Electronic Supplementary Information

Complexes of Peracetylated Cyclodextrin in a Non-Aqueous Aprotic Medium: The Role of Residual Water

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Contents:

NMR spectra of the water complexation experiments

Data used in the calculations of stability constants

Acquisition Time (sec)	1.8219	***Comment***	CDCl3 dried farma shim	***Date***	15 Sep 2014 10:51:12			***Date Stamp***	15 Sep 2014 10:51:12
File Name	CDCl3 dried.001.esp					***Frequency (MHz)***	300.13	***Nucleus***	1H
Number of Transients	4	***Origin***	spect	***Original Points Count***	8192	***Owner***	root	***Points Count***	65536
Pulse Sequence	zg	***Receiver Gain***	322.50	***SW(cyclical) (Hz)***	4496.40	***Solvent***	CDCl3	***Spectrum Offset (Hz)***	1944.7450
Spectrum Type	STANDARD	***Sweep Width (Hz)***	4496.33	***Temperature (degree C)***	22.560				

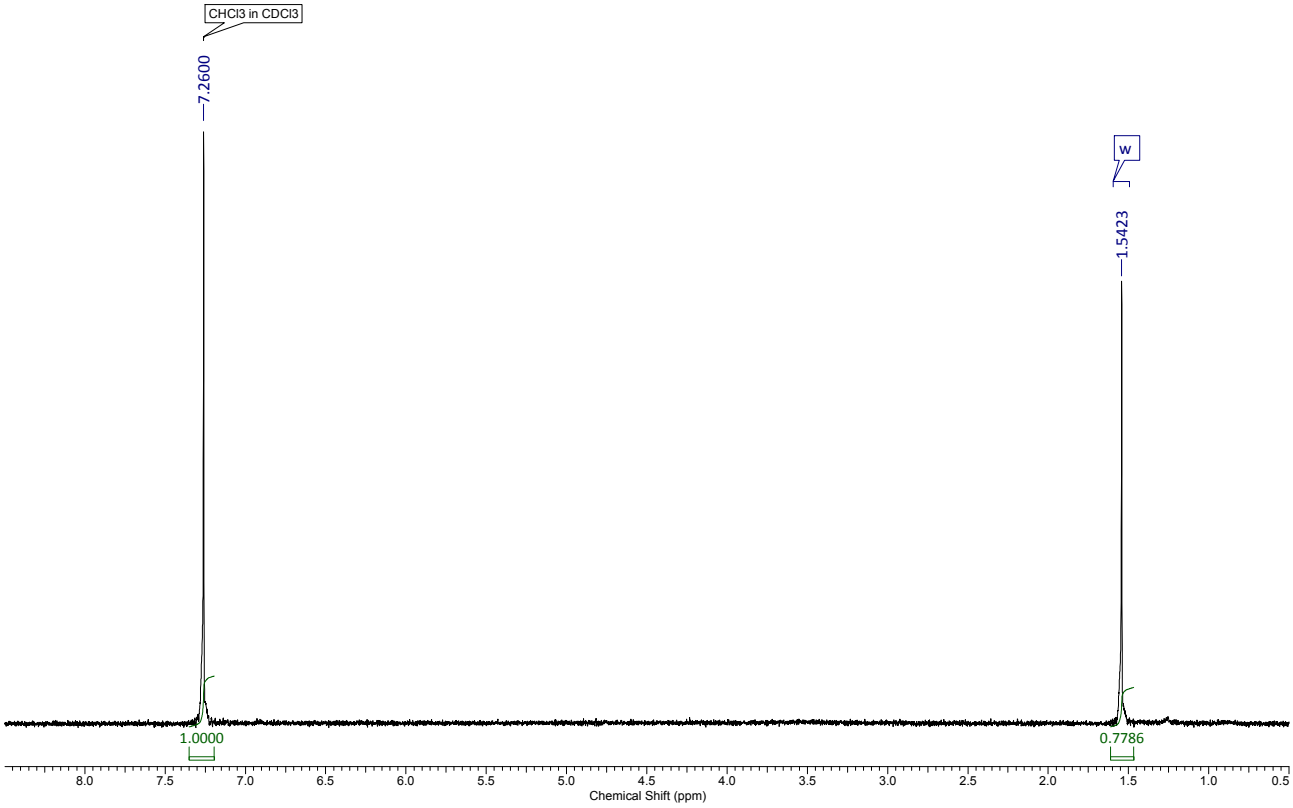


Figure S1.1.a. $CDCl_3$, water content ≤ 0.008%

Acquisition Time (sec)	3.6438	***Comment***	CDCl3 600ul satd water (10+1 ml) farma shim			***Date***	17 Nov 2014 14:43:28		
Date Stamp	17 Nov 2014 14:43:28			***File Name***	CDCl3_satdH2O.002.esp				
Frequency (MHz)	300.13	***Nucleus***	1H	***Number of Transients***	64	***Origin***	spect	***Original Points Count***	16384
Owner	root	***Points Count***	65536	***Pulse Sequence***	zg	***Receiver Gain***	362.00	***SW(cyclical) (Hz)***	4496.40
Solvent	CDCl3	***Spectrum Offset (Hz)***	1073.9510	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	4496.33	***Temperature (degree C)***	22.560

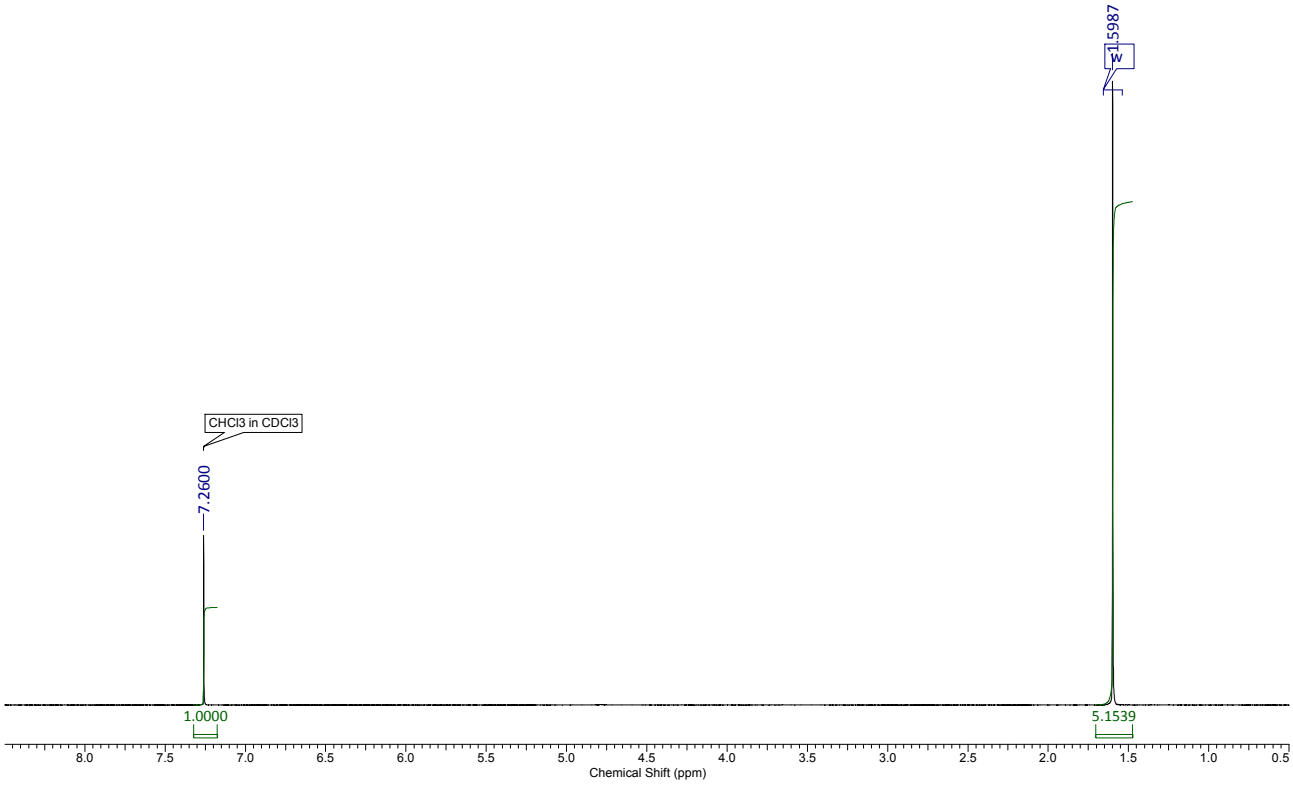


Figure S1.1.b. $CDCl_3$ saturated with water

Acquisition Time (sec)	3.6438	**Comment**	CDCl3 sat. D2O (2 + 0. ml) farma	**Date**	25 Feb 2015 10:46:40	**Date Stamp**	25 Feb 2015 10:46:40
File Name	CDCl3_satD2O.001.esp			**Frequency (MHz)**	300.13	**Nucleus**	1H
Origin	spect	**Original Points Count**	16384	**Owner**	root	**Points Count**	16384
Solvent	CDCl3	**Spectrum Offset (Hz)**	1074.7400	**Sweep Width (Hz)**	4496.13	**Temperature (degree C)**	22.660

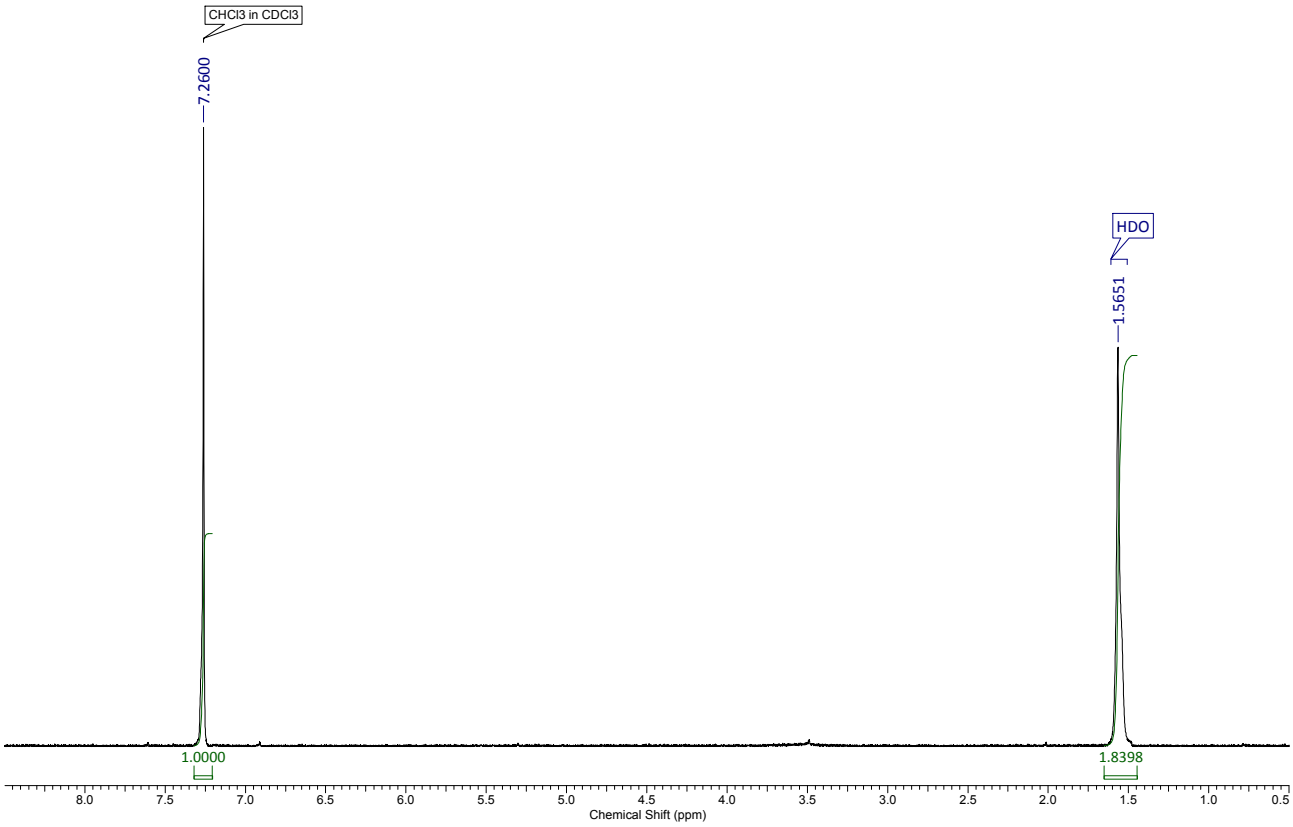


Figure S1.1.c. $CDCl_3$ saturated with D_2O

Acquisition Time (sec)	3.6438	**Comment**	1.34 mg perAcaCD new dried in 600ul CDCl3 farma shim			**Date**	13 Feb 2015 15:58:08
Date Stamp	13 Feb 2015 15:58:08			**File Name**	perAcaCD_newdried.001.esp		
Frequency (MHz)	300.13	**Nucleus**	1H	**Number of Transients**	64	**Origin**	spect
Original Points Count	16384	**Owner**	root	**Points Count**	65536	**Pulse Sequence**	zg
Receiver Gain	362.00	**SW(cyclical) (Hz)**	4496.40	**Solvent**	CHCl3 in CDCl3	**Spectrum Offset (Hz)**	1074.0195
Spectrum Type	STANDARD	**Sweep Width (Hz)**	4496.33	**Temperature (degree C)**	22.560		

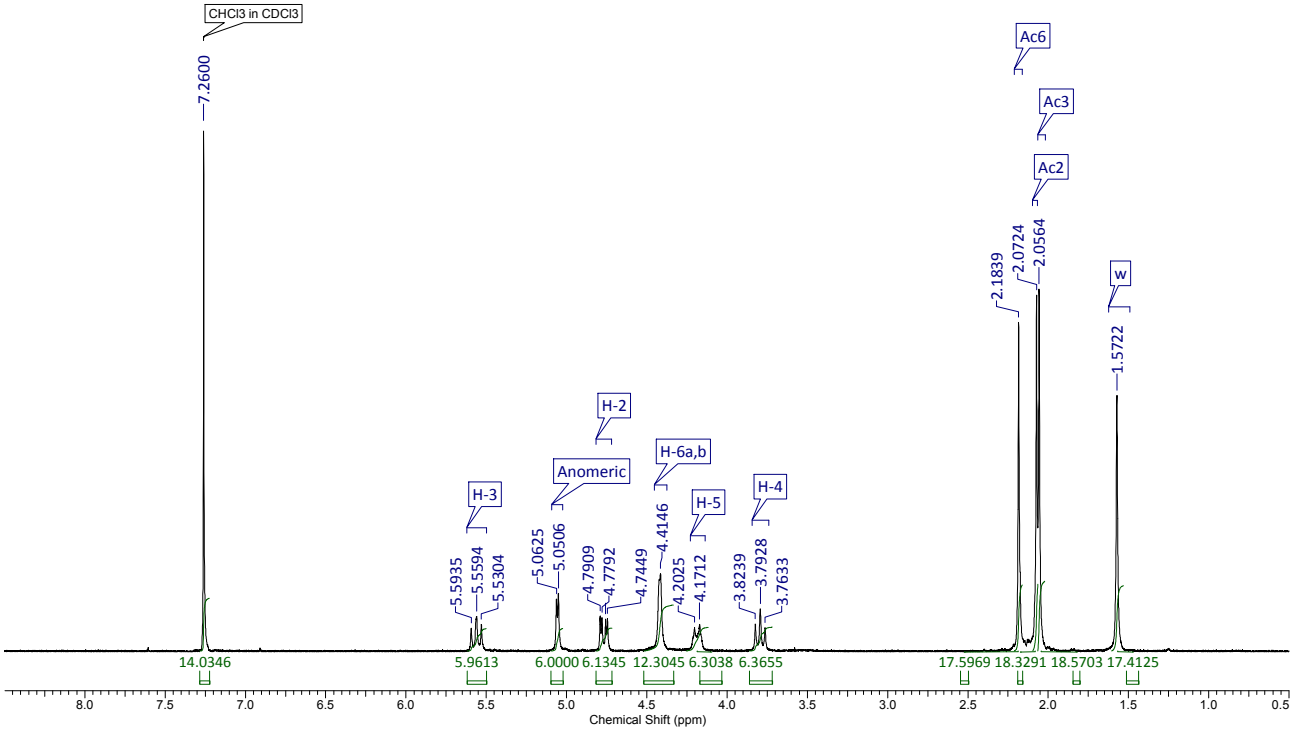


Figure S1.2.a. 1.3 mg of azeotropically dried peracetyl-αCD in dry $CDCl_3$

Acquisition Time (sec)	3.6438	***Comment***	1.3 mg perAcbCD_new dried in 600 ul CDCl3 farma shim			***Date***	25 Feb 2015 10:42:24
Date Stamp	25 Feb 2015 10:42:24			***File Name***	perAcbCD_newdried.001.esp		
Frequency (MHz)	300.13	***Nucleus***	1H	***Origin***	spect	***Original Points Count***	16384
Owner	root	***Points Count***	65536	***SW(cyclical) (Hz)***	4496.40	***Solvent***	CDCl3
Spectrum Offset (Hz)	1074.2942	***Sweep Width (Hz)***	4496.33	***Temperature (degree C)***	22.660		

