Electronic Supplementary Information (ESI)

Four imidazole derivative AIEE Luminophores: Sensitive detection of NACs explosives

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Contents

Synthesis procedures of compounds

M (M01)

First, benzil (9,10-phenanthreneqquinone) (0.42g, 2.00 mmol) and 4-(N,N-Diphenylamino)benzaldehyde (0.55 g, 2.00 mmol) were dissolved in anhydrous acetic acid (30 mL) at room temperature. 2-(4-Aminophenyl) acetonitrile (0.40 g, 3.00 mmol) The mixture was stirred for two hours at 25 ° C. Then, ammonium acetate (0.77 g, 10.00 mmol) was added and the mixture was heated to 120 ° C for 24 h. The final mixture was poured into cold saline water (200 mL), and neutralized with a NaOH aqueous solution. A large amount of precipitate was filtered, and washed with ethanol to give yellow compound.

M (0.65 g, 1.27 mmol). Yield: 64%. **^{1}H NMR (**400 MHz, $CDCl_3$**)** δ: 3.74 (s, 2H), 6.90 (d, 2H, *J* = 8.72 Hz), 7.06–7.11 (m, 10H), 7.24–7.32 (m, 14H), 7.63 (d, 2H, *J* = 7.80 Hz). **^{13}C NMR** (101 MHz, $CDCl_3$) δ: 148.11, 147.23, 146.87, 138.12, 137.13, 134.10, 131.16, 130.45, 130.43, 130.05, 129.73, 129.37, 129.16, 128.66, 128.53, 128.20, 127.41, 126.75, 125.04, 123.49, 121.98, 117.27, 23.36.

M01 (0.74 g, 1.28 mmol). Yield: 65%. **^{1}H NMR (400 MHz, $CDCl_3$)** δ: 8.93 (d, *J* = 8.0 Hz, 1H), 8.78 (dd, *J* = 27.7, 8.4 Hz, 2H), 7.79 (m, *J* = 8.0, 6.9, 1.1 Hz, 1H), 7.70 (m, *J* = 8.4, 7.0, 1.4 Hz, 1H), 7.67 – 7.58 (m, 4H), 7.55 (m, *J* = 7.5, 7.0, 1.2 Hz, 1H), 7.50 – 7.40 (m, 2H), 7.37 – 7.27 (m, 5H), 7.21 – 7.05 (m, 7H), 7.05 – 6.96 (m, 2H), 4.01 (d, *J* = 2.0 Hz, 2H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ: 150.85, 148.61, 147.12, 138.88, 131.76, 130.15, 129.99, 129.73, 129.42, 129.22, 128.27, 127.82, 127.37, 126.37, 125.74, 125.18, 124.91, 124.25, 123.69, 123.12, 122.89, 121.79, 120.54, 117.23, 23.67. **MS (ESI^{+}, 175.0 V, 25 °C):** *m*/*z* = 577.2390 ($[M+H]^{+}$), calcd for $C_{41}H_{28}N_4^{+}$ = 577.2386 (M^{+}).

M-MAP (M01-MAP).

M (M01) (1.00 mmol) and 4-(Dimethylamino)cinnamaldehyde (0.14 g, 1.00 mmol) were uniformly dispersed in ethanol (30 mL) at 80 °C. Soon afterwards, t-BuOK (0.11 g, 1.00 mmol) was added. The reaction system was monitored by TLC to notarize the completed reaction. The generated orange precipitate was filtered and further purified by column chromatography (petroleum ether:dichloromethane = 1:1, v/v) to get **M-MAP** (0.21 g, 0.20 mmol), Yield: 31%; **M01-MAP** (0.34 g, 0.41 mmol). Yield: 52%.

M-MAP: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 – 7.63 (m, 3H), 7.55 – 7.23 (m, 21H), 7.23 – 6.95 (m, 16H), 6.88 – 6.64 (m, 3H), 3.08 (dt, *J* = 466.7, 5.7, 0.0 Hz, 6H). **^{13}C NMR (101 MHz, $CDCl_3$)**

δ 131.24, 130.64, 130.35, 130.28, 129.68, 129.63, 129.59, 129.43, 128.34, 127.45, 126.71, 126.51, 126.49, 125.88, 125.30, 125.17, 125.07, 125.04, 124.27, 124.21, 123.77, 123.74, 123.49, 123.16, 123.11, 120.75, 120.32, 117.45, 112.02, 107.37, 107.06, 40.21, 40.13. **MS (ESI$^+$, 175.0 V, 25 °C):** *m*/*z* = 736.3452 ([M+H]$^+$), calcd for $C_{52}H_{41}N_5^+$ = 736.3434 (M^+).

M01-MAP: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.87 – 8.71 (m, 4H), 7.91 – 7.59 (m, 13H), 7.59 – 7.44 (m, 8H), 7.44 – 7.21 (m, 16H), 7.21 – 6.97 (m, 17H), 6.84 – 6.71 (m, 2H), 6.70 – 6.63 (m, 1H), 3.09 (d, *J* = 12.2 Hz, 6H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 163.42, 162.53, 160.97, 160.08, 148.19, 148.13, 147.27, 147.13, 146.86, 142.12, 139.21, 138.30, 137.86, 137.65, 137.09, 136.01, 134.22, 133.07, 132.59, 132.56, 131.96, 131.88, 131.44, 131.36, 131.21, 131.17, 130.54, 130.51, 130.43, 130.39, 130.31, 129.82, 129.76, 129.39, 129.05, 128.81, 128.77, 128.64, 128.57, 128.52, 128.37, 128.33, 128.30, 128.23, 127.70, 127.55, 127.44, 127.40, 126.76, 126.19, 126.11, 125.18, 125.07, 123.79, 123.60, 123.51, 123.49, 123.36, 123.27, 121.99, 121.56, 120.46, 120.35, 119.97, 117.93, 116.30, 116.01, 115.97, 115.90, 115.75, 115.69, 113.68, 112.34, 111.66, 111.58, 48.51, 48.37. **MS (ESI$^+$, 175.0 V, 25 °C):** *m*/*z* = 734.3296 ([M+H]$^+$), calcd for $C_{52}H_{39}N_5^+$ = 734.3278 (M^+).

M-IF (M01-IF).

The same method as that for the synthesis of **M-MAP** (**M01-MAP)** was used, except for substitution by (E)-3-(3-(4-fluorophenyl)-1-isopropyl-1H-indol-2-yl)acrylaldehyde (IF), to gain the orange **M-IF** (0.47 g, 0.55 mmol) (Yeild 47%); **M01-IF** (0.66 g, 0.61 mmol) (Yield 62%).

M-IF: ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.74 – 6.74 (m, 39H), 4.94 (m, *J* = 81.8, 7.0 Hz, 1H), 1.76 (dd, *J* = 34.7, 7.0 Hz, 6H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ: 163.42, 162.53, 160.97, 160.08, 148.19, 148.13, 147.27, 147.13, 146.86, 142.12, 139.21, 138.30, 137.86, 137.65, 137.09, 136.01, 134.22, 133.07, 132.59, 132.56, 131.96, 131.88, 131.44, 131.36, 131.21, 131.17, 130.54, 130.51, 130.43, 130.39, 130.31, 129.82, 129.76, 129.39, 129.05, 128.81, 128.77, 128.64, 128.57, 128.52, 128.37, 128.33, 128.30, 128.23, 127.70, 127.55, 127.44, 127.40, 126.76, 126.19, 126.11, 125.18, 125.07, 123.79, 123.60, 123.51, 123.49, 123.36, 123.27, 121.99, 121.56, 120.46, 120.35, 119.97, 117.93, 116.30, 116.01, 115.97, 115.90, 115.75, 115.69, 113.68, 112.34, 111.66, 111.58, 48.51, 48.37, 21.97, 21.85. **MS (ESI$^+$, 175.0 V, 25 °C):** *m*/*z* = 868.3826 ([M+H]$^+$), calcd for $C_{61}H_{46}FN_5^+$ = 868.3810 (M^+).

