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SUPPORTING INFORMATION

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Title: A Modular Synthesis of Multidentate S-, N- and O-Containing Meta- and Paracyclophanes
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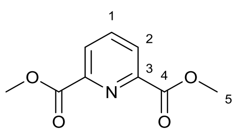
GENERAL EXPERIMENTAL

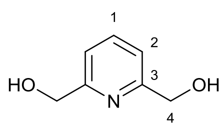
Anhydrous solvents and reagents were obtained as follows: DMF was dried three times over molecular sieves (3 Å), DMSO was left over molecular sieves (4 Å), THF was distilled from sodium wire and benzophenone, DCM was distilled from calcium hydride, methanol was dried over molecular sieves (4 Å). Dried Et_2O, THF and DCM were alternatively obtained from the PureSolv MD Solvent Purification System. Petrol or pet. ether refers to light petroleum which distils between 40 °C and 60 °C. All reactions were conducted in dry glassware under a nitrogen atmosphere, unless otherwise stated. All chemicals were used directly from the suppliers' vessel without further purification, unless otherwise stated. ^{1}H NMR spectra were recorded at 300, 400 or 500 MHz and ^{13}C NMR spectra at 75, 100 or 125 MHz on a Bruker AC300, AC400 or AC500 spectrometer. The splitting patterns for NMR spectra are designated as follows: s (singlet), br.s (broad singlet), d (doublet), t (triplet), q (quadruplet), quin (quintet), sext (sextet), sept. (septet), m (multiplet), or combinations thereof. Assignments were made with the aid of DEPT135, COSY, HMBC and HMQC experiments. Mass spectra were recorded on one of the following: Waters QTOF (ES, HRMS), Thermo Finnigan MAT95XP (GC/MS, EI, HRMS) or a Hewlett Packard 5971 MSD (GC/MS). Infrared spectra were recorded on a Bruker Alpha FT-IR.

Dimethyl pyridine-2,6-dicarboxylate:[1]



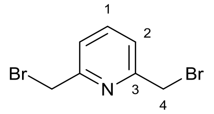
To methanol (300 mL) at 0 °C was added dropwise thionyl chloride (9.6 mL, 131.6 mmol) followed by pyridine 2,6-dicarboxylic acid (10 g, 59.8 mmol). The reaction was refluxed for 5 hours, after which the solid was dried by azeotropic removal of the solvent using toluene (3 x 200 mL), to give the *title compound* as a colourless powder (11.4 g, 98%; R_f = 0.65 (30% EtOAc in petrol); **m.p**. 117 – 120 °C, lit[1], m.p 120-122 °C), (found [ES^{+}] M^{+} + Na, 218.0421. $C_9H_9O_4NNa$ requires *M*, 218.0424); υ_{max} (ATR,) 3063 (w), 2850 (w), 1740 (s), 1571 (m), 1449 (m), 1290 (m), 1245 (s) and 1163 (m) cm^{-1}; δ_H ($CDCl_3$, 500 MHz) 4.02 (6H, s, C**H**$_3$, H-5), 8.03 (1H, t, J = 8.0 Hz, C**H**, H-1) and 8.31 (2H, d, J = 8.0 Hz, C**H**, H-2); δ_C ($CDCl_3$, 125 MHz) 53.17 (**C**H$_3$, C-5), 128.00 (**C**H, C-2), 138.34 (**C**H, C-1), 148.18 (**C**, C-3) and 165.02 (**C**, C-4); *m/z* (ES^{+}) 196.0 (M^{+} + H), 218.0 (M^{+} + Na).

Pyridine-2,6-diyldimethanol:[2]



$NaBH_4$ (9.49 g, 251 mmol) added in portions to a solution of pyridine ester (11.4 g, 58.3 mmol) in dry THF (100 mL) at room temperature ensuring the reaction does not get too hot. The reaction was left for 16 hours at room temperature. Saturated aqueous Na_2CO_3 solution (200 mL) was added dropwise, and the reaction was heated to 60 °C for 2 hours. On cooling to ambient temperature, the reaction mixture was taken to dryness *in vacuo*, azeotroping with MeOH. The fine colourless solid was extracted by Soxhlet extraction with chloroform for 16 hours. The solvent was removed *in vacuo*, resulting in a fine colourless crystalline product (3.85 g, 47%; R_f = 0.60 (EtOAc); **m.p.** 105 – 108 °C; lit[2], m.p 111-113 °C, (found [ES^{+}] M^{+} + Na, 162.0519. $C_7H_9O_2NNa$ requires *M*, 162.0525); υ_{max} (ATR): 3349 (m), 3097 (w), 2967 (w), 2895 (w), 1599 (m), 1469 (w), 1444 (m), 1220 (w), 1159 (m) and 1082 (s) cm^{-1}; δ_H ($CDCl_3$, 300 MHz) 4.79 (4H, s, C**H**$_2$, H-4), 7.20 (2H, d, J = 8.0 Hz, C**H**, H-2) and 7.71 (1H, t, J = 8.0 Hz, C**H**, H-1); δ_C ($CDCl_3$, 75 MHz) 64.38 (**C**H$_2$, C-4), 119.16 (**C**H, C-2), 137.44 (**C**H, C-1) and 158.40 (**C**, C-3); *m/z* (ES^{+}) 140 (M^{+} + H), 162 (M^{+} + Na), 178 (M^{+} + K), 317 (2M^{+} + K); *m/z* (ES^{-}) 265 (M^{-} + I).

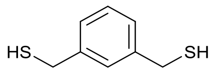
2,6-bis(Bromomethyl)pyridine (19):[2]



Pyridine-2,6-diyldimethanol (1.82 g, 13.1 mmol) and 33% HBr in acetic acid (26 mL, 2 mL/mmol) were heated at 100 °C for 90 minutes. The reaction was poured straight onto some ice, and neutralised with 1 M NaOH to pH 9. The precipitated product was collected as a pale brown solid (2.75 g, 80%); R_f = 0.32 (20% EtOAc in petrol); **m.p.** 81 – 83 °C, lit[2], m.p 80-82 °C found [ES^{+}] M^{+} + H 263.9019. $C_7H_8N^{79}Br_2$ requires *M*, 263.9018); υ_{max} (ATR) 3063 (w), 3020 (w), 2967 (w), 1570 (m), 1449 (m), 1203 (m), 817 (m) and 585 (s) cm^{-1}; δ_H ($CDCl_3$, 400 MHz) 4.54 (4H, s, C**H**$_2$, H-4), 7.38 (2H, d, J = 8.0 Hz, C**H**, H-2) and 7.71 (1H, t, J = 8.0 Hz, C**H**, H-1); δ_C ($CDCl_3$, 125 MHz) 33.37 (**C**H$_2$, C-4), 122.72 (**C**H, C-2), 138.04 (**C**H, C-1) and 156.55 (**C**, C-3); *m/z* (ES^{+}) 264 (M^{+} + H).

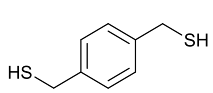
[1] N. W. Alcock, G. Clarkson, P. B. Glover, G. A. Lawrance, P. Moore, M. Napitupulu, *Dalton Trans.*, **2005**, 518-527.
[2] X.-M. Shi, R.-R. Tang, G.-L Gu., K.-l Huang., *Spectrochim. Acta, Part A*, **2009**, *72*, 198-203.

1,3-phenylenedimethanethiol (14):[3]



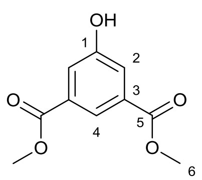
1,3-bis(bromomethyl)benzene (3.03 g, 11.5 mmol) and thiourea (1.75 g, 23.0 mmol) were dissolved in degassed, dry EtOH (30 mL) and stirred for 4 hours. The solvent was removed *in vacuo*, and the residual thiouronium salt was dissolved in degassed H_2O (30 mL). NaOH (1.83 g, 45.8 mmol) was added and the reaction stirred for 4 hours. The solution was cooled on an ice bath and 4 M HCl was added until the aqueous layer was acidic (pH 2). The solution was extracted with $CHCl_3$ (5 x 30 mL) and the combined organic extracts were dried over $MgSO_4$, and concentrated *in vacuo* to give **19** as a yellow oil (2.53 g, quant.), δ_H ($CDCl_3$, 300 MHz) 1.78 (2H, t, J = 7.5 Hz, S**H**), 3.75 (4H, d, J = 7.5 Hz, C**H**$_2$SH) and 7.18 – 7.32 (4H, m, Ar-**H**).

1,4-phenylenedimethanethiol (**17**)**:**[4]



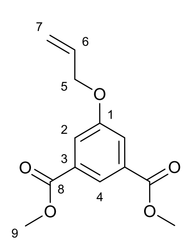
1,4-bis(bromomethyl)benzene (1.01 g, 3.8 mmol) and thiourea (582 mg, 7.6 mmol) were dissolved in degassed, dry EtOH (10 mL) and stirred for 4 hours. The solvent was removed *in vacuo* to afford the crude thiouronium salt as near-colourless crystals. To this solid was added 5 M NaOH (degassed aq., 3 mL) and the reaction was refluxed for 30 minutes. The solution was cooled on an ice bath and 4 M HCl was added until acidic (pH 2). The solution was extracted with $CHCl_3$ (5 x 10 mL), the combined organic extracts were dried over $MgSO_4$, and then concentrated *in vacuo* to give **17** as a thick yellow oil (650 mg, quant.), (found [EI] M, 170.0215. $C_8H_{10}S_2$ requires *M*, 170.0218); δ_H ($CDCl_3$, 400 MHz) 1.70 (2H, t, J = 7.0 Hz, CH_2S**H**), 3.67 (4H, d, J = 7.0 Hz, C**H**$_2$SH) and 7.22 (4H, s, Ar-**H**); δ_C ($CDCl_3$, 100 MHz) 28.58 (CH_2, **C**H_2SH), 128.31 (CH, **C**H, aryl) and 139.92 (C, **C**, aryl); *m/z* (EI) 170, 171 (M), 137(M – HS^-), 104 (M – $2HS^-$).

Dimethyl 5-hydroxyisophthalate[5]



5-Hydroxyisophthalic acid (10 g, 54.9 mmol) was dissolved in methanol (55 mL) to which was then added 98% H_2SO_4 (6.5 mL, 12.1 mmol, 0.22 eq.). The reaction was refluxed for 5 hours, allowed to cool, and concentrated to dryness *in vacuo*. EtOAc (150 mL) was added, and the organic extract washed (5% $NaHCO_3$; 2 x 80 mL; brine; 80 mL), dried over $MgSO_4$, filtered and concentrated *in vacuo*. The *title compound* was isolated as colourless crystalline solid in an essentially pure state (11.5 g, quant.), R_f = 0.57 (50% EtOAc in petrol), **m.p.** 158 – 159 °C [Ref: 160 – 161 °C[5]], (found [ES^-] M^- 209.0449. $C_{10}H_9O_5$ requires *M,* 209.0455); υ_{max} (ATR) 3354 (m), 2962 (w), 1698 (s), 1597 (m), 1428 (s), 1353 (s), 1299 (m), 1241 (s) and 1096 (m) cm^{-1}; δ_H (CD_3OD, 500 MHz) 3.91 (6H, s, CH_3, H-6), 7.59 (2H, d, J = 1.0 Hz, ArH, H-2) and 8.06 (1H, t, J = 1.0 Hz, ArH, H-2); δ_C (CD_3OD, 125 MHz) 52.99 (CH_3, C-6), 121.58 (CH, C-2), 122.51 (CH, C-4), 133.12 (C, C-3), 159.35 (C, C-1) and 167.71 (C, C-5); *m/z* (ES^+) 233 (M^+ + Na); *m/z* (ES^-) 209 (M^-).

Dimethyl 5-(allyloxy)isophthalate (22):[6]

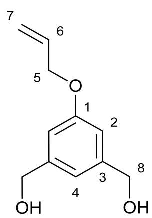


K_2CO_3 (10.3 g, 80.3 mmol) was added to a solution of dimethyl 5-hydroxyisophthalate (10.5 g, 49.6 mmol) in dry DMF (100 mL) at room temperature. After 2 hours, allyl bromide (4.25 mL, 50.2 mmol) was added and the reaction was warmed to 90 °C for 9 hours. On cooling to ambient temperature, the solvent was removed *in vacuo*, water (300 mL) was added and extracted with DCM (4 x 200 mL). The combined organic extracts were dried over $MgSO_4$, filtered, and concentrated *in vacuo* to give **22** as a colourless crystalline solid (12.4 g, quant.) in an essentially pure state; R_f = 0.50 (20% EtOAc in petrol); **m.p.** 59 – 60 °C, lit[5], m.p 68-69

[3] T. Sato, K. Nishiyama, Iitaka Y. Morita, *Bull. Chem. Soc. Jpn.*, **1985**, *58*, 2366-2369.
[4] W.-L.,Wang, J.-W. Xu,Y.-H. Lai, *J. Polym. Sci., Part A: Polym. Chem.*, **2006**, *44*, 4154-4164.
[5] A. K. Jain, V. V. Reddy, A. Paul, M. K Bhattacharya and S., *Biochemistry*, **2009**, *48*, 10693-10704.
[6] M. McWatt, G.-J. Boons, *Eur. J. Org. Chem.*, **2001**, *2001*, 2535-2545.

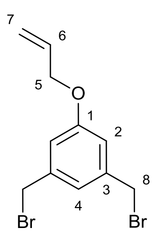
°C (found [ES^+] M^+ + Na, 273.0742. $C_{13}H_{14}O_5Na$ requires *M*, 273.0733); υ_{max} (ATR) 3089 (w), 2954 (w), 1732 (s), 1721 (s), 1593 (m), 1453 (m), 1433 (m), 1336 (s), 1237 (s), 1189 (m) cm^{-1}; δ_H ($CDCl_3$, 300 MHz) 3.95 (6H, s, C**H₃**, H-9), 4.63 (2H, d, *J* = 5.0 Hz, C**H₂**, H-5), 5.33 (1H, dd, *J* = 10.5, 1.0 Hz C**H₂**, H-7), 5.45 (1 H, dd, *J* = 17.0, 1.0 Hz, C**H₂**, H-7), 6.06 (1 H, ddt, *J* = 17.0, 10.5, 5.0 Hz, C**H**, H-6), 7.77 (2H, d, *J* = 1.0 Hz, Ar**H**,H-2) and 8.29 (1H, t, *J* = 1Hz, Ar**H**, H-4); δ_C ($CDCl_3$, 75 MHz) 52.40 (**C**H_3, C-9), 69.23 (**C**H, C-5), 118.18 (**C**H, C-7), 120.10 (**C**H, C-2), 123.11 (**C**H, C-4), 131.78 (**C**H, C-6), 132.40 (C, C-3), 158.65 (**C**, C-1) and 166.12 (**C**, C-8); *m/z* (ES^+) 251 (M^+ + H), 273 (M^+ + Na).

(5-(Allyloxy)-1,3-phenylene)dimethanol:[7]



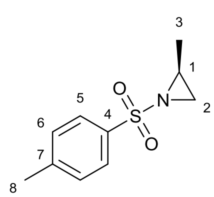
1 M Dibal-H in Et_2O (160 mL, 160 mmol) was added dropwise to a solution of dimethyl 5-(allyloxy)isophthalate (10.0 g, 34.0 mmol) in dry DCM (140 mL) at -78 °C. The reaction was stirred for 3 hours at -78 °C after which EtOAc (50 mL) was added and the reaction was allowed to warm to ambient temperature. Excess Dibal-H was quenched with water. The whole reaction mixture was filtered, dried over $MgSO_4$, filtered again and concentrated *in vacuo* giving *title compound* as a near-colourless solid (7.70 g, 99%); R_f = 0.17 (50% EtOAc in petrol); **m.p.** 50 – 52 °C, lit[6], m.p 54-54 °C (found [ES^+] M^+ + Na, 217.0841. $C_{11}H_{14}O_3Na$ requires *M*, 217.0835); υ_{max} (ATR): 3393 (m), 2927 (m), 1593 (m), 1421 (m), 1289 (m), 1151 (s), 1044 (s) and 987 (m) cm^{-1}; δ_H ($CDCl_3$, 500 MHz) 3.46 (2H, br. s, O**H**), 4.46 (2H, d, *J* = 5.5, 1.5 Hz, C**H₂**, H-5), 4.49 (4H, s, C**H₂**, H-8), 5.26 (1H, dd, *J* = 10.5, 1.0 Hz, C**H₂**, H-7), 5.38 (1H, dd, *J* = 17.0, 1.0 Hz, C**H₂**, H-7), 6.01 (1H, ddt, *J* = 17.0, 10.5, 5.5 Hz, C**H**, H-6), 6.73 (2H, s, Ar**H**, H-2) and 6.82 (1H, s, Ar**H**, H-4); δ_C ($CDCl_3$, 125 MHz) 64.58 (CH_2, C-8), 68.72 (CH_2, C-5), 112.14 (CH, C-2), 117.62 (CH, C-4 + CH_2, C-7), 133.08 (CH, C-6), 142.67 (C, C-3) and 158.71 (C, C-1); *m/z* (ES^+) 217 (M^+ + Na).

1-(Allyloxy)-3,5-bis(bromomethyl)benzene (23):[8]



Dry pyridine (100 µL, 1.2 mmol) added to a solution of (5-(Allyloxy)-1,3-phenylene)dimethanol (4.00 g, 20.6 mmol) in dry DCM (22 mL) at room temperature under N_2 before cooling to 0 °C. N_2 was replaced by a $CaCl_2$ tube and PBr_3 (704 µL, 7.5 mmol) was added dropwise. The reaction was allowed to warm up to room temperature and stirred for 24 hours. After quenching with water, the reaction was extracted with DCM (5 x 70 mL). The combined organic layers were dried over $MgSO_4$, filtered and concentrated in vacuo. The crude product was purified by flash column chromatography (DCM) to afford two products. The less polar material (R_f = 0.80) was collected as dark crystals (1.48 g, 22%), and identified as the title compound **23**, R_f = 0.80 (DCM); **m.p.** 38 – 40 °C, lit[7], m.p 38-39 °C (found [EI] M, 317.9251. $C_{11}H_{12}O^{79}Br_2$ requires M, 317.9249); δ_H ($CDCl_3$, 500 MHz) 4.44 (4H, s, CH_2, H-8), 4.55 (2H, d, J = 5.0 Hz, CH_2, H-5), 5.32 (1H, dd, J = 10.5, 1.0 Hz, CH_2, H-7), 5.44 (1H, dd, J = 17.0, 1.0 Hz, CH_2, H-7), 6.06 (1H, ddt, J = 17.0, 10.5, 5.0 Hz, CH, H-6), 6.89 (2H, d, J = 1.0 Hz, ArH, H-2) and 7.01 (1H, t, J = 1.0 Hz, ArH, H-4); δ_C ($CDCl_3$, 125 MHz) 32.82 (CH_2, C-8), 68.85 (CH_2, C-5), 115.37 (CH, C-2), 117.90 (CH_2, C-7), 121.89 (CH, C-4), 132.68 (CH, C-6), 139.51 (C, C-3) and 158.87 (C, C-1); m/z (GC-MS): 320 (M^+ + H), 239 (M^+ - Br), 159 (M^+ - 2Br).

(S)-2-methyl -1-tosylaziridine (3):[9]

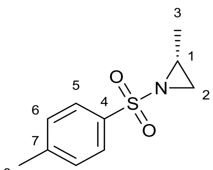


To a solution of (*S*)-alaninol (1.95 mL, 25 mmol) and tosyl chloride (5.72 g, 30 mmol) in dry DCM (200 mL) at −25 °C was added Et_3N (13.9 mL, 100 mmol). The reaction was stirred at −25 °C for 45 minutes, and then at room temperature for 3 hours. The reaction was again cooled to −25 °C, and mesyl chloride (2 mL, 26.3 mmol) was added dropwise over 10 minutes. The reaction was allowed to warm up to room temperature over 22 hours. The orange solution was washed with 0.5 M NaOH (2 x 20 mL), sat. $NaHCO_3$ (2 x 20 mL),

[7] N. L'Hermite, A. Giraud, O. Provot, J.-F. Peyrat , M. Alami, J.-D. Brion, *Tetrahedron*, **2006**, *62*, 11994-12002.
[8] Y. Hosokawa, S. Maki, T. Nagata, *Bull. Chem. Soc. Jpn.*, **2005**, *78*, 1773-1782.
[9] a) Y., Pei, K., Brade E. Brulé, L. Hagberg, Lake, C. Moberg *Eur. J. Org. Chem.*, **2005**, *2005*, 2835-2840; b) G. W. Daub, D. A. Heerding, L. E. Overman, *Tetrahedron*, **1988**, *44*, 3919-3930; c) G. Argouarch G. Stones C. L. Gibson, A. R., Kennedy, D. C. Sherrington, *Org. Biomol. Chem.*, **2003**, *1*, 4408-4417. (d) J. L.Vicario, D. Badia, L. Carrillo, *ARKIVOC*, **2007**, 4, 304-311.

dried over $MgSO_4$ and concentrated *in vacuo*. This left a brown oil (7.07 g) as a crude product which was purified by column chromatography (15% → 20% EtOAc in petrol) to afford the *title compound* **2** as a colourless waxy solid (3.80 g, 72%). **m.p**. 54 – 56 °C lit[8], m.p 58-59 °C; $[\alpha]_D$ = + 30 (c = 1.48, $CHCl_3$) lit[9c,d] $[\alpha]_D$ = +30.3 (c = 1.02, $CHCl_3$)(found C, 56.49; H, 6.14; N, 6.36%. $C_{10}H_{13}O_2NS$ requires C, 56.85; H, 6.20; N, 6.63%. Found [ES$^+$] M$^+$ + H, 212.0730. $C_{10}H_{14}O_2NS$ requires *M*, 212.0740); δ_H ($CDCl_3$, 400 MHz) 1.24 (3H, d, *J* = 6.0 Hz, CH_3, H-3), 2.02 (1H, d, *J* = 5.0 Hz, CH_2, H-2), 2.44 (3H, s, CH_3, H-8), 2.60 (1H, d, *J* = 7.0 Hz, CH_2, H-2), 2.82 (1H, dqd, *J* = 7.0, 6.0, 5.0 Hz, CH, H-1), 7.33 (2H d, *J* = 8.0 Hz, Ar-H, H-6) and 7.81 (2H, d, *J* = 8.0 Hz, Ar-H, H-5); δ_C ($CDCl_3$, 100 MHz) 17.05 (CH_3, C-3), 21.90 (CH_3, C-8), 35.00 (CH_2, C-2), 36.13 (CH, C-1), 128.05 (CH, C-5), 129.95 (CH, C-6), 135.56 (C, C-4) and 144.67 (C, C-7); *m/z* (ES$^+$) 212.0 (M$^+$ + H), 234.3 (M$^+$ + Na).

(*R*)-2-methyl-1-tosylaziridine (3)



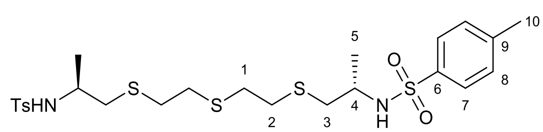
Preparation was analogous to **R-(3)**, using *(R)*-Alaninol (2.50 mL, 32.1 mmol), tosyl chloride (7.30 g, 38.3 mmol), Et_3N (19.8 mL, 142 mmol), and mesyl chloride (2.6 mL, 33.6 mmol), resulting in product as a colourless solid (4.77 g, 71%), R_f = 0.82 (50% EtOAc in hexane), $[\alpha]_D^{31}$ = 31 (c = 1.52, *$CHCl_3$*), **m.p.** 55 – 56 °C [Ref: 57 – 58 °C[10]], (found [ES$^+$] M$^+$ + H 212.0737. $C_{10}H_{14}O_2NS$ requires *M*, 212.0740); **υ_{max}** (ATR) 2998 (w), 2972 (w), 2967 (w), 1596 (m), 1451 (m), 1316 (m), 1307 (m), 1151 (s) and 1036 (m) cm^{-1}; δ_H ($CDCl_3$, 500 MHz) 1.25 (3H, d, *J* = 6.0 Hz, C**H**$_3$, H-3), 2.02 (1 H, d, *J* = 5.0 Hz, C**H**$_2$, H-2), 2.44 (3 H, s, C**H**$_3$, H-8), 2.60 (1H, d, *J* = 7.0 Hz, C**H**$_2$, H-2), 2.82 (1H, dqd, *J* = 7.0, 6.0, 5.0 Hz, C**H**, H-1), 7.33 (2H, d, *J* = 8.0 Hz, Ar**H**, H-6) and 7.82 (2H, d, *J* = 8.0 Hz, Ar**H**, H-5); δ_C ($CDCl_3$, 125 MHz) 16.69 (**C**H$_3$, C-3), 21.57 (**C**H$_3$, C-8), 34.68 (**C**H$_2$, C-2), 35.80 (**C**H, C-1), 127.70 (**C**H, C-5), 129.61 (**C**H, C-6), 135.18 (**C**, C-4) and 144.35 (C, C-7); *m/z* (ES$^+$) 234 (M$^+$ + Na), 266 (M$^+$ + Na,MeOH).

Thioether Linkers

General method for the formation of the dithiol spacer unit from the dithiol

Et_3N (2.1 eq.) was added slowly to the dithiol (1 eq.) in dry methanol (10 mL per mmol of thiol) at room temperature under nitrogen. After 10 minutes, 2-methyl-1-tosylaziridine (2.1 eq.) was added, the reaction stirred for 30 minutes, warmed to 35 °C and then stirred for 4.5 hours at this temperature. On cooling to room temperature, 0.1 M NaOH was added and the solvent removed *in vacuo* to about 1 mL. EtOAc was added and then washed with H_2O, 0.1 M NaOH and brine. The combined organic layers were dried over $MgSO_4$ and filtered to give the crude product which was purified by flash column chromatography (EtOAc:Pet. Ether) to give the desired product.

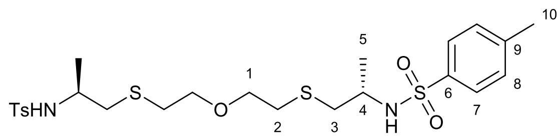
N,N'-(2S,2'S)-1,1'-(2,2'-thiobis(ethane-2,1-diyl)bis(sulfanediyl))bis(propane-2,1-diyl)bis(4-methylbenzenesulfonamide) (10):



Spacer **10** was prepared using the method described above starting from 2,2'-thiodiethanethiol (391 µL, 3.0 mmol), Et_3N (880 µL, 6.3 mmol), and *(S)*-2-methyl-1-tosylaziridine **3** (1.34 mg, 6.3 mmol) in dry methanol (30 mL). **10** (1.55 g, 90%) was isolated as fluffy colourless solid after column chromatography (20% EtOAc in petrol), R_f = 0.48 (40% EtOAc in petrol), $[\alpha]_D^{27}$ = -30 (c = 1.4, $CHCl_3$), m.p. 63.5 – 64.5 °C, (found C, 50.34; H, 6.45; N, 4.79%. $C_{24}H_{36}N_2O_4S_5$ requires C, 49.97; H, 6.29; N, 4.86%. Found [ES$^+$] M$^+$ + Na, 599.1178. $C_{24}H_{36}N_2NaO_4S_5$ requires *M*, 599.1171); υ_{max} (ATR) 3237 (m), 1708 (w), 1457 (w), 1327 (s), 1154 (s), 1076 (s) and 985 (s) cm^{-1}; δ_H ($CDCl_3$, 500 MHz) 1.11 (6H, d, *J* = 7.0 Hz, C**H**$_3$, H-5), 2.43 (6H, s, C**H**$_3$, H-10), 2.61 – 2.70 (12H, m, C**H**$_2$, H-1,2,3), 3.43 (2H, app. sept, *J* = 6.0 Hz, C**H**, H-4), 5.21 (2H, d, *J* = 7.0 Hz, N**H**), 7.31 (4H, d, *J* = 8.0 Hz, Ar**H**, H-8) and 7.78 (4H, d, *J* = 8.0 Hz, Ar**H**, H-7); δ_C ($CDCl_3$, 125 MHz) 20.41 (**C**H$_3$, C-5), 21.53 (**C**H$_3$, C-10), 32.03 (**C**H$_2$, C-1), 32.83 (**C**H$_2$, C-2), 39.34 (**C**H$_2$, C-3), 49.24 (**C**H, C-4), 127.04 (**C**H, C-7), 129.72 (**C**H, C-8), 137.52 (**C**, C-6) and 143.49 (**C**, C-9); *m/z* (ES$^+$) 576.9 (M$^+$ + H), 593.8 (M$^+$ + NH_4), 599.1 (M$^+$ + Na).

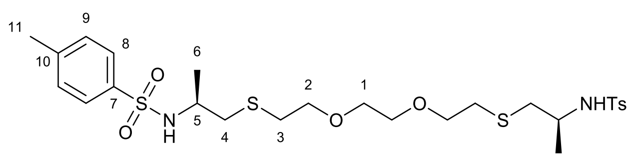
N,N'-(2S,2'S)-1,1'-(2,2'-oxybis(ethane-2,1-diyl)bis(sulfanediyl))bis(propane-2,1-diyl)bis(4-methylbenzenesulfonamide) (9):

[10] J. J. Farmer, F. C. Schroeder J. Meinwald, *Helv. Chim. Acta*, **2000**, *83*, 2594-2606.



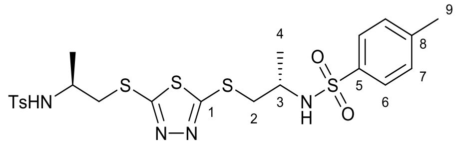
Spacer **9** was prepared using the method described above starting from 2,2'-oxydiethanethiol (375 µL, 3.0 mmol), Et_3N (880 µL, 6.3 mmol), and *(S)*-2-methyl-1-tosylaziridine **3** (1.31 g, 6.2 mmol) in dry methanol (30 mL). **9** (1.33 g, 79%) was isolated as viscous pale yellow oil after column chromatography (30% EtOAc in petrol), R_f = 0.43 (50% EtOAc in petrol); $[\alpha]_D^{32}$ = -24 (c = 1.43, $CHCl_3$), (found C, 51.06; H, 6.57; N, 4.79%. $C_{24}H_{36}N_2\ O_5S_4$ requires C, 51.40; H, 6.47; N, 5.00%. Found [ES$^+$] M$^+$ + Na, 583.1389. $C_{24}H_{36}O_5N_2S_4Na$ requires *M*, 583.1399); υ_{max} (ATR): 3270 (m), 2970 (w), 2921 (w), 2866 (w), 1453 (m), 1324 (m), 1155 (s), 1091 (s), 982 (m) and 900 (m) cm^{-1}; δ_H ($CDCl_3$, 500 MHz) 1.12 (6H, d, *J* = 6.5 Hz, C**H**$_3$, H-5), 2.42 (6H, s, C**H**$_3$, H-10), 2.53-2.69 (4H, m, C**H**$_2$, H-2), 2.64 (4H, d, *J* = 6.0 Hz, C**H**$_2$, H-3), 3.44 (2H, app. sept, *J* = 6.5 Hz, **C**H, H-4), 3.57 (4H, t, *J* = 6.5 Hz, C**H**$_2$, H-1), 5.34 (2H, d, *J* = 7.0 Hz, N**H**), 7.30 (4H, d, *J* = 8.0 Hz, C**H**, H-8) and 7.77 (4H, d, *J* = 8.0 Hz, C**H**, H-7); δ_C ($CDCl_3$, 125 MHz) 20.49 (**C**H$_3$, C-5), 21.47 (**C**H$_3$, C-10), 32.30 (**C**H$_2$, C-3), 39.77 (**C**H$_2$, C-2), 49.25 (**C**H, C-4), 70.49 (**C**H$_2$, C-1), 127.04 (**C**H, C-7), 129.61 (**C**H, C-8), 137.64 (**C**, C-6) and 143.29 (**C**, C-9); *m/z* (ES$^+$) 561.1 (M$^+$ + H), 578.0 (M$^+$ + NH$_4$), 583.0 (M$^+$ + Na).

N,N'-((2S,15S)-7,10-dioxa-4,13-dithiahexadecane-2,15-diyl)bis(4-methylbenzenesulfonamide) (8):



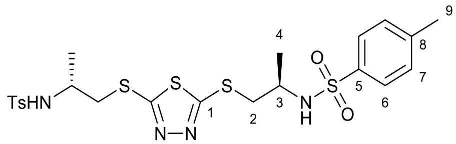
Spacer **8** was prepared using the method described above starting from 2,2'-(ethane-1,2-diylbis(oxy))diethanethiol (488 µL, 3.0 mmol), Et_3N (880 µL, 6.3 mmol), and *(S)*-2-methyl-1-tosylaziridine **3** (1.30 g, 6.2 mmol) in dry methanol (30 mL). **8** (1.56 g, 86%) was isolated as a viscous pale yellow oil after column chromatography (20% EtOAc in petrol), R_f = 0.35 (50% EtOAc in petrol), $[\alpha]_D^{27}$ = -20 (c = 5.62, $CHCl_3$), (found C, 51.83; H, 6.88; N, 4.51%. $C_{26}H_{40}O_6N_2S_4$ requires C, 51.63; H, 6.67; N, 4.63%. Found [ES$^+$] M$^+$ + Na, 627.1652. $C_{26}H_{40}O_6N_2NaS_4$ requires *M*, 627.1661); υ_{max} (ATR): 3267 (w), 2920 (w), 2866 (w), 1494 (w), 1324 (m), 1156 (s), 1092 (s), 662 (s) and 551 (s) cm^{-1}; δ_H ($CDCl_3$, 500 MHz) 1.11 (6H, d, *J* = 6.5 Hz, C**H**$_3$, H-6), 2.41 (6H, s, C**H**$_3$, H-11), 2.51 – 2.72 (8H, m, C**H**$_2$, H-3.4), 3.41 (2H, app. sept, *J* = 6.5 Hz, **C**H, H-5), 3.59 (4H, t, *J* = 6.0 Hz, C**H**$_2$, H-2), 3.62 (4H, s, C**H**$_2$, H-1), 5.43 (2H, d, *J* = 7.0, N**H**), 7.29 (4H, d, *J* = 8.0 Hz, C**H**, H-9) and 7.76 (4H, d, *J* = 8.0 Hz, C**H**, H-8); δ_C ($CDCl_3$, 125 MHz) 20.51 (**C**H$_3$, C-6), 21.45 (**C**H$_3$, C-11), 32.26 (**C**H$_2$, C-4), 39.68 (**C**H$_2$, C-3), 49.28 (**C**H, C-5), 70.17 (**C**H$_2$, C-1), 70.88 (**C**H$_2$, C-2), 127.02 (**C**H, C-8), 129.59 (**C**H, C-9), 137.66 (**C**, C-7) and 143.25 (**C**, C-10); *m/z* (ES$^+$) 605.1 (M$^+$ + H), 621.9 (M$^+$ + NH$_4$), 627.0 (M$^+$ + Na). On shaking with D_2O and NaOH: δ_H ($CDCl_3$, 400 MHz) 1.11 (6H, d, *J* = 6.5 Hz, C**H**$_3$, H-6), 2.40 (6H, s, C**H**$_3$, H-11), 2.52 – 2.68 (8H, m, C**H**$_2$, H-3,4), 3.40 (2H, app. sext, *J* = 6.5 Hz, **C**H, H-5), 3.59 (4H, t, *J* = 6.5 Hz, C**H**$_2$, H-2), 3.61 (4H, s, C**H**$_2$, H-1), 4.91 (2H, br. s, **H**DO), 7.28 (4H, d, *J* = 8.0 Hz, C**H**, H-9) and 7.76 (4H, d, *J* = 8.0 Hz, C**H**, H-8).

N,N'-(2S,2'S)-1,1'-(1,3,4-thiadiazole-2,5-diyl)bis(sulfanediyl)bis(propane-2,1-diyl)bis(4-methylbenzenesulfonamide) (11):



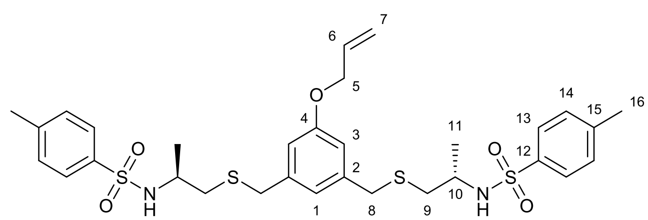
Spacer **11** was prepared using the method described above starting from 1,3,4-thiadiazole-2,5-dithiol (452 mg, 3.0 mmol), Et_3N (880 µL, 6.3 mmol), and *(S)*-2-methyl-1-tosylaziridine **3** (1.34 g, 6.3 mmol) in dry methanol (30 mL). **11** (1.40 g, 82%) was isolated as a colourless crystalline solid after column chromatography (30% EtOAc in petrol), R_f = 0.52 (60% EtOAc in petrol), $[\alpha]_D^{30}$ = -10 (c = 0.91, CH_2Cl_2), m.p. 76.5 – 77.5 °C, Found [ES$^+$] M$^+$ + Na, 595.0602. $C_{22}H_{28}O_4N_4NaS_5$ requires *M*, 595.0606); $\boldsymbol{\upsilon_{max}}$ (ATR): 3283 (m), 1738 (w), 1596 (w), 1378 (m), 1330 (m), 1151 (s) and 1045 (s) cm^{-1}; δ_H (CD_2Cl_2, 500 MHz) 1.21 (6H, d, *J* = 7.0 Hz, C**H**$_3$, H-4), 2.40 (6H, s, C**H**$_3$, H-9), 3.32 (4H, d, *J* = 6.0 Hz, C**H**$_2$, H-2), 3.70 (2H, app. sept, *J* = 7.0 Hz, **C**H, H-3), 5.49 (2H, d, *J* = 7Hz, N**H**), 7.28 (4H, d, *J* = 8.0 Hz, C**H**, H-7) and 7.69 (4H, d, *J* = 8.0 Hz, C**H**, H-6); δ_C ($CDCl_3$, 125 MHz) 21.67 (**C**H$_3$, C-4), 21.77 (**C**H_3, C-9), 40.75 (**C**H_2, C-2), 50.62 (**C**H, C-3), 127.58 (**C**H, C-6), 130.19 (**C**H, C-7), 138.10 (**C**, C-8), 144.18 (**C**, C-5) and 166.29 (**C**, C-1); *m/z* (ES^+) 573.3 (M^+ + H), 595.5 (M^+ + Na).

N,N'-(2R,2'R)-1,1'-(1,3,4-thiadiazole-2,5-diyl)bis(sulfanediyl)bis(propane-2,1-diyl)bis(4-methylbenzenesulfonamide) (12):



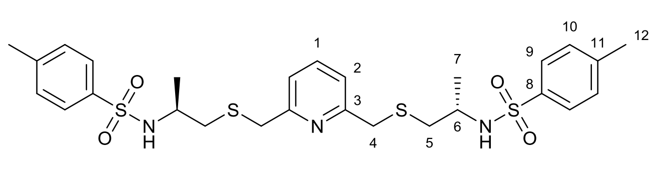
Spacer **12** was made following the standard method described above, starting from 1,3,4-thiadiazole-2,5-dithiol (360 mg, 2.4 mmol), Et_3N (700 µL, 5.0 mmol), and *(R)*-2-methyl-1-tosylaziridine (1.07 g, 5.1 mmol) in dry methanol (22 mL). **12** (839 mg, 61%) was isolated as a colourless powder after column chromatography (30% EtOAc in petrol), R_f = 0.71 (70% EtOAc in petrol), (found [ES^+] M^+ + Na, 595.0602. $C_{22}H_{28}O_4N_4NaS_5$ requires *M,* 595.0606); δ_H ($CDCl_3$, 500 MHz) 1.24 (6H, d, J = 6.5 Hz, C**H_3**, H-4), 2.41 (6H, s, C**H_3**, H-9), 3.31 (2H, dd, J = 14.5, 7.5 Hz, C**H_2**, H-2), 3.37 (2H, dd, J = 14.5, 4.5 Hz, C**H_2**, H-2), 3.75 (2 H, tqd, J = 7.5, 6.5, 4.5 Hz, C**H**, H-3), 5.42 (2H, d, J = 7.5 Hz, N**H**), 7.27 (4H, d, J = 8.0 Hz, C**H**, H-7) and 7.73 (4H, d, J = 8.0 Hz, C**H**, H-6); δ_C ($CDCl_3$, 75 MHz) 21.31 (**C**H_3, C-4), 21.53 (**C**H_3, C-9), 40.24 (**C**H_2, C-2), 49.99 (**C**H, C-3), 127.09 (**C**H, C-6), 129.66 (**C**H, C-7), 137.65 (**C**, C-8), 143.42 (**C**, C-5) and 165.59 (**C**, C-1); *m/z* (ES^+) 595.3 (M^+ + Na), 1167.6 ($2M^+$ + Na), 1739.9 ($3M^+$ + Na).

N,N'-((2S,2'S)-(((5-(allyloxy)-1,3-phenylene)bis(methylene))bis(sulfanediyl))bis(propane-2,1-diyl))bis(4-methylbenzenesulfonamide) (24):



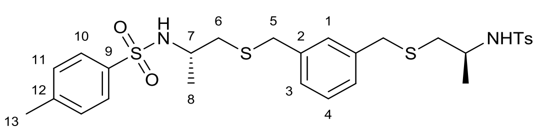
A solution of the dibromoether **23** (1.48 g, 4.6 mmol) and thiourea (714 mg, 9.4 mmol) in degassed ethanol (13 mL) were brought to reflux under N_2. After 30 minutes, the reaction was allowed to cool to room temperature and 5 M NaOH (degassed, 3.75 mL, 18.6 mmol) was added. The reaction mixture was then brought to reflux for 4 hours and cooled to room temperature. Once cool, (*S-S*) aziridine **3** (1.97 g, 9.3 mmol) was added and the reaction left to stir overnight. Aqueous 0.1 M NaOH was added until the reaction turned opaque, and the mixture reduced to dryness *in vacuo*. The residue was taken up in EtOAc (50 mL), and the organic extract was washed with H_2O (2 x 40 mL), 0.1 M NaOH (1 x 40 mL) and brine (1 x 40 mL). The organic extract was dried over $MgSO_4$, filtered and concentrated *in vacuo*. The crude product was purified by flash column chromatography (20% EtOAc in petrol) affording the *title compound* **24** as a viscous yellow oil (2.22 g, 74%), R_f = 0.65 (50% EtOAc in petrol), $[\alpha]_D^{32}$ = -24 (c = 2.02, $CHCl_3$), (found [ES^+] M^+ + Na, 671.1718. $C_{31}H_{40}O_5N_2NaS_4$ requires *M*, 671.1712); υ_{max} (ATR): 3267 (m, br), 2972 (w), 2922 (w), 2869 (w), 1593 (m), 1450 (m), 1422 (m), 1322 (m), 1298 (m) and 1153 (s) cm^{-1}; δ_H ($CDCl_3$, 500 MHz) 1.08 (6H, d, J = 6.0 Hz, C**H_3**, H-11), 2.42 (6H, s, C**H_3**, H-16), 2.43 (2H, dd, J = 14.0, 7.0 Hz, C**H_2**, H-9), 2.52 (2H, dd, J = 14.0, 5.5 Hz, C**H_2**, H-9), 3.41 (2H, dqd, J = 7.0, 6.0, 5.5 Hz, **C**H, H-10), 3.47 (2H, d, J = 14.0 Hz, C**H_2**, H-8), 3.54 (2H, d, J = 14.0 Hz, C**H_2**, H-8), 4.54 (2H, d, J = 5.0 Hz, C**H_2**, H-5), 4.72 (2H, br. s., N**H**), 5.29 (1H, d, J = 10.0 Hz, C**H_2**, H-7), 5.42 (1H, d, J = 17.0 Hz, C**H_2**, H-7), 6.05 (1H, ddt, J = 17.0, 11.0, 5.0 Hz, C**H**, H-6), 6.71 (2H, s, C**H**, H-3), 6.76 (1H, s, C**H**, H-1), 7.29 (4H, d, J = 8.0 Hz, C**H**, H-14) and 7.75 (4H, d, J = 8.0 Hz, C**H**, H-13); δ_C ($CDCl_3$, 125 MHz) 20.57 (**C**H_3, C-11), 21.47 (**C**H_3, C-16), 36.31 (**C**H_2, C-8), 38.26 (**C**H_2, C-9), 48.90 (**C**H, C-10), 68.73 (**C**H_2, C-5), 113.96 (**C**H, C-3), 117.68 (**C**H_2, C-7), 122.07 (**C**H, C-1), 127.01 (**C**H, C-13), 129.64 (**C**H, C-14), 133.06 (**C**H, C-6), 137.73 (**C**, C-12), 139.57 (**C**, C-2), 143.32 (**C**, C-15) and 158.96 (**C**, C-4); *m/z* (ES^+) 649 (M^+ + H), 671 (M^+ + Na), 687 (M^+ + K), 1319 ($2M^+$ + Na).

