Supporting Information

A structure-behaviour study of a family of "hybrid" merocyanines with an inverted solvatochromism

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TABLE OF CONTENTS

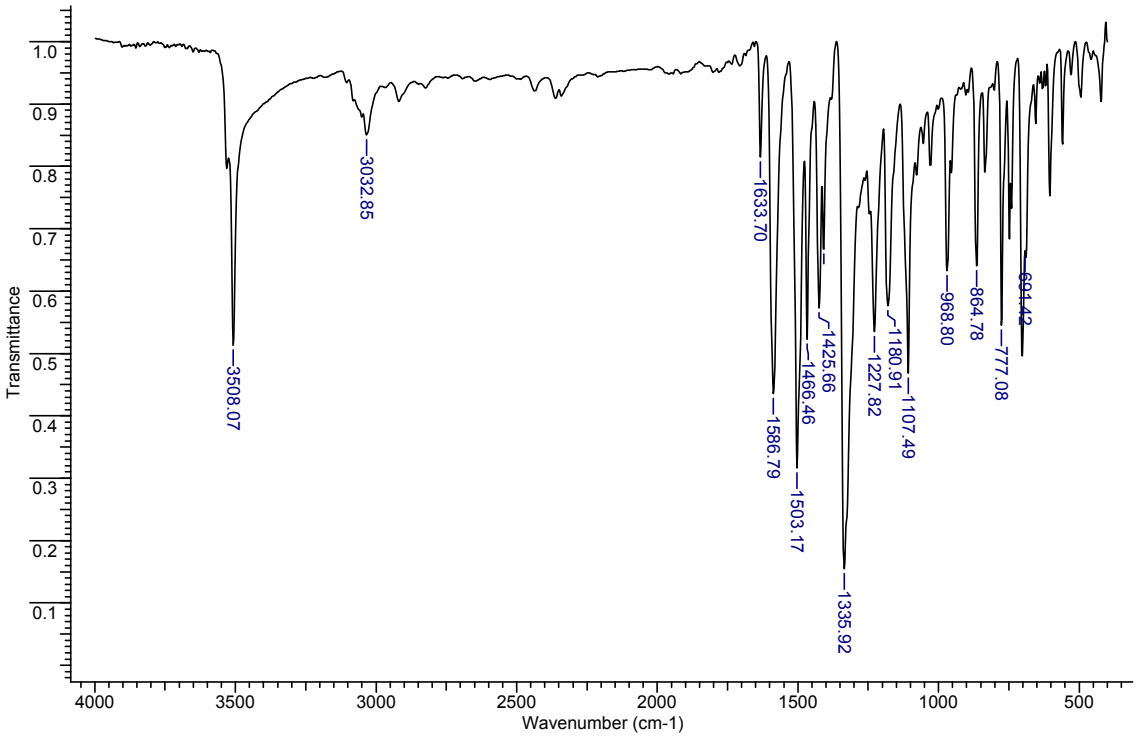

Figure S1. IR spectrum of **1b** (KBr pellet).

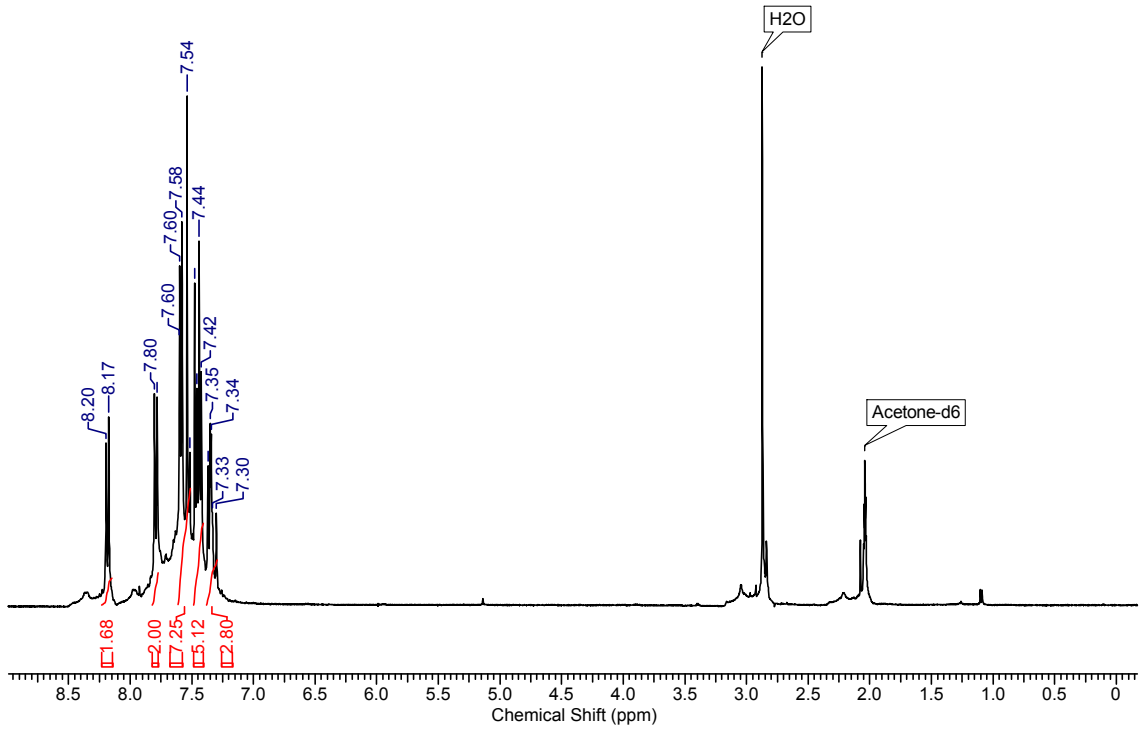

Figure S2. ^{1}H NMR spectrum of**1b**, measured in acetone-d_6 (400 MHz).

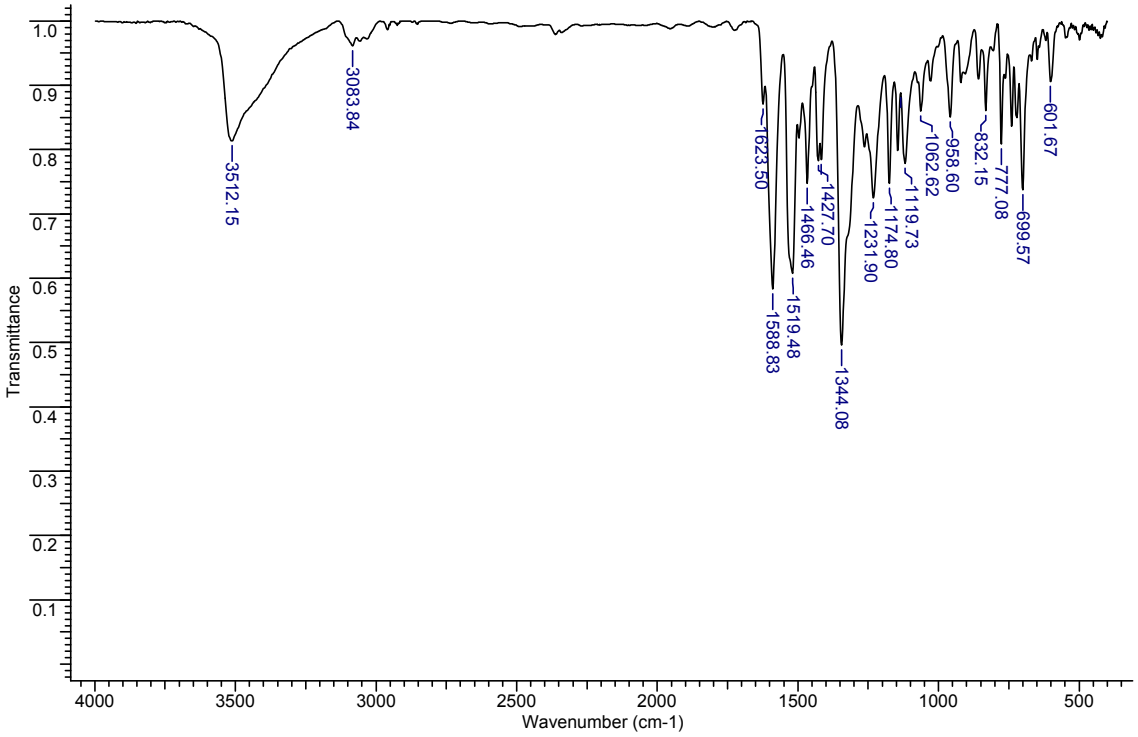

Figure S3. IR spectrum of **1g** (KBr pellet).

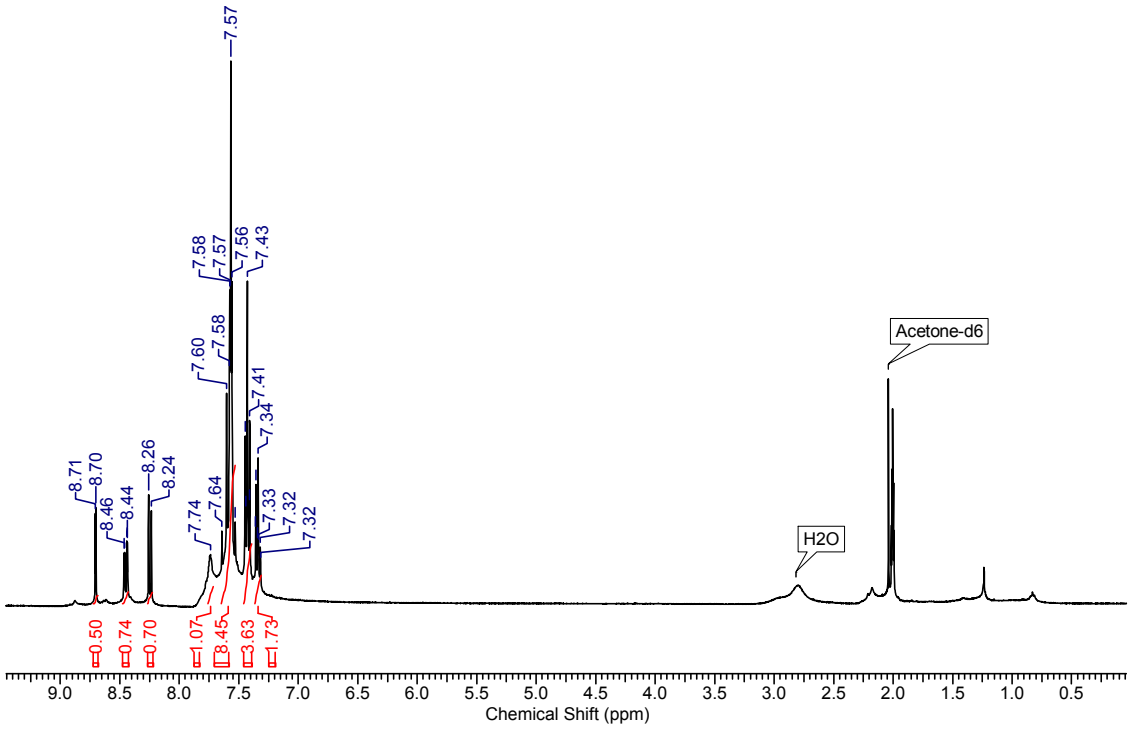

Figure S4. ^{1}H NMR spectrum of **1g**, measured in acetone-d_6 (400 MHz).

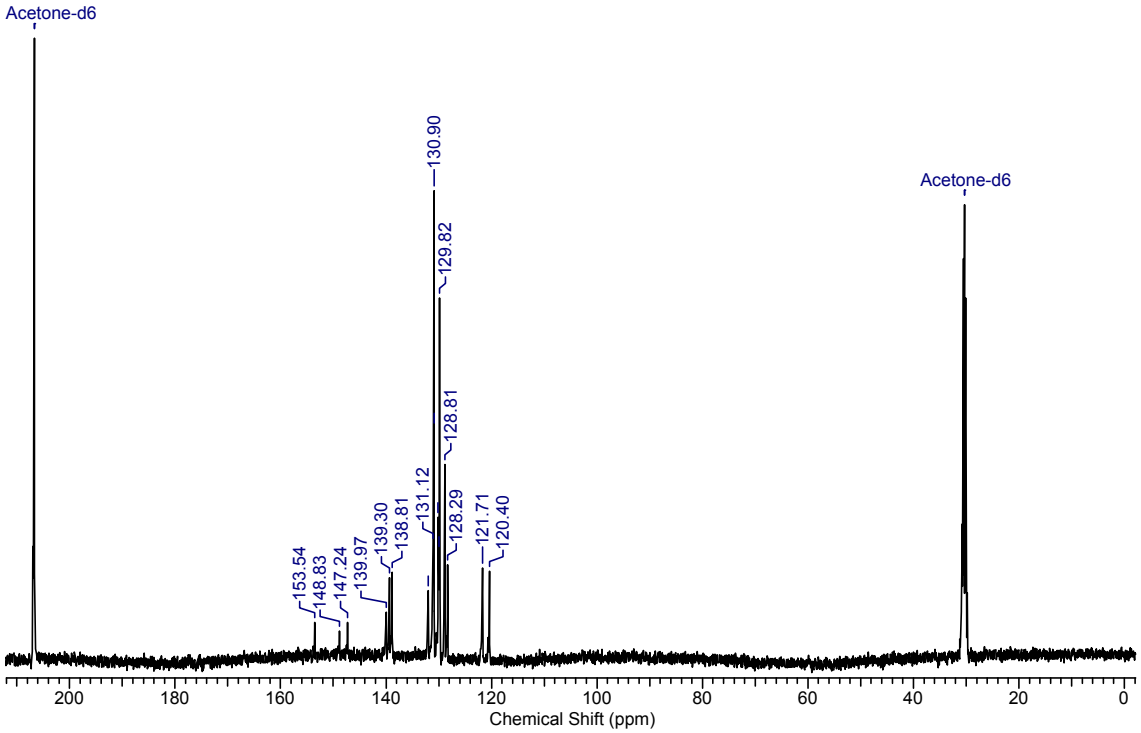

Figure S5. ^{13}C NMR spectrum of **1g**, measured in acetone-d_6 (100 MHz).

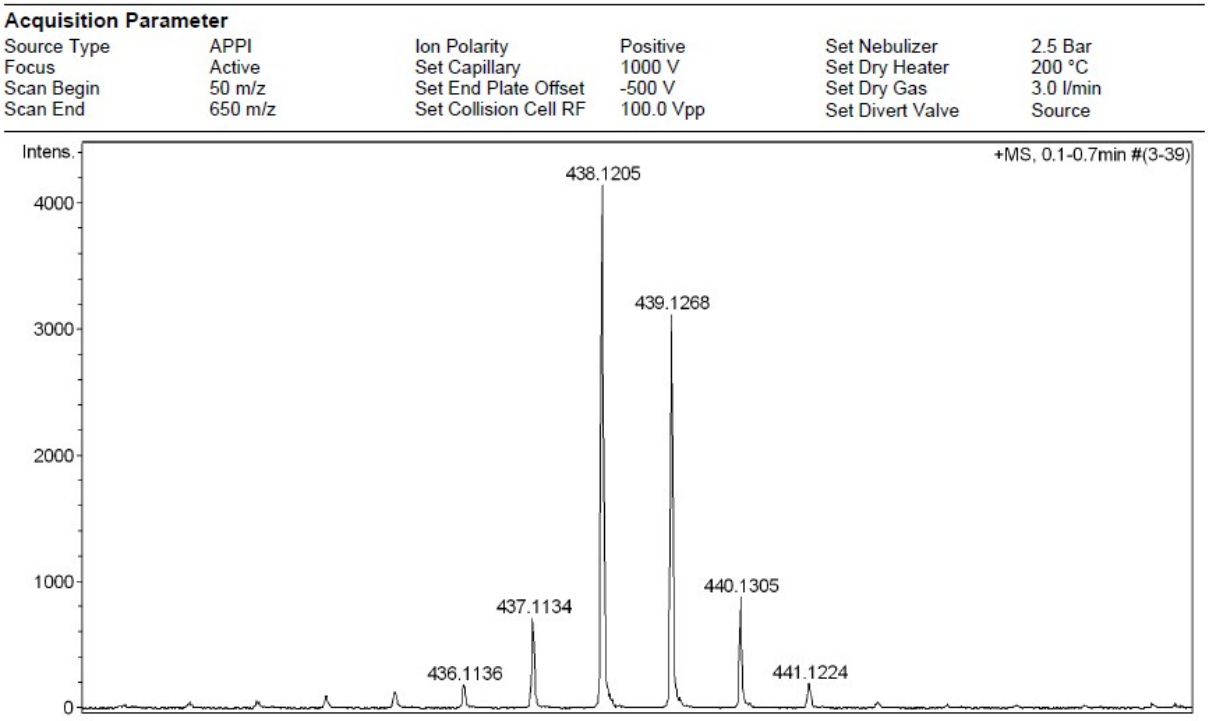

Figure S6. HRMS of **1g**.

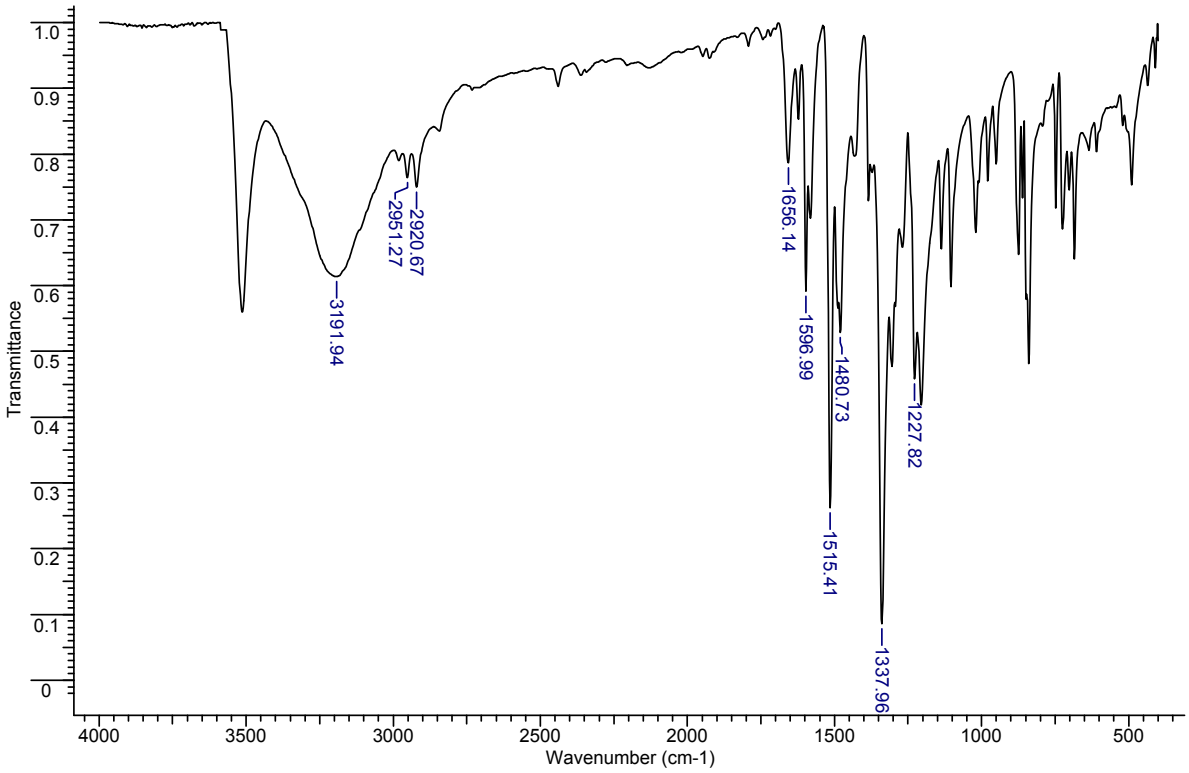

Figure S7. IR spectrum of **2c** (KBr pellet).

