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Functional lipids based on [12]aneN_3 and naphthalimide as effective non-viral gene vectors

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1. Fluorescence Spectra of 11a, 11b, 12a, 12b and 12c

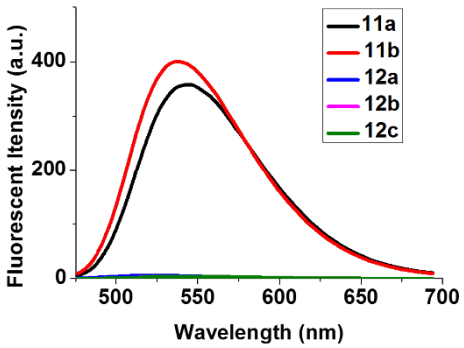


Figure 1S Fluorescence spectra of **11a**, **11b**, **12a**, **12b** and **12c** (1 x 10^{-5} M, Tris-HCl buffer, 1mM), λex = 465 nm.

2. EB displacement assay

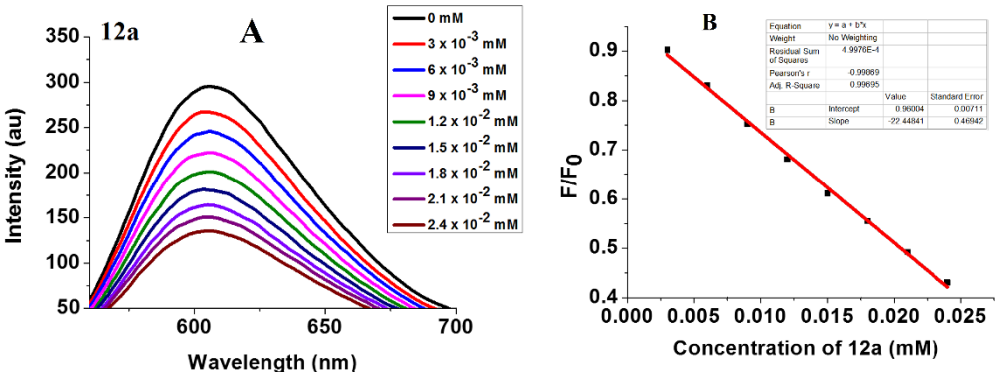


Figure 2SA)Fluorescence decrease and B) Fluorescence ratio changes at 608 nm inducedby **12a** through the displacement of CT-DNA-bound ethidium bromide in the buffer (5 mM Tris-HCl/50 mMNaCl, pH 7.4).λex = 537 nm.The binding constant $K_{app}$was calculated by the formula (K_{EB} × [EB] = K_{app} × [**12a**]) and given a result of4.88 × 10^6 M^{-1}, where K_{EB} = 1.0 × 10^6 M^{-1}, [EB] = 10 μM, and [**12a**] was the concentration at which a 50% reduction of the fluorescence had occurred.

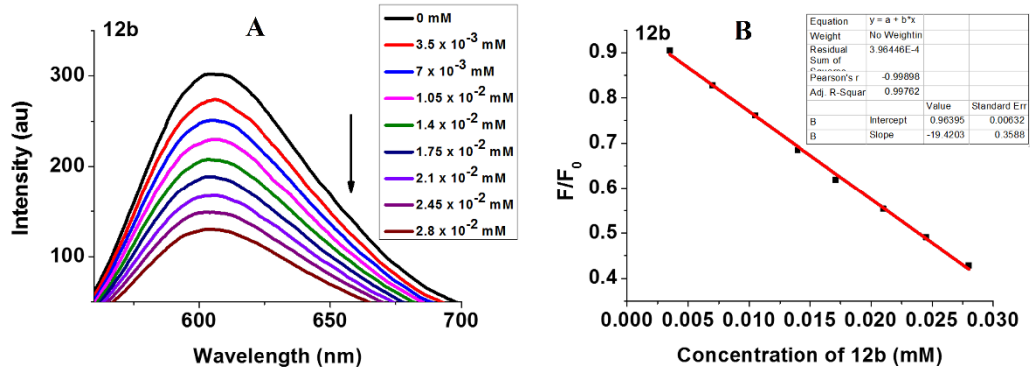


Figure 3SA) Fluorescence decrease and B) Fluorescence ratio changes at 608 nm inducedby **12b** through the displacement of CT-DNA-bound ethidium bromide in the buffer (5 mM Tris-HCl/50 mMNaCl, pH 7.4). λex = 537 nm. The binding constant $K_{app}$was calculated by the formula (K_{EB} × [EB] = K_{app} × [**12b**]) and given a result of4.18 × 10^6 M^{-1}, where K_{EB} = 1.0 × 10^6 M^{-1}, [EB] = 10 μM, and [**12b**] was the concentration at which a 50% reduction of the fluorescence had occurred.

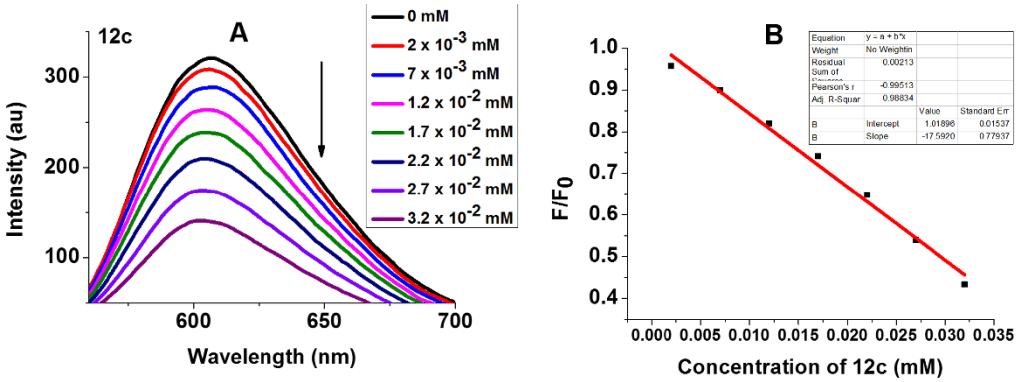


Figure 4SA) Fluorescence decrease and B) Fluorescence ratio changes at 608 nm inducedby **12c** through the displacement of CT-DNA-bound ethidium bromide in the buffer (5 mM Tris-HCl/50 mMNaCl, pH 7.4). λex = 537

nm. The binding constant $K_{app}$was calculated by the formula ($K_{EB} \times [EB] = K_{app} \times [\mathbf{12c}]$) and given a result of3.39 $\times 10^6$ M^{-1}, where K_{EB} = 1.0 $\times 10^6$ M^{-1}, [EB] = 10 μM, and [**12c**] was the concentration at which a 50% reduction of the fluorescence had occurred.

3. NMR, Ms, and IR data of compounds synthesized

2a, yield: 15%;^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58 (d, *J* = 7.3 Hz, 1H), 8.46 (d, *J* = 8.4 Hz, 1H), 8.05 (d, *J* = 8.0 Hz, 1H), 7.62 (t, *J* = 7.8 Hz, 1H), 6.75 (d, *J* = 8.6 Hz, 1H), 5.10 (s, 1H), 4.28 (t, *J* = 7.1 Hz, 2H), 4.19 (t, *J* = 6.3 Hz, 2H), 3.82-3.74 (m, 1H), 3.68-3.58 (m, 1H), 2.34-2.23 (m, 4H), 2.17-2.06 (m, 4H), 1.53-1.39 (m, 4H), 1.32-1.15 (m, 30H), 0.88 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.03, 164.69, 164.07, 148.46, 134.53, 131.30, 130.07, 125.89, 124.74, 120.26, 110.12, 104.77, 69.78, 62.54, 51.19, 37.40, 34.41, 33.86, 32.00, 30.57, 29.79, 29.75, 29.71, 29.58, 29.45, 29.35, 27.56, 25.02, 14.21; IR (KBr, cm^{-1}): 3432.48, 2923.25, 2850.91, 1653.07, 1634.74, 1569.16, 1383.98, 1362.77, 1111.05, 1018.46, 668.36, 652.93; HR-MS: m/z = 635.4418 ($[M+H]^+$). **2b**, yield: 23%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 (d, *J* = 6.9 Hz, 1H), 8.46 (d, *J* = 8.4 Hz, 1H), 8.04 (d, *J* = 8.5 Hz, 1H), 7.62 (t, *J* = 7.8 Hz, 1H), 6.75 (d, *J* = 8.6 Hz, 1H), 4.14 (t, *J* = 7.6 Hz, 2H), 3.81-3.74 (m, 1H), 3.68-3.59 (m, 1H), 2.30 (d, *J* = 12.3 Hz, 2H), 2.13 (d, *J* = 10.8 Hz, 2H), 1.74-1.68 (m, 2H), 1.60-1.22 (m, 34H), 0.88 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ163.70, 133.27, 132.08, 131.27, 131.16, 130.71, 130.25, 129.09, 128.14, 123.26, 122.39, 40.73, 29.78, 29.75, 29.74, 29.72, 29.68, 29.67, 29.63, 29.45, 28.17, 27.21, 14.20; IR (KBr, cm^{-1}): 3418.01, 2918.42, 2849.95, 1700.32, 1672.36, 1635.71, 1587.48, 1550.83, 1383.98, 1105.26, 773.49, 668.36, 652.93; HR-MS: m/z = 561.4061 ($[M+H]^+$).

3a, yield: 71%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60 (d, *J* = 7.1 Hz, 1H), 8.48 (d, *J* = 8.4 Hz, 1H), 8.09 (d, *J* = 7.9 Hz, 1H), 7.98 (s, 2H), 7.65 (t, *J* = 7.6 Hz, 1H), 7.51 (s, 1H), 6.78 (d, *J* = 8.6 Hz, 1H), 5.18-5.02 (m, 1H), 4.47 (s, 4H), 4.29 (t, *J* = 7.1 Hz, 2H), 4.19 (t, *J* = 6.3 Hz, 2H), 3.80-3.65 (m, 1H), 2.39 (d, *J* = 11.6 Hz, 2H), 2.34-2.18 (m, 4H), 2.13-2.05 (m, 2H), 1.86-1.78 (m, 4H), 1.72-1.52 (m, 4H), 1.25 (s, 26H), 0.88 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) 173.90, 163.65, 163.63, 133.43, 132.18, 131.36, 131.35, 131.21, 131.20, 130.45, 129.05, 128.18, 127.03, 123.06, 122.18, 73.73, 62.28, 58.98, 37.84, 34.36, 29.78, 29.74, 29.70, 29.56, 29.44, 29.34, 27.41, 25.00, 22.77, 14.21; IR (KBr, cm^{-1}): 34.28.62, 2924.21, 2852.84, 1737.94, 1703.22, 1649.21, 1635.71, 1585.55, 1466.93, 1383.98, 1234.50, 1178.56, 1106.22, 1028.10, 966.38, 780.24; HR-MS: m/z = 847.4876 ($[M-H]^+$). **3b**, yield: 74%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.61 (d, *J* = 7.2 Hz, 1H), 8.48 (d, *J* = 8.3 Hz, 1H), 8.15-8.05 (m, 1H), 8.04-7.93 (m, 2H), 7.70-7.59 (m, 1H), 7.51 (s, 1H), 6.85-6.72 (s, 1H), 5.19-5.05 (m, 1H), 4.47 (s, 4H), 4.15 (t, *J* = 7.6 Hz, 2H), 3.76-3.65 (m, 1H), 2.39 (d, *J* = 10.5 Hz, 2H), 2.29 (d, *J* = 11.2 Hz, 2H), 2.03-1.47 (m, 8H), 1.45-1.08 (m, 28H),

0.88 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) 173.56, 173.24, 170.62, 137.38, 137.27, 137.08, 136.90, 132.72, 132.07, 131.36, 130.92, 130.64, 130.35, 129.57, 129.20, 129.07, 127.23, 70.55, 64.46, 54.17, 54.11, 54.01, 41.70, 32.01, 30.35, 30.04, 29.78, 29.74, 29.68, 29.52, 29.45, 26.27, 22.78, 14.35, 14.21; IR (KBr, cm^{-1}): 3396.79, 2925.17, 2853.81, 2100.57, 1717.68, 1646.32, 1582.66, 1383.98, 1218.10, 1106.22, 1023.28, 863.18, 759.02; HR-MS: m/z = 847.4876 ($[M-H]^+$).

5a, yield: 71%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 (d, *J* = 7.1 Hz, 1H), 8.47 (d, *J* = 8.4 Hz, 1H), 8.09 (d, *J* = 8.4 Hz, 1H), 7.92 (s, 2H), 7.64 (t, *J* = 7.7 Hz, 1H), 7.38 (d, *J* = 6.4 Hz, 3H), 6.78 (d, *J* = 8.5 Hz, 1H), 5.57 (s, 4H), 5.08 (s, 1H), 5.05 (s, 1H), 4.28 (t, *J* = 6.9 Hz, 2H), 4.19 (t, *J* = 6.1 Hz, 2H), 3.79 (s, 4H), 3.72 (s, 1H), 3.33 (s, 16H), 2.44 (s, 6H), 2.40-2.30 (m, 2H), 2.30-2.21 (m, 4H), 2.13-2.06 (m, 2H), 1.89-1.81 (m, 12H), 1.79-1.72 (m, 2H), 1.68-1.52 (m, 4H), 1.45 (s, 36H), 1.25 (s, 30H), 0.87 (t, *J* = 6.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.72, 164.43, 163.75, 156.14, 148.73, 144.10, 136.53, 134.31, 132.11, 131.41, 130.98, 129.87, 128.95, 126.68, 124.30, 122.66, 122.58, 120.28, 109.58, 104.40, 79.12, 73.05, 62.32, 53.06, 50.78, 49.65, 46.52, 45.32, 43.72, 37.10, 34.16, 31.76, 29.92, 29.53, 29.50, 29.45, 29.32, 29.20, 29.10, 28.99, 28.38, 27.41, 27.05, 26.02, 24.80, 22.53, 14.03; IR (KBr, cm^{-1}): 3406.33, 3129.82, 2926.51, 2853.31, 1684.94, 1649.70, 1584.64, 1546.69, 1413.86, 1365.06, 1300.00, 1251.20, 1224.10, 1161.75, 1107.1045.18, 776.81; ESI-MS: m/z = 1667.8 ($[M+H]^+$). **5b**, yield: 41%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 (d, *J* = 7.3 Hz, 1H), 8.48 (d, *J* = 8.4 Hz, 1H), 8.08 (d, *J* = 8.4 Hz, 1H), 7.92 (s, 2H), 7.63 (t, *J* = 7.8 Hz, 1H), 7.38 (d, *J* = 6.1 Hz, 3H), 6.77 (d, *J* = 8.6 Hz, 1H), 5.57 (s, 4H), 5.15 (s, 1H), 5.09-5.01 (m, 1H), 4.19-4.10 (m, 2H), 3.79 (s, 4H), 3.71 (s, 1H), 3.33 (s, 16H), 2.66-2.29 (m, 10H), 2.24 (d, *J* = 10.3 Hz, 2H), 1.90-1.81 (m, 12H), 1.78-1.68 (m, 4H), 1.62-1.55 (m, 2H), 1.45 (s, 36H), 1.25 (s, 30H), 0.88 (t, *J* = 6.6 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.39, 164.35, 163.72, 156.07, 148.72 , 144.03, 136.54, 134.17 , 132.08 , 131.36, 130.80 , 129.81, 128.86 , 126.74, 124.20, 122.75, 122.62, 120.33, 109.69, 104.33, 79.04, 73.04 , 52.99, 50.77, 49.69, 46.48, 45.31, 43.71, 39.98, 31.71, 29.83, 29.48, 29.44, 29.37, 29.23, 29.14, 28.34, 28.09, 27.02, 26.03 , 22.48, 13.98; IR (KBr, cm^{-1}): 3409.04, 3124.40, 2926.51, 2853.31, 1687.65, 1646.99, 1584.64, 1543.98, 1457.43, 1413.86, 1381.33, 1365.06, 1297.29, 1248.49, 1221.39, 1164.46, 1104.82, 1050.60, 863.55, 774.10; ESI-MS: m/z = 1595.8 ($[M+H]^+$).

7a, yield: 57%; ^{1}H NMR (400 MHz, CD_3SOCD_3) δ 8.62-8.50 (m, 2H), 8.32 (d, *J* = 7.9 Hz, 1H), 8.21 (d, *J* = 7.9 Hz, 1H), 7.99 (m, 1H), 4.06 (t, *J* = 6.8 Hz, 2H), 2.82 (t, *J* = 6.8 Hz, 2H), 2.12 (brs,

2H).**7b**, yield: 83%;^{1}H NMR (400 MHz, $CDCl_3$) δ 8.66 (d, *J* = 6.6 Hz, 1H), 8.58 (d, *J* = 8.5 Hz, 1H), 8.42 (d, *J* = 7.9 Hz, 1H), 8.04 (d, *J* = 7.9 Hz, 1H), 7.84 (m, 1H), 4.53 (brs, 1H), 4.16 (t, *J* = 7.5 Hz, 2H), 3.15-3.09 (m, 2H), 1.79-1.68 (m, 2H), 1.48-1.35 (m, 13H), 1.28-1.22 (m, 2H).**7c**, yield: 48%;^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 (d, *J* = 7.3 Hz, 1H), 8.56 (d, *J* = 8.5 Hz, 1H), 8.41 (d, *J* = 7.9 Hz, 1H), 8.04 (t, *J* = 5.2 Hz, 1H), 7.89-7.80 (m, 1H), 4.51 (brs, 1H),4.24-4.06 (m, 2H), 3.12-3.07 (m, 2H), 1.73-1.71 (m, 2H), 1.44 (s, 13H), 1.28 (brs, 10H).

8b, yield: 86%; ^{1}H NMR (400 MHz, D_2O) δ 7.55 (d, *J* = 7.1 Hz, 1H), 7.46 (d, *J* = 8.3 Hz, 1H), 7.28-7.14 (m, 2H), 7.08 (t, *J* = 7.8 Hz, 1H), 3.53 ((t, *J* = 7.6 Hz, 2H), 2.95 ((t, *J* = 7.6 Hz, 2H), 1.74-1.61 (m, 2H), 1.61-1.09 (m, 6H); ^{13}C NMR (101 MHz, D_2O) 163.23, 163.18, 132.98, 131.95, 131.76, 131.34, 130.11, 129.59, 129.19, 128.56, 123.04, 122.26, 40.67, 40.46, 40.25, 40.05, 39.84, 39.63, 39.42, 39.11, 27.81, 27.39, 27.24, 26.63, 26.15, 25.85; IR (KBr, cm^{-1}): 3441.16, 3141.23, 2933.85, 2852.84, 1694.54, 1647.28, 1588.45, 1384.95, 1353.12, 1248.00, 1026.17, 1004.96, 848.72, 781.20, 734.91; HR-MS: m/z = 375.0702 ($[M+H]^+$).

8c, yield: 83%;^{1}H NMR (400 MHz, CD_3SOCD_3) δ 8.62-8.55 (m, 2H), 8.36 (d, *J* = 7.9 Hz, 1H), 8.25 (d, *J* = 7.9 Hz, 1H), 8.02 (dd, *J* = 8.5, 7.3 Hz, 1H), 7.70 (brs, 2H), 4.06-4.00 (m, 2H), 2.75 (dd, *J* = 14.6, 6.1 Hz, 2H), 1.63 (d, *J* = 7.3 Hz, 2H), 1.50 (d, *J* = 7.3 Hz, 2H), 1.29 (d, *J* = 23.4 Hz, 12H).

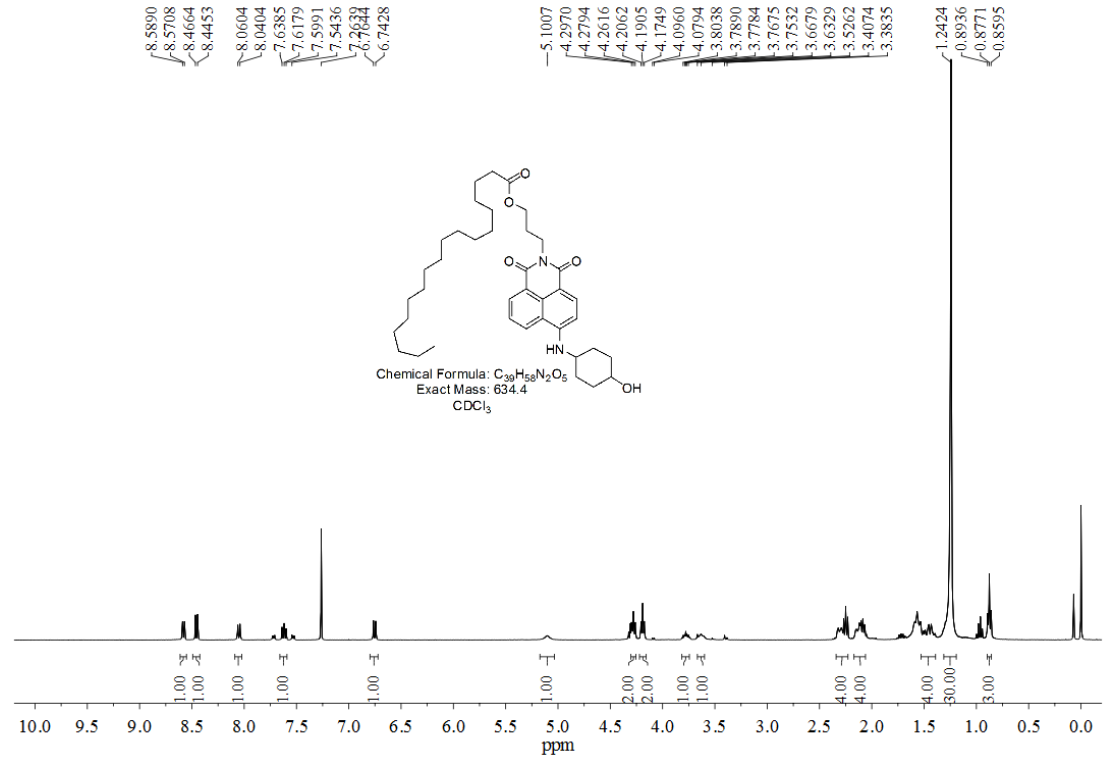
9a, yield: 57%;^{1}H NMR (400 MHz, CD_3SOCD_3) δ 8.66 (s, 1H), 8.58 (d, *J* = 7.9 Hz, 2H), 8.34 (d, *J* = 7.9 Hz, 1H), 8.23 (d, *J* = 7.9 Hz, 1H), 8.01 (t, *J* = 7.9 Hz, 1H), 7.62 (s, 2H), 7.47 (s, 1H), 4.50 (s, 4H), 4.28 (t, *J* = 5.7 Hz, 2H), 3.62 (t, *J* = 5.7 Hz, 2H); ^{13}C NMR (101 MHz, CD_3SOCD_3) 166.60, 163.79, 163.75, 136.94, 136.80, 136.24, 133.06, 132.01, 131.87, 131.42, 130.92, 129.50, 129.49, 129.34, 127.14, 123.64, 122.86, 55.43, 53.67, 39.43, 37.72; IR (KBr, cm^{-1}): 3447.91, 2253.92, 2094.78, 1701.29, 1663.68, 1636.67, 1383.98, 1375.30, 1344.44, 1052.21, 1027.14, 1006.89, 825.57, 763.84; HR-MS: m/z = 555.0499 ($[M+Na]^+$). **9b**, yield: 34%;^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64 (dd, *J* = 7.3, 1.1 Hz, 1H), 8.59 (dd, *J* = 8.5, 1.1 Hz, 1H), 8.40 (d, *J* = 7.9 Hz, 1H), 8.05 (d, *J* = 7.9 Hz, 1H), 7.85 (dd, *J* = 8.5, 7.3 Hz, 1H), 7.74 (d, *J* = 1.4 Hz, 2H), 7.41 (s, 1H), 6.40 (brs, 1H), 4.44 (s, 4H), 4.20 (t, *J* = 7.3 Hz, 2H), 3.50-3.44 (m, 2H), 1.82-1.75 (m, 2H), 1.72-1.63 (m, 2H), 1.51-1.46 (m, 2H), 0.89-0.81 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) 166.62, 163.80, 136.91, 136.22, 133.42, 132.12, 131.31, 131.20, 130.70, 130.43, 130.24, 129.04, 128.19, 126.53, 123.10, 122.23, 54.27, 40.17, 39.93, 29.78, 29.31, 27.81, 26.35, 26.25; IR (KBr, cm^{-1}): 3457.14,

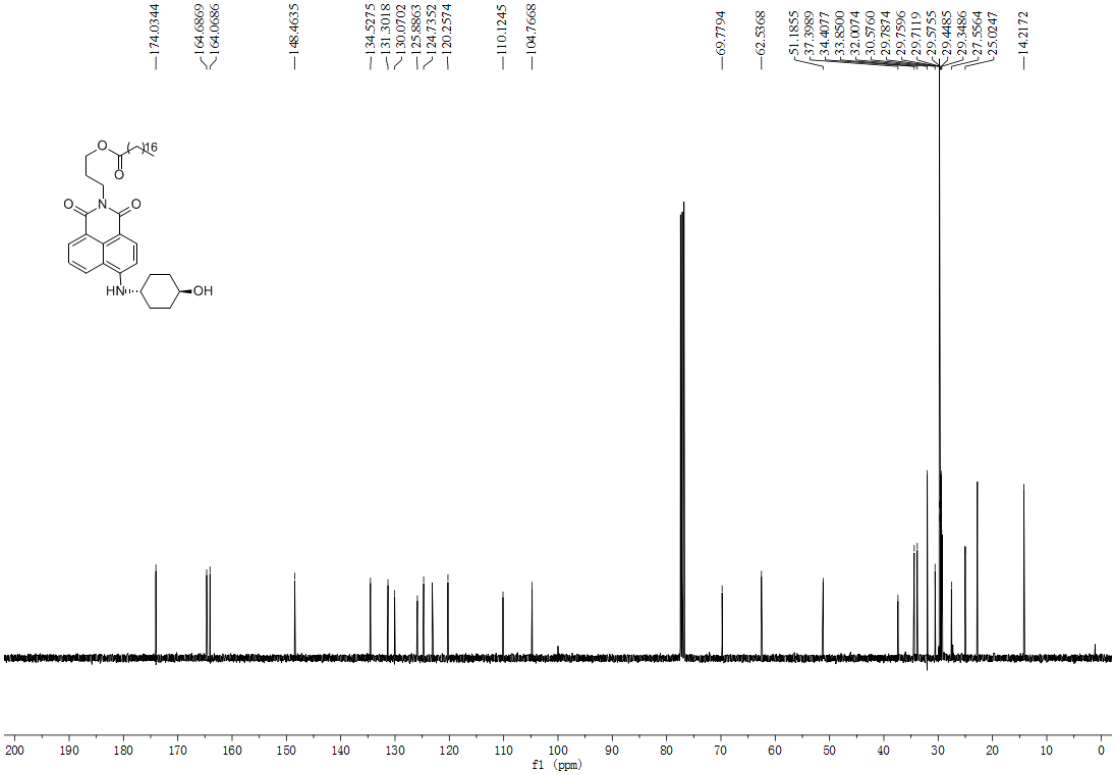
1698.34, 1103.87, 1008.67, 849.91, 783.21; HR-MS: m/z = 589.1035 ($[M+H]^+$). **9c**, yield: 48%;^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 (d, *J* = 7.3 Hz, 1H), 8.57 (d, *J* = 8.5 Hz, 1H), 8.40 (d, *J* = 7.9 Hz, 1H), 8.04 (d, *J* = 7.9 Hz, 1H), 7.84 (t, *J* = 7.9 Hz, 1H), 7.67 (s, 2H), 7.40 (s, 1H), 6.29-6.06 (brs, 1H), 4.42 (s, 4H), 4.16 (t, *J* = 7.6 Hz, 2H), 3.46 (dd, *J* = 13.1, 7.0 Hz, 2H), 1.76-1.69 (m, 2H), 1.66-1.60 (m, 2H), 1.46-1.31 (m, 10H), 0.90-0.84 (m, 2H).