N,N'-((2S,2'S)-((pyridine-2,6-diylbis(methylene))bis(sulfanediyl))bis(propane-2,1-diyl))bis(4-methylbenzenesulfonamide) (20):



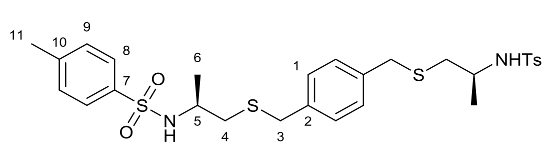
A solution of the dibromoether **19** (791 mg, 3.0 mmol) and thiourea (462 mg, 6.1 mmol) in degassed ethanol (7.5 mL) were brought to reflux under N_2. After 30 minutes, the reaction was allowed to cool to room temperature and 5 M NaOH (degassed, 2.4 mL, 12 mmol) was added. The reaction mixture was then brought to reflux for 4 hours and cooled to room temperature. Once cool, aziridine **2** (1.28 g, 6.1 mmol) was added and the reaction left to stir overnight at room temperature. Aqueous 0.1 M NaOH was added until the reaction turned opaque, and the mixture reduced to dryness *in vacuo*. The residue was taken up in EtOAc (25 mL), and the organic extract was washed with H_2O (2 x 20 mL), 0.1 M NaOH (1 x 20 mL) and brine (1 x 20 mL). The organic extract was dried over $MgSO_4$, filtered and concentrated *in vacuo*. The crude product was purified by flash column chromatography (40% EtOAc in petrol) affording the *title compound* **20** as a near-colourless crystalline solid (1.41 g, 89%), R_f = 0.67 (40% EtOAc in petrol), $[\alpha]_D^{32}$ = -65 (c = 2.14, $CHCl_3$), m.p. 88 – 90 °C, (found [ES^+] M^+ + Na, 616.1399. $C_{27}H_{35}O_4N_3NaS_4$ requires *M*, 616.1403); υ_{max} (ATR): 3246 (m), 3030 (w), 2989 (w), 2968 (w), 2926 (w), 2854 (w), 2773 (w), 2735 (w), 1594 (m), 1573 (m), 1431 (m), 1321 (s), 1156 (s) and 1140 (s) cm^{-1}; δ_H ($CDCl_3$, 300 MHz) 1.11 (6H, d, *J* = 6.5 Hz, C**H**$_3$, H-7), 2.41 (6H, s, C**H**$_3$, H-12), 2.60 (4H, app. d, *J* = 6.0 Hz, C**H**$_2$, H-5), 3.53 (2H, dqt, *J* = 7.0, 6.5, 6.0 Hz, **C**H, H-6), 3.71 (2H, d, *J* = 13.0 Hz, C**H**$_2$, H-4), 3.76 (2H, d, *J* = 13.0 Hz, C**H**$_2$, H-4), 6.12 (2H, d, *J* = 7.0 Hz, N**H**), 7.15 (2H, d, *J* = 7.0 Hz, C**H**, H-2), 7.28 (4H, d, *J* = 8.0 Hz, C**H**, H-10), 7.62 (1H, t, *J* = 7.0 Hz, C**H**, H-1) and 7.76 (4H, d, *J* = 8.0 Hz, C**H**, H-9); δ_C ($CDCl_3$, 125 MHz) 20.69 (**C**H$_3$, C-7), 21.46, 21.49 (**C**H$_3$, C-12), 37.88 (**C**H$_2$, C-4), 38.80 (**C**H$_2$, C-5), 49.58, 49.59 (**C**H, C-6), 121.58 (**C**H, C-2), 126.98 (**C**H, C-9), 129.59 (**C**H, C-10), 137.99 (**C**, C-8), 138.04 (**C**H), 143.14 (**C**, C-11) and 158.11 (**C**, C-3); *m/z* (ES^+) 593.8 (M^+ + H), 615.9 (M^+ + Na), 1187.7 ($2M^+$ + H), 1209.2 ($2M^+$ + Na), 1803.0 ($3M^+$ + Na).

N,N'-(2S,2'S)-1,1'-(1,3-phenylenebis(methylene))bis(sulfanediyl)bis(propane-2,1-diyl)bis(4-methylbenzenesulfonamide) (15):



Spacer **15** was prepared using the method described above starting from 1,3-phenylenedimethanethiol 209 (1.38 g, 8.1 mmol), Et_3N (2.4 mL, 17.2 mmol), and *(S)*-2-methyl-1-tosylaziridine 2 (3.59 g, 17.0 mmol) in dry methanol (80 mL). 14 (1.40 g, 61%) was isolated as a pale oil after column chromatography (40% EtOAc in petrol), R_f = 0.48 (40% EtOAc in petrol), $[\alpha]_D^{25}$ = - 22 (c = 1.425, $CHCl_3$), m.p. 77 – 78 °C, (found C, 55.54; H, 6.20; N, 4.51; S, 20.78%. $C_{28}H_{36}N_2O_4S_4$.½H_2O requires C, 55.88; H, 6.20; N, 4.65; S, 21.31%. Found [ES^+] M^+ + Na, 615.1446. $C_{28}H_{36}N_2NaO_4S_4$ requires *M*, 615.1450); υ_{max} (ATR): 3270 (m), 2972 (w), 2920 (w), 1598 (m), 1494 (w), 1421 (m), 1324 (s), 1155 (s), 1091 (s) and 982 (m) cm^{-1}; δ_H ($CDCl_3$, 500 MHz) 1.10 (6H, d, *J* = 7.0 Hz, CH_3, H-8), 2.42 (6H, s, CH_3, H-13), 2.43 (2H, dd, *J* = 13.5, 6.5 Hz, CH_2, H-6), 2.52 (2H, dd, *J* = 13.5, 5.5 Hz, CH_2, H-6), 3.41 (2H, m, CH, H-7), 3.52 (2H, d, *J* = 14.0 Hz, CH_2, H-5), 3.58 (2H, d, *J* = 14.0 Hz, CH_2, H-5), 5.29 (2H, d, *J* = 7.0 Hz, NH), 7.12 (2H, dd, *J* = 8.0, 1.0 Hz, CH, H-3), 7.18 (1H, br.t, *J* = 1.0 Hz, CH, H-1), 7.24 (1H, t, *J* = 8.0 Hz, CH, H-4), 7.30 (4H, d, *J* = 8.0 Hz, CH, H-11) and 7.78 (4H, d, *J* = 8.0 Hz, CH, H-11); δ_C ($CDCl_3$, 125 MHz) 20.62 (CH_3, C-8), 21.52 (CH_3, C-13), 36.24 (CH_2, C-6), 38.25 (CH_2, C-5), 48.87 (CH, C-7), 127.04 (CH, C-10), 127.69 (CH, C-3), 128.91 (CH, C-4), 129.49 (CH, C-1), 129.68 (CH, C-11), 137.70 (C, C-9), 138.19 (C, C-2) and 143.38 (C, C-12); *m/z* (ES^+) 610.8 (M^+ + NH_4), 615.4 (M^+ + Na).

N,N'-(2S,2'S)-1,1'-(1,4-phenylenebis(methylene))bis(sulfanediyl)bis(propane-2,1-diyl)bis(4-methylbenzenesulfonamide) (18):



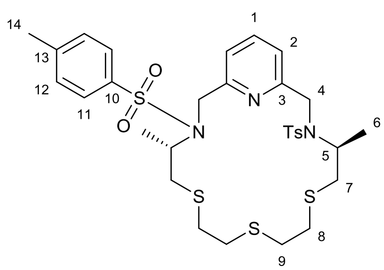
Spacer **18** was prepared using the method described above starting from 1,4-phenylenedimethanethiol (450 mg, 2.6 mmol), Et_3N (859 μL, 6.2 mmol), and (*S*)-2-methyl-1-tosylaziridine **2** (1.31 g, 6.2 mmol) in dry methanol (30 mL). **18** (1.39 g, 89%) was isolated as a pale yellow oil after column chromatography (30% EtOAc in petrol), R_f = 0.63 (50% EtOAc in petrol), $[\alpha]_D^{31}$ = -15 (c = 1.82, $CHCl_3$), (found [ES^+] M^+ + Na, 615.1462. $C_{28}H_{36}O_4N_2NaS_4$ requires *M,* 615.1450); υ_{max} (ATR): 3264 (w), 2920 (w), 1597 (w), 1422 (m), 1324 (m), 1154 (s) and 1091 (s) cm^{-1}; δ_H ($CDCl_3$, 400 MHz) 1.09 (6H, d, *J* = 7.0 Hz, C**H**$_3$, H-6), 2.39 (2H, dd, *J* = 13.5, 6.5 Hz, C**H**$_2$, H-4), 2.43 (6H, s, C**H**$_3$, H-11), 2.47 (2H, dd, *J* = 13.5, 6.0 Hz, C**H**$_2$, H-4), 3.31 – 3.44 (2H, m, **C**H, H-5), 3.47 (2H, d, *J* = 13.0 Hz, C**H**$_2$, H-3), 3.54 (2H, d, *J* = 13.0 Hz, C**H**$_2$, H-3), 5.11 (2H, d, *J* = 7.0 Hz, N**H**), 7.15 (4H, s, C**H**, H-1), 7.31 (4H, d, *J* = 8.0 Hz, C**H**, H-9) and 7.77 (4H, d, *J* = 8.0 Hz, C**H**, H-8); δ_C ($CDCl_3$, 100 MHz) 20.61 (**C**H$_3$, C-6), 21.46 (**C**H$_3$, C-11), 35.97 (**C**H$_2$, C-4), 38.12 (**C**H_2, C-3), 48.73 (**C**H, C-5), 127.01 (**C**H, C-8), 128.96 (**C**H, C-1), 129.61 (**C**H, C-9), 136.61 (**C**, C-2), 137.50 (**C**, C-7) and 143.33 (**C**, C-10); *m/z* (ES^+) 593.0 (M^+ + H), 615.4 (M^+ + Na), 631.3 (M^+ + K).

Macrocyclisation Reactions

General Method for the synthesis of the macrocycles

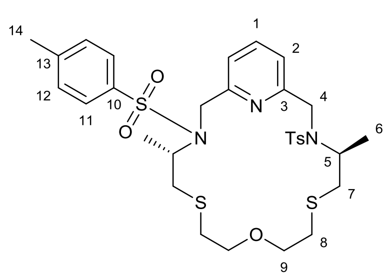
The ditosamide (1 eq.) was dissolved in dry DMF (300 mL/mmol dithiol) under N_2. After 10 minutes of stirring, 2,6-bis(bromomethyl)pyridine **19** (1 eq.) and Cs_2CO_3 (5 eq.) were added and the reaction was left to stir for 48 hours at room temperature. The solvent was removed *in vacuo* and the residue dissolved in dichloromethane which was washed with H_2O (6 times). The combined organic extracts were dried over $MgSO_4$, filtered and the solvent removed *in vacuo*. The crude product was purified by flash column chromatography (EtOAc: Pet. Ether) to yield the desired product.

(4S,14S)-4,14-Dimethyl-3,15-bis-(toluene-4-sulfonyl)-6,9,12-trithia-3,15,21-triaza-bicyclo[15.3.1]henicosa-1(20),17(21),18-triene (30)



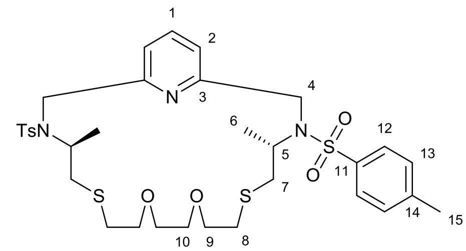
Using the general method described above, starting from ditosamide **10** (111 mg, 193 μmol), 2,6-bis(bromomethyl)pyridine (56.4 mg, 213 μmol), and Cs_2CO_3 (315 mg, 969 μmol), **30** was isolated as a near-colourless glass (77.7 mg, 59%) after column chromatography (20% EtOAc in petrol), R_f = 0.63 (60% EtOAc in petrol), (found C, 55.15; H, 6.23; N, 6.06%. $C_{31}H_{41}O_4N_3S_5$ requires C, 54.75; H, 6.08; N, 6.18%. Found [ES^+] M^+ + H, 680.1764. $C_{31}H_{42}O_4N_3S_5$ requires *M*, 680.1773); υ_{max} (ATR): 2921 (w), 1594 (w), 1576 (w), 1331 (m), 1150 (s), 1089 (m), 867 (m) and 813 (m) cm^{-1}; δ_H ($CDCl_3$, 500 MHz) 1.05 (6H, d, *J* = 6.0 Hz, C**H**$_3$, H-6), 2.43 (6H, s, C**H**$_3$, H-14), 2.53 (2H, dd, *J* = 13.0, 9.0 Hz, C**H**$_2$, H-7), 2.57 – 2.70 (8H, m, C**H**$_2$, H-8,9), 2.86 (2H, dd, *J* = 13.0, 6.0 Hz, C**H**$_2$, H-7), 3.93 (2H, app. sext., *J* = 7.0 Hz, C**H**, H-5), 4.46 (4H, br.s., C**H**$_2$, H-4), 7.29 (4H, d, *J* = 8.0 Hz, C**H**, H-12), 7.49 (2H, d, *J* = 8.0 Hz, C**H**, H-2), 7.69 (1H, t, *J* = 8.0 Hz, C**H**, H-1) and 7.72 (4H, d, *J* = 8.0 Hz, C**H**, H-11); δ_C ($CDCl_3$, 125 MHz) 18.28 (**C**H_3, C-6), 21.49 (**C**H_3, C-14), 32.03 (**C**H_2, C-9), 33.28 (**C**H_2, C-8), 37.67 (**C**H_2, C-7), 49.45 (**C**H_2, C-4), 54.85 (**C**H, C-5), 121.89 (**C**H, C-2), 127.12 (**C**H, C-11), 129.64 (**C**H, C-12), 137.32 (**C**H, C-1), 137.70 (**C**, C-10), 143.31 (**C**, C-13) and 157.43 (**C**, C-3); *m/z* (ES^+) 680.4 (M^+ + H), 701.9 (M^+ + Na).

(4S,14S)-4,14-Dimethyl-3,15-bis-(toluene-4-sulfonyl)-9-oxa-6,12-dithia-3,15,21-triaza-bicyclo[15.3.1]henicosa-1(20),17(21),18-triene (31)

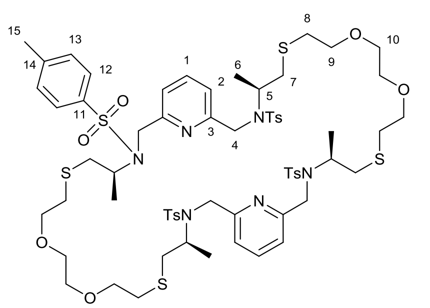


Using the general method described above, starting from ditosamide **9** (107 mg, 190 μmol), 2,6-bis(bromomethyl)pyridine (51.3 mg, 194 μmol), and Cs_2CO_3 (3078 mg, 942 μmol) **31** was isolated as a pale yellow oil (121 mg, 96%) after purification by column chromatography (40% EtOAc in petrol), R_f = 0.54 (60% EtOAc in petrol), $[\alpha]_D^{29}$ = + 75 (c = 1.15, $CHCl_3$), (found C, 56.32; H, 6.53; N, 6.05%. $C_{31}H_{41}O_4N_3S_5$ requires C, 56.08; H, 6.22; N, 6.33%. Found [ES^+] M^+ + H, 664.1998. $C_{31}H_{42}N_3O_5S_4$ requires *M*, 664.2002); υ_{max} (ATR): 3971, 3921, 2854, 1594, 1333, 1152, 1090 and 870 cm^{-1}; δ_H ($CDCl_3$, 500 MHz) 1.13 (6H, d, *J* = 7.0 Hz, C**H**$_3$, H-6), 2.36 – 2.48 (4H, m, C**H**$_2$, H-8), 2.42 (6H, s, C**H**$_3$, H-14), 2.67 (2H, dd, *J* = 13.0, 8.0 Hz, C**H**$_2$, H-7), 2.84 (2H, dd, *J* = 13.0, 6.0 Hz, C**H**$_2$, H-7), 3.45 (4H, t, *J* = 6.0 Hz, C**H**$_2$, H-9), 3.93 (2H, app. sext., *J* = 7.0 Hz, C**H**, H-5), 4.40 (2H, d, *J* = 16.0 Hz, C**H**$_2$, H-4), 4.47 (2H, d, *J* = 16.0 Hz, C**H**$_2$, H-4), 7.26 (4H, d, *J* = 7.0 Hz, C**H**, H-12), 7.52 (2H, d, *J* = 8.0 Hz, C**H**, H-2), 7.68 (1H, t, *J* = 8.0 Hz, C**H**, H-1) and 7.70 (4H, d, J = 8.0 Hz, C**H**, H-11); δ_C ($CDCl_3$, 125 MHz) 18.15 (**C**H_3, C-6), 21.49 (**C**H_3, C-14), 32.03 (**C**H_2, C-8), 38.19 (**C**H_2, C-7), 49.74 (**C**H_2, C-4), 55.04 (**C**H, C-5), 71.68 (**C**H_2, C-9), 121.75 (**C**H, C-2), 127.26 (**C**H, C-11), 129.57 (**C**H, C-12), 137.15 (**C**H, C-1), 137.82 (**C**, C-10), 143.24 (**C**, C-13) and 157.31 (**C**, C-3); *m/z* (ES^+) 664.3 (M^+ + H), 686.2 (M^+ + Na), 772.2 (M^+ + K).

(4S,17S)-4,17-Dimethyl-3,18-bis-(toluene-4-sulfonyl)-9,12-dioxa-6,15-dithia-3,18,24-triaza-bicyclo[18.3.1]tetracosa-1(23),20(24),21-triene (32)

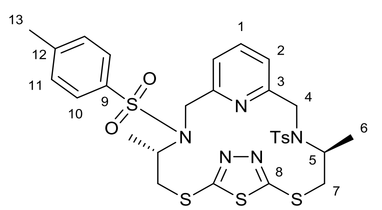


Using the general method described above, starting from ditosamide **8** (106 mg, 176 μmol), 2,6-bis(bromomethyl)pyridine (49.6 mg, 187 μmol), and Cs_2CO_3 (301 mg, 924 μmol) were isolated two products. The less polar product **32** (R_f = 0.43) was isolated as a near-colourless solid foam (55.1 mg, 44%) after purification by column chromatography (30% EtOAc in petrol), R_f = 0.43 (40% EtOAc in petrol), m.p. 45 – 47 °C, (found [ES^+] M^+ + H, 708.2279. $C_{33}H_{46}O_6N_3S_4$ requires *M*, 708.2264); υ_{max} (ATR): 2922 (w), 2872 (w), 1596 (w), 1455 (m), 1334 (m), 1158 (s) and 1091 (s) cm^{-1}; δ_H ($CDCl_3$, 500 MHz) 1.11 (6H, d, J = 7.0 Hz, C**H**$_3$, H-6), 2.43 (6H, s, C**H**$_3$, H-15), 3.44 – 2.54 (4H, m, C**H**$_2$, H-8), 2.60 (2H, dd, J = 13.0, 8.0 Hz, C**H**$_2$, H-7), 2.73 (2H, dd, J = 13.0, 6.0 Hz, C**H**$_2$, H-7), 3.51 (4H, s, C**H**$_2$, H-10), 3.52 – 3.59 (4H, m, C**H**$_2$, H-9), 3.96 (2H, app. sext. J = 7.0 Hz, C**H**, H-5), 4.42 (4H, s, C**H**$_2$, H-4), 7.29 (4H, d, J = 8.0 Hz, C**H**, H-13, tosyl), 7.53 (2H, d, J = 8.0 Hz, C**H**, H-2), 7.69 (1H, t, J = 8.0 Hz, C**H**, H-1), 7.73 (4H, d, J = 8.0 Hz, C**H**, H-12); δ_C ($CDCl_3$, 125 MHz) 18.47 (**C**H_3, C-6), 21.53 (**C**H_3, C-15), 31.86 (**C**H_2, C-8), 37.59 (**C**H_2, C-7), 49.52 (CH_2, **C**H_2, C-4), 54.70 (**C**H, C-5), 70.44 (**C**H_2, C-10), 71.37 (**C**H_2, C-9), 122.00 (**C**H, C-2), 127.23 (**C**H, C-12), 129.59 (**C**H, C-13), 137.39 (**C**H, C-1), 137.69 (**C**, C-11), 143.26 (**C**, C-14), 157.36 (**C**, C-3); *m/z* (ES^+) 708.0 (M^+ + H), 730.3 (M^+ + Na), 746.1 (M^+ + K).

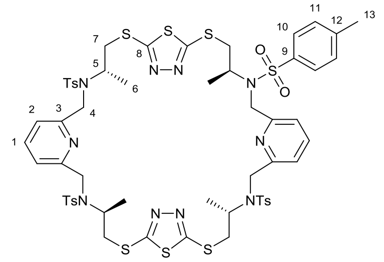


Further elution afforded a second fraction, analysed as dimer product **(33)** as a pale yellow oil (4.9 mg, 4%), Rf = 0.22 (40% EtOAc in petrol), δH (CDCl3, 400 MHz) 1.04 (12H, d, J = 7.0 Hz, CH_3, H-6), 2.34 (4H, dd, J = 13.0, 9.0 Hz, CH_2, H-7), 2.43 (12H, s, CH_3, H-15), 2.51 – 2.60 (12H, m, CH2, H-7 + CH_2, H-8), 3.48 – 3.57 (16H, CH_2, H-10 + CH_2, H-9), 3.99 – 4.10 (4H, m, CH, H-5), 4.37 (4H, d, J = 16.0 Hz, CH_2, H-4), 4.49 (4H, d, J = 16.0 Hz, CH2, H-4), 7.30 (8H, d, J = 8.0 Hz, CH, H-13, tosyl), 7.54 (4H, d, J = 8.0 Hz, CH, H-2), 7.69 (2H, t, J = 8.0 Hz, CH, H-1) and 7.72 (8H, d, J = 8.0 Hz, CH, H-12); m/z (ES+) 1415.3 (M^+ + H), 1437.2 (M^+ + Na), 1453.2 (M^+ + K).

(4S,13S)-4,13-Dimethyl-3,14-bis-(toluene-4-sulfonyl)-6,11,21-trithia-3,8,9,14,20-pentaaza-tricyclo[14.3.1.1^{7,10}]henicosa-1(19),7,9,16(20),17-pentaene (29)

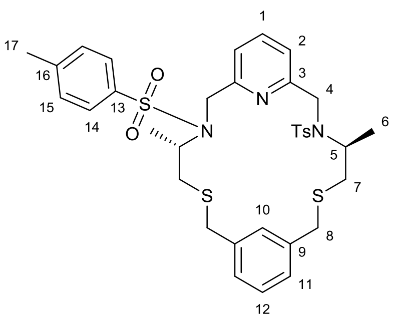


Using the general method described above, starting from ditosamide **12** (703 mg, 1.2 mmol), 2,6-bis(bromomethyl)pyridine (324 mg, 1.2 mmol), and Cs_2CO_3 (2.01 g, 6.2 mmol) were isolated two products. The less polar product **29** (R_f = 0.57) was isolated as a solid colourless foam (322 mg, 39%) after purification by column chromatography (40% EtOAc in petrol), R_f = 0.57 (50% EtOAc in petrol), 0.26 (40% EtOAc in petrol), $[\alpha]_D^{29}$ = + 78 (c = 3.06, $CHCl_3$), m.p. 87.0 – 89.0 °C, (found C, 51.98; H, 5.07; N, 9.81; S, 22.76%. $C_{29}H_{33}N_5O_4S_5$ requires C, 51.53; H, 4.92; N, 10.36; S, 23.72%. Found [ES^+] M^+ + H, 676.1215. $C_{29}H_{34}O_4N_5S_5$ requires *M*, 676.1209); υ_{max} (ATR): 2927 (w), 1595 (m), 1575 (w), 1456 (m), 1334 (s), 1151 (s). 1089 (m), 924 (w) and 873 (m) cm^{-1}; δ_H ($CDCl_3$, 400 MHz) 1.28 (6H, d, J = 7.0 Hz, C**H**$_3$, H-6), 2.46 (6H, s, C**H**$_3$, H-13), 3.36 (2H, dd, J = 14.0, 8.0 Hz, C**H**$_2$, H-7), 3.54 (2H, dd, J = 14.0, 7.0 Hz, C**H**$_2$, H-7), (2H, app. sext. J = 7.0 Hz, C**H**, H-5), 4.36 (4H, s, C**H**$_2$, H-4), 7.33 (4H, d, J = 8.0 Hz, C**H**, H-11), 7.35 (2H, d, J = 8.0 Hz, C**H**, H-2), 7.59 (1H, t, J = 8.0 Hz, C**H**, H-1) and 7.77 (4H, d, J = 8.0 Hz, C**H**, H-10); δ_C ($CDCl_3$, 125 MHz) 16.86, 16.98 (**C**H_3, C-6), 21.47, 21.57 (**C**H_3, C-13), 40.40 (**C**H_2, C-7), 53.09 (**C**H_2, C-4), 54.82, 54.98 (**C**H, C-5), 121.68 (**C**H, C-2), 127.22, 127.33 (**C**H, C-10), 129.44, 129.82 (**C**H, C-11), 137.47 (**C**H, C-1), 138.02 (**C**, C-9), 143.73 (**C**, C-12), 156.26 (**C**, C-3) and 165.15 (**C**, C-8); *m/z* (ES^+) 698.5 (M^+ + Na), 714.4 (M^+ + K).



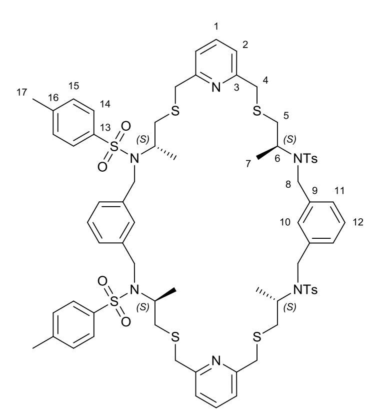
Further elution afforded a second fraction, the dimer product **(34)** as a pale yellow solid foam (28.2 mg, 3%), R_f = 0.18 (40% EtOAc in petrol), m.p. 118 – 122 °C (decomp.), δ_H ($CDCl_3$, 400 MHz) 1.19 (12H, d, J = 7.0 Hz, CH_3, H-6), 2.38 (12H, s, CH_3, H-13), 3.30 (4H, dd, J = 14.0, 10.0 Hz, CH_2, H-7), 3.53 (4H, dd, J = 14.0, 5.0 Hz, CH_2, H-7), 4.17 – 4.24 (4H, m, CH, H-5), 4.27 (4H, d, J = 16.0 Hz, CH_2, H-4), 4.51 (4H, d, J = 16.0 Hz, CH_2, H-4), 7.18 (8H, d, J = 8.0 Hz, CH, H-11), 7.42 (4H, d, J = 8.0 Hz, CH, H-2), 7.58 (8H, d, J = 8.0 Hz, CH, H-10) and 7.64 (2H, t, J = 8.0 Hz, CH, H-1); δ_C ($CDCl_3$, MHz) 18.70 (CH_3, C-6), 21.53 (CH_3, C-13), 38.11 (CH_2, C-7), 50.27 (CH_2, C-4), 54.86 (CH, C-5), 122.61 (CH, C-2), 127.30 (CH, C-10), 129.46 (CH, C-11), 137.47 (CH, C-1 + C, C-9), 143.41 (C, C-12), 156.74 (C, C-3) and 164.56 (C, C-8); *m/z* (ES^+) 1368.9 (M^+ + NH_4), 1373.8 (M^+ + Na).

(4S,16S)-4,16-Dimethyl-3,17-bis-(toluene-4-sulfonyl)-6,14-dithia-3,17,23-triaza-tricyclo[17.3.1.1^{8,12}]tetracosa-1(22),8,10,12(24),19(23),20-hexaene (26)



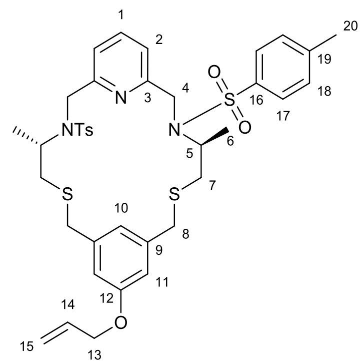
Using the general method described above, starting from ditosamide **15** (856 mg, 1.4 mmol), 2,6-bis(bromomethyl)pyridine (379 mg, 1.4 mmol), and Cs_2CO_3 (2.41 g, 7.4 mmol) were isolated two products. The less polar compound **26** (Rf = 0.54) was the *title compound* isolated as a colourless foam (377 mg, 41%) after purification by column chromatography (40% EtOAc in petrol), R_f = 0.54 (60% EtOAc in petrol). $[\alpha]_D^{29}$ = - 9 (c = 1.78, $CHCl_3$), m.p. 141 – 143 °C, (found C, 57.69; H, 5.69; N, 5.54; S, 17.25%. $C_{35}H_{41}N_3O_4S_4.½CH_2Cl_2$ requires C, 57.74; H, 5.73; Cl, 4.80; N, 5.69; S, 17.37%. Found [ES^+] M^+ + Na, 718.1868. $C_{35}H_{41}O_4N_3NaS_4$ requires *M*, 718.1872); $\boldsymbol{\upsilon_{max}}$ (ATR): 2975 (w), 1594 (w), 1465 (w), 1333 (m), 1148 (s), 1088 (m), 1015 (w) and 815 (m) cm^{-1}; δ_H ($CDCl_3$, 500 MHz) 1.00 (6H, d, J = 7.0 Hz, C**H**$_3$, H-6), 2.21 (2H, dd, J = 13.0, 9.0 Hz, C**H**$_2$, H-7), 2.42 (6H, s, C**H**$_3$, H-17), 2.51 (2H, dd, J = 10.0, 6.0 Hz, C**H**$_2$, H-7), 3.54 (2H, d, J = 14.0 Hz, C**H**$_2$, H-8), 3.58 (2H, d, J = 14.0 Hz, C**H**$_2$, H-8), 3.96 (2H, m, C**H**, H-5), 4.21 (2H, d, J = 16.0 Hz, C**H**$_2$, H-4), 4.35 (2H, d, J = 16.0 Hz, C**H**$_2$, H-4), 7.06 (2H, d, J = 8.0 Hz, C**H**, H-11), 7.17 (1H, s, C**H**, H-10), 7.18 (1H, t, J = 7.0 Hz, C**H**, H-12), 7.26 (4H, d, J = 8.0 Hz, C**H**, H-15), 7.34 (2H, d, J = 8.0 Hz, C**H**, H-2), 7.55 (1H, t, J = 8.0 Hz, C**H**, H-1) and 7.67 (4H, d, J = 8.0 Hz, C**H**, H-14); δ_C ($CDCl_3$, 125 MHz) 18.32 (**C**H$_3$, C-6), 21.51 (**C**H$_3$, C-17), 35.62 (**C**H$_2$, C-7), 36.25 (**C**H$_2$, C-8), 48.93 (**C**H$_2$, C-4), 54.53 (**C**H, C-5), 121.64 (**C**H, C-2), 127.15 (**C**H, C-14), 127.65 (**C**H, C-11), 128.73 (**C**H, C-12), 129.17 (**C**H, C-10), 129.55 (**C**H, C-15), 137.05 (**C**H, C-1), 137.96 (**C**, C-13), 138.43 (**C**, C-9), 143.12 (**C**, C-16) and 157.09 (**C**, C-3); *m/z* (ES^+) 718.5 (M^+ + Na), 734.7 (M^+ + K).

Further elution afforded a second fraction, dimer-type product **35**, isolated as a near-colourless foam (154 mg, 8%), R_f = 0.32 (60% EtOAc in petrol), $[\alpha]_D^{32}$ = -18 (c = 2.61, $CHCl_3$), m.p. 162 – 167 °C, υ_{max} (ATR): 3025 (w), 2976 (w), 2921 (w), 1593 (m, 1493 (w), 1454 (m), 1332 (m), 1215 (w), 1150 (s) and 1089 (s) cm^{-1}; δ_H ($CDCl_3$, 500 MHz) 1.00 (12H, d, J = 7.0 Hz, CH_3, H-6), 2.21 (4H, dd, J = 13.0, 9.0 Hz, CH_2, H-7), 2.42 (12H, s, CH_3, H-17), 2.52 (4H, dd, J = 13.0, 6.0 Hz, CH_2, H-7), 3.54 (4H, d, J = 14.0 Hz, CH_2, H-8), 3.58 (4H, d, J = 14.0 Hz, CH_2, H-8), 3.96 (4H, app. sext, J = 7.0 Hz, CH, H-5), 4.22 (4H, d, J = 16.0 Hz, CH_2, H-4), 4.35 (4H, d, J = 16.0 Hz, CH_2, H-4), 7.07 (2H, d, J = 7.5 Hz, CH, H-11), 7.17 (1H, br. s. , CH, H-10), 7.18 (2H, t, J = 7.5 Hz, CH, H-12), 7.26 (8H, d, J = 8.5 Hz, CH, H-15), 7.34 (4H, d, J = 7.5 Hz, CH, H-2), 7.55 (2H, t, J = 7.5 Hz, CH, H-1) and 7.67 (8H, d, J = 8.5 Hz, CH, H-14); δ_C ($CDCl_3$, 125 MHz) 18.32 (CH_3, C-6), 21.51 (CH_3, C-17), 35.62 (CH_2, C-7), 36.26 (CH_2, C-8), 48.93 (CH_2, C-4), 54.53 (CH, C-5), 121.64 (CH, C-2), 127.15 (CH, C-14), 127.65 (CH, C-11), 128.73



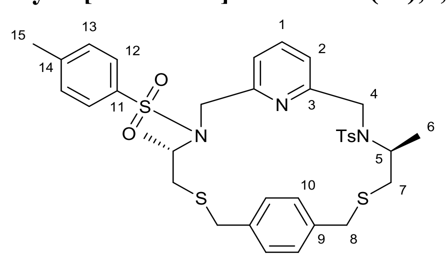
(CH, C-12), 129.17 (CH, C-10), 129.55 (CH, C-15), 137.04 (CH, C-1), 137.97 (C, C-13), 138.43 (C, C-9), 143.11 (C, C-16) and 157.09 (C, C-3); *m/z* (ES^+) 1391 (M^+ + H), 1413 (M^+ + Na); *m/z* (ES^-) 1425 (M^- + Cl).

(4S,16S)-10-allyloxy-4,16-Dimethyl-3,17-bis-(toluene-4-sulfonyl)-6,14-dithia-3,17,23-triaza-tricyclo[17.3.1.1^{8,12}]tetracosa-1(22),8,10,12(24),19(23),20-hexaene (28)

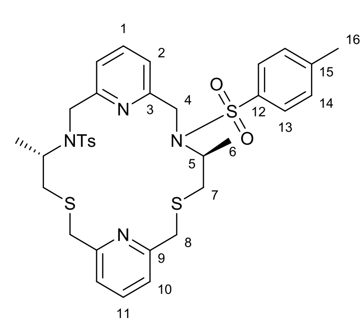


Using the general method described above, starting from ditosamide **24** (2.19 g, 3.4 mmol), 2,6-bis(bromomethyl)pyridine (890 mg, 3.4 mmol), and Cs_2CO_3 (5.53 g, 17.0 mmol) **28** was isolated as a near-colourless foam (2.13 g, 84%) after purification by column chromatography (20% EtOAc in petrol), R_f = 0.56 (50% EtOAc in petrol), $[\alpha]_D^{32}$ = -5.3 (c = 2.17, $CHCl_3$), m.p. 139 – 143 °C, (found [ES^+] M^+ + H, 752.2307. $C_{38}H_{46}O_5N_3S_4$ requires *M*, 752.2315); υ_{max} (ATR): 2977 (w), 2921 (w), 1591 (m), 1453 (m), 1331 (m), 1145 (s), 1089 (m), 864 (m) cm^{-1}; δ_H ($CDCl_3$, 400 MHz) 1.01 (6H, d, *J* = 6.5 Hz, C**H$_3$**, H-6), 2.21 (2H, dd, *J* = 12.5, 9.0 Hz, C**H$_2$**, H-7), 2.42 (6H, s, C**H$_3$**, H-20), 2.53 (2H, dd, *J* = 12.5, 6.0 Hz, C**H$_2$**, H-7), 3.50 (2H, d, *J* = 14.0 Hz,C**H$_2$**, H-8), 3.55 (2H, d, *J* = 14.0 Hz, C**H$_2$**, H-8), 3.96 (2 H, app. sext, *J* = 7.0 Hz, C**H**, H-5), 4.22 (2H, d, *J* = 16.0 Hz, C**H$_2$**, H-4), 4.38 (2H, d, *J* = 16.0 Hz, C**H$_2$**, H-4), 4.49 (2H, d, *J* = 4.5 Hz, C**H$_2$**, H-13), 5.29 (1H, d, *J* = 10.0 Hz, C**H$_2$**, H-15), 5.42 (1H, d, *J* = 17.0 Hz, C**H$_2$**, H-15), 6.05 (1H, ddt, *J* = 17.0, 10.0, 4.5 Hz, C**H**, H-14), 6.67 (2H, s, C**H**, H-11), 6.76 (1H, s, C**H**, H-10), 7.27 (4H, d, *J* = 8.0 Hz, C**H**, H-18), 7.34 (2H, d, *J* = 7.5 Hz, C**H**, H-2), 7.55 (1H, t, *J* = 7.5 Hz, C**H**, H-1) and 7.68 (4H, d, *J* = 8.0 Hz, C**H**, H-17); δ_C ($CDCl_3$, 125 MHz) 18.26 (**C**H$_3$, C-6), 21.44, 21.47 (**C**H$_3$, C-20), 35.72 (**C**H$_2$, C-7), 36.37 (**C**H$_2$, C-8), 49.01 (**C**H$_2$, C-4), 54.59 (**C**H, C-5), 68.63 (**C**H$_2$, C-13), 113.93 (**C**H, C-11), 117.68 (**C**H$_2$, C-15), 121.57 (**C**H, C-10), 121.79 (**C**H, C-2), 127.07 (**C**H, C-17), 129.51 (**C**H, C-18), 132.97 (**C**H, C-14), 136.95 (**C**H, C-1), 137.93 (**C**, C-16), 139.84 (**C**, C-9), 143.09 (**C**, C-19), 157.02 (**C**, C-3) and 158.73 (**C**, C-12); *m/z* (ES^+) 752 (M^+ + H), 774 (M^+ + Na), 790 (M^+ + K).

(5S,15S)-5,15-Dimethyl-6,14-bis-(toluene-4-sulfonyl)-3,17-dithia-6,14,24-triaza-tricyclo[17.2.2.1^{8,12}]tetracosa-1(22),8,10,12(24),19(23),20-hexaene (27)



Using the general method described above, starting from ditosamide **18** (672 mg, 1.1 mmol), 2,6-bis(bromomethyl)pyridine (366 mg, 1.4 mmol), and Cs_2CO_3 (1.51 g, 4.6 mmol) was isolated the *title compound* (269 mg, 34%) as a pale yellow oil after purification by column chromatography (30% EtOAc in petrol), R_f = 0.69 (50% EtOAc in petrol), $[\alpha]_D^{30}$ = + 6 (c = 1.46, $CHCl_3$), (found [ES^+] M^+ + H, 696.2064. $C_{35}H_{42}O_4N_3S_4$ requires *M*, 696.2053. Found [ES^+] M^+ + Na, 718.1872. $C_{35}H_{41}O_4N_3NaS_4$ requires *M*, 718.1872); υ_{max} (ATR): 2921 (w), 2951 (w), 1594 (m), 1575 (w), 1455 (m), 1330 (s), 1151 (s) and 1090 (s) cm^{-1}; δ_H ($CDCl_3$, 500 MHz) 0.80 (6H, d, *J* = 6.5 Hz, C**H$_3$**, H-6), 2.17 (2H, dd, *J* = 12.5, 7.0 Hz, C**H$_2$**, H-7), 2.45 (6H, s, C**H$_3$**, H-15), 2.52 (2H, dd, *J* = 12.5, 8.5 Hz, C**H$_2$**, H-7), 3.47 (2H, d, *J* = 14.0 Hz, C**H**$_2$, H-8), 3.55 (2H, d, *J* = 14.0 Hz, C**H**$_2$, H-8), 3.94 (2H, ddq, *J* = 8.5, 7.0, 6.5, C**H**, H-5), 3.99 (2H, d, *J* = 16.0 Hz, C**H**$_2$, H-4), 4.49 (2H, d, *J* = 16.0 Hz, C**H**$_2$, H-4), 7.11 (4H, s, C**H**, H-10), 7.31 (4H, d, *J* = 8.0 Hz, C**H**, H-13), 7.50 (2H, d, *J* = 7.5 Hz, C**H**, H-2), 7.62 (1H, t, *J* = 7.5 Hz, C**H**, H-1) and 7.73 (4H, d, *J* = 8.0 Hz, C**H**, H-12); δ_C ($CDCl_3$, 125 MHz) 20.25 (**C**H$_3$, C-6), 21.50, 21.54 (**C**H$_3$, C-15), 34.51 (**C**H$_2$, C-5), 36.09 (**C**H$_2$, C-8), 48.80 (**C**H$_2$, C-4), 53.52, 53.58 (**C**H, C-5), 122.10 (**C**H, C-2), 127.23 (**C**H, C-12), 128.96 (**C**H, C-10), 129.45 (**C**H, C-13), 136.85 (**C**, C-9), 137.11 (**C**H, C-1), 137.71 (**C**, C-11), 143.11 (**C**, C-14) and 157.42 (**C**, C-3); *m/z* (ES^+) 696.6 (M^+ + H), 718.6 (M^+ + Na), 734.6 (M^+ + K), 1414.1 ($2M^+$ + Na).

