

Electronic supplementary Information (ESI)

Table S1 Spectroscopic data of AFPO in different solvents.

Solvents	λ_a (nm)	$\bar{\nu}_a$ (cm ⁻¹) ^a	λ_f (nm)	$\bar{\nu}_f$ (cm ⁻¹) ^b	$\Delta\bar{\nu}$ (cm ⁻¹) ^c	$\bar{\nu}_a + \bar{\nu}_f/2$ (cm ⁻¹) ^d	$\bar{\nu}_a + \bar{\nu}_f$ (cm ⁻¹)
Hexane	348	28735	420	23809	4926	26272	52545
p-xylene	349	28653	423	23640	4956	26146	52293
Toluene	352	28409	428	23364	4934	25886	51773
Ether	352	28409	429	23310	5099	25859	51719
Diethylamine	356	28089	434	23041	5048	25565	51131
1,4-Dioxane	357	28011	435	22988	5022	25499	50999
Chlorobenzene	359	27855	440	22727	5127	25291	50582
Tetrahydrofuran	362	27624	446	22421	5202	25022	50045
Ethyl acetate	362	27624	446	22421	5202	25022	50045
Chloroform	360	27777	442	22624	5153	25201	50402
Dichloromethane	364	27472	449	22271	5200	24872	49744
Dimethyl formamide	364	27472	452	22123	5348	24798	49596
Dimethylsulphoxide	365	27397	456	21929	5467	24663	49327
Acetonitrile	368	27173	459	21786	5387	24480	48960
Butanol	372	26881	464	21551	5329	24216	48433
Propanol	375	26666	469	21321	5344	23994	47988
Ethanol	376	26595	472	21186	5409	23891	47782
Methanol	378	26455	476	21008	5446	23731	47463

^a Absorption maxima.

^b Fluorescence maxima.

^c Stokes shift.

^d Arithmetic mean of absorption maxima and fluorescence maxima.

Table S2 Spectroscopic data of FHPO in different solvents.

Solvents	λ_a (nm)	$\bar{\nu}_a$ (cm ⁻¹) ^a	λ_f (nm)	$\bar{\nu}_f$ (cm ⁻¹) ^b	$\Delta\bar{\nu}$ (cm ⁻¹) ^c	$\bar{\nu}_a + \bar{\nu}_f/2$ (cm ⁻¹) ^d	$\bar{\nu}_a + \bar{\nu}_f$ (cm ⁻¹)
Hexane	350	28571	425	23529	5042	26050	52100
p-xylene	352	28409	428	23364	5044	25886	51773
Toluene	353	28328	430	23255	5072	25792	51584
Ether	356	28089	435	22988	5101	25539	51078
Diethylamine	357	28011	438	22831	5180	25421	50842
1,4-Dioxane	359	27855	440	22727	5127	25291	50582
Chlorobenzene	362	27624	446	22421	5202	25022	50045
Tetrahydrofuran	362	27624	447	22371	5252	24997	49995
Ethyl acetate	363	27548	448	22321	5226	24934	49869
Chloroform	364	27472	450	22222	5250	24847	49694
Dichloromethane	366	27322	454	22026	5295	24674	49348
Dimethyl formamide	369	27100	459	21786	5313	24443	48886
Dimethylsulphoxide	370	27027	462	21645	5382	24336	48672
Acetonitrile	371	26954	464	21551	5402	24252	48505
Butanol	372	26881	466	21459	5422	24170	48340
Propanol	375	26666	472	21186	5480	23926	47853
Ethanol	377	26525	476	21008	5516	23766	47533
Methanol	379	26385	480	20833	5551	23609	47218

^a Absorption maxima.

^b Fluorescence maxima.

^c Stokes shift.

^d Arithmetic mean of absorption maxima and fluorescence maxima.

