

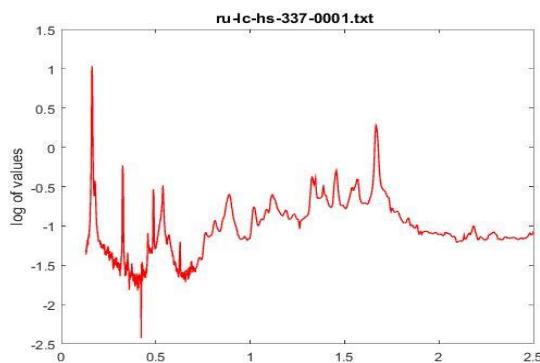
Supplementary Material

Asymmetric flavone-based liquid crystals

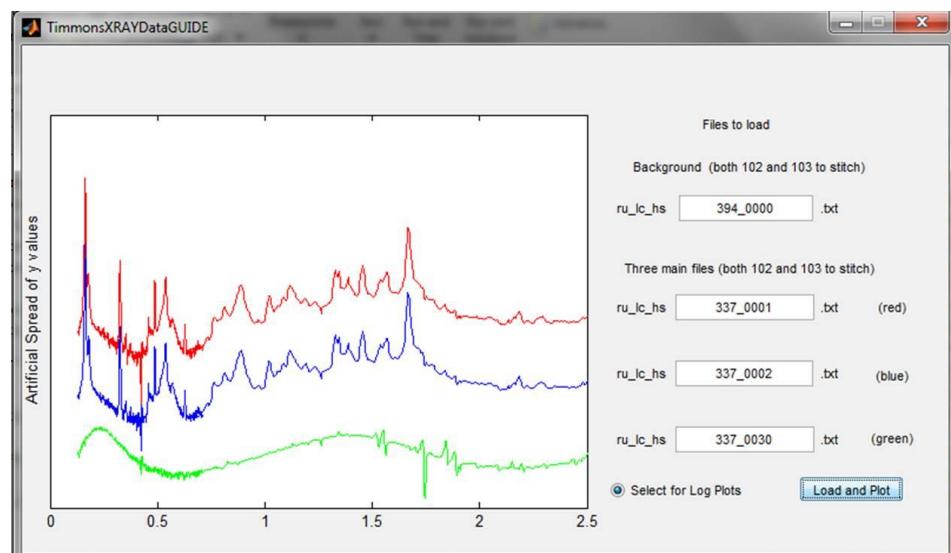
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PXRD data:

Summary of subtraction of background data and plot creation: experimental data was imported, stored in two data files (based on two time intervals), along with background noise data in a third file, into a Matlab file, followed by concatenation into one data set and subtraction of the corresponding background noise. Results were plotted with [q (\AA^{-1})] as horizontal axis and log of [I (arbitrary units)] on the vertical axis. Example: imported and concatenated data in ru_lc_hs103_337_0001.txt and ru_lc_hs102_337_0001.txt, subtracted background data contained in ru_lc_hs103_394_000.txt and plotted time versus log data (as pictured).



The picture below shows a graphical user interface (GUI) that was developed in order to compare data from three different data files. Picture shown using data from samples ru_lc_hs_337_0001.txt, ru_lc_hs_337_0002.txt, and ru_lc_hs_337_0030.txt, background in ru_lc_hs_394_0000.txt



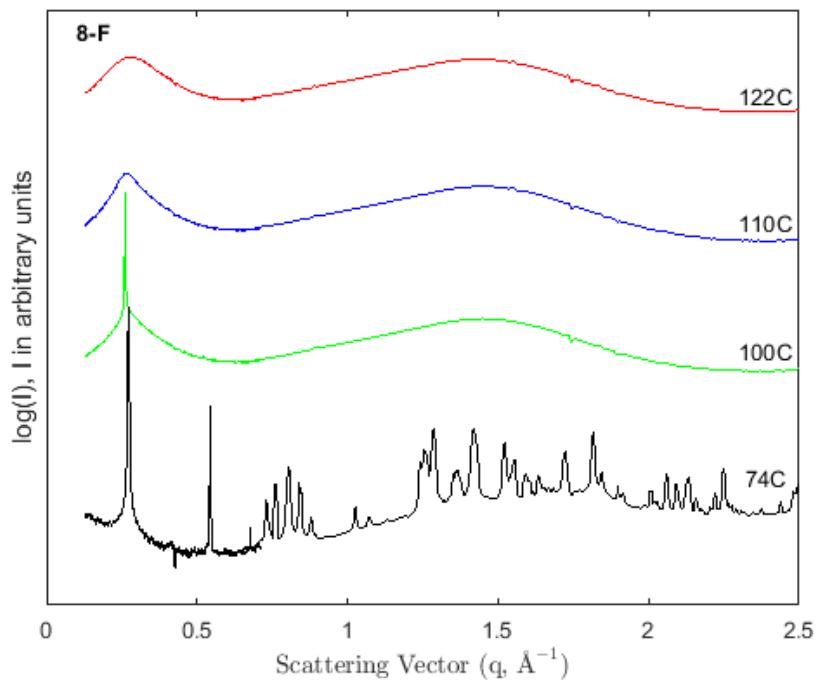


Figure S1. PXRD data of **8-F** at four temperatures. Curves have been offset vertically for clarity.

