

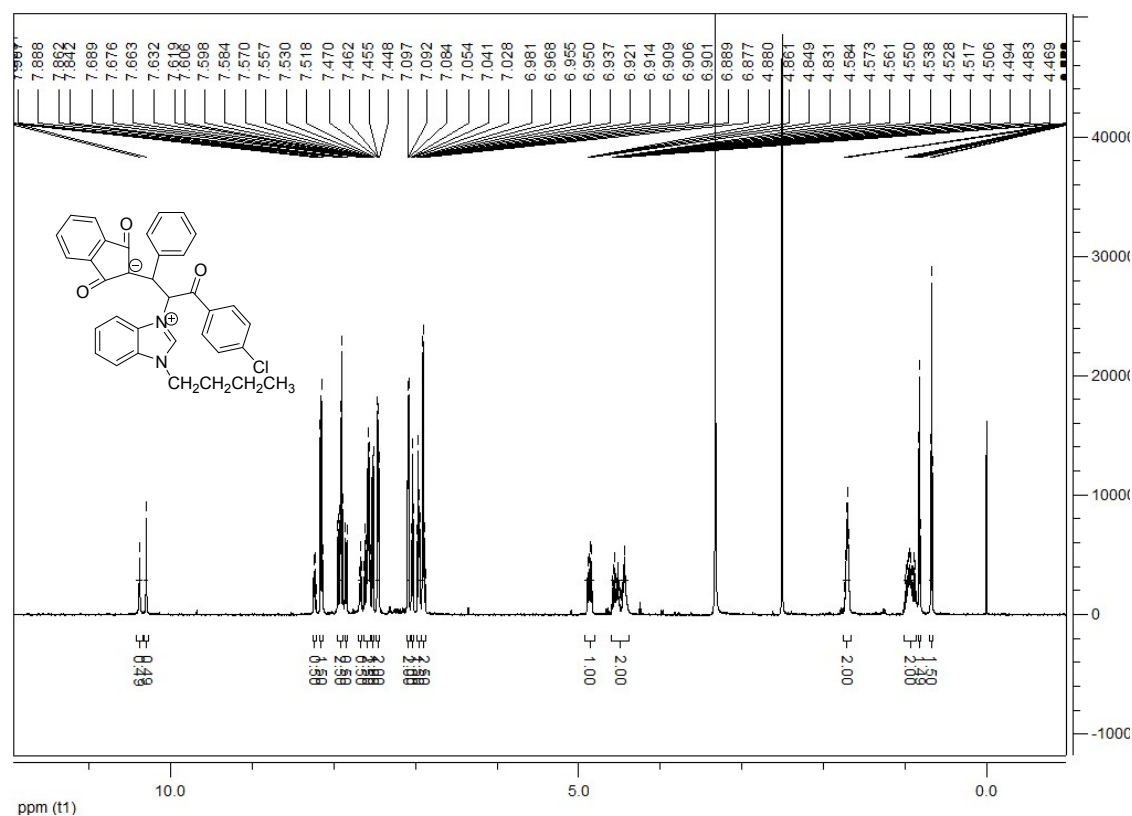
**Formation of zwitterionic salts via three-component reaction of benzimidazolium  
bromides, aromatic aldehydes and 1,3-indanedione**

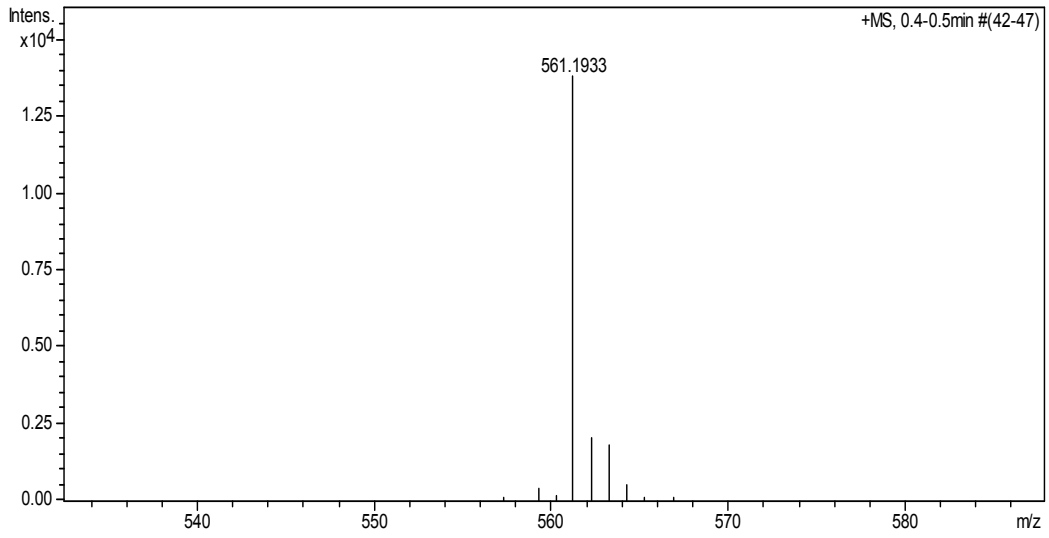
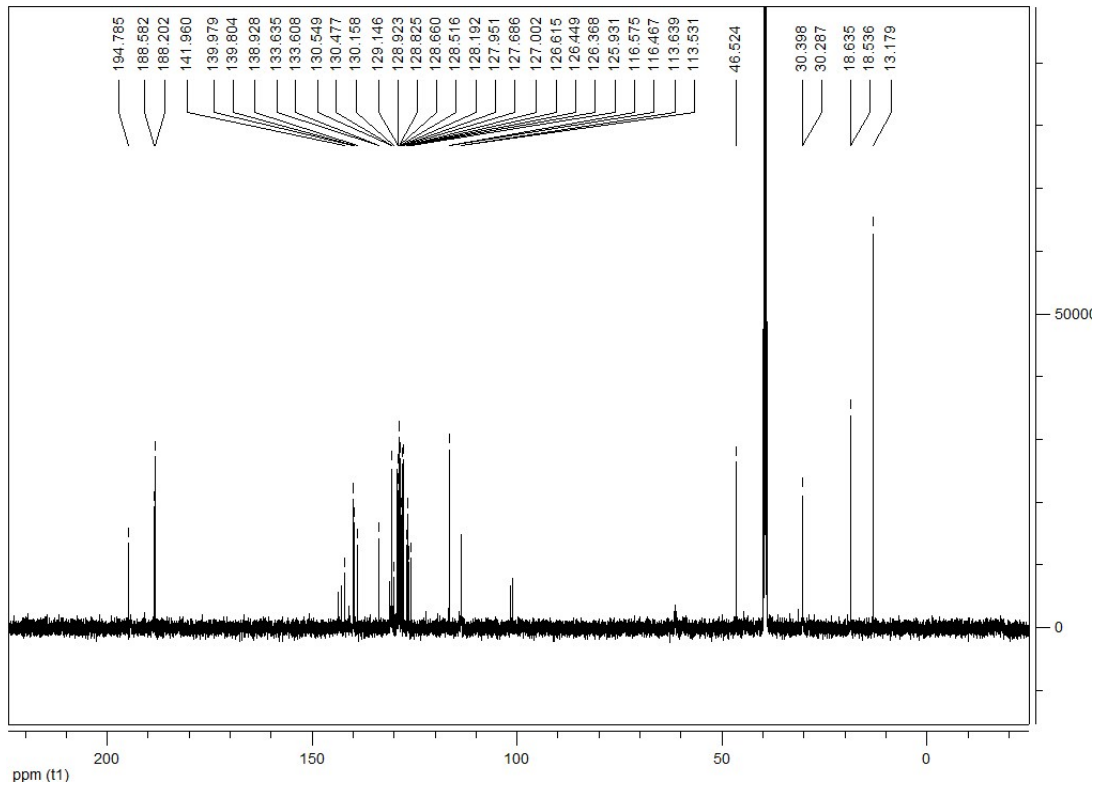
Gong Jin, Jing Sun, Chao-Guo Yan\*

**Supporting Information**

**<sup>1</sup>H NMR, <sup>13</sup>C NMR and HRMS spectra of the prepared compounds** 2-43

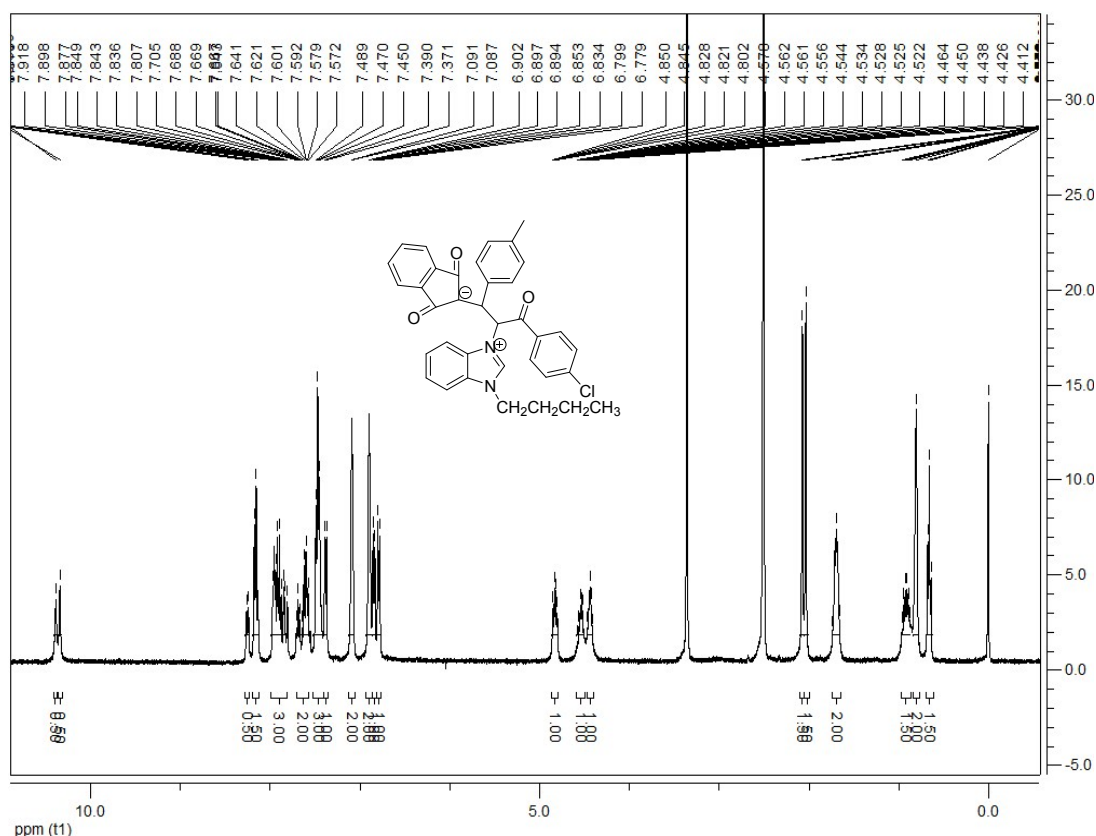
**2-(2-(1-butyl-1H-benzo[d]imidazol-3-ium-3-yl)-3-(4-chlorophenyl)-3-oxo-1-phenylpropyl)-1,3-dioxo-2,3-dihydro-1H-inden-2-ide (1a):** yellow solid, 88%, m.p. 168~170°C; <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ: A-conformation: 10.30 (s, 1H, CH), 8.17~8.14 (m, 2H, ArH), 7.96~7.89 (m, 2H, ArH), 7.86~7.84 (m, 1H, ArH), 7.69~7.66 (m, 1H, ArH), 7.63~7.56 (m, 2H, ArH), 7.52 (d, *J* = 7.2 Hz, 1H, ArH), 7.47~7.45 (m, 2H, ArH), 7.10~7.08 (m, 2H, ArH), 7.05~7.03 (m, 1H, ArH), 6.98~6.94 (m, 1H, ArH), 6.92~6.88 (m, 3H, ArH, CH), 4.88~4.83 (m, 1H, CH), 4.58~4.42 (m, 2H, CH), 1.74~1.69 (m, 2H, CH), 0.99~0.88 (m, 2H, CH), 0.83~0.81 (m, 3H, CH<sub>3</sub>); B-conformation: 10.38 (s, 1H, CH), 8.25~8.22 (m, 1H, ArH), 0.67 (t, *J* = 7.2 Hz, 3H, CH<sub>3</sub>). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ: 194.8, 188.6, 188.2, 142.0, 140.0, 139.8, 138.9, 133.6, 130.5, 130.2, 129.1, 128.9, 128.8, 128.7, 128.5, 128.2, 128.0, 127.7, 127.0, 126.6, 126.5, 126.4, 125.9, 116.6, 116.5, 113.7, 113.5, 46.5, 30.4, 30.3, 18.6, 18.5, 13.2; IR (KBr) ν: 3051, 2959, 1691, 1598, 1533, 1427, 1317, 1206, 1088, 1004, 961, 859, 810, 729 cm<sup>-1</sup>; MS (*m/z*): HRMS (ESI) Calcd. for C<sub>35</sub>H<sub>30</sub>ClN<sub>2</sub>O<sub>3</sub> ([M+H]<sup>+</sup>): 561.1939. Found: 561.1933.

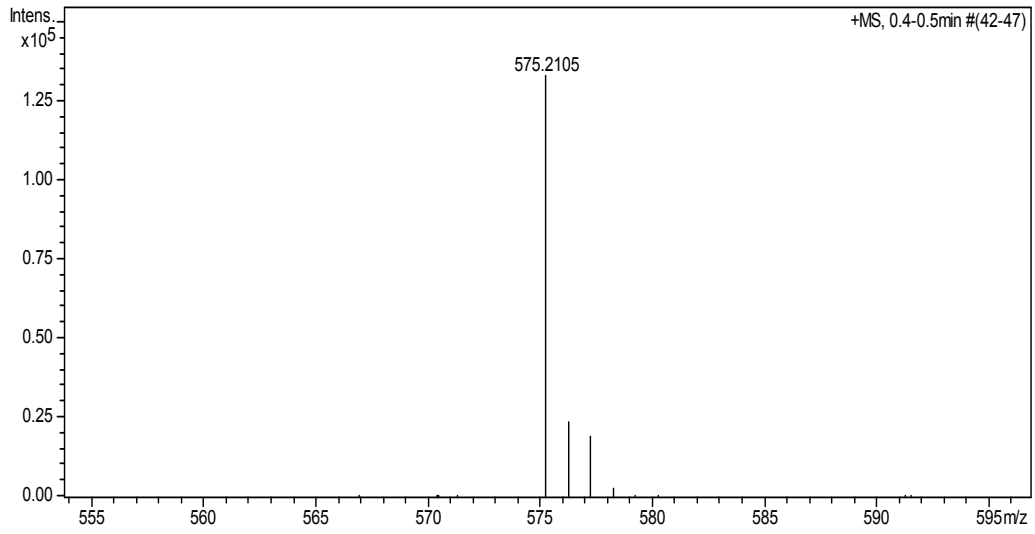
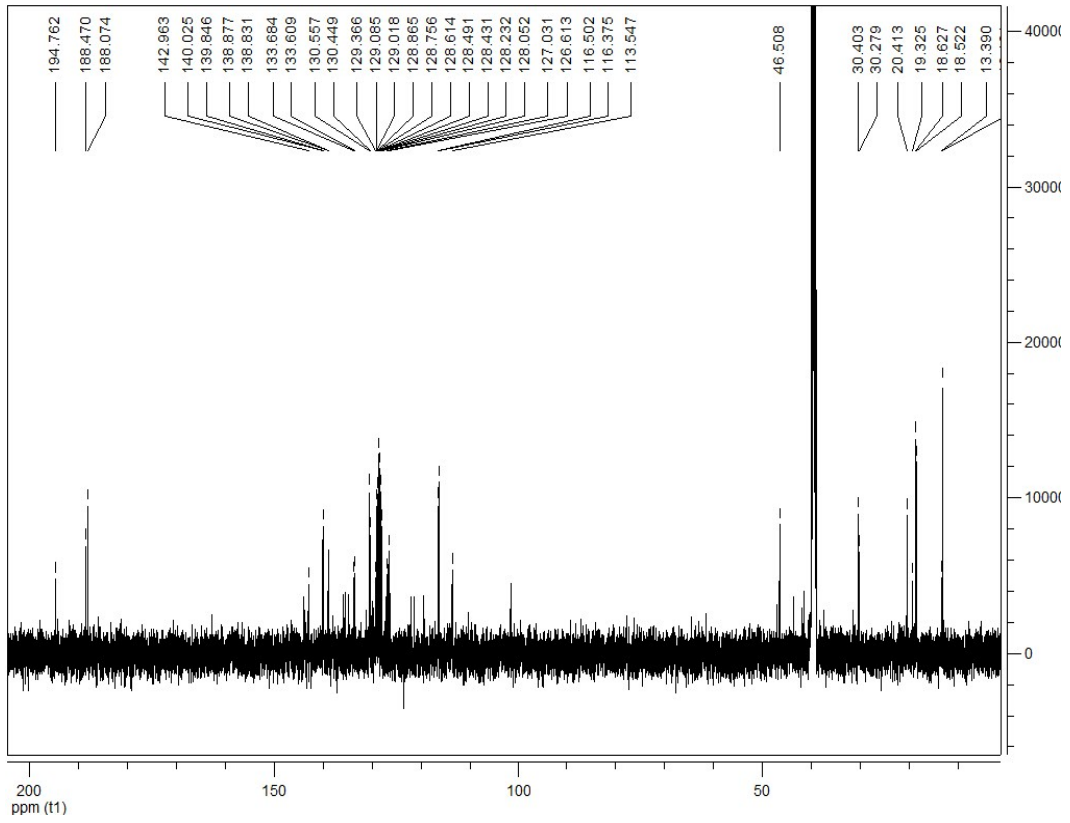




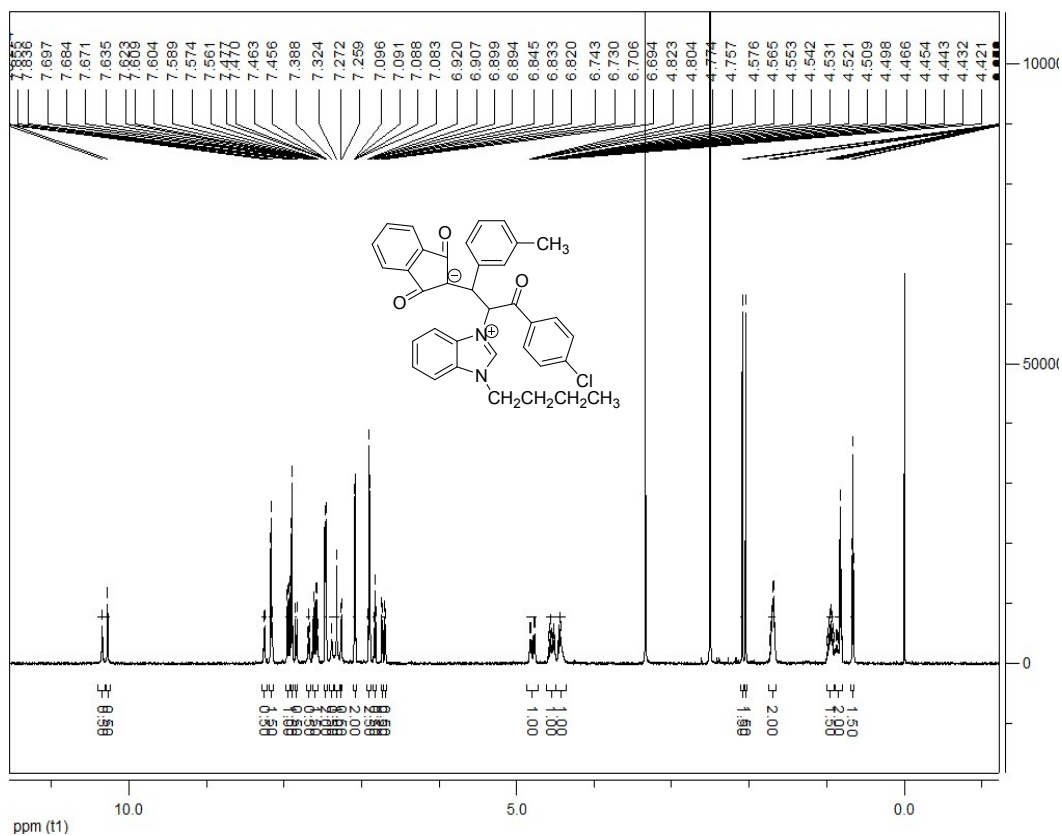
**2-(2-(1-butyl-1H-benzo[d]imidazol-3-ium-3-yl)-3-(4-chlorophenyl)-3-oxo-1-(p-tolyl)propyl)-**

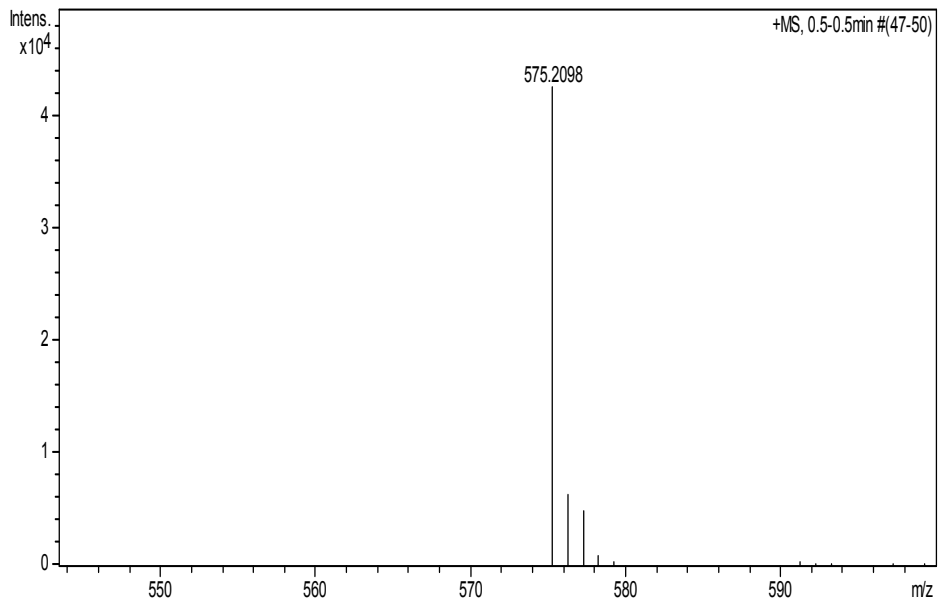
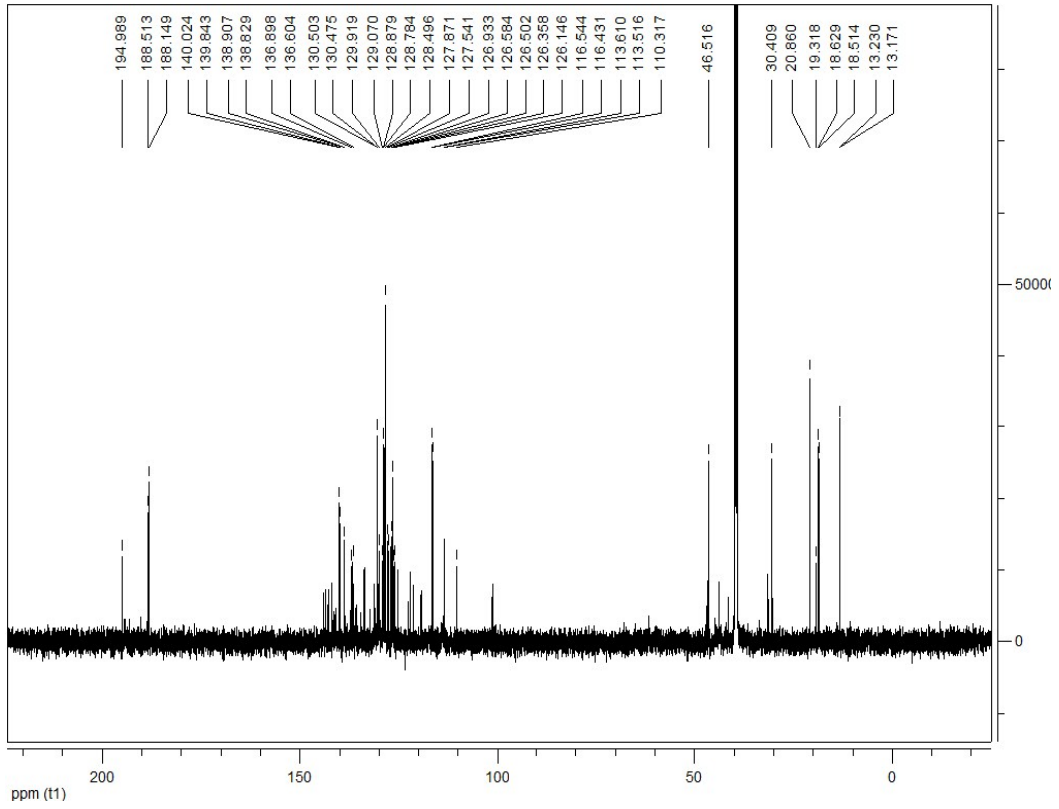
**1,3-dioxo-2,3-dihydro-1H-inden-2-ide (1b):** yellow solid, 82%, m.p. 179~181 °C; <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ: A-conformation: 10.34 (s, 1H, CH), 8.25 (d, *J* = 8.0 Hz, 1H, ArH), 8.18~8.13 (m, 1H, ArH), 7.97~7.81 (m, 3H, ArH), 7.70~7.57 (m, 2H, ArH), 7.49~7.45 (m, 3H, ArH), 7.38 (d, *J* = 7.6 Hz, 1H, ArH), 7.09 (brs, 2H, ArH), 6.90~6.89 (m, 2H, ArH, CH), 6.84 (d, *J* = 7.6 Hz, 1H, ArH), 6.79 (d, *J* = 8.0 Hz, 1H, ArH), 4.85~4.80 (m, 1H, CH), 4.58~4.52 (m, 1H, CH), 4.46~4.40 (m, 1H, CH), 2.07 (s, 3H, CH<sub>3</sub>), 1.74~1.66 (m, 2H, CH), 0.96~0.87 (m, 3H, CH<sub>3</sub>), 0.81 (brs, 2H, CH); B-conformation: 10.39 (s, 1H, CH), 2.03 (s, 3H, CH<sub>3</sub>), 0.66 (t, *J* = 7.2 Hz, 3H, CH<sub>3</sub>). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ: 194.8, 188.5, 188.1, 143.0, 140.0, 139.8, 138.9, 138.8, 133.7, 133.6, 130.6, 130.4, 129.4, 129.1, 129.0, 128.9, 128.8, 128.6, 128.5, 128.4, 128.2, 128.1, 127.0, 126.6, 116.5, 116.4, 113.5, 46.5, 30.4, 30.3, 20.4, 19.3, 18.6, 18.5, 13.4, 13.2; IR (KBr) ν: 3036, 2957, 1690, 1601, 1535, 1426, 1208, 1091, 1004, 963, 860, 822, 731 cm<sup>-1</sup>; MS (*m/z*): HRMS (ESI) Calcd. for C<sub>36</sub>H<sub>32</sub>ClN<sub>2</sub>O<sub>3</sub> ([M+H]<sup>+</sup>): 575.2096. Found: 575.2105.



