Supporting Information

Synthesis of [1,2,3]triazolo[5,1-*a*]isoquinoline derivatives via a selective cascade cyclization sequence of 1,2-bis(phenylethynyl)benzene derivatives

Shipeng Tao, Qinquan Hu, Huan Li, Shan Ma, Yunfeng Chen*

School of Chemical and Environmental Engineering, Wuhan Institute of Technology, Wuhan 430073, P. R. China

Email: chyfch@hotmail.com

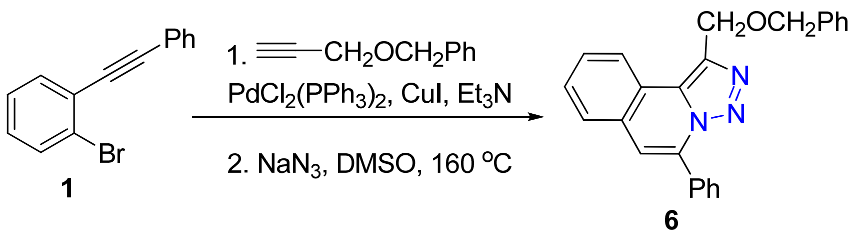
Table of contents

I. General Methods and materials:

All of the reaction were carried out in 25mL round-bottom flasks with air condensers. Unless otherwise noted, all commercial reagents and solvents were obtained from the commercial provider and used without further purification. ^{1}H NMR and ^{13}C NMR spectra were recorded on Varian 600 MHz and 400 MHz spectrometers. Chemical shifts were reported relative to internal tetramethylsilane (TMS) (0.00 ppm) or $CDCl_3$ (7.26 ppm) for ^{1}H, $CDCl_3$ (77.0 ppm) for ^{13}C and d^6-DMSO (2.5 ppm) for ^{1}H, (39.5 ppm) for ^{13}C. Flash column chromatography was performed on 200-300 mesh silica gel. Analytical thin layer chromatography was performed with precoated glass baked plates (250μ) and visualized by fluorescence. MS were measured on a Finnigan Trace MS spectrometer. Melting points were measured on a melting point tester RY-1G apparatus and uncorrected. All the products had passed the infrared detector.

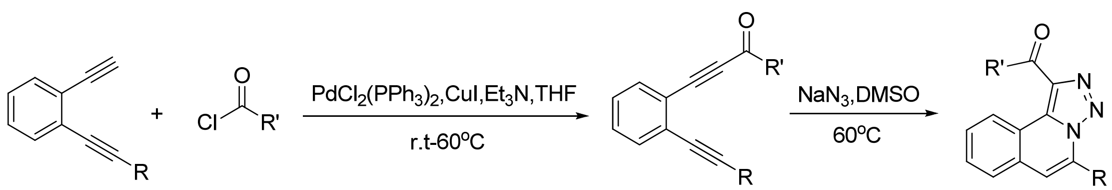
II. Experimental

Typical experimental procedure for synthesis of **3**, **4**, **6**, **9**, **10** and **13**.



1-bromo-2-(phenylethynyl)benzene [1](257 mg, 1 mmol), $PdCl_2(PPh_3)_2$ (35 mg, 0.05 mmol), CuI (12 mg, 0.06 mmol) were added to a pear-shaped Schlenk tube charged with a magnetic stirrer. The tube was evacuated and backfilled with argon and then degassed Et_3N/THF (6 mL, V/V, 1:1) was introduced, then ((prop-2-ynyloxy)methyl)benzene[2] (175 mg, 1.2 mmol) was introduced, the mixtures were heating at 80 °C for 5-6 hours. Then poured into water and extracted with EtOAc, the organic layer further washed with brine and dried with anhydrous Na_2SO_4. After filtration, the organic layer was concentrated under reduced pressure and the residue was eluted through a short flash column chromatography (silica gel), the obtained solution was removed the solvent to give an oil. The oil were redissolved in DMSO, and then NaN_3 (195 mg, 3 mmol) was added. The solution was heating at 160 °C. The reaction was monitored by TLC, after the completion of the reaction, the mixture was poured into water and extracted with EtOAc. The organic layer was washed with brine and dried with anhydrous Na_2SO_4. Concentration under reduced pressure and purification of the residue by flash chromatography on silica gel gives the target product **6** as white solid (231 mg, yield 64%)[3][4].

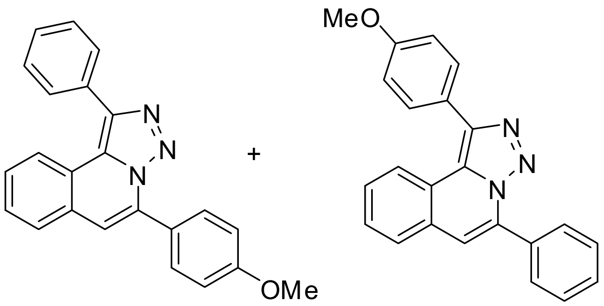
Typical experimental procedure for synthesis of **15a**.



1-Ethynyl-2-(phenylethynyl)benzene (202 mg, 1 mmol), $PdCl_2(PPh_3)_2$ (35 mg, 0.05 mmol), CuI (19 mg, 0.1 mmol) were added to a pear-shaped Schlenk tube charged with a magnetic stirrer. The tube was evacuated and backfilled with argon and then degassed Et_3N and THF (6 mL, V/V, 1:1) was introduced, then the 2-chlorobenzoyl chloride (262 mg, 1.5 mmol) was introduced, the mixtures were heating at 60 °C for 2 hours. Then the reaction mixture cooled to room temperature, next filtrated with short flash column chromatography (silica gel), and the column was eluted with EtOAc, the combined solution was removed the solvent under reduced pressure to give an oil[5], which needn't further purification and redissolve in DMSO (5 mL), and then NaN_3 (130 mg, 2 mmol) were added, the mixture was heating at 60°C. The reaction was monitored by TLC, after the completion of the reaction, the mixture was poured into water and extracted with EtOAc. The organic layer was washed with brine and dried with anhydrous Na_2SO_4. Concentration under reduced pressure and purification of the residue by flash chromatography on silica gel gives **15a** as white solid (82% yield for two steps).

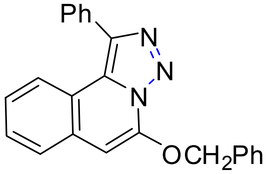
III. Compounds Characterization

5-(4-methoxyphenyl)-1-phenyl-[1,2,3]triazolo[5,1-a]isoquinoline （**3,4**）



White solid, [1]H NMR (600 MHz, $CDCl_3$) δ 8.13-8.18 (m, 1H), 7.96 (d, *J* = 7.8 Hz, 1H), 7.93 (d, *J* = 9.0 Hz, 1H), 7.77 (d, *J* = 7.8 Hz, 1H), 7.70 -7.74 (m, 1H), 7.68 (d, *J* = 9.0 Hz, 1H), 7.47-7.58 (m, 4H), 7.35-7.41 (m, 1H), 7.14 (s, 1H), 7.08 (d, *J* = 8.4 Hz, 1H), 7.04 (d, *J* = 8.4 Hz, 1H), 3.89 (s, 1H), 3.86 (s, 2H); [13]C NMR (100 MHz, $CDCl_3$) δ 160.6, 159.8, 140.9, 140.8, 135.8, 135.6, 132.3, 132.1, 130.9, 130.7, 129.9, 129.7, 129.6, 129.3, 128.8, 128.7, 128.6, 128.6, 128.5, 128.3, 127.8, 127.5, 127.4, 127.3, 124.5, 124.4, 123.0, 122.9, 122.8, 122.6, 115.8, 115.1, 114.1, 113.8, 55.2; ESI-MS(*m/z*): 351.5$[C_{23}H_{17}N_3O]^+$; HRMS (ESI): calcd. $[C_{23}H_{17}N_3O+H]^+$: 352.1444, found: 352.1447; IR(KBr): 2913, 1602, 1066, 1027, 898, 825, 763㎝$^{-1}$.

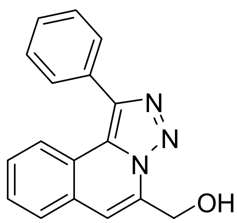
5-(benzyloxy)-1-phenyl-[1,2,3]triazolo[5,1-a]isoquinoline（**6**）



White solid, mp: 136-138 ℃, [1]H NMR (600 MHz, $CDCl_3$) δ8.37-8.49 (m, 1H), 7.95 (d, *J* = 7.8 Hz, 2H), 7.80-7.82 (m, 1H), 7.59-7.66 (m, 2H), 7.49-7.59 (m, 3H), 7.38 (d, *J* = 7.8 Hz, 2H), 7.31-7.34

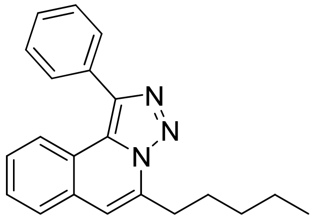
(m, 2H), 7.26-7.30 (m, 1H), 7.24 (d, *J* = 4.2 Hz, 1H), 5.24 (s, 2H), 4.65 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.6, 137.2, 135.9, 132.1, 131.3, 129.9, 129.4, 129.3, 128.9, 128.6, 128.3, 128.2, 128.1, 127.8, 127.6, 127.3, 127.2, 125.0, 124.9, 122.7, 116.2, 116.0,71.9, 64.3; ESI-MS(*m/z*): 365.4[$C_{24}H_{19}N_3O$]$^+$; HRMS (ESI): calcd. [$C_{24}H_{19}N_3O$ +H]$^+$: 366.1601, found: 366.1605; IR(KBr): 2863, 1558, 1068, 985, 943, 902, 850, 734, 698 ㎝$^{-1}$.

(1-phenyl-[1,2,3]triazolo[5,1-a]isoquinolin-5-yl)methanol (**9**)



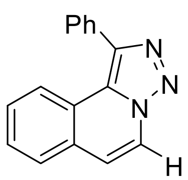
Yellow solid, mp: 160-164 ℃, ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.51 (d, *J* = 7.8 Hz, 1H), 7.88 (d, *J* = 4.8 Hz, 2H), 7.81 (d, *J* = 7.8 Hz, 1H), 7.67-7.71 (m, 1H), 7.62-7.66 (m, 1H), 7.51 (d, *J* = 4.8 Hz, 3H), 7.23 (s, 1H), 5.35 (s, 2H), 3.29 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.8, 135.9, 132.0, 130.7, 129.82, 129.80, 129.3, 129.0, 128.8, 128.5, 127.3, 124.9, 122.8, 116.3, 57.5; ESI-MS(*m/z*): 275.3[$C_{17}H_{13}N_3O$]$^+$; HRMS (ESI): calcd. [$C_{17}H_{13}N_3O$ +H]$^+$: 276.1132, found: 276.1132; IR(KBr): 3415, 2854, 1558, 1002, 767, 690, 578, 487 ㎝$^{-1}$.

5-pentyl-1-phenyl-[1,2,3]triazolo[5,1-a]isoquinoline (**11**)



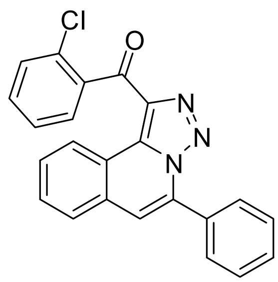
White solid, mp: 162-164 ℃, ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.64 (s, 1H), 7.97 (d, *J* = 7.8 Hz, 1H), 7.57-7.62 (m, 1H), 7.49-7.53 (m, 1H), 7.26 (s, 1H), 7.20-7.25 (m, 2H), 7.15-7.18 (m, 1H), 7.10 (d, *J* = 7.8 Hz, 2H), 4.57 (s, 2H), 3.15-3.25 (m, 2H), 1.63-1.75 (m, 2H), 1.48-1.42 (m, 2H), 0.85-0.95 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.1, 132.0, 128.5, 127.9, 127.1, 126.4, 126.1, 126.0, 122.9, 33.9, 32.5, 29.5, 23.1, 14.0; ESI-MS(*m/z*): 315.4$[C_{21}H_{21}N_3]^+$; HRMS (ESI): calcd. $[C_{21}H_{21}N_3+H]^+$: 316.1808, found: 316.1810; IR(KBr): 2911, 1511, 969, 845, 782㎝$^{-1}$.

1-phenyl-[1,2,3]triazolo[5,1-a]isoquinoline（**13**）



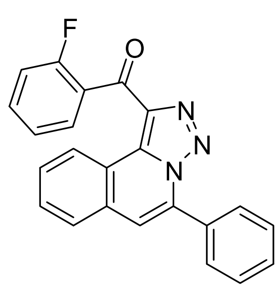
Yellow solid, mp: 186-190 □,^{1}H NMR (600 MHz, $CDCl_3$) δ 8.52 (s, 1H), 8.16 (d, *J* = 7.2 Hz, 1H), 7.98 (d, *J* = 6.6 Hz, 2H), 7.81 (d, *J* = 6.6 Hz, 1H), 7.61-7.67 (m, 2H), 7.50-7.57 (m, 3H), 7.23 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.9, 133.2, 132.1, 129.8, 129.5, 129.4, 129.2, 129.1, 128.4, 127.5, 126.0, 123.8, 123.7, 122.2,115.7, 115.5; ESI-MS(*m/z*): 245.2$[C_{16}H_{11}N_3]^+$; HRMS (ESI): calcd. $[C_{16}H_{11}N_3+H]^+$: 246.1026, found: 246.1026; IR(KBr): 3052, 1560, 987, 962, 848, 765, 671, 541 ㎝$^{-1}$.

