Electronic Supplementary Material (ESI) for New Journal of Chemistry.

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Encapsulation of monoamine neurotransmitters and trace amines by amphiphilic anionic calix[5]arene micelles

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Electronic Supplementary Information

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Table S1. Diffusion coefficients ($D_{\mathbf{1}\mathrm{free}}$), hydrodynamic radii ($R_h$) and aggregation numbers (N) of the species present at 298 K in D_2O solutions of calixarene **1** at different concentrations. Data were calculated from DOSY experiments, using the SCH_2 resonance (δ = 2.87 ppm) as the probe signal.

C (mM)	$D_{\mathbf{1}\mathrm{free}} \times 10^{-10}$ (m^2/s)	R_h (Å)	N
10	0.82 ± 0.03	24.4 ± 0.9	14.3
7.5	0.82 ± 0.05	24.4 ± 1.4	14.3
5	0.94 ± 0.08	21.2 ± 1.6	9.5
2	1.17 ± 0.10	17.0 ± 1.3	4.9
1	1.62 ± 0.10	12.3 ± 0.7	1.8
0.8	1.78 ± 0.08	11.2 ± 0.5	1.4
0.64	1.89 ± 0.05	10.5 ± 0.2	1.2
0.5	1.94 ± 0.07	10.3 ± 0.4	1.1
0.4	1.98 ± 0.07	10.1 ± 0.4	1
0.3	2.04 ± 0.10	9.8 ± 0.5	0.9
0.2	1.99 ± 0.08	10.0 ± 0.5	1

Table S2. Chemical shifts (ppm) of neurotransmitters **2**–**7** (10 mM) prior and after binding to calixarene **1** (10 mM) and relative complexation induced shifts (cis). ^{1}H NMR spectra were recorded in D_2O (500 MHz, 298 K).[a]

Proton	δ (ppm)	δ_{bound} (ppm)	cis ($\Delta\delta$, ppm)
Pea·HCl (**2**)			
α-CH_2	3.16	3.01	0.15
		(–0.62)	(3.78)
β-CH_2	2.88	2.74	0.14
		(–0.81)	(3.69)
ArH(2,6)	7.21	6.91	0.30
		(4.75)	(2.46)
ArH(4)	7.23	6.76	0.47
		(6.54)	(0.69)
ArH(3,5)	7.30	7.02	0.28
		(6.29)	(1.01)
Tyrm·HCl (**3**)			
α-CH_2	3.10	2.94	0.16
β-CH_2	2.79	2.57	0.22
ArH(3,5)	7.08	6.86	0.22
ArH(2,6)	6.77	6.61	0.16
Dopa·HCl (**4**)			
α-CH_2	3.10	2.94	0.16
β-CH_2	2.75	2.51	0.24
ArH(6)	6.78	6.62	0.16
ArH(3)	6.71	6.61	0.10
ArH(5)	6.63	6.38	0.25
Sert·HCl (**5**)			
α-CH_2	3.18	3.03	0.15
β-CH_2	2.98	2.76	0.22
ArH(7)	7.29	6.96	0.33
ArH(2)	7.15	6.95	0.20
ArH(4)	6.96	6.83	0.13
ArH(6)	6.74	6.54	0.20
Hist·2HCl (**6**)			
α-CH_2	3.22	3.14	0.08
β-CH_2	3.03	2.88	0.15
ArH(2)	8.51	8.37	0.19
ArH(4)	7.26	7.14	0.12
Nore·HCl (**7**)			
CH_2N	3.10	2.94	0.16
CHO	4.75	4.65	0.10
ArH(6)	6.82	6.67	0.15
ArH(3)	6.83	6.77	0.06
ArH(5)	6.74	6.58	0.16

[a] Values in parenthesis refer to the chemical shifts of the *endo*-cavity included phenethylammonium ions (Pea·$H^{+}\subset$**1**).

