Supporting Information for

Detecting a Peroxide-based Explosive via Molecular Gelation

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I. General Experimental

Commercially available reagents and solvents for the synthetic procedures were obtained from Sigma-Aldrich, Acros Organic, and Fisher Scientific and used as received. The syntheses were adapted from published literature procedures[1] as described in section II.

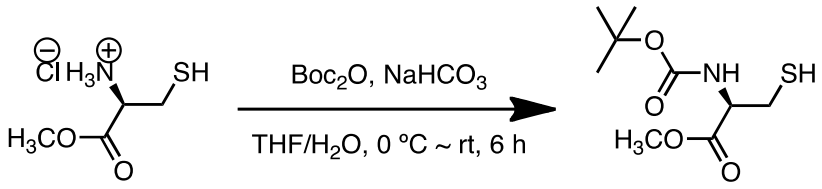
Synthesis of TATP:[2] All operations should be carried out behind a blast shield in the fume hood. TATP was synthesized on a 100-200 mg scale. A 4 mL vial was charged with a stir bar and placed in an ice-water bath. Acetone (200 µL) and H_2O_2 (30%, 276 µL) were added to the vial. Concentrated H_2SO_4 (20 µL) was added to the solution drop-wise. The vial was capped and the homogeneous solution was stirred overnight at rt. The white precipitate was filtered and washed with H_2O (3 x 20 mL), and dried under air for 30-60 min. The typical yield was ~35-60% and the product was characterized by ^1H and ^{13}C NMR spectroscopy. The product was stored at 4 ℃ and used without further purification.

NMR Spectroscopy: ^1H and ^{13}C NMR spectra for all compounds were acquired at rt in DMSO-d_6 or $CDCl_3$ on a Varian vnmrs 500 operating at 500 and 126 MHz or a Varian MR 400 operating at 400 and 100 MHz, respectively. The chemical shift data are reported in units of δ (ppm) relative to tetramethylsilane (TMS) and referenced with residual solvent. Multiplicities are reported as follows: singlet (s), doublet (d), doublet of doublets (dd), triplet (t), quartet (q), quintet (quin), multiplet (m) and broad resonance (br).

Mass Spectrometry: HRMS data was obtained on a Micromass Autospec Ultima Magnetic Sector mass spectrometer.

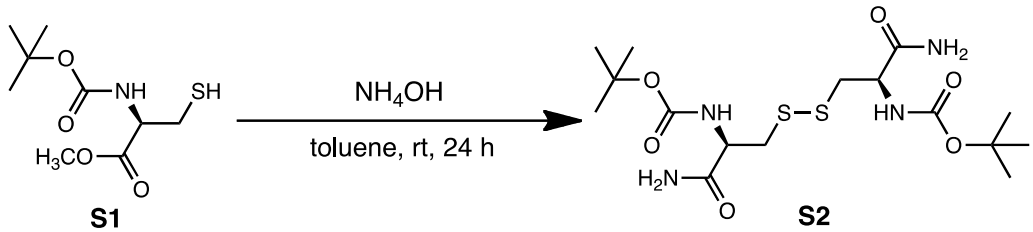
General Procedure for cgc Determination: A 4 mL vial was charged with ~2-3 mg of **2-7** and 0.30 mL MeOH. The mixture was sonicated while heating to the boiling point of MeOH and then allowed to cool to rt. The vial was inverted to examine if a stable gel formed. If a stable gel formed, 0.10 mL of MeOH was added and the procedure was repeated until an unstable gel was formed. The last concentration of the stable gel was recorded as critical gelation concentration (cgc).

II. Syntheses



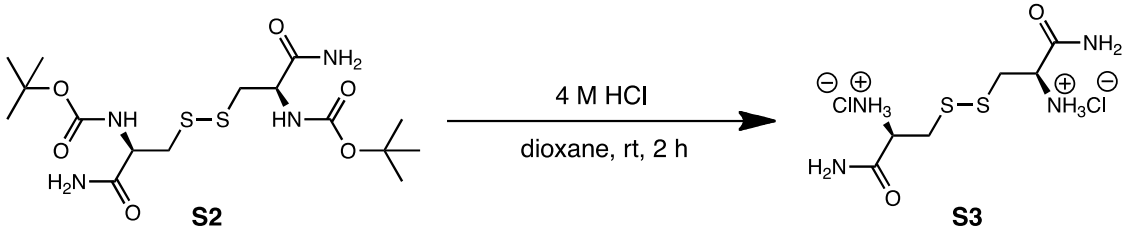
S1

S1: A 250 mL round-bottom flask was charged with a stir bar, L-cysteine methyl ester (2.005 g, 11.73 mmol) and THF (15 mL) and cooled to 0 ℃. To this solution, an aqueous solution of $NaHCO_3$ (2.3 M, 15 mL) was added, followed by the addition of di-*t*-butyl dicarbonate (2.427 g, 11.13 mmol). The ice-water bath was then removed and the solution was stirred at rt. After 6 h, the solution was concentrated under reduced pressure and the residue was adjusted to ~ pH 4 with saturated aqueous solution of citric acid. The mixture was then extracted with CH_2Cl_2 (3 x 30 mL). The organic layers were combined, washed with brine (50 mL), dried over $MgSO_4$, filter and concentrated in vacuo to give a colorless oil (2.577 g, 94%). HRMS (ESI): Calcd for $C_9H_{17}NO_4S$, 258.0770 $[M + Na]^+$; Found 258.0770 .



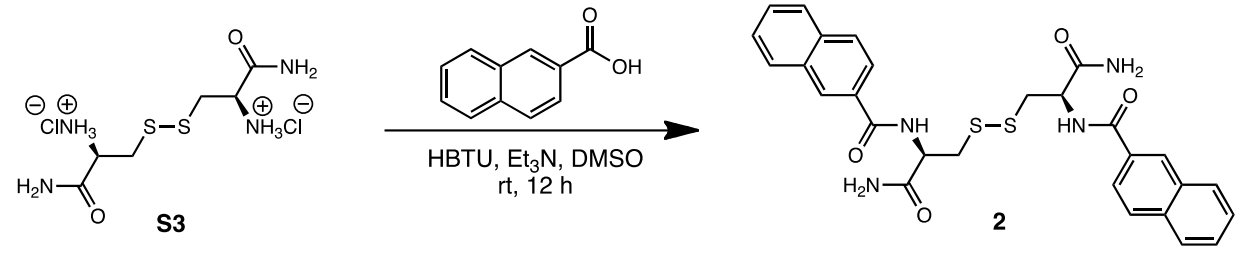
S1 **S2**

S2[1a]**:** A 250 mL round-bottom flask was charged with a stir bar, **S1** (5.199 g, 22.12 mmol), toluene (15 mL) and NH_4OH (aq) (30%, 15 mL) and the heterogeneous mixture was stirred at rt. After 24 h, the reaction was concentrated under reduced pressure. The solid residue was filtered and the white solid was washed with H_2O (3 x 20 mL), MeOH (3 x 20 mL) and dried in vacuo to give a white solid (3.334 g, 69%). HRMS (ESI): Calcd for $C_{16}H_{31}N_4O_6S_2$, 461.1499 $[M + Na]^+$; Found 461.1501.

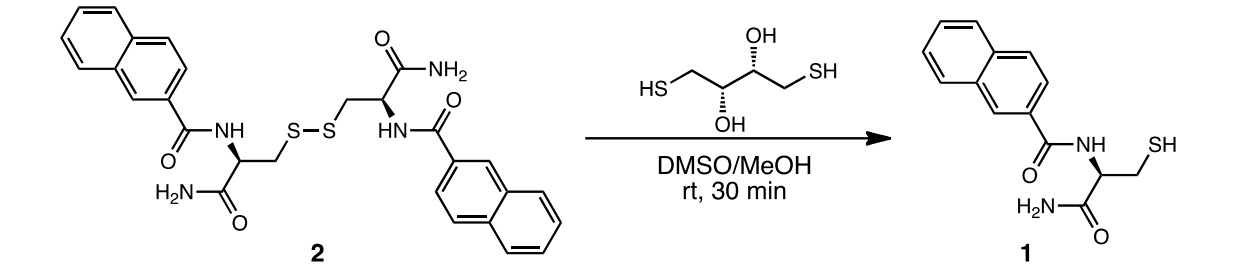


S2 **S3**

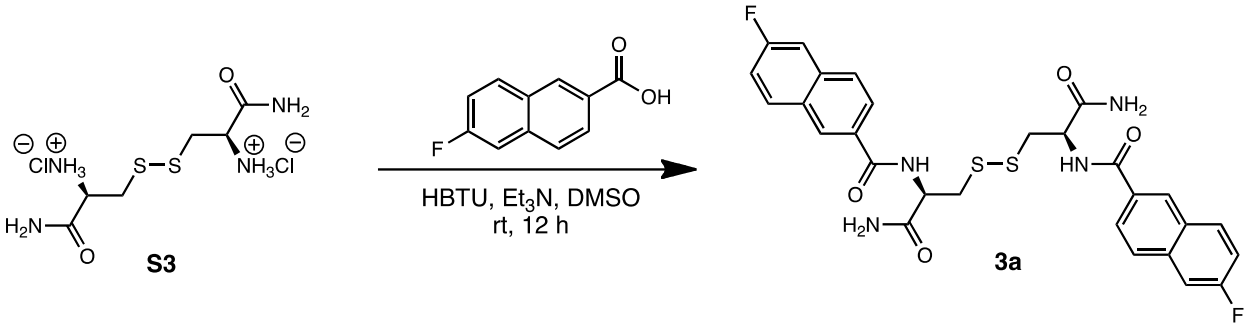
S3[1b]**:** A 50 mL round-bottom flask was charged with a stir bar, **S2** (795 mg, 1.82 mmol) and dioxane (10 mL). To this mixture, HCl (10 mL, 4 M in dioxane) was added over 10 min and the mixture was stirred at rt. After 2 h, the solvent was evaporated under reduced pressure. The solid residue was filtered and the white solid was washed with acetone (3 x 20 mL) and dried in vacuo to give a white solid (535 mg, 95%). HRMS (ESI): Calcd for $C_6H_{14}N_4O_2S_2$, 239.0636 $[M + H]^+$; Found 239.0637.



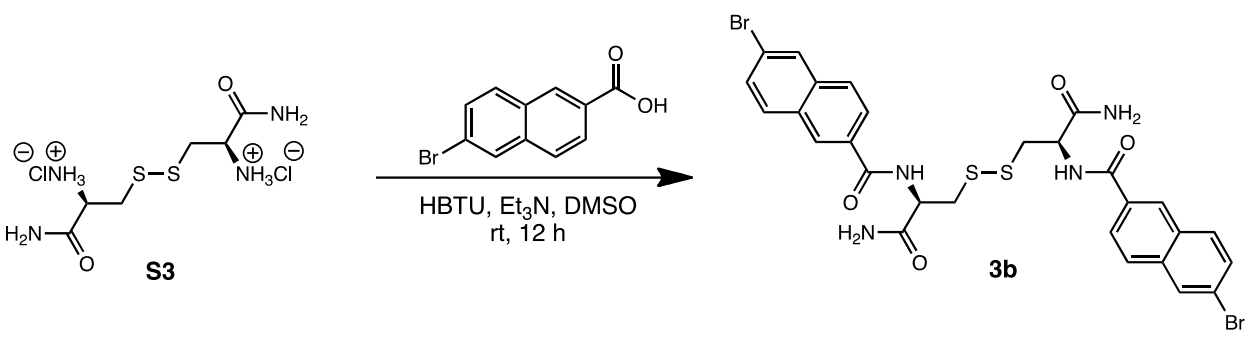
2[1c]**:** A 50 mL round-bottom flask was charged with a stir bar, 2-naphthoic acid (111 mg, 0.645 mmol), HBTU (245 mg, 0.646 mmol) and anhydrous DMSO (10 mL). The solution was stirred at rt for 30 min. Sequentially, **S3** (100 mg, 0.323 mmol) and Et_3N (179 µL, 1.29 mmol) were added and the solution was stirred at rt. After 12 h, the solution was poured into H_2O (100 mL). The resulting precipitate was filtered and washed with H_2O (3 x 20 mL), MeOH (3 x 20 mL) and dried in vacuo to give a white solid (113 mg, 64%). HRMS (ESI): Calcd for $C_{28}H_{26}N_4O_4S_2$, 547.1468 $[M + H]^+$; Found 547.1473.



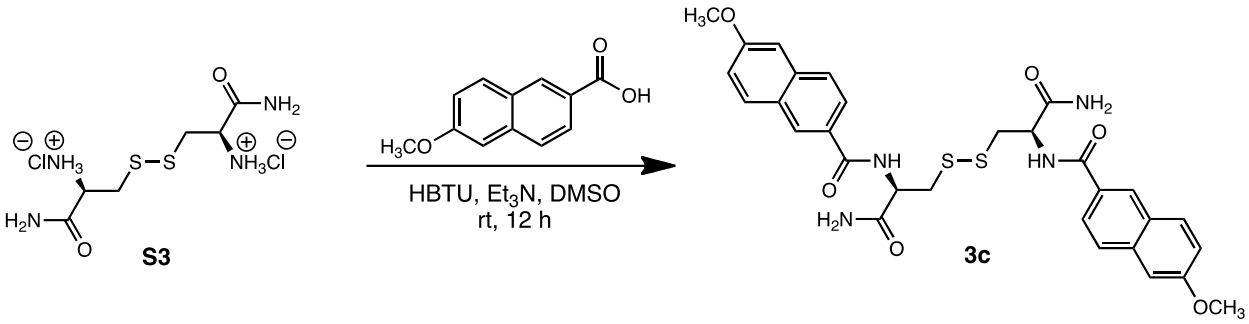
1: A 50 mL round-bottom flask was charged with a stir bar, **2** (200 mg, 0.366 mmol) and anhydrous DMSO (10 mL). To this mixture, a solution of dithiolthreitol (1.85 M, 1 mL MeOH) was added and the solution was stirred at rt. After 30 min, the mixture was poured into H_2O (100 mL) and extracted with EtOAc (3 x 30 mL). The organic layers were combined, washed with brine (2 x 30 mL), dried over $MgSO_4$, filtered and concentrated in vacuo to give a white solid (91 mg, 45%). HRMS (ESI): Calcd for $C_{14}H_{14}N_2O_2S$, 297.0674 $[M + Na]^+$; Found 297.0672.



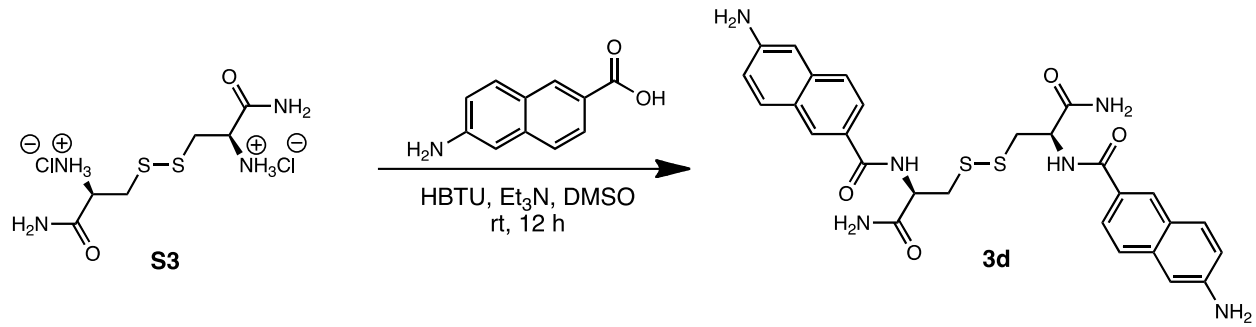
3a: A 50 mL round-bottom flask was charged with a stir bar, 6-fluoro-2-naphthoic acid (123 mg, 0.647 mmol), HBTU (245 mg, 0.646 mmol) and anhydrous DMSO (10 mL). The solution was stirred at rt for 30 min. Sequentially, **S3** (100 mg, 0.323 mmol) and Et_3N (179 µL, 1.29 mmol) were added and the solution was stirred at rt. After 12 h, the solution was poured into H_2O (100 mL). The resulting precipitate was filtered and washed with H_2O (3 x 20 mL), MeOH (3 x 20 mL) and dried in vacuo to give a white solid (92 mg, 49%). HRMS (ESI): Calcd for $C_{28}H_{26}N_4O_6S_2$, 583.1280 $[M + H]^+$; Found 583.1301.



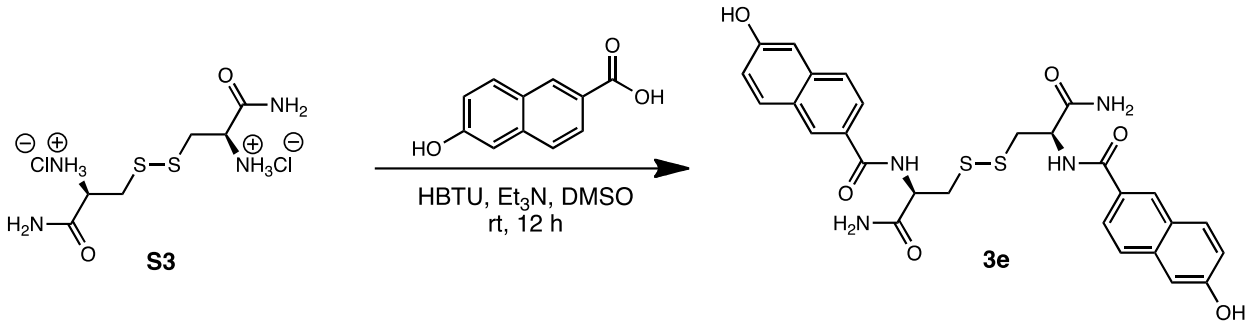
3b: A 50 mL round-bottom flask was charged with a stir bar, 6-bromo-2-naphthoic acid (162 mg, 0.645 mmol), HBTU (245 mg, 0.646 mmol) and anhydrous DMSO (10 mL). The solution was stirred at rt for 30 min. Sequentially, **S3** (100 mg, 0.323 mmol) and Et_3N (179 µL, 1.29 mmol) were added and the solution was stirred at rt. After 12 h, the solution was poured into H_2O (100 mL). The resulting precipitate was filtered and washed with H_2O (3 x 20 mL), MeOH (3 x 20 mL) and dried in vacuo to give a white solid (138 mg, 61%). HRMS (ESI): Calcd for $C_{28}H_{24}Br_2N_4O_4S_2$, 724.9498 $[M + Na]^+$; Found 724.9483.



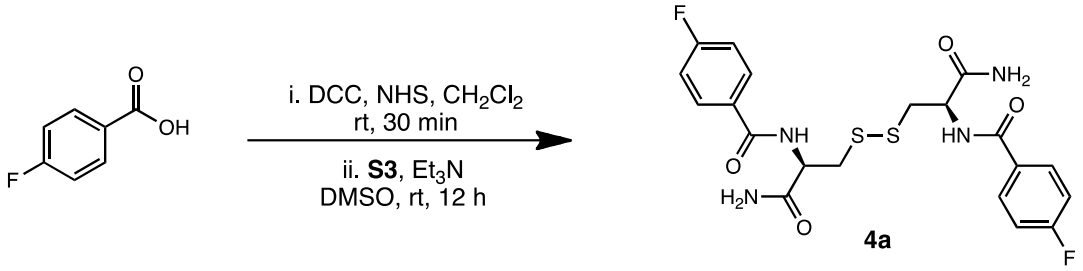
3c: A 50 mL round-bottom flask was charged with a stir bar, 6-methoxy-2-naphthoic acid (130 mg, 0.644 mmol), HBTU (245 mg, 0.646 mmol) and anhydrous DMSO (10 mL). The solution was stirred at rt for 30 min. Sequentially, **S3** (100 mg, 0.323 mmol) and Et_3N (179 µL, 1.29 mmol) were added and the solution was stirred at rt. After 12 h, the solution was poured into H_2O (100 mL). The resulting precipitate was filtered and washed with H_2O (3 x 20 mL), MeOH (3 x 20 mL) and dried in vacuo to give a white solid (115 mg, 59%). HRMS (ESI): Calcd for $C_{30}H_{30}N_4O_6S_2$, 607.1685 $[M + H]^+$; Found 607.1685.



