# Supporting Information

## Metal-free construction of aminated isoquinoline frameworks from 2-(2-oxo-2-arylethyl) benzonitrile in an aqueous medium

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## X-Ray Crystallographic Studies

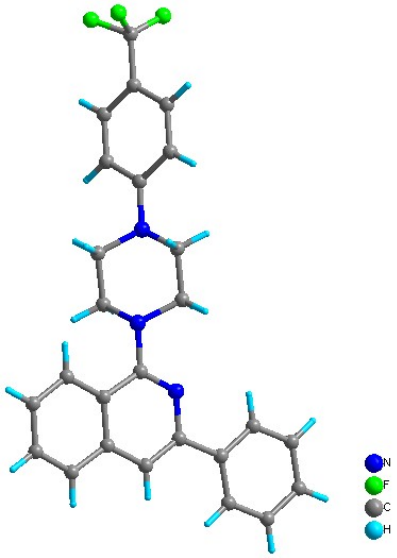
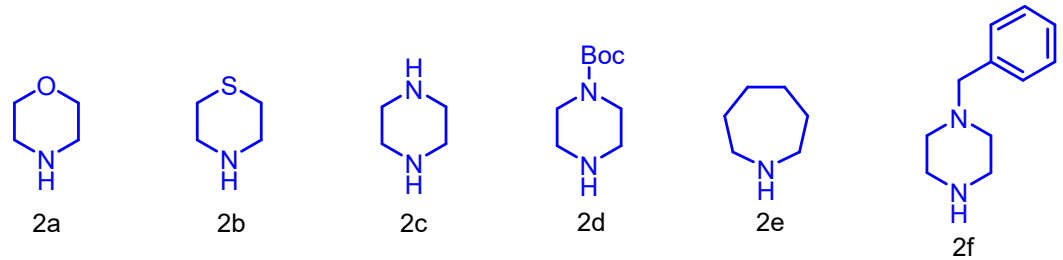
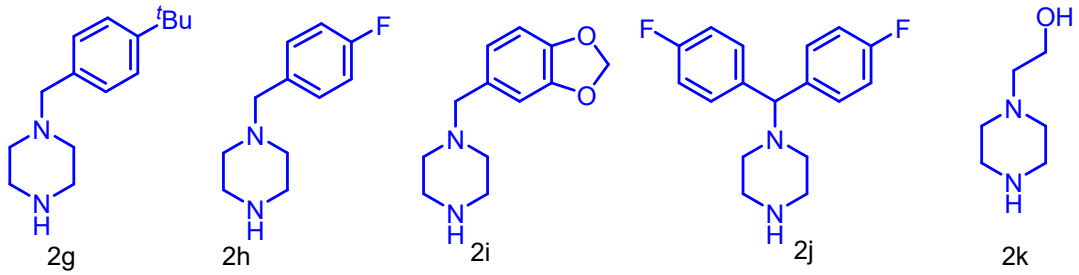