(2-chlorophenyl)(5-phenyl-[1,2,3]triazolo[5,1-a]isoquinolin-1-yl)methanone (**15a**)



Yellow solid, mp: 181-184 ℃, ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.94 (d, *J* = 3.0 Hz, 1H), 7.88-7.95 (m, 3H), 7.80-7.82 (m, 2H), 7.59-7.62 (m, 1H), 7.52 (s, 3H), 7.41-7.50 (m, 3H), 7.24-7.40 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.7, 139.9, 139.8, 136.0, 134.8, 131.72, 131.67, 131.6, 131.3, 131.1, 130.1, 123.0, 129.8, 129.7, 128.9, 128.5, 128.3, 127.3, 126.4, 122.3, 118.0; ESI-MS(*m/z*): 383.1$[C_{23}H_{14}ClN_3O]^+$, 385.1$[C_{23}H_{14}ClN_3O+2]^+$(3:1); HRMS (ESI): calcd. $[C_{23}H_{14}ClN_3O+H]^+$: 384.0898, found: 384.0902; IR(KBr): 1656, 1521, 1064, 941, 858㎝$^{-1}$.

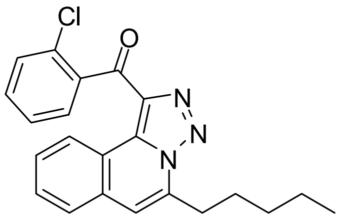
(2-fluorophenyl)(5-phenyl-[1,2,3]triazolo[5,1-a]isoquinolin-1-yl)methanone (**15b**)



White solid, mp: 180-181 ℃, ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.75-9.78 (m, 1H), 7.93-7.94 (m, 2H), 7.92 (s, 1H), 7.74-7.85 (m, 3H), 7.50-7.54 (m, 4H), 7.42 (s, 1H), 7.26-7.30 (m, 1H), 7.16-7.20 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 186.5, 160.6(d, *J* = 168 Hz), 139.9, 135.8, 134.4, 133.2, 133.1, 133.0, 131.5(d, *J* = 5 Hz), 131.1, 130.9, 130.0, 129.8, 129.6, 128.6, 128.5, 128.4, 127.9, 127.8, 127.2, 127.1, 123.9(d, *J* = 16 Hz), 122.1, 117.8 (d, *J* = 12 Hz), 116.3, 116.1, 116.0; ESI-MS(*m/z*): 368.4$[C_{23}H_{14}FN_3O+1]^+$; HRMS (ESI): calcd. $[C_{23}H_{14}FN_3O+H]^+$: 368.1194, found: 368.1196;

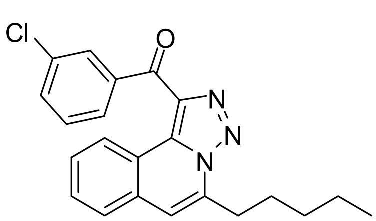
IR(KBr): 1654, 1519, 1070, 912, 806, 755, 526 ㎝$^{-1}$.

(2-chlorophenyl)(5-pentyl-[1,2,3]triazolo[5,1-a]isoquinolin-1-yl)methanone (**15c**)



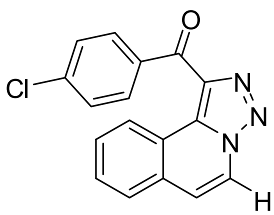
Yellow solid, mp: 122-126 ℃, ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.88 (d, *J* = 7.8 Hz, 1H), 7.84 (d, *J* = 6.6 Hz, 1H), 7.73-7.81 (m, 2H), 7.61 (d, *J* = 6.6 Hz, 1H), 7.50 (d, *J* = 7.8 Hz, 1H), 7.43-7.48 (m, 1H), 7.39-7.43 (m, 1H), 7.22 (s, 1H), 3.30-3.40 (m, 2H), 1.86-2.02 (m, 2H), 1.43-1.52 (m, 2H), 1.34-1.44 (m, 2H), 0.90-0.94 (m, 3H); ^{13}C NMR (100 MHz, d^{6}-DMSO) δ 188.0, 152.2, 136.5, 135.7, 131.6, 131.4, 131.3, 130.0, 129.5, 129.2, 128.1, 127.4, 127.2, 126.9, 126.8, 123.7, 122.8, 122.4, 120.9, 115.8, 30.8, 30.0, 26.0, 21.7, 13.7; ESI-MS(*m/z*): 377.2$[C_{22}H_{20}ClN_3O]^+$; HRMS (ESI): calcd. $[C_{22}H_{20}ClN_3O+H]^+$: 378.1368, found: 378.1374; IR(KBr): 2925, 1654, 1511, 991, 906 ㎝$^{-1}$.

(3-chlorophenyl)(5-pentyl-[1,2,3]triazolo[5,1-a]isoquinolin-1-yl)methanone (**15d**)



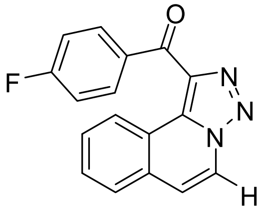
White solid, mp: 94-95 ℃, ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.45 (d, *J* = 8.4 Hz, 1H), 8.16 (s, 1H), 8.06 (d, *J* = 7.8 Hz, 1H), 7.71 (d, *J* = 7.8 Hz, 1H), 7.55-7.67 (m, 2H), 7.48 (d, *J* = 7.8 Hz, 1H), 7.35-7.40 (m, 1H), 7.09 (s, 1H), 3.20-3.35 (m, 2H), 1.81-1.93 (m, 2H), 1.27-1.46 (m, 4H), 0.82-0.92 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 186.7, 140.1, 139.3, 136.8, 134.6, 134.2, 132.4, 131.4, 130.8, 130.8, 129.3, 129.1, 127.9, 127.4, 126.6, 121.7, 115.5, 31.5, 30.8, 26.6, 22.4, 14.0; ESI-MS(*m/z*): 377.1[$C_{22}H_{20}ClN_3O$]$^+$, 379.1[$C_{22}H_{20}ClN_3O$+2]$^+$(3:1); HRMS (ESI): calcd. [$C_{22}H_{20}ClN_3O$+H]$^+$: 378.1368, found: 378.1372; IR(KBr): 2944, 1643, 1511, 946, 858㎝$^{-1}$.

[1,2,3]triazolo[5,1-a]isoquinolin-1-yl(4-chlorophenyl)methanone (**15e**)



White solid, mp: 183-184 ℃, ^{1}H NMR (600 MHz,$CDCl_3$) δ 9.57-9.61 (m, 1H), 8.64 (d, *J* = 7.8 Hz, 1H), 8.23 (d, *J* = 8.4 Hz, 2H), 7.87-7.91 (m, 1H), 7.75-7.83 (m, 2H), 7.52 (d, J = 8.4Hz, 2H), 7.44 (d, *J* = 7.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 186.7, 139.2, 136.6, 134.2, 132.3, 131.0, 129.1, 128.5, 127.9, 127.4, 122.9, 122.3, 118.3; ESI-MS(*m/z*): 307.2[$C_{17}H_{10}ClN_3O$]$^+$, 309.2[$C_{17}H_{10}ClN_3O$+2]$^+$ (3:1); HRMS (ESI): calcd. [$C_{17}H_{10}ClN_3O$+H]$^+$: 308.0585, found: 308.0586; IR(KBr): 3091, 1645, 1569, 952, 840, 792, 754, 667㎝$^{-1}$.

[1,2,3]triazolo[5,1-a]isoquinolin-1-yl(4-fluorophenyl)methanone (**15f**)



Yellow solid, mp: 153-154 ℃, ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.54-9.68 (m, 1H), 8.65 (d, *J* = 7.2

Hz, 1H), 8.30-8.35 (m, 2H), 7.87-7.90 (m, 1H), 7.75-7.85 (m, 2H), 7.44 (d, *J* = 7.2 Hz, 1H), 7.20-7.27 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 186.5, 165.2(d, *J* = 153 Hz), 139.4, 134.5, 134.2, 133.5(d, *J* = 12 Hz), 130.9, 129.2, 127.9, 127.4, 123.0, 122.3, 118.3, 115.3(d, *J* = 22 Hz); ESI-MS(*m/z*): 291.1$[C_{17}H_{10}FN_3O]^+$; HRMS (ESI): calcd. $[C_{17}H_{10}FN_3O+H]^+$: 292.0881, found: 292.0882; IR(KBr): 3083, 1656, 1554, 927, 889, 786, 744, 657㎝$^{-1}$.

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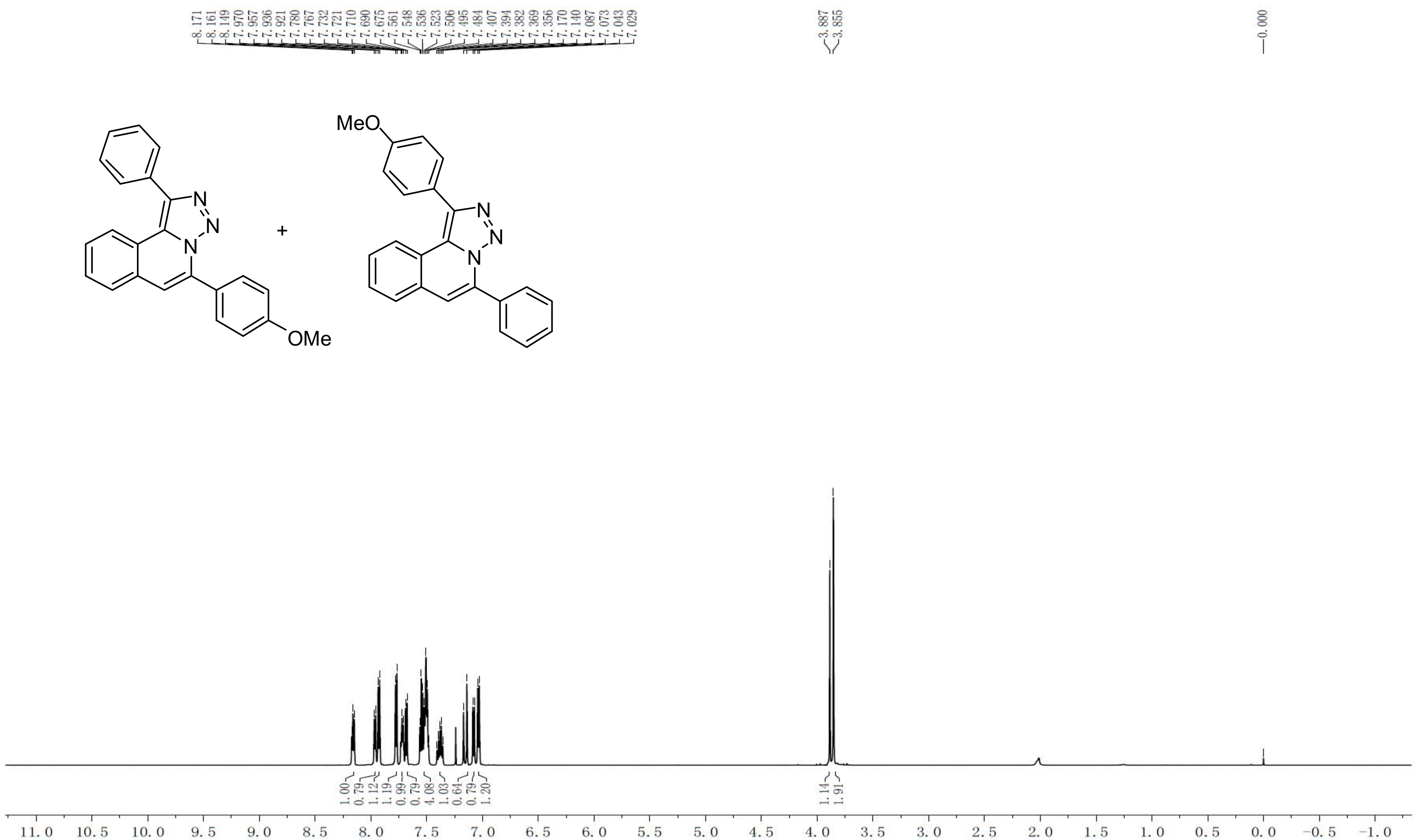

