

Electronic Supplementary Information

**Relationship between crystal shape and unit cell shape:  
crystal shape modification via co-crystallization toward  
SXRD-suitable crystals**

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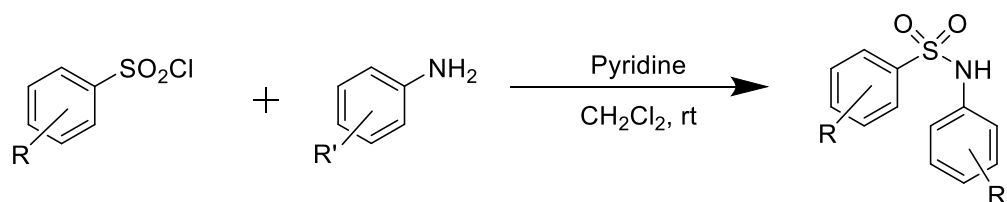
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## 1. Experimental



Scheme S1

### Characteristic Data of synthesized sulfonamides in this paper (1–11)

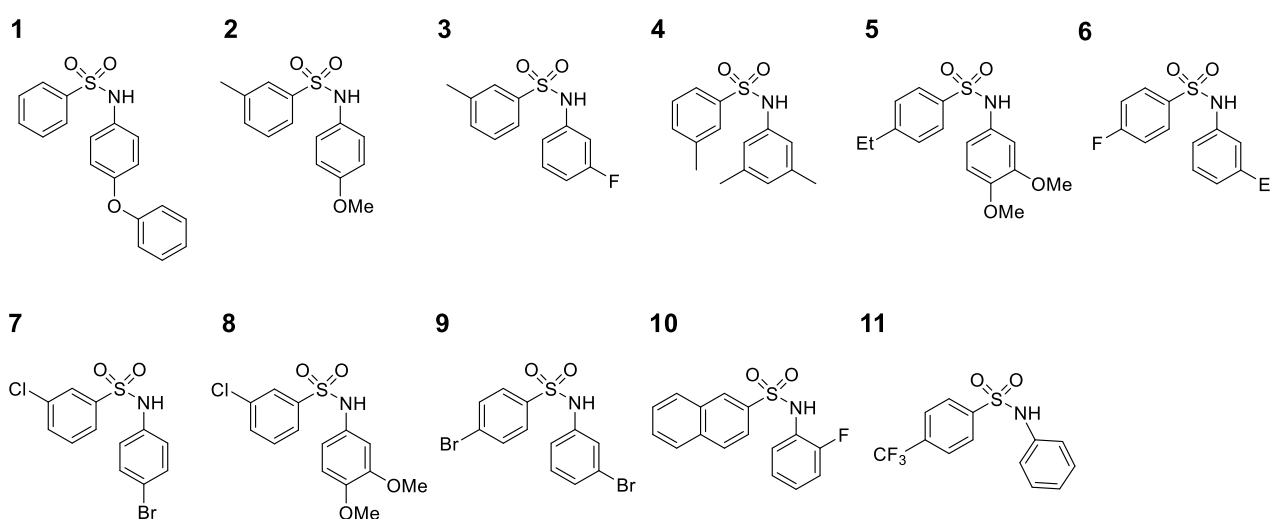


Fig S1 Molecular structures of **1–11**

***N*-(4-Phenoxyphenyl)benzenesulfonamide (1).**<sup>s1</sup> Yield: 479.8 mg (1.47 mmol), 73.6%. Color, Habit: colorless, prism crystals. M.p.: 109–110 °C. <sup>1</sup>H NMR (400 MHz, 298 K, CDCl<sub>3</sub>) (ppm): δ 7.75 (dd, *J* = 8.5, 1.1, 2H), 7.56 (ddt, *J* = 7.4, 7.3, 1.4, 1H), 7.46 (dd, *J* = 7.5, 7.3, 2H), 7.33 (dd, *J* = 8.1, 7.9, 2H), 7.11 (ddt, *J* = 7.4, 7.3, 1.4, 1H), 7.01 (d, *J* = 8.9, 2H), 6.95 (dd, *J* = 8.6, 1.1, 2H), 6.87 (d, *J* = 9.2, 2H), 6.57 (brs, 1H).

***N*-(4-Methoxyphenyl)-3-methylbenzenesulfonamide (2).**<sup>s2</sup> Yield: 416.4 mg (1.5 mmol), 79.4%. Color, Habit: colorless, prism crystals. M.p.: 82 °C. <sup>1</sup>H NMR (400 MHz, 298 K, CDCl<sub>3</sub>) (ppm): δ 7.52 (s, 1H), 7.46 (d, *J* = 7.6, 1H), 7.35–7.28 (m, 2H), 6.97 (d, *J* = 8.7, 2H), 6.76 (d, *J* = 8.9, 2H), 6.46 (brs, 1H), 3.77 (s, 3H), 2.36 (s, 3H).

**4-Acetyl-*N*-(3-fluorophenyl)benzenesulfonamide (3).** Yield: 360.2 mg (1.23 mmol), 67.2%. M.p.: 95–96 °C. <sup>1</sup>H NMR (400 MHz, 298 K, CDCl<sub>3</sub>) (ppm): δ 7.65–7.59 (m, 2H), 7.38–7.32 (m, 2H), 7.18 (ddd, *J* = 8.1, 8.0, 6.4, 1H), 7.07 (brs, 1H), 6.90 (dt, *J* = 10.0, 2.3, 1H), 6.84–6.76 (m, 2H), 2.37 (s, 3H). <sup>13</sup>C NMR (100 MHz,

298 K, CDCl<sub>3</sub>) (ppm):  $\delta$  163.0 (d,  $J_{\text{CF}} = 246.3$ ), 139.5, 138.5, 138.1 (d,  $J_{\text{CF}} = 10.5$ ), 134.2, 130.5 (d,  $J_{\text{CF}} = 9.6$ ), 129.0, 127.5, 124.4, 116.3 (d,  $J_{\text{CF}} = 2.9$ ), 112.0 (d,  $J_{\text{CF}} = 21.1$ ), 108.2 (d,  $J_{\text{CF}} = 24.9$ ), 21.3. FT-IR (KBr, cm<sup>-1</sup>): 3245, 3071, 2976, 2900, 1615, 1499, 1420, 1615, 1499, 1420, 1327, 1136, 984, 913, 700, 566, 511. MS (FAB):  $m/z$  266[M+H]<sup>+</sup>. Anal. Calcd. for C<sub>14</sub>H<sub>12</sub>FNO<sub>3</sub>S: C, 57.33; H, 4.12; N, 4.78, Found: C, 59.03; H, 4.4; N, 5.27.

***N*-(3,5-Dimethylphenyl)-3-methylbenzenesulfonamide (4).** Yield: 301 mg (1.09 mmol), 52%. Color, Habit: brown, prism crystals. M.p.: 126–127 °C. <sup>1</sup>H NMR (400 MHz, 298 K, CDCl<sub>3</sub>) (ppm):  $\delta$  7.61 (s, 1H), 7.58 (d,  $J = 6.4$ , 1H), 7.34–7.29 (m, 2H), 6.74 (s, 1H), 6.68 (s, 2H), 6.61 (brs, 1H), 2.36 (s, 3H), 2.22 (s, 6H). <sup>13</sup>C NMR (100 MHz, 298 K, CDCl<sub>3</sub>) (ppm):  $\delta$  139.2, 139.1, 139.0, 136.2, 133.7, 128.8, 127.6, 127.1, 124.4, 119.2, 21.3, 21.2. FT-IR (KBr, cm<sup>-1</sup>): 3230, 2917, 1598, 1478, 1401, 1323, 1217, 1151, 1095, 698, 650, 596, 505, 423. MS (FAB):  $m/z$  276[M+H]<sup>+</sup>. Anal. Calcd. for C<sub>15</sub>H<sub>17</sub>NO<sub>2</sub>S: C, 65.43; H, 6.22; N, 5.09, Found: C, 65.48; H, 6.06; N, 5.15.

***N*-(3,4-Dimethoxyphenyl)-4-ethylbenzenesulfonamide (5).** Yield: 361 mg (1.12 mmol), 57%. Color, Habit: brown, amorphous. M.p.: 91 °C. <sup>1</sup>H NMR (400 MHz, 298 K, CDCl<sub>3</sub>) (ppm):  $\delta$  7.62 (d,  $J = 8.6$ , 2H), 7.25 (d,  $J = 8.6$ , 2H), 6.71–6.66 (m, 2H), 6.52 (dd,  $J = 8.5$ , 2.5, 1H), 6.38 (brs, 1H), 3.83 (s, 3H), 3.77 (s, 3H), 6.28 (q,  $J = 7.6$ , 2H), 1.23 (t,  $J = 7.6$ , 3H). <sup>13</sup>C NMR (100 MHz, 298 K, CDCl<sub>3</sub>) (ppm):  $\delta$  149.9, 149.2, 147.5, 136.1, 129.2, 128.4, 127.5, 116.0, 111.1, 108.1, 56.0, 55.9, 28.8, 15.1. MS (FAB):  $m/z$  321[M]<sup>+</sup>. Anal. Calcd. for C<sub>16</sub>H<sub>19</sub>NO<sub>4</sub>S: C, 59.80; H, 5.96; N, 4.36, Found: C, 59.6; H, 5.89; N, 4.36.

***N*-(3-Ethylphenyl)-4-fluorobenzenesulfonamide (6).** Yield: 420 mg (1.5 mmol), 75.2%. Color, Habit: brown, liquid. <sup>1</sup>H NMR (400 MHz, 298 K, CDCl<sub>3</sub>) (ppm):  $\delta$  7.81–7.75 (m, 2H), 7.18–7.07 (m, 3H), 6.97 (d,  $J = 7.8$ , 1H), 6.88 (d,  $J = 8.5$ , 2H), 6.75 (brs, 1H), 2.56 (q,  $J = 7.6$ , 2H), 1.15 (t,  $J = 7.6$ , 3H). <sup>13</sup>C NMR (100 MHz, 298 K, CDCl<sub>3</sub>) (ppm):  $\delta$  165.2 (d,  $J_{\text{CF}} = 255.0$ ), 145.9, 136.0, 135.0, 135.0, 130.0 (d,  $J_{\text{CF}} = 9.6$ ), 129.3, 125.4, 121.5, 119.2, 116.2 (d,  $J_{\text{CF}} = 23.0$ ), 28.6, 15.4. FT-IR (KBr, cm<sup>-1</sup>): 3263, 2967, 1592, 1494, 1469, 1407, 1336, 1238, 1153, 1091, 838, 697, 564, 543. MS (FAB):  $m/z$  280[M+H]<sup>+</sup>. HRMS (FAB):  $m/z$  [M+H]<sup>+</sup> calcd for C<sub>14</sub>H<sub>15</sub>FNO<sub>2</sub>S: 280.0808; found: 280.0808.

***N*-(4-Bromophenyl)-3-chlorobenzenesulfonamide (7).**<sup>s1</sup> Yield: 542 mg (1.56 mmol), 82.6%. Color, Habit: colorless, prism crystals. M.p.: 103–104 °C. <sup>1</sup>H NMR (400 MHz, 298 K, CDCl<sub>3</sub>) (ppm):  $\delta$  7.78 (dd,  $J = 2.0$ , 1.8, 1H), 7.61 (ddd,  $J = 7.8$ , 1.7, 1.0, 1H), 7.53 (ddd,  $J = 8.0$ , 2.0, 1.0, 1H), 7.42–7.37 (m, 3H), 6.97 (d,  $J = 8.8$ , 2H), 6.82 (brs, 1H).

**3-Chloro-*N*-(3,4-dimethoxyphenyl)benzenesulfonamide (8).** Yield: 576 mg (1.76 mmol), 87%. Color, Habit: colorless, prism crystals. M.p.: 126–127 °C. <sup>1</sup>H NMR (400 MHz, 298 K, CDCl<sub>3</sub>) (ppm):  $\delta$  7.73 (dd,  $J = 1.7$ , 1.7, 1H), 7.55 (ddd,  $J = 7.8$ , 1.7, 1.0, 1H), 7.52 (ddd,  $J = 8.0$ , 2.1, 1.0, 1H), 7.37 (t,  $J = 8.0$ , 1H),

6.73–6.69 (m, 2H), 6.50 (dd,  $J = 8.5, 2.4$ , 1H), 6.35 (brs, 1H), 3.84 (s, 3H), 3.81 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz, 298 K,  $\text{CDCl}_3$ ) (ppm):  $\delta$  149.3, 147.8, 140.5, 135.2, 133.1, 130.2, 128.5, 127.4, 125.5, 116.2, 111.2, 108.3, 56.0, 56.0. FT–IR (KBr,  $\text{cm}^{-1}$ ): 3225, 3006, 2356, 1513, 1343, 1269, 1231, 1172, 1022, 967, 679, 635, 586. MS (FAB):  $m/z$  327 $[\text{M}]^+$ . Anal. Calcd. for  $\text{C}_{14}\text{H}_{14}\text{ClNO}_4\text{S}$ : C, 51.30; H, 4.31; N, 4.27, Found: C, 50.82; H, 4.25; N, 4.28.

**4-Bromo-*N*-(3-bromophenyl)benzenesulfonamide (9).** Yield: 467 mg (1.19 mmol), 60%. M.p.: 113–114 °C.  $^1\text{H}$  NMR (400 MHz, 298 K,  $\text{CDCl}_3$ ) (ppm):  $\delta$  7.65–7.59 (m, 4H), 7.30–7.26 (m, 2H), 7.13 (t,  $J = 8.0$ , 1H), 7.00 (ddd,  $J = 8.1, 2.1, 1.0$ , 1H), 6.50 (brs, 1H).  $^{13}\text{C}$  NMR (100 MHz, 298 K,  $\text{CDCl}_3$ ) (ppm):  $\delta$  137.7, 137.3, 132.5, 130.8, 128.8, 128.7, 128.5, 124.3, 123.0, 119.8. MS (FAB):  $m/z$  391 $[\text{M}+\text{H}]^+$ . Anal. Calcd. for  $\text{C}_{12}\text{H}_9\text{Br}_2\text{NO}_2\text{S}$ : C, 36.86; H, 2.32; N, 3.58, Found: C, 36.82; H, 2.37; N, 3.6.

***N*-(2-Fluorophenyl)naphthalene-2-sulfonamide (10).** Yield: 461.1 mg (1.53 mmol), 76.5%. M.p.: 111–112 °C.  $^1\text{H}$  NMR (400 MHz, 298 K,  $\text{CDCl}_3$ ) (ppm):  $\delta$  8.36 (d,  $J = 1.4$ , 1H), 7.90 (s, 1H), 7.88 (s, 1H), 7.86 (s, 1H), 7.74 (dd,  $J = 8.7, 2.8$ , 1H), 7.67–7.56 (m, 3H), 7.11–7.00 (m, 2H), 6.91 (ddd,  $J = 10.1, 8.1, 1.8$ , 1H), 6.82 (brs, 1H).  $^{13}\text{C}$  NMR (100 MHz, 298 K,  $\text{CDCl}_3$ ) (ppm):  $\delta$  153.9 (d,  $J_{\text{CF}} = 244.4$ ), 136.3 (d,  $J_{\text{CF}} = 66.1$ ), 132.0, 129.5, 129.3, 129.1, 128.9, 127.9, 127.6, 126.2 (d,  $J_{\text{CF}} = 7.7$ ), 124.8 (d,  $J_{\text{CF}} = 4.8$ ), 124.6, 124.5, 123.2, 122.0, 115.4 (d,  $J_{\text{CF}} = 19.2$ ). FT–IR (KBr,  $\text{cm}^{-1}$ ): 3264, 3066, 1592, 1494, 1406, 1337, 1253, 1163, 901, 827, 797, 750, 680, 564, 486. MS (FAB):  $m/z$  302 $[\text{M}+\text{H}]^+$ . Anal. Calcd. for  $\text{C}_{16}\text{H}_{12}\text{FNO}_2\text{S}$ : C, 63.77; H, 4.01; N, 4.65, Found: C, 63.63; H, 3.75; N, 4.64.

