# Molybdate sulfuric acid (MSA): an efficient solid acid catalyst for the synthesis of diversely functionalized fused imidazo[1,2-a]pyrimidines under solvent-free condition.

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Supporting Information

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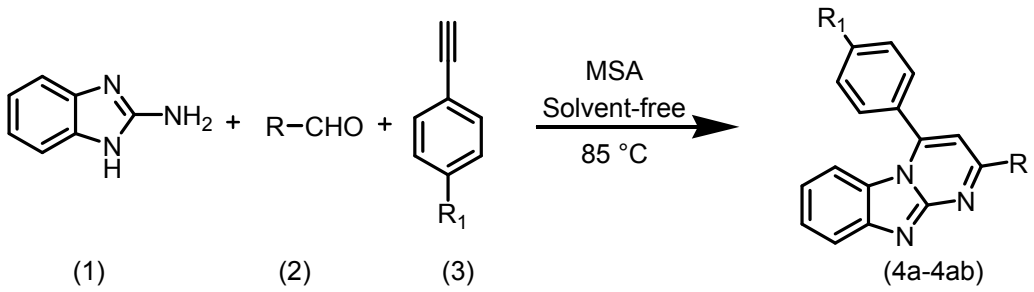
**General procedures for the synthesis of imidazo[1,2-*a*]pyrimidines (4):**



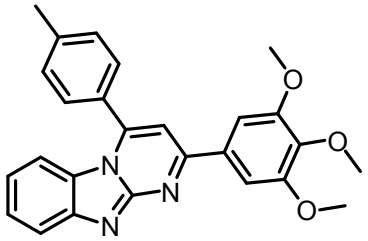

(1) (2) (3) (4a-4ab)

**Procedure: Synthesis of 2-(3,4,5-Trimethoxyphenyl)-4-*p*-tolylbenzo[4,5]imidazo[1,2-*a*]-pyrimidine (4a)**

A mixture of 1*H*-benzo[*d*]imidazol-2-amine (1, 1 mmol), 3,4,5-trimethoxybenzaldehyde (2a, 1mmol) and 1-ethynyl-4-methylbenzene (3a, 1.5 mmol) and MSA (15 mol %) was stirred at 85 °C under solvent-free condition for 2 h. The progress of the reaction was monitored by TLC. After completion of the reaction, the mixture was washed with ethyl acetate and filtered to recover the catalyst. The filtrate was evaporated, and the crude product was purified by flash column chromatography on silica gel (200−300mesh) with ethyl acetate and hexane as eluent to afford the product **4a** in excellent yield (87%). The MSA catalyst was reused by the way of addition of ethyl acetate to the reaction mixture and filtration followed by drying in a vacuum oven every time. Compounds **4b-4ab** were also synthesized by adopting this procedure.

## Spectral data of the compounds

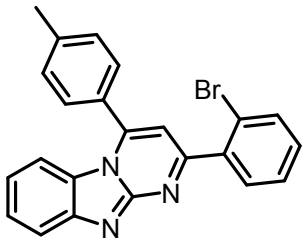
2-(3,4,5-Trimethoxyphenyl)-4-*p*-tolylbenzo[4,5]imidazo[1,2-a]-pyrimidine **(4a)**



**(4a)**

Yield 87%; yellow solid; Mp: 258-260 $^{o}$C; $^{1}$H NMR (400 MHz, $CDCl_3$): δ 7.91 (d, *J*=8.1, 1H), 7.54-7.56 (m, 4H), 7.47 (d, *J*=8.1 Hz, 2H), 7.42 (t, *J*=7.7 Hz, 1H), 7.16 (s, 1H), 7.01 (t, *J*=7.6 Hz, 1H), 6.73 (d, *J*=8.1 Hz, 1H), 3.97 (s, 6H), 3.93 (s, 3H), 2.56 (s, 3H), $^{13}$C NMR (100 MHz, $CDCl_3$): δ 160.30, 153.53, 149.45, 145.50, 141.49, 131.97, 130.07, 128.35, 125.89, 121.08, 120.03, 114.63, 105.04, 61.04, 56.45, 21.72; HRMS (ESI, m/z): calcd for $C_{26}H_{23}N_3O_3$ ($M+H^+$) 425.1739, found: 425.1738.

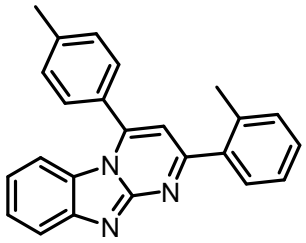
2-(2-Bromophenyl)-4-p-tolylbenzo[4,5]imidazo[1,2-a]-pyrimidine (**4b**)



**(4b)**

Yield 82%; yellow solid; Mp: 220-222 $^{o}$C; $^{1}$H NMR (400 MHz, $CDCl_3$): δ 7.99 (d, *J*=8.1 Hz, 1H), 7.85 (d, *J*=7.7 Hz, 1H), 7.67 (d, *J*=8.1 Hz, 1H), 7.53 (d, *J*=8.1 Hz, 2H), 7.43-7.48 (m, 4H), 7.31 (t, *J*=7.5 Hz, 1H), 7.17 (s, 1H), 7.06 (t, *J*=6.9 Hz, 1H), 6.87 (d, *J*=8.4 Hz, 1H), 2.54 (s, 3H), $^{13}$C NMR (100 MHz, $CDCl_3$): δ 162.85, 148.58, 145.43, 141.55, 139.32, 133.63, 132.04, 131.15, 130.08, 129.47, 128.31, 127.88, 127.43, 126.02, 121.47, 121.32, 120.46, 114.95, 109.89, 21.74; HRMS (ESI, m/z): calcd for $C_{23}H_{16}BrN_3$ ($M+H^+$) 413.0527, found: 413.0528.

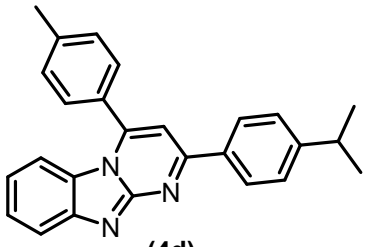
2-(2-Methylphenyl)-4-p-tolylbenzo[4,5]imidazo[1,2-a]-pyrimidine (**4c**)



**(4c)**

Yield 81%; yellow solid; Mp: 162-164 °C; $^1$H NMR (400 MHz, $CDCl_3$): δ 7.96 (d, *J*=8.1 Hz, 1H), 7.62 (d, *J*=7.7 Hz, 1H), 7.50 (d, *J*=8.1 Hz, 2H), 7.42 (d, *J*=7.7 Hz, 3H), 7.23-7.35 (m, 3H), 7.02 (t, *J*=7.7 Hz, 1H), 6.92 (s, 1H), 6.82 (d, *J*=8.1 Hz, 1H), 2.63 (s, 3H), 2.52 (s, 3H), $^{13}$C NMR (100 MHz, $CDCl_3$): δ 164.57, 149.10, 145.35, 141.42, 137.87, 137.08, 131.48, 130.00, 129.78, 129.70, 129.48, 128.21, 126.02, 125.80, 121.01, 120.19, 114.78, 109.16, 21.65, 21.05; HRMS (ESI, m/z): calcd for $C_{24}H_{19}N_3$ ($M+H^+$) 349.1579, found: 349.1580.

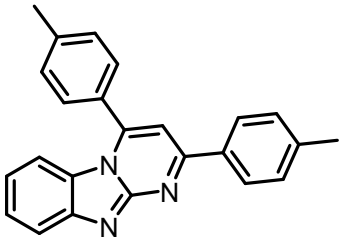
2-(4-Isopropylphenyl)-4-p-tolylbenzo[4,5]imidazo[1,2-a]-pyrimidine (**4d**)



**(4d)**

Yield 86%; yellow solid; Mp: 166-168 °C; $^1$H NMR (400 MHz, $CDCl_3$): δ 8.21 (d, *J*=8.4 Hz, 2H), 7.94 (s, 1H), 7.50 (d, *J*=8.1 Hz, 2H), 7.44 (d, *J*=7.7 Hz, 2H), 7.40 (d, *J*=7.3 Hz, 1H), 7.35 (d, *J*=8.1 Hz, 2H), 7.18 (s, 1H), 6.99 (t, *J*=7.3 Hz, 1H), 6.75 (d, *J*=8.1 Hz, 1H), 2.93-3.00 (m, 1H), 2.54 (s, 3H), 1.28 (d, *J*=7.0 Hz, 6H), $^{13}$C NMR (100 MHz, $CDCl_3$): δ 161.06, 152.63, 141.37, 134.38, 130.04, 128.34, 127.94, 127.10, 125.76, 120.93, 120.08, 114.69, 105.30, 34.18, 23.86, 21.72; HRMS (ESI, m/z): calcd for $C_{26}H_{23}N_3$ ($M+H^+$) 377.1892, found: 377.1894.

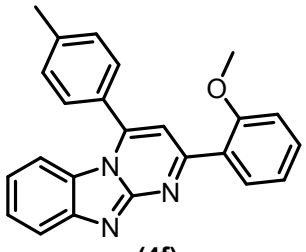
2-(4-Methylphenyl)-4-p-tolylbenzo[4,5]imidazo[1,2-a]-pyrimidine (**4e**)



**(4e)**

Yield 80%; yellow solid; Mp: 238-240 °C; $^1$H NMR (400 MHz, $CDCl_3$): δ 8.14 (d, *J*=8.1 Hz, 2H), 7.92 (d, *J*=8.1 Hz, 1H), 7.49 (d, *J*=8.1 Hz, 2H), 7.43 (d, *J*=8.1 Hz, 2H), 7.38 (d, *J*=7.7 Hz, 1H), 7.24 (d, *J*=8.1 Hz, 2H), 7.14 (s, 1H), 6.98 (t, *J*=8.1 Hz, 1H), 6.73 (d, *J*=8.1 Hz, 1H), 2.53 (s, 3H), 2.36 (s, 3H), $^{13}$C NMR (100 MHz, $CDCl_3$): δ 160.95, 149.39, 141.73, 141.33, 133.90, 129.99, 129.74, 129.63, 128.30, 127.72, 125.71, 120.86, 120.03, 114.65, 105.20, 21.69, 21.52; HRMS (ESI, m/z): calcd for $C_{24}H_{19}N_3$ ($M+H^+$) 349.1579, found: 349.1579.

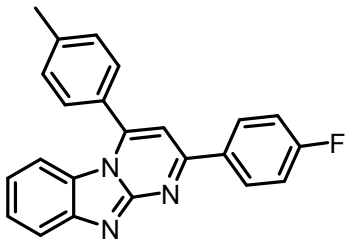
2-(2-Methoxyphenyl)-4-p-tolylbenzo[4,5]imidazo[1,2-a]-pyrimidine **(4f)**



**(4f)**

Yield 78%; yellow solid; Mp: 156-158 °C; $^1$H NMR (400 MHz, $CDCl_3$): δ 8.26 (d, *J*=8.1, 1H), 7.95 (d, *J* =8.1 Hz, 1H), 7.51 (d, *J*=8.1 Hz, 2H), 7.48 (s, 1H), 7.41-7.44 (m, 4H), 7.11 (t, *J*=7.3 Hz, 1H), 7.02 (d, *J*=7.7 Hz, 1H), 6.98 (d, *J*=8.1 Hz, 1H), 6.77 (d, *J*=8.1 Hz, 1H), 3.88 (s, 3H), 2.53 (s, 3H), $^{13}$C NMR (100 MHz, $CDCl_3$): δ 161.23, 158.06, 147.93, 145.36, 141.14, 132.14, 131.99, 129.95, 128.41, 126.68, 125.64, 121.32, 120.76, 120.05, 114.75, 111.53, 110.16, 55.70, 21.68; HRMS (ESI, m/z): calcd for $C_{24}H_{19}N_3O$ ($M+H^+$) 365.1528, found: 365.1529.

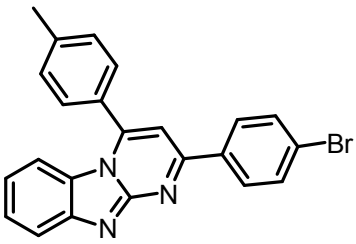
2-(4-Flurophenyl)-4-p-tolylbenzo[4,5]imidazo[1,2-a]-pyrimidine (**4g**)



**(4g)**

Yield 81%; yellow solid; Mp: 240-242 °C; $^1$H NMR (400 MHz, $CDCl_3$): δ 8.21-8.24 (m, 2H), 7.90 (d, *J*=7.3 Hz, 1H), 7.51 (d, *J*=7.7 Hz, 2H), 7.44 (d, *J*=7.7 Hz, 2H), 7.39 (t, *J*=7.7 Hz, 1H), 7.11 (t, *J*=7.3 Hz, 3H), 6.98 (t, *J*=7.3 Hz, 1H), 6.73 (d, *J*=8.4 Hz, 1H), 2.54 (s, 3H), $^{13}$C NMR (100 MHz, $CDCl_3$): δ 166.05, 163.54, 159.72, 149.77, 141.49, 132.84, 130.03, 129.90, 129.82, 129.57, 128.27, 125.87, 121.08, 120.06, 116.03, 115.82, 114.72, 104.96, 21.70; HRMS (ESI, m/z): calcd for $C_{23}H_{16}FN_3$ ($M+H^+$) 353.1328, found: 353.1330.

2-(4-Bromophenyl)-4-p-tolylbenzo[4,5]imidazo[1,2-a]-pyrimidine (**4h**)

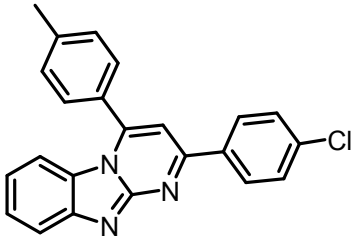


**(4h)**

Yield 84%; yellow solid; Mp: 240-242 °C; $^1$H NMR (400 MHz, $CDCl_3$): δ 8.09 (d, *J*=8.4 Hz,

2H), 7.92 (s, 1H), 7.57 (d, *J*=8.1 Hz, 2H), 7.52 (d, *J*=8.1 Hz, 2H), 7.45 (d, *J*=7.7 Hz, 2H), 7.40 (t, *J*=6.4 Hz, 1H), 7.12 (s, 1H), 7.00 (t, *J*=7.3 Hz, 1H), 6.75 (d, *J*=8.4 Hz, 1H), 2.55 (s, 3H), $^{13}$C NMR (100 MHz, $CDCl_3$): δ 159.66, 149.94, 141.57, 135.55, 132.11, 130.09, 129.23, 128.30, 126.00, 121.25, 120.15, 114.80, 104.92, 21.75; HRMS (ESI, m/z): calcd for $C_{23}H_{16}BrN_3$ ($M+H^+$) 413.0527, found: 413.0526.

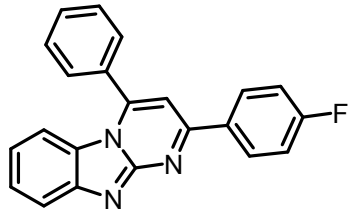
2-(4-Chlorophenyl)-4-p-tolylbenzo[4,5]imidazo[1,2-a]-pyrimidine (**4i**)




**(4i)**

Yield 81%; yellow solid; Mp: 206-208 $^{o}$C; $^{1}$H NMR (400 MHz, $CDCl_3$): δ 8.17 (d, *J*=7.0 Hz, 2H), 7.91 (d, J=7.0 Hz, 1H), 7.41-7.51 (m, 8H), 7.12 (s, 1H), 7.00 (t, *J*=7.3 Hz, 1H), 6.74 (d, *J*=7.3 Hz, 1H), 2.55 (s, 3H), $^{13}$C NMR (100 MHz, $CDCl_3$): δ 159.63, 149.89, 141.56, 137.52, 130.09, 129.15, 129.03, 128.29, 125.99, 121.22, 120.18, 114.77, 104.97, 21.75; HRMS (ESI, m/z): calcd for $C_{23}H_{16}ClN_3$ ($M+H^+$) 369.1032, found: 369.1031.

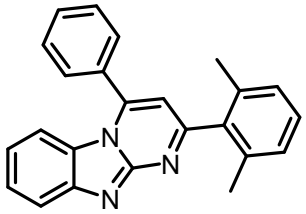
2-(4-Fluorophenyl)-4-phenylbenzo[4,5]imidazo[1,2-a]-pyrimidine **(4j)**




**(4j)**

Yield 80%; yellow solid; Mp: 197-199 $^{o}$C; $^{1}$H NMR (400 MHz, $CDCl_3$): δ 8.21-8.24 (m, 2H), 7.89 (d, *J* =8.1 Hz, 1H), 7.64-7.71 (m, 5H), 7.39 (t, *J*=7.5 Hz, 1H), 7.11 (t, *J*=8.4 Hz, 3H), 6.97 (t, *J*=7.7 Hz, 1H), 6.62 (d, *J*=8.4 Hz, 1H), $^{13}$C NMR (100 MHz, $CDCl_3$): δ 159.73, 151.96, 149.47, 145.47, 136.93, 132.47, 131.13, 129.93, 129.83, 129.41, 128.40, 127.38, 125.91, 121.20, 120.12, 116.05, 115.83, 114.56, 104.90; HRMS (ESI, m/z): calcd for $C_{22}H_{14}FN_3$ ($M+H^+$) 339.1171, found: 339.1172.

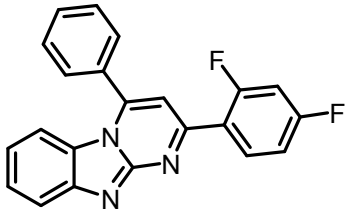
2-(2,6-Dimethylphenyl)-4-phenylbenzo[4,5]imidazo[1,2-a]-pyrimidine **(4k)**



**(4k)**

Yield 76%; yellow solid; Mp: 190-192 °C; $^1$H NMR (400 MHz, $CDCl_3$): δ 8.02 (d, *J*=8.4, 1H), 7.63-7.70 (m, 5H), 7.47 (t, *J* =7.3 Hz, 1H), 7.22 (d, *J*=7.3 Hz, 1H), 7.12 (d, *J*=7.7 Hz, 2H), 7.06 (t, *J*=8.1 Hz, 1H), 6.80 (d, *J*=8.1 Hz, 1H), 6.74 (s, 1H), 2.25 (s, 6H), $^{13}$C NMR (100 MHz, $CDCl_3$): δ 162.98, 154.59, 147.80, 138.65, 135.43, 132.24, 131.22, 129.44, 128.79, 128.39, 127.92, 126.03, 121.33, 120.47, 114.82, 109.92, 20.42; HRMS (ESI, m/z): calcd for $C_{24}H_{19}N_3$ ($M+H^+$) 349.1579, found: 349.1580.

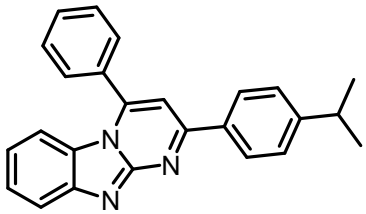
2-(2,4-diluorophenyl)-4-phenylbenzo[4,5]imidazo[1,2-a]-pyrimidine **(4l)**



**(4l)**

Yield 74%; yellow solid; Mp: 252-254 °C; $^1$H NMR (400 MHz, $CDCl_3$): δ 8.49-8.55 (m, 1H), 8.96 (d, *J*=8.1 Hz, 1H), 7.62-7.73 (m, 5H), 7.45 (t, *J*=8.1 Hz, 1H), 7.34 (s, 1H), 7.08 (t, *J*=8.4 Hz, 1H), 7.03 (t, *J*=8.5 Hz, 1H), 6.90-6.95 (m, 1H), 6.71 (d, *J*=8.4, 1H), $^{13}$C NMR (100 MHz, $CDCl_3$): δ 160.46, 156.92, 151.67, 149.24, 145.41, 133.23, 133.13, 132.42, 131.16, 129.44, 128.43, 126.12, 121.35, 120.27, 114.73, 112.48, 108.52, 108.39, 104.66 ; HRMS (ESI, m/z): calcd for $C_{22}H_{13}F_2N_3$ ($M+H^+$) 357.1077, found: 357.1075.

2-(4-Isopropylphenyl)-4-phenylbenzo[4,5]imidazo[1,2-a]-pyrimidine **(4m)**

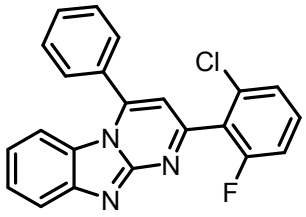


**(4m)**

Yield 81%; yellow solid; Mp: 166-168 °C; $^1$H NMR (400 MHz, $CDCl_3$): δ 8.21 (d, *J*=8.4 Hz, 2H), 7.93 (d, *J* =7.7, Hz, 1H), 7.61-7.71 (m, 5H), 7.40 (t, *J*=7.7 Hz, 1H), 7.35 (d, *J*=8.1 Hz, 2H), 7.20 (s, 1H), 6.98 (t, *J*=7.7 Hz, 1H), 6.65 (d, *J*=8.4 Hz, 1H), 2.93-3.0 (m, 1H), 1.28 (d,

*J*=6.6 Hz, 6H), $^{13}$C NMR (100 MHz, $CDCl_3$): δ 161.06, 152.69, 149.18, 134.30, 132.69, 131.04, 129.42, 128.47, 127.95, 127.11, 125.80, 121.04, 120.13, 114.54, 105.23, 34.17, 23.85; HRMS (ESI, m/z): calcd for $C_{25}H_{21}N_3$ (M+H+) 363.1735, found: 363.1736.

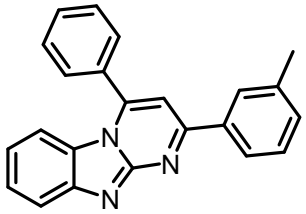
2-(2-chloro-6-fluorolphenyl)-4-phenylbenzo[4,5]imidazo[1,2-a]-pyrimidine **(4n)**




**(4n)**

Yield 75%; yellow solid; Mp: 248-250 $^{o}$C; $^{1}$H NMR (400 MHz, $CDCl_3$): δ 8.02 (d, *J*=7.3, 1H), 7.64-7.71 (m, 5H), 7.47 (t, *J*=7.3, 1H), 7.34-7.40 (m, 1H), 7.31 (d, *J* =8.1 Hz, 1H), 7.13 (t, *J* =8.1 Hz, 1H), 7.06 (t, *J*=8.4 Hz, 1H), 6.88 (s, 1H), 6.78 (d, *J*=8.4 Hz, 1H), $^{13}$C NMR (100 MHz, $CDCl_3$): δ 161.77, 159.26, 157.27, 151.50, 149.23, 145.43, 133.96, 132.08, 131.26, 131.17, 129.45, 128.40, 126.23, 125.90, 121.61, 120.67, 114.91, 114.83, 114.61, 110.11; HRMS (ESI, m/z): calcd for $C_{22}H_{13}ClFN_3$ ($M+H^+$) 373.0782, found: 373.0784.

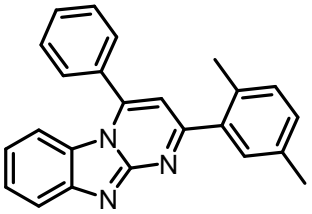
2-(3-Methylphenyl)-4-phenylbenzo[4,5]imidazo[1,2-a]-pyrimidine **(4o)**




**(4o)**

Yield 82%; yellow solid; Mp: 248-250 $^{o}$C; $^{1}$H NMR (400 MHz, $CDCl_3$): δ 8.16 (s, 1H), 8.03 (d, *J*=7.7, 1H), 7.94 (d, *J*=8.1, 1H), 7.62-7.72 (m, 5H), 7.42 (t, *J* =7.7 Hz, 1H), 7.37 (t, *J* =7.7 Hz, 1H), 7.30 (d, *J*=7.7 Hz, 1H), 7.22 (s, 1H), 6.99 (t, *J*=7.7 Hz, 1H), 6.66 (d, *J*=8.4 Hz, 1H), 2.44 (s, 3H), $^{13}$C NMR (100 MHz, $CDCl_3$): δ 161.21, 149.27, 145.60, 138.73, 136.61, 132.67, 132.14, 131.09, 129.44, 128.83, 128.57, 128.47, 125.88, 124.97, 121.13, 120.23, 114.59, 105.42, 21.57; HRMS (ESI, m/z): calcd for $C_{23}H_{17}N_3$ ($M+H^+$) 335.1422, found: 335.1421.

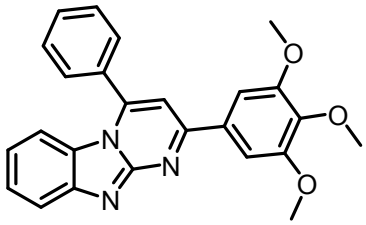
2-(2,5-Dimethylphenyl)-4-phenylbenzo[4,5]imidazo[1,2-a]-pyrimidine **(4p)**



**(4p)**

Yield 79%; yellow solid; Mp: 156-158 °C; $^1$H NMR (400 MHz, $CDCl_3$): δ 7.98 (d, *J*=8.1, 1H), 7.62-7.72 (m, 5H), 7.49 (s, 1H), 7.45 (t, *J* =8.2 Hz, 1H), 7.21 (d, *J*=8.1 Hz, 1H), 7.18 (d, *J*=7.7 Hz, 1H), 7.03 (t, *J*=8.4 Hz, 1H), 6.97 (s, 1H), 6.72 (d, *J*=8.4 Hz, 1H), 2.60 (s, 3H), 2.37 (s, 3H), $^{13}$C NMR (100 MHz, $CDCl_3$): δ 164.87, 151.87, 148.76, 145.44, 137.72, 135.67, 134.01, 132.54, 131.56, 131.13, 130.65, 130.54, 129.48, 128.96, 128.45, 127.42, 125.93, 121.19, 120.39, 114.68, 109.24, 21.02, 20.67; HRMS (ESI, m/z): calcd for $C_{24}H_{19}N_3$ ($M+H^+$) 349.1579, found: 349.1579.

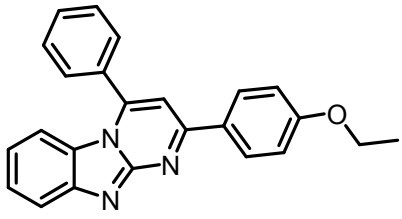
2-(3,4,5-Trimethoxyphenyl)-4-phenylbenzo[4,5]imidazo[1,2-a]-pyrimidine **(4q)**



**(4q)**

Yield 84%; yellow solid; Mp: 230-232 °C; $^1$H NMR (400 MHz, $CDCl_3$): δ 7.88 (d, *J*=8.4 Hz, 1H), 7.67-7.71 (m, 5H), 7.53 (s, 2H), 7.39 (t, *J*=7.3 Hz, 1H), 7.16 (s, 1H), 6.97 (t, *J*=7.7 Hz, 1H), 6.62 (d, *J*=8.4 Hz, 1H), 3.95 (s, 6H), 3.93 (s, 3H), $^{13}$C NMR (100 MHz, $CDCl_3$): δ; 160.15, 153.40, 149.08, 145.33, 140.98, 132.45, 131.75, 129.34, 128.70, 128.40, 127.38, 125.80, 121.08, 119.89, 114.42, 104.92, 60.94, 56.33; HRMS (ESI, m/z): calcd for $C_{25}H_{21}N_3O_3$ (M+H+) 411.1582, found: 411.1581.

2-(4-Ethoxyphenyl)-4-phenylbenzo[4,5]imidazo[1,2-a]-pyrimidine **(4r)**

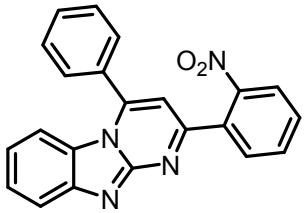


**(4r)**

Yield 82%; yellow solid; Mp: 202-204 °C; $^1$H NMR (400 MHz, $CDCl_3$): δ 8.18 (d, *J*=7.7,

2H), 7.90 (s, 1H), 7.61-7.65 (m, 5H), 7.37 (s, 1H), 7.10 (s, 1H), 6.89-6.96 (m, 3H), 6.61 (d, *J*=7.7 Hz, 1H), 4.0 (q, *J*=7.0 Hz, 2H), 1.39 (t, *J*=7.0 Hz, 3H), $^{13}$C NMR (100 MHz, $CDCl_3$): δ 161.71, 160.49, 148.90, 145.44, 132.63, 130.93, 129.42, 129.31, 128.78, 128.42, 125.59, 120.78, 119.87, 114.61, 114.41, 104.84, 63.61, 14.74; HRMS (ESI, m/z): calcd for $C_{24}H_{19}N_3O$ ($M+H^+$) 365.1528, found: 365.1529.

