

Rational Optimization and Action Mechanism of Novel Imidazole (or Imidazolium)-Labeled 1,3,4-Oxadiazole Thioethers as Promising Antibacterial Agents Against Plant Bacterial Diseases

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1. Characterization data for tatget compounds

2-((5-(1*H*-imidazol-1-yl)pentyl)thio)-5-(2,4-dichlorophenyl)-1,3,4-oxadiazole (A₅)

A light yellow liquid, yield 67.9%; ¹H NMR (500 MHz, CDCl₃) δ 7.89 (d, *J* = 8.5 Hz, 1H, Ar-6-H), 7.55 (d, *J* = 2.0 Hz, 1H, Ar-3-H), 7.46 (s, 1H, Imidazole-2-H), 7.38 (dd, *J* = 8.5, 2.1 Hz, 1H, Ar-5-H), 7.05 (s, 1H, Imidazole-5-H), 6.90 (s, 1H, Imidazole-4-H), 3.95 (t, *J* = 7.0 Hz, 2H, N-CH₂), 3.26 (t, *J* = 7.1 Hz, 2H, S-CH₂), 1.92-1.80 (m, 4H, N-CH₂CH₂ & S-CH₂CH₂), 1.49-1.43 (m, 2H, S-(CH₂)₂CH₂); ¹³C NMR (126 MHz, CDCl₃) δ 165.3, 163.4, 138.2, 137.2, 133.8, 131.7, 131.3, 129.7, 127.7, 121.5, 118.8, 46.8, 32.3, 30.6, 28.9, 25.6; HRMS (ESI) [M+H]⁺calcd for C₁₆H₁₆Cl₂N₄OS: 383.0495, found: 383.0488.

2-((6-(1*H*-imidazol-1-yl)hexyl)thio)-5-(2,4-dichlorophenyl)-1,3,4-oxadiazole (A₆)

A yellow liquid, yield 49.1%; ¹H NMR (500 MHz, CDCl₃) δ 7.85 (d, *J* = 8.5 Hz, 1H, Ar-6-H), 7.51 (d, *J* = 1.9 Hz, 1H, Ar-3-H), 7.41 (s, 1H, Imidazole-2-H), 7.33 (dd, *J* = 8.4, 2.0 Hz, 1H, Ar-5-H), 6.99 (s, 1H, Imidazole-5-H), 6.86 (s, 1H, Imidazole-4-H), 3.89 (t, *J* = 7.1 Hz, 2H, N-CH₂), 3.23 (t, *J* = 7.3 Hz, 2H, S-CH₂), 1.83-1.72 (m, 4H, N-CH₂CH₂ & S-CH₂CH₂), 1.48-1.42 (m, 2H, N-(CH₂)₂CH₂), 1.34-1.26 (m, 2H, S-(CH₂)₂CH₂); ¹³C NMR (126 MHz, CDCl₃) δ 165.4, 163.3, 138.0, 137.0, 133.7, 131.6, 131.2, 129.4, 127.6, 121.4, 118.8, 46.9, 32.4, 30.9, 29.1, 28.0, 26.0; HRMS (ESI) [M+H]⁺calcd for C₁₇H₁₈Cl₂N₄OS: 397.0651, found: 397.0643.

2-((7-(1*H*-imidazol-1-yl)heptyl)thio)-5-(2,4-dichlorophenyl)-1,3,4-oxadiazole (A₇)

A light yellow solid, yield 79.3%, m. p. 41.1-42.6 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.86 (d, *J* = 8.5, 1H, Ar-6-H), 7.52 (d, *J* = 2.3 Hz, 1H, Ar-3-H), 7.46 (s, 1H, Imidazole-2-H), 7.34 (dd, *J* = 8.5, 2.1 Hz, 1H, Ar-5-H), 7.01 (s, 1H, Imidazole-5-H), 6.87 (s, 1H, Imidazole-4-H), 3.89 (t, *J* = 7.1 Hz, 2H, N-CH₂), 3.24 (t, *J* = 7.3 Hz, 2H, S-CH₂), 1.87-1.65 (m, 4H, N-CH₂CH₂ & S-CH₂CH₂), 1.49-1.17 (m, 6H, N-(CH₂)₂CH₂CH₂CH₂); ¹³C NMR (126 MHz, CDCl₃) δ 165.5, 163.3, 138.0, 137.1, 133.7, 131.6, 131.2, 129.3, 127.6, 121.5, 118.8, 47.0, 32.5, 31.0, 29.2, 28.5, 28.4, 26.4; HRMS (ESI) [M+H]⁺calcd for C₁₈H₂₀Cl₂N₄OS: 411.0808, found: 411.0800.

2-((8-(1*H*-imidazol-1-yl)octyl)thio)-5-(2,4-dichlorophenyl)-1,3,4-oxadiazole

(A₈)

A yellow liquid, yield 77.5%; ¹H NMR (500 MHz, CDCl₃) δ 7.88 (d, *J* = 8.5 Hz, 1H, Ar-6-H), 7.54 (d, *J* = 2.0 Hz, 1H, Ar-3-H), 7.46 (s, 1H, Imidazole-2-H), 7.37 (dd, *J* = 8.5, 2.1 Hz, 1H, Ar-5-H), 7.03 (s, 1H, Imidazole-5-H), 6.89 (s, 1H, Imidazole-4-H), 3.91 (t, *J* = 7.1 Hz, 2H, N-CH₂), 3.27 (t, *J* = 7.1 Hz, 2H, S-CH₂), 1.90-1.66 (m, 4H, N-CH₂CH₂ & S-CH₂CH₂), 1.45-1.40 (m, 2H, N-(CH₂)₂CH₂), 1.37-1.21 (m, 6H, N-(CH₂)₃CH₂CH₂CH₂); ¹³C NMR (126 MHz, CDCl₃) δ 165.6, 163.3, 138.1, 137.1, 133.8, 131.6, 131.3, 129.3, 127.7, 121.6, 118.9, 47.1, 32.6, 31.1, 29.3, 28.9, 28.8, 28.5, 26.5; HRMS (ESI) [M+H]⁺calcd for C₁₉H₂₂Cl₂N₄OS: 425.0964, found: 425.0954.

2-((5-(1*H*-imidazol-1-yl)pentyl)oxy)-5-(2,4-dichlorophenyl)-1,3,4-oxadiazole

(B₅)

A yellow liquid, yield 58.3%; ¹H NMR (500 MHz, CDCl₃) δ 7.72 (d, *J* = 8.4 Hz, 1H, Ar-6-H), 7.52 (d, *J* = 1.3 Hz, 1H, Ar-3-H), 7.44 (s, 1H, Imidazole-2-H), 7.36 (dd, *J* = 8.2, 2.4 Hz, 1H, Ar-5-H), 7.02 (s, 1H, Imidazole-5-H), 6.89 (s, 1H, Imidazole-4-H), 3.94 (t, *J* = 7.1 Hz, 2H, N-CH₂), 3.80 (t, *J* = 6.9 Hz, 2H, O-CH₂), 1.87-1.81 (m, 4H, N-CH₂CH₂ & O-CH₂CH₂), 1.41-1.35 (m, 2H, O-(CH₂)₂CH₂); ¹³C NMR (126 MHz, CDCl₃) δ 153.1, 150.8, 137.9, 137.1, 133.4, 131.5, 130.6, 129.6, 127.7, 121.3, 118.8, 46.8, 45.8, 30.6, 27.8, 23.5; HRMS (ESI) [M+H]⁺calcd for C₁₆H₁₆Cl₂N₄O₂: 367.0723, found: 367.0715.

2-((6-(1*H*-imidazol-1-yl)hexyl)oxy)-5-(2,4-dichlorophenyl)-1,3,4-oxadiazole

(B₆)

A light yellow liquid, yield 71.0%; ¹H NMR (500 MHz, CDCl₃) δ 7.72 (d, *J* = 8.5 Hz, 1H, Ar-6-H), 7.51 (d, *J* = 2.0 Hz, 1H, Ar-3-H), 7.45 (s, 1H, Imidazole-2-H), 7.35 (dd, *J* = 8.5, 2.0 Hz, 1H, Ar-5-H), 7.02 (s, 1H, Imidazole-5-H), 6.88 (s, 1H, Imidazole-4-H), 3.91 (t, *J* = 7.1 Hz, 2H, N-CH₂), 3.79 (t, *J* = 7.0 Hz, 2H, O-CH₂), 1.82-1.75 (m, 4H, N-CH₂CH₂ & O-CH₂CH₂), 1.43-1.30 (m, 4H, N-(CH₂)₂CH₂CH₂); ¹³C NMR (126 MHz, CDCl₃) δ 153.1, 150.7, 137.8, 137.1, 133.4, 131.4, 130.6, 129.5, 127.7, 121.3, 118.8, 47.0, 45.9, 31.0, 28.1, 26.1, 25.9; HRMS (ESI) [M+H]⁺calcd for C₁₇H₁₈Cl₂N₄O₂: 381.0880, found: 381.0872.

2-((8-(1*H*-imidazol-1-yl)octyl)oxy)-5-(2,4-dichlorophenyl)-1,3,4-oxadiazole

(B₈)

A yellow liquid, yield 77.4%; ^1H NMR (500 MHz, CDCl_3) δ 7.72 (d, J = 8.5 Hz, 1H, Ar-6-H), 7.52 (d, J = 2.0 Hz, 1H, Ar-3-H), 7.43 (s, 1H, Imidazole-2-H), 7.35 (dd, J = 8.6, 2.0 Hz, 1H, Ar-5-H), 7.02 (s, 1H, Imidazole-5-H), 6.88 (s, 1H, Imidazole-4-H), 3.90 (t, J = 7.1 Hz, 2H, N- CH_2), 3.79 (t, J = 7.1 Hz, 2H, O- CH_2), 1.80-1.72 (m, 4H, N- CH_2CH_2 & O- CH_2CH_2), 1.33-1.28 (m, 8H, N-(CH_2) $_2\text{CH}_2\text{CH}_2\text{CH}_2$); ^{13}C NMR (126 MHz, CDCl_3) δ 153.1, 150.6, 137.8, 137.1, 133.4, 131.5, 130.6, 129.4, 127.6, 121.4, 118.9, 47.1, 46.2, 31.1, 29.0, 28.9, 28.2, 26.5, 26.3; HRMS (ESI) $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{19}\text{H}_{22}\text{Cl}_2\text{N}_4\text{O}_2$: 409.1193, found: 409.1185.

2-((6-(1*H*-imidazol-1-yl)hexyl)thio)-5-(2,4-dichlorophenyl)-1,3,4-thiadiazole (C₆)

A white solid, yield 97.5%, m. p. 95.8-97.1 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.24 (d, J = 8.6 Hz, 1H, Ar-6-H), 7.53 (d, J = 2.1 Hz, 1H, Ar-3-H), 7.46 (s, 1H, Imidazole-2-H), 7.39 (dd, J = 8.6, 2.1 Hz, 1H, Ar-5-H), 7.06 (s, 1H, Imidazole-5-H), 6.91 (s, 1H, Imidazole-4-H), 3.93 (t, J = 7.1 Hz, 2H, N- CH_2), 3.36 (t, J = 7.4 Hz, 2H, S- CH_2), 1.87-1.77 (m, 4H, N- CH_2CH_2 & S- CH_2CH_2), 1.53-1.49 (m, 2H, N-(CH_2) $_2\text{CH}_2$), 1.39-1.30 (m, 2H, S-(CH_2) $_2\text{CH}_2$); ^{13}C NMR (126 MHz, CDCl_3) δ 167.7, 162.7, 137.2, 133.0, 131.6, 130.5, 129.7, 128.1, 127.6, 118.9, 47.0, 33.9, 31.0, 29.2, 28.3, 26.2; HRMS (ESI) $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{17}\text{H}_{18}\text{Cl}_2\text{N}_4\text{S}_2$: 413.0423, found: 413.0415.

2-((8-(1*H*-imidazol-1-yl)octyl)thio)-5-(2,4-dichlorophenyl)-1,3,4-thiadiazole (C₈)

A light yellow solid, yield 95.0%, m. p. 32.8-34.8 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.24 (d, J = 8.6 Hz, 1H, Ar-6-H), 7.53 (d, J = 2.0 Hz, 1H, Ar-3-H), 7.45 (s, 1H, Imidazole-2-H), 7.39 (dd, J = 8.6, 2.2 Hz, 1H, Ar-5-H), 7.04 (s, 1H, Imidazole-5-H), 6.89 (s, 1H, Imidazole-4-H), 3.91 (t, J = 7.1 Hz, 2H, N- CH_2), 3.36 (t, J = 7.4 Hz, 2H, S- CH_2), 1.86-1.80 (m, 2H, N- CH_2CH_2), 1.78-1.73 (m, 2H, S- CH_2CH_2), 1.50-1.40 (m, 2H, N-(CH_2) $_2\text{CH}_2$), 1.36-1.27 (m, 6H, N-(CH_2) $_3\text{CH}_2\text{CH}_2\text{CH}_2$); ^{13}C NMR (126 MHz, CDCl_3) δ 167.9, 162.6, 137.2, 133.0, 131.6, 130.5, 129.5, 128.0, 127.7, 118.9, 47.1, 34.2, 31.2, 29.3, 28.9, 28.8, 28.7, 26.6; HRMS (ESI) $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{19}\text{H}_{22}\text{Cl}_2\text{N}_4\text{S}_2$: 441.0736, found: 441.0727.

2-((10-(1*H*-imidazol-1-yl)decyl)thio)-5-(2,4-dichlorophenyl)-1,3,4-thiadiazole (C₁₀)

A light yellow solid, yield 43.8%, m. p. 53.6-55.0 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.23 (d, J = 8.6 Hz, 1H, Ar-6-H), 7.52 (d, J = 2.1 Hz, 1H, Ar-3-H), 7.44 (s,

1H, Imidazole-2-H), 7.37 (dd, $J = 8.6, 2.0$ Hz, 1H, Ar-5-H), 7.03 (s, 1H, Imidazole-5-H), 6.88 (s, 1H, Imidazole-4-H), 3.90 (t, $J = 7.1$ Hz, 2H, N-CH₂), 3.36 (t, $J = 7.4$ Hz, 2H, S-CH₂), 1.84-1.80 (m, 2H, N-CH₂CH₂), 1.78-1.73 (m, 2H, S-CH₂CH₂), 1.48-1.40 (m, 2H, N-(CH₂)₂CH₂), 1.29-1.26 (m, 10H, S-(CH₂)₃CH₂CH₂CH₂CH₂CH₂); ¹³C NMR (126 MHz, CDCl₃) δ 168.0, 162.5, 137.1, 133.0, 131.6, 130.4, 129.5, 128.0, 127.6, 118.9, 47.1, 34.3, 31.2, 29.4, 29.3, 29.1, 29.0, 28.8, 26.6; HRMS (ESI) [M+H]⁺calcd for C₂₁H₂₆Cl₂N₄S₂: 469.1049, found: 469.1038.

2-((6-(1H-imidazol-1-yl)hexyl)thio)-5-(4-(trifluoromethyl)phenyl)-1,3,4-oxadiazole (E₂)

A yellow liquid, yield 66.0%; ¹H NMR (500 MHz, CDCl₃) δ 8.08 (d, $J = 8.1$ Hz, 2H, Ar-3,5-H), 7.71 (d, $J = 8.3$ Hz, 2H, Ar-2,6-H), 7.44 (s, 1H, Imidazole-2-H), 7.01 (s, 1H, Imidazole-5-H), 6.87 (s, 1H, Imidazole-4-H), 3.90 (t, $J = 7.1$ Hz, 2H, N-CH₂), 3.25 (t, $J = 7.1$ Hz, 2H, S-CH₂), 1.84-1.73 (m, 4H, N-CH₂CH₂ & S-CH₂CH₂), 1.53-1.39 (m, 2H, N-(CH₂)₂CH₂), 1.34-1.28 (m, 2H, S-(CH₂)₂CH₂); ¹³C NMR (126 MHz, CDCl₃) δ 165.5, 164.6, 137.1, 133.1 (q, $^2J_{C-F} = 33.4$ Hz), 129.4, 126.9, 126.8, 126.1 (q, $^3J_{C-F} = 3.4$ Hz), 123.6 (q, $^1J_{C-F} = 289.6$ Hz). 118.9, 47.0, 32.4, 30.9, 29.0, 28.1, 26.0; ¹⁹F NMR (376 MHz, CDCl₃) δ -63.1 (s, -CF₃); HRMS (ESI) [M+H]⁺calcd for C₁₈H₁₉F₃N₄OS: 397.1304, found: 397.1296.

2-((6-(1H-imidazol-1-yl)hexyl)thio)-5-(4-fluorophenyl)-1,3,4-oxadiazole (E₃)

A light yellow liquid, yield 70.0%; ¹H NMR (500 MHz, CDCl₃) δ 7.84-7.75 (m, 2H, Ar-2,6-H), 7.30 (s, 1H, Imidazole-2-H), 7.05-6.94 (m, 2H, Ar-3,5-H), 6.96 (s, 1H, Imidazole-5-H), 6.82 (s, 1H, Imidazole-4-H), 3.84 (t, $J = 6.2$ Hz, 2H, N-CH₂), 3.17 (t, $J = 6.2$ Hz, 2H, S-CH₂), 1.77-1.65 (m, 4H, N-CH₂CH₂ & S-CH₂CH₂), 1.43-1.34 (m, 2H, N-(CH₂)₂CH₂), 1.39-1.27 (m, 2H, S-(CH₂)₂CH₂); ¹³C NMR (126 MHz, CDCl₃) δ 164.4, 164.2 (d, $^1J_{C-F} = 253.8$ Hz), 164.0, 136.7, 128.9, 128.5 (d, $^3J_{C-F} = 8.9$ Hz), 119.6 (d, $^4J_{C-F} = 3.1$ Hz), 118.4, 116.0 (d, $^2J_{C-F} = 22.5$ Hz), 46.4, 31.9, 30.5, 28.6, 27.6, 25.5; ¹⁹F NMR (376 MHz, CDCl₃) δ -106.9 (s, Ar-F); HRMS (ESI) [M+H]⁺calcd for C₁₇H₁₉FN₄OS: 347.1336, found: 347.1329.

2-((6-(1H-imidazol-1-yl)hexyl)thio)-5-(4-chlorophenyl)-1,3,4-oxadiazole (E₄)

A light yellow solid, yield 49.9%, m. p. 81.5-83.5 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.82 (d, $J = 6.5$ Hz, 2H, Ar-2,6-H), 7.52 (s, 1H, Imidazole-2-H), 7.36 (m, $J = 6.4$ Hz, 2H, Ar-3,5-H), 7.06 (s, 1H, Imidazole-5-H), 6.92 (s, 1H, Imidazole-4-H), 3.84 (t, $J = 6.2$ Hz, 2H, N-CH₂), 3.17 (t, $J = 6.2$ Hz, 2H, S-CH₂), 1.77-1.65 (m, 4H, N-

CH₂CH₂ & S-CH₂CH₂), 1.43-1.34 (m, 2H, N-(CH₂)₂CH₂), 1.28-1.23 (m, S-(CH₂)₂CH₂); ¹³C NMR (126 MHz, CDCl₃) δ 164.7, 164.5, 137.6, 136.9, 129.2, 129.1, 127.7, 121.9, 118.7, 46.7, 32.1, 30.7, 28.8, 27.8, 25.8; HRMS (ESI) [M+H]⁺calcd for C₁₇H₁₉ClN₄OS: 363.1041, found: 363.1032.

2-((6-(1*H*-imidazol-1-yl)hexyl)thio)-5-(3-chlorophenyl)-1,3,4-oxadiazole (E₅)

A yellow liquid, yield 69.0%; ¹H NMR (500 MHz, CDCl₃) δ 7.96 (t, *J* = 1.8 Hz, 1H, Ar-2-H), 7.88-7.86 (m, 1H, Ar-6-H), 7.49-7.36 (m, 3H, Ar-4,5-H & Imidazole-2-H), 7.02 (s, 1H, Imidazole-5-H), 6.88 (s, 1H, Imidazole-4-H), 3.91 (t, *J* = 7.1 Hz, 2H, N-CH₂), 3.26 (t, *J* = 7.3 Hz, 2H, S-CH₂), 1.85-1.75 (m, 4H, N-CH₂CH₂ & S-CH₂CH₂), 1.54-1.42 (m, 2H, N-(CH₂)₂CH₂), 1.40-1.27 (m, 2H, S-(CH₂)₂CH₂); ¹³C NMR (126 MHz, CDCl₃) δ 165.0, 164.6, 137.1, 135.2, 131.7, 130.5, 129.5, 126.6, 125.3, 124.8, 118.8, 46.9, 32.4, 30.9, 29.1, 28.0, 26.0; HRMS (ESI) [M+H]⁺calcd for C₁₇H₁₉ClN₄OS: 363.1041, found: 363.1032.

2-((6-(1*H*-imidazol-1-yl)hexyl)thio)-5-(2-chlorophenyl)-1,3,4-oxadiazole (E₆)

A yellow liquid, yield 62.0%; ¹H NMR (500 MHz, CDCl₃) δ 7.87 (d, *J* = 7.8, 1.6 Hz, 1H, Ar-6-H), 7.48-7.31 (m, 3H, Imidazole-2-H & Ar-3,5-H & Ar-3-H), 7.36-7.30 (m, 1H, Ar-4-H), 6.98 (s, 1H, Imidazole-5-H), 6.85 (s, 1H, Imidazole-4-H), 3.87 (t, *J* = 7.1 Hz, 2H, N-CH₂), 3.21 (t, *J* = 7.3 Hz, 2H, S-CH₂), 1.81-1.70 (m, 4H, N-CH₂CH₂ & S-CH₂CH₂), 1.46-1.40 (m, 2H, N-(CH₂)₂CH₂), 1.33-1.22 (m, 2H, S-(CH₂)₂CH₂); ¹³C NMR (126 MHz, CDCl₃) δ 165.0, 163.9, 137.0, 132.8, 132.3, 131.2, 130.8, 129.3, 127.1, 122.8, 118.7, 46.8, 32.3, 30.8, 29.1, 27.9, 25.9; HRMS (ESI) [M+H]⁺calcd for C₁₇H₁₉ClN₄OS: 363.1041, found: 363.1033.

2-((6-(1*H*-imidazol-1-yl)hexyl)thio)-5-phenyl-1,3,4-oxadiazole (E₇)

A light yellow liquid, yield 93.7%; ¹H NMR (500 MHz, CDCl₃) δ 8.03-7.94 (m, 2H, Ar-2,6-H), 7.52-7.42 (m, 4H, Imidazole-2-H & Ar-3,5-H & Ar-4-H), 7.03 (s, 1H, Imidazole-5-H), 6.89 (s, 1H, Imidazole-4-H), 3.92 (t, *J* = 7.1 Hz, 2H, N-CH₂), 3.26 (t, *J* = 7.3 Hz, 2H, S-CH₂), 1.86-1.76 (m, 4H, N-CH₂CH₂ & S-CH₂CH₂), 1.52-1.46 (m, 2H, N-(CH₂)₂CH₂), 1.39-1.29 (m, 2H, S-(CH₂)₂CH₂); ¹³C NMR (126 MHz, CDCl₃) δ 165.8, 164.5, 137.1, 131.8, 129.5, 129.2, 126.7, 123.7, 118.8, 47.0, 32.4, 31.0, 29.2, 28.1, 26.1; HRMS (ESI) [M+H]⁺calcd for C₁₇H₂₀N₄OS: 329.1431, found: 329.1422.

2-((6-(1*H*-imidazol-1-yl)hexyl)thio)-5-(*p*-tolyl)-1,3,4-oxadiazole (E₈)

A light yellow solid, yield 92.6%, m. p. 66.0-67.9 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.86 (d, *J* = 6.7 Hz, 2H, Ar-2,6-H), 7.44 (s, 1H, Imidazole-2-H), 7.27 (d, *J* =

7.5 Hz, 2H, Ar-3,5-H), 7.03 (s, 1H, Imidazole-5-H), 6.89 (s, 1H, Imidazole-4-H), 3.91 (t, $J = 7.1$ Hz, 2H, N-CH₂), 3.24 (t, $J = 7.3$ Hz, 2H, S-CH₂), 2.39 (s, 3H, -CH₃), 1.85-1.74 (m, 4H, N-CH₂CH₂ & S-CH₂CH₂), 1.54-1.43 (m, 2H, N-(CH₂)₂CH₂), 1.39-1.25 (m, 2H, S-(CH₂)₂CH₂); ¹³C NMR (126 MHz, CDCl₃) δ 165.8, 164.0, 142.2, 137.0, 129.7, 129.4, 126.5, 120.8, 118.8, 46.8, 32.3, 30.9, 29.0, 28.0, 26.0, 21.6; HRMS (ESI) [M+H]⁺calcd for C₁₈H₂₂N₄OS: 343.1587, found: 343.1579.

2-(((6-(1*H*-imidazol-1-yl)hexyl)thio)-5-(3-methoxyphenyl)-1,3,4-oxadiazole (E₉)

A light yellow solid, yield 59.0%, m. p. 69.3-71.1 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.51-7.48 (m, 2H, Ar-6-H & Imidazole-2-H), 7.45 (dd, $J = 2.5, 1.5$ Hz, 1H, Ar-5-H), 7.33 (t, $J = 8.0$ Hz, 1H, Ar-2-H), 7.00-6.98 (m, 2H, Imidazole-5-H & Ar-4-H), 6.86 (s, 1H, Imidazole-4-H), 3.88 (t, $J = 7.1$ Hz, 2H, N-CH₂), 3.80 (s, 3H, -OCH₃), 3.21 (t, $J = 7.3$ Hz, 2H, S-CH₂), 1.82-1.69 (m, 4H, N-CH₂CH₂ & S-CH₂CH₂), 1.46-1.40 (m, 2H, N-(CH₂)₂CH₂), 1.33-1.23 (m, 2H, S-(CH₂)₂CH₂); ¹³C NMR (126 MHz, CDCl₃) δ 165.5, 164.4, 159.8, 137.1, 130.1, 129.2, 124.6, 118.9, 118.8, 118.0, 111.1, 55.5, 46.9, 32.2, 30.8, 29.0, 27.9, 25.9; HRMS (ESI) [M+H]⁺calcd for C₁₈H₂₂N₄O₂S: 359.1536, found: 359.1526.

2-(((6-(1*H*-imidazol-1-yl)hexyl)thio)-5-(furan-2-yl)-1,3,4-oxadiazole (E₁₀)

A light yellow solid, yield 52.4%, m. p. 56.8-58.4 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.59 (dd, $J = 1.8, 0.8$ Hz, 1H, Furan-5-H), 7.42 (s, 1H, Imidazole-2-H), 7.07 (dd, $J = 3.5, 0.7$ Hz, 1H, Furan-3-H), 7.00 (s, 1H, Imidazole-5-H), 6.86 (s, 1H, Imidazole-4-H), 6.55 (dd, $J = 3.6, 1.8$ Hz, 1H, Furan-4-H), 3.89 (t, $J = 7.1$ Hz, 2H, N-CH₂), 3.23 (t, $J = 7.1$ Hz, 2H, S-CH₂), 1.85-1.68 (m, 4H, N-CH₂CH₂ & S-CH₂CH₂), 1.52-1.39 (m, 2H, N-(CH₂)₂CH₂), 1.37-1.25 (m, 2H, S-(CH₂)₂CH₂); ¹³C NMR (126 MHz, CDCl₃) δ 163.9, 158.5, 145.7, 139.1, 137.1, 129.4, 118.8, 113.87, 112.2, 46.9, 32.4, 30.9, 29.0, 28.0, 26.0; HRMS (ESI) [M+H]⁺calcd for C₁₅H₁₈N₄OS: 319.1223, found: 319.1216.

2-(((6-(1*H*-imidazol-1-yl)hexyl)thio)-5-(pyridin-3-yl)-1,3,4-oxadiazole (E₁₁)

A light yellow solid, yield 55.4%, m. p. 60.1-62.0 °C; ¹H NMR (500 MHz, CDCl₃) δ 9.07 (d, $J = 1.9$ Hz, 1H, Pyridine-2-H), 8.61 (dd, $J = 4.8, 1.1$ Hz, 1H, Pyridine-6-H), 8.15-8.13 (m, 1H, Pyridine-4-H), 7.48 (s, 1H, Imidazole-2-H), 7.33 (dd, $J = 8.0, 4.9$ Hz, 1H, Pyridine-5-H), 6.94 (s, 1H, Imidazole-5-H), 6.82 (s, 1H, Imidazole-4-H), 3.83 (t, $J = 6.9$ Hz, 2H, N-CH₂), 3.15 (t, $J = 7.2$ Hz, 2H, S-CH₂),

1.81-1.59 (m, 4H, N-CH₂CH₂ & S-CH₂CH₂), 1.40-1.34 (m, 2H, N-(CH₂)₂CH₂), 1.25-1.19 (m, 2H, S-(CH₂)₂CH₂); ¹³C NMR (126 MHz, CDCl₃) δ 165.1, 163.3, 152.1, 147.3, 137.0, 133.6, 128.8, 123.6, 119.9, 118.8, 46.8, 32.1, 30.6, 28.7, 27.7, 25.7; HRMS (ESI) [M+H]⁺calcd for C₁₆H₁₉N₅OS: 330.1383, found: 330.1375.

2-((6-(1*H*-imidazol-1-yl)hexyl)thio)-5-(4-chlorobenzyl)-1,3,4-oxadiazole (E₁₂)

A yellow liquid, yield 72.9%; ¹H NMR (500 MHz, CDCl₃) δ 7.45 (s, 1H, Imidazole-2-H), 7.34-7.28 (m, 2H, Ar-3,5-H), 7.22 (dd, *J* = 11.6, 5.2 Hz, 2H, Ar-2,6-H), 7.05 (s, 1H, Imidazole-5-H), 6.89 (s, 1H, Imidazole-4-H), 4.13 (s, 2H, Ar-CH₂), 3.91 (t, *J* = 7.1 Hz, 2H, N-CH₂), 3.17 (t, *J* = 7.1 Hz, 2H, S-CH₂), 1.81-1.69 (m, 4H, N-CH₂CH₂ & S-CH₂CH₂), 1.47-1.41 (m, 2H, N-(CH₂)₂CH₂), 1.35-1.27 (m, 2H, S-(CH₂)₂CH₂); ¹³C NMR (126 MHz, CDCl₃) δ 165.9, 165.2, 137.2, 132.2, 130.3, 129.6, 129.3, 129.2, 118.9, 47.0, 32.3, 31.4, 31.0, 29.1, 28.1, 26.1; HRMS (ESI) [M+H]⁺calcd for C₁₈H₂₁ClN₄OS: 377.1197, found: 377.1189.

2-((6-(1*H*-imidazol-1-yl)hexyl)thio)-5-(phenoxymethyl)-1,3,4-oxadiazole (E₁₃)

A light yellow liquid, yield 97.8%; ¹H NMR (500 MHz, CDCl₃) δ 7.46 (s, 1H, Imidazole-2-H), 7.29-7.24 (m, 2H, Ar-3,5-H), 7.01 (s, 1H, Imidazole-5-H), 6.99-6.94 (m, 3H, Ar-4-H & Ar-2,6-H), 6.86 (s, 1H, Imidazole-4-H), 5.16 (s, 2H, O-CH₂), 3.87 (t, *J* = 7.1 Hz, 2H, N-CH₂), 3.17 (t, *J* = 7.1 Hz, 2H, S-CH₂), 1.79-1.68 (m, 4H, N-CH₂CH₂ & S-CH₂CH₂), 1.45-1.37 (m, 2H, N-(CH₂)₂CH₂), 1.32-1.23 (m, 2H, S-(CH₂)₂CH₂); ¹³C NMR (126 MHz, CDCl₃) δ 166.1, 163.2, 157.4, 137.1, 129.7, 129.2, 122.1, 118.8, 114.7, 59.6, 46.8, 32.2, 30.8, 28.9, 27.9, 25.9; HRMS (ESI) [M+H]⁺calcd for C₁₈H₂₂N₄O₂S: 359.1536, found: 359.1527.

2-((6-(1*H*-imidazol-1-yl)hexyl)thio)-5-methyl-1,3,4-oxadiazole (E₁₄)

A light yellow liquid, yield 91.6%; ¹H NMR (500 MHz, CDCl₃) δ 7.37 (s, 1H, Imidazole-2-H), 6.94 (s, 1H, Imidazole-5-H), 6.82 (s, 1H, Imidazole-4-H), 3.84 (t, *J* = 7.1 Hz, 2H, N-CH₂), 3.10 (t, *J* = 7.3 Hz, 2H, S-CH₂), 2.41 (s, 3H, C-CH₃), 1.72-1.66 (m, 4H, N-CH₂CH₂ & S-CH₂CH₂), 1.41-1.35 (m, 2H, N-(CH₂)₂CH₂), 1.27-1.20 (m, 2H, S-(CH₂)₂CH₂); ¹³C NMR (126 MHz, CDCl₃) δ 165.4, 164.7, 136.9, 129.2, 118.6, 46.7, 33.6, 30.7, 28.8, 27.9, 25.8, 15.5; HRMS (ESI) [M+H]⁺calcd for C₁₂H₁₈N₄OS: 267.1274, found: 267.1268.

2-((6-(1*H*-1,2,4-triazol-1-yl)hexyl)thio)-5-(2,4-dichlorophenyl)-1,3,4-oxadiazole (F₂)

A light yellow liquid, yield 81.1%; ^1H NMR (500 MHz, CDCl_3) δ 8.03 (s, 1H, Triazole-5-H), 7.90 (s, 1H, Triazole-3-H), 7.87 (d, $J = 8.5$ Hz, 1H, Ar-6-H), 7.53 (d, $J = 2.0$ Hz, 1H, Ar-3-H), 7.35 (dd, $J = 8.5, 2.0$ Hz, 1H, Ar-5-H), 4.15 (t, $J = 7.1$ Hz, 2H, N- CH_2), 3.25 (t, $J = 7.3$ Hz, 2H, S- CH_2), 1.93-1.79 (m, 4H, N- CH_2CH_2 & S- CH_2CH_2), 1.54-1.43 (m, 2H, N- $(\text{CH}_2)_2\text{CH}_2$), 1.39-1.28 (m, 2H, S- $(\text{CH}_2)_2\text{CH}_2$); ^{13}C NMR (126 MHz, CDCl_3) δ 165.4, 163.4, 152.0, 142.9, 138.1, 133.8, 131.6, 131.3, 127.7, 121.5, 49.6, 32.4, 29.7, 29.1, 28.0, 26.0; HRMS (ESI) $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{16}\text{H}_{17}\text{Cl}_2\text{N}_5\text{OS}$: 398.0604, found: 398.0596.

2-(2,4-dichlorophenyl)-5-((6-(pyridin-4-yloxy)hexyl)thio)-1,3,4-oxadiazole (F₃)

A light yellow solid, yield 52.6%, m. p. 39.7-41.6 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.40 (dd, $J = 4.9, 1.4$ Hz, 2H, Pyridine-2,6-H), 7.90 (d, $J = 8.5$ Hz, 1H, Ar-6-H), 7.56 (d, $J = 2.0$ Hz, 1H, Ar-3-H), 7.38 (dd, $J = 8.5, 2.1$ Hz, 1H, Ar-5-H), 6.78 (dd, $J = 4.8, 1.5$ Hz, 2H, Pyridine-3,5-H), 4.00 (t, $J = 6.4$ Hz, 2H, N- CH_2), 3.31 (t, $J = 6.4$ Hz, 2H, S- CH_2), 1.92-1.80 (m, 4H, N- CH_2CH_2 & S- CH_2CH_2), 1.61-1.47 (m, 4H, N- $(\text{CH}_2)_2\text{CH}_2$ & S- $(\text{CH}_2)_2\text{CH}_2$); ^{13}C NMR (126 MHz, CDCl_3) δ 165.6, 165.2, 163.4, 151.1, 138.2, 133.9, 131.7, 131.3, 127.8, 121.6, 110.4, 67.8, 32.6, 29.4, 28.9, 28.4, 25.6; HRMS (ESI) $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{19}\text{H}_{19}\text{Cl}_2\text{N}_3\text{O}_2\text{S}$: 424.0648, found: 424.0638.

2-(2,4-dichlorophenyl)-5-((6-(piperidin-1-yl)hexyl)thio)-1,3,4-oxadiazole (F₄)

A yellow liquid, yield 86.7%; ^1H NMR (500 MHz, CDCl_3) δ 7.89 (d, $J = 8.5$ Hz, 1H, Ar-6-H), 7.55 (d, $J = 2.0$ Hz, 1H, Ar-3-H), 7.37 (dd, $J = 8.5, 2.1$ Hz, 1H, Ar-5-H), 3.28 (t, $J = 6.7$ Hz, 2H, S- CH_2), 2.36 (s, 4H, Piperidine-2,6-H), 2.27 (t, $J = 6.7$ Hz, 2H, N- CH_2), 1.88-1.80 (m, 2H, S- CH_2CH_2), 1.59-1.55 (m, 4H, Piperidine-3,5-H), 1.50-1.41 (m, 6H, Piperidine-4-H & N- CH_2CH_2 & S- $(\text{CH}_2)_2\text{CH}_2$), 1.37-1.31 (m, 2H, N- $(\text{CH}_2)_2\text{CH}_2$); ^{13}C NMR (126 MHz, CDCl_3) δ 165.7, 163.3, 138.1, 133.8, 131.7, 131.3, 127.7, 121.7, 59.5, 54.7, 32.7, 29.4, 28.6, 27.2, 26.8, 26.0, 24.5; HRMS (ESI) $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{19}\text{H}_{25}\text{Cl}_2\text{N}_3\text{OS}$: 414.1168, found: 414.1161.

4-(6-((5-(2,4-dichlorophenyl)-1,3,4-oxadiazol-2-yl)thio)hexyl)morpholine (F₅)

A yellow liquid, yield 97.7%; ^1H NMR (500 MHz, CDCl_3) δ 7.90 (d, $J = 8.5$ Hz, 1H, Ar-6-H), 7.56 (d, $J = 2.0$ Hz, 1H, Ar-3-H), 7.38 (d, $J = 8.5, 2.1$ Hz, 1H, Ar-5-H), 3.71 (t, $J = 7.3$ Hz, 4H, Morpholine-3,5-H), 3.29 (t, $J = 7.1$ Hz, 2H, S- CH_2), 2.48-2.37 (m, 4H, Morpholine-2,6-H), 2.32 (t, $J = 7.1$ Hz, 2H, N- CH_2), 1.89-1.82 (m, 2H, S- CH_2CH_2), 1.54-1.45 (m, 4H, S- $(\text{CH}_2)_2\text{CH}_2$ & N- CH_2CH_2), 1.41-1.31 (m, 2H, N- $(\text{CH}_2)_2\text{CH}_2$).

(CH₂)₂CH₂); ¹³C NMR (126 MHz, CDCl₃) δ 165.6, 163.4, 138.1, 133.9, 131.7, 131.3, 127.7, 121.7, 67.1, 59.1, 53.9, 32.7, 29.4, 28.6, 27.0, 26.5; HRMS (ESI) [M+H]⁺calcd for C₁₈H₂₃Cl₂N₃O₂S: 416.0961, found: 416.0953.

6-((5-(2,4-dichlorophenyl)-1,3,4-oxadiazol-2-yl)thio)-N,N-diethylhexan-1-amine (F₆)

A light yellow liquid, yield 96.9%; ¹H NMR (500 MHz, CDCl₃) δ 7.90 (d, *J* = 8.5 Hz, 1H, Ar-6-H), 7.56 (d, *J* = 2.0 Hz, 1H, Ar-3-H), 7.38 (dd, *J* = 8.5, 2.1 Hz, 1H, Ar-5-H), 3.29 (t, *J* = 7.1 Hz, 2H, S-CH₂), 2.80 (q, *J* = 7.2 Hz, 4H, 2N-CH₂CH₃), 2.67 (t, *J* = 7.1 Hz, 2H, N-CH₂), 1.93-1.82 (m, 2H, S-CH₂CH₂), 1.69-1.62 (m, 2H, S-(CH₂)₂CH₂), 1.57-1.45 (m, 2H, N-CH₂CH₂), 1.44-1.33 (m, 2H, N-(CH₂)₂CH₂), 1.20 (t, *J* = 7.2 Hz, 6H, 2N-CH₂CH₃); ¹³C NMR (126 MHz, CDCl₃) δ 165.6, 163.4, 138.2, 133.9, 131.7, 131.3, 127.7, 121.6, 52.2, 46.8, 32.5, 29.3, 28.3, 26.8, 25.2, 10.3; HRMS (ESI) [M+H]⁺calcd for C₁₈H₂₅Cl₂N₃OS: 402.1168, found: 402.1163.

1-(6-((5-(2,4-dichlorophenyl)-1,3,4-oxadiazol-2-yl)thio)hexyl)-3-ethyl-1*H*-imidazol-3-ium iodide (G₂)

A light yellow liquid, yield 97.8%; ¹H NMR (500 MHz, CDCl₃) δ 9.99 (s, 1H, Imidazole-2-H), 7.84 (d, *J* = 8.5 Hz, 1H, Ar-6-H), 7.59 (t, *J* = 1.7 Hz, 1H, Ar-3-H), 7.55 (t, *J* = 1.7 Hz, 1H, Imidazole-4-H), 7.49 (d, *J* = 2.0 Hz, 1H, Imidazole-5-H), 7.35 (dd, *J* = 8.5, 2.2 Hz, 1H, Ar-5-H), 4.40-4.34 (m, 4H, N⁺-CH₂ & N-CH₂), 3.23 (t, *J* = 7.1 Hz, 2H, S-CH₂), 1.97-1.91 (m, 2H, N-CH₂CH₂), 1.87-1.75 (m, 2H, S-CH₂CH₂), 1.56 (t, *J* = 7.4 Hz, 3H, -CH₂CH₃), 1.53-1.46 (m, 2H, N-(CH₂)₂CH₂), 1.42-1.36 (m, 2H, S-(CH₂)₂CH₂); ¹³C NMR (126 MHz, CDCl₃) δ 165.4, 163.1, 138.0, 135.8, 133.5, 131.5, 131.1, 127.7, 122.6, 122.1, 121.2, 49.9, 45.4, 32.2, 29.9, 28.8, 27.6, 25.3, 15.7; HRMS (ESI) [M-I]⁺calcd for C₁₉H₂₃Cl₂N₄OS: 402.1168, found: 402.1163.

1-(6-((5-(2,4-dichlorophenyl)-1,3,4-oxadiazol-2-yl)thio)hexyl)-3-propyl-1*H*-imidazol-3-ium iodide (G₃)

A light yellow liquid, yield 85.6%; ¹H NMR (500 MHz, CDCl₃) δ 9.91 (s, 1H, Imidazole-2-H), 7.81 (d, *J* = 8.5 Hz, 1H, Ar-6-H), 7.61 (s, 1H, Imidazole-4-H), 7.51 (s, 1H, Imidazole-4-H), 7.46 (d, *J* = 2.0 Hz, 1H, Ar-3-H), 7.32 (dd, *J* = 8.5, 2.0 Hz, 1H, Ar-5-H), 4.34 (t, *J* = 7.4 Hz, 2H, N⁺-CH₂), 4.25 (t, *J* = 7.3 Hz, 2H, N-CH₂), 3.20 (t, *J* = 7.3 Hz, 2H, S-CH₂), 1.95-1.85 (m, 4H, N-CH₂CH₂ & N⁺-CH₂CH₂), 1.83-1.72 (m, 2H, S-CH₂CH₂), 1.49-1.43 (m, 2H, N-(CH₂)₂CH₂), 1.38-1.32 (m, 2H, S-(CH₂)₂CH₂), 0.89 (t, *J* = 7.4 Hz, 3H, -CH₃); ¹³C NMR (126 MHz, CDCl₃) δ 165.4,

163.0, 137.9, 135.9, 133.4, 131.4, 131.0, 127.6, 122.5, 122.3, 121.1, 51.4, 49.8, 32.1, 29.9, 28.7, 27.5, 25.2, 23.6, 10.7; HRMS (ESI) $[M-I]^+$ calcd for $C_{20}H_{25}Cl_2N_4OS$: 439.1121, found: 439.1113.

3-butyl-1-(6-((5-(2,4-dichlorophenyl)-1,3,4-oxadiazol-2-yl)thio)hexyl)-1H-imidazol-3-ium iodide (G₄)

A light yellow liquid, yield 97.5%; 1H NMR (400 MHz, $CDCl_3$) δ 10.16 (s, 1H, Imidazole-2-H), 7.88 (d, $J = 8.5$ Hz, 1H, Ar-6-H), 7.57 (t, $J = 1.7$ Hz, 1H, Imidazole-4-H), 7.54 (d, $J = 2.0$ Hz, 1H, Ar-3-H), 7.44 (t, $J = 1.7$ Hz, 1H, Imidazole-5-H), 7.38 (dd, $J = 8.5, 2.1$ Hz, 1H, Ar-5-H), 4.40 (t, $J = 7.4$ Hz, 2H, N^+-CH_2), 4.34 (t, $J = 7.4$ Hz, 2H, N- CH_2), 3.26 (t, $J = 7.4$ Hz, 2H, S- CH_2), 2.01-1.94 (m, 2H, $N^+-CH_2CH_2$), 1.93-1.81 (m, 4H, N- CH_2CH_2 & S- CH_2CH_2), 1.57-1.50 (m, 2H, $N^+-(CH_2)_2CH_2$), 1.44-1.32 (m, 4H, N- $(CH_2)_2CH_2$ & S- $(CH_2)_2CH_2$), 0.94 (t, $J = 7.4$ Hz, 3H, $-CH_3$); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.6, 163.3, 138.1, 136.5, 133.7, 131.6, 131.3, 127.8, 122.5, 122.2, 121.4, 50.1, 50.0, 32.2, 32.1, 30.0, 28.9, 27.7, 25.4, 19.6, 13.6; HRMS (ESI) $[M-I]^+$ calcd for $C_{21}H_{27}Cl_2N_4OS$: 453.1277, found: 453.1269.

1-(6-((5-(2,4-dichlorophenyl)-1,3,4-oxadiazol-2-yl)thio)hexyl)-3-pentyl-1H-imidazol-3-ium iodide (G₅)

A light yellow liquid, yield 85.3%; 1H NMR (500 MHz, $CDCl_3$) δ 10.11 (s, 1H, Imidazole-2-H), 7.87 (d, $J = 8.5$ Hz, 1H, Ar-6-H), 7.59 (t, $J = 1.6$ Hz, 1H, Imidazole-4-H), 7.53 (d, $J = 2.0$ Hz, 1H, Ar-3-H), 7.45 (t, $J = 1.6$ Hz, 1H, Imidazole-5-H), 7.37 (dd, $J = 8.5, 2.0$ Hz, 1H, Ar-5-H), 4.39 (t, $J = 7.4$ Hz, 2H, N^+-CH_2), 4.32 (t, $J = 7.5$ Hz, 2H, N- CH_2), 3.25 (t, 7.5 Hz, 2H, S- CH_2), 2.03-1.77 (m, 6H, N- CH_2CH_2 & $N^+-CH_2CH_2$ & S- CH_2CH_2), 1.55-1.49 (m, 2H, $N^+-(CH_2)_2CH_2$), 1.44-1.38 (m, 2H, N- $(CH_2)_2CH_2$), 1.36-1.23 (m, 4H, $N^+-(CH_2)_3CH_2$ & S- $(CH_2)_2CH_2$), 0.85 (t, $J = 6.9$ Hz, 3H, $-CH_3$); ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.6, 163.3, 138.1, 136.4, 133.7, 131.6, 131.2, 127.8, 122.6, 122.2, 121.4, 50.3, 50.0, 32.3, 30.0, 28.9, 28.3, 27.6, 25.4, 22.1, 13.9; HRMS (ESI) $[M-I]^+$ calcd for $C_{22}H_{29}Cl_2N_4OS$: 467.1434, found: 467.1426.

1-(6-((5-(2,4-dichlorophenyl)-1,3,4-oxadiazol-2-yl)thio)hexyl)-3-hexyl-1H-imidazol-3-ium bromide (G₆)

A light yellow liquid, yield 91.9%; 1H NMR (500 MHz, $CDCl_3$) δ 10.47 (s, 1H, Imidazole-2-H), 7.88 (d, $J = 8.5$ Hz, 1H, Ar-6-H), 7.54 (d, $J = 2.1$ Hz, 1H, Ar-3-H), 7.49 (t, $J = 1.7$ Hz, 1H, Imidazole-4-H), 7.38 (dd, $J = 8.5, 1.9$ Hz, 1H, Ar-5-H), 7.35 (t, $J = 1.6$ Hz, 1H, Imidazole-5-H), 4.40 (t, $J = 7.4$ Hz, 2H, N^+-CH_2), 4.32 (t, $J = 7.3$ Hz,

2H, N-CH₂), 3.27 (t, J = 7.4 Hz, 2H, S-CH₂), 1.98-1.94 (m, 2H, N⁺-CH₂CH₂), 1.93-1.79 (m, 4H, N-CH₂CH₂ & S-CH₂CH₂), 1.55-1.49 (m, 2H, N⁺-(CH₂)₂CH₂), 1.44-1.38 (m, 2H, N-(CH₂)₂CH₂), 1.36-1.19 (m, 6H, N⁺-(CH₂)₃CH₂CH₂ & S-(CH₂)₂CH₂), 0.84 (t, J = 6.9 Hz, 3H, -CH₃); ¹³C NMR (126 MHz, CDCl₃) δ 165.6, 138.1, 137.4, 133.7, 131.6, 131.3, 127.8, 122.2, 121.8, 50.3, 50.0, 32.3, 31.2, 30.3, 30.0, 29.0, 27.7, 26.0, 25.4, 22.5, 14.0; HRMS (ESI) [M-Br]⁺calcd for C₂₃H₃₁Cl₂N₄OS: 481.1590, found: 481.1582.

1-(6-((5-(2,4-dichlorophenyl)-1,3,4-oxadiazol-2-yl)thio)hexyl)-3-heptyl-1H-imidazol-3-ium bromide (G₇)

A light yellow liquid, yield 69.9%; ¹H NMR (500 MHz, CDCl₃) δ 10.51 (d, J = 9.4 Hz, 1H, Imidazole-2-H), 7.88 (d, J = 8.5 Hz, 1H, Ar-6-H), 7.56-7.48 (m, 2H, Ar-3-H & Imidazole-4-H), 7.38-7.36 (m, 2H, Ar-5-H & Imidazole-5-H), 4.40 (t, J = 7.4 Hz, 2H, N⁺-CH₂), 4.31 (t, J = 7.4 Hz, 2H, N-CH₂), 3.26 (t, J = 7.2 Hz, 2H, S-CH₂), 1.99-1.80 (m, 6H, N-CH₂CH₂ & N⁺-CH₂CH₂ & S-CH₂CH₂), 1.56-1.49 (m, 2H, N⁺-(CH₂)₂CH₂), 1.44-1.38 (m, 2H, N-(CH₂)₂CH₂), 1.34-1.15 (m, 8H, N⁺-(CH₂)₃CH₂CH₂CH₂ & S-(CH₂)₂CH₂), 0.83 (t, J = 6.8 Hz, 3H, -CH₃); ¹³C NMR (126 MHz, CDCl₃) δ 165.6, 163.3, 138.1, 137.3, 133.7, 131.6, 131.3, 127.8, 122.3, 121.9, 121.4, 50.2, 50.0, 32.3, 31.6, 30.4, 30.0, 29.0, 28.7, 27.7, 26.3, 25.4, 22.6, 14.1; HRMS (ESI) [M-Br]⁺calcd for C₂₄H₃₃Cl₂N₄OS: 495.1747, found: 495.1736.

1-(6-((5-(2,4-dichlorophenyl)-1,3,4-oxadiazol-2-yl)thio)hexyl)-3-octyl-1H-imidazol-3-ium bromide (G₈)

A light yellow liquid, yield 71.2%; ¹H NMR (500 MHz, CDCl₃) δ 10.51 (s, 1H, Imidazole-2-H), 7.88 (d, J = 8.7 Hz, 1 H, Ar-6-H), 7.54 (d, J = 2.0 Hz, 1H, Ar-3-H), 7.50 (t, J = 1.7 Hz, 1H, Imidazole-4-H), 7.38 (dd, J = 8.5, 1.9 Hz, 1H, Ar-5-H), 7.35 (t, J = 1.7 Hz, 1H, Imidazole-5-H), 4.40 (t, J = 7.4 Hz, 2H, N⁺-CH₂), 4.31 (t, J = 7.4 Hz, 2H, N-CH₂), 3.25 (t, J = 7.4 Hz, 2H, S-CH₂), 1.98-1.92 (m, 2H, N⁺-CH₂CH₂), 1.90-1.81 (m, 4H, N-CH₂CH₂ & S-CH₂CH₂), 1.55-1.49 (m, 2H, N⁺-(CH₂)₂CH₂), 1.44-1.38 (m, 2H, N-(CH₂)₂CH₂), 1.33-1.15 (m, 10H, N⁺-(CH₂)₃CH₂CH₂CH₂CH₂ & S-(CH₂)₂CH₂), 0.83 (t, J = 7.0 Hz, 3H, -CH₃); ¹³C NMR (126 MHz, CDCl₃) δ 165.59, 163.3, 138.1, 137.4, 133.7, 131.6, 131.3, 127.8, 122.2, 121.8, 121.4, 50.3, 50.0, 32.3, 31.7, 30.4, 30.0, 29.2, 29.0, 27.7, 26.3, 25.4, 22.7, 14.2; HRMS (ESI) [M-Br]⁺calcd for C₂₅H₃₅Cl₂N₄OS: 509.1903, found: 509.1895.

3-allyl-1-(6-((5-(2,4-dichlorophenyl)-1,3,4-oxadiazol-2-yl)thio)hexyl)-1H-imidazol-3-ium bromide (G₉)

A yellow liquid, yield 80.0%; ¹H NMR (500 MHz, CDCl₃) δ 10.31 (s, 1H, Imidazole-2-H), 7.87 (d, *J* = 8.6 Hz, 1H, Ar-6-H), 7.57 (s, 1H, Imidazole-4-H), 7.52 (d, *J* = 1.9 Hz, 1H, Ar-3-H), 7.41 (s, 1H, Imidazole-5-H), 7.36 (dd, *J* = 8.5, 1.7 Hz, 1H, Ar-5-H), 6.04-5.96 (m, 1H, -CH=CH₂), 5.43 (t, *J* = 7.5 Hz, 2H, N⁺-CH₂), 5.00 (d, *J* = 6.4 Hz, 2H, -CH=CH₂), 4.37 (t, *J* = 7.4 Hz, 2H, N-CH₂), 3.24 (t, *J* = 7.4 Hz, 2H, S-CH₂), 1.97-1.91 (m, 2H, N-CH₂CH₂), 1.85-1.79 (m, 2H, S-CH₂CH₂), 1.53-1.48 (m, 2H, N-(CH₂)₂CH₂), 1.43-1.37 (m, 2H, S-(CH₂)₂CH₂); ¹³C NMR (126 MHz, CDCl₃) δ 165.5, 163.3, 138.1, 137.0, 133.7, 131.6, 131.2, 130.0, 127.8, 122.7, 122.5, 121.9, 121.4, 52.2, 50.1, 32.3, 30.0, 28.9, 27.7, 25.5; HRMS (ESI) [M-Br]⁺calcd for C₂₀H₂₃Cl₂N₄OS: 437.0964, found: 437.0956.

1-(6-((5-(2,4-dichlorophenyl)-1,3,4-oxadiazol-2-yl)thio)hexyl)-3-(4-(trifluoromethyl)benzyl)-1H-imidazol-3-ium bromide (G₁₀)

A light yellow liquid, yield 89.0%; ¹H NMR (500 MHz, CDCl₃) δ 10.55 (s, 1H, Imidazole-2-H), 7.86 (d, *J* = 7.5 Hz, 1H, 1-Ar-6-H), 7.72 (d, *J* = 7.8 Hz, 2H, 2-Ar-3,5-H), 7.62-7.46 (m, 5H, 1-Ar-3-H & 2-Ar-2,6-H & Imidazole-4-H & Imidazole-5-H), 7.37 (dd, *J* = 8.5, 2.0 Hz, 1H, 1-Ar-5-H), 5.78 (s, 2H, N⁺-CH₂), 4.32 (t, *J* = 7.4 Hz, 2H, N-CH₂), 3.23 (t, *J* = 7.3 Hz, 2H, S-CH₂), 2.00-1.77 (m, 4H, N-CH₂CH₂ & S-CH₂CH₂), 1.55-1.34 (m, 4H, N-(CH₂)₂CH₂ & S-(CH₂)₂CH₂); ¹³C NMR (126 MHz, CDCl₃) δ 165.6, 163.3, 138.2, 137.3, 137.1, 133.7, 131.6, 131.5 (q, ²*J*_{C-F} = 32.7 Hz), 131.3, 129.6, 127.8, 126.3 (q, ³*J*_{C-F} = 3.4 Hz), 123.7 (q, ¹*J*_{C-F} = 273.1 Hz), 122.5, 122.3, 121.3, 52.5, 50.3, 32.2, 29.8, 28.9, 27.6, 25.4; ¹⁹F NMR (471 MHz, CDCl₃) δ -62.7 (s, -CF₃); HRMS (ESI) [M-Br]⁺calcd for C₂₅H₂₄Cl₂FN₄OS: 555.0994, found: 555.0983.

1-(6-((5-(2,4-dichlorophenyl)-1,3,4-oxadiazol-2-yl)thio)hexyl)-3-(3-nitrobenzyl)-1H-imidazol-3-ium chloride (G₁₁)

A yellow liquid, yield 64.7%; ¹H NMR (500 MHz, CDCl₃) δ 10.62 (s, 1H, Imidazole-2-H), 8.43 (s, 1H, 2-Ar-2-H), 8.19-8.01 (m, 2H, 2-Ar-4,6-H), 7.87 (d, *J* = 8.5 Hz, 1H, 1-Ar-6-H), 7.75 (s, 1H, Imidazole-4-H), 7.55 (t, *J* = 8.0 Hz, 1H, 2-Ar-5-H), 7.52 (d, *J* = 1.9 Hz, 1H, 1-Ar-3-H), 7.48 (s, 1H, Imidazole-5-H), 7.36 (dd, *J* = 8.5, 2.0 Hz, 1H, 1-Ar-5-H), 5.90 (s, 2H, N⁺-CH₂), 4.32 (t, *J* = 7.4 Hz, 2H, N-CH₂), 3.22 (t, *J* = 7.3 Hz, 2H, S-CH₂), 1.95-1.90 (m, 2H, N-CH₂CH₂), 1.83-1.77 (m, 2H, S-CH₂CH₂), 1.51-1.45 (m, 2H, N-(CH₂)₂CH₂), 1.41-1.36 (m, 2H, S-(CH₂)₂CH₂); ¹³C

NMR (126 MHz, CDCl₃) δ 165.6, 163.3, 148.4, 138.2, 137.6, 136.1, 135.8, 133.7, 131.6, 131.3, 130.7, 127.8, 124.2, 124.0, 122.6, 122.5, 121.4, 52.0, 50.2, 32.2, 29.8, 29.0, 27.7, 25.5; HRMS (ESI) [M-Cl]⁺calcd for C₂₄H₂₄Cl₂N₅O₂S: 532.0971, found: 532.0958.

