

Supplementary Information

New naphthalene-linked pyrazoline-thiazole hybrids as prominent anti-lung and anti-breast cancer agents

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2 **3-(4-Chlorophenyl)-1-(naphthalen-2-yl)prop-2-en-1-one (A1)** [33]. Yield: 90%. ¹H
3 NMR (600 MHz, CDCl₃): 7.42 (2H, d, *J* = 8.04 Hz), 7.56-7.63 (4H, m), 7.67 (1H, d, *J* =
4 15.54 Hz), 7.82 (1H, d, *J* = 15.66 Hz), 7.90 (1H, d, *J* = 7.92 Hz), 7.95 (1H, d, *J* = 8.52
5 Hz), 8.00 (1H, d, *J* = 8.28 Hz), 8.10 (1H, d, *J* = 8.58 Hz), 7.53 (1H, s). ¹³C NMR (150
6 MHz, CDCl₃): 122.57 (CH), 124.46 (CH), 126.90 (CH), 127.89 (CH), 128.50 (C),
7 128.69 (CH), 129.31 (2CH), 129.56 (CH), 129.68 (2CH), 130.15 (CH), 132.61 (CH),
8 133.51 (C), 135.43 (C), 135.62 (C), 136.47 (C), 143.28 (CH), 189.93 (C). For
9 C₁₉H₁₃ClO: MS (FAB) [M+H]⁺: *m/z* = 293.0.

10 **3-(4-Chlorophenyl)-1-(2-methoxynaphthalen-1-yl)prop-2-en-1-one (A2)** [34, 35]:
11 Yield: 90%. ¹H NMR (600 MHz, CDCl₃): 3.82 (3H, s), 7.09 (1H, d, *J* = 17.22 Hz), 7.27
12 (1H, d, *J* = 16.32 Hz), 7.31-7.34 (3H, m), 7.37 (1H, t, *J* = 7.68 Hz), 7.41-7.46 (3H, s),
13 7.69 (1H, d, *J* = 7.68 Hz), 7.83 (1H, d, *J* = 8.16 Hz), 7.94 (1H, d, *J* = 9.06 Hz). ¹³C NMR
14 (150 MHz, CDCl₃): 56.79 (CH₃), 113.28 (CH), 124.06 (CH), 124.22 (CH), 127.60 (CH),
15 128.16 (CH), 128.89 (CH), 129.19 (2CH), 129.26 (CH), 129.65 (2CH), 131.48 (2C),
16 131.52 (C), 133.24 (C), 136.48 (C), 143.90 (CH), 154.32 (C), 196.98 (C). For
17 C₂₀H₁₅ClO₂: MS (FAB⁺) [M+H]⁺: *m/z* = 322.9.

18 **5-(4-Chlorophenyl)-3-(naphthalen-2-yl)-4,5-dihydro-1H-pyrazole-1-**
19 **carbothioamide (B1)** [37]: Yield: 86%. ¹H NMR (600 MHz, CDCl₃): 3.31 (1H, dd, *J*_{AB}
20 = 17.52 Hz, *J*_{AX} = 3.84 Hz), 3.94 (1H, dd, *J*_{BA} = 17.40 Hz, *J*_{BX} = 11.40 Hz), 6.06 (1H, dd,
21 *J*_{BX} = 11.52 Hz, *J*_{AX} = 3.72 Hz), 6.19 (1H, bs), 7.20 (3H, d, *J* = 8.82 Hz), 7.30 (2H, d, *J*
22 = 8.82 Hz), 7.52-7.57 (2H, m), 7.83-7.88 (3H, m), 7.95 (1H, s), 8.00 (1H, d, *J* = 8.79
23 Hz). ¹³C NMR (150 MHz, CDCl₃): 43.11 (CH₂), 63.36 (CH), 123.10 (CH), 127.05
24 (2CH), 127.07 (CH), 127.80 (CH), 127.95 (CH), 128.02 (CH), 128.08 (CH), 128.55

(CH), 128.77 (C), 129.14 (2CH), 132.96 (C), 133.48 (C), 134.51 (C), 140.40 (C), 155.89 (C), 176.83 (C). For C₂₀H₁₆ClN₃S: MS (FAB) [M+H]⁺: m/z = 365.9.

5-(4-Chlorophenyl)-3-(2-methoxynaphthalen-1-yl)-4,5-dihydro-1H-pyrazole-1-

carbothioamide (B2): Yield: 86%. ¹H NMR (600 MHz, CDCl₃): 3.24 (1H, dd, *J*_{AB} = 18.12 Hz, *J*_{AX} = 3.24 Hz), 3.92 (3H, s), 3.95 (1H, dd, *J*_{BA} = 20.64 Hz, *J*_{BX} = 9.12 Hz), 6.04 (1H, dd, *J*_{BX} = 11.52 Hz, *J*_{AX} = 3.00 Hz), 7.03 (1H, bs), 7.30 (1H, d, *J* = 9.54 Hz), 7.36 (4H, s), 7.41 (1H, t, *J* = 6.54 Hz), 7.53 (1H, t, *J* = 8.04 Hz), 7.83 (1H, d, *J* = 7.50 Hz), 7.94 (1H, d, *J* = 9.00 Hz), 7.99 (1H, d, *J* = 8.28 Hz). ¹³C NMR (150 MHz, CDCl₃): 47.13 (CH₂), 56.37 (CH₃), 62.74 (CH), 112.66 (C), 123.71 (CH), 124.36 (CH), 127.49 (3CH), 127.99 (CH), 128.45 (CH), 128.98 (3CH), 132.03 (C), 132.10 (C), 133.40 (C), 140.53 (C), 156.05 (C), 156.49 (C), 177.09 (C). HRMS (FAB) calcd. for C₂₁H₁₈ClN₃OS [M+H]⁺: m/z = 396.0937, found: 396.0926.

1-(4-(4-(Cyanophenyl)thiazole-2-yl)-3-(naphthalen-2-yl)-5-(4-chlorophenyl)-2-

pyrazoline (BTT-1): Yield: 92%. ¹H NMR (600 MHz, DMSO-*d*₆): 3.53 (1H, dd, *J*_{AB} = 17.64 Hz, *J*_{AX} = 6.48 Hz), 4.20 (1H, dd, *J*_{BA} = 17.70 Hz, *J*_{BX} = 11.76 Hz), 5.78 (1H, dd, *J*_{BX} = 12.48 Hz, *J*_{AX} = 6.60 Hz), 7.45 (2H, d, *J* = 9.18 Hz), 7.49 (2H, d, *J* = 9.24 Hz), 7.57-7.60 (2H, m), 7.68 (1H, s), 7.83 (2H, d, *J* = 7.20 Hz), 7.90 (2H, d, *J* = 8.52 Hz), 7.97-8.02 (3H, m), 8.06 (1H, d, *J* = 8.55 Hz), 8.20 (1H, s). ¹³C NMR (150 MHz, DMSO-*d*₆): 42.85 (CH₂), 63.51 (CH), 108.49 (C), 119.13 (C, C≡N), 123.08 (CH), 126.05 (2CH), 126.90 (CH), 127.18 (CH), 127.28 (CH), 127.76 (CH), 128.32 (CH), 128.37 (C), 128.43 (2CH), 128.60 (2CH), 128.64 (2CH), 132.12 (C), 132.64 (2CH), 132.77 (C), 135.67 (C), 138.46 (C), 140.57 (C), 148.74 (C), 153.45 (C), 164.46 (C). HRMS (FAB) calcd. for C₂₉H₁₉ClN₄S [M+H]⁺: m/z = 490.0999, found: 490.1019.

1-(4-(4-(Nitrophenyl)thiazole-2-yl)-3-(naphthalen-2-yl)-5-(4-chlorophenyl)-2-

pyrazoline (BTT-2): Yield: 90%. ¹H NMR (600 MHz, DMSO-*d*₆): 3.55 (1H, dd, $J_{AB} = 17.76$ Hz, $J_{AX} = 6.60$ Hz), 4.20 (1H, dd, $J_{BA} = 17.10$ Hz, $J_{BX} = 12.48$ Hz), 5.79 (1H, dd, $J_{BX} = 10.50$ Hz, $J_{AX} = 6.60$ Hz), 7.46 (2H, d, $J = 9.84$ Hz), 7.51 (2H, d, $J = 8.58$ Hz), 7.58-7.61 (2H, m), 7.75 (1H, s), 7.97-8.02 (5H, m), 8.06 (1H, d, $J = 8.70$ Hz), 8.21 (1H, s), 8.24 (2H, d, $J = 9.54$ Hz). ¹³C NMR (150 MHz, DMSO-*d*₆): 42.66 (CH₂), 63.68 (CH), 109.37 (CH), 122.99 (CH), 124.06 (2CH), 126.32 (2CH), 126.90 (CH), 127.18 (CH), 127.29 (C), 127.77 (CH), 128.30 (CH), 128.39 (CH), 128.47 (CH), 128.63 (2CH), 128.77 (2CH), 132.18 (C), 132.79 (C), 133.55 (C), 140.37 (C), 140.46 (C), 146.28 (C), 148.44 (C), 153.53 (C), 164.49 (C). HRMS (FAB) calcd. for C₂₈H₁₉ClN₄O₂S [M+H]⁺ :m/z = 510.0926 found: 510.0917.

1-(4-(4-(Fluorophenyl)thiazole-2-yl)-3-(naphthalen-2-yl)-5-(4-chlorophenyl)-2-

pyrazoline (BTT-3) [42]: Yield: 88%. ¹H NMR (600 MHz, DMSO-*d*₆): 3.51 (1H, dd, $J_{AB} = 17.76$ Hz, $J_{AX} = 6.60$ Hz), 4.19 (1H, dd, $J_{BA} = 18.06$ Hz, $J_{BX} = 12.12$ Hz), 5.79 (1H, dd, $J_{BX} = 12.18$ Hz, $J_{AX} = 6.30$ Hz), 7.20 (2H, d, $J = 8.58$ Hz), 7.35 (1H, s), 7.44 (2H, d, $J = 8.58$ Hz), 7.48 (2H, d, $J = 8.22$ Hz), 7.57-7.60 (2H, m), 7.75-7.77 (2H, m), 7.96-8.02 (3H, m), 8.06 (1H, d, $J = 8.61$ Hz), 8.20 (1H, s). ¹³C NMR (150 MHz, DMSO-*d*₆): 42.95 (CH₂), 64.02 (CH), 104.54 (CH), 115.31 (CH), 115.44 (CH), 123.18 (CH), 126.87 (CH), 127.05 (CH), 127.24 (CH), 127.41 (CH), 127.48 (CH), 127.75 (C), 128.34 (CH), 128.42 (2CH), 128.58 (2CH), 128.62 (2CH), 131.01 (C), 132.05 (C), 132.79 (C), 133.48 (C), 140.75 (C), 149.42 (C), 153.04 (C), 160.79 (C), 164.29 (C). HRMS (FAB) calcd. for C₂₈H₁₉ClFN₃S [M+H]⁺ :m/z = 483.0956 found: 483.0972.

1-(4-(4-(Chlorophenyl)thiazole-2-yl)-3-(naphthalen-2-yl)-5-(4-chlorophenyl)-2-

pyrazoline (BTT-4) [42]: Yield: 84%. ¹H NMR (600 MHz, DMSO-*d*₆): 3.52 (1H, dd,

$J_{AB} = 18.06$ Hz, $J_{AX} = 6.60$ Hz), 4.19 (1H, dd, $J_{BA} = 17.10$ Hz, $J_{BX} = 11.22$ Hz), 5.77 (1H, dd, $J_{BX} = 11.82$ Hz, $J_{AX} = 6.54$ Hz), 7.44 (5H, t, $J = 8.52$ Hz), 7.48 (2H, d, $J = 8.58$ Hz), 7.58-7.59 (2H, m), 7.74 (2H, d, $J = 8.22$ Hz), 7.96-8.02 (3H, m), 8.06 (1H, d, $J = 8.37$ Hz), 8.20 (1H, s). ^{13}C NMR (150 MHz, DMSO- d_6): 43.30 (CH₂), 63.69 (CH), 105.92 (CH), 123.14 (CH), 126.87 (CH), 127.07 (CH), 127.19 (2CH), 127.26 (C), 128.36 (CH), 128.39 (CH), 128.41 (2CH), 128.57 (3CH), 128.66 (3CH), 131.98 (C), 132.09 (C), 132.79 (C), 133.26 (C), 133.47 (C), 140.66 (C), 149.24 (C), 153.15 (C), 164.35 (C). HRMS (FAB) calcd. for C₂₈H₁₉Cl₂N₃S [M+H]⁺ :m/z = 499.0660 found: 499.0667.

1-(4-(4-(Bromophenyl)thiazole-2-yl)-3-(naphthalen-2-yl)-5-(4-chlorophenyl)-2-

pyrazoline (BTT-5): Yield: 88%. ^1H NMR (600 MHz, DMSO- d_6): 3.52 (1H, dd, $J_{AB} = 17.76$ Hz, $J_{AX} = 6.42$ Hz), 4.19 (1H, dd, $J_{BA} = 17.58$ Hz, $J_{BX} = 11.76$ Hz), 5.77 (1H, dd, $J_{BX} = 11.88$ Hz, $J_{AX} = 6.42$ Hz), 7.44 (3H, d, $J = 6.84$ Hz), 7.48 (2H, d, $J = 9.42$ Hz), 7.56-7.59 (4H, m), 7.68 (2H, d, $J = 8.76$ Hz), 7.96-8.01 (3H, m), 8.06 (1H, d, $J = 8.67$ Hz), 8.19 (1H, s). ^{13}C NMR (150 MHz, DMSO- d_6): 42.93 (CH₂), 63.71 (CH), 105.50 (CH), 120.70 (C), 123.07 (CH), 126.89 (CH), 127.09 (CH), 127.22 (2CH), 127.46 (2CH), 127.76 (CH), 128.34 (CH), 128.38 (CH), 128.40 (CH), 128.57 (2CH), 128.66 (2CH), 131.47 (C), 132.07 (C), 132.79 (C), 133.48 (C), 133.59 (C), 140.66 (C), 149.28 (C), 153.15 (C), 164.35 (C). HRMS (FAB⁺) calcd. for C₂₈H₁₉BrClN₃S [M+H]⁺ :m/z = 543.0135 found: 543.0172.

1-(4-(4-(Methylphenyl)thiazole-2-yl)-3-(naphthalen-2-yl)-5-(4-chlorophenyl)-2-

pyrazoline (BTT-6): Yield: 86%. ^1H NMR (600 MHz, DMSO- d_6): 2.29 (3H, s), 3.50 (1H, dd, $J_{AB} = 17.52$ Hz, $J_{AX} = 6.84$ Hz), 4.18 (1H, dd, $J_{BA} = 17.10$ Hz, $J_{BX} = 11.52$ Hz), 5.76 (1H, dd, $J_{BX} = 12.84$ Hz, $J_{AX} = 6.42$ Hz), 7.17 (2H, d, $J = 8.16$ Hz), 7.28 (1H, s), 7.44 (2H, d, $J = 10.32$ Hz), 7.48 (2H, d, $J = 9.42$ Hz), 7.57-7.59 (2H, m), 7.61 (2H, d, J

= 7.74 Hz), 7.96-8.01 (3H, m), 8.06 (1H, d, $J = 8.67$ Hz), 8.19 (1H, s). ^{13}C NMR (150 MHz, DMSO- d_6): 20.60 (CH₃), 42.57 (CH₂), 63.64 (CH), 103.62 (CH), 123.04 (CH), 125.44 (2CH), 126.85 (CH), 126.97 (CH), 127.22 (CH), 127.73 (C), 128.34 (CH), 128.40 (CH), 128.47 (CH), 128.53 (2CH), 128.67 (2CH), 129.07 (2CH), 131.78 (C), 132.05 (C), 132.82 (C), 133.45 (C), 136.84 (C), 140.82 (C), 150.58 (C), 152.86 (C), 164.13 (C). HRMS (FAB⁺) calcd. for C₂₉H₂₂ClN₃S [M+H]⁺ :m/z = 479.1207 found: 479.1223.

1-(4-(4-(Methoxyphenyl)thiazole-2-yl)-3-(naphthalen-2-yl)-5-(4-chlorophenyl)-2-

pyrazoline (BTT-7) [42]: Yield: 88%. ^1H NMR (600 MHz, DMSO- d_6): 3.50 (1H, dd, $J_{AB} = 17.82$ Hz, $J_{AX} = 6.78$ Hz), 3.77 (3H, s), 4.18 (1H, dd, $J_{BA} = 17.40$ Hz, $J_{BX} = 11.76$ Hz), 5.76 (1H, dd, $J_{BX} = 11.94$ Hz, $J_{AX} = 6.60$ Hz), 6.93 (2H, d, $J = 9.48$ Hz), 7.19 (1H, s), 7.45 (2H, d, $J = 8.58$ Hz), 7.48 (2H, d, $J = 8.04$ Hz), 7.58-7.59 (2H, m), 7.65 (2H, d, $J = 8.28$ Hz), 7.96-8.01 (3H, m), 8.06 (1H, d, $J = 8.79$ Hz), 8.19 (1H, s). ^{13}C NMR (150 MHz, DMSO- d_6): 42.93 (CH₂), 55.03 (CH₃), 63.80 (CH), 102.11 (CH), 113.97 (2CH), 123.03 (CH), 126.81 (2CH), 126.86 (C), 126.97 (CH), 127.19 (C), 127.31 (CH), 127.74 (CH), 128.34 (CH), 128.42 (CH), 128.48 (CH), 128.55 (2CH), 128.67 (2CH), 132.06 (C), 132.77 (C), 133.48 (C), 140.89 (C), 150.35 (C), 152.78 (C), 158.86 (C), 164.17 (C). HRMS (FAB⁺) calcd. for C₂₉H₂₂ClN₃OS [M+H]⁺ :m/z = 495.1172 found: 495.1172.

1-(4-(4-(Trifluoromethylphenyl)thiazole-2-yl)-3-(naphthalen-2-yl)-5-(4-

chlorophenyl)-2-pyrazoline (BTT-8): Yield: 84%. ^1H NMR (600 MHz, DMSO- d_6): 3.54 (1H, dd, $J_{AB} = 17.34$ Hz, $J_{AX} = 6.30$ Hz), 4.20 (1H, dd, $J_{BA} = 17.70$ Hz, $J_{BX} = 11.76$ Hz), 5.79 (1H, dd, $J_{BX} = 12.00$ Hz, $J_{AX} = 6.60$ Hz), 7.46 (2H, d, $J = 8.40$ Hz), 7.50 (2H, d, $J = 8.64$ Hz), 7.59-7.62 (3H, m), 7.74 (2H, d, $J = 8.28$ Hz), 7.94 (2H, d, $J = 8.16$ Hz), 7.97-8.02 (3H, m), 8.07 (1H, d, $J = 8.55$ Hz), 8.21 (1H, s). ^{13}C NMR (150 MHz, DMSO-

d_6): 43.13 (CH₂), 63.61 (CH), 107.18 (CH), 123.05 (CH), 125.53 (C), 126.01 (2CH), 126.89 (CH), 127.12 (CH), 127.24 (CH), 127.76 (C), 128.37 (2CH), 128.45 (2CH), 128.48 (CH), 128.59 (2CH), 128.75 (2CH), 132.16 (C), 132.78 (2C), 133.50 (C), 138.09 (C), 140.58 (C), 148.94 (C), 153.34 (C), 164.44 (C). HRMS (FAB⁺) calcd. for C₂₉H₁₉ClF₃N₃S [M+H]⁺: m/z = 533.0923 found: 533.0940.

1-(4-(4-(Trifluoromethoxyphenyl)thiazole-2-yl)-3-(naphthalen-2-yl)-5-(4-chlorophenyl)-2-pyrazoline (BTT-9): Yield: 86%. ¹H NMR (600 MHz, DMSO- d_6): 3.53 (1H, dd, J_{AB} = 17.28 Hz, J_{AX} = 6.00 Hz), 4.20 (1H, dd, J_{BA} = 17.82 Hz, J_{BX} = 12.30 Hz), 5.77 (1H, dd, J_{BX} = 12.30 Hz, J_{AX} = 7.02 Hz), 7.37 (2H, d, J = 8.28 Hz), 7.45 (3H, d, J = 7.14 Hz), 7.49 (2H, d, J = 8.28 Hz), 7.58-7.60 (2H, m), 7.84 (2H, d, J = 9.24 Hz), 7.97-8.02 (3H, m), 8.07 (1H, d, J = 8.28 Hz), 8.20 (1H, s). ¹³C NMR (150 MHz, DMSO- d_6): 43.12 (CH₂), 63.82 (CH), 105.70 (CH), 121.16 (2CH), 123.01 (CH), 126.88 (CH), 127.09 (CH), 127.20 (2CH), 127.74 (CH), 128.35 (CH), 128.38 (CH), 128.41 (CH), 128.57 (2CH), 128.65 (2CH), 132.10 (2C), 132.78 (2C), 133.50 (C), 133.67 (C), 140.64 (C), 147.56 (C), 149.01 (C), 153.17 (C), 164.40 (C). HRMS (FAB⁺) calcd. for C₂₉H₁₉ClF₃N₃OS [M+H]⁺: m/z = 549.0903 found: 549.0889.

1-(4-(4-(Methylsulfonylphenyl)thiazole-2-yl)-3-(naphthalen-2-yl)-5-(4-chlorophenyl)-2-pyrazoline (BTT-10): Yield: 82%. ¹H NMR (600 MHz, DMSO- d_6): 3.22 (3H, s), 3.50 (1H, dd, J_{AB} = 17.82 Hz, J_{AX} = 6.78 Hz), 4.21 (1H, dd, J_{BA} = 17.52 Hz, J_{BX} = 11.76 Hz), 5.79 (1H, dd, J_{BX} = 12.06 Hz, J_{AX} = 7.02 Hz), 7.47 (2H, d, J = 8.76 Hz), 7.51 (2H, d, J = 7.98 Hz), 7.59-7.60 (2H, m), 7.67 (1H, s), 7.92 (2H, d, J = 8.52 Hz), 7.98 (3H, d, J = 8.28 Hz), 7.99-8.03 (2H, m), 8.07 (1H, d, J = 8.52 Hz), 8.22 (1H, s). ¹³C NMR (150 MHz, DMSO- d_6): 43.00 (CH₃), 43.63 (CH₂), 63.72 (CH), 108.08 (CH), 123.03 (CH), 126.03 (2CH), 126.89 (CH), 127.13 (CH), 127.25 (CH), 127.42 (2CH),

127.75 (C), 128.34 (CH), 128.37 (CH), 128.43 (CH), 128.58 (2CH), 128.79 (2CH),
132.14 (C), 132.77 (C), 133.52 (C), 138.88 (C), 139.25 (C), 140.52 (C), 148.81 (C),
153.36 (C), 164.40 (C). HRMS (FAB⁺) calcd. for C₂₉H₂₂ClN₃O₂S₂ [M+H]⁺ :m/z =
543.0842 found: 543.0842.

1-(4-(4-(Cyanophenyl)thiazole-2-yl)-3-(2-methoxynaphthalen-1-yl)-5-(4-

chlorophenyl)-2-pyrazoline (BTP-1): Yield: 83%. ¹H NMR (600 MHz, CDCl₃): 3.46
(1H, dd, *J*_{AB} = 18.00 Hz, *J*_{AX} = 6.72 Hz), 3.96 (3H, s), 3.99 (1H, dd, *J*_{BA} = 18.18 Hz, *J*_{BX}
= 12.30 Hz), 5.67 (1H, dd, *J*_{BX} = 12.03 Hz, *J*_{AX} = 7.02 Hz), 6.97 (1H, s), 7.31 (1H, d, *J* =
11.04 Hz), 7.37-7.42 (3H, m), 7.51-7.56 (3H, m), 7.62 (2H, d, *J* = 7.92 Hz), 7.78 (2H, d,
J = 7.92 Hz), 7.84 (1H, d, *J* = 9.60 Hz), 7.93 (1H, d, *J* = 11.40 Hz), 8.24 (1H, d, *J* = 8.52
Hz). ¹³C NMR (150 MHz, CDCl₃): 47.44 (CH₂), 56.72 (CH₃), 63.82 (CH), 106.79 (CH),
110.96 (C), 112.66 (CH), 114.36 (CH), 119.46 (C, C≡N), 124.25 (CH), 124.33 (CH),
126.24 (2CH), 128.31 (3CH), 128.90 (2CH), 129.17 (CH), 131.71 (2C), 132.42 (2CH),
132.47 (C), 133.52 (C), 139.07 (C), 140.40 (C), 149.71 (C), 152.05 (C), 156.08 (C),
165.72 (C). HRMS (FAB⁺) calcd. for C₃₀H₂₁ClN₄OS [M+H]⁺ :m/z = 520.1125, found:
520.1104.

1-(4-(4-(Nitrophenyl)thiazole-2-yl)-3-(2-methoxynaphthalen-1-yl)-5-(4-

chlorophenyl)-2-pyrazoline (BTP-2): Yield: 84%. ¹H NMR (600 MHz, CDCl₃): 3.47
(1H, dd, *J*_{AB} = 17.46 Hz, *J*_{AX} = 6.48 Hz), 3.97 (3H, s), 3.99 (1H, dd, *J*_{BA} = 18.06 Hz, *J*_{BX}
= 12.24 Hz), 5.68 (1H, dd, *J*_{BX} = 11.64 Hz, *J*_{AX} = 7.08 Hz), 7.03 (1H, s), 7.31 (1H, d, *J* =
9.06 Hz), 7.38-7.42 (3H, m), 7.52-7.56 (3H, m), 7.81-7.84 (3H, m), 7.93 (1H, d, *J* = 8.01
Hz), 8.20 (2H, d, *J* = 9.06 Hz), 8.24 (1H, d, *J* = 11.28 Hz). ¹³C NMR (150 MHz, CDCl₃):
47.60 (CH₂), 56.56 (CH₃), 63.98 (CH), 107.56 (CH), 112.74 (C), 114.28 (CH), 123.99
(2CH), 124.19 (CH), 124.29 (CH), 126.26 (2CH), 127.73 (CH), 128.32 (3CH), 128.90

(2CH), 129.14 (C), 131.65 (CH), 132.42 (C), 133.66 (C), 140.36 (C), 140.88 (C), 146.73 (C), 149.34 (C), 152.20 (C), 156.01 (C), 165.80 (C). HRMS (FAB⁺) calcd. for C₂₉H₂₁N₄ClS [M+H]⁺: m/z = 540.1023, found: 540.1022.

1-(4-(4-(Fluorophenyl)thiazole-2-yl)-3-(2-methoxynaphthalen-1-yl)-5-(4-

chlorophenyl)-2-pyrazoline (BTP-3): Yield: 85%. ¹H NMR (600 MHz, CDCl₃): 3.44

(1H, dd, *J*_{AB} = 17.76 Hz, *J*_{AX} = 6.48 Hz), 3.96 (3H, s), 3.98 (1H, dd, *J*_{BA} = 18.06 Hz, *J*_{BX} = 11.82 Hz), 5.69 (1H, bs), 6.74 (1H, s), 7.03 (2H, t, *J* = 9.00 Hz), 7.31 (1H, d, *J* = 9.00 Hz), 7.37-7.42 (3H, m), 7.52-7.55 (3H, m), 7.65-7.68 (2H, m), 7.83 (1H, d, *J* = 7.50 Hz),

7.93 (1H, d, *J* = 9.54 Hz), 8.25 (1H, d, *J* = 8.52 Hz). ¹³C NMR (150 MHz, CDCl₃): 47.44

(CH₂), 56.56 (CH₃), 63.82 (CH), 102.96 (CH), 112.77 (C), 115.21 (CH), 115.42 (CH),

124.11 (CH), 127.55 (2CH, d, *J* = 10.14 Hz), 127.71 (CH), 128.28 (2CH), 128.39 (3CH),

128.80 (3CH), 129.16 (C), 131.56 (C), 132.54 (C), 133.41 (C), 140.58 (C), 156.05 (2C),

161.65 (C), 163.35 (C), 165.67 (C). HRMS (FAB⁺) calcd. for C₂₉H₂₁ClFN₃OS [M+H]⁺

: m/z = 513.1071, found: 513.1078.

1-(4-(4-(Chlorophenyl)thiazole-2-yl)-3-(2-methoxynaphthalen-1-yl)-5-(4-

chlorophenyl)-2-pyrazoline (BTP-4): Yield: 88%. ¹H NMR (600 MHz, CDCl₃): 3.45

(1H, dd, *J*_{AB} = 18.06 Hz, *J*_{AX} = 6.54 Hz), 3.96 (3H, s), 3.98 (1H, dd, *J*_{BA} = 18.00 Hz, *J*_{BX} = 12.00 Hz), 5.68 (1H, bs), 6.80 (1H, s), 7.30 (3H, d, *J* = 9.06 Hz), 7.36-7.41 (3H, m),

7.52-7.56 (3H, m), 7.63 (2H, d, *J* = 7.02 Hz), 7.83 (1H, d, *J* = 7.02 Hz), 7.93 (1H, d, *J* =

10.02 Hz), 8.25 (1H, d, *J* = 8.04 Hz). ¹³C NMR (150 MHz, CDCl₃): 47.42 (CH₂), 56.39

(CH₃), 63.92 (CH), 103.81 (CH), 112.76 (C), 124.13 (CH), 124.38 (CH), 127.17 (2CH),

127.76 (C), 128.27 (CH), 128.42 (3CH), 128.61 (3CH), 128.82 (3CH), 129.18 (C),

131.59 (C), 132.48 (C), 133.44 (C), 140.53 (C), 156.05 (2C), 158.21 (C), 165.65 (C).

HRMS (FAB⁺) calcd. for C₂₉H₂₁Cl₂N₃OS [M+H]⁺: m/z = 529.0782, found: 529.0782.

1-(4-(4-(Bromophenyl)thiazole-2-yl)-3-(2-methoxynaphthalen-1-yl)-5-(4-

chlorophenyl)-2-pyrazoline (BTP-5): Yield: 86%. ¹H NMR (600 MHz, CDCl₃): 3.44

(1H, dd, $J_{AB} = 17.70$ Hz, $J_{AX} = 6.66$ Hz), 3.95 (3H, s), 3.97 (1H, dd, $J_{BA} = 18.30$ Hz, J_{BX}

= 11.88 Hz), 5.67 (1H, dd, $J_{BX} = 12.18$ Hz, $J_{AX} = 6.66$ Hz), 6.81 (1H, s), 7.30 (1H, d, $J =$

9.18 Hz), 7.37 (2H, d, $J = 8.76$ Hz), 7.39-7.41 (1H, m), 7.45 (2H, d, $J = 9.06$ Hz), 7.51-

7.57 (5H, m), 7.82 (1H, d, $J = 8.52$ Hz), 7.92 (1H, d, $J = 9.18$ Hz), 8.25 (1H, d, $J = 8.76$

Hz). ¹³C NMR (150 MHz, CDCl₃): 47.19 (CH₂), 56.13 (CH₃), 64.15 (CH), 104.09 (CH),

112.58 (C), 121.37 (C), 124.15 (CH), 127.47 (3CH), 127.75 (2CH), 128.28 (2CH),

128.80 (3CH), 129.16 (C), 131.58 (3CH), 132.52 (C), 133.46 (C), 134.00 (C), 140.55

(C), 150.45 (C), 151.68 (C), 156.05 (C), 165.63 (C). HRMS (FAB⁺) calcd. for

C₂₉H₂₁BrClN₃OS [M+H]⁺ :m/z = 573.0266, found: 575.0257.