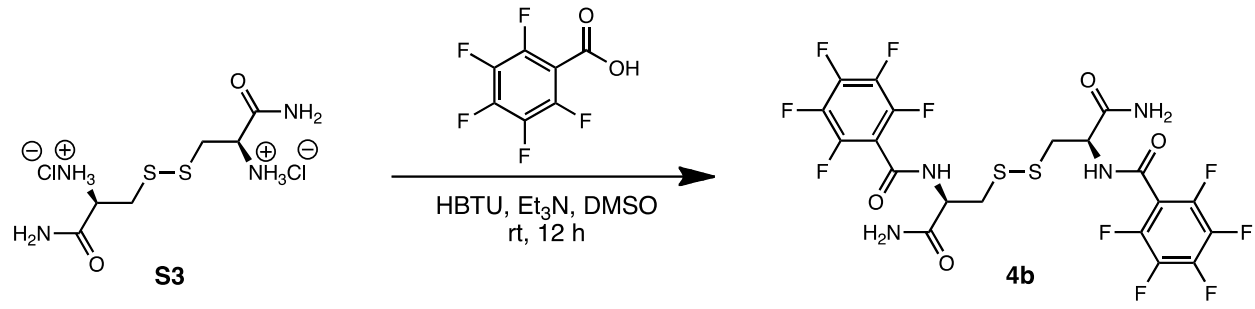
3d: A 50 mL round-bottom flask was charged with stir bar, 6-amino-2-naphthoic acid (0.300 g, 1.60 mmol), HBTU (0.608 g, 1.79 mmol) and anhydrous DMSO (15 mL). The solution was stirred at rt for 30 min. Sequentially, **S3** (0.249 g, 0.801 mmol) and Et_3N (0.47 mL, 3.2 mmol) were added and the solution was stirred at rt. After 12 h the solution was poured into H_2O (150 mL). The resulting precipitate was filtered, washed with H_2O (3 x 10 mL), MeOH (3 x 10 mL) and acetone (3 x 10 mL) to give a light brown solid (0.282 g, 61%). HRMS (ESI): Calcd for $C_{28}H_{28}N_6O_4S_2$, 599.1511 $[M + Na]^+$; Found 599.1509.



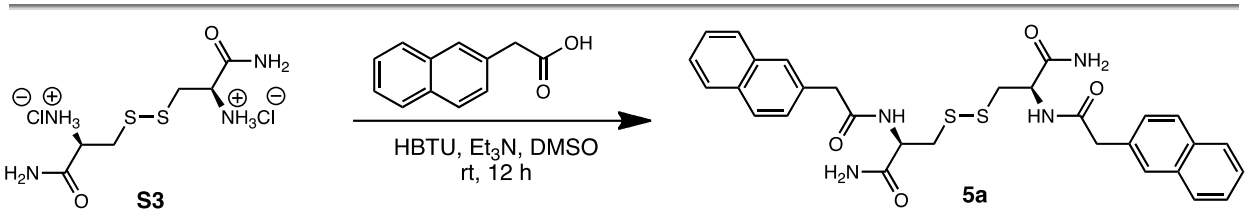
3e: A 50 mL round-bottom flask was charged with stir bar, 6-hydroxy-2-naphthoic acid (0.158 g, 0.839 mmol) and HBTU (0.318 g, 0.838 mmol) and anhydrous DMSO (10 mL). The solution was stirred at rt for 30 min. Sequentially, **S3** (0.130 g, 0.418 mmol) and Et_3N (0.26 mL, 1.8 mmol) were added and the solution was stirred at rt. After 12 h the solution was poured into H_2O (100 mL). The resulting precipitate was filtered, washed with H_2O (3 x 10 mL) and hexanes (3 x 10 mL). The crude product was recrystallized from MeOH/EtOAc (95:5) to give a white solid (0.077 g, 32%). HRMS (ESI): Calcd for $C_{28}H_{26}N_4O_6S_2$, 579.1367 $[M + H]^+$; Found 579.1378.



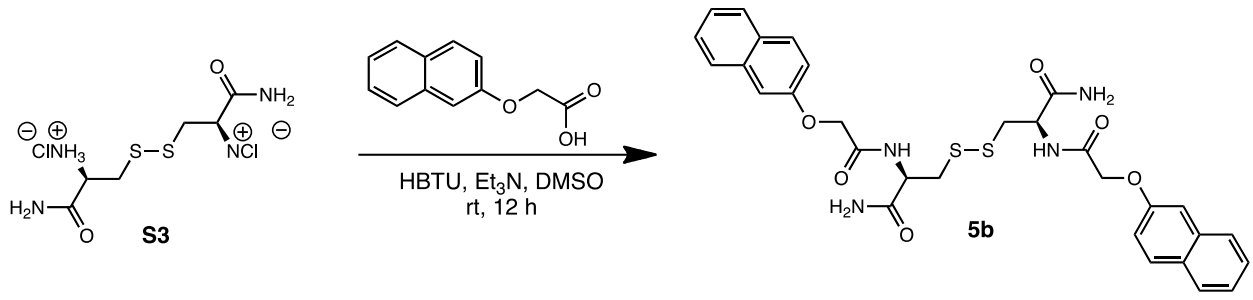
4a: In a 20 mL vial, 4-fluorobenzoic acid (0.200 g, 1.44 mmol) and N-hydroxysuccinimide (NHS, 0.164 g, 1.43 mmol) were dissolved in CH_2Cl_2 (10.0 mL) at rt. To this solution, N,N'-dicyclohexylcarbodiimide (DCC, 0.198 g, 0.960 mmol) was added and the solution was stirred at rt for 30 min. The precipitate was removed via filtration and the filtrate, which contains the intermediate, was evaporated under reduced pressure to obtain a white solid that was submitted to the next reaction without further purification. The solid obtained from previous step and **S3** (0.222 g, 0.714 mmol) were dissolved in anhydrous DMSO (10 mL) and stirred for 10 min at rt. Then Et_3N (4.0 mL, 2.9 mmol) was added at rt. After 12 h the reaction was poured into H_2O (100 mL). The resulting precipitate was filtered, washed with H_2O (3 x 10 mL), hexanes (2 x 10 mL), and cyclohexane/EtOH (1:1, 2 x 20 mL). The crude product was recrystallized from MeOH to give a white solid (0.139 g, 46%). HRMS (ESI): Calcd for $C_{20}H_{20}F_2N_4O_4S_2$, 505.0792 $[M + Na]^+$; Found 505.0784.



4b: A 50 mL round-bottom flask was charged with a stir bar, pentafluorobenzoic acid (72 mg, 0.34 mmol), HBTU (129 mg, 0.340 mmol) and anhydrous DMSO (10 mL). The solution was stirred at rt for 30 min. Sequentially, **S3** (53 mg, 0.17 mmol) and Et_3N (95 µL, 0.68 mmol) were added and the solution was stirred at rt. After 12 h, the solution was poured into H_2O (100 mL). The resulting precipitate was filtered and washed with H_2O (3 x 20 mL) and dried in vacuo to give a pale brown solid (29 mg, 27%). HRMS (ESI): Calcd for $C_{20}H_{12}F_{10}N_4O_4S_2$, 627.0213 $[M + H]^+$; Found 627.0220.

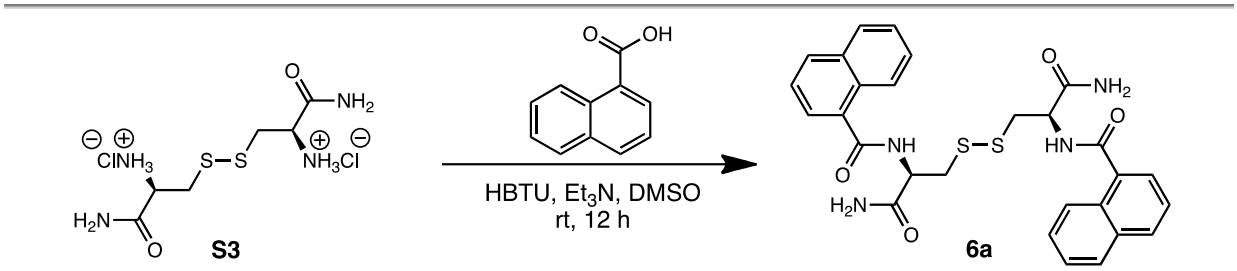


5a: A 50 mL round-bottom flask was charged with a stir bar, 2-naphthaleneacetic acid (120 mg, 0.645 mmol), HBTU (245 mg, 0.646 mmol) and anhydrous DMSO (10 mL). The solution was stirred at rt for 30 min. Sequentially, **S3** (100 mg, 0.323 mmol) and Et_3N (179 µL, 1.29 mmol) were added and the solution was stirred at rt. After 12 h, the solution was poured into H_2O (100 mL). The resulting precipitate was filtered and washed with H_2O (3 x 20 mL), MeOH (3 x 20 mL) and dried in vacuo to give a white solid (114 mg, 62%). HRMS (ESI): Calcd for $C_{30}H_{30}N_4O_4S_2$, 597.1606 $[M + H]^+$; Found 597.1605.



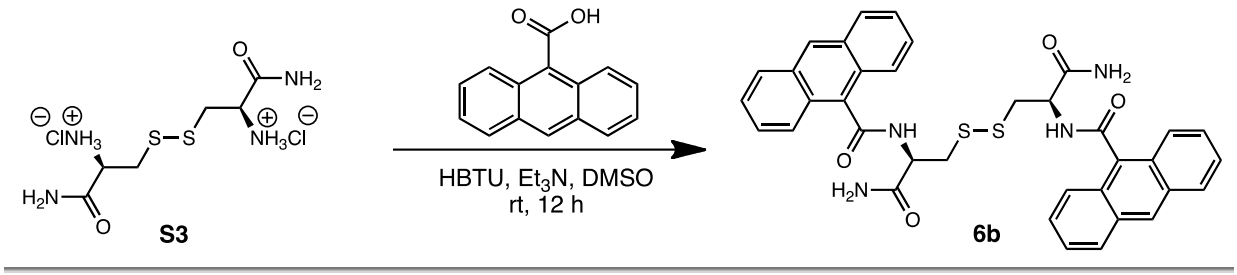
5b: A 50 mL round-bottom flask was charged with a stir bar, 2-naphthoxyacetic acid (130 mg, 0.644 mmol), HBTU (245 mg, 0.646 mmol) and anhydrous DMSO (10 mL). The solution was stirred at rt for 30 min. Sequentially, **S3** (100 mg, 0.323 mmol) and Et_3N (179 µL, 1.29 mmol) were added and the solution

was stirred at rt. After 12 h, the solution was poured into H_2O (100 mL). The resulting precipitate was filtered and washed with H_2O (3 x 20 mL), MeOH (3 x 20 mL) and dried in vacuo to give a white solid (158 mg, 81%). HRMS (ESI): Calcd for $C_{30}H_{30}N_4O_6S_2$, 629.1504 $[M + Na]^+$; Found 629.1500. Elemental Analysis: Calcd. for $C_{30}H_{30}N_4O_6S_2$: C, 59.39; H, 4.98; N, 9.23; O, 15.82; S, 10.57; Found: C, 59.50; H, 4.93; N, 9.21; O, 15.94; S, 10.42.



S3 6a

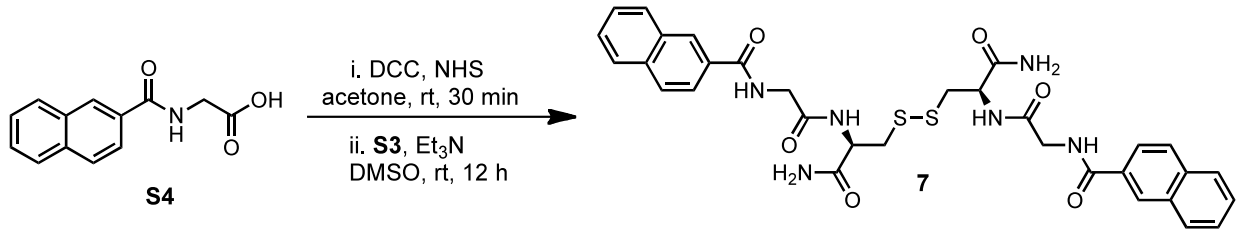
6a: A 50 mL round-bottom flask was charged with a stir bar, 1-naphthoic acid (111 mg, 0.645 mmol), HBTU (245 mg, 0.646 mmol) and anhydrous DMSO (10 mL). The solution was stirred at rt for 30 min. Sequentially, **S3** (100 mg, 0.323 mmol) and Et_3N (179 µL, 1.29 mmol) were added and the solution was stirred at rt. After 12 h, the solution was poured into H_2O (100 mL). The resulting precipitate was filtered and washed with H_2O (3 x 20 mL), MeOH (3 x 20 mL) and dried in vacuo to give a brown solid (102 mg, 58%). HRMS (ESI): Calcd for $C_{28}H_{26}N_4O_4S_2$, 547.1474 $[M + H]^+$; Found 547.1474.



S3 6b

6b: A 50 mL round-bottom flask was charged with a stir bar, 9-anthracenecarboxylic acid (143 mg, 0.644 mmol), HBTU (245 mg, 0.646 mmol) and anhydrous DMSO (10 mL). The solution was stirred at rt for 30 min. Sequentially, **S3** (100 mg, 0.323 mmol) and Et_3N (179 µL, 1.29 mmol) were added and the solution was stirred at rt. After 12 h, the solution was poured into H_2O (100 mL). The resulting precipitate was filtered and washed with H_2O (3 x 20 mL), MeOH (3 x 20 mL) and dried in vacuo to give a pale yellow solid (80 mg, 38%). HRMS (ESI): Calcd for $C_{36}H_{30}N_4O_4S_2$, 669.1606 $[M + Na]^+$; Found 669.1604.

S4: In a 20 mL vial, 2-naphthoic acid (0.150 g, 0.871 mmol) and NHS (0.101 g, 0.869 mmol) were dissolved in CH_2Cl_2 (10.0 mL) at rt. To this solution, DCC (0.198 g, 0.960 mmol) was added and the final solution was stirred at rt for 30 min. The precipitate was removed via filtration and the filtrate, which contains the intermediate, was evaporated under reduced pressure to obtain a white solid that was submitted to the next reaction without further purification. Glycine (0.065 g, 0.87 mmol) and $NaHCO_3$ (0.146 g, 1.74 mmol) were dissolved in H_2O (6.0 mL) at rt and the solid obtained previously was dissolved in acetone (9.0 mL) and added to the aqueous solution. After 12 h, the reaction was evaporated under reduced pressure, and the residue re-dissolved in H_2O (~10 mL). The insoluble solid was filtered off and the filtrate was acidified to pH = 3 with dilute HCl to obtain a white precipitate. The solid was filtered, washed with H_2O (3 x 10 mL), hexanes (2 x 10 mL), CH_2Cl_2 (2 x 10 mL) and dried under vacuum to give a white solid (0.145 g; 72%). HRMS (ESI): Calcd for $C_{13}H_{11}NO_3$, 230.0812 $[M + H]^+$; Found 230.0815.



7: In a 20 mL vial, **S4** (0.130 g, 0.567 mmol) and NHS (0.065 g, 0.57 mmol) were dissolved in acetone (12.0 mL) at rt. To this solution, DCC (0.129 g, 0.625 mmol) was added and the final solution was stirred at rt for 30 min. The precipitate was removed via filtration and the filtrate, which contains the intermediate, was evaporated under reduced pressure to obtain a white solid that was submitted to the next reaction without further purification. The solid obtained from previous step and **S3** (0.088 g, 0.28 mmol) were dissolved in anhydrous DMSO (15 mL) and stirred for 10 min at rt. Then Et_3N (0.16 mL, 1.1 mmol) was added at rt. After 12 h, the reaction was poured into H_2O (100 mL). The resulting precipitate was filtered, washed with H_2O (3 x 10 mL), hexanes (2 x 10 mL), and cyclohexane/EtOH (1:1, 2 x 20 mL) to give a white solid (0.124 g, 66%). HRMS (ESI): Calcd for $C_{32}H_{32}N_6O_6S_2$, 683.1722 $[M + Na]^+$; Found 683.1720.

III. ^{1}H and ^{13}C NMR Spectra

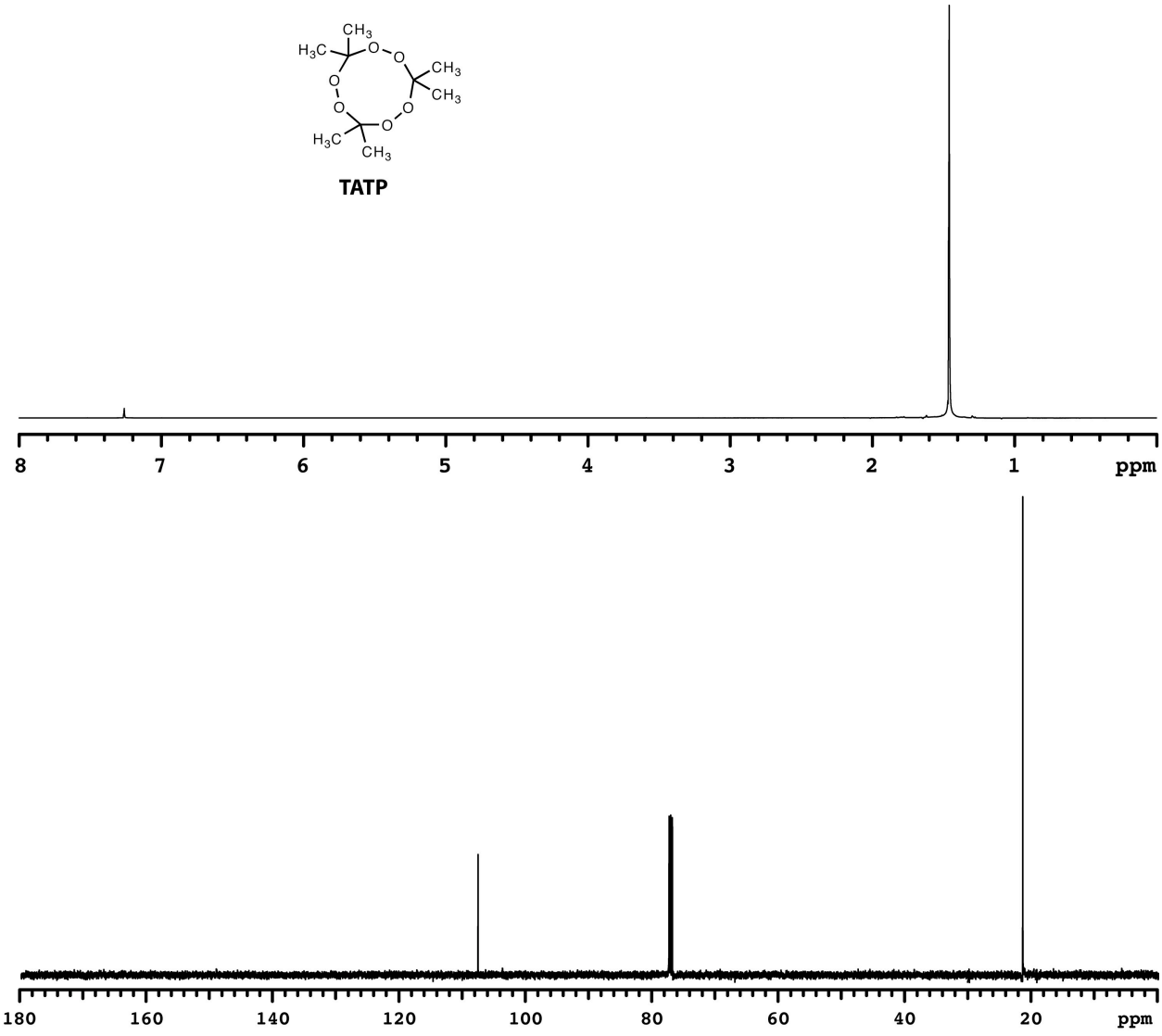


Figure S1. ^{1}H and ^{13}C NMR spectra of **TATP.** ^{1}H NMR ($CDCl_3$, 500 MHz): δ 1.46. ^{13}C NMR ($CDCl_3$, 125 MHz): δ 107.72, 21.54.