M01-IF: ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.98 – 8.71 (m, 3H), 7.91 – 7.82 (m, 2H), 7.82 – 7.75 (m,

1H), 7.74 – 7.64 (m, 2H), 7.63 – 7.42 (m, 9H), 7.38 – 7.27 (m, 8H), 7.26 – 7.04 (m, 10H), 7.04 – 6.96 (m, 2H), 5.08 (p, J = 7.0 Hz, 1H), 1.83 (d, J = 7.0 Hz, 6H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ: 163.46, 157.67, 150.81, 148.57, 147.13, 142.80, 139.20, 137.13, 134.64, 132.53, 131.98, 131.90, 130.83, 130.51, 130.12, 129.87, 129.43, 129.20, 128.52, 128.27, 128.18, 127.85, 127.36, 127.07, 126.39, 125.72, 125.20, 124.91, 124.26, 123.89, 123.68, 123.14, 122.86, 121.80, 120.64, 120.61, 120.51, 116.36, 116.02, 115.81, 112.37, 111.38, 48.42, 21.89. **MS (ESI+, 175.0 V, 25 °C):** m/z = 866.3673 ([M+H]$^+$), calcd for $C_{61}H_{44}N_5^+$ = 866.3653 (M^+).

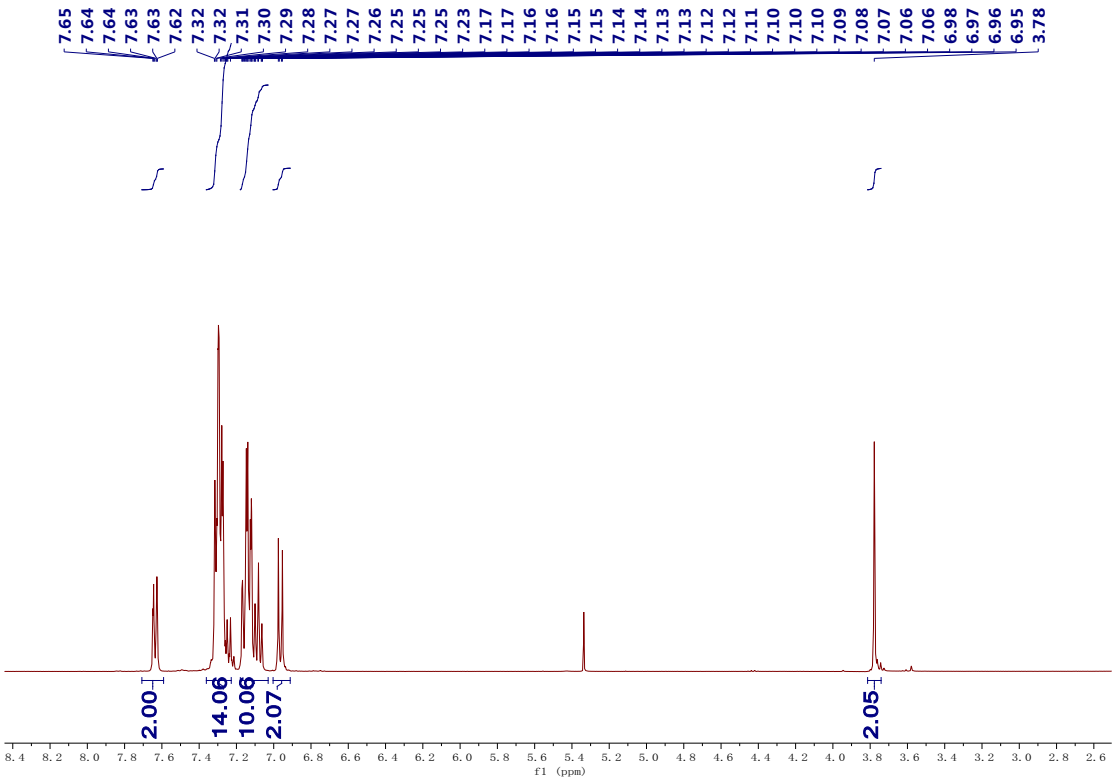

Figure S1 1H NMR spectrum of M in CDCl3.

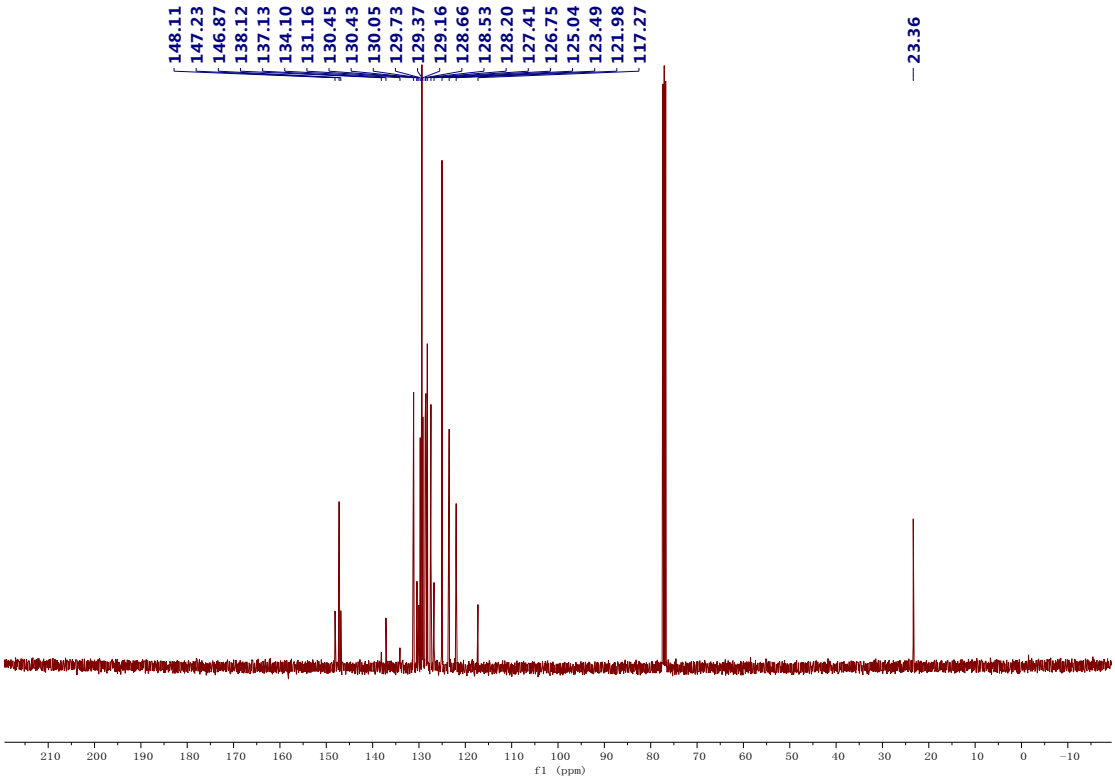

Figure S2 13C NMR spectrum of M in CDCl3.

