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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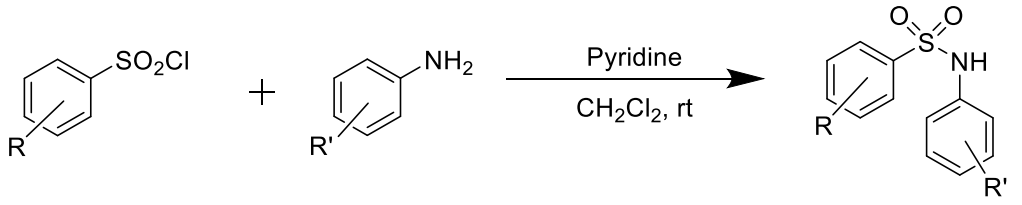
Table of Contents

1. Experimental



Scheme S1

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

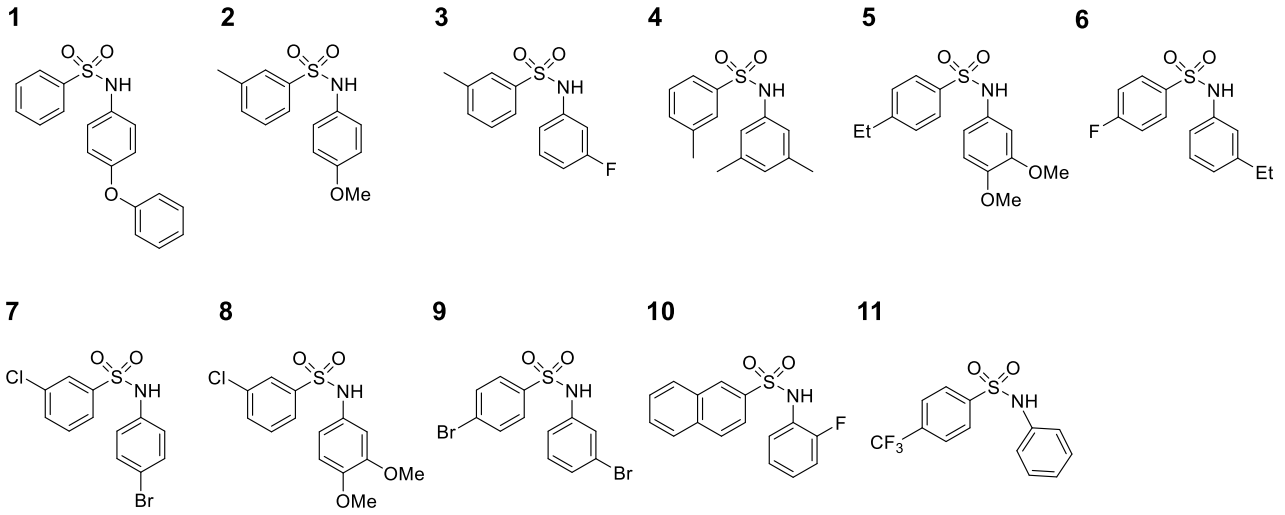


Fig S1 Molecular structures of **1−11**

***N*-(4-Phenoxyphenyl)benzenesulfonamide (1).**[s1] Yield: 479.8 mg (1.47 mmol), 73.6%. Color, Habit: colorless, prism crystals. M.p.: 109−110 °C. ^{1}H NMR (400 MHz, 298 K, $CDCl_3$) (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).** [s2] Yield: 416.4 mg (1.5 mmol), 79.4%. Color, Habit: colorless, prism crystals. M.p.: 82 °C. ^{1}H NMR (400 MHz, 298 K, $CDCl_3$) (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. ^{1}H NMR (400 MHz, 298 K, $CDCl_3$) (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). ^{13}C NMR (100 MHz,

298 K, $CDCl_3$) (ppm): δ 163.0 (d, J_{CF} = 246.3), 139.5, 138.5, 138.1 (d, J_{CF} = 10.5), 134.2, 130.5 (d, J_{CF} = 9.6), 129.0, 127.5, 124.4, 116.3 (d, J_{CF} = 2.9), 112.0 (d, J_{CF} = 21.1), 108.2 (d, J_{CF} = 24.9), 21.3. FT–IR (KBr, cm^{-1}): 3245, 3071, 2976, 2900, 1615, 1499, 1420, 1615, 1499, 1420, 1327, 1136, 984, 913, 700, 566, 511. MS (FAB): *m/z* 266$[M+H]^+$. Anal. Calcd. for $C_{14}H_{12}FNO_3S$: 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. ^{1}H NMR (400 MHz, 298 K, $CDCl_3$) (ppm): δ 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). ^{13}C NMR (100 MHz, 298 K, $CDCl_3$) (ppm): δ 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^{-1}): 3230, 2917, 1598, 1478, 1401, 1323, 1217, 1151, 1095, 698, 650, 596, 505, 423. MS (FAB): *m/z* 276$[M+H]^+$. Anal. Calcd. for $C_{15}H_{17}NO_2S$: 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. ^{1}H NMR (400 MHz, 298 K, $CDCl_3$) (ppm): δ 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). ^{13}C NMR (100 MHz, 298 K, $CDCl_3$) (ppm): δ 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$[M]^+$. Anal. Calcd. for $C_{16}H_{19}NO_4S$: 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. ^{1}H NMR (400 MHz, 298 K, $CDCl_3$) (ppm): δ 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). ^{13}C NMR (100 MHz, 298 K, $CDCl_3$) (ppm): δ 165.2 (d, J_{CF} = 255.0), 145.9, 136.0, 135.0, 135.0, 130.0 (d, J_{CF} = 9.6), 129.3, 125.4, 121.5, 119.2, 116.2 (d, J_{CF} = 23.0), 28.6, 15.4. FT–IR (KBr, cm^{-1}): 3263, 2967, 1592, 1494, 1469, 1407, 1336, 1238, 1153, 1091, 838, 697, 564, 543. MS (FAB): *m/z* 280$[M+H]^+$. HRMS (FAB): *m/z* $[M+H]^+$ calcd for $C_{14}H_{15}FNO_2S$: 280.0808; found:280.0808.

***N*-(4-Bromophenyl)-3-chlorobenzenesulfonamide (7).**[s1] Yield: 542 mg (1.56 mmol), 82.6%. Color, Habit: colorless, prism crystals. M.p.: 103−104 °C. ^{1}H NMR (400 MHz, 298 K, $CDCl_3$) (ppm): δ 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. ^{1}H NMR (400 MHz, 298 K, $CDCl_3$) (ppm): δ 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}C NMR (100 MHz, 298 K, $CDCl_3$) (ppm): δ 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, cm^{-1}): 3225, 3006, 2356, 1513, 1343, 1269, 1231, 1172, 1022, 967, 679, 635, 586. MS (FAB): *m/z* 327$[M]^+$. Anal. Calcd. for $C_{14}H_{14}ClNO_4S$: 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}H NMR (400 MHz, 298 K, $CDCl_3$) (ppm): δ 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}C NMR (100 MHz, 298 K, $CDCl_3$) (ppm): δ 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$[M+H]^+$. Anal. Calcd. for $C_{12}H_9Br_2NO_2S$: 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}H NMR (400 MHz, 298 K, $CDCl_3$) (ppm): δ 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}C NMR (100 MHz, 298 K, $CDCl_3$) (ppm): δ 153.9 (d, J_{CF} = 244.4), 136.3 (d, J_{CF} = 66.1), 132.0, 129.5, 129.3, 129.1, 128.9 127.9, 127.6, 126.2 (d, J_{CF} = 7.7), 124.8 (d, J_{CF} = 4.8), 124.6, 124.5, 123.2, 122.0, 115.4 (d, J_{CF} = 19.2). FT–IR (KBr, cm^{-1}): 3264, 3066, 1592, 1494, 1406, 1337, 1253, 1163, 901, 827, 797, 750, 680, 564, 486. MS (FAB): *m/z* 302$[M+H]^+$. Anal. Calcd. for $C_{16}H_{12}FNO_2S$: 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).** [s3] Yield: 342.7 mg (1.14 mmol), 62.6%. M.p.: 138−139 °C. ^{1}H NMR (400 MHz, 298 K, $CDCl_3$) (ppm): δ 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}C NMR (100 MHz, 298 K, $CDCl_3$) (ppm): δ 142.6, 136.6, 134.9, 134.6, 129.6,127.8, 126.2 (q, J_{CF} = 3.8), 124.5, 122.3. FT–IR (KBr, cm^{-1}): 3254, 3095, 3047, 1935, 1594, 1406, 1329, 1165, 1065, 1017, 845, 752, 718, 694, 604, 540, 430. MS (FAB): *m/z* 302$[M+H]^+$. Anal. Calcd. for $C_{13}H_{10}F_3NO_2S$: 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.

