

Supporting Information

Characteristic Hydrogen Bonding Observed in the Crystals of Aromatic Sulfonamides: 1D chain Assembly of Molecules and Chiral Discrimination on Crystallization

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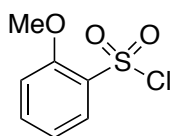
1. Experimental

General Comments.

All of the starting materials, except for 2-methoxybenzenesulfonyl chloride (**S5**), and solvents were purchased from Sigma–Aldrich Japan (Tokyo, Japan), FUJIFILM Wako Pure Chemical Co. (Osaka, Japan), nacalai tesque, INC. (Kyoto, Japan), and TCI Co., Ltd. (Tokyo, Japan). All commercially available reagents and solvents were used without further purification. 2-Methoxybenzenesulfonylchloride (**S5**) was synthesized according to a modified procedure based on a literature report.^{S1a} The synthesis and crystallization of sulfonamides was carried out according to procedure, **TP-S** and **TP-C**. FT-IR spectra were recorded on a JASCO FT/IR-4100 using KBr tablets. ¹H-NMR spectra were recorded on a JEOL JNM-AL400 (400 MHz) spectrometer. Chemical shifts (δ) are given from TMS (0 ppm) in CDCl₃ and coupling constants are expressed in hertz (Hz). The following abbreviations are used: s = singlet, brs = broad singlet, d = doublet, dd = double doublet, ddd = double double doublet, t = triplet, dt = double triplet, td = triple doublet, m = multiplet. ¹³C-NMR spectra were recorded on a JEOL JNM-AL400 (100 MHz) spectrometer. Chemical shifts (δ) are given from ¹³CDCl₃ (77.0 ppm). Mass spectroscopy and high-resolution mass spectroscopy were measured on a JEOL JMS-AM SYSTEM II-50.

Synthesis and Characteristic Data of a Sulfonyl chloride

2-Methoxybenzenesulfonylchloride (**S5**).^{S1b}



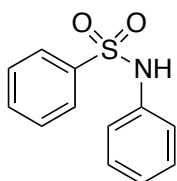
A mixture of 2-methoxybenzenethiol (3 mmol, 0.538 mL), 30% H₂O₂ (9 mmol, 0.9 mL), and ZrCl₄ (3 mmol, 699 mg) was stirred in MeCN (15 mL) at 25 °C for 10 min. The reaction mixture was quenched by adding H₂O (10 mL), and extracted with EtOAc (4 × 5 mL). The extract was dried with anhydrous MgSO₄ and the filtrate was evaporated under vacuum to afford **S5** as orange

crystals (610 mg, 98 %).

¹H NMR (400 MHz, CDCl₃): δ 7.69 (ddd, J = 8.0, 1.8, 0.2 Hz, 1H), 7.69 (ddd, J = 9.2, 7.3, 1.7 Hz, 1H), 7.14–7.09 (m, 2H), 4.07 (s, 3H).

Synthesis and Characteristic Data of Sulfonamides

N-Phenylbenzenesulfonamide (S1A1).^{S2}



Color, Habit: Colorless, prism crystals. Mp: 112.0 °C (lit: 109–110 °C)

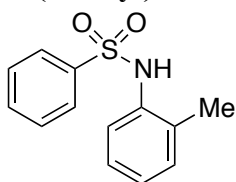
¹H NMR (400 MHz, CDCl₃): δ 7.76 (m, 2H), 7.79–7.76 (m, 1H), 7.46–7.42 (m, 2H), 7.26–7.22 (m, 2H), 7.14–7.10 (m, 1H), 7.09–7.05 (m, 2H).

¹³C{¹H} NMR (100 MHz, CDCl₃): δ 139.0, 136.3, 133.0, 129.3, 129.0, 127.2, 125.5, 121.8.

IR (KBr pellet): 3207, 1597, 1475, 1446, 1415, 1331, 1305, 1155, 1093, 929, 906, 754, 726, 581, 552 cm⁻¹.

Crystallization procedure: **TP-S**.

N-(*o*-Tolyl)benzenesulfonamide (S1A2).^{S3}



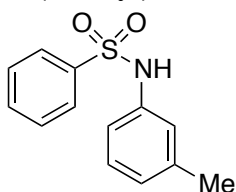
Color, Habit: Colorless, prism crystals. Mp: 128.0–129.0 °C (lit: 126.3 °C)

¹H NMR (400 MHz, CDCl₃): δ 7.75–7.72 (m, 2 H), 7.55 (t, *J* = 7.4 Hz, 1 H), 7.44 (t, *J* = 8.0 Hz, 2 H), 7.31 (d, *J* = 7.7 Hz, 1 H), 7.09 (dd, *J* = 5.04, 1.03, 2 H), 6.34 (s, 1 H), 1.98 (s, 3 H).

IR (KBr pellet): (neat, cm⁻¹): 3433, 3217, 1491, 1448, 1406, 1327, 1154, 1093, 917, 756, 729, 553 cm⁻¹.

Crystallization procedure: **TP-S**

N-(*m*-tolyl)benzenesulfonamide (S1A3).^{S4}



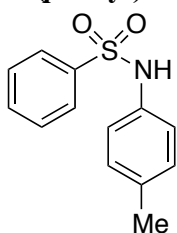
Color, Habit: Colorless, prism crystals. Mp: 94.5–95.0 °C (lit: 94.5–95.5 °C)

¹H NMR (400 MHz, CDCl₃): δ 7.79–7.76 (m, 2H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.44 (t, *J* = 7.9 Hz, 2H), 7.11 (t, *J* = 7.9 Hz, 1H), 6.94–6.83 (m, 3H), 2.27 (s, 3H).

IR (KBr pellet): 3336, 3228, 1594, 1497, 1396, 1303, 1262, 1152, 1095, 1023, 948, 839, 796, 697, 570, 548 cm⁻¹.

Crystallization procedure: **TP-S** (form I) and **TP-C** (Solvent A/ Solvent B: Ethyl acetate/MeOH, form II).

N-(*p*-tolyl)benzenesulfonamide (S1A4).^{S3}



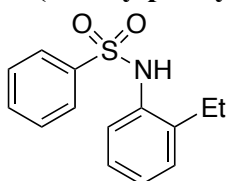
Color, Habit: Colorless, prism crystals. Mp: 125.0–126.0 °C (lit: 102.9 °C)

¹H NMR (400 MHz, CDCl₃): δ 7.74 (d, *J* = 7.6 Hz, 2 H), 7.53 (t, *J* = 7.4 Hz, 1 H), 7.43 (t, *J* = 7.7 Hz, 2 H), 7.04 (d, *J* = 8.5 Hz, 2 H), 6.93 (d, *J* = 8.4 Hz, 2 H), 6.40 (brs, 1 H), 2.28 (s, 3 H).

IR (KBr pellet): 3336, 3228, 1594, 1497, 1396, 1302, 1262, 1152, 1095, 1023, 948, 697, 570 cm⁻¹.

Crystallization procedure: **TP-S**.

N-(2-Ethylphenyl)benzenesulfonamide (S1A5).^{S5}



Color, Habit: Colorless, platelet crystals. Mp: 115.0–115.5 °C (lit: 110–111 °C)

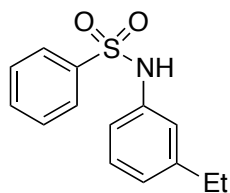
¹H NMR (400 MHz, CDCl₃): δ 7.75–7.71 (m, 2H), δ 7.54 (ddt, *J* = 8.1, 6.8, 1.3 Hz, 1H), δ 7.46–7.41 (m, 2H), δ 7.34–7.29 (m, 1H), δ 7.17–7.11 (m, 3H), 6.34 (brs, 1H), 2.34 (q, *J* = 7.6 Hz, 2H), 1.02 (t, *J* = 7.6 Hz, 3H).

¹³C{¹H} NMR (100 MHz, CDCl₃): δ 139.5, 137.1, 133.6, 133, 129, 128.9, 127.2, 126.8, 126.6, 124.4, 23.6, 14.1.

IR (KBr pellet): 3240, 1496, 1455, 1413, 1329, 1090, 910, 756, 733, 688, 670, 608, 552 cm⁻¹.

Crystallization procedure: **TP-S**.

N-(3-Ethylphenyl)benzenesulfonamide (S1A6).



Color, Habit: Colorless, prism crystals. Mp: 58.0–59.0 °C

MS (FAB⁺): *m/z*: 262 [*M*+H]⁺, 284 [*M*+Na]⁺.

¹H NMR (400 MHz, CDCl₃): δ 7.80–7.77 (m, 2H), 7.53 (t, *J* = 7.6 Hz, 2H), δ 7.43 (t, *J* = 7.8 Hz, 2H), δ 7.13 (dd, *J* = 7.8 Hz, 1H), δ 7.94 (d, *J* = 8.0 Hz, 1H), δ 6.89–6.85 (m, 3H), 2.55 (q, *J* = 7.6 Hz, 2H), 1.14 (t, *J* = 7.6 Hz, 3H).

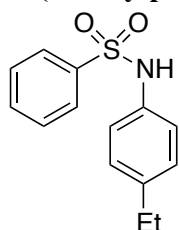
¹³C{¹H} NMR (100 MHz, CDCl₃): δ 145.8, 139.1, 136.3, 133.0, 129.3, 129.1, 127.4, 125.2, 121.4, 119.2, 28.7, 15.5.

IR (KBr pellet): 3270, 2954, 2867, 1606, 1593, 1502, 1446, 1413, 1330, 1290, 1169, 1151, 1090, 938, 873, 790, 756, 718, 694, 587, 552, 446 cm⁻¹.

Anal. Calcd. for C₁₄H₁₅NO₂S: C, 64.34; H, 5.79; N, 5.36. Found: C, 64.28; H, 5.72; N, 5.31.

Crystallization procedure: **TP-S**.

N-(4-Ethylphenyl)benzenesulfonamide (S1A7).



Color, Habit: Colorless, platelet crystals. Mp: 83.0–84.0 °C (lit^{S6}: 82–83 °C)

MS (FAB⁺): *m/z*: 262 [*M*+H]⁺, 284 [*M*+Na]⁺.

¹H NMR (400 MHz, CDCl₃): δ 7.76–7.73 (m, 2H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.46–7.41 (m, 2H), 7.09–7.05 (m, 2H), 7.76–7.73 (m, 2H), 6.96 (d, *J* = 8.6 Hz, 2H), 6.42 (brs, 1H), 2.58 (q, *J* = 7.6 Hz, 2H), 1.18 (t, *J* = 7.7 Hz, 3H).

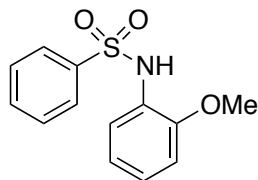
¹³C{¹H} NMR (100 MHz, CDCl₃): δ 142.0, 139.1, 133.7, 132.9, 129.0, 128.7, 127.2, 122.5, 28.2, 15.4.

IR (KBr pellet): 3244, 1511, 1454, 1393, 1330, 1154, 1091, 912, 729, 579 cm⁻¹.

Anal. Calcd. for C₁₄H₁₅NO₂S: C, 64.34; H, 5.79; N, 5.36. Found: C, 64.16; H, 5.72; N, 5.33.

Crystallization procedure: **TP-S** (form I) and **TP-C** (Solvent A/ Solvent B: MeOH/*c*-hexane, form II).

N-(2-Methoxyphenyl)benzenesulfonamide (S1A8).^{S3}



Color, Habit: Colorless, block crystals. Mp: 91.0 °C (lit^{S7}: 87–89 °C)

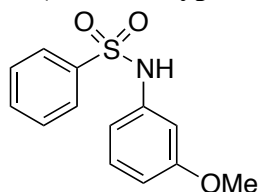
¹H NMR (400 MHz, CDCl₃): δ = 7.75 (d, *J* = 8.1 Hz, 2 H), 7.53 (d, *J* = 7.9 Hz, 1 H), 7.49 (d, *J* = 7.3 Hz, 1 H), 7.42–7.38 (m, 2 H), 7.04 (t, *J* = 7.6 Hz, 1 H), 6.99 (brs, 1 H), 6.91 (t, *J* = 7.6 Hz, 1 H), 6.72 (t, *J* = 8.1 Hz, 1 H), 3.61 (s, 3 H).

IR (KBr pellet): 3256, 3066, 3015, 2938, 1602, 1497, 1468, 1446, 1397, 1340, 1298, 1258, 1170, 1110, 1092, 1045, 1026, 940, 911, 782, 751, 731, 686, 613,

578, 543 cm⁻¹.

Crystallization procedure: **TP-S**.

N-(3-Methoxyphenyl)benzenesulfonamide (S1A9).^{S8}



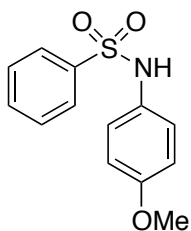
Color, Habit: Colorless, prism crystals. Mp: 77.5–81.0 °C (lit^{S7}: 79.5–81.5 and 82.5–83.5 °C)

¹H NMR (400 MHz, CDCl₃): δ 7.80 – 7.78 (m, 2H), 7.54 (dt, *J* = 6.6, 1.2 Hz, 1H), 7.47–7.43 (m, 2H), 7.12 (t, *J* = 8.1 Hz, 1H), 6.68–6.64 (m, 2H), 6.62 (ddd, *J* = 7.9, 2.1, 1.0 Hz, 1H), 6.49 (brs, 1H), 3.74 (s, 3H).

IR (KBr pellet): 3256, 3015, 2965, 1611, 1499, 1448, 1412, 1331, 1286, 1149, 1090, 1051, 945, 898, 776, 727, 689, 661, 592, 551 cm⁻¹.

Crystallization procedure: **TP-S**, and the crude oil was washed with *n*-hexane and dried in vacuo.

N-(4-Methoxyphenyl)benzenesulfonamide (S1A10).^{S3}



Color, Habit: Colorless, prism crystals. Mp: 95.5–96.5 °C (lit^{S7}: 93–94.5 and 88–89 °C)

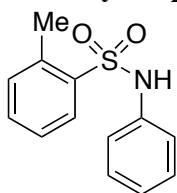
¹H NMR (400 MHz, CDCl₃): δ 7.71–7.68 (m, 2 H), 7.54 (dt, *J* = 6.9, 1.3 Hz, 1 H), 7.46–7.41 (m, 2 H), 6.96 (d, *J* = 8.7 Hz, 2 H), 6.76 (d, *J* = 8.9 Hz, 2 H), 6.35 (brs, 1H), 3.76 (s, 3 H).

IR (KBr pellet): 3256, 3005, 2934, 2841, 1614, 1507, 1467, 1446, 1400, 1334, 1289, 1248, 1153, 1090, 1038, 916, 827, 760, 723, 687, 634, 583, 543, 514 cm⁻¹

1.

Crystallization procedure: **TP-S** and **TP-C** (Solvent A/ Solvent B: chloroform/toluene, form I; MeOH/THF, form II).

2-Methyl-*N*-phenylbenzenesulfonamide (S2A1).^{S4}



Color, Habit: Colorless, prism crystals. Mp: 139–142 °C.

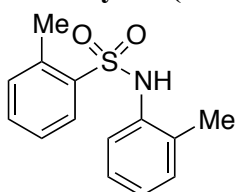
¹H NMR (400 MHz, CDCl₃): δ 7.97 (d, *J* = 8.1 Hz, 1H), 7.43 (td, *J* = 7.3, 1.4 Hz, 1H), 7.28 (d, *J* = 7.6 Hz, 2H), 7.22 (t, *J* = 7.4 Hz, 2sH), 7.07 (t, *J* = 7.4 Hz, 1H), 7.03–6.99 (m, 2H), 6.75 (brs, 1H), 2.66 (s, 3H).

¹³C {¹H} NMR (100 MHz, CDCl₃): δ 137.3, 137.2, 136.4, 133.2, 132.6, 130.0, 129.3, 126.3, 125.0, 120.6, 20.4.

IR (KBr pellet): 3280, 1600, 1492, 1477, 1409, 1331, 1317, 1299, 1281, 1221, 1157, 1130, 1065, 920, 758, 694, 588 cm⁻¹.

Crystallization procedure: **TP-S**.

2-Methyl-*N*-(*o*-tolyl)benzenesulfonamide (S2A2).



Color, Habit: Pale red powder. Mp: 108–111 °C

HRMS (FAB) *m/z*: Calcd for C₁₄H₁₅NNaO₂S 293.0722 [*M*+Na]⁺; Found 284.0721 [*M*+Na]⁺.

¹H NMR (400 MHz, CDCl₃): δ 7.90 (d, *J* = 7.9 Hz, 1H), 7.45 (td, *J* = 7.7, 1.3 Hz, 1H), 7.30–7.26 (m, 2H), 7.13–7.04 (m, 4H), 6.82 (s, 1H), 6.79 (d, *J* = 8.0 Hz, 1H), 6.52 (s, 1H), 2.65 (s, 3H), 2.25 (s, 3H).

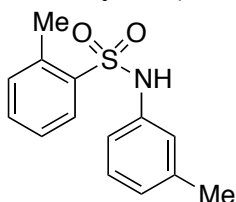
¹³C {¹H} NMR (100 MHz, CDCl₃): δ 138.1, 137.3, 134.5, 133.2, 132.7, 131.0, 130.8, 129.9, 127.0, 126.4, 126.0, 123.3, 20.6, 17.7.

IR (KBr pellet): 3260, 1495, 1471, 1401, 1330, 1164, 1108, 1066, 913, 758, 690, 574 cm⁻¹.

Anal. Calcd. for C₁₄H₁₅NO₂S: C, 64.34; H, 5.79; N, 5.36. Found: C, 60.10; H, 5.56; N, 4.58.

Crystallization procedure: **TP-S** and **TP-C** (Solvent A/ Solvent B = chloroform/toluene).

2-Methyl-*N*-(*m*-tolyl)benzenesulfonamide (S2A3).^{S4}



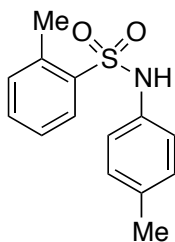
Color, Habit: Pale red platelet crystals. Mp: 122.0–123.0 °C.

¹H NMR (400 MHz, CDCl₃): δ 7.96 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.43 (td, *J* = 7.6, 1.3 Hz, 1H), 7.29–7.26 (m, 2H), 7.09 (t, *J* = 7.8 Hz, 1H), 6.89 (d, *J* = 7.6 Hz, 1H), 6.82 (s, 1H), 6.79 (d, *J* = 7.9 Hz, 1H), 6.49 (brs, 1H), 2.65 (s, 3H), 2.25 (s, 3H).

IR (KBr pellet): 3268, 33085, 2919, 1585, 1496 1395, 1333, 1231, 1161, 1089, 1046, 944, 912, 861, 795, 696, 639, 595, 546 cm⁻¹.

Crystallization procedure: **TP-S**.

2-Methyl-*N*-(*p*-tolyl)benzenesulfonamide (S2A4).^{S3}



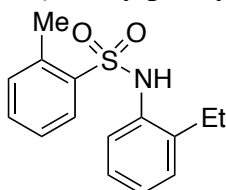
Color, Habit: White powder. Mp: 127.0–128.5 °C. (lit: 126.9 °C)

¹H NMR (400 MHz, CDCl₃): δ 7.92 (dd, *J* = 7.9, 1.4 Hz, 1 H), 7.42 (td, *J* = 7.6, 1.4 Hz, 1 H), 7.30–7.24 (m, 2 H), 7.01 (d, *J* = 8.0 Hz, 2 H), 7.00 (d, *J* = 8.4 Hz, 2 H), 6.44 (brs, 1H), 2.64 (s, 3 H), 2.25 (s, 3 H).

IR (KBr pellet): 3256, 3103, 3025, 2922, 2860, 1614, 1511, 1461, 1393, 1325, 1302, 1156, 1130, 1067, 921, 843, 813, 772, 713, 688, 589, 529, 498, 441 cm⁻¹.

Crystallization procedure: **TP-S** and **TP-C** (Solvent A/ Solvent B = chloroform/toluene).

N-(2-Ethylphenyl)-2-methylbenzenesulfonamide (S2A5).



Color, Habit: Colorless, block crystals. Mp: 91.0–91.5 °C.

MS (FAB⁺): *m/z*: 276 [*M*+H]⁺, 298 [*M*+Na]⁺.

¹H NMR (400 MHz, CDCl₃): δ 7.94–7.92 (m, 1H), 7.45 (td, *J* = 7.3, 1.4 Hz, 1H), 7.31–7.28 (m, 2H), 7.17–7.15 (m, 1H), 7.13–7.03 (m, 3H), 6.35 (brs, 1H), 2.61 (s, 3H), 2.53 (q, *J* = 7.6 Hz, 2H), 1.15 (t, *J* = 7.6 Hz, 3H).

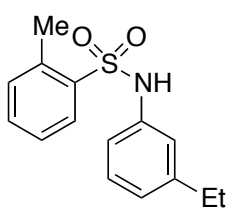
¹³C{¹H} NMR (100 MHz, CDCl₃): δ 138.2, 137.3, 136.8, 133.9, 133.2, 132.7, 129.9, 129.0, 126.8, 126.4, 126.2, 123.4, 23.9, 20.6, 14.2.

IR (KBr pellet): 3269, 1583, 1497, 1410, 1326, 1288, 1157, 1130, 1076, 930, 756, 692, 596 cm⁻¹.

Anal. Calcd. for C₁₅H₁₇NO₂S: C, 65.43; H, 6.22; N, 5.09. Found: C, 65.15; H, 6.10; N, 5.0s.

Crystallization procedure: **TP-S**.

N-(3-Ethylphenyl)-2-methylbenzenesulfonamide (S2A6).



Color, Habit: Colorless, prism crystals. Mp: 77.0–78.0 °C.

HRMS (FAB) *m/z*: Calcd for C₁₅H₁₇NNaO₂S 298.0878 [*M*+Na]⁺; Found 298.0879 [*M*+Na]⁺.

¹H NMR (400 MHz, CDCl₃): δ 7.96–7.90 (m, 1H), 7.43 (t, *J* = 7.7 Hz, 1H), 7.30–7.25 (m, 2H), 7.11 (td, *J* = 7.8, 0.9 Hz, 1H), 6.91–6.80 (m, 3H), 6.66 (brs, 1H), 2.65 (s, 3H), 2.53 (q, *J* = 7.7 Hz, 2H), 1.12 (t, *J* = 7.6 Hz, 3H).

¹³C{¹H} NMR (100 MHz, CDCl₃): δ 145.8, 137.5, 137.3, 136.4, 133.2, 132.6, 130.2, 129.3, 126.3, 124.8, 120.3, 118.0, 28.7, 20.5, 15.4.

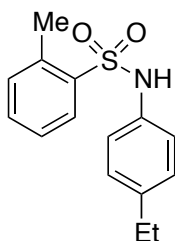
IR (KBr pellet): 3254, 1607, 1592, 1473, 1412, 1326, 1153, 1132, 1063, 943, 790, 762, 698, 593, 561 cm⁻¹.

HRMS (FAB) *m/z*: Calcd for C₁₅H₁₇NNaO₃S 279.0878 [*M*+Na]⁺; Found 279.0879 [*M*+Na]⁺.

Anal. Calcd. for C₁₅H₁₇NO₂S: C, 65.43; H, 6.22; N, 5.09. Found: C, 65.12; H, 6.10; N, 4.89.

Crystallization procedure: **TP-S**.

N-(4-Ethylphenyl)-2-methylbenzenesulfonamide (S2A7).



Color, Habit: Colorless, prism crystals. Mp: 92.0 °C.

MS (FAB⁺): *m/z*: 276 [*M*+H]⁺, 298 [*M*+Na]⁺.

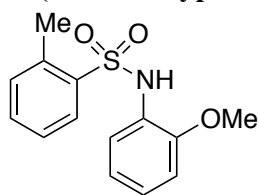
¹H NMR (400 MHz, CDCl₃): δ 7.94 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.43 (td, *J* = 7.7, 1.4 Hz, 1H), 7.30–7.24 (m, 2H), 7.04 (d, *J* = 8.4, 2H), 6.91 (d, *J* = 8.5, 2H), 6.50 (brs, 1H), 2.64 (s, 3H), 2.55 (q, *J* = 7.7 Hz, 2H), 1.16 (d, *J* = 7.6 Hz, 3H).

¹³C{¹H} NMR (100 MHz, CDCl₃): δ 141.5, 137.5, 137.1, 133.7, 133, 132.5, 130, 128.7, 126.3, 121.5, 28.2, 20.4, 15.4.

IR (KBr pellet): 3257, 1512, 1461, 1395, 1320, 1158, 1133, 1064, 931, 689, 589 cm⁻¹.

Anal. Calcd. for C₁₅H₁₇NO₂S: C, 65.43; H, 6.22; N, 5.09. Found: C, 65.13; H, 6.17; N, 5.07.

Crystallization procedure: **TP-S**.

***N*-(2-Methoxyphenyl)-2-methylbenzenesulfonamide (S2A8).**

Color, Habit: Colorless, block crystals. Mp: 110.0–112.0 °C.

MS (FAB⁺): *m/z*: 278 [*M*+H]⁺, 300 [*M*+Na]⁺.

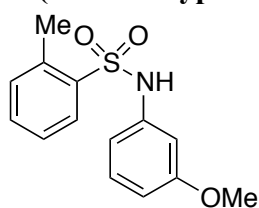
¹H NMR (400 MHz, CDCl₃): δ 7.93 (d, *J* = 7.9, 1H), 7.39 (t, *J* = 8.6 Hz, 2H), 7.26–7.21 (m, 3H), 7.14 (brs, 1H), 6.98 (t, *J* = 7.9, 1H), 6.76 (d, *J* = 8.1, 1H), 3.74 (s, 3H), 2.67 (s, 3H).

¹³C{¹H} NMR (100 MHz, CDCl₃): δ 149.0, 137.4, 133, 132.5, 130.2, 126.1, 126.0, 124.8, 121.1, 119.9, 110.5, 55.7, 20.2.

IR (KBr pellet): 3282, 3006, 2970, 2935, 1596, 1503, 1444, 1396, 1334, 1288, 1254, 1160, 1114, 1029, 927, 749, 692, 594 cm⁻¹.

Anal. Calcd. for C₁₄H₁₅NO₃S: C, 60.63; H, 5.45; N, 5.05. Found: C, 60.46; H, 5.45; N, 5.07.

Crystallization procedure: **TP-S**.

***N*-(3-Methoxyphenyl)-2-methylbenzenesulfonamide (S2A9).**

Color, Habit: Red prism crystals. Mp: 108.0–109.0 °C.

MS (FAB⁺): *m/z*: 278 [*M*+H]⁺, 300 [*M*+Na]⁺.

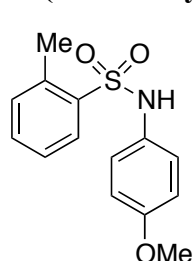
¹H NMR (400 MHz, CDCl₃): δ 7.99 (dd, *J* = 7.0, 1.5, 1H), 7.44 (td, *J* = 7.4, 1.4 Hz, 1H), 7.30–7.26 (m, 3H), 7.12–7.08 (m, 2H), 6.62–6.54 (m, 1H), 3.71 (s, 3H), 2.66 (s, 3H).