1-(4-(4-(Methylphenyl)thiazole-2-yl)-3-(2-methoxynaphthalen-1-yl)-5-(4-

chlorophenyl)-2-pyrazoline (BTP-6): Yield: 87%. ¹H NMR (600 MHz, CDCl₃): 2.34

(3H, s), 3.44 (1H, dd, $J_{AB} = 17.82$ Hz, $J_{AX} = 6.66$ Hz), 3.95 (3H, s), 3.98 (1H, bs), 5.69

(1H, dd, $J_{BX} = 11.52$ Hz, $J_{AX} = 6.54$ Hz), 6.75 (1H, s), 7.15 (2H, d, $J = 10.02$ Hz), 7.29

(1H, d, $J = 10.02$ Hz), 7.36 (2H, d, $J = 8.04$ Hz), 7.40 (1H, d, $J = 7.32$ Hz), 7.54 (3H, d,

$J = 7.98$ Hz), 7.59 (2H, d, $J = 8.04$ Hz), 7.82 (1H, d, $J = 7.02$ Hz), 7.92 (1H, d, $J = 8.52$

Hz), 8.26 (1H, d, $J = 8.52$ Hz). ¹³C NMR (150 MHz, CDCl₃): 21.48 (CH₃), 47.43 (CH₂),

56.41 (CH₃), 64.29 (CH), 102.77 (CH), 112.81 (C), 124.13 (CH), 124.44 (CH), 125.83

(2CH), 127.73 (CH), 128.23 (CH), 128.48 (3CH), 128.74 (2CH), 129.14 (3CH), 131.49

(C), 132.40 (C), 132.57 (C), 133.33 (C), 137.21 (C), 140.71 (C), 151.29 (C), 151.54 (C),

154.96 (C), 165.45 (C). HRMS (FAB⁺) calcd. for C₃₀H₂₄ClN₃OS [M+H]⁺ :m/z =

509.1328, found: 509.1329.

1-(4-(4-(Methoxyphenyl)thiazole-2-yl)-3-(2-methoxynaphthalen-1-yl)-5-(4-chlorophenyl)-2-pyrazoline (BTP-7): Yield: 85%. ^1H NMR (600 MHz, CDCl_3): 3.43 (1H, dd, $J_{AB} = 18.18$ Hz, $J_{AX} = 6.90$ Hz), 3.82 (3H, s), 3.95 (3H, s), 3.97 (1H, d, $J_{BX} = 11.76$ Hz), 5.69 (1H, dd, $J_{BX} = 11.28$ Hz, $J_{AX} = 7.02$ Hz), 6.67 (1H, s), 6.88 (2H, d, $J = 9.54$ Hz), 7.30 (1H, d, $J = 9.54$ Hz), 7.37 (2H, d, $J = 8.52$ Hz), 7.40 (1H, d, $J = 7.44$ Hz), 7.53-7.55 (3H, m), 7.64 (2H, d, $J = 9.30$ Hz), 7.82 (1H, d, $J = 8.04$ Hz), 7.92 (1H, d, $J = 9.03$ Hz), 8.26 (1H, d, $J = 8.52$ Hz). ^{13}C NMR (150 MHz, CDCl_3): 47.48 (CH_2), 55.40 (CH_3), 56.37 (CH_3), 64.06 (CH), 101.69 (CH), 112.81 (C), 113.86 (2CH), 124.13 (CH), 124.44 (CH), 127.15 (2CH), 127.69 (2CH), 128.25 (2CH), 128.44 (2CH), 128.77 (2CH), 129.19 (C), 131.59 (C), 132.59 (C), 133.41 (C), 140.82 (C), 151.37 (C), 156.01 (2C), 159.17 (C), 165.55 (C). HRMS (FAB $^+$) calcd. for $\text{C}_{30}\text{H}_{24}\text{ClN}_3\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$:m/z = 525.1281, found: 525.1278.

1-(4-(4-(Trifluoromethylphenyl)thiazole-2-yl)-3-(2-methoxynaphthalen-1-yl)-5-(4-chlorophenyl)-2-pyrazoline (BTP-8): Yield: 84%. ^1H NMR (600 MHz, CDCl_3): 3.45 (1H, dd, $J_{AB} = 18.06$ Hz, $J_{AX} = 6.78$ Hz), 3.96 (3H, s), 3.99 (1H, dd, $J_{BA} = 17.94$ Hz, $J_{BX} = 11.76$ Hz), 5.68 (1H, dd, $J_{BX} = 11.76$ Hz, $J_{AX} = 6.54$ Hz), 6.92 (1H, s), 7.31 (1H, d, $J = 8.76$ Hz), 7.38 (2H, d, $J = 8.28$ Hz), 7.41 (1H, t, $J = 7.32$ Hz), 7.52-7.56 (3H, m), 7.59 (2H, d, $J = 8.04$ Hz), 7.79 (2H, d, $J = 8.04$ Hz), 7.83 (1H, d, $J = 8.04$ Hz), 7.93 (1H, d, $J = 9.06$ Hz), 8.25 (1H, d, $J = 7.98$ Hz). ^{13}C NMR (150 MHz, CDCl_3): 47.41 (CH_2), 56.55 (CH_3), 63.99 (CH), 105.51 (CH), 112.80 (C), 124.15 (CH), 124.35 (CH), 125.47 (C, CF_3), 125.99 (2CH), 127.75 (2CH), 128.31 (2CH), 128.39 (3CH), 128.84 (3CH), 129.17 (C), 131.61 (C), 132.49 (C), 133.49 (C), 138.30 (C), 140.48 (C), 150.15 (C), 151.86 (C), 156.06 (C), 165.72 (C). HRMS (FAB $^+$) calcd. for $\text{C}_{30}\text{H}_{21}\text{ClF}_3\text{N}_3\text{OS}$ $[\text{M}+\text{H}]^+$:m/z = 563.1066, found: 563.1046.

1-(4-(4-(Trifluoromethoxyphenyl)thiazole-2-yl)-3-(2-methoxynaphthalen-1-yl)-5-

(4-chlorophenyl)-2-pyrazoline (BTP-9): Yield: 88%. ¹H NMR (600 MHz, CDCl₃):

3.44 (1H, dd, $J_{AB} = 17.64$ Hz, $J_{AX} = 6.30$ Hz), 3.96 (3H, s), 3.98 (1H, dd, $J_{BA} = 17.88$ Hz, $J_{BX} = 11.82$ Hz), 5.67 (1H, dd, $J_{BX} = 11.58$ Hz, $J_{AX} = 6.54$ Hz), 6.80 (1H, s), 7.18 (2H, d, $J = 8.04$ Hz), 7.30 (1H, d, $J = 9.06$ Hz), 7.37 (2H, d, $J = 8.52$ Hz), 7.40 (1H, t, $J = 7.56$ Hz), 7.51-7.56 (3H, m), 7.70 (2H, d, $J = 8.82$ Hz), 7.83 (1H, d, $J = 7.56$ Hz), 7.92 (1H, d, $J = 8.82$ Hz), 8.25 (1H, d, $J = 8.52$ Hz). ¹³C NMR (150 MHz, CDCl₃): 47.49 (CH₂), 56.40 (CH₃), 63.84 (CH), 104.00 (CH), 112.76 (C), 120.97 (2CH), 124.11 (CH), 124.38 (CH), 127.21 (2CH), 127.73 (2CH), 128.29 (2CH), 128.36 (2CH), 128.82 (2CH), 129.16 (C), 131.57 (C), 132.53 (C), 133.43 (C), 133.83 (C), 140.56 (C), 148.48 (C), 150.20 (C), 151.69 (C), 156.06 (C), 165.69 (C). HRMS (FAB⁺) calcd. for C₃₀H₂₁ClF₃N₃O₂S [M+H]⁺ :m/z = 579.1000, found: 579.0995.

1-(4-(4-(Methylsulfonylphenyl)thiazole-2-yl)-3-(2-methoxynaphthalen-1-yl)-5-(4-

chlorophenyl)-2-pyrazoline (BTP-10): Yield: 80%. ¹H NMR (600 MHz, CDCl₃): 3.22

(3H, s), 3.56 (1H, dd, $J_{AB} = 17.76$ Hz, $J_{AX} = 6.72$ Hz), 3.99 (3H, s), 4.00 (1H, dd, $J_{BA} = 18.00$ Hz, $J_{BX} = 11.76$ Hz), 5.68 (1H, dd, $J_{BX} = 11.94$ Hz, $J_{AX} = 6.78$ Hz), 6.99 (1H, s), 7.31 (1H, d, $J = 9.06$ Hz), 7.38 (1H, d, $J = 8.04$ Hz), 7.41 (2H, t, $J = 7.50$ Hz), 7.52-7.56 (3H, m), 7.83 (1H, d, $J = 8.52$ Hz), 7.86 (2H, d, $J = 8.52$ Hz), 7.90 (2H, d, $J = 8.76$ Hz), 7.94 (1H, d, $J = 8.82$ Hz), 8.25 (1H, d, $J = 8.82$ Hz). ¹³C NMR (150 MHz, CDCl₃): 44.78 (CH₃), 47.26 (CH₂), 56.71 (CH₃), 63.84 (CH), 106.91 (CH), 112.80 (C), 124.16 (CH), 124.29 (CH), 126.49 (2CH), 127.72 (2CH), 127.76 (CH), 128.32 (CH), 128.37 (2CH), 128.85 (3CH), 129.16 (CH), 131.66 (C), 132.46 (C), 133.54 (C), 138.78 (C), 140.06 (C), 140.38 (C), 149.57 (C), 152.07 (C), 156.09 (C), 165.76 (C). HRMS (FAB⁺) calcd. for C₃₀H₂₄ClN₃O₃S₂ [M+H]⁺ :m/z = 573.0938, found: 573.0948.

1 Supplementary Figures

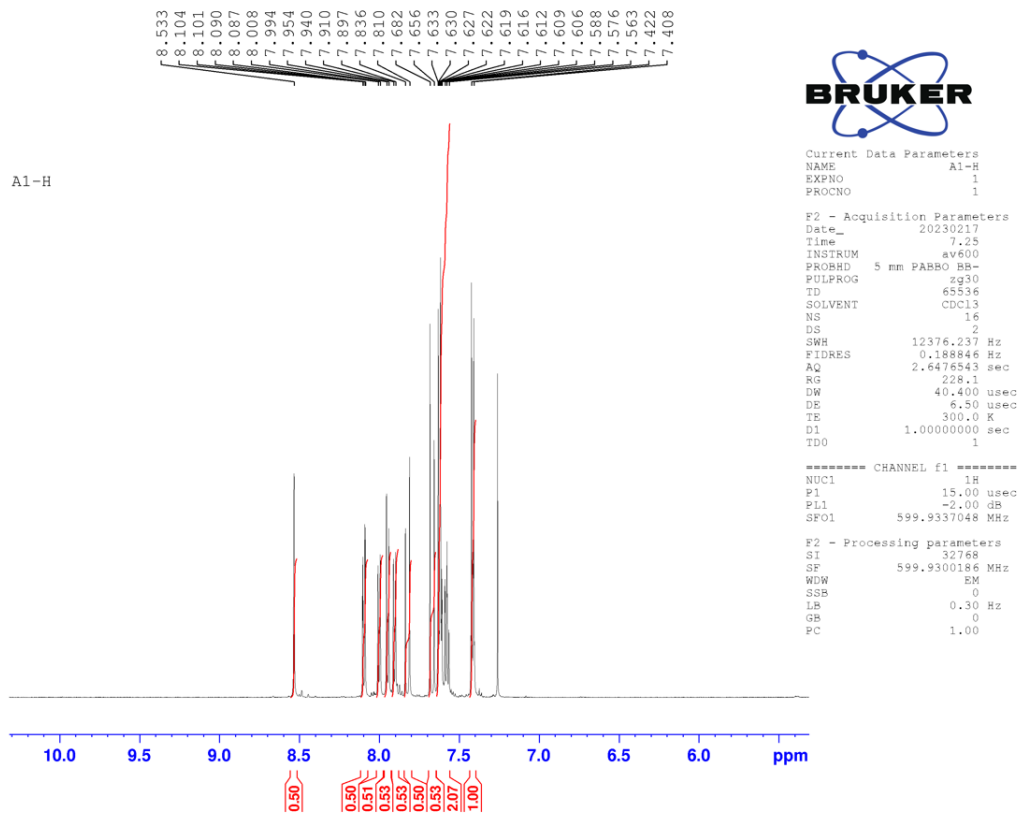
- 2 Figure S1: ^1H NMR Spectrum of **A1**
- 3 Figure S2: ^{13}C NMR Spectrum of **A1**
- 4 Figure S3: Mass Spectrum of **A1**
- 5 Figure S4: ^1H NMR Spectrum of **A2**
- 6 Figure S5: ^{13}C NMR Spectrum of **A2**
- 7 Figure S6: Mass Spectrum of **A2**
- 8 Figure S7: ^1H NMR Spectrum of **B1**
- 9 Figure S8: ^{13}C NMR Spectrum of **B1**
- 10 Figure S9: Mass Spectrum of **B1**
- 11 Figure S10: ^1H NMR Spectrum of **B2**
- 12 Figure S11: ^{13}C NMR Spectrum of **B2**
- 13 Figure S12: Mass Spectrum of **B2**
- 14 Figure S13: ^1H NMR Spectrum of **BTT-1**
- 15 Figure S14: ^{13}C NMR Spectrum of **BTT-1**
- 16 Figure S15: Mass Spectrum of **BTT-1**
- 17 Figure S16: ^1H NMR Spectrum of **BTT-2**
- 18 Figure S17: ^{13}C NMR Spectrum of **BTT-2**
- 19 Figure S18: Mass Spectrum of **BTT-2**
- 20 Figure S19: ^1H NMR Spectrum of **BTT-3**
- 21 Figure S20: ^{13}C NMR Spectrum of **BTT-3**
- 22 Figure S21: Mass Spectrum of **BTT-3**
- 23 Figure S22: ^1H NMR Spectrum of **BTT-4**
- 24 Figure S23: ^{13}C NMR Spectrum of **BTT-4**

- 1 Figure S24: Mass Spectrum of **BTT-4**
- 2 Figure S25: ^1H NMR Spectrum of **BTT-5**
- 3 Figure S26: ^{13}C NMR Spectrum of **BTT-5**
- 4 Figure S27: Mass Spectrum of **BTT-5**
- 5 Figure S28: ^1H NMR Spectrum of **BTT-6**
- 6 Figure S29: ^{13}C NMR Spectrum of **BTT-6**
- 7 Figure S30: Mass Spectrum of **BTT-6**
- 8 Figure S31: ^1H NMR Spectrum of **BTT-7**
- 9 Figure S32: ^{13}C NMR Spectrum of **BTT-7**
- 10 Figure S33: Mass Spectrum of **BTT-7**
- 11 Figure S34: ^1H NMR Spectrum of **BTT-8**
- 12 Figure S35: ^{13}C NMR Spectrum of **BTT-8**
- 13 Figure S36: Mass Spectrum of **BTT-8**
- 14 Figure S37: ^1H NMR Spectrum of **BTT-9**
- 15 Figure S38: ^{13}C NMR Spectrum of **BTT-9**
- 16 Figure S39: Mass Spectrum of **BTT-9**
- 17 Figure S40: ^1H NMR Spectrum of **BTT-10**
- 18 Figure S41: ^{13}C NMR Spectrum of **BTT-10**
- 19 Figure S42: Mass Spectrum of **BTT-10**
- 20 Figure S43: ^1H NMR Spectrum of **BTP-1**
- 21 Figure S44: ^{13}C NMR Spectrum of **BTP-1**
- 22 Figure S45: Mass Spectrum of **BTP-1**
- 23 Figure S46: ^1H NMR Spectrum of **BTP-2**
- 24 Figure S47: ^{13}C NMR Spectrum of **BTP-2**

- 1 Figure S48: Mass Spectrum of **BTP-2**
- 2 Figure S49: ^1H NMR Spectrum of **BTP-3**
- 3 Figure S50: ^{13}C NMR Spectrum of **BTP-3**
- 4 Figure S51: Mass Spectrum of **BTP-3**
- 5 Figure S52: ^1H NMR Spectrum of **BTP-4**
- 6 Figure S53: ^{13}C NMR Spectrum of **BTP-4**
- 7 Figure S54: Mass Spectrum of **BTP-4**
- 8 Figure S55: ^1H NMR Spectrum of **BTP-5**
- 9 Figure S56: ^{13}C NMR Spectrum of **BTP-5**
- 10 Figure S57: Mass Spectrum of **BTP-5**
- 11 Figure S58: ^1H NMR Spectrum of **BTP-6**
- 12 Figure S59: ^{13}C NMR Spectrum of **BTP-6**
- 13 Figure S60: Mass Spectrum of **BTP-6**
- 14 Figure S61: ^1H NMR Spectrum of **BTP-7**
- 15 Figure S62: ^{13}C NMR Spectrum of **BTP-7**
- 16 Figure S63: Mass Spectrum of **BTP-7**
- 17 Figure S64: ^1H NMR Spectrum of **BTP-8**
- 18 Figure S65: ^{13}C NMR Spectrum of **BTP-8**
- 19 Figure S66: Mass Spectrum of **BTP-8**
- 20 Figure S67: ^1H NMR Spectrum of **BTP-9**
- 21 Figure S68: ^{13}C NMR Spectrum of **BTP-9**
- 22 Figure S69: Mass Spectrum of **BTP-9**
- 23 Figure S70: ^1H NMR Spectrum of **BTP-10**
- 24 Figure S71: ^{13}C NMR Spectrum of **BTP-10**

1 Figure S72: Mass Spectrum of **BTP-10**

2



3

4 Figure S1. ¹H NMR Spectrum of **A1**

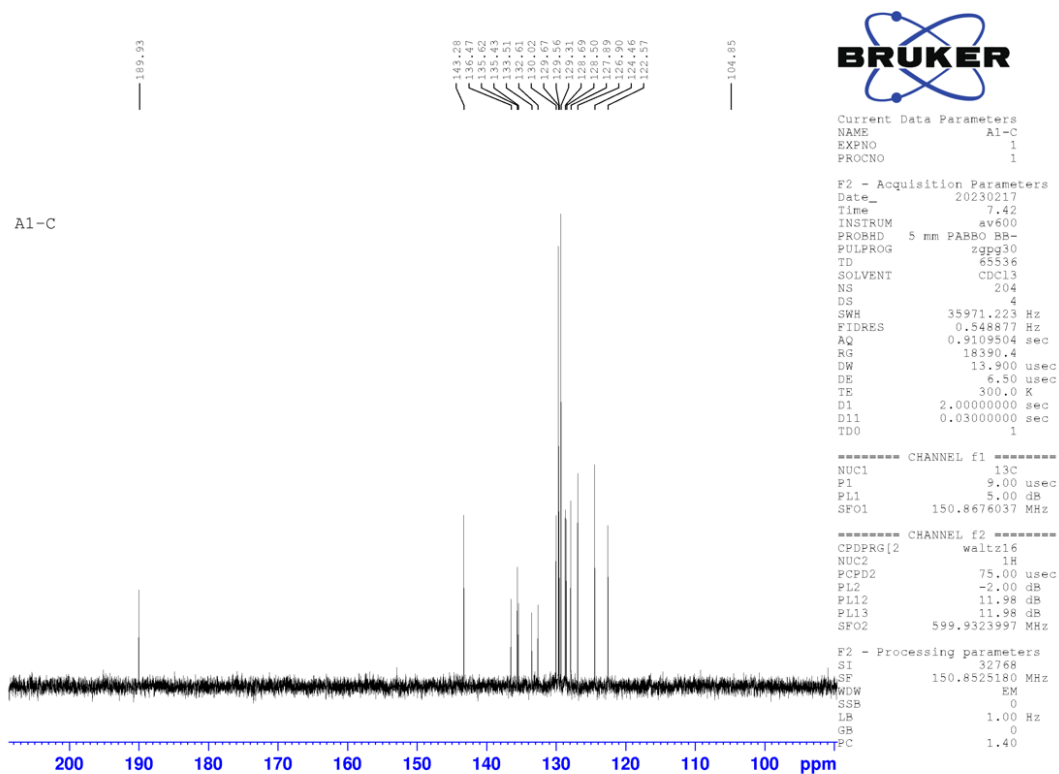


Figure S2. ^{13}C NMR Spectrum of A1

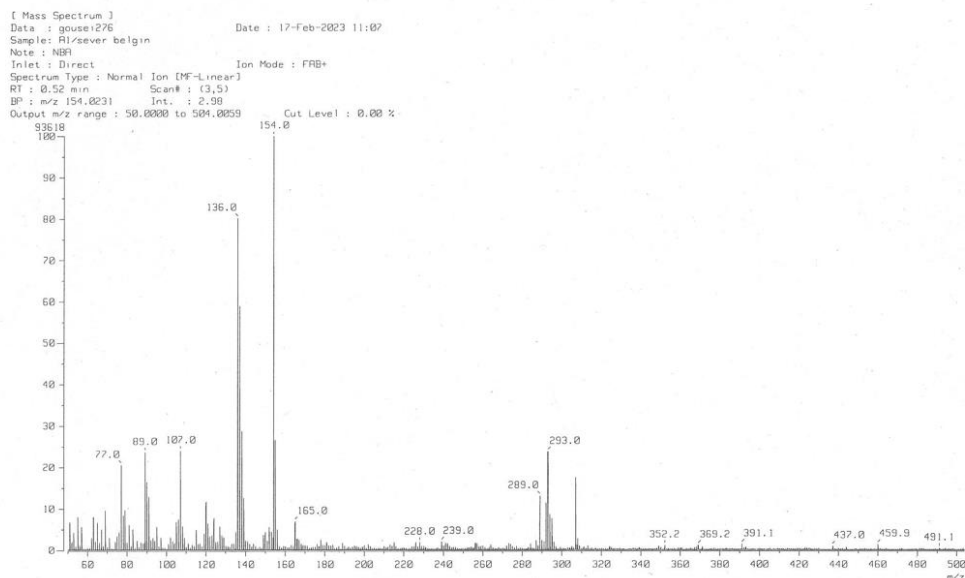
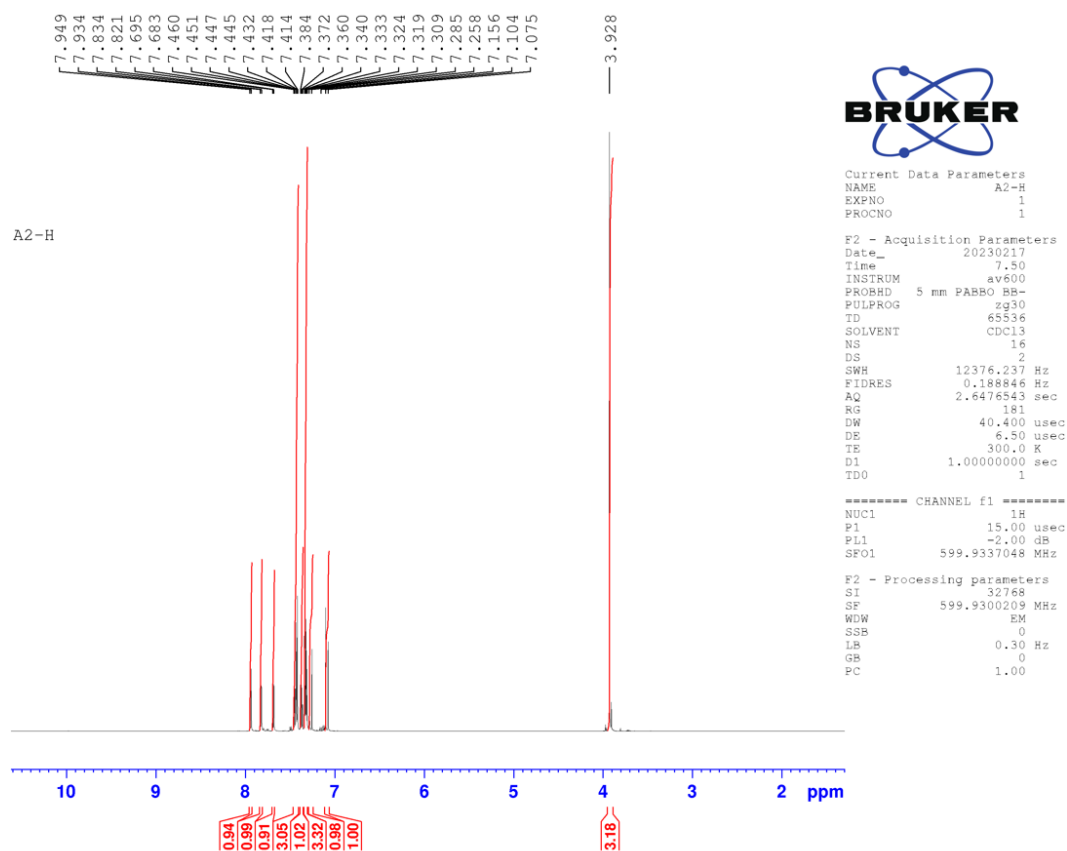


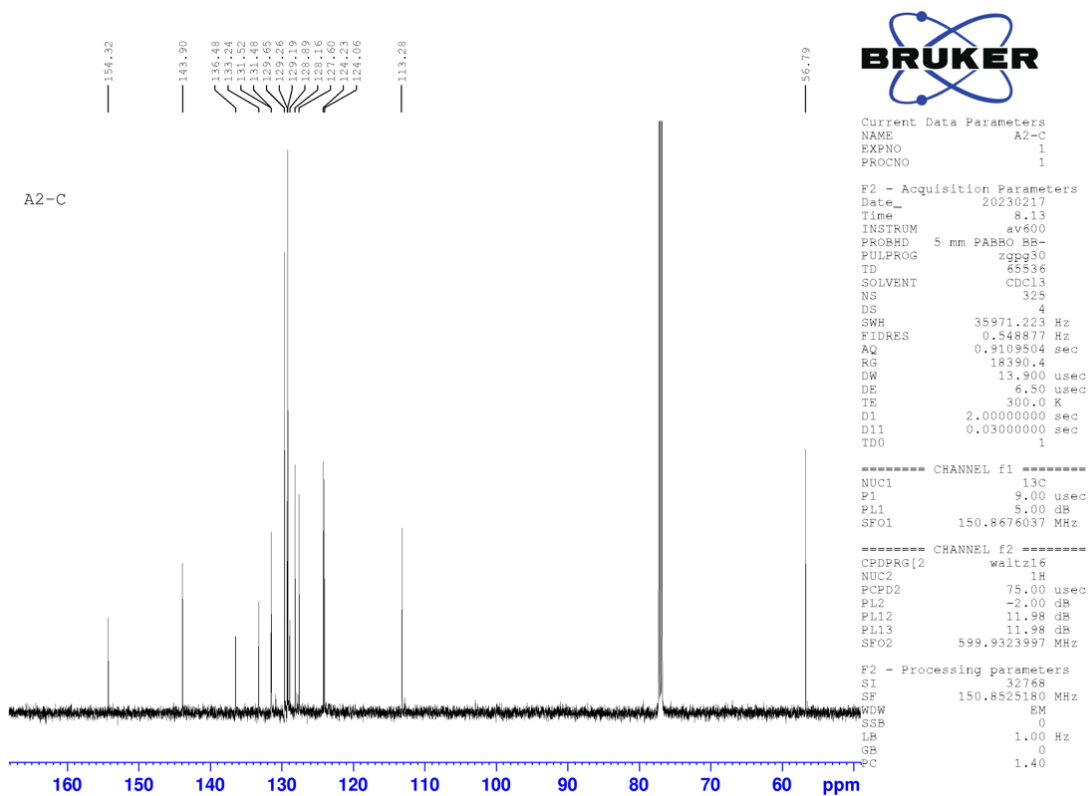
Figure S3: Mass Spectrum of A1

1



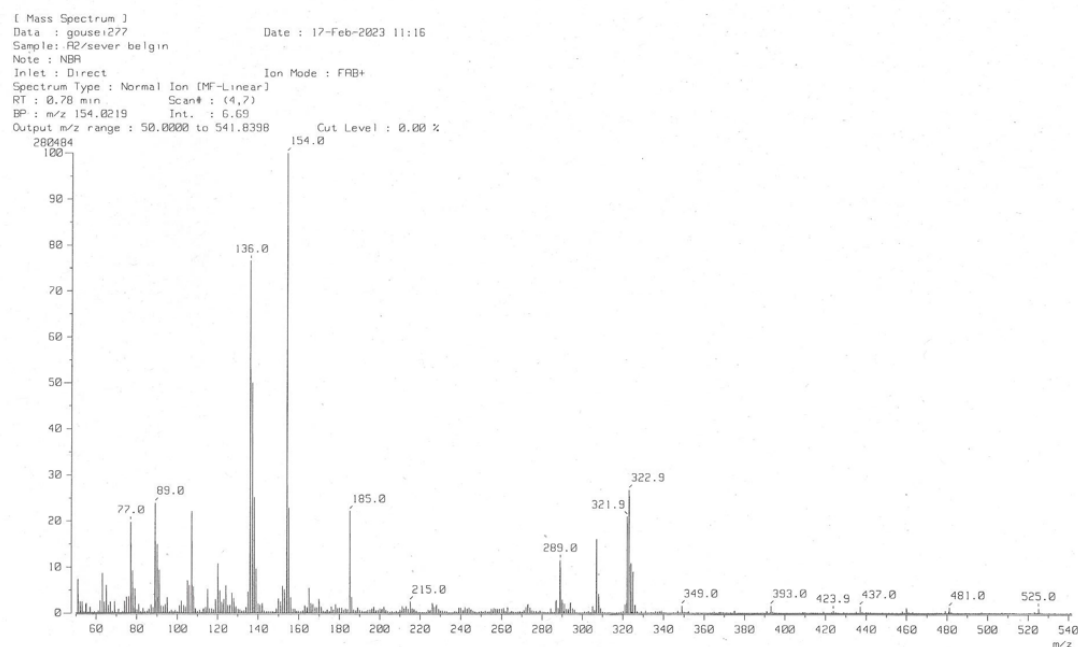
2

3 **Figure S4:** ^1H NMR Spectrum of A2



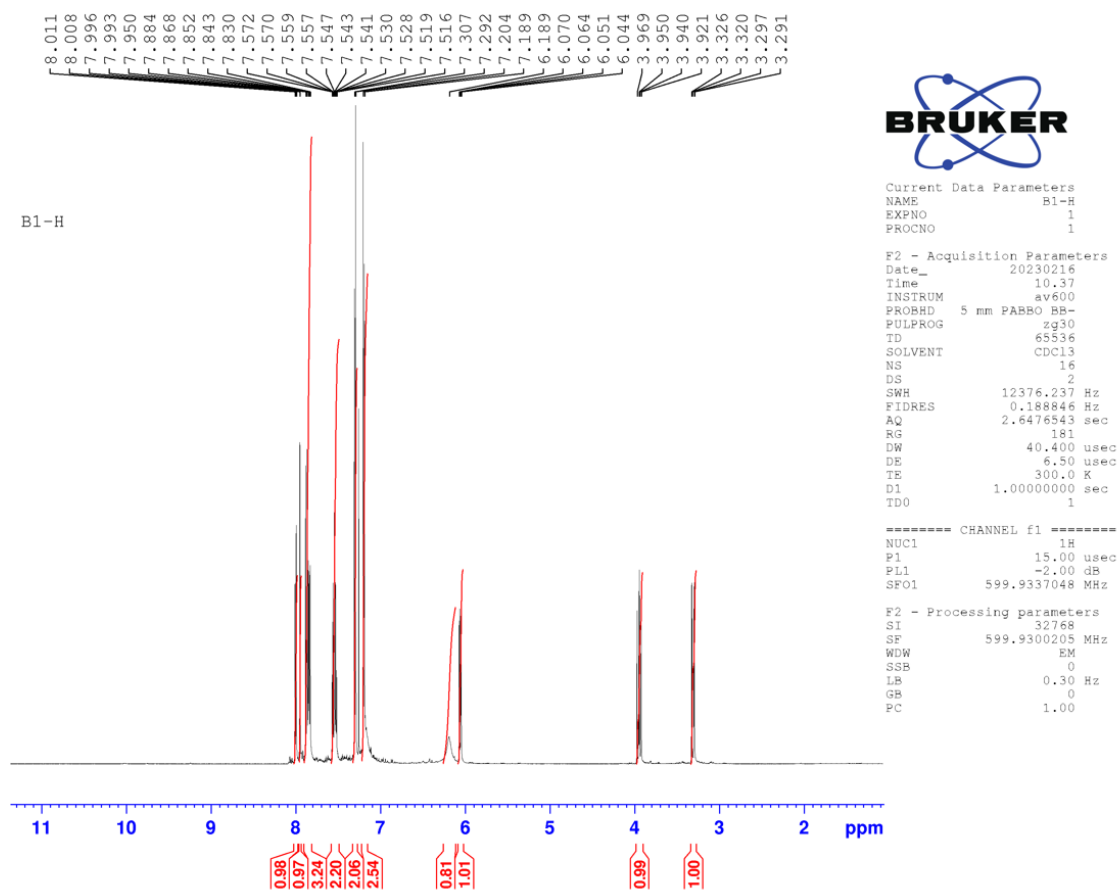
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2 **Figure S5:** ^{13}C NMR Spectrum of A2