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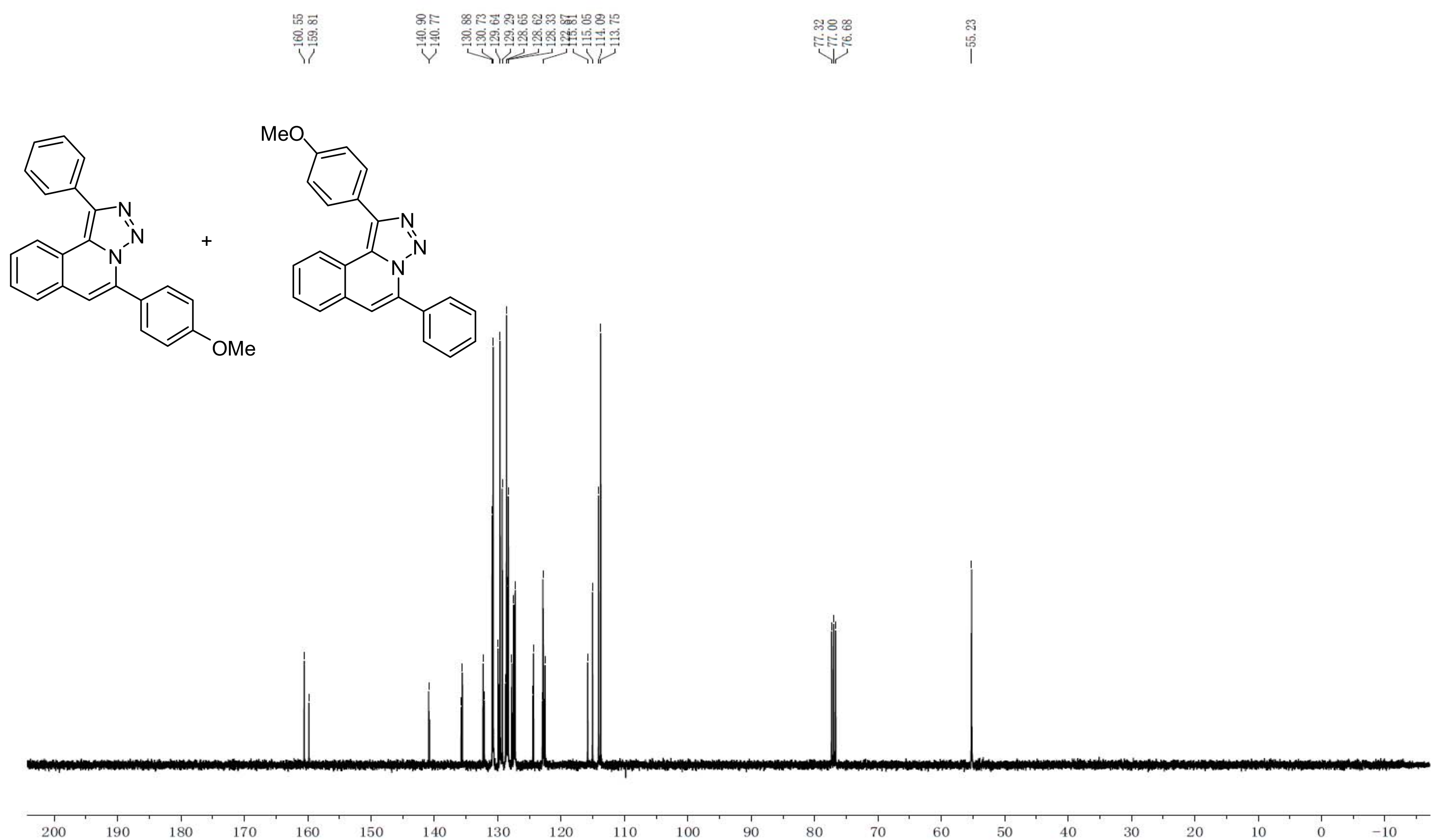

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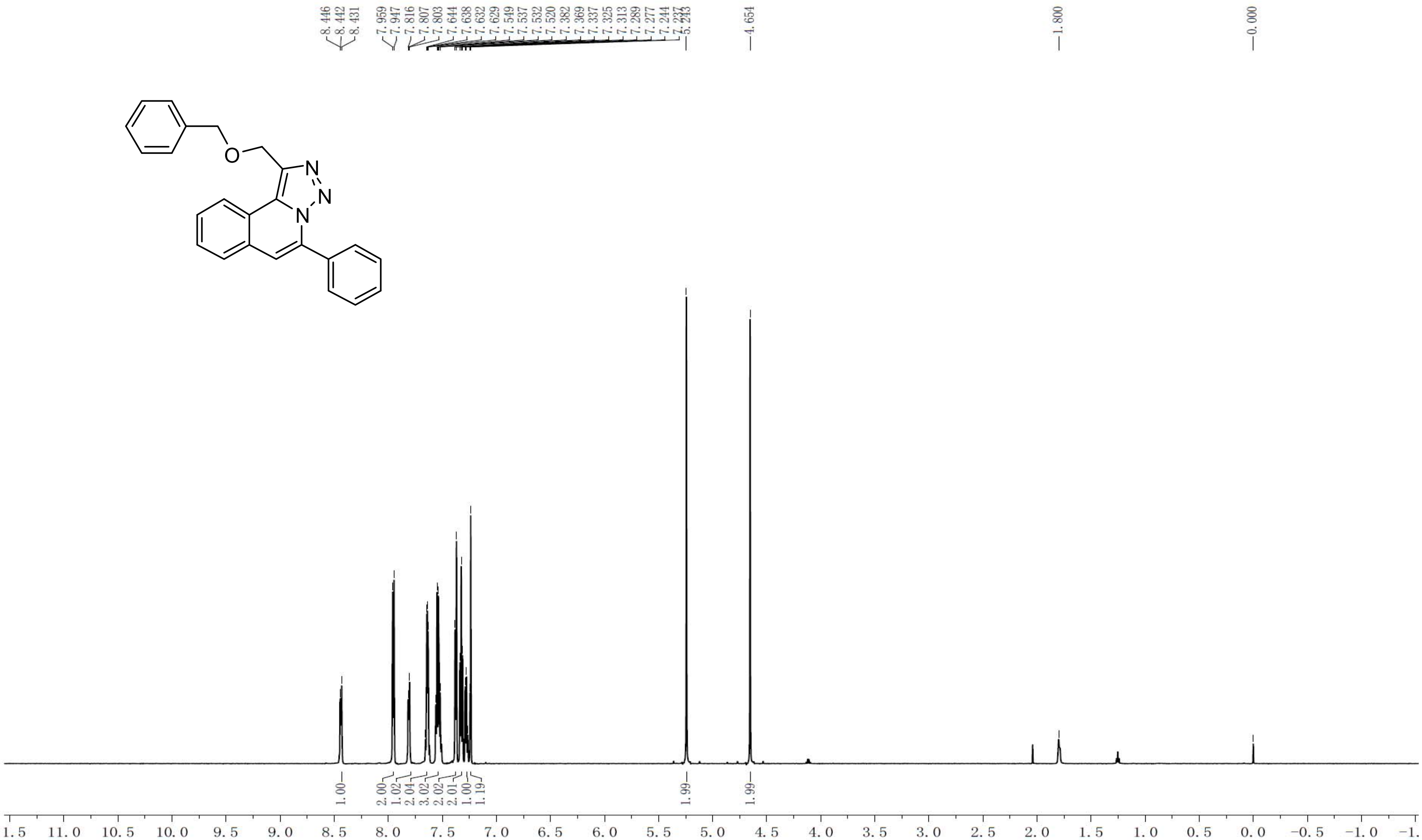
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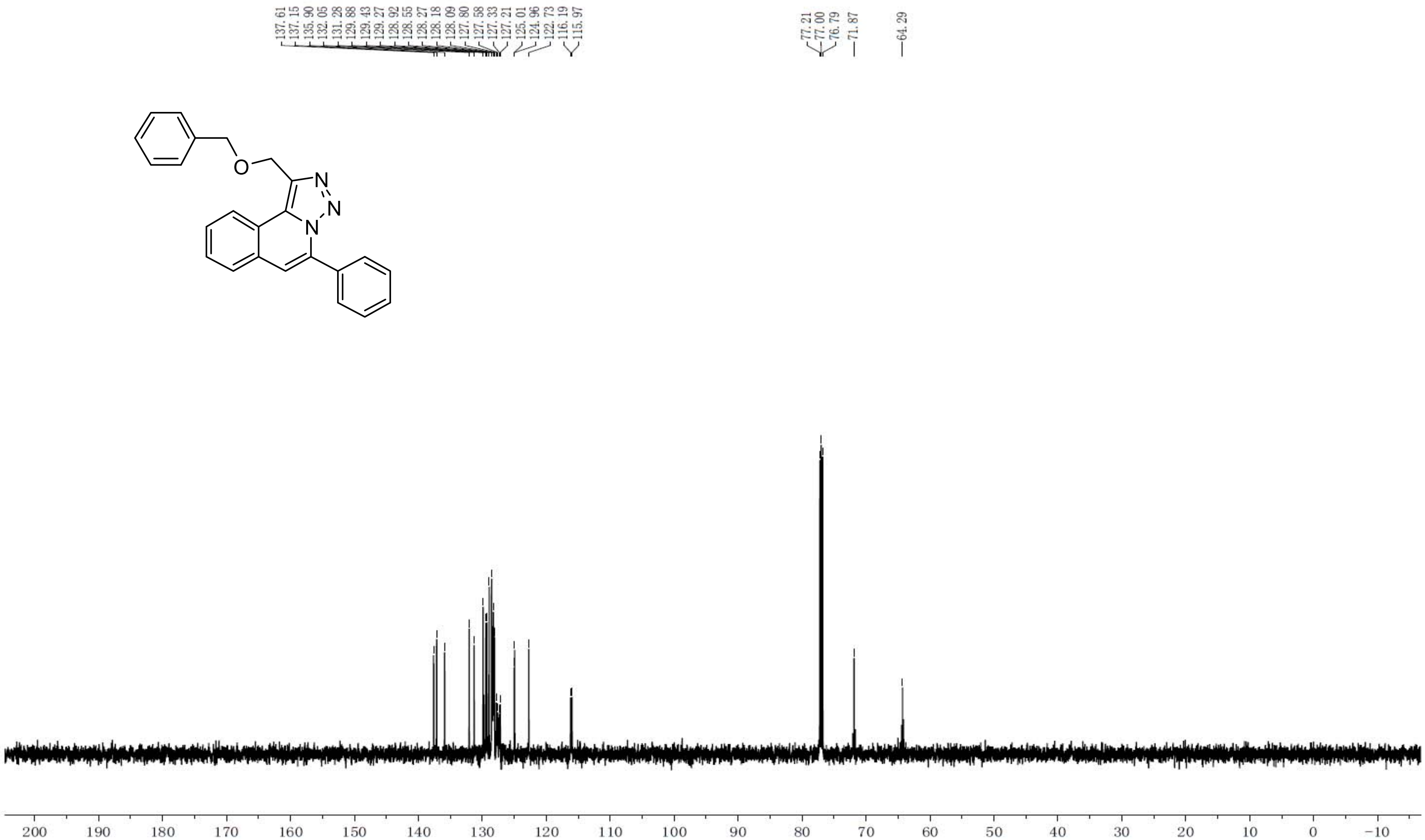