3-(3-chlorobenzyl)-1-(6-((5-(2,4-dichlorophenyl)-1,3,4-oxadiazol-2-yl)thio)hexyl)-1H-imidazol-3-ium chloride (G₁₂)

A light yellow solid, yield 66.9%, m. p. 56.5-58.1 °C; ¹H NMR (500 MHz, CDCl₃) δ 10.86 (s, 1H, Imidazole-2-H), 7.88 (d, J = 8.6 Hz, 1H, 1-Ar-6-H), 7.54 (d, J = 1.9 Hz, 1H, 1-Ar-3-H), 7.49-7.41 (m, 3H, Imidazole-4-H & 2-Ar-2,6-H), 7.38-7.36 (m, 2H, 1-Ar-5-H & Imidazole-5-H), 7.30 (dd, J = 8.3, 5.5 Hz, 2H, 2-Ar-4,5-H), 5.64 (s, 2H, N⁺-CH₂), 4.33 (t, J = 7.4 Hz, 2H, N-CH₂), 3.23 (t, J = 7.4 Hz, 2H, S-CH₂), 1.97-1.91 (m, 2H, N-CH₂CH₂), 1.85-1.79 (m, 2H, S-CH₂CH₂), 1.53-1.47 (m, 2H, N-(CH₂)₂CH₂), 1.42-1.36 (m, 2H, S-(CH₂)₂CH₂); ¹³C NMR (126 MHz, CDCl₃) δ 165.6, 163.3, 138.2, 138.0, 135.4, 135.1, 133.7, 131.6, 131.3, 130.9, 129.7, 129.0, 127.8, 127.5, 122.2, 121.9, 121.4, 52.6, 50.1, 32.2, 29.9, 29.0, 27.7, 25.5; HRMS (ESI) [M-Cl]⁺calcd for C₂₄H₂₄Cl₃N₄OS: 521.0731, found: 521.0723.

1-(6-((5-(2,4-dichlorophenyl)-1,3,4-oxadiazol-2-yl)thio)hexyl)-3-(3-methylbenzyl)-1H-imidazol-3-ium chloride (G₁₃)

A light yellow liquid, yield 74.0%; ¹H NMR (500 MHz, CDCl₃) δ 10.80 (s, 1H, Imidazole-2-H), 7.86 (d, J = 8.6 Hz, 1H, 1-Ar-6-H), 7.52 (d, J = 1.9 Hz, 1H, 1-Ar-3-H), 7.46 (s, 1H, Imidazole-4-H), 7.36 (dd, J = 8.5, 2.0 Hz, 1H, 1-Ar-5-H), 7.24-7.12 (m, Imidazole-5-H & 2-Ar-2,4,5,6-H), 5.50 (s, 2H, N⁺-CH₂), 4.34 (t, J = 7.2 Hz, 2H, N-CH₂), 3.24 (t, J = 7.2 Hz, 2H, S-CH₂), 2.29 (s, 3H, 2-Ar-CH₃), 2.00-1.74 (m, 4H, N-CH₂CH₂ & S-CH₂CH₂), 1.53-1.35 (m, 4H, S-(CH₂)₂CH₂ & N-(CH₂)₂CH₂); ¹³C NMR (126 MHz, CDCl₃) δ 165.5, 163.3, 139.4, 138.1, 137.7, 133.7, 133.1, 131.6, 131.2, 130.3, 129.6, 129.3, 127.7, 126.1, 122.2, 121.7, 121.4, 53.4, 50.0, 32.2, 30.1, 29.0, 27.7, 25.5, 21.4; HRMS (ESI) [M-Cl]⁺calcd for C₂₅H₂₇Cl₂N₄OS: 501.1277, found: 501.1267.

1-(6-((5-(2,4-dichlorophenyl)-1,3,4-oxadiazol-2-yl)thio)hexyl)-3-(2-methylbenzyl)-1H-imidazol-3-ium chloride (G₁₄)

A yellow liquid, yield 81.3%; ¹H NMR (500 MHz, CDCl₃) δ 10.60 (s, 1H, Imidazole-2-H), 7.84 (d, J = 8.6 Hz, 1H, 1-Ar-6-H), 7.51 (d, J = 1.9 Hz, 1H, 1-Ar-3-H), 7.49 (s, 1H, Imidazole-4-H), 7.35 (dd, J = 8.5, 2.0 Hz, 1H, 1-Ar-5-H), 7.27-7.22

(m, 2H, 2-Ar-3-H & 2-Ar-6-H), 7.17 (t, $J = 7.8$ Hz, 2H, 2-Ar-4,5-H), 7.05 (s, 1H, Imidazole-5-H), 5.58 (s, 2H, N^+-CH_2), 4.36 (t, $J = 7.4$ Hz, 2H, $N-CH_2$), 3.24 (t, $J = 7.3$ Hz, 2H, $S-CH_2$), 2.28 (s, 3H, Ar- CH_3), 1.95-1.89 (m, 2H, $N-CH_2CH_2$), 1.83-1.77 (m, 2H, $S-CH_2CH_2$), 1.51-1.46 (m, 2H, $N-(CH_2)_2CH_2$), 1.41-1.35 (m, 2H, $S-(CH_2)_2CH_2$); ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.5, 163.3, 138.1, 137.7, 137.2, 133.7, 131.6, 131.3, 131.2, 131.0, 130.1, 129.8, 127.7, 127.0, 122.2, 121.5, 121.4, 51.6, 50.0, 32.2, 30.0, 29.0, 27.7, 25.4, 19.3; HRMS (ESI) $[M-Cl]^+$ calcd for $C_{25}H_{27}Cl_2N_4OS$: 501.1277, found: 501.1266.

1-(6-((5-(2,4-dichlorophenyl)-1,3,4-oxadiazol-2-yl)thio)hexyl)-3-(4-methylbenzyl)-1H-imidazol-3-ium chloride (G_{15})

A light yellow liquid, yield 78.0%; 1H NMR (500 MHz, $CDCl_3$) δ 10.56 (s, 1H, Imidazole-2-H), 7.83 (d, $J = 8.5$ Hz, 1H, 1-Ar-6-H), 7.50 (d, $J = 2.1$ Hz, 1H, 1-Ar-3-H), 7.44 (t, $J = 1.5$ Hz, 1H, Imidazole-4-H), 7.34 (dd, $J = 8.5, 2.1$ Hz, 1H, 1-Ar-5-H), 7.30 (d, $J = 8.0$ Hz, 2H, 2-Ar-2,6-H), 7.26 (t, $J = 1.7$ Hz, 1H, Imidazole-5-H), 7.11 (d, $J = 7.9$ Hz, 2H, 2-Ar-3,5-H), 5.48 (s, 2H, N^+-CH_2), 4.31 (t, $J = 7.4$ Hz, 2H, $N-CH_2$), 3.20 (t, $J = 7.3$ Hz, 2H, $S-CH_2$), 2.27 (s, 3H, 2-Ar- CH_3), 1.92-1.86 (m, 2H, $N-CH_2CH_2$), 1.83-1.74 (m, 2H, $S-CH_2CH_2$), 1.49-1.43 (m, 2H, $N-(CH_2)_2CH_2$), 1.38-1.32 (m, 2H, $S-(CH_2)_2CH_2$); ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.5, 163.2, 139.4, 138.1, 137.3, 133.7, 131.6, 131.2, 130.3, 130.1, 129.0, 127.7, 122.2, 121.7, 121.4, 53.2, 49.9, 32.2, 29.9, 28.9, 27.7, 25.5, 21.2; HRMS (ESI) $[M-Cl]^+$ calcd for $C_{25}H_{27}Cl_2N_4OS$: 501.1277, found: 501.1264.

1-(6-((5-(2,4-dichlorophenyl)-1,3,4-oxadiazol-2-yl)thio)hexyl)-3-(3-methoxybenzyl)-1H-imidazol-3-ium chloride (G_{16})

A yellow liquid, yield 79.6%; 1H NMR (500 MHz, $CDCl_3$) δ 10.71 (s, 1H, Imidazole-2-H), 7.82 (d, $J = 8.5$ Hz, 1H, 1-Ar-6-H), 7.51 (s, 1H, Imidazole-4-H), 7.48 (d, $J = 2.1$ Hz, 1H, 1-Ar-3-H), 7.36 (s, 1H, Imidazole-5-H), 7.33 (dd, $J = 8.5, 2.0$ Hz, 1H, 1-Ar-5-H), 7.19 (t, $J = 7.9$ Hz, 1H, 2-Ar-5-H), 7.04-6.93 (m, 2H, 2-Ar-2,4-H), 6.80 (dd, $J = 8.2, 2.1$ Hz, 1H, 2-Ar-6-H), 5.49 (s, 2H, N^+-CH_2), 4.29 (t, $J = 7.1$ Hz, 2H, $N-CH_2$), 3.72 (s, 3H, $-OCH_3$), 3.20 (t, $J = 7.3$ Hz, 2H, $S-CH_2$), 1.95-1.83 (m, 2H, $N-CH_2CH_2$), 1.80-1.74 (m, 2H, $S-CH_2CH_2$), 1.47-1.41 (m, 2H, $N-(CH_2)_2CH_2$), 1.36-1.30 (m, 2H, $S-(CH_2)_2CH_2$); ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.4, 163.2, 160.2, 138.0, 137.4, 134.7, 133.6, 131.5, 131.2, 130.4, 127.7, 122.3, 121.9, 121.3, 121.0, 114.9,

114.5, 55.6, 53.2, 49.9, 32.2, 29.9, 28.9, 27.6, 25.4; HRMS (ESI) $[M-Cl]^+$ calcd for $C_{25}H_{27}Cl_2N_4O_2S$: 517.1226, found: 517.1215.

3-(2,6-dichlorobenzyl)-1-(6-((5-(2,4-dichlorophenyl)-1,3,4-oxadiazol-2-yl)thio)hexyl)-1*H*-imidazol-3-ium chloride (G₁₇)

A light yellow solid, yield 48.3%, m. p. 77.3-78.5 °C; ¹H NMR (500 MHz, CDCl₃) δ 10.88 (s, 1H, Imidazole-2-H), 7.87 (d, *J* = 8.7 Hz, 1H, 1-Ar-6-H), 7.55 (d, *J* = 2.0 Hz, 1H, 1-Ar-6-H), 7.49 (t, *J* = 1.7 Hz, 1H, Imidazole-4-H), 7.42-7.30 (m, 4H, 2-Ar-3,5-H & 1-Ar-5-H & 2-Ar-4-H), 7.12 (t, *J* = 1.9 Hz, 1H, Imidazole-5-H), 5.84 (s, 2H, N⁺-CH₂), 4.45 (t, *J* = 7.3 Hz, 2H, N-CH₂), 3.24 (t, *J* = 7.3 Hz, 2H, S-CH₂), 2.00-1.90 (m, 2H, N-CH₂CH₂), 1.85-1.80 (m, 2H, S-CH₂CH₂), 1.54-1.48 (m, 2H, N-(CH₂)₂CH₂), 1.44-1.37 (m, 2H, S-(CH₂)₂CH₂); ¹³C NMR (126 MHz, CDCl₃) δ 165.6, 163.3, 138.8, 138.1, 136.9, 133.8, 132.1, 131.6, 131.3, 129.3, 128.8, 127.8, 122.4, 121.4, 121.0, 50.1, 48.5, 32.3, 30.0, 29.0, 27.7, 25.4; HRMS (ESI) $[M-Cl]^+$ calcd for $C_{24}H_{23}Cl_4N_4OS$: 555.0341, found: 555.0331.

3-(3,4-dichlorobenzyl)-1-(6-((5-(2,4-dichlorophenyl)-1,3,4-oxadiazol-2-yl)thio)hexyl)-1*H*-imidazol-3-ium chloride (G₁₈)

A yellow liquid, yield 78.6%; ¹H NMR (500 MHz, CDCl₃) δ 10.46 (s, 1H, Imidazole-2-H), 7.82 (d, *J* = 7.3 Hz, 1H, 1-Ar-6-H), 7.66 (d, *J* = 1.9 Hz, 1H, 2-Ar-5-H), 7.60 (s, 1H, Imidazole-4-H), 7.52-7.45 (m, 3H, 1-Ar-3-H & 1-Ar-5-H & Imidazole-5-H), 7.39-7.32 (m, 2H, 2-Ar-2,6-H), 5.67 (s, 2H, N⁺-CH₂), 4.28 (t, *J* = 7.1 Hz, 2H, N-CH₂), 3.20 (t, *J* = 7.1 Hz, 2H, S-CH₂), 1.95-1.83 (m, 2H, N-CH₂CH₂), 1.82-1.72 (m, 2H, S-CH₂CH₂), 1.51-1.39 (m, 2H, N-(CH₂)₂CH₂), 1.37-1.31 (m, 2H, S-(CH₂)₂CH₂); ¹³C NMR (126 MHz, CDCl₃) δ 165.5, 163.2, 138.1, 137.2, 134.1, 133.6, 133.5, 133.1, 131.6, 131.6, 131.4, 131.2, 131.0, 128.8, 127.7, 122.4, 121.3, 51.7, 50.0, 32.2, 29.8, 28.9, 27.6, 25.5; HRMS (ESI) $[M-Cl]^+$ calcd for $C_{24}H_{23}Cl_4N_4OS$: 555.0341, found: 555.0331.

2. Toxicity of compounds A₆ and G₈ towards rice plants

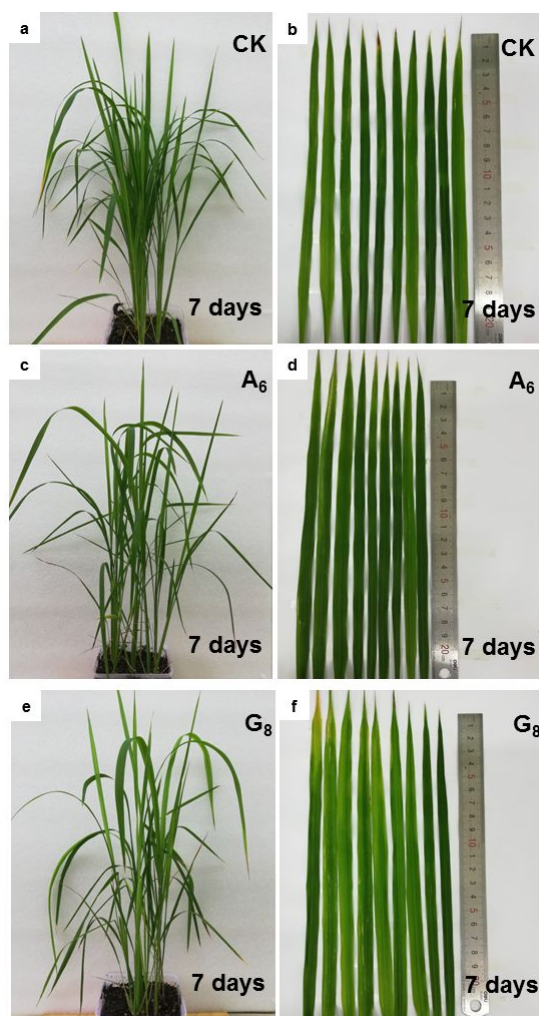


Figure Sa. Toxicity of compounds A₆ (c, d) and G₈ (e, f) towards rice plants, blank control (a, b).

The result showed that compounds A₆ and G₈ are non-toxic towards rice plants after treating them with the drug concentration of 200 µg/mL for 7 days, respectively.

3. SEM images of compounds A₆ and G₈ against *Xoo* and *Xac* at the drug concentration of 2×EC₅₀ and 5×EC₅₀ values

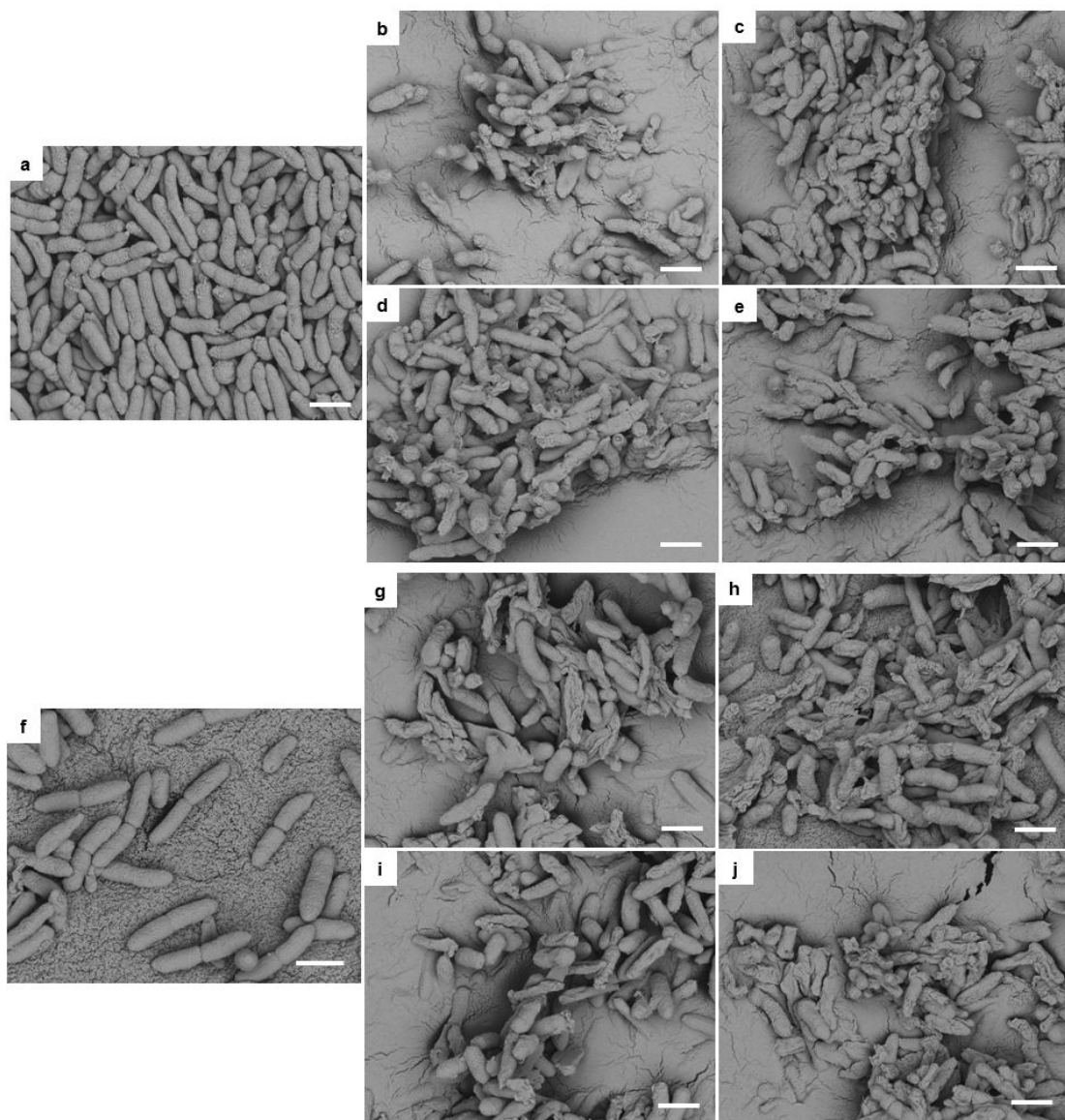


Figure Sb. SEM images of compounds A₆ and G₈ at the drug concentration of 2×EC₅₀ and 5×EC₅₀ values against *Xoo* (a: blank control; b: A₆, 2×EC₅₀; c: A₆, 5×EC₅₀; d: G₈, 2×EC₅₀; e: G₈, 5×EC₅₀) and *Xac* (f: blank control; g: A₆, 2×EC₅₀; h: A₆, 5×EC₅₀; i: G₈, 2×EC₅₀; j: G₈, 5×EC₅₀), scale bars for (a-j) are 1 μm.

4. TEM images of compounds A₆ and G₈ against *Xoo* and *Xac* at the drug concentration of 2×EC₅₀ and 5×EC₅₀ values

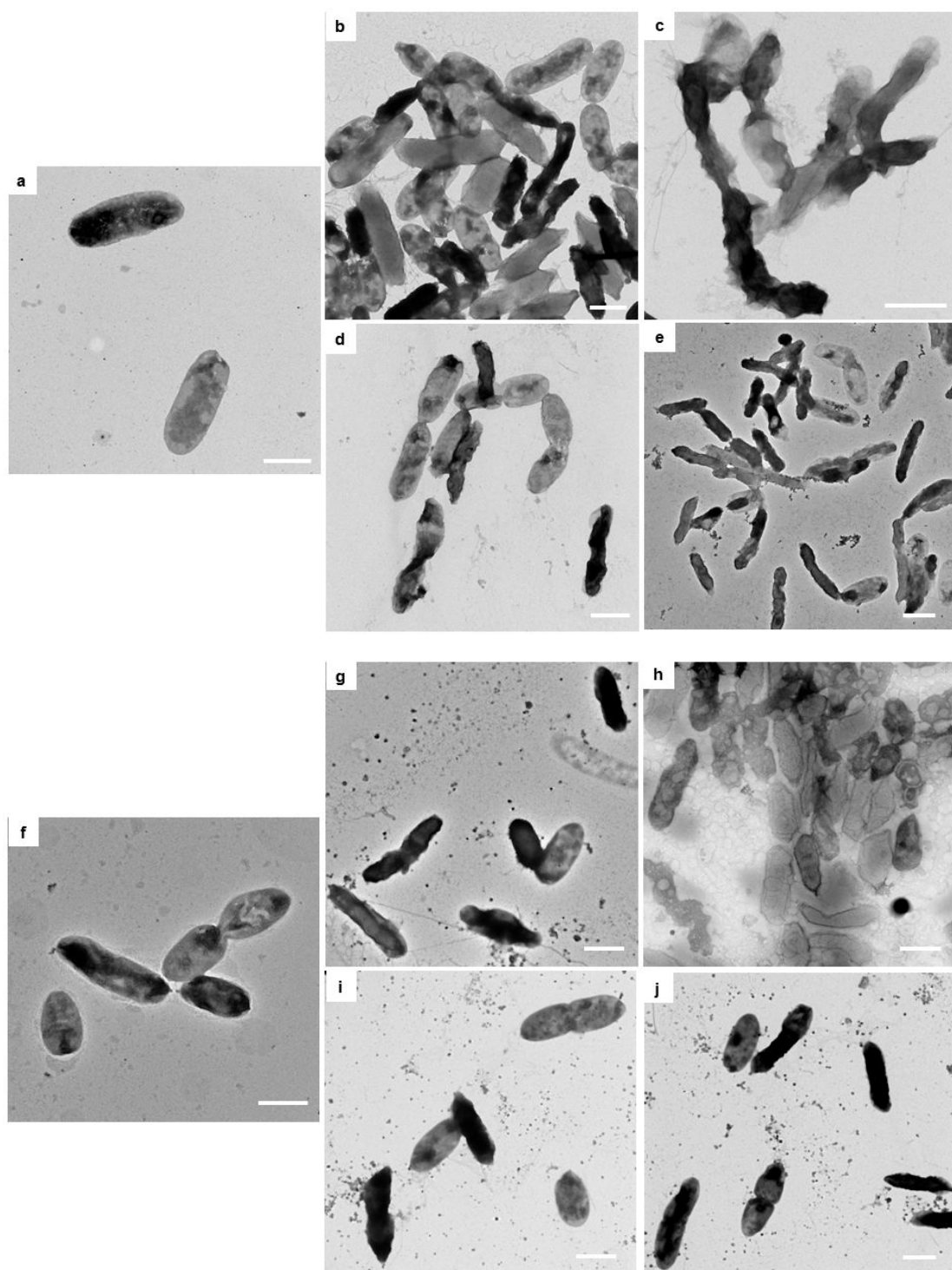
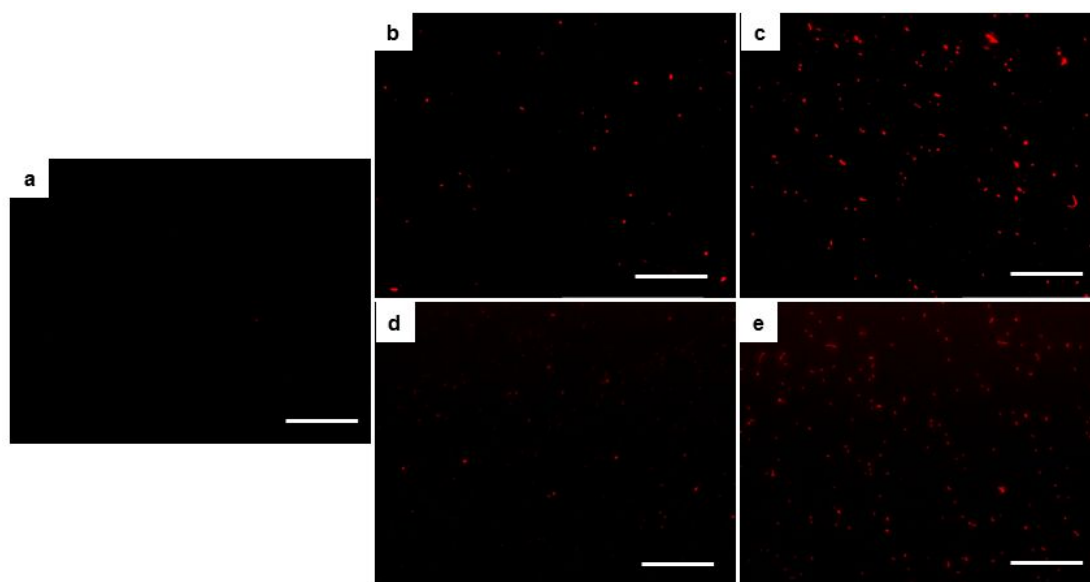


Figure Sc. TEM images of compounds A_6 and G_8 at the drug concentration of $2 \times EC_{50}$ and $5 \times EC_{50}$ values against *Xoo* (a: blank control; b: A_6 , $2 \times EC_{50}$; c: A_6 , $5 \times EC_{50}$; d: G_8 , $2 \times EC_{50}$; e: G_8 , $5 \times EC_{50}$) and *Xac* (f: blank control; g: A_6 , $2 \times EC_{50}$; h: A_6 , $5 \times EC_{50}$; i: G_8 , $2 \times EC_{50}$; j: G_8 , $5 \times EC_{50}$), scale bars for (a-j) are 1 μm .

In this assay, 1.5 mL *Xoo* (or *Xac*) cells incubated at the logarithmic phase were centrifuged and washed with PBS (pH = 7.0), and re-suspended in 1.5 mL of PBS buffer (pH = 7.0). After that, bacteria *Xoo* (or *Xac*) were incubated with compounds **A₆** or **G₈** at concentration of $2\times EC_{50}$ and $5\times EC_{50}$, and an equivalent volume of DMSO (solvent control) for 4 h at room temperature. After incubation, samples were prepared by drop-casting the aqueous solution on the carbon-coated copper grid, and then were negatively stained with a phosphotungstic acid solution. Finally, transmission electron microscopy (TEM) measurements were carried out on a FEI Talos F200C electron microscope operating at an acceleration voltage of 120 kV.

5. FM images of compounds **A₆** and **G₈** against *Xoo* and *Xac* at the drug concentration of $2\times EC_{50}$ and $5\times EC_{50}$ values



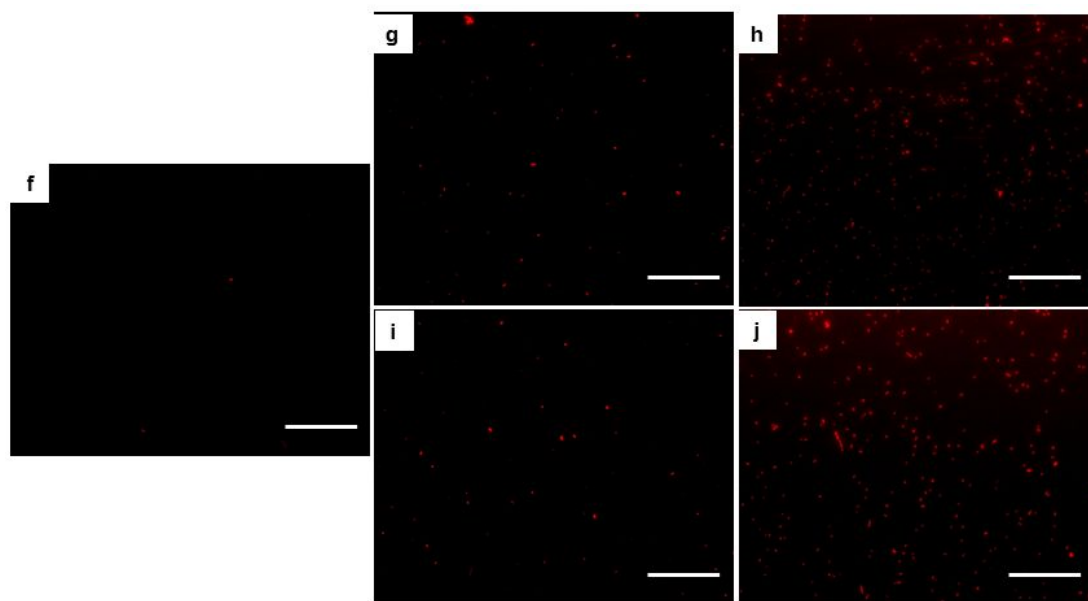


Figure Sd. FM images of compounds A_6 and G_8 at the drug concentration of $2\times EC_{50}$ and $5\times EC_{50}$ values against *Xoo* (a: blank control; b: A_6 , $2\times EC_{50}$; c: A_6 , $5\times EC_{50}$; d: G_8 , $2\times EC_{50}$; e: G_8 , $5\times EC_{50}$) and *Xac* (f: blank control; g: A_6 , $2\times EC_{50}$; h: A_6 , $5\times EC_{50}$; i: G_8 , $2\times EC_{50}$; j: G_8 , $5\times EC_{50}$), scale bars for (a-j) are 50 μm .

We investigated the effect of compounds A_6 and G_8 on membrane permeability using the membrane impermeable DNA probe propidium iodide (PI) to label DNA in cells in which the membrane is compromised. In this method, 200 μL of solvent NB (1.5 g beef extract, 2.5 g peptone, 0.5 g yeast powder, 5.0 g glucose, and 500 mL distilled water; pH = 7.0-7.2) containing *Xoo* (or *Xac*) incubated on the phase of logarithmic growth were washed 3 times with buffer (PBS, pH = 7.0). Following the final wash, the bacteria were pelleted and then re-suspended in 200 μL of PBS buffer (pH= 7.0). The diluted cells were then treated with compounds A_6 and G_8 at concentration of $2\times EC_{50}$ and $5\times EC_{50}$, and an equivalent volume of DMSO (solvent control) incubating for 4 h at room temperature. And then 5 μL of 10 $\mu g/mL$ PI were added to the solution and incubated for 15 min in the dark at room temperature. The samples were imaged and collected by fluorescent spectroscopy (EVOS™ FL Auto Imaging System AMAFD1000).

6. 1H NMR, ^{19}F NMR, ^{13}C NMR and HRMS Spectra of A_1 , A_4 - A_8 , B_4 - B_6 , B_8 , C_5 - C_6 , C_8 , C_{10} , D_6 , E_1 - E_{14} , F_1 - F_6 and G_1 - G_{18} (Figure S1 to S162)

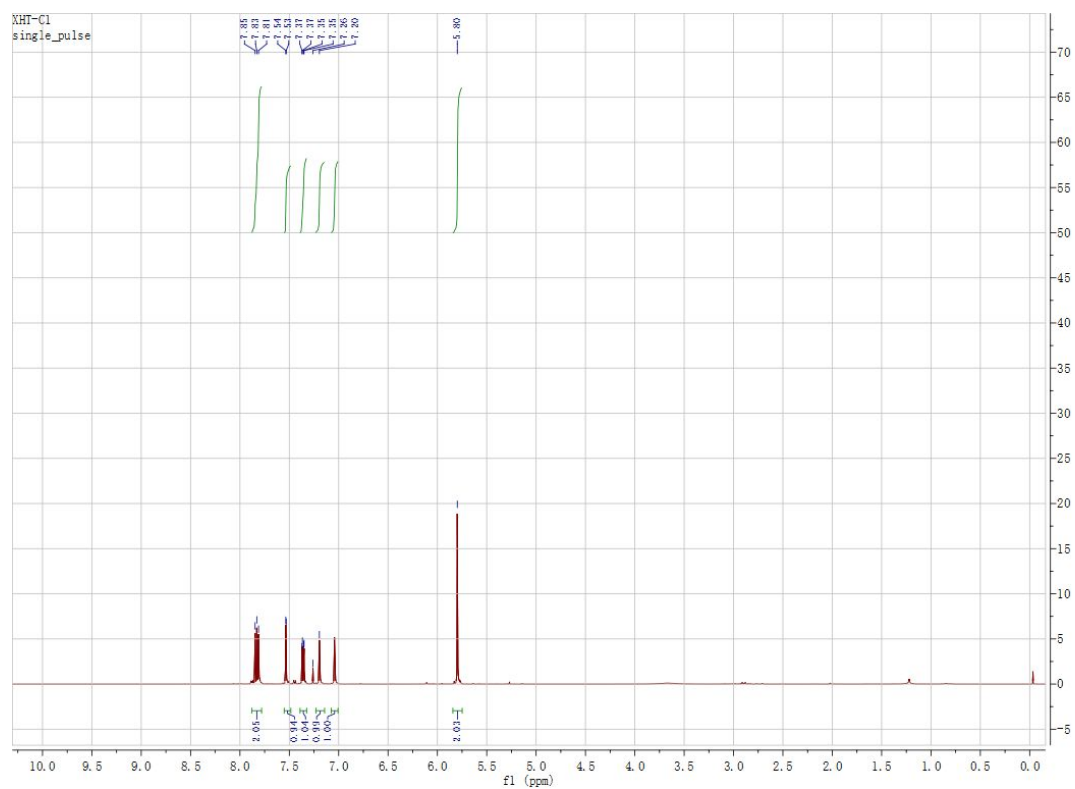


Figure S1. ¹H NMR Spectrum (CDCl₃, 500 MHz) of A₁.

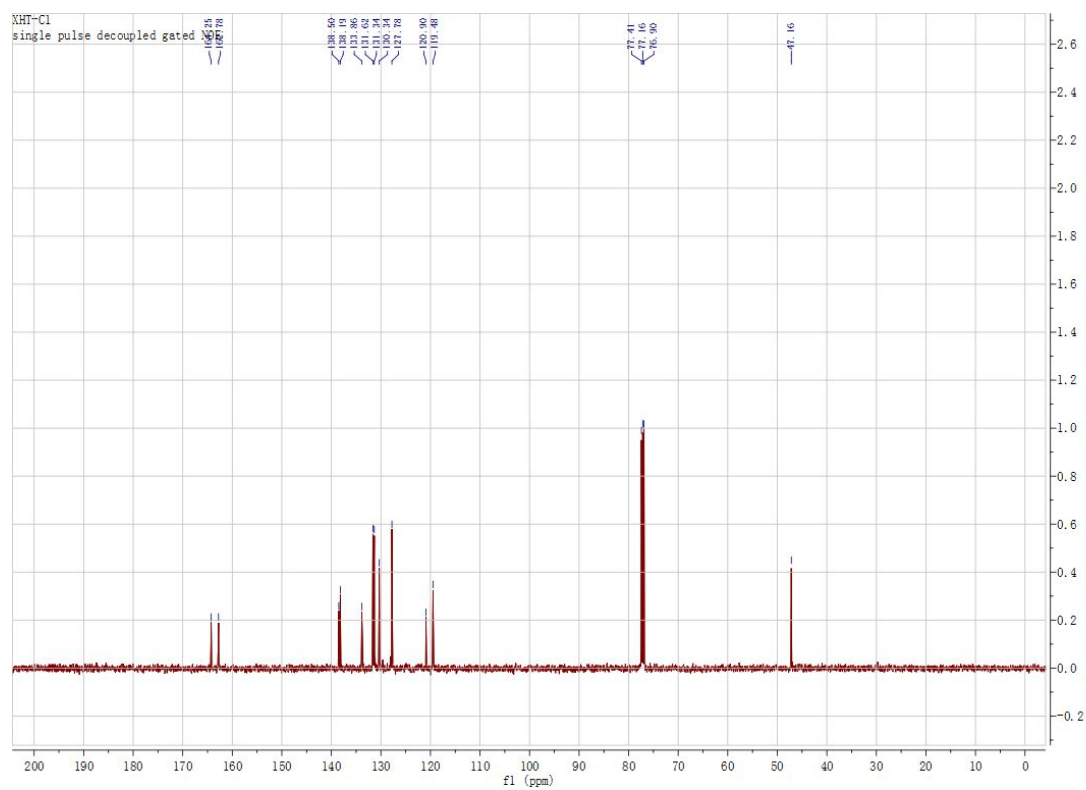


Figure S2. ¹³C NMR Spectrum (CDCl₃, 126 MHz) of A₁.

2018122858 #87 RT: 0.84 AV: 1 NL: 5.16E8
T: FTMS + p ESI Full ms [100.0000-1000.0000]

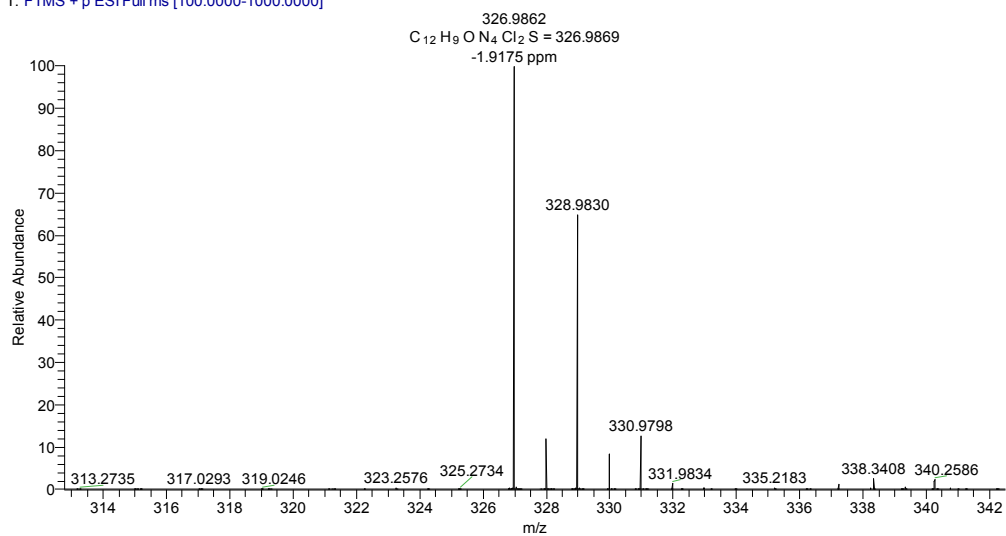


Figure S3. HRMS Spectrum of A₁.

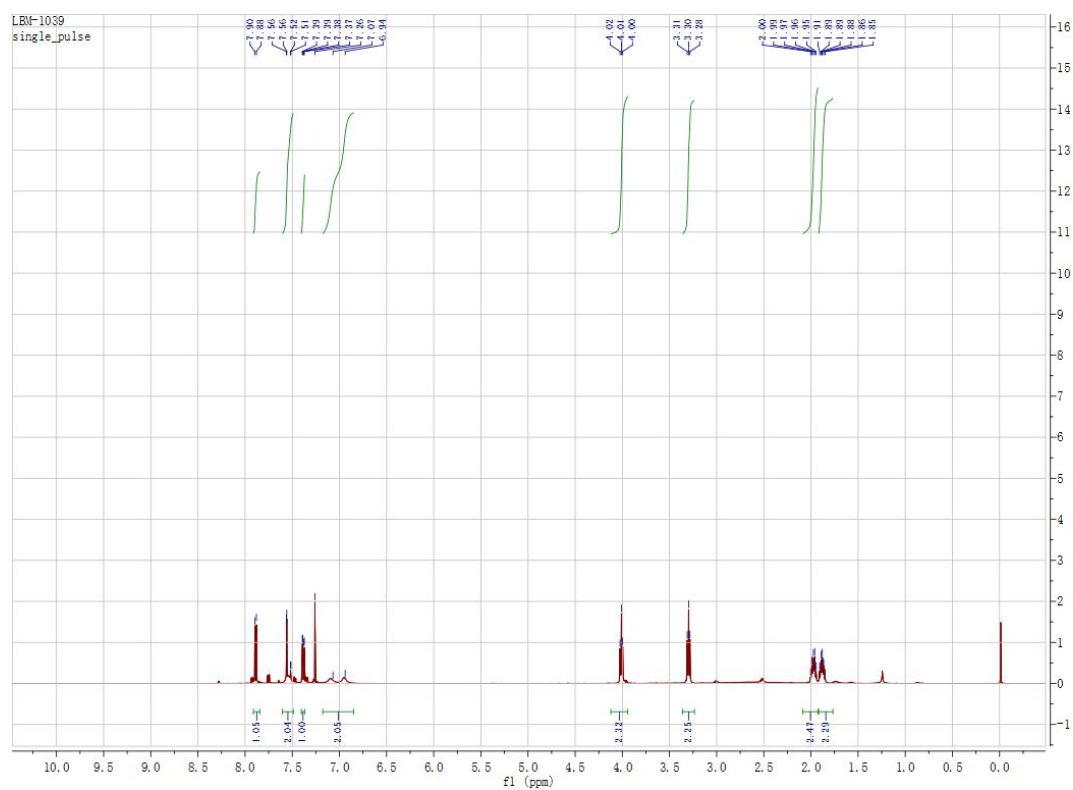


Figure S4. 1H NMR Spectrum ($CDCl_3$, 500 MHz) of A₄.

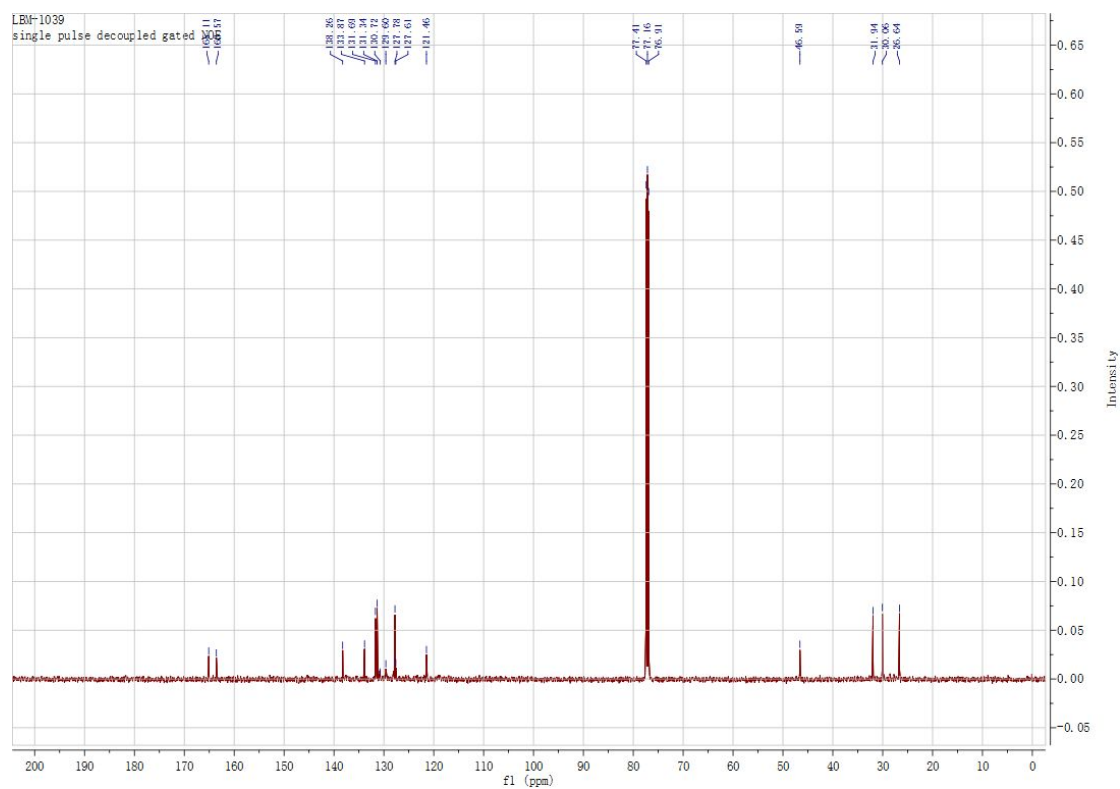


Figure S5. ^{13}C NMR Spectrum (CDCl_3 , 126 MHz) of A_4 .

2018122835 #93 RT: 0.89 AV: 1 NL: 2.37E9
T: FTMS + p ESI Full ms [100.0000-1000.0000]

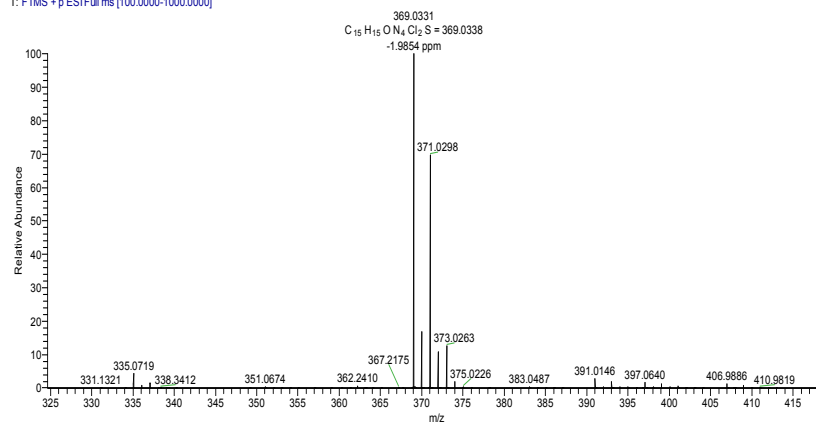


Figure S6. HRMS Spectrum of A_4 .

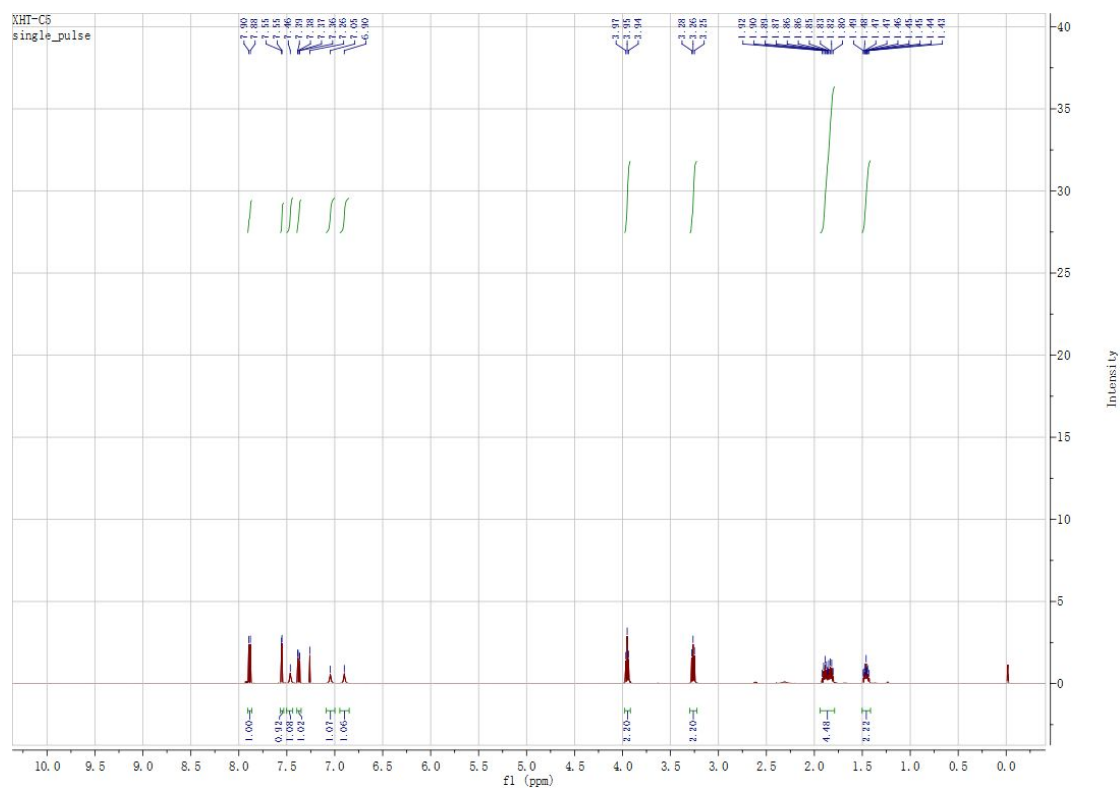


Figure S7. ¹H NMR Spectrum (CDCl₃, 500 MHz) of A₅.

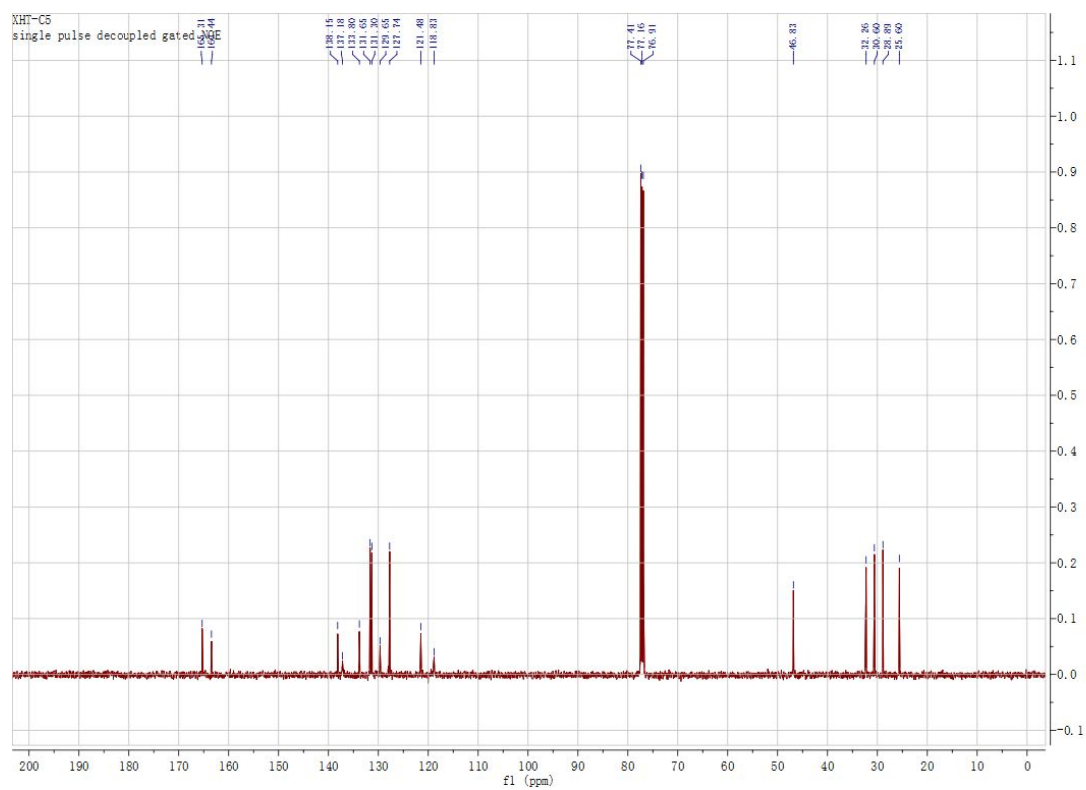


Figure S8. ¹³C NMR Spectrum (CDCl₃, 126 MHz) of A₅.

2018122851#103 RT: 0.99 AV: 1 NL: 3.27E9
T: FTMS + p ESI Full ms [100.0000-1000.0000]

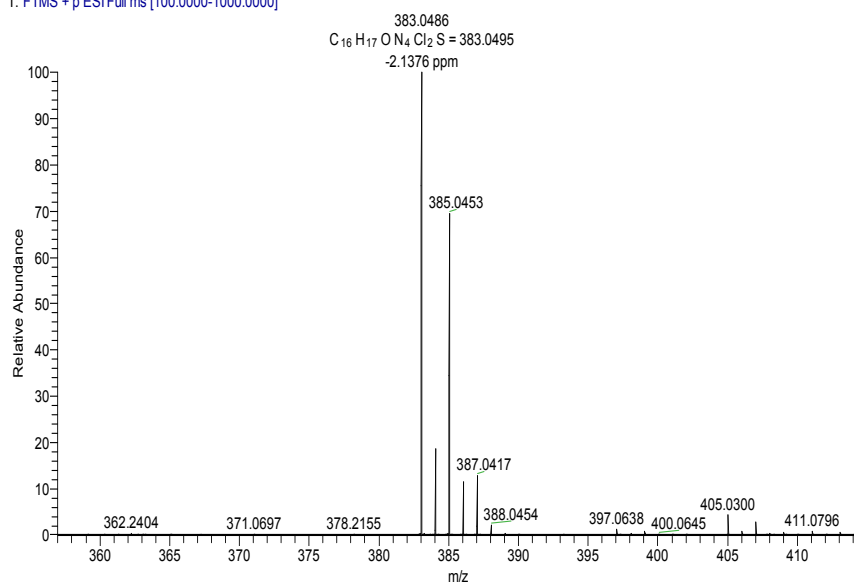


Figure S9. HRMS Spectrum of A₅.

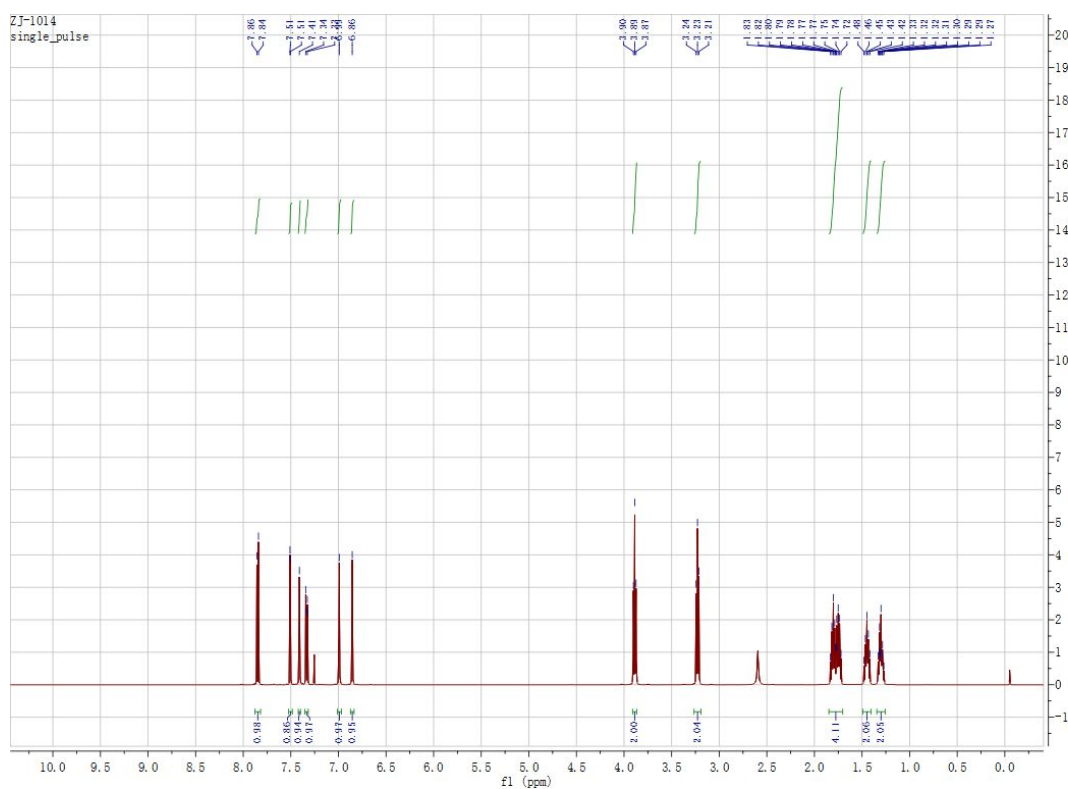


Figure S10. ¹H NMR Spectrum (CDCl₃, 500 MHz) of A₆.

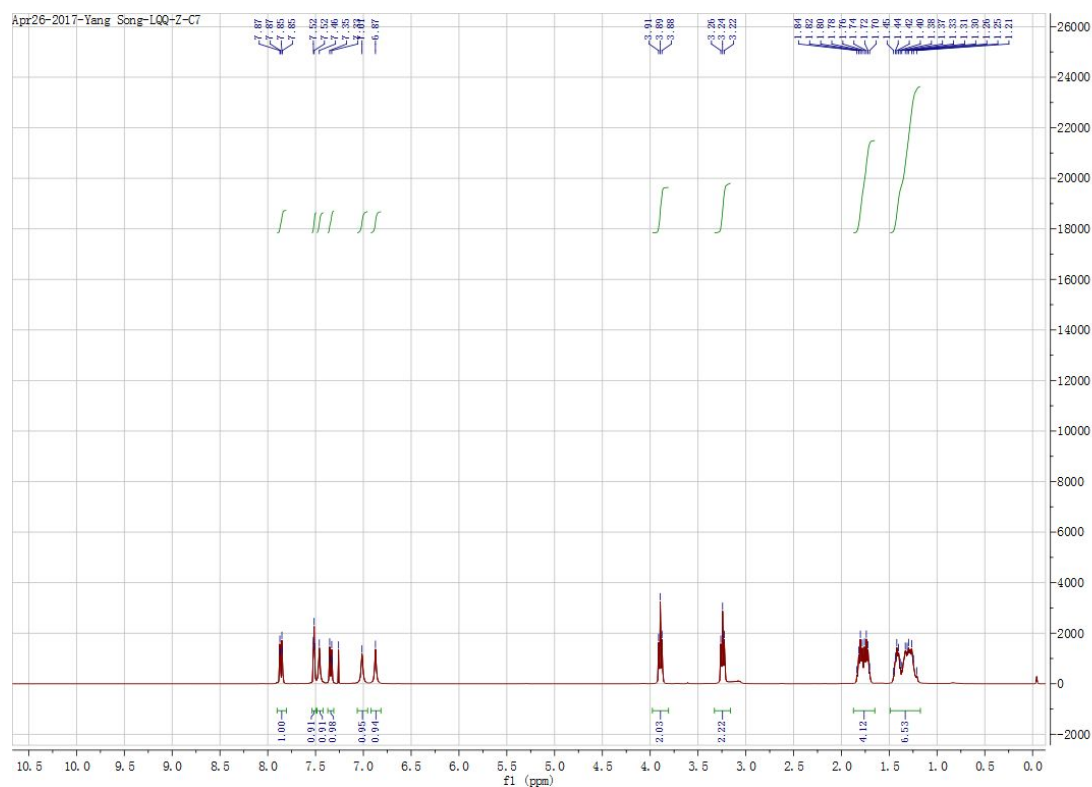


Figure S13. ^1H NMR Spectrum (CDCl_3 , 500 MHz) of A_7 .