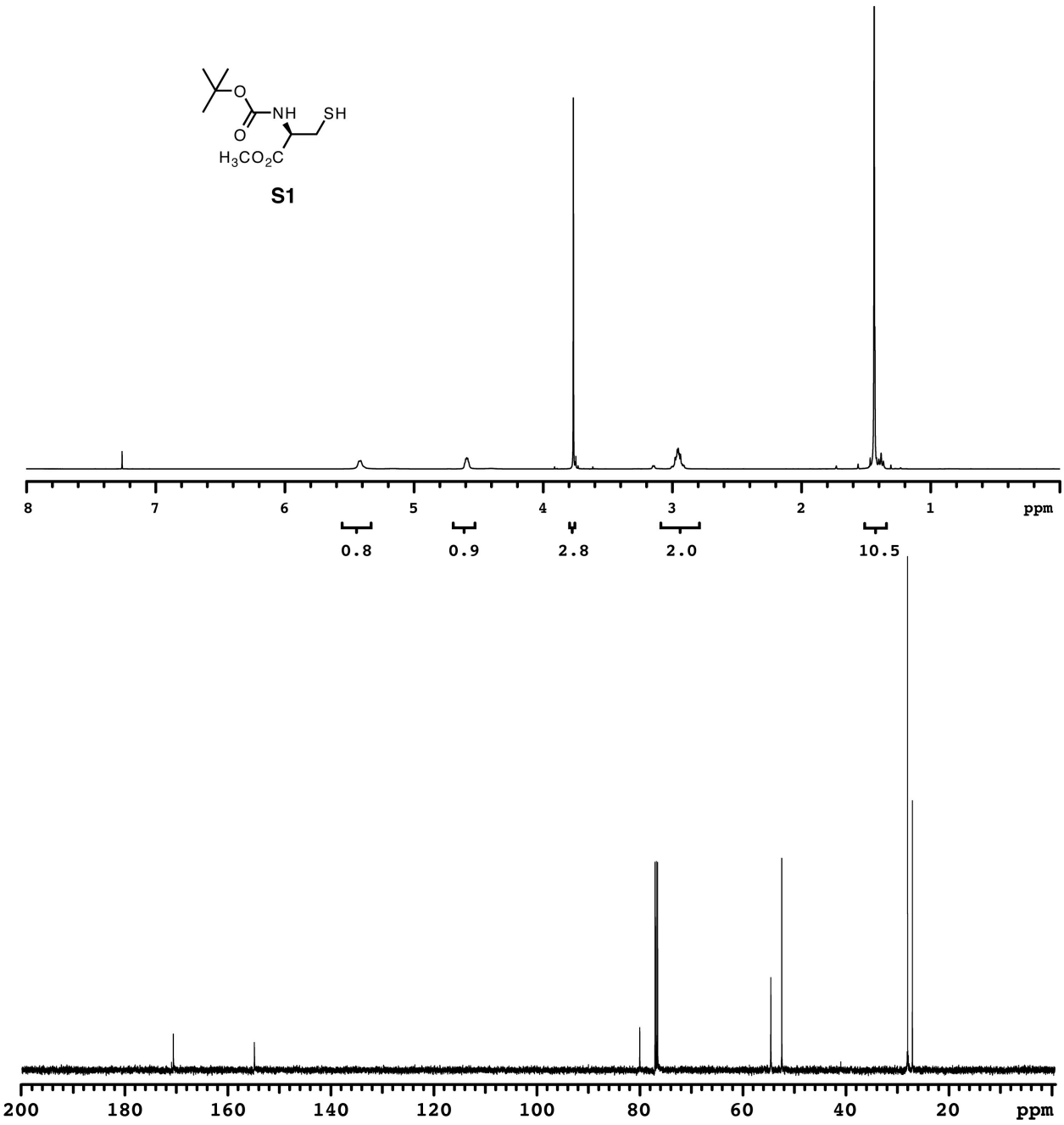


Figure S2. ^{1}H and ^{13}C NMR spectra of **S1**. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 5.42 (brs, 1H), 4.59 (brs, 1H), 3.77 (s, 3H), 2.95 (m, 2H), 1.43-1.37 (m, 10H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ 170.52, 154.79, 79.96, 54.52, 52.39, 27.98, 27.03.

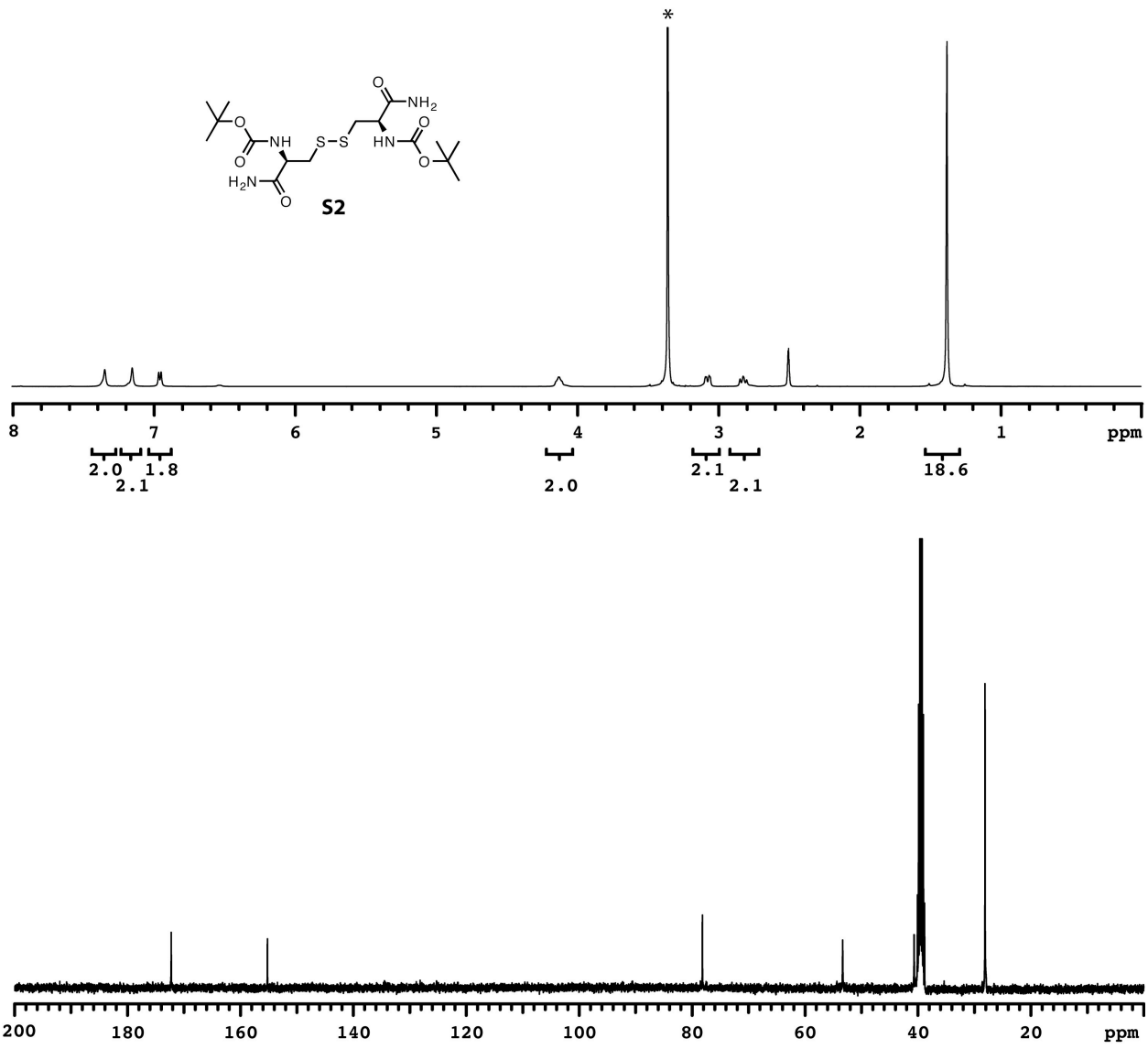


Figure S3. ^{1}H and ^{13}C NMR spectra of **S2**. ^{1}H NMR (DMSO-d_6, 400 MHz): δ 7.33 (brs, 2H), 7.14 (brs, 2H), 6.94 (brm, 2H), 4.13 (brs, 2H), 3.08 (m, 2H), 2.83 (m, 2H), 1.38 (s, 18H). ^{13}C NMR (DMSO-d_6, 100 MHz): δ 172.30, 155.26, 78.22, 53.38, 40.72, 28.16. *denotes H_2O.

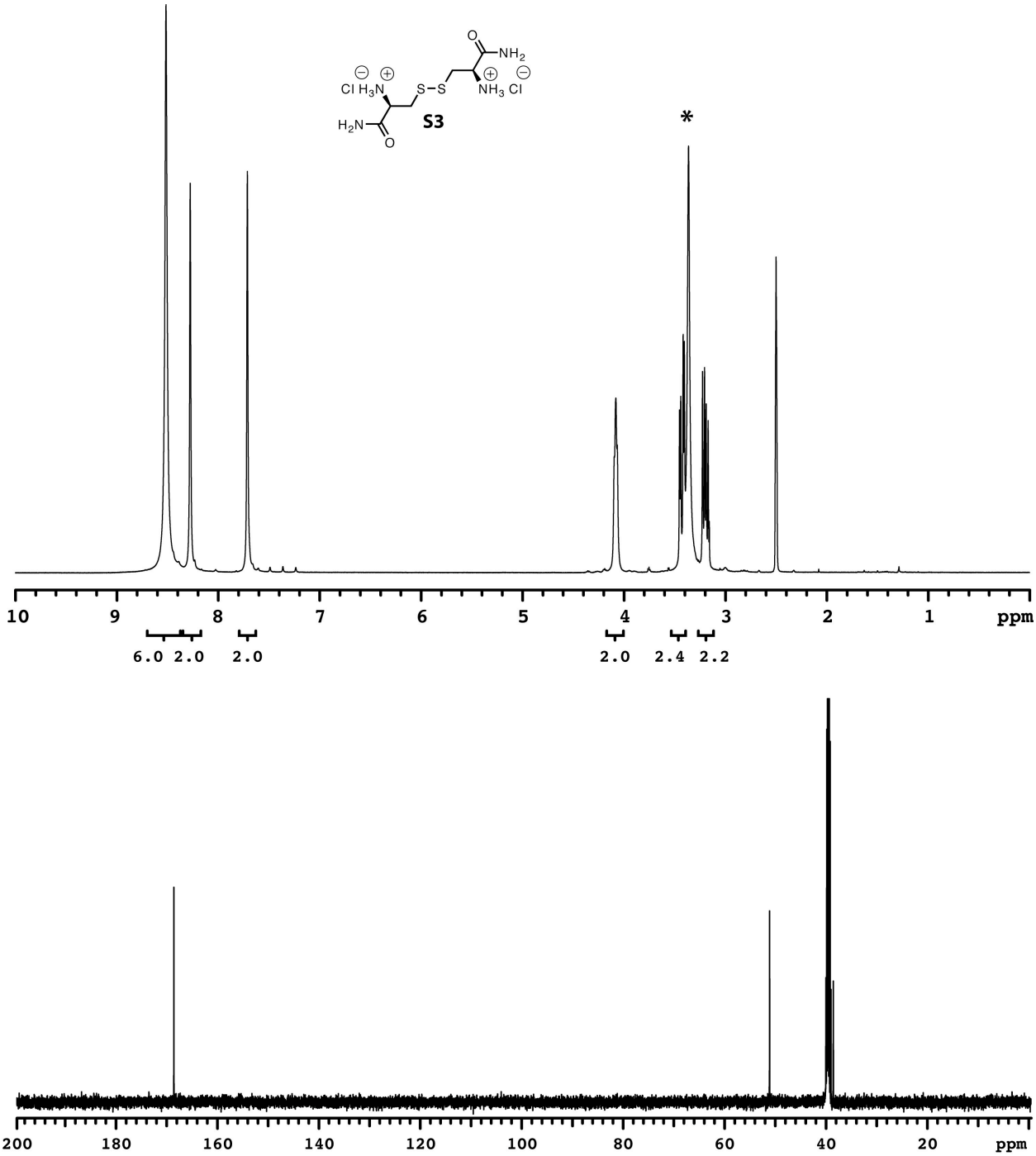


Figure S4. ^{1}H and ^{13}C NMR spectra of **S3**. ^{1}H NMR (DMSO-d_6, 400 MHz): δ 8.52 (brs, 6H), 8.28 (s, 2H), 7.71 (s, 2H), 4.08 (brm, 2H), 3.46-3.40 (m, 2H), 3.20 (m, 2H). ^{13}C NMR (DMSO-d_6, 125 MHz): δ 168.57, 51.10, 38.54. *denotes H_2O.

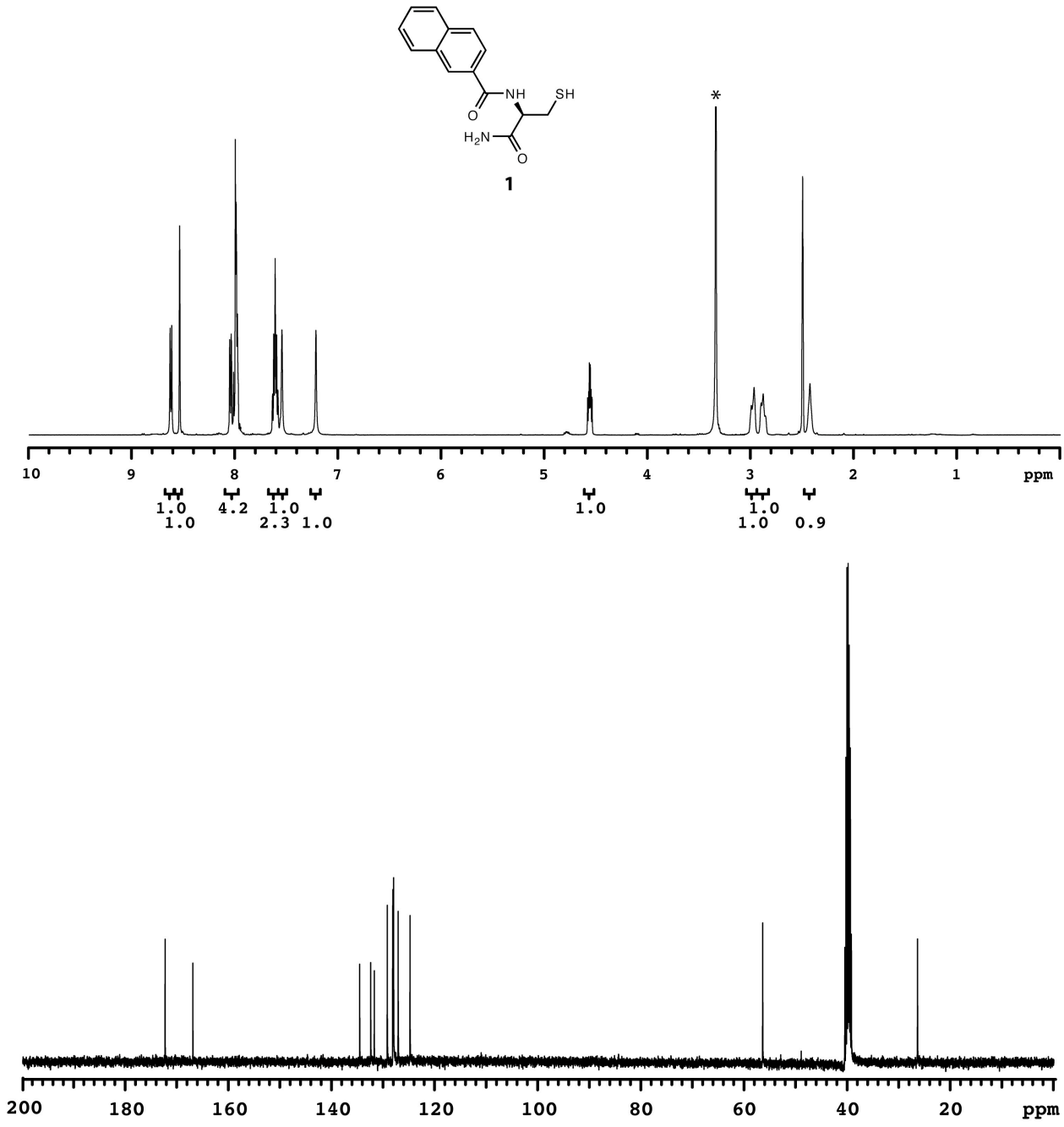


Figure S5. ^{1}H and ^{13}C NMR spectra of **1**. ^{1}H NMR (DMSO-d_6, 500 MHz): δ 8.63 (d, J = 7.5 Hz, 1H), 8.54 (s, 1H), 8.06-7.98 (m, 4H), 7.62 (m, 2H), 7.55 (s, 1H), 7.22 (s, 1H), 4.56 (m, 1H), 2.98 (m, 1H), 2.89 (m, 1H), 2.43 (brs, 1H). ^{13}C NMR (DMSO-d_6, 125 MHz): δ 171.95, 166.56, 134.22, 132.08, 131.38, 128.87, 127.82, 127.78, 127.67, 127.64, 126.75, 124.45, 56.07, 26.04. *denotes H_2O.

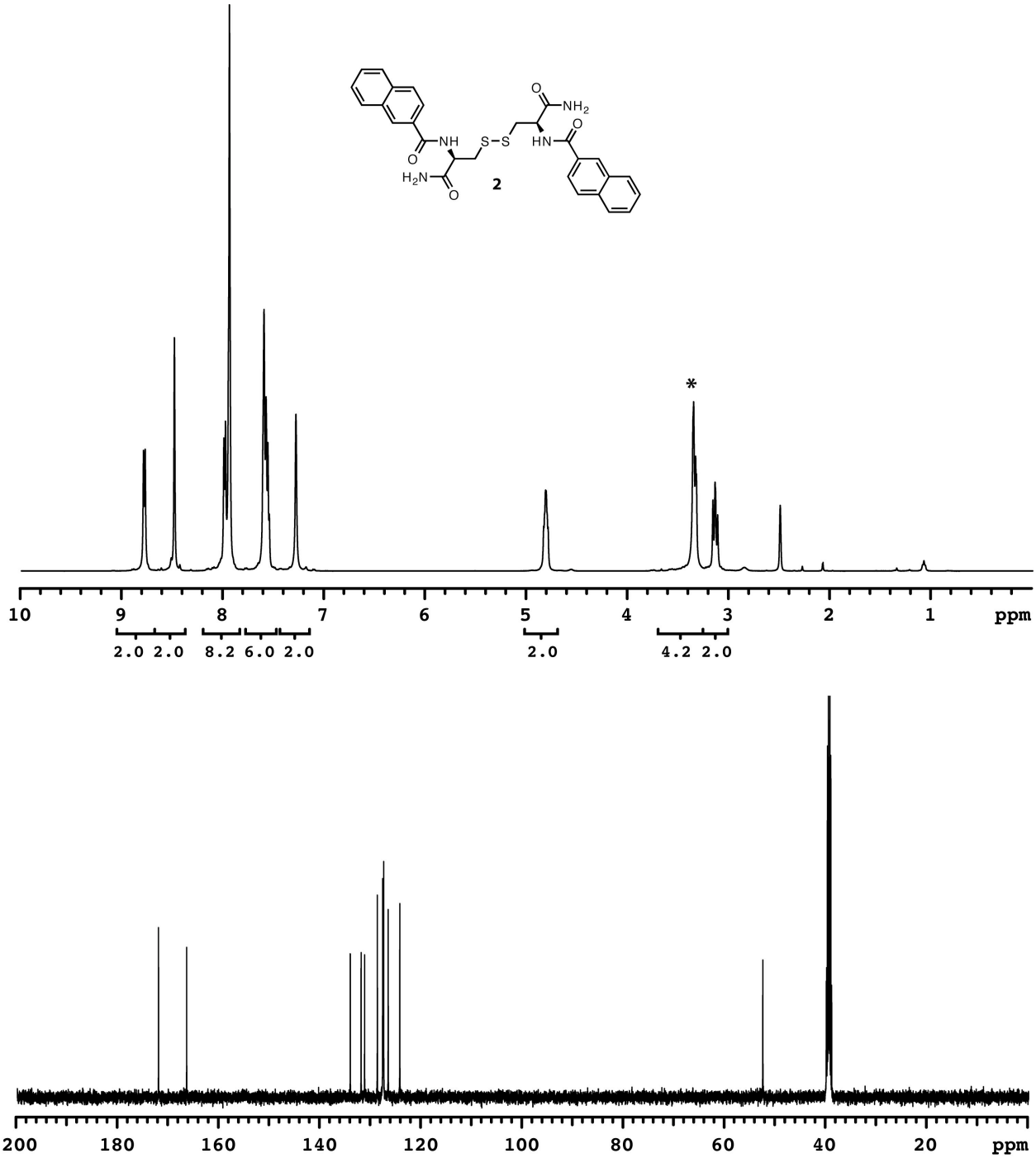


Figure S6. ^{1}H and ^{13}C NMR spectra of **2**. ^{1}H NMR (DMSO-d_6, 500 MHz): δ 8.78 (d, J = 8.0 Hz, 2H), 8.49 (s, 2H), 8.00-7.95 (m, 8H), 7.60-7.55 (m, 6H), 7.29 (s, 2H), 4.82 (m, 2H), 3.33 (m, 2H), 3.15 (m, 2H). ^{13}C NMR (DMSO-d_6, 125 MHz): δ 172.08, 166.52, 134.17, 132.03, 131.34, 128.82, 127.77, 127.71, 127.58, 126.68, 124.38, 52.61, 40.05. One aromatic carbon was not resolved. *denotes H_2O.