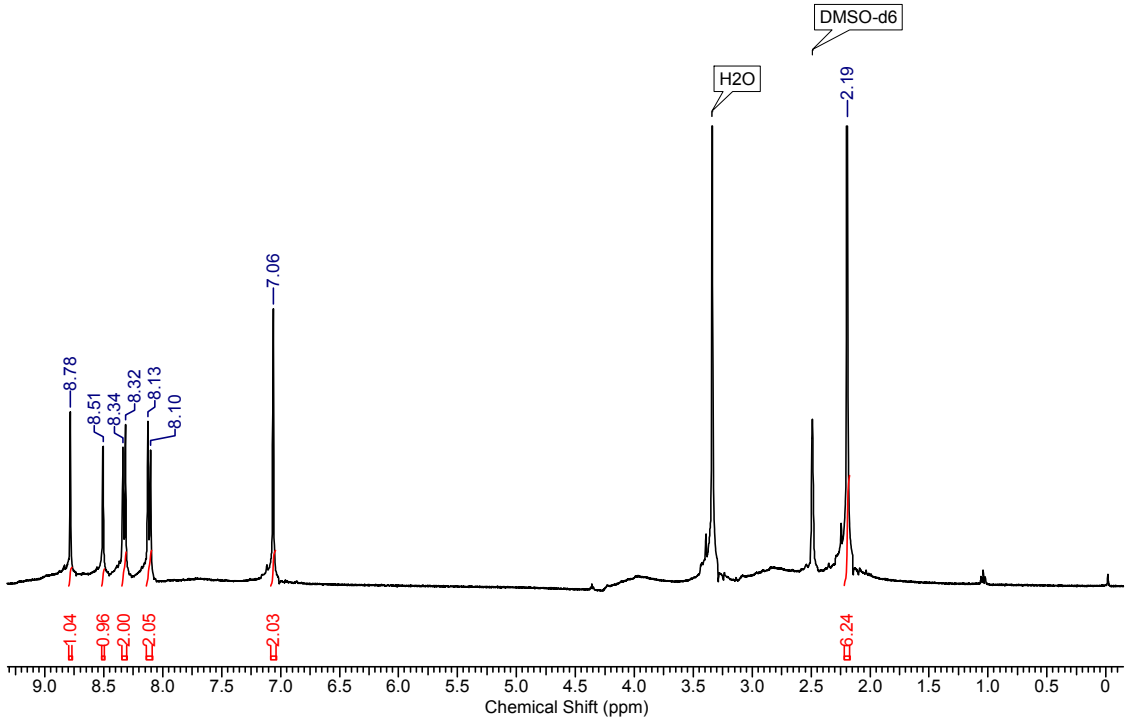

Figure S8. ^{1}H NMR spectrum of **2c**, measured in DMSO-d_6 (400 MHz).

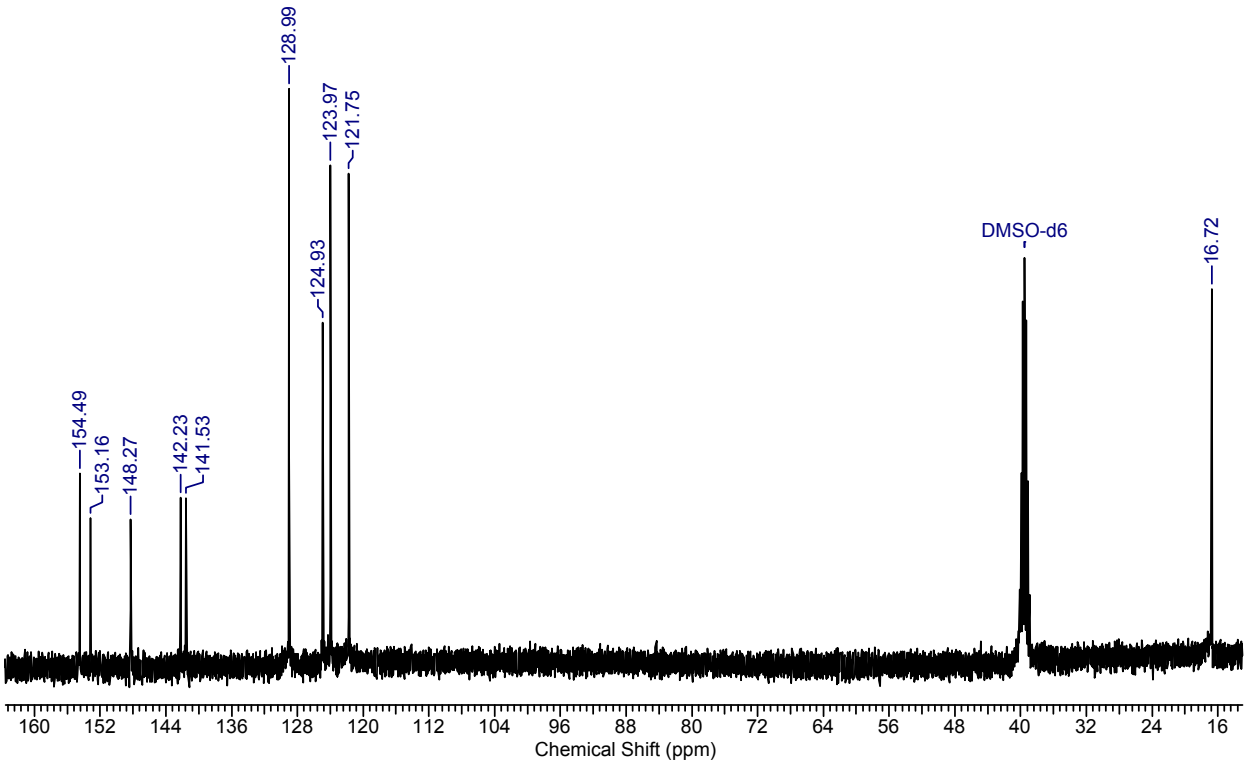

Figure S9. ^{13}C NMR spectrum of **2c**, measured in DMSO-d_6 (100 MHz).

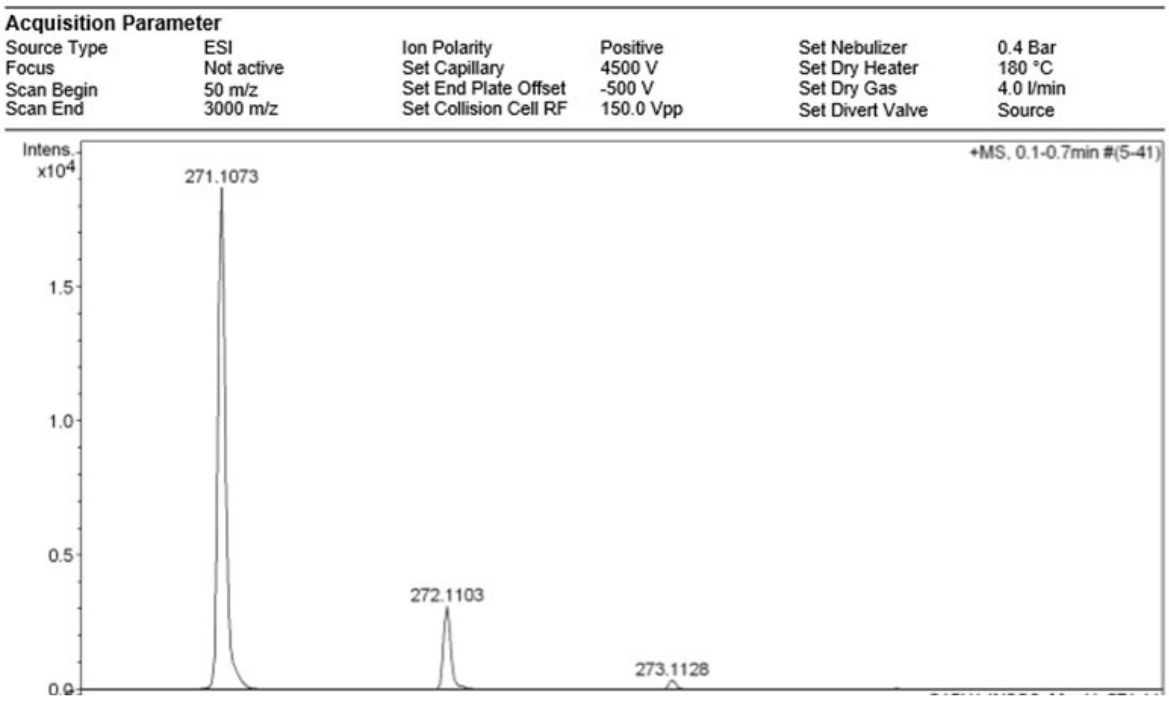

Figure S10. HRMS of **2c**.

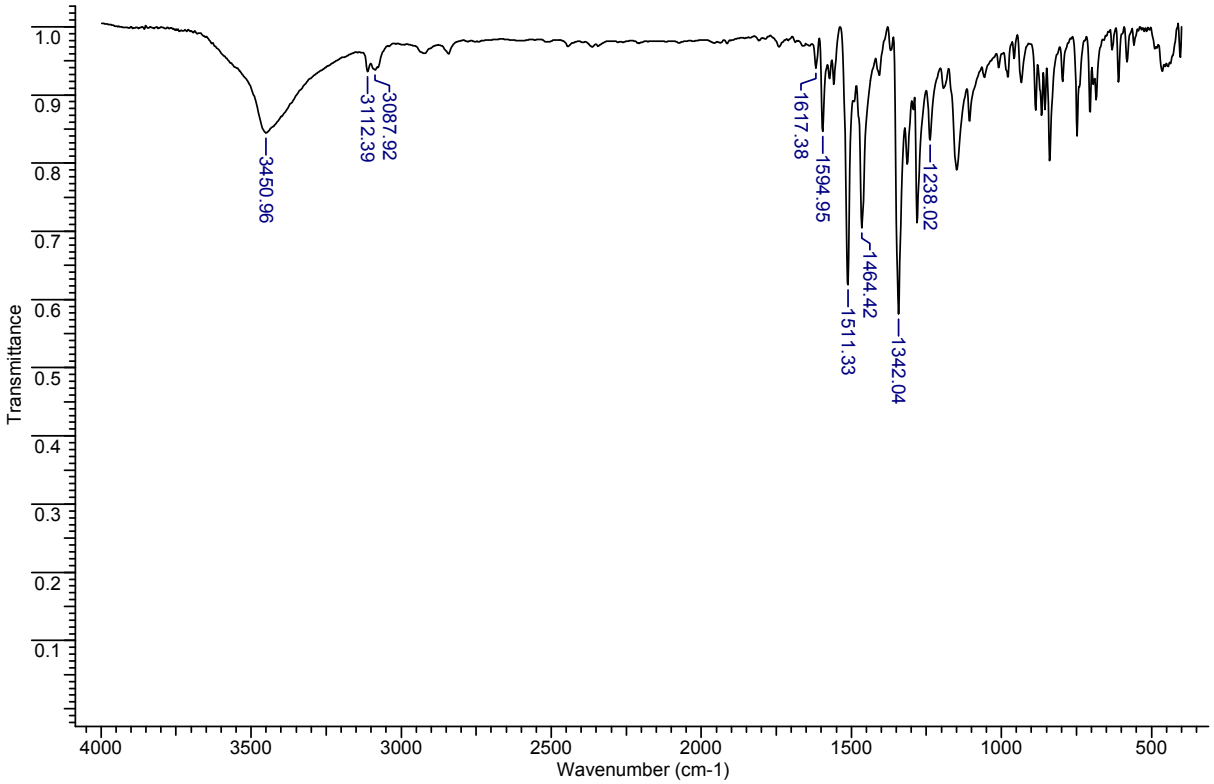

Figure S11. IR spectrum of **2d** (KBr pellet).

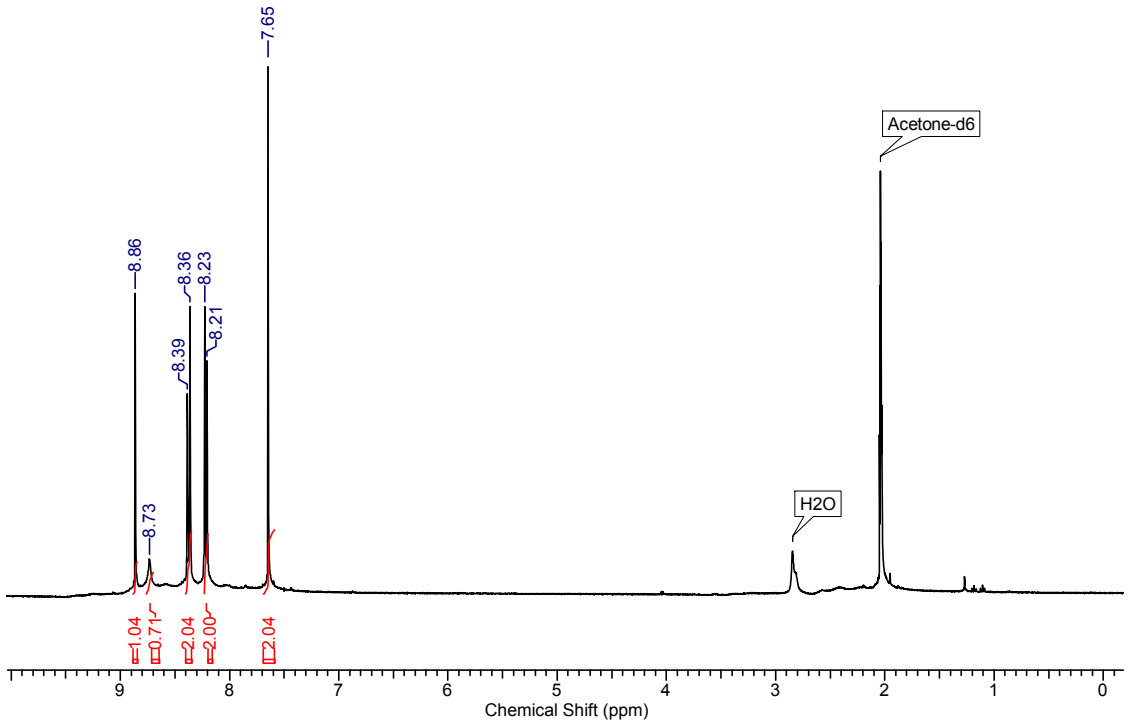

Figure S12. ^{1}H NMR spectrum of **2d**, measured in acetone-d_6 (400 MHz).

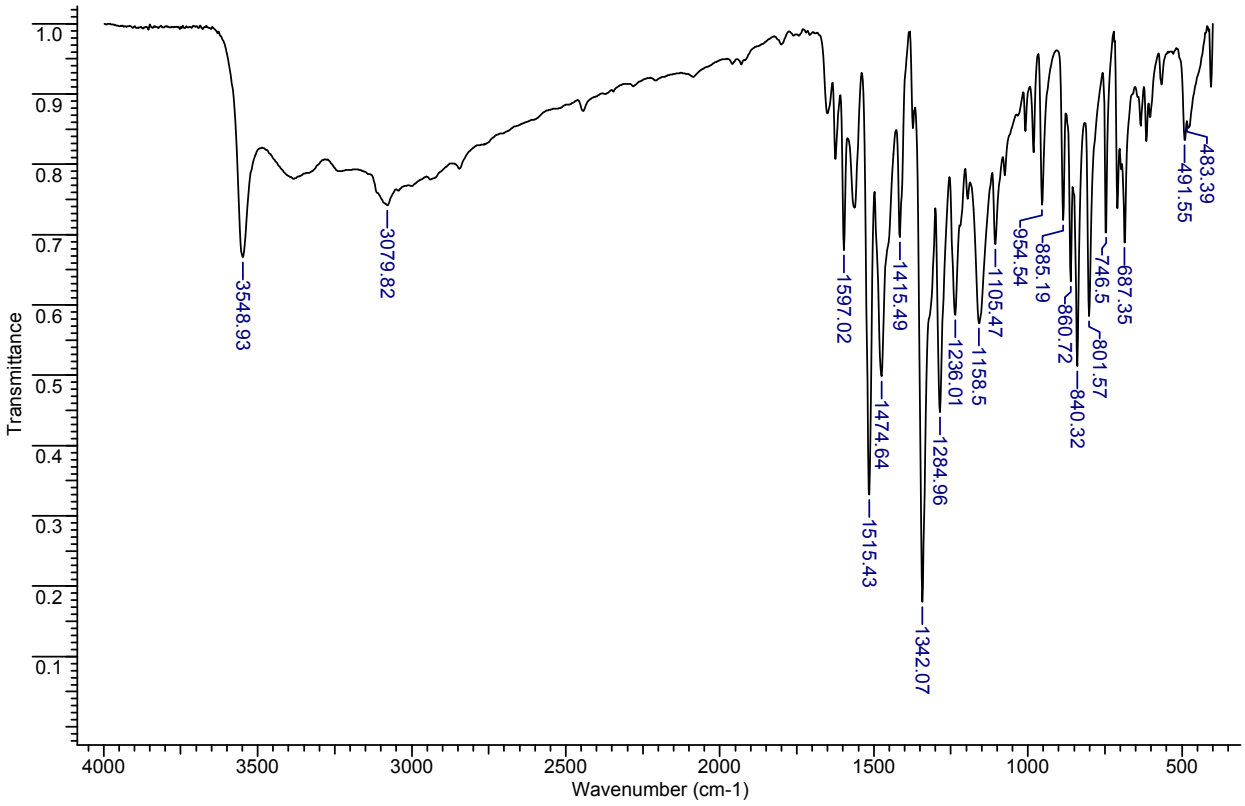

Figure S13. IR spectrum of **2e** (KBr pellet).

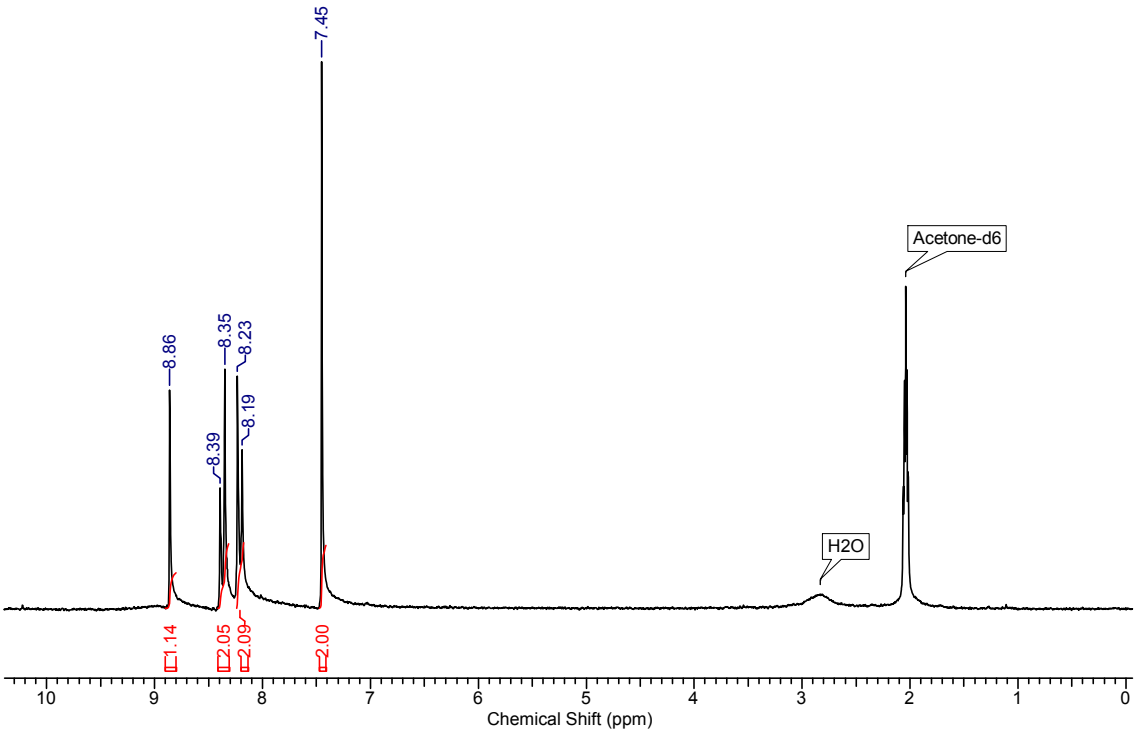

Figure S14. ^{1}H NMR spectrum of **2e**, measured in acetone-d_6 (200 MHz).

