Supplementary data for

Redox properties of alkyl-substituted 4-aryl-2,4-dioxobutanoic acids

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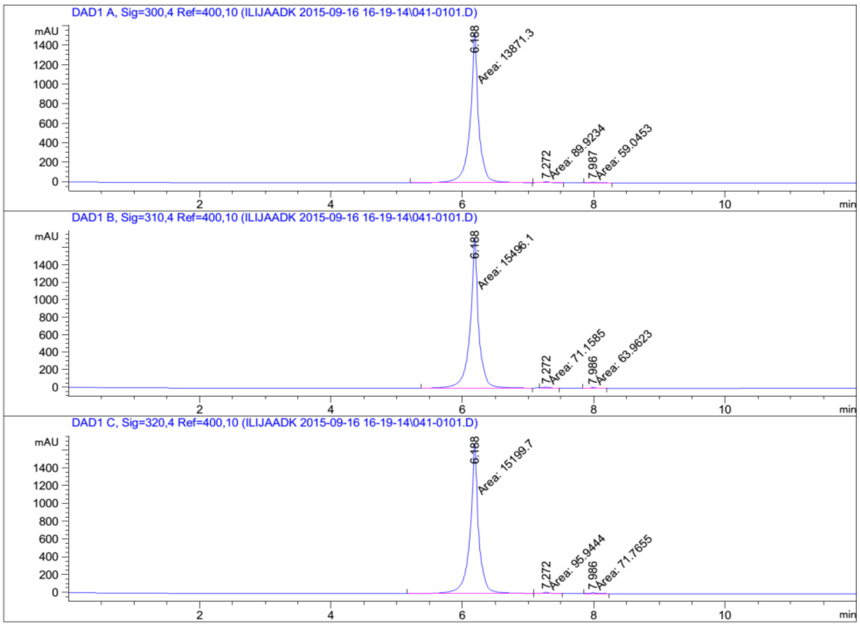


Signal 1: DAD1 A, Sig=300,4 Ref=400,10

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.188	MM	0.1499	1.38713e4	1542.77527	98.9375
2	7.272	MM	0.1237	89.92340	12.11744	0.6414
3	7.987	MM	0.1303	59.04533	7.55190	0.4211
Totals :				1.40203e4	1562.44460	

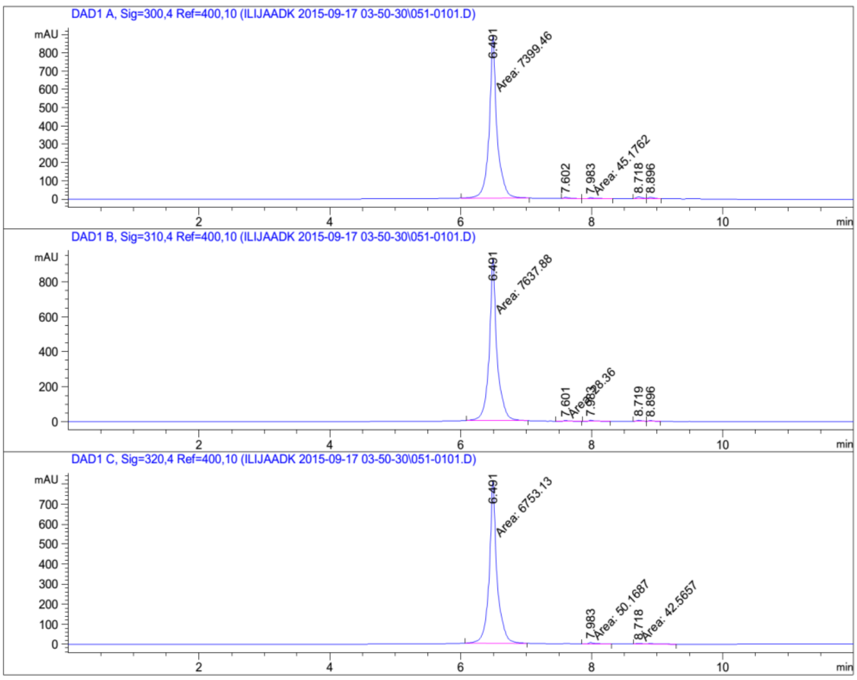
Signal 2: DAD1 B, Sig=310,4 Ref=400,10

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.188	MM	0.1498	1.54961e4	1723.59949	99.1356
2	7.272	MM	0.0992	71.15846	11.95799	0.4552
3	7.986	MM	0.1170	63.96226	9.10771	0.4092
Totals :				1.56312e4	1744.66518	

Signal 3: DAD1 C, Sig=320,4 Ref=400,10

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.188	MM	0.1498	1.51997e4	1690.71960	98.9087
2	7.272	MM	0.1266	95.94437	12.63321	0.6243
3	7.986	MM	0.1167	71.76546	10.25321	0.4670
Totals :				1.53674e4	1713.60602	

Fig. S1. Chromatogram for the assessment of compound **1** purity, with the tables showing the detector response at three wavelengths



Signal 1: DAD1 A, Sig=300,4 Ref=400,10

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.491	MM	0.1384	7399.45605	891.22644	97.3957
2	7.602	BB	0.0747	43.75071	8.13640	0.5759
3	7.983	MM	0.1336	45.17621	5.63593	0.5946
4	8.718	BV	0.0936	63.11792	10.00004	0.8308
5	8.896	VB	0.0746	45.81448	8.81991	0.6030
Totals :				7597.31538	923.81872	

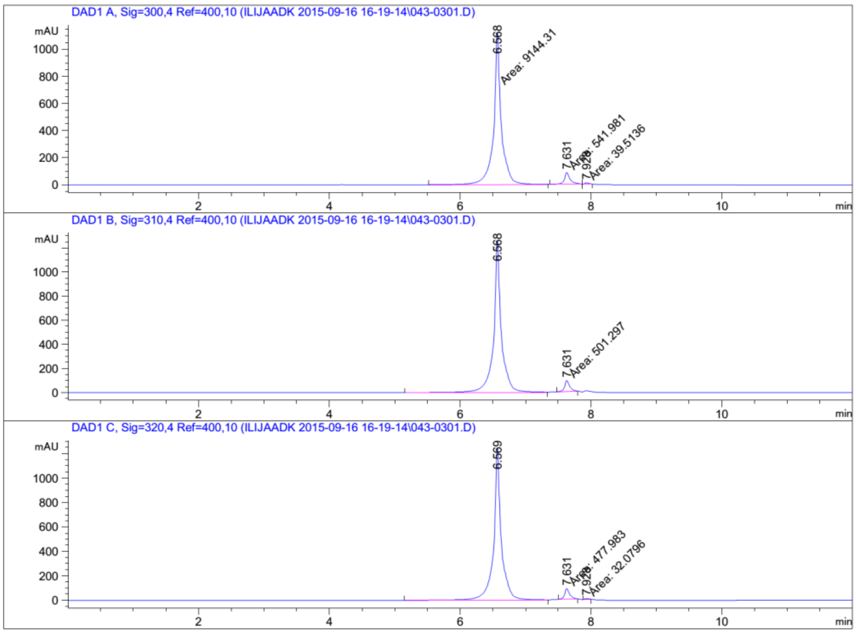
Signal 2: DAD1 B, Sig=310,4 Ref=400,10

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.491	MM	0.1368	7637.88330	930.65759	98.2398
2	7.601	MM	0.1015	28.35998	4.65668	0.3648
3	7.983	BB	0.0900	44.02977	6.75667	0.5663
4	8.719	VV	0.0939	37.49060	5.91716	0.4822
5	8.896	VB	0.0739	26.97103	5.25505	0.3469
Totals :				7774.73468	953.24315	

Signal 3: DAD1 C, Sig=320,4 Ref=400,10

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.188	MM	0.1498	1.51997e4	1690.71960	98.9087
2	7.272	MM	0.1266	95.94437	12.63321	0.6243
3	7.986	MM	0.1167	71.76546	10.25321	0.4670
Totals :				1.53674e4	1713.60602	

Fig. S2. Chromatogram for the assessment of compound **2** purity, with the tables showing the detector response at three wavelengths.