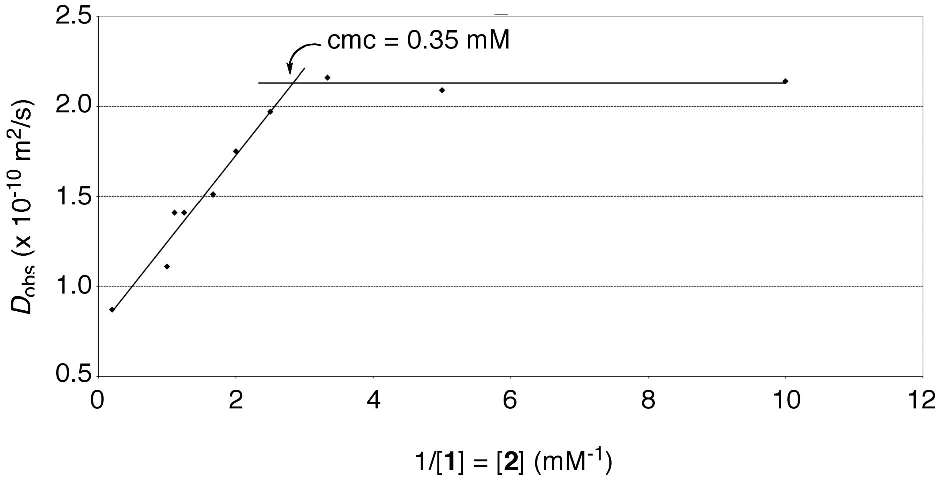


Figure S1. Plot of the diffusion coefficients (D_{obs}) of the calixarene-Pea·HCl surfactant *vs* 1/[**1**] = [**2**]. Data were calculated using the isochronous $ArCH_2Ar$ resonances (δ 4.35 ppm) of the monomers and the aggregated species.