***N*-Phenyl-4-(trifluoromethyl)benzenesulfonamide (11).** <sup>s3</sup> Yield: 342.7 mg (1.14 mmol), 62.6%. M.p.: 138–139 °C.  $^1\text{H}$  NMR (400 MHz, 298 K,  $\text{CDCl}_3$ ) (ppm):  $\delta$  7.88 (d,  $J = 8.2$ , 2H), 7.71 (d,  $J = 8.5$ , 2H), 7.29 (d,  $J = 7.3$ , 2H), 7.18 (ddt,  $J = 7.3, 7.3, 1.1$ , 1H), 7.07 (dd,  $J = 8.5, 1.4$ , 2H), 6.64 (brs, 1H).  $^{13}\text{C}$  NMR (100 MHz, 298 K,  $\text{CDCl}_3$ ) (ppm):  $\delta$  142.6, 136.6, 134.9, 134.6, 129.6, 127.8, 126.2 (q,  $J_{\text{CF}} = 3.8$ ), 124.5, 122.3. FT–IR (KBr,  $\text{cm}^{-1}$ ): 3254, 3095, 3047, 1935, 1594, 1406, 1329, 1165, 1065, 1017, 845, 752, 718, 694, 604, 540, 430. MS (FAB):  $m/z$  302 $[\text{M}+\text{H}]^+$ . Anal. Calcd. for  $\text{C}_{13}\text{H}_{10}\text{F}_3\text{NO}_2\text{S}$ : C, 51.83; H, 3.35; N, 4.65, Found: C, 51.75; H, 3.3; N, 4.68.