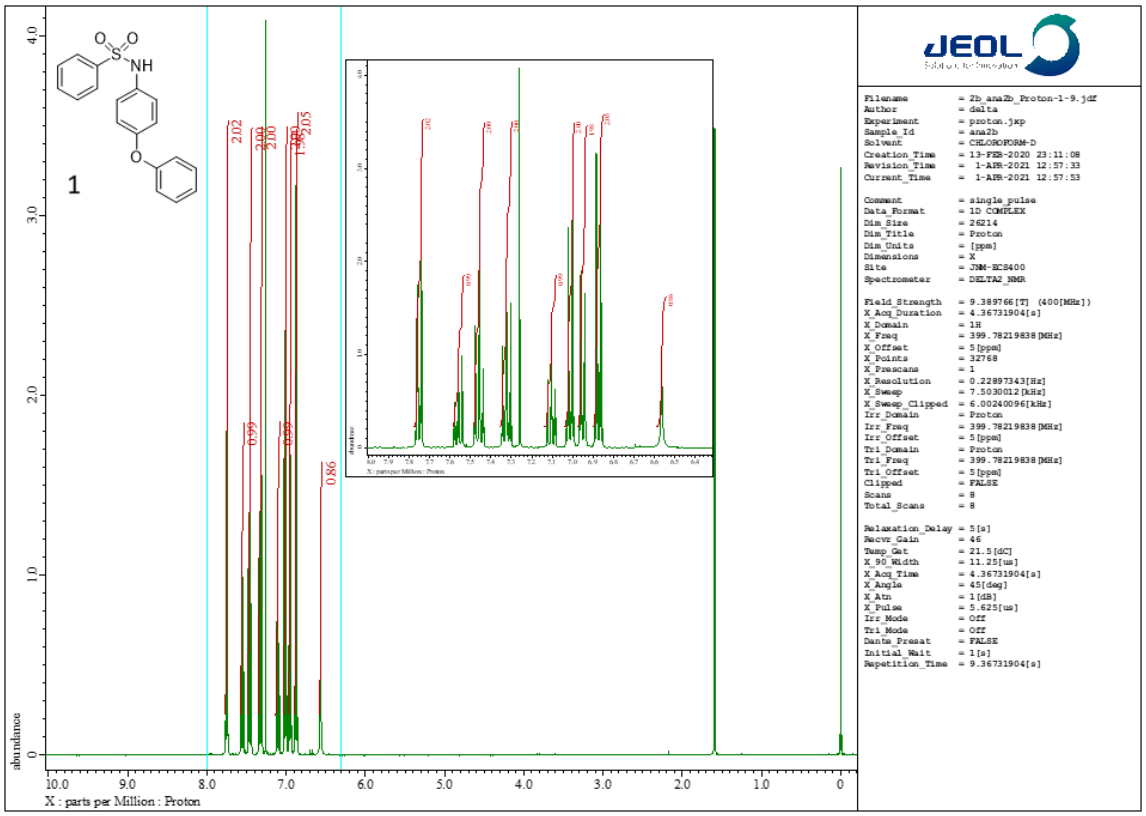


Fig S2 ^{1}H NMR Spectra of **1**

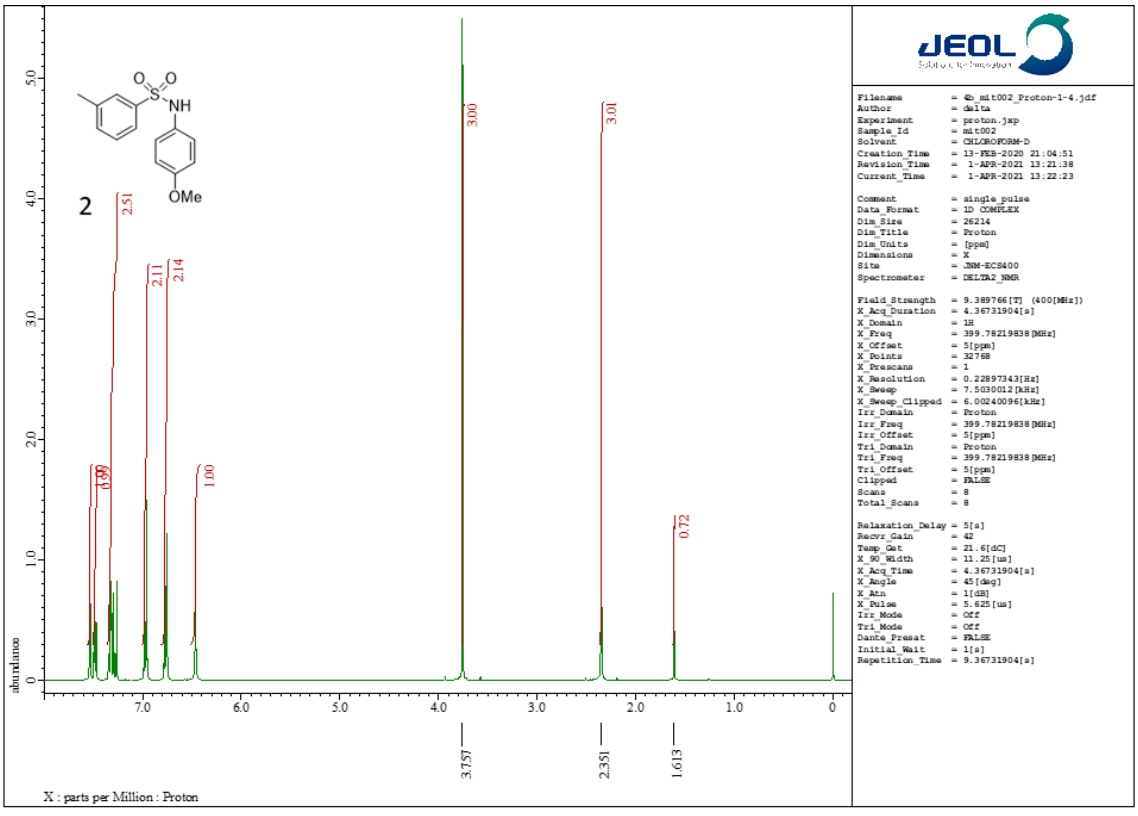


Fig S3 ^{1}H NMR Spectra of **2**

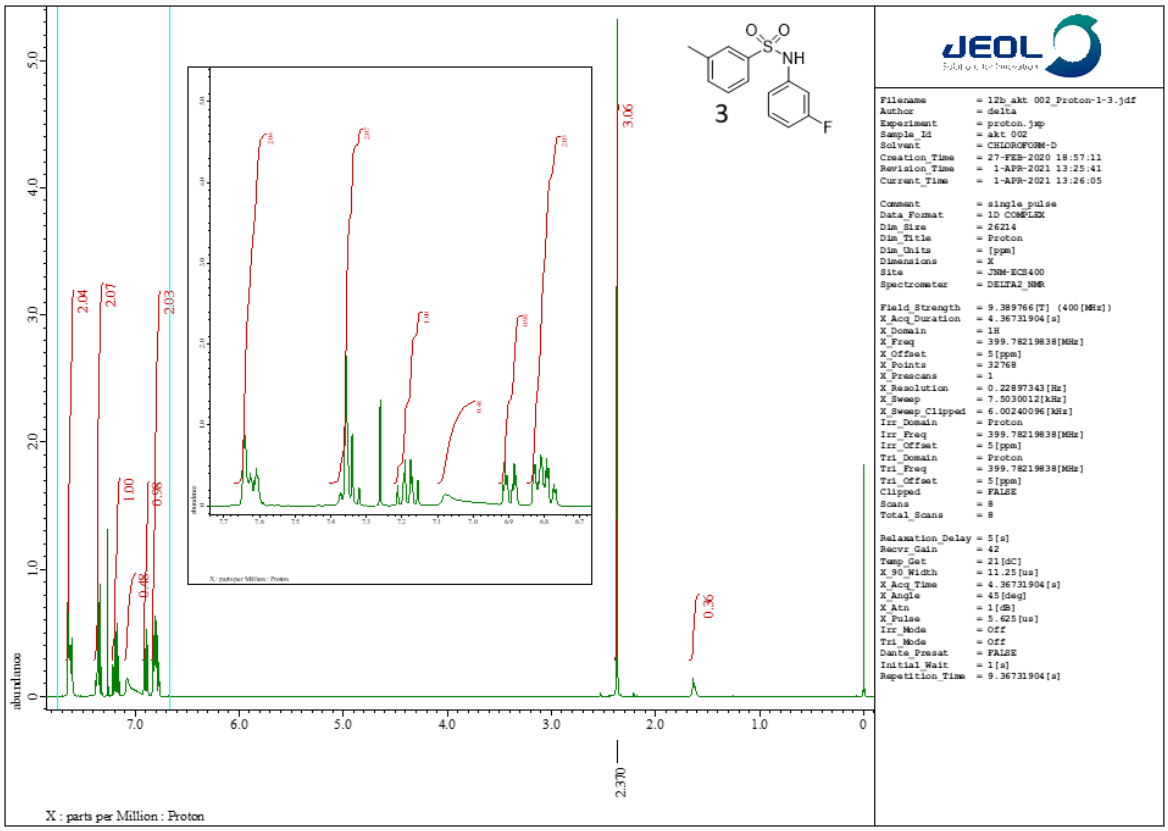


Fig S4 ^{1}H NMR Spectra of **3**

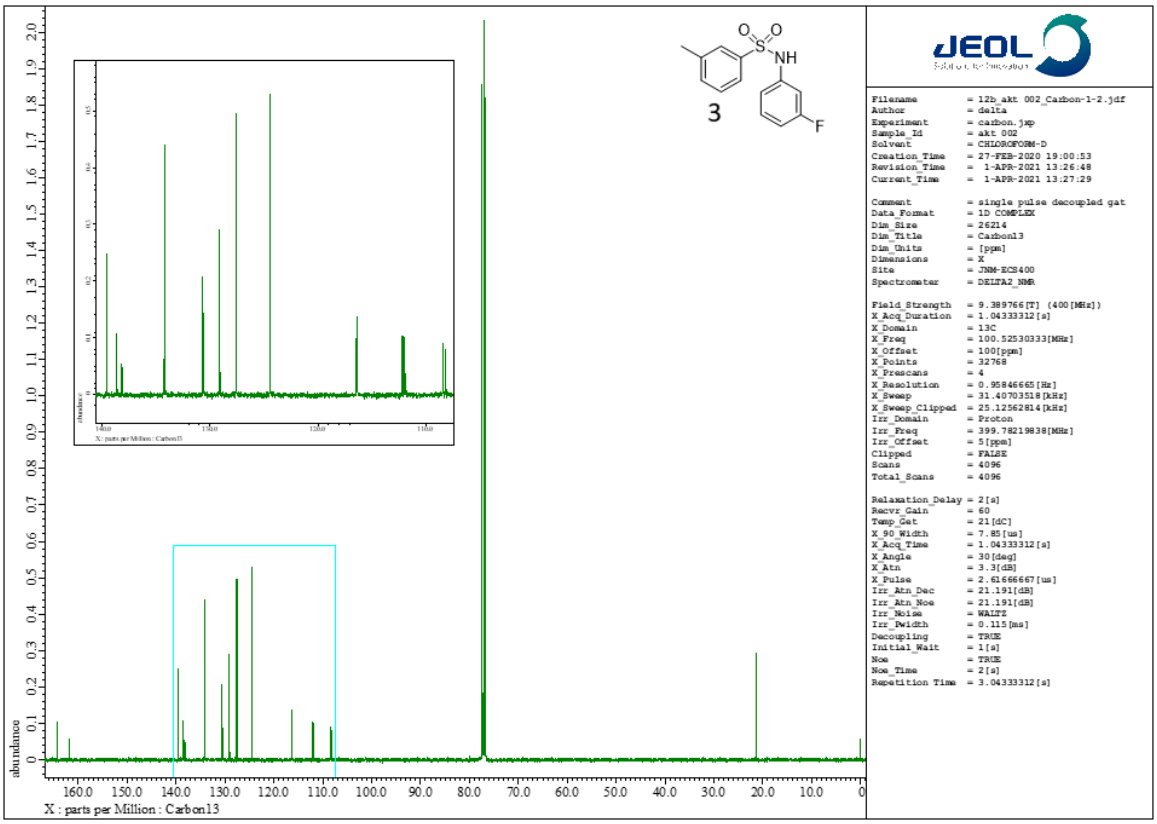


Fig S5 ^{13}C NMR Spectra of **3**

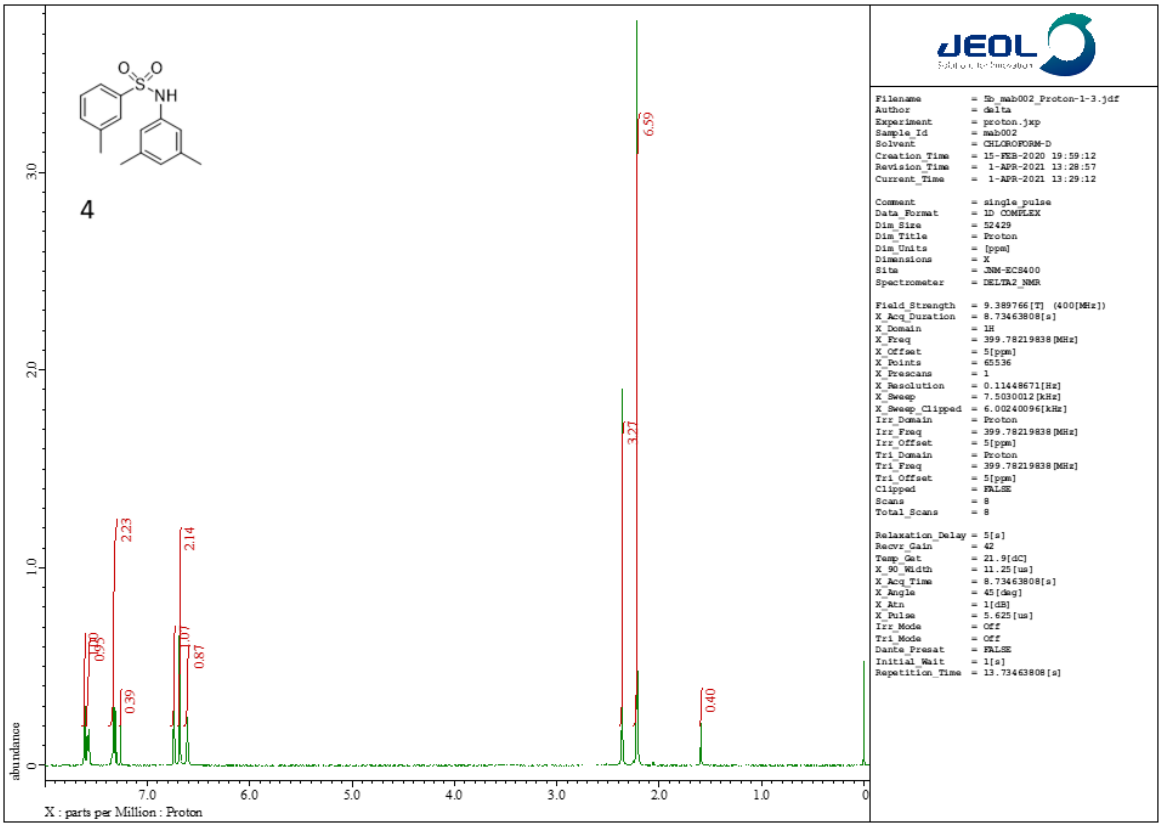


Fig S6 ^{1}H NMR Spectra of **4**

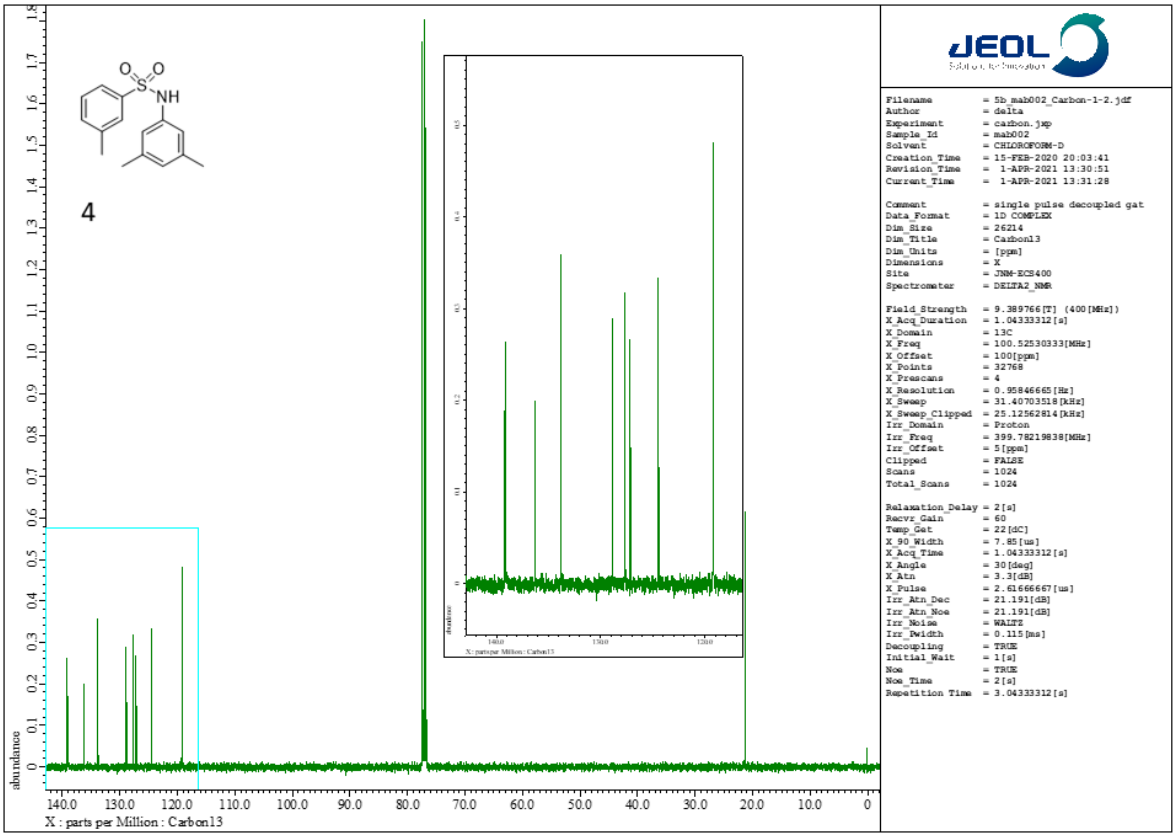


Fig S7 ^{13}C NMR Spectra of **4**

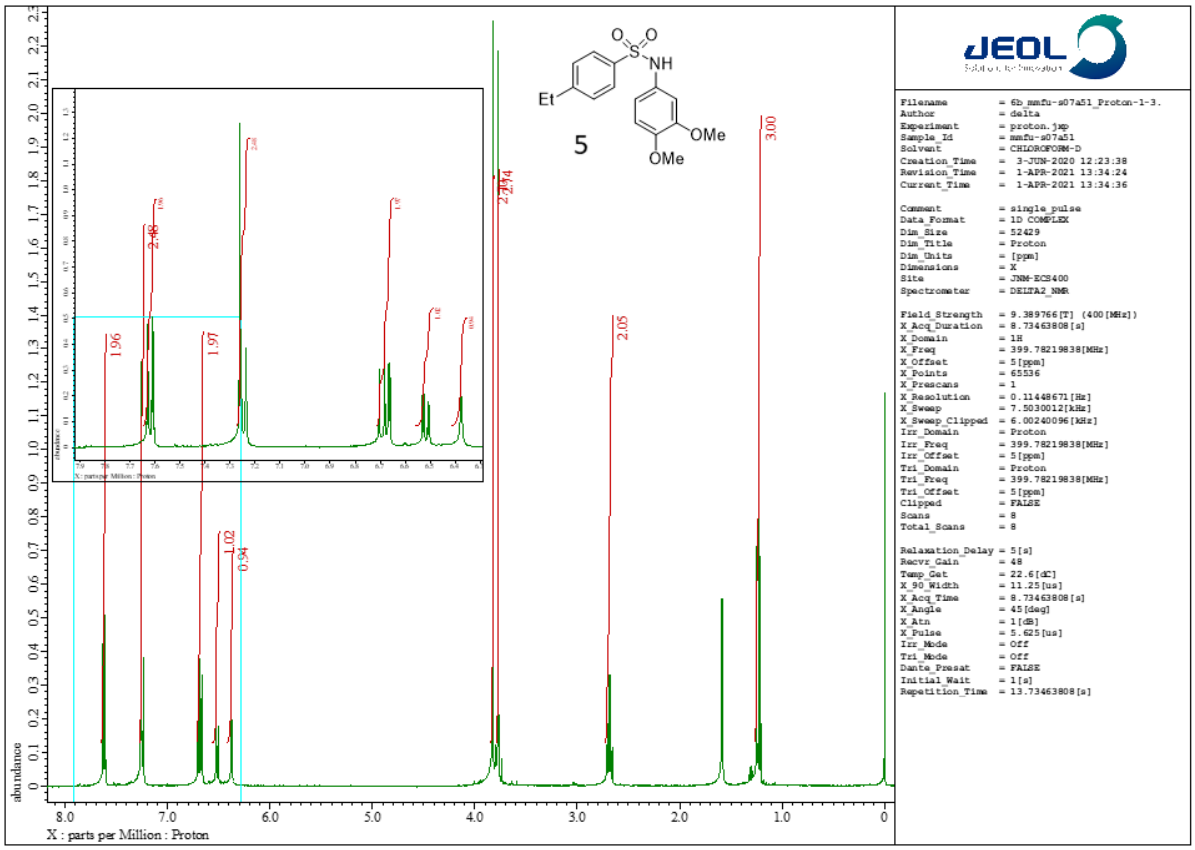


Fig S8 ^{1}H NMR Spectra of **5**

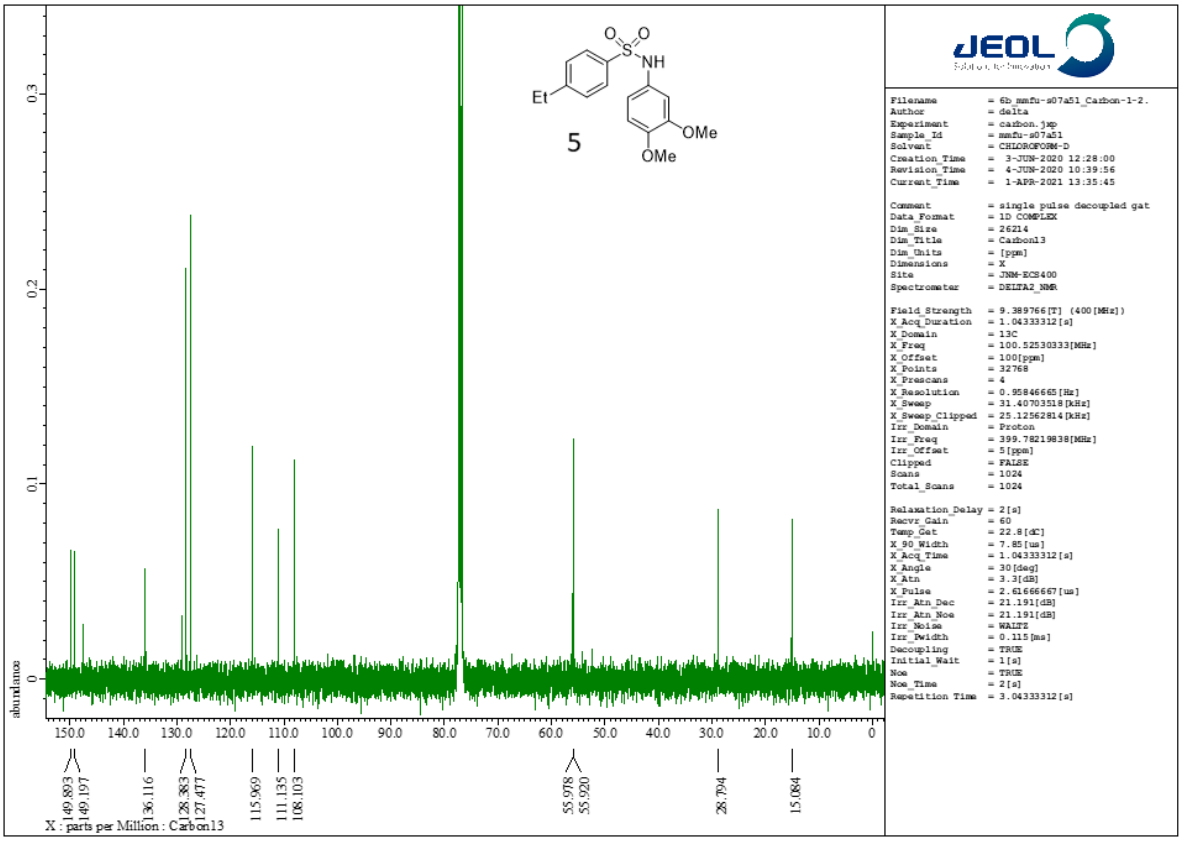


Fig S9 ^{13}C NMR Spectra of **5**

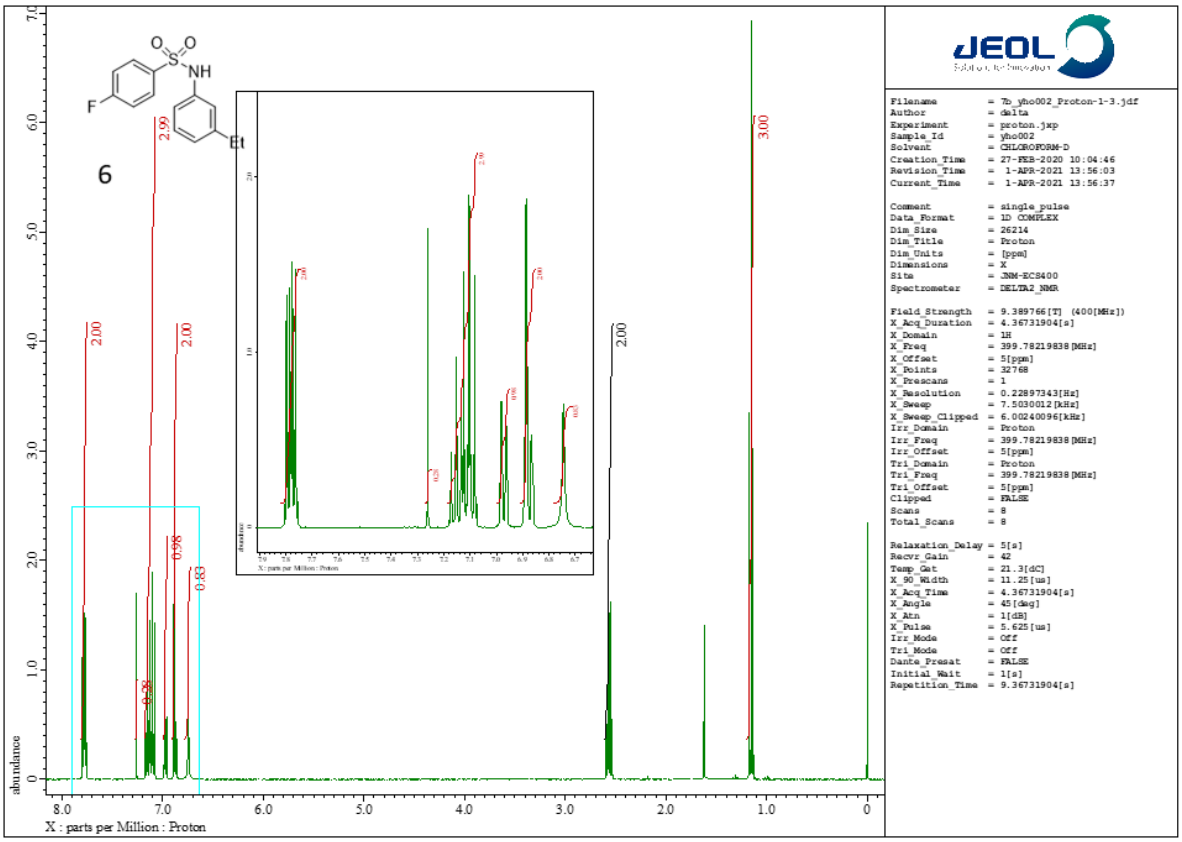


Fig S10 ^{1}H NMR Spectra of **6**

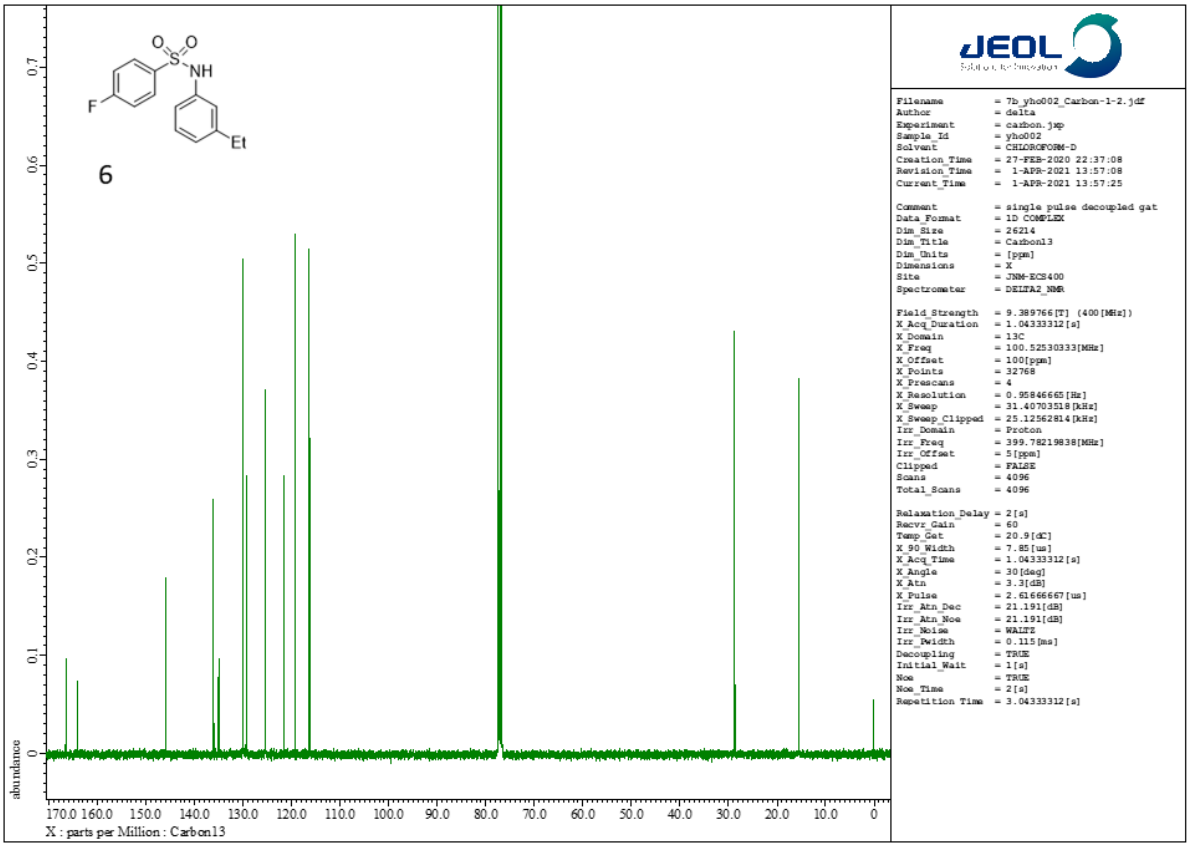


Fig S11 ^{13}C NMR Spectra of **6**

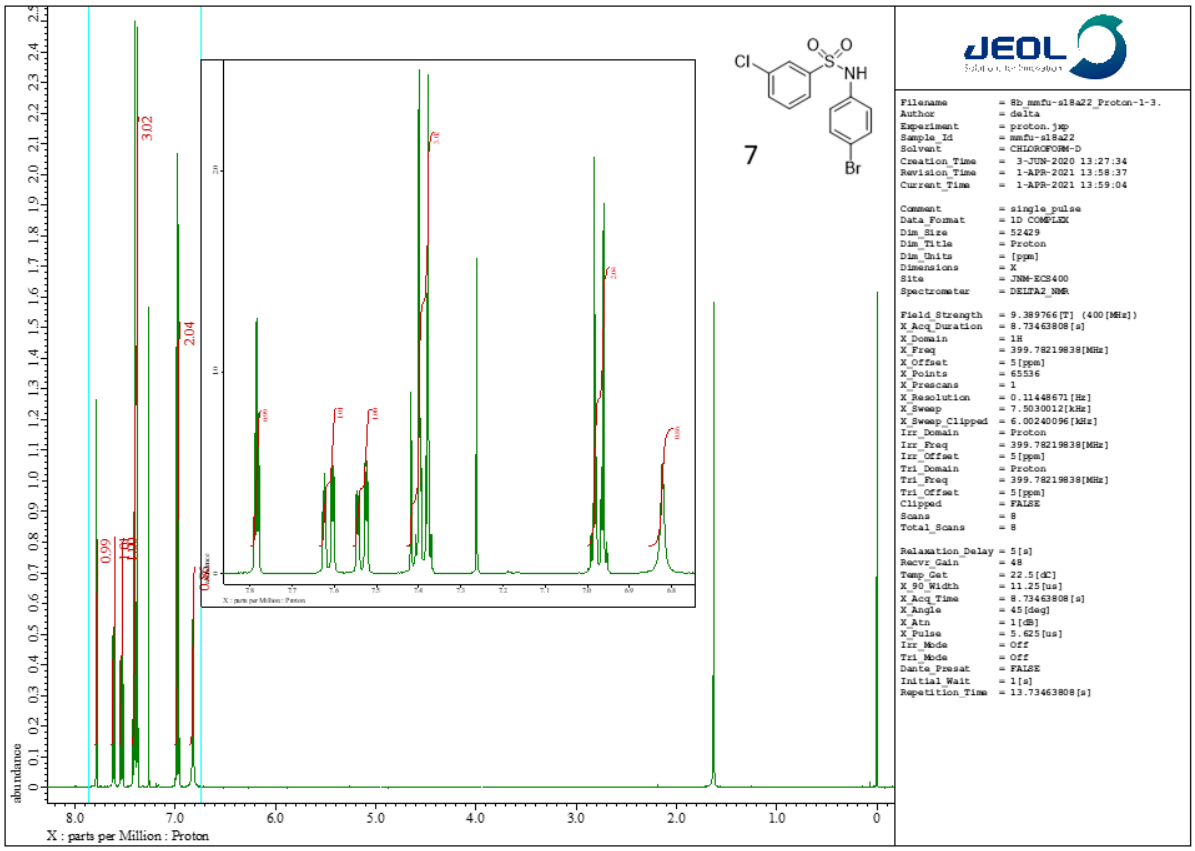


Fig S12 ^{1}H NMR Spectra of **7**

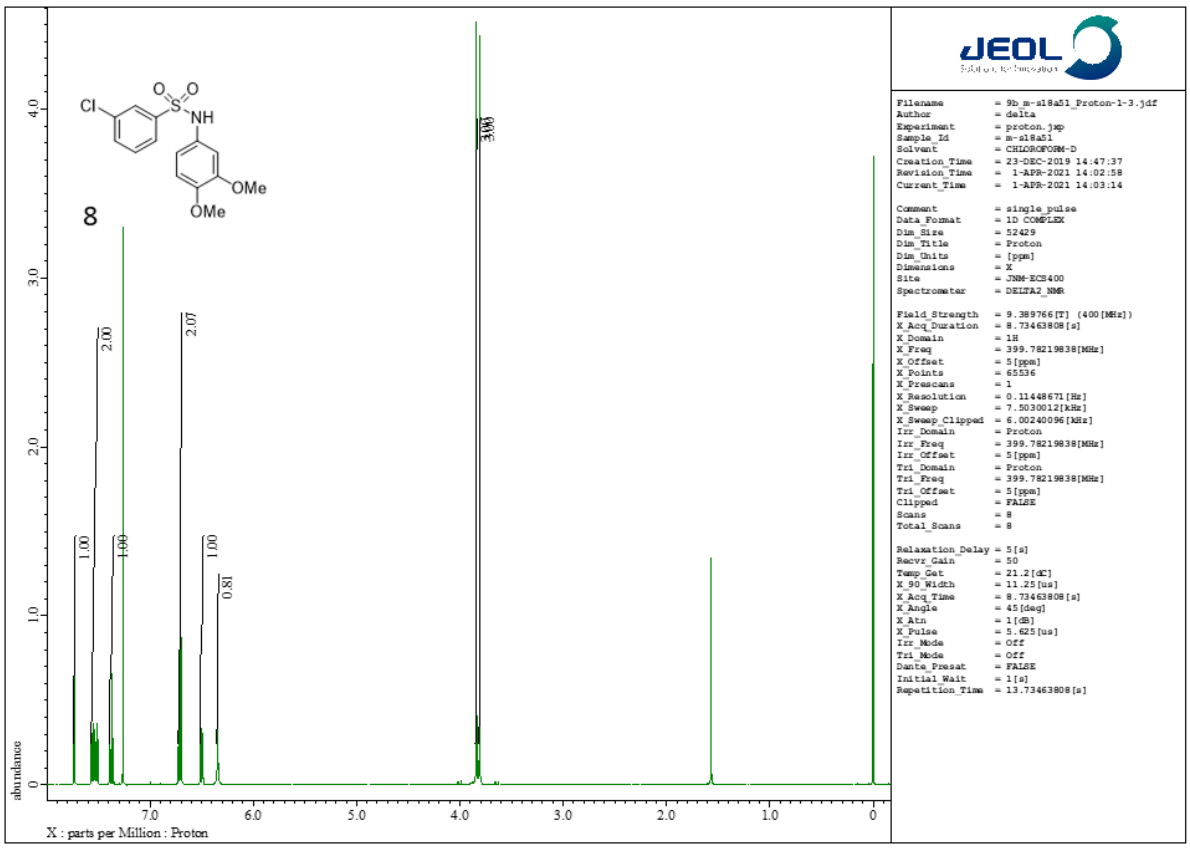


