Electronic Supplementary Material (ESI) for Nanoscale.

SUPPORTING INFORMATION

for the paper

Tridentate Benzylthiols on Gold(111): Control of Self-Assembly Geometry

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Content

STM: image processing and analysis

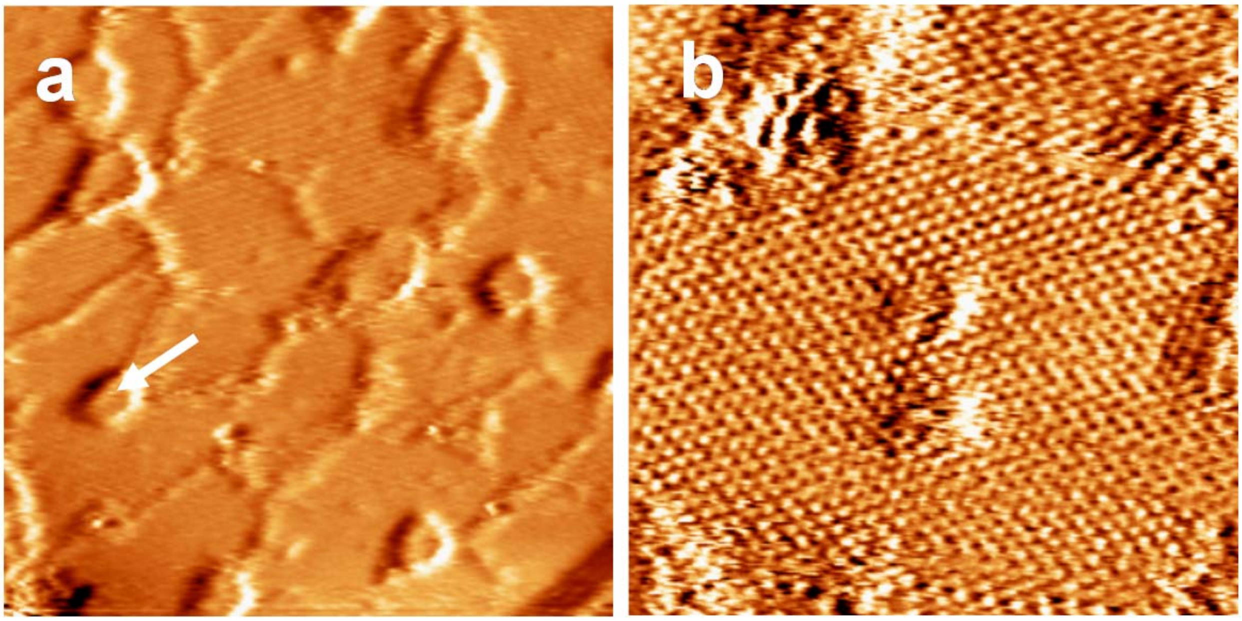

Figure SI1. STM images of 1-octanethiol deposited from 0.1M DMF solution. (a) Low resolution and (b) high resolution STM images (a): 59×59 nm; (b):20×20 nm; V_t = 700 mV, I_t = 0.1 nA of **C_8SH** SAMs on Au(111). The white arrow in figure (a) indicates an etch pit in **C_8SH** SAMs.

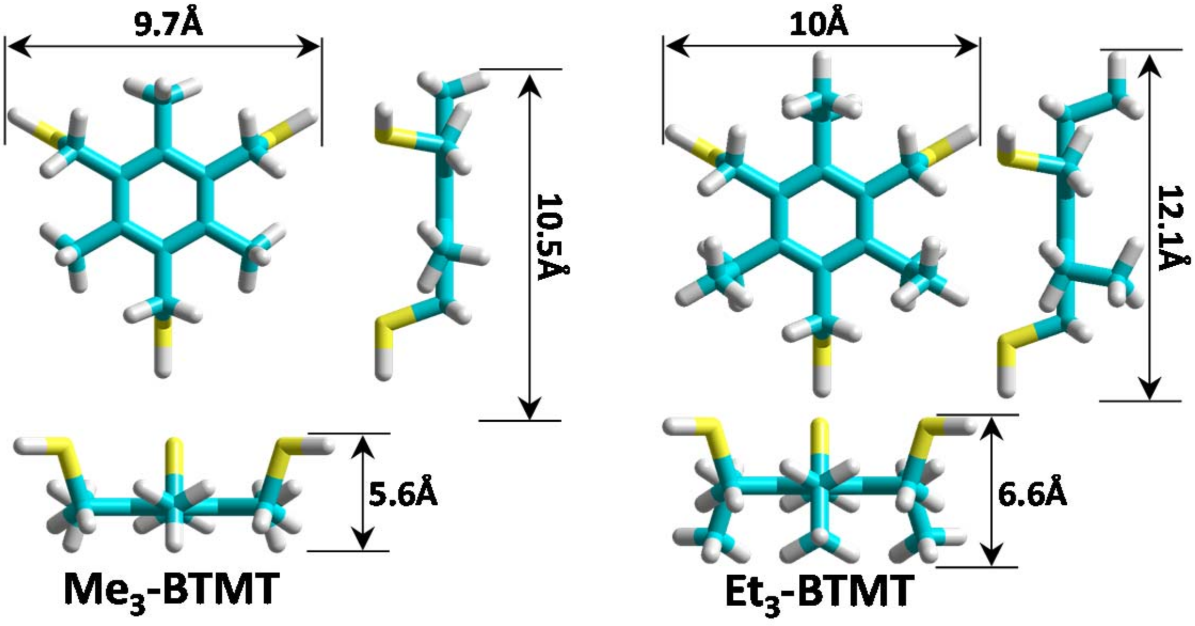

Figure SI2. DFT (B3LYP/6-31G(d)) calculated molecular dimensions of **Me_3-BTMT** and **Et_3-BTMT**.

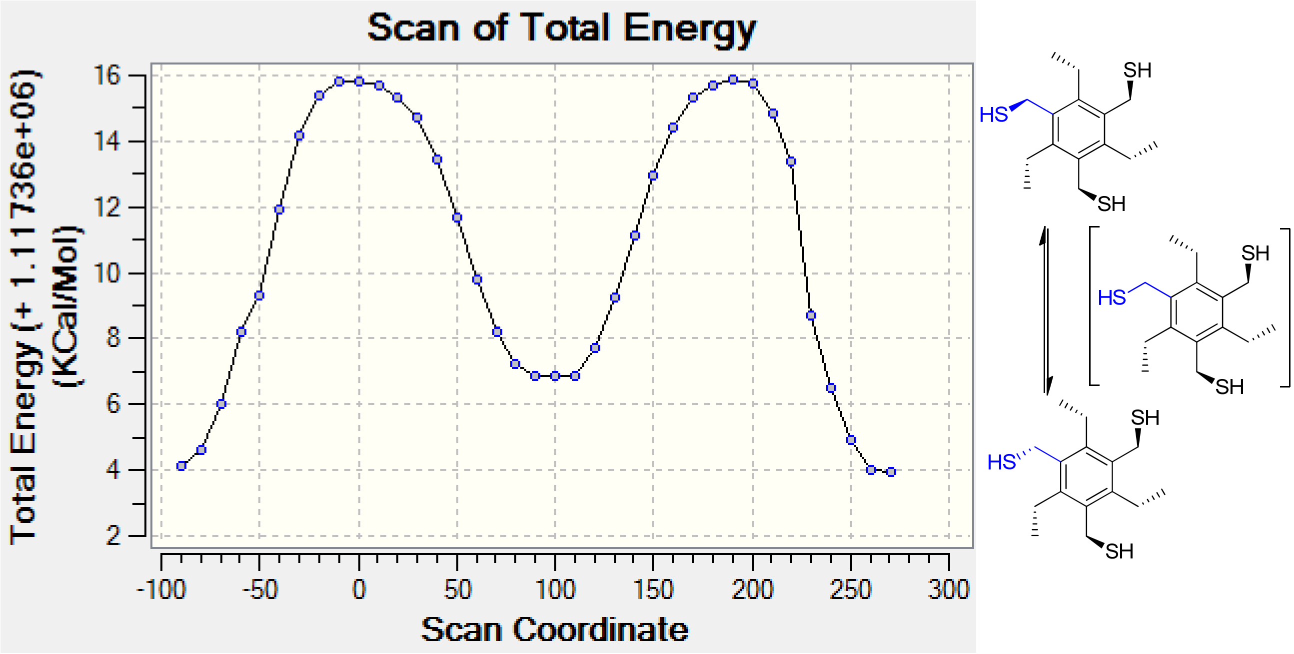

Figure SI3. Interconversion between *syn* and *anti* conformers of **Et$_3$-BTMT** calculated at B3LYP/6-31G(d) level. Scan coordinate corresponds to the C-C-C-S dihedral angle (°); all other coordinate were allowed to fully relax.