## 2. NMR spectra of compound 1–11.

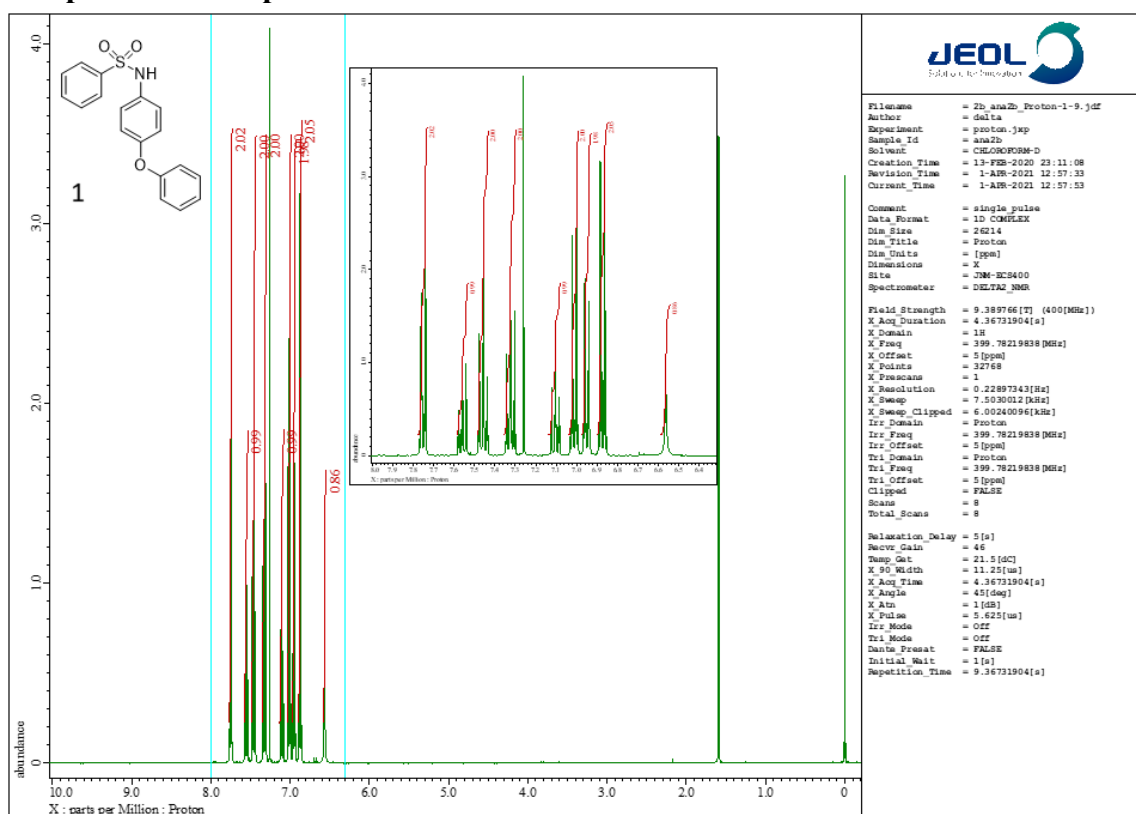


Fig S2 <sup>1</sup>H NMR Spectra of **1**

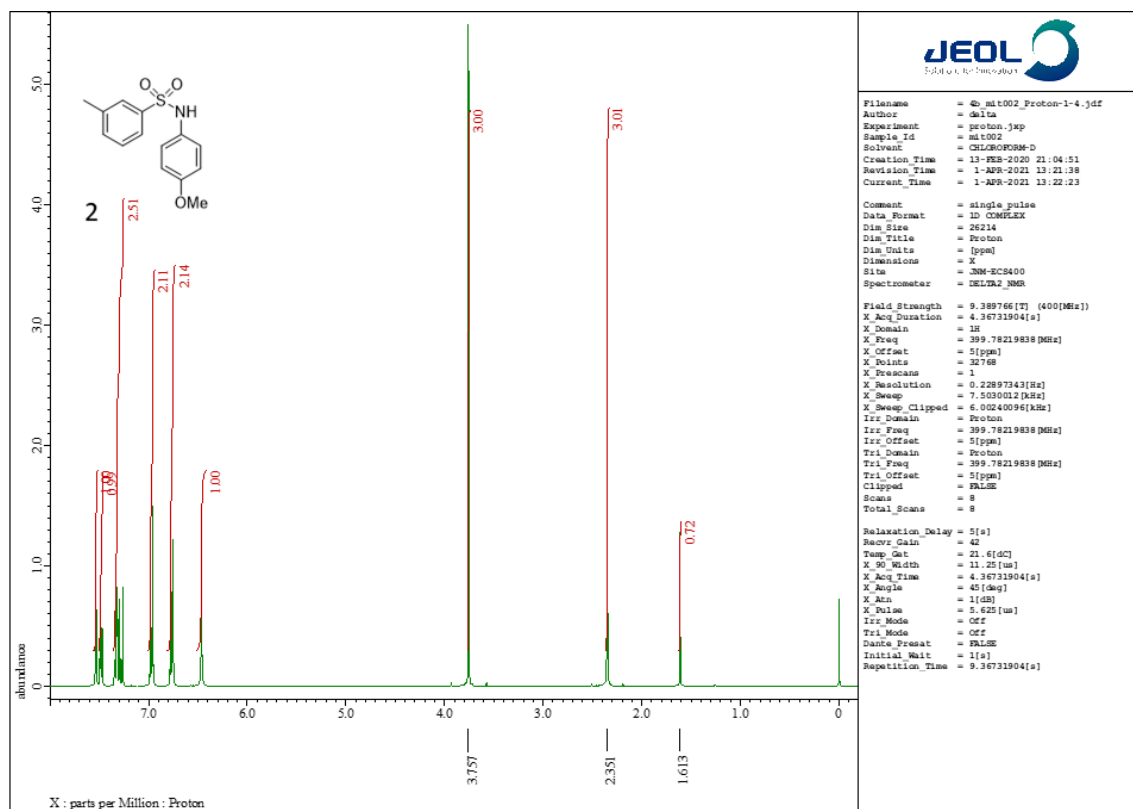


Fig S3 <sup>1</sup>H NMR Spectra of **2**

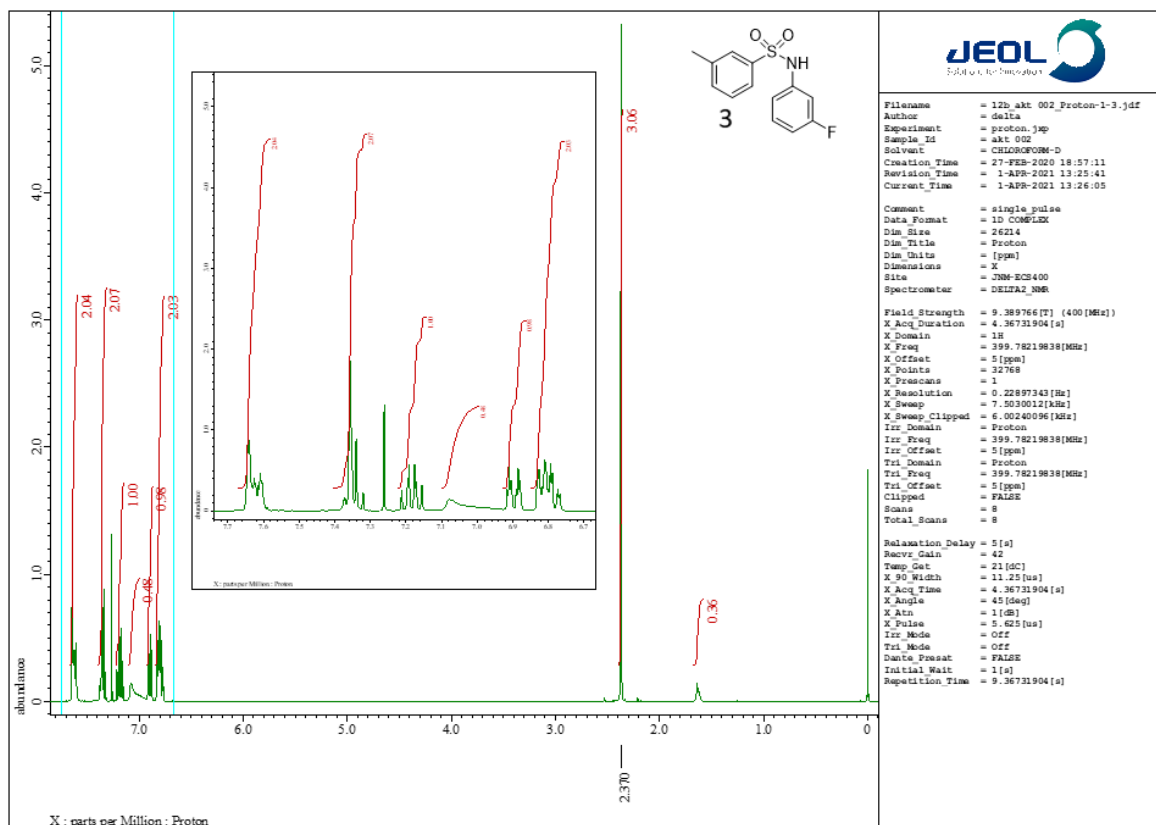


Fig S4 <sup>1</sup>H NMR Spectra of **3**

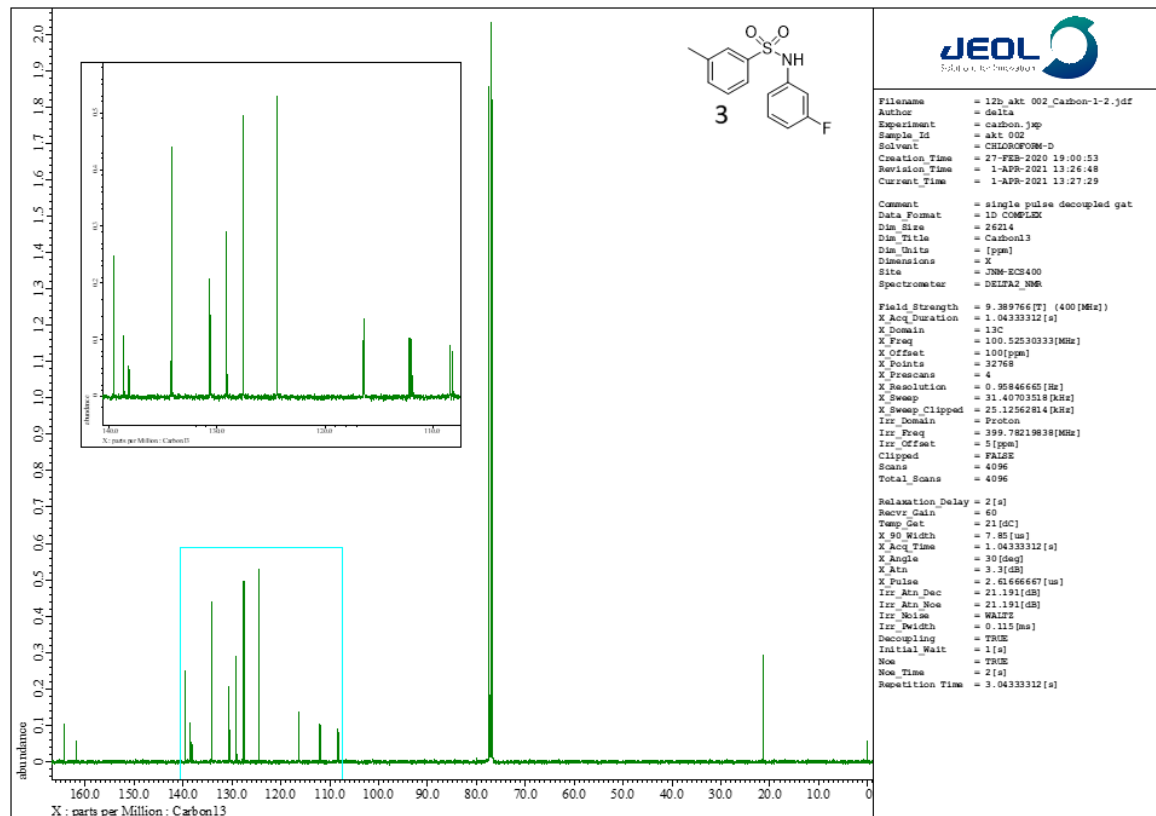


Fig S5 <sup>13</sup>C NMR Spectra of **3**

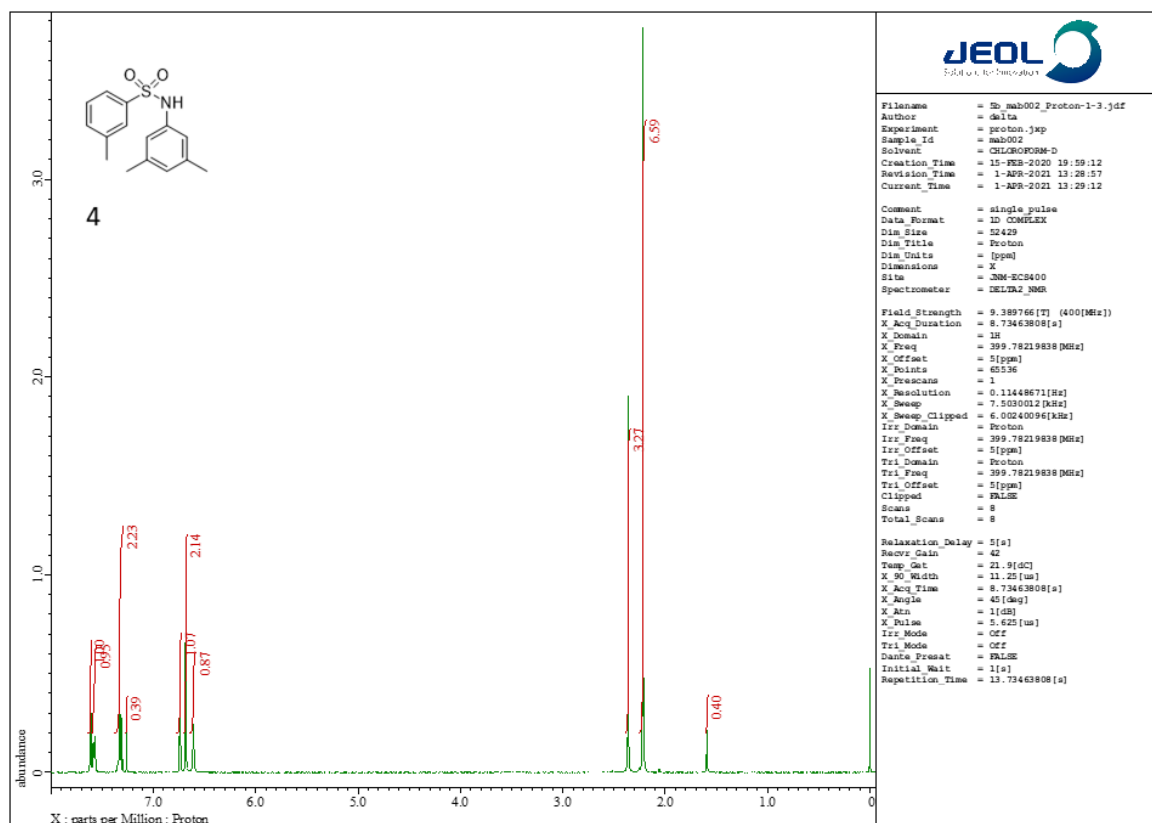


Fig S6 <sup>1</sup>H NMR Spectra of **4**

