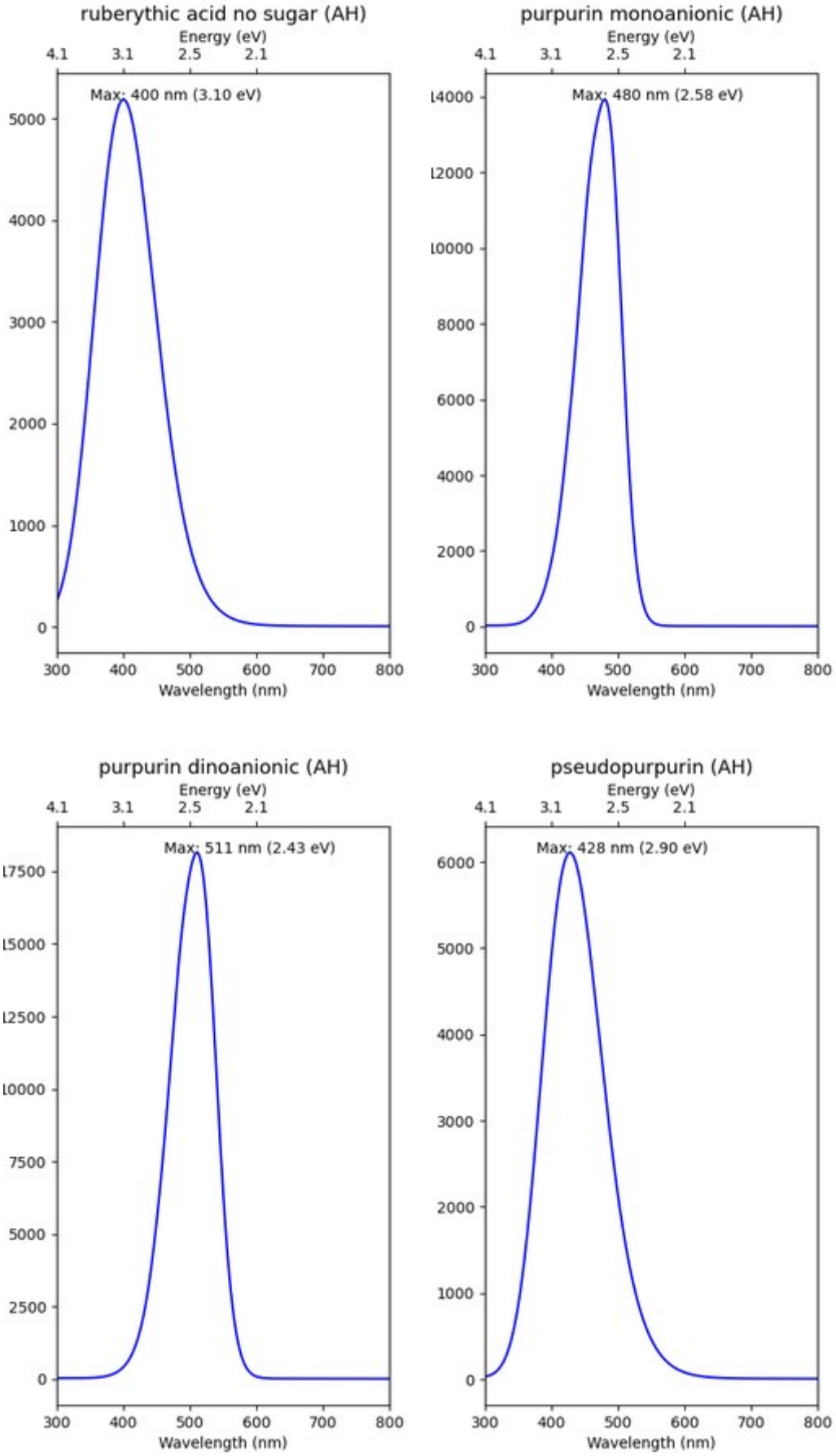

munjistin (AHAS)
Energy (eV)
4.1
3.1
2.5
2.1
Max: 399 nm (3.11 eV)
3500
3000
2500
2000
1500
1000
500
0
300
400
500
600
700
800
Wavelength (nm)

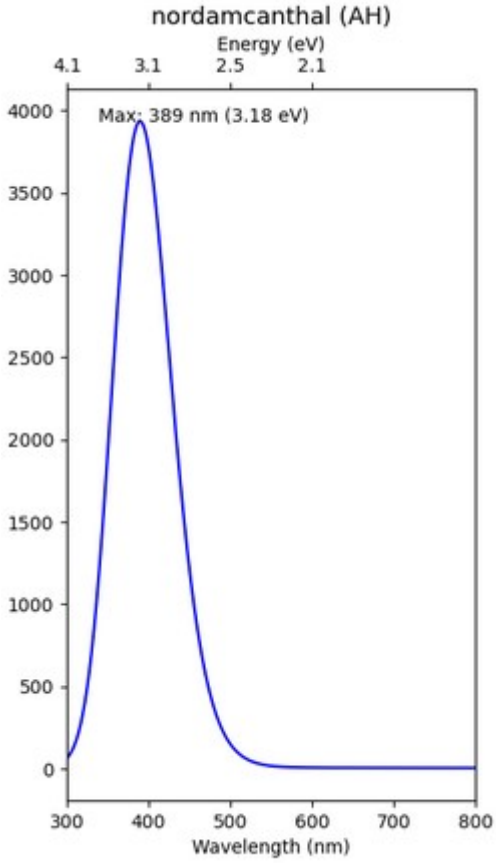

lucidine primeveroside (AHAS)
Energy (eV)
4.1
3.1
2.5
2.1
Max: 400 nm (3.10 eV)
5000
4000
3000
2000
1000
0
300
400
500
600
700
800
Wavelength (nm)