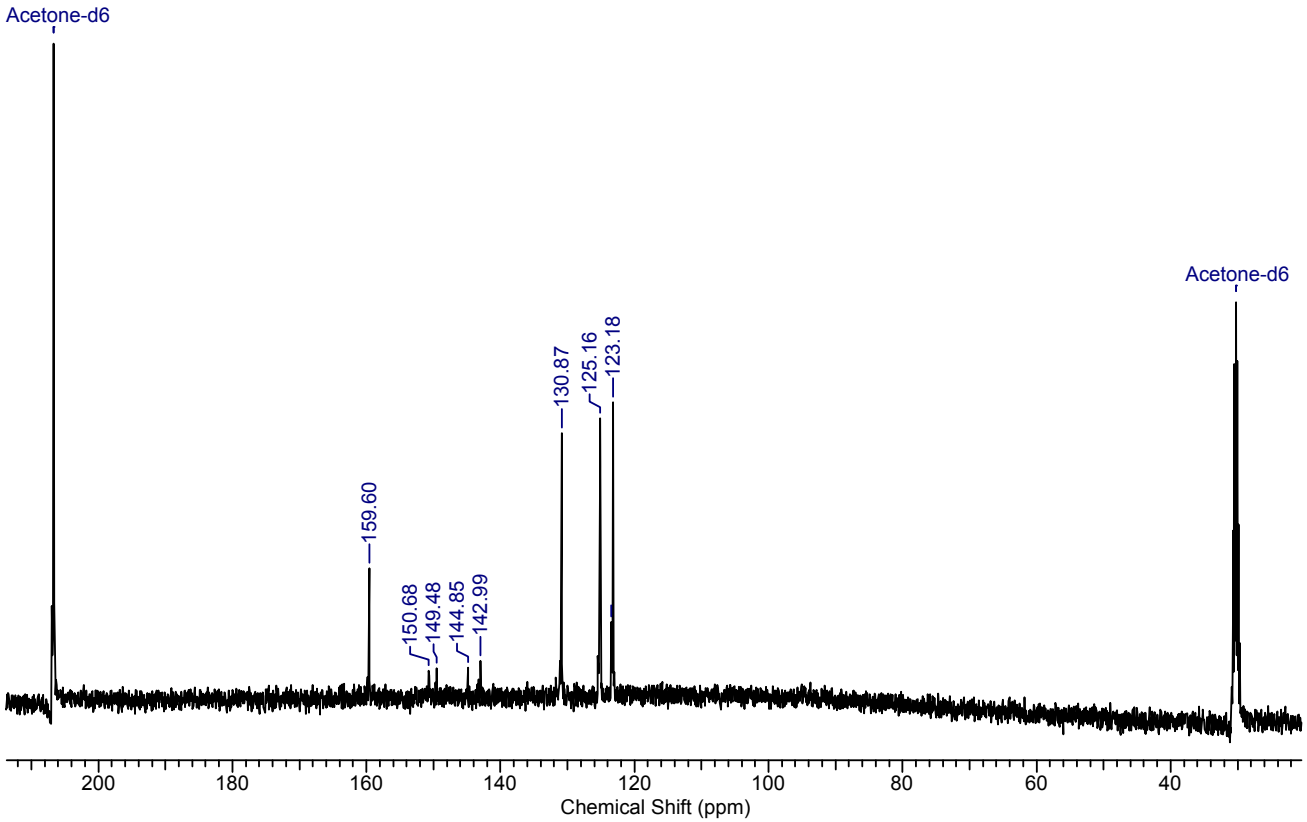

Figure S15. ^{13}C NMR spectrum of **2e**, measured in acetone-d_6 (100 MHz).

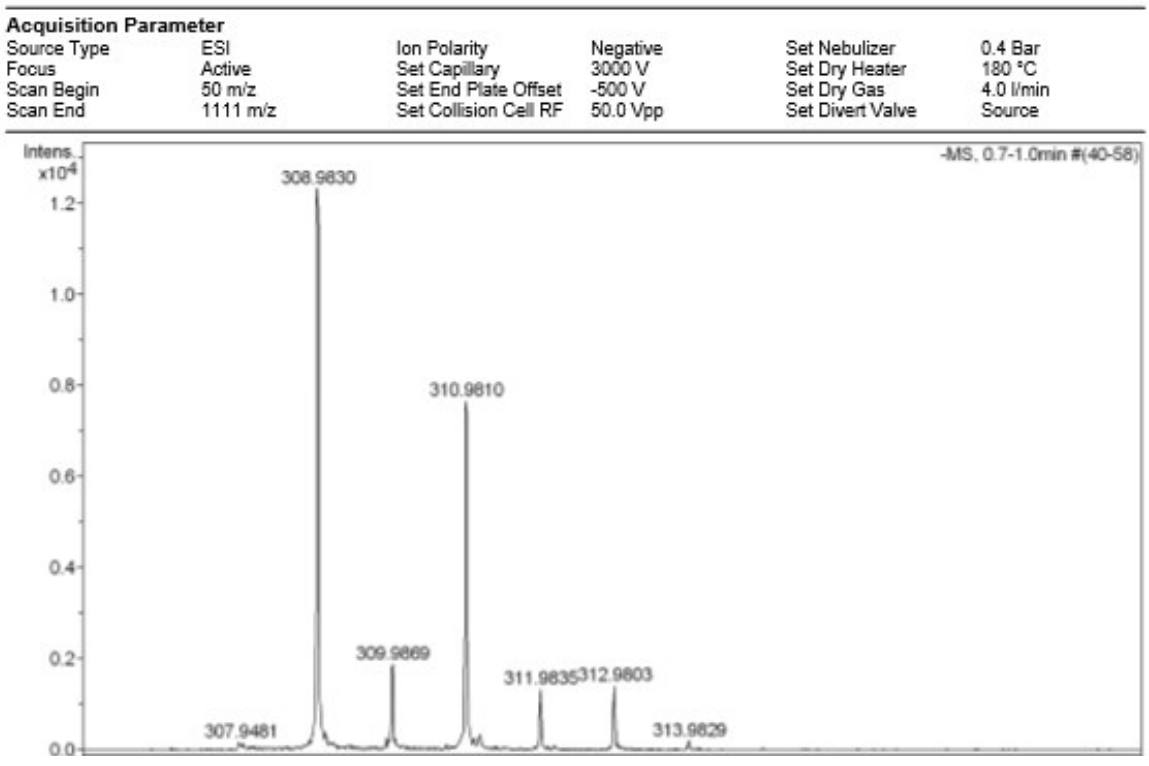

Figure S16. HRMS of **2e**.

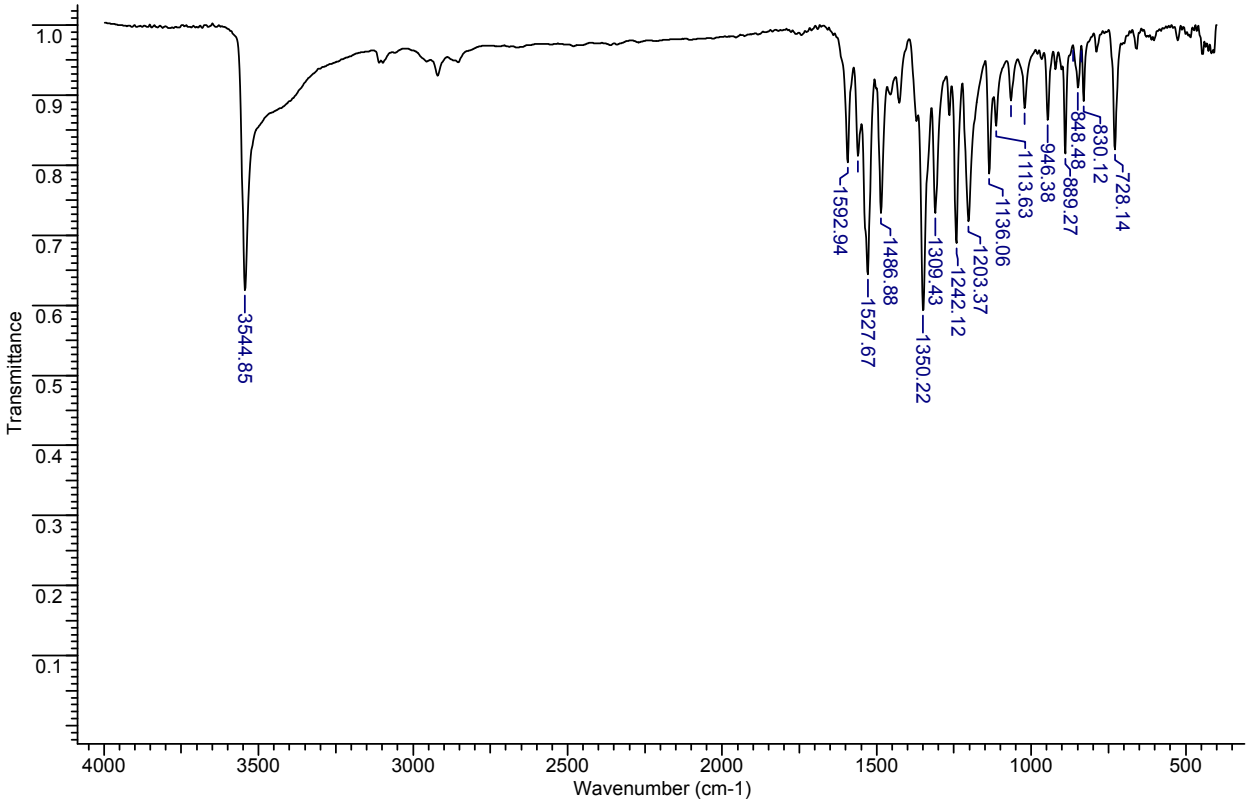

Figure S17. IR spectrum of **2h** (KBr pellet).

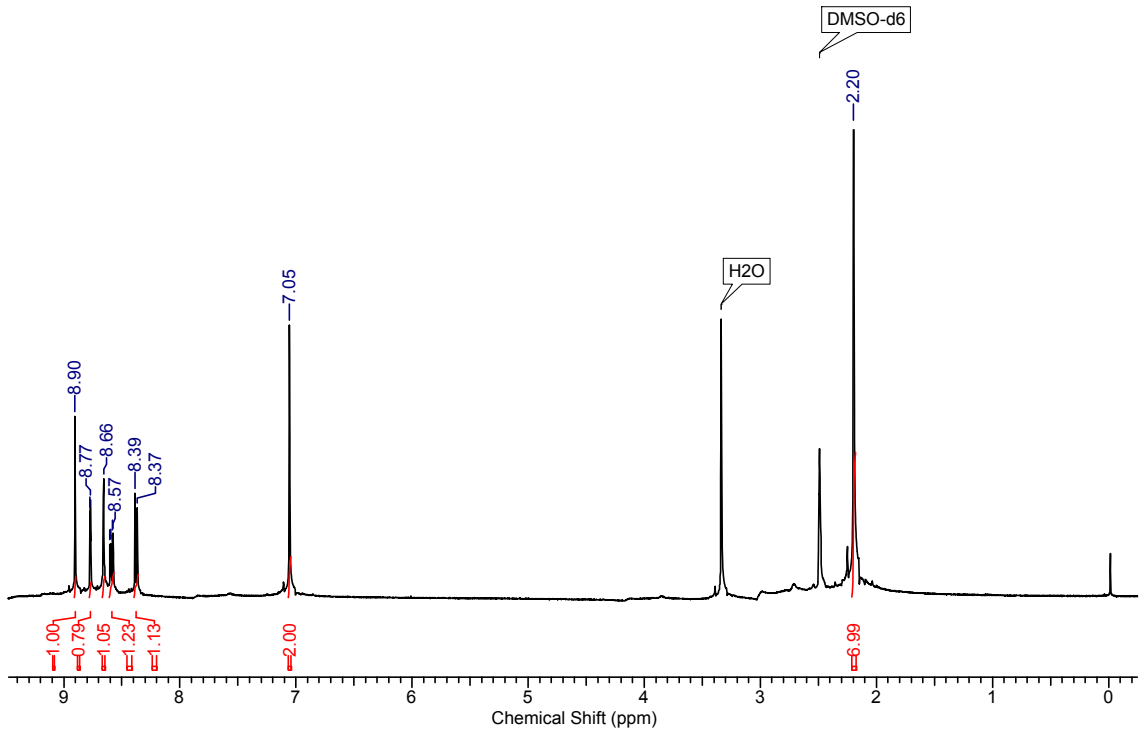

Figure S18. ^{1}H NMR spectrum of **2h**, measured in DMSO-d_6 (400 MHz).

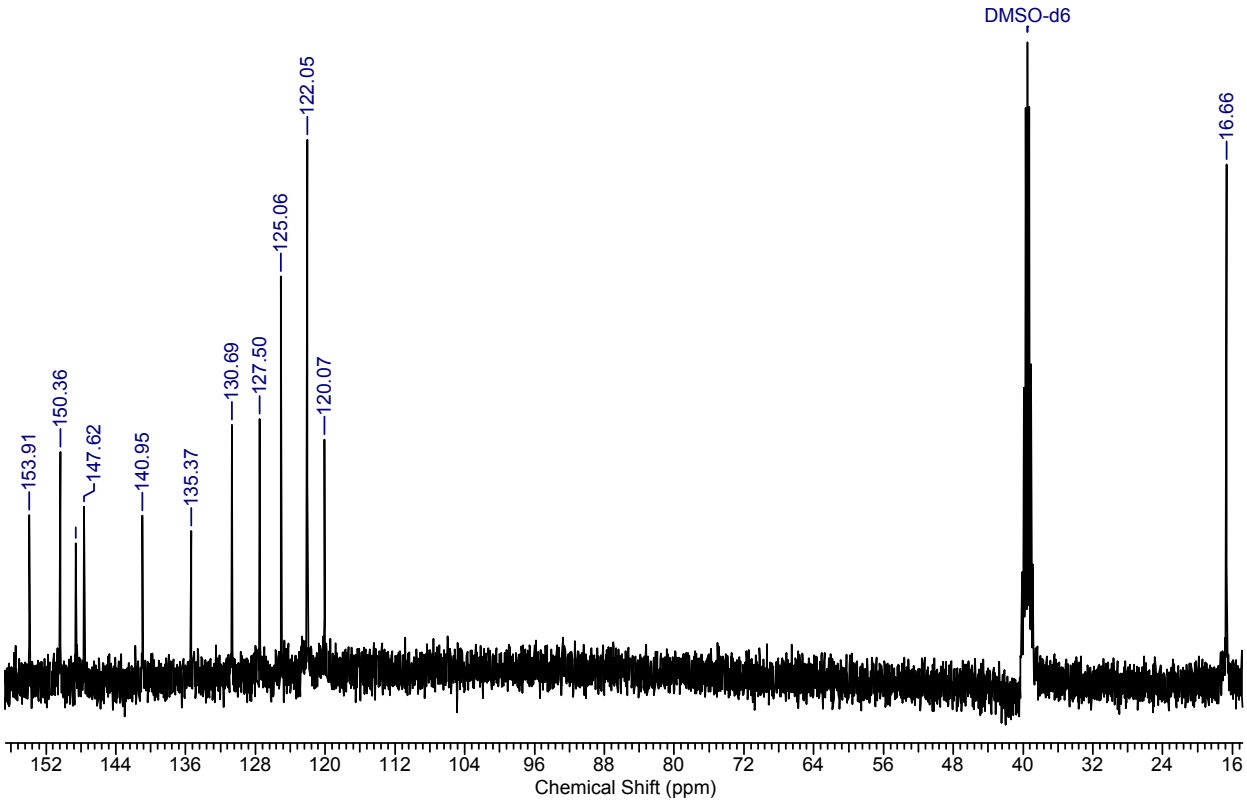

Figure S19. ^{13}C NMR spectrum of **2h**, measured in DMSO-d_6 (100 MHz).

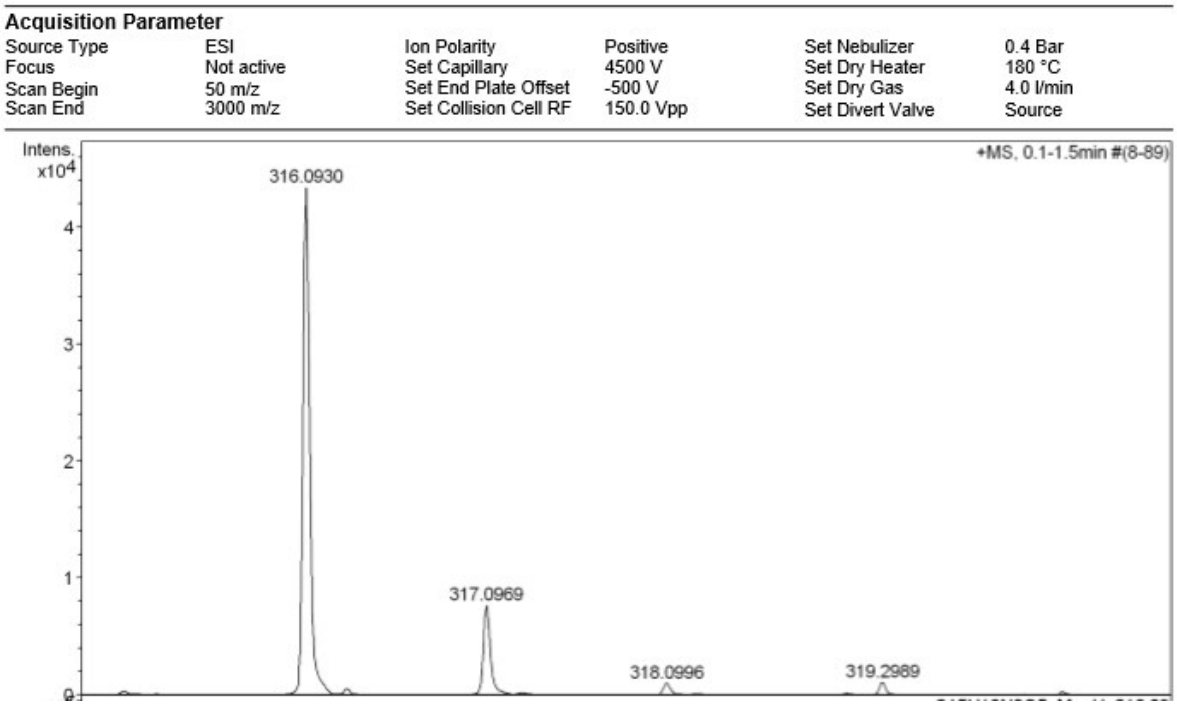

Figure S20. HRMS of **2h**.