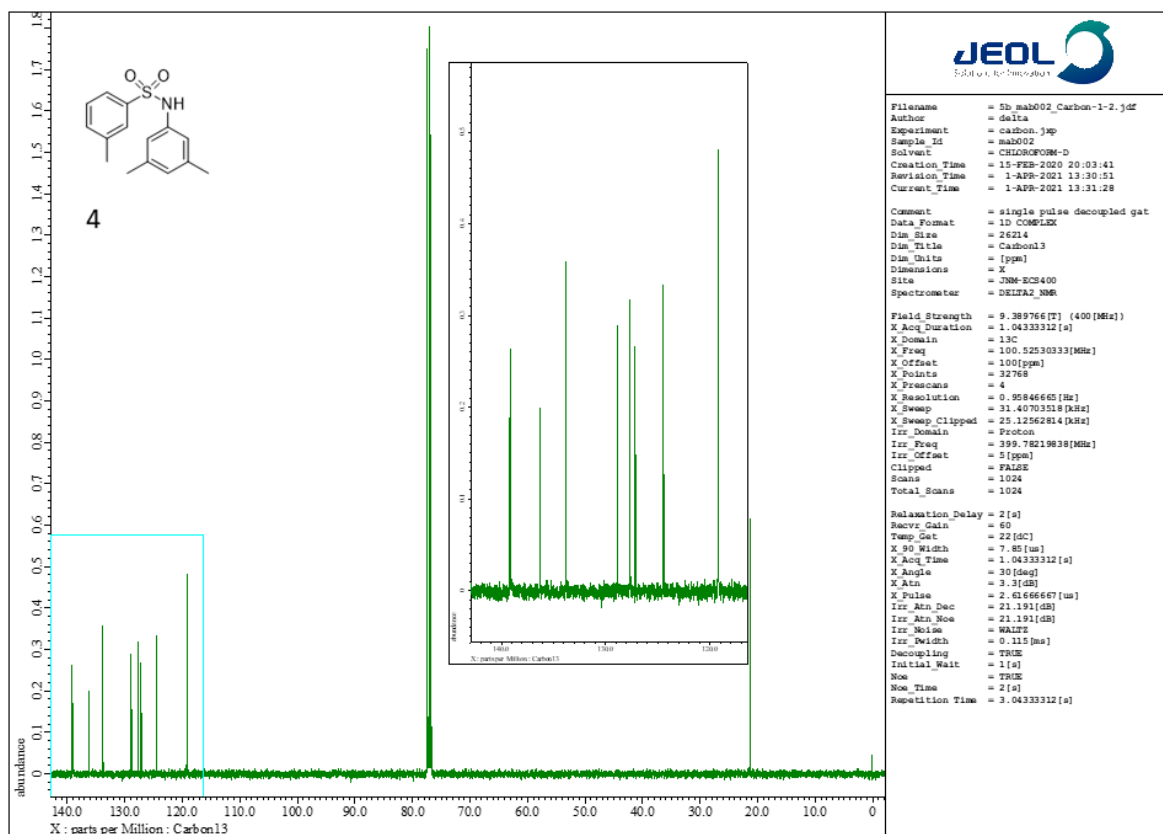


Fig S7 <sup>13</sup>C NMR Spectra of **4**

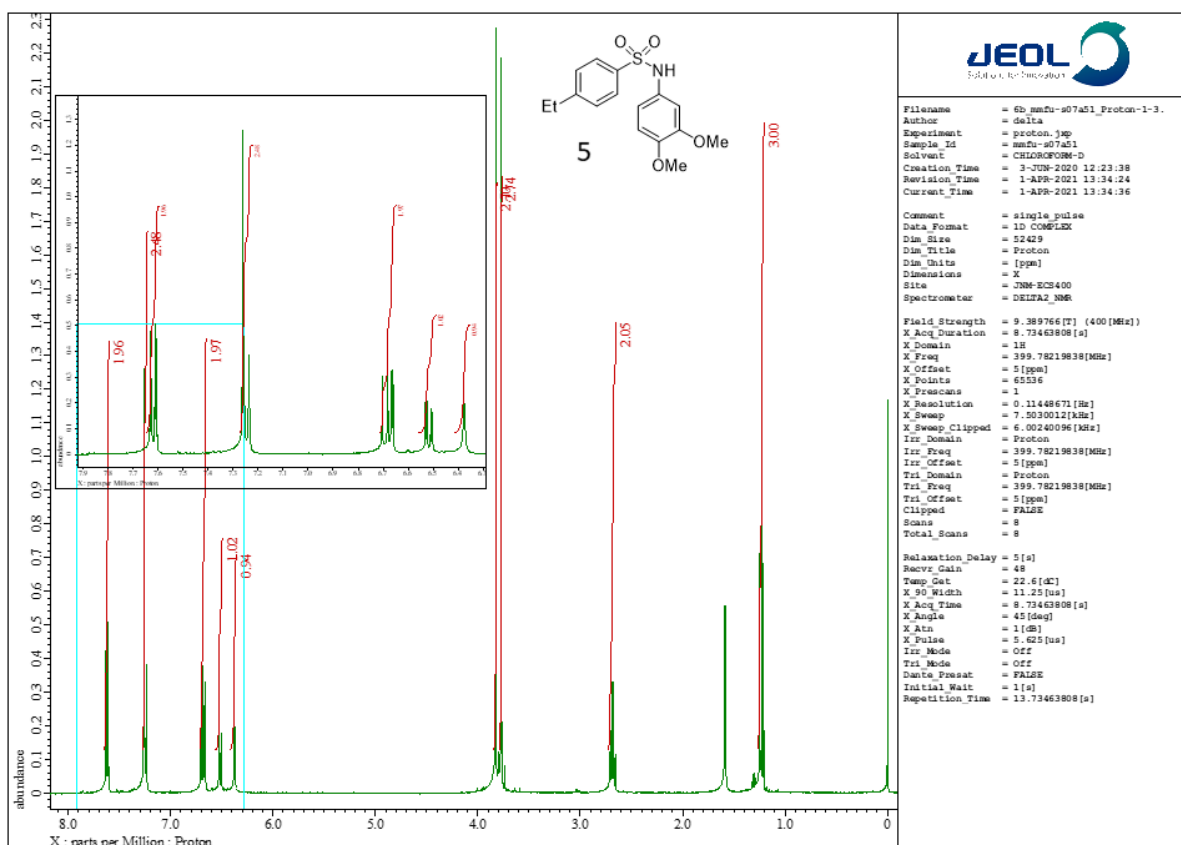


Fig S8 <sup>1</sup>H NMR Spectra of **5**

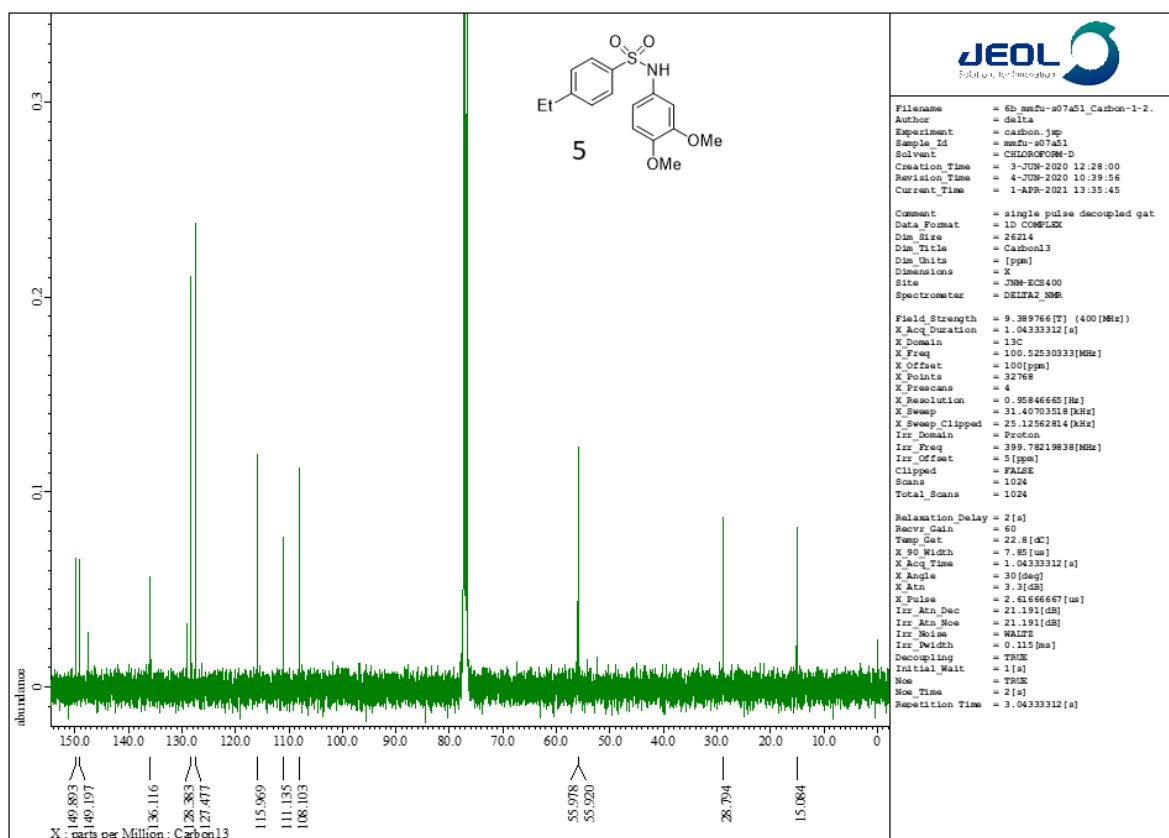


Fig S9 <sup>13</sup>C NMR Spectra of **5**



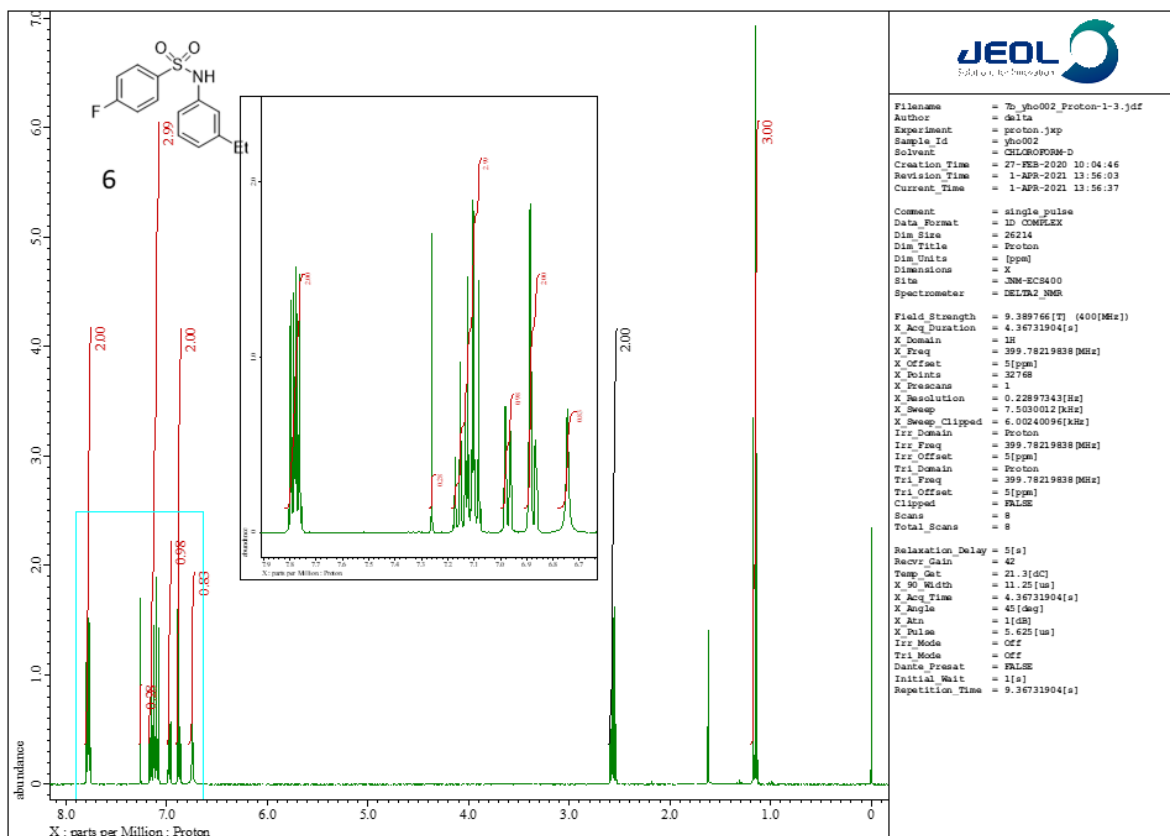


Fig S10 <sup>1</sup>H NMR Spectra of **6**

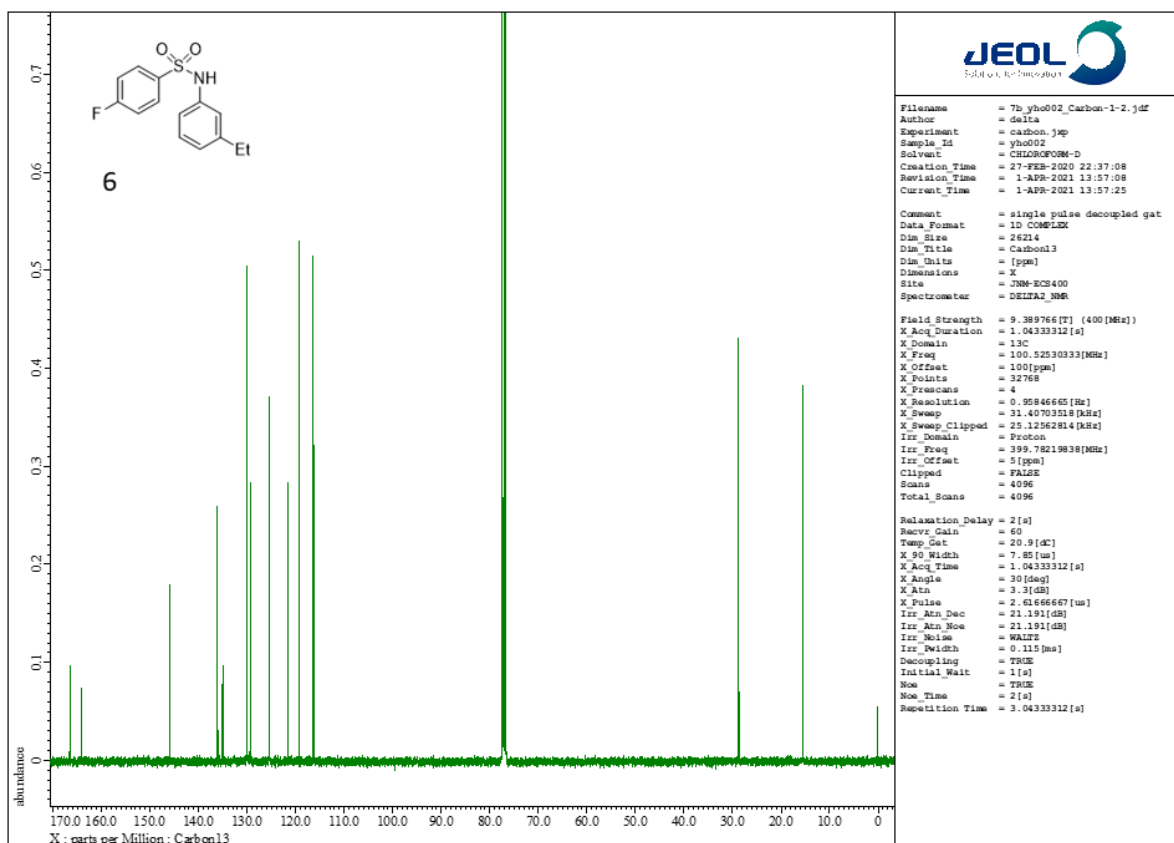
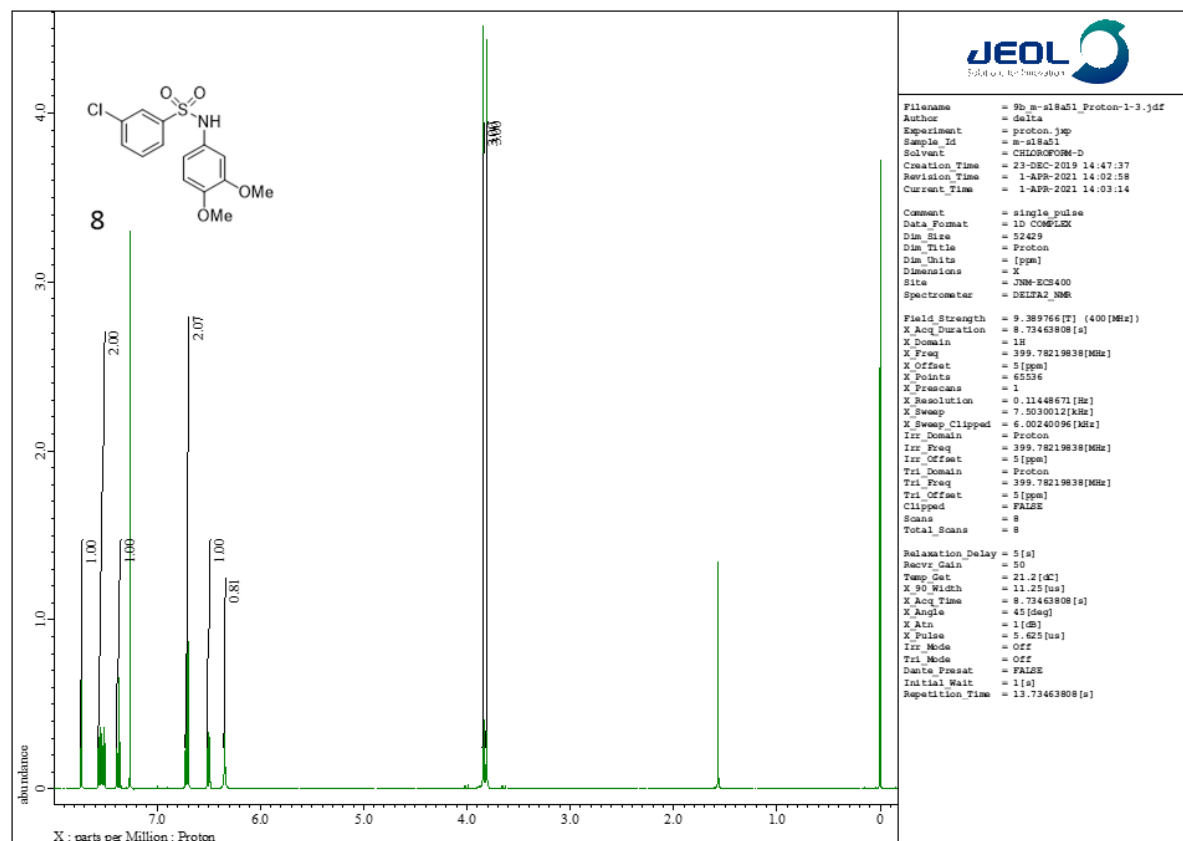
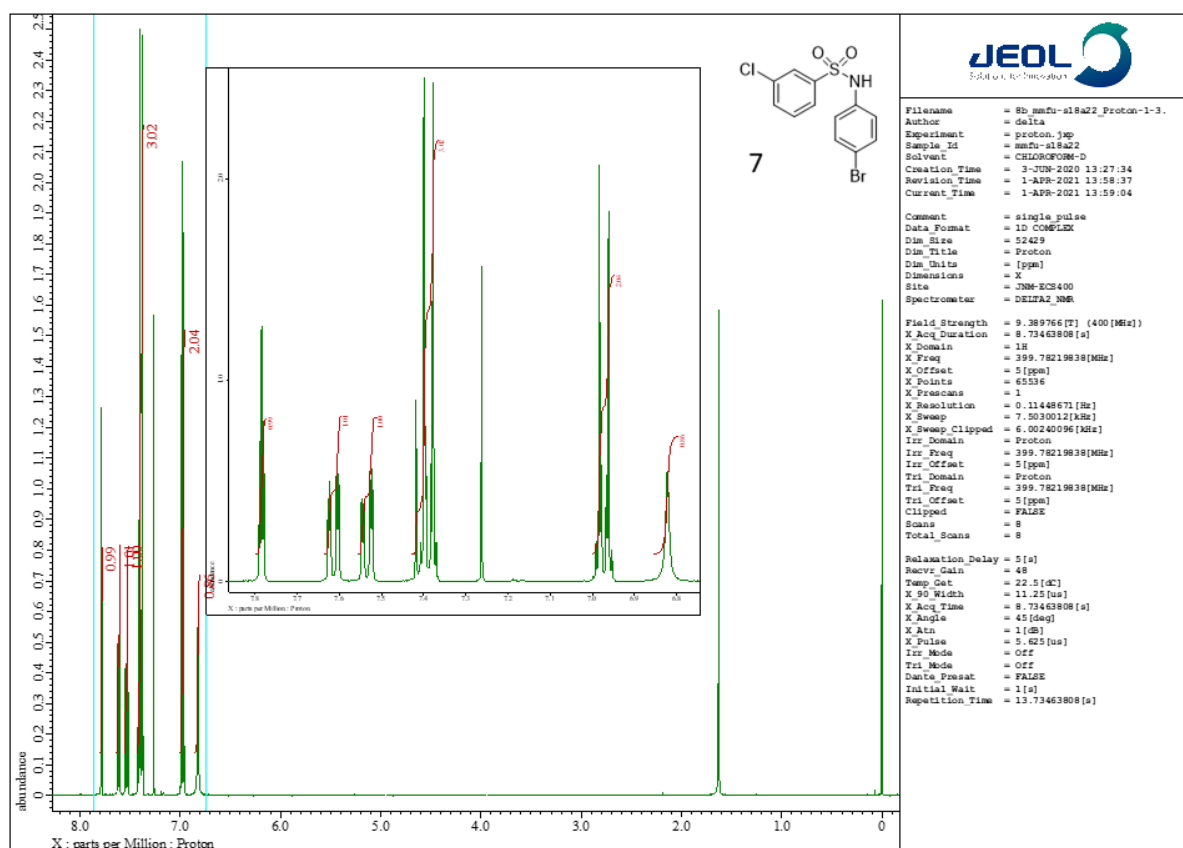