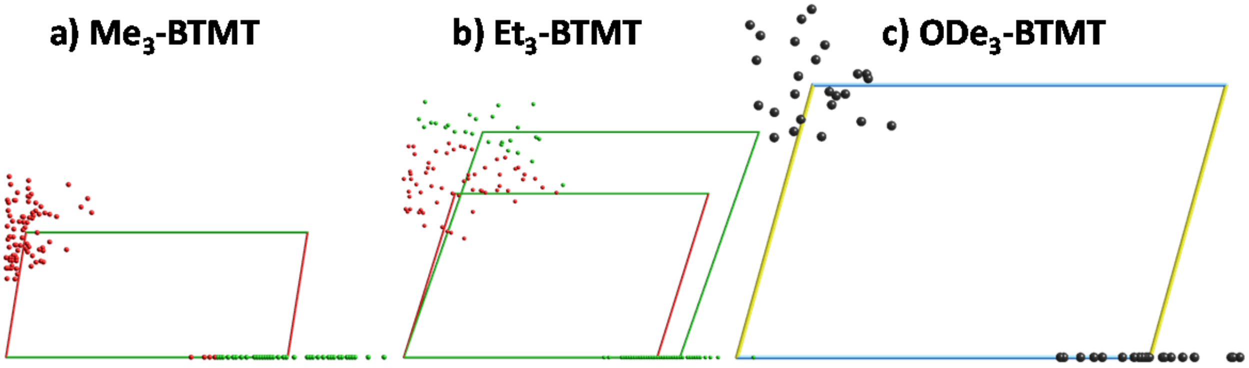

Figure SI4. Pair correlation analysis of the nearest three-point contacts determined for monolayers of: a) **Me$_3$-BTMT**, b) **Et$_3$-BTMT** and 3) **ODe$_3$-BTMT**. Relative orientations of all possible trios of molecules (manually determined from high-contrast spots in STM images) was plotted in the same coordinates, providing both the average intermolecular distances and the relative orientation of two contacts emanating from the same origin (an angle of a "local unit cell"). Intermolecular separations larger than 1.6 nm (for **Me$_3$-BTMT** and **Et$_3$-BTMT**) and 3 nm (for **ODe$_3$-BTMT**) were excluded from the analysis. The red color for molecular positions and "unit cell" vectors bars correspond to intermolecular separations that are only possible for *standing up* orientation of molecules (<0.9 nm for **Me$_3$-BTMT** and <1.0 nm for **Et$_3$-BTMT**). Green color for molecular separations and average "unit cell vectors" represent distances at which the neighboring molecules can either lie down or stand up on the surface. The other colors do not bear any internal assignment. Average "unit cells" were: (a) *a*=0.5±0.2 nm, *b*=1.1±0.4 nm, α =80°±10°; (b) *a*=0.7±0.2 nm, *b*=1.0±0.3 nm, α=73°±20°; *a*=0.9±0.2 nm, *b*=1.1±0.3 nm, α =75°±20°; (c) *a*=1.7±0.5 nm, *b*=2.5±0.5 nm, α =75°±20°.

Synthesis.

1,3,5-Trimethyl-2,4,6-tris(chloromethyl)benzene. To a one-neck round-bottom flask equipped with a stir bar were added mesitylene (21.6 g, 0.180 mol), paraformaldehyde (32.4 g, 1.08 mol), concentrated hydrochloric acid (156 g, 1.58 mol) and sodium chloride (5.61 g, 0.100 mol). A cooler condenser was connected to the flask, and the mixture was refluxed for 12 h under vigorous stirred. After cooling down to r.t., the liquid part was decanted, and another portions of paraformaldehyde (32.4 g, 1.08 mol), concentrated hydrochloric acid (156 g, 1.58 mol), sodium chloride (5.61 g, 0.100 mol), and zinc chloride (24.6 g, 0.180 mol) were added to the reaction mass. The mixture was refluxed for another 24 h under vigorous stirring. After cooling to room temperature, the precipitate was filtered and washed a several times with water and concentrated under reduced pressure. The crude material was recrystallized from dichloromethane/toluene mixture to give the desired product (22.8 g, 48%) with NMR spectral data identical to that previously reported.[1]

*1,3,5-Trimethyl-2,4,6-tris(S-acetylthiomethyl)benzene.*1,3,5-trimethyl-2,4,6-tris(chloromethyl)benzene (1.0 g, 3.8 mmol) and potassium thioacetate (3.0 g, 26 mol) were dissolved in DMF (10 mL) and stirred at r.t. for 4 h. The reaction mixture was poured into water (100 mL), resulting in significant precipitation. The solid material was collected by filtration, washed with H_2O (200 mL), and dried under reduced pressure to give the desired product as yellow powder (1.42 g, 98%). ^{1}H NMR (300 MHz, DMSO-d6): $\delta =$ 4.15 (6H, s), 2.36 (9H, s), 2.20 (9H, s).

1,3,5-Trimethyl-2,4,6-tris(hydrothiomethyl)benzene [**Me_3-BTMT**]. 1,4-Dioxane and distilled H_2O were purged with bubbling N_2 before use. In a 50 mL two-neck round-bottom flask equipped with a stir bar, 1,3,5-trimethyl-2,4,6-tris(S-acetylthiomethyl)benzene (0.250 g, 0.65 mmol) was dissolved in 1,4-dioxane (15 mL). The flask was equipped with a condenser and a rubber septum, and the system was flushed with N_2 gas for ~30 min. Sodium hydroxide (0.143 g, 3.58 mmol) was dissolved in H_2O (1 mL) and added dropwise to the solution at r.t. The mixture was refluxed under N_2 for 2 h and then cooled to r.t. 2M HCl (2.1 mL, 4.2 mmol) was added dropwise, and the mixture was stirred at r.t. for 1 h under N_2. H_2O was added, and the product was extracted with chloroform. The organic layer was washed with H_2O several times and dried over $MgSO_4$, followed by filtration and solvent evaporation to give the desired product as a white powder (0.165 g, 98%). NMR spectral data is identical to that reported earlier.[2]

1,3,5-Triethyl-2,4,6-tris(bromomethyl)benzene. To a 250 mL one-neck round-bottom flask equipped with a stir bar were added 1,3,5-triethylbenzene (3.93 g, 24.2 mmol), paraformaldehyde (8.75 g, 292 mmol), zinc bromide (9.69 g, 43.0 mmol), and 33% wt hydrogen bromide solution in acetic acid (55 mL; 0.30 mol). A cooler condenser was connected to the flask, and the mixture was heated to 100°C for 22 h under vigorous stirred. The mixture dissolved completely once heated, and in 3 h no precipitate was observed. Overnight heating resulted in formation of a precipitate, indicating that the reaction has completed. After cooling to room temperature, the precipitate was filtered and washed several times with water (400 mL). To remove possible zinc residues, the crude product was suspended in 1.5 M HCl (14 mL conc. HCl in 100 mL H_2O) and kept under stirring for 30 min. The solid product was filtered, washed with water until the wash solution had a neutral pH, then resuspended in 0.5 M aqueous $NaHCO_3$ (5.336 g in 100 mL H_2O) and kept stirred for 20 min. The material was filtered, washed with H_2O until neutral pH, and dried under reduced pressure to give the desired product as a white

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[1]. K. Mizoguchi, T. Higashihara and M. Ueda, *Macromolecules*, 2010, **43**, 2832– 2839.

[2] M. C. Aversa, A. Baratucci, P. Bonaccorsi, C. Faggi and T. Papalia, *J. Org. Chem*. 2007, **72**, 4486–4496.

powder (9.99 g, 93%). m.p.=168–169°C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 4.58 (6H, s), 2.94 (6H, q, J = 7.6 Hz), 1.35 (9H, t, J = 7.6 Hz). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 144.97, 132.63, 28.56, 22.73, 15.62.

1,3,5-Triethyl-2,4,6-tris(S-acetylthiomethyl)benzene. In a 250 mL one-neck round-bottom flask equipped with a stir bar, potassium thioacetate (9.09 g, 79.6 mmol) was dissolved in dimethylformamide (100 mL). 1,3,5-Triethyl-2,4,6-tris(bromomethyl)benzene (4.95 g, 11.2 mmol) was added to this solution and stirred at room temperature under N_2 for 3 h. The reaction mixture was poured into water (200 mL) and the resulting precipitate was collected by filtration, washed with H_2O, and dried under reduced pressure to give the pure product as a white powder (4.74 g, 99%). m.p.=148–149°C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 4.17 (6H, s), 2.60 (6H, q, J = 7.6 Hz), 2.36 (9H, s), 1.22 (9H, t, J = 7.6 Hz). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 196.03, 143.15, 130.24, 30.32, 28.42, 23.29, 15.68. m/z (ESI^{+} HRMS) for $C_{21}H_{30}O_3S_3$: 449.1249 $(M+Na)^{+}$, found 449.1240.

1,3,5-Triethyl-2,4,6-tris(hydrothiomethyl)benzene) [**Et$_3$-BTMT**]. 1,4-Dioxane and distilled H_2O were purged with bubbling Ar before use. In a 100 mL two-neck round-bottom flask equipped with a stir bar, 1,3,5-Triethyl-2,4,6-tris(S-acetylthiomethyl)benzene (0.716 g, 1.68 mmol) was dissolved in 1,4-dioxane (50 mL). The flask was equipped with a condenser and a rubber septum, and the system was flushed with Ar gas for ~30 min. Sodium hydroxide (0.393 g, 9.82 mmol) was dissolved in H_2O (3 mL) and added dropwise to the solution at r.t. The mixture was refluxed under Ar for 3 h, then cooled to r.t. 2M HCl (5 mL, 10.0 mmol) was added dropwise, and the mixture was stirred at r.t. for 1 h under Ar. H_2O was added, and the product was extracted with chloroform. The organic layer was washed with H_2O several times and dried over $MgSO_4$, followed by filtration and solvent evaporation to give the desired product as a white powder (0.504 g, 100%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.76 (6H, d, J = 6.4 Hz), 2.86 (6H, q, J = 7.6 Hz), 1.70 (3H, t, J = 6.2 Hz), 1.27 (9H, t, J = 7.6 Hz). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 140.21, 135.48, 22.81, 22.77, 16.12.

1,3,5-Tris(acetyloxy)benzene. Acetic anhydride (70 mL, 0.7 mol) was added to a solution of phloroglucinol dihydrate (11.89 g, 73 mmol) in pyridine (50 mL) at r.t. under vigorous stirring. [Note: exothermic reaction!] In 1.5 h, ice (ca. 400 mL) was added to the reaction mixture resulting in formation of precipitate, and stirring continued for another 1 h to destroy the excess Ac_2O. The resulting solid material was filtered, washed with H_2O, and dried under reduced pressure to afford 1,3,5-tris(acetyloxy)benzene (17.01 g) as a light gray powder. Yield: 93%. m.p.=105–106°C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 6.84 (3H, s), 2.28 (9H, s). ^{13}C NMR (75 MHz, CDCl3): δ = 168.56, 151.07, 112.75, 21.08.