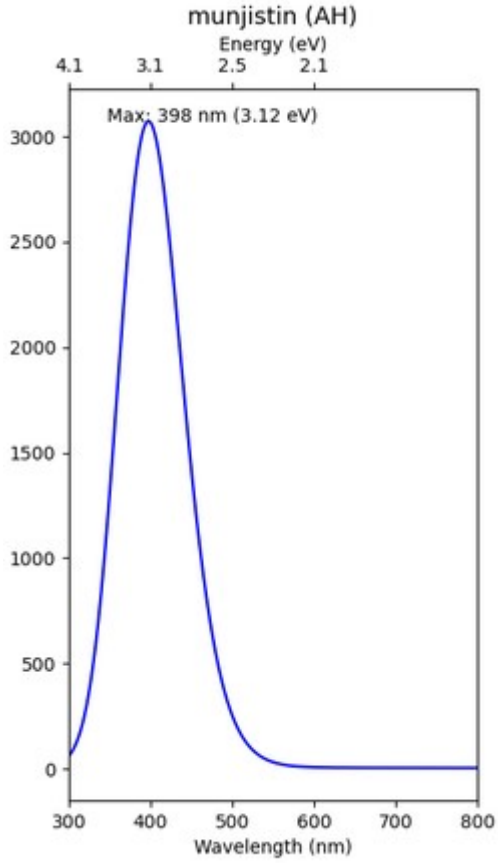

galiosin (AHAS)
Energy (eV)
4.1
3.1
2.5
2.1
Max: 429 nm (2.89 eV)
3500
3000
2500
2000
1500
1000
500
0
300
400
500
600
700
800
Wavelength (nm)

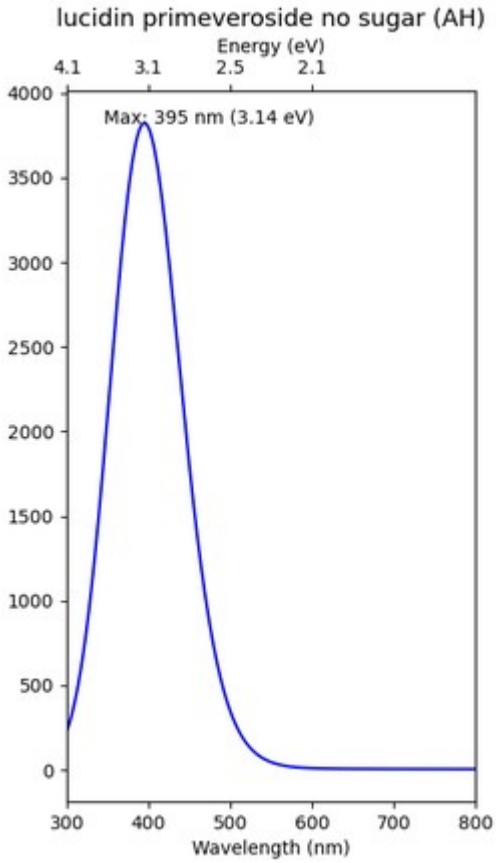

alizarin monoanionic (AHAS)
Energy (eV)
4.1
3.1
2.5
2.1
Max: 495 nm (2.50 eV)
6000
5000
4000
3000
2000
1000
0
300
400
500
600
700
800
Wavelength (nm)

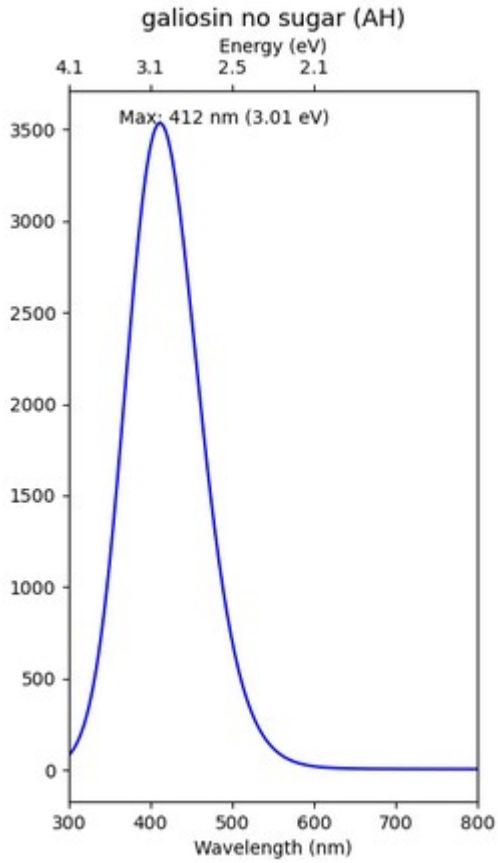
SI.13. Computed individual spectra using Adiabatic Hessian (AH) method.

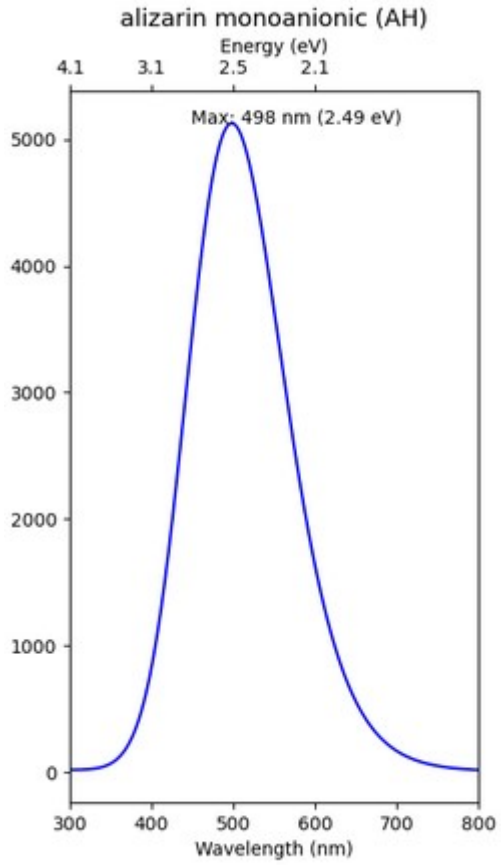



nordamcanthal (AH)
Energy (eV)
4.1
3.1
2.5
2.1
Max: 389 nm (3.18 eV)
4000
3500
3000
2500
2000
1500
1000
500
0
300
400
500
600
700
800
Wavelength (nm)