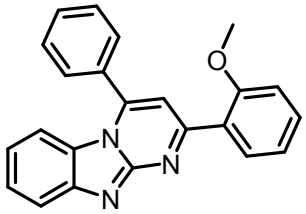
2-(2-Nitrophenyl)-4-phenylbenzo[4,5]imidazo[1,2-a]-pyrimidine **(4s)**




**(4s)**

Yield 71%; yellow solid; Mp: 218-220 $^{o}$C; $^{1}$H NMR (400 MHz, $CDCl_3$): δ 7.95 (d, *J*=7.7, 2H), 7.19 (d, *J* =6.2 Hz, 1H), 7.61-7.68 (m, 4H), 7.55 (t, *J*=7.3 Hz, 1H), 7.45 (t, *J*=6.6 Hz, 2H), 7.05 (t, *J*=7.7 Hz, 2H), 6.79 (s, 1H), 6.75 (d, *J*=7.7 Hz, 1H), $^{13}$C NMR (100 MHz, $CDCl_3$): δ 160.59, 149.57, 148.42, 145.24, 133.62, 133.24, 131.89, 131.56, 131.37, 130.68, 129.48, 128.36, 126.32, 124.74, 121.83, 120.38, 114.93, 107.89; HRMS (ESI, m/z): calcd for $C_{22}H_{14}N_4O_2$ ($M+H^+$) 366.1116, found: 366.1117.

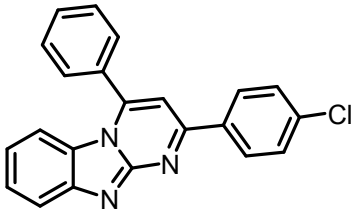
2-(2-Methoxyphenyl)-4-phenylbenzo[4,5]imidazo[1,2-a]-pyrimidine **(4t)**




**(4t)**

Yield 79%; yellow solid; Mp: 160-162 $^{o}$C; $^{1}$H NMR (400 MHz, $CDCl_3$): δ 8.27 (d, *J*=8.1, 1H), 7.95 (d, *J* =8.4 Hz, 1H), 7.62-7.70 (m, 5H), 7.50 (s, 1H), 7.40-7.45 (m, 2H), 7.12 (t, *J*=7.7 Hz, 1H), 6.98 (d, *J*=8.4 Hz, 2H), 6.68 (d, *J*=8.4 Hz, 1H), 3.87 (s, 3H), $^{13}$C NMR (100 MHz, $CDCl_3$): δ 161.26, 158.07, 152.28, 147.64, 145.37, 132.88, 132.20, 131.98, 130.85, 129.32, 128.53, 127.41, 126.62, 125.68, 121.33, 120.87, 120.12, 114.59, 111.54, 110.10, 55.71; HRMS (ESI, m/z): calcd for $C_{23}H_{17}N_3O$ ($M+H^+$) 351.13716, found: 351.13716.

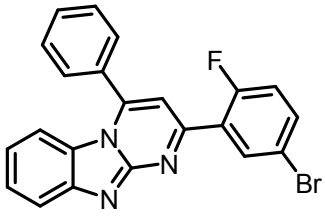
2-(4-Chlorophenyl)-4-phenylbenzo[4,5]imidazo[1,2-a]-pyrimidine **(4u)**




**(4u)**

Yield 85%; yellow solid; Mp: 198-200 °C; $^1$H NMR (400 MHz, $CDCl_3$): δ 8.16 (d, *J*=8.8 Hz, 2H), 7.90 (d, *J* =8.1 Hz, 1H), 7.63-7.73 (m, 5H), 7.42 (d, *J*=8.8 Hz, 3H), 7.14 (s, 1H), 6.98 (t, *J*=8.1 Hz, 1H), 6.64 (d, *J*=8.4 Hz, 1H), $^{13}$C NMR (100 MHz, $CDCl_3$): δ 159.66, 151.93, 149.62, 145.57, 137.61, 135.07, 132.49, 131.20, 129.48, 129.18, 129.06, 128.44, 127.44, 126.05, 121.35, 120.25, 114.63, 104.92; HRMS (ESI, m/z): calcd for $C_{22}H_{14}ClN_3$ ($M+H^+$) 355.0876, found: 355.0877.

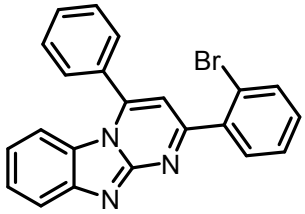
2-(2-Fluoro,5-bromophenyl)-4-phenylbenzo[4,5]imidazo[1,2-a]-pyrimidine **(4v)**




**(4v)**

Yield 81%; yellow solid; Mp: 195-197 °C; $^1$H NMR (400 MHz, $CDCl_3$): δ 8.64 (d, *J*=6.6, 1H), 7.97 (d, *J*=6.6, 1H), 7.64-7.72 (m, 5H), 7.54-7.57 (m, 1H), 7.46 (t, *J*=7.3, 1H), 7.36 (s, 1H), 7.02-7.09 (m, 2H), 6.73 (d, *J*=7.7 Hz, 1H), $^{13}$C NMR (100 MHz, $CDCl_3$): δ 161.71, 156.25, 149.49, 145.56, 135.42, 134.25, 131.27, 129.52, 128.46, 126.30, 121.59, 118.52, 118.26, 114.86, 108.59, 108.45; HRMS (ESI, m/z): calcd for $C_{22}H_{13}BrFN_3$ ($M+H^+$) 417.0276, found: 417.0278.

2-(2-Bromophenyl)-4-phenylbenzo[4,5]imidazo[1,2-a]-pyrimidine **(4w)**

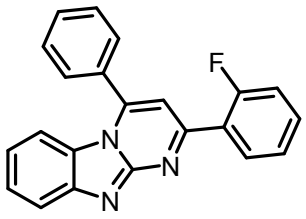



**(4w)**

Yield 80%; yellow solid; Mp: 188-190 °C; $^1$H NMR (400 MHz, $CDCl_3$): δ 7.98 (s, 1H), 7.83 (d, *J* =7.3 Hz, 1H), 7.61-7.65 (m, 6H), 7.43 (t, *J*=7.0 Hz, 2H), 7.28 (t, *J*=7.7 Hz, 1H), 7.17 (s, 1H), 7.01 (t, *J*=7.3 Hz, 1H), 6.75 (d, *J*=7.7 Hz, 1H), $^{13}$C NMR (100 MHz, $CDCl_3$): δ 162.75,

148.32, 139.18, 133.58, 132.35, 131.95, 131.15, 129.39, 128.33, 127.84, 125.95, 121.42, 121.37, 114.85, 109.83; HRMS (ESI, m/z): calcd for $C_{22}H_{14}BrN_3$ ($M+H^+$) 399.0371, found: 399.0373.

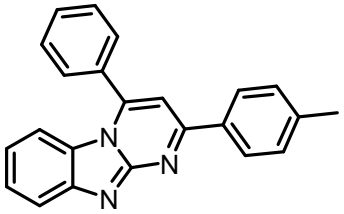
2-(2-Fluorophenyl)-4-phenylbenzo[4,5]imidazo[1,2-a]-pyrimidine **(4x)**




**(4x)**

Yield 78%; yellow solid; Mp: 172-174 $^oC$; $^1H$ NMR (400 MHz, $CDCl_3$): δ 8.47 (s, 1H), 8.00 (s, 1H), 7.63-7.69 (m, 5H), 7.45-7.50 (m, 2H), 7.39 (s, 1H), 7.33 (t, *J*=7.7 Hz, 1H), 7.14-7.19 (m, 1H), 7.01 (t, *J*=7.7 Hz, 1H), 6.76 (s, 1H), $^{13}C$ NMR (100 MHz, $CDCl_3$): δ 160.05, 157.68, 149.23, 147.32, 145.79, 132.69, 132.60, 131.52, 131.01, 129.28, 128.31, 125.80, 124.79, 121.26, 116.48, 116.25, 108.95, 108.82; HRMS (ESI, m/z): calcd for $C_{22}H_{14}FN_3$ ($M+H^+$) 339.1171, found: 339.1172.

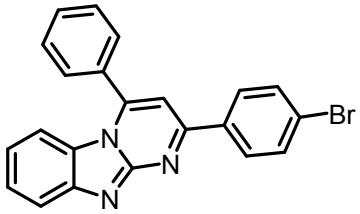
2-(4-Methylphenyl)-4-phenylbenzo[4,5]imidazo[1,2-a]-pyrimidine **(4y)**




**(4y)**

Yield 83%; yellow solid; Mp: 190-192 $^oC$; $^1H$ NMR (400 MHz, $CDCl_3$): δ 8.17 (d, *J*=8.4 Hz, 2H), 7.93 (d, *J* =8.4 Hz, 1H), 7.61-7.66 (m, 3H), 7.38-7.41 (m, 1H), 7.33 (d, *J*=8.1 Hz, 1H), 7.27 (d, *J*=8.1 Hz, 2H), 7.19 (s, 1H), 7.16 (d, *J*=8.1 Hz, 1H), 6.98 (t, *J*=7.7 Hz, 1H), 6.64 (d, *J*=8.4 Hz, 1H), 2.39 (s, 3H), $^{13}C$ NMR (100 MHz, $CDCl_3$): δ 161.09, 152.29, 149.19, 145.52, 141.88, 133.92, 132.69, 131.06, 129.71, 128.42, 128.99, 128.47, 127.80, 127.53, 126.67, 125.84, 121.06, 120.14, 114.53, 105.23, 21.55; HRMS (ESI, m/z): calcd for $C_{23}H_{17}N_3$ ($M+H^+$) 335.1422, found: 335.1421.

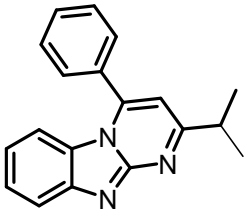
2-(4-Bromophenyl)-4-phenylbenzo[4,5]imidazo[1,2-a]-pyrimidine **(4z)**




**(4z)**

Yield 84%; yellow solid; Mp: 210-212 °C; $^{1}$H NMR (400 MHz, $CDCl_3$): δ 8.12 (d, *J*=6.6 Hz, 2H), 7.96 (s, 1H), 7.65-7.72 (m, 5H), 7.59 (d, *J*=7.3 Hz, 2H), 7.42 (s, 1H), 7.17 (s, 1H), 7.00 (t, *J*=7.7 Hz, 1H), 3.69 (d, *J*=7.0 Hz, 1H), $^{13}$C NMR (100 MHz, $CDCl_3$): δ 160.61, 152.40, 151.45, 138.47, 136.25, 135.58, 133.78, 132.25, 129.68, 128.18, 127.88, 125.71, 122.62, 116.54, 114.68, 103.02; HRMS (ESI, m/z): calcd for $C_{22}H_{14}BrN_3$ ($M+H^+$) 399.0371, found: 399.0372.

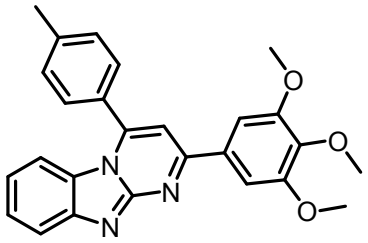
2-Isopropyl-4-phenylbenzo[4,5]imidazo[1,2-*a*]pyrimidine (**4ab**)

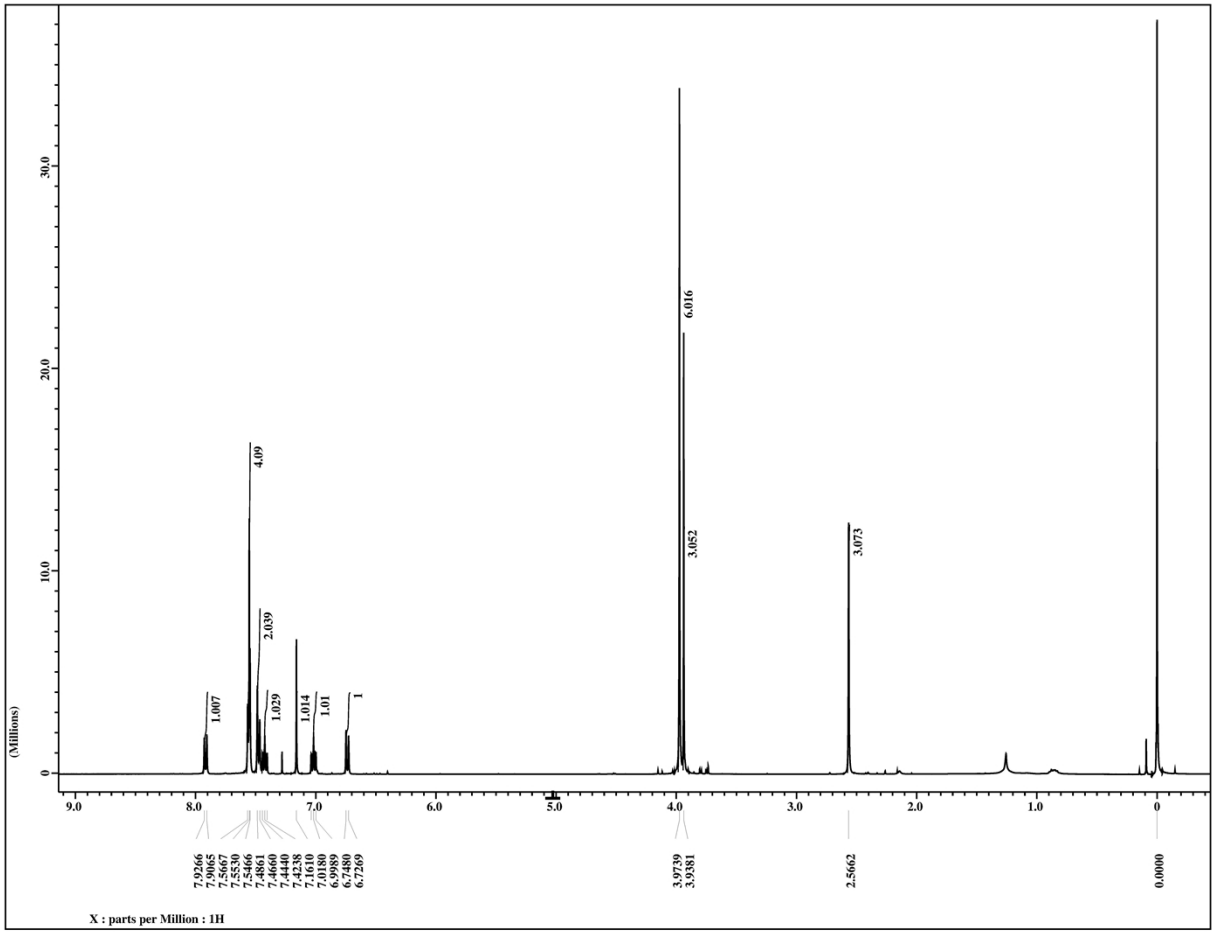


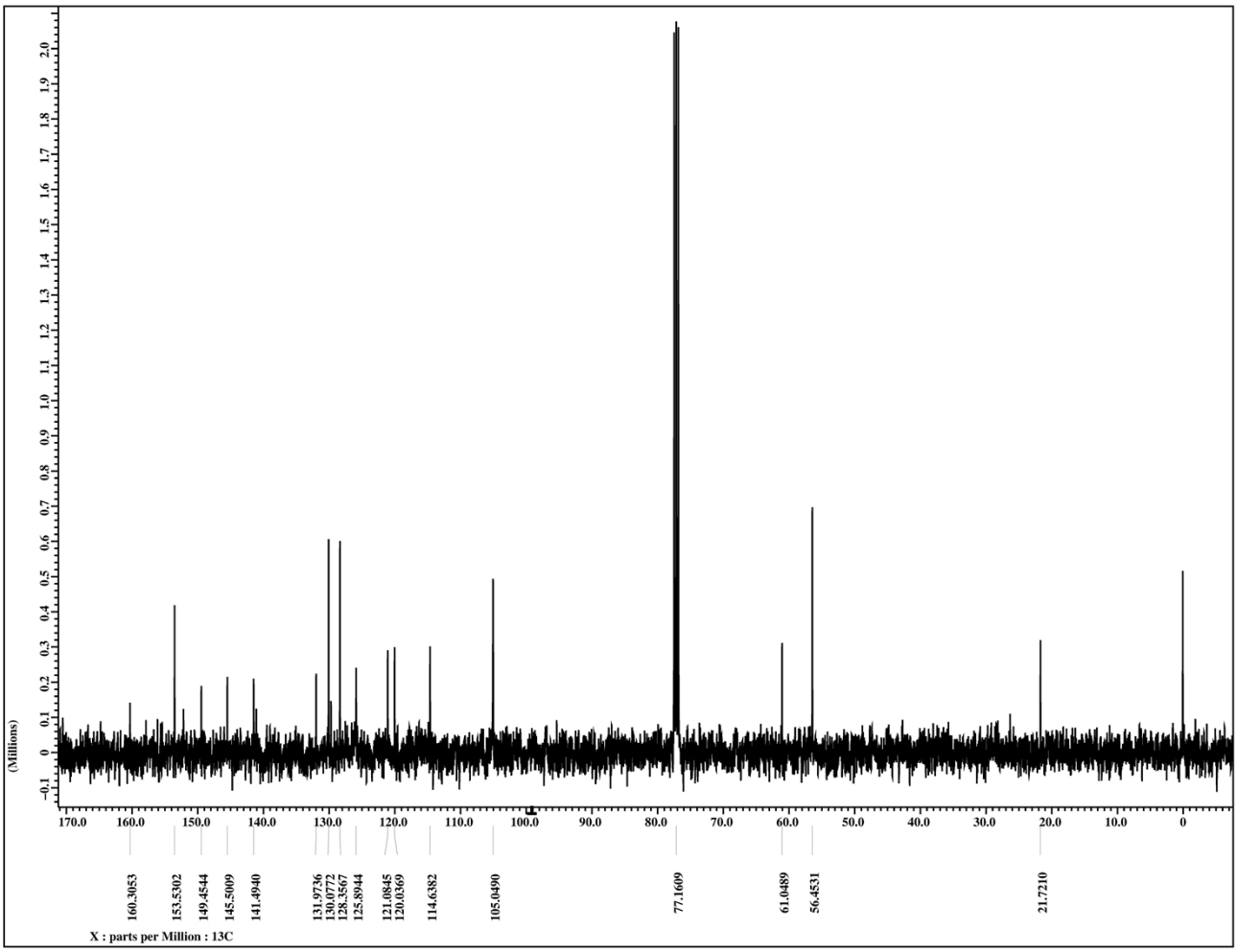

**(4ab)**

Yield 52%; yellow solid; Mp: 193-195 °C; $^{1}$H NMR (400 MHz, $CDCl_3$): δ 7.98 (br, 1H), 7.66−7.60 (m, 5H), 7.43 (s, 1H), 7.02 (t, *J* = 7.6 Hz, 1H), 6.69 (s, 2H), 3.23 (m, 1H), 1.43 (d, *J* = 6.2 Hz, 6H), $^{13}$C NMR (100 MHz, $CDCl_3$): δ 173.49, 148.88, 132.67, 130.89, 129.26, 128.81, 128.13, 127.78, 125.46, 120.67, 120.09, 114.39, 106.88, 37.13, 21.52; HRMS (ESI, m/z): calcd for $C_{19}H_{17}N_3$ ($M+H^+$) 287.1422, found: 287.1424.

$^{1}$H NMR and $^{13}$C NMR spectra of the compounds

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1.5
1.4
1.3
1.2
1.1
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0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
-0.1
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
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153.5302
149.4544
145.5009
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131.9736
130.0772
128.3567
125.8944
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21.7210
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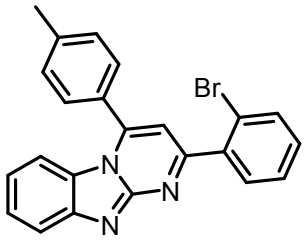
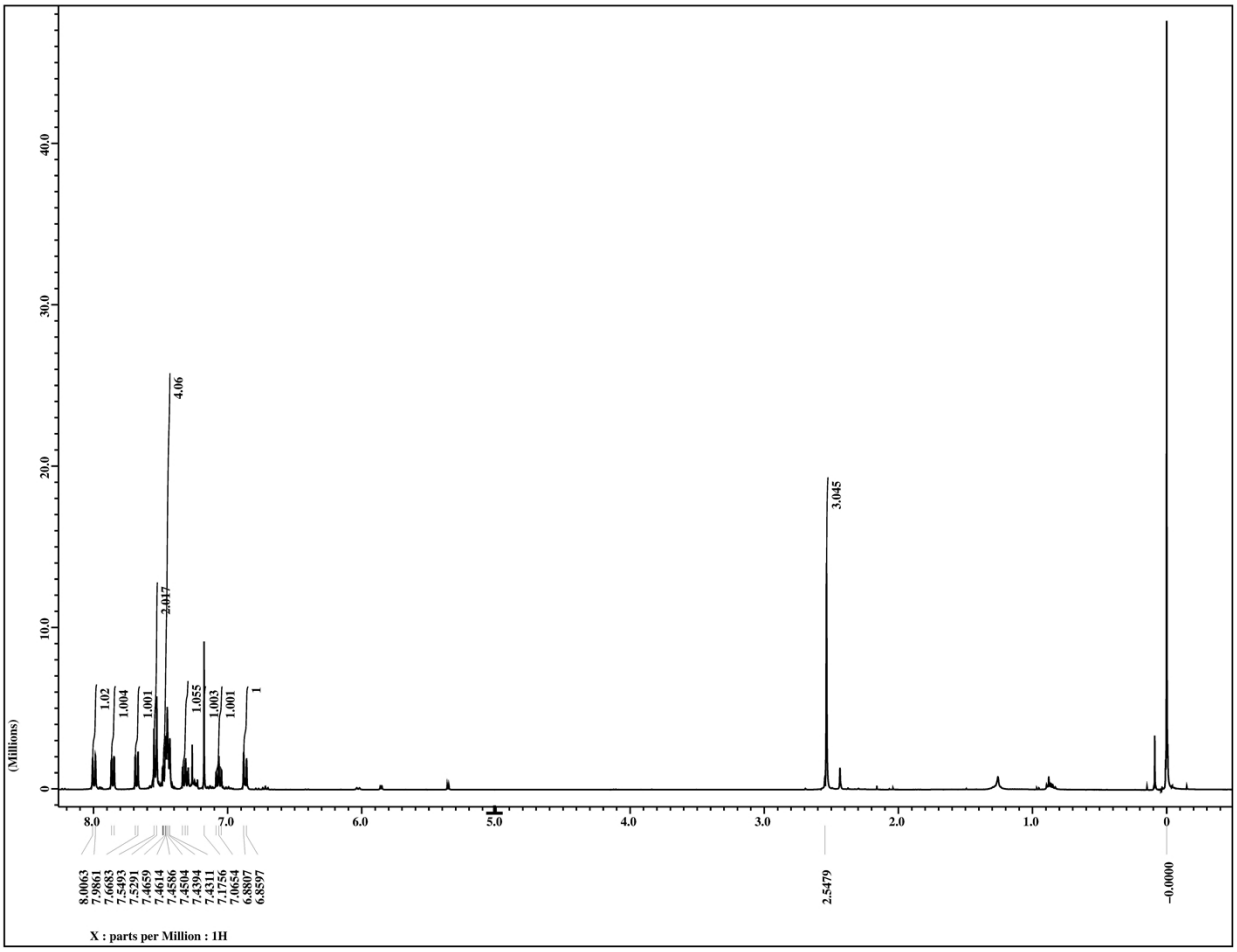

Br
N
N
N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7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
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7.9861
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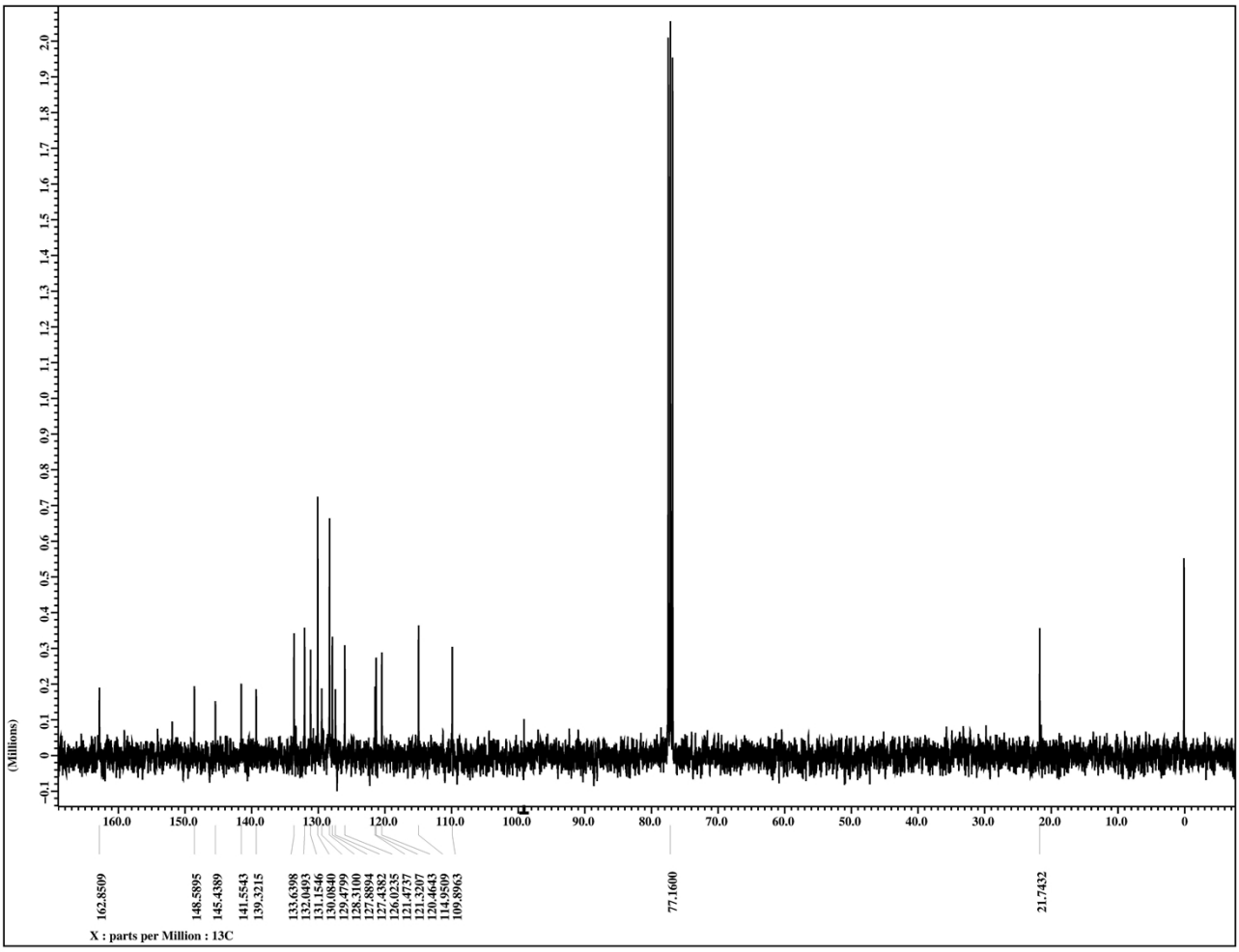
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0.4
0.3
0.2
0.1
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130.0
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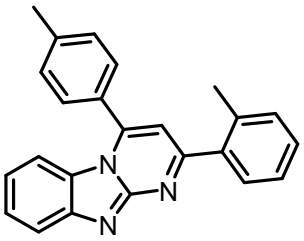