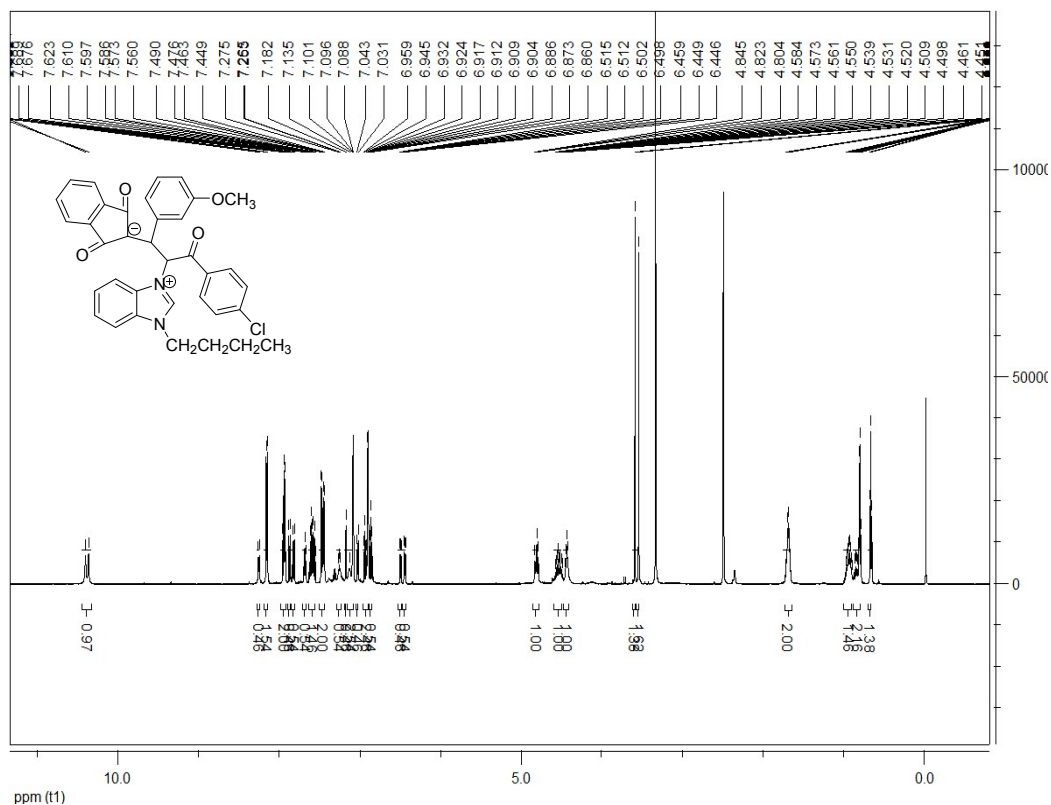


**2-(2-(1-butyl-1H-benzo[d]imidazol-3-ium-3-yl)-3-(4-chlorophenyl)-3-oxo-1-(m-tolyl)propyl)-1,3-dioxo-2,3-dihydro-1H-inden-2-ide (1c):** yellow solid, 65%, m.p. 174~176°C; <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ: A-conformation: 10.27 (s, 1H, CH), 8.26 (d, *J* = 8.4 Hz, 1H, ArH), 8.18~8.15 (m, 1H, ArH), 7.97~7.92 (m, 1H, ArH), 7.91~7.90 (m, 1H, ArH), 7.86~7.84 (m, 1H, ArH), 7.70~7.67 (m, 1H, ArH), 7.64~7.56 (m, 1H, ArH), 7.48~7.46 (m, 2H, ArH), 7.32 (s, 1H, ArH), 7.27 (d, *J* = 7.8 Hz, 1H, ArH), 7.10~7.08 (m, 2H, ArH), 6.92~6.89 (m, 2H, ArH, CH), 6.74 (d, *J* = 7.5 Hz, 1H, ArH), 6.70 (d, *J* = 7.4 Hz, 1H, ArH), 4.82~4.76 (m, 1H, CH), 4.58~4.50 (m, 1H, CH), 4.47~4.42 (m, 1H, CH), 2.09 (s, 3H, CH<sub>3</sub>), 1.73~1.66 (m, 2H, CH), 0.99~0.91 (m, 3H, CH<sub>3</sub>), 0.88~0.81 (m, 2H, CH); B-conformation: 10.34 (s, 1H, CH), 7.39 (brs, 1H, ArH), 6.84~6.82 (m, 1H, ArH), 2.04 (s, 3H, CH<sub>3</sub>), 0.66 (t, *J* = 7.2 Hz, 3H, CH<sub>3</sub>). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ: 195.0, 188.5, 188.1, 140.0, 139.8, 138.9, 138.8, 136.9, 136.6, 130.5, 129.9, 129.1, 128.9, 128.8, 128.5, 127.9, 127.5, 126.9, 126.6, 126.5, 126.4, 126.1, 116.5, 116.4, 113.6, 113.5, 110.3, 46.5, 30.4, 20.9, 19.3, 18.6, 18.5, 13.2; IR (KBr) ν: 3032, 2962, 1688, 1607, 1538, 1486, 1425, 1209, 1089, 1007, 967, 850, 730 cm<sup>-1</sup>; MS (*m/z*): HRMS (ESI) Calcd. for C<sub>36</sub>H<sub>32</sub>ClN<sub>2</sub>O<sub>3</sub> ([M+H]<sup>+</sup>): 575.2096. Found: 575.2098.

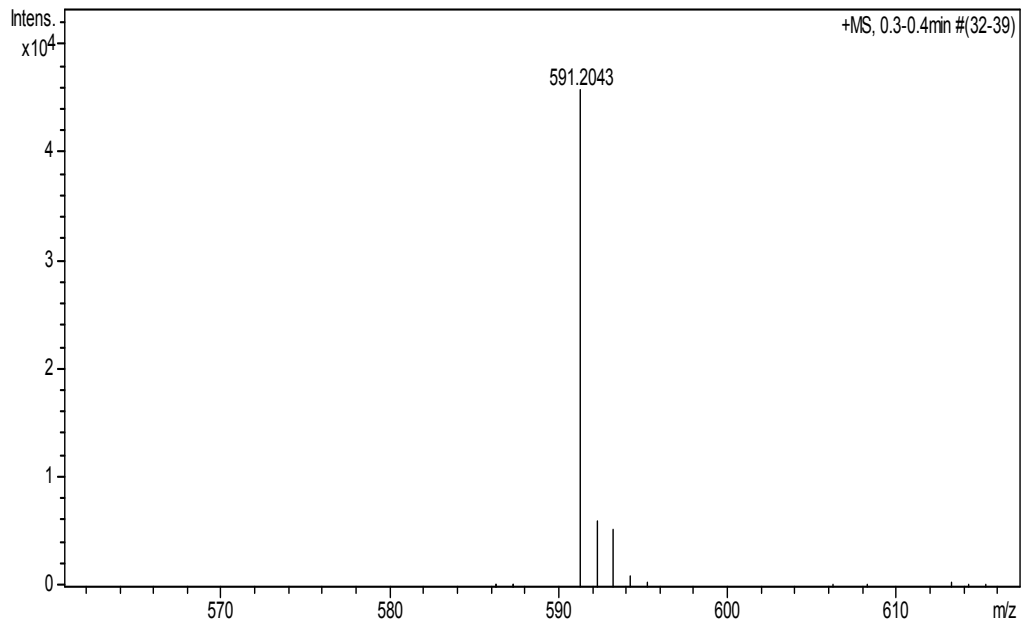
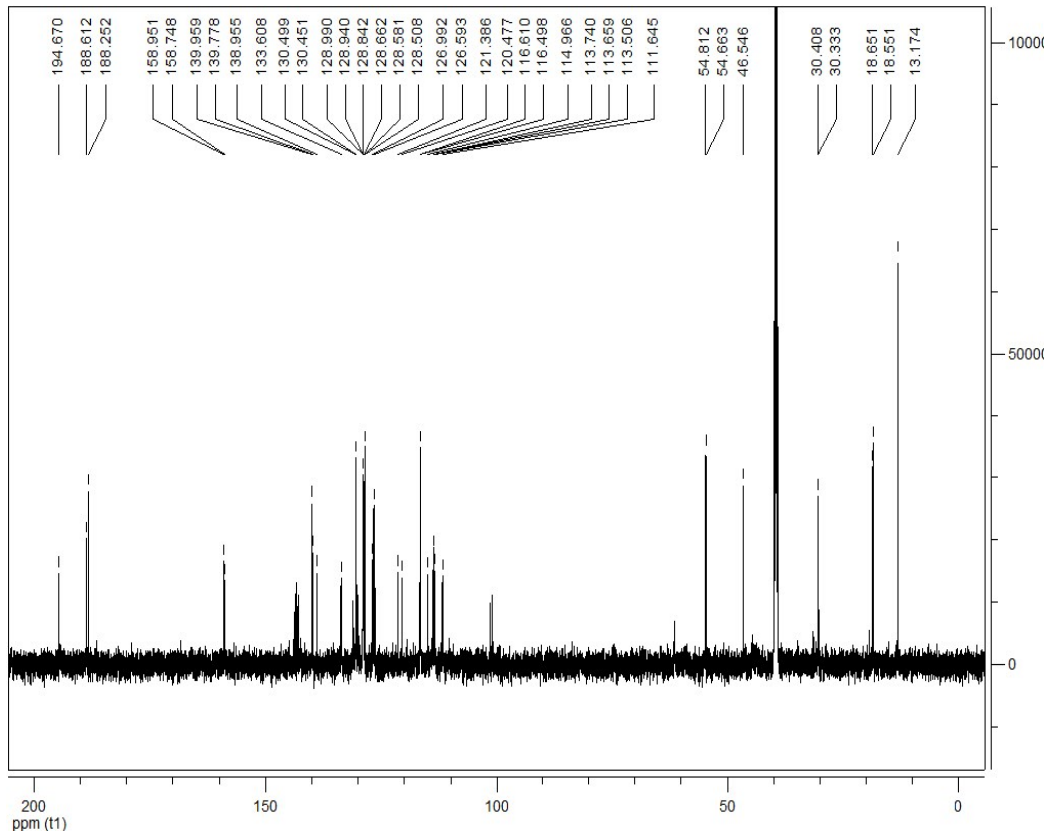




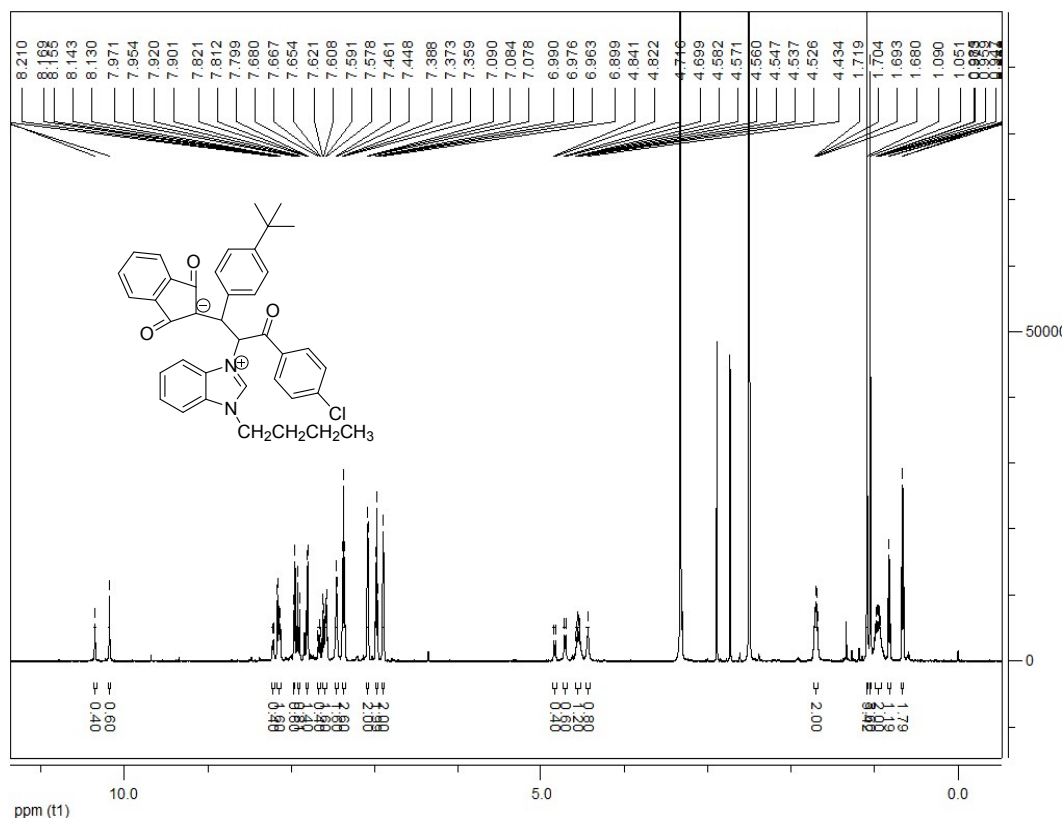
**2-(2-(1-butyl-1H-benzo[d]imidazol-3-ium-3-yl)-3-(4-chlorophenyl)-1-(3-methoxyphenyl)-3-oxopropyl)-1,3-dioxo-2,3-dihydro-1H-inden-2-ide (1d):** yellow solid, 90%, m.p. 156~158°C; <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ: A-conformation: 10.40~10.37 (m, 1H, CH), 8.16 (d, *J* = 8.5 Hz, 2H, ArH), 7.96~7.93 (m, 2H, ArH), 7.84~7.82 (m, 1H, ArH), 7.70~7.68 (m, 1H, ArH), 7.62~7.56 (m, 1H, ArH), 7.49~7.45 (m, 2H, ArH), 7.28~7.25 (m, 1H, ArH), 7.14~7.09 (m, 3H, ArH), 6.96~6.90 (m, 2H, ArH), 6.89~6.86 (m, 1H, ArH), 6.46~6.45 (m, 1H, CH), 4.84~4.80 (m, 1H, CH), 4.58~4.50 (m, 1H, CH), 4.46~4.43 (m, 1H, CH), 3.55 (s, 3H, OCH<sub>3</sub>), 1.74~1.67 (m, 2H, CH), 0.99~0.91 (m, 1H, CH), 0.88~0.80 (m, 4H, CH); B-conformation: δ: 8.26 (d, *J* = 8.4 Hz, 1H, ArH), 7.89~7.87 (m, 1H, ArH), 7.18 (brs, 1H, ArH), 7.04~7.03 (m, 1H, ArH), 6.52~6.50 (m, 1H, CH), 3.60 (s, 3H, OCH<sub>3</sub>), 0.68 (t, *J* = 7.2 Hz, 3H, CH<sub>3</sub>). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ: 194.7, 188.6, 188.3, 159.0, 158.7, 140.0, 139.8, 139.0, 133.6, 130.5, 129.0, 128.9, 128.8, 128.7, 128.6, 128.5, 127.0, 126.6, 121.4, 120.5, 116.6, 116.5, 115.0, 113.7, 113.5, 111.6, 54.8, 54.7, 46.5, 30.4, 30.3, 18.7, 18.5, 13.2; IR (KBr) ν: 2967, 2873, 1691, 1643, 1601, 1528, 1425, 1349, 1222, 1165, 1087, 983, 837, 733 cm<sup>-1</sup>; MS (*m/z*): HRMS (ESI) Calcd. for C<sub>36</sub>H<sub>32</sub>ClN<sub>2</sub>O<sub>4</sub> ([M+H]<sup>+</sup>): 591.2045. Found: 591.2043.

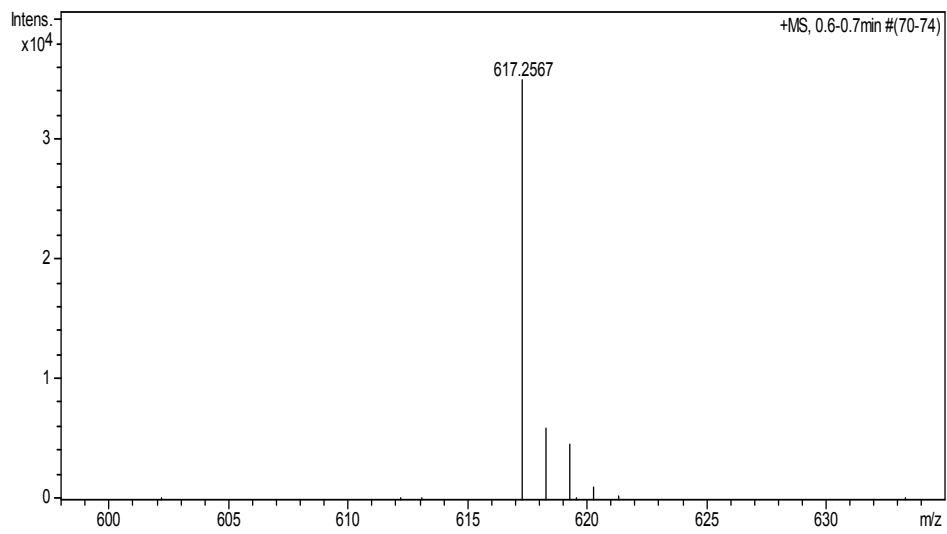
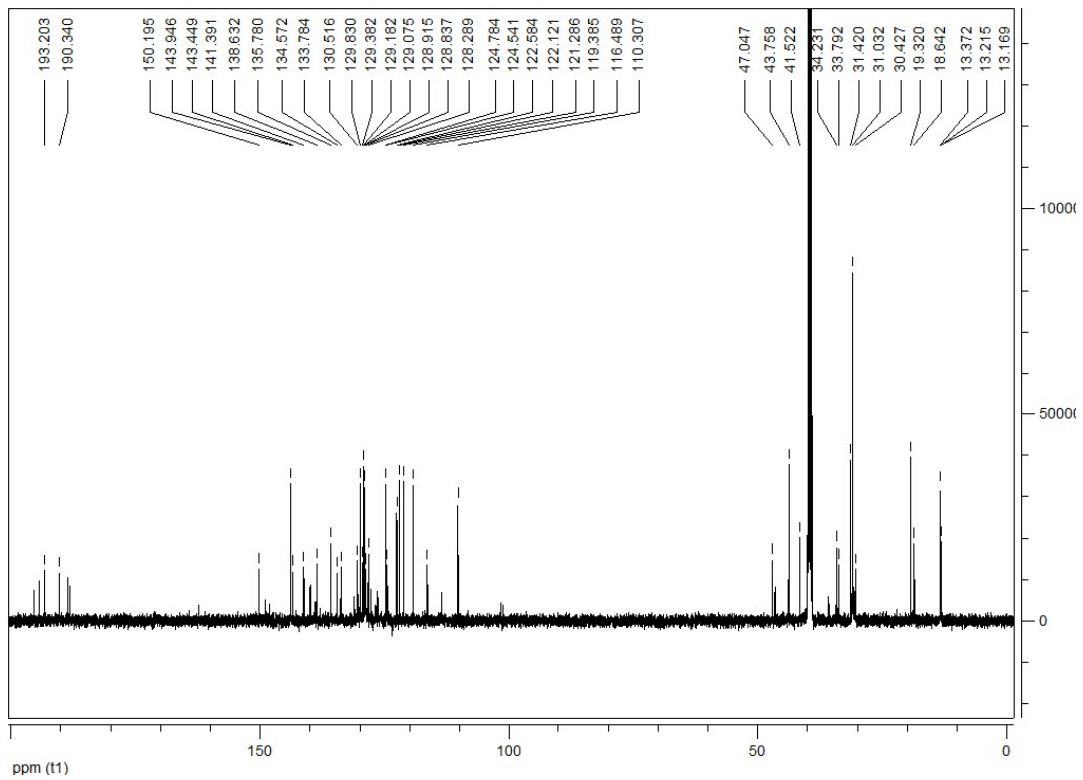