¹³C{¹H} NMR (100 MHz, CDCl₃): δ 160.4, 137.7, 137.4, 137.3, 133.3, 132.7, 130.2, 130.2, 126.4, 55.4, 20.5, 20.2.

IR (KBr pellet): 3260, 3006, 2975, 2930, 2829, 1603, 1504, 1397, 1320, 1262, 1199, 1155, 1038, 986, 872, 842, 769, 757, 685, 639, 588, 561, 492 cm⁻¹.

Anal. Calcd. for C₁₄H₁₅NO₃S: C, 60.63; H, 5.45; N, 5.05. Found: C, 60.51; H, 5.34; N, 5.03.

Crystallization procedure: **TP-S**.

***N*-(4-Methoxyphenyl)-2-methylbenzenesulfonamide (S2A10).**

Color, Habit: purple prism crystals. Mp: 125.0–126.0 °C.

HRMS (FAB) *m/z*: Calcd for C₁₄H₁₅NNaO₃S 300.0670 [*M*+Na]⁺; Found 300.0671 [*M*+Na]⁺.

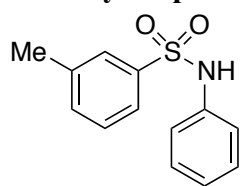
¹H NMR (400 MHz, CDCl₃): δ 7.85 (dd, 8.0, 1.3 Hz, 1H), 7.43 (td, *J* = 7.6, 1.4 Hz, 1H), 7.31–7.21 (m, 2H), 6.95–6.90 (m, 2H), 6.76–6.71 (m, 2H), 6.34 (brs, 1H), 3.74 (s, 3H), 2.63 (s, 3H).

¹³C{¹H} NMR (100 MHz, CDCl₃): δ 157.9, 137.3, 137.1, 133.0, 132.5, 130.1, 128.6, 126.3, 125.1, 114.4, 55.4, 20.5.

IR (KBr pellet): 3275, 3004, 2985, 1608, 1509, 1321, 1286, 1156, 1134, 1029, 909, 758, 691, 598, 544 cm⁻¹.

Anal. Calcd. for C₁₄H₁₅NO₃S: C, 60.63; H, 5.45; N, 5.05. Found: C, 60.32; H, 5.46; N, 5.02.

Crystallization procedure: **TP-S**.

3-Methyl-*N*-phenylbenzenesulfonamide (S3A1).^{S9}

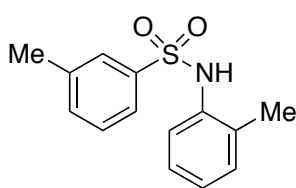
Color, Habit: Colorless, block crystals. Mp: 96.0–97.0 °C (lit: 88–90 °C).

¹H NMR (400 MHz, CDCl₃): δ 7.58–7.54 (m, 2H), 7.35–7.29 (m, 2H), 7.27–7.22 (m, 2H), 7.12 (t, *J* = 7.3, 1H), 7.06 (d, *J* = 7.3, 2H), 6.48 (brs, 1H), 2.35 (s, 3H).

IR (KBr pellet): 3257, 1598, 1483, 1415, 1336, 1214, 1153, 907, 758, 704 cm⁻¹.

Crystallization procedure: **TP-S**.

3-Methyl-*N*-(*o*-tolyl)benzenesulfonamide (S3A2).



Color, Habit: White powder. Mp: 117.0–118.0 °C.

MS (FAB⁺): m/z: 262 [M+H]⁺, 284 [M+Na]⁺.

¹H NMR (400 MHz, CDCl₃): δ 7.54–7.51 (m, 2H), 7.36–7.28 (m, 3H), 7.17–7.12 (m, 1H), 7.10–7.08 (m, 2H), 6.28 (brs, 1H), 2.35 (s, 3H), 2.00 (s, 3H).

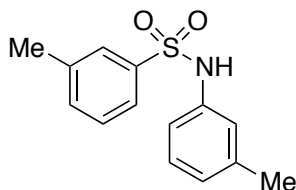
¹³C{¹H} NMR (100 MHz, CDCl₃): δ 139.4, 139.2, 134.4, 133.7, 131.3, 130.8, 128.8, 127.5, 127.0, 126.3, 124.4, 124.2, 21.3, 17.5.

IR (KBr pellet): 3267, 1496, 1395, 1332, 1161, 914, 756, 697, 686 cm⁻¹.

Anal. Calcd. for C₁₄H₁₅NO₂S: C, 64.34; H, 5.79; N, 5.36. Found: C, 64.09; H, 5.72; N, 5.28.

Crystallization procedure: **TP-S** and **TP-C** (Solvent A/ Solvent B = chloroform/*c*-hexane).

3-Methyl-*N*-(*m*-tolyl)benzenesulfonamide (S3A3).



Color, Habit: Colorless, prism crystals. Mp: 102.0–104.0 °C.

MS (FAB⁺): m/z: 262 [M+H]⁺, 284 [M+Na]⁺.

¹H NMR (400 MHz, CDCl₃): δ 7.59 (s, 1H), 7.56 (d, *J* = 7.1, 1H), 7.35–7.29 (m, 2H), 7.11 (t, *J* = 7.8, 1H), 6.93 (d, *J* = 7.6, 1H), 6.89 (s, 1H), 6.85 (d, *J* = 8.0, 1H), 6.51 (brs, 1H), 2.36 (s, 3H), 2.27 (s, 3H).

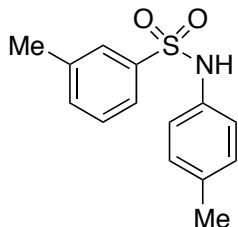
¹³C{¹H} NMR (100 MHz, CDCl₃): δ 139.4, 139.3, 139.0, 136.4, 133.9, 129.2, 128.9, 127.7, 126.4, 124.5, 122.4, 118.7, 21.42, 21.38.

IR (KBr pellet): 3232, 1608, 1590, 1499, 1475, 1403, 1330, 1305, 1165, 1147, 1096, 784, 810, 619, 592 cm⁻¹.

Anal. Calcd. for C₁₄H₁₅NO₂S: C, 64.34; H, 5.79; N, 5.36. Found: C, 64.22; H, 5.73; N, 5.38.

Crystallization procedure: **TP-S**.

3-Methyl-*N*-(*p*-tolyl)benzenesulfonamide (S3A4).^{S10}



Color, Habit: Colorless, prism crystals. Mp: 109.5–110.5 °C (lit: 98–100 °C).

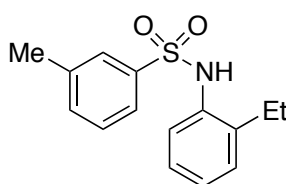
MS (FAB⁺): m/z: 262 [M+H]⁺, 284 [M+Na]⁺.

¹H NMR (400 MHz, CDCl₃): δ 7.56 (s, 1H), 7.51 (d, *J* = 6.7, 1H), 7.34–7.28 (m, 2H), 7.04 (d, *J* = 8.0, 2H), 6.93 (d, *J* = 8.5, 2H), 6.34 (brs, 1H), 2.36 (s, 3H), 2.28 (s, 3H).

IR (KBr pellet): 3271, 3025, 2921, 2858, 1610, 1509, 1475, 1394, 1338, 1297, 1219, 1152, 1098, 919, 820, 790, 695, 618, 585, 499 cm⁻¹.

Crystallization procedure: **TP-S**.

N-(2-Ethylphenyl)-3-methylbenzenesulfonamide (S3A5).



Color, Habit: Colorless, block crystals. Mp: 112.0 °C.

MS (FAB⁺): m/z: 276 [M+H]⁺, 298 [M+Na]⁺.

¹H NMR (400 MHz, CDCl₃): δ 7.54–7.51 (m, 2H), 7.36–7.28 (m, 3H), 7.15–7.12 (m, 3H), 6.30 (brs, 1H), 2.37 (q, *J* = 7.6, 2H), 2.35 (s, 3H), 1.04 (t, *J* = 7.6, 3H).

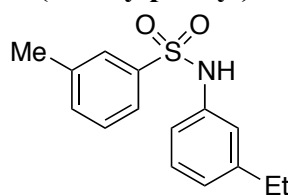
¹³C{¹H} NMR (100 MHz, CDCl₃): δ 139.5, 139.3, 137.2, 133.9, 133.9, 129.0, 129, 127.6, 126.9, 126.6, 124.4, 23.8, 21.4, 14.2.

IR (KBr pellet): 3263, 1491, 1398, 1333, 1226, 1160, 1088, 914, 792, 749, 696, 646, 594 cm⁻¹.

Anal. Calcd. for C₁₅H₁₇NO₂S: C, 65.43; H, 6.22; N, 5.09. Found: C, 65.18; H, 6.15; N, 5.08.

Crystallization procedure: **TP-S**.

***N*-(3-Ethylphenyl)-3-methylbenzenesulfonamide (S3A6).**



Color, Habit: White powder. Mp: 82.5–83.5 °C.

MS (FAB⁺): *m/z*: 276 [*M*+H]⁺, 298 [*M*+Na]⁺.

¹H NMR (400 MHz, CDCl₃): δ 7.58–7.54 (m, 2H), 7.33–7.31 (m, 2H), 7.15 (t, *J* = 7.7 Hz, 1H), 7.95 (d, *J* = 7.6 Hz, 3H), 6.88–6.85 (m, 2H), 6.43 (brs, 1H), 2.56 (q, *J* = 7.6, 2H), 2.35 (s, 3H), 1.15 (t, *J* = 7.7, 3H).

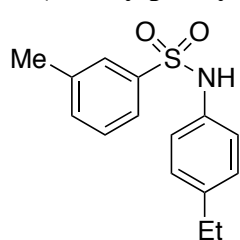
¹³C{¹H} NMR (100 MHz, CDCl₃): δ 145.8, 139.2, 139.0, 136.4, 133.8, 129.3, 128.9, 127.7, 125.2, 124.5, 121.4, 119.2, 28.7, 21.4, 15.5.

IR (KBr pellet): 3243, 2966, 1604, 1460, 1332, 1304, 1155, 1086, 798, 790, 757, 705, 643, 564 cm⁻¹.

Anal. Calcd. for C₁₅H₁₇NO₂S: C, 65.43; H, 6.22; N, 5.09. Found: C, 65.22; H, 6.17; N, 5.08.

Crystallization procedure: **TP-S** and **TP-C** (Solvent A/ Solvent B = MeOH/MeOH).

***N*-(4-Ethylphenyl)-3-methylbenzenesulfonamide (S3A7).**



Color, Habit: Colorless, prism crystals. Mp: 78.0–79.0 °C.

MS (FAB⁺): *m/z*: 276 [*M*+H]⁺, 298 [*M*+Na]⁺.

¹H NMR (400 MHz, CDCl₃): δ 7.56–7.52 (m, 2H), 7.33–7.29 (m, 2H), 7.07 (d, *J* = 8.5 Hz, 2H), 6.96 (d, *J* = 8.2 Hz, 2H), 6.38 (brs, 1H), 2.58 (q, *J* = 7.8, 2H), 2.35 (s, 3H), 1.18 (t, *J* = 7.6, 3H).

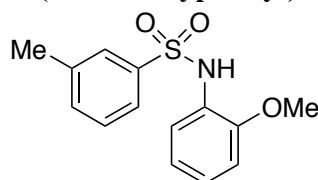
¹³C{¹H} NMR (100 MHz, CDCl₃): δ 142.1, 139.2, 139.1, 133.84, 133.78, 128.9, 128.8, 127.7, 124.5, 122.6, 28.3, 21.4, 15.6.

IR (KBr pellet): 3243, 2959, 2929, 2870, 1614, 1516, 1475, 1339, 1284, 1225, 1151, 1086, 931, 828, 687, 585 cm⁻¹.

Anal. Calcd. for C₁₅H₁₇NO₂S: C, 65.43; H, 6.22; N, 5.09. Found: C, 65.32; H, 6.19; N, 5.04.

Crystallization procedure: **TP-S** (form I) and **TP-C** (Solvent A/ Solvent B: chloroform/*c*-hexane, form II).

***N*-(2-Methoxyphenyl)-3-methylbenzenesulfonamide (S3A8).**



Color, Habit: Colorless, block crystals. Mp: 93.5–94.5 °C.

MS (FAB⁺): *m/z*: 278 [*M*+H]⁺, 300 [*M*+Na]⁺.

¹H NMR (400 MHz, CDCl₃): δ 7.58–7.54 (m, 2H), 7.51 (dd, *J* = 7.8, 1.9, 1H), 7.31–7.25 (m, 2H), 7.03 (td, *J* = 7.6, 1.6, 1H), 6.99 (brs, 1H), 6.90 (td, *J* = 7.6, 1.4 Hz, 1H), 6.73 (dd, *J* = 8.2, 1.1 Hz, 1H), 3.63 (s, 3H), 2.37

(s, 3H).

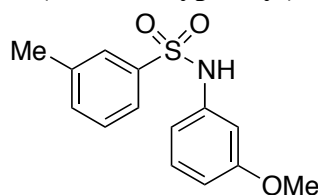
¹³C{¹H} NMR (100 MHz, CDCl₃): δ 149.6, 139.1, 139.0, 133.7, 128.6, 127.7, 126.0, 125.4, 124.4, 121.3, 121.2, 110.6, 55.7, 21.3.

IR (KBr pellet): 3249, 2046, 3014, 2948, 2838, 1588, 1498, 1405, 1337, 1257, 1164, 1115, 1090, 1046, 1029, 936, 917, 861, 784, 757, 704, 667, 589, 553, 513, 485, 434 cm⁻¹.

Anal. Calcd. for C₁₄H₁₅NO₃S: C, 60.63; H, 5.45; N, 5.05. Found: C, 60.51; H, 5.46; N, 5.04.

Crystallization procedure: **TP-S** and **TP-C** (Solvent A/ Solvent B = chloroform/MeOH).

***N*-(3-Methoxyphenyl)-3-methylbenzenesulfonamide (S3A9).**



Color, Habit: Colorless, block crystals. Mp: 88 °C.

MS (FAB⁺): *m/z*: 278 [*M*+H]⁺, 300 [*M*+Na]⁺.

¹H NMR (400 MHz, CDCl₃): δ 7.62–7.58 (m, 2H), 7.35–7.30 (m, 2H), 7.13 (t, *J* = 8.0, 1H), 6.68–6.58 (m, 3H), 3.75 (s, 3H), 2.36 (s, 3H).

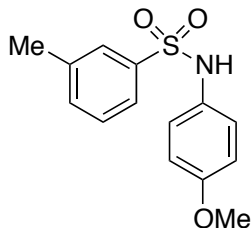
¹³C{¹H} NMR (100 MHz, CDCl₃): δ 160.4, 139.4, 138.9, 137.8, 134.0, 130.1, 129.0, 127.7, 124.5, 113.4, 111.0, 107.0, 55.4, 21.4.

IR (KBr pellet): 3241, 2997, 2961, 1606, 1597, 1496, 1439, 1407, 1328, 1309, 1278, 1151, 1042, 969, 845, 781, 594, 567 cm^{-1} .

Anal. Calcd. for $\text{C}_{14}\text{H}_{15}\text{NO}_3\text{S}$: C, 60.63; H, 5.45; N, 5.05. Found: C, 60.53; H, 5.45; N, 5.06.

Crystallization procedure: **TP-S**.

***N*-(4-Methoxyphenyl)-3-methylbenzenesulfonamide (S3A10).**



Color, Habit: Colorless, prism crystals. Mp: 85.0–86.0 °C.

MS (FAB⁺): m/z : 278 [$M+H$]⁺, 300 [$M+Na$]⁺.

¹H NMR (400 MHz, CDCl_3): δ 7.52 (s, 1H), 7.46 (d, $J = 7.6$, 1H), 7.35–7.28 (m, 2H), 6.6 (d, $J = 9.2$, 2H), 6.77 (d, $J = 8.9$, 2H), 6.16 (brs, 1H), 3.77 (s, 3H), 2.36 (s, 3H).

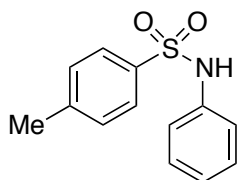
¹³C{¹H} NMR (100 MHz, CDCl_3): δ 158.1, 139.2, 138.9, 133.7, 128.8, 127.7, 125.72, 125.67, 124.5, 114.5, 55.5, 21.4.

IR (KBr pellet): 3278, 3013, 2970, 2841, 1889, 1610, 1512, 1397, 1225, 1291, 1252, 1216, 1153, 1031, 911, 822, 788, 701, 683, 634, 581, 554, 519, 465 cm^{-1} .

Anal. Calcd. for $\text{C}_{14}\text{H}_{15}\text{NO}_3\text{S}$: C, 60.63; H, 5.45; N, 5.05. Found: C, 60.72; H, 5.47; N, 5.06.

Crystallization procedure: **TP-S** and **TP-C** (Solvent A/ Solvent B: chloroform/*c*-hexane).

4-Methyl-*N*-phenylbenzenesulfonamide (S4A1).^{S11}



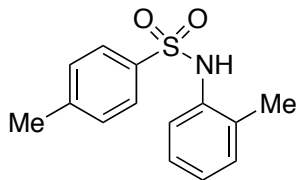
Color, Habit: Colorless, block crystals. Mp: 102–104 °C (lit: 104–105 °C).

¹H NMR (400 MHz, CDCl_3): δ 7.65–7.62 (m, 2H), 7.24–7.21 (m, 4H), 7.11 (7, $J = 7.8$, 1H), 7.06–7.04 (m, 2H), 6.55 (brs, 1H), 2.38 (s, 3H).

IR (KBr pellet): 3250, 1598, 1483, 1416, 1338, 1289, 1159, 1091, 913, 756, 694, 661, 565, 542, 421 cm^{-1} .

Crystallization procedure: **TP-S** and **TP-C** (Solvent A/ Solvent B: chloroform/toluene).

4-Methyl-*N*-(*o*-tolyl)benzenesulfonamide (S4A2).^{S12}



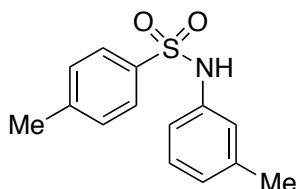
Color, Habit: Pale yellow powder. Mp: 108–109 °C (lit: 108–109 °C).

¹H NMR (400 MHz, CDCl_3): δ 7.60 (d, $J = 8.4$ Hz, 2H), 7.30 (d, $J = 7.7$ Hz, 1H), 7.22 (d, $J = 8.6$ Hz, 2H), 7.16–7.12 (m, 1H), 7.09–7.07 (m, 2H), 6.26 (br s, 1H), 2.39 (s, 3H), 2.00 (s, 3H).

IR (KBr pellet): 3277, 3037, 2979, 2925, 1922, 1808, 1673, 1599, 1489, 1397, 1331, 1164, 1092, 949, 904, 817, 765, 678, 570, 534, 451 cm^{-1} .

Crystallization procedure: **TP-S** and **TP-C** (Solvent A/ Solvent B: chloroform/*c*-hexane).

4-Methyl-*N*-(*m*-tolyl)benzenesulfonamide (S4A3).^{S8}



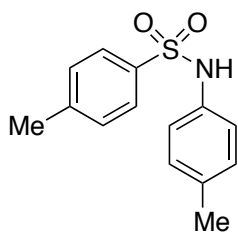
Color, Habit: Colorless, prism crystals. Mp: 114.5–116.5 °C (lit^{S7}: 114–115.5 and lit⁷: 110–112 °C).

¹H NMR (400 MHz, CDCl_3): δ 7.65 (d, $J = 8.2$ Hz, 2H), 7.23 (d, $J = 8.0$ Hz, 2H), 7.11 (t, $J = 7.6$ Hz, 1H), 6.93–6.90 (m, 2H), 6.84 (d, $J = 7.8$ Hz, 1H), 6.49 (brs, 1H), 2.38 (s, 3H), 2.2 (s, 3H).

IR (KBr pellet): 3251, 1593, 1504, 1399, 1330, 1306, 1288, 1158, 1093, 956, 901, 813, 784, 658, 567, 544, 424 cm^{-1} .

Crystallization procedure: **TP-S** and **TP-C** (Solvent A/ Solvent B: chloroform/*c*-hexane).

4-Methyl-*N*-(*p*-tolyl)benzenesulfonamide (S4A4).^{S11}

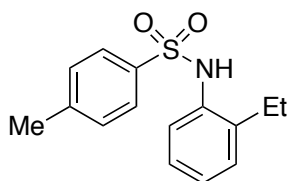


Color, Habit: Pale yellow powder. Mp: 119.5–120.5 °C (lit: 118–118.7 °C).
¹H NMR (400 MHz, CDCl₃): δ 7.61 (d, *J* = 8.2 Hz, 2H), 7.22 (d, *J* = 8.0 Hz, 2H), 7.04 (d, *J* = 8.0 Hz, 2H), 6.93 (d, *J* = 8.4 Hz, 2H), 6.29 (brs, 1H), 2.38 (s, 3H), 2.28 (s, 3H).

IR (KBr pellet): 3235, 3028, 2924, 2864, 1798, 1508, 1457, 1396, 1335, 1161, 1092, 911, 810, 705, 593, 551, 526, 502, cm⁻¹.

Crystallization procedure: **TP-S** and **TP-C** (Solvent A/ Solvent B: ethyl acetate/chloroform, form I; MeOH/*c*-hexane, form II).

N-(2-Ethylphenyl)-4-methylbenzenesulfonamide (S4A5).



Color, Habit: Colorless, block crystals. Mp: 136 °C.

MS (FAB⁺): *m/z*: 276 [*M*+H]⁺, 298 [*M*+Na]⁺.

¹H NMR (400 MHz, CDCl₃): δ 7.61 (d, *J* = 8.2, 2H), 7.32–7.30 (m, 1H), 7.23–7.21 (m, 2H), 7.16–7.11 (m, 3H), 6.31 (brs, 1H), 2.39 (s, 3H), 2.35 (q, *J* = 7.6 Hz, 2H), 1.04 (t, *J* = 7.8 Hz, 3H).

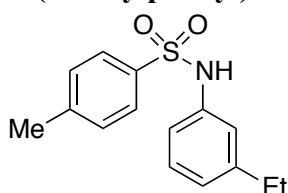
¹³C{¹H} NMR (100 MHz, CDCl₃): δ 143.9, 137.0, 136.7, 134.0, 129.7, 129.0, 127.4, 126.9, 126.5, 124.2, 23.8, 21.7, 14.2.

IR (KBr pellet): 3314, 2968, 2897, 2843, 1928, 1815, 1659, 1596, 1492, 1456, 1403, 1325, 1157, 1090, 949, 925, 819, 660, 766, 706, 660, 629, 576, 533 cm⁻¹.

Anal. Calcd. for C₁₅H₁₇NO₂S: C, 65.43; H, 6.22; N, 5.09. Found: C, 65.33; H, 6.18; N, 5.13.

Crystallization procedure: **TP-S** and **TP-C** (Solvent A/ Solvent B: MeOH/toluene).

N-(3-Ethylphenyl)-4-methylbenzenesulfonamide (S4A6).



Color, Habit: Colorless, prism crystals. Mp: 82–83 °C.

MS (FAB⁺): *m/z*: 276 [*M*+H]⁺, 298 [*M*+Na]⁺.

¹H NMR (400 MHz, CDCl₃): δ 7.64 (dt, *J* = 8.2, 1.7, 2H), 7.23–7.21 (m, 2H), 7.14 (t, *J* = 7.8, 2H), 6.97–6.93 (m, 1H), 6.89–6.84 (m, 2H), 6.46 (brs, 1H), 2.56 (q, *J* = 7.6 Hz, 2H), 2.38 (s, 3H), 1.15 (t, *J* = 7.6 Hz, 3H).

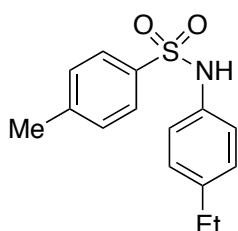
¹³C{¹H} NMR (100 MHz, CDCl₃): δ 145.7, 143.8, 136.4, 136.1, 129.6, 129.1, 127.3, 125.0, 121.1, 118.8, 28.7, 21.5, 15.4.

IR (KBr pellet): 3240, 1591, 1496, 1408, 1334, 1168, 1155, 1091, 936, 809, 791, 702, 564, 543 cm⁻¹.

Anal. Calcd. for C₁₅H₁₇NO₂S: C, 65.43; H, 6.22; N, 5.09. Found: C, 65.34; H, 6.19; N, 5.04.

Crystallization procedure: **TP-S**.

N-(4-Ethylphenyl)-4-methylbenzenesulfonamide (S4A7).^{S13}



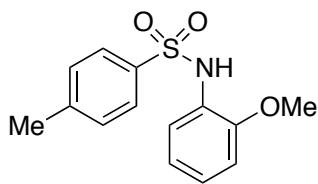
Color, Habit: Colorless, block crystals. Mp: 94.0–95.0 °C (lit: 90–92 °C)

¹H NMR (400 MHz, CDCl₃): δ 7.62 (d, *J* = 8.4 Hz, 2H), 7.22 (d, *J* = 8.5 Hz, 2H), 7.07 (d, *J* = 8.4 Hz, 2H), 6.95 (d, *J* = 8.5 Hz, 2H), 6.26 (brs, 1H), 2.58 (q, *J* = 7.7 Hz, 2H), 2.39 (s, 3H), 1.18 (t, *J* = 7.4 Hz, 3H)

IR (KBr pellet): 3238, 2957, 1511, 1459, 1397, 1336, 1159, 1092, 915, 809, 692, 587, 556, 516 cm⁻¹.

Crystallization procedure: **TP-S**.

***N*-(2-Methoxyphenyl)-4-methylbenzenesulfonamide (S4A8).**^{S9}



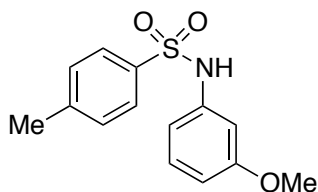
Color, Habit: Colorless, prism crystals. Mp: 129.5–132.0 °C

¹H NMR (400 MHz, CDCl₃): δ 7.64 (d, *J* = 8.2 Hz, 2H), 7.52 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.19 (d, *J* = 8.5 Hz, 1H), 7.02 (td, *J* = 7.6, 1.8 Hz, 1H), 6.99 (br. s, 1H), 6.89 (td, *J* = 7.8, 1.4 Hz, 1H), 6.73 (d, *J* = 8.0 Hz, 1H), 3.64 (s, 3H), 2.36 (s, 3H)

IR (KBr pellet): 3333, 3010, 2967, 1595, 1498, 1445, 1398, 1335, 1257, 1160, 1115, 1091, 1026, 932, 823, 781, 755, 628, 555, 536, 460 cm⁻¹.

Crystallization procedure: **TP-S**.