1,3,5-Tris(decyloxy)benzene [**ODe$_3$-B**]. In a 500 mL one-neck round-bottom flask equipped with a stir bar, 1-bromodecane (40 mL, 190 mmol) was added to a solution of 1,3,5-tris(acetyloxy)benzene (13.4 g, 50 mmol) in DMF (150 mL) at -5°C under vigorous stirring. 60% NaH in mineral oil (17.9 g, 440 mmol) was added in one portion, and the reaction mixture was stirred for 20 min, followed by addition of H_2O (6 mL) at -5°C dropwise over a period of 1 h. [Note: because of released H_2, it is important to use a relatively large volume flask as used here.] The reaction mixture was allowed to slowly warm to heat to r.t and kept under vigorous stirring overnight. After 21 h, the reaction mixture was heated to 50°C and stirred for another 2 h. Brine was added, and the product was extracted into ethyl acetate. The organic layer was washed with H_2O and concentrated under reduced pressure to afford a crude product consisting of target material and excess of 1-bromodecane, which was removed by distillation using Büchi Glass Oven B-585 under reduced pressure (0.25 mbar) at 100°C. The residue from the reaction flask was filtered through silica gel using hexane as an eluent, affording 1,3,5-tris(decyloxy)benzene as a light yellow liquid (16.21 g, 56%). The compound contains an impurity of mineral oil (from

NaH) and can be used as is in further synthesis. For analytical purposes, it was purified by column chromatography (SiO_2; hexane – hexane/CH_2Cl_2 (2:1) gradient). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 6.06 (3H, s), 3.90 (6H, t, J = 6.6 Hz), 1.75 (6H, p), 1.52–1.20 (42H, m), 0.88 (9H, t, J = 6.6 Hz). ^{13}C NMR (75 MHz, CDCl3): δ = 160.93, 93.72, 67.99, 31.91, 29.59, 29.57, 29.39, 29.33, 29.25, 26.06, 22.69, 14.13. m/z (ESI$^+$ HRMS) for $C_{36}H_{66}O_3$: 547.50847 $(M+H)^+$, found 547.50915.

1,3,5-Tris(decyloxy)-2,4,6-tris(bromomethyl)benzene. To a 100 mL one-neck round-bottom flask equipped with a stir bar were added 1,3,5-tris(decyloxy)benzene (2.97 g, 5.43 mmol), paraformaldehyde (2.57 g, 85.7 mmol), zinc bromide (2.30 g, 10.2 mmol), and 33% wt hydrogen bromide solution in acetic acid (20 mL; 110 mmol). A condenser was connected to the flask, and the mixture was heated to 55°C for 91 h under vigorous stirring. A higher temperature should be avoided; a partial dealkylation was observed when the reaction was performed at~70°C. The reaction mass was cooled to room temperature, H_2O was added, and the product was extracted to ethyl acetate. The organic layer was washed with H_2O until the wash solution was at neutral pH, dried over $MgSO_4$, filtered and concentrated under reduced pressure. The crude product was purified by column chromatography on silica using hexane and dichloromethane to afford the desired product as a colorless oil (0.71 g, 16%). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 4.58 (6H, s), 4.25 (6H, t, J = 6.9 Hz), 1.93 (6H, p, J = 6.9 Hz), 1.6–1.2 (42H, m), 0.89 (9H, t, J = 6.8 Hz). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 159.50, 123.15, 75.04, 31.91, 30.31, 29.61, 29.58, 29.50, 29.34, 25.82, 23.11, 22.71, 14.15.

1,3,5-Tris(decyloxy)-2,4,6-tris(S-acetylthiomethyl)benzene. In a 10 mL one-neck round-bottom flask equipped with a stir bar, potassium thioacetate (97 mg, 0.85 mmol) was dissolved in dimethylformamide (1 mL) and mixed with 1,3,5-tris(decyloxy)-2,4,6-tris(bromomethyl)benzene (71 mg, 0.090 mmol) dissolved in dimethylformamide (1 mL). The reaction mixture was stirred at room temperature for 2 days. H_2O was added, and the product was extracted to chloroform. The organic layer was washed with H_2O a few times, dried over $MgSO_4$, filtered and concentrated under reduced pressure to afford the desired product as a yellow oil (51 mg, 75%). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 4.17 (6H, s), 3.79 (6H, t, J = 6.8 Hz), 2.33 (9H, s), 1.80 (6H, p), 1.51–1.21 (42H, m), 0.88 (9H, t). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 195.37, 157.84, 120.37, 75.40, 31.92, 30.24, 30.22, 29.62, 29.58, 29.52, 29.35, 25.89, 23.41, 22.70, 14.14. m/z (ESI$^+$ MS) for $C_{45}H_{78}O_6S_3$: 833.4858 $(M+Na)^+$, found 833.4852.

1,3,5-Tris(decyloxy)-2,4,6-tris(hydrothiomethyl)benzene [**ODe$_3$-BTMT**]. 1,4-Dioxane and distilled H_2O were degassed with bubbling Ar before use. In a 100 mL two-neck round-bottom flask equipped with a stir bar, 1,3,5-tris(decyloxy)-2,4,6-tris(S-acetylthiomethyl)benzene (0.90 g, 1.1 mmol) was dissolved in 1,4-dioxane (15 mL). The flask was equipped with a condenser and a rubber septum, and the system was flushed with N_2 for ~30 min. 2.9 M aqueous sodium hydroxide (2.3 mL, 6.7 mmol) was added dropwise to the reaction at r.t. The mixture was refluxed under N_2 for 2 h, then cooled to r.t. 2M HCl (3.8 mL, 7.6 mmol) was added dropwise, and the mixture was stirred at r.t. for 1 h under nitrogen. H_2O was added, and the product was extracted with dichloromethane. The organic layer was washed with H_2O several times and dried over $MgSO_4$, followed by filtration and solvent evaporation to yield the desired product as a light yellow oil (0.64 g, 84%). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 3.95 (6H, t, J = 6.6), 3.69 (6H, d, J = 7.8 Hz), 2.23 (3H, t, J = 7.8 Hz), 1.86 (6H, p, J = 7.2 Hz), 1.6–1.2 (42H, m), 0.89 (9H, t, J = 6.5 Hz). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 155.49, 125.73, 75.15, 31.87, 30.44, 29.57, 29.55, 29.49, 29.30, 26.03, 22.66, 18.18, 14.10. m/z (APCI$^-$ HRMS) for $C_{39}H_{72}O_3S_3$: 683.45708 $(M–H)^-$, found 683.45550.

Spectral data.

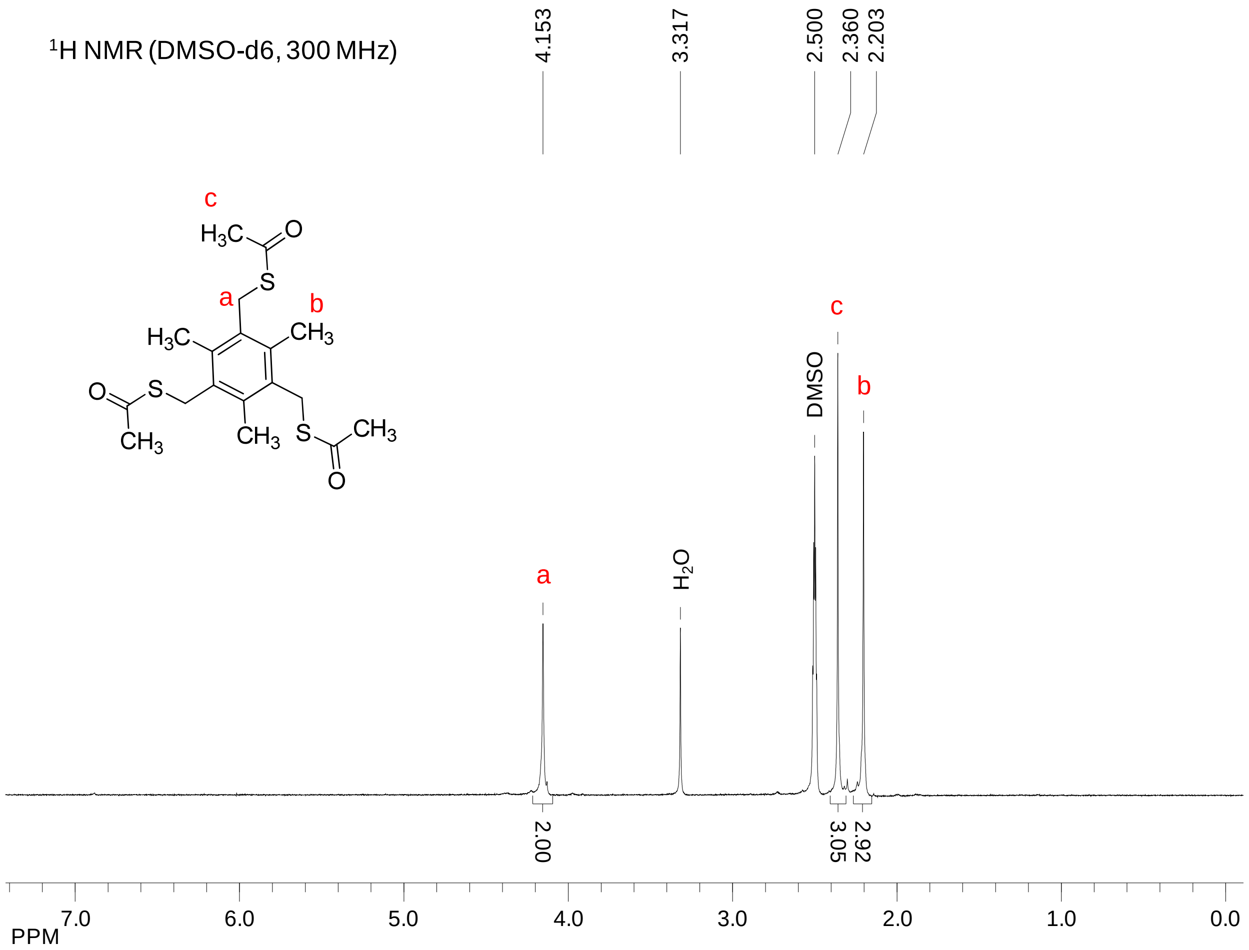
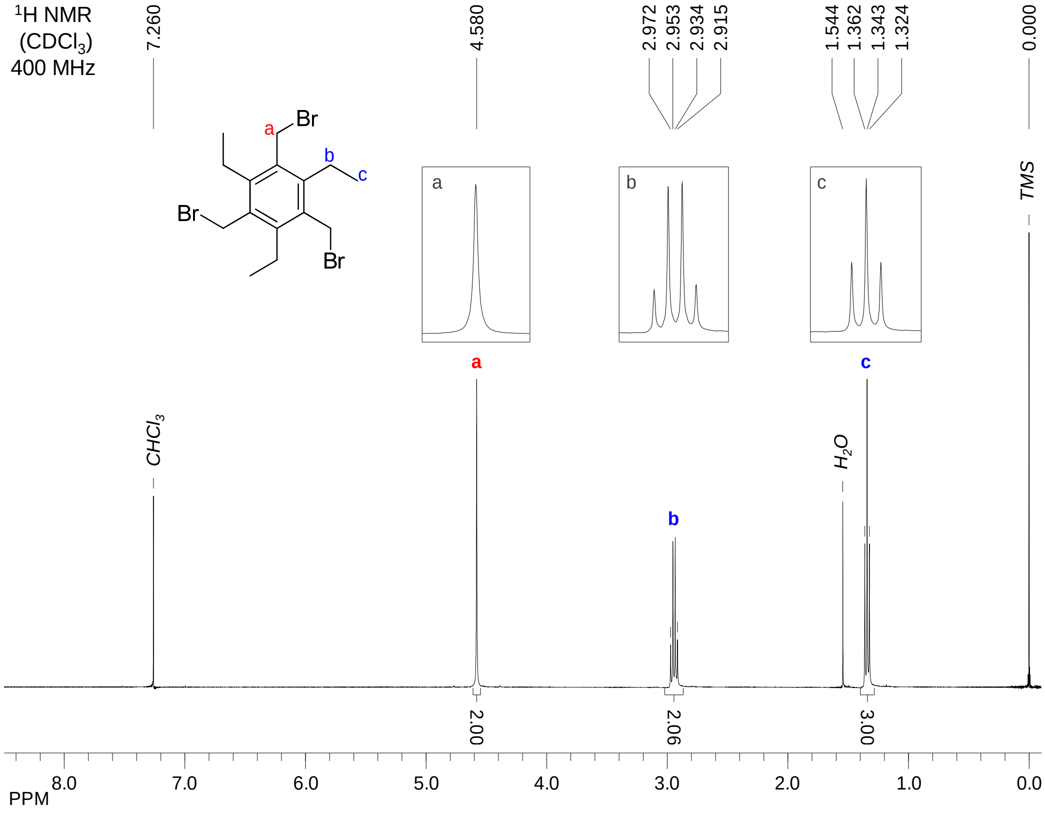