Fig S13 ^{1}H NMR Spectra of **8**

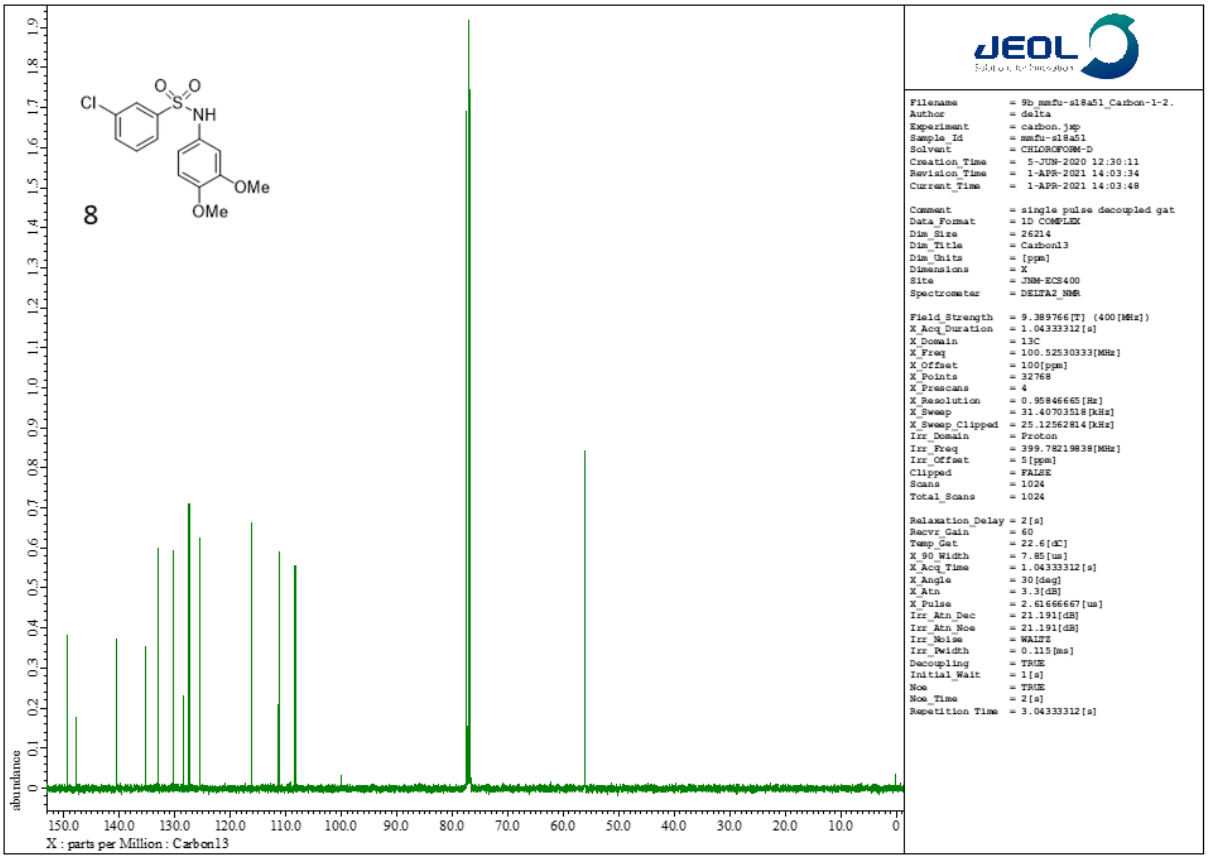


Fig S14 ^{13}C NMR Spectra of **8**

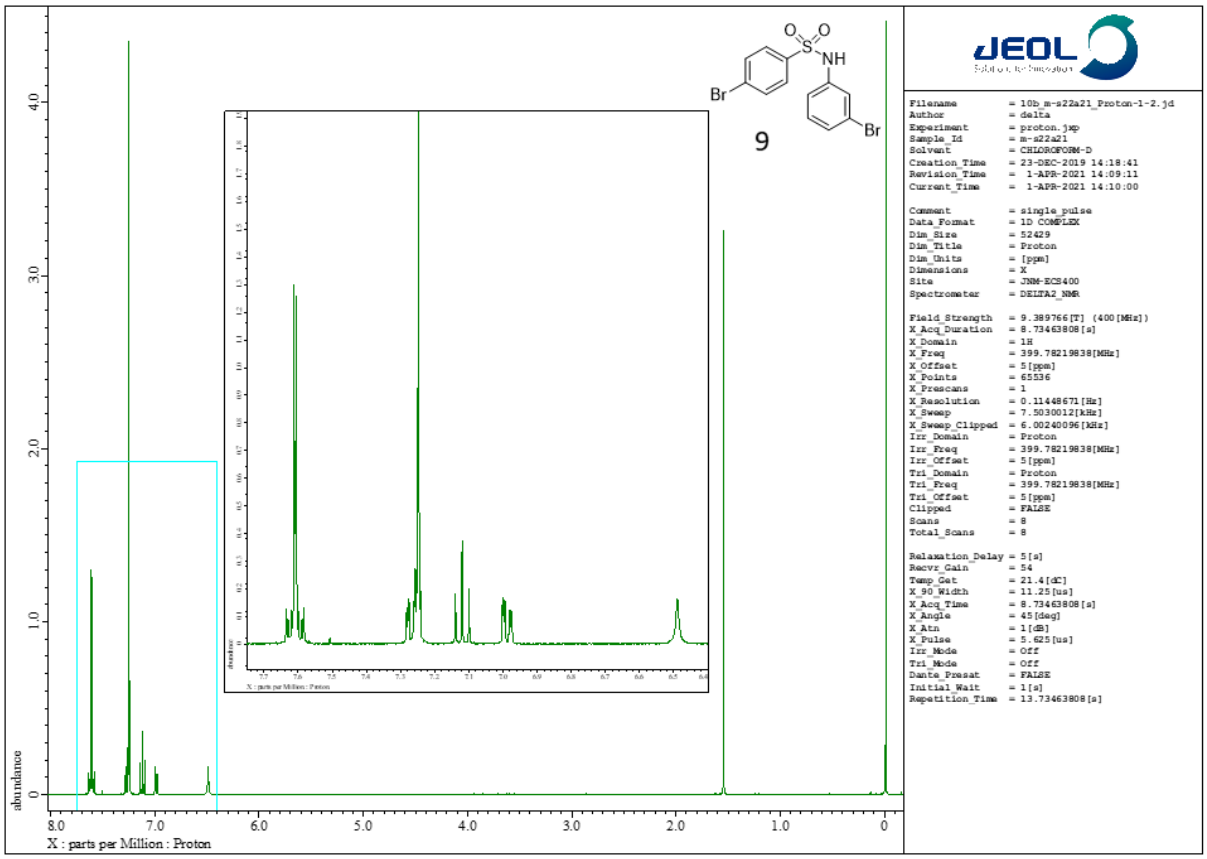


Fig S15 ^{1}H NMR Spectra of **9**

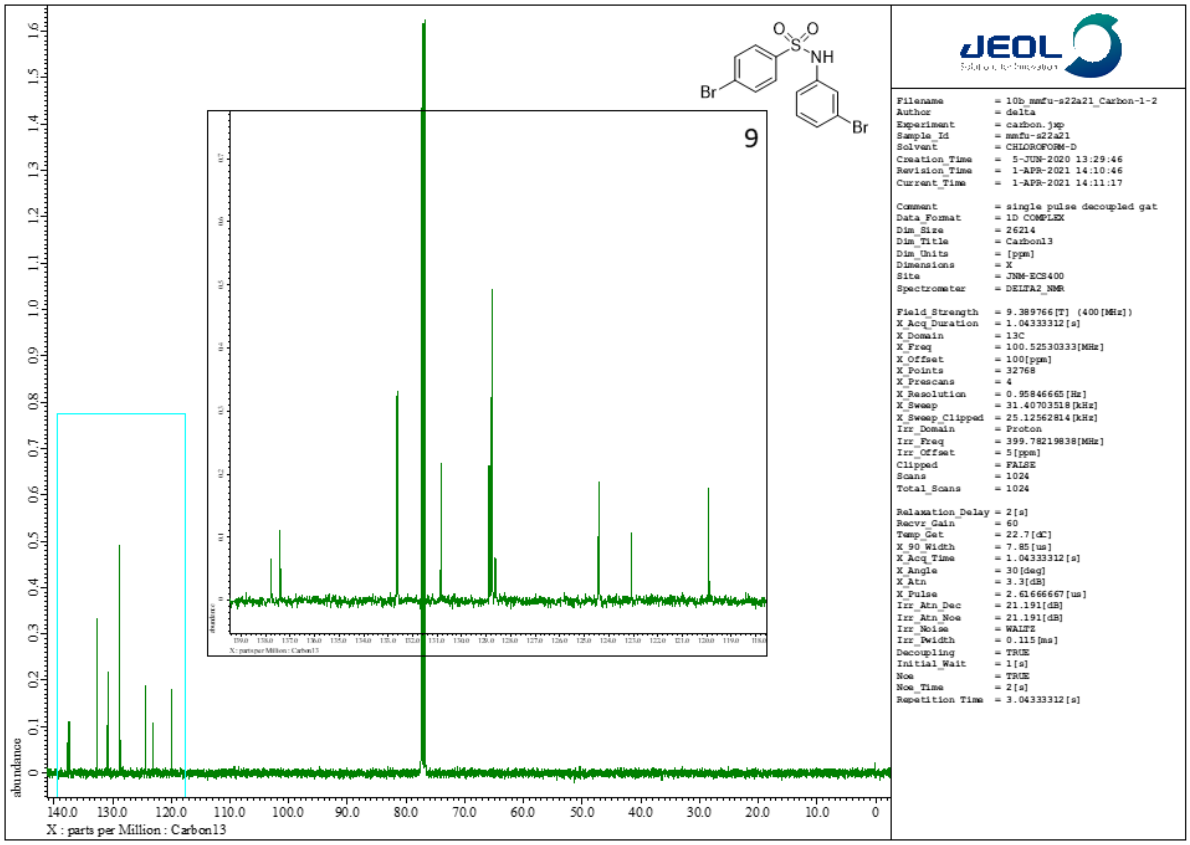


Fig S16 ^{13}C NMR Spectra of **9**

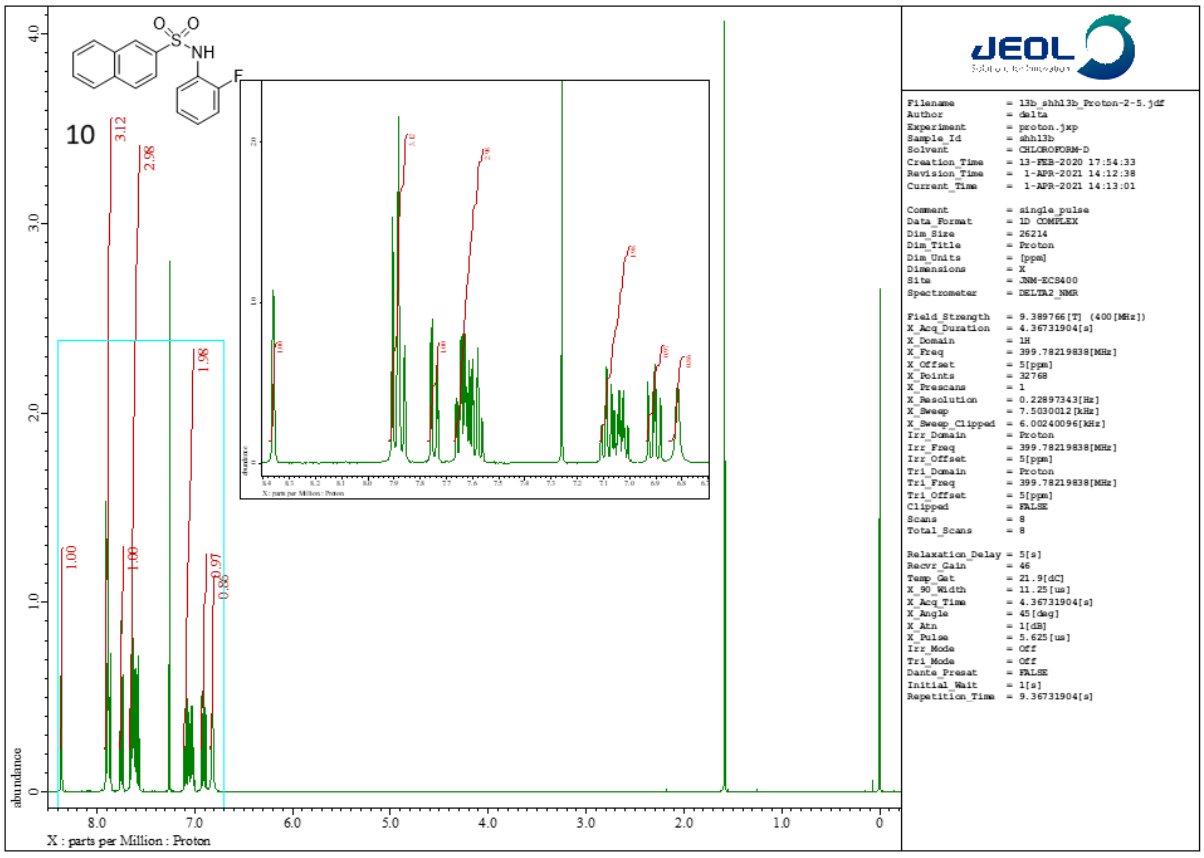


Fig S17 ^{1}H NMR Spectra of **10**

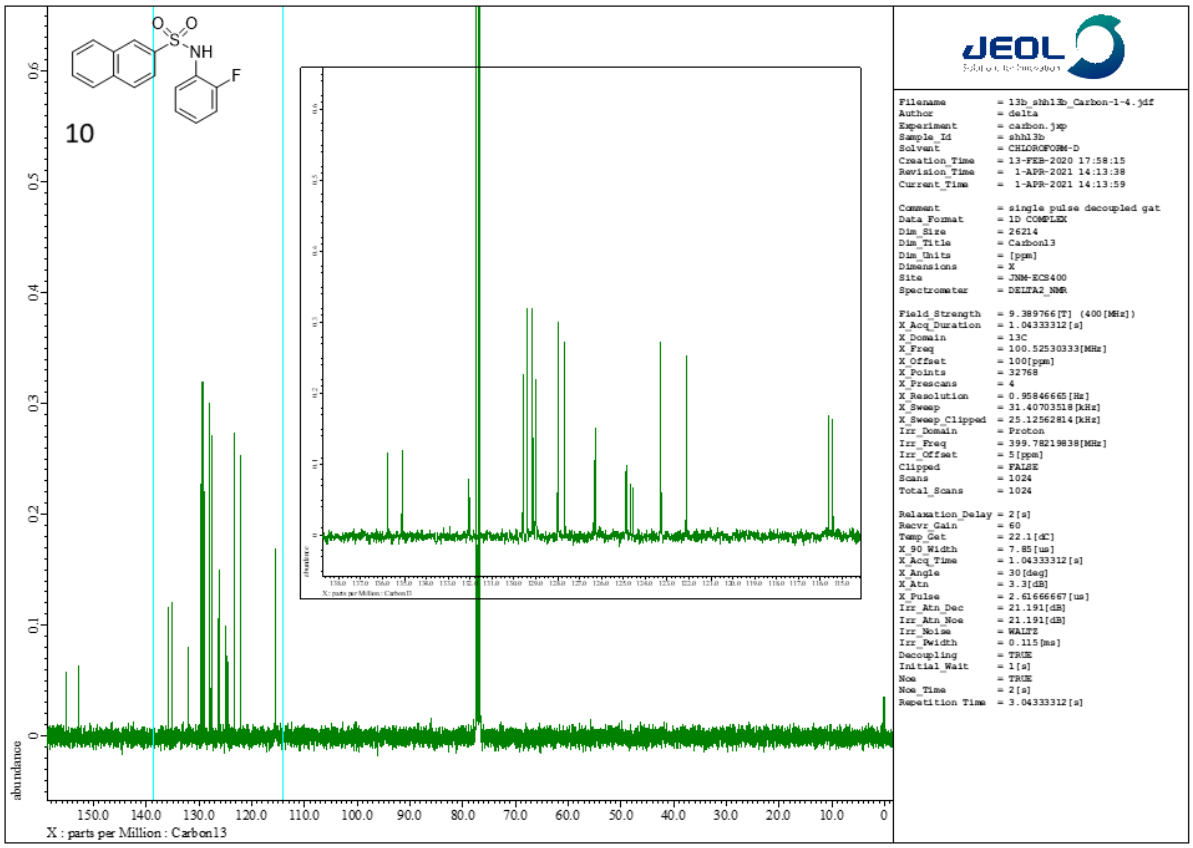


Fig S18 ^{13}C NMR Spectra of **10**

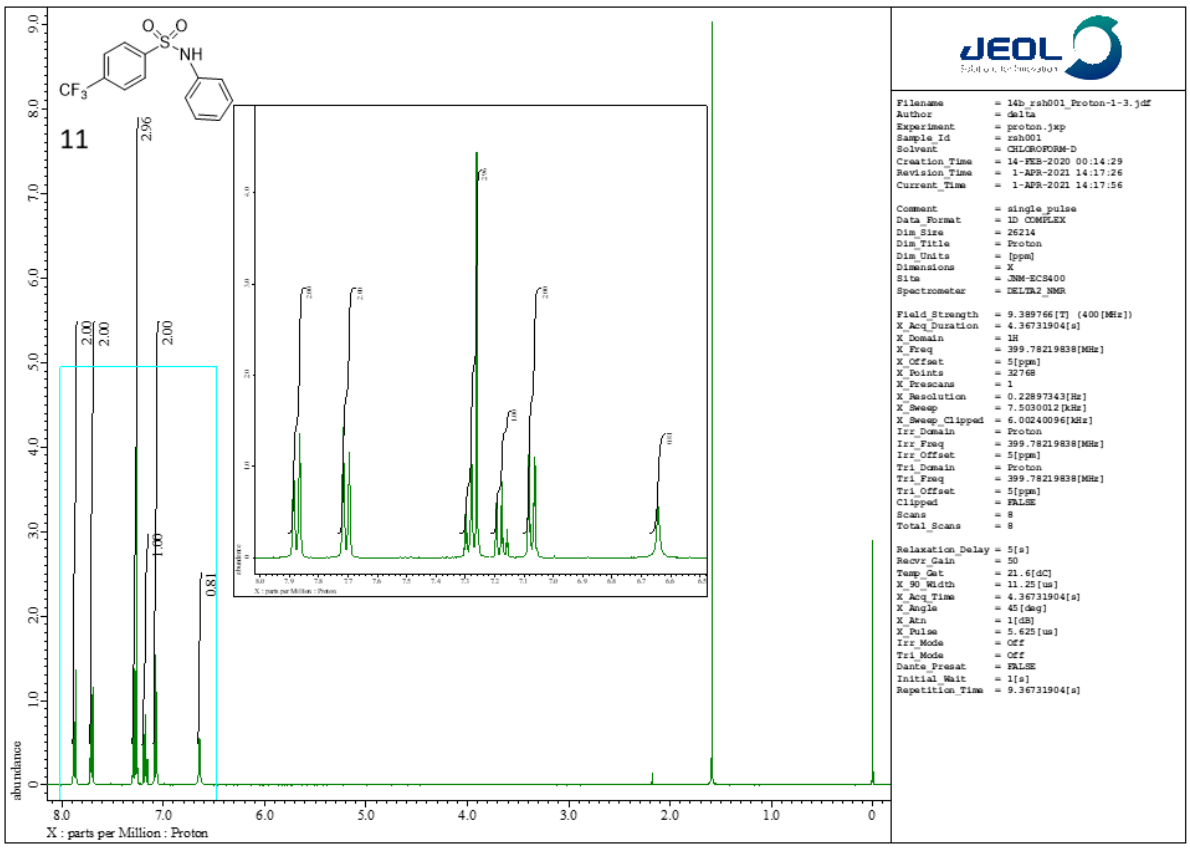


Fig S19 ^{1}H NMR Spectra of **11**

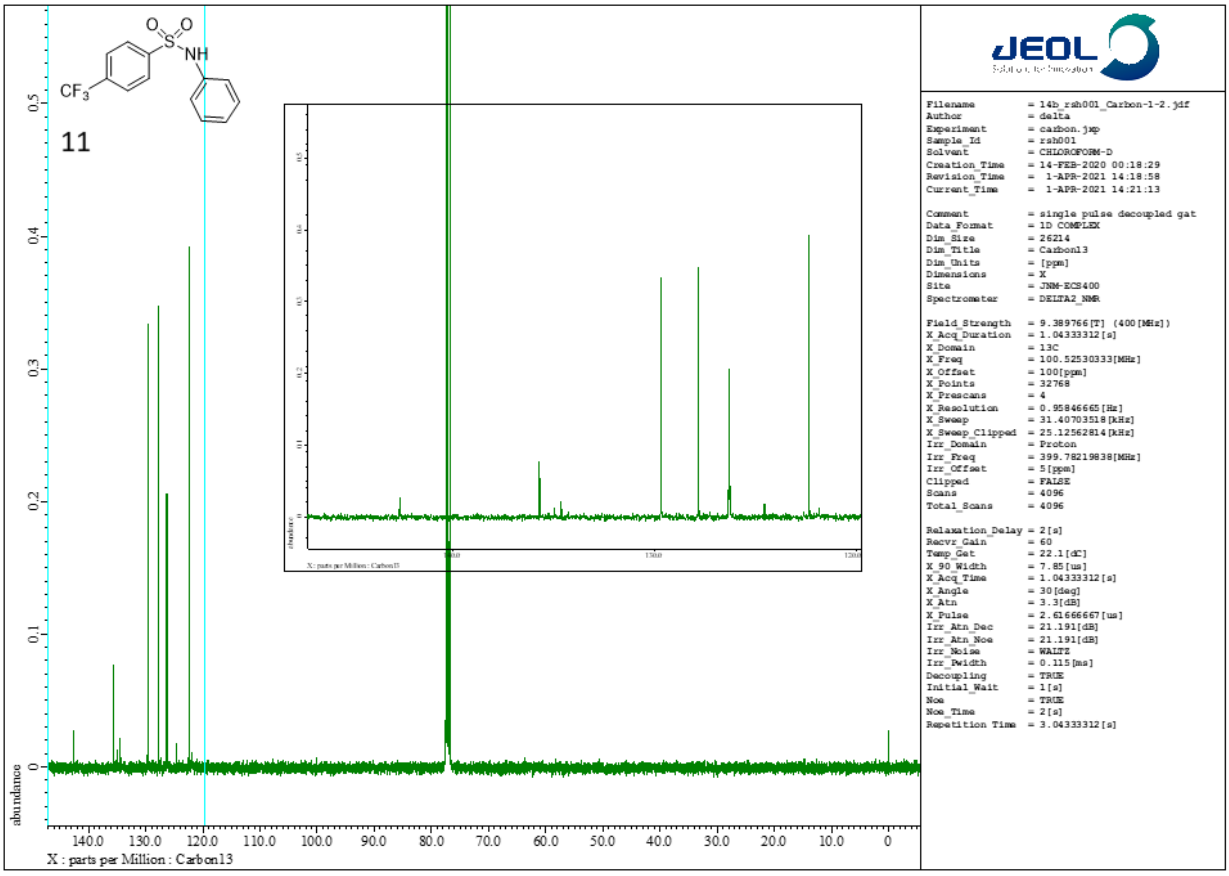


Fig S20 ^{13}C NMR Spectra of **11**

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	$C_{18}H_{15}NO_3S$	$C_{14}H_{15}NO_3S$	$C_{13}H_{12}FNO_2S$	$C_{15}H_{17}NO_2S$	$C_{12}H_9BrClNO_2S$	$C_{14}H_{14}ClNO_4S$	$C_{12}H_9Br_2NO_2S$	$C_{16}H_{12}FNO_2S$	$C_{13}H_{10}F_3NO_2S$
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	$P2_12_12_1$	$P2_12_12_1$	$P2_1/n$	$P\bar{1}$	$Pbca$	$P2_1/n$	$Pna2_1$	$Pbca$	$Pna2_1$