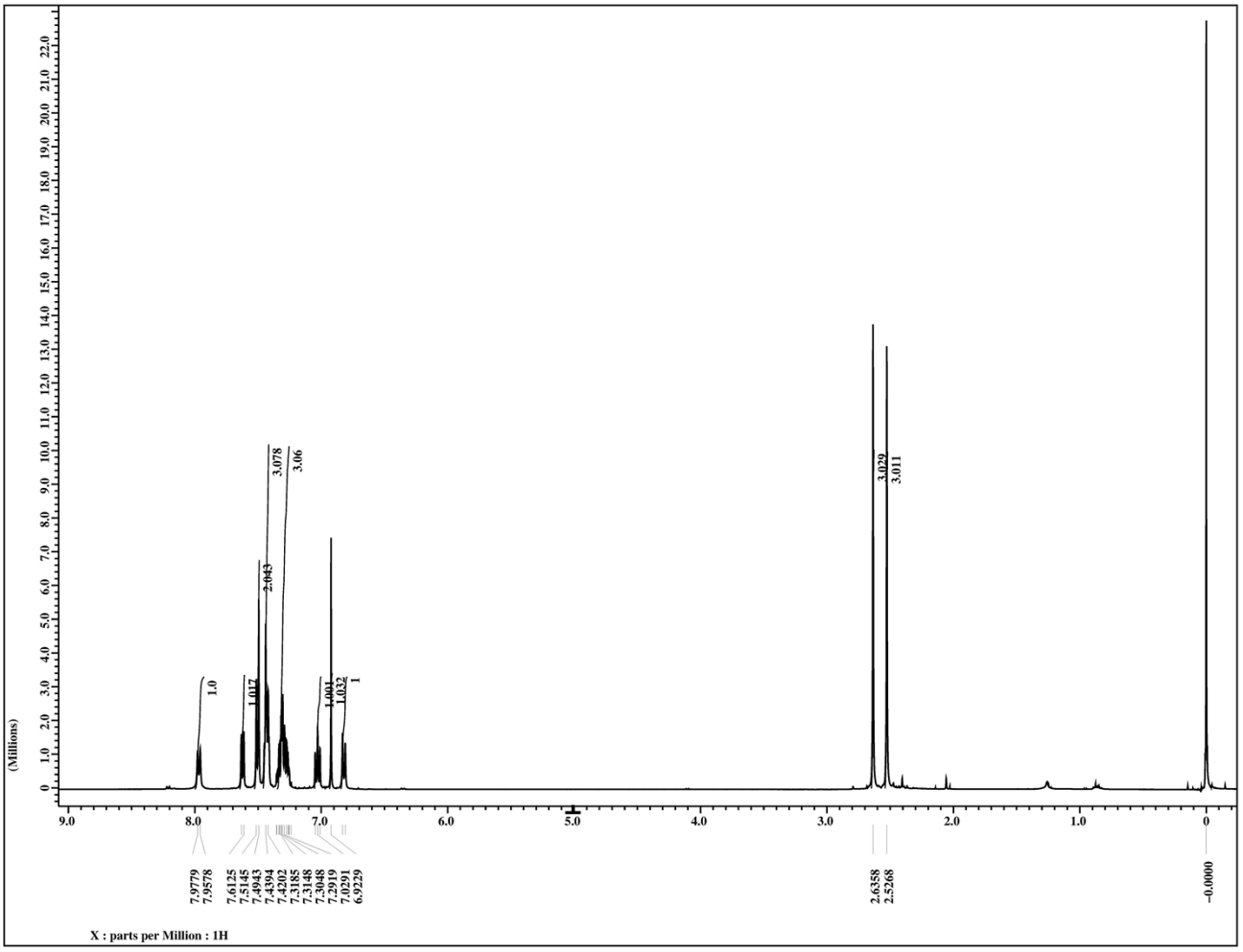
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5.0
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3.0
2.0
1.0
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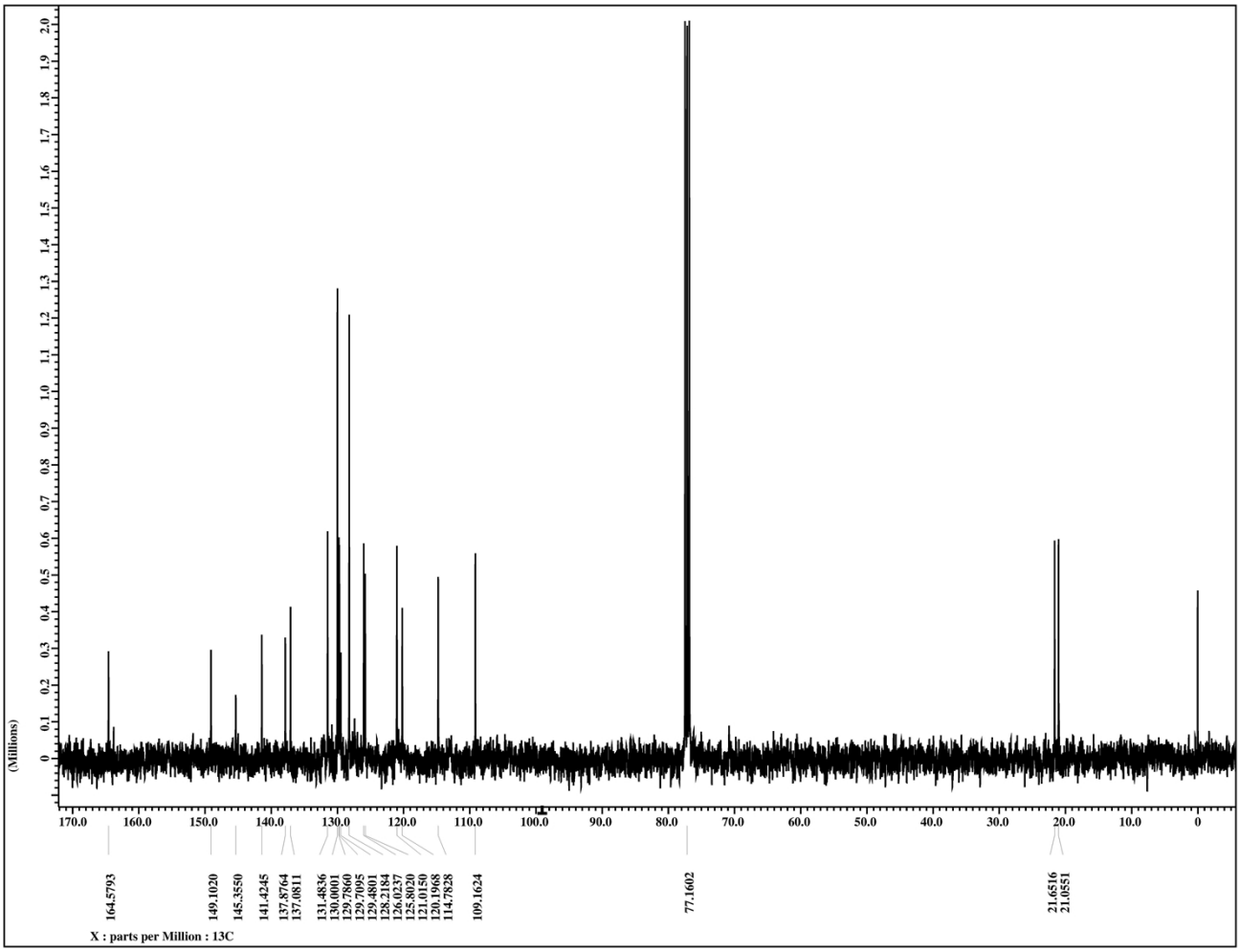
X : parts per Million : 1H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1.2
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0.6
0.5
0.4
0.3
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140.0
130.0
120.0
110.0
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90.0
80.0
70.0
60.0
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40.0
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10.0
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129.4801
128.2184
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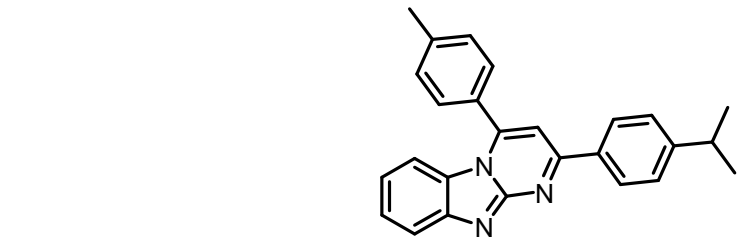
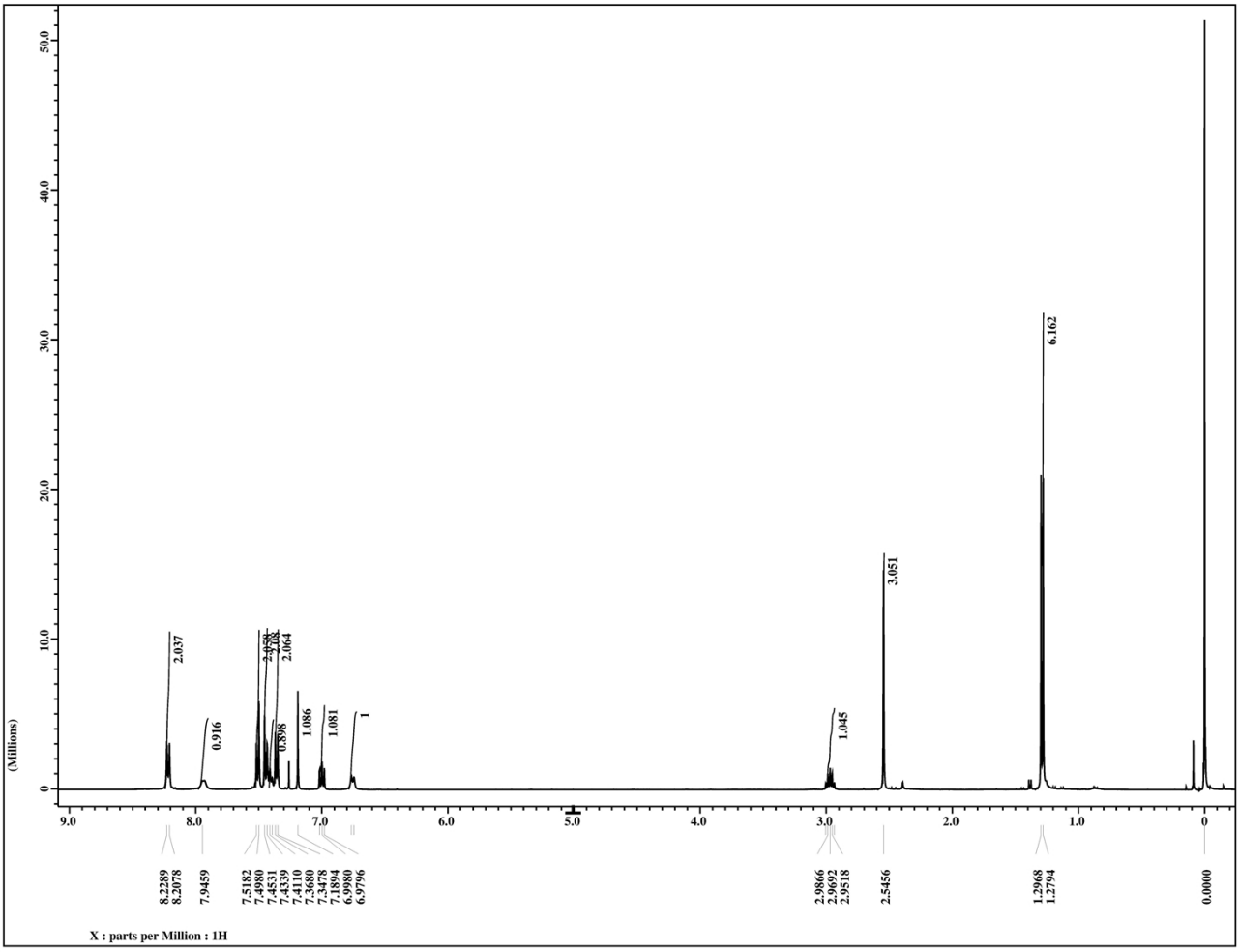
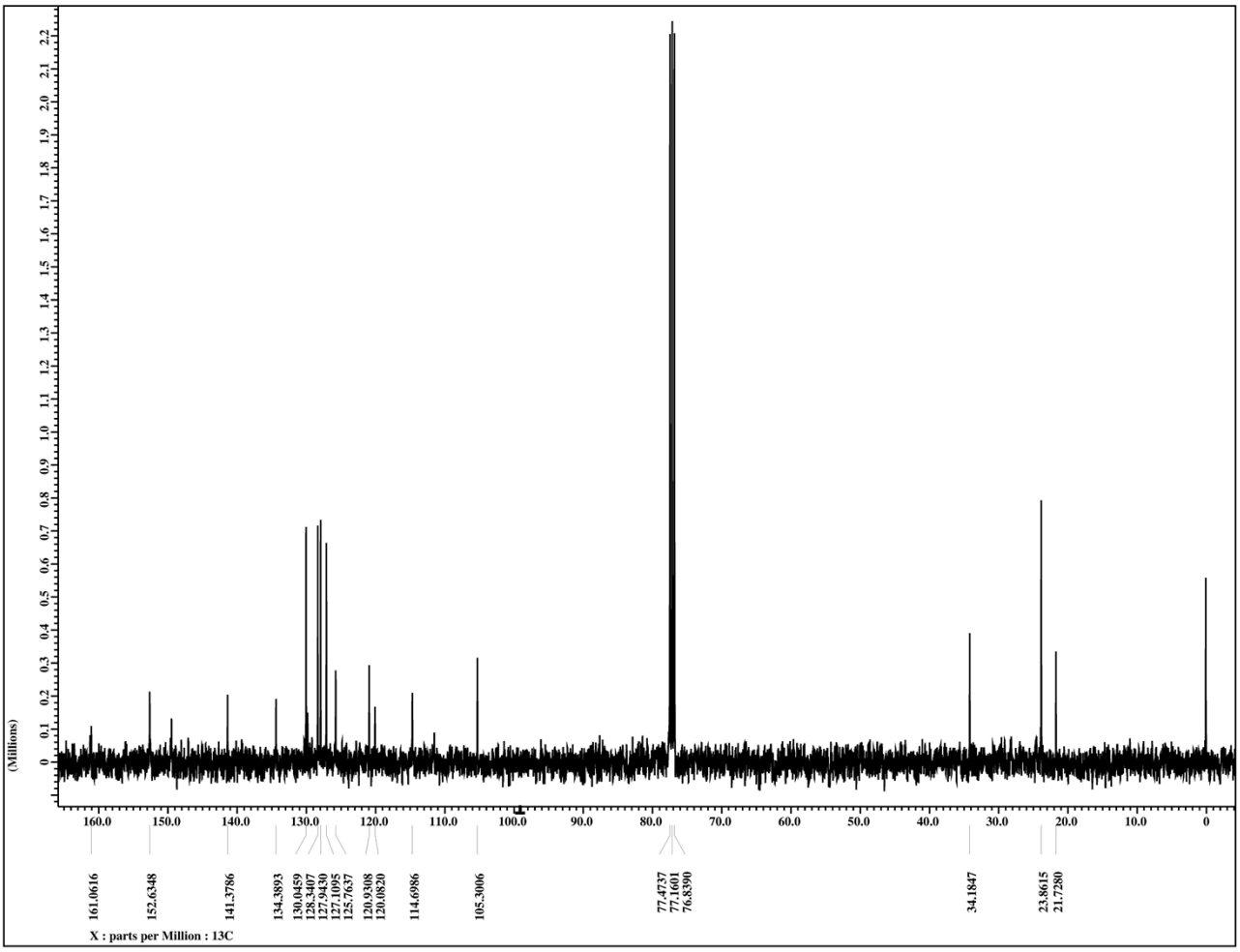
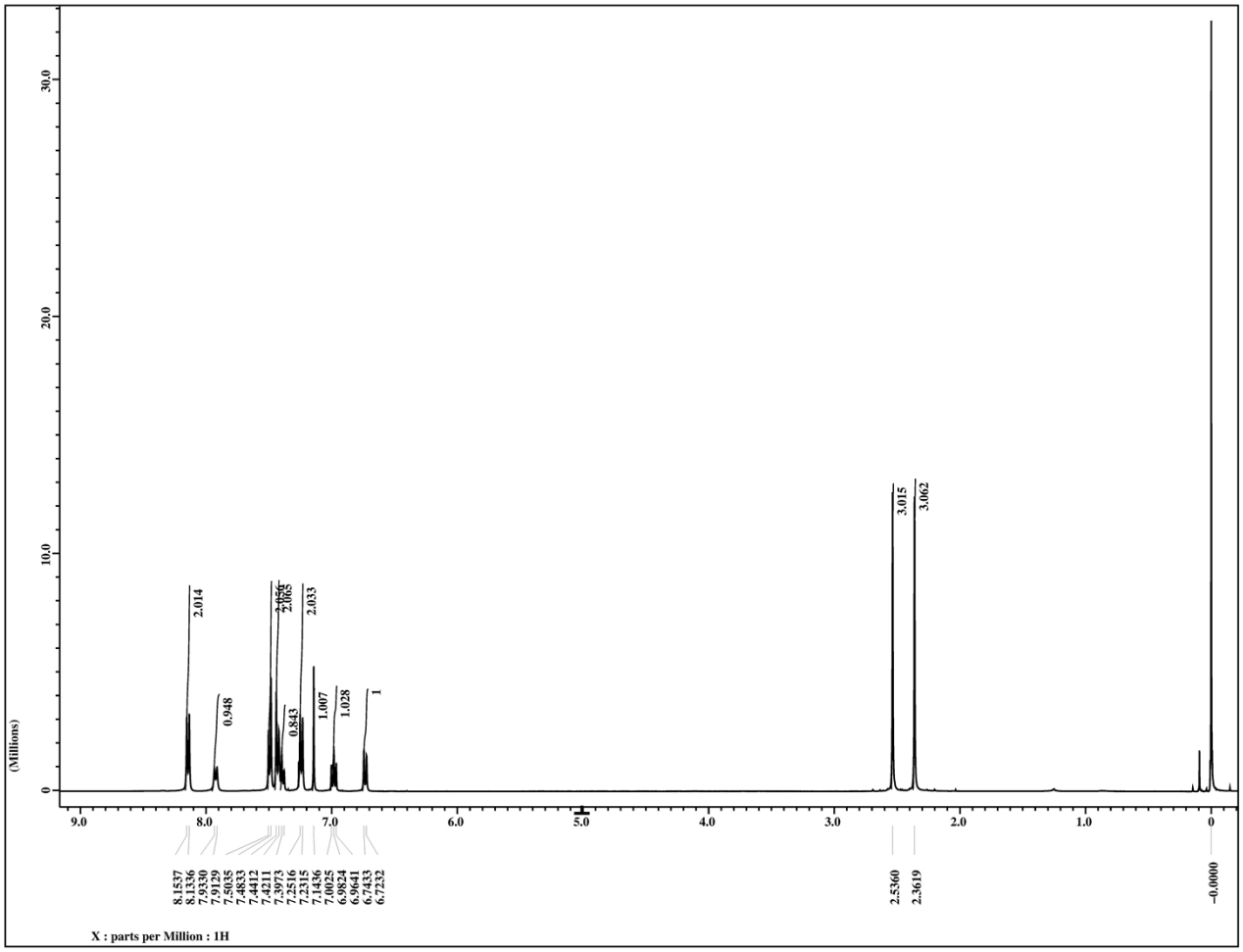
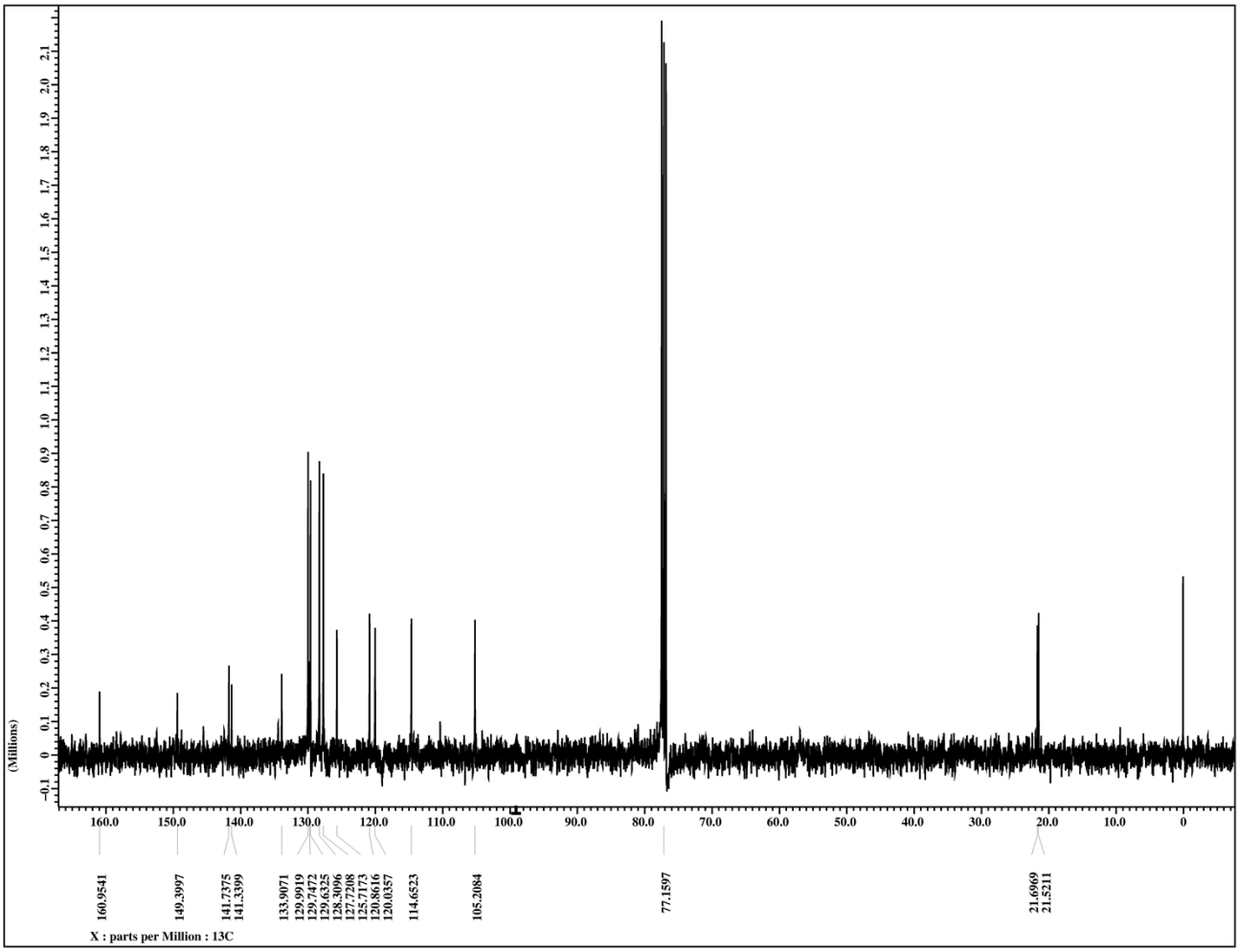
114.7828
109.1624
77.1602
21.6516
21.0551
X : parts per Million : 13C

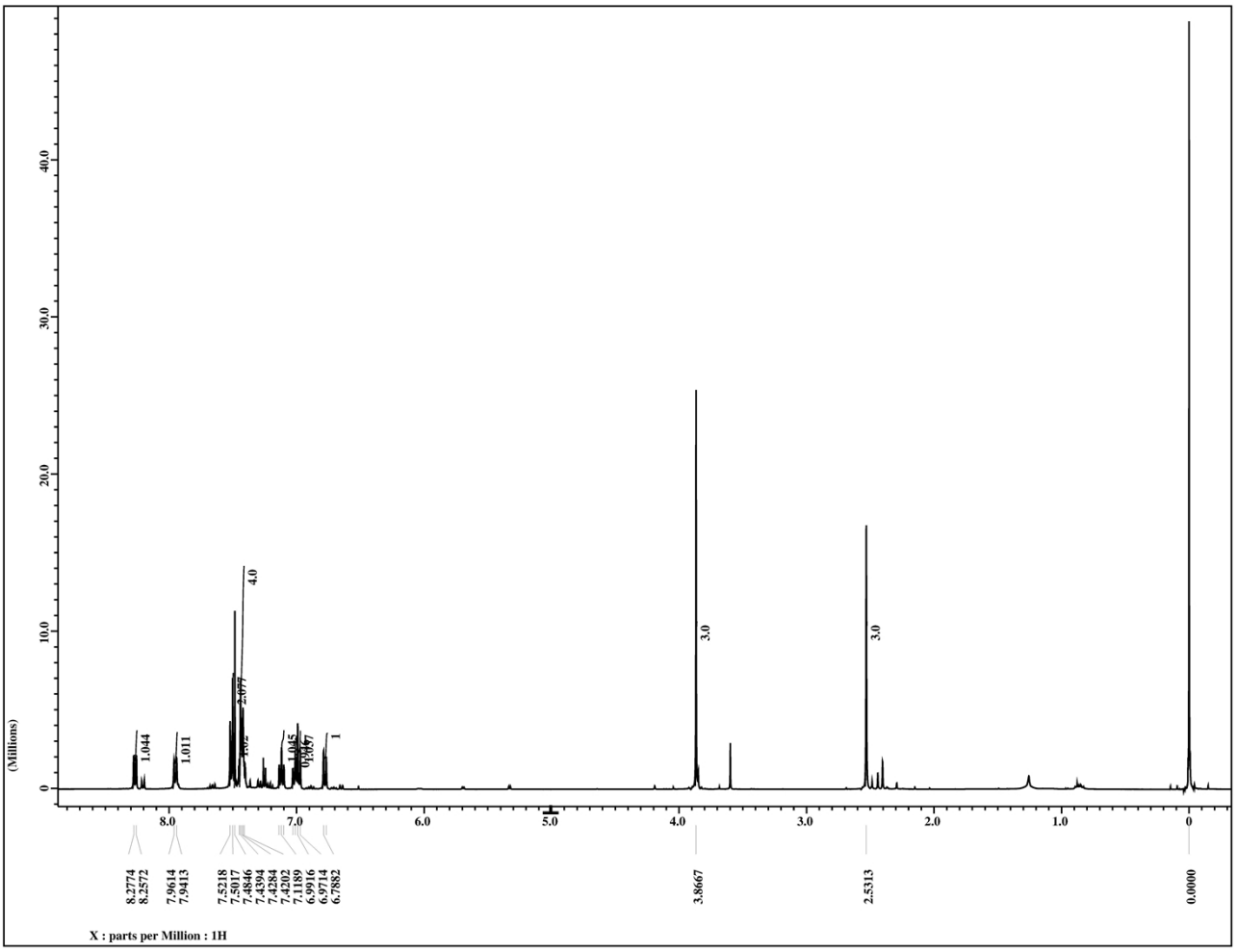


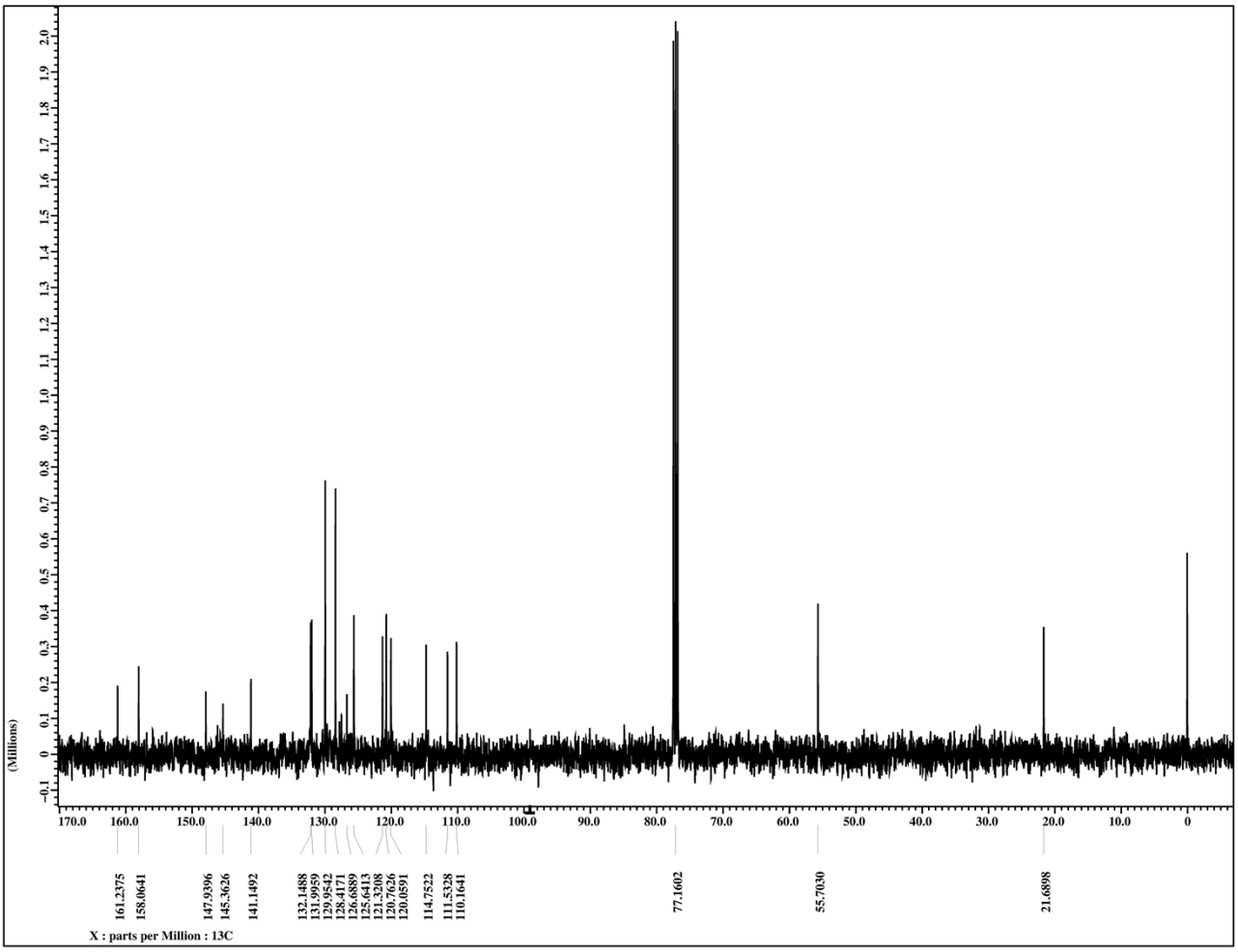

(Millions)
50.0
40.0
30.0
20.0
10.0
0
2.037
0.916
2.064
1.086
1.081
1
1.045
3.051
6.162
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.2289
8.2078
7.9459
7.5182
7.4980
7.4531
7.4339
7.4110
7.3680
7.3478
7.1894
6.9980
6.9796
2.9866
2.9692
2.9518
2.5456
1.2968
1.2794
0.0000
X : parts per Million : 1H