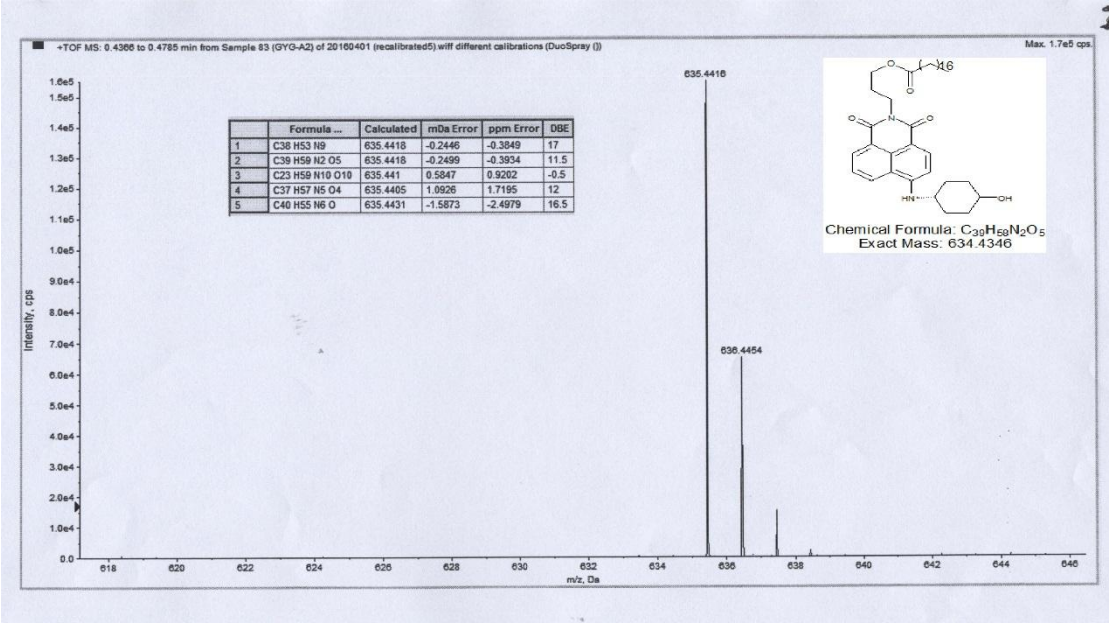
10a, yield: 30%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 (d, *J* = 7.4 Hz, 1H), 8.60 (d, *J* = 8.6 Hz, 1H), 8.48 (d, *J* = 7.9 Hz, 1H), 8.10 (d, *J* = 7.9 Hz, 1H), 7.90 (m, 1H), 7.63 (s, 2H), 7.35 (s, 2H), 7.29 (m, 1H), 5.51 (s, 4H), 4.53-4.48 (m, 2H), 3.86-3.81 (m, 2H), 3.75 (s, 4H), 3.43-3.18 (m, 16H), 2.48-2.25 (m, 8H), 1.90-1.75 (m, 12H), 1.44 (s, 36H); ^{13}C NMR (101 MHz, $CDCl_3$) δ166.34, 164.05, 156.18, 144.22, 136.41, 136.36, 133.33, 132.18, 131.43, 131.14, 130.45, 130.35, 129.80, 128.90, 128.73, 128.10, 126.79, 125.18, 122.57, 122.50, 121.62, 79.16, 53.22, 49.73, 46.76, 45.35, 43.81, 39.74, 39.57, 28.42, 26.07; IR (KBr, cm^{-1}): 3411.75, 2969.88, 2931.93, 1687.65, 1590.06, 1478.92, 1413.86, 1365.06, 1232.23, 1172.59, 1047.89, 779.52; ESI-MS: m/z = 1351.3 ($[M+H]^+$). **10b**, yield: 53%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64 (dd, *J* = 7.3, 1.0 Hz, 1H), 8.58 (d, *J* = 8.5 Hz, 1H), 8.40 (d, *J* = 7.9 Hz, 1H), 8.05 (d, *J* = 7.9 Hz, 1H), 7.85 (dd, *J* = 8.5, 7.3 Hz, 1H), 7.72 (s, 2H), 7.36 (s, 2H), 7.29 (s, 1H), 6.765 (brs, 1H), 5.52 (s, 4H), 4.18 (s, 2H), 3.73 (s, 4H), 3.45-3.22 (m, 18H), 2.41 (brs, 6H), 1.80 (brs, 12H), 1.68-1.58 (m, 4H), 1.51-1.40 (m, 36H), 1.26 (s, 4H), 0.90-0.81 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.14, 163.42, 163.39, 156.18, 144.24, 136.82, 136.35, 133.10, 131.83, 131.03, 130.98, 130.41,130.12, 129.80, 128.74, 127.99, 126.96, 122.87, 122.60,122.01, 79.18, 53.45, 53.24, 49.80, 46.80, 45.35, 43.86, 40.07, 39.87, 28.41, 27.70, 27.16, 26.34, 26.27, 26.60; IR (KBr, cm^{-1}): 3381.93, 2931.93, 1693.07, 1665.96, 1590.06, 1416.57, 1236.35, 1164.46, 1050.60, 782.23; ESI-MS: m/z = 1407.7 ($[M+H]^+$). **10c**, yield: 49%;^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 (dd, *J* = 7.3, 1.0 Hz, 1H), 8.57 (dd, *J* = 8.5, 1.0 Hz, 1H), 8.41 (d, *J* = 7.9 Hz, 1H), 8.04 (d, *J* = 7.9 Hz, 1H), 7.85 (dd, *J* = 8.5, 7.4 Hz, 1H), 7.67 (s, 2H), 7.36 (s, 2H), 7.29 (s, 1H), 6.53 (s, 1H), 5.52 (s, 4H), 4.23-4.09 (m, 2H), 3.74 (s, 4H), 3.98-3.27 (m, 18H), 2.42 (brs, 8H), 1.94-1.79 (m, 12H), 1.78-1.65 (m, 2H), 1.61-1.56 (m, 2H), 1.45-1.38 (m, 36H), 1.38-1.21 (m, 10H), 0.88-0.84 (m, 2H);^{13}C NMR (101 MHz, $CDCl_3$) δ166.08, 163.25, 126.22, 156.13, 144.24, 136.84, 136.34, 132.91, 131.71, 130.90, 130.32, 129.92, 129.71, 128.67, 127.91, 126.87, 122.91, 122.60, 122.05, 79.12, 53.44, 53.19, 49.87, 46.82, 45.35, 43.87, 40.39, 40.17, 29.51, 29.43, 29.25, 29.11, 28.39, 27.87, 27.14, 26.92, 26.85, 26.04; IR (KBr, cm^{-1}): 3436.14, 2929.22, 1687.65,

1660.54, 1598.19, 1411.14, 1359.64, 1245.78, 1172.59, 1447.89, 782.23; ESI-MS: m/z = 1463.7 ($[M+H]^+$).

4. NMR, Ms, and IR spectra of compounds synthesized







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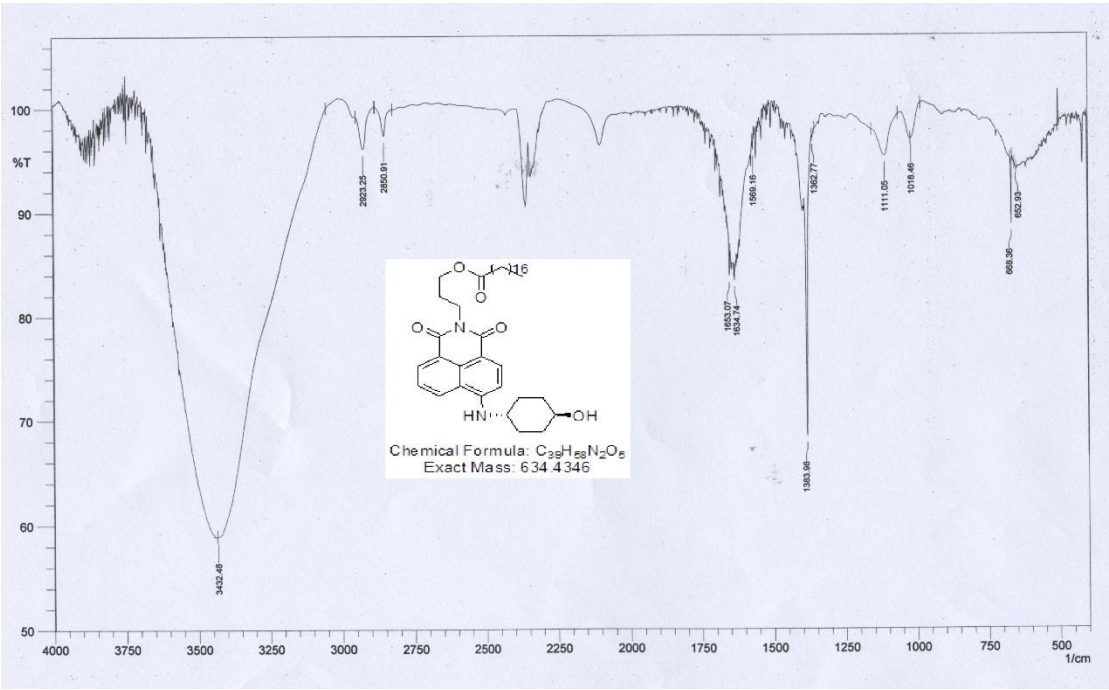
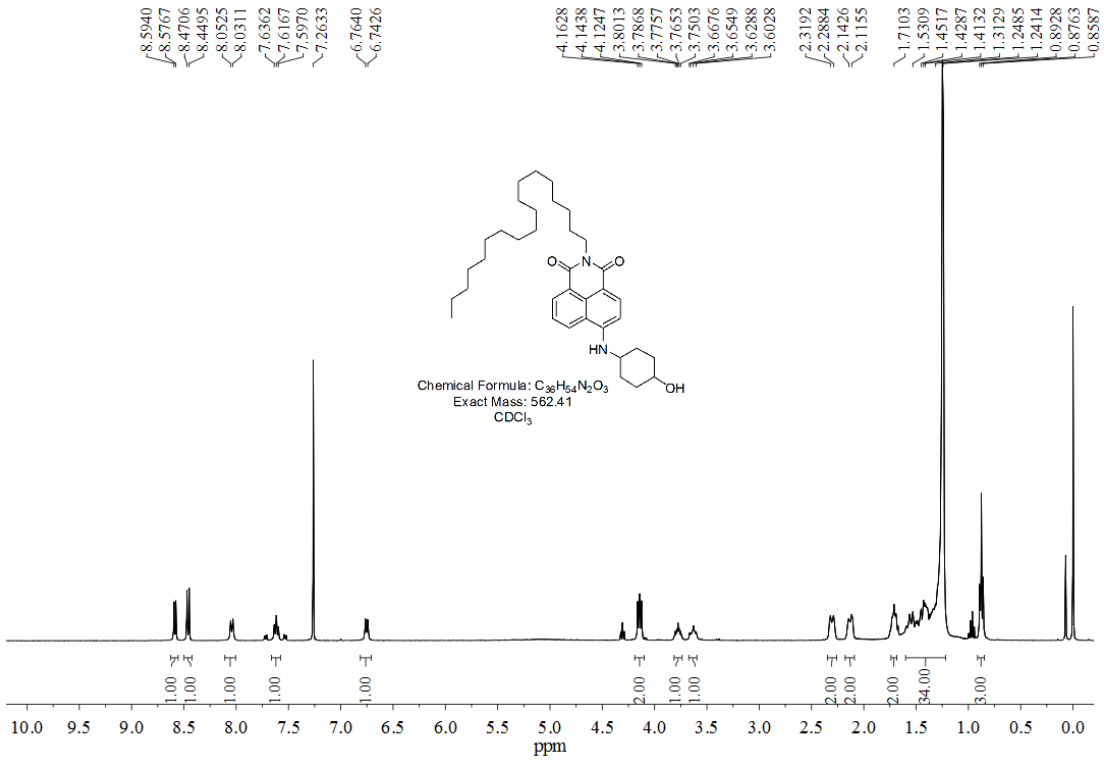
1	C38 H53 N9	635.4418	-0.2446	-0.3849	17
2	C39 H59 N2 O5	635.4418	-0.2499	-0.3934	11.5
3	C23 H59 N10 O10	635.441	0.5847	0.9202	-0.5
4	C37 H57 N5 O4	635.4405	1.0926	1.7195	12
5	C40 H55 N6 O	635.4431	-1.5873	-2.4979	16.5

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3.7757
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Exact Mass: 562.41
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3.00
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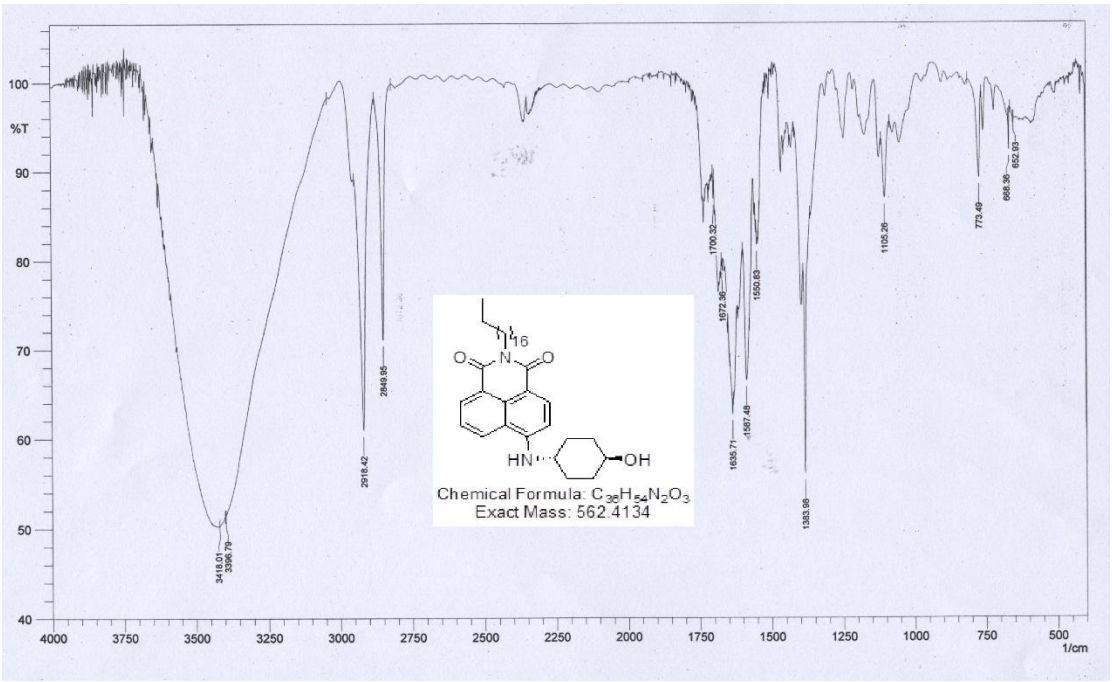
ppm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50
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3396.79
2918.42
2849.95
1700.32
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1635.71
1587.48
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1383.98
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Exact Mass: 562.4134
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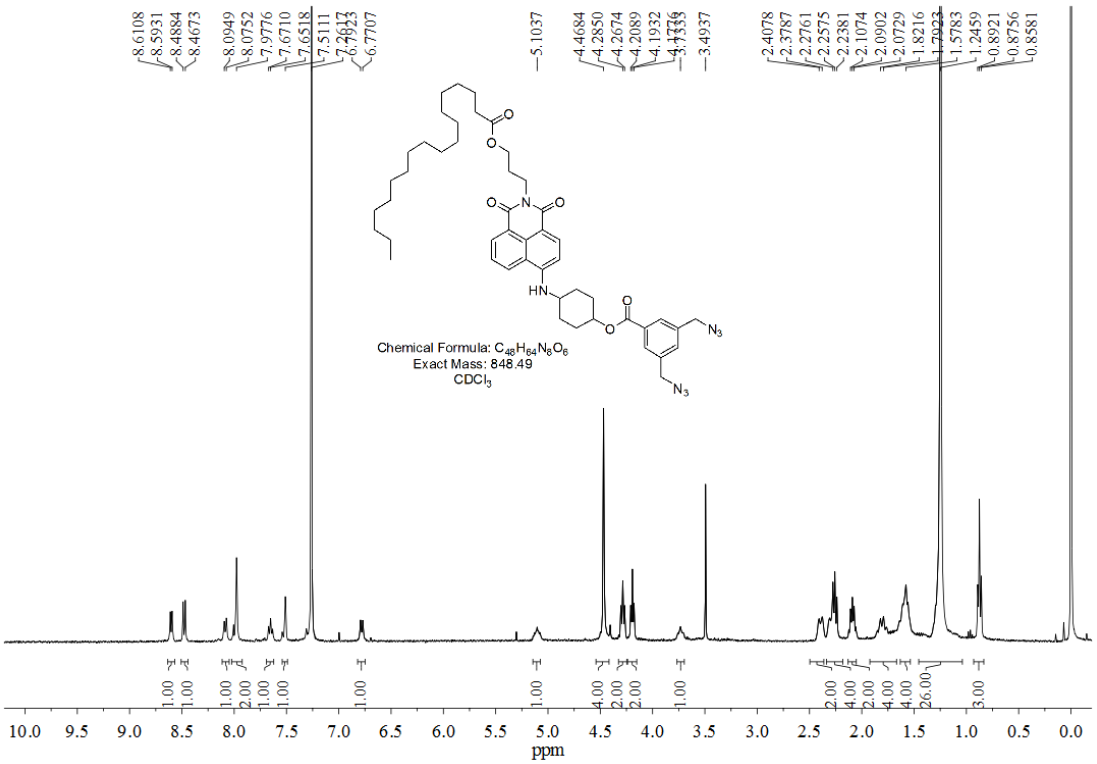

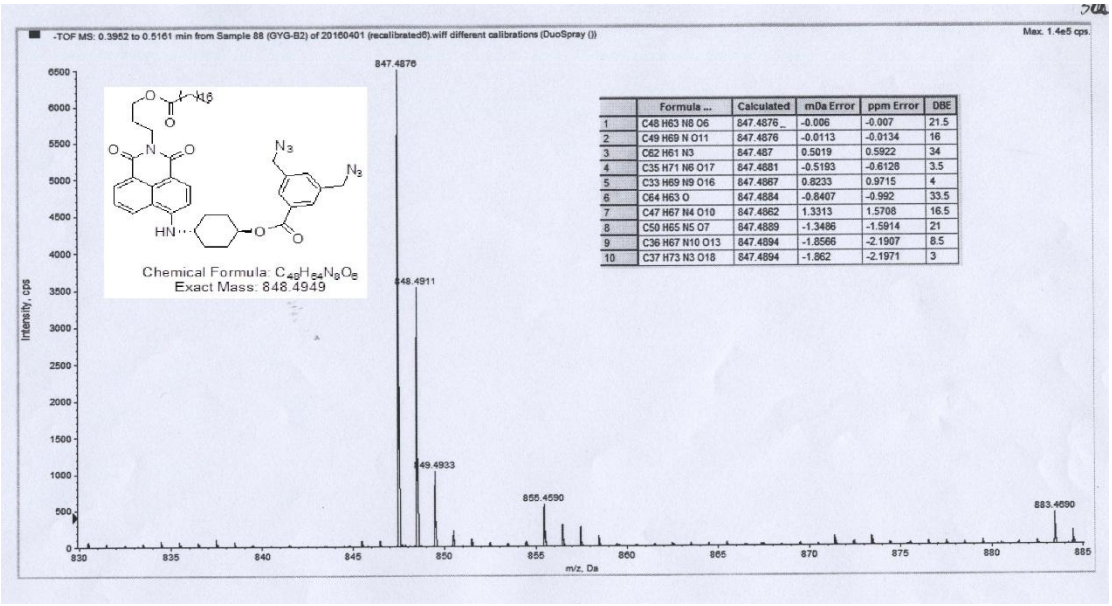

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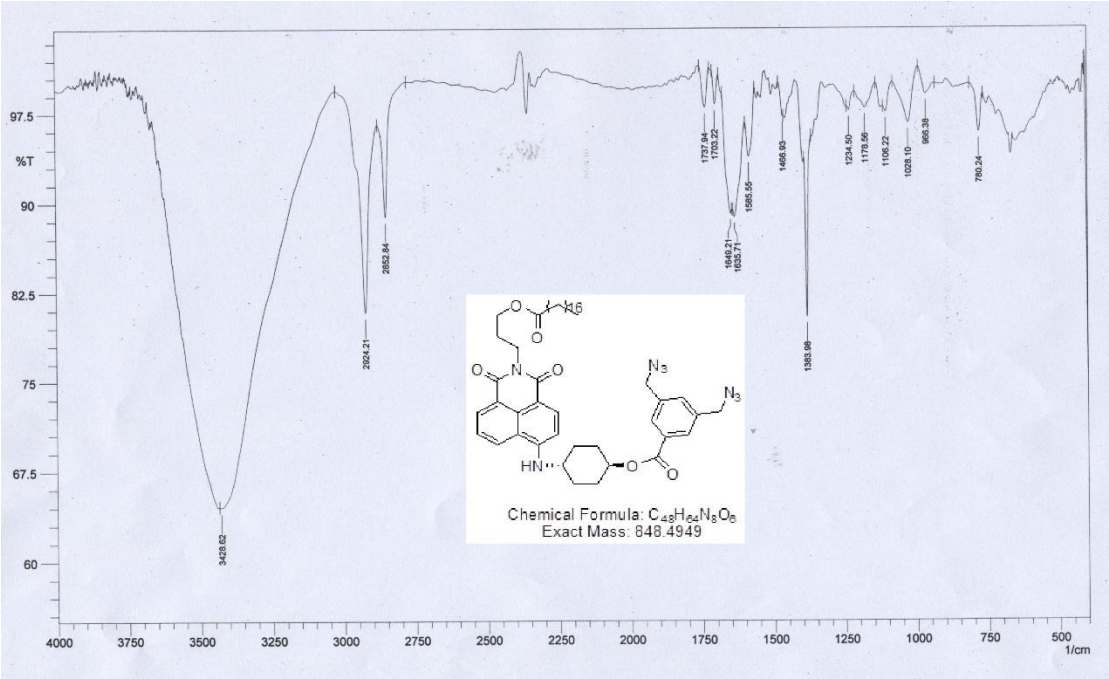
3	C62 H61 N3	847.487	0.5019	0.5922	34
4	C35 H71 N6 O17	847.4881	-0.5193	-0.6128	3.5
5	C33 H69 N9 O16	847.4867	0.8233	0.9715	4
6	C64 H63 O	847.4884	-0.8407	-0.992	33.5
7	C47 H67 N4 O10	847.4862	1.3313	1.5708	16.5
8	C50 H65 N5 O7	847.4889	-1.3486	-1.5914	21
9	C36 H67 N10 O13	847.4894	-1.8566	-2.1907	8.5
10	C37 H73 N3 O18	847.4894	-1.862	-2.1971	3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1000
750
500
1/cm
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2924.21
2852.84
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1703.22
1646.21
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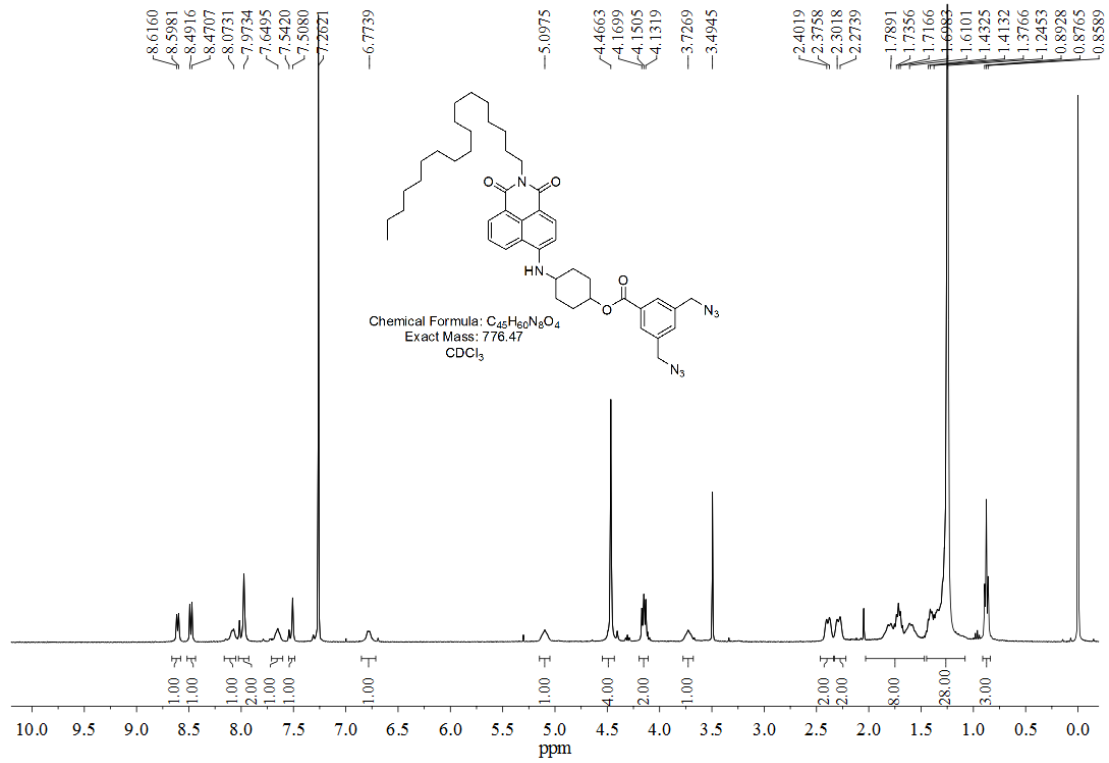
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3.00
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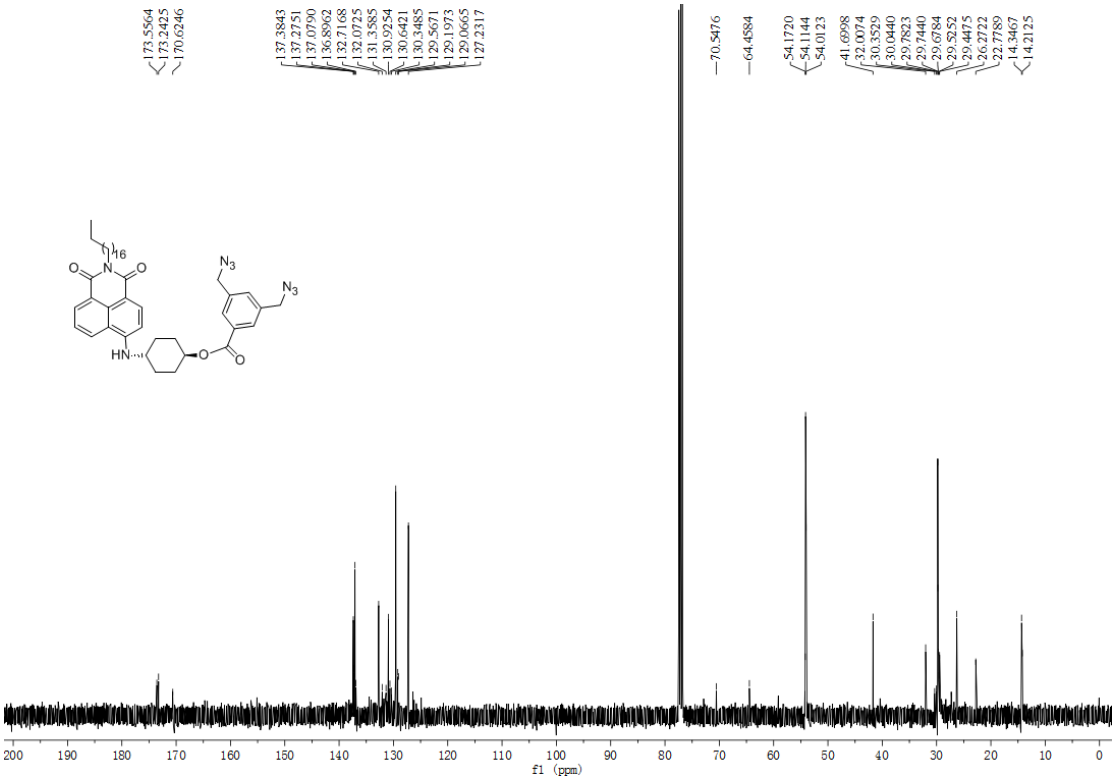
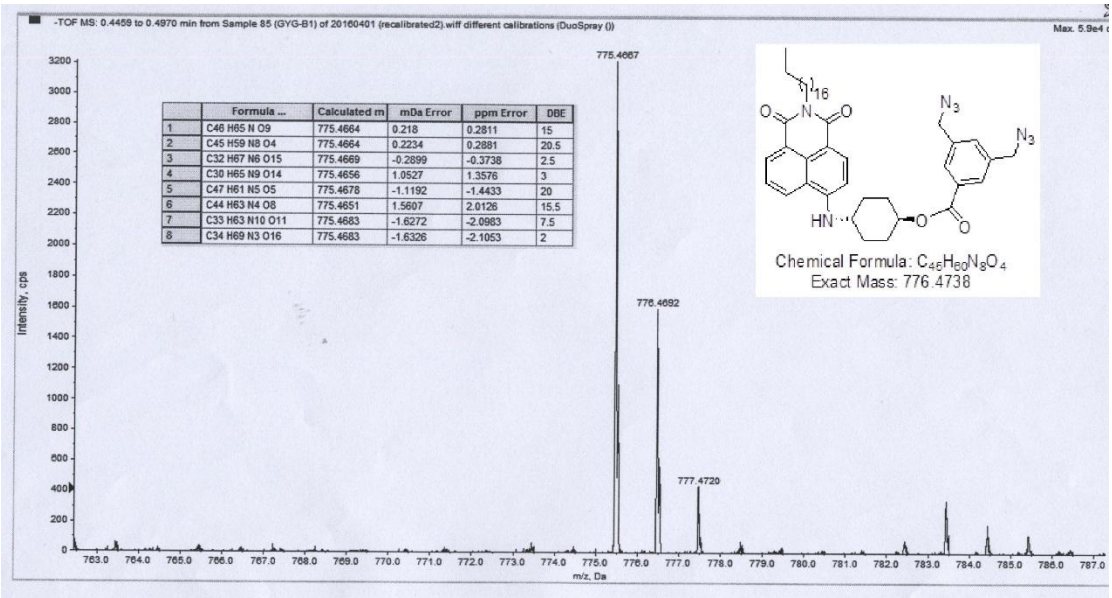
ppm





