Electronic Supplementary Information for Dalton Transactions

The assembly of rotaxane-like ternary dye/cyclodextrin/surface complexes on aluminium trihydroxide or goethite

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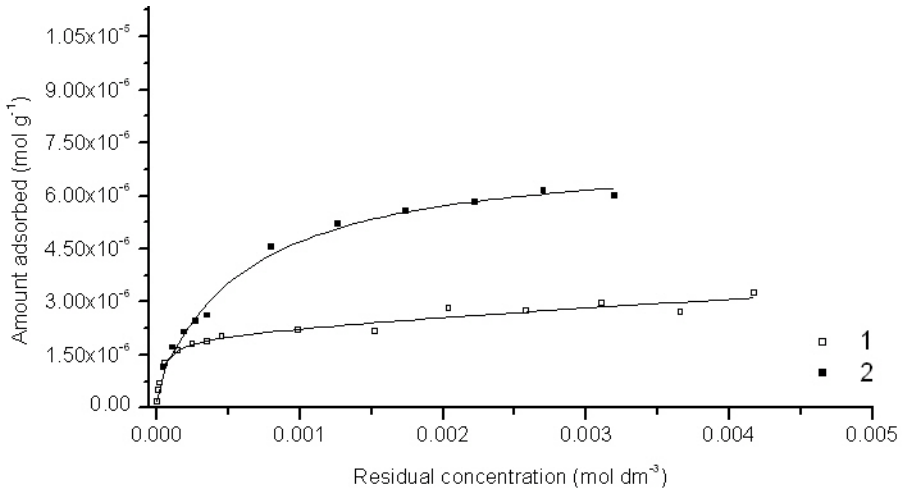
Contents

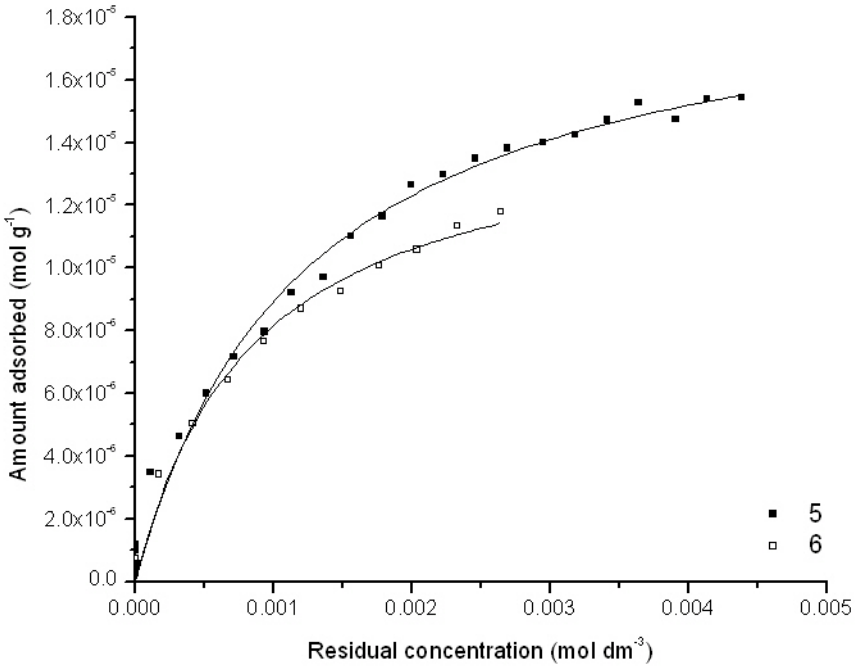
Data for isotherms of compounds **1** and **2** on ATH



Compound **1**		Compound **2**	
Residual concentration (mol dm^{-3})	**Amount adsorbed (mol g^{-1})**	**Residual concentration (mol dm^{-3})**	**Amount adsorbed (mol g^{-1})**
4.10E-06	1.63E-07	4.57E-05	1.16E-06
1.27E-05	4.85E-07	1.15E-04	1.72E-06
2.55E-05	6.98E-07	1.90E-04	2.14E-06
5.67E-05	1.25E-06	2.70E-04	2.45E-06
1.50E-04	1.63E-06	3.57E-04	2.62E-06
2.51E-04	1.80E-06	7.99E-04	4.57E-06
3.54E-04	1.88E-06	1.27E-03	5.20E-06
4.56E-04	2.02E-06	1.74E-03	5.55E-06
9.87E-04	2.19E-06	2.22E-03	5.82E-06
1.53E-03	2.17E-06	2.70E-03	6.15E-06
2.04E-03	2.80E-06	3.20E-03	5.99E-06

2.58E-03	2.74E-06	-	-
3.11E-03	2.97E-06	-	-
3.66E-03	2.70E-06	-	-
4.17E-03	3.24E-06	-	-

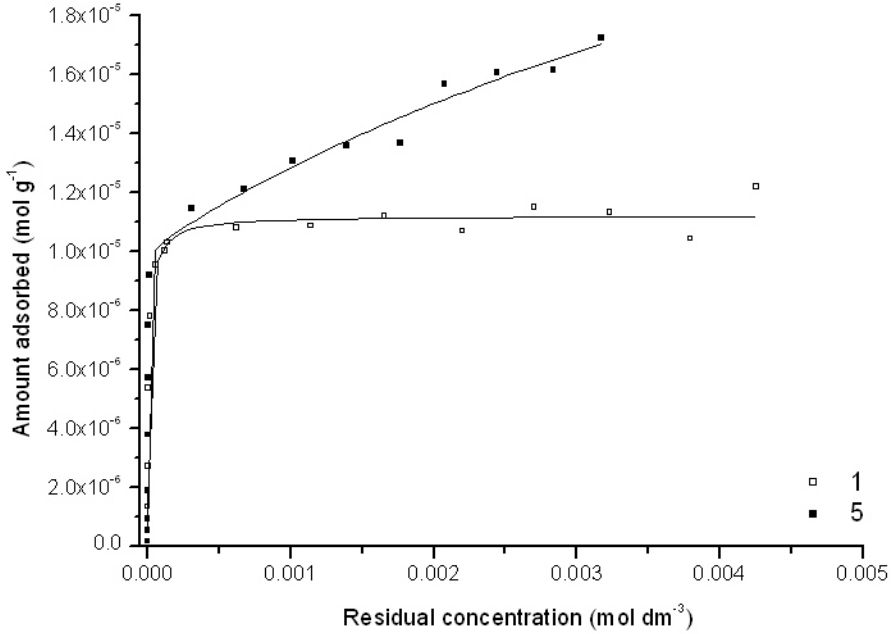
Data for Figure 3 – isotherms of **5** and **6** on ATH

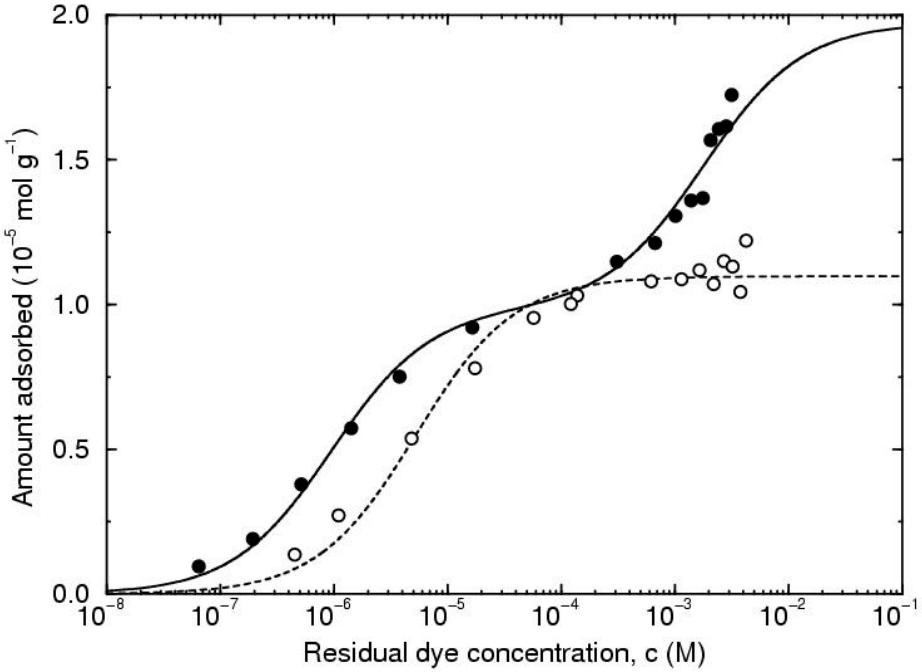


Compound **5**		Compound **6**	
Residual concentration (mol dm^{-3})	**Amount adsorbed (mol g^{-1})**	**Residual concentration (mol dm^{-3})**	**Amount adsorbed (mol g^{-1})**
2.43E-06	4.37E-07	7.67E-07	2.48E-07
8.16E-06	5.50E-07	1.25E-06	5.04E-07
8.55E-07	9.76E-07	2.10E-06	7.50E-07
2.10E-06	1.20E-06	3.78E-06	9.75E-07
1.10E-04	3.49E-06	6.23E-06	1.18E-06
3.16E-04	4.62E-06	1.72E-04	3.42E-06
5.11E-04	5.99E-06	4.17E-04	5.03E-06

