ELECTRONIC SUPPORTING INFORMATION

Novel hetarylazo dyes containing tetrazole and hydroquinoline moieties: Spectral characteristics, solvatochromism and photochemistry

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(A)

Display Report

Analysis Info

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Comment	C13H17N7O mH 288.156 clb added		

Acquisition Parameter

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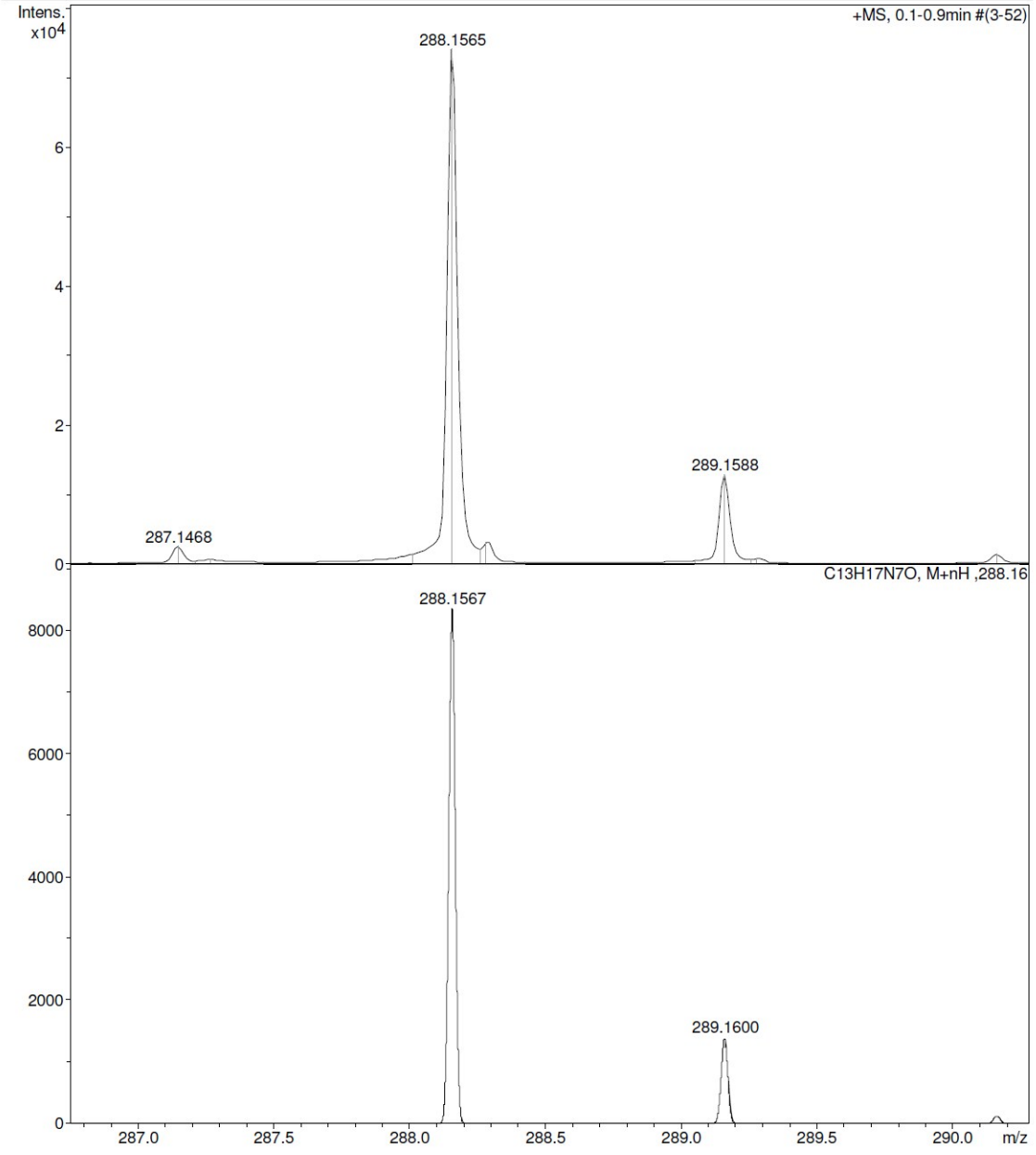
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