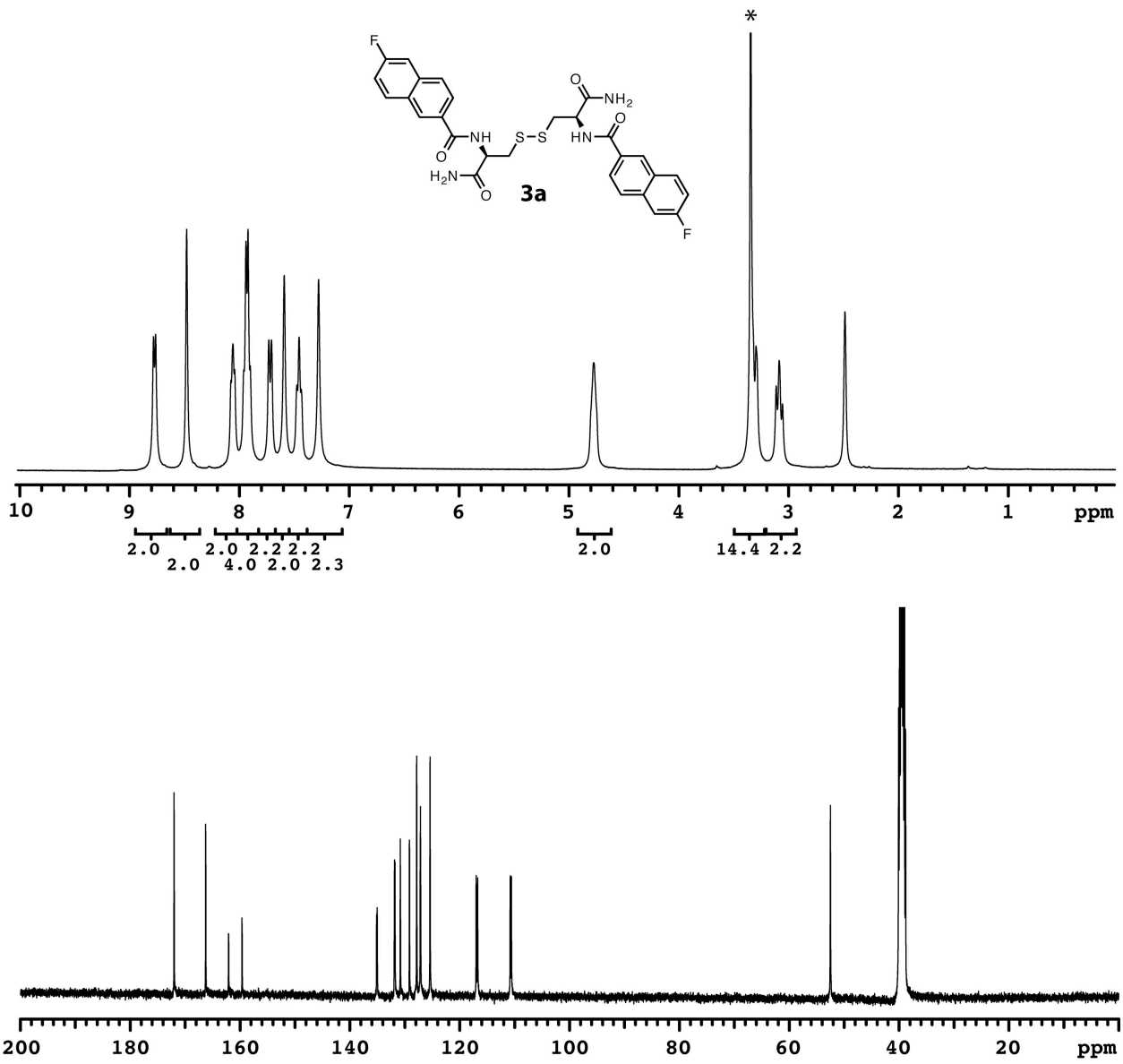


Figure S7. ^{1}H and ^{13}C NMR spectra of **3a**. ^{1}H NMR (DMSO-d_6, 400 MHz): δ 8.78 (d, J = 7.6 Hz, 2H), 8.49 (s, 2H), 8.07 (m, 2H), 7.94 (m, 4H), 7.73 (d, J = 9.6 Hz, 2H), 7.61 (s, 2H), 7.47 (m, 2H), 7.29 (s, 2H), 4.79 (brs, 2H), 3.31-3.26 (m, 2H), 3.10 (m, 2H). ^{13}C NMR (DMSO-d_6, 100 MHz): δ 172.50 (d, $J_{F\text{-}C}$ = 3.1 Hz), 166.30 (d, $J_{F\text{-}C}$ = 3.1 Hz), 160.90 (d, $J_{F\text{-}C}$ = 248 Hz), 135.17 (dd, $J_{F\text{-}C}$ = 3.1 Hz and 7.0 Hz), 131.88 (d, $J_{F\text{-}C}$ = 6.6 Hz), 130.85, 129.19 (d, $J_{F\text{-}C}$ = 2.7 Hz), 127.87, 127.19, 125.43, 116.90 (d, $J_{F\text{-}C}$ = 25.2 Hz), 110.73 (d, $J_{F\text{-}C}$ = 20.5), 52.53. One aliphatic proton was not resolved with DMSO. *denotes H_2O.

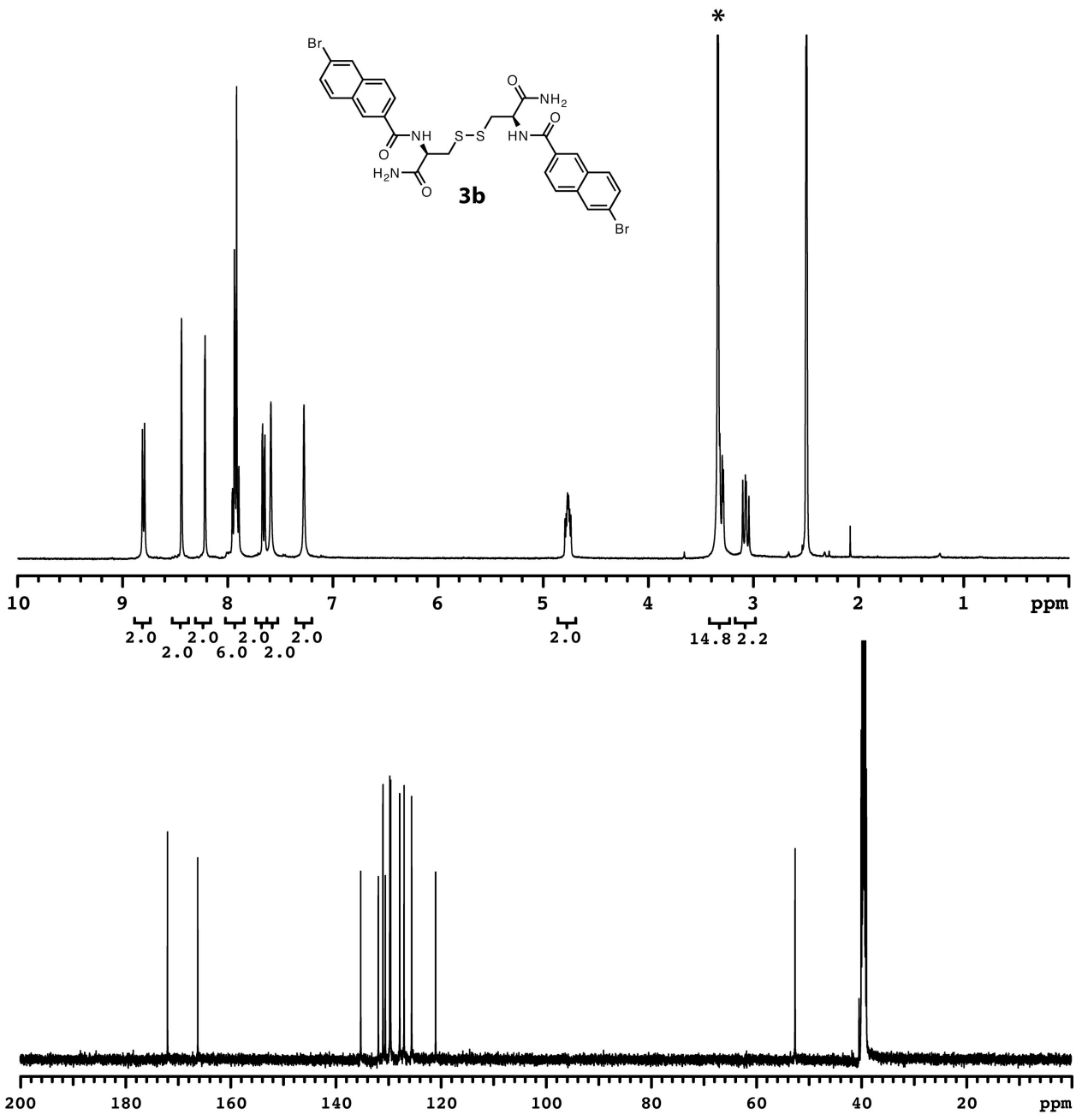


Figure S8. ^{1}H and ^{13}C NMR spectra of **3b**. ^{1}H NMR (DMSO-d_6, 400 MHz): δ 8.81 (d, J = 8.4 Hz, 2H), 8.44 (s, 2H), 8.22 (s, 2H), 7.96-7.90 (m, 6H), 7.66 (m, 2H), 7.59 (s, 2H), 7.28 (s, 2H), 4.77 (m, 2H), 3.31-3.25 (m, 2H), 3.08 (m, 2H). ^{13}C NMR (DMSO-d_6, 125 MHz): δ 171.97, 166.21, 135.21, 131.85, 130.97, 130.52, 129.67, 129.52, 127.78, 126.96, 125.51, 120.96, 52.57, 40.41. *denotes H_2O.

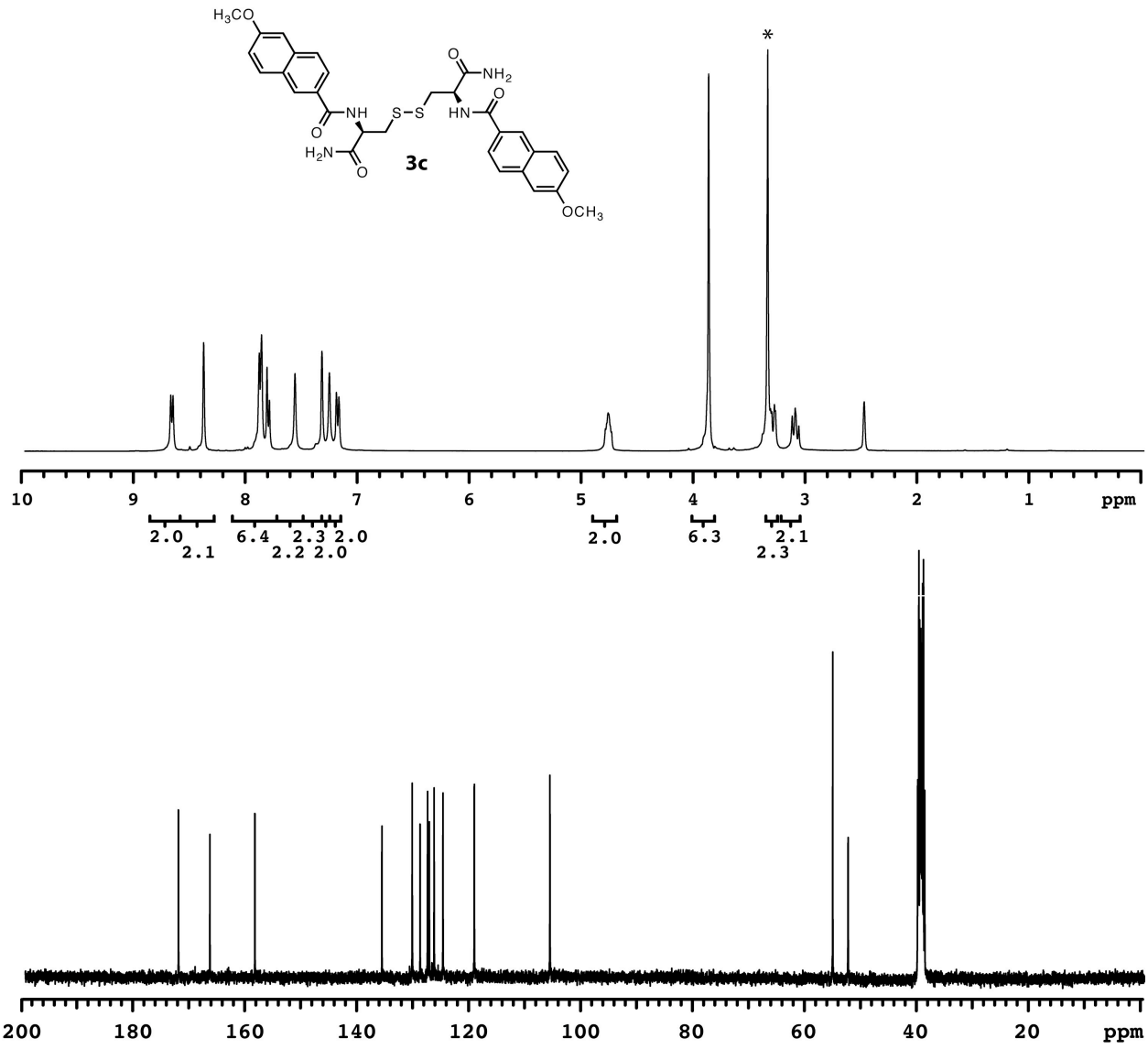


Figure S9. ^{1}H and ^{13}C NMR spectra of **3c**. ^{1}H NMR (DMSO-d_6, 400 MHz): δ 8.69 (d, J = 8.0 Hz, 2H), 8.40 (s, 2H), 7.91-7.81 (m, 6H), 7.59 (s, 2H), 7.35 (s, 2H), 7.28 (s, 2H), 7.21 (d, J = 8.8 Hz, 2H), 4.79 (brm, 2H), 3.89 (s, 6H), 3.36-3.29 (m, 2H), 3.12 (m, 2H). ^{13}C NMR (DMSO-d_6, 100 MHz): δ 172.20, 166.58, 158.54, 135.85, 130.44, 129.03, 127.69, 127.38, 126.52, 124.94, 119.34, 105.83, 55.31, 52.56, 40.05. *denotes H_2O.

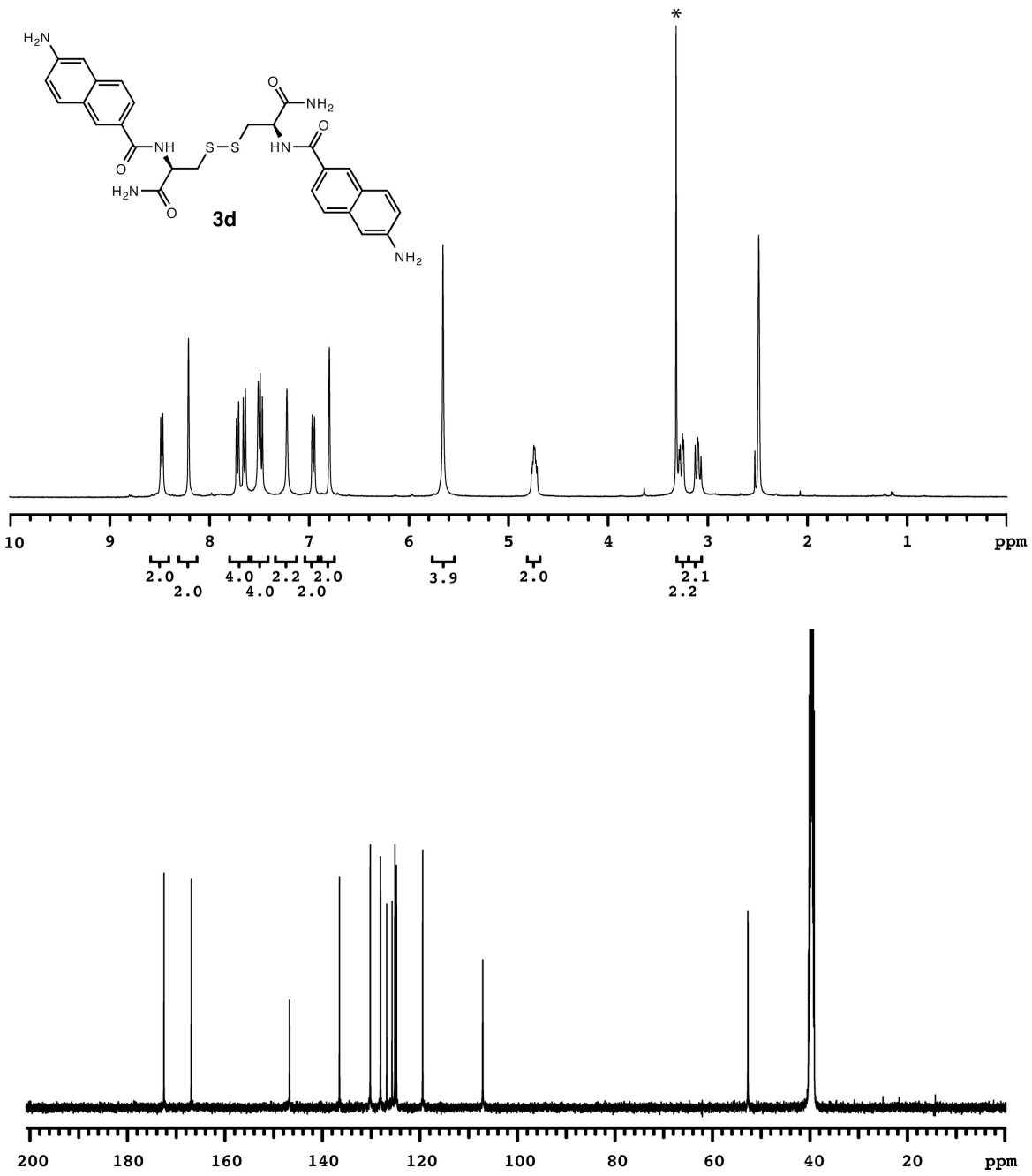


Figure S10. ^{1}H and ^{13}C NMR spectra of **3d**. ^{1}H NMR (DMSO-d_6, 400 MHz): δ 8.49 (d, J = 8.0 Hz, 2H), 8.22 (s, 2H), 7.78-7.60 (m, 4H), 7.57-7.43 (m, 4H), 7.24 (s, 2H), 6.97 (d, J = 12.8 Hz, 2H), 6.81 (s, 2H), 5.67 (s, 4H), 4.75 (brm, 2H), 3.28 (m, 2H), 3.11 (m, 2H). ^{13}C NMR (DMSO-d_6, 125 MHz): δ 172.82, 167.22, 147.07, 136.81, 130.51, 128.39, 127.13, 126.04, 125.45, 125.12, 119.76, 107.43, 53.03, 40.58. *denotes H_2O.