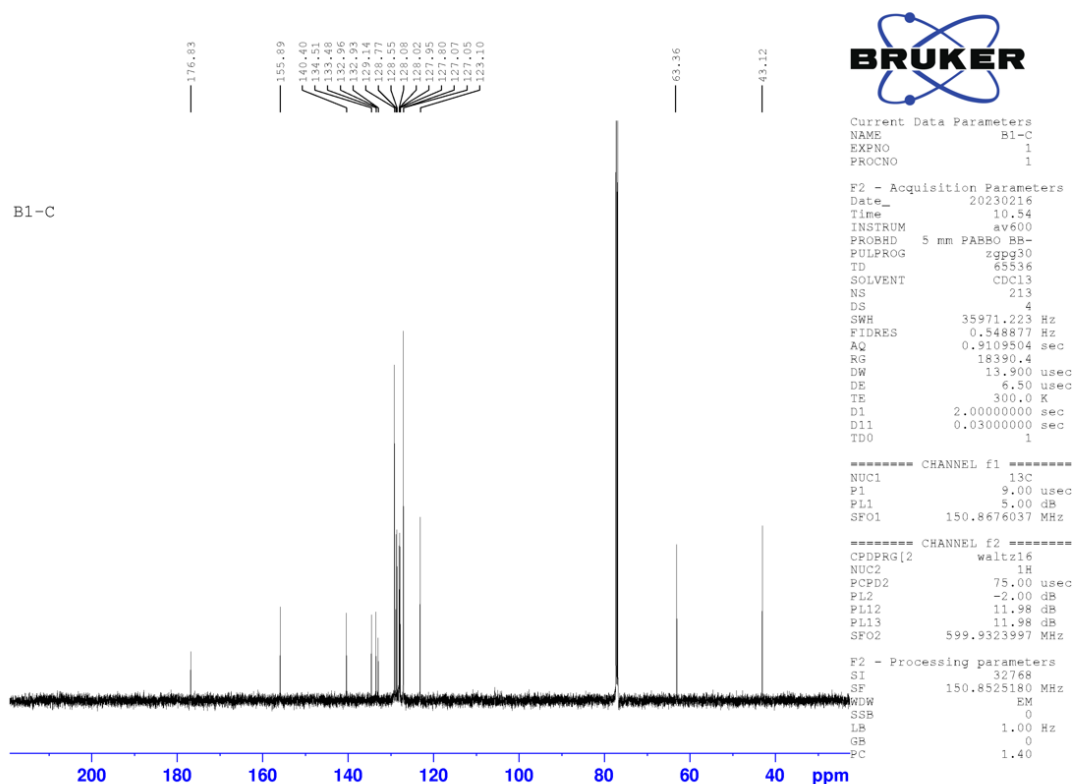
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4 **Figure S6:** Mass Spectrum of A2



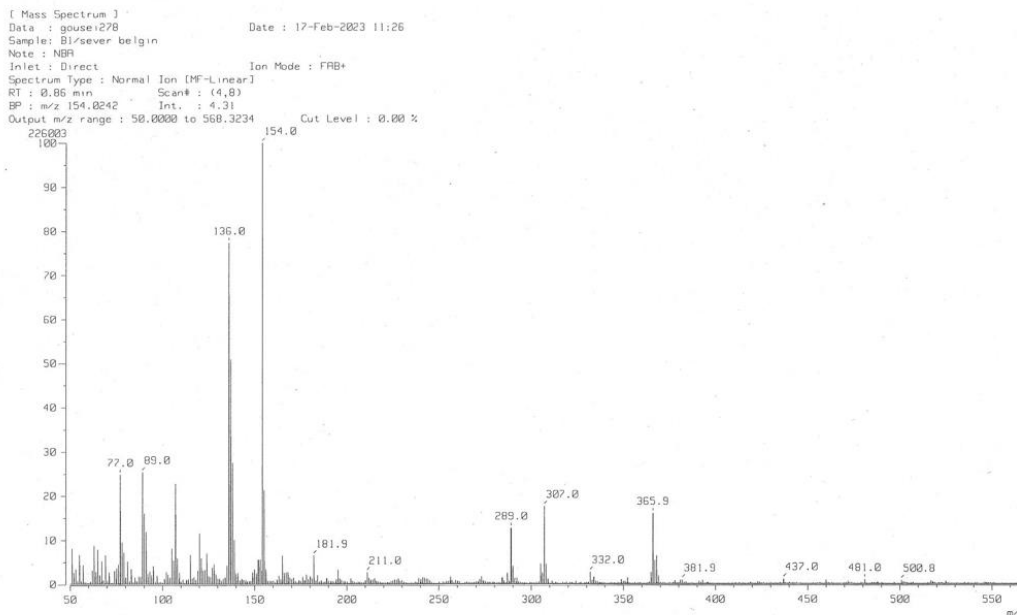
1

2 **Figure S7:** ^1H NMR Spectrum of **B1**



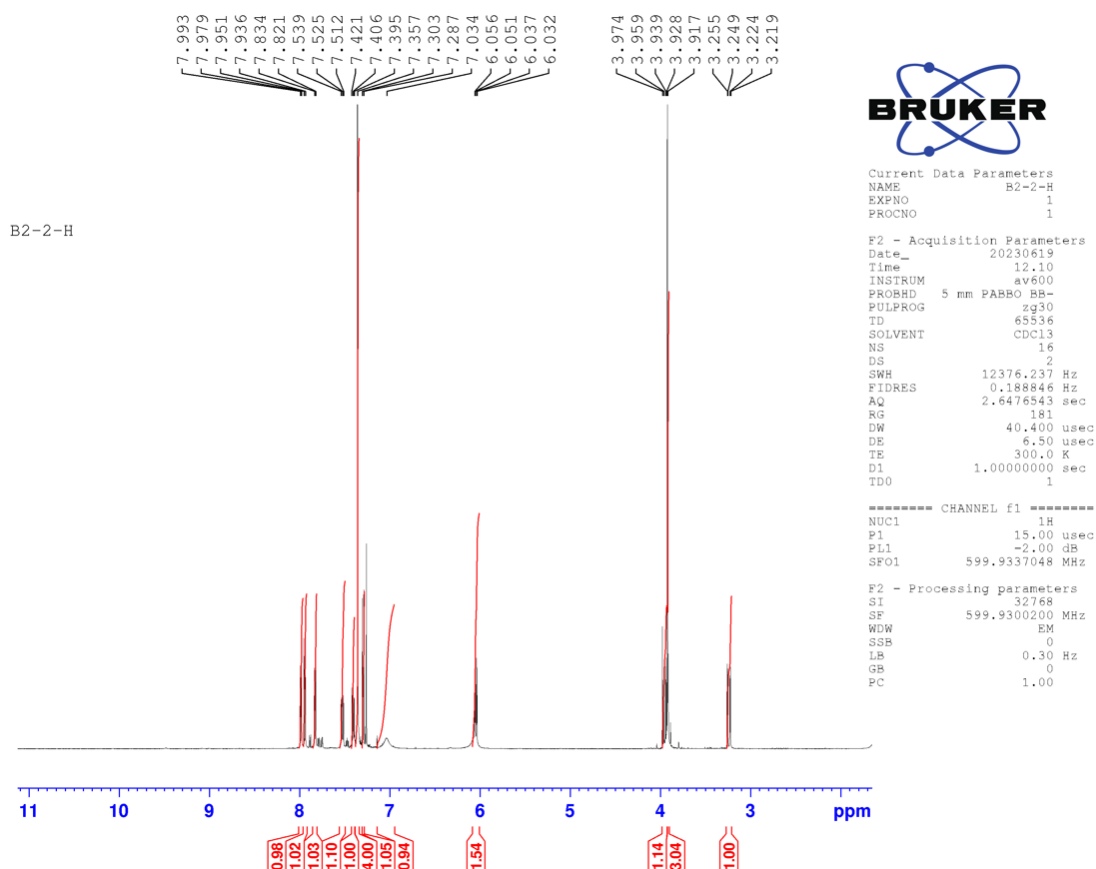
1

2 **Figure S8:** ^{13}C NMR Spectrum of **B1**



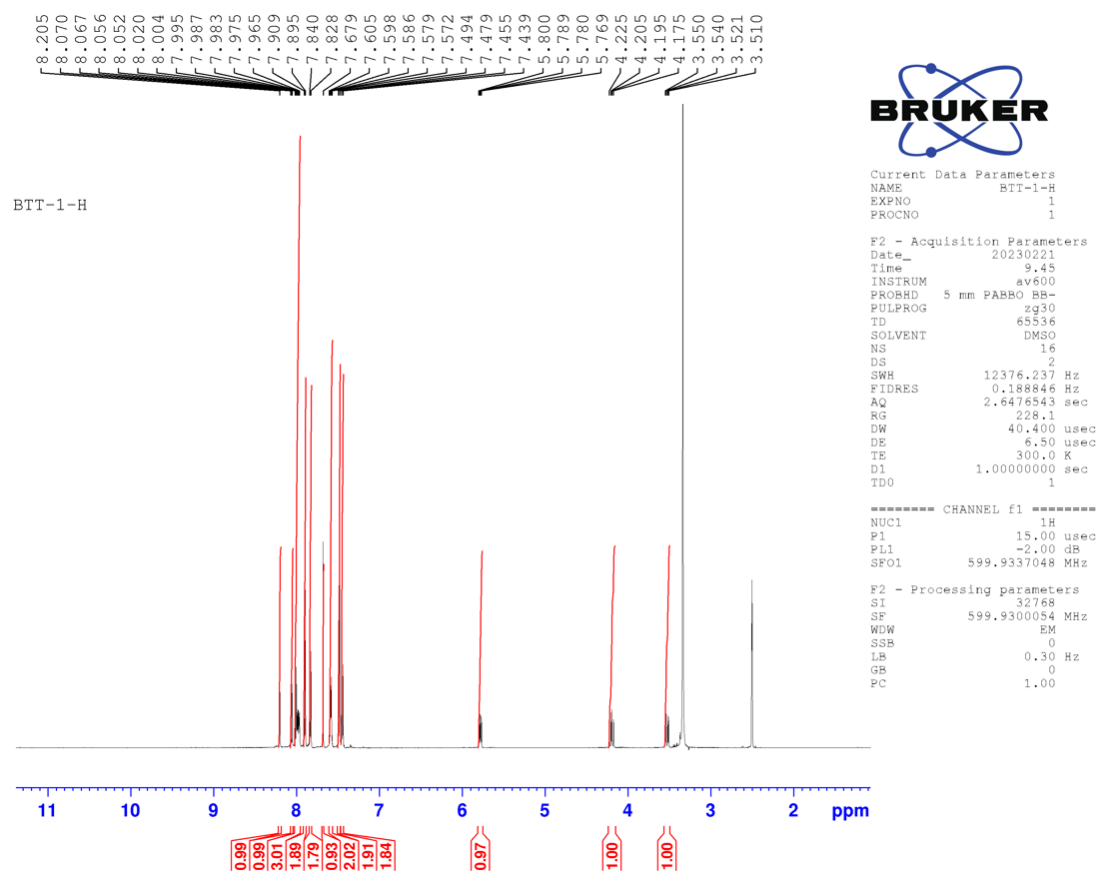
3

4 **Figure S9:** Mass Spectrum of **B1**



1

2 **Figure S10:** ^1H NMR Spectrum of **B2**



1

2 **Figure S13:** ^1H NMR Spectrum of **BTT-1**

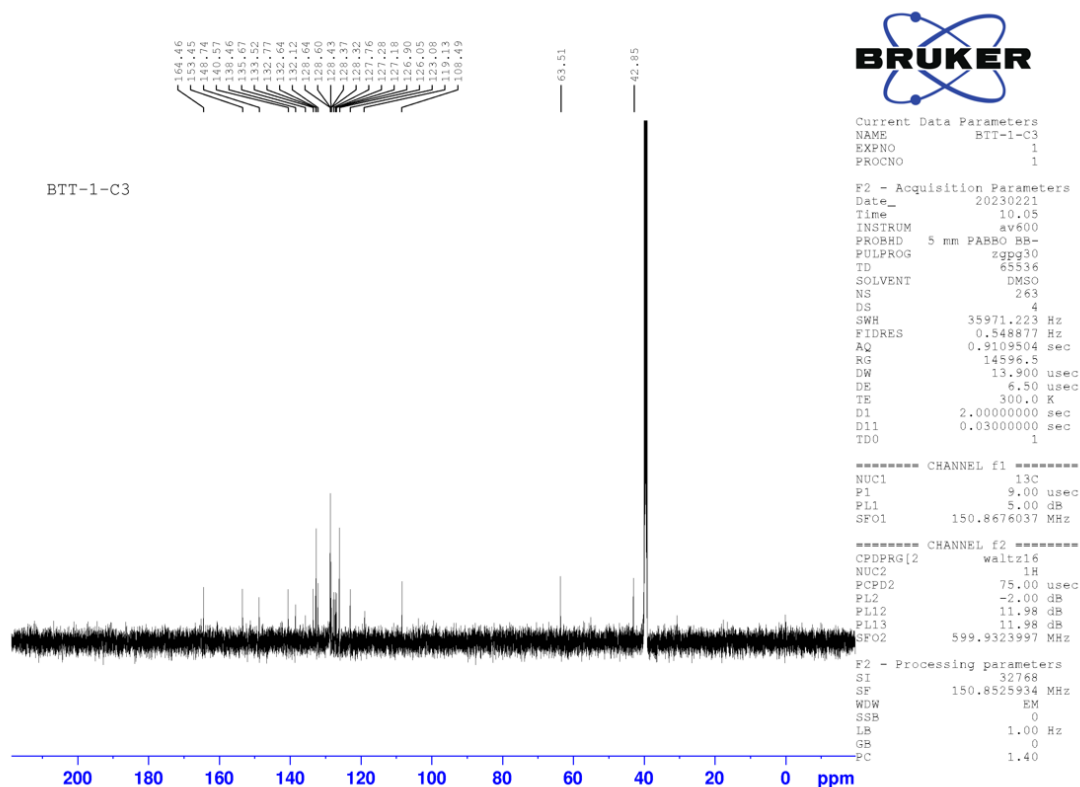


Figure S14: ^{13}C NMR Spectrum of BTT-1

[Elemental Composition]

Data : gousei244 Date : 03-Feb-2023 14:08 Page: 1

Sample: BTT-1/sever belgin

Note : NBA

Inlet : Direct Ion Mode : FAB+

RT : 1.25 min Scan#: (3,9)

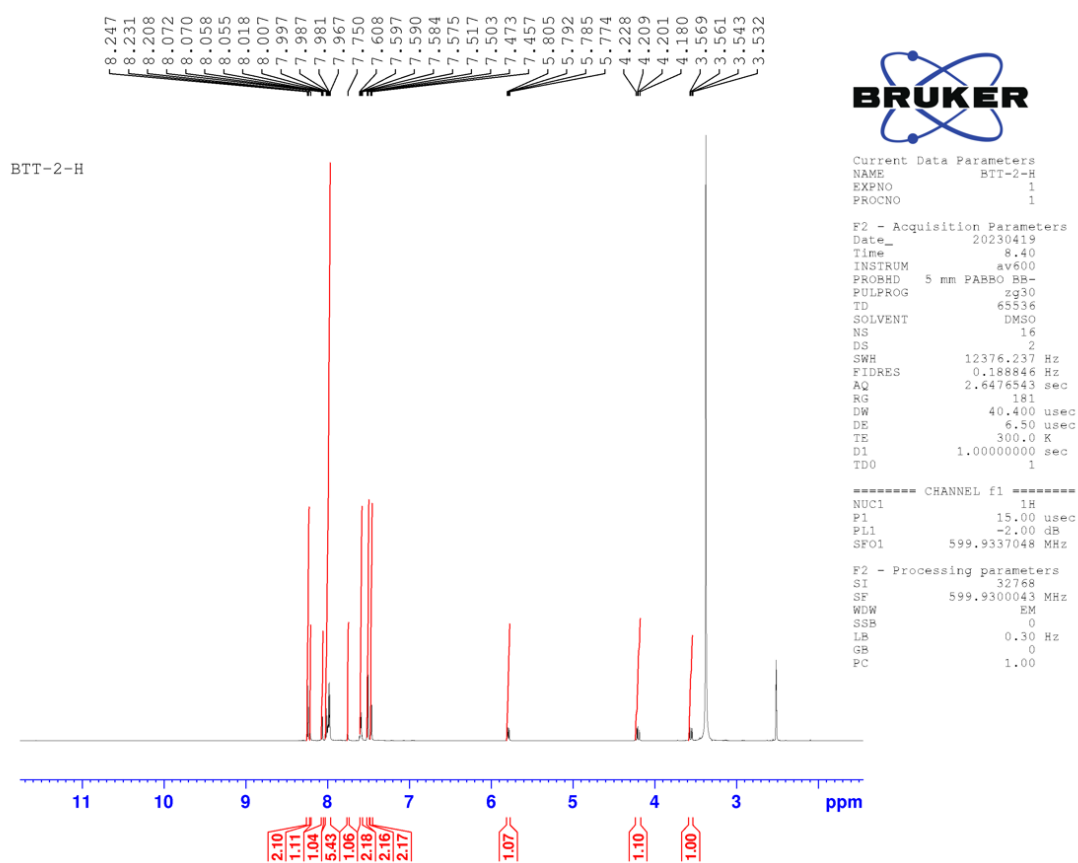
Elements : C 100/0, H 100/0, N 5/3, Cl 2/0, S 2/0

Mass Tolerance : 20ppm, 10mmu if m/z < 500, 20mmu if m/z > 1000

Unsaturation (U.S.) : -0.5 - 150.0

Observed m/z	Int%	Err [ppm / mmu]	U.S. Composition
490.0999	11.7	-19.2 / -9.4	31.5 C 34 H 12 N 5
		+2.7 / +1.3	27.0 C 32 H 15 N 4 Cl
		-4.2 / -2.0	23.0 C 29 H 19 N 4 Cl S
		+17.8 / +8.7	18.5 C 27 H 22 N 3 Cl 2 S
		-11.0 / -5.4	19.0 C 26 H 23 N 4 Cl S 2
		+14.6 / +7.2	19.5 C 25 H 21 N 5 Cl S 2
		+10.9 / +5.3	14.5 C 24 H 26 N 3 Cl 2 S 2
491.1089	12.1	-16.6 / -8.1	31.0 C 34 H 13 N 5
		-20.3 / -10.0	26.0 C 33 H 18 N 3 Cl
		+5.3 / +2.6	26.5 C 32 H 16 N 4 Cl
		-1.6 / -0.8	22.5 C 29 H 20 N 4 Cl S
		+20.3 / +10.0	18.0 C 27 H 23 N 3 Cl 2 S
		-8.4 / -4.1	18.5 C 26 H 24 N 4 Cl S 2
		+17.2 / +8.4	19.0 C 25 H 22 N 5 Cl S 2
		+13.4 / +6.6	14.0 C 24 H 27 N 3 Cl 2 S 2

Figure S15: Mass Spectrum of BTT-1



1

2 **Figure S16:** ^1H NMR Spectrum of **BTT-2**

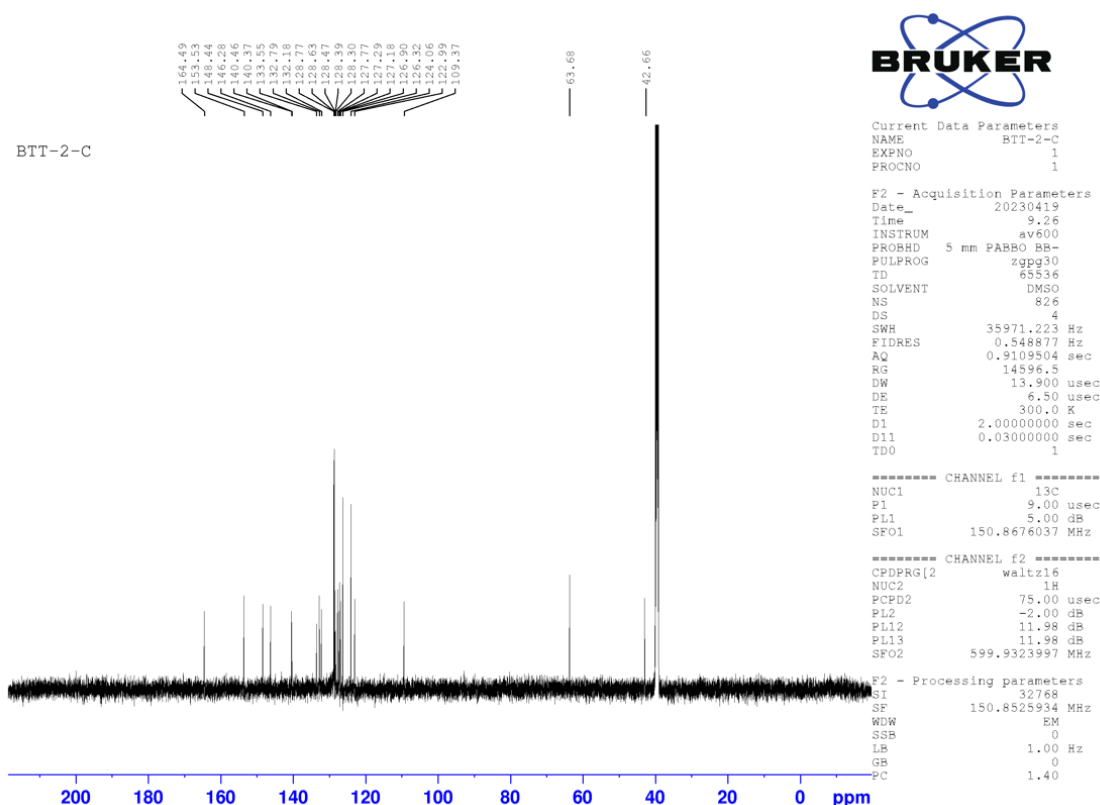


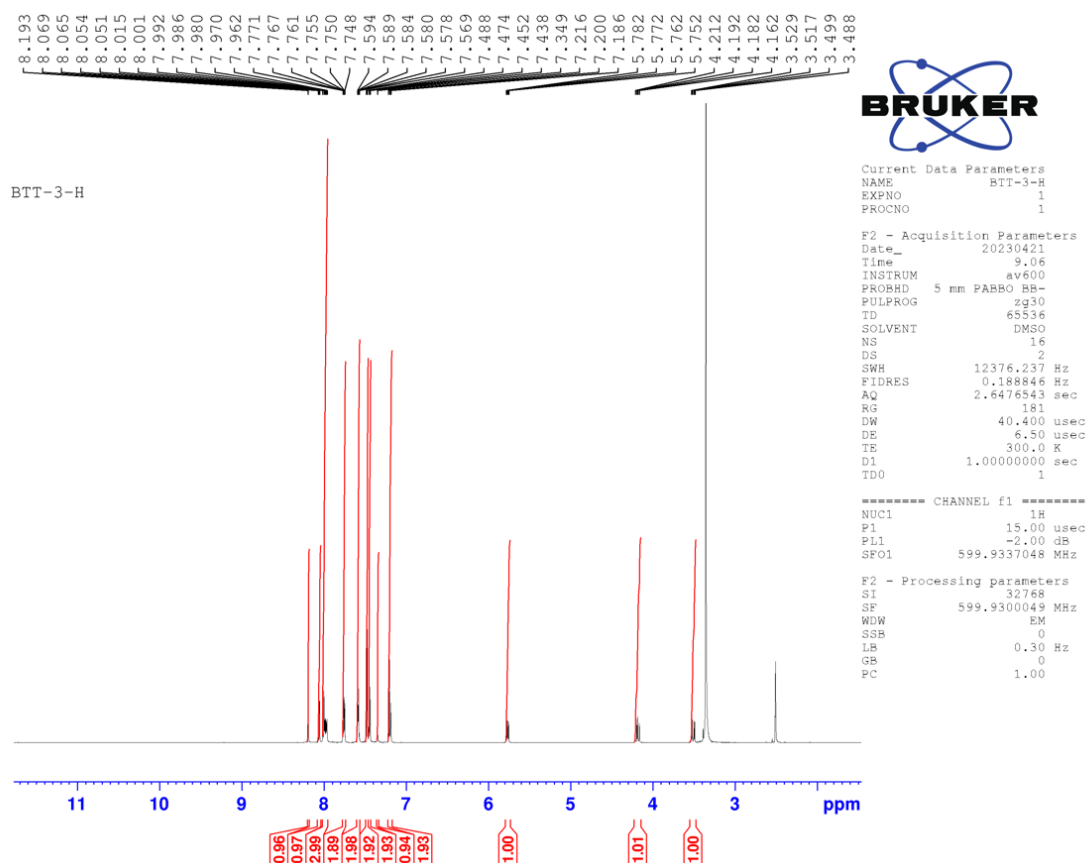
Figure S17: ^{13}C NMR Spectrum of BTT-2

[Elemental Composition]
 Date : 03-Feb-2023 14:25
 Data : gousei245
 Sample: BTT-2/sever belgin
 Note : NBA
 Inlet : Direct
 RT : 1.63 min
 Elements : C 100/0, H 100/0, O 3/1, N 5/3, Cl 2/0, S 2/0
 Mass Tolerance : 20ppm, 10mmu if m/z < 500, 20mmu if m/z > 1000
 Unsaturation (U.S.) : -0.5 - 150.0

Ion Mode : FAB+
 Scan#: (5,10)

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
510.0926	50.5	+9.3 / +4.7	30.5	C 34 H 12 O 3 N 3
		-12.8 / -6.5	30.5	C 33 H 12 O 2 N 5
		-16.3 / -8.3	25.5	C 32 H 17 O 2 N 3 Cl
		+8.3 / +4.2	26.0	C 31 H 15 O 2 N 4 Cl
		-17.3 / -8.8	21.0	C 29 H 20 O N 4 Cl 2
		+7.4 / +3.7	21.5	C 28 H 18 O N 5 Cl 2
		+2.7 / +1.4	26.5	C 31 H 16 O 3 N 3 S
		-19.4 / -9.9	26.5	C 30 H 16 O 2 N 5 S
		+1.7 / +0.9	22.0	C 28 H 19 O 2 N 4 Cl S
		+0.7 / +0.4	17.5	C 25 H 22 O N 5 Cl 2 S
		-4.0 / -2.0	22.5	C 28 H 20 O 3 N 3 S 2
		-4.9 / -2.5	18.0	C 25 H 23 O 2 N 4 Cl S 2
		+19.7 / +10.1	18.5	C 24 H 21 O 2 N 5 Cl S 2
		+16.2 / +8.2	13.5	C 23 H 26 O 2 N 3 Cl 2 S 2
		-5.9 / -3.0	13.5	C 22 H 26 O N 5 Cl 2 S 2
511.0974	36.4	+3.4 / +1.7	30.0	C 34 H 13 O 3 N 3
		-18.6 / -9.5	30.0	C 33 H 13 O 2 N 5
		+2.4 / +1.2	25.5	C 31 H 16 O 2 N 4 Cl
		+1.5 / +0.7	21.0	C 28 H 19 O N 5 Cl 2
		-3.2 / -1.7	26.0	C 31 H 17 O 3 N 3 S
		-4.2 / -2.1	21.5	C 28 H 20 O 2 N 4 Cl S
		+16.8 / +8.6	17.0	C 26 H 23 O 2 N 3 Cl 2 S
		-5.1 / -2.6	17.0	C 25 H 23 O N 5 Cl 2 S
		-9.8 / -5.0	22.0	C 28 H 21 O 3 N 3 S 2
		+14.8 / +7.6	22.5	C 27 H 19 O 3 N 4 S 2
		-10.8 / -5.5	17.5	C 25 H 24 O 2 N 4 Cl S 2
		+13.8 / +7.1	18.0	C 24 H 22 O 2 N 5 Cl S 2
		+10.2 / +5.2	13.0	C 23 H 27 O 2 N 3 Cl 2 S 2
		-11.7 / -6.0	13.0	C 22 H 27 O N 5 Cl 2 S 2