7.12E-04	7.17E-06	6.70E-04	6.43E-06
9.33E-04	7.97E-06	9.30E-04	7.65E-06
1.13E-03	9.21E-06	1.20E-03	8.71E-06
1.36E-03	9.71E-06	1.48E-03	9.24E-06
1.56E-03	1.10E-05	1.76E-03	1.01E-05
1.79E-03	1.16E-05	2.04E-03	1.06E-05
1.99E-03	1.27E-05	2.33E-03	1.13E-05
2.23E-03	1.30E-05	2.64E-03	1.18E-05
2.46E-03	1.35E-05		
2.69E-03	1.38E-05		
2.95E-03	1.40E-05		
3.18E-03	1.43E-05		
3.41E-03	1.47E-05		
3.64E-03	1.53E-05		
3.91E-03	1.47E-05		
4.13E-03	1.54E-05		
4.38E-03	1.54E-05		

Data for Figure 4 – isotherms of **1** and **5** on goethite (plotted on a log scale)

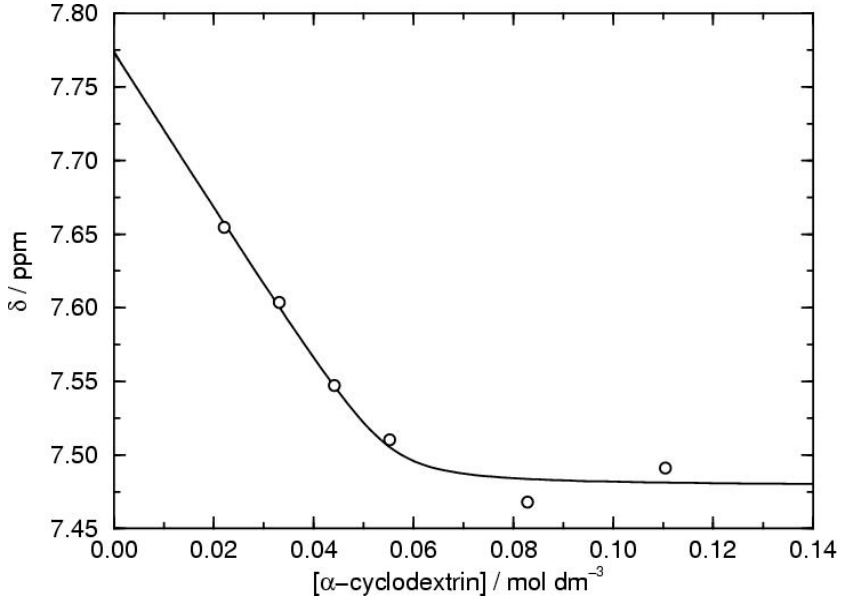




Compound **1**			Compound **5**		
Residual concentration (mol dm^{-3})	**Log Residual concentration**	**Amount adsorbed (mol g^{-1})**	**Residual concentration (mol dm^{-3})**	**Log Residual concentration**	**Amount adsorbed (mol g^{-1})**
4.52E-07	-6.345	1.36E-06	6.45E-08	-7.190	1.90E-07
1.10E-06	-5.960	2.72E-06	6.45E-08	-7.190	9.50E-07
4.84E-06	-5.315	5.37E-06	1.94E-07	-6.713	1.90E-06
1.75E-05	-4.758	7.80E-06	5.16E-07	-6.287	3.79E-06
5.73E-05	-4.242	9.53E-06	1.42E-06	-5.848	5.72E-06
1.39E-04	-3.858	1.03E-05	3.77E-06	-5.423	7.51E-06

1.222E-04	-3.913	1.00E-05	1.65E-05	-4.781	9.20E-06
6.197E-04	-3.208	1.08E-05	3.10E-04	-3.509	1.15E-05
1.144E-03	-2.942	1.09E-05	6.73E-04	-3.172	1.21E-05
1.656E-03	-2.781	1.12E-05	1.02E-03	-2.992	1.31E-05
2.201E-03	-2.657	1.07E-05	1.39E-03	-2.856	1.36E-05
2.702E-03	-2.568	1.15E-05	1.77E-03	-2.752	1.37E-05
3.231E-03	-2.491	1.13E-05	2.07E-03	-2.683	1.57E-05
3.794E-03	-2.421	1.04E-05	2.44E-03	-2.612	1.61E-05
4.252E-03	-2.371	1.22E-05	2.84E-03	-2.547	1.62E-05
-	-	-	3.17E-03	-2.498	1.72E-05

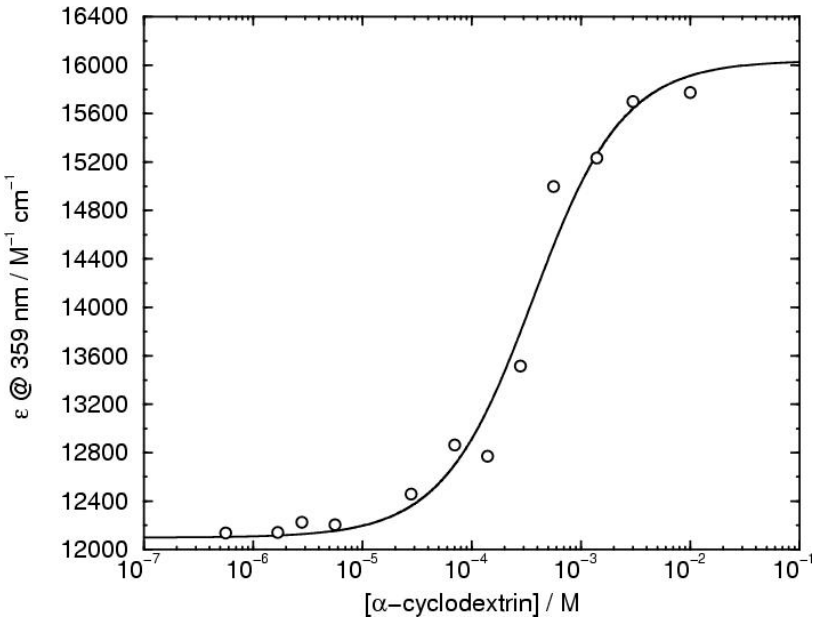
Data for Figure 5 – NMR data for formation of **5**: α-CD complex



Dye **5** concentration fixed at 0.05 mol dm^{-3}

α-CD concentration (mol dm^{-3})	**Variation of the chemical shift of 5 δ (ppm)**
0.4	7.6546
0.6	7.6037
0.8	7.5471
1	7.5103
1.5	7.4680
2	7.4911

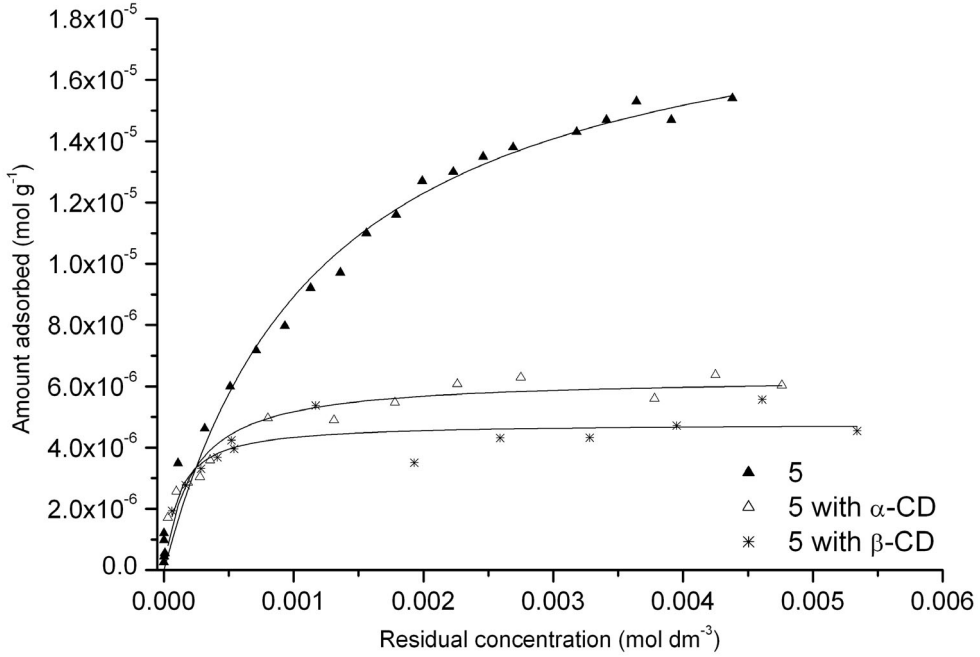
Data for Figure 6 – UV/Vis data for formation of **5**: α-CD complex