Figure SI5. ^{1}H NMR spectrum of 1,3,5-trimethyl-2,4,6-tris(S-acetylthiomethyl)benzene.



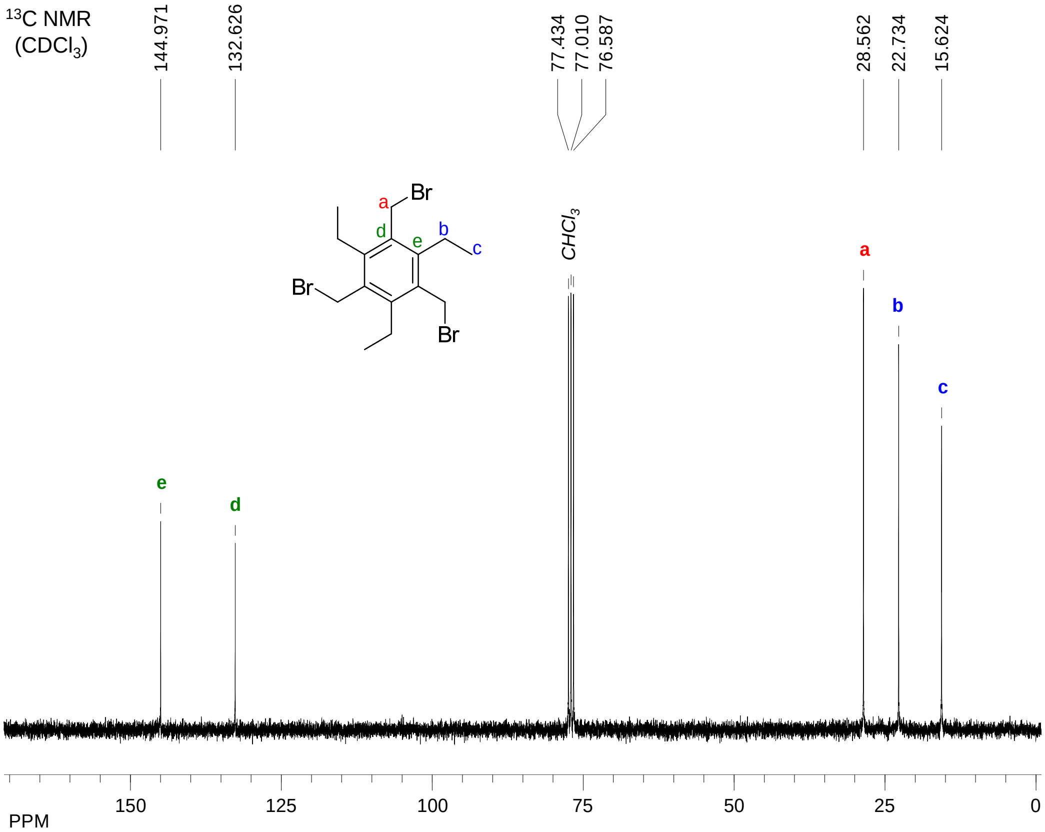


Figure SI6. ^{1}H (top) and ^{13}C (bottom) NMR spectra of 1,3,5-triethyl-2,4,6-tris(bromomethyl)benzene.

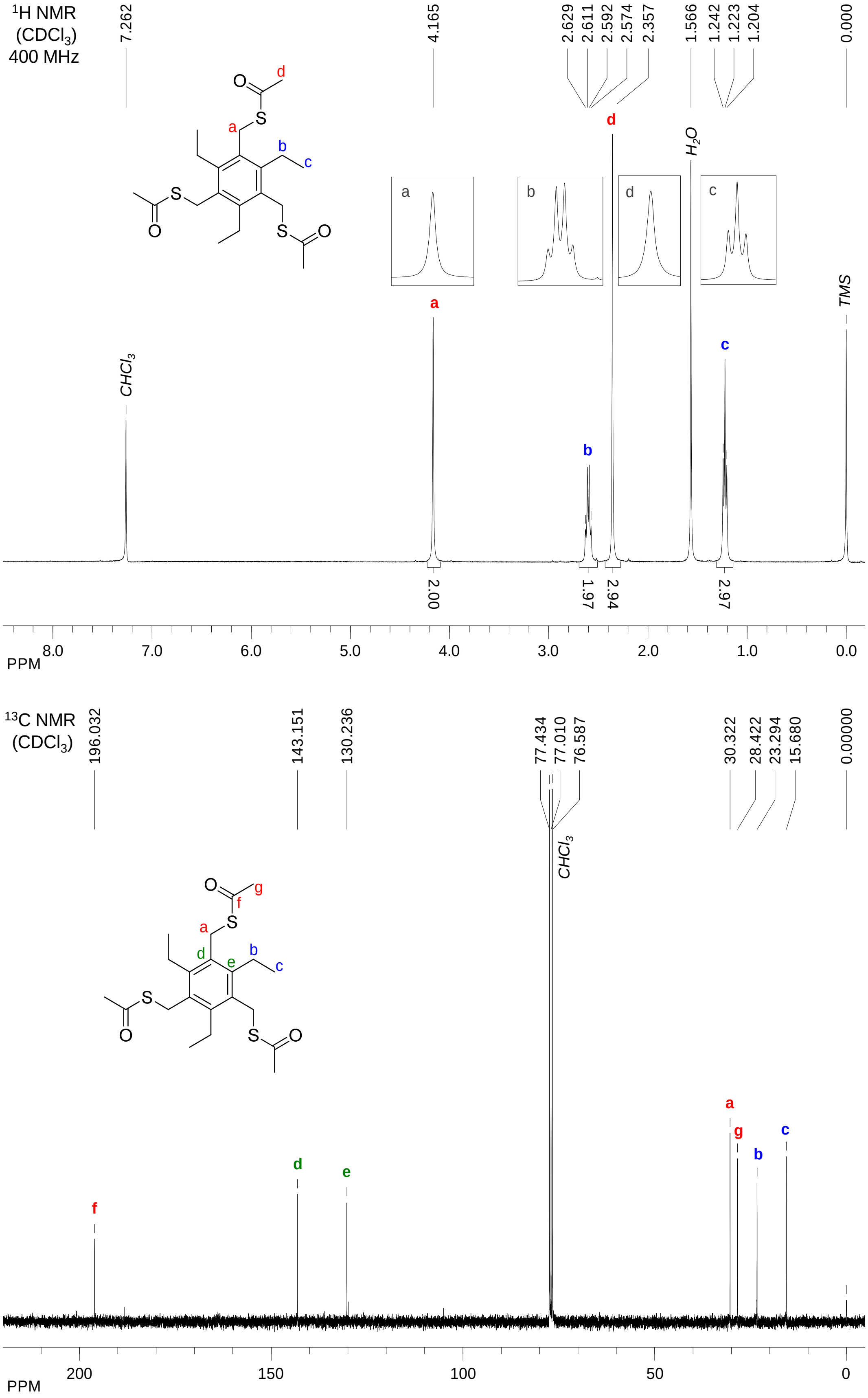
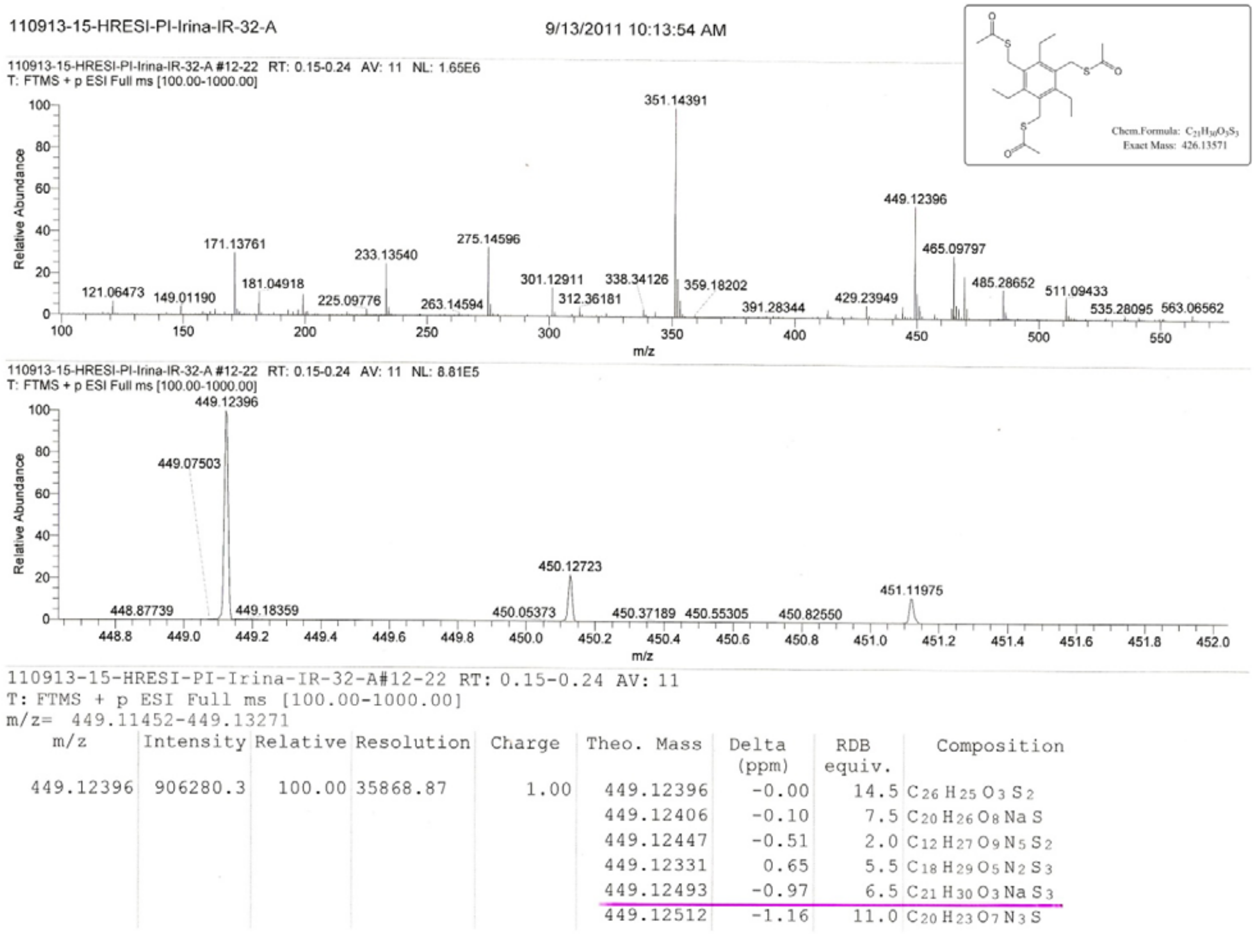