Signal 1: DAD1 A, Sig=300,4 Ref=400,10

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.568	MM	0.1354	9144.30762	1125.57922	94.0211
2	7.631	MM	0.1035	541.98132	87.25426	5.5726
3	7.928	MM	0.0752	39.51355	8.76017	0.4063
Totals :				9725.80249	1221.59366	

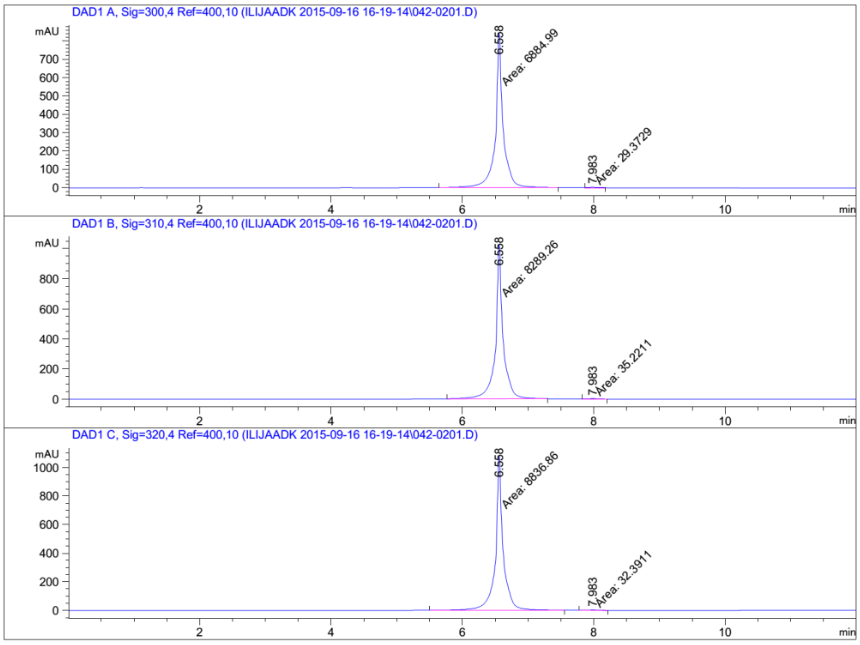
Signal 2: DAD1 B, Sig=310,4 Ref=400,10

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.568	BV	0.1105	1.04653e4	1265.41760	95.4289
2	7.631	MM	0.0912	501.29694	91.58324	4.5711
Totals :				1.09666e4	1357.00084	

Signal 3: DAD1 C, Sig=320,4 Ref=400,10

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.569	BV	0.1125	1.03210e4	1247.92981	95.2907
2	7.631	MM	0.0909	477.98343	87.68449	4.4131
3	7.928	MM	0.0651	32.07959	8.20785	0.2962
Totals :				1.08310e4	1343.82214	

Fig. S3. Chromatogram for the assessment of compound **3** purity, with the tables showing the detector response at three wavelengths.



Signal 1: DAD1 A, Sig=300,4 Ref=400,10

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.558	MM	0.1359	6884.98584	844.67102	99.5752
2	7.983	MM	0.1335	29.37285	3.66623	0.4248
Totals :				6914.35869	848.33725	

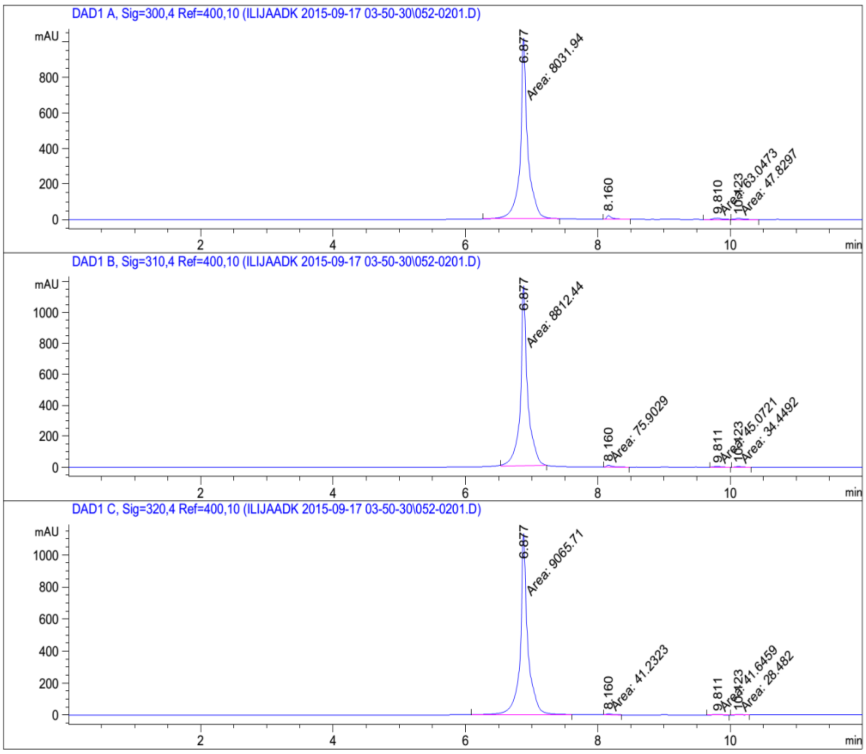
Signal 2: DAD1 B, Sig=310,4 Ref=400,10

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.558	MM	0.1343	8289.25977	1029.00488	99.5769
2	7.983	MM	0.1359	35.22105	4.31915	0.4231
Totals :				8324.48082	1033.32404	

Signal 3: DAD1 C, Sig=320,4 Ref=400,10

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.558	MM	0.1359	8836.85742	1083.69934	99.6348
2	7.983	MM	0.1194	32.39113	4.52258	0.3652
Totals :				8869.24855	1088.22192	

Fig. S4. Chromatogram for the assessment of compound **4** purity, with the tables showing the detector response at three wavelengths.



Signal 1: DAD1 A, Sig=300,4 Ref=400,10

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.877	MM	0.1312	8031.94043	1020.67456	97.2473
2	8.160	BV	0.0785	116.47652	21.05224	1.4102
3	9.810	MM	0.1373	63.04733	7.65068	0.7634
4	10.123	MM	0.1081	47.82969	7.37333	0.5791
Totals :				8259.29396	1056.75080	

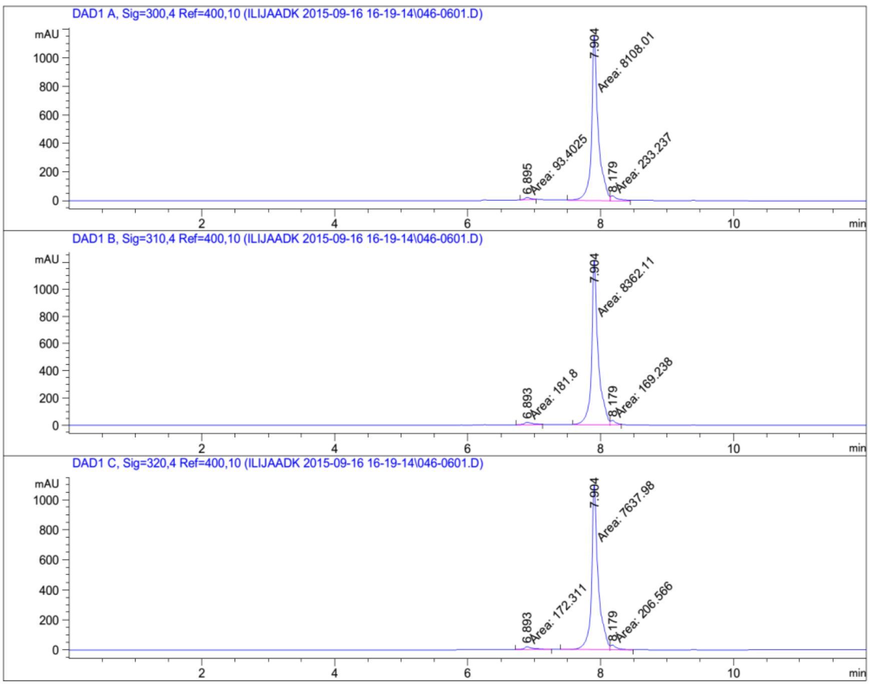
Signal 2: DAD1 B, Sig=310,4 Ref=400,10

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.877	MM	0.1261	8812.43652	1164.66846	98.2669
2	8.160	MM	0.0959	75.90292	13.19241	0.8464
3	9.811	MM	0.1394	45.07211	5.38910	0.5026
4	10.123	MM	0.1095	34.44922	5.24225	0.3841
Totals :				8967.86077	1188.49222	

Signal 3: DAD1 C, Sig=320,4 Ref=400,10

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.877	MM	0.1330	9065.71289	1136.19385	98.7865
2	8.160	MM	0.0936	41.23225	7.34139	0.4493
3	9.811	MM	0.1716	41.64587	4.04555	0.4538
4	10.123	MM	0.1264	28.48196	3.75556	0.3104
Totals :				9177.07297	1151.33635	

Fig. S5. Chromatogram for the assessment of compound **5** purity, with the tables showing the detector response at three wavelengths.