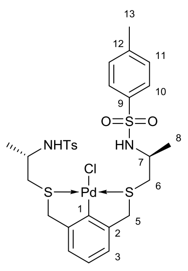


(5S,15S)-5,15-Dimethyl-6,14-bis-(toluene-4-sulfonyl)-3,17-dithia-6,14,23,24-tetraaza-tricyclo[17.3.1.1^{8,12}]tetracosa-1(22),8,10,12(24),19(23),20-hexaene (25)

Using the general method described above, starting from ditosamide **20** (478 mg, 806 μmol), 2,6-bis(bromomethyl)pyridine (213 mg, 810 μmol), and

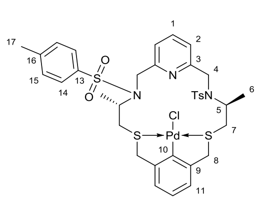
Cs_2CO_3 (1.34 g, 4.1 mmol) **25** was isolated as a viscous, colourless oil (477 mg, 85%) after purification by column chromatography (50% EtOAc in petrol), R_f = 0.72 (80% EtOAc in petrol), $[\alpha]_D^{28}$ = 62 ° (c = 2, $CHCl_3$), (found [ES$^+$] M$^+$ + Na, 719.1825. $C_{34}H_{40}O_4N_4NaS_4$ requires *M*, 719.1825), υ_{max} (ATR): 2972 (w),2924 (w), 1591 (m), 1573 (m), 1493 (w), 1453 m), 1332 (s), 1152 (s), 1089 (s), 993 (m) cm^{-1}; δ_H ($CDCl_3$, 400 MHz) 1.01 (6H, d, *J* = 6.5 Hz, C**H₃**, H-6), 2.37 (6H, s, C**H₃**, H-16), 2.58 (2H, dd, *J* = 13.0, 8.0 Hz, C**H**$_2$, H-7), 2.70 (2 H, dd, *J* = 13.0, 6.5 Hz, C**H**$_2$, H-7), 3.54 (2H, d, *J* = 13.5 Hz, C**H**$_2$, H-8), 3.64 (2H, d, *J* = 13.5 Hz, C**H**$_2$, H-8), 4.00 (2H, dquin, *J* = 8.0, 6.5 Hz, C**H**, H-5), 4.32 (2H, d, *J* = 16.5 Hz, C**H**$_2$, H-4), 4.45 (2H, d, *J* = 16.5 Hz, C**H**$_2$, H-4), 7.06 (2H, d, *J* = 8.0 Hz, C**H**, H-10), 7.21 (2H, d, *J* = 8.0 Hz, C**H**, H-2), 7.41 (4H, d, *J* = 8.0 Hz, C**H**, H-14), 7.54 (1H, t, *J* = 8.0 Hz, C**H**, H-11), 7.58 (1H, t, *J* = 8.0 Hz, C**H**, H-1) and 7.65 (4H, d, *J* = 8.0 Hz, C**H**, H-13); δ_C ($CDCl_3$, 100 MHz) 18.61 (**C**H_3, C-6), 21.46 (**C**H_3, C-16), 35.99 (**C**H_2, C-7), 37.95 (**C**H_2, C-8), 49.22 (**C**H_2, C-4), 54.53 (**C**H, C-5), 121.02 (**C**H, C-10), 121.75 (**C**H, C-2), 127.16 (**C**H, C-13), 129.50 (**C**H, C-14), 137.07 (**C**H, C-1), 137.50 (**C**H, C-11), 137.79 (**C**, C-12), 143.12 (**C**, C-15), 157.09 (**C**, C-3) and 157.88 (**C**, C-9); *m/z* (ES$^+$) 697 (M$^+$ + H), 719 (M$^+$ + Na); *m/z* (ES$^-$) 731 (M$^-$ + Cl).

Palladium complexed spacer (36)



A solution of the spacer **15** (103 mg, 173 µmol) and $PdCl_2(CH_3CN)_2$ (45.5 mg, 175 µmol) in dry CH_3CN (70 mL) was brought to reflux for 24 hours. After an additional period at room temperature for 24 hours, the solvent was removed *in vacuo* to leave the desired product 298 (121 mg, 95%) as a yellow powder; δ_H ($CDCl_3$, 500 MHz) 1.17 (6H, d, *J* = 6.0 Hz, CH_3, H-8), 2.36 (6H, s, CH_3, H-13), 3.46 (2H, br.s, CH_2, H-6 + 2H, CH, H-7), 3.73 (2H, br.s, CH_2, H-6), 4.13 (2H, br.s, CH_2, H-5), 4.31 (2H, br.s, CH_2, H-5), 6.80 – 6.94 (3H, m, CH, H-3,4), 7.24 (4H, d, *J* = 7.0 Hz, CH, H-11) and 7.77 (4H, d, *J* = 6.0 Hz, CH, H-10); δ_C ($CDCl_3$, 75 MHz) 20.59 (CH_3, C-7), 21.40 (CH_3, C-13), 46.25 (CH_2, C-6), 48.39 (CH_2, C-5), 48.47 (CH, C-7), 122.54 (CH, C-3), 124.81 (CH, C-4),126.91 (CH, C-10), 129.61 (CH, C-11), 137.92 (C, C-9), 143.23 (C, C-12), 148.13 (C, C-2) and 158.99 (C, C-1); *m/z* (ES$^+$) 695.1, 696.1, 697.1, 698.1, 699.1, 700.1, 701.0, 702.1 (M$^+$ - Cl).

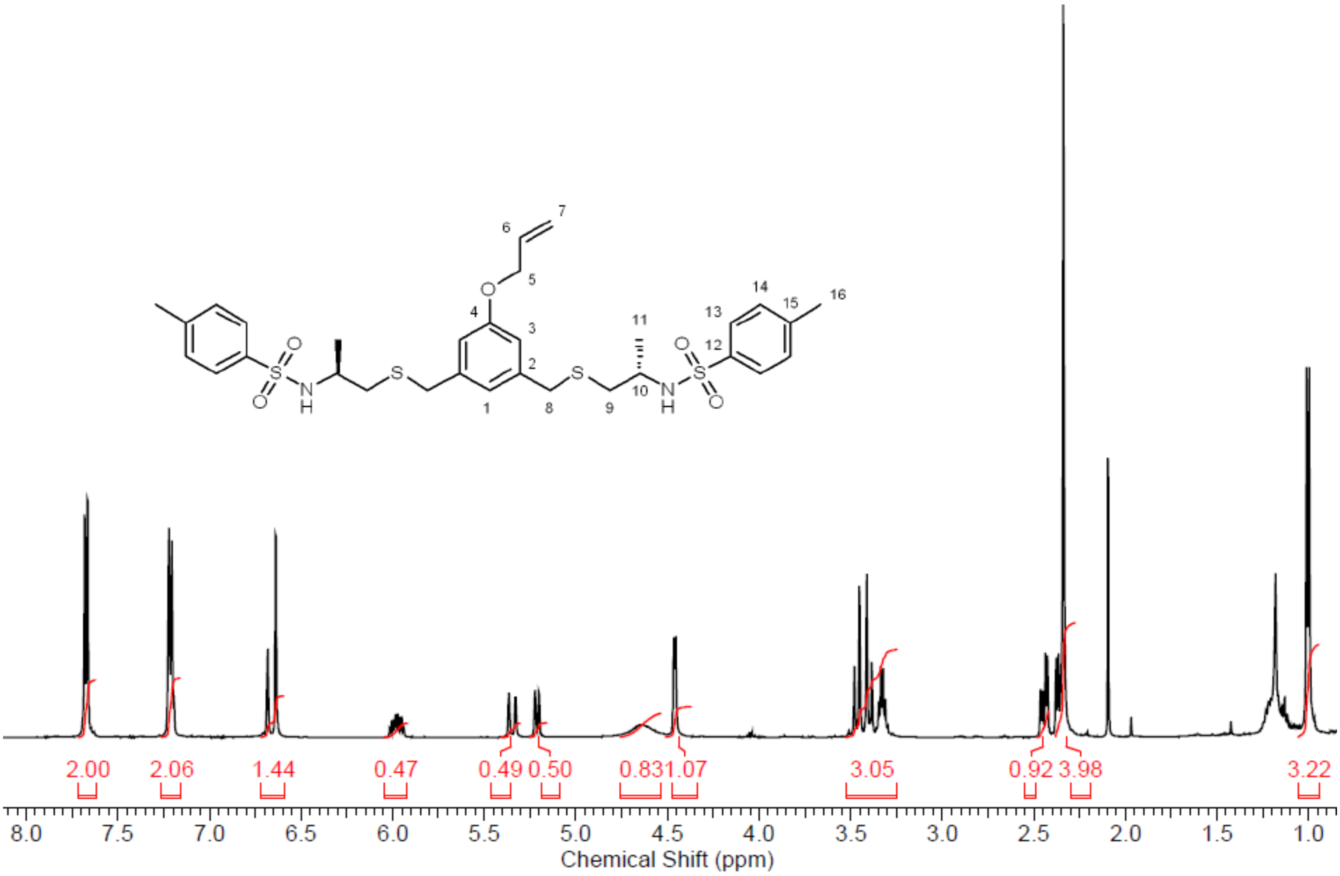
Palladium complexed macrocycle (37)

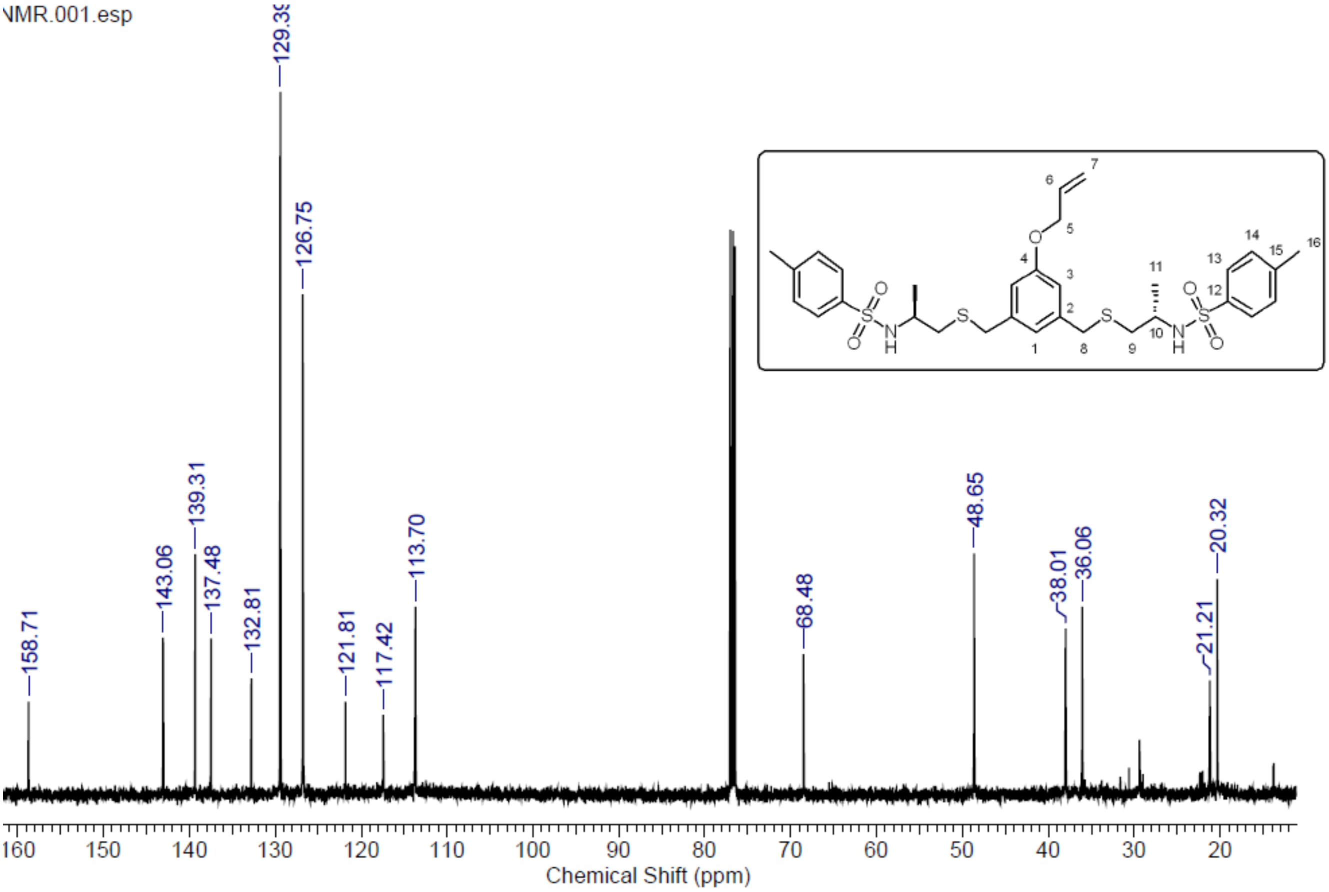


A solution of the macrocycle **26** (102 mg, 160 µmol) and $PdCl_2(CH_3CN)_2$ (41.2 mg, 159 µmol) in dry CH_3CN (40 mL) was brought to reflux for 24 hours. The solvent was removed *in vacuo* to leave the *title compound* **37** (122 mg, quant.) as a dark yellow powder; (found C, 46.75; H, 4.78; N, 4.62; Cl, 7.39; S, 13.83; Pd, 12.94%. $C_{35}H_{40}ClN_3O_4PdS_4$.HCl requires C, 48.14; H, 4.73; N, 4.81; Cl, 8.12; S, 14.69; Pd, 12.19%. Found [ES$^+$] M$^+$ - Cl, 800.0928. $C_{35}H_{40}O_4N_3PdS_4$ requires *M*, 800.0931); δ_H ($CDCl_3$, 500 MHz) Spectrum showed formation of the *title compound*, key peaks reported as follows 1.11 (6H, d, *J* = 7.0 Hz, CH_3, H-6), 1.52 (6H, d, *J* = 6.5 Hz, CH_3, H-6), 2.44 (6H, s, CH_3, H-17), 2.45 (6H, s, CH_3, H-17), 2.92 (2H, dd, *J* = 14.5, 6.5 Hz, CH_2, H-7), 3.46 (2H, dd, *J* = 14.5, 6.0 Hz, CH_2, H-7), 3.83 (2H, d, *J* = 16.0 Hz, CH_2), 4.10 (2H, d, *J* = 15.5 Hz, CH_2), 4.21 (2H, d, *J* = 16.5 Hz, CH_2), 4.31 (2H, d, *J* = 16.5 Hz, CH_2), 4.40 (2H, d, *J* = 15.5 Hz, CH_2), 4.51 (2H, d, *J* = 16.0 Hz, CH_2); *m/z* (ES$^+$) 798.4 799.4,800.2, 802.6, 803.8, 804.6, 805.4 (M$^+$ - Cl).

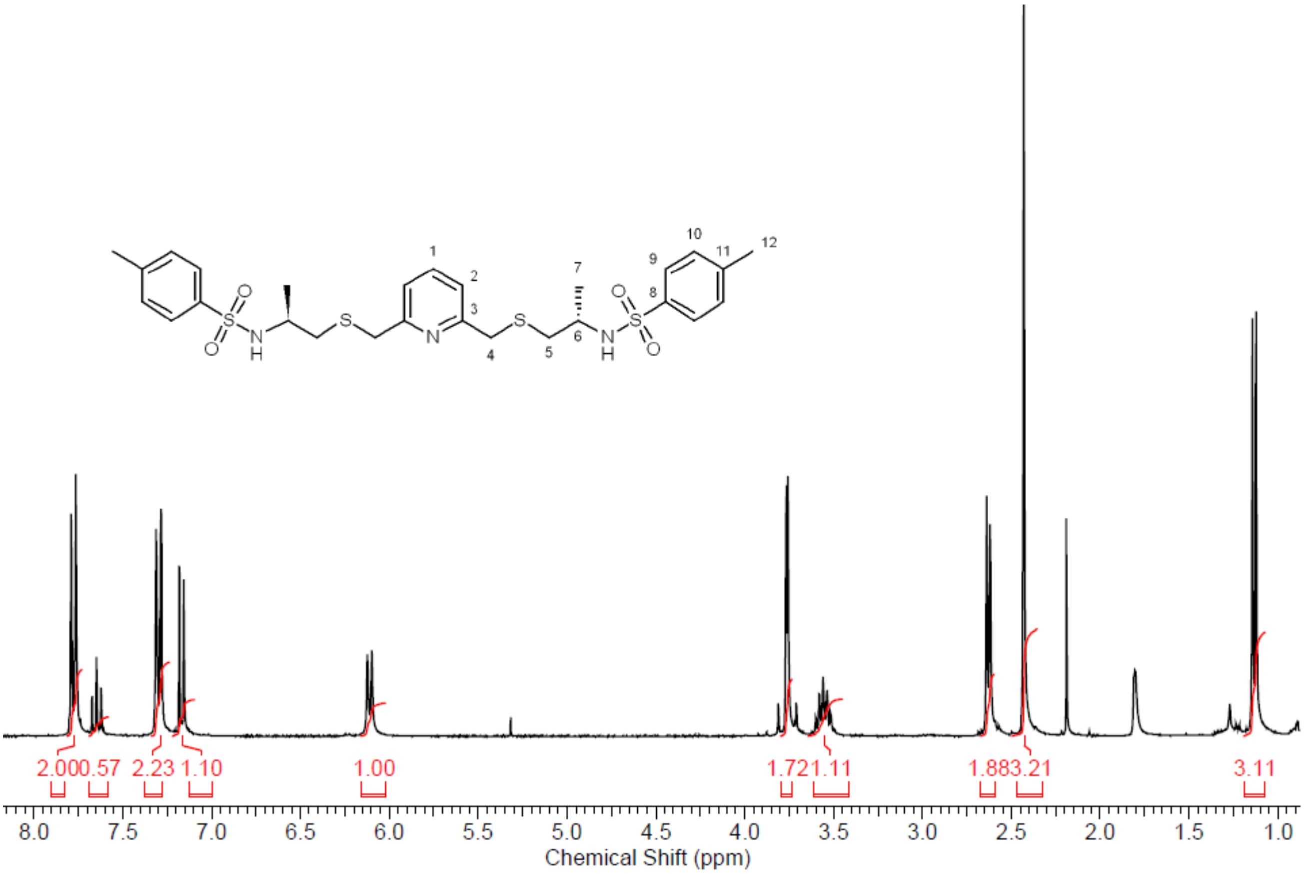
NMR Spectra

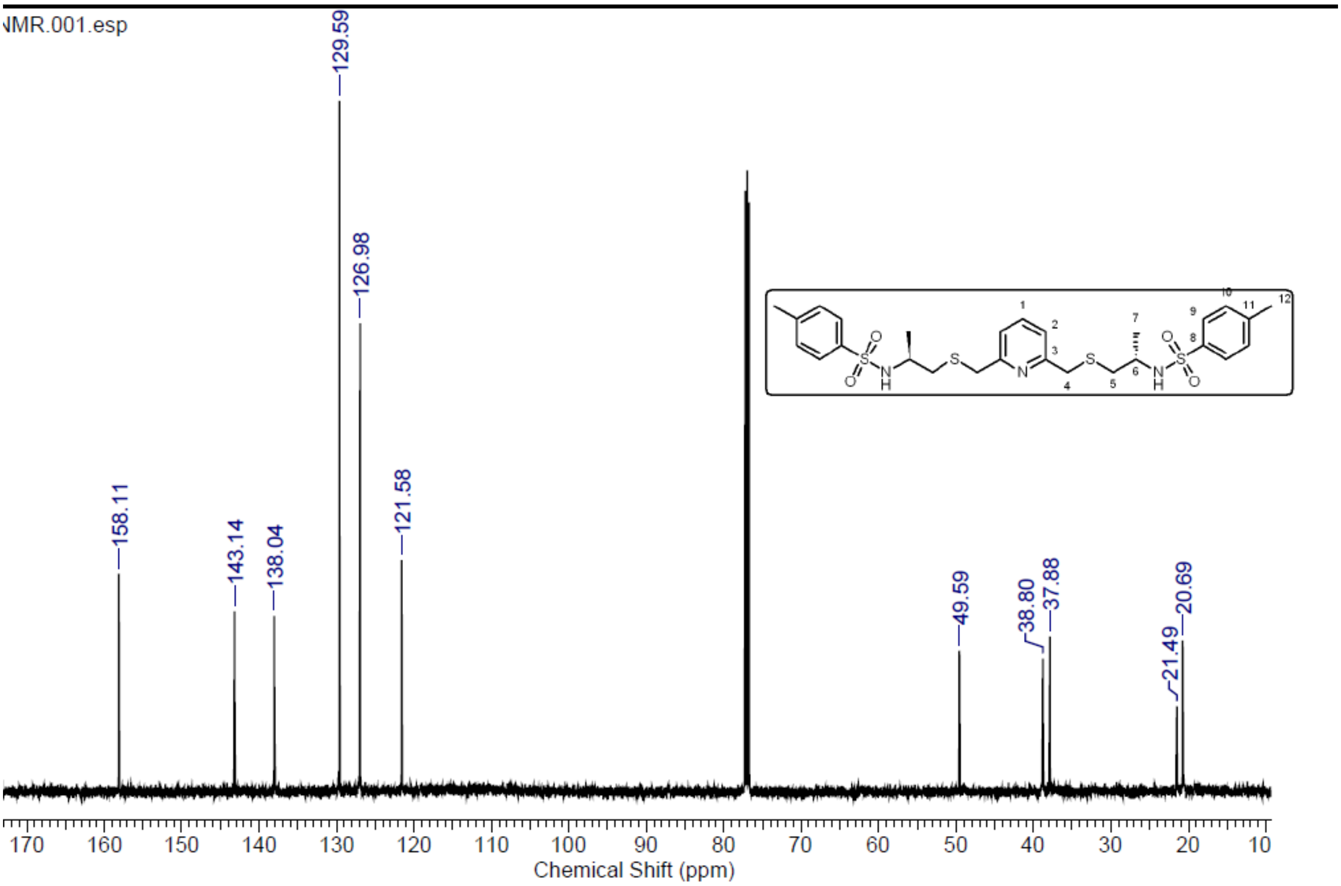
N,N'-((2S,2'S)-(((5-(allyloxy)-1,3-phenylene)bis(methylene))bis(sulfanediyl))bis(propane-2,1-diyl))bis(4-methylbenzenesulfonamide) (24)



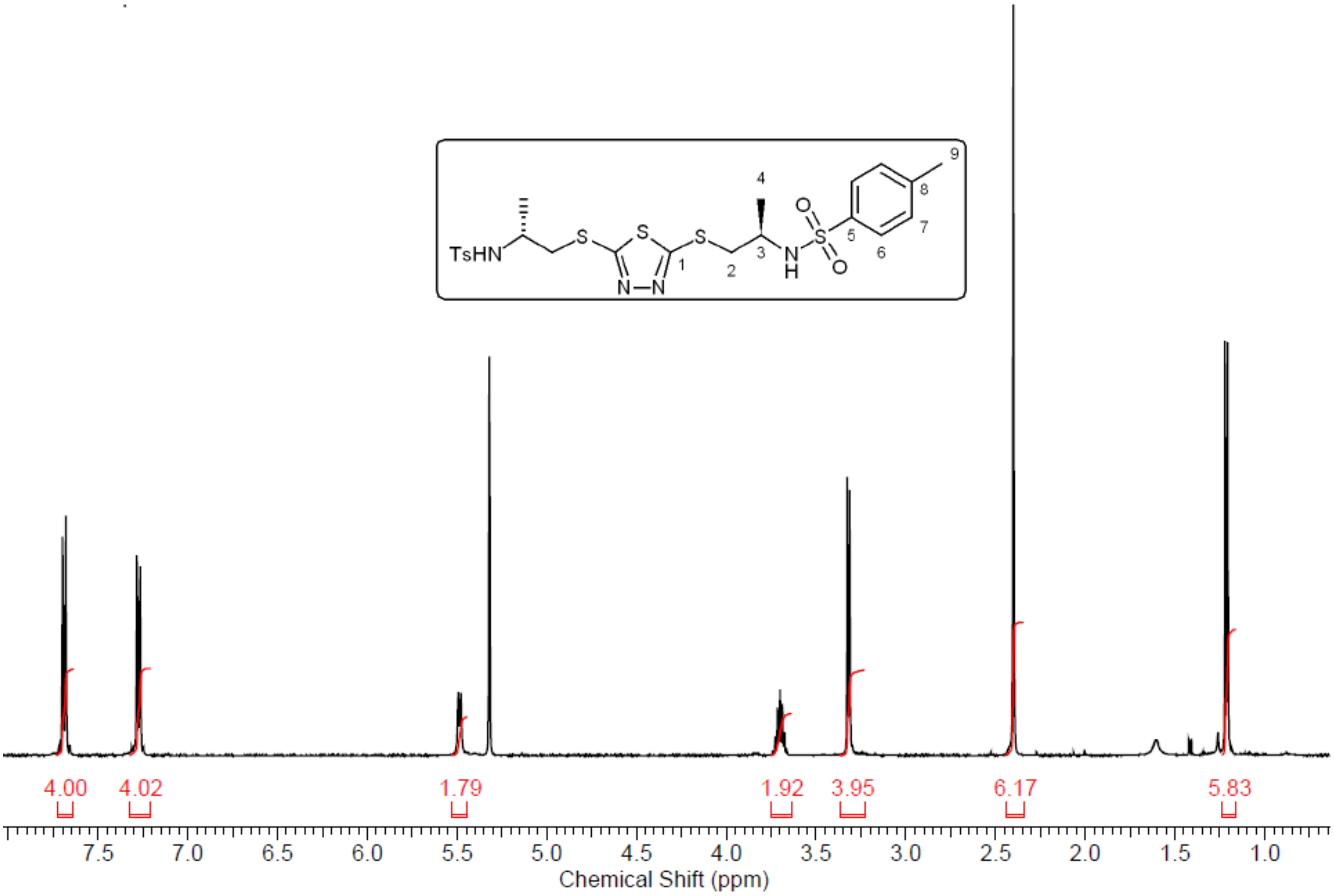


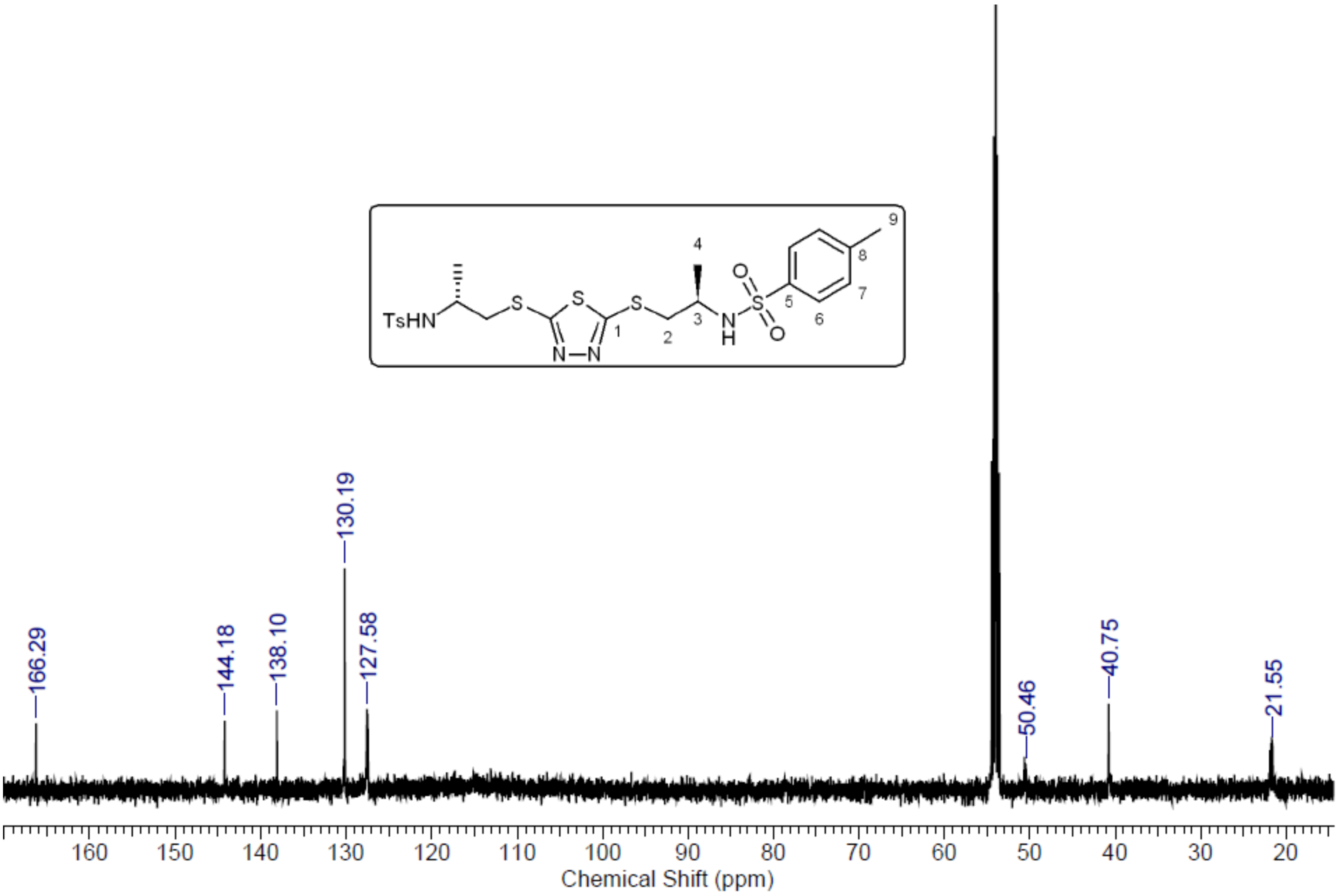
N,N'-((2S,2'S)-((pyridine-2,6-diylbis(methylene))bis(sulfanediyl))bis(propane-2,1-diyl))bis(4-methylbenzenesulfonamide) (20):



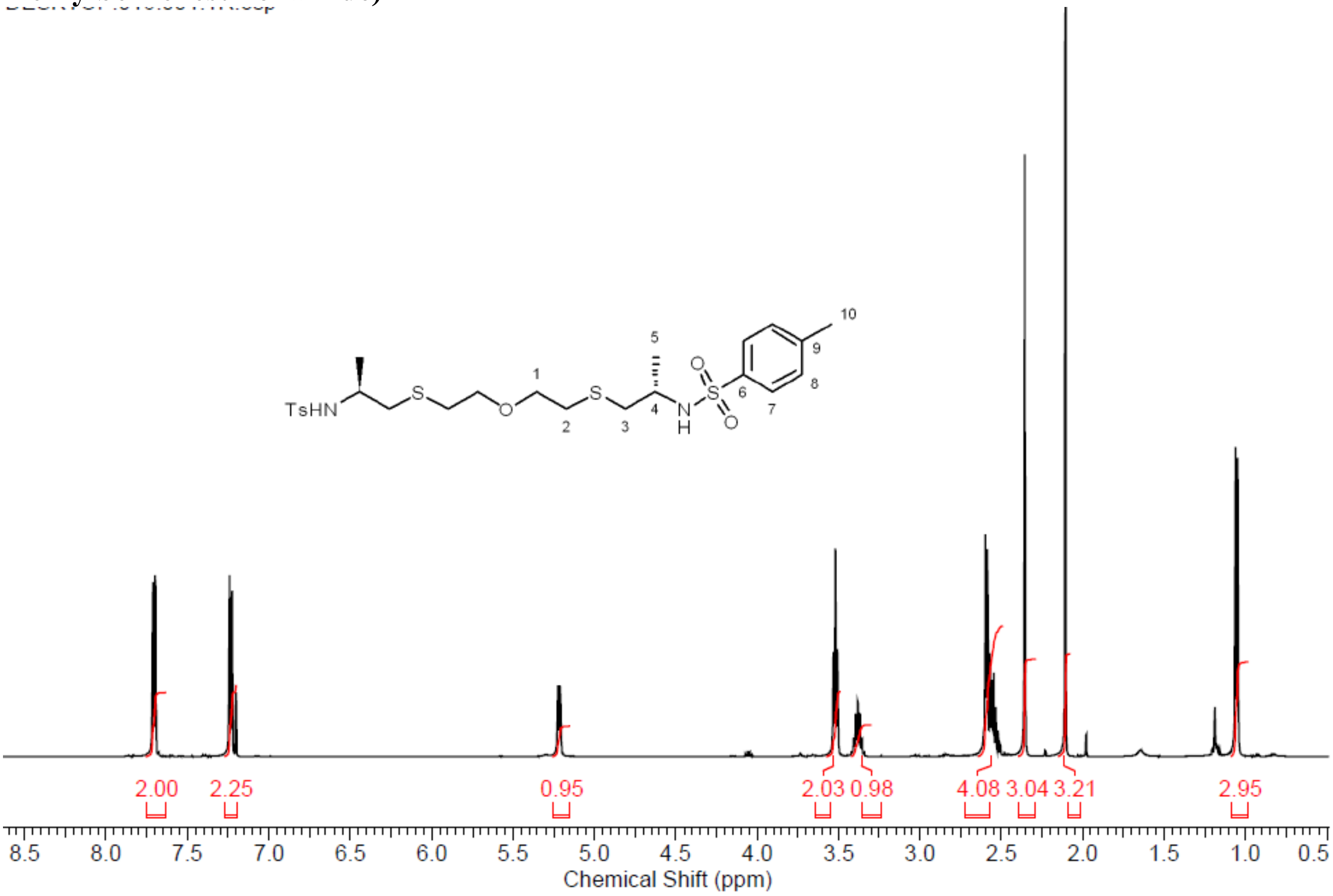


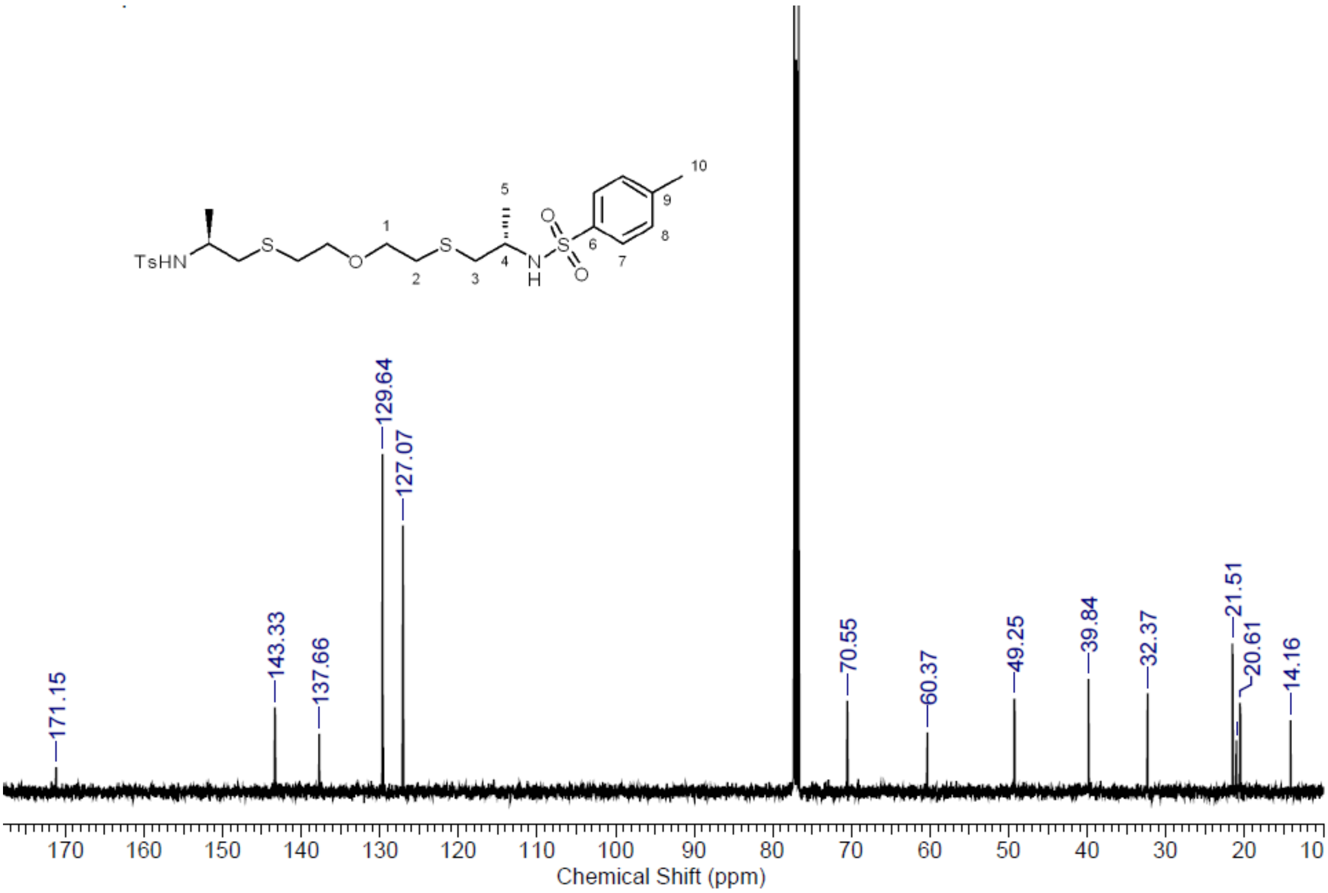
N,N'-(2R,2'R)-1,1'-(1,3,4-thiadiazole-2,5-diyl)bis(sulfanediyl)bis(propane-2,1-diyl)bis(4-methylbenzenesulfonamide) (12):



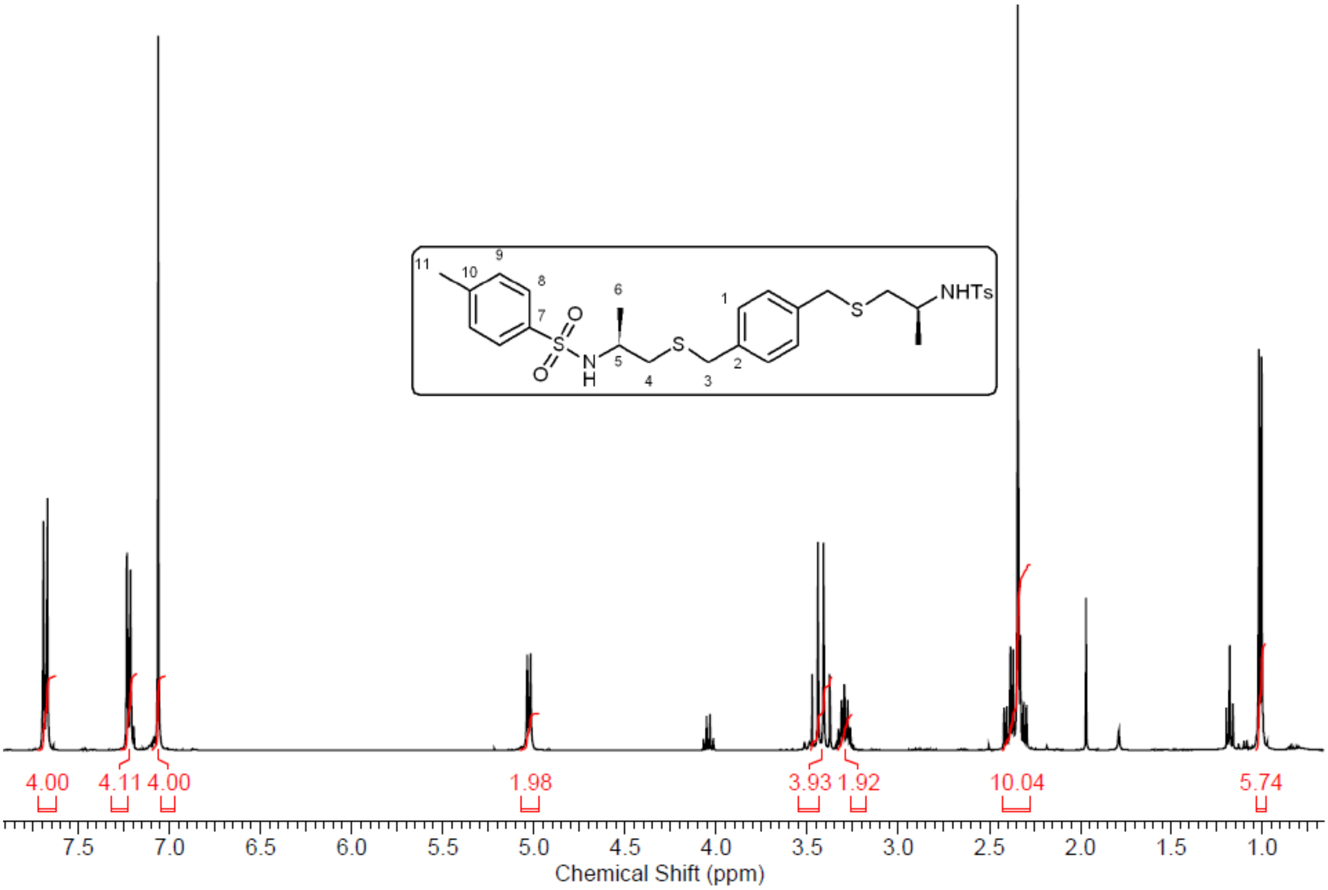


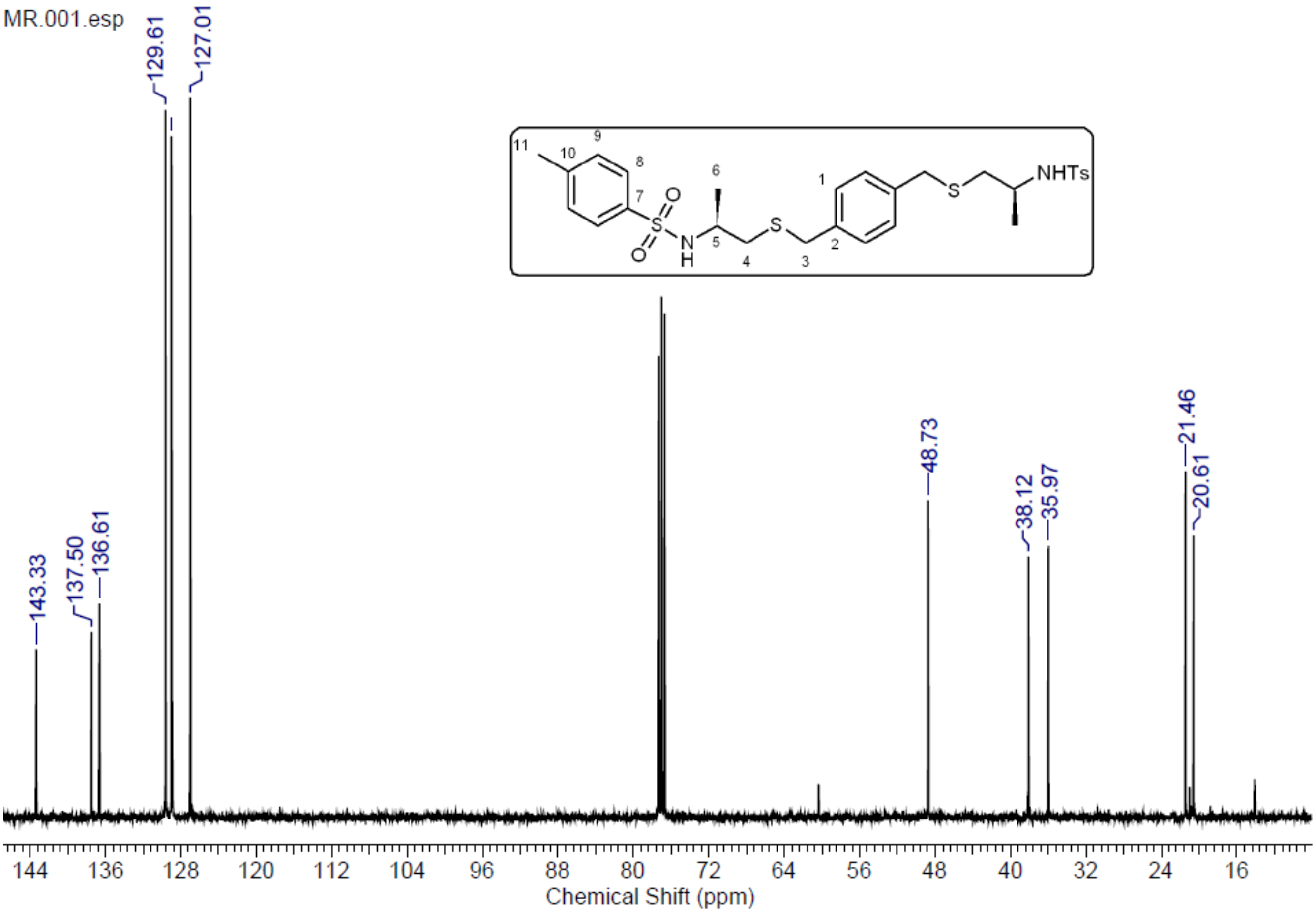
N,N'-(2S,2'S)-1,1'-(2,2'-oxybis(ethane-2,1-diyl)bis(sulfanediyl))bis(propane-2,1-diyl)bis(4-methylbenzenesulfonamide)