***N*-(3-Methoxyphenyl)-4-methylbenzenesulfonamide (S4A9).**^{S8}



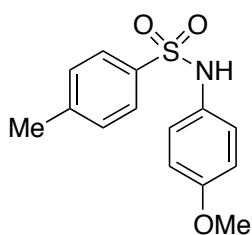
Color, Habit: Colorless, orange block crystals. Mp: 66.5–67.5 °C (lit: light yellow liquid)

¹H NMR (400 MHz, CDCl₃): δ 7.68 (d, *J* = 8.0 Hz, 2H), δ 7.23 (d, *J* = 8.2 Hz, 2H), 7.11 (t, *J* = 7.8 Hz, 1H), 6.69–6.58 (m, 4H), 3.74 (s, 3H), 2.38 (s, 3H).

IR (KBr pellet): 3236, 2006, 2956, 2834, 1612, 1496, 1409, 1334, 1287, 1152, 1092, 1052, 948, 899, 864, 810, 774, 703, 565, 543 cm⁻¹.

Crystallization procedure: **TP-S** and **TP-C** (Solvent A/ Solvent B: ethyl acetate/acetonitrile).

***N*-(4-Methoxyphenyl)-4-methylbenzenesulfonamide (S4A10).**^{S9}



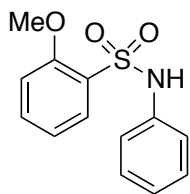
Color, Habit: Colorless, prism crystals. Mp: 115.5–116.5 °C (lit³: 112–114 °C)

¹H NMR (400 MHz, CDCl₃): δ 7.56 (d, *J* = 7.7 Hz, 2H), 7.22 (d, *J* = 8.0 Hz, 2H), 7.96 (d, *J* = 8.2 Hz, 2H), 6.77 (d, *J* = 8.0 Hz, 2H), 6.18 (brs, 1H), 3.76 (s, 3H), 2.39 (s, 3H)

IR (KBr pellet): 3270, 3011, 2963, 2838, 1508, 1396, 1335, 1290, 1253, 1219, 1160, 1092, 1030, 911, 812, 681, 555, 540 cm⁻¹.

Crystallization procedure: **TP-S**.

2-Methoxy-*N*-phenylbenzenesulfonamide (S5A1).



Color, Habit: Colorless, platelet crystals. Mp: 161.0–163.0 °C.

MS (FAB+): *m/z*: 264 [*M*+H]⁺.

¹H NMR (400 MHz, CDCl₃): δ 7.82 (d, *J* = 7.8 Hz, 1H), 7.48 (ddd, *J* = 9.2, 7.4, 1.7 Hz, 1H), 7.21–7.17 (m, 2H), 7.08–7.03 (m, 3H), 7.01–6.96 (m, 3H), 4.04 (s, 3H).

¹³C{¹H} NMR (100 MHz, CDCl₃): δ 156.2, 136.8, 135.0, 131.1, 129.3,

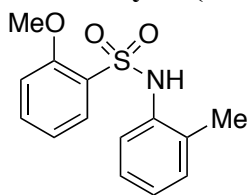
126.3, 125.4, 121.4, 120.8, 112.1, 76.8, 56.5.

IR (KBr pellet): 3254, 2967, 1595, 1481, 1416, 1331, 1282, 1226, 1155, 1138, 1072, 1018, 922, 801, 762, 705, 574, 536 cm⁻¹.

Anal. Calcd. for C₁₃H₁₃NO₃S: C, 59.30; H, 4.98; N, 5.32 Found: C, 59.19; H, 4.94; N, 5.24.

Crystallization procedure: **TP-S** (form I) and **TP-C** (Solvent A/ Solvent B: MeOH/chloroform, form II).

2-Methoxy-*N*-(*o*-tolyl)benzenesulfonamide (S5A2).



Color, Habit: White powder. Mp: 148.0–149.0 °C.

HRMS (FAB) *m/z*: Calcd for C₁₄H₁₆NO₃S 278.0851 [*M*+H]⁺; Found 278.0851 [*M*+H]⁺.

¹H NMR (400 MHz, CDCl₃): δ 7.85 (t, *J* = 8.1 Hz, 2H), 7.52 (t, *J* = 7.9 Hz, 2H), 7.18 (d, *J* = 7.7 Hz, 1H), 7.10 (d, *J* = 7.1 Hz, 1H), 7.06–6.97 (m, 4H), 6.76 (brs, 1H), 4.01 (s, 3H), 2.26 (s, 3H).

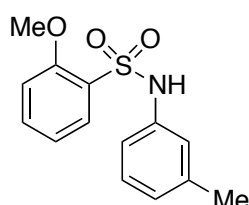
¹³C{¹H} NMR (100 MHz, CDCl₃): δ 156.0, 134.9, 134.8, 130.8, 130.7, 130.4, 127.2, 126.7, 125.4, 122.1, 120.6, 112.0, 56.2, 17.5.

IR (KBr pellet): 3259, 2959, 2934, 2834, 1594, 1490, 1408, 1324, 1281, 1158, 1018, 921, 755, 595, 579, 535, 425 cm⁻¹.

Anal. Calcd. for C₁₄H₁₅NO₃S: C, 60.63; H, 5.45; N, 5.05. Found: C, 59.10; H, 5.27; N, 4.11.

Crystallization procedure: **TP-S** and **TP-C** (Solvent A/ Solvent B = chloroform/*n*-hexane).

2-Methoxy-*N*-(*m*-tolyl)benzenesulfonamide (S5A3).



Color, Habit: Colorless, platelet crystals. Mp: 151.0–151.5 °C.

MS (FAB⁺): *m/z*: 278 [*M*+H]⁺, 300 [*M*+Na]⁺.

¹H NMR (400 MHz, CDCl₃): δ 7.82 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.49 (ddd, *J* = 9.4, 7.6, 1.8 Hz, 1H), 7.06 (t, *J* = 7.8 Hz, 1H), 7.01–6.97 (m, 2H), 6.91 (s, 1H), 6.88–6.82 (m, 3H), 4.04 (s, 3H), 2.25 (s, 3H).

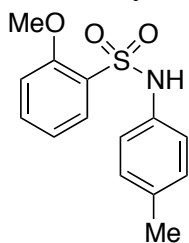
¹³C{¹H} NMR (100 MHz, CDCl₃): δ 156.3, 139.2, 136.7, 135.0, 131.1, 129.0, 126.4, 126.0, 122.0, 120.7, 118.2, 112.1, 56.5, 21.4.

IR (KBr pellet): 3256, 2968, 2938, 2839, 1611, 1590, 1496, 1401, 1323, 1153, 1070, 1018, 952, 909, 891, 796, 751, 708, 616, 579, 555, 543, 502, 445 cm⁻¹.

Anal. Calcd. for C₁₄H₁₅NO₃S: C, 60.63; H, 5.45; N, 5.05. Found: C, 60.34; H, 5.40; N, 5.01.

Crystallization procedure: **TP-S**.

2-Methoxy-*N*-(*p*-tolyl)benzenesulfonamide (S5A4).



Color, Habit: Colorless, block crystals. Mp: 195.0–197.0 °C.

MS (FAB⁺): *m/z*: 278 [*M*+H]⁺, 300 [*M*+Na]⁺.

¹H NMR (400 MHz, CDCl₃): δ 7.78 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.48 (ddd, *J* = 9.2, 7.6, 1.8 Hz, 1H), 7.02–6.93 (m, 6H), 6.86 (brs, 1H), 4.05 (s, 3H), 2.22 (s, 3H).

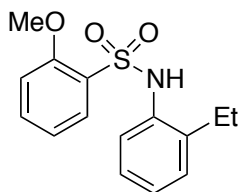
¹³C{¹H} NMR (100 MHz, CDCl₃): δ 156.1, 135.3, 134.9, 134.0, 131.1, 129.8, 126.4, 122.0, 120.8, 112.1, 56.5, 20.9.

IR (KBr pellet): 3249, 3108, 3026, 2975, 2942, 2867, 1591, 1510, 1481, 1432, 1397, 1328, 1301, 1281, 1157, 1071, 924, 815, 769, 802, 598, 564, 528 cm⁻¹.

Anal. Calcd. for C₁₄H₁₅NO₃S: C, 60.63; H, 5.45; N, 5.05. Found: C, 60.59; H, 5.47; N, 5.03.

Crystallization procedure: **TP-S**.

N-(2-Ethylphenyl)-2-methoxybenzenesulfonamide (S5A5).



Color, Habit: Colorless, platelet crystals. Mp: 122.5–123.5 °C.

HRMS (FAB) *m/z*: Calcd for C₁₅H₁₇NNaO₃S 314.0827 [*M*+Na]⁺; Found 314.0827 [*M*+Na]⁺.

¹H NMR (400 MHz, CDCl₃): δ 7.86 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.55–7.50 (m, 1H), 7.15 (dt, *J* = 7.3, 2.1 Hz, 2H), 7.08–7.00 (m, 4H), 6.77 (brs, 1H), 4.01 (s, 3H), 2.64 (q, *J* = 7.6 Hz, 2H), 1.17 (t, *J* = 7.6 Hz, 3H).

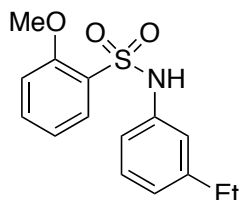
¹³C{¹H} NMR (100 MHz, CDCl₃): δ 156.2, 136.8, 134.9, 134.3, 130.9, 129.1, 127.5, 126.7, 125.9, 122.7, 120.8, 112.1, 56.4, 23.9, 14.4.

IR (KBr pellet): 3277, 2974, 1591, 1496, 1482, 1415, 1331, 1283, 1165, 1135, 1018, 919, 749, 706, 592 cm^{-1} .

Anal. Calcd. for $\text{C}_{15}\text{H}_{17}\text{NO}_3\text{S}$: C, 61.83; H, 5.88; N, 4.81. Found: C, 61.52; H, 5.78; N, 4.80.

Crystallization procedure: **TP-S**.

***N*-(3-Ethylphenyl)-2-methoxybenzenesulfonamide (S5A6).**



Color, Habit: Colorless, block crystals. Mp: 139.5–141.0 °C.

HRMS (FAB) m/z : Calcd for $\text{C}_{15}\text{H}_{17}\text{NNaO}_3\text{S}$ 314.0827 $[M+\text{Na}]^+$; Found 314.0826 $[M+\text{Na}]^+$.

^1H NMR (400 MHz, CDCl_3): δ 7.82 (dd, $J = 7.8, 1.6$ Hz, 1H), 7.48 (ddd, $J = 9.2, 7.6, 1.6$ Hz, 1H), 7.09 (t, $J = 7.6$ Hz, 1H), 7.00–6.96 (m, 2H), 6.91–6.84 (m, 4H), 4.04 (s, 3H), 2.53 (q, $J = 7.6$ Hz, 2H), 1.12 (t, $J = 7.6$ Hz, 3H).

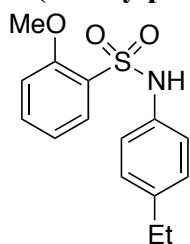
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 156.2, 145.6, 136.8, 134.9, 131.1, 129.1, 126.4, 124.9, 120.9, 120.7, 118.6, 112.1, 56.5, 28.7, 15.4.

IR (KBr pellet): 3283, 2965, 2930, 1592, 1473, 1435, 1405, 1333, 1285, 1158, 1132, 1069, 1022, 988, 942, 895, 881, 856, 756, 701, 650, 631, 576, 534, 454 cm^{-1} .

Anal. Calcd. for $\text{C}_{15}\text{H}_{17}\text{NO}_3\text{S}$: C, 61.83; H, 5.88; N, 4.81. Found: C, 61.51; H, 5.77; N, 4.76.

Crystallization procedure: **TP-S** and **TP-C** (Solvent A/ Solvent B: chloroform/MeOH).

***N*-(4-Ethylphenyl)-2-methoxybenzenesulfonamide (S5A7).**



Color, Habit: Colorless, prism crystals. Mp: 164 °C.

MS (FAB⁺): m/z : 292 $[M+\text{H}]^+$, 314 $[M+\text{Na}]^+$.

^1H NMR (400 MHz, CDCl_3): δ 7.79 (dd, $J = 7.8, 1.4$ Hz, 1H), 7.51–7.47 (m, 1H), 7.02–6.96 (m, 6H), 6.84 (brs, 1H), 4.05 (s, 3H), 2.53 (q, $J = 7.8$ Hz, 2H), 1.14 (t, $J = 7.6$ Hz, 3H).

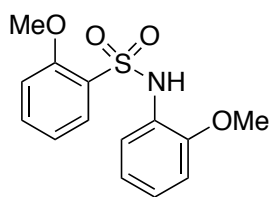
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 156.1, 141.7, 134.8, 134.1, 131.0, 128.6, 126.6, 122.2, 120.9, 112.1, 56.5, 28.2, 15.4.

IR (KBr pellet): 3257, 2963, 2871, 1595, 1514, 1482, 1434, 1401, 1334, 1287, 1661, 1132, 1070, 1018, 927, 832, 801, 753, 700, 594, 565, 551 cm^{-1} .

Anal. Calcd. for $\text{C}_{15}\text{H}_{17}\text{NO}_3\text{S}$: C, 61.83; H, 5.88; N, 4.81. Found: C, 61.67; H, 5.79; N, 4.79.

Crystallization procedure: **TP-S**.

2-Methoxy-*N*-(2-methoxyphenyl)benzenesulfonamide (S5A8).



Color, Habit: Colorless, block crystals. Mp: 101.0–103.0 °C.

MS (FAB⁺): m/z : 294 $[M+\text{H}]^+$, 316 $[M+\text{Na}]^+$.

^1H NMR (400 MHz, CDCl_3): δ 7.88 (d, $J = 7.8$ Hz, 1H), 7.61 (brs, 3H), 7.51 (d, $J = 8.0$ Hz, 1H), 7.46 (t, $J = 7.8$ Hz, 1H), 6.98–6.92 (m, 3H), 6.82 (t, $J = 8.0$ Hz, 1H), 6.75 (d, $J = 8.0$ Hz, 1H), 3.95 (s, 3H), 3.77 (s, 3H).

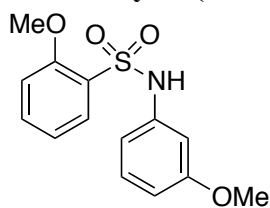
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 156.5, 148.9, 134.8, 131.1, 126.7, 126.6, 124.5, 121.2, 120.3, 119.9, 111.8, 110.5, 56.1, 55.9.

IR (KBr pellet): 3319, 2976, 2949, 2841, 1591, 1498, 1479, 1399, 1340, 1281, 1254, 1162, 1112, 069, 1020, 898, 851, 708, 652 cm^{-1} .

Anal. Calcd. for $\text{C}_{14}\text{H}_{15}\text{NO}_4\text{S}$: C, 57.32; H, 5.15; N, 4.77. Found: C, 57.14; H, 5.10; N, 4.78.

Crystallization procedure: **TP-S** (form II) and **TP-C** (Solvent A/ Solvent B: ethyl acetate/ethyl acetate, form I).

2-Methoxy-*N*-(3-methoxyphenyl)benzenesulfonamide (S5A9).



Color, Habit: White powder. Mp: 141.0–142.0 °C.

HRMS (FAB) *m/z*: Calcd for C₁₄H₁₅NNaO₄S 316.0619 [*M*+Na]⁺; Found 316.0619 [*M*+Na]⁺.

¹H NMR (400 MHz, CDCl₃): δ 7.84 (dd, *J* = 8.0, 1.8 Hz, 1H), 7.49 (ddd, *J* = 9.2, 7.6, 1.8 Hz, 1H), 7.08 (t, *J* = 8.0 Hz, 1H), 7.01–6.97 (m, 2H), 6.90 (brs, 1H), 6.69 (t, *J* = 2.3, 1H), 6.59 (dd, *J* = 8.2, 2.3, 2H), 4.03 (s, 3H), 3.72 (s,

3H).

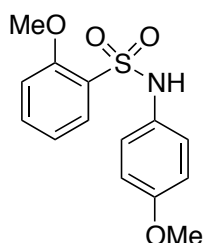
¹³C{¹H} NMR (100 MHz, CDCl₃): δ 160.2, 156.2, 138.0, 135.0, 131.1, 129.9, 126.3, 120.8, 113.3, 112.1, 110.8, 107.0, 56.5, 55.3.

IR (KBr pellet): 3255, 2936, 2837, 1610, 1506, 1479, 1328, 1282, 1155, 1135, 1056, 863, 781, 757, 699, 592 cm⁻¹.

Anal. Calcd. for C₁₄H₁₅NO₄S: C, 57.32; H, 5.15; N, 4.77. Found: C, 57.01; H, 5.05; N, 4.71.

Crystallization procedure: **TP-S** and **TP-C** (Solvent A/ Solvent B: chloroform/*n*-hexane).

2-Methoxy-*N*-(4-methoxyphenyl)benzenesulfonamide (S5A10).



Color, Habit: Colorless, prism crystals. Mp: 153.5–155.0 °C.

MS (FAB⁺): *m/z*: 294 [*M*+H]⁺, 316 [*M*+Na]⁺.

¹H NMR (400 MHz, CDCl₃): δ 7.73 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.49 (ddd, *J* = 9.2, 7.3, 1.6 Hz, 1H), 7.03 (d, *J* = 8.2 Hz, 1H), 7.00–6.94 (m, 3H), 6.81 (brs, 1H), 6.71 (d, *J* = 9.2, 2H), 4.07 (s, 3H), 3.71 (s, 3H).

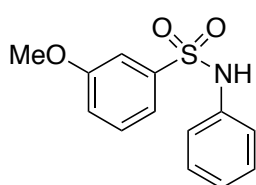
¹³C{¹H} NMR (100 MHz, CDCl₃): δ 157.9, 156.1, 134.8, 131.0, 129.2, 126.5, 124.8, 120.9, 114.4, 112.1, 56.6, 55.4.

IR (KBr pellet): 3245, 3019, 2972, 2846, 1591, 1510, 1483, 1469, 1442, 1397, 1324, 1289, 1250, 1161, 1137, 1069, 1029, 1109, 911, 824, 800, 754, 707, 634 cm⁻¹.

Anal. Calcd. for C₁₄H₁₅NO₄S: C, 57.32; H, 5.15; N, 4.77. Found: C, 57.19; H, 5.06; N, 4.76.

Crystallization procedure: **TP-S**.

3-Methoxy-*N*-phenylbenzenesulfonamide (S6A1).



Color, Habit: Pale orange powder. Mp: 104.5–105.0 °C.

MS (FAB⁺): *m/z*: 264 [*M*+H]⁺, 286 [*M*+Na]⁺.

¹H NMR (400 MHz, CDCl₃): δ 7.34–7.33 (m, 2H), 7.28–7.21 (m, 5H), 7.14 (t, *J* = 7.4, 1H), 7.08–7.04 (m, 3H), 6.50 (brs, 1H), 3.74 (s, 3H).

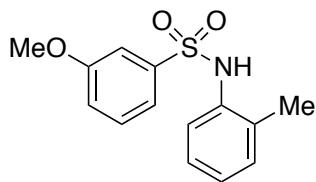
¹³C{¹H} NMR (100 MHz, CDCl₃): δ 159.8, 140.1, 136.4, 130.1, 129.4, 125.8, 122.2, 119.8, 119.4, 111.7, 55.7.

IR (KBr pellet): 3256, 2015, 1965, 1611, 1499, 1448, 1412, 1330, 1286, 1165, 1149, 1090, 1051, 645, 697, 864, 776, 727, 689, 661, 592, 551 cm⁻¹.

Anal. Calcd. for C₁₃H₁₃NO₃S: C, 59.30; H, 4.98; N, 5.32. Found: C, 59.04; H, 4.93; N, 5.24.

Crystallization procedure: **TP-S** and **TP-C** (Solvent A/ Solvent B: ethyl acetate/*c*-hexane).

3-Methoxy-*N*-(*o*-tolyl)benzenesulfonamide (S6A2).



Color, Habit: Colorless, block crystals. Mp: 74.0–75.0 °C.

MS (FAB⁺): *m/z*: 278 [*M*+H]⁺, 300 [*M*+Na]⁺.

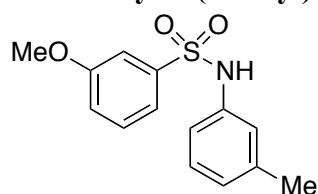
¹H NMR (400 MHz, CDCl₃): δ 7.36–7.32 (m, 3H), 7.17–7.14 (m, 2H), 7.10–7.05 (m, 3H), 6.29 (brs, 1H), 3.72 (s, 3H), 1.98 (s, 3H).

¹³C{¹H} NMR (100 MHz, CDCl₃): δ 159.8, 140.7, 134.5, 131.7, 130.9, 130.1, 127.1, 126.5, 124.8, 119.9, 119.3, 111.5, 55.6, 17.6.

IR (KBr pellet): 3255, 3001, 1596, 2341, 1486, 1396, 1333, 1251, 1157, 1038, 913, 855, 763, 695, 286, 526 cm⁻¹.

Anal. Calcd. for C₁₄H₁₅NO₃S: C, 60.63; H, 5.45; N, 5.05. Found: C, 60.67; H, 5.47; N, 5.10.
Crystallization procedure: **TP-S**.

3-Methoxy-*N*-(*m*-tolyl)benzenesulfonamide (S6A3).



Color, Habit: Colorless, block crystals. Mp: 89.0–90.0 °C.

MS (FAB⁺): m/z: 278 [M+H]⁺, 300 [M+Na]⁺.

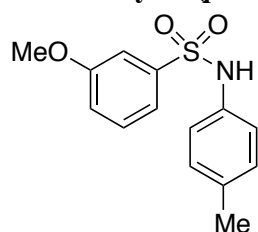
¹H NMR (400 MHz, CDCl₃): δ 7.36–7.31 (m, 2H), 7.24–7.22 (m, 1H), 7.12 (t, *J* = 7.8, 1H), 7.07–7.04 (m, 1H), 6.94 (d, *J* = 7.6, 1H), 6.90 (s, 1H), 6.85 (d, *J* = 8.0, 1H), 6.39 (brs, 1H), 3.75 (s, 3H), 2.28 (s, 3H).

¹³C{¹H} NMR (100 MHz, CDCl₃): δ 159.8, 140.2, 139.5, 136.3, 130.1, 129.2, 126.5, 122.6, 119.8, 119.5, 118.8, 111.7, 55.7, 21.4.

IR (KBr pellet): 3284, 3090, 3011, 2963, 2833, 1608, 1484, 1325, 1254, 1155, 1098, 1035, 956, 885, 849, 791, 699, 605, 516, 442 cm⁻¹.

Anal. Calcd. for C₁₄H₁₅NO₃S: C, 60.63; H, 5.45; N, 5.05. Found: C, 60.35; H, 5.43; N, 5.01.
Crystallization procedure: **TP-S**.

3-Methoxy-*N*-(*p*-tolyl)benzenesulfonamide (S6A4).



Color, Habit: Colorless, block crystals. Mp: 93.0–94.0 °C.

MS (FAB⁺): m/z: 278 [M+H]⁺, 300 [M+Na]⁺.

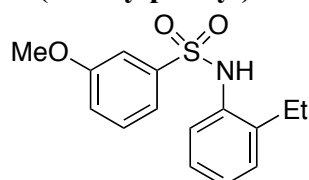
¹H NMR (400 MHz, CDCl₃): δ 7.35–7.29 (m, 2H), 7.20–7.19 (m, 1H), 7.07–7.04 (m, 3H), 6.94 (d, *J* = 8.5, 2H), 6.28 (brs, 1H), 3.75 (s, 3H), 2.28 (s, 3H).

¹³C{¹H} NMR (100 MHz, CDCl₃): δ 159.8, 140.1, 135.7, 133.7, 130.1, 130.0, 122.6, 119.7, 119.5, 111.7, 55.6, 20.9.

IR (KBr pellet): 3222, 1596, 1509, 1481, 1333, 1290, 1249, 1160, 1043, 782, 707, 582, 506 cm⁻¹.

Anal. Calcd. for C₁₄H₁₅NO₃S: C, 60.63; H, 5.45; N, 5.05. Found: C, 60.47; H, 5.39; N, 4.98.
Crystallization procedure: **TP-S**.

N-(2-Ethylphenyl)-3-methoxybenzenesulfonamide (S6A5).



Color, Habit: Colorless, block crystals. Mp: 65.0–66.0 °C.

MS (FAB⁺): m/z: 292 [M+H]⁺, 314 [M+Na]⁺.

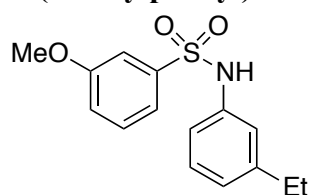
¹H NMR (400 MHz, CDCl₃): δ 7.36–7.32 (m, 3H), 7.17–7.12 (m, 4H), 7.08–7.05 (m, 1H), 6.30 (brs, 1H), 3.72 (s, 3H), 2.35 (q, *J* = 7.6, 2H), 1.03 (t, *J* = 7.6, 3H).

¹³C{¹H} NMR (100 MHz, CDCl₃): δ 159.8, 140.6, 137.3, 133.8, 130.1, 129.0, 126.9, 126.7, 124.6, 119.8, 119.3, 111.5, 55.6, 23.7, 14.2.

IR (KBr pellet): 3281, 2972, 2941, 2898, 2841, 1595, 1489, 1458, 1433, 1408, 1337, 1290, 1247, 1159, 1040, 918, 852, 794, 750, 687, 606, 519 cm⁻¹.

Anal. Calcd. for C₁₅H₁₇NO₃S: C, 61.83; H, 5.88; N, 4.81. Found: C, 61.74; H, 5.78; N, 4.78.
Crystallization procedure: **TP-S**.

N-(3-Ethylphenyl)-3-methoxybenzenesulfonamide (S6A6).



Color, Habit: Pale red, prism crystals. Mp: 53.0–54.0 °C.

MS (FAB⁺): m/z: 292 [M+H]⁺, 314 [M+Na]⁺.

¹H NMR (400 MHz, CDCl₃): δ 7.34–7.33 (m, 2H), 7.21–7.19 (m, 1H), 7.16 (t, *J* = 8.2, 1H), 7.07–7.04 (m, 1H), 6.98 (d, *J* = 7.6, 1H), 6.89–6.87 (m, 2H), 6.36 (brs, 1H), 3.74 (s, 3H), 2.57 (q, *J* = 7.6, 2H), 1.15 (t, *J* = 7.6, 3H).

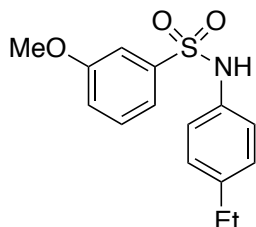
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 159.8, 145.8, 140.1, 136.4, 130.1, 129.3, 125.3, 121.6, 119.8, 119.5, 119.3, 111.7, 55.6, 28.7, 15.5.

IR (KBr pellet): 3247, 2966, 2871, 1608, 1471, 1402, 1329, 1256, 1149, 1102, 1031, 944, 881, 860, 793, 703, 597, 533, cm^{-1} .

Anal. Calcd. for $\text{C}_{15}\text{H}_{17}\text{NO}_3\text{S}$: C, 61.83; H, 5.88; N, 4.81. Found: C, 61.60; H, 5.81; N, 4.80.

Crystallization procedure: **TP-S**.