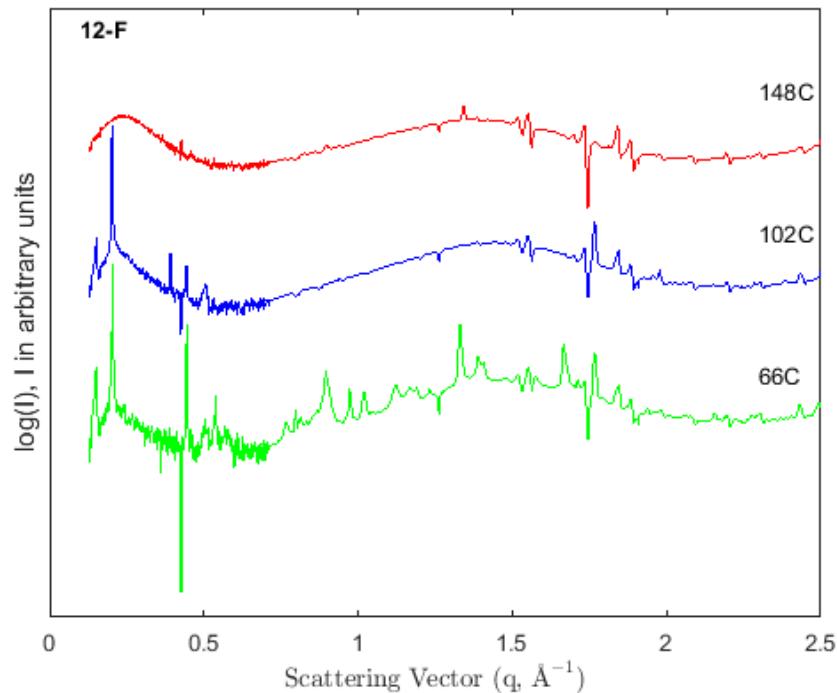


Figure S2. PXRD data of **12-F** at three temperatures. Curves have been offset vertically for clarity.

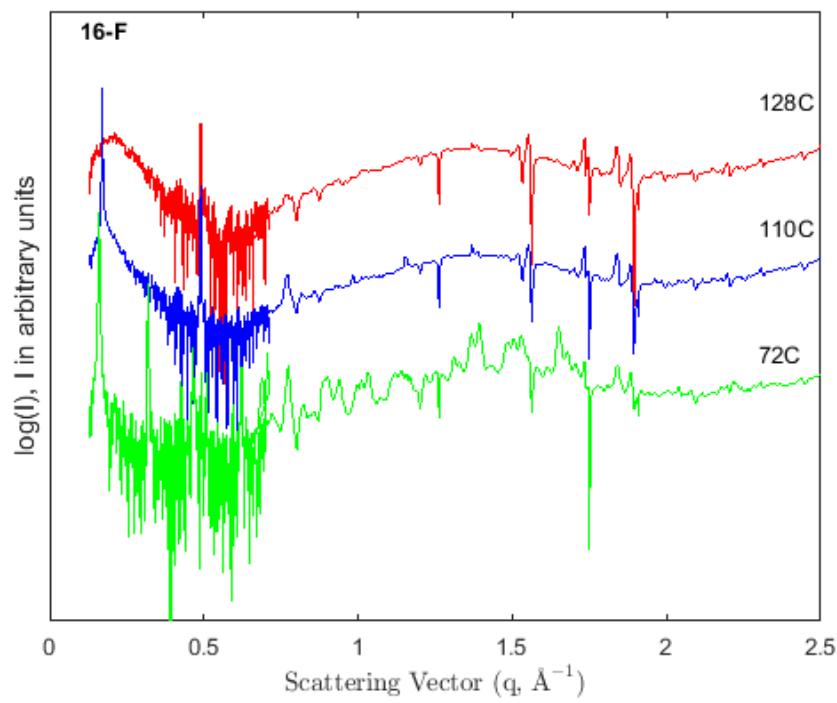


Figure S3. PXRD data of **16-F** at three temperatures. Curves have been offset vertically for clarity.

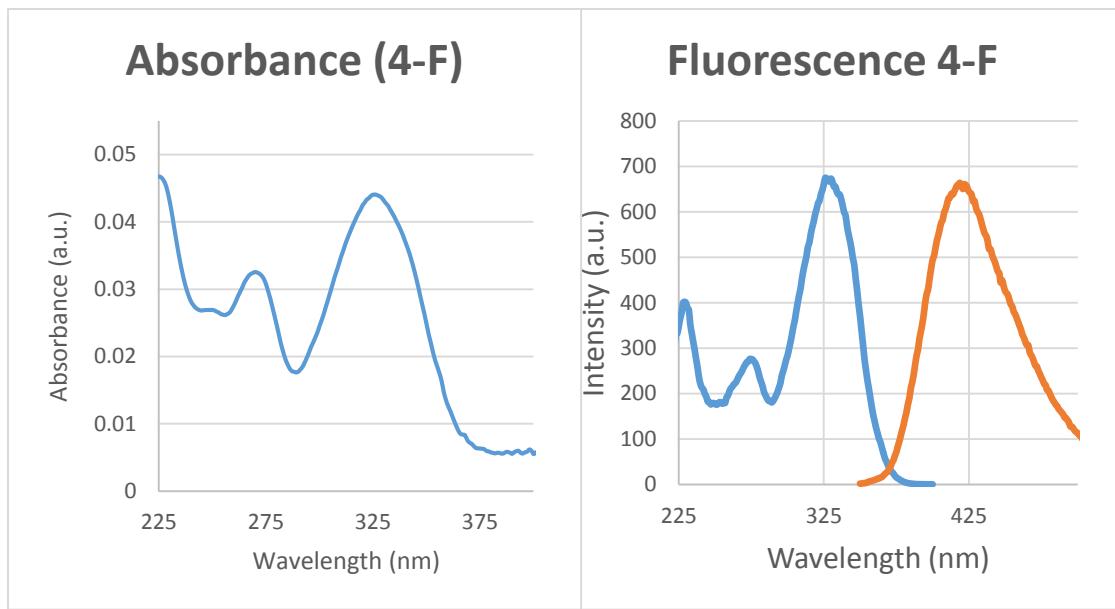


Figure S4. Absorbance spectra for **4-F** in methanol (2.68×10^{-6} M).