Dye **5** concentration fixed at 7 x 10^{-5} M

α-CD concentration (M)	**Change in extinction coefficient (ε) of 5 at 359 nm**
5.60E-07	12138
1.68E-06	12142
2.80E-06	12225
5.60E-06	12206
2.80E-05	12458
7.00E-05	12863
1.40E-04	12770
2.80E-04	13516
5.60E-04	14998
1.40E-03	15234
3.00E-03	15700
1.00E-02	15775

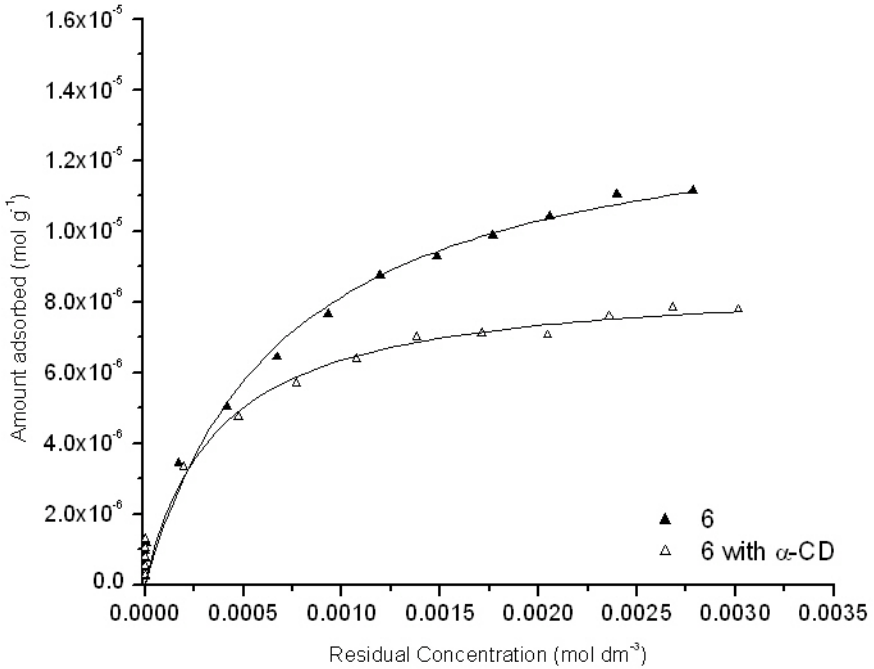
Data for Figure 8 – isotherms of compound **5** with α- and β-CD on ATH



Compound **5**		Compound **5** and α-CD		Compound **5** and β-CD	
Residual concentration (mol dm^{-3})	**Amount adsorbed (mol g^{-1})**	**Residual concentration (mol dm^{-3})**	**Amount adsorbed (mol g^{-1})**	**Residual concentration (mol dm^{-3})**	**Amount adsorbed (mol g^{-1})**
2.43E-06	4.37E-07	5.21E-04	4.24E-06	8.02E-04	4.96E-06
8.16E-06	5.50E-07	1.17E-03	5.37E-06	1.31E-03	4.89E-06
8.55E-07	9.76E-07	1.93E-03	3.51E-06	1.78E-03	5.47E-06

2.10E-06	1.20E-06	2.59E-03	4.32E-06	2.26E-03	6.07E-06
1.10E-04	3.49E-06	3.28E-03	4.32E-06	2.75E-03	6.29E-06
3.16E-04	4.62E-06	3.95E-03	4.72E-06	3.78E-03	5.59E-06
5.11E-04	5.99E-06	4.61E-03	5.57E-06	4.25E-03	6.37E-06
7.12E-04	7.17E-06	5.34E-03	4.54E-06	4.76E-03	6.03E-06
9.33E-04	7.97E-06	6.16E-05	1.94E-06	3.16E-05	1.71E-06
1.13E-03	9.21E-06	1.69E-04	2.78E-06	9.72E-05	2.56E-06
1.36E-03	9.71E-06	2.87E-04	3.31E-06	1.86E-04	2.85E-06
1.56E-03	1.10E-05	4.12E-04	3.68E-06	2.79E-04	3.04E-06
1.79E-03	1.16E-05	5.41E-04	3.95E-06	3.57E-04	3.59E-06
1.99E-03	1.27E-05				
2.23E-03	1.30E-05				
2.46E-03	1.35E-05				
2.69E-03	1.38E-05				
2.95E-03	1.40E-05				
3.18E-03	1.43E-05				
3.41E-03	1.47E-05				
3.64E-03	1.53E-05				
3.91E-03	1.47E-05				
4.13E-03	1.54E-05				
4.38E-03	1.54E-05				

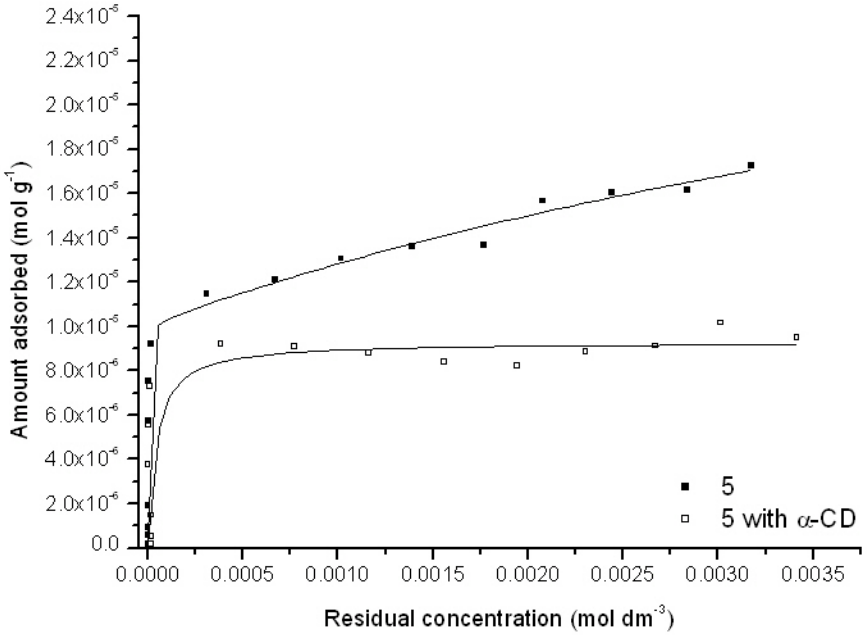
Data for Figure 10 – isotherm of compound **6** with α-CD on ATH



Compound **6**		Compound **6** and α-CD	
Residual concentration (mol dm^{-3})	**Amount adsorbed (mol g^{-1})**	**Residual concentration (mol dm^{-3})**	**Amount adsorbed (mol g^{-1})**
7.67E-07	2.48E-07	3.99E-07	2.58E-07
1.25E-06	5.04E-07	6.05E-07	5.20E-07
2.10E-06	7.50E-07	8.18E-07	7.82E-07
3.78E-06	9.75E-07	1.26E-06	1.04E-06
6.23E-06	1.18E-06	2.26E-06	1.28E-06
1.72E-04	3.42E-06	2.00E-04	3.32E-06
4.17E-04	5.03E-06	4.75E-04	4.76E-06

6.70E-04	6.43E-06	7.71E-04	5.69E-06
9.30E-04	7.65E-06	1.08E-03	6.37E-06
1.20E-03	8.71E-06	1.38E-03	7.02E-06
1.48E-03	9.24E-06	1.71E-03	7.13E-06
1.76E-03	1.01E-05	2.05E-03	7.07E-06
2.04E-03	1.06E-05	2.36E-03	7.58E-06
2.33E-03	1.13E-05	2.68E-03	7.85E-06
2.64E-03	1.18E-05	3.02E-03	7.79E-06