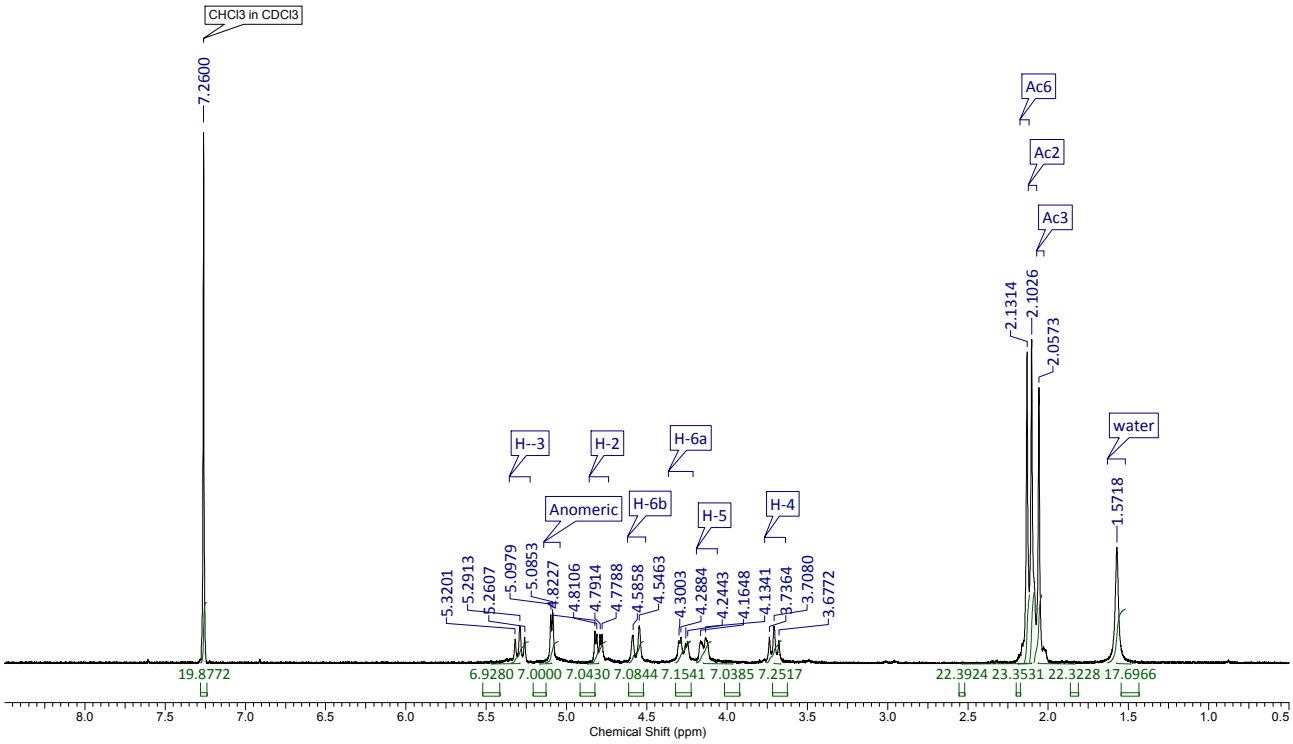


Figure S1.2.b. 1.3 mg of azeotropically dried peracetyl-βCD in dry $CDCl_3$

Acquisition Time (sec)	3.6438	***Comment***	1.46 mg perAcgCD in 600ul CDCl3 farma shim			***Date***	13 Feb 2015 16:36:32
Date Stamp	13 Feb 2015 16:36:32			***File Name***	perAcgCD_newdried.001.esp		
Frequency (MHz)	300.13	***Nucleus***	1H	***Origin***	spect	***Original Points Count***	16384
Owner	root	***Points Count***	65536	***SW(cyclical) (Hz)***	4496.40	***Solvent***	CDCl3
Spectrum Offset (Hz)	1074.0197	***Sweep Width (Hz)***	4496.33	***Temperature (degree C)***	22.660		

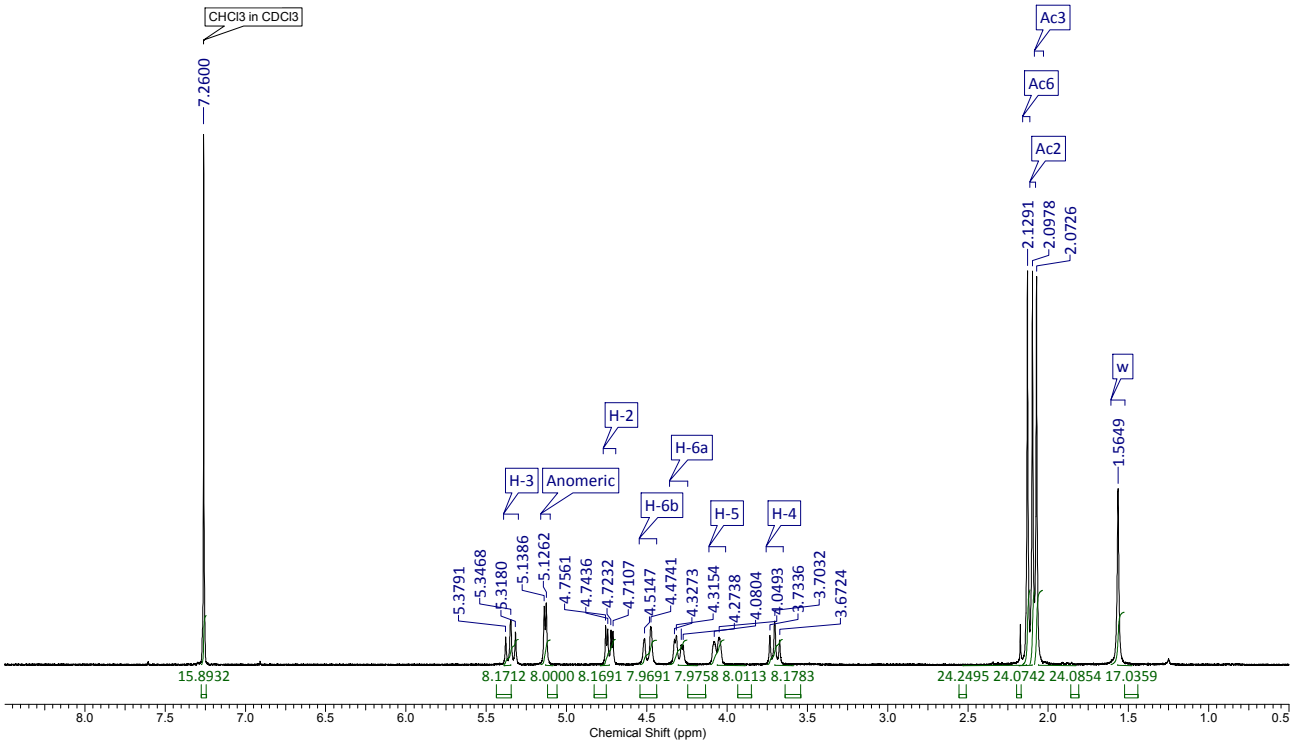


Figure S1.2.c. 1.46 mg of azeotropically dried peracetyl-γCD in dry $CDCl_3$

Acquisition Time (sec)	3.6438	***Comment***	31.34 mg perAcaCD new dried in 600 ul CDCl3 farma shim			***Date***	13 Feb 2015 16:08:48		
Date Stamp	13 Feb 2015 16:08:48			***File Name***	perAcaCD_newdried.002.esp				
Frequency (MHz)	300.13	***Nucleus***	1H	***Number of Transients***	64	***Origin***	spect	***Original Points Count***	16384
Owner	root	***Points Count***	65536	***Pulse Sequence***	zg	***Receiver Gain***	90.50	***SW(cyclical) (Hz)***	4496.40
Solvent	CDCl3	***Spectrum Offset (Hz)***	1074.1226	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	4496.27	***Temperature (degree C)***	22.460

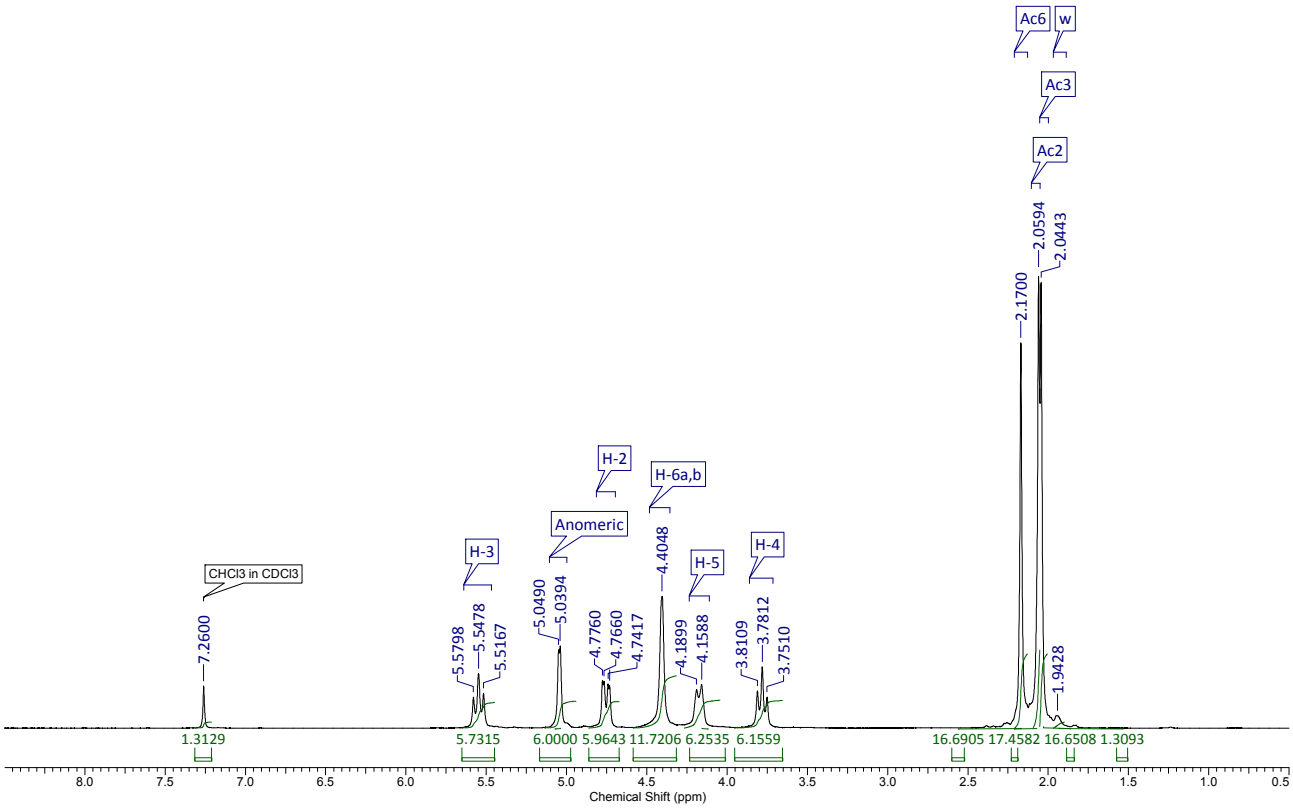


Figure S1.3.a. 31 mg of azeotropically dried peracetyl-αCD in dry $CDCl_3$

Acquisition Time (sec)	3.6438	***Comment***	32.1 mg perAcbCD new dried in 600 ul CDCl3 farma shim			***Date***	25 Feb 2015 11:14:24		
Date Stamp	25 Feb 2015 11:14:24			***File Name***	perAcbCD_newdried.002.esp				
Frequency (MHz)	300.13	***Nucleus***	1H	***Number of Transients***	64	***Origin***	spect	***Original Points Count***	16384
Owner	root	***Points Count***	65536	***Pulse Sequence***	zg	***Receiver Gain***	90.50	***SW(cyclical) (Hz)***	4496.40
Solvent	CDCl3	***Spectrum Offset (Hz)***	1074.0195	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	4496.33	***Temperature (degree C)***	22.560

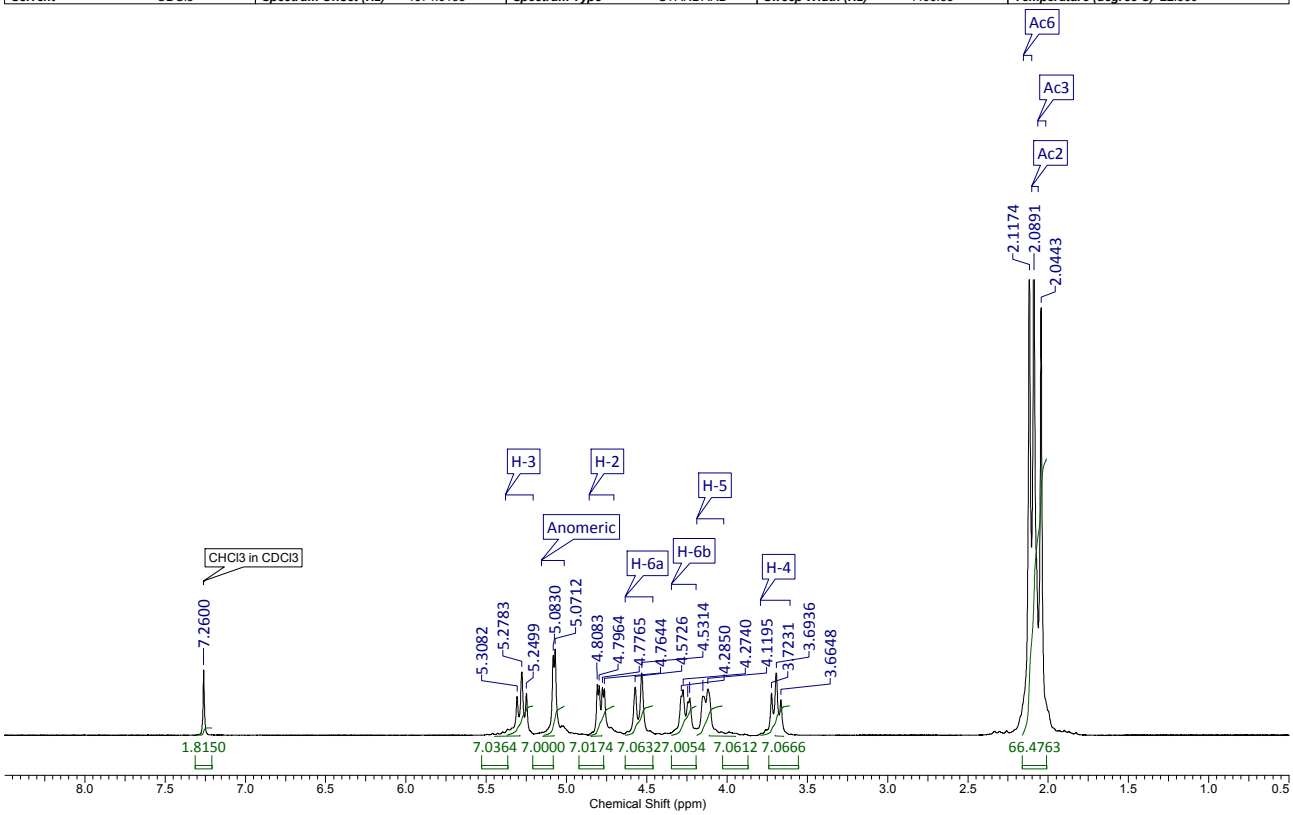


Figure S1.3.b. 31 mg of azeotropically dried peracetyl-βCD in dry $CDCl_3$

Acquisition Time (sec)	3.6438	***Comment***	31.76 mg perAcgCD new dried in 600 ul CDCl3 farma shim			***Date***	13 Feb 2015 16:47:12		
Date Stamp	13 Feb 2015 16:47:12			***File Name***	perAcgCD_newdried.002.esp				
Frequency (MHz)	300.13	***Nucleus***	1H	***Number of Transients***	64	***Origin***	spect	***Original Points Count***	16384
Owner	root	***Points Count***	65536	***Pulse Sequence***	zg	***Receiver Gain***	90.50	***SW(cyclical) (Hz)***	4496.40
Solvent	CDCl3	***Spectrum Offset (Hz)***	1074.1567	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	4496.33	***Temperature (degree C)***	22.460