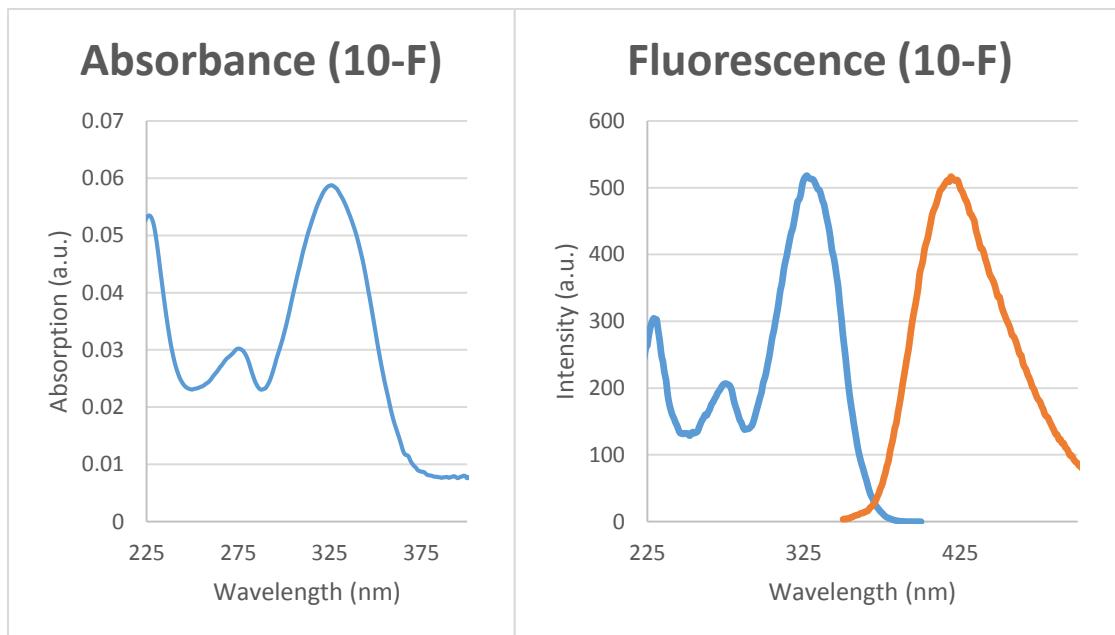


Figure S5. Absorbance spectra for **10-F** in methanol (3.39×10^{-6} M).

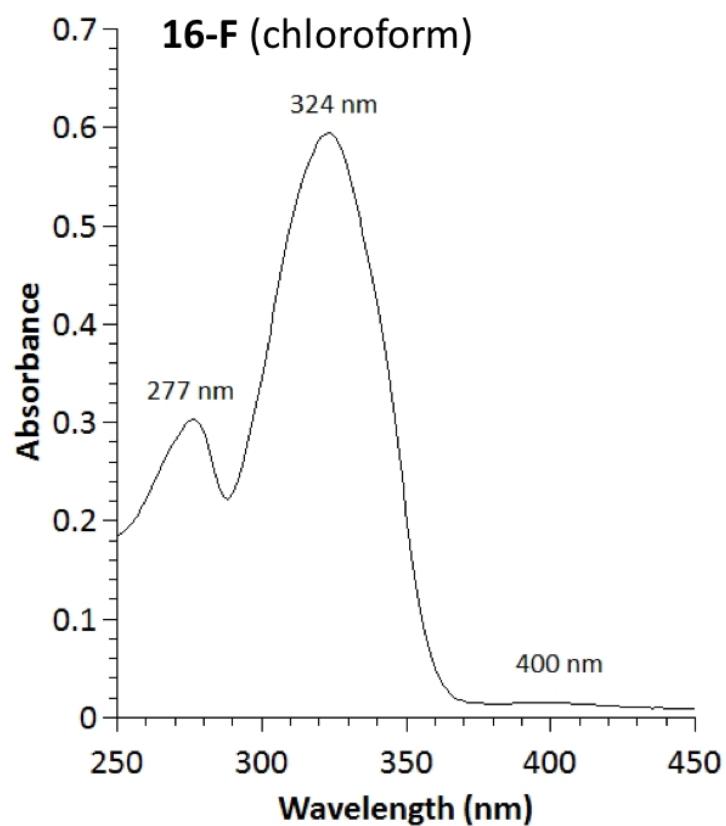


Figure S6. Absorbance spectra for **16-F** in chloroform.

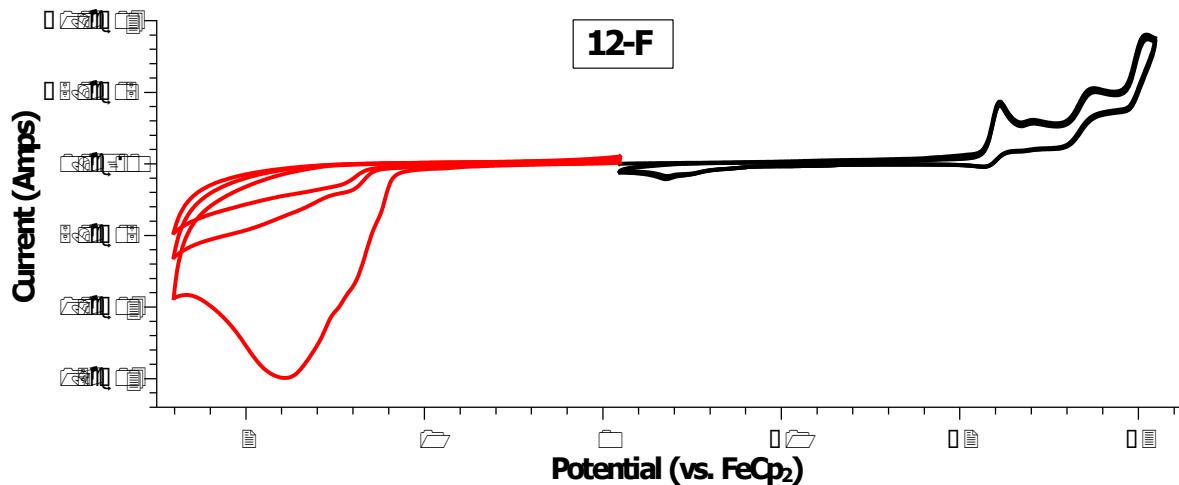


Figure S7. Overlay of oxidative and reductive cyclic voltammograms of ~2 mM **12-F** in MeCN containing 0.1M TBAPF₆.