(B)

Display Report

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Comment	C14H17N7O mH 300.156 clb added		

Acquisition Parameter

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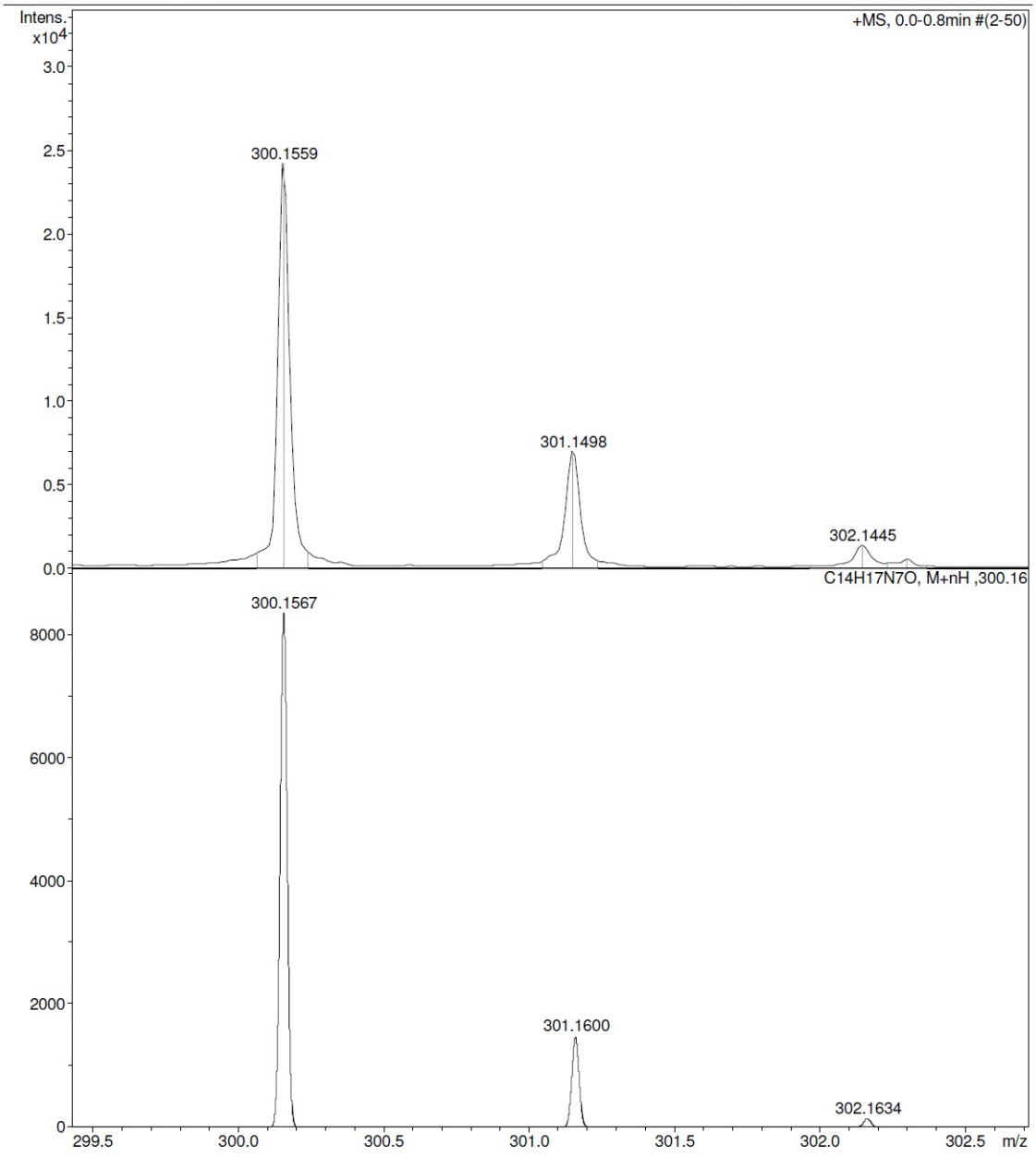
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



Bruker Compass DataAnalysis 4.0 printed: 01.09.2016 12:57:06 Page 1 of 1

Figure S1 HRMS spectra of dyes **3** (A) and **4** (B).