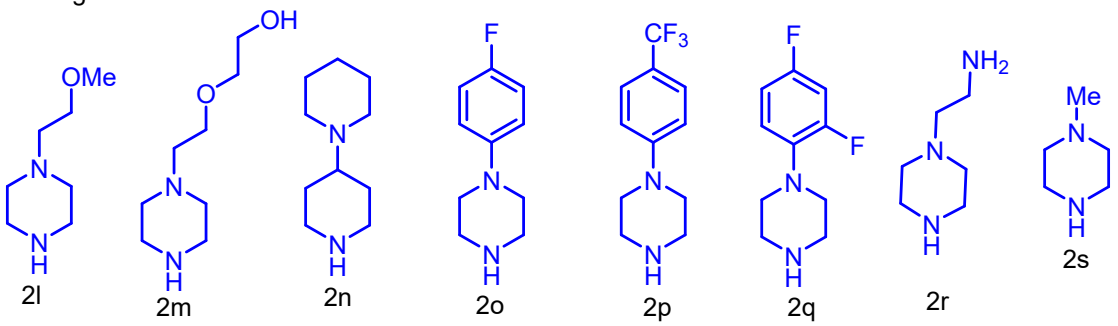

**Figure I**. ORTEP structure of compound **3p.** CCDC No. 2204378

| | |
|---|---|
| Empirical formula | $C_{26}H_{22}F_3N_3$ |
| Formula weight | 433.46 |
| Temperature/K | 298 |
| Crystal system | monoclinic |
| Space group | $P2_1/n$ |
| $a$/Å | 9.7050(10) |
| $b$/Å | 16.0805(14) |
| $c$/Å | 13.7744(13) |
| $\alpha$/° | 90 |
| $\beta$/° | 93.165(9) |
| $\gamma$/° | 90 |
| Volume/Å$^3$ | 2146.4(4) |
| $Z$ | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.341 |
| $\mu$/mm$^{-1}$ | 0.098 |
| $F$(000) | 904.0 |
| Crystal size/mm$^3$ | 0.055 × 0.032 × 0.023 |
| Radiation | Mo Kα ($\lambda$ = 0.71073) |
| 2Θ range for data collection/° | 5.066 to 65.708 |
| Index ranges | $-14 \leq h \leq 12$, $-23 \leq k \leq 22$, $-17 \leq l \leq 19$ |
| Reflections collected | 31693 |
| Independent reflections | 7578 [$R_{int}$ = 0.0535, $R_{sigma}$ = 0.0593] |
| Data/restraints/parameters | 7578/3/317 |
| Goodness-of-fit on F$^2$ | 0.993 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0773, $wR_2$ = 0.1970 |
| Final R indexes [all data] | $R_1$ = 0.1977, $wR_2$ = 0.2869 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.39/-0.20 |

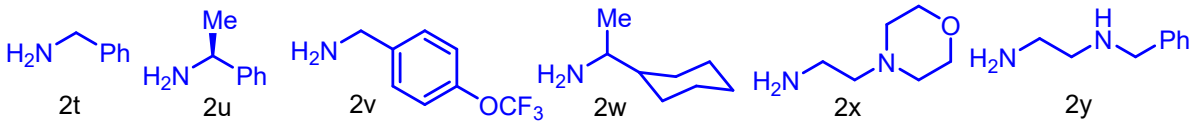
Secondary amine



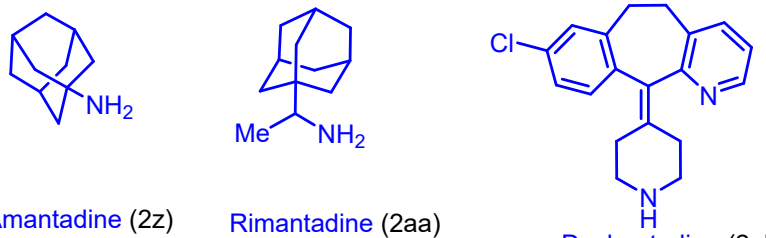




Primary amine




Drugs



## EXPERIMENTAL SECTION

### General Information and Method

$^{1}H$ NMR (400 MHz) and $^{13}C\{H\}$NMR (100 MHz) spectra were recorded in $CDCl_3$ and $(CD_3)_2SO$. Chemical shifts for protons and carbons are reported in ppm from tetramethylsilane and are referenced to the carbon resonance of the solvent. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublet), coupling constants in Hertz and integration. High-resolution mass spectra were recorded on q-TOF electrospray mass spectrometer. Crystal structure analysis was accomplished on single needles X-ray diffractometer. TLC analysis was performed on commercially prepared 60 $F_{254}$ silica gel plates and visualized by either UV irradiation or by staining with $I_2$. All purchased chemicals were used as received. All melting points are uncorrected.