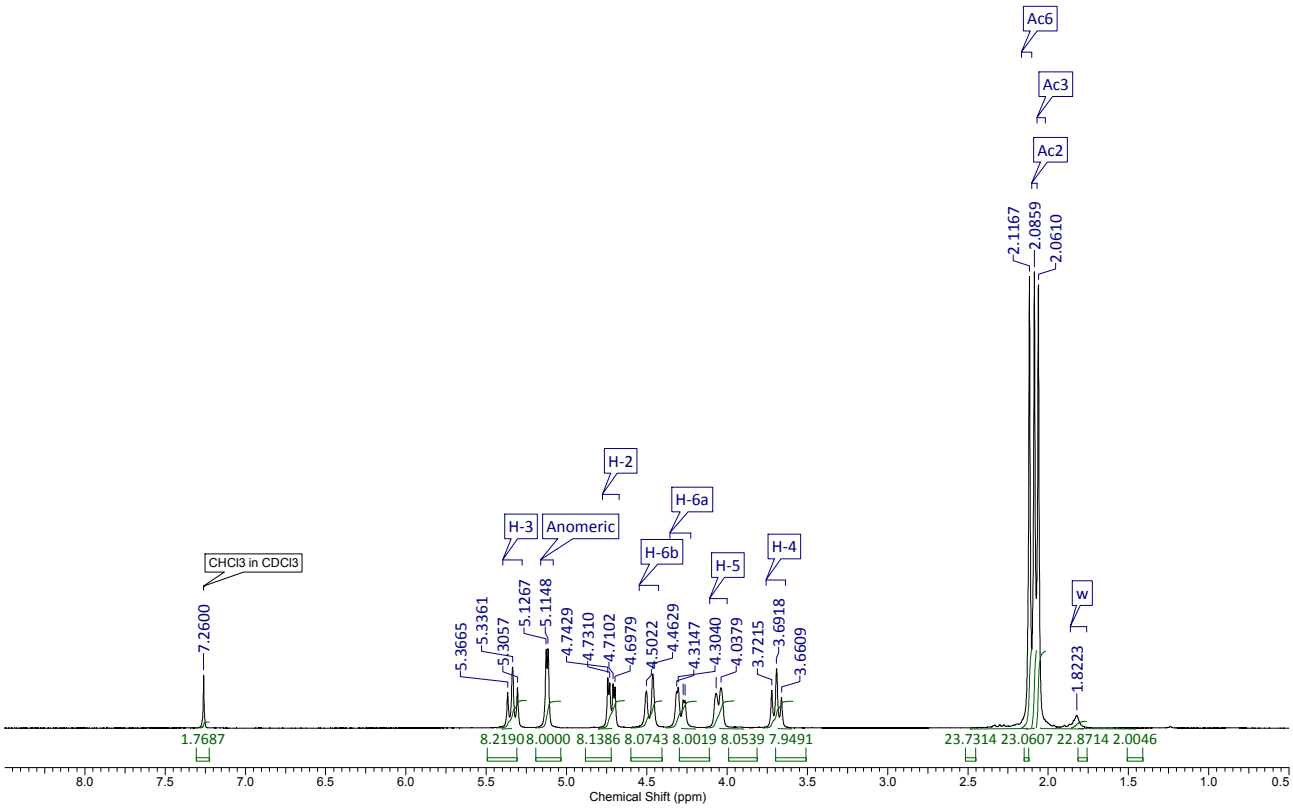


Figure S1.3.c. 31 mg of azeotropically dried peracetyl-γCD in dry $CDCl_3$

Acquisition Time (sec)	3.6438	***Comment***	31.34 mg perAcaCD new dried in 600 ul CDCl3 + 300ul CDCl3 saturated with D2O farma shim						
Date	13 Feb 2015 16:23:44			***Date Stamp***	13 Feb 2015 16:23:44				
File Name	perAcaCD_newdried.003.esp							***Frequency (MHz)***	300.13
Nucleus	1H	***Number of Transients***	64	***Origin***	spect			***Original Points Count***	16384
Owner	root	***Points Count***	65536	***Pulse Sequence***	zg			***Receiver Gain***	90.50
SW(cyclical) (Hz)	4496.40	***Solvent***	CHCl3 in CDCl3	***Spectrum Offset (Hz)***	1074.1567			***Spectrum Type***	STANDARD
Sweep Width (Hz)	4496.33	***Temperature (degree C)***	22.560						

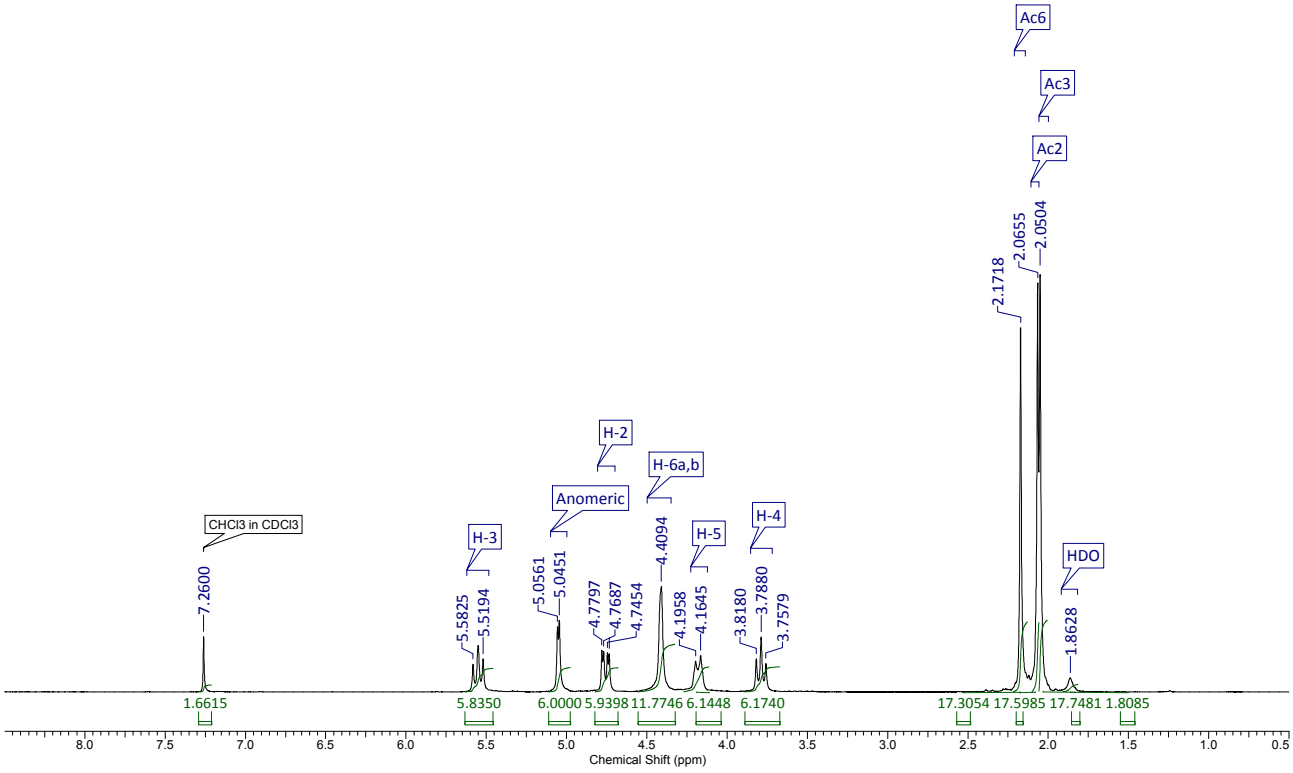


Figure S1.4.a. ~21 mg/600 µL of azeotropically dried peracetyl-αCD in $CDCl_3$ saturated with D_2O

Acquisition Time (sec)	3.6438	***Comment***	32.1 mg perAcbCD new dried in 600 ul CDCl3 + 300ul CDCl3 saturated with D2O farma shim				
Date	25 Feb 2015 11:25:04			***Date Stamp***	25 Feb 2015 11:25:04		
File Name	perAcbCD_newdried.003.esp					***Frequency (MHz)***	300.13
Nucleus	1H	***Number of Transients***	64	***Origin***	spect	***Original Points Count***	16384
Owner	root	***Points Count***	65536	***Pulse Sequence***	zg	***Receiver Gain***	90.50
SW(cyclical) (Hz)	4496.40	***Solvent***	CDCl3	***Spectrum Offset (Hz)***	1074.0883	***Spectrum Type***	STANDARD
Sweep Width (Hz)	4496.33	***Temperature (degree C)***	22.460				

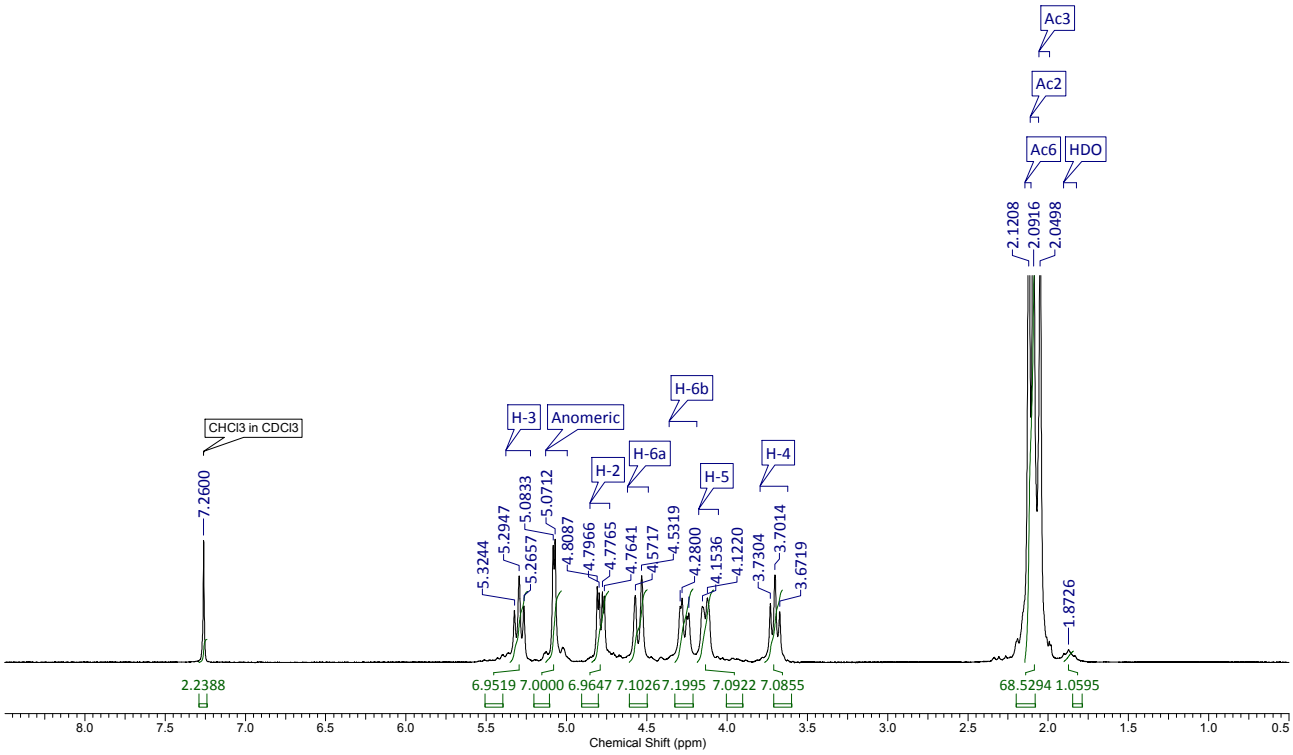


Figure S1.4.b. ~21 mg/600 µL of azeotropically dried peracetyl-βCD in $CDCl_3$ saturated with D_2O

Acquisition Time (sec)	3.6438	***Comment***	31.76 mg perAcgCD new dried in 600 ul CDCl3 + 300ul CDCl3 saturated with D2O farma shim				
Date	13 Feb 2015 16:57:52			***Date Stamp***	13 Feb 2015 16:57:52		
File Name	perAcgCD_newdried.003.esp					***Frequency (MHz)***	300.13
Nucleus	1H	***Number of Transients***	64	***Origin***	spect	***Original Points Count***	16384
Owner	root	***Points Count***	65536	***Pulse Sequence***	zg	***Receiver Gain***	90.50
SW(cyclical) (Hz)	4496.40	***Solvent***	CDCl3	***Spectrum Offset (Hz)***	1074.0883	***Spectrum Type***	STANDARD
Sweep Width (Hz)	4496.33	***Temperature (degree C)***	22.360				

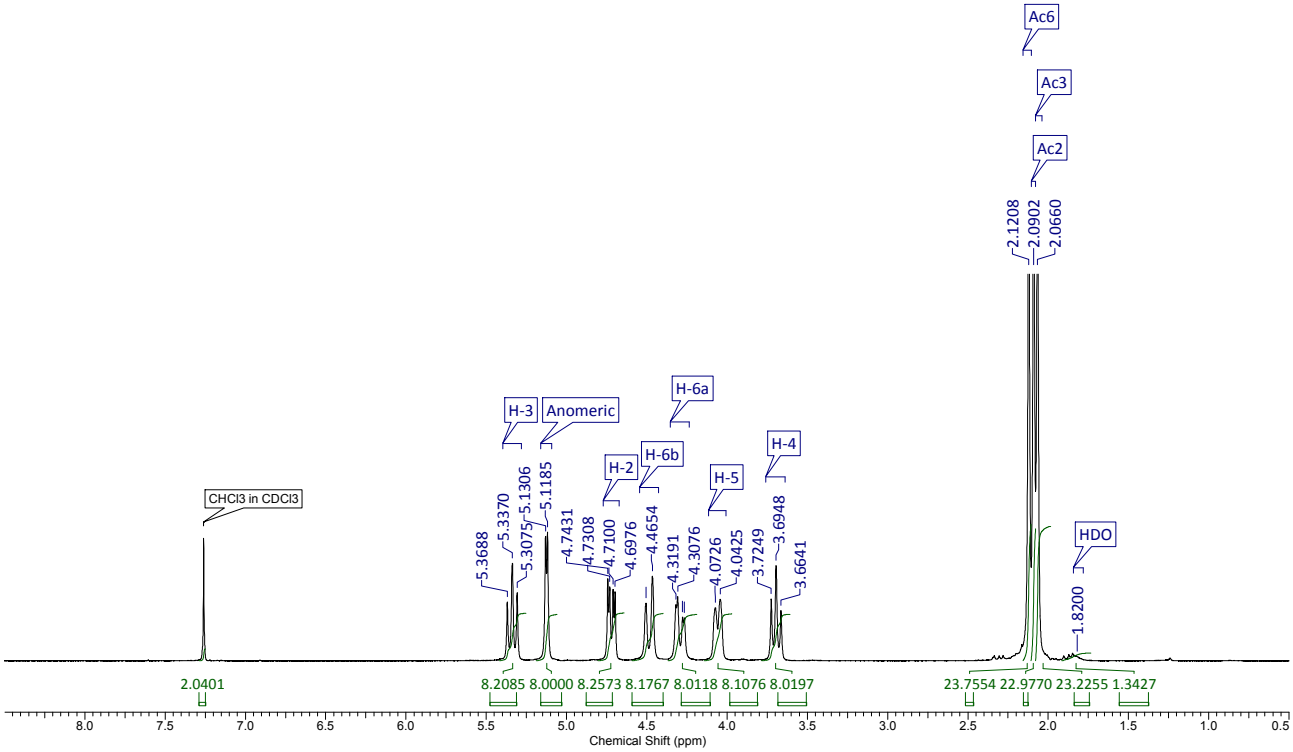


Figure S1.4.c. ~21 mg/600 µL of azeotropically dried peracetyl-γCD in $CDCl_3$ saturated with D_2O

Acquisition Time (sec)	3.6438	***Comment***	perAcgCD dried at 80°C for 4days and half day in the essiccator (5,2mg in 800 ul CDCl3) farma shim				
Date	01 Dec 2014 17:32:00			***Date Stamp***	01 Dec 2014 17:32:00		
File Name	CDCL3_perAcgCD_D2O.001.esp					***Frequency (MHz)***	300.13
Nucleus	1H	***Number of Transients***	64	***Origin***	spect	***Original Points Count***	16384
Owner	root	***Points Count***	65536	***Pulse Sequence***	zg	***Receiver Gain***	362.00
SW(cyclical) (Hz)	4496.40	***Solvent***	CDCl3 satd with D2O	***Spectrum Offset (Hz)***	1074.0195	***Spectrum Type***	STANDARD
Sweep Width (Hz)	4496.33	***Temperature (degree C)***	22.360				