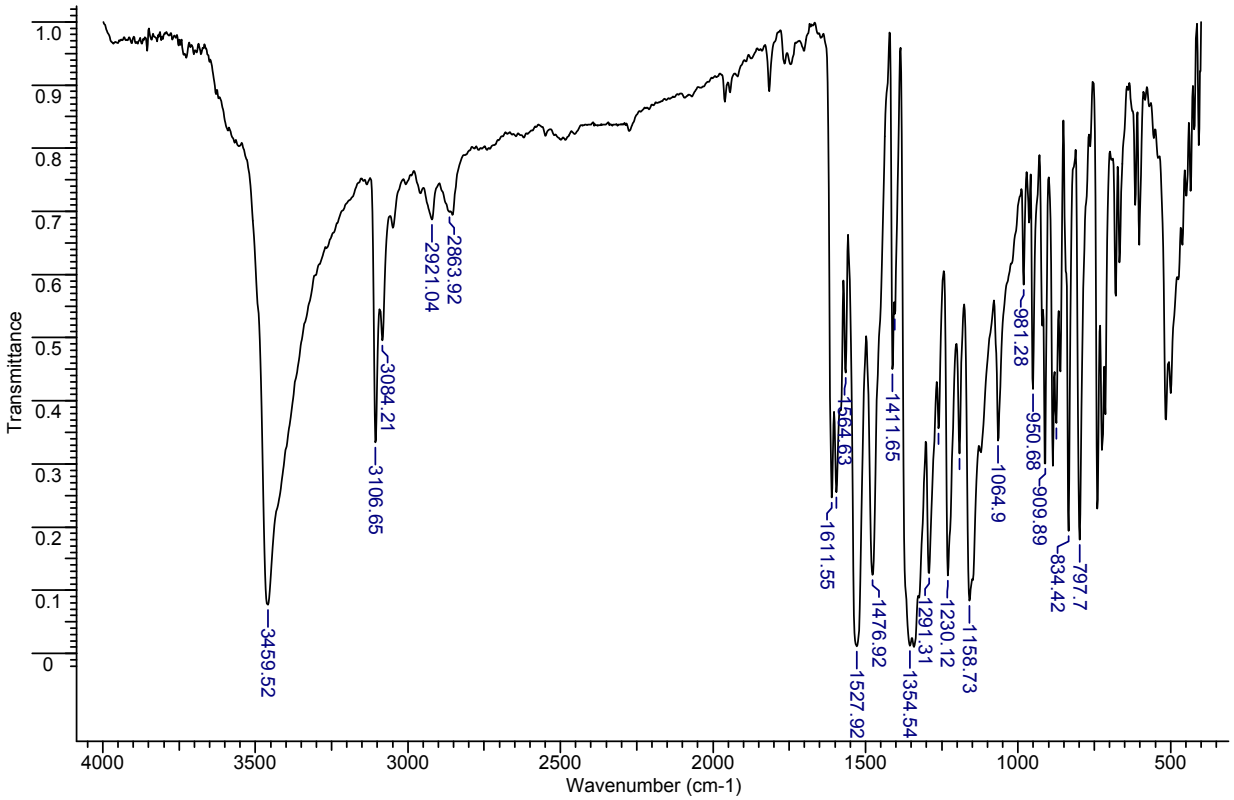

Figure S21. IR spectrum of **2i** (KBr pellet).

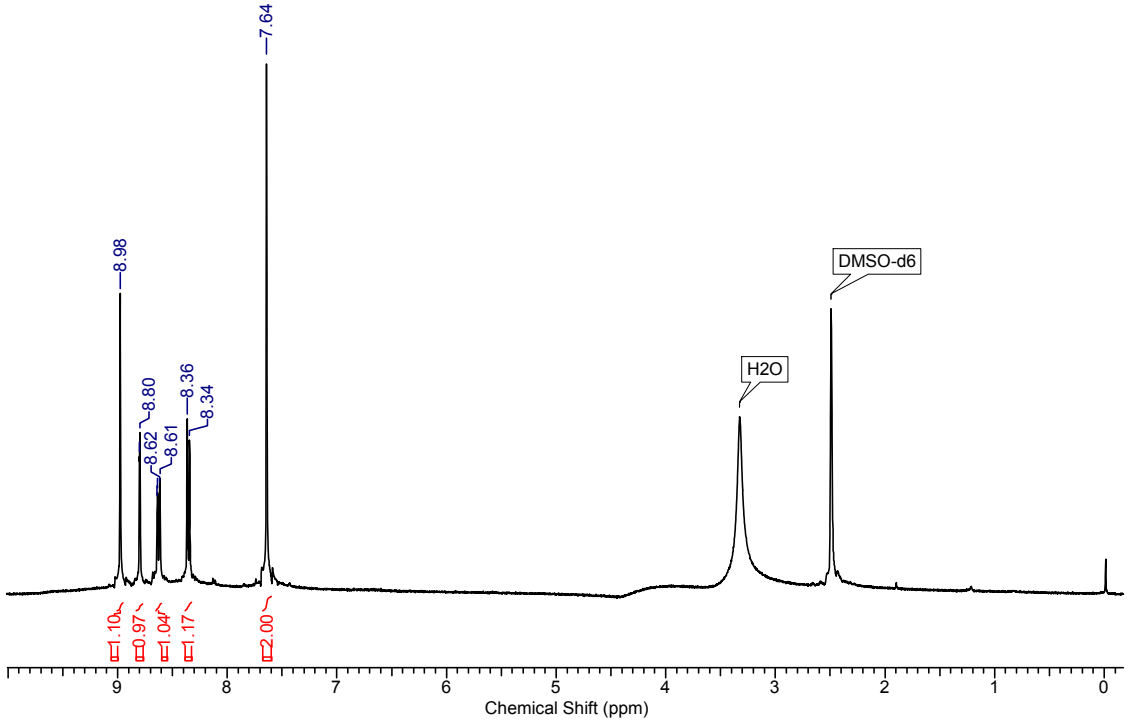

Figure S22. ^{1}H NMR spectrum of **2i**, measured in DMSO-d_6 (400 MHz).

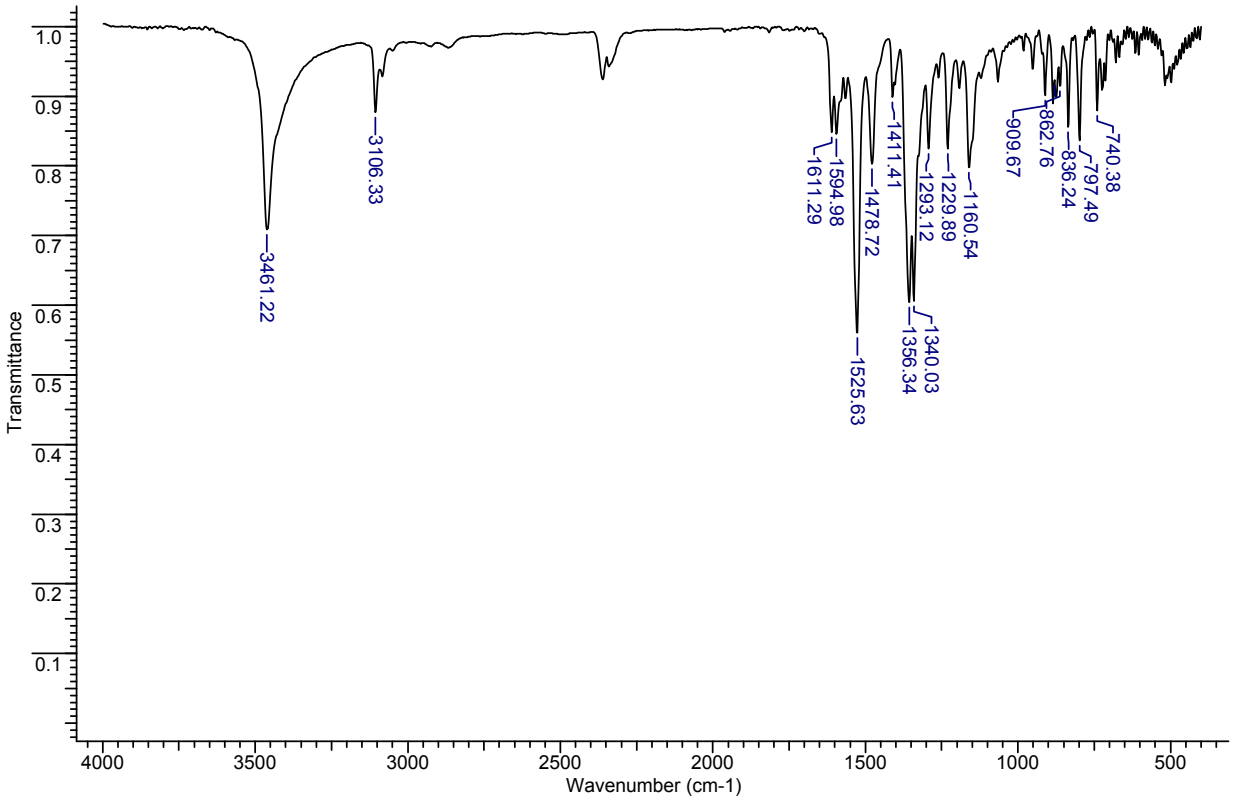

Figure S23. IR spectrum of **2j** (KBr pellet).

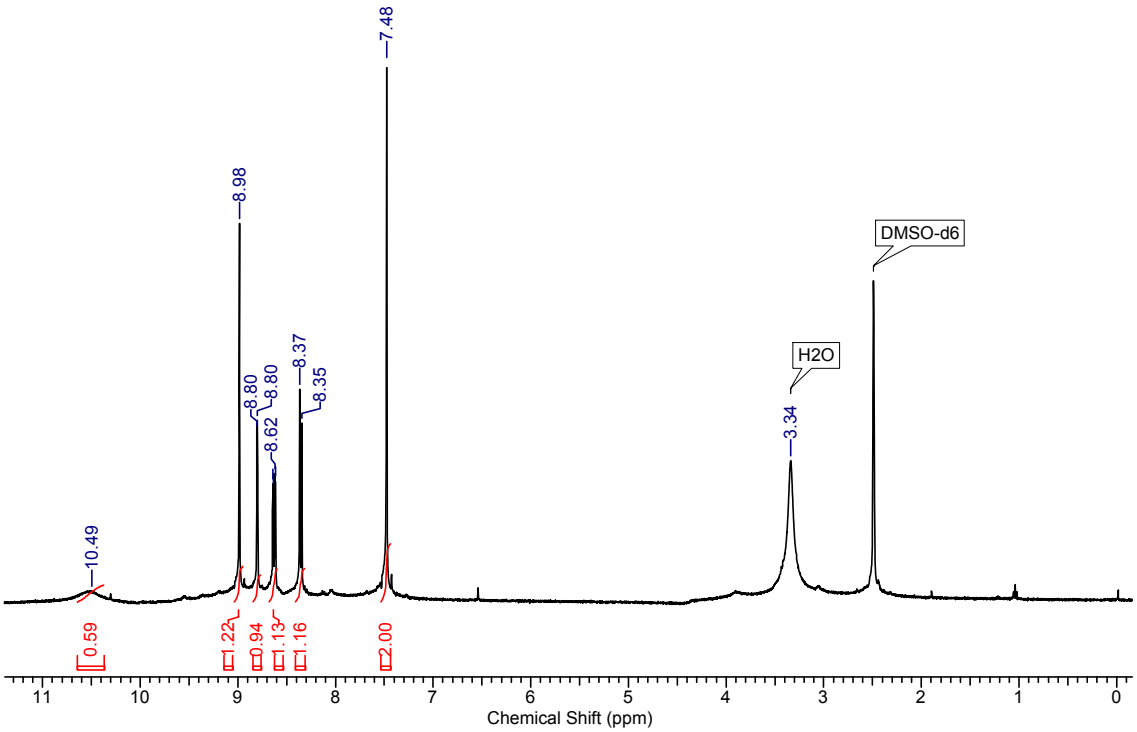

Figure S24. ^{1}H NMR spectrum of **2j**, measured in DMSO-d_6 (400 MHz).

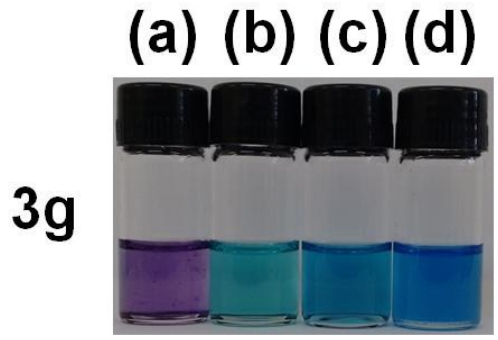

Figure S25. Solutions of compound **3g** in ethane-1,2-diol (a), DMA (b), ethyl acetate, (c) and toluene (d).

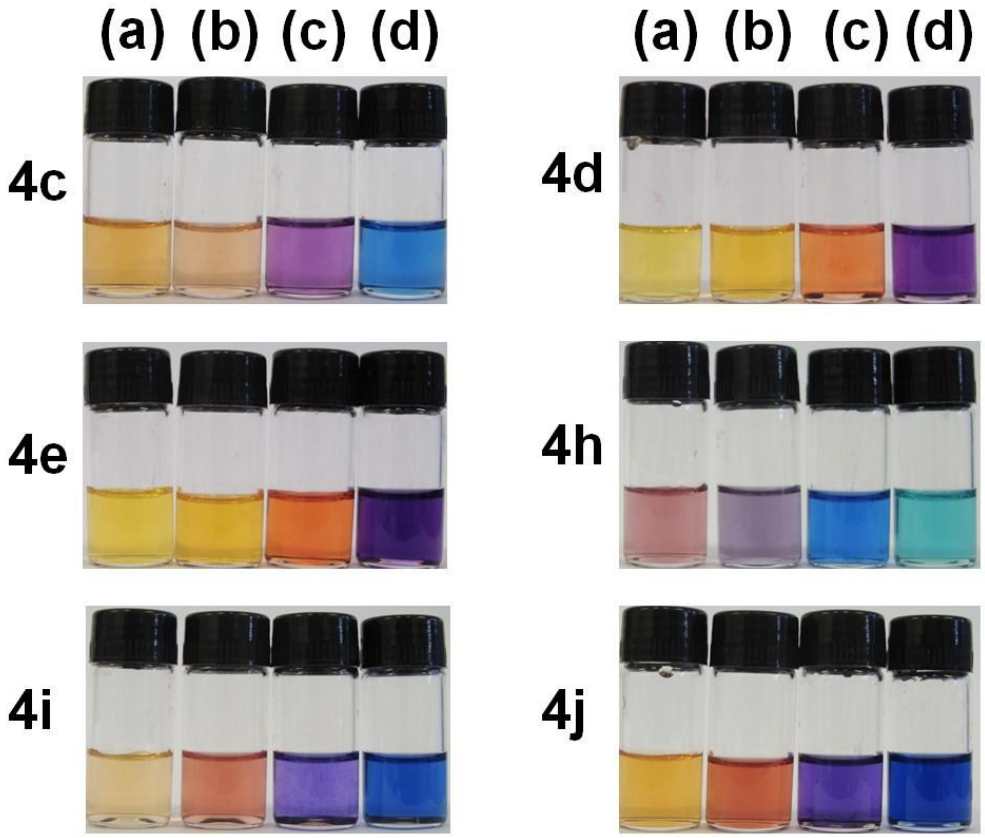

Figure S26. Solutions of compouds **4c**-**4e** and **4h**-**4j** in (a) water, (b) methanol, (c) decan-1-ol, and (d) *N,N*-dimethylformamide.

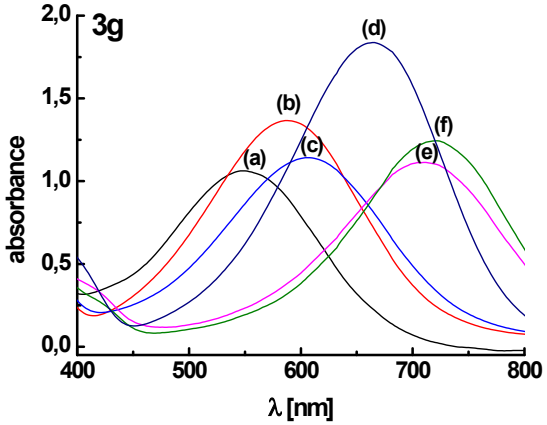

Figure S27. UV-vis spectra for **3g** obtained in methanol (a), ethanol (b), benzyl alcohol (c), ethyl acetate (d), DMSO, (e) and DMA (f).

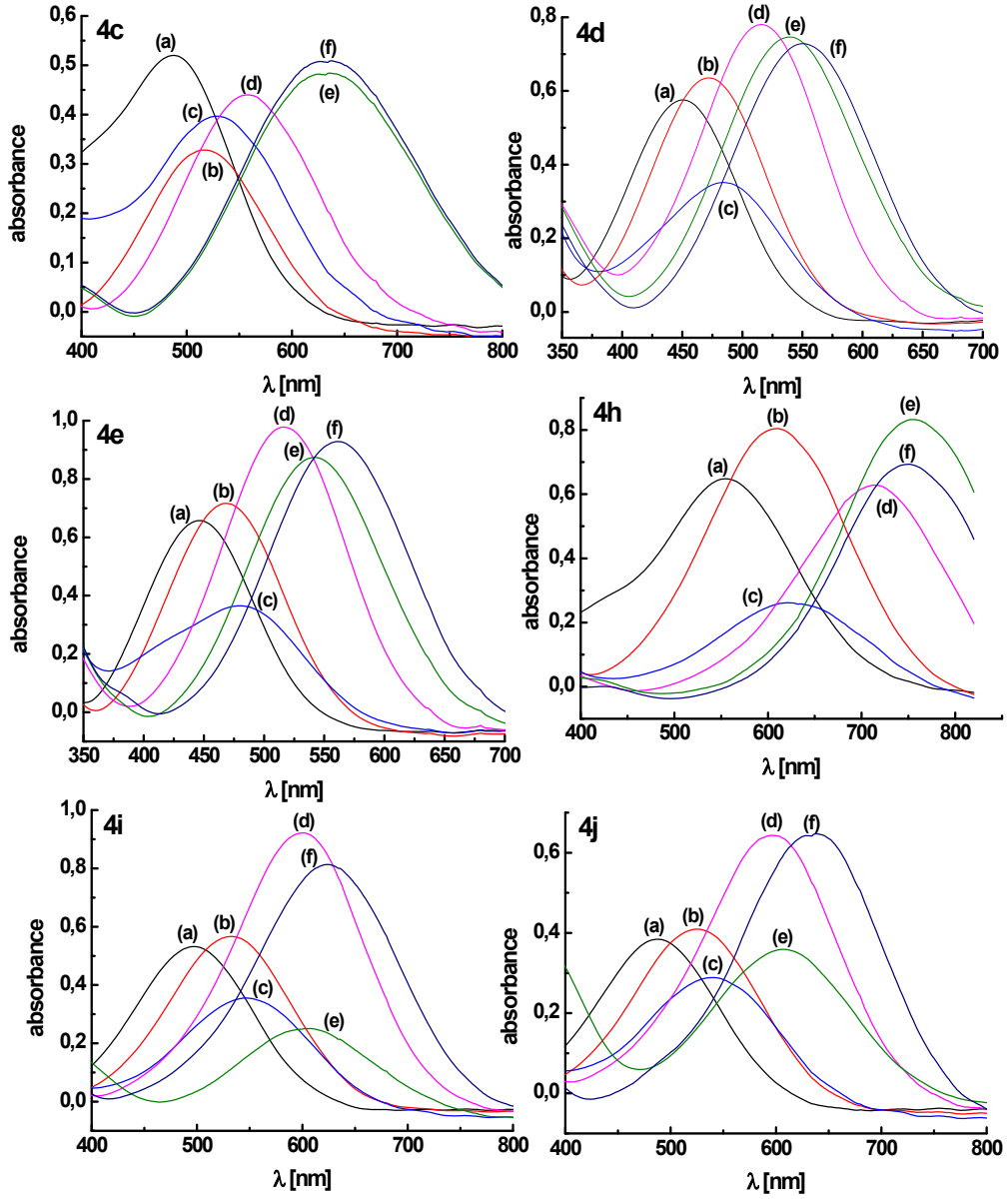

Figure S28. UV-vis spectra for **4c-4e** and **4h-4j** obtained in methanol (a), ethanol (b), benzyl alcohol (c), ethyl acetate (d), DMSO, (e) and DMA (f).