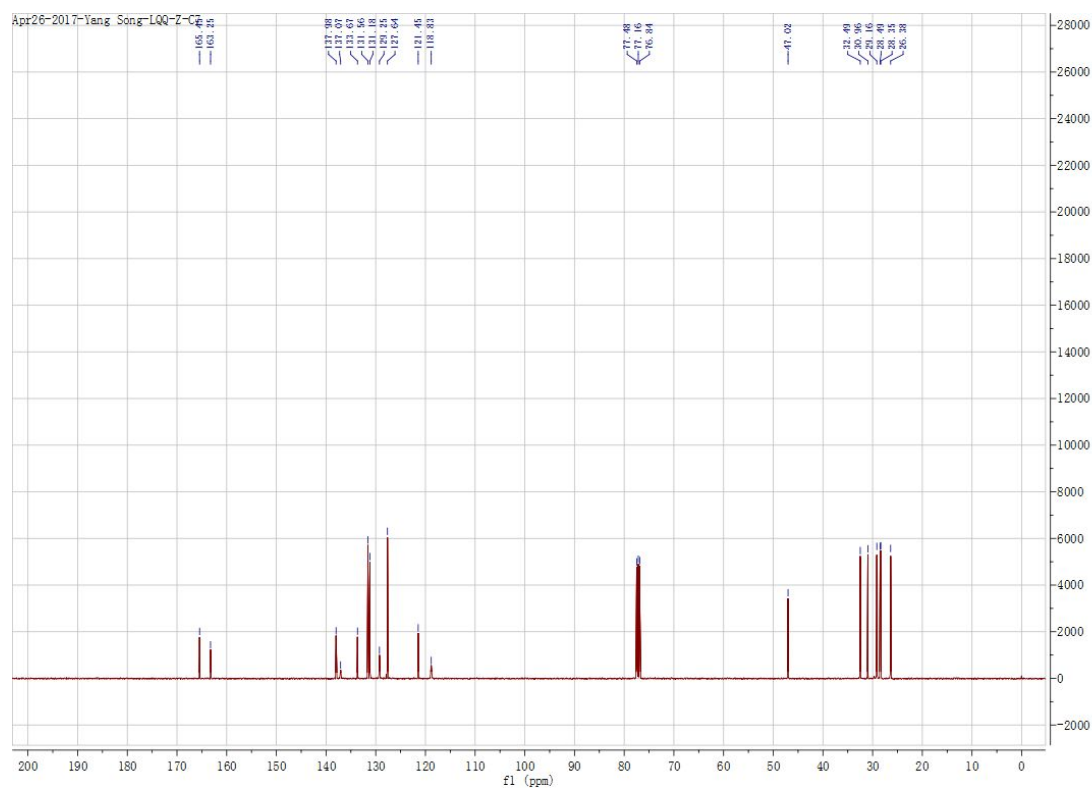


Figure S14. ^{13}C NMR Spectrum (CDCl_3 , 126 MHz) of A_7 .

2018122859 #91 RT: 0.88 AV: 1 NL: 6.01E8
T: FTMS + p ESI Full ms [100.0000-1000.0000]

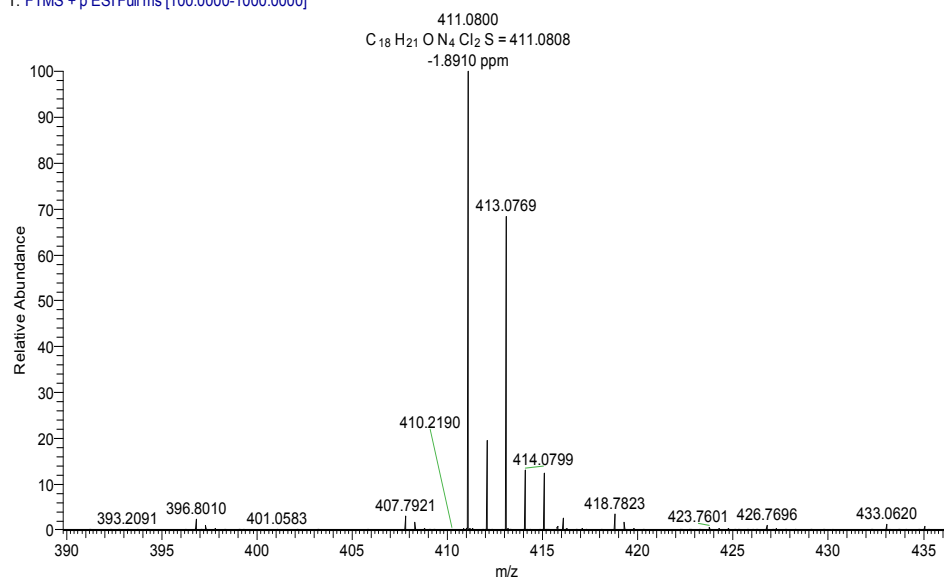


Figure S15. HRMS Spectrum of A₇.

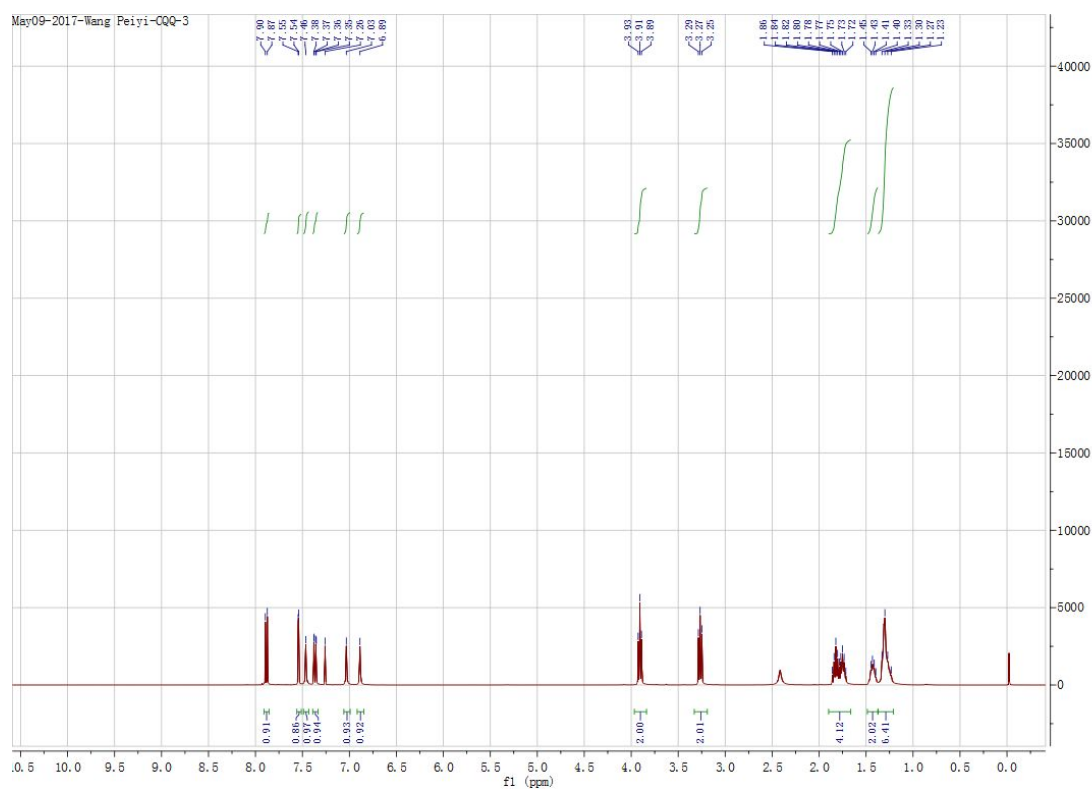


Figure S16. ¹H NMR Spectrum (CDCl₃, 500 MHz) of A₈.

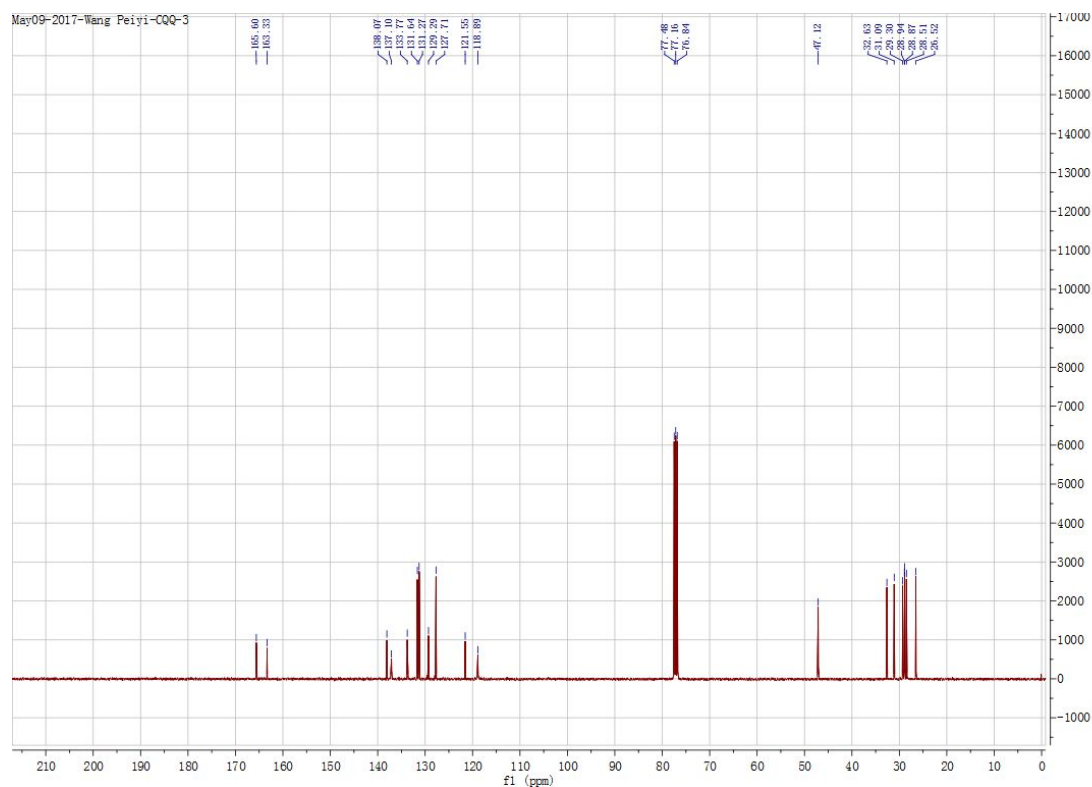


Figure S17. ^{13}C NMR Spectrum (CDCl_3 , 126 MHz) of A_8 .

2018122837 #87 RT: 0.84 AV: 1 NL: 1.22E9
T: FTMS + p ESI Full ms [100.0000-1000.0000]

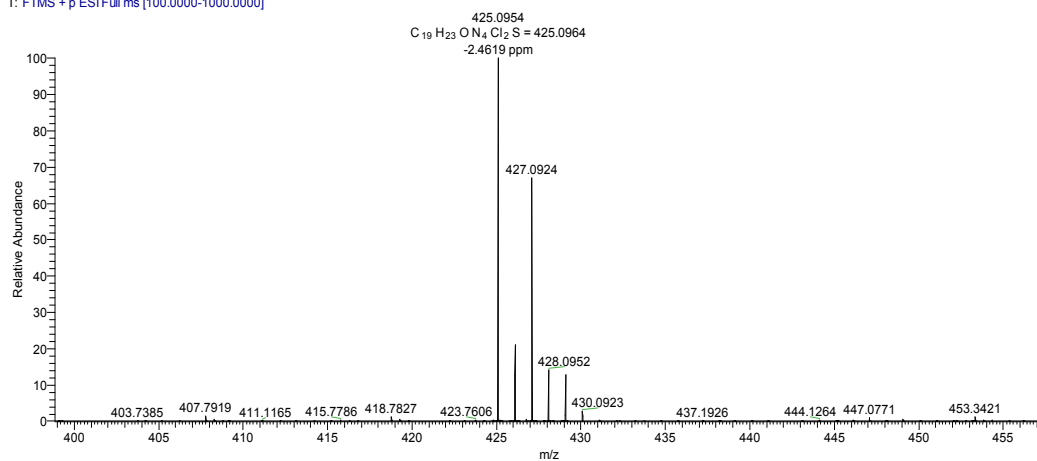


Figure S18. HRMS Spectrum of A_8 .

2018122831 #91 RT: 0.88 AV: 1 NL: 2.29E9
T: FTMS + p ESI Full ms [100.0000-1000.0000]

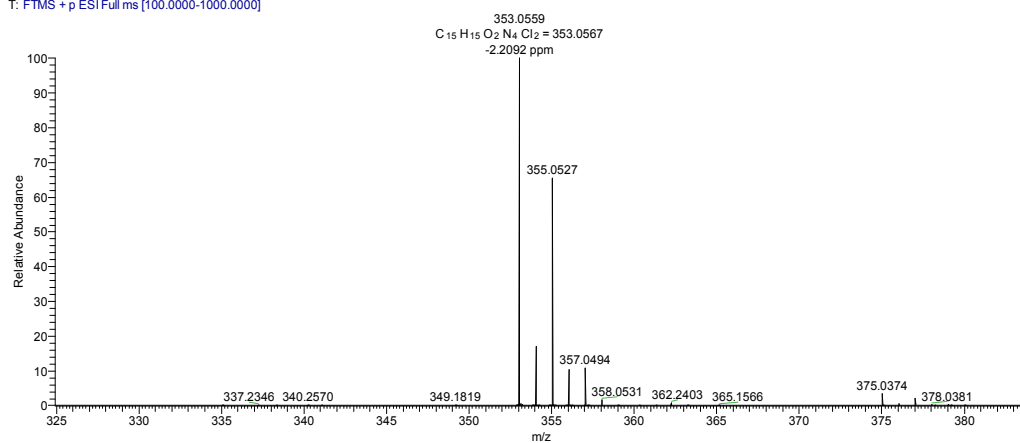


Figure S21. HRMS Spectrum of B₄.

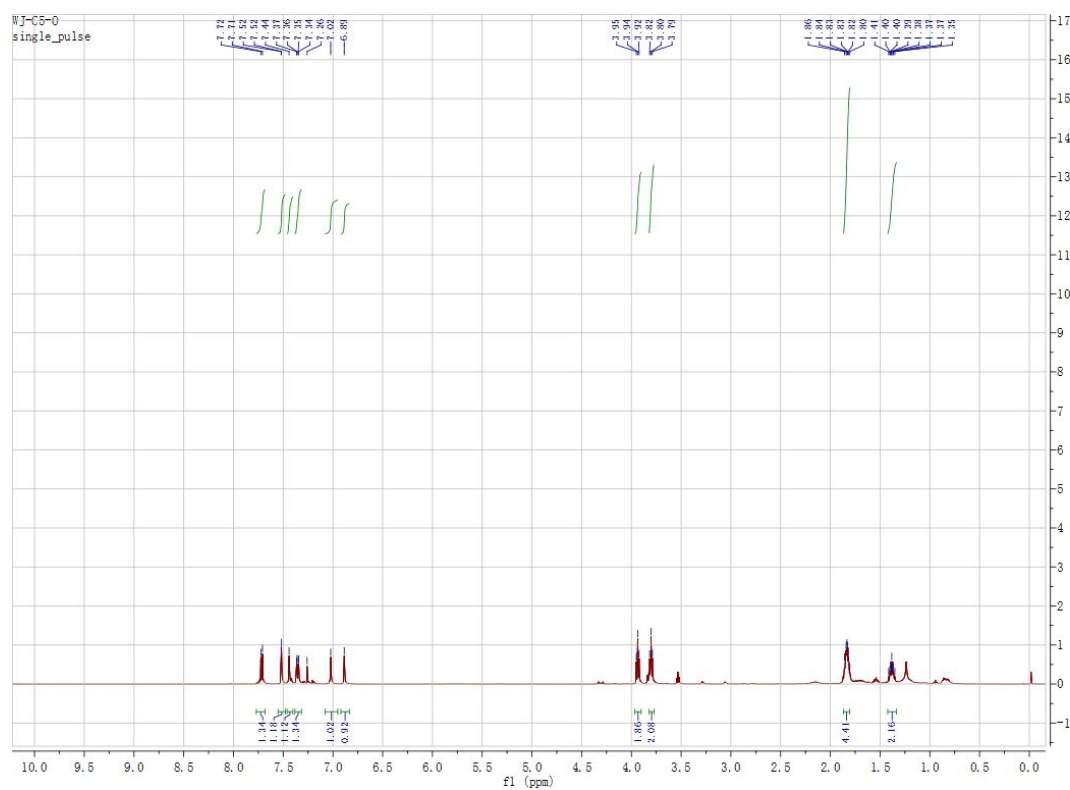


Figure S22. ¹H NMR Spectrum (CDCl₃, 500 MHz) of B₅.

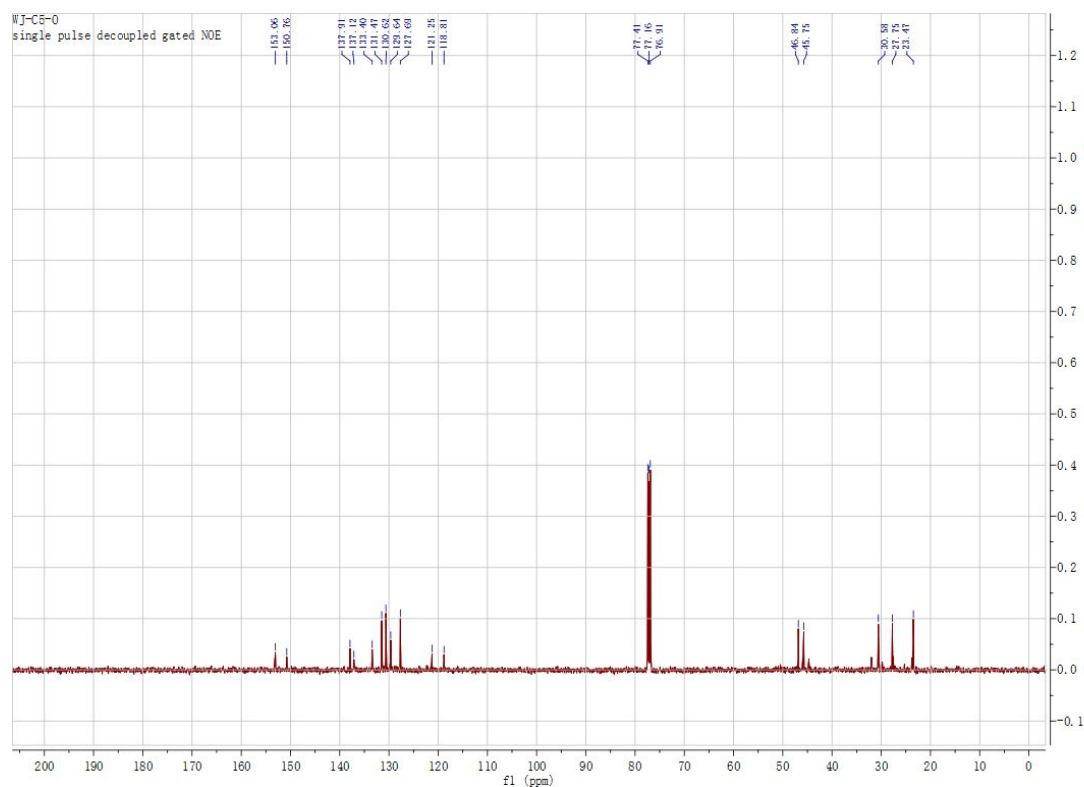


Figure S23. ^{13}C NMR Spectrum (CDCl_3 , 126 MHz) of B_5 .

2018122832#85 RT: 0.82 AV: 1 NL: 8.06E8
T: FTMS + p ESI Full ms [100.0000-1000.0000]

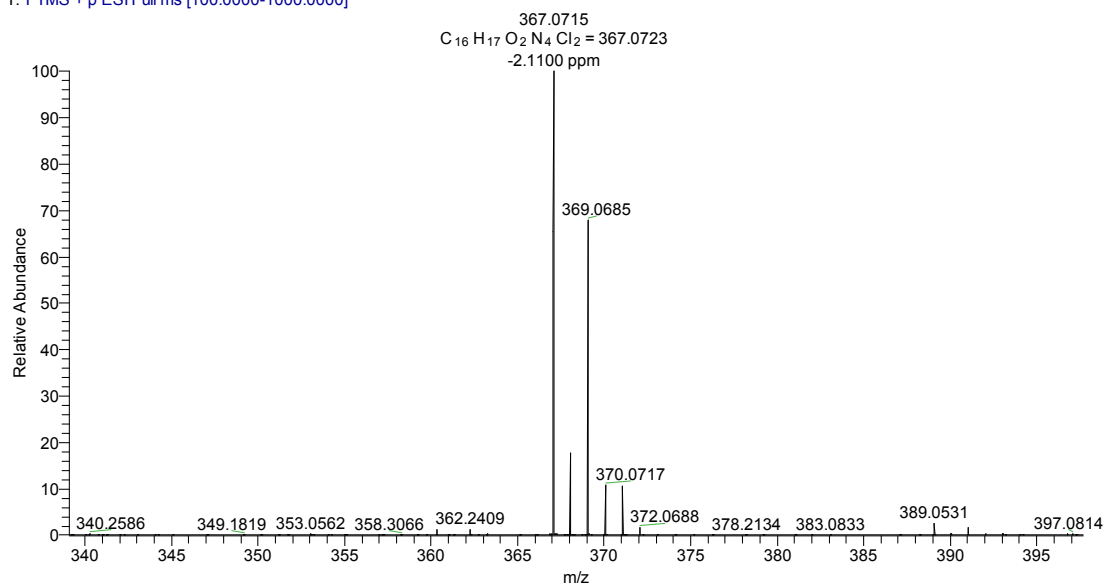


Figure S24 HRMS Spectrum of B_5 .

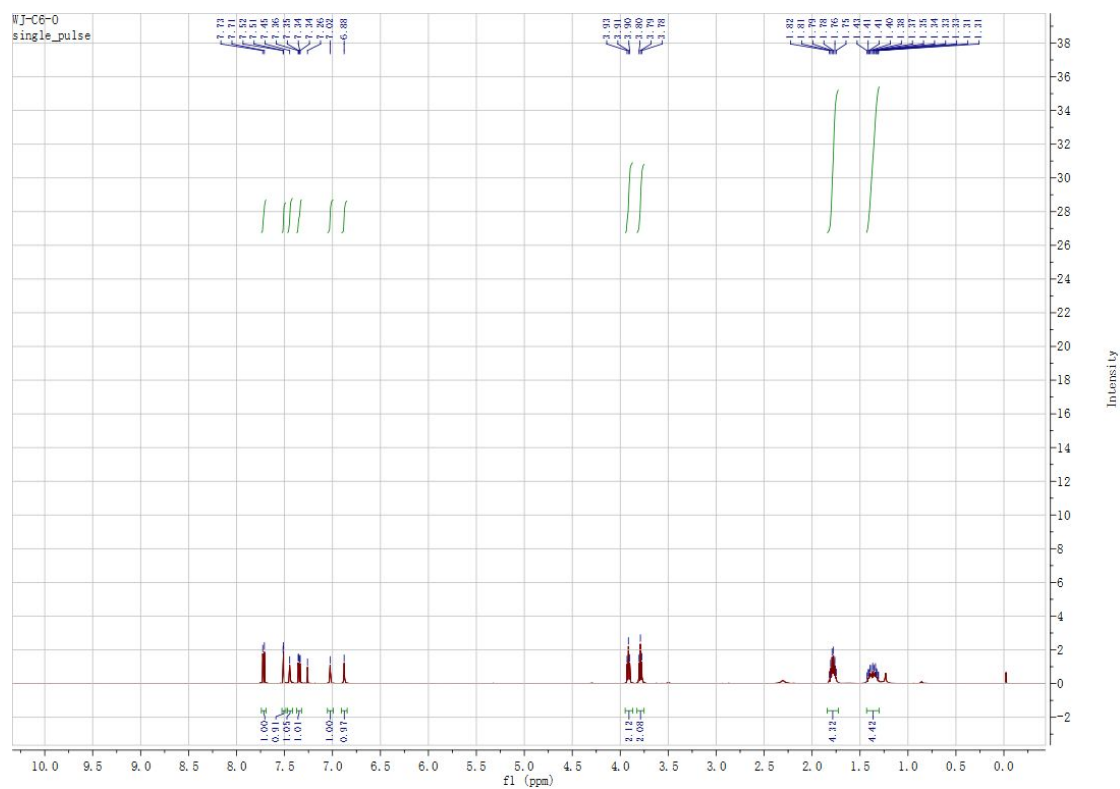


Figure S25. ^1H NMR Spectrum (CDCl_3 , 500 MHz) of B_6 .

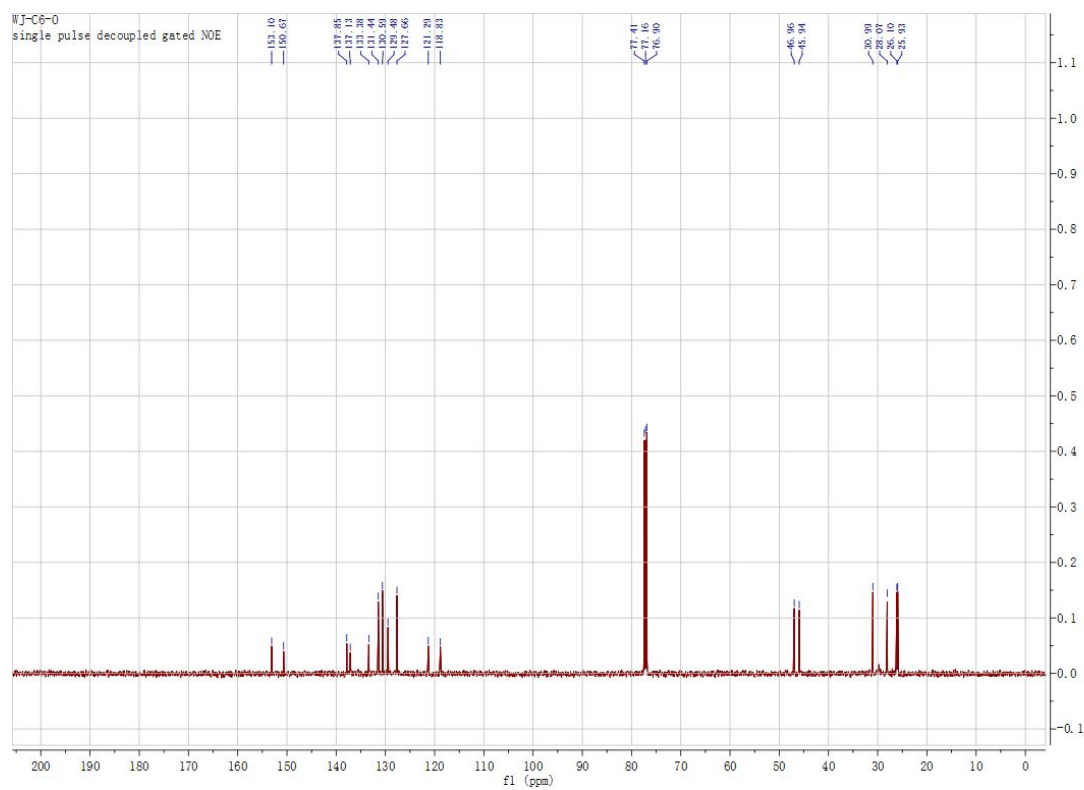


Figure S26. ^{13}C NMR Spectrum (CDCl_3 , 126 MHz) of B_6 .

2018122833 #89 RT: 0.86 AV: 1 NL: 2.50E9
T: FTMS + p ESI Full ms [100.0000-1000.0000]

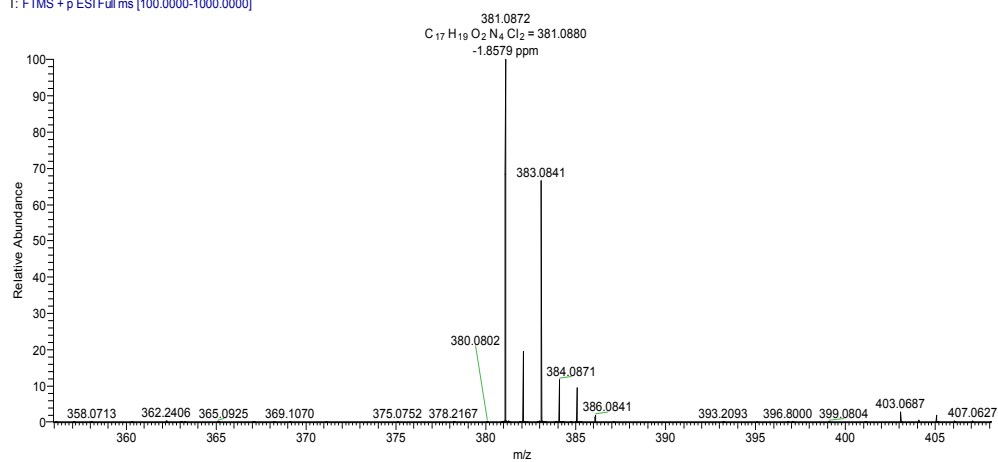


Figure S27. HRMS Spectrum of B₆.

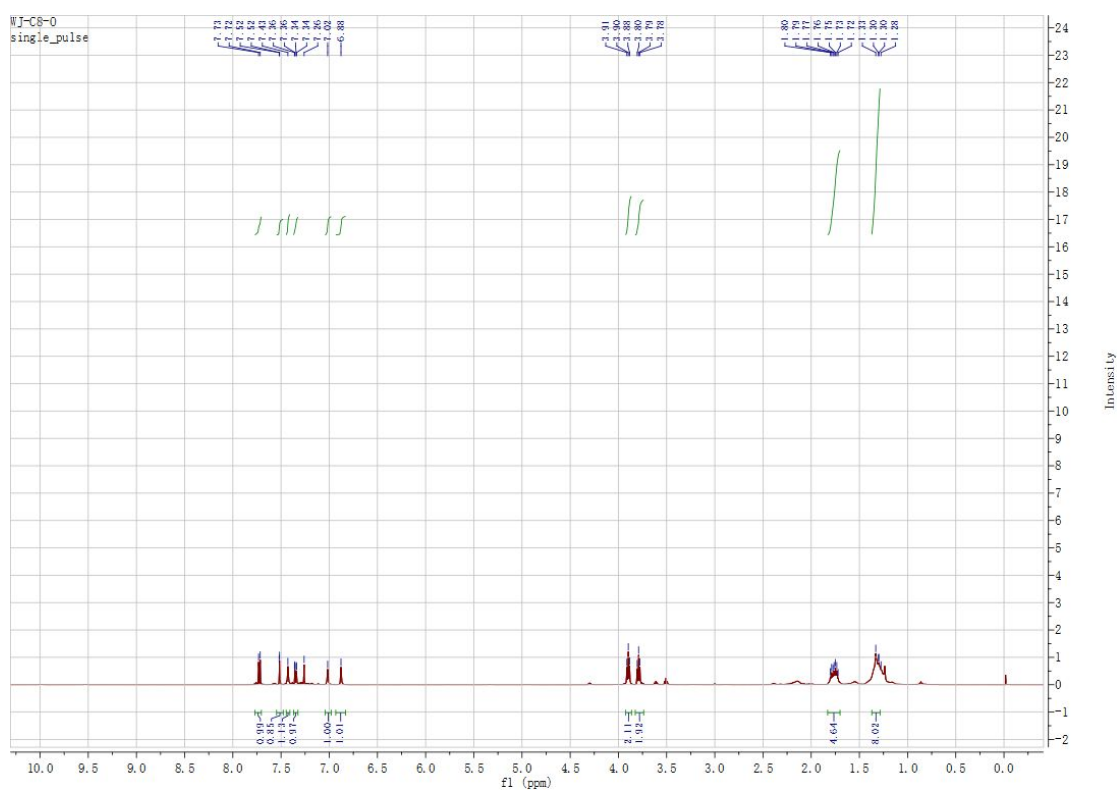


Figure S28. ¹H NMR Spectrum (CDCl₃, 500 MHz) of B₈.

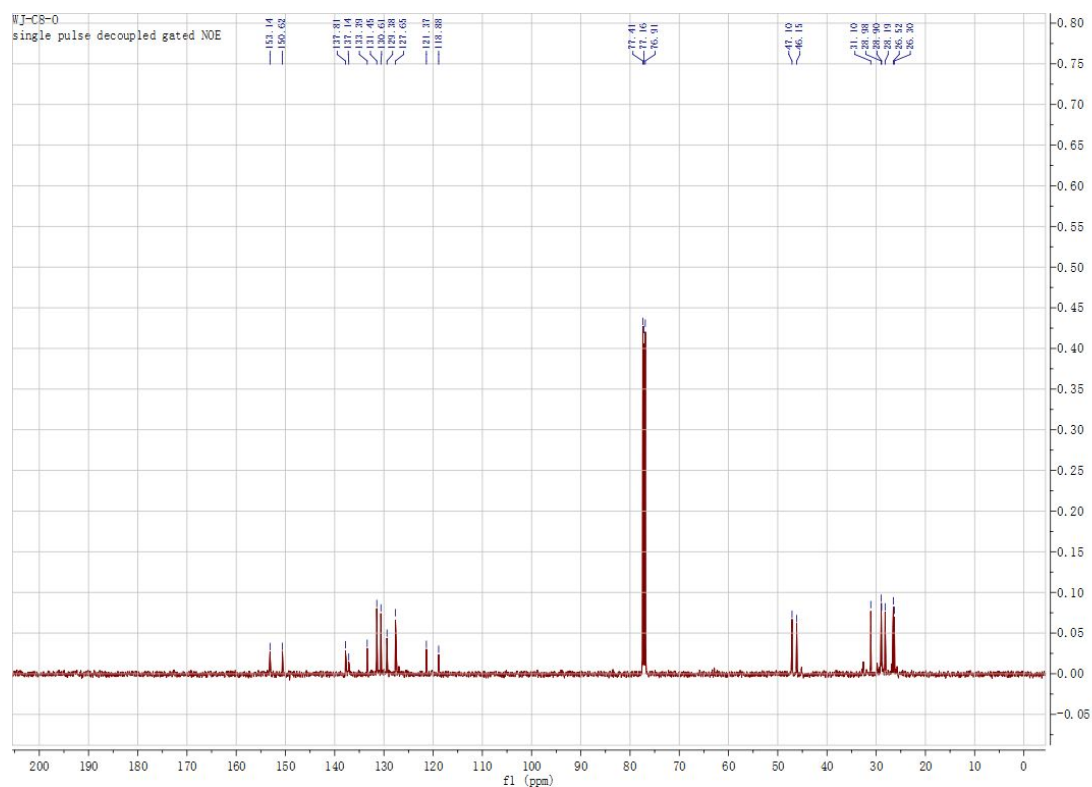


Figure S29. ^{13}C NMR Spectrum (CDCl_3 , 126 MHz) of B_8 .

2018122834 #97 RT: 0.94 AV: 1 NL: 5.12E8
T: FTMS + p ESI Full ms [100.0000-1000.0000]

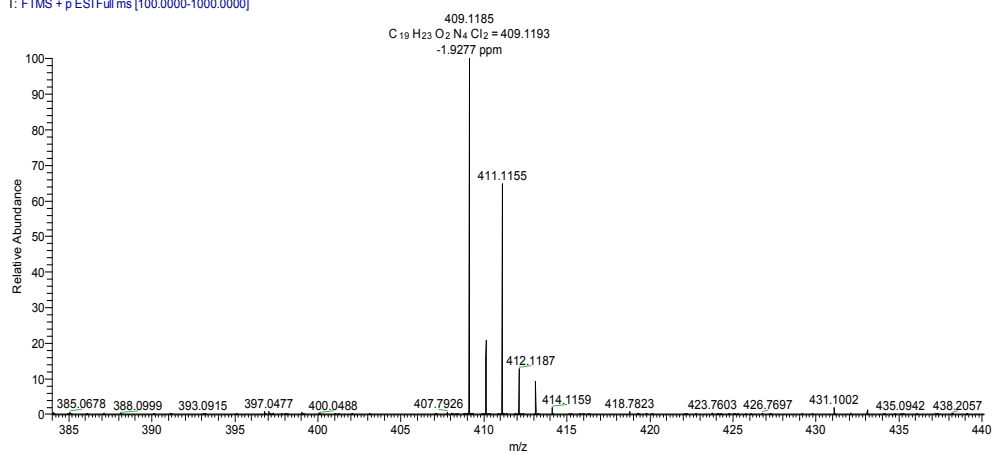


Figure S30. HRMS Spectrum of B_8 .

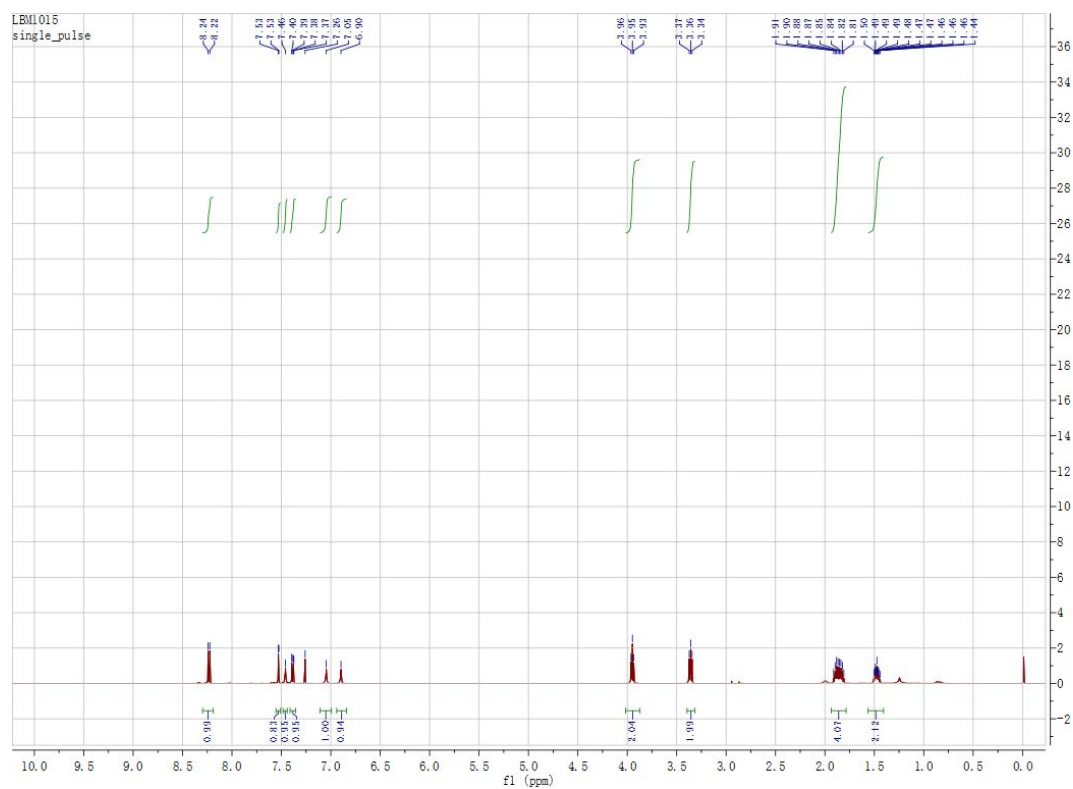


Figure S31. ^1H NMR Spectrum (CDCl_3 , 500 MHz) of C_5 .

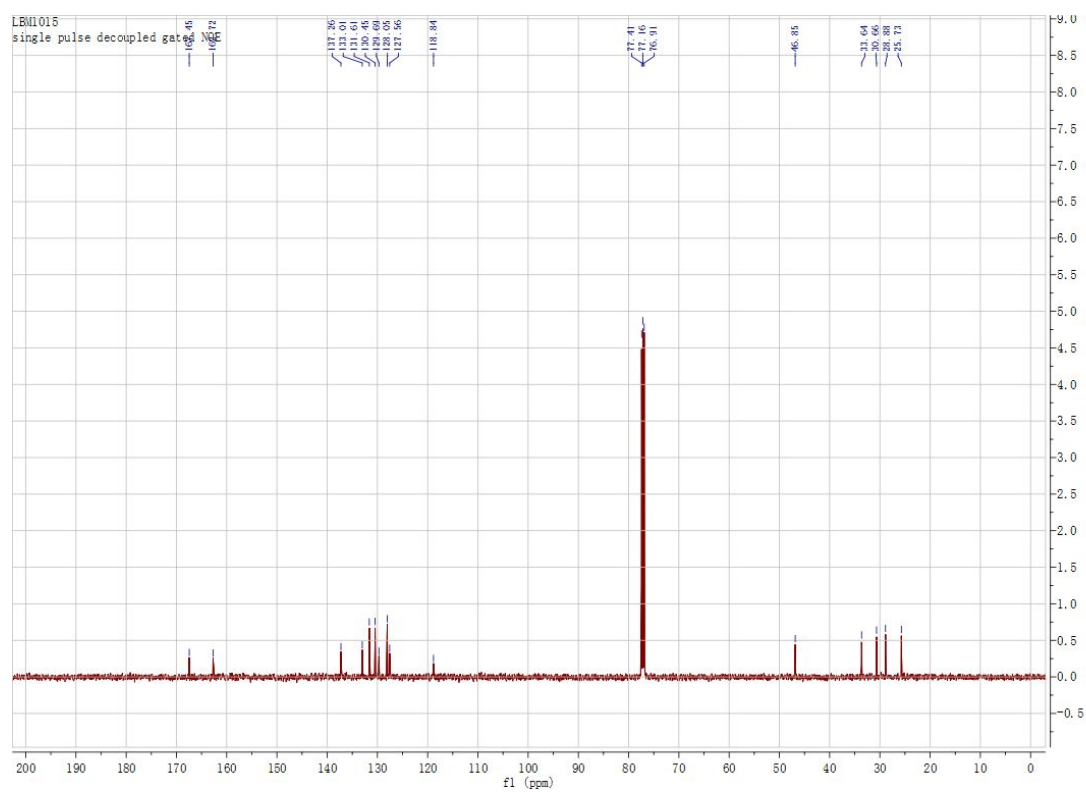


Figure S32. ^{13}C NMR Spectrum (CDCl_3 , 126 MHz) of C_5 .

2018122826 #113 RT: 1.09 AV: 1 NL: 3.85E8
T: FTMS + p ESI Full ms [100.0000-1000.0000]

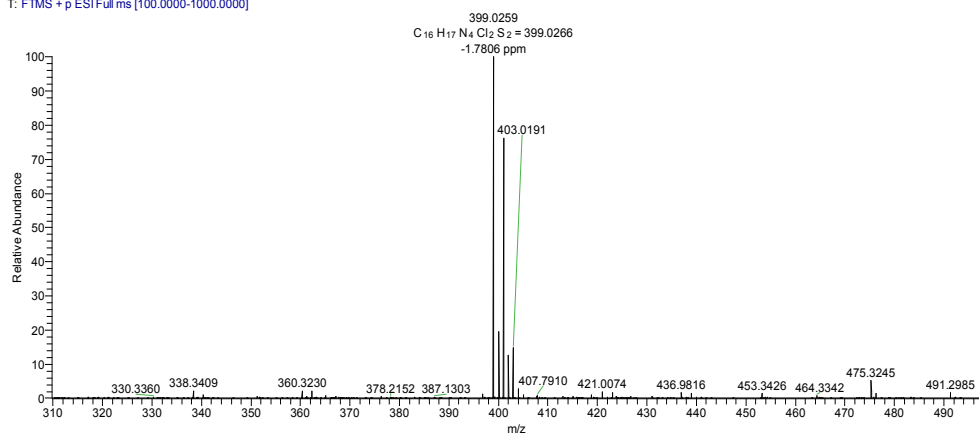


Figure S33. HRMS Spectrum of C_5 .

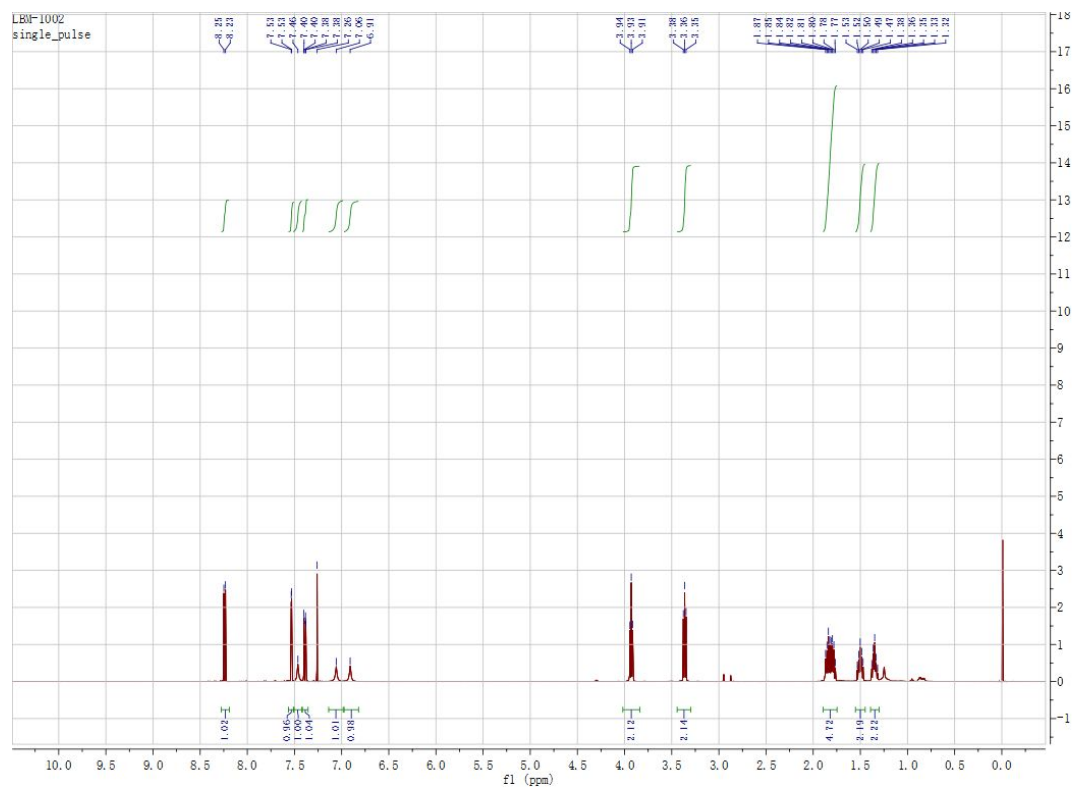


Figure S34. 1H NMR Spectrum ($CDCl_3$, 500 MHz) of C_6 .

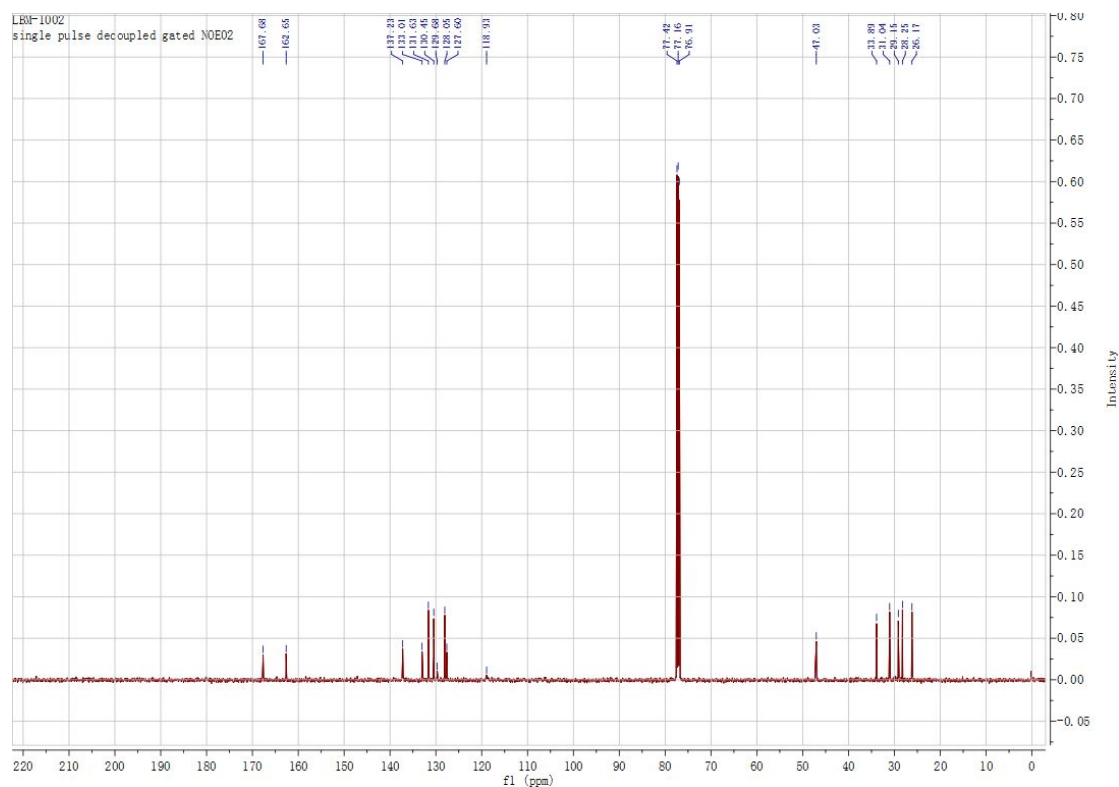


Figure S35. ^{13}C NMR Spectrum (CDCl_3 , 126 MHz) of C_6 .

2018122828#119 RT: 1.15 AV: 1 NL: 3.49E8
T: FTMS + p ESI Full ms [100.0000-1000.0000]

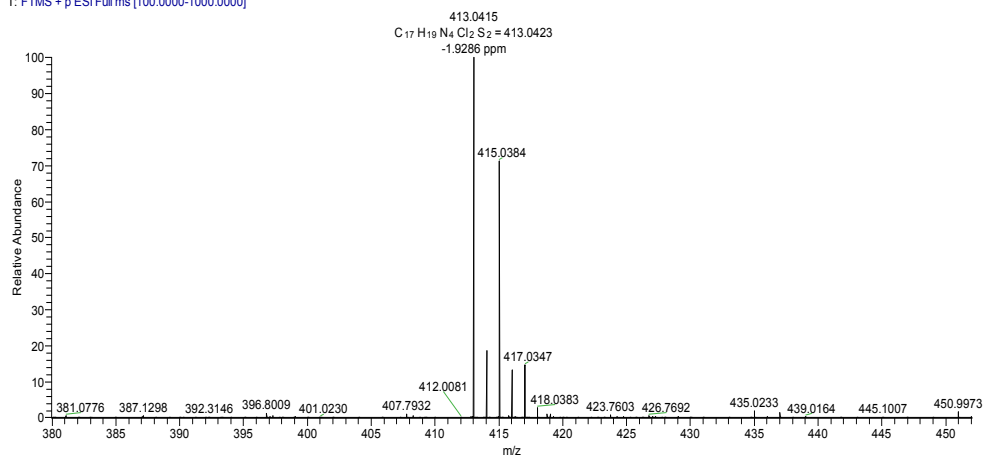


Figure S36. HRMS Spectrum of C_6 .

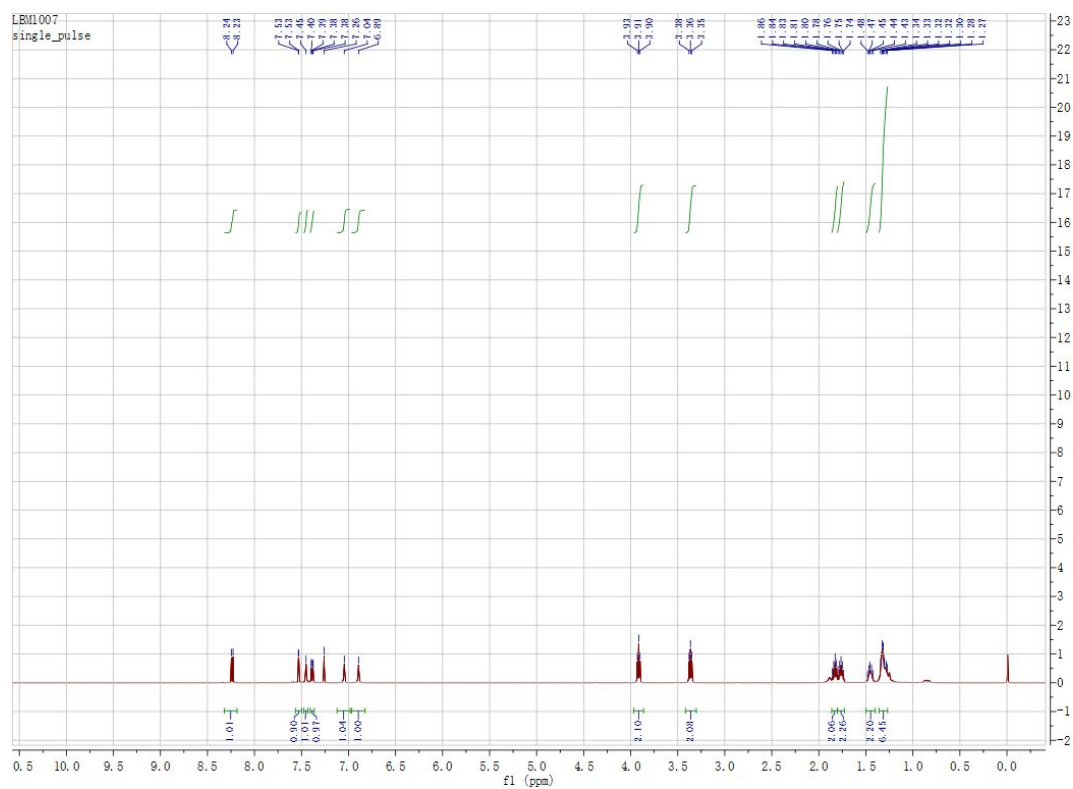


Figure S37. ^1H NMR Spectrum (CDCl_3 , 500 MHz) of C_8 .

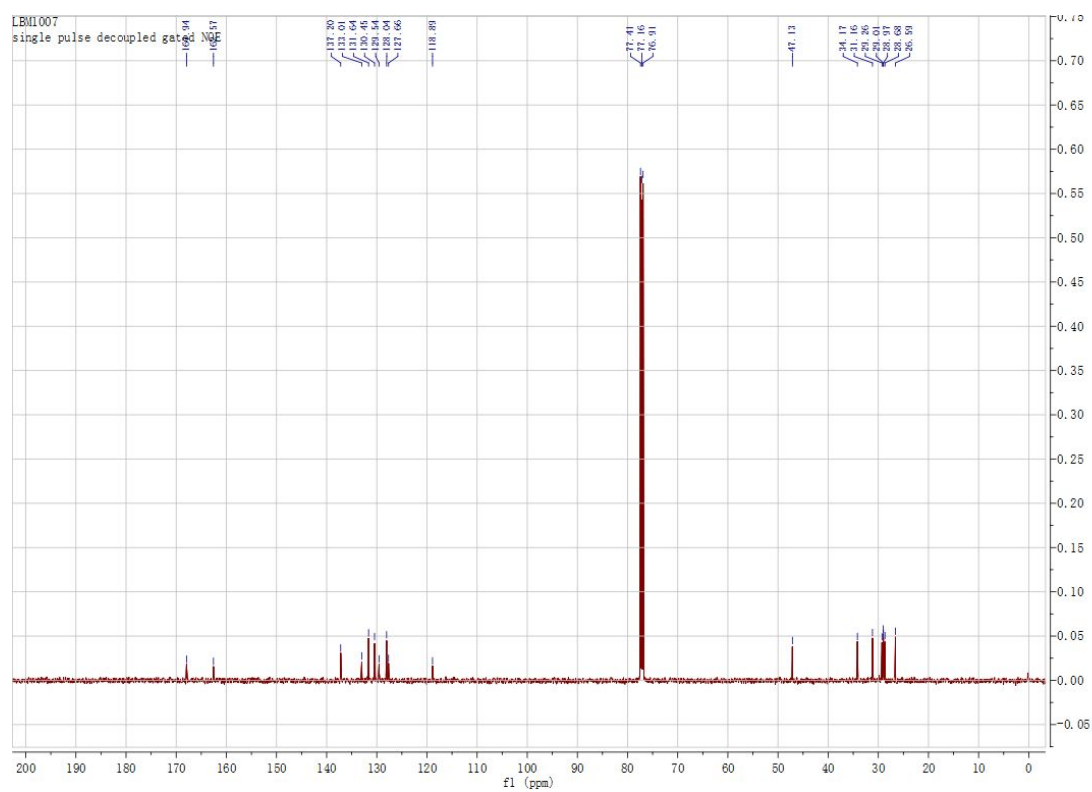


Figure S38. ^{13}C NMR Spectrum (CDCl_3 , 126 MHz) of C_8 .

2018122829 #113 RT: 1.09 AV: 1 NL: 2.90E9
T: FTMS + p ESI Full ms [100.0000-1000.0000]

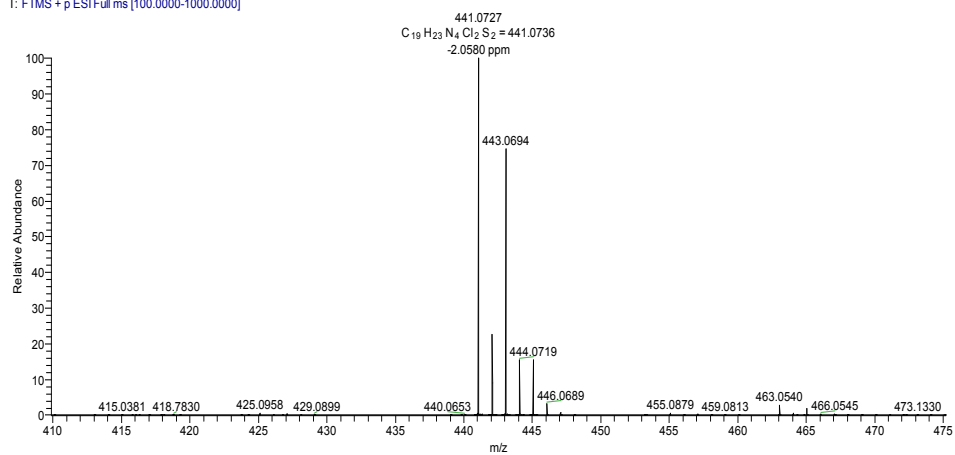


Figure S39. HRMS Spectrum of C_8 .

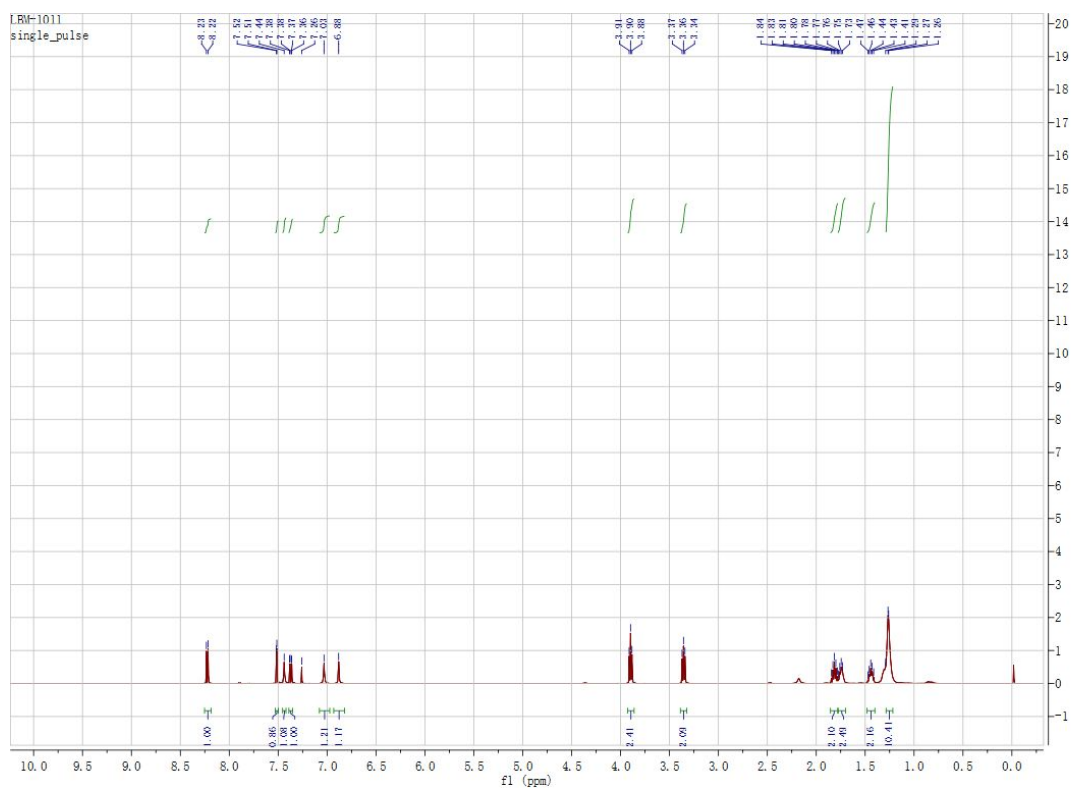


Figure S40. 1H NMR Spectrum (CDCl₃, 500 MHz) of C_{10} .