***N*-(4-Ethylphenyl)-3-methoxybenzenesulfonamide (S6A7).**



Color, Habit: White powder. Mp: 77–81 °C.

HRMS (FAB) m/z : Calcd for $\text{C}_{15}\text{H}_{17}\text{NNaO}_3\text{S}$ 314.0827 [$M+\text{Na}$] $^+$; Found 314.0827 [$M+\text{Na}$] $^+$.

^1H NMR (400 MHz, CDCl_3): δ 7.34–7.33 (m, 2H), 7.20–7.18 (m, 1H), 7.09–7.04 (m, 3H), 6.98 (d, $J = 8.5$, 2H), 6.46 (brs, 1H), 3.74 (s, 3H), 2.58 (q, $J = 7.6$, 2H), 1.18 (t, $J = 7.6$, 3H).

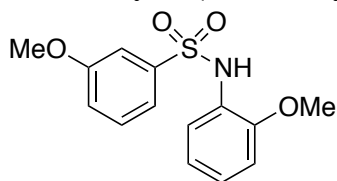
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 159.8, 142.0, 140.2, 133.9, 130.1, 128.7, 122.7, 119.8, 119.5, 111.6, 55.6, 28.3, 15.6.

IR (KBr pellet): 3249, 3072, 3029, 2961, 1602, 1512, 1490, 1459, 1396, 1331, 1256, 1156, 1101, 1029, 918, 791, 696, 680, 655, 642, 581, 506 cm^{-1} .

Anal. Calcd. for $\text{C}_{15}\text{H}_{17}\text{NO}_3\text{S}$: C, 61.83; H, 5.88; N, 4.81. Found: C, 61.20; H, 5.75; N, 4.78.

Crystallization procedure: **TP-S**.

3-Methoxy-*N*-(2-methoxyphenyl)benzenesulfonamide (S6A8).



Color, Habit: Colorless, prism crystals. Mp: 104.5–105.5 °C.

MS (FAB $^+$): m/z : 294 [$M+\text{H}$] $^+$, 316 [$M+\text{Na}$] $^+$.

^1H NMR (400 MHz, CDCl_3): δ 7.54 (dd, $J = 7.90$, 1.60, 1H), 7.36–7.28 (m, 2H), 7.20 (t, $J = 1.83$, 1H), 7.07–7.00 (m, 2H), 6.98 (brs, 1H), 6.91 (t, $J = 7.90$, 1H), 6.74 (d, $J = 8.13$, 1H), 3.73 (s, 3H), 3.63 (s, 3H).

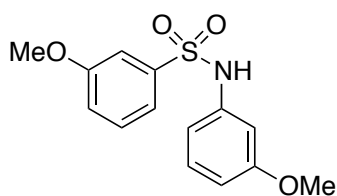
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 159.7, 140.6, 134.4, 131.7, 130.8, 130.1, 127.0, 126.5, 124.7, 119.8, 119.2, 111.4, 55.6, 17.5.

IR (KBr pellet): 3279, 3016, 1600, 1513, 1483, 1396, 1323, 1289, 1253, 1215, 1156, 1031, 908, 853, 821, 786, 697, 634, 584, 523 cm^{-1} .

Anal. Calcd. for $\text{C}_{14}\text{H}_{15}\text{NO}_4\text{S}$: C, 57.32; H, 5.15; N, 4.77. Found: C, 57.18; H, 5.06; N, 4.77.

Crystallization procedure: **TP-S** (form I) and **TP-C** (Solvent A/ Solvent B: ethyl acetate/chloroform, form II).

3-Methoxy-*N*-(3-methoxyphenyl)benzenesulfonamide (S6A9).



Color, Habit: Colorless, block crystals. Mp: 44.0–45.0 °C.

MS (FAB $^+$): m/z : 294 [$M+\text{H}$] $^+$, 316 [$M+\text{Na}$] $^+$.

^1H NMR (400 MHz, CDCl_3): δ 7.39–7.32 (m, 2H), 7.27–7.26 (m, 1H), 7.13 (t, $J = 8.0$, 1H), 7.06 (dt, $J = 7.6$, 1.8, 1H), 7.00–6.60 (m, 4H), 3.76 (s, 3H), 3.75 (s, 3H).

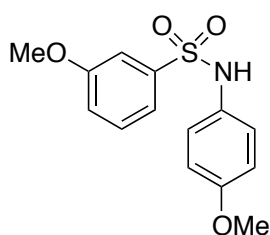
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 160.3, 159.8, 140.0, 137.5, 130.1, 119.7, 119.4, 113.7, 111.7, 111.2, 107.4, 99.9, 55.6, 55.3.

IR (KBr pellet): 3246, 3064, 3008, 2970, 2841, 1607, 1474, 1435, 1394, 1322, 1282, 1243, 1148, 1041, 951, 885, 778, 700, 606, 583, 517 cm^{-1} .

Anal. Calcd. for $\text{C}_{14}\text{H}_{15}\text{NO}_4\text{S}$: C, 57.32; H, 5.15; N, 4.77. Found: C, 57.02; H, 5.05; N, 4.67.

Crystallization procedure: **TP-S** (form I) and **TP-C** (Solvent A/ Solvent B: chloroform/*c*-hexane, form II).

3-Methoxy-*N*-(4-methoxyphenyl)benzenesulfonamide (S6A10).



Color, Habit: Purple, prism crystals. Mp: 102–105 °C.

MS (FAB⁺): m/z: 294 [*M*+H]⁺, 316 [*M*+Na]⁺.

¹H NMR (400 MHz, CDCl₃): δ 7.33 (t, *J* = 8.0, 1H), 7.39–7.32 (m, 2H), 7.29–7.26 (m, 1H), 7.18 (dd, *J* = 2.4, 1.3, 1H), 7.05 (ddd, *J* = 8.1, 2.6, 1.3, 1H), 6.98 (d, *J* = 8.9, 2H), 6.77 (d, *J* = 8.9, 2H), 6.44 (brs, 1H), 3.76 (s, 3H), 3.75 (s, 3H).

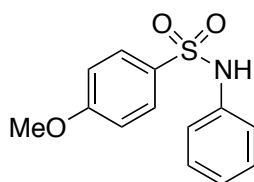
¹³C{¹H} NMR (100 MHz, CDCl₃): δ 159.8, 158.1, 140.1, 130.0, 128.9, 125.7, 119.6, 119.6, 114.5, 111.8, 55.7, 55.5.

IR (KBr pellet): 3279, 3016, 1600, 1513, 1483, 1396, 1323, 1289, 1253, 1156, 1031, 908, 853, 821, 786, 697, 679, 634, 584, 523 cm⁻¹.

Anal. Calcd. for C₁₄H₁₅NO₄S: C, 57.32; H, 5.15; N, 4.77. Found: C, 57.27; H, 5.15; N, 4.85.

Crystallization procedure: **TP-S**.

4-Methoxy-*N*-phenylbenzenesulfonamide (S7A1).^{S2}



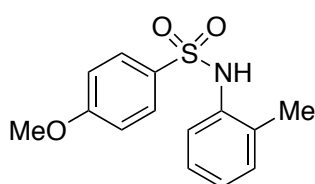
Color, Habit: Colorless, prism crystals. Mp: 108.0–108.5 °C (lit: 105–106 °C)

¹H NMR (400 MHz, CDCl₃): δ 7.70 (t, *J* = 8.9, 2H), 7.22–7.22 (m, 2H), 7.05–7.13 (m, 3H), 6.89 (t, *J* = 9.2, 2H), 6.64 (brs, 1H), 3.82 (s, 3H).

IR (KBr pellet): 3257, 2988, 2946, 1599, 1494, 1338, 1266, 1162, 1092, 1018, 922, 898, 835, 755, 698, 568, 554 cm⁻¹.

Crystallization procedure: **TP-S** and **TP-C** (Solvent A/ Solvent B: toluene/*c*-hexane).

4-Methoxy-*N*-(*o*-tolyl)benzenesulfonamide (S7A2).



Color, Habit: Colorless, prism crystals. Mp: 111–113 °C.

HRMS (FAB) m/z: Calcd for C₁₄H₁₅NNaO₃S 300.0670 [*M*+Na]⁺; Found 300.0670 [*M*+Na]⁺.

¹H NMR (400 MHz, CDCl₃): δ 7.65 (d, *J* = 9.0, 2H), 7.31 (d, *J* = 7.9, 2H), 7.17–7.12 (m, 1H), 7.10–7.05 (m, 2H), 6.88 (d, *J* = 8.9, 2H), 6.28 (brs, 1H), 3.84 (s, 3H), 2.01 (s, 3H).

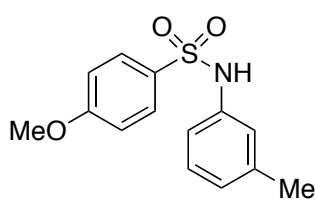
¹³C{¹H} NMR (100 MHz, CDCl₃): δ 163.1, 134.6, 131.2, 131.2, 130.8, 129.3, 127.0, 126.2, 124.3, 114.1, 55.6, 17.6.

IR (KBr pellet): 3264, 1595, 1499, 1396, 1333, 1308, 1263, 1155, 1095, 1030, 908, 832, 802, 761, 698, 569, 541 cm⁻¹.

Anal. Calcd. for C₁₄H₁₅NO₃S: C, 60.63; H, 5.45; N, 5.05. Found: C, 60.25; H, 5.45; N, 4.99.

Crystallization procedure: **TP-S**.

4-Methoxy-*N*-(*m*-tolyl)benzenesulfonamide (S7A3).



Color, Habit: Pale red powder. Mp: 70–72 °C.

MS (FAB⁺): m/z: 278 [*M*+H]⁺, 300 [*M*+Na]⁺.

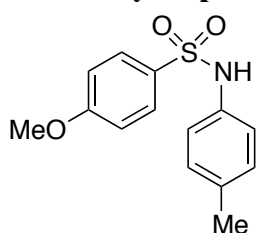
¹H NMR (400 MHz, CDCl₃): δ 7.71 (d, *J* = 8.9, 2H), 7.11 (t, *J* = 7.8, 2H), 6.93–6.87 (m, 2H), 6.84 (d, *J* = 8.0, 2H), 6.52 (brs, 1H), 3.84 (s, 3H), 2.27 (s, 3H).

¹³C{¹H} NMR (100 MHz, CDCl₃): δ 163.1, 139.3, 136.5, 130.7, 129.4, 129.1, 126.1, 122.1, 118.4, 114.1, 55.6, 21.3.

IR (KBr pellet): 3336, 3228, 1594, 1497, 1396, 1303, 1262, 1152, 1095, 1023, 948, 697, 570, 549 cm⁻¹.

Anal. Calcd. for C₁₄H₁₅NO₃S: C, 60.63; H, 5.45; N, 5.05. Found: C, 60.66; H, 5.47; N, 5.04.
Crystallization procedure: **TP-S** (form I) and **TP-C** (Solvent A/ Solvent B: MeOH/*c*-hexane, form II).

4-Methoxy-*N*-(*p*-tolyl)benzenesulfonamide (S7A4).^{S12}



Color, Habit: Colorless, prism crystals. Mp: 99.0–100.0 °C (lit: 94.6–96.6 °C)

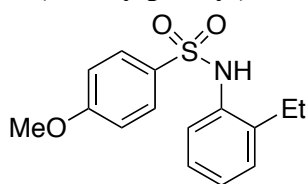
¹H NMR (400 MHz, CDCl₃): δ 7.66 (d, *J* = 8.9, 2H), 7.04 (d, *J* = 8.0, 2H), 6.93 (d, *J* = 8.5, 2H), 6.88 (d, *J* = 9.0, 2H), 6.38 (brs, 1H), 3.83 (s, 3H), 2.28 (s, 3H).

¹³C{¹H} NMR (100 MHz, CDCl₃): δ 163.0, 135.4, 133.8, 130.6, 129.8, 129.4, 122.4, 114.1, 55.6, 20.9.

IR (KBr pellet): 3276, 1602, 1502, 1437, 1391, 1331, 1271, 1220, 1158, 1093, 1020, 906, 832, 802, 767, 685, 567, 532, 500 cm⁻¹.

Crystallization procedure: **TP-S**.

N-(2-Ethylphenyl)-4-methoxybenzenesulfonamide (S7A5).



Color, Habit: Colorless, block crystals. Mp: 106–109 °C.

MS (FAB⁺): *m/z*: 292 [*M*+H]⁺, 314 [*M*+Na]⁺.

¹H NMR (400 MHz, CDCl₃): δ 7.66 (d, *J* = 8.9, 2H), 7.33–7.30 (m, 1H), 7.16–7.11 (m, 3H), 6.88 (d, *J* = 9.2, 2H), 6.25 (brs, 1H), 3.83 (s, 3H), 2.37 (q, *J* = 7.6, 2H), 1.08 (t, *J* = 7.8, 3H).

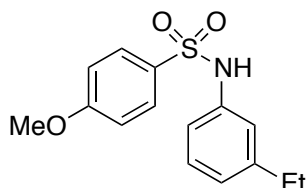
¹³C{¹H} NMR (100 MHz, CDCl₃): δ 163.2, 136.9, 134, 131.2, 129.4, 129.0, 126.9, 126.4, 124.2, 114.2, 55.7, 23.8, 14.2.

IR (KBr pellet): 3281, 3099, 3007, 2970, 2840, 1595, 1492, 1457, 1442, 1401, 1332, 1261, 1153, 1093, 1029, 912, 837, 801, 751, 673, 563 cm⁻¹.

Anal. Calcd. for C₁₅H₁₇NO₃S: C, 61.83; H, 5.88; N, 4.81. Found: C, 61.68; H, 5.81; N, 4.81.

Crystallization procedure: **TP-S** and **TP-C** (Solvent A/ Solvent B: chloroform/toluene).

N-(3-Ethylphenyl)-4-methoxybenzenesulfonamide (S7A6).



Color, Habit: Colorless, block crystals. Mp: 62.0–63.0 °C.

MS (FAB⁺): *m/z*: 292 [*M*+H]⁺, 314 [*M*+Na]⁺.

¹H NMR (400 MHz, CDCl₃): δ 7.71–7.67 (m, 2H), 7.14 (t, *J* = 7.8, 1H), 6.95 (d, *J* = 7.7, 1H), 6.29 (brs, 1H), 6.91–6.84 (m, 4H), 3.83 (s, 3H), 2.57 (q, *J* = 7.6, 2H), 1.16 (t, *J* = 7.7, 3H).

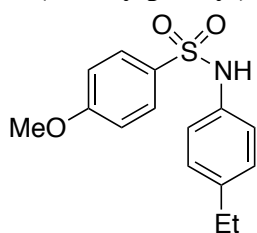
¹³C{¹H} NMR (100 MHz, CDCl₃): δ 163.2, 145.8, 136.6, 130.7, 129.5, 129.2, 125.0, 121.2, 118.9, 114.2, 55.7, 28.7, 15.5.

IR (KBr pellet): 3237, 1594, 1497, 1404, 1334, 1266, 1148, 1093, 1028, 933, 841, 697, 571, 551 cm⁻¹.

Anal. Calcd. for C₁₅H₁₇NO₃S: C, 61.83; H, 5.88; N, 4.81. Found: C, 61.60; H, 5.78; N, 4.80.

Crystallization procedure: **TP-S**.

N-(4-Ethylphenyl)-4-methoxybenzenesulfonamide (S7A7).



Color, Habit: Colorless, prism crystals. Mp: 103.0–104.0 °C.

MS (FAB⁺): *m/z*: 292 [*M*+H]⁺, 314 [*M*+Na]⁺.

¹H NMR (400 MHz, CDCl₃): δ 7.67 (d, *J* = 8.9, 2H), 7.06 (d, *J* = 8.2, 2H), 6.96 (d, *J* = 8.5, 2H), 6.89 (d, *J* = 8.9, 2H), 6.34 (brs, 1H), 3.83 (s, 3H), 2.58 (q, *J* = 7.8, 2H), 1.18 (t, *J* = 7.6, 3H).

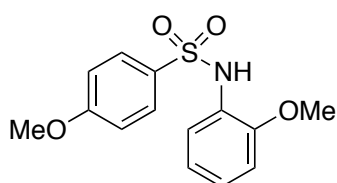
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 163.2, 145.8, 136.6, 130.7, 129.5, 129.2, 125.0, 121.2, 118.9, 114.2, 55.7, 28.7, 15.5.

IR (KBr pellet): 3269, 2970, 2934, 1602, 1577, 1508, 1390, 1328, 1271, 1221, 1179, 1153, 1093, 1021, 908, 833, 581, 547 cm^{-1} .

Anal. Calcd. for $\text{C}_{15}\text{H}_{17}\text{NO}_3\text{S}$: C, 61.83; H, 5.88; N, 4.81. Found: C, 61.74; H, 5.81; N, 4.74.

Crystallization procedure: **TP-S** (form I) and **TP-C** (Solvent A/ Solvent B: MeOH/ethyl acetate, form II).

4-Methoxy-*N*-(2-methoxyphenyl)benzenesulfonamide (S7A8).^{S14}



Color, Habit: Pale purple powder. Mp: 102.5–103.5 °C (lit^{S15}: 85.5–87 °C)

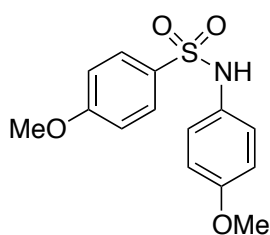
^1H NMR (400 MHz, CDCl_3): δ 7.69 (d, $J = 9.0$, 2H), 7.51 (dd, $J = 7.9$, 1.6, 1H), 7.03 (td, $J = 8.1$, 1.6, 1H), 6.98 (brs, 1H), 6.91–6.84 (m, 3H), 6.73 (dd, $J = 8.1$, 1.1, 2H), 3.81 (s, 3H), 3.66 (s, 3H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ 163.0, 149.4, 130.9, 129.4, 126.1, 125.2, 121.1, 121.0, 113.9, 110.5, 55.6, 55.5.

IR (KBr pellet): 3444, 3238, 1595, 1498, 1338, 1259, 1158, 1115, 1094, 1026, 913, 838, 757, 690, 567 cm^{-1} .

Crystallization procedure: **TP-S** (form I) and **TP-C** (Solvent A/ Solvent B: chloroform/*n*-hexane, form II).

4-Methoxy-*N*-(4-methoxyphenyl)benzenesulfonamide (S7A10).^{S2}



Color, Habit: Colorless, prism crystals. Mp: 104 °C (lit: 99 °C)

^1H NMR (400 MHz, CDCl_3): δ 7.62 (d, $J = 8.9$ Hz, 2H), 6.96 (d, $J = 8.9$ Hz, 2H), 6.88 (d, $J = 9.2$ Hz, 2H), 6.76 (d, $J = 8.9$ Hz, 2H), 6.32 (brs, 1H), 3.84 (s, 3H), 3.76 (s, 3H).

IR (KBr pellet): 3258, 3007, 2846, 1596, 1507, 1389, 1335, 1261, 1238, 1159, 092, 1026, 898, 835, 822, 803, 768 681, 566, 543 cm^{-1} .

Crystallization procedure: **TP-S** (form I and form II).

Crystallographic Data of Sulfonamides

X-ray data were collected on a Rigaku XtaLAB P200 diffractometer with multi-layer mirror monochromated MoK α ($\lambda = 0.71075\text{\AA}$) or CuK α ($\lambda = 1.54187\text{\AA}$) radiation.

Table S1. Crystallographic parameters for structures of the sulfonamides.

(a) S1A1–S1A10

Compound	S1A1 ^{S16}	S1A2 ^{S17}	S1A3-I ^{S18}	S1A3-II	S1A4 ^{S19}	S1A5	S1A6
Formula	C ₁₂ H ₁₃ NO ₂ S	C ₁₃ H ₁₃ NO ₂ S	C ₁₃ H ₁₃ NO ₂ S	C ₁₃ H ₁₃ NO ₂ S	C ₁₃ H ₁₃ NO ₂ S	C ₁₄ H ₁₅ NO ₂ S	C ₁₄ H ₁₅ NO ₂ S
M_r	235.30	247.31	247.31	247.31	247.31	261.34	261.34
Crystal system	tetragonal	orthorhombic	orthorhombic	monoclinic	monoclinic	monoclinic	monoclinic
Space group (= S.G.)	$P4_32_12$	$P2_12_12_1$	$P2_12_12_1$	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P2_1/n$
$a / \text{\AA}$	8.7353(13)	6.4385(2)	8.6328(9)	12.7352(5)	10.7631(8)	7.8407(15)	11.00206(11)
$b / \text{\AA}$	8.7353(13)	8.5072(3)	8.7196(9)	6.0173(2)	9.5973(6)	23.289(3)	8.41173(6)
$c / \text{\AA}$	29.975(7)	21.7857(8)	32.503(4)	16.6467(6)	23.7034(18)	7.2981(13)	14.03426(12)
$\alpha / \text{deg.}$	90	90	90	90	90	90	90
$\beta / \text{deg.}$	90	90	90	110.148(4)	101.147(2)	110.207(5)	101.6482(9)
$\gamma / \text{deg.}$	90	90	90	90	90	90	90
$V / \text{\AA}^3$	2287.3(7)	1193.28(7)	2446.6(5)	1197.60(8)	2402.3(3)	1250.6(4)	1272.071(19)
Z	8	4	8	4	8	4	4
Z'	1	1	2	1	2	1	1
Temperature (= T) / K	293	103	93	102	93	93	293
Goodness-of-fit on F^2 (= S)	1.123	1.036	1.076	1.014	1.049	0.964	1.096
R_1 [$I > 2\sigma(I)$] on F	0.0874	0.0283	0.0314	0.0354	0.0296	0.0416	0.0297
wR_2 (all data) on F^2	0.2059	0.0699	0.0819	0.1077	0.0804	0.1110	0.0833
Reflection collected (all data)	19533	9584	19767	18369	38440	20891	16084
No. of reflections [$I > 2\sigma(I)$]	1897	2544	4727	2274	4827	2227	2209
R_{int}	0.1798	0.0335	0.0392	0.0443	0.0279	0.0881	0.0444
Abs. corr.	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan
Flack parameter	0.04(9)	0.06(3)	0.02(3)	-	-	-	-
Radiation type	MoK α	MoK α	MoK α	MoK α	MoK α	MoK α	CuK α
T_{max}	0.434	0.468	0.805	0.829	0.904	0.734	0.543
T_{min}	0.948	0.974	0.955	0.992	0.977	0.992	0.643
$2\theta_{\text{max}}$	27.341	27.497	27.530	27.495	27.496	27.577	68.107
μ / mm^{-1}	0.267	0.259	0.253	0.258	0.258	0.252	2.207
CCDC No.	1894035	1894011	1894046	1894047	1894023	1894084	1894081

(a) (continued)

Compound	S1A7-I	S1A7-II	S1A8-I	S1A8-II ^{S20}	S1A9	S1A10-I	S1A10-II	S1A10-III ^{S21}
Formula	C ₁₄ H ₁₅ NO ₂ S	C ₁₄ H ₁₅ NO ₂ S	C ₁₃ H ₁₃ NO ₃ S	C ₁₃ H ₁₃ N ₁ O ₃ S ₁	C ₁₃ H ₁₃ NO ₃ S	C ₁₃ H ₁₃ NO ₃ S	C ₁₃ H ₁₃ NO ₃ S	C ₁₃ H ₁₃ NO ₃ S
<i>M_r</i>	261.34	261.34	263.31	263.31	263.31	263.31	263.31	263.30
Crystal system	orthorhombic	monoclinic	monoclinic	monoclinic	monoclinic	orthorhombic	monoclinic	orthorhombic
S.G.	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> 2 ₁ / <i>c</i>	<i>Aba</i> 2	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> 2 ₁ 2 ₁ 2 ₁
<i>a</i> / Å	11.1936(7)	13.2426(3)	10.3968(12)	8.7705(2)	8.4455(7)	22.3076(7)	8.4131(3)	5.3094(5)
<i>b</i> / Å	12.5067(7)	5.21342(13)	8.7575(10)	28.1684(7)	22.1496(14)	15.1093(5)	5.22145(19)	8.5309(10)
<i>c</i> / Å	18.6821(11)	18.0818(5)	14.1708(17)	10.7256(3)	7.4601(6)	7.3966(2)	28.3568(10)	27.925(3)
<i>α</i> / deg.	90	90	90	90	90	90	90	90
<i>β</i> / deg.	90	91.563(2)	99.530(4)	105.968(1)	116.099(11)	90	91.954(3)	90
<i>γ</i> / deg.	90	90	90	90	90	90	90	90
<i>V</i> / Å ³	2615.4(3)	1247.89(5)	1272.4(3)	2547.530	1253.2(2)	2493.04(13)	1244.95(8)	1264.8(2)
<i>Z</i>	8	4	4	8	4	8	4	4
<i>Z'</i>	2	1	1	2	1	1	1	1
<i>T</i>	293	102	93	296	93	293	102	296(2)
<i>S</i>	1.038	1.071	1.064	1.02	1.064	1.125	1.050	1.021
<i>R</i> ₁	0.0303	0.0380	0.0298	0.0466	0.0486	0.0239	0.0314	0.0608
<i>wR</i> ₂	0.0658	0.0971	0.0788	0.113	0.1209	0.0760	0.0835	0.1308
Reflection collected	21440	20117	19969	6318	21394	9770	20089	7272
No. of reflections	5302	2694	2621	4145	2642	2579	2527	1503
<i>R</i> _{int}	0.0317	0.0413	0.0243	0.043	0.0754	0.0202	0.0395	0.0595
Abs. corr.	multi-scan	multi-scan	multi-scan	-	multi-scan	multi-scan	multi-scan	multi-scan
Flack parameter	0.38(2) ^a	-	-	-	-	0.47(2) ^a	-	0.09(16)
Radiation type	MoKα	MoKα	MoKα	MoKα	MoKα	MoKα	MoKα	MoKα
<i>T</i> _{max}	0.920	0.792	0.900	-	0.800	0.637	0.833	0.961
<i>T</i> _{min}	0.988	0.991	0.948	-	0.997	0.938	0.991	0.970
2 <i>θ</i> _{max}	27.520	29.751	27.427	-	29.714	27.479	27.495	26.00
<i>μ</i> / mm ⁻¹	0.241	0.252	0.253	0.25	0.257	0.259	0.259	0.255
CCDC No.	1894085	1894086	1894056	YUPXIR	1894042	1894027	1894028	IJJUT

^aThe final Flack parameter indicated that the structure is inversion-twin.