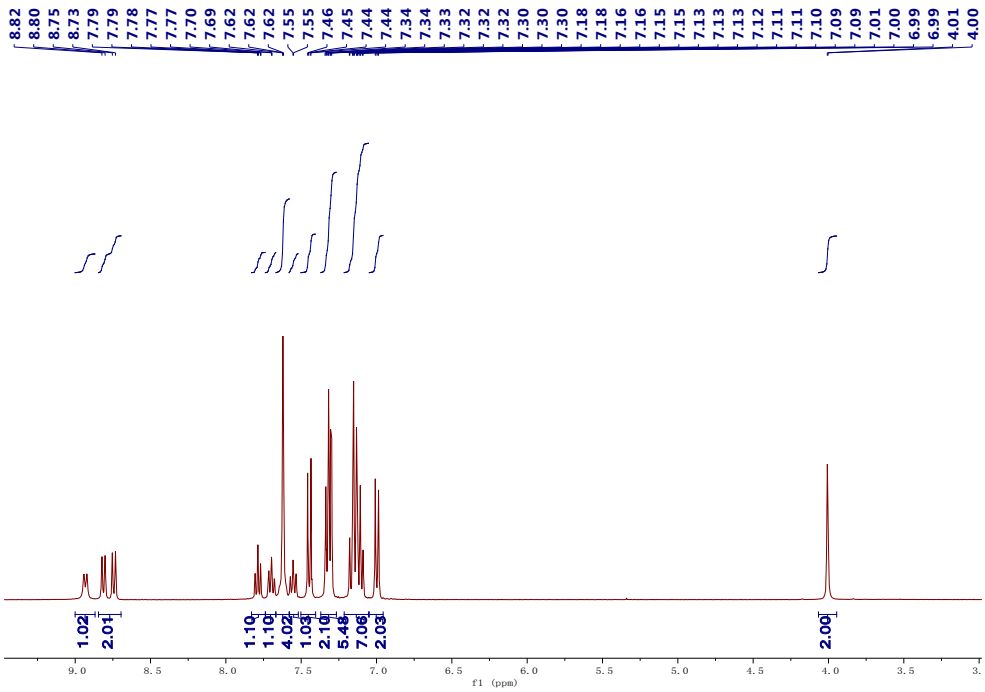

Figure S3 1H NMR spectrum of M01 in CDCl3.

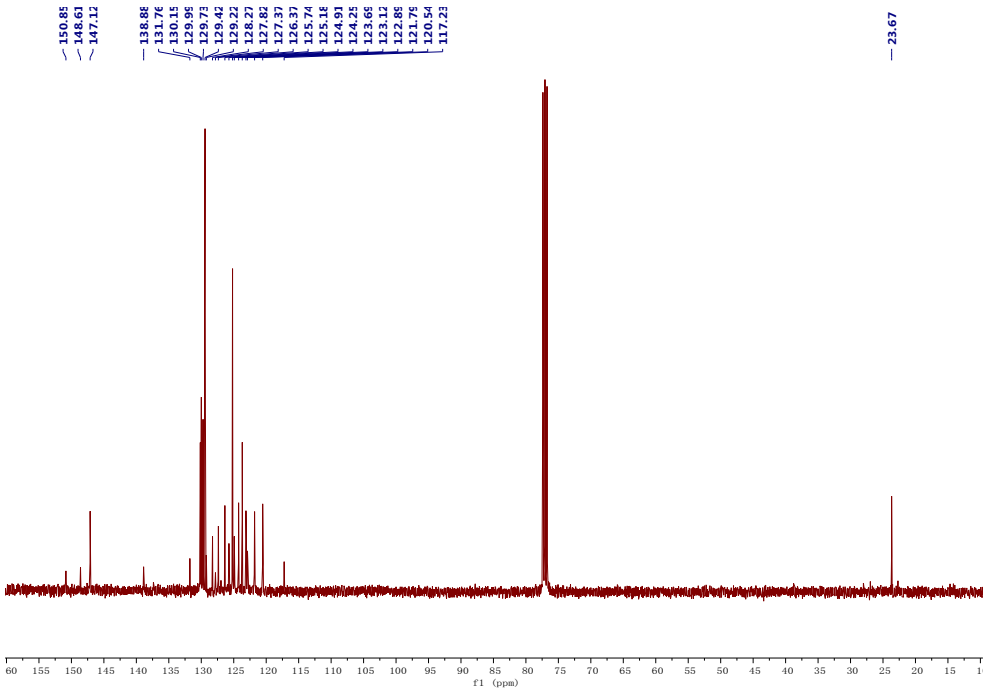

Figure S4 13C NMR spectrum of M01 in CDCl3.

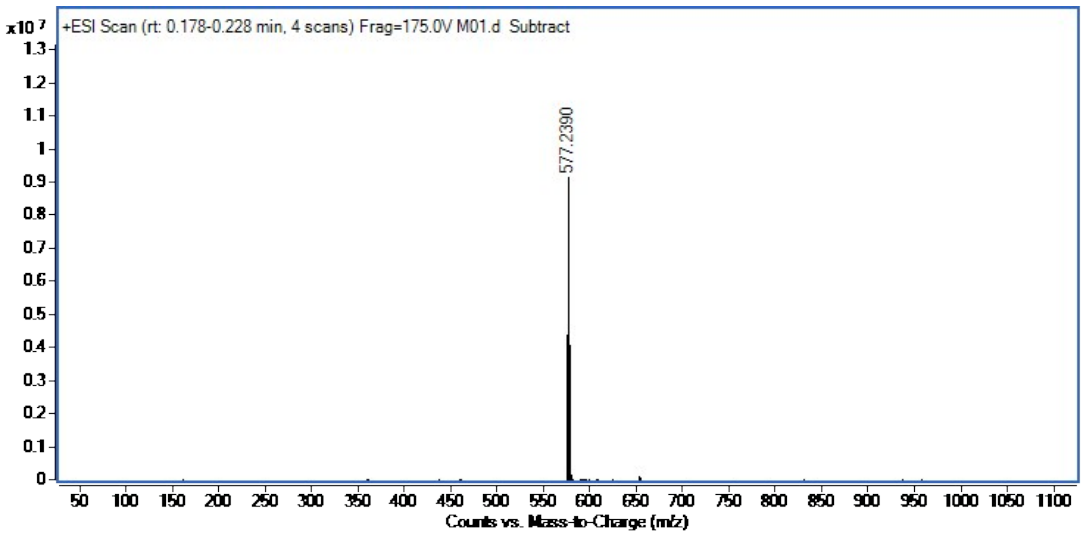

Figure S5 HRMS spectrum of M01.