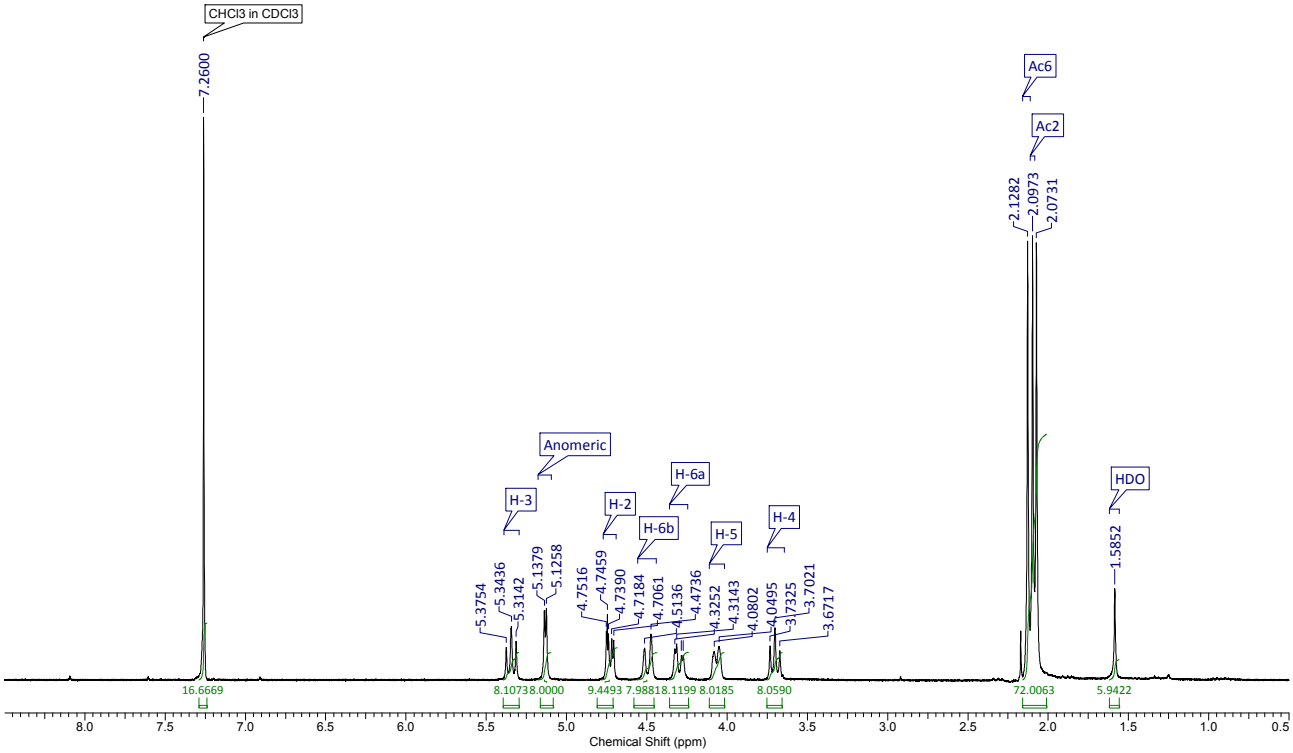


Figure S1.4.d. ~5 mg of heat & vacuum dried peracetyl-γCD in $CDCl_3$ saturated with D_2O (~1: 6)

Acquisition Time (sec)	3.6438	***Comment***	perAcgCD dried at 80°C for 4days and half day in the essiccator (10,2mg in 800 ul CDCl3)				
Date	01 Dec 2014 17:42:40			***Date Stamp***	01 Dec 2014 17:42:40		
File Name	CDCL3_perAcgCD_D2O.002.esp					***Frequency (MHz)***	300.13
Nucleus	1H	***Number of Transients***	64	***Origin***	spect	***Original Points Count***	16384
Owner	root	***Points Count***	65536	***Pulse Sequence***	zg	***Receiver Gain***	181.00
SW(cyclical) (Hz)	4496.40	***Solvent***	CDCl3 satd with D2O	***Spectrum Offset (Hz)***	1074.4313	***Spectrum Type***	STANDARD
Sweep Width (Hz)	4496.33	***Temperature (degree C)***	22.360				

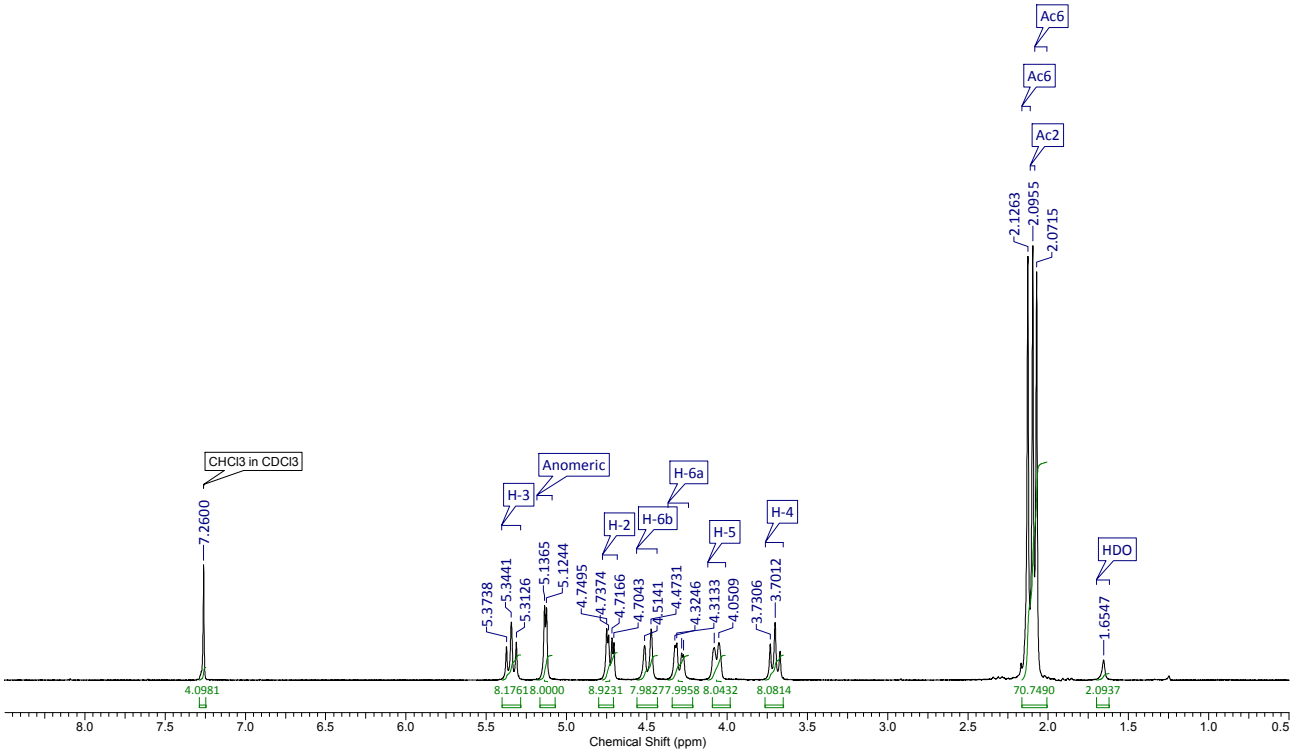


Figure S1.4.e. ~10 mg of heat & vacuum dried peracetyl-γCD in $CDCl_3$ saturated with D_2O (~1:2)

Acquisition Time (sec)	3.6438	***Comment***	perAcgCD dried at 80°C for 4days and half day in the essiccator (50mg in 600 ul CDCl3) farma shim				
Date	01 Dec 2014 17:55:28			***Date Stamp***	01 Dec 2014 17:55:28		
File Name	CDCL3_perAcgCD_D2O.003.esp					***Frequency (MHz)***	300.13
Nucleus	1H	***Number of Transients***	64	***Origin***	spect	***Original Points Count***	16384
Owner	root	***Points Count***	65536	***Pulse Sequence***	zg	***Receiver Gain***	57.00
SW(cyclical) (Hz)	4496.40	***Solvent***	CDCl3 satd with D2O	***Spectrum Offset (Hz)***	1073.9510	***Spectrum Type***	STANDARD
Sweep Width (Hz)	4496.33	***Temperature (degree C)***	22.660				

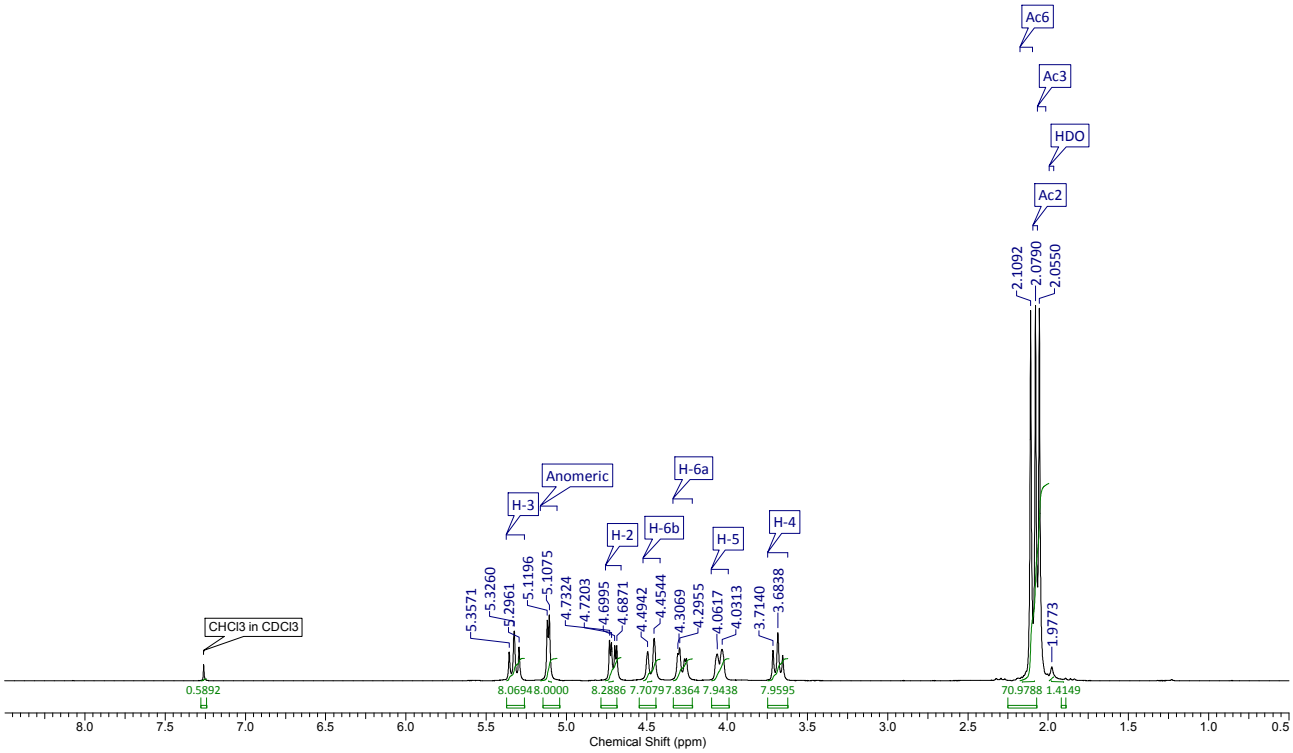


Figure S1.4.f. ~50 mg of heat & vacuum dried peracetyl-γCD in $CDCl_3$ saturated with D_2O (~1:1)

Acquisition Time (sec)	3.6438	***Comment***	peracetyl aCD A+ 1ul DEHT			***Date***	30 Sep 2014 16:21:52
Date Stamp	30 Sep 2014 16:21:52			***File Name***	peracetyl aCD_DEHT.011.fid		
Frequency (MHz)	300.13	***Nucleus***	1H	***Number of Transients***	64	***Origin***	spect
Owner	root	***Points Count***	65536	***Pulse Sequence***	zg	***Receiver Gain***	90.50
Solvent	CDCl3			***Spectrum Offset (Hz)***	1074.2941	***Spectrum Type***	STANDARD
Temperature (degree C)	22.660						

Original Points Count	16384		
SW(cyclical) (Hz)	4496.40		
Sweep Width (Hz)	4496.33		

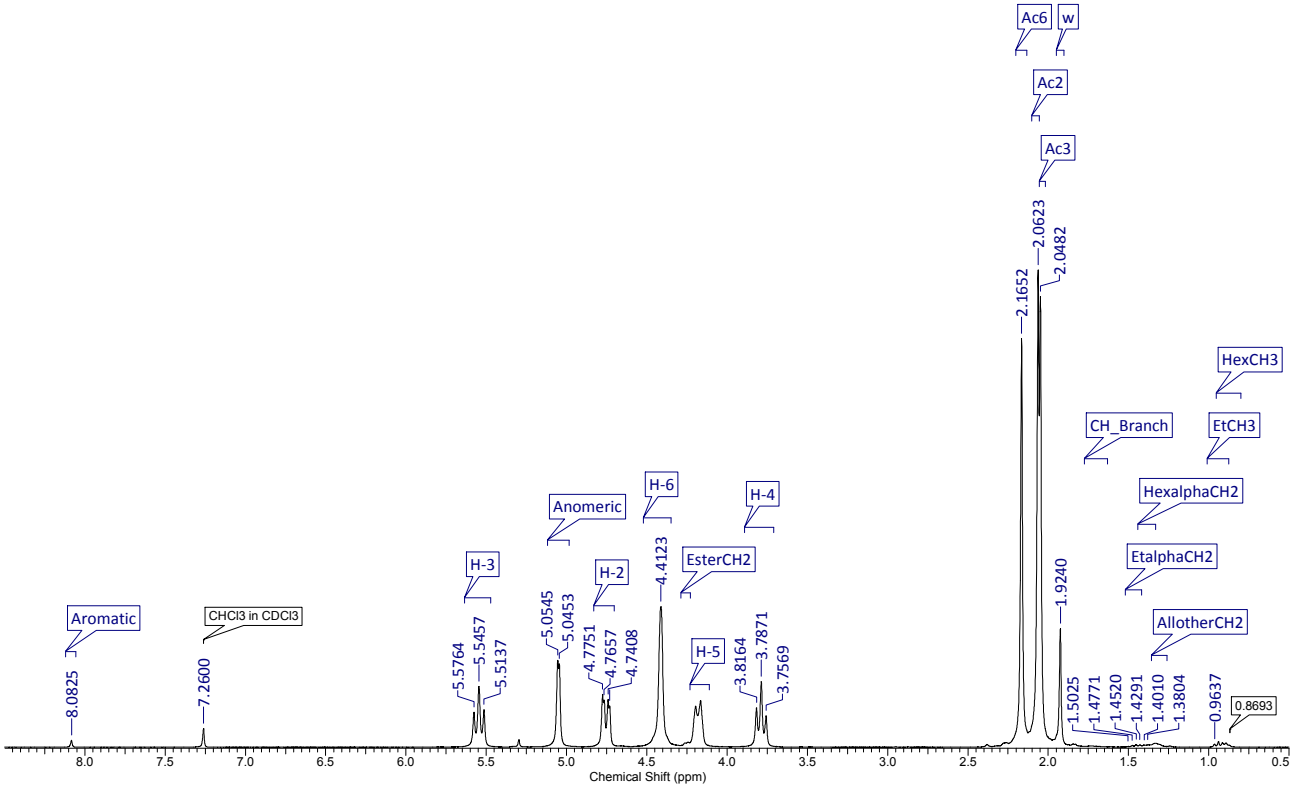


Figure S2.1.a. Peracetyl-αCD, ~23:1 host:guest ratio

Acquisition Time (sec)	3.6438	***Comment***	peracetyl aCD B + 7 ul DEHT			***Date***	30 Sep 2014 18:04:16
Date Stamp	30 Sep 2014 18:04:16			***File Name***	peracetyl aCD_DEHT.071.fid		
Frequency (MHz)	300.13	***Nucleus***	1H	***Number of Transients***	64	***Origin***	spect
Owner	root	***Points Count***	65536	***Pulse Sequence***	zg	***Receiver Gain***	90.50
Solvent	CDCl3	***Spectrum Offset (Hz)***	1074.7059	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	4496.33