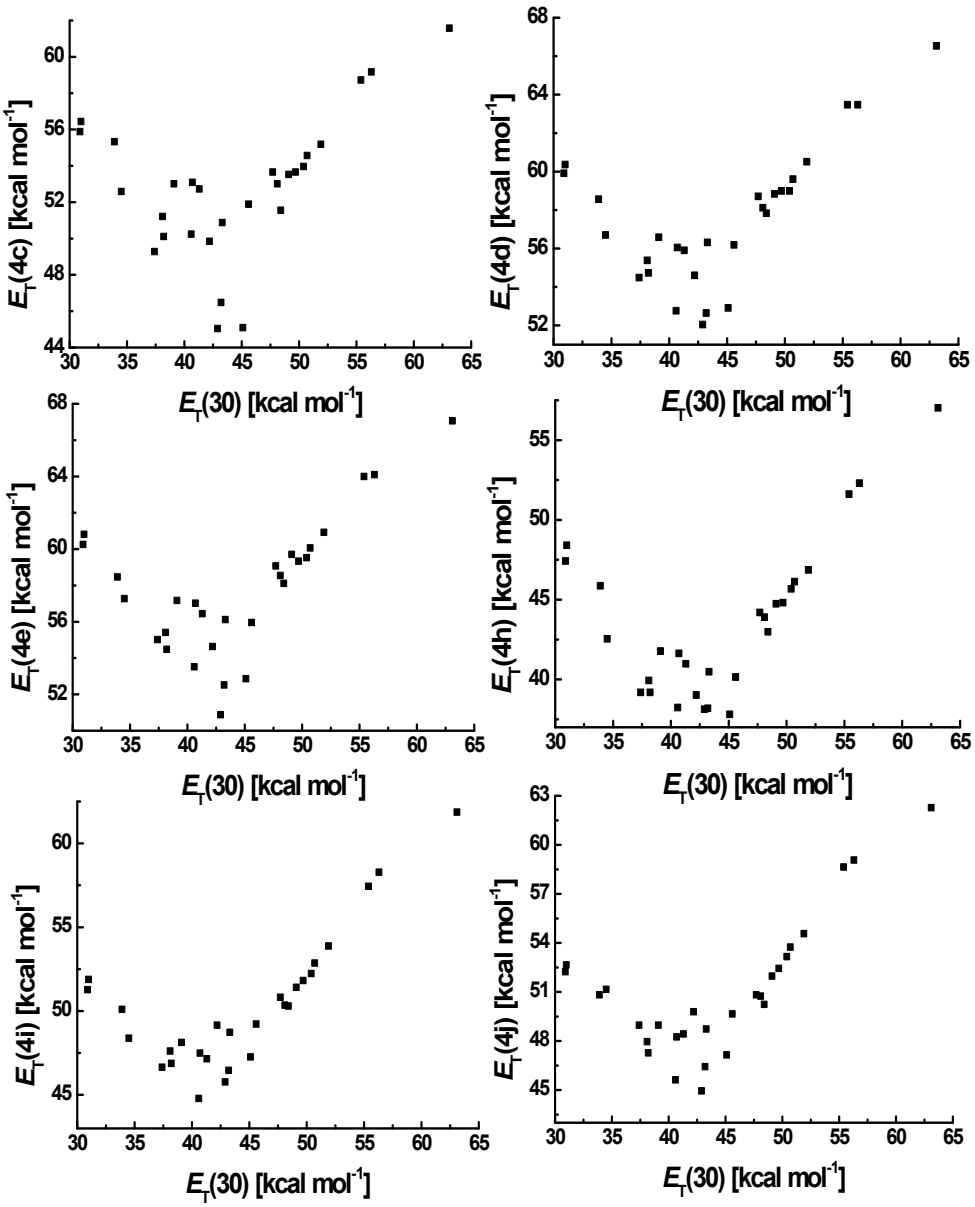

Figure S29. E_T(dye) values for **4c-4e** and **4h-4j** as a function of E_T(30) values.

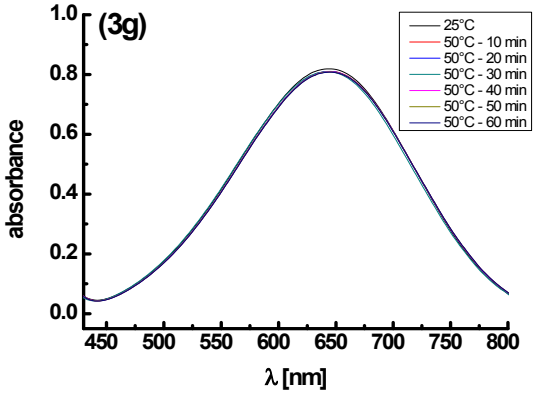

Figure S30. Investigation of the possible *cis-trans* isomerization of compound **3g**.

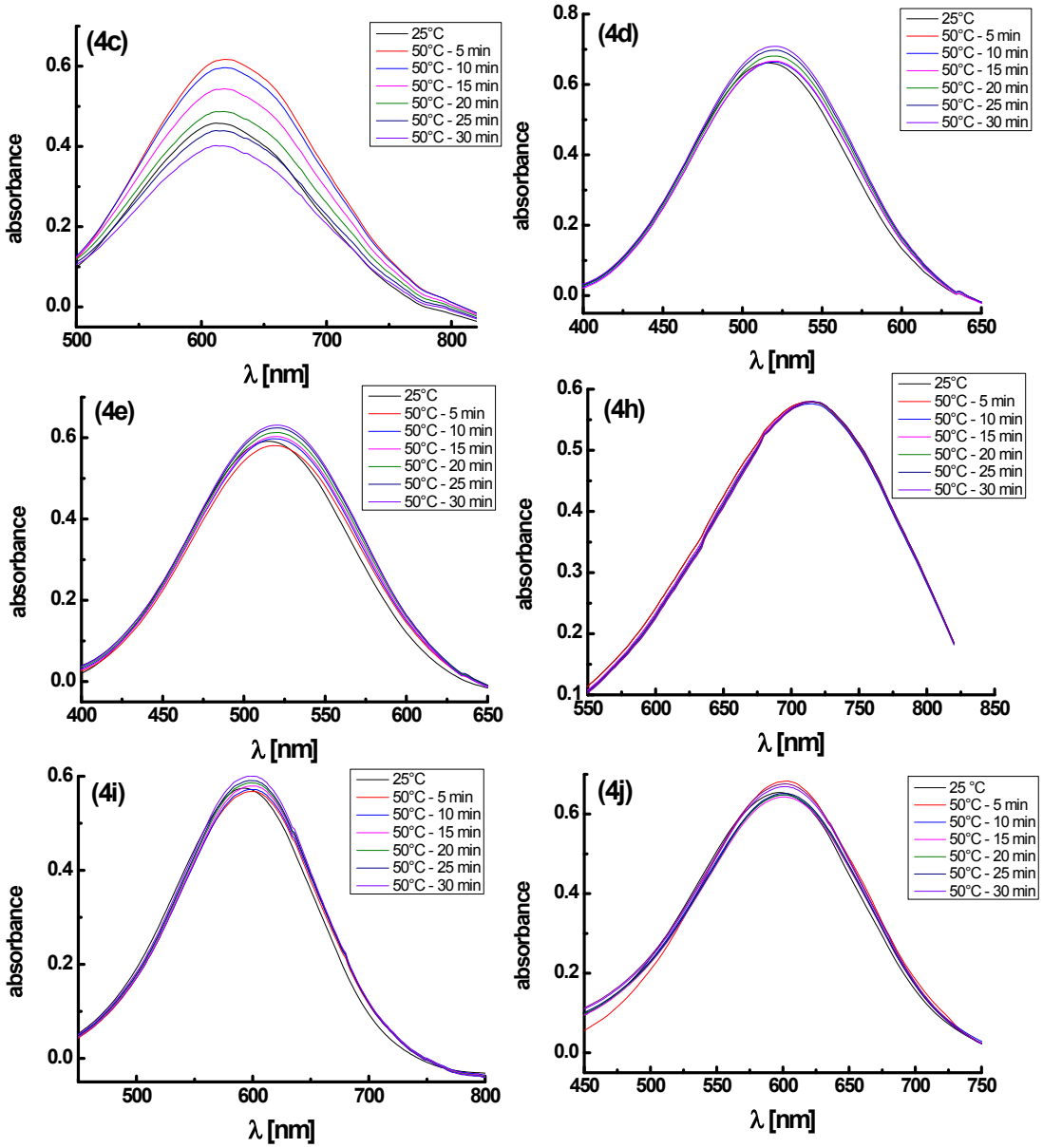

Figure S31. Investigation of the possible *cis-trans* isomerization of compounds **4c**-**4e** and **4h**-**4j**.

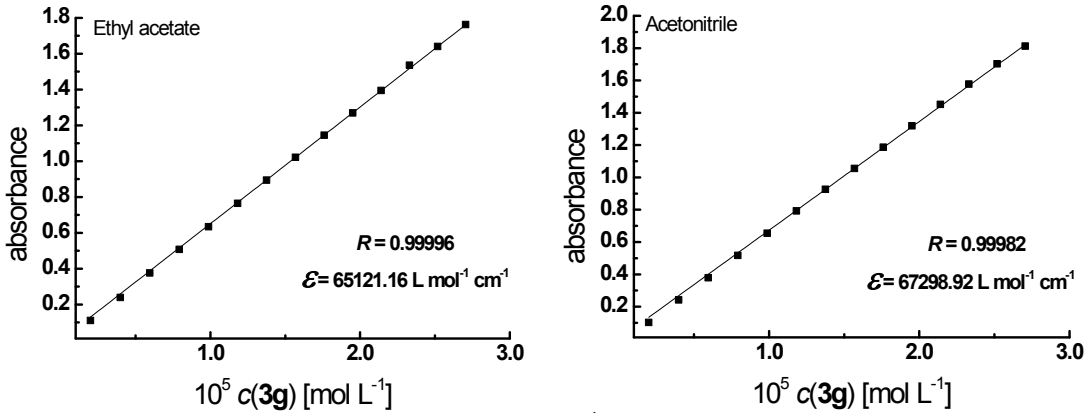

Figure S32. Experiments used to discard the possible aggregation of **3g** in ethyl acetate and acetonitrile.

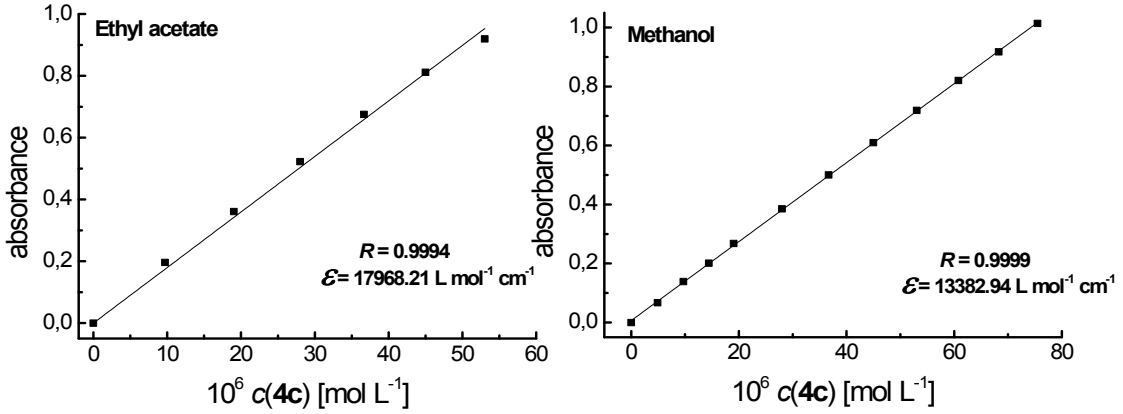

Figure S33. Experiments used to discard the possible aggregation of **4c** in ethyl acetate and methanol.

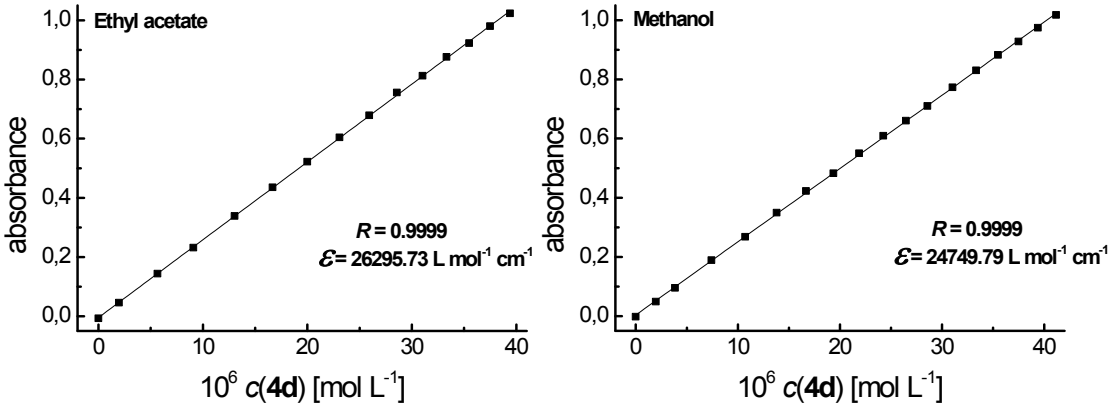

Figure S34. Experiments used to discard the possible aggregation of **4d** in ethyl acetate and methanol.

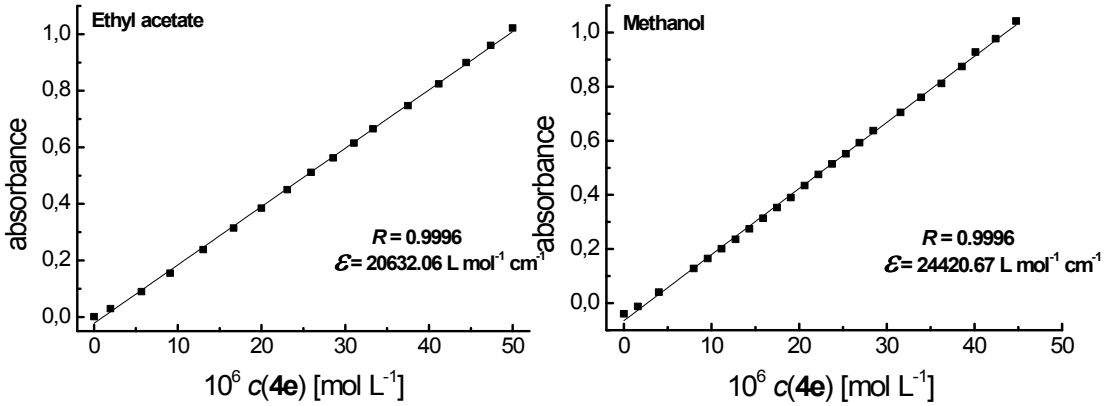

Figure S35. Experiments used to discard the possible aggregation of **4e** in ethyl acetate and methanol.

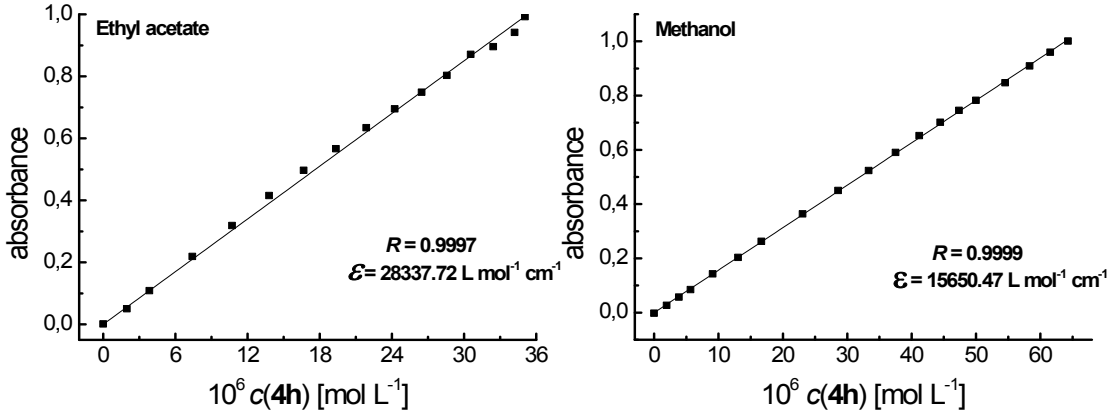

Figure S36. Experiments used to discard the possible aggregation of **4h** in ethyl acetate and methanol.

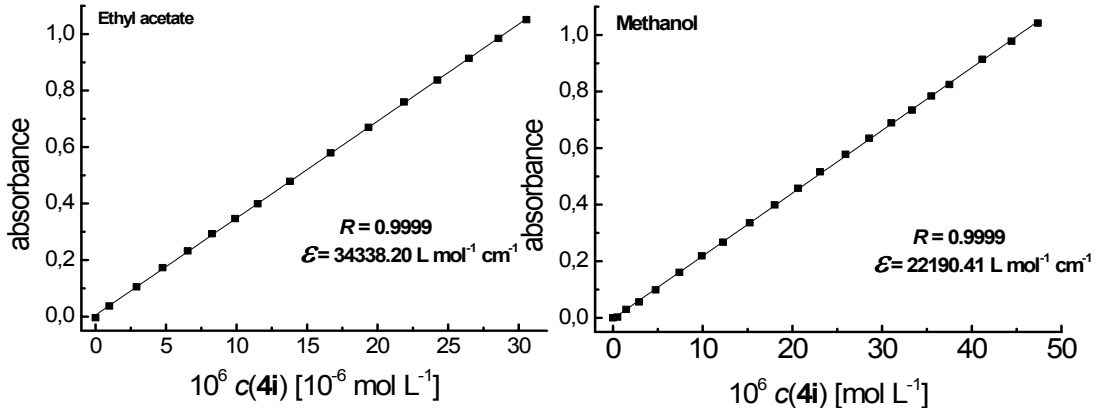

Figure S37. Experiments used to discard the possible aggregation of **4i** in ethyl acetate and methanol.