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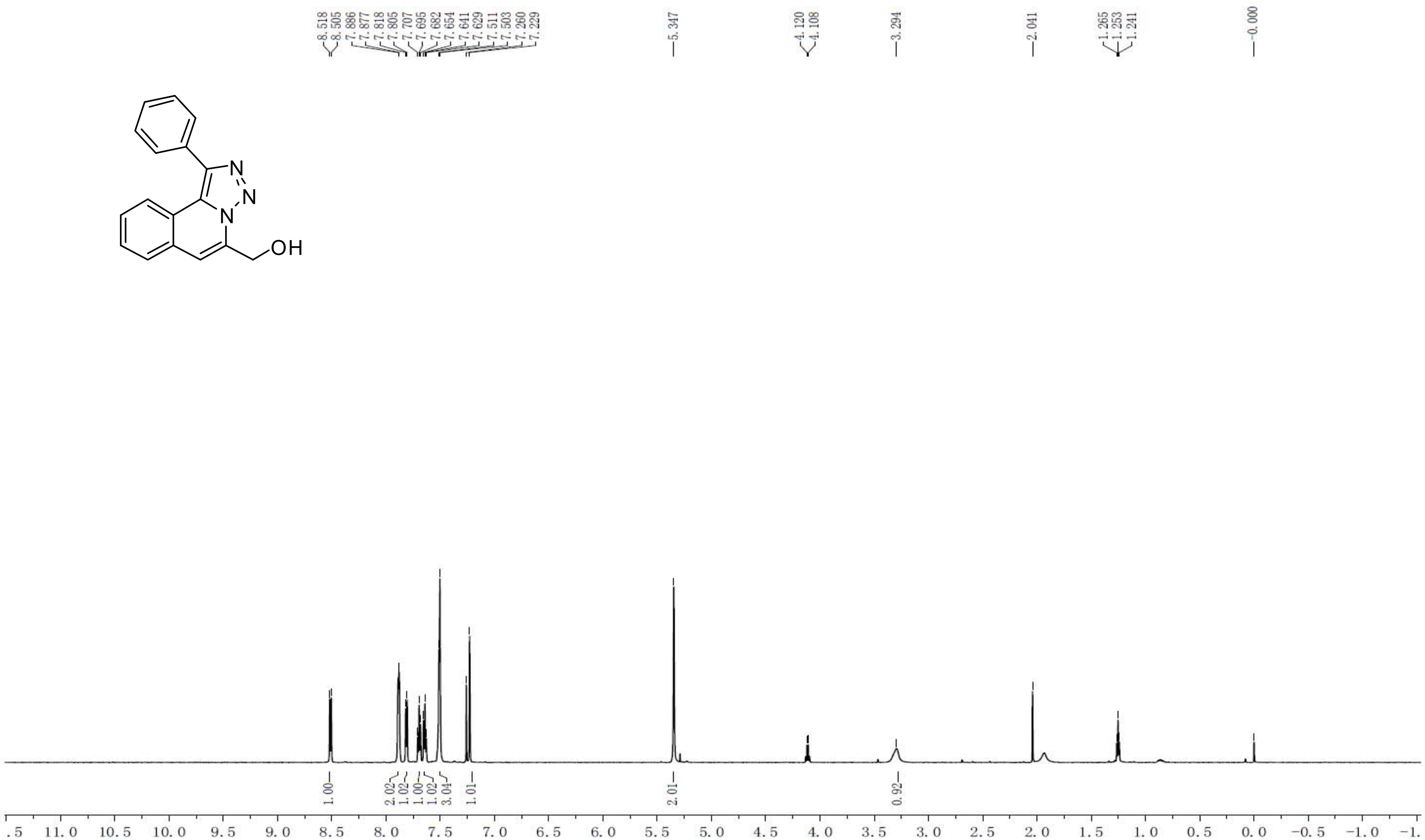

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2.01
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N
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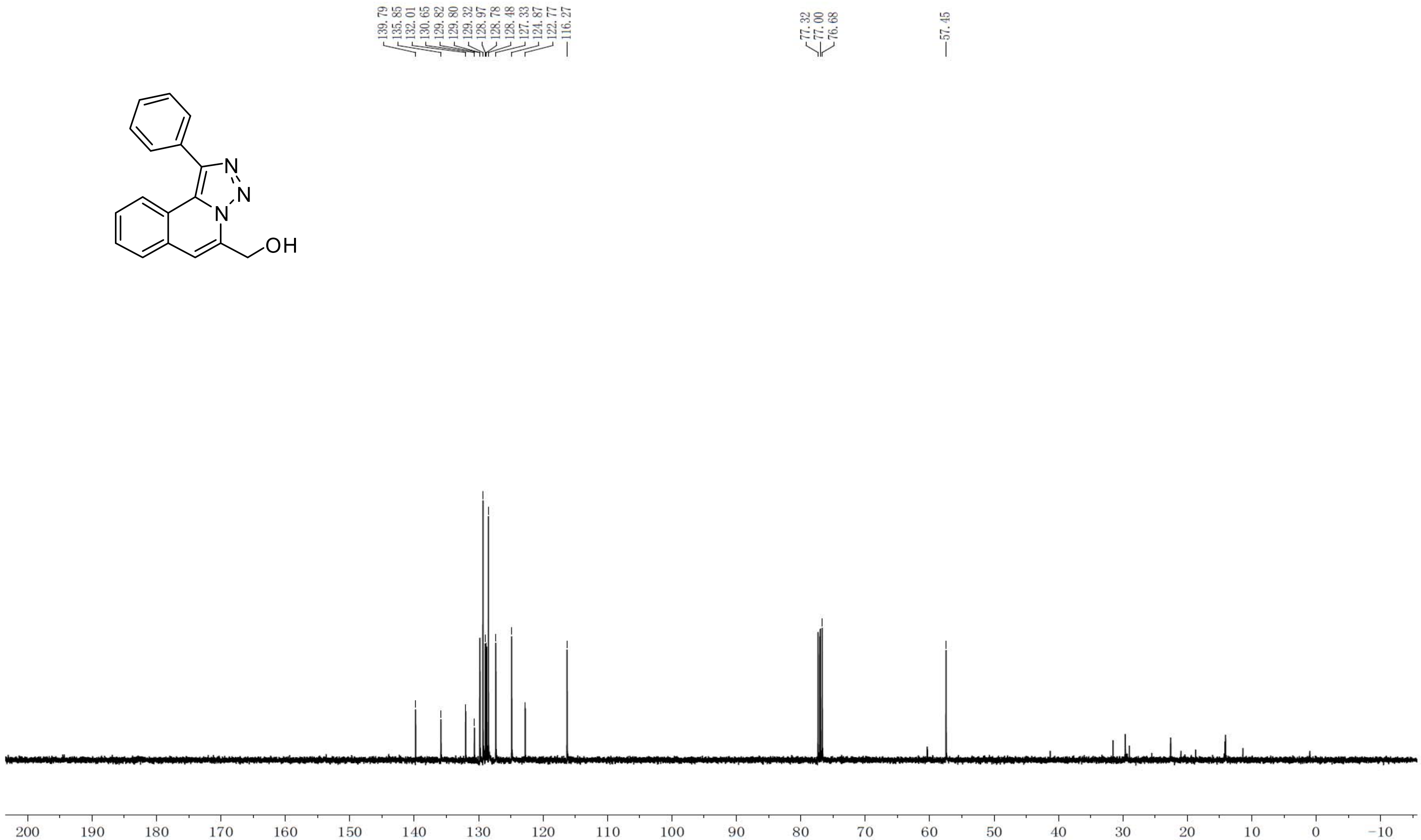
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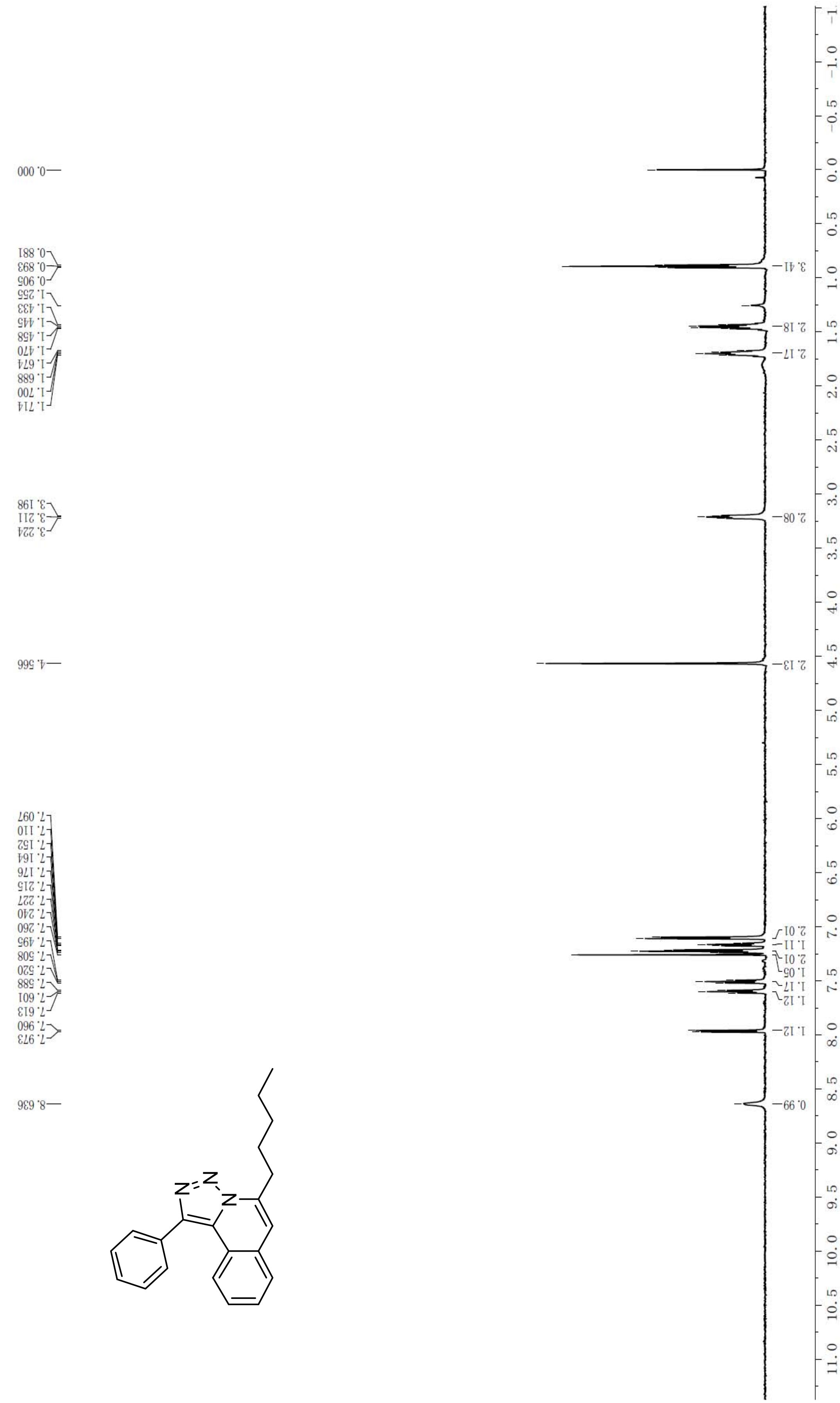
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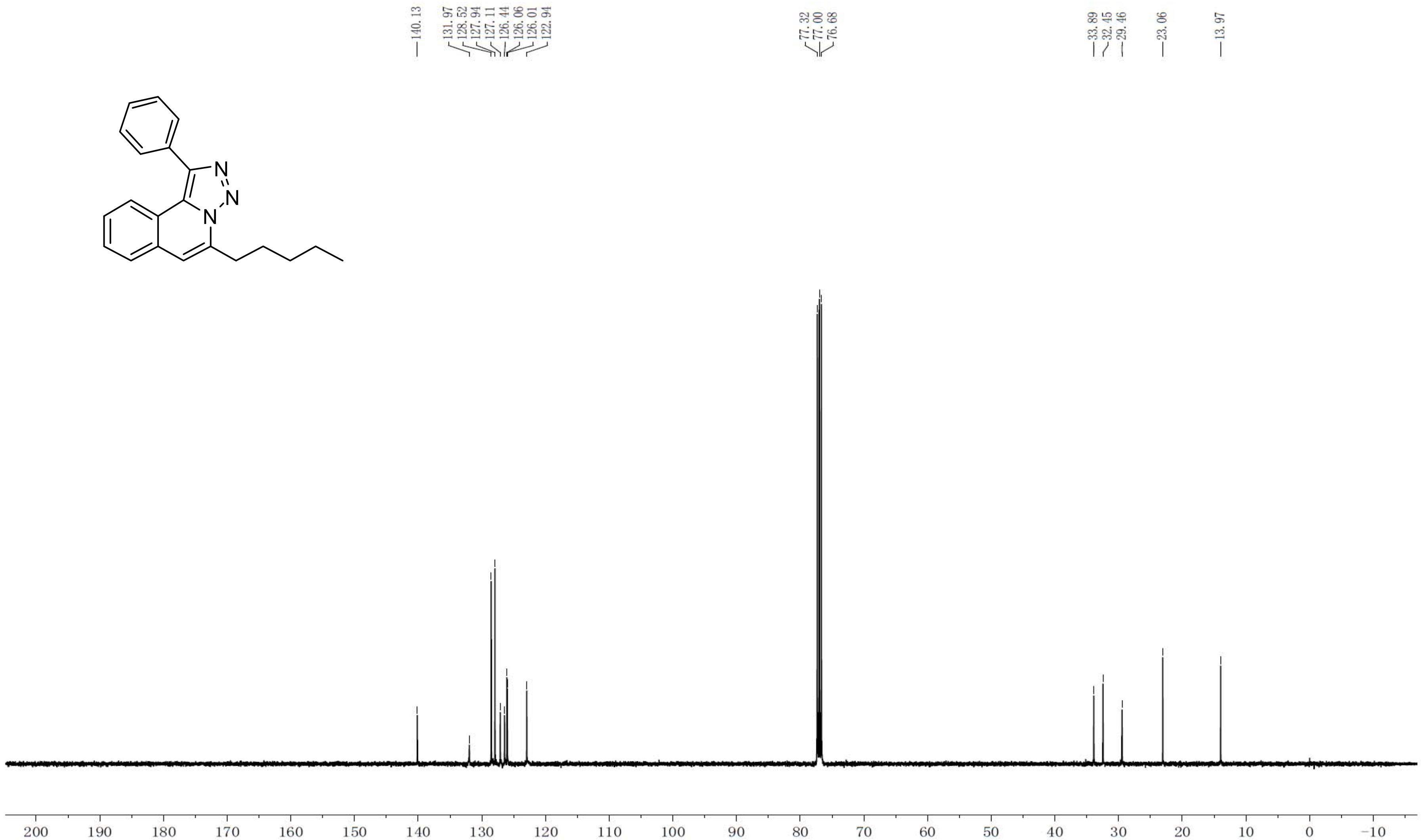
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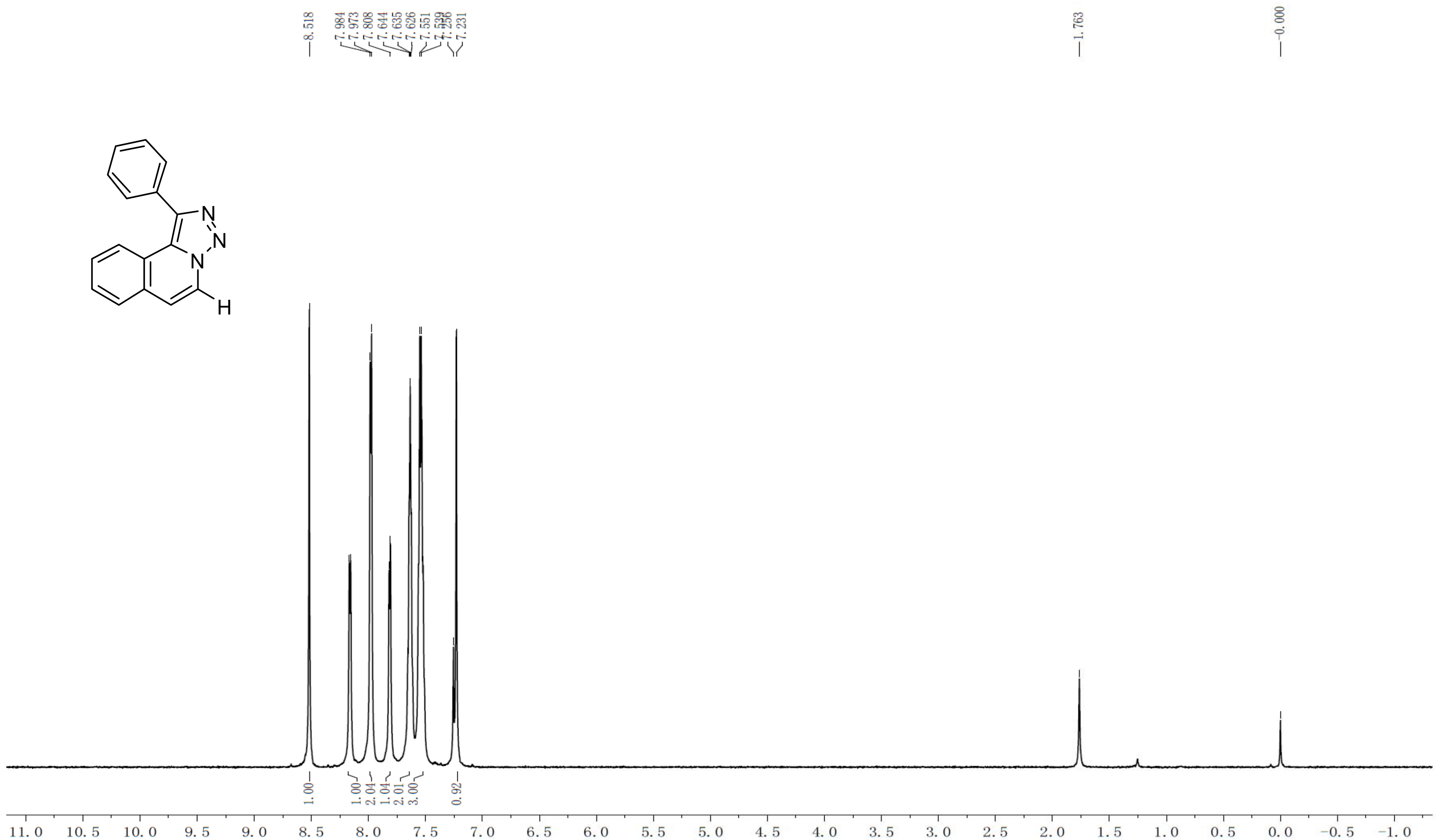