munjistin (AH)
Energy (eV)
4.1
3.1
2.5
2.1
Max: 398 nm (3.12 eV)
3000
2500
2000
1500
1000
500
0
300
400
500
600
700
800
Wavelength (nm)


lucidin primeveroside no sugar (AH)
Energy (eV)
4.1
3.1
2.5
2.1
Max: 395 nm (3.14 eV)
4000
3500
3000
2500
2000
1500
1000
500
0
300
400
500
600
700
800
Wavelength (nm)


galiosin no sugar (AH)
Energy (eV)
4.1
3.1
2.5
2.1
Max: 412 nm (3.01 eV)
3500
3000
2500
2000
1500
1000
500
0
300
400
500
600
700
800
Wavelength (nm)



SI.14. Optimized geometries

Molecule: ruberythric acid
Energy: -1944.943126905704

64

C	-6.091078	-3.231837	2.897012
C	-7.428469	-3.032728	3.315471
C	-7.722342	-2.013833	4.203197
C	-6.718169	-1.166292	4.661766
C	-5.410722	-1.330191	4.252988
C	-1.982328	0.238003	4.701104
C	-0.679965	0.063549	4.263682
C	-0.369703	-0.974274	3.391493
C	-1.362777	-1.834886	2.956792
C	-2.673868	-1.663104	3.390230
C	-3.718642	-2.583285	2.908947
C	-5.086494	-2.376917	3.363035
H	0.649970	-1.110004	3.050771
H	-1.135450	-2.646098	2.276690
H	0.098252	0.737504	4.602247
C	-4.374180	-0.411758	4.751420
C	-2.986783	-0.620351	4.270041
H	-2.238036	1.040604	5.381443

O	-3.432719	-3.503413	2.133451
O	-4.635890	0.492153	5.529066
O	-5.847196	-4.233196	2.060388
H	-4.866332	-4.201700	1.887672
H	-8.735756	-1.874462	4.554763
O	-8.312447	-3.888526	2.785600
C	-10.432990	-4.593540	2.049792
O	-10.021000	-4.013897	4.357899
C	-10.547395	-5.315443	4.612643
C	-10.107190	-6.082102	2.273302
C	-9.884636	-6.393494	3.774347
O	-10.169309	-4.216422	0.727777
H	-9.389707	-4.728724	0.465613
O	-8.993557	-6.468093	1.504673
H	-10.961329	-6.660947	1.915413
H	-8.227686	-6.384453	2.095090
O	-8.498192	-6.465663	4.058346
H	-10.361079	-7.344049	4.018120
H	-8.290929	-7.359835	4.343240
H	-6.959713	-0.368448	5.352059
C	-10.386153	-5.537372	6.098749
H	-11.619626	-5.326921	4.376059
O	-11.055209	-6.743152	6.410583
H	-10.837588	-4.700327	6.643989
H	-9.325525	-5.598727	6.355750
C	-9.698055	-3.706731	3.039781
H	-11.499606	-4.440179	2.235218
H	-9.942588	-2.653206	2.875995
C	-11.126456	-7.031933	7.758408
C	-12.111579	-8.178338	7.936118
C	-12.116898	-8.640204	9.388093
C	-10.715624	-8.804231	9.985678
C	-9.857311	-7.613675	9.616628
O	-9.843872	-7.377264	8.221055
H	-11.485821	-6.155544	8.327133
H	-8.823941	-7.790017	9.916245
H	-10.229637	-6.726035	10.146256
O	-10.073514	-9.983476	9.550247
H	-10.707131	-10.703152	9.651885
H	-10.819612	-8.817635	11.079928
O	-12.864140	-9.831347	9.517206
H	-12.781856	-10.296049	8.672892
H	-12.620590	-7.863775	9.973228
O	-11.792181	-9.288683	7.123733
H	-11.992204	-9.058220	6.210817
H	-13.111796	-7.804908	7.684449

Molecule: Ruberythric acid with glucose replaced by methoxyl
Energy: -877.817932981778

29

C	-5.40764165749113	3.40839709494715	-1.44621766916911
C	-4.31894641393323	2.58708559249548	-1.83360651872284
C	-4.27277575220136	1.27189586760537	-1.40745955192567
C	-5.28151932702352	0.75351441808880	-0.60034854249714
C	-6.34429903497130	1.53736809432476	-0.20304282637621
C	-6.41232915753662	2.88319953813531	-0.62767633497945
C	-7.51198410824387	3.74606129424290	-0.22180876471955
C	-8.55353977673397	3.18717709438907	0.65742994386088
C	-8.49797937432696	1.85274896413879	1.07555212531637
C	-7.38820645939771	0.96180780468918	0.65767440298041
C	-9.60217439235256	4.00150259885745	1.07389373147591
C	-10.59035072310744	3.49358426959097	1.89913184443683
C	-10.53828185106400	2.16659063219540	2.31185486640211
C	-9.49711493781541	1.35111848485178	1.90136678133259
O	-7.57734050905812	4.92281620795077	-0.59822717175264
O	-7.35109565409614	-0.20225521231555	1.02497255824740
O	-5.42206099952205	4.66159494689433	-1.88142060498332
O	-3.40347177835925	3.18392193477324	-2.60172219511068
H	-3.44806411950646	0.63631399469825	-1.70058555436663
H	-5.23526997021424	-0.27744128993362	-0.27384884341954
H	-9.63026009883806	5.03218617989863	0.74345785404819
H	-11.40475290620329	4.13098387517242	2.22268877920207
H	-11.31366006839464	1.76927351258073	2.95641701085611
H	-9.44321273272574	0.31645295825892	2.21615956906235
H	-6.24983422380709	5.06502843074463	-1.49933649399074
C	-2.27308178375929	2.42283078409803	-3.00079820399976
H	-1.65701530195711	3.09428514442104	-3.59392872512567
H	-2.57488399244492	1.56546089506777	-3.60782567132427
H	-1.71028289491435	2.07731588913793	-2.12979579475798