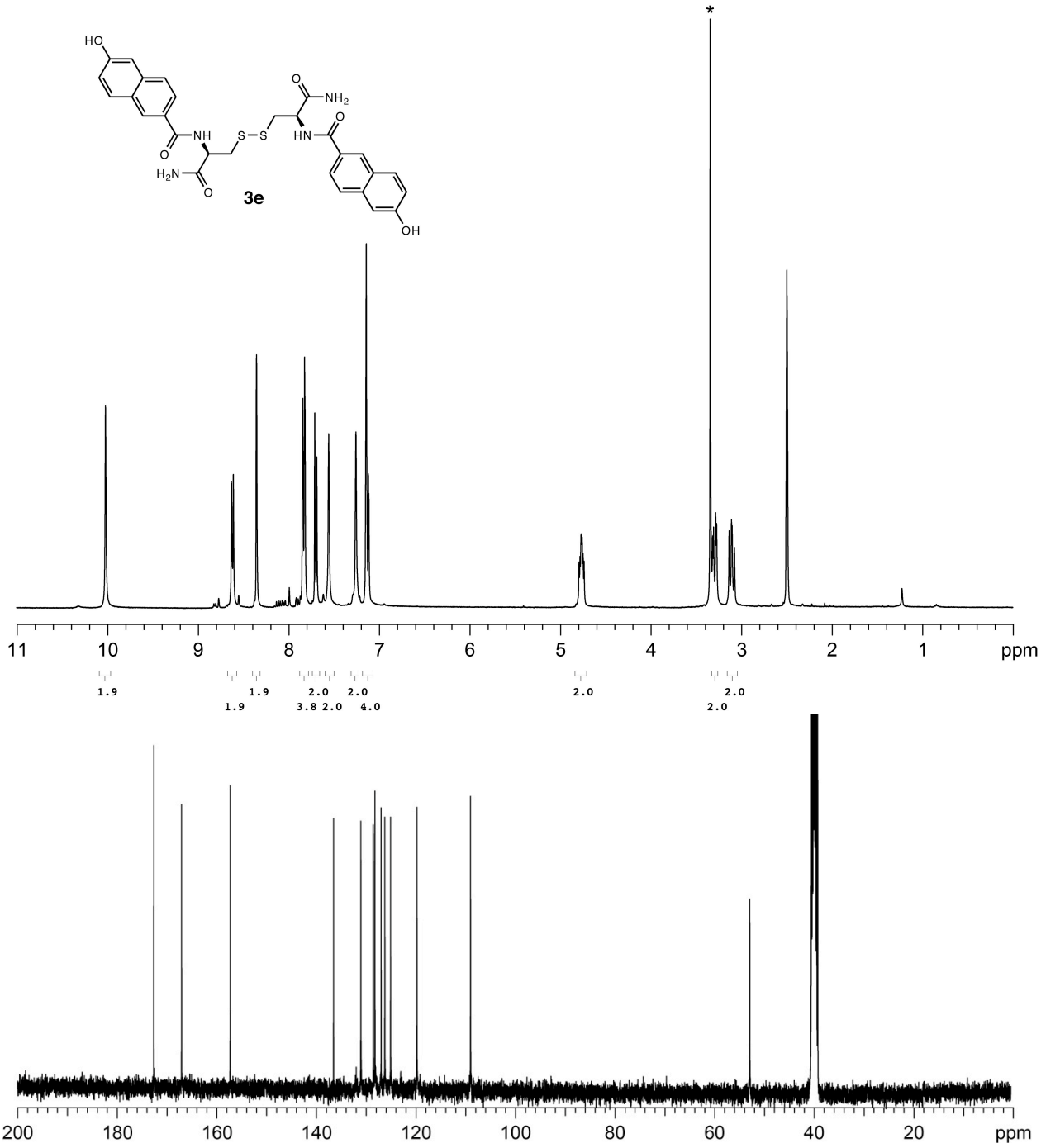


Figure S11. ^{1}H and ^{13}C NMR spectra of **3e**. ^{1}H NMR (DMSO-d_6, 400 MHz): δ 10.03 (s, 2H), 8.62 (d, J = 8.4 Hz, 2H), 8.36 (s, 2H), 7.84 (d, J = 8.8 Hz, 4H), 7.70 (d, J = 8.4 Hz, 2H), 7.56 (s, 2H), 7.26 (s, 2H), 7.15-7.12 (m, 4H), 4.77 (m, 2H), 3.30 (m, 2H), 3.11 (m, 2H). ^{13}C NMR (DMSO-d_6, 100 MHz): δ 172.64, 167.06, 157.31, 136.53, 131.06, 128.56, 128.23, 126.98, 126.24, 125.08, 119.80, 109.02, 52.95, 40.50. *denotes H_2O.

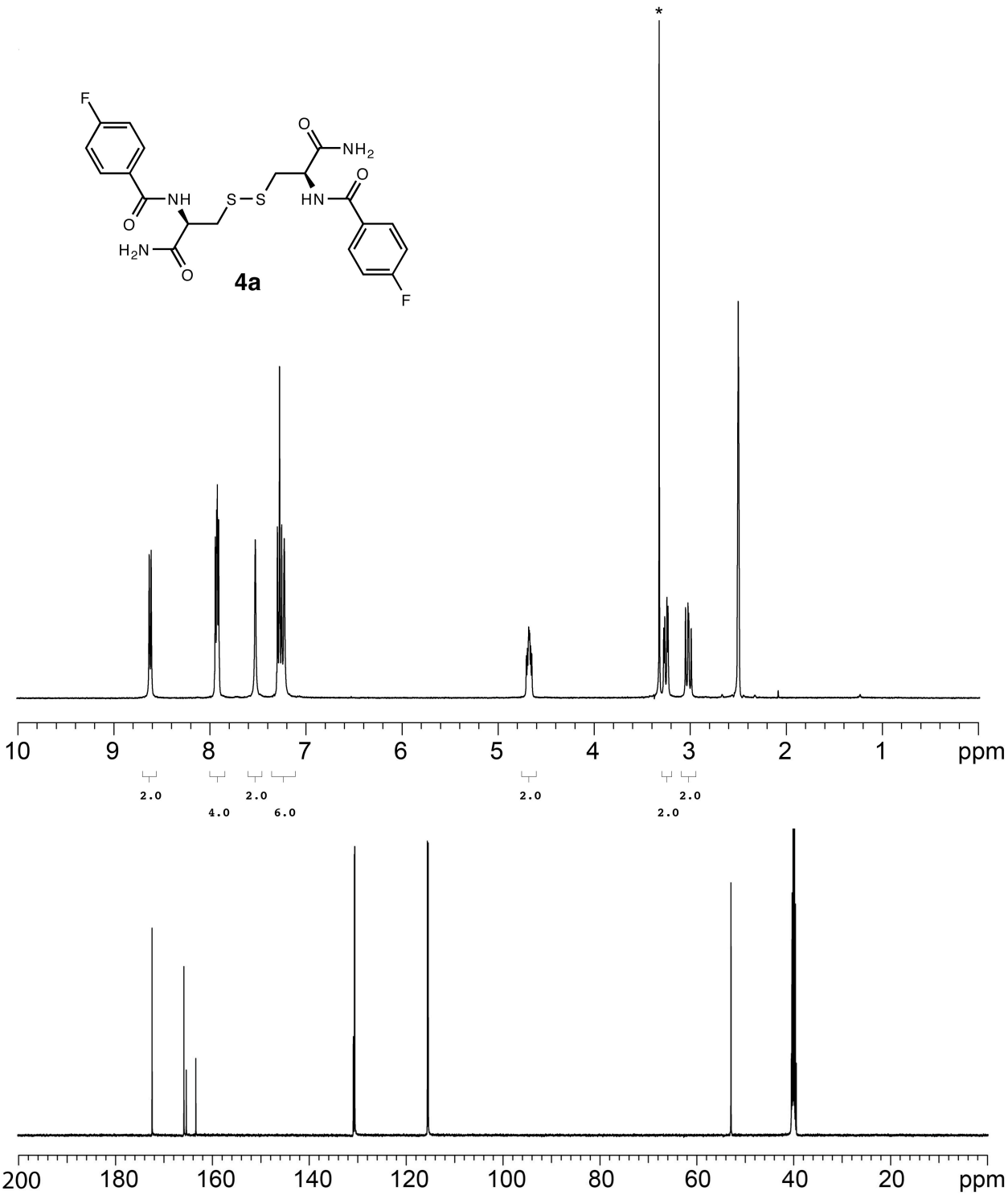


Figure S12. ^{1}H and ^{13}C NMR spectra of **4a**. ^{1}H NMR (DMSO-d_6, 400 MHz): δ 8.62 (d, J = 5.0 Hz, 2H), 7.92 (m, 4H), 7.53 (s, 2H), 7.30-7.23 (m, 6H), 4.68 (m, 2H), 3.26 (m, 2H), 3.02 (m, 2H). ^{13}C NMR (DMSO-d_6, 125 MHz): δ 172.46, 165.88, 164.40 (d, $J_{F\text{-}C}$ = 247 Hz), 130.91 (d, $J_{F\text{-}C}$ = 2.9 Hz), 130.64 (d, $J_{F\text{-}C}$ = 8.8 Hz), 115.53 (d, $J_{F\text{-}C}$ = 21 Hz), 52.94, 40.35. *denotes H_2O.

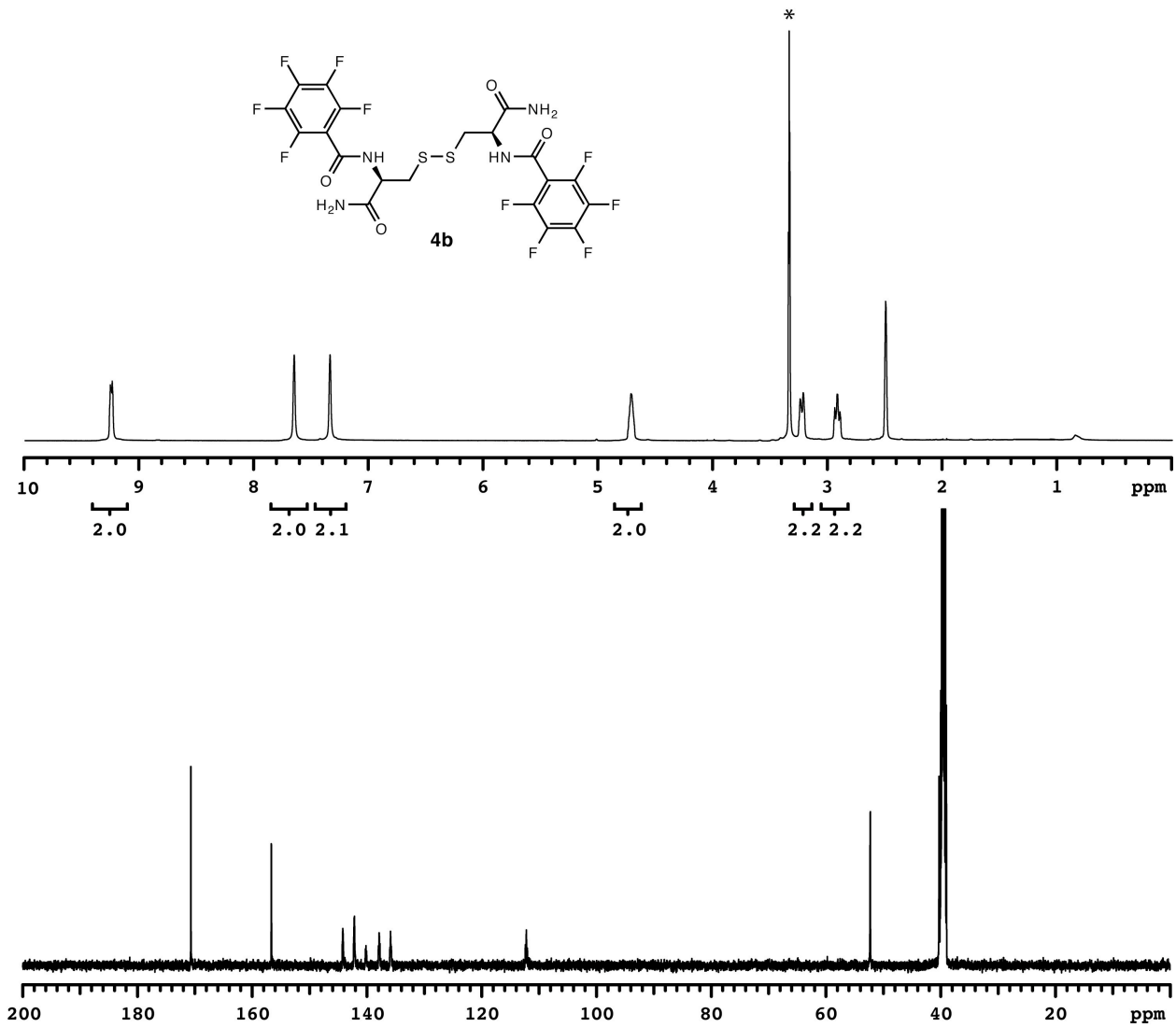


Figure S13. ^{1}H and ^{13}C NMR spectra of **4b**. ^{1}H NMR (DMSO-d_6, 500 MHz): δ 9.25 (m, 2H), 7.65 (s, 2H), 7.34 (m, 2H), 4.72 (m, 2H), 3.23 (m, 2H), 2.92 (m, 2H). ^{13}C NMR (DMSO-d_6, 125 MHz): δ 170.68, 156.66, 143.19 (d, $J_{F\text{-}C}$ = 255 Hz), 141.17 (d, $J_{F\text{-}C}$ = 251 Hz), 136.87 (d, $J_{F\text{-}C}$ = 243 Hz), 112.22 (m), 52.26, 40.27. *denotes H_2O.

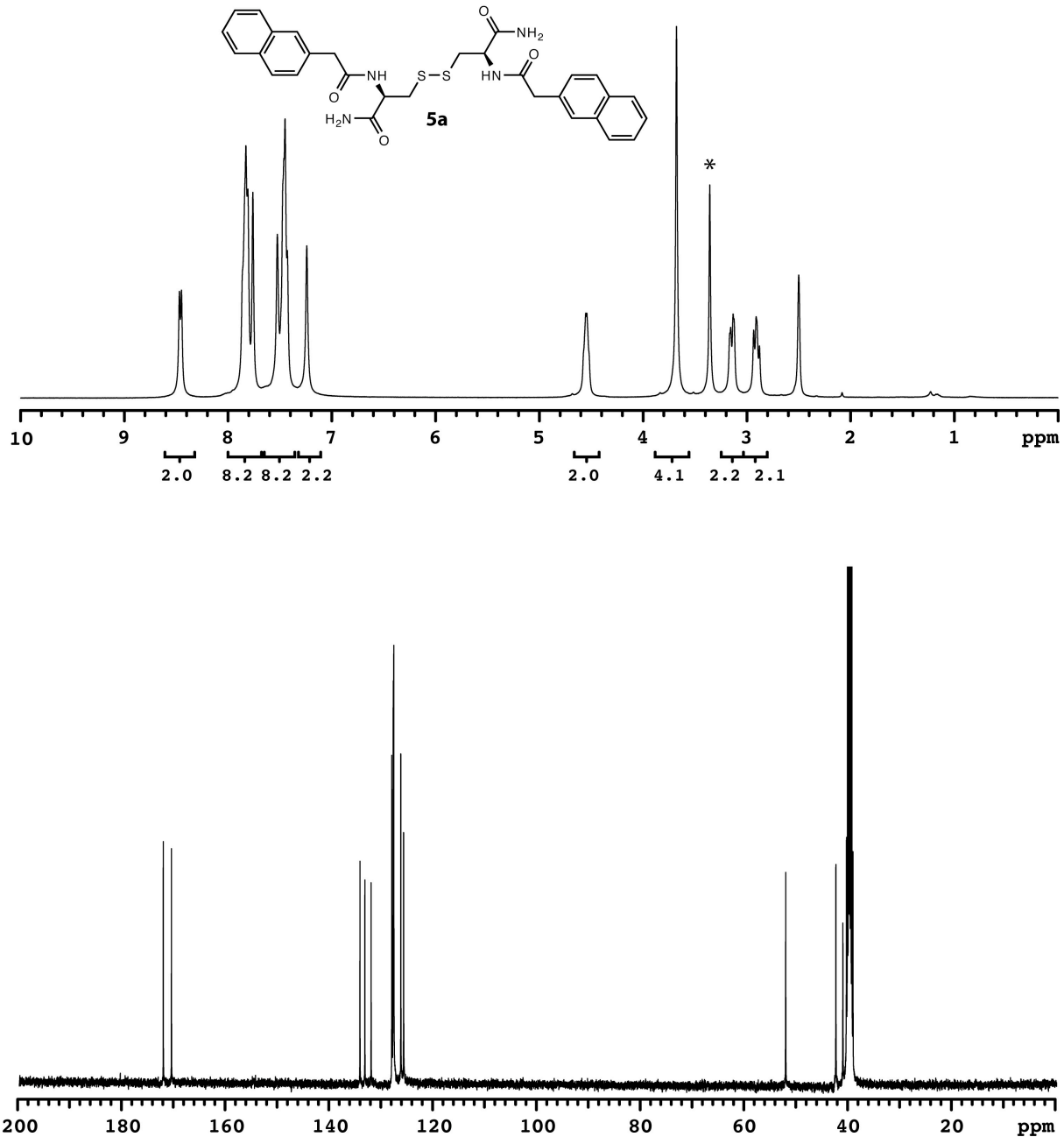


Figure S14. ^{1}H and ^{13}C NMR spectra of **5a**. ^{1}H NMR (DMSO-d_6, 400 MHz): δ 8.45 (d, J = 8.0 Hz, 2H), 7.86-7.76 (m, 8H), 7.51-7.42 (m, 8H), 7.23 (s, 2H), 4.54 (brm, 2H), 3.67 (s, 4H), 3.18-3.10 (m, 2H), 2.95-2.84 (m, 2H). ^{13}C NMR (DMSO-d_6, 100 MHz): δ 171.82, 170.25, 133.91, 132.96, 131.76, 127.77, 127.52, 127.47, 127.42, 127.38, 126.04, 125.49, 51.84, 42.17, 40.82. *denotes H_2O.