Figure SI7. ^{1}H (top) and ^{13}C (bottom) NMR spectra of 1,3,5-triethyl-2,4,6-tris(S-acetylthiomethyl)benzene.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m/z= 449.11452-449.13271

m/z	Intensity	Relative	Resolution	Charge	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
449.12396	906280.3	100.00	35868.87	1.00	449.12396	-0.00	14.5	$C_{26}H_{25}O_3S_2$
					449.12406	-0.10	7.5	$C_{20}H_{26}O_8NaS$
					449.12447	-0.51	2.0	$C_{12}H_{27}O_9N_5S_2$
					449.12331	0.65	5.5	$C_{18}H_{29}O_5N_2S_3$
					449.12493	-0.97	6.5	$C_{21}H_{30}O_3NaS_3$
					449.12512	-1.16	11.0	$C_{20}H_{23}O_7N_3S$

Figure SI8. Mass spectrum of 1,3,5-triethyl-2,4,6-tris(S-acetylthiomethyl)benzene.

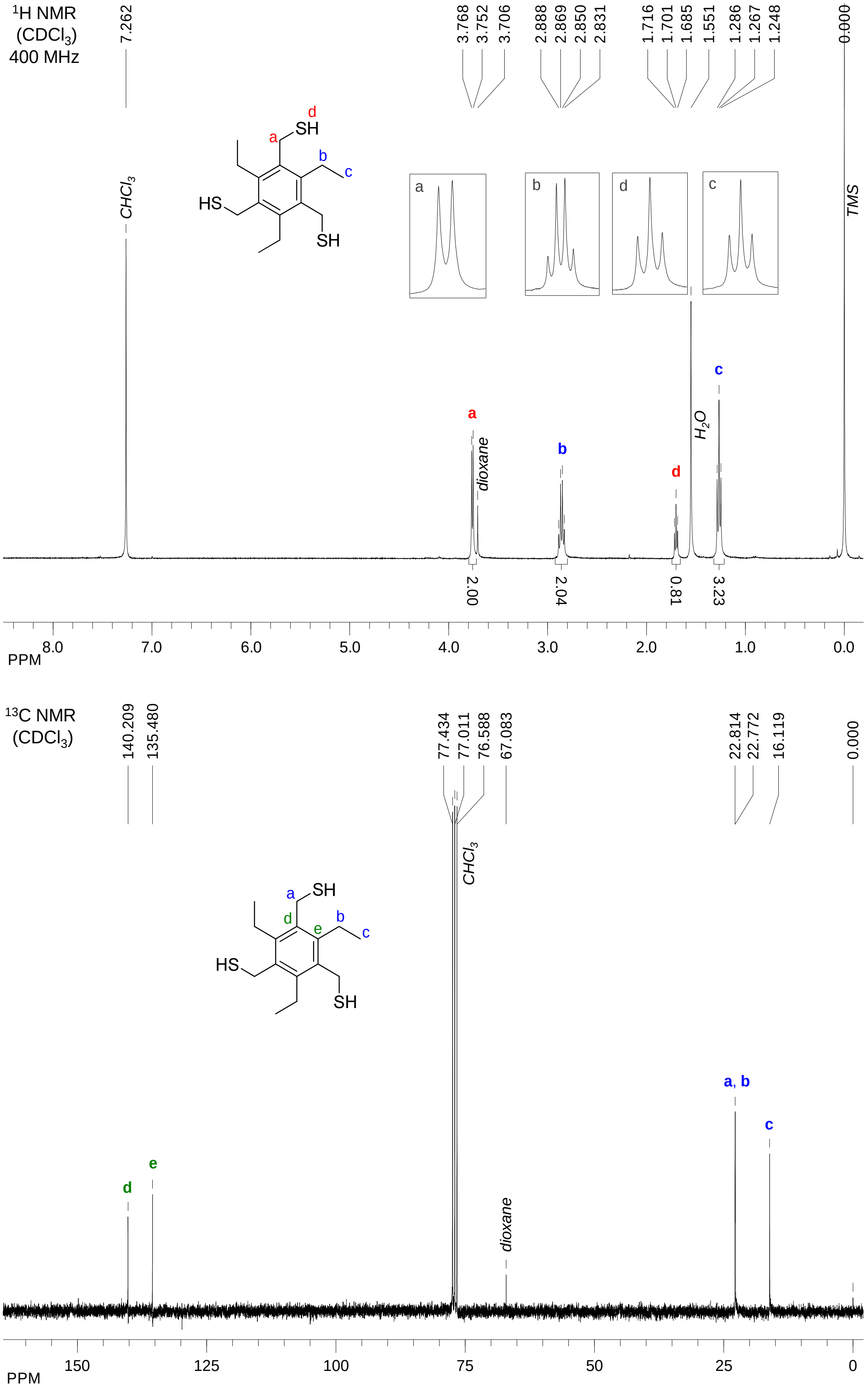

Figure SI9. ^{1}H (top) and ^{13}C (bottom) NMR spectra of 1,3,5-triethyl-2,4,6-tris(hydrothiomethyl)benzene) [**Et$_3$-BTMT**].