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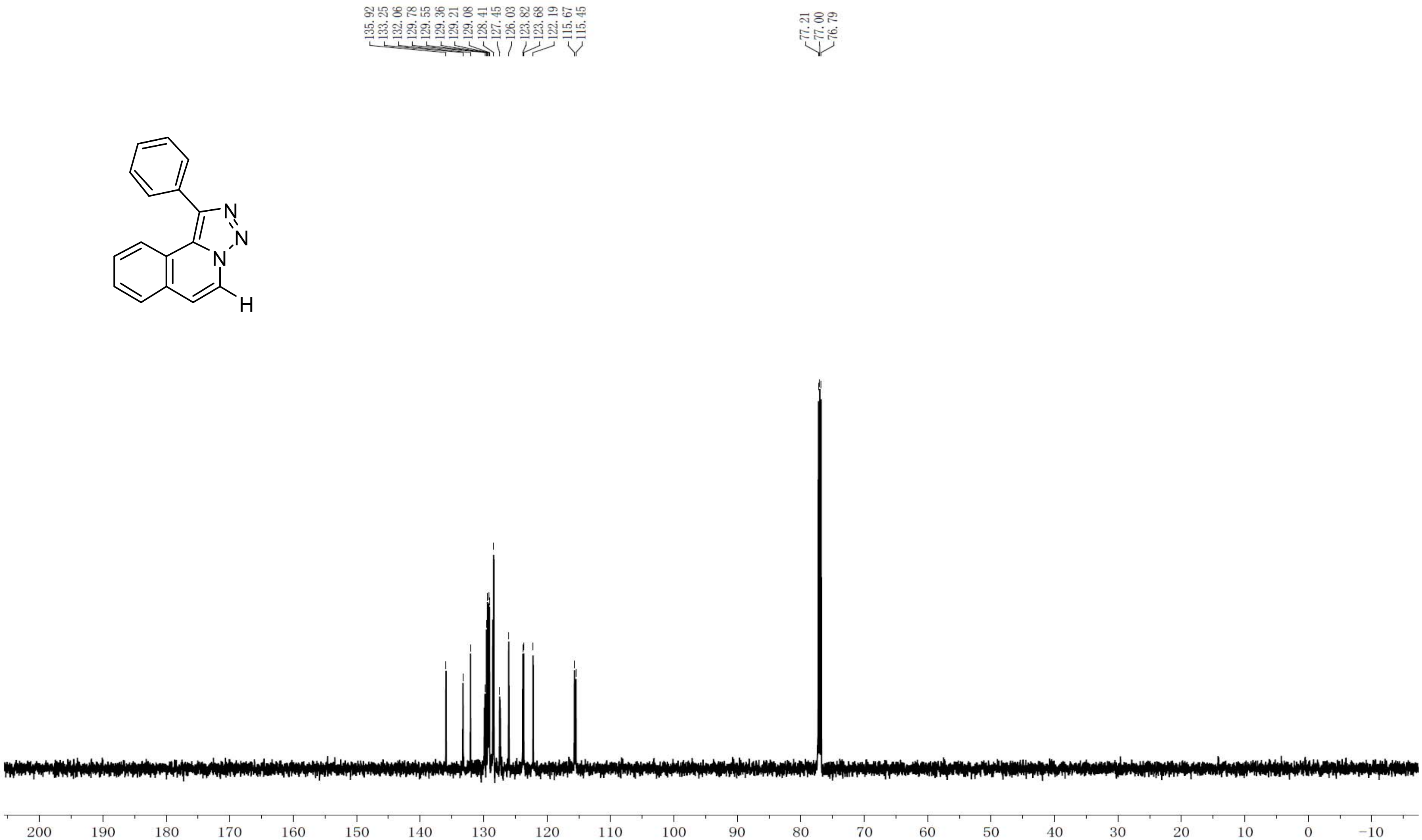
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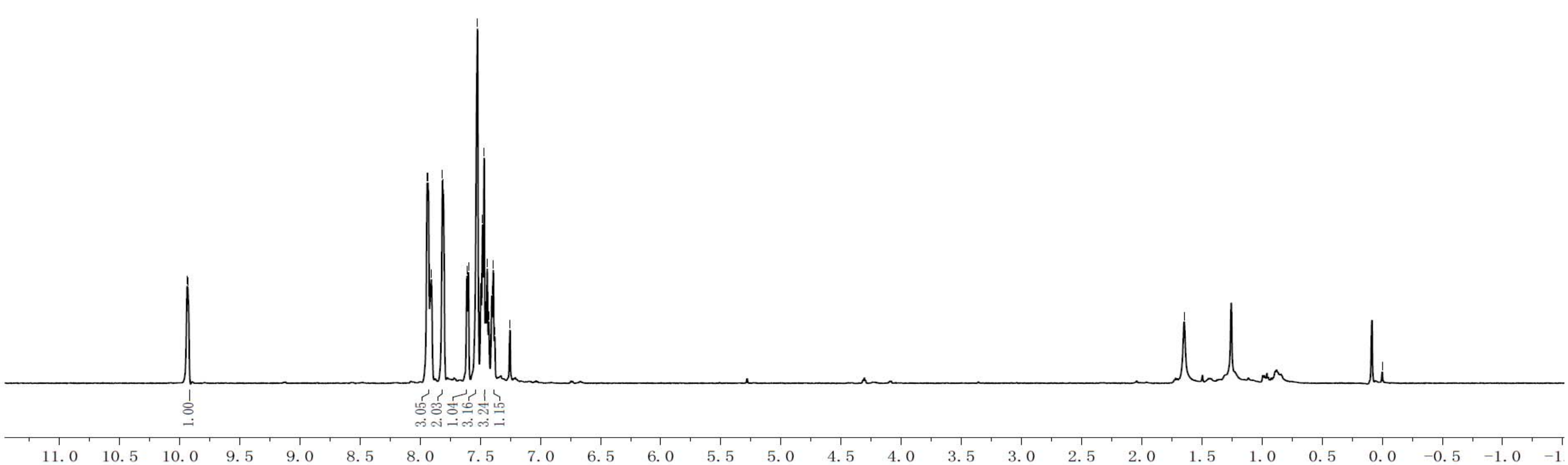

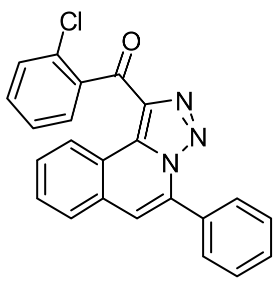

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1.00
3.05
2.03
1.04
3.16
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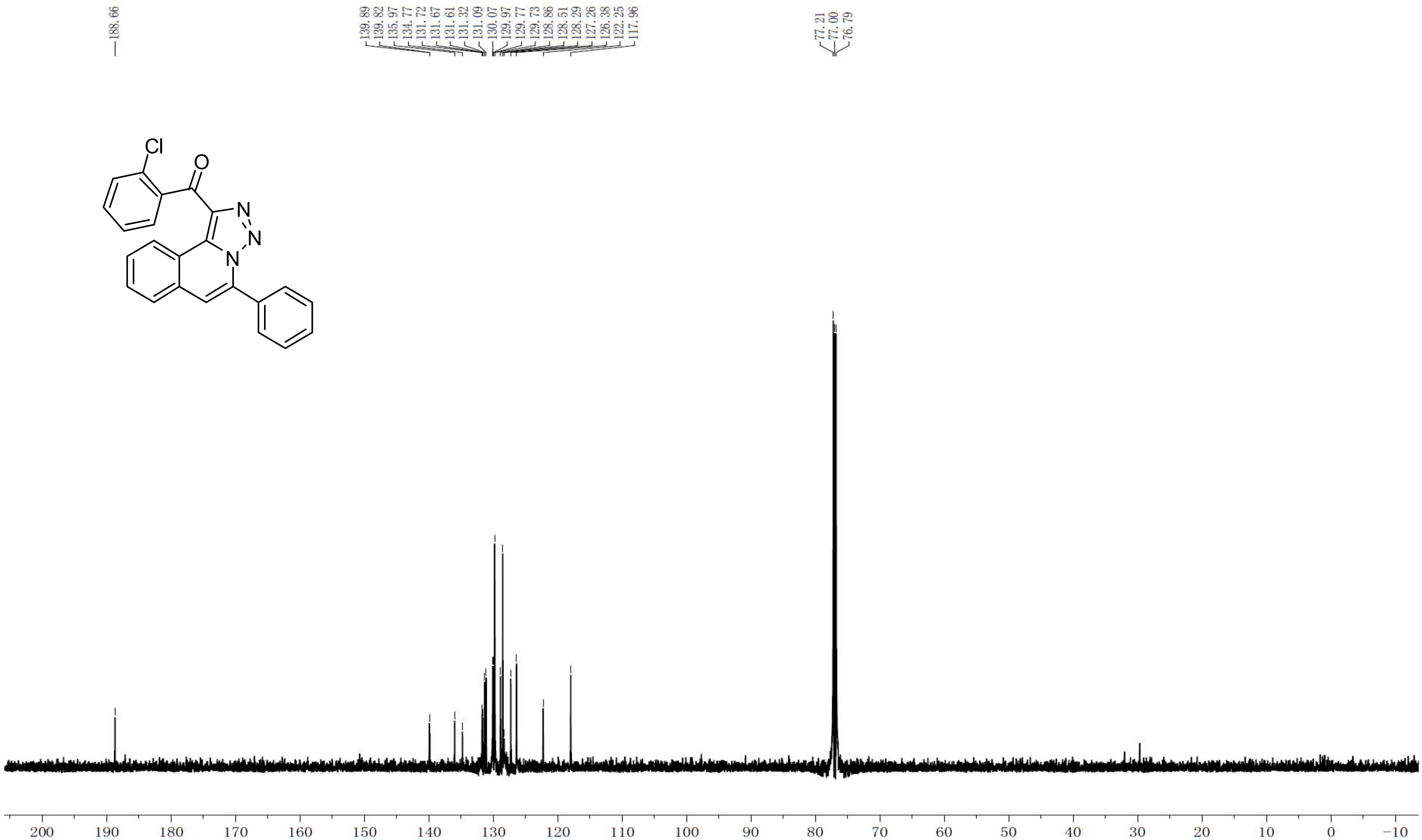