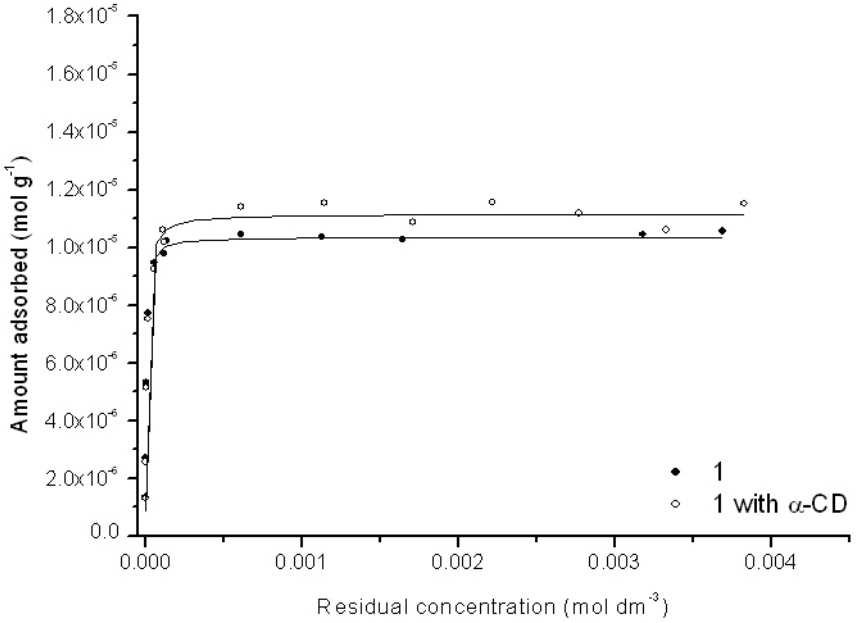
Data for Figure 11 – isotherm of compound **5** with α-CD on goethite



Compound **5**		Compound **5** and α-CD	
Residual concentration (mol dm^{-3})	**Amount adsorbed (mol g^{-1})**	**Residual concentration (mol dm^{-3})**	**Amount adsorbed (mol g^{-1})**
6.45E-08	1.90E-07	1.63E-05	1.62E-07
1.94E-07	5.73E-07	1.62E-05	5.36E-07
6.45E-08	9.50E-07	1.63E-05	1.48E-06
1.94E-07	1.90E-06	7.42E-07	3.76E-06
5.16E-07	3.79E-06	2.07E-06	5.53E-06
1.42E-06	5.72E-06	8.26E-06	7.30E-06
3.77E-06	7.51E-06	3.84E-04	9.22E-06

1.66E-05	9.20E-06	7.69E-04	9.07E-06
3.10E-04	1.15E-05	1.16E-03	8.80E-06
6.73E-04	1.21E-05	1.56E-03	8.40E-06
1.02E-03	1.31E-05	1.94E-03	8.20E-06
1.39E-03	1.36E-05	2.30E-03	8.88E-06
1.77E-03	1.37E-05	2.67E-03	9.13E-06
2.08E-03	1.57E-05	3.01E-03	1.02E-05
2.44E-03	1.61E-05	3.41E-03	9.49E-06
2.84E-03	1.62E-05		
3.17E-03	1.72E-05		

Data for Figure 12 – isotherm of compound **1** with α-CD on goethite



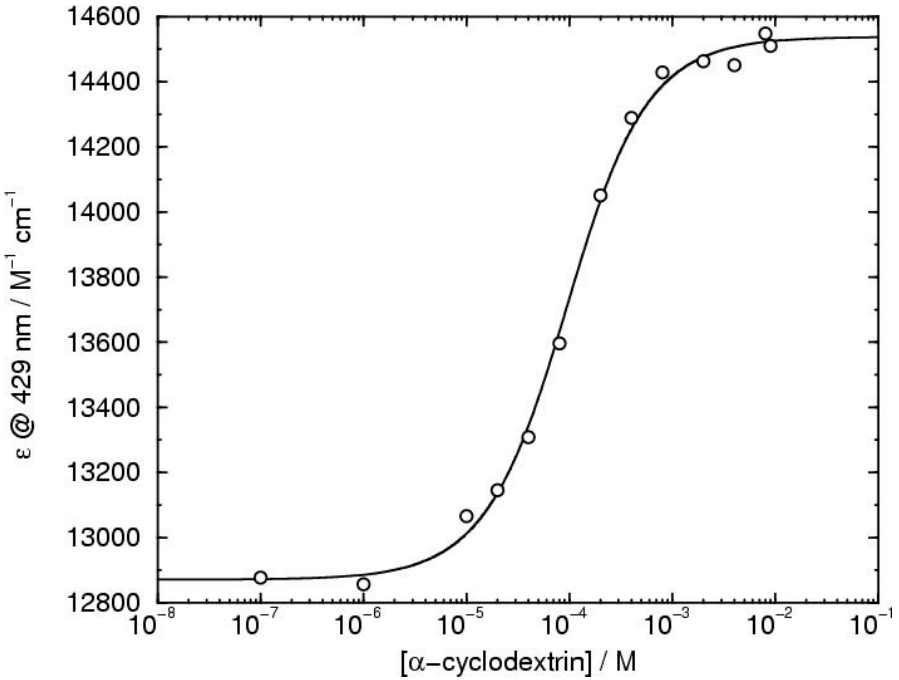
Compound **1**		Compound **1** and α-CD	
Residual concentration (mol dm^{-3})	**Amount adsorbed (mol g^{-1})**	**Residual concentration (mol dm^{-3})**	**Amount adsorbed (mol g^{-1})**
4.19E-07	1.35E-06	6.13E-07	1.29E-06
1.16E-06	2.69E-06	1.58E-06	2.57E-06
4.94E-06	5.32E-06	5.26E-06	5.13E-06
1.73E-05	7.73E-06	1.59E-05	7.52E-06
5.60E-05	9.46E-06	5.10E-05	9.25E-06
1.37E-04	1.02E-05	1.18E-04	1.02E-05

1.20E-04	9.78E-06	1.12E-04	1.06E-05
6.09E-04	1.05E-05	6.12E-04	1.14E-05
1.13E-03	1.04E-05	1.15E-03	1.15E-05
1.64E-03	1.03E-05	1.71E-03	1.09E-05
3.18E-03	1.05E-05	2.22E-03	1.16E-05
3.69E-03	1.06E-05	2.77E-03	1.12E-05
		3.33E-03	1.06E-05
		3.83E-03	1.15E-05

Data for UV/Vis for formation of **4**: α-CD complex

Dye **4** concentration = 9 x 10^{-5} M
Wavelength selected = 351 nm

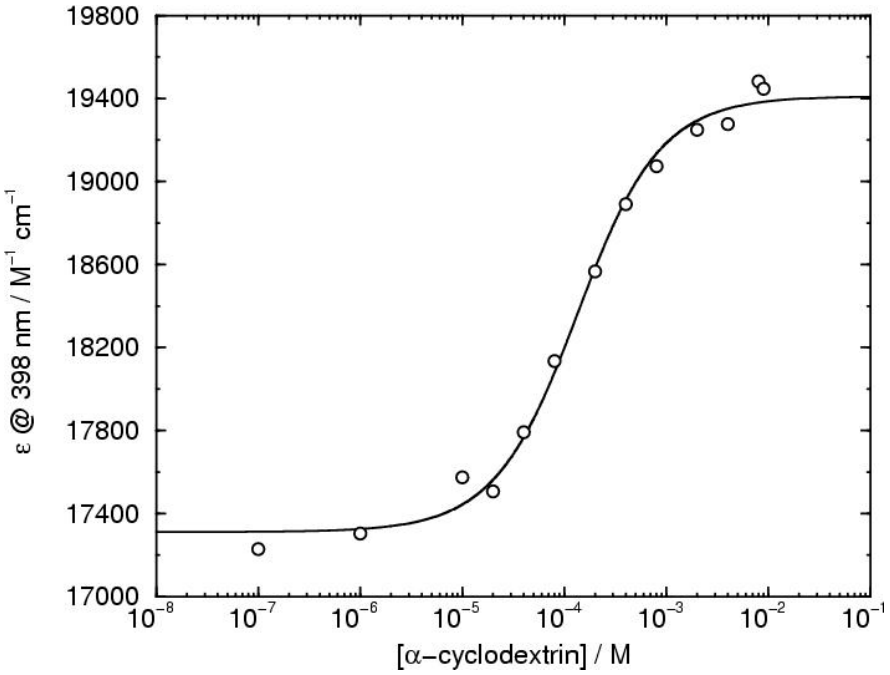
α-CD concentration (M)	Change in extinction coefficient (ε) of **4** at 359 nm
1.00E-07	14296.53
1.00E-06	14287.39
1.00E-05	14379.46
2.00E-04	15018.07
4.00E-04	15051.37
6.00E-04	15183.03
8.00E-04	15256.74
1.00E-03	15256.74
2.00E-03	15324.28
4.00E-03	15588.72
6.00E-03	15303.47
8.00E-03	15287.52
1.00E-02	15487.8