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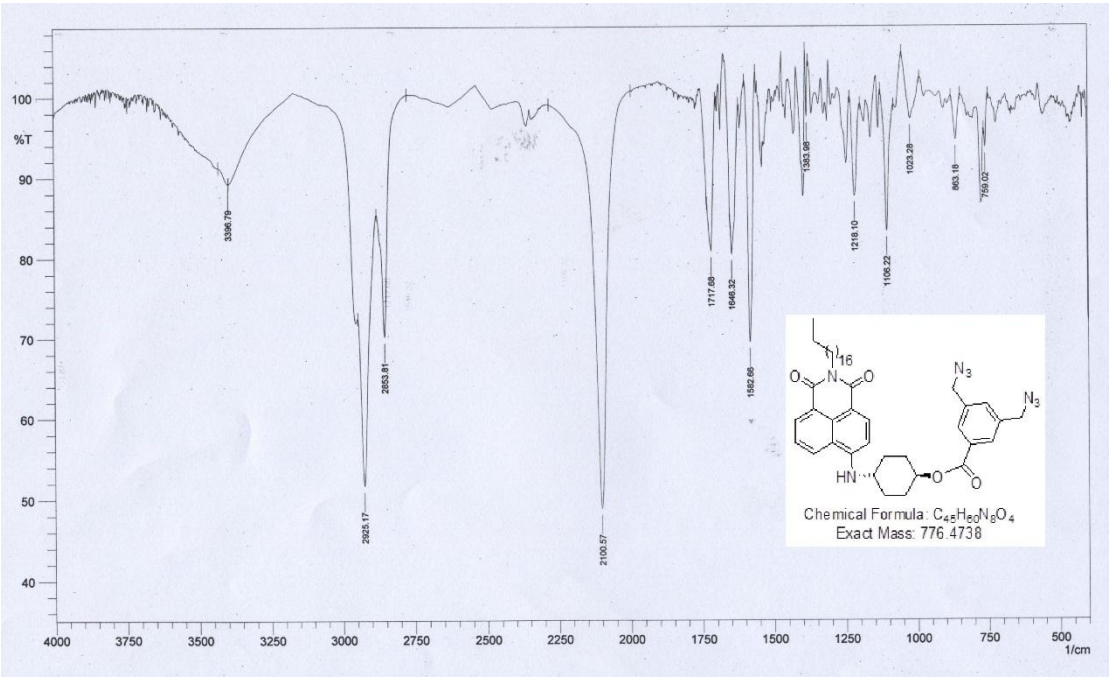
2	C45 H59 N8 O4	775.4664	0.2234	0.2881	20.5
3	C32 H67 N6 O15	775.4669	-0.2899	-0.3738	2.5
4	C30 H65 N9 O14	775.4656	1.0527	1.3576	3
5	C47 H61 N5 O5	775.4678	-1.1192	-1.4433	20
6	C44 H63 N4 O8	775.4651	1.5607	2.0126	15.5
7	C33 H63 N10 O11	775.4683	-1.6272	-2.0983	7.5
8	C34 H69 N3 O16	775.4683	-1.6326	-2.1053	2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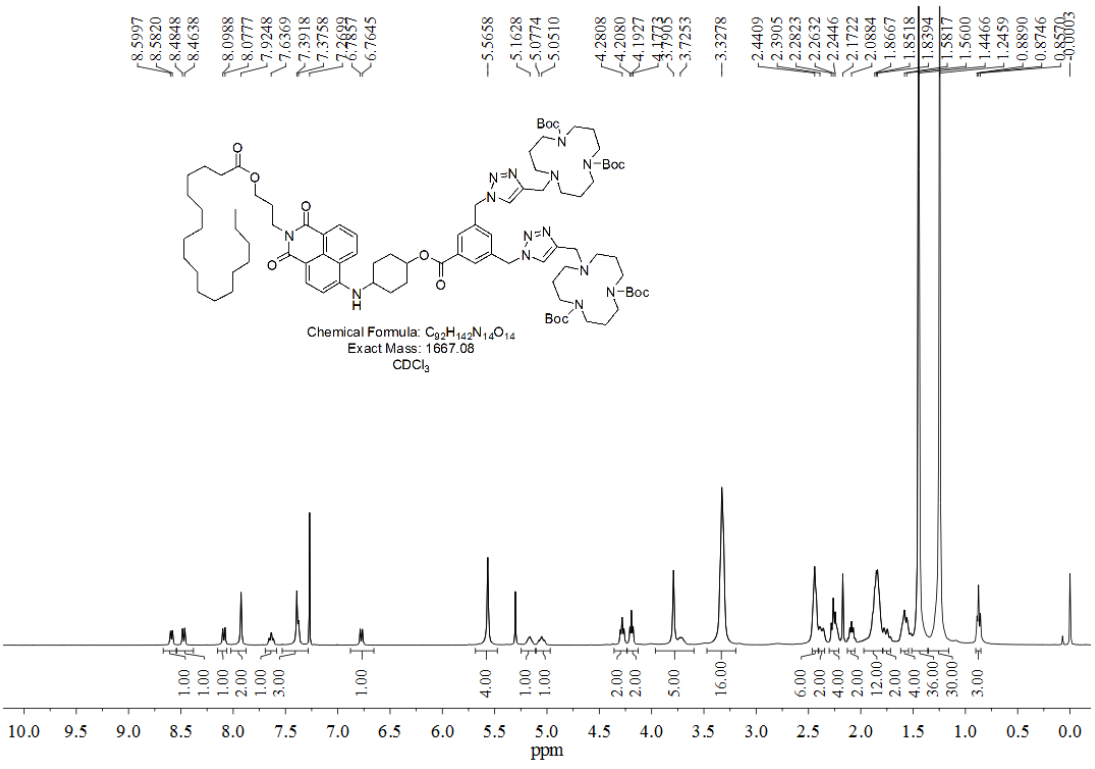
Chemical Formula: C45H60N8O4
Exact Mass: 776.4738
1/cm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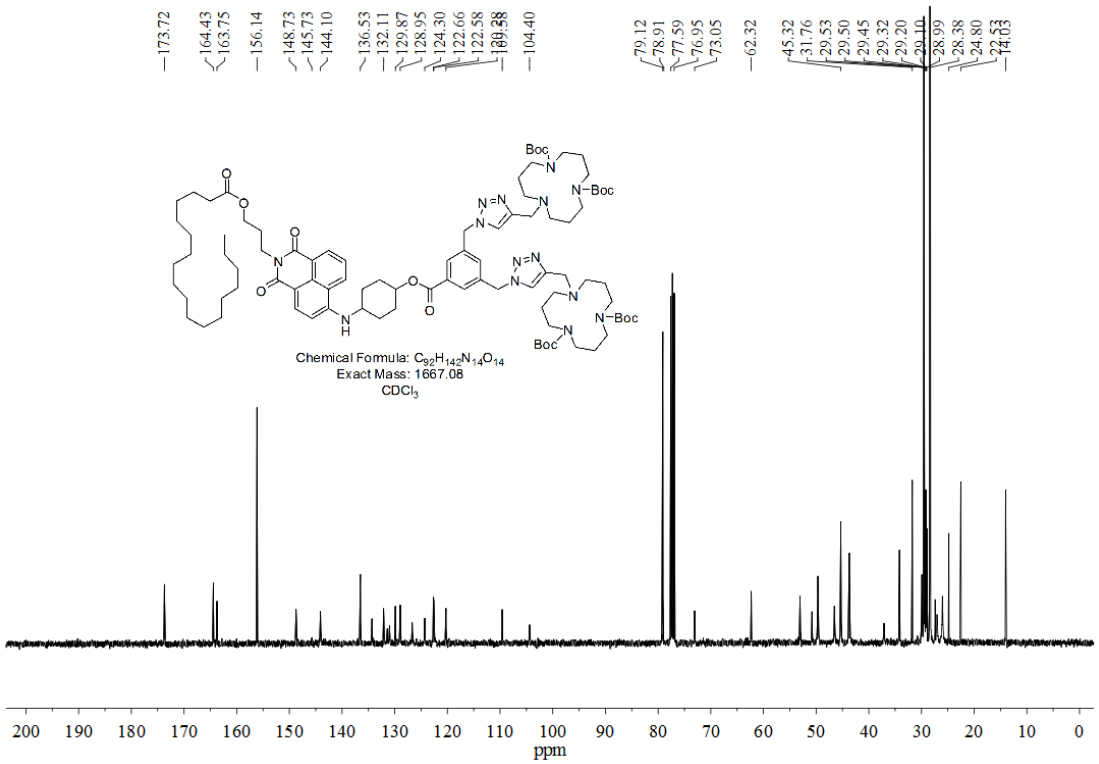
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79.12
78.91
77.59
76.95
73.05
62.32
45.32
31.76
29.53
29.50
29.45
29.32
29.20
29.10
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28.38
24.80
22.53
14.03
Boc
N-Boc
Chemical Formula: C92H142N14O14
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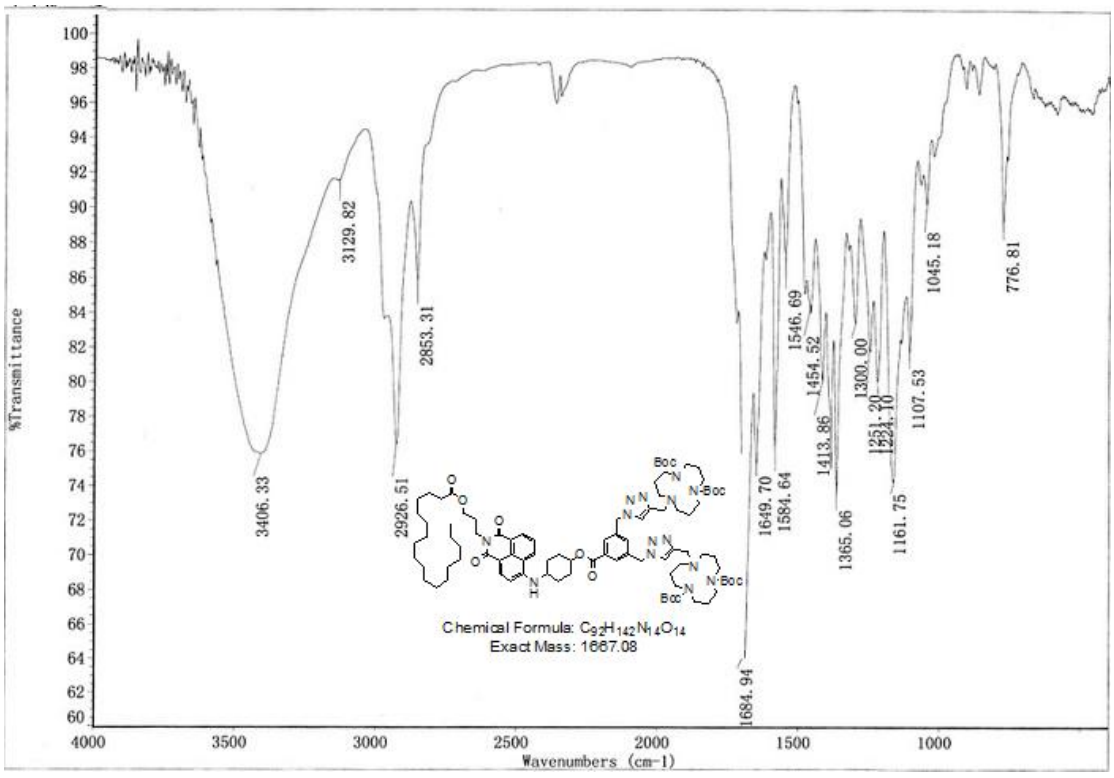
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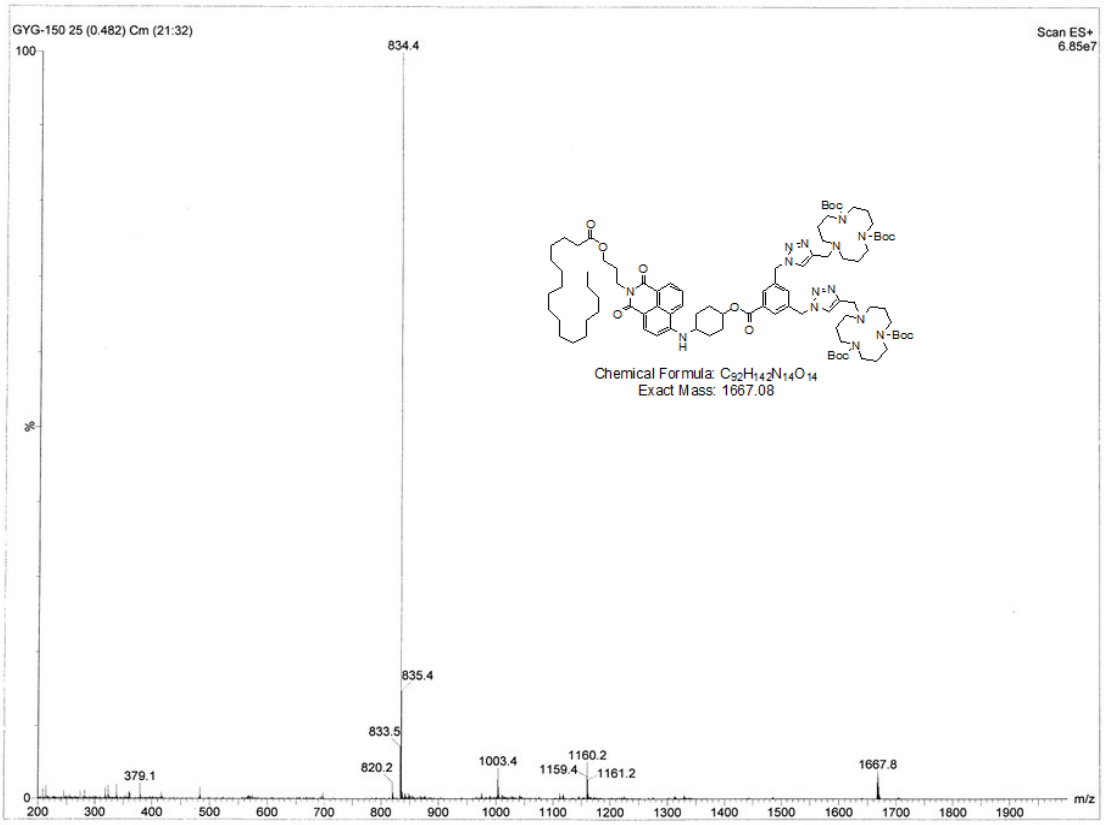
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379.1
1003.4
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1160.2
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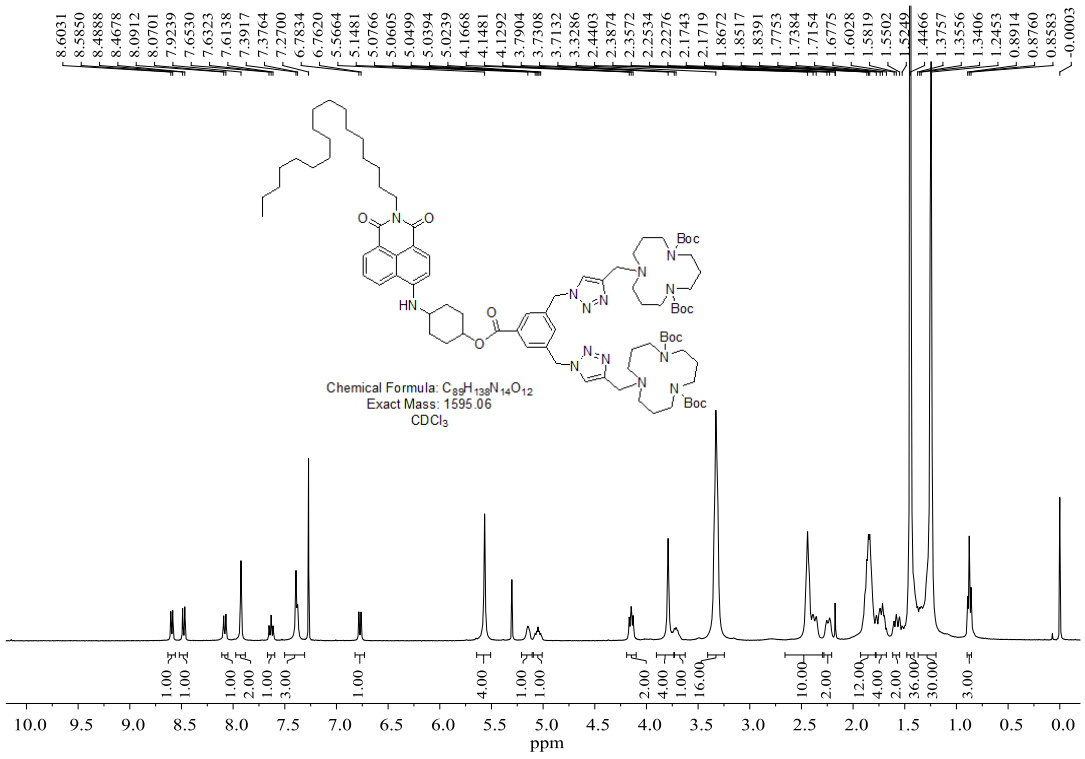
m/z
Chemical Formula: C92H142N14O14
Exact Mass: 1667.08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Exact Mass: 1595.06
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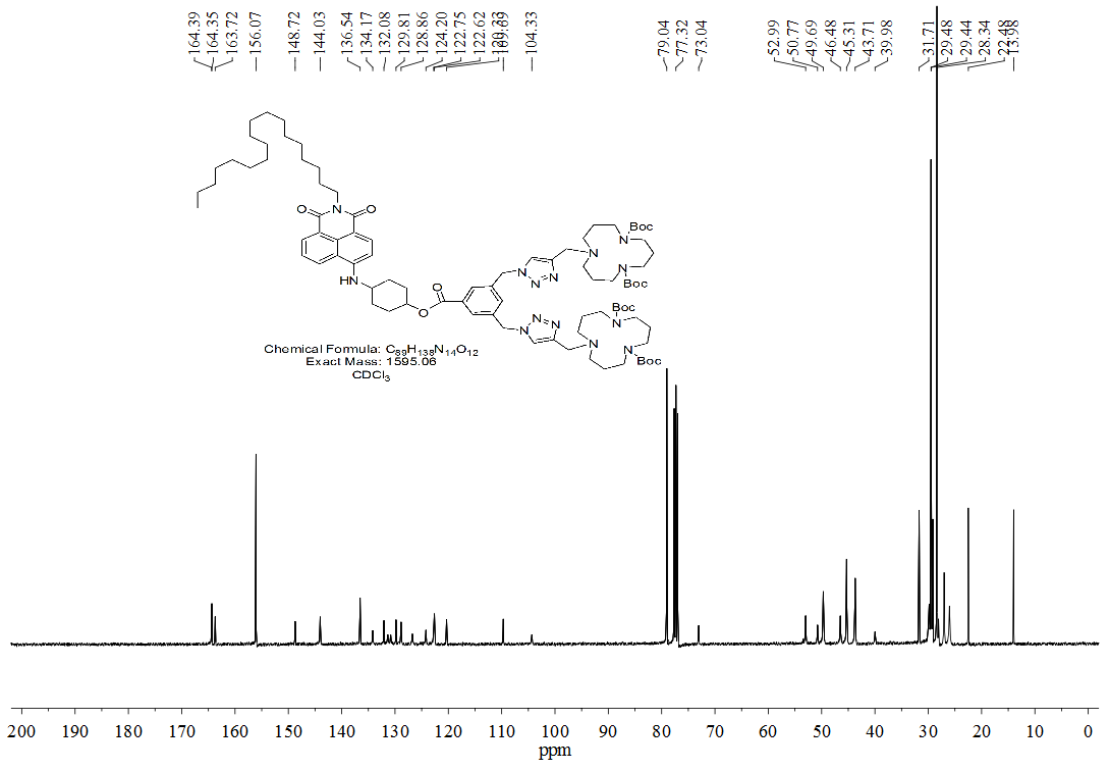
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52.99
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49.69
46.48
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43.71
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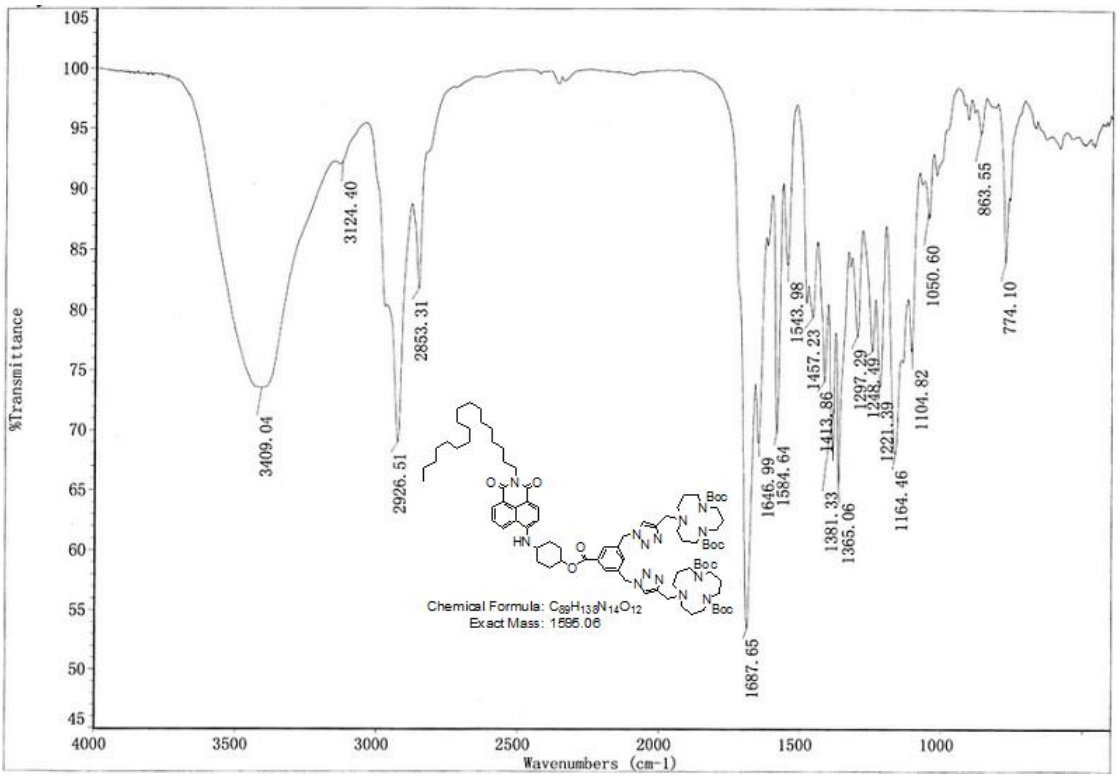
CDCl3
ppm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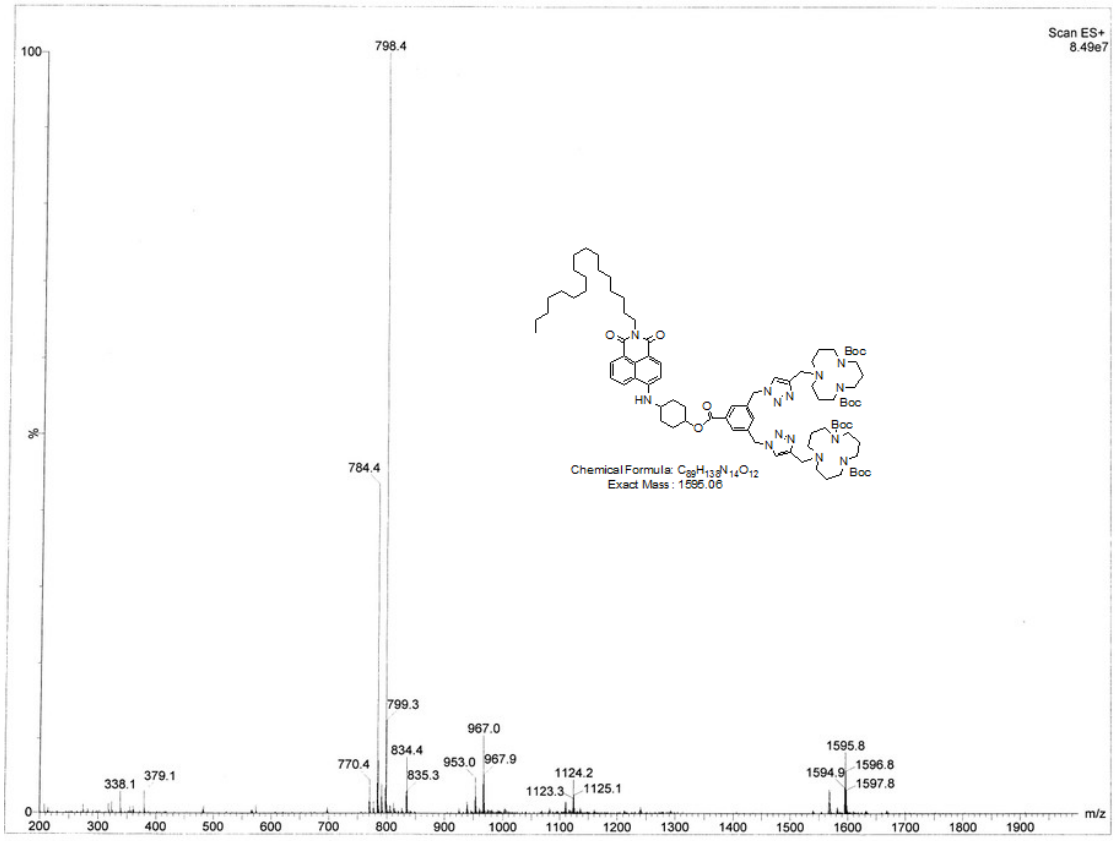
Chemical Formula: C89H138N14O12
Exact Mass: 1595.06
Wavenumbers (cm-1)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1125.1
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1594.9
1596.8
1597.8
m/z
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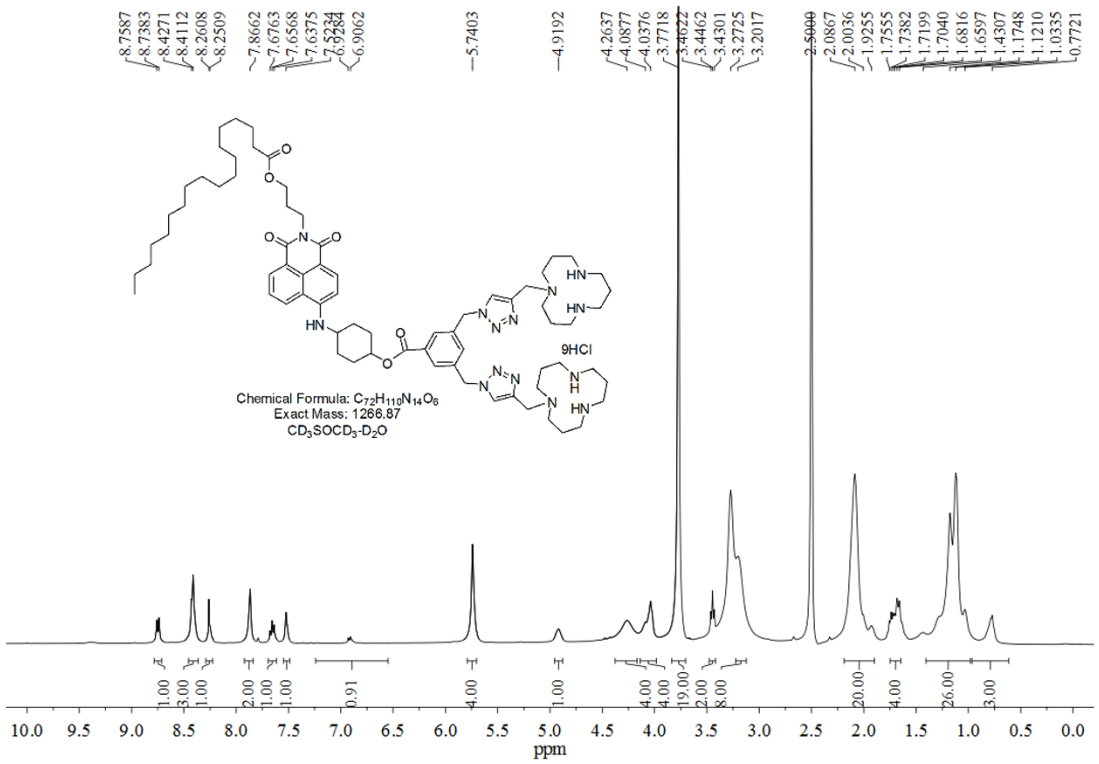
Boc
HN
Chemical Formula: C89H138N14O12
Exact Mass: 1595.06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8.4271
8.4112
8.2608
8.2509
7.8662
7.6763
7.6568
7.6375
7.5234
6.9384
6.9062
5.7403
4.9192
4.2637
4.0877
4.0376
3.7718
3.4622
3.4462
3.4301
3.2725
3.2017
2.5000
2.0867
2.0036
1.9255
1.7555
1.7382
1.7199
1.7040
1.6816
1.6597
1.4307
1.1748
1.1210
1.0335
0.7721
HN
9HCl
Chemical Formula: C72H110N14O6
Exact Mass: 1266.87
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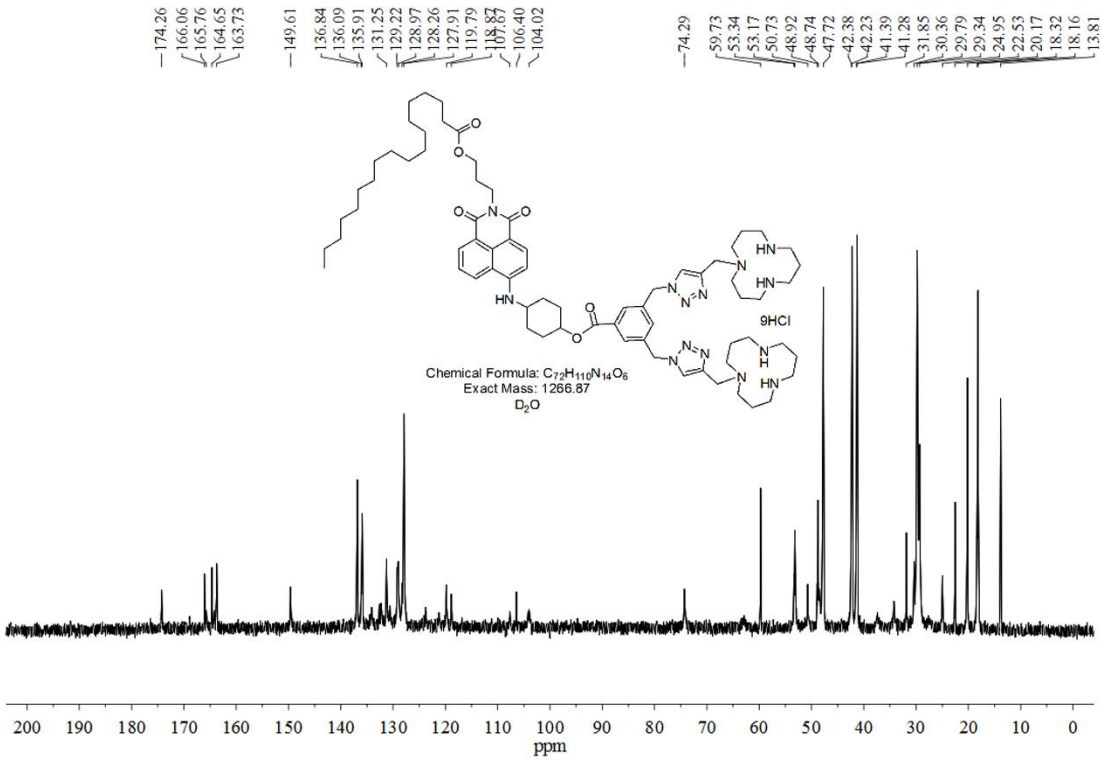
3.00
1.00
2.00
1.00
1.00
0.91
4.00
1.00
4.00
4.00
19.00
2.00
8.00
20.00
4.00
26.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm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131.25
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128.26
127.91
119.79
118.87
107.67
106.40
104.02
74.29
59.73
53.34
53.17
50.73
48.92
48.74
47.72
42.38
42.23
41.39
41.28
31.85
30.36
29.79
29.34
24.95
22.53
20.17
18.32
18.16
13.81
9HCl
Chemical Formula: C72H110N14O6
Exact Mass: 1266.87
D2O
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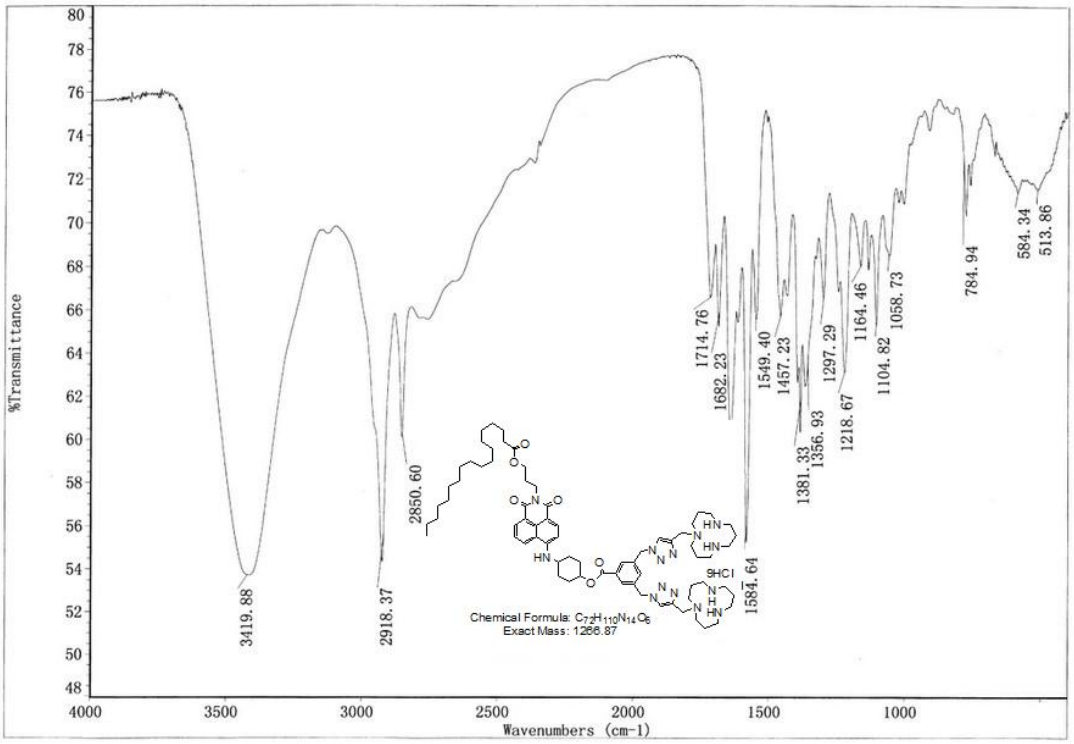
ppm