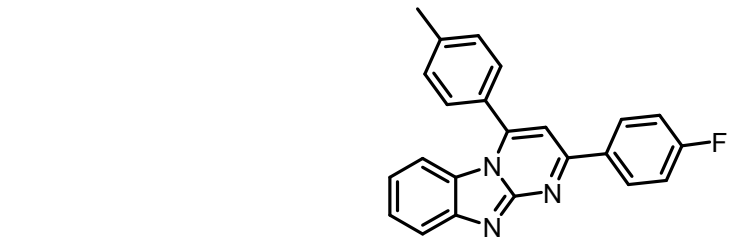

(Millions)
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8 1.9 2.0 2.1 2.2
160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
161.0616
152.6348
141.3786
134.3893
130.0459
128.3407
127.9430
127.1095
125.7637
120.9308
120.0820
114.6986
105.3006
77.4737
77.1601
76.8390
34.1847
23.8615
21.7280
X : parts per Million : 13C

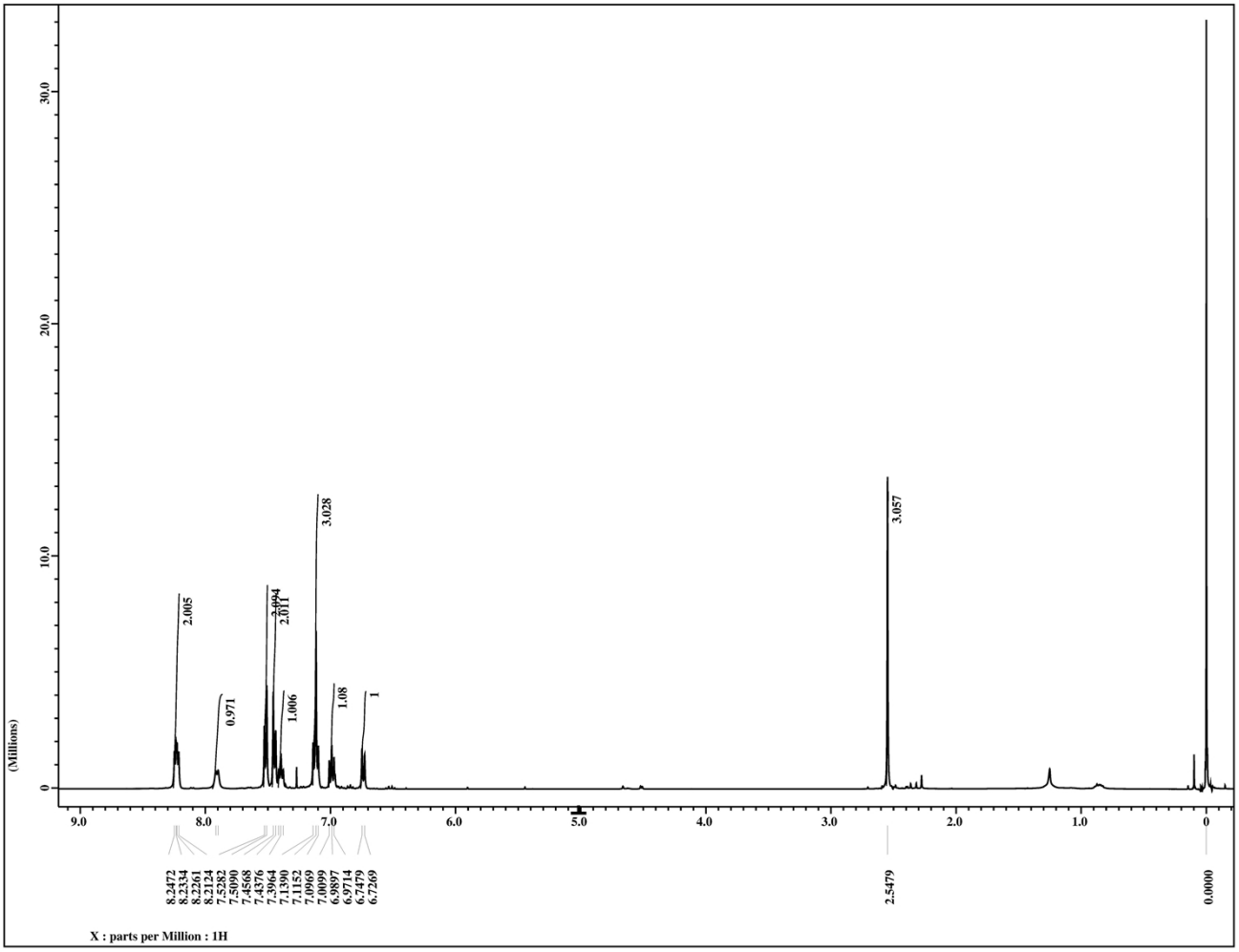

(Millions)
30.0
20.0
10.0
0
2.014
0.948
2.033
0.843
1.007
1.028
1
3.015
3.062
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.1537
8.1336
7.9330
7.9129
7.5035
7.4833
7.4412
7.4211
7.3973
7.2516
7.2315
7.1436
7.0025
6.9824
6.9641
6.7433
6.7232
2.5360
2.3619
-0.0000
X : parts per Million : 1H

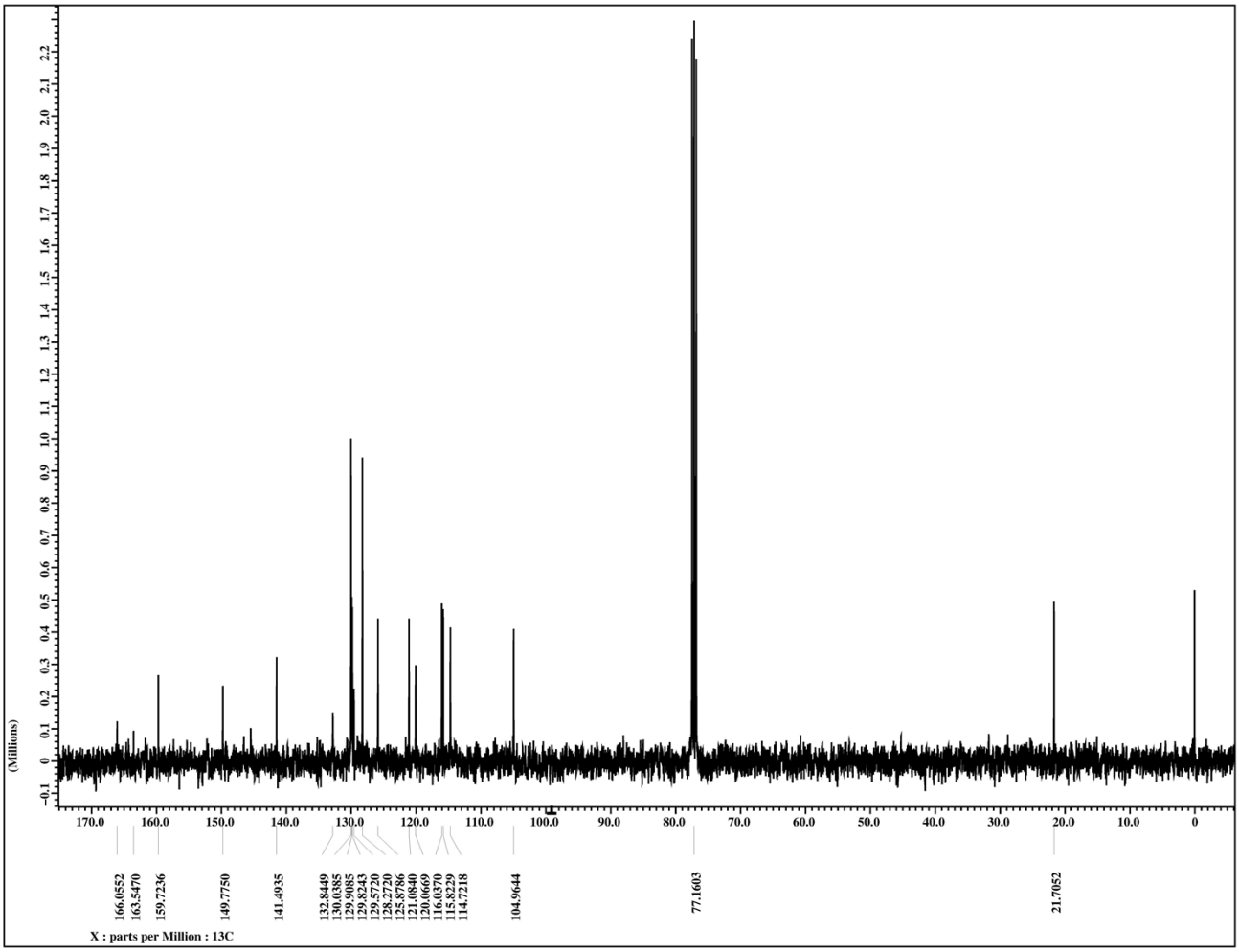

(Millions)
160.9541
149.3997
141.7375
141.3399
133.9071
129.9919
129.7472
129.4325
129.3006
127.7208
125.7173
120.8616
120.0357
114.6523
105.2084
77.1597
21.6969
21.5211
X : parts per Million : 13C

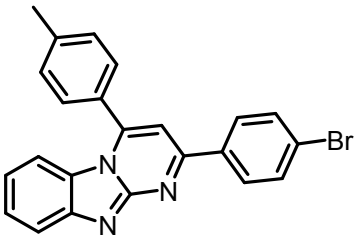

(Millions)
40.0
30.0
20.0
10.0
0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
1.044
1.011
4.0
2.077
1.045
0.947
1
3.0
3.0
8.2774
8.2572
7.9614
7.9413
7.5218
7.5017
7.4846
7.4394
7.4284
7.4102
7.1189
6.9916
6.9714
6.7882
3.8667
2.5313
0.0000
X : parts per Million : 1H

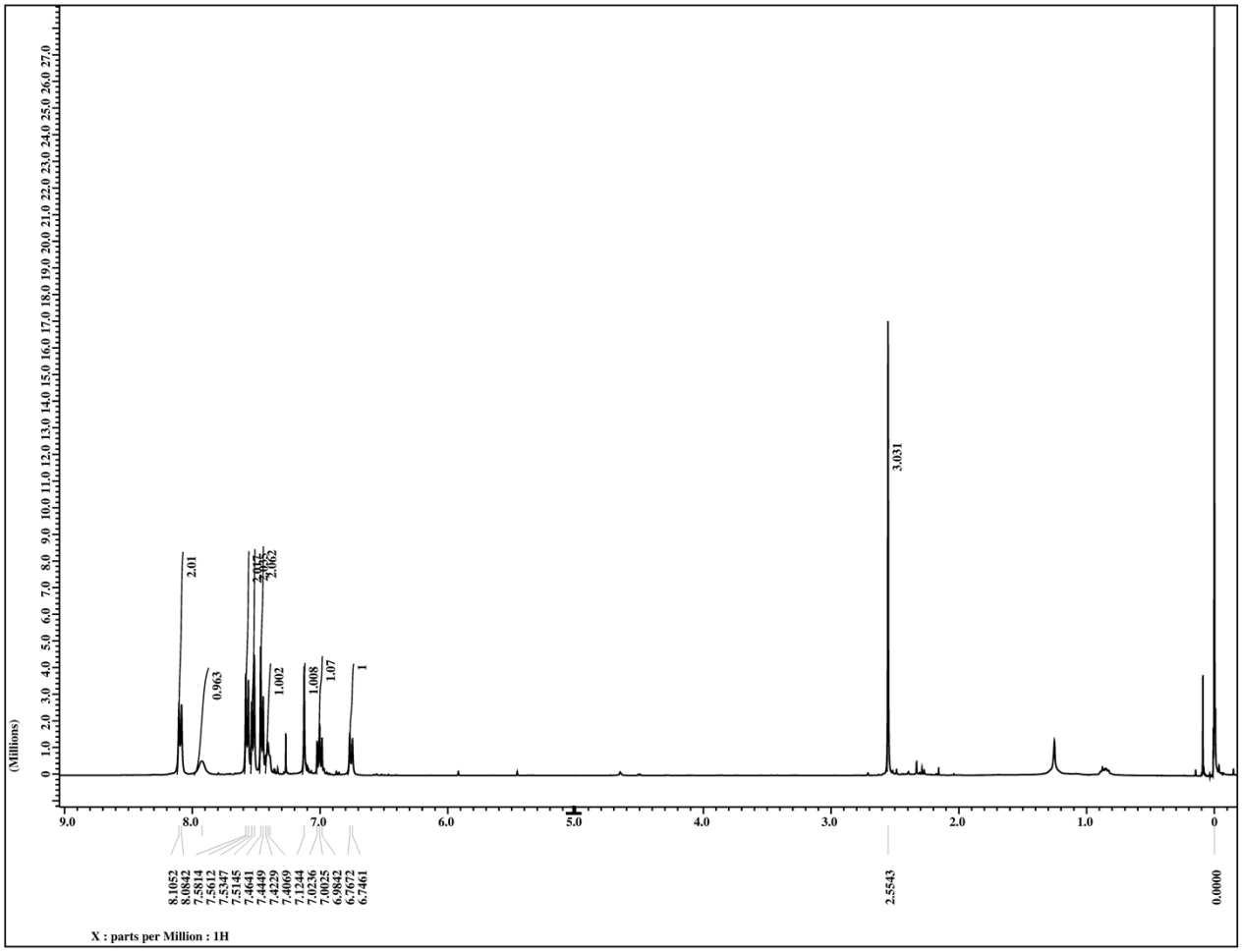

(Millions)
X : parts per Million : 13C
161.2375
158.0641
147.9396
145.3626
141.1492
132.1488
131.9959
129.3542
128.4171
126.6889
125.6413
121.3208
120.7626
120.0591
114.7522
111.5328
110.1641
77.1602
55.7030
21.6898

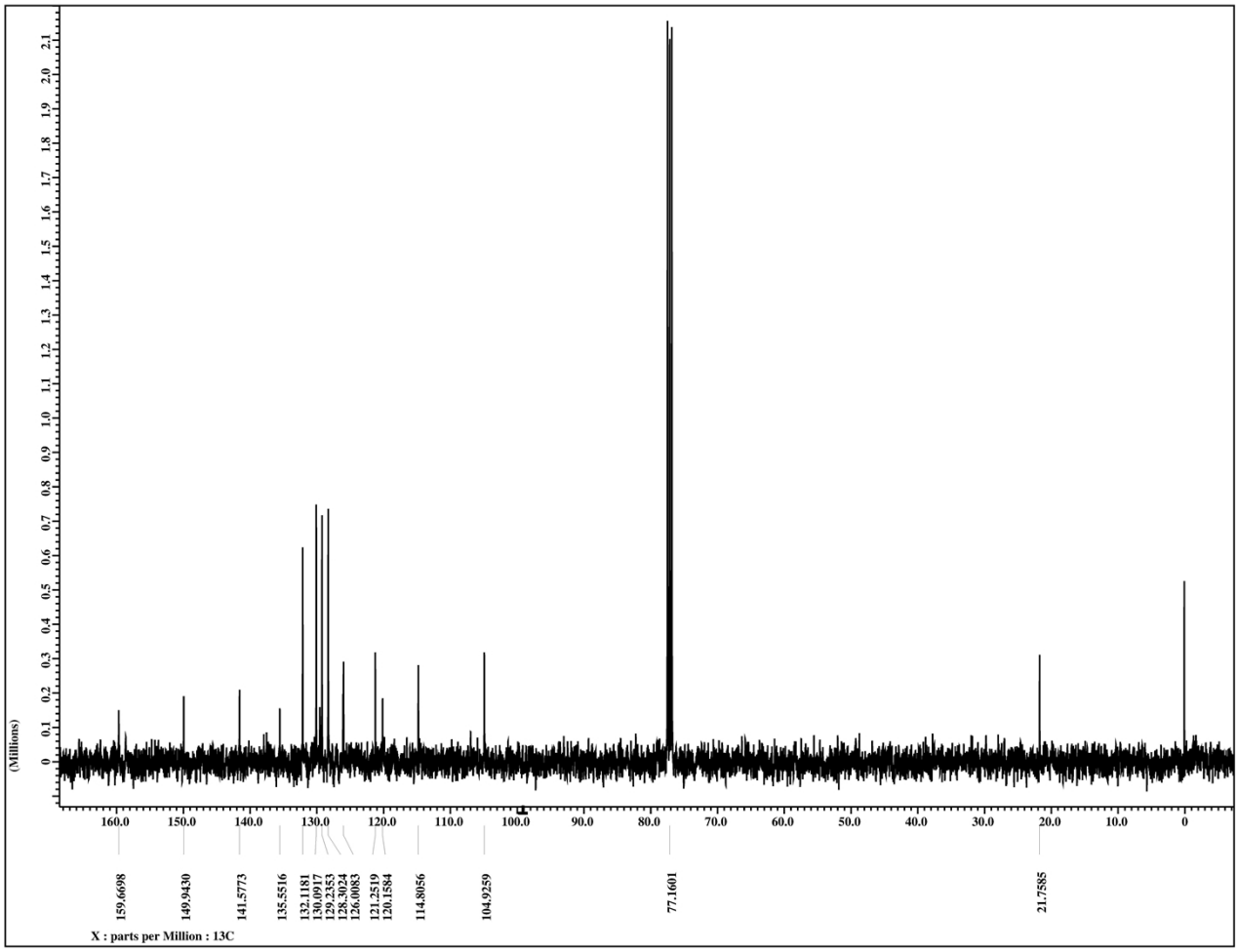

F
N
N
N

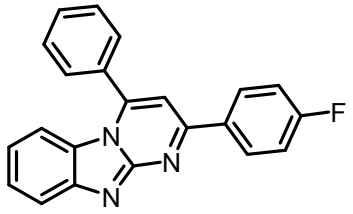

(Millions)
30.0
20.0
10.0
0
2.005
0.971
2.004
2.011
1.006
3.028
1.08
1
3.057
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.2472
8.2334
8.2261
8.2124
7.5282
7.5090
7.4568
7.4376
7.3964
7.3390
7.1152
7.0969
7.0099
6.9897
6.9714
6.7479
6.7269
2.5479
0.0000
X : parts per Million : 1H

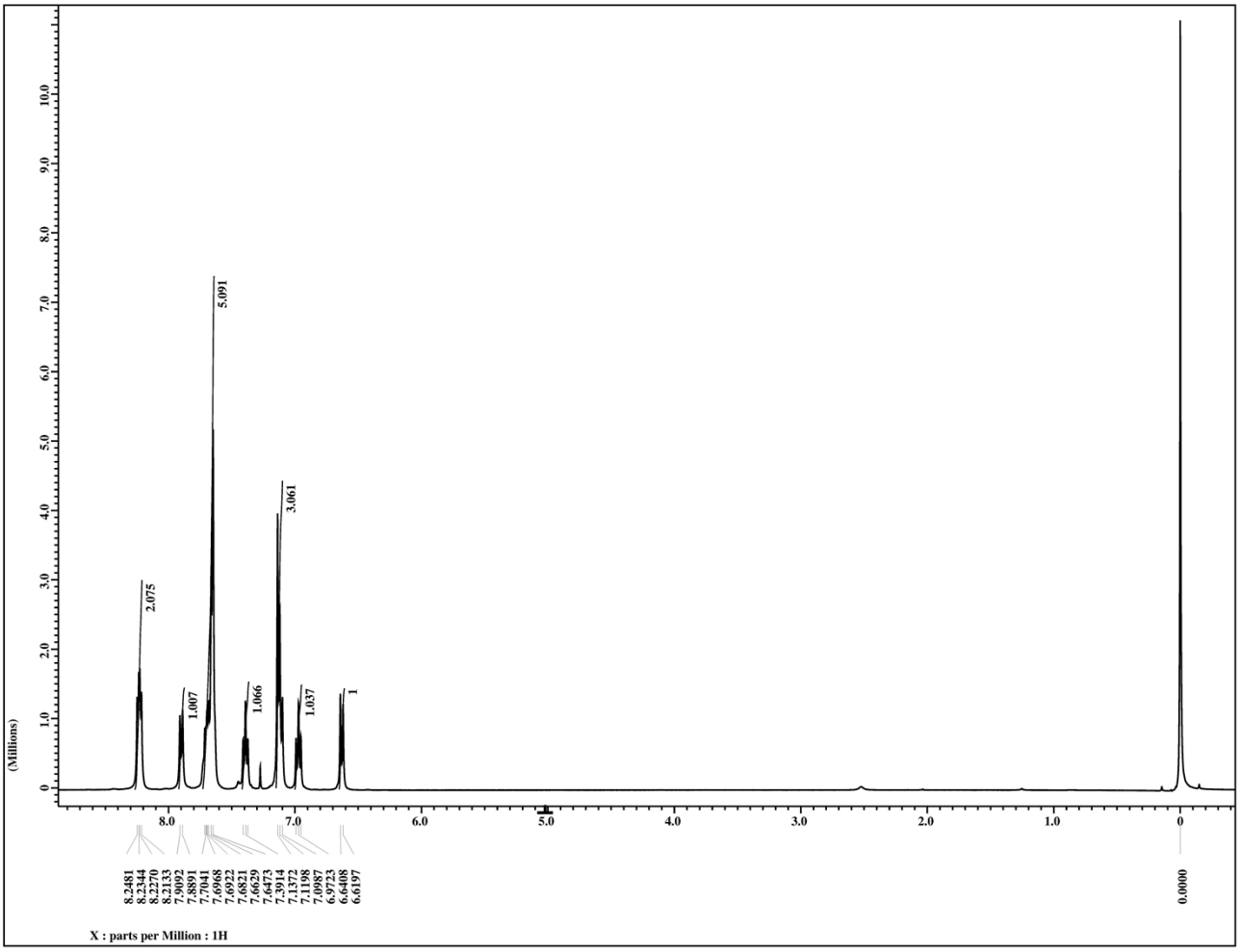

(Millions)
X : parts per Million : 13C
166.0552
163.5470
159.7236
149.7750
141.4935
132.8449
130.0385
129.9085
129.8243
129.5720
128.2720
125.8786
121.0840
120.0669
116.0370
115.8229
114.7218
104.9644
77.1603
21.7052

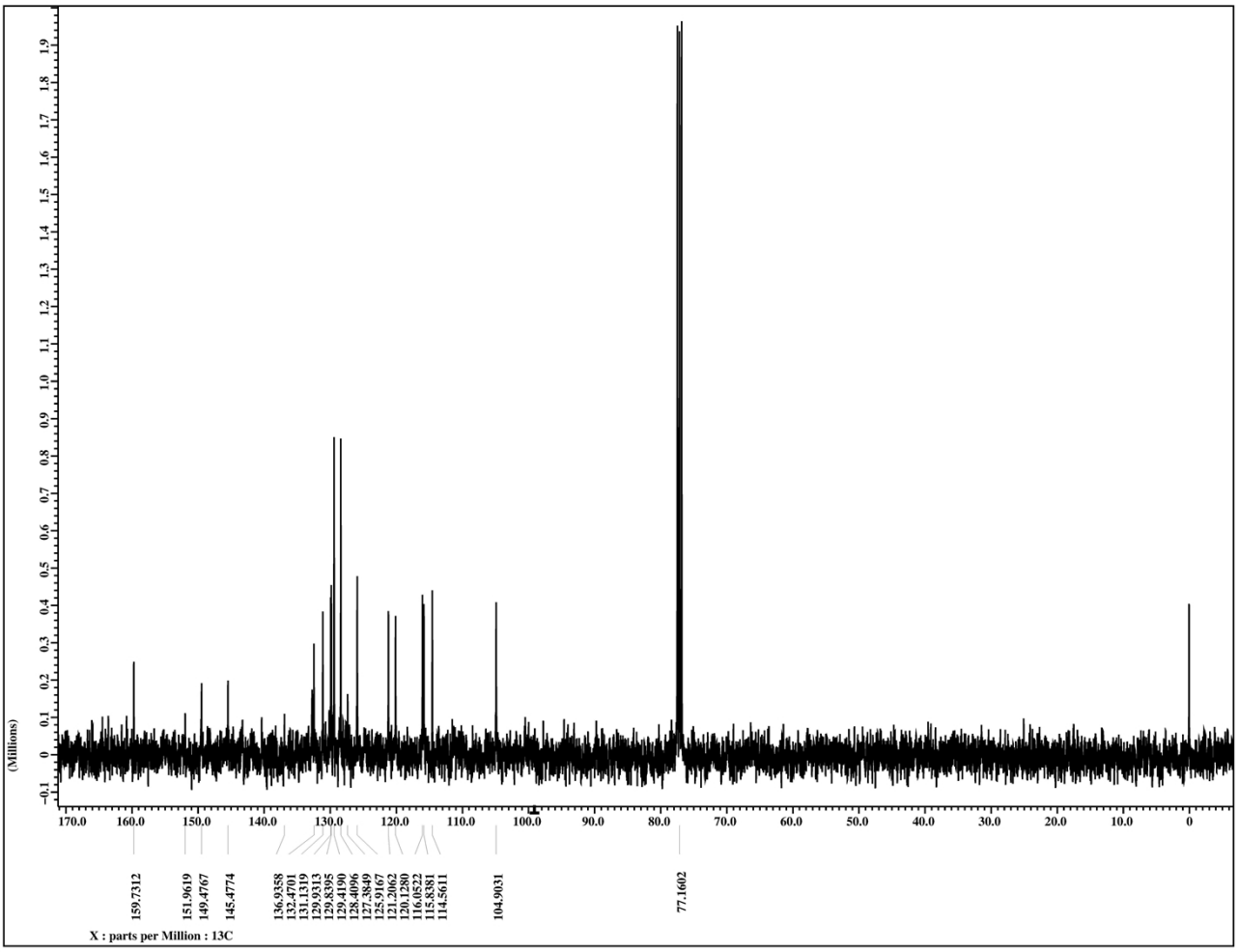

Br
N
N
N

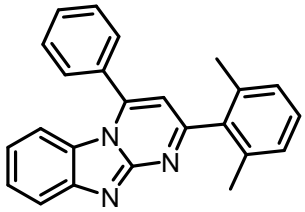

(Millions)
2.01
0.963
1.002
1.008
1.07
1
3.031
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.1052
8.0842
7.5814
7.5612
7.5347
7.5145
7.4641
7.4449
7.4229
7.4069
7.1244
7.0236
7.0025
6.9842
6.7672
6.7461
2.5543
0.0000
X : parts per Million : 1H