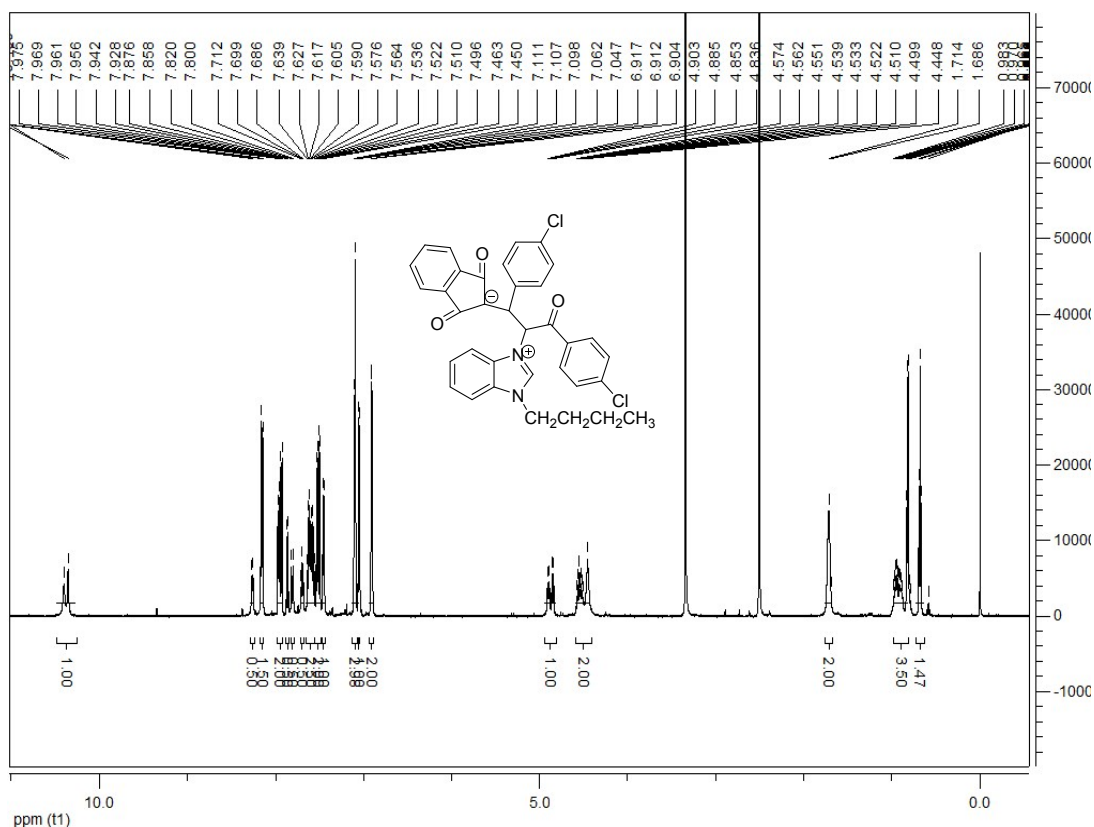


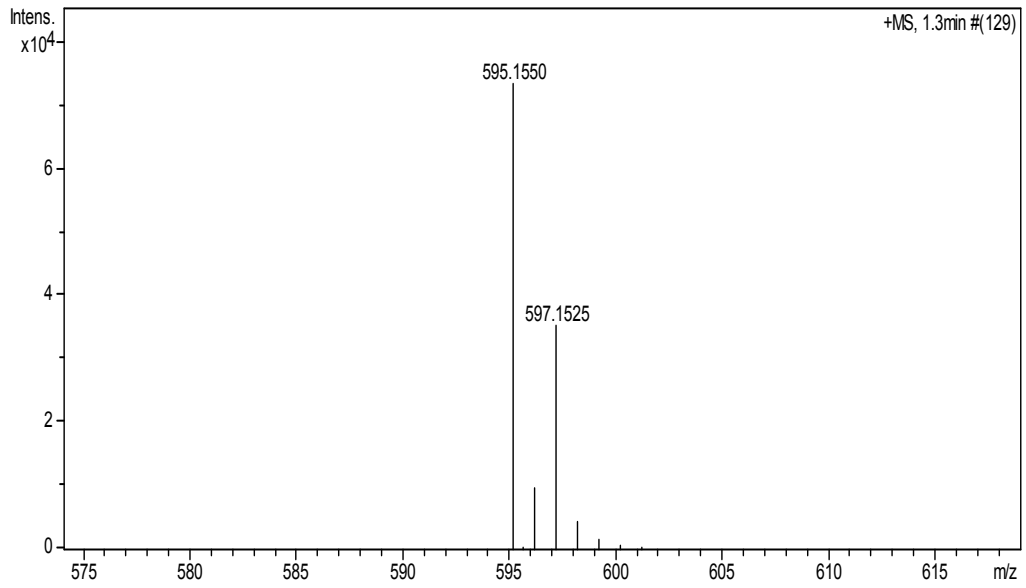
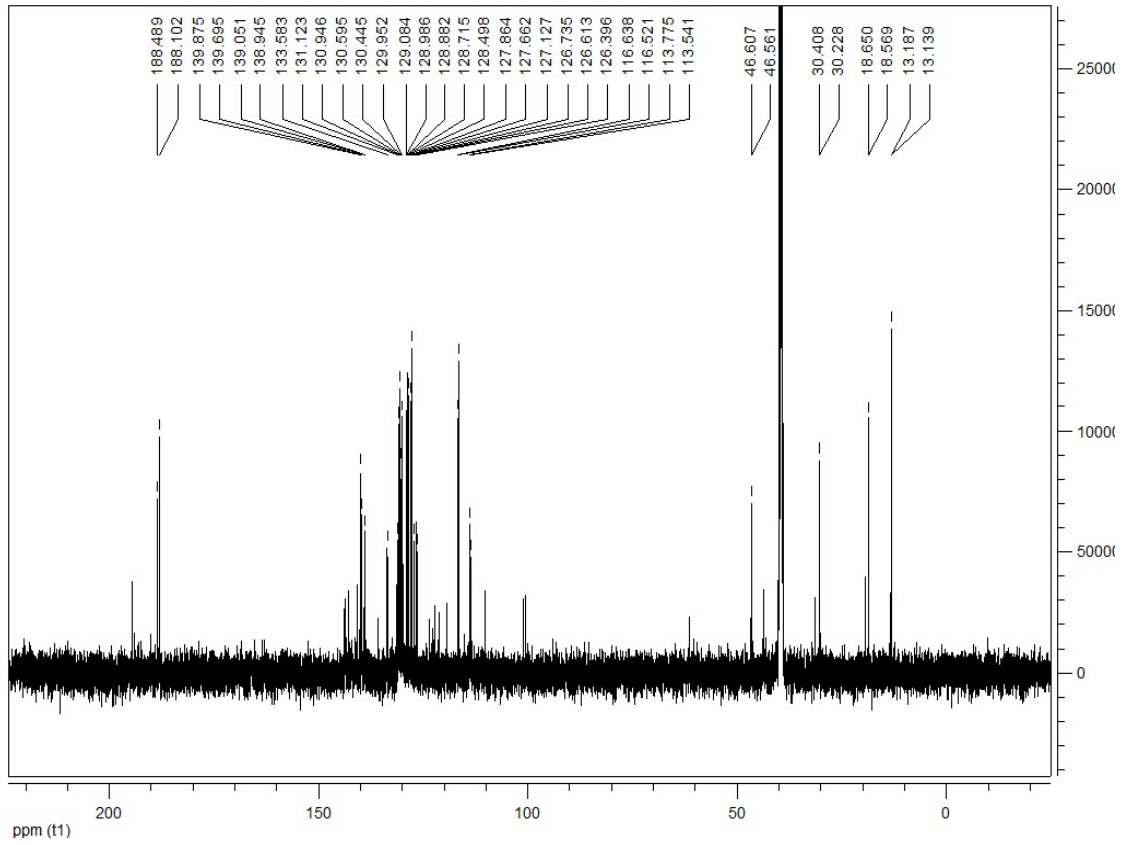
**2-(1-(4-(tert-butyl)phenyl)-2-(1-butyl-1H-benzo[d]imidazol-3-ium-3-yl)-3-(4-chlorophenyl)-3-oxopropyl)-1,3-dioxo-2,3-dihydro-1H-inden-2-ide (1e):** yellow solid, 80%, m.p. 183~185°C; <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ: A-conformation: 10.18 (s, 1H, CH), 8.17~8.13 (m, 2H, ArH), 7.97~7.95 (m, 1H, ArH), 7.82~7.80 (m, 1H, ArH), 7.62~7.58 (m, 2H, ArH), 7.46~7.45 (m, 2H, ArH), 7.39~7.36 (m, 3H, ArH), 7.09~7.08 (m, 2H, ArH), 6.99~6.96 (m, 2H, ArH), 6.90 (brs, 2H, ArH, CH), 4.71 (d, *J* = 10.6 Hz, 1H, CH), 4.58~4.53 (m, 2H, CH), 1.72~1.68 (m, 2H, CH), 1.09 (s, 9H, 3CH<sub>3</sub>), 0.98~0.93 (m, 2H, CH), 0.66 (t, *J* = 7.2 Hz, 3H, CH<sub>3</sub>); B-conformation: 10.35 (s, 1H, CH), 8.22~8.21 (m, 1H, ArH), 7.92~7.90 (m, 2H, ArH), 7.68~7.65 (m, 1H, ArH), 4.83 (d, *J* = 11.4 Hz, 1H, CH), 4.43 (brs, 2H, CH), 1.05 (s, 9H, 3CH<sub>3</sub>), 0.82 (t, *J* = 7.2 Hz, 3H, CH<sub>3</sub>). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ: 193.2, 190.4, 150.2, 143.9, 143.4, 141.4, 138.6, 135.8, 134.6, 133.8, 130.5, 129.8, 129.4, 129.2, 129.1, 128.9, 128.8, 128.3, 124.8, 124.5, 122.6, 122.1, 121.3, 119.4, 116.5, 110.3, 47.0, 43.8, 41.5, 34.2, 33.8, 31.4, 31.0, 30.4, 19.3, 18.6, 13.4, 13.2, 13.2; IR (KBr) ν: 3054, 2962, 2872, 1688, 1599, 1533, 1425, 1317, 1271, 1210, 1093, 1004, 963, 842, 726 cm<sup>-1</sup>; MS (*m/z*): HRMS (ESI) Calcd. for C<sub>39</sub>H<sub>38</sub>ClN<sub>2</sub>O<sub>3</sub> ([M+H]<sup>+</sup>): 617.2565. Found: 617.2567.



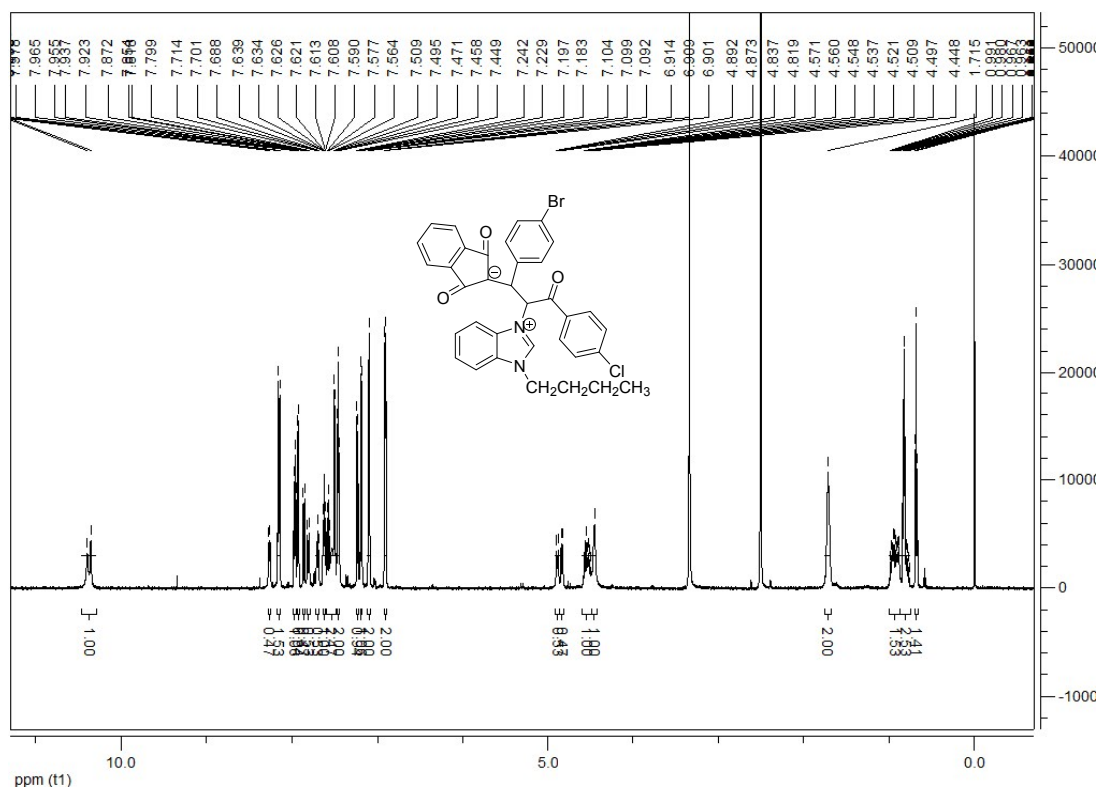


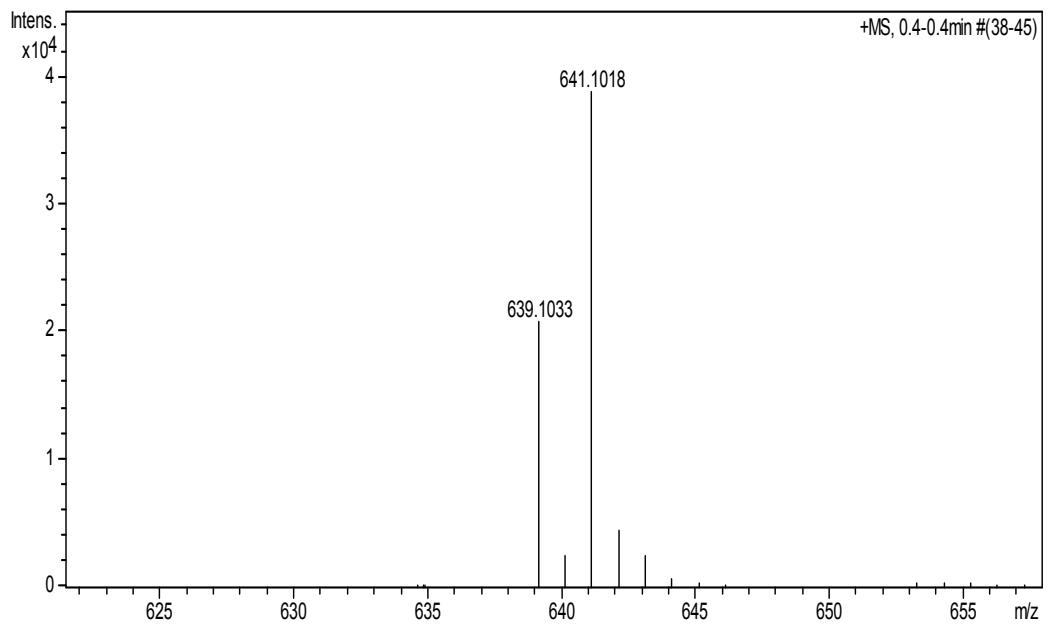
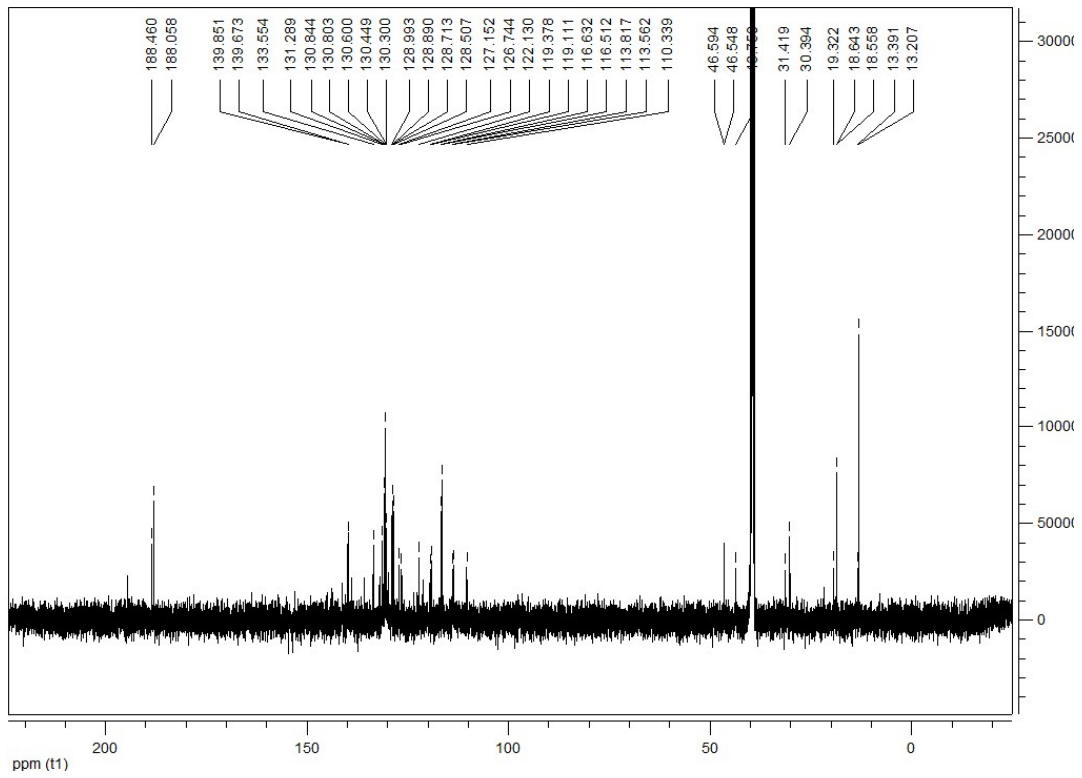
**2-(2-(1-butyl-1H-benzo[d]imidazol-3-ium-3-yl)-1,3-bis(4-chlorophenyl)-3-oxopropyl)-1,3-dioxo-2,3-dihydro-1H-inden-2-ide (**1f**):** yellow solid, 80%, m.p. 174~176°C; <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ: A-conformation: 10.40~10.35 (m, 1H, CH), 8.26 (d, *J* = 8.4 Hz, 1H, ArH), 8.17~8.14 (m, 1H, ArH), 7.98~7.93 (m, 2H, ArH), 7.82~7.80 (m, 1H, ArH), 7.64~7.56 (m, 3H, ArH), 7.54~7.50 (m, 2H, ArH), 7.46 (d, *J* = 7.8 Hz, 1H, ArH), 7.11~7.09 (m, 3H, ArH), 7.05 (d, *J* = 9.0 Hz, 1H, ArH), 6.92~6.90 (m, 2H, ArH, CH), 4.90~4.84 (m, 1H, CH), 4.57~4.45 (m, 2H, CH), 1.71 (brs, 2H, CH), 0.97~0.82 (m, 5H, CH); B-conformation: 7.88~7.86 (m, 1H, ArH), 7.71~7.69 (m, 1H, ArH), 0.68 (t, *J* = 7.2 Hz, 3H, CH<sub>3</sub>). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ: 188.5, 188.1, 139.9, 139.7, 139.0, 138.9, 133.9, 131.1, 130.9, 130.6, 130.4, 130.0, 129.1, 129.0, 128.9, 128.7, 128.5, 127.9, 127.7, 127.1, 126.7, 126.6, 126.4, 116.6, 116.5, 113.8, 113.5, 46.6, 30.4, 30.3, 18.6, 13.2, 13.1; IR (KBr) ν: 3039, 2957, 1690, 1599, 1536, 1485, 1426, 1208, 1087, 1006, 963, 825, 732 cm<sup>-1</sup>; MS (*m/z*): HRMS (ESI) Calcd. for C<sub>35</sub>H<sub>29</sub>Cl<sub>2</sub>N<sub>2</sub>O<sub>3</sub> ([M+H]<sup>+</sup>): 595.1550. Found: 595.1550.





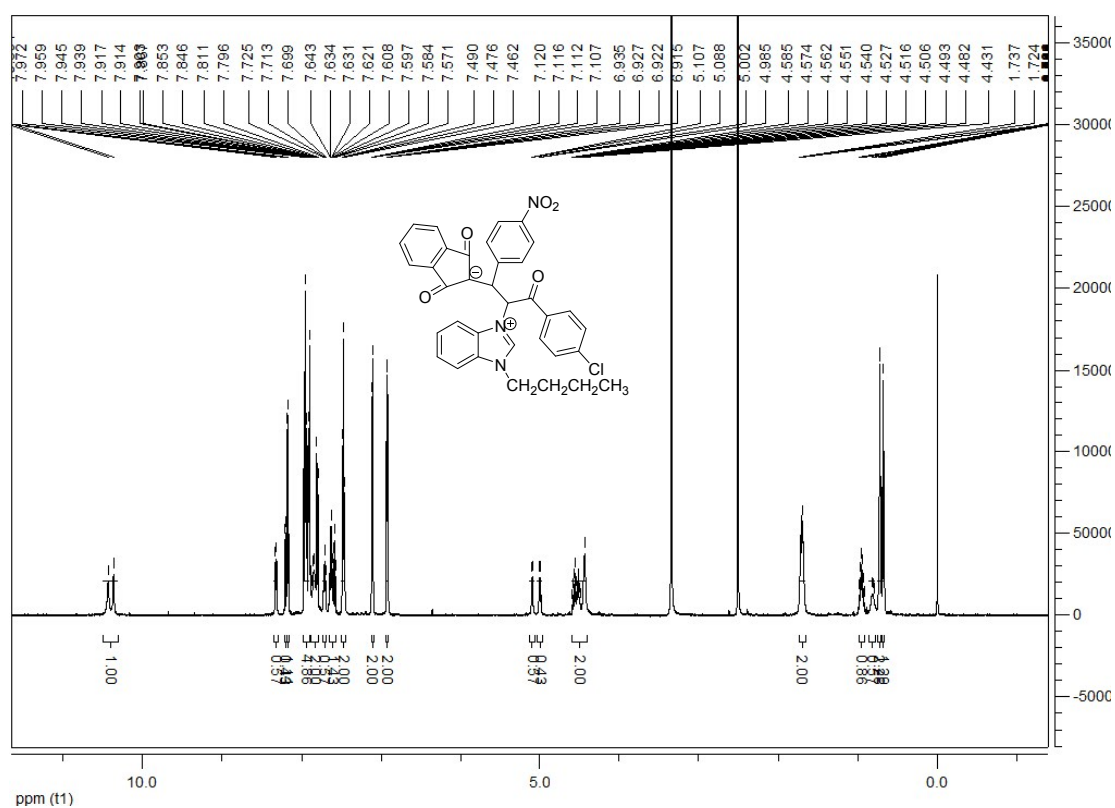
**2-(1-(4-bromophenyl)-2-(1-butyl-1H-benzo[d]imidazol-3-ium-3-yl)-3-(4-chlorophenyl)-3-oxopropyl)-1,3-dioxo-2,3-dihydro-1H-inden-2-ide (1g):** yellow solid, 90%, m.p. 194~196°C; <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ: A-conformation: 10.40~10.36 (m, 1H, CH), 8.17~8.14 (m, 2H, ArH), 7.98~7.96 (m, 2H, ArH), 7.82~7.80 (m, 1H, ArH), 7.71~7.69 (m, 1H, ArH), 7.64~7.61 (m, 1H, ArH), 7.59~7.50 (m, 2H, ArH), 7.47~7.45 (m, 2H, ArH), 7.19 (d, *J* = 8.3 Hz, 2H, ArH), 7.10~7.09 (m, 2H, ArH), 6.91~6.90 (m, 2H, ArH, CH), 4.88 (d, *J* = 11.4 Hz, 1H, CH), 4.57~4.50 (m, 1H, CH), 4.45 (brs, 1H, CH), 1.72 (brs, 2H, CH), 0.99~0.88 (m, 2H, CH), 0.80 (t, *J* = 7.2 Hz, 3H, CH<sub>3</sub>); B-conformation: δ: 8.26 (d, *J* = 8.4 Hz, 1H, ArH), 7.94~7.92 (m, 2H, ArH), 7.87~7.85 (m, 1H, ArH), 7.24 (d, *J* = 8.3 Hz, 2H, ArH), 4.83 (d, *J* = 10.8 Hz, 1H, CH), 0.68 (t, *J* = 7.2 Hz, 3H, CH<sub>3</sub>). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ: 188.5, 188.1, 139.9, 139.7, 133.6, 131.3, 130.8, 130.6, 130.4, 130.3, 129.0, 128.9, 128.7, 128.5, 127.2, 126.7, 122.1, 119.4, 119.1, 116.6, 116.5, 113.8, 113.6, 110.3, 46.6, 46.5, 43.7, 31.4, 30.4, 19.3, 18.6, 13.4, 13.2; IR (KBr) ν: 3049, 2965, 1690, 1601, 1533, 1426, 1276, 1206, 1083, 1004, 962, 857, 813, 729 cm<sup>-1</sup>; MS (*m/z*): HRMS (ESI) Calcd. for C<sub>35</sub>H<sub>29</sub>BrClN<sub>2</sub>O<sub>3</sub> ([M+H]<sup>+</sup>): 639.1045. Found: 639.1033.