Fig S11 <sup>13</sup>C NMR Spectra of **6**



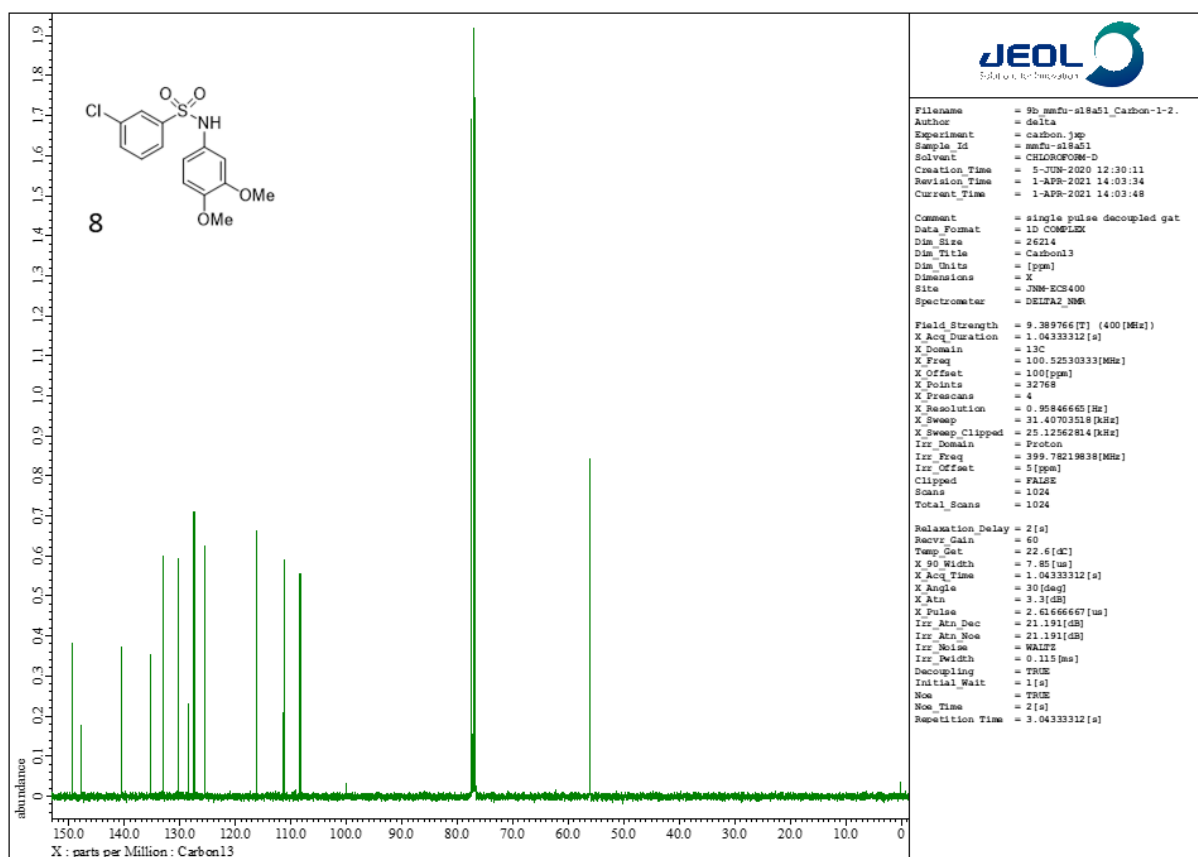


Fig S14 <sup>13</sup>C NMR Spectra of **8**

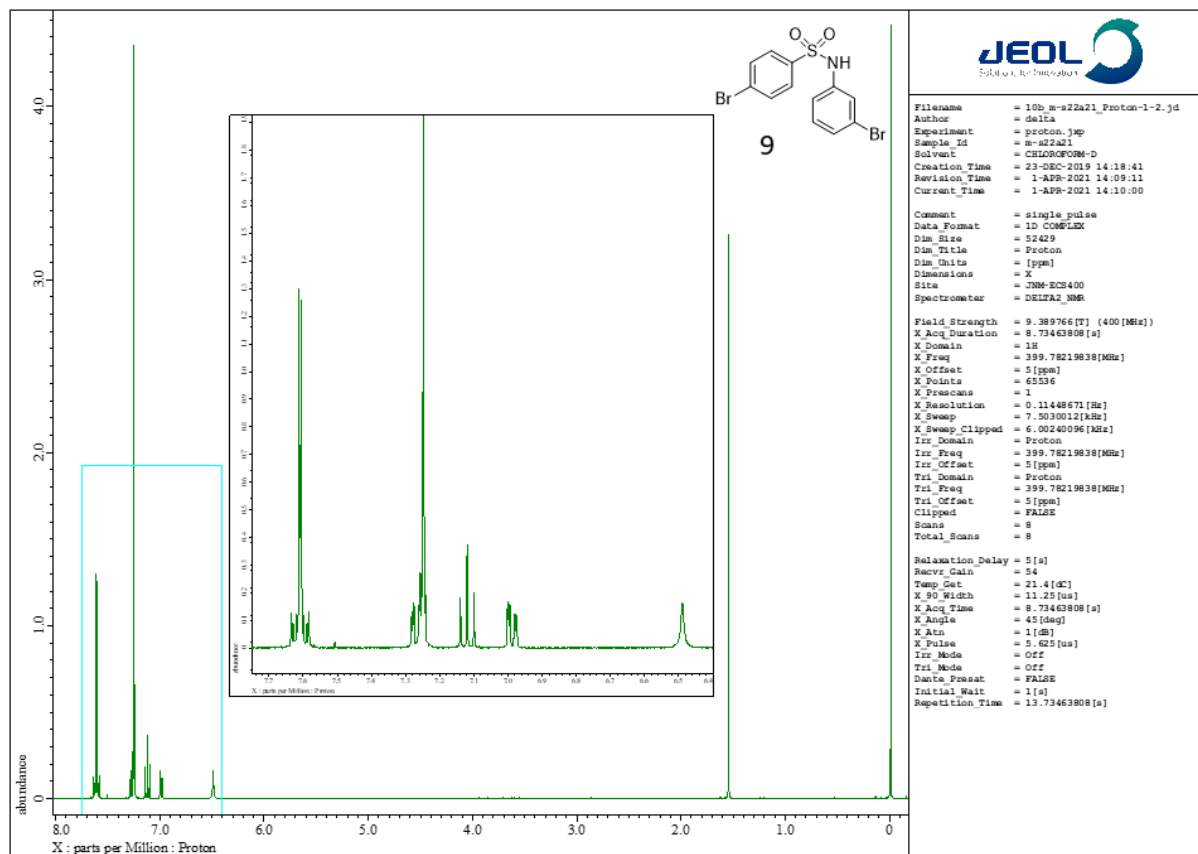


Fig S15 <sup>1</sup>H NMR Spectra of **9**

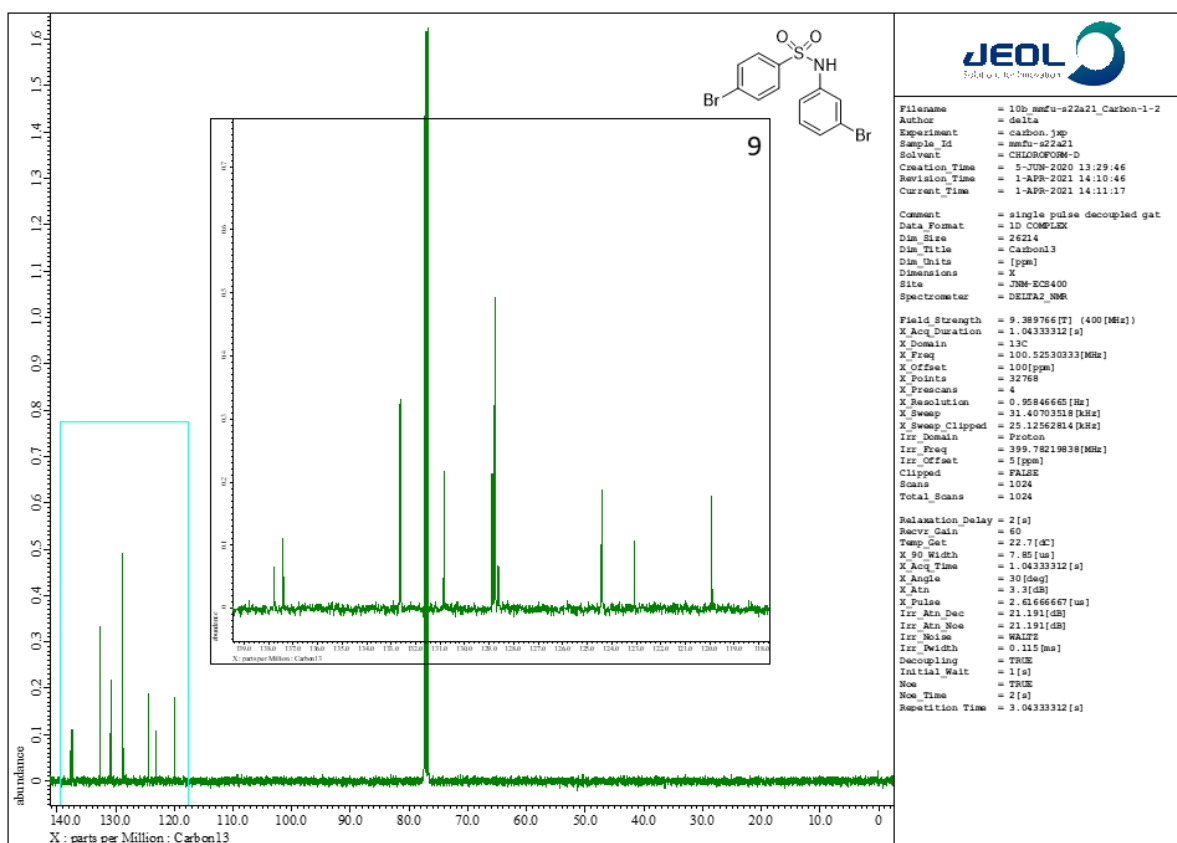


Fig S16 <sup>13</sup>C NMR Spectra of **9**

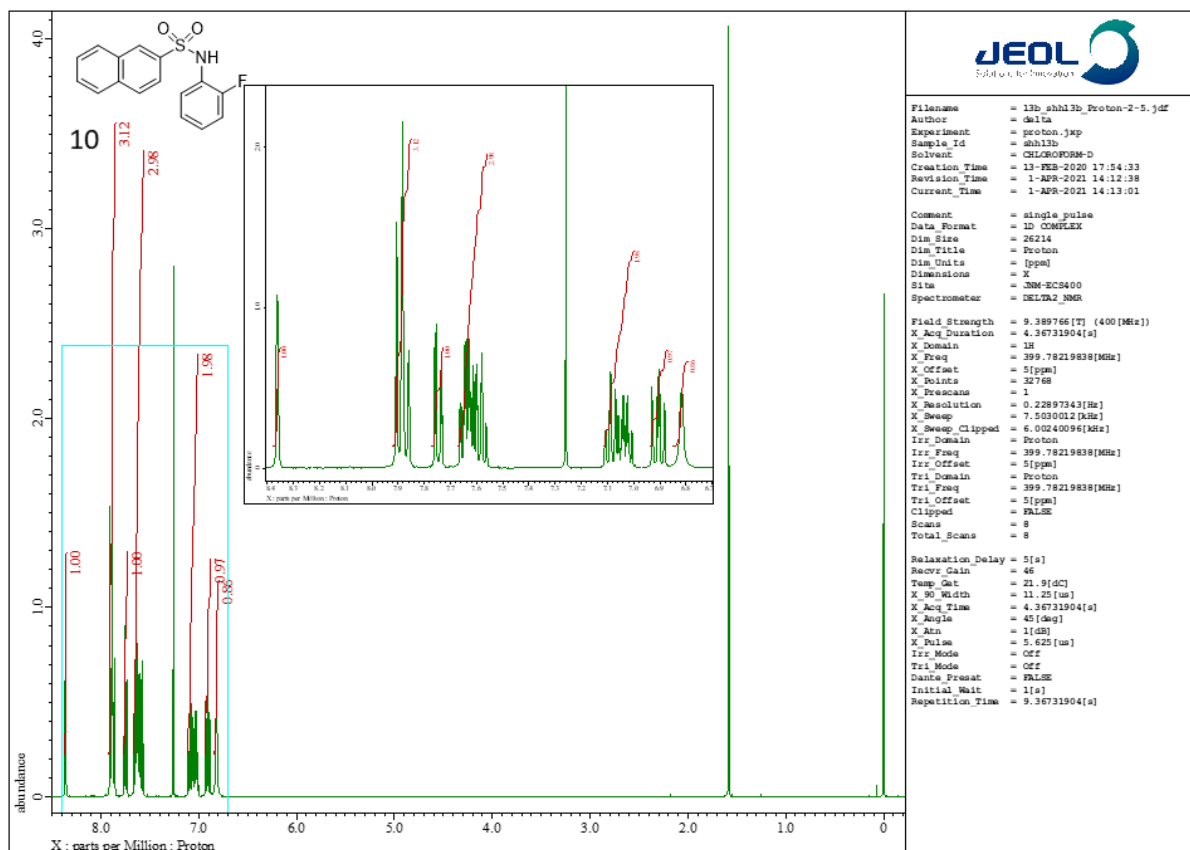


Fig S17 <sup>1</sup>H NMR Spectra of **10**

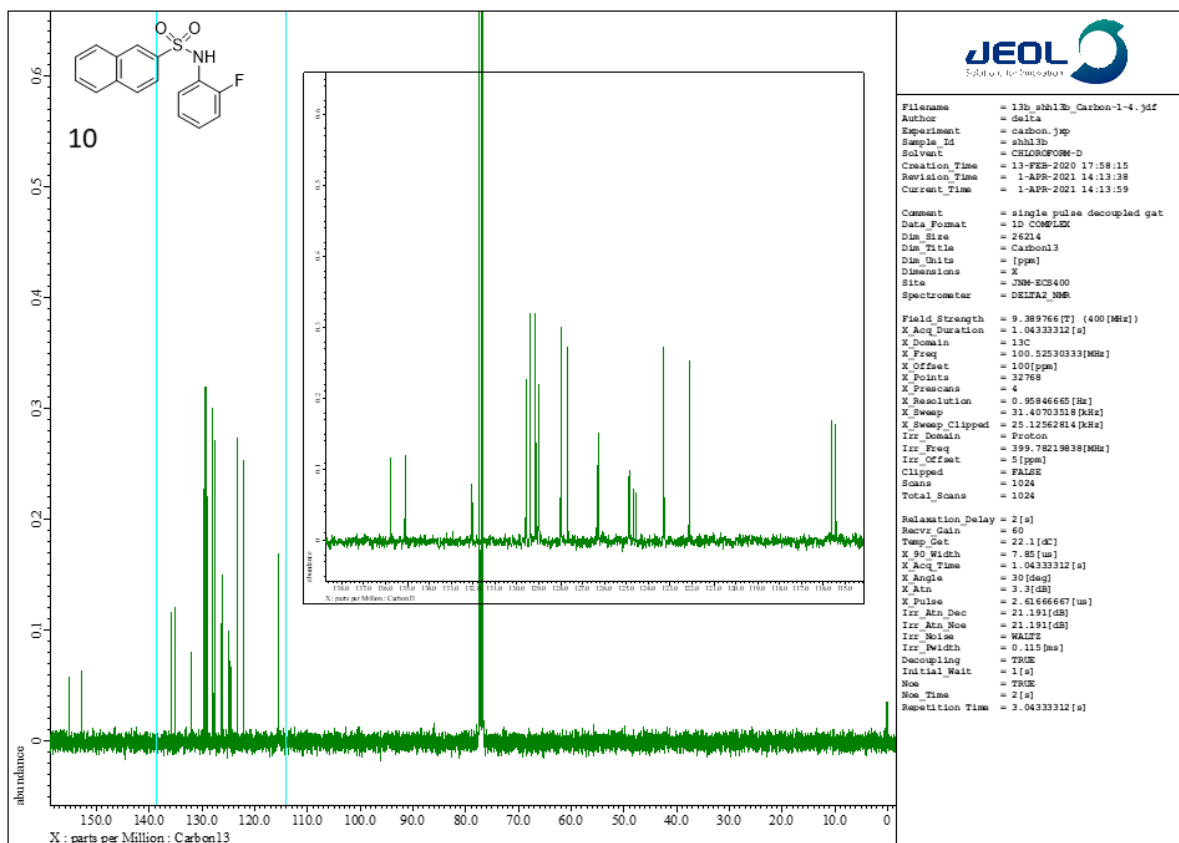


Fig S18 <sup>13</sup>C NMR Spectra of 10

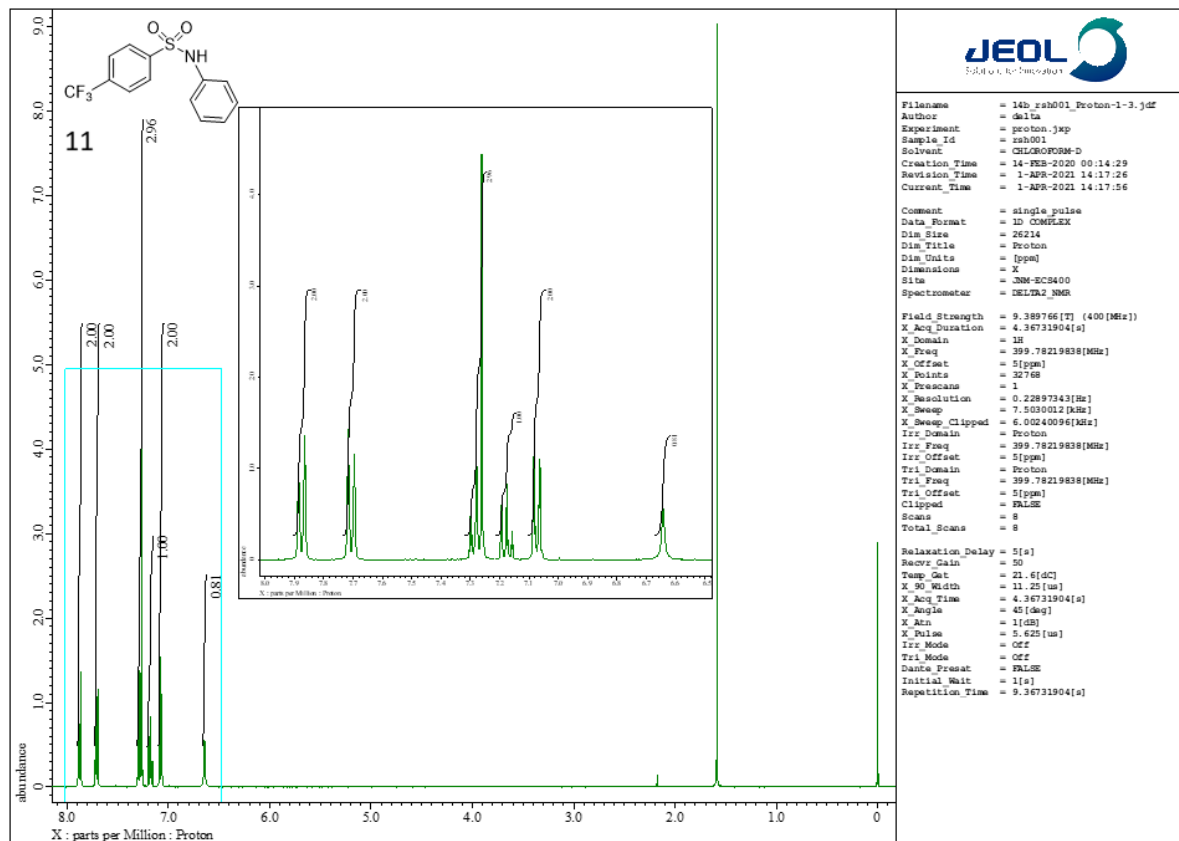


Fig S19 <sup>1</sup>H NMR Spectra of 11

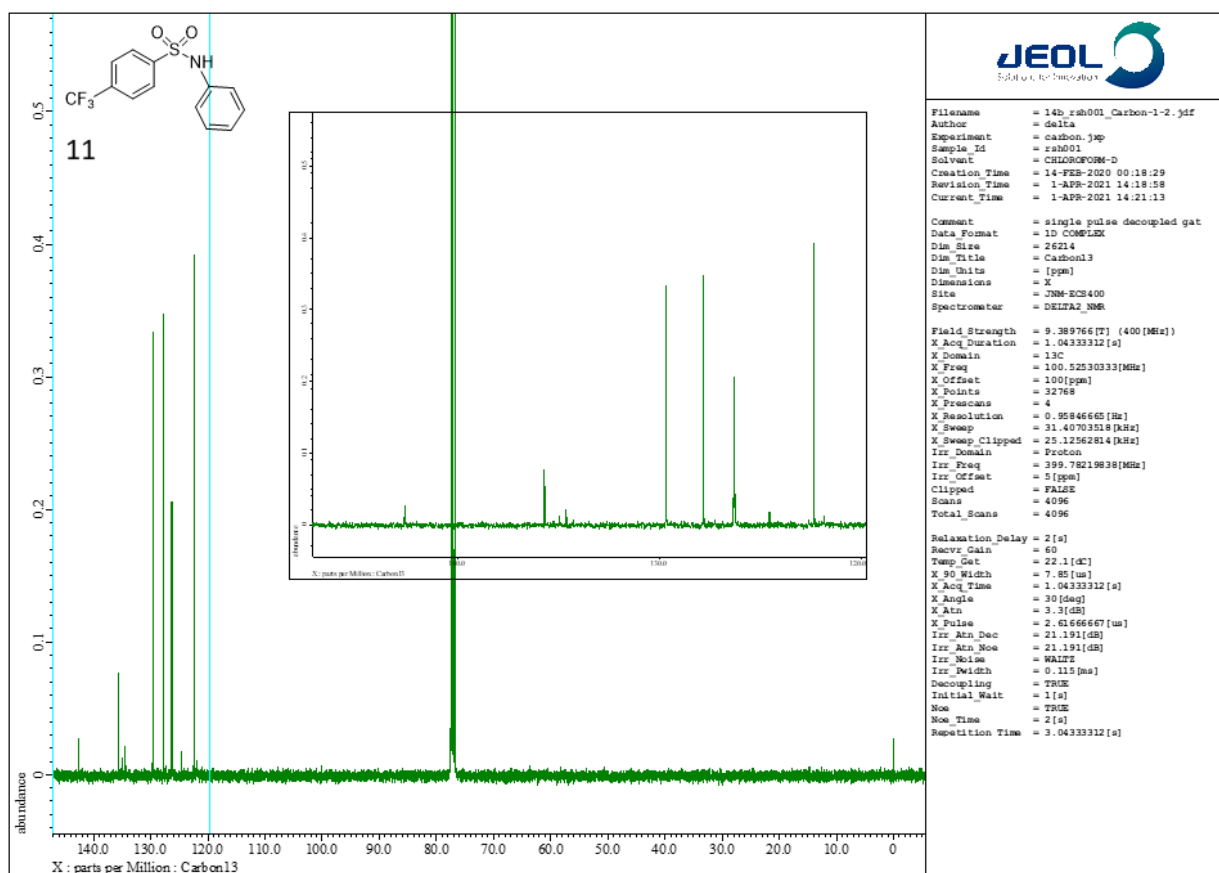


Fig S20 <sup>13</sup>C NMR Spectra of **11**

### 3. Crystal structures

**Table S1.** Crystallographic parameters for structures of the synthesized sulfonamides in this paper (**1–11**)

|                                                                              | 1                                                     | 2                                                     | 3                                                  | 4                                                 | 7                                                    | 8                                                   | 9                                                                | 10                                                 | 11                                                               |
|------------------------------------------------------------------------------|-------------------------------------------------------|-------------------------------------------------------|----------------------------------------------------|---------------------------------------------------|------------------------------------------------------|-----------------------------------------------------|------------------------------------------------------------------|----------------------------------------------------|------------------------------------------------------------------|
| Formula                                                                      | C <sub>18</sub> H <sub>15</sub> NO <sub>3</sub> S     | C <sub>14</sub> H <sub>15</sub> NO <sub>3</sub> S     | C <sub>13</sub> H <sub>12</sub> FNO <sub>2</sub> S | C <sub>15</sub> H <sub>17</sub> NO <sub>2</sub> S | C <sub>12</sub> H <sub>9</sub> BrClNO <sub>2</sub> S | C <sub>14</sub> H <sub>14</sub> ClNO <sub>4</sub> S | C <sub>12</sub> H <sub>9</sub> Br <sub>2</sub> NO <sub>2</sub> S | C <sub>16</sub> H <sub>12</sub> FNO <sub>2</sub> S | C <sub>13</sub> H <sub>10</sub> F <sub>3</sub> NO <sub>2</sub> S |
| Formula weight                                                               | 325.38                                                | 277.34                                                | 265.3                                              | 275.36                                            | 346.63                                               | 327.78                                              | 391.08                                                           | 301.33                                             | 301.28                                                           |
| Crystal system                                                               | orthorhombic                                          | orthorhombic                                          | monoclinic                                         | triclinic                                         | orthorhombic                                         | monoclinic                                          | orthorhombic                                                     | orthorhombic                                       | monoclinic                                                       |
| Space group                                                                  | <i>P</i> 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub> | <i>P</i> 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub> | <i>P</i> 2 <sub>1</sub> / <i>n</i>                 | <i>P</i> $\bar{1}$                                | <i>Pbca</i>                                          | <i>P</i> 2 <sub>1</sub> / <i>n</i>                  | <i>Pna</i> 2 <sub>1</sub>                                        | <i>Pbca</i>                                        | <i>Pna</i> 2 <sub>1</sub>                                        |
| <i>a</i> /Å                                                                  | 8.79899(6)                                            | 5.3169(5)                                             | 9.1750(5)                                          | 9.0097(5)                                         | 22.990(4)                                            | 8.4505(4)                                           | 9.9580(4)                                                        | 11.5492(5)                                         | 5.0813(4)                                                        |
| <i>b</i> /Å                                                                  | 12.17385(9)                                           | 8.3453(8)                                             | 5.9502(3)                                          | 12.3524(7)                                        | 15.918(3)                                            | 13.5240(6)                                          | 21.7896(10)                                                      | 7.5883(4)                                          | 20.4639(13)                                                      |
| <i>c</i> /Å                                                                  | 15.22942(12)                                          | 29.723(3)                                             | 22.5000(13)                                        | 12.9152(7)                                        | 7.3032(15)                                           | 13.0184(6)                                          | 6.0999(3)                                                        | 31.0045(14)                                        | 12.2504(9)                                                       |
| $\alpha$ /°                                                                  | 90                                                    | 90                                                    | 90                                                 | 82.341(5)                                         | 90                                                   | 90                                                  | 90                                                               | 90                                                 | 90                                                               |
| $\beta$ /°                                                                   | 90                                                    | 90                                                    | 95.764(5)                                          | 84.612(5)                                         | 90                                                   | 100.599(5)                                          | 90                                                               | 90                                                 | 90.757(6)                                                        |
| $\gamma$ /°                                                                  | 90                                                    | 90                                                    | 90                                                 | 84.720(5)                                         | 90                                                   | 90                                                  | 90                                                               | 90                                                 | 90                                                               |
| <i>V</i> /Å <sup>3</sup>                                                     | 1631.34(2)                                            | 1318.8(2)                                             | 1222.13(12)                                        | 1413.62(14)                                       | 2672.7(9)                                            | 1462.42(12)                                         | 1323.56(10)                                                      | 2717.2(2)                                          | 1273.72(16)                                                      |
| <i>Z</i>                                                                     | 4                                                     | 4                                                     | 4                                                  | 4                                                 | 8                                                    | 4                                                   | 4                                                                | 8                                                  | 4                                                                |
| <i>T</i> /K                                                                  | 93                                                    | 93                                                    | 93                                                 | 93                                                | 120                                                  | 93                                                  | 93                                                               | 93                                                 | 93                                                               |
| $\mu$ /mm <sup>-1</sup>                                                      | 1.884                                                 | 0.248                                                 | 0.27                                               | 0.226                                             | 3.432                                                | 0.418                                               | 6.292                                                            | 0.253                                              | 0.291                                                            |
| <sup>a</sup> GOF on <i>F</i> <sup>2</sup>                                    | 1.089                                                 | 1.012                                                 | 1.073                                              | 1.016                                             | 1.063                                                | 1.036                                               | 1.086                                                            | 1.029                                              | 1.092                                                            |
| Reflections collected (all <i>c</i> 20883                                    |                                                       | 10788                                                 | 18973                                              | 45577                                             | 21467                                                | 23555                                               | 10151                                                            | 21952                                              | 20381                                                            |
| Independent reflections <i>I</i> > 2969                                      |                                                       | 2849                                                  | 2185                                               | 3711                                              | 1883                                                 | 2589                                                | 2590                                                             | 2425                                               | 2450                                                             |
| Restraints/parameters                                                        | 0/268                                                 | 0/232                                                 | 0/173                                              | 0/351                                             | 0/199                                                | 0/194                                               | 1/167                                                            | 0/194                                              | 0/185                                                            |
| <i>R</i> <sub>int</sub>                                                      | 0.0466                                                | 0.0174                                                | 0.1129                                             | 0.1726                                            | 0.1150                                               | 0.0775                                              | 0.0451                                                           | 0.0668                                             | 0.1046                                                           |
| <sup>b</sup> <i>R</i> <sub>1</sub> [on <i>F</i> , <i>I</i> > 2σ( <i>I</i> )] | 0.0292                                                | 0.0241                                                | 0.0510                                             | 0.0774                                            | 0.0410                                               | 0.0418                                              | 0.0259                                                           | 0.0385                                             | 0.0676                                                           |
| <sup>c</sup> <i>wR</i> <sub>2</sub> (on <i>F</i> <sup>2</sup> , all data)    | 0.0745                                                | 0.063                                                 | 0.1440                                             | 0.2176                                            | 0.0764                                               | 0.0969                                              | 0.0541                                                           | 0.0907                                             | 0.1812                                                           |
| Flack parameter                                                              | 0.003(6)                                              | 0.012(18)                                             | -                                                  | -                                                 | -                                                    | -                                                   | -                                                                | -                                                  | -                                                                |
| <i>T</i> <sub>min</sub>                                                      | 0.709                                                 | 0.910                                                 | 0.094                                              | 0.553                                             | 1.000                                                | 0.396                                               | 0.409                                                            | 0.749                                              | 0.290                                                            |
| <i>T</i> <sub>max</sub>                                                      | 0.844                                                 | 0.993                                                 | 0.989                                              | 0.998                                             | 1.000                                                | 0.988                                               | 0.686                                                            | 0.995                                              | 0.957                                                            |
| Largest diff. peak/hole/eÅ                                                   | 0.24/-0.48                                            | 0.23/-0.30                                            | 0.56/-0.53                                         | 0.68/-0.69                                        | 0.83/-0.68                                           | 0.60/-0.45                                          | 0.41/-0.35                                                       | 0.40/-0.42                                         | 0.83/-0.47                                                       |

<sup>a</sup>GOF = [Σw(*F*<sub>o</sub><sup>2</sup> - *F*<sub>c</sub><sup>2</sup>)/(*N*<sub>o</sub> - *N*<sub>v</sub>)]<sup>1/2</sup> (*N*<sub>o</sub>; number of observations, *N*<sub>v</sub>; number of variables), <sup>b</sup>*R*<sub>1</sub> = Σ ||*F*<sub>o</sub>| - |*F*<sub>c</sub>|| / Σ |*F*<sub>o</sub>|, <sup>c</sup>*wR*<sub>2</sub> = [Σ(w(*F*<sub>o</sub><sup>2</sup> - *F*<sub>c</sub><sup>2</sup>)/Σw(*F*<sub>o</sub><sup>2</sup>))]<sup>1/2</sup>.

**Table S2.** Crystallographic parameters for structures of the co-crystals (**1c–11c**)

|                                                                              | <b>1c</b>                                                                    | <b>2c</b>                                                       | <b>3c</b>                                                        | <b>4c</b>                                                          | <b>5c</b>                                                                       | <b>6c</b>                                                        | <b>7c</b>                                                           | <b>8c</b>                                                                       | <b>9c</b>                                                                       | <b>10c</b>                                                                      | <b>11c</b>                                                                     |
|------------------------------------------------------------------------------|------------------------------------------------------------------------------|-----------------------------------------------------------------|------------------------------------------------------------------|--------------------------------------------------------------------|---------------------------------------------------------------------------------|------------------------------------------------------------------|---------------------------------------------------------------------|---------------------------------------------------------------------------------|---------------------------------------------------------------------------------|---------------------------------------------------------------------------------|--------------------------------------------------------------------------------|
| Formula                                                                      | C <sub>56</sub> H <sub>46</sub> N <sub>6</sub> O <sub>6</sub> S <sub>2</sub> | C <sub>24</sub> H <sub>23</sub> N <sub>3</sub> O <sub>3</sub> S | C <sub>23</sub> H <sub>20</sub> FN <sub>3</sub> O <sub>2</sub> S | C <sub>25</sub> H <sub>24.82</sub> N <sub>3</sub> O <sub>2</sub> S | C <sub>20</sub> H <sub>19</sub> Cl <sub>3</sub> N <sub>2</sub> O <sub>4</sub> S | C <sub>24</sub> H <sub>22</sub> FN <sub>3</sub> O <sub>2</sub> S | C <sub>17</sub> H <sub>13</sub> BrClN <sub>2</sub> O <sub>2</sub> S | C <sub>20</sub> H <sub>19</sub> Cl <sub>4</sub> N <sub>2</sub> O <sub>4</sub> S | C <sub>22</sub> H <sub>17</sub> Br <sub>2</sub> N <sub>3</sub> O <sub>2</sub> S | C <sub>88</sub> H <sub>68</sub> F <sub>3</sub> N <sub>11</sub> O <sub>6</sub> S | C <sub>23</sub> H <sub>18</sub> F <sub>3</sub> N <sub>3</sub> O <sub>2</sub> S |
| Formula weight                                                               | 963.14                                                                       | 433.52                                                          | 421.49                                                           | 431.37                                                             | 489.8                                                                           | 435.52                                                           | 424.72                                                              | 525.25                                                                          | 547.26                                                                          | 1528.75                                                                         | 457.46                                                                         |