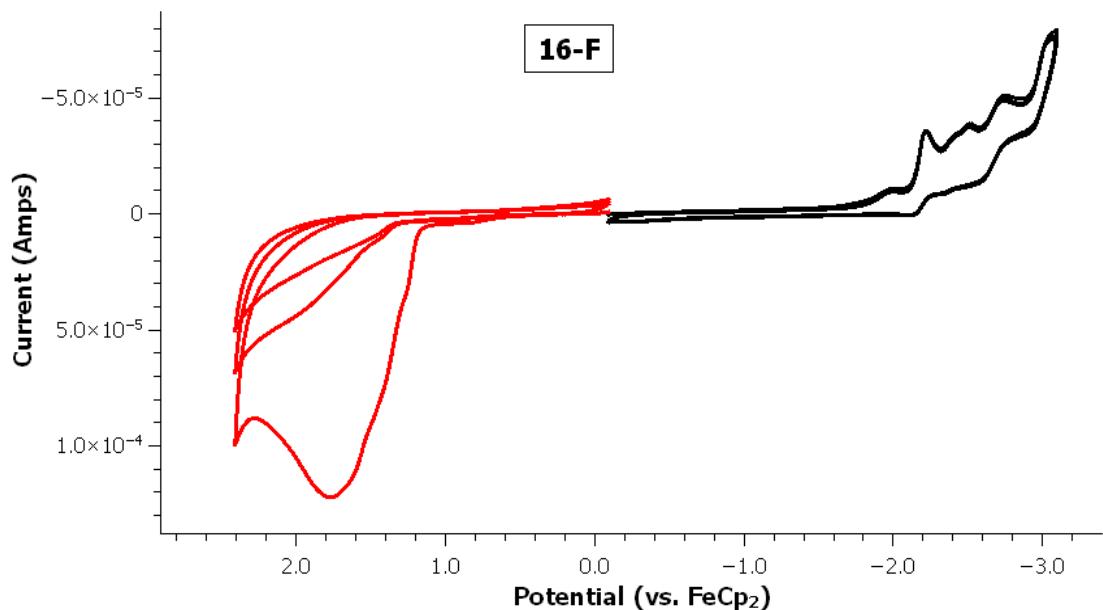
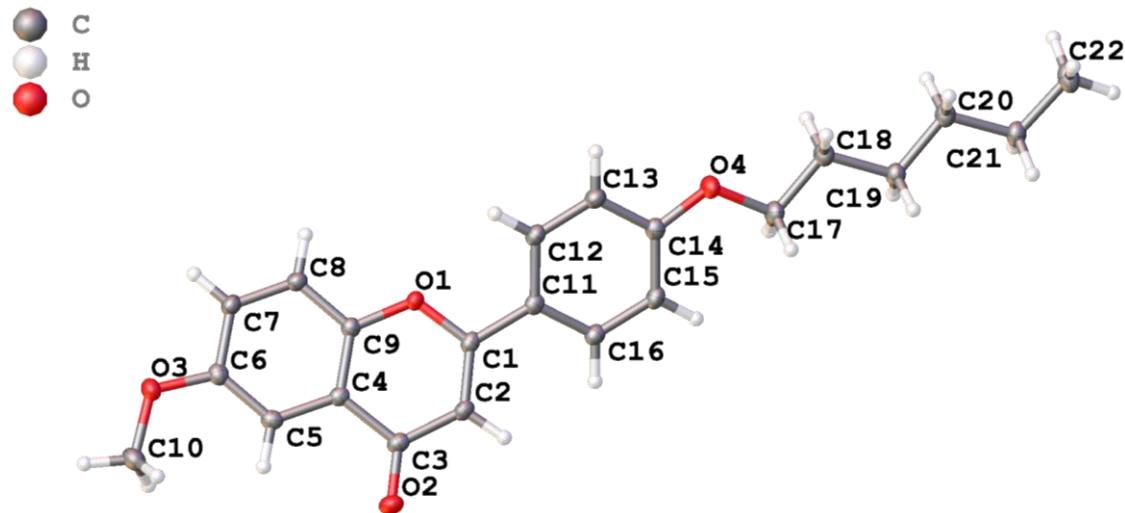


Figure S8. Overlay of oxidative and reductive cyclic voltammograms of ~2 mM **16-F** in MeCN containing 0.1M TBAPF₆.

Table S1. Crystal data and structure refinement for **6-F**.

Identification code	cs1933
Empirical formula	C ₂₂ H ₂₄ O ₄
Formula weight	352.41
Temperature	100(1) K
Wavelength	0.7107 Å
Crystal system	monoclinic
Space group	P 1 2 ₁ /n 1
Unit cell dimensions	$a = 13.1720(8)$ Å $\alpha = 90^\circ$. $b = 8.6248(3)$ Å $\beta = 111.235(7)^\circ$. $c = 17.2374(10)$ Å $\gamma = 90^\circ$.
Volume	1825.32(17) Å ³
Z	4
Density (calculated)	1.282 Mg/m ³
Absorption coefficient	0.087 mm ⁻¹
F(000)	752
Crystal size	0.572 x 0.3161 x 0.1408 mm ³
Theta range for data collection	3.89 to 32.42°.
Index ranges	-18≤h≤19, -11≤k≤12, -24≤l≤22
Reflections collected	18655
Independent reflections	6032 [R(int) = 0.0393]
Completeness to theta = 31.00°	99.3 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.90449
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	6032 / 0 / 237
Goodness-of-fit on F ²	1.023
Final R indices [I>2sigma(I)]	R1 = 0.0490, wR2 = 0.1116
R indices (all data)	R1 = 0.0732, wR2 = 0.1268
Largest diff. peak and hole	0.408 and -0.242 e.Å ⁻³



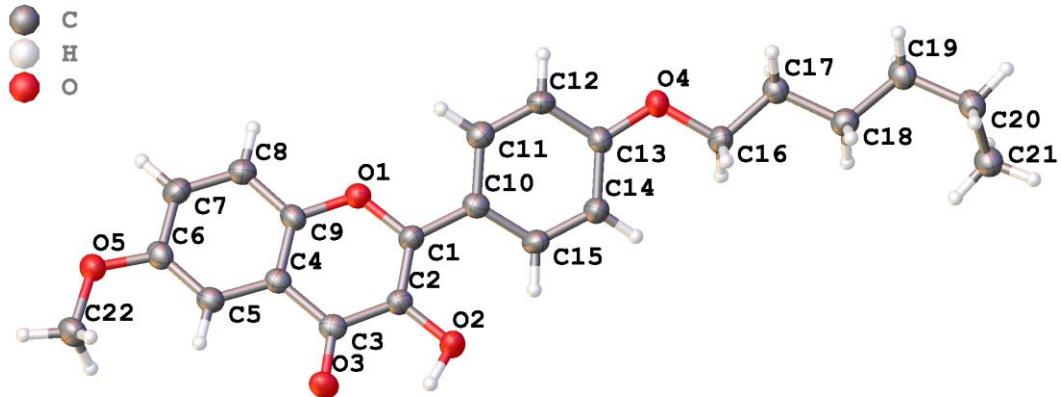
6-F

Table S2. Bond lengths [Å] and angles [°] for **6-F**.