Absorption spectra of dyes 4 and 5 in different solvents at different concentrations

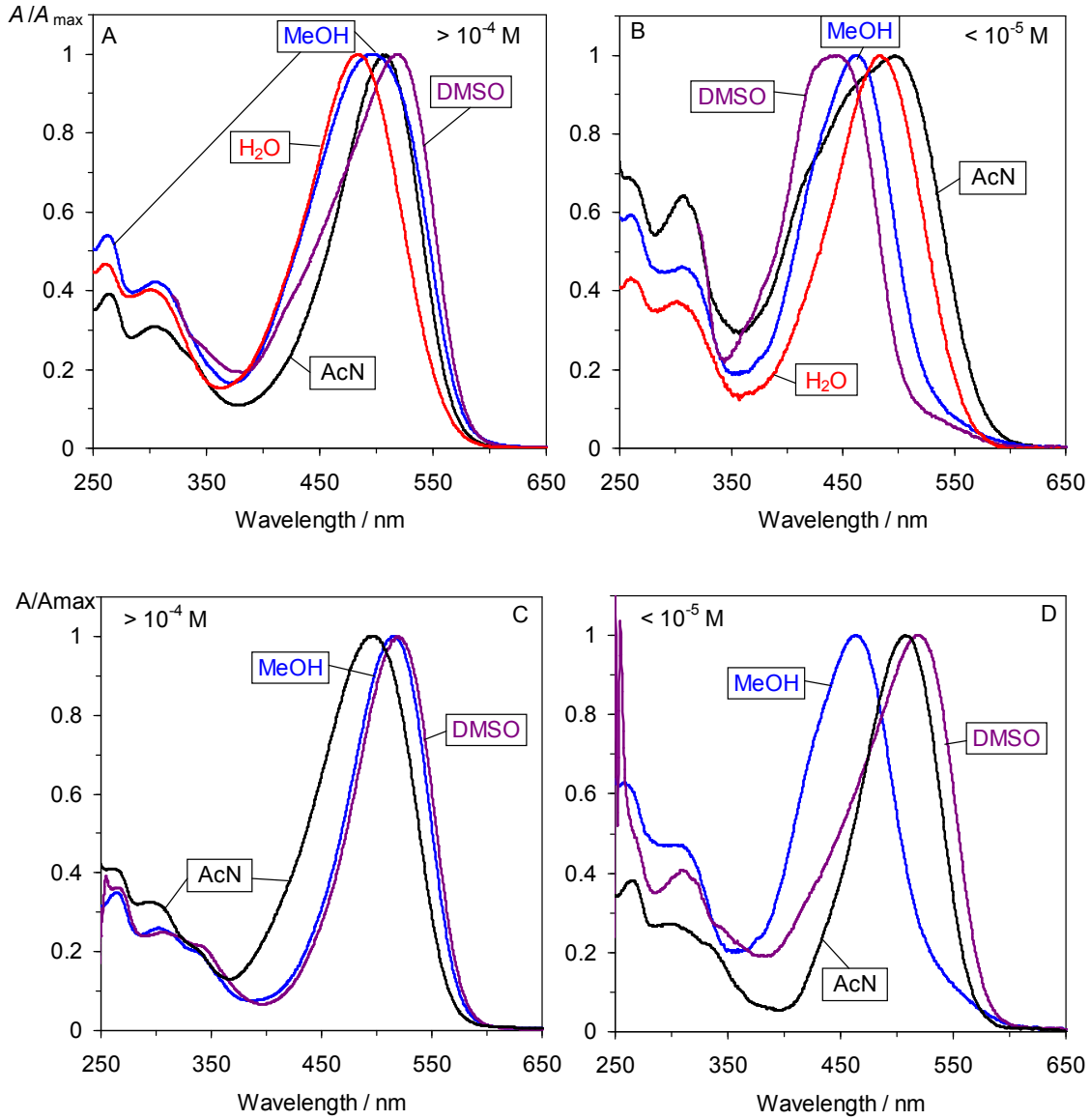


Figure S2 Normalized absorption spectra of dyes **4** (A, B) and **5** (C, D) at concentrations > 1 × 10^{-4} M (A, C) and < 1 × 10^{-5} M (B, D) in different solvents.