(b) S2A1–S2A10

Compound	S2A1	S2A2	S2A3	S2A4	S2A5	S2A6	S2A7	S2A8	S2A9	S2A10
Formula	C ₁₃ H ₁₃ N O ₂ S	C ₁₄ H ₁₅ N O ₂ S	C ₁₄ H ₁₅ N O ₂ S	C ₁₄ H ₁₅ N O ₂ S	C ₁₅ H ₁₇ N O ₂ S	C ₁₅ H ₁₇ N O ₂ S	C ₁₅ H ₁₇ N O ₂ S	C ₁₄ H ₁₅ N O ₃ S	C ₁₄ H ₁₅ N O ₃ S	C ₁₄ H ₁₅ N O ₃ S
<i>M_r</i>	247.31	261.34	261.34	261.34	275.36	275.36	275.36	277.34	277.34	277.34
Crystal system	monoclinic	triclinic	monoclinic	monoclinic	monoclinic	monoclinic	triclinic	monoclinic	monoclinic	monoclinic
S.G.	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> -1	<i>P</i> 2 ₁ / <i>c</i>	<i>C</i> 2/ <i>c</i>	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> -1	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁ / <i>c</i>
<i>a</i> / Å	8.8379 (5)	7.8936 (4)	12.624 (3)	14.462 (4)	7.9198 (15)	14.6985 (8)	8.56190 (10)	15.3081 (4)	12.6212 (13)	8.6918 (9)
<i>b</i> / Å	9.1086 (4)	8.0827 (4)	6.4513 (14)	13.827 (3)	15.802 (3)	17.4783 (6)	11.23040 (10)	10.6973 (2)	11.1179 (10)	19.2661 (19)
<i>c</i> / Å	15.1509 (9)	10.3808 (5)	16.276 (4)	14.690 (4)	21.921 (5)	11.0240 (6)	29.1636 (4)	17.5100 (4)	9.5157 (11)	7.9012 (8)
<i>α</i> / deg.	90	77.449 (4)	90	90	90	90	93.8980 (10)	90	90	90
<i>β</i> / deg.	105.161 (6)	85.766 (4)	104.235 (7)	114.857 (8)	95.028 (8)	98.568 (5)	90.5980 (10)	112.245 (3)	100.890 (4)	94.497 (3)
<i>γ</i> / deg.	90	75.782 (4)	90	90	90	90	96.8290 (10)	90	90	90
<i>V</i> / Å ³	1177.21 (11)	626.53 (6)	1284.8 (5)	2665.4 (12)	2732.8 (10)	2800.5 (2)	2777.36 (6)	2653.95 (12)	1311.2 (2)	1319.0 (2)
<i>Z</i>	4	2	4	8	8	8	8	8	4	4
<i>Z'</i>	1	1	1	1	2	2	4	2	1	1
<i>T</i>	93	103	293	93	93	103	93	103	93	93
<i>S</i>	1.062	1.101	1.033	1.044	1.084	1.009	1.026	1.061	1.032	1.055
<i>R</i> ₁	0.0628	0.0562	0.0295	0.0559	0.0299	0.0432	0.0362	0.0312	0.0282	0.0344
<i>wR</i> ₂	0.1786	0.1573	0.0841	0.1544	0.0932	0.0918	0.0886	0.0826	0.0758	0.0939
Reflection collected	18444	19902	19975	42489	41091	44250	96916	41016	20886	21682
No. of reflections	2440	2491	2548	2534	5384	4409	10312	5376	2654	2651
<i>R</i> _{int}	0.1281	0.0732	0.0261	0.1112	0.0353	0.0821	0.0421	0.0369	0.0236	0.0324
Abs. corr.	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan
Flack parameter	-	-	-	-	-	-	-	-	-	-
Radiation type	MoKα	MoKα	MoKα	MoKα	MoKα	MoKα	MoKα	MoKα	MoKα	MoKα
<i>T</i> _{max}	0.514	0.540	0.912	0.565	0.887	0.736	0.712	0.748	0.940	0.891
<i>T</i> _{min}	0.947	0.985	0.985	0.988	0.934	0.998	0.993	0.961	0.988	0.985
2 <i>θ</i> _{max}	27.493	27.499	27.527	27.507	27.487	27.498	27.497	27.499	27.483	27.540
<i>μ</i> / mm ⁻¹	0.263	0.251	0.245	0.236	0.234	0.228	0.230	0.247	0.250	0.248
CCDC No.	1894030	1894029	1894049	1894034	1894031	1894057	1894033	1894012	1894050	1894032

(c) S3A1–S3A10

Compound	S3A1	S3A2	S3A3	S3A4 ^{S22}	S3A5	S3A6	S3A7-I	S3A7-II	S3A8	S3A9	S3A10
Formula	C ₁₃ H ₁₃ NO ₂ S	C ₁₄ H ₁₅ NO ₂ S	C ₁₄ H ₁₅ NO ₂ S	C ₁₄ H ₁₅ NO ₂ S	C ₁₅ H ₁₇ NO ₂ S	C ₁₅ H ₁₇ NO ₂ S	C ₁₅ H ₁₇ NO ₂ S	C ₁₅ H ₁₇ NO ₂ S	C ₁₄ H ₁₅ NO ₃ S	C ₁₄ H ₁₅ NO ₃ S	C ₁₄ H ₁₅ NO ₃ S
<i>M_r</i>	247.31	261.34	261.34	261.34	275.36	275.36	275.36	275.36	277.34	277.34	277.34
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic	orthorhombic	monoclinic	monoclinic	orthorhombic
S.G.	<i>P2₁/c</i>	<i>P2₁/c</i>	<i>P2₁/c</i>	<i>P2₁/c</i>	<i>P2₁/n</i>	<i>P2₁/c</i>	<i>P2₁/n</i>	<i>P2₁2₁2₁</i>	<i>P2₁/n</i>	<i>P2₁/c</i>	<i>P2₁2₁2₁</i>
<i>a</i> / Å	10.4536 (9)	8.1205 (15)	9.4829 (2)	11.0818 (3)	8.1746 (11)	8.393(2))	10.7708 (8)	5.70611 (11)	8.1244 (14)	10.256 (3)	5.3169 (5)
<i>b</i> / Å	12.8332 (11)	20.614 (3)	8.6573 (2)	10.0252 (2)	14.6820 (16)	18.022 (5)	6.6015 (6)	9.3187 (2)	14.8024 (18)	14.160 (3)	8.3453 (8)
<i>c</i> / Å	9.3394 (9)	8.1391 (14)	16.0675 (4)	23.8926 (6)	11.6322 (13)	10.030 (3)	20.120 (3)	26.0563 (5)	11.3357 (18)	10.402 (3)	29.723 (3)
α / deg.	90	90	90	90	90	90	90	90	90	90	90
β / deg.	104.706 (2)	106.054 (5)	97.203 (2)	103.044 (2)	103.399 (3)	108.698 (7)	97.451 (9)	90	103.682 (5)	119.072 (8)	90
γ / deg.	90	90	90	90	90	90	90	90	90	90	90
<i>V</i> / Å ³	1211.87 (19)	1309.3 (4)	1308.67 (5)	2585.91 (11)	1358.1 (3)	1437.1 (7)	1418.5 (3)	1385.51 (5)	1324.6 (4)	1320.3 (6)	1318.8 (2)
<i>Z</i>	4	4	4	8	4	4	4	4	4	4	4
<i>Z'</i>	1	1	1	2	1	1	1	1	1	1	1
<i>T</i>	93	93	103	103	93	93	93	103	93	93	93
<i>S</i>	1.203	0.986	1.059	1.032	1.040	1.022	1.061	1.057	1.080	1.088	1.012
<i>R</i> ₁	0.0332	0.0577	0.0351	0.0376	0.0280	0.0340	0.0845	0.0257	0.0277	0.0309	0.0241
<i>wR</i> ₂	0.1047	0.1534	0.0963	0.1001	0.0789	0.0888	0.2026	0.0699	0.0775	0.0899	0.0630
Reflection collected	19705	22032	21247	39298	21584	22892	21794	23074	21190	21221	10788
No. of reflections	2513	2392	2684	4999	2774	2618	2065	3470	2755	2624	2849
<i>R</i> _{int}	0.0323	0.0818	0.0435	0.0477	0.0203	0.0463	0.0949	0.0315	0.0210	0.0457	0.0174
Abs. corr.	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan
Flack parameter	-	-	-	-	-	-	-	-0.007 (16)	-	-	0.012 (18)
Radiation type	MoK α	MoK α	MoK α	MoK α	MoK α	MoK α	MoK α	MoK α	MoK α	MoK α	MoK α
<i>T</i> _{max}	0.873	0.520	0.820	0.866	0.935	0.921	0.401	0.764	0.890	0.805	0.910
<i>T</i> _{min}	0.960	0.976	0.986	0.988	0.981	0.987	0.991	0.964	0.942	0.933	0.993
2 θ _{max}	27.490	27.538	27.496	27.500	27.463	27.530	27.500	29.694	27.477	27.502	27.517
μ / mm ⁻¹	0.255	0.240	0.240	0.243	0.235	0.222	0.225	0.231	0.247	0.248	0.248
CCDC No.	189403 7	189408 9	189401 3	189401 4	189407 4	189405 8	189401 9	189401 5	189405 9	189406 0	189406 1

(d) S4A1–S4A10

Compound	S4A1-I ^{S23}	S4A1-II ^{S24}	S4A2 ^{S25}	S4A3 ^{S26}	S4A4-I ^{S27}	S4A4-II	S4A5	S4A6	S4A7	S4A8 ^{S28}	S4A9	S4A10 ^{S29}
Formula	C ₁₃ H ₁₃ NO ₂ S	C ₁₃ H ₁₃ N ₁ O ₂ S ₁	C ₁₄ H ₁₅ NO ₂ S	C ₁₄ H ₁₅ NO ₂ S	C ₁₄ H ₁₅ NO ₂ S	C ₁₄ H ₁₅ NO ₂ S	C ₁₅ H ₁₇ NO ₂ S	C ₁₅ H ₁₇ NO ₂ S	C ₁₅ H ₁₇ NO ₂ S	C ₁₄ H ₁₅ NO ₃ S	C ₁₄ H ₁₅ NO ₃ S	C ₁₄ H ₁₅ NO ₃ S
M_r	247.31	247.31	261.34	261.34	261.34	261.34	275.36	275.36	275.36	277.34	277.34	277.34
Crystal system	triclinic	monoclinic	orthorhombic	monoclinic	triclinic	monoclinic	orthorhombic	monoclinic	monoclinic	orthorhombic	monoclinic	monoclinic
S.G.	<i>P</i> -1	<i>P</i> 2 ₁ / <i>c</i>	<i>Pbca</i>	<i>C</i> 2/ <i>c</i>	<i>P</i> -1	<i>P</i> 2 ₁ / <i>n</i>	<i>Pbca</i>	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁ / <i>n</i>	<i>Pbca</i>	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁
$a / \text{Å}$	10.196 6(2)	8.770(2)	14.900 6(15)	13.715 8(3)	8.5707 9(14)	5.3029 (5)	13.005 5(2)	8.6240 (11)	9.2520 (13)	12.587 3(15)	8.2872 (3)	8.9928 (2)
$b / \text{Å}$	10.935 1(2)	9.768(2)	14.651 1(16)	14.780 2(3)	8.6521 8(15)	16.106 1(12)	11.440 88(17)	13.769 2(14)	8.1230 (10)	11.443 1(13)	13.876 8(6)	5.2181 8(13)
$c / \text{Å}$	13.241 9(2)	16.234 (5)	12.130 2(13)	13.044 3(3)	9.1751 7(15)	15.824 7(11)	18.323 4(3)	12.063 5(15)	19.313 (3)	18.369 (2)	11.904 2(5)	15.003 6(4)
$\alpha / \text{deg.}$	68.053 7(17)	90	90	90	87.103 2(13)	90	90	90	90	90	90	90
$\beta / \text{deg.}$	86.782 7(15)	113.20 0 (2)	90	95.449 2(19)	78.048 8(14)	98.058 (8)	90	104.33 0(4)	99.501 (5)	90	98.376 (4)	102.75 4(3)
$\gamma / \text{deg.}$	66.889 2(18)	90	90	90	74.130 5(15)	90	90	90	90	90	90	90
$V / \text{Å}^3$	1252.4 7(5)	1278.2 34	2648.1 (5)	2632.4 2(10)	640.26 3(19)	1338.2 3(19)	2726.4 2(7)	1387.9 (3)	1431.5 (3)	2645.8 (5)	1354.3 8(10)	686.69 (3)
Z	4	4	8	8	2	4	8	4	4	8	4	2
Z'	2	1	1	1	1	1	1	1	1	1	1	1
T	103	283- 303	93	103	103	103	93	93	93	93	93	100
S	1.049	1.1	1.047	1.074	1.030	1.045	1.058	1.023	1.101	1.024	1.027	1.062
R_1	0.0435	0.0706	0.0294	0.0326	0.0304	0.0752	0.0325	0.0309	0.0302	0.0335	0.0354	0.0315
wR_2	0.1144	0.217	0.0831	0.0876	0.0865	0.1897	0.0863	0.0819	0.0827	0.0854	0.0952	0.0772
Reflection collected	40543	2278	39911	20652	20864	10895	41755	22171	22343	20119	21130	11400
No. of reflections	4596	2041	2709	2763	2747	1511	3295	2745	2994	2390	2625	2958
R_{int}	0.0415	0.096	0.0219	0.0337	0.0301	0.1259	0.0320	0.0282	0.0209	0.0450	0.0403	0.0409
Abs. corr.	multi-scan	ψ -scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan
Flack parameter	-	-	-	-	-	-	-	-	-	-	-	-0.03 (3)
Radiation type	MoK α	CuK α	MoK α	MoK α	MoK α	MoK α	MoK α	MoK α	MoK α	MoK α	MoK α	MoK α
T_{max}	0.720	0.42	0.848	0.679	0.844	0.257	0.758	0.919	0.861	0.829	0.644	0.432
T_{min}	0.985	0.336	0.949	0.959	0.955	0.998	0.913	0.989	0.929	0.952	0.993	0.953
$2\theta_{\text{max}}$	27.500		27.479	27.495	27.499	27.491	29.635	27.501	27.535	27.515	27.493	27.499
μ / mm^{-1}	0.247	2.17	0.238	0.239	0.246	0.235	0.234	0.230	0.223	0.248	0.242	0.238
CCDC No.	18940 91	FAXB UB01	18940 90	18940 55	18940 25	18940 26	18940 83	18940 62	18940 63	18940 64	18940 45	18940 16

(e) S5A1–S5A10

Compound	S5A1-I	S5A1-II	S5A2	S5A3	S5A4	S5A5	S5A6	S5A7	S5A8-I	S5A8-II	S5A9	S5A10
Formula	C ₁₃ H ₁₃ N O ₃ S	C ₁₃ H ₁₃ N O ₃ S	C ₁₄ H ₁₅ N O ₃ S	C ₁₄ H ₁₅ N O ₃ S	C ₁₄ H ₁₅ N O ₃ S	C ₁₅ H ₁₇ N O ₃ S	C ₁₅ H ₁₇ N O ₃ S	C ₁₅ H ₁₇ N O ₃ S	C ₁₄ H ₁₅ N O ₄ S	C ₁₄ H ₁₅ N O ₄ S	C ₁₄ H ₁₅ N O ₄ S	C ₁₄ H ₁₅ N O ₄ S
M_r	263.31	263.31	277.34	277.34	277.34	291.36	291.36	291.36	293.34	293.34	293.34	293.34
Crystal system	triclinic	monoclinic	triclinic	monoclinic	monoclinic	triclinic	triclinic	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic
S.G.	<i>P</i> -1	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> -1	<i>P</i> 2 ₁ / <i>n</i>	<i>I</i> ₂ / <i>a</i>	<i>P</i> -1	<i>P</i> -1	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁ / <i>n</i>	<i>C</i> 2/ <i>c</i>
$a / \text{Å}$	8.774 (2)	8.96158 (15)	8.57970 (10)	8.8443 (2)	26.2413 (8)	7.750 (2)	8.3129 (18)	11.8793 (13)	13.4431 (5)	13.8784 (4)	10.4234 (18)	19.924 (3)
$b / \text{Å}$	11.661 (3)	17.2901 (2)	11.6725 (2)	13.5478 (3)	10.3800 (3)	8.813 (19)	8.6039 (19)	13.7310 (14)	22.7591 (10)	23.7917 (6)	9.0202 (14)	12.0627 (17)
$c / \text{Å}$	13.504 (4)	8.97366 (18)	14.7785 (2)	23.2774 (9)	20.6867 (6)	11.286 (3)	11.599 (2)	9.2476 (11)	18.4941 (7)	8.4589 (2)	15.535 (3)	12.0327 (18)
$\alpha / \text{deg.}$	105.359 (8)	90	109.673 2(14)	90	90	93.512 (7)	93.828 (4)	90	90	90	90	90
$\beta / \text{deg.}$	92.258 (5)	110.442 (2)	90.1789 (12)	98.341 (3)	104.481 (3)	109.311 (7)	103.019 (3)	108.241 (3)	101.033 (4)	101.748 (3)	102.037 (6)	97.408 (4)
$\gamma / \text{deg.}$	103.338 (6)	90	104.146 6(13)	90	90	102.630 (5)	117.096 (4)	90	90	90	90	90
$V / \text{Å}^3$	1288.9 (6)	1302.88 (4)	1345.44 (4)	2759.61 (14)	5455.7 (3)	702.4 (3)	705.7 (3)	1432.6 (3)	5553.7 (4)	2734.54 (13)	1428.5 (4)	2867.8 (7)
Z	4	4	4	8	16	2	2	4	16	8	4	8
Z'	2	1	2	2	1	1	1	1	2	4	1	1
T	93	293	93	93	93	93	93	93	93	93	93	93
S	1.167	1.059	1.017	1.076	1.043	1.087	1.074	1.033	1.034	1.053	1.062	1.073
R_1	0.0334	0.0331	0.0370	0.0564	0.0331	0.0283	0.0275	0.0364	0.0456	0.0310	0.0686	0.0298
wR_2	0.1056	0.0921	0.0980	0.1480	0.0890	0.0861	0.0737	0.0985	0.1075	0.0842	0.1934	0.0800
Reflection collected	43151	30842	43059	86625	43520	23141	22974	23030	87938	44627	22703	22635
No. of reflections	5189	2217	5511	4553	6217	2879	3001	2537	9157	5634	2680	2941
R_{int}	0.0437	0.0234	0.0594	0.0784	0.0374	0.0292	0.0190	0.0598	0.0918	0.0324	0.0632	0.0281
Abs. corr.	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan
Flack parameter	-	-	-	-	-	-	-	-	-	-	-	-
Radiation type	MoK α	CuK α	MoK α	MoK α	MoK α	MoK α	MoK α	MoK α	MoK α	MoK α	MoK α	MoK α
T_{max}	0.828	0.149	0.741	0.797	0.884	0.859	0.888	0.861	0.785	0.670	0.732	0.828
T_{min}	0.956	0.641	0.973	0.995	0.985	0.967	0.958	0.986	0.957	0.937	0.991	0.931
$2\theta_{\text{max}}$	27.477	68.246	27.497	27.500	39.220	27.410	27.402	27.463	27.499	27.497	27.517	27.481
μ / mm^{-1}	0.250	2.221	0.243	0.237	0.060	0.237	0.236	0.232	0.245	0.249	0.238	0.237
CCDC No.	189406 5	189403 6	189408 2	189404 0	189406 6	189406 7	189406 8	189406 9	189407 0	189407 1	189403 9	189407 2

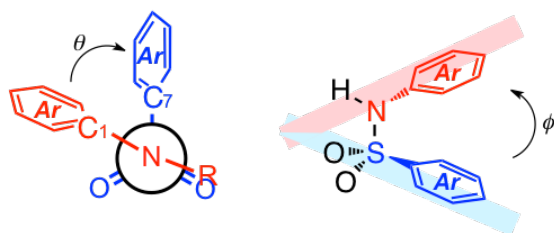
(f) S6A1–S6A10

Compound	S6A1	S6A2	S6A3	S6A4	S6A5	S6A6	S6A7	S6A8-I	S6A8-II	S6A9-I	S6A9-II	S6A10
Formula	C ₁₃ H ₁₃ N O ₃ S	C ₁₄ H ₁₅ N O ₃ S	C ₁₄ H ₁₅ N O ₃ S	C ₁₄ H ₁₅ N O ₃ S	C ₁₅ H ₁₇ N O ₃ S	C ₁₅ H ₁₇ N O ₃ S	C ₁₅ H ₁₇ N O ₃ S	C ₁₄ H ₁₅ N O ₄ S	C ₁₄ H ₁₅ N O ₄ S	C ₁₄ H ₁₅ N O ₄ S	C ₁₄ H ₁₅ N O ₄ S	C ₁₄ H ₁₅ N O ₄ S
<i>M_r</i>	263.31	277.34	277.34	277.34	291.36	291.36	291.36	293.34	293.34	293.34	293.34	293.34
Crystal system	monoclinic	orthorhombic	monoclinic	monoclinic	monoclinic	monoclinic	triclinic	monoclinic	triclinic	monoclinic	monoclinic	orthorhombic
S.G.	<i>P2₁/n</i>	<i>Pbca</i>	<i>P2₁/c</i>	<i>P2₁/n</i>	<i>P2₁/n</i>	<i>P-1</i>	<i>P2₁/c</i>	<i>P-1</i>	<i>P2₁/c</i>	<i>P2₁/c</i>	<i>P2₁/c</i>	<i>P2₁2₁2₁</i>
<i>a</i> / Å	9.5468 (9)	14.532 (2)	10.5927 (16)	9.529 7(4)	10.2318 (2)	8.0566 (8)	11.8008 (11)	8.5516 (14)	8.7580 (2)	12.8863 (9)	8.57126 (16)	5.3301 (5)
<i>b</i> / Å	7.0557 (6)	14.227 (2)	13.1257 (19)	6.8423 (3)	12.7612 (3)	8.5669 (10)	14.9057 (12)	9.3740 (16)	9.6939 (2)	11.0722 (9)	16.1509 (3)	8.4345 (9)
<i>c</i> / Å	18.1976 (18)	12.680 (2)	9.6636 (14)	20.9182 (11)	10.9784 (2)	11.4372 (9)	8.4100 (7)	10.3578 (17)	15.9532 (4)	10.1103 0(11)	10.0059 (2)	29.603 (3)
<i>α</i> / deg.	90	90	90	90	90	90	78.172 (11)	90	103.192 (2)	90	90	90
<i>β</i> / deg.	93.507 (4)	90	98.563 (5)	94.929 (5)	91.970 (2)	70.150 (9)	103.485 (3)	105.948 (2)	93.769 (2)	107.903 (3)	90.9787 (17)	90
<i>γ</i> / deg.	90	90	90	90	90	90	85.073 (12)	90	114.090 (2)	90	90	90
<i>V</i> / Å ³	1223.5 (2)	2621.5 (7)	1328.6 (3)	1358.93 (11)	1432.60 (5)	726.62 (13)	1438.5 (2)	671.80 (19)	1351.48 (5)	1372.68 (15)	1384.95 (5)	1330.9 (2)
<i>Z</i>	4	8	4	4	4	2	4	2	4	4	4	4
<i>Z'</i>	1	1	1	1	1	1	1	1	1	1	1	1
<i>T</i>	93	93	93	103	103	93	93	93	102	93	103	93
<i>S</i>	1.061	1.036	1.126	1.049	1.077	1.066	1.135	1.085	1.050	1.115	1.066	1.114
<i>R</i> ₁	0.0282	0.0320	0.0292	0.0503	0.0325	0.0277	0.0296	0.0263	0.0315	0.0282	0.0311	0.0240
<i>wR</i> ₂	0.0792	0.0849	0.0913	0.1413	0.0886	0.0773	0.1020	0.0750	0.0809	0.0824	0.0831	0.0685
Reflection collected	19020	19799	21213	21282	23306	23882	23091	22390	21087	21773	22486	10592
No. of reflections	2542	2599	2748	2592	3356	3018	2890	2776	2719	2859	2887	2868
<i>R</i> _{int}	0.0210	0.0326	0.0231	0.0694	0.0392	0.0223	0.0251	0.0237	0.0429	0.0230	0.0398	0.0210
Abs. corr.	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan
Flack parameter	-	-	-	-	-	-	-	-	-	-	-	-
Radiation type	MoKα	MoKα	MoKα	MoKα	MoKα	MoKα	MoKα	MoKα	MoKα	MoKα	MoKα	MoKα
<i>T</i> _{max}	0.888	0.871	0.886	0.281	0.735	0.900	0.878	0.920	0.789	0.891	0.864	0.905
<i>T</i> _{min}	0.946	0.963	0.952	0.974	0.950	0.984	0.966	0.968	0.988	0.940	0.983	0.972
2θ _{max}	27.460	27.526	27.485	27.493	29.723	27.471	27.440	27.468	27.488	27.488	27.499	27.496
μ / mm ⁻¹	0.264	0.250	0.247	0.241	0.232	0.229	0.231	0.253	0.252	0.248	0.246	0.256
CCDC No.	1894073	1894020	1894048	1894017	1894104	1894075	1894076	1894021	1894022	1894043	1894044	1894038

(g) S7A1–S7A10

Compound	S7 A1 ^{S16}	S7A2	S7A3-I	S7A3- II	S7 A4 ^{S30}	S7A5	S7A6	S7A7-I	S7A7- II	S7A8-I	S7A8- II	S7A10- I ^{S31}	S7A10- II
Formula	C ₁₃ H ₁₃ NO ₃ S	C ₁₄ H ₁₅ NO ₃ S	C ₁₄ H ₁₅ NO ₃ S	C ₁₄ H ₁₅ NO ₃ S	C ₁₄ H ₁₅ NO ₃ S	C ₁₅ H ₁₇ NO ₃ S	C ₁₅ H ₁₇ NO ₃ S	C ₁₅ H ₁₇ NO ₃ S	C ₁₅ H ₁₇ NO ₃ S	C ₁₄ H ₁₅ NO ₄ S	C ₁₄ H ₁₆ NO _{4.5} S	C ₁₄ H ₁₅ NO ₄ S	C ₁₄ H ₁₅ NO ₄ S
<i>M_r</i>	263.31	277.34	277.34	277.34	277.34	291.36	291.36	291.36	291.36	293.34	302.34	293.34	293.34
Crystal system	orthorh ombic	triclinic	monocl inic	triclinic	monocl inic	monocl inic	orthorh ombic	monocl inic	monocl inic	monocl inic	monocl inic	monocl inic	monocl inic
S.G.	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> -1	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> -1	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> bca	<i>P</i> 2 ₁	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> 2 ₁ / <i>c</i>	<i>C</i> 2/ <i>c</i>	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁ / <i>n</i>
<i>a</i> / Å	5.1875 9(15)	7.9387 (13)	11.976 9(8)	7.5752 (3)	14.538 (4)	16.868 2(4)	11.454 6(7)	8.9158 (14)	18.502 3(4)	17.156 3(5)	17.544 0(5)	14.667 4(4)	10.136 2(2)
<i>b</i> / Å	14.512 7(4)	8.1134 (13)	10.114 2(7)	12.291 4(4)	5.2457 (11)	15.276 3(4)	15.323 2(10)	4.9848 (9)	10.110 3(2)	15.439 1(4)	9.2494 2)	5.2309 0(13)	13.511 1(2)
<i>c</i> / Å	16.527 5(5)	10.632 9(16)	22.722 2(16)	14.939 7(5)	17.571 (4)	11.028 9(3)	16.578 3(11)	15.924 (3)	23.540 5(5)	10.575 1(3)	17.394 8(5)	18.208 7(5)	10.371 3(2)
<i>α</i> / deg.	90	94.010 (3)	90	85.867 (3)	90	90	90	90	90	90	90	90	90
<i>β</i> / deg.	90	95.832 (5)	99.029 (3)	80.753 (3)	95.077 (6)	90.494 (2)	90	92.870 (5)	98.040 6(19)	91.563 (2)	100.25 0(3)	98.799 3)	108.83 8(2)
<i>γ</i> / deg.	90	105.95 5(5)	90	78.007 (3)	90	90	90	90	90	90	90	90	90
<i>V</i> / Å ³	1244.2 9(6)	651.64 (18)	2718.4 (3)	1341.9 1(8)	1334.7 (6)	2841.8 6(13)	2909.8 (3)	706.8 (2)	4360.2 8(16)	2800.0 7(14)	2777.6 3(13)	1380.6 0(6)	1344.2 8(5)
<i>Z</i>	4	2	8	4	4	8	8	2	12	8	8	4	4
<i>Z'</i>	1	1	2	2	1	2	1	1	3	2	1	1	1
<i>T</i>	93	93	93	103	93	93	93	93	102	93	103	93	93
<i>S</i>	1.050	1.247	1.054	1.018	1.016	1.177	1.060	1.001	1.028	1.149	1.035	1.078	1.045
<i>R</i> ₁	0.0288	0.0307	0.0327	0.0649	0.0557	0.0665	0.0293	0.0404	0.0372	0.0540	0.0309	0.0378	0.0303
<i>wR</i> ₂	0.0671	0.1111	0.0908	0.1749	0.1425	0.1986	0.0808	0.1018	0.0902	0.1335	0.0816	0.1099	0.0848
Reflection collected	20007	21532	42481	43701	20446	47725	22166	11728	67739	43316	21270	20675	21562
No. of reflections	2559	2773	5534	3653	2351	5930	2904	2858	7744	5446	2912	2861	3294
<i>R</i> _{int}	0.0497	0.0239	0.0205	0.0995	0.1197	0.0716	0.0267	0.0704	0.0529	0.0656	0.0440	0.0604	0.0226
Abs. corr.	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan
Flack parameter	0.07(3)	-	-	-	-	-	-	-	-	-	-	-	-
Radiation type	MoKα	MoKα	MoKα	MoKα	MoKα	MoKα	MoKα	MoKα	MoKα	MoKα	MoKα	MoKα	MoKα
<i>T</i> _{max}	0.687	0.774	0.938	0.826	0.513	0.709	0.906	0.747	0.883	0.227	0.721	0.709	0.853
<i>T</i> _{min}	0.992	0.965	0.988	0.998	0.993	0.969	0.966	0.995	0.993	0.959	0.964	0.990	0.911
2θ _{max}	27.497	27.426	27.472	27.499	27.522	27.487	27.531	27.416	27.499	27.498	27.499	27.495	29.815
μ/mm ⁻¹	0.259	0.251	0.241	0.244	0.245	0.234	0.229	0.235	0.229	0.243	0.250	0.247	0.253
CCDC No.	189404 1	189407 7	189405 1	189405 2	189402 4	189401 8	189407 8	189408 7	189408 8	189405 3	189405 4	189407 9	189408 0

Table S2. The absolute values of the torsion angles of the sulfonamide bond (θ) and dihedral angles of the two benzene rings (ϕ), and the angles around N atoms.