O(1)-C(1)	1.3626(14)	C(3)-C(4)	1.4785(16)	C(13)-C(14)	1.3993(17)
O(1)-C(9)	1.3741(14)	C(4)-C(5)	1.4116(17)	C(14)-C(15)	1.3991(17)
O(2)-C(3)	1.2380(14)	C(4)-C(9)	1.3896(15)	C(15)-C(16)	1.3979(17)
O(3)-C(6)	1.3657(15)	C(5)-C(6)	1.3861(17)	C(17)-C(18)	1.5123(17)
O(3)-C(10)	1.4338(15)	C(6)-C(7)	1.4097(16)	C(18)-C(19)	1.5250(18)
O(4)-C(14)	1.3633(14)	C(7)-C(8)	1.3762(17)	C(19)-C(20)	1.5285(17)
O(4)-C(17)	1.4392(15)	C(8)-C(9)	1.3990(16)	C(20)-C(21)	1.5218(18)
C(1)-C(2)	1.3584(16)	C(11)-C(12)	1.4099(16)	C(21)-C(22)	1.5240(18)
C(1)-C(11)	1.4711(17)	C(11)-C(16)	1.3980(16)		
C(2)-C(3)	1.4474(17)	C(12)-C(13)	1.3822(17)		
C(1)-O(1)-C(9)	119.38(9)	O(1)-C(9)-C(4)	122.81(10)		
C(6)-O(3)-C(10)	117.28(10)	O(1)-C(9)-C(8)	115.80(10)		
C(14)-O(4)-C(17)	119.28(9)	C(4)-C(9)-C(8)	121.39(11)		
O(1)-C(1)-C(11)	111.34(10)	C(12)-C(11)-C(1)	119.55(11)		
C(2)-C(1)-O(1)	121.91(11)	C(16)-C(11)-C(1)	121.76(10)		
C(2)-C(1)-C(11)	126.75(11)	C(16)-C(11)-C(12)	118.69(11)		
C(1)-C(2)-C(3)	122.32(11)	C(13)-C(12)-C(11)	120.55(11)		
O(2)-C(3)-C(2)	123.39(11)	C(12)-C(13)-C(14)	120.25(11)		
O(2)-C(3)-C(4)	122.02(11)	O(4)-C(14)-C(13)	114.44(10)		
C(2)-C(3)-C(4)	114.59(10)	O(4)-C(14)-C(15)	125.41(11)		
C(5)-C(4)-C(3)	121.61(10)	C(15)-C(14)-C(13)	120.16(11)		
C(9)-C(4)-C(3)	118.93(11)	C(16)-C(15)-C(14)	119.18(11)		
C(9)-C(4)-C(5)	119.46(11)	C(15)-C(16)-C(11)	121.17(11)		
C(6)-C(5)-C(4)	119.28(11)	O(4)-C(17)-C(18)	106.37(10)		
O(3)-C(6)-C(5)	125.75(11)	C(17)-C(18)-C(19)	112.79(10)		
O(3)-C(6)-C(7)	114.07(11)	C(18)-C(19)-C(20)	112.74(10)		
C(5)-C(6)-C(7)	120.17(11)	C(21)-C(20)-C(19)	113.07(10)		
C(8)-C(7)-C(6)	120.89(11)	C(20)-C(21)-C(22)	113.26(11)		
C(7)-C(8)-C(9)	118.75(11)				

Table S3. Crystal data and structure refinement for **6-F-OH**.

Identification code	DT270b
Empirical formula	C ₂₂ H ₂₄ O ₅
Formula weight	368.41
Temperature	100.00(10) K
Wavelength	1.5418 Å
Crystal system	triclinic
Space group	P -1
Unit cell dimensions	$a = 7.5634(7)$ Å $\alpha = 89.108(7)^\circ$. $b = 10.1766(9)$ Å $\beta = 86.251(7)^\circ$. $c = 12.0988(9)$ Å $\gamma = 81.306(8)^\circ$.
Volume	918.55(14) Å ³
Z	2
Density (calculated)	1.332 Mg/m ³
Absorption coefficient	0.765 mm ⁻¹
F(000)	392
Crystal size	0.1268 x 0.0581 x 0.0167 mm ³
Theta range for data collection	3.66 to 72.63°.
Index ranges	-8<=h<=9, -12<=k<=12, -14<=l<=13
Reflections collected	10503
Independent reflections	3559 [R(int) = 0.0677]
Completeness to theta = 67.50°	99.5 %
Absorption correction	Gaussian
Max. and min. transmission	1.047 and 0.953
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3559 / 0 / 249
Goodness-of-fit on F ²	1.019
Final R indices [I>2sigma(I)]	R1 = 0.0686, wR2 = 0.1598
R indices (all data)	R1 = 0.1243, wR2 = 0.1948
Largest diff. peak and hole	0.275 and -0.296 e.Å ⁻³



6-F-OH

Table S4. Bond lengths [\AA] and angles [$^\circ$] for **6-F-OH**.