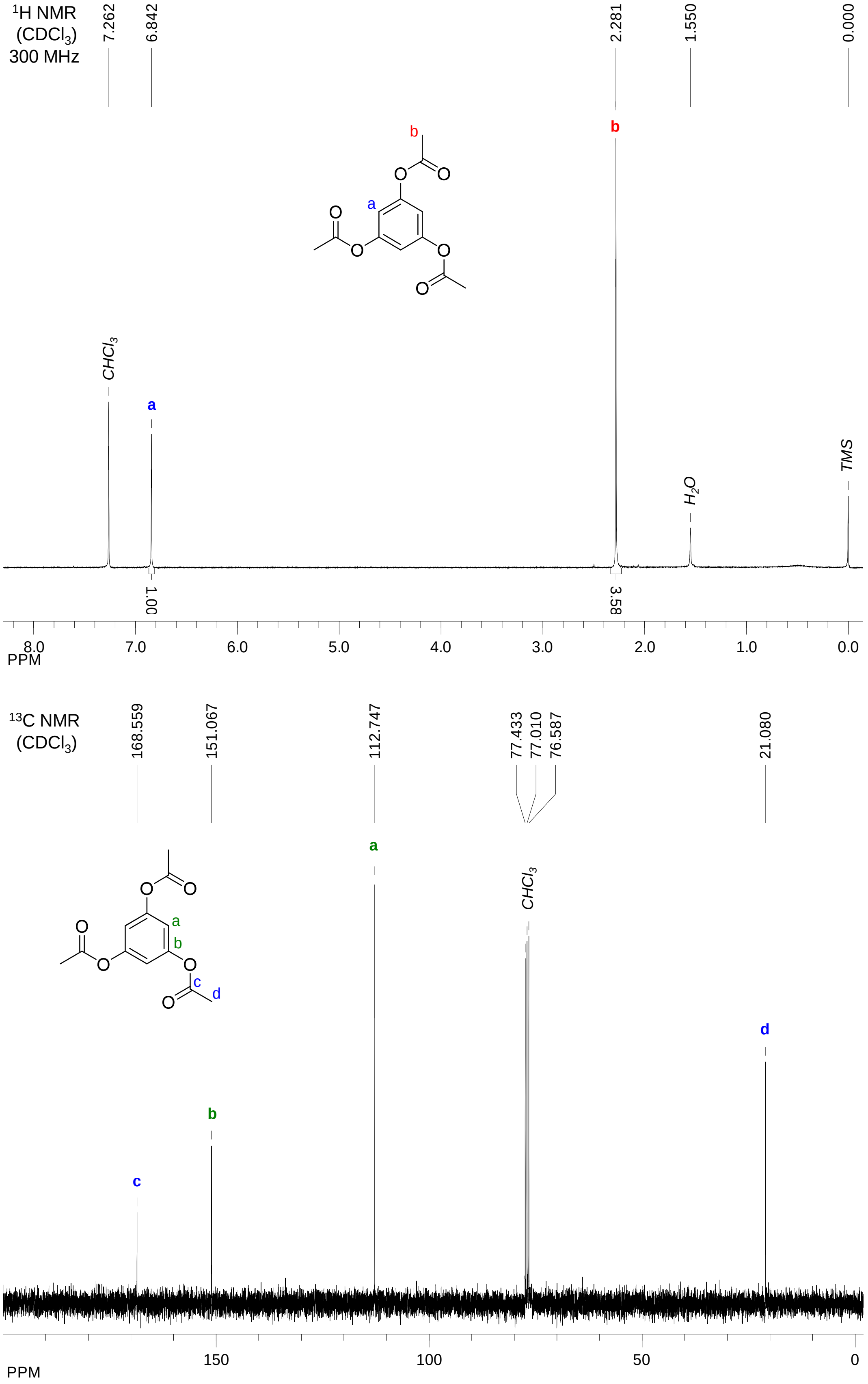

Figure SI10. ^{1}H (top) and ^{13}C (bottom) NMR spectra of 1,3,5-tris(acetyloxy)benzene.

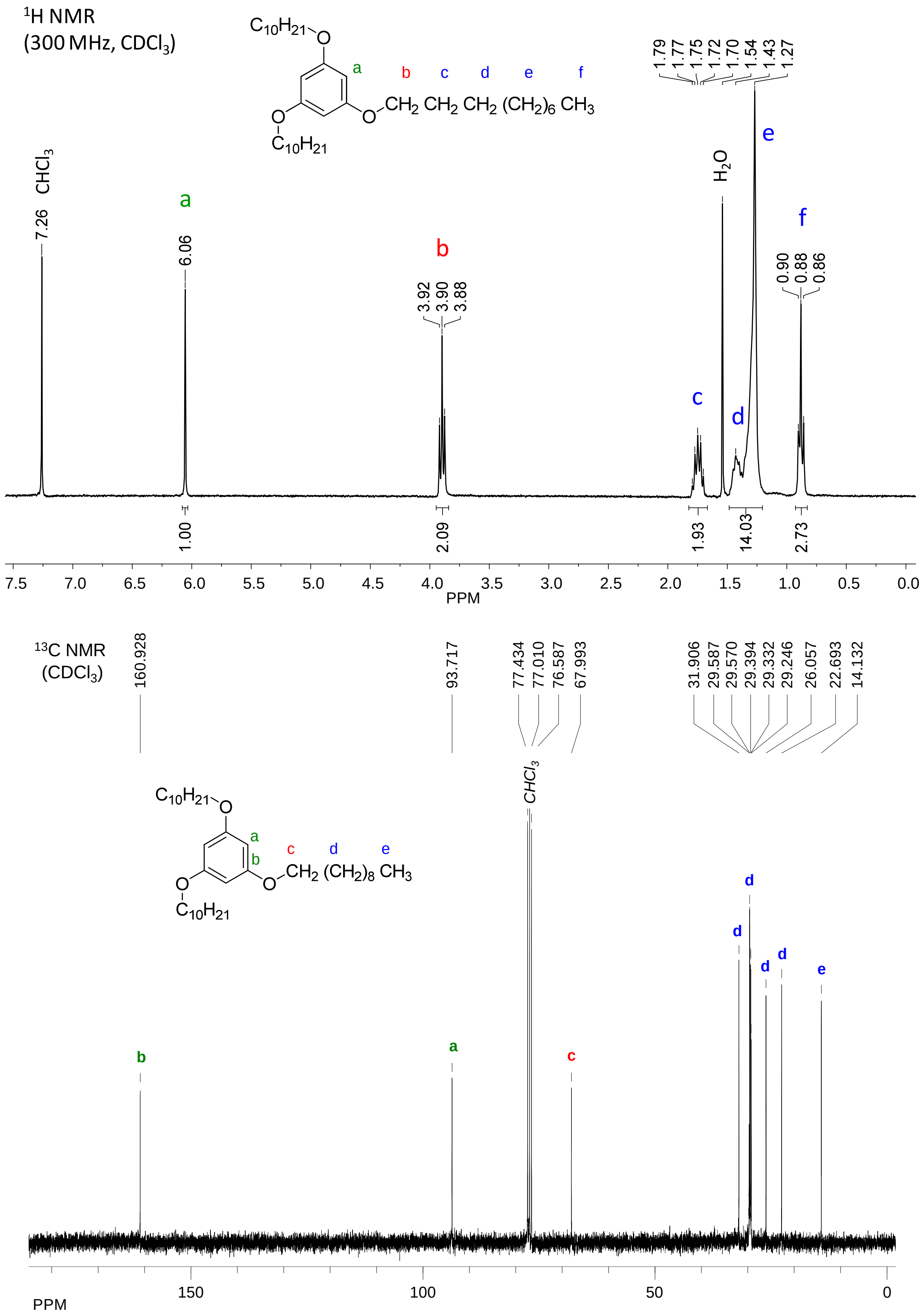

Figure SI11. ^{1}H (top) and ^{13}C (bottom) NMR spectra of 1,3,5-tris(decyloxy)benzene.

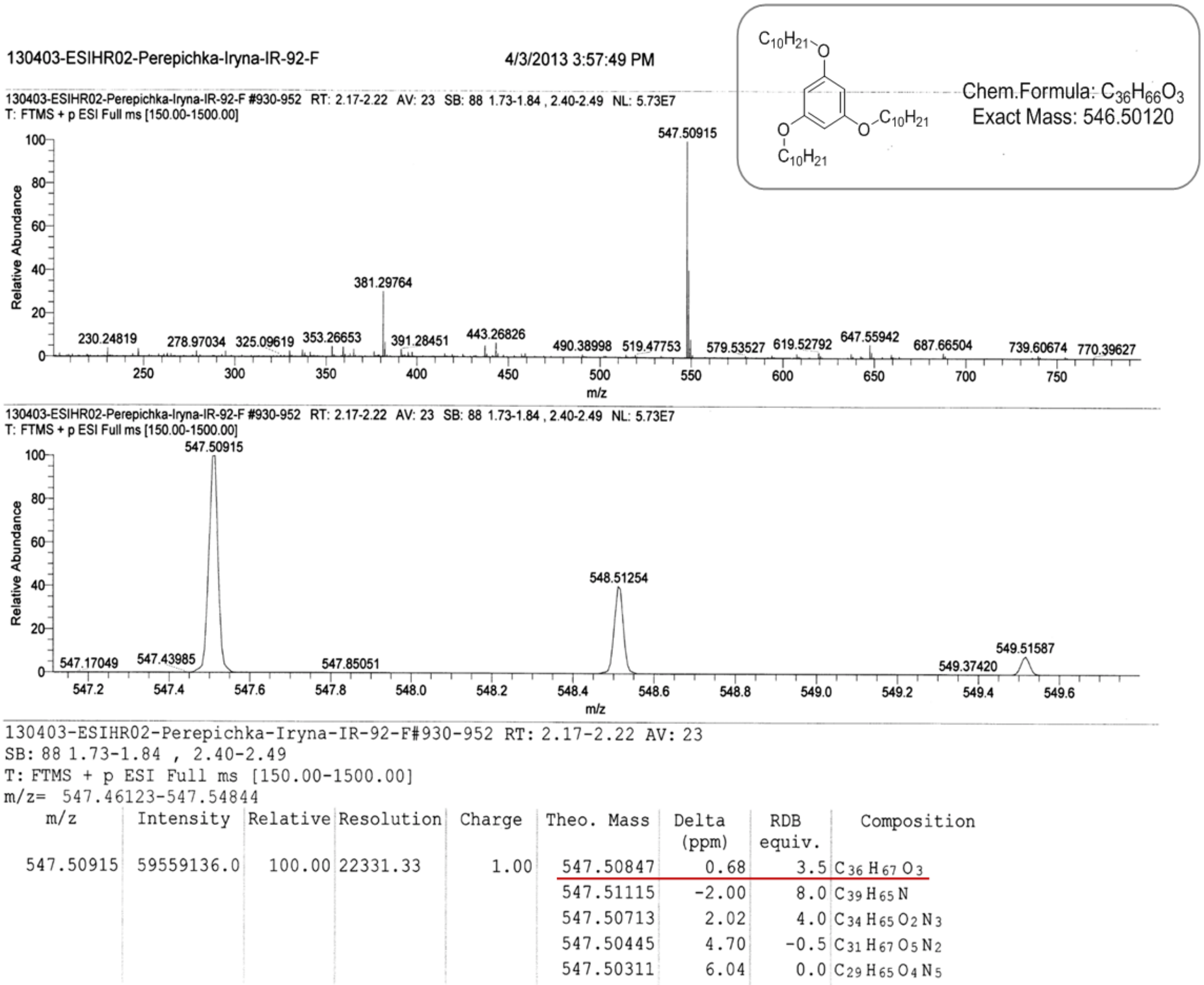

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Figure SI12. Mass spectrum of 1,3,5-tris(decyloxy)benzene.