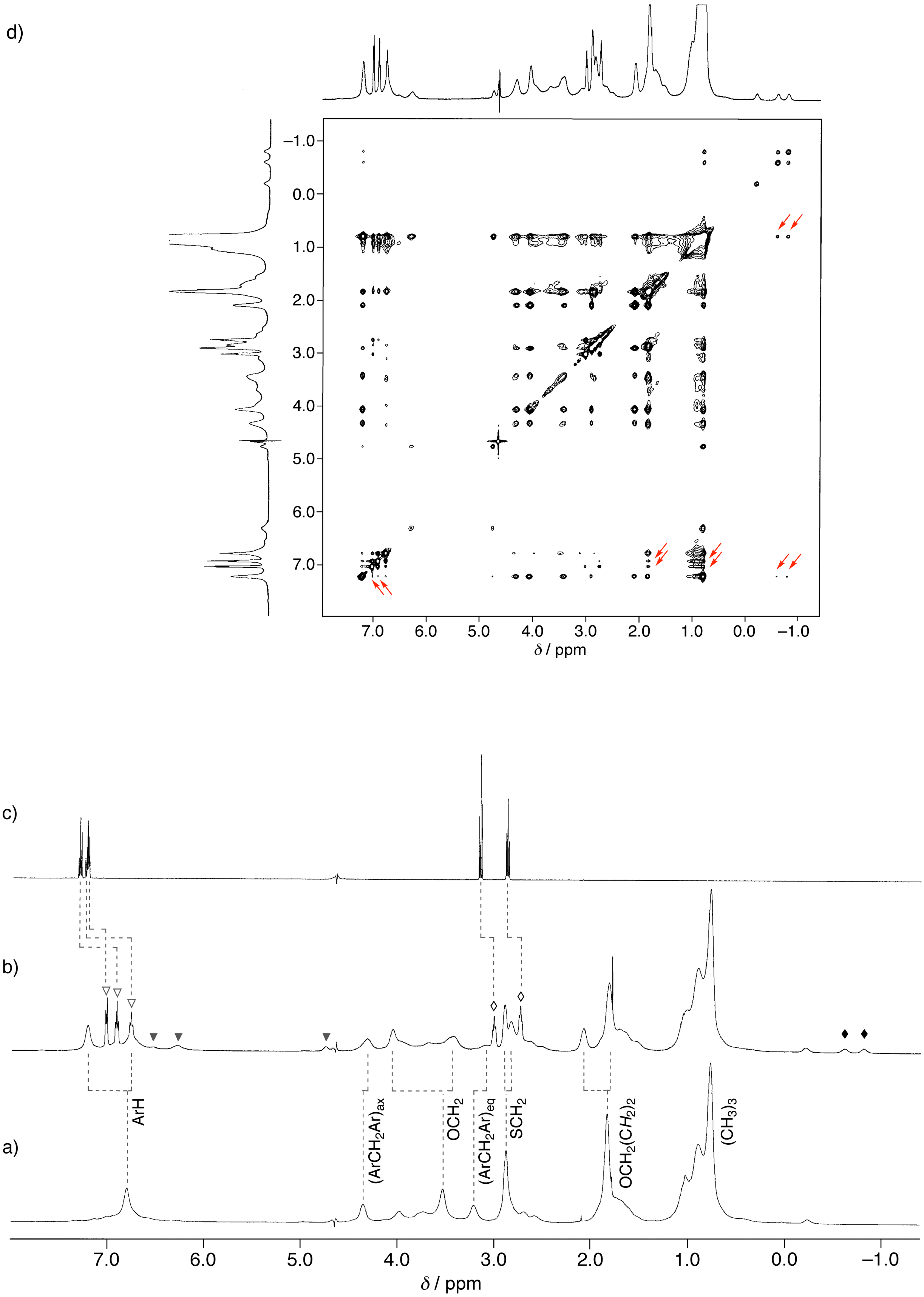
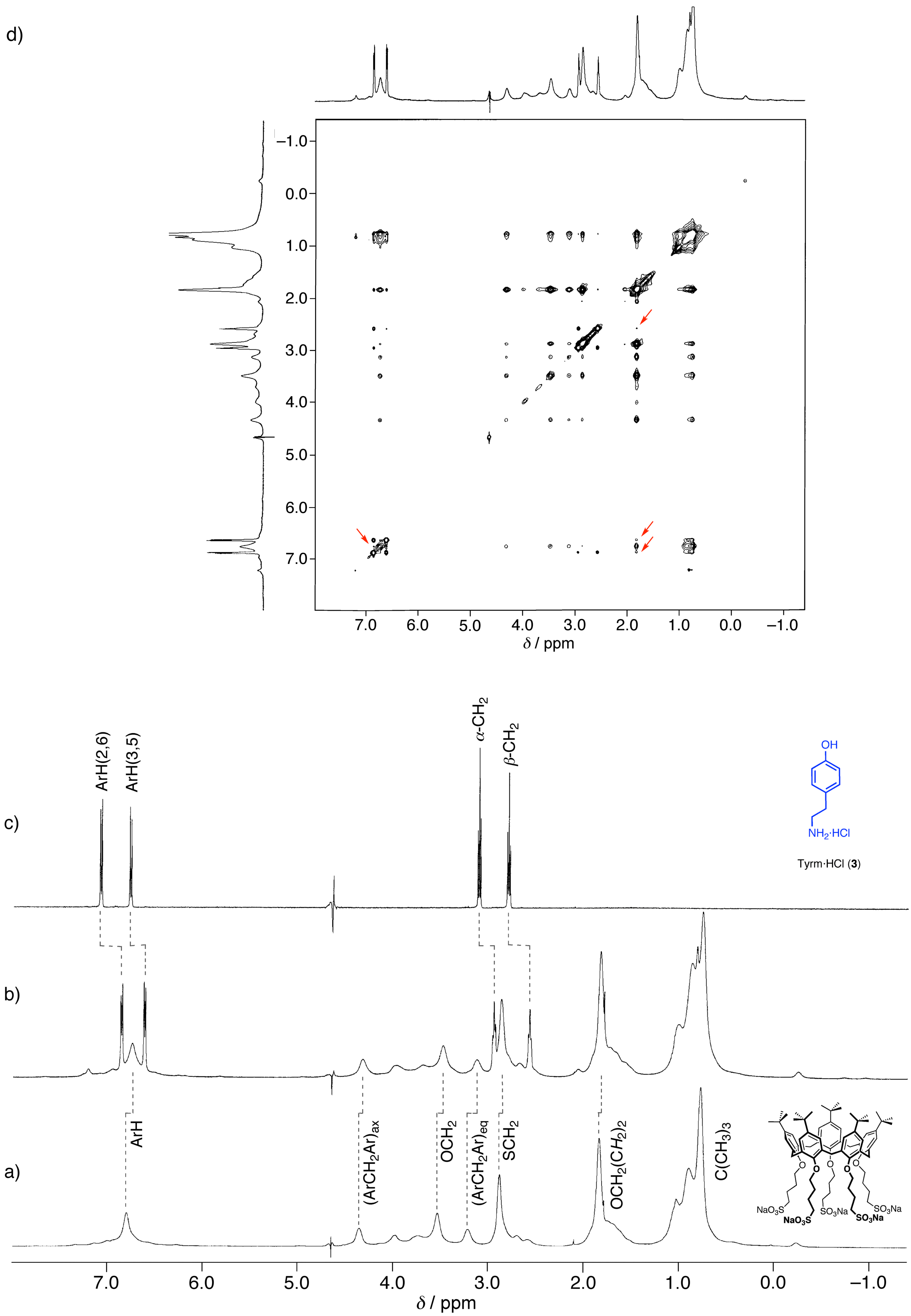