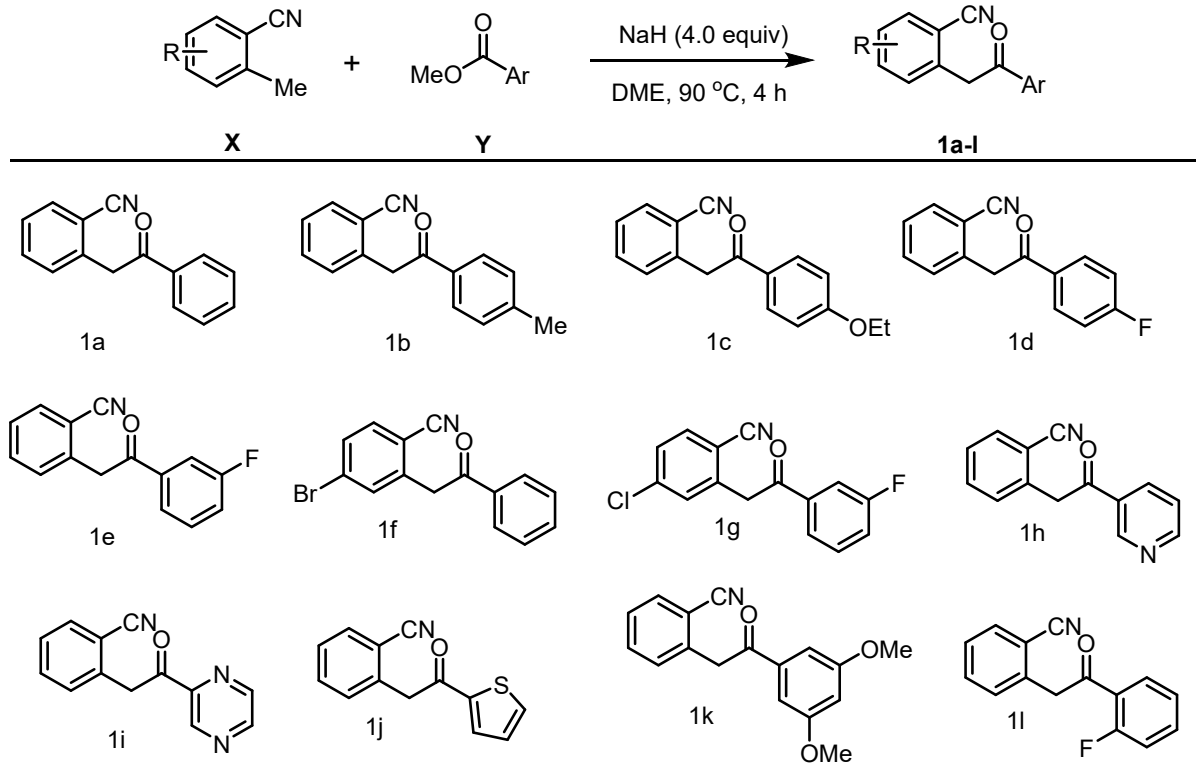
### Reagents

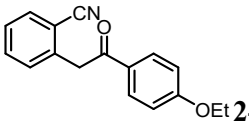
All reagents were used directly as obtained commercially unless otherwise noted. HPLC grade ACN, THF, DMF, DMSO, MeOH, dioxane, hexane, ethyl acetate, and DCM were purchased from Merck Chemical Co. Sodium hydride, Aryl ester, 2-Methyl benzonitrile derivatives, Primary/Secondary amines, and Drugs were purchased from Sigma-Aldrich Chemical Co., Inc.

### General procedure for the preparation of 2-(2-oxo-2-arylethyl)benzonitrile (1a-l)

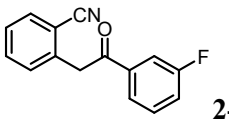
To probe the viability of the designed tandem strategy, 2-(2-oxo-2-arylethyl)benzonitrile **1a-l** were readily prepared by standard reported general procedure[1]. Initially, sodium hydride (4.0 equiv) was added to dimethoxyethane (DME) under a nitrogen atmosphere and stirred at room temperature for 20 min then aryl ester 1.0 equiv, (10.0 mol) and 2-methylbenzonitrile 1.0 equiv, were added drop-wise via syringe and reaction mixture stirred at 90 $^{o}C$ for 4 hours. After the complete consumption of starting material, the reaction was monitored by TLC and cooled to room temperature, quenched in the brine solution. The mixture was extracted with ethyl acetate (2×40 mL). The combined organic layers were dried over anhydrous $Na_2SO_4$, filtered, and concentrated under a rotary evaporator. The residue was purified by column chromatography using (100-200) silica gel, furnishing the corresponding products

as white solids. The structure and purity of the starting materials **1a-1l** were confirmed by spectral data $^{1}$H NMR, $^{13}$C NMR and HRMS.