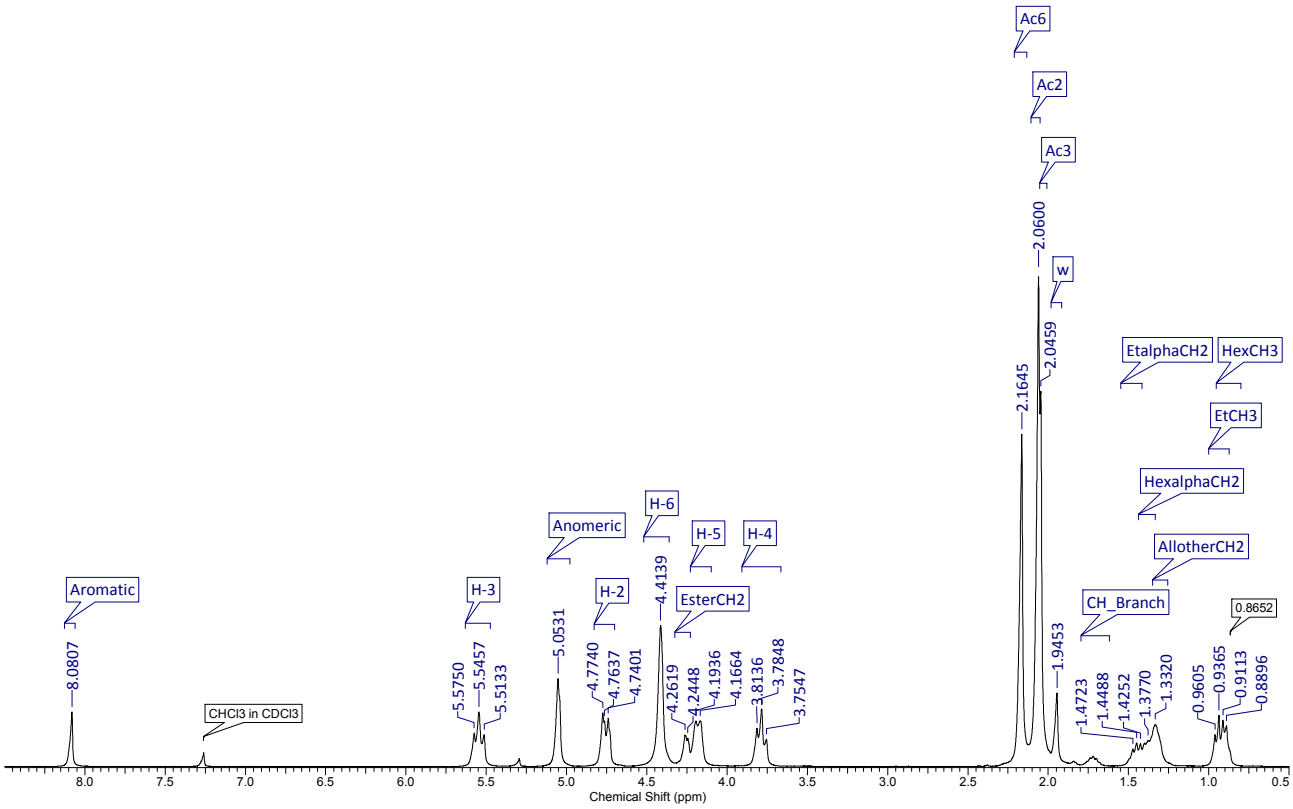


Figure S2.1.b. Peracetyl-αCD, ~1.4:1 host:guest ratio

Acquisition Time (sec)	3.6438	***Comment***	peracetyl aCD C_last addition of DEHT farma shim			***Date***	30 Sep 2014 19:08:16
Date Stamp	30 Sep 2014 19:08:16			***File Name***	peracetyl aCD_DEHT\131.esp		
Frequency (MHz)	300.13	***Nucleus***	1H	***Number of Transients***	64	***Origin***	spect
Owner	root	***Points Count***	65536	***Pulse Sequence***	zg	***Receiver Gain***	35.90
Solvent	CDCl3			***Spectrum Offset (Hz)***	1075.3918	***Spectrum Type***	STANDARD
Temperature (degree C)	22.760						

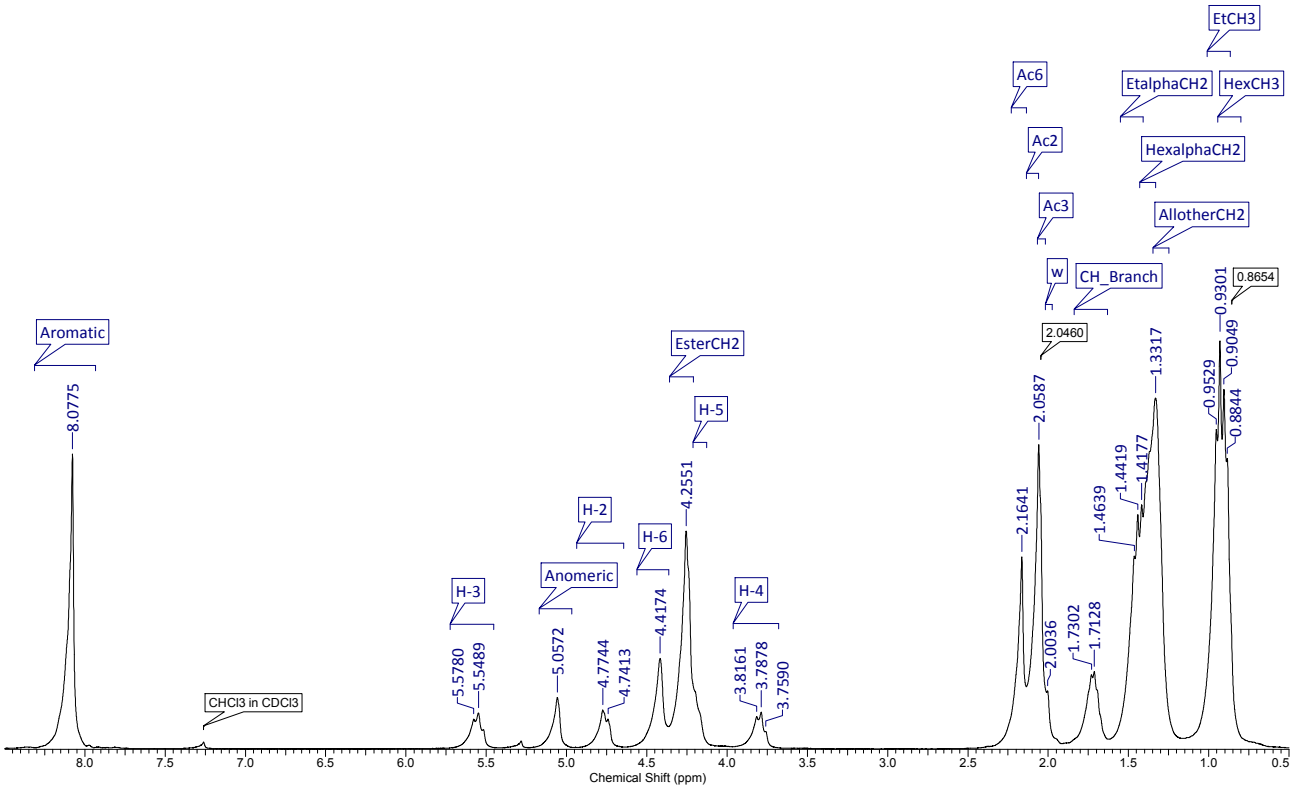


Figure S2.1.c. Peracetyl-αCD, ~1:10 host:guest ratio

Acquisition Time (sec)	3.6438	***Comment***	perACbCD A +1ul DEHT farma shim			***Date***	10 Nov 2014 10:29:36		
Date Stamp	10 Nov 2014 10:29:36			***File Name***	perAcbCD_DEHT5.011.esp				
Frequency (MHz)	300.13	***Nucleus***	1H	***Number of Transients***	64	***Origin***	spect	***Original Points Count***	16384
Owner	root	***Points Count***	65536	***Pulse Sequence***	zg	***Receiver Gain***	71.80	***SW(cyclical) (Hz)***	4496.40
Solvent	CDCl3			***Spectrum Offset (Hz)***	1074.1567	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	4496.33
Temperature (degree C)	22.660								

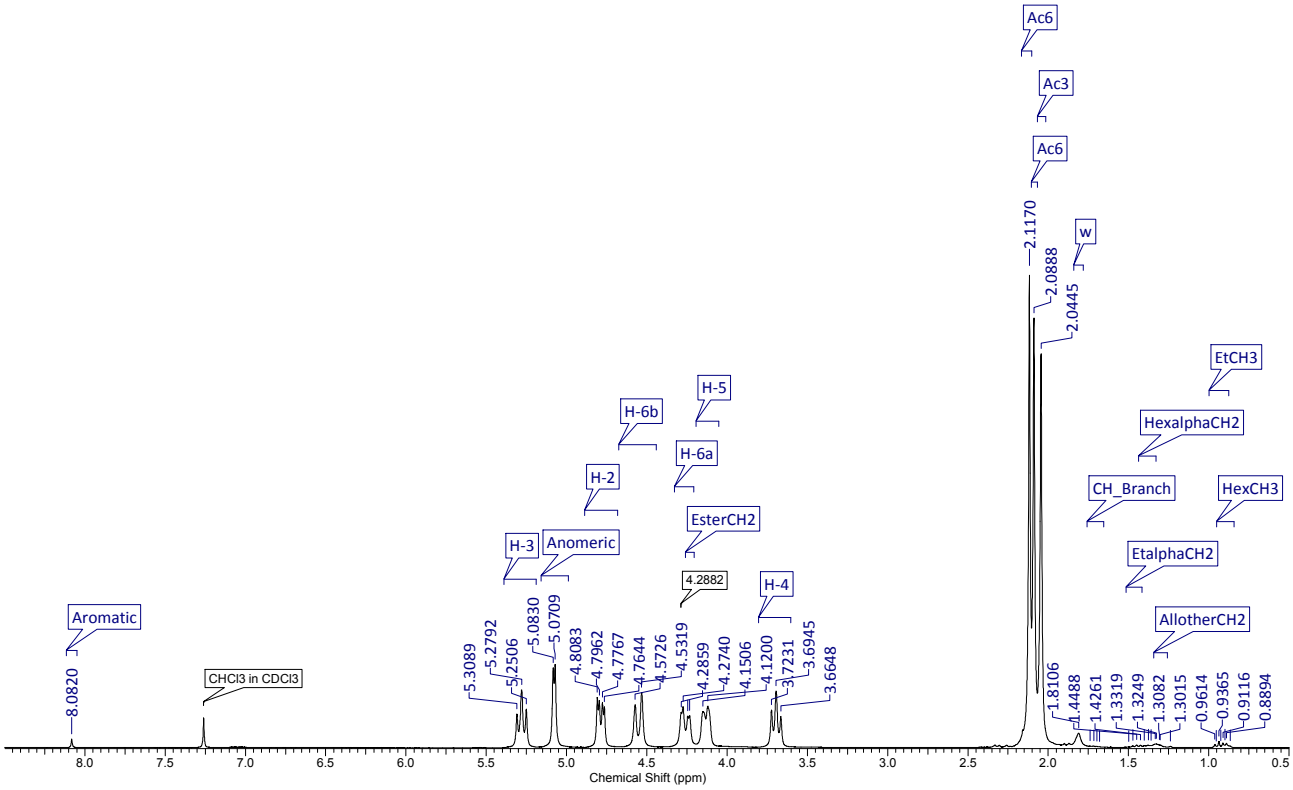


Figure S2.2.a. Peracetyl-βCD, ~20:1 host:guest ratio

Acquisition Time (sec)	3.6438	***Comment***	perACbCD B + 8ul DEHT farma shim			***Date***	10 Nov 2014 11:48:32		
Date Stamp	10 Nov 2014 11:48:32			***File Name***	perAcbCD_DEHT5.071.esp				
Frequency (MHz)	300.13	***Nucleus***	1H	***Number of Transients***	64	***Origin***	spect	***Original Points Count***	16384
Owner	root	***Points Count***	65536	***Pulse Sequence***	zg	***Receiver Gain***	71.80	***SW(cyclical) (Hz)***	4496.40
Solvent	CDCL3			***Spectrum Offset (Hz)***	1074.0883	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	4496.33
Temperature (degree C)	22.460								

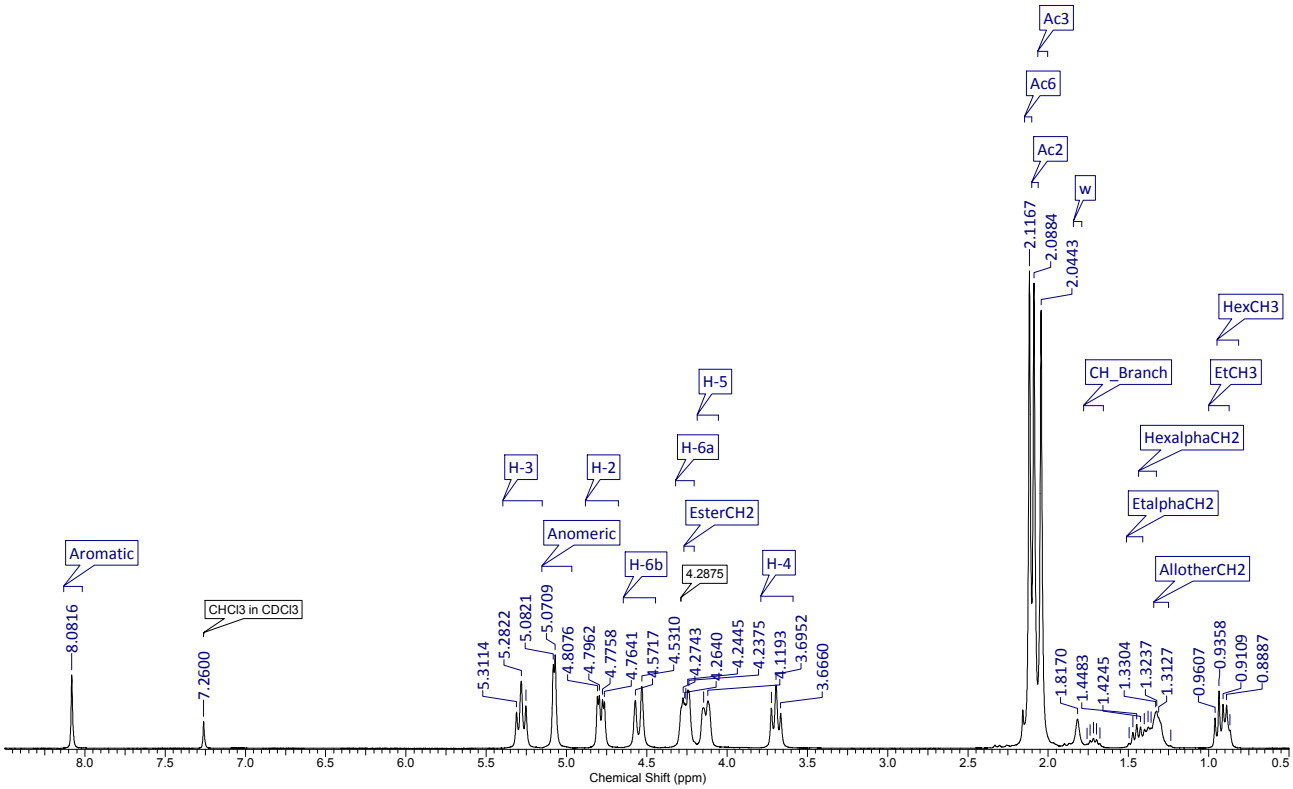


Figure S2.2.b. Peracetyl-βCD, ~1.2:1 host:guest ratio

Acquisition Time (sec)	3.6438	***Comment***	perAcbCD C + 102ul DEHT farma shim			***Date***	10 Nov 2014 13:05:20		
Date Stamp	10 Nov 2014 13:05:20			***File Name***	perAcbCD_DEHT5.131\.esp				
Frequency (MHz)	300.13	***Nucleus***	1H	***Number of Transients***	64	***Origin***	spect	***Original Points Count***	16384
Owner	root	***Points Count***	65536	***Pulse Sequence***	zg	***Receiver Gain***	35.90	***SW(cyclical) (Hz)***	4496.40
Solvent	CDCl3			***Spectrum Offset (Hz)***	1074.1567	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	4496.33
Temperature (degree C)	22.560								