a/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)
b/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)
c/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)
α/°	90	90	90	82.341(5)	90	90	90	90	90
β/°	90	90	95.764(5)	84.612(5)	90	100.599(5)	90	90	90.757(6)
γ/°	90	90	90	84.720(5)	90	90	90	90	90
V/Å^3	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)
Z	4	4	4	4	8	4	4	8	4
T /K	93	93	93	93	120	93	93	93	93
μ/mm^{-1}	1.884	0.248	0.27	0.226	3.432	0.418	6.292	0.253	0.291
[a]GOF on F^2	1.089	1.012	1.073	1.016	1.063	1.036	1.086	1.029	1.092
Reflections collected (all d	20883	10788	18973	45577	21467	23555	10151	21952	20381
Independent reflections $I>$	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
R_{int}	0.0466	0.0174	0.1129	0.1726	0.1150	0.0775	0.0451	0.0668	0.1046
[b]R_1 [on F, $I>2\sigma(I)$]	0.0292	0.0241	0.0510	0.0774	0.0410	0.0418	0.0259	0.0385	0.0676
[c]wR_2 (on F^2, 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)	-	-	-	-	-	-	-
T_{min}	0.709	0.910	0.094	0.553	1.000	0.396	0.409	0.749	0.290
T_{max}	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

[a]GOF =$[\Sigma w(F_o^2-F_c^2)^2/(N_o-N_v)]^{1/2}$ (N_o; number of observations, N_v; number of variables), [b]$R_1 = \Sigma\ ||F_o| - |F_c|| / \Sigma\ |F_o|$, [c]$wR_2 = [\ \Sigma(w(F_o^2 - F_c^2)^2\ )/\Sigma w(F_o^2)^2]^{1/2}$.

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

	1c	**2c**	**3c**	**4c**	**5c**	**6c**	**7c**	**8c**	**9c**	**10c**	**11c**
Formula	$C_{56}H_{46}N_6O_6S_2$	$C_{24}H_{23}N_3O_3S$	$C_{23}H_{20}FN_3O_2S$	C25H24.82N3O2S	$C_{20}H_{19}Cl_3N_2O_4S$	$C_{24}H_{22}FN_3O_2S$	$C_{17}H_{13}BrClN_2O_2S$	$C_{20}H_{19}Cl_4N_2O_4S$	$C_{22}H_{17}Br_2N_3O_2S$	$C_{88}H_{68}F_3N_{11}O_6S$	$C_{23}H_{18}F_3N_3O_2S$