Signal 1: DAD1 A, Sig=300,4 Ref=400,10

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.895	MM	0.1019	93.40249	15.26987	1.1074
2	7.904	MM	0.1164	8108.01123	1161.14124	96.1274
3	8.179	MM	0.1122	233.23743	34.65784	2.7652
Totals :				8434.65115	1211.06895	

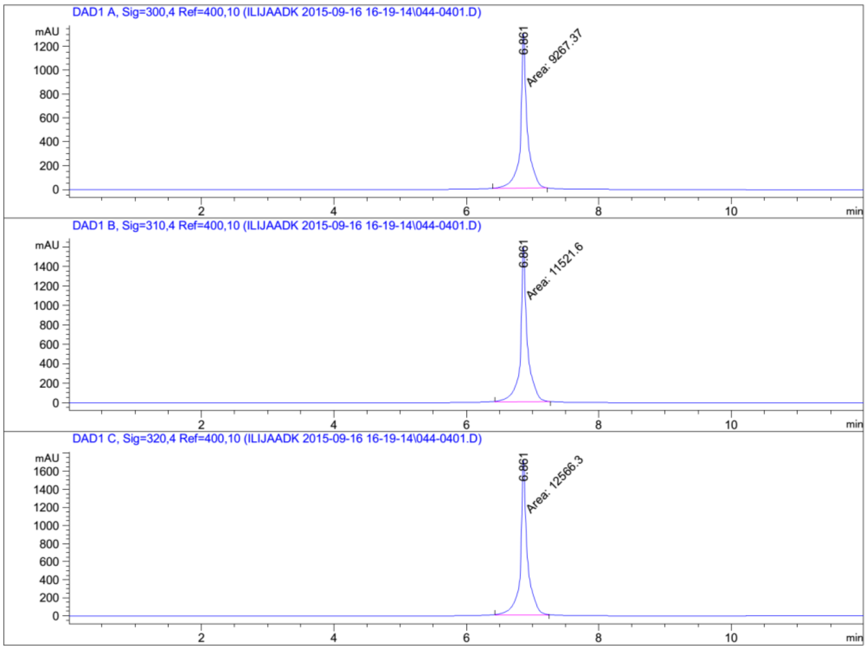
Signal 2: DAD1 B, Sig=310,4 Ref=400,10

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.893	MM	0.1523	181.80042	19.89683	2.0865
2	7.904	MF	0.1147	8362.10840	1214.82483	95.9712
3	8.179	FM	0.0895	169.23830	31.51430	1.9423
Totals :				8713.14711	1266.23596	

Signal 3: DAD1 C, Sig=320,4 Ref=400,10

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.893	MM	0.1620	172.31148	17.72326	2.1494
2	7.904	MF	0.1155	7637.97559	1101.79370	95.2740
3	8.179	FM	0.1095	206.56557	31.44277	2.5766
Totals :				8016.85263	1150.95973	

Fig. S6. Chromatogram for the assessment of compound **6** purity, with the tables showing the detector response at three wavelengths.



Signal 1: DAD1 A, Sig=300,4 Ref=400,10

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.861	MM	0.1185	9267.36816	1303.51819	100.0000
Totals :				9267.36816	1303.51819	

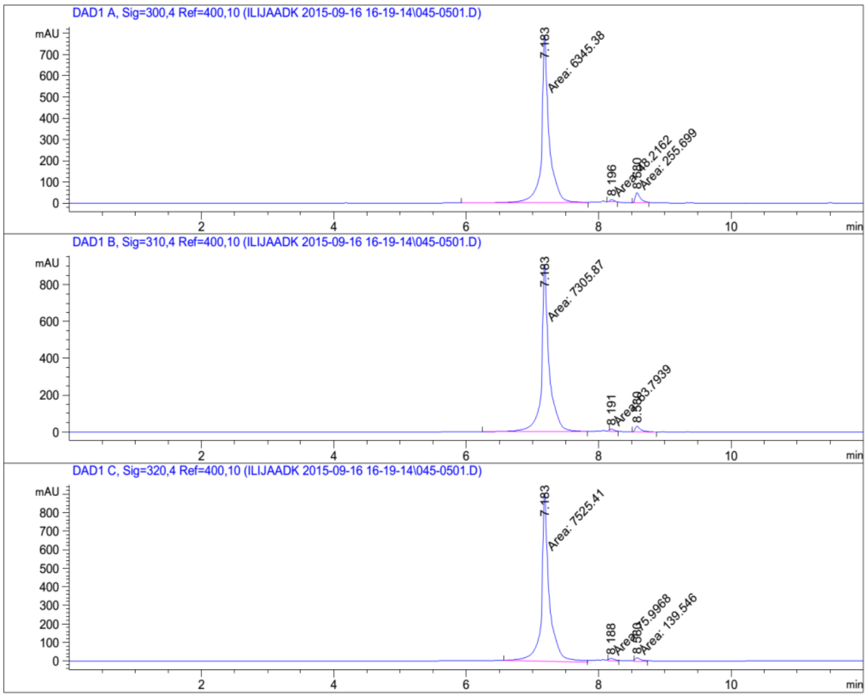
Signal 2: DAD1 B, Sig=310,4 Ref=400,10

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.861	MM	0.1199	1.15216e4	1601.59851	100.0000
Totals :				1.15216e4	1601.59851	

Signal 3: DAD1 C, Sig=320,4 Ref=400,10

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.861	MM	0.1211	1.25663e4	1729.70715	100.0000
Totals :				1.25663e4	1729.70715	

Fig. S7. Chromatogram for the assessment of compound **7** purity, with the tables showing the detector response at three wavelengths.



Signal 1: DAD1 A, Sig=300,4 Ref=400,10

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.183	MM	0.1338	6345.37500	790.56934	95.4294
2	8.196	MM	0.0748	48.21621	10.74792	0.7251
3	8.580	MM	0.0883	255.69875	48.24373	3.8455
Totals :				6649.28996	849.56099	

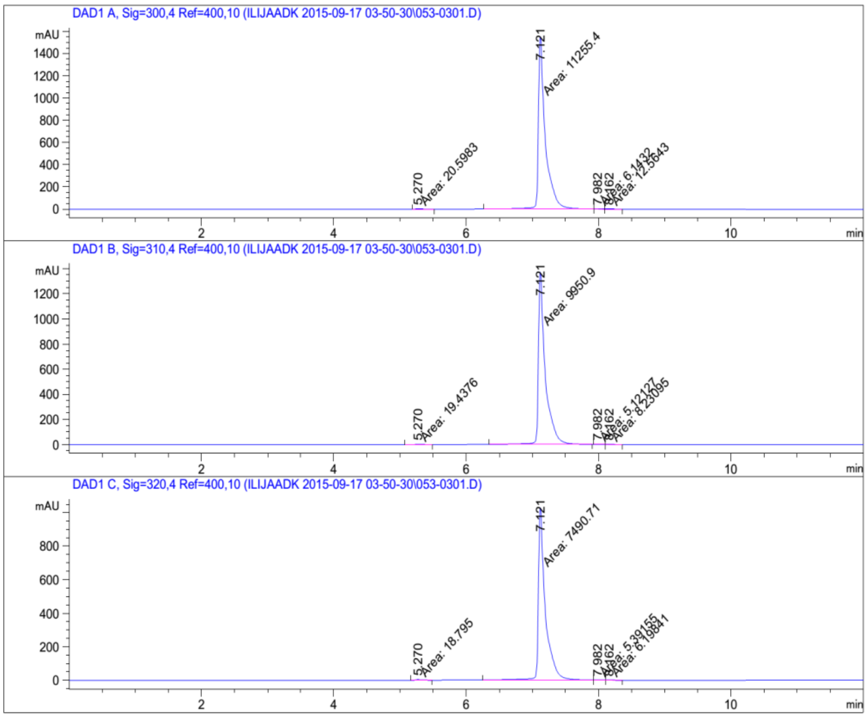
Signal 2: DAD1 B, Sig=310,4 Ref=400,10

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.183	MM	0.1336	7305.87354	911.51147	96.7396
2	8.191	MM	0.0764	63.79385	13.90957	0.8447
3	8.580	BB	0.0839	182.43127	31.36720	2.4156
Totals :				7552.09866	956.78825	

Signal 3: DAD1 C, Sig=320,4 Ref=400,10

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.183	MM	0.1379	7525.41113	909.51855	97.2156
2	8.188	MM	0.0982	75.99679	12.90106	0.9817
3	8.580	MM	0.1109	139.54582	20.97921	1.8027
Totals :				7740.95374	943.39883	

Fig. S8. Chromatogram for the assessment of compound **8** purity, with the tables showing the detector response at three wavelengths.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.270	MM	0.1076	20.59832	3.18970	0.1824
2	7.121	MM	0.1205	1.12554e4	1556.25171	99.6520
3	7.982	MM	0.0917	6.14320	1.11701	0.0544
4	8.162	MM	0.1114	12.56429	1.87958	0.1112
Totals :				1.12947e4	1562.43800	

Signal 2: DAD1 B, Sig=310,4 Ref=400,10

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.270	MM	0.0926	19.43761	3.49813	0.1947
2	7.121	MM	0.1205	9950.90234	1375.92627	99.6716
3	7.982	MM	0.0745	5.12127	1.14633	0.0513
4	8.162	MM	0.0911	8.23095	1.50506	0.0824
Totals :				9983.69218	1382.07579	

Signal 3: DAD1 C, Sig=320,4 Ref=400,10

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.270	MM	0.0944	18.79499	3.31737	0.2499
2	7.121	MM	0.1210	7490.70850	1032.15369	99.5960
3	7.982	MM	0.0718	5.39155	1.25197	0.0717
4	8.162	MM	0.0935	6.19841	1.10505	0.0824
Totals :				7521.09344	1037.82807	

Fig. S9. Chromatogram for the assessment of compound **9** purity, with the tables showing the detector response at three wavelengths.