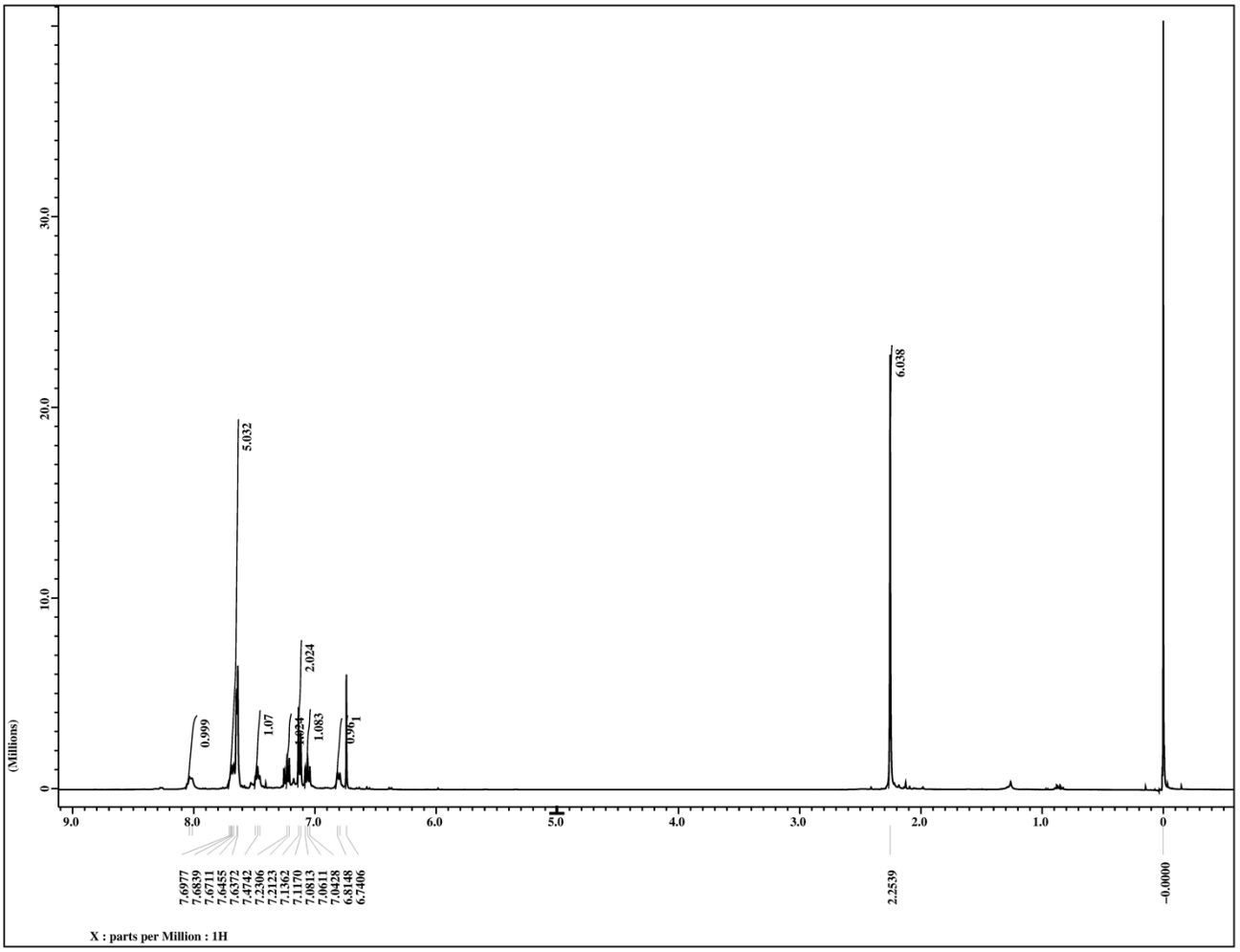

(Millions)
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8 1.9 2.0 2.1
160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
159.6698
149.9430
141.5773
135.5516
132.1181
130.0917
129.2353
128.3024
126.0083
121.2519
120.1584
114.8056
104.9259
77.1601
21.7585
X : parts per Million : 13C

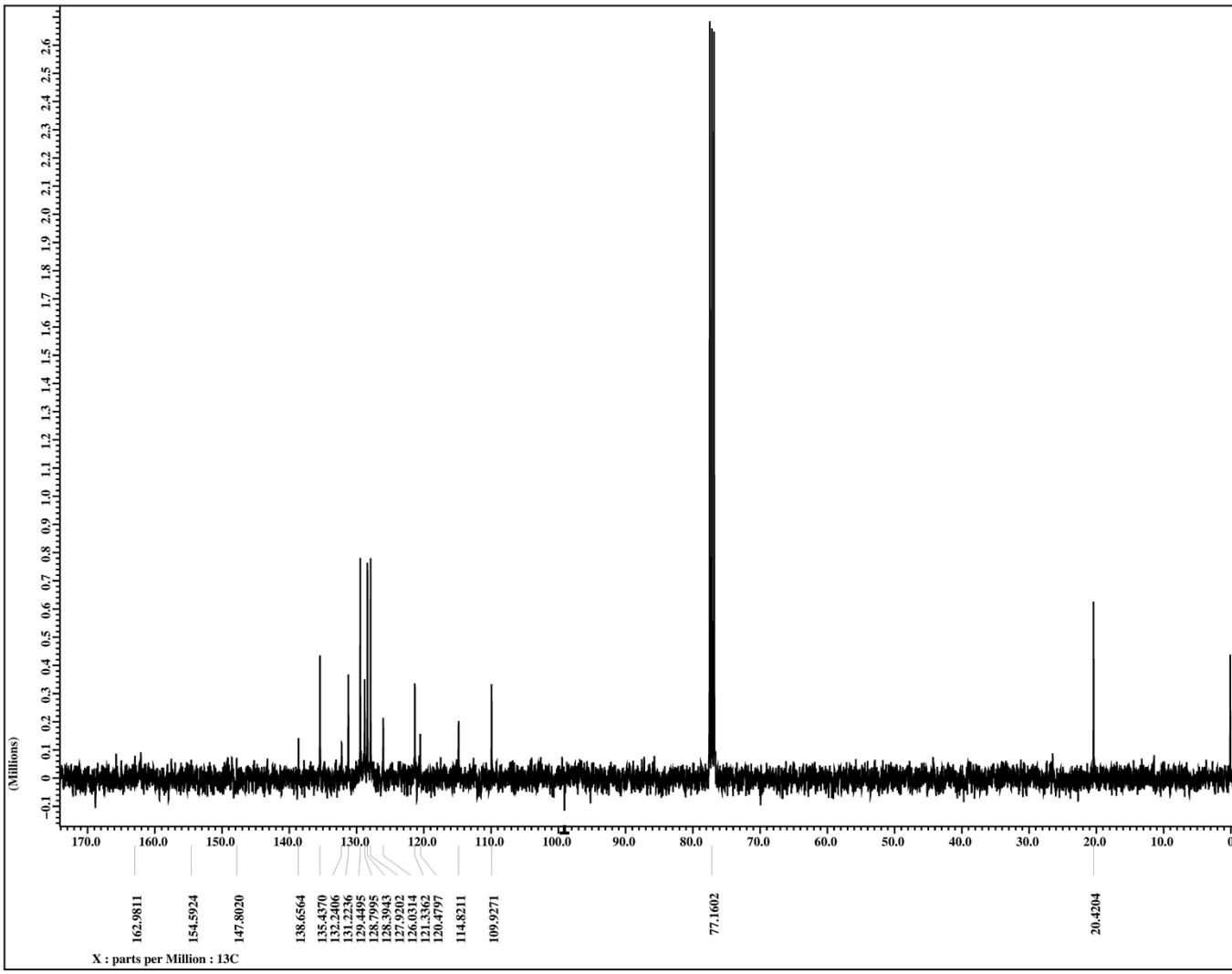

F
N
N
N

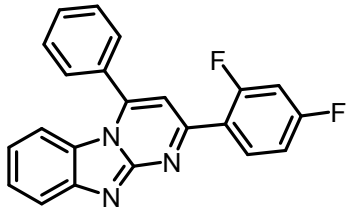

(Millions)
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
2.075
1.007
5.091
1.066
3.061
1.037
1
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.2481
8.2344
8.2270
8.2133
7.9092
7.8891
7.7044
7.6968
7.6922
7.6821
7.6629
7.6473
7.3914
7.1372
7.1198
7.0987
6.9723
6.6408
6.6197
0.0000
X : parts per Million : 1H

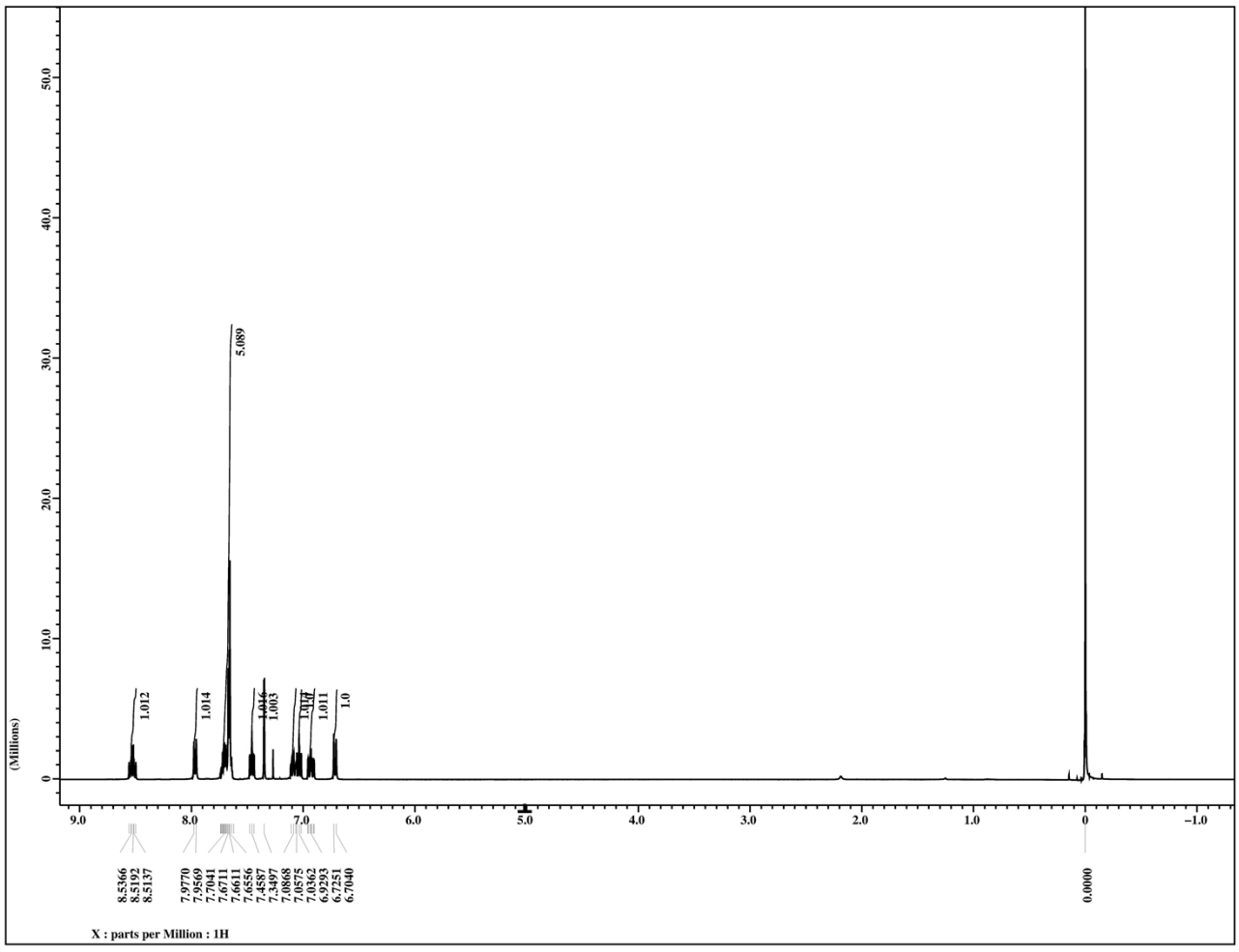

(Millions)
159.7312
151.9619
149.4767
145.4774
136.9358
132.4701
131.1319
129.9313
129.8395
129.4190
129.4096
127.3849
125.9167
121.2062
120.1280
116.0522
115.8381
114.5611
104.9031
77.1602
X : parts per Million : 13C

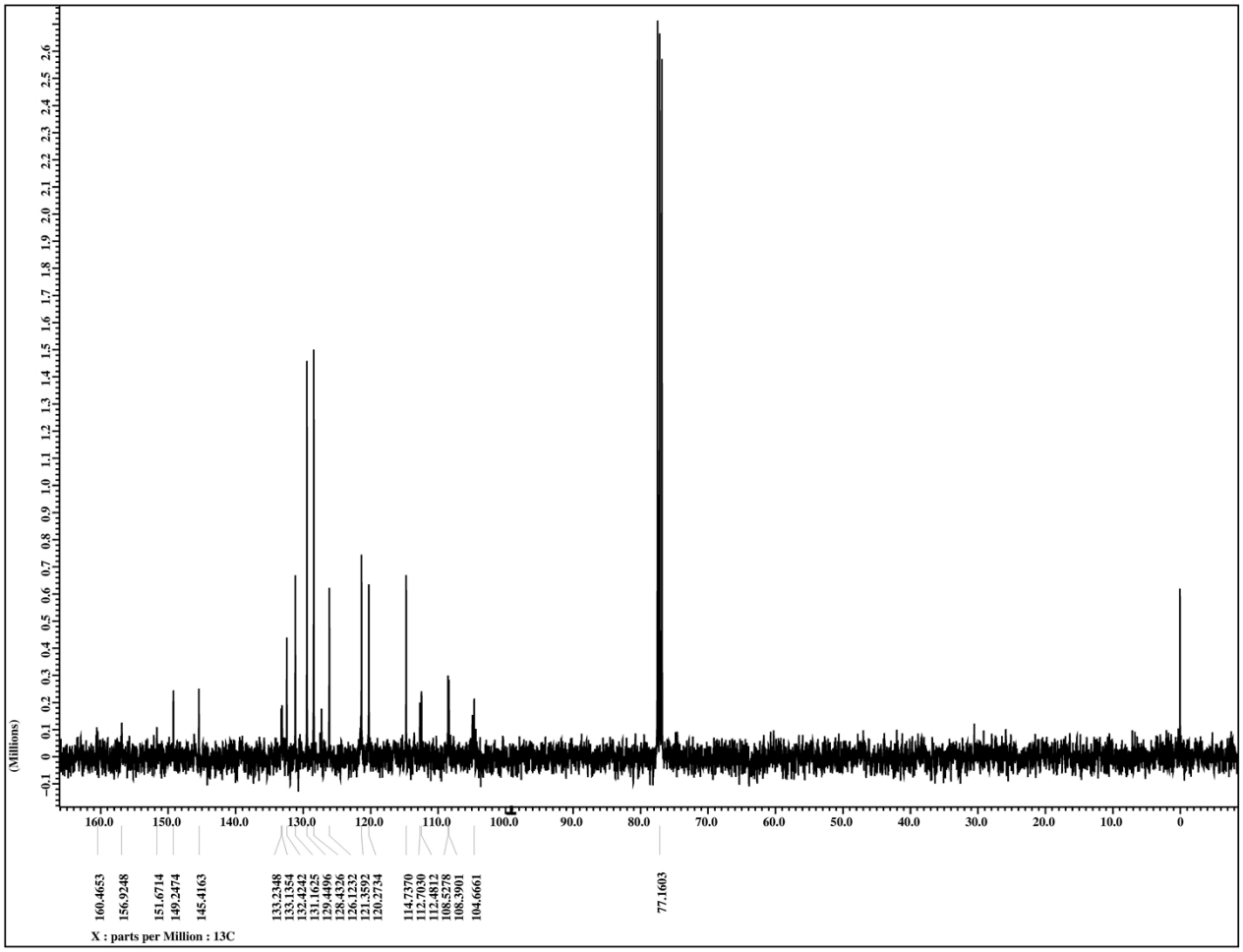


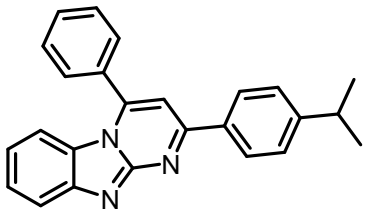

(Millions)
30.0
20.0
10.0
0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
0.999
5.032
1.07
2.024
1.083
0.96
6.038
7.6977
7.6839
7.6711
7.6455
7.6372
7.4742
7.2306
7.2123
7.1162
7.1070
7.0813
7.0611
7.0428
6.8148
6.7406
2.2539
-0.0000
X : parts per Million : 1H

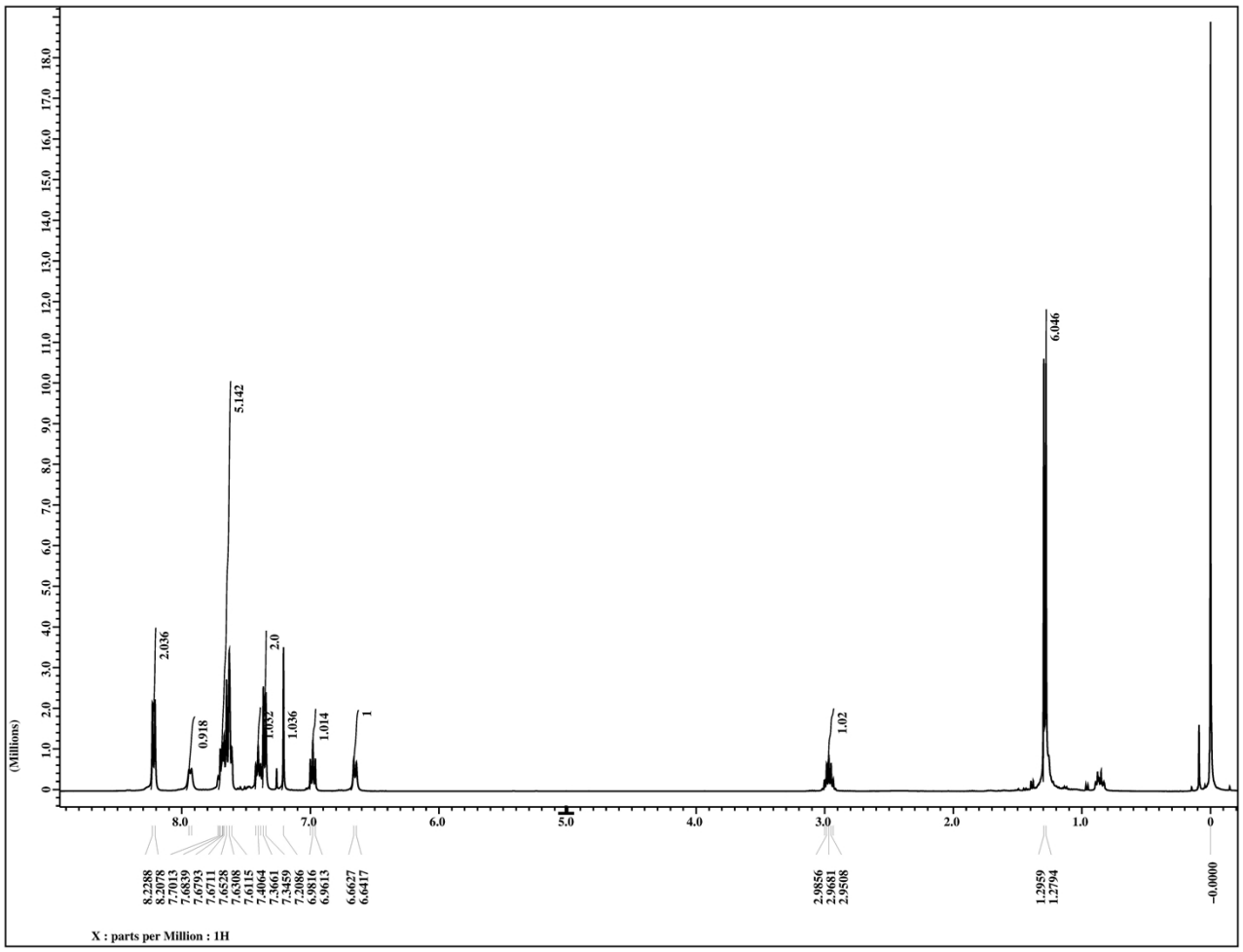

(Millions)
2.6
2.5
2.4
2.3
2.2
2.1
2.0
1.9
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
−0.1
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
162.9811
154.5924
147.8020
138.6564
135.4370
132.2406
131.2236
129.4495
128.7995
128.3943
127.9202
126.0314
121.3362
120.4797
114.8211
109.9271
77.1602
20.4204
X : parts per Million : 13C

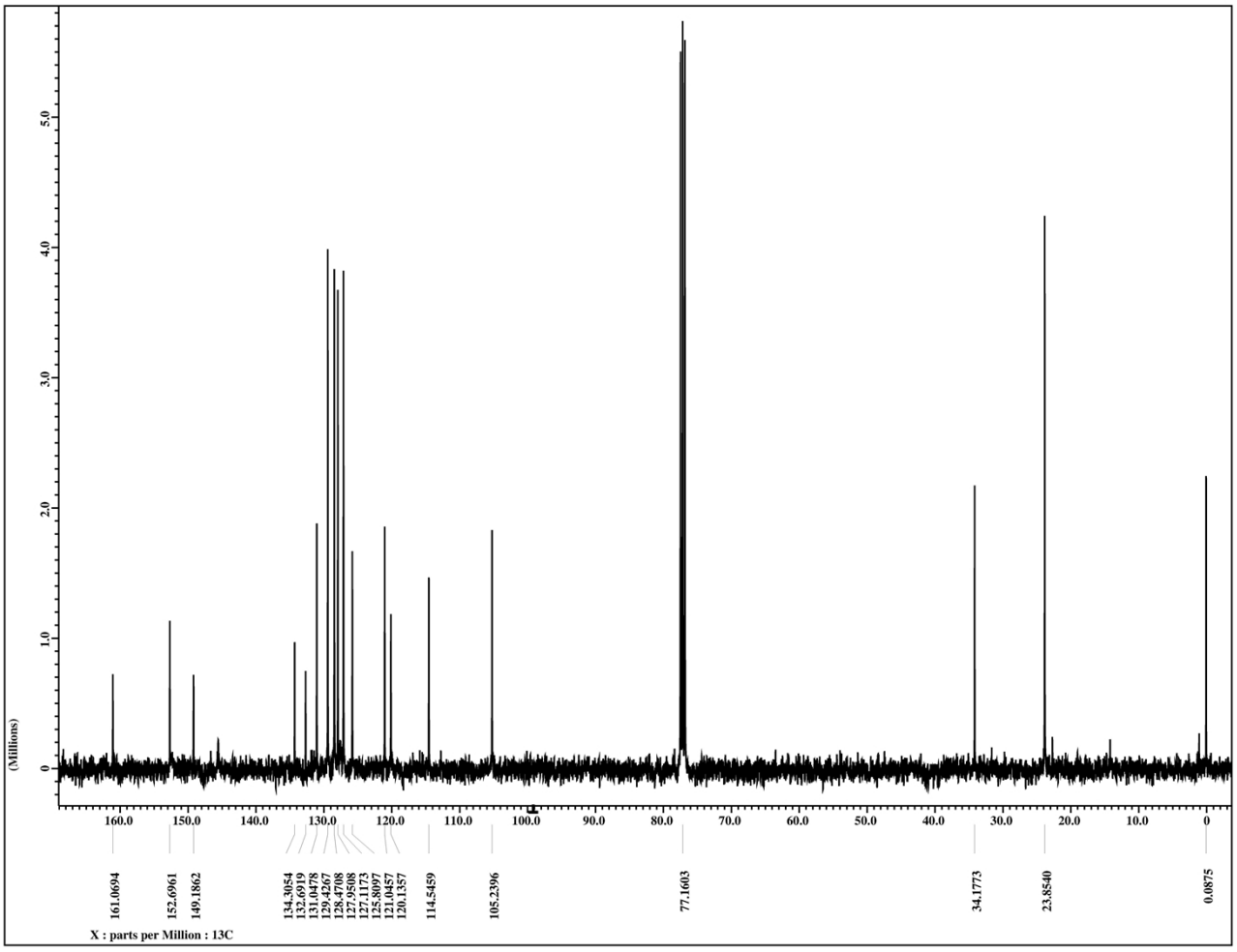

F
F
N
N
N

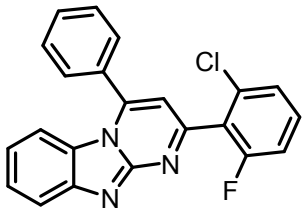

(Millions)
50.0
40.0
30.0
20.0
10.0
0
5.089
1.012
1.014
1.004
1.003
1.007
1.011
1.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−1.0
8.5366
8.5192
8.5137
7.9770
7.9569
7.7041
7.6711
7.6611
7.6456
7.4587
7.3497
7.0868
7.0575
7.0362
6.9293
6.7251
6.7040
0.0000
X : parts per Million : 1H