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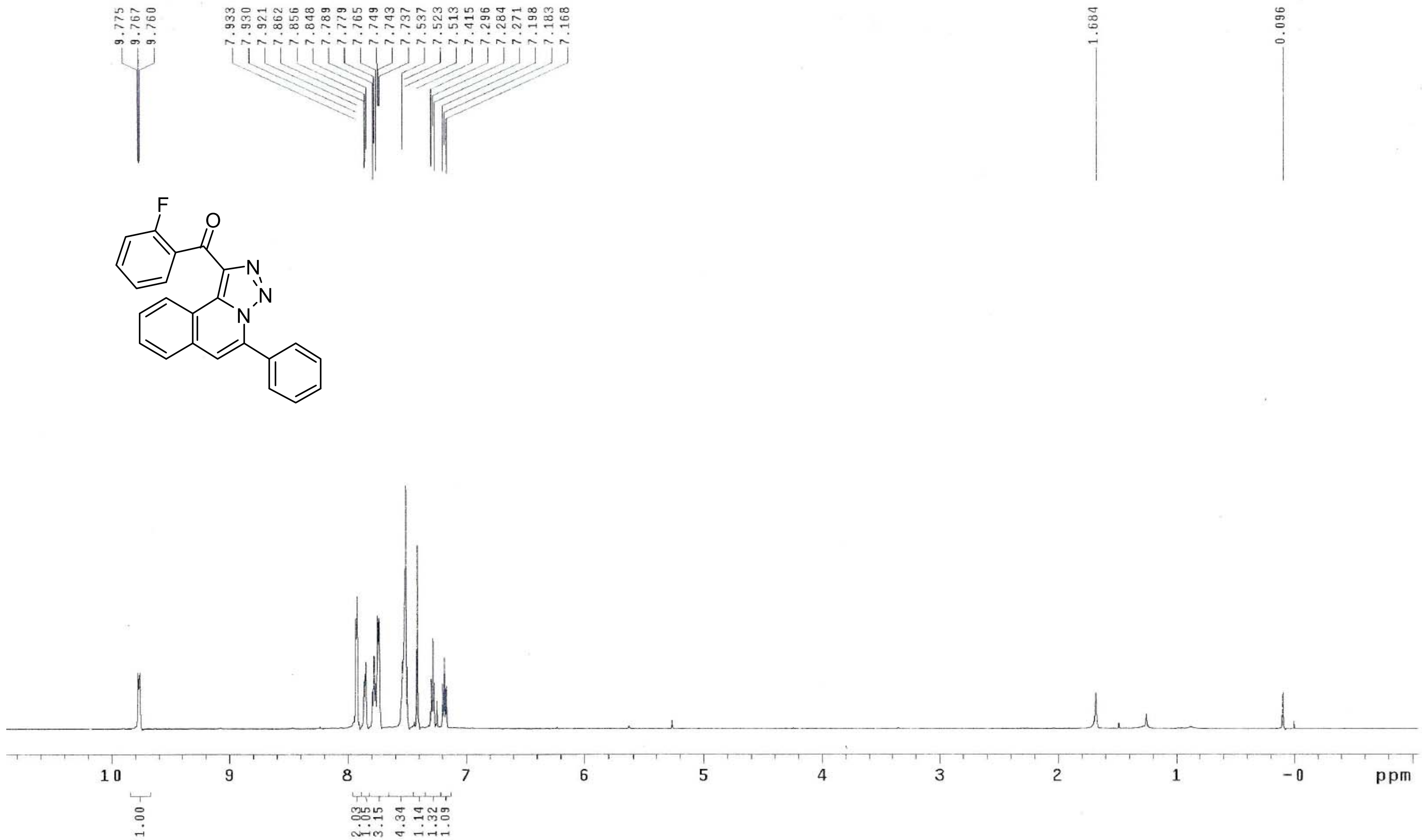
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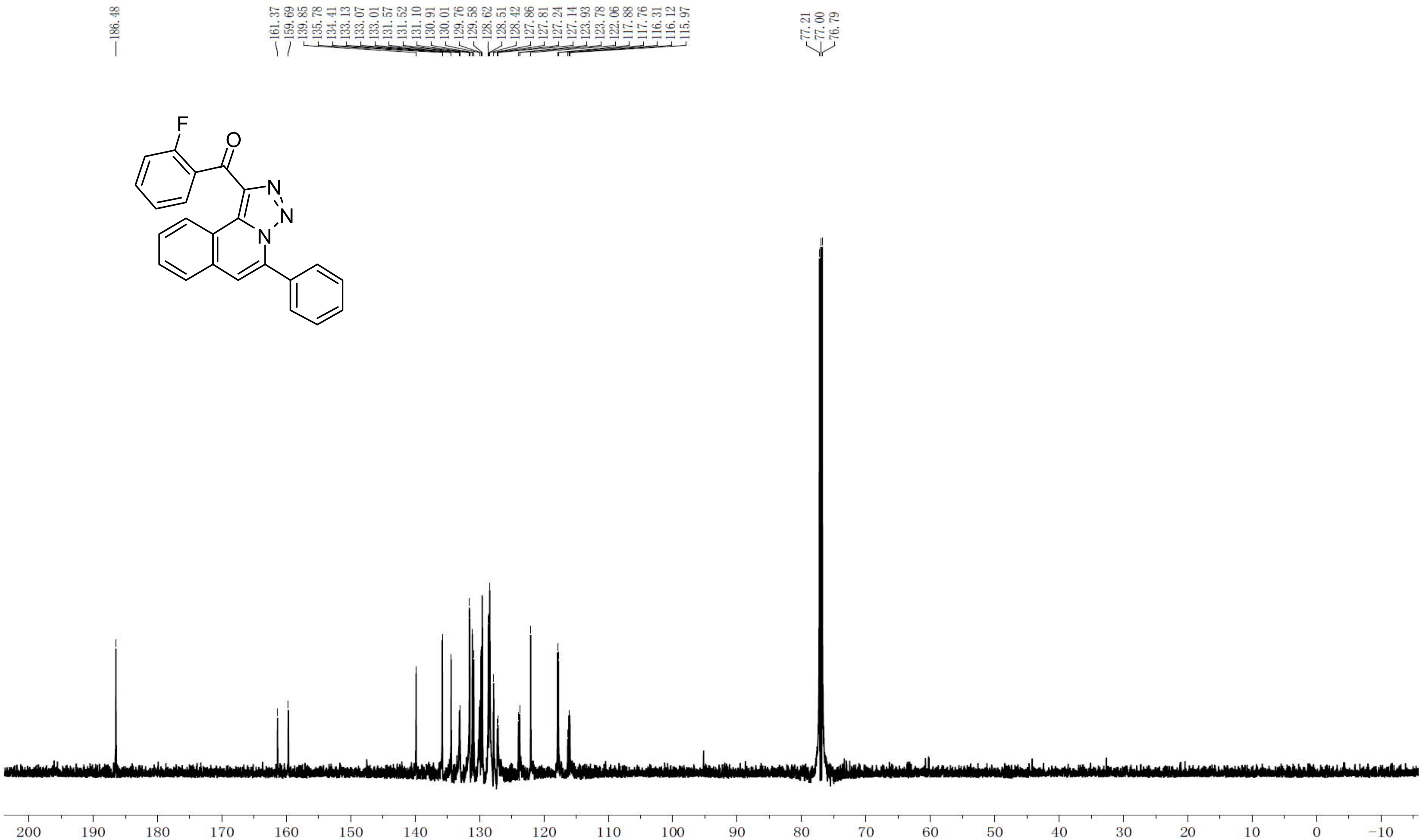
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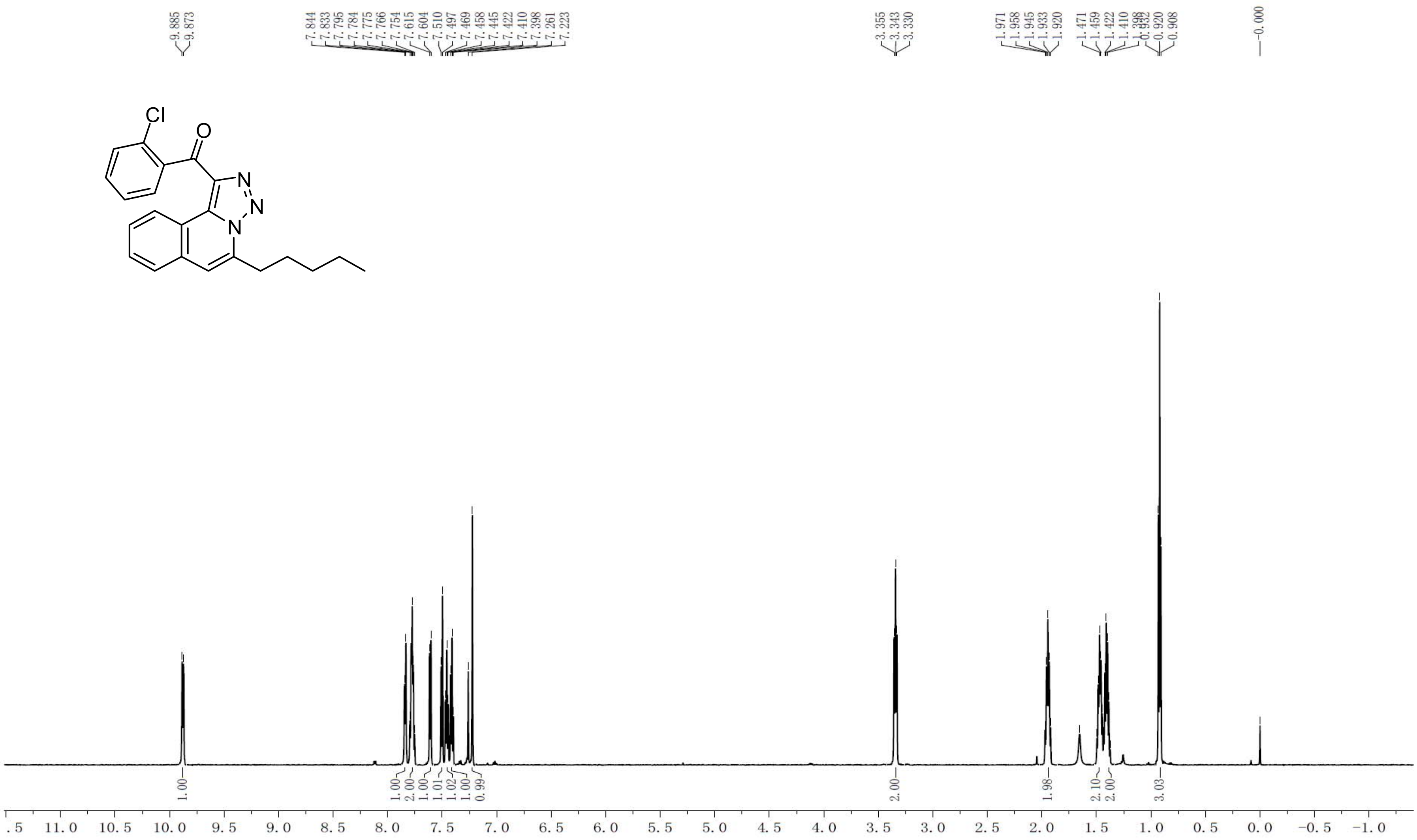