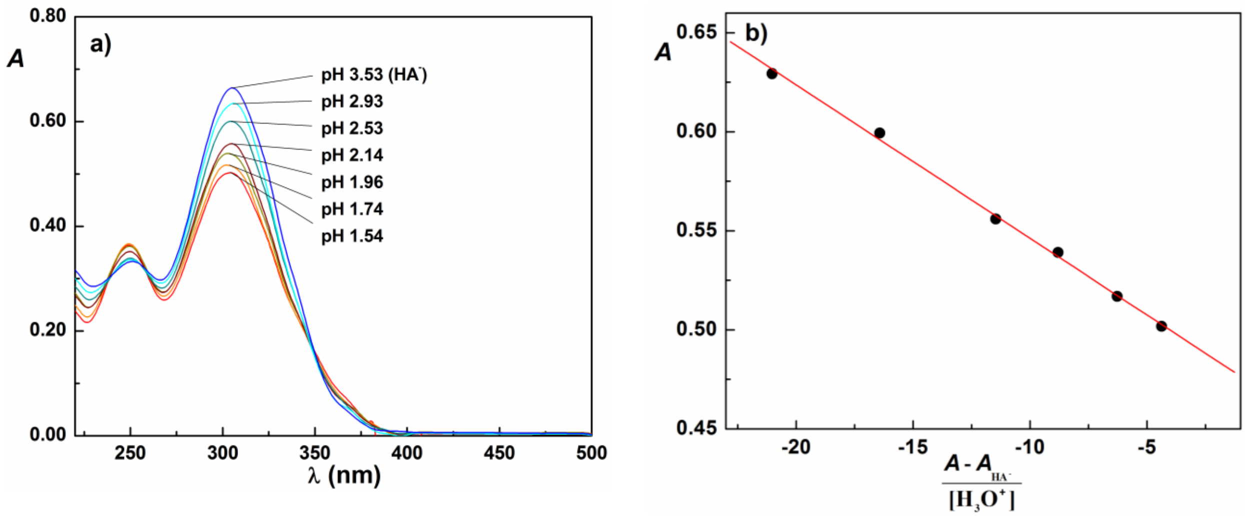


Fig. S10. Absorption spectra of compound **2** used for K_{a1} determination in solutions of different acidity, pH values are indicated; b) Spectrophotometric determination of K_{a1} according to Equation 1; c_2=5.023×10^{-5} M; λ= 302.9 nm; t = 25 °C, I = 0.1 M (NaCl); scan speed 500 nm/min.

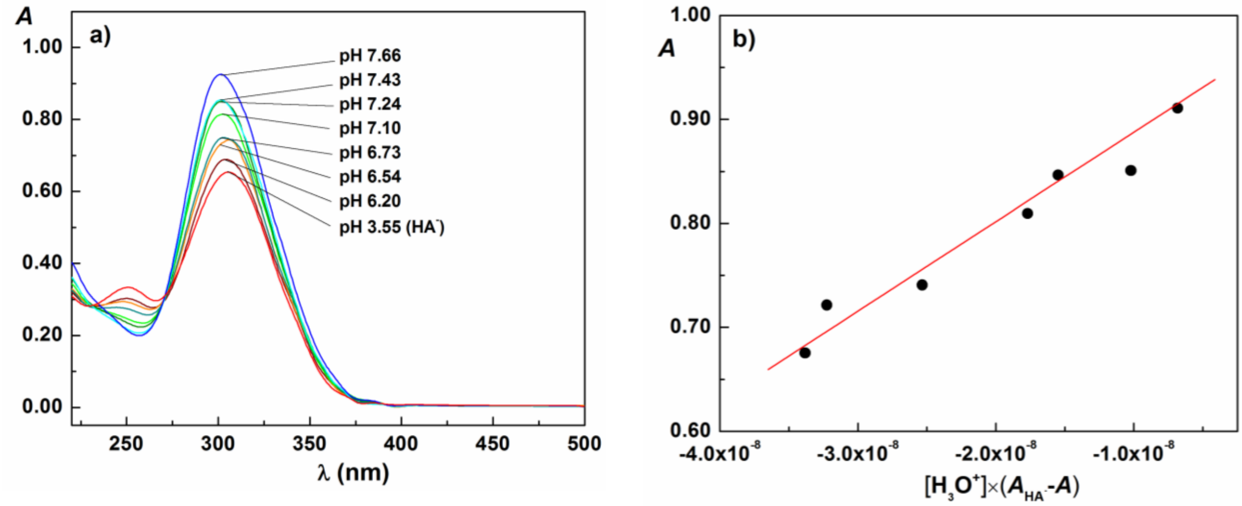


Fig. S11. Absorption spectra of compound **2** used for K_{a2} determination in solutions of different acidity, pH values are indicated; b) Spectrophotometric determination of K_{a2} according to Equation 2; c_2=5.023×10^{-5} M; λ= 299.5 nm; t = 25 °C, I = 0.1 M (NaCl); scan speed 500 nm/min.

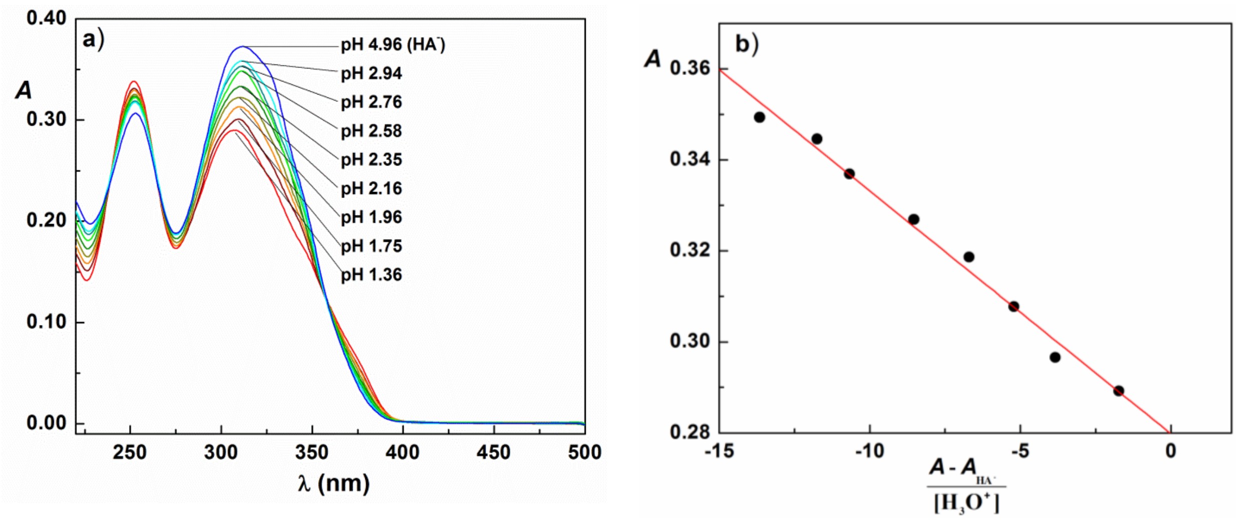


Fig. S12. Absorption spectra of compound **3** used for K_{a1} determination in solutions of different acidity, pH values are indicated; b) Spectrophotometric determination of K_{a1} according to Equation 1; c_3=4.908×10^{-5} M; λ= 305.4 nm; t = 25 °C, I = 0.1 M (NaCl); scan speed 500 nm/min.

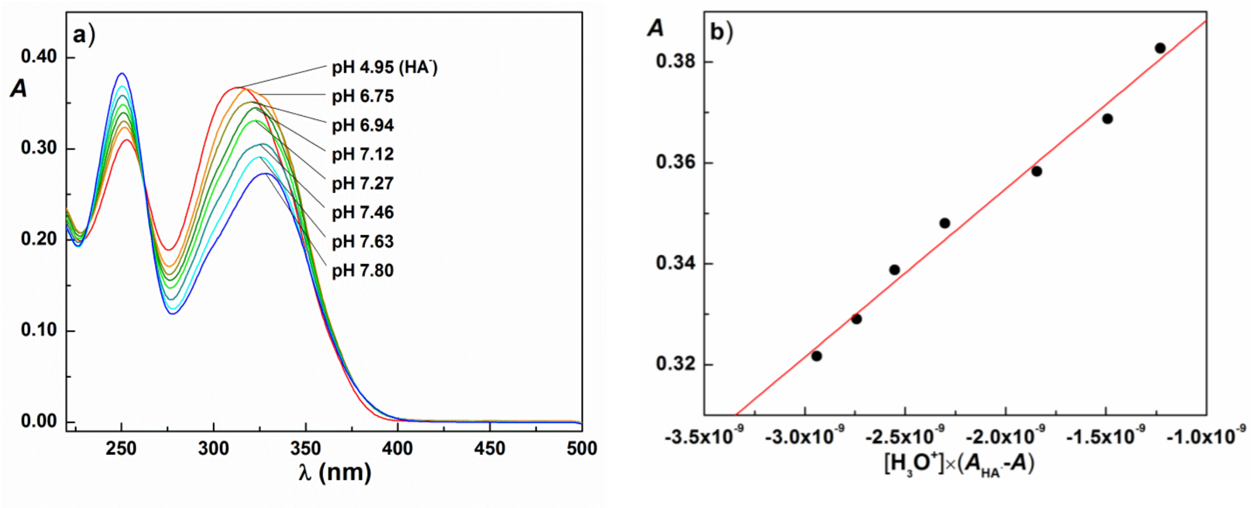


Fig. S13. Absorption spectra of compound **3** used for K_{a2} determination in solutions of different acidity, pH values are indicated; b) Spectrophotometric determination of K_{a2} according to Equation 2; c_3=4.908×10^{-5} M; λ= 250.0 nm; t = 25 °C, I = 0.1 M (NaCl); scan speed 500 nm/min.