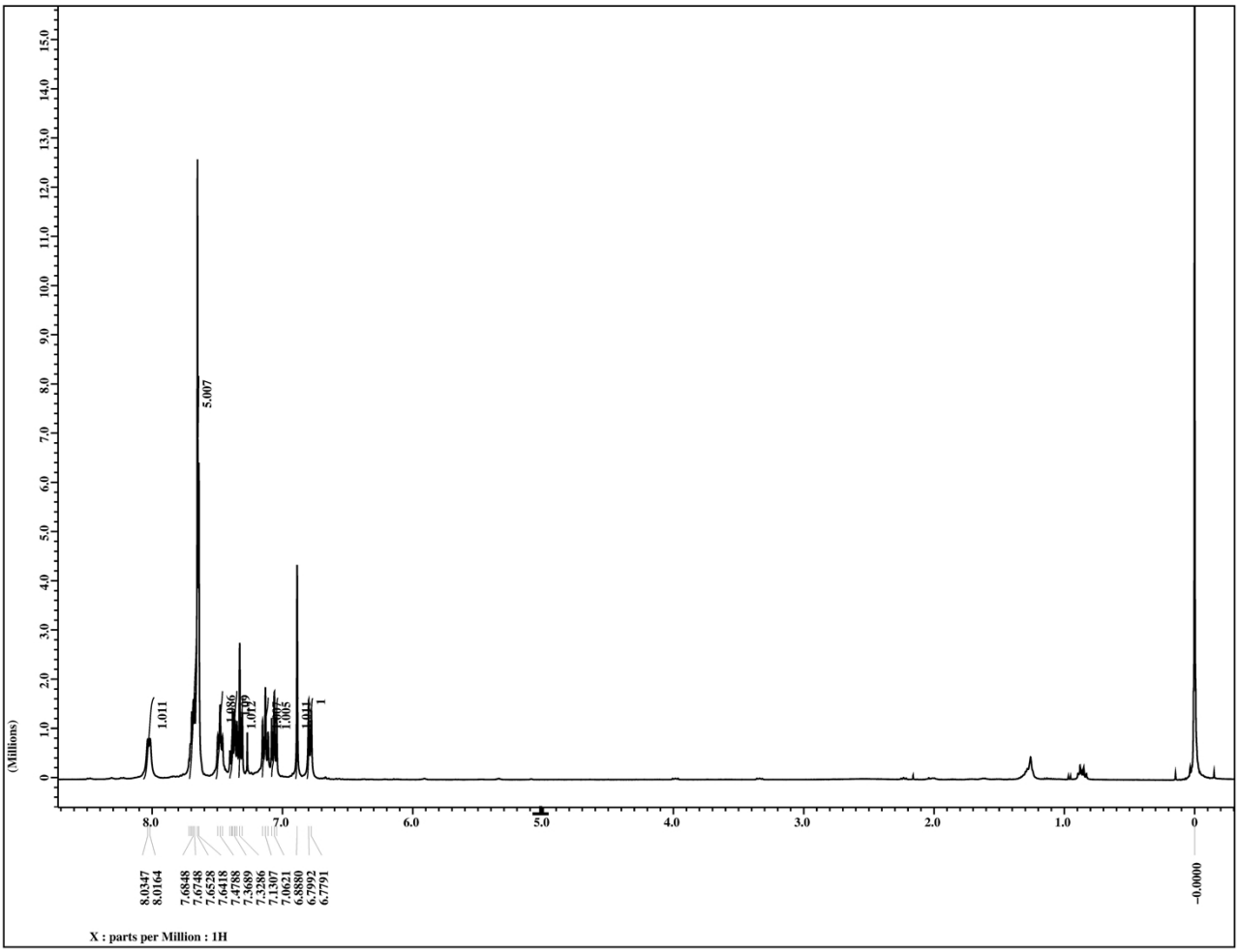

(Millions)
160.4653
156.9248
151.6714
149.2474
145.4163
133.2348
133.1354
132.4242
131.1625
129.4496
128.4326
126.1232
121.3592
120.2734
114.7370
112.7030
112.4812
108.5278
106.3901
104.6661
77.1603
X : parts per Million : 13C

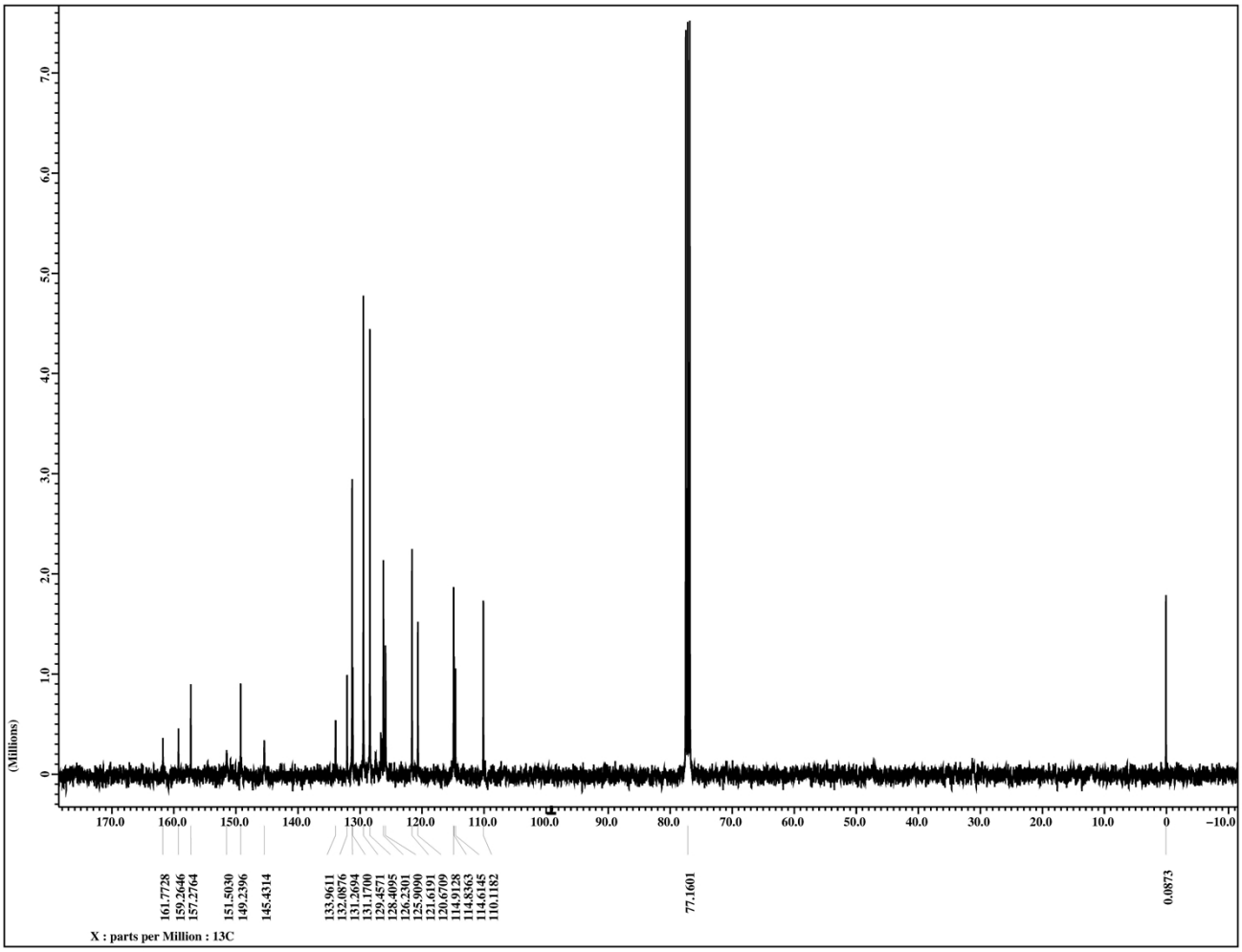


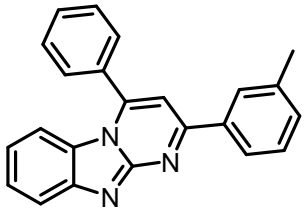

(Millions)
2.036
0.918
5.142
2.0
1.052
1.036
1.014
1
1.02
6.046
8.2288
8.2078
7.7013
7.6839
7.6793
7.6711
7.6528
7.6498
7.6115
7.4064
7.3661
7.3459
7.2086
6.9816
6.9613
6.6627
6.6417
2.9856
2.9681
2.9508
1.2959
1.2794
-0.0000
X : parts per Million : 1H

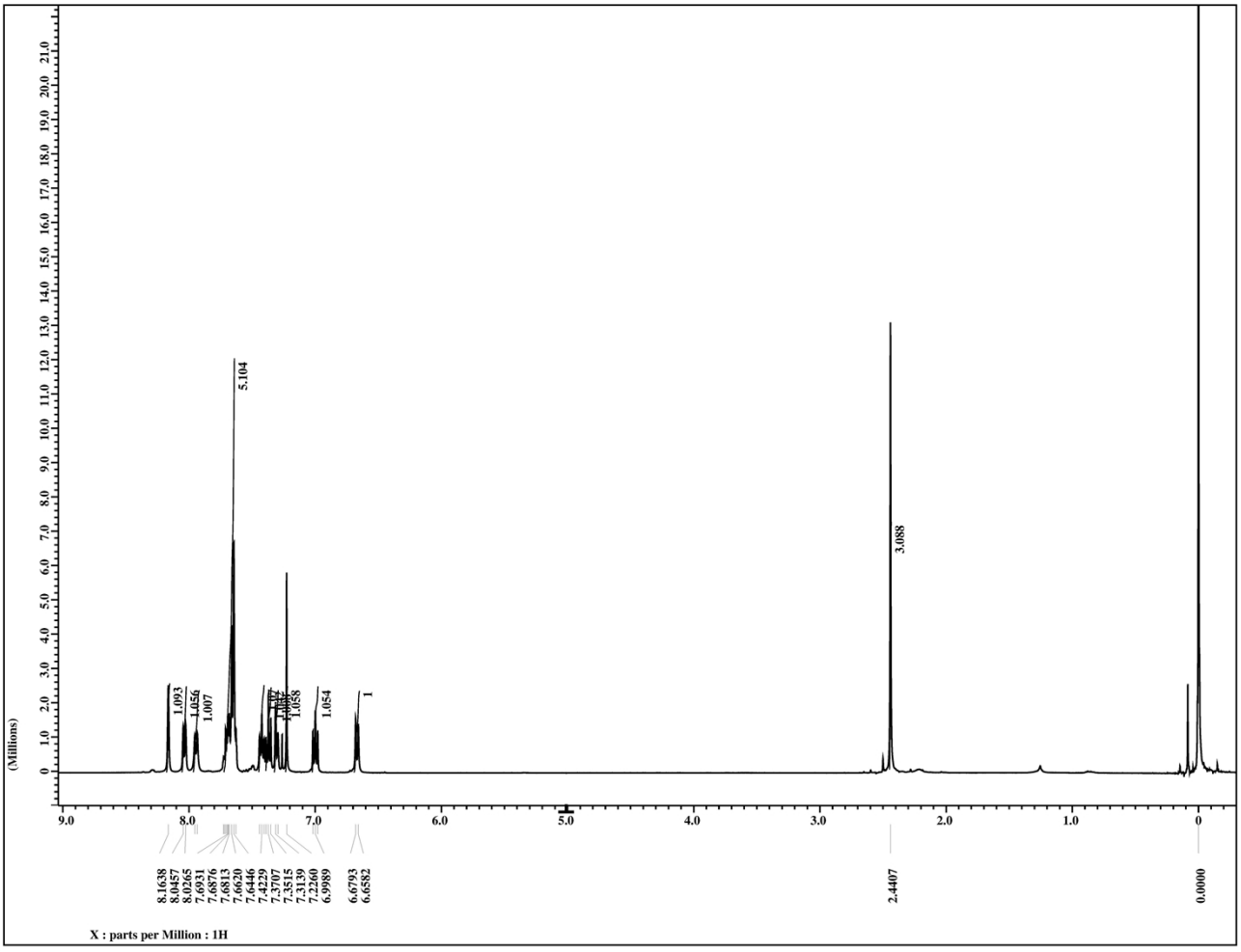

(Millions)
0
1.0
2.0
3.0
4.0
5.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
161.0694
152.6961
149.1862
134.3054
132.6919
131.0478
129.4267
128.4708
127.9508
127.1173
125.8097
121.0457
120.1357
114.5459
105.2396
77.1603
34.1773
23.8540
0.0875
X : parts per Million : 13C

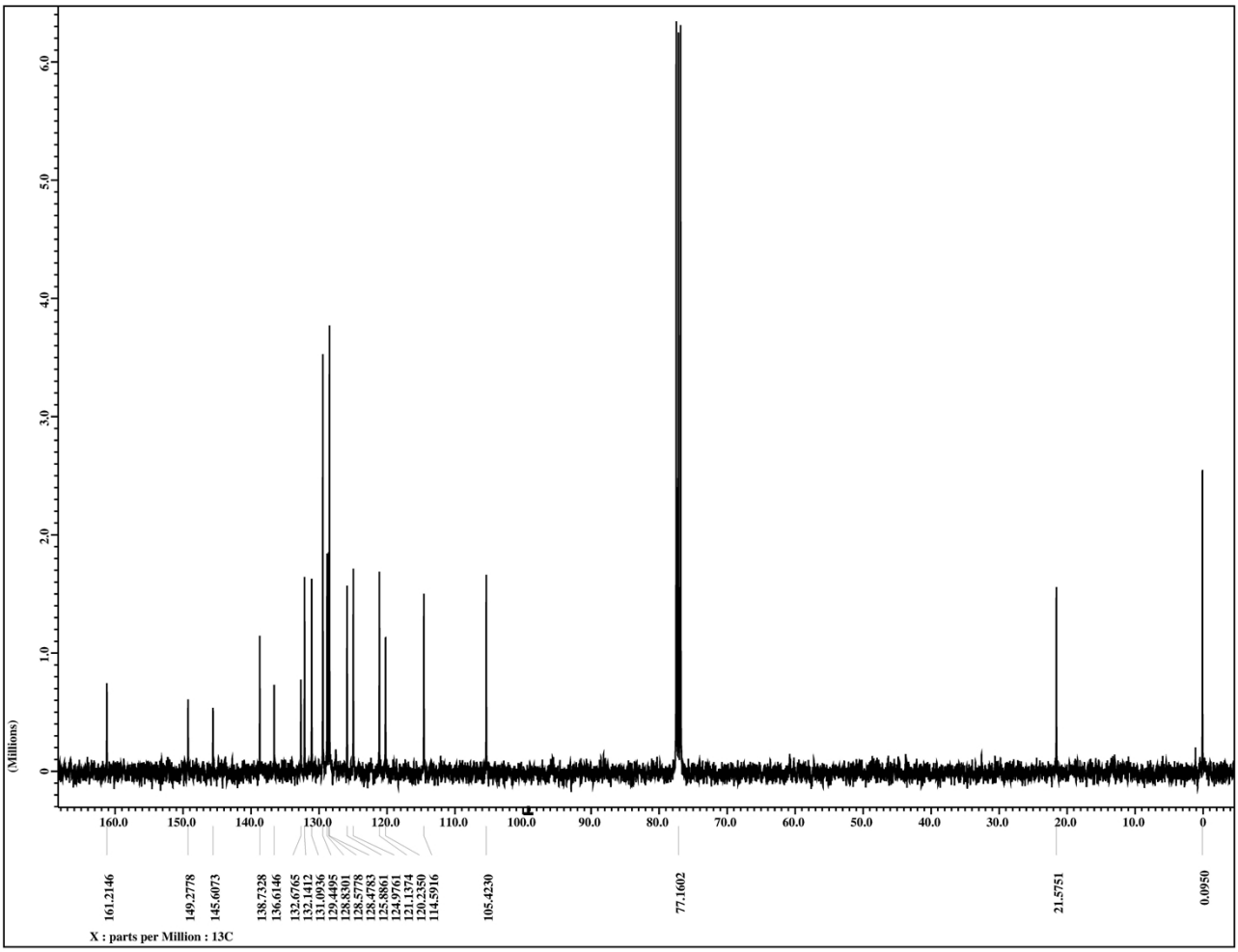

Cl
N
N
N
F


(Millions)
5.007
1.011
8.0347
8.0164
7.6848
7.6748
7.6528
7.6418
7.4788
7.3689
7.3286
7.1007
7.0621
6.8880
6.7992
6.7791
-0.0000
X : parts per Million : 1H


(Millions)
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0
161.7728
159.2646
157.2764
151.5030
149.2396
145.4314
133.9611
132.0876
131.2694
131.1700
129.4571
128.4095
126.2301
125.6990
123.6191
120.6709
114.9128
114.8363
114.6145
110.1182
77.1601
0.0873
X : parts per Million : 13C




(Millions)
5.104
3.088
1.093
1.056
1.007
1.058
1.054
1
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.1638
8.0457
8.0265
7.6931
7.6876
7.6813
7.6620
7.6446
7.4229
7.3707
7.3515
7.3139
7.2760
6.9989
6.6793
6.6582
2.4407
0.0000
X : parts per Million : 1H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4.0
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2.0
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140.0
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120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
161.2146
149.2778
145.6073
138.7328
136.6146
132.6765
132.1412
131.0936
129.4495
128.8301
128.5778
128.4783
125.8861
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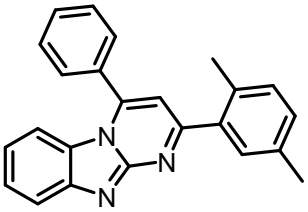
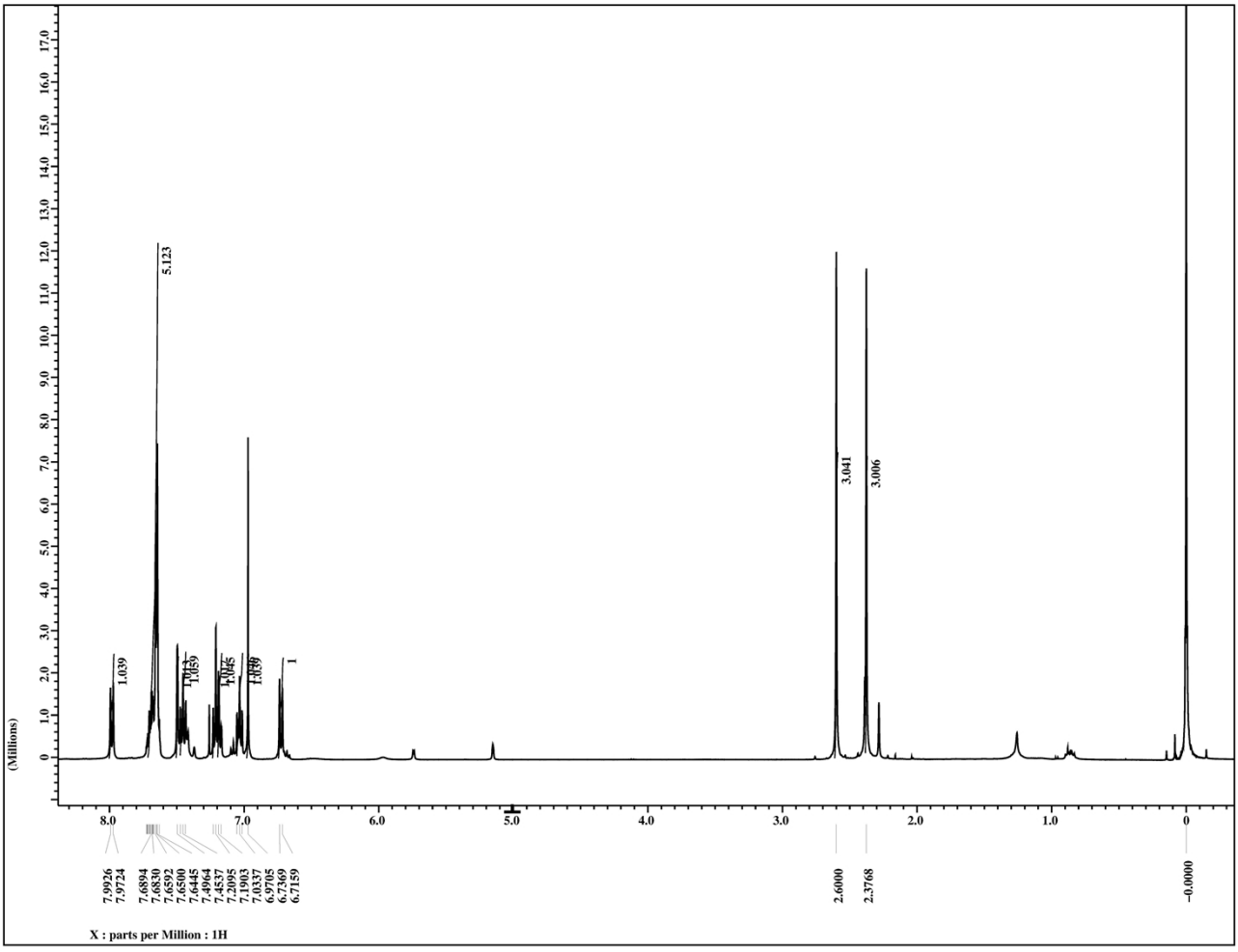
121.1374
120.2580
114.5916
105.4230
77.1602
21.5751
0.0950
X : parts per Million : 13C

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3.041
3.006
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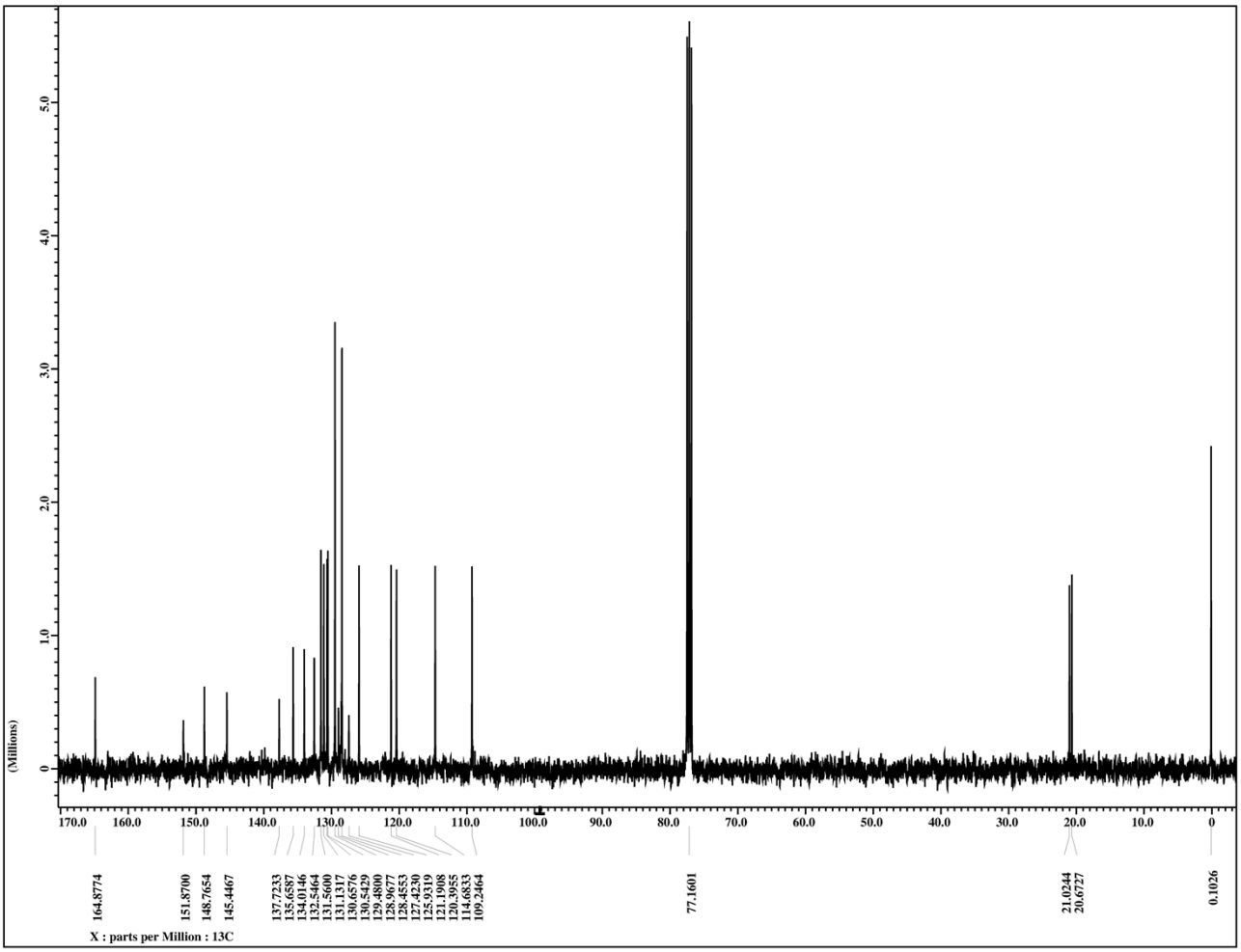
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.9926
7.9724
7.6894
7.6830
7.6592
7.6500
7.6445
7.4964
7.4837
7.2095
7.1903
7.0337
6.9705
6.7369
6.7159
2.6000
2.3768
-0.0000
X : parts per Million : 1H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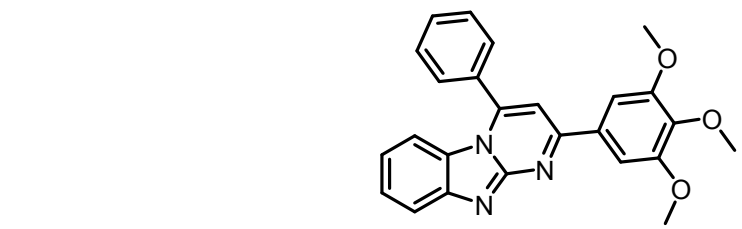
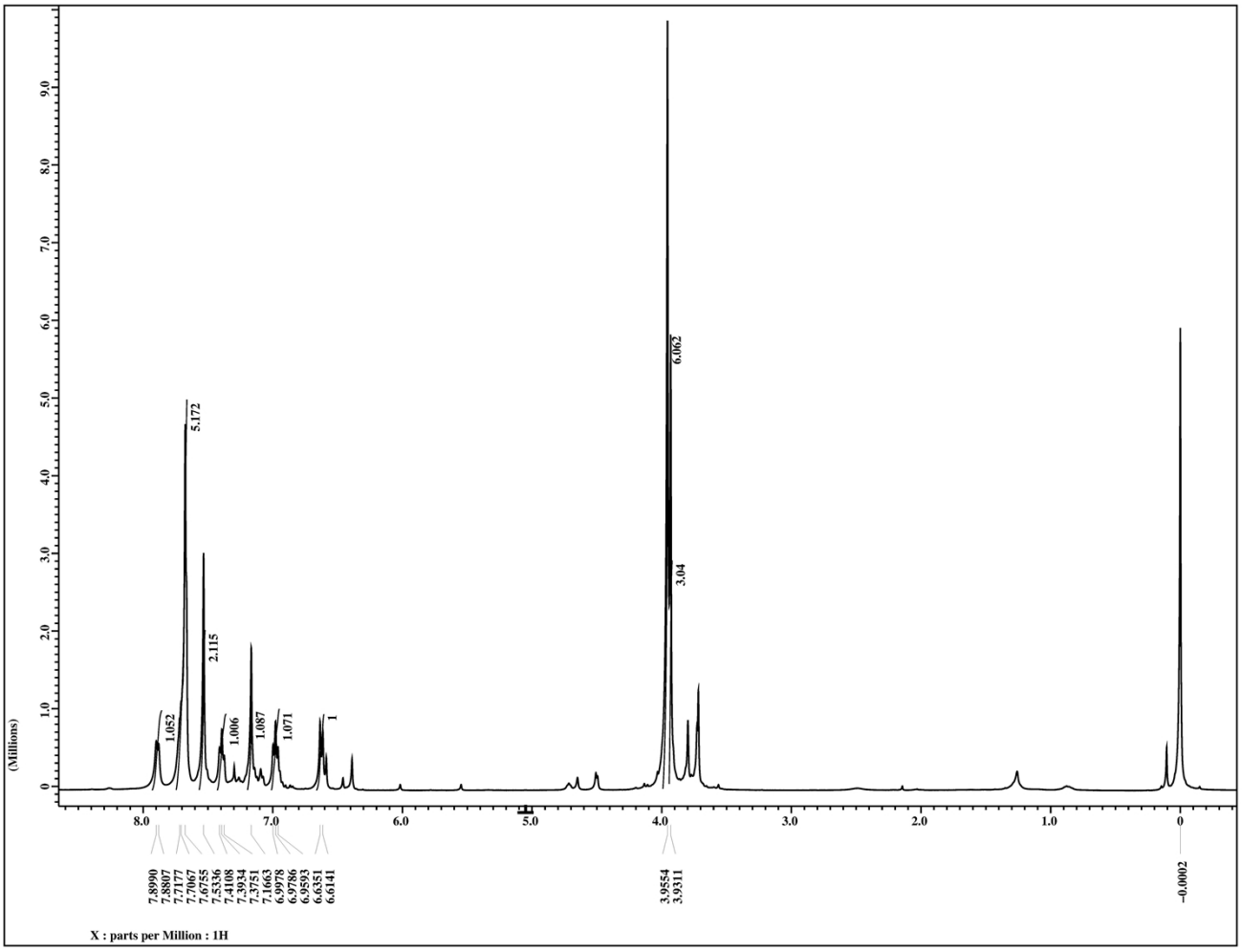
4.0
3.0
2.0
1.0
0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
164.8774
151.8700
148.7654
145.4467
137.7233
135.6587
134.0146
132.5464
131.5600
131.1177
130.6576
130.5429
129.4800
128.9677
128.4553
127.4230
125.9319
121.1908
120.3955
114.6833
109.2464
77.1601
21.0244
20.6727
0.1026
X : parts per Million : 13C