%Transmittance
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4000 3500 3000 2500 2000 1500 1000
Wavenumbers (cm-1)
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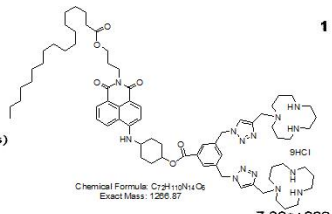
2918.37
2850.60
1714.76
1682.23
1584.64
1549.40
1457.23
1381.33
1356.93
1297.29
1218.67
1164.46
1104.82
1058.73
784.94
584.34
513.86
9HCl
Chemical Formula: C72H110N14O6
Exact Mass: 1266.87

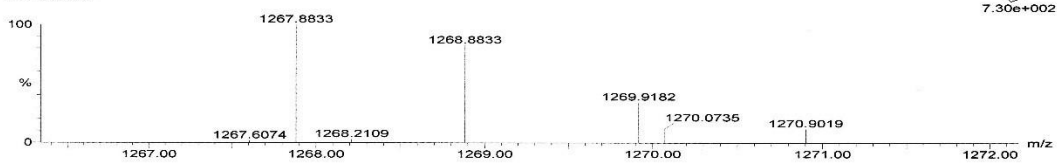
Elemental Composition Report 1

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

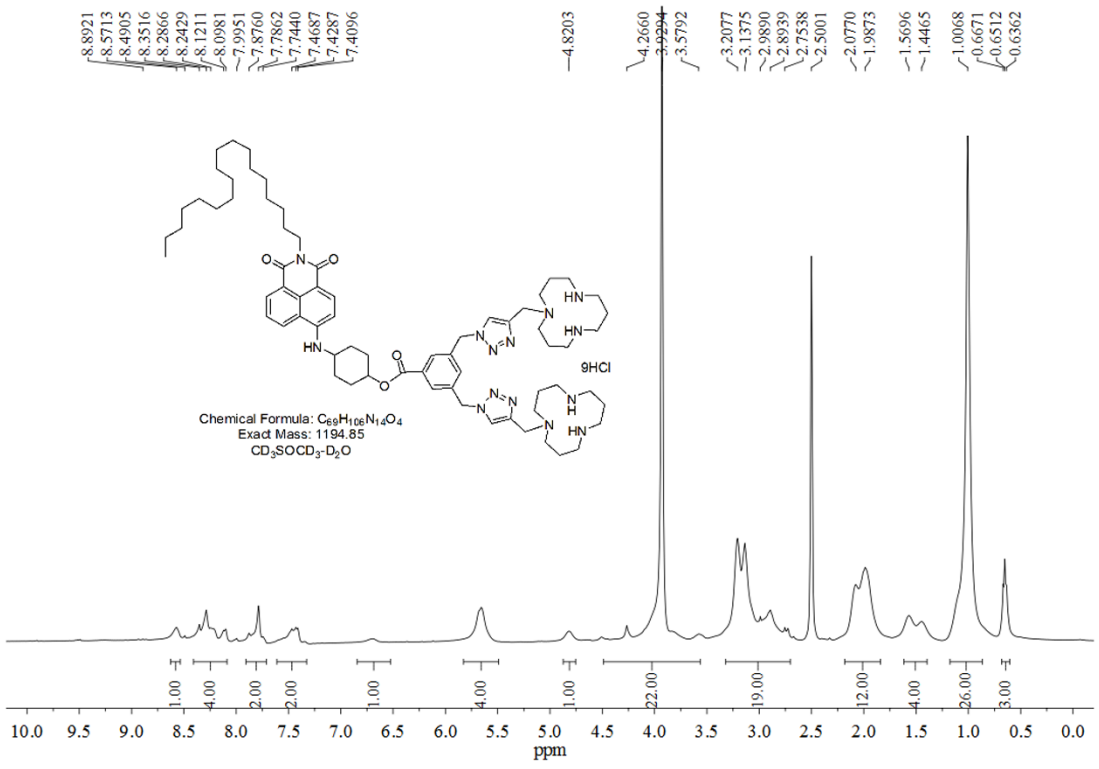
Monoisotopic Mass, Even Electron Ions
8482 formula(e) evaluated with 33 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-100 H: 0-120 N: 0-15 O: 0-10 I: 0-4

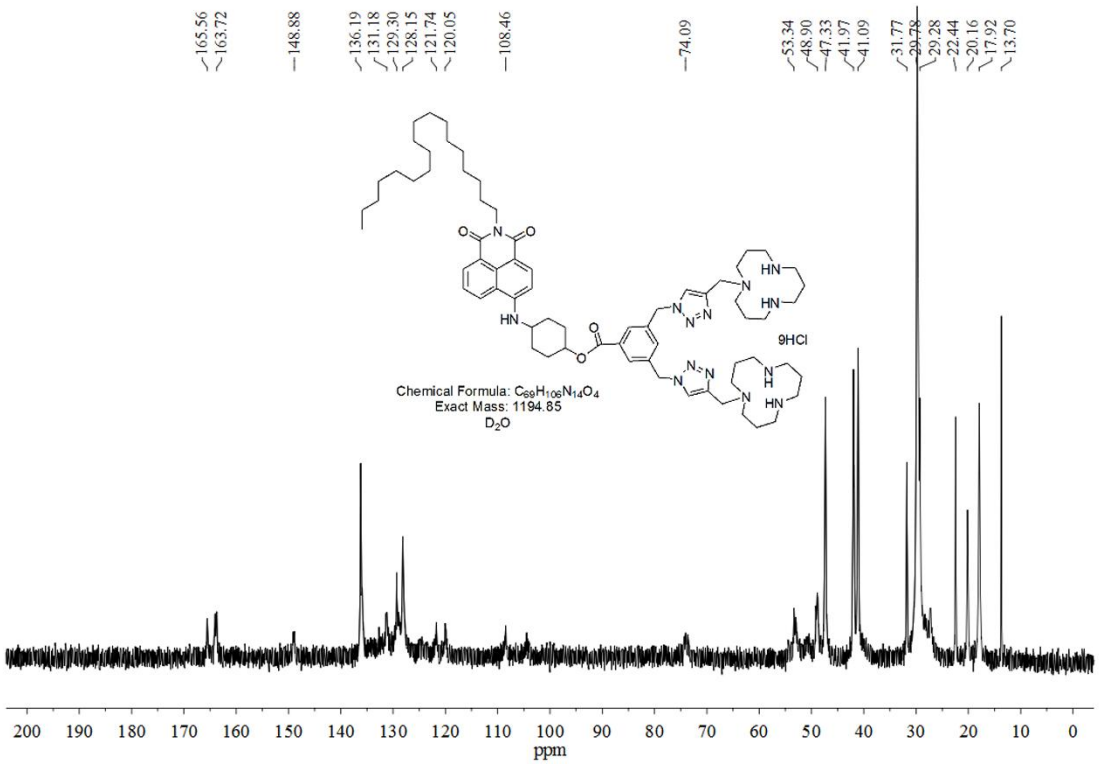


GYG-152 17 (0.315)
TOF MS ES+
7.30e+002



Minimum:		5.0	5.0	-1.5		
Maximum:				50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
1267.8833	1267.8832	0.1	0.1	40.5	24.1	C44 H21 N15 O8 I3
	1267.8838	-0.5	-0.4	27.5	28.1	C46 H38 N3 O8 I4
	1267.8838	-0.5	-0.4	23.5	1.2	C76 H115 N8 O8
	1267.8827	0.6	0.5	47.5	6.4	C59 H25 N3 O7 I3
	1267.8825	0.8	0.6	33.5	28.2	C43 H30 N13 O2 I4
	1267.8843	-1.0	-0.8	20.5	63.4	C31 H34 N15 O9 I4
	1267.8846	-1.3	-1.0	35.5	9.1	C92 H115 O3
	1267.8819	1.4	1.1	40.5	8.3	C58 H34 N O I4
	1267.8819	1.4	1.1	36.5	7.4	C88 H111 N6 O
	1267.8851	-1.8	-1.4	32.5	23.2	C47 H34 N7 O4 I4
	1267.8851	-1.8	-1.4	28.5	2.0	C77 H111 N12 O4
	1267.8811	2.2	1.7	28.5	33.7	C42 H34 N9 O6 I4
	1267.8811	2.2	1.7	24.5	0.5	C72 H111 N14 O6
	1267.8859	-2.6	-2.1	39.5	19.6	C48 H25 N9 O10 I3
	1267.8806	2.7	2.1	31.5	5.9	C87 H115 N2 O5
	1267.8804	2.9	2.3	17.5	0.2	C71 H120 N12 I
	1267.8865	-3.2	-2.5	22.5	2.1	C80 H119 N2 O10
	1267.8865	-3.2	-2.5	37.5	18.9	C48 H30 N11 I4
	1267.8800	3.3	2.6	48.5	8.8	C55 H21 N9 O5 I3
	1267.8798	3.5	2.8	19.5	0.2	C71 H115 N10 O10
	1267.8798	3.5	2.8	23.5	39.8	C41 H38 N5 O10 I4
	1267.8872	-3.9	-3.1	44.5	15.7	C49 H21 N13 O6 I3
	1267.8878	-4.5	-3.5	31.5	18.9	C51 H38 N O6 I4
	1267.8878	-4.5	-3.5	27.5	3.1	C81 H115 N6 O6
	1267.8787	4.6	3.6	43.5	11.7	C54 H25 N5 O9 I3
	1267.8784	4.9	3.9	29.5	39.8	C38 H30 N15 O4 I4
	1267.8883	-5.0	-3.9	24.5	47.9	C36 H34 N13 O7 I4
	1267.8779	5.4	4.3	32.5	4.5	C83 H111 N8 O3
	1267.8779	5.4	4.3	36.5	14.4	C53 H34 N3 O3 I4
	1267.8891	-5.8	-4.6	32.5	4.4	C82 H111 N10 O2
	1267.8892	-5.9	-4.7	36.5	15.1	C52 H34 N5 O2 I4
	1267.8773	6.0	4.7	49.5	11.7	C51 H17 N15 O3 I3
	1267.8771	6.2	4.9	24.5	46.6	C37 H34 N11 O8 I4

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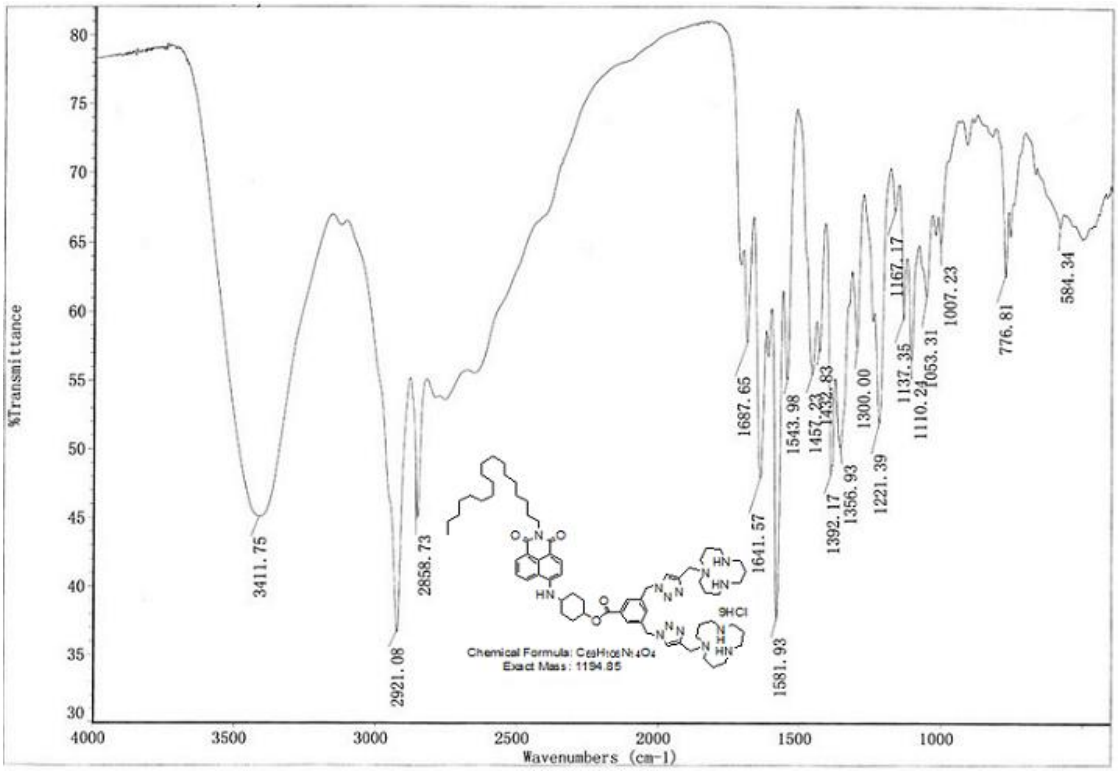
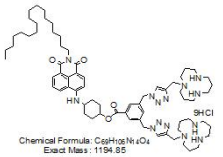
131.18
129.30
128.15
121.74
120.05
108.46
74.09
53.34
48.90
47.33
41.97
41.09
31.77
29.78
29.28
22.44
20.16
17.92
13.70
9HCl
Chemical Formula: C69H106N14O4
Exact Mass: 1194.85
D2O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm


%Transmittance
80 75 70 65 60 55 50 45 40 35 30
4000 3500 3000 2500 2000 1500 1000
Wavenumbers (cm-1)
3411.75
2921.08
2858.73
1687.65
1641.57
1581.93
1543.98
1457.22
1432.83
1392.17
1356.93
1300.00
1221.39
1167.17
1137.35
1110.24
1053.31
1007.23
776.81
584.34
9HCl
Chemical Formula: C69H106N14O4
Exact Mass: 1194.85

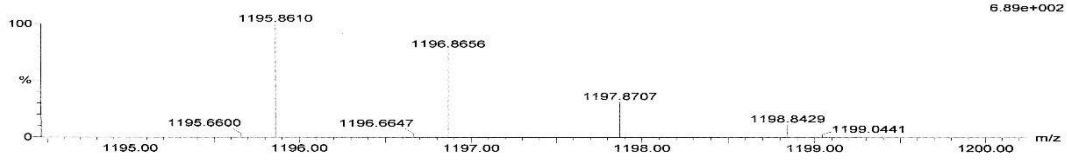
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

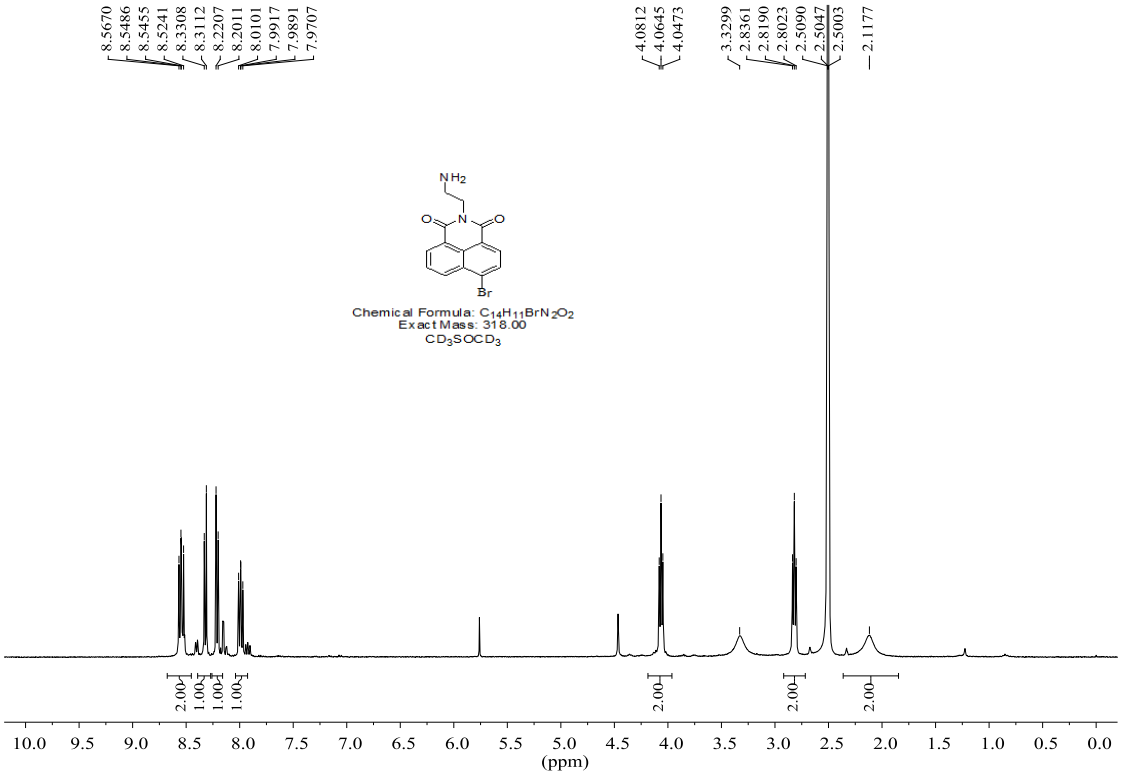
Monoisotopic Mass, Even Electron Ions
8189 formula(e) evaluated with 36 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-100 H: 0-120 N: 0-15 O: 0-10 I: 0-4

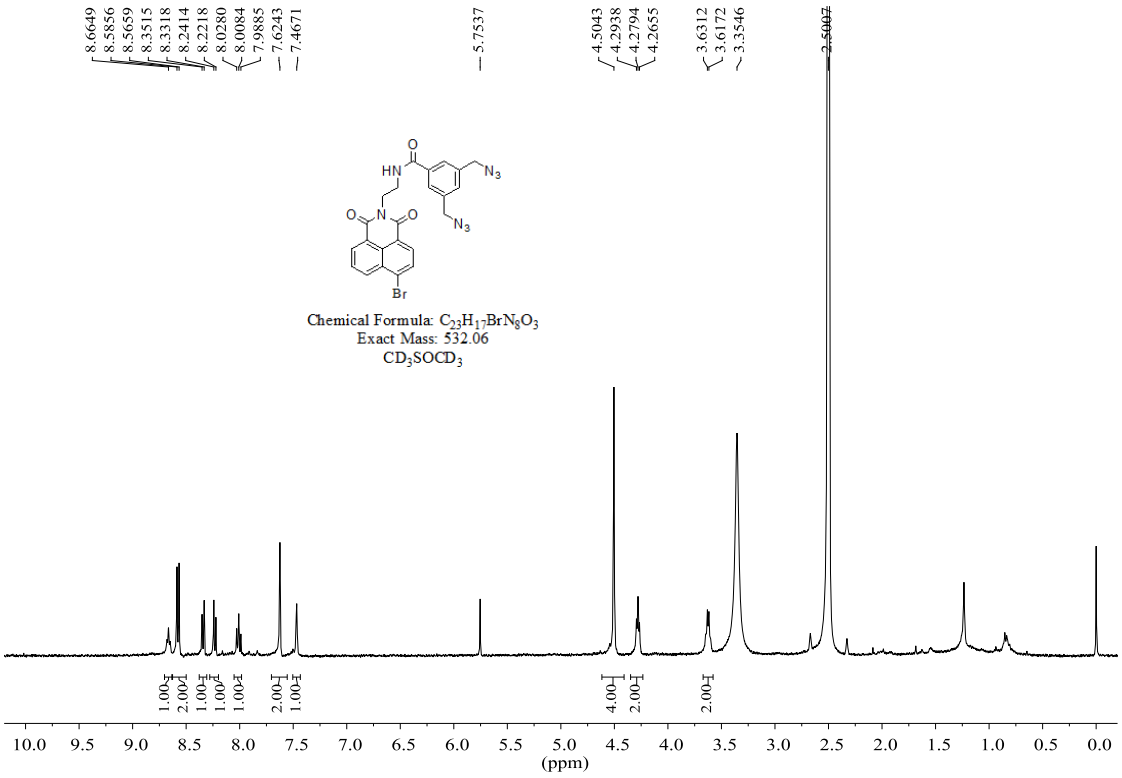


GYG-153 7 (0.130)
TOF MS ES+



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
Minimum:				-1.5		
Maximum:		5.0	5.0	50.0		
1195.8610	1195.8611	-0.1	-0.1	3.5	1.7	C56 H120 N14 O5 I
	1195.8613	-0.3	-0.3	17.5	1.0	C72 H115 N4 O10
	1195.8613	-0.3	-0.3	32.5	25.7	C40 H26 N13 I4
	1195.8607	0.3	0.3	34.5	26.6	C40 H21 N11 O10 I3
	1195.8616	-0.6	-0.5	46.5	5.2	C56 H21 N3 O5 I3
	1195.8619	-0.9	-0.8	15.5	1.1	C72 H120 N6 I
	1195.8600	1.0	0.8	27.5	31.0	C39 H30 N9 O4 I4
	1195.8600	1.0	0.8	23.5	1.0	C69 H107 N14 O4
	1195.8621	-1.1	-0.9	39.5	21.8	C41 H17 N15 O6 I3
	1195.8595	1.5	1.3	30.5	7.2	C84 H111 N2 O3
	1195.8627	-1.7	-1.4	26.5	25.7	C43 H34 N3 O6 I4
	1195.8627	-1.7	-1.4	22.5	1.8	C73 H111 N8 O6
	1195.8589	2.1	1.8	47.5	7.4	C52 H17 N9 O3 I3
	1195.8632	-2.2	-1.8	19.5	60.0	C28 H30 N15 O7 I4
	1195.8586	2.4	2.0	22.5	36.9	C38 H34 N5 O8 I4
	1195.8586	2.4	2.0	18.5	0.4	C68 H111 N10 O8
	1195.8635	-2.5	-2.1	34.5	10.6	C89 H111 O
	1195.8640	-3.0	-2.5	27.5	2.8	C74 H107 N12 O2
	1195.8640	-3.0	-2.5	31.5	20.9	C44 H30 N7 O2 I4
	1195.8579	3.1	2.6	11.5	0.1	C67 H120 N8 O2 I
	1195.8575	3.5	2.9	42.5	10.1	C51 H21 N5 O7 I3
	1195.8647	-3.7	-3.1	38.5	17.5	C45 H21 N9 O8 I3
	1195.8573	3.7	3.1	28.5	37.0	C35 H26 N15 O2 I4
	1195.8651	-4.1	-3.4	7.5	0.3	C61 H120 N12 O3 I
	1195.8568	4.2	3.5	31.5	5.7	C80 H107 N8 O
	1195.8568	4.2	3.5	35.5	12.6	C50 H30 N3 O I4
	1195.8653	-4.3	-3.6	21.5	2.8	C77 H115 N2 O8
	1195.8562	4.8	4.0	48.5	10.1	C48 H13 N15 O I3
	1195.8658	-4.8	-4.0	14.5	0.1	C62 H111 N14 O9
	1195.8659	-4.9	-4.1	18.5	52.0	C32 H34 N9 O9 I4
	1195.8560	5.0	4.2	23.5	43.5	C34 H30 N11 O6 I4
	1195.8661	-5.1	-4.3	43.5	13.8	C46 H17 N13 O4 I3
	1195.8554	5.6	4.7	26.5	4.3	C79 H111 N4 O5
	1195.8667	-5.7	-4.8	26.5	4.0	C78 H111 N6 O4
	1195.8667	-5.7	-4.8	30.5	16.8	C48 H34 N O4 I4
	1195.8552	5.8	4.9	12.5	0.1	C63 H116 N14 I