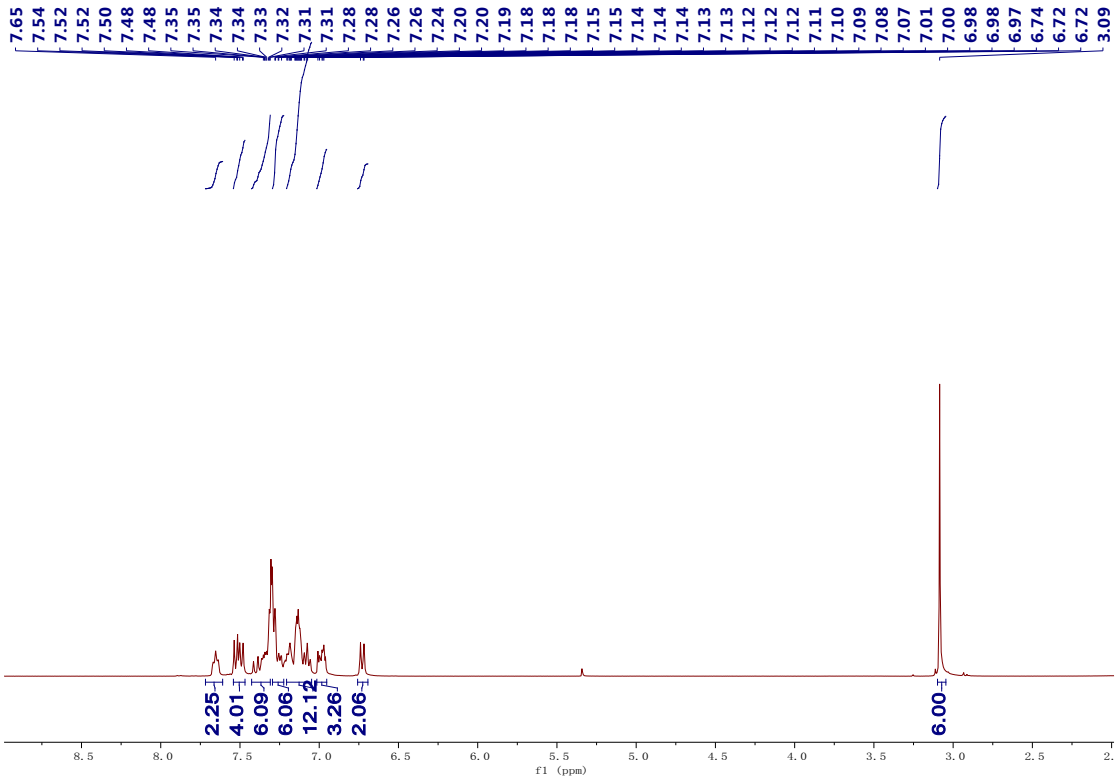

Figure S6 1H NMR spectrum of M-MAP in CDCl3.

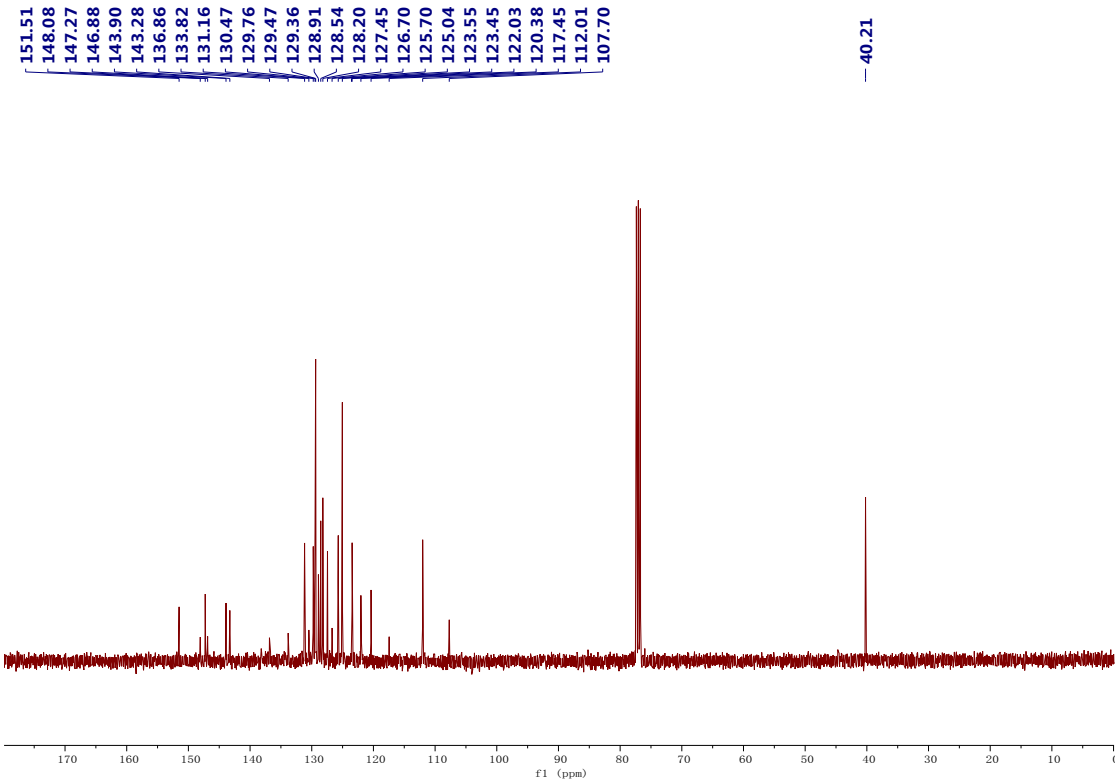

Figure S7 13C NMR spectrum of M-MAP in CDCl3.

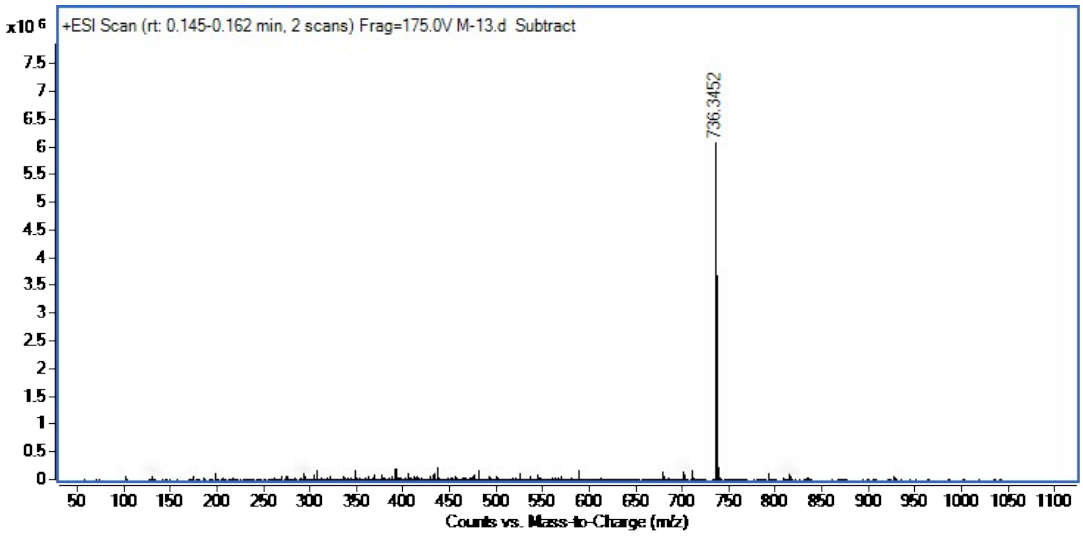

Figure S8 HRMS spectrum of M-MAP.