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	$P2_1/n$	$C2/c$	$P2_1/c$	$P2_1/c$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P2_1/c$	$P\bar{1}$
a/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)
b/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)
c/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)
α/°	90	90	90	90	85.3760(13)	80.489(4)	93.998(4)	85.3760(13)	76.2980(2)	90	82.9508(16)
β/°	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)
γ/°	90	90	90	90	80.6487(14)	87.660(3)	108.500(5)	80.6487(14)	71.5990(2)	90	76.4332(18)
V/Å^3	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)
Z	4	8	4	4	2	4	2	2	4	4	4
T /K	93	93	93	93	93	93	93	93	93	93	93
μ/mm^{-1}	0.17	0.172	0.194	0.173	0.514	0.189	2.695	0.631	3.845	0.171	0.206
[a]GOF on F^2	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 $I>2\sigma(I)$	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
R_{int}	0.1335	0.0684	0.0928	0.0465	0.0432	0.1223	0.0715	0.0432	0.0732	0.0763	0.0554
[b]R_1 [on F, $I>2\sigma(I)$]	0.057	0.0421	0.0632	0.0665	0.037	0.0951	0.0330	0.037	0.0538	0.0538	0.0484
[c]wR_2 (on F^2, 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	-	-	-	-	-	-	-	-	-	-	-
T_{min}	0.780	0.150	0.267	0.652	0.720	0.804	0.763	0.749	0.765	0.762	0.85
T_{max}	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^{-3}	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

[a]GOF =$[\Sigma w(F_o^2-F_c^2)^2/(N_o-N_v)]^{1/2}$ (N_o; number of observations, N_v; number of variables), [b]$R_1 = \Sigma\ ||F_o| - |F_c|| / \Sigma\ |F_o|$, [c]$wR_2 = [\ \Sigma(w(F_o^2 - F_c^2)^2\ )/\Sigma w(F_o^2)^2]^{1/2}$.

4. The difference Fourier map

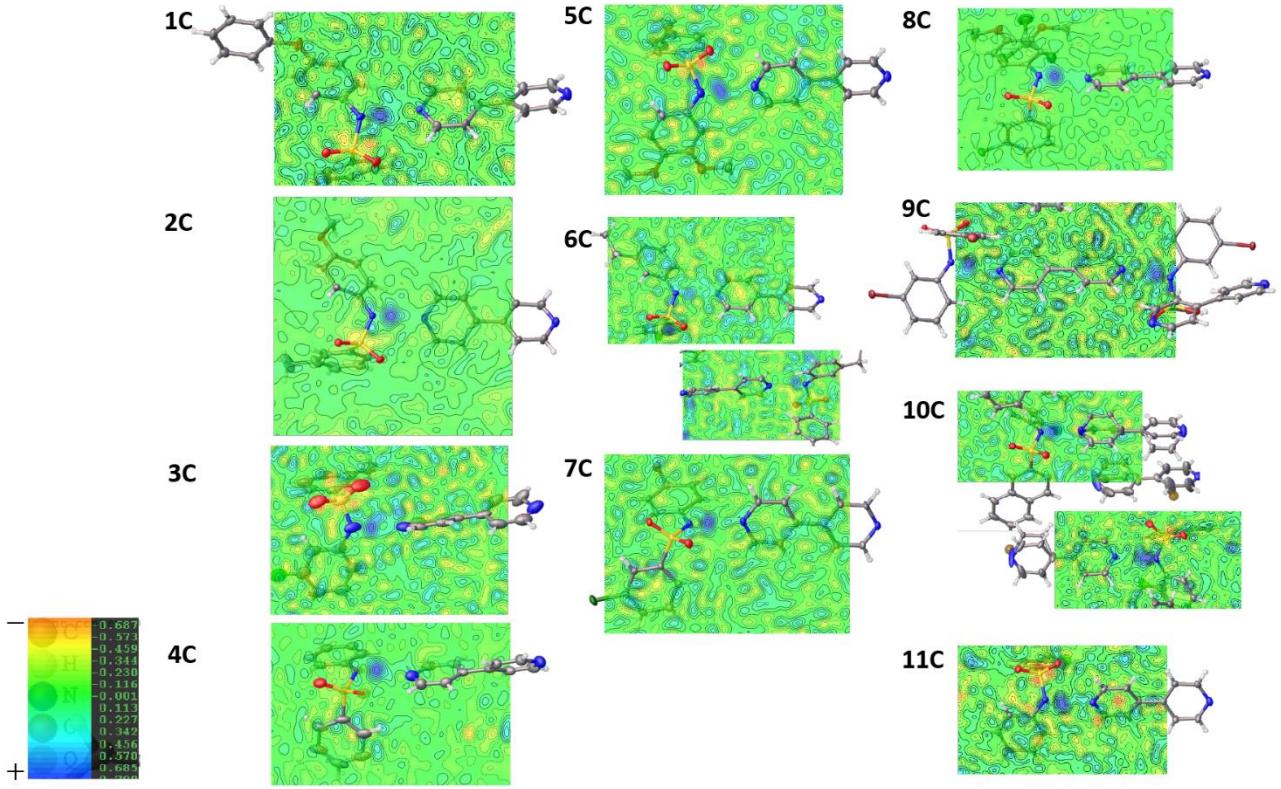


Fig S21 Difference Fourier map of the hydrogen-bonded section of the co-crystals of **1c-11c** calculated using Olex2. The blue area between the sulfonamide and **dpy** molecules indicates the location of the hydrogen.