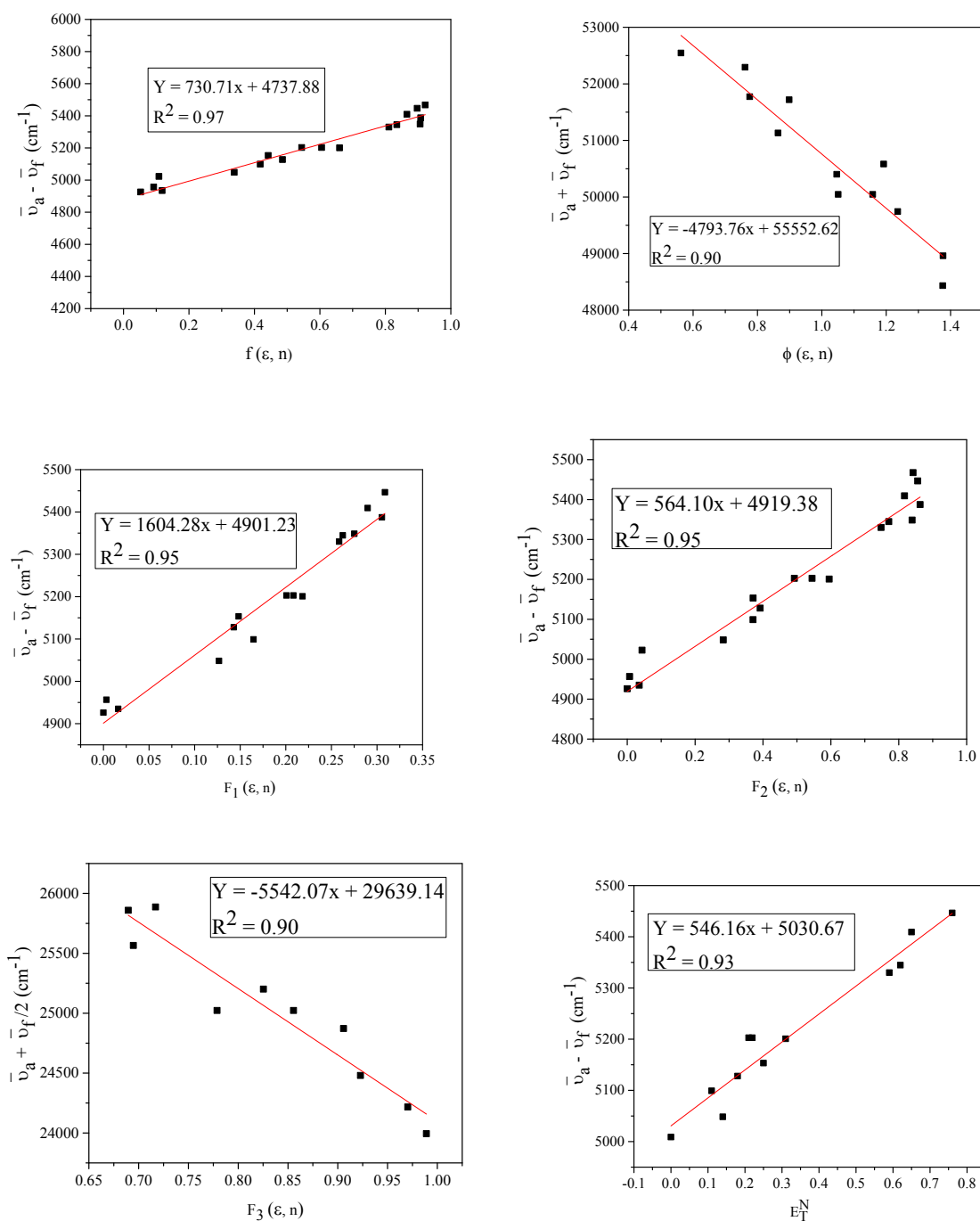
Table S3 Kamlet-Abboud-Taft solvent parameters.

Solvents	α	β	π^*
Hexane	0	0	-0.11
p-xylene	0	0	0.43
Toluene	0	0.11	0.54
Ether	0	0.47	0.24
Diethylamine	0	0.71	0.09
1,4-Dioxane	0	0.37	0.55
Chlorobenzene	0	0.07	0.68
Tetrahydrofuran	0	0.55	0.58
Ethyl acetate	0	0.45	0.55
Chloroform	0.2	0.1	0.69
Dichloromethane	0.3	0	0.82
Dimethyl formamide	0	0.69	0.88
Dimethylsulphoxide	0	0.76	1
Acetonitrile	0.19	0.31	0.75
Butanol	0.79	0.88	0.47
Propanol	0.76	0.84	0.48
Ethanol	0.83	0.77	0.54
Methanol	0.93	0.62	0.6

Table S4 Catalan solvent parameters.