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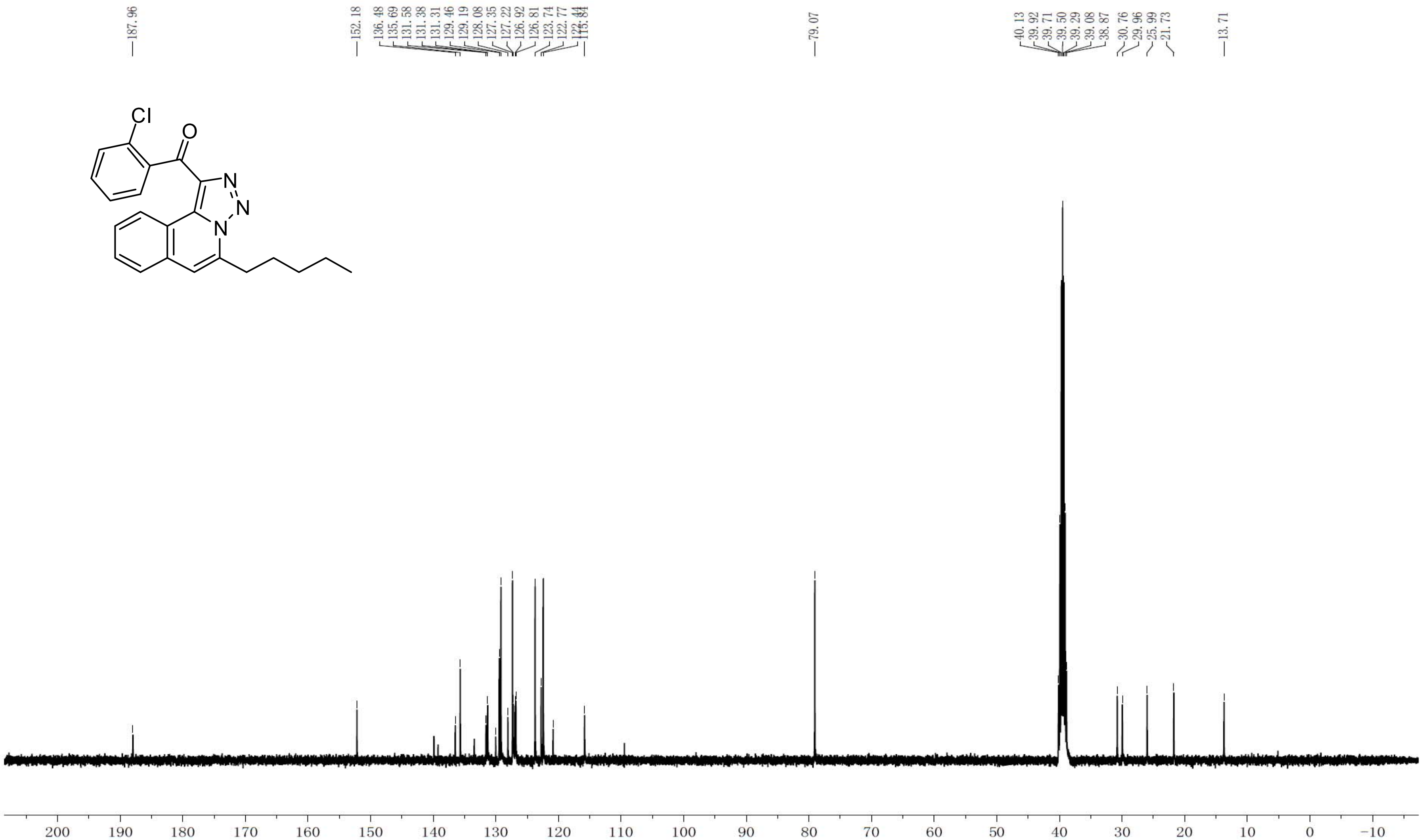
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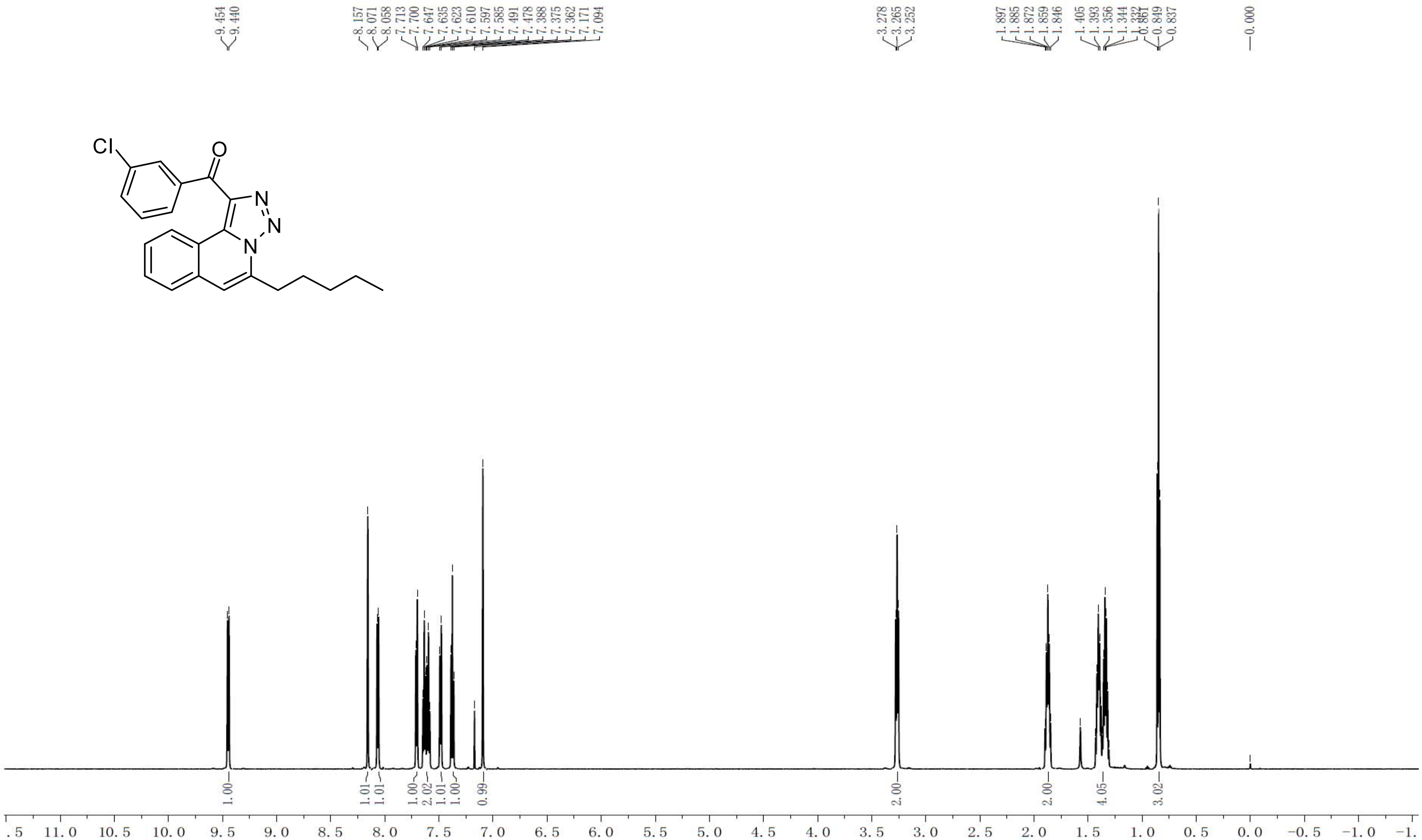

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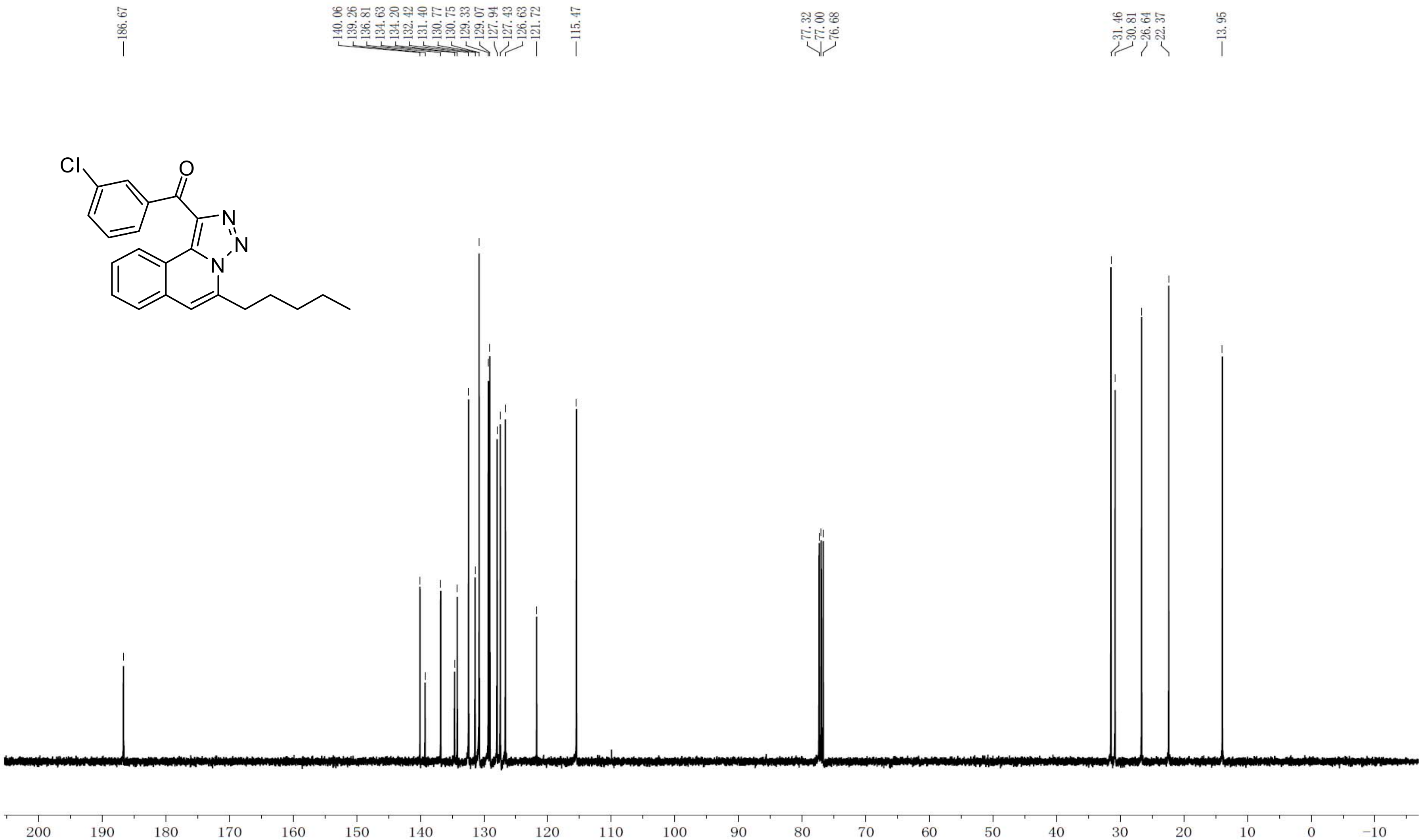