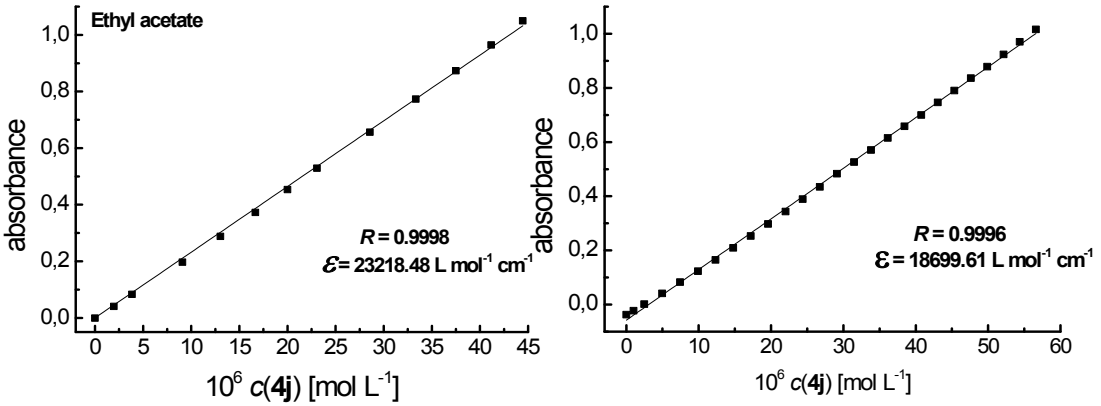

Figure S38. Experiments used to discard the possible aggregation of **4j** in ethyl acetate and methanol.

Table S1. Correlation coefficients b, c, d,e, and p obtained from Catalán multiparametric analysis, correlation coefficient (*r*) and standard deviation (S.D.) by the treatment of E_T(dye) values for compounds **3b, 4c-4e**, **4h-4j** in 30 solvents and **3g** in 31 solvents.

Dye	constant	a	b	c	d	*r*	S.D.
3b	68.60	16.58	-4.88	-14.14	-7.86	0.98	0.74
3g	56.20	15.63	-3.31	-9.89	-7.32	0.99	0.58
4c	65.02	13.09	-5.39	-10.81	-6.75	0.94	1.49
4d	67.28	12.90	-2.86	-10.27	-5.31	0.97	0.83
4e	67.68	13.81	-3.11	-9.85	-6.04	0.96	1.02
4h	52.45	17.07	-4.71	-7.32	-7.08	0.98	1.00
4i	58.39	14.64	-2.81	-10.89	-2.78	0.97	0.99
4j	60.90	14.79	-3.52	-12.42	-3.48	0.96	1.20
3b	68.60	16.58	-4.88	-14.14	-7.86	0.98	0.74

Table S2. Influence of parameters b, c, d, and e using Catalán multiparametric strategy.

Dye	constant	a	b	c	d	*r*	S.D.
	69.24	-	-0.55	-16.03	-6.33	0.64	3.18
	63.85	14.36	-	-8.85	-9.72	0.94	1.40
3b	58.97	16.81	-3.63	-	-9.52	0.95	1.23
	73.98	15.21	-8.12	-26.33	-	0.86	2.14
	63.98	-	-3.66	-21.72	-1.82	0.49	3.88
	52.83	15.73	-	-6.36	-8.59	0.97	1.11
3g	49.49	16.24	-2.68	-	-8.41	0.98	0.90
	60.65	12.81	-5.55	-20.74	-	0.90	1.96
	71.75	-	-5.70	-20.99	-2.13	0.55	3.08
	59.03	13.25	-	-4.83	-8.40	0.87	2.13
4c	57.59	13.77	-4.67	-	-7.85	0.92	1.65
	67.58	10.73	-6.92	-19.21	-	0.85	2.22
	73.91	-	-3.16	-20.31	-0.76	0.47	3.32
	64.10	12.99	-	-7.09	-6.18	0.95	1.16
4d	60.22	13.55	-2.17	-	-6.36	0.90	1.09
	69.30	11.04	-4.07	-16.89	-	0.91	1.55
	77.78	-	-3.42	-20.60	-1.17	0.46	3.60
	64.23	13.91	-	-6.41	-6.99	0.94	1.35
4e	60.90	14.43	-2.44	-	-7.05	0.95	1.22
	69.97	11.70	-4.47	-17.38	-	0.89	1.81
	61.55	-	-5.12	-21.10	-0,84	0.42	4.53
	47.23	17.85	-	-2.10	-8.52	0.94	1.67
4h	47.42	18.16	-4.21	-	-7.83	0.97	1.11
	55.14	15.23	-6.30	-16.14	-	0.91	2.01
	66.91	-	-3.15	-22.28	2.37	0.40	3.78
	55.27	14.72	-	-7.77	-3.64	0.89	1.26
4i	50.90	15.32	-2.07	-	-3.89	0.95	1.24
	59.44	13.66	-3.44	-14.36	-	0.95	1.19
	68.50	-	-3.87	-23.94	1.73	0.43	3.88
	56.99	14.90	-	-8.52	-4.55	0.93	1.55
4j	52.36	15.57	-2.69	-	-4.74	0.93	1.47
	62.22	13.57	-4.31	-16.76	-	0.94	1.46

Table S3. Correlation coefficients a, b, s, and p obtained from the Kamlet-Abboud-Taft multiparametric, correlation coefficient (*r*) and standard deviation (S.D.) by the treatment of E_T(dye) values for compounds **3b, 4c-4e**, **4h-4j** in 30 solvents and **3g** in 31 solvents.

Dye	constant	a	b	s	*r*	S.D.
3b	57.98	9.57	-8.51	-5.62	0.96	1.13
3g	48.09	10.67	-8.48	-3.26	0.90	1.84
4c	56.07	10.47	-10.99	-2.51	0.94	1.46
4d	59.13	9.60	-7.26	-2.23	0.94	1.26
4e	59.65	10.42	-8.21	-2.35	0.95	1.26
4h	45.30	12.21	-9.99	-1.66	0.89	2.24
4i	49.82	10.27	-6.34	-0.08	0.90	1.84
4j	51.21	10.53	-7.41	-0.58	0.88	2.02

Table S4. Influence of parameters a, b, and s using Kamlet-Abboud-Taft multiparametric strategy.

Dye	constant	a	b	s	*r*	S.D.
	58.53	-	-1.30	-8.09	0.66	2.99
3b	56.41	4.99	-	-8.21	0.80	2.36
	55.55	11.06	-10.87	-	0.88	1.92
	48.13	-	-1.16	-3.77	0.31	4.05
3g	45.82	7.13	-	-4.89	0.74	2.88
	46.57	10.98	-9.39	-	0.88	2.04
	55.98	-	-3.70	-2.58	0.34	3.98
4c	52.60	6.40	-	-4.09	0.66	3.18
	54.73	10.48	-11.42	-	0.92	1.60
	59.04	-	-0.58	-2.28	0.19	3.62
4d	56.83	6.91	-	-3.27	0.79	2.25
	57.93	9.61	-7.65	-	0.92	1.39
	59.56	-	-1.50	-1.73	0.15	4.86
4e	57.06	7.38	-	-3.52	0.78	2.46
	58.40	10.43	-8.61	-	0.93	1.40
	45.19	-	-0.94	-1.33	0.10	4.95
4h	42.14	8.51	-	-3.09	0.72	3.40
	44.42	12.22	-10.28	-	0.89	2.25
	49.73	-	0.80	-0.14	0.06	4.07
4i	47.82	7.92	-	-0.98	0.80	2.44
	49.78	10.27	-6.35	-	0.90	1.81
	51.12	-	-0.08	-0.64	0.04	4.23
4j	48.87	7.79	-	-1.64	0.76	2.76
	50.90	10.53	-7.51	-	0.88	1.99

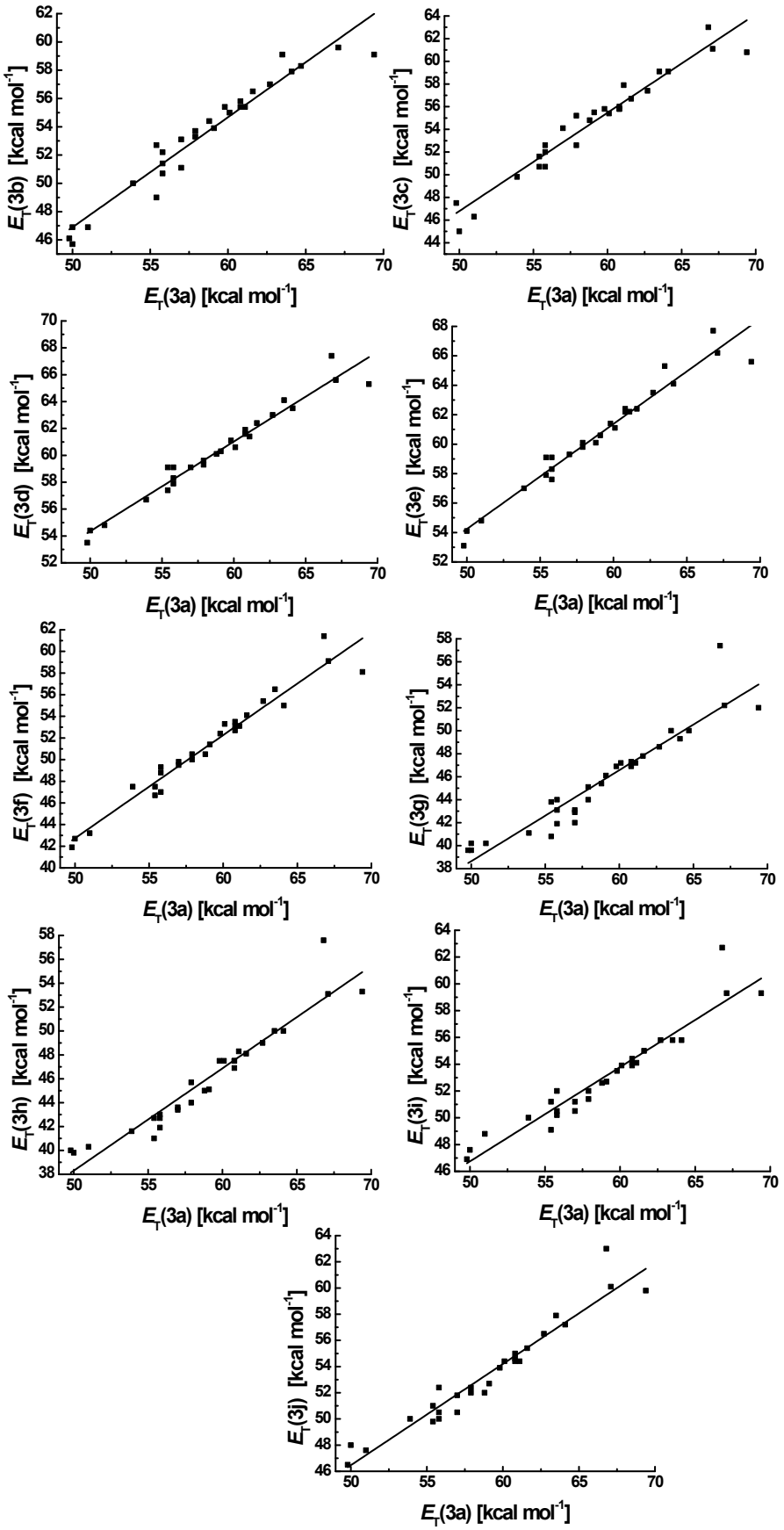

Figure S39. Linear plot of E_T (dye) *vs.* E_T(**3a**) values for compounds **3b**-**3j**.

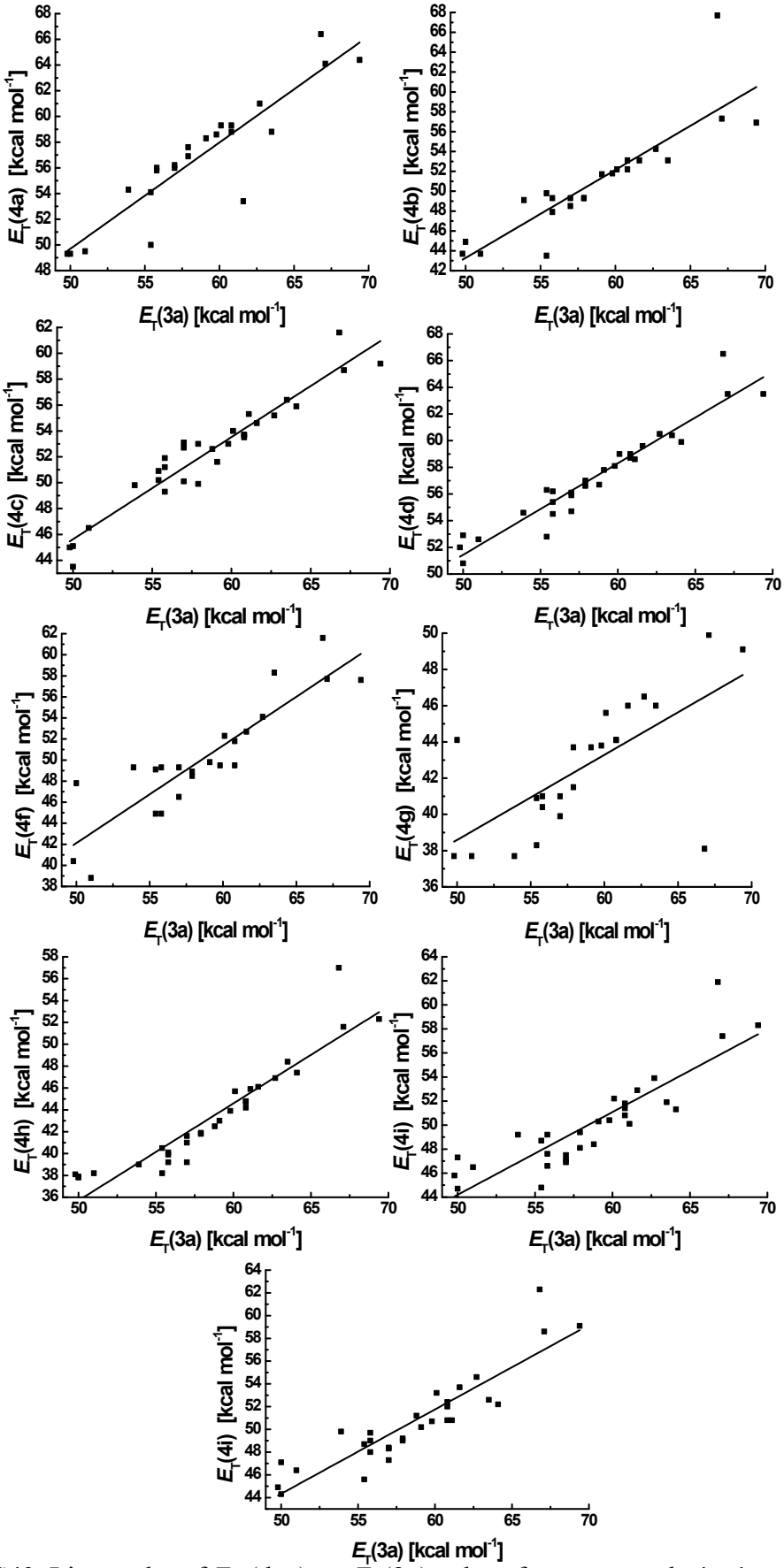

Figure S40. Linear plot of E_T (dye) *vs.* E_T(**3a**) values for compounds **4a**-**4c** and **4d**-**4j**.

Table S5. Bond lengths (Å) and angles (°) for compound **1b**.

C(1)-C(2)	1.3949(19)
C(1)-C(6)	1.4005(19)
C(1)-C(7)	1.4688(17)
C(2)-C(3)	1.3813(19)
C(2)-H(2)	0.9500
C(3)-C(4)	1.382(2)
C(3)-H(3)	0.9500
C(4)-C(5)	1.3874(19)
C(4)-N(1)	1.4608(16)
C(5)-C(6)	1.3863(18)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-C(8)	1.3290(19)
C(7)-H(7)	0.9500
C(8)-C(9)	1.4651(16)
C(8)-H(8)	0.9500
C(9)-C(10)	1.3933(18)
C(9)-C(14)	1.4025(17)
C(10)-C(11)	1.3955(16)
C(10)-H(10)	0.9500
C(11)-C(12)	1.4043(17)
C(11)-C(15A)	1.4900(17)
C(12)-O(3)	1.3703(14)
C(12)-C(13)	1.4070(17)
C(13)-C(14)	1.3927(16)
C(13)-C(15B)	1.4899(16)
C(14)-H(14)	0.9500
C(15A)-C(16A)	1.3965(18)
C(15A)-C(20A)	1.4025(17)
C(15B)-C(20B)	1.3932(19)
C(15B)-C(16B)	1.3950(18)
C(16A)-C(17A)	1.385(2)
C(16A)-H(16A)	0.9500
C(16B)-C(17B)	1.3956(19)
C(16B)-H(16B)	0.9500
C(17A)-C(18A)	1.383(2)

C(17A)-H(17A)	0.9500
C(17B)-C(18B)	1.382(2)
C(17B)-H(17B)	0.9500
C(18A)-C(19A)	1.386(2)
C(18A)-H(18A)	0.9500
C(18B)-C(19B)	1.383(2)
C(18B)-H(18B)	0.9500
C(19A)-C(20A)	1.388(2)
C(19A)-H(19A)	0.9500
C(19B)-C(20B)	1.3879(19)
C(19B)-H(19B)	0.9500
C(20A)-H(20A)	0.9500
C(20B)-H(20B)	0.9500
N(1)-O(1)	1.2202(18)
N(1)-O(2)	1.2268(17)
O(3)-H(1O)	0.8669

C(2)-C(1)-C(6)	118.20(12)
C(2)-C(1)-C(7)	118.83(12)
C(6)-C(1)-C(7)	122.97(12)
C(3)-C(2)-C(1)	121.25(13)
C(3)-C(2)-H(2)	119.4
C(1)-C(2)-H(2)	119.4
C(2)-C(3)-C(4)	118.78(13)
C(2)-C(3)-H(3)	120.6
C(4)-C(3)-H(3)	120.6
C(3)-C(4)-C(5)	122.05(12)
C(3)-C(4)-N(1)	118.86(12)
C(5)-C(4)-N(1)	119.08(12)
C(6)-C(5)-C(4)	118.13(13)
C(6)-C(5)-H(5)	120.9
C(4)-C(5)-H(5)	120.9
C(5)-C(6)-C(1)	121.42(13)
C(5)-C(6)-H(6)	119.3
C(1)-C(6)-H(6)	119.3
C(8)-C(7)-C(1)	125.44(12)
C(8)-C(7)-H(7)	117.3
C(1)-C(7)-H(7)	117.3

C(7)-C(8)-C(9)	127.11(12)
C(7)-C(8)-H(8)	116.4
C(9)-C(8)-H(8)	116.4
C(10)-C(9)-C(14)	117.74(11)
C(10)-C(9)-C(8)	118.08(11)
C(14)-C(9)-C(8)	124.16(12)
C(9)-C(10)-C(11)	122.54(11)
C(9)-C(10)-H(10)	118.7
C(11)-C(10)-H(10)	118.7
C(10)-C(11)-C(12)	118.03(11)
C(10)-C(11)-C(15A)	119.53(11)
C(12)-C(11)-C(15A)	122.38(11)
O(3)-C(12)-C(11)	121.60(11)
O(3)-C(12)-C(13)	117.30(10)
C(11)-C(12)-C(13)	121.05(11)
C(14)-C(13)-C(12)	118.56(11)
C(14)-C(13)-C(15B)	120.29(11)
C(12)-C(13)-C(15B)	121.04(10)
C(13)-C(14)-C(9)	121.84(12)
C(13)-C(14)-H(14)	119.1
C(9)-C(14)-H(14)	119.1
C(16A)-C(15A)-C(20A)	117.80(12)
C(16A)-C(15A)-C(11)	119.82(11)
C(20A)-C(15A)-C(11)	122.37(11)
C(20B)-C(15B)-C(16B)	118.40(12)
C(20B)-C(15B)-C(13)	119.84(11)
C(16B)-C(15B)-C(13)	121.75(12)
C(17A)-C(16A)-C(15A)	121.43(12)
C(17A)-C(16A)-H(16A)	119.3
C(15A)-C(16A)-H(16A)	119.3
C(15B)-C(16B)-C(17B)	120.33(13)
C(15B)-C(16B)-H(16B)	119.8
C(17B)-C(16B)-H(16B)	119.8
C(18A)-C(17A)-C(16A)	119.94(13)
C(18A)-C(17A)-H(17A)	120.0
C(16A)-C(17A)-H(17A)	120.0
C(18B)-C(17B)-C(16B)	120.51(13)
C(18B)-C(17B)-H(17B)	119.7

C(16B)-C(17B)-H(17B)	119.7
C(17A)-C(18A)-C(19A)	119.78(13)
C(17A)-C(18A)-H(18A)	120.1
C(19A)-C(18A)-H(18A)	120.1
C(17B)-C(18B)-C(19B)	119.48(13)
C(17B)-C(18B)-H(18B)	120.3
C(19B)-C(18B)-H(18B)	120.3
C(18A)-C(19A)-C(20A)	120.34(13)
C(18A)-C(19A)-H(19A)	119.8
C(20A)-C(19A)-H(19A)	119.8
C(18B)-C(19B)-C(20B)	120.26(14)
C(18B)-C(19B)-H(19B)	119.9
C(20B)-C(19B)-H(19B)	119.9
C(19A)-C(20A)-C(15A)	120.68(13)
C(19A)-C(20A)-H(20A)	119.7
C(15A)-C(20A)-H(20A)	119.7
C(19B)-C(20B)-C(15B)	120.96(13)
C(19B)-C(20B)-H(20B)	119.5
C(15B)-C(20B)-H(20B)	119.5
O(1)-N(1)-O(2)	122.89(12)
O(1)-N(1)-C(4)	119.03(12)
O(2)-N(1)-C(4)	118.09(13)
C(12)-O(3)-H(1O)	109.0

Table S6. Torsion angles (°) for compound **1b**.