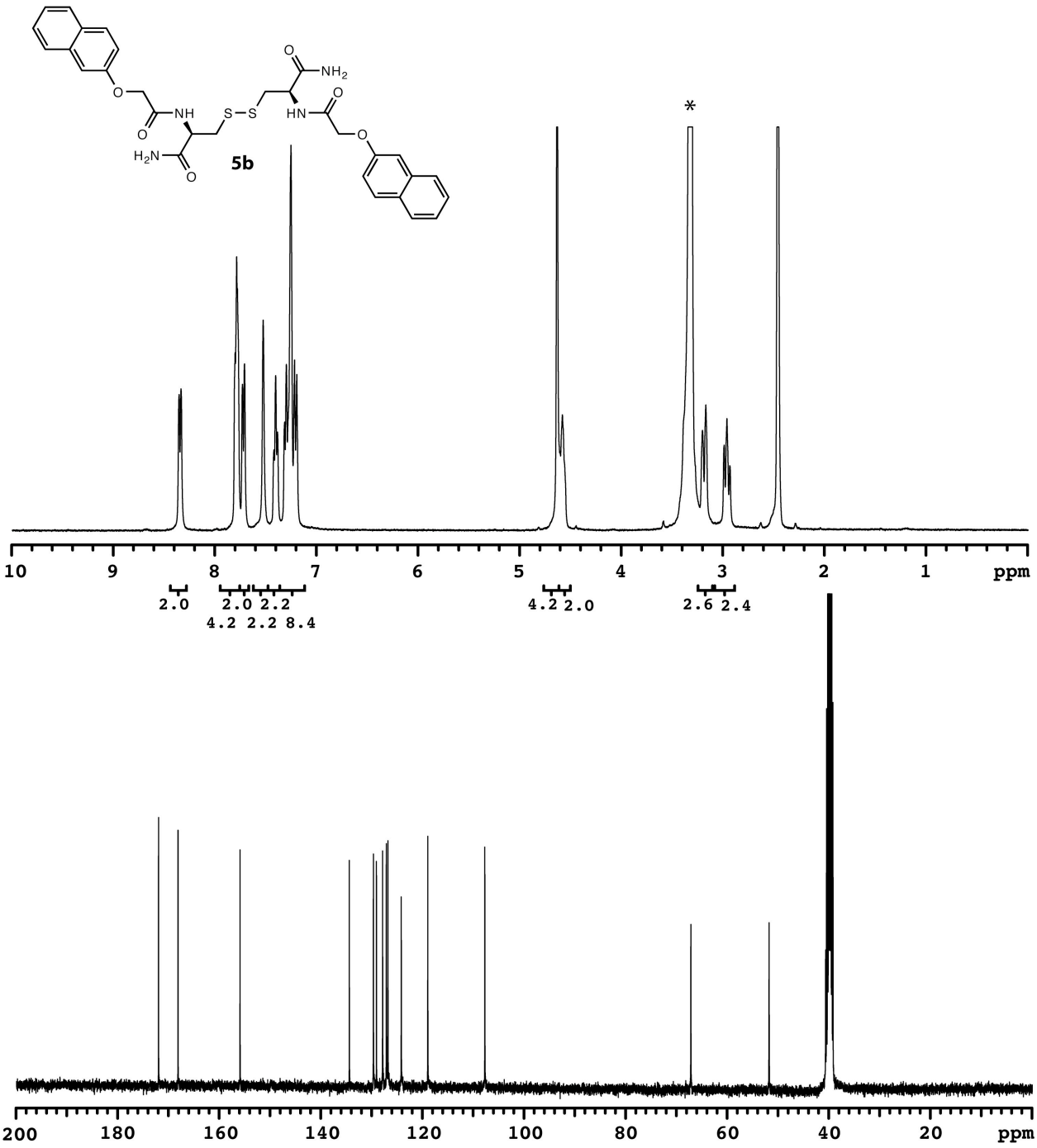


Figure S15. ^{1}H and ^{13}C NMR spectra of **5b**. ^{1}H NMR (DMSO-d_6, 400 MHz): δ 8.38 (d, J = 7.6 Hz, 2H), 7.84-7.82 (m, 4H), 7.76 (d, J = 8.0 Hz, 2H), 7.57 (s, 2H), 7.44 (m, 2H), 7.36-7.24 (m, 8H), 4.67 (s, 4H), 4.62 (s, 2H), 3.23 (m, 2H), 3.00 (m, 2H). ^{13}C NMR (DMSO-d_6, 100 MHz): δ 171.63, 167.80, 155.59, 134.08, 129.34, 128.74, 127.52, 126.79, 126.47, 123.85, 118.63, 107.40, 66.84, 51.44, 40.31. *denotes H_2O.

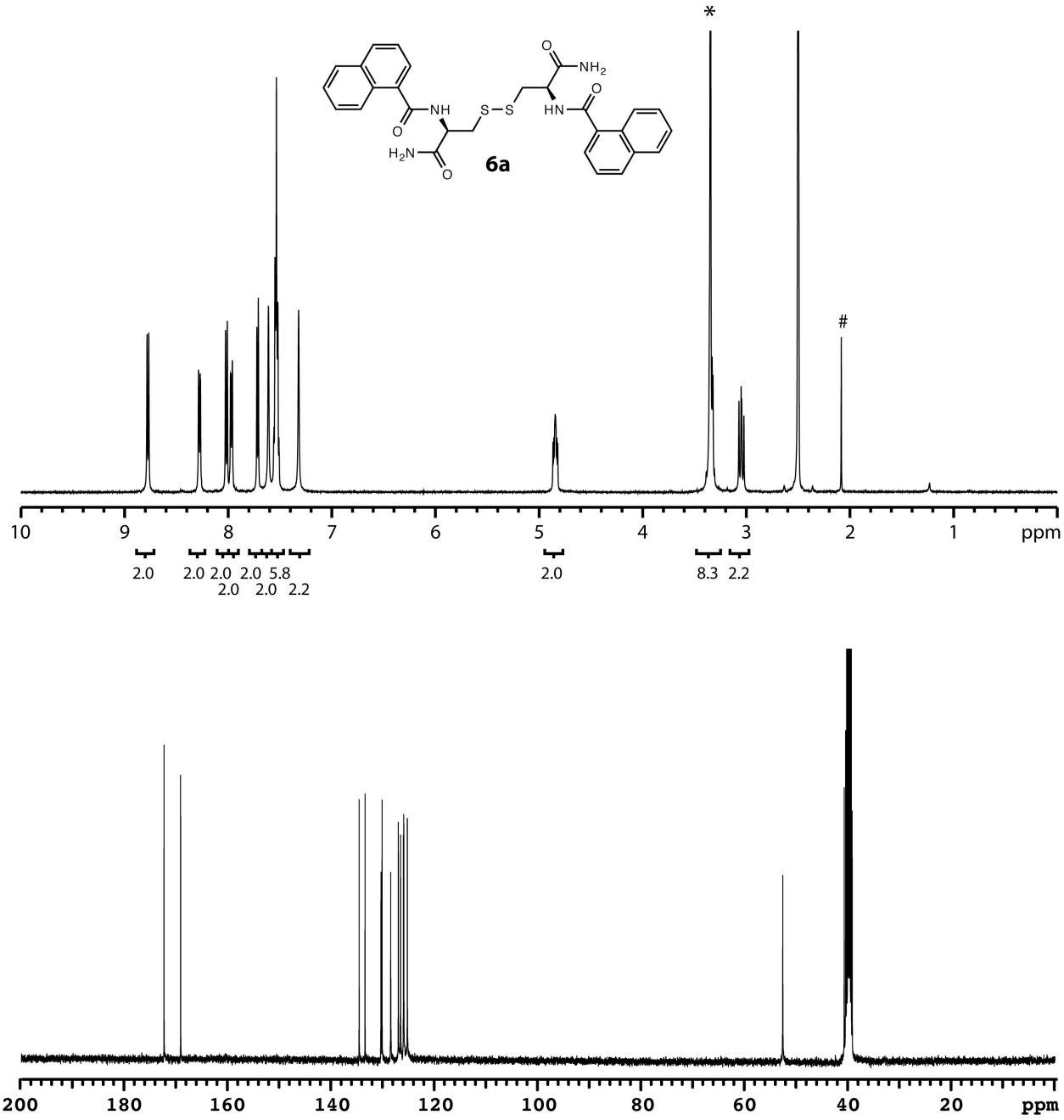


Figure S16. ^{1}H and ^{13}C NMR spectra of **6a**. ^{1}H NMR (DMSO-d_6, 500 MHz): δ 8.78 (d, J = 8.5 Hz, 2H), 8.28 (d, J = 8.0 Hz, 2H), 8.02 (d, J = 8.5 Hz, 2H), 7.97 (m, 2H), 7.72 (d, J = 7.0 Hz, 2H), 7.61 (s, 2H), 7.56-7.51 (m, 6H), 7.32 (s, 2H), 4.81 (m, 2H), 3.43-3.28 (m, 2H), 3.01 (m, 2H). ^{13}C NMR (DMSO-d_6, 100 MHz): δ 172.00, 168.79, 134.26, 133.11, 130.02, 129.82, 128.15, 126.67, 126.23, 125.68, 125.62, 124.94, 52.30, 40.41. *denotes H_2O. #denotes acetone.

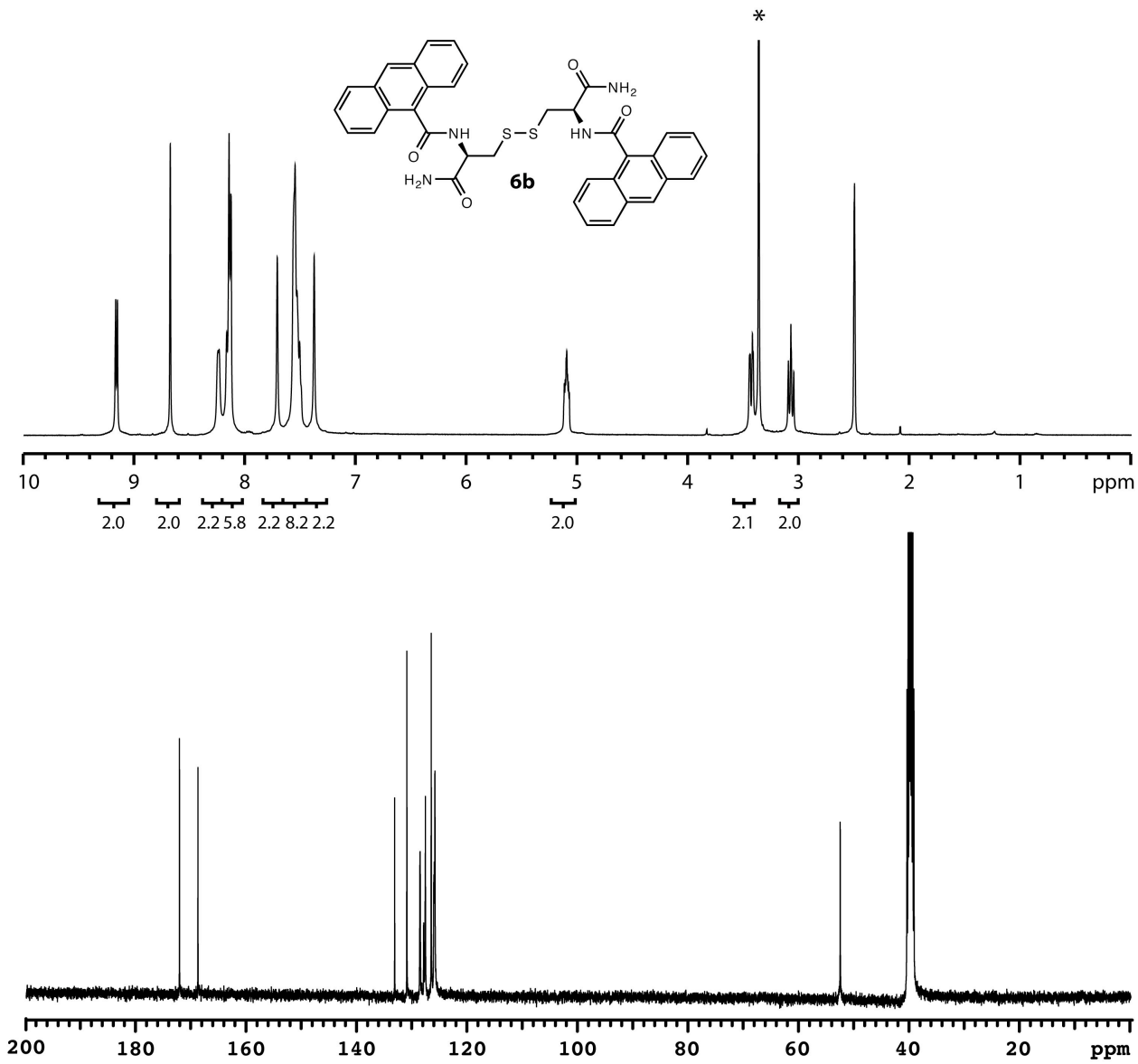


Figure S17. ^{1}H and ^{13}C NMR spectra of **6b**. ^{1}H NMR (DMSO-d_6, 500 MHz): δ 9.16 (d, J = 8.0 Hz, 2H), 8.68 (s, 2H), 8.24 (brm, 2H), 8.17-8.13 (m, 6H), 7.71 (s, 2H), 7.55-7.51 (brm, 8H), 7.38 (s, 2H), 5.10 (m, 2H), 3.43 (m, 2H), 3.07 (m, 2H). ^{13}C NMR (DMSO-d_6, 100 MHz): δ 171.82, 168.48, 132.87, 130.66, 128.27, 127.62, 127.31, 126.25, 125.70, 125.58, 52.22. *denotes H_2O.

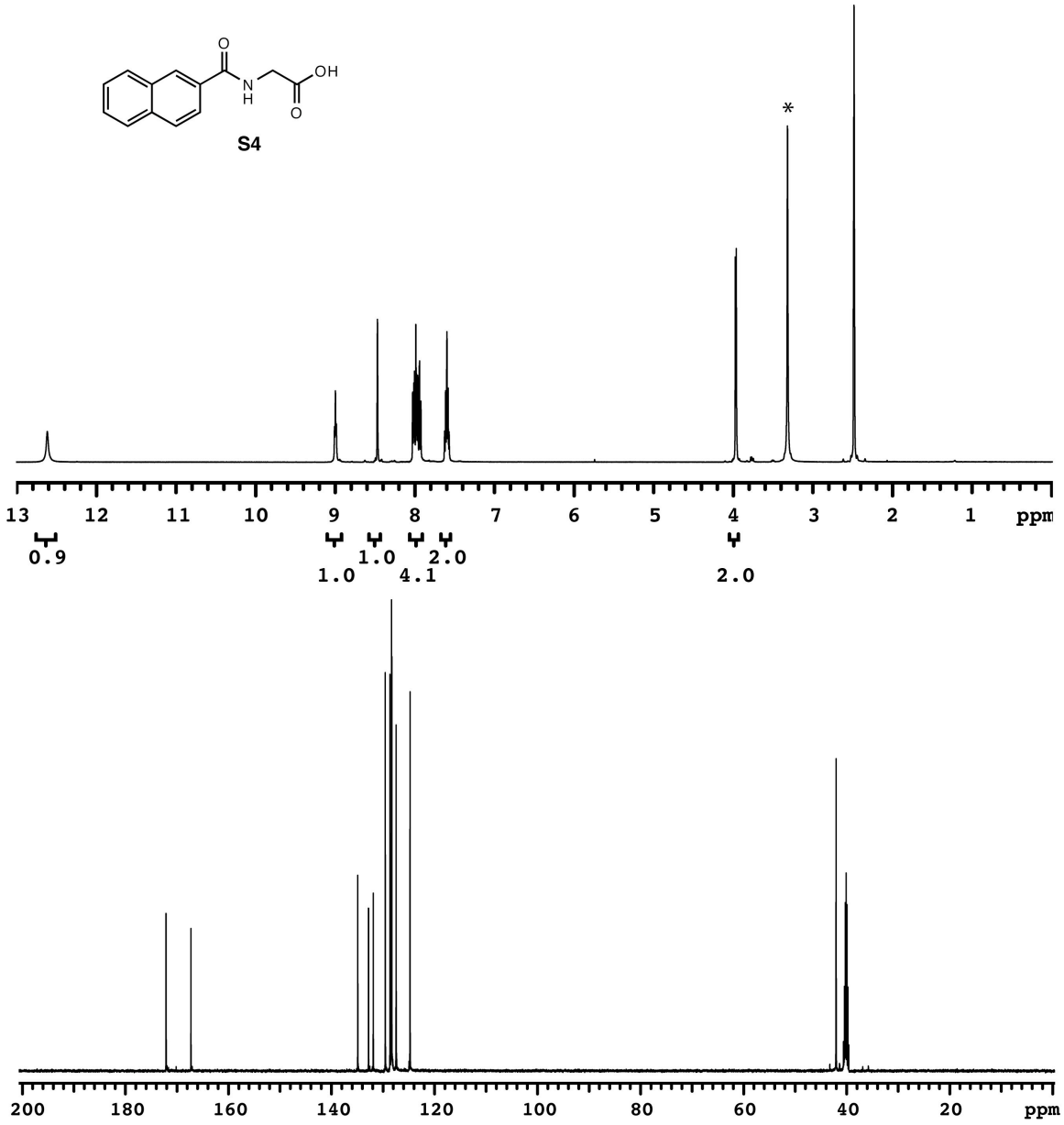


Figure S18. ^{1}H and ^{13}C NMR spectra of **S4**. ^{1}H NMR (DMSO-d_6, 500 MHz): δ 12.63 (s, 1H), 9.02 (t, J = 6.0 Hz, 1H), 8.49 (s, 1H), 8.04-7.94 (m, 4H), 7.60 (m, 2H), 3.99 (d, J = 5.0 Hz, 2H). ^{13}C NMR (DMSO-d_6, 125 MHz): δ 171.89, 167.06, 134.68, 132.59, 131.67, 129.34, 128.43, 128.28, 128.13, 128.09, 127.24, 124.54, 41.83. *denotes H_2O.

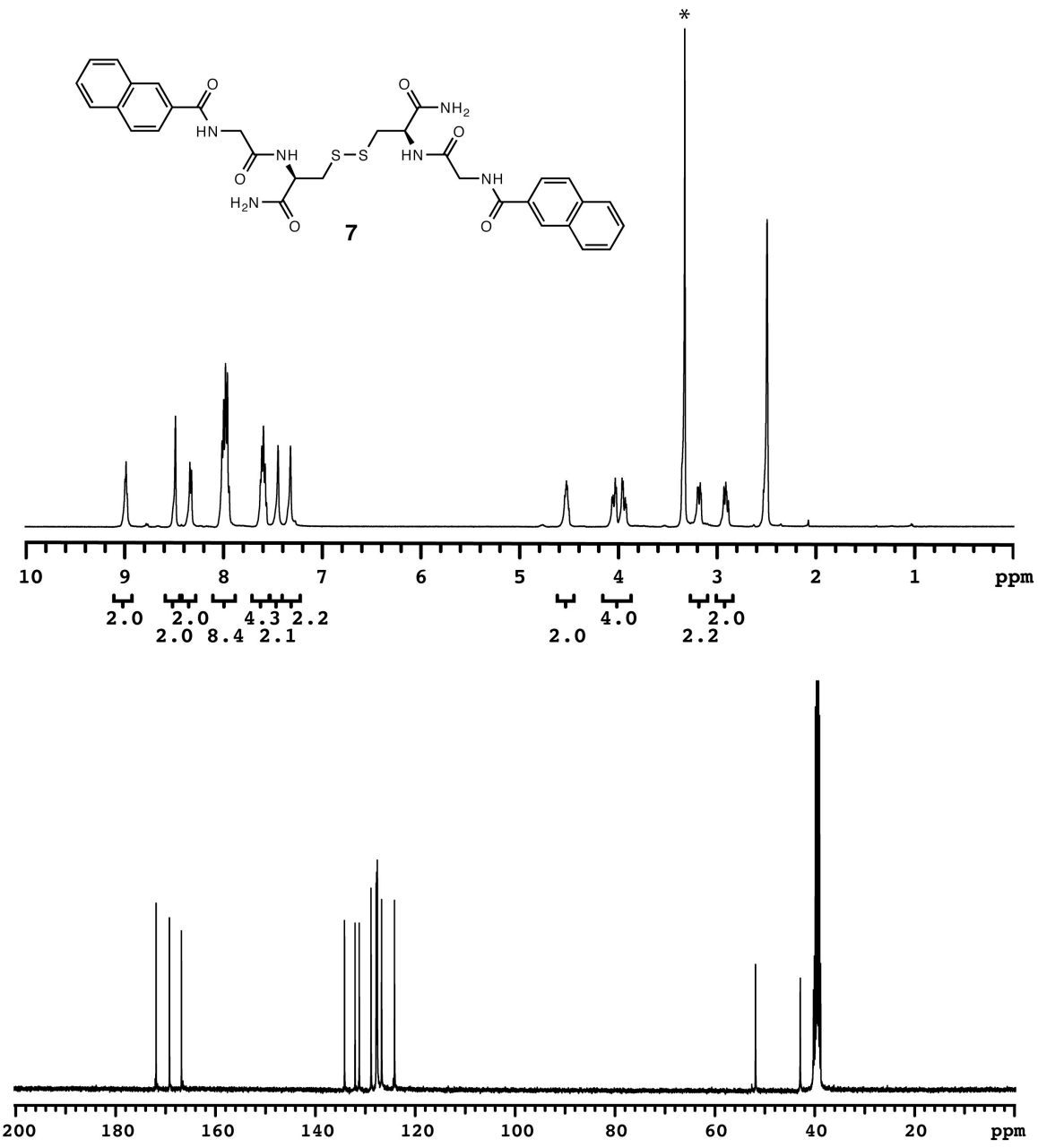


Figure S19. ^{1}H and ^{13}C NMR spectra of **7**. ^{1}H NMR (DMSO-d_6, 500 MHz): δ 8.99 (m, 2H), 8.49 (s, 2H), 8.34 (d, J = 8.5 Hz, 2H), 8.02-7.95 (m, 8H), 7.63-7.57 (m, 4H), 7.45 (s, 2H), 7.33 (s, 2H), 4.50 (brm, 2H), 4.12-3.88 (m, 4H), 3.19 (m, 2H), 2.92 (m, 2H). ^{13}C NMR (DMSO-d_6, 100 MHz): δ 172.37, 169.69, 167.29, 134.64, 132.53, 131.68, 129.32, 128.31, 128.20, 128.13, 128.06, 127.20, 124.62, 52.34, 43.38, 40.73. *denotes H_2O.