Gaussian deconvolution of the spectra for 3 and 4 in various solvents

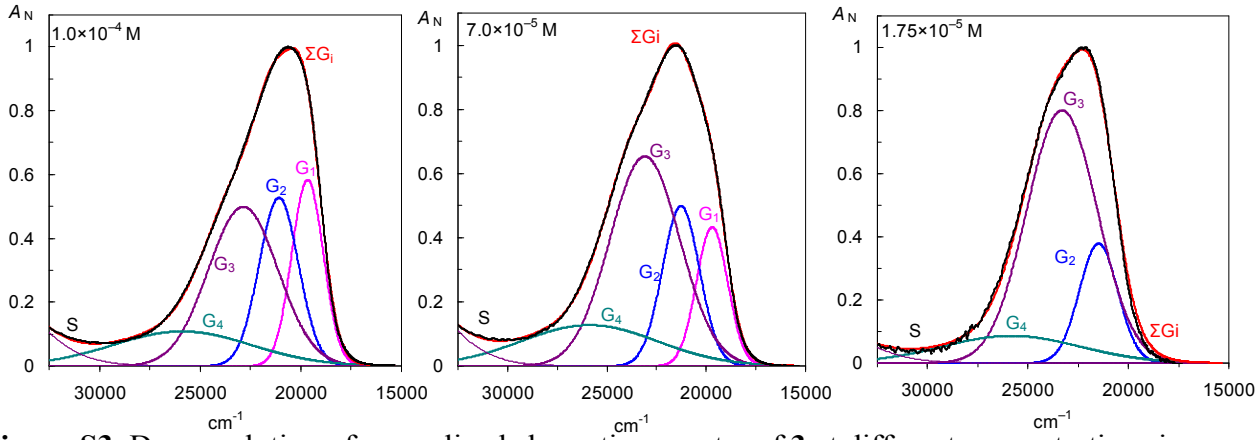


Figure S3. Deconvolution of normalized absorption spectra of **3** at different concentrations in MeOH.

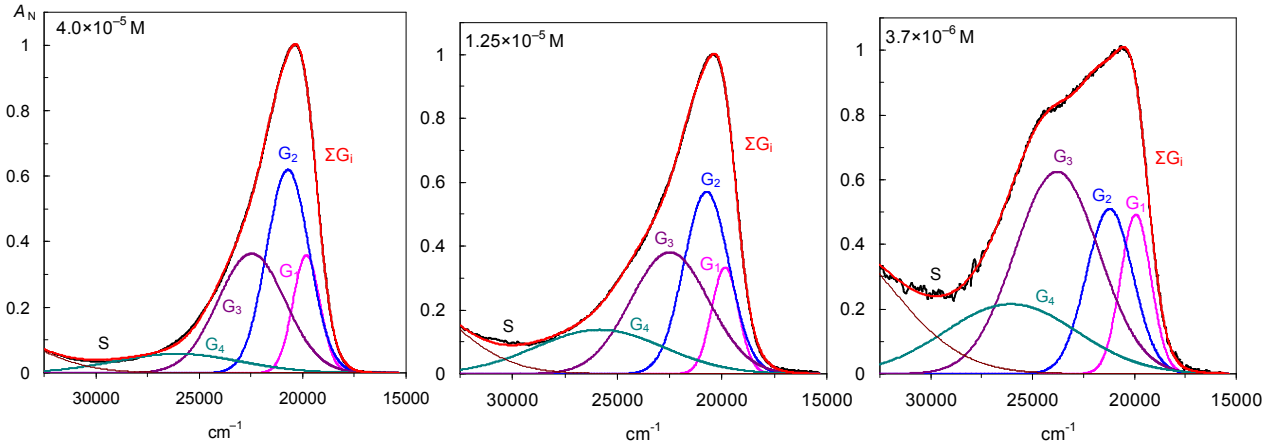


Figure S4. Gaussian deconvolution of normalized absorption spectra of dye **3** at different concentrations in ACN.