Figure S18: Mass Spectrum of BTT-2



1

2 **Figure S19:** ^1H NMR Spectrum of BTT-3

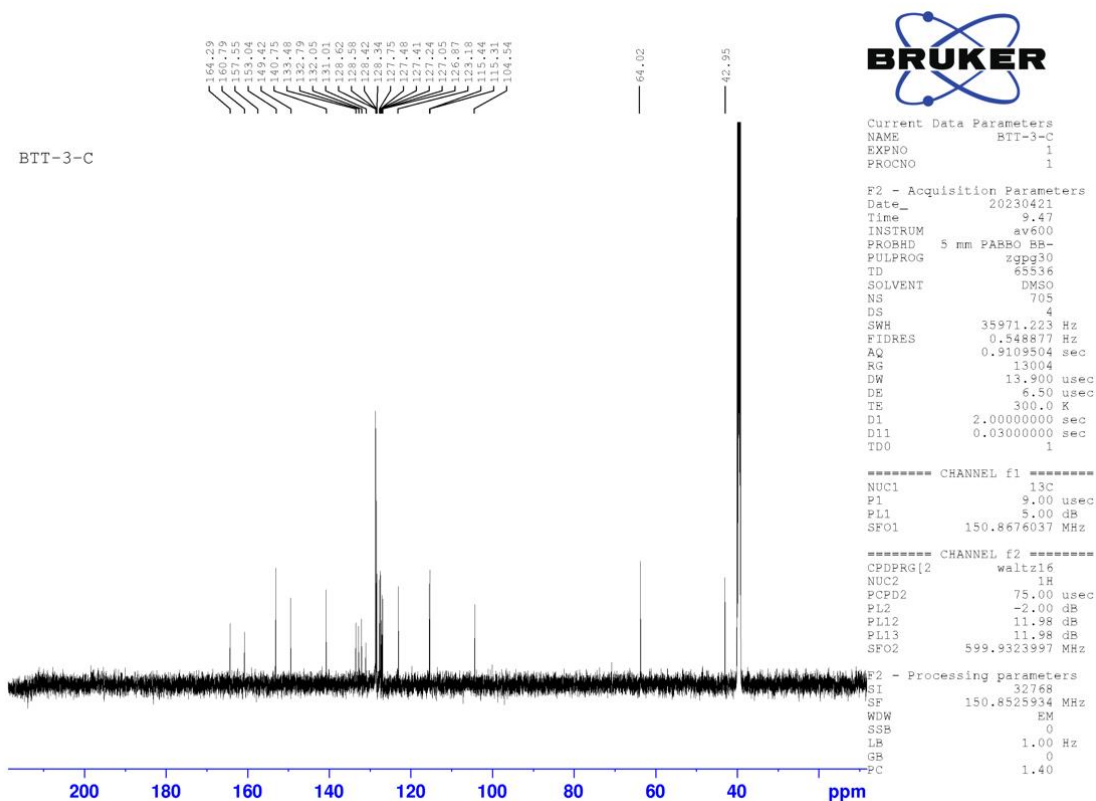


Figure S20: ^{13}C NMR Spectrum of BTT-3

[Elemental Composition]

Data : gousei262 Date : 07-Feb-2023 08:55 Page: 1

Sample: BTT-3/sever belgin

Note : NBA

Inlet : Direct Ion Mode : FAB+

RT : 2.00 min Scan#: (7,11)

Elements : C 100/0, H 100/0, N 4/2, Cl 2/0, F 2/0, S 2/0

Mass Tolerance : 20ppm, 10mmu if m/z < 500, 20mmu if m/z > 1000

Unsaturation (U.S.) : -0.5 - 150.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
483.0956	100.0	+6.9 / +3.3	33.5	C 37 H 11 N 2
		-18.7 / -9.0	29.5	C 33 H 12 N 4 F
		+3.5 / +1.7	25.0	C 31 H 15 N 3 Cl F
		+0.1 / +0.1	16.5	C 25 H 19 N 4 Cl 2 F 2
		-0.1 / +0.0	29.5	C 34 H 15 N 2 S
		-3.5 / -1.7	21.0	C 28 H 19 N 3 Cl F S
		+18.8 / +9.1	16.5	C 26 H 22 N 2 Cl 2 F S
		-6.8 / -3.3	12.5	C 22 H 23 N 4 Cl 2 F 2 S
		-7.1 / -3.4	25.5	C 31 H 19 N 2 S 2
		+19.0 / +9.2	26.0	C 30 H 17 N 3 S 2
		-10.4 / -5.0	17.0	C 25 H 23 N 3 Cl F S 2
		+15.6 / +7.5	17.5	C 24 H 21 N 4 Cl F S 2
		+11.8 / +5.7	12.5	C 23 H 26 N 2 Cl 2 F S 2
		-13.8 / -6.7	8.5	C 19 H 27 N 4 Cl 2 F 2 S 2

Figure S21: Mass Spectrum of BTT-3

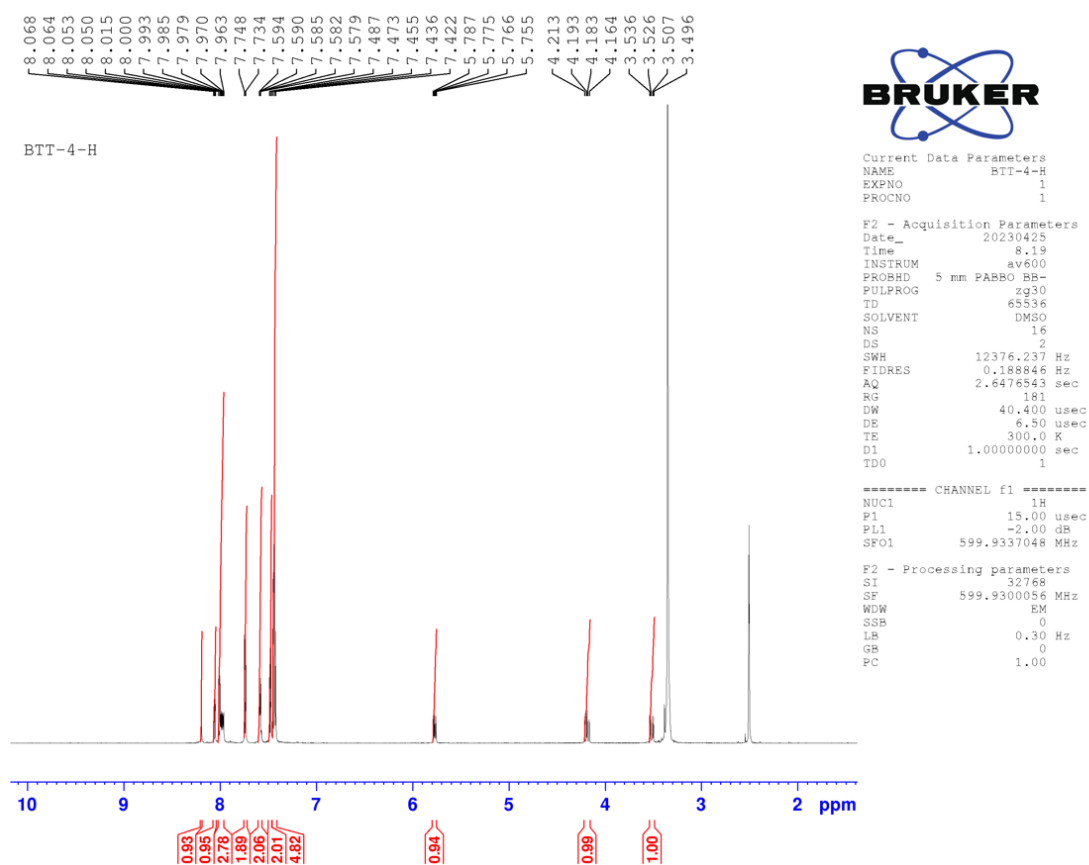


Figure S22: ^1H NMR Spectrum of **BTT-4**

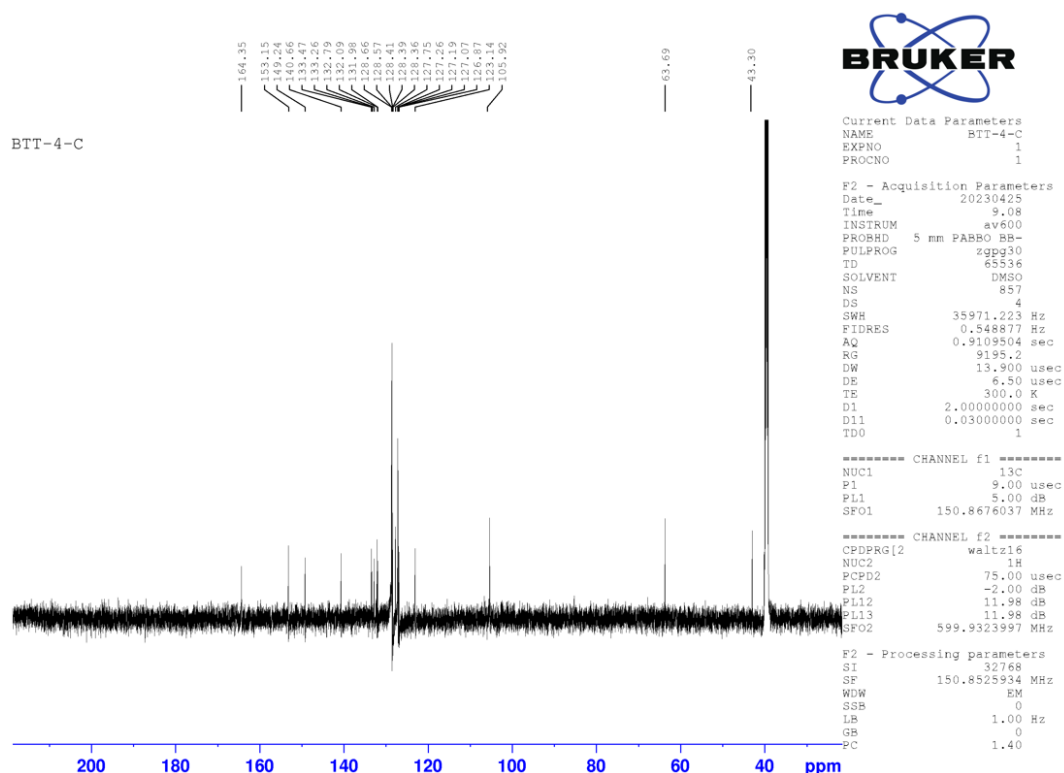


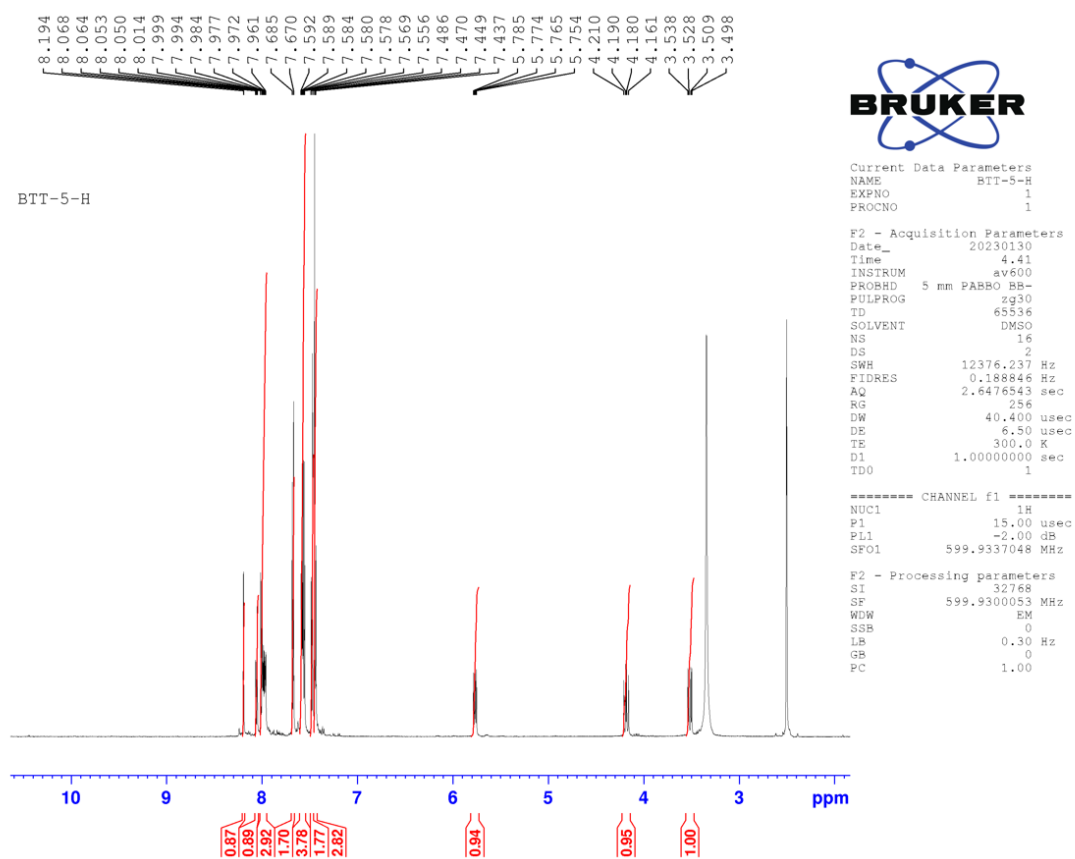
Figure S23: ^{13}C NMR Spectrum of BTT-4

[Elemental Composition]
Data : gousei263
Sample: BTT-4/sever belgin
Note : NBA
Inlet : Direct
RT : 1.13 min
Elements : C 100/0, H 100/0, N 4/2, Cl 3/1, S 2/0
Mass Tolerance : 20ppm, 10mmu if m/z < 500, 20mmu if m/z > 1000
Unsaturation (U.S.) : -0.5 - 150.0

Date : 07-Feb-2023 09:10
Page: 1
Ion Mode : FAB+
Scan#: (3,8)

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
499.0660	23.2	-18.2 / -9.1	29.5	C 33 H 12 N 4 Cl
		+3.4 / +1.7	25.0	C 31 H 15 N 3 Cl 2
		-3.4 / -1.7	21.0	C 28 H 19 N 3 Cl 2 S
		+18.1 / +9.1	16.5	C 26 H 22 N 2 Cl 3 S
		-10.2 / -5.1	17.0	C 25 H 23 N 3 Cl 2 S 2
		+15.0 / +7.5	17.5	C 24 H 21 N 4 Cl 2 S 2
		+11.4 / +5.7	12.5	C 23 H 26 N 2 Cl 3 S 2

Figure S24: Mass Spectrum of BTT-4



1

2 **Figure S25:** ^1H NMR Spectrum of **BTT-5**

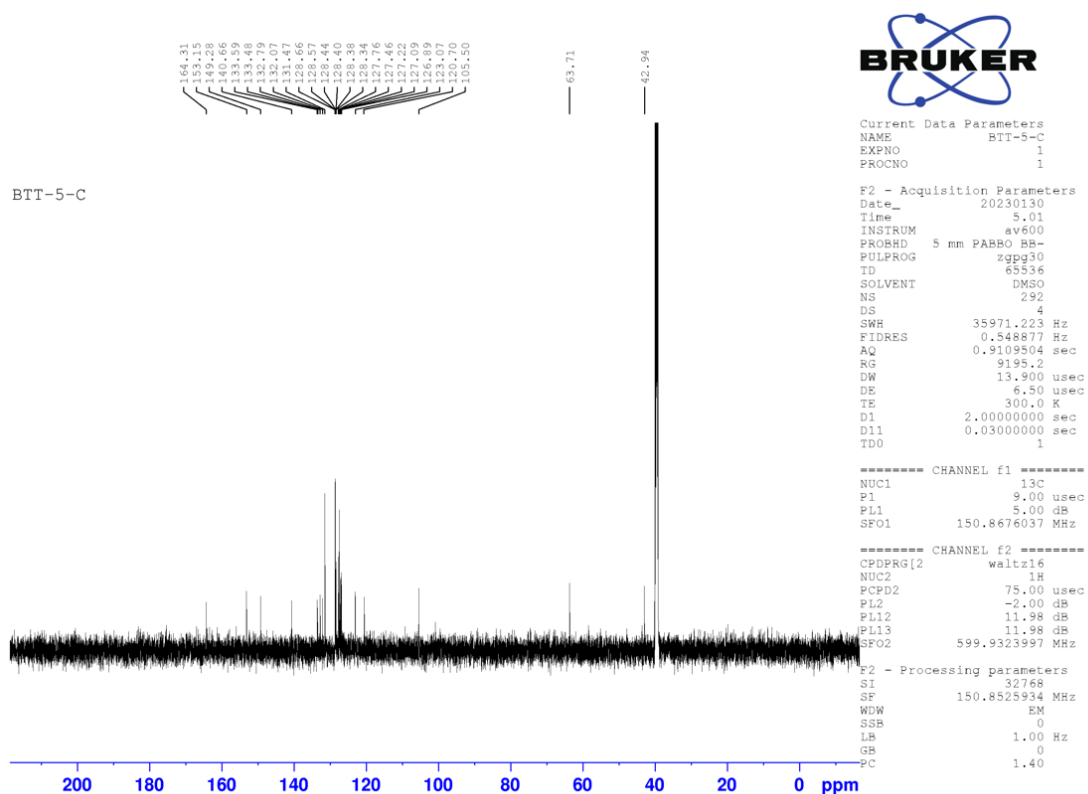


Figure S26: ^{13}C NMR Spectrum of **BTT-5**

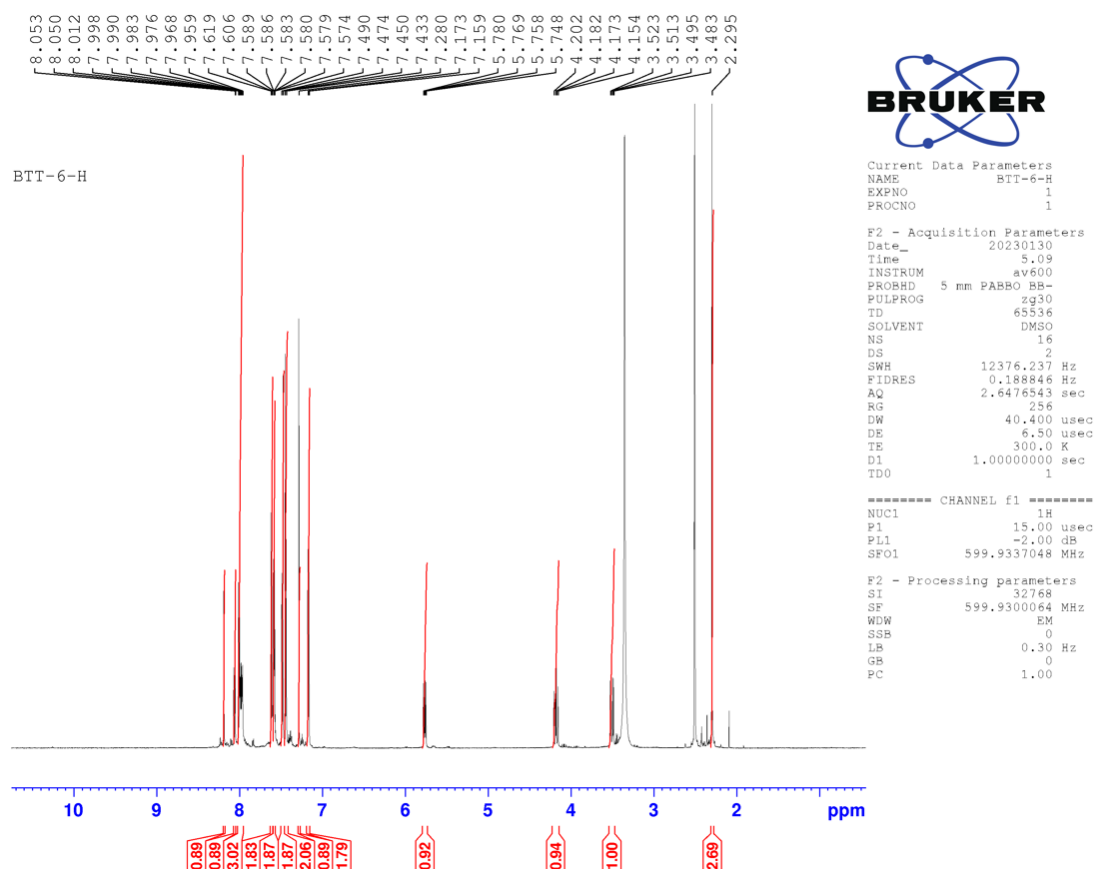
[Elemental Composition]
 Date : 30-Jan-2023 16:09
 Data : gousei240
 Sample: BTT-5/sever belgin
 Note : NBA
 Inlet : Direct
 RT : 1.50 min
 Elements : C 100/0, H 100/0, N 4/2, Cl 2/0, Br 2/0, S 2/0
 Mass Tolerance : 20ppm, 10mmu if m/z < 500, 20mmu if m/z > 1000
 Unsaturation (U.S.) : -0.5 - 150.0

Page: 1

Ion Mode : FAB+
 Scan#: (4,10)

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
544.0172	8.6	-8.2 / -4.5	24.5	C 31 H 16 N 3 Cl Br
		+14.9 / +8.1	25.0	C 30 H 14 N 4 Cl Br
		+11.6 / +6.3	20.0	C 29 H 19 N 2 Cl 2 Br
		+4.0 / +2.2	18.0	C 28 H 22 N 2 Br 2
		+14.0 / +7.6	41.0	C 40 H 4 N 2 S
		-14.4 / -7.8	20.5	C 28 H 20 N 3 Cl Br S
		+8.7 / +4.7	21.0	C 27 H 18 N 4 Cl Br S
		+5.4 / +2.9	16.0	C 26 H 23 N 2 Cl 2 Br S
		-2.2 / -1.2	14.0	C 25 H 26 N 2 Br 2 S
		+7.8 / +4.3	37.0	C 37 H 8 N 2 S 2
		+2.5 / +1.4	17.0	C 24 H 22 N 4 Cl Br S 2
		-0.8 / -0.5	12.0	C 23 H 27 N 2 Cl 2 Br S 2
		-8.4 / -4.6	10.0	C 22 H 30 N 2 Br 2 S 2
		+14.7 / +8.0	10.5	C 21 H 28 N 3 Br 2 S 2
543.0135	8.3	-12.7 / -6.9	31.5	C 34 H 9 N 4 Cl 2
		-0.4 / -0.2	25.0	C 31 H 15 N 3 Cl Br
		+19.4 / +10.5	20.5	C 29 H 18 N 2 Cl 2 Br
		+11.8 / +6.4	18.5	C 28 H 21 N 2 Br 2
		-18.9 / -10.2	27.5	C 31 H 13 N 4 Cl 2 S
		-6.6 / -3.6	21.0	C 28 H 19 N 3 Cl Br S
		+16.5 / +9.0	21.5	C 27 H 17 N 4 Cl Br S
		+13.1 / +7.1	16.5	C 26 H 22 N 2 Cl 2 Br S
		+5.6 / +3.0	14.5	C 25 H 25 N 2 Br 2 S
		+15.6 / +8.5	37.5	C 37 H 7 N 2 S 2
		-12.9 / -7.0	17.0	C 25 H 23 N 3 Cl Br S 2
		+10.3 / +5.6	17.5	C 24 H 21 N 4 Cl Br S 2
		+6.9 / +3.8	12.5	C 23 H 26 N 2 Cl 2 Br S 2
		-0.6 / -0.3	10.5	C 22 H 29 N 2 Br 2 S 2

Figure S27: Mass Spectrum of **BTT-5**



1

2 **Figure S28:** ^1H NMR Spectrum of **BTI-6**

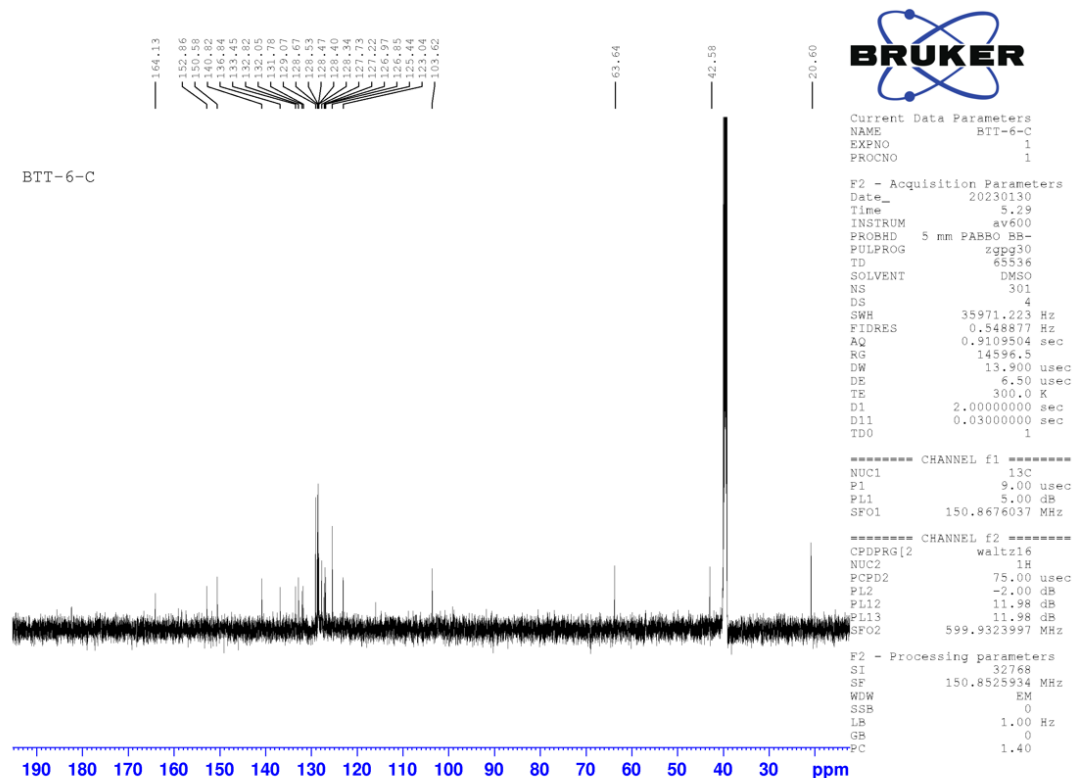


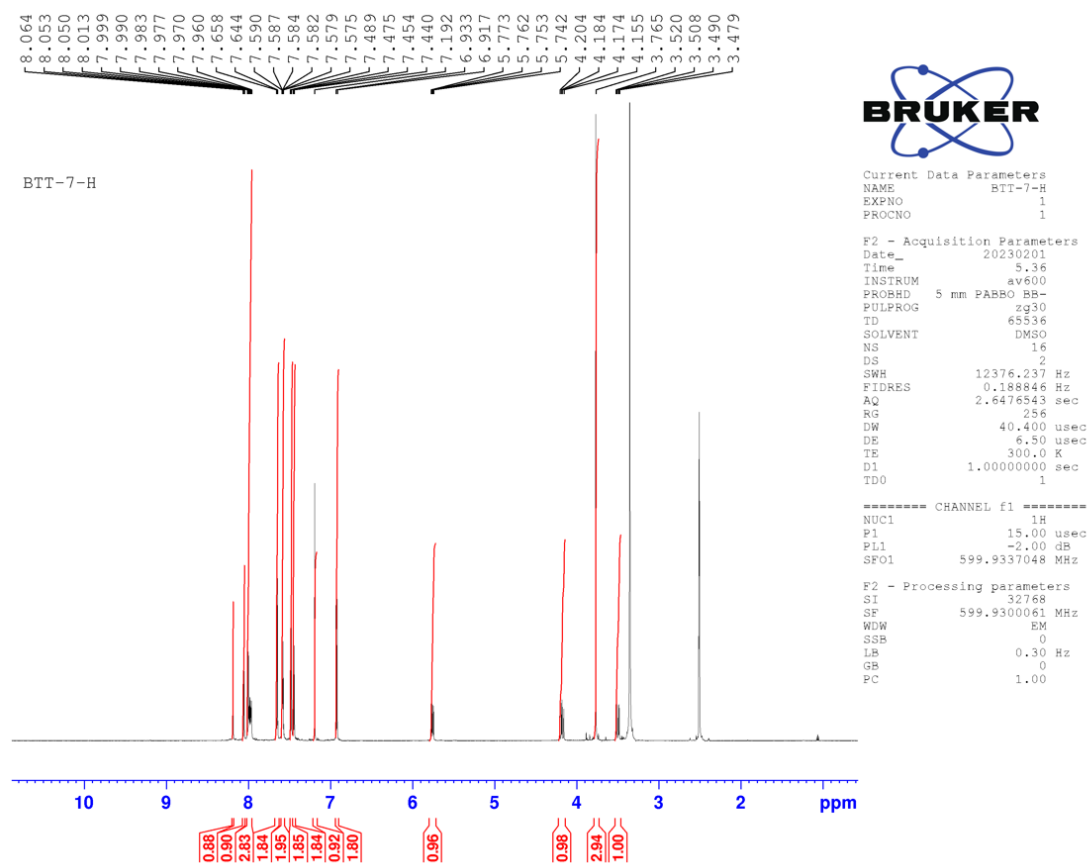
Figure S29: ^{13}C NMR Spectrum of BTT-6

[Elemental Composition]
Data : gousei241
Sample: BTT-6/sever belgin
Note : NBA
Inlet : Direct
RT : 1.88 min
Elements : C 100/0, H 100/0, N 4/2, Cl 2/0, S 2/0
Mass Tolerance : 20ppm, 10mmu if m/z < 500, 20mmu if m/z > 1000
Unsaturation (U.S.) : -0.5 - 150.0

Date : 30-Jan-2023 16:32
Page: 1
Ion Mode : FAB+
Scan#: (5,12)

Observed m/z	Int%	Err [ppm / mmu]	U.S.	Composition
480.1268	12.9	+0.1 / +0.1	24.5	C 32 H 19 N 3 Cl
		-6.9 / -3.3	20.5	C 29 H 23 N 3 Cl S
		+19.3 / +9.3	21.0	C 28 H 21 N 4 Cl S
		+15.5 / +7.4	16.0	C 27 H 26 N 2 Cl 2 S
		-13.9 / -6.7	16.5	C 26 H 27 N 3 Cl S 2
		+12.3 / +5.9	17.0	C 25 H 25 N 4 Cl S 2
		+8.4 / +4.1	12.0	C 24 H 30 N 2 Cl 2 S 2
479.1207	13.9	-18.8 / -9.0	29.5	C 34 H 15 N 4
		+3.6 / +1.7	25.0	C 32 H 18 N 3 Cl
		-3.4 / -1.6	21.0	C 29 H 22 N 3 Cl S
		+19.0 / +9.1	16.5	C 27 H 25 N 2 Cl 2 S
		-10.4 / -5.0	17.0	C 26 H 26 N 3 Cl S 2
		+15.8 / +7.6	17.5	C 25 H 24 N 4 Cl S 2
		+12.0 / +5.7	12.5	C 24 H 29 N 2 Cl 2 S 2