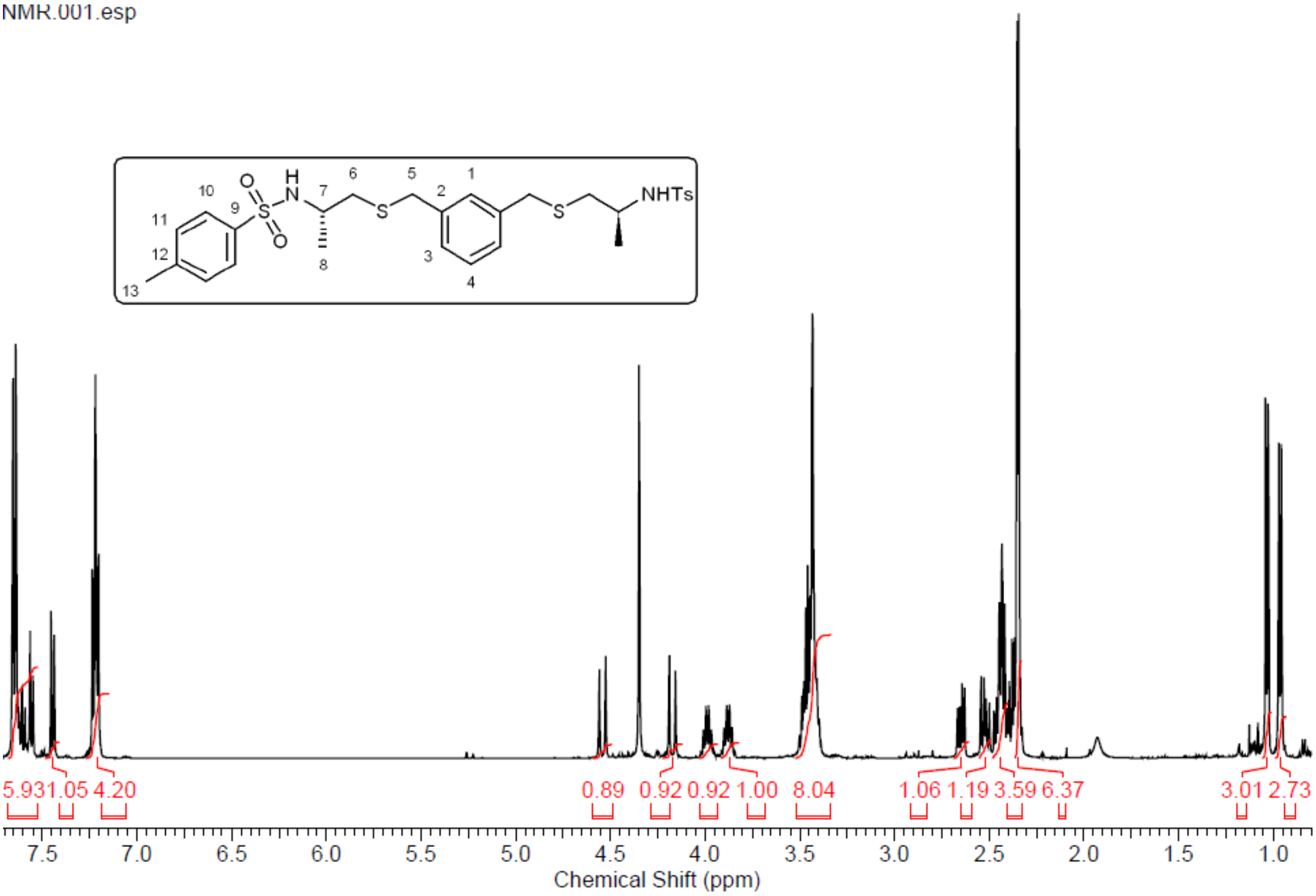


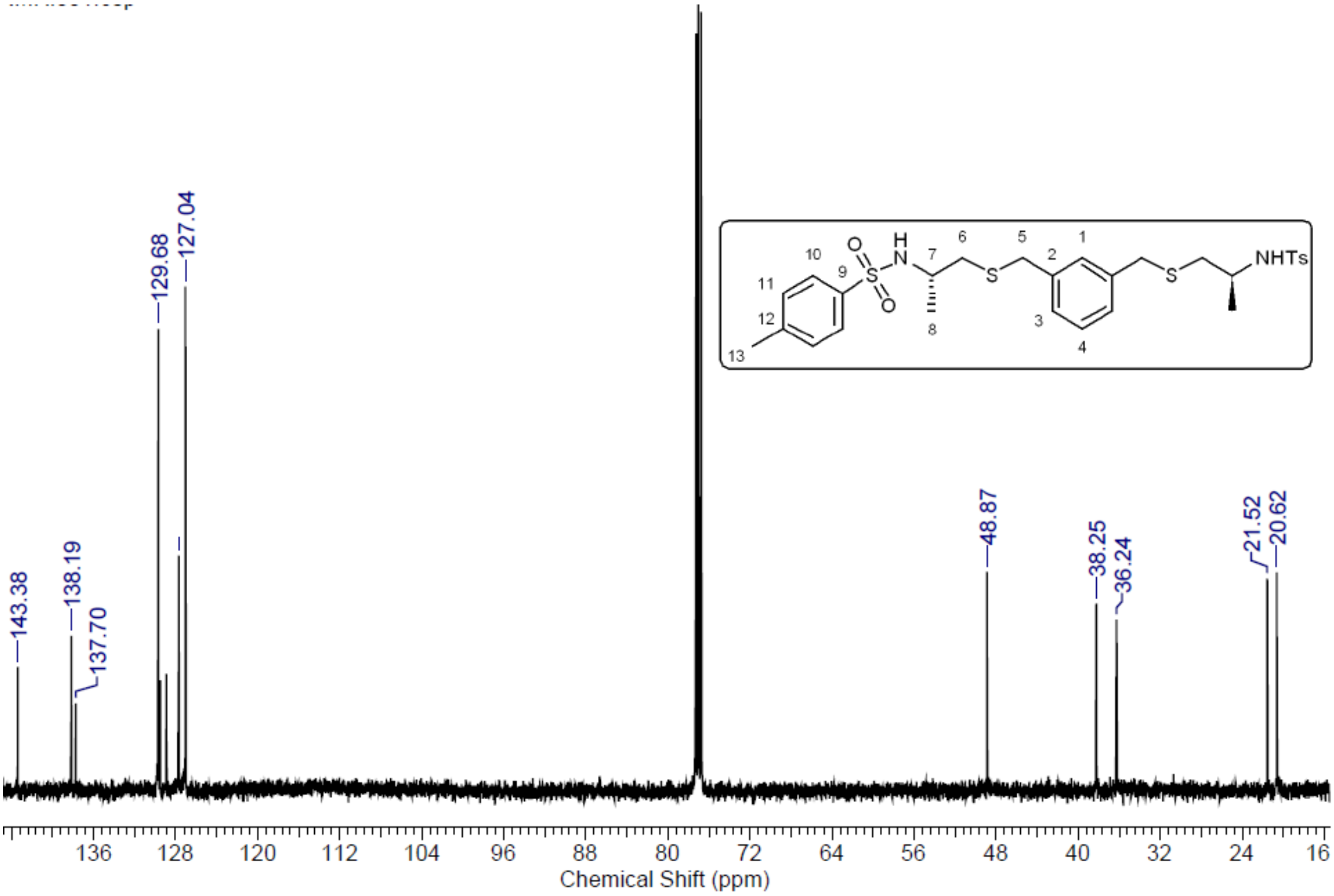
N,N'-(2S,2'S)-1,1'-(1,4-phenylenebis(methylene))bis(sulfanediyl)bis(propane-2,1-diyl)bis(4-methylbenzenesulfonamide) (18):



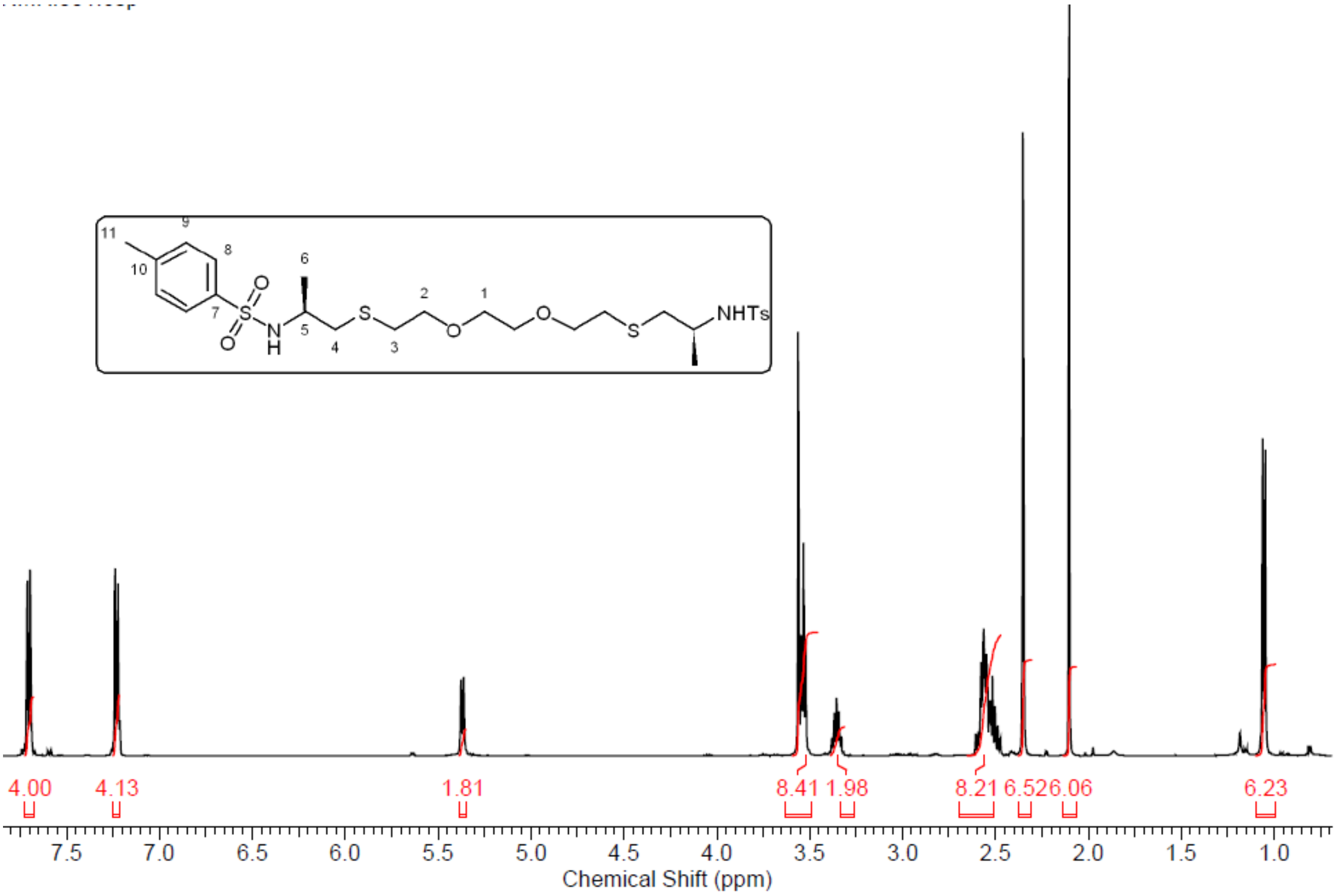


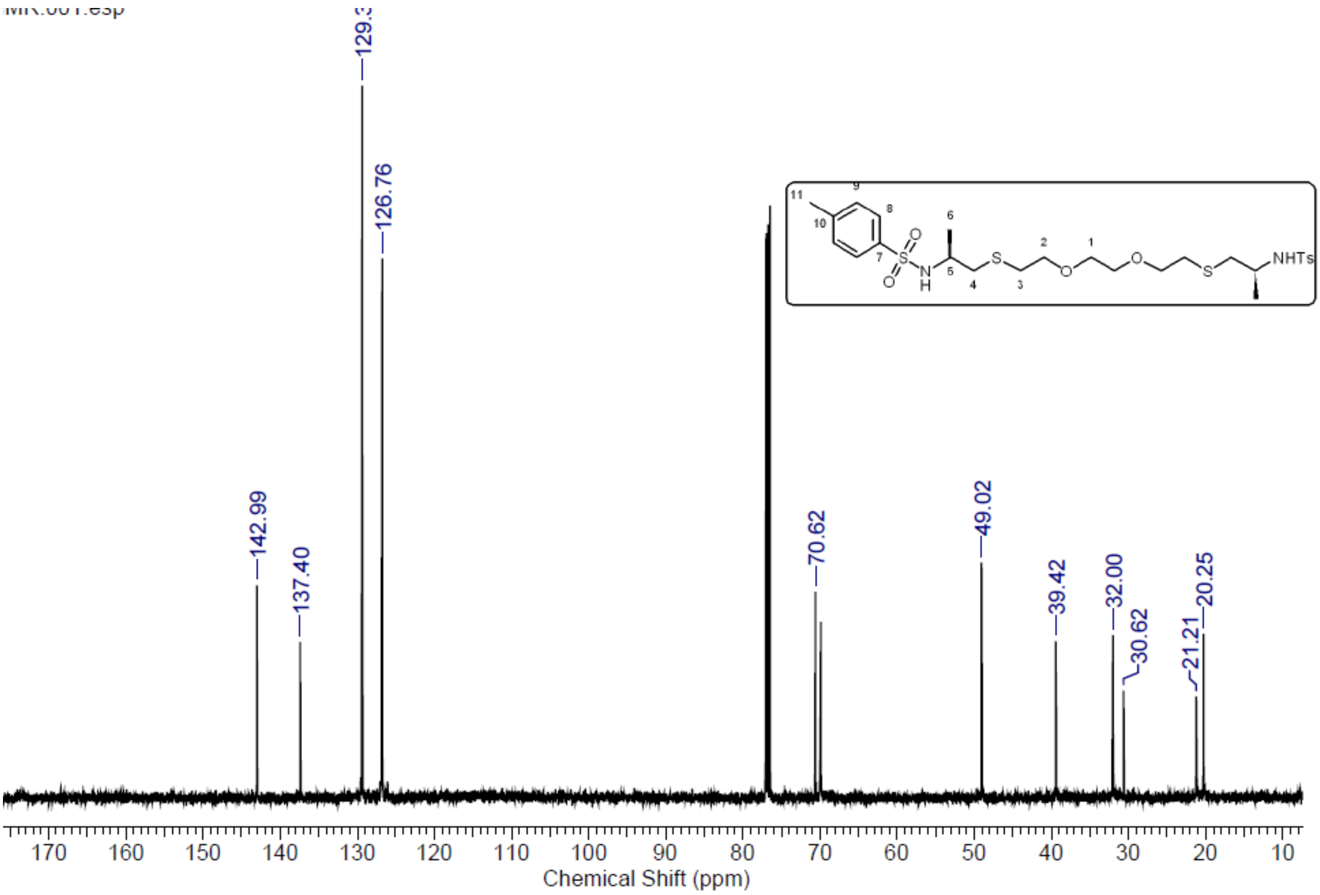
N,N'-(2S,2'S)-1,1'-(1,3-phenylenebis(methylene))bis(sulfanediyl)bis(propane-2,1-diyl)bis(4-methylbenzenesulfonamide) (15):



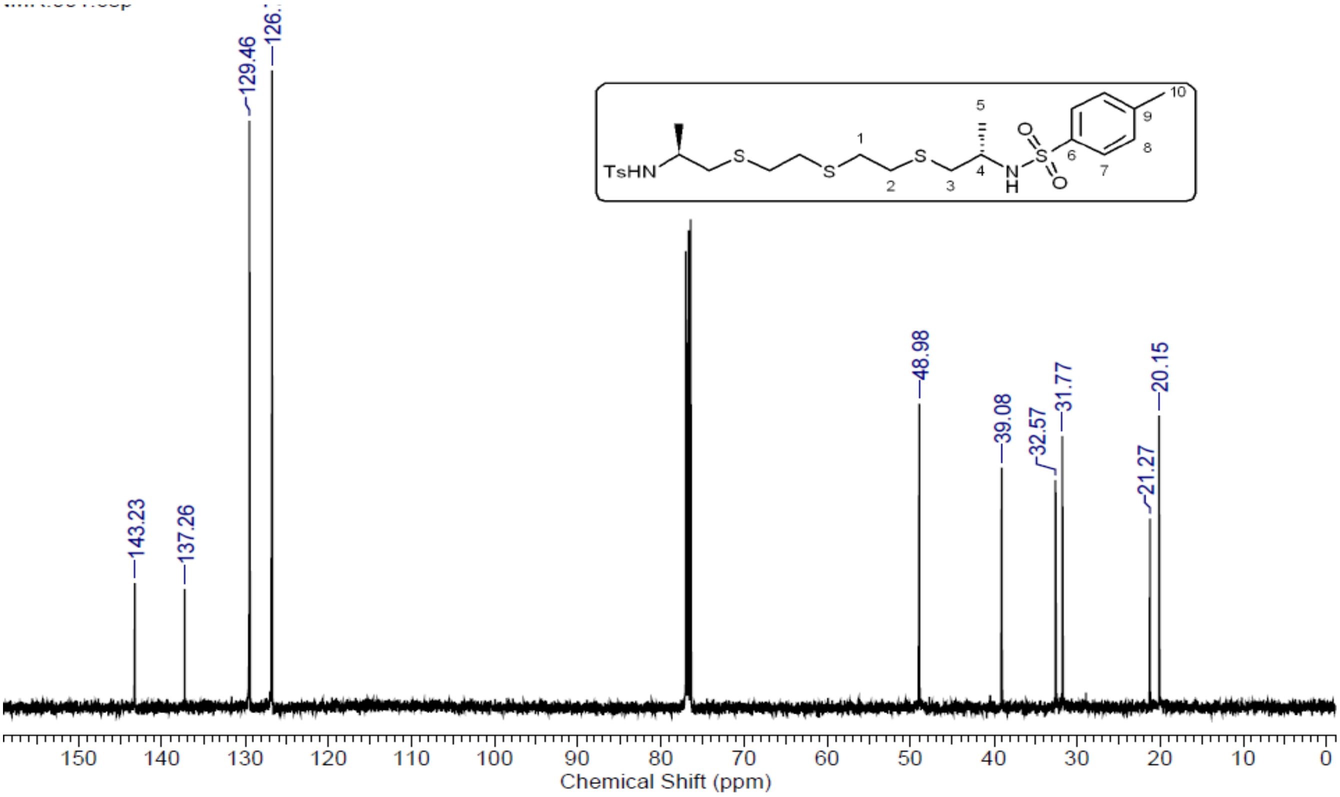


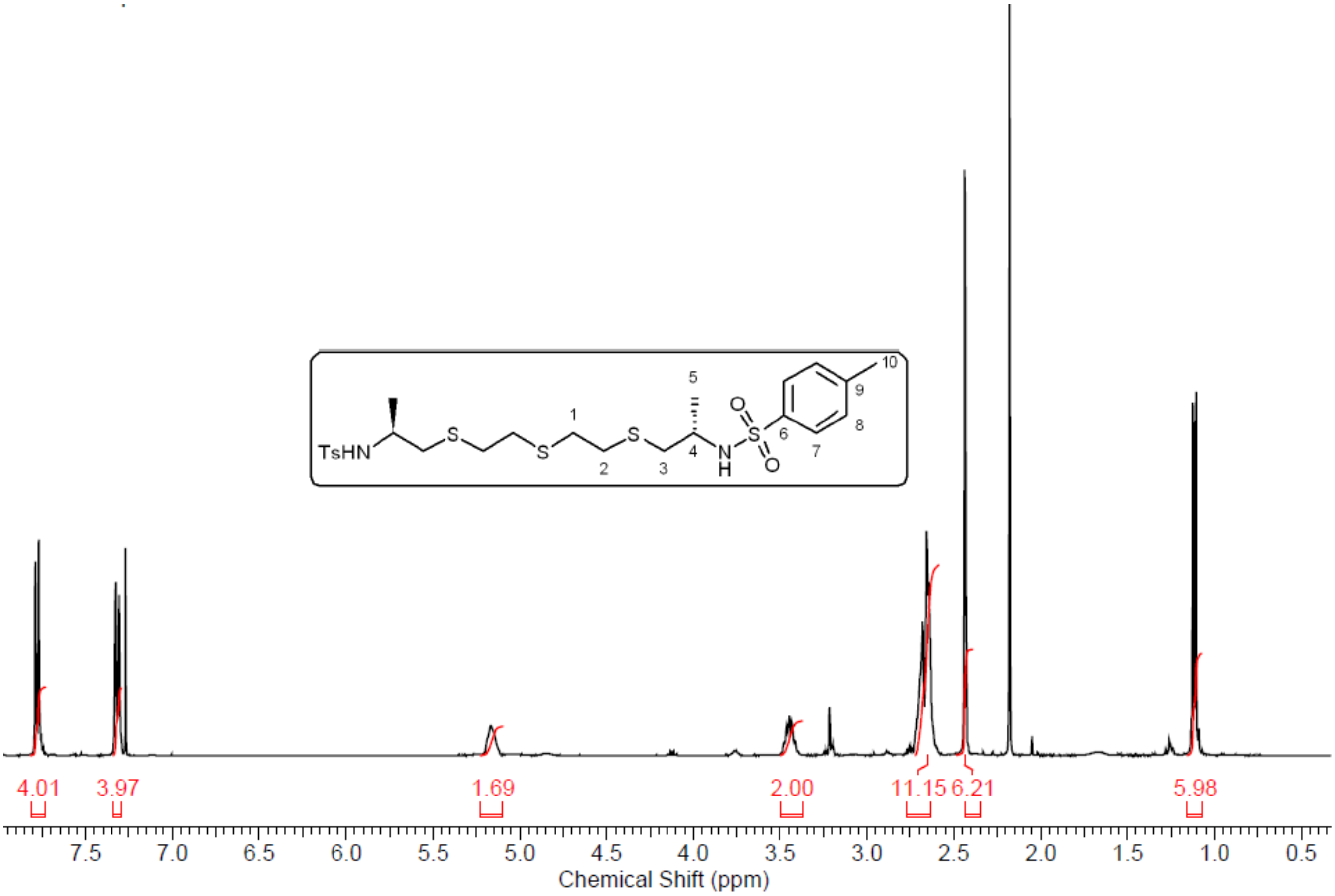
N,N'-((2S,15S)-7,10-dioxa-4,13-dithiahexadecane-2,15-diyl)bis(4-methylbenzenesulfonamide) (8):





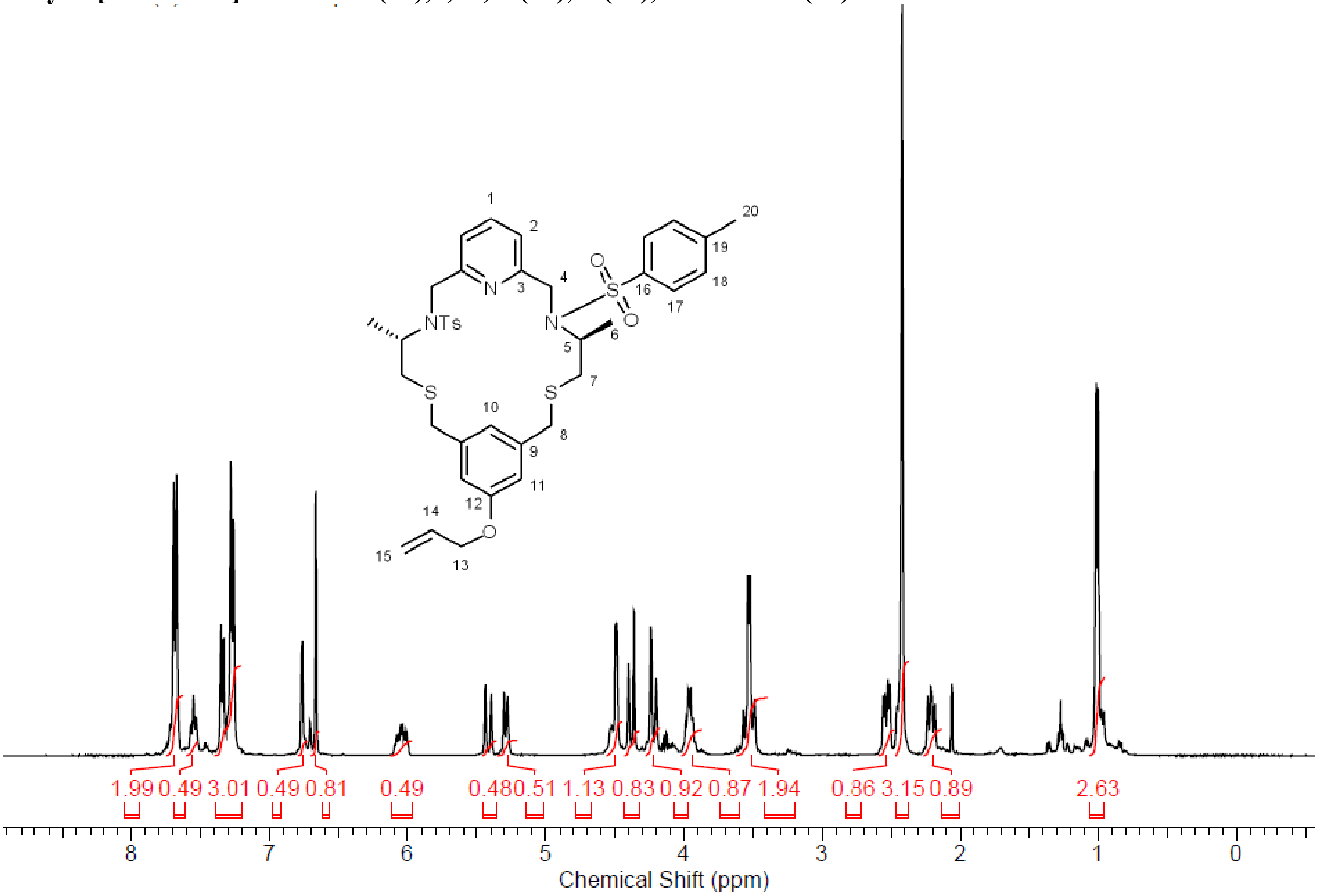
N,N'-(2S,2'S)-1,1'-(2,2'-thiobis(ethane-2,1-diyl)bis(sulfanediyl))bis(propane-2,1-diyl)bis(4-methylbenzenesulfonamide)(10):

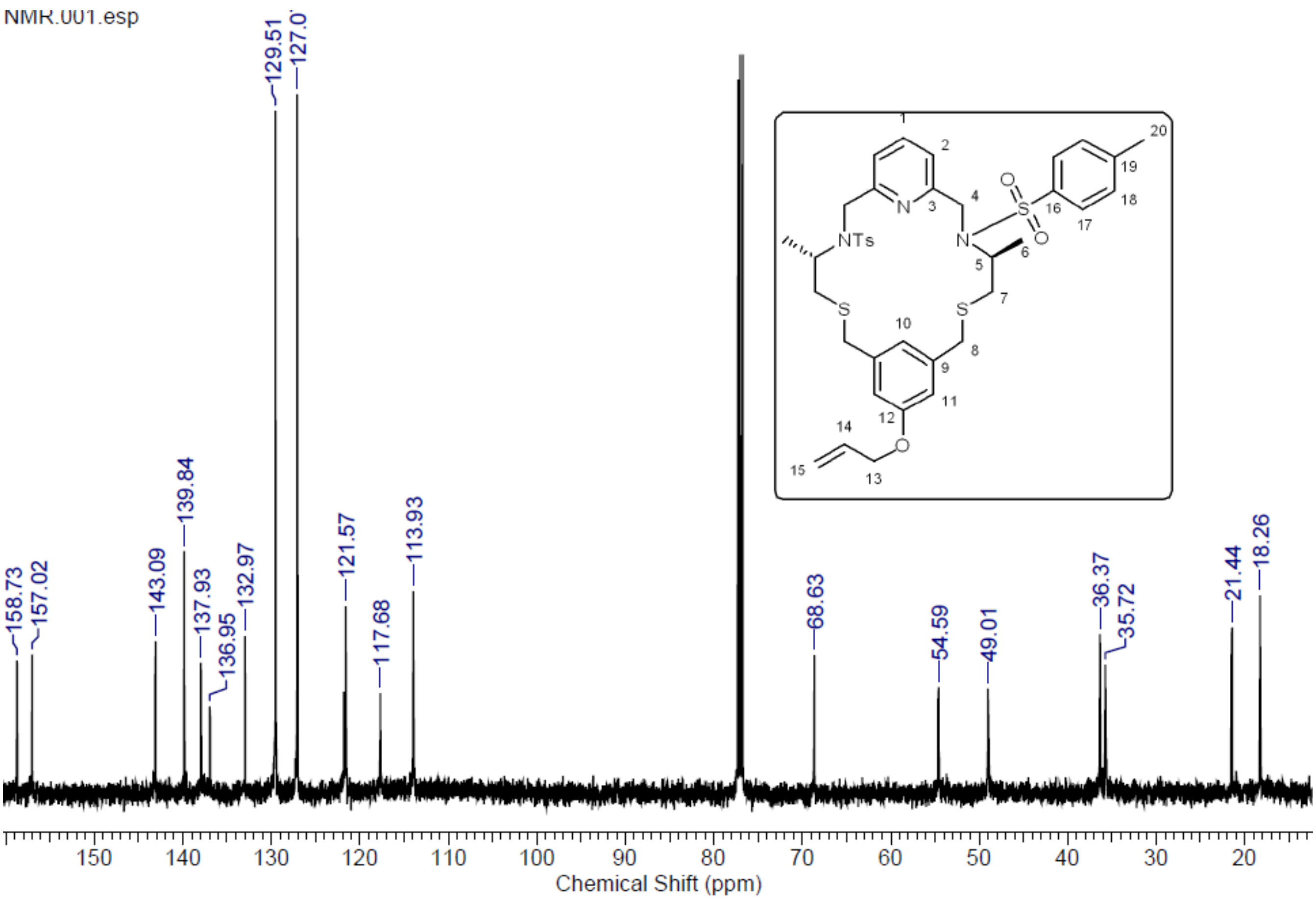




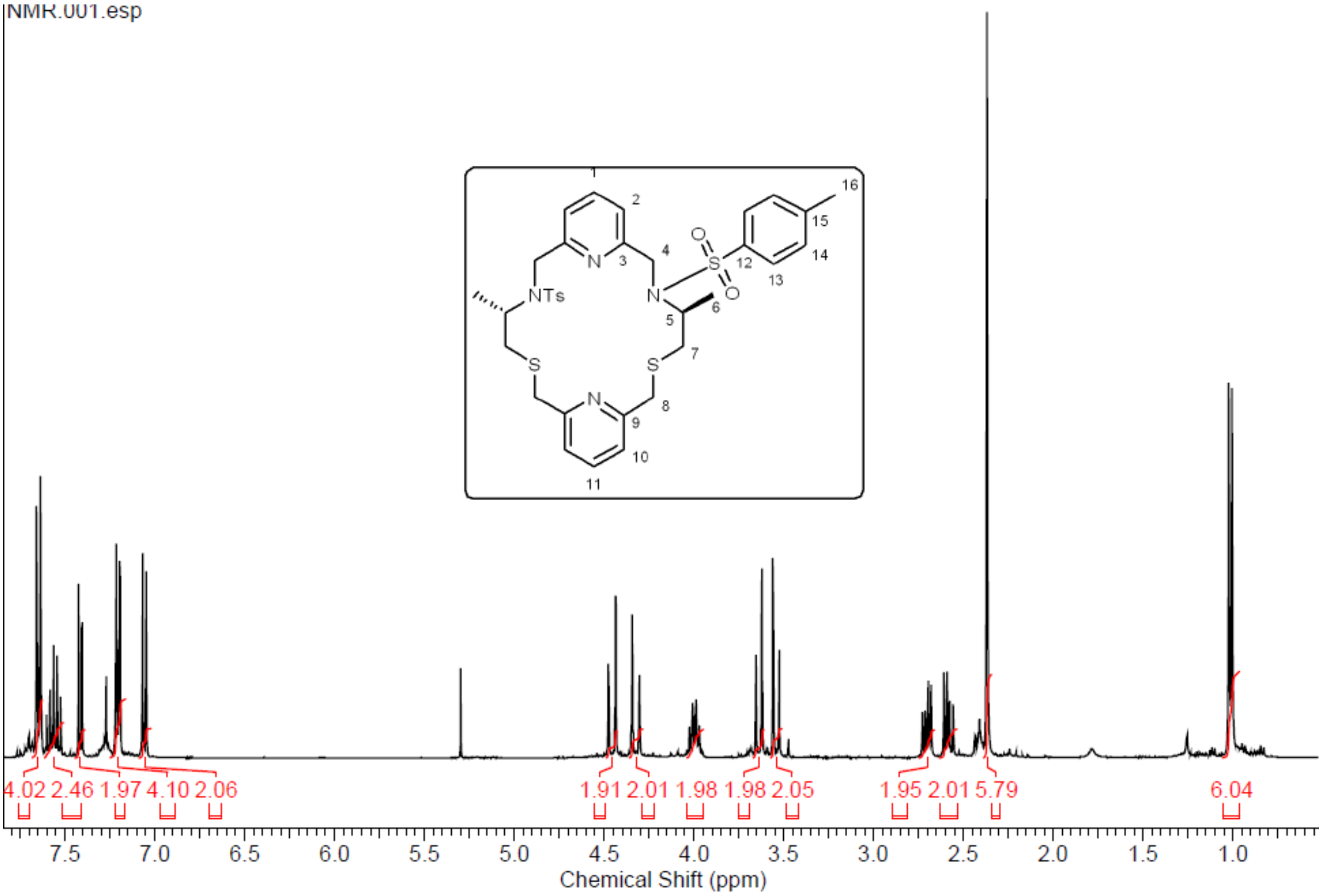
Macrocycles:

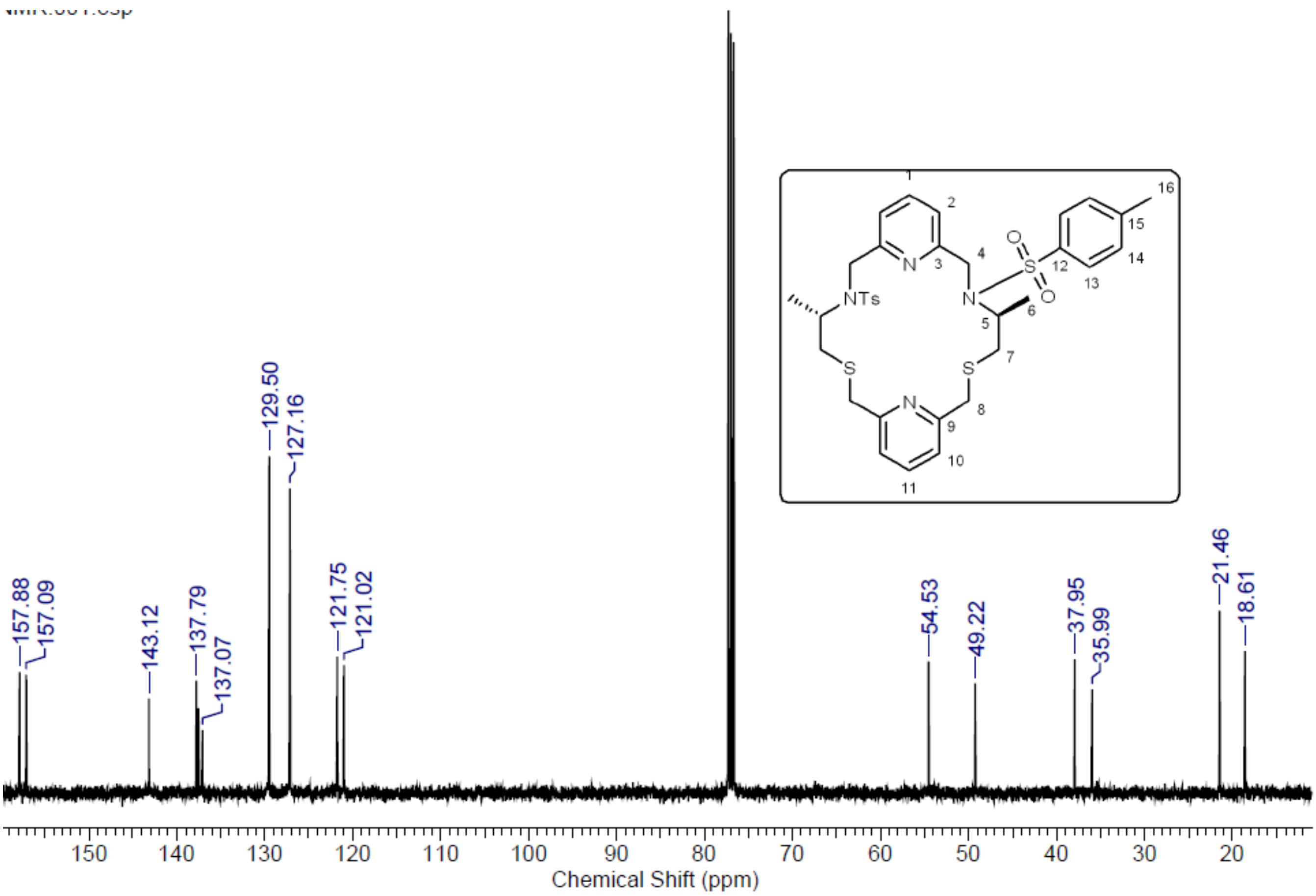
(4S,16S)-10-allyloxy-4,16-Dimethyl-3,17-bis-(toluene-4-sulfonyl)-6,14-dithia-3,17,23-triaza-tricyclo[17.3.1.1^{8,12}]tetracosa-1(22),8,10,12(24),19(23),20-hexaene (28)

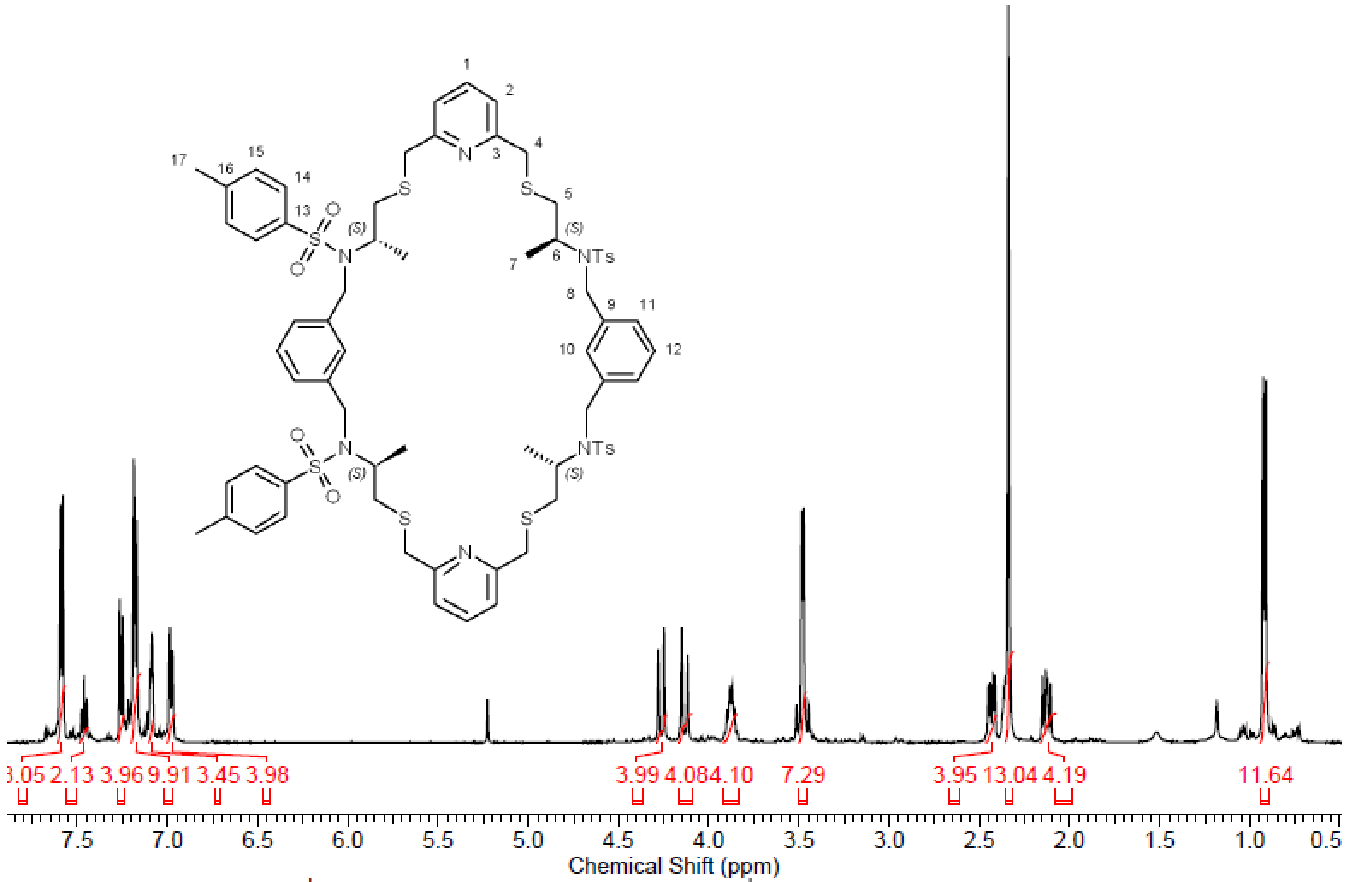




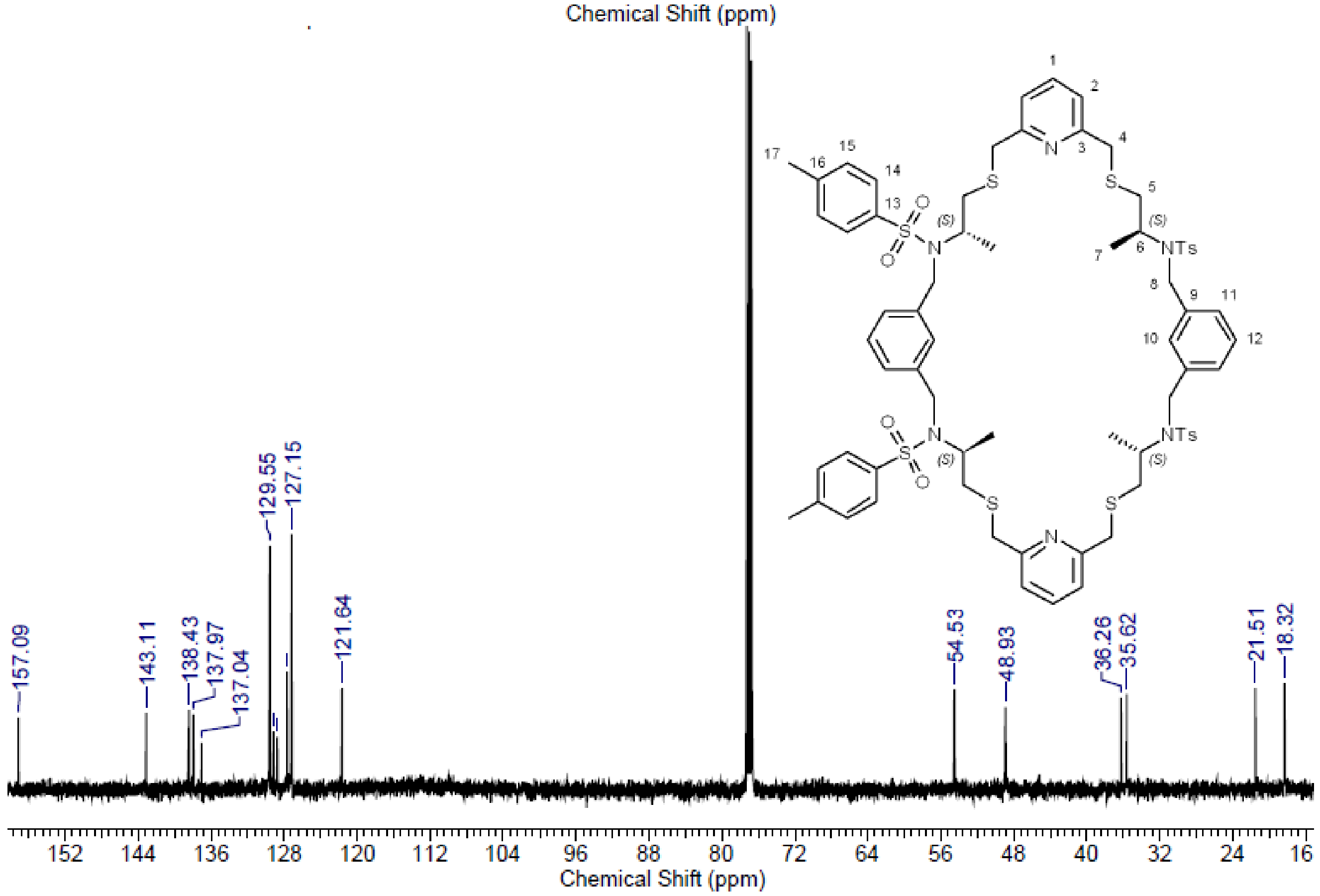
(5S,15S)-5,15-Dimethyl-6,14-bis-(toluene-4-sulfonyl)-3,17-dithia-6,14,23,24-tetraaza-tricyclo[17.3.1.1^{8,12}]tetracosa-1(22),8,10,12(24),19(23),20-hexaene (25)