O
O
O
N
N
N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5.0
4.0
3.0
2.0
1.0
0
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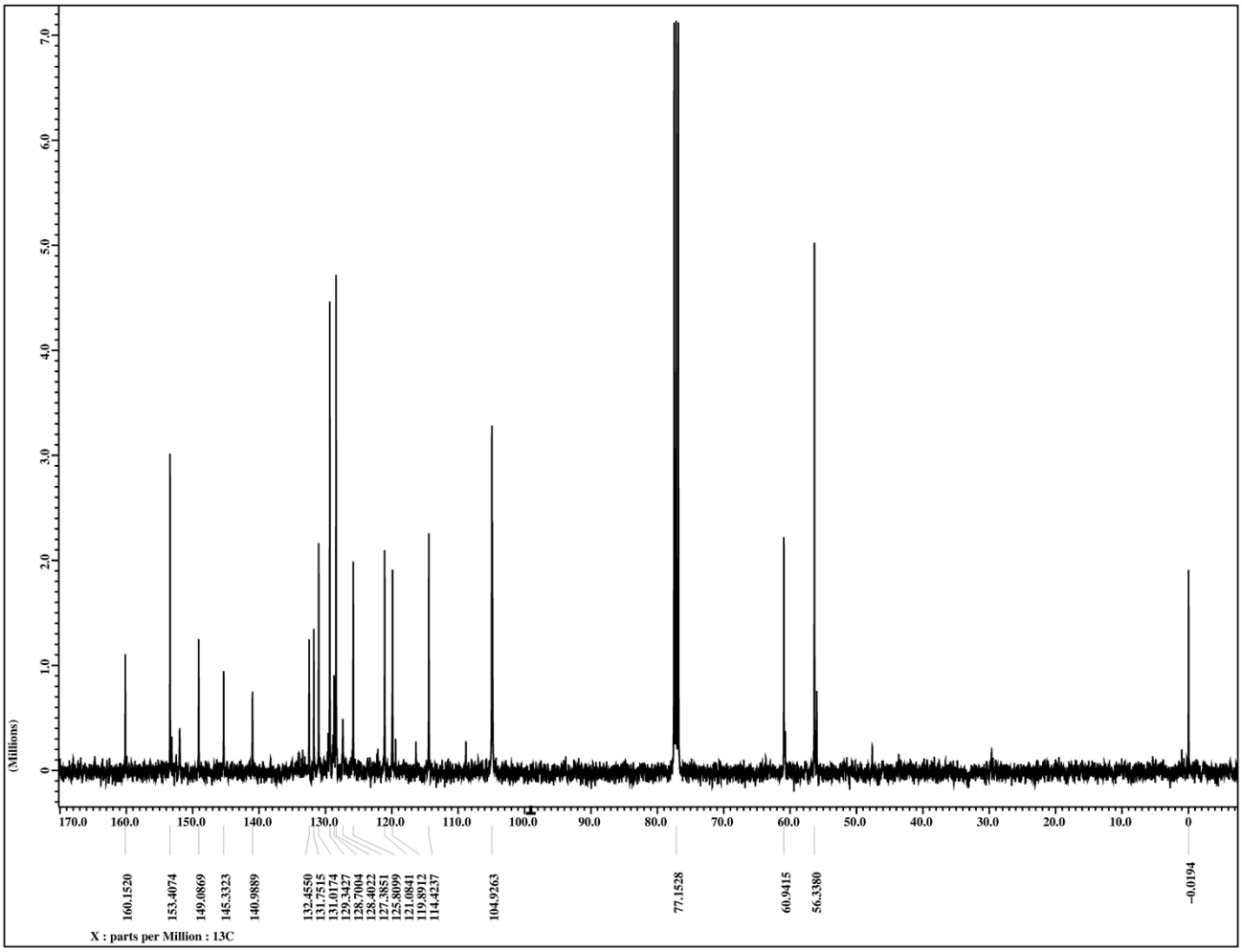
6.062
3.04
2.115
1.052
1.006
1.087
1.071
1
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.8990
7.8807
7.7177
7.7067
7.6455
7.5356
7.4108
7.3934
7.3751
7.1663
6.9978
6.9786
6.9593
6.6351
6.6141
3.9554
3.9311
-0.0002
X : parts per Million : 1H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6.0
5.0
4.0
3.0
2.0
1.0
0
170.0
160.0
150.0
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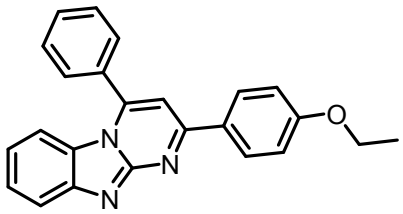
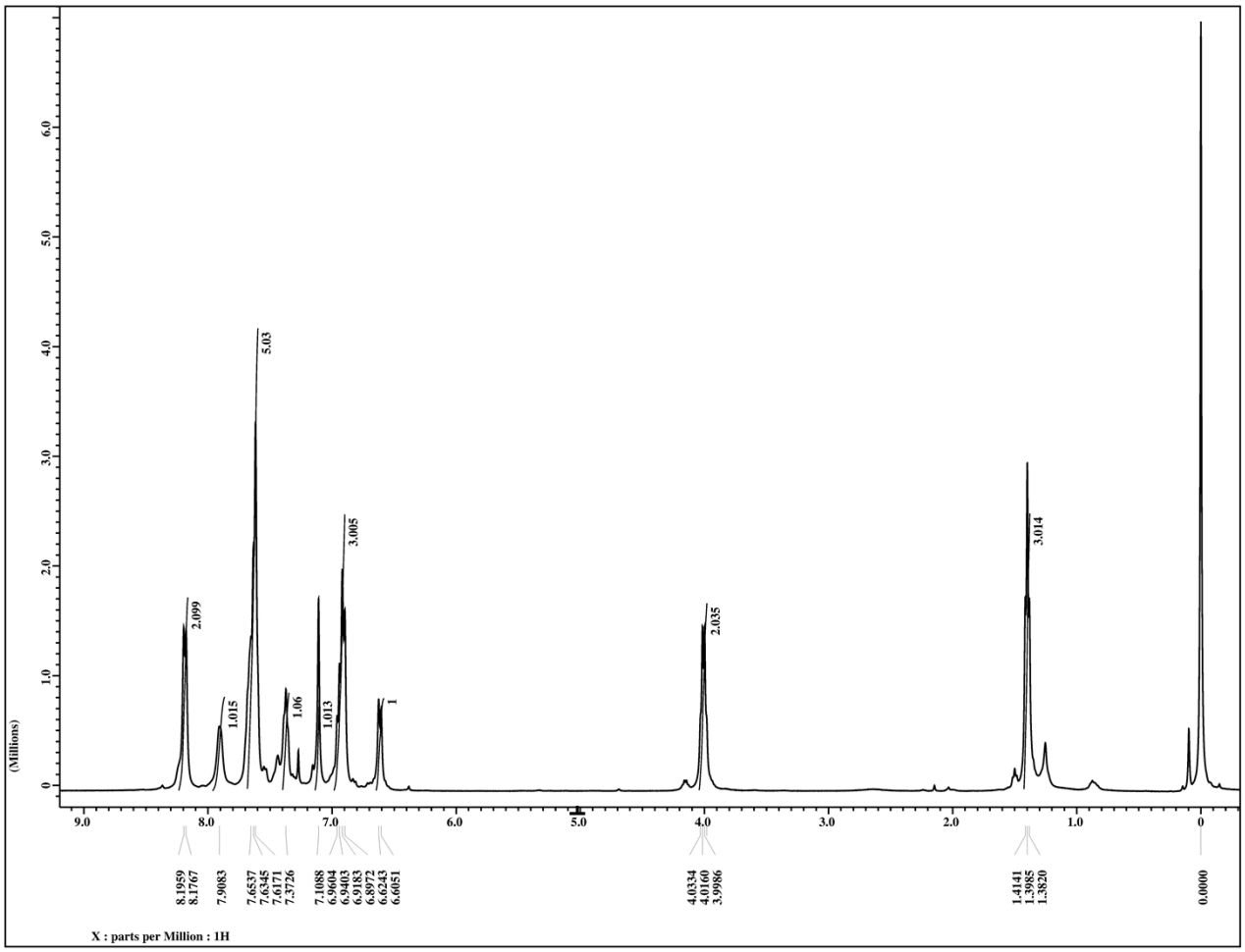
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
160.1520
153.4074
149.0869
145.3323
140.9889
132.4550
131.7515
131.0174
129.3427
128.7004
128.4022
127.3851
125.8099
121.0841
119.8912
114.4237
104.9263
77.1528
60.9415
56.3380
−0.0194
X : parts per Million : 13C


N
N
N
O


(Millions)
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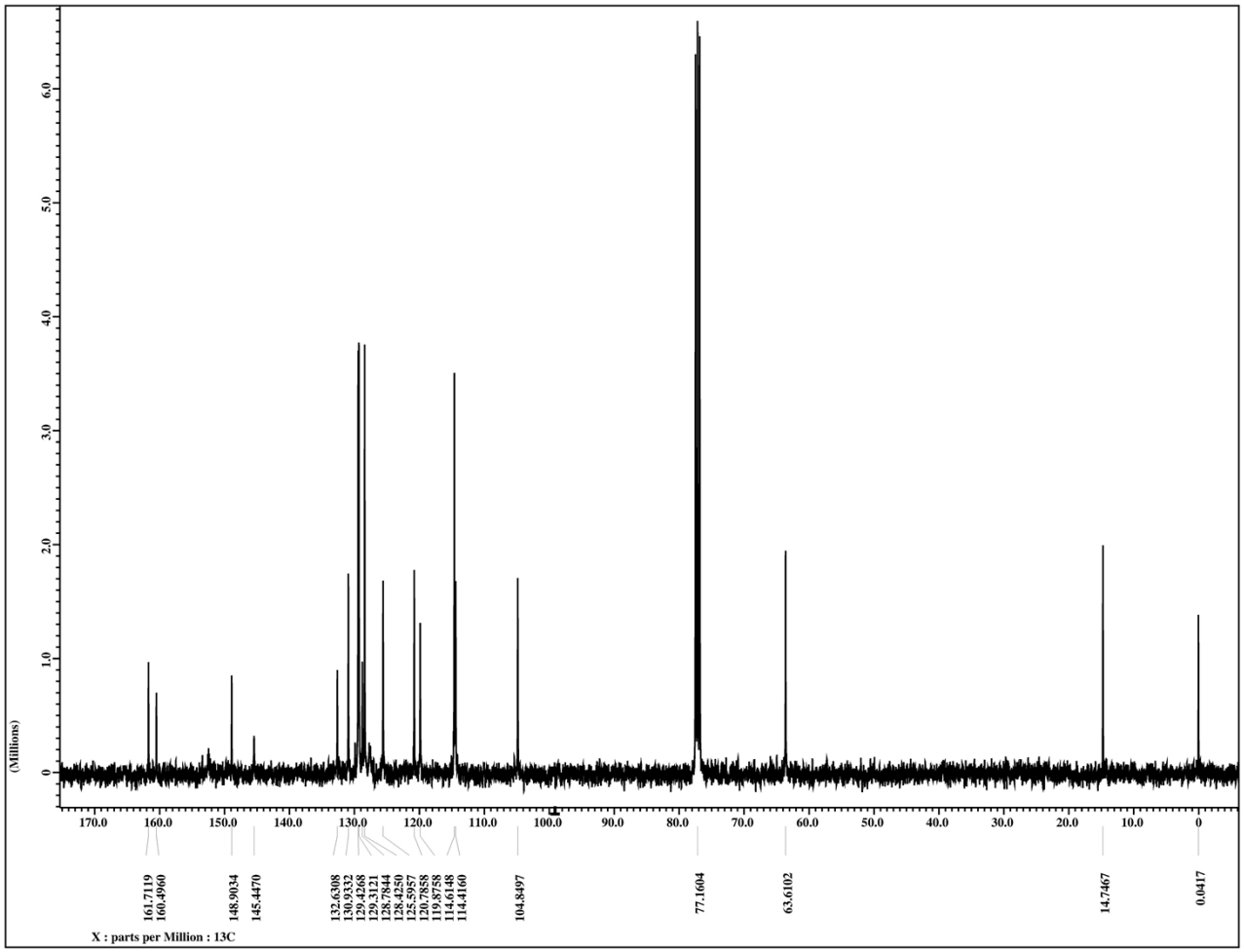
5.0
4.0
3.0
2.0
1.0
0
2.099
1.015
5.03
1.06
1.013
3.005
1
2.035
3.014
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.1959
8.1767
7.9083
7.6537
7.6345
7.6171
7.3726
7.1088
6.9604
6.9403
6.9183
6.8972
6.6243
6.6051
4.0334
4.0160
3.9986
1.4141
1.3985
1.3820
0.0000
X : parts per Million : 1H


(Millions)
0
1.0
2.0
3.0
4.0
5.0
6.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
161.7119
160.4960
148.9034
145.4470
132.6308
130.9332
129.4268
129.1121
128.7944
128.4250
125.5957
120.7858
119.8758
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114.4160
104.8497
77.1604
63.6102
14.7467
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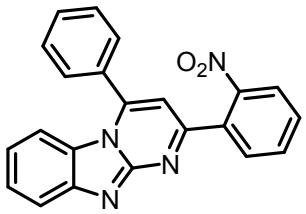
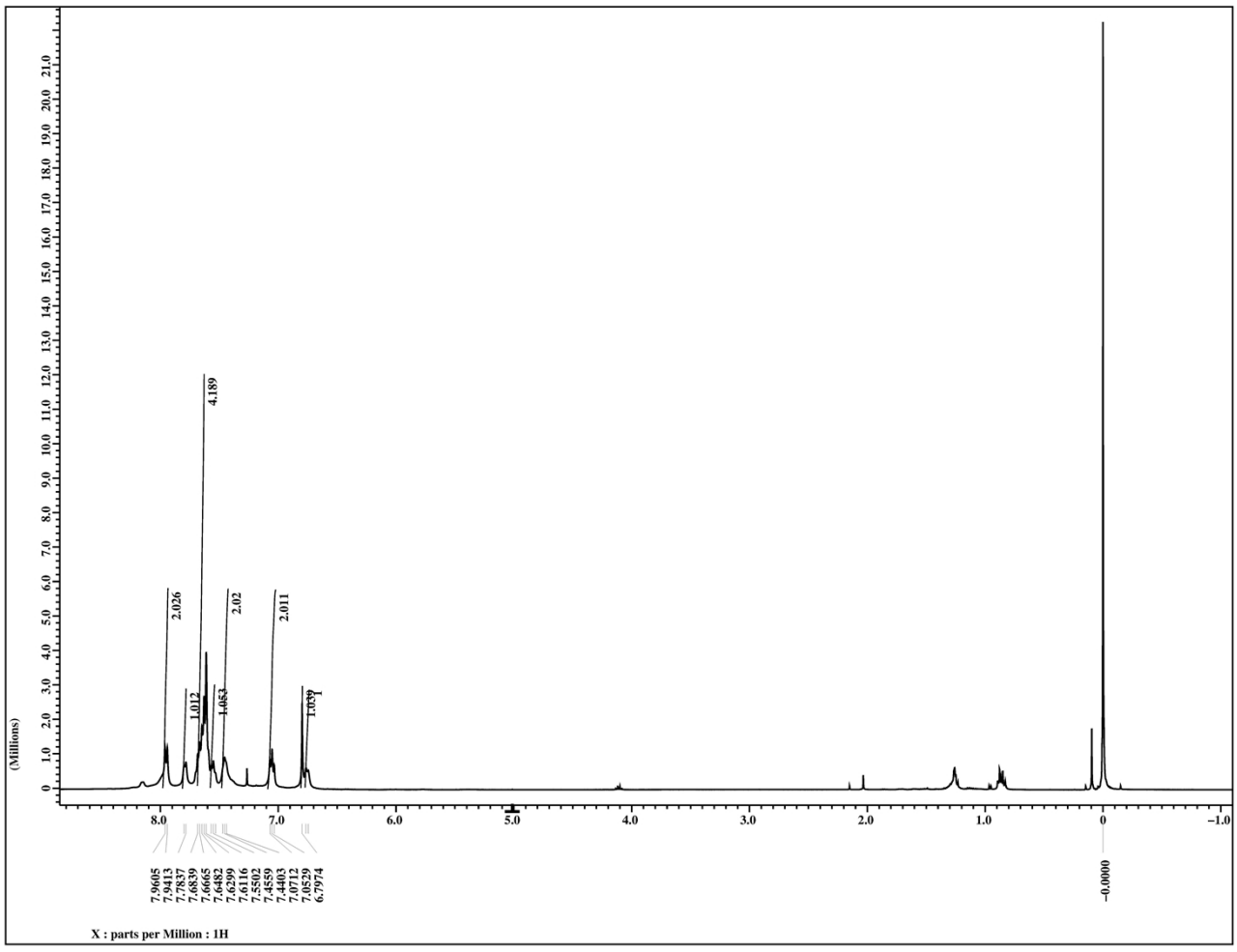
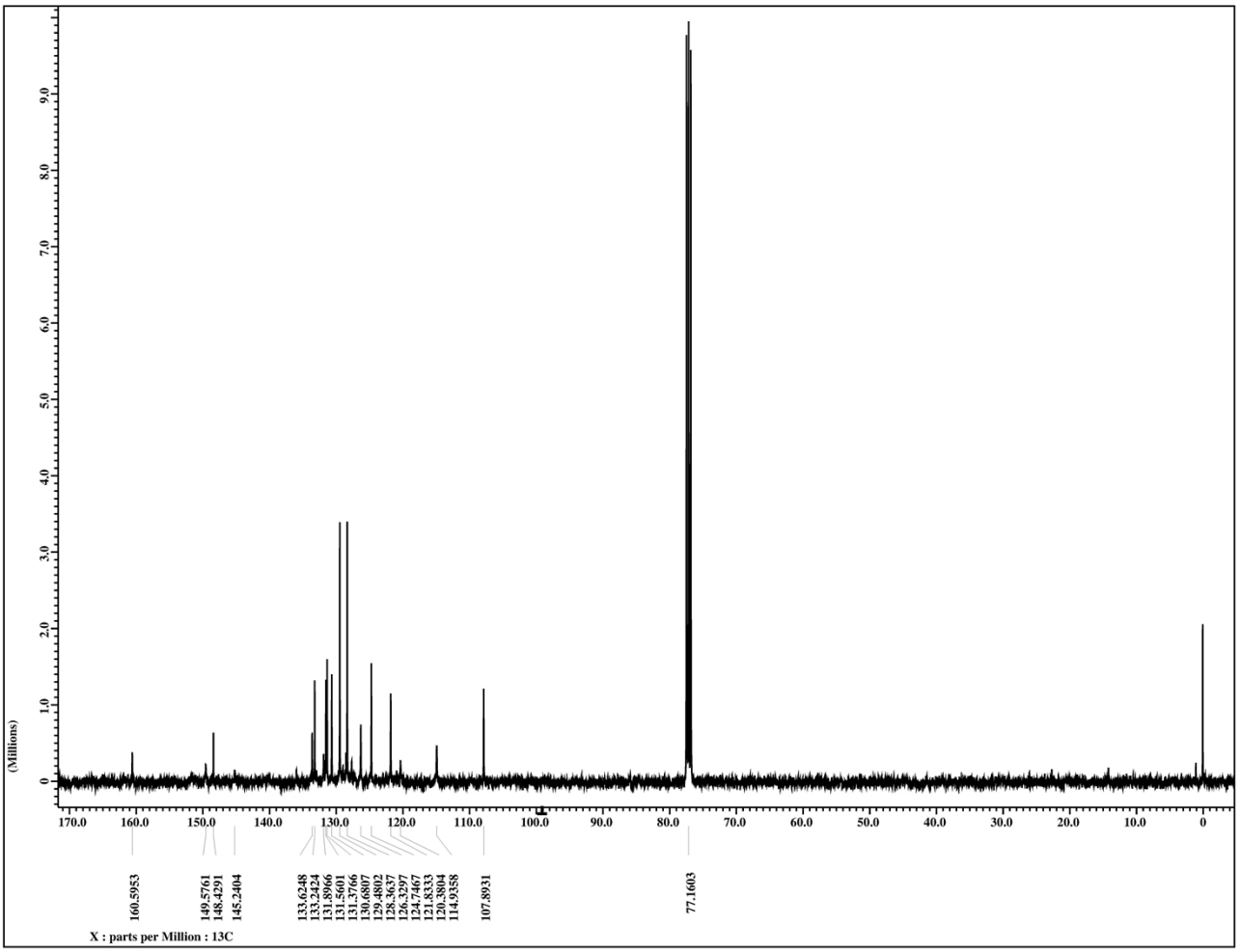
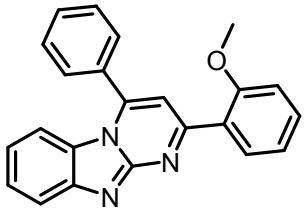
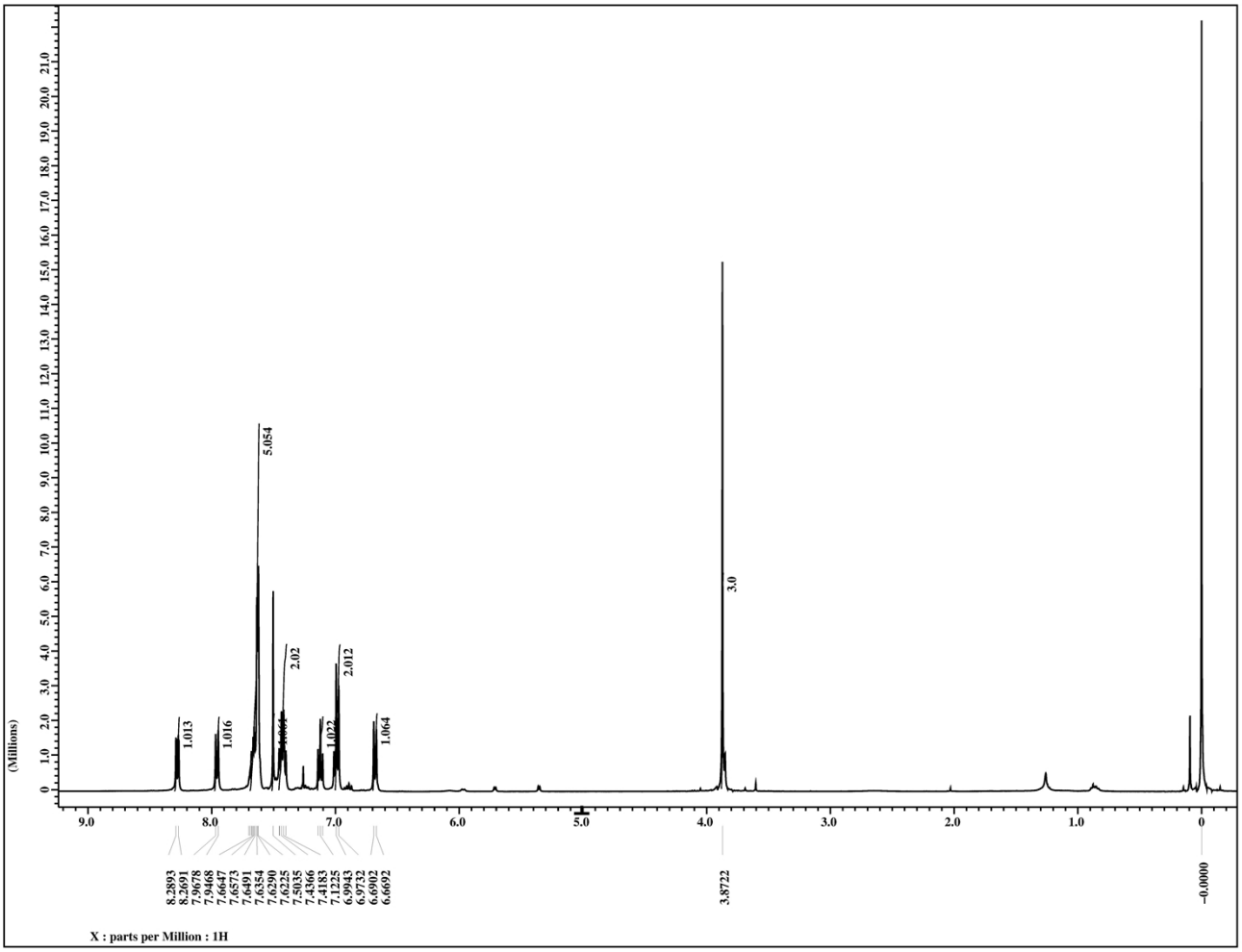
X : parts per Million : 13C


O2N
N
N
N


(Millions)
4.189
2.026
2.02
2.011
1.012
1.053
1.039
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−1.0
7.9605
7.9413
7.7837
7.6839
7.6665
7.6482
7.6299
7.6116
7.5502
7.4559
7.4403
7.0712
7.0529
6.7974
−0.0000
X : parts per Million : 1H


(Millions)
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
160.5953
149.5761
148.4291
145.2404
133.6248
133.2424
131.8966
131.5401
131.3766
130.6807
129.4802
128.3637
126.3297
124.7467
121.8333
120.3804
114.9358
107.8931
77.1603
X : parts per Million : 13C


O
N
N
N


(Millions)
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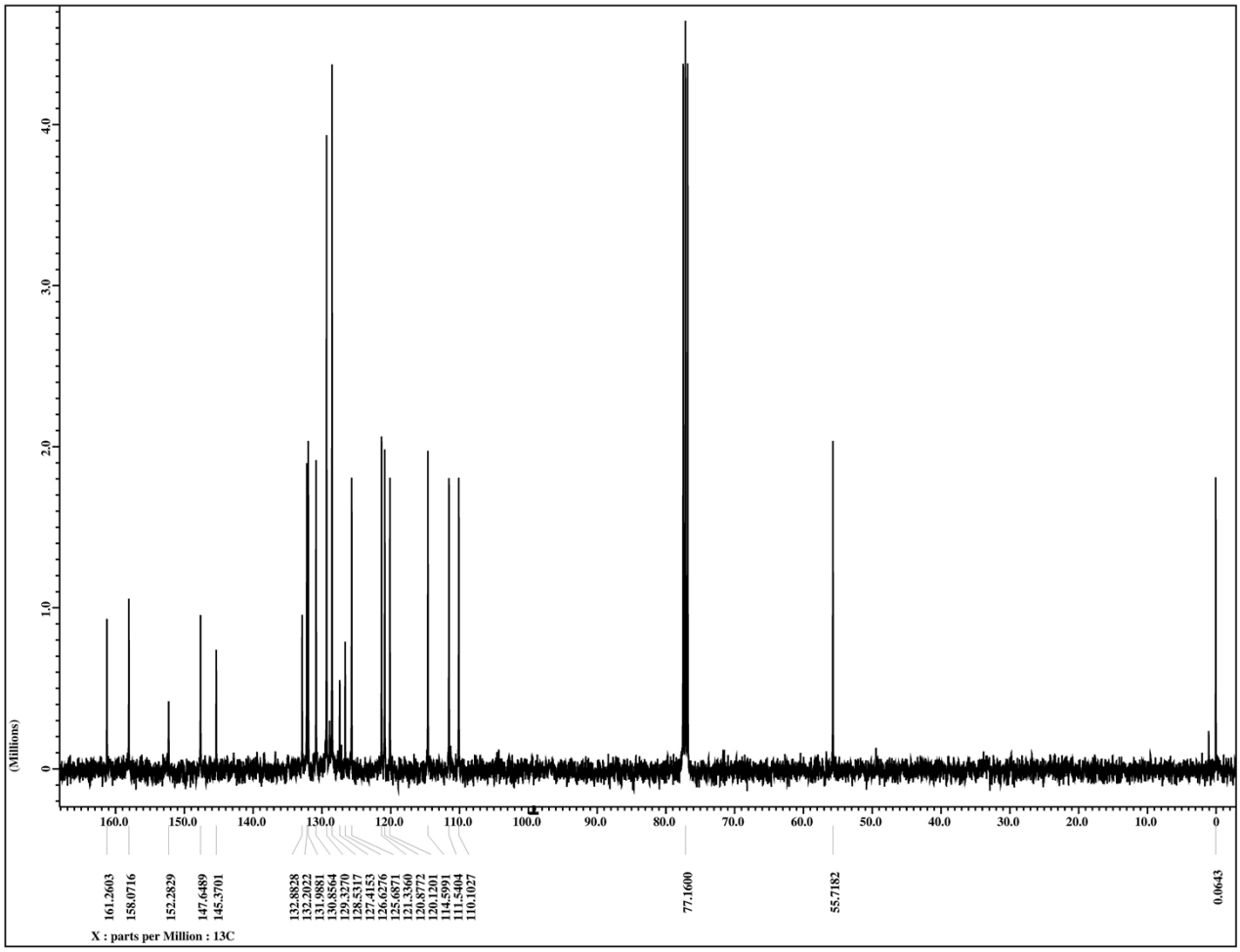
1.016
5.054
2.02
2.012
1.064
3.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.2893
8.2691
7.9678
7.9468
7.6647
7.6573
7.6491
7.6354
7.6290
7.6225
7.5035
7.4366
7.4183
7.1225
6.9943
6.9732
6.6902
6.6692
3.8722
-0.0000
X : parts per Million : 1H