C(6)-C(1)-C(2)-C(3)	-4.4(2)
C(7)-C(1)-C(2)-C(3)	176.02(13)
C(1)-C(2)-C(3)-C(4)	1.9(2)
C(2)-C(3)-C(4)-C(5)	1.7(2)
C(2)-C(3)-C(4)-N(1)	-177.47(13)
C(3)-C(4)-C(5)-C(6)	-2.6(2)
N(1)-C(4)-C(5)-C(6)	176.55(13)
C(4)-C(5)-C(6)-C(1)	0.0(2)
C(2)-C(1)-C(6)-C(5)	3.4(2)
C(7)-C(1)-C(6)-C(5)	-177.00(13)
C(2)-C(1)-C(7)-C(8)	-173.59(14)
C(6)-C(1)-C(7)-C(8)	6.8(2)
C(1)-C(7)-C(8)-C(9)	-175.46(12)
C(7)-C(8)-C(9)-C(10)	168.74(13)
C(7)-C(8)-C(9)-C(14)	-9.5(2)
C(14)-C(9)-C(10)-C(11)	4.05(19)
C(8)-C(9)-C(10)-C(11)	-174.31(12)
C(9)-C(10)-C(11)-C(12)	-0.74(19)
C(9)-C(10)-C(11)-C(15A)	176.74(12)
C(10)-C(11)-C(12)-O(3)	173.50(12)
C(15A)-C(11)-C(12)-O(3)	-3.90(19)
C(10)-C(11)-C(12)-C(13)	-3.68(19)
C(15A)-C(11)-C(12)-C(13)	178.92(12)
O(3)-C(12)-C(13)-C(14)	-172.71(12)
C(11)-C(12)-C(13)-C(14)	4.59(19)
O(3)-C(12)-C(13)-C(15B)	3.48(18)
C(11)-C(12)-C(13)-C(15B)	-179.22(12)
C(12)-C(13)-C(14)-C(9)	-1.12(19)
C(15B)-C(13)-C(14)-C(9)	-177.34(12)
C(10)-C(9)-C(14)-C(13)	-3.09(19)
C(8)-C(9)-C(14)-C(13)	175.16(12)
C(10)-C(11)-C(15A)-C(16A)	-39.38(17)
C(12)-C(11)-C(15A)-C(16A)	137.98(13)
C(10)-C(11)-C(15A)-C(20A)	139.40(13)
C(12)-C(11)-C(15A)-C(20A)	-43.23(18)

C(14)-C(13)-C(15B)-C(20B)	46.15(18)
C(12)-C(13)-C(15B)-C(20B)	-129.97(13)
C(14)-C(13)-C(15B)-C(16B)	-133.90(14)
C(12)-C(13)-C(15B)-C(16B)	49.98(18)
C(20A)-C(15A)-C(16A)-C(17A)	0.8(2)
C(11)-C(15A)-C(16A)-C(17A)	179.65(12)
C(20B)-C(15B)-C(16B)-C(17B)	1.7(2)
C(13)-C(15B)-C(16B)-C(17B)	-178.29(13)
C(15A)-C(16A)-C(17A)-C(18A)	0.9(2)
C(15B)-C(16B)-C(17B)-C(18B)	0.4(2)
C(16A)-C(17A)-C(18A)-C(19A)	-1.8(2)
C(16B)-C(17B)-C(18B)-C(19B)	-2.0(2)
C(17A)-C(18A)-C(19A)-C(20A)	1.1(2)
C(17B)-C(18B)-C(19B)-C(20B)	1.4(2)
C(18A)-C(19A)-C(20A)-C(15A)	0.6(2)
C(16A)-C(15A)-C(20A)-C(19A)	-1.5(2)
C(11)-C(15A)-C(20A)-C(19A)	179.64(13)
C(18B)-C(19B)-C(20B)-C(15B)	0.7(2)
C(16B)-C(15B)-C(20B)-C(19B)	-2.2(2)
C(13)-C(15B)-C(20B)-C(19B)	177.71(12)
C(3)-C(4)-N(1)-O(1)	-178.53(15)
C(5)-C(4)-N(1)-O(1)	2.3(2)
C(3)-C(4)-N(1)-O(2)	1.5(2)
C(5)-C(4)-N(1)-O(2)	-177.68(14)

Table S7. Bond lengths (Å) and angles (°) for compound **2c**.

O(3)-C(12)	1.3725(14)
O(3)-H(100)	0.9721
N(8)-C(7)	1.2734(17)
N(8)-C(9)	1.4209(15)
O(1W)-H(1W)	0.9370
O(1W)-H(2W)	0.7804
O(1)-N(1)	1.2224(17)
O(2)-N(1)	1.2164(16)
N(1)-C(4)	1.4667(16)
C(9)-C(14)	1.3880(17)
C(9)-C(10)	1.3933(17)
C(12)-C(13)	1.3966(18)
C(12)-C(11)	1.4023(18)
C(13)-C(14)	1.3881(17)
C(13)-C(16)	1.5030(18)
C(14)-H(14)	0.9500
C(10)-C(11)	1.3888(17)
C(10)-H(10)	0.9500
C(11)-C(15)	1.5019(17)
C(1)-C(6)	1.3945(18)
C(1)-C(2)	1.3965(18)
C(1)-C(7)	1.4699(17)
C(7)-H(7)	0.9500
C(2)-C(3)	1.3772(18)
C(2)-H(2)	0.9500
C(4)-C(5)	1.3768(19)
C(4)-C(3)	1.3868(18)
C(5)-C(6)	1.3830(18)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(3)-H(3)	0.9500
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800

C(15)-H(15C)	0.9800

C(12)-O(3)-H(100)	115.1
C(7)-N(8)-C(9)	120.85(10)
H(1W)-O(1W)-H(2W)	106.5
O(2)-N(1)-O(1)	123.20(12)
O(2)-N(1)-C(4)	118.71(12)
O(1)-N(1)-C(4)	118.09(12)
C(14)-C(9)-C(10)	118.92(11)
C(14)-C(9)-N(8)	116.04(11)
C(10)-C(9)-N(8)	125.03(11)
O(3)-C(12)-C(13)	118.36(11)
O(3)-C(12)-C(11)	120.25(11)
C(13)-C(12)-C(11)	121.37(11)
C(14)-C(13)-C(12)	117.94(11)
C(14)-C(13)-C(16)	120.72(11)
C(12)-C(13)-C(16)	121.34(11)
C(9)-C(14)-C(13)	122.03(11)
C(9)-C(14)-H(14)	119.0
C(13)-C(14)-H(14)	119.0
C(11)-C(10)-C(9)	120.89(11)
C(11)-C(10)-H(10)	119.6
C(9)-C(10)-H(10)	119.6
C(10)-C(11)-C(12)	118.79(11)
C(10)-C(11)-C(15)	120.77(11)
C(12)-C(11)-C(15)	120.44(11)
C(6)-C(1)-C(2)	119.57(11)
C(6)-C(1)-C(7)	119.29(11)
C(2)-C(1)-C(7)	121.13(11)
N(8)-C(7)-C(1)	121.30(11)
N(8)-C(7)-H(7)	119.3
C(1)-C(7)-H(7)	119.3
C(3)-C(2)-C(1)	120.47(12)
C(3)-C(2)-H(2)	119.8
C(1)-C(2)-H(2)	119.8
C(5)-C(4)-C(3)	122.60(12)
C(5)-C(4)-N(1)	118.65(12)
C(3)-C(4)-N(1)	118.75(12)

C(4)-C(5)-C(6)	118.44(12)
C(4)-C(5)-H(5)	120.8
C(6)-C(5)-H(5)	120.8
C(5)-C(6)-C(1)	120.46(12)
C(5)-C(6)-H(6)	119.8
C(1)-C(6)-H(6)	119.8
C(2)-C(3)-C(4)	118.44(12)
C(2)-C(3)-H(3)	120.8
C(4)-C(3)-H(3)	120.8
C(13)-C(16)-H(16A)	109.5
C(13)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(13)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(11)-C(15)-H(15A)	109.5
C(11)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(11)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5

Table S8. Torsion angles (°) for compound **2c**.

C(7)-N(8)-C(9)-C(14)	-155.34(11)
C(7)-N(8)-C(9)-C(10)	25.41(18)
O(3)-C(12)-C(13)-C(14)	178.77(10)
C(11)-C(12)-C(13)-C(14)	-2.80(18)
O(3)-C(12)-C(13)-C(16)	-1.65(18)
C(11)-C(12)-C(13)-C(16)	176.78(11)
C(10)-C(9)-C(14)-C(13)	-0.35(18)
N(8)-C(9)-C(14)-C(13)	-179.65(11)
C(12)-C(13)-C(14)-C(9)	2.24(18)
C(16)-C(13)-C(14)-C(9)	-177.34(12)
C(14)-C(9)-C(10)-C(11)	-1.07(18)
N(8)-C(9)-C(10)-C(11)	178.16(11)
C(9)-C(10)-C(11)-C(12)	0.51(18)
C(9)-C(10)-C(11)-C(15)	-179.68(11)
O(3)-C(12)-C(11)-C(10)	179.87(10)
C(13)-C(12)-C(11)-C(10)	1.47(18)
O(3)-C(12)-C(11)-C(15)	0.06(18)
C(13)-C(12)-C(11)-C(15)	-178.34(11)
C(9)-N(8)-C(7)-C(1)	178.97(10)
C(6)-C(1)-C(7)-N(8)	160.04(12)
C(2)-C(1)-C(7)-N(8)	-21.27(18)
C(6)-C(1)-C(2)-C(3)	-0.95(19)
C(7)-C(1)-C(2)-C(3)	-179.64(11)
O(2)-N(1)-C(4)-C(5)	-2.22(19)
O(1)-N(1)-C(4)-C(5)	178.19(13)
O(2)-N(1)-C(4)-C(3)	177.85(13)
O(1)-N(1)-C(4)-C(3)	-1.73(19)
C(3)-C(4)-C(5)-C(6)	0.58(19)
N(1)-C(4)-C(5)-C(6)	-179.34(11)
C(4)-C(5)-C(6)-C(1)	-1.26(19)
C(2)-C(1)-C(6)-C(5)	1.45(19)
C(7)-C(1)-C(6)-C(5)	-179.83(11)
C(1)-C(2)-C(3)-C(4)	0.28(19)
C(5)-C(4)-C(3)-C(2)	-0.1(2)
N(1)-C(4)-C(3)-C(2)	179.83(11)

Table S9. Hydrogen bonds for compound **2c** (Å and °).

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(3)-H(100)...O(1W)#1	0.97	1.89	2.7739(15)	150
O(1W)-H(1W)...N(8)#2	0.94	2.00	2.9361(15)	173
O(1W)-H(2W)...O(3)#3	0.78	2.12	2.8967(15)	174

Symmetry transformations used to generate equivalent atoms:

#1 x-1, y, z #2 x+1/2, -y+1/2, z+1/2 #3 -x+1, -y,- z+1

Table S10. Bond lengths (Å) and angles (°) for compound **2d**.

C(1)-C(2)	1.397(3)
C(1)-C(6)	1.401(3)
C(1)-C(7)	1.477(3)
C(2)-C(3)	1.384(3)
C(2)-H(3)	0.9500
C(3)-C(4)	1.389(3)
C(3)-H(4)	0.9500
C(4)-C(5)	1.381(3)
C(4)-N(1)	1.477(3)
C(5)-C(6)	1.388(3)
C(5)-H(5)	0.9500
C(6)-H(2)	0.9500
C(7)-N(8)	1.272(3)
C(7)-H(6)	0.9500
C(9)-C(14)	1.396(3)
C(9)-C(10)	1.398(3)
C(9)-N(8)	1.421(3)
C(10)-C(11)	1.379(3)
C(10)-H(1)	0.9500
C(11)-C(12)	1.397(3)
C(11)-Br(1)	1.899(2)
C(12)-O(3)	1.354(2)
C(12)-C(13)	1.396(3)
C(13)-C(14)	1.383(3)
C(13)-Br(2)	1.895(2)
C(14)-H(8)	0.9500
C(21)-C(26)	1.393(3)
C(21)-C(22)	1.395(3)
C(21)-C(27)	1.468(3)
C(22)-C(23)	1.385(3)
C(22)-H(9)	0.9500
C(23)-C(24)	1.378(3)
C(23)-H(16)	0.9500
C(24)-C(25)	1.387(3)
C(24)-N(21)	1.464(3)
C(25)-C(26)	1.377(3)

C(25)-H(10)	0.9500
C(26)-H(11)	0.9500
C(27)-N(28)	1.268(3)
C(27)-H(15)	0.9500
C(29)-C(34)	1.394(3)
C(29)-C(30)	1.395(3)
C(29)-N(28)	1.417(3)
C(30)-C(31)	1.387(3)
C(30)-H(14)	0.9500
C(31)-C(32)	1.390(3)
C(31)-Br(22)	1.893(2)
C(32)-O(23)	1.349(3)
C(32)-C(33)	1.396(3)
C(33)-C(34)	1.379(3)
C(33)-Br(21)	1.894(2)
C(34)-H(34)	0.9500
N(1)-O(1)	1.218(3)
N(1)-O(2)	1.229(3)
N(21)-O(22)	1.219(3)
N(21)-O(21)	1.222(3)
O(3)-H(3O)	0.6916
O(23)-H(23O)	0.7723

C(2)-C(1)-C(6)	119.4(2)
C(2)-C(1)-C(7)	121.3(2)
C(6)-C(1)-C(7)	119.3(2)
C(3)-C(2)-C(1)	120.7(2)
C(3)-C(2)-H(3)	119.6
C(1)-C(2)-H(3)	119.6
C(2)-C(3)-C(4)	118.4(2)
C(2)-C(3)-H(4)	120.8
C(4)-C(3)-H(4)	120.8
C(5)-C(4)-C(3)	122.5(2)
C(5)-C(4)-N(1)	118.8(2)
C(3)-C(4)-N(1)	118.6(2)
C(4)-C(5)-C(6)	118.5(2)
C(4)-C(5)-H(5)	120.7
C(6)-C(5)-H(5)	120.7

C(5)-C(6)-C(1)	120.4(2)
C(5)-C(6)-H(2)	119.8
C(1)-C(6)-H(2)	119.8
N(8)-C(7)-C(1)	122.4(2)
N(8)-C(7)-H(6)	118.8
C(1)-C(7)-H(6)	118.8
C(14)-C(9)-C(10)	118.38(19)
C(14)-C(9)-N(8)	117.19(19)
C(10)-C(9)-N(8)	124.40(19)
C(11)-C(10)-C(9)	119.9(2)
C(11)-C(10)-H(1)	120.1
C(9)-C(10)-H(1)	120.1
C(10)-C(11)-C(12)	122.9(2)
C(10)-C(11)-Br(1)	119.85(16)
C(12)-C(11)-Br(1)	117.21(16)
O(3)-C(12)-C(13)	118.99(19)
O(3)-C(12)-C(11)	124.82(19)
C(13)-C(12)-C(11)	116.18(19)
C(14)-C(13)-C(12)	122.1(2)
C(14)-C(13)-Br(2)	119.81(16)
C(12)-C(13)-Br(2)	118.10(16)
C(13)-C(14)-C(9)	120.5(2)
C(13)-C(14)-H(8)	119.7
C(9)-C(14)-H(8)	119.7
C(26)-C(21)-C(22)	119.9(2)
C(26)-C(21)-C(27)	121.3(2)
C(22)-C(21)-C(27)	118.8(2)
C(23)-C(22)-C(21)	120.5(2)
C(23)-C(22)-H(9)	119.8
C(21)-C(22)-H(9)	119.8
C(24)-C(23)-C(22)	118.0(2)
C(24)-C(23)-H(16)	121.0
C(22)-C(23)-H(16)	121.0
C(23)-C(24)-C(25)	123.0(2)
C(23)-C(24)-N(21)	118.8(2)
C(25)-C(24)-N(21)	118.2(2)
C(26)-C(25)-C(24)	118.3(2)
C(26)-C(25)-H(10)	120.8

C(24)-C(25)-H(10)	120.8
C(25)-C(26)-C(21)	120.3(2)
C(25)-C(26)-H(11)	119.9
C(21)-C(26)-H(11)	119.9
N(28)-C(27)-C(21)	122.1(2)
N(28)-C(27)-H(15)	118.9
C(21)-C(27)-H(15)	118.9
C(34)-C(29)-C(30)	118.99(19)
C(34)-C(29)-N(28)	123.41(19)
C(30)-C(29)-N(28)	117.5(2)
C(31)-C(30)-C(29)	119.8(2)
C(31)-C(30)-H(14)	120.1
C(29)-C(30)-H(14)	120.1
C(30)-C(31)-C(32)	121.97(19)
C(30)-C(31)-Br(22)	119.67(17)
C(32)-C(31)-Br(22)	118.34(16)
O(23)-C(32)-C(31)	125.70(19)
O(23)-C(32)-C(33)	117.2(2)
C(31)-C(32)-C(33)	117.05(19)
C(34)-C(33)-C(32)	122.1(2)
C(34)-C(33)-Br(21)	119.35(16)
C(32)-C(33)-Br(21)	118.49(16)
C(33)-C(34)-C(29)	119.98(19)
C(33)-C(34)-H(34)	120.0
C(29)-C(34)-H(34)	120.0
O(1)-N(1)-O(2)	123.5(2)
O(1)-N(1)-C(4)	118.4(2)
O(2)-N(1)-C(4)	118.05(19)
C(7)-N(8)-C(9)	119.68(19)
O(22)-N(21)-O(21)	122.9(2)
O(22)-N(21)-C(24)	119.3(2)
O(21)-N(21)-C(24)	117.8(2)
C(27)-N(28)-C(29)	118.6(2)
C(12)-O(3)-H(3O)	108.8
C(32)-O(23)-H(23O)	113.0

Table S11. Torsion angles (°) for compound **2d**.