O(1)-C(1)	1.378(4)	C(2)-C(3)	1.437(4)	C(11)-C(12)	1.382(5)
O(1)-C(9)	1.369(4)	C(3)-C(4)	1.454(5)	C(12)-C(13)	1.401(5)
O(2)-C(2)	1.366(4)	C(4)-C(5)	1.408(4)	C(13)-C(14)	1.400(5)
O(3)-C(3)	1.251(4)	C(4)-C(9)	1.384(5)	C(14)-C(15)	1.373(4)
O(4)-C(13)	1.357(4)	C(5)-C(6)	1.384(5)	C(16)-C(17)	1.500(4)
O(4)-C(16)	1.443(4)	C(6)-C(7)	1.405(5)	C(17)-C(18)	1.521(4)
O(5)-C(6)	1.362(4)	C(7)-C(8)	1.366(5)	C(18)-C(19)	1.526(4)
O(5)-C(22)	1.441(4)	C(8)-C(9)	1.399(5)	C(19)-C(20)	1.528(5)
C(1)-C(2)	1.367(5)	C(10)-C(11)	1.399(5)	C(20)-C(21)	1.520(5)
C(1)-C(10)	1.460(4)	C(10)-C(15)	1.404(5)		
C(9)-O(1)-C(1)	120.5(3)			C(7)-C(8)-C(9)	118.5(3)
C(13)-O(4)-C(16)	117.4(3)			O(1)-C(9)-C(4)	122.4(3)
C(6)-O(5)-C(22)	117.3(3)			O(1)-C(9)-C(8)	116.4(3)
O(1)-C(1)-C(10)	112.1(3)			C(4)-C(9)-C(8)	121.2(3)
C(2)-C(1)-O(1)	119.9(3)			C(11)-C(10)-C(1)	119.7(3)
C(2)-C(1)-C(10)	127.9(3)			C(11)-C(10)-C(15)	117.6(3)
O(2)-C(2)-C(1)	119.9(3)			C(15)-C(10)-C(1)	122.6(3)
O(2)-C(2)-C(3)	117.9(3)			C(12)-C(11)-C(10)	121.3(3)
C(1)-C(2)-C(3)	122.3(3)			C(11)-C(12)-C(13)	120.1(3)
O(3)-C(3)-C(2)	120.8(3)			O(4)-C(13)-C(12)	115.8(3)
O(3)-C(3)-C(4)	123.2(3)			O(4)-C(13)-C(14)	124.8(3)
C(2)-C(3)-C(4)	116.1(3)			C(14)-C(13)-C(12)	119.3(3)
C(5)-C(4)-C(3)	121.3(3)			C(15)-C(14)-C(13)	119.8(3)
C(9)-C(4)-C(3)	118.8(3)			C(14)-C(15)-C(10)	121.8(3)
C(9)-C(4)-C(5)	119.9(3)			O(4)-C(16)-C(17)	107.8(3)
C(6)-C(5)-C(4)	119.0(3)			C(16)-C(17)-C(18)	111.8(3)
O(5)-C(6)-C(5)	125.2(3)			C(17)-C(18)-C(19)	113.0(3)
O(5)-C(6)-C(7)	115.0(3)			C(18)-C(19)-C(20)	113.3(3)
C(5)-C(6)-C(7)	119.8(3)			C(21)-C(20)-C(19)	113.5(3)
C(8)-C(7)-C(6)	121.6(3)				

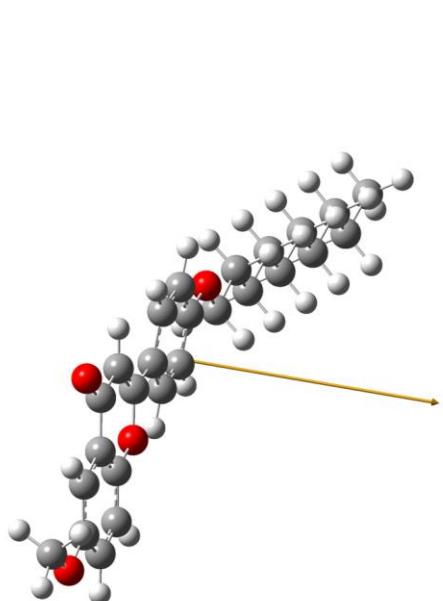
DFT Calculations were performed with Gaussian 09¹⁹ and GaussView 5²⁰ was used to visualize the structures. All atoms were optimized and checked for imaginary frequencies using the 6-31(g) basis set on all atoms.

	Zero Point Energy Corrected Energy (au)	Number of Imaginary Frequencies	Dipole Moment (Debye)
Flavone	-1310.127989	0	5.1126
Isoflavone	-1310.121466	0	3.0844

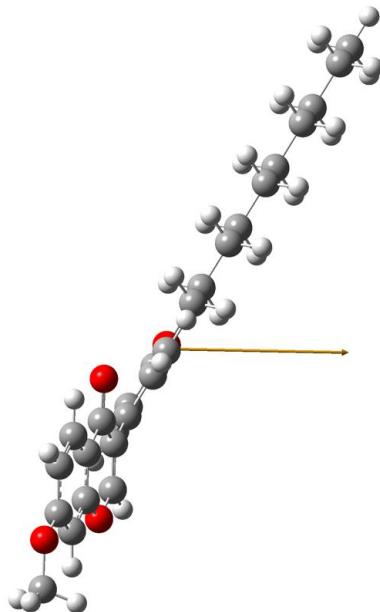
Flavone	Exact polarizability:	515.811	-13.624	281.75	1.408	-0.756	149.861
	Approx polarizability:	615.468	20.58	490.385	3.965	0.033	219.676