Data for UV/Vis for formation of **6**: α-CD complex

Dye **6** concentration = 3.5 x 10^{-5} M
Wavelength selected = 429 nm

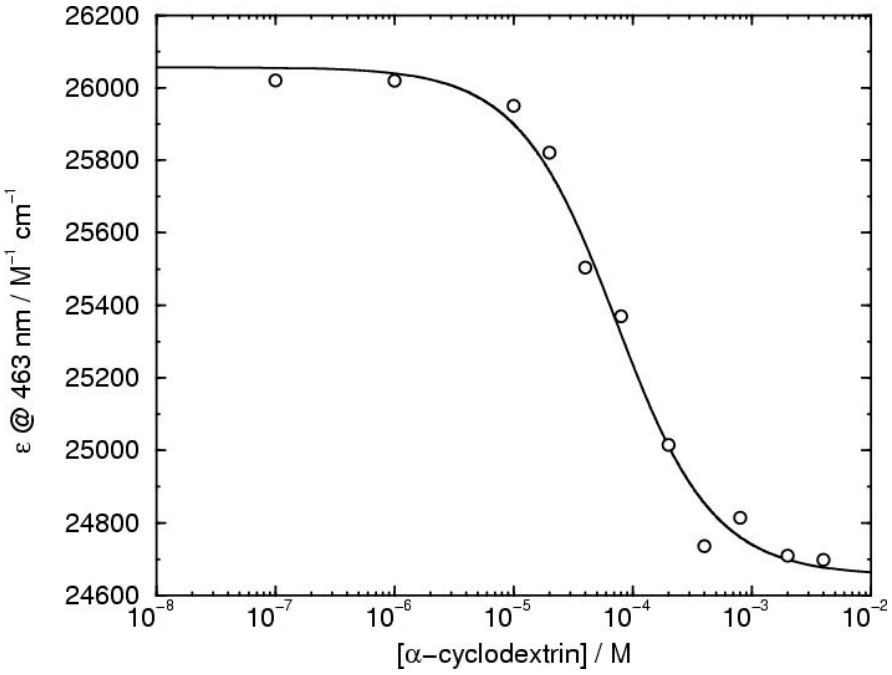
α-CD concentration (M)	Change in extinction coefficient (ε) of **6** at 429 nm
1.00E-07	12876
1.00E-06	12857
1.00E-05	13066
2.00E-05	13146
4.00E-05	13308
8.00E-05	13596
2.00E-04	14053
4.00E-04	14288
8.00E-04	14427
2.00E-03	14463
4.00E-03	14451
8.00E-03	14548
9.00E-03	14513



Data for UV/Vis for formation of **7**: α-CD complex

Dye **7** concentration = 3.5 x 10^{-5} M
Wavelength selected = 398 nm

α-CD concentration (M)	Change in extinction coefficient (ε) of **7** at 398 nm
1.00E-07	17229
1.00E-06	17303
1.00E-05	17574
2.00E-05	17506
4.00E-05	17791
8.00E-05	18134
2.00E-04	18566
4.00E-04	18891
8.00E-04	19074
2.00E-03	19249
4.00E-03	19277
8.00E-03	19483
9.00E-03	19446



Data for UV/Vis for formation of **8**: α-CD complex

Dye **8** concentration = 1.75 x 10^{-5} M
Wavelength selected = 463 nm

α-CD concentration (M)	Change in extinction coefficient (ε) of **8** at 463 nm
1.00E-07	26020
1.00E-06	26019
1.00E-05	25950
2.00E-05	25821
4.00E-05	25504
8.00E-05	25270
2.00E-04	25015
4.00E-04	24736
8.00E-04	24814
2.00E-03	24710
4.00E-03	24698

Data for UV/Vis for formation of **9**: α-CD complex

Dye **9** concentration = 6 x 10^{-5} M
Wavelength selected = 379 nm

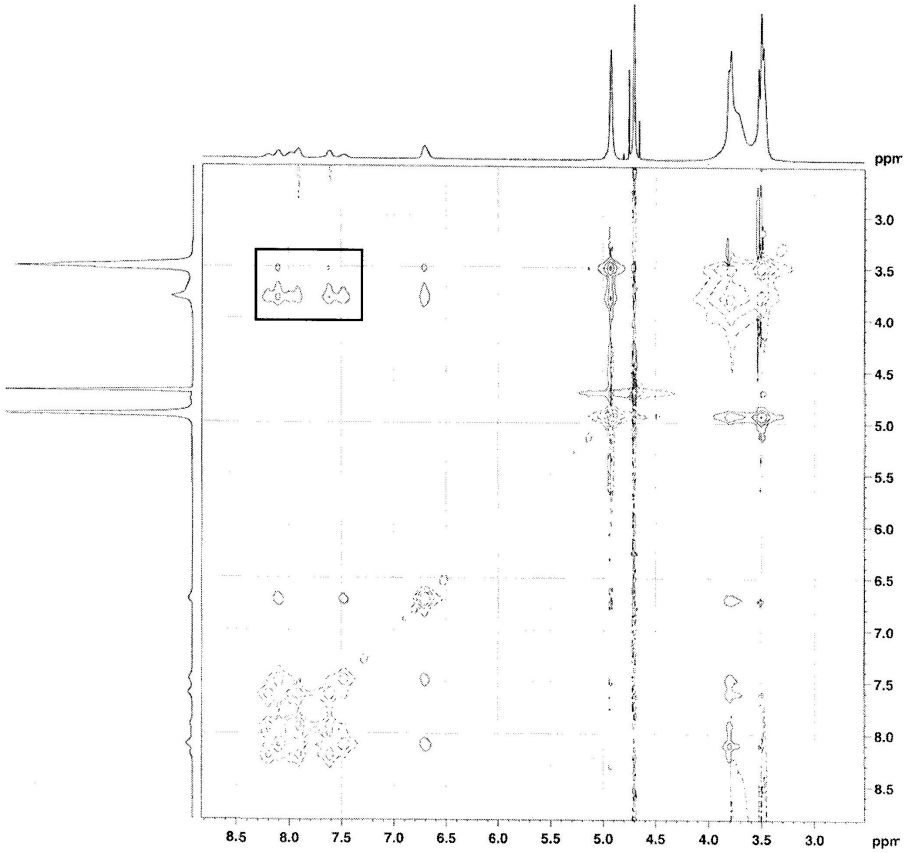
α-CD concentration (M)	Change in extinction coefficient (ε) of **9** at 379 nm
1.00E-07	12892
1.00E-06	12904
1.00E-05	12943
2.00E-04	12962
4.00E-04	13029
6.00E-04	13281
8.00E-04	13433
1.00E-03	13456
2.00E-03	13585
4.00E-03	13687
6.00E-03	13151
8.00E-03	13581
1.00E-02	13435

Data for UV/Vis for formation of **10**: α-CD complex

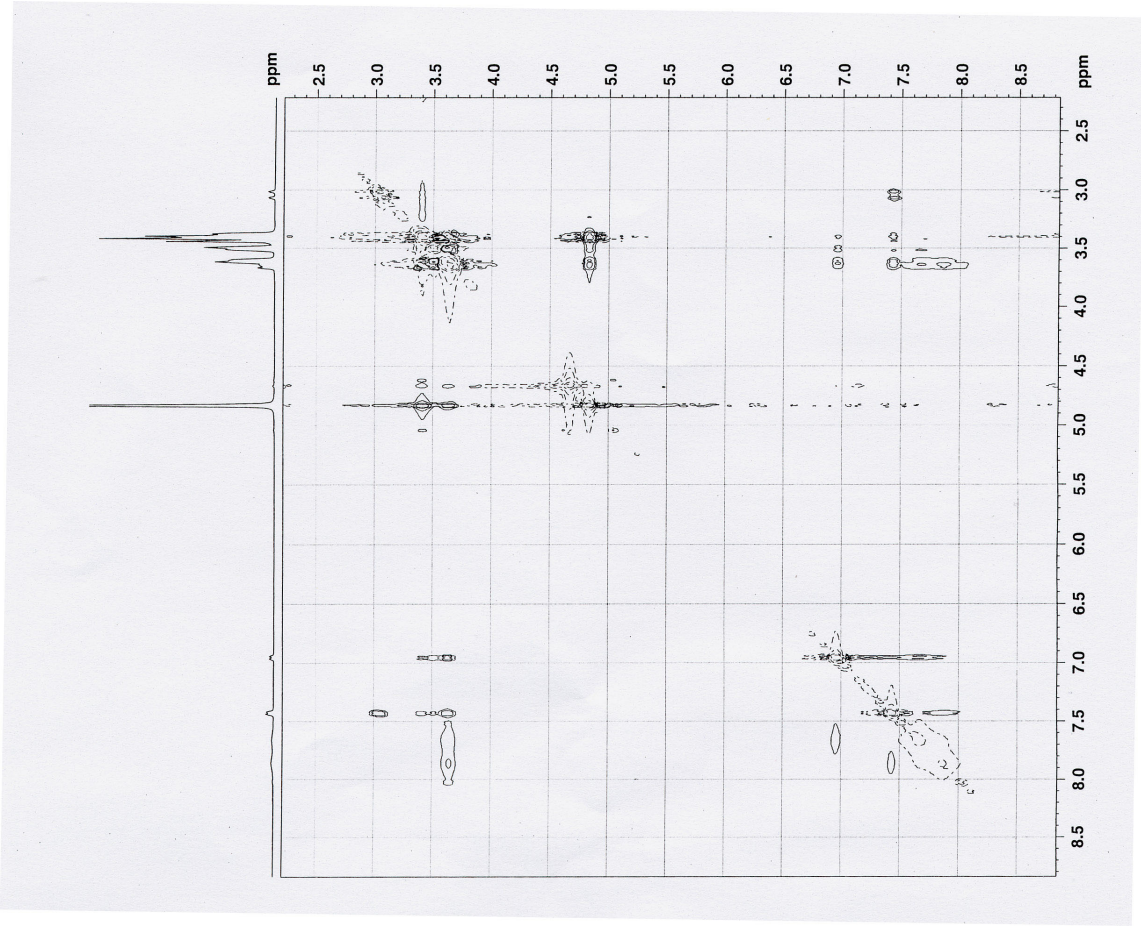
Dye **10** concentration = 6 x 10^{-5} M