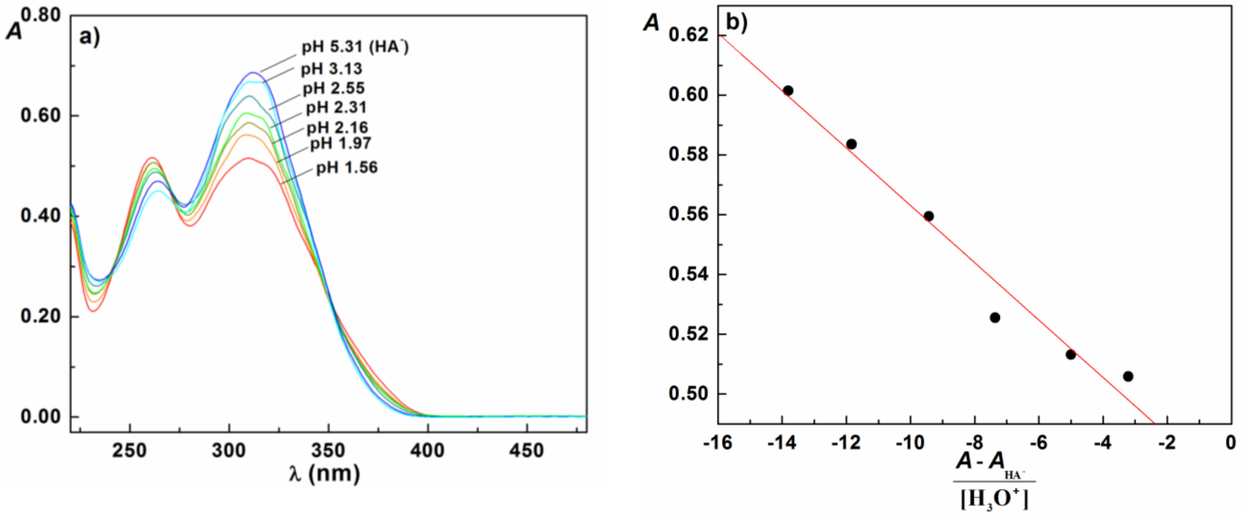


Fig. S14. Absorption spectra of compound **5** used for K_{a1} determination in solutions of different acidity, pH values are indicated; b) Spectrophotometric determination of K_{a1} according to Equation 1; c_5=6.021×10^{-5}M; λ= 312.3 nm; t = 25 °C, I = 0.1 M (NaCl); scan speed 500 nm/min.

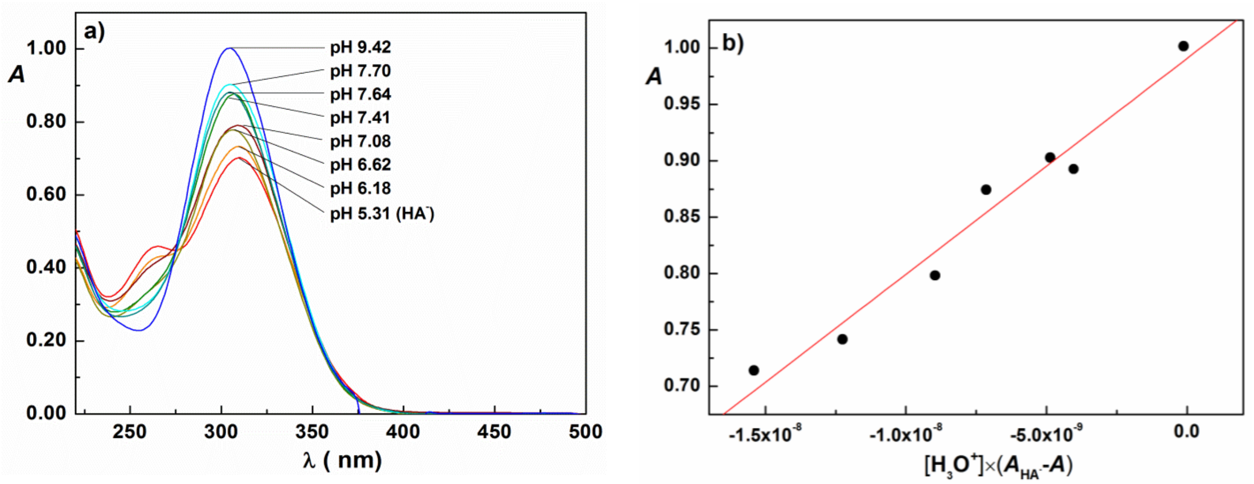


Fig. S15. Absorption spectra of compound **5** used for K_{a2} determination in solutions of different acidity, pH values are indicated; b) Spectrophotometric determination of K_{a2} according to Equation 2; c_5=6.021×10^{-5}M; λ= 305.9 nm; t = 25 °C, I = 0.1 M (NaCl); scan speed 500 nm/min.

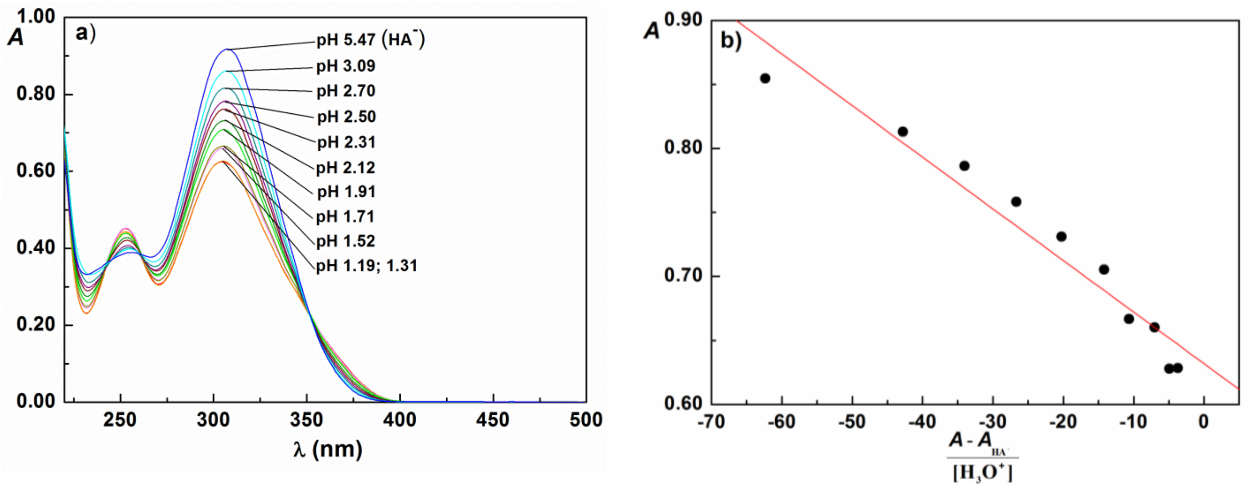


Fig. S16. Absorption spectra of compound **6** used for K_{a1} determination in solutions of different acidity, pH values are indicated; b) Spectrophotometric determination of K_{a1} according to Equation 1; c_6=9.014×10^{-5} M; λ= 306.3 nm; t = 25 °C, I = 0.1 M (NaCl); scan speed 500 nm/min.

Figure S11.