Figure S30: Mass Spectrum of BTT-6



1

2 **Figure S31:** ^1H NMR Spectrum of **BTT-7**

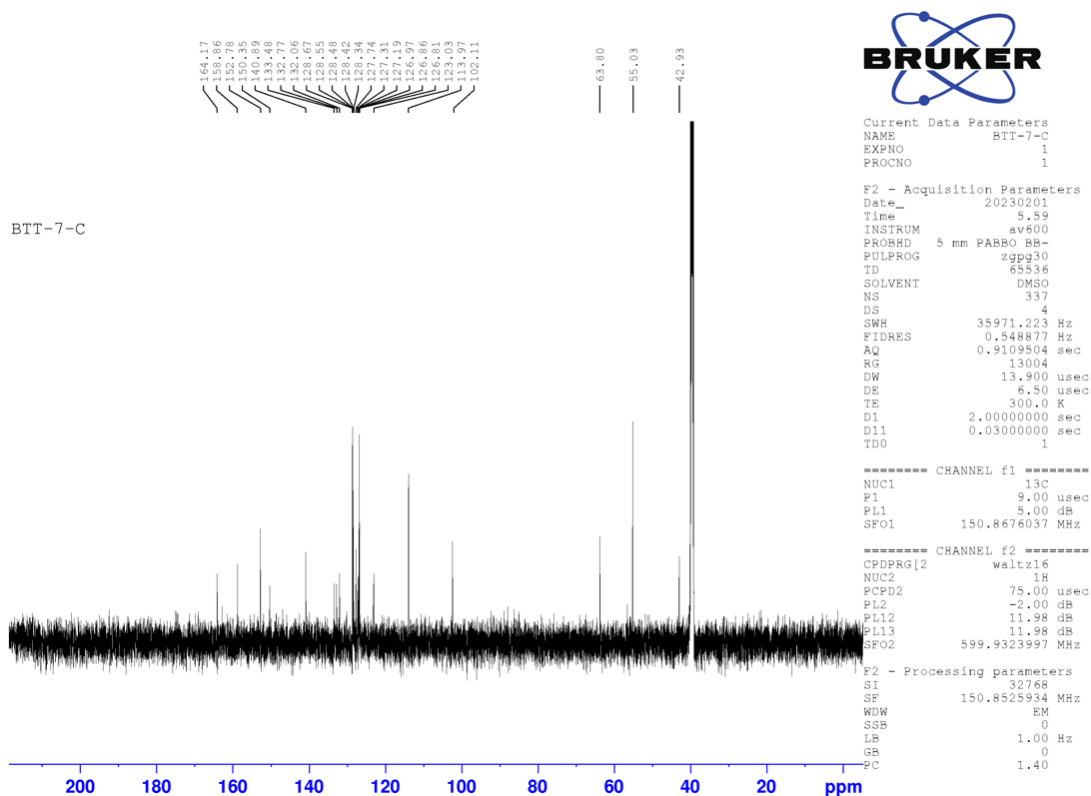


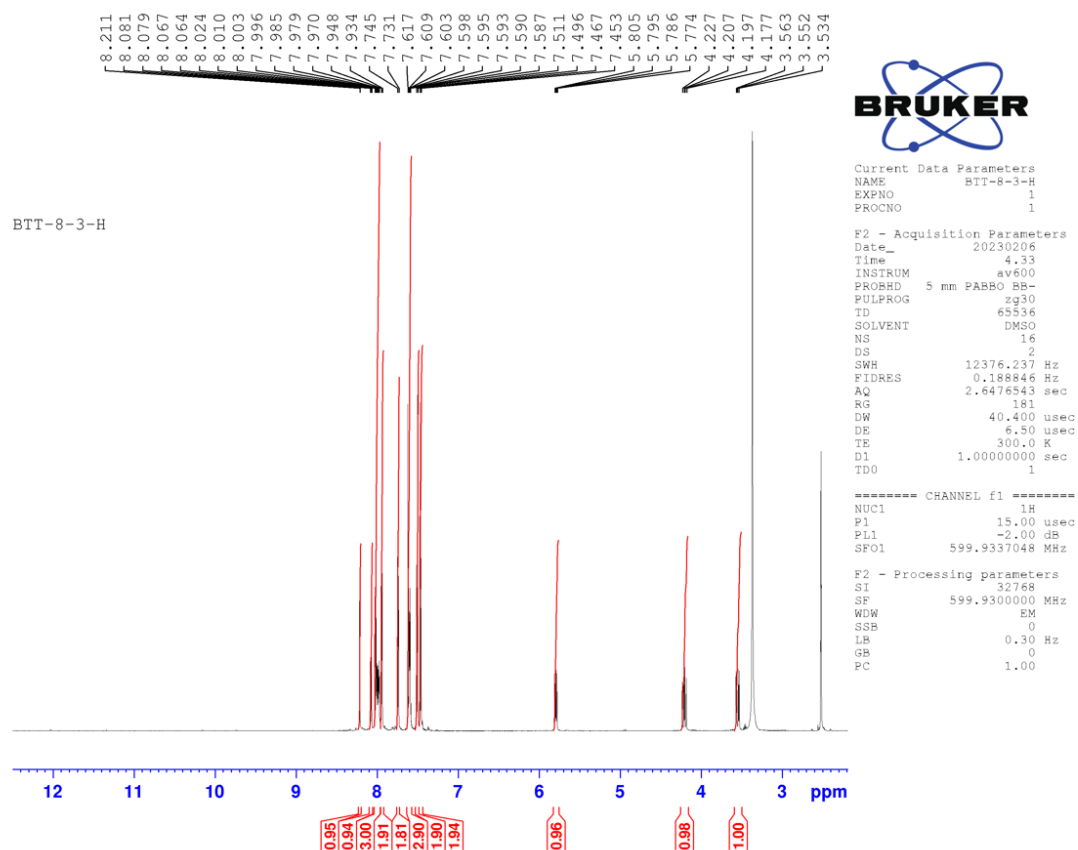
Figure S32: ^{13}C NMR Spectrum of BTT-7

[Elemental Composition]
Data : gousei242
Sample: BTT-7/sever belgin
Note : NBA
Inlet : Direct
RT : 1.75 min
Elements : C 100/0, H 100/0, O 2/0, N 4/2, Cl 2/0, S 2/0
Mass Tolerance : 20ppm, 10mmu if m/z < 500, 20mmu if m/z > 1000
Unsaturation (U.S.) : -0.5 - 150.0

Date : 01-Feb-2023 15:35
Page: 1
Ion Mode : FAB+
Scan#: (4,12)

Observed m/z	Int%	Err(ppm / mmu)	U.S.	Composition
495.1172	35.8	+7.7 / +3.8	29.5	C 35 H 15 O 2 N 2
		-14.9 / -7.4	29.5	C 34 H 15 O N 4
		-18.6 / -9.2	24.5	C 33 H 20 O N 2 Cl
		+6.8 / +3.3	25.0	C 32 H 18 O N 3 Cl
		-19.6 / -9.7	20.0	C 30 H 23 N 3 Cl 2
		+5.8 / +2.9	20.5	C 29 H 21 N 4 Cl 2
		+0.9 / +0.5	25.5	C 32 H 19 O 2 N 2 S
		+0.0 / +0.0	21.0	C 29 H 22 O N 3 Cl S
		-1.0 / -0.5	16.5	C 26 H 25 N 4 Cl 2 S
		-5.9 / -2.9	21.5	C 29 H 23 O 2 N 2 S 2
		+19.5 / +9.7	22.0	C 28 H 21 O 2 N 3 S 2
		-6.9 / -3.4	17.0	C 26 H 26 O N 3 Cl S 2
		+18.5 / +9.2	17.5	C 25 H 24 O N 4 Cl S 2
		+14.8 / +7.3	12.5	C 24 H 29 O N 2 Cl 2 S 2
		-7.8 / -3.9	12.5	C 23 H 29 N 4 Cl 2 S 2
496.1177	34.3	-7.0 / -3.5	29.0	C 35 H 16 O 2 N 2
		+18.4 / +9.1	29.5	C 34 H 14 O 2 N 3
		-8.0 / -4.0	24.5	C 32 H 19 O N 3 Cl
		+17.4 / +8.6	25.0	C 31 H 17 O N 4 Cl
		+13.7 / +6.8	20.0	C 30 H 22 O N 2 Cl 2
		-9.0 / -4.4	20.0	C 29 H 22 N 4 Cl 2
		-13.8 / -6.8	25.0	C 32 H 20 O 2 N 2 S
		+11.6 / +5.7	25.5	C 31 H 18 O 2 N 3 S
		-14.8 / -7.3	20.5	C 29 H 23 O N 3 Cl S
		+10.6 / +5.2	21.0	C 28 H 21 O N 4 Cl S
		+6.9 / +3.4	16.0	C 27 H 26 O N 2 Cl 2 S
		-15.8 / -7.8	16.0	C 26 H 26 N 4 Cl 2 S
		+4.8 / +2.4	21.5	C 28 H 22 O 2 N 3 S 2
		+3.8 / +1.9	17.0	C 25 H 25 O N 4 Cl S 2
		+0.1 / +0.0	12.0	C 24 H 30 O N 2 Cl 2 S 2

Figure S33: Mass Spectrum of BTT-7



1

2 **Figure S34:** ^1H NMR Spectrum of **BTT-8**

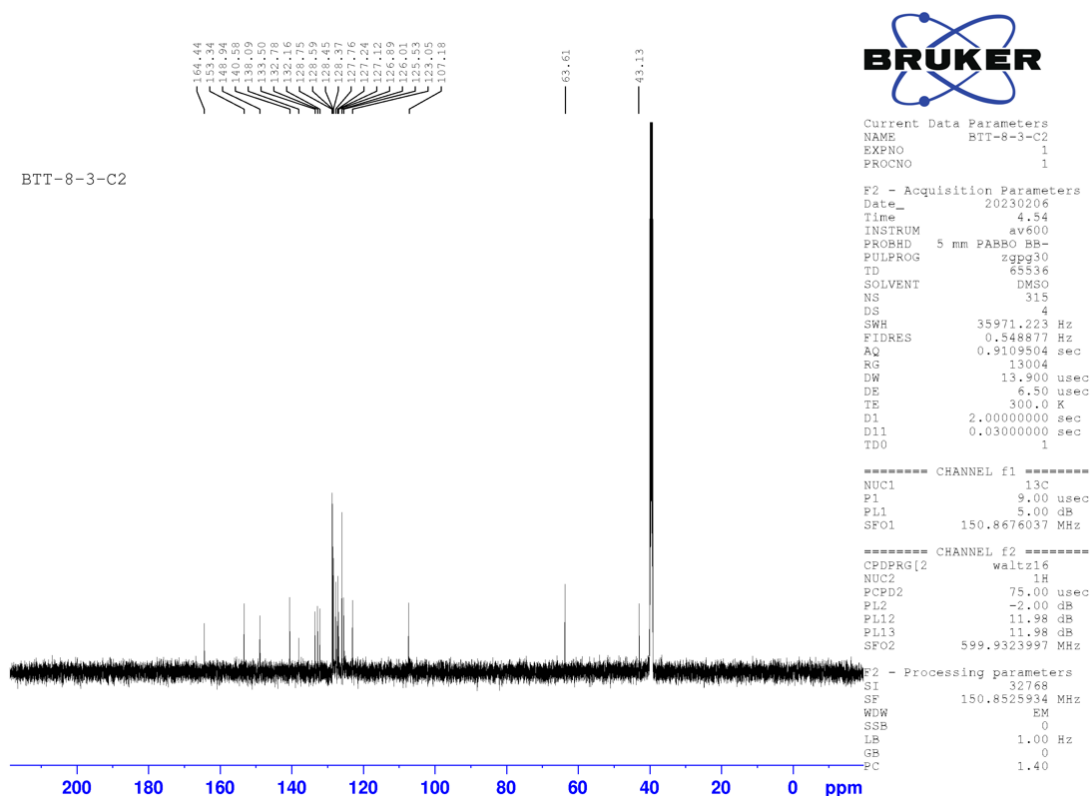


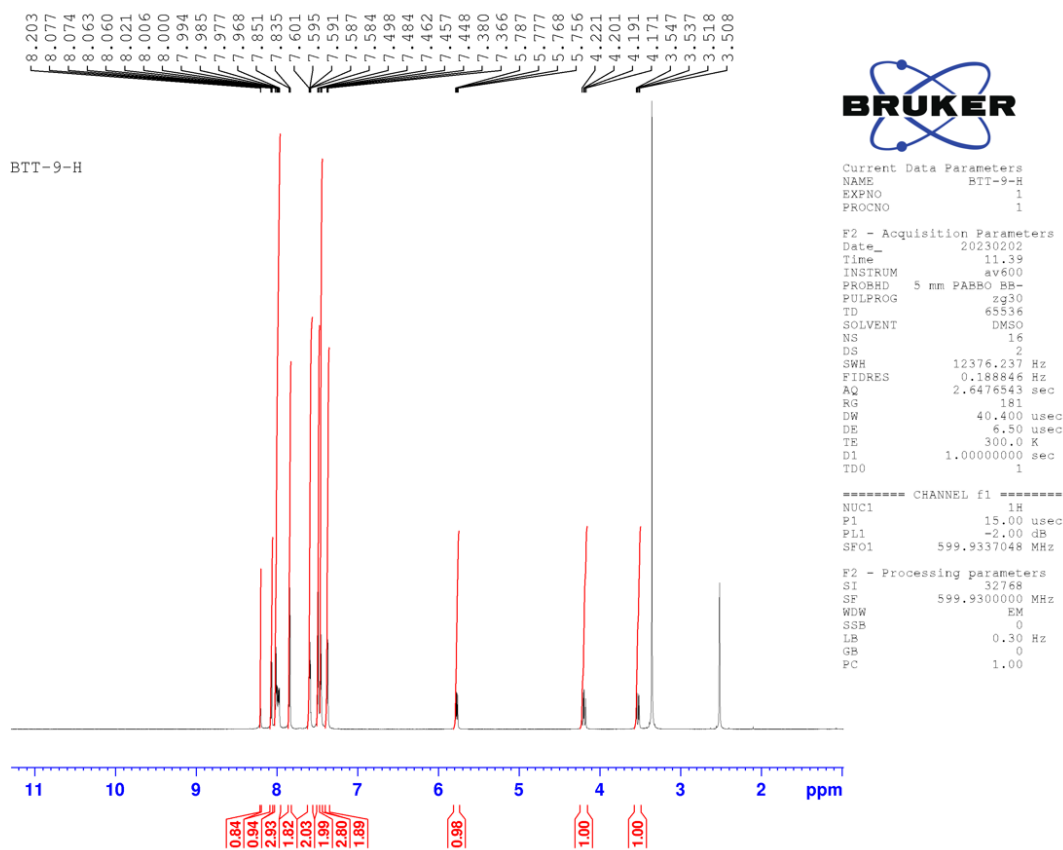
Figure S35: ^{13}C NMR Spectrum of BTT-8

[Elemental Composition]
Data : gousei243
Sample: BTT-8/sever belgin
Note : NBA
Inlet : Direct
RT : 1.75 min
Elements : C 100/0, H 100/0, N 4/2, Cl 2/0, F 4/2, S 2/0
Mass Tolerance : 20ppm, 10mmu if m/z < 500, 20mmu if m/z > 1000
Unsaturation (U.S.) : -0.5 - 150.0

Date : 01-Feb-2023 15:54
Page: 1
Ion Mode : FAB+
Scan#: (6,10)

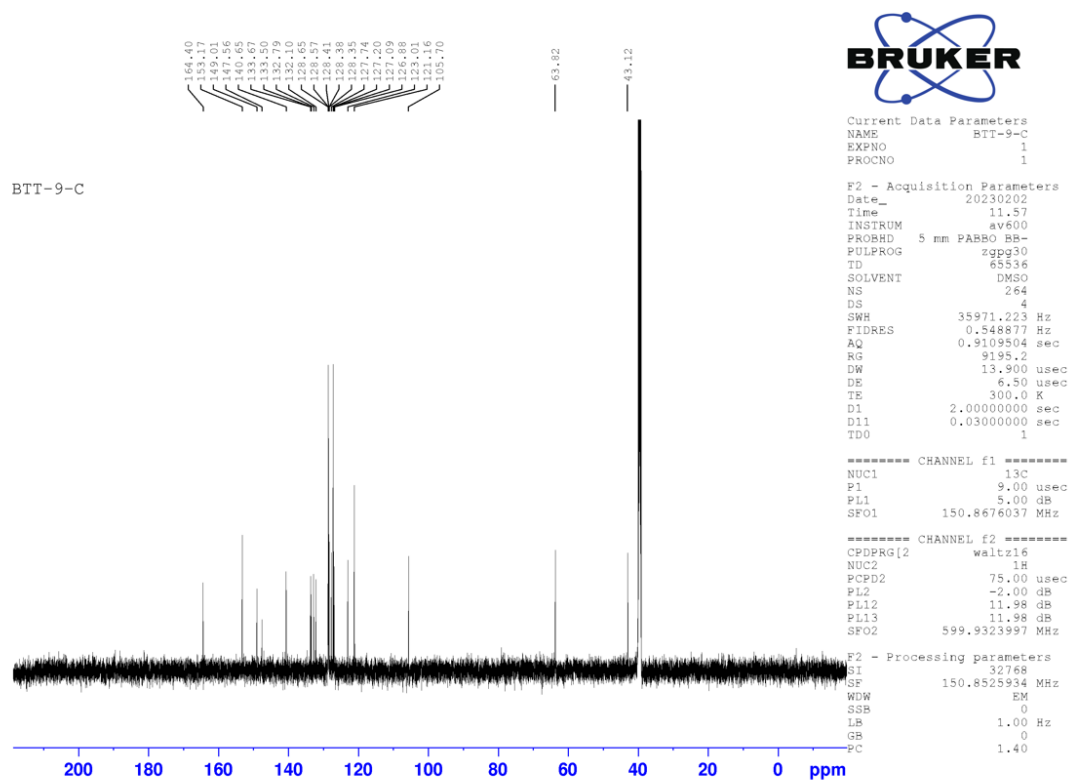
Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
533.0923	20.1	+6.1 / +3.3	33.5	C 38 H 11 N 2 F 2
		-17.1 / -9.1	29.5	C 34 H 12 N 4 F 3
		+3.0 / +1.6	25.0	C 32 H 15 N 3 Cl F 3
		+0.0 / +0.0	16.5	C 26 H 19 N 4 Cl 2 F 4
		-0.2 / -0.1	29.5	C 35 H 15 N 2 F 2 S
		-3.3 / -1.7	21.0	C 29 H 19 N 3 Cl F 3 S
		+16.9 / +9.0	16.5	C 27 H 22 N 2 Cl 2 F 3 S
		-6.3 / -3.4	12.5	C 23 H 23 N 4 Cl 2 F 4 S
		-6.5 / -3.5	25.5	C 32 H 19 N 2 F 2 S 2
		+17.0 / +9.1	26.0	C 31 H 17 N 3 F 2 S 2
		-9.6 / -5.1	17.0	C 26 H 23 N 3 Cl F 3 S 2
		+14.0 / +7.5	17.5	C 25 H 21 N 4 Cl F 3 S 2
		+10.6 / +5.6	12.5	C 24 H 26 N 2 Cl 2 F 3 S 2
		-12.7 / -6.7	8.5	C 20 H 27 N 4 Cl 2 F 4 S 2
534.1013	17.6	+8.2 / +4.4	33.0	C 38 H 12 N 2 F 2
		-14.9 / -8.0	29.0	C 34 H 13 N 4 F 3
		-18.4 / -9.8	24.0	C 33 H 18 N 2 Cl F 3
		+5.2 / +2.8	24.5	C 32 H 16 N 3 Cl F 3
		+2.1 / +1.1	16.0	C 26 H 20 N 4 Cl 2 F 4
		+1.9 / +1.0	29.0	C 35 H 16 N 2 F 2 S
		-1.1 / -0.6	20.5	C 29 H 20 N 3 Cl F 3 S
		+19.0 / +10.1	16.0	C 27 H 23 N 2 Cl 2 F 3 S
		-4.2 / -2.2	12.0	C 23 H 24 N 4 Cl 2 F 4 S
		-4.4 / -2.3	25.0	C 32 H 20 N 2 F 2 S 2
		+19.2 / +10.2	25.5	C 31 H 18 N 3 F 2 S 2
		-7.4 / -4.0	16.5	C 26 H 24 N 3 Cl F 3 S 2
		+16.1 / +8.6	17.0	C 25 H 22 N 4 Cl F 3 S 2
		+12.7 / +6.8	12.0	C 24 H 27 N 2 Cl 2 F 3 S 2
		-10.5 / -5.6	8.0	C 20 H 28 N 4 Cl 2 F 4 S 2

Figure S36: Mass Spectrum of BTT-8



1

2 **Figure S37: ^1H NMR Spectrum of BTT-9**



1

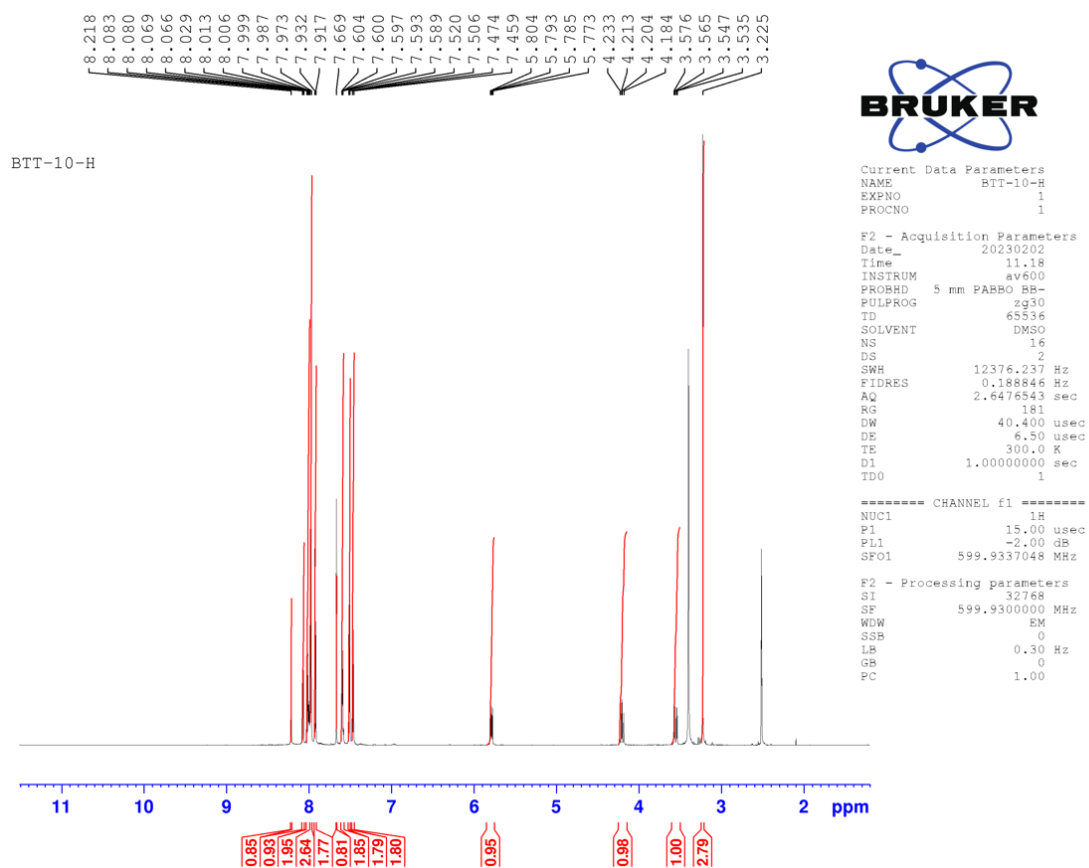
2 **Figure S38:** ^{13}C NMR Spectrum of BTT-9

[Elemental Composition]
 Date : 03-Feb-2023 14:45 Page: 1
 Data : gousei246
 Sample: BTT-9/sever belgin
 Note : NBA
 Inlet : Direct Ion Mode : FAB+
 RT : 0.88 min Scan#: (2,7)
 Elements : C 100/0, H 100/0, O 2/0, N 4/2, Cl 2/0, F 4/2, S 2/0
 Mass Tolerance : 20ppm, 10mmu if m/z < 500, 20mmu if m/z > 1000
 Unsaturation (U.S.) : -0.5 - 150.0

Observed m/z	Int%	Err [ppm / mmu]	U.S.	Composition
549.0903	100.0	+11.6 / +6.4	33.5	C 38 H 11 O N 2 F 2
		-8.8 / -4.8	33.5	C 37 H 11 N 4 F 2
		-12.2 / -6.7	28.5	C 36 H 16 N 2 Cl F 2
		+10.7 / +5.9	29.0	C 35 H 14 N 3 Cl F 2
		-4.8 / -2.7	24.5	C 31 H 16 O 2 N 4 Cl F 2
		-8.2 / -4.5	19.5	C 30 H 21 O 2 N 2 Cl 2 F 2
		+14.7 / +8.1	20.0	C 29 H 19 O 2 N 3 Cl 2 F 2
		+9.6 / +5.2	29.5	C 35 H 12 O 2 N 2 F 3
		-10.9 / -6.0	29.5	C 34 H 12 O N 4 F 3
		-14.2 / -7.8	24.5	C 33 H 17 O N 2 Cl F 3
		+8.7 / +4.8	25.0	C 32 H 15 O N 3 Cl F 3
		-15.1 / -8.3	20.0	C 30 H 20 N 3 Cl 2 F 3
		+7.8 / +4.3	20.5	C 29 H 18 N 4 Cl 2 F 3
		+2.6 / +1.4	30.0	C 35 H 11 N 3 F 4
		-13.0 / -7.1	25.5	C 31 H 13 O 2 N 4 F 4
		-16.3 / -9.0	20.5	C 30 H 18 O 2 N 2 Cl F 4
		+6.6 / +3.6	21.0	C 29 H 16 O 2 N 3 Cl F 4
		-17.2 / -9.4	16.0	C 27 H 21 O N 3 Cl 2 F 4
		+5.7 / +3.1	16.5	C 26 H 19 O N 4 Cl 2 F 4
		+5.5 / +3.0	29.5	C 35 H 15 O N 2 F 2 S
		-15.0 / -8.2	29.5	C 34 H 15 N 4 F 2 S
		-18.3 / -10.0	24.5	C 33 H 20 N 2 Cl F 2 S
		+4.6 / +2.5	25.0	C 32 H 18 N 3 Cl F 2 S
		-11.0 / -6.0	20.5	C 28 H 20 O 2 N 4 Cl F 2 S
		-14.3 / -7.9	15.5	C 27 H 25 O 2 N 2 Cl 2 F 2 S
		+8.6 / +4.7	16.0	C 26 H 23 O 2 N 3 Cl 2 F 2 S
		+3.4 / +1.9	25.5	C 32 H 16 O 2 N 2 F 3 S
		-17.0 / -9.4	25.5	C 31 H 16 O N 4 F 3 S
		+2.5 / +1.4	21.0	C 29 H 19 O N 3 Cl F 3 S
		+1.6 / +0.9	16.5	C 26 H 22 N 4 Cl 2 F 3 S
		-3.6 / -2.0	26.0	C 32 H 15 N 3 F 4 S
		+19.4 / +10.6	26.5	C 31 H 13 N 4 F 4 S
		-19.1 / -10.5	21.5	C 28 H 17 O 2 N 4 F 4 S
		+16.0 / +8.8	21.5	C 30 H 18 N 2 Cl F 4 S
		+0.4 / +0.2	17.0	C 26 H 20 O 2 N 3 Cl F 4 S
		-0.4 / -0.2	12.5	C 23 H 23 O N 4 Cl 2 F 4 S
		-0.6 / -0.4	25.5	C 32 H 19 O N 2 F 2 S 2
		-1.5 / -0.8	21.0	C 29 H 22 N 3 Cl F 2 S 2
		-17.1 / -9.4	16.5	C 25 H 24 O 2 N 4 Cl F 2 S 2
		+18.0 / +9.9	16.5	C 27 H 25 N 2 Cl 2 F 2 S 2
		+2.5 / +1.3	12.0	C 23 H 27 O 2 N 3 Cl 2 F 2 S 2
		-2.7 / -1.5	21.5	C 29 H 20 O 2 N 2 F 3 S 2
		-3.6 / -2.0	17.0	C 26 H 23 O N 3 Cl F 3 S 2
		+19.3 / +10.6	17.5	C 25 H 21 O N 4 Cl F 3 S 2
		+16.0 / +8.8	12.5	C 24 H 26 O N 2 Cl 2 F 3 S 2
		-4.5 / -2.5	12.5	C 23 H 26 N 4 Cl 2 F 3 S 2
		-9.7 / -5.3	22.0	C 29 H 19 N 3 F 4 S 2
		+13.2 / +7.3	22.5	C 28 H 17 N 4 F 4 S 2
		+9.9 / +5.4	17.5	C 27 H 22 N 2 Cl F 4 S 2
		-5.7 / -3.1	13.0	C 23 H 24 O 2 N 3 Cl F 4 S 2
		+17.2 / +9.4	13.5	C 22 H 22 O 2 N 4 Cl F 4 S 2
		+13.9 / +7.6	8.5	C 21 H 27 O 2 N 2 Cl 2 F 4 S 2
		-6.6 / -3.6	8.5	C 20 H 27 O N 4 Cl 2 F 4 S 2

1

2 **Figure S39: Mass Spectrum of BTT-9**



1

2 **Figure S40: ^1H NMR Spectrum of BTT-10**

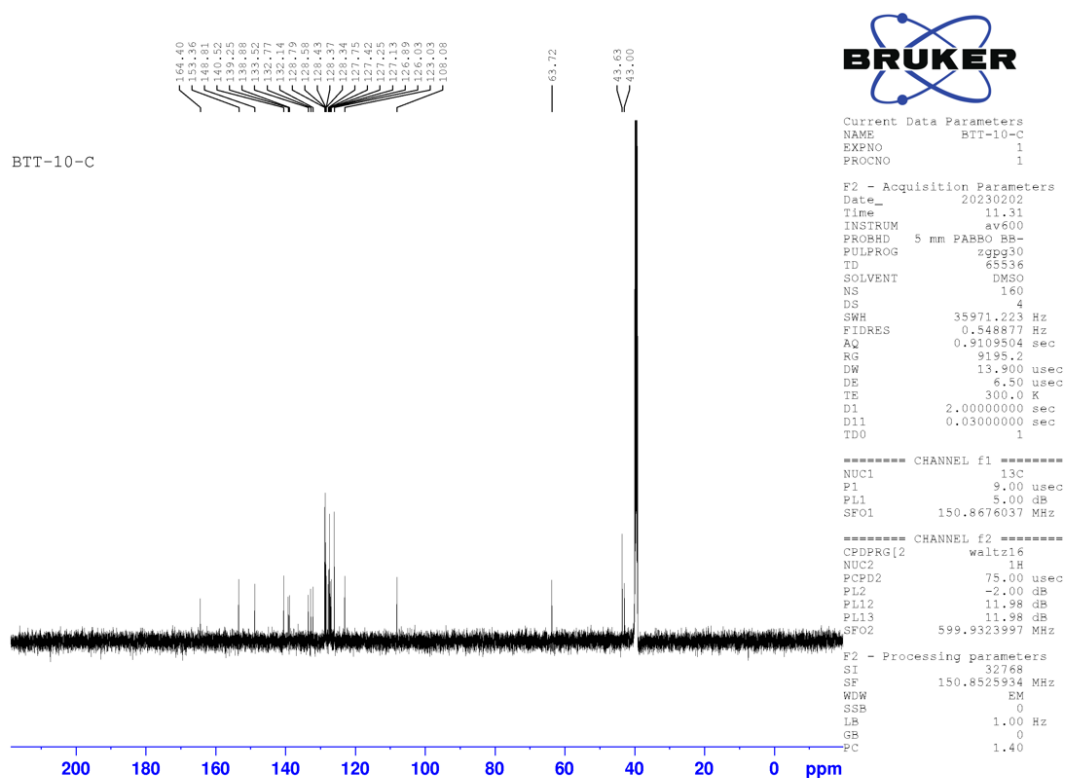


Figure S41: ^{13}C NMR Spectrum of BTT-10

[Elemental Composition]

Data : gousei247 Date : 03-Feb-2023 15:10 Page: 1

Sample: BTT-10/sever belgin

Note : NBA

Inlet : Direct Ion Mode : FAB+

RT : 1.25 min Scan#: (3,9)