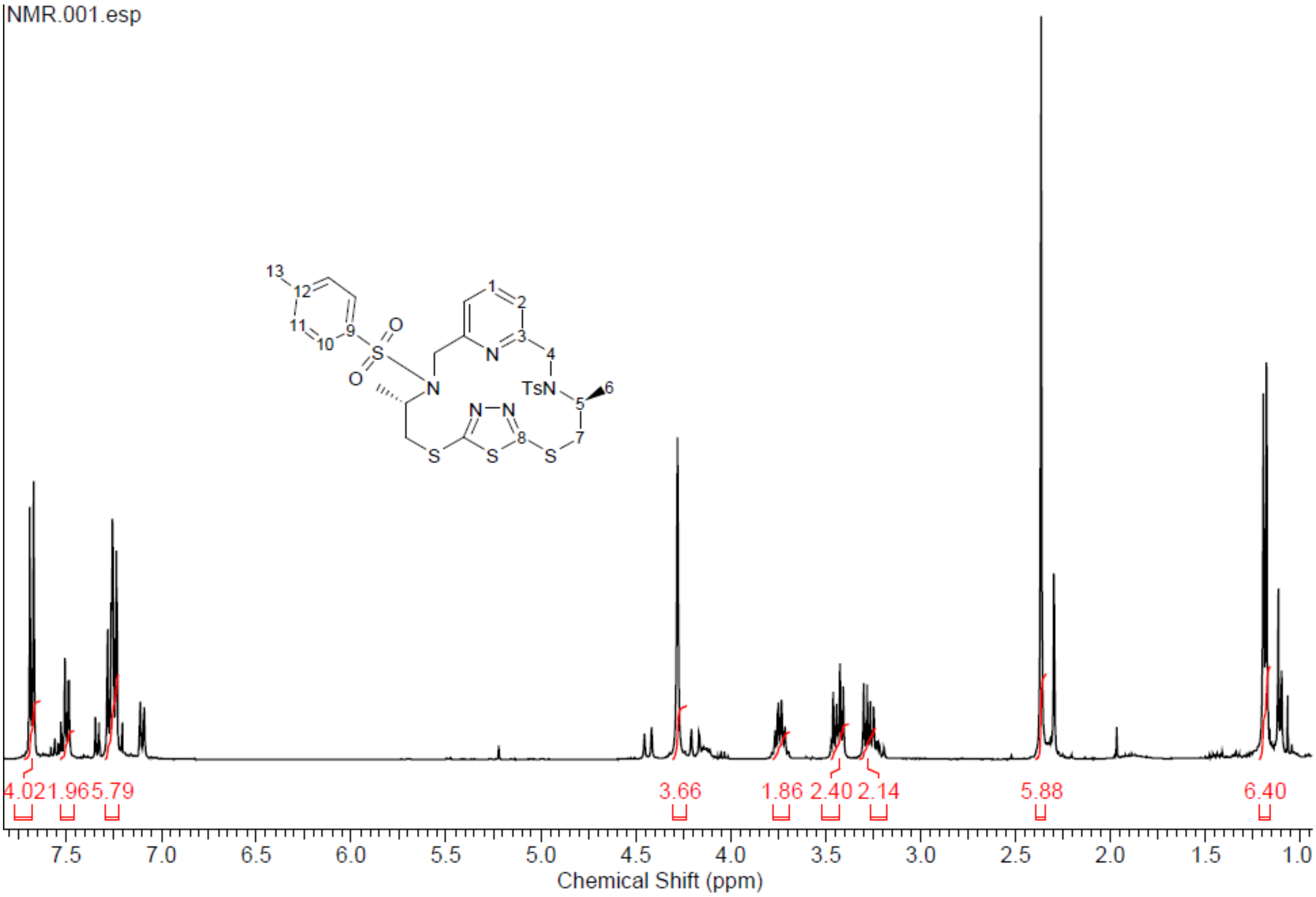


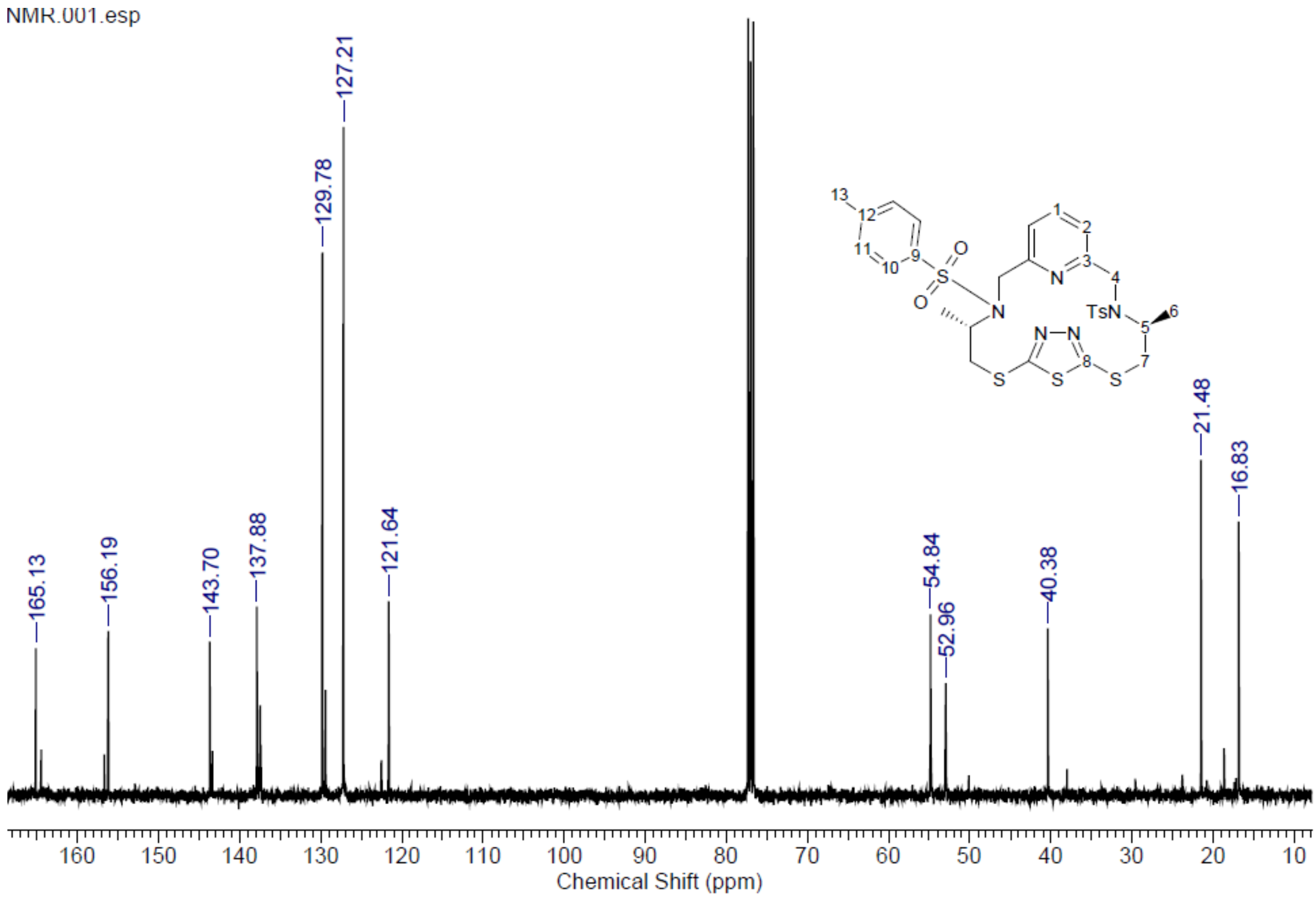
3.05 2.13 3.96 9.91 3.45 3.98
3.99 4.08 4.10
7.29
3.95 13.04 4.19
11.64
Chemical Shift (ppm)



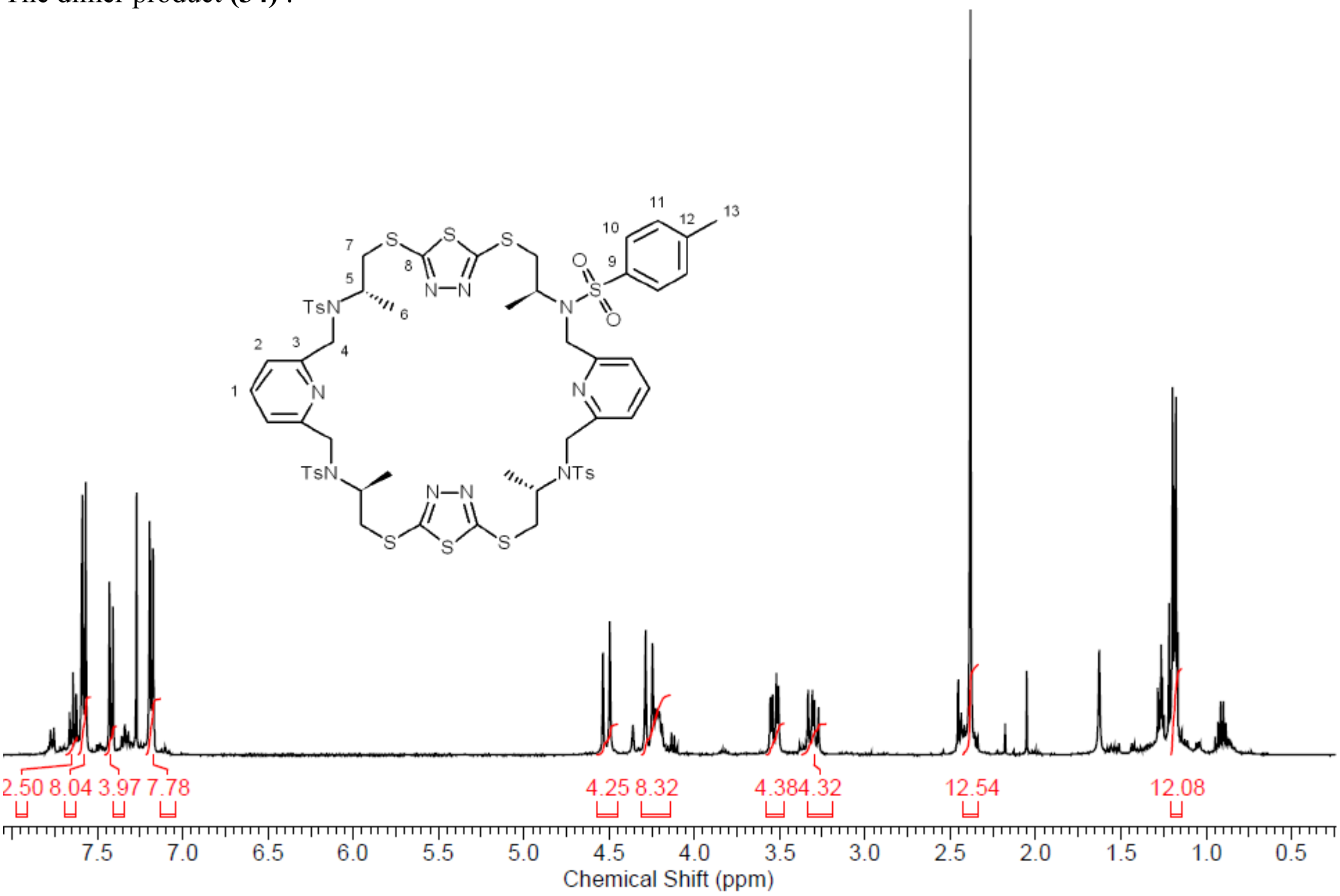
157.09
143.11
138.43
137.97
137.04
129.55
127.15
121.64
54.53
48.93
36.26
35.62
21.51
18.32
Chemical Shift (ppm)

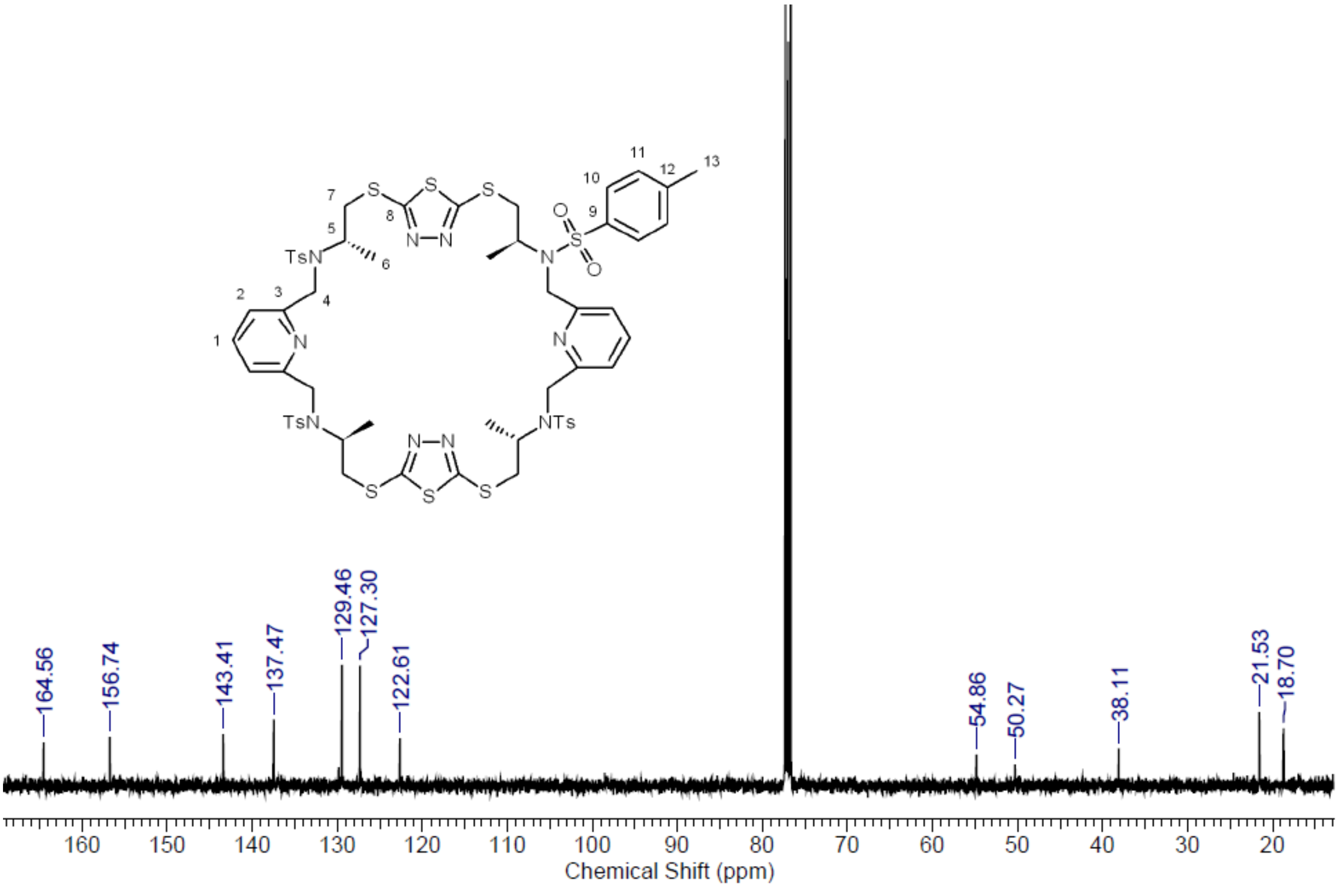
(4S,13S)-4,13-Dimethyl-3,14-bis-(toluene-4-sulfonyl)-6,11,21-trithia-3,8,9,14,20-pentaaza-tricyclo[14.3.1.1^{7,10}]henicosa-1(19),7,9,16(20),17-pentaene (29)



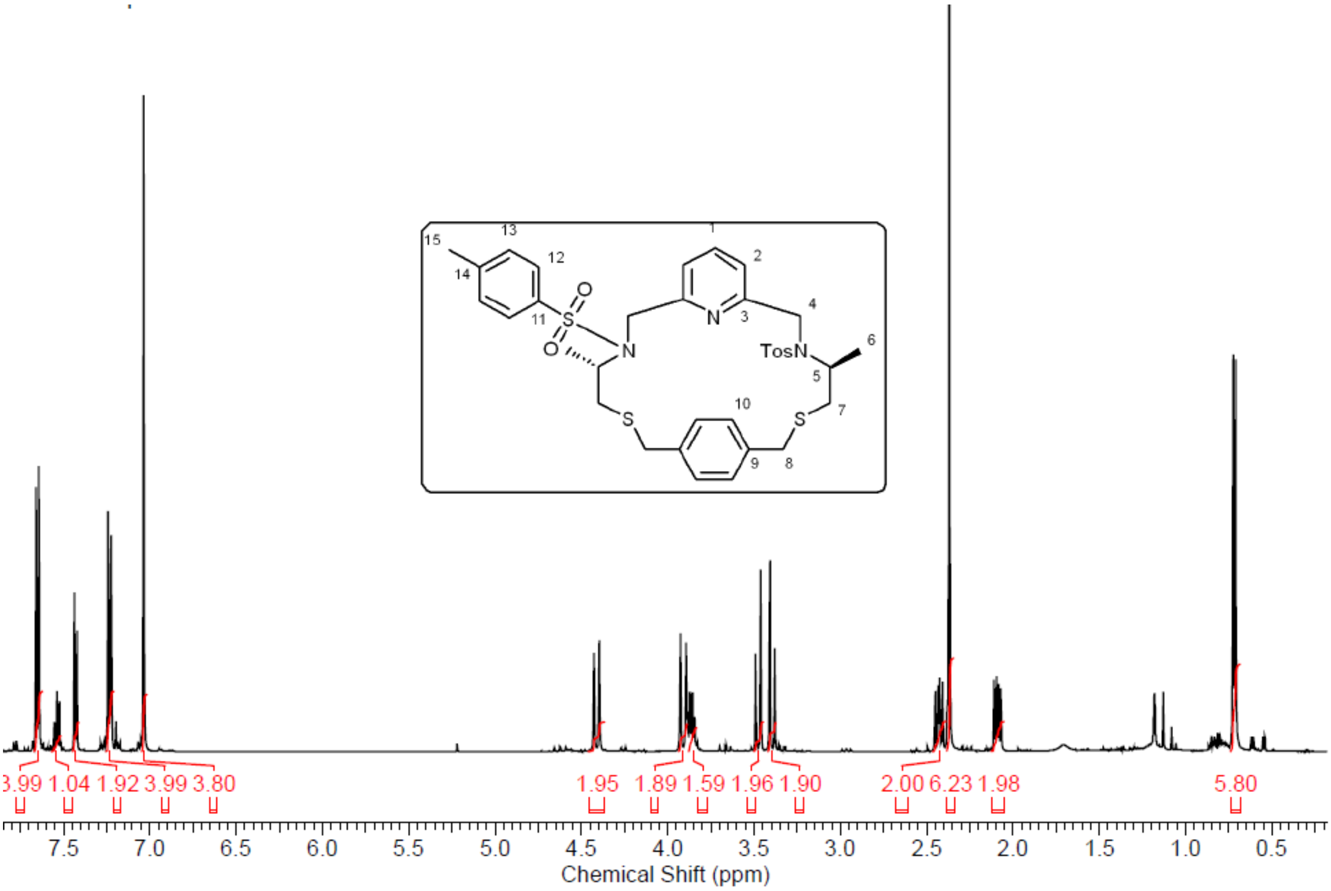


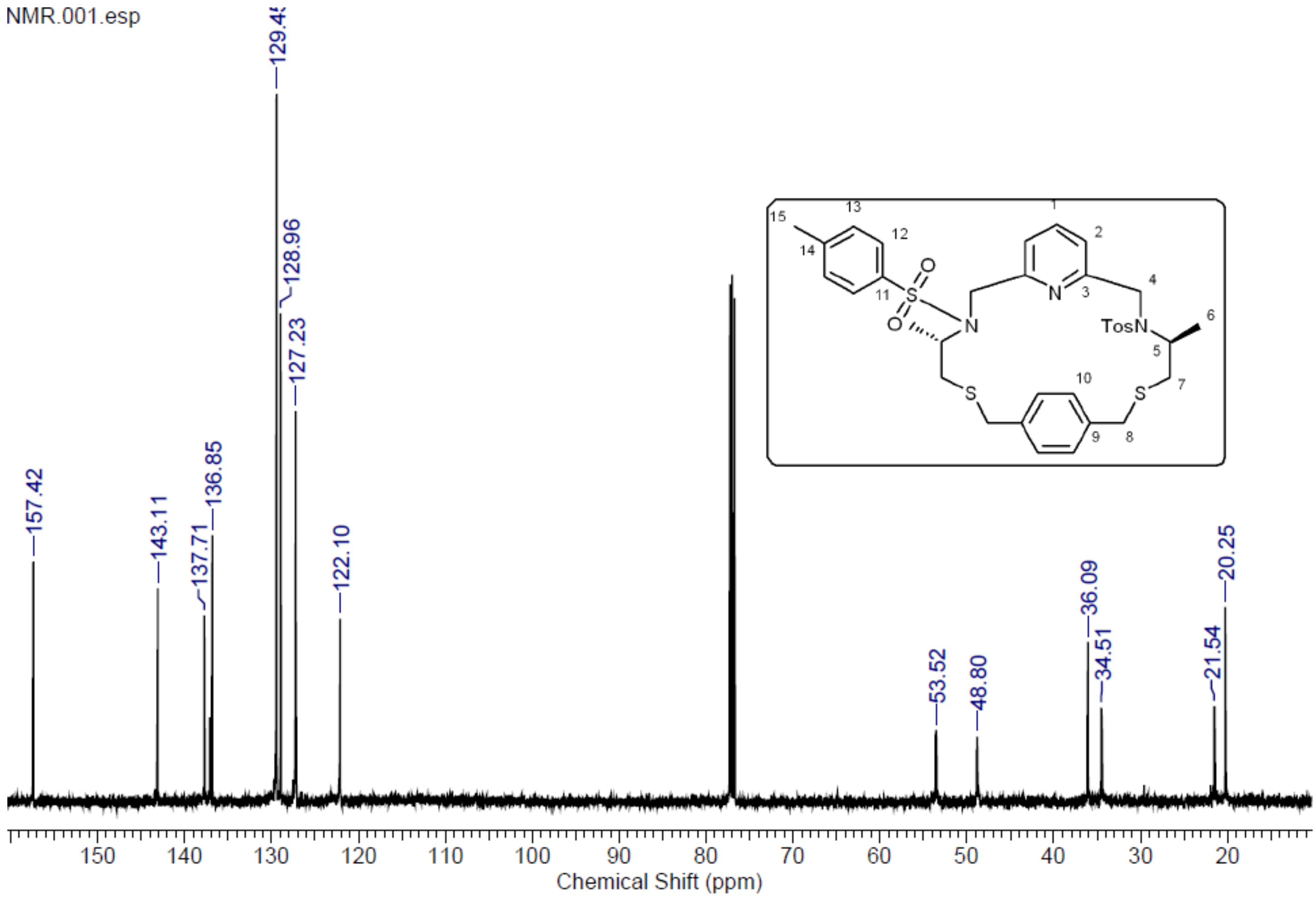
The dimer product **(34)** :



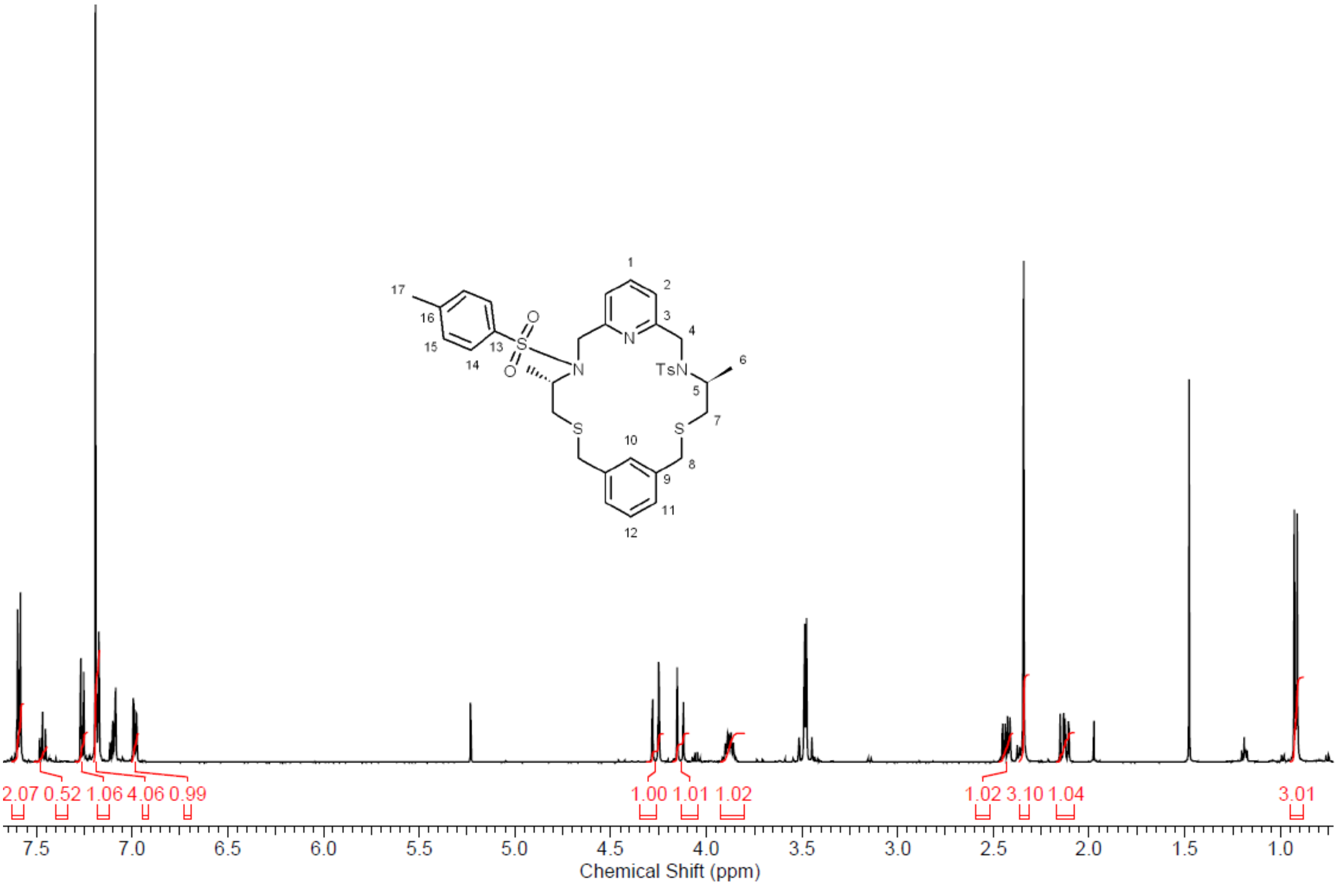


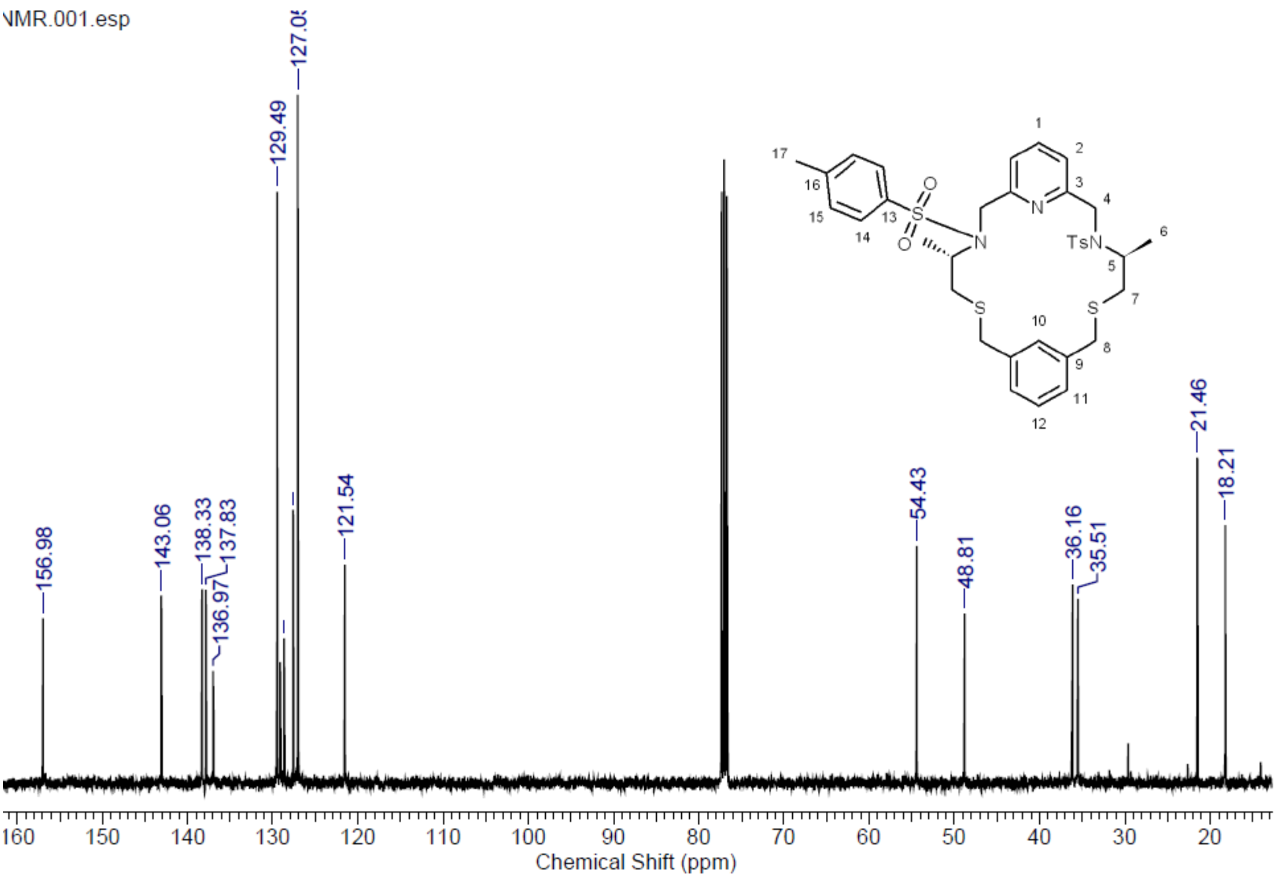
(5S,15S)-5,15-Dimethyl-6,14-bis-(toluene-4-sulfonyl)-3,17-dithia-6,14,24-triaza-tricyclo[17.2.2.1^{8,12}]tetracosa-1(22),8,10,12(24),19(23),20-hexaene (27)



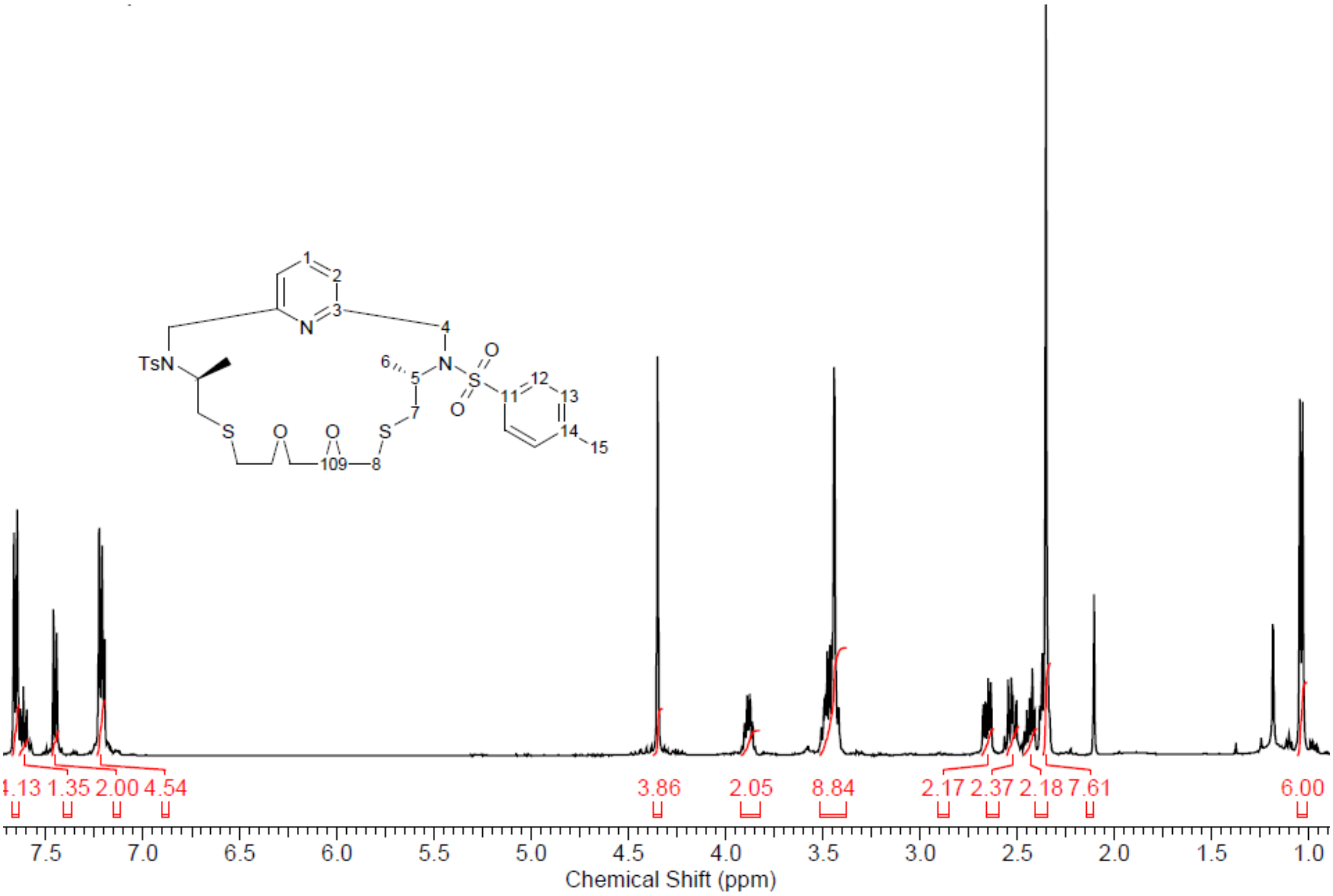


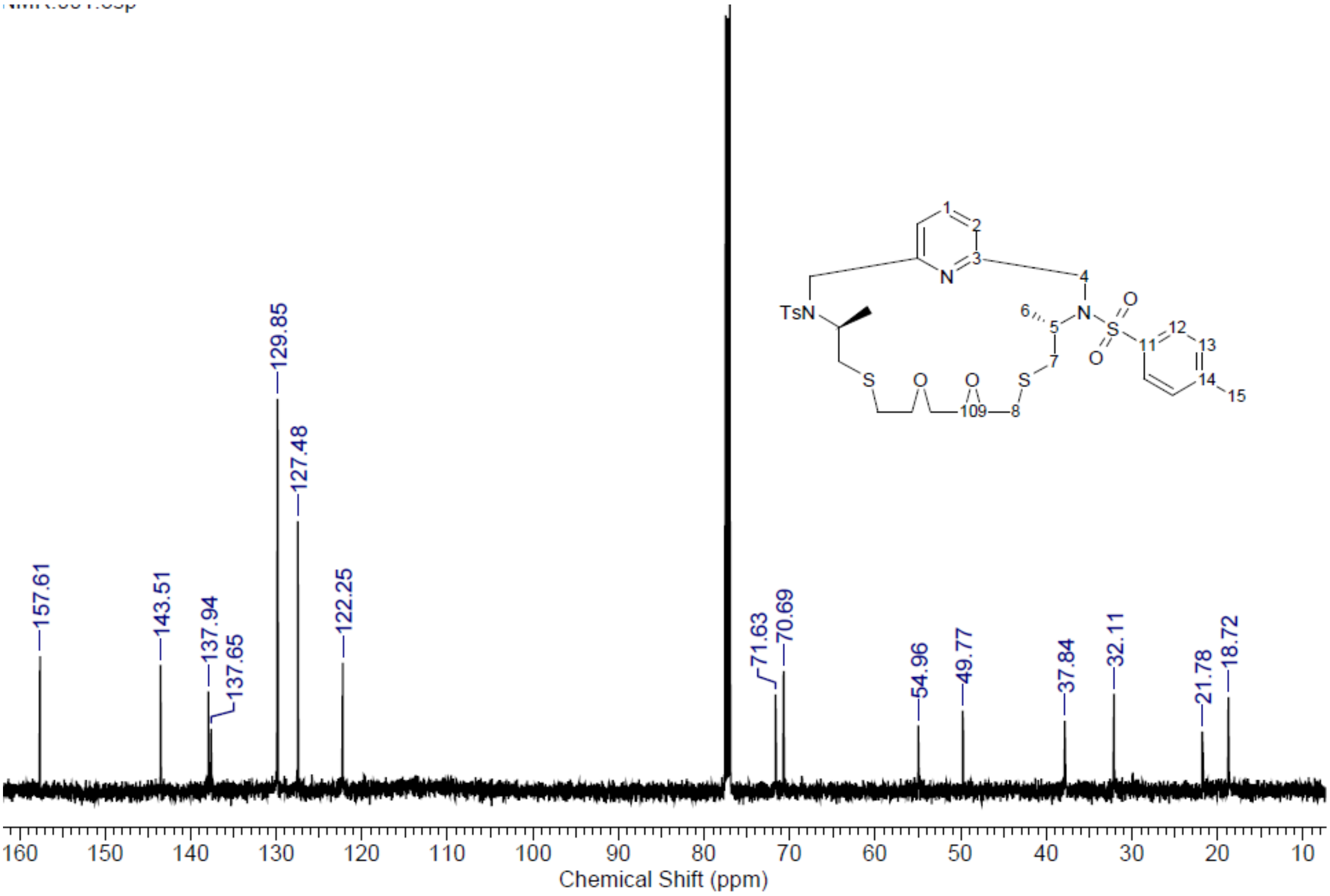
(5S,15S)-5,15-Dimethyl-6,14-bis-(toluene-4-sulfonyl)-3,17-dithia-6,14,23,24-tetraaza-tricyclo[17.3.1.1^{8,12}]tetracosa-1(22),8,10,12(24),19(23),20-hexaene (26)