Figure S2. [1]H NMR spectra (500 MHz, 298 K, D_2O) of: (a) [**1**] = 10 mM, (b) [**1**] = [**2**] = 10 mM and (c) [**2**] = 10 mM. (d) The 2D NOESY spectrum (500 MHz, 298 K, D_2O) of [**1**] = [**2**] = 10 mM.



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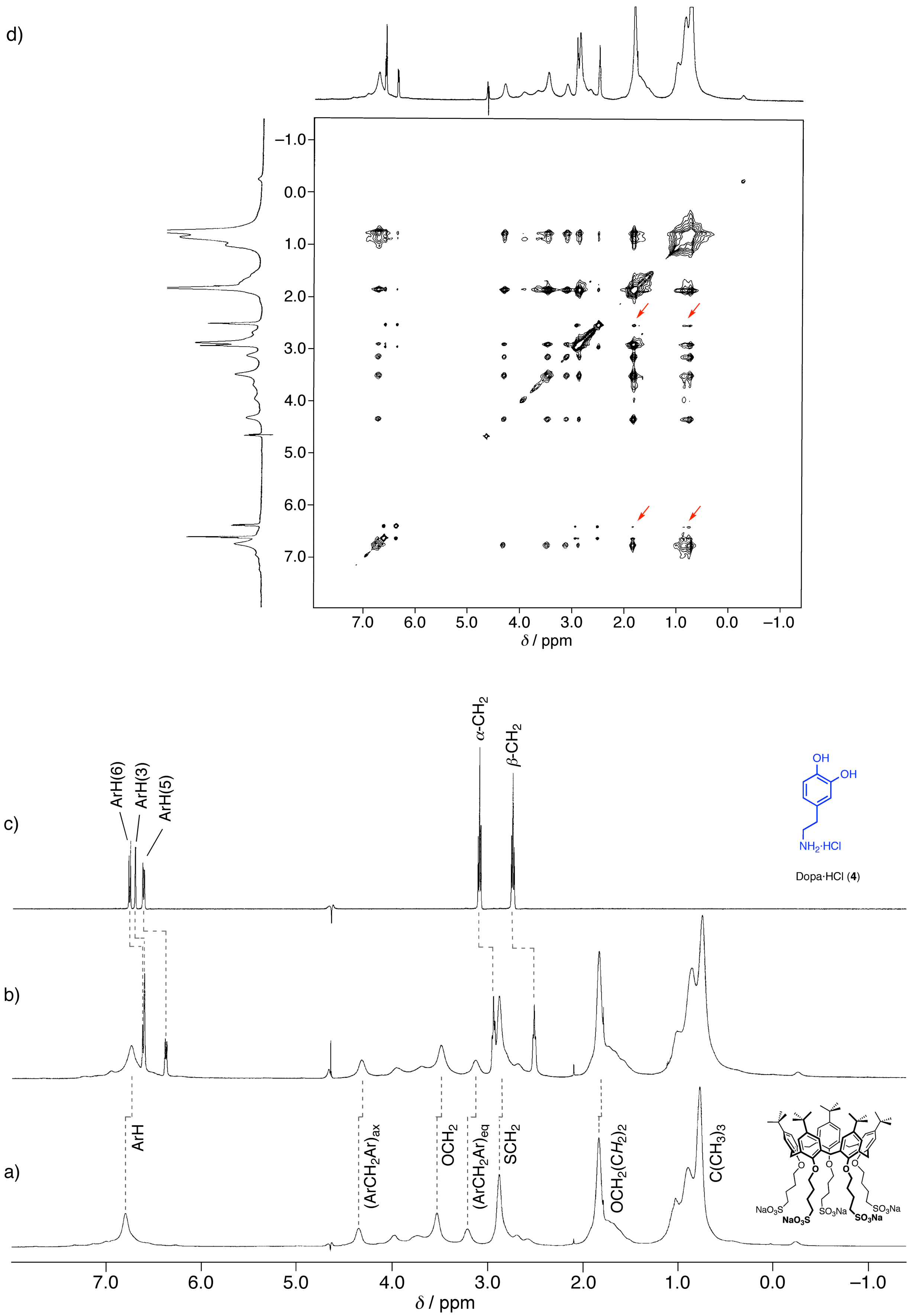