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7.4671
5.7537
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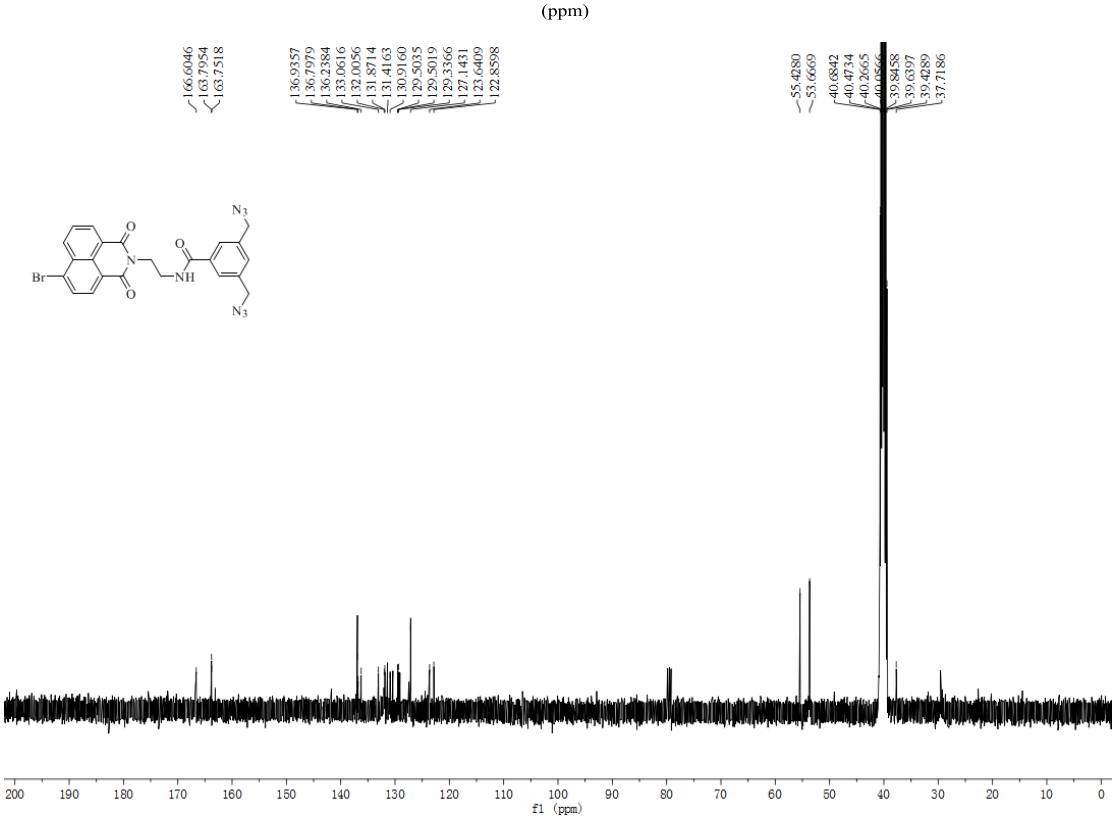
Chemical Formula: C23H17BrN8O3
Exact Mass: 532.06
CD3SOCD3
(ppm)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136.7979
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133.0616
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131.8714
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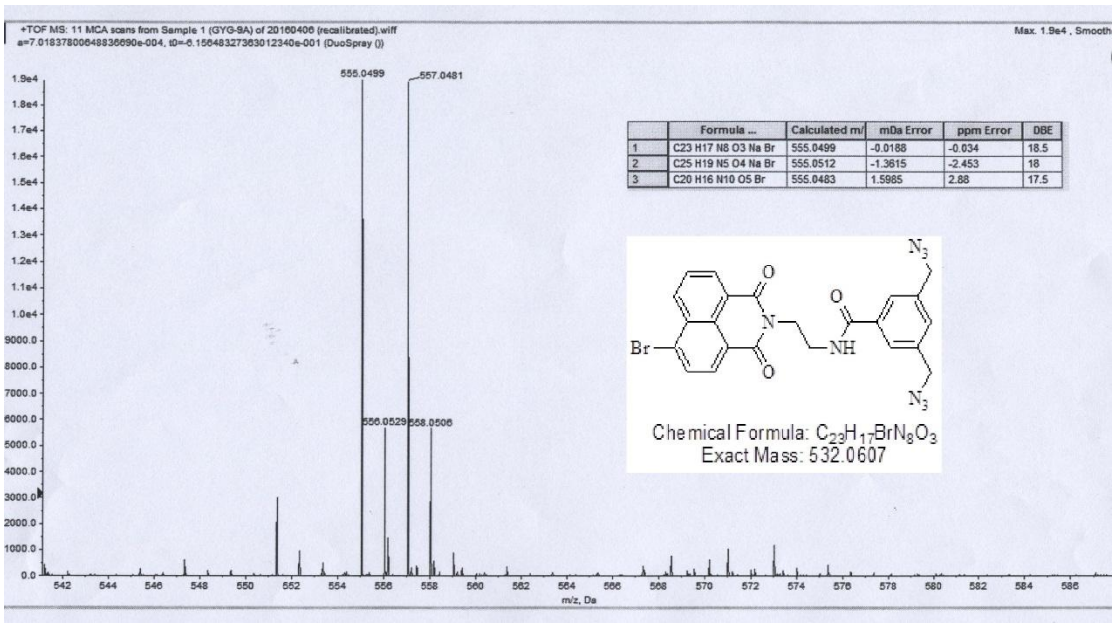
37.7186
f1 (ppm)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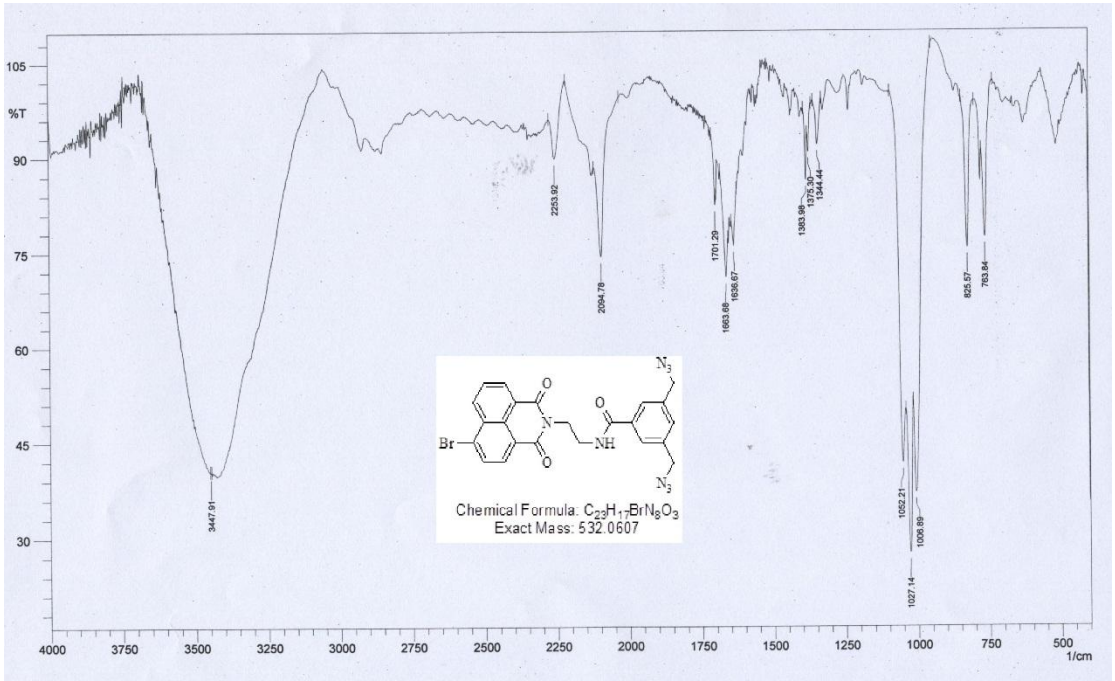
a=7.018378006848836690e-004, t0=-6.156483273630123 40e-001 (DuoSpray ())
Max. 1.9e4 , Smooth
555.0499
557.0481
556.0529
558.0506
m/z, Da
Formula ... | Calculated m/ | mDa Error | ppm Error | DBE
1 | C23 H17 N8 O3 Na Br | 555.0499 | -0.0188 | -0.034 | 18.5
2 | C25 H19 N5 O4 Na Br | 555.0512 | -1.3615 | -2.453 | 18
3 | C20 H16 N10 O5 Br | 555.0483 | 1.5985 | 2.88 | 17.5
Chemical Formula: C23H17BrN8O3
Exact Mass: 532.0607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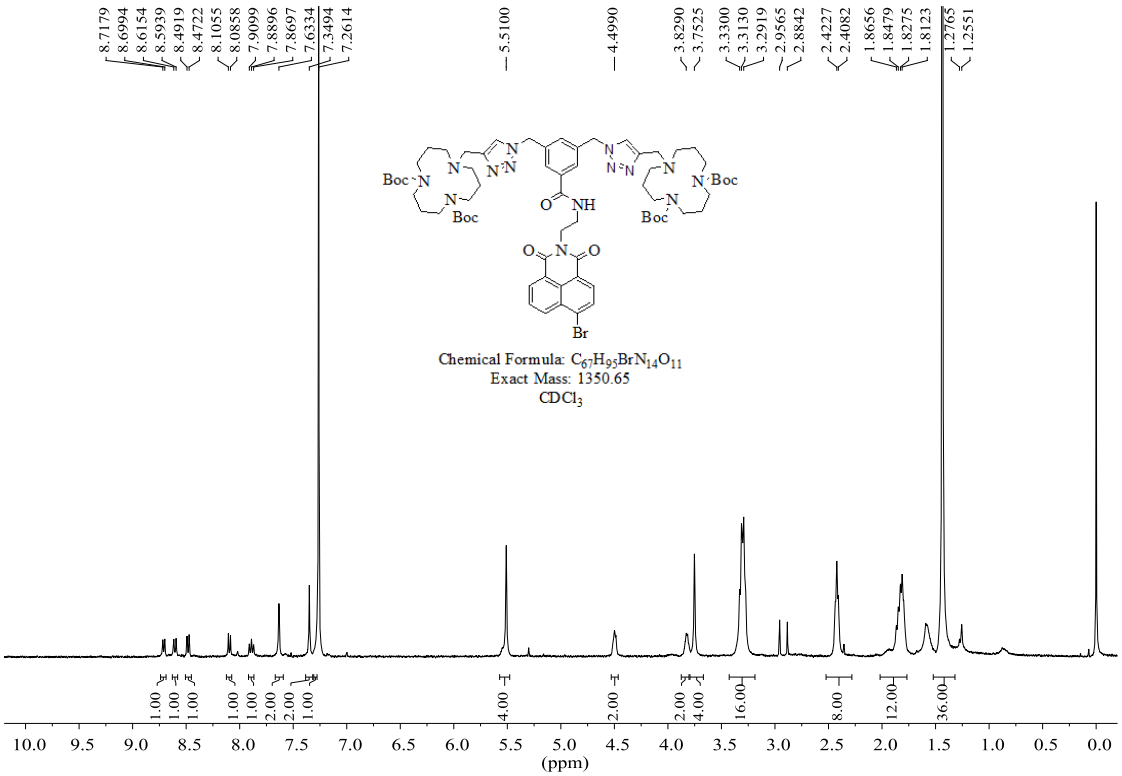
2253.92
2094.78
1701.29
1663.68
1636.67
1383.99
1375.30
1344.44
1052.21
1027.14
1006.89
825.57
763.84
1/cm
Chemical Formula: C23H17BrN8O3
Exact Mass: 532.0607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8.4919
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7.8697
7.6334
7.3494
7.2614
5.5100
4.4990
3.8290
3.7525
3.3300
3.3130
3.2919
2.9565
2.8842
2.4227
2.4082
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1.8479
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1.8123
1.2765
1.2551
Boc
NH
Br
Chemical Formula: C67H95BrN14O11
Exact Mass: 1350.65
CDCl3
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1.00
1.00
1.00
1.00
2.00
2.00
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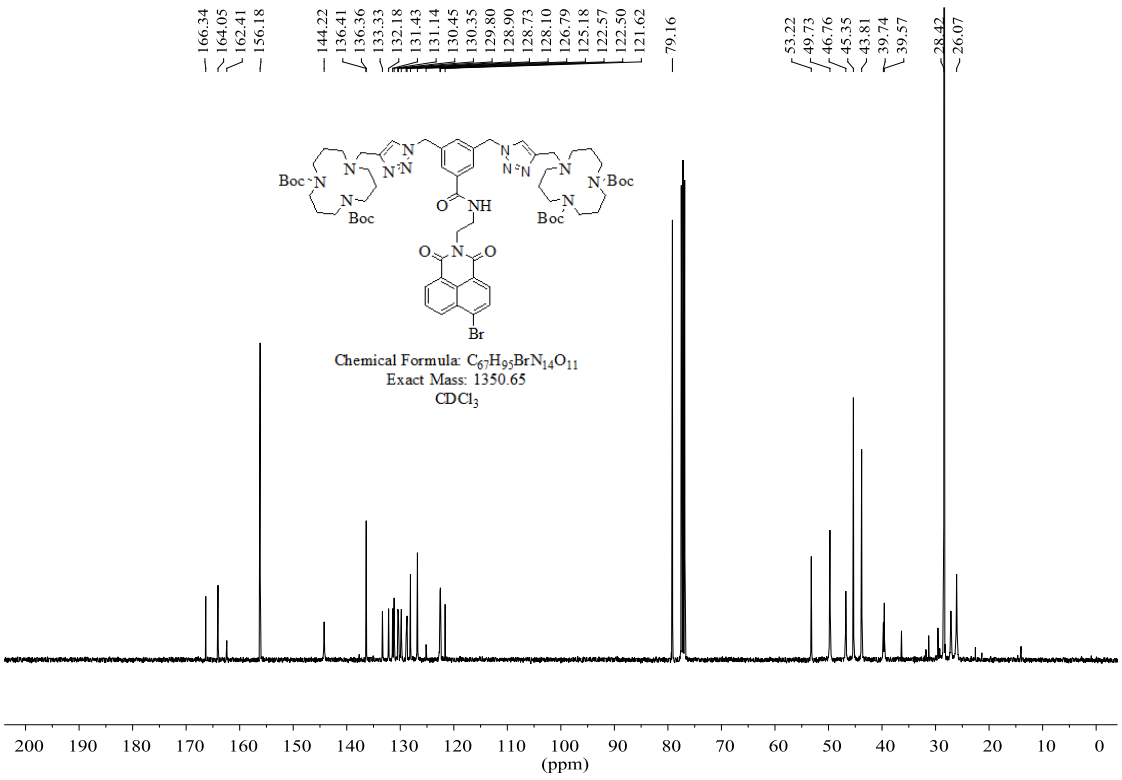
36.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)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122.57
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121.62
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45.35
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Boc
NH
Br
Chemical Formula: C67H95BrN14O11
Exact Mass: 1350.65
CDCl3
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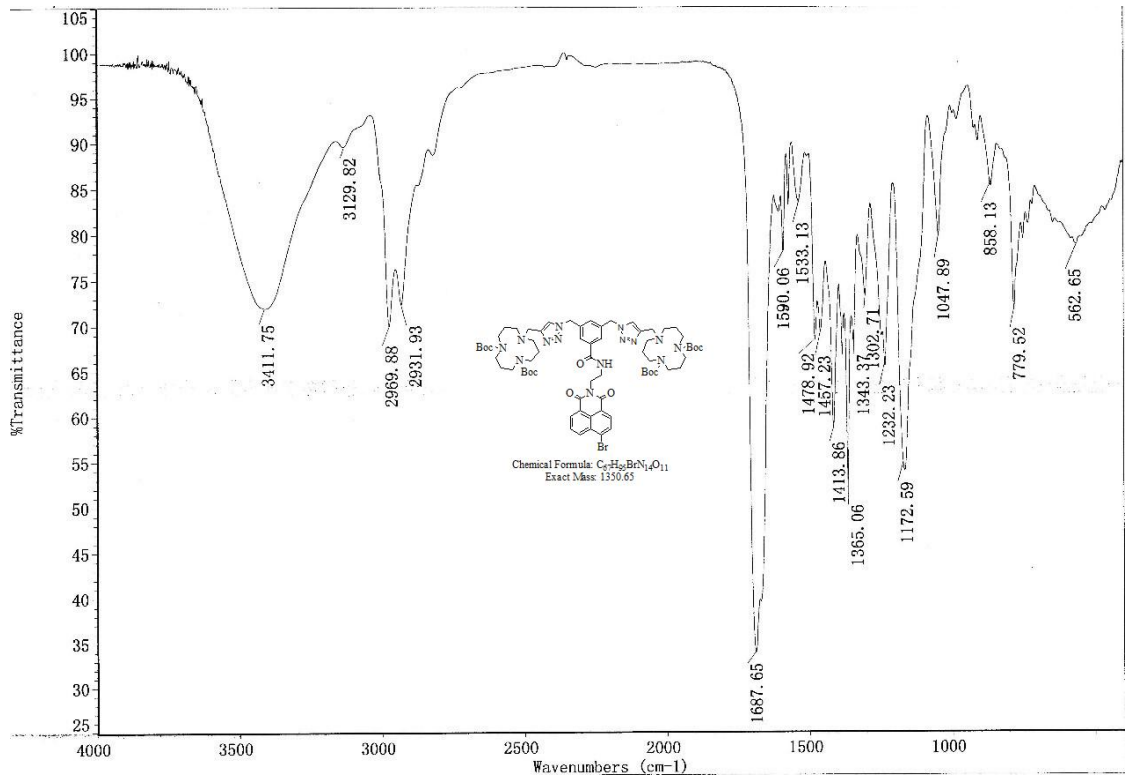
(ppm)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Wavenumbers (cm-1)
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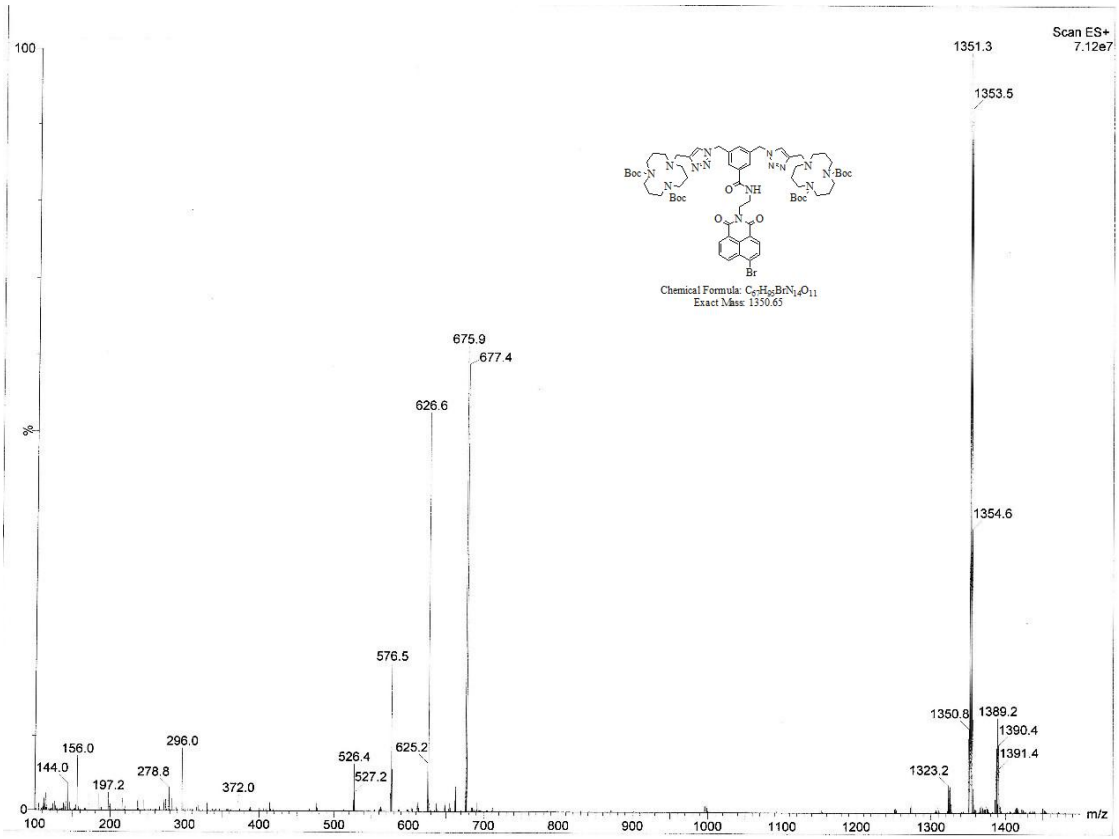
Exact Mass: 1350.65


Scan ES+
7.12e7
%
m/z
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197.2
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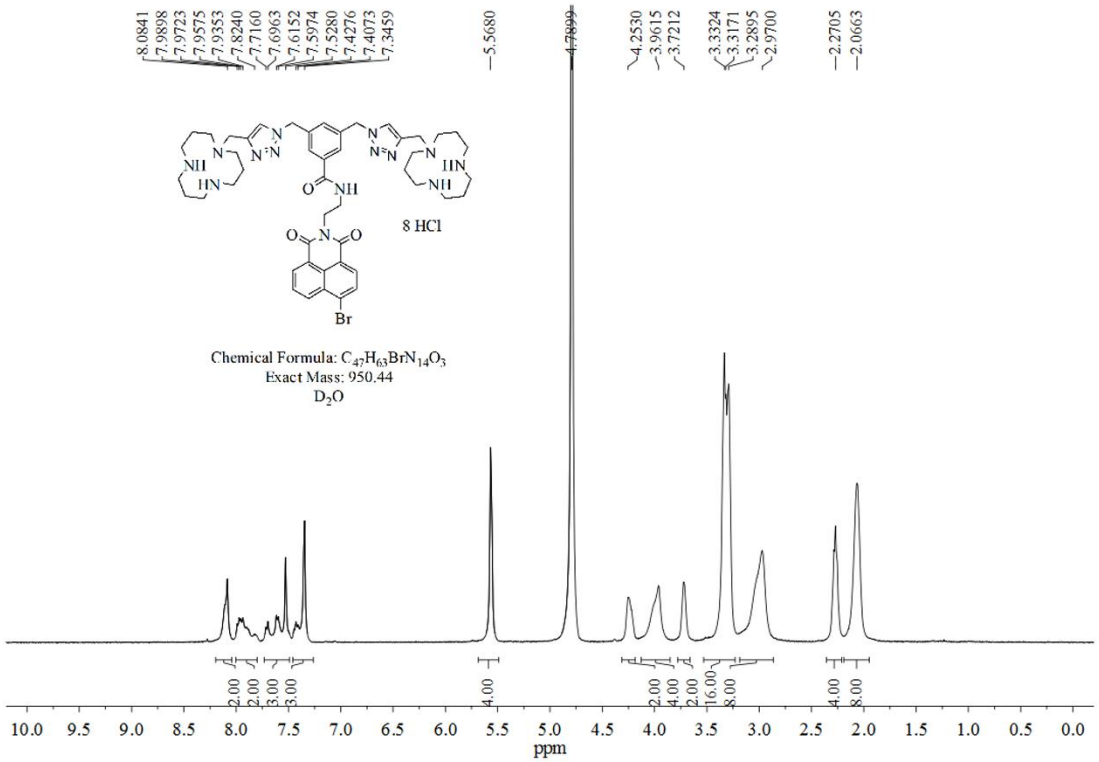
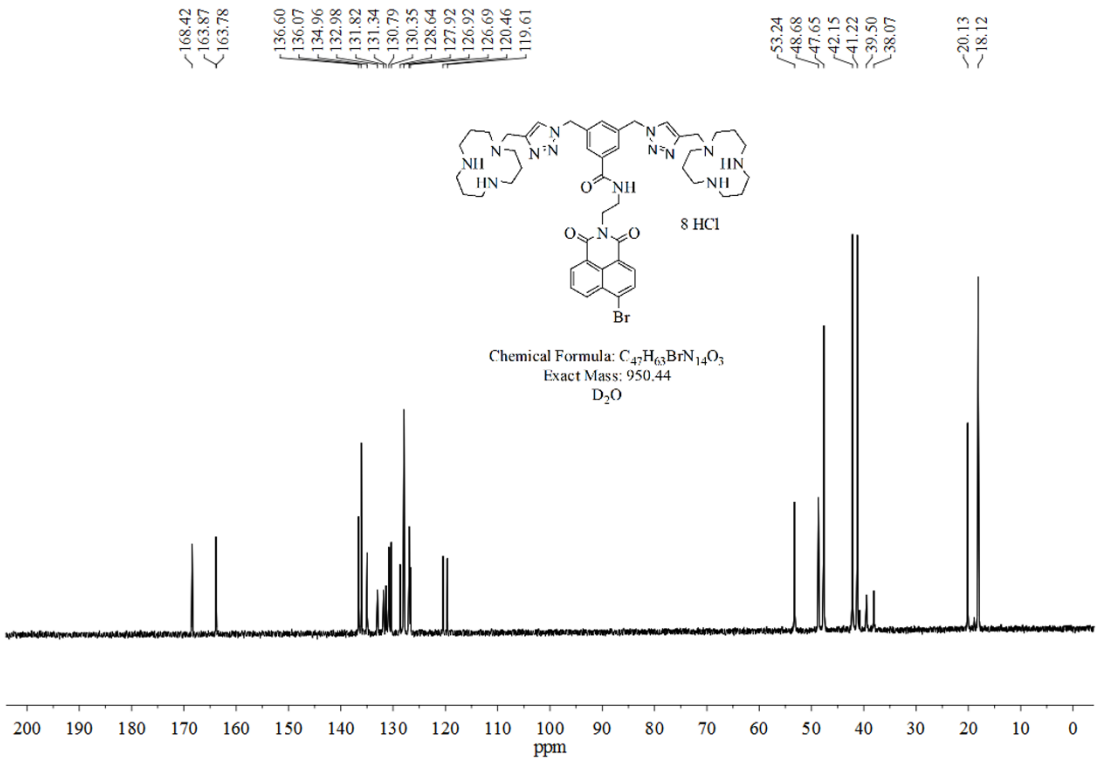
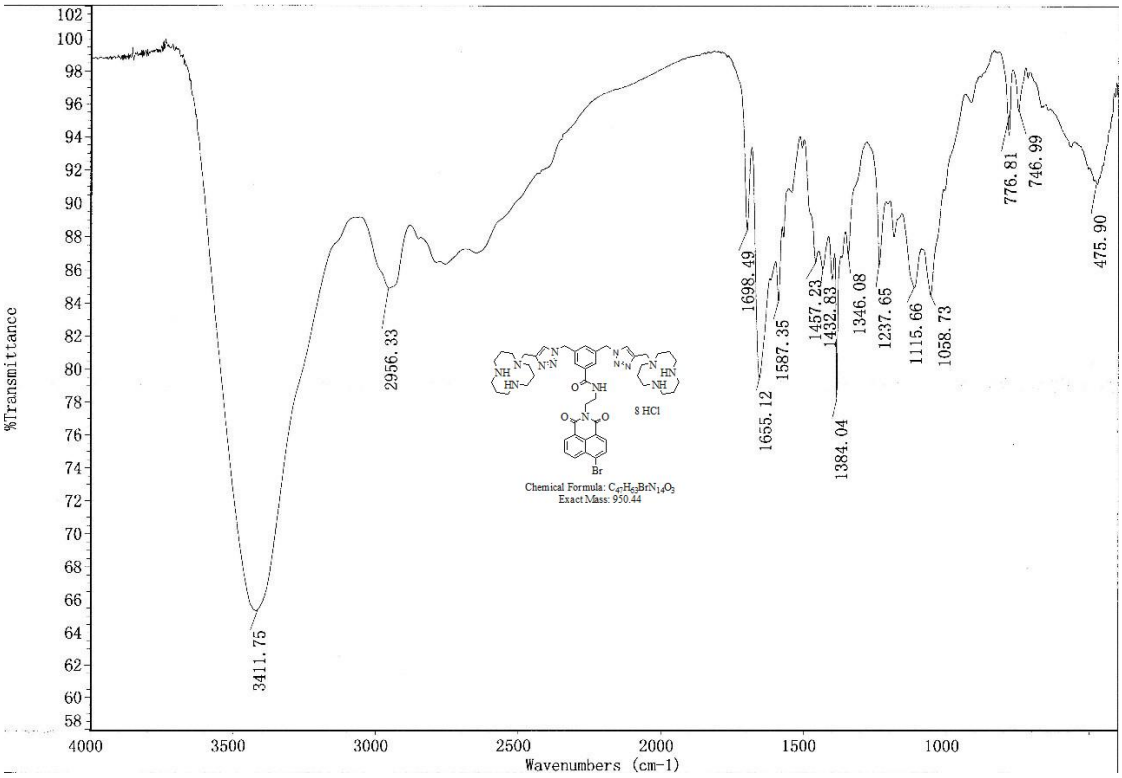
1350.8
1389.2
1390.4
1391.4
1323.2
Chemical Formula: C68H92BrN14O11
Exact Mass: 1350.65