Molecule: alizarin_monoanionic.xyz
Energy: -1296.597450140063

31

C	2.09549226699071	0.76553987762188	0.55402563001255
C	3.25022582714545	-0.10706559565290	0.45560168640416
C	2.96709583705528	-1.45102671693993	0.11749090559954
C	1.68435315829292	-1.90437780789172	-0.11260052246208
C	0.58128885687232	-1.06162082250658	-0.02483528982095
C	0.80262475167439	0.30327422672971	0.31460379097663
C	-0.30592300440690	1.23265434456348	0.42683399586793
C	-1.66636797458703	0.72931562946882	0.17242225868592
C	-1.87783978573859	-0.61372269838201	-0.16170289155899
C	-0.74603946158382	-1.57370574755399	-0.27673321565433
C	-2.74774951029284	1.60123129140241	0.27053619411593
C	-4.03353360856948	1.14534874736494	0.04002729141637
C	-4.24625645728688	-0.18918523507706	-0.29091135092257
C	-3.17471703600421	-1.06066613265389	-0.39054971037408
O	-0.13138123395534	2.42553990245570	0.72854693003299
O	-0.97176384672795	-2.74840309484202	-0.57590809763593

O 2.33731962615458 2.03412351572642 0.88384286759012
O 4.42052235799774 0.32821322548610 0.67229078868224
H 3.80963384587398 -2.13052382290315 0.04111186483580
H 1.51554416930678 -2.94385637779624 -0.36994235903063
H -2.56355019596612 2.63645923513417 0.52949543096900
H -4.87242769194191 1.82700232751605 0.11800206290068
H -5.25313352577300 -0.54807746176817 -0.47123244162364
H -3.32512073550890 -2.10201245937723 -0.64685440474610
H 1.43935472097688 2.47264001406118 0.91439259565140
O 3.52487347513334 3.72485256366868 -1.46629506528275
H 2.74236184914389 3.31700209873735 -1.08313526324909
H 4.24390439044399 3.41282432758206 -0.87601575754403
O 5.39543199287427 2.74392335167212 0.29756641278364
H 4.96513053507645 1.86388659220572 0.48177429150355
H 6.24351640732980 2.52950270194797 -0.10154862812327

Molecule: alizarin_neutral.xyz
Energy: -837.843016007538
26
C -5.43140321663462 3.30642687769580 -1.42294385045615
C -4.35403895326397 2.46386105146881 -1.77571338930577
C -4.32509489205431 1.16009665133133 -1.31860333871728
C -5.34012849760864 0.66894173350352 -0.50709407082492
C -6.39805283760335 1.47724305267249 -0.13916520383779
C -6.44913705969553 2.81047909782007 -0.59967919842915
C -7.54657447274260 3.69370075415184 -0.22853198029130
C -8.60049673073165 3.16924723297537 0.65689993661549
C -8.55890322191371 1.84753821489001 1.11451450415997
C -7.45312300038979 0.93641662965104 0.73121544374931
C -9.64562610888268 4.00379186167859 1.04071050296821
C -10.64342211286375 3.52852972053434 1.87391128729753
C -10.60452996667369 2.21440099937420 2.32691794695588
C -9.56739752271178 1.37862719479265 1.94787223264486
O -7.59812754818271 4.85869232908090 -0.63979488727795
O -7.42699484848848 -0.21592873966836 1.13391929638452
O -5.42674005794093 4.54910269854569 -1.89206275820568
O -3.40449911708241 3.00436874884750 -2.55307353914961
H -3.49295659509857 0.52386121790216 -1.60240531085180
H -5.30753253234378 -0.35322019926191 -0.15294994237198
H -9.66318108706045 5.02431920089943 0.67946449584933
H -11.45482002406549 4.18180036939784 2.17236557320143
H -11.38691203283391 1.84284517407070 2.97833762761808
H -9.52438010220419 0.35350682541086 2.29396095580977
H -6.25388175686031 4.97135120050293 -1.53247414786582
H -2.71533570406863 2.35211010173216 -2.73112818566919

Molecule: galiosin.xyz
Energy: -2208.152431649668
67
C -5.76760867269799 2.19343793037947 0.75242114234666
C -6.99096859997711 1.62579322430758 0.33627389484906