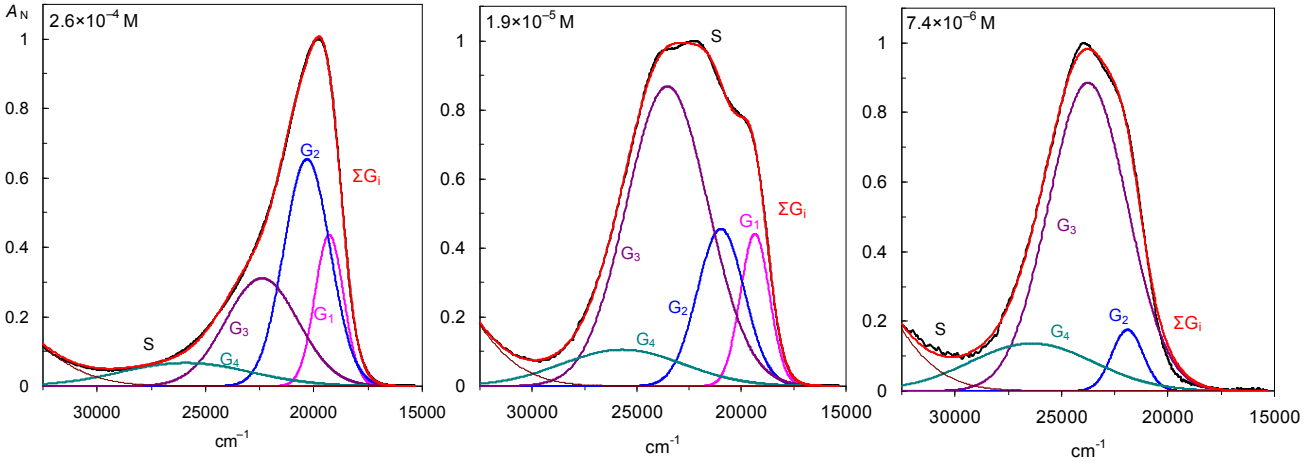


Figure S5. Gaussian deconvolution of normalized absorption spectra of dye **3** at different concentrations in DMSO.

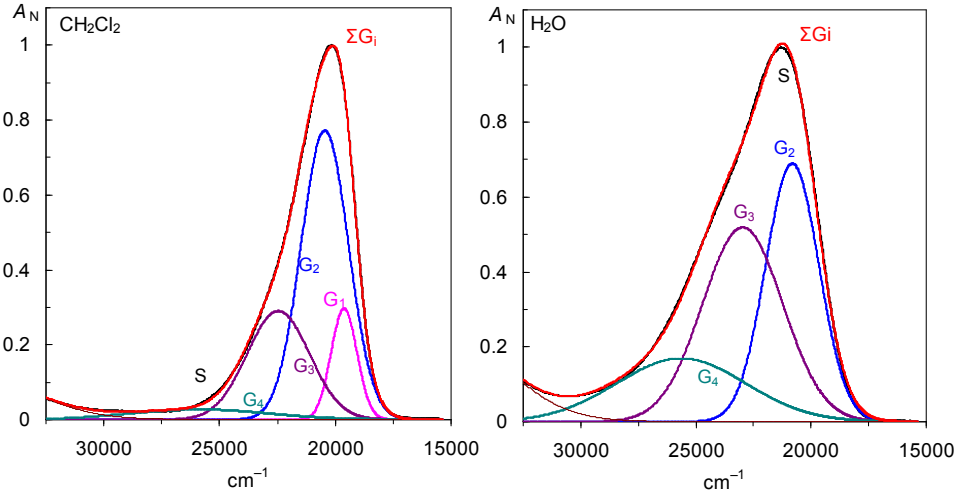


Figure S6. Gaussian deconvolution of normalized absorption spectra of dye **3** in CH_2Cl_2 and water