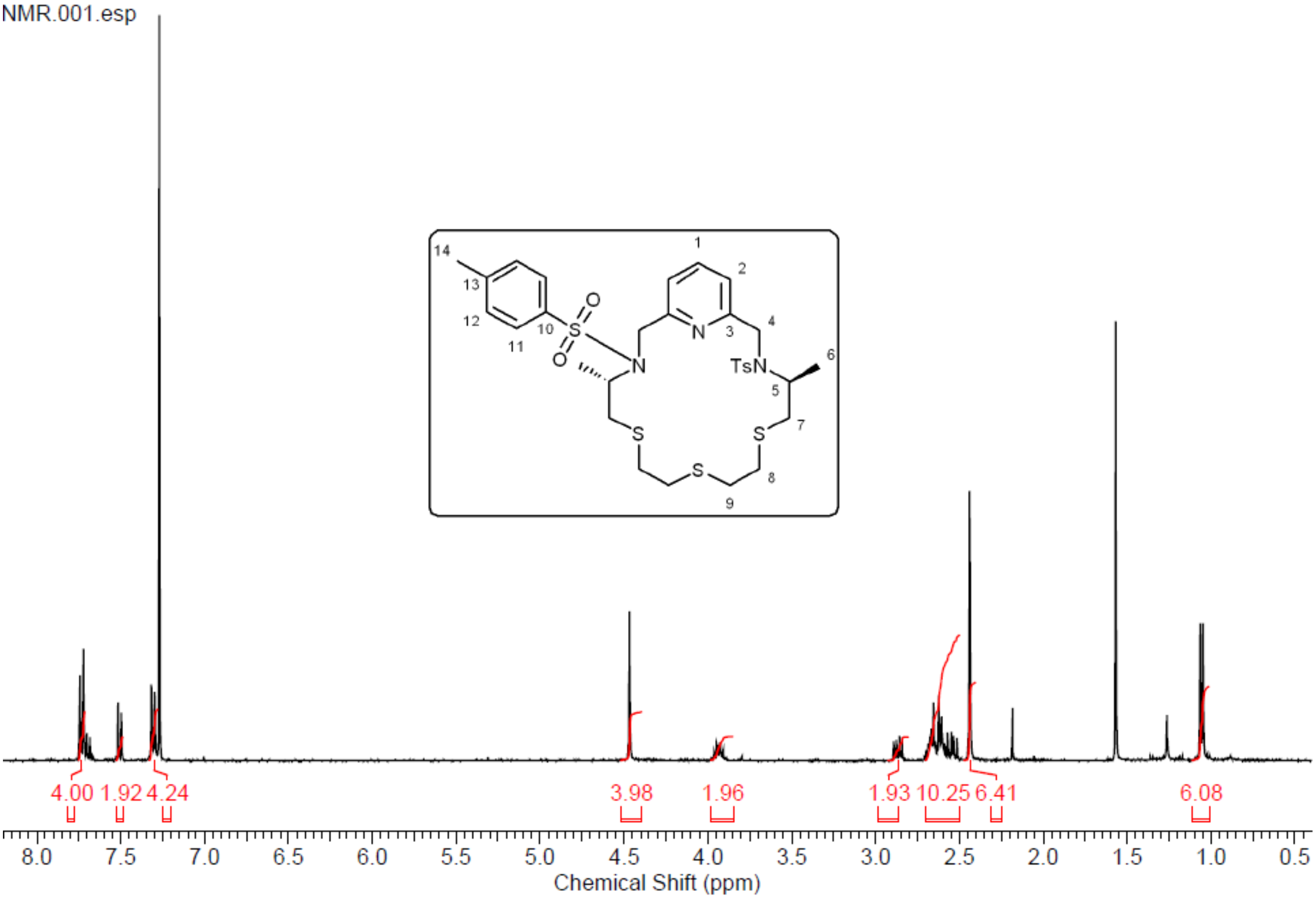


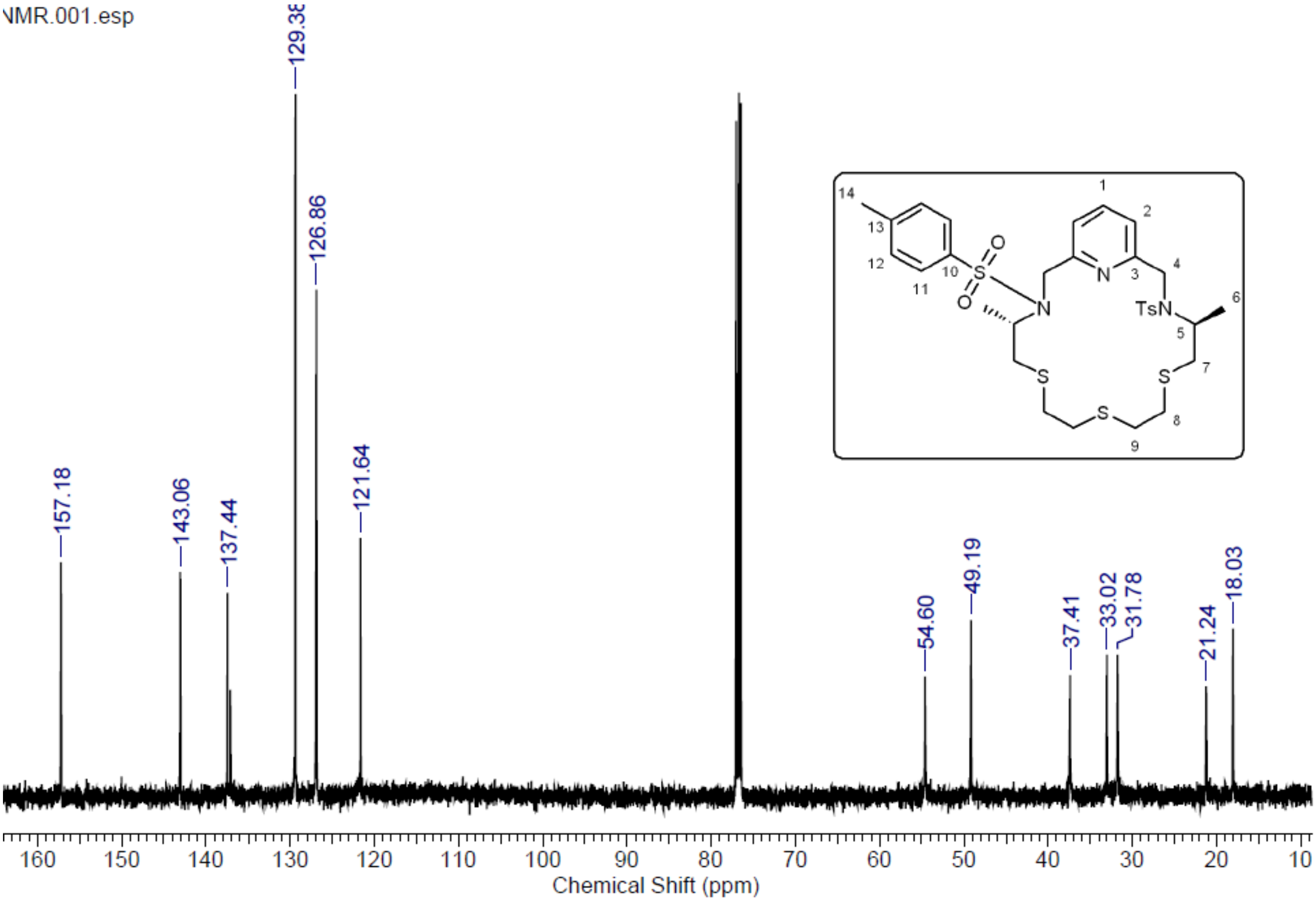
(4S,17S)-4,17-Dimethyl-3,18-bis-(toluene-4-sulfonyl)-9,12-dioxa-6,15-dithia-3,18,24-triaza-bicyclo[18.3.1]tetracosa-1(23),20(24),21-triene (32)



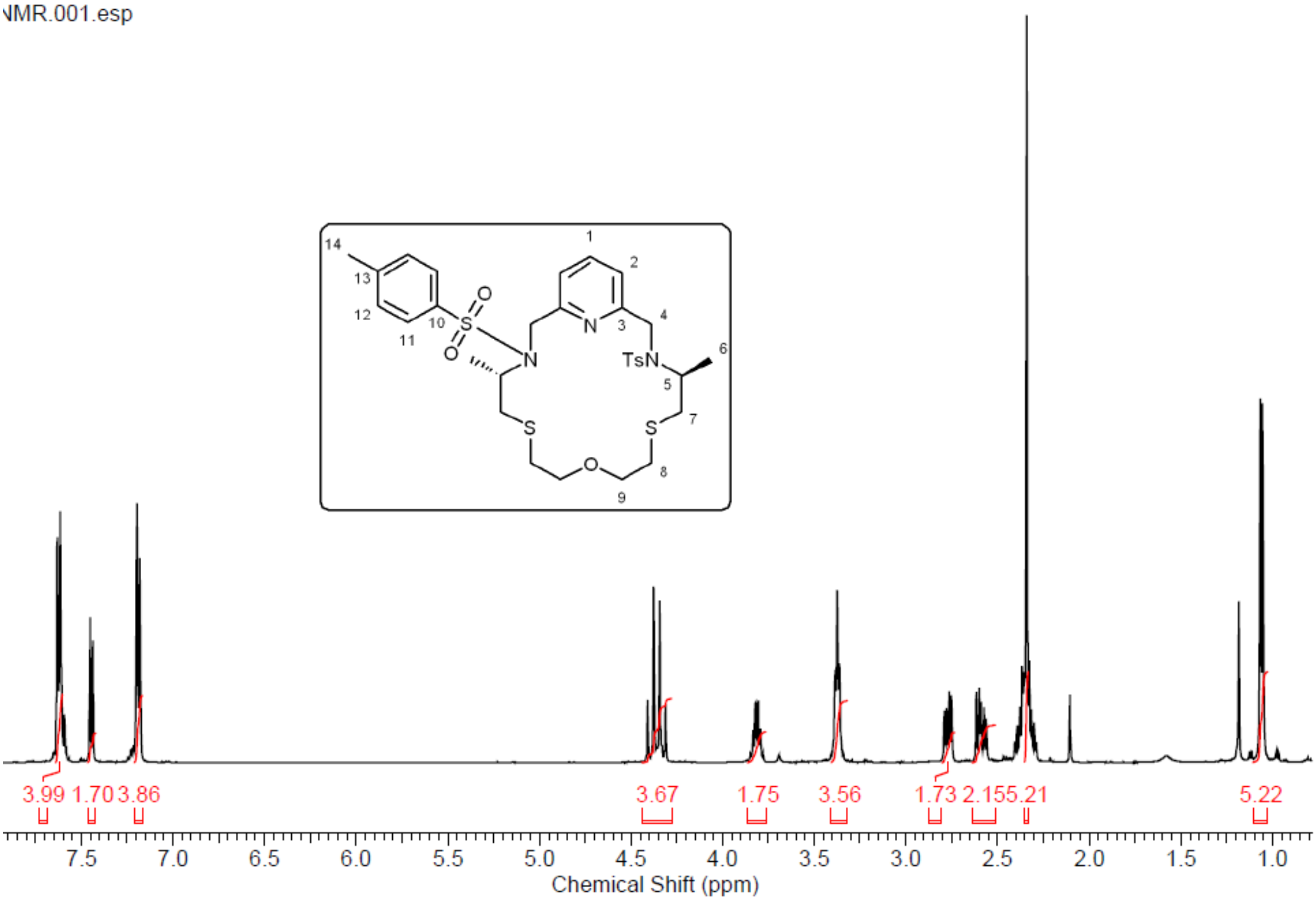


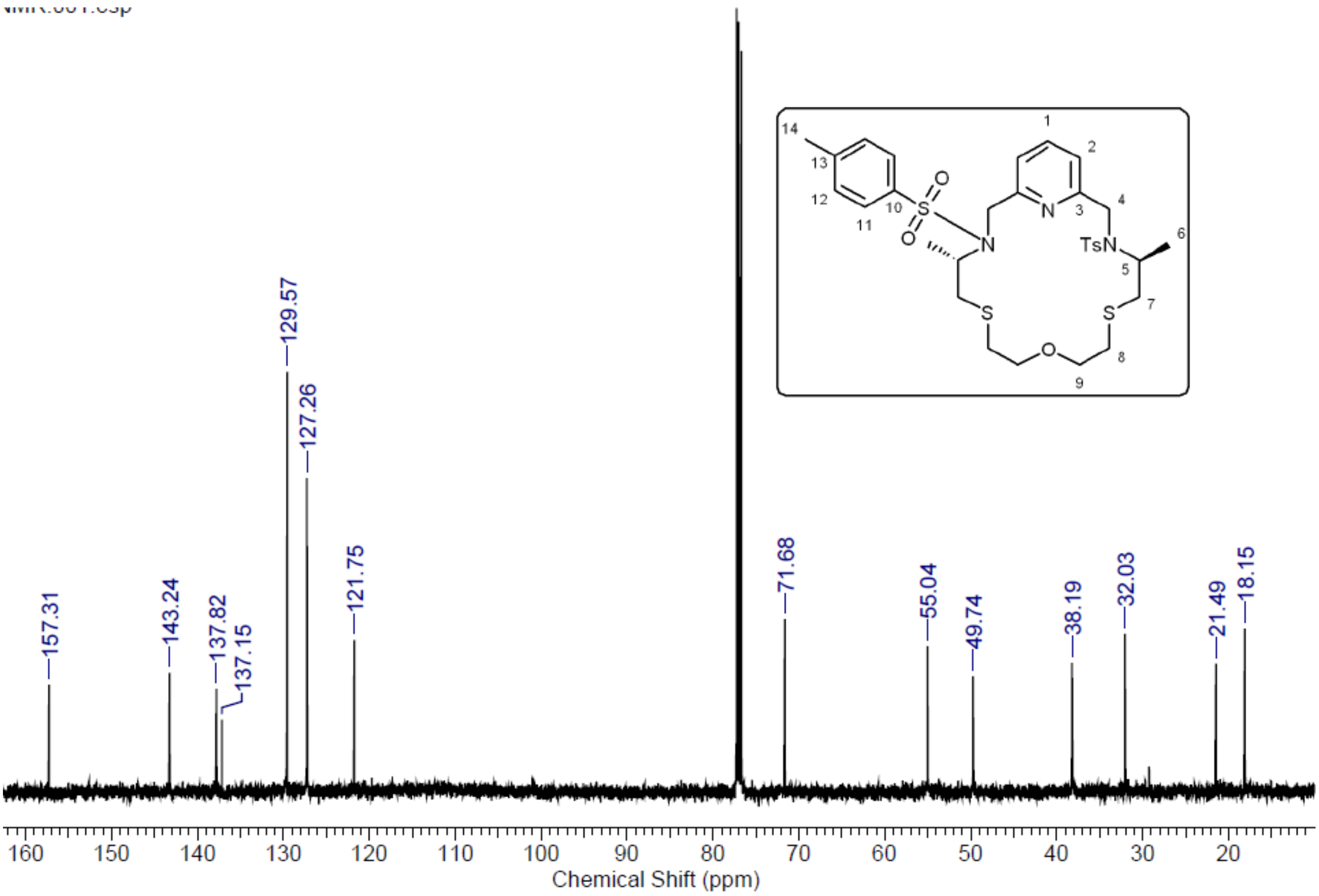
(4S,14S)-4,14-Dimethyl-3,15-bis-(toluene-4-sulfonyl)-6,9,12-trithia-3,15,21-triaza-bicyclo[15.3.1]henicosa-1(20),17(21),18-triene (30)



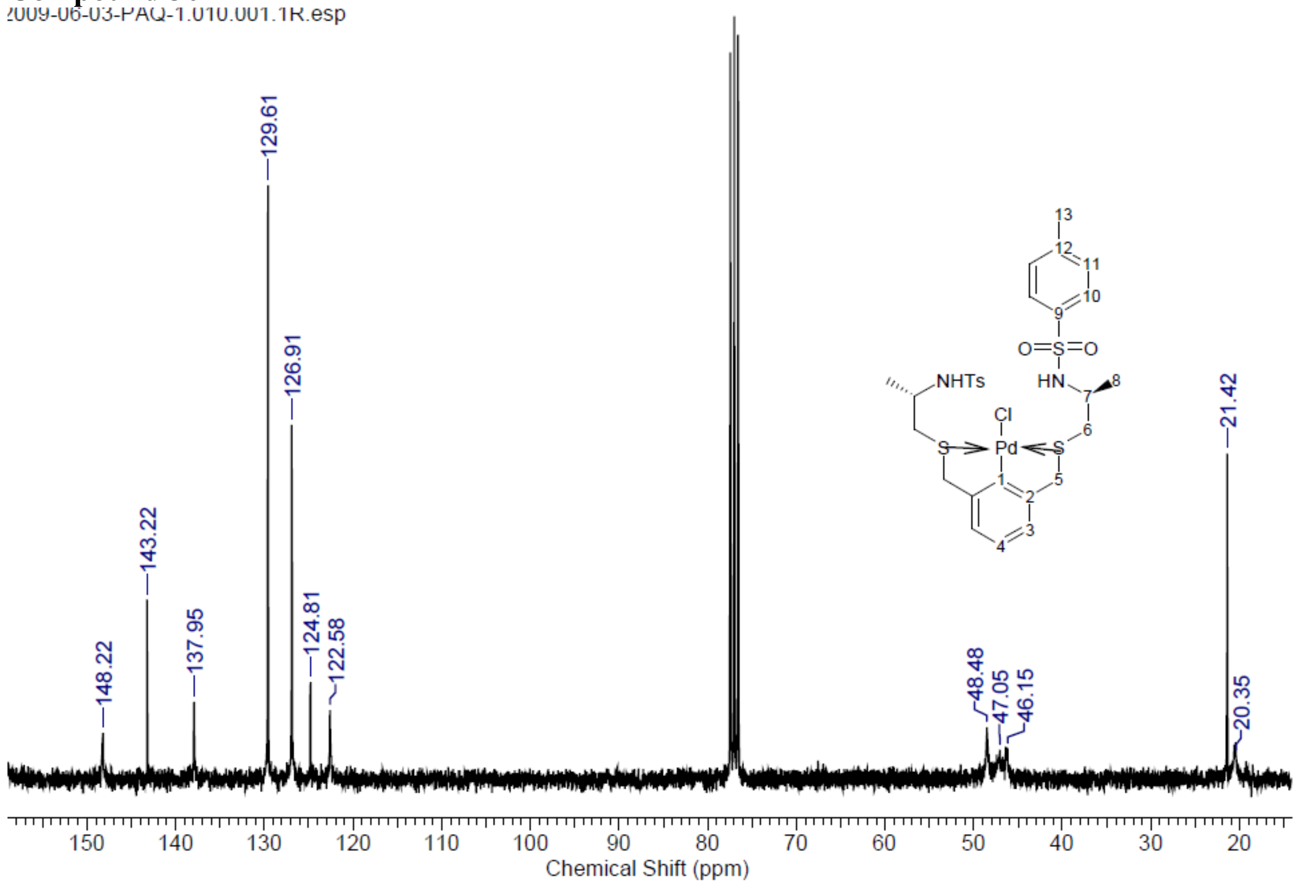


(4S,14S)-4,14-Dimethyl-3,15-bis-(toluene-4-sulfonyl)-9-oxa-6,12-dithia-3,15,21-triaza-bicyclo[15.3.1]henicosa-1(20),17(21),18-triene (31)





Compound 36



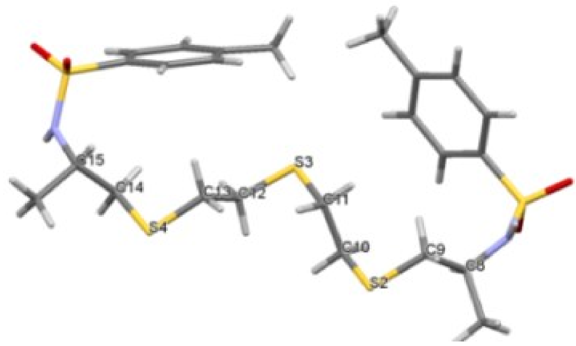
2009-06-03-PAQ-1.010.001.1R.esp
148.22
143.22
137.95
129.61
126.91
124.81
122.58
48.48
47.05
46.15
21.42
20.35
NHTs
Cl
Pd
S
HN
O=S=O
13
12
11
10
9
8
7
6
5
4
3
2
1
150 140 130 120 110 100 90 80 70 60 50 40 30 20
Chemical Shift (ppm)

X-Ray Structures

Tosamide 10:

As to be expected, the torsion angles about C15-C14-S4-C13 and C10-S2-C9-C8 were close to orthogonality (99.4(1)° and 85.5(5)° respectively) whereas those about S4-C13-C12-S3 and S3-C11-C10-S2 (176.6(3)° and 179.4(7)° respectively) indicated an *anti*-periplanar disposition of the sulphur substituents with respect to each other). In addition the methylene groups within the central thioether chain adopt a gauche conformation (e.g. C13-C12-S3-C11=68.3(5)°) which is also typical of such systems.

X-ray crystal structure of *bis*-tosamide 10.



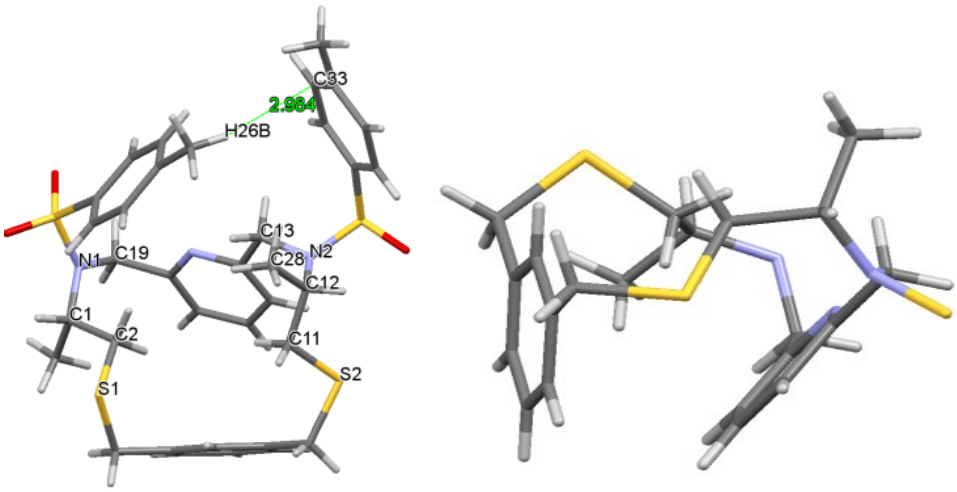
Torsion angles: C15-C14-S4-C13 = 99.41°; S4-C13-C12-S3=176.6(3)°; C12-S3-C11-C10=72.6(7)°; C13-C12-S3-C11=68.3(5)°; S3-C11-C10-S2=179.4(7)°; C10-S2-C9-C8=85.5(5)°

Macrocycles **26** and **28**:

For (*S*,*S*)-**26** there is a noticeable tilt of the pyridine ring towards the aromatic ring in the linker (angle between the mean planes of each ring = 40.2°) and a relatively short H26B-C33 separation of 2.98(4) Å, which may be indicative of π−π and CH-π interactions respectively.[17] The C19-N1-C1-C2 and C13-N2-C12-C11 torsion angles (75.8(2)° and 78.23° respectively) are such that the C27/C28 methyl groups adopt a pseudo *trans*-diaxial disposition with respect the macrocyclic core (C27-C1-C2-S1= −72.6(9)°; C28-C12-C11-S2=−161.4(5)°) resulting in large C27-C28 separation of 8.0(4) Å.

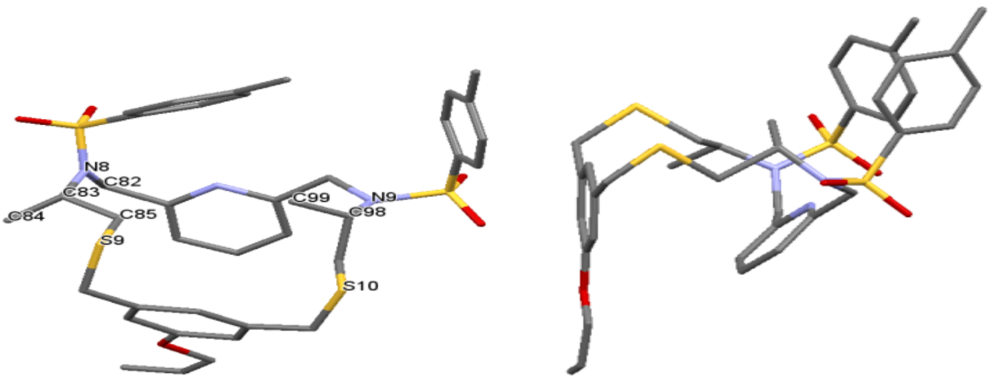
Not unexpectedly, there is considerable disorder about the allyloxy-group in (*S*,*S*)-**28a**,**b**. Both of these structures exhibit the "pac man" motif as observed for (*S*,*S*)-**26**, and, once again, the pyridine and aromatic linker residues are tilted towards one another. In both (*S*,*S*)-**28a** and (*S*,*S*)-**28b** the ring sulphur atoms are *exo*-disposed, but in both of these cases the linker, S9 to S10 and S1to S2, adopt a boat-boat conformation. Rotation about C83-C85 in (*S*,*S*)-**28a** generates **(***S*,*S*)-**28b** with a concomitant conformational change within the macrocycle such that the methyl groups associated with the core now point towards each other ((*S*,*S*)-**28a**: C84-C99= 6.6(2) Å; (*S*,*S*)-**28b**: C8-C23=3.8(6) Å). While C85 was inward-pointing in (*S*,*S*)-**28a** (C82-N8-C83-C85=71.5(1)°) C9, the analogous atom in **28b**, points to the outside macrocyclic ring (C6-N2-C7-C9=-82.9(2) °).

X-ray structure of (*S*,*S*)-26 (Hydrogens omitted for clarity).

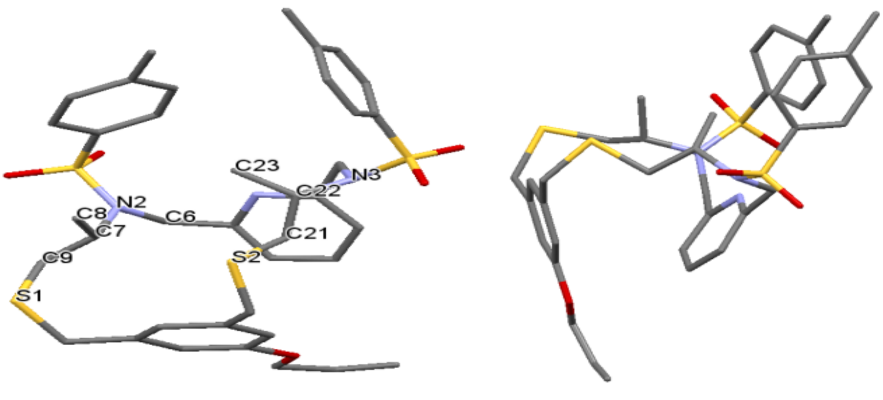


Representative distance: C27-C28 = 8.0(4); H26B-C-33=2.98(4) Å. Torsion angles: N2-C12-C11-S2=−32.6(1)°; N1-C1-C2-S1=161.6(2)°; N2-C12-C11-S2= −32.6(1)°; C19-N1-C1-C27=−50.5(5)°; C19-N1-C1-C2=75.8(2)°; C27-C1-C2-S1=−72.6(9)°; C28-C12-C11-S2=−161.4(5)°; C13-N2-C12-C11=78.2(3)°.

X-ray structure of (*S*,*S*)-28a and (*S*,*S*)-28b (Hydrogens omitted for clarity).



(*S*,*S*)-**28a**



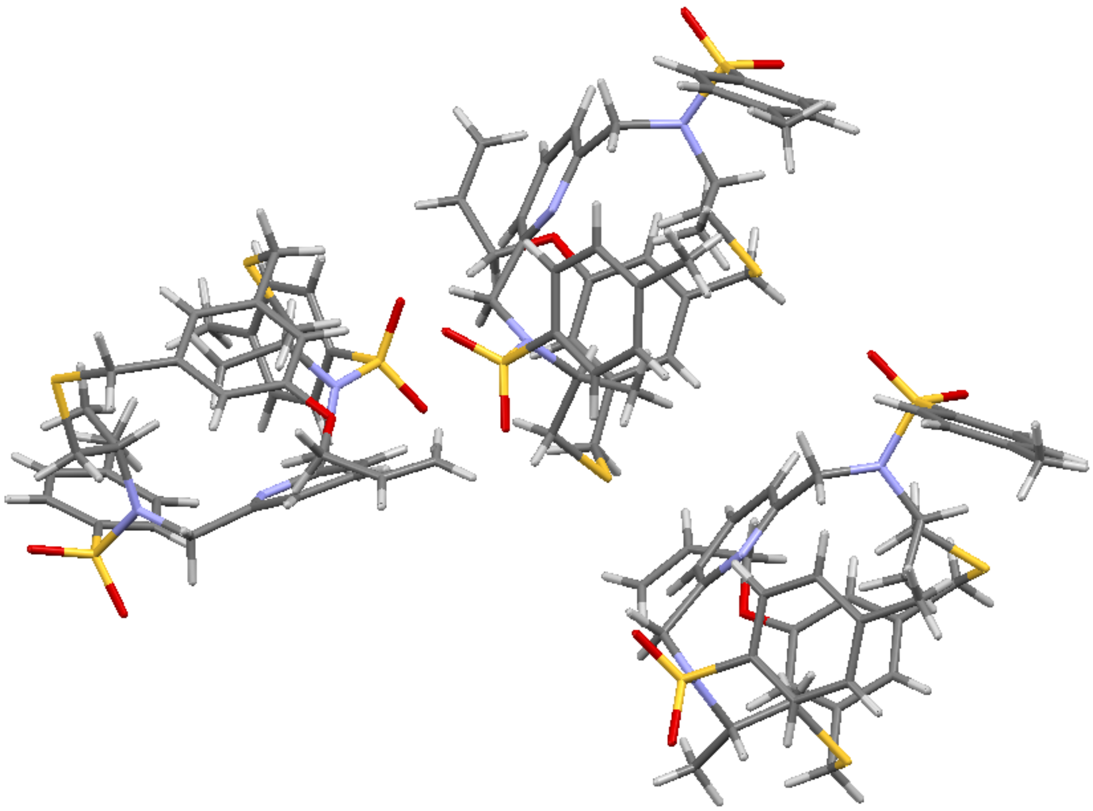
(S,S)-28b

*(*S,S)-**28a**: Distance: C84-C99 = 6.624 Å; Torsion angles: N8-C83-C85-S9=170.61°; N9-C-98-C-97-S10=156.32°; C82-N8-C83-C84=-55.90°; C82-N8-C83-C85=71.51°. (S,S)-**28b**: Distance: C8-C23=3.876 Å. Torsion angles: N2-C7-C9-S1=176.0°; N3-C23-C22-S2=166.8(4)°; C6-N2-C7-C8=149.37°; C6-N2-C7-C9=-82.92°.

X-Ray crystallographic data

Crystal data and structure refinement for 28 (UoM code: s3334bm).

CCDC 1411546



Identification code	s3334bm
Empirical formula	C38 H45 N3 O5 S4
Formula weight	752.01
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 16.764(3) A alpha = 90 deg. b = 23.931(4) A beta = 90 deg. c = 27.815(5) A gamma = 90 deg.
Volume	11159(3) A^3
Z, Calculated density	12, 1.343 Mg/m^3
Absorption coefficient	0.303 mm^-1
F(000)	4776
Crystal size	0.50 x 0.50 x 0.40 mm
Theta range for data collection	1.42 to 25.03 deg.

Limiting indices	-19<=h<=19, -28<=k<=28, -33<=l<=33
Reflections collected / unique	80756 / 19696 [R(int) = 0.0461]
Completeness to theta = 25.03	99.9 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	19696 / 199 / 1420
Goodness-of-fit on F^2	1.018
Final R indices [I>2sigma(I)]	R1 = 0.0362, wR2 = 0.0755
R indices (all data)	R1 = 0.0400, wR2 = 0.0770
Absolute structure parameter	-0.02(3)
Largest diff. peak and hole	0.517 and -0.236 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for s3334bm. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
S(1)	1956(1)	2893(1)	6477(1)	31(1)
S(2)	-1054(1)	3378(1)	7180(1)	26(1)
S(3)	2535(1)	3455(1)	8213(1)	29(1)
S(4)	-2115(1)	3599(1)	8907(1)	23(1)
O(1)	-146(1)	942(1)	7369(1)	31(1)
O(2)	2825(1)	3178(1)	8631(1)	40(1)
O(3)	3089(1)	3643(1)	7856(1)	37(1)
O(4)	-2216(1)	3288(1)	9343(1)	28(1)
O(5)	-2750(1)	3608(1)	8563(1)	31(1)
N(1)	524(1)	2779(1)	8565(1)	24(1)
N(2)	1897(1)	3030(1)	7961(1)	26(1)
N(3)	-1328(1)	3344(1)	8635(1)	25(1)
C(1)	-223(2)	2680(1)	8712(1)	25(1)
C(2)	-612(2)	2175(1)	8637(1)	27(1)
C(3)	-236(2)	1765(1)	8375(1)	29(1)
C(4)	526(2)	1873(1)	8202(1)	28(1)
C(5)	890(2)	2375(1)	8314(1)	23(1)
C(6)	1750(2)	2480(1)	8172(1)	30(1)
C(7)	1622(2)	3103(1)	7452(1)	28(1)
C(8)	1373(2)	3693(1)	7331(1)	30(1)
C(9)	2256(2)	2870(1)	7106(1)	31(1)
C(10)	1551(2)	2196(1)	6392(1)	31(1)
C(11)	783(2)	2071(1)	6656(1)	26(1)
C(12)	149(2)	2440(1)	6651(1)	27(1)

C(13)	-564(2)	2312(1)	6883(1)	24(1)
C(14)	-639(2)	1802(1)	7115(1)	25(1)
C(15)	-6(2)	1429(1)	7120(1)	27(1)
C(16)	706(2)	1558(1)	6892(1)	28(1)
C(17)	485(2)	549(1)	7411(1)	30(1)
C(18)	237(2)	96(1)	7746(1)	33(1)
C(19)	-453(2)	48(1)	7959(1)	42(1)
C(20)	-1248(2)	2721(1)	6871(1)	27(1)
C(21)	-1048(2)	3109(1)	7792(1)	26(1)
C(22)	-1144(2)	3586(1)	8152(1)	25(1)
C(23)	-434(2)	3981(1)	8164(1)	30(1)
C(24)	-653(2)	3165(1)	8943(1)	25(1)
C(25)	2003(2)	4054(1)	8411(1)	28(1)
C(26)	1517(2)	4015(1)	8812(1)	29(1)
C(27)	1094(2)	4481(1)	8955(1)	31(1)
C(28)	1134(2)	4980(1)	8706(1)	30(1)
C(29)	1645(2)	5012(1)	8309(1)	35(1)
C(30)	2087(2)	4555(1)	8164(1)	34(1)
C(31)	625(2)	5472(1)	8846(1)	39(1)
C(32)	-1890(2)	4297(1)	9061(1)	26(1)
C(33)	-2190(2)	4732(1)	8792(1)	33(1)
C(34)	-1983(2)	5274(1)	8906(1)	40(1)
C(35)	-1470(2)	5388(1)	9290(1)	38(1)
C(36)	-1174(2)	4942(1)	9551(1)	35(1)
C(37)	-1379(2)	4399(1)	9445(1)	29(1)
C(38)	-1254(2)	5982(1)	9417(1)	50(1)
S(5)	3734(1)	1421(1)	9382(1)	44(1)
S(6)	6934(1)	1738(1)	9977(1)	34(1)
S(7)	2805(1)	1039(1)	7680(1)	26(1)
S(8)	7521(1)	1158(1)	8232(1)	27(1)
O(6)	5040(1)	3781(1)	9095(1)	46(1)
O(7)	2761(1)	1257(1)	7203(1)	32(1)
O(8)	2161(1)	1140(1)	8006(1)	32(1)
O(9)	8118(1)	984(1)	8571(1)	34(1)
O(10)	7764(1)	1423(1)	7795(1)	35(1)
N(4)	5503(1)	1828(1)	7947(1)	24(1)
N(5)	3609(1)	1301(1)	7929(1)	28(1)
N(6)	6902(1)	1589(1)	8497(1)	28(1)
C(39)	5896(2)	2250(1)	8155(1)	23(1)
C(40)	5561(2)	2770(1)	8231(1)	29(1)
C(41)	4792(2)	2869(1)	8068(1)	34(1)
C(42)	4386(2)	2437(1)	7849(1)	31(1)
C(43)	4749(2)	1925(1)	7806(1)	26(1)
C(44)	4299(2)	1419(1)	7616(1)	30(1)
C(45)	3763(2)	1118(1)	8436(1)	31(1)
C(46)	4481(2)	741(1)	8473(1)	39(1)
C(47)	3821(2)	1634(1)	8757(1)	32(1)
C(48)	3660(2)	2109(2)	9646(1)	44(1)
C(49)	4408(2)	2456(1)	9614(1)	32(1)
C(50)	5116(2)	2277(1)	9831(1)	32(1)
C(51)	5801(2)	2605(1)	9803(1)	28(1)
C(52)	5775(2)	3107(1)	9554(1)	29(1)
C(53)	5070(2)	3284(1)	9339(1)	32(1)
C(54)	4390(2)	2956(1)	9367(1)	34(1)
C(55)	5601(3)	4149(2)	9110(2)	39(1)
C(56)	5329(4)	4667(3)	8858(2)	45(2)
C(57)	4628(7)	4733(6)	8670(7)	52(3)
C(55B)	4390(4)	4050(3)	8906(2)	34(2)
C(56B)	4510(8)	4621(6)	8697(8)	39(2)
C(57B)	5204(6)	4864(4)	8658(3)	43(2)
C(58)	6558(2)	2441(1)	10062(1)	30(1)
C(59)	7250(2)	1755(1)	9350(1)	31(1)
C(60)	6628(2)	1509(1)	9004(1)	30(1)
C(61)	6417(2)	907(1)	9131(1)	33(1)

C(62)	6761(2)	2144(1)	8290(1)	29(1)
C(63)	2934(2)	306(1)	7651(1)	25(1)
C(64)	3403(2)	73(1)	7293(1)	28(1)
C(65)	3520(2)	-496(1)	7288(1)	29(1)
C(66)	3172(2)	-842(1)	7635(1)	26(1)
C(67)	2707(2)	-599(1)	7989(1)	28(1)
C(68)	2586(2)	-26(1)	8001(1)	28(1)
C(69)	3297(2)	-1464(1)	7622(1)	35(1)
C(70)	6971(2)	551(1)	8076(1)	26(1)
C(71)	7132(2)	47(1)	8299(1)	31(1)
C(72)	6679(2)	-416(1)	8193(1)	33(1)
C(73)	6052(2)	-388(1)	7864(1)	28(1)
C(74)	5929(2)	115(1)	7631(1)	30(1)
C(75)	6371(2)	586(1)	7733(1)	29(1)
C(76)	5519(2)	-880(1)	7765(1)	36(1)
S(9)	1815(1)	3855(1)	3590(1)	30(1)
S(10)	-1322(1)	3576(1)	3869(1)	33(1)
S(10B)	-1423(1)	3187(1)	4280(1)	28(1)
S(11)	3138(1)	4007(1)	5258(1)	31(1)
S(12)	-1666(1)	3849(1)	5569(1)	27(1)
O(11)	757(1)	1438(1)	3921(1)	36(1)
O(12)	3212(1)	3786(1)	5734(1)	38(1)
O(13)	3830(1)	4228(1)	5022(1)	41(1)
O(14)	-1626(1)	3592(1)	6031(1)	37(1)
O(15)	-2316(1)	3723(1)	5254(1)	36(1)
N(7)	1180(1)	3255(1)	5316(1)	25(1)
N(8)	2771(1)	3512(1)	4925(1)	31(1)
N(9)	-845(1)	3691(1)	5279(1)	26(1)
C(77)	397(2)	3142(1)	5354(1)	26(1)
C(78)	68(2)	2634(1)	5227(1)	32(1)
C(79)	560(2)	2229(1)	5041(1)	33(1)
C(80)	1366(2)	2336(1)	4993(1)	32(1)
C(81)	1652(2)	2850(1)	5139(1)	26(1)
C(82)	2538(2)	2974(1)	5131(1)	32(1)
C(83)	2759(2)	3602(1)	4396(1)	28(1)
C(84)	3265(2)	3170(1)	4136(1)	37(1)
C(85)	1897(2)	3634(1)	4215(1)	28(1)
C(86)	1735(2)	3187(1)	3281(1)	31(1)
C(87)	1049(2)	2831(1)	3448(1)	26(1)
C(88)	268(2)	3033(1)	3434(1)	29(1)
C(89)	-361(2)	2709(1)	3593(1)	29(1)
C(90)	-224(2)	2168(1)	3757(1)	28(1)
C(91)	553(2)	1961(1)	3772(1)	30(1)
C(92)	1184(2)	2299(1)	3621(1)	28(1)
C(93)	125(2)	1084(1)	4076(1)	33(1)
C(94)	463(2)	528(1)	4200(1)	36(1)
C(95)	1213(2)	385(1)	4167(1)	40(1)
C(96)	-1195(2)	2944(1)	3608(1)	41(1)
C(97)	-950(4)	3358(3)	4456(2)	35(1)
C(99)	-66(4)	4194(3)	4652(2)	44(1)
C(97B)	-582(4)	3651(3)	4391(2)	30(1)
C(99B)	-108(5)	4458(3)	4845(3)	37(2)
C(98)	-786(2)	3937(2)	4793(1)	45(1)
C(100)	-109(2)	3607(1)	5560(1)	28(1)
C(101)	2430(2)	4552(1)	5269(1)	30(1)
C(102)	2476(2)	4986(1)	4942(1)	37(1)
C(103)	1930(2)	5419(1)	4964(1)	42(1)
C(104)	1335(2)	5429(1)	5311(1)	36(1)
C(105)	1298(2)	4988(1)	5636(1)	32(1)
C(106)	1829(2)	4548(1)	5615(1)	31(1)
C(107)	749(2)	5905(1)	5345(1)	46(1)
C(108)	-1633(2)	4581(1)	5643(1)	25(1)
C(109)	-2022(2)	4924(1)	5313(1)	28(1)
C(110)	-1957(2)	5494(1)	5354(1)	29(1)

C(111)	-1511(2)	5738(1)	5721(1)	27(1)
C(112)	-1118(2)	5385(1)	6046(1)	29(1)
C(113)	-1179(2)	4809(1)	6009(1)	26(1)
C(114)	-1459(2)	6357(1)	5770(1)	39(1)

Table 3. Bond lengths [A] and angles [deg] for s3334bm.