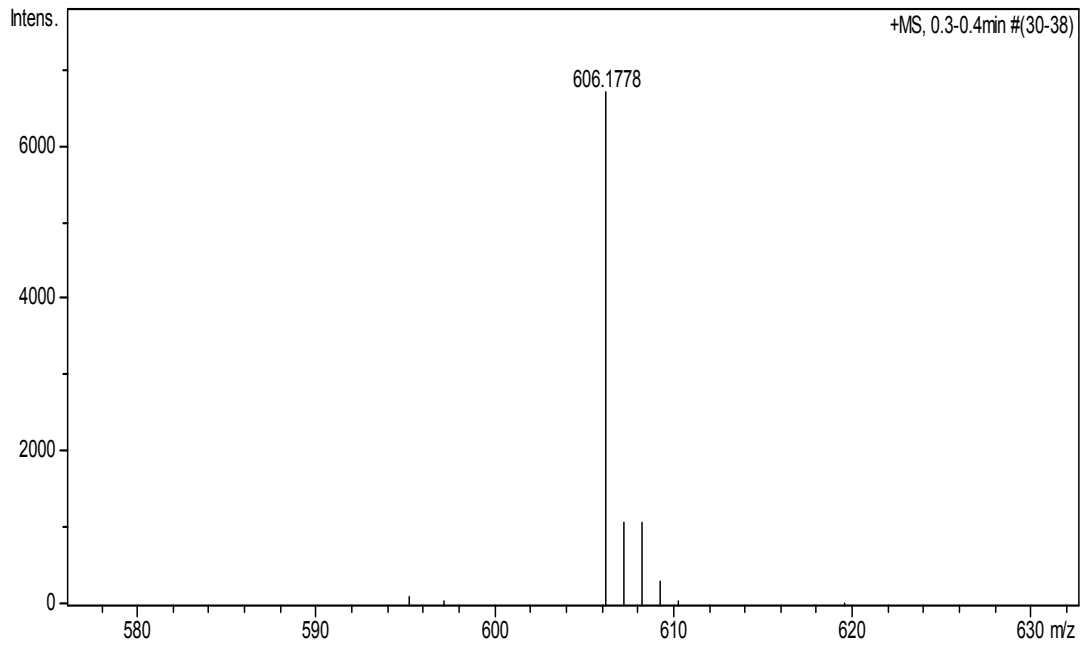
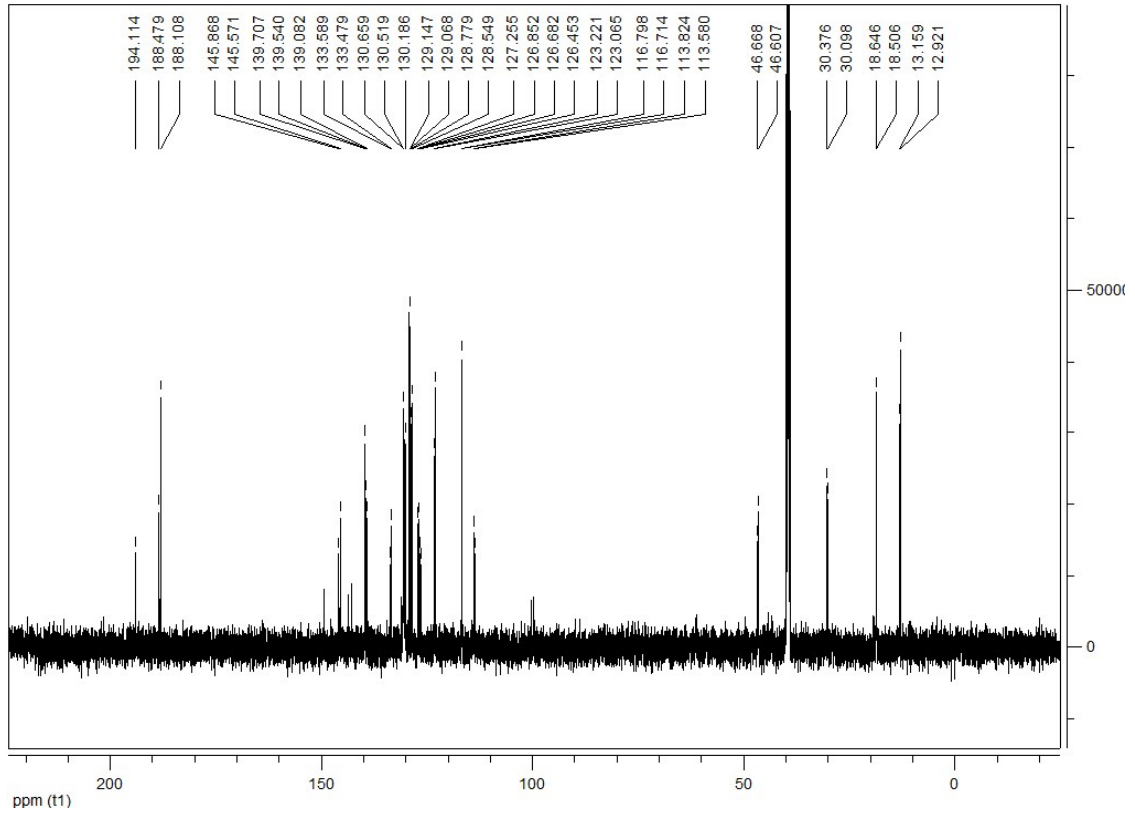


**2-(2-(1-butyl-1H-benzo[d]imidazol-3-ium-3-yl)-3-(4-chlorophenyl)-1-(4-nitrophenyl)-3-**

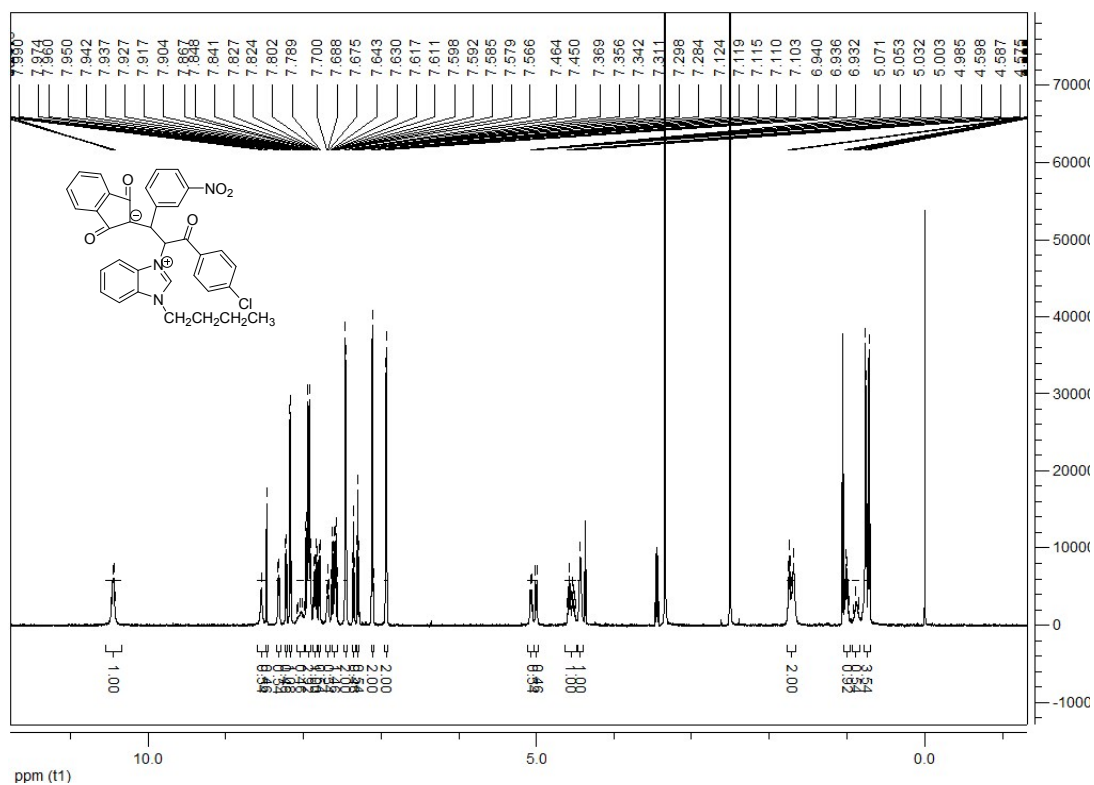
**oxopropyl)-1,3-dioxo-2,3-dihydro-1H-inden-2-ide (1h):** yellow solid, 90%, m.p. 153~155°C; <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ: A-conformation: 10.36 (s, 1H, CH), 8.32 (d, *J* = 8.4 Hz, 1H, ArH), 8.18 (d, *J* = 8.4 Hz, 2H, ArH), 7.97~7.90 (m, 4H, ArH), 7.88~7.80 (m, 2H, ArH), 7.72~7.70 (m, 1H, ArH), 7.64~7.57 (m, 1H, ArH), 7.49~7.46 (m, 2H, ArH), 7.12~7.11 (m, 2H, ArH), 6.94~6.92 (m, 2H, ArH, CH), 5.10 (d, *J* = 11.4 Hz, 1H, CH), 4.58~4.43 (m, 2H, CH), 1.74~1.69 (m, 2H, CH), 0.82~0.80 (m, 1H, CH), 0.74~0.72 (m, 4H, CH); B-conformation: δ: 10.43 (s, 1H, CH), 8.20 (d, *J* = 8.4 Hz, 1H, ArH), 4.99 (d, *J* = 10.2 Hz, 1H, CH), 0.98~0.92 (m, 2H, CH), 0.69~0.66 (m, 3H, CH<sub>3</sub>). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ: 194.1, 188.5, 188.1, 145.9, 145.6, 139.7, 139.5, 139.1, 133.6, 133.5, 130.7, 130.5, 130.2, 129.1, 128.8, 128.5, 127.3, 126.9, 126.7, 126.5, 123.2, 123.1, 116.8, 116.7, 113.8, 113.6, 46.7, 46.6, 30.4, 30.1, 18.6, 18.5, 13.2, 12.9; IR (KBr) ν: 3039, 2957, 1690, 1599, 1537, 1487, 1425, 1275, 1207, 1092, 1007, 964, 828, 731 cm<sup>-1</sup>; MS (*m/z*): HRMS (ESI) Calcd. for C<sub>35</sub>H<sub>29</sub>ClN<sub>3</sub>O<sub>5</sub> ([M+H]<sup>+</sup>): 606.1790. Found: 606.1778.

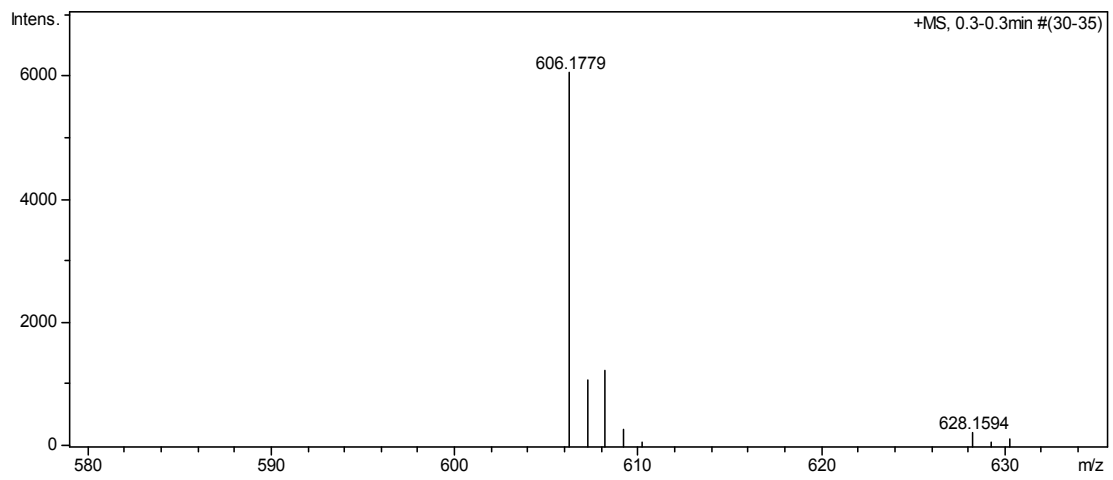
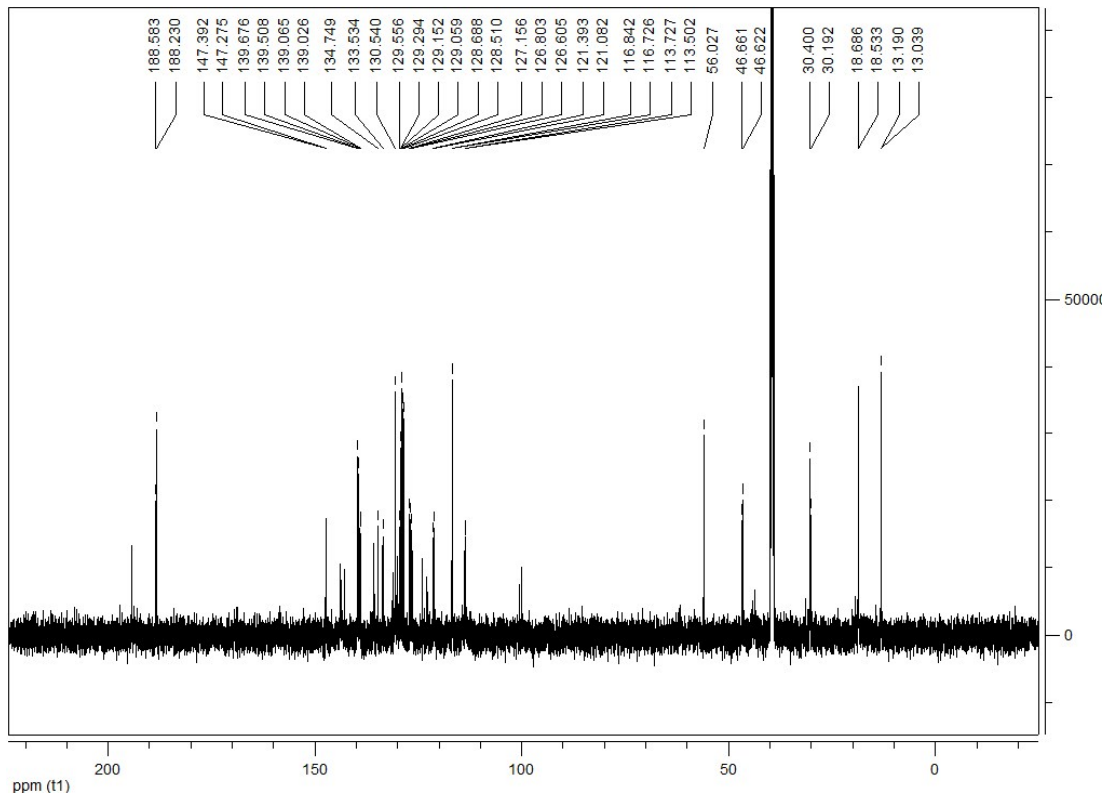




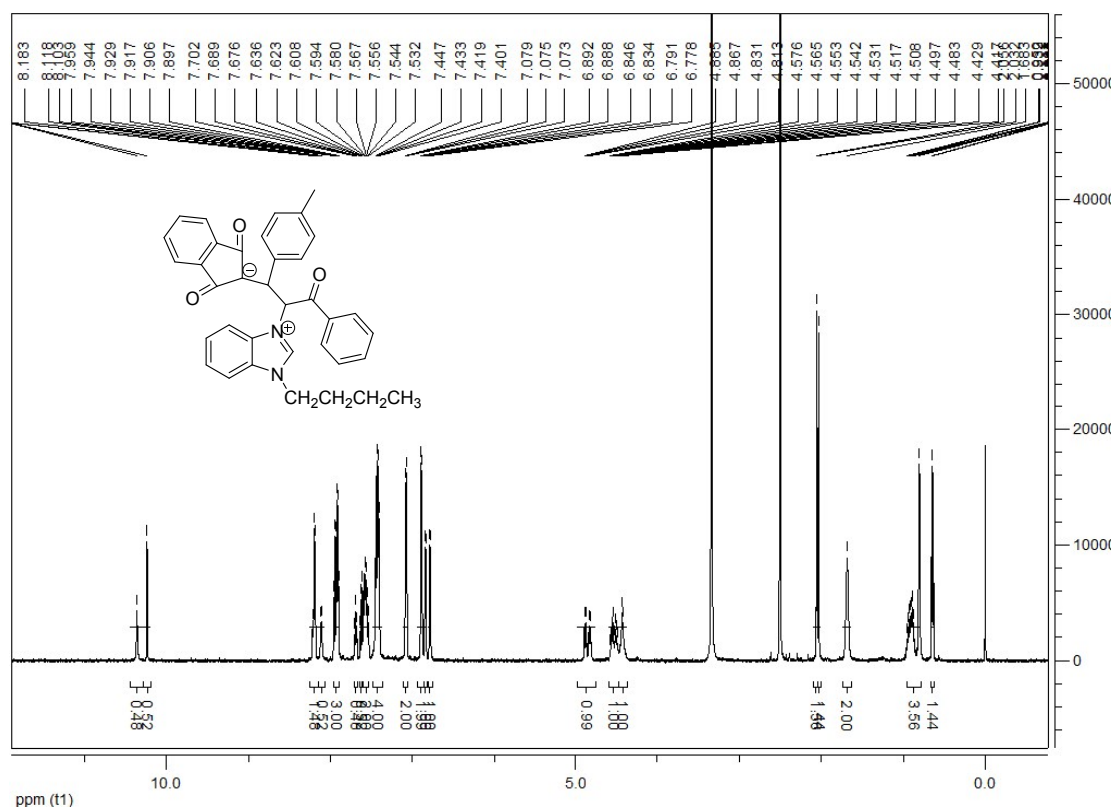


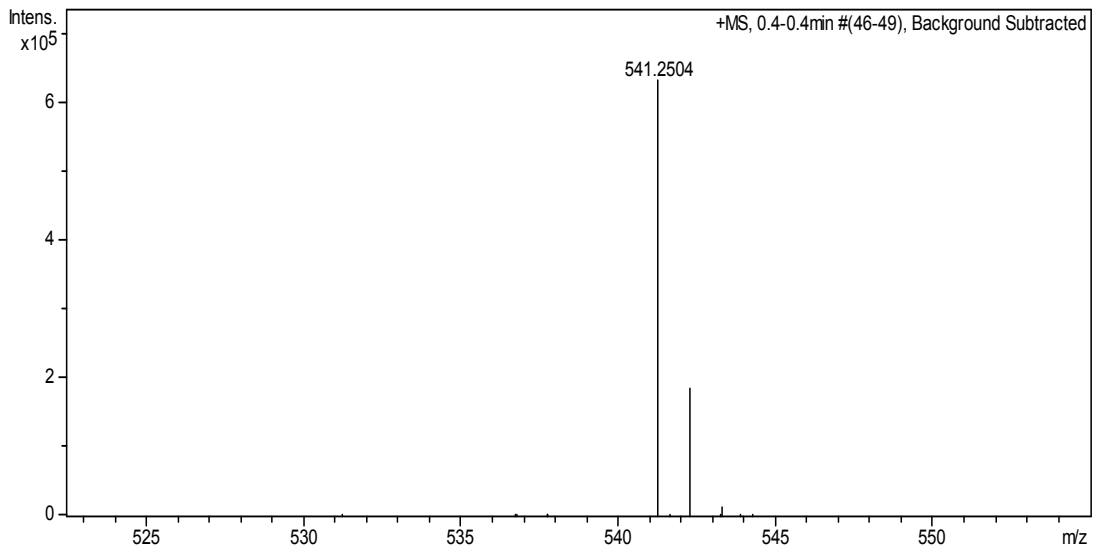
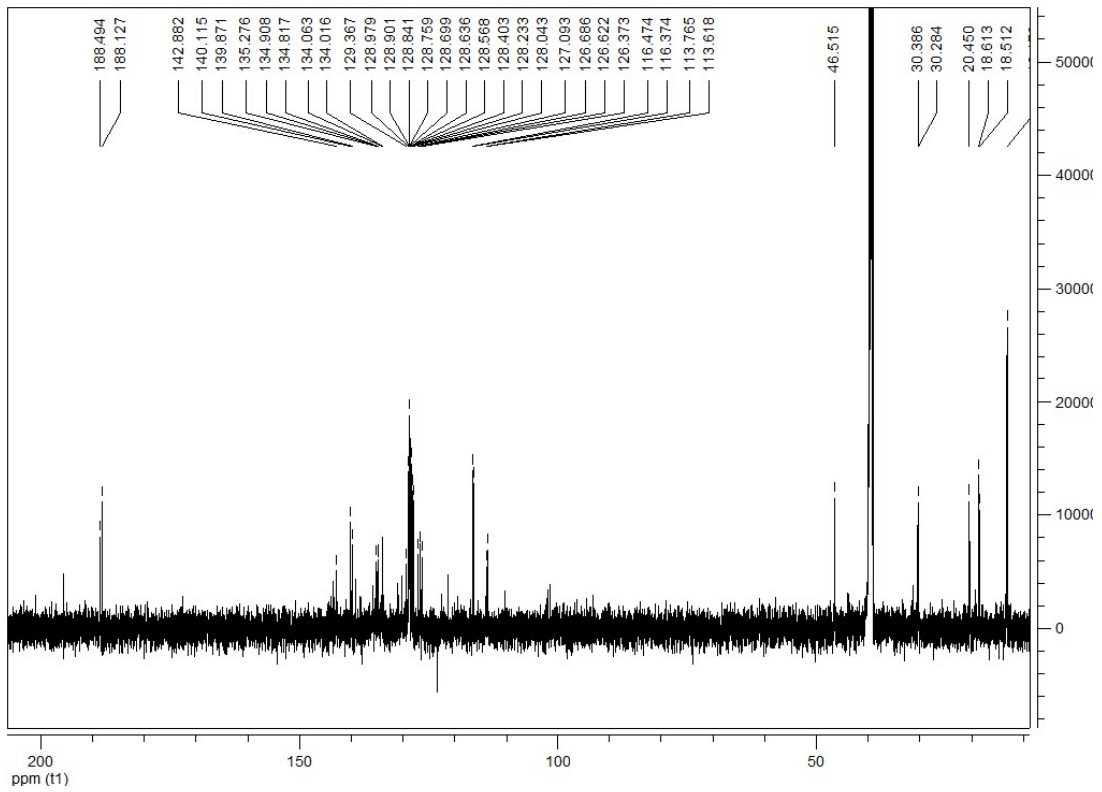
**2-(2-(1-butyl-1H-benzo[d]imidazol-3-ium-3-yl)-3-(4-chlorophenyl)-1-(3-nitrophenyl)-3-oxopropyl)-1,3-dioxo-2,3-dihydro-1H-inden-2-ide (1i):** yellow solid, 84%, m.p. 143~145°C; <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ: A-conformation: 10.47~10.42 (m, 1H, CH), 8.54 (brs, 1H, ArH), 8.32 (d, *J* = 8.4 Hz, 1H, ArH), 8.17 (d, *J* = 8.4 Hz, 2H, ArH), 7.97~7.90 (m, 2H, ArH), 7.87~7.82 (m, 1H, ArH), 7.80~7.79 (m, 1H, ArH), 7.70~7.68 (m, 1H, ArH), 7.63~7.57 (m, 1H, ArH), 7.46 (d, *J* = 8.4 Hz, 2H, ArH), 7.31~7.28 (m, 1H, ArH), 7.12~7.10 (m, 2H, ArH), 6.94~6.93 (m, 2H, ArH, CH), 5.06 (d, *J* = 10.8 Hz, 1H, CH), 4.60~4.49 (m, 1H, CH), 4.43 (brs, 1H, CH), 1.75~1.69 (m, 2H, CH), 0.92~0.85 (m, 1H, CH), 0.77~0.71 (m, 4H, CH); B-conformation: δ: 8.47 (s, 1H, ArH), 8.22 (d, *J* = 8.4 Hz, 1H, ArH), 8.09~7.99 (m, 1H, ArH), 7.37~7.34 (m, 1H, ArH), 4.99 (d, *J* = 10.8 Hz, 1H, CH), 1.03~0.97 (m, 2H, CH). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ: 188.6, 188.2, 147.4, 147.3, 139.7, 139.5, 139.1, 139.0, 134.7, 133.5, 130.5, 129.6, 129.3, 129.2, 129.1, 128.7, 128.5, 127.2, 126.8, 126.6, 121.4, 121.1, 116.8, 116.7, 113.7, 113.5, 56.0, 46.7, 46.6, 30.4, 30.2, 18.7, 18.5, 13.2, 13.1; IR (KBr) *v*: 2991, 1691, 1599, 1535, 1418, 1280, 1210, 1062, 1008, 959, 891, 853, 725 cm<sup>-1</sup>; MS (*m/z*): HRMS (ESI) Calcd. for C<sub>35</sub>H<sub>29</sub>ClN<sub>3</sub>O<sub>5</sub> ([M+H]<sup>+</sup>): 606.1790. Found: 606.1779.