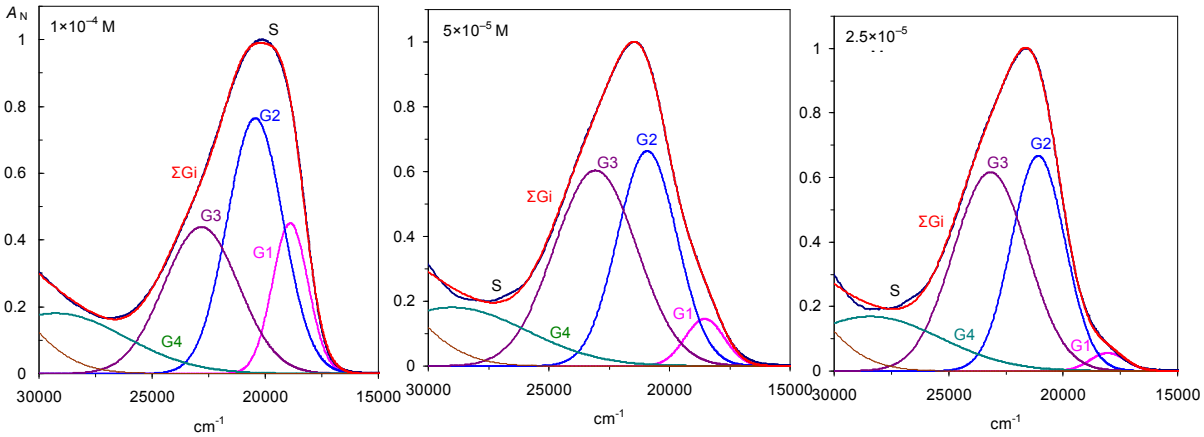


Figure S7. Gaussian deconvolution of normalized absorption spectra of dye **4** at different concentrations in MeOH.

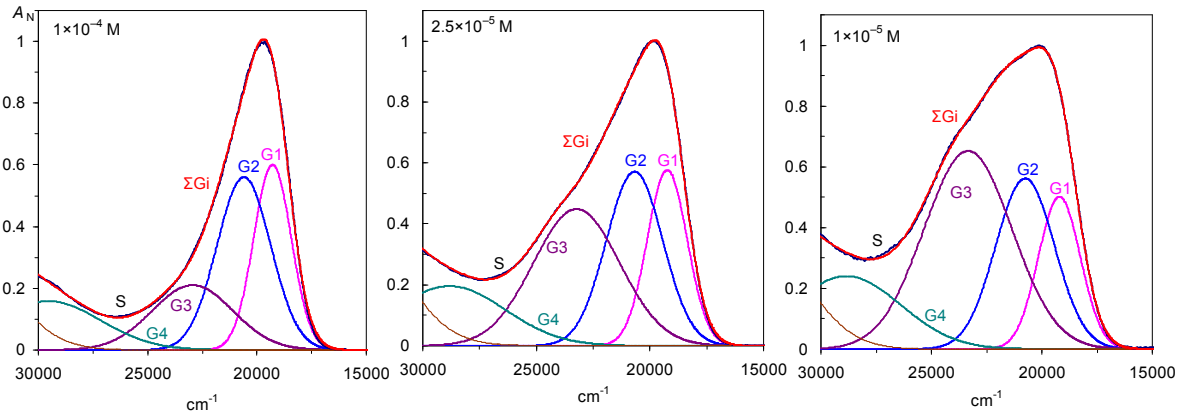


Figure S8. Gaussian deconvolution of normalized absorption spectra of dye **4** at different concentrations in AcN.

Table S1. Parameters of the Gaussian functions (wavenumbers, FWMH in cm^{-1} and *H* - height) in deconvolution of the normalized absorption spectra for **3** in various solvents at different concentrations