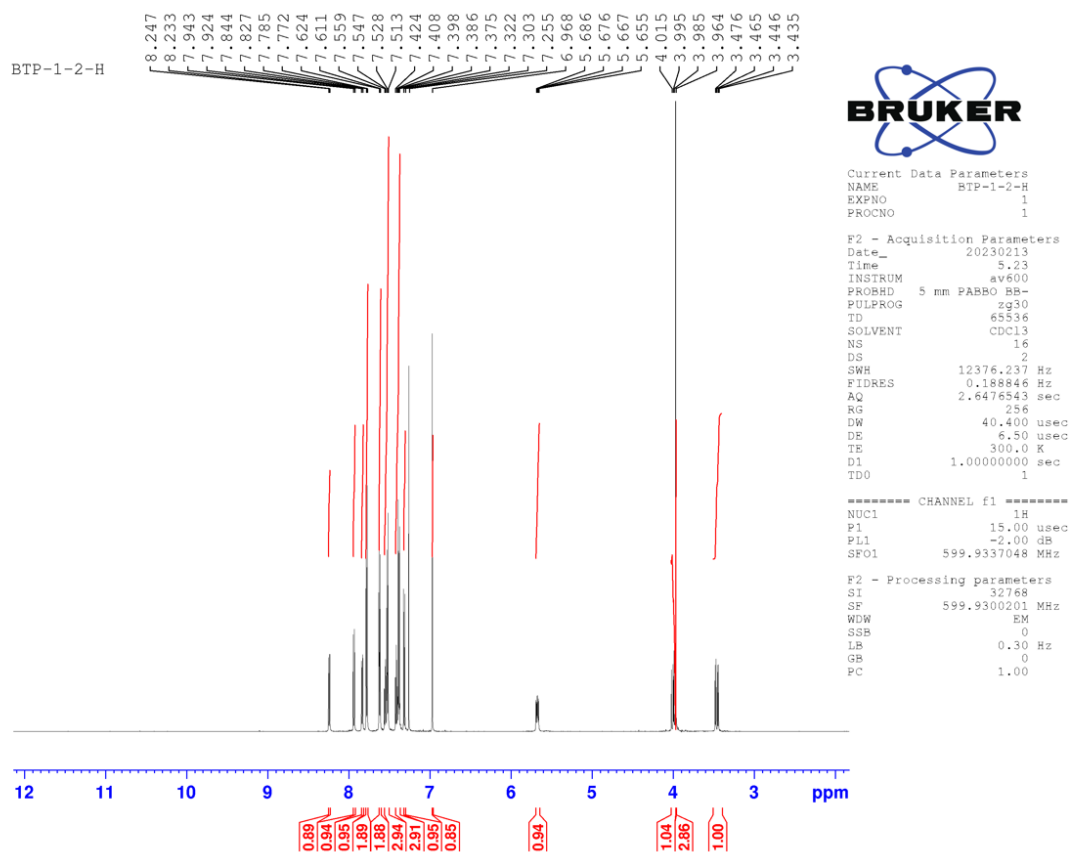
Elements : C 100/0, H 100/0, O 3/1, N 4/2, Cl 2/0, S 3/1

Mass Tolerance : 20ppm, 10mmu if m/z < 500, 20mmu if m/z > 1000

Unsaturation (U.S.) : -0.5 - 150.0

Observed m/z	Int%	Err [ppm / mmu]	U.S.	Composition
543.0842	52.2	+7.0 / +3.8	30.5	C 35 H 15 O 3 N 2 S
		-13.6 / -7.4	30.5	C 34 H 15 O 2 N 4 S
		-17.0 / -9.2	25.5	C 33 H 20 O 2 N 2 Cl S
		+6.2 / +3.3	26.0	C 32 H 18 O 2 N 3 Cl S
		-17.9 / -9.7	21.0	C 30 H 23 O N 3 Cl 2 S
		+5.3 / +2.9	21.5	C 29 H 21 O N 4 Cl 2 S
		+0.8 / +0.5	26.5	C 32 H 19 O 3 N 2 S 2
		-19.8 / -10.8	26.5	C 31 H 19 O 2 N 4 S 2
		-0.1 / +0.0	22.0	C 29 H 22 O 2 N 3 Cl S 2
		+19.7 / +10.7	17.5	C 27 H 25 O 2 N 2 Cl 2 S 2
		-1.0 / -0.5	17.5	C 26 H 25 O N 4 Cl 2 S 2
		-5.4 / -2.9	22.5	C 29 H 23 O 3 N 2 S 3
		+17.8 / +9.7	23.0	C 28 H 21 O 3 N 3 S 3
		-6.3 / -3.4	18.0	C 26 H 26 O 2 N 3 Cl S 3
		+16.9 / +9.2	18.5	C 25 H 24 O 2 N 4 Cl S 3
		+13.5 / +7.3	13.5	C 24 H 29 O 2 N 2 Cl 2 S 3
		-7.2 / -3.9	13.5	C 23 H 29 O N 4 Cl 2 S 3

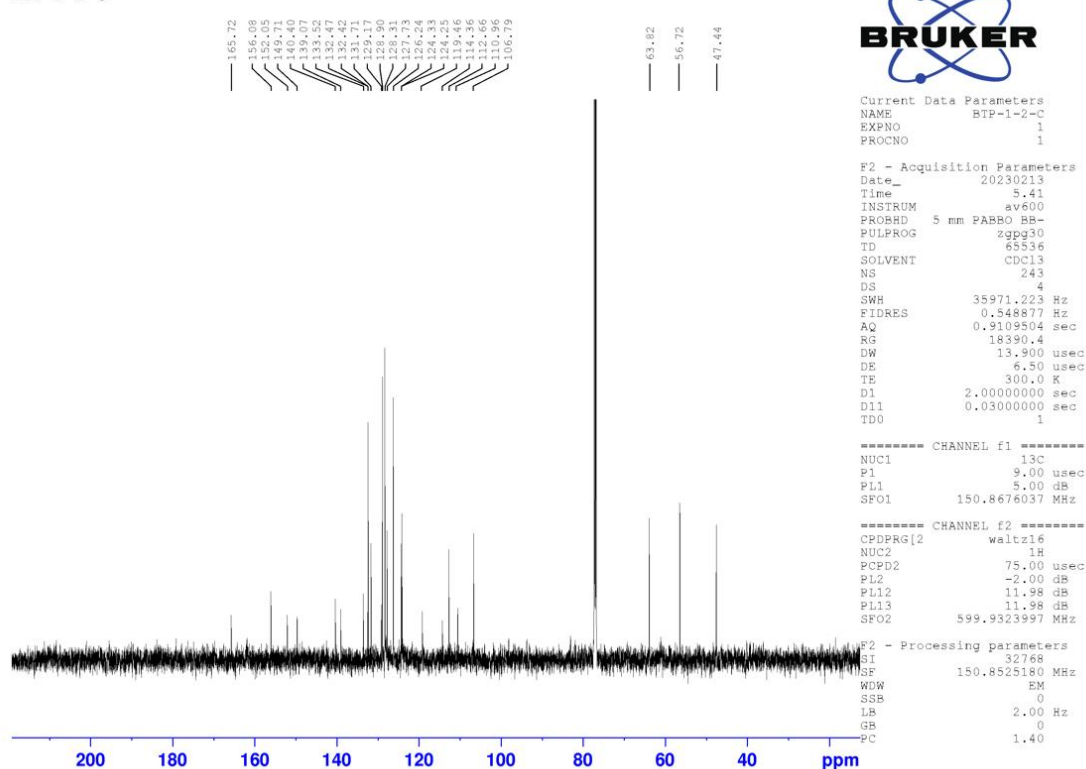
Figure S42: Mass Spectrum of BTT-10



1

2 **Figure S43:** ^1H NMR Spectrum of **BTP-1**

BTP-1-2-C



1

2 **Figure S44:** ^{13}C NMR Spectrum of BTP-1

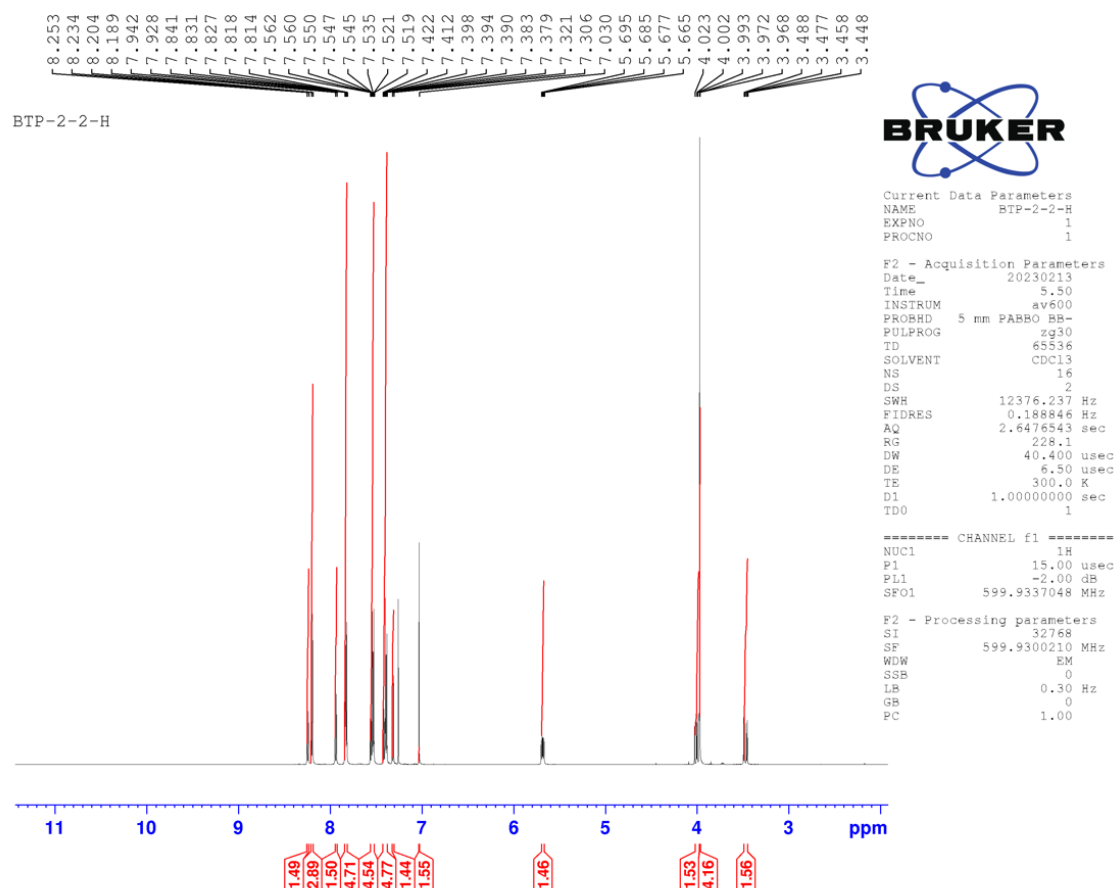
[Elemental Composition]
Data : gousei260
Sample: BTP-1/sever belgin
Note : NBA
Inlet : Direct
RT : 1.88 min
Elements : C 100/0, H 100/0, O 2/0, N 5/3, Cl 2/0, S 2/0
Mass Tolerance : 20ppm, 10mmu if m/z < 500, 20mmu if m/z > 1000
Unsaturation (U.S.) : -0.5 - 150.0

Date : 03-Feb-2023 18:38
Page: 1
Ion Mode : FAB+
Scan#: (7,10)

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
520.1104	100.0	+3.5 / +1.8	31.5	C 36 H 14 O 2 N 3
		-18.1 / -9.4	31.5	C 35 H 14 O N 5
		+2.5 / +1.3	27.0	C 33 H 17 O N 4 Cl
		+1.6 / +0.8	22.5	C 30 H 20 N 5 Cl 2
		-3.0 / -1.6	27.5	C 33 H 18 O 2 N 3 S
		-3.9 / -2.0	23.0	C 30 H 21 O N 4 Cl S
		+16.7 / +8.7	18.5	C 28 H 24 O N 3 Cl 2 S
		-4.9 / -2.5	18.5	C 27 H 24 N 5 Cl 2 S
		-9.5 / -4.9	23.5	C 30 H 22 O 2 N 3 S 2
		+14.7 / +7.6	24.0	C 29 H 20 O 2 N 4 S 2
		-10.4 / -5.4	19.0	C 27 H 25 O N 4 Cl S 2
		+13.8 / +7.2	19.5	C 26 H 23 O N 5 Cl S 2
		+10.2 / +5.3	14.5	C 25 H 28 O N 3 Cl 2 S 2
		-11.4 / -5.9	14.5	C 24 H 28 N 5 Cl 2 S 2

3

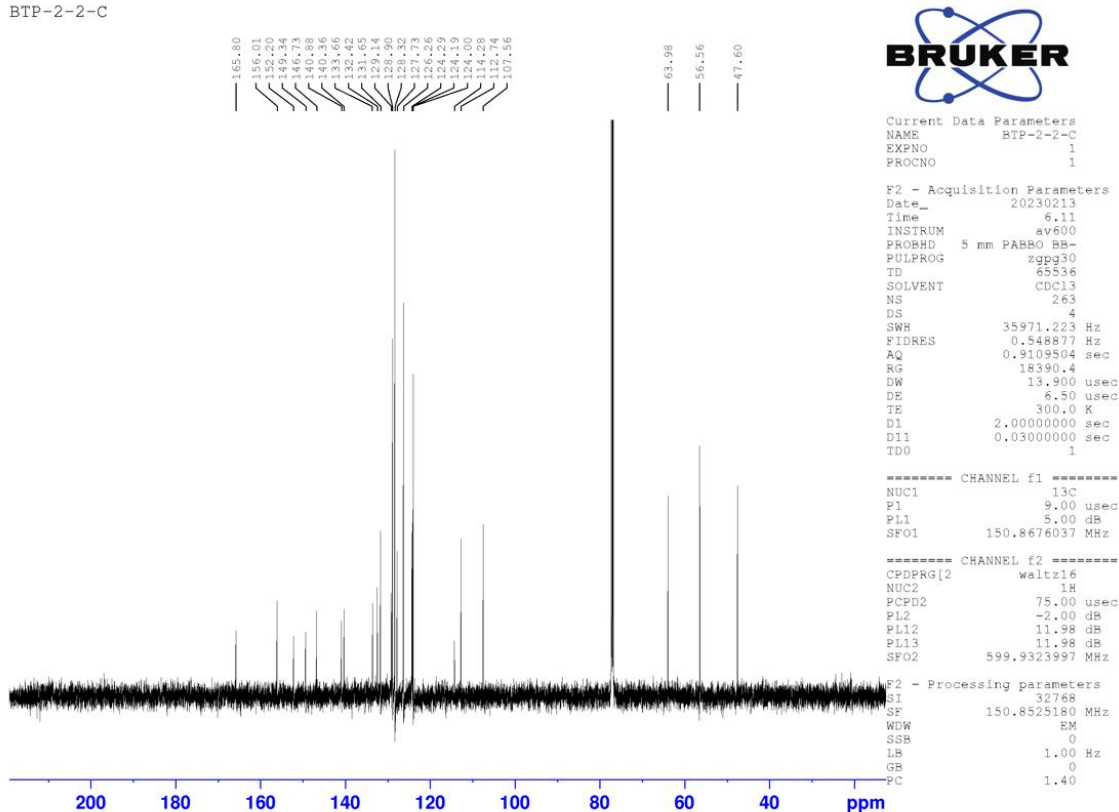
4 **Figure S45:** Mass Spectrum of BTP-1



1

2 **Figure S46:** ^1H NMR Spectrum of **BTP-2**

BTP-2-2-C



1

2 **Figure S47:** ^{13}C NMR Spectrum of **BTP-2**

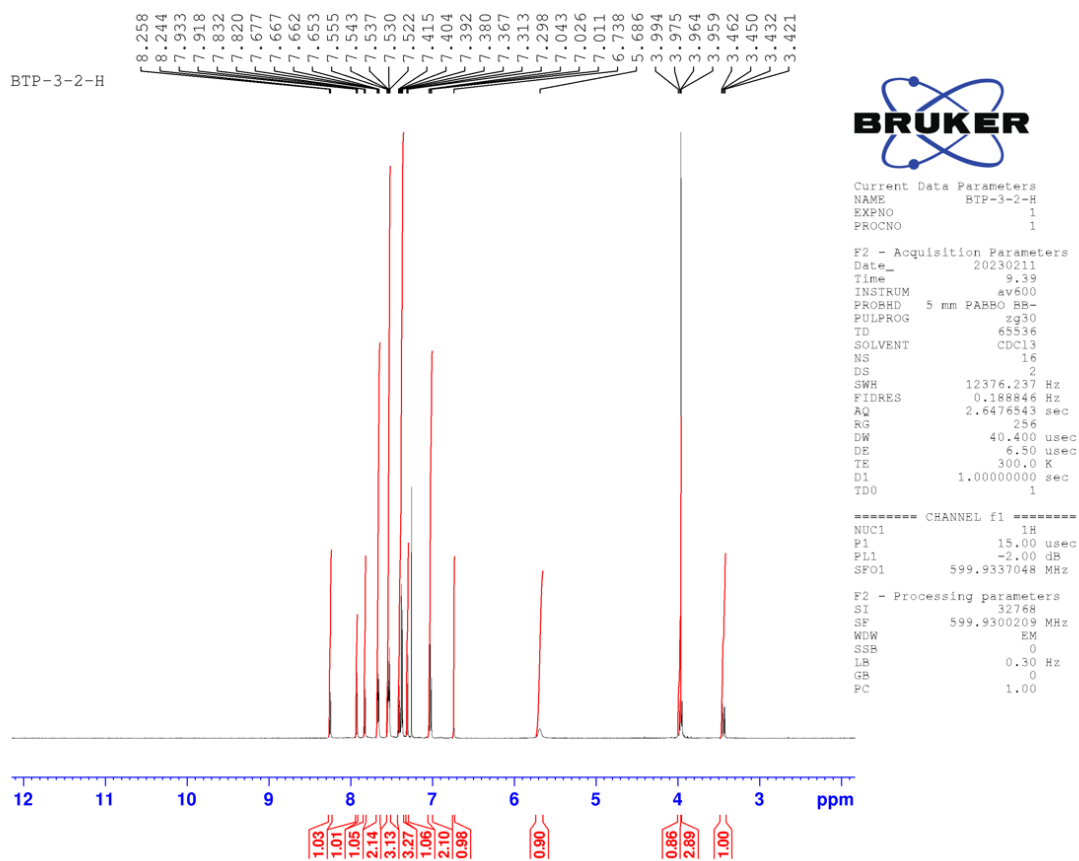
[Elemental Composition]
Data : gousei261
Sample: BTP-2/sever belgin
Note : NEA
Inlet : Direct
RT : 1.38 min
Elements : C 100/0, H 100/0, O 4/2, N 5/3, Cl 2/0, S 2/0
Mass Tolerance : 20ppm, 10mmu if m/z < 500, 20mmu if m/z > 1000
Unsaturation (U.S.) : -0.5 - 150.0

Date : 06-Feb-2023 14:39
Page: 1
Ion Mode : FAB+
Scan#: (4,9)

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
540.1022	41.7	+6.9 / +3.7	30.5	C 35 H 14 O 4 N 3
		-13.9 / -7.5	30.5	C 34 H 14 O 3 N 5
		-17.3 / -9.3	25.5	C 33 H 19 O 3 N 3 Cl
		+6.0 / +3.3	26.0	C 32 H 17 O 3 N 4 Cl
		-18.2 / -9.8	21.0	C 30 H 22 O 2 N 4 Cl 2
		+5.1 / +2.8	21.5	C 29 H 20 O 2 N 5 Cl 2
		+0.7 / +0.4	26.5	C 32 H 18 O 4 N 3 S
		-0.2 / -0.1	22.0	C 29 H 21 O 3 N 4 Cl S
		+19.7 / +10.6	17.5	C 27 H 24 O 3 N 3 Cl 2 S
		-1.1 / -0.6	17.5	C 26 H 24 O 2 N 5 Cl 2 S
		-5.6 / -3.0	22.5	C 29 H 22 O 4 N 3 S 2
		+17.7 / +9.6	23.0	C 28 H 20 O 4 N 4 S 2
		-6.5 / -3.5	18.0	C 26 H 25 O 3 N 4 Cl S 2
		+16.8 / +9.1	18.5	C 25 H 23 O 3 N 5 Cl S 2
		+13.4 / +7.3	13.5	C 24 H 28 O 3 N 3 Cl 2 S 2
		-7.4 / -4.0	13.5	C 23 H 28 O 2 N 5 Cl 2 S 2

3

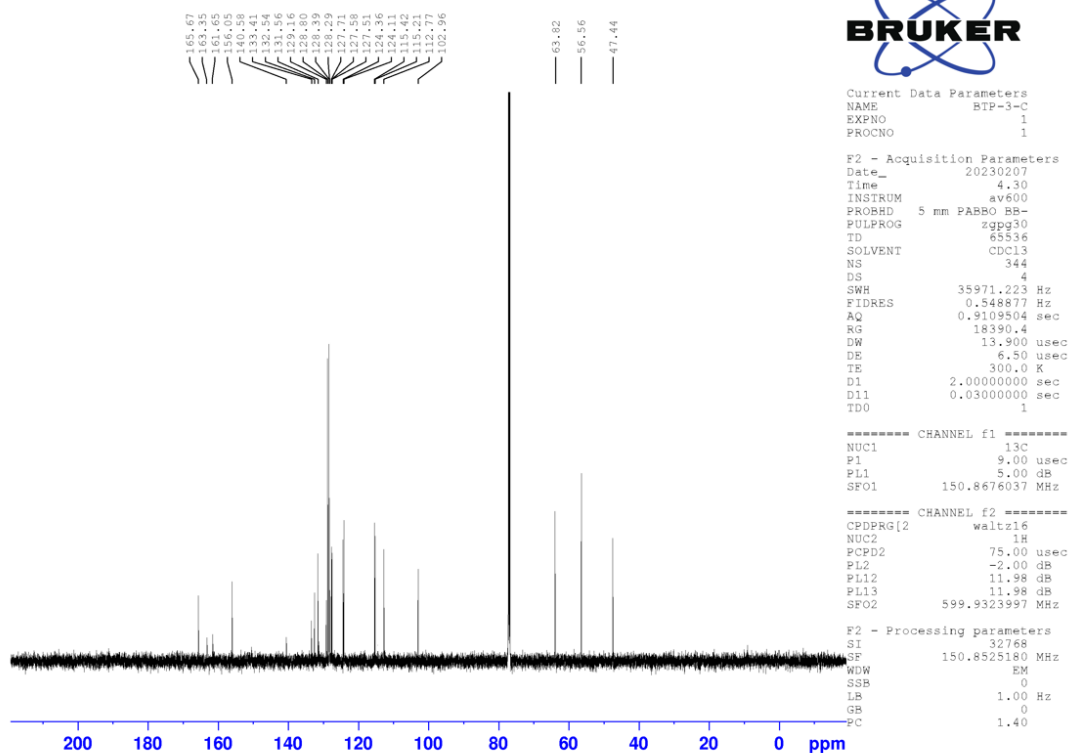
4 **Figure S48:** Mass Spectrum of **BTP-2**



1

2 **Figure S49:** ^1H NMR Spectrum of **BTP-3**

BTP-3-C



1

2 **Figure S50:** ^{13}C NMR Spectrum of **BTP-3**

[Elemental Composition]
 Date : 07-Feb-2023 15:45
 Data : gousei264
 Sample: BTP-3/sever belgin
 Note : NBA
 Inlet : Direct
 RT : 1.63 min
 Elements : C 100/0, H 100/0, O 2/0, N 4/2, Cl 2/0, F 2/0, S 2/0
 Mass Tolerance : 20ppm, 10mmu if m/z < 500, 20mmu if m/z > 1000
 Unsaturation (U.S.) : -0.5 - 150.0

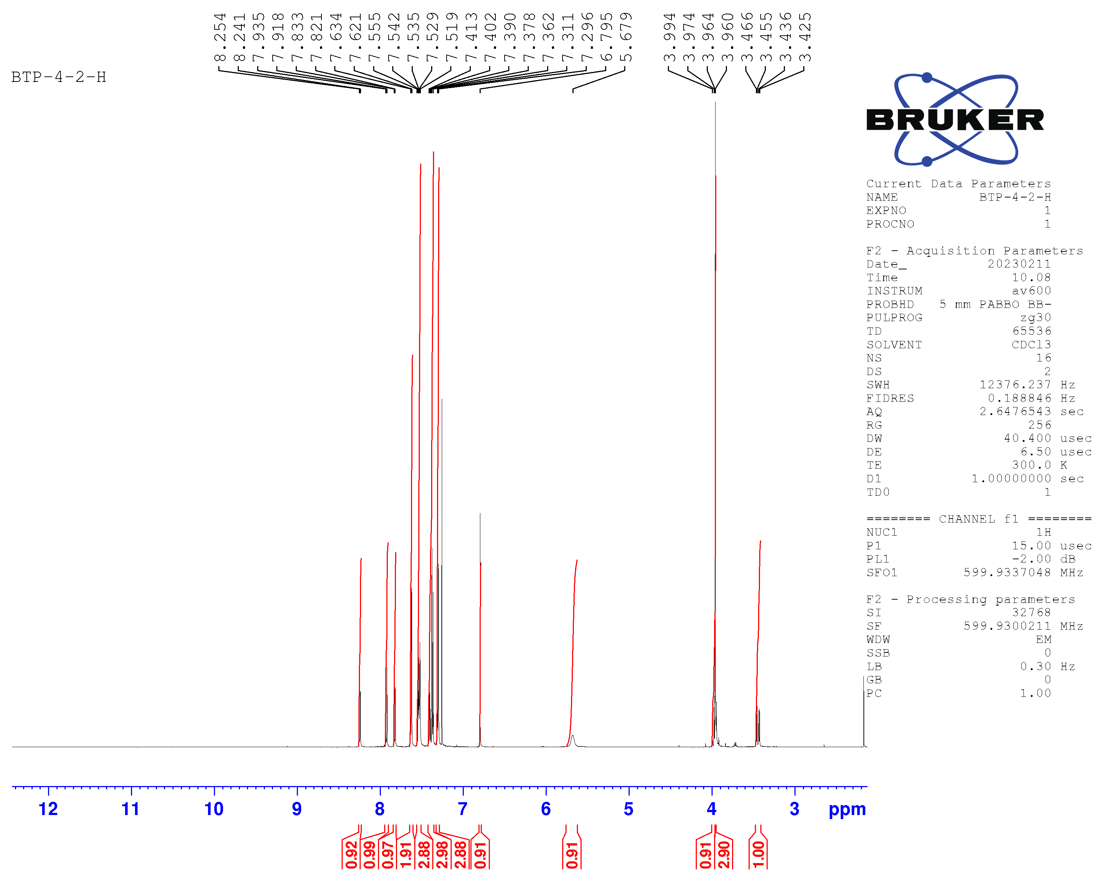
Page: 1

Ion Mode : FAB+
 Scan#: (5,10)

Observed m/z	Int%	Err [ppm / mmu]	U.S.	Composition
513.1071	100.0	+8.3 / +4.3	33.5	C 38 H 13 O N 2
		-13.6 / -7.0	33.5	C 37 H 13 N 4
		-17.1 / -8.8	28.5	C 36 H 18 N 2 Cl
		+7.4 / +3.8	29.0	C 35 H 16 N 3 Cl
		-9.3 / -4.8	24.5	C 31 H 18 O 2 N 4 Cl
		-12.9 / -6.6	19.5	C 30 H 23 O 2 N 2 Cl 2
		+11.6 / +6.0	20.0	C 29 H 21 O 2 N 3 Cl 2
		+6.1 / +3.1	29.5	C 35 H 14 O 2 N 2 F
		-15.8 / -8.1	29.5	C 34 H 14 O N 4 F
		-19.4 / -9.9	24.5	C 33 H 19 O N 2 Cl F
		+5.1 / +2.6	25.0	C 32 H 17 O N 3 Cl F
		+4.2 / +2.2	20.5	C 29 H 20 N 4 Cl 2 F
		-1.4 / -0.7	30.0	C 35 H 13 N 3 F 2
		-18.0 / -9.3	25.5	C 31 H 15 O 2 N 4 F 2
		+19.6 / +10.0	25.5	C 33 H 16 N 2 Cl F 2
		+2.9 / +1.5	21.0	C 29 H 18 O 2 N 3 Cl F 2
		+2.0 / +1.0	16.5	C 26 H 21 O N 4 Cl 2 F 2
		+1.7 / +0.9	29.5	C 35 H 17 O N 2 S
		+0.8 / +0.4	25.0	C 32 H 20 N 3 Cl S
		-15.9 / -8.1	20.5	C 28 H 22 O 2 N 4 Cl S
		-19.4 / -10.0	15.5	C 27 H 27 O 2 N 2 Cl 2 S
		+5.1 / +2.6	16.0	C 26 H 25 O 2 N 3 Cl 2 S
		-0.5 / -0.2	25.5	C 32 H 18 O 2 N 2 F S
		-1.4 / -0.7	21.0	C 29 H 21 O N 3 Cl F S
		+19.5 / +10.0	16.5	C 27 H 24 O N 2 Cl 2 F S
		-2.4 / -1.2	16.5	C 26 H 24 N 4 Cl 2 F S
		-7.9 / -4.1	26.0	C 32 H 17 N 3 F 2 S
		+16.6 / +8.5	26.5	C 31 H 15 N 4 F 2 S
		+13.0 / +6.7	21.5	C 30 H 20 N 2 Cl F 2 S
		-3.7 / -1.9	17.0	C 26 H 22 O 2 N 3 Cl F 2 S
		+17.3 / +8.9	12.5	C 24 H 25 O 2 N 2 Cl 2 F 2 S
		-4.6 / -2.4	12.5	C 23 H 25 O N 4 Cl 2 F 2 S
		-4.8 / -2.5	25.5	C 32 H 21 O N 2 S 2
		+19.7 / +10.1	26.0	C 31 H 19 O N 3 S 2
		-5.8 / -3.0	21.0	C 29 H 24 N 3 Cl S 2
		+18.7 / +9.6	21.5	C 28 H 22 N 4 Cl S 2
		+15.2 / +7.8	16.5	C 27 H 27 N 2 Cl 2 S 2
		-1.5 / -0.8	12.0	C 23 H 29 O 2 N 3 Cl 2 S 2
		-7.1 / -3.6	21.5	C 29 H 22 O 2 N 2 F S 2
		+17.5 / +9.0	22.0	C 28 H 20 O 2 N 3 F S 2
		-8.0 / -4.1	17.0	C 26 H 25 O N 3 Cl F S 2
		+16.5 / +8.5	17.5	C 25 H 23 O N 4 Cl F S 2
		+12.9 / +6.6	12.5	C 24 H 28 O N 2 Cl 2 F S 2
		-9.0 / -4.6	12.5	C 23 H 28 N 4 Cl 2 F S 2
		-14.5 / -7.4	22.0	C 29 H 21 N 3 F 2 S 2
		+10.0 / +5.1	22.5	C 28 H 19 N 4 F 2 S 2
		+6.4 / +3.3	17.5	C 27 H 24 N 2 Cl F 2 S 2
		-10.2 / -5.2	13.0	C 23 H 26 O 2 N 3 Cl F 2 S 2
		+14.3 / +7.3	13.5	C 22 H 24 O 2 N 4 Cl F 2 S 2
		+10.7 / +5.5	8.5	C 21 H 29 O 2 N 2 Cl 2 F 2 S 2
		-11.2 / -5.7	8.5	C 20 H 29 O N 4 Cl 2 F 2 S 2