C(6)-C(1)-C(2)-C(3)	-1.2(3)
C(7)-C(1)-C(2)-C(3)	179.5(2)
C(1)-C(2)-C(3)-C(4)	-0.9(3)
C(2)-C(3)-C(4)-C(5)	1.7(3)
C(2)-C(3)-C(4)-N(1)	-178.6(2)
C(3)-C(4)-C(5)-C(6)	-0.3(4)
N(1)-C(4)-C(5)-C(6)	180.0(2)
C(4)-C(5)-C(6)-C(1)	-1.8(3)
C(2)-C(1)-C(6)-C(5)	2.6(3)
C(7)-C(1)-C(6)-C(5)	-178.1(2)
C(2)-C(1)-C(7)-N(8)	-21.3(3)
C(6)-C(1)-C(7)-N(8)	159.4(2)
C(14)-C(9)-C(10)-C(11)	1.8(3)
N(8)-C(9)-C(10)-C(11)	179.6(2)
C(9)-C(10)-C(11)-C(12)	0.2(3)
C(9)-C(10)-C(11)-Br(1)	-177.79(16)
C(10)-C(11)-C(12)-O(3)	-179.4(2)
Br(1)-C(11)-C(12)-O(3)	-1.3(3)
C(10)-C(11)-C(12)-C(13)	-0.9(3)
Br(1)-C(11)-C(12)-C(13)	177.17(16)
O(3)-C(12)-C(13)-C(14)	178.1(2)
C(11)-C(12)-C(13)-C(14)	-0.5(3)
O(3)-C(12)-C(13)-Br(2)	-1.0(3)
C(11)-C(12)-C(13)-Br(2)	-179.62(16)
C(12)-C(13)-C(14)-C(9)	2.6(3)
Br(2)-C(13)-C(14)-C(9)	-178.34(16)
C(10)-C(9)-C(14)-C(13)	-3.2(3)
N(8)-C(9)-C(14)-C(13)	178.86(19)
C(26)-C(21)-C(22)-C(23)	-1.5(4)
C(27)-C(21)-C(22)-C(23)	179.6(2)
C(21)-C(22)-C(23)-C(24)	0.3(4)
C(22)-C(23)-C(24)-C(25)	1.0(4)
C(22)-C(23)-C(24)-N(21)	-177.3(2)
C(23)-C(24)-C(25)-C(26)	-1.1(4)
N(21)-C(24)-C(25)-C(26)	177.2(2)

C(24)-C(25)-C(26)-C(21)	-0.2(4)
C(22)-C(21)-C(26)-C(25)	1.4(4)
C(27)-C(21)-C(26)-C(25)	-179.7(2)
C(26)-C(21)-C(27)-N(28)	-1.9(4)
C(22)-C(21)-C(27)-N(28)	177.0(2)
C(34)-C(29)-C(30)-C(31)	-3.2(3)
N(28)-C(29)-C(30)-C(31)	-179.3(2)
C(29)-C(30)-C(31)-C(32)	1.0(3)
C(29)-C(30)-C(31)-Br(22)	179.37(17)
C(30)-C(31)-C(32)-O(23)	-179.3(2)
Br(22)-C(31)-C(32)-O(23)	2.3(3)
C(30)-C(31)-C(32)-C(33)	2.3(3)
Br(22)-C(31)-C(32)-C(33)	-176.13(16)
O(23)-C(32)-C(33)-C(34)	178.0(2)
C(31)-C(32)-C(33)-C(34)	-3.4(3)
O(23)-C(32)-C(33)-Br(21)	-5.1(3)
C(31)-C(32)-C(33)-Br(21)	173.47(16)
C(32)-C(33)-C(34)-C(29)	1.3(3)
Br(21)-C(33)-C(34)-C(29)	-175.58(16)
C(30)-C(29)-C(34)-C(33)	2.1(3)
N(28)-C(29)-C(34)-C(33)	177.9(2)
C(5)-C(4)-N(1)-O(1)	-1.5(3)
C(3)-C(4)-N(1)-O(1)	178.8(2)
C(5)-C(4)-N(1)-O(2)	178.0(2)
C(3)-C(4)-N(1)-O(2)	-1.7(3)
C(1)-C(7)-N(8)-C(9)	-178.53(19)
C(14)-C(9)-N(8)-C(7)	-156.4(2)
C(10)-C(9)-N(8)-C(7)	25.7(3)
C(23)-C(24)-N(21)-O(22)	-177.1(2)
C(25)-C(24)-N(21)-O(22)	4.6(3)
C(23)-C(24)-N(21)-O(21)	3.5(3)
C(25)-C(24)-N(21)-O(21)	-174.9(2)
C(21)-C(27)-N(28)-C(29)	-175.4(2)
C(34)-C(29)-N(28)-C(27)	24.5(3)
C(30)-C(29)-N(28)-C(27)	-159.6(2)

Table S12. Hydrogen bonds for compound **2d** (Å and °).

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(3)-H(3O)...O(2)#1	0.69	2.42	2.944(2)	134
O(3)-H(3O)...Br(1)	0.69	2.63	3.0925(16)	126
O(23)-H(23O)...O(21)#2	0.77	2.08	2.660(2)	132
O(23)-H(23O)...Br(22)	0.77	2.68	3.1287(17)	119

Symmetry transformations used to generate equivalent atoms:

#1 x, y, z-1 #2 x, y, z+1

Table S13. Bond lengths (Å) and angles (°) for compound **2e**.

C(1)-C(6)	1.3953(17)
C(1)-C(2)	1.3962(17)
C(1)-C(7)	1.4713(16)
C(2)-C(3)	1.3878(17)
C(2)-H(2)	0.9500
C(3)-C(4)	1.3794(18)
C(3)-H(3)	0.9500
C(4)-C(5)	1.3874(18)
C(4)-N(1)	1.4675(16)
C(5)-C(6)	1.3852(17)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-N(8)	1.2724(16)
C(7)-H(7)	0.9500
C(9)-C(10)	1.3909(17)
C(9)-C(14)	1.3969(16)
C(9)-N(8)	1.4179(15)
C(10)-C(11)	1.3835(16)
C(10)-H(10)	0.9500
C(11)-C(12)	1.3956(17)
C(11)-Cl(1)	1.7273(12)
C(12)-O(3)	1.3480(14)
C(12)-C(13)	1.4008(17)
C(13)-C(14)	1.3861(16)
C(13)-Cl(2)	1.7311(12)
C(14)-H(14)	0.9500
N(1)-O(2)	1.2150(18)
N(1)-O(1)	1.2230(17)
O(1W)-H(1W)	0.8671
O(1W)-H(2W)	0.9339
O(3)-H(3O)	0.8585
C(6)-C(1)-C(2)	119.89(11)
C(6)-C(1)-C(7)	120.94(11)
C(2)-C(1)-C(7)	119.14(11)
C(3)-C(2)-C(1)	120.21(11)

C(3)-C(2)-H(2)	119.9
C(1)-C(2)-H(2)	119.9
C(4)-C(3)-C(2)	118.36(11)
C(4)-C(3)-H(3)	120.8
C(2)-C(3)-H(3)	120.8
C(3)-C(4)-C(5)	122.96(11)
C(3)-C(4)-N(1)	118.42(11)
C(5)-C(4)-N(1)	118.62(12)
C(6)-C(5)-C(4)	118.05(11)
C(6)-C(5)-H(5)	121.0
C(4)-C(5)-H(5)	121.0
C(5)-C(6)-C(1)	120.50(12)
C(5)-C(6)-H(6)	119.8
C(1)-C(6)-H(6)	119.8
N(8)-C(7)-C(1)	121.01(11)
N(8)-C(7)-H(7)	119.5
C(1)-C(7)-H(7)	119.5
C(10)-C(9)-C(14)	119.49(10)
C(10)-C(9)-N(8)	115.62(10)
C(14)-C(9)-N(8)	124.89(11)
C(11)-C(10)-C(9)	120.18(11)
C(11)-C(10)-H(10)	119.9
C(9)-C(10)-H(10)	119.9
C(10)-C(11)-C(12)	122.02(11)
C(10)-C(11)-Cl(1)	118.61(10)
C(12)-C(11)-Cl(1)	119.36(9)
O(3)-C(12)-C(11)	120.55(11)
O(3)-C(12)-C(13)	122.97(11)
C(11)-C(12)-C(13)	116.46(10)
C(14)-C(13)-C(12)	122.77(11)
C(14)-C(13)-Cl(2)	118.82(9)
C(12)-C(13)-Cl(2)	118.41(9)
C(13)-C(14)-C(9)	119.05(11)
C(13)-C(14)-H(14)	120.5
C(9)-C(14)-H(14)	120.5
O(2)-N(1)-O(1)	122.99(13)
O(2)-N(1)-C(4)	118.82(12)
O(1)-N(1)-C(4)	118.18(12)

C(7)-N(8)-C(9)	120.48(10)
H(1W)-O(1W)-H(2W)	104.9
C(12)-O(3)-H(3O)	112.7

Table S14. Torsion angles (°) for compound **2e**.

C(6)-C(1)-C(2)-C(3)	1.76(18)
C(7)-C(1)-C(2)-C(3)	179.54(11)
C(1)-C(2)-C(3)-C(4)	-1.77(19)
C(2)-C(3)-C(4)-C(5)	0.55(19)
C(2)-C(3)-C(4)-N(1)	-178.96(11)
C(3)-C(4)-C(5)-C(6)	0.7(2)
N(1)-C(4)-C(5)-C(6)	-179.80(11)
C(4)-C(5)-C(6)-C(1)	-0.72(19)
C(2)-C(1)-C(6)-C(5)	-0.48(19)
C(7)-C(1)-C(6)-C(5)	-178.23(12)
C(6)-C(1)-C(7)-N(8)	-21.16(18)
C(2)-C(1)-C(7)-N(8)	161.07(12)
C(14)-C(9)-C(10)-C(11)	-0.65(18)
N(8)-C(9)-C(10)-C(11)	-179.78(11)
C(9)-C(10)-C(11)-C(12)	1.75(19)
C(9)-C(10)-C(11)-Cl(1)	-177.37(9)
C(10)-C(11)-C(12)-O(3)	179.79(11)
Cl(1)-C(11)-C(12)-O(3)	-1.09(16)
C(10)-C(11)-C(12)-C(13)	-1.72(18)
Cl(1)-C(11)-C(12)-C(13)	177.39(9)
O(3)-C(12)-C(13)-C(14)	179.13(11)
C(11)-C(12)-C(13)-C(14)	0.69(18)
O(3)-C(12)-C(13)-Cl(2)	-1.05(16)
C(11)-C(12)-C(13)-Cl(2)	-179.49(9)
C(12)-C(13)-C(14)-C(9)	0.33(18)
Cl(2)-C(13)-C(14)-C(9)	-179.50(9)
C(10)-C(9)-C(14)-C(13)	-0.36(17)
N(8)-C(9)-C(14)-C(13)	178.69(11)
C(3)-C(4)-N(1)-O(2)	-6.6(2)
C(5)-C(4)-N(1)-O(2)	173.83(14)
C(3)-C(4)-N(1)-O(1)	173.78(13)
C(5)-C(4)-N(1)-O(1)	-5.74(19)
C(1)-C(7)-N(8)-C(9)	177.62(11)
C(10)-C(9)-N(8)-C(7)	-154.68(12)
C(14)-C(9)-N(8)-C(7)	26.24(18)

Table S15. Hydrogen bonds for compound **2e** (Å and °).

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1W)-H(1W)...O(3)#1	0.87	2.09	2.9412(17)	166
O(1W)-H(1W)...Cl(1)#1	0.87	2.96	3.4388(15)	117
O(1W)-H(2W)...N(8)#2	0.93	2.01	2.9160(16)	162
O(3)-H(3O)...O(1W)#3	0.86	1.95	2.7246(16)	150
O(3)-H(3O)...Cl(2)	0.86	2.56	2.9839(10)	111

Symmetry transformations used to generate equivalent atoms:

#1 -x+1, -y, -z+1 #2 x+1/2, -y+1/2, z+1/2 #3 x-1, y, z

Table S16. Bond lengths (Å) and angles (°) for compound **2h**.

C(1)-C(6)	1.401(2)
C(1)-C(2)	1.402(2)
C(1)-C(7)	1.473(2)
C(6)-C(5)	1.377(2)
C(6)-H(6)	0.9500
C(5)-C(4)	1.385(2)
C(5)-H(5)	0.9500
C(4)-C(3)	1.374(2)
C(4)-N(2)	1.469(2)
C(3)-C(2)	1.379(2)
C(3)-H(3)	0.9500
C(2)-N(1)	1.470(2)
C(7)-N(8)	1.2730(19)
C(7)-H(7)	0.9500
C(9)-C(10)	1.393(2)
C(9)-C(14)	1.400(2)
C(9)-N(8)	1.4181(19)
C(10)-C(11)	1.389(2)
C(10)-H(10)	0.9500
C(11)-C(12)	1.399(2)
C(11)-C(15)	1.507(2)
C(12)-O(5)	1.3663(18)
C(12)-C(13)	1.403(2)
C(13)-C(14)	1.380(2)
C(13)-C(16)	1.509(2)
C(14)-H(14)	0.9500
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-H(16A)	0.9800

C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
N(1)-O(1)	1.2092(19)
N(1)-O(2)	1.2221(19)
N(2)-O(4)	1.2218(18)
N(2)-O(3)	1.2257(18)
O(5)-H(5O)	0.8067

C(6)-C(1)-C(2)	115.74(14)
C(6)-C(1)-C(7)	119.91(13)
C(2)-C(1)-C(7)	124.29(14)
C(5)-C(6)-C(1)	122.39(14)
C(5)-C(6)-H(6)	118.8
C(1)-C(6)-H(6)	118.8
C(6)-C(5)-C(4)	118.60(15)
C(6)-C(5)-H(5)	120.7
C(4)-C(5)-H(5)	120.7
C(3)-C(4)-C(5)	122.01(14)
C(3)-C(4)-N(2)	118.13(14)
C(5)-C(4)-N(2)	119.86(14)
C(4)-C(3)-C(2)	117.71(14)
C(4)-C(3)-H(3)	121.1
C(2)-C(3)-H(3)	121.1
C(3)-C(2)-C(1)	123.47(14)
C(3)-C(2)-N(1)	114.98(13)
C(1)-C(2)-N(1)	121.51(13)
N(8)-C(7)-C(1)	119.91(14)
N(8)-C(7)-H(7)	120.0
C(1)-C(7)-H(7)	120.0
C(10)-C(9)-C(14)	118.60(14)
C(10)-C(9)-N(8)	116.28(14)
C(14)-C(9)-N(8)	125.11(14)
C(11)-C(10)-C(9)	121.73(15)

C(11)-C(10)-H(10)	119.1
C(9)-C(10)-H(10)	119.1
C(10)-C(11)-C(12)	117.90(14)
C(10)-C(11)-C(15)	121.71(14)
C(12)-C(11)-C(15)	120.39(14)
O(5)-C(12)-C(11)	122.19(14)
O(5)-C(12)-C(13)	115.85(14)
C(11)-C(12)-C(13)	121.95(14)
C(14)-C(13)-C(12)	118.17(14)
C(14)-C(13)-C(16)	121.37(14)
C(12)-C(13)-C(16)	120.47(14)
C(13)-C(14)-C(9)	121.65(14)
C(13)-C(14)-H(14)	119.2
C(9)-C(14)-H(14)	119.2
C(11)-C(15)-H(15A)	109.5
C(11)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(11)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(13)-C(16)-H(16A)	109.5
C(13)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(13)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
O(1)-N(1)-O(2)	123.49(16)
O(1)-N(1)-C(2)	117.27(15)
O(2)-N(1)-C(2)	119.22(14)
O(4)-N(2)-O(3)	124.16(14)
O(4)-N(2)-C(4)	118.30(14)
O(3)-N(2)-C(4)	117.53(14)
C(7)-N(8)-C(9)	120.87(14)

C(12)-O(5)-H(5O)	107.6

Table S17. Torsion angles (°) for compound **2h**.

C(2)-C(1)-C(6)-C(5)	1.7(2)
C(7)-C(1)-C(6)-C(5)	178.95(15)
C(1)-C(6)-C(5)-C(4)	-2.1(2)
C(6)-C(5)-C(4)-C(3)	0.0(2)
C(6)-C(5)-C(4)-N(2)	179.84(14)
C(5)-C(4)-C(3)-C(2)	2.3(2)
N(2)-C(4)-C(3)-C(2)	-177.58(14)
C(4)-C(3)-C(2)-C(1)	-2.7(2)
C(4)-C(3)-C(2)-N(1)	175.31(14)
C(6)-C(1)-C(2)-C(3)	0.7(2)
C(7)-C(1)-C(2)-C(3)	-176.39(15)
C(6)-C(1)-C(2)-N(1)	-177.13(15)
C(7)-C(1)-C(2)-N(1)	5.8(2)
C(6)-C(1)-C(7)-N(8)	11.1(2)
C(2)-C(1)-C(7)-N(8)	-171.90(15)
C(14)-C(9)-C(10)-C(11)	0.4(2)
N(8)-C(9)-C(10)-C(11)	179.12(14)
C(9)-C(10)-C(11)-C(12)	0.6(2)
C(9)-C(10)-C(11)-C(15)	-178.47(15)
C(10)-C(11)-C(12)-O(5)	179.79(14)
C(15)-C(11)-C(12)-O(5)	-1.1(2)
C(10)-C(11)-C(12)-C(13)	-1.2(2)
C(15)-C(11)-C(12)-C(13)	177.92(15)
O(5)-C(12)-C(13)-C(14)	179.79(14)
C(11)-C(12)-C(13)-C(14)	0.7(2)
O(5)-C(12)-C(13)-C(16)	0.2(2)
C(11)-C(12)-C(13)-C(16)	-178.95(16)
C(12)-C(13)-C(14)-C(9)	0.4(2)
C(16)-C(13)-C(14)-C(9)	-179.99(16)
C(10)-C(9)-C(14)-C(13)	-0.9(2)

N(8)-C(9)-C(14)-C(13)	-179.49(15)
C(3)-C(2)-N(1)-O(1)	34.3(2)
C(1)-C(2)-N(1)-O(1)	-147.70(18)
C(3)-C(2)-N(1)-O(2)	-143.82(16)
C(1)-C(2)-N(1)-O(2)	34.2(2)
C(3)-C(4)-N(2)-O(4)	178.07(15)
C(5)-C(4)-N(2)-O(4)	-1.8(2)
C(3)-C(4)-N(2)-O(3)	-1.9(2)
C(5)-C(4)-N(2)-O(3)	178.25(15)
C(1)-C(7)-N(8)-C(9)	-179.94(13)
C(10)-C(9)-N(8)-C(7)	177.03(15)
C(14)-C(9)-N(8)-C(7)	-4.4(2)

Table S18. Hydrogen bonds for compound **2h** (Å and °).

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(5)-H(5O)...O(3)#1	0.81	2.17	2.8353(16)	139.7

Symmetry transformations used to generate equivalent atoms:

#1 x, y, z+1