C/10^{-5} M	MeOH			
	G1(19780±100) *H* (FWMH)	G2(21340±250) *H* (FWMH)	G3(23060±50) *H* (FWMH)	G4(25850±60) *H* (FWMH)
0.38	0	0.26 (2257)	0.70 (4142)	0.18 (8043)
1.74	0	0.35 (2257)	0.80 (4142)	0.086 (8043)
5.20	0.11 (1857)	0.35 (2257)	0.76 (4142)	0.16 (8043)
7.00	0.43 (1852)	0.50 (2201)	0.65 (4146)	0.13 (8031)
8.70	0.58 (1880)	0.53 (2267)	0.54 (4210)	0.11 (8047)
10.5	0.59 (1840)	0.54 (2303)	0.49 (4071)	0.10 (8050)
41.8	0.57 (1802)	0.52(2190)	0.36 (3964)	0.07 (8082)
	ACN			
	G1(19850±100) *H* (FWMH)	G2(20850±250) *H* (FWMH)	G3(22850±400) *H* (FWMH)	G4(25950±100) *H* (FWMH)
0.37	0.49 (1760)	0.51 (2688)	0.62 (4862)	0.22 (7608)
0.55	0.47 (1725)	0.49 (2630)	0.43 (4876)	0.19 (7304)
0.83	0.34 (1510)	0.56 (2445)	0.41 (4465)	0.17 (7148)
1.86	0.38 (1583)	0.57 (2502)	0.36 (4148)	0.11 (7044)
2.80	0.34 (1516)	0.62 (2489)	0.36 (3994)	0.09 (7052)
4.18	0.36 (1526)	0.62 (2419)	0.36 (3825)	0.06 (7080)
41.8	0.33 (1532)	0.64 (2378)	0.37 (3640)	0.05 (7113)
	DMSO			
	G1(19350±50) *H* (FWMH)	G2(20850±500) *H* (FWMH)	G3(23110±500) *H* (FWMH)	G4(25820±500) *H* (FWMH)
0.74	0	0.18 (1722)	0.89 (4356)	0.14 (6830)
1.54	0.33 (1711)	0.37 (2407)	0.88 (4364)	0.11 (6830)
1.91	0.44 (1638)	0.45 (2650)	0.87 (4601)	0.11 (6848)
2.35	0.55 (1652)	0.55 (2656)	0.80 (4633)	0.11 (6859)
2.90	0.53 (1641)	0.56 (2661)	0.61 (4680)	0.11 (6889)
4.18	0.50 (1633)	0.59 (2648)	0.40 (4446)	0.09 (6958)
7.32	0.52 (1639)	0.58 (2509)	0.37 (4380)	0.07 (6907)
10.0	0.48 (1596)	0.60 (2464)	0.34 (4180)	0.07 (6916)
26.1	0.44 (1556)	0.65 (2518)	0.31 (3943)	0.07 (7042)
	CH_2Cl_2			
	G1(19620) *H* (FWMH)	G2(20451) *H* (FWMH)	G3(22464) *H* (FWMH)	G4(25820±500) *H* (FWMH)
5–0.1	0.30 (1318)	0.77 (2412)	0.29 (3167)	0.03 (7038)
	H_2O			
	G1 *H* (FWMH)	G2(20810) *H* (FWMH)	G3(22970) *H* (FWMH)	G4(25867) *H* (FWMH)
5–0.1	0	0.69 (2729)	0.52 (4110)	0.17 (6589)

Table S2. Parameters of the Gaussian functions (wavenumbers, FWMH in cm^{-1} and *H* - height) in deconvolution of the normalized absorption spectra for **4** in various solvents at different concentrations

C/10^{-5} M	MeOH			
	G1(18600 ± 300) *H* (FWMH/cm^{-1})	G2(20750 ± 300) *H* (FWMH/cm^{-1})	G3(23000 ± 200) *H* (FWMH/cm^{-1})	G4(28940 ± 300) *H* (FWMH/cm^{-1})
10	0.45 (1860)	0.37 (2910)	0.28 (3890)	0.21 (7230)
7.5	0.40 (1860)	0.35 (2910)	0.31 (3890)	0.22 (7230)
5	0.15 (1900)	0.32 (2900)	0.41 (4032)	0.22 (7250)
2.5	0.06 (1830)	0.33 (2750)	0.43 (3790)	0.22 (7230)
	ACN			
	G1(19240 ± 40) *H* (FWMH/cm^{-1})	G2(20650 ± 100) *H* (FWMH/cm^{-1})	G3(23100 ± 200) *H* (FWMH/cm^{-1})	G4(29050 ± 250) *H* (FWMH/cm^{-1})
10	0.60 (2020)	0.56 (2900)	0.21 (4330)	0.16 (5680)
5	0.59 (2000)	0.58 (2790)	0.30 (4330)	0.16 (5680)
2.5	0.58 (2070)	0.57(2920)	0.45 (4470)	0.20 (5740)
1	0.50 (2240)	0.56 (3140)	0.65 (4690)	0.24 (5790)
DMSO				
	G1(18810 ± 150) *H* (FWMH/cm^{-1})	G2(20660 ± 100 *H* (FWMH/cm^{-1})	G3(22600 ± 400 *H* (FWMH/cm^{-1})	G4(26600 ± 700) *H* (FWMH/cm^{-1})
10	0.55 (1710)	0.58 (2560)	0.42 (4010)	0.18 (6910)
7.5	0.58 (1730)	0.55 (2540)	0.50 (4020)	0.21 (7060)
5	0.58 (1830)	0.48 (2590)	0.72 (3920)	0.31 (7050)
2.5	0.16 (2220)	0.33 (1860)	0.79 (3730)	0.32 (6870)
1	0.05 (1850)	0.37 (1870)	0.73 (3410)	0.35 (6750)