1

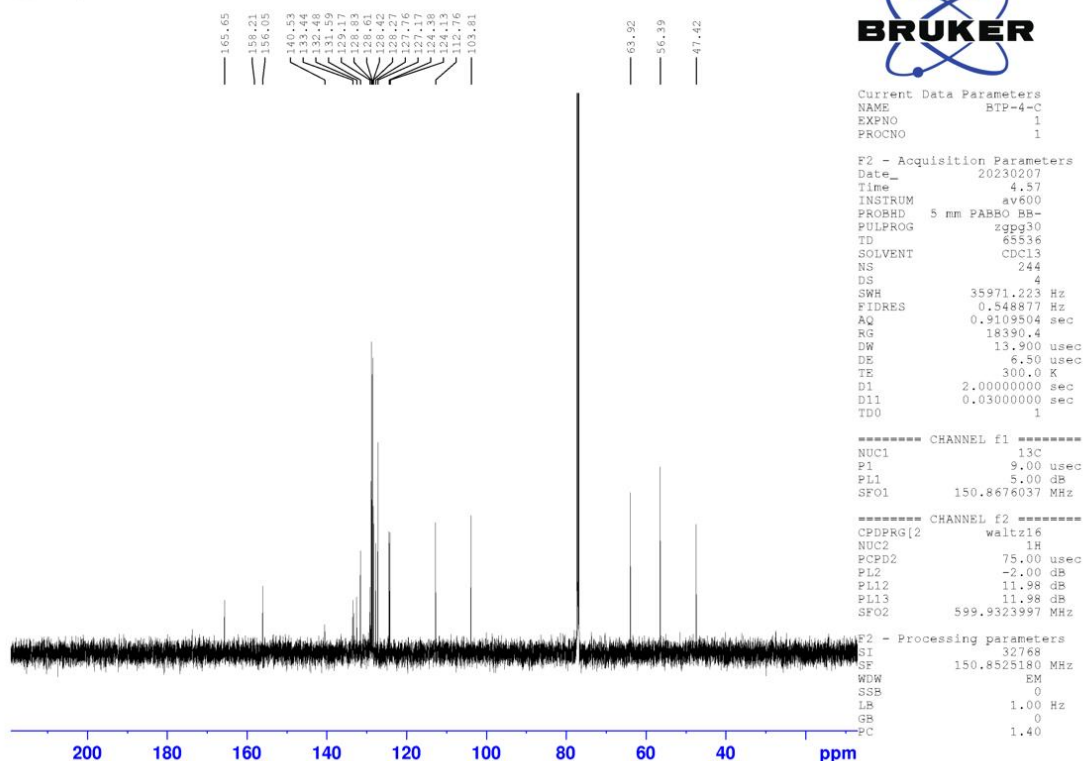
2 **Figure S51: Mass Spectrum of BTP-3**



1

2 **Figure S52:** ^1H NMR Spectrum of **BTP-4**

BTP-4-C



1

2 **Figure S53:** ^{13}C NMR Spectrum of BTP-4

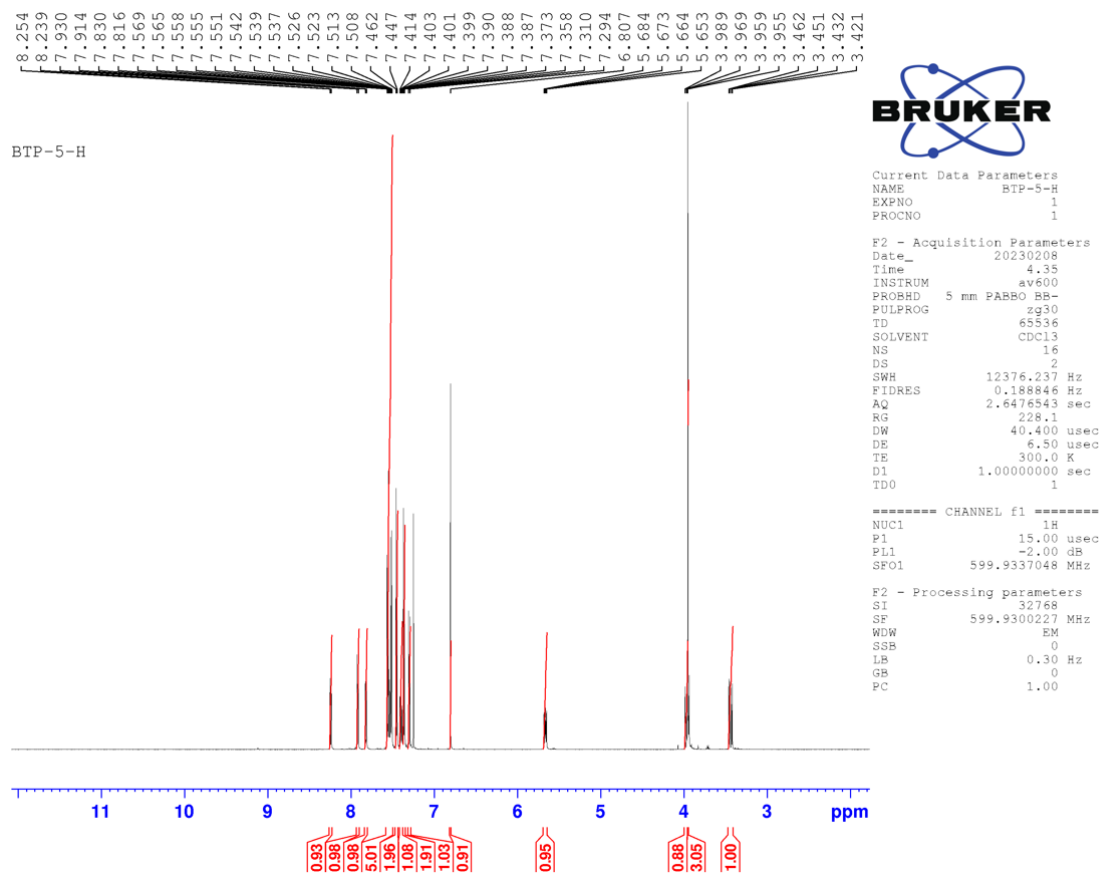
[Elemental Composition]
Data : gousei265
Sample: BTP-4/sever belgin
Note : NBA
Inlet : Direct
RT : 0.75 min
Elements : C 100/0, H 100/0, O 2/0, N 4/2, Cl 3/1, S 2/0
Mass Tolerance : 20ppm, 10mmu if m/z < 500, 20mmu if m/z > 1000
Unsaturation (U.S.) : -0.5 - 150.0

Date : 07-Feb-2023 16:00
Page: 1
Ion Mode : FAB+
Scan#: (2,6)

Observed m/z	Int%	Err(ppm / mmu)	U.S.	Composition
529.0782	100.0	+7.3 / +3.9	29.5	C 35 H 14 O 2 N 2 Cl
		-13.9 / -7.4	29.5	C 34 H 14 O N 4 Cl
		-17.4 / -9.2	24.5	C 33 H 19 O N 2 Cl 2
		+6.4 / +3.4	25.0	C 32 H 17 O N 3 Cl 2
		-18.3 / -9.7	20.0	C 30 H 22 N 3 Cl 3
		+5.5 / +2.9	20.5	C 29 H 20 N 4 Cl 3
		+0.9 / +0.5	25.5	C 32 H 18 O 2 N 2 Cl S
		+0.0 / +0.0	21.0	C 29 H 21 O N 3 Cl 2 S
		-0.9 / -0.5	16.5	C 26 H 24 N 4 Cl 3 S
		-5.4 / -2.9	21.5	C 29 H 22 O 2 N 2 Cl S 2
		+18.3 / +9.7	22.0	C 28 H 20 O 2 N 3 Cl S 2
		-6.4 / -3.4	17.0	C 26 H 25 O N 3 Cl 2 S 2
		+17.4 / +9.2	17.5	C 25 H 23 O N 4 Cl 2 S 2
		+14.0 / +7.4	12.5	C 24 H 28 O N 2 Cl 3 S 2
		-7.3 / -3.9	12.5	C 23 H 28 N 4 Cl 3 S 2

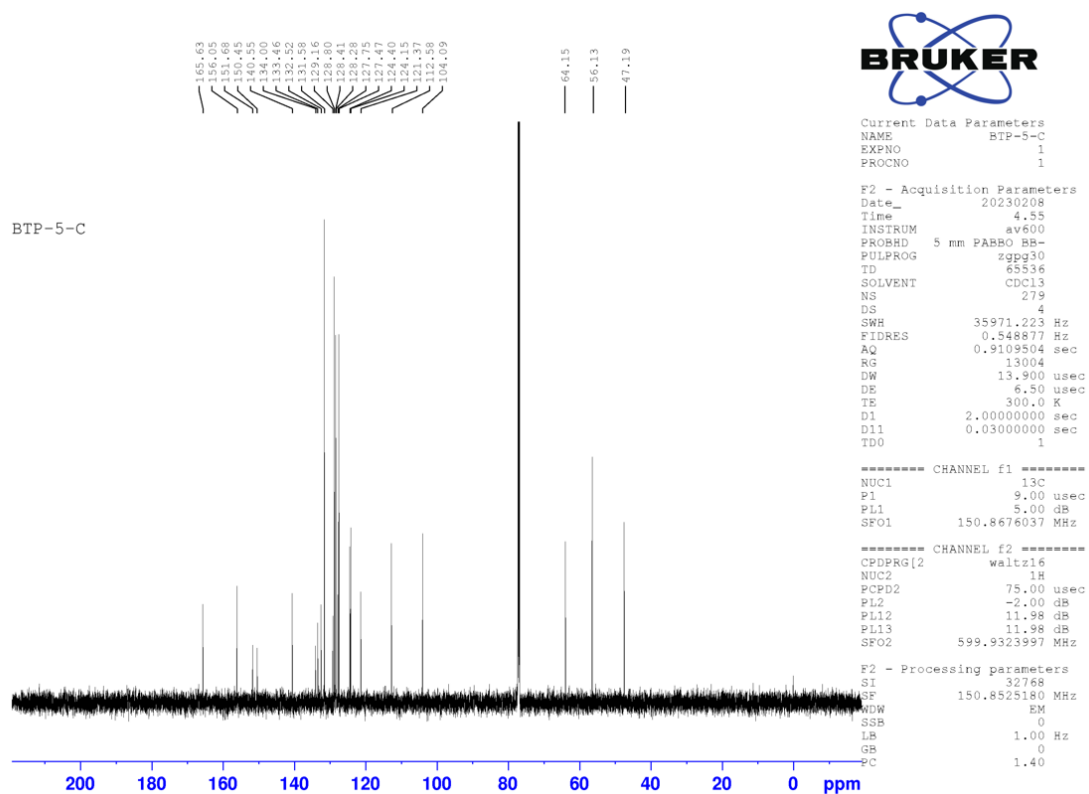
3

4 **Figure S54:** Mass Spectrum of BTP-4



1

2 **Figure S55: ^1H NMR Spectrum of BTP-5**



1

2 **Figure S56:** ^{13}C NMR Spectrum of BTP-5

[Elemental Composition]
 Date : 08-Feb-2023 16:20
 Page: 1
 Data : gousei266
 Sample: BTP-5/sever belgin
 Note : NBA
 Inlet : Direct
 Ion Mode : FAB+
 RT : 1.88 min
 Scan#: (7,10)
 Elements : C 100/0, H 100/0, O 2/0, N 4/2, Cl 2/0, Br 2/0, S 2/0
 Mass Tolerance : 20ppm, 10mmu if m/z < 500, 20mmu if m/z > 1000
 Unsaturation (U.S.) : -0.5 - 150.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
573.0266	62.7	-10.7 / -6.1	45.0	C 44 H 3 N 3
		+11.2 / +6.4	45.5	C 43 H N 4
		+8.0 / +4.6	40.5	C 42 H 6 N 2 Cl
		-6.9 / -4.0	36.0	C 38 H 8 O 2 N 3 Cl
		+15.0 / +8.6	36.5	C 37 H 6 O 2 N 4 Cl
		+11.9 / +6.8	31.5	C 36 H 11 O 2 N 2 Cl 2
		-7.8 / -4.4	31.5	C 35 H 11 O N 4 Cl 2
		+4.7 / +2.7	29.5	C 35 H 14 O 2 N 2 Br
		-14.9 / -8.5	29.5	C 34 H 14 O N 4 Br
		-18.1 / -10.4	24.5	C 33 H 19 O N 2 Cl Br
		+3.8 / +2.2	25.0	C 32 H 17 O N 3 Cl Br
		-19.0 / -10.9	20.0	C 30 H 22 N 3 Cl 2 Br
		+3.0 / +1.7	20.5	C 29 H 20 N 4 Cl 2 Br
		+15.4 / +8.8	18.5	C 29 H 23 O N 2 Br 2
		-4.2 / -2.4	18.5	C 28 H 23 N 4 Br 2
		-7.4 / -4.2	13.5	C 27 H 28 N 2 Cl Br 2
		+14.6 / +8.4	14.0	C 26 H 26 N 3 Cl Br 2
		-0.4 / -0.2	9.5	C 22 H 28 O 2 N 4 Cl Br 2
		-3.5 / -2.0	4.5	C 21 H 33 O 2 N 2 Cl 2 Br 2
		+18.4 / +10.5	5.0	C 20 H 31 O 2 N 3 Cl 2 Br 2
		-16.6 / -9.5	41.0	C 41 H 7 N 3 S
		+5.3 / +3.1	41.5	C 40 H 5 N 4 S
		+2.1 / +1.2	36.5	C 39 H 10 N 2 Cl S
		-12.8 / -7.3	32.0	C 35 H 12 O 2 N 3 Cl S
		+9.2 / +5.3	32.5	C 34 H 10 O 2 N 4 Cl S
		+6.0 / +3.4	27.5	C 33 H 15 O 2 N 2 Cl 2 S
		-13.6 / -7.8	27.5	C 32 H 15 O N 4 Cl 2 S
		-1.2 / -0.7	25.5	C 32 H 18 O 2 N 2 Br S
		-2.0 / -1.2	21.0	C 29 H 21 O N 3 Cl Br S
		+19.9 / +11.4	21.5	C 28 H 19 O N 4 Cl Br S
		+16.7 / +9.6	16.5	C 27 H 24 O N 2 Cl 2 Br S
		-2.9 / -1.7	16.5	C 26 H 24 N 4 Cl 2 Br S
		+9.5 / +5.5	14.5	C 26 H 27 O N 2 Br 2 S
		-10.1 / -5.8	14.5	C 25 H 27 N 4 Br 2 S
		-13.3 / -7.6	9.5	C 24 H 32 N 2 Cl Br 2 S
		+8.7 / +5.0	10.0	C 23 H 30 N 3 Cl Br 2 S
		-6.2 / -3.6	5.5	C 19 H 32 O 2 N 4 Cl Br 2 S
		-9.4 / -5.4	0.5	C 18 H 37 O 2 N 2 Cl 2 Br 2 S
		+12.5 / +7.2	1.0	C 17 H 35 O 2 N 3 Cl 2 Br 2 S
		+19.1 / +10.9	37.5	C 38 H 9 O N 2 S 2
		-0.5 / -0.3	37.5	C 37 H 9 N 4 S 2
		-3.7 / -2.1	32.5	C 36 H 14 N 2 Cl S 2
		+18.2 / +10.4	33.0	C 35 H 12 N 3 Cl S 2
		-18.7 / -10.7	28.0	C 32 H 16 O 2 N 3 Cl S 2
		+3.3 / +1.9	28.5	C 31 H 14 O 2 N 4 Cl S 2
		+0.1 / +0.0	23.5	C 30 H 19 O 2 N 2 Cl 2 S 2
		-19.5 / -11.2	23.5	C 29 H 19 O N 4 Cl 2 S 2
		-7.1 / -4.1	21.5	C 29 H 22 O 2 N 2 Br S 2
		+14.9 / +8.5	22.0	C 28 H 20 O 2 N 3 Br S 2
		-7.9 / -4.5	17.0	C 26 H 25 O N 3 Cl Br S 2
		+14.0 / +8.0	17.5	C 25 H 23 O N 4 Cl Br S 2
		+10.8 / +6.2	12.5	C 24 H 28 O N 2 Cl 2 Br S 2
		-8.8 / -5.0	12.5	C 23 H 28 N 4 Cl 2 Br S 2
		+3.7 / +2.1	10.5	C 23 H 31 O N 2 Br 2 S 2
		-15.9 / -9.1	10.5	C 22 H 31 N 4 Br 2 S 2

1

2 **Figure S57: Mass Spectrum of BTP-5**

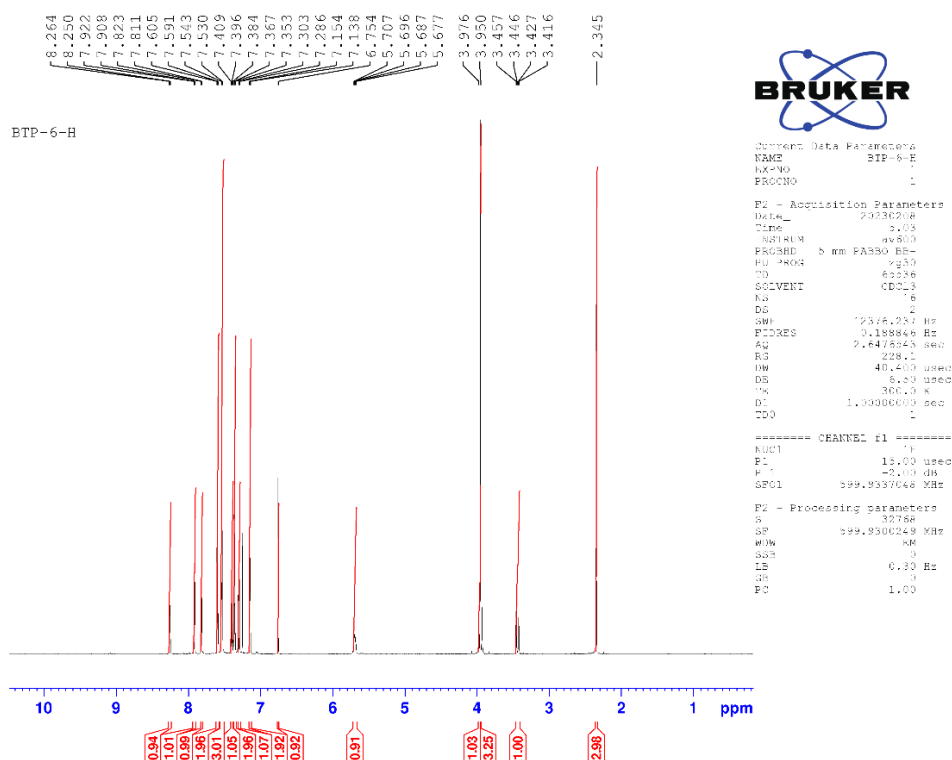


Figure S58: ^1H NMR Spectrum of BTP-6

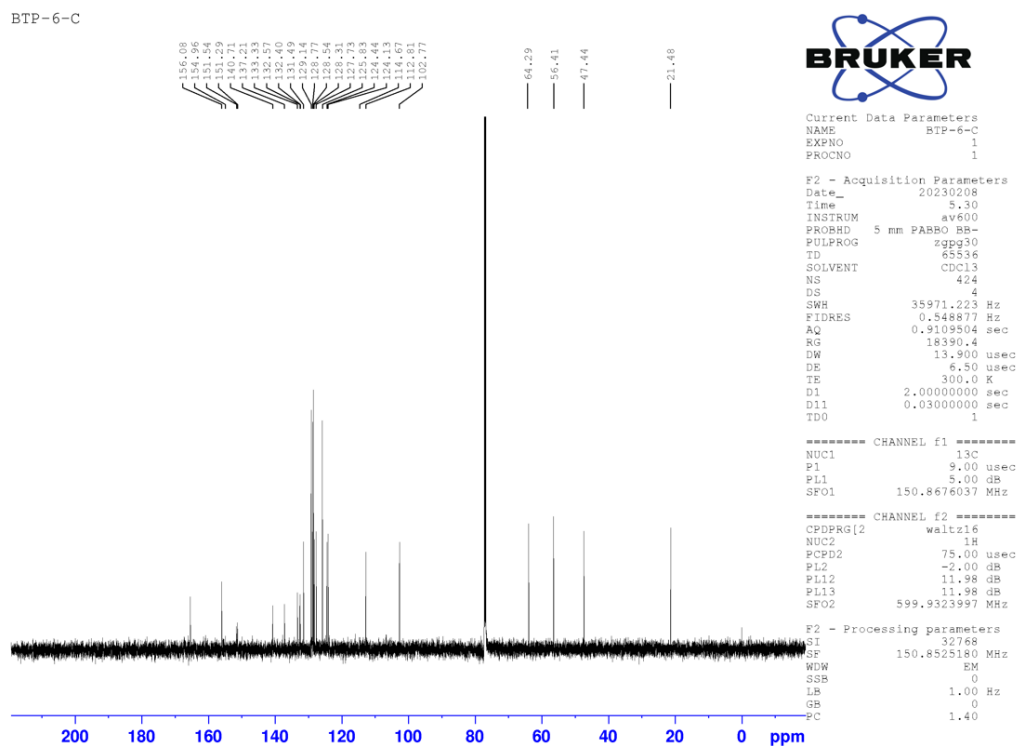


Figure S59: ^{13}C NMR Spectrum of BTP-6

[Elemental Composition]

Data : gousei267

Sample: BTP-6/sever belgin

Note : NBA

Inlet : Direct

RT : 1.38 min

Elements : C 100/0, H 100/0, O 2/0, N 4/2, Cl 2/0, S 2/0

Mass Tolerance : 20ppm, 10mmu if m/z < 500, 20mmu if m/z > 1000

Unsaturation (U.S.) : -0.5 - 150.0

Date : 08-Feb-2023 16:38

Page: 1

Observed m/z

Int%

Err[ppm / mmu]

U.S. Composition

509.1328

100.0

+7.4 / +3.7

29.5 C 36 H 17 O 2 N 2

-14.7 / -7.5

29.5 C 35 H 17 O N 4

-18.3 / -9.3

24.5 C 34 H 22 O N 2 Cl

+6.4 / +3.3

25.0 C 33 H 20 O N 3 Cl

-19.3 / -9.8

20.0 C 31 H 25 N 3 Cl 2

+5.4 / +2.8

20.5 C 30 H 23 N 4 Cl 2

+0.7 / +0.4

25.5 C 33 H 21 O 2 N 2 S

-0.2 / -0.1

21.0 C 30 H 24 O N 3 Cl S

-1.2 / -0.6

16.5 C 27 H 27 N 4 Cl 2 S

-5.9 / -3.0

21.5 C 30 H 25 O 2 N 2 S 2

+18.8 / +9.6

22.0 C 29 H 23 O 2 N 3 S 2

-6.8 / -3.5

17.0 C 27 H 28 O N 3 Cl S 2

+17.9 / +9.1

17.5 C 26 H 26 O N 4 Cl S 2

+14.3 / +7.3

12.5 C 25 H 31 O N 2 Cl 2 S 2

-7.8 / -4.0

12.5 C 24 H 31 N 4 Cl 2 S 2

Figure S60: Mass Spectrum of BTP-6

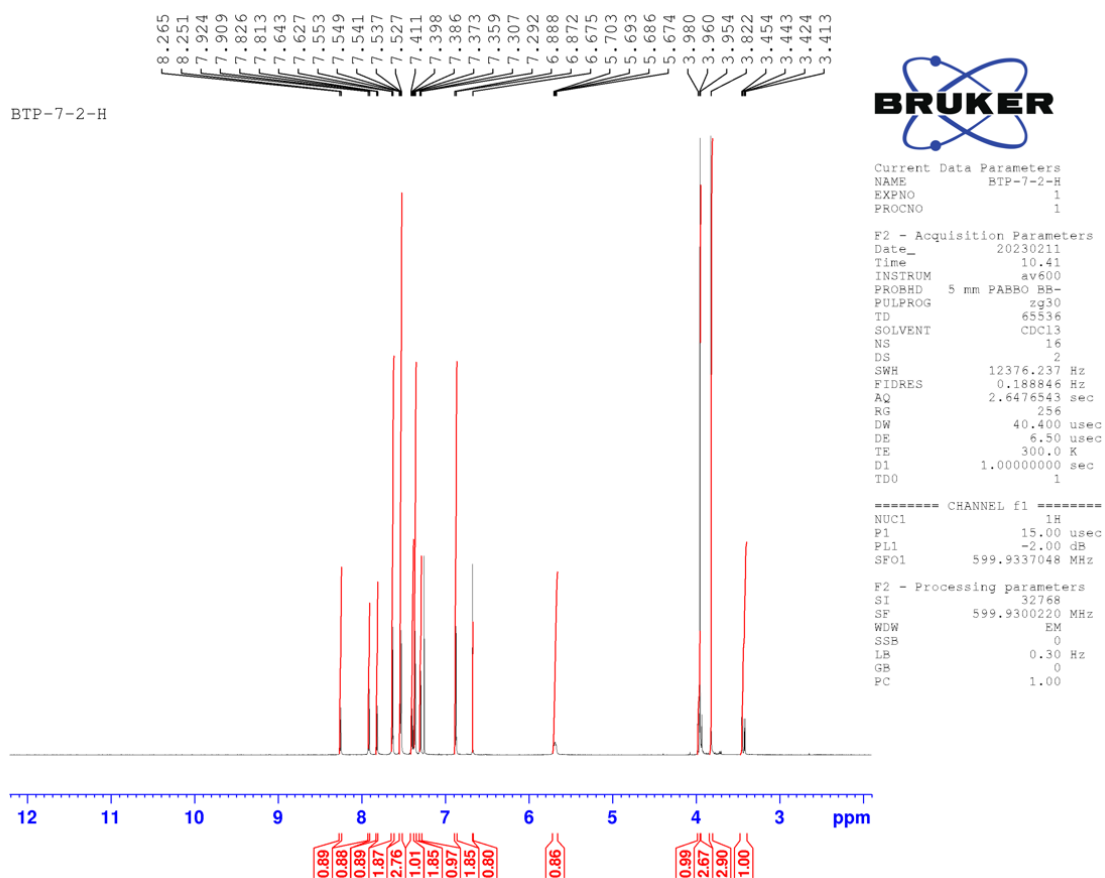


Figure S61: ¹H NMR Spectrum of BTP-7

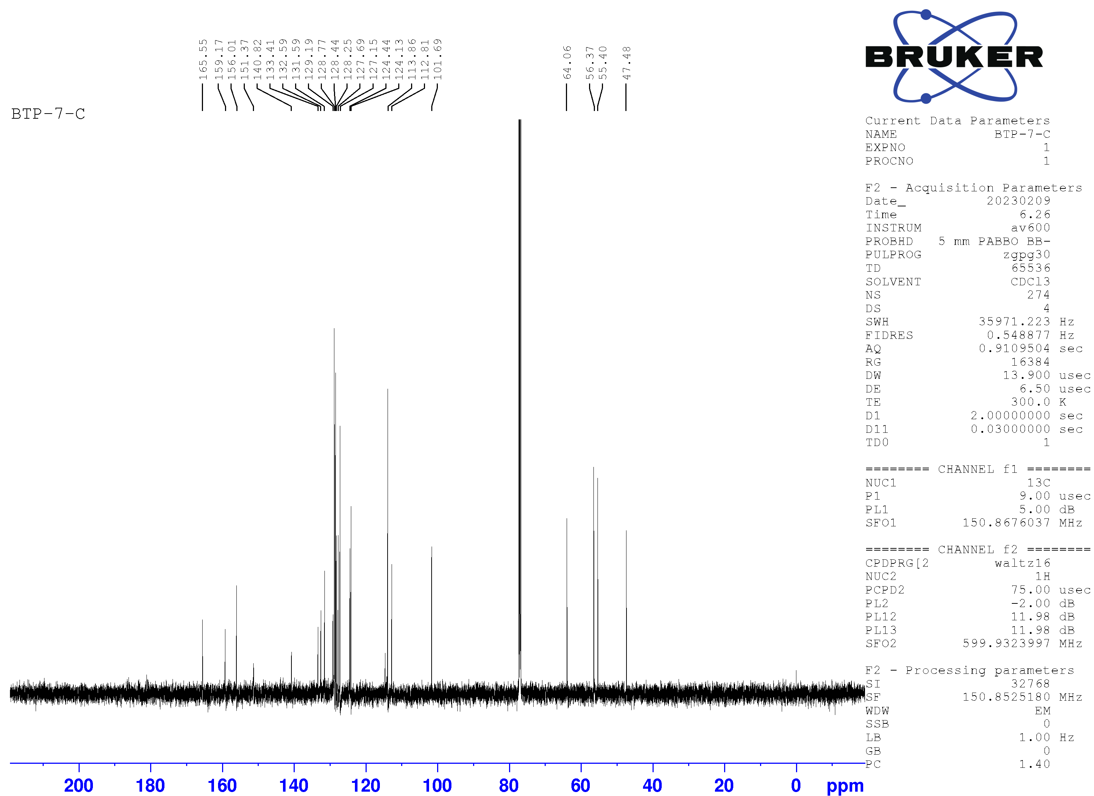


Figure S62: ^{13}C NMR Spectrum of BTP-7

[Elemental Composition]
Data : gousei270
Sample: BTP-7/sever belgin
Note : NBA
Inlet : Direct
RT : 1.13 min
Elements : C 100/0, H 100/0, O 3/1, N 4/2, Cl 2/0, S 2/0
Mass Tolerance : 20ppm, 10mmu if m/z < 500, 20mmu if m/z > 1000
Unsaturation (U.S.) : -0.5 - 150.0

Date : 09-Feb-2023 16:23
Page: 1
Ion Mode : FAB+
Scan#: (3,8)

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
525.1281	99.6	+7.9 / +4.1	29.5	C 36 H 17 O 3 N 2
		-13.5 / -7.1	29.5	C 35 H 17 O 2 N 4
		-17.0 / -8.9	24.5	C 34 H 22 O 2 N 2 Cl
		+6.9 / +3.6	25.0	C 33 H 20 O 2 N 3 Cl
		-17.9 / -9.4	20.0	C 31 H 25 O N 3 Cl 2
		+6.0 / +3.2	20.5	C 30 H 23 O N 4 Cl 2
		+1.5 / +0.8	25.5	C 33 H 21 O 3 N 2 S
		-19.9 / -10.5	25.5	C 32 H 21 O 2 N 4 S
		+0.5 / +0.3	21.0	C 30 H 24 O 2 N 3 Cl S
		-0.4 / -0.2	16.5	C 27 H 27 O N 4 Cl 2 S
		-5.0 / -2.6	21.5	C 30 H 25 O 3 N 2 S 2
		+19.0 / +10.0	22.0	C 29 H 23 O 3 N 3 S 2
		-5.9 / -3.1	17.0	C 27 H 28 O 2 N 3 Cl S 2
		+18.1 / +9.5	17.5	C 26 H 26 O 2 N 4 Cl S 2
		+14.6 / +7.6	12.5	C 25 H 31 O 2 N 2 Cl 2 S 2
		-6.8 / -3.6	12.5	C 24 H 31 O N 4 Cl 2 S 2