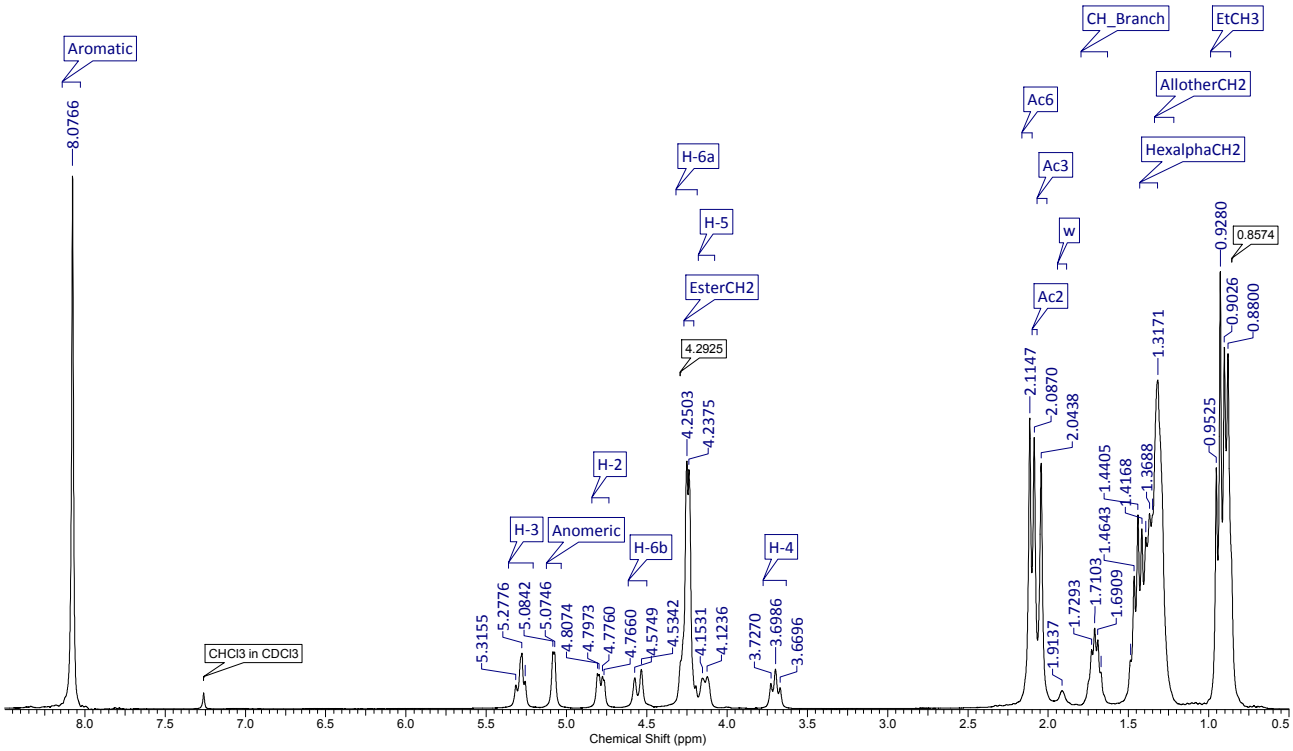


Figure S2.2.c. Peracetyl-βCD, ~1:10 host:guest ratio

Acquisition Time (sec)	3.6438	***Comment***	perAcgCD new dried + 50 ul DEHT in 700ul CDCl3						
Date	13 Feb 2015 17:23:28	***Date Stamp***	13 Feb 2015 17:23:28	***File Name***	perAcgCD_DEHT_dried.011.esp				
Frequency (MHz)	300.13	***Nucleus***	1H	***Origin***	spect	***Original Points Count***	16384		
Owner	root	***Points Count***	65536	***SW(cyclical) (Hz)***	4496.40	***Solvent***	CDCl3		
Spectrum Offset (Hz)	1074.4313	***Sweep Width (Hz)***	4496.33	***Temperature (degree C)***	22.660				

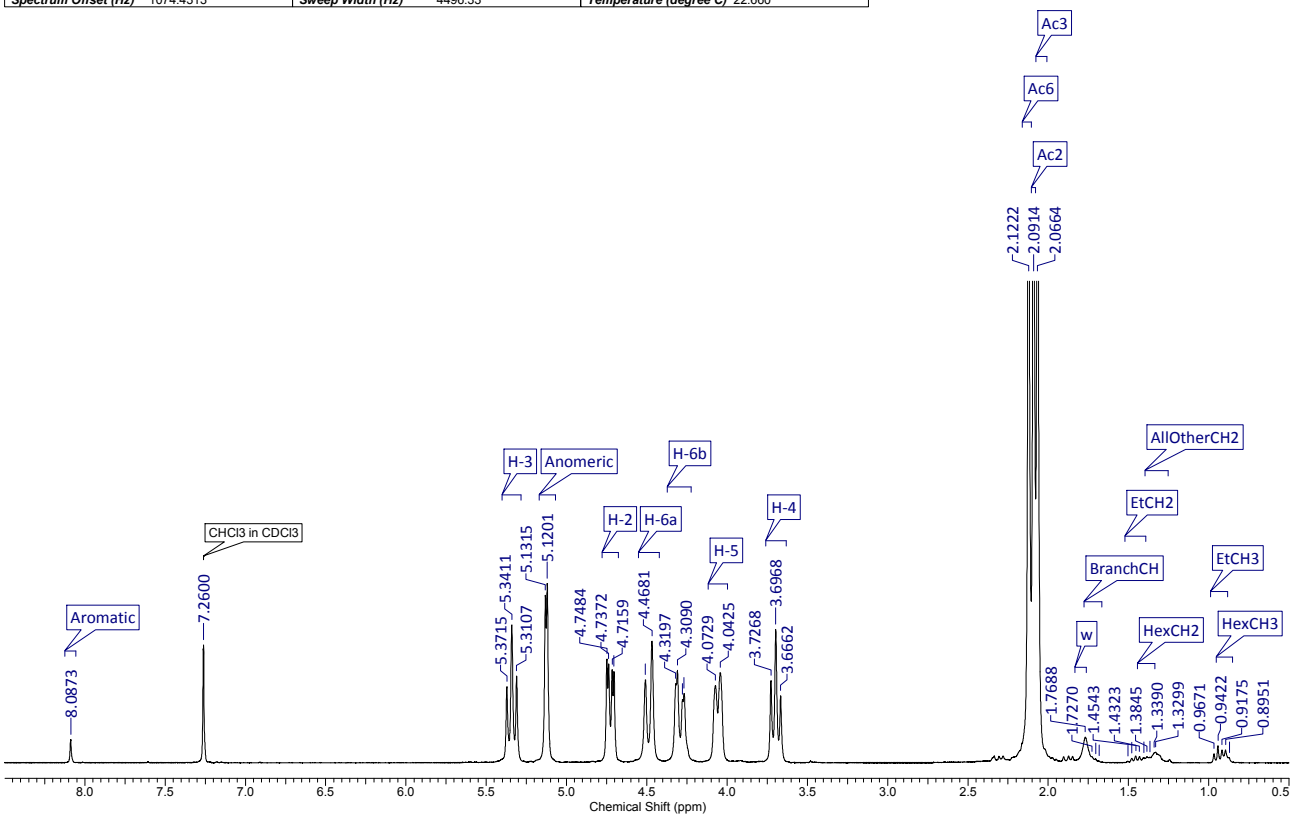


Figure S2.3.a. Peracetyl-γCD, ~13:1 host:guest ratio

Acquisition Time (sec)	3.6438	***Comment***	perAcgCD new dried + 450 ul DEHT in 700ul CDCl3				
Date	13 Feb 2015 18:23:12			***Date Stamp***	13 Feb 2015 18:23:12		
File Name	perAcgCD_DEHT_dried.071.esp					***Frequency (MHz)***	300.13
Nucleus	1H	***Number of Transients***	64	***Origin***	spect	***Original Points Count***	16384
Owner	root	***Points Count***	65536	***Pulse Sequence***	zg	***Receiver Gain***	114.00
SW(cyclical) (Hz)	4496.40	***Solvent***	CDCl3	***Spectrum Offset (Hz)***	1073.7452	***Spectrum Type***	STANDARD
Sweep Width (Hz)	4496.33	***Temperature (degree C)***	22.660				

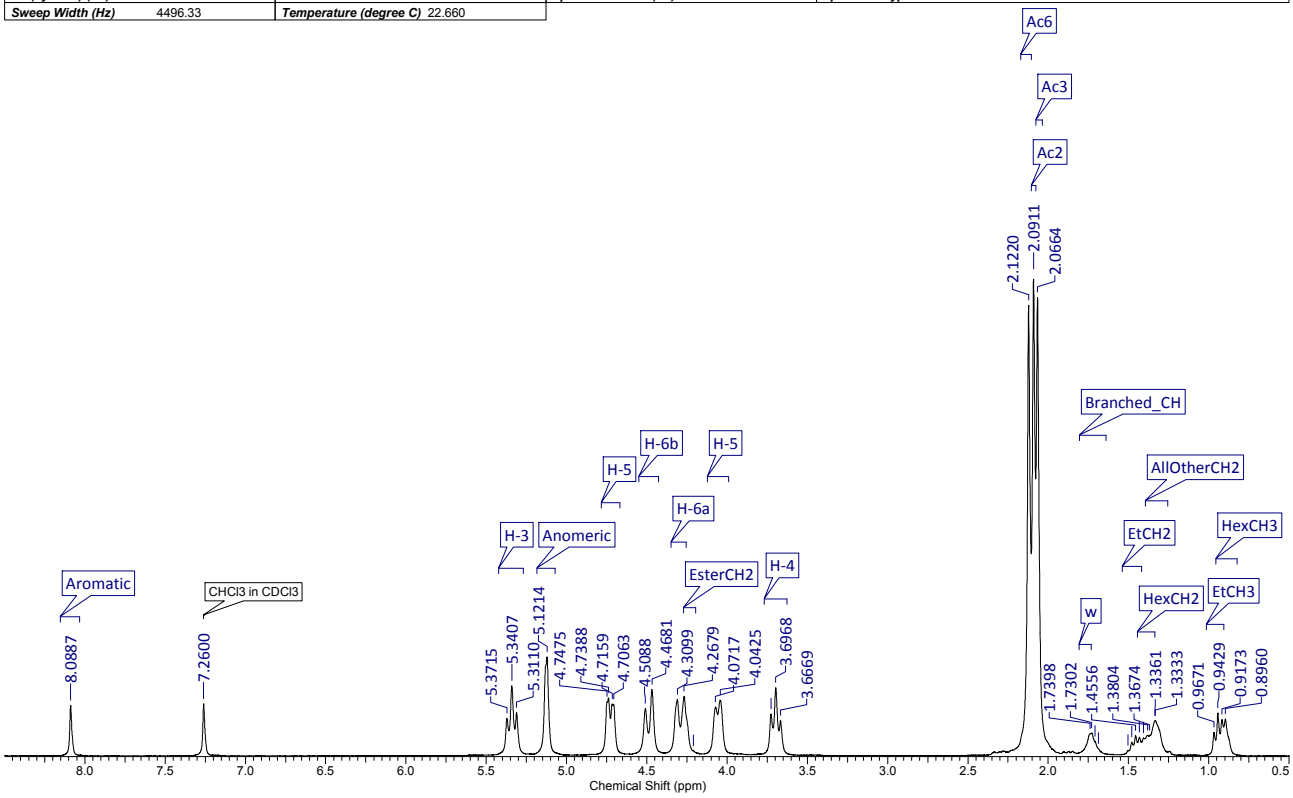


Figure S2.3.b. Peracetyl-γCD, ~1.3:1 host:guest ratio

Acquisition Time (sec)	3.6438	***Comment***	perAcgCD new dried + 3700 ul DEHT in 700ul CDCl3				
Date	16 Feb 2015 12:24:48	***Date Stamp***	16 Feb 2015 12:24:48	***File Name***	perAcgCD_newdried.131.esp		
Frequency (MHz)	300.13	***Nucleus***	1H	***Origin***	spect	***Original Points Count***	16384
Owner	root	***Points Count***	65536	***SW(cyclical) (Hz)***	4496.40	***Solvent***	CDCl3
Spectrum Offset (Hz)	1074.0881	***Sweep Width (Hz)***	4496.33	***Temperature (degree C)***	22.660		

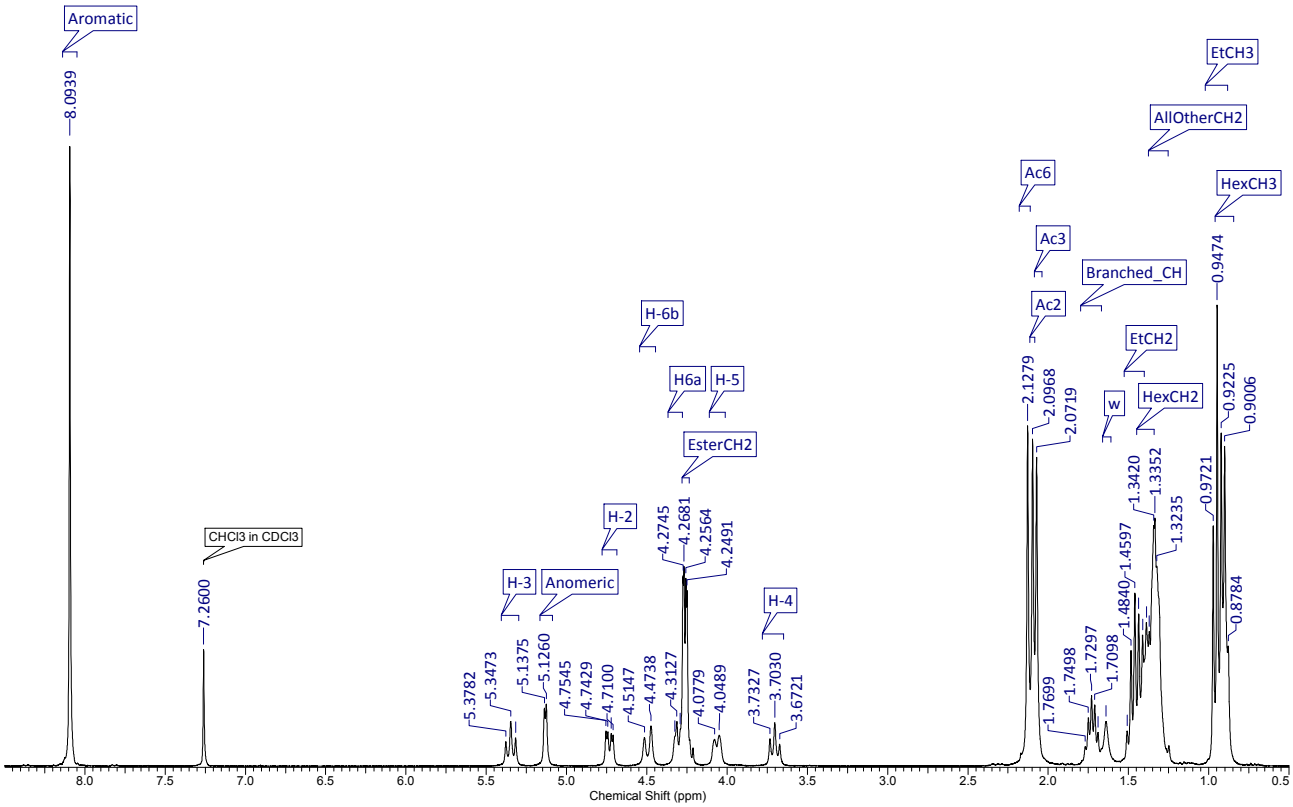


Figure S2.3.c. Peracetyl-γCD, ~1:17 host:guest ratio

Table S1.a1. Peracetyl-αCD/water, water proton shifts*,**

c_water [M]	c_CD [M]	Water δ
0.0039159	0.0036037	1.7025
0.0084344	0.0071876	1.7763
0.0135885	0.0107517	1.8424
0.0181937	0.0142962	1.8552
0.0233774	0.0178212	1.8938
0.0303678	0.0213271	1.9434
0.0364552	0.0248138	1.9672
0.0426298	0.0284199	1.9830
0.0725241	0.0390489	2.0726

Table S1.a2. Peracetyl-αCD/water, peracetyl cyclodextrin proton shifts

c_CD [M]	c_water [M]	alpha-Ac3	alpha-Ac2	alpha-Ac6	alpha-Ac4	alpha-Ac5
0.000990	0.001104	2.0564	2.0724	2.1839	3.7934	4.1868
0.003604	0.003916	2.0605	2.0735	2.1698	3.7995	4.1932
0.007188	0.008434	2.0552	2.0699	2.1691	3.7944	4.1875
0.010752	0.013589	2.0520	2.0669	2.1677	3.7912	4.1839
0.014296	0.018194	2.0516	2.0664	2.1670	3.7911	4.1837
0.017821	0.023377	2.0502	2.0651	2.1650	3.7892	4.1821
0.018069	0.035792	2.0470	2.0626	2.1720	3.7840	4.1829
0.021327	0.030368	2.0471	2.0621	2.1641	3.7862	4.1788
0.022983	0.058100	2.0443	2.0594	2.1700	3.7810	4.1744
0.024814	0.036455	2.0459	2.0610	2.1634	3.7851	4.1775
0.028420	0.042630	2.0328	2.0605	2.1629	3.7846	4.1769
0.039049	0.072524	2.0365	2.0518	2.1565	3.7755	4.1680

c_CD [M]	c_water [M]	alpha-Ac6a	alpha-Ac6b	alpha-Ac2	alpha-Ac1	alpha-Ac3
0.000990	0.001104	4.4146	4.4146	4.7679	5.0565	5.5611
0.003604	0.003916	4.4222	4.4280	4.7604	5.0589	5.5508
0.007188	0.008434	4.4148	4.4220	4.7584	5.0554	5.5484
0.010752	0.013589	4.4112	4.4190	4.7565	5.0529	5.5474
0.014296	0.018194	4.4112	4.4196	4.7560	5.0525	5.5469
0.017821	0.023377	4.4100	4.4170	4.7541	5.0505	5.5445
0.018069	0.035792	4.4048	4.4144	4.7571	5.0480	5.5506
0.021327	0.030368	4.4062	4.4148	4.7521	5.0480	5.5436
0.022983	0.058100	4.4048	4.4048	4.7539	5.0442	5.5481
0.024814	0.036455	4.4050	4.4139	4.7513	5.0468	5.5429
0.028420	0.042630	4.4050	4.4132	4.7508	5.0464	5.5423
0.039049	0.072524	4.3950	4.3996	4.7434	5.0380	5.5358

* concentrations are calculated values in all tables

** Not all data was used in the stability constant calculations, in all cases the out-of tolerance points were removed during the nonlinear fitting. Usually, not less than 9 were used in calculations.