α-CD concentration (M)	Change in extinction coefficient (ε) of **10**
1.00E-07	13745
1.00E-06	13982
1.00E-05	13984
2.00E-04	14097
4.00E-04	14085
6.00E-04	14482
8.00E-04	15106
1.00E-03	15137
2.00E-03	16192

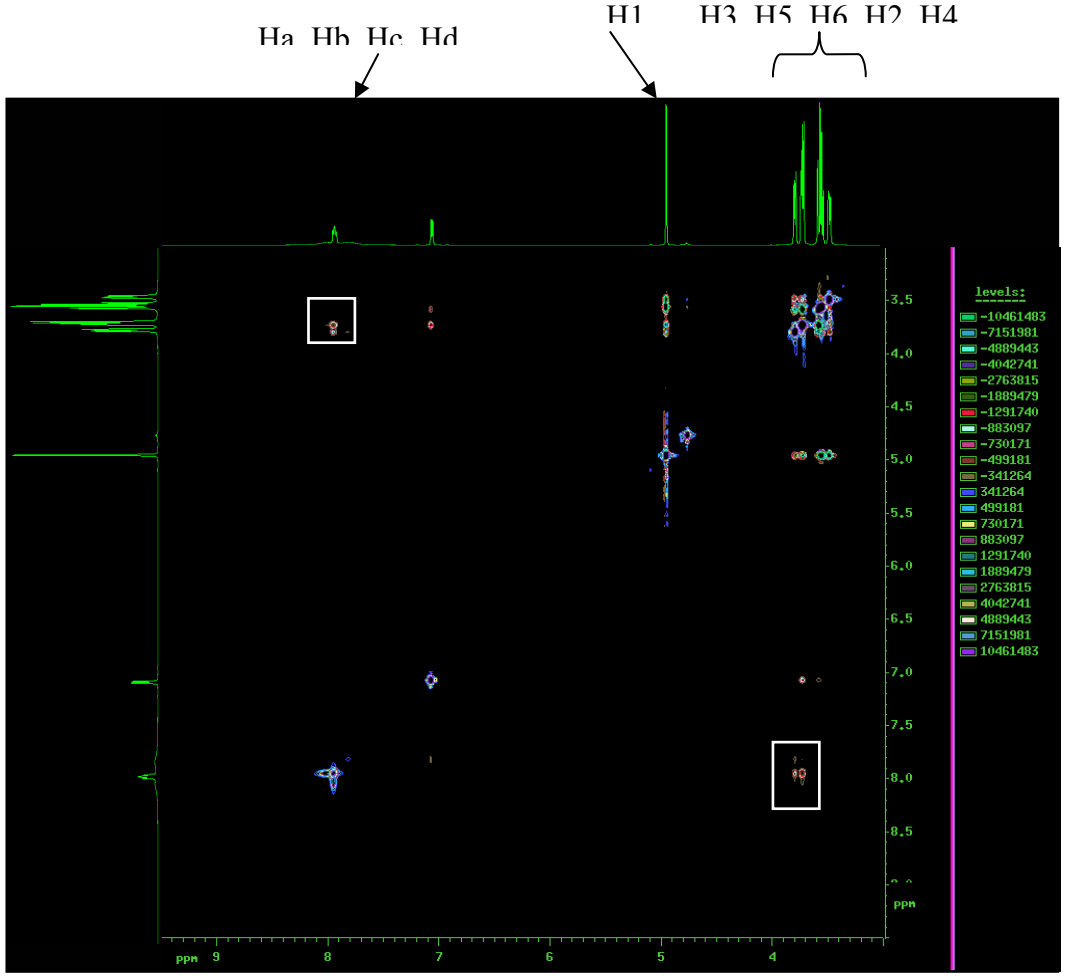
ROESY NMR spectrum of **3** and α-cyclodextrin (0.05 mol dm^{-3}) in D_2O



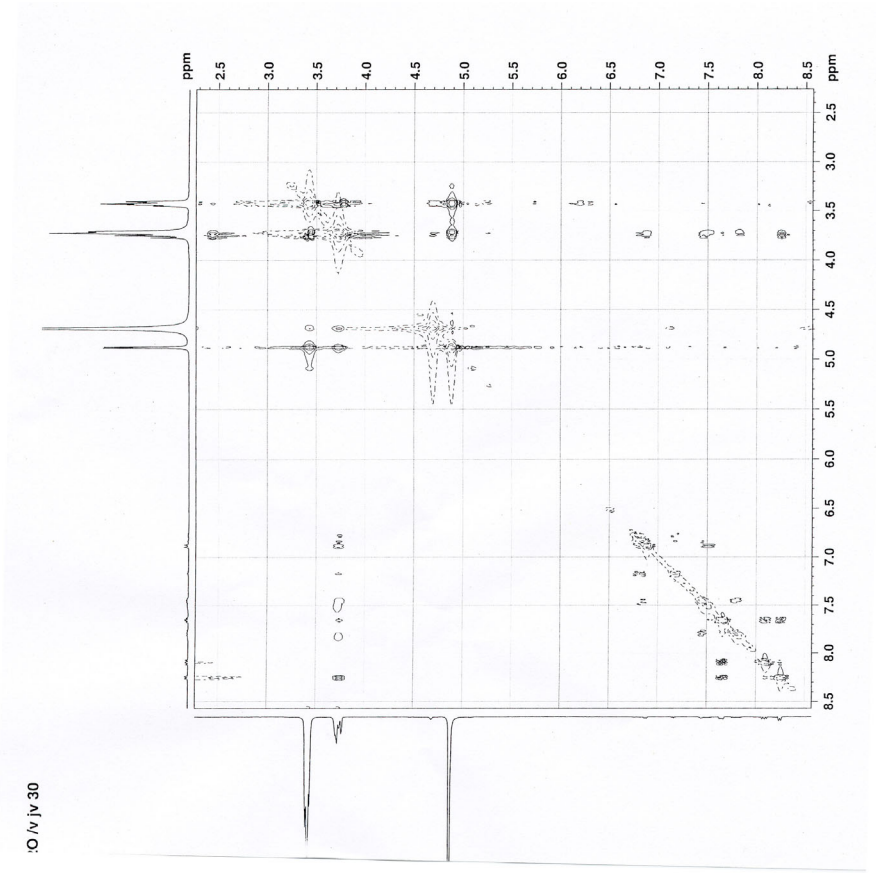
ROESY NMR spectrum of **4** and α-cyclodextrin (0.05 mol dm^{-3}) in D_2O



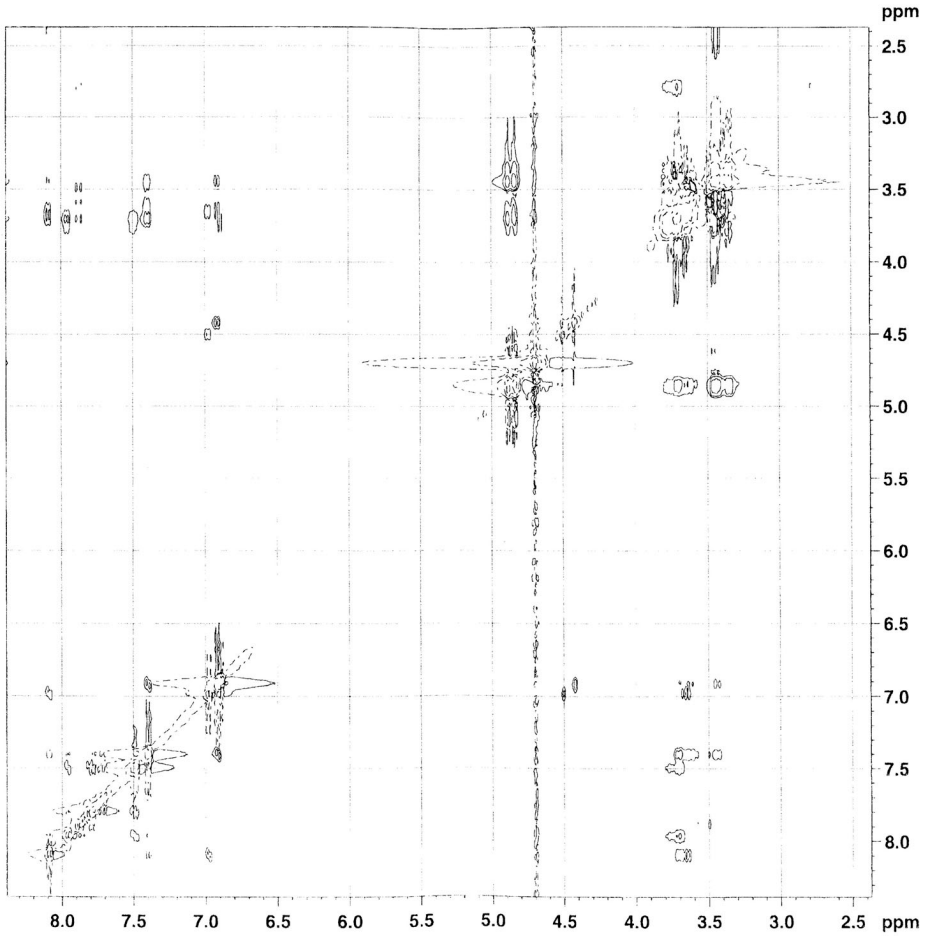
ROESY NMR spectrum of **5** and α-cyclodextrin (0.05 mol dm^{-3}) in D_2O