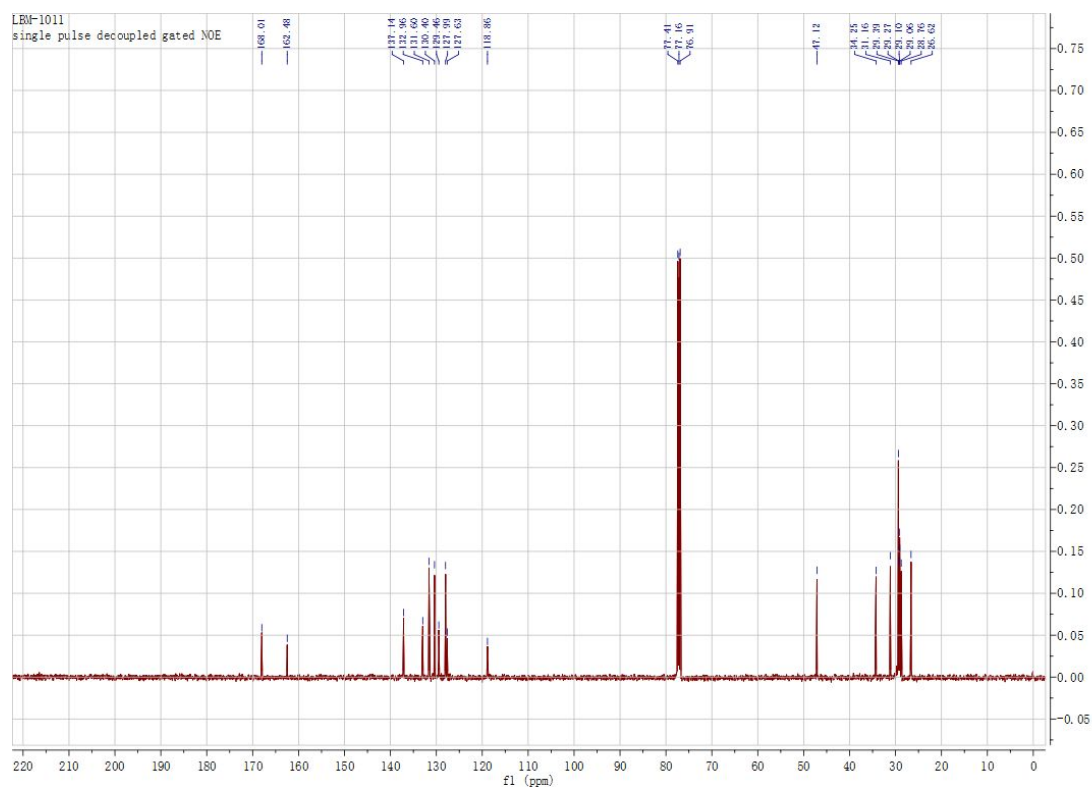


Figure S41. ^{13}C NMR Spectrum (CDCl_3 , 126 MHz) of C_{10} .

2018122830 #155 RT: 1.49 AV: 1 NL: 4.28E9
T: FTMS + p ESI Full ms [100.0000-1000.0000]

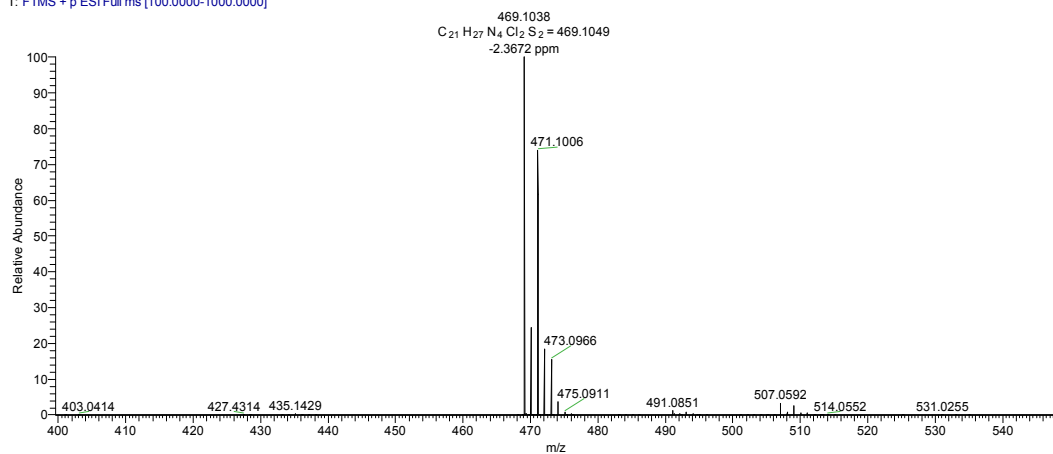


Figure S42. HRMS Spectrum of C_{10} .

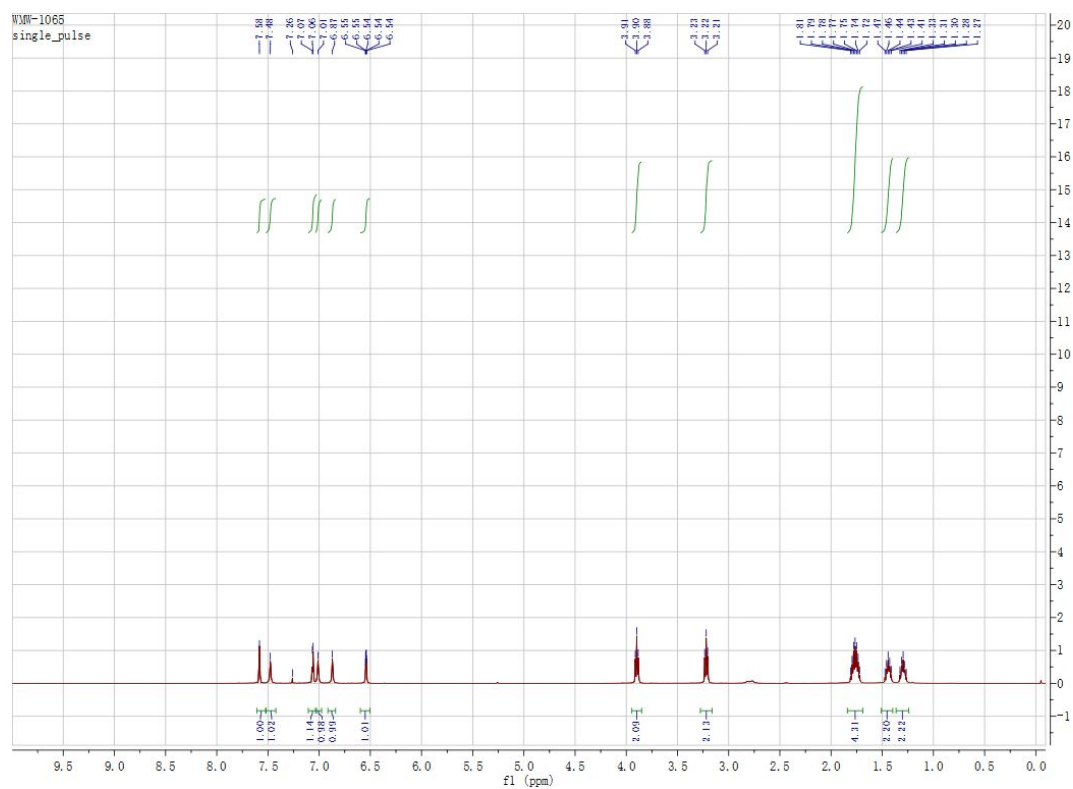


Figure S43. ^1H NMR Spectrum (CDCl_3 , 500 MHz) of D_6 .

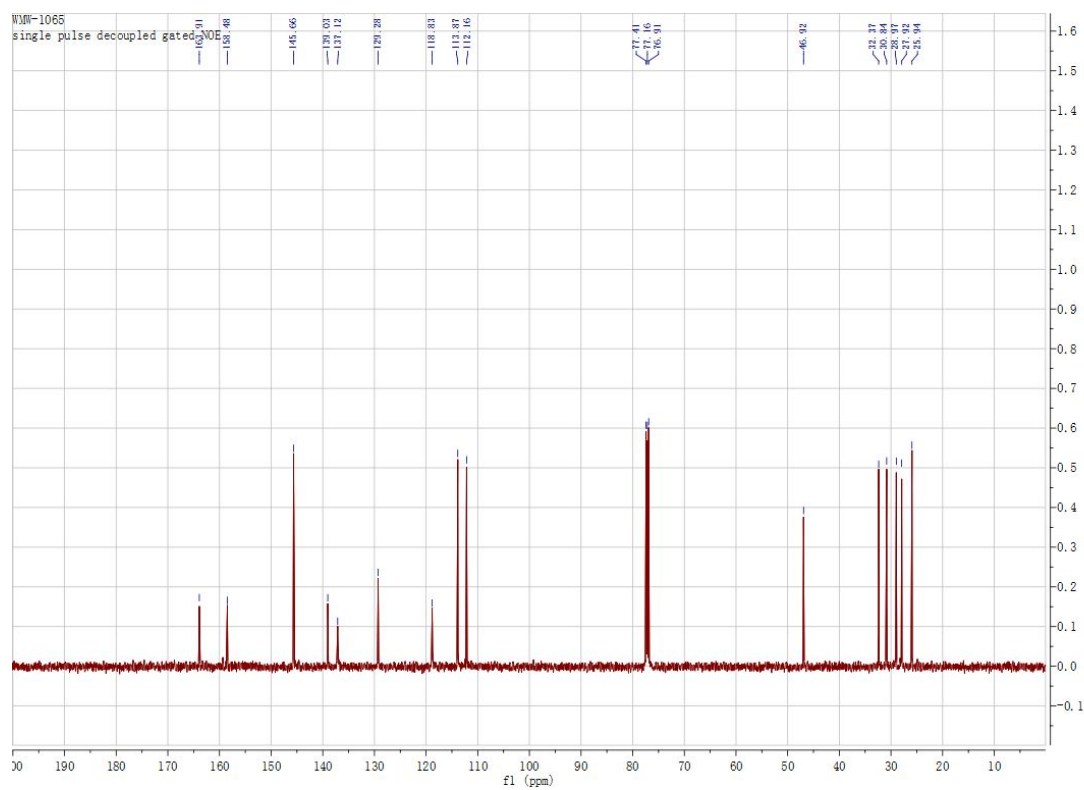


Figure S44. ^{13}C NMR Spectrum (CDCl_3 , 126 MHz) of D_6 .

2019011101_190111150012 #83 RT: 0.81 AV: 1 NL: 8.55E5
T: FTMS + p ESI Full ms [100.0000-1000.0000]

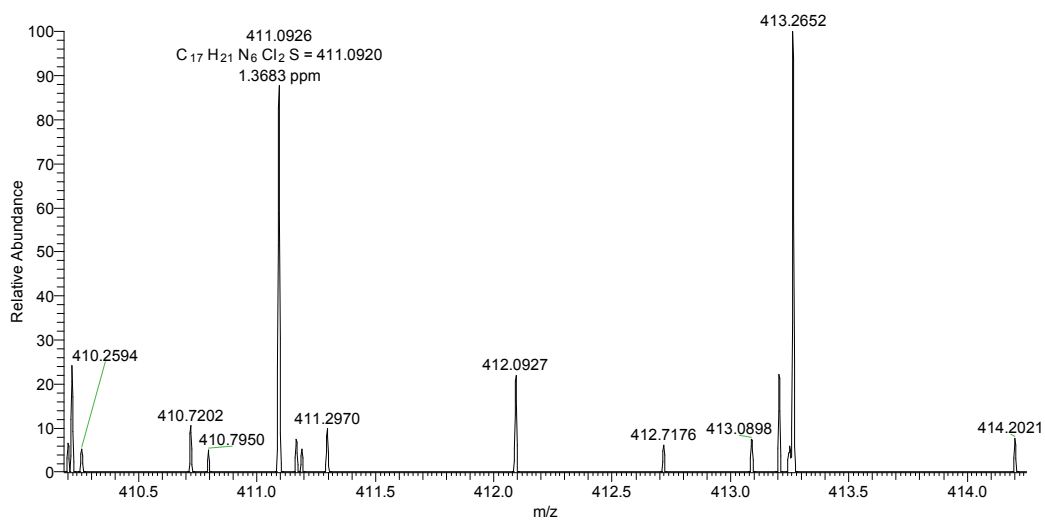


Figure S45. HRMS Spectrum of D₆.

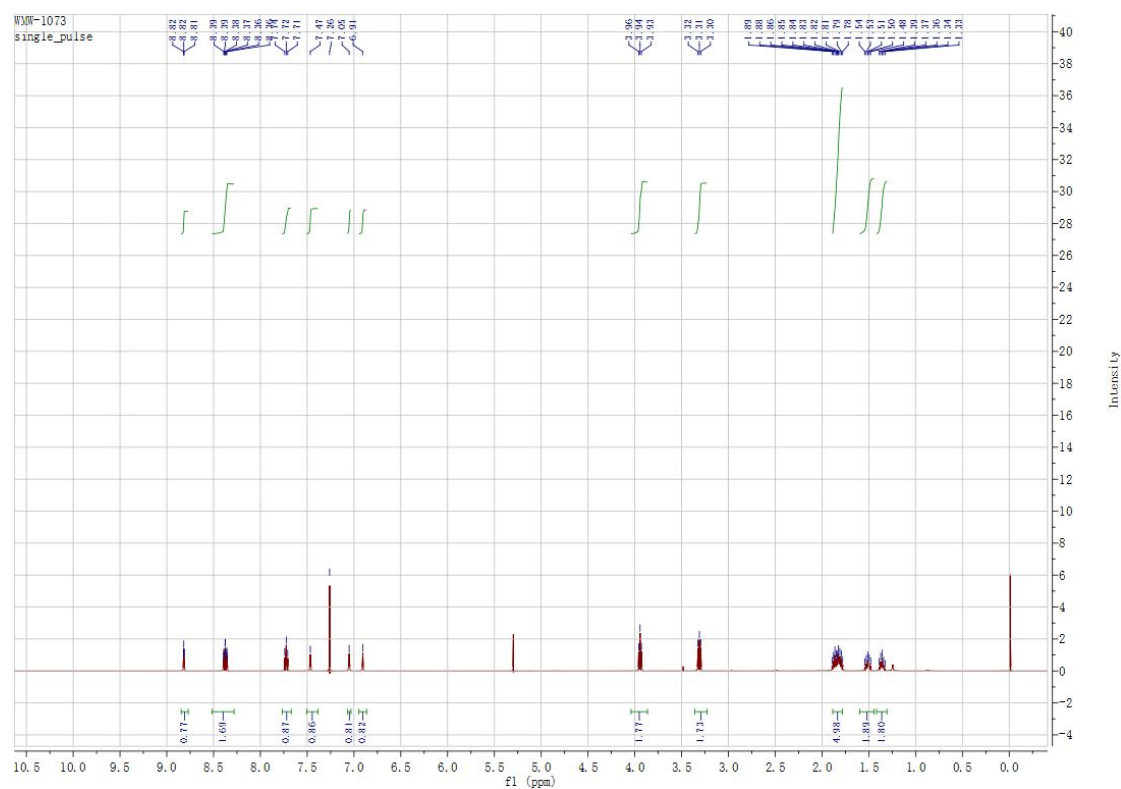


Figure S46. ¹H NMR Spectrum (CDCl₃, 500 MHz) of E₁.

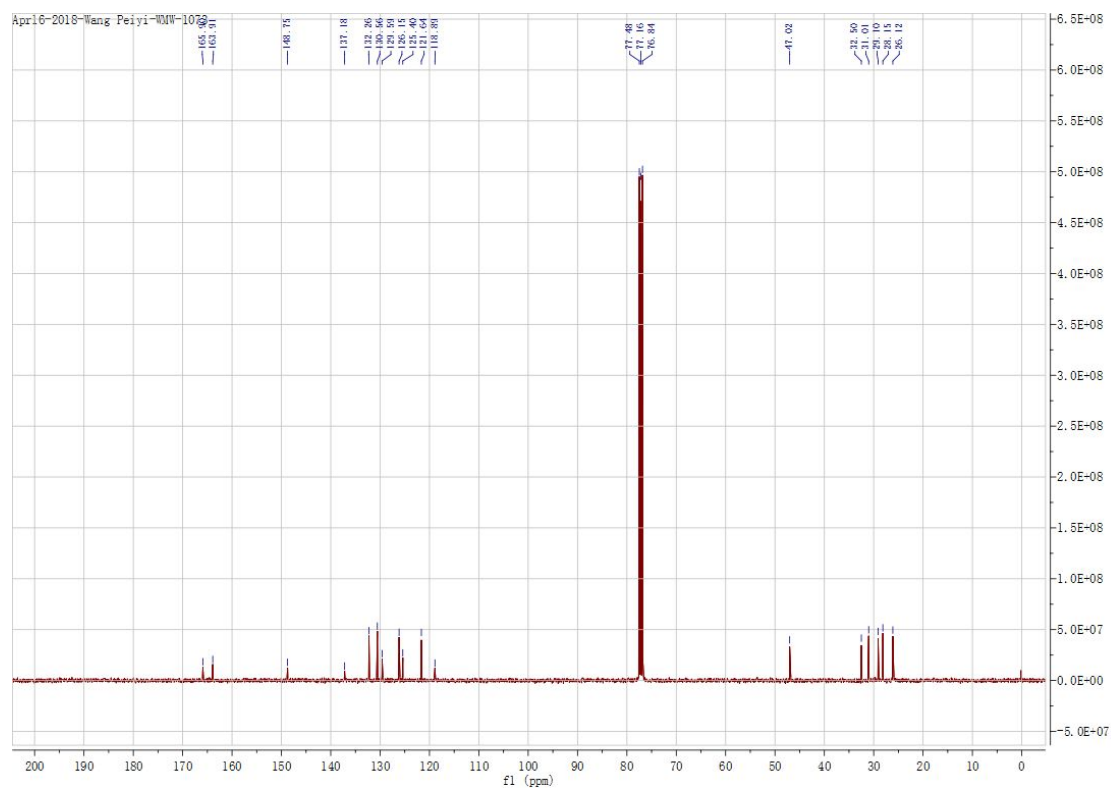


Figure S47. ^{13}C NMR Spectrum (CDCl_3 , 126 MHz) of E_1 .

2018122827 #93 RT: 0.90 AV: 1 NL: 1.84E9
T: FTMS + p ESIFul.ms [100.0000-1000.0000]

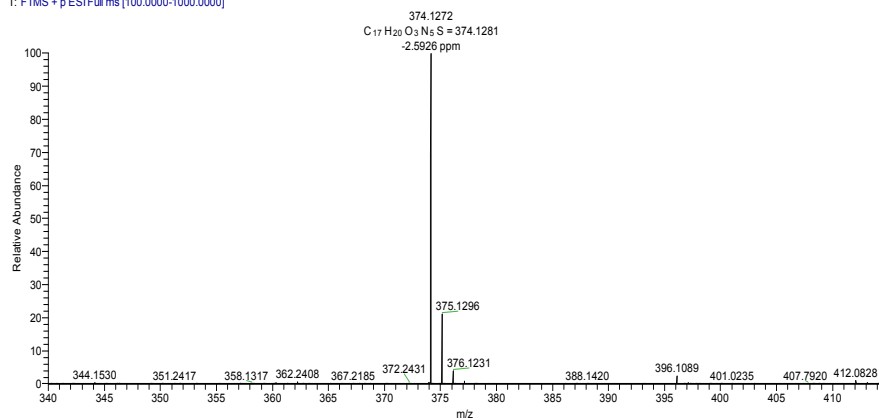


Figure S48. HRMS Spectrum of E_1 .

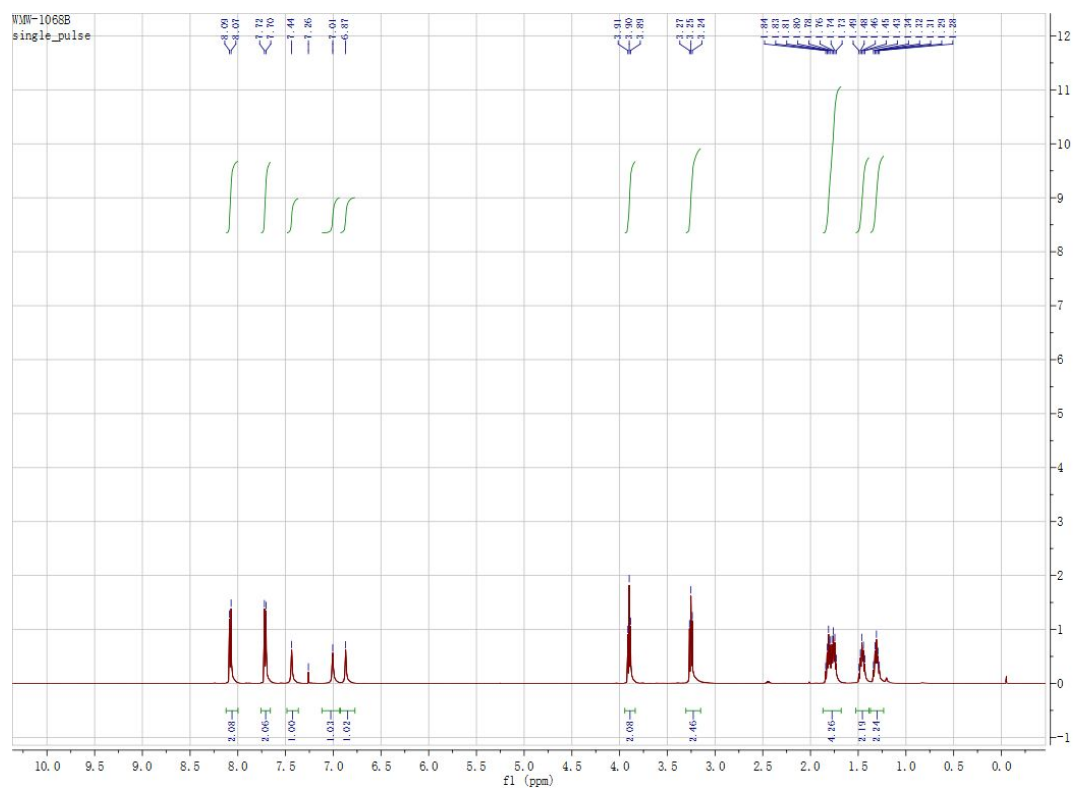


Figure S49. ^1H NMR Spectrum (CDCl_3 , 500 MHz) of E_2 .

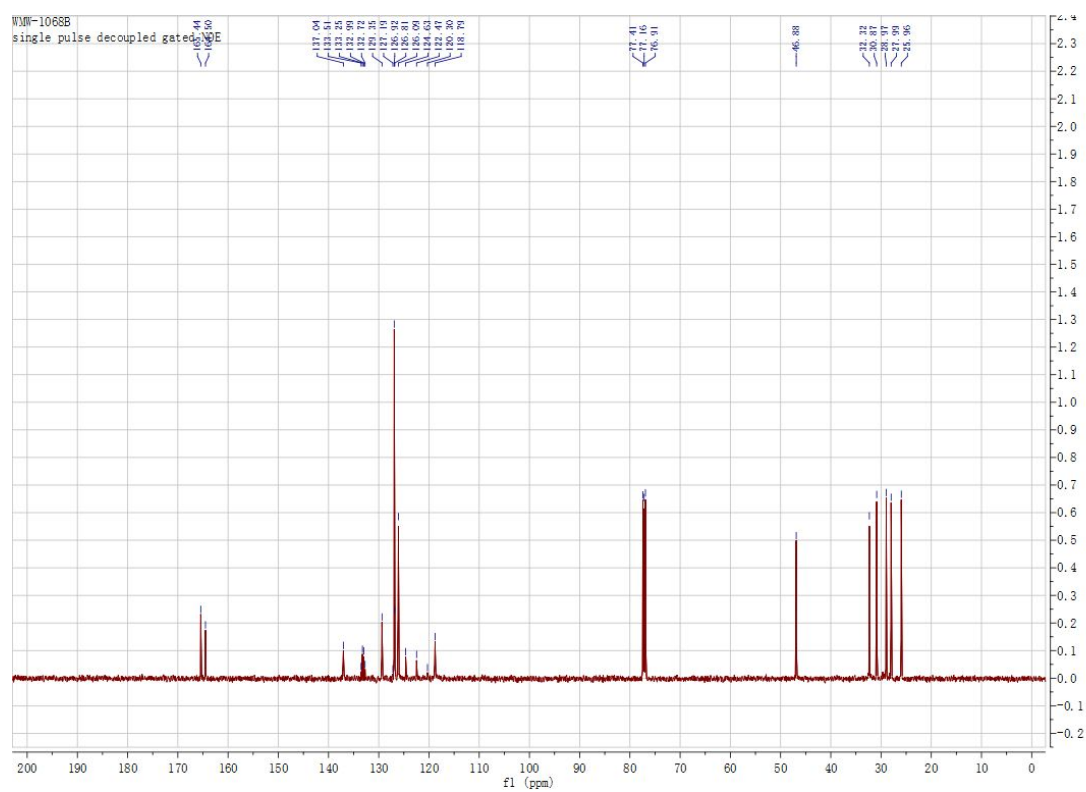


Figure S50. ^{13}C NMR Spectrum (CDCl_3 , 126 MHz) of E_2 .

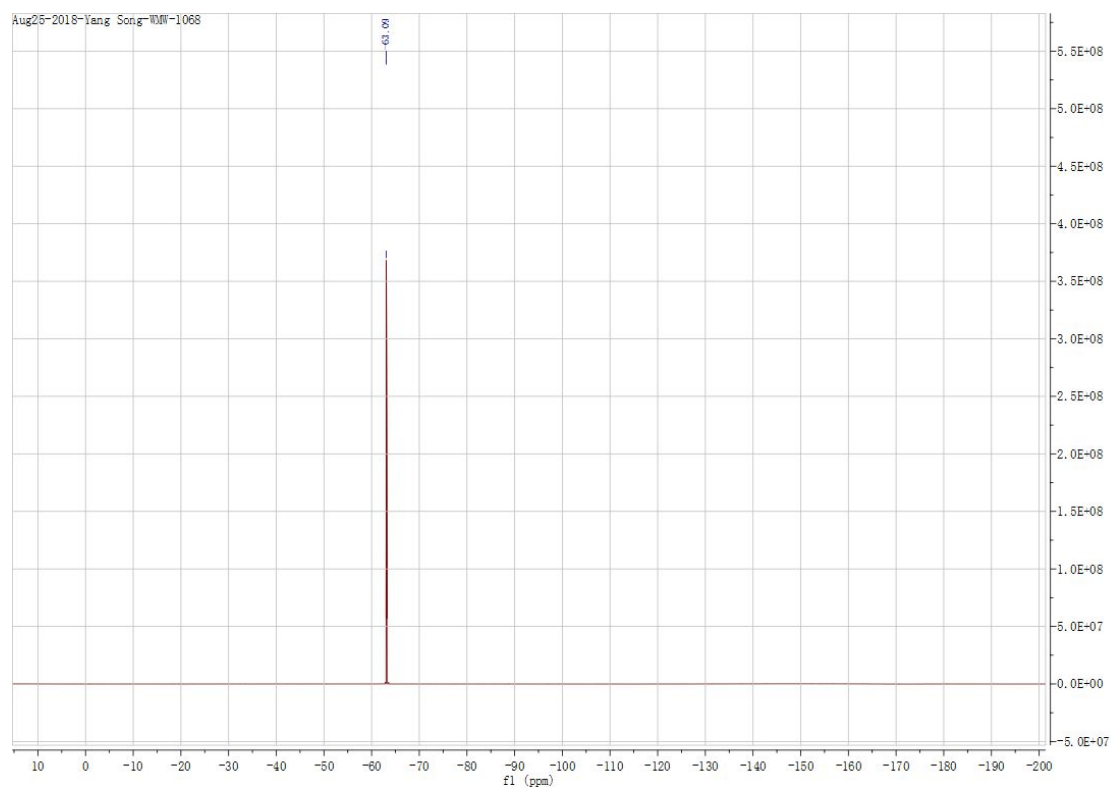


Figure S51. ^{19}F NMR Spectrum (CDCl_3 , 471 MHz) of E_2 .

2018122848 #87 RT: 0.84 AV: 1 NL: 3.27E9
T: FTMS + p ESI Full ms [100.0000-1000.0000]

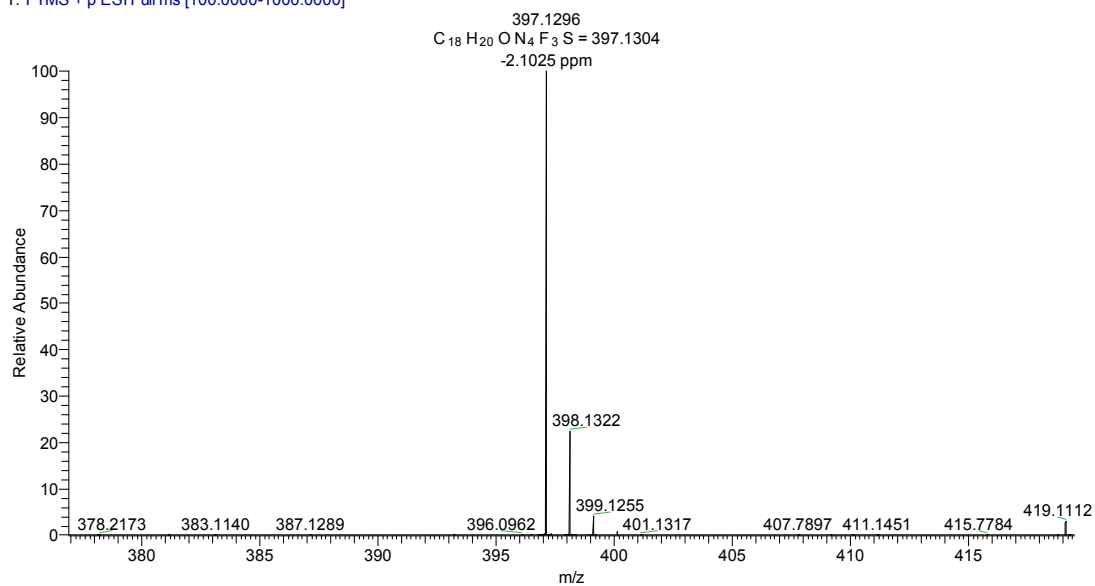


Figure S52. HRMS Spectrum of E_2 .

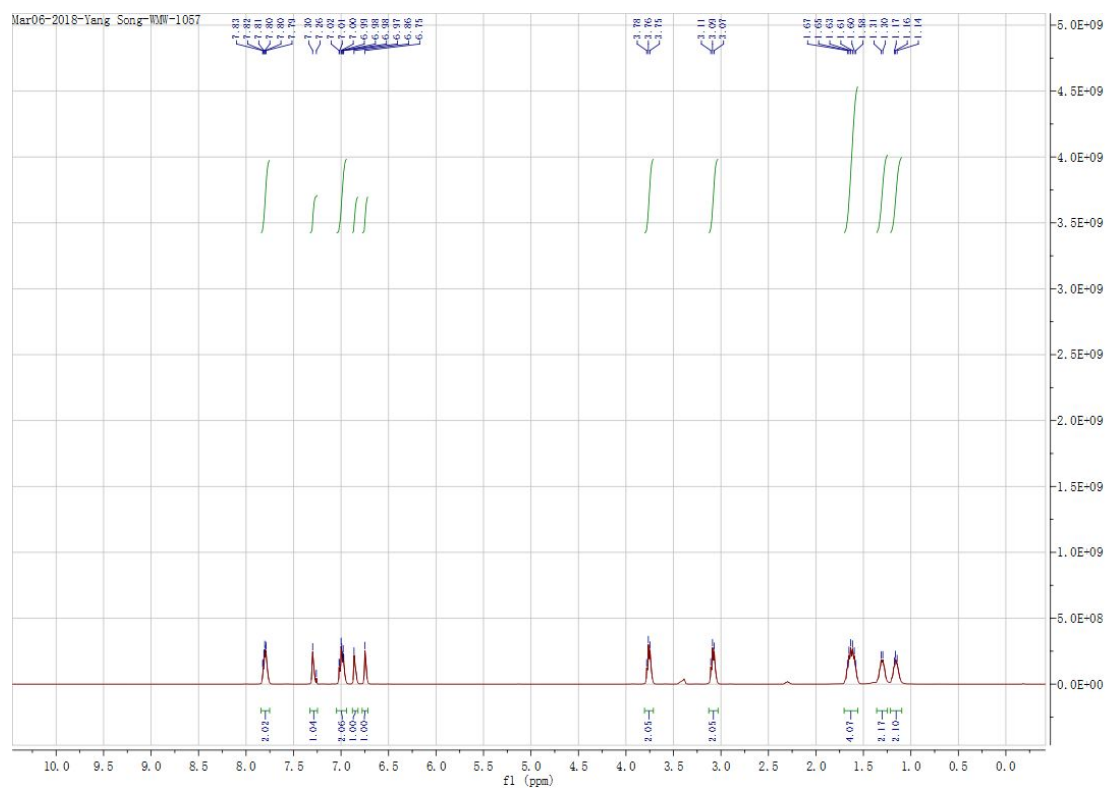


Figure S53. ^1H NMR Spectrum (CDCl_3 , 400 MHz) of E_3 .

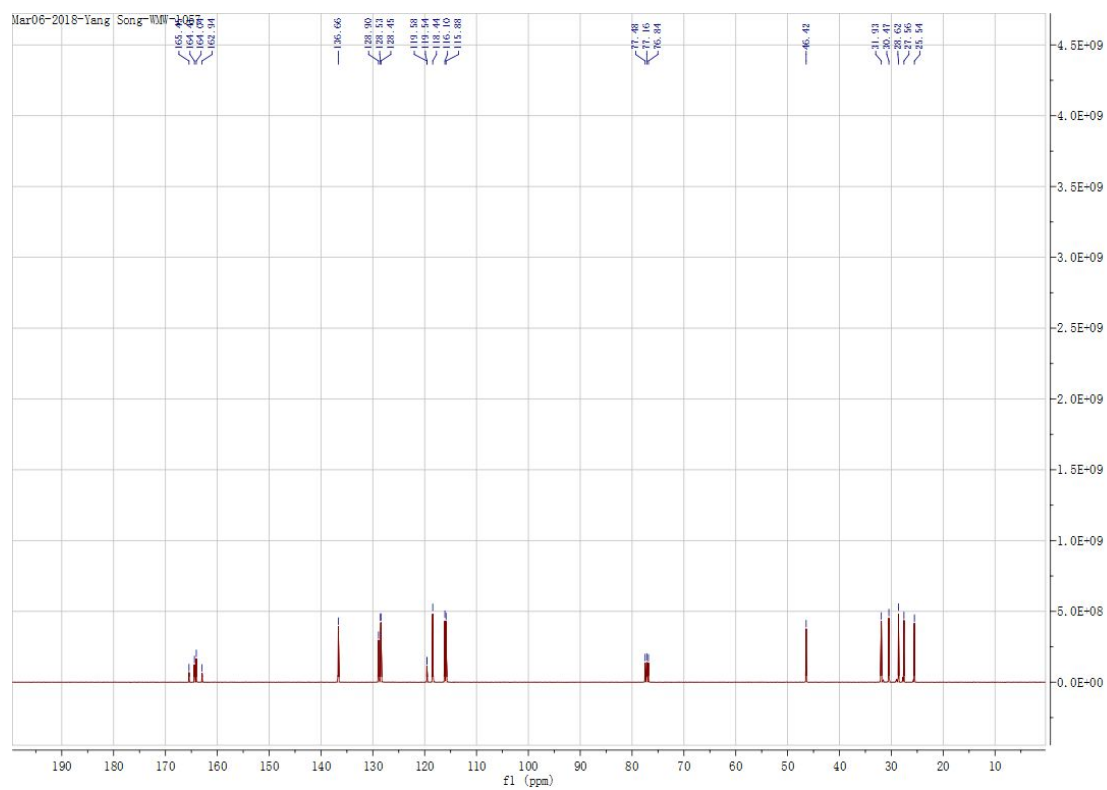


Figure S54. ^{13}C NMR Spectrum (CDCl_3 , 101 MHz) of E_3 .

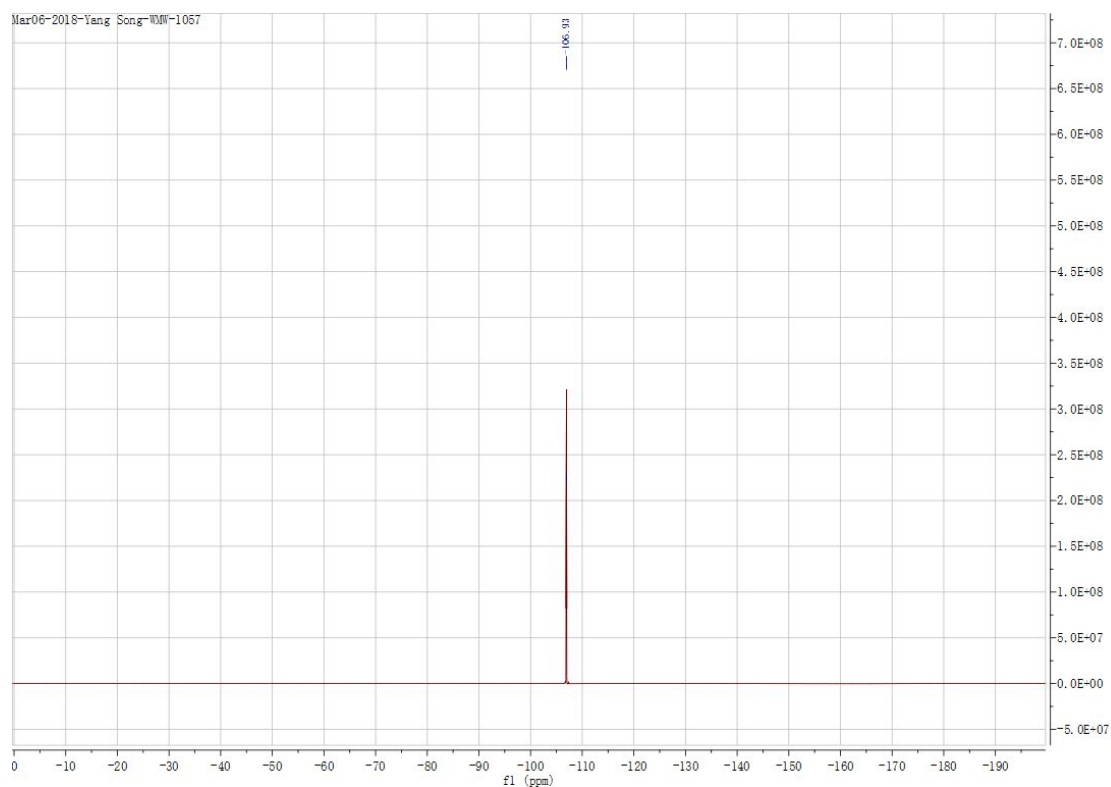


Figure S55. ^{19}F NMR Spectrum (CDCl_3 , 376 MHz) of E_3 .

2018122844 #93 RT: 0.90 AV: 1 NL: 4.53E9
T: FTMS + p ESI Full ms [100.0000-1000.0000]

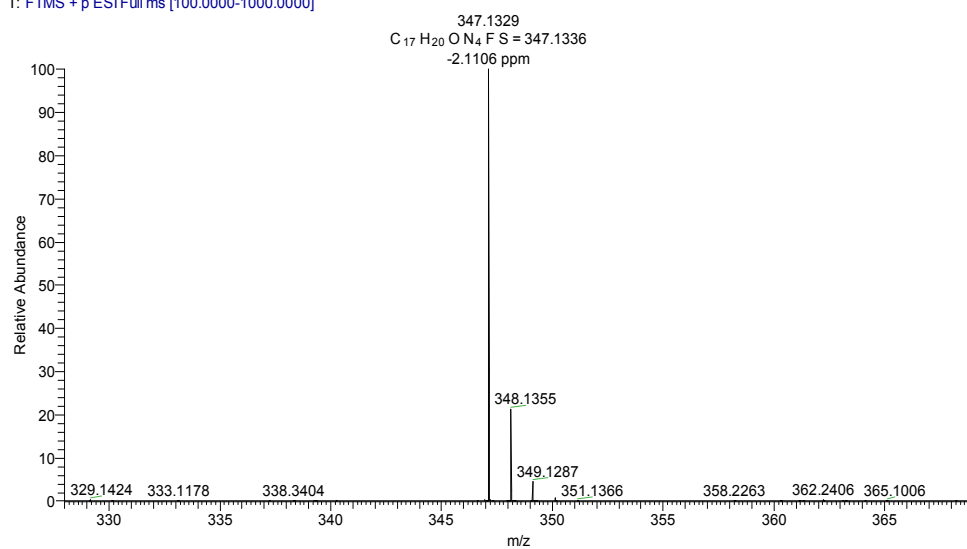


Figure S56. HRMS Spectrum of E_3 .

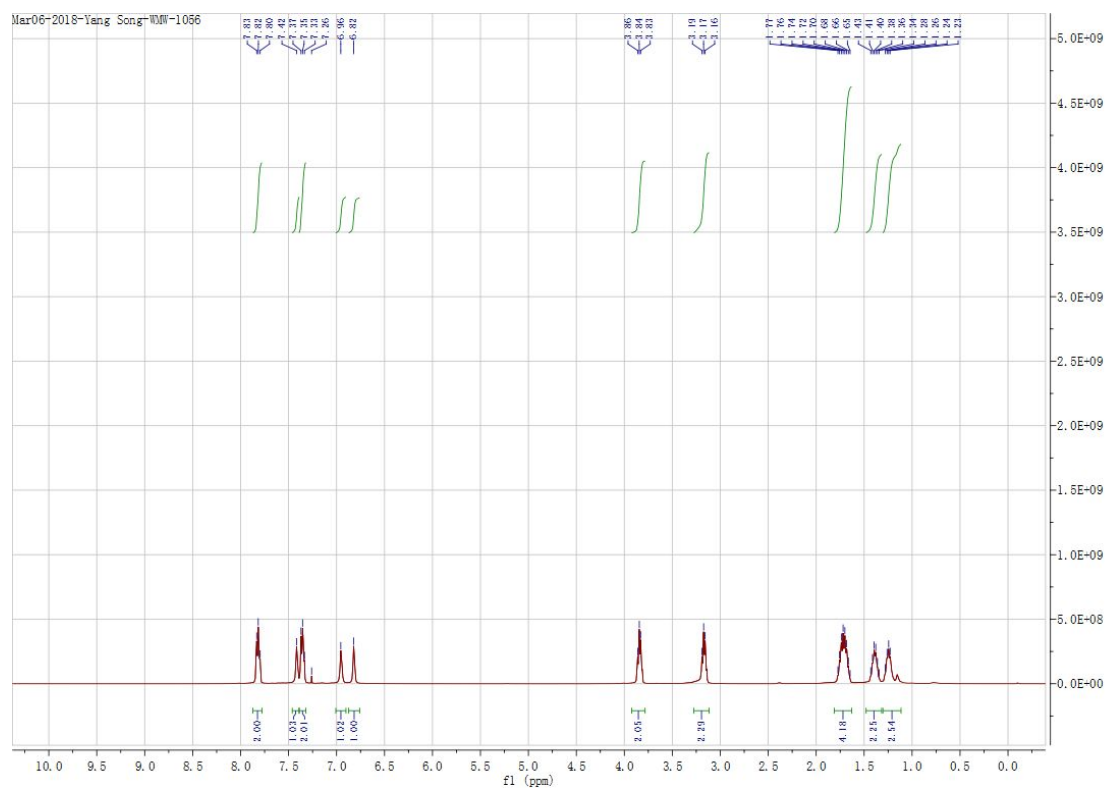


Figure S57. ^1H NMR Spectrum (CDCl_3 , 400 MHz) of E_4 .

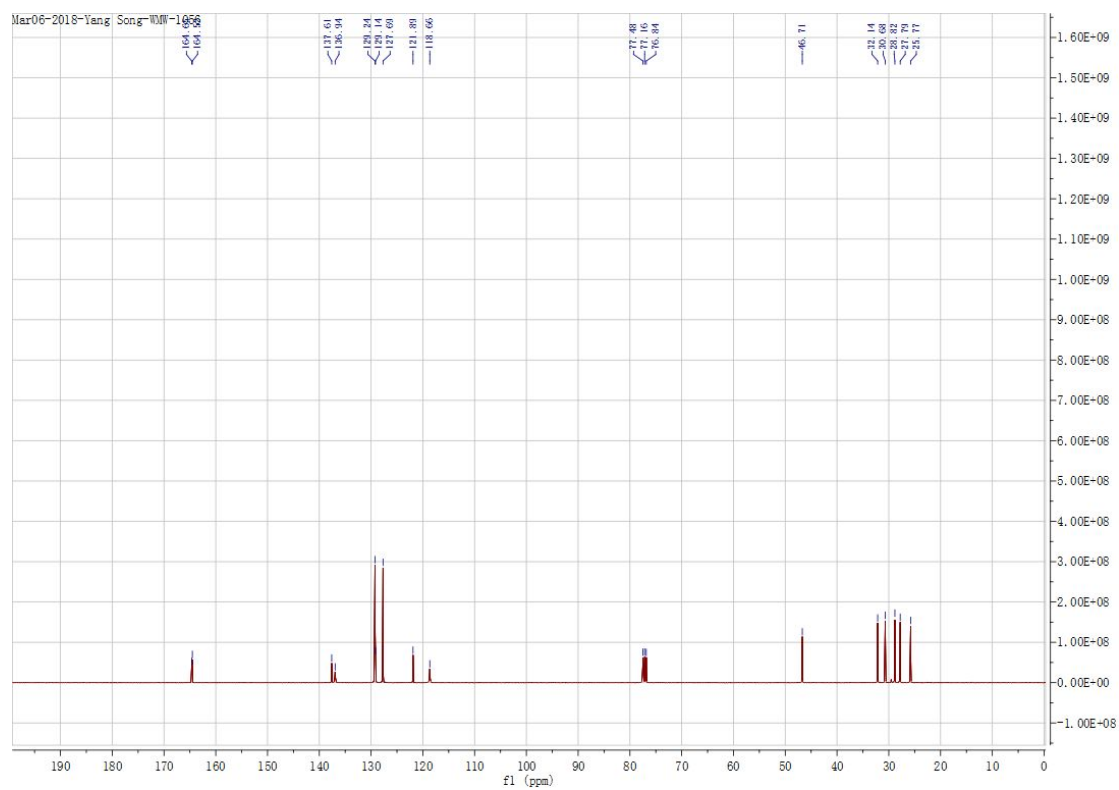


Figure S58. ^{13}C NMR Spectrum (CDCl_3 , 101 MHz) of E_4 .

2018122843 #91 RT: 0.88 AV: 1 NL: 3.75E9
T: FTMS + p ESI Full ms [100.0000-1000.0000]

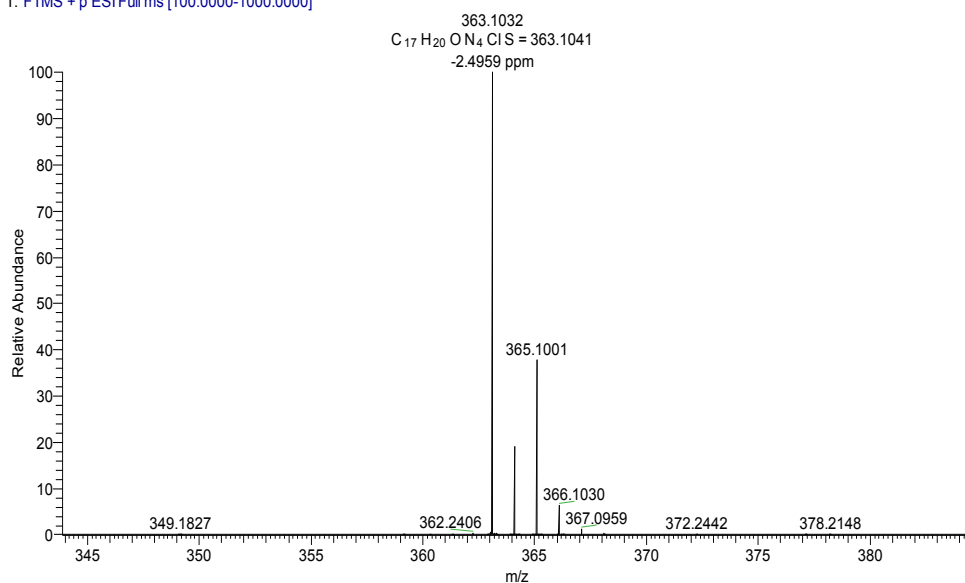


Figure S59. HRMS Spectrum of E₄.

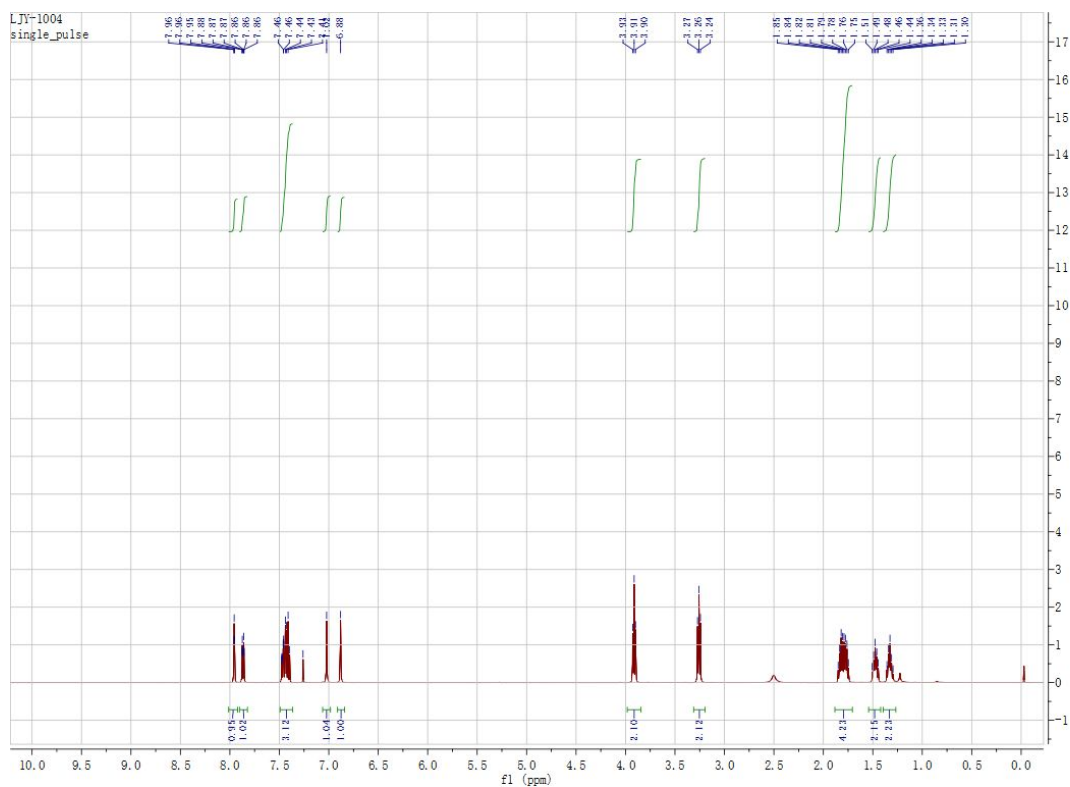


Figure S60. ¹H NMR Spectrum (CDCl₃, 500 MHz) of E₅.

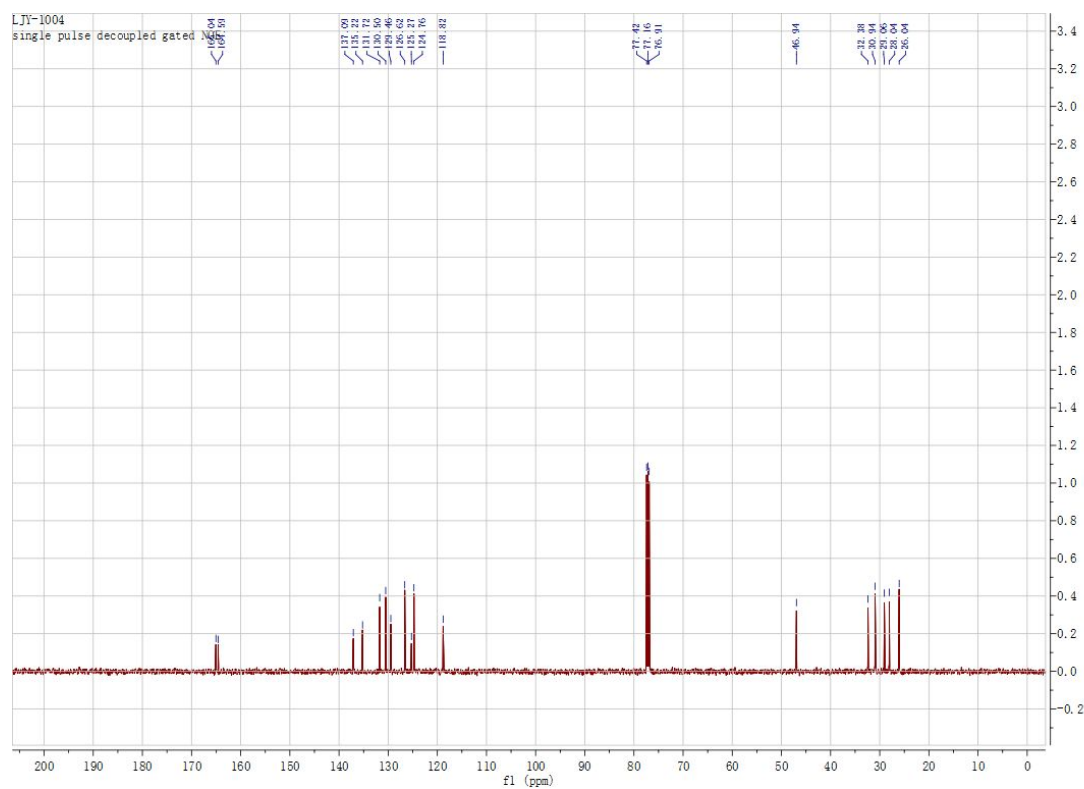


Figure S61. ^{13}C NMR Spectrum (CDCl_3 , 126 MHz) of E_5 .

2018122839 #85 RT: 0.82 AV: 1 NL: 1.61E9
T: FTMS + p ESI Full ms [100.0000-1000.0000]

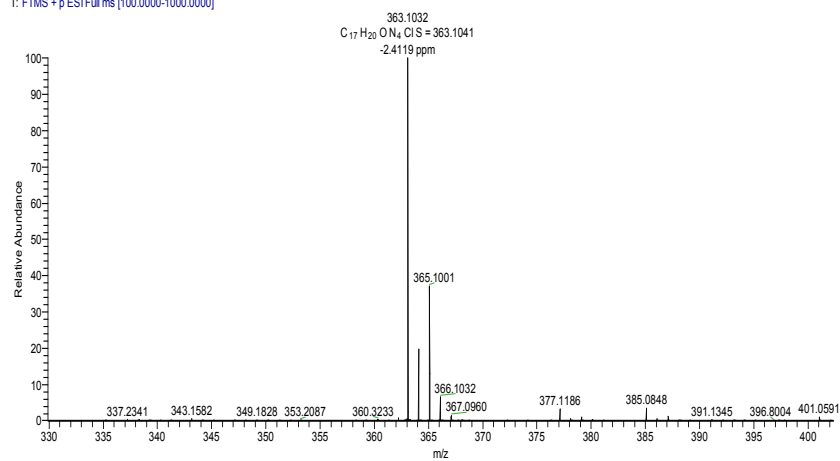


Figure S62. HRMS Spectrum of E_5 .

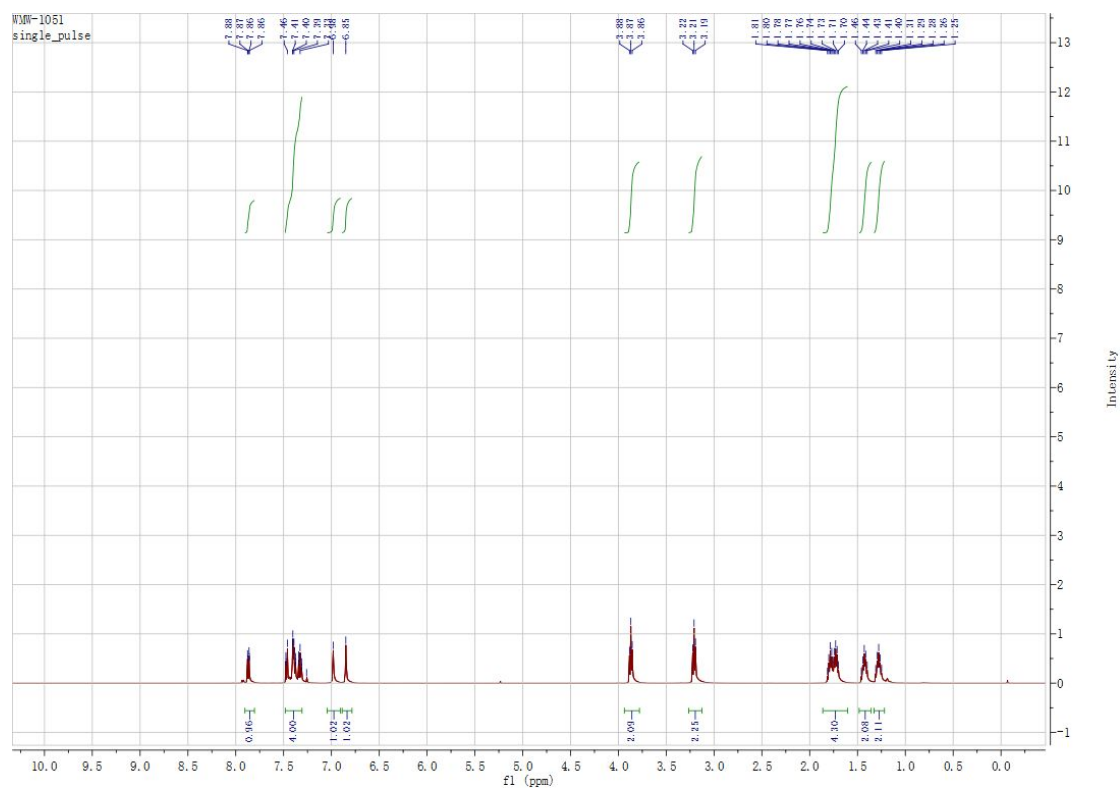


Figure S63. ^1H NMR Spectrum (CDCl_3 , 500 MHz) of E_6 .