IV. In situ Gelation in a 4 mL Vial

A 4 mL vial was charged with **1** (5 mg, 0.018 mmol), TsOH (124 mg, 0.65 mmol, 36 equiv.) and MeOH (0.25 mL). Then TATP (0.25 mL, 45 mM in MeOH) was added to the vial. The mixture was shaken for 1-2 s and allowed to sit at rt. After 30 min, the vial was inverted and a stable gel was formed.

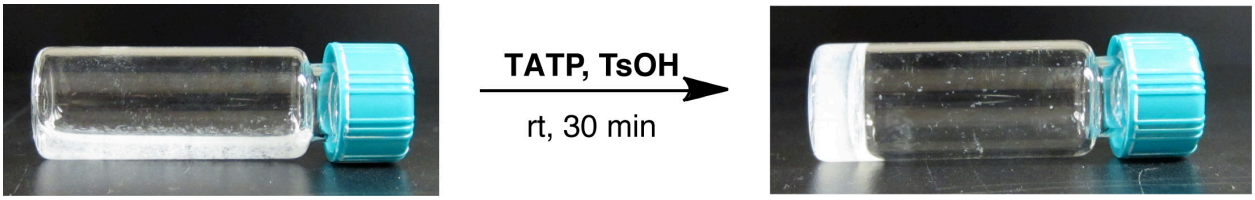
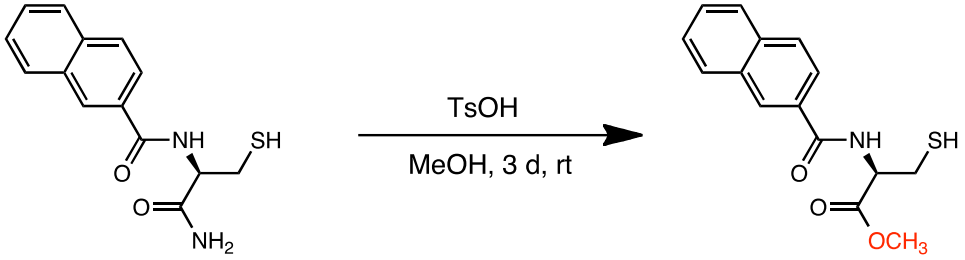


Figure S20. In situ gel formation triggered by oxidation of **1** under TATP/TsOH conditions.

V. Reaction of 1 under Acidic Conditions



1 **S5**

A 20 mL vial was charged with **1** (11 mg, 0.040 mmol), TsOH (275 mg, 1.45 mmol) and MeOH (5 mL). After 3 d at rt, the solution was concentrated under reduced pressure. H_2O (20 mL) was added to the oily residue to generate a white suspension. The mixture was extracted with EtOAc (3 x 20 mL). The organic layers were combined, washed with brine (30 mL) and dried over $MgSO_4$, filtered and concentrated in vacuo to give a crude oil. The crude product was further purified via column chromatography (hexanes/EtOAc 1:1) to give a white solid of **S5** (9 mg, 78%). HRMS (EI): Calcd for $C_{15}H_{15}NO_3S$, 289.0773 M^+; Found 289.0771.

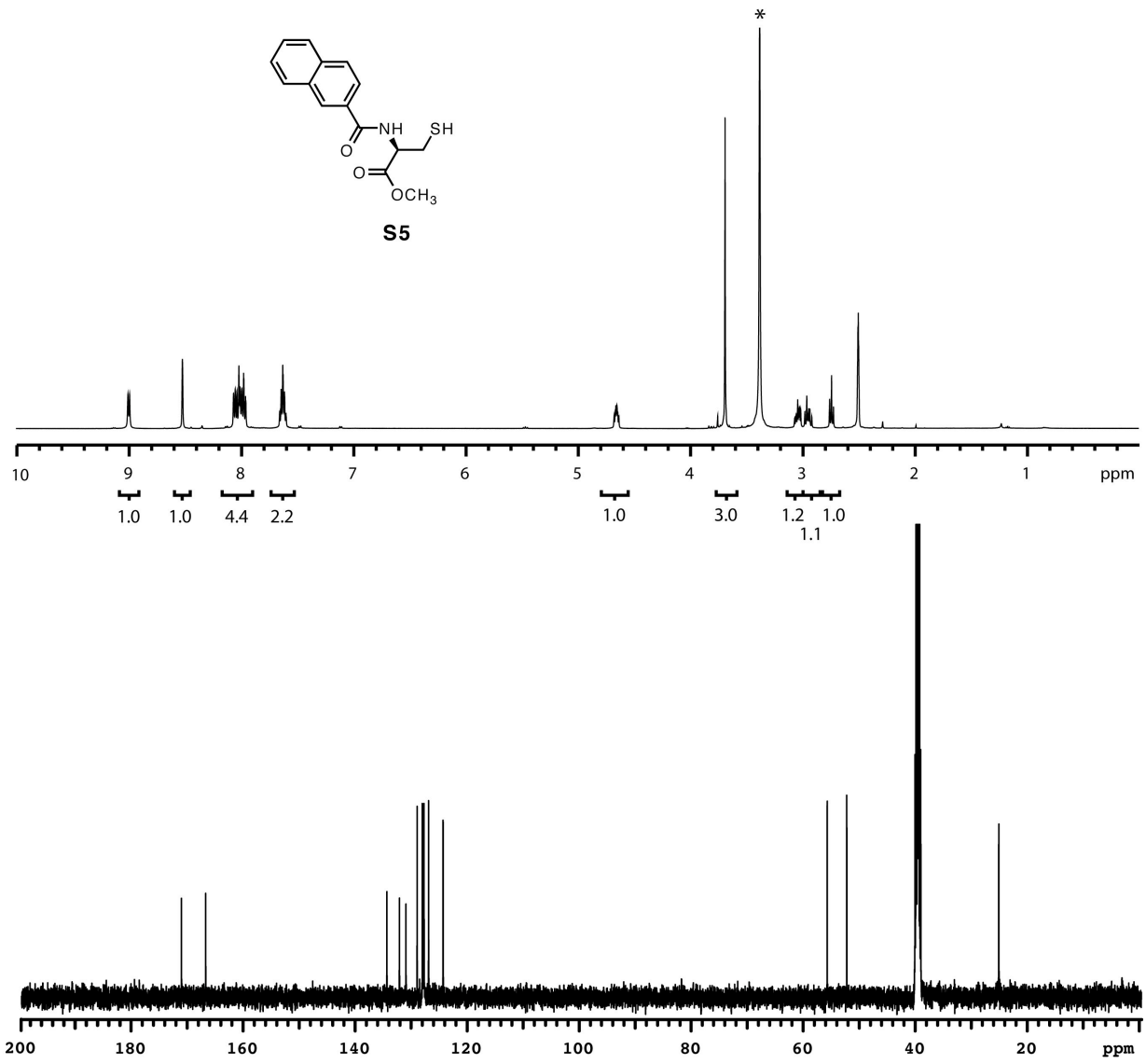


Figure S21. ^{1}H and ^{13}C NMR spectra of **S5**. ^{1}H NMR (DMSO-d_6, 500 MHz): δ 9.01 (d, J = 7.5 Hz, 1H), 8.52 (s, 1H), 8.06-7.95 (m, 4H), 7.63 (m, 2H), 4.65 (m, 1H), 3.69 (s, 3H), 3.04 (m, 1H), 2.94 (m, 1H), 2.74 (t, J = 8.5 Hz, 1H). ^{13}C NMR (DMSO-d_6, 125 MHz): δ 171.00, 166.68, 134.32, 132.08, 130.92, 128.92, 127.98, 127.90, 127.83, 127.69, 126.87, 124.28, 55.69, 52.20, 25.05. *denotes H_2O.

VI. Gelation Tests of 2-7

Table S1. Cgcs of **2, 3a, 4a** and **5b**.

Compound	cgc in MeOH (mM)	cgc in 1/1 (v/v) DMSO/H_2O (mM)	Compound	cgc in MeOH (mM)	cgc in 1/1 (v/v) DMSO/H_2O (mM)
2	4.6	0.55	**5a**	--	--
3a	6.5*	3.4	**5b**	8.5	1.5
3b	--	--	**6a**	--	--
3c	--	--	**6b**	--	--
3d	--	--	**7a**	--	--
3e	--	--	**7b**	--	--
4a	25	1.9	**7c**	--	--
4b	--	--			

(--) indicates nongelator under all conditions examined.

* Gelation was not observed for **3a** in MeOH via the general procedure on page S2. A stable gel was formed when a heated solution of **3a** was cooled to rt and then sonicated for ~ 30 s.

VII. Rate Measurements of TATP Degradation under Acidic Conditions

(1) Determining the reaction order in TATP

An NMR tube was charged with TATP (0.50 mL of 0.0491 M in CD_3OD) and 1,4-dioxane (10 μL) as an internal standard. Then TsOH (50 μL of 9.0 M in CD_3OD) was added and the NMR tube was capped and inverted twice to ensure complete mixing. ^1H NMR spectra were acquired over time to monitor the change in [TATP] (Figure S22). The same procedure was applied to three other samples where $[TATP]_0$ = 0.0614 M, 0.0369 M, 0.0246 M.

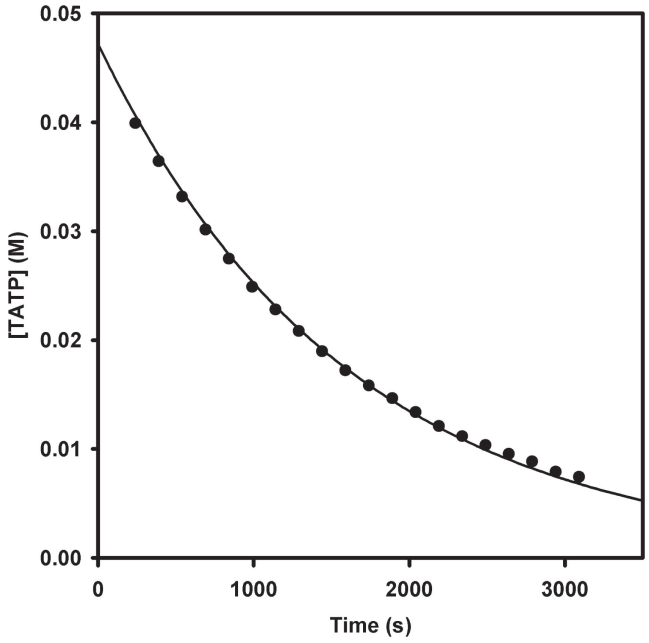


Figure S22. Plot of [TATP] versus time fit to $[TATP] = [TATP]_0e^{-k_{obs}t}$, where $[TATP]_0 = 4.72 \pm 0.06 \times 10^{-2}$ and $k_{obs} = 6.26 \pm 0.08 \times 10^{-4}$.

Table S2. Rate constants of TATP degradation at different $[TATP]_0$.

Run	$[TATP]_0$ (M)	k_{obs} (s^{-1})
A	$5.79 \pm 0.07 \times 10^{-2}$	$6.13 \pm 0.01 \times 10^{-4}$
B	$4.72 \pm 0.06 \times 10^{-2}$	$6.26 \pm 0.08 \times 10^{-4}$
C	$3.61 \pm 0.02 \times 10^{-2}$	$6.23 \pm 0.05 \times 10^{-4}$
D	$2.39 \pm 0.01 \times 10^{-2}$	$6.28 \pm 0.06 \times 10^{-4}$

(2) Determining reaction order in TsOH

A NMR tube was charged with TATP (0.50 mL of 0.0450 M in CD_3OD) and 1,4-dioxane (10 μL) as an internal standard. Then TsOH (40 μL of 9.0 M in CD_3OD) was added and the NMR tube was capped and inverted twice to ensure complete mixing. ^1H NMR spectra were acquired over time to monitor the change in [TATP]. The same procedure was applied to three other samples where $[TsOH]_0$ = 0.137 M, 0.350 M, 0.451 M and 0.578 M respectively.

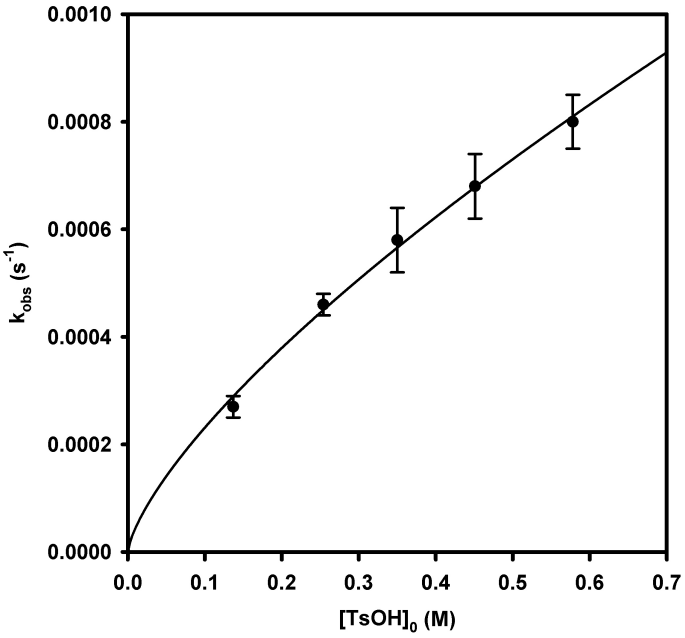


Figure S23. Plot of k_{obs} versus [TsOH] for the TsOH-induced TATP degradation ([TATP] = 0.0450 M), fit to $k_{obs} = a[TsOH]^n$, where a = 1.20 ± 0.04 x 10^{-3} and n = 0.72 ± 0.03.

Table S3. Data for the plot in Figure S23.

$[TsOH]_0$ (M)	k_{obs} (s^{-1})
0.578	0.00080 ± 0.00005
0.451	0.00068 ± 0.00007
0.350	0.00058 ± 0.00006
0.254	0.00046 ± 0.00002
0.137	0.00027 ± 0.00002

VIII. Rate Measurement of Oxidation of 1 with H_2O_2

(1) Determining the reaction order in **1**

An NMR tube was charged with **1** (0.50 mL of 5.48 mM in CD_3OD) and 1,3-dinitrobenzene (10 μL of 0.30 M in CD_3OD) as an internal standard. Then H_2O_2 (50 μL of 2.0 M in H_2O) was added and the NMR tube was capped and inverted twice to ensure complete mixing. ^1H NMR spectra were acquired over time to monitor the change in [**1**] (Figure S24). The same procedure was applied to another sample where $[\mathbf{1}]_0$ = 3.32 mM.

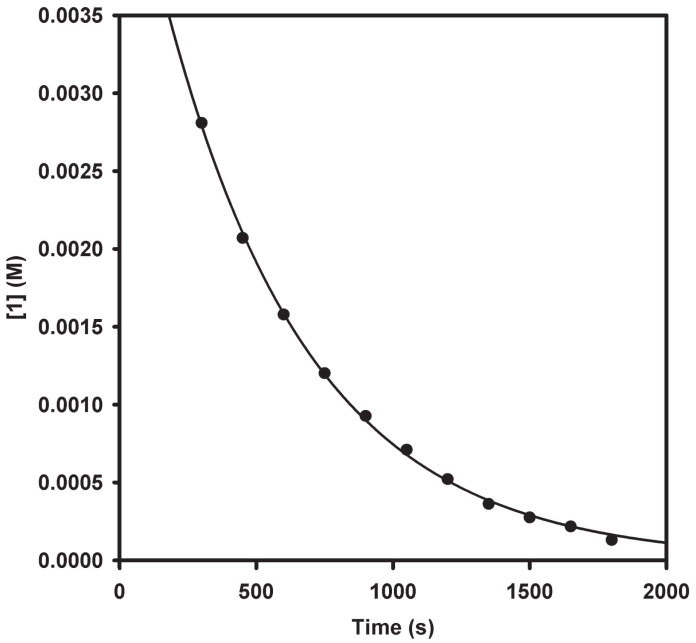


Figure S24. Plot of [**1**] versus time, fit to $[\mathbf{1}] = [\mathbf{1}]_0 e^{-k_{obs}t}$, where $[\mathbf{1}]_0 = 4.8 \pm 0.1 \times 10^{-3}$ and $k_{obs} = 1.7 \pm 0.2 \times 10^{-3}$.

Table S4. Rate constants of thiol oxidation at different $[\mathbf{1}]_0$.

Run	$[\mathbf{1}]_0$ (M)	k_{obs} (s^{-1})
A	$4.8 \pm 0.1 \times 10^{-3}$	$1.7 \pm 0.2 \times 10^{-3}$
B	$3.2 \pm 0.1 \times 10^{-3}$	$1.8 \pm 0.1 \times 10^{-3}$

(2) Determining the reaction order in H_2O_2

An NMR tube was charged with **1** (0.50 mL, 3.65 mM in CD_3OD) and 1,3-dinitrobenzene (10 μL, 0.30 M in CD_3OD) as an internal standard. Then H_2O_2 (50 μL, 2.0 M in H_2O) was added and the NMR tube was capped and inverted twice to ensure complete mixing. ^1H NMR spectra were acquired over time to monitor the change in [**1**]. The same procedure was applied to two other samples where $[H_2O_2]_0$ = 0.0904 and 0.271 M respectively. The reported data represent an average of 3 runs.

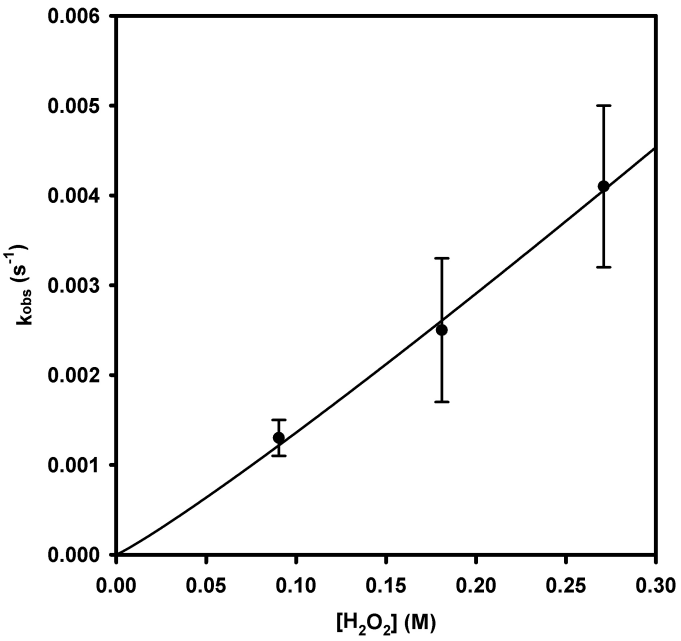
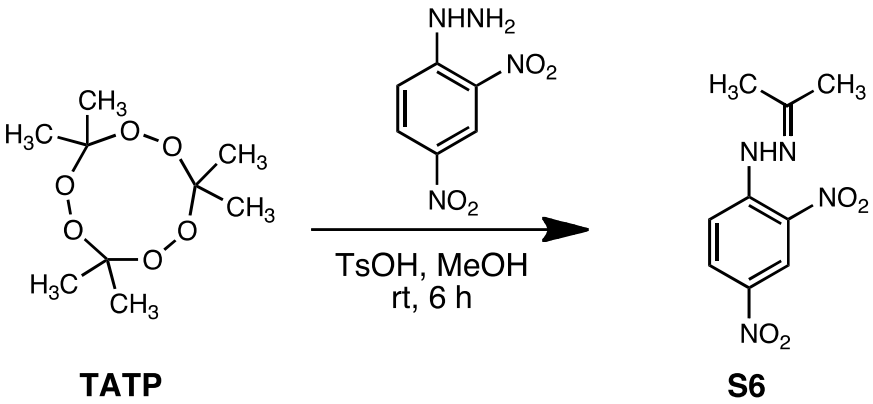


Figure S25. Plot of k_{obs} versus $[H_2O_2]$ for the oxidation of **1** by H_2O_2 ([**1**] = 0.00365 M), fit to $k_{obs} = a[H_2O_2]^n$, where a = 1.7 ± 0.3 x 10^{-2} and n = 1.1 ± 0.1.