Figure S63: Mass Spectrum of BTP-7

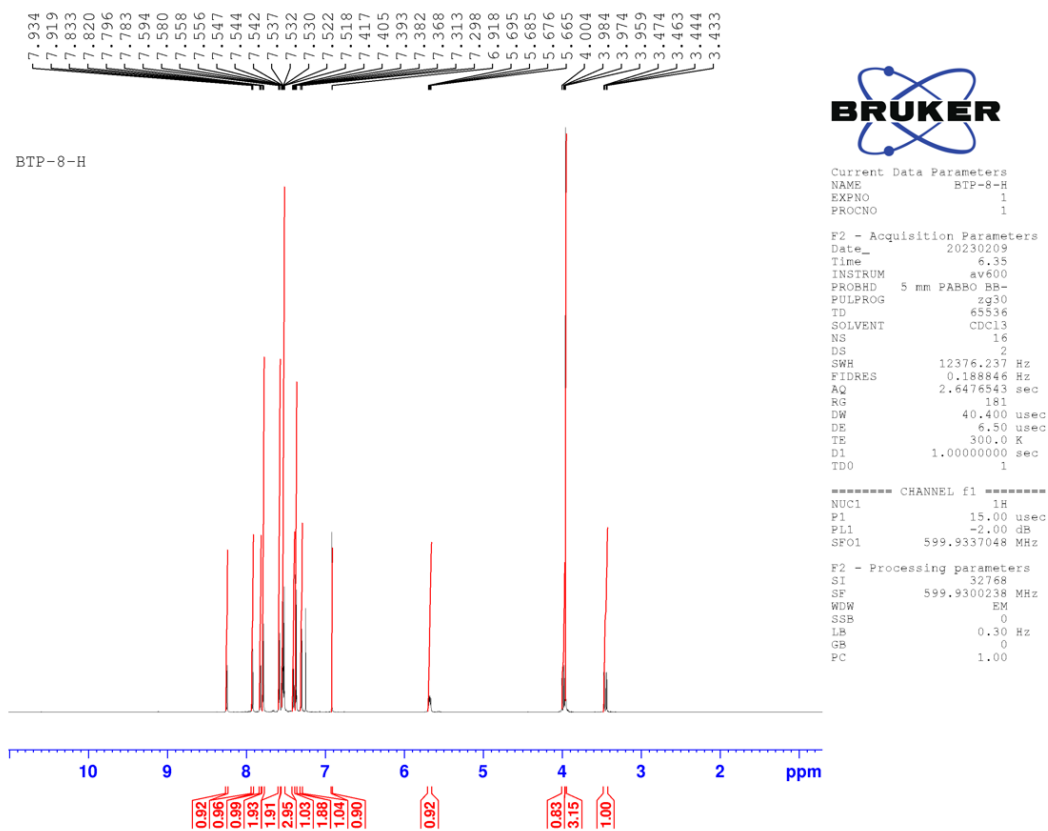


Figure S64: ^1H NMR Spectrum of BTP-8

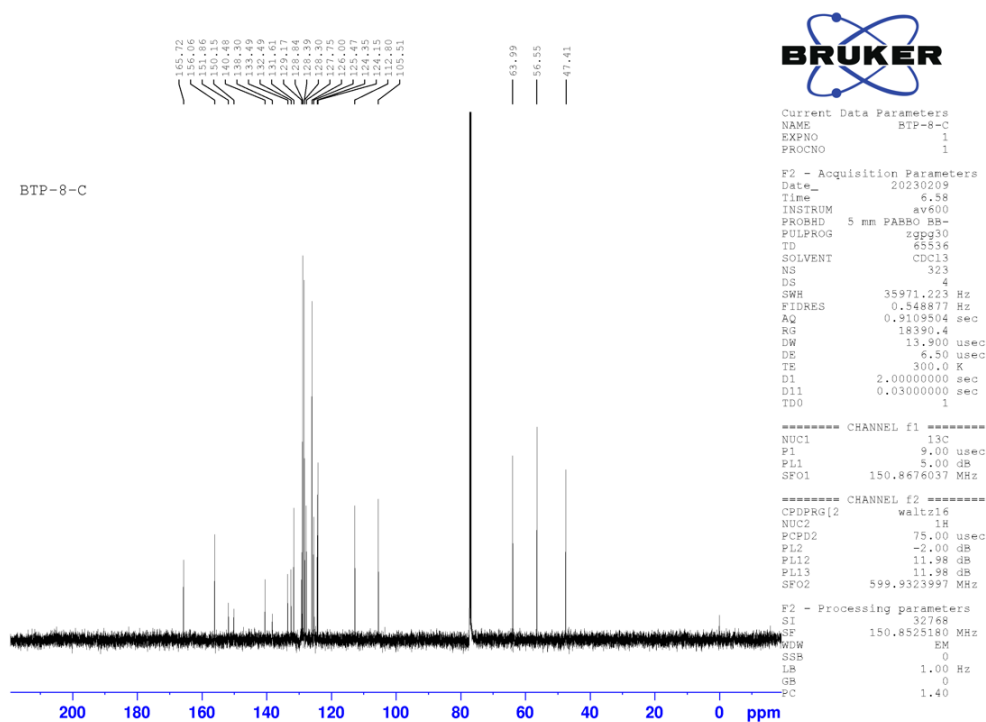


Figure S65: ^{13}C NMR Spectrum of BTP-8

[Elemental Composition]
 Date : 09-Feb-2023 16:39 Page: 1
 Data : gousei271
 Sample: BTP-8/sever belgin
 Note : NBA
 Inlet : Direct Ion Mode : FAB+
 RT : 1.25 min Scan#: (3,9)
 Elements : C 100/0, H 100/0, O 2/0, N 4/2, Cl 2/0, F 4/2, S 2/0
 Mass Tolerance : 20ppm, 10mmu if m/z < 500, 20mmu if m/z > 1000
 Unsaturation (U.S.) : -0.5 - 150.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
563.1066	100.0	+12.4 / +7.0	33.5	C 39 H 13 O N 2 F 2
		-7.6 / -4.3	33.5	C 38 H 13 N 4 F 2
		-10.8 / -6.1	28.5	C 37 H 18 N 2 Cl F 2
		+11.5 / +6.5	29.0	C 36 H 16 N 3 Cl F 2
		-3.7 / -2.1	24.5	C 32 H 18 O 2 N 4 Cl F 2
		-6.9 / -3.9	19.5	C 31 H 23 O 2 N 2 Cl 2 F 2
		+15.4 / +8.7	20.0	C 30 H 21 O 2 N 3 Cl 2 F 2
		+10.4 / +5.8	29.5	C 36 H 14 O 2 N 2 F 3
		-9.6 / -5.4	29.5	C 35 H 14 O N 4 F 3
		-12.8 / -7.2	24.5	C 34 H 19 O N 2 Cl F 3
		+9.5 / +5.3	25.0	C 33 H 17 O N 3 Cl F 3
		-13.7 / -7.7	20.0	C 31 H 22 N 3 Cl 2 F 3
		+8.6 / +4.9	20.5	C 30 H 20 N 4 Cl 2 F 3
		-18.8 / -10.6	29.5	C 37 H 15 N 2 F 4
		+3.6 / +2.0	30.0	C 36 H 13 N 3 F 4
		-11.6 / -6.5	25.5	C 32 H 15 O 2 N 4 F 4
		-14.9 / -8.4	20.5	C 31 H 20 O 2 N 2 Cl F 4
		+7.5 / +4.2	21.0	C 30 H 18 O 2 N 3 Cl F 4
		-15.7 / -8.9	16.0	C 28 H 23 O N 3 Cl 2 F 4
		+6.6 / +3.7	16.5	C 27 H 21 O N 4 Cl 2 F 4
		+6.4 / +3.6	29.5	C 36 H 17 O N 2 F 2 S
		-13.6 / -7.6	29.5	C 35 H 17 N 4 F 2 S
		-16.8 / -9.5	24.5	C 34 H 22 N 2 Cl F 2 S
		+5.5 / +3.1	25.0	C 33 H 20 N 3 Cl F 2 S
		-9.7 / -5.4	20.5	C 29 H 22 O 2 N 4 Cl F 2 S
		-12.9 / -7.3	15.5	C 28 H 27 O 2 N 2 Cl 2 F 2 S
		+9.4 / +5.3	16.0	C 27 H 25 O 2 N 3 Cl 2 F 2 S
		+4.4 / +2.5	25.5	C 33 H 18 O 2 N 2 F 3 S
		-15.6 / -8.8	25.5	C 32 H 18 O N 4 F 3 S
		-18.8 / -10.6	20.5	C 31 H 23 O N 2 Cl F 3 S
		+3.5 / +2.0	21.0	C 30 H 21 O N 3 Cl F 3 S
		-19.7 / -11.1	16.0	C 28 H 26 N 3 Cl 2 F 3 S
		+2.6 / +1.5	16.5	C 27 H 24 N 4 Cl 2 F 3 S
		-2.4 / -1.4	26.0	C 33 H 17 N 3 F 4 S
		+19.9 / +11.2	26.5	C 32 H 15 N 4 F 4 S
		-17.6 / -9.9	21.5	C 29 H 19 O 2 N 4 F 4 S
		+16.7 / +9.4	21.5	C 31 H 20 N 2 Cl F 4 S
		+1.5 / +0.8	17.0	C 27 H 22 O 2 N 3 Cl F 4 S
		+0.6 / +0.3	12.5	C 24 H 25 O N 4 Cl 2 F 4 S
		+0.4 / +0.2	25.5	C 33 H 21 O N 2 F 2 S 2
		-19.5 / -11.0	25.5	C 32 H 21 N 4 F 2 S 2
		-0.5 / -0.3	21.0	C 30 H 24 N 3 Cl F 2 S 2
		-15.6 / -8.8	16.5	C 26 H 26 O 2 N 4 Cl F 2 S 2
		+18.6 / +10.5	16.5	C 28 H 27 N 2 Cl 2 F 2 S 2
		-18.9 / -10.6	11.5	C 25 H 31 O 2 N 2 Cl 2 F 2 S 2
		+3.4 / +1.9	12.0	C 24 H 29 O 2 N 3 Cl 2 F 2 S 2
		-1.6 / -0.9	21.5	C 30 H 22 O 2 N 2 F 3 S 2
		-2.5 / -1.4	17.0	C 27 H 25 O N 3 Cl F 3 S 2
		+19.8 / +11.2	17.5	C 26 H 23 O N 4 Cl F 3 S 2
		+16.6 / +9.3	12.5	C 25 H 28 O N 2 Cl 2 F 3 S 2
		-3.4 / -1.9	12.5	C 24 H 28 N 4 Cl 2 F 3 S 2
		-8.4 / -4.7	22.0	C 30 H 21 N 3 F 4 S 2
		+13.9 / +7.8	22.5	C 29 H 19 N 4 F 4 S 2
		+10.7 / +6.0	17.5	C 28 H 24 N 2 Cl F 4 S 2
		-4.5 / -2.5	13.0	C 24 H 26 O 2 N 3 Cl F 4 S 2

1

2 **Figure S66: Mass Spectrum of BTP-8**

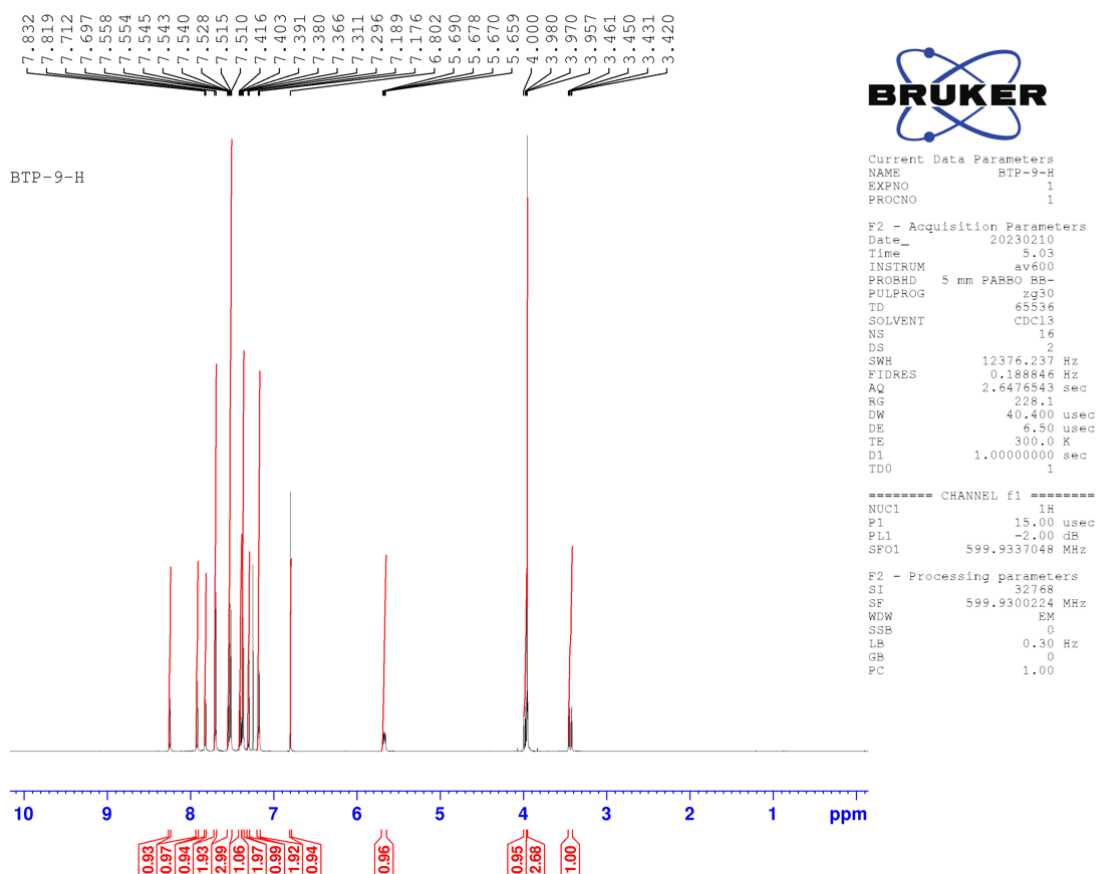
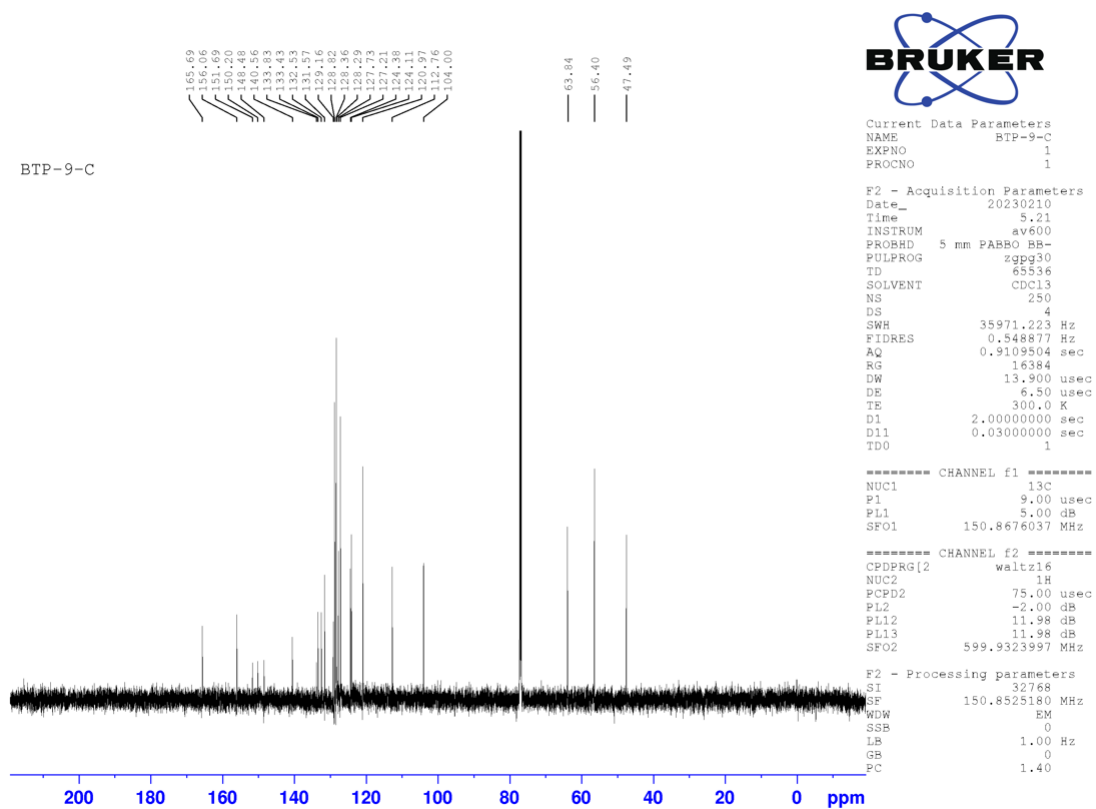


Figure S67: ^1H NMR Spectrum of BTP-9



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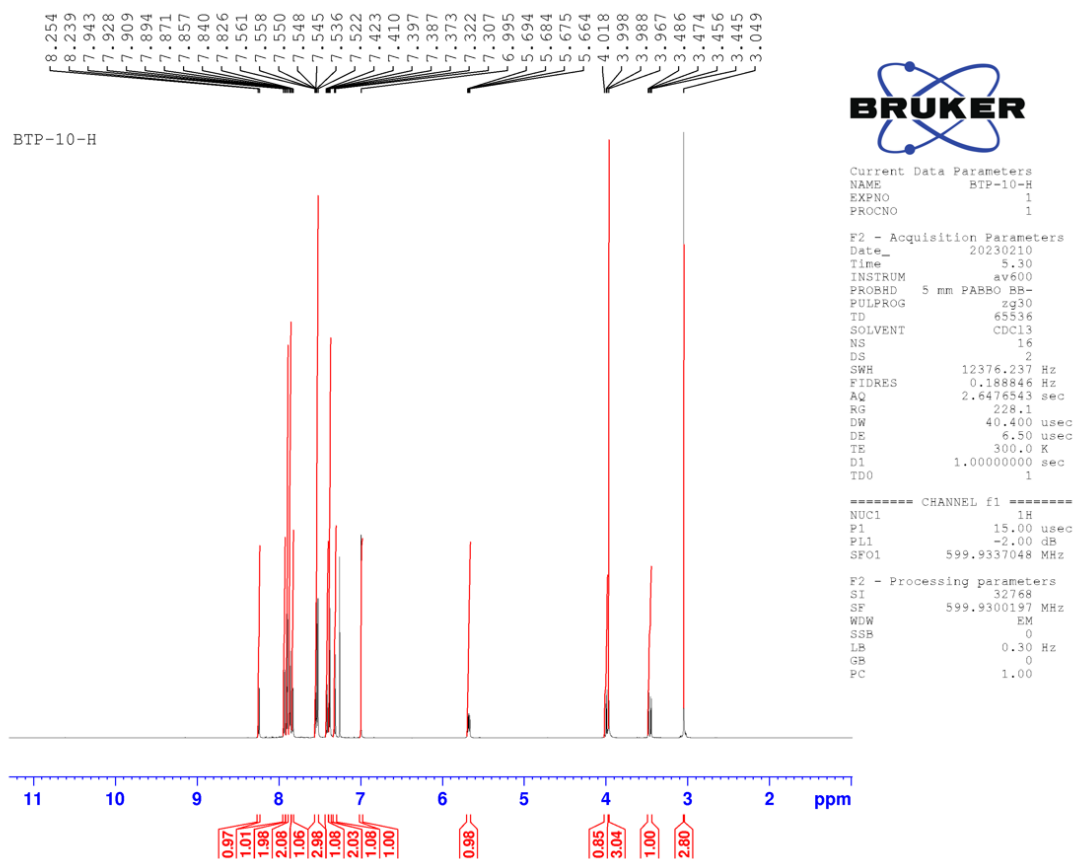
2 **Figure S68:** ^{13}C NMR Spectrum of **BTP-9**

[Elemental Composition]
 Date : 10-Feb-2023 14:15 Page: 1
 Data : gousei272
 Sample: BTP-9/sever belgin
 Note : NBA
 Inlet : Direct Ion Mode : FAB+
 RT : 1.00 min Scan#: (2,8)
 Elements : C 100/0, H 100/0, O 3/1, N 4/2, Cl 2/0, F 4/2, S 2/0
 Mass Tolerance : 20ppm, 10mmu if m/z < 500, 20mmu if m/z > 1000
 Unsaturation (U.S.) : -0.5 - 150.0

Observed m/z	Int%	Err(ppm / mmu)	U.S.	Composition
579.1000	100.0	+9.4 / +5.5	33.5	C 39 H 13 O 2 N 2 F 2
		-10.0 / -5.8	33.5	C 38 H 13 O N 4 F 2
		-13.1 / -7.6	28.5	C 37 H 18 O N 2 Cl F 2
		+8.6 / +5.0	29.0	C 36 H 16 O N 3 Cl F 2
		-6.2 / -3.6	24.5	C 32 H 18 O 3 N 4 Cl F 2
		-9.3 / -5.4	19.5	C 31 H 23 O 3 N 2 Cl 2 F 2
		+12.4 / +7.2	20.0	C 30 H 21 O 3 N 3 Cl 2 F 2
		+7.5 / +4.3	29.5	C 36 H 14 O 3 N 2 F 3
		-11.9 / -6.9	29.5	C 35 H 14 O 2 N 4 F 3
		-15.1 / -8.7	24.5	C 34 H 19 O 2 N 2 Cl F 3
		+6.6 / +3.8	25.0	C 33 H 17 O 2 N 3 Cl F 3
		-15.9 / -9.2	20.0	C 31 H 22 O N 3 Cl 2 F 3
		+5.8 / +3.3	20.5	C 30 H 20 O N 4 Cl 2 F 3
		+0.9 / +0.5	30.0	C 36 H 13 O N 3 F 4
		-13.9 / -8.1	25.5	C 32 H 15 O 3 N 4 F 4
		+19.4 / +11.2	25.5	C 34 H 16 O N 2 Cl F 4
		-17.1 / -9.9	20.5	C 31 H 20 O 3 N 2 Cl F 4
		+4.7 / +2.7	21.0	C 30 H 18 O 3 N 3 Cl F 4
		-17.9 / -10.4	16.0	C 28 H 23 O 2 N 3 Cl 2 F 4
		+3.8 / +2.2	16.5	C 27 H 21 O 2 N 4 Cl 2 F 4
		+3.6 / +2.1	29.5	C 36 H 17 O 2 N 2 F 2 S
		-15.8 / -9.1	29.5	C 35 H 17 O N 4 F 2 S
		-18.9 / -11.0	24.5	C 34 H 22 O N 2 Cl F 2 S
		+2.8 / +1.6	25.0	C 33 H 20 O N 3 Cl F 2 S
		-12.0 / -6.9	20.5	C 29 H 22 O 3 N 4 Cl F 2 S
		-15.2 / -8.8	15.5	C 28 H 27 O 3 N 2 Cl 2 F 2 S
		+6.6 / +3.8	16.0	C 27 H 25 O 3 N 3 Cl 2 F 2 S
		+1.6 / +1.0	25.5	C 33 H 18 O 3 N 2 F 3 S
		-17.8 / -10.3	25.5	C 32 H 18 O 2 N 4 F 3 S
		+0.8 / +0.5	21.0	C 30 H 21 O 2 N 3 Cl F 3 S
		+19.4 / +11.2	16.5	C 28 H 24 O 2 N 2 Cl 2 F 3 S
		+0.0 / +0.0	16.5	C 27 H 24 O N 4 Cl 2 F 3 S
		-5.0 / -2.9	26.0	C 33 H 17 O N 3 F 4 S
		+16.8 / +9.7	26.5	C 32 H 15 O N 4 F 4 S
		-19.7 / -11.4	21.5	C 29 H 19 O 3 N 4 F 4 S
		+13.6 / +7.9	21.5	C 31 H 20 O N 2 Cl F 4 S
		-1.2 / -0.7	17.0	C 27 H 22 O 3 N 3 Cl F 4 S
		+17.4 / +10.1	12.5	C 25 H 25 O 3 N 2 Cl 2 F 4 S
		-2.0 / -1.2	12.5	C 24 H 25 O 2 N 4 Cl 2 F 4 S
		-2.2 / -1.3	25.5	C 33 H 21 O 2 N 2 F 2 S 2
		+19.5 / +11.3	26.0	C 32 H 19 O 2 N 3 F 2 S 2
		-3.0 / -1.8	21.0	C 30 H 24 O N 3 Cl F 2 S 2
		+18.7 / +10.8	21.5	C 29 H 22 O N 4 Cl F 2 S 2
		-17.8 / -10.3	16.5	C 26 H 26 O 3 N 4 Cl F 2 S 2
		+15.5 / +9.0	16.5	C 28 H 27 O N 2 Cl 2 F 2 S 2
		+0.7 / +0.4	12.0	C 24 H 29 O 3 N 3 Cl 2 F 2 S 2
		-4.2 / -2.4	21.5	C 30 H 22 O 3 N 2 F 3 S 2
		+17.5 / +10.2	22.0	C 29 H 20 O 3 N 3 F 3 S 2
		-5.0 / -2.9	17.0	C 27 H 25 O 2 N 3 Cl F 3 S 2
		+16.7 / +9.7	17.5	C 26 H 23 O 2 N 4 Cl F 3 S 2
		+13.5 / +7.8	12.5	C 25 H 28 O 2 N 2 Cl 2 F 3 S 2
		-5.9 / -3.4	12.5	C 24 H 28 O N 4 Cl 2 F 3 S 2
		-10.8 / -6.2	22.0	C 30 H 21 O N 3 F 4 S 2
		+10.9 / +6.3	22.5	C 29 H 19 O N 4 F 4 S 2
		+7.8 / +4.5	17.5	C 28 H 24 O N 2 Cl F 4 S 2

1

2 **Figure S69: Mass Spectrum of BTP-9**



1

2 **Figure S70: ^1H NMR Spectrum of BTP-10**

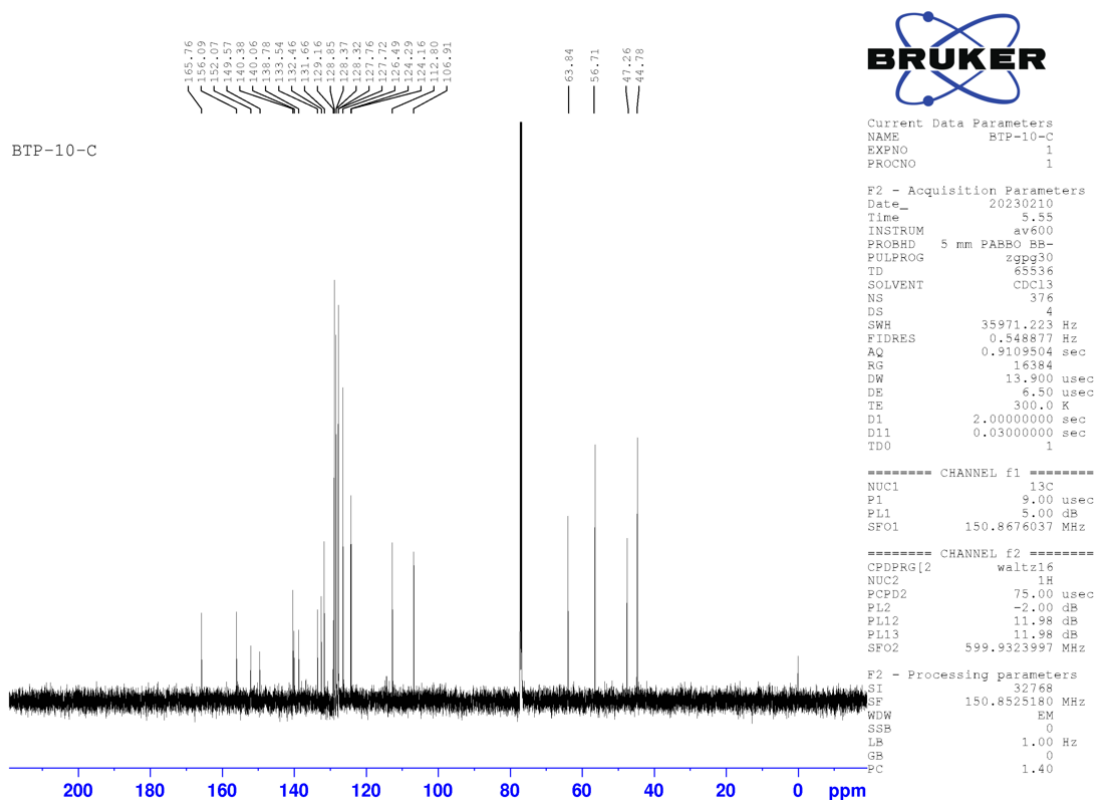


Figure S71: ^{13}C NMR Spectrum of BTP-10

[Elemental Composition]
Data : gousei273
Sample: BTP-10/sever belgin
Note : NBA
Inlet : Direct
RT : 1.00 min
Elements : C 100/0, H 100/0, O 4/2, N 4/2, Cl 2/0, S 3/1
Mass Tolerance : 20ppm, 10mmu if m/z < 500, 20mmu if m/z > 1000
Unsaturation (U.S.) : -0.5 - 150.0

Date : 10-Feb-2023 14:32
Ion Mode : FAB+
Scan#: (2,8)

Page: 1

Observed m/z	Int%	Err [ppm / mmu]	U.S.	Composition
573.0938	97.8	+5.1 / +2.9	30.5	C 36 H 17 O 4 N 2 S
		-14.5 / -8.3	30.5	C 35 H 17 O 3 N 4 S
		-17.7 / -10.2	25.5	C 34 H 22 O 3 N 2 Cl S
		+4.2 / +2.4	26.0	C 33 H 20 O 3 N 3 Cl S
		-18.6 / -10.6	21.0	C 31 H 25 O 2 N 3 Cl 2 S
		+3.4 / +1.9	21.5	C 30 H 23 O 2 N 4 Cl 2 S
		-0.8 / -0.5	26.5	C 33 H 21 O 4 N 2 S 2
		-1.7 / -1.0	22.0	C 30 H 24 O 3 N 3 Cl S 2
		+17.1 / +9.8	17.5	C 28 H 27 O 3 N 2 Cl 2 S 2
		-2.5 / -1.4	17.5	C 27 H 27 O 2 N 4 Cl 2 S 2
		-6.7 / -3.8	22.5	C 30 H 25 O 4 N 2 S 3
		+15.2 / +8.7	23.0	C 29 H 23 O 4 N 3 S 3
		-7.5 / -4.3	18.0	C 27 H 28 O 3 N 3 Cl S 3
		+14.4 / +8.3	18.5	C 26 H 26 O 3 N 4 Cl S 3
		+11.2 / +6.4	13.5	C 25 H 31 O 3 N 2 Cl 2 S 3
		-8.4 / -4.8	13.5	C 24 H 31 O 2 N 4 Cl 2 S 3

Figure S72: Mass Spectrum of BTP-10