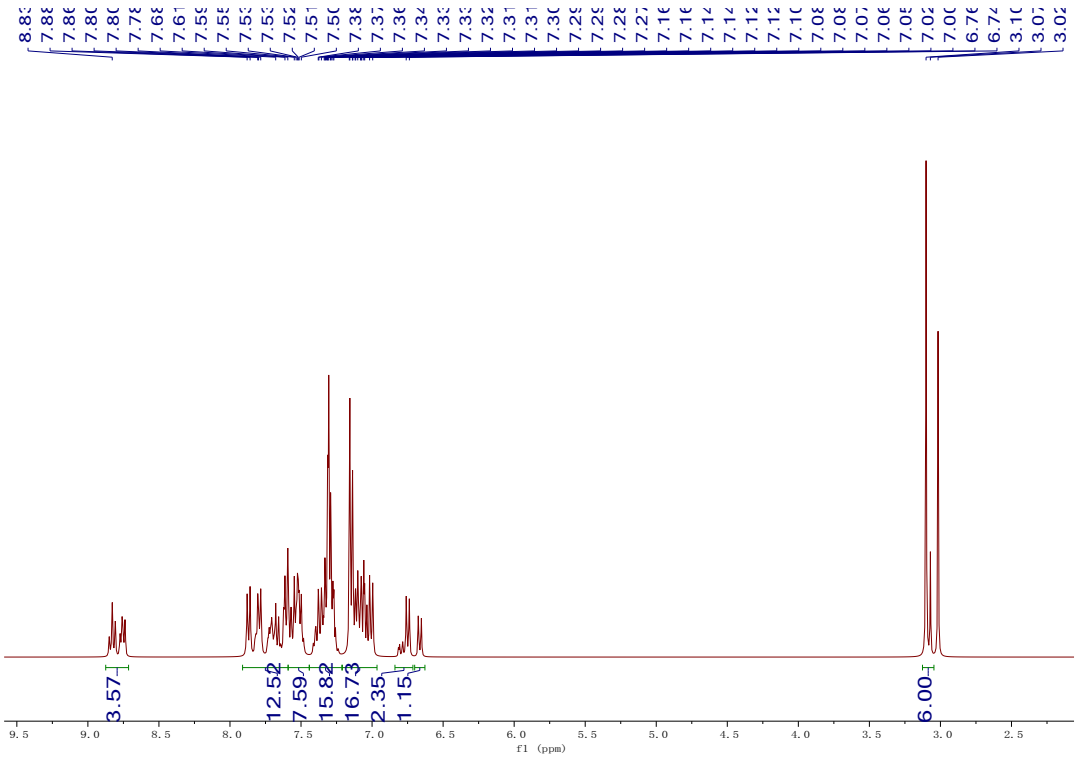

Figure S9 1H NMR spectrum of M01-MAP in CDCl3.

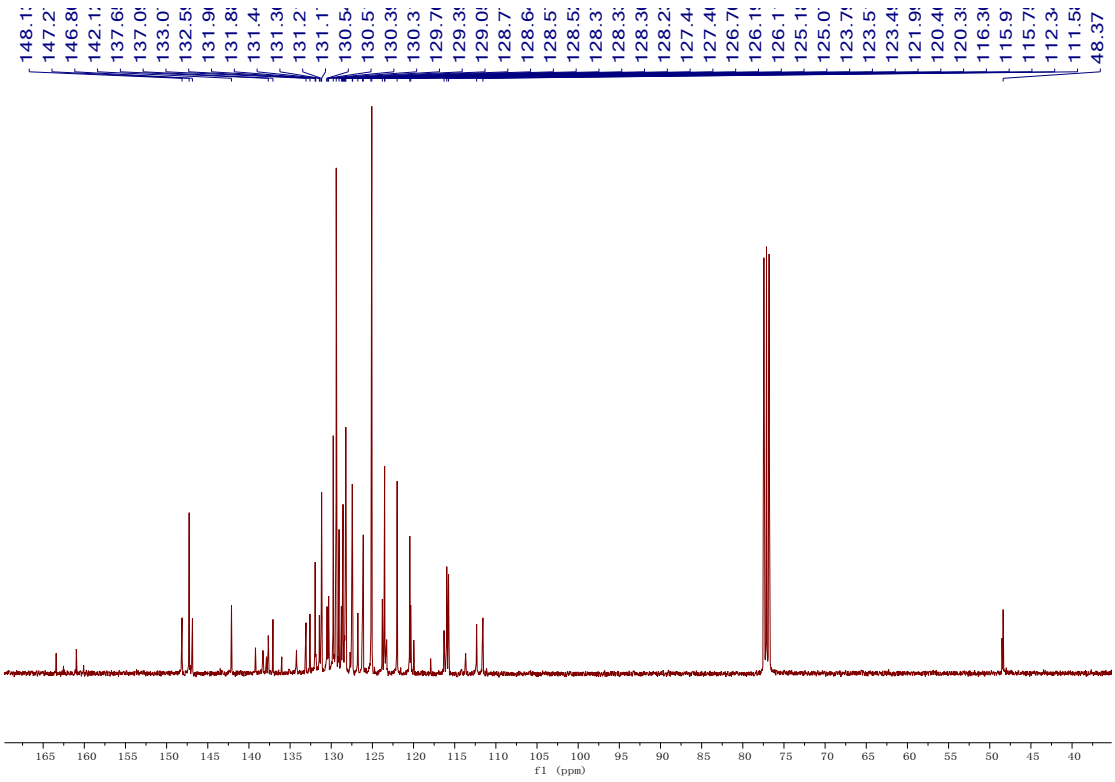

Figure S10 13C NMR spectrum of M01-MAP in CDCl3.

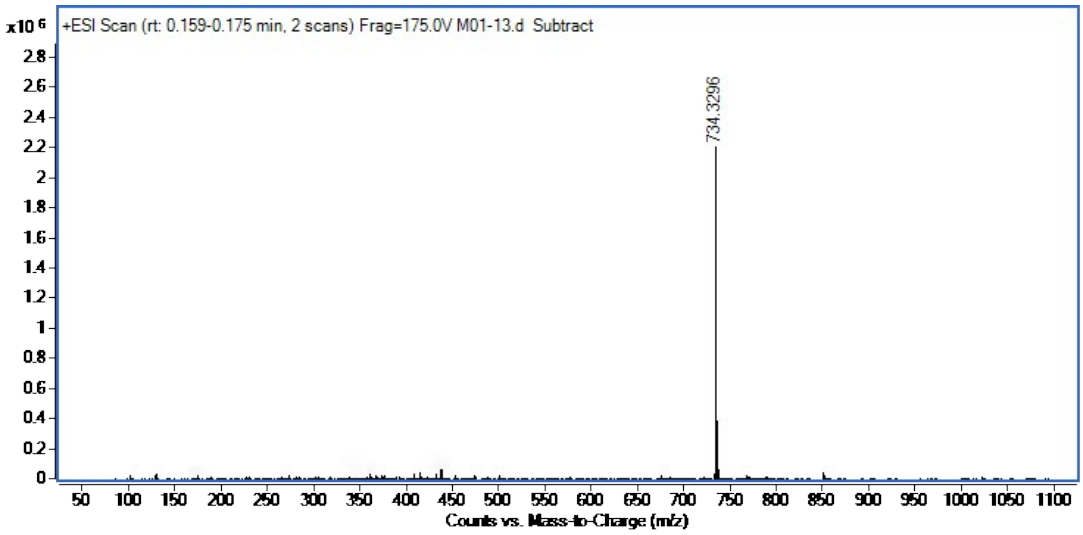

Figure S11 HRMS spectrum of M01-MAP.