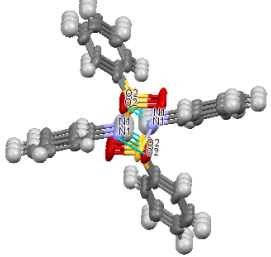
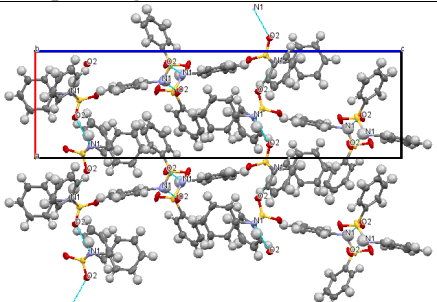
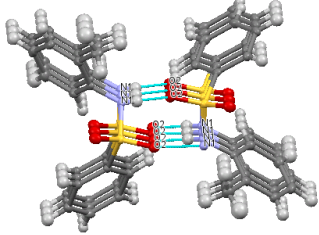
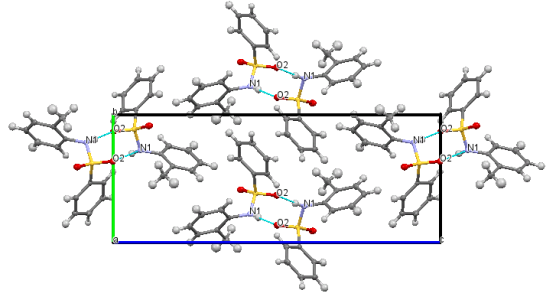
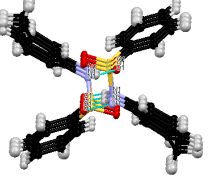
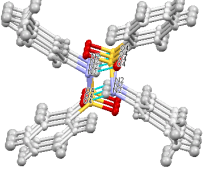
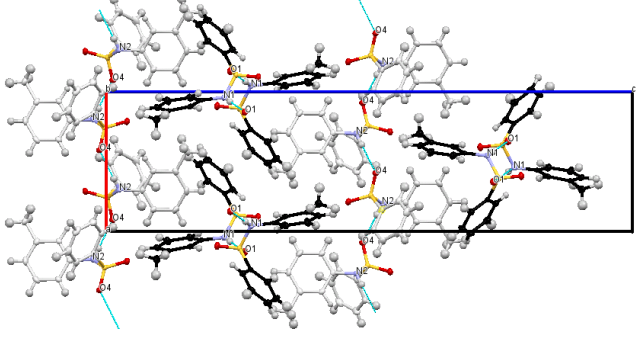
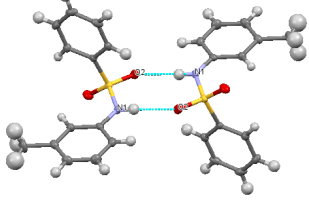
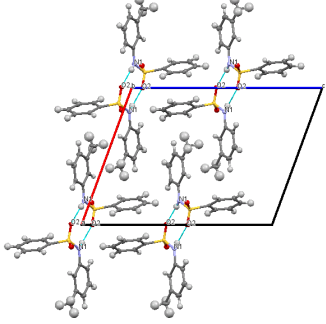
Compound	No. of asymmetric molecule	[degree]		The angles around N [degree]				
		θ	ϕ	(a) \angle SNC	(b) \angle SNH	(c) \angle CNH	Sum of the angles	
S1A1	1	-	57.42	63.84	120.3	103.0	108.0	331.3
S1A2	1	+	72.33	60.85	119.1	111.9	115.0	346.1
S1A3-I	1	+	57.23	66.75	121.8	109.0	115.8	346.5
S1A3-I	1	-	55.13	67.52	121.4	108.6	114.9	344.8
S1A3-II	1	+	63.33	88.75	127.5	112.2	118.2	357.9
S1A4	1	-	58.51	76.52	123.2	109.1	113.7	345.9
S1A4	1	+	55.51	74.82	121.2	110.4	116.1	347.6
S1A5	1	-	72.98	43.82	121.3	107.1	115.0	343.3
S1A6	1	+	66.59	87.32	127.1	110.8	114.8	352.6
S1A7-I	1	+	57.15	71.56	120.4	106.9	115.3	342.6
S1A7-I	2	-	54.74	68.61	119.8	110.7	114.0	344.5
S1A7-II	1	-	65.50	46.40	118.7	109.2	114.0	341.9
S1A8-I	1	-	61.51	43.15	117.0	106.4	114.6	338.0
S1A8-II ^{S20}	1	+	67.26	88.15	-	-	-	-
S1A8-II ^{S20}	2	-	81.18	44.50	-	-	-	-
S1A9	1	+	62.19	71.60	122.9	107.6	117.1	347.6
S1A10-I	1	-	61.08	71.62	122.5	111.7	115.7	349.9
S1A10-II	1	-	66.60	58.37	120.4	111.5	113.8	345.7
S1A10-III ^{S21}	1 (disordered)	+	70.32	54.51	-	-	-	-
S1A10-III ^{S21}	1 (disordered)	+	70.32	62.87	-	-	-	-
S2A1	1	-	51.04	76.01	125.5	112.6	119.1	357.2
S2A2	1	-	76.29	48.11	121.8	110.0	117.8	349.6
S2A3	1	-	62.19	89.26	127.4	115.0	115.8	358.2
S2A4	1	+	47.05	73.36	123.7	114.4	114.9	353.0
S2A5	1	-	75.58	72.86	127.1	111.7	118.2	356.9
S2A5	2	+	78.21	72.84	127.0	112.7	118.8	358.6
S2A6	1	+	53.64	80.06	126.1	113.0	116.0	355.0
S2A6	2	+	54.42	83.10	125.3	111.3	116.5	353.1
S2A7	1	-	48.22	65.63	120.9	111.3	115.2	347.4
S2A7	2	-	54.72	84.69	125.7	112.0	117.5	355.1
S2A7	3	-	58.58	87.03	127.4	110.2	118.4	356.0
S2A7	4	-	62.09	85.00	127.2	114.0	116.2	357.4
S2A8	1	-	56.87	71.49	122.6	110.9	116.7	350.3

Compound	No. of asymmetric molecule	[degree]		The angles around N [degree]			Sum of the angles	
		θ	φ	(a) \angle SNC	(b) \angle SNH	(c) \angle CNH		
S2A8	2	-	58.65	83.30	124.7	112.6	117.1	354.4
S2A9	1	+	78.24	72.36	128.0	114.7	117.2	359.9
S2A10	1	-	54.29	64.97	119.6	112.8	117.8	350.1
S3A1	1	-	54.96	68.26	122.9	108.0	114.4	345.3
S3A2	1	-	63.30	46.75	119.7	110.4	112.8	342.8
S3A3	1	-	62.55	76.09	124.6	111.3	113.1	349.0
S3A4	1	+	64.48	81.64	125.3	109.4	114.2	348.9
S3A4	2	-	54.35	69.51	122.2	110.8	115.1	348.1
S3A5	1	-	66.05	51.65	120.3	109.2	118.1	347.6
S3A6	1	-	60.49	46.42	119.6	110.0	114.7	344.3
S3A7-I	1 (disordered, major)	+	63.15	61.18	122.1	105.9	114.6	342.5
S3A7-I	1 (disordered, minor)	+	65.10	79.76	-	-	-	-
S3A7-II	1	+	63.10	89.47	125.4	112.9	116.1	354.5
S3A8	1	-	66.92	56.24	119.5	109.3	114.4	343.2
S3A9	1	+	63.91	74.40	125.2	109.0	115.4	349.6
S3A10	1	+	71.30	56.29	122.7	109.4	115.5	347.6
S4A1-I	1	+	50.67	65.60	122.4	109.4	113.7	345.5
S4A1-I	2	+	61.30	81.63	125.9	94.1	130.0	350.1
S4A1-II ^{S24}	1	-	51.60	68.40	-	-	-	-
S4A2	1	+	61.43	44.22	118.8	108.6	116.6	343.9
S4A3	1	+	59.35	87.15	126.5	113.6	119.1	359.2
S4A4-I	1	-	61.06	69.04	123.2	109.5	115.0	347.7
S4A4-II	1	+	63.87	60.69	120.4	110.9	113.2	344.5
S4A5	1	-	56.46	70.06	123.4	111.3	120.2	355.0
S4A6	1	+	63.04	72.96	124.9	110.5	114.4	349.8
S4A7	1	+	60.72	69.83	121.6	109.2	115.3	346.1
S4A8	1	-	56.65	70.84	122.8	109.2	120.9	352.8
S4A9	1	+	60.30	65.30	122.8	108.6	113.2	344.6
S4A10	1	-	71.18	63.05	121.8	113.6	110.5	346.0
S5A1-I	1	-	48.72	65.67	119.9	112.2	111.7	343.8
S5A1-I	2	+	61.02	78.91	121.1	111.5	115.5	348.1
S5A1-II	1	+	70.94	83.58	128.4	113.6	116.7	358.7
S5A2	1 (disordered)	+	71.12	70.97	122.2	113.9	117.7	353.8
S5A2	1 (disordered)	+	57.17	69.69	125.3	113.9	108.5	347.7
S5A2	2	+	70.01	71.08	122.0	110.9	120.6	353.5
S5A3	1	+	56.08	79.93	122.3	110.8	114.4	347.5
S5A3	2	-	58.19	79.76	122.4	112.7	114.0	349.1
S5A4	1	+	51.80	77.22	124.3	113.6	114.2	352.1
S5A4	2	-	54.45	80.78	123.6	112.0	115.5	351.1
S5A5	1	-	66.62	76.73	123.9	110.5	118.2	352.5
S5A6	1	+	46.50	72.45	123.0	110.4	111.9	345.2

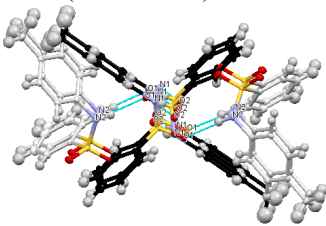
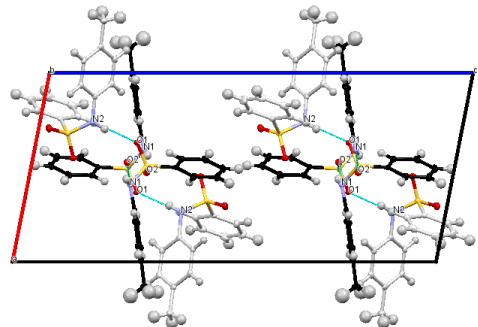
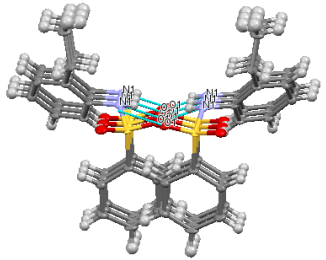
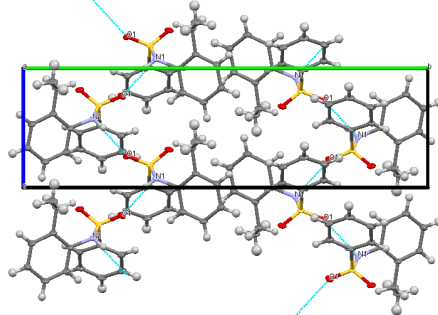
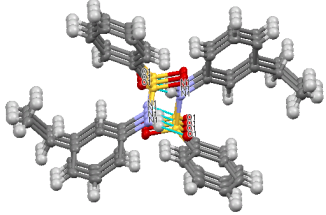
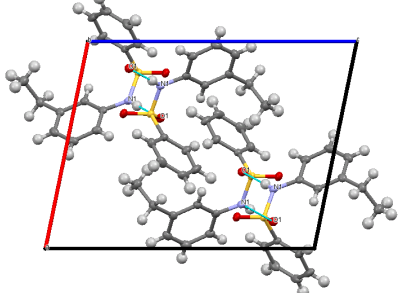
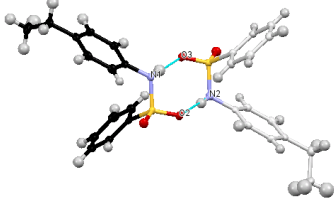
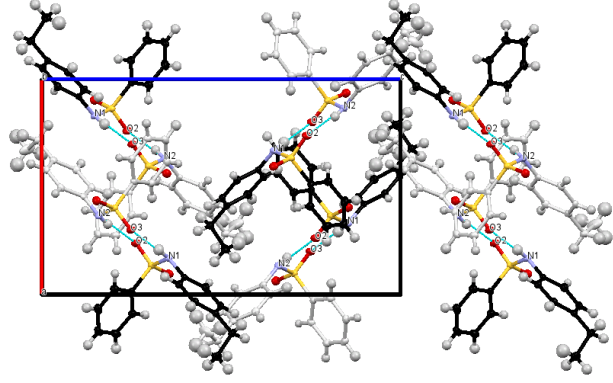
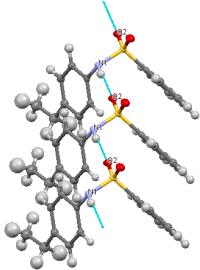
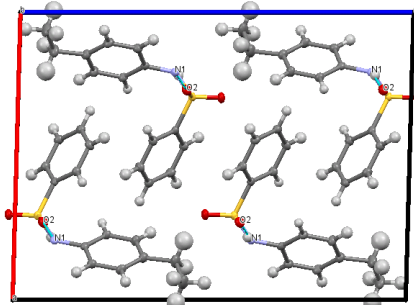
Compound	No. of asymmetric molecule	[degree]		The angles around N [degree]			Sum of the angles	
		θ	φ	(a) \angle SNC	(b) \angle SNH	(c) \angle CNH		
S5A7	1	+	53.34	78.48	124.6	112.0	114.2	350.8
S5A8-I	1	+	66.78	75.92	122.7	107.1	112.5	342.3
S5A8-I	2	-	59.96	74.79	122.3	109.2	113.2	344.7
S5A8-I	3	-	57.40	68.39	120.5	108.7	113.7	343.0
S5A8-I	4	-	61.84	77.07	123.9	105.3	114.7	343.9
S5A8-II	1	+	60.83	72.00	121.1	108.8	110.7	340.6
S5A8-II	2	+	64.92	70.60	120.7	108.6	111.1	340.4
S5A9	1	-	50.24	68.03	120.4	109.7	115.1	345.1
S5A10	1	-	51.81	64.65	118.9	111.3	115.6	345.8
S6A1	1	+	59.64	55.38	119.6	110.8	113.2	343.7
S6A2	1	+	67.45	43.92	120.1	109.3	118.3	347.7
S6A3	1	+	59.45	74.75	124.4	109.3	114.2	347.9
S6A4	1	+	57.41	48.29	118.7	109.6	113.2	341.5
S6A5	1	-	66.05	51.65	120.3	109.2	118.1	347.6
S6A6	1	-	55.47	78.34	122.8	108.1	113.8	344.7
S6A7	1	+	56.82	75.96	122.8	108.7	115.1	346.6
S6A8-I	1	-	67.06	74.43	122.1	110.0	114.7	346.7
S6A8-II	1	+	72.85	75.10	126.9	113.5	115.4	355.8
S6A9-I	1	+	66.96	85.98	127.3	114.7	114.7	356.7
S6A9-II	1	+	59.36	55.79	121.6	108.1	115.9	345.6
S6A10	1	+	67.32	56.21	121.9	111.1	113.2	346.2
S7A1	1	+	71.88	57.19	122.3	109.2	115.2	346.8
S7A2	1	+	74.10	42.70	120.2	112.0	115.4	347.6
S7A3-I	1	-	53.18	79.54	124.5	109.4	114.5	348.3
S7A3-I	2	+	51.20	73.59	122.6	108.7	116.5	347.9
S7A3-II	1	-	69.81	68.28	125.3	113.7	108.9	347.9
S7A3-II	2	+	66.14	66.36	121.9	110.7	111.5	344.1
S7A4	1 (disordered, major)	-	65.78	49.56	121.4	107.8	117.2	346.5
S7A4	1 (disordered, minor)	-	65.78	63.23	-	-	-	-
S7A5	1	+	64.83	70.41	122.1	114.4	114.9	351.3
S7A5	2	-	66.02	68.00	122.7	111.0	114.8	348.5
S7A6	1	-	57.41	68.22	121.9	110.0	114.7	346.6
S7A7-I	1	-	65.94	40.59	117.6	108.6	117.2	343.5
S7A7-II	1	+	61.78	89.98	126.2	109.6	116.7	352.4
S7A7-II	2	-	60.52	88.43	125.6	112.2	116.3	354.1
S7A7-II	3	+	60.59	88.16	127.3	113.1	117.4	357.9
S7A8-I	1	-	66.68	68.92	121.2	109.2	114.2	344.6
S7A8-I	2	+	64.88	70.88	121.5	109.7	116.1	347.3
S7A8-II	1	+	59.35	87.15	126.5	113.6	119.1	359.2
S7A10-I	1	-	64.50	58.17	121.1	111.0	115.2	347.3
S7A10-II	1	-	58.33	44.41	116.8	110.1	116.0	342.9

Table S3 Hydrogen bonding patterns and crystal packings.

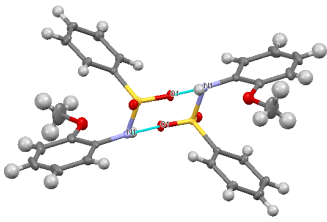
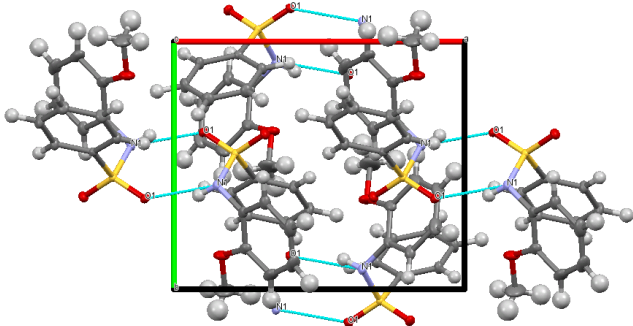
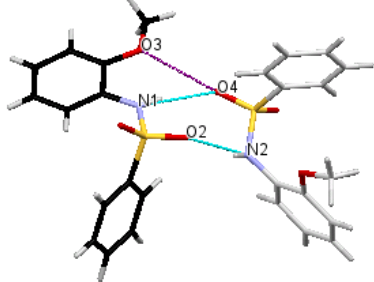
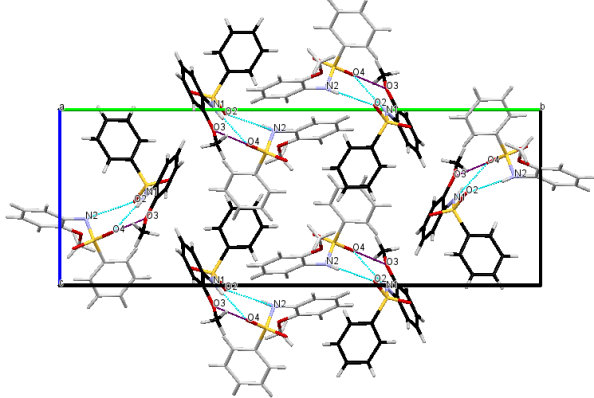
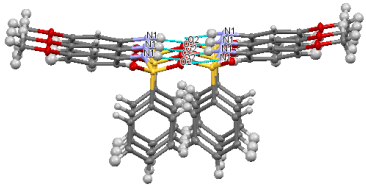
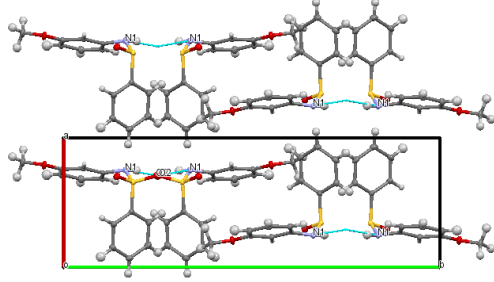
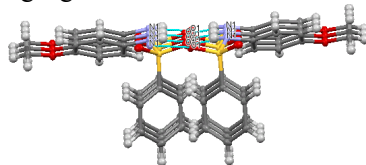
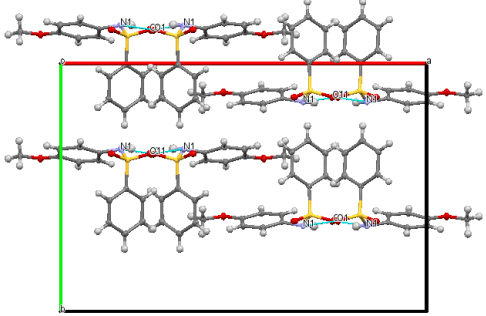
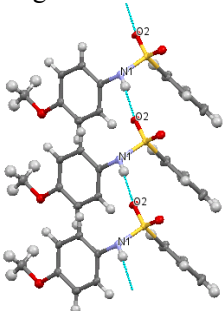
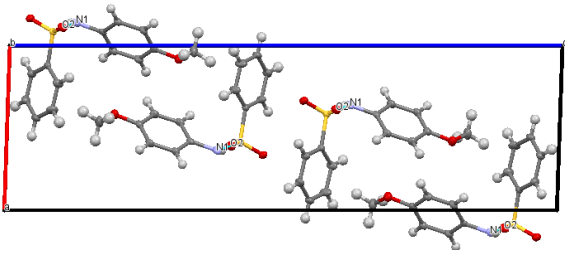
View along the selected axis (shown in parentheses in the cells). Dashed lines indicate intermolecular and intramolecular interactions. Colors of dashed lines: NH...O=S, light blue, NH ...OMe or NH...OH(water), purple. Colors of atoms: C, gray spheres; O, red spheres; N, violet spheres; S, orange spheres; and H, light gray spheres.