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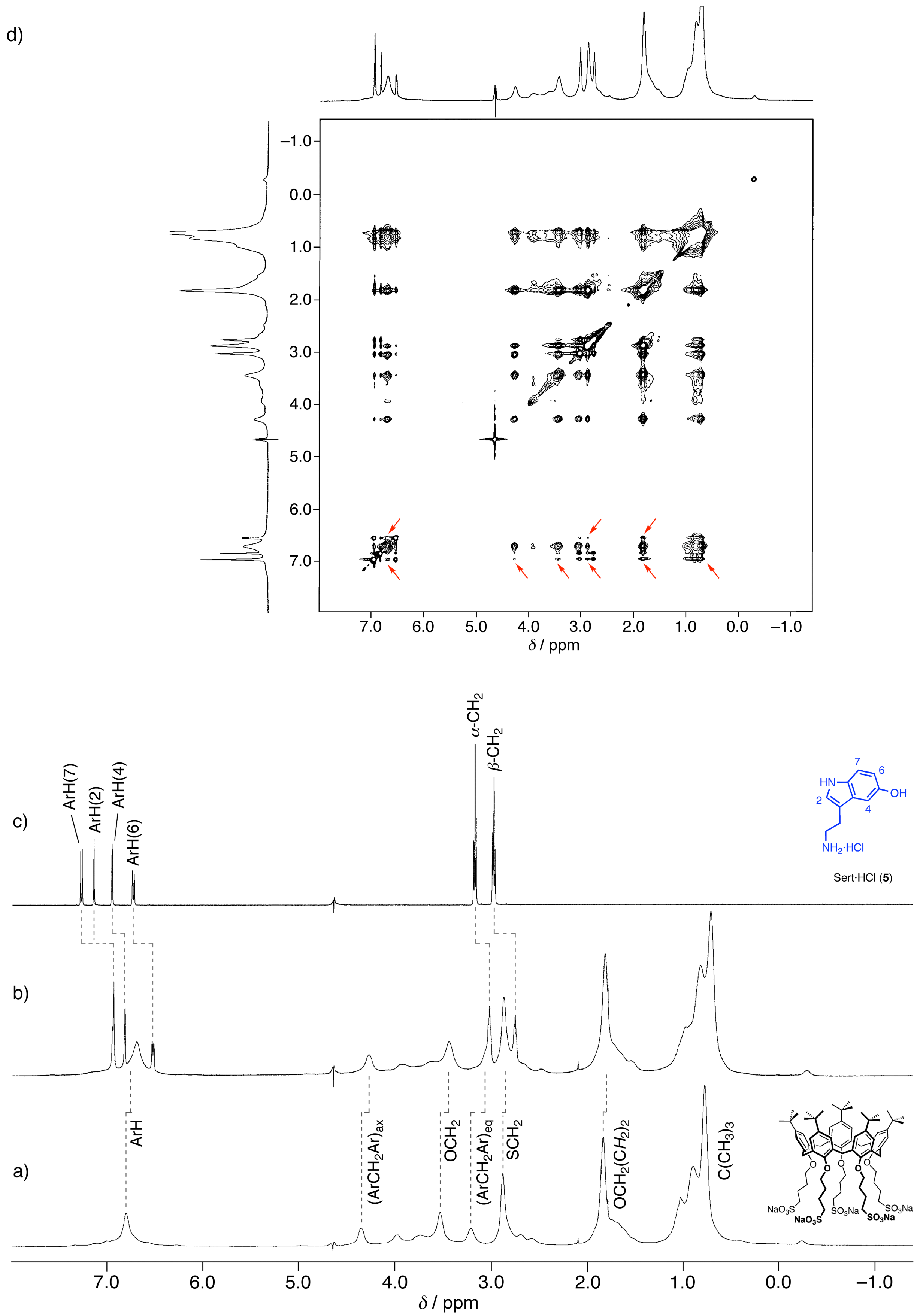