Table S1.b. Peracetyl-αCD/1,4-bis(2-ethylhexyl)benzene-1,4-dicarboxylate, guest proton shifts[#]

c_guest [M]	c_CD [M]	Hexyl-CH3	Ethyl-CH3	Hex-alphaCH2	Et-CH2	Branch-CH	Ester-CH2	Aromatic-CH
0.001066	0.024072	0.8693	0.9637	1.3896	1.4771	1.7025	4.2578	8.0825
0.002130*	0.024052	0.8700	0.9630	1.3871	1.4691	1.7024	4.2727	8.0852
0.004253*	0.024012	0.8651	0.9607	1.3857	1.4805	1.7141	4.2528	8.0866
0.006369	0.023972	0.8690	0.9620	1.3860	1.4819	1.7158	4.2546	8.0820
0.008478*	0.023932	0.8648	0.9632	1.3879	1.4517	1.7240	4.2552	8.0830
0.012675	0.023853	0.8625	0.9591	1.3864	1.4714	1.7162	4.2519	8.0809
0.016845	0.023775	0.8652	0.9605	1.3770	1.4723	1.7067	4.2533	8.0807
0.023048*	0.023658	0.8670	0.9616	1.3865	1.4737	1.7240	4.2546	8.0820
0.033252	0.023466	0.8667	0.9582	1.3858	1.4689	1.7232	4.2506	8.0795
0.045281	0.023240	0.8685	0.9593	1.3851	1.4705	1.7279	4.2525	8.0804
0.064821	0.022872	0.8627	0.9596	1.3854	1.4712	1.7178	4.2530	8.0800
0.102103	0.022170	0.8615	0.9575	1.3827	1.4668	1.7143	4.2508	8.0790
0.186014	0.020591	0.8654	0.9529	1.3810	1.4639	1.7215	4.2551	8.0775

when the multiplet could not be used always the less overlapping relevant signal was used

* removed from 2:1 calculations

Table S1.c. Peracetyl-αCD/1,4-bis(2-ethylhexyl) benzene-1,4-dicarboxylate cyclodextrin proton shifts

c_CD [M]	c_guest [M]	alpha-Ac3	alpha-Ac2	alpha-Ac6	alpha-H4	alpha-H5
0.0243605	0.0010660	2.0482	2.0523	2.1652	3.7868	4.1800
0.0243403	0.0021301	2.0479	2.0621	2.1654	3.7864	4.1797
0.0242998	0.0042532	2.0465	2.0600	2.1654	3.7860	4.1803
0.0242595	0.0063692	2.0468	2.0610	2.1654	3.7855	4.1795
0.0242194	0.0084782	2.0495	2.0621	2.1663	3.7871	4.1820
0.0241394	0.0126754	2.0460	2.0598	2.1647	3.7850	4.1790
0.0240600	0.0168449	2.0459	2.0600	2.1645	3.7844	4.1800
0.0239419	0.0230480	2.0482	2.0612	2.1657	3.7863	4.1840
0.0237476	0.0332523	2.0453	2.0589	2.1636	3.7840	4.1800
0.0235185	0.0452808	2.0472	2.0603	2.1647	3.7853	4.1845
0.0231464	0.0648209	2.0463	2.0598	2.1645	3.7849	4.1820
0.0224364	0.1021029	2.0462	2.0596	2.1647	3.7840	4.1810
0.0208383	0.1860139	2.0460	2.0587	2.1641	3.7880	4.1790

c_CD [M]	c_guest [M]	alpha-H6a	alpha-H6b	alpha-H2	alpha-H1	alpha-H3
0.0243605	0.0010660	4.4123	4.4123	4.7533	5.0499	5.5453
0.0243403	0.0021301	4.4119	4.4119	4.7532	5.0494	5.5453
0.0242998	0.0042532	4.4139	4.4139	4.7567	5.0529	5.5451
0.0242595	0.0063692	4.4142	4.4142	4.7602	5.0538	5.5454
0.0242194	0.0084782	4.4155	4.4155	4.7583	5.0545	5.5462
0.0241394	0.0126754	4.4144	4.4144	4.7563	5.0529	5.5437
0.0240600	0.0168449	4.4139	4.4139	4.7593	5.0531	5.5447
0.0239419	0.0230480	4.4160	4.4160	4.7583	5.0549	5.5458
0.0237476	0.0332523	4.4139	4.4139	4.7561	5.0529	5.5439
0.0235185	0.0452808	4.4151	4.4151	4.7577	5.0545	5.5456
0.0231464	0.0648209	4.4148	4.4148	4.7596	5.0538	5.5454
0.0224364	0.1021029	4.4169	4.4169	4.7596	5.0561	5.5538
0.0208383	0.1860139	4.4174	4.4174	4.7579	5.0572	5.5634

Table S2.a1. Peracetyl-βCD/water water proton shifts

c_water [M]	c_CD [M]	Water δ
0.0038176	0.0036037	1.6609
0.0081900	0.0071876	1.7116
0.0133052	0.0107517	1.7560
0.0177344	0.0142962	1.7797
0.0222107	0.0178212	1.8241
0.0291092	0.0213271	1.8570
0.0359426	0.0248833	1.8680
0.0432463	0.0284890	1.8888
0.0806911	0.0424398	1.9763
0.1936385	0.0628017	2.0159

Table S2.a2. Peracetyl-βCD/water cyclodextrin proton shifts

c_CD [M]	c_water [M]	beta-Ac3	beta-Ac2	beta-Ac6	beta-H4	beta-H5
0.000939	0.001045	2.0573	2.1026	2.1314	3.7072	4.1494
0.003604	0.003818	2.0559	2.0970	2.1263	3.7089	4.1410
0.007188	0.008190	2.0550	2.0968	2.1258	3.7061	4.1397
0.010752	0.013305	2.0499	2.0922	2.1210	3.7023	4.1367
0.014296	0.017734	2.0497	2.0920	2.1208	3.7013	4.1365
0.017821	0.022211	2.0486	2.0897	2.1187	3.7300	4.1343
0.021327	0.029109	2.0447	2.0867	2.1153	3.6968	4.1308
0.024883	0.035943	2.0435	2.0856	2.1144	3.6956	4.1365
0.028489	0.043246	2.0422	2.0847	2.1133	3.6930	4.1319
0.042440	0.080691	2.0310	2.0744	2.1023	3.6818	4.1182
0.062802	0.193639	2.0214	2.0641	2.0915	3.6726	4.1085

c_CD [M]	c_water [M]	beta-H6a	beta-H6b	beta-H2	beta-H1	beta-H3
0.000939	0.001045	4.2727	4.5661	4.8800	5.0916	5.2907
0.003604	0.003818	4.2726	4.5530	4.7918	5.0824	5.3060
0.007188	0.008190	4.2706	4.5480	4.7924	5.0824	5.3015
0.010752	0.013305	4.2666	4.5540	4.7884	5.0789	5.2954
0.014296	0.017734	4.2662	4.5520	4.7882	5.0788	5.2953
0.017821	0.022211	4.2648	4.5485	4.7849	5.0756	5.2969
0.021327	0.029109	4.2607	4.5471	4.7821	5.0729	5.2898
0.024883	0.035943	4.2595	4.5466	4.7814	5.0723	5.2883
0.028489	0.043246	4.2576	4.5447	4.7805	5.0710	5.2855
0.042440	0.080691	4.2459	4.5352	4.7708	5.0616	5.2709
0.062802	0.193639	4.2360	4.5251	4.7599	5.0513	5.2627

Table S2.b. Peracetyl-βCD/1,4-bis(2-ethylhexyl) benzene-1,4-dicarboxylate, guest proton shifts[#]

c_guest [M]	c_CD [M]	Hexyl-CH3	Ethyl-CH3	Hex-alphaCH2	Et-CH2	Branch-CH	Ester-CH2	Aromatic-CH
0.001066	0.024072	0.8655	0.9607	1.4721	1.3913	1.7081	4.2329	8.0820
0.002130	0.024052	0.8661	0.9605	1.4714	1.3906	1.7088	4.2330	8.0814
0.004253[*]	0.024012	0.8658	0.9593	1.4714	1.3659	1.7175	4.2343	8.0807
0.006369	0.023972	0.8673	0.9607	1.4723	1.3833	1.7165	4.2439	8.0823
0.008478	0.023932	0.8658	0.9607	1.4721	1.3705	1.7107	4.2455	8.0818
0.012675	0.023853	0.8656	0.9586	1.4705	1.3765	1.7062	4.2358	8.0802
0.016845[**]	0.023775	0.8688	0.9607	1.4723	1.3902	1.7187	4.2500	8.0816
0.023048	0.023658	0.8670	0.9605	1.4725	1.3668	1.7085	4.2370	8.0811
0.033252	0.023466	0.8635	0.9580	1.4700	1.3644	1.7160	4.2349	8.0793
0.045281	0.023240	0.8649	0.9586	1.4707	1.3649	1.7163	4.2361	8.0800
0.064821	0.022872	0.8635	0.9586	1.4703	1.3764	1.7160	4.2370	8.0801
0.102103	0.022170	0.8616	0.9564	1.4684	1.3749	1.7139	4.2354	8.0788
0.186014	0.020591	0.8574	0.9525	1.4643	1.3698	1.7100	4.2375	8.0786

when the multiplet could not be used always the less overlapping relevant signal was used

[*] removed from 1:2 calculations

[**] removed from 1:1 and 2:1 calculations

Table S2.c. Peracetyl-βCD/1,4-bis(2-ethylhexyl) benzene-1,4-dicarboxylate cyclodextrin proton shifts

c_CD [M]	c_guest [M]	beta-Ac3	beta-Ac2	beta-Ac6	beta-H4	beta-H5
0.0207979	0.0010660	2.0445	2.0888	2.1170	3.6941	4.1353
0.0207806	0.0021301	2.0436	2.0879	2.1160	3.6932	4.1318
0.0207461	0.0042532	2.0431	2.0875	2.1156	3.6931	4.1337
0.0207117	0.0063692	2.0450	2.0891	2.1167	3.6954	4.1331
0.0206774	0.0084782	2.0475	2.0904	2.1172	3.6976	4.1384
0.0206091	0.0126754	2.0431	2.0870	2.1151	3.6932	4.1332
0.0205413	0.0168449	2.0443	2.0884	2.1167	3.6950	4.1330
0.0204405	0.0230480	2.0445	2.0884	2.1165	3.6955	4.1356
0.0202746	0.0332523	2.0457	2.0866	2.1147	3.6937	4.1344
0.0200790	0.0452808	2.0438	2.0875	2.1156	3.6953	4.1360
0.0197613	0.0648209	2.0440	2.0879	2.1160	3.6956	4.1334
0.0191551	0.1021029	2.0440	2.0875	2.1154	3.6964	4.1342
0.0177908	0.1860139	2.0438	2.0870	2.1147	3.6984	4.1384

c_CD [M]	c_guest [M]	beta-H6a	beta-H6b	beta-H2	beta-H1	beta-H3
0.0207979	0.0010660	4.2594	4.5522	4.7864	5.0770	5.2756
0.0207806	0.0021301	4.2839	4.5506	4.7855	5.0760	5.2790
0.0207461	0.0042532	4.2845	4.5502	4.7847	5.0754	5.2794
0.0207117	0.0063692	4.2831	4.5522	4.7895	5.0789	5.2825
0.0206774	0.0084782	4.2839	4.5554	4.7918	5.0824	5.2848
0.0206091	0.0126754	4.2825	4.5505	4.7843	5.0752	5.2789
0.0205413	0.0168449	4.2600	4.5513	4.7859	5.0765	5.2822
0.0204405	0.0230480	4.2864	4.5519	4.7859	5.0766	5.2832
0.0202746	0.0332523	4.2845	4.5505	4.7842	5.0753	5.2809
0.0200790	0.0452808	4.2848	4.5515	4.7852	5.0764	5.2838
0.0197613	0.0648209	4.2880	4.5520	4.7860	5.0771	5.2837
0.0191551	0.1021029	4.2893	4.5526	4.7858	5.0776	5.2842
0.0177908	0.1860139	4.2925	4.5545	4.7867	5.0794	5.2838

Table S3.a1. Peracetyl-γCD/water water proton shifts

c_water [M]	c_CD [M]	Water δ
0.0038033	0.0036037	1.6680
0.0080206	0.0071876	1.7190
0.0126228	0.0107517	1.7430
0.0174527	0.0142962	1.7760
0.0219705	0.0178212	1.8000
0.0287624	0.0214669	1.8430
0.0353124	0.0253004	1.8710
0.0415519	0.0290419	1.8890
0.0764351	0.0495687	2.0290
0.1276147	0.0758860	2.0290

Table S3.a2. Peracetyl-γCD/water cyclodextrin proton shifts

c_CD [M]	c_water [M]	gamma-Ac3	gamma-Ac2	gamma-Ac6	gamma-H4	gamma-H5
0.001207	0.001349	2.0575	2.0978	2.1291	3.7031	4.0649
0.003604	0.003803	2.0720	2.0960	2.1270	3.7010	4.0650
0.007188	0.008021	2.0700	2.0940	2.1250	3.6990	4.0620
0.010752	0.012623	2.0670	2.0920	2.1220	3.6970	4.0580
0.014296	0.017453	2.0650	2.0900	2.1200	3.6950	4.0570
0.017821	0.021971	2.0640	2.0880	2.1190	3.6930	4.0550
0.020925	0.047605	2.0727	2.0960	2.1285	3.7022	4.0631
0.021467	0.028762	2.0610	2.0860	2.1170	3.6900	4.0510
0.022983	0.046542	2.0610	2.0859	2.1167	3.6914	4.0526
0.025300	0.035312	2.0600	2.0840	2.1150	3.6890	4.0510
0.029042	0.041552	2.0580	2.0830	2.1130	3.6880	4.0500
0.049569	0.076435	2.0460	2.0700	2.1000	3.6750	4.0340
0.075886	0.127615	2.0290	2.0530	2.0820	3.6600	4.0210

c_CD [M]	c_water [M]	gamma-H6a	gamma-H6b	gamma-H2	gamma-H1	gamma-H3
0.001207	0.001349	4.3004	4.4944	4.7334	5.1324	5.3480
0.003604	0.003803	4.2980	4.4940	4.7280	5.1310	5.3440
0.007188	0.008021	4.2960	4.4920	4.7260	5.1290	5.3420
0.010752	0.012623	4.2930	4.4890	4.7240	5.1260	5.3390
0.014296	0.017453	4.2920	4.4870	4.7230	5.1240	5.3380
0.017821	0.021971	4.2890	4.4850	4.7210	5.1230	5.3180
0.020925	0.047605	4.2992	4.4937	4.7320	5.1314	5.3470
0.021467	0.028762	4.2870	4.4810	4.7190	5.1200	5.3340
0.022983	0.046542	4.2885	4.4825	4.7205	5.1208	5.3361
0.025300	0.035312	4.2860	4.4810	4.7170	5.1190	5.3320
0.029042	0.041552	4.2840	4.4790	4.7160	5.1170	5.3310
0.049569	0.076435	4.2710	4.4640	4.7020	5.1040	5.3180
0.075886	0.127615	4.2550	4.4490	4.6850	5.0890	5.3180

Table S3.b. Peracetyl-γCD/1,4-bis(2-ethylhexyl) benzene-1,4-dicarboxylate, guest proton shifts[#]