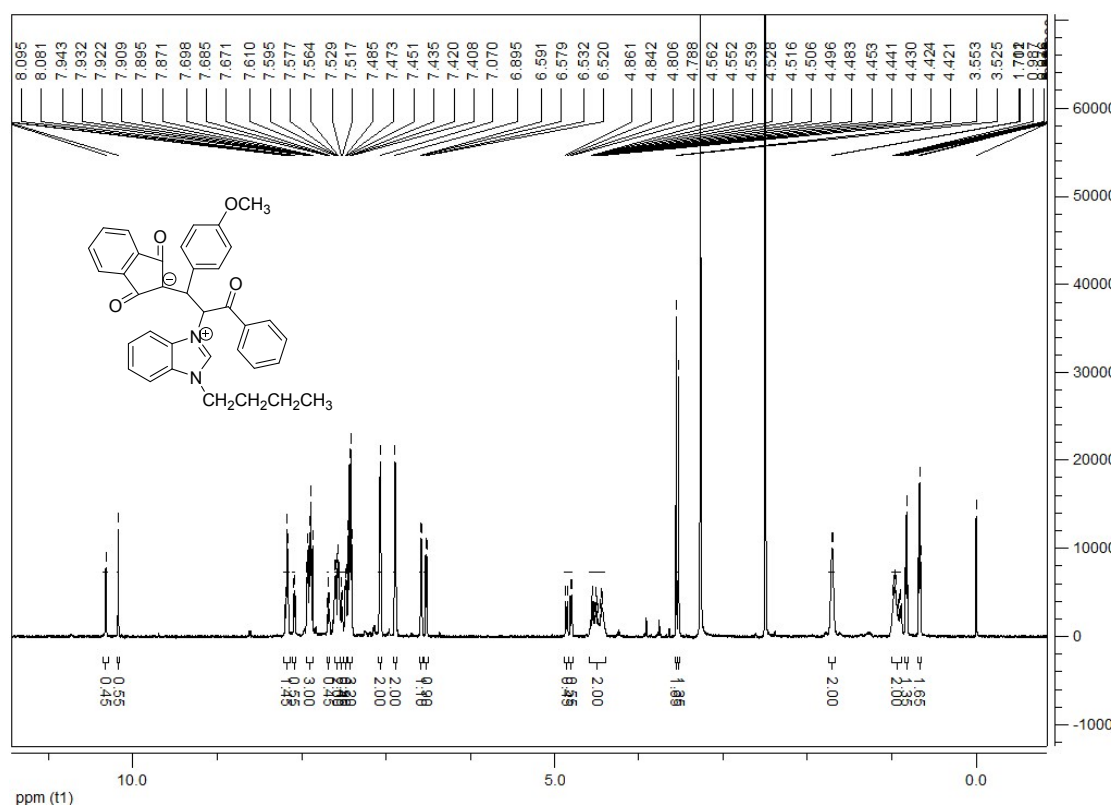


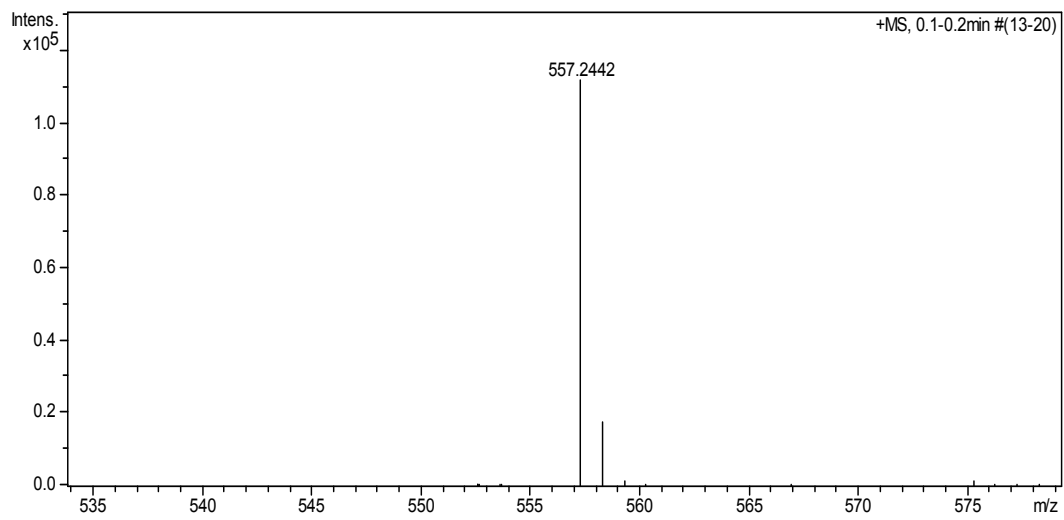
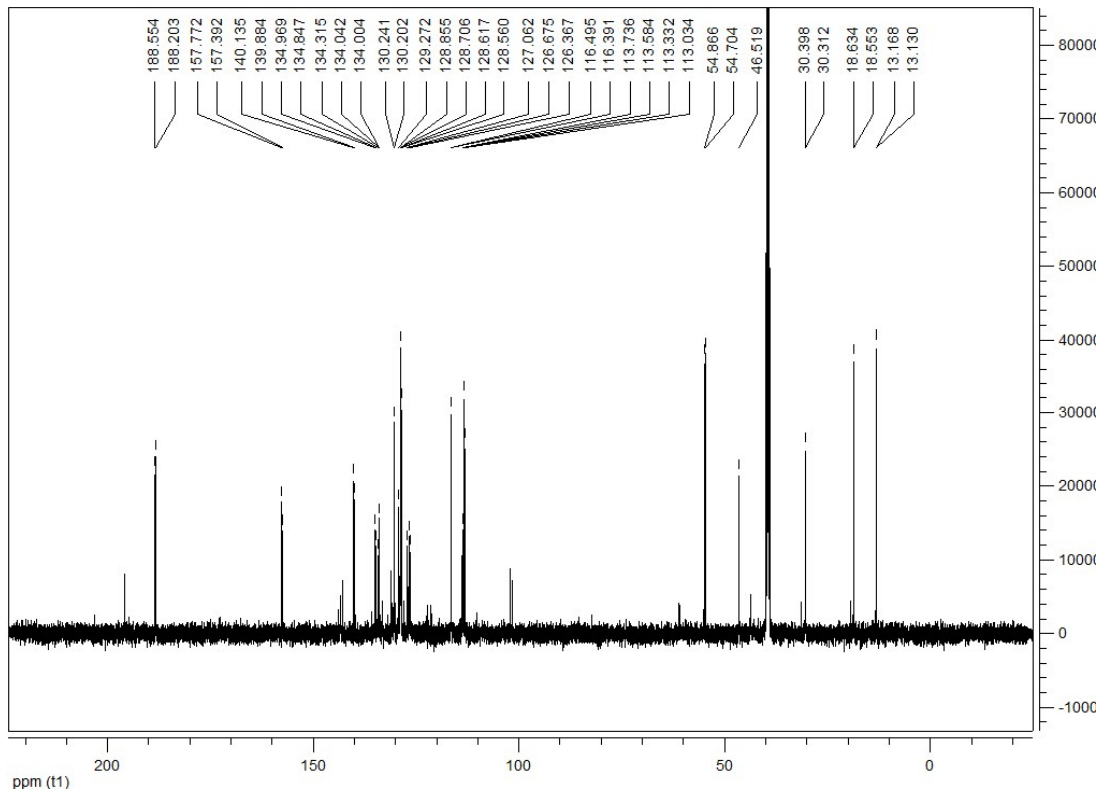
**2-(2-(1-butyl-1H-benzo[d]imidazol-3-ium-3-yl)-3-oxo-3-phenyl-1-(p-tolyl)propyl)-1,3-dioxo-2,3-dihydro-1H-inden-2-ide (1j):** yellow solid, 80%, m.p. 171~173°C; <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ: A-conformation: 10.24 (s, 1H, CH), 8.21~8.18 (m, 1H, ArH), 8.11 (d, *J* = 8.6 Hz, 1H, ArH), 7.96~7.90 (m, 3H, ArH), 7.64~7.61 (m, 1H, ArH), 7.59~7.53 (m, 2H, ArH), 7.45~7.40 (m, 4H, ArH), 7.08~7.07 (m, 2H, ArH), 6.89~6.88 (m, 2H, ArH, CH), 6.84 (d, *J* = 7.2 Hz, 1H, ArH), 6.78 (d, *J* = 7.8 Hz, 1H, ArH), 4.88~4.81 (m, 1H, CH), 4.58~4.48 (m, 1H, CH), 4.43~4.42 (m, 1H, CH), 2.06 (s, 3H, CH<sub>3</sub>), 1.68 (brs, 2H, CH), 0.95~0.80 (m, 5H, CH); B-conformation: δ: 10.36 (s, 1H, CH), 7.00~7.68 (m, 1H, ArH), 2.03 (s, 3H, CH<sub>3</sub>), 0.64 (t, *J* = 7.2 Hz, 3H, CH<sub>3</sub>). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ: 188.5, 188.1, 142.9, 140.1, 139.9, 135.3, 134.9, 134.8, 134.1, 134.0, 129.4, 129.0, 128.9, 128.8, 128.7, 128.6, 128.4, 128.2, 128.0, 127.1, 126.7, 126.6, 126.4, 116.5, 116.4, 113.8, 113.6, 46.5, 30.4, 30.3, 20.4, 18.6, 18.5, 13.2; IR (KBr) ν: 3032, 2959, 1686, 1608, 1535, 1429, 1209, 1005, 962, 827, 733 cm<sup>-1</sup>; MS (*m/z*): HRMS (ESI) Calcd. for C<sub>36</sub>H<sub>33</sub>N<sub>2</sub>O<sub>3</sub> ([M+H]<sup>+</sup>): 541.2486. Found: 541.2504.



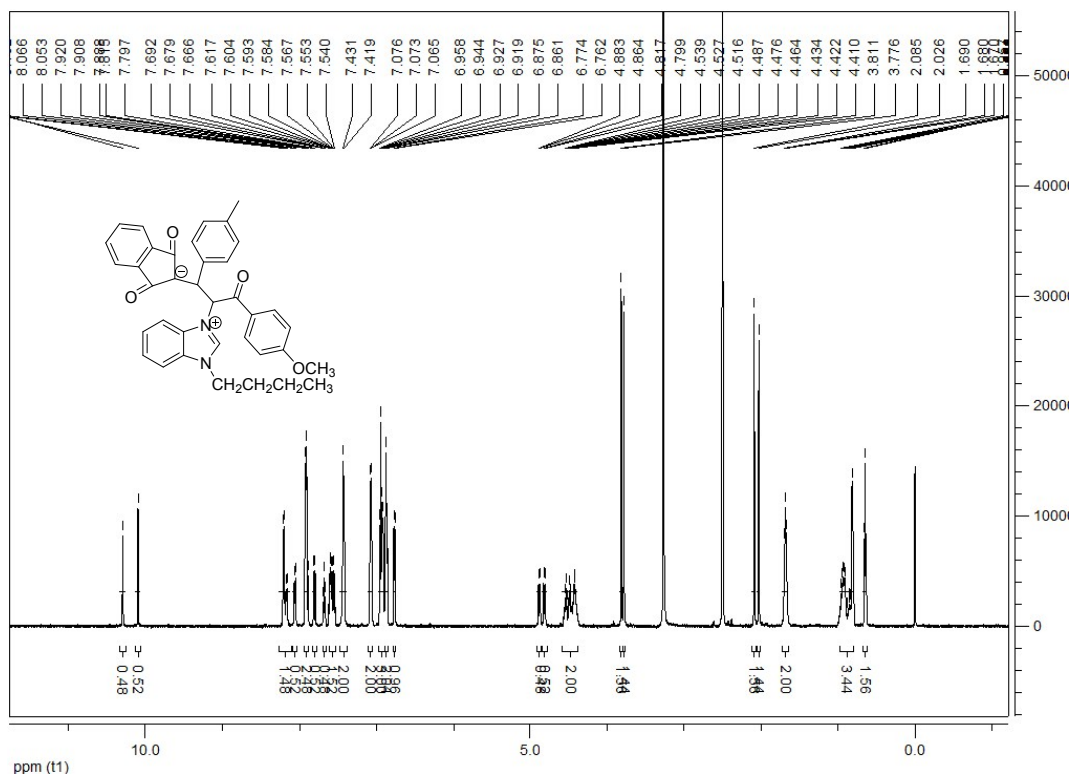


**2-(2-(1-butyl-1H-benzo[d]imidazol-3-ium-3-yl)-1-(4-methoxyphenyl)-3-oxo-3-phenylpropyl)-1,3-dioxo-2,3-dihydro-1H-inden-2-ide (1k):** yellow solid, 80%, m.p. 174~176°C;  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO-}d_6$ )  $\delta$ : A-conformation: 10.17 (s, 1H, CH), 8.19~8.16 (m, 1H, ArH), 8.09 (d,  $J = 8.4\text{Hz}$ , 1H, ArH), 7.94~7.87 (m, 3H, ArH), 7.61~7.56 (m, 2H, ArH), 7.45~7.41 (m, 5H, ArH), 7.07 (brs, 2H, ArH), 6.90 (brs, 2H, ArH, CH), 6.58 (d,  $J = 7.2\text{ Hz}$ , 2H, ArH), 4.80 (d,  $J = 10.8\text{ Hz}$ , 1H, CH), 4.56~4.42 (m, 2H, CH), 3.55 (s, 3H,  $\text{OCH}_3$ ), 1.71~1.70 (m, 2H, CH), 0.99~0.90 (m, 2H, CH), 0.67 (t,  $J = 7.2\text{ Hz}$ , 3H,  $\text{CH}_3$ ); A-conformation: 10.32 (s, 1H, CH), 7.70~7.67 (m, 1H, ArH), 7.53~7.52 (m, 1H, ArH), 7.48~7.47 (m, 2H, ArH), 6.53 (d,  $J = 7.2\text{ Hz}$ , 2H, ArH), 4.85 (d,  $J = 11.4\text{Hz}$ , 1H, CH), 3.52 (s, 3H,  $\text{OCH}_3$ ), 0.82 (t,  $J = 7.2\text{ Hz}$ , 3H,  $\text{CH}_3$ ).  $^{13}\text{C}$  NMR (150 MHz,  $\text{DMSO-}d_6$ )  $\delta$ : 188.6, 188.2, 157.8, 157.4, 140.1, 139.9, 135.0, 134.8, 134.3, 134.0, 130.2, 129.3, 128.9, 128.7, 128.6, 127.1, 126.7, 126.4, 116.5, 116.4, 113.7, 113.6, 113.3, 113.0, 54.9, 54.7, 46.5, 30.4, 30.3, 18.6, 13.2, 13.1; IR (KBr)  $\nu$ : 3032, 2958, 1684, 1607, 1535, 1426, 1249, 1209, 1177, 1037, 964, 840, 729  $\text{cm}^{-1}$ ; MS ( $m/z$ ): HRMS (ESI) Calcd. for  $\text{C}_{36}\text{H}_{33}\text{N}_2\text{O}_4$  ( $[\text{M}+\text{H}]^+$ ): 557.2435. Found: 557.2442.

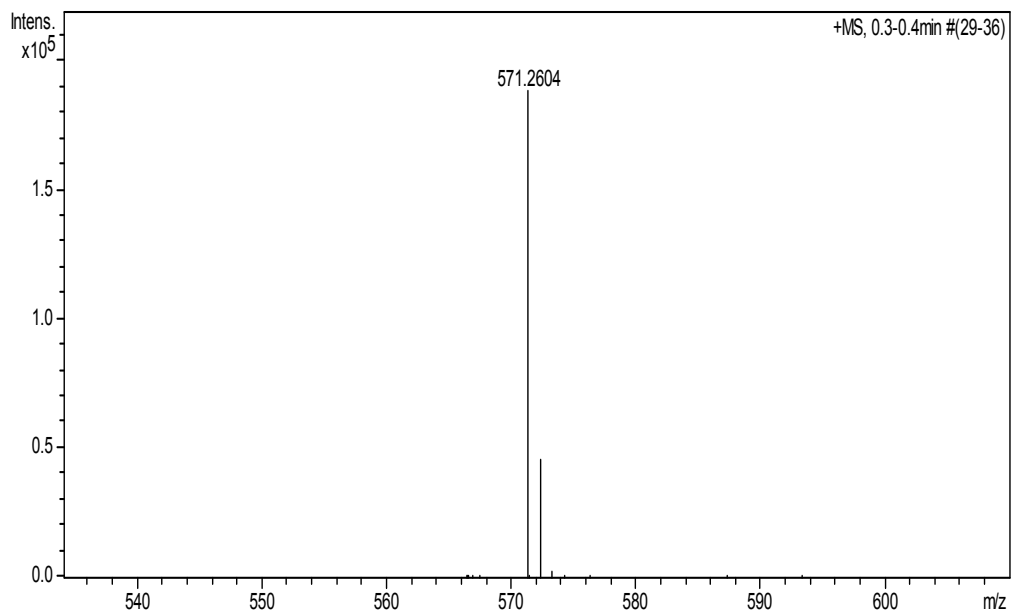
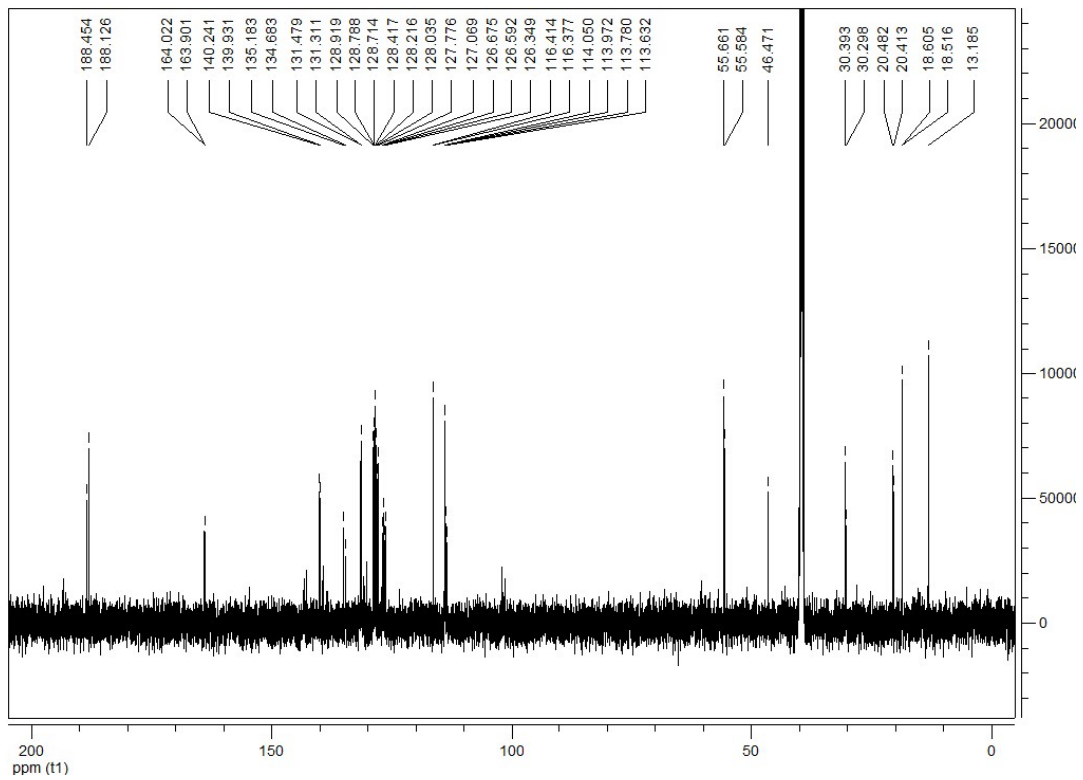




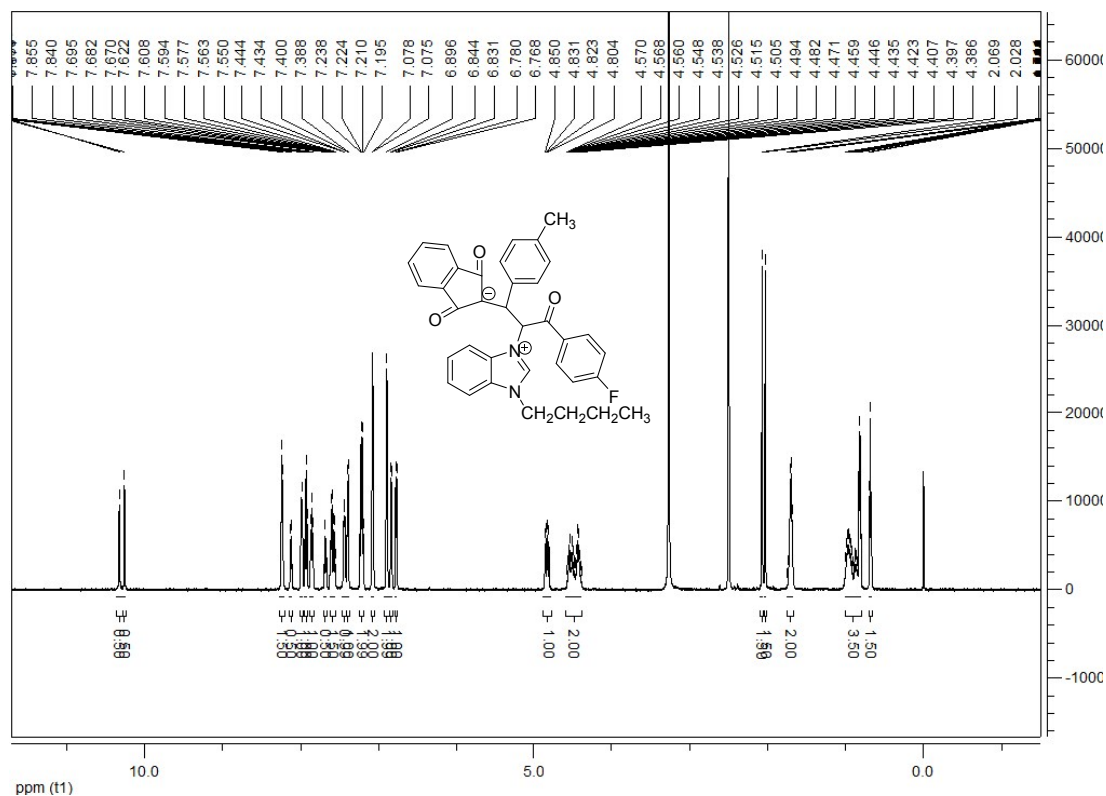
**2-(2-(1-butyl-1H-benzo[d]imidazol-3-ium-3-yl)-3-(4-methoxyphenyl)-3-oxo-1-(p-tolyl)propyl)-1,3-dioxo-2,3-dihydro-1H-inden-2-ide (11)**: yellow solid, 80%, m.p. 177~179°C; <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ: A-conformation: 10.10 (s, 1H, CH), 8.21~8.16 (m, 1H, ArH), 8.06 (d, *J* = 7.8 Hz, 1H, ArH), 7.92~7.89 (m, 2H, ArH), 7.82~7.80 (m, 1H, ArH), 7.62~7.54 (m, 2H, ArH), 7.43~7.42 (m, 2H, ArH), 7.08~7.07 (m, 2H, ArH), 6.96~6.92 (m, 3H, ArH), 6.88~6.86 (m, 3H, ArH, CH), 4.81 (d, *J* = 10.8 Hz, 1H, CH), 4.54~4.41 (m, 2H, CH), 3.81 (s, 3H, OCH<sub>3</sub>), 2.08 (s, 3H, CH<sub>3</sub>), 1.69~1.67 (m, 2H, CH), 0.96~0.80 (m, 2H, CH), 0.64 (t, *J* = 7.2 Hz, 3H, CH<sub>3</sub>); B-conformation: 10.29 (s, 1H, CH), 7.69~7.67 (m, 1H, ArH), 6.77 (d, *J* = 7.2 Hz, 2H, CH), 4.87 (d, *J* = 11.4 Hz, 1H, CH), 3.78 (s, 3H, OCH<sub>3</sub>), 2.03 (s, 3H, CH<sub>3</sub>). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ: 188.5, 188.1, 164.0, 163.9, 140.2, 139.9, 135.2, 134.7, 131.5, 131.3, 128.9, 128.8, 128.7, 128.4, 128.2, 128.0, 127.8, 127.1, 126.7, 126.6, 126.3, 116.4, 114.0, 113.8, 113.6, 55.7, 55.6, 46.5, 30.4, 30.3, 20.5, 20.4, 18.6, 18.5, 13.2; IR (KBr) ν: 3026, 2958, 1674, 1601, 1534, 1424, 1317, 1270, 1208, 1171, 1021, 962, 828, 732 cm<sup>-1</sup>; MS (*m/z*): HRMS (ESI) Calcd. for C<sub>37</sub>H<sub>35</sub>N<sub>2</sub>O<sub>4</sub> ([M+H]<sup>+</sup>): 571.2591. Found: 571.2604.