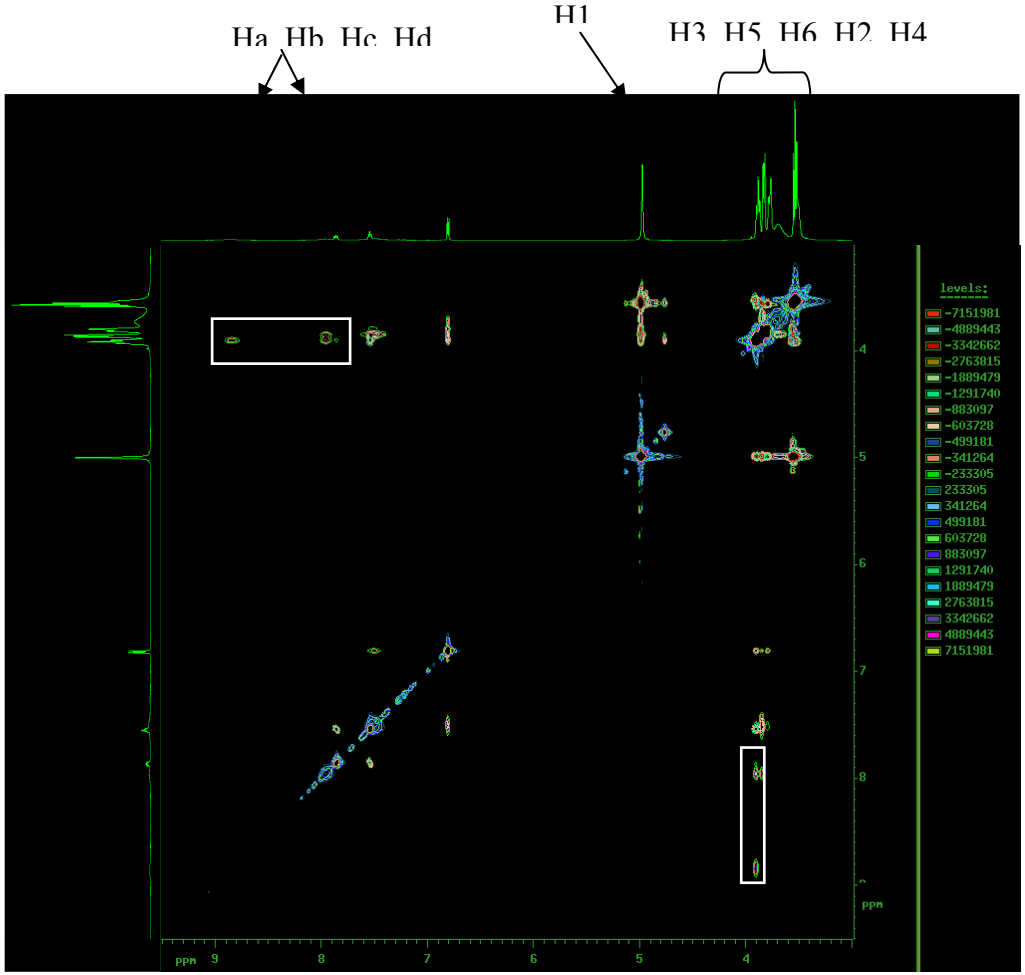
ROESY NMR spectrum of **6** and α-cyclodextrin (0.05 mol dm^{-3}) in D_2O



ROESY NMR spectrum of **9** and α-cyclodextrin (0.05 mol dm^{-3}) in D_2O



ROESY NMR spectrum of **10** and α-cyclodextrin (0.05 mol dm^{-3}) in D_2O



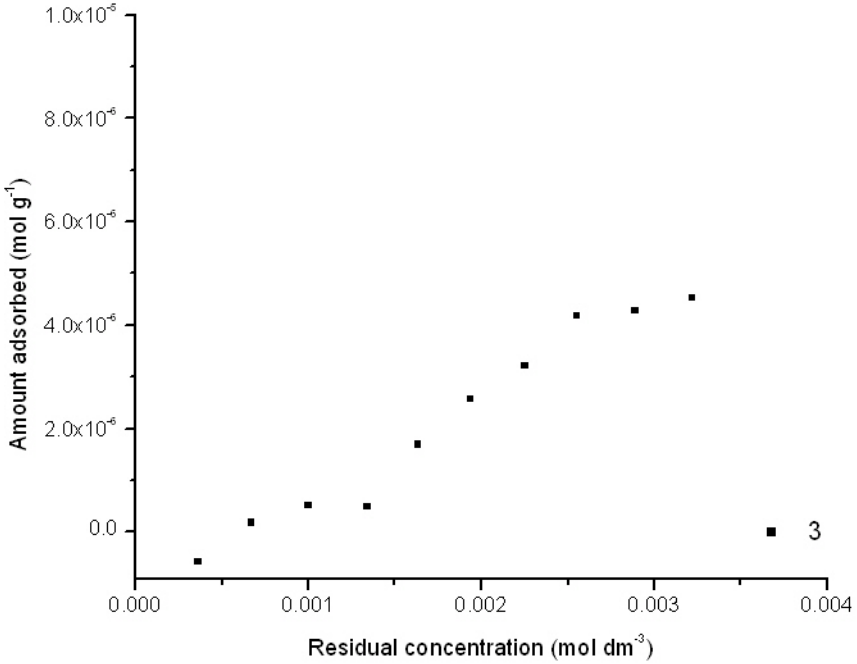
Dye	ROD	Hue	Chroma	Best LF performance[a]	Worst LF performance[b]
3	1.64-0.83	91-37	103-64	HP Premium paper (polymeric coat, swellable)	PR 101 (alumina coat, microporous)
4	1.39-0.81	101-86	89-63	SEC premium glossy paper (silica coat, microporous)	PR 101 (alumina coat, microporous)
5	1.13-.047	102-89	79-41	SEC premium glossy paper (silica coat, microporous)	PR 101 (alumina coat, microporous)
6	2.06-1.89	34-26	89-77	HP Premium paper (polymeric coat, swellable)	HG 201 (alumina coat, microporous, acidic)
9	1.46-0.73	95-82	96-62	SEC premium glossy paper (silica coat, microporous)	PR 101 (alumina coat, microporous)
10	0.59-0.2	112-107	24-16	Printasia (polymer coating)	PR 101 (alumina coat, microporous)

Summary of light fastness properties for dyes **3**-**6**, **9** and **10** after printing onto papers described on supplementary page 32.
[a] and [b] - Smallest and greatest % lost of reflected optical density respectively.