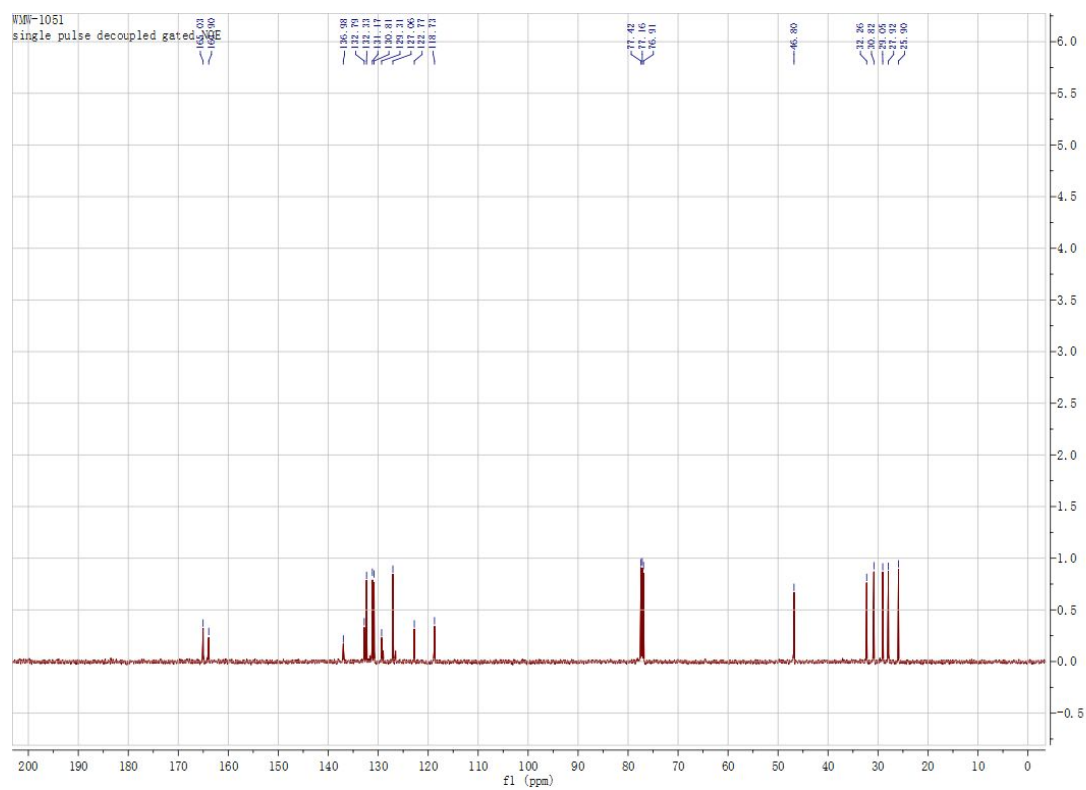


Figure S64. ^{13}C NMR Spectrum (CDCl_3 , 126 MHz) of E_6 .

2018122842 #77 RT: 0.74 AV: 1 NL: 1.84E9
T: FTMS + p ESI Full ms [100.0000-1000.0000]

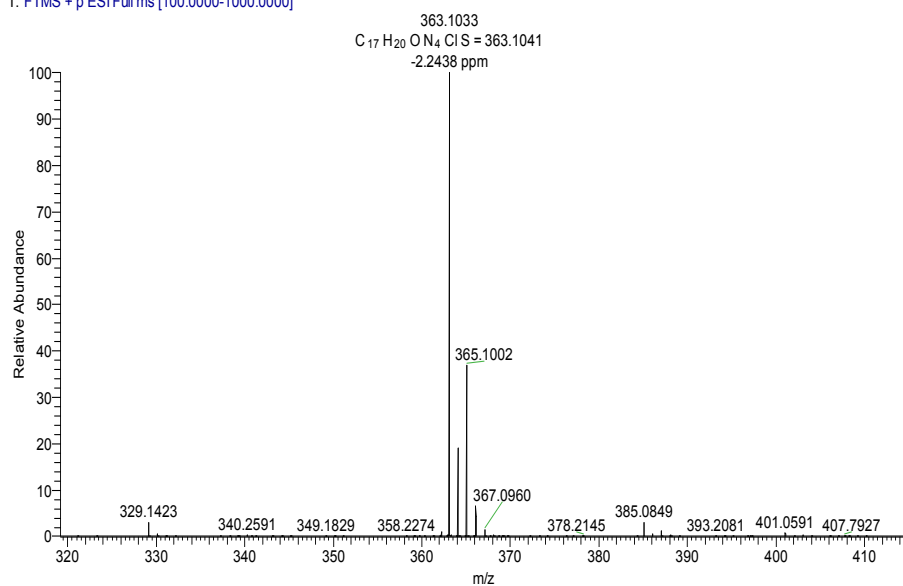


Figure S65. HRMS Spectrum of E₆.

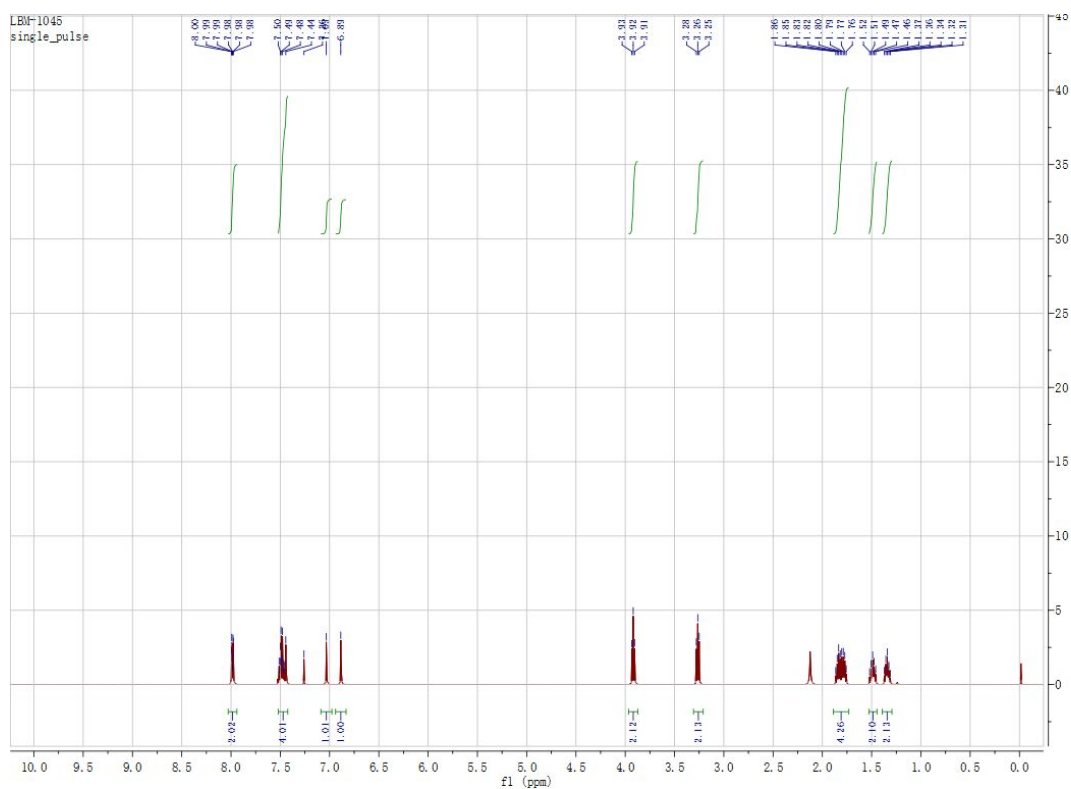


Figure S66. ¹H NMR Spectrum (CDCl₃, 500 MHz) of E₇.

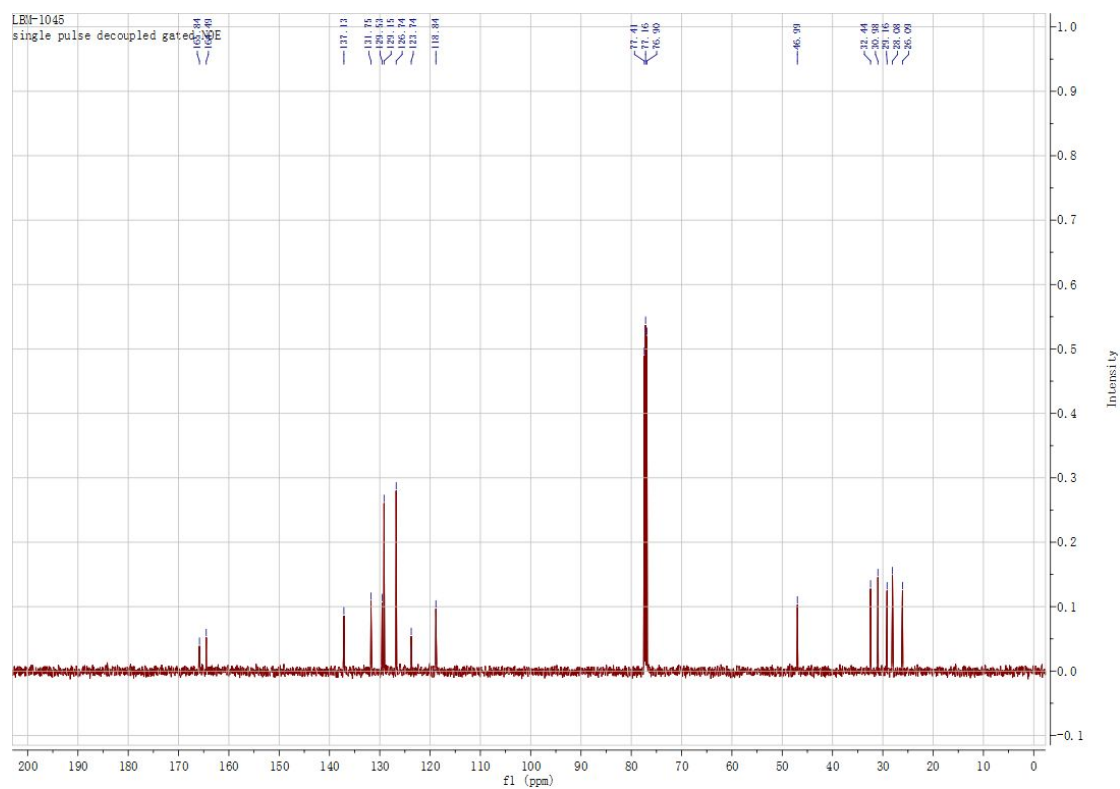


Figure S67. ^{13}C NMR Spectrum (CDCl_3 , 126 MHz) of E_7 .

2018122836 #93 RT: 0.90 AV: 1 NL: 4.46E9
T: FTMS + p ESI Full ms [100.0000-1000.0000]

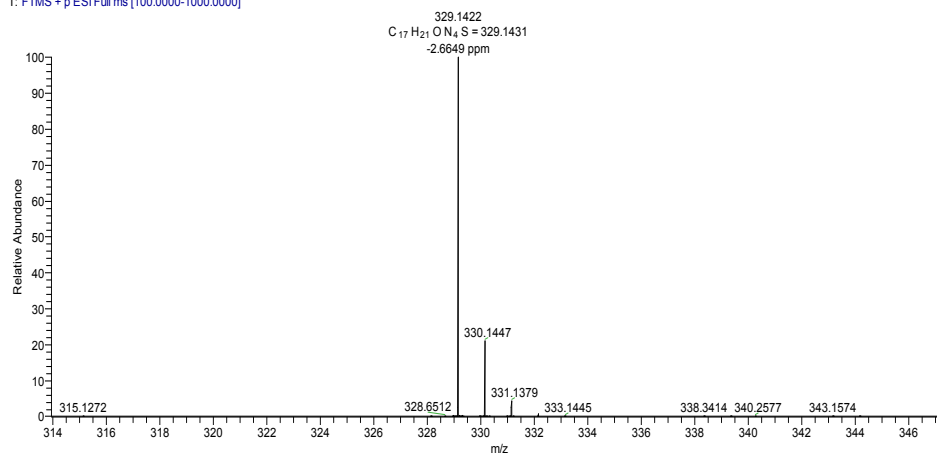


Figure S68. HRMS Spectrum of E_7 .

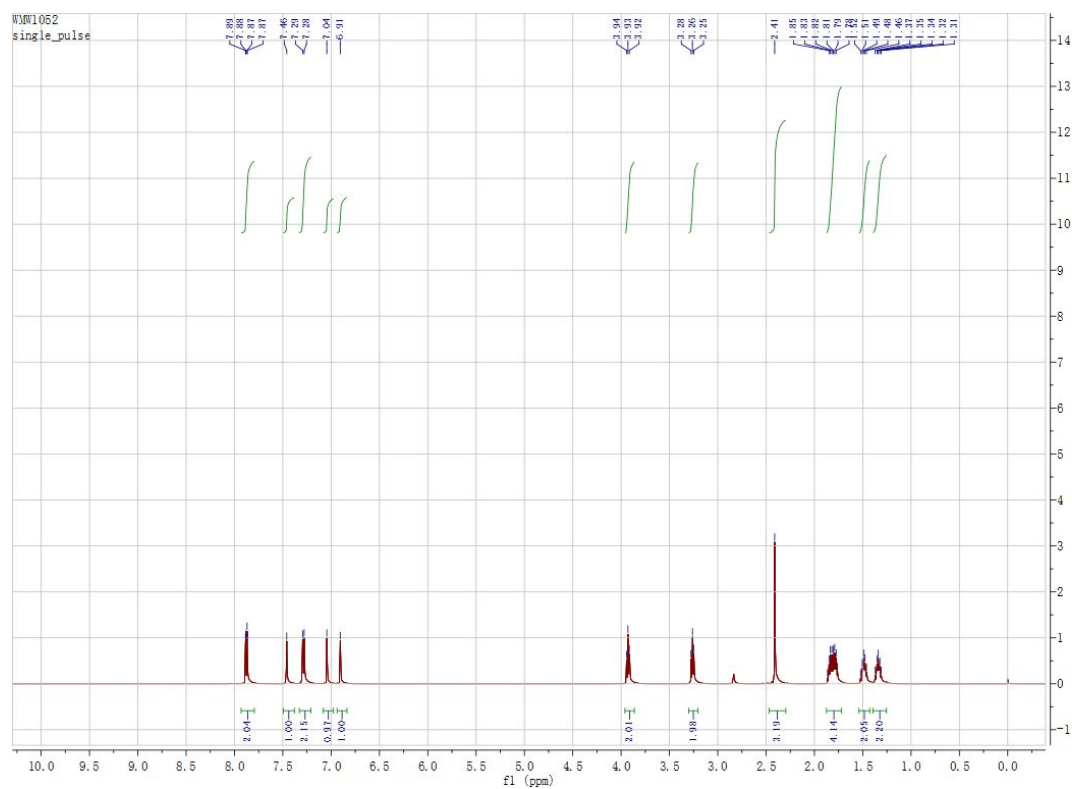


Figure S69. ^1H NMR Spectrum (CDCl_3 , 500 MHz) of E_8 .

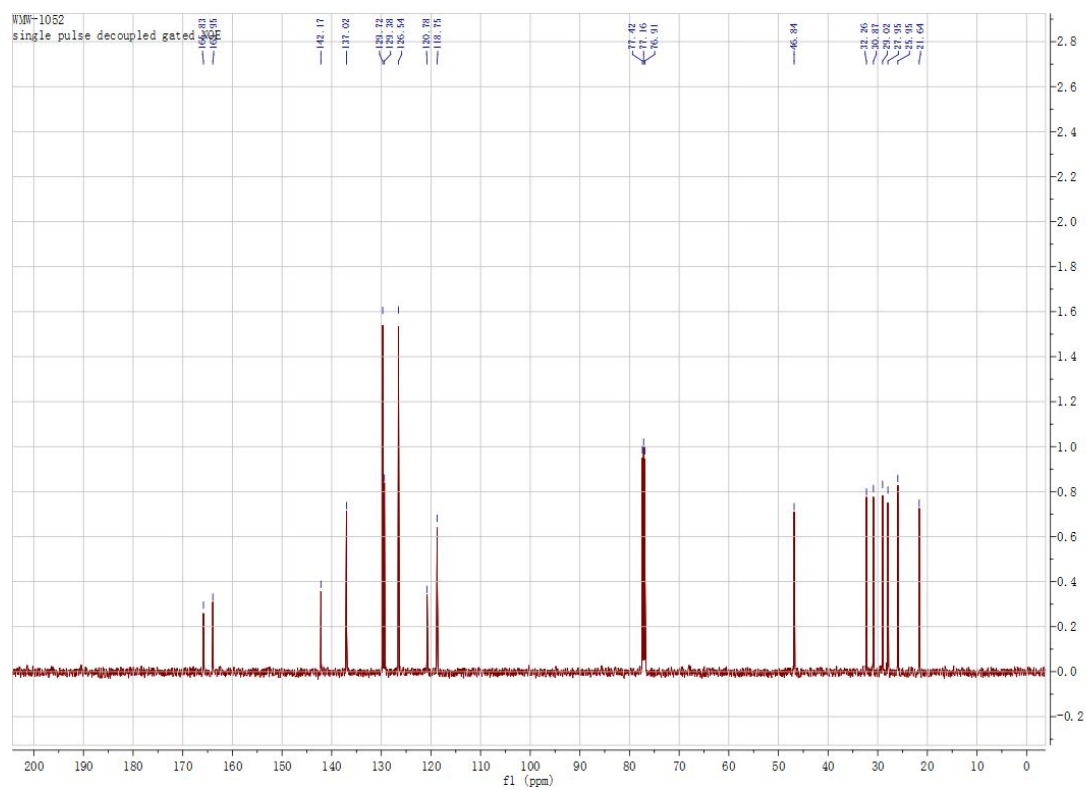


Figure S70. ^{13}C NMR Spectrum (CDCl_3 , 126 MHz) of E_8 .

2018122838 #109 RT: 1.05 AV: 1 NL: 1.01E10
T: FTMS + p ESI Full ms [100.0000-1000.0000]

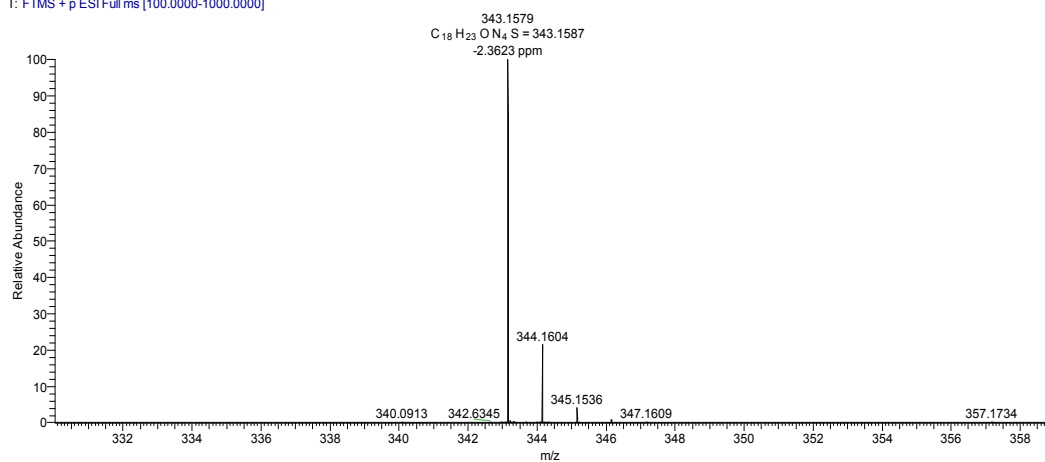


Figure S71. HRMS Spectrum of E₈.

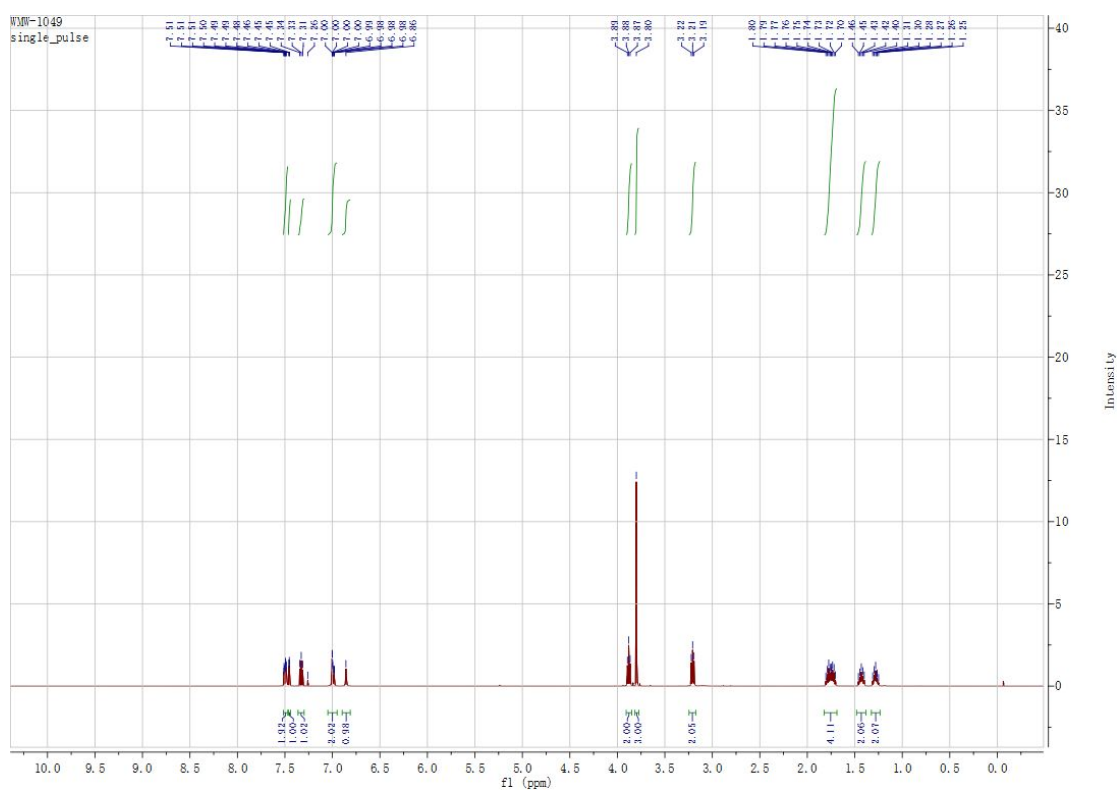


Figure S72. 1H NMR Spectrum (CDCl₃, 500 MHz) of E₉.

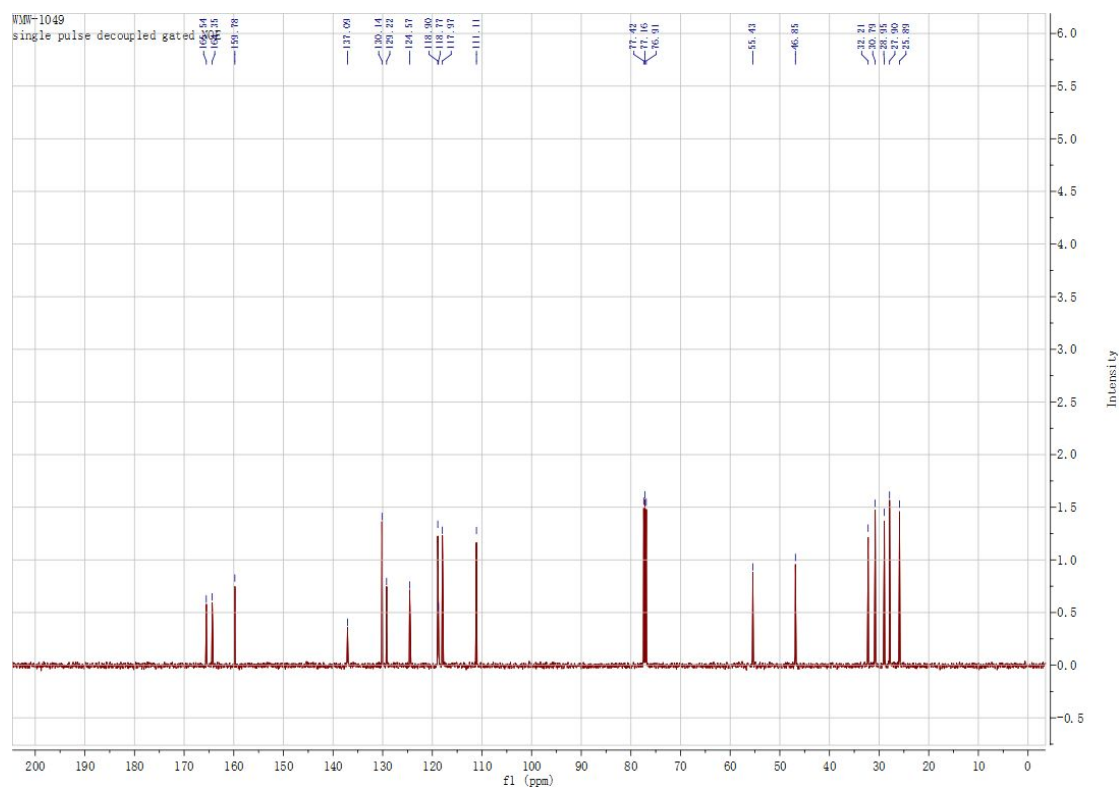


Figure S73. ^{13}C NMR Spectrum (CDCl_3 , 126 MHz) of **E**₉.

2018122840 #91 RT: 0.88 AV: 1 NL: 2.99E9
T: FTMS + p ESI Full ms [100.0000-1000.0000]

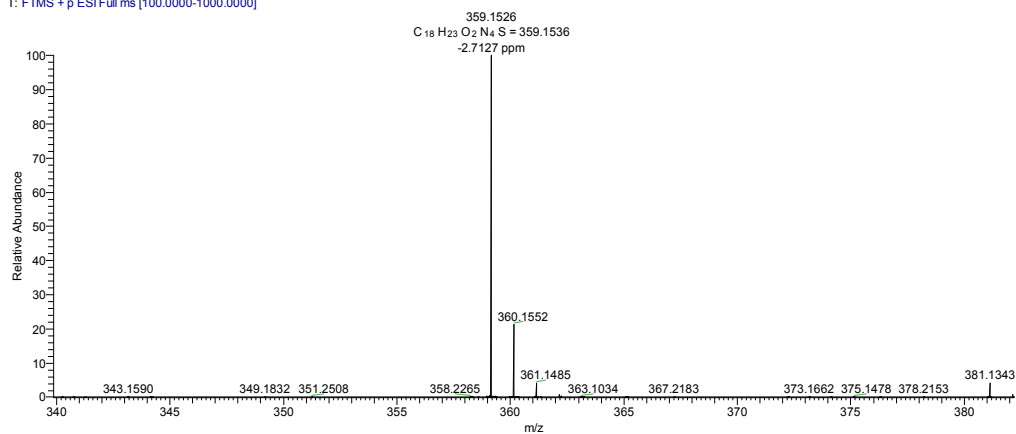


Figure S74. HRMS Spectrum of **E**₉.

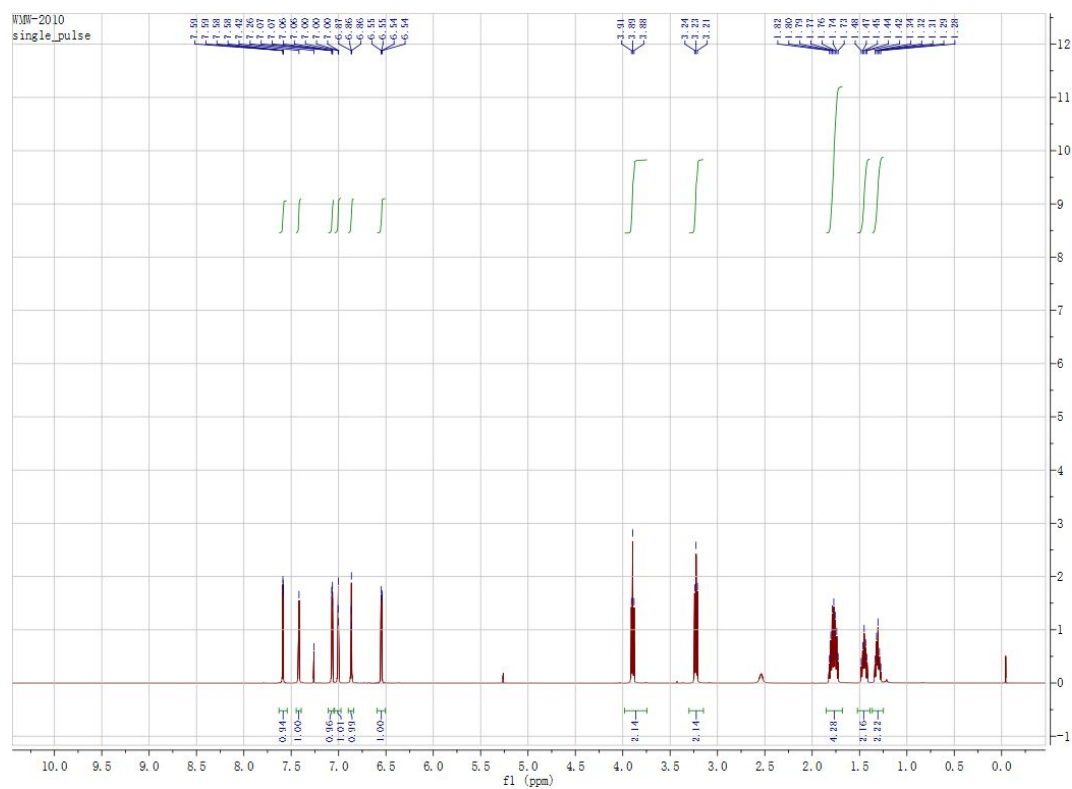


Figure S75. ^1H NMR Spectrum (CDCl_3 , 500 MHz) of E_{10} .

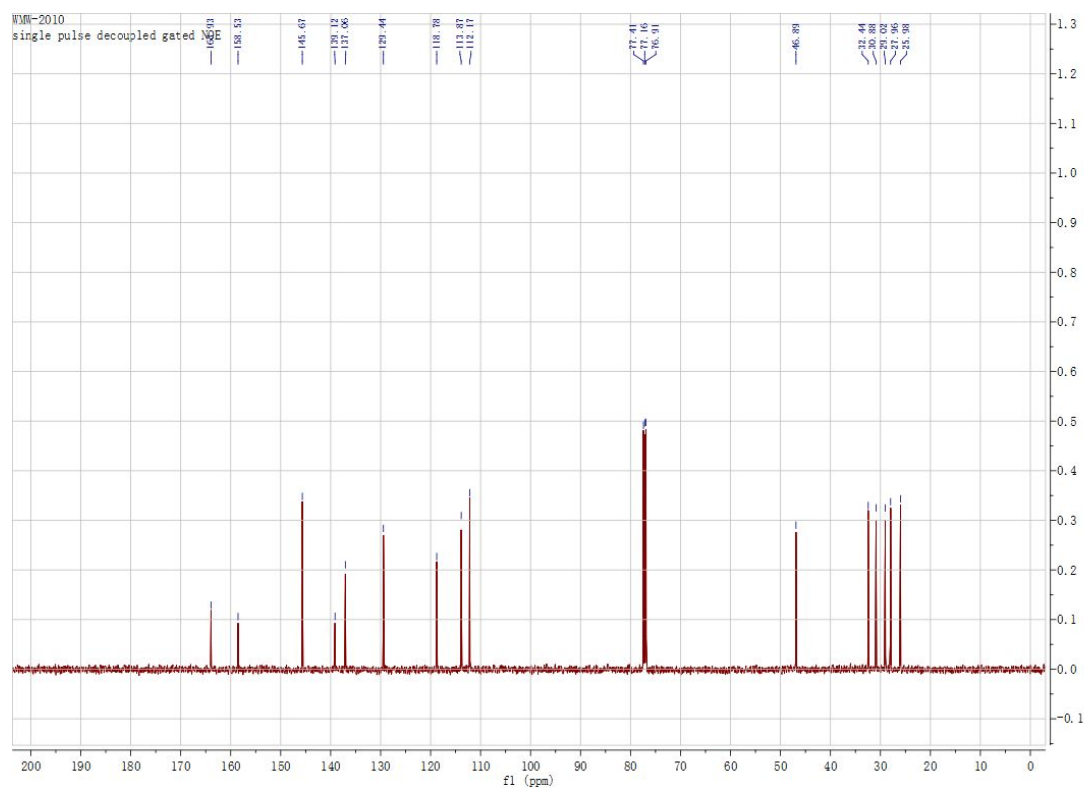


Figure S76. ^{13}C NMR Spectrum (CDCl_3 , 126 MHz) of E_{10} .

2018122846 #83 RT: 0.80 AV: 1 NL: 3.52E9
T: FTMS + p ESI Full ms [100.0000-1000.0000]

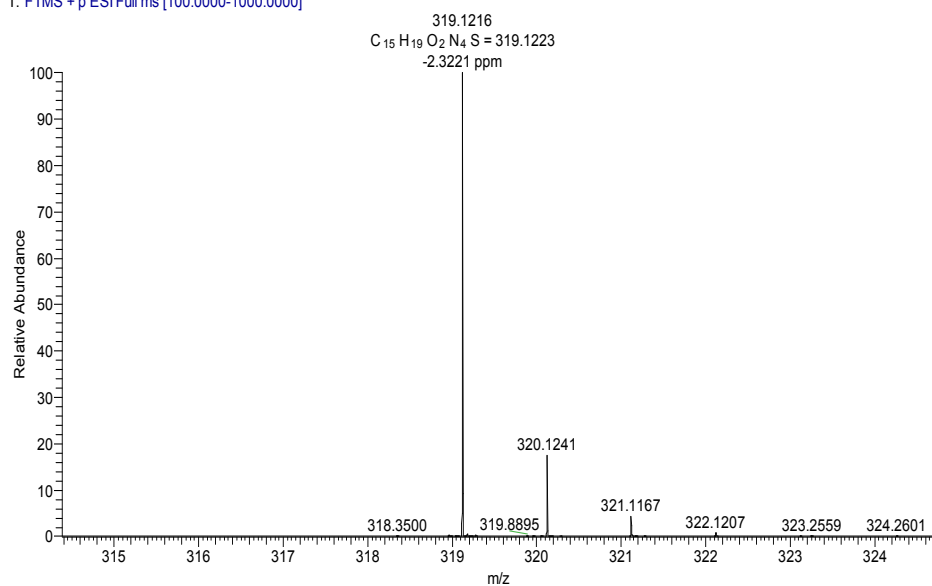


Figure S77. HRMS Spectrum of E₁₀.

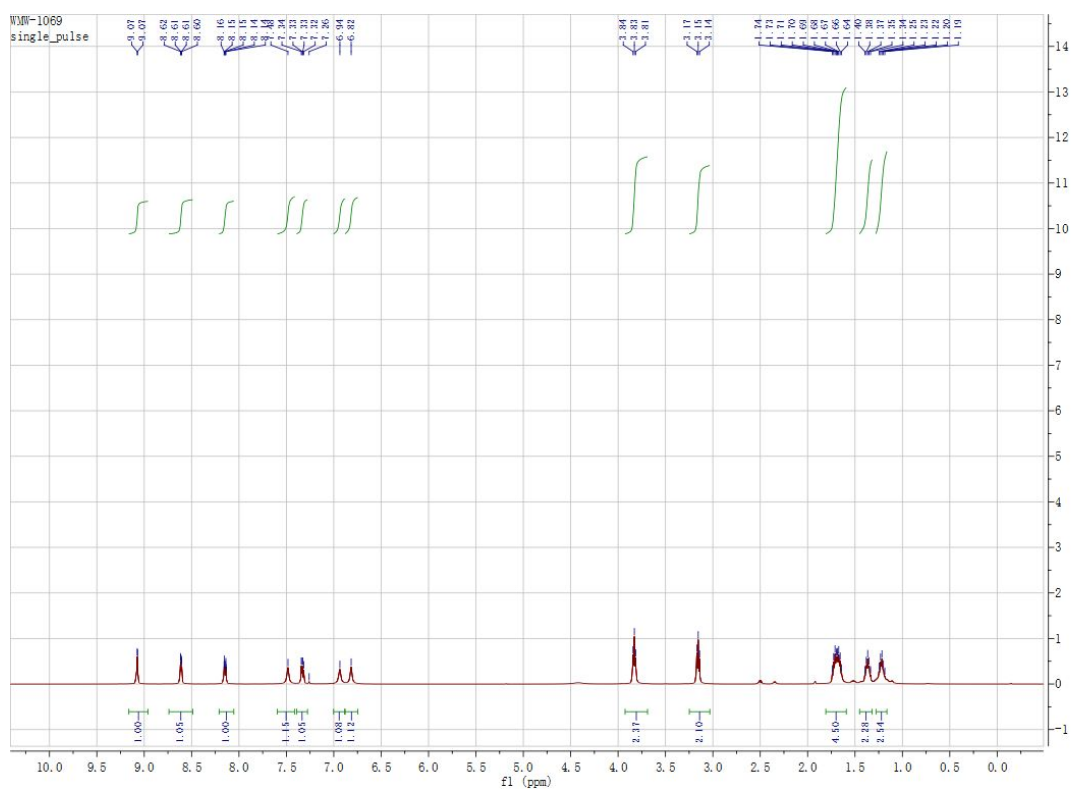


Figure S78. ¹H NMR Spectrum (CDCl₃, 500 MHz) of E₁₁.

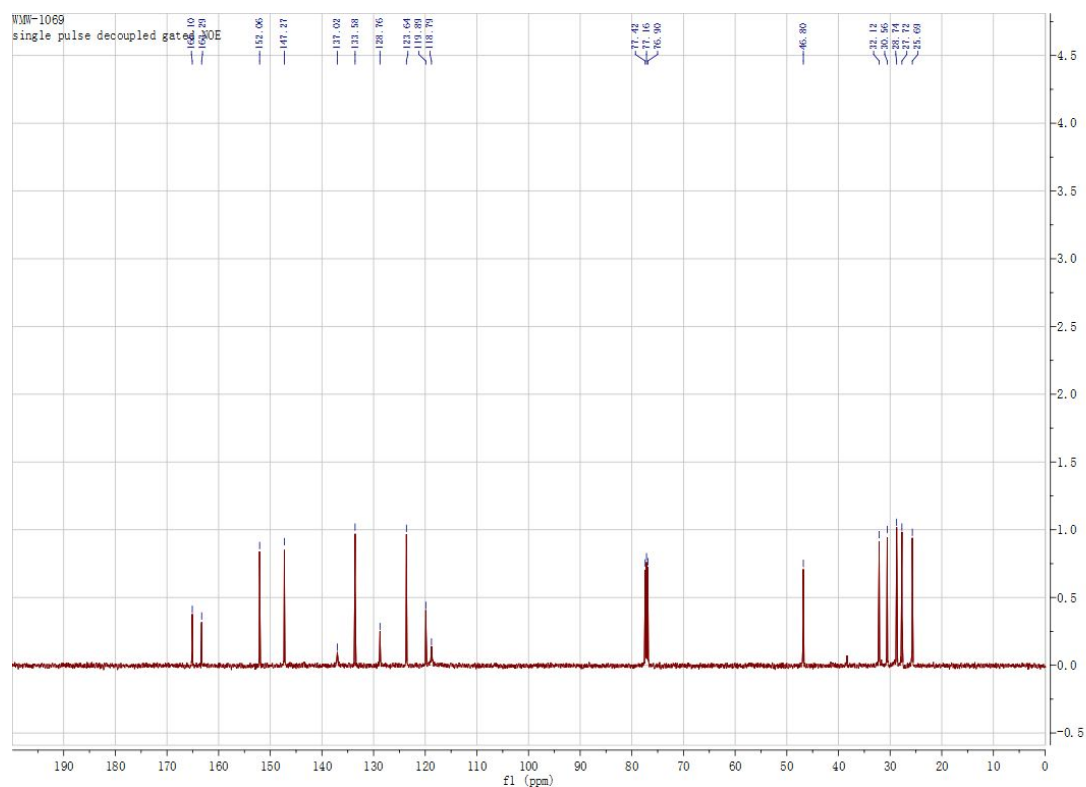


Figure S79. ^{13}C NMR Spectrum (CDCl_3 , 126 MHz) of E_{11} .

2018122849 #87 RT: 0.84 AV: 1 NL: 2.13E9
T: FTMS + p ESI Full ms [100.0000-1000.0000]

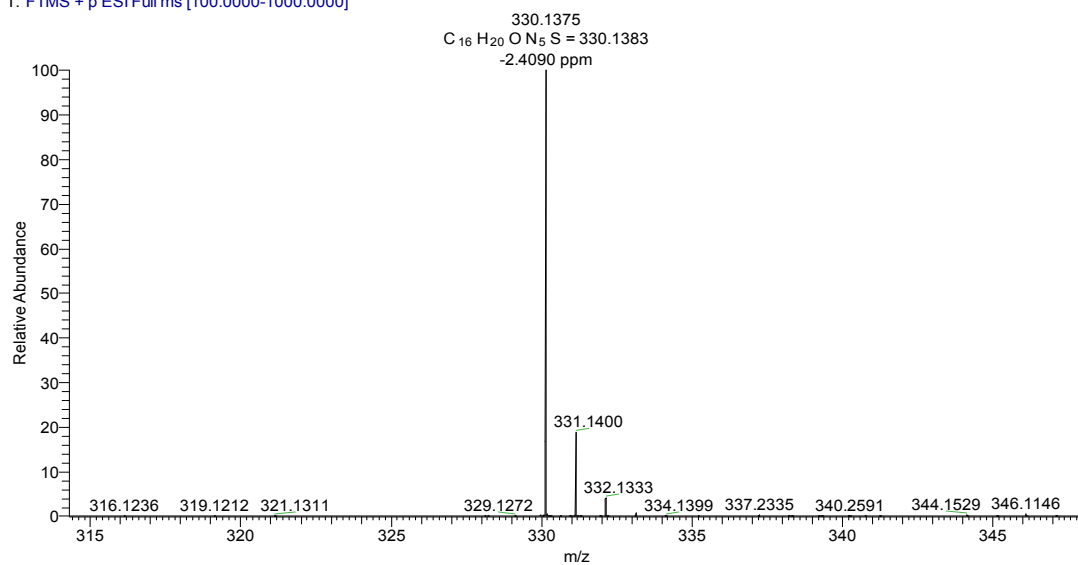


Figure S80. HRMS Spectrum of E_{11} .

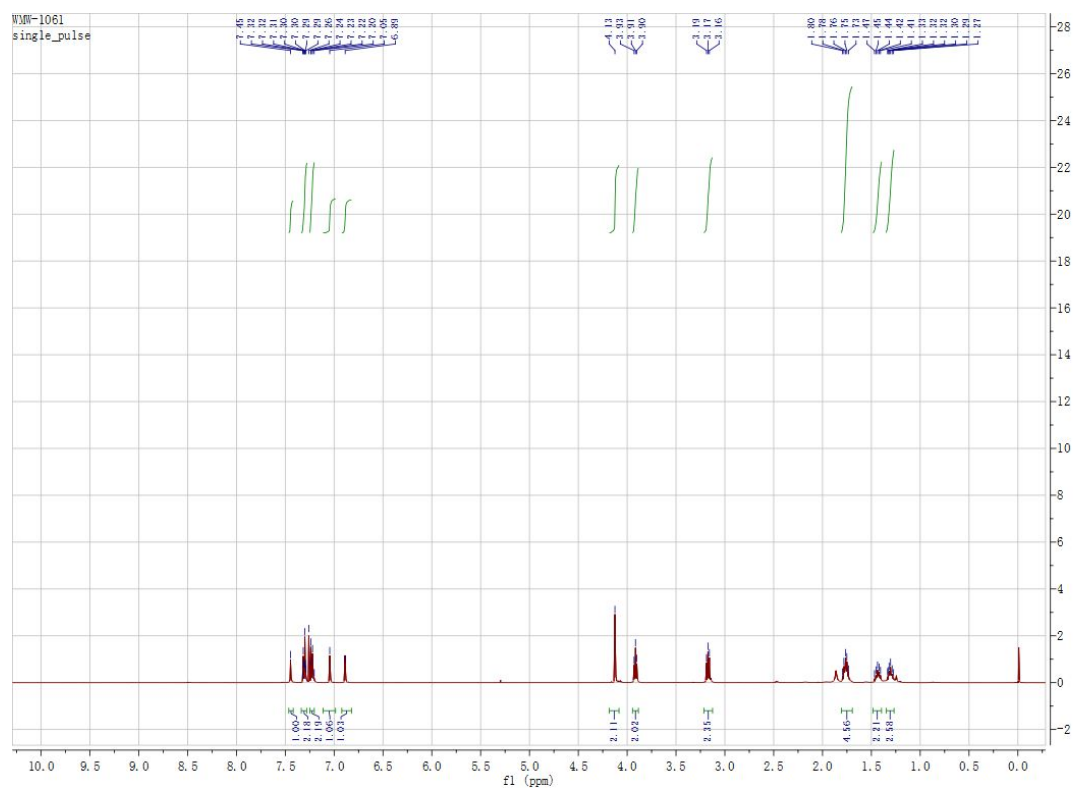


Figure S81. ^1H NMR Spectrum (CDCl_3 , 500 MHz) of E_{12} .

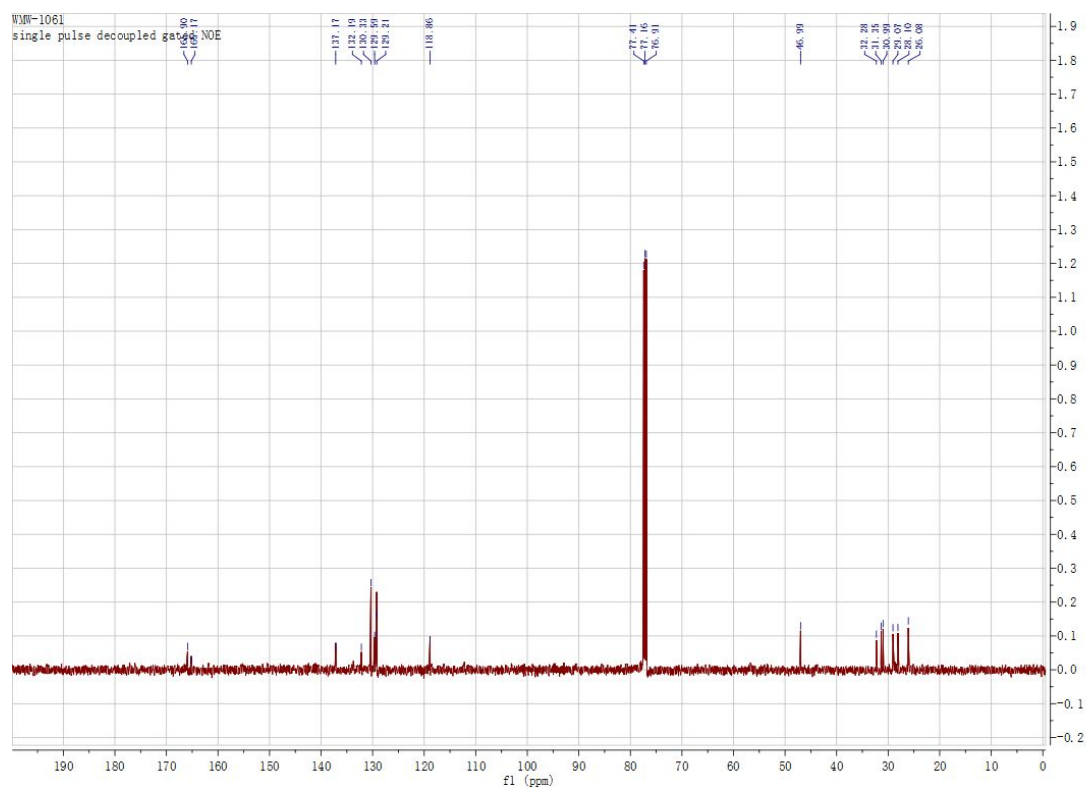


Figure S82. ^{13}C NMR Spectrum (CDCl_3 , 126 MHz) of E_{12} .

2018122845 #101 RT: 0.97 AV: 1 NL: 3.80E9
T: FTMS + p ESI Full ms [100.0000-1000.0000]

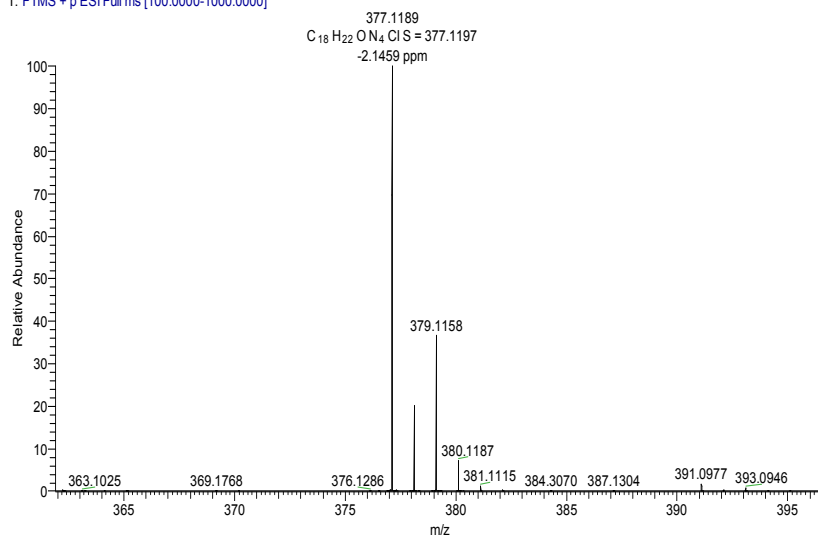


Figure S83. HRMS Spectrum of E₁₂.



Figure S84. ¹H NMR Spectrum (CDCl₃, 500 MHz) of E₁₃.

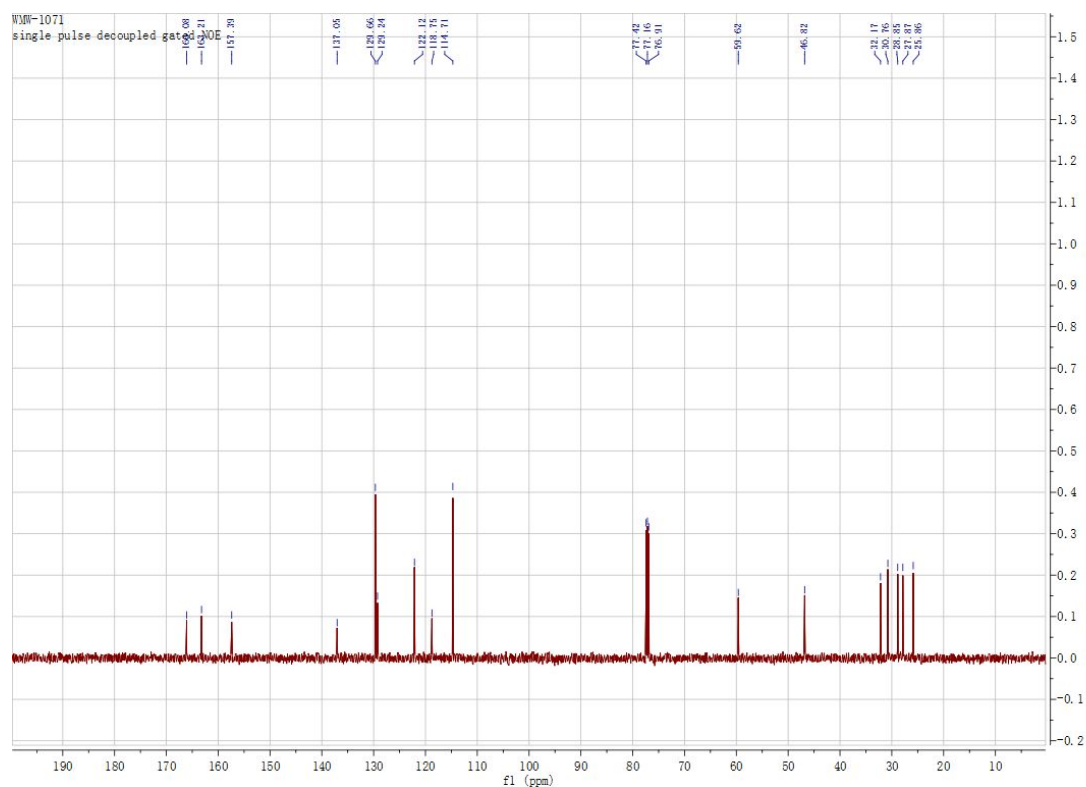


Figure S85. ^{13}C NMR Spectrum (CDCl_3 , 126 MHz) of E_{13} .

2018122850 #87 RT: 0.84 AV: 1 NL: 1.62E9
T: FTMS + p ESI Full ms [100.0000-1000.0000]

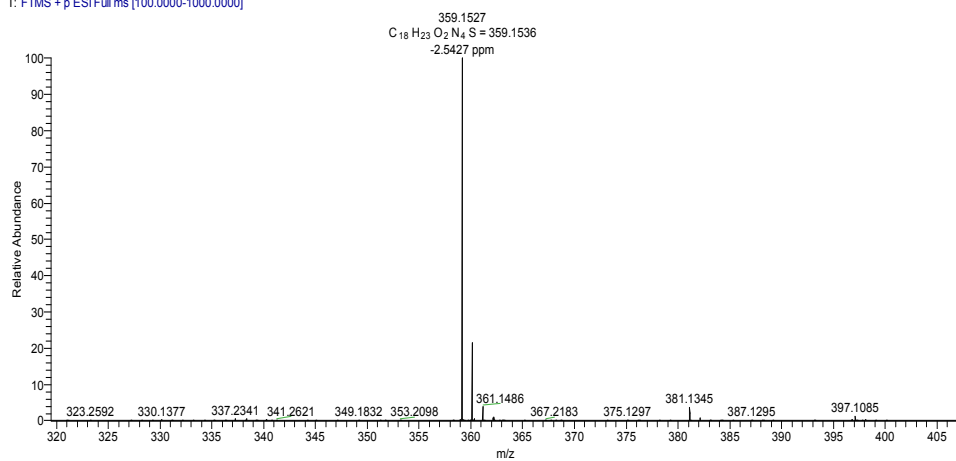


Figure S86. HRMS Spectrum of E_{13} .

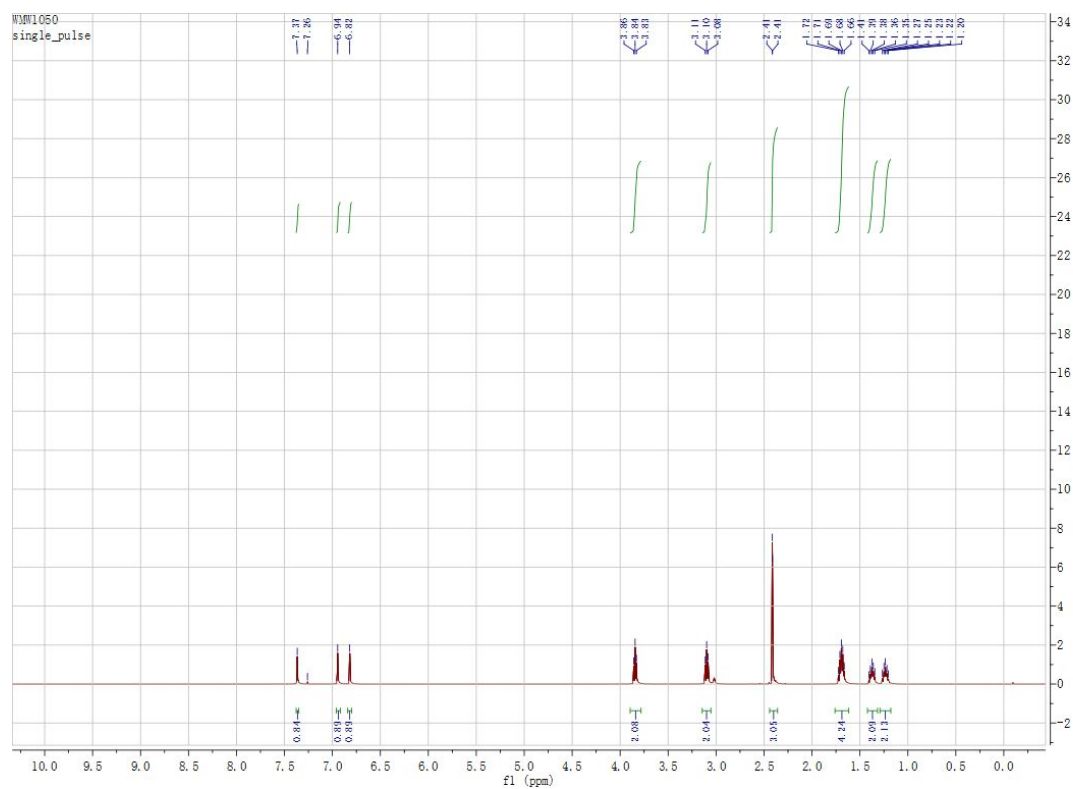


Figure S87. ^1H NMR Spectrum (CDCl_3 , 500 MHz) of E_{14} .

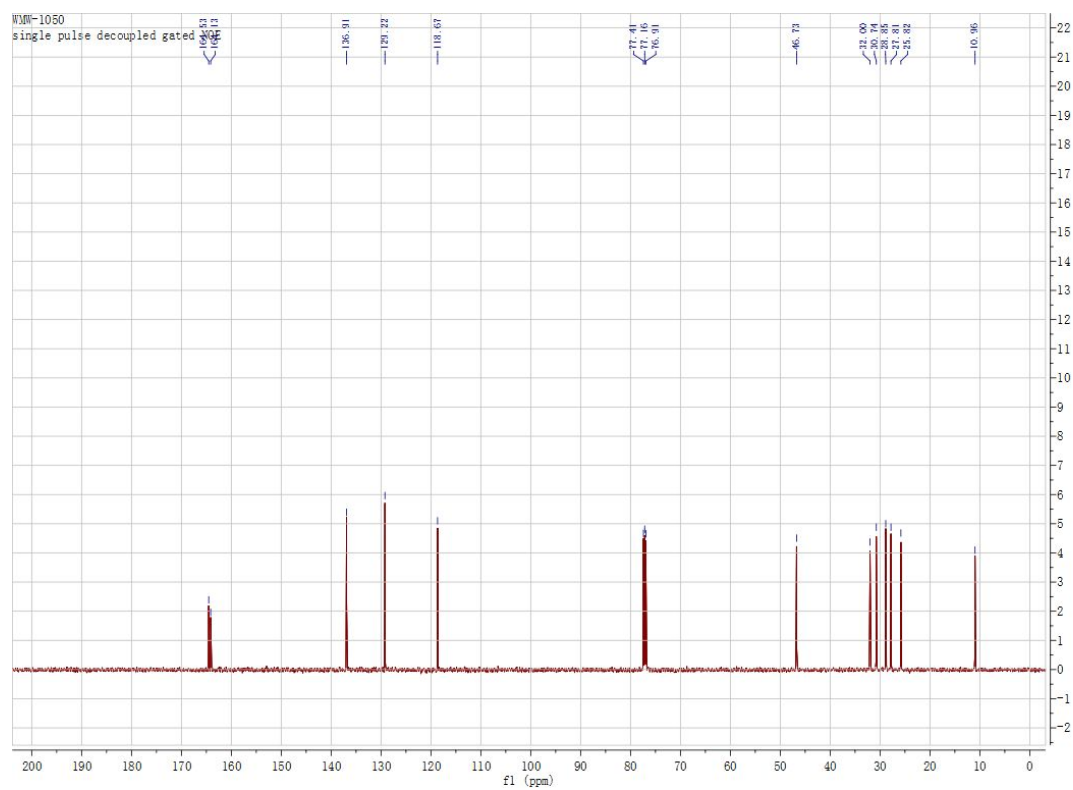


Figure S88. ^{13}C NMR Spectrum (CDCl_3 , 126 MHz) of E_{14} .