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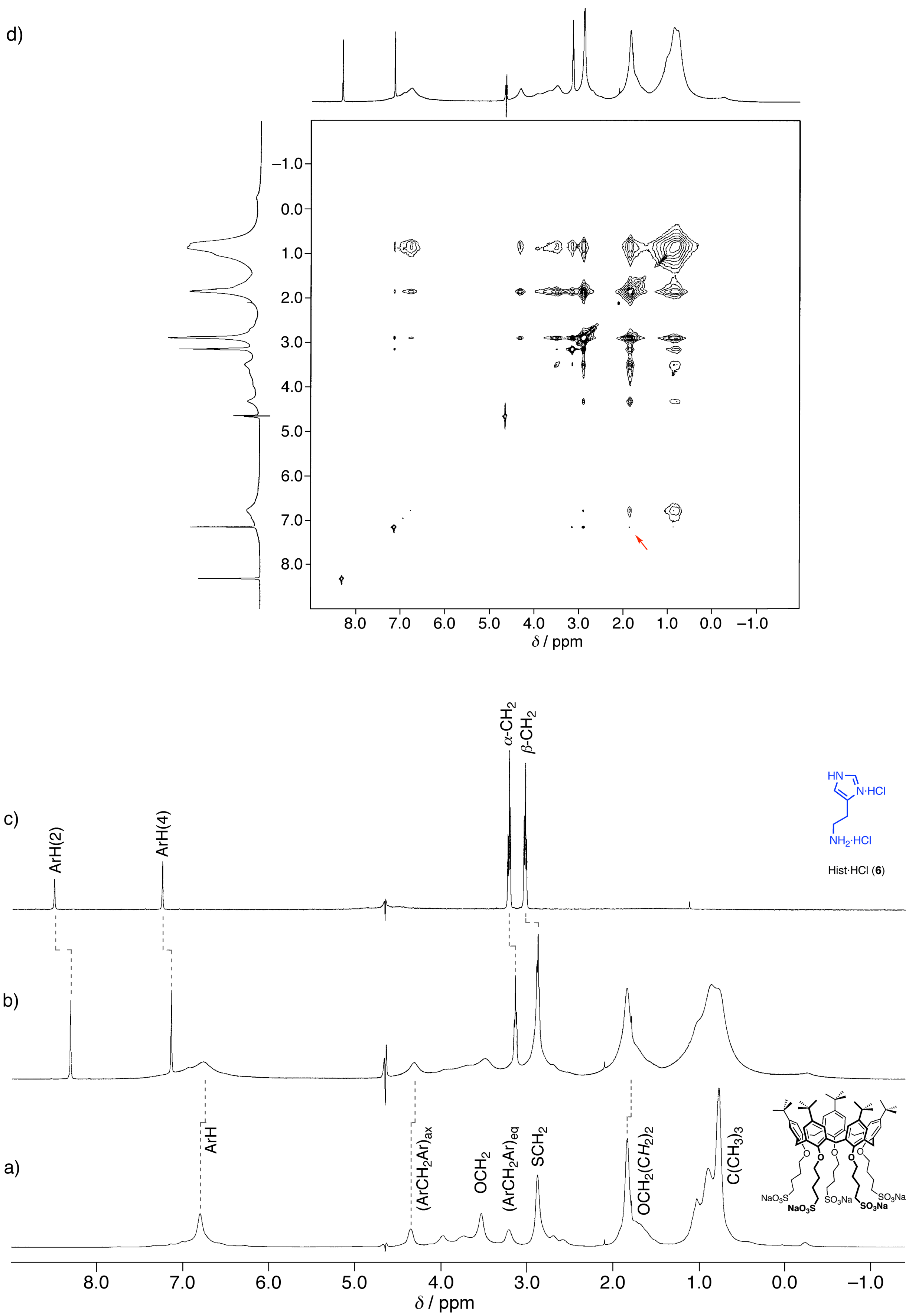