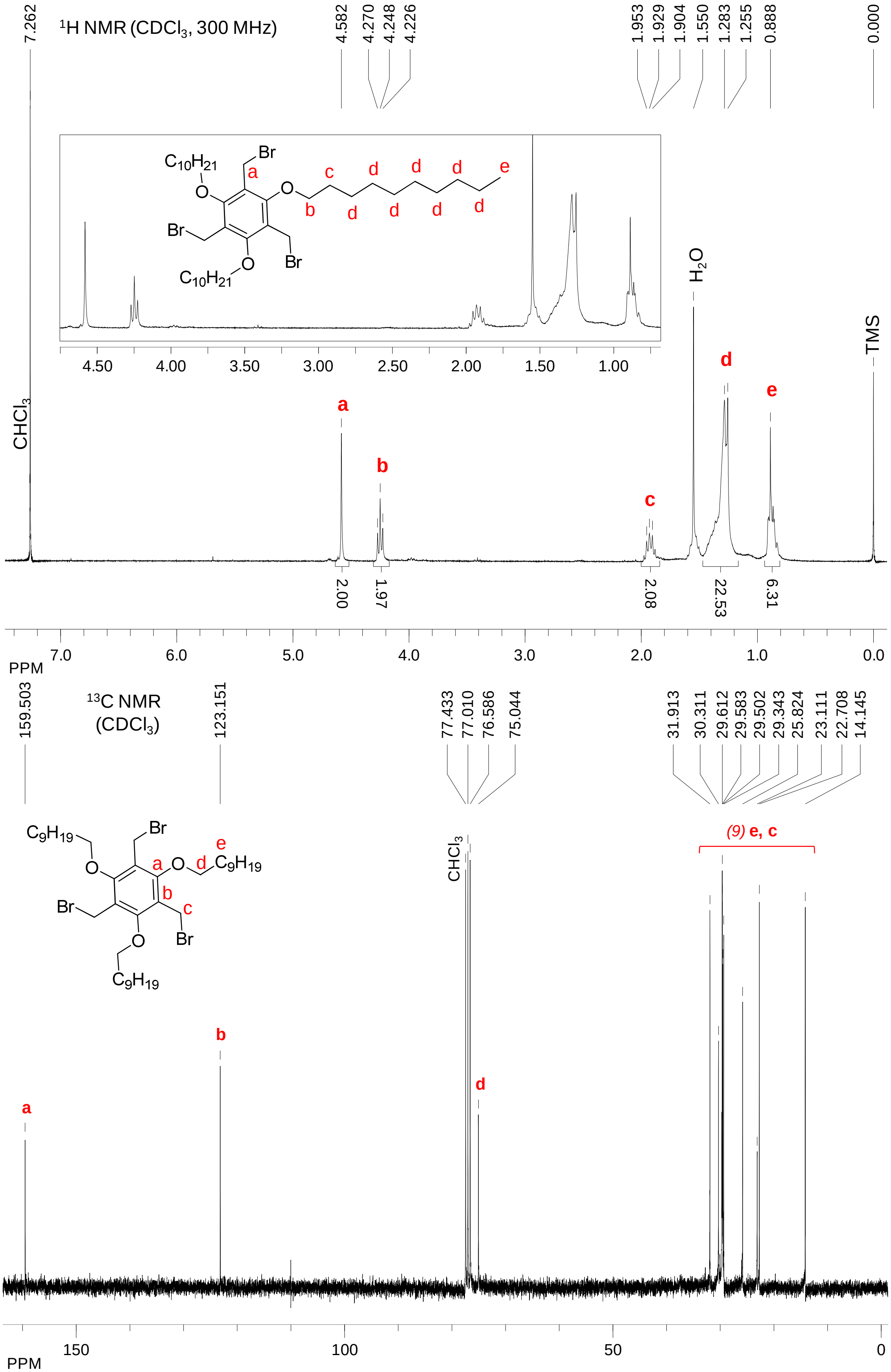


Figure SI13. ^{1}H (top) and ^{13}C (bottom) NMR spectra of 1,3,5-tris(decyloxy)-2,4,6-tris(bromomethyl)benzene.

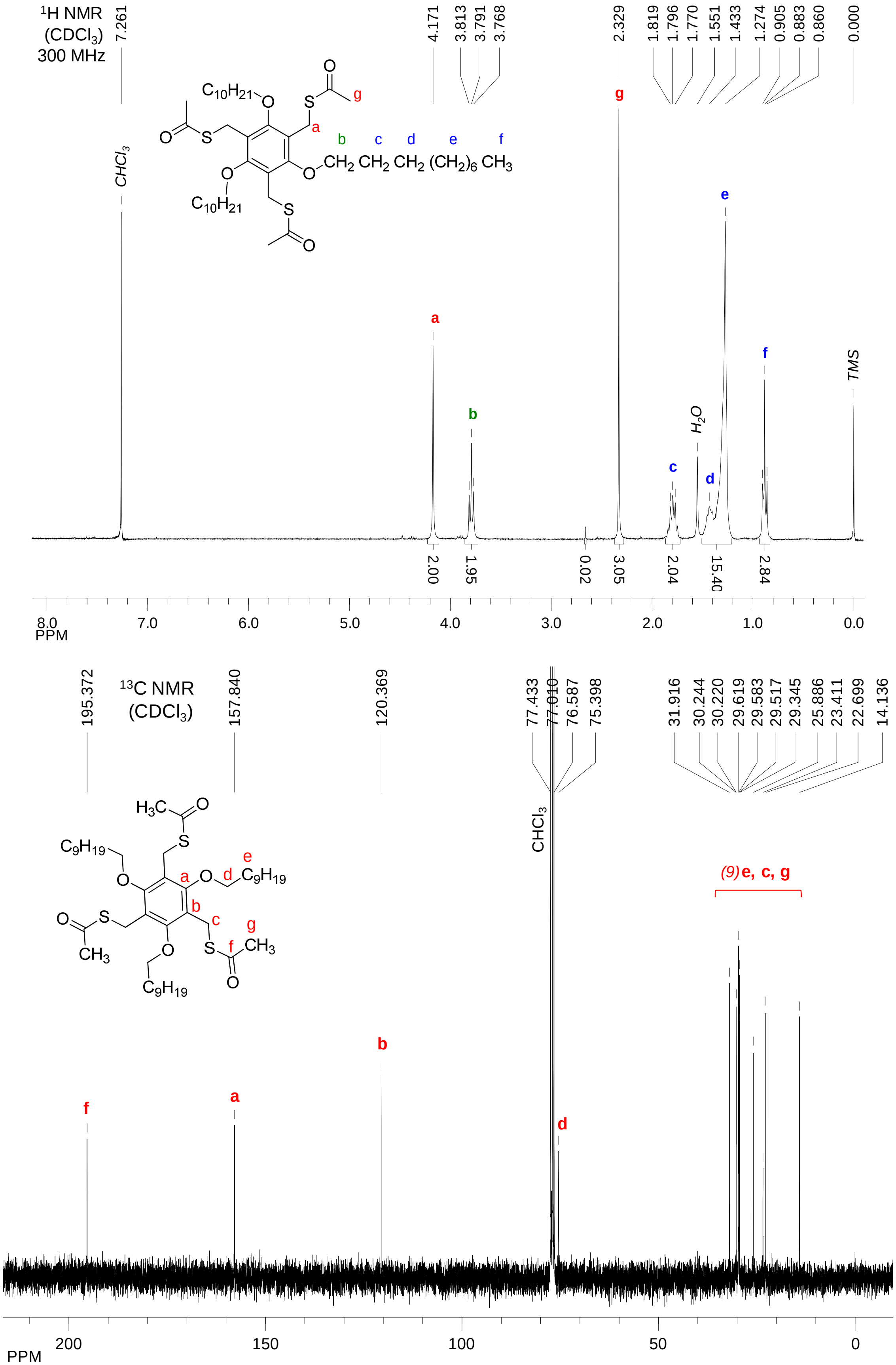
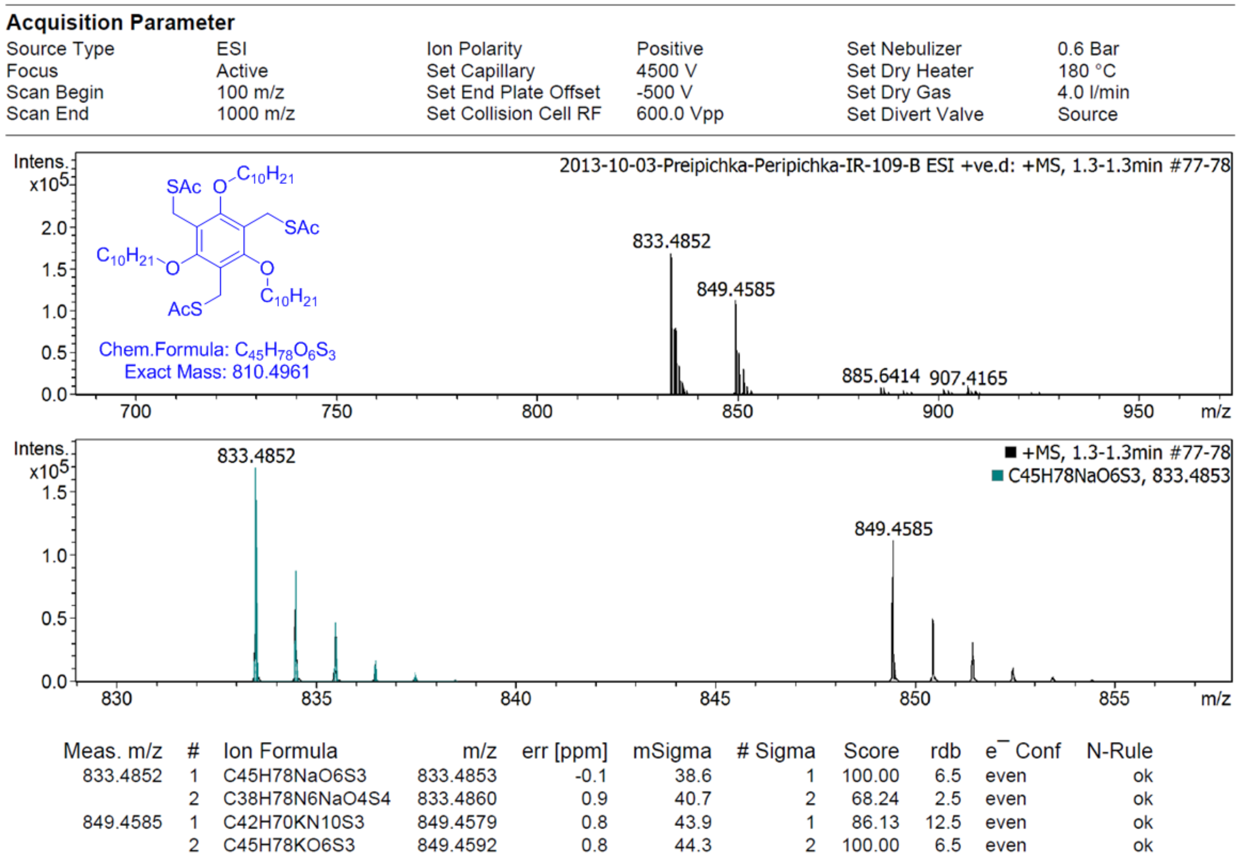