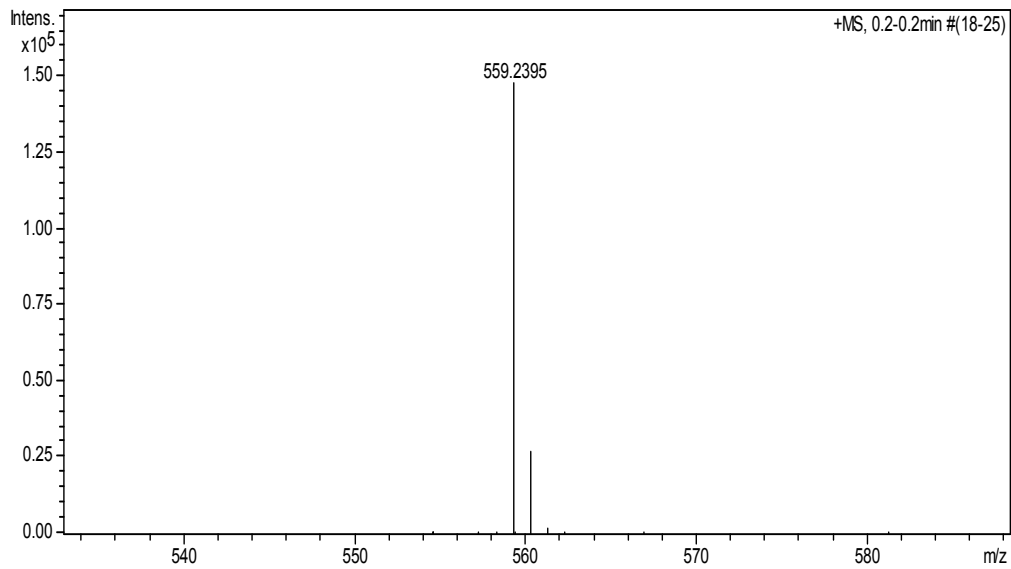
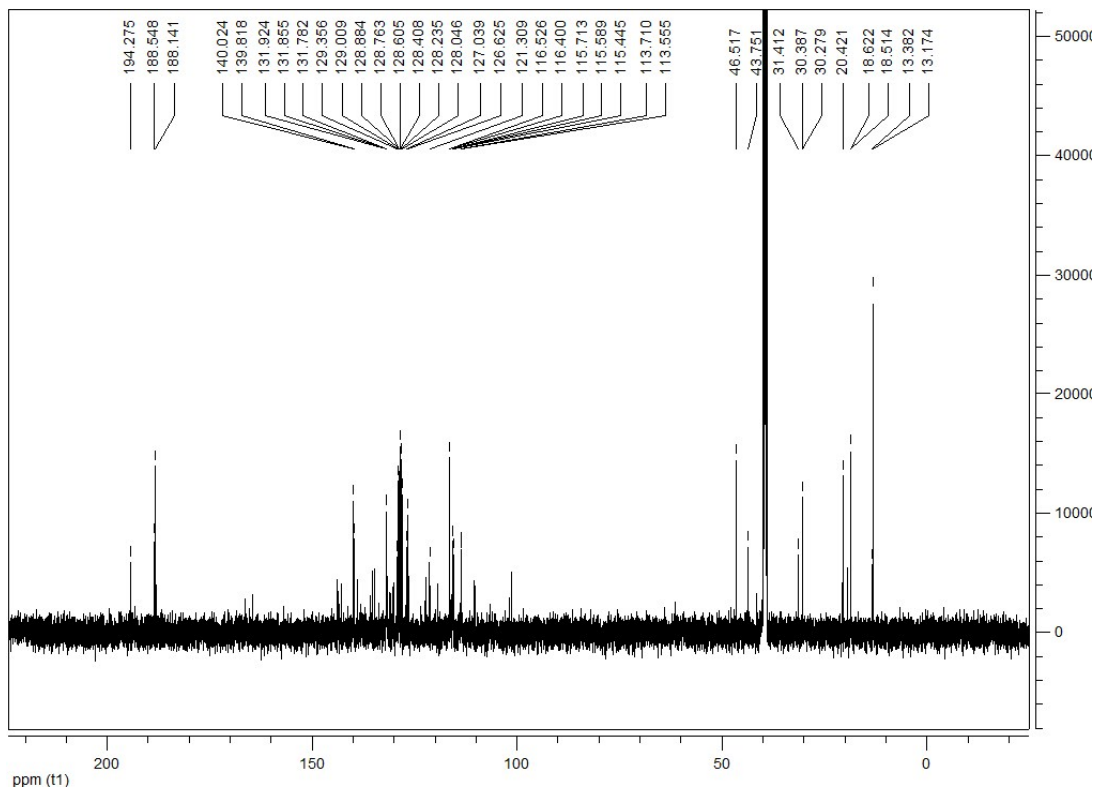




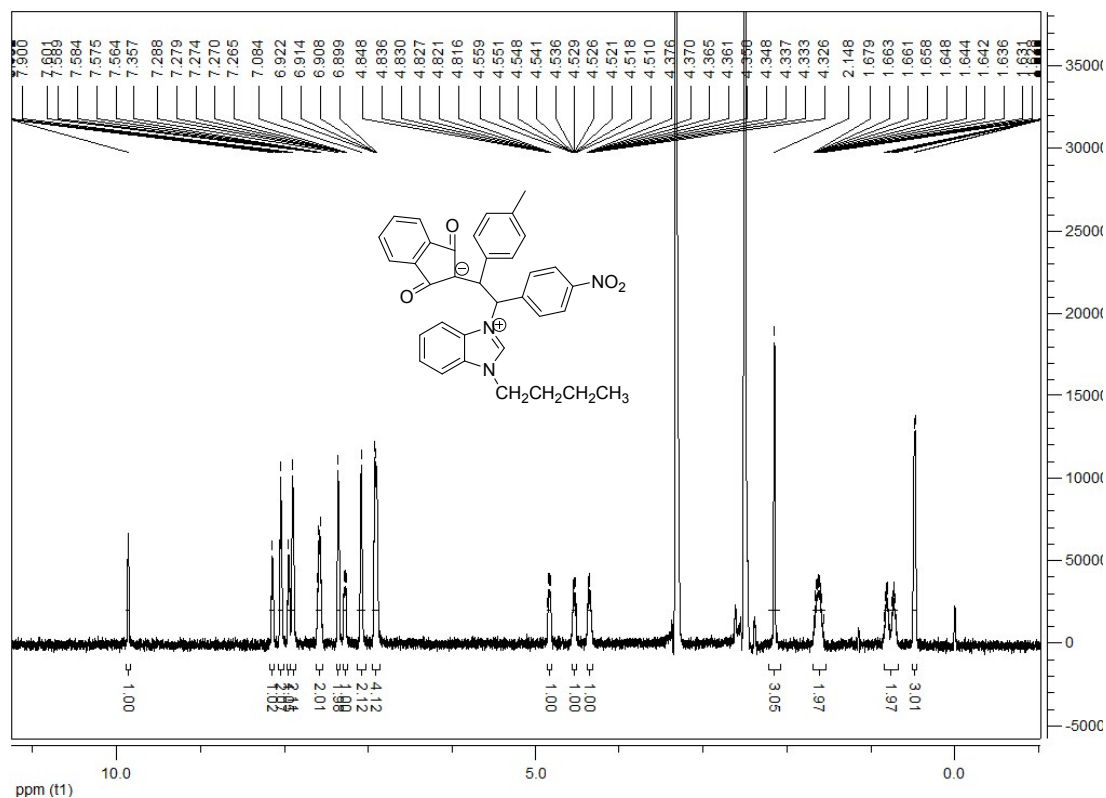


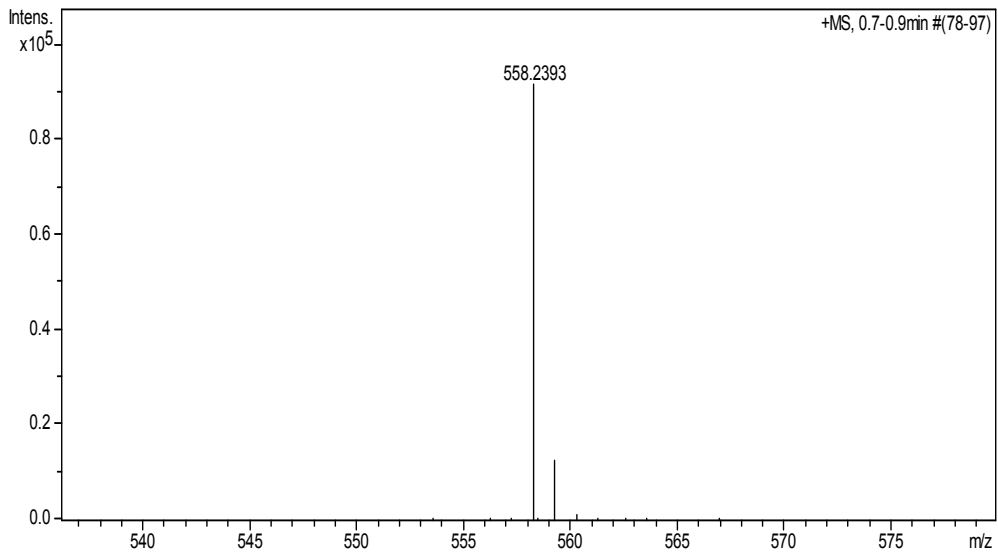
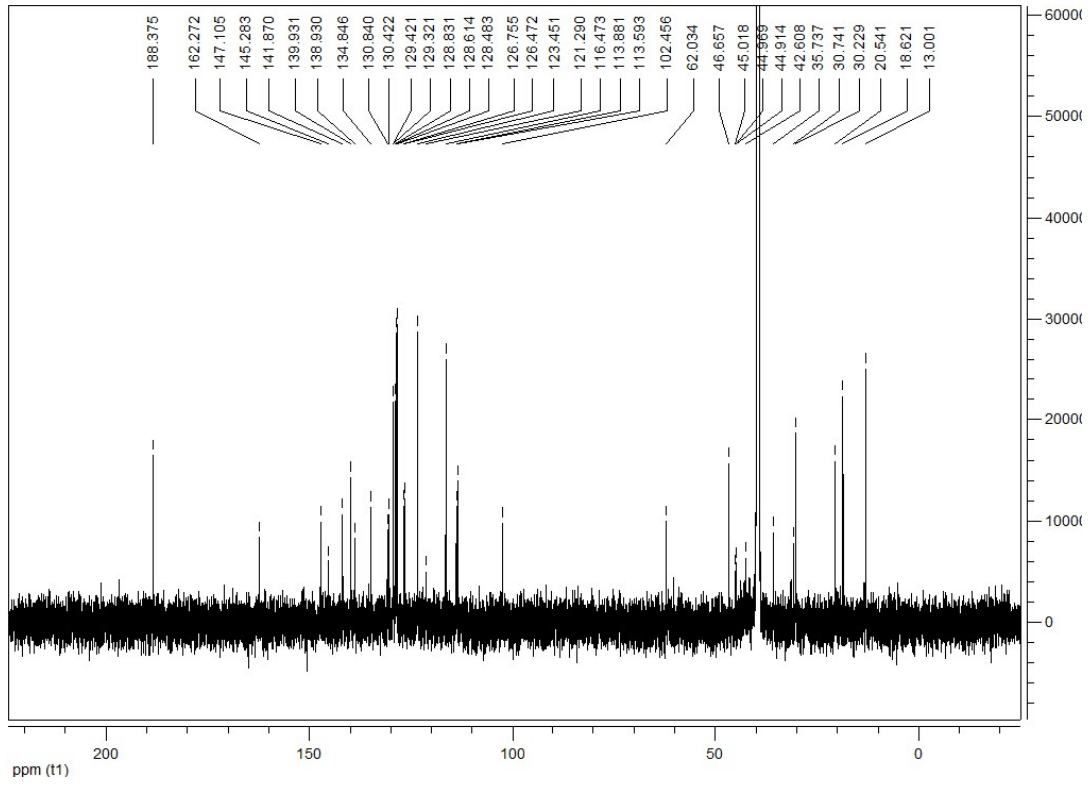
**2-(2-(1-butyl-1H-benzo[d]imidazol-3-ium-3-yl)-3-(4-fluorophenyl)-3-oxo-1-(p-tolyl)propyl)-1,3-dioxo-2,3-dihydro-1H-inden-2-ide (1m):** yellow solid, 85%, m.p. 183~185°C;  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO-}d_6$ )  $\delta$ : A-conformation: 10.26 (s, 1H, CH), 8.24~8.23 (m, 2H, ArH), 8.00~7.98 (m, 1H, ArH), 7.94~7.92 (m, 1H, ArH), 7.87~7.84 (m, 1H, ArH), 7.62~7.55 (m, 2H, ArH), 7.44 (d,  $J = 6.0\text{Hz}$ , 1H, ArH), 7.39 (d,  $J = 7.2\text{ Hz}$ , 1H, ArH), 7.24~7.20 (m, 2H, ArH), 7.08 (brs, 2H, ArH), 6.90 (brs, 2H, ArH, CH), 6.84 (d,  $J = 7.8\text{ Hz}$ , 1H, ArH), 6.77 (d,  $J = 7.2\text{ Hz}$ , 1H, ArH), 4.85~4.80 (m, 1H, CH), 4.57~4.39 (m, 2H, CH), 2.07 (s, 3H,  $\text{CH}_3$ ), 1.74~1.66 (m, 2H, CH), 1.00~0.80 (m, 5H, CH); B-conformation:  $\delta$ : 10.32 (s, 1H, CH), 8.12 (d,  $J = 8.4\text{ Hz}$ , 1H, ArH), 7.70~7.67 (m, 1H, ArH), 2.03 (s, 3H,  $\text{CH}_3$ ), 0.68 (t,  $J = 7.2\text{ Hz}$ , 3H,  $\text{CH}_3$ ).  $^{13}\text{C}$  NMR (150 MHz,  $\text{DMSO-}d_6$ )  $\delta$ : 194.3, 188.5, 188.2, 140.0, 139.8, 131.9, 131.8, 129.4, 129.0, 128.9, 128.8, 128.6, 128.4, 128.2, 128.0, 127.0, 126.6, 121.3, 116.5, 116.4, 115.7, 115.6, 115.4, 113.7, 113.6, 46.5, 43.7, 31.4, 30.4, 30.3, 20.4, 18.6, 18.5, 13.4, 13.2; IR (KBr)  $\nu$ : 3036, 2959, 1689, 1603, 1536, 1425, 1276, 1237, 1210, 1161, 964, 828, 731  $\text{cm}^{-1}$ ; MS ( $m/z$ ): HRMS (ESI) Calcd. for  $\text{C}_{36}\text{H}_{32}\text{FN}_2\text{O}_3$  ( $[\text{M}+\text{H}]^+$ ): 559.2391. Found: 559.2395.





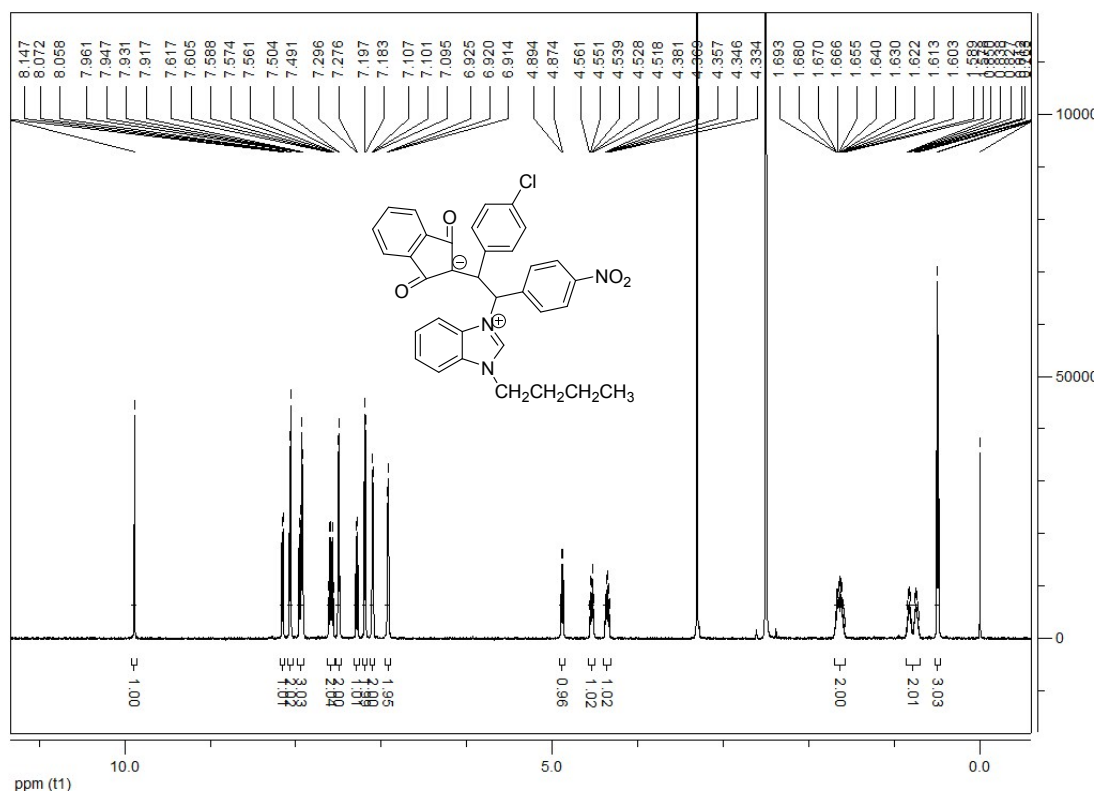
**2-(2-(1-butyl-1H-benzo[d]imidazol-3-ium-3-yl)-2-(4-nitrophenyl)-1-(p-tolyl)ethyl)-1,3-dioxo-2,3-dihydro-1H-inden-2-ide (2a):** yellow solid, 65%, m.p. 210~212°C; <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ: 9.86 (s, 1H, CH), 8.15~8.13 (m, 1H, ArH), 8.05~8.03 (m, 2H, ArH), 7.96~7.94 (m, 1H, ArH), 7.90 (brs, 2H, ArH), 7.60~7.56 (m, 2H, ArH), 7.36 (brs, 2H, ArH), 7.29~7.26 (m, 1H, CH), 7.08 (s, 2H, ArH), 6.92~6.90 (m, 4H, ArH, CH), 4.85~4.82 (m, 1H, CH), 4.56~4.51 (m, 1H, CH), 4.38~4.33 (m, 1H, CH), 2.15 (brs, 3H, CH<sub>3</sub>), 1.68~1.57 (m, 2H, CH), 0.84~0.69 (m, 2H, CH), 0.48~0.47 (m, 3H, CH<sub>3</sub>); <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ: 188.4, 162.3, 147.1, 145.3, 141.9, 139.9, 138.9, 134.8, 130.8, 130.4, 129.4, 129.3, 128.8, 128.6, 128.5, 126.8, 126.5, 123.4, 121.3, 116.5, 113.9, 113.6, 102.5, 62.0, 46.7, 45.0, 42.6, 35.7, 30.7, 30.2, 20.5, 18.6, 13.0; IR (KBr) ν: 2960, 2780, 1607, 1527, 1431, 1345, 1255, 1182, 1118, 1010, 964, 886, 821, 725 cm<sup>-1</sup>; MS (*m/z*): HRMS (ESI) Calcd. for C<sub>35</sub>H<sub>32</sub>N<sub>3</sub>O<sub>4</sub> ([M+H]<sup>+</sup>): 558.2387. Found: 558.2393.

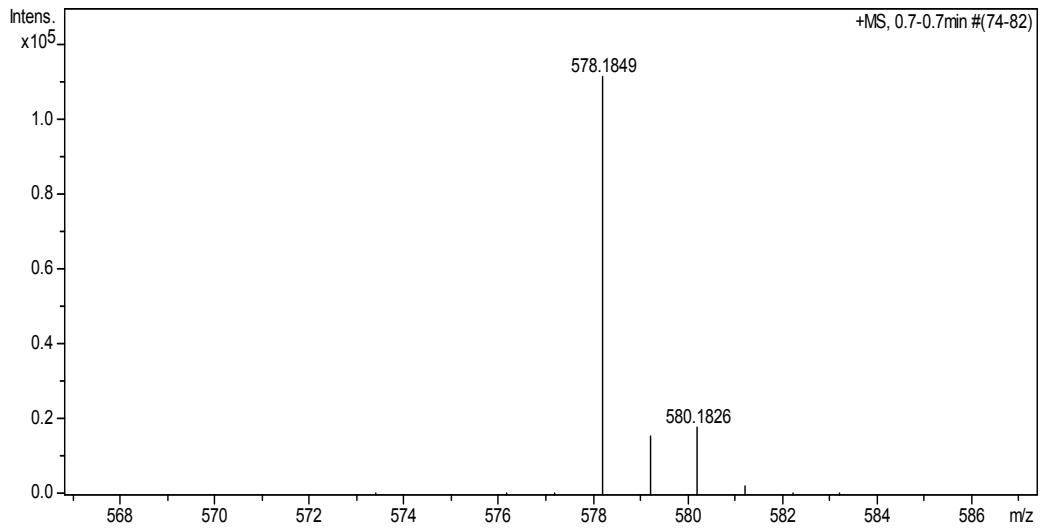
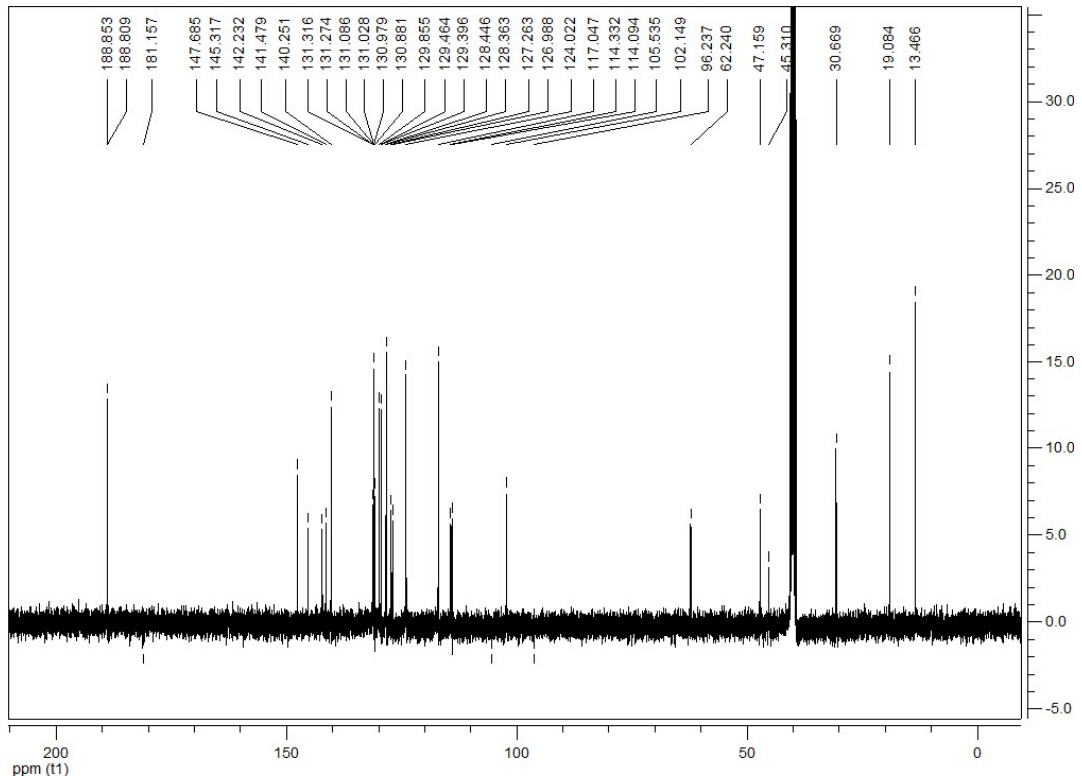




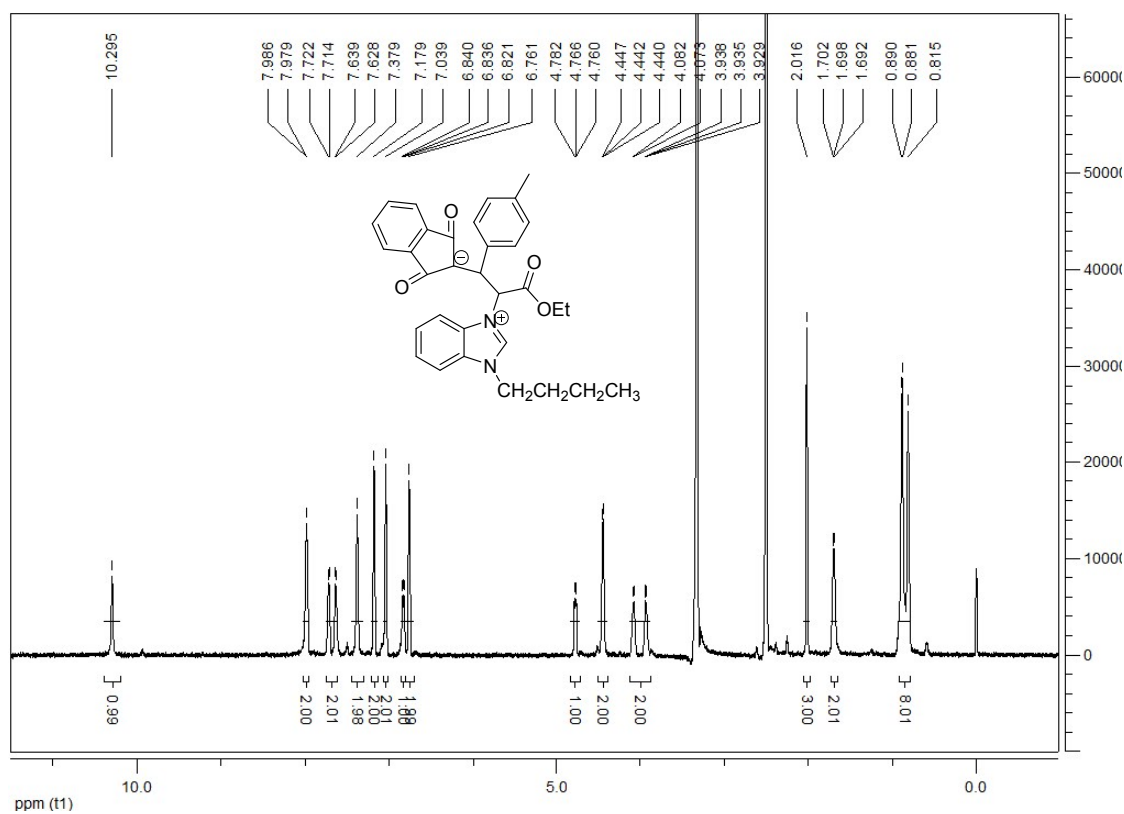
**2-(2-(1-butyl-1H-benzo[d]imidazol-3-ium-3-yl)-1-(4-chlorophenyl)-2-(4-nitrophenyl)ethyl)-**

**1,3-dioxo-2,3-dihydro-1H-inden-2-ide (2b):** yellow solid, 70%, m.p. 225~227°C; <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ: 9.88 (s, 1H, CH), 8.15 (d, *J* = 7.8 Hz, 1H, ArH), 8.07~8.06 (m, 2H, ArH), 7.96~7.92 (m, 3H, ArH), 7.62~7.56 (m, 2H, ArH), 7.50 (d, *J* = 7.8 Hz, 2H, ArH), 7.30~7.29 (m, 1H, ArH), 7.19 (d, *J* = 8.4 Hz, 2H, ArH), 7.11~7.10 (m, 2H, ArH), 6.92~6.91 (m, 2H, ArH, CH), 4.88 (d, *J* = 11.9 Hz, 1H, CH), 4.56~4.52 (m, 1H, CH), 4.38~4.33 (m, 1H, CH), 1.69~1.58 (m, 2H, CH), 0.85~0.72 (m, 2H, CH), 0.49 (t, *J* = 7.2 Hz, 3H, CH<sub>3</sub>); <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>) δ: 188.9, 188.8, 181.2, 147.7, 145.3, 142.2, 141.5, 140.2, 131.3, 131.1, 131.0, 130.9, 129.9, 129.5, 129.4, 128.4, 128.4, 127.3, 127.0, 124.0, 117.0, 114.3, 114.1, 105.5, 102.1, 96.2, 62.2, 47.2, 45.3, 30.7, 19.1, 13.5; IR (KBr) ν: 3055, 2958, 2870, 1608, 1531, 1427, 1345, 1258, 1189, 1099, 1015, 963, 862, 817, 733 cm<sup>-1</sup>; MS (*m/z*): HRMS (ESI) Calcd. for C<sub>34</sub>H<sub>29</sub>ClN<sub>3</sub>O<sub>4</sub> ([M+H]<sup>+</sup>): 578.1841. Found: 578.1849.