5. The BFDH models of sulfonamides and co-crystals

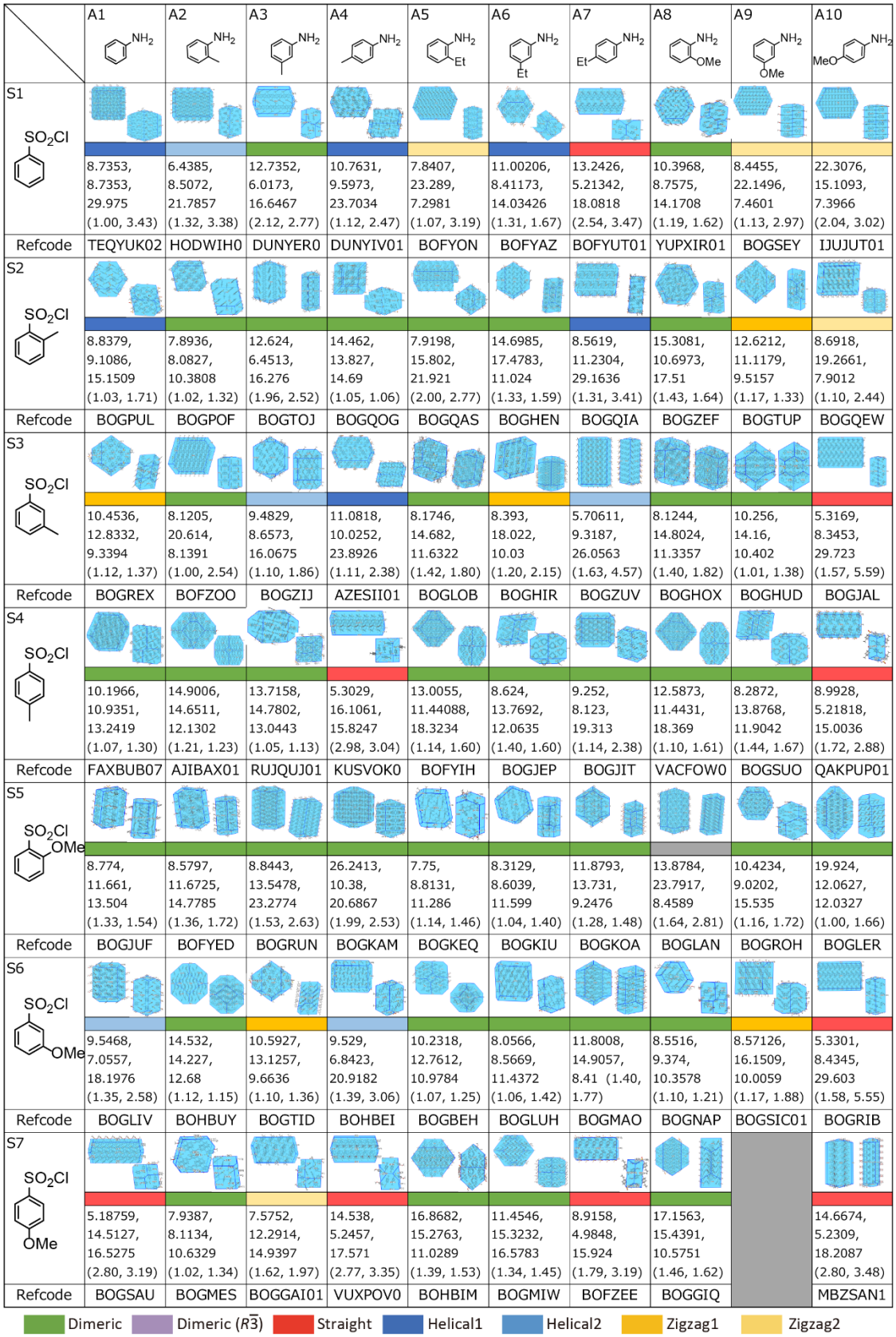


Fig S22 The BFDH model calculated using Mercury for the crystals in Fig 7. In each frame, the left-hand model is the front view of the widest face, and the right-hand model is the left figure rotated 90° horizontally.

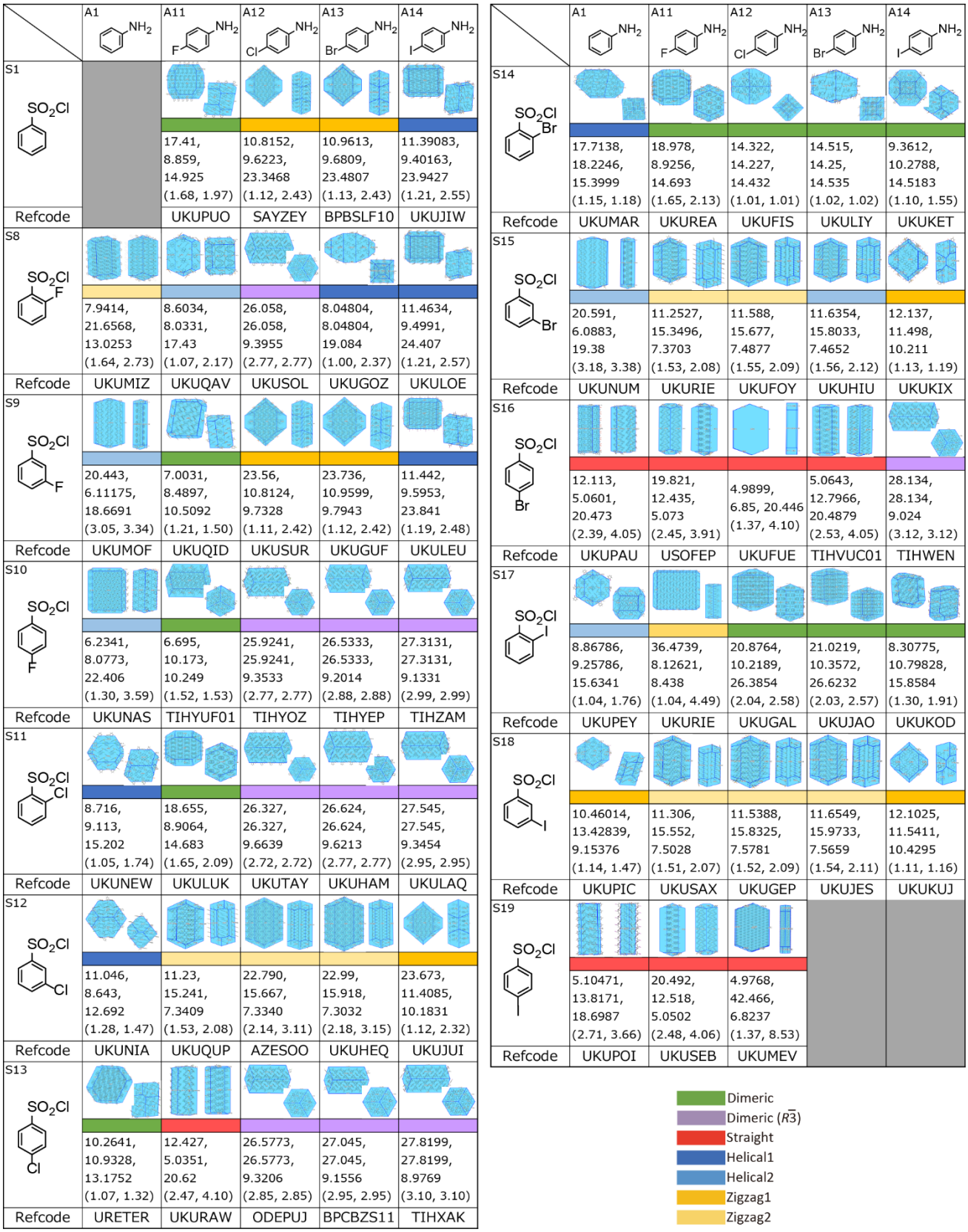
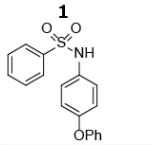
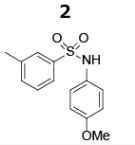
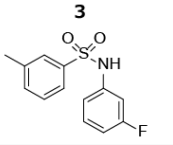
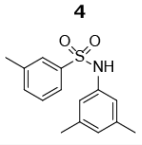
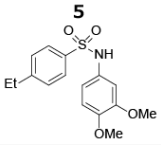
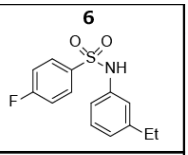
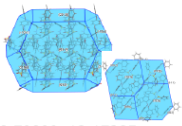
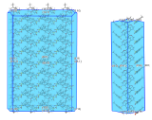
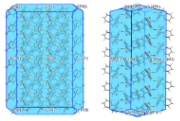
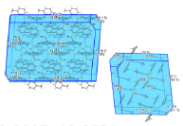
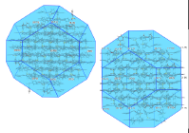
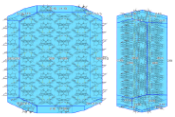
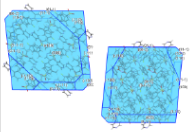
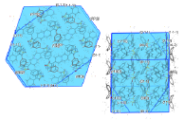
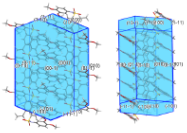
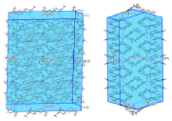


Fig S23 The BFDH model calculated using Mercury for the crystals in Fig 8. In each frame, the left-hand model is the front view of the widest face, and the right-hand model is the left figure rotated 90° horizontally.

	1	2	3	4	5	6
						
Sulfonamide	 8.79899, 12.17385, 15.22942 (1.38, 1.73)	 5.3169, 8.3453, 29.723 (1.57, 5.59)	 9.175, 5.9502, 22.5 (1.54, 3.78)	 9.0097, 12.3524, 12.9152 (1.37, 1.43)		
HB pattern	Helical1	Straight	Helical2	Helical1	amorphous	liquid
CCDC No./Refcode	2087464	BOGJAL	2087467	2087469		
	1c	2c	3c	4c	5c	6c
Cocrystal	 14.8313, 16.0368, 20.2334 (1.08, 1.36)	 31.8179, 8.1924, 17.861 (2.18, 3.88)	 10.2247, 13.3486, 15.0139 (1.31, 1.47)	 12.6562, 11.1186, 15.7821 (1.14, 1.42)	 8.3499, 11.4704, 13.571 (1.37, 1.63)	 10.0096, 12.4631, 17.7972 (1.25, 1.78)
CCDC No./Refcode	2087465	2087466	2087468	2087470	2087471	2087472

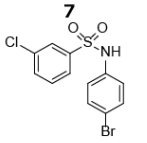
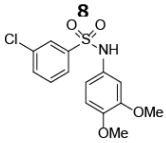
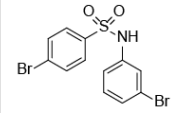
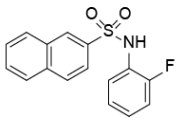
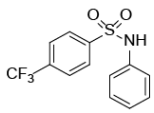
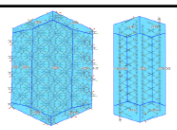
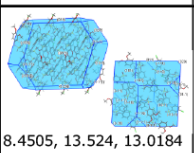
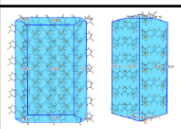
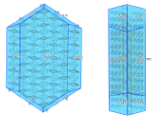
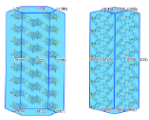
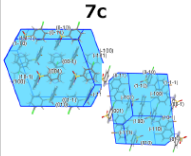
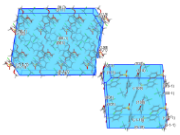
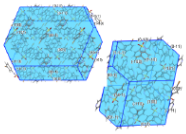
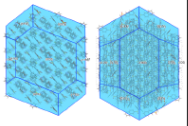
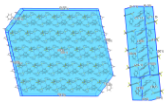
	7	8	9	10	11
					
Sulfonamide	 22.99, 15.918, 7.3032 (2.18, 3.15)	 8.4505, 13.524, 13.0184 (1.54, 1.60)	 9.958, 21.7896, 6.0999 (1.63, 3.57)	 11.5492, 7.5883, 31.0045 (1.52, 4.09)	 5.0813, 20.4639, 12.2504 (2.41, 4.03)
HB pattern	Zigzag2	Other	Helical2	Zigzag1	Straight
CCDC No./Refcode	UKUHEQ	2087474	2087476	2087478	2087480
	7c	8c	9c	10c	11c
Cocrystal	 8.4205, 9.8122, 11.2928 (1.17, 1.34)	 8.56656, 11.3193, 12.12655 (1.32, 1.42)	 11.7276, 14.3853, 16.9385 (1.23, 1.44)	 15.701, 30.2586, 17.029 (1.08, 1.93)	 8.24881, 9.01501, 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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