S(1)-C(10)	1.815(3)
S(1)-C(9)	1.819(3)
S(2)-C(21)	1.819(3)
S(2)-C(20)	1.822(3)
S(3)-O(2)	1.425(2)
S(3)-O(3)	1.431(2)
S(3)-N(2)	1.634(2)
S(3)-C(25)	1.775(3)
S(4)-O(5)	1.4305(18)
S(4)-O(4)	1.4325(18)
S(4)-N(3)	1.638(2)
S(4)-C(32)	1.768(3)
O(1)-C(15)	1.376(3)
O(1)-C(17)	1.420(3)
N(1)-C(1)	1.340(3)
N(1)-C(5)	1.341(3)
N(2)-C(6)	1.461(3)
N(2)-C(7)	1.499(3)
N(3)-C(24)	1.483(3)
N(3)-C(22)	1.493(3)
C(1)-C(2)	1.388(4)
C(1)-C(24)	1.509(4)
C(2)-C(3)	1.376(4)
C(2)-H(2)	0.9500
C(3)-C(4)	1.389(4)
C(3)-H(3)	0.9500
C(4)-C(5)	1.382(4)
C(4)-H(4)	0.9500
C(5)-C(6)	1.517(3)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(8)	1.512(4)
C(7)-C(9)	1.539(4)
C(7)-H(7)	1.0000
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-C(11)	1.512(4)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(12)	1.383(4)
C(11)-C(16)	1.398(4)
C(12)-C(13)	1.392(4)
C(12)-H(12)	0.9500
C(13)-C(14)	1.387(4)
C(13)-C(20)	1.508(4)
C(14)-C(15)	1.387(4)
C(14)-H(14)	0.9500
C(15)-C(16)	1.387(4)
C(16)-H(16)	0.9500
C(17)-C(18)	1.490(4)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900

C(18)-C(19)	1.304(4)
C(18)-H(18)	0.9500
C(19)-H(19A)	0.9500
C(19)-H(19B)	0.9500
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(21)-C(22)	1.527(3)
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(22)-C(23)	1.521(4)
C(22)-H(22)	1.0000
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(25)-C(26)	1.386(4)
C(25)-C(30)	1.388(4)
C(26)-C(27)	1.380(4)
C(26)-H(26)	0.9500
C(27)-C(28)	1.382(4)
C(27)-H(27)	0.9500
C(28)-C(29)	1.400(4)
C(28)-C(31)	1.506(4)
C(29)-C(30)	1.382(4)
C(29)-H(29)	0.9500
C(30)-H(30)	0.9500
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-C(33)	1.377(4)
C(32)-C(37)	1.389(4)
C(33)-C(34)	1.381(4)
C(33)-H(33)	0.9500
C(34)-C(35)	1.397(4)
C(34)-H(34)	0.9500
C(35)-C(36)	1.384(4)
C(35)-C(38)	1.508(4)
C(36)-C(37)	1.376(4)
C(36)-H(36)	0.9500
C(37)-H(37)	0.9500
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800
S(5)-C(48)	1.808(4)
S(5)-C(47)	1.818(3)
S(6)-C(58)	1.811(3)
S(6)-C(59)	1.825(3)
S(7)-O(8)	1.4297(19)
S(7)-O(7)	1.4298(19)
S(7)-N(5)	1.641(2)
S(7)-C(63)	1.767(3)
S(8)-O(9)	1.4359(19)
S(8)-O(10)	1.432(2)
S(8)-N(6)	1.637(2)
S(8)-C(70)	1.775(3)
O(6)-C(55)	1.290(6)
O(6)-C(53)	1.369(3)
O(6)-C(55B)	1.371(6)
N(4)-C(39)	1.339(3)
N(4)-C(43)	1.345(3)
N(5)-C(44)	1.474(3)
N(5)-C(45)	1.500(3)
N(6)-C(62)	1.467(3)

N(6)-C(60)	1.496(3)
C(39)-C(40)	1.380(4)
C(39)-C(62)	1.518(4)
C(40)-C(41)	1.388(4)
C(40)-H(40)	0.9500
C(41)-C(42)	1.379(4)
C(41)-H(41)	0.9500
C(42)-C(43)	1.375(4)
C(42)-H(42)	0.9500
C(43)-C(44)	1.520(4)
C(44)-H(44A)	0.9900
C(44)-H(44B)	0.9900
C(45)-C(46)	1.506(4)
C(45)-C(47)	1.526(4)
C(45)-H(45)	1.0000
C(46)-H(46A)	0.9800
C(46)-H(46B)	0.9800
C(46)-H(46C)	0.9800
C(47)-H(47A)	0.9900
C(47)-H(47B)	0.9900
C(48)-C(49)	1.507(4)
C(48)-H(48A)	0.9900
C(48)-H(48B)	0.9900
C(49)-C(54)	1.378(4)
C(49)-C(50)	1.400(4)
C(50)-C(51)	1.393(4)
C(50)-H(50)	0.9500
C(51)-C(52)	1.387(4)
C(51)-C(58)	1.511(4)
C(52)-C(53)	1.390(4)
C(52)-H(52)	0.9500
C(53)-C(54)	1.386(4)
C(54)-H(54)	0.9500
C(55)-C(56)	1.496(8)
C(55)-H(55A)	0.9900
C(55)-H(55B)	0.9900
C(56)-C(57)	1.296(11)
C(56)-H(56)	0.9500
C(57)-H(57A)	0.9500
C(57)-H(57B)	0.9500
C(55B)-C(56B)	1.498(12)
C(55B)-H(55C)	0.9900
C(55B)-H(55D)	0.9900
C(56B)-C(57B)	1.305(12)
C(56B)-H(56B)	0.9500
C(57B)-H(57C)	0.9500
C(57B)-H(57D)	0.9500
C(58)-H(58A)	0.9900
C(58)-H(58B)	0.9900
C(59)-C(60)	1.536(4)
C(59)-H(59A)	0.9900
C(59)-H(59B)	0.9900
C(60)-C(61)	1.525(4)
C(60)-H(60)	1.0000
C(61)-H(61A)	0.9800
C(61)-H(61B)	0.9800
C(61)-H(61C)	0.9800
C(62)-H(62A)	0.9900
C(62)-H(62B)	0.9900
C(63)-C(64)	1.386(4)
C(63)-C(68)	1.386(4)
C(64)-C(65)	1.377(4)
C(64)-H(64)	0.9500
C(65)-C(66)	1.399(4)

C(65)-H(65)	0.9500
C(66)-C(67)	1.384(4)
C(66)-C(69)	1.503(4)
C(67)-C(68)	1.385(4)
C(67)-H(67)	0.9500
C(68)-H(68)	0.9500
C(69)-H(69A)	0.9800
C(69)-H(69B)	0.9800
C(69)-H(69C)	0.9800
C(70)-C(71)	1.382(4)
C(70)-C(75)	1.390(4)
C(71)-C(72)	1.376(4)
C(71)-H(71)	0.9500
C(72)-C(73)	1.395(4)
C(72)-H(72)	0.9500
C(73)-C(74)	1.383(4)
C(73)-C(76)	1.504(4)
C(74)-C(75)	1.379(4)
C(74)-H(74)	0.9500
C(75)-H(75)	0.9500
C(76)-H(76A)	0.9800
C(76)-H(76B)	0.9800
C(76)-H(76C)	0.9800
S(9)-C(86)	1.819(3)
S(9)-C(85)	1.822(3)
S(10)-C(96)	1.690(3)
S(10)-C(97)	1.824(5)
S(10B)-C(97B)	1.820(7)
S(10B)-C(96)	1.993(4)
S(11)-O(12)	1.430(2)
S(11)-O(13)	1.434(2)
S(11)-N(8)	1.624(2)
S(11)-C(101)	1.763(3)
S(12)-O(14)	1.425(2)
S(12)-O(15)	1.430(2)
S(12)-N(9)	1.640(2)
S(12)-C(108)	1.764(3)
O(11)-C(91)	1.363(3)
O(11)-C(93)	1.425(3)
N(7)-C(77)	1.344(3)
N(7)-C(81)	1.344(3)
N(8)-C(82)	1.462(3)
N(8)-C(83)	1.487(3)
N(9)-C(100)	1.475(3)
N(9)-C(98)	1.479(4)
C(77)-C(78)	1.381(4)
C(77)-C(100)	1.511(4)
C(78)-C(79)	1.374(4)
C(78)-H(78)	0.9500
C(79)-C(80)	1.381(4)
C(79)-H(79)	0.9500
C(80)-C(81)	1.381(4)
C(80)-H(80)	0.9500
C(81)-C(82)	1.514(4)
C(82)-H(82A)	0.9900
C(82)-H(82B)	0.9900
C(83)-C(84)	1.519(4)
C(83)-C(85)	1.532(4)
C(83)-H(83)	1.0000
C(84)-H(84A)	0.9800
C(84)-H(84B)	0.9800
C(84)-H(84C)	0.9800
C(85)-H(85A)	0.9900
C(85)-H(85B)	0.9900

C(86)-C(87)	1.504(4)
C(86)-H(86A)	0.9900
C(86)-H(86B)	0.9900
C(87)-C(92)	1.380(4)
C(87)-C(88)	1.396(4)
C(88)-C(89)	1.381(4)
C(88)-H(88)	0.9500
C(89)-C(90)	1.391(4)
C(89)-C(96)	1.508(4)
C(90)-C(91)	1.393(4)
C(90)-H(90)	0.9500
C(91)-C(92)	1.396(4)
C(92)-H(92)	0.9500
C(93)-C(94)	1.486(4)
C(93)-H(93A)	0.9900
C(93)-H(93B)	0.9900
C(94)-C(95)	1.305(4)
C(94)-H(94)	0.9500
C(95)-H(95A)	0.9500
C(95)-H(95B)	0.9500
C(96)-H(96A)	0.9900
C(96)-H(96B)	0.9900
C(97)-C(98)	1.694(7)
C(97)-H(97A)	0.9900
C(97)-H(97B)	0.9900
C(99)-C(98)	1.410(6)
C(99)-H(99A)	0.9800
C(99)-H(99B)	0.9800
C(99)-H(99C)	0.9800
C(97B)-C(98)	1.355(7)
C(97B)-H(97C)	0.9900
C(97B)-H(97D)	0.9900
C(99B)-C(98)	1.693(8)
C(99B)-H(99D)	0.9800
C(99B)-H(99E)	0.9800
C(99B)-H(99F)	0.9800
C(98)-H(98)	1.0000
C(100)-H(10C)	0.9900
C(100)-H(10D)	0.9900
C(101)-C(102)	1.382(4)
C(101)-C(106)	1.392(4)
C(102)-C(103)	1.386(4)
C(102)-H(102)	0.9500
C(103)-C(104)	1.387(4)
C(103)-H(103)	0.9500
C(104)-C(105)	1.393(4)
C(104)-C(107)	1.507(4)
C(105)-C(106)	1.379(4)
C(105)-H(105)	0.9500
C(106)-H(106)	0.9500
C(107)-H(10E)	0.9800
C(107)-H(10F)	0.9800
C(107)-H(10G)	0.9800
C(108)-C(113)	1.383(4)
C(108)-C(109)	1.392(4)
C(109)-C(110)	1.375(4)
C(109)-H(109)	0.9500
C(110)-C(111)	1.394(4)
C(110)-H(110)	0.9500
C(111)-C(112)	1.400(4)
C(111)-C(114)	1.491(4)
C(112)-C(113)	1.387(4)
C(112)-H(112)	0.9500
C(113)-H(113)	0.9500

C(114)-H(11A)	0.9800
C(114)-H(11B)	0.9800
C(114)-H(11C)	0.9800

C(10)-S(1)-C(9)	101.60(13)
C(21)-S(2)-C(20)	97.84(12)
O(2)-S(3)-O(3)	119.39(12)
O(2)-S(3)-N(2)	106.46(12)
O(3)-S(3)-N(2)	108.84(12)
O(2)-S(3)-C(25)	107.13(12)
O(3)-S(3)-C(25)	106.68(12)
N(2)-S(3)-C(25)	107.87(11)
O(5)-S(4)-O(4)	118.98(11)
O(5)-S(4)-N(3)	107.24(11)
O(4)-S(4)-N(3)	107.07(11)
O(5)-S(4)-C(32)	107.88(12)
O(4)-S(4)-C(32)	108.09(11)
N(3)-S(4)-C(32)	107.02(11)
C(15)-O(1)-C(17)	118.4(2)
C(1)-N(1)-C(5)	117.3(2)
C(6)-N(2)-C(7)	115.6(2)
C(6)-N(2)-S(3)	119.96(18)
C(7)-N(2)-S(3)	122.18(17)
C(24)-N(3)-C(22)	118.3(2)
C(24)-N(3)-S(4)	117.05(16)
C(22)-N(3)-S(4)	115.89(16)
N(1)-C(1)-C(2)	123.2(2)
N(1)-C(1)-C(24)	116.1(2)
C(2)-C(1)-C(24)	120.6(2)
C(3)-C(2)-C(1)	119.1(2)
C(3)-C(2)-H(2)	120.5
C(1)-C(2)-H(2)	120.5
C(2)-C(3)-C(4)	118.1(3)
C(2)-C(3)-H(3)	120.9
C(4)-C(3)-H(3)	120.9
C(5)-C(4)-C(3)	119.3(3)
C(5)-C(4)-H(4)	120.3
C(3)-C(4)-H(4)	120.3
N(1)-C(5)-C(4)	122.9(2)
N(1)-C(5)-C(6)	116.8(2)
C(4)-C(5)-C(6)	120.3(2)
N(2)-C(6)-C(5)	114.5(2)
N(2)-C(6)-H(6A)	108.6
C(5)-C(6)-H(6A)	108.6
N(2)-C(6)-H(6B)	108.6
C(5)-C(6)-H(6B)	108.6
H(6A)-C(6)-H(6B)	107.6
N(2)-C(7)-C(8)	114.0(2)
N(2)-C(7)-C(9)	109.7(2)
C(8)-C(7)-C(9)	112.9(2)
N(2)-C(7)-H(7)	106.6
C(8)-C(7)-H(7)	106.6
C(9)-C(7)-H(7)	106.6
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-S(1)	113.65(19)
C(7)-C(9)-H(9A)	108.8
S(1)-C(9)-H(9A)	108.8
C(7)-C(9)-H(9B)	108.8
S(1)-C(9)-H(9B)	108.8

H(9A)-C(9)-H(9B)	107.7
C(11)-C(10)-S(1)	115.97(19)
C(11)-C(10)-H(10A)	108.3
S(1)-C(10)-H(10A)	108.3
C(11)-C(10)-H(10B)	108.3
S(1)-C(10)-H(10B)	108.3
H(10A)-C(10)-H(10B)	107.4
C(12)-C(11)-C(16)	119.7(2)
C(12)-C(11)-C(10)	121.5(2)
C(16)-C(11)-C(10)	118.8(2)
C(11)-C(12)-C(13)	120.9(2)
C(11)-C(12)-H(12)	119.5
C(13)-C(12)-H(12)	119.5
C(14)-C(13)-C(12)	119.2(2)
C(14)-C(13)-C(20)	120.7(2)
C(12)-C(13)-C(20)	120.0(2)
C(13)-C(14)-C(15)	120.1(2)
C(13)-C(14)-H(14)	119.9
C(15)-C(14)-H(14)	119.9
O(1)-C(15)-C(16)	124.4(2)
O(1)-C(15)-C(14)	114.9(2)
C(16)-C(15)-C(14)	120.7(2)
C(15)-C(16)-C(11)	119.3(2)
C(15)-C(16)-H(16)	120.4
C(11)-C(16)-H(16)	120.4
O(1)-C(17)-C(18)	109.0(2)
O(1)-C(17)-H(17A)	109.9
C(18)-C(17)-H(17A)	109.9
O(1)-C(17)-H(17B)	109.9
C(18)-C(17)-H(17B)	109.9
H(17A)-C(17)-H(17B)	108.3
C(19)-C(18)-C(17)	126.5(3)
C(19)-C(18)-H(18)	116.8
C(17)-C(18)-H(18)	116.8
C(18)-C(19)-H(19A)	120.0
C(18)-C(19)-H(19B)	120.0
H(19A)-C(19)-H(19B)	120.0
C(13)-C(20)-S(2)	114.45(18)
C(13)-C(20)-H(20A)	108.6
S(2)-C(20)-H(20A)	108.6
C(13)-C(20)-H(20B)	108.6
S(2)-C(20)-H(20B)	108.6
H(20A)-C(20)-H(20B)	107.6
C(22)-C(21)-S(2)	110.45(17)
C(22)-C(21)-H(21A)	109.6
S(2)-C(21)-H(21A)	109.6
C(22)-C(21)-H(21B)	109.6
S(2)-C(21)-H(21B)	109.6
H(21A)-C(21)-H(21B)	108.1
N(3)-C(22)-C(23)	112.6(2)
N(3)-C(22)-C(21)	108.8(2)
C(23)-C(22)-C(21)	113.3(2)
N(3)-C(22)-H(22)	107.3
C(23)-C(22)-H(22)	107.3
C(21)-C(22)-H(22)	107.3
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
N(3)-C(24)-C(1)	109.9(2)
N(3)-C(24)-H(24A)	109.7
C(1)-C(24)-H(24A)	109.7

N(3)-C(24)-H(24B)	109.7
C(1)-C(24)-H(24B)	109.7
H(24A)-C(24)-H(24B)	108.2
C(26)-C(25)-C(30)	121.0(3)
C(26)-C(25)-S(3)	119.4(2)
C(30)-C(25)-S(3)	119.6(2)
C(27)-C(26)-C(25)	118.8(3)
C(27)-C(26)-H(26)	120.6
C(25)-C(26)-H(26)	120.6
C(28)-C(27)-C(26)	121.9(3)
C(28)-C(27)-H(27)	119.1
C(26)-C(27)-H(27)	119.1
C(27)-C(28)-C(29)	118.2(3)
C(27)-C(28)-C(31)	121.3(3)
C(29)-C(28)-C(31)	120.5(3)
C(30)-C(29)-C(28)	121.0(3)
C(30)-C(29)-H(29)	119.5
C(28)-C(29)-H(29)	119.5
C(29)-C(30)-C(25)	119.0(3)
C(29)-C(30)-H(30)	120.5
C(25)-C(30)-H(30)	120.5
C(28)-C(31)-H(31A)	109.5
C(28)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(28)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(33)-C(32)-C(37)	120.7(2)
C(33)-C(32)-S(4)	120.2(2)
C(37)-C(32)-S(4)	119.0(2)
C(32)-C(33)-C(34)	119.5(3)
C(32)-C(33)-H(33)	120.3
C(34)-C(33)-H(33)	120.3
C(33)-C(34)-C(35)	120.9(3)
C(33)-C(34)-H(34)	119.5
C(35)-C(34)-H(34)	119.5
C(36)-C(35)-C(34)	118.2(3)
C(36)-C(35)-C(38)	121.1(3)
C(34)-C(35)-C(38)	120.8(3)
C(35)-C(36)-C(37)	121.7(3)
C(35)-C(36)-H(36)	119.2
C(37)-C(36)-H(36)	119.2
C(36)-C(37)-C(32)	119.0(3)
C(36)-C(37)-H(37)	120.5
C(32)-C(37)-H(37)	120.5
C(35)-C(38)-H(38A)	109.5
C(35)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(35)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(48)-S(5)-C(47)	97.97(14)
C(58)-S(6)-C(59)	101.82(13)
O(8)-S(7)-O(7)	119.22(11)
O(8)-S(7)-N(5)	106.74(11)
O(7)-S(7)-N(5)	107.08(11)
O(8)-S(7)-C(63)	106.85(12)
O(7)-S(7)-C(63)	109.02(12)
N(5)-S(7)-C(63)	107.38(12)
O(9)-S(8)-O(10)	119.23(11)
O(9)-S(8)-N(6)	109.19(11)
O(10)-S(8)-N(6)	106.42(11)
O(9)-S(8)-C(70)	106.57(12)
O(10)-S(8)-C(70)	107.63(12)

N(6)-S(8)-C(70)	107.26(12)
C(55)-O(6)-C(53)	123.4(3)
C(55)-O(6)-C(55B)	105.7(4)
C(53)-O(6)-C(55B)	128.9(3)
C(39)-N(4)-C(43)	117.3(2)
C(44)-N(5)-C(45)	118.4(2)
C(44)-N(5)-S(7)	117.94(17)
C(45)-N(5)-S(7)	115.21(17)
C(62)-N(6)-C(60)	115.8(2)
C(62)-N(6)-S(8)	119.78(18)
C(60)-N(6)-S(8)	122.55(18)
N(4)-C(39)-C(40)	123.1(2)
N(4)-C(39)-C(62)	116.7(2)
C(40)-C(39)-C(62)	120.1(2)
C(39)-C(40)-C(41)	118.9(3)
C(39)-C(40)-H(40)	120.6
C(41)-C(40)-H(40)	120.6
C(42)-C(41)-C(40)	118.4(3)
C(42)-C(41)-H(41)	120.8
C(40)-C(41)-H(41)	120.8
C(43)-C(42)-C(41)	119.2(3)
C(43)-C(42)-H(42)	120.4
C(41)-C(42)-H(42)	120.4
N(4)-C(43)-C(42)	123.0(2)
N(4)-C(43)-C(44)	115.5(2)
C(42)-C(43)-C(44)	121.4(2)
N(5)-C(44)-C(43)	109.6(2)
N(5)-C(44)-H(44A)	109.7
C(43)-C(44)-H(44A)	109.7
N(5)-C(44)-H(44B)	109.7
C(43)-C(44)-H(44B)	109.7
H(44A)-C(44)-H(44B)	108.2
N(5)-C(45)-C(46)	112.1(2)
N(5)-C(45)-C(47)	108.9(2)
C(46)-C(45)-C(47)	113.2(2)
N(5)-C(45)-H(45)	107.5
C(46)-C(45)-H(45)	107.5
C(47)-C(45)-H(45)	107.5
C(45)-C(46)-H(46A)	109.5
C(45)-C(46)-H(46B)	109.5
H(46A)-C(46)-H(46B)	109.5
C(45)-C(46)-H(46C)	109.5
H(46A)-C(46)-H(46C)	109.5
H(46B)-C(46)-H(46C)	109.5
C(45)-C(47)-S(5)	109.10(18)
C(45)-C(47)-H(47A)	109.9
S(5)-C(47)-H(47A)	109.9
C(45)-C(47)-H(47B)	109.9
S(5)-C(47)-H(47B)	109.9
H(47A)-C(47)-H(47B)	108.3
C(49)-C(48)-S(5)	114.9(2)
C(49)-C(48)-H(48A)	108.5
S(5)-C(48)-H(48A)	108.5
C(49)-C(48)-H(48B)	108.5
S(5)-C(48)-H(48B)	108.5
H(48A)-C(48)-H(48B)	107.5
C(54)-C(49)-C(50)	119.9(3)
C(54)-C(49)-C(48)	119.3(3)
C(50)-C(49)-C(48)	120.7(3)
C(51)-C(50)-C(49)	120.1(3)
C(51)-C(50)-H(50)	119.9
C(49)-C(50)-H(50)	119.9
C(52)-C(51)-C(50)	119.4(3)
C(52)-C(51)-C(58)	119.3(2)

C(50)-C(51)-C(58)	121.2(3)
C(51)-C(52)-C(53)	120.3(3)
C(51)-C(52)-H(52)	119.9
C(53)-C(52)-H(52)	119.9
O(6)-C(53)-C(54)	119.3(3)
O(6)-C(53)-C(52)	120.5(3)
C(54)-C(53)-C(52)	120.1(3)
C(49)-C(54)-C(53)	120.1(3)
C(49)-C(54)-H(54)	119.9
C(53)-C(54)-H(54)	119.9
O(6)-C(55)-C(56)	109.1(5)
O(6)-C(55)-H(55A)	109.9
C(56)-C(55)-H(55A)	109.9
O(6)-C(55)-H(55B)	109.9
C(56)-C(55)-H(55B)	109.9
H(55A)-C(55)-H(55B)	108.3
C(57)-C(56)-C(55)	124.6(8)
C(57)-C(56)-H(56)	117.7
C(55)-C(56)-H(56)	117.7
C(56)-C(57)-H(57A)	120.0
C(56)-C(57)-H(57B)	120.0
H(57A)-C(57)-H(57B)	120.0
O(6)-C(55B)-C(56B)	118.1(7)
O(6)-C(55B)-H(55C)	107.8
C(56B)-C(55B)-H(55C)	107.8
O(6)-C(55B)-H(55D)	107.8
C(56B)-C(55B)-H(55D)	107.8
H(55C)-C(55B)-H(55D)	107.1
C(57B)-C(56B)-C(55B)	123.9(11)
C(57B)-C(56B)-H(56B)	118.1
C(55B)-C(56B)-H(56B)	118.1
C(56B)-C(57B)-H(57C)	120.0
C(56B)-C(57B)-H(57D)	120.0
H(57C)-C(57B)-H(57D)	120.0
C(51)-C(58)-S(6)	118.16(19)
C(51)-C(58)-H(58A)	107.8
S(6)-C(58)-H(58A)	107.8
C(51)-C(58)-H(58B)	107.8
S(6)-C(58)-H(58B)	107.8
H(58A)-C(58)-H(58B)	107.1
C(60)-C(59)-S(6)	113.14(19)
C(60)-C(59)-H(59A)	109.0
S(6)-C(59)-H(59A)	109.0
C(60)-C(59)-H(59B)	109.0
S(6)-C(59)-H(59B)	109.0
H(59A)-C(59)-H(59B)	107.8
N(6)-C(60)-C(61)	114.2(2)
N(6)-C(60)-C(59)	109.5(2)
C(61)-C(60)-C(59)	112.0(2)
N(6)-C(60)-H(60)	106.9
C(61)-C(60)-H(60)	106.9
C(59)-C(60)-H(60)	106.9
C(60)-C(61)-H(61A)	109.5
C(60)-C(61)-H(61B)	109.5
H(61A)-C(61)-H(61B)	109.5
C(60)-C(61)-H(61C)	109.5
H(61A)-C(61)-H(61C)	109.5
H(61B)-C(61)-H(61C)	109.5
N(6)-C(62)-C(39)	113.7(2)
N(6)-C(62)-H(62A)	108.8
C(39)-C(62)-H(62A)	108.8
N(6)-C(62)-H(62B)	108.8
C(39)-C(62)-H(62B)	108.8
H(62A)-C(62)-H(62B)	107.7

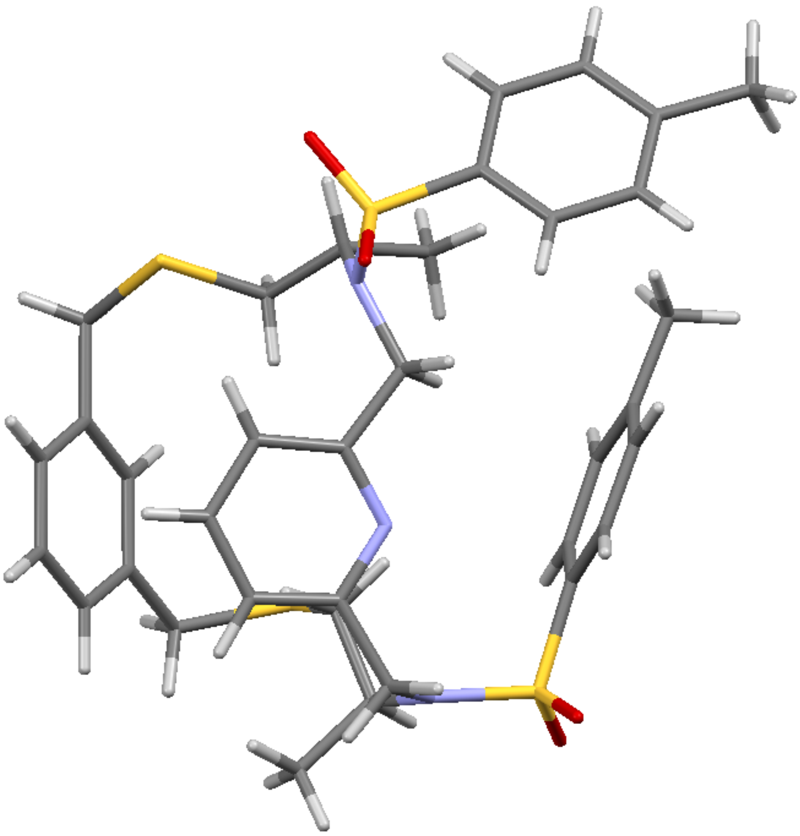
C(64)-C(63)-C(68)	120.8(2)
C(64)-C(63)-S(7)	120.1(2)
C(68)-C(63)-S(7)	119.1(2)
C(65)-C(64)-C(63)	119.2(2)
C(65)-C(64)-H(64)	120.4
C(63)-C(64)-H(64)	120.4
C(64)-C(65)-C(66)	121.2(3)
C(64)-C(65)-H(65)	119.4
C(66)-C(65)-H(65)	119.4
C(67)-C(66)-C(65)	118.5(2)
C(67)-C(66)-C(69)	120.8(2)
C(65)-C(66)-C(69)	120.7(2)
C(66)-C(67)-C(68)	121.1(2)
C(66)-C(67)-H(67)	119.5
C(68)-C(67)-H(67)	119.5
C(67)-C(68)-C(63)	119.3(2)
C(67)-C(68)-H(68)	120.4
C(63)-C(68)-H(68)	120.4
C(66)-C(69)-H(69A)	109.5
C(66)-C(69)-H(69B)	109.5
H(69A)-C(69)-H(69B)	109.5
C(66)-C(69)-H(69C)	109.5
H(69A)-C(69)-H(69C)	109.5
H(69B)-C(69)-H(69C)	109.5
C(71)-C(70)-C(75)	120.2(2)
C(71)-C(70)-S(8)	120.2(2)
C(75)-C(70)-S(8)	119.6(2)
C(72)-C(71)-C(70)	120.0(3)
C(72)-C(71)-H(71)	120.0
C(70)-C(71)-H(71)	120.0
C(71)-C(72)-C(73)	121.1(3)
C(71)-C(72)-H(72)	119.4
C(73)-C(72)-H(72)	119.4
C(74)-C(73)-C(72)	117.6(2)
C(74)-C(73)-C(76)	120.5(2)
C(72)-C(73)-C(76)	122.0(3)
C(73)-C(74)-C(75)	122.3(3)
C(73)-C(74)-H(74)	118.8
C(75)-C(74)-H(74)	118.8
C(74)-C(75)-C(70)	118.7(3)
C(74)-C(75)-H(75)	120.7
C(70)-C(75)-H(75)	120.7
C(73)-C(76)-H(76A)	109.5
C(73)-C(76)-H(76B)	109.5
H(76A)-C(76)-H(76B)	109.5
C(73)-C(76)-H(76C)	109.5
H(76A)-C(76)-H(76C)	109.5
H(76B)-C(76)-H(76C)	109.5
C(86)-S(9)-C(85)	101.55(13)
C(96)-S(10)-C(97)	94.9(2)
C(97B)-S(10B)-C(96)	100.8(2)
O(12)-S(11)-O(13)	119.27(12)
O(12)-S(11)-N(8)	107.00(12)
O(13)-S(11)-N(8)	108.26(12)
O(12)-S(11)-C(101)	108.39(12)
O(13)-S(11)-C(101)	106.24(13)
N(8)-S(11)-C(101)	107.13(12)
O(14)-S(12)-O(15)	119.83(12)
O(14)-S(12)-N(9)	107.67(11)
O(15)-S(12)-N(9)	106.75(11)
O(14)-S(12)-C(108)	108.84(12)
O(15)-S(12)-C(108)	107.78(12)
N(9)-S(12)-C(108)	105.01(12)
C(91)-O(11)-C(93)	116.9(2)

C(77)-N(7)-C(81)	117.3(2)
C(82)-N(8)-C(83)	120.7(2)
C(82)-N(8)-S(11)	121.27(18)
C(83)-N(8)-S(11)	117.70(18)
C(100)-N(9)-C(98)	118.8(2)
C(100)-N(9)-S(12)	118.25(17)
C(98)-N(9)-S(12)	114.53(18)
N(7)-C(77)-C(78)	123.1(2)
N(7)-C(77)-C(100)	115.5(2)
C(78)-C(77)-C(100)	121.4(2)
C(79)-C(78)-C(77)	118.6(3)
C(79)-C(78)-H(78)	120.7
C(77)-C(78)-H(78)	120.7
C(78)-C(79)-C(80)	119.5(3)
C(78)-C(79)-H(79)	120.3
C(80)-C(79)-H(79)	120.3
C(79)-C(80)-C(81)	118.5(3)
C(79)-C(80)-H(80)	120.7
C(81)-C(80)-H(80)	120.7
N(7)-C(81)-C(80)	123.0(3)
N(7)-C(81)-C(82)	116.2(2)
C(80)-C(81)-C(82)	120.7(2)
N(8)-C(82)-C(81)	116.1(2)
N(8)-C(82)-H(82A)	108.3
C(81)-C(82)-H(82A)	108.3
N(8)-C(82)-H(82B)	108.3
C(81)-C(82)-H(82B)	108.3
H(82A)-C(82)-H(82B)	107.4
N(8)-C(83)-C(84)	111.4(2)
N(8)-C(83)-C(85)	110.2(2)
C(84)-C(83)-C(85)	113.9(2)
N(8)-C(83)-H(83)	107.0
C(84)-C(83)-H(83)	107.0
C(85)-C(83)-H(83)	107.0
C(83)-C(84)-H(84A)	109.5
C(83)-C(84)-H(84B)	109.5
H(84A)-C(84)-H(84B)	109.5
C(83)-C(84)-H(84C)	109.5
H(84A)-C(84)-H(84C)	109.5
H(84B)-C(84)-H(84C)	109.5
C(83)-C(85)-S(9)	113.53(18)
C(83)-C(85)-H(85A)	108.9
S(9)-C(85)-H(85A)	108.9
C(83)-C(85)-H(85B)	108.9
S(9)-C(85)-H(85B)	108.9
H(85A)-C(85)-H(85B)	107.7
C(87)-C(86)-S(9)	114.12(18)
C(87)-C(86)-H(86A)	108.7
S(9)-C(86)-H(86A)	108.7
C(87)-C(86)-H(86B)	108.7
S(9)-C(86)-H(86B)	108.7
H(86A)-C(86)-H(86B)	107.6
C(92)-C(87)-C(88)	118.8(2)
C(92)-C(87)-C(86)	120.4(2)
C(88)-C(87)-C(86)	120.9(2)
C(89)-C(88)-C(87)	120.9(3)
C(89)-C(88)-H(88)	119.5
C(87)-C(88)-H(88)	119.5
C(88)-C(89)-C(90)	120.0(3)
C(88)-C(89)-C(96)	120.5(3)
C(90)-C(89)-C(96)	119.4(2)
C(91)-C(90)-C(89)	119.7(3)
C(91)-C(90)-H(90)	120.2
C(89)-C(90)-H(90)	120.2

O(11)-C(91)-C(90)	124.8(2)
O(11)-C(91)-C(92)	115.6(2)
C(90)-C(91)-C(92)	119.6(3)
C(87)-C(92)-C(91)	121.0(3)
C(87)-C(92)-H(92)	119.5
C(91)-C(92)-H(92)	119.5
O(11)-C(93)-C(94)	108.6(2)
O(11)-C(93)-H(93A)	110.0
C(94)-C(93)-H(93A)	110.0
O(11)-C(93)-H(93B)	110.0
C(94)-C(93)-H(93B)	110.0
H(93A)-C(93)-H(93B)	108.4
C(95)-C(94)-C(93)	125.9(3)
C(95)-C(94)-H(94)	117.1
C(93)-C(94)-H(94)	117.1
C(94)-C(95)-H(95A)	120.0
C(94)-C(95)-H(95B)	120.0
H(95A)-C(95)-H(95B)	120.0
C(89)-C(96)-S(10)	117.6(2)
C(89)-C(96)-S(10B)	108.3(2)
S(10)-C(96)-S(10B)	46.57(10)
C(89)-C(96)-H(96A)	107.9
S(10)-C(96)-H(96A)	107.9
S(10B)-C(96)-H(96A)	68.3
C(89)-C(96)-H(96B)	107.9
S(10)-C(96)-H(96B)	107.9
S(10B)-C(96)-H(96B)	143.0
H(96A)-C(96)-H(96B)	107.2
C(98)-C(97)-S(10)	108.4(3)
C(98)-C(97)-H(97A)	110.0
S(10)-C(97)-H(97A)	110.0
C(98)-C(97)-H(97B)	110.0
S(10)-C(97)-H(97B)	110.0
H(97A)-C(97)-H(97B)	108.4
C(98)-C(99)-H(99A)	109.5
C(98)-C(99)-H(99B)	109.5
C(98)-C(99)-H(99C)	109.5
C(98)-C(97B)-S(10B)	104.6(4)
C(98)-C(97B)-H(97C)	110.8
S(10B)-C(97B)-H(97C)	110.8
C(98)-C(97B)-H(97D)	110.8
S(10B)-C(97B)-H(97D)	110.8
H(97C)-C(97B)-H(97D)	108.9
C(98)-C(99B)-H(99D)	109.5
C(98)-C(99B)-H(99E)	109.5
H(99D)-C(99B)-H(99E)	109.5
C(98)-C(99B)-H(99F)	109.5
H(99D)-C(99B)-H(99F)	109.5
H(99E)-C(99B)-H(99F)	109.5
C(97B)-C(98)-C(99)	77.0(4)
C(97B)-C(98)-N(9)	124.8(4)
C(99)-C(98)-N(9)	119.0(3)
C(97B)-C(98)-C(99B)	105.9(4)
C(99)-C(98)-C(99B)	29.4(3)
N(9)-C(98)-C(99B)	105.0(3)
C(97B)-C(98)-C(97)	34.1(3)
C(99)-C(98)-C(97)	110.1(4)
N(9)-C(98)-C(97)	99.7(3)
C(99B)-C(98)-C(97)	139.4(4)
C(97B)-C(98)-H(98)	113.8
C(99)-C(98)-H(98)	109.2
N(9)-C(98)-H(98)	109.2
C(99B)-C(98)-H(98)	92.6
C(97)-C(98)-H(98)	109.2

N(9)-C(100)-C(77)	111.7(2)
N(9)-C(100)-H(10C)	109.3
C(77)-C(100)-H(10C)	109.3
N(9)-C(100)-H(10D)	109.3
C(77)-C(100)-H(10D)	109.3
H(10C)-C(100)-H(10D)	107.9
C(102)-C(101)-C(106)	120.0(3)
C(102)-C(101)-S(11)	120.4(2)
C(106)-C(101)-S(11)	119.6(2)
C(101)-C(102)-C(103)	119.8(3)
C(101)-C(102)-H(102)	120.1
C(103)-C(102)-H(102)	120.1
C(104)-C(103)-C(102)	121.2(3)
C(104)-C(103)-H(103)	119.4
C(102)-C(103)-H(103)	119.4
C(103)-C(104)-C(105)	118.0(3)
C(103)-C(104)-C(107)	121.7(3)
C(105)-C(104)-C(107)	120.2(3)
C(106)-C(105)-C(104)	121.5(3)
C(106)-C(105)-H(105)	119.3
C(104)-C(105)-H(105)	119.3
C(105)-C(106)-C(101)	119.5(3)
C(105)-C(106)-H(106)	120.3
C(101)-C(106)-H(106)	120.3
C(104)-C(107)-H(10E)	109.5
C(104)-C(107)-H(10F)	109.5
H(10E)-C(107)-H(10F)	109.5
C(104)-C(107)-H(10G)	109.5
H(10E)-C(107)-H(10G)	109.5
H(10F)-C(107)-H(10G)	109.5
C(113)-C(108)-C(109)	120.7(2)
C(113)-C(108)-S(12)	119.6(2)
C(109)-C(108)-S(12)	119.6(2)
C(110)-C(109)-C(108)	119.6(2)
C(110)-C(109)-H(109)	120.2
C(108)-C(109)-H(109)	120.2
C(109)-C(110)-C(111)	121.2(2)
C(109)-C(110)-H(110)	119.4
C(111)-C(110)-H(110)	119.4
C(110)-C(111)-C(112)	118.2(2)
C(110)-C(111)-C(114)	120.8(3)
C(112)-C(111)-C(114)	120.9(2)
C(113)-C(112)-C(111)	121.2(2)
C(113)-C(112)-H(112)	119.4
C(111)-C(112)-H(112)	119.4
C(108)-C(113)-C(112)	119.1(2)
C(108)-C(113)-H(113)	120.4
C(112)-C(113)-H(113)	120.4
C(111)-C(114)-H(11A)	109.5
C(111)-C(114)-H(11B)	109.5
H(11A)-C(114)-H(11B)	109.5
C(111)-C(114)-H(11C)	109.5
H(11A)-C(114)-H(11C)	109.5
H(11B)-C(114)-H(11C)	109.5

Crystal data and structure refinement for 26 (UoM code: s3313m).
CCDC 1411542



Identification code	s3313m
Empirical formula	C36 H43 Cl2 N3 O4 S4
Formula weight	780.87
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 10.9439(14) A alpha = 90 deg. b = 17.302(2) A beta = 90 deg. c = 19.969(3) A gamma = 90 deg.
Volume	3781.2(8) A^3
Z, Calculated density	4, 1.372 Mg/m^3
Absorption coefficient	0.435 mm^-1
F(000)	1640
Crystal size	0.50 x 0.40 x 0.25 mm
Theta range for data collection	2.04 to 28.27 deg.
Limiting indices	-14<=h<=14, -22<=k<=22, -26<=l<=15
Reflections collected / unique	23961 / 8896 [R(int) = 0.0802]

Completeness to theta = 25.00	100.0 %
Absorption correction	None
Max. and min. transmission	0.8990 and 0.8118
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8896 / 0 / 446
Goodness-of-fit on F^2	0.743
Final R indices [I>2sigma(I)]	R1 = 0.0470, wR2 = 0.0636
R indices (all data)	R1 = 0.0756, wR2 = 0.0694
Absolute structure parameter	-0.07(5)
Largest diff. peak and hole	0.522 and -0.350 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for s3313m. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	8516(3)	11192(2)	9843(2)	17(1)
C(2)	7114(3)	11265(2)	9805(2)	17(1)
C(3)	6435(3)	12652(2)	9133(2)	25(1)
C(4)	5691(3)	12172(2)	8652(2)	18(1)
C(5)	6209(3)	11902(2)	8054(2)	23(1)
C(6)	5520(3)	11466(2)	7606(2)	25(1)
C(7)	4317(3)	11288(2)	7756(2)	23(1)
C(8)	3786(3)	11540(2)	8346(2)	18(1)
C(9)	4486(3)	11981(2)	8782(2)	18(1)
C(10)	2471(3)	11357(2)	8509(2)	20(1)
C(11)	2917(3)	10420(2)	9604(1)	20(1)
C(12)	2742(3)	9667(2)	9988(2)	17(1)
C(13)	4823(3)	9045(2)	9854(2)	18(1)
C(14)	5667(3)	9330(2)	9305(2)	14(1)
C(15)	5305(3)	9442(2)	8647(2)	16(1)
C(16)	6157(3)	9700(2)	8188(2)	19(1)
C(17)	7337(3)	9845(2)	8411(2)	17(1)
C(18)	7624(3)	9716(2)	9071(2)	15(1)
C(19)	8891(3)	9854(2)	9346(2)	21(1)
C(20)	7887(3)	9755(2)	11079(2)	16(1)
C(21)	7178(3)	10289(2)	11408(2)	22(1)
C(22)	6142(3)	10045(2)	11743(2)	22(1)
C(23)	5822(3)	9272(2)	11774(2)	24(1)
C(24)	6541(3)	8741(2)	11434(2)	21(1)
C(25)	7572(3)	8978(2)	11079(2)	18(1)
C(26)	4728(3)	9009(2)	12176(2)	31(1)
C(27)	9145(3)	11567(2)	9242(2)	27(1)
C(28)	2959(3)	9792(2)	10741(2)	25(1)
C(29)	2766(3)	7747(2)	10349(2)	15(1)
C(30)	1703(3)	7831(2)	10723(2)	16(1)
C(31)	1654(3)	7545(2)	11367(2)	18(1)
C(32)	2663(3)	7184(2)	11655(2)	17(1)
C(33)	3709(3)	7094(2)	11268(2)	17(1)

C(34)	3769(3)	7363(2)	10616(2)	17(1)
C(35)	2628(3)	6919(2)	12377(1)	24(1)
C(36)	2601(3)	1433(2)	2743(2)	31(1)
Cl(1)	1626(1)	958(1)	2174(1)	36(1)
Cl(2)	3928(1)	1785(1)	2339(1)	39(1)
N(1)	8924(2)	10379(1)	9928(1)	16(1)
N(2)	3503(2)	9050(1)	9692(1)	15(1)
N(3)	6804(2)	9458(1)	9522(1)	15(1)
O(1)	9714(2)	10690(1)	11048(1)	25(1)
O(2)	9966(2)	9371(1)	10580(1)	28(1)
O(3)	1678(2)	8331(1)	9304(1)	19(1)
O(4)	3741(2)	7768(1)	9161(1)	20(1)
S(1)	6552(1)	12233(1)	9966(1)	24(1)
S(2)	2207(1)	10372(1)	8789(1)	20(1)
S(3)	9242(1)	10051(1)	10665(1)	19(1)
S(4)	2885(1)	8198(1)	9561(1)	16(1)

Table 3. Bond lengths [A] and angles [deg] for s3313m.