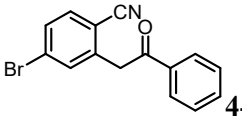



**2-(2-(4-Ethoxyphenyl)-2-oxoethyl)benzonitrile (1c).** The product was obtained as pale-yellow solid (1.51 g, 57%): mp 105–106 °C: $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, $J$ = 8.9 Hz, 2H), 7.67 (d, $J$ = 8.9 Hz, 1H), 7.54 (t, $J$ = 7.7 Hz, 1H), 7.37 (d, $J$ = 7.6 Hz, 2H), 6.94 (d, $J$ = 8.9 Hz, 2H), 4.48 (s, 2H), 4.10 (q, $J$ = 7.0 Hz, 2H), 1.44 (t, $J$ = 7.0 Hz, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 194.0, 163.4, 139.4, 132.9, 131.1, 130.9, 129.12, 127.6, 118.3, 114.5, 113.5, 63.6, 43.3, 14.6; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{17}H_{16}NO_2$ 266.1176, found 266.1178.

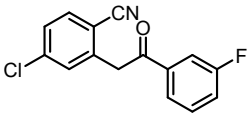


**2-(2-(3-Fluorophenyl)-2-oxoethyl)benzonitrile (1e).** The product was obtained as off pale-yellow solid (1.31 g, 55%): mp 107-108 °C: $^{1}$H NMR (400 MHz $CDCl_3$) δ 7.84 (d, $J$ = 7.7 Hz, 1H), 7.70 (t, $J$ = 7.0 Hz, 2H), 7.58 (t, $J$ = 7.6 Hz, 1H), 7.49 (dd, $J$ = 13.5, 8.0 Hz, 1H), 7.43 – 7.35 (m, 2H), 7.30 (t, $J$ = 8.2 Hz, 1H), 4.52 (s, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 194.4, 163.0 (d, $J$ = 248.5 Hz, 1C), 138.3 (d, $J$ = 5.8 Hz, 1C), 133.0, 132.9, 131.1, 130.7 (d, $J$ = 7.7 Hz, 1C), 127.9, 124.2, 120.9(d,

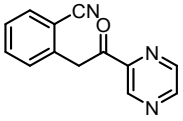
*J* = 21.2Hz, 1C), 117.9, 115.3, 115.1, 113.7, 43.7; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{15}H_{11}FNO$ 240.0819, found 240.0837.



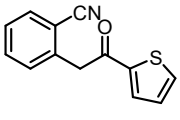

**4-Bromo-2-(2-oxo-2-phenylethyl)benzonitrile (1f).** The product was obtained as light-brown solid (1.08 g, 36%): mp119-120 °C: $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.03 (d, *J* = 8.6 Hz, 2H), 7.62 (t, *J* = 7.4 Hz, 1H), 7.58 – 7.48 (m, 5H), 4.51 (s, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 194.7, 140.4, 136.0, 134.5, 134.0, 133.8, 131.2, 129.0, 128.5, 128.0, 117.4, 112.7, 43.4; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{15}H_{11}Br^{81}NO$ 301.9998, found 301.9988.




**4-Chloro-2-(2-(3-fluorophenyl)-2-oxoethyl)benzonitrile (1g).** The product was obtained as light-brown solid (1.15 g, 42%): mp 123-124 °C: $^1$H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, *J* = 7.8 Hz, 1H), 7.74 – 7.67 (m, 1H), 7.63 (d, *J* = 8.2 Hz, 1H), 7.51 (td, *J* = 8.0, 5.5 Hz, 1H), 7.40 (dd, *J* = 10.0, 1.8 Hz, 2H), 7.33 (td, *J* = 8.2, 2.6 Hz, 1H), 4.49 (s, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 193.6, 163.0 (d, *J* = 248.5 Hz, 1C), 139.9, 139.6, 133.9, 131.6, 130.7 (d, *J* = 7.7 Hz, 1C), 128.4, 124.2, 121.1(d, *J* = 21.2Hz, 1C), 117.2, 115.3, 115.1, 112.2, 43.6; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{15}H_{10}ClFNO$ 274.0429, found 274.0437.