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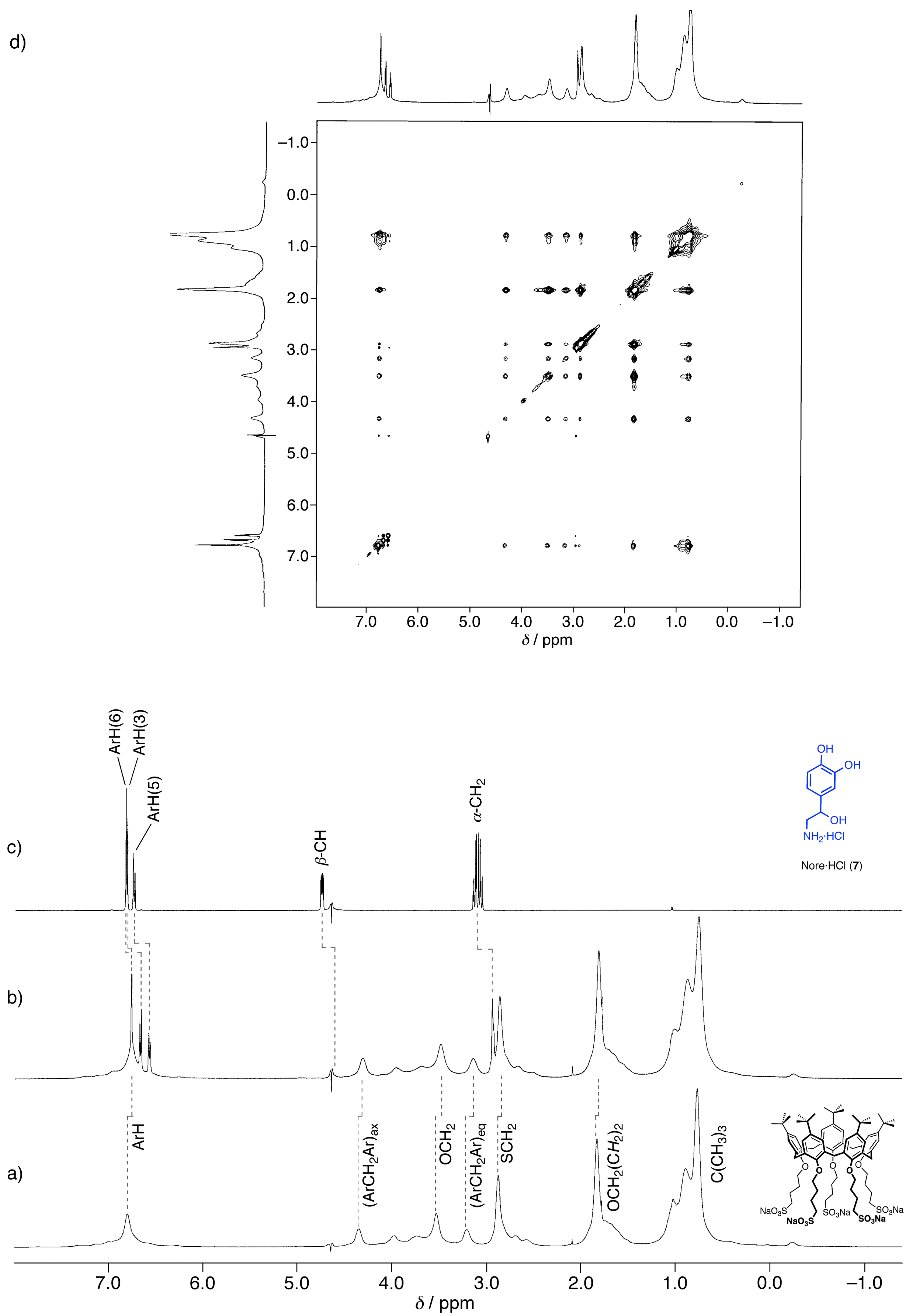

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