Compound	HB pattern	Crystal packing
S1A1	Helical 1 	 (b)
S1A2	Helical 2 	 (a)
S1A3-I	Helical 1 ($Z'=2$) ^a  (+)-synclinal and  (-)-synclinal	 (b)
S1A3-II	Dimeric 	 (b)

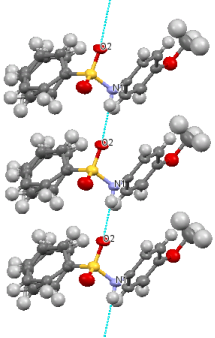
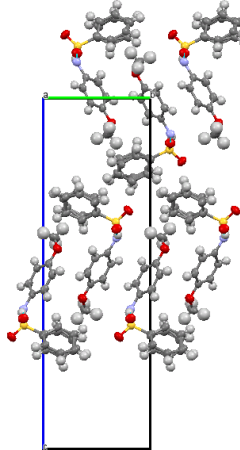
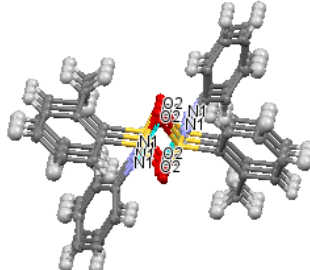
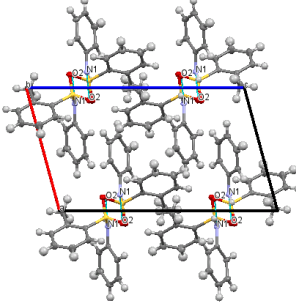
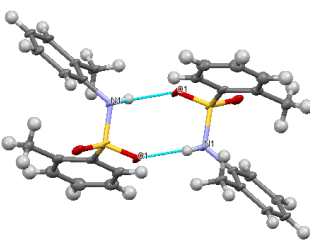
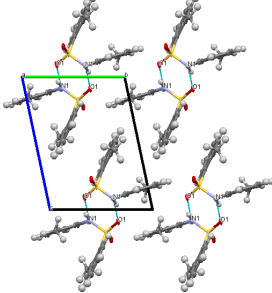
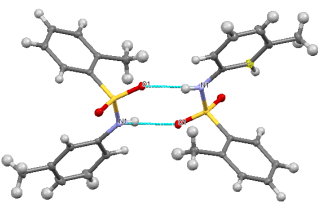
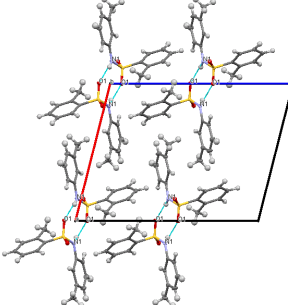
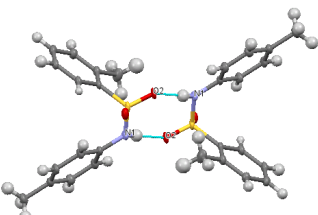
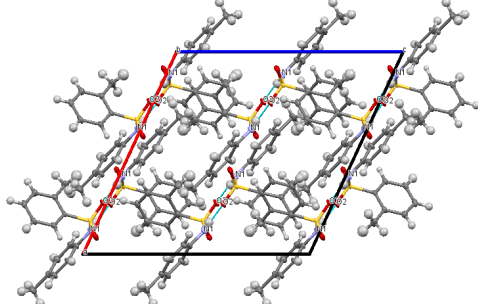
(Table S3)

Compound	HB pattern	Crystal packing
S1A4	Helical-1 ($Z' = 2$) ^a Helical (molecule A) and side chain (molecule B) 	 (b)
S1A5	Zigzag-2 	 (a)
S1A6	Helical-1 	 (b)
S1A7-I	Dimeric ($Z' = 2$) ^a  *pseudo-inversion	 (b)
S1A7-II	Straight 	 (b)

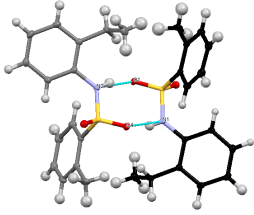
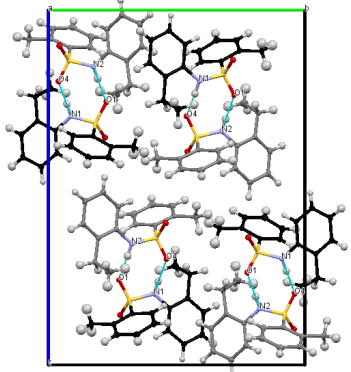
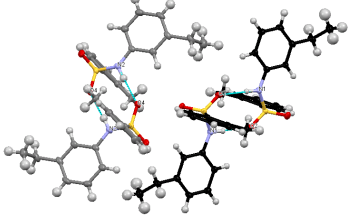
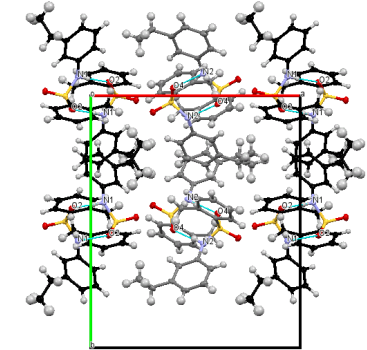
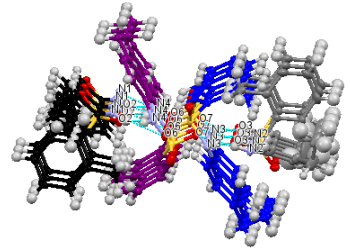
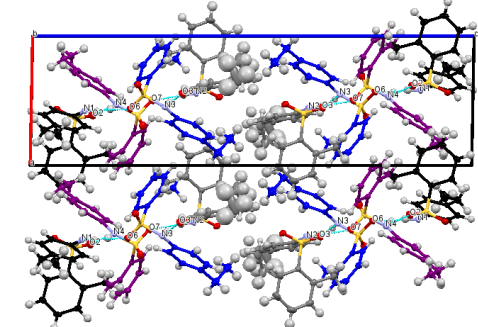
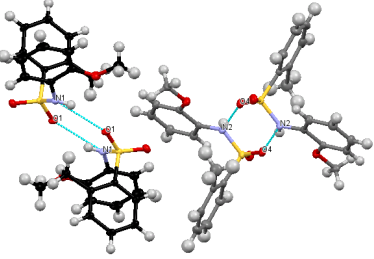
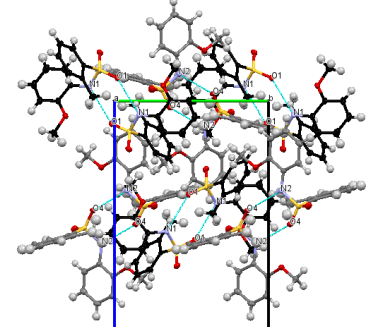
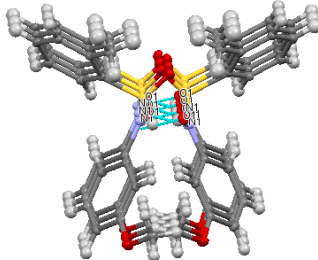
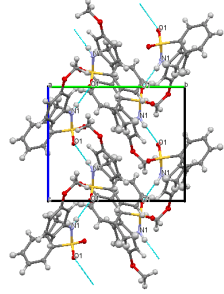
(Table S3)

Compound	HB pattern	Crystal packing
S1A8-I	Dimeric 	 (c)
S1A8-II ^{S20} [YUPXIR]	Dimeric ($Z' = 2$) ^a  *pseudo-inversion	 (a)
S1A9	Zigzag-2 	 (c)
S1A10-I	Zigzag-2 	 (c)
S1A10-II	Straight 	 (b)

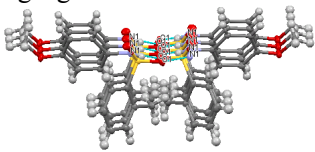
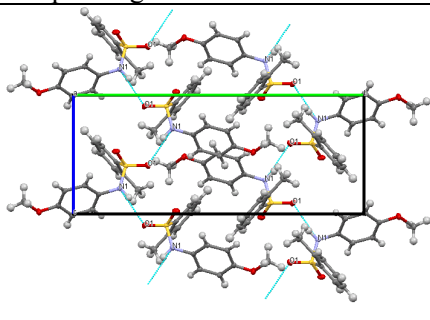
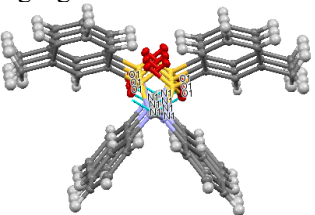
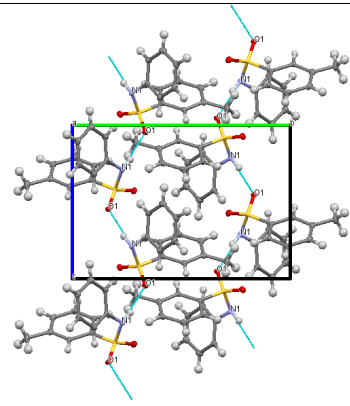
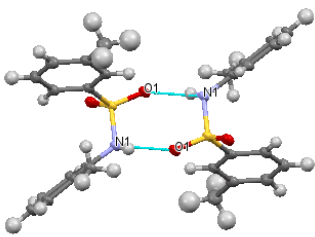
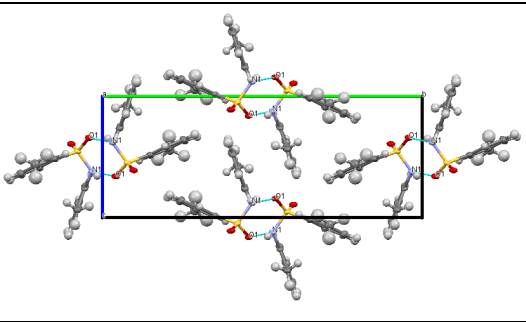
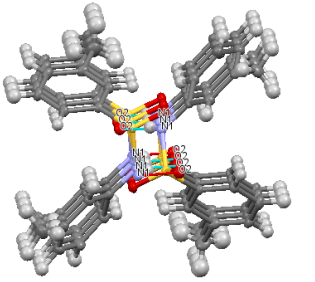
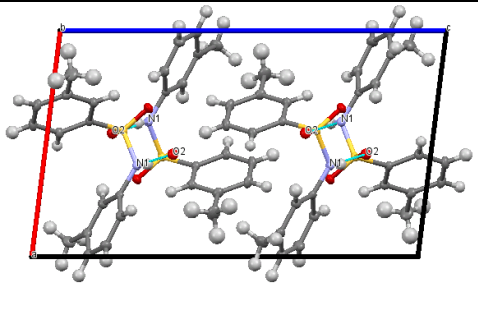
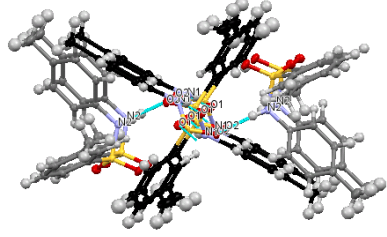
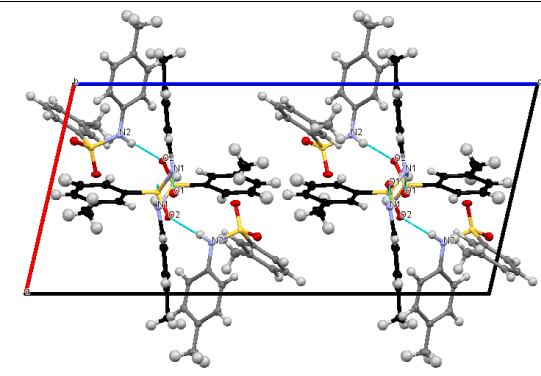
(Table S3)

Compound	HB pattern	Crystal packing
S1A10-III ^{S21} [IJUJUT]	Straight 	 (b)
S2A1	Helical-1 	 (b)
S2A2	Dimeric 	 (a)
S2A3	Dimeric 	 (b)
S2A4	Dimeric 	 (b)

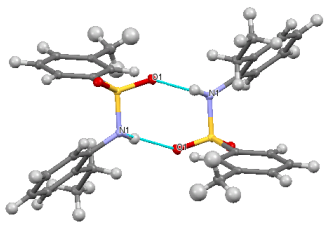
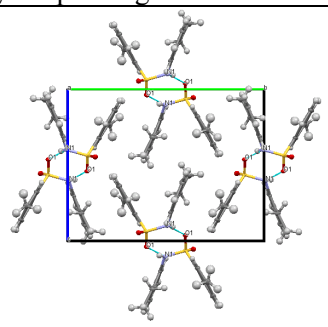
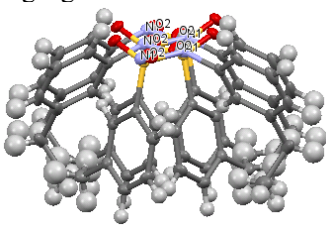
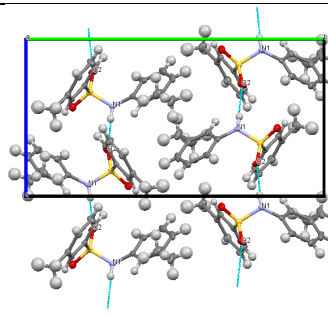
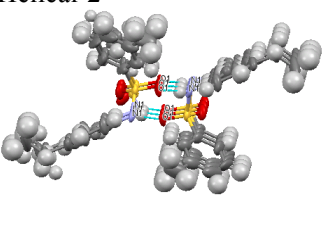
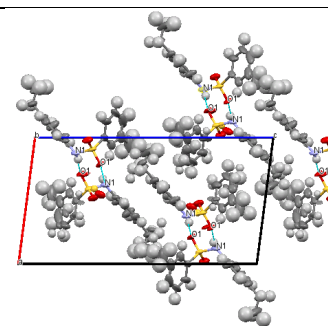
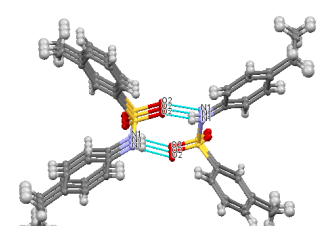
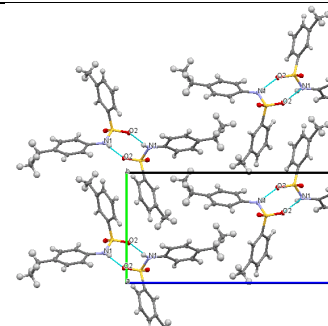
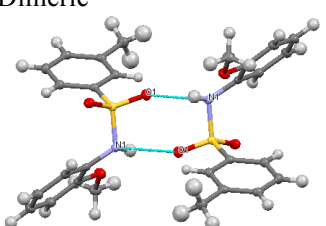
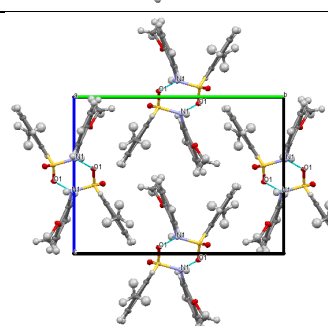
(Table S3)

Compound	HB pattern	Crystal packing
S2A5	Dimeric ($Z' = 2$) ^a  *pseudo-inversion	 (a)
S2A6	Dimeric ($Z' = 2$) ^a 	 (c)
S2A7	Helical-1+2 ($Z' = 4$) ^a 	 (b)
S2A8	Dimeric ($Z' = 2$) ^a 	 (a)
S2A9	Zigzag-1 	 (a)

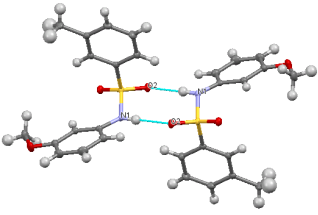
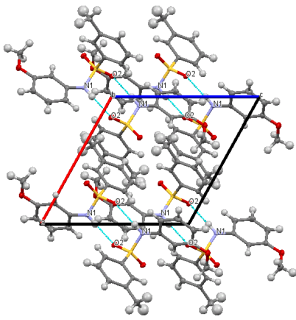
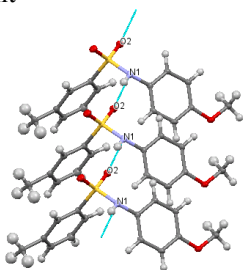
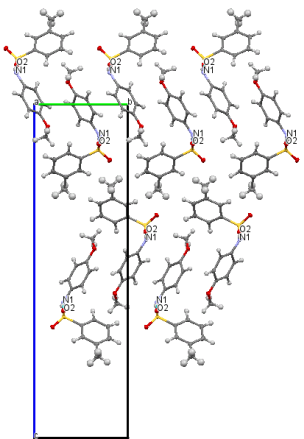
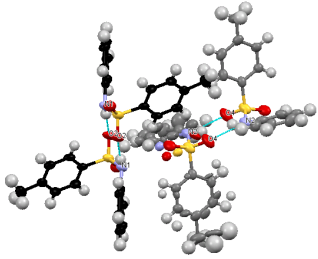
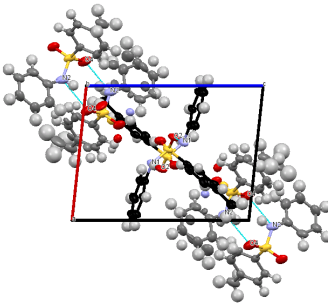
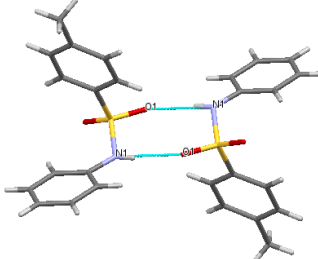
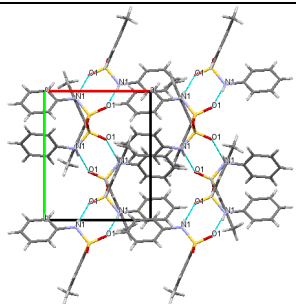
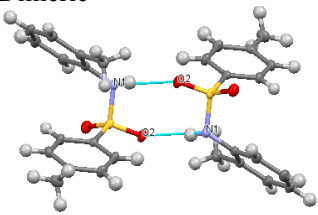
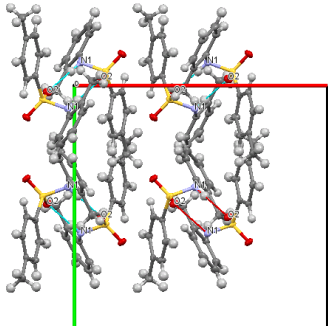
(Table S3)

Compound	HB pattern	Crystal packing
S2A10	Zigzag-2 	 (a)
S3A1	Zigzag-1 	 (a)
S3A2	Dimeric 	 (a)
S3A3	Helical-2 	 (b)
S3A4	Helical-1 ($Z' = 2$) ^a Helical (molecule A) and side chain (molecule B) 	 (b)

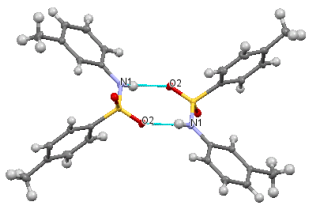
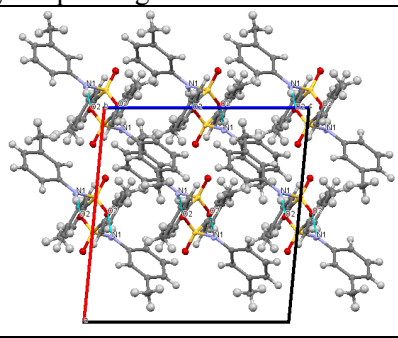
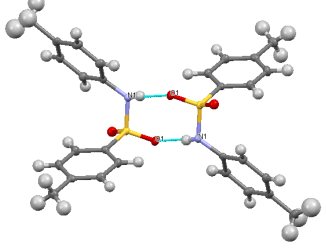
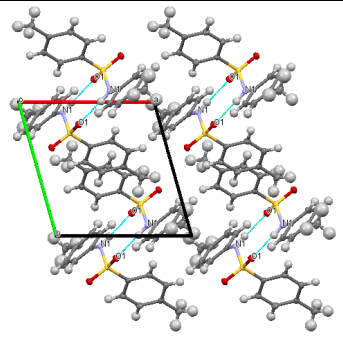
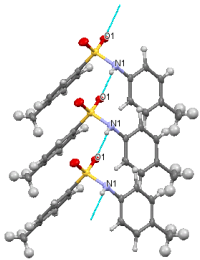
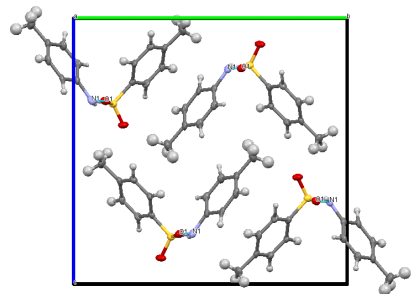
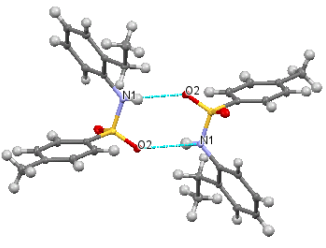
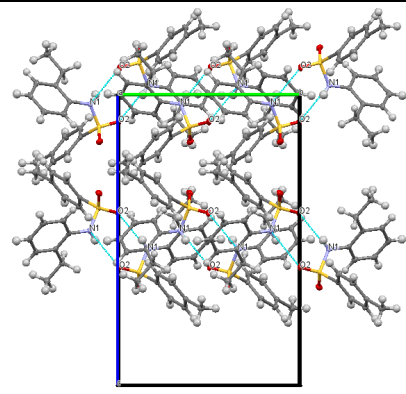
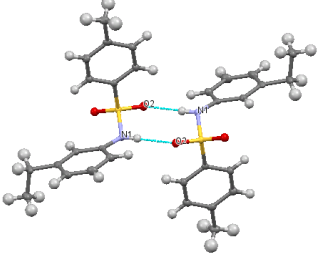
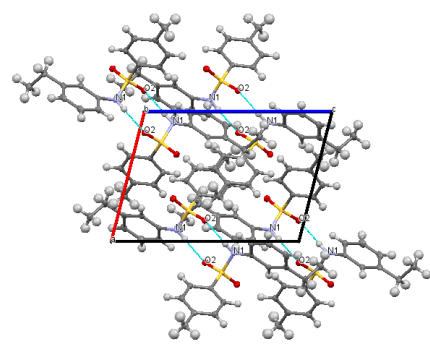
(Table S3)

Compound	HB pattern	Crystal packing
S3A5	Dimeric 	 (a)
S3A6	Zigzag-1 	 (a)
S3A7-I	Helical-2 	 (b)
S3A7-II	Helical-2 	 (a)
S3A8	Dimeric 	 (a)

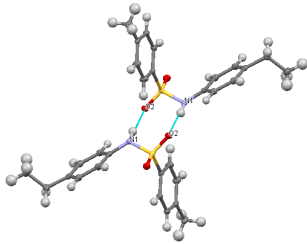
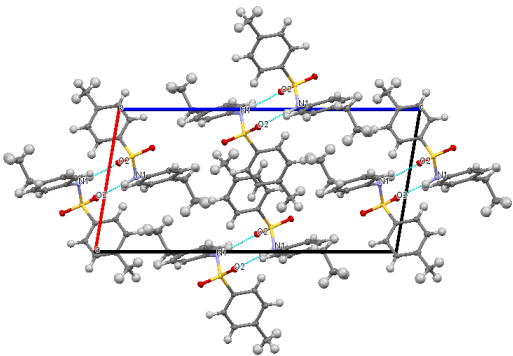
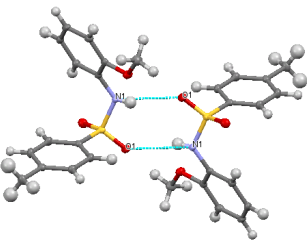
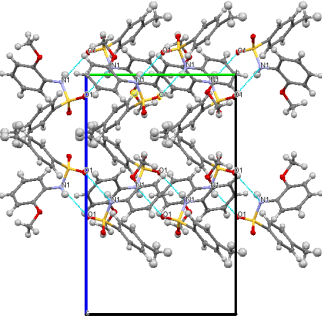
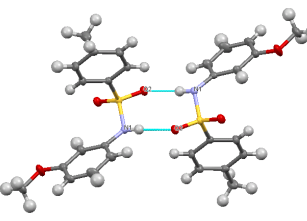
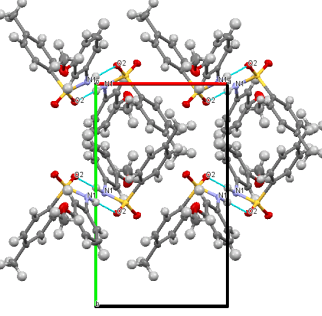
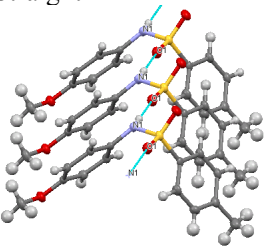
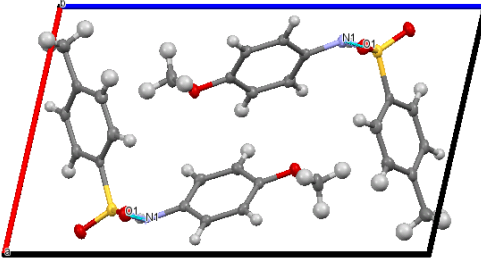
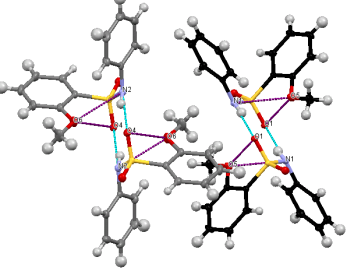
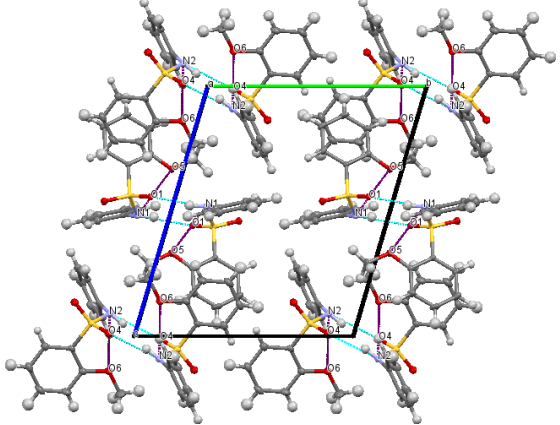
(Table S3)

Compound	HB pattern	Crystal packing
S3A9	Dimeric 	Crystal packing  (b)
S3A10	Straight 	Crystal packing  (a)
S4A1-I	Dimeric ($Z' = 2$) ^a 	Crystal packing  (b)
S4A1-II ^{S24} [FABUB01]	Dimeric 	Crystal packing  (c)
S4A2	Dimeric 	Crystal packing  (c)

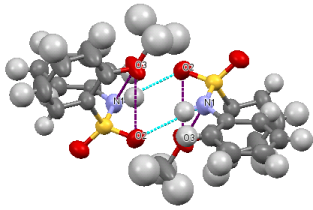
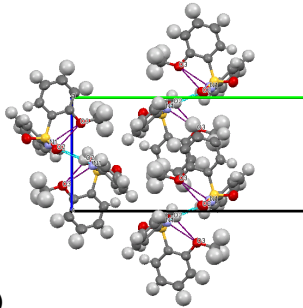
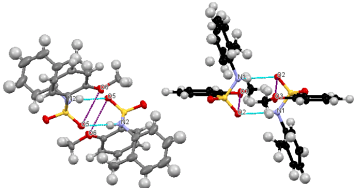
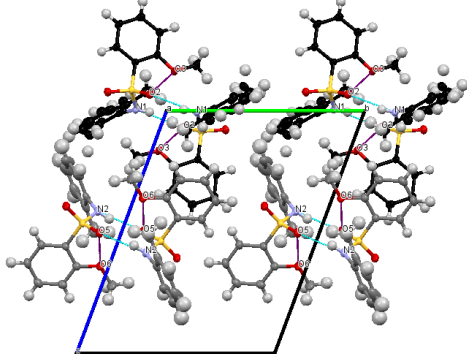
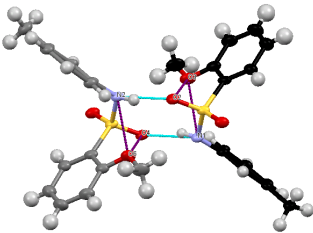
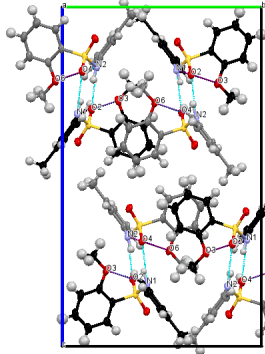
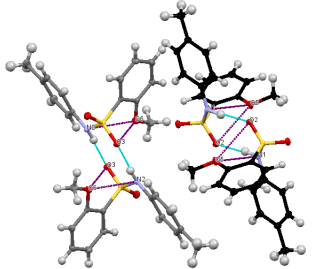
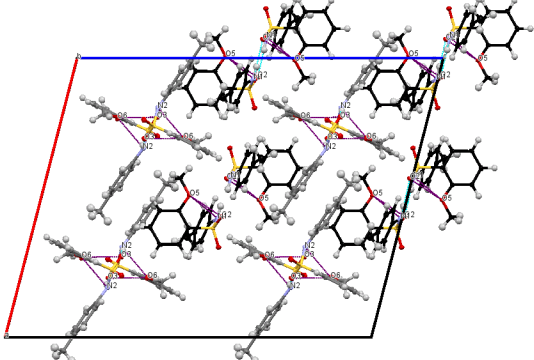
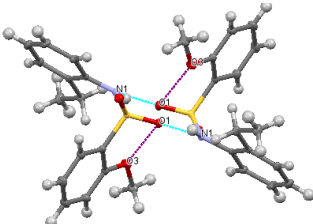
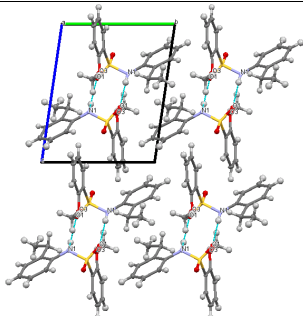
(Table S3)