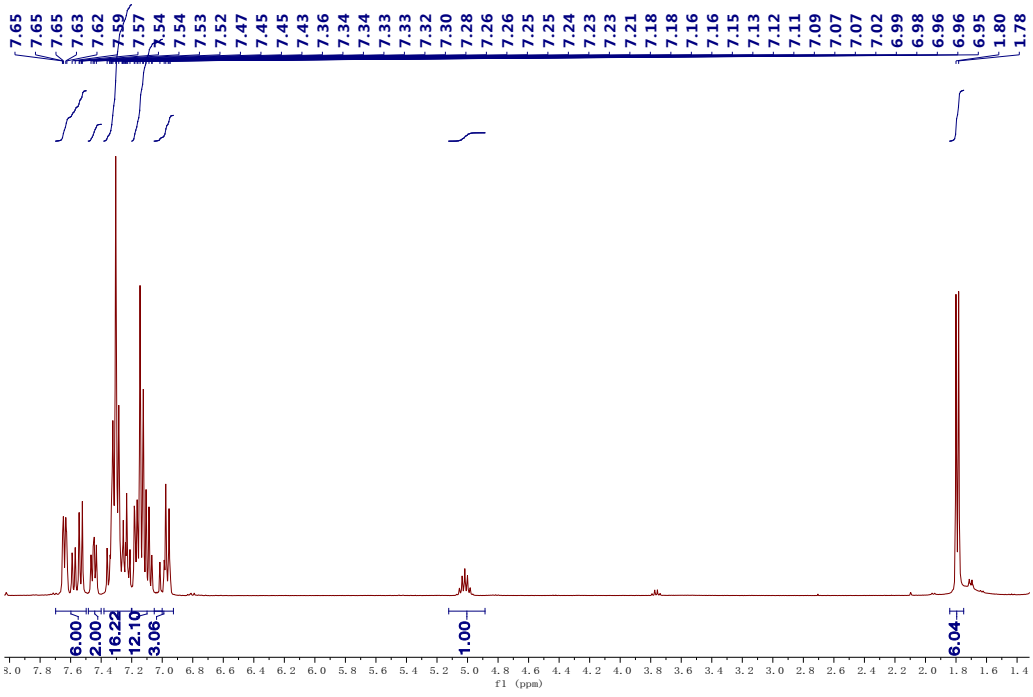

Figure S12 1H NMR spectrum of M-IF in CDCl3.

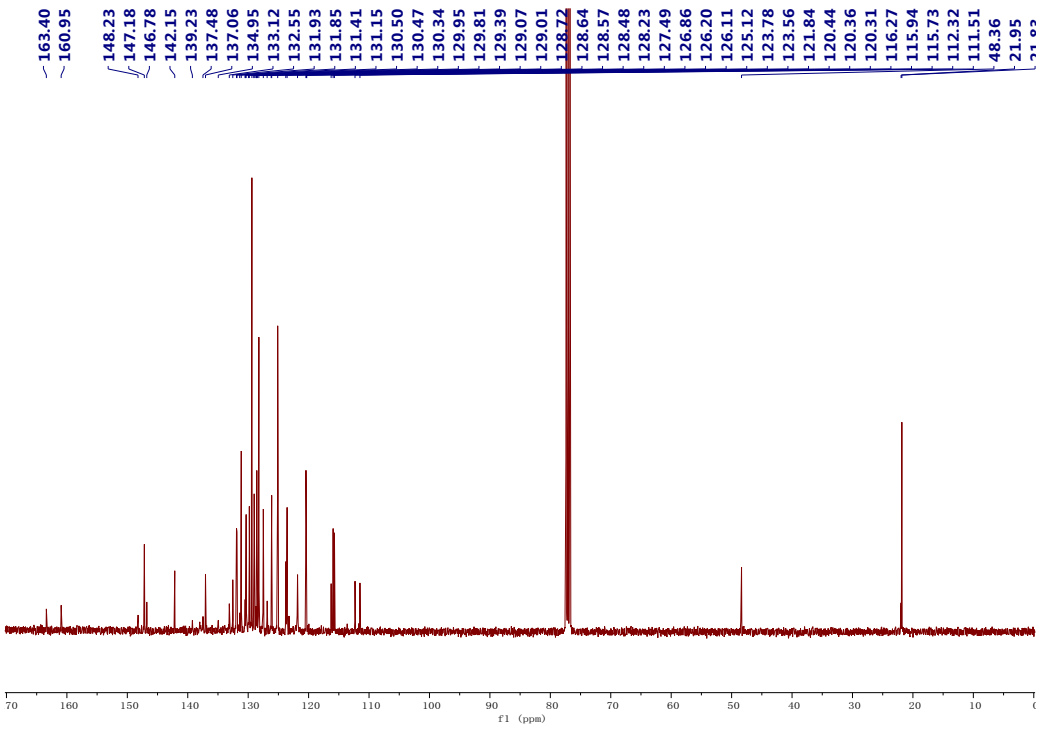

Figure S13 13C NMR spectrum of M-IF in CDCl3.

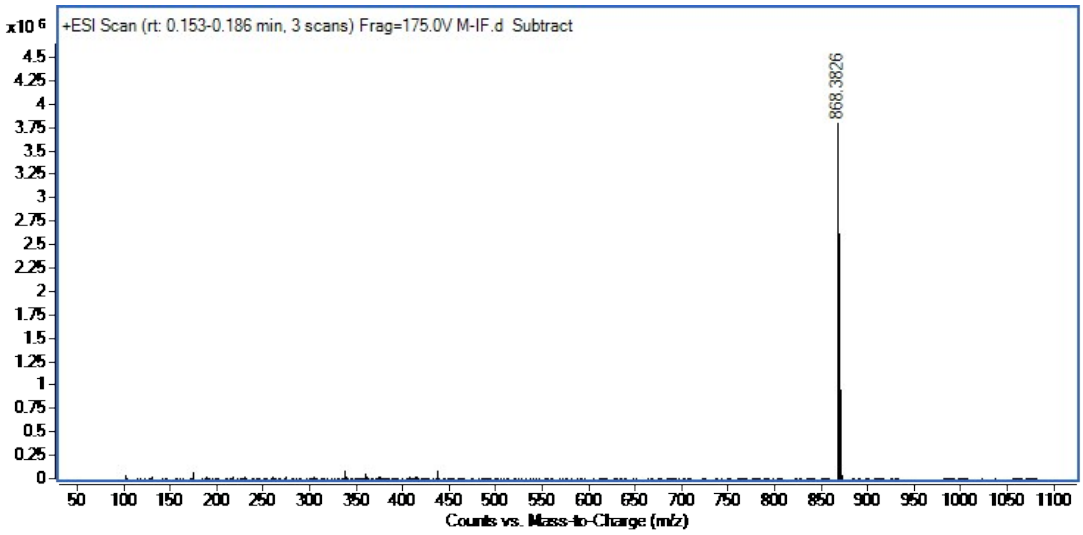

Figure S14 HRMS spectrum of M-IF.