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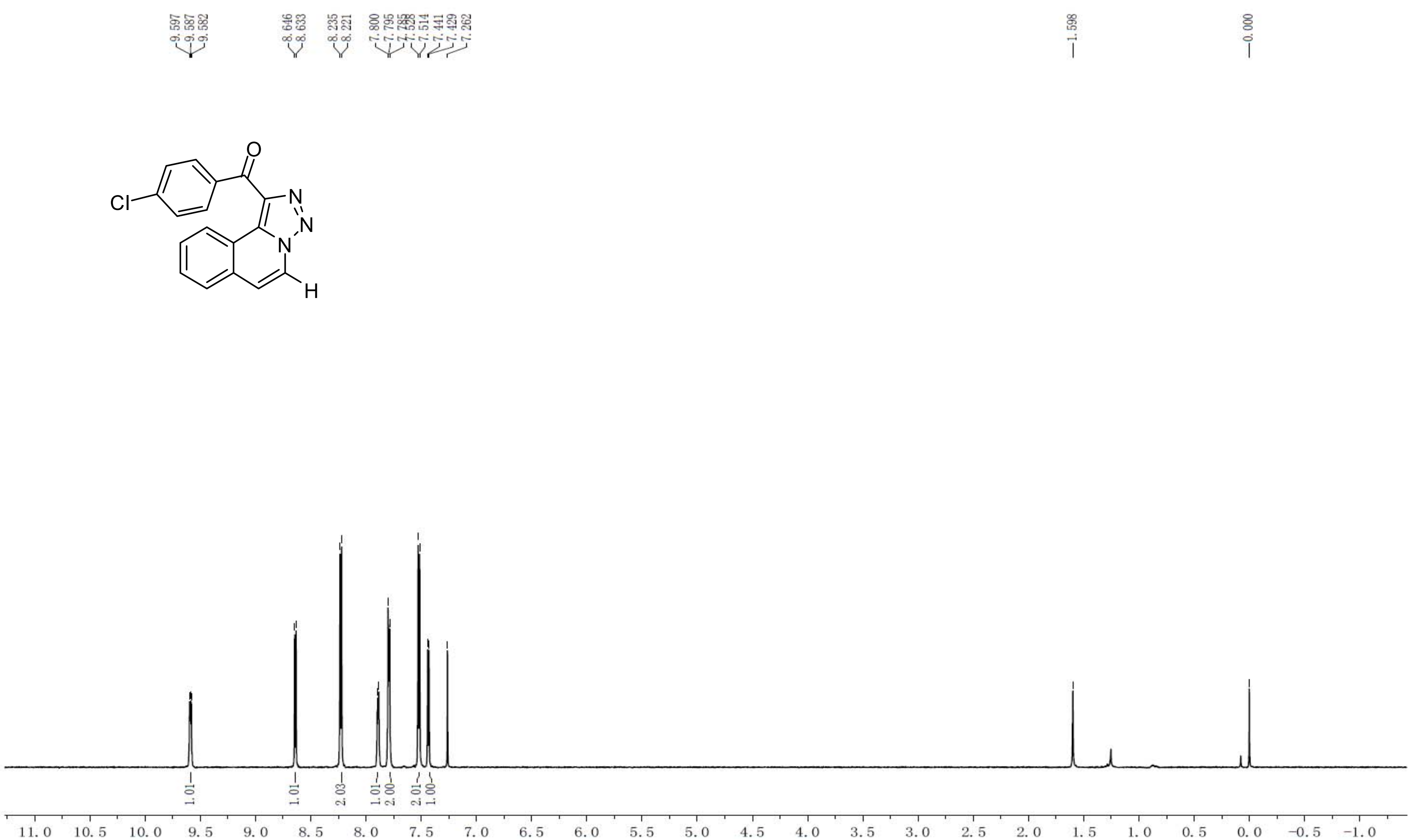
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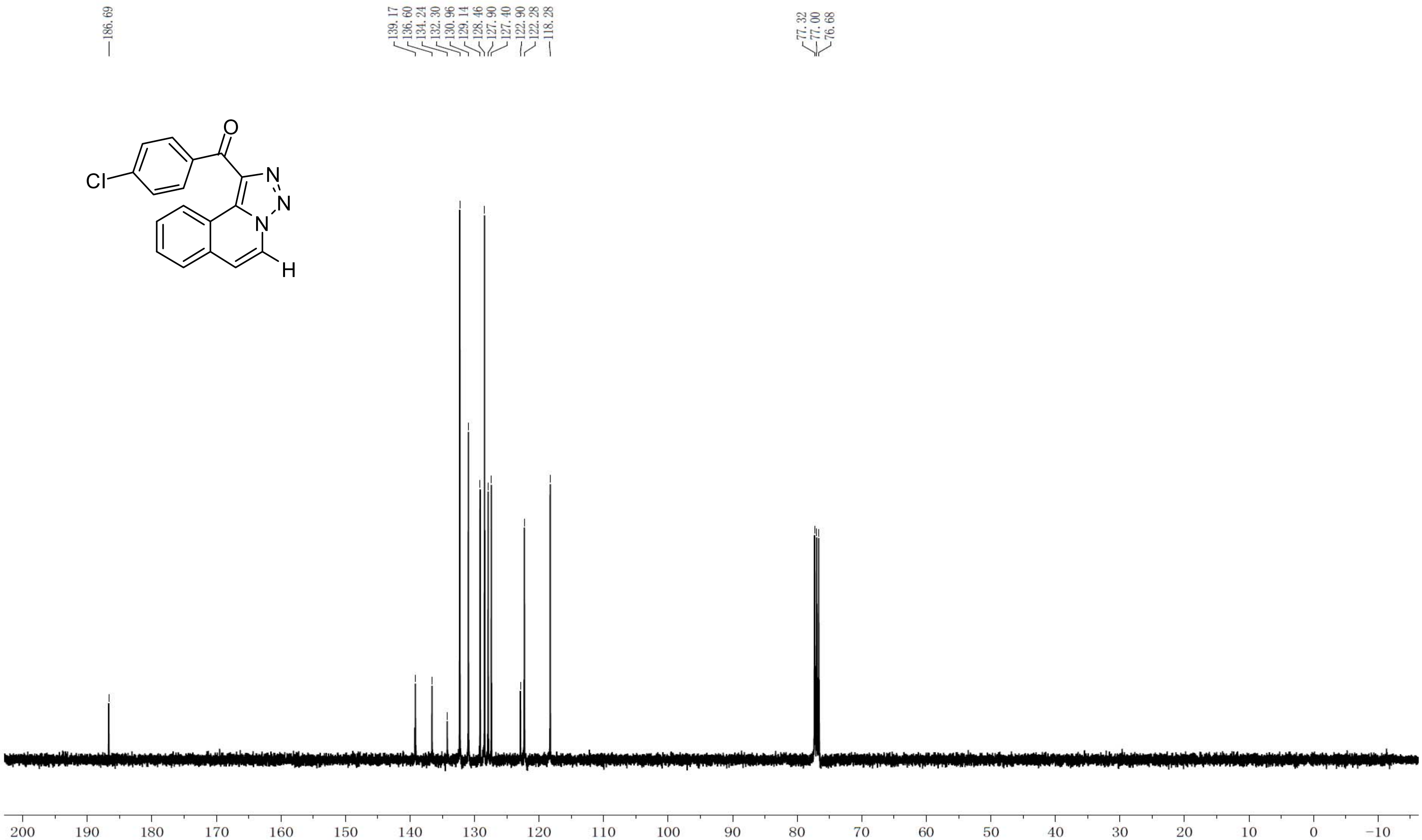

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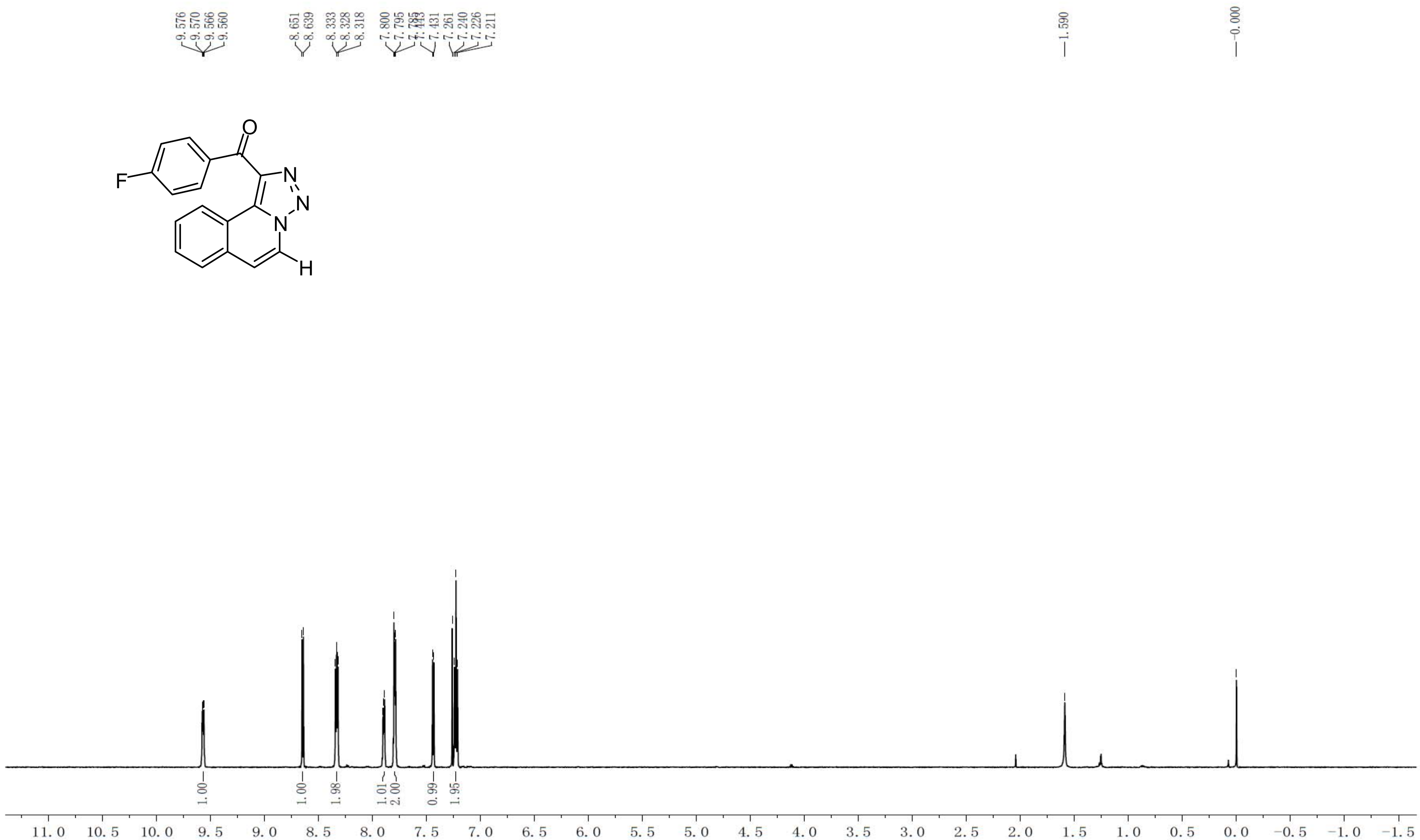

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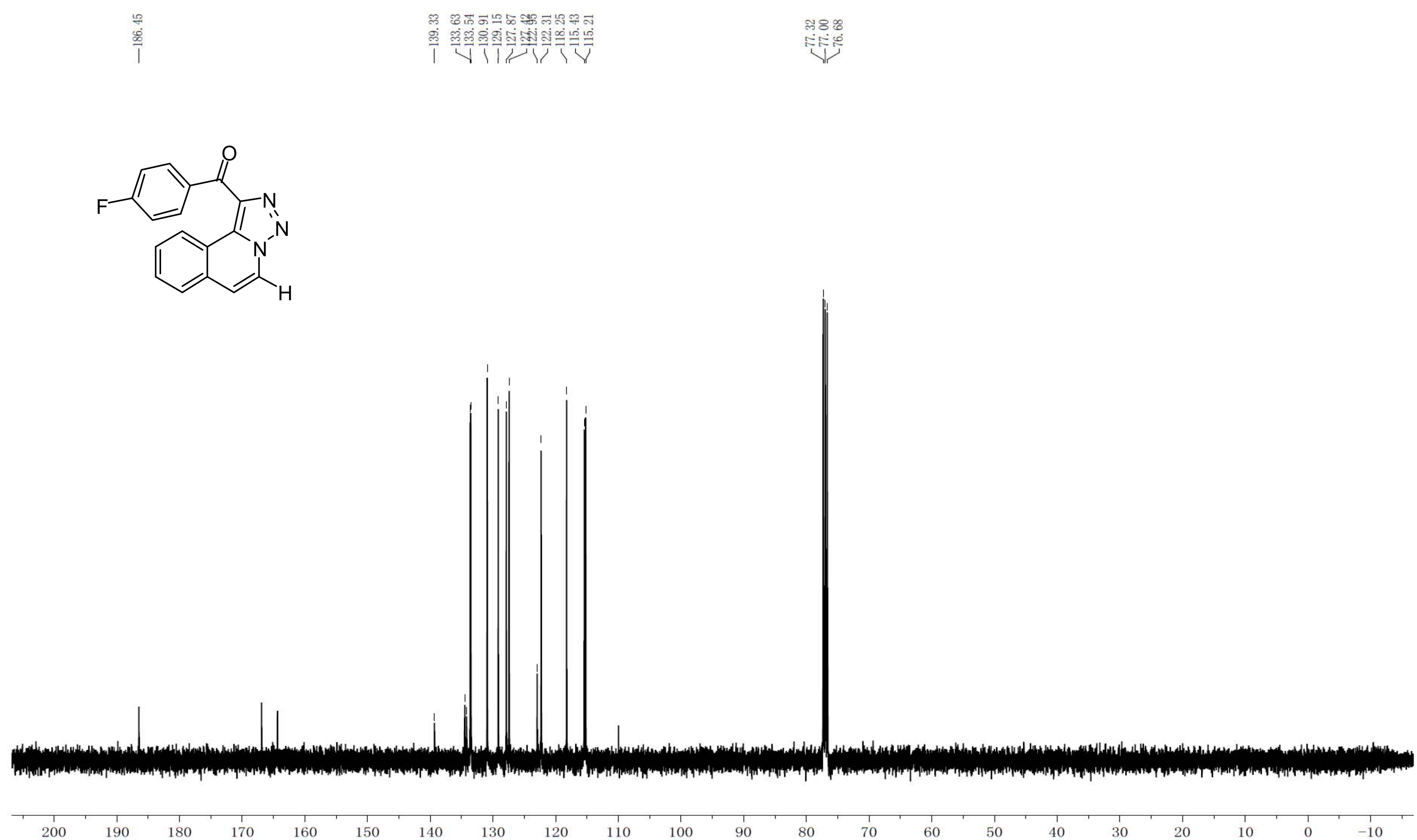
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200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10