C	-6.99501484217373	0.39292775975978	-0.31852499609137
C	-5.79450795934596	-0.32583990318096	-0.50592234942876
C	-4.59066112642368	0.24325323783361	-0.12297802813815
C	-0.99961949206263	-0.87562656248342	0.36575960757550
C	0.12263197211861	-0.49680048907520	1.08047138556744
C	0.14013485515620	0.72266571212742	1.75173250723493
C	-0.96379244472631	1.55717018765403	1.71021843567419
C	-2.10549688455939	1.16958775257781	1.01709095283266
C	-3.28387920086269	2.07656697018842	0.98145897337316
C	-4.55403082228920	1.51166501188017	0.52071860173014
H	1.02130736045370	1.02128677874287	2.30779261850664
H	-0.95838208174614	2.51416524860088	2.21663711927722
H	0.98840074976258	-1.14766511029504	1.11526842110913
C	-3.30956699722152	-0.45613030043221	-0.42586551462900
C	-2.11931013033154	-0.04884165772734	0.34322725905623
H	-1.02763620715356	-1.81525016095021	-0.17203206385709
O	-3.15063039772808	3.23139821341645	1.36191797277857
O	-3.22557252327849	-1.32349269719494	-1.27588025568596
O	-5.79283218458211	3.35646743699844	1.37749452982541
H	-6.78435751824463	3.59113917561684	1.43786428823680
C	-8.28649973797116	2.30171790554733	0.64058151281851
O	-8.26106780090634	3.40165927157899	1.24081252991130
O	-9.35504556272323	1.71596000382641	0.28612442597882
O	-8.12136244313283	-0.13204484612655	-0.76269945443978
H	-8.83758284133483	0.53310474041709	-0.44640173698000
O	-5.93376443946187	-1.56697531645881	-1.05827392136011
C	-5.72906237580375	-2.65524035372560	-0.16532941838624
C	-6.08127077187038	-3.94046491650443	-0.91157099068082
C	-6.68926495982977	-4.92229283888881	0.08685968673957
C	-7.84451694753814	-2.86179853207928	0.82649331126041
O	-6.47796264744965	-2.51165945904421	0.99896822101713
O	-4.96923525808650	-4.49611146097520	-1.57962127192638
H	-6.81528064795517	-3.71975149721330	-1.69040736759618
H	-4.24903172592512	-4.60808092483172	-0.94686311537183
O	-6.88232055576154	-6.18623974656062	-0.49504533473916
H	-6.09278649403850	-6.36737979323922	-1.02040014220084
C	-8.01547328697242	-4.37502916695567	0.61451390080025
H	-6.00370138648768	-5.00091068025631	0.94262272612594
H	-4.68567144586812	-2.67633401119266	0.16024595688301
O	-9.02984139678993	-4.63035742898843	-0.33162811218386
H	-8.25163586901655	-4.87173222626749	1.56454229122660
H	-9.83378274219917	-4.15497311052317	-0.06121006351941
C	-8.55038131732629	-2.28492294240645	2.03728219267003
H	-8.21607134149923	-2.37275409689389	-0.07888780561585
O	-9.95035548704533	-2.49112891169151	2.01845358328362
H	-8.31956097728835	-1.21649321728653	2.10377635670879
H	-8.18686816151073	-2.77412684378286	2.94298087219784
C	-10.62860187640663	-1.88158895290503	0.97205069292577
C	-11.64160452890193	-0.86297087274885	1.48939227116627
C	-12.51768229591942	-0.37947634605520	0.34030542539895
C	-13.08974369548700	-1.55520452771825	-0.43385720312533

C	-11.96653889474309	-2.47189825545370	-0.86980325133333
O	-11.25849168850463	-2.93312899704483	0.26720046228241
H	-11.29271265095480	-1.93735490049171	-1.55274405132030
H	-12.35759366393623	-3.35244638346264	-1.37891013859410
H	-9.93129339660868	-1.36433366640769	0.29971682786990
O	-13.54158682335164	0.49841590794436	0.76142934096261
H	-11.89808904782088	0.20624500164225	-0.35009662261415
H	-14.06514182787154	0.05141882719337	1.43775969837494
O	-10.98250507406014	0.19277459629363	2.14424442700481
H	-12.26694703014384	-1.36106881507537	2.23941730859469
H	-10.48739324948234	0.72101646564473	1.49181902928394
O	-13.77681680597821	-1.12536420480985	-1.58669350407750
H	-13.76341300362528	-2.11696755786850	0.23095093364774
H	-14.36167267649664	-0.40759467689816	-1.31570498121217

Molecule: Galiosin with glucose replaced by methoxyl
Energy: -1141.003122254734

32

C	-5.20281523133832	3.17961755315085	-1.68651058071273
C	-4.13766491295172	2.39206158006379	-2.13030365640145
C	-4.06784071427494	1.08898575816558	-1.68887059395632
C	-5.02422081546737	0.54398329578658	-0.80013794407272
C	-6.09498361636236	1.31187190806127	-0.37246433441019
C	-6.18088911378651	2.66173090031040	-0.81201593279735
C	-7.24980978452478	3.53094338915652	-0.37866174591130
C	-8.25621663092780	3.00752240671035	0.55861178095971
C	-8.21979216374363	1.67104563252231	0.95928880768831
C	-7.17170600866701	0.74432059008094	0.46684804264973
C	-9.25094978135237	3.85182459514187	1.04153698054660
C	-10.20192383772040	3.36863266291554	1.92327552531536
C	-10.16720118700484	2.03690899207555	2.32357393606161
C	-9.18224487070644	1.19193955061162	1.84158440726613
O	-7.33350470127287	4.70909556034321	-0.76818390421136
O	-7.22952482394947	-0.44045824183733	0.75052492704032
O	-5.26269760675774	4.43464975188988	-2.12191033663370
C	-3.07898970822010	2.96770733087276	-3.06225679447273
H	-9.26515416042448	4.88486280480261	0.71785367510728
H	-10.97385212371477	4.02885903540029	2.30097370604563
H	-10.91219698456050	1.65948009175132	3.01423774910812
H	-9.14267793248360	0.15329940246729	2.14474362411476
H	-6.08106739874512	4.82668371175163	-1.69780670483015
O	-2.12461560716535	3.54252687923024	-2.50486190303528
O	-3.06341484466550	0.30557326424144	-2.10036551667791
O	-3.27865668645640	2.80280678159181	-4.28049327870511
H	-3.21072812256048	-0.57220015503238	-1.71001907209426
O	-4.79398961808867	-0.75641983726348	-0.47517769917176
C	-4.30185196733748	-0.97849754108306	0.85076185081927
H	-4.10945041612035	-2.04689255773425	0.92757131576059
H	-5.04470910507982	-0.68397701742463	1.59106423157815
H	-3.37297952356861	-0.42297807872062	1.00399943803280