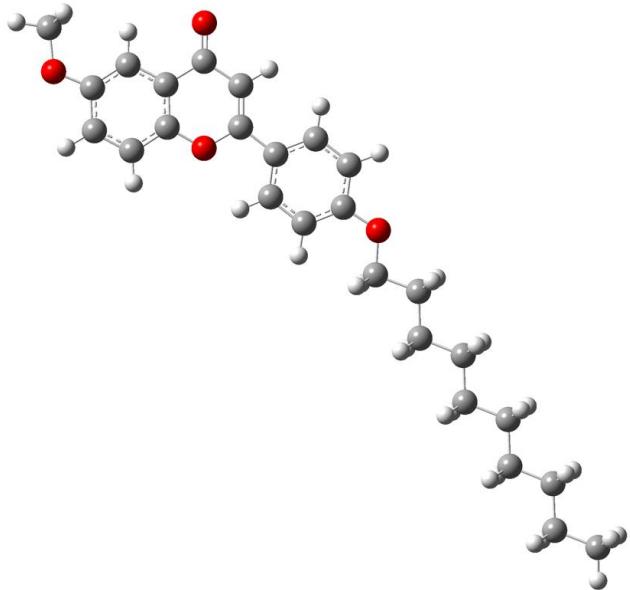
Isoflavone	Exact polarizability:	501.089	-4.816	256.368	-13.057	-5.613	161.84
	Approx polarizability:	578.208	19.009	457.357	-27.93	-21.371	245.113

Dipole vector for Flavone:



Dipole vector for Isoflavone:





Flavone Coordinates:

TITLE	Flavone						
REMARK	1	File	created	by	GaussView	5.0.9	
HETATM	1	C	0	6.067	-2.243	-0.079	C
HETATM	2	C	0	5.76	-0.877	-0.028	C
HETATM	3	C	0	6.764	0.096	0.021	C
HETATM	4	C	0	8.112	-0.308	0.019	C
HETATM	5	C	0	8.426	-1.663	-0.032	C
HETATM	6	C	0	7.399	-2.632	-0.081	C
HETATM	7	H	0	5.265	-2.97	-0.117	H
HETATM	8	H	0	8.861	0.473	0.058	H
HETATM	9	H	0	7.68	-3.677	-0.121	H
HETATM	10	C	0	6.398	1.526	0.077	C
HETATM	11	O	0	7.268	2.436	0.127	O
HETATM	12	C	0	4.972	1.794	0.074	C
HETATM	13	H	0	4.677	2.832	0.13	H
HETATM	14	C	0	4.029	0.81	0.016	C
HETATM	15	O	0	4.407	-0.529	-0.031	O
HETATM	16	C	0	2.572	0.975	-0.002	C
HETATM	17	C	0	1.722	-0.141	0.105	C
HETATM	18	C	0	1.981	2.253	-0.126	C
HETATM	19	C	0	0.333	0.001	0.093	C

HETATM	20	H	0	2.156	-1.128	0.199	H
HETATM	21	C	0	0.602	2.405	-0.14	C
HETATM	22	H	0	2.603	3.135	-0.226	H
HETATM	23	C	0	-0.233	1.278	-0.03	C
HETATM	24	H	0	-0.29	-0.88	0.18	H
HETATM	25	H	0	0.142	3.381	-0.239	H
HETATM	26	O	0	-1.592	1.535	-0.058	O
HETATM	27	C	0	-2.541	0.425	0.048	C
HETATM	28	H	0	-2.39	-0.093	1.004	H
HETATM	29	H	0	-2.36	-0.288	-0.768	H
HETATM	30	C	0	-3.939	1.022	-0.044	C
HETATM	31	H	0	-4.032	1.555	-0.999	H
HETATM	32	H	0	-4.054	1.771	0.75	H
HETATM	33	C	0	-5.04	-0.048	0.075	C
HETATM	34	H	0	-4.944	-0.57	1.039	H
HETATM	35	H	0	-4.899	-0.811	-0.706	H
HETATM	36	C	0	-6.46	0.537	-0.045	C
HETATM	37	H	0	-6.559	1.051	-1.013	H
HETATM	38	H	0	-6.601	1.307	0.729	H
HETATM	39	C	0	-7.568	-0.523	0.084	C
HETATM	40	H	0	-7.419	-1.299	-0.682	H
HETATM	41	H	0	-7.474	-1.03	1.057	H
HETATM	42	C	0	-8.987	0.057	-0.051	C
HETATM	43	H	0	-9.136	0.836	0.712	H
HETATM	44	H	0	-9.082	0.559	-1.026	H
HETATM	45	O	0	9.717	-2.174	-0.04	O
HETATM	46	C	0	10.83	-1.24	0.005	C
HETATM	47	H	0	11.724	-1.862	-0.013	H
HETATM	48	H	0	10.821	-0.573	-0.865	H
HETATM	49	H	0	10.808	-0.643	0.924	H
HETATM	50	C	0	-10.096	-1.003	0.083	C
HETATM	51	H	0	-9.944	-1.785	-0.677	H
HETATM	52	H	0	-10.004	-1.502	1.06	H
HETATM	53	C	0	-11.516	-0.426	-0.06	C
HETATM	54	H	0	-11.669	0.357	0.699	H
HETATM	55	H	0	-11.609	0.072	-1.037	H
HETATM	56	C	0	-12.625	-1.485	0.075	C
HETATM	57	H	0	-12.472	-2.267	-0.683	H
HETATM	58	H	0	-12.532	-1.983	1.052	H
HETATM	59	C	0	-14.039	-0.9	-0.07	C

HETATM	60	H	0	-14.806	-1.677	0.027	H
HETATM	61	H	0	-14.232	-0.141	0.698	H
HETATM	62	H	0	-14.169	-0.422	-1.049	H
END							
CONECT	1	2	6	7			
CONECT	2	1	3	15			
CONECT	3	2	4	10			
CONECT	4	3	5	8			
CONECT	5	4	6	45			
CONECT	6	1	5	9			
CONECT	7	1					
CONECT	8	4					
CONECT	9	6					
CONECT	10	3	11	12			
CONECT	11	10					
CONECT	12	10	13	14			
CONECT	13	12					
CONECT	14	12	15	16			
CONECT	15	2	14				
CONECT	16	14	17	18			
CONECT	17	16	19	20			
CONECT	18	16	21	22			
CONECT	19	17	23	24			
CONECT	20	17					
CONECT	21	18	23	25			
CONECT	22	18					
CONECT	23	19	21	26			
CONECT	24	19					
CONECT	25	21					
CONECT	26	23	27				
CONECT	27	26	28	29	30		
CONECT	28	27					
CONECT	29	27					
CONECT	30	27	31	32	33		
CONECT	31	30					
CONECT	32	30					
CONECT	33	30	34	35	36		
CONECT	34	33					
CONECT	35	33					
CONECT	36	33	37	38	39		