Figure SI14. ^{1}H (top) and ^{13}C (bottom) NMR spectra of 1,3,5-tris(decyloxy)-2,4,6-tris(S-acetylthiomethyl)benzene.



Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
833.4852	1	C45H78NaO6S3	833.4853	-0.1	38.6	1	100.00	6.5	even	ok
	2	C38H78N6NaO4S4	833.4860	0.9	40.7	2	68.24	2.5	even	ok
849.4585	1	C42H70KN10S3	849.4579	0.8	43.9	1	86.13	12.5	even	ok
	2	C45H78KO6S3	849.4592	0.8	44.3	2	100.00	6.5	even	ok

Figure SI15. Mass spectrum of 1,3,5-tris(decyloxy)-2,4,6-tris(S-acetylthiomethyl)benzene.

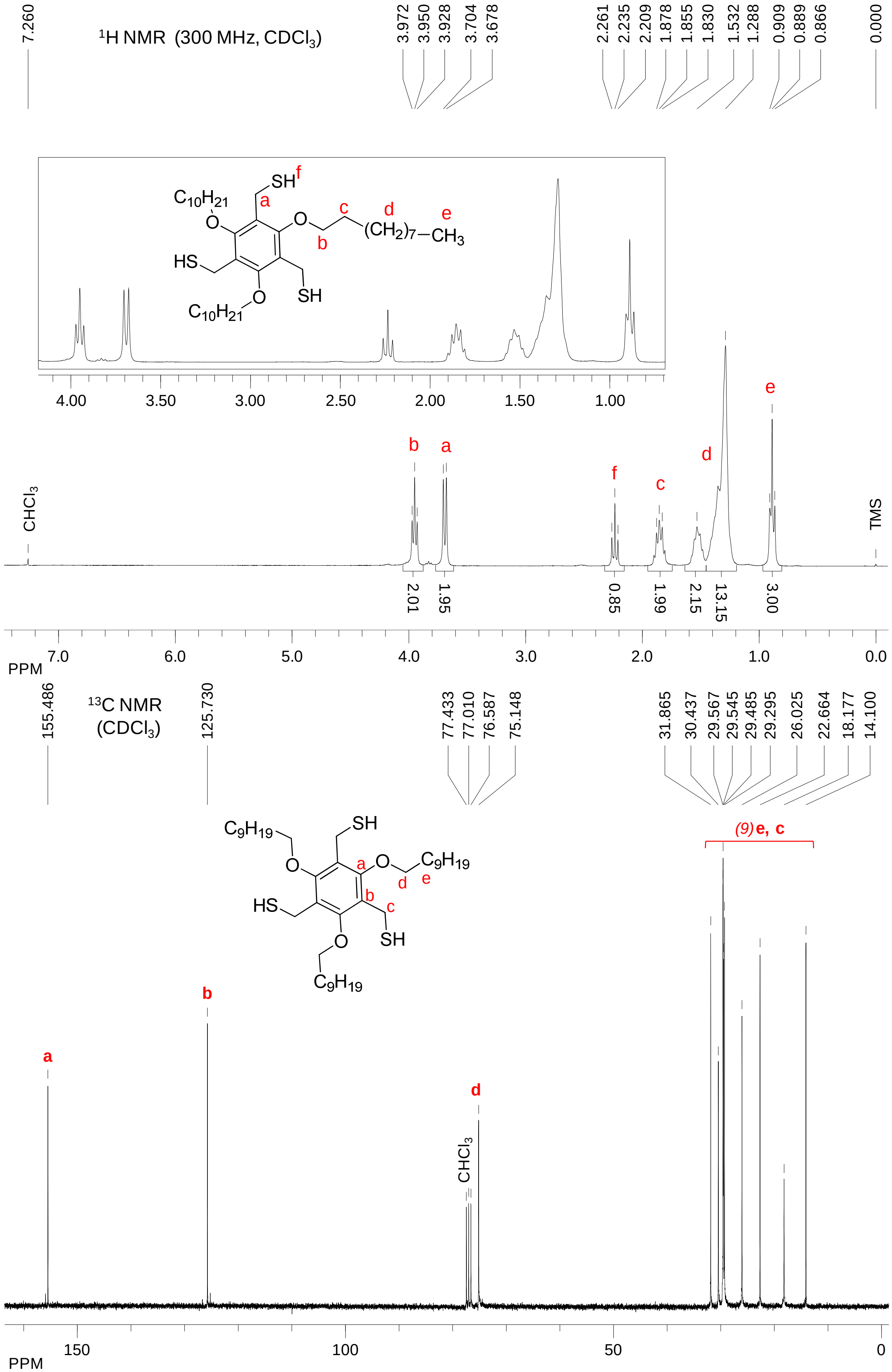
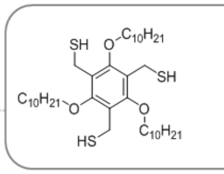


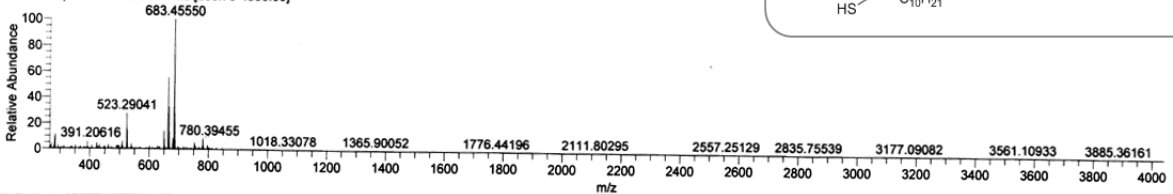
Figure SI16. ^{1}H (top) and ^{13}C (bottom) NMR spectra of 1,3,5-tris(decyloxy)-2,4,6-tris(hydrothiomethyl)benzene [**ODe$_3$-BTMT**].

130516-08HRAPCI-Perepichka-Iryna-IR99 5/16/2013 6:25:16 PM



Chem.Formula: $C_{39}H_{72}O_3S_3$
Exact Mass: 684.46436

130516-08HRAPCI-Perepichka-Iryna-IR99 #233-247 RT: 0.69-0.73 AV: 15 NL: 3.18E6
T: FTMS - p APCI corona Full ms [266.70-4000.00]



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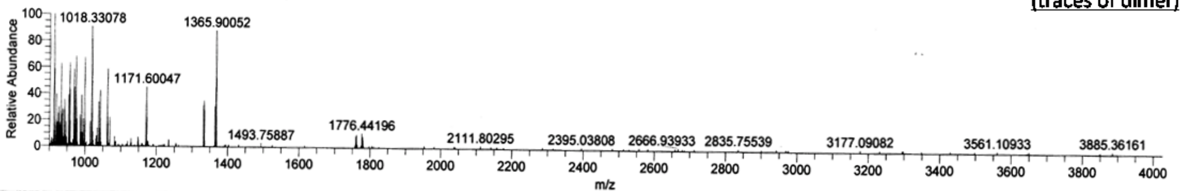
   m/z        Intensity  Relative Resolution  Charge  Theo. Mass   Delta     RDB      Composition
                                                                   (ppm)    equiv.
 683.45550   3184846.3   100.00  20599.29      1.00   683.45708    -2.32       4.5  C39 H71 O3 S3
                                                      683.45371     2.61       9.5  C42 H67 O3 S2
```

130516-08HRAPCI-Perepichka-Iryna-IR99 #233-247 RT: 0.69-0.73 AV: 15 NL: 1.52E4
T: FTMS - p APCI corona Full ms [266.70-4000.00]

(traces of dimer)



```
   m/z        Intensity Relative Resolution  Charge  Theo. Mass   Delta     RDB      Composition
                                                                  (ppm)    equiv.
 1365.90052    13374.0   100.00 15018.20      1.00  1365.89992     0.44      17.5  C85 H137 O S6
                                                    1365.89905     1.08      18.5  C84 H133 O6 S4
                                                    1365.90242    -1.39      13.5  C81 H137 O6 S5
                                                    1365.90579    -3.86       8.5  C78 H141 O6 S6
```

Figure SI17. Mass spectrum of 1,3,5-tris(decyloxy)-2,4,6-tris(hydrothiomethyl)benzene.