2018122841 #63 RT: 0.61 AV: 1 NL: 8.33E8
T: FTMS + p ESI Full ms [100.0000-1000.0000]

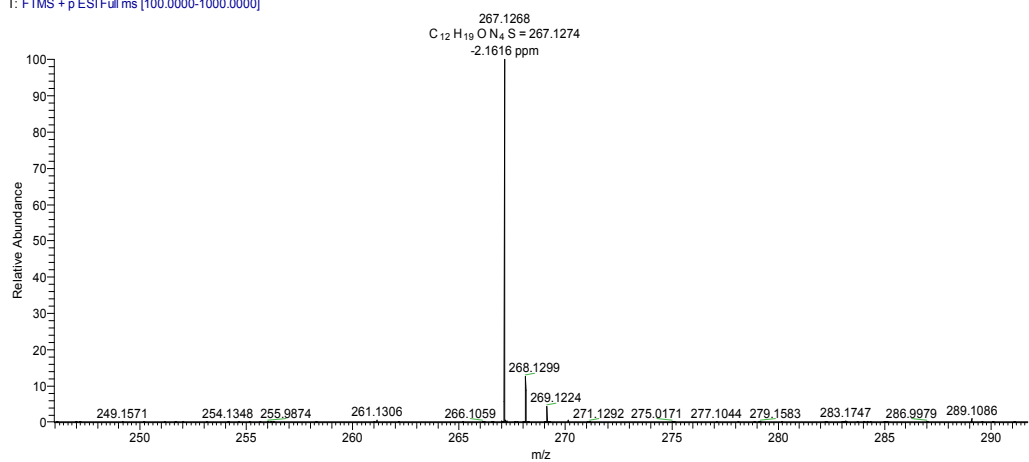


Figure S89. HRMS Spectrum of E₁₄.

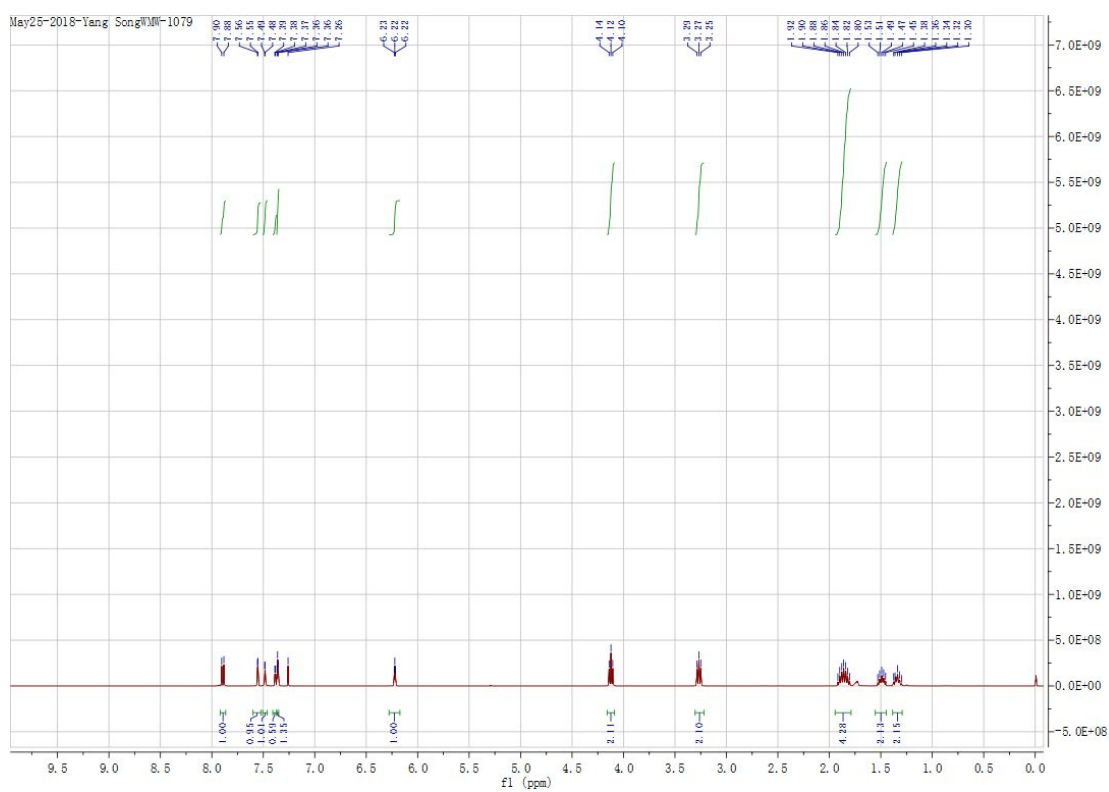


Figure S90. ¹H NMR Spectrum (CDCl₃, 400 MHz) of F₁.

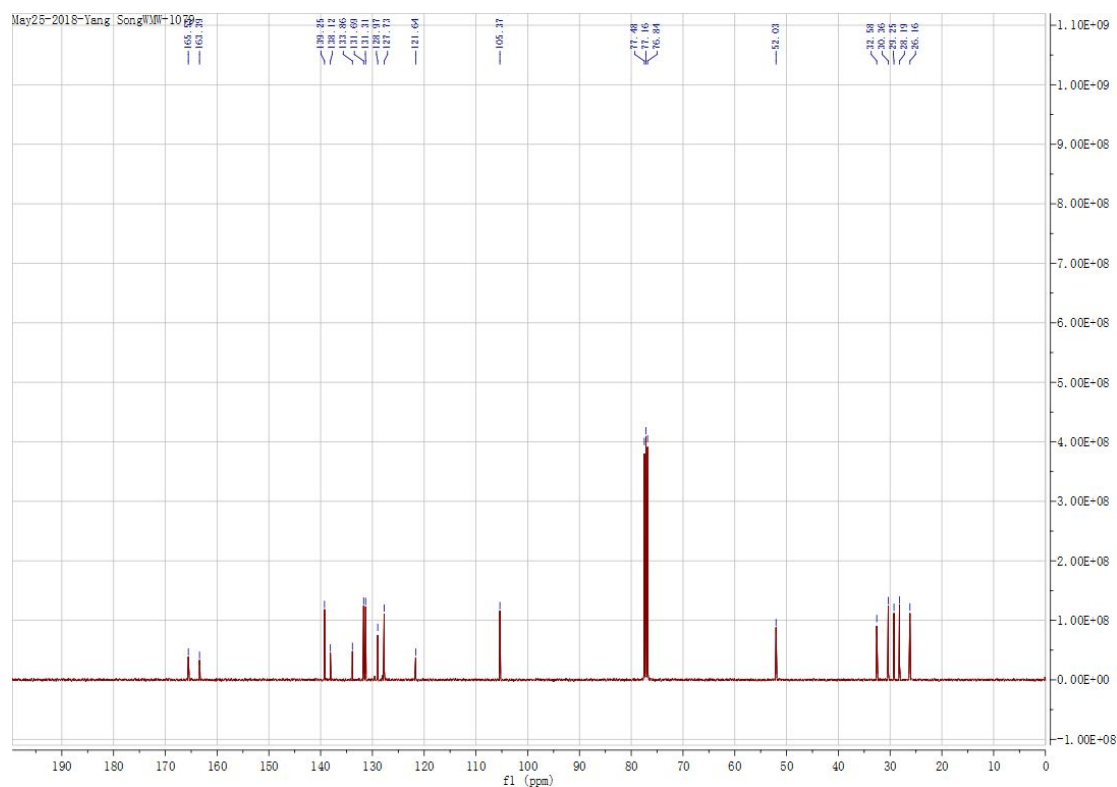


Figure S91. ^{13}C NMR Spectrum (CDCl_3 , 101 MHz) of F_1 .

2018122854 #105 RT: 1.02 AV: 1 NL: 1.00E8
T: FTMS + p ESI Full ms [100.0000-1000.0000]

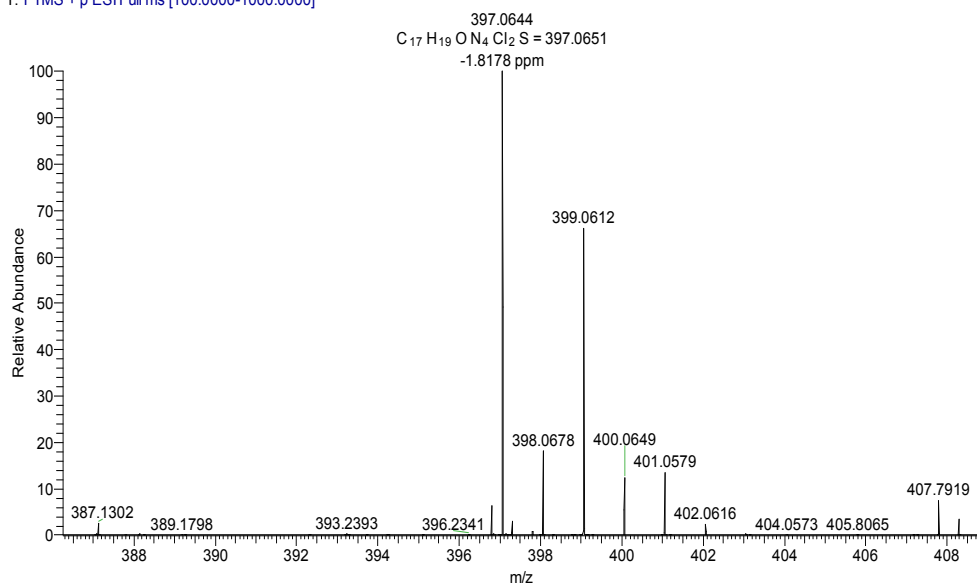


Figure S92. HRMS Spectrum of F_1 .

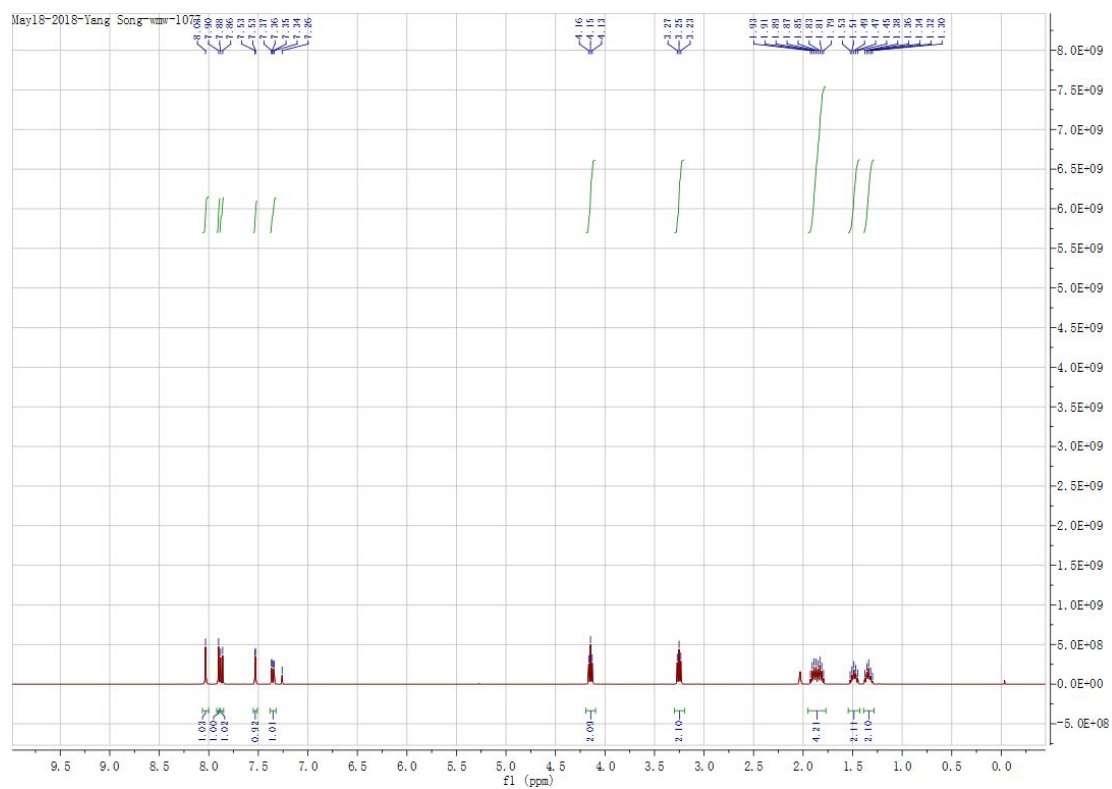


Figure S93. ^1H NMR Spectrum (CDCl_3 , 400 MHz) of F_2 .

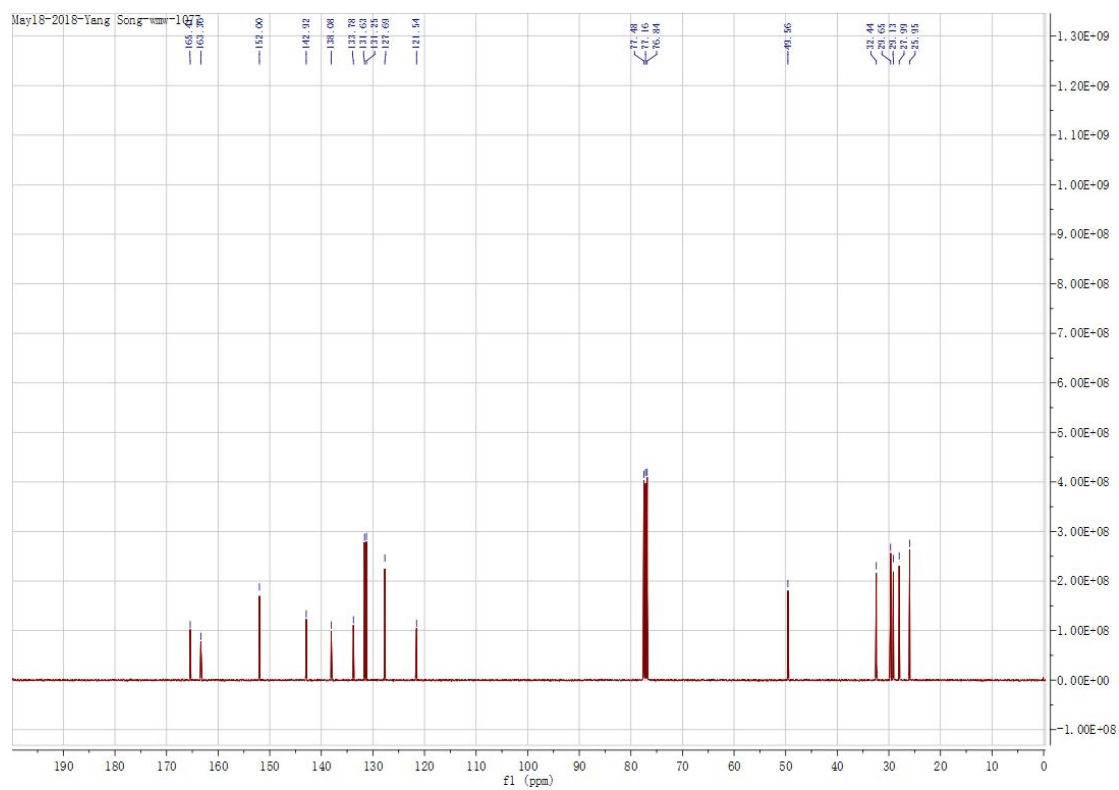


Figure S94. ^{13}C NMR Spectrum (CDCl_3 , 101 MHz) of F_2 .

2018122852 #99 RT: 0.96 AV: 1 NL: 2.74E8
T: FTMS + p ESI Full ms [100.0000-1000.0000]

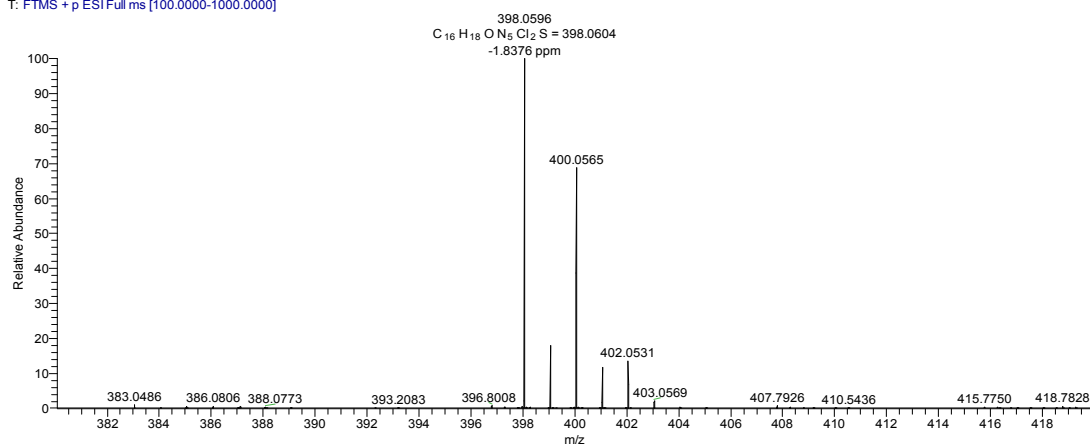


Figure S95. HRMS Spectrum of F₂.

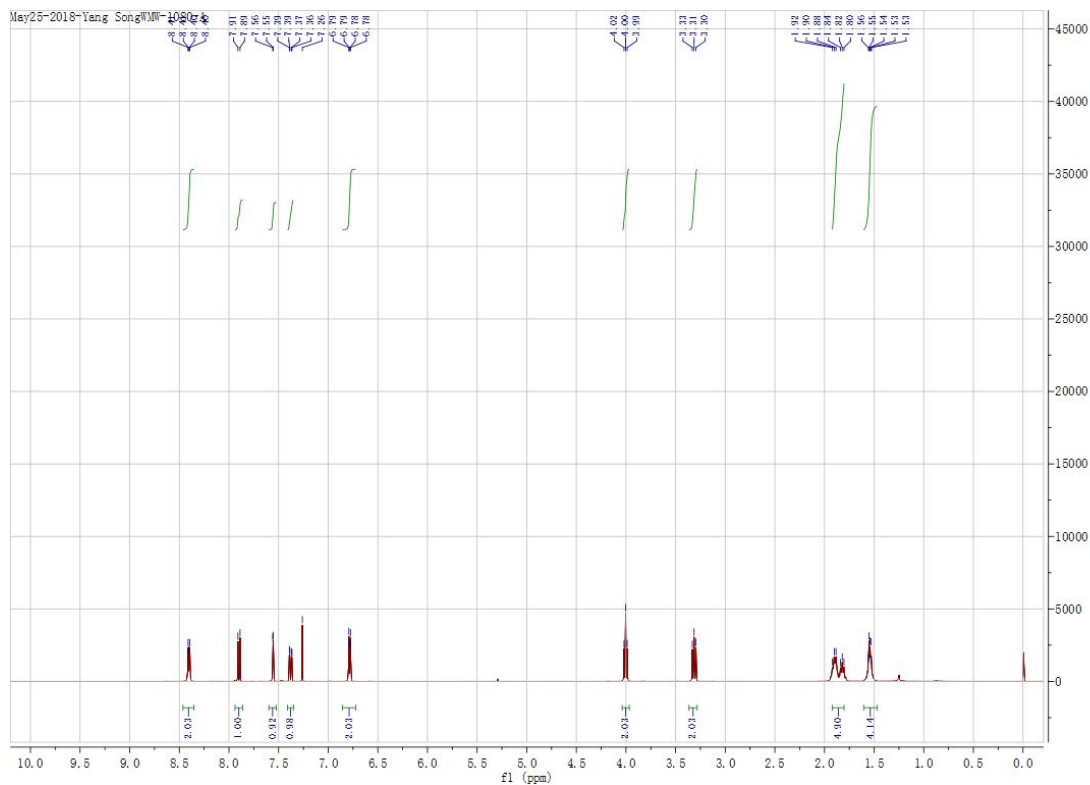


Figure S96. ¹H NMR Spectrum (CDCl₃, 400 MHz) of F₃.

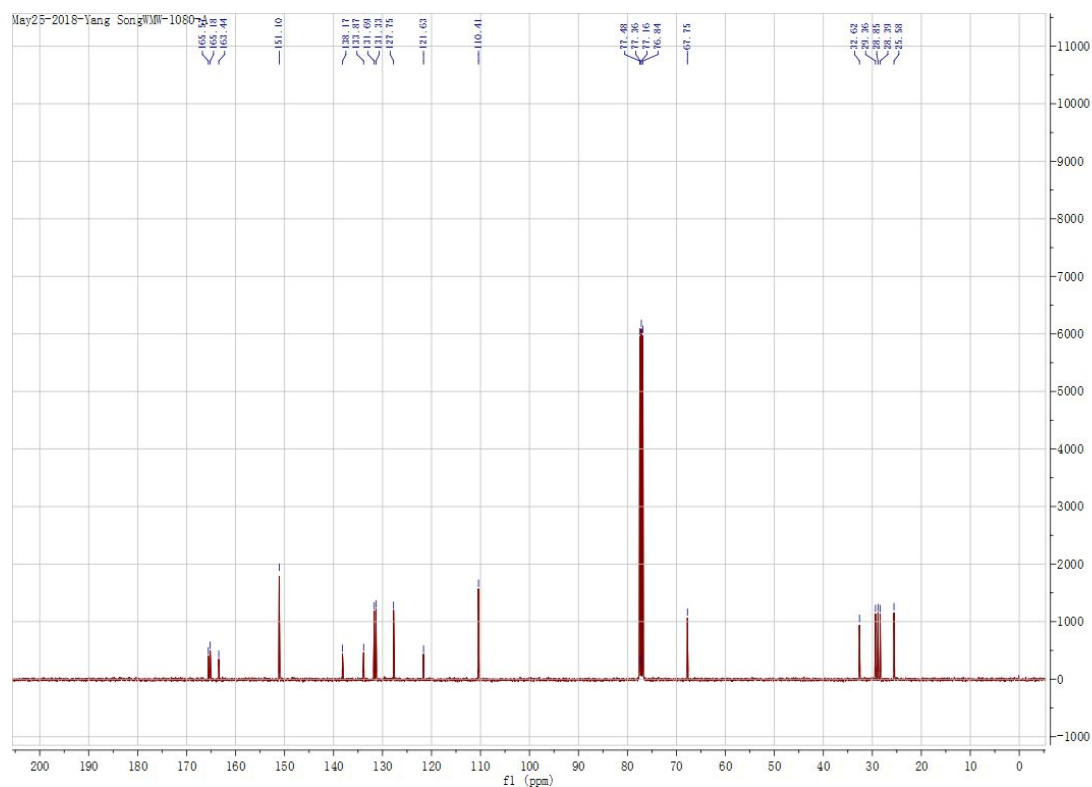


Figure S97. ^{13}C NMR Spectrum (CDCl_3 , 101 MHz) of F_3 .

2018122855 #93 RT: 0.90 AV: 1 NL: 1.75E9
T: FTMS + p ESI Full ms [100.0000-1000.0000]

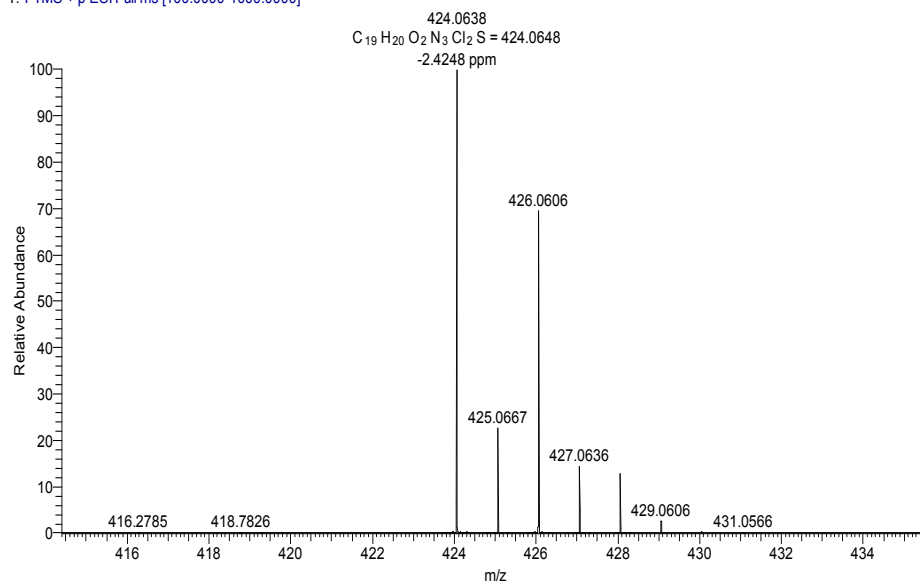


Figure S98. HRMS Spectrum of F_3 .

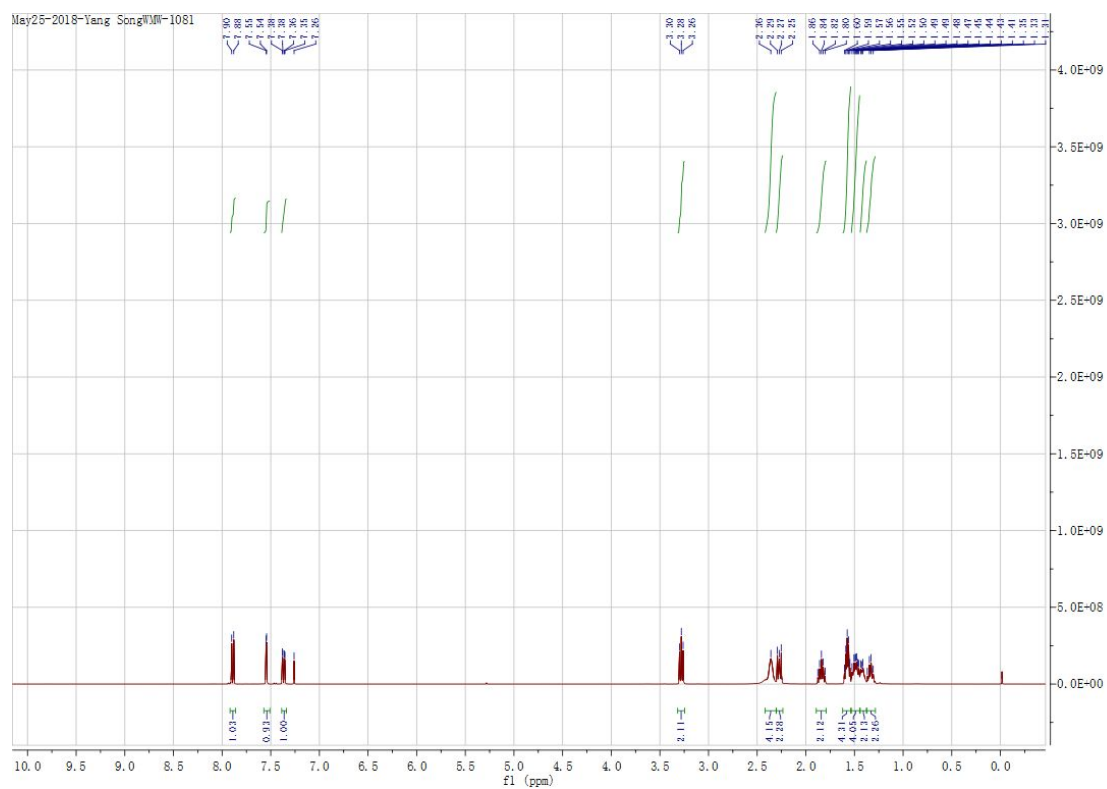


Figure S99. ^1H NMR Spectrum (CDCl_3 , 400 MHz) of F_4 .

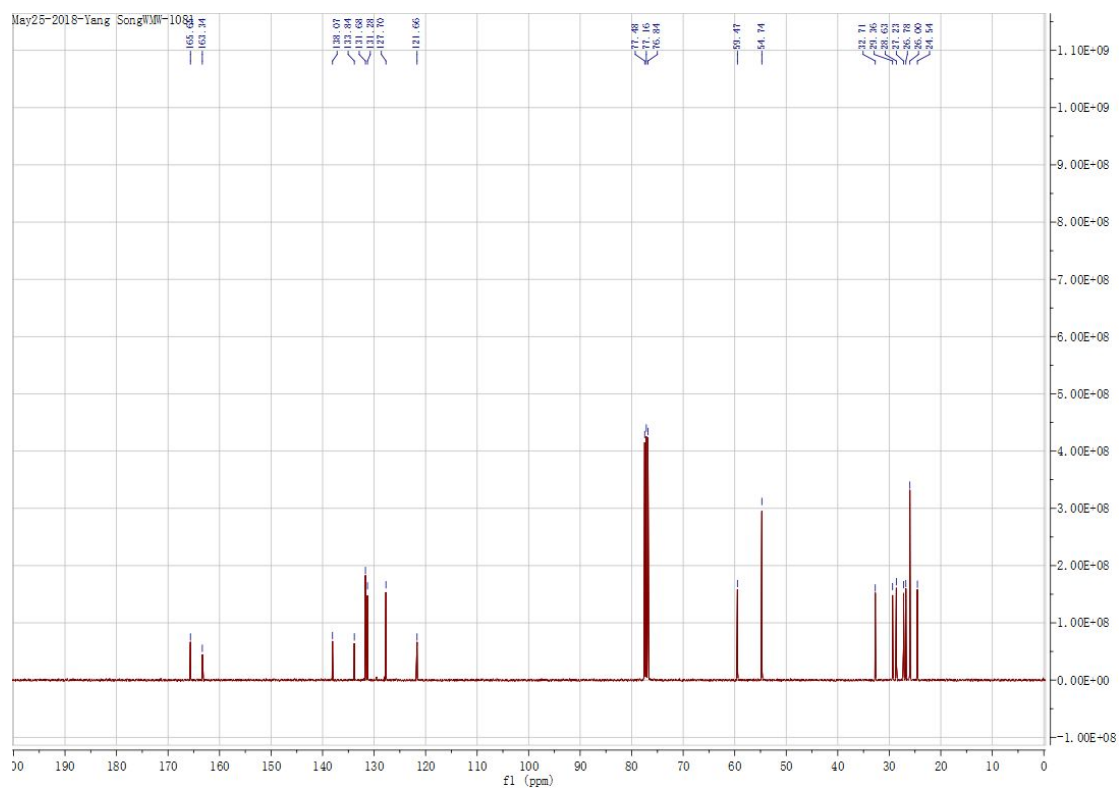


Figure S100. ^{13}C NMR Spectrum (CDCl_3 , 101 MHz) of F_4 .

2018122856 #75 RT: 0.72 AV: 1 NL: 7.40E8
T: FTMS + p ESIFull ms [100.0000-1000.0000]

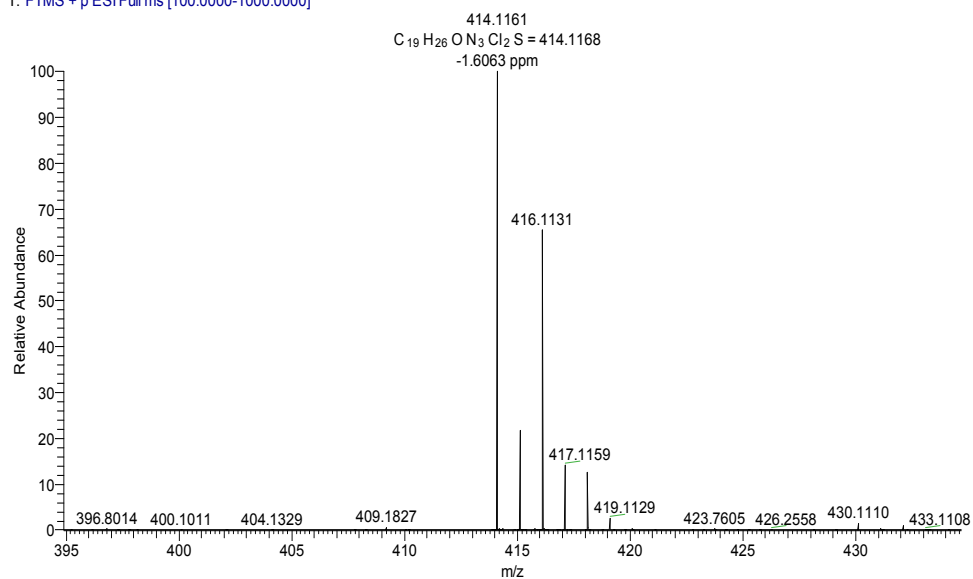


Figure S101. HRMS Spectrum of F₄.

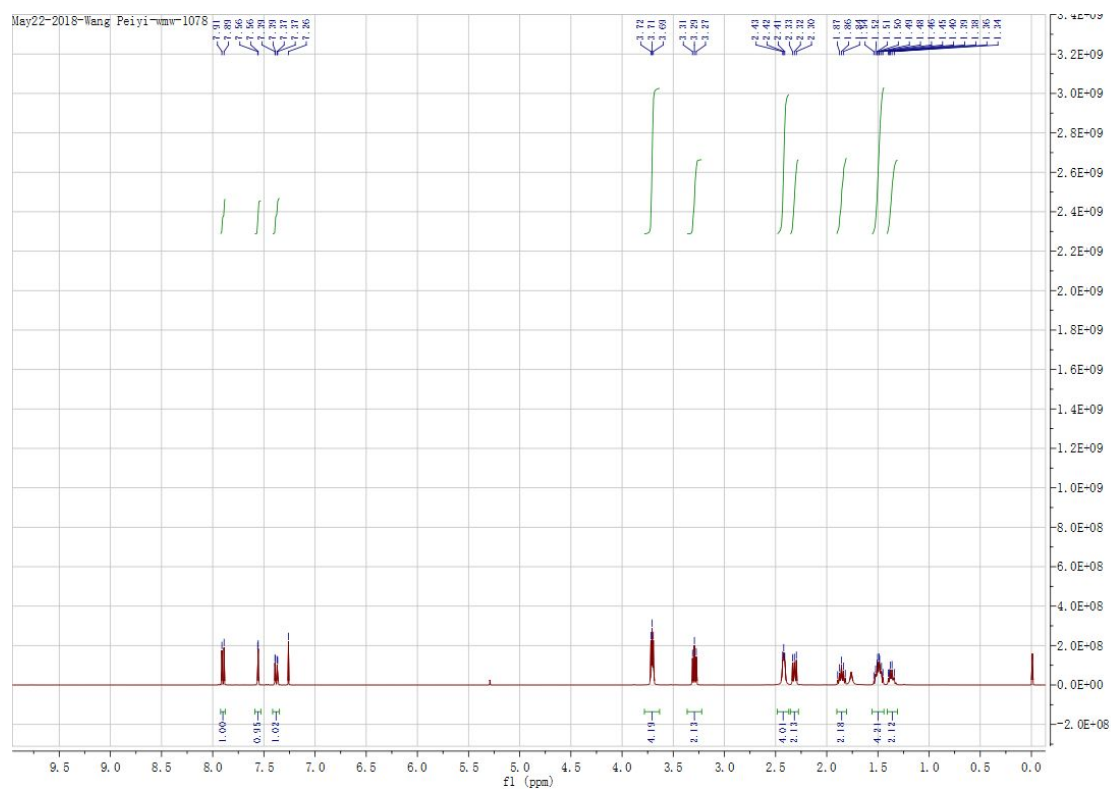


Figure S102. ¹H NMR Spectrum (CDCl₃, 400 MHz) of F₅.

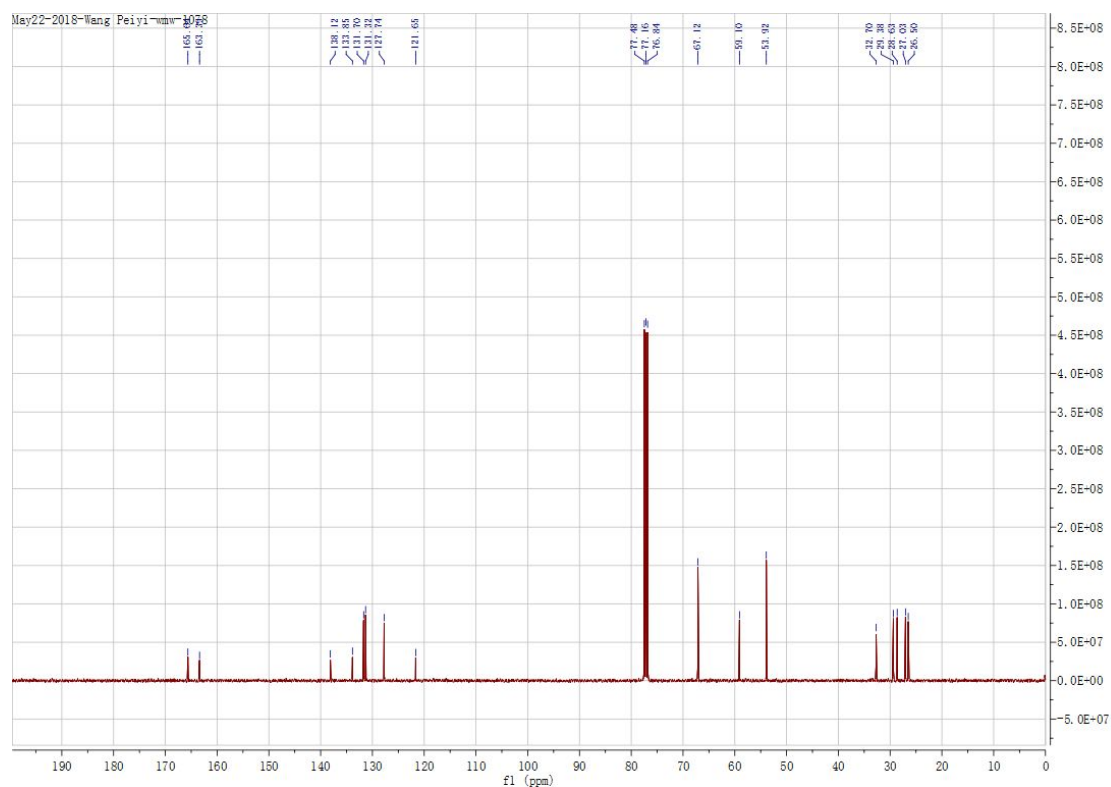


Figure S103. ^{13}C NMR Spectrum (CDCl_3 , 101 MHz) of F_5 .

2018122853 #85 RT: 0.82 AV: 1 NL: 2.98E8
T: FTMS + p ESI Full ms [100.0000-1000.0000]

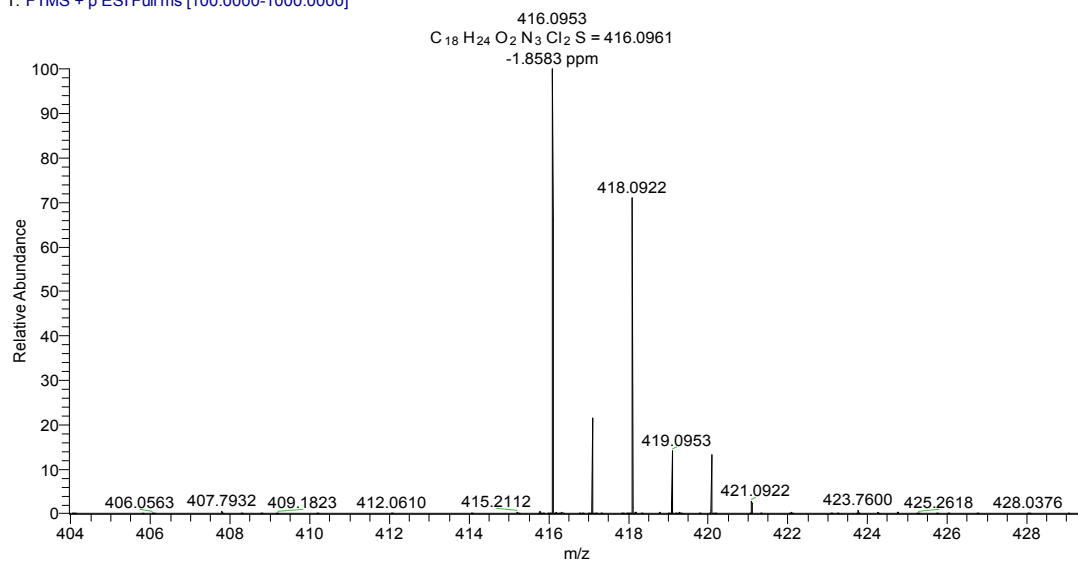


Figure S104. HRMS Spectrum of F_5 .

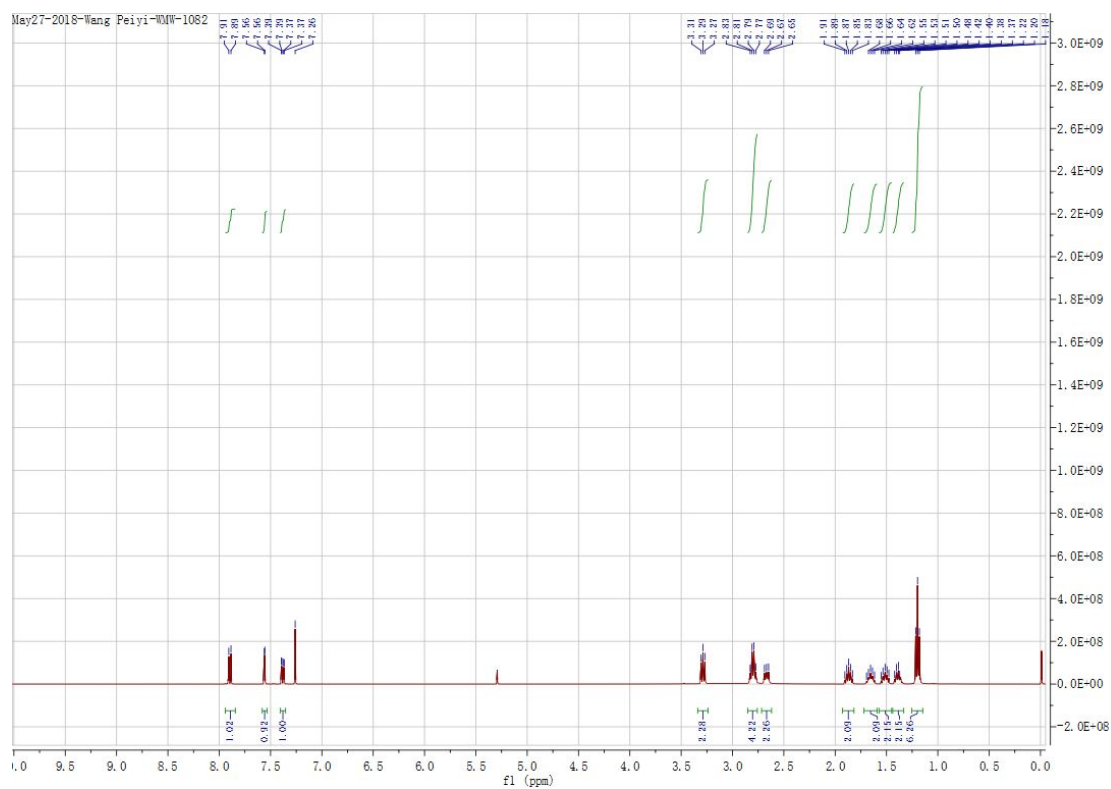


Figure S105. ^1H NMR Spectrum (CDCl_3 , 400 MHz) of F_6 .

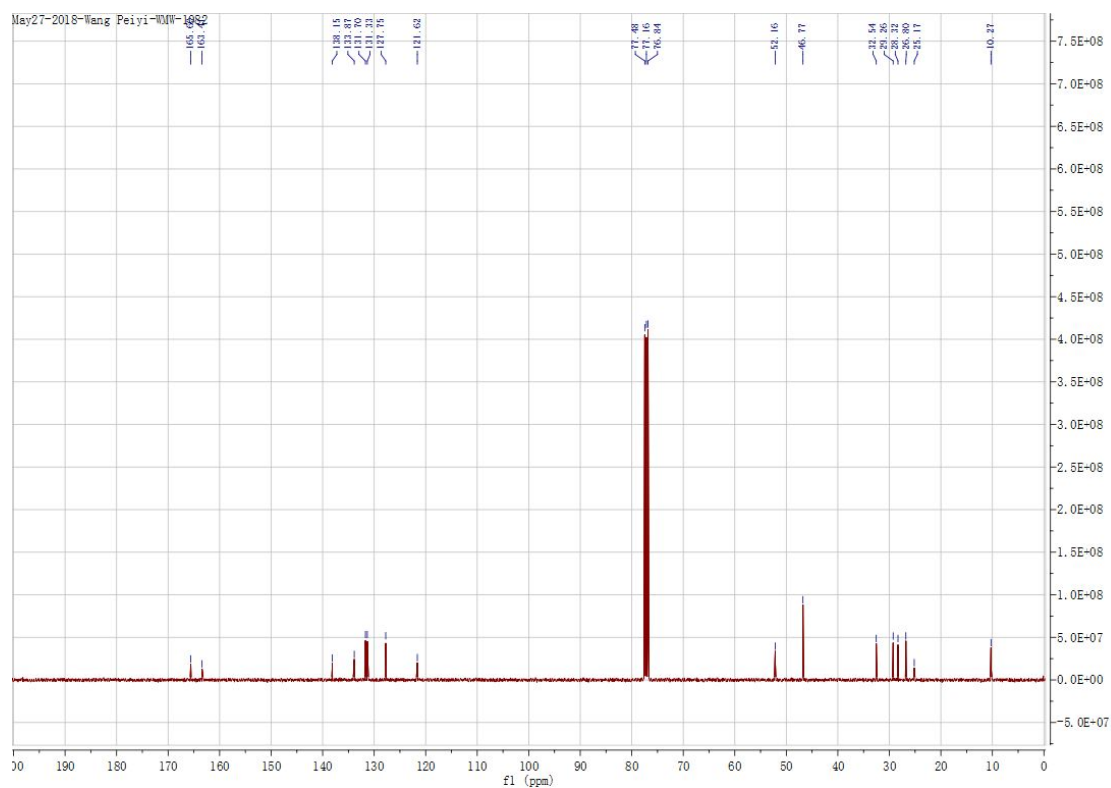


Figure S106. ^{13}C NMR Spectrum (CDCl_3 , 101 MHz) of F_6 .

2018122857 #93 RT: 0.90 AV: 1 NL: 6.15E8
T: FTMS + p ESI Full ms [100.0000-1000.0000]

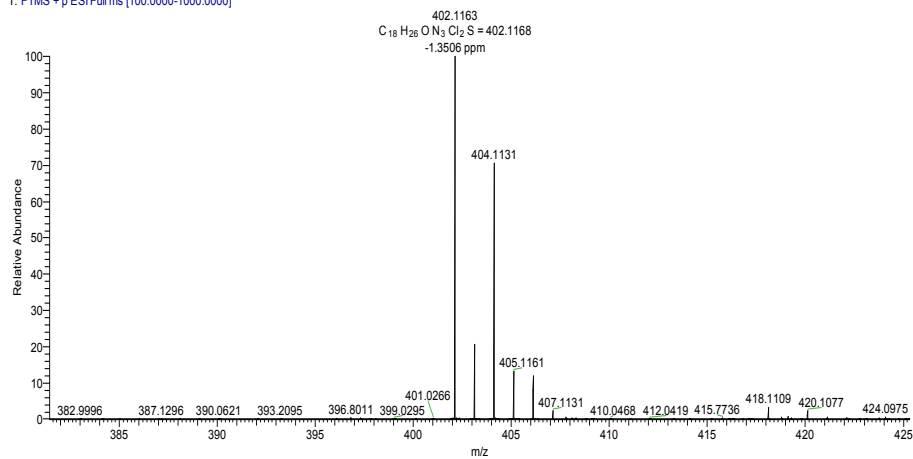


Figure 107. HRMS Spectrum of F₆.

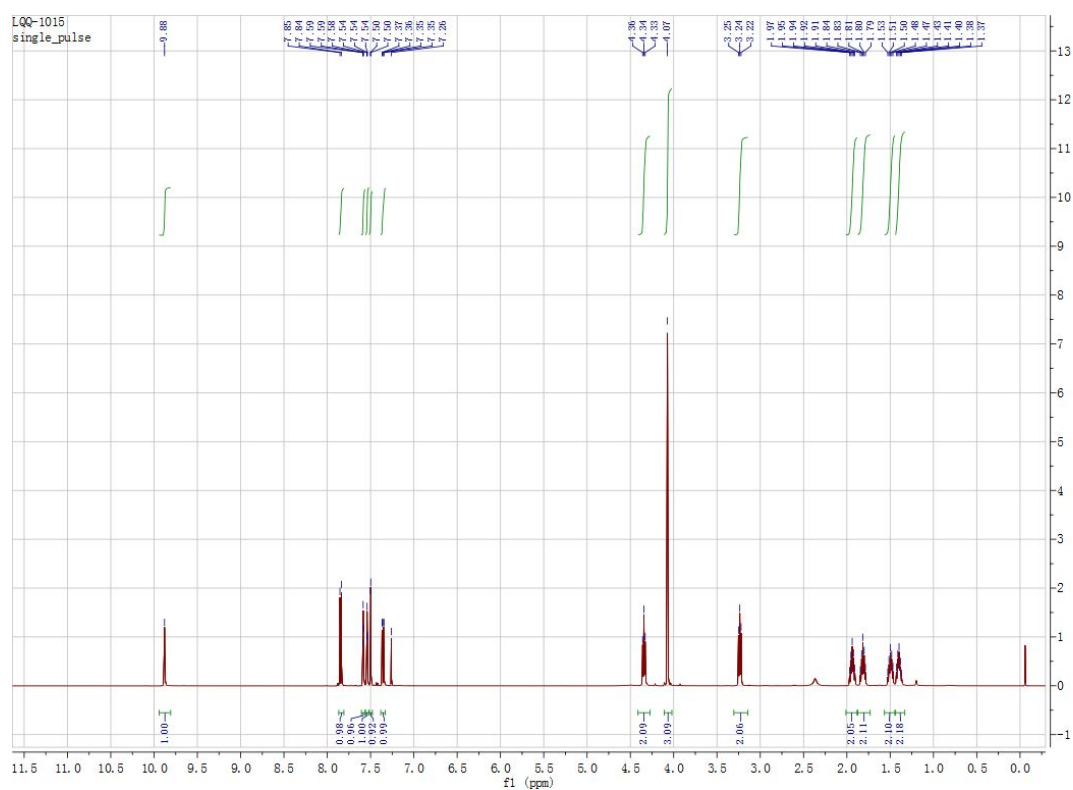


Figure S108. ¹H NMR Spectrum (CDCl₃, 500 MHz) of G₁.

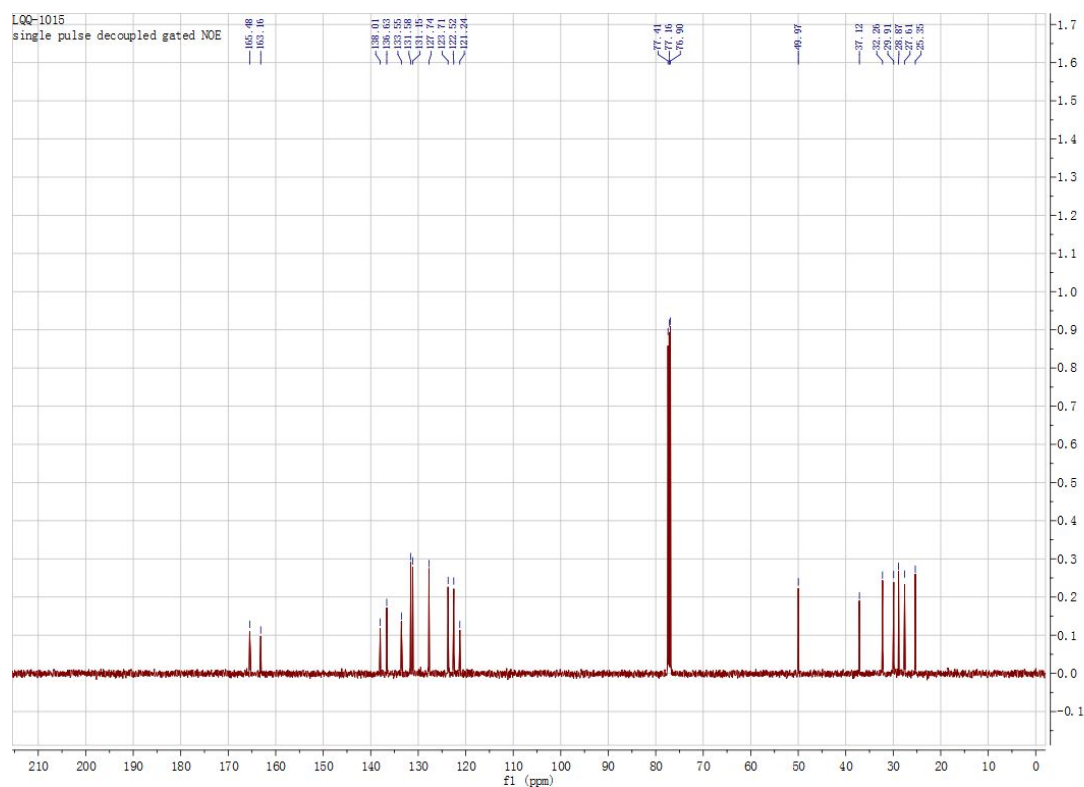


Figure S109. ^{13}C NMR Spectrum (CDCl_3 , 126 MHz) of G_1 .

2018122807 #95 RT: 0.91 AV: 1 NL: 1.41E8
T: FTMS + p ESI Full ms [100.0000-1000.0000]

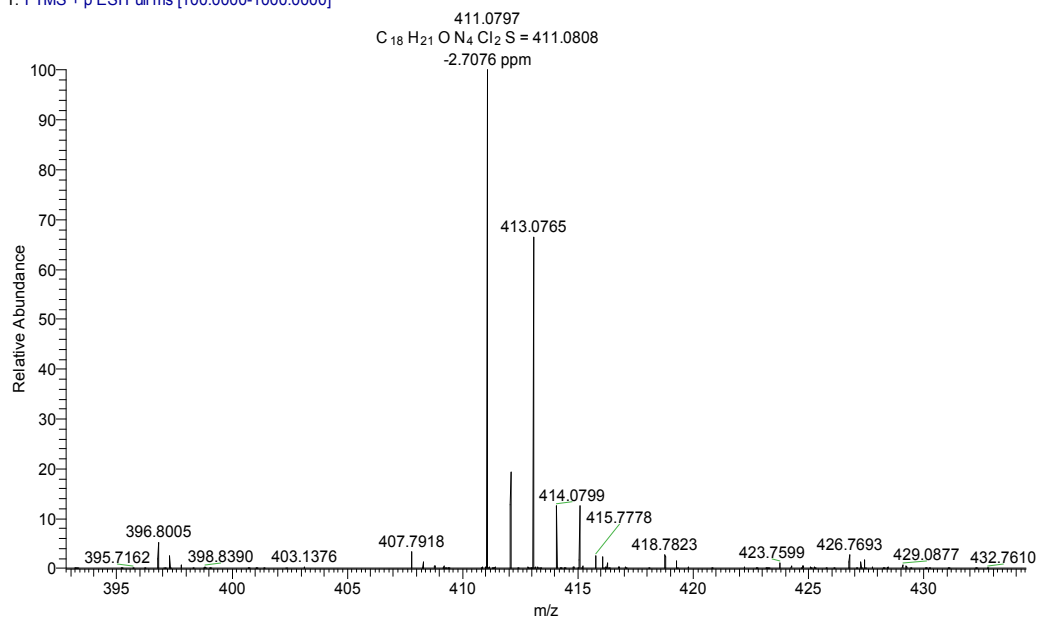


Figure S110. HRMS Spectrum of G_1 .

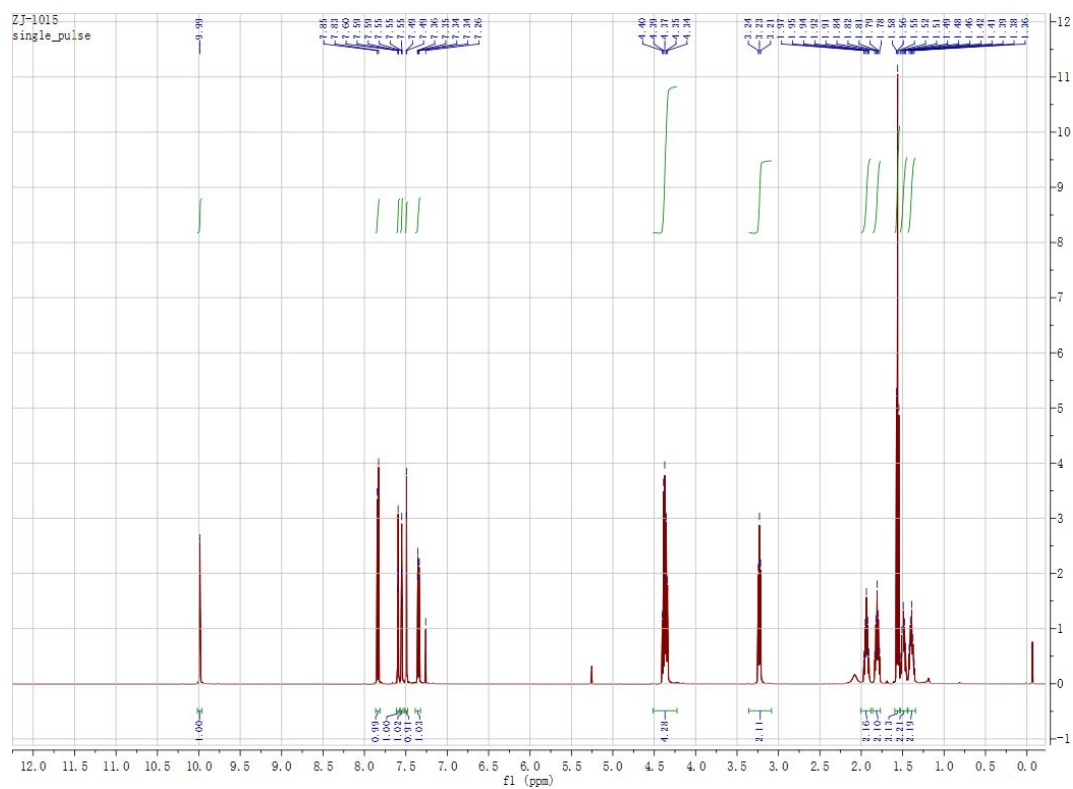


Figure S111. ^1H NMR Spectrum (CDCl_3 , 500 MHz) of G_2 .