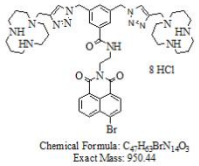

8.0841
7.9898
7.9723
7.9575
7.9353
7.8240
7.7160
7.6963
7.6152
7.5974
7.5280
7.4276
7.4073
7.3459
5.5680
4.7899
4.2530
3.9615
3.7212
3.3324
3.3171
3.2895
2.9700
2.2705
2.0663
8 HCl
Br
Chemical Formula: C47H63BrN14O3
Exact Mass: 950.44
D2O
2.00
2.00
3.00
3.00
4.00
2.00
4.00
2.00
16.00
8.00
4.00
8.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm


168.42
163.87
163.78
136.60
136.07
134.96
132.98
131.82
131.34
130.79
130.35
128.64
127.92
126.92
126.69
120.46
119.61
53.24
48.68
47.65
42.15
41.22
39.50
38.07
20.13
18.12
8 HCl
Br
Chemical Formula: C47H63BrN14O3
Exact Mass: 950.44
D2O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm



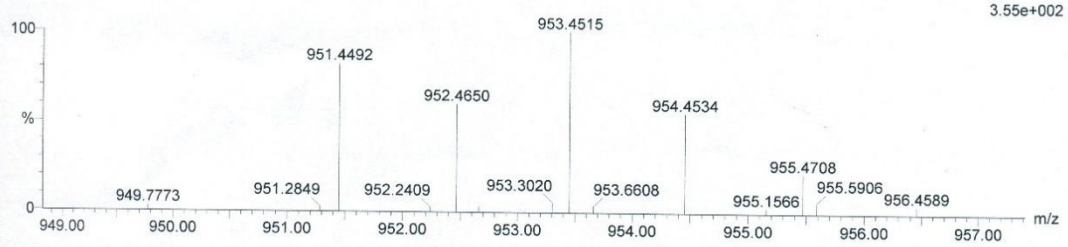
Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 3.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

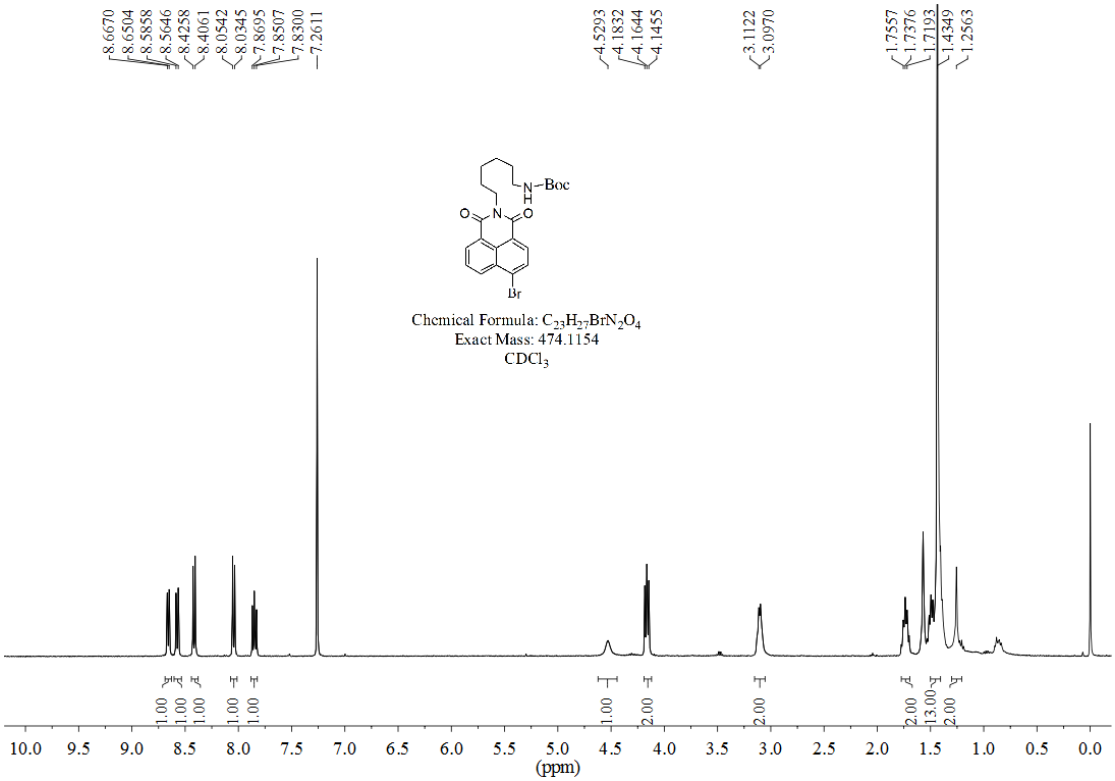


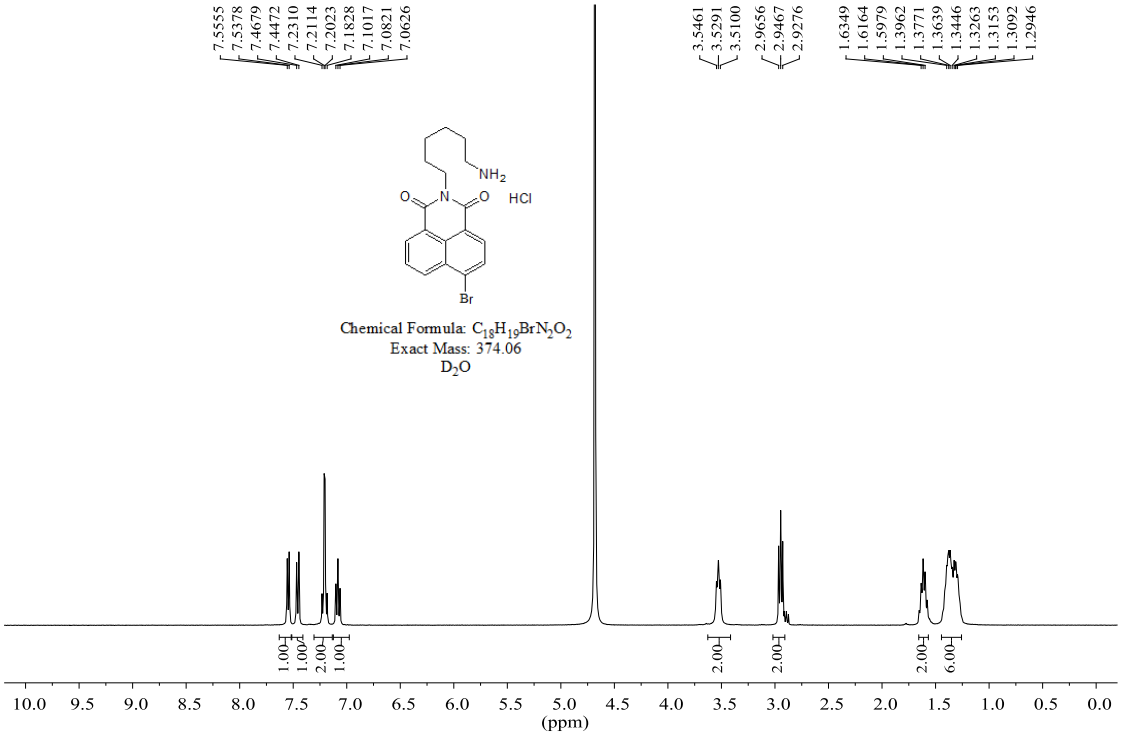
Monoisotopic Mass, Even Electron Ions
855 formula(e) evaluated with 3 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-50 H: 0-70 N: 0-15 O: 0-5 S: 0-2 Br: 0-1

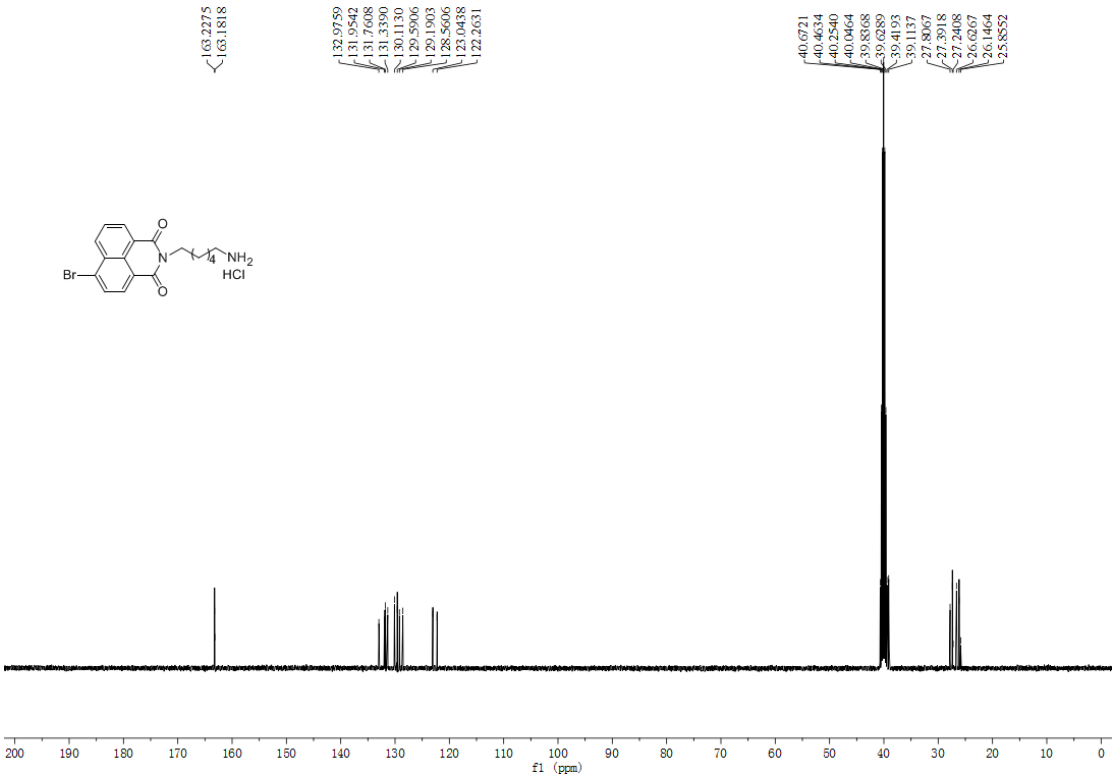
HHY-032 19 (0.351)
TOF MS ES+

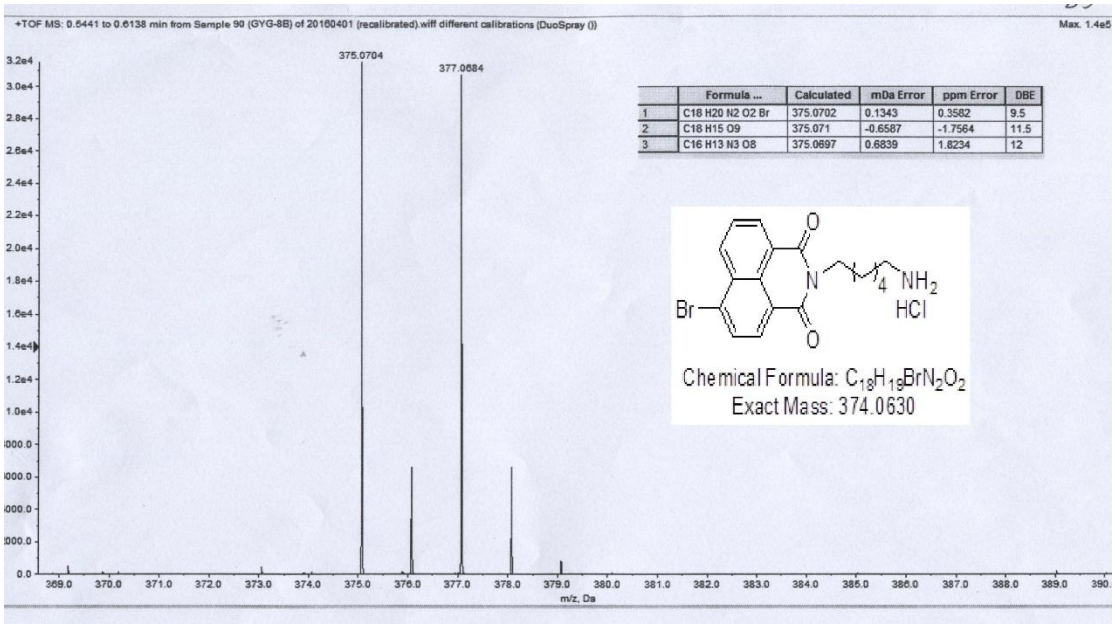


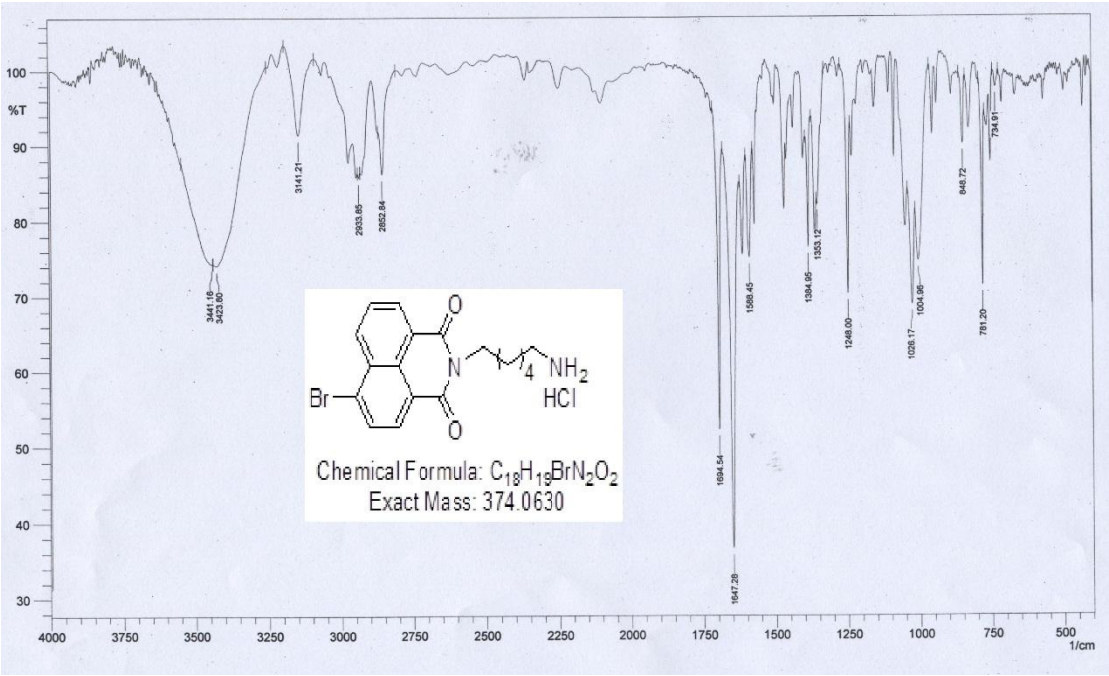
Minimum:				-1.5		
Maximum:		5.0	3.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
951.4492	951.4486	0.6	0.6	23.5	2.2	C48 H63 N12 O5 S2
	951.4503	-1.1	-1.2	17.5	4.1	C44 H68 N14 O3 S Br
	951.4469	2.3	2.4	22.5	3.0	C47 H64 N14 O3 Br

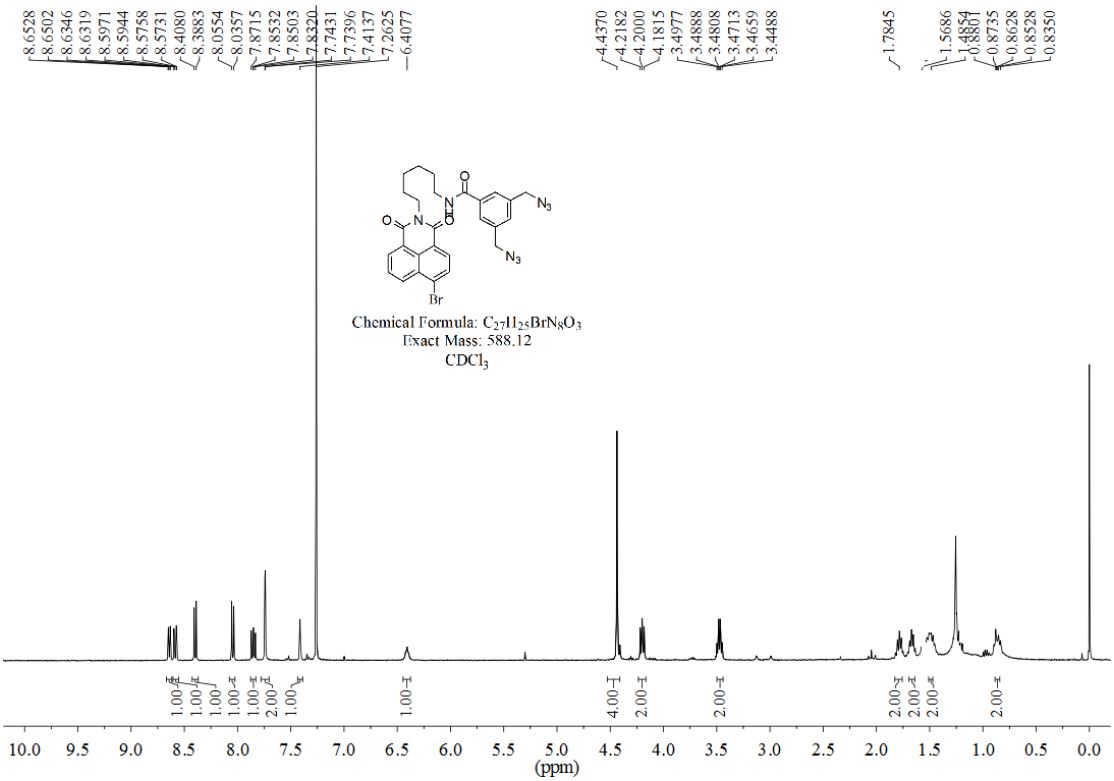

8.6670
8.6504
8.5858
8.5646
8.4258
8.4061
8.0542
8.0345
7.8695
7.8507
7.8300
7.2611
4.5293
4.1832
4.1644
4.1455
3.1122
3.0970
1.7557
1.7376
1.7193
1.4349
1.2563
N–Boc
Br
Chemical Formula: C23H27BrN2O4
Exact Mass: 474.1154
CDCl3
(ppm)

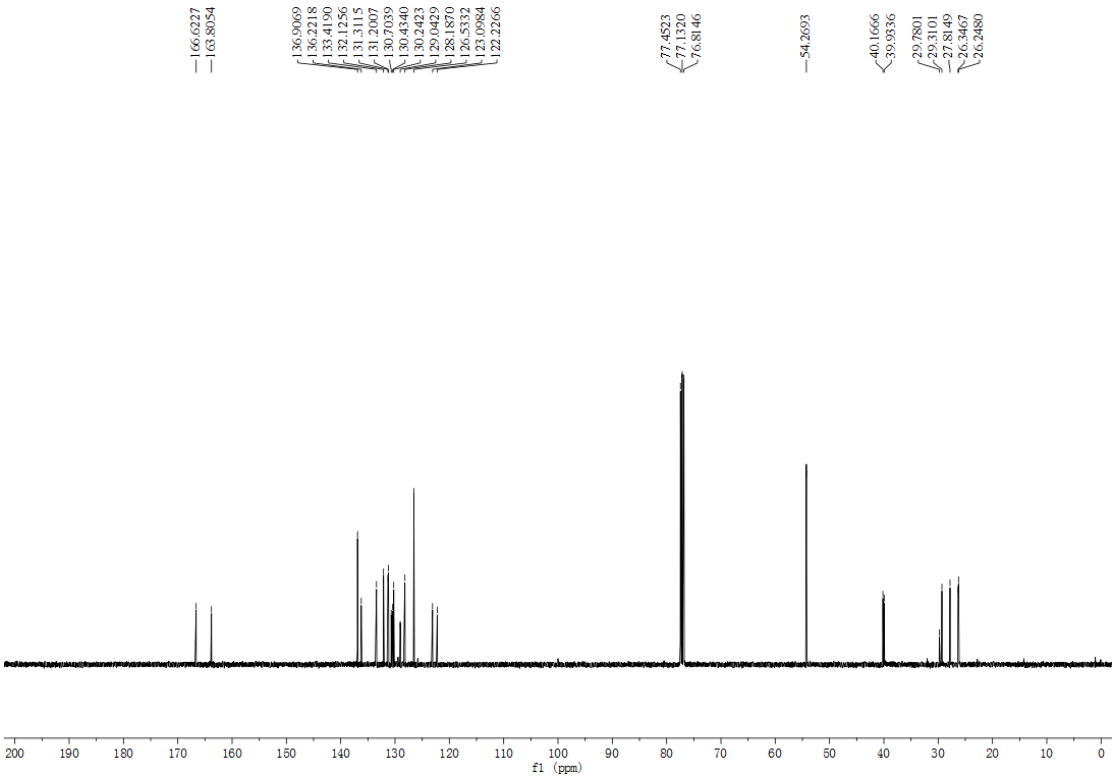

7.5555
7.5378
7.4679
7.4472
7.2310
7.2114
7.2023
7.1828
7.1017
7.0821
7.0626
3.5461
3.5291
3.5100
2.9656
2.9467
2.9276
1.6349
1.6164
1.5979
1.3962
1.3771
1.3639
1.3446
1.3263
1.3153
1.3092
1.2946
NH2
HCl
Br
Chemical Formula: C18H19BrN2O2
Exact Mass: 374.06
D2O
(ppm)

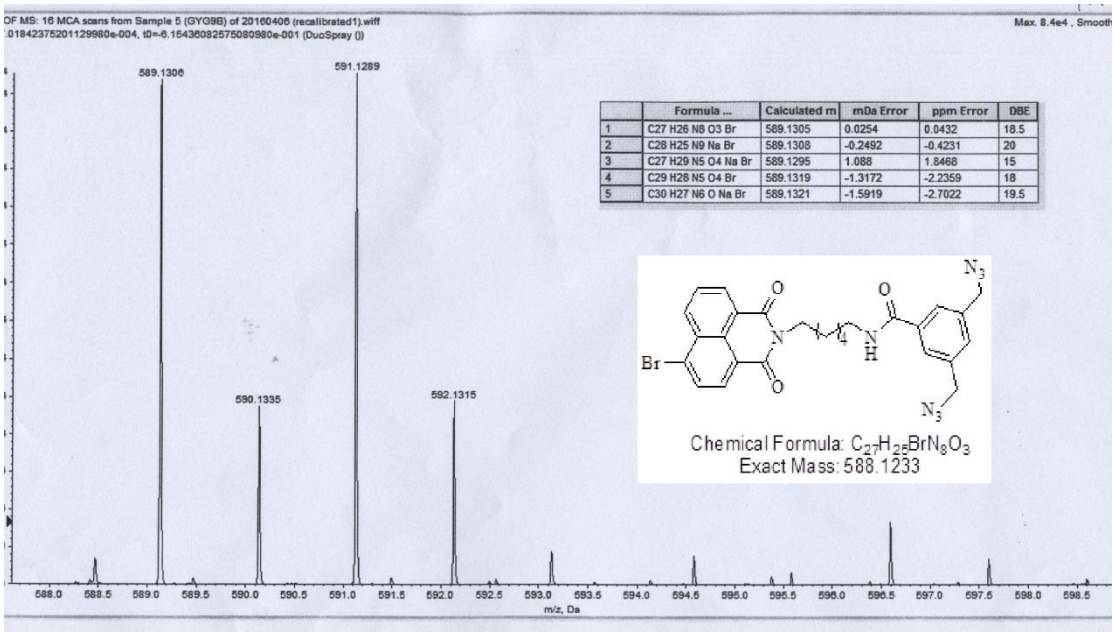

163.2275
163.1818
132.9759
131.9542
131.7608
131.3390
130.1130
129.5906
129.1903
128.5606
123.0438
122.2631
40.6721
40.4634
40.2540
40.0464
39.8368
39.6289
39.4193
39.1137
27.8067
27.3918
27.2408
26.6267
26.1464
25.8852
Br
N
4
NH2
HCl
O
O
f1 (ppm)

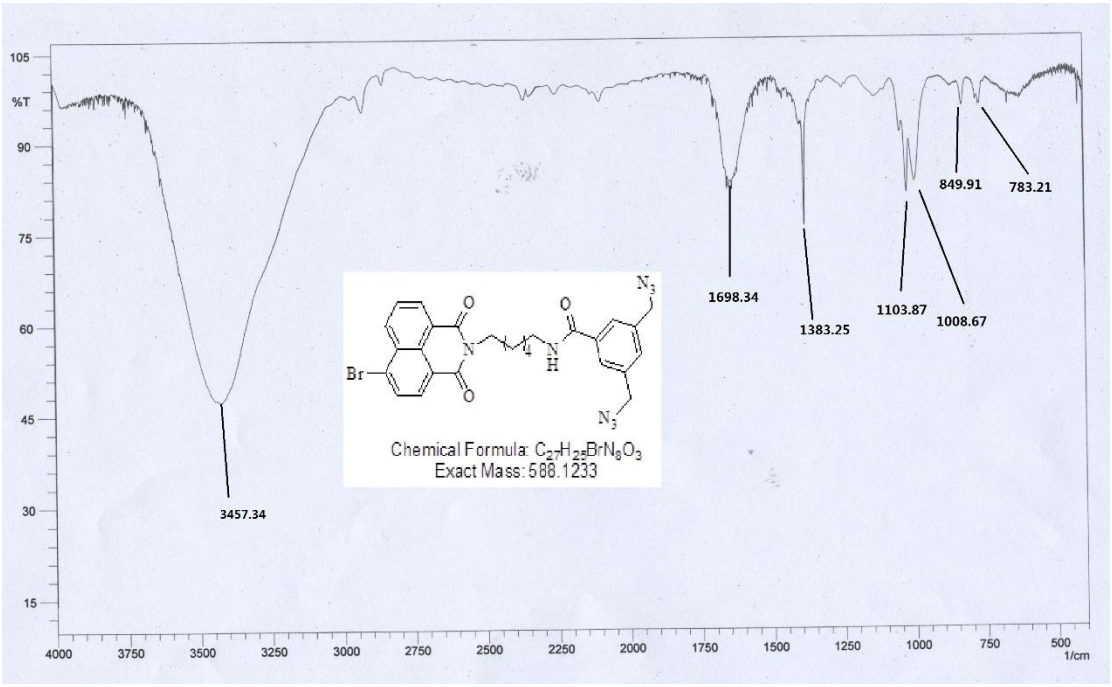

+TOF MS: 0.5441 to 0.6138 min from Sample 90 (GYG-8B) of 20160401 (recalibrated).wiff different calibrations (DuoSpray ())
Max. 1.4e5
375.0704
377.0684
m/z, Da
Formula ... | Calculated | mDa Error | ppm Error | DBE
1 | C18 H20 N2 O2 Br | 375.0702 | 0.1343 | 0.3582 | 9.5
2 | C18 H15 O9 | 375.071 | -0.6587 | -1.7564 | 11.5
3 | C16 H13 N3 O8 | 375.0697 | 0.6839 | 1.8234 | 12
Br
N
4
NH2
HCl
O
O
Chemical Formula: C18H19BrN2O2
Exact Mass: 374.0630