Molecule: lucidine.xyz
Energy: -953.126335211700
30

C	-4.857511	1.627720	-0.093297
C	-3.533101	2.164908	0.102616
C	-2.411656	1.222667	0.289276
C	-5.096039	0.239973	-0.106143
C	-3.980763	-0.720924	0.078295
C	-1.127960	1.721035	0.480400
C	-0.063859	0.852937	0.660401
C	-0.275691	-0.521154	0.651687
C	-1.551657	-1.024710	0.460979
C	-2.625328	-0.160670	0.278602
C	-5.950296	2.502579	-0.271379
C	-7.248018	2.016277	-0.461614
C	-7.442759	0.633352	-0.458723
C	-6.365843	-0.247472	-0.288542
H	-6.547519	-1.314402	-0.298216
H	-0.976993	2.793146	0.486240
H	0.934701	1.246764	0.808991
H	0.557267	-1.199468	0.794386
H	-1.732602	-2.092413	0.452084
O	-3.322675	3.388496	0.117955
O	-4.172943	-1.923433	0.066828
O	-5.772968	3.820127	-0.247719
H	-4.792441	3.958126	-0.107455
O	-8.652670	0.088428	-0.609164
H	-9.270844	0.814266	-0.859500
C	-8.372625	2.999487	-0.595703
O	-9.440055	2.420458	-1.342427
H	-8.012194	3.901940	-1.094946
H	-8.725424	3.290089	0.401453
H	-10.247592	2.910593	-1.156095

Molecule: lucidine_primeveroside.xyz
Energy: -2059.378150005619
68

C	-4.219674	-3.264137	3.509404
C	-5.437236	-3.220307	4.208511
C	-6.189241	-2.055507	4.120279
C	-5.698385	-0.923689	3.462366
C	-4.485758	-0.961741	2.821873
C	-2.213444	1.268754	0.743439
C	-1.004395	1.201673	0.071563
C	-0.272976	0.019065	0.069842
C	-0.751856	-1.094680	0.738964
C	-1.965971	-1.035200	1.414393
C	-2.458971	-2.232209	2.120903
C	-3.726596	-2.147578	2.815369
H	0.673694	-0.032328	-0.454907

H	-0.191749	-2.021147	0.746333
H	-0.628467	2.072493	-0.452484
C	-3.997758	0.253514	2.128510
C	-2.702558	0.155991	1.417685
H	-2.793329	2.183166	0.754045
O	-1.797834	-3.280726	2.112875
O	-4.635967	1.290646	2.141355
O	-3.538622	-4.410568	3.530690
H	-2.708724	-4.246547	2.996555
C	-8.601286	-2.429155	4.397851
C	-9.015296	-2.174406	2.938497
O	-8.623128	-3.801072	4.657294
C	-9.944900	-4.303835	4.819568
C	-10.109535	-3.207271	2.563842
C	-10.883980	-3.626309	3.802127
O	-7.956953	-2.261751	2.027923
H	-9.434795	-1.166171	2.881566
H	-7.986526	-3.170235	1.685286
O	-9.461089	-4.322006	1.970040
H	-10.793018	-2.752176	1.841445
H	-10.005484	-4.649976	1.249365
O	-11.945941	-4.506803	3.510495
H	-11.282338	-2.710798	4.257483
H	-12.666978	-3.993234	3.132396
C	-9.842308	-7.326612	6.590881
C	-8.668302	-6.732478	7.413302
O	-9.372387	-8.387279	5.782299
C	-8.510372	-9.261927	6.486477
C	-7.157877	-8.608873	6.778176
C	-7.323014	-7.085691	6.802251
O	-8.835233	-5.345385	7.562423
H	-8.700776	-7.215094	8.400869
H	-8.004180	-5.019588	7.931453
O	-6.305463	-6.492780	7.585734
H	-7.264683	-6.713805	5.778189
H	-5.685695	-6.012528	7.000542
O	-6.701743	-9.078437	8.029588
H	-6.045660	-8.431197	8.325038
H	-8.399902	-10.151101	5.867002
H	-8.964531	-9.560593	7.440593
H	-6.431588	-8.869074	5.998083
O	-7.364538	-1.892855	4.792316
H	-9.310942	-1.916982	5.059026
C	-5.852318	-4.427610	4.995900
O	-4.845964	-4.886712	5.892427
H	-6.141914	-5.230555	4.307804
H	-6.718019	-4.190395	5.603910
H	-4.092848	-5.185214	5.366526
C	-9.846833	-5.822250	4.715521
H	-10.290762	-4.067540	5.831267
O	-10.542112	-6.444139	5.791683

H	-8.792033	-6.086625	4.720941
H	-10.277817	-6.183057	3.783315
H	-10.593982	-7.715698	7.289618
H	-6.294968	-0.021408	3.449674

Molecule: lucidin primeveroside with glucose replaced by methoxyl.xyz
Energy: -992.275801789786

33

C	-5.19781825352267	3.57189464962303	-1.70928035003456
C	-4.08621588739360	2.84205367257668	-2.13057279350271
C	-3.93543493015318	1.53114473033328	-1.67283178813931
C	-4.86680976233156	0.94385343894252	-0.81276279184469
C	-5.95862459897508	1.67660323487429	-0.40077071732362
C	-6.14870984852333	2.99899423174346	-0.83168959683595
C	-7.28614296163406	3.77794072597918	-0.39324515856271
C	-8.25178811389801	3.15757255931082	0.53521220492498
C	-8.08227519267351	1.83914823771348	0.97237067875831
C	-6.93406791769632	1.02825157121391	0.51230379066086
C	-9.34153462996805	3.89742717994554	0.97949922774773
C	-10.25488876670369	3.33310116969293	1.85465873512771
C	-10.08607621305071	2.02366003483954	2.29046683026794
C	-9.00388987674104	1.28002984204261	1.85020122591306
O	-7.45761032669719	4.94488738608637	-0.77515452784124
O	-6.79231944164526	-0.12783835121647	0.86719923612589
O	-5.34643504052684	4.82049551684970	-2.14307634298042
C	-3.06430106591597	3.42540893606493	-3.06246920914673
H	-4.75574469400601	-0.07071931307137	-0.45843326620753
H	-9.46185593326799	4.91587412801702	0.63238913141193
H	-11.10199725243612	3.91427456590316	2.19955937763483
H	-10.80116542583354	1.58350516235274	2.97545734685673
H	-8.85899312738493	0.25905443556154	2.18092328793306
H	-6.18778190704425	5.15524145286221	-1.72387600725711
O	-3.02309907622864	2.76247203970639	-4.31695321639858
H	-2.07918159267480	3.39677163382575	-2.58195950582297
H	-3.30810987899541	4.46546425840308	-3.26835015208637
H	-2.72274412831621	1.86172828057511	-4.15085541247050
O	-2.84583614075176	0.89430179670449	-2.12278616459739
C	-2.61132778265757	-0.44514952779711	-1.70666776423732
H	-3.42541839039445	-1.09922299188062	-2.02674025084556
H	-2.49563010692459	-0.49866500004141	-0.62198256103935
H	-1.68558173503307	-0.74662968773702	-2.19043349618834