| Crystal system                                                               | monoclinic                                                                   | monoclinic                                                      | monoclinic                                                       | monoclinic                                                         | triclinic                                                                       | triclinic                                                        | triclinic                                                           | triclinic                                                                       | triclinic                                                                       | monoclinic                                                                      | triclinic                                                                      |
| Space group                                                                  | <i>P</i> 2 <sub>1</sub> / <i>n</i>                                           | <i>C</i> 2/ <i>c</i>                                            | <i>P</i> 2 <sub>1</sub> / <i>c</i>                               | <i>P</i> 2 <sub>1</sub> / <i>c</i>                                 | <i>P</i> $\bar{1}$                                                              | <i>P</i> $\bar{1}$                                               | <i>P</i> $\bar{1}$                                                  | <i>P</i> $\bar{1}$                                                              | <i>P</i> $\bar{1}$                                                              | <i>P</i> 2 <sub>1</sub> / <i>c</i>                                              | <i>P</i> $\bar{1}$                                                             |
| <i>a</i> /Å                                                                  | 14.8313(5)                                                                   | 31.8179(11)                                                     | 10.2247(6)                                                       | 12.6908(4)                                                         | 8.56656(14)                                                                     | 10.0096(3)                                                       | 8.4205(5)                                                           | 8.56656(14)                                                                     | 9.9673(2)                                                                       | 15.7030(5)                                                                      | 8.24874(18)                                                                    |
| <i>b</i> /Å                                                                  | 16.0368(7)                                                                   | 8.1924(3)                                                       | 13.3486(6)                                                       | 11.0757(3)                                                         | 11.31930(19)                                                                    | 12.4631(6)                                                       | 9.8122(5)                                                           | 11.31930(19)                                                                    | 15.2825(5)                                                                      | 30.2596(8)                                                                      | 9.01497(18)                                                                    |
| <i>c</i> /Å                                                                  | 20.2334(7)                                                                   | 17.8610(6)                                                      | 15.0139(13)                                                      | 15.7411(5)                                                         | 12.12655(19)                                                                    | 17.7972(7)                                                       | 11.2928(6)                                                          | 12.12655(19)                                                                    | 15.6422(4)                                                                      | 17.0294(6)                                                                      | 29.4840(6)                                                                     |
| <i>α</i> /°                                                                  | 90                                                                           | 90                                                              | 90                                                               | 90                                                                 | 85.3760(13)                                                                     | 80.489(4)                                                        | 93.998(4)                                                           | 85.3760(13)                                                                     | 76.2980(2)                                                                      | 90                                                                              | 82.9508(16)                                                                    |
| <i>β</i> /°                                                                  | 91.974(3)                                                                    | 103.002(3)                                                      | 98.168(7)                                                        | 91.683(3)                                                          | 87.7729(13)                                                                     | 73.938(3)                                                        | 101.829(5)                                                          | 87.7729(13)                                                                     | 79.7290(19)                                                                     | 111.871(4)                                                                      | 83.6918(18)                                                                    |
| <i>γ</i> /°                                                                  | 90                                                                           | 90                                                              | 90                                                               | 90                                                                 | 80.6487(14)                                                                     | 87.660(3)                                                        | 108.500(5)                                                          | 80.6487(14)                                                                     | 71.5990(2)                                                                      | 90                                                                              | 76.4332(18)                                                                    |
| <i>V</i> /Å <sup>3</sup>                                                     | 4809.6(3)                                                                    | 4536.4(3)                                                       | 2028.4(2)                                                        | 2211.61(12)                                                        | 1156.08(3)                                                                      | 2104.19(15)                                                      | 856.87(9)                                                           | 1156.08(3)                                                                      | 2182.6371(10)                                                                   | 7509.4(5)                                                                       | 2107.72(8)                                                                     |
| <i>Z</i>                                                                     | 4                                                                            | 8                                                               | 4                                                                | 4                                                                  | 2                                                                               | 4                                                                | 2                                                                   | 2                                                                               | 4                                                                               | 4                                                                               | 4                                                                              |
| <i>T</i> /K                                                                  | 93                                                                           | 93                                                              | 93                                                               | 93                                                                 | 93                                                                              | 93                                                               | 93                                                                  | 93                                                                              | 93                                                                              | 93                                                                              | 93                                                                             |
| <i>μ</i> /mm <sup>-1</sup>                                                   | 0.17                                                                         | 0.172                                                           | 0.194                                                            | 0.173                                                              | 0.514                                                                           | 0.189                                                            | 2.695                                                               | 0.631                                                                           | 3.845                                                                           | 0.171                                                                           | 0.206                                                                          |
| <sup>a</sup> GOF on <i>F</i> <sup>2</sup>                                    | 1.022                                                                        | 1.058                                                           | 1.030                                                            | 1.071                                                              | 1.046                                                                           | 1.052                                                            | 1.067                                                               | 1.046                                                                           | 1.118                                                                           | 1.065                                                                           | 1.104                                                                          |
| Reflections collected (all data)                                             | 77886                                                                        | 33592                                                           | 31848                                                            | 34413                                                              | 37159                                                                           | 67401                                                            | 27568                                                               | 37159                                                                           | 70946                                                                           | 113014                                                                          | 70682                                                                          |
| Independent reflections <i>I</i> > 2σ( <i>I</i> )                            | 7152                                                                         | 4641                                                            | 2687                                                             | 4400                                                               | 4709                                                                            | 7272                                                             | 3221                                                                | 4709                                                                            | 7616                                                                            | 11645                                                                           | 7960                                                                           |
| Restraints/parameters                                                        | 0/639                                                                        | 0/284                                                           | 0/275                                                            | 6/314                                                              | 0/288                                                                           | 0/563                                                            | 0/221                                                               | 0/288                                                                           | 0/549                                                                           | 1/1212                                                                          | 18/611                                                                         |
| <i>R</i> <sub>int</sub>                                                      | 0.1335                                                                       | 0.0684                                                          | 0.0928                                                           | 0.0465                                                             | 0.0432                                                                          | 0.1223                                                           | 0.0715                                                              | 0.0432                                                                          | 0.0732                                                                          | 0.0763                                                                          | 0.0554                                                                         |
| <sup>b</sup> <i>R</i> <sub>1</sub> [on <i>F</i> , <i>I</i> > 2σ( <i>I</i> )] | 0.057                                                                        | 0.0421                                                          | 0.0632                                                           | 0.0665                                                             | 0.037                                                                           | 0.0951                                                           | 0.0330                                                              | 0.037                                                                           | 0.0538                                                                          | 0.0538                                                                          | 0.0484                                                                         |
| <sup>c</sup> <i>wR</i> <sub>2</sub> (on <i>F</i> <sup>2</sup> , all data)    | 0.1376                                                                       | 0.1135                                                          | 0.162                                                            | 0.1841                                                             | 0.1000                                                                          | 0.2847                                                           | 0.0715                                                              | 0.1                                                                             | 0.1609                                                                          | 0.1367                                                                          | 0.1257                                                                         |
| Flack parameter                                                              | -                                                                            | -                                                               | -                                                                | -                                                                  | -                                                                               | -                                                                | -                                                                   | -                                                                               | -                                                                               | -                                                                               | -                                                                              |
| <i>T</i> <sub>min</sub>                                                      | 0.780                                                                        | 0.150                                                           | 0.267                                                            | 0.652                                                              | 0.720                                                                           | 0.804                                                            | 0.763                                                               | 0.749                                                                           | 0.765                                                                           | 0.762                                                                           | 0.85                                                                           |
| <i>T</i> <sub>max</sub>                                                      | 0.990                                                                        | 0.966                                                           | 0.992                                                            | 0.979                                                              | 0.993                                                                           | 0.991                                                            | 0.828                                                               | 0.910                                                                           | 0.877                                                                           | 0.980                                                                           | 0.986                                                                          |
| Largest diff. peak/hole/eÅ <sup>-3</sup>                                     | 0.35/-0.51                                                                   | 0.35/-0.60                                                      | 0.30/-0.41                                                       | 1.75/-0.41                                                         | 0.78/-0.68                                                                      | 1.75/-0.74                                                       | 0.48/-0.57                                                          | 0.78/-0.68                                                                      | 1.12/-0.76                                                                      | 0.59/-0.62                                                                      | 0.37/-0.43                                                                     |

<sup>a</sup>GOF = [Σw(*F*<sub>o</sub><sup>2</sup> - *F*<sub>c</sub><sup>2</sup>)/(*N*<sub>o</sub> - *N*<sub>v</sub>)]<sup>1/2</sup> (*N*<sub>o</sub>; number of observations, *N*<sub>v</sub>; number of variables), <sup>b</sup>*R*<sub>1</sub> = Σ ||*F*<sub>o</sub>|| - ||*F*<sub>c</sub>|| / Σ ||*F*<sub>o</sub>||, <sup>c</sup>*wR*<sub>2</sub> = [Σ(w(*F*<sub>o</sub><sup>2</sup> - *F*<sub>c</sub><sup>2</sup>)<sup>2</sup>)/Σw(*F*<sub>o</sub><sup>2</sup>)]<sup>1/2</sup>.