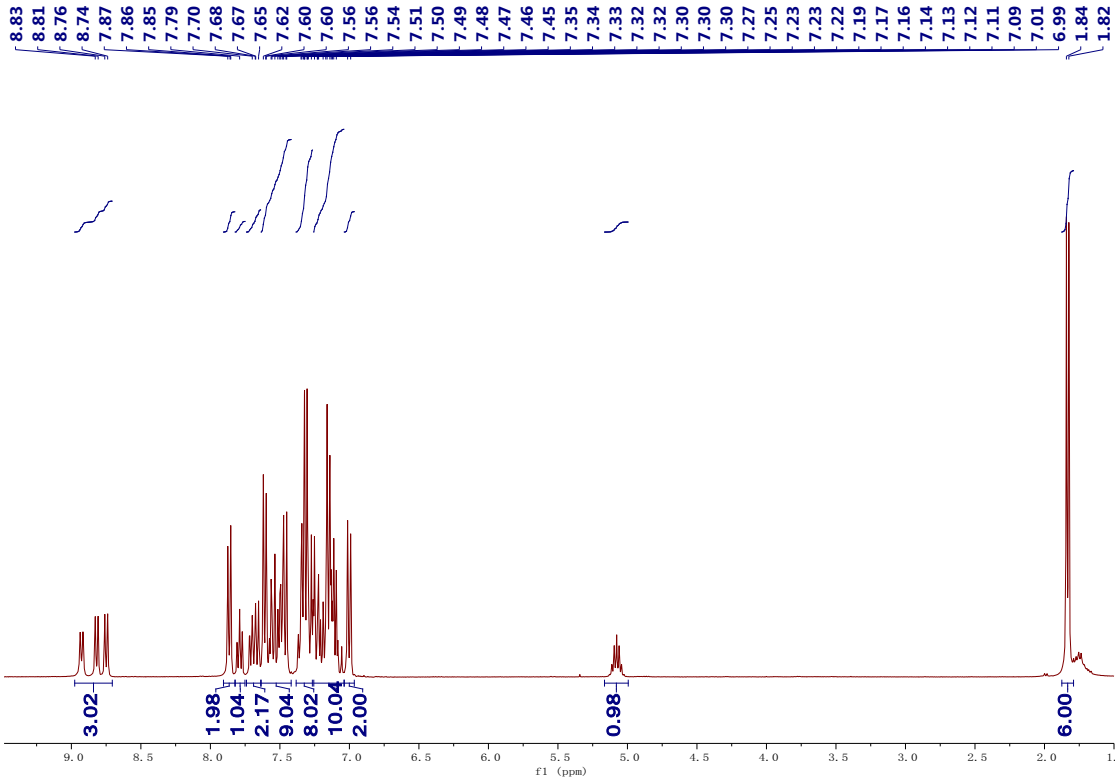

Figure S15 1H NMR spectrum of M01-IF in CDCl3.

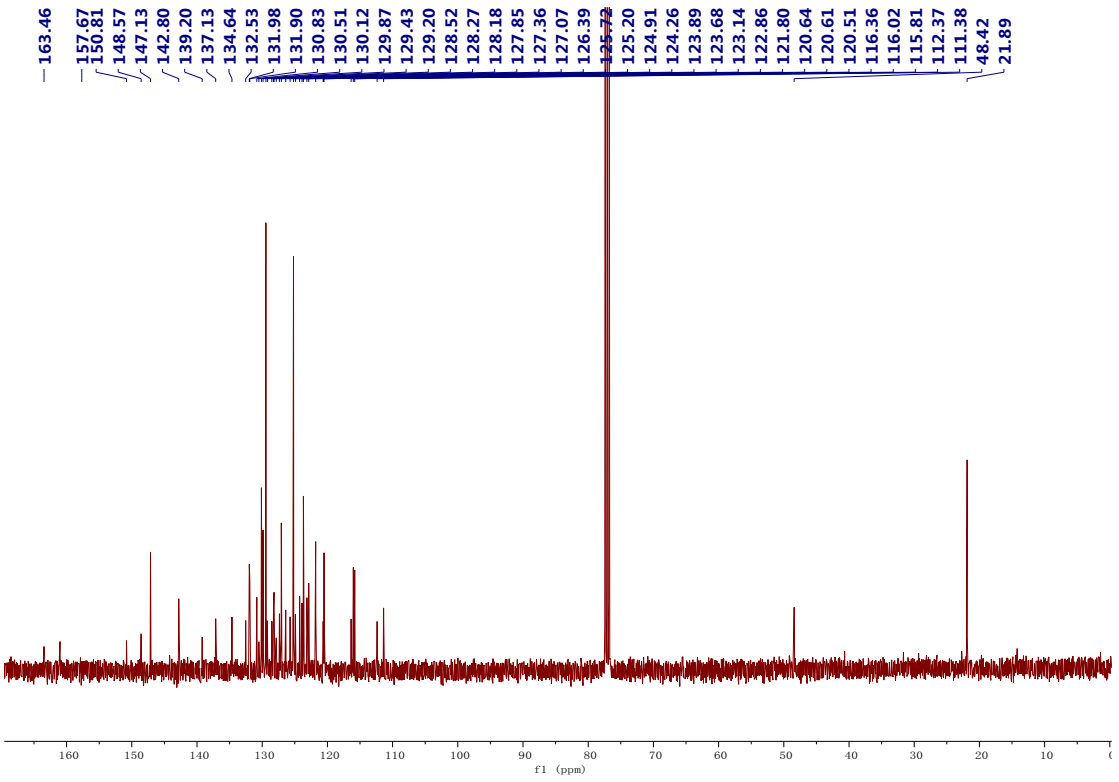

Figure S16 13C NMR spectrum of M01-IF in CDCl3.

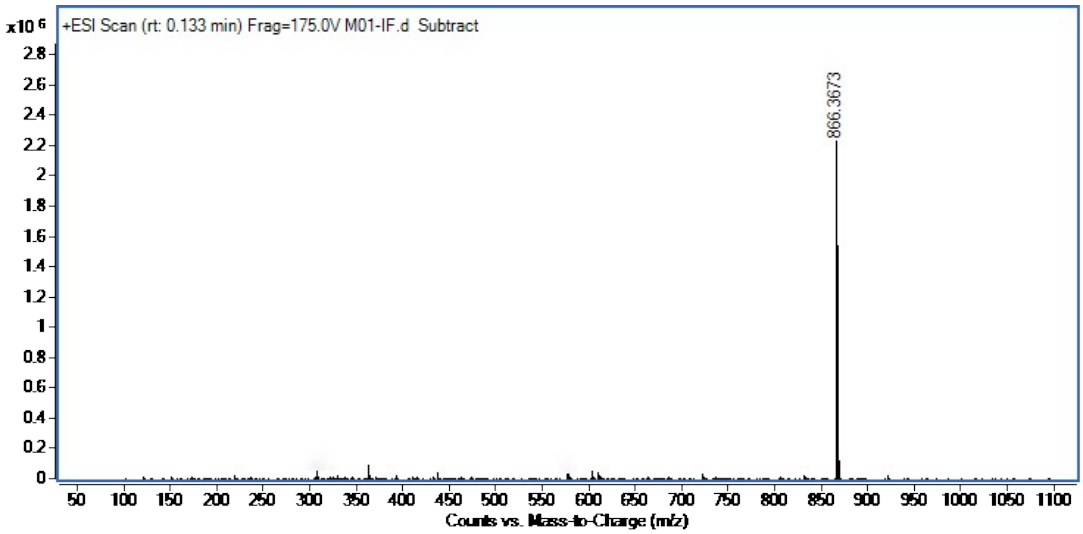

Figure S17 HRMS spectrum of M01-IF.