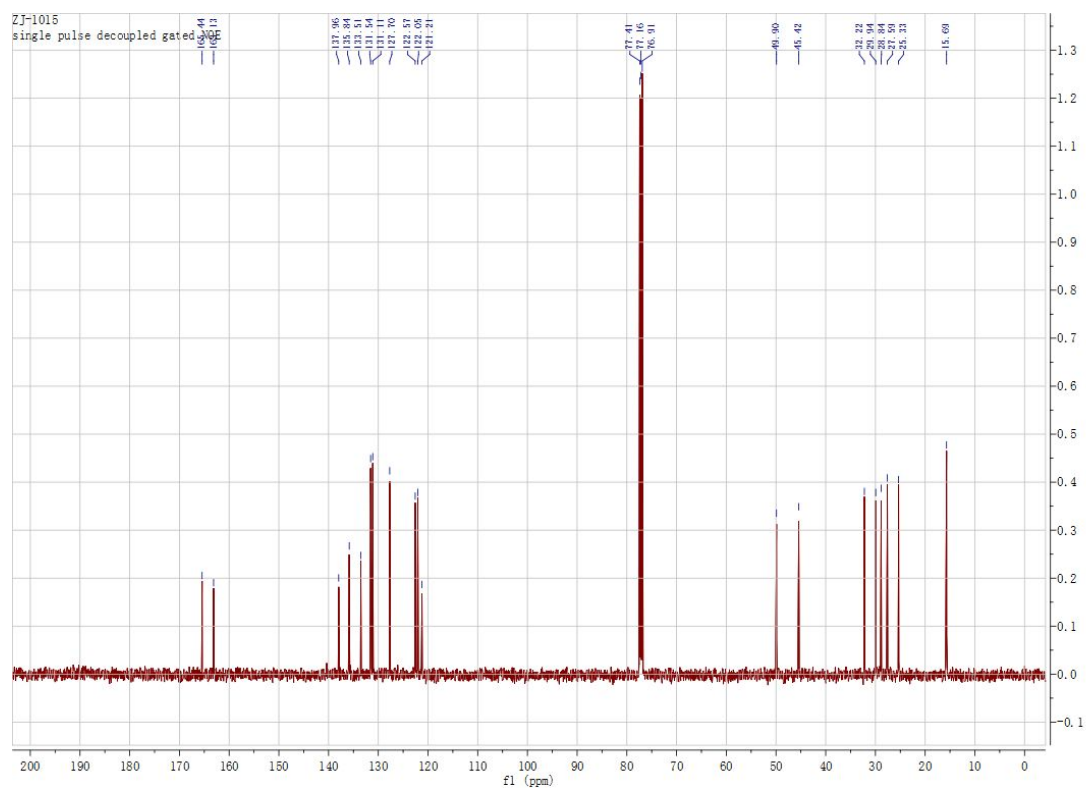


Figure S112. ^{13}C NMR Spectrum (CDCl_3 , 126 MHz) of G_2 .

2018122808 #75 RT: 0.72 AV: 1 NL: 6.49E8
T: FTMS + p ESI Full ms [100.0000-1000.0000]

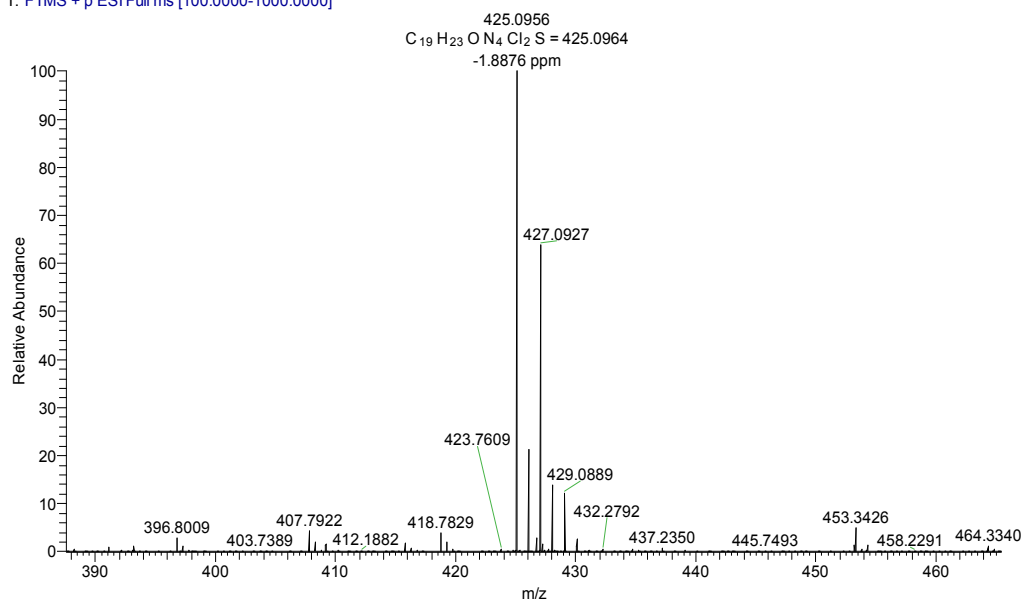


Figure S113. HRMS Spectrum of G_2 .



Figure S114. 1H NMR Spectrum (CDCl₃, 500 MHz) of G_3 .

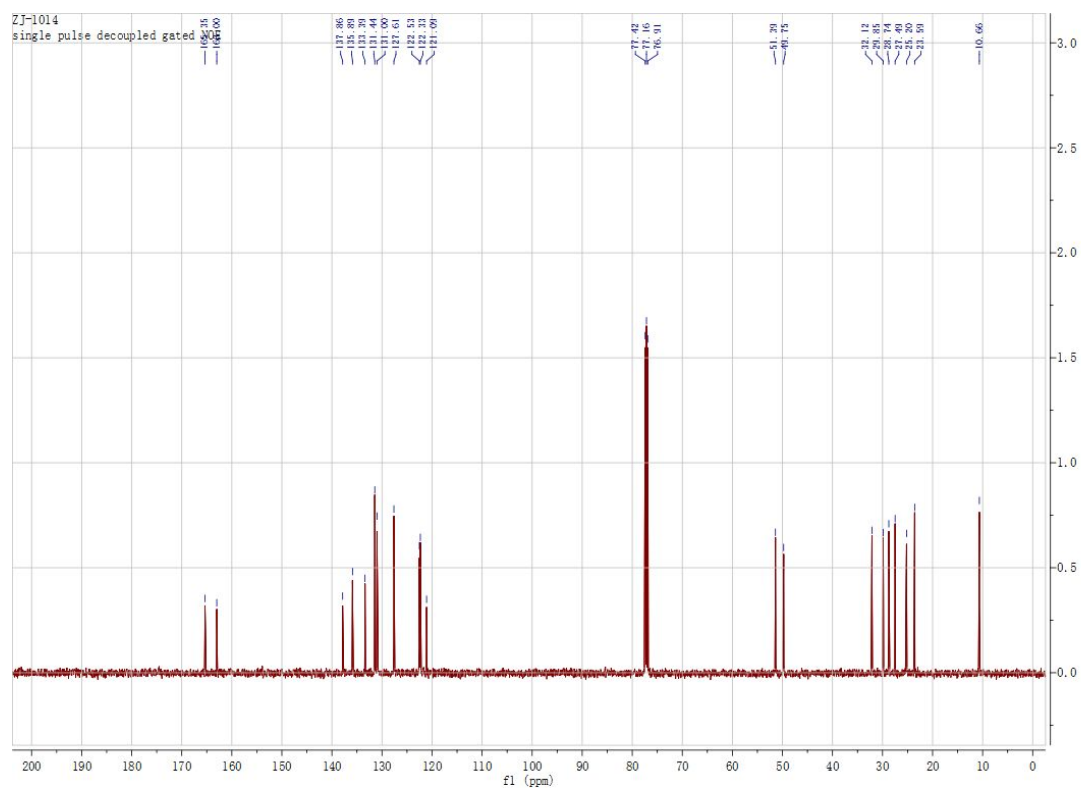


Figure S115. ^{13}C NMR Spectrum (CDCl_3 , 126 MHz) of G_3 .

2018122809 #95 RT: 0.91 AV: 1 NL: 1.04E8
T: FTMS + p ESI Full ms [100.0000-1000.0000]

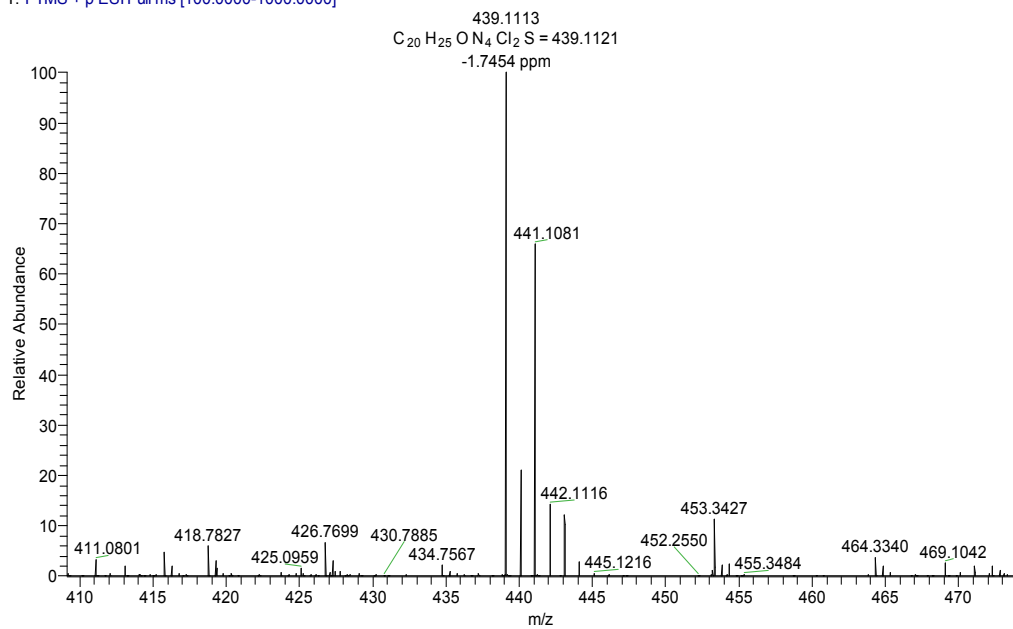


Figure S116. HRMS Spectrum of G_3 .

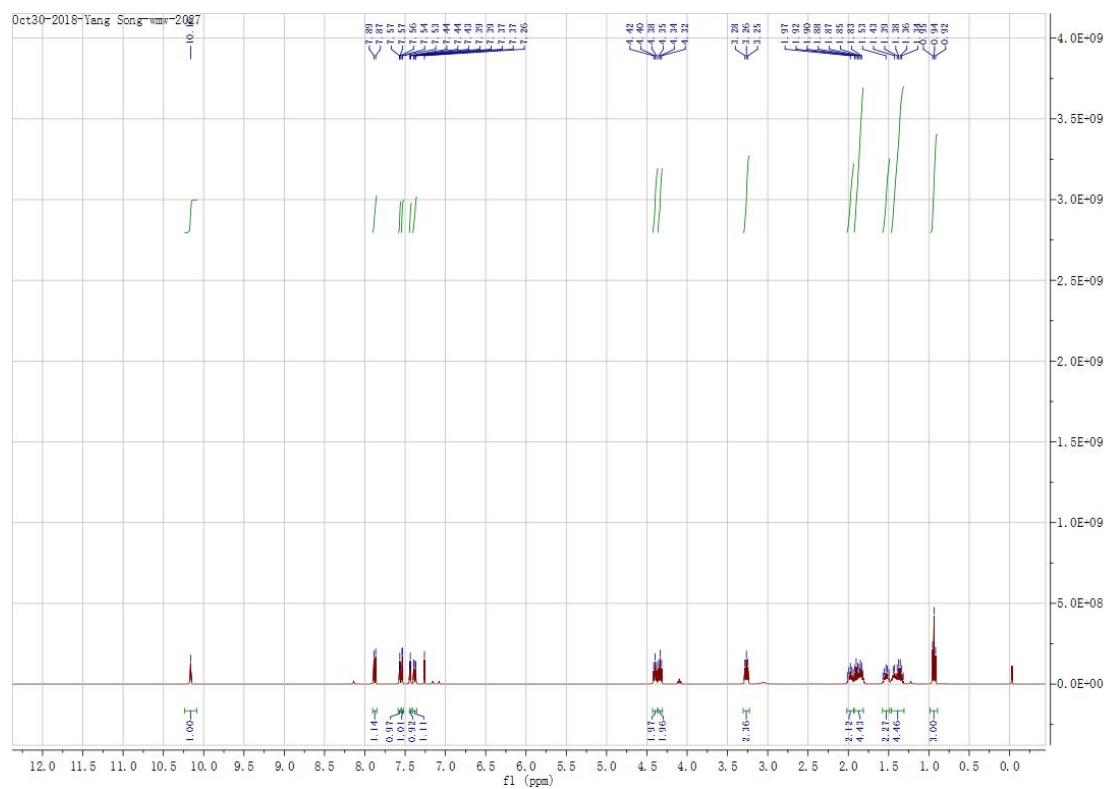


Figure S117. ^1H NMR Spectrum (CDCl_3 , 400 MHz) of G_4 .

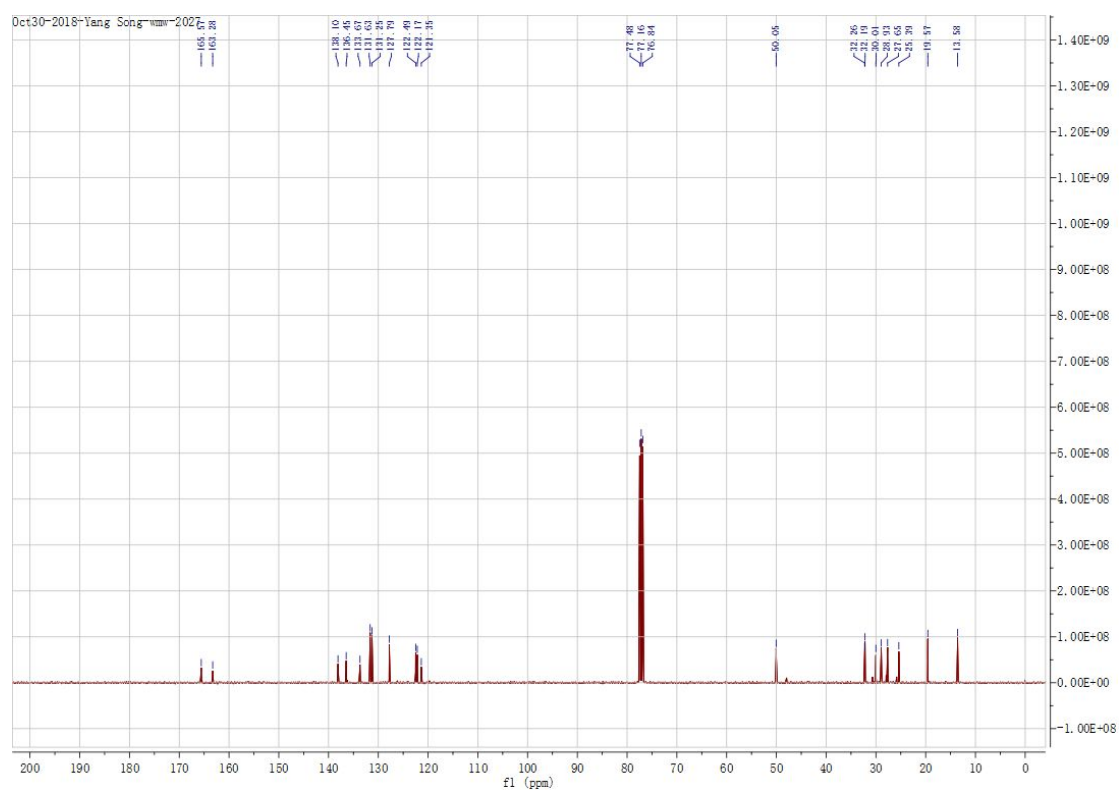


Figure S118. ^{13}C NMR Spectrum (CDCl_3 , 101 MHz) of G_4 .

2018122810 #97 RT: 0.93 AV: 1 NL: 8.18E7
T: FTMS + p ESI Full ms [100.0000-1000.0000]

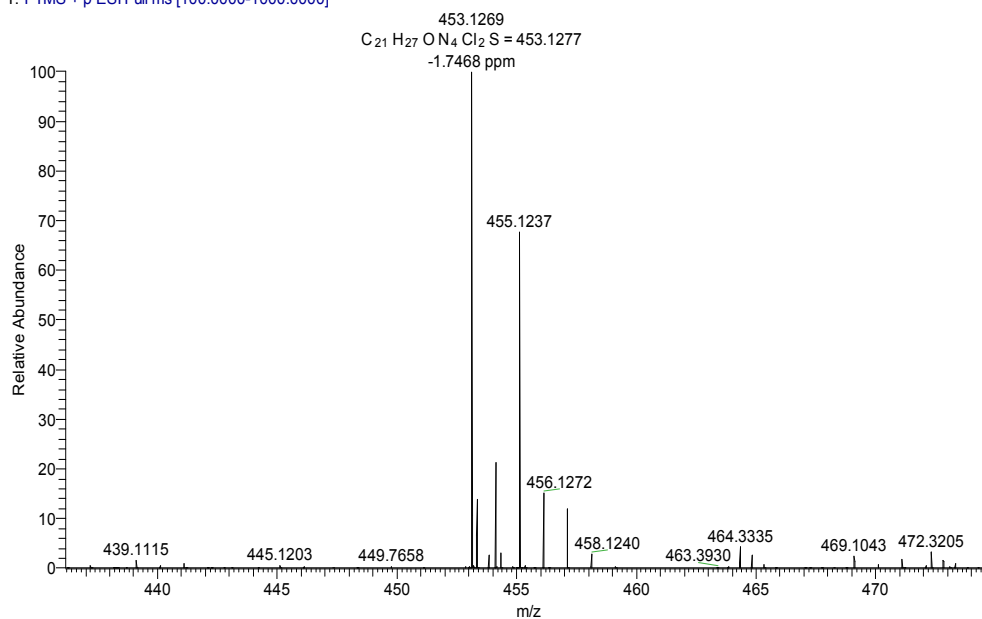


Figure S119. HRMS Spectrum of G₄.

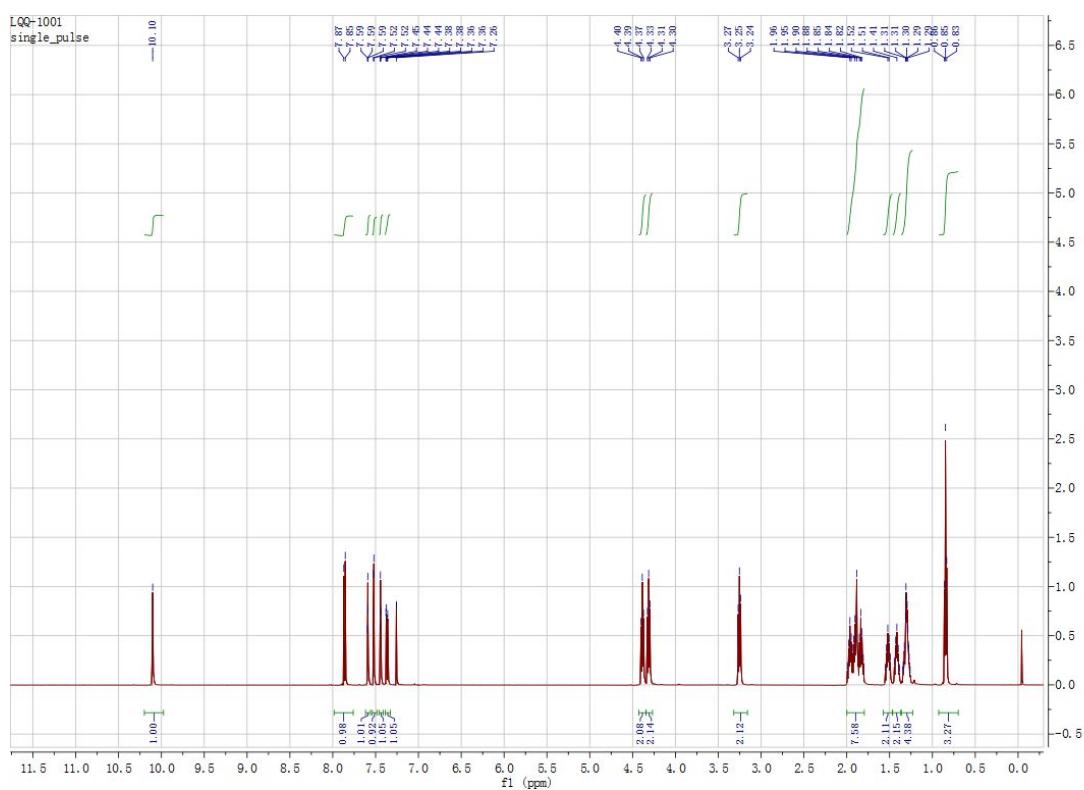


Figure S120. ¹H NMR Spectrum (CDCl₃, 500 MHz) of G₅.

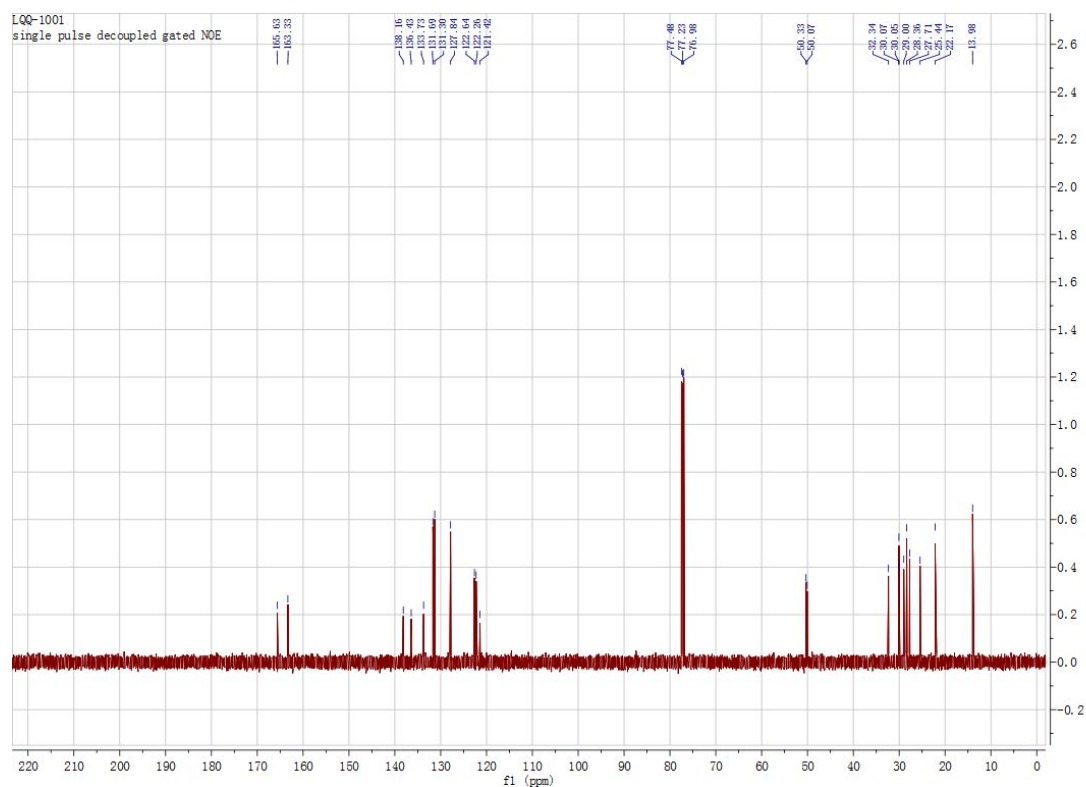


Figure S121. ¹³C NMR Spectrum (CDCl₃, 126 MHz) of G₅.

2018122811 #75 RT: 0.72 AV: 1 NL: 8.11E7
T: FTMS + p ESI Full ms [100.0000-1000.0000]

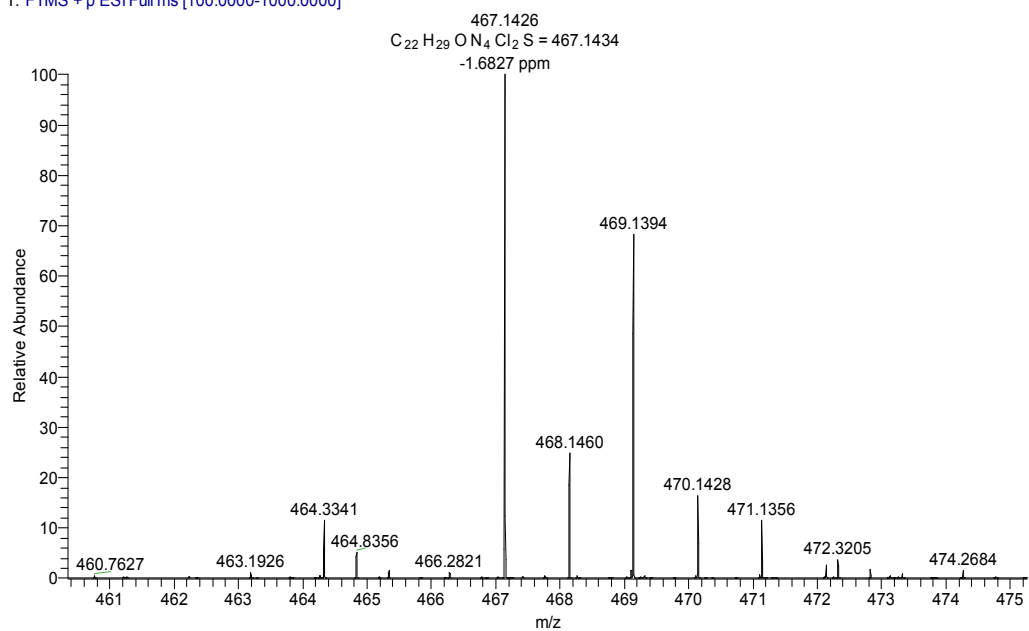


Figure S122. HRMS Spectrum of G₅.

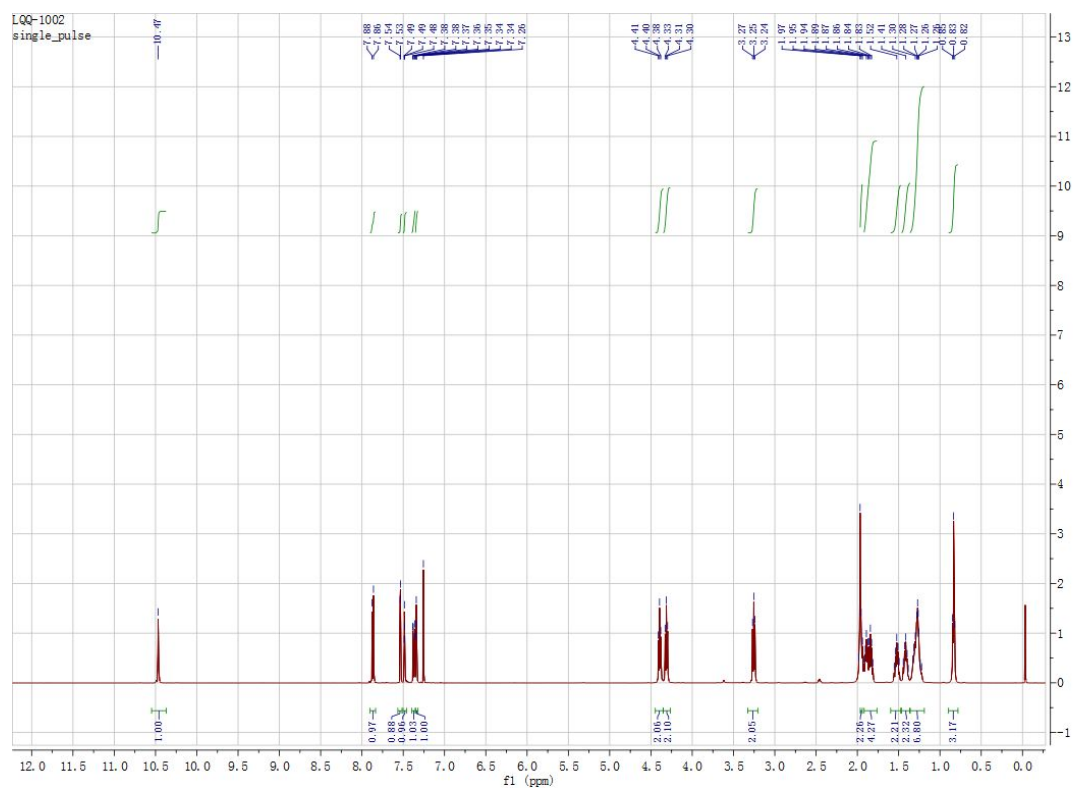


Figure S123. ¹H NMR Spectrum (CDCl₃, 500 MHz) of G₆.

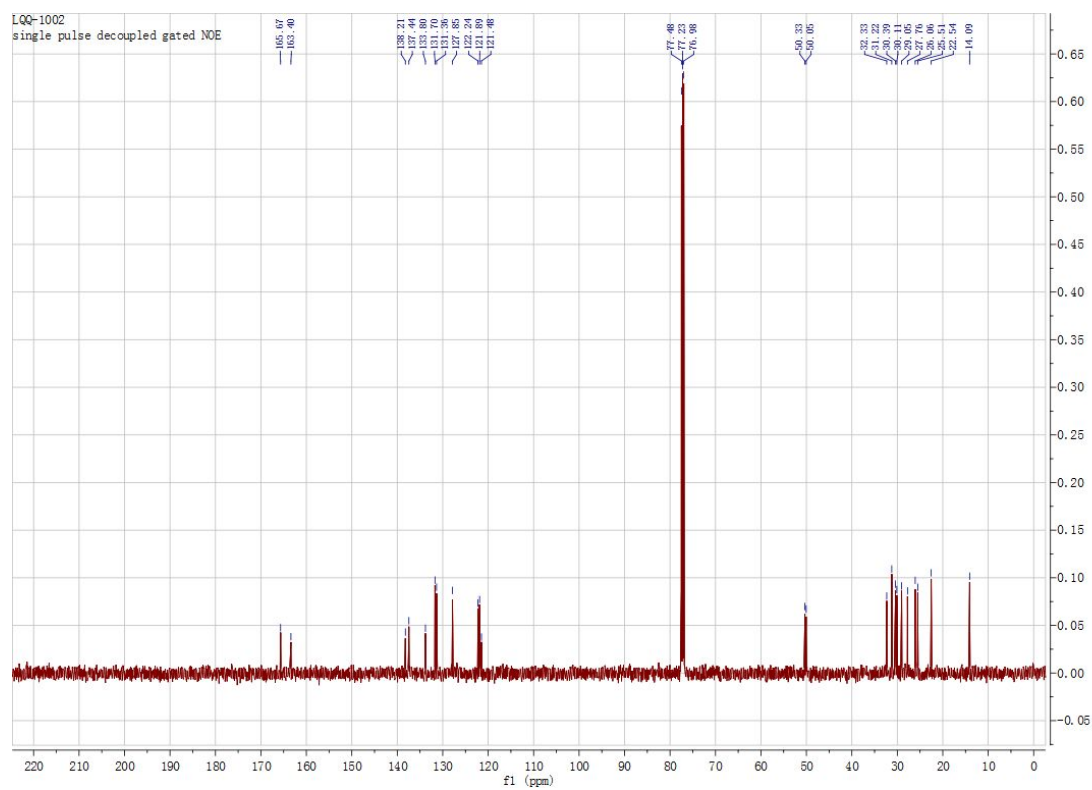


Figure S124. ¹³C NMR Spectrum (CDCl₃, 126 MHz) of G₆.

2018122812 #93 RT: 0.90 AV: 1 NL: 2.28E8
T: FTMS + p ESI Full ms [100.0000-1000.0000]

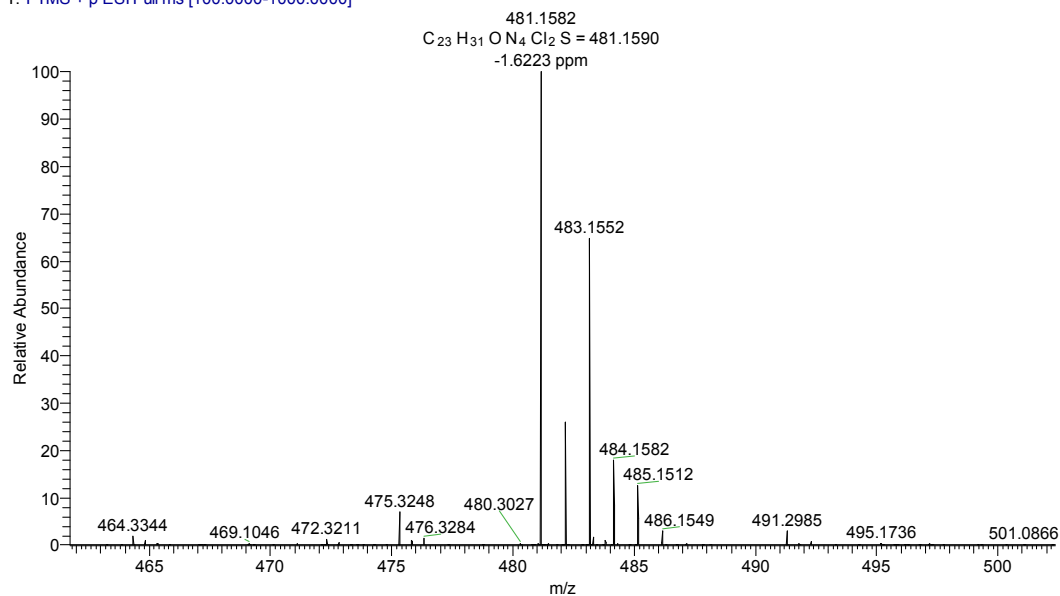


Figure S125. HRMS Spectrum of G_6 .

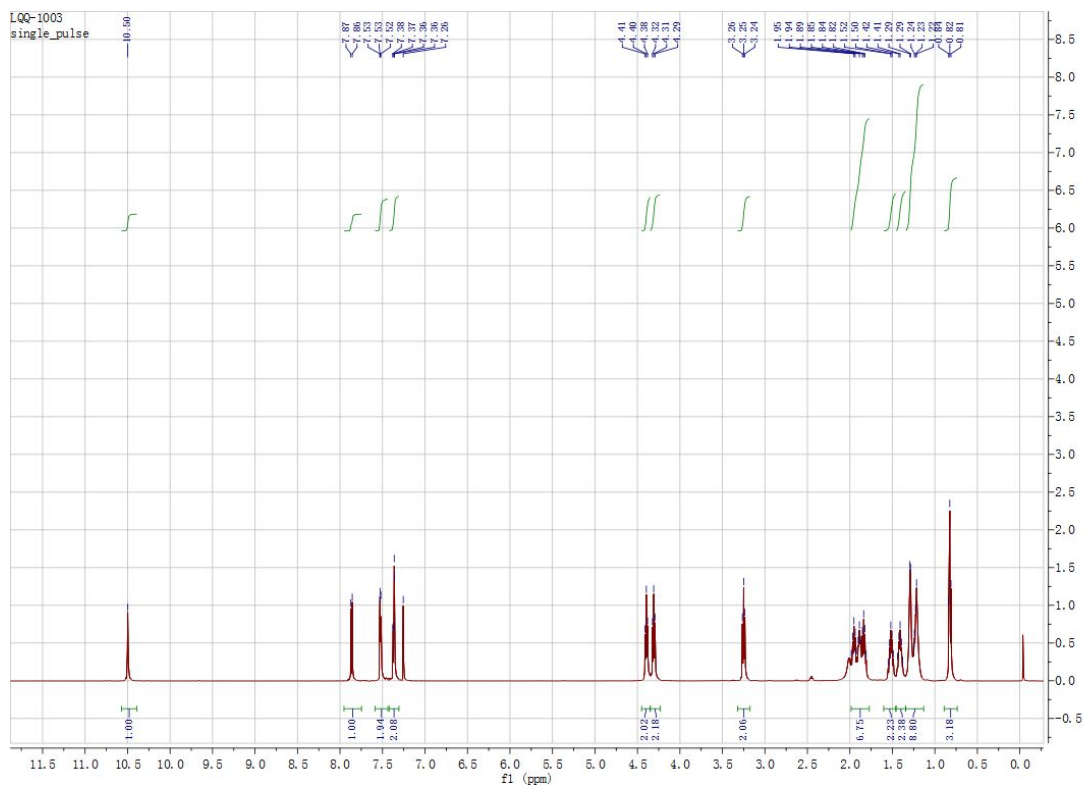


Figure S126. 1H NMR Spectrum ($CDCl_3$, 500 MHz) of G_7 .

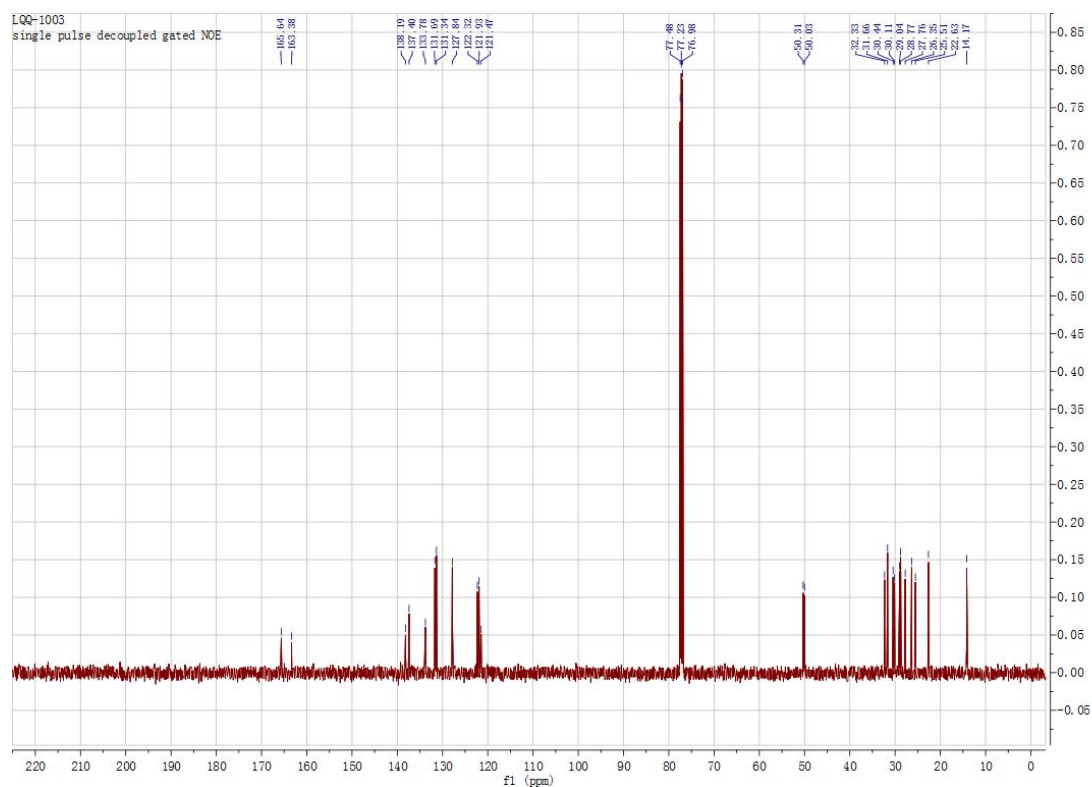


Figure S127. ^{13}C NMR Spectrum (CDCl_3 , 126 MHz) of G_7 .

2018122813 #99 RT: 0.96 AV: 1 NL: 2.79E8
T: FTMS + p ESI Full ms [100.0000-1000.0000]

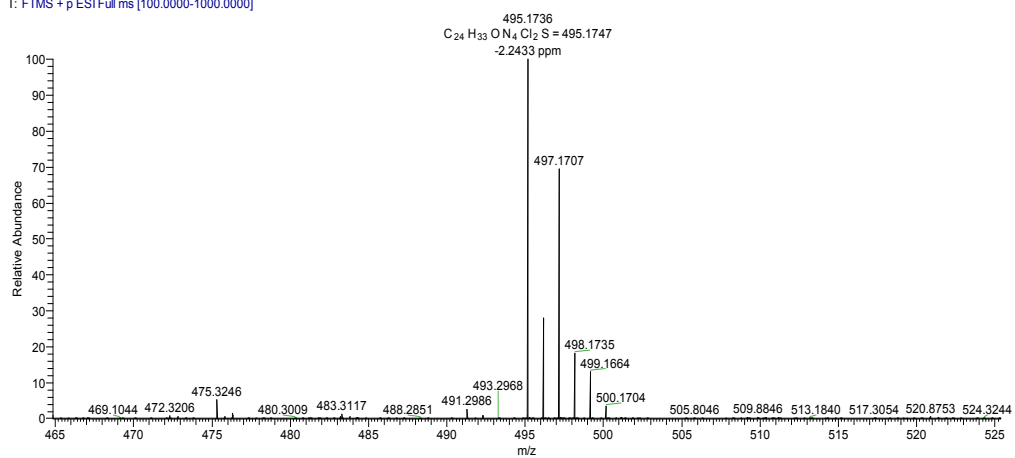


Figure S128. HRMS Spectrum of G_7 .

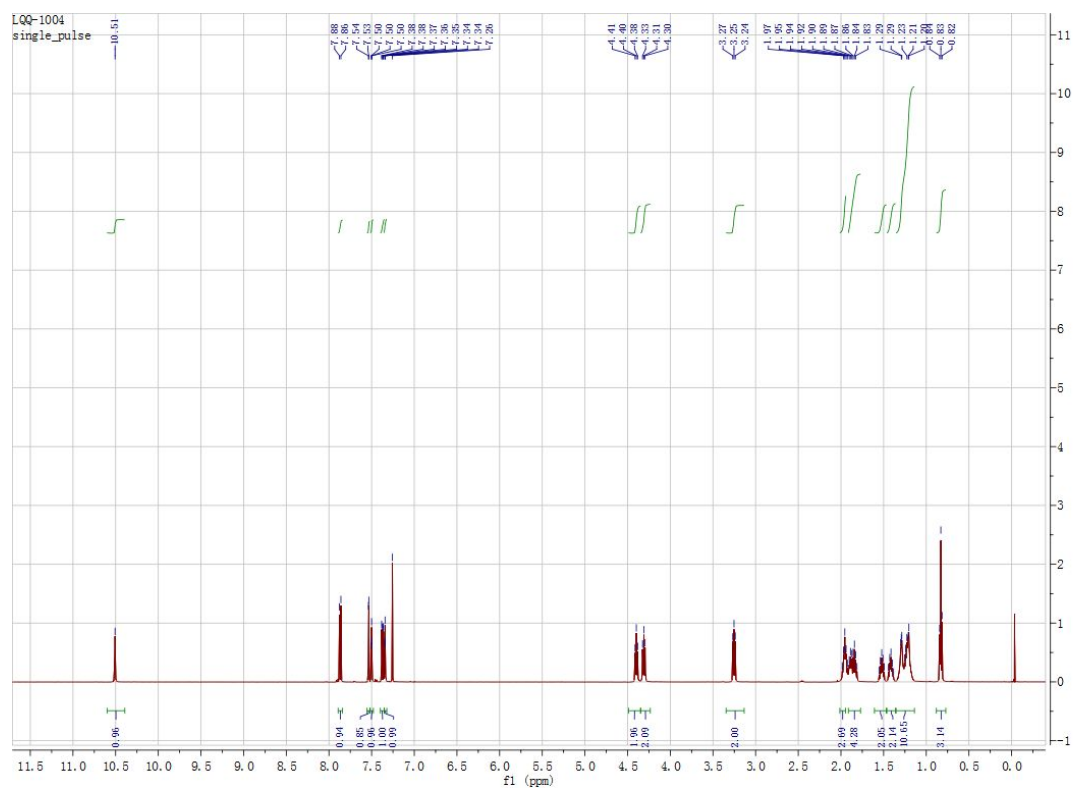


Figure S129. ^1H NMR Spectrum (CDCl_3 , 500 MHz) of G_8 .

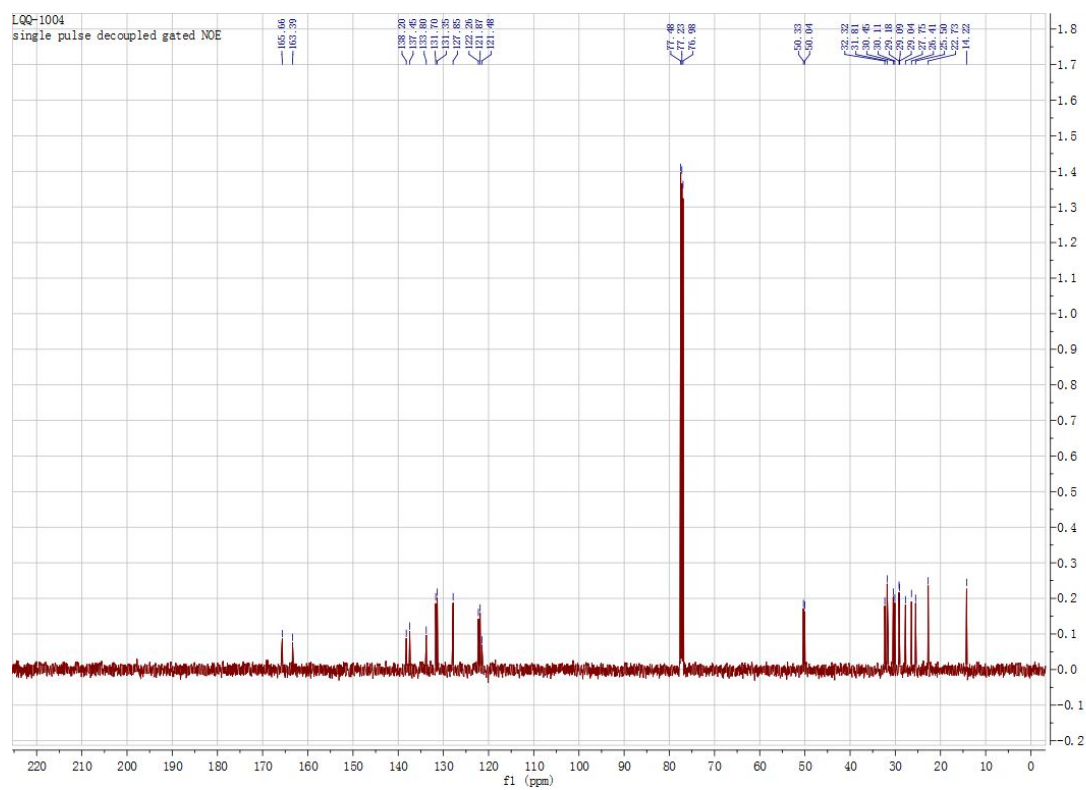


Figure S130. ^{13}C NMR Spectrum (CDCl_3 , 126 MHz) of G_8 .

2018122814 #101 RT: 0.97 AV: 1 NL: 2.73E8
T: FTMS + p ESI Full ms [100.0000-1000.0000]

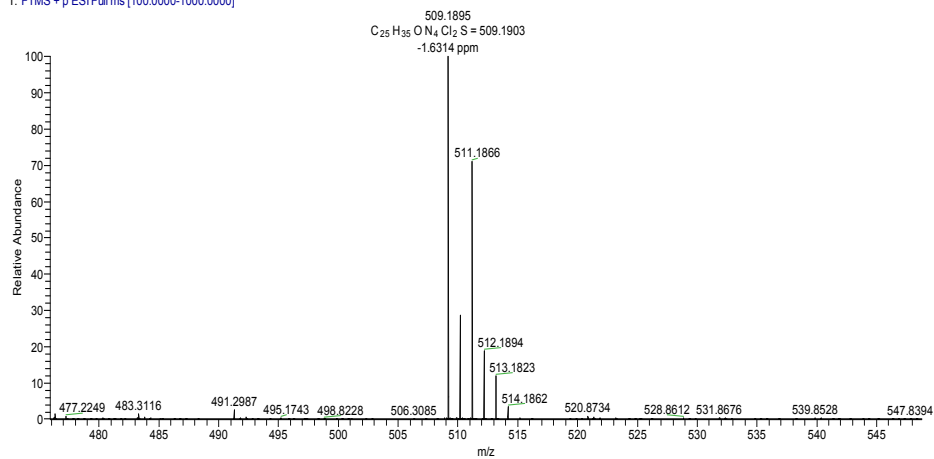


Figure S131. HRMS Spectrum of G_8 .

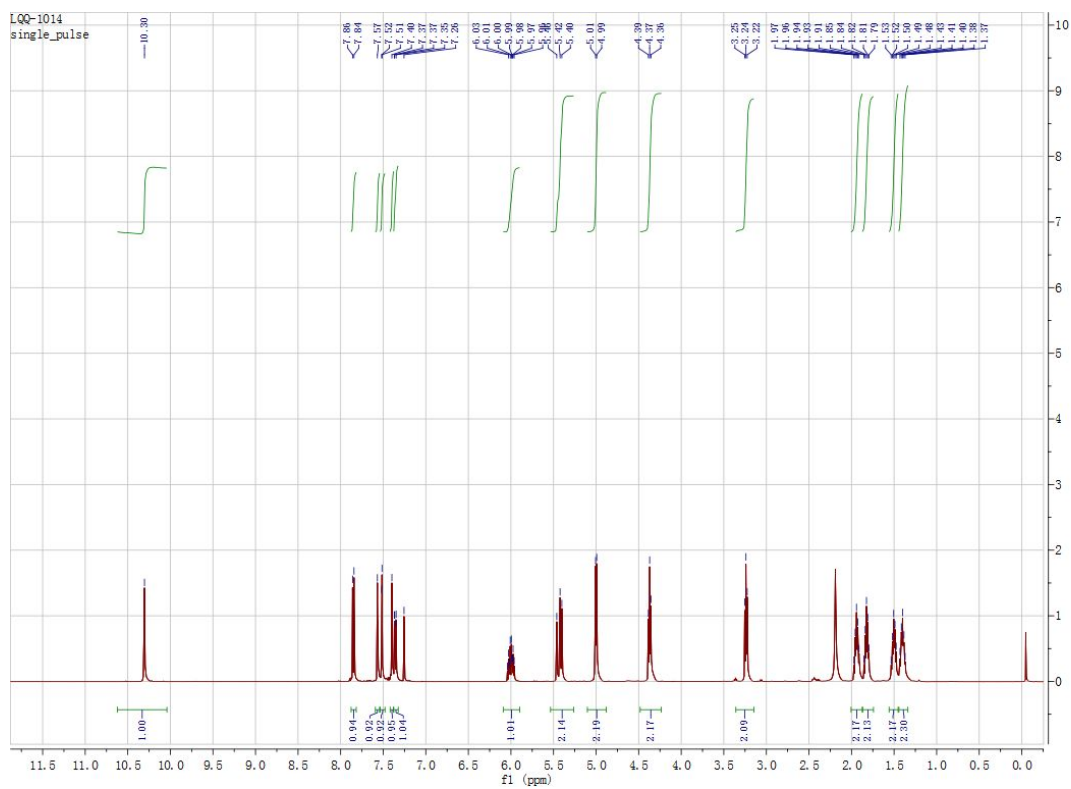


Figure S132. 1H NMR Spectrum ($CDCl_3$, 500 MHz) of G_9 .

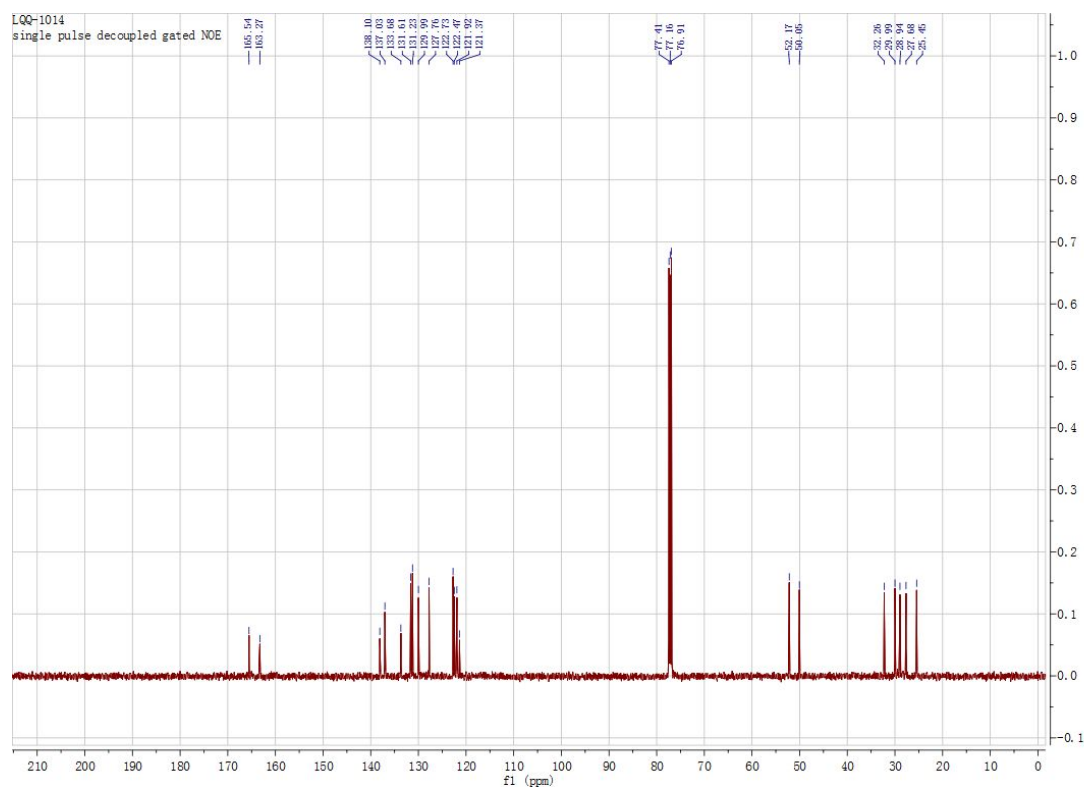


Figure S133. ^{13}C NMR Spectrum (CDCl_3 , 126 MHz) of G_9 .

2018122824 #81 RT: 0.78 AV: 1 NL: 4.88E8
T: FTMS + p ESI Full ms [100.0000-1000.0000]

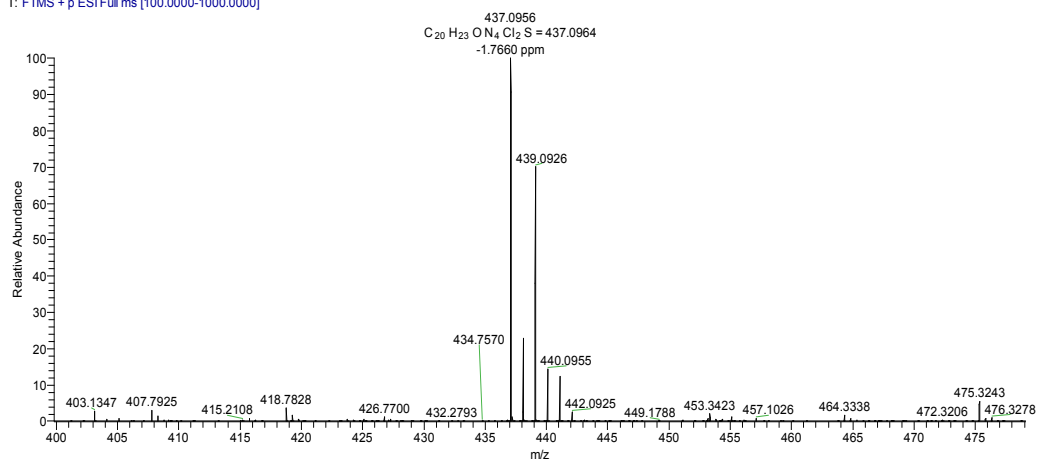


Figure S134. HRMS Spectrum of G_9 .

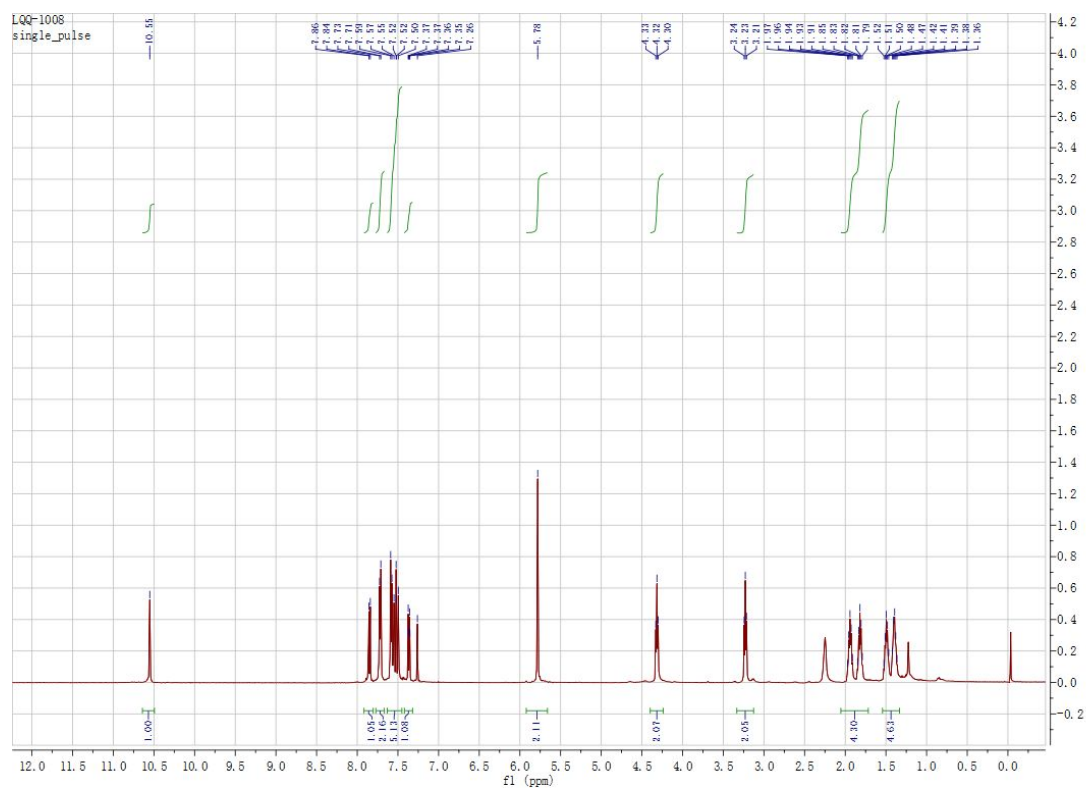


Figure S135. ¹H NMR Spectrum (CDCl₃, 500 MHz) of G₁₀.