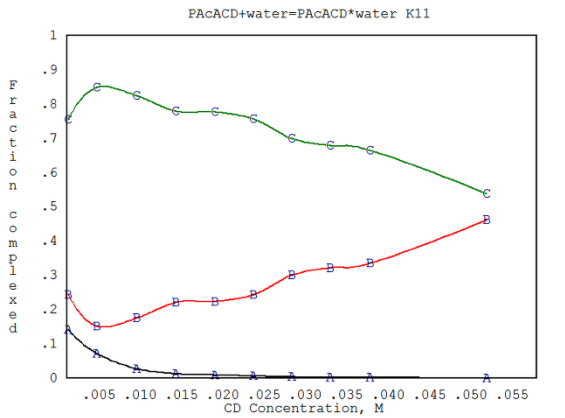
c_guest [M]	c_CD [M]	Hexyl-CH3	Ethyl-CH3	Hex-alphaCH2	Et-CH2	Branch-CH	Ester-CH2	Aromatic-CH
0.001338	0.016768	0.8750	0.9671	1.4065	1.5041	1.6831	4.2440	8.0883
0.002725	0.015526	0.8750	0.9671	1.4065	1.5041	1.6831	4.2443	8.0873
0.003921	0.014455	0.8729	0.9664	1.4062	1.5039	1.6838	4.2420	8.0873
0.005203	0.013308	0.8743	0.9671	1.4065	1.5018	1.6849	4.2432	8.0880
0.006296	0.012329	0.8761	0.9678	1.4060	1.5066	1.6867	4.2440	8.0884
0.007239	0.011485	0.8730	0.9678	1.4067	1.5082	1.6915	4.2440	8.0887
0.008062	0.010749	0.8740	0.9671	1.4060	1.5025	1.6872	4.2450	8.0887
0.009007	0.009902	0.8750	0.9676	1.4065	1.5027	1.6865	4.2450	8.0887
0.010175	0.008856	0.8740	0.9678	1.4081	1.5039	1.6874	4.2480	8.0889
0.011397	0.007763	0.8750	0.9680	1.4074	1.5059	1.6874	4.2460	8.0894
0.012556	0.006725	0.8757	0.9701	1.4101	1.5050	1.6715	4.2466	8.0919
0.014997[*]	0.004540	0.8777	0.9712	1.4108	1.5071	1.6595	4.2487	8.0932
0.016926[**]	0.002813	0.8784	0.9357	1.3671	1.4600	1.6399	4.2491	8.0939

when the multiplet could not be used always the less overlapping relevant signal was used
[*] removed from 1:1 and 2:1 calculations
[**] removed from 1:2 calculations

Table S3.c. Peracetyl-γCD/1,4-bis(2-ethylhexyl) benzene-1,4-dicarboxylate cyclodextrin proton shifts

c_CD [M]	c_guest [M]	gamma-Ac3	gamma-Ac2	gamma-Ac6	gamma-H4	gamma-H5
0.0167679	0.0013379	2.0664	2.0914	2.1222	3.6966	4.0577
0.0155258	0.0027253	2.0653	2.0902	2.1211	3.6959	4.0565
0.0144550	0.0039214	2.0653	2.0904	2.1213	3.6961	4.0567
0.0133078	0.0052029	2.0658	2.0907	2.1215	3.6964	4.0570
0.0123293	0.0062959	2.0662	2.0911	2.1220	3.6971	4.0579
0.0114848	0.0072392	2.0667	2.0914	2.1222	3.6972	4.0577
0.0107486	0.0080616	2.0664	2.0911	2.1220	3.6967	4.0571
0.0099023	0.0090070	2.0667	2.0914	2.1222	3.6970	4.0573
0.0088563	0.0101754	2.0669	2.0916	2.1224	3.6977	4.0580
0.0077629	0.0113968	2.0678	2.0927	2.1236	3.6989	4.0589
0.0067251	0.0125560	2.0699	2.0948	2.1256	3.7005	4.0621
0.0045400	0.0149968	2.0710	2.0959	2.1270	3.7014	4.0620
0.0028134	0.0169255	2.0719	2.0968	2.1279	3.7026	4.0634

c_CD [M]	c_guest [M]	gamma-H6a	gamma-H6b	gamma-H2	gamma-H1	gamma-H3
0.0167679	0.0013379	4.2936	4.4882	4.7265	5.1258	5.3412
0.0155258	0.0027253	4.2927	4.4677	4.7257	5.1251	5.3403
0.0144550	0.0039214	4.2982	4.4879	4.7260	5.1252	5.3406
0.0133078	0.0052029	4.2882	4.4883	4.7265	5.1256	5.3409
0.0123293	0.0062959	4.2895	4.4894	4.7270	5.1260	5.3414
0.0114848	0.0072392	4.2896	4.4894	4.7278	5.1264	5.3419
0.0107486	0.0080616	4.2889	4.4885	4.7271	5.1270	5.3411
0.0099023	0.0090070	4.2676	4.4887	4.7274	5.1217	5.3413
0.0088563	0.0101754	4.2888	4.4891	4.7277	5.1219	5.3414
0.0077629	0.0113968	4.2897	4.4911	4.7291	5.1276	5.3430
0.0067251	0.0125560	4.3110	4.4922	4.7297	5.1297	5.3453
0.0045400*	0.0149968	4.3090	4.4930	4.7312	5.1308	5.3463
0.0028134**	0.0169255	4.3120	4.4943	4.7323	5.1317	5.3480



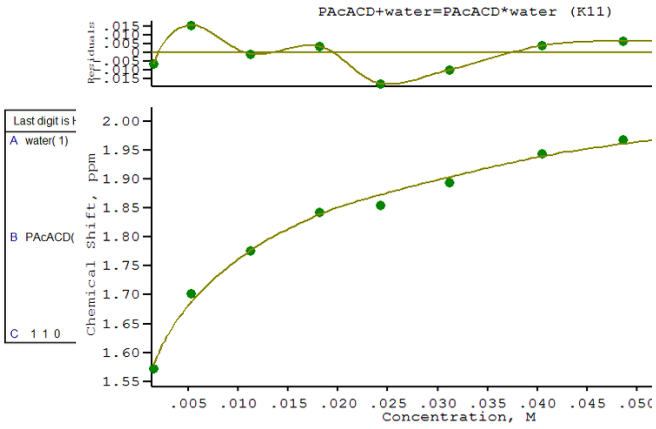
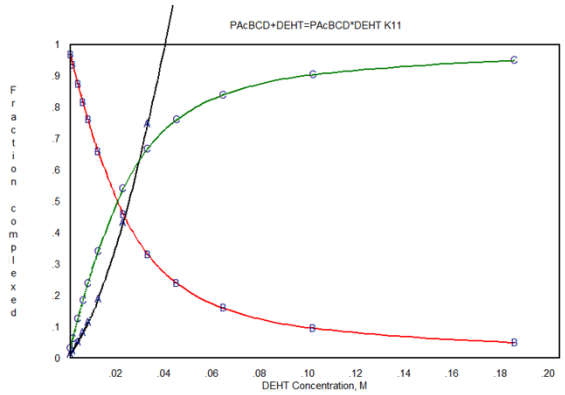
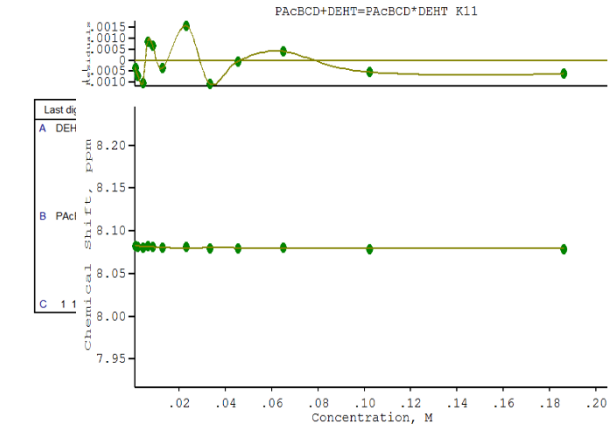
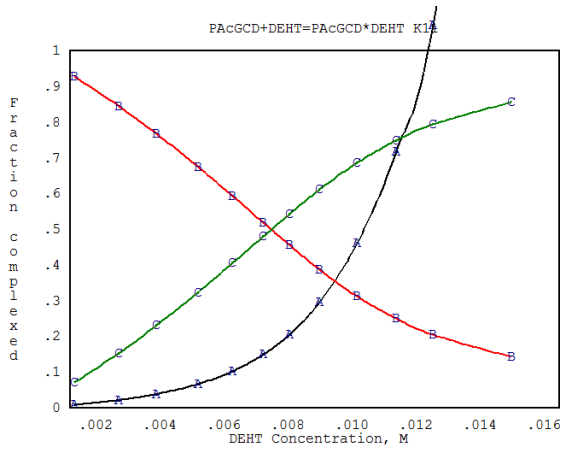


Figure S3.1. Simulated concentration curves for peracetyl CDs and water systems as 1:1 association







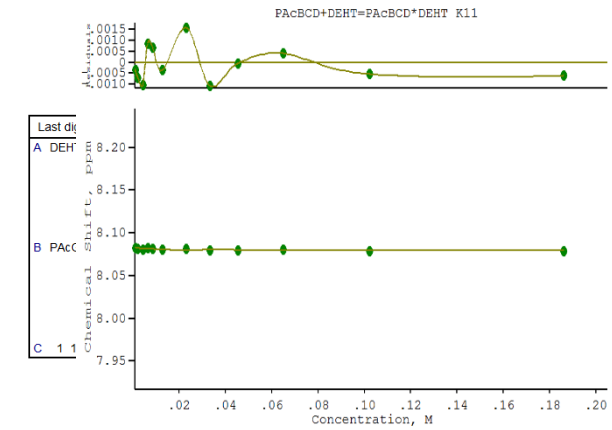


Figure S3.2. Calculated chemical shifts of peracetyl CDs and water systems.

Upper graphs show the deviation of measured and calculated shifts.

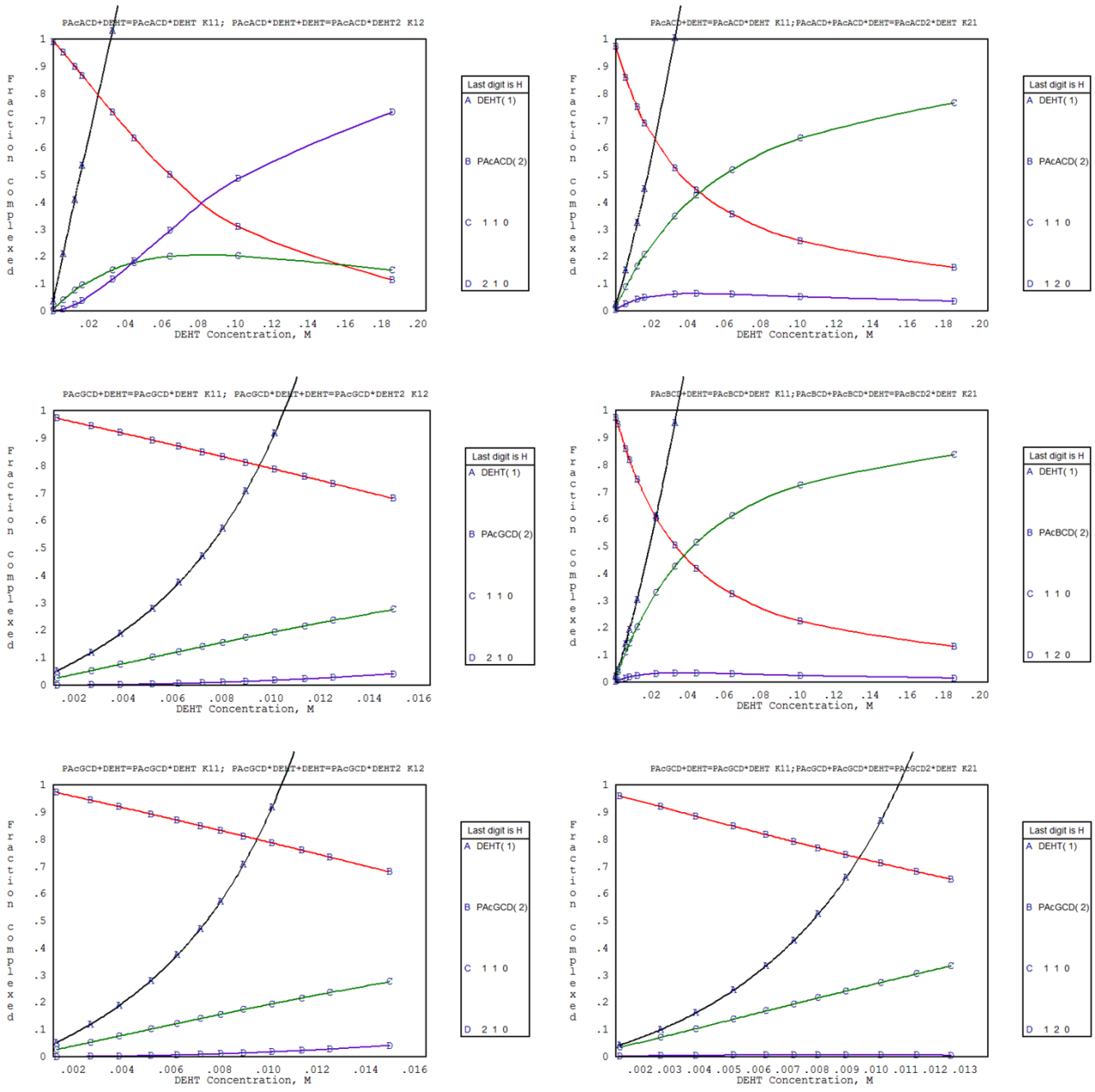


Figure S3.3. Simulated concentration curves for 1:2 (left), and 2:1 complexes (right).

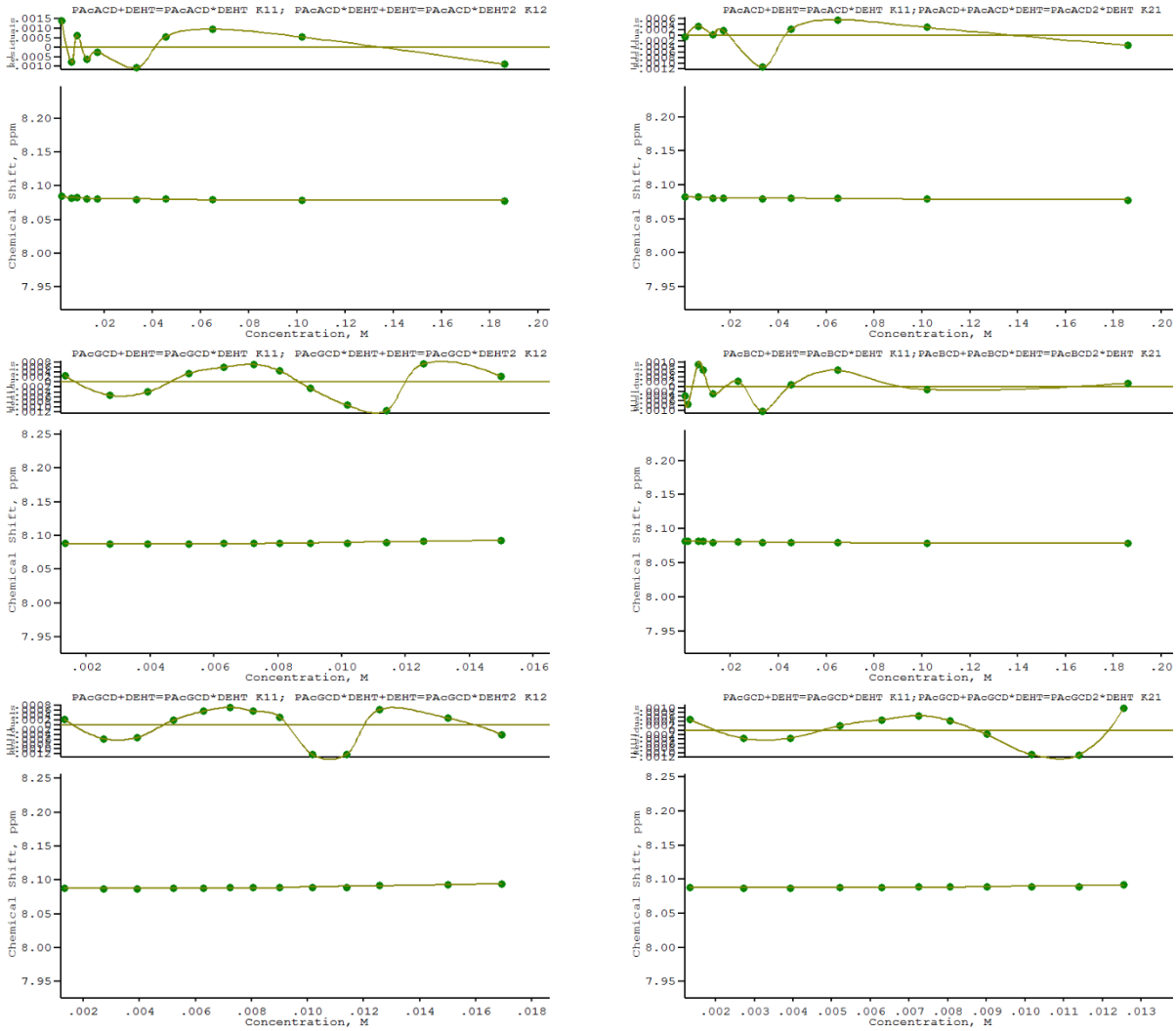


Figure S3.4. Measured and calculated chemical shifts for peracetyl CD and bis(2-ethylhexyl) benzene-1,4-dicarboxylate 1:2 (left) and 2:1 (right) systems. Upper graphs show the deviation between measured and calculated shifts.