CONECT	37	36			
CONECT	38	36			
CONECT	39	36	40	41	42
CONECT	40	39			
CONECT	41	39			
CONECT	42	39	43	44	50
CONECT	43	42			
CONECT	44	42			
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CONECT	46	45	47	48	49
CONECT	47	46			
CONECT	48	46			
CONECT	49	46			
CONECT	50	42	51	52	53
CONECT	51	50			
CONECT	52	50			
CONECT	53	50	54	55	56
CONECT	54	53			
CONECT	55	53			
CONECT	56	53	57	58	59
CONECT	57	56			
CONECT	58	56			
CONECT	59	56	60	61	62
CONECT	60	59			
CONECT	61	59			
CONECT	62	59			



Isoflavone Coordinates:

TITLE	Isoflavone						
REMARK	1	File	created	by	GaussView	5.0.9	
HETATM	1	C	0	-8.253	-0.352	0.365	C
HETATM	2	C	0	-6.86	-0.313	0.248	C
HETATM	3	C	0	-6.159	0.837	-0.139	C
HETATM	4	C	0	-6.915	1.998	-0.421	C
HETATM	5	C	0	-8.293	1.993	-0.316	C
HETATM	6	C	0	-8.966	0.812	0.079	C
HETATM	7	H	0	-8.725	-1.275	0.671	H
HETATM	8	H	0	-6.374	2.888	-0.72	H
HETATM	9	C	0	-4.693	0.835	-0.248	C
HETATM	10	O	0	-4.06	1.876	-0.564	O
HETATM	11	C	0	-4.031	-0.457	0.04	C
HETATM	12	C	0	-4.799	-1.507	0.439	C
HETATM	13	O	0	-6.176	-1.489	0.548	O
HETATM	14	C	0	-2.565	-0.631	-0.095	C
HETATM	15	C	0	-2.028	-1.862	-0.535	C
HETATM	16	C	0	-1.664	0.401	0.226	C
HETATM	17	C	0	-0.655	-2.064	-0.621	C
HETATM	18	H	0	-2.696	-2.661	-0.84	H

HETATM	19	C	0	-0.281	0.209	0.138	C
HETATM	20	H	0	-2.048	1.365	0.529	H
HETATM	21	C	0	0.227	-1.028	-0.278	C
HETATM	22	H	0	-0.242	-3.005	-0.965	H
HETATM	23	H	0	0.381	1.027	0.394	H
HETATM	24	O	0	1.58	-1.323	-0.396	O
HETATM	25	O	0	-10.342	0.915	0.155	O
HETATM	26	C	0	-11.115	-0.25	0.557	C
HETATM	27	H	0	-12.153	0.08	0.544	H
HETATM	28	H	0	-10.979	-1.076	-0.15	H
HETATM	29	H	0	-10.84	-0.576	1.566	H
HETATM	30	H	0	-4.415	-2.475	0.726	H
HETATM	31	H	0	-8.887	2.873	-0.529	H
HETATM	32	C	0	2.567	-0.296	-0.078	C
HETATM	33	H	0	2.42	0.571	-0.736	H
HETATM	34	H	0	2.434	0.033	0.963	H
HETATM	35	C	0	3.943	-0.917	-0.283	C
HETATM	36	H	0	4.017	-1.273	-1.319	H
HETATM	37	H	0	4.03	-1.8	0.363	H
HETATM	38	C	0	5.084	0.073	0.018	C
HETATM	39	H	0	4.988	0.443	1.05	H
HETATM	40	H	0	4.99	0.954	-0.636	H
HETATM	41	C	0	6.481	-0.547	-0.167	C
HETATM	42	H	0	6.578	-0.921	-1.198	H
HETATM	43	H	0	6.577	-1.425	0.49	H
HETATM	44	C	0	7.627	0.437	0.127	C
HETATM	45	H	0	7.524	0.818	1.155	H
HETATM	46	H	0	7.534	1.312	-0.535	H
HETATM	47	C	0	9.025	-0.183	-0.046	C
HETATM	48	H	0	9.128	-0.566	-1.073	H
HETATM	49	H	0	9.119	-1.056	0.618	H
HETATM	50	C	0	10.172	0.802	0.246	C
HETATM	51	H	0	10.08	1.673	-0.42	H
HETATM	52	H	0	10.067	1.187	1.272	H
HETATM	53	C	0	11.571	0.181	0.079	C
HETATM	54	H	0	11.664	-0.69	0.746	H
HETATM	55	H	0	11.677	-0.205	-0.946	H
HETATM	56	C	0	12.718	1.166	0.37	C
HETATM	57	H	0	12.624	2.036	-0.297	H
HETATM	58	H	0	12.61	1.553	1.394	H
HETATM	59	C	0	14.11	0.537	0.203	C
HETATM	60	H	0	14.905	1.261	0.418	H
HETATM	61	H	0	14.241	-0.315	0.881	H

HETATM	62	H		0	14.257	0.172	-0.821	H
END								
CONECT	1		2	6		7		
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CONECT	3		2	4		9		
CONECT	4		3	5		8		
CONECT	5		4	6		31		
CONECT	6		1	5		25		
CONECT	7		1					
CONECT	8		4					
CONECT	9		3	10		11		
CONECT	10		9					
CONECT	11		9	12		14		
CONECT	12		11	13		30		
CONECT	13		2	12				
CONECT	14		11	15		16		
CONECT	15		14	17		18		
CONECT	16		14	19		20		
CONECT	17		15	21		22		
CONECT	18		15					
CONECT	19		16	21		23		
CONECT	20		16					
CONECT	21		17	19		24		
CONECT	22		17					
CONECT	23		19					
CONECT	24		21	32				
CONECT	25		6	26				
CONECT	26		25	27	28		29	
CONECT	27		26					
CONECT	28		26					
CONECT	29		26					
CONECT	30		12					
CONECT	31		5					
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CONECT	37		35					
CONECT	38		35	39	40		41	
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CONECT	41		38	42	43		44	

CONECT	42	41			
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CONECT	47	44	48	49	50
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CONECT	62	59			