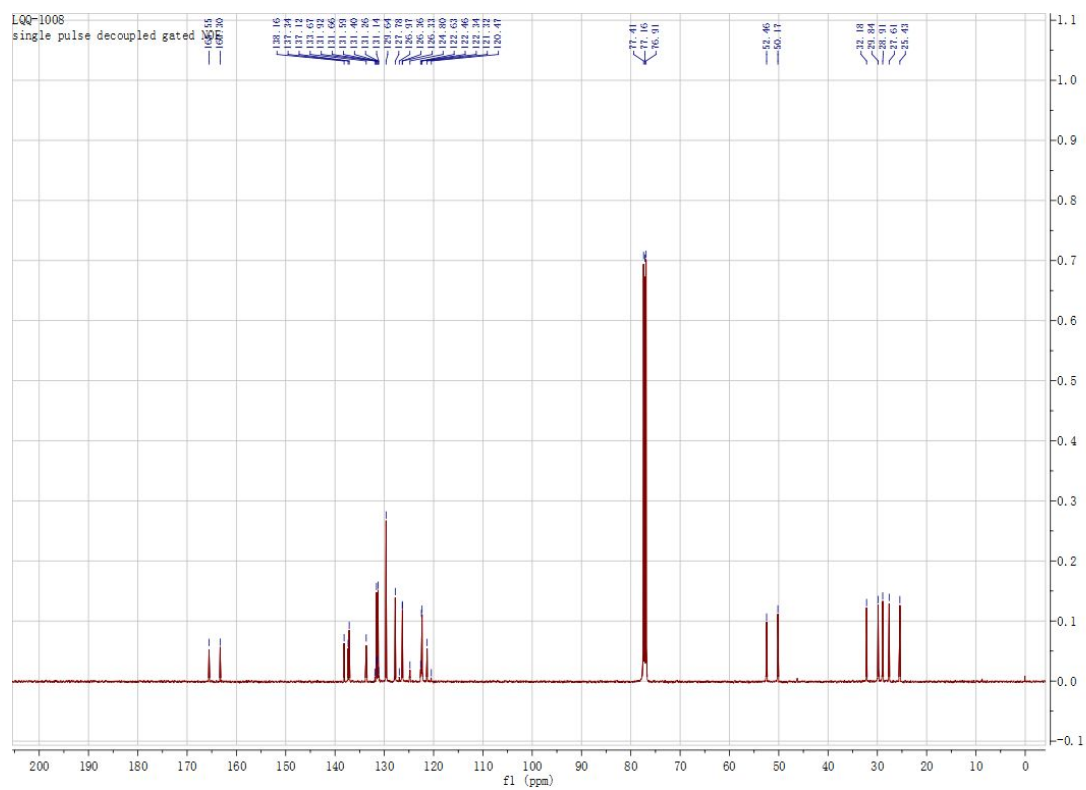


Figure S136. ¹³C NMR Spectrum (CDCl₃, 126 MHz) of G₁₀.

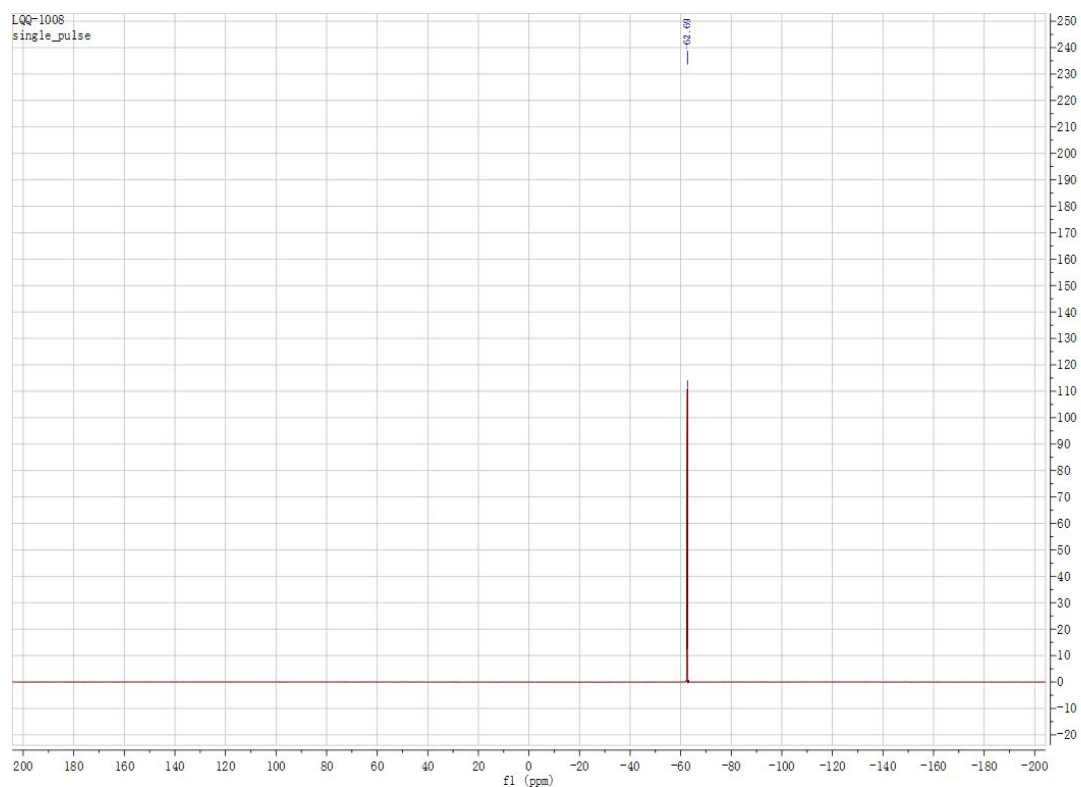


Figure S137. ^{19}F NMR Spectrum (CDCl_3 , 471 MHz) of G_{10} .

2018122818 #77 RT: 0.74 AV: 1 NL: 3.60E8
T: FTMS + p ESI Full ms [100.0000-1000.0000]

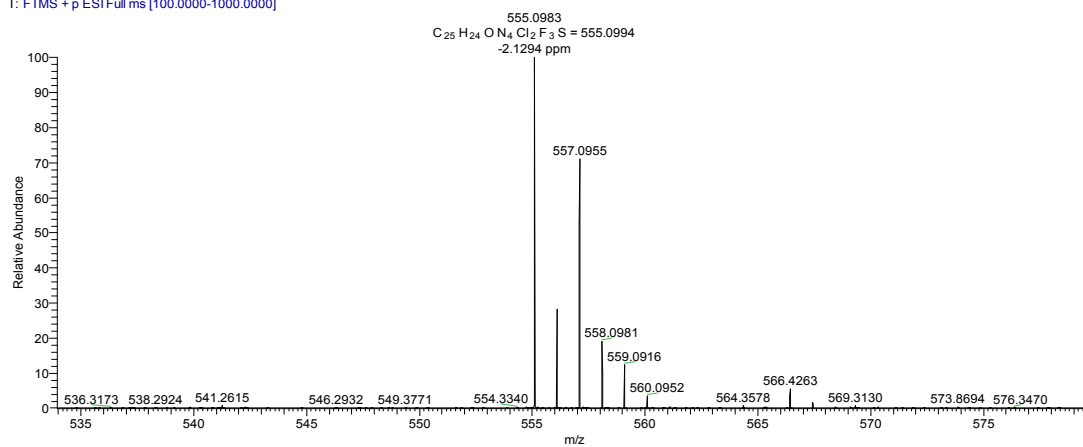


Figure S138. HRMS Spectrum of G_{10} .

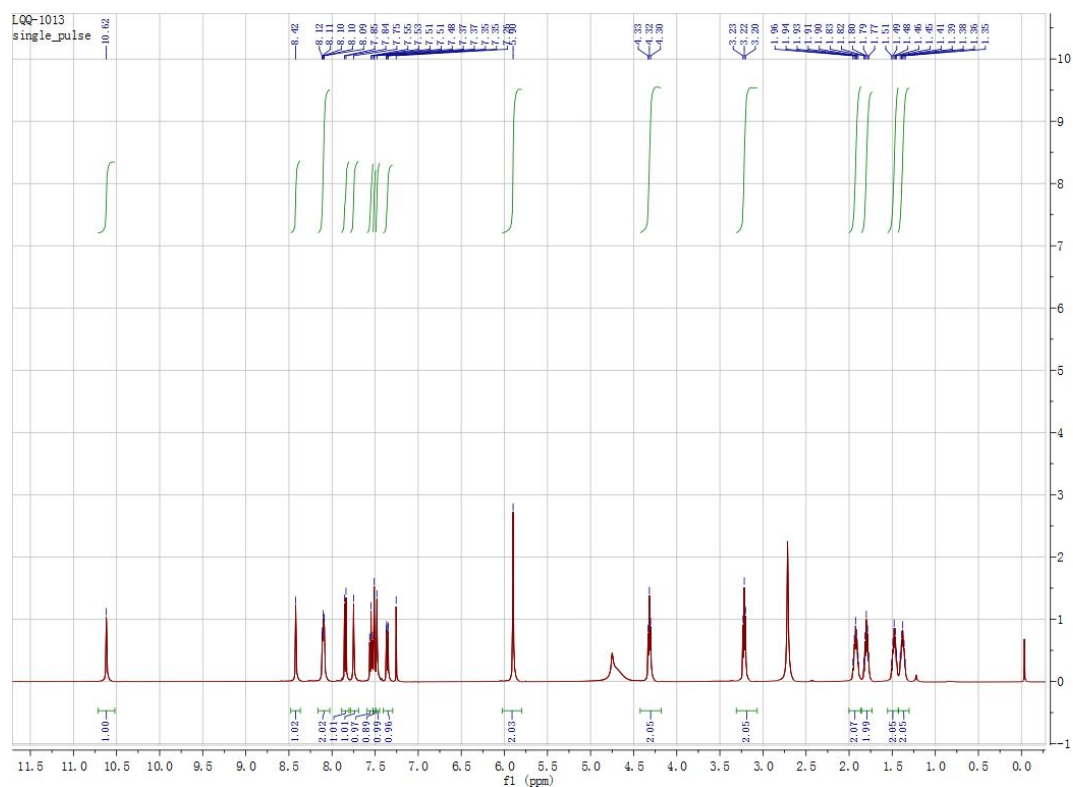


Figure S139. ^1H NMR Spectrum (CDCl_3 , 500 MHz) of G_{11} .

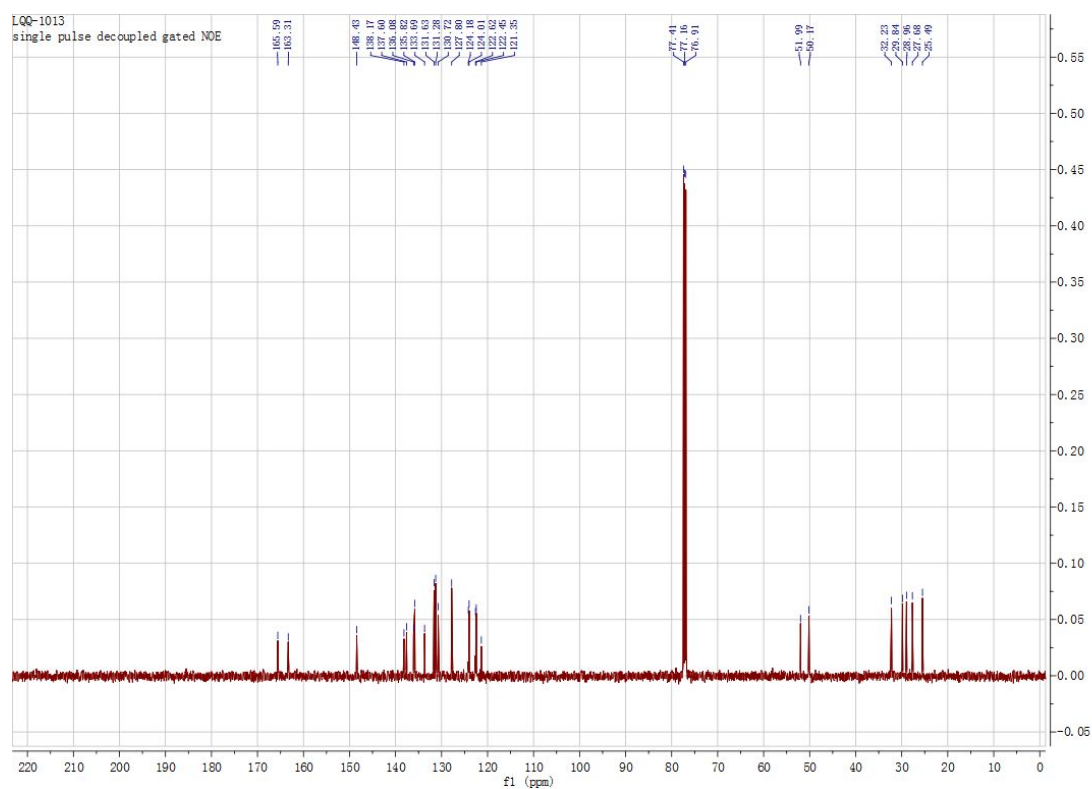


Figure S140. ^{13}C NMR Spectrum (CDCl_3 , 126 MHz) of G_{11} .

2018122823 #79 RT: 0.76 AV: 1 NL: 4.13E8
T: FTMS + p ESI Full ms [100.0000-1000.0000]

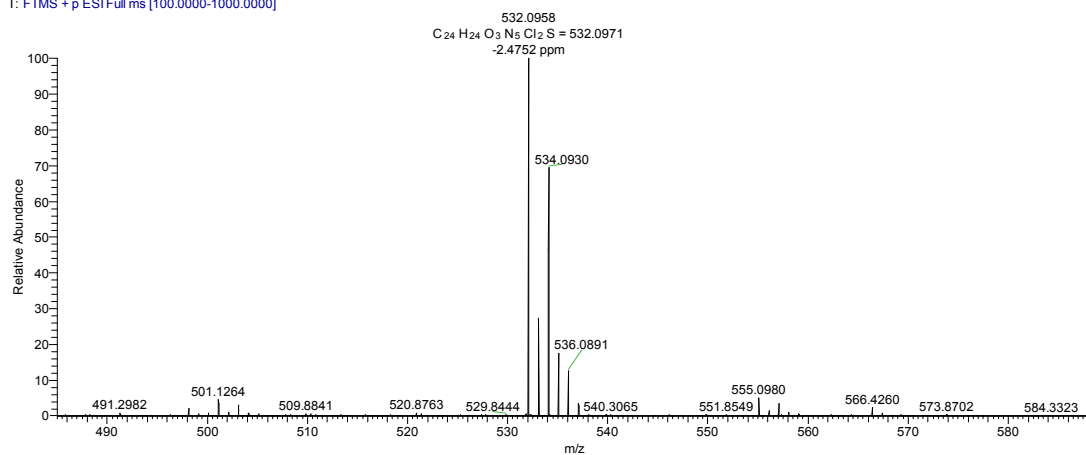


Figure S141. HRMS Spectrum of G₁₁.

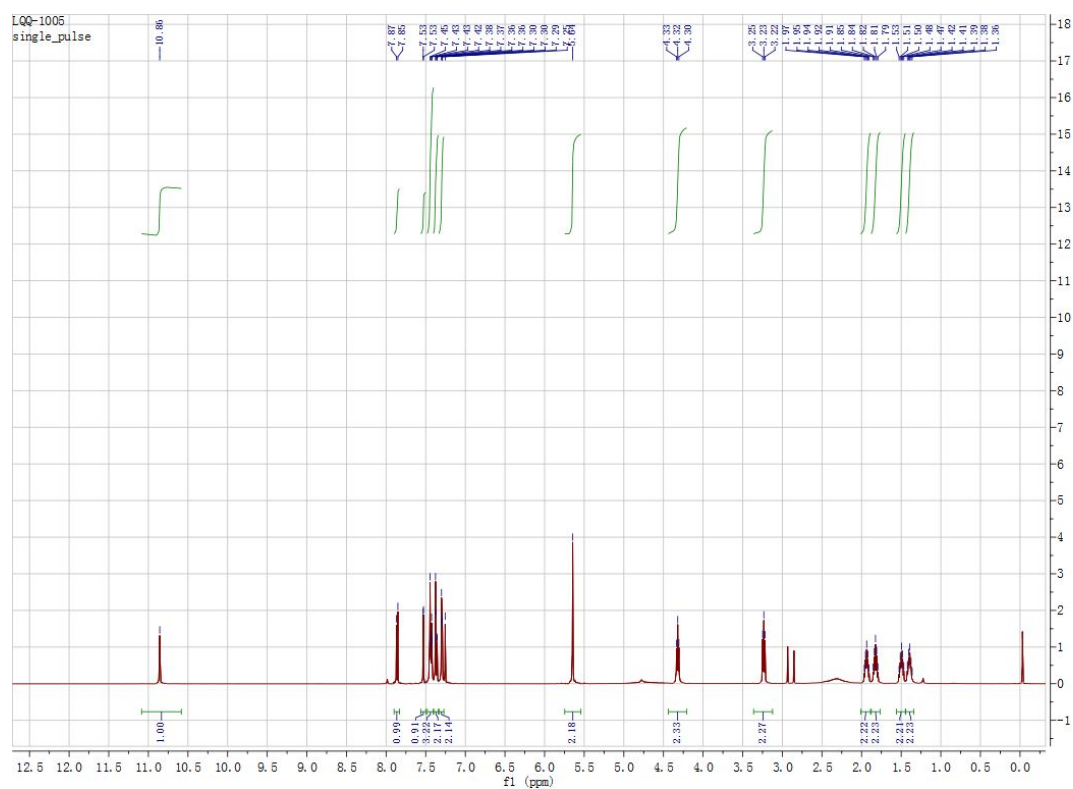


Figure S142. ¹H NMR Spectrum (CDCl₃, 500 MHz) of G₁₂.

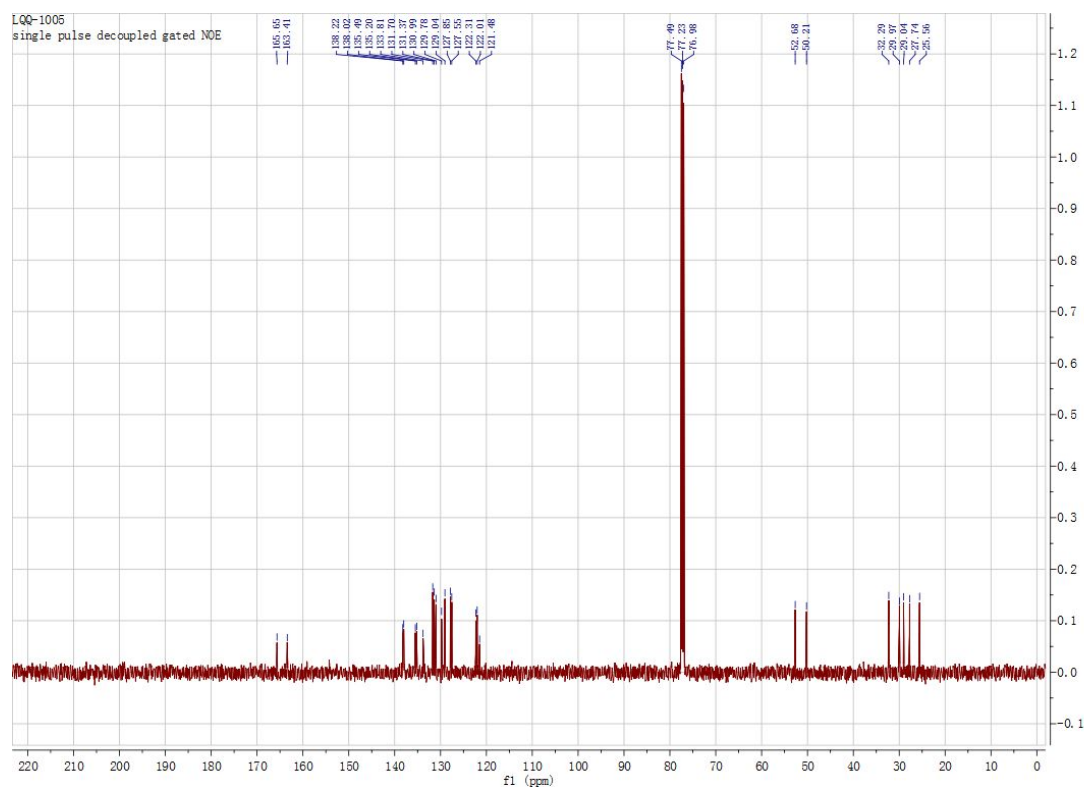


Figure S143. ^{13}C NMR Spectrum (CDCl_3 , 126 MHz) of G_{12} .

2018122815 #75 RT: 0.72 AV: 1 NL: 2.81E7
T: FTMS + p ESI Full ms [100.0000-1000.0000]

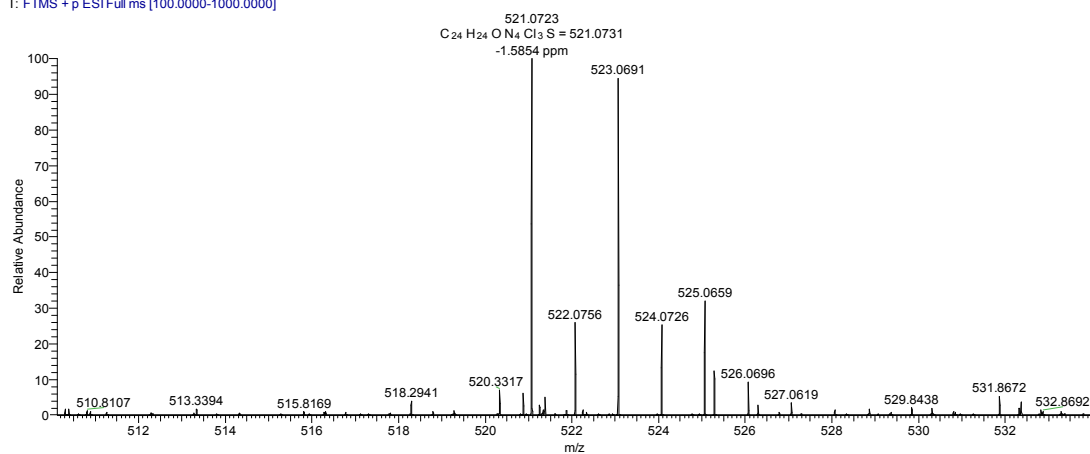


Figure S144. HRMS Spectrum of G_{12} .

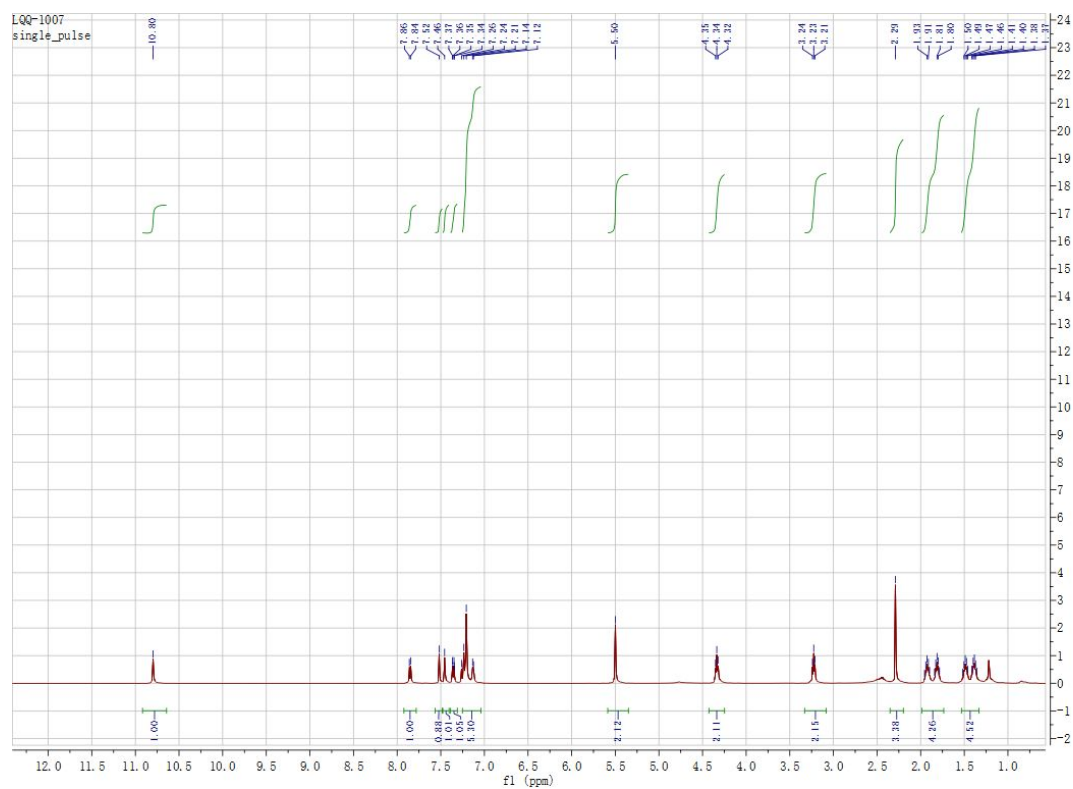


Figure S145. ^1H NMR Spectrum (CDCl_3 , 500 MHz) of G_{13} .

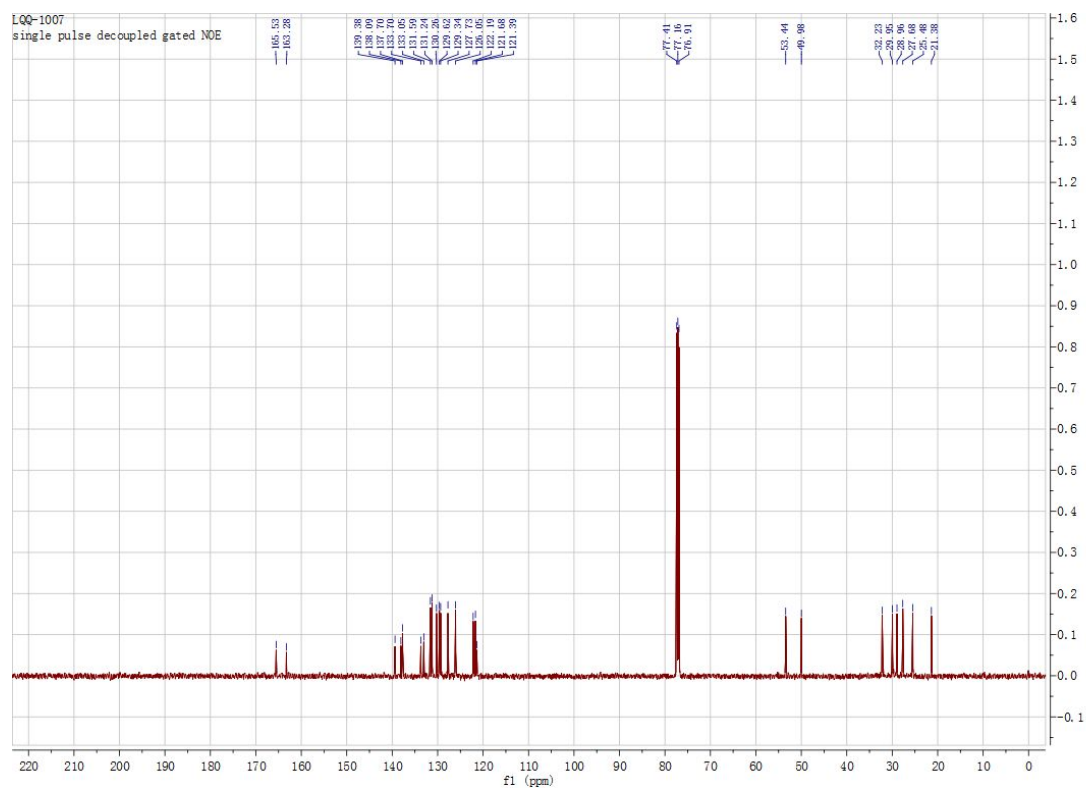


Figure S146. ^{13}C NMR Spectrum (CDCl_3 , 126 MHz) of G_{13} .

2018122817 #85 RT: 0.82 AV: 1 NL: 4.62E8
T: FTMS + p ESI Full ms [100.0000-1000.0000]

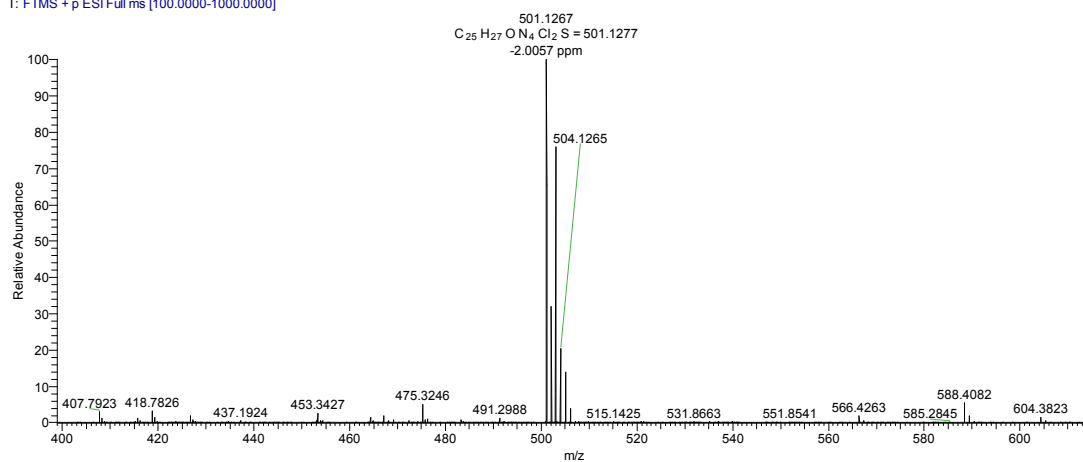


Figure S147. HRMS Spectrum of G₁₃.

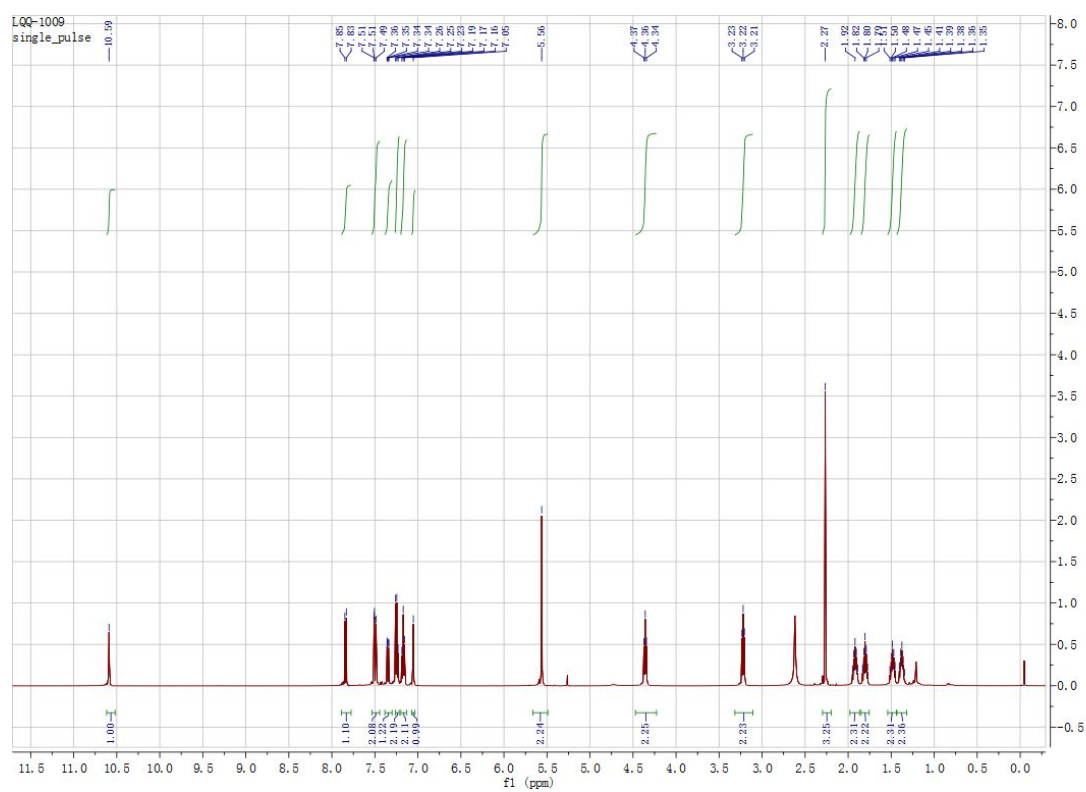


Figure S148. ¹H NMR Spectrum (CDCl₃, 500 MHz) of G₁₄.

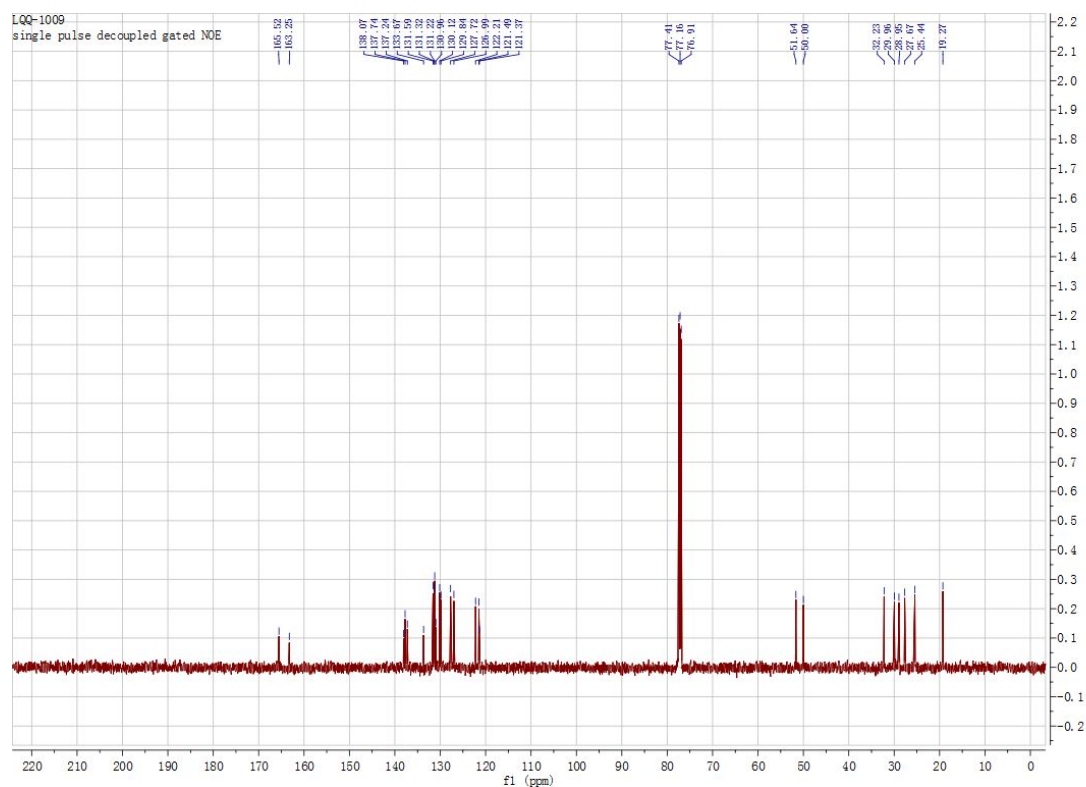


Figure S149. ^{13}C NMR Spectrum (CDCl_3 , 126 MHz) of G_{14} .

2018122819 #79 RT: 0.76 AV: 1 NL: 5.52E8
T: FTMS + p ESI Full ms [100.0000-1000.0000]

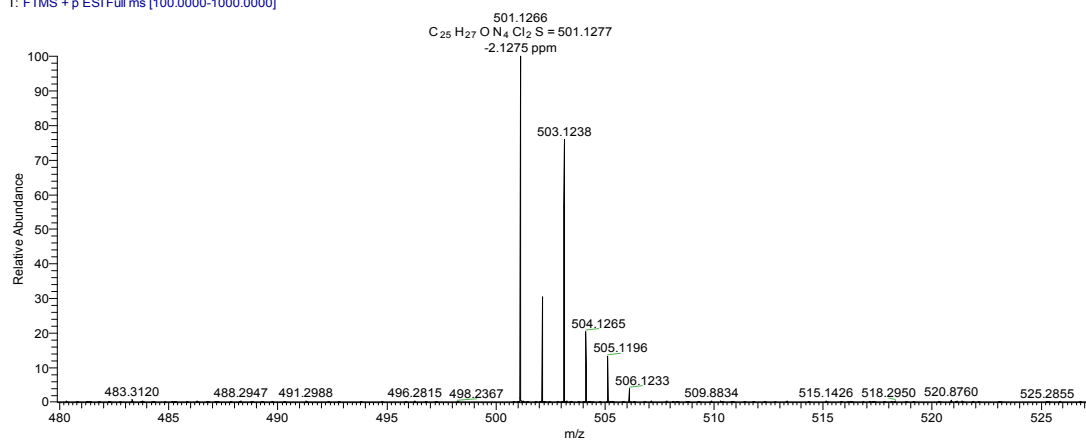


Figure S150. HRMS Spectrum of G_{14} .

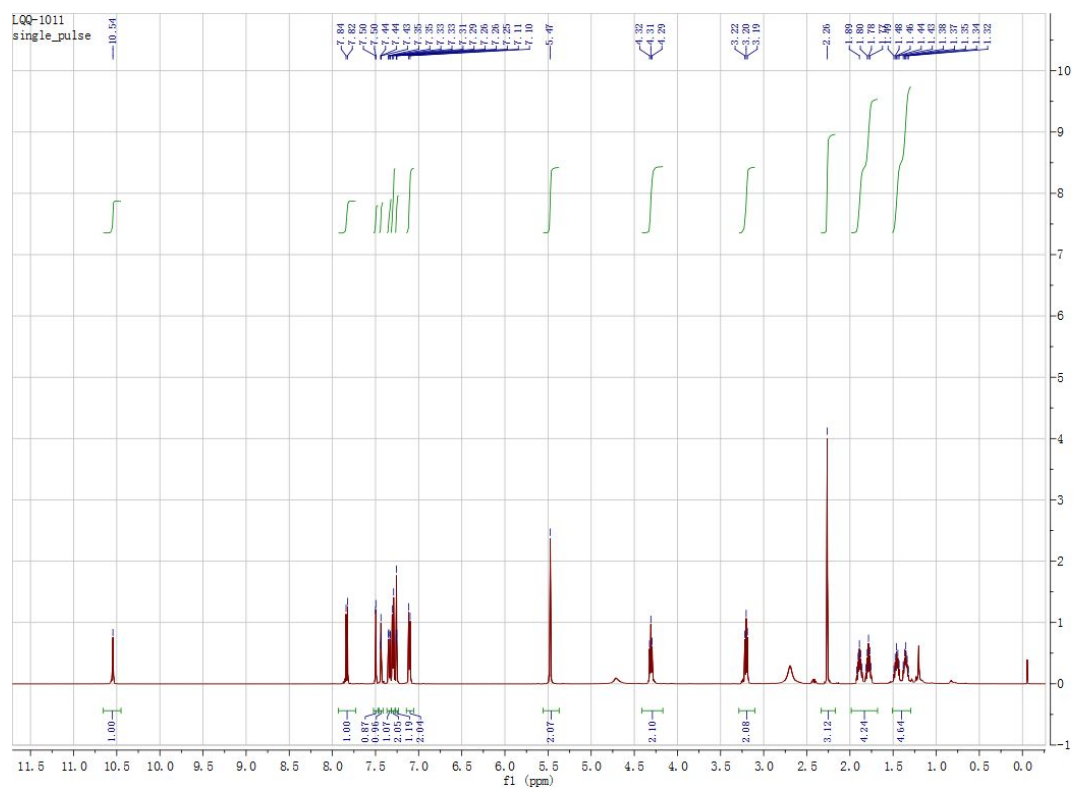


Figure S151. ¹H NMR Spectrum (CDCl₃, 500 MHz) of G₁₅.

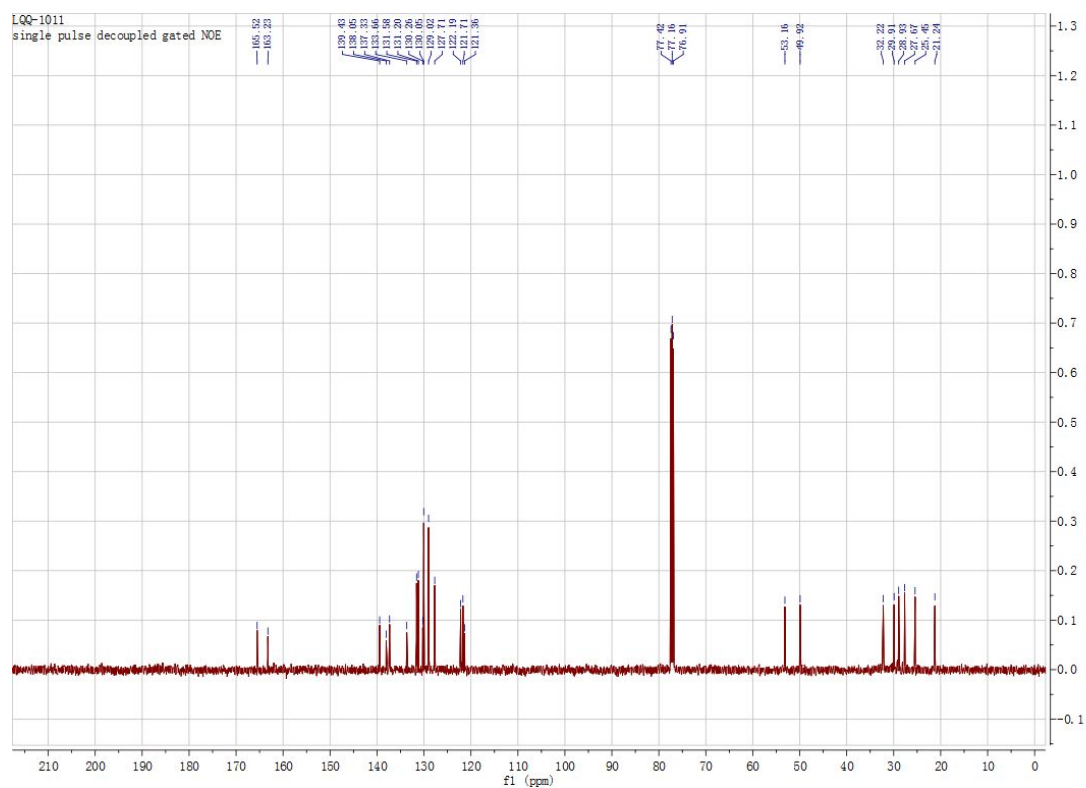


Figure S152. ¹³C NMR Spectrum (CDCl₃, 126 MHz) of G₁₅.

2018122821 #81 RT: 0.78 AV: 1 NL: 9.03E8
T: FTMS + p ESI Full ms [100.0000-1000.0000]

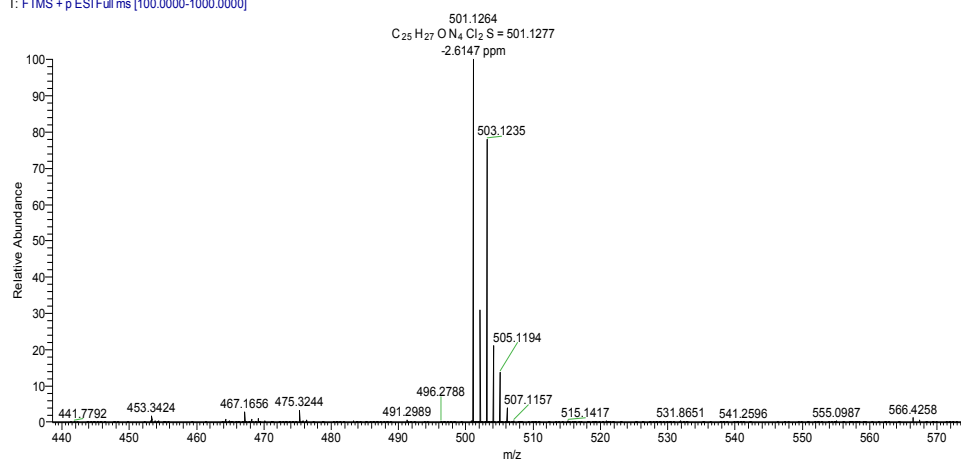


Figure S153. HRMS Spectrum of G₁₅.

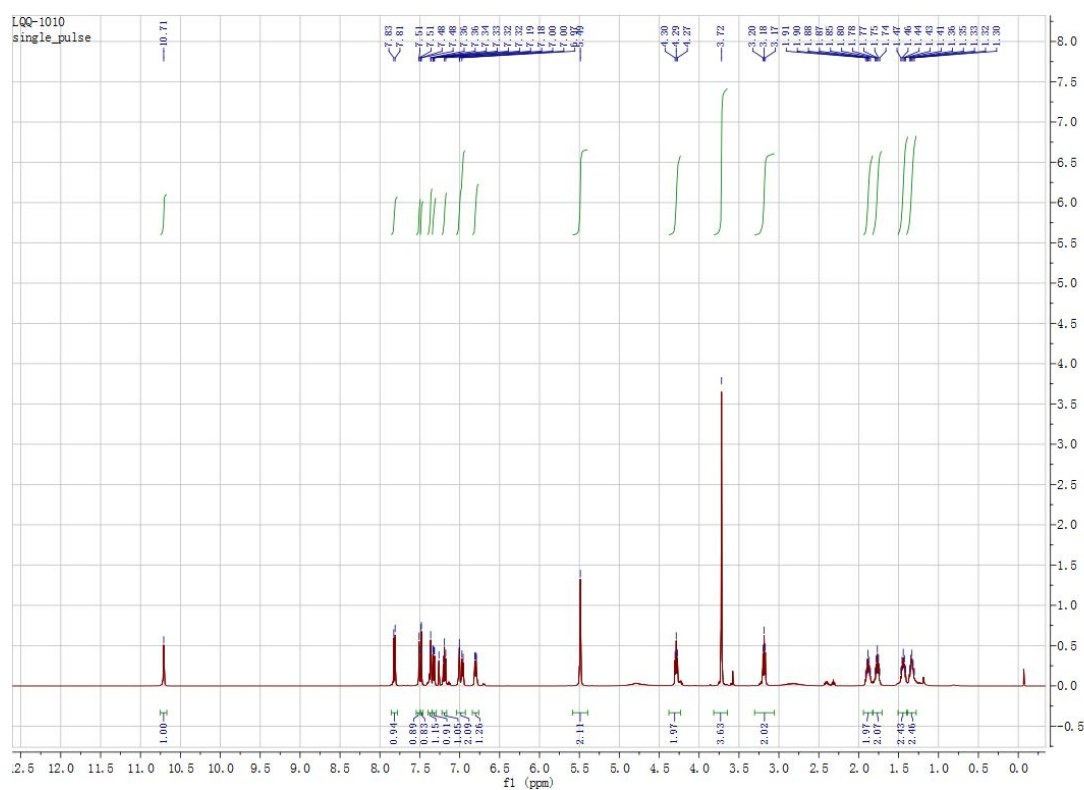


Figure S154. ¹H NMR Spectrum (CDCl₃, 500 MHz) of G₁₆.

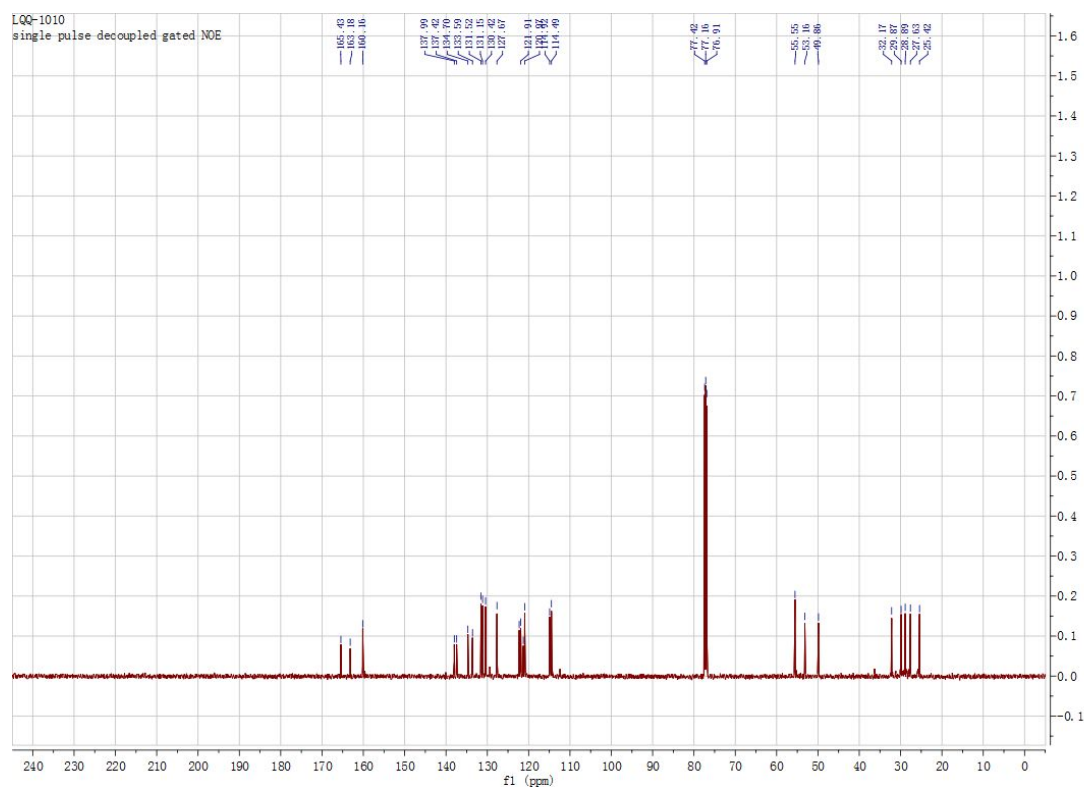


Figure S155. ^{13}C NMR Spectrum (CDCl_3 , 126 MHz) of G_{16} .

2018122820 #77 RT: 0.74 AV: 1 NL: 1.70E8
T: FTMS + p ESI Full ms [100.0000-1000.0000]

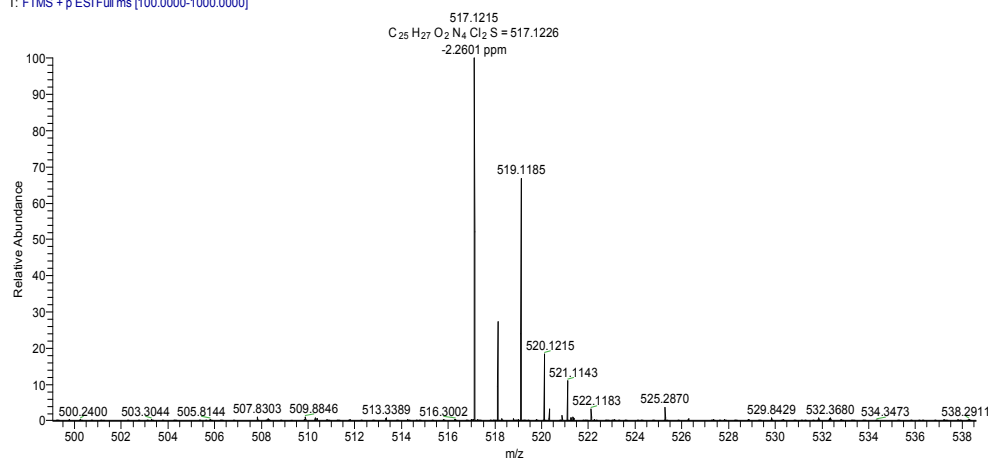


Figure S156. HRMS Spectrum of G_{16} .

2018122816 #95 RT: 0.92 AV: 1 NL: 6.52E7
T: FTMS + p ESI Full ms [100.0000-1000.0000]

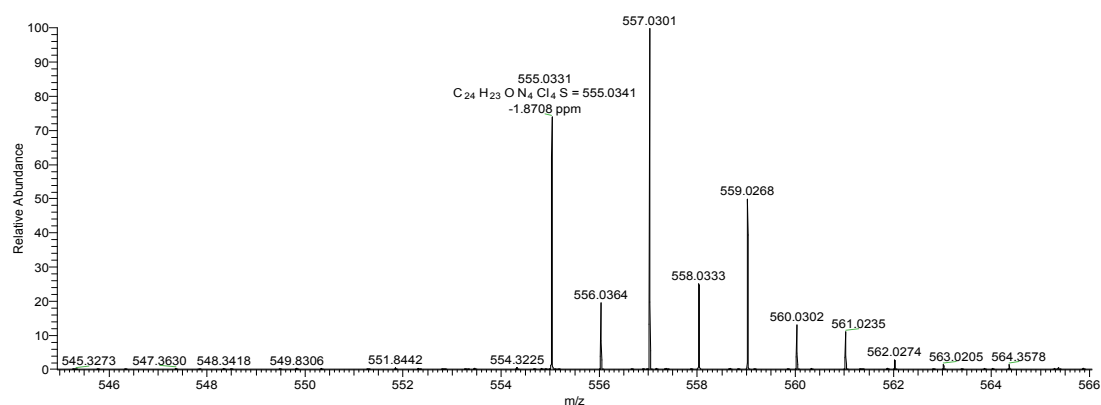


Figure S159. HRMS Spectrum of G₁₇.

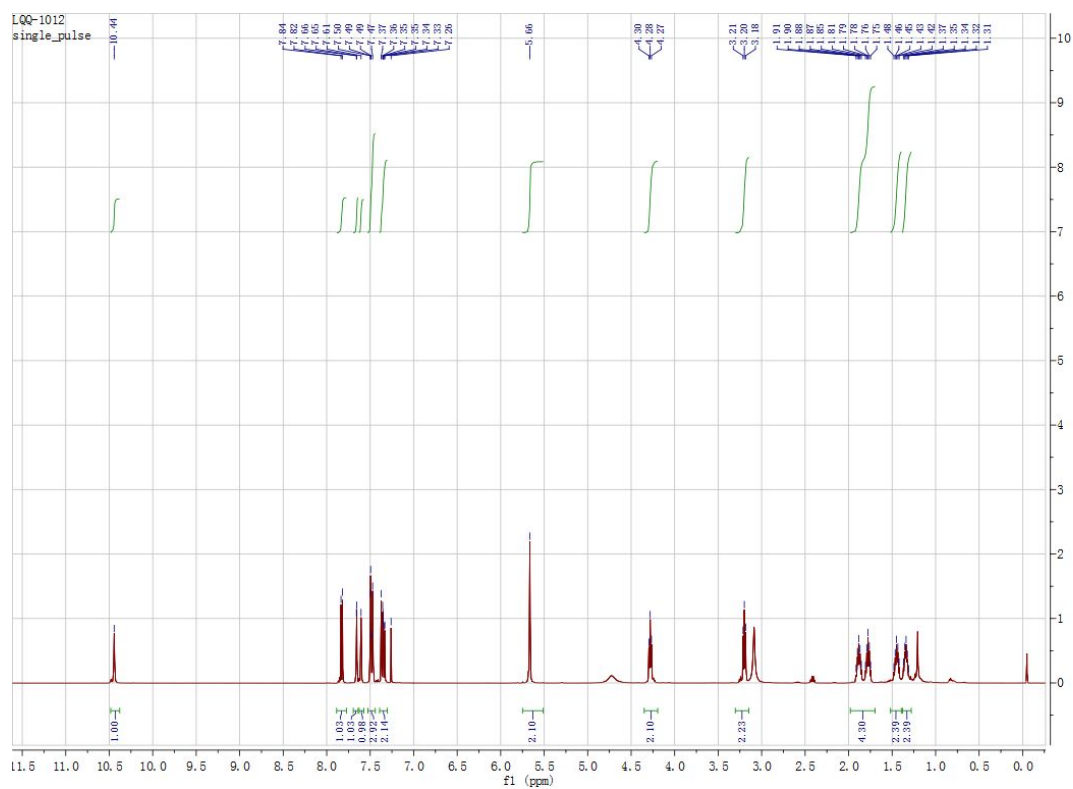


Figure S160. ¹H NMR Spectrum (CDCl₃, 500 MHz) of G₁₈.

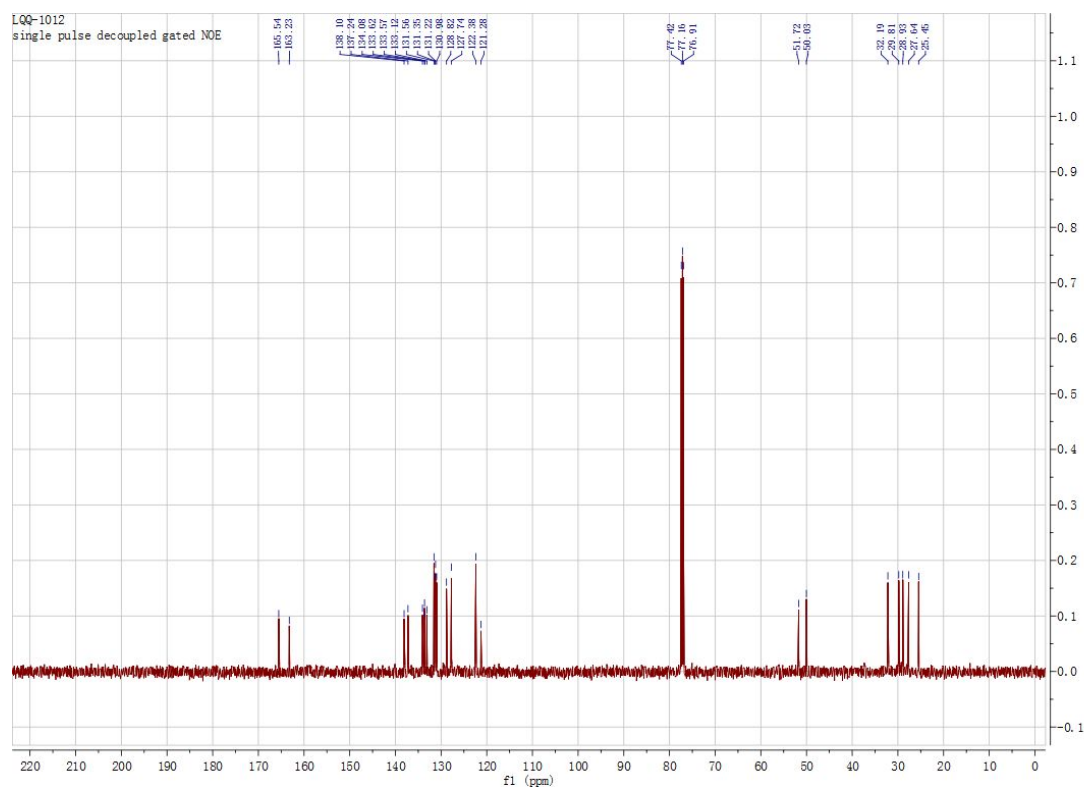


Figure S161. ^{13}C NMR Spectrum (CDCl_3 , 126 MHz) of G_{18} .

2018122822 #141 RT: 1.36 AV: 1 NL: 4.54E6
T: FTMS + p ESI Full ms [100.0000-1000.0000]

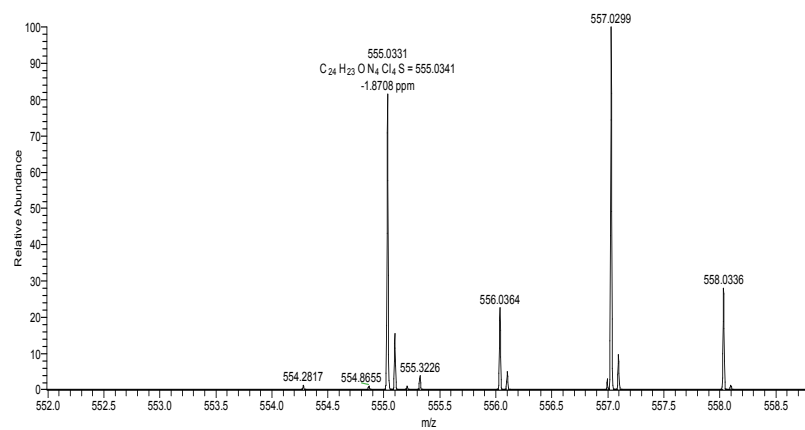


Figure S162. HRMS Spectrum of G_{18} .