Paper	Commercial name	Description	Type
SEC Premium	Epson Premium Glossy Photo Paper	Silica coating	microporous
PR 101	Canon Photo Paper Pro	Alumina coating	microporous
HG 201	High Gloss Photo Film	Alumina coating	microporous
HP Premium	HP Premium Plus Photo Paper	Polymer coating	swellable
Printasia	Ilford Printasia Photo Glossy Paper	Polymer coating	swellable
PGPP	Epson Premium Glossy Photo Paper	Silica	microporous
Non commercial media	Development media	Alumina	microporous

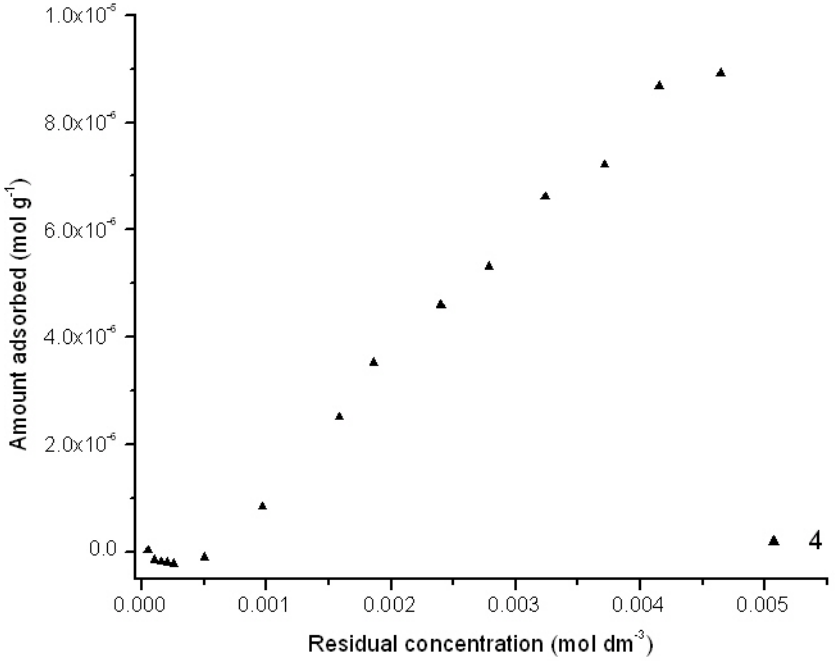
Paper types used for ink jet tests.

Data for isotherms of **3** on ATH



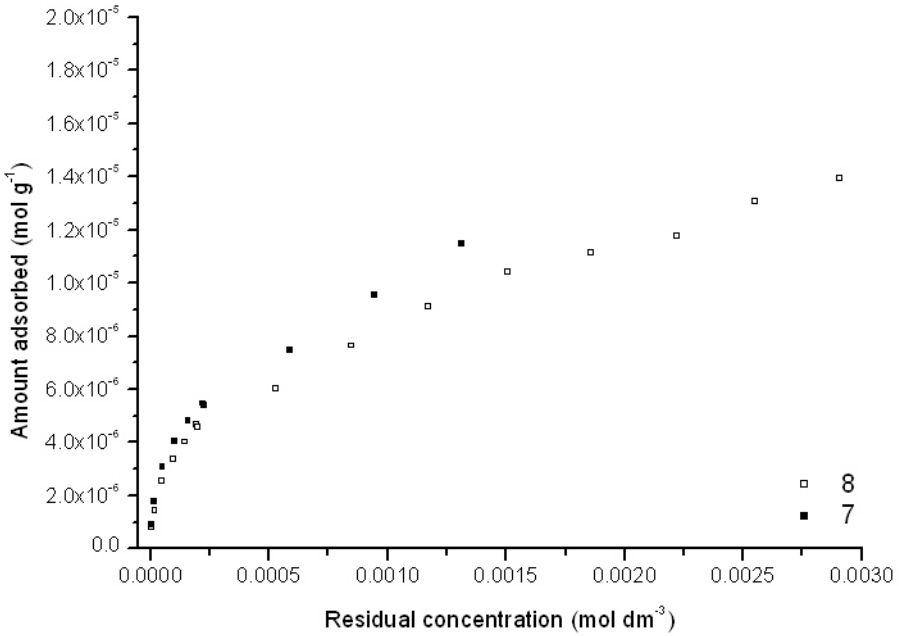
Compound **3**	
Residual concentration (mol dm^{-3})	**Amount adsorbed (mol g^{-1})**
6.73E-04	1.77E-07
1.00E-03	5.08E-07
1.34E-03	4.84E-07
1.63E-03	1.69E-06
1.94E-03	2.57E-06
2.25E-03	3.22E-06
2.55E-03	4.18E-06
2.89E-03	4.27E-06
3.22E-03	4.53E-06

Data for isotherms of **4** on ATH



Compound **4**	
Residual concentration (mol dm^{-3})	**Amount adsorbed (mol g^{-1})**
4.90E-05	2.45E-08
1.06E-04	-1.44E-07
1.58E-04	-1.89E-07
2.08E-04	-2.08E-07
2.59E-04	-2.28E-07
5.04E-04	-1.05E-07
9.66E-04	8.40E-07
1.58E-03	2.51E-06
1.86E-03	3.52E-06
2.40E-03	4.60E-06
2.79E-03	5.32E-06
3.24E-03	6.62E-06
3.71E-03	7.21E-06
4.15E-03	8.68E-06
4.64E-03	8.93E-06

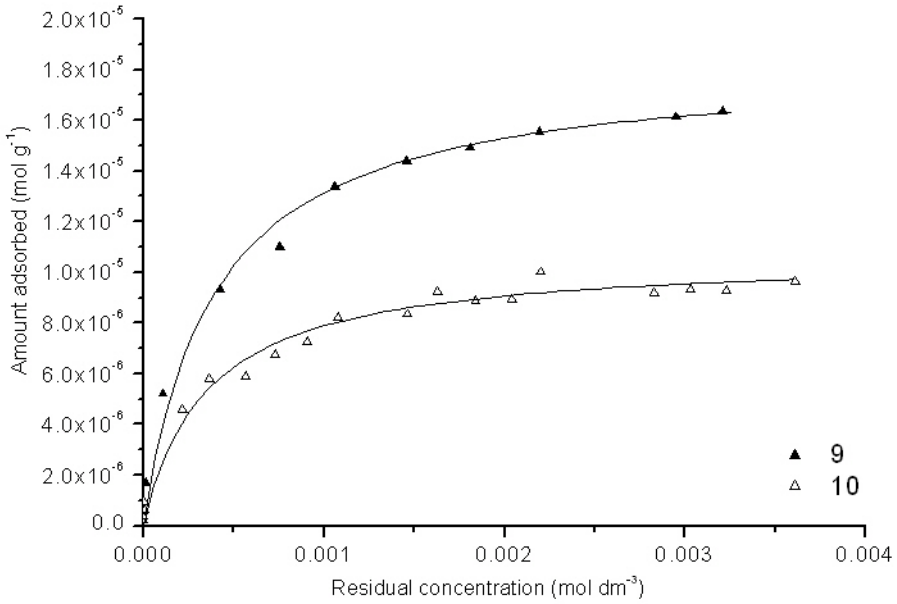
Data for isotherms of **7** and **8** on ATH



Compound **7**		Compound **8**	
Residual concentration (mol dm^{-3})	**Amount adsorbed (mol g^{-1})**	**Residual concentration (mol dm^{-3})**	**Amount adsorbed (mol g^{-1})**
5.95E-06	8.09E-07	6.37E-06	9.24E-07
1.84E-05	1.44E-06	1.50E-05	1.79E-06
4.98E-05	2.56E-06	5.08E-05	3.09E-06
9.42E-05	3.37E-06	1.01E-04	4.05E-06
1.43E-04	4.03E-06	1.58E-04	4.82E-06
1.96E-04	4.68E-06	2.20E-04	5.47E-06
2.01E-04	4.58E-06	2.28E-04	5.40E-06

5.27E-04	6.02E-06	5.86E-04	7.47E-06
8.48E-04	7.64E-06	9.46E-04	9.55E-06
1.17E-03	9.11E-06	1.31E-03	1.15E-05
1.51E-03	1.04E-05		
1.86E-03	1.11E-05		
2.22E-03	1.17E-05		
2.55E-03	1.31E-05		
2.91E-03	1.40E-05		

Data for isotherms of **9** and **10** on ATH



Compound **9**		Compound **10**	
Residual concentration (mol dm^{-3})	**Amount adsorbed (mol g^{-1})**	**Residual concentration (mol dm^{-3})**	**Amount adsorbed (mol g^{-1})**
1.25E-05	1.68E-06	0.00E+00	1.99E-07
1.08E-04	5.21E-06	1.05E-06	3.77E-07
4.25E-04	9.34E-06	0.00E+00	5.96E-07
7.55E-04	1.10E-05	7.80E-06	6.08E-07
1.06E-03	1.34E-05	2.26E-06	9.44E-07
1.46E-03	1.44E-05	2.17E-04	4.58E-06

1.81E-03	1.49E-05	3.66E-04	5.79E-06
2.20E-03	1.55E-05	5.66E-04	5.91E-06
2.95E-03	1.61E-05	7.32E-04	6.76E-06
3.21E-03	1.64E-05	9.09E-04	7.27E-06
		1.08E-03	8.20E-06
		1.46E-03	8.35E-06
		1.63E-03	9.21E-06
		1.84E-03	8.85E-06
		2.04E-03	8.91E-06
		2.20E-03	1.00E-05
		2.83E-03	9.20E-06
		3.03E-03	9.32E-06
		3.23E-03	9.28E-06
		3.61E-03	9.64E-06