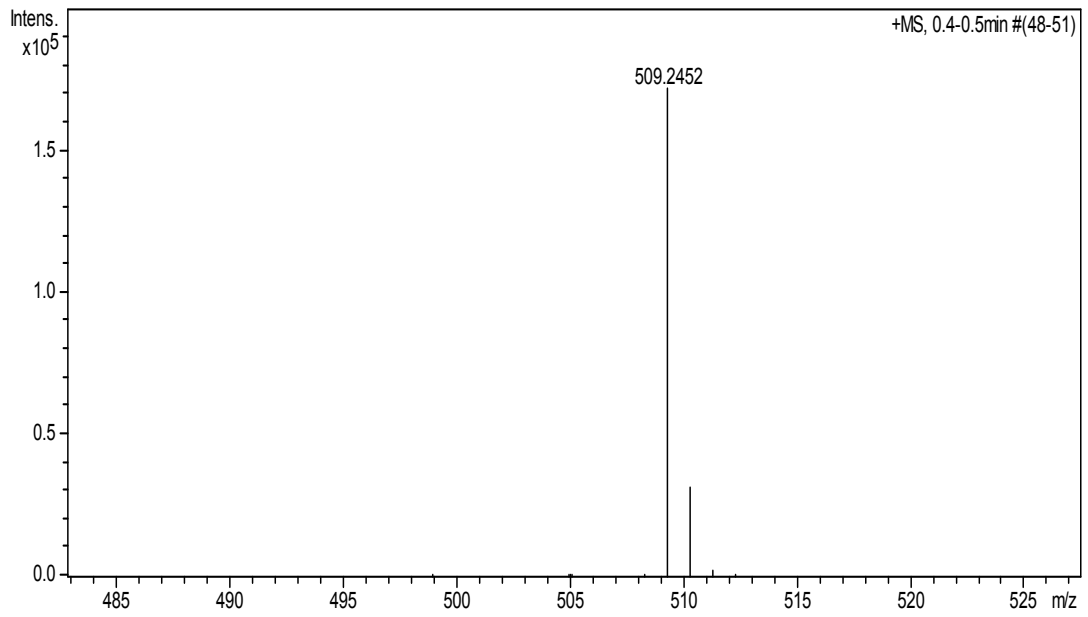
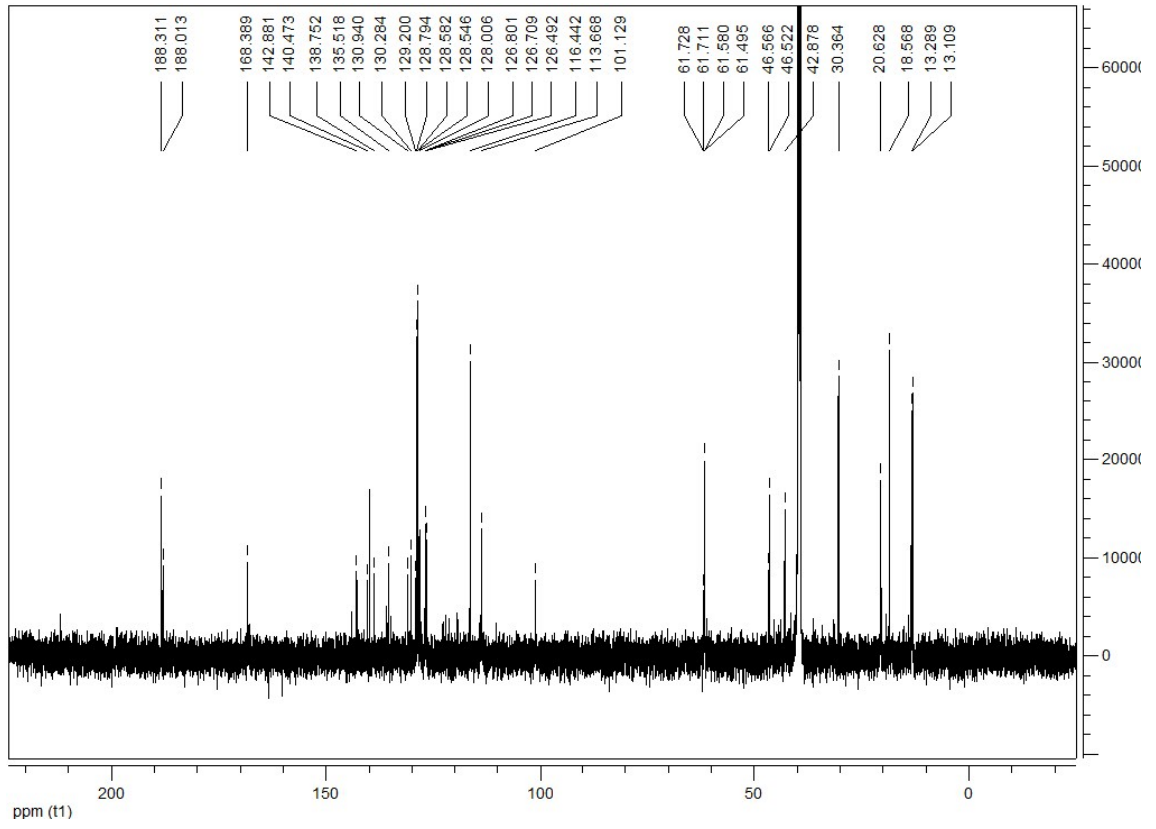




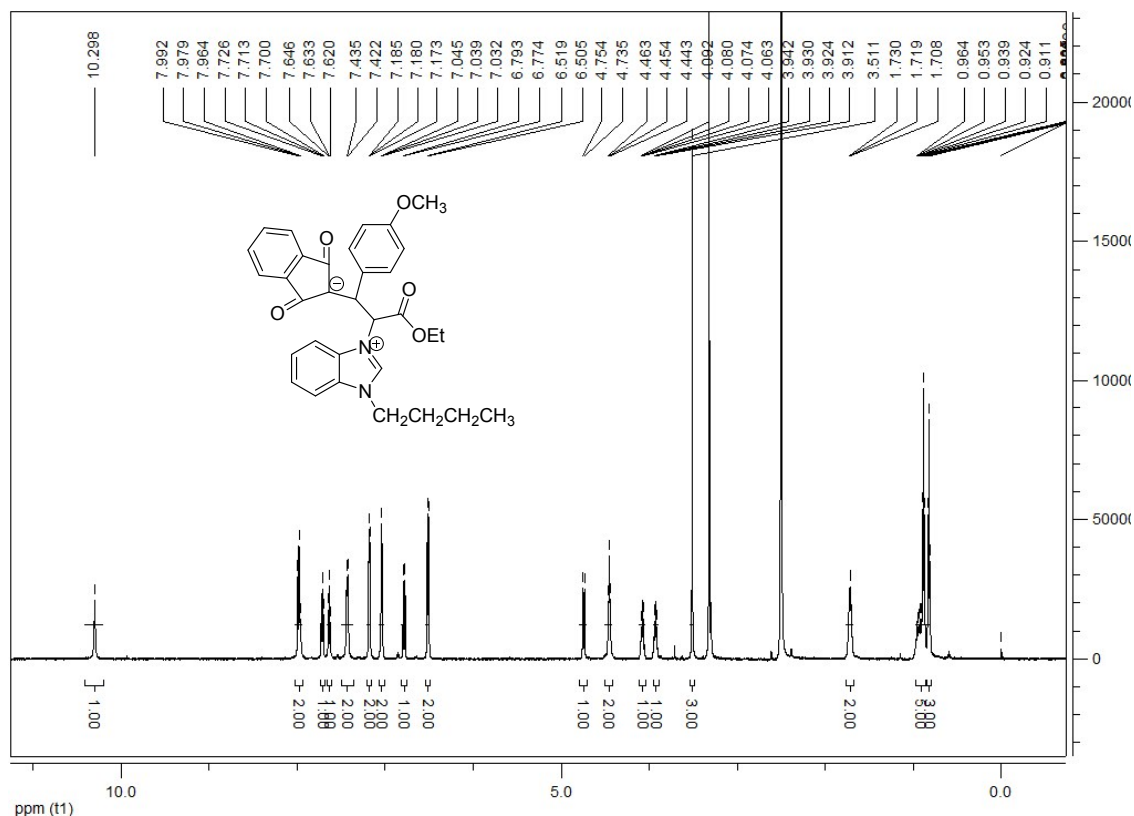
**2-(2-(1-butyl-1H-benzo[d]imidazol-3-ium-3-yl)-3-ethoxy-3-oxo-1-(p-tolyl)propyl)-1,3-dioxo-2,3-dihydro-1H-inden-2-ide (2c):** yellow solid, 65%, m.p. 175~177°C; <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ: 10.30 (s, 1H, CH), 7.99~7.98 (m, 2H, ArH), 7.72~7.63 (m, 2H, ArH), 7.38 (s, 2H, ArH), 7.18 (s, 2H, ArH), 7.04 (s, 2H, ArH), 6.84~6.82 (m, 1H, CH), 6.76 (s, 2H, ArH), 4.78~4.76 (m, 1H, CH), 4.45~4.44 (m, 2H, CH), 4.08~3.93 (m, 2H, CH), 2.02 (s, 3H, CH<sub>3</sub>), 1.70~1.69 (m, 2H, CH), 0.89~0.82 (m, 8H, CH); <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ: 188.3, 188.0, 168.4, 142.9, 140.5, 138.8, 135.5, 130.9, 130.3, 129.2, 128.8, 128.6, 128.0, 126.8, 126.7, 126.5, 116.4, 113.7, 101.1, 61.7, 61.6, 61.5, 46.6, 46.5, 42.9, 30.4, 20.6, 18.6, 13.3, 13.1; IR (KBr) ν: 3027, 2960, 1734, 1609, 1535, 1426, 1318, 1199, 1030, 826, 733 cm<sup>-1</sup>; MS (*m/z*): HRMS (ESI) Calcd. for C<sub>32</sub>H<sub>33</sub>N<sub>2</sub>O<sub>4</sub> ([M+H]<sup>+</sup>): 509.2435. Found: 509.2452.

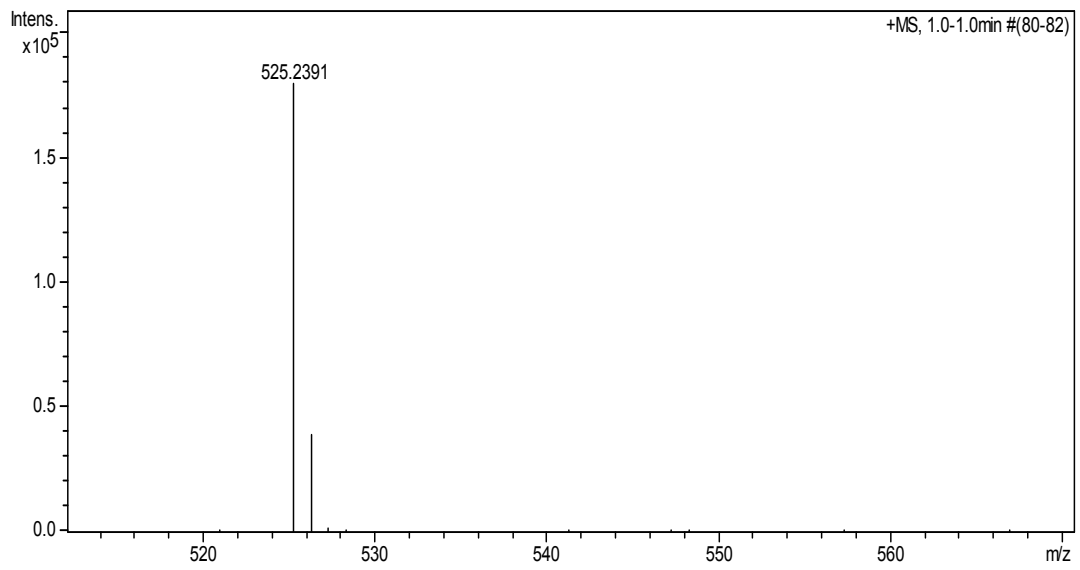
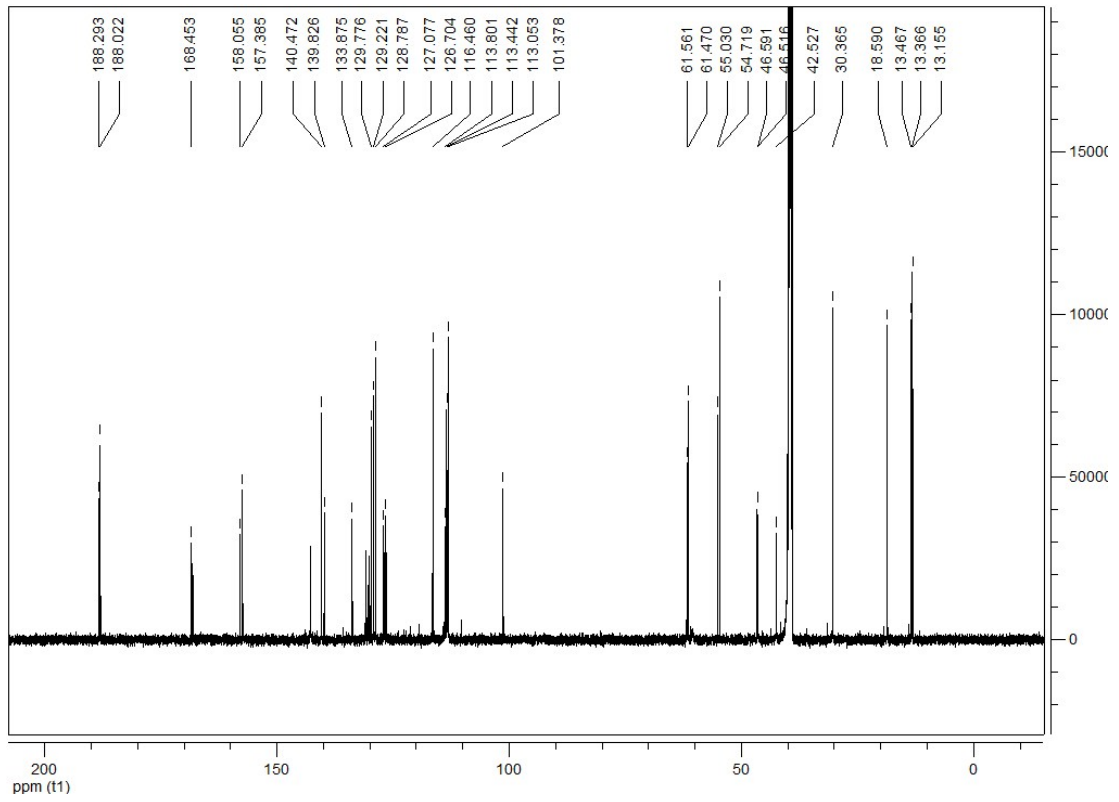






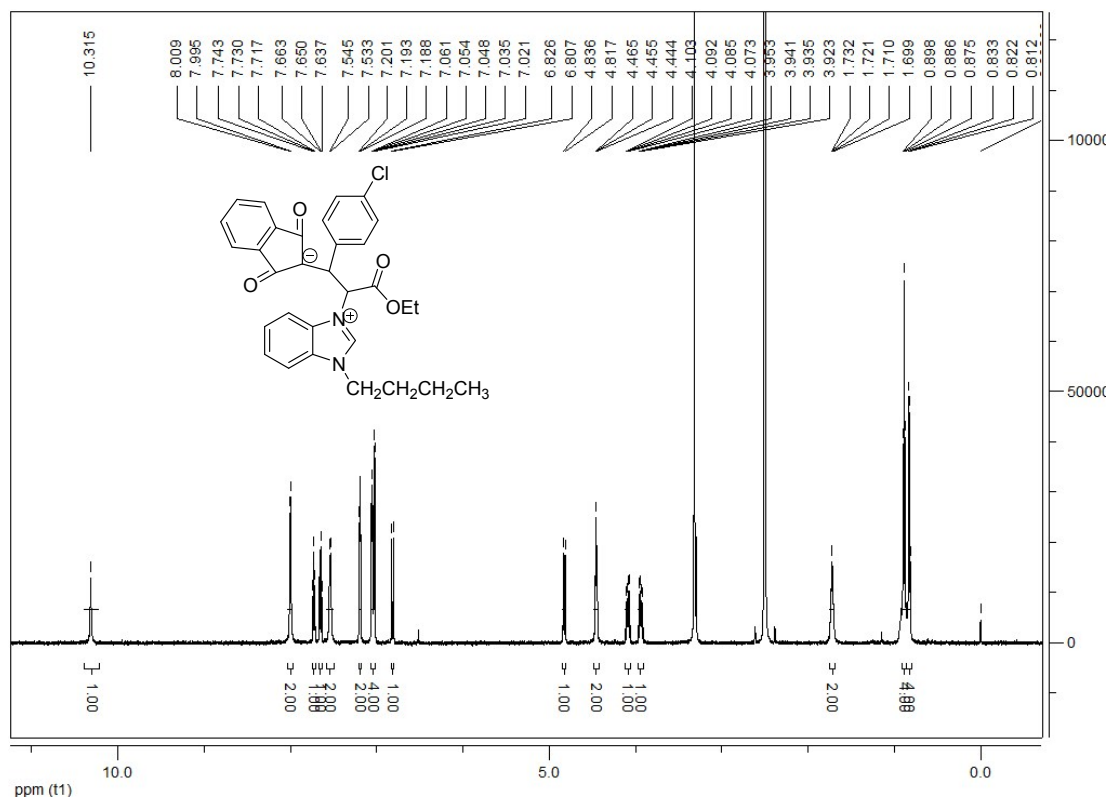
**2-(2-(1-butyl-1H-benzo[d]imidazol-3-ium-3-yl)-3-ethoxy-1-(4-methoxyphenyl)-3-oxopropyl)-1,3-dioxo-2,3-dihydro-1H-inden-2-ide (2d):** yellow solid, 70%, m.p. 170~172°C; <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ: 10.30 (s, 1H, CH), 7.99~7.96 (m, 2H, ArH), 7.73~7.70 (m, 1H, ArH), 7.65~7.62 (m, 1H, ArH), 7.43 (d, *J* = 7.8 Hz, 2H, ArH), 7.18~7.17 (m, 2H, ArH), 7.04~7.03 (m, 2H, ArH), 6.78 (d, *J* = 11.4 Hz, 1H, CH), 6.51 (d, *J* = 8.4 Hz, 2H, ArH), 4.74 (d, *J* = 11.4 Hz, 1H, CH), 4.46~4.44 (m, 2H, CH), 4.10~4.05 (m, 1H, CH), 3.95~3.90 (m, 1H, CH), 3.51 (s, 3H, OCH<sub>3</sub>), 1.74~1.70 (m, 2H, CH), 0.96~0.87 (m, 5H, CH), 0.82 (t, *J* = 7.2 Hz, 3H, CH<sub>3</sub>); <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ: 188.2, 188.0, 168.4, 158.0, 157.3, 140.4, 139.8, 133.8, 129.7, 129.2, 128.7, 127.0, 126.7, 116.4, 113.8, 113.4, 113.0, 101.3, 61.5, 61.4, 55.0, 54.7, 46.5, 42.5, 30.3, 18.5, 13.4, 13.3, 13.1; IR (KBr) ν: 3020, 2962, 1737, 1610, 1538, 1429, 1250, 1191, 1031, 842, 736 cm<sup>-1</sup>; MS (*m/z*): HRMS (ESI) Calcd. for C<sub>32</sub>H<sub>33</sub>N<sub>2</sub>O<sub>5</sub> ([M+H]<sup>+</sup>): 525.2384. Found: 525.2391.

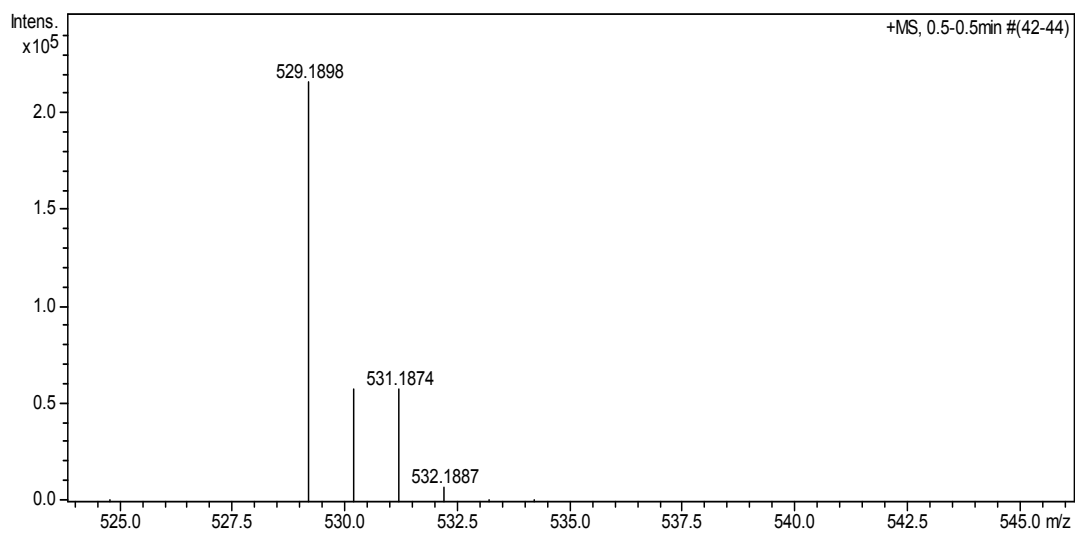
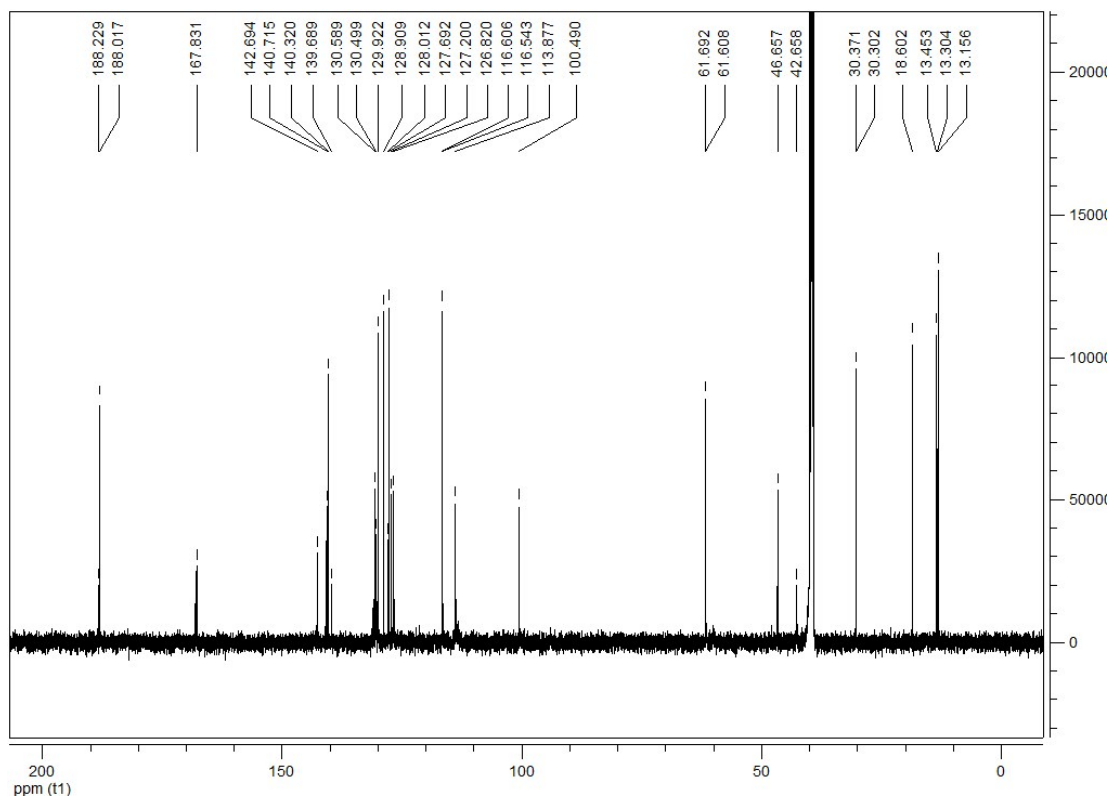