Molecule: munjistine.xyz
Energy: -1026.682918339696
28

C	-5.53728875642919	1.67931864855782	-0.23143970579570
C	-4.22615742660558	2.20694480284845	-0.02654637826664
C	-3.09998253726915	1.26489774731656	0.15615262981006

C	-5.77371236834307	0.28250104102381	-0.25138217514481
C	-4.65603842641271	-0.68051236779681	-0.05374554104987
C	-1.81670986540972	1.76691506077834	0.34259430639138
C	-0.74720684992185	0.90348677498287	0.51356828509631
C	-0.95039133117178	-0.47224461575478	0.50222565987286
C	-2.22483781325034	-0.97996522984966	0.31807006361919
C	-3.30356816317749	-0.11924920918637	0.14339973563297
C	-6.63720528458823	2.56165086260987	-0.42638170735261
C	-7.93471776728669	2.06631991283830	-0.64003182548851
C	-8.14595933985640	0.64641710158108	-0.65018031300537
C	-7.02562502229860	-0.21393533038144	-0.45137327760399
H	-1.67076845257638	2.83957920338835	0.35043495901642
H	0.25023701232033	1.30254009899467	0.65665325198309
H	-0.11279854167701	-1.14647163796224	0.63695989318158
H	-2.40228517775134	-2.04831852790507	0.30649442688941
O	-3.99538602481185	3.43600234445679	0.00037344635460
O	-4.84804131446000	-1.88339534591663	-0.05523800277372
O	-6.40797417590195	3.86292627936791	-0.40348723399674
H	-5.41742475827716	3.95891090507525	-0.23907637339707
C	-9.09528026579866	2.96559944922749	-0.86055961177815
H	-7.19461469963465	-1.28314922859372	-0.46415816607177
O	-9.04412985455493	4.18231267689105	-0.88693947485650
O	-10.24895222736640	2.34396051722805	-1.03964768834452
O	-9.30014174065002	0.13396433423899	-0.83267569273811
H	-10.04517882683900	1.31860373194105	-0.98073349018377

Molecule: nordamcanthal.xyz
Energy: -951.903528714651
28

C	-5.28446582181150	2.86869858093023	-1.48123171153536
C	-4.28876040990814	1.90728482690141	-1.78029636495583
C	-4.38333088013137	0.61299589443026	-1.21811115451449
C	-5.45174944726299	0.28776008296208	-0.39036159472809
C	-6.41272060117508	1.23069973930965	-0.11493539316111
C	-6.36700198327178	2.53937178874067	-0.64113610863220
C	-7.42254523265422	3.50796089807170	-0.31085743215647
C	-8.50270552413031	3.06640760901891	0.61708557808091
C	-8.55596546620277	1.77219029128799	1.13688728951297
C	-7.52060932414091	0.78982152110778	0.78954974103798
C	-9.48970130610289	3.98120350570789	0.96809624984556
C	-10.51274709028897	3.61137231124389	1.82415946987070
C	-10.56514396062910	2.31915420986457	2.33792825968047
C	-9.58942554327762	1.40245009980260	1.99408890144239
O	-7.45644998789940	4.64286026350623	-0.75600145565624
O	-7.54644388085942	-0.34694380022695	1.22025859058547
O	-5.22568384782095	4.09987927531136	-1.97559682144674
C	-3.17579146257535	2.19900168610715	-2.65308938050551
H	-5.52329126091056	-0.70432351999173	0.03396399208005
H	-4.44028185124254	4.23661216453493	-2.51770126234204
H	-9.61118069402111	0.39210735715300	2.38300556248855
H	-11.36779060288586	2.03195391248700	3.00685060100620

H	-9.44056736141050	4.98303005600874	0.56127483541037
H	-11.27594139431796	4.33188122136732	2.09441518572131
O	-3.47120818730254	-0.30876340663595	-1.46269577819509
H	-2.79837961244083	0.10018470222274	-2.07267750249986
O	-2.29424673626474	1.38733604670514	-2.92106292636526
H	-3.10455052906047	3.19540268207134	-3.11540937006864