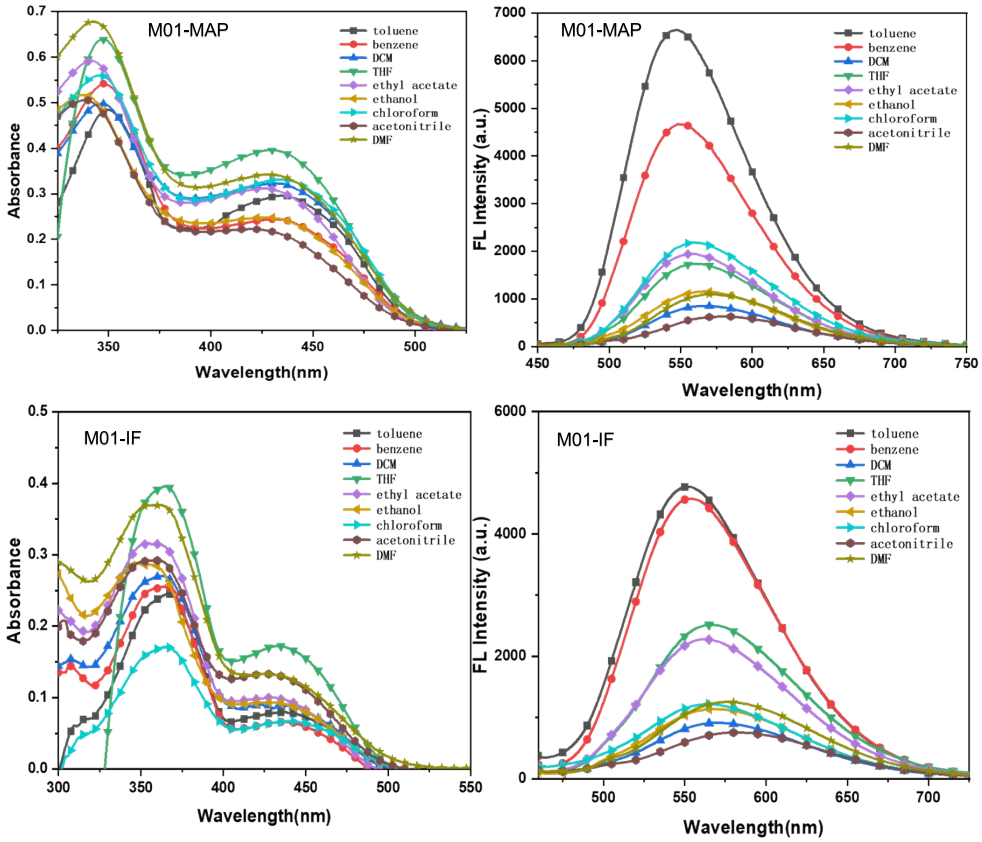

Figure S18 The UV-vis and fluorescence spectra of the compounds in different solvents (10.0 μM).

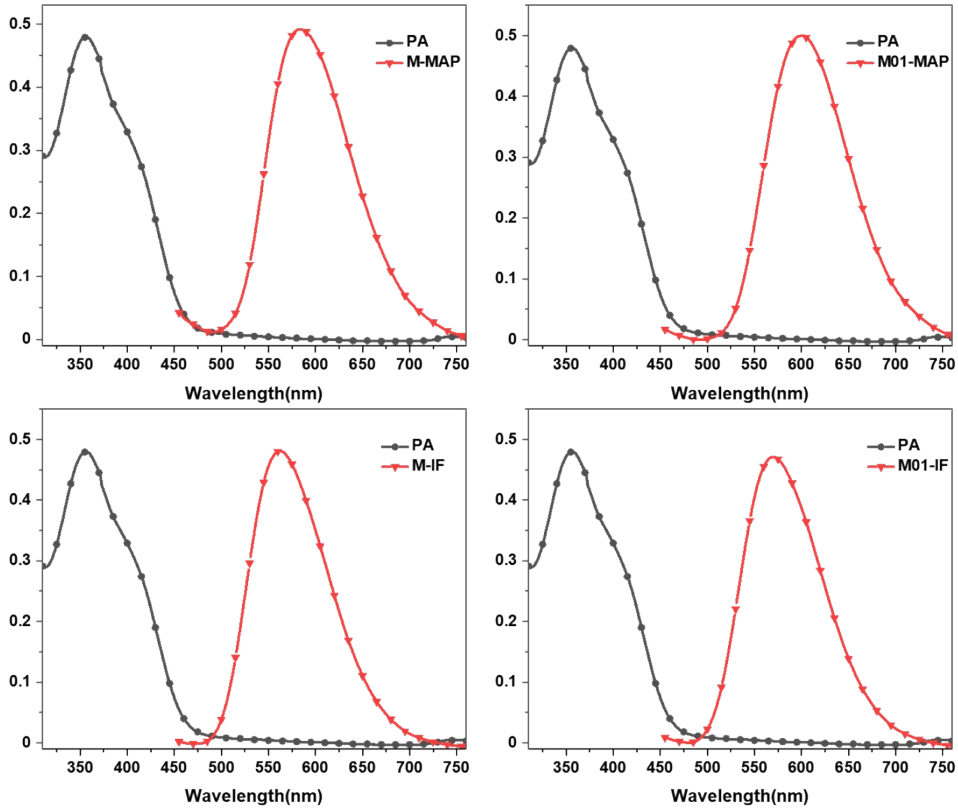

Figure S19 Normalized absorption spectrum of PA and the fluorescence spectra in THF-water (f_w = 90%) mixture solution.

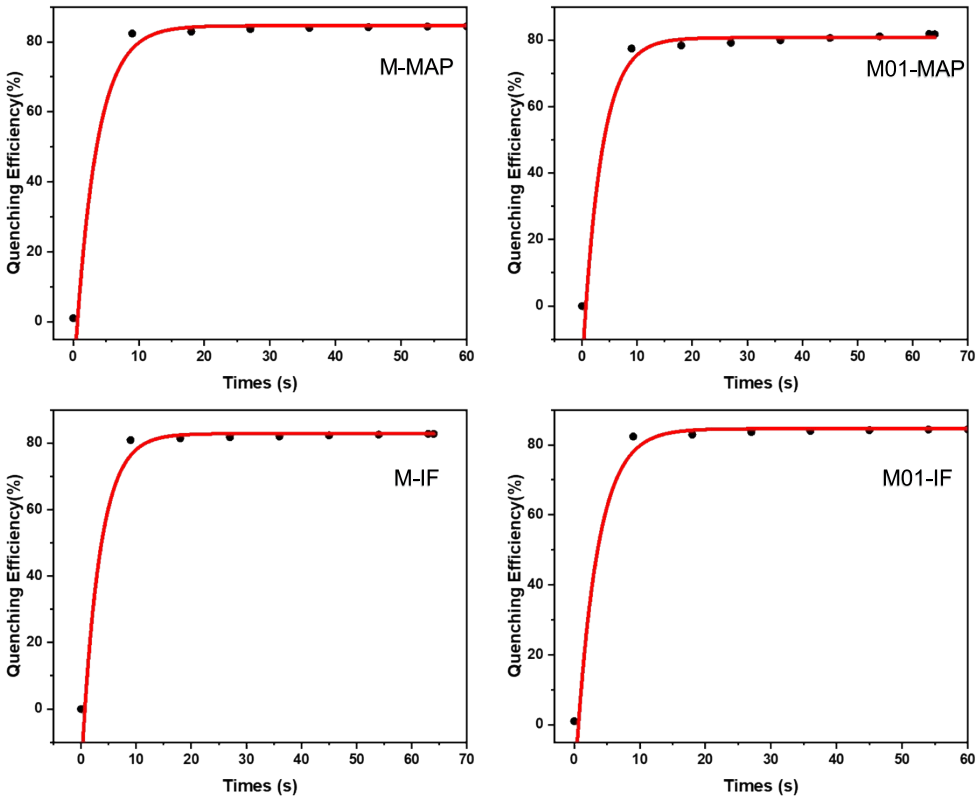

Figure S20 Time dependent fluorescence quenching efficiency response to PA (8 eq.)