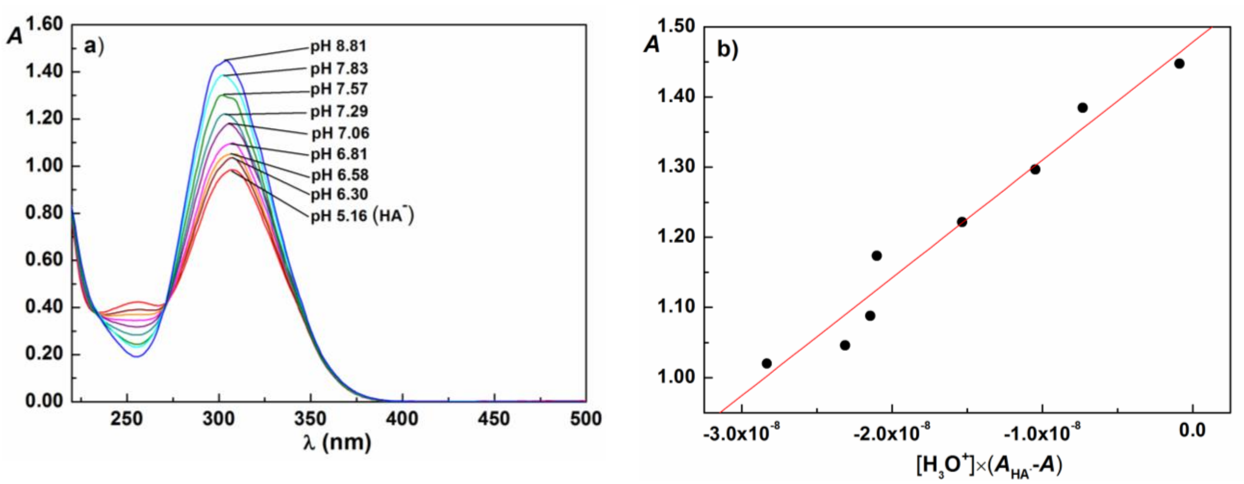


Fig. S17. Absorption spectra of compound **6** used for K_{a2} determination in solutions of different acidity, pH values are indicated; b) Spectrophotometric determination of K_{a2} according to Equation 2; c_6=9.014×10^{-5} M; λ= 303.7 nm; t = 25 °C, I = 0.1 M (NaCl); scan speed 500 nm/min.

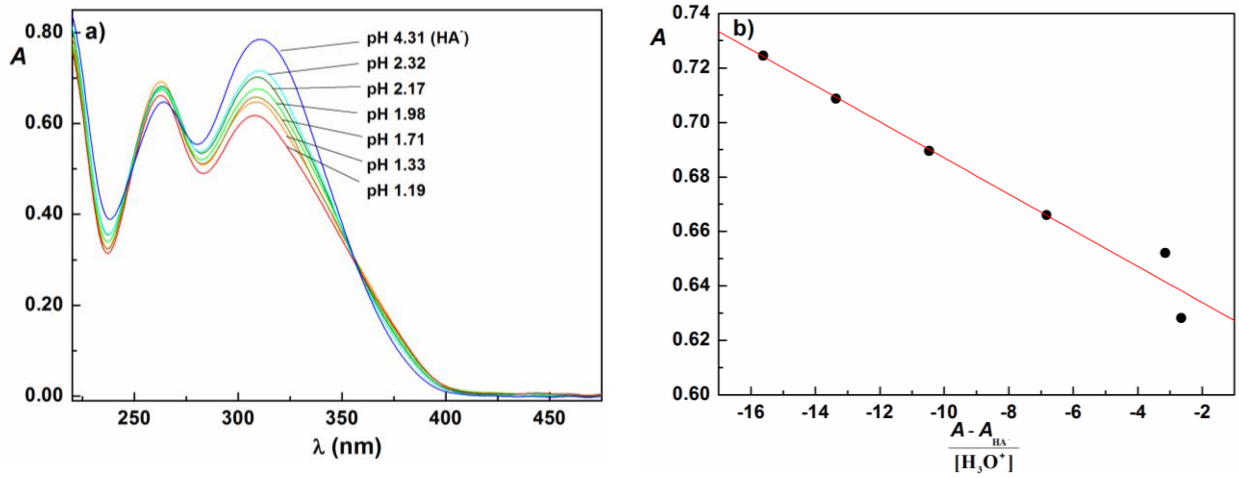


Fig. S18. Absorption spectra of compound **8** used for K_{a1} determination in solutions of different acidity, pH values are indicated; b) Spectrophotometric determination of K_{a1} according to Equation 1; c_8=5.904×10^{-5}M; λ= 308.8 nm; t = 25 °C, I = 0.1 M (NaCl); scan speed 500 nm/min.

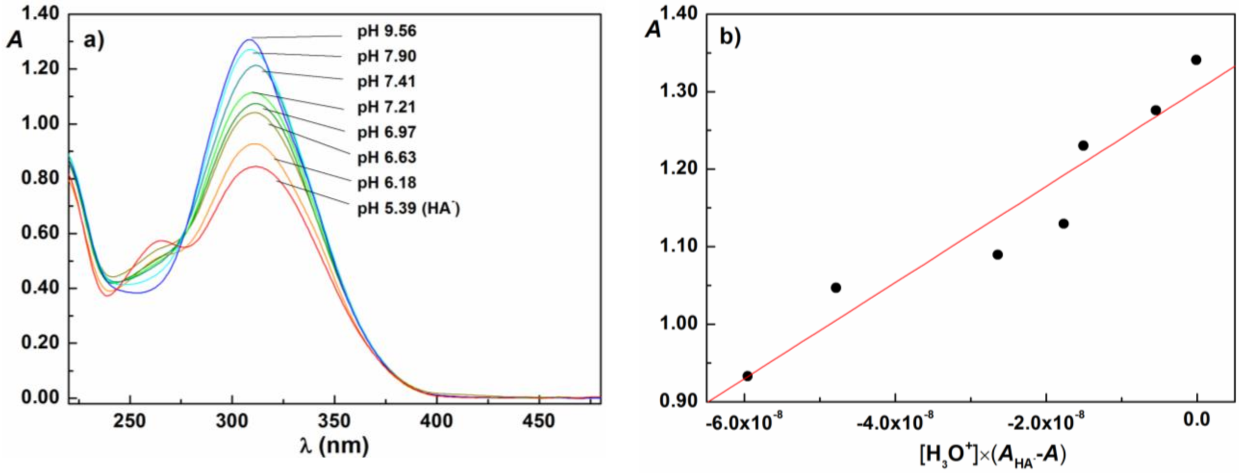


Fig. S19. Absorption spectra of compound **8** used for K_{a2} determination in solutions of different acidity, pH values are indicated; b) Spectrophotometric determination of K_{a2} according to Equation 2; c_8=5.904×10^{-5} M; λ= 308.0 nm; t = 25 °C, I = 0.1 M (NaCl); scan speed 500 nm/min.

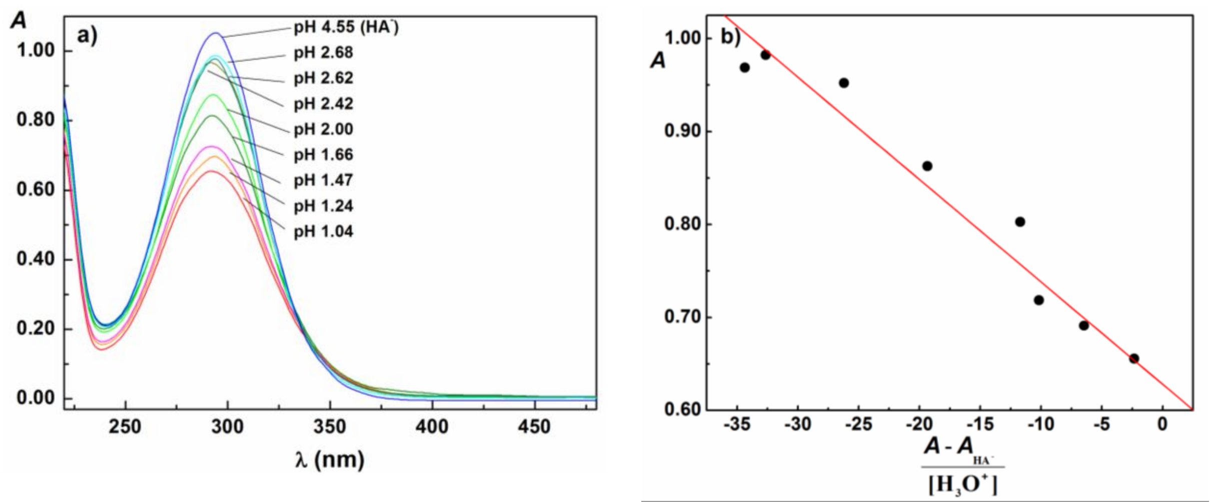


Fig. S20. Absorption spectra of compound **9** used for K_{a1} determination in solutions of different acidity, pH values are indicated; b) Spectrophotometric determination of K_{a1} according to Equation 1; c_9=6.066×10^{-5} M; λ= 293.0 nm; t = 25 °C, I = 0.1 M (NaCl); scan speed 500 nm/min.