#### 4. The difference Fourier map

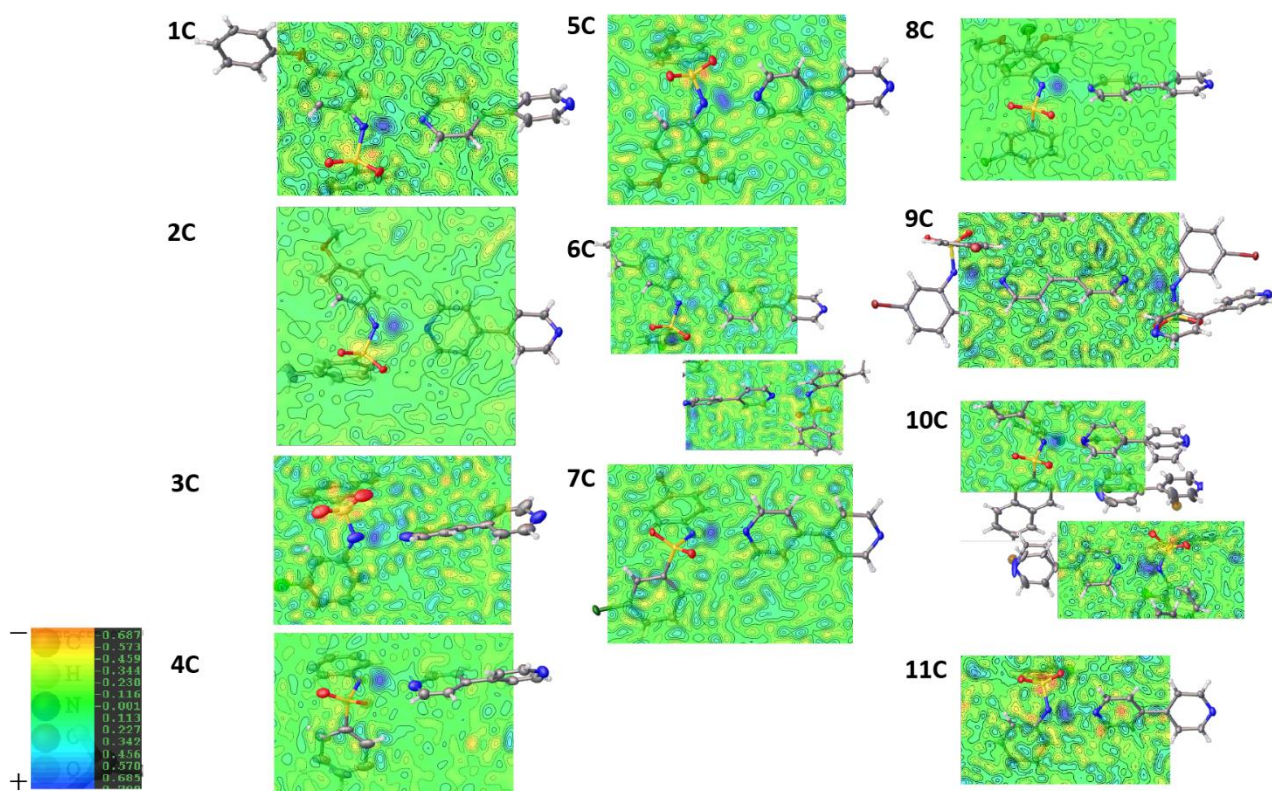


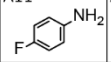
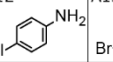
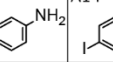
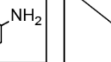
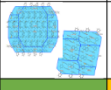
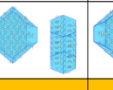
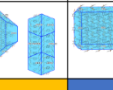
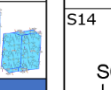
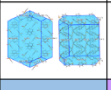
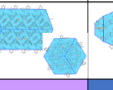
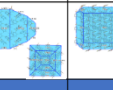
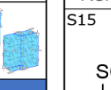
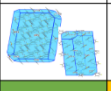
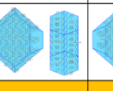
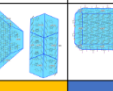
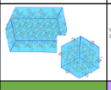
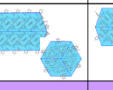
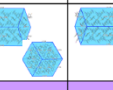
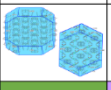
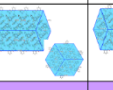
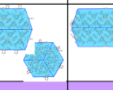
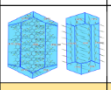
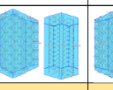
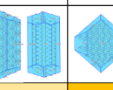
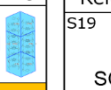
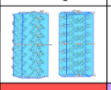
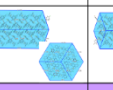
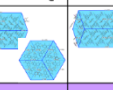
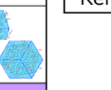
Fig S21 Difference Fourier map of the hydrogen-bonded section of the co-crystals of **1c-11c** calculated using Olex2. The blue area between the sulfonamide and **dpy** molecules indicates the location of the hydrogen.

## 5. The BFDH models of sulfonamides and co-crystals

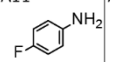
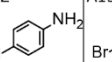
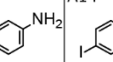
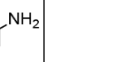
|                                                                                           | A1<br>                                                | A2<br>                                                | A3<br>                                                | A4<br>                                               | A5<br>                                                 | A6<br>                                                | A7<br>                                               | A8<br>                                                | A9<br>                                                | A10<br>                                              |
|-------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------|
| S1<br>   | <br>8.7353,<br>8.7353,<br>29.975<br>(1.00, 3.43)      | <br>6.4385,<br>8.5072,<br>21.7857<br>(1.32, 3.38)     | <br>12.7352,<br>6.0173,<br>16.6467<br>(2.12, 2.77)    | <br>10.7631,<br>9.5973,<br>23.7034<br>(1.12, 2.47)   | <br>7.8407,<br>23.289,<br>7.2981<br>(1.07, 3.19)       | <br>11.00206,<br>8.41173,<br>14.03426<br>(1.31, 1.67) | <br>13.2426,<br>5.21342,<br>18.0818<br>(2.54, 3.47) | <br>10.3968,<br>8.7575,<br>14.1708<br>(1.19, 1.62)    | <br>8.4455,<br>22.1496,<br>7.4601<br>(1.13, 2.97)     | <br>22.3076,<br>15.1093,<br>7.3966<br>(2.04, 3.02)   |
| Refcode                                                                                   | TEQYUK02                                                                                                                               | HODWIH0                                                                                                                                | DUNYER0                                                                                                                                | DUNYIV01                                                                                                                              | BOFYON                                                                                                                                  | BOFYAZ                                                                                                                                 | BOFYUT01                                                                                                                               | YUPXIR01                                                                                                                                 | BOGSEY                                                                                                                                   | IJUJUT01                                                                                                                                |
| S2<br>   | <br>8.8379,<br>9.1086,<br>15.1509<br>(1.03, 1.71)     | <br>7.8936,<br>8.0827,<br>10.3808<br>(1.02, 1.32)     | <br>12.624,<br>6.4513,<br>16.276<br>(1.96, 2.52)      | <br>14.462,<br>13.827,<br>14.69<br>(1.05, 1.06)      | <br>7.9198,<br>15.802,<br>21.921<br>(2.00, 2.77)       | <br>14.6985,<br>17.4783,<br>11.024<br>(1.33, 1.59)    | <br>8.5619,<br>11.2304,<br>29.1636<br>(1.31, 3.41)  | <br>15.3081,<br>10.6973,<br>17.51<br>(1.43, 1.64)     | <br>12.6212,<br>11.1179,<br>9.5157<br>(1.17, 1.33)    | <br>8.6918,<br>19.2661,<br>7.9012<br>(1.10, 2.44)    |
| Refcode                                                                                   | BOGPUL                                                                                                                                 | BOGPOF                                                                                                                                 | BOGTOJ                                                                                                                                 | BOGQOG                                                                                                                                | BOGQAS                                                                                                                                  | BOGHEN                                                                                                                                 | BOGQIA                                                                                                                                 | BOGZEF                                                                                                                                   | BOGTUP                                                                                                                                   | BOGQEW                                                                                                                                  |
| S3<br>   | <br>10.4536,<br>12.8332,<br>9.3394<br>(1.12, 1.37)    | <br>8.1205,<br>20.614,<br>8.1391<br>(1.00, 2.54)      | <br>9.4829,<br>8.6573,<br>16.0675<br>(1.10, 1.86)     | <br>11.0818,<br>10.0252,<br>23.8926<br>(1.11, 2.38)  | <br>8.1746,<br>14.682,<br>11.6322<br>(1.42, 1.80)      | <br>8.393,<br>18.022,<br>10.03<br>(1.20, 2.15)        | <br>5.70611,<br>9.3187,<br>26.0563<br>(1.63, 4.57)  | <br>8.1244,<br>14.8024,<br>11.3357<br>(1.40, 1.82)    | <br>10.256,<br>14.16,<br>10.402<br>(1.01, 1.38)       | <br>5.3169,<br>8.3453,<br>29.723<br>(1.57, 5.59)     |
| Refcode                                                                                   | BOGREX                                                                                                                                 | BOFZOO                                                                                                                                 | BOGZIJ                                                                                                                                 | AZESII01                                                                                                                              | BOGLOB                                                                                                                                  | BOGHIR                                                                                                                                 | BOGZUV                                                                                                                                 | BOGHOX                                                                                                                                   | BOGHUD                                                                                                                                   | BOGJAL                                                                                                                                  |
| S4<br> | <br>10.1966,<br>10.9351,<br>13.2419<br>(1.07, 1.30) | <br>14.9006,<br>14.6511,<br>12.1302<br>(1.21, 1.23) | <br>13.7158,<br>14.7802,<br>13.0443<br>(1.05, 1.13) | <br>5.3029,<br>16.1061,<br>15.8247<br>(2.98, 3.04) | <br>13.0055,<br>11.44088,<br>18.3234<br>(1.14, 1.60) | <br>8.624,<br>13.7692,<br>12.0635<br>(1.40, 1.60)   | <br>9.252,<br>8.123,<br>19.313<br>(1.14, 2.38)    | <br>12.5873,<br>11.4431,<br>18.369<br>(1.10, 1.61)  | <br>8.2872,<br>13.8768,<br>11.9042<br>(1.44, 1.67)  | <br>8.9928,<br>5.21818,<br>15.0036<br>(1.72, 2.88) |
| Refcode                                                                                   | FAXBUB07                                                                                                                               | AJIBAX01                                                                                                                               | RUJQUJ01                                                                                                                               | KUSVOK0                                                                                                                               | BOFYIH                                                                                                                                  | BOGJEP                                                                                                                                 | BOGJIT                                                                                                                                 | VACFOW0                                                                                                                                  | BOGSUO                                                                                                                                   | QAKPUP01                                                                                                                                |
| S5<br> | <br>8.774,<br>11.661,<br>13.504<br>(1.33, 1.54)     | <br>8.5797,<br>11.6725,<br>14.7785<br>(1.36, 1.72)  | <br>8.8443,<br>13.5478,<br>23.2774<br>(1.53, 2.63)  | <br>26.2413,<br>10.38,<br>20.6867<br>(1.99, 2.53)  | <br>7.75,<br>8.8131,<br>11.286<br>(1.14, 1.46)       | <br>8.3129,<br>8.6039,<br>11.599<br>(1.04, 1.40)    | <br>11.8793,<br>13.731,<br>9.2476<br>(1.28, 1.48) | <br>13.8784,<br>23.7917,<br>8.4589<br>(1.64, 2.81)  | <br>10.4234,<br>9.0202,<br>15.535<br>(1.16, 1.72)   | <br>19.924,<br>12.0627,<br>12.0327<br>(1.00, 1.66) |
| Refcode                                                                                   | BOGJUF                                                                                                                                 | BOFYED                                                                                                                                 | BOGRUN                                                                                                                                 | BOGKAM                                                                                                                                | BOGKEQ                                                                                                                                  | BOGKIU                                                                                                                                 | BOGKOA                                                                                                                                 | BOGLAN                                                                                                                                   | BOGROH                                                                                                                                   | BOGLER                                                                                                                                  |
| S6<br> | <br>9.5468,<br>7.0557,<br>18.1976<br>(1.35, 2.58)   | <br>14.532,<br>14.227,<br>12.68<br>(1.12, 1.15)     | <br>10.5927,<br>13.1257,<br>9.6636<br>(1.10, 1.36)  | <br>9.529,<br>6.8423,<br>20.9182<br>(1.39, 3.06)   | <br>10.2318,<br>12.7612,<br>10.9784<br>(1.07, 1.25)  | <br>8.0566,<br>8.5669,<br>11.4372<br>(1.06, 1.42)   | <br>11.8008,<br>14.9057,<br>8.41<br>(1.40, 1.77)  | <br>8.5516,<br>9.374,<br>10.3578<br>(1.10, 1.21)    | <br>8.57126,<br>16.1509,<br>10.0059<br>(1.17, 1.88) | <br>5.3301,<br>8.4345,<br>29.603<br>(1.58, 5.55)   |
| Refcode                                                                                   | BOGLIV                                                                                                                                 | BOHBUY                                                                                                                                 | BOGTID                                                                                                                                 | BOHBEI                                                                                                                                | BOGBEH                                                                                                                                  | BOGLUH                                                                                                                                 | BOGMAO                                                                                                                                 | BOGNAP                                                                                                                                   | BOGSIC01                                                                                                                                 | BOGRIB                                                                                                                                  |
| S7<br> | <br>5.18759,<br>14.5127,<br>16.5275<br>(2.80, 3.19) | <br>7.9387,<br>8.1134,<br>10.6329<br>(1.62, 1.97)   | <br>7.5752,<br>12.2914,<br>14.9397<br>(2.77, 3.35)  | <br>14.538,<br>5.2457,<br>17.571<br>(2.77, 3.35)   | <br>16.8682,<br>15.2763,<br>11.0289<br>(1.39, 1.53)  | <br>11.4546,<br>15.3232,<br>16.5783<br>(1.34, 1.45) | <br>8.9158,<br>4.9848,<br>15.924<br>(1.79, 3.19)  | <br>17.1563,<br>15.4391,<br>10.5751<br>(1.46, 1.62) |                                                                                                                                          | <br>14.6674,<br>5.2309,<br>18.2087<br>(2.80, 3.48) |
| Refcode                                                                                   | BOGSAU                                                                                                                                 | BOGMES                                                                                                                                 | BOGGAI01                                                                                                                               | VUXPOV0                                                                                                                               | BOHBIM                                                                                                                                  | BOGMIW                                                                                                                                 | BOFZEE                                                                                                                                 | BOGGIQ                                                                                                                                   |                                                                                                                                          | MBZSAN1                                                                                                                                 |