Molecule: pseudopurpurine.xyz
Energy: -1101.871813487737
29

C	-5.98512852099425	1.38209676347813	-0.28838667547226
C	-4.68706935405129	2.01472115313249	-0.01098618460472
C	-3.51895987307294	1.11818875320324	0.15719448768795
C	-6.10052604249366	-0.04951541106771	-0.35938824275316
C	-4.96599688656252	-0.88913324178401	-0.16773422776613
C	-2.26537949142955	1.67651074372487	0.39301159804799
C	-1.15695768786899	0.86501777065726	0.55241771052908
C	-1.29232269343337	-0.51871627690197	0.48027949676083
C	-2.53375701227174	-1.08235725159722	0.24860987519735
C	-3.65413536029932	-0.27056135545506	0.08412025658199
C	-7.11222341392472	2.13966157965206	-0.48272818082881
C	-8.40042591460702	1.52636130489404	-0.76302987529148
C	-8.51234565348475	0.12192855306248	-0.84430908658533
C	-7.35279760869982	-0.65655354360416	-0.62706027173491
H	-2.17821524829369	2.75448792988329	0.44715732921364
H	-0.18366389860321	1.30619606580568	0.73332220673265
H	-0.42436287872765	-1.15587743179486	0.60488126735391
H	-2.65454626355127	-2.15658743334131	0.18972904356102
O	-4.54520323969129	3.22630837664685	0.08105743179403
O	-5.03928848972810	-2.14506047382273	-0.21119401530888
O	-7.16125224488413	3.46970207830482	-0.44291865527510
H	-8.10677781473403	3.66707747919496	-0.62343623171377
O	-9.36593895301963	2.34324119546310	-0.92266585807373
H	-10.43919694524581	1.32257147062944	-1.18322821618829
O	-7.42879011585277	-1.97126335733454	-0.67311564794547
H	-6.47823664966580	-2.29696610139979	-0.49202530966778
C	-9.82981512737187	-0.47951696535257	-1.15990060628137
O	-10.82288599259936	0.39131143521989	-1.31312631915917
O	-10.04770062483729	-1.66766380949668	-1.28784709881005

Molecule: purpurin_monoanionic.xyz
Energy: -2059.264579259574

26

C	-5.01423454489245	1.41691221078699	-0.08156840585369
C	-3.74530859253235	2.08182041152585	0.08993912886510
C	-2.55088993357431	1.24573255206866	0.27343324263453
C	-5.09775898254131	-0.01304412844363	-0.06403088536772
C	-3.95959664880473	-0.82275859222842	0.11839289717133
C	-1.30478743818292	1.84926688452038	0.43392373776505
C	-0.17118303818669	1.07731538594033	0.60731069453449

C	-0.27396619045423	-0.31136753387434	0.62364019694448
C	-1.50624422628712	-0.92005836481342	0.46594400456103
C	-2.65566619597121	-0.15359118019034	0.28863307695650
C	-6.15285243243494	2.18638030821158	-0.26430656021725
C	-7.48202332874302	1.57229642728435	-0.45323794888364
C	-7.50955919236432	0.15863585419298	-0.42358515095219
C	-6.37350033398099	-0.60813098775622	-0.23792921280393
H	-8.46432411028636	-0.33861700355199	-0.55576026365316
H	-1.24281901733105	2.93041625928833	0.41951695624897
H	0.79520427782022	1.55212426004035	0.73036967401344
H	0.61419633721130	-0.91791080262534	0.75962950037602
H	-1.59902524453512	-1.99884034153210	0.47631258408654
O	-3.64987780522650	3.32756354785506	0.08365285943879
O	-4.01555880869723	-2.08743636531464	0.13977902286321
O	-6.10908953884256	3.50804468830703	-0.28143551447098
H	-5.13832335412352	3.73523612545404	-0.14166621782246
O	-8.48474728459358	2.29777923561013	-0.62472572692861
O	-6.47665384355827	-1.93764310201099	-0.22342043350970
H	-5.52952052888669	-2.26679574874463	-0.07672125599616

Molecule: purpurin_dianionic.xyz
Energy: -2058.918427253842
25

C	-0.71248430244730	0.64564869399404	-0.00137410547404
C	0.44822264119037	1.48933944103099	-0.00250767763616
C	1.77002477117609	0.80691218576196	-0.00277287398226
C	-0.54936774951954	-0.79799579893750	-0.00089806134994
C	0.70180169181733	-1.42826723632616	-0.00134163472626
C	2.93226520751425	1.58351566992504	-0.00364711805889
C	4.18282124912506	0.99852262703255	-0.00398545327496
C	4.30005090166666	-0.39294557601424	-0.00345471538132
C	3.16450045403055	-1.17590630224907	-0.00260067645912
C	1.89241779215911	-0.59033030470490	-0.00223672333531
C	-2.03118332640747	1.21562432379271	-0.00071914462758
C	-3.23136982709983	0.26685837633807	-0.00030108829954
C	-2.98782902013875	-1.11965391703316	0.00028572843084
C	-1.70823166026689	-1.63879023322834	0.00003215363219
O	0.44543467986084	2.73907598770849	-0.00269128032415
O	0.84495703280456	-2.71322604390910	-0.00074194058610
O	-2.29608438040093	2.43068913124258	-0.00152356454767
O	-4.37837665144201	0.75908790549753	-0.00004430505040
O	-1.54539660815081	-2.95687211111271	0.00057759005221
H	-3.83254480670138	-1.80212860521641	0.00091102857354
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H	3.23398782060577	-2.25681539147699	-0.00218512752865
H	-0.49754642422574	-3.07769879904849	0.00024209174412

Molecule: rubiadin_primeveroside.xyz
Energy: -1984.221251211675

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C	-4.98556719792448	1.38125418207949	-2.22306217088846
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C	-7.79850094324300	2.83783358281252	1.85458011237001
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C	-3.49069737963004	-1.40593457890963	-0.52133579526195
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C	-4.12056798911374	-3.15495155201236	0.89759761658837
C	-2.87555304730033	-3.98415431471201	0.56317958475271
C	-1.75839897754827	-3.08393963494743	0.04764799749994
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H	-3.89783363307749	-2.52596467397509	1.77247674253547
C	-5.82014560907884	2.47041605530203	-1.94541768648050
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H	-6.21353324279967	-3.32669216512378	1.32445458723506
C	-5.77203827261096	-5.99594456300506	2.35278091722590
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C	-7.81543616794961	-7.00725092266888	2.82291343777413
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C	-7.21336491117605	-7.96979108723138	3.83673648640130
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H	-4.95497509639751	-6.36528991817032	4.28193467166324
H	-3.67323135577415	-7.68525801780786	2.14843708556274
H	-6.59184066547083	4.08161802875852	-2.49097472298817

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