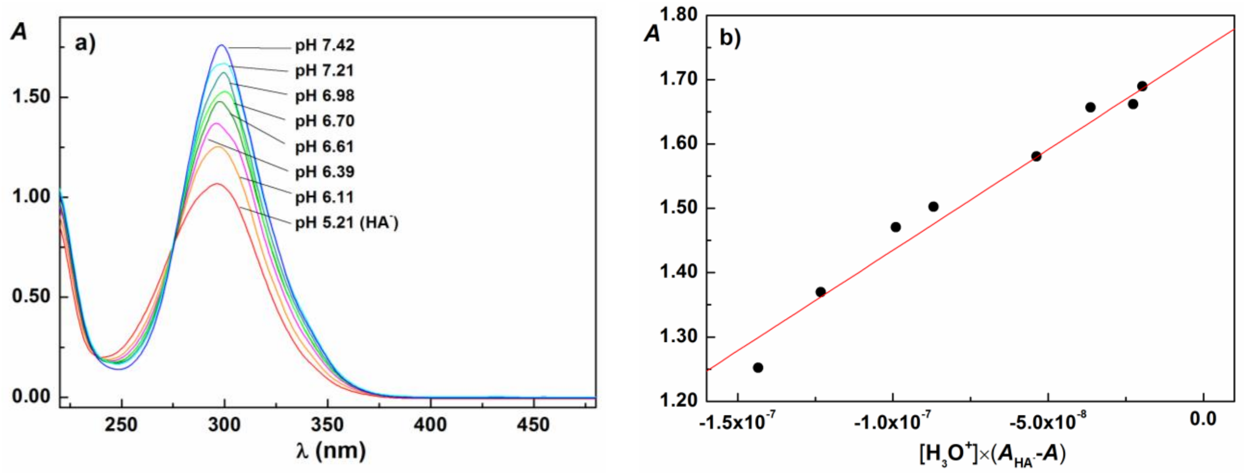


Fig. S21. Absorption spectra of compound **9** used for K_{a2} determination in solutions of different acidity, pH values are indicated; b) Spectrophotometric determination of K_{a2} according to Equation 2; c_9=6.066×10^{-5} M; λ= 296.0 nm; t = 25 °C, I = 0.1 M (NaCl); scan speed 500 nm/min.

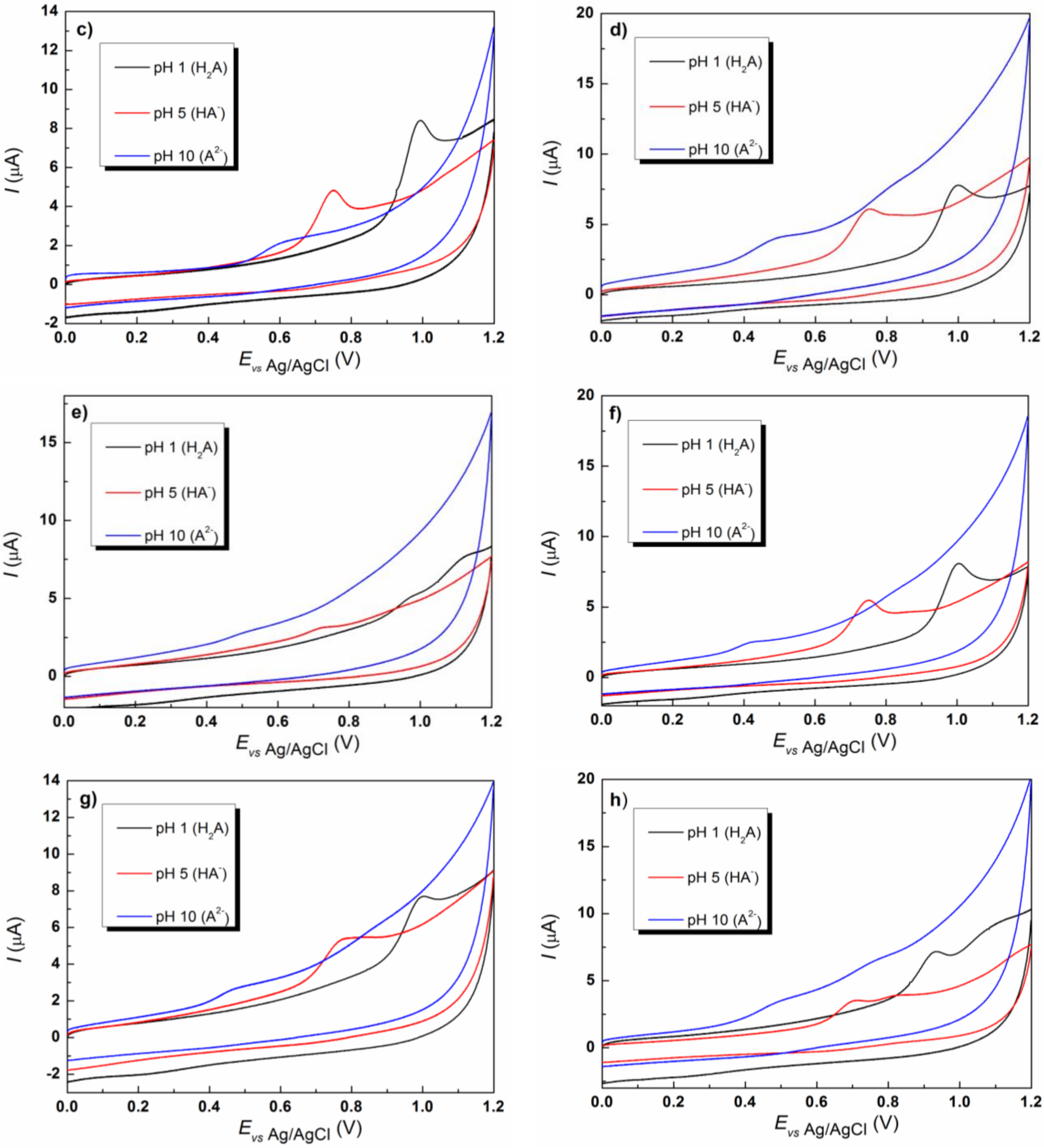


Fig. S22. Cyclic voltammograms of compounds **1-3** and **5-9** in Britton-Robinson buffer at pH 1, pH 5, and pH 10. a) **1**, c_1= 5.46×10^{-5} M; b) **2**, c_2 = 4.61×10^{-5} M; c) **3**, c_3 = 6.54×10^{-5} M; d) **5**, c_5 = 6.58×10^{-5} M; e) **6**, c_6 = 4.09×10^{-5} M; f) **7**, c_7 = 5.22×10^{-5} M; g) **8**, c_8 = 4.06×10^{-5} M; h) **9**, c_9 = 4.43×10^{-5} M; scan rate 100 mV/s, t=25±1 ºC.

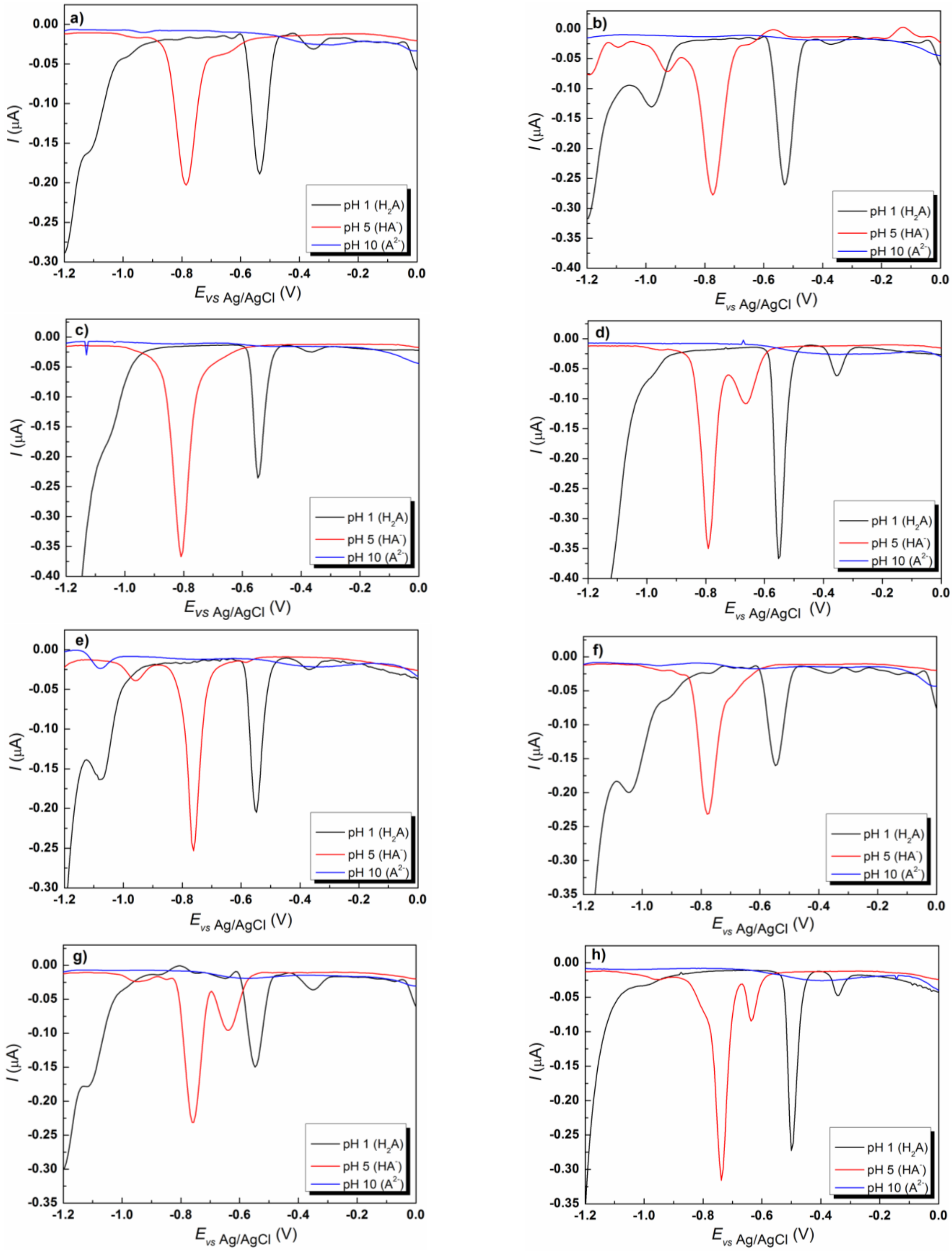
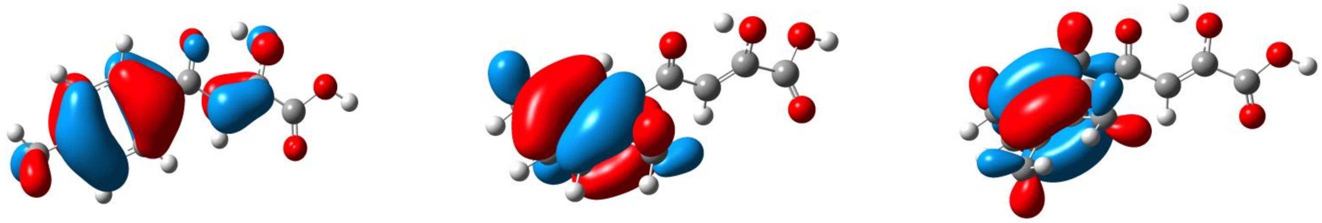
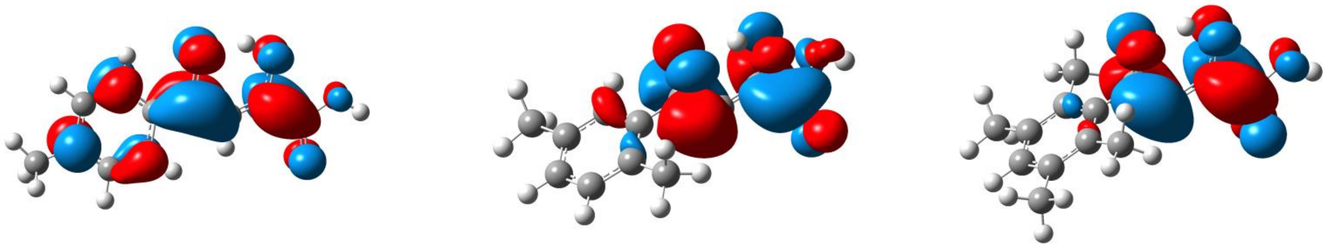