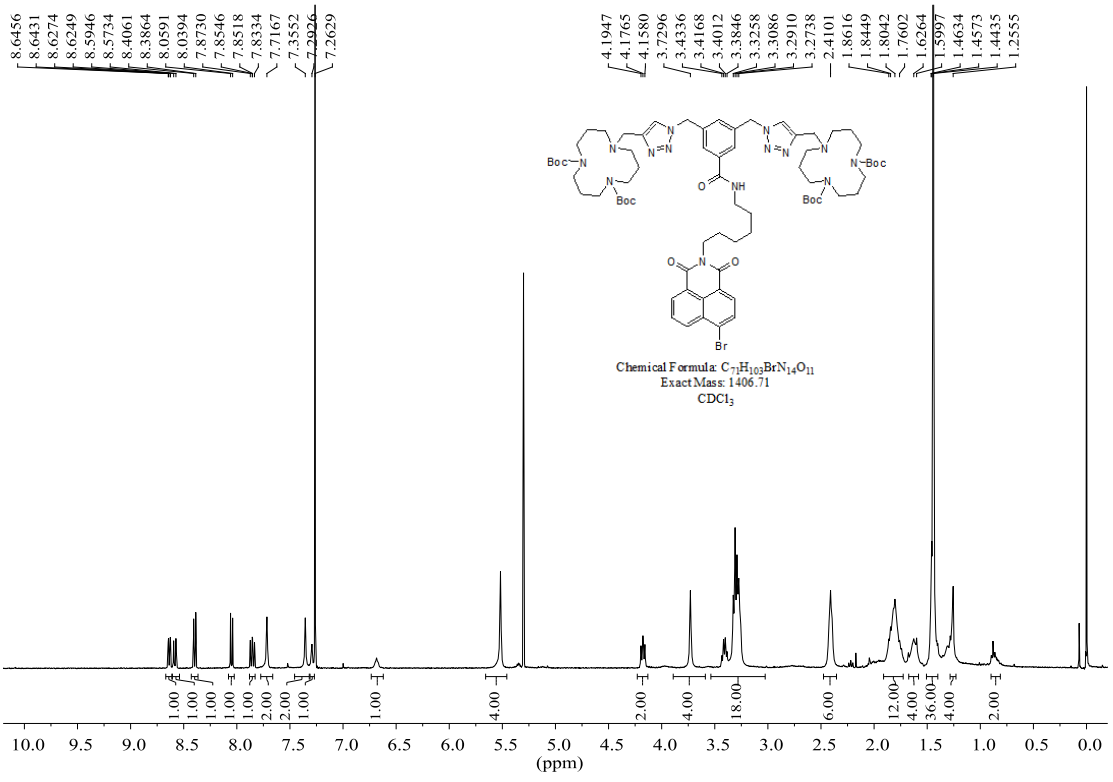

%T
100
90
80
70
60
50
40
30
4000
3750
3500
3250
3000
2750
2500
2250
2000
1750
1500
1250
1000
750
500
1/cm
3441.16
3420.80
3141.21
2933.85
2852.84
1694.54
1647.28
1588.45
1384.65
1353.12
1248.00
1028.17
1004.96
848.72
781.20
734.91
Br
O
N
4
NH2
HCl
Chemical Formula: C18H19BrN2O2
Exact Mass: 374.0630

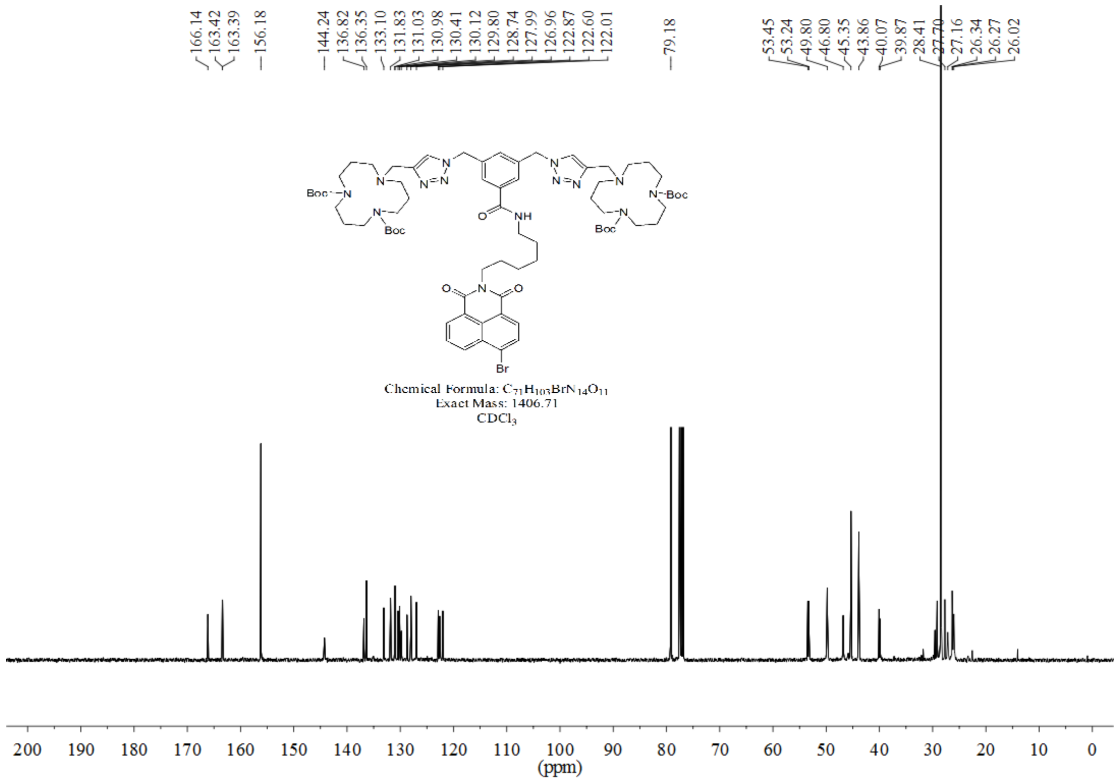

8.6528
8.6502
8.6346
8.6319
8.5971
8.5944
8.5758
8.5731
8.4080
8.3883
8.0554
8.0357
7.8715
7.8532
7.8503
7.8320
7.7431
7.7396
7.4137
7.2625
6.4077
4.4370
4.2182
4.2000
4.1815
3.4977
3.4888
3.4808
3.4713
3.4659
3.4488
1.7845
1.5686
1.4854
0.8801
0.8735
0.8628
0.8528
0.8350
N3
N3
Br
Chemical Formula: C27H25BrN8O3
Exact Mass: 588.12
CDCl3
1.00
1.00
1.00
1.00
2.00
1.00
1.00
4.00
2.00
2.00
2.00
2.00
2.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
(ppm)

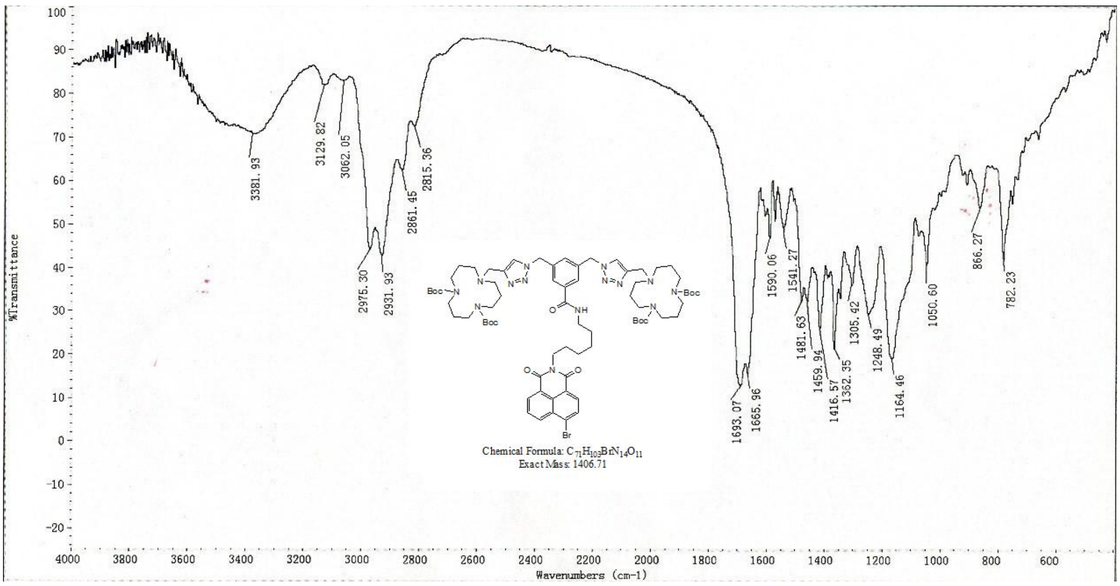

166.6227
163.8054
136.9069
136.2218
133.4190
132.1256
131.3115
131.2007
130.7039
130.4340
130.2423
129.0429
128.1870
126.5332
123.0984
122.2266
77.4523
77.1320
76.8146
54.2693
40.1666
39.9336
29.7801
29.3101
27.8149
26.3467
26.2480
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

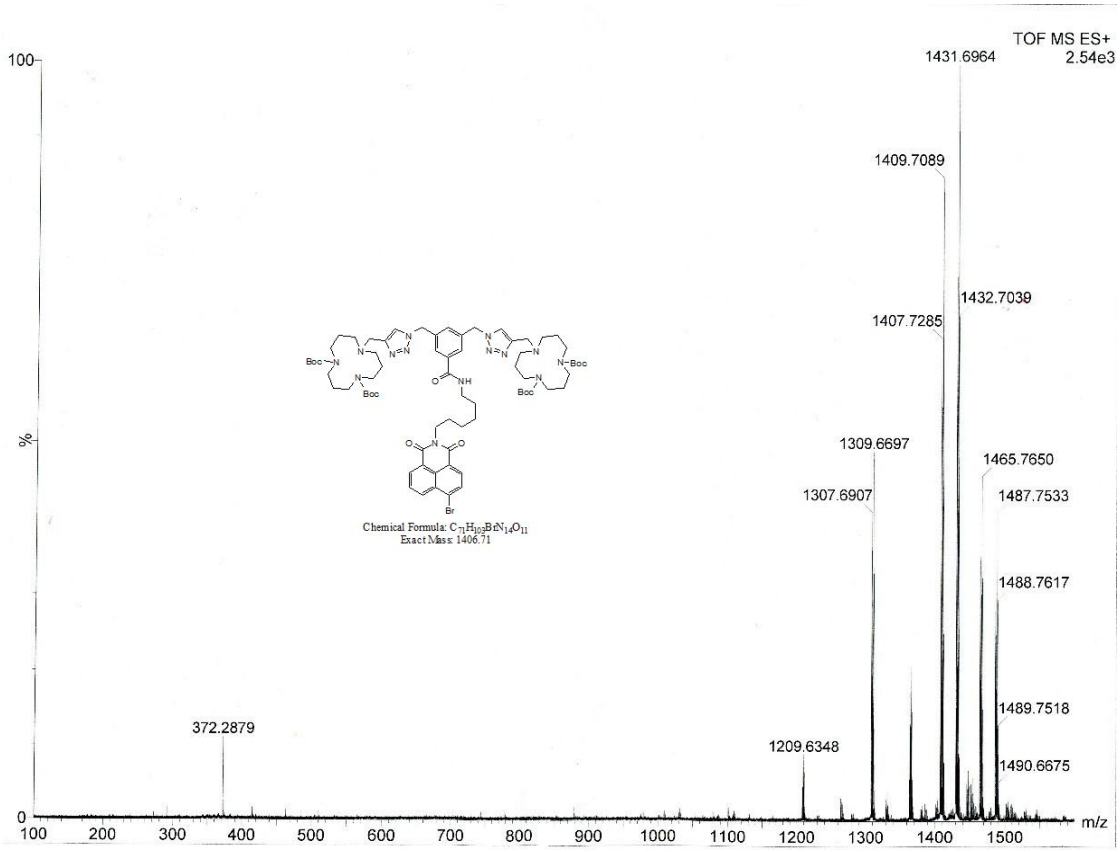

OF MS: 16 MCA scans from Sample 5 (GYG9B) of 20160406 (recalibrated1).wiff
.018423752011299 80e-004, t0=-6.154360825750809 80e-001 (DuoSpray ())
Max. 8.4e4 , Smooth
589.1306
591.1289
590.1335
592.1315
Formula ... | Calculated m | mDa Error | ppm Error | DBE
1 | C27 H26 N8 O3 Br | 589.1305 | 0.0254 | 0.0432 | 18.5
2 | C28 H25 N9 Na Br | 589.1308 | -0.2492 | -0.4231 | 20
3 | C27 H29 N5 O4 Na Br | 589.1295 | 1.088 | 1.8468 | 15
4 | C29 H28 N5 O4 Br | 589.1319 | -1.3172 | -2.2359 | 18
5 | C30 H27 N6 O Na Br | 589.1321 | -1.5919 | -2.7022 | 19.5
Br
O
N
4
N
H
O
O
N3
N3
Chemical Formula: C27H25BrN8O3
Exact Mass: 588.1233
588.0 588.5 589.0 589.5 590.0 590.5 591.0 591.5 592.0 592.5 593.0 593.5 594.0 594.5 595.0 595.5 596.0 596.5 597.0 597.5 598.0 598.5
m/z, Da

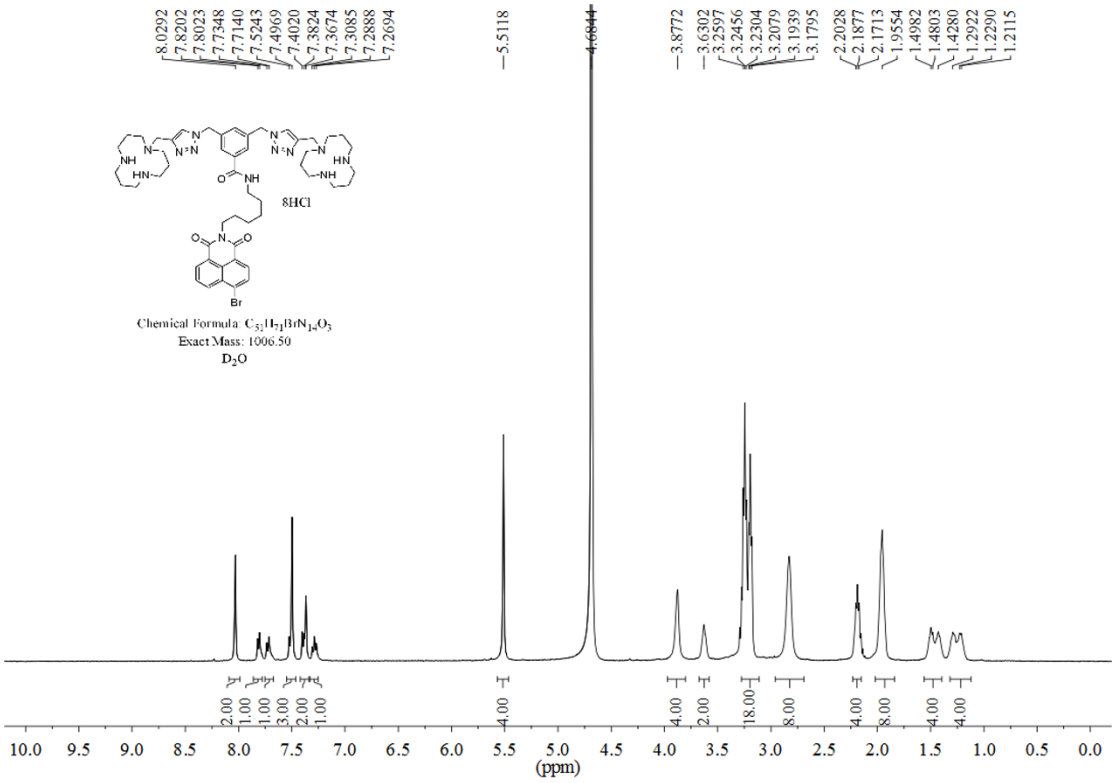

%T
105
90
75
60
45
30
15
4000
3750
3500
3250
3000
2750
2500
2250
2000
1750
1500
1250
1000
750
500
1/cm
3457.34
1698.34
1383.25
1103.87
1008.67
849.91
783.21
Chemical Formula: C27H25BrN8O3
Exact Mass: 588.1233

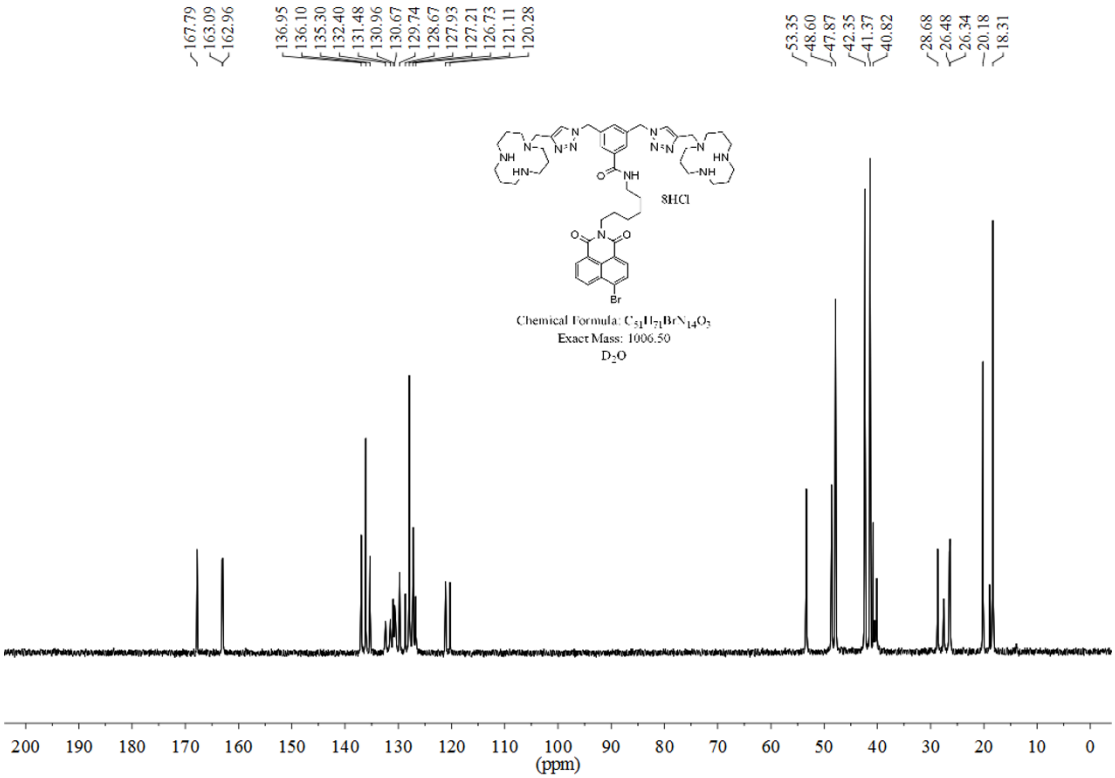

8.6456
8.6431
8.6274
8.6249
8.5946
8.5734
8.4061
8.3864
8.0591
8.0394
7.8730
7.8546
7.8518
7.8334
7.7167
7.3552
7.2926
7.2629
4.1947
4.1765
4.1580
3.7296
3.4336
3.4168
3.4012
3.3846
3.3258
3.3086
3.2910
3.2738
2.4101
1.8616
1.8449
1.8042
1.7602
1.6264
1.5997
1.4634
1.4573
1.4435
1.2555
Chemical Formula: C71H103BrN14O11
Exact Mass: 1406.71
CDCl3
1.00
1.00
1.00
1.00
1.00
1.00
2.00
2.00
1.00
1.00
4.00
2.00
4.00
18.00
6.00
12.00
4.00
36.00
4.00
2.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
(ppm)

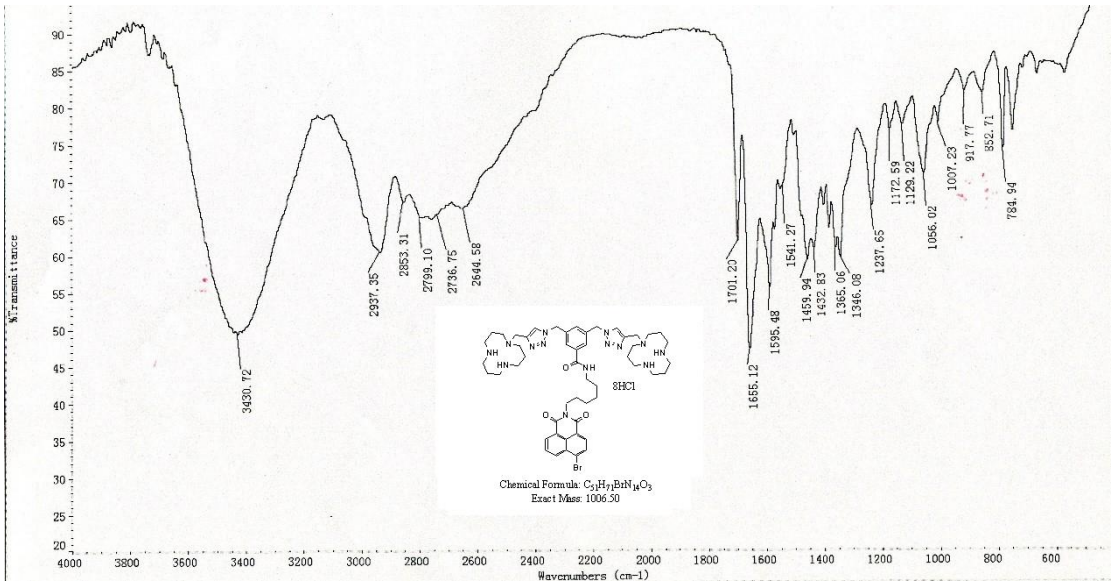

166.14
163.42
163.39
156.18
144.24
136.82
136.35
133.10
131.83
131.03
130.98
130.41
130.12
129.80
128.74
127.99
126.96
122.87
122.60
122.01
79.18
53.45
53.24
49.80
46.80
45.35
43.86
40.07
39.87
28.41
27.70
27.16
26.34
26.27
26.02
Chemical Formula: $C_{71}H_{103}BrN_{14}O_{11}$
Exact Mass: 1406.71
$CDCl_3$
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)


%Transmittance
Wavenumbers (cm-1)
3381.93
3129.82
3062.05
2975.30
2931.93
2861.45
2815.36
1693.07
1665.96
1590.06
1541.27
1481.63
1459.94
1416.57
1362.35
1305.42
1248.49
1164.46
1050.60
866.27
782.23
Chemical Formula: $C_{71}H_{103}BrN_{14}O_{11}$
Exact Mass: 1406.71


TOF MS ES+
2.54e3
1431.6964
1409.7089
1432.7039
1407.7285
1309.6697
1465.7650
1307.6907
1487.7533
1488.7617
1489.7518
372.2879
1209.6348
1490.6675
%
m/z
Chemical Formula: C71H103BrN14O11
Exact Mass: 1406.71


8HCl
Chemical Formula: C51H71BrN14O3
Exact Mass: 1006.50
D2O
(ppm)

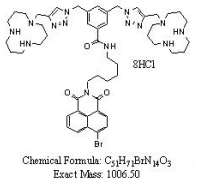

167.79
163.09
162.96
136.95
136.10
135.30
132.40
131.48
130.96
130.67
129.74
128.67
127.93
127.21
126.73
121.11
120.28
53.35
48.60
47.87
42.35
41.37
40.82
28.68
26.48
26.34
20.18
18.31
8HCl
Br
Chemical Formula: C51H71BrN14O5
Exact Mass: 1006.50
D2O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)


%Transmittance
3430.72
2937.35
2853.31
2799.10
2736.75
2644.58
1701.20
1655.12
1595.48
1541.27
1459.94
1432.83
1365.06
1346.08
1237.65
1172.59
1129.22
1056.02
1007.23
917.77
852.71
784.94
8HCl
Br
Chemical Formula: C51H71BrN14O5
Exact Mass: 1006.50
4000 3800 3600 3400 3200 3000 2800 2600 2400 2200 2000 1800 1600 1400 1200 1000 800 600
Wavenumbers (cm-1)

Elemental Composition Report **Page 1**

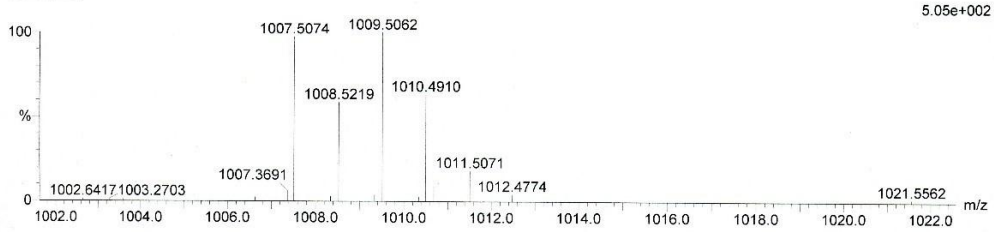
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
695 formula(e) evaluated with 6 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-55 H: 0-80 N: 0-15 O: 0-10 Br: 0-1