 Dimeric 
  Dimeric ( $R\bar{3}$ ) 
  Straight 
  Helical1 
  Helical2 
  Zigzag1 
  Zigzag2

Fig S22 The BFDH model calculated using Mercury for the crystals in Fig 7. In each frame, the left-hand model is the front view of the widest face, and the right-hand model is the left figure rotated 90° horizontally.

|                                                                                            | A1<br> | A11<br>                                               | A12<br>                                            | A13<br>                                              | A14<br>                                              |
|--------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------|
| S1<br>    |                                                                                         | <br>17.41,<br>8.859,<br>14.925<br>(1.68, 1.97)        | <br>10.8152,<br>9.6223,<br>23.3468<br>(1.12, 2.43) | <br>10.9613,<br>9.6809,<br>23.4807<br>(1.13, 2.43)   | <br>11.39083,<br>9.40163,<br>23.9427<br>(1.21, 2.55) |
| Refcode                                                                                    |                                                                                         | UKUPUO                                                                                                                                 | SAYZEY                                                                                                                              | BPBSLF10                                                                                                                              | UKUJIW                                                                                                                                |
| S8<br>    |        | <br>7.9414,<br>21.6568,<br>13.0253<br>(1.64, 2.73)    | <br>8.6034,<br>8.0331,<br>17.43<br>(1.07, 2.17)    | <br>26.058,<br>26.058,<br>9.3955<br>(2.77, 2.77)     | <br>8.04804,<br>8.04804,<br>19.084<br>(1.00, 2.37)   |
| Refcode                                                                                    | UKUMIZ                                                                                  | UKUQAV                                                                                                                                 | UKUSOL                                                                                                                              | UKUGOZ                                                                                                                                | UKULOE                                                                                                                                |
| S9<br>    |        | <br>20.443,<br>6.11175,<br>18.6691<br>(3.05, 3.34)    | <br>7.0031,<br>8.4897,<br>10.5092<br>(1.21, 1.50)  | <br>23.56,<br>10.8124,<br>9.7328<br>(1.11, 2.42)     | <br>23.736,<br>10.9599,<br>9.7943<br>(1.12, 2.42)    |
| Refcode                                                                                    | UKUMOF                                                                                  | UKUQID                                                                                                                                 | UKUSUR                                                                                                                              | UKUGUF                                                                                                                                | UKULEU                                                                                                                                |
| S10<br>  |       | <br>6.2341,<br>8.0773,<br>22.406<br>(1.30, 3.59)     | <br>6.695,<br>10.173,<br>10.249<br>(1.52, 1.53)   | <br>25.9241,<br>25.9241,<br>9.3533<br>(2.77, 2.77)  | <br>26.5333,<br>26.5333,<br>9.2014<br>(2.88, 2.88)  |
| Refcode                                                                                    | UKUNAS                                                                                  | TIHYUF01                                                                                                                               | TIHYOZ                                                                                                                              | TIHYEP                                                                                                                                | TIHZAM                                                                                                                                |
| S11<br> |      | <br>8.716,<br>9.113,<br>15.202<br>(1.05, 1.74)      | <br>18.655,<br>8.9064,<br>14.683<br>(1.65, 2.09) | <br>26.327,<br>26.327,<br>9.6639<br>(2.72, 2.72)   | <br>26.624,<br>26.624,<br>9.3454<br>(2.77, 2.77)   |
| Refcode                                                                                    | UKUNEW                                                                                  | UKULUK                                                                                                                                 | UKUTAY                                                                                                                              | UKUHAM                                                                                                                                | UKUQAQ                                                                                                                                |
| S12<br> |      | <br>11.046,<br>8.643,<br>12.692<br>(1.28, 1.47)     | <br>11.23,<br>15.241,<br>7.3409<br>(1.53, 2.08)  | <br>22.790,<br>15.667,<br>7.3340<br>(2.14, 3.11)   | <br>22.99,<br>15.918,<br>7.3032<br>(2.18, 3.15)    |
| Refcode                                                                                    | UKUNIA                                                                                  | UKUQUP                                                                                                                                 | AZESOO                                                                                                                              | UKUHEQ                                                                                                                                | UKUJUI                                                                                                                                |
| S13<br> |      | <br>10.2641,<br>10.9328,<br>13.1752<br>(1.07, 1.32) | <br>12.427,<br>5.0351,<br>20.62<br>(2.47, 4.10)  | <br>26.5773,<br>26.5773,<br>9.3206<br>(2.85, 2.85) | <br>27.045,<br>27.045,<br>9.1556<br>(2.95, 2.95)   |
| Refcode                                                                                    | URETER                                                                                  | UKURAW                                                                                                                                 | ODEPUJ                                                                                                                              | BPCBZS11                                                                                                                              | TIHXAK                                                                                                                                |

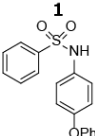
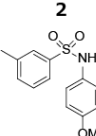
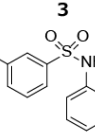
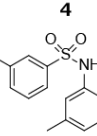
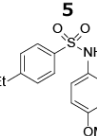
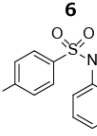
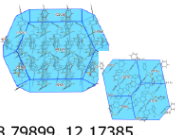
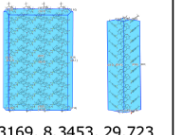
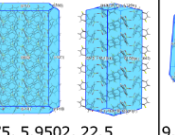
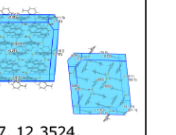
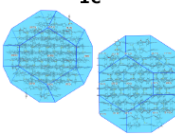
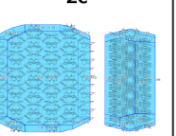
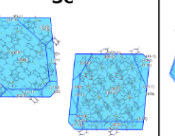
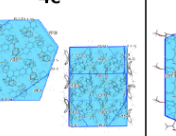
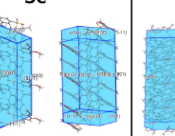
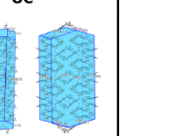
|                                                                                            | A1<br>                                                 | A11<br>                                            | A12<br>                                              | A13<br>                                              | A14<br>                                               |
|--------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------|
| S14<br>   | <br>17.7138,<br>18.2246,<br>15.3999<br>(1.15, 1.18)     | <br>18.978,<br>8.9256,<br>14.693<br>(1.65, 2.13)   | <br>14.322,<br>14.227,<br>14.432<br>(1.01, 1.01)     | <br>14.515,<br>14.25,<br>14.535<br>(1.02, 1.02)      | <br>9.3612,<br>10.2788,<br>14.5183<br>(1.10, 1.55)    |
| Refcode                                                                                    | UKUMAR                                                                                                                                   | UKUREA                                                                                                                                | UKUFIS                                                                                                                                  | UKULIY                                                                                                                                  | UKUKET                                                                                                                                   |
| S15<br>   | <br>20.591,<br>6.0883,<br>19.38<br>(3.18, 3.38)         | <br>11.2527,<br>15.3496,<br>7.3703<br>(1.53, 2.08) | <br>11.588,<br>15.677,<br>7.4877<br>(1.55, 2.09)     | <br>11.6354,<br>15.8033,<br>7.4652<br>(1.56, 2.12)   | <br>12.137,<br>11.498,<br>10.211<br>(1.13, 1.19)      |
| Refcode                                                                                    | UKUNUM                                                                                                                                   | UKURIE                                                                                                                                | UKUFOY                                                                                                                                  | UKUHIU                                                                                                                                  | UKUKIX                                                                                                                                   |
| S16<br>   | <br>12.113,<br>5.0601,<br>20.473<br>(2.39, 4.05)        | <br>19.821,<br>12.435,<br>5.073<br>(2.45, 3.91)    | <br>4.9899,<br>6.85,<br>20.446<br>(1.37, 4.10)       | <br>5.0643,<br>12.7966,<br>20.4879<br>(2.53, 4.05)   | <br>28.134,<br>28.134,<br>9.024<br>(3.12, 3.12)       |
| Refcode                                                                                    | UKUPAU                                                                                                                                   | USOFEP                                                                                                                                | UKUFUE                                                                                                                                  | TIHVUC01                                                                                                                                | TIHWEN                                                                                                                                   |
| S17<br>  | <br>8.86786,<br>9.25786,<br>15.6341<br>(1.04, 1.76)    | <br>36.4739,<br>8.12621,<br>8.438<br>(1.04, 4.49) | <br>20.8764,<br>10.2189,<br>26.3854<br>(2.04, 2.58) | <br>21.0219,<br>10.3572,<br>26.6232<br>(2.03, 2.57) | <br>8.30775,<br>10.79828,<br>15.8584<br>(1.30, 1.91) |
| Refcode                                                                                    | UKUPEY                                                                                                                                   | UKURIE                                                                                                                                | UKUGAL                                                                                                                                  | UKUJAO                                                                                                                                  | UKUKOD                                                                                                                                   |
| S18<br> | <br>10.46014,<br>13.42839,<br>9.15376<br>(1.14, 1.47) | <br>11.306,<br>15.552,<br>7.5028<br>(1.51, 2.07) | <br>11.5388,<br>15.8325,<br>7.5781<br>(1.52, 2.09) | <br>11.6549,<br>15.9733,<br>7.5659<br>(1.54, 2.11) | <br>12.1025,<br>11.5411,<br>10.4295<br>(1.11, 1.16) |
| Refcode                                                                                    | UKUPIC                                                                                                                                   | UKUSAX                                                                                                                                | UKUGEP                                                                                                                                  | UKUJES                                                                                                                                  | UKUKUJ                                                                                                                                   |
| S19<br> | <br>5.10471,<br>13.8171,<br>18.6987<br>(2.71, 3.66)   | <br>20.492,<br>12.518,<br>5.0502<br>(2.48, 4.06) | <br>4.9768,<br>42.466,<br>6.8237<br>(1.37, 8.53)   |                                                                                                                                         |                                                                                                                                          |
| Refcode                                                                                    | UKUPOI                                                                                                                                   | UKUSEB                                                                                                                                | UKUMEV                                                                                                                                  |                                                                                                                                         |                                                                                                                                          |

 Dimeric  
 Dimeric ( $R\bar{3}$ )  
 Straight  
 Helical1  
 Helical2  
 Zigzag1  
 Zigzag2

Fig S23 The BFDH model calculated using Mercury for the crystals in Fig 8. In each frame, the left-hand model is the front view of the widest face, and the right-hand model is the left figure rotated 90° horizontally.



|                  |                                                                                                                                  |                                                                                                                              |                                                                                                                                |                                                                                                                                 |                                                                                                                                |                                                                                                                                  |
|------------------|----------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------|
|                  |                                                 |                                             |                                               |                                                |                                             |                                               |
| Sulfonamide      | <br>8.79899, 12.17385,<br>15.22942 (1.38, 1.73) | <br>5.3169, 8.3453, 29.723<br>(1.57, 5.59)  | <br>9.175, 5.9502, 22.5<br>(1.54, 3.78)       | <br>9.0097, 12.3524,<br>12.9152 (1.37, 1.43)  |                                                                                                                                |                                                                                                                                  |
| HB pattern       | Helical1                                                                                                                         | Straight                                                                                                                     | Helical2                                                                                                                       | Helical1                                                                                                                        | amorphous                                                                                                                      | liquid                                                                                                                           |
| CCDC No./Refcode | 2087464                                                                                                                          | BOGJAL                                                                                                                       | 2087467                                                                                                                        | 2087469                                                                                                                         |                                                                                                                                |                                                                                                                                  |
| Cocrystal        | <br>14.8313, 16.0368,<br>20.2334 (1.08, 1.36)   | <br>31.8179, 8.1924, 17.861<br>(2.18, 3.88) | <br>10.2247, 13.3486,<br>15.0139 (1.31, 1.47) | <br>12.6562, 11.1186,<br>15.7821 (1.14, 1.42) | <br>8.3499, 11.4704, 13.571<br>(1.37, 1.63) | <br>10.0096, 12.4631,<br>17.7972 (1.25, 1.78) |
| CCDC No./Refcode | 2087465                                                                                                                          | 2087466                                                                                                                      | 2087468                                                                                                                        | 2087470                                                                                                                         | 2087471                                                                                                                        | 2087472                                                                                                                          |

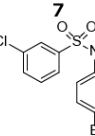
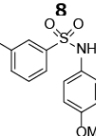
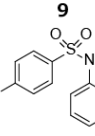
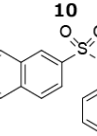
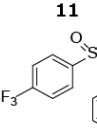
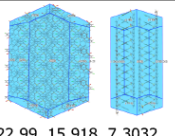
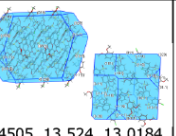
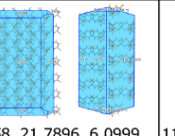
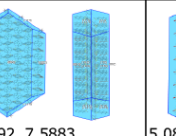
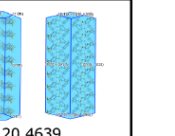
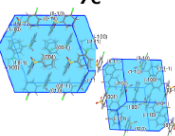
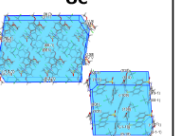
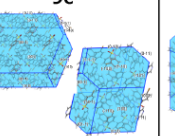
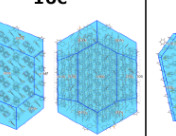
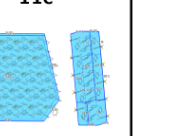
|                  |                                                                                                                                |                                                                                                                                   |                                                                                                                                  |                                                                                                                                  |                                                                                                                                    |
|------------------|--------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------|
|                  |                                              |                                                 |                                                |                                                |                                                |
| Sulfonamide      | <br>22.99, 15.918, 7.3032<br>(2.18, 3.15)   | <br>8.4505, 13.524, 13.0184<br>(1.54, 1.60)    | <br>9.958, 21.7896, 6.0999<br>(1.63, 3.57)    | <br>11.5492, 7.5883,<br>31.0045 (1.52, 4.09) | <br>5.0813, 20.4639,<br>12.2504 (2.41, 4.03)  |
| HB pattern       | Zigzag2                                                                                                                        | Other                                                                                                                             | Helical2                                                                                                                         | Zigzag1                                                                                                                          | Straight                                                                                                                           |
| CCDC No./Refcode | UKUHEQ                                                                                                                         | 2087474                                                                                                                           | 2087476                                                                                                                          | 2087478                                                                                                                          | 2087480                                                                                                                            |
| Cocrystal        | <br>8.4205, 9.8122, 11.2928<br>(1.17, 1.34) | <br>8.56656, 11.3193,<br>12.12655 (1.32, 1.42) | <br>11.7276, 14.3853,<br>16.9385 (1.23, 1.44) | <br>15.701, 30.2586, 17.029<br>(1.08, 1.93)  | <br>8.24881, 9.01501,<br>29.4839 (1.09, 3.57) |
| CCDC No./Refcode | 2087473                                                                                                                        | 2087475                                                                                                                           | 2087477                                                                                                                          | 2087479                                                                                                                          | 2087481                                                                                                                            |

Fig S24 The BFDH model calculated using Mercury for the crystals in Fig 12. In each frame, the left-hand model is the front view of the widest face, and the right-hand model is the left figure rotated 90° horizontally.

## 6. References

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