Fig. S23. Differential pulse voltammograms of comp. **2-9** in Britton-Robinson buffer at pH 1, pH 5, and pH 10; a) **2**, c_2 = 4.61×10^{-5} M; b) **3**, c_3 = 6.54×10^{-5} M; c) **4**, c_4 = 4.77×10^{-5} M d) **5**, c_5 = 6.58×10^{-5} M; e) **6**, c_6 = 4.09×10^{-5} M; f) **7**, c_7 = 5.22×10^{-5} M; g) **8**, c_8 = 4.06×10^{-5} M; h) **9**, c_9 = 4.43×10^{-5} M; scan rate 13 mV/s, *t*=25±1 ºC.



Compound **4** Compound **6** Compound **9**

Fig. S24. HOMO orbitals of H_2A form of compounds **4**, **6** and **9** plotted on isocontour level 0.03.



Compound **4** Compound **6** Compound **9**

Fig. S 25. LUMO orbitals of H_2A form of compounds **4**, **6** and **9** plotted on isocontour level 0.03.

Table SI. Energies of FMOs (given in Hartree), and dipoles (given in Debye) for molecular and monoanionic form of compounds **1**-**9**.

	Neutral (H_2A)				**Anion (HA^-)**			
Compound	HOMO	LUMO	HOMO-LUMO gap	Dipole	HOMO	LUMO	HOMO-LUMO gap	Dipole
1	-0.3470	0.0367	0.3837	2.7040	-0.3321	0.0625	0.3946	20.1289
2	-0.3359	0.0406	0.3764	2.3366	-0.3274	0.0670	0.3944	20.7147
3	-0.3363	0.0377	0.3740	2.8168	-0.3266	0.0625	0.3891	22.3967
4	-0.3360	0.0394	0.3754	3.2365	-0.3244	0.0641	0.3885	22.8528
5	-0.3299	0.0417	0.3716	2.8786	-0.3213	0.0683	0.3896	23.1538
6	-0.3236	0.0401	0.3638	2.6851	-0.3172	0.0670	0.3842	21.9031
7	-0.3300	0.0403	0.3703	3.3452	-0.3199	0.0641	0.3840	24.8252
8	-0.3196	0.0425	0.3621	3.1584	-0.3129	0.0687	0.3816	24.0766
9	-0.3100	0.0448	0.3548	2.4134	-0.3063	0.0778	0.3840	22.9021

Table SII. Energies of FMOs (given in Hartree), and dipole moments (given in Debye) for radical anion and radical cation derived from molecular form (H_2A) or monoanionic form (HA^-) of compounds **1-9**. Energies of αSOMO and αLUMO are shown.

	Radical anion from H_2A				**Radical cation from H_2A**			
Compound	SOMO	LUMO	SOMO-LUMO gap	Dipole	SOMO	LUMO	SOMO-LUMO gap	Dipole
1	0.0757	0.2471	0.1713	5.1253	-0.3009	-0.1600	0.1409	2.2888
2	0.0767	0.2475	0.1708	5.6837	-0.2996	-0.1579	0.1417	3.0584
3	0.0756	0.2459	0.1703	6.6132	-0.2989	-0.1576	0.1413	3.3480
4	0.0765	0.2458	0.1693	7.3901	-0.2970	-0.1551	0.1419	2.9073
5	0.0774	0.2465	0.1691	7.7582	-0.2761	-0.1313	0.1449	2.9050
6	0.0766	0.2443	0.1677	7.0045	-0.2975	-0.1555	0.1421	3.4272
7	0.0763	0.2452	0.1690	8.6434	-0.2749	-0.1306	0.1443	3.1645
8	0.0772	0.2461	0.1689	8.8467	-0.2751	-0.1316	0.1435	1.9357
9	0.0784	0.2537	0.1754	8.6062	-0.2532	-0.0821	0.1711	10.3233
	Radical dianion from HA^-							
Compound	SOMO	LUMO	SOMO-LUMO gap	Dipole				
1	0.1658	0.3866	0.2208	12.3478				
2	0.1685	0.3824	0.2138	14.5640				
3	0.1641	0.3836	0.2195	15.5722				
4	0.1645	0.3812	0.2167	15.8690				
5	0.1669	0.3779	0.2109	17.5080				
6	0.1664	0.3836	0.2172	16.0213				
7	0.1631	0.3817	0.2186	18.6586				
8	0.1665	0.3795	0.2130	19.1801				
9	0.1875	0.3529	0.1654	23.1287				

Table SIII. Intercorrelation matrix (*r* values) between oxidation/reduction potentials at pH 1 and at pH 5 and descriptors extracted from QM calculations. Indicator variable (*I*) is also included. ‘Molecular’ refer to neutral form of compounds; ‘anion’ refer to anionic form of compounds (deprotonated carboxyl group); ‘RA’ refer to radical anion/dianion (derived from neutral/anionic form); ‘RC’ refer to radical cation derived from neutral form.

E_{ox}-pH_1		**E_{red}-pH_1**	
HOMO molecular	-0.6797	HOMO molecular	0.3250
LUMO molecular	-0.5739	LUMO molecular	0.2916
HOMO-LUMO gap/molecular	0.6876	HOMO-LUMO gap/molecular	-0.3233
Dipole molecular	0.3642	Dipole molecular	-0.6104
SOMO (RC)	-0.6565	SOMO (RA)	0.3298
LUMO (RC)	-0.7924	LUMO (RA)	0.8713
SOMO-LUMO gap/RC	-0.9352	SOMO-LUMO gap/RA	0.9361
Dipole RC	-0.9519	Dipole RA	-0.0503
I	-0.7908	*I*	0.5906
E_{ox}-pH_5		**E_{red}-pH_5**	
HOMO molecular	-0.4092	HOMO anion	0.8213
LUMO molecular	-0.3958	LUMO anion	0.7433
HOMO-LUMO gap/molecular	0.3999	HOMO-LUMO gap/anion	-0.6495
Dipole molecular	0.4117	Dipole molecular	-0.3518
SOMO (RC)	-0.4353	SOMO dianion (RA)	0.6858
LUMO (RC)	-0.6048	LUMO dianion (RA)	-0.6739
SOMO-LUMO gap/cation (RC)	-0.8283	SOMO-LUMO gap/dianion (RA)	-0.6869
Dipole (RC)	-0.9067	Dipole dianion (RA)	0.7311
I	-0.5295	*I*	0.9533