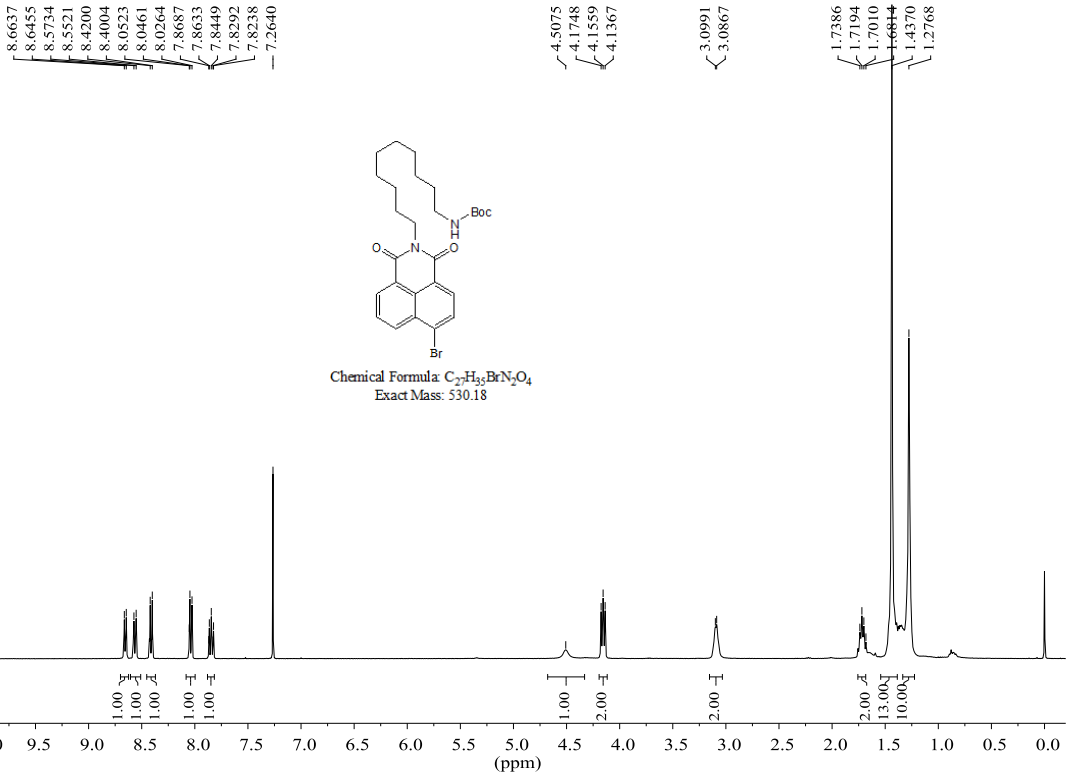


Chemical Formula: $C_{51}H_{71}BrN_{14}O_3$
Exact Mass: 1006.50

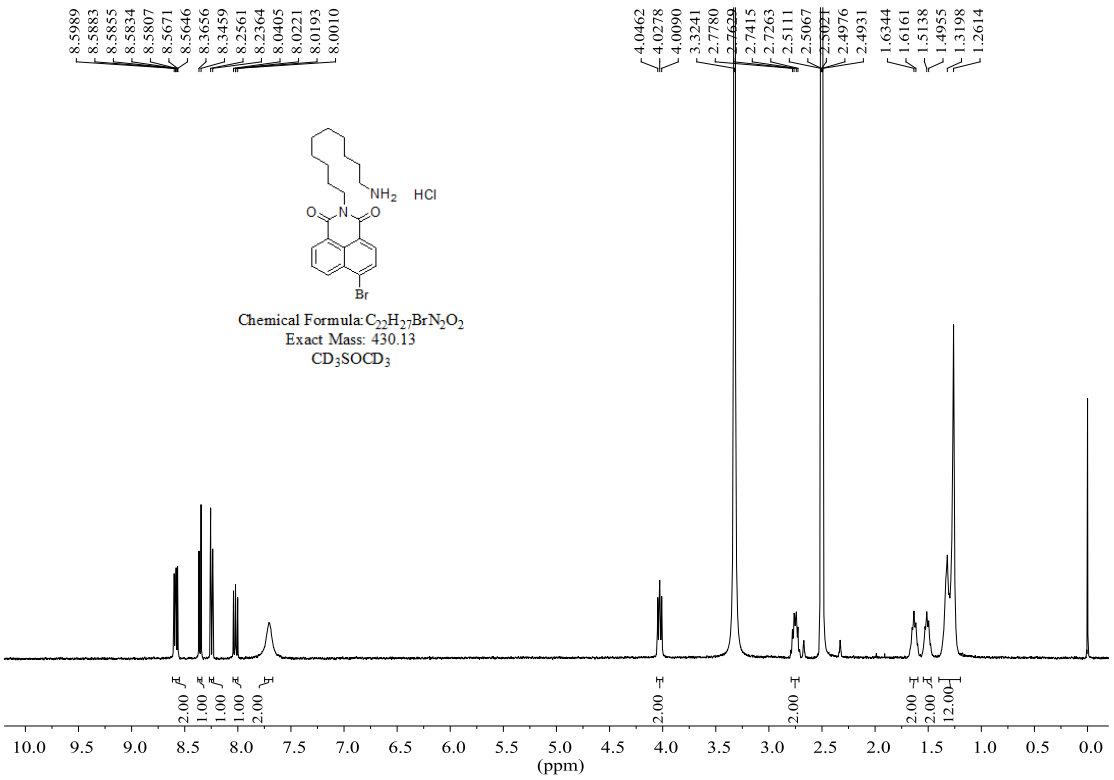
HYY-053 24 (0.444)
TOF MS ES+

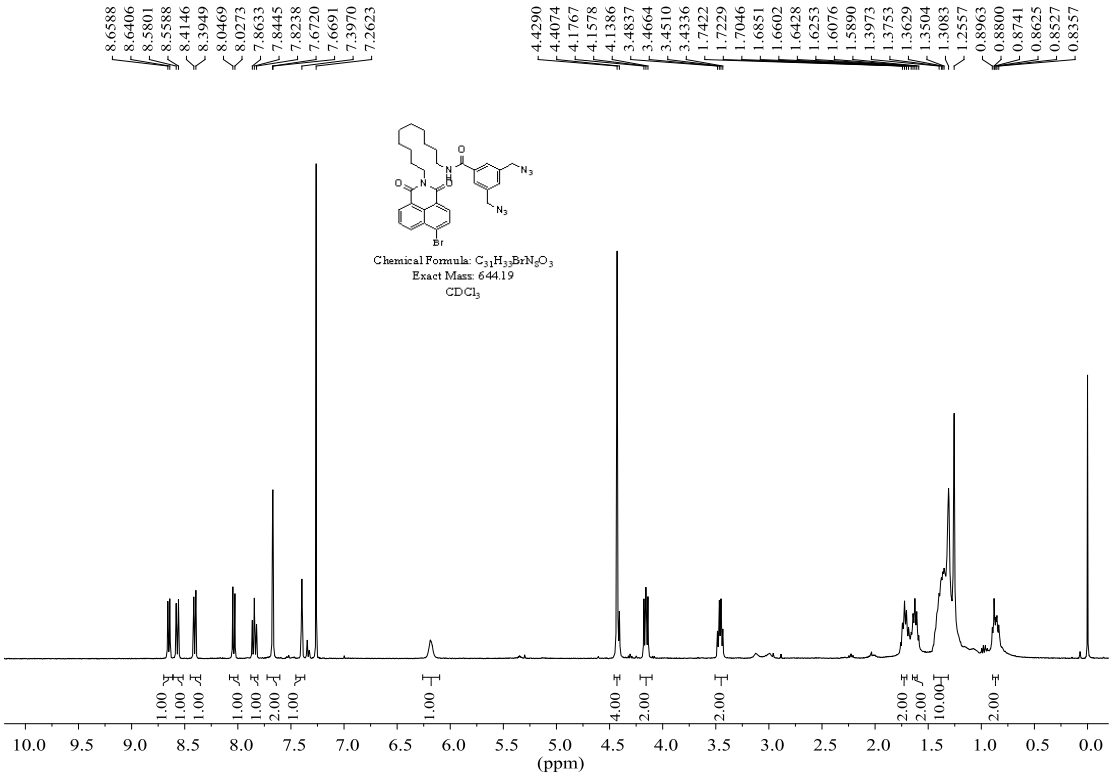


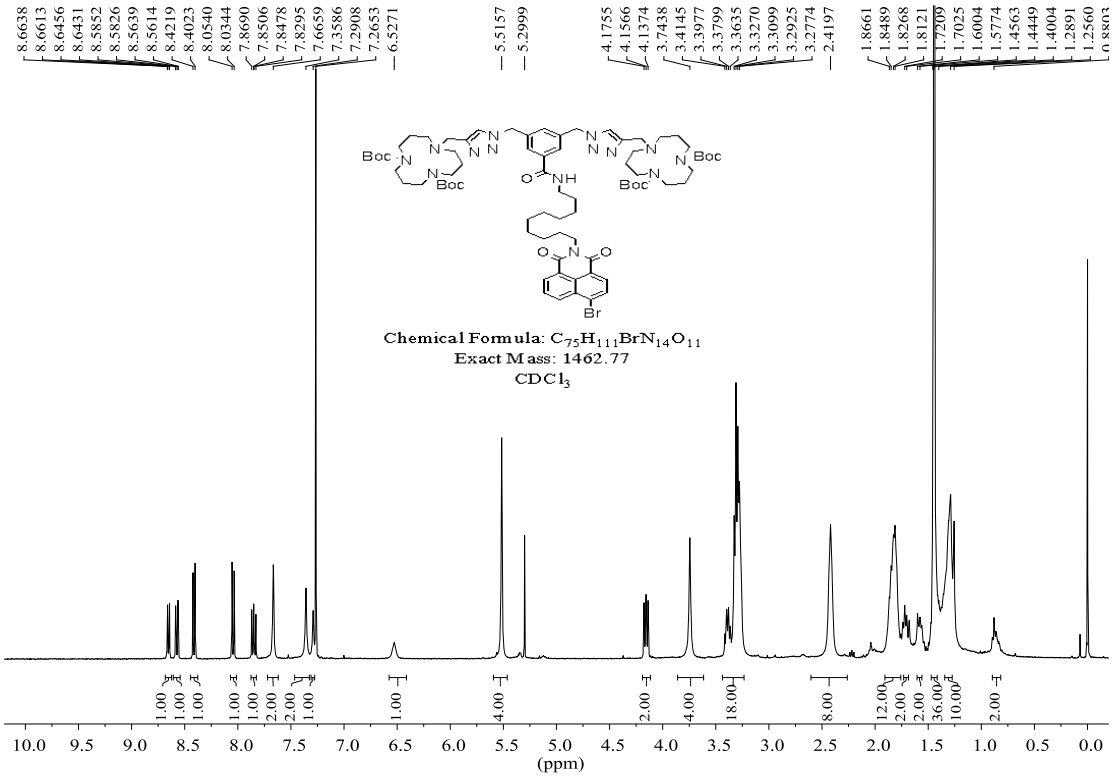
Minimum:				-1.5		
Maximum:		5.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
1007.5074	1007.5082	-0.8	-0.8	17.5	0.1	C50 H76 N10 O7 Br
	1007.5095	-2.1	-2.1	22.5	0.3	C51 H72 N14 O3 Br
	1007.5103	-2.9	-2.9	24.5	0.2	C51 H67 N12 O10
	1007.5042	3.2	3.2	13.5	0.7	C45 H76 N12 O9 Br
	1007.5109	-3.5	-3.5	16.5	0.3	C54 H80 N4 O9 Br
	1007.5122	-4.8	-4.8	21.5	0.7	C55 H76 N8 O5 Br

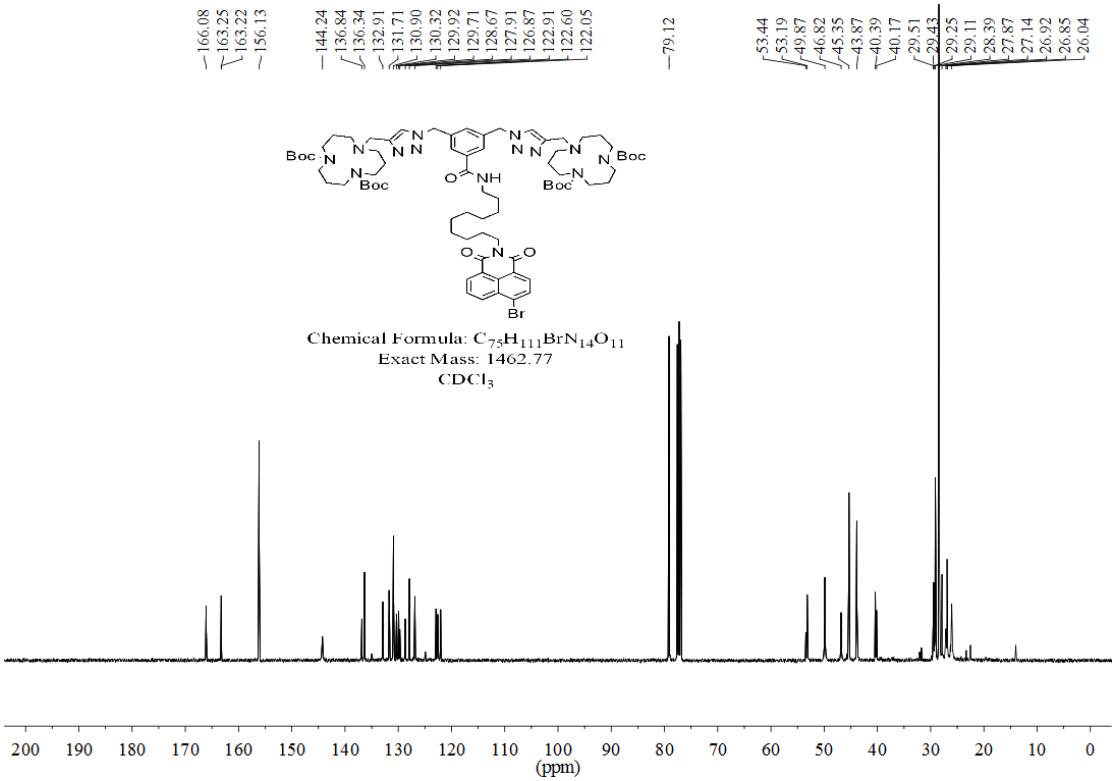


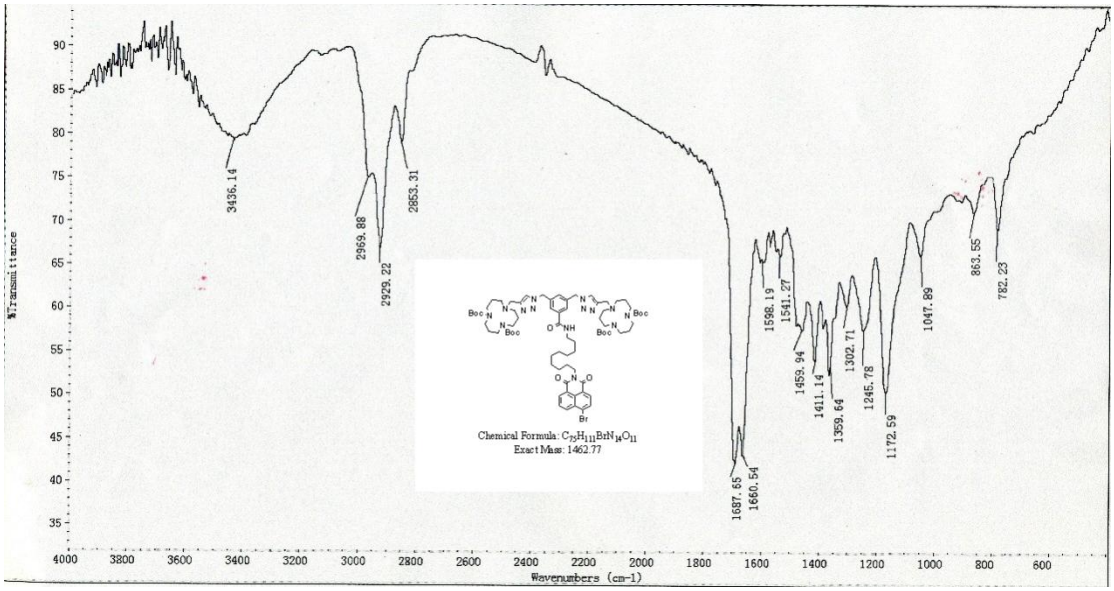
Chemical Formula: $C_{27}H_{35}BrN_2O_4$
Exact Mass: 530.18

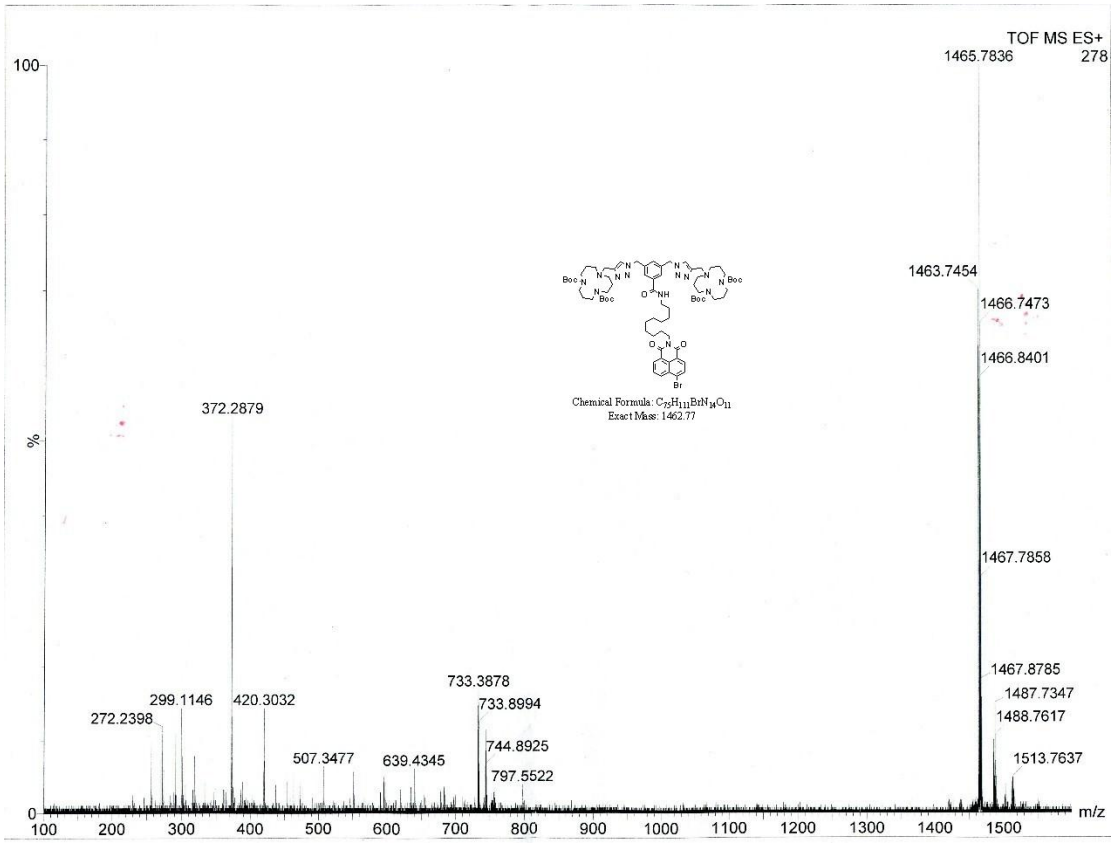

8.5989
8.5883
8.5855
8.5834
8.5807
8.5671
8.5646
8.3656
8.3459
8.2561
8.2364
8.0405
8.0221
8.0193
8.0010
4.0462
4.0278
4.0090
3.3241
2.7780
2.7629
2.7415
2.7263
2.5111
2.5067
2.5027
2.4976
2.4931
1.6344
1.6161
1.5138
1.4955
1.3198
1.2614
NH2 HCl
O
N
O
Br
Chemical Formula: C22H27BrN2O2
Exact Mass: 430.13
CD3SOCD3
2.00
1.00
1.00
1.00
2.00
2.00
2.00
2.00
2.00
12.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)

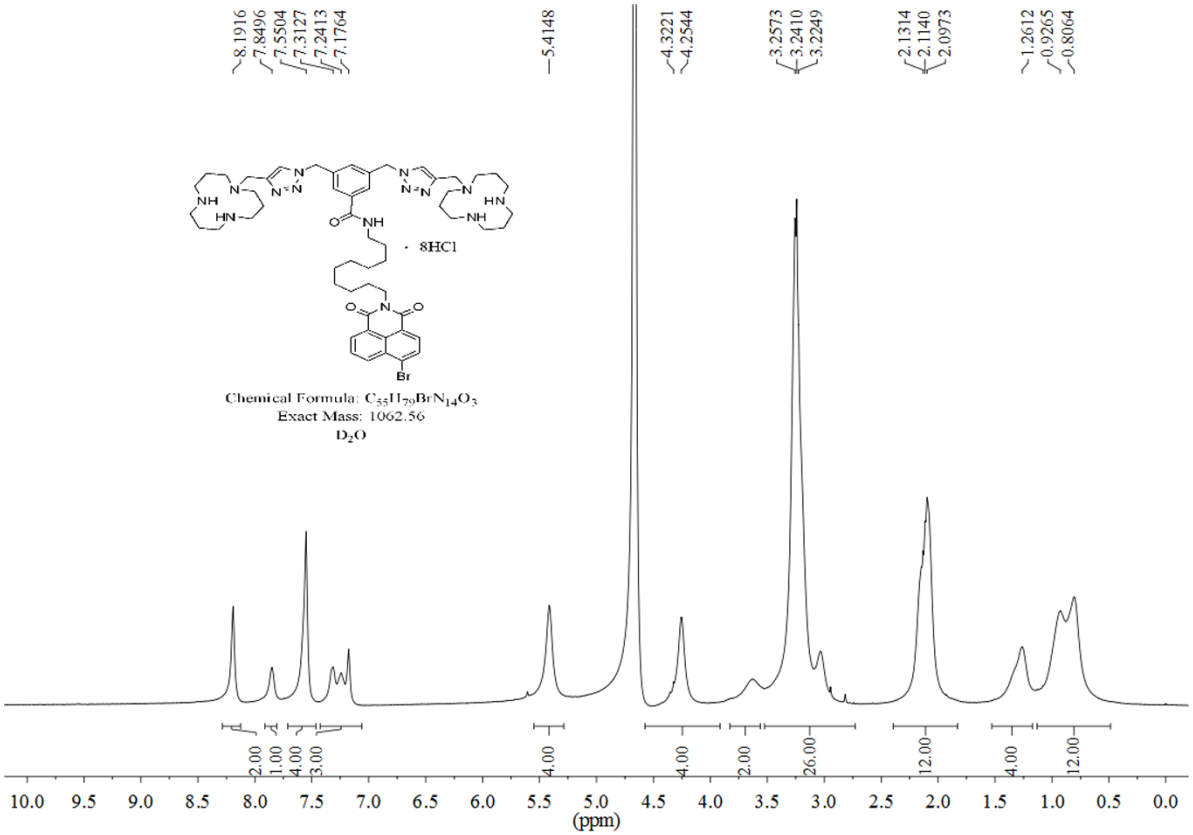

8.6588
8.6406
8.5801
8.5588
8.4146
8.3949
8.0469
8.0273
7.8633
7.8445
7.8238
7.6720
7.6691
7.3970
7.2623
4.4290
4.4074
4.1767
4.1578
4.1386
3.4837
3.4664
3.4510
3.4336
1.7422
1.7229
1.7046
1.6851
1.6602
1.6428
1.6253
1.6076
1.5890
1.3973
1.3753
1.3629
1.3504
1.3083
1.2557
0.8963
0.8800
0.8741
0.8625
0.8527
0.8357
O
N
O
N3
N3
Br
Chemical Formula: C31H33BrN6O3
Exact Mass: 644.19
CDCl3
1.00
1.00
1.00
1.00
1.00
2.00
1.00
1.00
4.00
2.00
2.00
2.00
2.00
10.00
2.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)

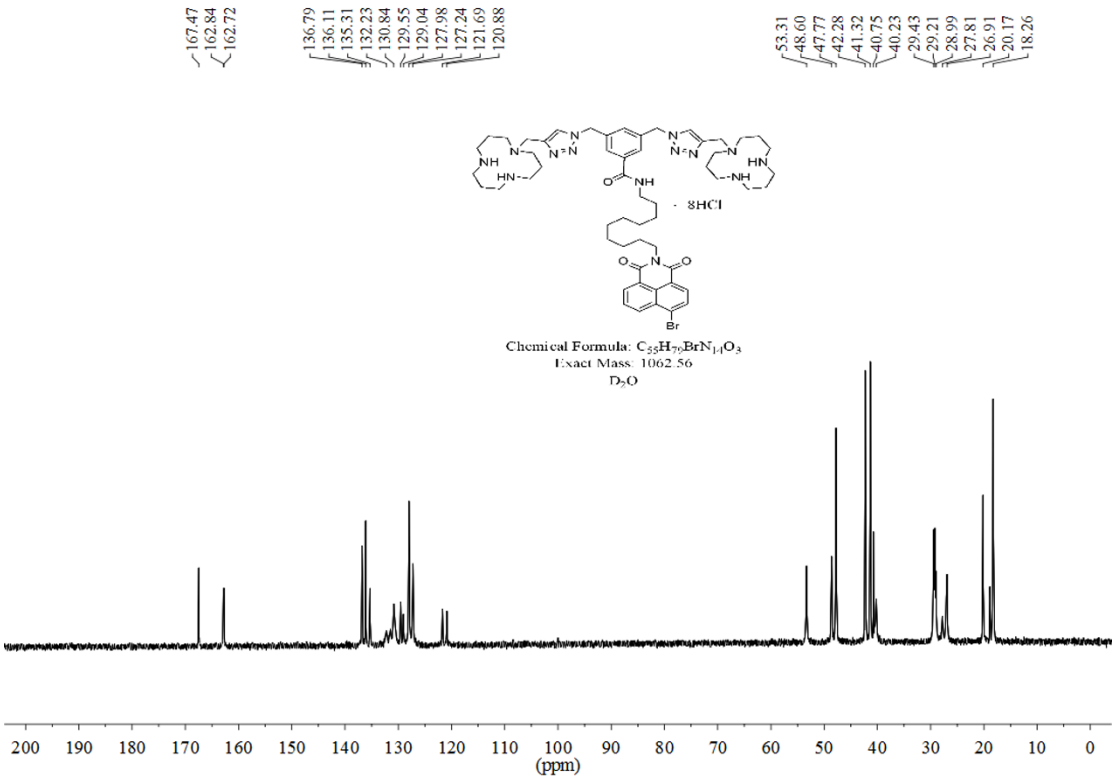

Chemical Formula: $C_{75}H_{111}BrN_{14}O_{11}$
Exact Mass: 1462.77
$CDCl_3$
(ppm)

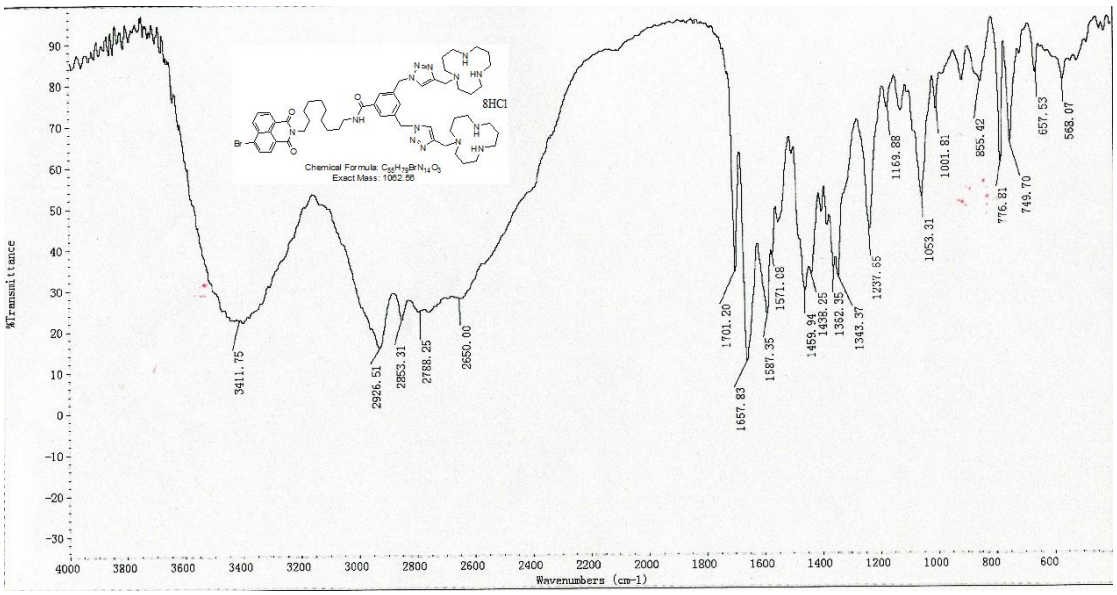

Chemical Formula: $C_{75}H_{111}BrN_{14}O_{11}$
Exact Mass: 1462.77
$CDCl_3$
(ppm)


%Transmittance
Wavenumbers (cm-1)
3436.14
2969.88
2929.22
2853.31
1687.65
1660.54
1598.19
1541.27
1459.94
1411.14
1359.64
1302.71
1245.78
1172.59
1047.89
863.55
782.23
Chemical Formula: C75H111BrN14O11
Exact Mass: 1462.77


TOF MS ES+
278
%
m/z
1465.7836
1463.7454
1466.7473
1466.8401
1467.7858
1467.8785
1487.7347
1488.7617
1513.7637
372.2879
733.3878
733.8994
299.1146
420.3032
272.2398
507.3477
639.4345
744.8925
797.5522
Chemical Formula: C75H111BrN14O11
Exact Mass: 1462.77


8.1916
7.8496
7.5504
7.3127
7.2413
7.1764
5.4148
4.3221
4.2544
3.2573
3.2410
3.2249
2.1314
2.1140
2.0973
1.2612
0.9265
0.8064
· 8HCl
Chemical Formula: C55H79BrN14O3
Exact Mass: 1062.56
D2O
2.00
1.00
4.00
3.00
4.00
4.00
2.00
26.00
12.00
4.00
12.00
(ppm)


167.47
162.84
162.72
136.79
136.11
135.31
132.23
130.84
129.55
129.04
127.98
127.24
121.69
120.88
53.31
48.60
47.77
42.28
41.32
40.75
40.23
29.43
29.21
28.99
27.81
26.91
20.17
18.26
· 8HCl
Chemical Formula: C55H79BrN14O3
Exact Mass: 1062.56
D2O
(ppm)

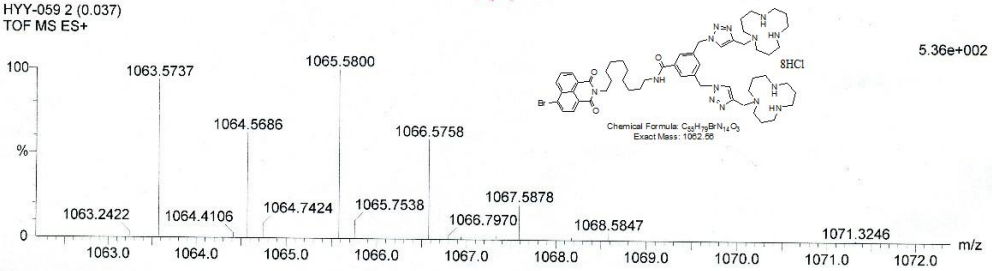


Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
447 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-55 H: 0-80 N: 0-15 O: 0-10 Br: 0-1

HYY-059 2 (0.037)
TOF MS ES+



Minimum:				-1.5		
Maximum:		5.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
1063.5737	1063.5729	0.8	0.8	24.5	0.1	C55 H75 N12 O10
	1063.5721	1.6	1.5	22.5	0.1	C55 H80 N14 O3 Br