C(1)-N(1)	1.485(4)
C(1)-C(27)	1.527(4)
C(1)-C(2)	1.541(4)
C(1)-H(1)	1.0000
C(2)-S(1)	1.812(3)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(4)	1.509(4)
C(3)-S(1)	1.819(3)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(9)	1.384(4)
C(4)-C(5)	1.402(4)
C(5)-C(6)	1.392(4)
C(5)-H(5)	0.9500
C(6)-C(7)	1.384(4)
C(6)-H(6)	0.9500
C(7)-C(8)	1.385(4)
C(7)-H(7)	0.9500
C(8)-C(9)	1.389(4)
C(8)-C(10)	1.509(4)
C(9)-H(9)	0.9500
C(10)-S(2)	1.815(3)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(12)	1.525(4)
C(11)-S(2)	1.806(3)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-N(2)	1.478(4)
C(12)-C(28)	1.538(4)
C(12)-H(12)	1.0000
C(13)-N(2)	1.481(4)
C(13)-C(14)	1.516(4)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-N(3)	1.337(4)
C(14)-C(15)	1.386(4)
C(15)-C(16)	1.381(4)
C(15)-H(15)	0.9500
C(16)-C(17)	1.388(4)
C(16)-H(16)	0.9500
C(17)-C(18)	1.374(4)

C(17)-H(17)	0.9500
C(18)-N(3)	1.347(4)
C(18)-C(19)	1.510(4)
C(19)-N(1)	1.476(4)
C(19)-H(19A)	0.9900
C(19)-H(19B)	0.9900
C(20)-C(21)	1.375(4)
C(20)-C(25)	1.387(4)
C(20)-S(3)	1.773(3)
C(21)-C(22)	1.383(4)
C(21)-H(21)	0.9500
C(22)-C(23)	1.383(4)
C(22)-H(22)	0.9500
C(23)-C(24)	1.387(4)
C(23)-C(26)	1.512(4)
C(24)-C(25)	1.394(4)
C(24)-H(24)	0.9500
C(25)-H(25)	0.9500
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-C(34)	1.389(4)
C(29)-C(30)	1.390(4)
C(29)-S(4)	1.761(3)
C(30)-C(31)	1.379(4)
C(30)-H(30)	0.9500
C(31)-C(32)	1.392(4)
C(31)-H(31)	0.9500
C(32)-C(33)	1.390(4)
C(32)-C(35)	1.513(4)
C(33)-C(34)	1.384(4)
C(33)-H(33)	0.9500
C(34)-H(34)	0.9500
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36)-Cl(1)	1.762(3)
C(36)-Cl(2)	1.768(4)
C(36)-H(36A)	0.9900
C(36)-H(36B)	0.9900
N(1)-S(3)	1.616(3)
N(2)-S(4)	1.641(2)
O(1)-S(3)	1.440(2)
O(2)-S(3)	1.427(2)
O(3)-S(4)	1.437(2)
O(4)-S(4)	1.439(2)

N(1)-C(1)-C(27)	110.8(3)
N(1)-C(1)-C(2)	112.5(3)
C(27)-C(1)-C(2)	112.1(3)
N(1)-C(1)-H(1)	107.0
C(27)-C(1)-H(1)	107.0
C(2)-C(1)-H(1)	107.0
C(1)-C(2)-S(1)	113.9(2)
C(1)-C(2)-H(2A)	108.8
S(1)-C(2)-H(2A)	108.8
C(1)-C(2)-H(2B)	108.8
S(1)-C(2)-H(2B)	108.8

H(2A)-C(2)-H(2B)	107.7
C(4)-C(3)-S(1)	113.6(2)
C(4)-C(3)-H(3A)	108.9
S(1)-C(3)-H(3A)	108.9
C(4)-C(3)-H(3B)	108.9
S(1)-C(3)-H(3B)	108.9
H(3A)-C(3)-H(3B)	107.7
C(9)-C(4)-C(5)	117.7(3)
C(9)-C(4)-C(3)	121.8(3)
C(5)-C(4)-C(3)	120.5(3)
C(6)-C(5)-C(4)	120.6(3)
C(6)-C(5)-H(5)	119.7
C(4)-C(5)-H(5)	119.7
C(7)-C(6)-C(5)	119.8(3)
C(7)-C(6)-H(6)	120.1
C(5)-C(6)-H(6)	120.1
C(6)-C(7)-C(8)	120.8(3)
C(6)-C(7)-H(7)	119.6
C(8)-C(7)-H(7)	119.6
C(7)-C(8)-C(9)	118.4(3)
C(7)-C(8)-C(10)	121.2(3)
C(9)-C(8)-C(10)	120.4(3)
C(4)-C(9)-C(8)	122.6(3)
C(4)-C(9)-H(9)	118.7
C(8)-C(9)-H(9)	118.7
C(8)-C(10)-S(2)	114.5(2)
C(8)-C(10)-H(10A)	108.6
S(2)-C(10)-H(10A)	108.6
C(8)-C(10)-H(10B)	108.6
S(2)-C(10)-H(10B)	108.6
H(10A)-C(10)-H(10B)	107.6
C(12)-C(11)-S(2)	111.1(2)
C(12)-C(11)-H(11A)	109.4
S(2)-C(11)-H(11A)	109.4
C(12)-C(11)-H(11B)	109.4
S(2)-C(11)-H(11B)	109.4
H(11A)-C(11)-H(11B)	108.0
N(2)-C(12)-C(11)	110.2(2)
N(2)-C(12)-C(28)	113.9(3)
C(11)-C(12)-C(28)	110.6(2)
N(2)-C(12)-H(12)	107.2
C(11)-C(12)-H(12)	107.2
C(28)-C(12)-H(12)	107.2
N(2)-C(13)-C(14)	115.8(3)
N(2)-C(13)-H(13A)	108.3
C(14)-C(13)-H(13A)	108.3
N(2)-C(13)-H(13B)	108.3
C(14)-C(13)-H(13B)	108.3
H(13A)-C(13)-H(13B)	107.4
N(3)-C(14)-C(15)	123.4(3)
N(3)-C(14)-C(13)	112.7(3)
C(15)-C(14)-C(13)	123.9(3)
C(16)-C(15)-C(14)	118.7(3)
C(16)-C(15)-H(15)	120.6
C(14)-C(15)-H(15)	120.6
C(15)-C(16)-C(17)	118.4(3)
C(15)-C(16)-H(16)	120.8
C(17)-C(16)-H(16)	120.8
C(18)-C(17)-C(16)	119.3(3)
C(18)-C(17)-H(17)	120.3
C(16)-C(17)-H(17)	120.3
N(3)-C(18)-C(17)	122.9(3)
N(3)-C(18)-C(19)	114.9(3)
C(17)-C(18)-C(19)	122.2(3)

N(1)-C(19)-C(18)	113.9(2)
N(1)-C(19)-H(19A)	108.8
C(18)-C(19)-H(19A)	108.8
N(1)-C(19)-H(19B)	108.8
C(18)-C(19)-H(19B)	108.8
H(19A)-C(19)-H(19B)	107.7
C(21)-C(20)-C(25)	120.8(3)
C(21)-C(20)-S(3)	120.0(2)
C(25)-C(20)-S(3)	119.2(2)
C(20)-C(21)-C(22)	119.3(3)
C(20)-C(21)-H(21)	120.4
C(22)-C(21)-H(21)	120.4
C(21)-C(22)-C(23)	121.6(3)
C(21)-C(22)-H(22)	119.2
C(23)-C(22)-H(22)	119.2
C(22)-C(23)-C(24)	118.4(3)
C(22)-C(23)-C(26)	121.0(3)
C(24)-C(23)-C(26)	120.6(3)
C(23)-C(24)-C(25)	120.9(3)
C(23)-C(24)-H(24)	119.6
C(25)-C(24)-H(24)	119.6
C(20)-C(25)-C(24)	119.1(3)
C(20)-C(25)-H(25)	120.5
C(24)-C(25)-H(25)	120.5
C(23)-C(26)-H(26A)	109.5
C(23)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(23)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(1)-C(27)-H(27A)	109.5
C(1)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(1)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(12)-C(28)-H(28A)	109.5
C(12)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(12)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(34)-C(29)-C(30)	120.3(3)
C(34)-C(29)-S(4)	119.8(3)
C(30)-C(29)-S(4)	119.7(2)
C(31)-C(30)-C(29)	119.7(3)
C(31)-C(30)-H(30)	120.1
C(29)-C(30)-H(30)	120.1
C(30)-C(31)-C(32)	121.0(3)
C(30)-C(31)-H(31)	119.5
C(32)-C(31)-H(31)	119.5
C(33)-C(32)-C(31)	118.3(3)
C(33)-C(32)-C(35)	121.1(3)
C(31)-C(32)-C(35)	120.6(3)
C(34)-C(33)-C(32)	121.6(3)
C(34)-C(33)-H(33)	119.2
C(32)-C(33)-H(33)	119.2
C(33)-C(34)-C(29)	119.0(3)
C(33)-C(34)-H(34)	120.5
C(29)-C(34)-H(34)	120.5
C(32)-C(35)-H(35A)	109.5
C(32)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(32)-C(35)-H(35C)	109.5

H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
Cl(1)-C(36)-Cl(2)	111.40(18)
Cl(1)-C(36)-H(36A)	109.3
Cl(2)-C(36)-H(36A)	109.3
Cl(1)-C(36)-H(36B)	109.3
Cl(2)-C(36)-H(36B)	109.3
H(36A)-C(36)-H(36B)	108.0
C(19)-N(1)-C(1)	119.1(2)
C(19)-N(1)-S(3)	120.4(2)
C(1)-N(1)-S(3)	120.1(2)
C(12)-N(2)-C(13)	117.8(2)
C(12)-N(2)-S(4)	118.7(2)
C(13)-N(2)-S(4)	115.6(2)
C(14)-N(3)-C(18)	117.3(3)
C(2)-S(1)-C(3)	103.33(15)
C(11)-S(2)-C(10)	99.55(14)
O(2)-S(3)-O(1)	119.76(14)
O(2)-S(3)-N(1)	107.47(14)
O(1)-S(3)-N(1)	106.88(14)
O(2)-S(3)-C(20)	106.38(14)
O(1)-S(3)-C(20)	105.95(14)
N(1)-S(3)-C(20)	110.26(14)
O(3)-S(4)-O(4)	118.84(13)
O(3)-S(4)-N(2)	106.99(13)
O(4)-S(4)-N(2)	106.55(13)
O(3)-S(4)-C(29)	108.85(15)
O(4)-S(4)-C(29)	108.30(14)
N(2)-S(4)-C(29)	106.67(13)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for s3313m.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	17(2)	15(2)	18(2)	-3(2)	1(2)	-3(2)
C(2)	14(2)	18(2)	19(2)	1(2)	2(2)	-1(2)
C(3)	15(2)	23(2)	35(2)	4(2)	-4(2)	-2(2)
C(4)	20(2)	10(2)	23(2)	3(2)	1(2)	3(2)
C(5)	16(2)	23(2)	30(2)	8(2)	6(2)	1(2)
C(6)	34(2)	25(2)	15(2)	2(2)	6(2)	2(2)
C(7)	28(2)	20(2)	22(2)	1(2)	-3(2)	-3(2)
C(8)	18(2)	16(2)	19(2)	1(2)	-5(2)	3(2)
C(9)	22(2)	14(2)	19(2)	0(2)	0(2)	4(2)
C(10)	16(2)	20(2)	23(2)	4(2)	-6(2)	0(1)
C(11)	19(2)	13(2)	27(2)	0(2)	-1(2)	1(2)
C(12)	10(2)	21(2)	21(2)	-1(2)	-2(2)	-1(2)
C(13)	13(2)	23(2)	17(2)	4(2)	-2(2)	1(2)
C(14)	13(2)	11(2)	18(2)	0(2)	2(2)	0(1)
C(15)	13(2)	20(2)	15(2)	-4(2)	-2(2)	3(1)
C(16)	25(2)	16(2)	16(2)	-3(2)	1(2)	1(2)
C(17)	18(2)	12(2)	22(2)	-1(2)	8(2)	-7(1)
C(18)	14(2)	8(2)	23(2)	-3(2)	6(2)	-1(1)
C(19)	14(2)	20(2)	28(2)	-4(2)	4(2)	-2(1)
C(20)	15(2)	16(2)	16(2)	4(1)	1(2)	1(2)
C(21)	25(2)	21(2)	19(2)	0(2)	-3(2)	-4(2)

C(22)	20(2)	29(2)	19(2)	-9(2)	2(2)	6(2)
C(23)	17(2)	37(2)	17(2)	1(2)	-2(2)	-5(2)
C(24)	22(2)	19(2)	24(2)	2(2)	-2(2)	-5(2)
C(25)	17(2)	19(2)	19(2)	-3(2)	-1(2)	5(1)
C(26)	26(2)	48(2)	19(2)	7(2)	4(2)	-2(2)
C(27)	14(2)	26(2)	41(2)	6(2)	3(2)	-1(2)
C(28)	26(2)	26(2)	22(2)	1(2)	6(2)	-2(2)
C(29)	15(2)	14(2)	17(2)	4(2)	0(2)	-4(2)
C(30)	15(2)	13(2)	21(2)	0(2)	-4(2)	1(1)
C(31)	18(2)	18(2)	19(2)	-1(2)	6(2)	-4(2)
C(32)	27(2)	6(2)	18(2)	-1(1)	0(2)	-3(2)
C(33)	20(2)	11(2)	20(2)	3(2)	-3(2)	1(1)
C(34)	12(2)	14(2)	24(2)	-2(2)	5(2)	-1(1)
C(35)	32(2)	17(2)	23(2)	0(2)	1(2)	4(2)
C(36)	48(3)	27(2)	18(2)	-1(2)	-4(2)	-2(2)
Cl(1)	49(1)	38(1)	22(1)	-2(1)	0(1)	-16(1)
Cl(2)	24(1)	47(1)	45(1)	-2(1)	-6(1)	5(1)
N(1)	13(2)	13(1)	23(2)	0(1)	4(1)	0(1)
N(2)	11(2)	15(1)	18(2)	2(1)	1(1)	1(1)
N(3)	17(2)	12(1)	17(2)	-3(1)	3(1)	0(1)
O(1)	18(1)	28(1)	29(2)	2(1)	-8(1)	-9(1)
O(2)	16(1)	23(1)	46(2)	14(1)	4(1)	6(1)
O(3)	14(1)	22(1)	20(1)	3(1)	-7(1)	-7(1)
O(4)	19(1)	23(1)	18(1)	-2(1)	5(1)	1(1)
S(1)	21(1)	23(1)	28(1)	-8(1)	-4(1)	6(1)
S(2)	18(1)	18(1)	24(1)	2(1)	-4(1)	-3(1)
S(3)	11(1)	20(1)	28(1)	4(1)	-2(1)	0(1)
S(4)	14(1)	17(1)	17(1)	2(1)	0(1)	-2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for s3313m.

	x	y	z	U(eq)
H(1)	8786	11482	10250	20
H(2A)	6746	10907	10135	20
H(2B)	6840	11102	9354	20
H(3A)	6060	13171	9170	29
H(3B)	7268	12719	8948	29
H(5)	7037	12018	7954	28
H(6)	5874	11291	7199	30
H(7)	3850	10989	7449	28
H(9)	4123	12158	9186	22
H(10A)	1968	11453	8106	23
H(10B)	2189	11716	8863	23
H(11A)	3801	10524	9551	24
H(11B)	2556	10852	9862	24
H(12)	1869	9509	9932	21
H(13A)	5062	8510	9971	21
H(13B)	4954	9369	10256	21
H(15)	4486	9343	8514	19
H(16)	5941	9777	7732	23
H(17)	7941	10031	8109	21
H(19A)	9249	9351	9477	25
H(19B)	9408	10073	8986	25
H(21)	7397	10821	11405	26
H(22)	5638	10417	11958	27
H(24)	6329	8209	11444	26
H(25)	8052	8613	10840	22
H(26A)	4999	8832	12618	47

H(26B)	4320	8584	11942	47
H(26C)	4157	9441	12230	47
H(27A)	10019	11447	9253	41
H(27B)	9031	12128	9261	41
H(27C)	8787	11366	8828	41
H(28A)	2982	9290	10969	37
H(28B)	2294	10105	10927	37
H(28C)	3738	10060	10808	37
H(30)	1013	8084	10535	20
H(31)	921	7595	11618	22
H(33)	4400	6842	11456	20
H(34)	4484	7285	10355	20
H(35A)	3032	6416	12415	36
H(35B)	1777	6873	12523	36
H(35C)	3053	7297	12658	36
H(36A)	2841	1070	3102	37
H(36B)	2159	1870	2952	37

Table 6. Torsion angles [deg] for s3313m.

N(1)-C(1)-C(2)-S(1)	161.6(2)
C(27)-C(1)-C(2)-S(1)	-72.7(3)
S(1)-C(3)-C(4)-C(9)	58.2(4)
S(1)-C(3)-C(4)-C(5)	-121.7(3)
C(9)-C(4)-C(5)-C(6)	0.8(5)
C(3)-C(4)-C(5)-C(6)	-179.3(3)
C(4)-C(5)-C(6)-C(7)	-0.8(5)
C(5)-C(6)-C(7)-C(8)	0.1(5)
C(6)-C(7)-C(8)-C(9)	0.6(5)
C(6)-C(7)-C(8)-C(10)	179.3(3)
C(5)-C(4)-C(9)-C(8)	-0.1(5)
C(3)-C(4)-C(9)-C(8)	180.0(3)
C(7)-C(8)-C(9)-C(4)	-0.5(5)
C(10)-C(8)-C(9)-C(4)	-179.2(3)
C(7)-C(8)-C(10)-S(2)	76.5(3)
C(9)-C(8)-C(10)-S(2)	-104.8(3)
S(2)-C(11)-C(12)-N(2)	71.6(3)
S(2)-C(11)-C(12)-C(28)	-161.4(2)
N(2)-C(13)-C(14)-N(3)	167.5(3)
N(2)-C(13)-C(14)-C(15)	-13.0(4)
N(3)-C(14)-C(15)-C(16)	-0.2(5)
C(13)-C(14)-C(15)-C(16)	-179.6(3)
C(14)-C(15)-C(16)-C(17)	-0.7(4)
C(15)-C(16)-C(17)-C(18)	1.0(4)
C(16)-C(17)-C(18)-N(3)	-0.4(5)
C(16)-C(17)-C(18)-C(19)	179.4(3)
N(3)-C(18)-C(19)-N(1)	-55.0(4)
C(17)-C(18)-C(19)-N(1)	125.2(3)
C(25)-C(20)-C(21)-C(22)	0.2(5)
S(3)-C(20)-C(21)-C(22)	-178.2(2)
C(20)-C(21)-C(22)-C(23)	2.1(5)
C(21)-C(22)-C(23)-C(24)	-2.6(5)
C(21)-C(22)-C(23)-C(26)	176.4(3)
C(22)-C(23)-C(24)-C(25)	0.9(5)
C(26)-C(23)-C(24)-C(25)	-178.1(3)
C(21)-C(20)-C(25)-C(24)	-1.8(5)
S(3)-C(20)-C(25)-C(24)	176.6(2)
C(23)-C(24)-C(25)-C(20)	1.2(5)
C(34)-C(29)-C(30)-C(31)	1.3(4)
S(4)-C(29)-C(30)-C(31)	-173.4(2)
C(29)-C(30)-C(31)-C(32)	1.2(4)
C(30)-C(31)-C(32)-C(33)	-2.3(4)

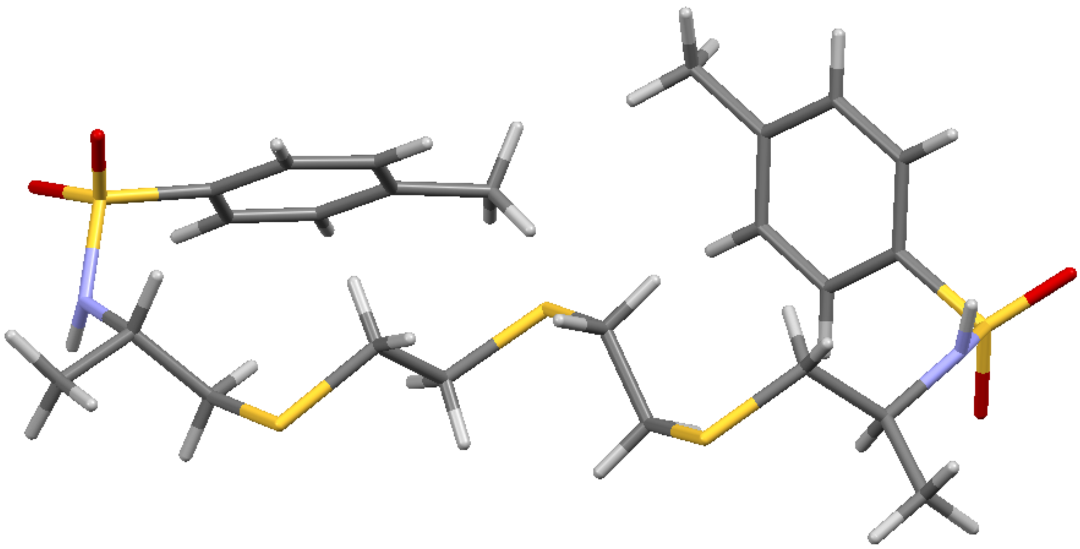
C(30)-C(31)-C(32)-C(35)	176.0(3)
C(31)-C(32)-C(33)-C(34)	0.9(5)
C(35)-C(32)-C(33)-C(34)	-177.3(3)
C(32)-C(33)-C(34)-C(29)	1.5(5)
C(30)-C(29)-C(34)-C(33)	-2.6(4)
S(4)-C(29)-C(34)-C(33)	172.1(2)
C(18)-C(19)-N(1)-C(1)	-62.8(4)
C(18)-C(19)-N(1)-S(3)	109.8(3)
C(27)-C(1)-N(1)-C(19)	-50.6(4)
C(2)-C(1)-N(1)-C(19)	75.8(3)
C(27)-C(1)-N(1)-S(3)	136.8(2)
C(2)-C(1)-N(1)-S(3)	-96.8(3)
C(11)-C(12)-N(2)-C(13)	78.2(3)
C(28)-C(12)-N(2)-C(13)	-46.8(3)
C(11)-C(12)-N(2)-S(4)	-134.1(2)
C(28)-C(12)-N(2)-S(4)	100.8(3)
C(14)-C(13)-N(2)-C(12)	-104.2(3)
C(14)-C(13)-N(2)-S(4)	107.2(3)
C(15)-C(14)-N(3)-C(18)	0.8(4)
C(13)-C(14)-N(3)-C(18)	-179.7(2)
C(17)-C(18)-N(3)-C(14)	-0.5(4)
C(19)-C(18)-N(3)-C(14)	179.7(3)
C(1)-C(2)-S(1)-C(3)	93.5(2)
C(4)-C(3)-S(1)-C(2)	53.5(3)
C(12)-C(11)-S(2)-C(10)	175.5(2)
C(8)-C(10)-S(2)-C(11)	70.9(3)
C(19)-N(1)-S(3)-O(2)	26.0(2)
C(1)-N(1)-S(3)-O(2)	-161.4(2)
C(19)-N(1)-S(3)-O(1)	155.8(2)
C(1)-N(1)-S(3)-O(1)	-31.7(3)
C(19)-N(1)-S(3)-C(20)	-89.5(2)
C(1)-N(1)-S(3)-C(20)	83.0(2)
C(21)-C(20)-S(3)-O(2)	160.5(3)
C(25)-C(20)-S(3)-O(2)	-17.9(3)
C(21)-C(20)-S(3)-O(1)	32.1(3)
C(25)-C(20)-S(3)-O(1)	-146.4(3)
C(21)-C(20)-S(3)-N(1)	-83.2(3)
C(25)-C(20)-S(3)-N(1)	98.3(3)
C(12)-N(2)-S(4)-O(3)	41.3(2)
C(13)-N(2)-S(4)-O(3)	-170.4(2)
C(12)-N(2)-S(4)-O(4)	169.4(2)
C(13)-N(2)-S(4)-O(4)	-42.3(2)
C(12)-N(2)-S(4)-C(29)	-75.1(2)
C(13)-N(2)-S(4)-C(29)	73.3(2)
C(34)-C(29)-S(4)-O(3)	161.7(2)
C(30)-C(29)-S(4)-O(3)	-23.6(3)
C(34)-C(29)-S(4)-O(4)	31.2(3)
C(30)-C(29)-S(4)-O(4)	-154.1(2)
C(34)-C(29)-S(4)-N(2)	-83.1(3)
C(30)-C(29)-S(4)-N(2)	91.6(3)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for s3313m [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)

Crystal data and structure refinement for 10 (UoM code: s3119m).
CCDC 1411557



Identification code	s3119m
Empirical formula	C24 H36 N2 O4 S5
Formula weight	576.85
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 5.9470(5) A alpha = 90 deg. b = 17.8499(16) A beta = 90 deg. c = 27.203(3) A gamma = 90 deg.
Volume	2887.7(4) A^3
Z, Calculated density	4, 1.327 Mg/m^3
Absorption coefficient	0.433 mm^-1
F(000)	1224
Crystal size	0.30 x 0.20 x 0.10 mm
Theta range for data collection	1.36 to 28.28 deg.
Limiting indices	-7<=h<=7, -23<=k<=23, -35<=l<=35
Reflections collected / unique	25072 / 6868 [R(int) = 0.0805]
Completeness to theta = 25.00	100.0 %
Absorption correction	None

Max. and min. transmission	0.9580 and 0.8810
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6868 / 0 / 328
Goodness-of-fit on F^2	0.879
Final R indices [I>2sigma(I)]	R1 = 0.0585, wR2 = 0.1153
R indices (all data)	R1 = 0.1157, wR2 = 0.1452
Absolute structure parameter	-0.07(11)
Largest diff. peak and hole	0.422 and -0.425 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for s3119m.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	9936(8)	5624(2)	11025(2)	28(1)
C(2)	8316(8)	5981(2)	11298(2)	35(1)
C(3)	6701(9)	6414(3)	11065(2)	39(1)
C(4)	6702(8)	6494(2)	10560(2)	36(1)
C(5)	8319(9)	6129(3)	10294(2)	39(1)
C(6)	9962(8)	5692(2)	10517(2)	34(1)
C(7)	4941(9)	6974(3)	10312(2)	57(2)
C(8)	10618(10)	3697(3)	11073(2)	45(2)
C(9)	8131(9)	3564(3)	10988(2)	36(1)
C(10)	7604(11)	3670(3)	9976(2)	47(2)
C(11)	5528(10)	4153(3)	9981(2)	50(2)
C(12)	4849(8)	4290(3)	8972(2)	36(1)
C(13)	2571(9)	3936(3)	8963(2)	50(2)
C(14)	1752(10)	4019(3)	7944(2)	47(1)
C(15)	-706(8)	4099(2)	7827(2)	31(1)
C(16)	-33(9)	5985(3)	8006(2)	38(1)
C(17)	125(10)	5876(3)	8514(2)	50(2)
C(18)	1822(11)	6216(3)	8776(2)	58(2)
C(19)	3389(11)	6668(3)	8546(2)	51(2)
C(20)	3214(10)	6778(3)	8043(2)	55(2)
C(21)	1537(9)	6431(3)	7769(2)	42(1)
C(22)	5327(11)	7011(4)	8836(2)	82(2)
C(23)	11856(10)	2998(3)	11217(3)	95(3)
C(24)	-1642(10)	3381(3)	7598(2)	50(2)
N(1)	10945(7)	4267(2)	11459(1)	35(1)
N(2)	-1057(7)	4722(2)	7478(1)	31(1)
O(1)	12403(6)	5438(2)	11795(1)	47(1)
O(2)	13795(5)	4959(2)	10989(1)	39(1)
O(3)	-2497(5)	5943(2)	7230(1)	40(1)
O(4)	-3884(6)	5340(2)	7997(1)	48(1)
S(1)	11980(2)	5073(1)	11330(1)	33(1)
S(2)	7591(4)	2979(1)	10463(1)	68(1)
S(3)	5402(3)	4851(1)	9504(1)	64(1)
S(4)	2225(4)	3336(1)	8429(1)	85(1)
S(5)	-2077(2)	5509(1)	7665(1)	33(1)

Table 3. Bond lengths [A] and angles [deg] for s3119m.

C(1)-C(2)	1.373(6)
C(1)-C(6)	1.387(6)
C(1)-S(1)	1.770(5)
C(2)-C(3)	1.386(7)
C(2)-H(2)	0.9500
C(3)-C(4)	1.383(7)
C(3)-H(3)	0.9500
C(4)-C(5)	1.368(7)
C(4)-C(7)	1.510(7)
C(5)-C(6)	1.390(6)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-N(1)	1.475(7)
C(8)-C(23)	1.500(7)
C(8)-C(9)	1.516(7)
C(8)-H(8)	1.0000
C(9)-S(2)	1.799(5)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-C(11)	1.506(7)
C(10)-S(2)	1.810(4)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-S(3)	1.801(5)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(13)	1.495(7)
C(12)-S(3)	1.791(5)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-S(4)	1.818(6)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-C(15)	1.503(7)
C(14)-S(4)	1.818(5)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-N(2)	1.478(5)
C(15)-C(24)	1.530(6)
C(15)-H(15)	1.0000
C(16)-C(21)	1.385(7)
C(16)-C(17)	1.398(6)
C(16)-S(5)	1.750(5)
C(17)-C(18)	1.378(8)
C(17)-H(17)	0.9500
C(18)-C(19)	1.381(8)
C(18)-H(18)	0.9500
C(19)-C(20)	1.387(7)
C(19)-C(22)	1.524(8)
C(20)-C(21)	1.390(7)
C(20)-H(20)	0.9500
C(21)-H(21)	0.9500
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9800

C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
N(1)-S(1)	1.604(4)
N(1)-H(1N)	0.8308
N(2)-S(5)	1.612(4)
N(2)-H(2N)	0.86(5)
O(1)-S(1)	1.442(3)
O(2)-S(1)	1.438(3)
O(3)-S(5)	1.435(3)
O(4)-S(5)	1.438(3)

C(2)-C(1)-C(6)	120.4(5)
C(2)-C(1)-S(1)	119.1(4)
C(6)-C(1)-S(1)	120.6(4)
C(1)-C(2)-C(3)	119.9(5)
C(1)-C(2)-H(2)	120.1
C(3)-C(2)-H(2)	120.1
C(4)-C(3)-C(2)	120.8(5)
C(4)-C(3)-H(3)	119.6
C(2)-C(3)-H(3)	119.6
C(5)-C(4)-C(3)	118.4(5)
C(5)-C(4)-C(7)	121.5(5)
C(3)-C(4)-C(7)	120.1(5)
C(4)-C(5)-C(6)	122.0(5)
C(4)-C(5)-H(5)	119.0
C(6)-C(5)-H(5)	119.0
C(1)-C(6)-C(5)	118.5(5)
C(1)-C(6)-H(6)	120.8
C(5)-C(6)-H(6)	120.8
C(4)-C(7)-H(7A)	109.5
C(4)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(4)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
N(1)-C(8)-C(23)	108.9(5)
N(1)-C(8)-C(9)	110.2(4)
C(23)-C(8)-C(9)	112.9(4)
N(1)-C(8)-H(8)	108.2
C(23)-C(8)-H(8)	108.2
C(9)-C(8)-H(8)	108.2
C(8)-C(9)-S(2)	112.7(4)
C(8)-C(9)-H(9A)	109.0
S(2)-C(9)-H(9A)	109.0
C(8)-C(9)-H(9B)	109.0
S(2)-C(9)-H(9B)	109.0
H(9A)-C(9)-H(9B)	107.8
C(11)-C(10)-S(2)	112.3(4)
C(11)-C(10)-H(10A)	109.1
S(2)-C(10)-H(10A)	109.1
C(11)-C(10)-H(10B)	109.1
S(2)-C(10)-H(10B)	109.1
H(10A)-C(10)-H(10B)	107.9
C(10)-C(11)-S(3)	115.0(4)
C(10)-C(11)-H(11A)	108.5
S(3)-C(11)-H(11A)	108.5
C(10)-C(11)-H(11B)	108.5
S(3)-C(11)-H(11B)	108.5
H(11A)-C(11)-H(11B)	107.5
C(13)-C(12)-S(3)	114.5(4)
C(13)-C(12)-H(12A)	108.6
S(3)-C(12)-H(12A)	108.6
C(13)-C(12)-H(12B)	108.6
S(3)-C(12)-H(12B)	108.6

H(12A)-C(12)-H(12B)	107.6
C(12)-C(13)-S(4)	111.3(4)
C(12)-C(13)-H(13A)	109.4
S(4)-C(13)-H(13A)	109.4
C(12)-C(13)-H(13B)	109.4
S(4)-C(13)-H(13B)	109.4
H(13A)-C(13)-H(13B)	108.0
C(15)-C(14)-S(4)	111.6(4)
C(15)-C(14)-H(14A)	109.3
S(4)-C(14)-H(14A)	109.3
C(15)-C(14)-H(14B)	109.3
S(4)-C(14)-H(14B)	109.3
H(14A)-C(14)-H(14B)	108.0
N(2)-C(15)-C(14)	110.2(4)
N(2)-C(15)-C(24)	108.5(4)
C(14)-C(15)-C(24)	111.1(4)
N(2)-C(15)-H(15)	109.0
C(14)-C(15)-H(15)	109.0
C(24)-C(15)-H(15)	109.0
C(21)-C(16)-C(17)	119.6(5)
C(21)-C(16)-S(5)	120.0(4)
C(17)-C(16)-S(5)	120.2(5)
C(18)-C(17)-C(16)	119.9(6)
C(18)-C(17)-H(17)	120.0
C(16)-C(17)-H(17)	120.0
C(17)-C(18)-C(19)	121.2(5)
C(17)-C(18)-H(18)	119.4
C(19)-C(18)-H(18)	119.4
C(18)-C(19)-C(20)	118.6(6)
C(18)-C(19)-C(22)	120.8(6)
C(20)-C(19)-C(22)	120.6(7)
C(21)-C(20)-C(19)	121.3(6)
C(21)-C(20)-H(20)	119.4
C(19)-C(20)-H(20)	119.4
C(16)-C(21)-C(20)	119.4(5)
C(16)-C(21)-H(21)	120.3
C(20)-C(21)-H(21)	120.3
C(19)-C(22)-H(22A)	109.5
C(19)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(19)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(8)-C(23)-H(23A)	109.5
C(8)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(8)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(15)-C(24)-H(24A)	109.5
C(15)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(15)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(8)-N(1)-S(1)	121.0(3)
C(8)-N(1)-H(1N)	120.8
S(1)-N(1)-H(1N)	109.8
C(15)-N(2)-S(5)	120.5(3)
C(15)-N(2)-H(2N)	115(3)
S(5)-N(2)-H(2N)	118(3)
O(2)-S(1)-O(1)	119.9(2)
O(2)-S(1)-N(1)	107.5(2)
O(1)-S(1)-N(1)	106.3(2)

O(2)-S(1)-C(1)	106.9(2)
O(1)-S(1)-C(1)	106.3(2)
N(1)-S(1)-C(1)	109.7(2)
C(9)-S(2)-C(10)	100.7(2)
C(12)-S(3)-C(11)	101.8(2)
C(14)-S(4)-C(13)	101.7(2)
O(3)-S(5)-O(4)	120.1(2)
O(3)-S(5)-N(2)	106.1(2)
O(4)-S(5)-N(2)	107.2(2)
O(3)-S(5)-C(16)	107.2(2)
O(4)-S(5)-C(16)	106.7(2)
N(2)-S(5)-C(16)	109.2(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for s3119m.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	28(3)	22(2)	33(3)	4(2)	-4(2)	-10(2)
C(2)	37(3)	34(3)	32(3)	3(2)	5(2)	-6(3)
C(3)	37(3)	35(3)	46(3)	0(2)	6(3)	-2(3)
C(4)	32(3)	30(3)	45(3)	6(2)	-6(3)	-11(2)
C(5)	52(4)	34(3)	31(3)	8(2)	-7(3)	-13(3)
C(6)	43(3)	30(3)	29(3)	-1(2)	4(2)	-9(2)
C(7)	48(4)	57(4)	66(4)	22(3)	-5(3)	-3(3)
C(8)	52(4)	23(3)	59(4)	2(3)	18(3)	-4(3)
C(9)	49(3)	38(3)	22(2)	3(2)	-2(3)	4(3)
C(10)	82(5)	41(3)	17(2)	1(2)	1(3)	1(3)
C(11)	60(4)	63(4)	26(3)	7(3)	-8(3)	1(3)
C(12)	45(3)	40(3)	23(2)	5(2)	-4(2)	-5(3)
C(13)	49(4)	53(3)	49(3)	26(3)	-3(3)	-6(3)
C(14)	54(4)	34(3)	52(3)	15(2)	-20(3)	6(3)
C(15)	35(3)	32(3)	27(3)	6(2)	4(2)	-1(2)
C(16)	51(4)	26(3)	36(3)	0(2)	-3(3)	17(3)
C(17)	66(4)	53(4)	30(3)	-3(3)	2(3)	25(3)
C(18)	69(5)	67(4)	39(3)	-18(3)	-16(4)	36(4)
C(19)	59(4)	48(3)	46(4)	-19(3)	-21(3)	33(3)
C(20)	54(4)	31(3)	80(4)	-2(3)	-19(4)	14(3)
C(21)	50(4)	32(3)	44(3)	-2(2)	-14(3)	12(3)
C(22)	75(6)	80(5)	90(5)	-43(4)	-48(4)	28(4)
C(23)	31(4)	32(3)	223(9)	-6(5)	6(5)	2(3)
C(24)	57(4)	40(3)	52(3)	9(3)	-14(3)	-13(3)
N(1)	32(3)	43(3)	29(2)	7(2)	9(2)	10(2)
N(2)	35(2)	34(2)	24(2)	7(2)	6(2)	6(2)
O(1)	36(2)	67(2)	37(2)	-10(2)	-10(2)	3(2)
O(2)	28(2)	46(2)	44(2)	-2(2)	5(2)	-5(2)
O(3)	41(2)	40(2)	39(2)	13(2)	-10(2)	5(2)
O(4)	47(2)	50(2)	47(2)	11(2)	18(2)	14(2)
S(1)	27(1)	41(1)	32(1)	-2(1)	-4(1)	-3(1)
S(2)	145(2)	32(1)	28(1)	-1(1)	-13(1)	-5(1)
S(3)	105(1)	50(1)	36(1)	-1(1)	-25(1)	3(1)
S(4)	129(2)	36(1)	88(1)	22(1)	-77(1)	-10(1)
S(5)	34(1)	36(1)	30(1)	8(1)	3(1)	11(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic

displacement parameters (A^2 x 10^3) for s3119m.

	x	y	z	U(eq)
H(2)	8301	5931	11646	41
H(3)	5580	6659	11255	47
H(5)	8318	6175	9946	47
H(6)	11077	5446	10326	41
H(7A)	5507	7487	10279	85
H(7B)	3569	6976	10512	85
H(7C)	4606	6769	9986	85
H(8)	11288	3890	10761	54
H(9A)	7373	4052	10940	43
H(9B)	7476	3326	11284	43
H(10A)	8948	3992	10011	56
H(10B)	7708	3411	9654	56
H(11A)	5438	4408	10304	60
H(11B)	4193	3824	9952	60
H(12A)	5013	4608	8676	43
H(12B)	5998	3890	8952	43
H(13A)	1407	4332	8959	60
H(13B)	2360	3635	9266	60
H(14A)	2359	4510	8048	56
H(14B)	2569	3861	7644	56
H(15)	-1546	4207	8138	38
H(17)	-938	5567	8678	60
H(18)	1917	6139	9121	70
H(20)	4260	7097	7882	66
H(21)	1469	6499	7423	50
H(22A)	6139	6615	9011	123
H(22B)	4734	7374	9073	123
H(22C)	6356	7265	8609	123
H(23A)	13467	3106	11242	143
H(23B)	11611	2610	10967	143
H(23C)	11298	2820	11535	143
H(24A)	-3266	3434	7549	75
H(24B)	-1348	2957	7817	75
H(24C)	-910	3293	7280	75
H(1N)	10042	4306	11691	17(12)
H(2N)	-150(80)	4730(30)	7230(18)	50(17)

Table 6. Torsion angles [deg] for s3119m.

C(6)-C(1)-C(2)-C(3)	-0.3(7)
S(1)-C(1)-C(2)-C(3)	-180.0(3)
C(1)-C(2)-C(3)-C(4)	-0.2(7)
C(2)-C(3)-C(4)-C(5)	0.7(7)
C(2)-C(3)-C(4)-C(7)	-179.5(4)
C(3)-C(4)-C(5)-C(6)	-0.9(7)
C(7)-C(4)-C(5)-C(6)	179.3(4)
C(2)-C(1)-C(6)-C(5)	0.1(7)
S(1)-C(1)-C(6)-C(5)	179.8(3)
C(4)-C(5)-C(6)-C(1)	0.5(7)
N(1)-C(8)-C(9)-S(2)	171.5(3)
C(23)-C(8)-C(9)-S(2)	-66.5(6)
S(2)-C(10)-C(11)-S(3)	-179.5(3)
S(3)-C(12)-C(13)-S(4)	-176.6(2)
S(4)-C(14)-C(15)-N(2)	172.9(3)
S(4)-C(14)-C(15)-C(24)	-66.8(5)

C(21)-C(16)-C(17)-C(18)	0.7(7)
S(5)-C(16)-C(17)-C(18)	176.0(4)
C(16)-C(17)-C(18)-C(19)	-0.1(8)
C(17)-C(18)-C(19)-C(20)	0.5(8)
C(17)-C(18)-C(19)-C(22)	-177.0(5)
C(18)-C(19)-C(20)-C(21)	-1.5(8)
C(22)-C(19)-C(20)-C(21)	176.0(5)
C(17)-C(16)-C(21)-C(20)	-1.6(7)
S(5)-C(16)-C(21)-C(20)	-177.0(4)
C(19)-C(20)-C(21)-C(16)	2.1(8)
C(23)-C(8)-N(1)-S(1)	123.5(4)
C(9)-C(8)-N(1)-S(1)	-112.2(4)
C(14)-C(15)-N(2)-S(5)	-104.9(4)
C(24)-C(15)-N(2)-S(5)	133.3(4)
C(8)-N(1)-S(1)-O(2)	-41.4(4)
C(8)-N(1)-S(1)-O(1)	-170.9(4)
C(8)-N(1)-S(1)-C(1)	74.6(4)
C(2)-C(1)-S(1)-O(2)	-163.1(3)
C(6)-C(1)-S(1)-O(2)	17.2(4)
C(2)-C(1)-S(1)-O(1)	-34.0(4)
C(6)-C(1)-S(1)-O(1)	146.3(4)
C(2)-C(1)-S(1)-N(1)	80.6(4)
C(6)-C(1)-S(1)-N(1)	-99.1(4)
C(8)-C(9)-S(2)-C(10)	-85.6(4)
C(11)-C(10)-S(2)-C(9)	-73.1(4)
C(13)-C(12)-S(3)-C(11)	68.3(4)
C(10)-C(11)-S(3)-C(12)	72.7(4)
C(15)-C(14)-S(4)-C(13)	-99.4(4)
C(12)-C(13)-S(4)-C(14)	-76.9(4)
C(15)-N(2)-S(5)-O(3)	-171.9(3)
C(15)-N(2)-S(5)-O(4)	-42.4(4)
C(15)-N(2)-S(5)-C(16)	72.8(4)
C(21)-C(16)-S(5)-O(3)	-29.0(4)
C(17)-C(16)-S(5)-O(3)	155.6(4)
C(21)-C(16)-S(5)-O(4)	-158.9(4)
C(17)-C(16)-S(5)-O(4)	25.7(5)
C(21)-C(16)-S(5)-N(2)	85.5(4)
C(17)-C(16)-S(5)-N(2)	-89.8(4)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for s3119m [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1N)...O(3)#1	0.83	2.15	2.957(5)	162.4
N(2)-H(2N)...O(1)#2	0.86(5)	2.04(5)	2.875(5)	162(5)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1/2,-y+1,z+1/2   #2 -x+3/2,-y+1,z-1/2