Compound	HB pattern	Crystal packing
S4A3	Dimeric 	 (b)
S4A4-I	Dimeric 	 (c)
S4A4-II	Straight 	 (a)
S4A5	Dimeric 	 (a)
S4A6	Dimeric 	 (b)

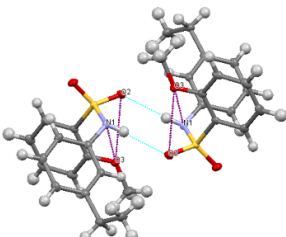
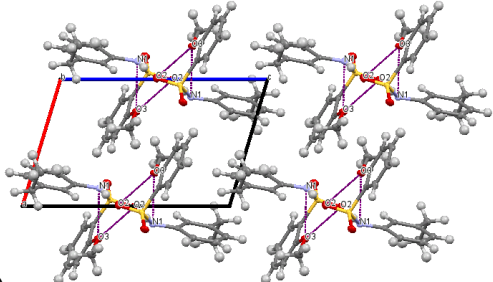
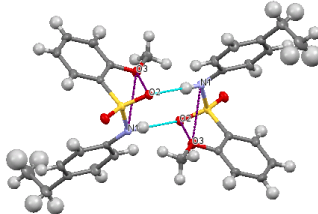
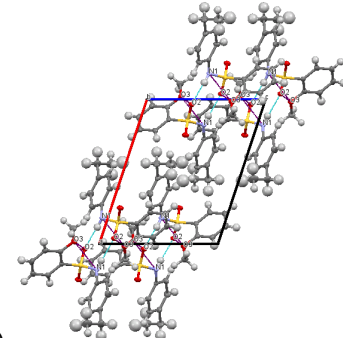
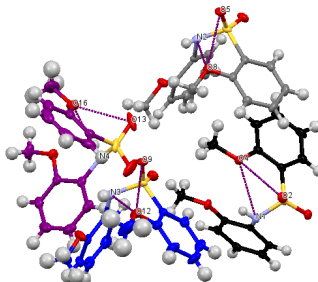
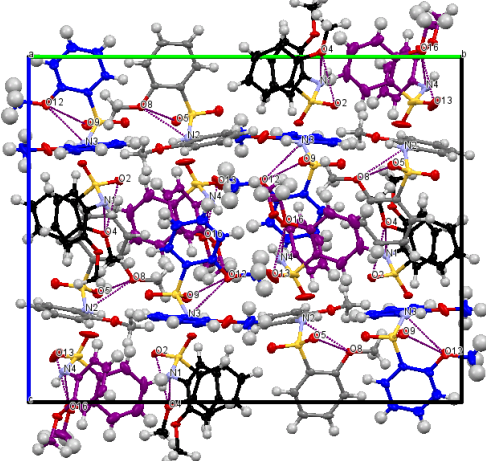
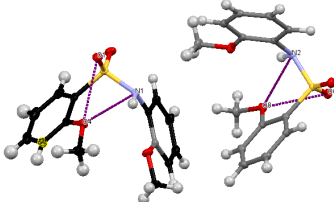
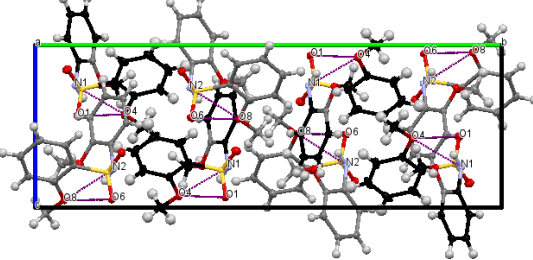
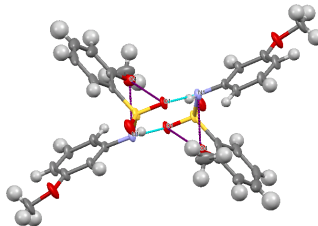
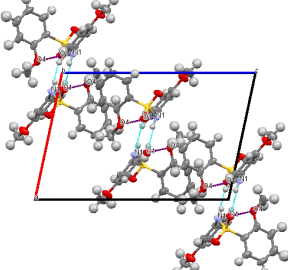
(Table S3)

Compound	HB pattern	Crystal packing
S4A7	Dimeric 	Crystal packing  (b)
S4A8	Dimeric 	Crystal packing  (a)
S4A9	Dimeric 	Crystal packing  (c)
S4A10	Straight 	Crystal packing  (b)
S5A1-I	Dimeric ($Z' = 2$) ^a 	Crystal packing  (a)

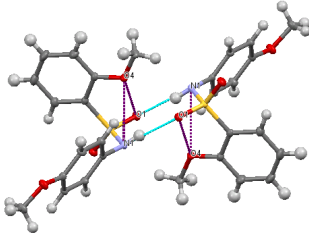
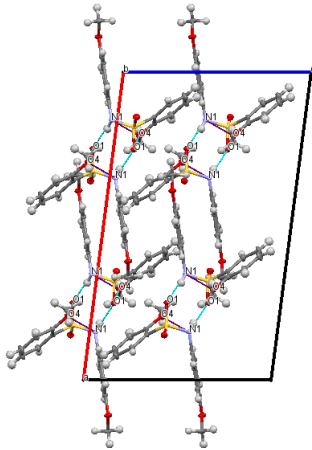
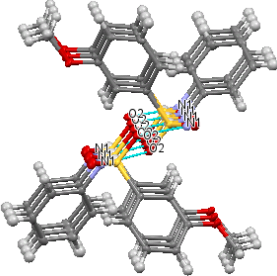
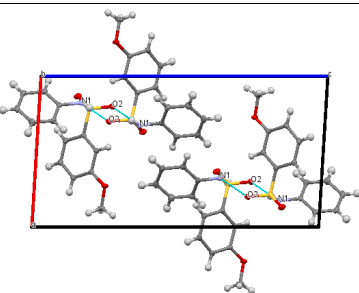
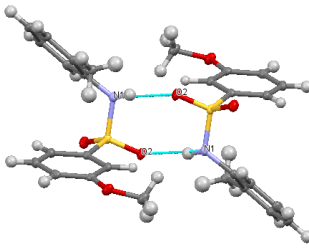
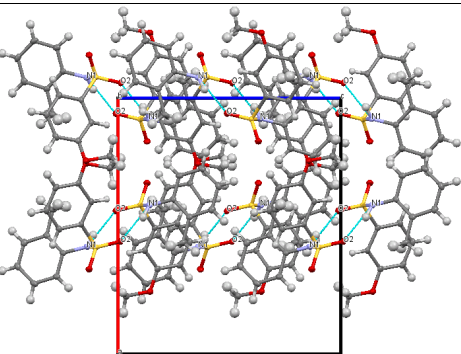
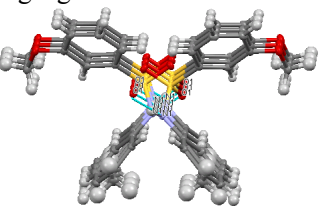
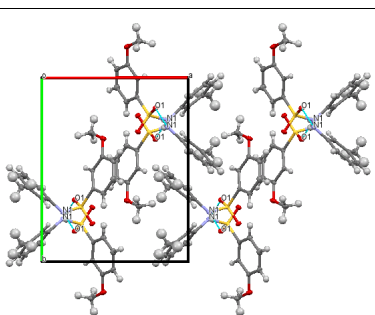
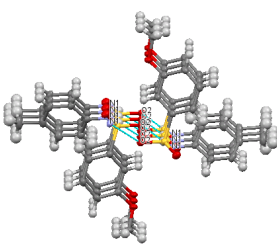
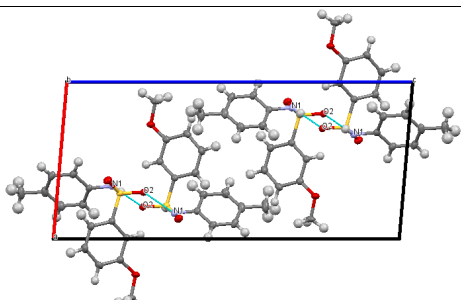
(Table S3)

Compound	HB pattern	Crystal packing
S5A1-II	Dimeric 	 (a)
S5A2	Dimeric ($Z' = 2$) ^a 	 (a)
S5A3	Dimeric ($Z' = 2$) ^a *pseudo-inversion 	 (a)
S5A4	Dimeric ($Z' = 2$) ^a 	 (b)
S5A5	Dimeric 	 (a)

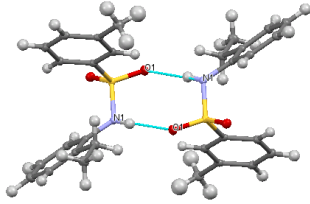
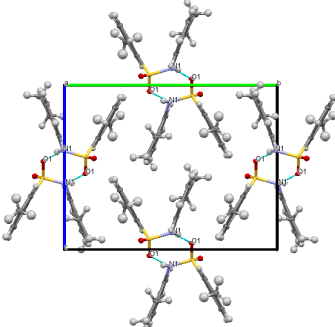
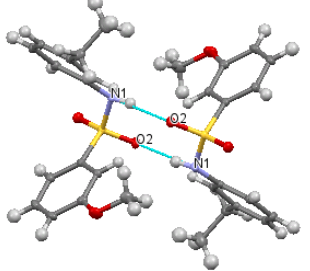
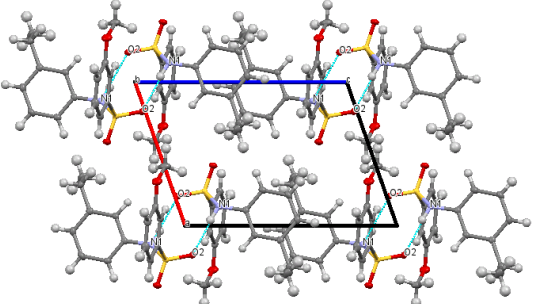
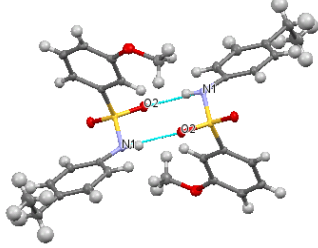
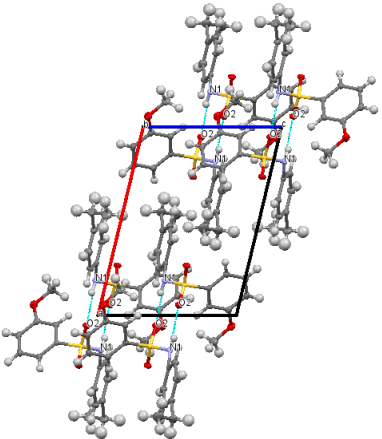
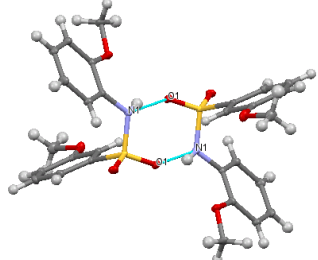
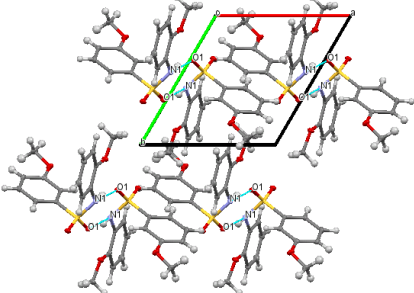
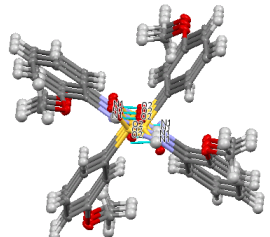
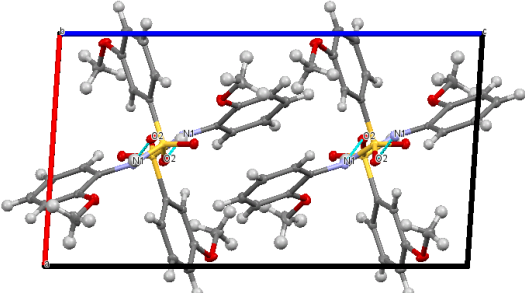
(Table S3)

Compound	HB pattern	Crystal packing
S5A6	Dimeric 	Crystal packing  (b)
S5A7	Dimeric 	Crystal packing  (b)
S5A8-I	NH...OMe ($Z' = 4$) ^a 	Crystal packing  (a)
S5A8-II	NH...OMe ($Z' = 2$) ^a 	Crystal packing  (a)
S5A9	Dimeric 	Crystal packing  (b)

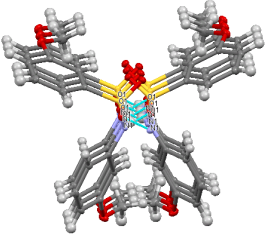
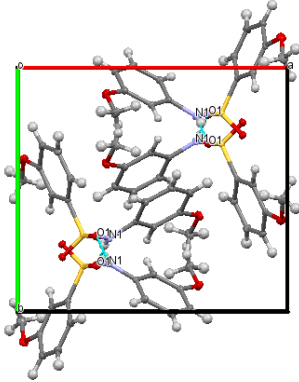
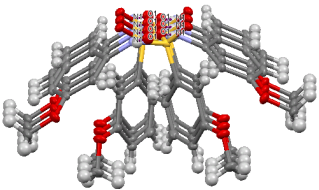
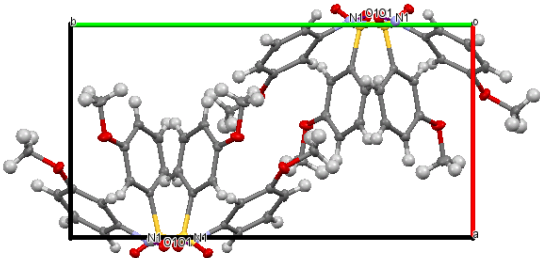
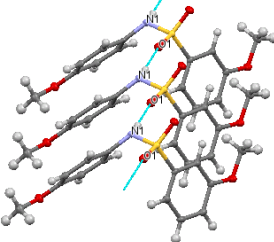
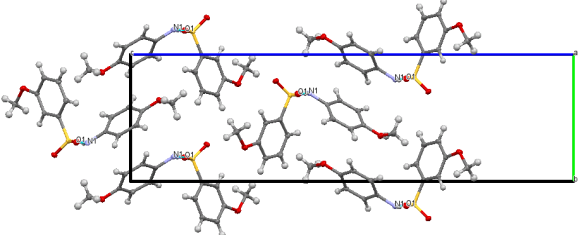
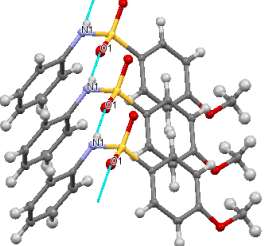
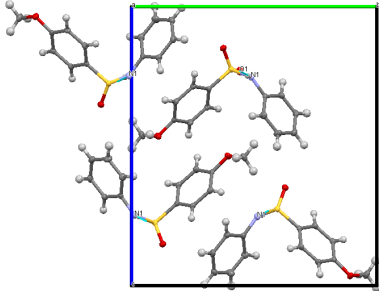
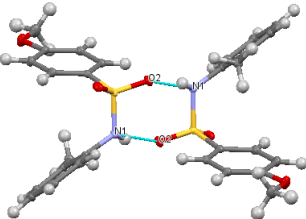
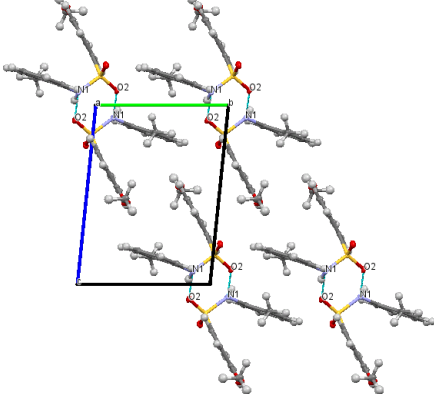
(Table S3)

Compound	HB pattern	Crystal packing
S5A10	Dimeric 	 (b)
S6A1	Helical-2 	 (b)
S6A2	Dimeric 	 (b)
S6A3	Zigzag-1 ^b 	 (c)
S6A4	Helical-2 	 (b)

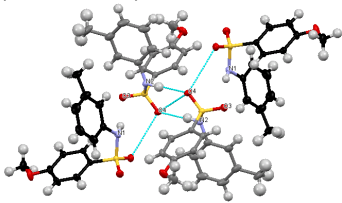
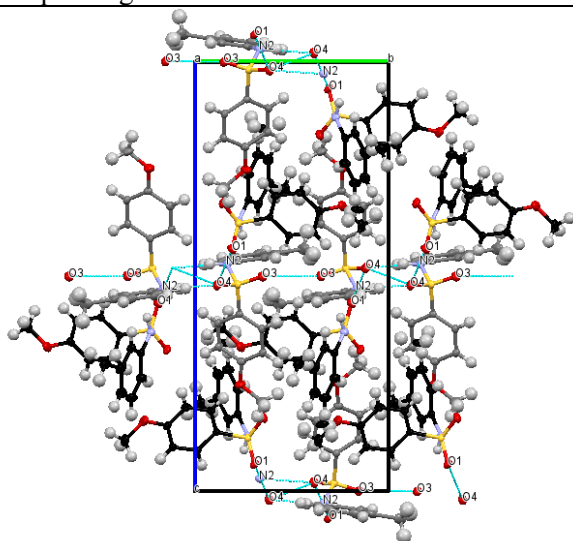
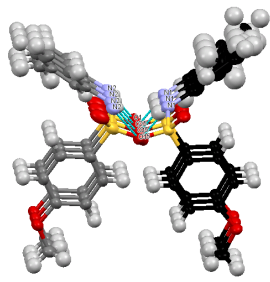
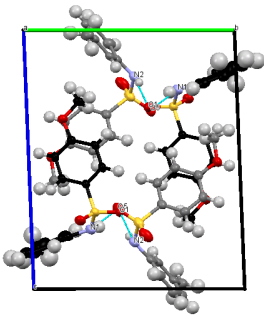
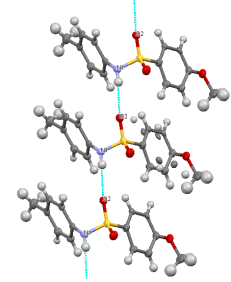
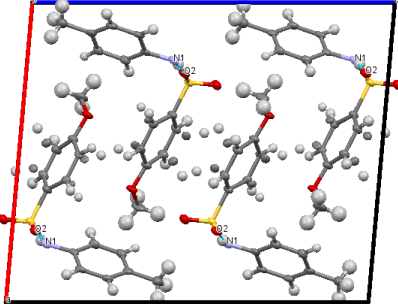
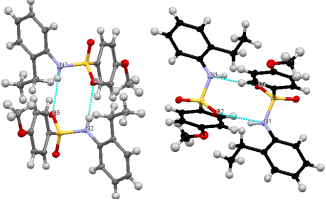
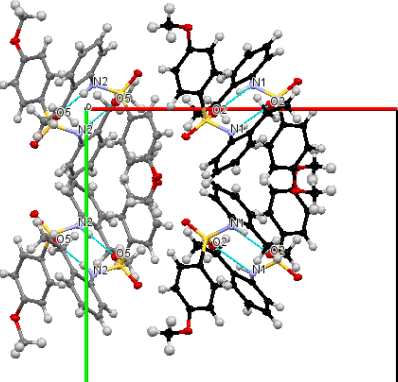
(Table S3)

Compound	HB pattern	Crystal packing
S6A5	Dimeric 	 (a)
S6A6	Dimeric 	 (b)
S6A7	Dimeric 	 (b)
S6A8-I	Dimeric 	 (c)
S6A8-II	Helical-1 	 (b)

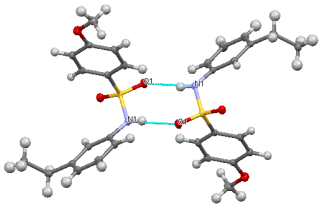
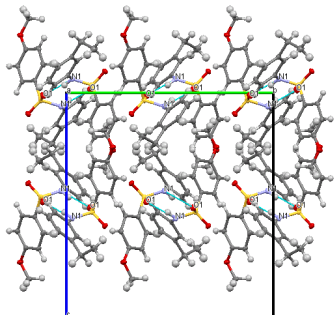
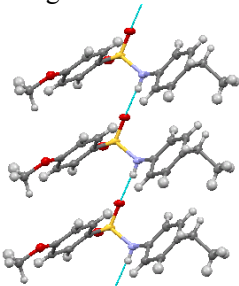
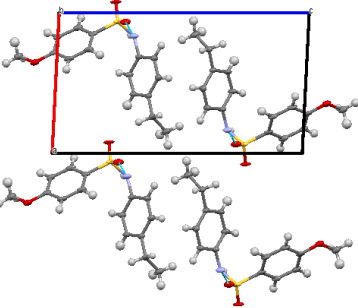
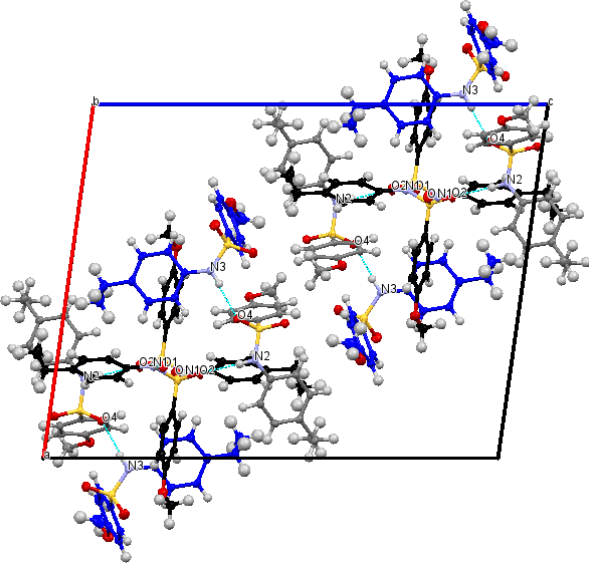
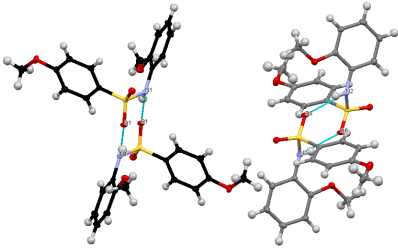
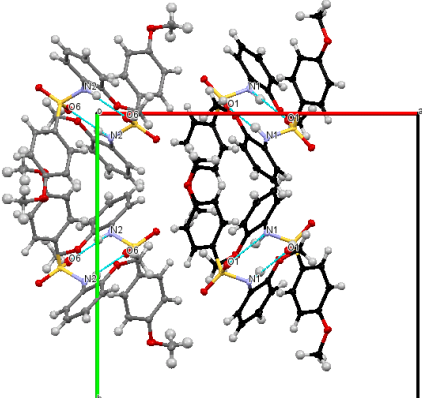
(Table S3)

Compound	HB pattern	Crystal packing
S6A9-I	Zigzag-1 	Crystal packing  (c)
S6A9-II	Zigzag-1 	 (c)
S6A10	Straight 	 (a)
S7A1	Straight 	 (a)
S7A2	Dimeric 	 (a)

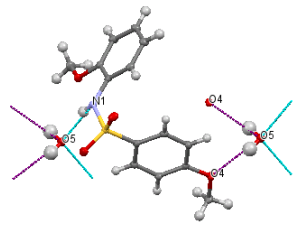
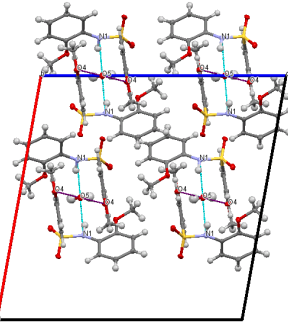
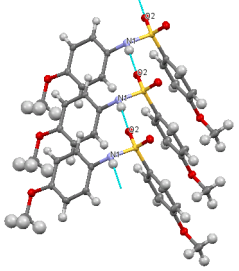
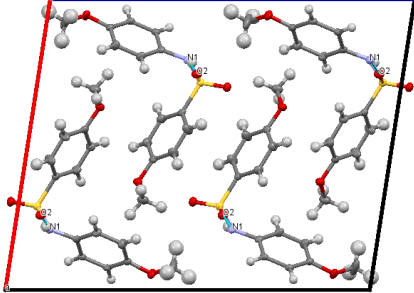
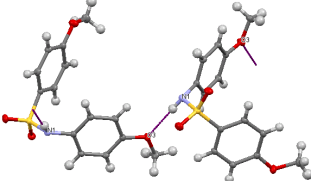
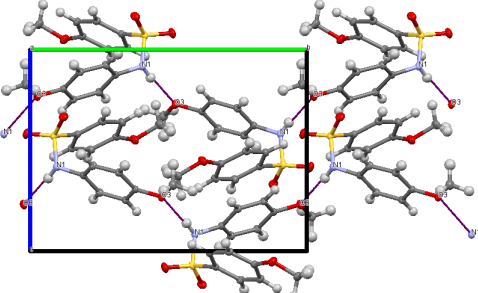
(Table S3)

Compound	HB pattern	Crystal packing
S7A3-I	Dimeric ($Z' = 2$) ^a Side chain (molecule A), Dimeric (molecule B) 	 <p>(a)</p>
S7A3-II	Zigzag-2 ($Z' = 2$) ^{a,b} *pseudo-glide 	 <p>(a)</p>
S7A4	Straight 	 <p>(b)</p>
S7A5	Dimeric ($Z' = 2$) ^a 	 <p>(c)</p>

(Table S3)

Compound	HB pattern	Crystal packing
S7A6	Dimeric 	Crystal packing  (a)
S7A7-I	Straight 	 (b)
S7A7-II	Helical-1 ($Z' = 3$) ^a Helical (molecule A, black), side chains (molecule B, light gray; molecule C, blue)	 (b)
S7A8-I	Dimeric ($Z' = 2$) ^a 	 (c)

(Table S3)

Compound	HB pattern	Crystal packing
S7A8-II	NH...Solvent 	 (b)
S7A10-I	Staright 	 (b)
S7A10-II	NH...OMe 	 (a)

^a Colors of carbon atoms: molecule A, black; molecule B, light gray, molecule C, blue; molecule D, purple ^b The distance between the amide proton and the oxygen is slightly larger than the sum of van der Waals radii.

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