Table S5. Data for the plot in Figure S25.

$[H_2O_2]_0$ (M)	k_{obs} (s^{-1})
0.0904	1.3 ± 0.4 x 10^{-3}
0.181	2.5 ± 0.8 x 10^{-3}
0.271	4.1 ± 0.9 x 10^{-3}

IX. Characterization of TATP Degradation Products



TATP **S6**

A 20 mL vial was charged with a stir bar, TATP (30 mg, 0.14 mmol), 2,4-dinitrophenylhydrazine (59 mg, 0.30 mmol), TsOH (959 mg, 5.05 mmol) and MeOH (3 mL). The mixture was stirred at rt. After 6 h, the heterogeneous mixture became homogeneous. The solution was poured into H_2O (~50 mL) and the resulting precipitate was filtered and washed with H_2O (3 x 20 mL) and dried in vacuo to give an orange solid **S6** (27 mg, 28%). Average yield was ~30% based on 2 runs. HRMS (EI): Calcd for $C_9H_{10}N_4O_4$, 238.0702 M^+; Found 238.0703.

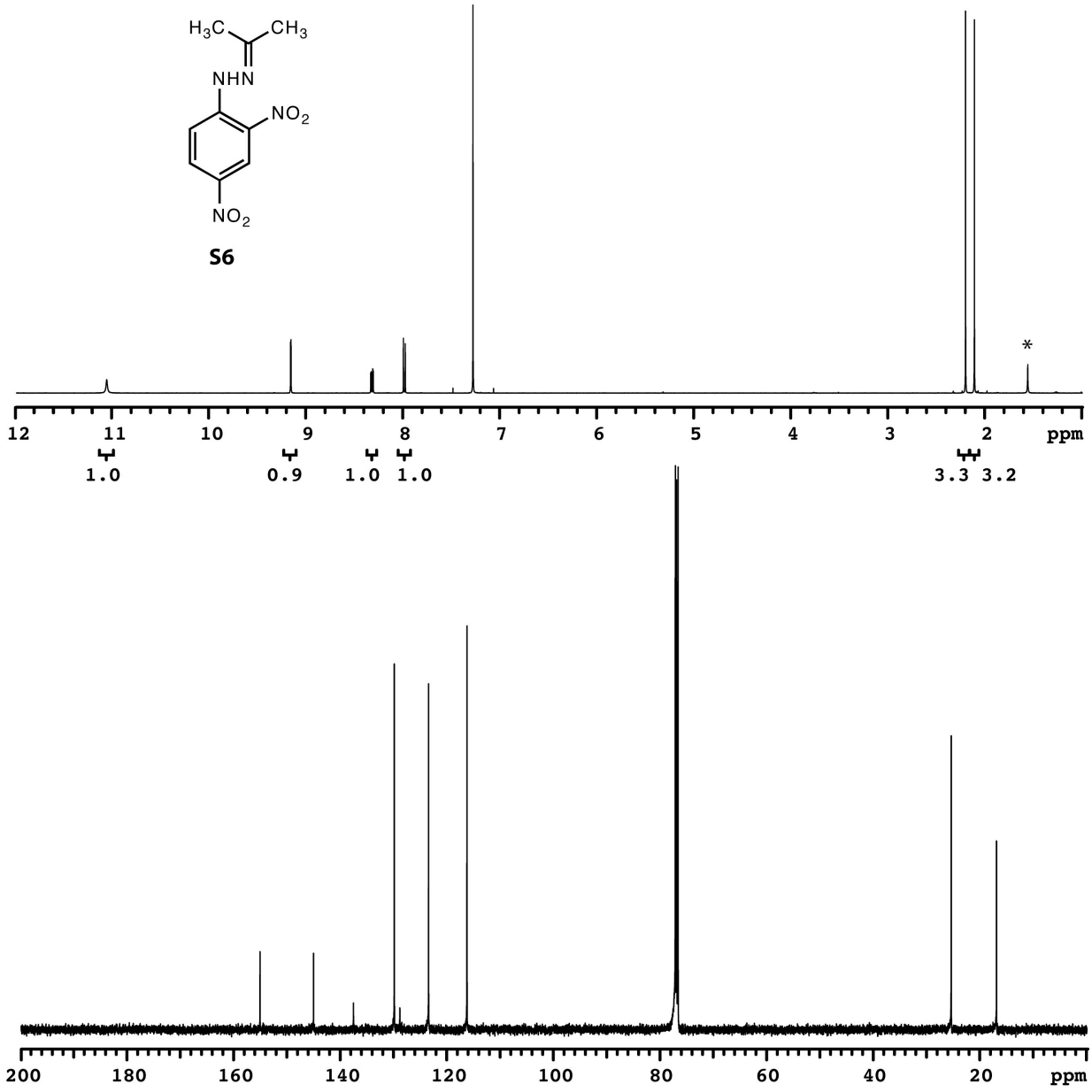
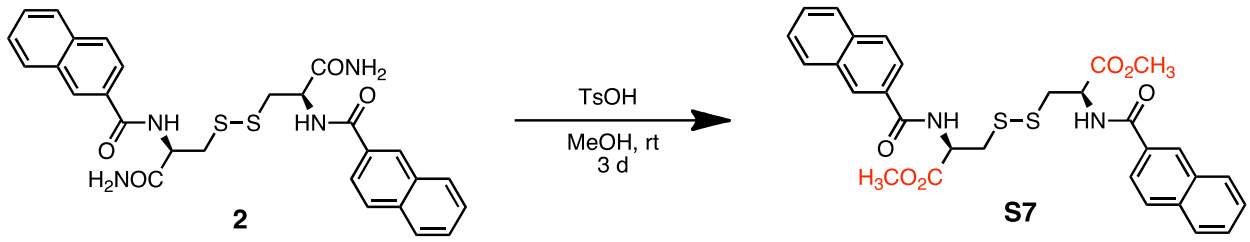


Figure S26. ^{1}H and ^{13}C NMR spectra of **S6**. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 11.04 (brs, 1H), 9.14 (d, *J* = 2.5 Hz, 1H), 8.30 (m, 1H), 7.97 (d, *J* = 9.5 Hz, 1H), 2.18 (s, 3H), 2.09 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ 154.93, 144.88, 137.38, 129.72, 128.69, 123.29, 116.10, 25.24, 16.75. *denotes H_2O.

X. Reaction of 2 under Acidic Conditions



A 20 mL vial was charged with **2** (67 mg, 0.12 mmol), TsOH (839 mg, 4.3 mmol) and MeOH (5 mL). The reaction conversion at 5 and 24 h were ~ 10% and ~ 33%, respectively, as determined by ^{1}H NMR spectroscopy. After 3 d at rt, the undissolved **2** was removed by filtration and dried in vacuo (20 mg, 30%). The filtrate was concentrated under reduced pressure. H_2O (50 mL) was added to the oily residue to generate a white precipitate. The precipitate was isolated by filtration, washed with H_2O (3 x 20 mL) and dried in vacuo to give a white solid **S7** (36 mg, 50%). HRMS (EI): Calcd for **S7** $C_{30}H_{28}N_2O_6S_2$, 576.1389 M^+; Found, 576.1389.

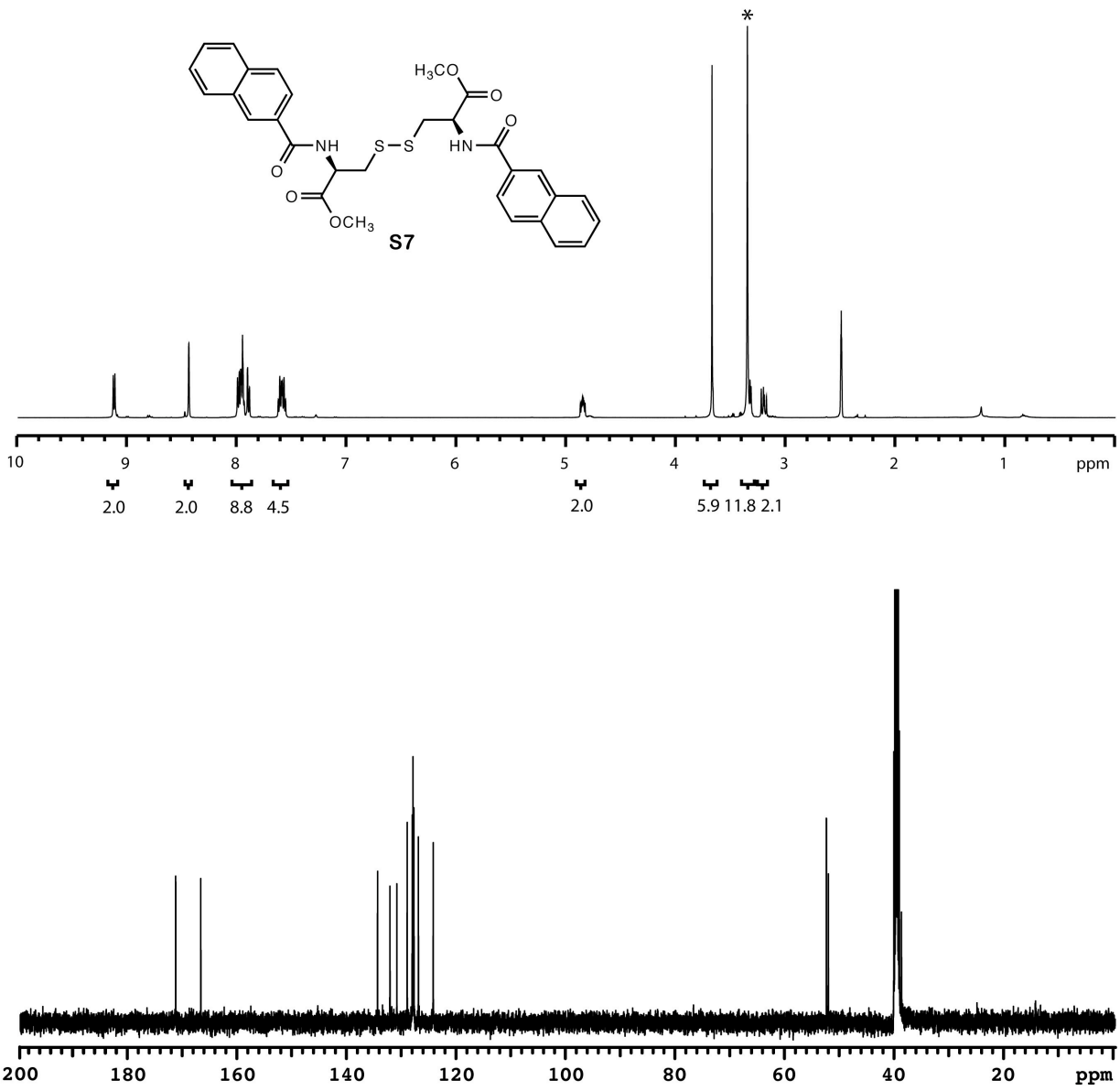


Figure S27. ^{1}H and ^{13}C NMR spectra of **S7**. ^{1}H NMR (DMSO-d_6, 500 MHz): δ 9.13 (d, J = 7.5 Hz, 2H), 8.44 (s, 2H), 8.00-7.89 (m, 8H), 7.63-7.56 (m, 4H), 4.85 (m, 2H), 3.68 (s, 6H), 3.35-3.32 (m, 2H), 3.20 (m, 2H). ^{13}C NMR (DMSO-d_6, 125 MHz): δ 171.15, 166.57, 134.28, 132.02, 130.77, 128.88, 127.96, 127.81, 127.64, 126.83, 124.12, 52.32, 51.97, 38.62. One aromatic carbon was not resolved. *denotes H_2O.

XI. Optimization of TATP Sensing Conditions in a Small Tube

Note that for experimental convenience, optimizations were performed with a stock solution of TATP. Also all reagents were combined in a 4 mL vial before transferring to the small tube.

(1) Optimization of [TsOH]

A 4 mL vial was charged with **1** (2 mg, 0.007 mmol), TsOH (different amounts as shown below) and MeOH (0.15 mL). Then TATP (0.15 mL of 45 mM in MeOH) was added to the vial. The mixture was shaken for 1-2 s and transferred to a small tube (4.6 mm I.D.). After 10 min, the tube was inverted to examine for gel formation.

Table S6. Optimization of [TsOH]

Equiv. of TsOH	6.1	13.7	25.2	36.7
At 10 min	Solution	Unstable gel	Gel	Gel
Equiv. of TsOH	49.0	61.3	73.5	85.8
At 10 min	Gel	Solution*	Solution*	Solution*

* The solution is attributed to the background reaction of **2** with TsOH in MeOH to generate **S7**.

(2) Optimization of [**1**]

A 4 mL vial was charged with MeOH (0.15 mL), **1** (different amounts as shown below) and TsOH (36 equiv. to **1**). Then TATP (0.15 mL, 45 mM in MeOH) was added to the vial. The mixture was shaken for 1-2 s and transferred to a small tube (4.6 mm I.D.). The sample was inverted to examine for gelation every 5 min.

Table S7. Optimization of [**1**]

[1] (mM)	12 mM	24 mM	36 mM
Observed Gelation	> 60 min	15 min	10 min

(3) Detection limit

A 4 mL vial was charged with **1** (3 mg, 0.011 mmol), TsOH (77 mg, 0.41 mmol, 37 equiv.) and MeOH (0.15 mL). Then TATP (0.15 mL, different concentrations in MeOH) was added to the vial to generate the final [TATP] as shown below. The mixture was shaken for 1-2 s and transferred to a small tube (4.6 mm I.D.). The sample was inverted to examine for gelation every 5 min.

Table S8. Gelation time at various final [TATP]

[TATP] (mM)	4.5 mM	14 mM	32 mM	45 mM	180 mM
Observed Gelation	~ 30 min	10-15 min	5-10 min	5-10 min	~ 2 min

XII. TATP Detection at Different Sample Volumes

A 4 mL vial was charged with **1** (4 mg, 14 mmol), TsOH (99 mg, 0.52 mol) and MeOH (0.20 mL). Then TATP (0.20 mL of 45 mM in MeOH) was added to the vial. The mixture was shaken for 1-2 s and allowed to sit at rt. After 30 min, the vial was inverted and a stable gel was formed (Figure S28, left).

The procedure described above was repeated with all reagents increased by a factor of 10. A stable gel was observed after 30 min (Figure S28, right).

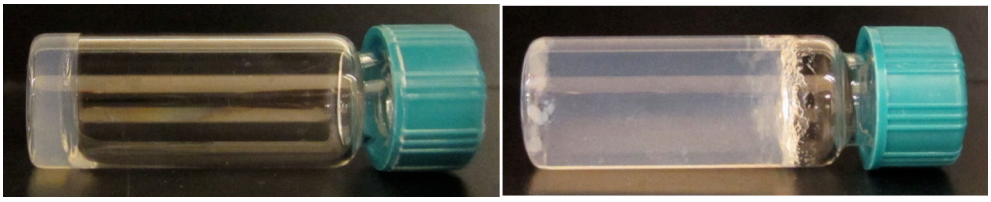


Figure S28. (left) A 0.4 mL gel of **1** triggered by 2 mg TATP and (right) a 4 mL gel of **1** triggered by 20 mg TATP.

XIII. Cgc Measurements in an NMR Tube

An NMR tube was charged with a suspension of **2** (0.30 mL, 4.6 mM in MeOH), heated to the boiling point of MeOH and then allowed to cool to room temperature. The tube was inverted to examine whether a stable gel formed. If a stable gel formed, 0.10 mL of MeOH was added and the procedure was repeated until an unstable gel was observed. The last concentration of a stable gel was recorded as the cgc.

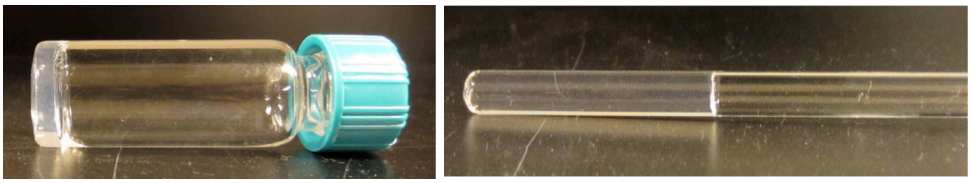


Figure S29. Gels of **2** at cgc (left) in a 4 mL vial and (right) in an NMR tube, both at a volume of 0.50 mL.

Table S9. Cgcs of **2** in a 4 mL vial and an NMR tube.

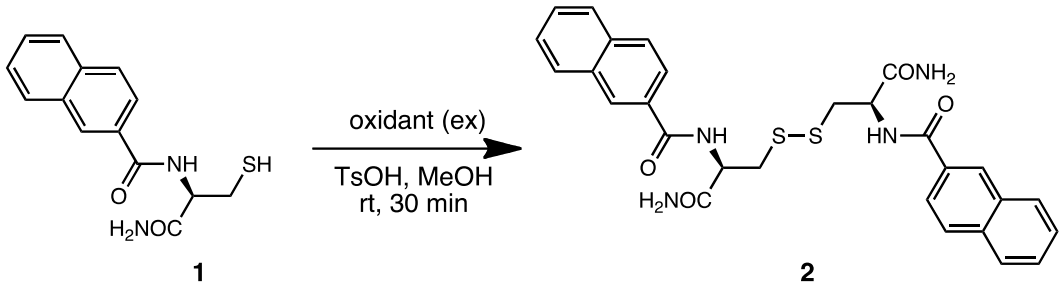
cgc in a 4 mL vial (mM)	cgc in an NMR tube (mM)
4.6	2.0

XIV. In situ Gelation in a Small Tube

A 4 mL vial was charged with **1** (3 mg, 0.011 mmol), TsOH (75 mg, 0.39 mmol, 36 equiv.) and MeOH (0.15 mL). Then TATP (0.15 mL, 45 mM in MeOH) was added to the vial. The mixture was shaken for 1-2 s and transferred to a small tube. After 8 min, the sample was inverted and a stable gel was observed.

Figure S30. In situ gel formation triggered by the oxidation of **1** under TATP/TsOH conditions in a small tube.

XV. Sensor Selectivity

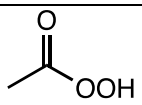
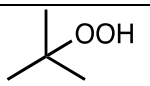
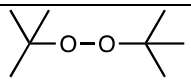
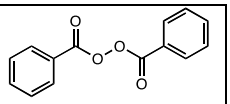


1 **2**

A 4 mL vial was charged with **1** (2 mg, 0.007 mmol) and MeOH (1 mL). An excess amount of oxidant (10 equiv.) was added. Note that organic oxidants (e.g., NaOCl, peroxides) were added without dilution. Inorganic oxidants were added as aqueous solutions (0.1 mL, ~ 0.7 M in H_2O). After 30 min, the vial was inverted to check for gelation.

For screenings performed under acidic conditions, the same procedures were repeated except that TsOH (13 mg, 0.068 mmol) was added prior to the addition of oxidants.

Table S10. In situ gel screenings of **1** towards various oxidants.

[TsOH] (M)	**NaOCl**				
0	Gel	Gel	Gel	Solution	Solution
0.068	Gel	Gel	Gel	Gel	Solution
	K_2CrO_4	**$K_2Cr_2O_4$**	**$KClO_3$**	**KI**	**$NaNO_2$**
0	Gel	Gel	Solution	Solution	Solution
0.068	Gel	Gel	Solution	Solution	Solution

XVI. References:

1. (a) Lin, Y. A.; Chalker, J. M.; Floyd, N.; Bernardes, G. J. L.; Davis, B. G. *J. Am. Chem. Soc*. **2008**, *130*, 9642-9643. (b) Yanagisawa, H.; Ishihara, S.; Ando, A.; Kanazaki, T.; Miyamoto, S.; Koike, H.; Iijima, Y.; Oizumi, K.; Matsushita, Y.; Hata, T. *J. Med. Chem*. **1987**, *30*, 1984-1991. (c) Han, G.; Tamaki, M.; Hruby, V. J. *J. Peptide Res*. **2001**, *58*, 338-341.

2. (a) Matyas, R.; Pachman, J. *Propellants Explos. Pyrotech*. **2010**, *35*, 31-37. (b) Bellamy, A. J. *J. Forensic Sci.* **1999**, *44*, 603-608.