(Millions)
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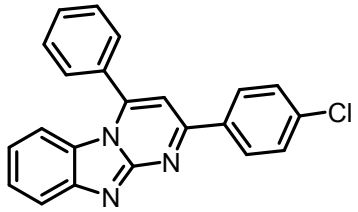
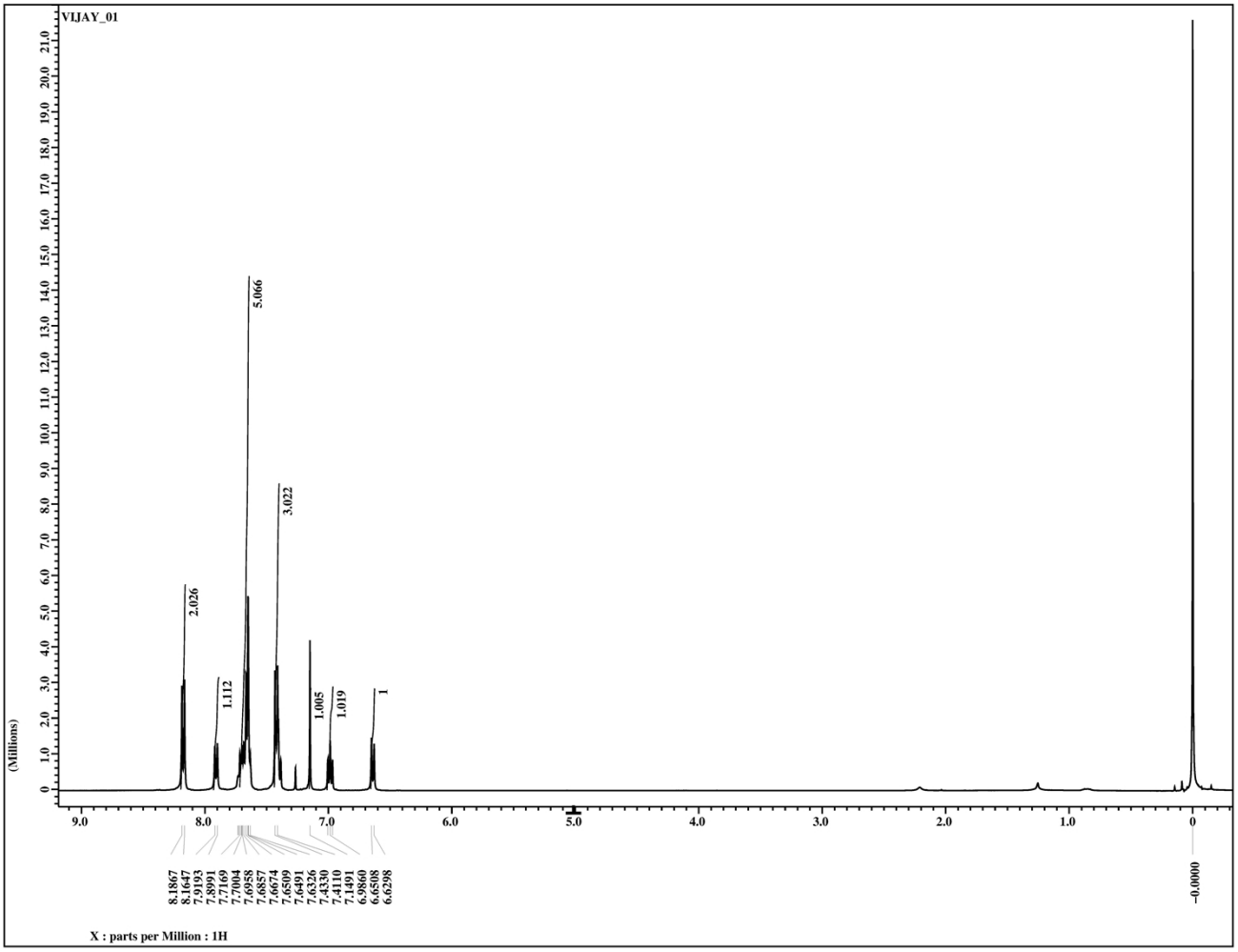
3.0
2.0
1.0
0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
161.2603
158.0716
152.2829
147.6489
145.3701
132.8828
132.2022
131.9681
130.8854
129.3270
128.5317
127.4153
126.6276
125.6871
121.3360
120.8772
120.1201
114.5991
111.5404
110.1027
77.1600
55.7182
0.0643
X : parts per Million : 13C


Cl
N
N
N


VIJAY_01
(Millions)
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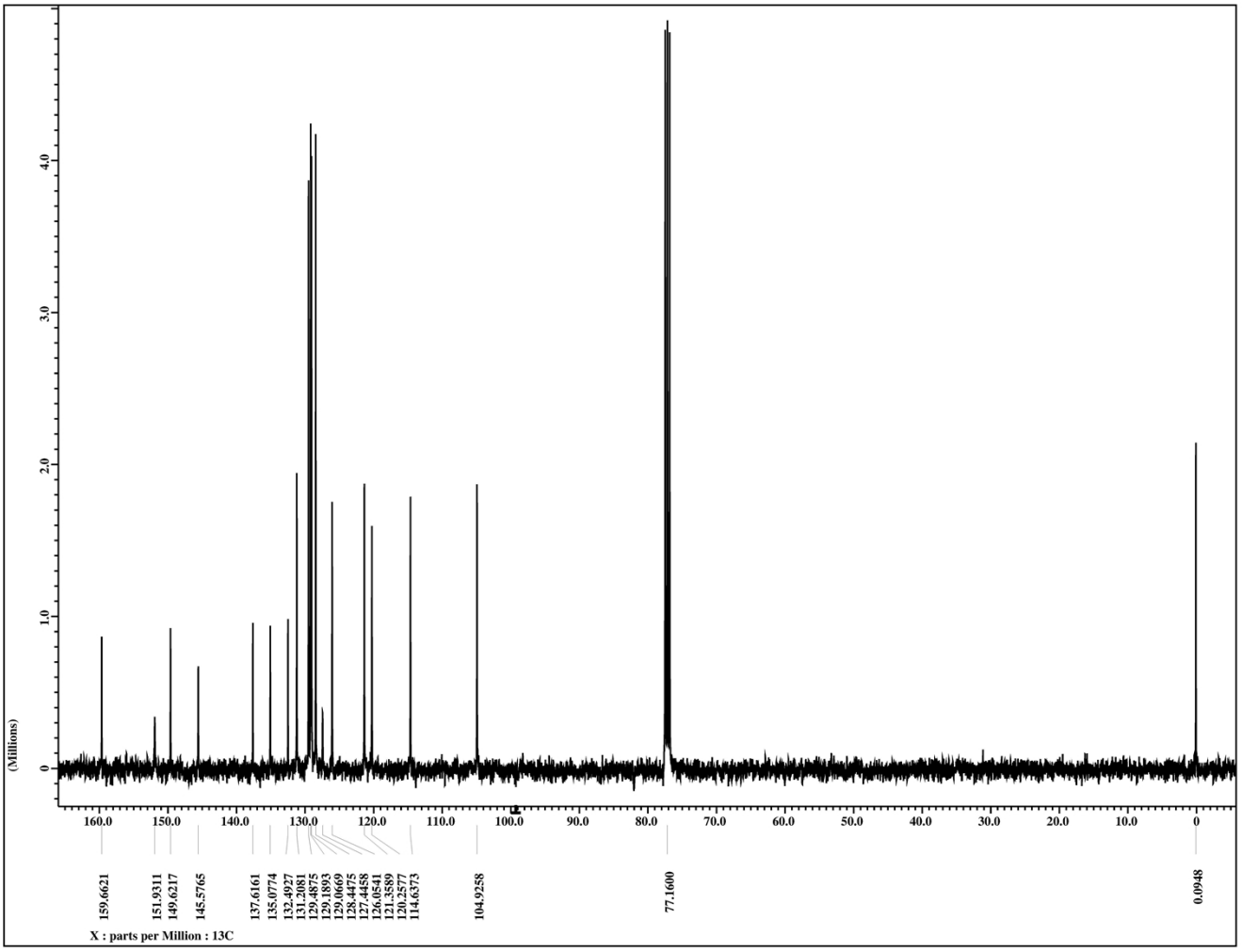
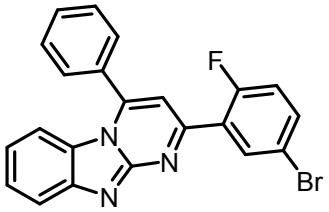
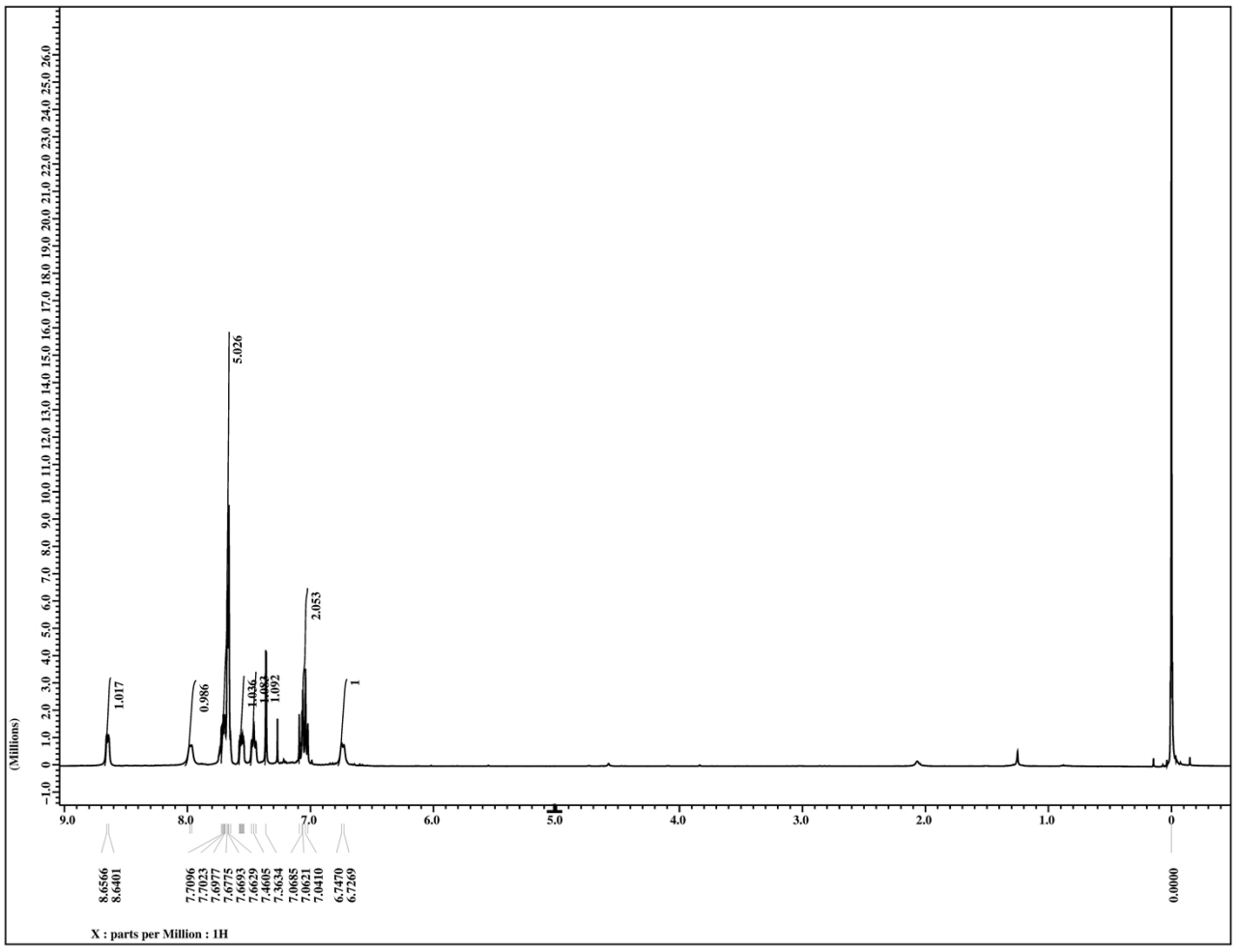
3.022
2.026
1.112
1.005
1.019
1
-0.0000
X : parts per Million : 1H


(Millions)
4.0
3.0
2.0
1.0
0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
159.6621
151.9311
149.6217
145.5765
137.6161
135.0774
132.4927
131.2081
129.4875
129.1893
129.0669
128.4475
127.4458
126.0541
121.3589
120.2577
114.6373
104.9258
77.1600
0.0948
X : parts per Million : 13C


F
N
N
N
Br


(Millions)
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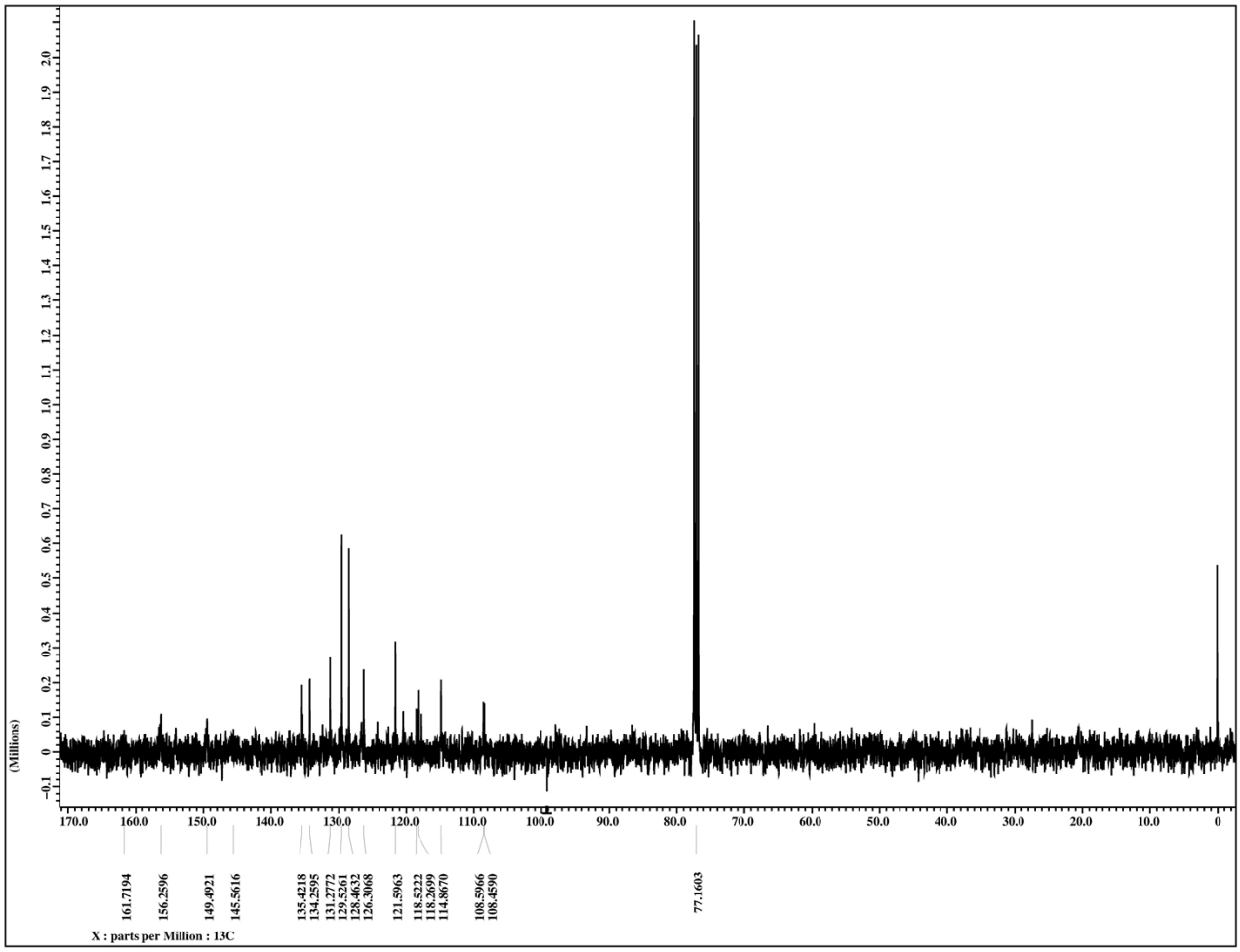
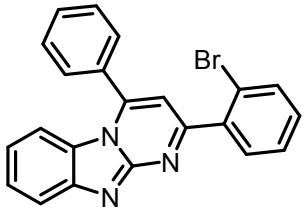
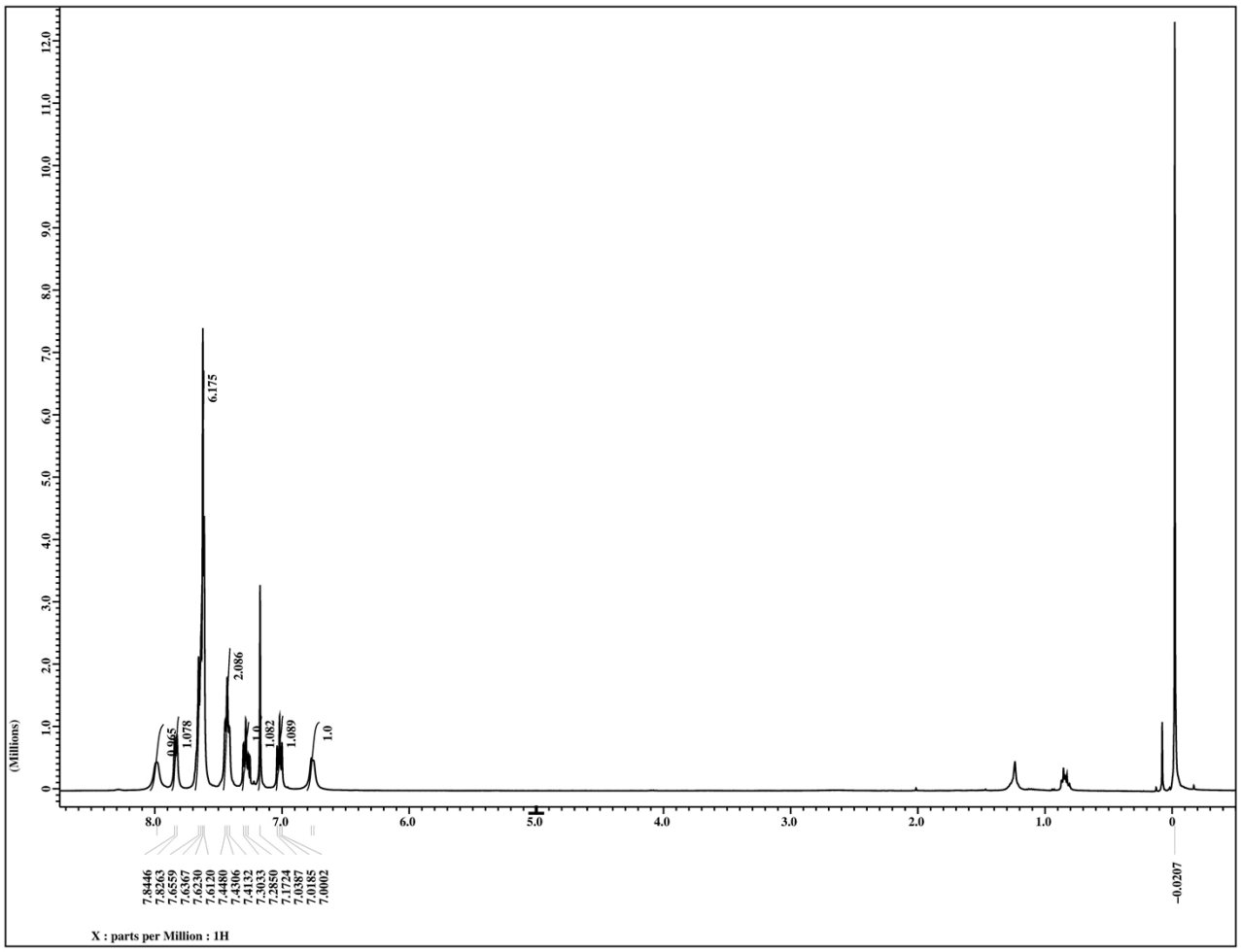
0.986
5.026
1.036
1.083
1.092
2.053
1
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.6566
8.6401
7.7096
7.7023
7.6977
7.6775
7.6693
7.6629
7.4605
7.3634
7.0685
7.0621
7.0410
6.7470
6.7269
0.0000
X : parts per Million : 1H


(Millions)
2.0
1.9
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
-0.1
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
161.7194
156.2596
149.4921
145.5616
135.4218
134.2595
131.2772
129.5261
128.4632
126.3068
121.5963
118.5222
118.2699
114.8670
108.5966
108.4590
77.1603
X : parts per Million : 13C


Br
N
N
N


(Millions)
6.175
2.086
1.0
1.082
1.089
1.0
0.965
1.078
7.8446
7.8263
7.6559
7.6367
7.6230
7.6120
7.4480
7.4406
7.4132
7.3033
7.2850
7.1724
7.0387
7.0185
7.0002
-0.0207
X : parts per Million : 1H

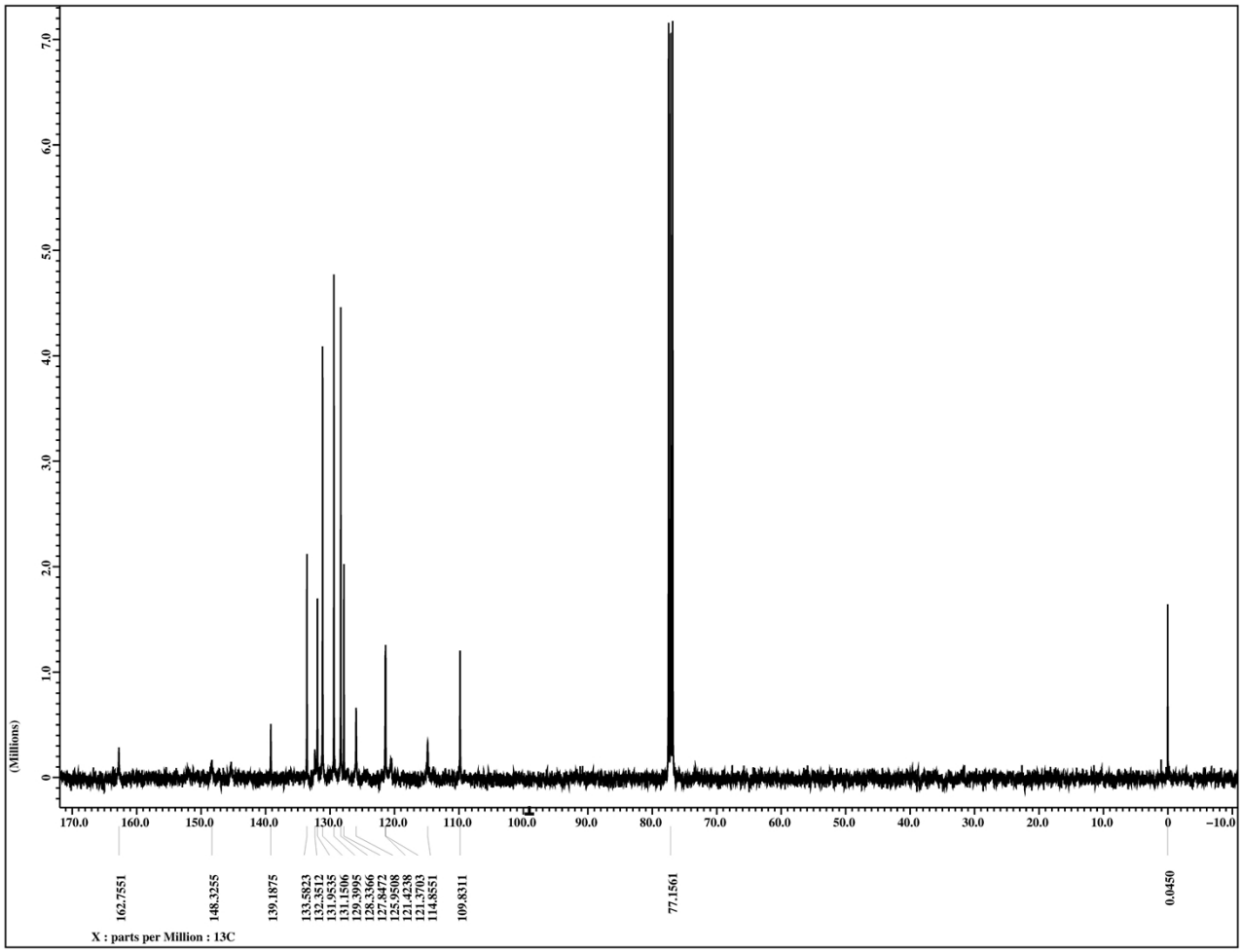

(Millions)
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
−10.0
162.7551
148.3255
139.1875
133.5823
132.3512
131.1535
131.1506
129.3995
128.3366
127.8472
125.9508
121.4238
121.3703
114.8551
109.8311
77.1561
0.0450
X : parts per Million : 13C

Figure S2

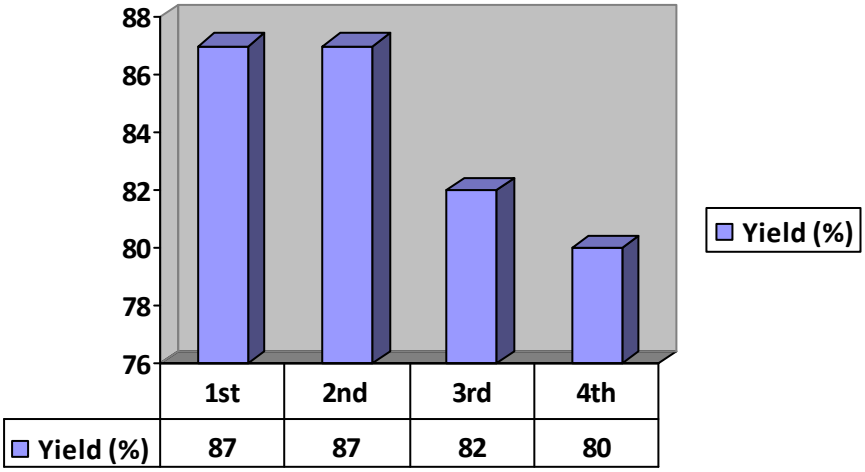



**Figure S2**: Reusability of the MSA catalyst.