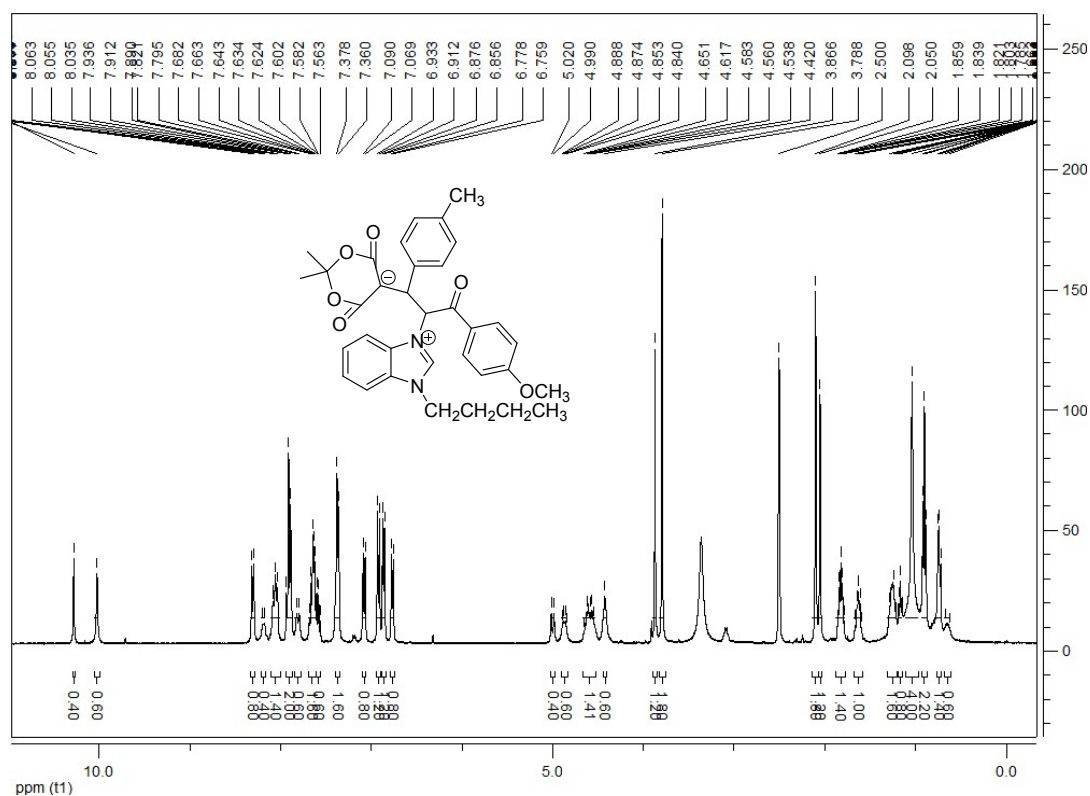
**2-(2-(1-butyl-1H-benzo[d]imidazol-3-ium-3-yl)-1-(4-chlorophenyl)-3-ethoxy-3-oxopropyl)-**

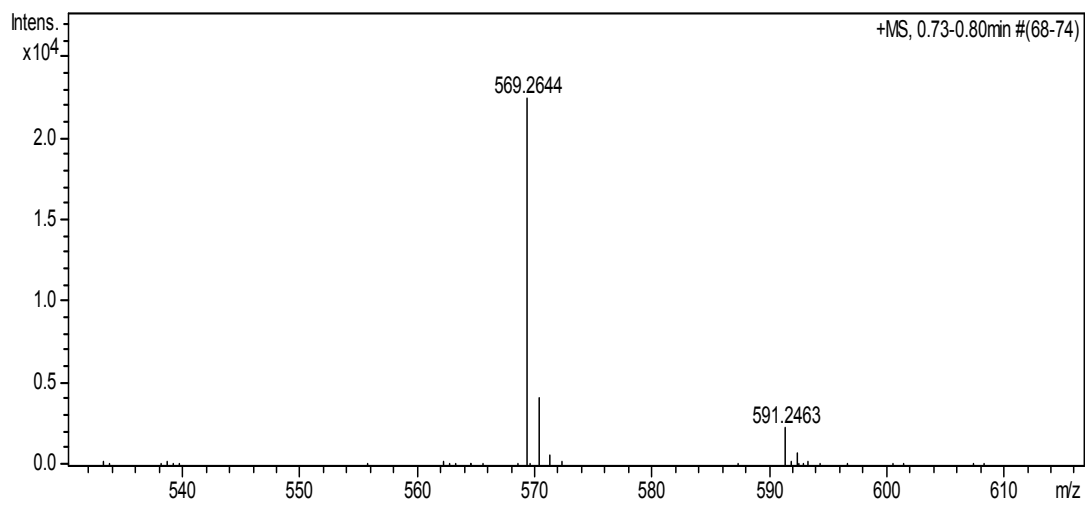
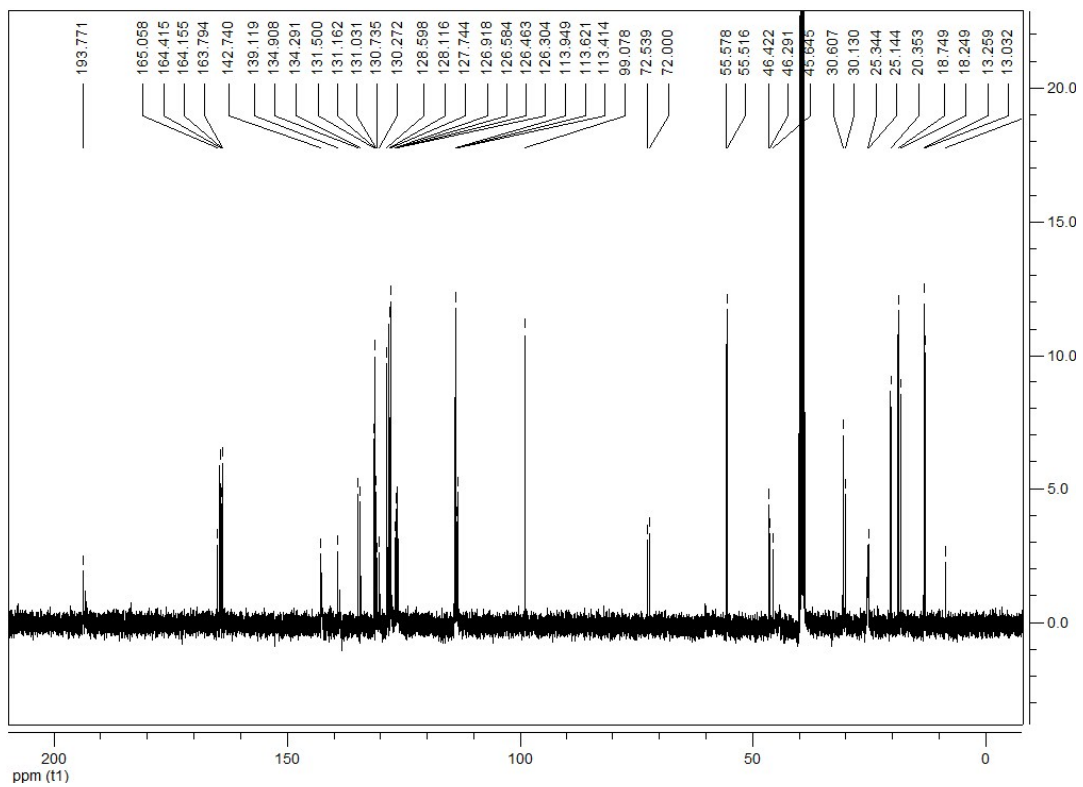
**1,3-dioxo-2,3-dihydro-1H-inden-2-ide (2e):** yellow solid, 68%, m.p. 176~178°C; <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ: 10.32 (s, 1H, CH), 8.00 (d, *J* = 8.4 Hz, 2H, ArH), 7.74~7.72 (m, 1H, ArH), 7.66~7.64 (m, 1H, ArH), 7.54 (d, *J* = 7.2 Hz, 2H, ArH), 7.20~7.19 (m, 2H, ArH), 7.06~7.02 (m, 4H, ArH), 6.82 (d, *J* = 11.4 Hz, 1H, CH), 4.83 (d, *J* = 11.4 Hz, 1H, CH), 4.46~4.44 (m, 2H, CH), 4.12~4.06 (m, 1H, CH), 3.96~3.91 (m, 1H, CH), 1.73~1.70 (m, 2H, CH), 0.90~0.88 (m, 4H, CH), 0.86~0.81 (m, 4H, CH); <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) δ: 188.2, 188.0, 167.8, 142.6, 140.7, 140.3, 139.6, 130.5, 130.4, 129.9, 128.9, 128.0, 127.6, 127.1, 126.8, 116.6, 116.5, 113.8, 100.4, 61.6, 46.6, 42.6, 30.3, 18.6, 13.4, 13.3, 13.1; IR (KBr) ν: 3050, 2964, 2924, 1732, 1624, 1532, 1485, 1425, 1318, 1199, 1100, 867, 733 cm<sup>-1</sup>; MS (*m/z*): HRMS (ESI) Calcd. for C<sub>31</sub>H<sub>30</sub>ClN<sub>2</sub>O<sub>4</sub> ([M+H]<sup>+</sup>): 529.1889. Found: 529.1898.



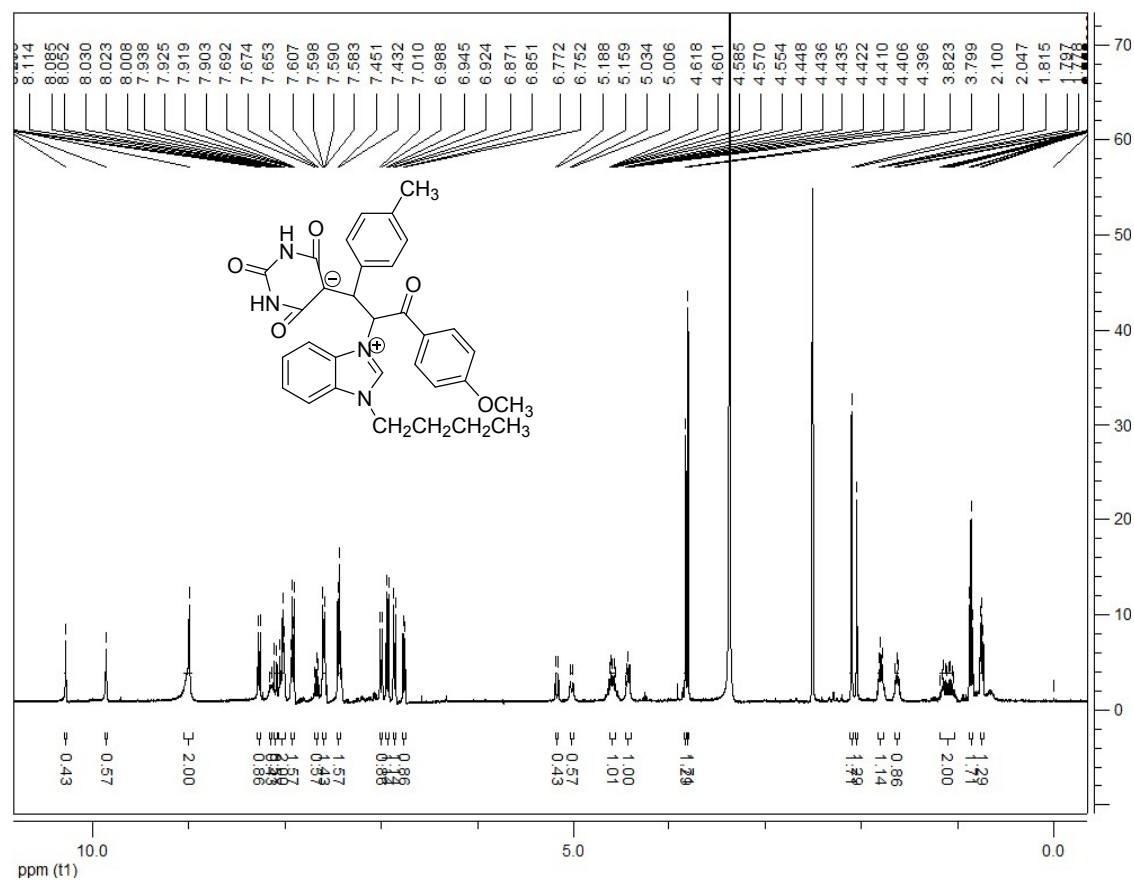


**5-(2-(1-butyl-1H-benzo[d]imidazol-3-ium-3-yl)-3-(4-methoxyphenyl)-3-oxo-1-(p-tolyl)propyl)-2,2-dimethyl-4,6-dioxo-1,3-dioxan-5-ide (2f):** white solid, 80%, m.p. 196~198°C; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ: A-conformation: 10.02 (s, 1H, CH), 8.08~8.04 (m, 1H, ArH), 7.94~7.89 (m, 2H, ArH), 7.82~7.80 (m, 1H, ArH), 7.68~7.62 (m, 2H, ArH), 7.60~7.56 (m, 1H, ArH), 7.38~7.36 (m, 2H, ArH, CH), 6.92 (d, *J* = 8.4 Hz, 2H, ArH), 6.87 (d, *J* = 7.7 Hz, 2H, ArH), 4.89~4.84 (m, 1H, CH), 4.65~4.54 (m, 1H, CH), 4.42 (brs, 1H, CH), 3.79 (s, 3H, OCH<sub>3</sub>), 2.10 (s, 3H, CH<sub>3</sub>), 1.86~1.78 (m, 1H, CH), 1.66~1.60 (m, 1H, CH), 1.28~1.22 (m, 1H, CH), 1.04 (brs, 4H, CH), 0.92~0.88 (m, 3H, CH<sub>3</sub>), 0.75~0.72 (m, 1H, CH), 0.67~0.62 (m, 1H, CH); B-conformation: 10.28 (s, 1H, CH), 8.31 (d, *J* = 8.6 Hz, 2H, ArH), 8.20~8.18 (m, 1H, ArH), 7.08 (d, *J* = 8.4 Hz, 2H, ArH), 6.77 (d, *J* = 7.7 Hz, 2H, ArH), 5.01 (d, *J* = 11.8 Hz, 1H, CH), 3.87 (s, 3H, OCH<sub>3</sub>), 2.05 (s, 3H, CH<sub>3</sub>), 1.18~1.17 (m, 2H, CH). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>) δ: 193.7, 165.0, 164.4, 164.1, 163.7, 142.7, 139.1, 134.9, 134.2, 131.4, 131.1, 131.0, 130.7, 130.2, 128.5, 128.1, 127.7, 126.9, 126.5, 126.4, 126.3, 113.9, 113.6, 113.4, 99.0, 72.5, 72.0, 55.5, 55.5, 46.4, 46.2, 45.6, 30.6, 30.1, 25.3, 25.1, 20.3, 18.7, 18.2, 13.2, 13.0; IR (KBr) ν: 2957, 1673, 1599, 1511, 1434, 1382, 1319, 1260, 1170, 1104, 1030, 920, 757 cm<sup>-1</sup>; MS (*m/z*): HRMS (ESI) Calcd. for C<sub>34</sub>H<sub>37</sub>N<sub>2</sub>O<sub>6</sub> ([M+H]<sup>+</sup>): 569.2646. Found: 569.2644.

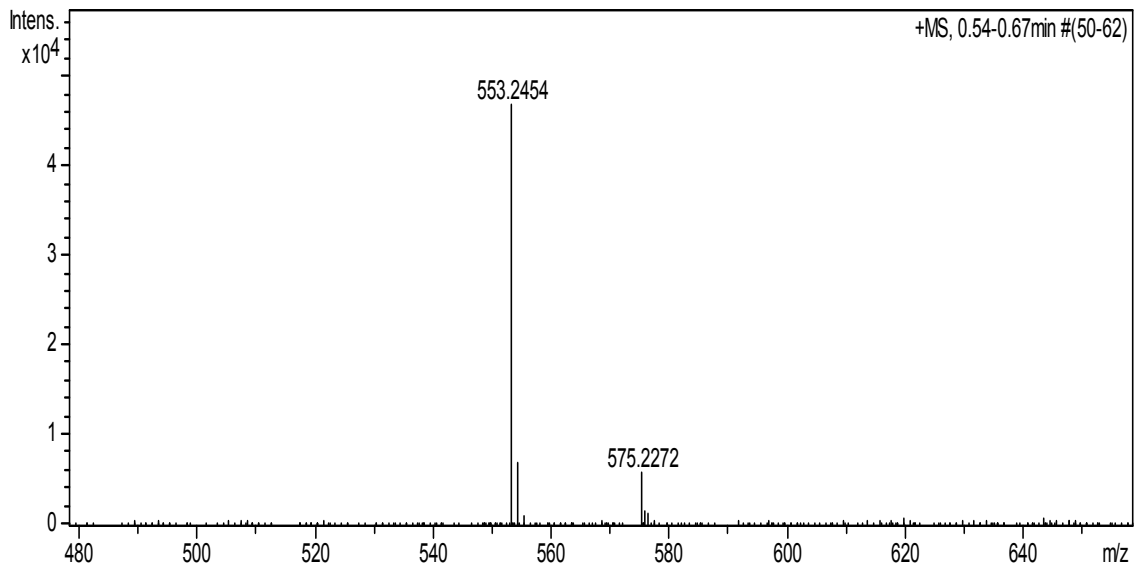
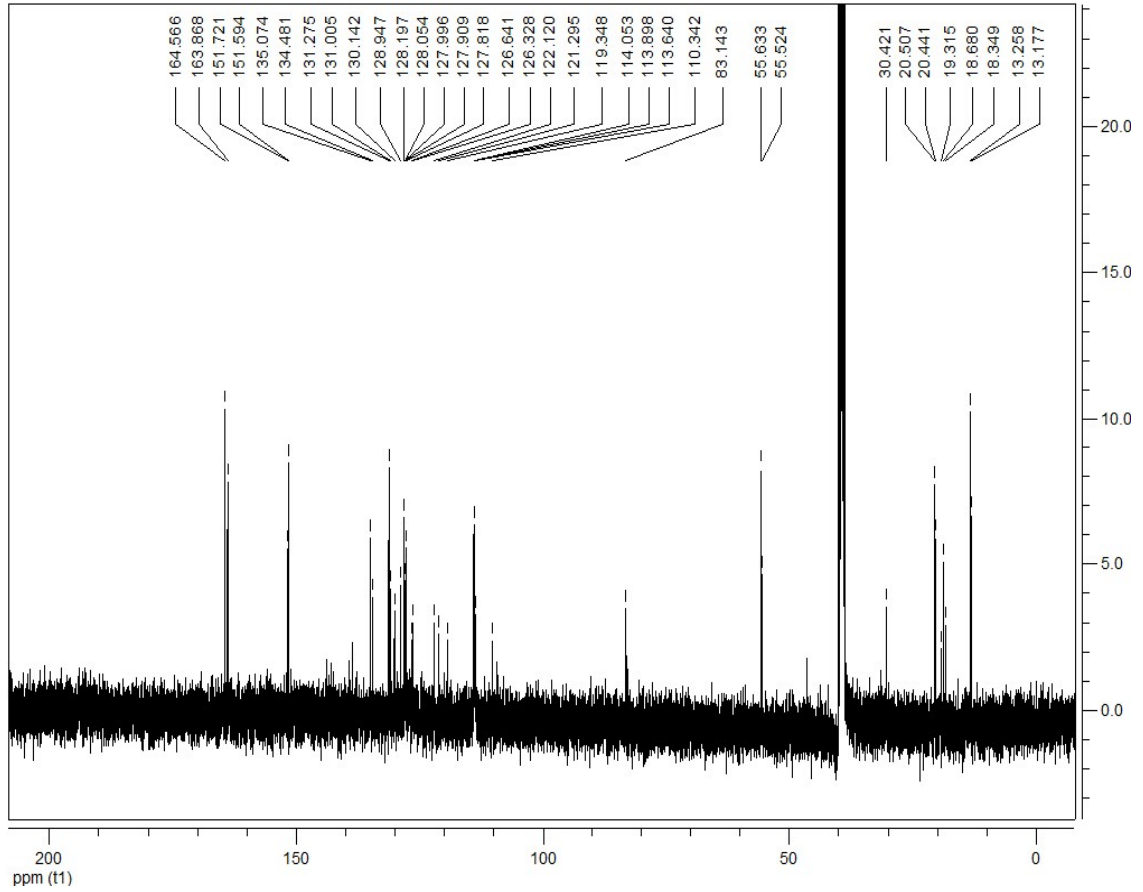




**5-(2-(1-butyl-1H-benzo[d]imidazol-3-ium-3-yl)-3-(4-methoxyphenyl)-3-oxo-1-(p-tolyl)propyl)-2,4,6-trioxohexahydropyrimidin-5-ide (2g):** white solid, 91%, m.p. 205~207°C; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ: A-conformation: 9.86 (s, 1H, CH), 9.00 (s, 2H, NH), 8.11~8.08 (m, 1H, ArH), 8.05~8.01 (m, 2H, ArH), 7.94~7.90 (m, 2H, ArH), 7.69~7.65 (m, 1H, ArH), 7.61~7.58 (m, 1H, ArH), 7.45~7.43 (m, 2H, ArH, CH), 6.93 (d, *J* = 8.6 Hz, 2H, ArH), 6.86 (d, *J* = 7.9 Hz, 2H, ArH), 5.02 (d, *J* = 11.3 Hz, 1H, CH), 4.62~4.55 (m, 1H, CH), 4.45~4.40 (m, 1H, CH), 3.80 (s, 3H, OCH<sub>3</sub>), 2.10 (s, 3H, CH<sub>3</sub>), 1.82~1.78 (m, 2H, CH), 1.18~1.04 (m, 2H, CH), 0.88~0.84 (m, 3H, CH<sub>3</sub>); B-conformation: 10.28 (s, 1H, CH), 8.27 (d, *J* = 8.8 Hz, 2H, ArH), 8.16~8.13 (m, 1H, ArH), 7.00 (d, *J* = 8.6 Hz, 2H, ArH), 5.17 (d, *J* = 11.6 Hz, 1H, CH), 3.82 (s, 3H, OCH<sub>3</sub>), 2.05 (s, 3H, CH<sub>3</sub>), 1.65~1.61 (m, 2H, CH), 0.76~0.73 (m, 3H, CH<sub>3</sub>). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>) δ: 164.5, 163.8, 151.7, 151.5, 135.0, 134.4, 131.2, 131.0, 130.1, 128.9, 128.1, 128.0, 127.9, 127.9, 127.8, 126.6, 126.3, 122.1, 121.2, 119.3, 114.0, 113.8, 113.6, 110.3, 83.1, 55.6, 55.5, 30.4, 20.5, 20.4, 19.3, 18.6, 18.3, 13.2, 13.1; IR (KBr) ν: 2958, 1685, 1574, 1455, 1389, 1244, 1174, 973, 847 cm<sup>-1</sup>; MS (*m/z*): HRMS (ESI) Calcd. for C<sub>32</sub>H<sub>33</sub>N<sub>4</sub>O<sub>5</sub> ([M+H]<sup>+</sup>): 553.2445. Found: 553.2454.







**5-(2-(1-butyl-1H-benzo[d]imidazol-3-ium-3-yl)-3-(4-methoxyphenyl)-3-oxo-1-(p-tolyl)propyl)-1,3-dimethyl-2,4,6-trioxohexahydropyrimidin-5-ide (2h):** yellow solid, 95%, m.p. 178~180°C; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ: A-conformation: 9.86 (s, 1H, CH), 8.18~8.16 (m, 1H, ArH), 8.07~8.04 (m, 2H, ArH), 8.00~7.94 (m, 2H, ArH), 7.71~7.66 (m, 1H, ArH), 7.62~7.59 (m, 1H, ArH), 7.44~7.39 (m, 2H, ArH, CH), 6.95 (d, *J* = 8.6 Hz, 2H, ArH), 6.86 (d, *J* = 7.6 Hz, 2H, ArH), 5.16 (d, *J* = 11.4 Hz, 1H, CH), 4.62~4.52 (m, 1H, CH), 4.47~4.42 (m, 1H, CH), 3.80 (s, 3H, OCH<sub>3</sub>), 3.13~3.06 (m, 6H, 2CH<sub>3</sub>), 2.09 (s, 3H, CH<sub>3</sub>), 1.80~1.71 (m, 2H, CH), 1.06~0.93 (m, 2H, CH), 0.82~0.79 (m, 3H, CH<sub>3</sub>); A-conformation: δ: 10.26 (s, 1H, CH), 8.23~8.21 (m, 1H, ArH), 8.11~8.09 (m, 1H, ArH), 7.82~7.80 (m, 1H, ArH), 7.00 (d, *J* = 8.6 Hz, 2H, ArH), 6.75 (d, *J* = 7.6 Hz, 2H, ArH), 5.25 (d, *J* = 11.4 Hz, 1H, CH), 3.83 (s, 3H, OCH<sub>3</sub>), 2.04 (s, 3H, CH<sub>3</sub>), 1.64~1.60 (m, 2H, CH), 0.74~0.71 (m, 3H, CH<sub>3</sub>). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>) δ: 193.7, 163.9, 162.1, 161.6, 152.3, 152.2, 142.9, 142.5, 138.4, 135.0, 134.4, 131.3, 130.9, 130.8, 130.0, 128.7, 128.1, 128.0, 127.8, 126.4, 126.3, 114.0, 113.5, 83.5, 55.6, 46.3, 45.5, 30.3, 30.2, 26.7, 20.4, 18.4, 18.2, 13.2, 13.1; IR (KBr) ν: 2938, 2744, 2676, 1668, 1581, 1435, 1383, 1315, 1268, 1163, 1031, 915, 845, 752 cm<sup>-1</sup>; MS (m/z): HRMS (ESI) Calcd. for C<sub>34</sub>H<sub>37</sub>N<sub>4</sub>O<sub>5</sub> ([M+H]<sup>+</sup>): 581.2758. Found: 581.2765.