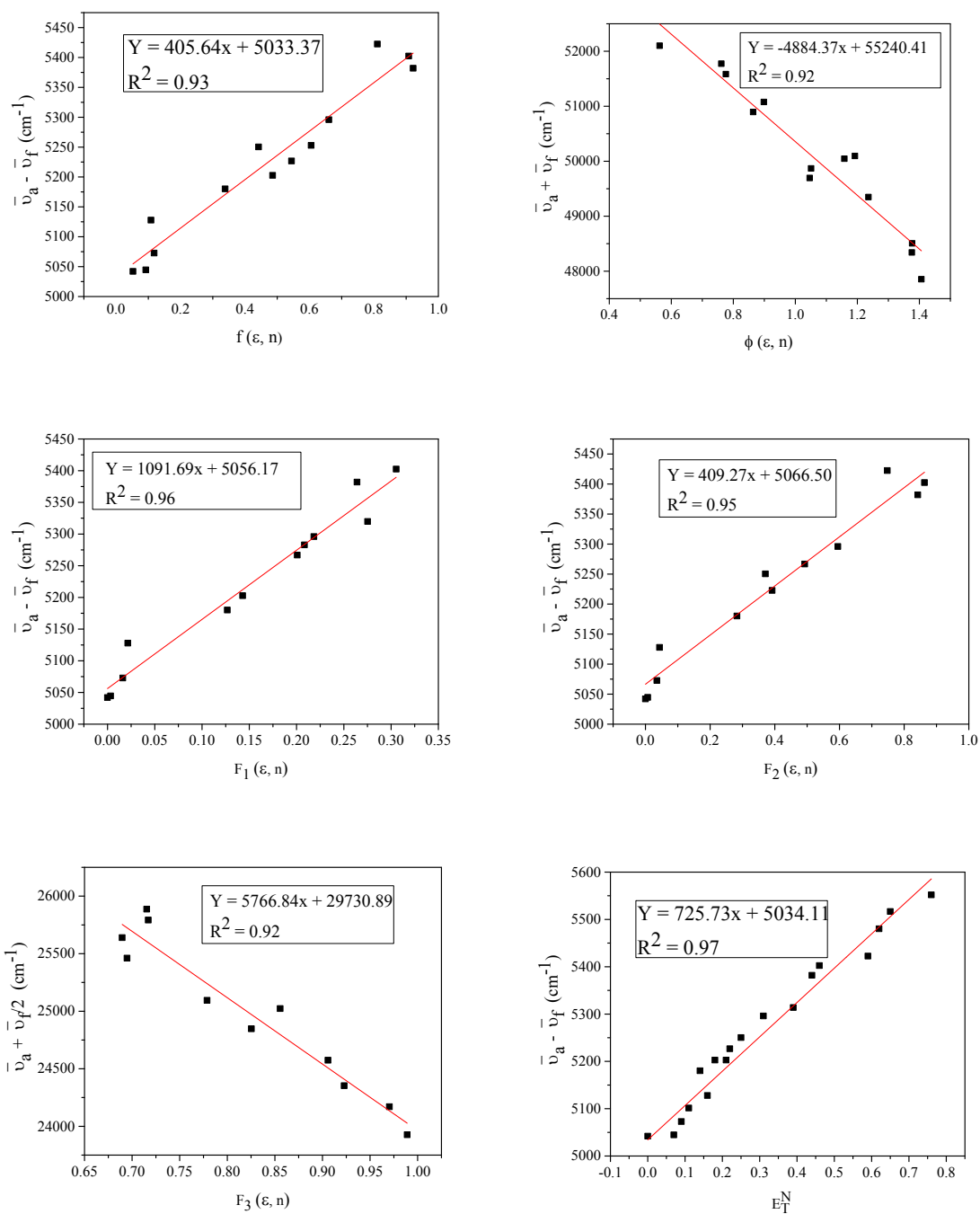
Solvents	SA	SB	SP	SdP
Hexane	0	0.056	0.616	0.519
p-xylene	0	0.16	0.778	0.175
Toluene	0	0.128	0.782	0.284
Ether	0	0.562	0.617	0.385
Diethylamine	0	0.885	0.66	0.617
1,4-Dioxane	0	0.444	0.737	0.312
Chlorobenzene	0	0.182	0.833	0.537
Tetrahydrofuran	0	0.591	0.714	0.634
Ethyl acetate	0	0.542	0.656	0.603
Chloroform	0.047	0.071	0.783	0.614
Dichloromethane	0.04	0.178	0.761	0.769
Dimethyl formamide	0.031	0.613	0.759	0.977
Dimethylsulphoxide	0.83	1.000	0.072	0.647
Acetonitrile	0.044	0.286	0.645	0.974
Butanol	0.341	0.809	0.674	0.655
Propanol	0.367	0.782	0.658	0.748
Ethanol	0.4	0.658	0.633	0.783
Methanol	0.605	0.545	0.608	0.904

Figure S1 Solvatochromic linear plots of AFPO.