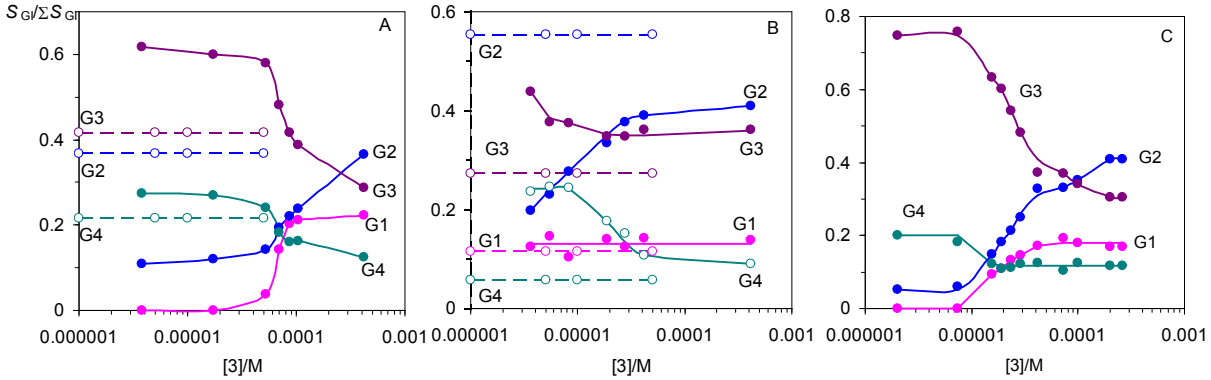


Figure S9 Contributions of Gaussian components into the visible absorption band at different concentrations of dye **3** in (A) MeOH (solid lines) and H_2O (dashed lines), (B) ACN (solid lines) and CH_2Cl_2 (dashed lines) and (C) DMSO

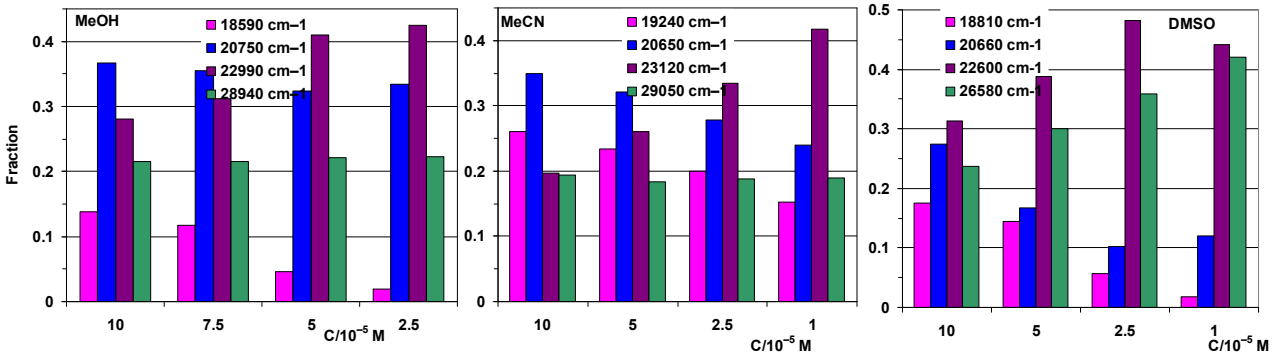


Figure S10. Contributions of Gaussian components into the visible absorption band at different concentrations of **4** in MeOH, ACN and DMSO.