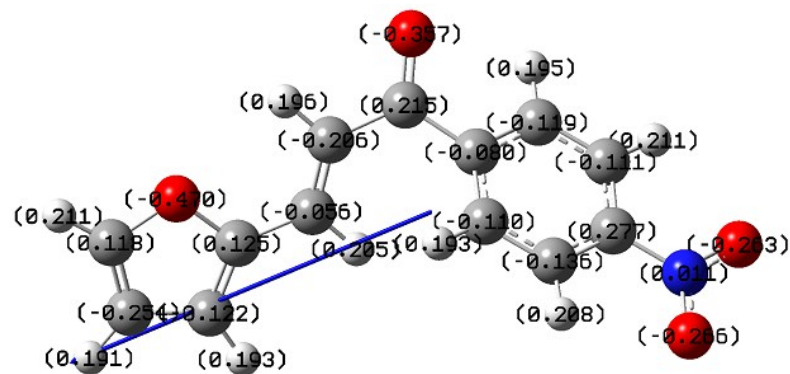
Solvatochromic linear plots of $\bar{\nu}_a - \bar{\nu}_f$ vs $f(\epsilon, n)$, $\bar{\nu}_a + \bar{\nu}_f$ vs $\phi(\epsilon, n)$ (Bilot-Kawski), $(\bar{\nu}_a - \bar{\nu}_f)$ vs $F_1(\epsilon, n)$ (Lippert-Mataga), $F_2(\epsilon, n)$ (Bakhshiev), $(\bar{\nu}_a + \bar{\nu}_f)/2$ vs $F_3(\epsilon, n)$ (Kawski-Chamma-Viallet) and $(\bar{\nu}_a - \bar{\nu}_f)$ vs $E_T^N(\epsilon, n)$ (Reichardt) for AFPO.

Figure S2 Solvatochromic linear plots of FHPO.

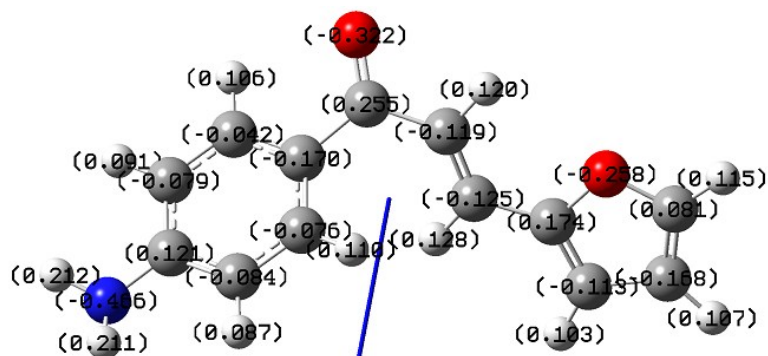


Solvatochromic linear plots of $\bar{\nu}_a - \bar{\nu}_f$ vs $f(\epsilon, n)$, $\bar{\nu}_a + \bar{\nu}_f$ vs $\phi(\epsilon, n)$ (Bilot-Kawski), $(\bar{\nu}_a - \bar{\nu}_f)$ vs $F_1(\epsilon, n)$ (Lippert-Mataga), $F_2(\epsilon, n)$ (Bakhshiev), $(\bar{\nu}_a + \bar{\nu}_f)/2$ vs $F_3(\epsilon, n)$ (Kawski-Chamma-Viallet) and $(\bar{\nu}_a - \bar{\nu}_f)$ vs $E_T^N(\epsilon, n)$ (Reichardt) for FHPO.

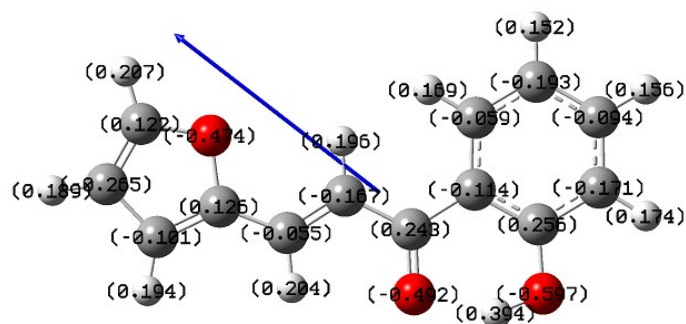
Figure S3 Mulliken charge density of FNPO, AFPO and FHPO



FNPO



AFPO



FHPO