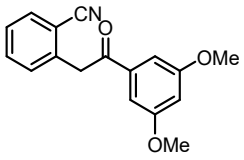



**2-(2-Oxo-2-(pyrazin-2-yl)ethyl)benzonitrile (1i).** The product was obtained as light-brown solid (0.69 g, 31%): mp 165-166 °C: $^1$H NMR (400 MHz, $CDCl_3$) δ 9.25 (s, 1H), 8.79 (d, *J* = 2.4 Hz, 1H), 8.72 – 8.66 (m, 1H), 7.69 (d, *J* = 7.1 Hz, 1H), 7.56 (t, *J* = 8.3 Hz, 1H), 7.43 – 7.33 (m, 2H), 4.77 (s, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 196.6, 148.4, 146.9, 144.0, 143.7, 138.2, 133.0, 132.9, 131.2, 127.8, 117.9, 114.0, 43.20; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{13}H_{10}N_3O$ 224.0818, found 224.0823.




**2-(2-Oxo-2-(thiophen-2-yl)ethyl)benzonitrile (1j).** The product was obtained as brown solid (1.3 g, 56%): mp123-124 °C: $^1$H NMR (400 MHz, $CDCl_3$) δ 7.90 (dd, *J* = 3.8, 1.1 Hz, 1H),

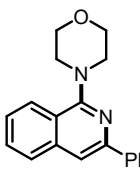
7.71 – 7.64 (m, 2H), 7.57 (td, *J* = 7.7, 1.4 Hz, 1H), 7.45 (d, *J* = 7.3 Hz, 1H), 7.38 (t, *J* = 8.2 Hz, 1H), 7.17 (dd, *J* = 4.9, 3.8 Hz, 1H), 4.46 (s, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) *δ* 188.5, 143.4, 138.0, 134.9, 133.0, 132.9, 131.0, 128.5, 127.8, 118.0, 113.5, 44.0; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{13}H_{10}NOS$ 228.0478, found 228.0480.




**2-(2-(3,5-dimethoxyphenyl)-2-oxoethyl)benzonitrile (1k).** The product was obtained as white solid (1.2 g, 44%): mp109-110 °C: $^1$H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 6.9 Hz, 1H), 7.57 (t, *J* = 8.4 Hz, 1H), 7.39 (t, *J* = 8.2 Hz, 2H), 7.18 (d, *J* = 2.3 Hz, 2H), 6.69 (t, *J* = 2.3 Hz, 1H), 4.51 (s, 2H), 3.85 (s, 6H); $^{13}$C NMR (100 MHz, $CDCl_3$) *δ* 195.2, 161.0, 138.5, 138.1, 132.8, 132.8, 131.0, 127.6, 118.0, 113.6, 106.2, 106.0, 55.7, 43.7; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{17}H_{16}NO_3$ 282.1125, found 282.1136.

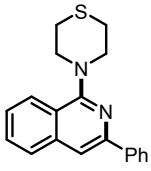
**General procedure for the synthesis of functionalized 1-amino-3-arylisoquinoline (3, 4, and 5)**

In an oven-dried 10 mL sealed tube, a mixture of 2-(arylethyl)benzonitrile **1** (0.5 mmol) and corresponding amine **2** (0.6 mmol) in 2 mL of distilled $H_2O$ was heated at 100 °C for 4h. The progression of the reaction was monitored by TLC analysis; after the complete consumption of starting material, the reaction was cooled to room temperature. The reaction mixture was diluted with ethyl acetate (10 mL). The layers were separated, and the organic layer was dried over $Na_2SO_4$. The organic layer was concentrated under reduced pressure. The crude material so obtained was purified by column chromatography on silica gel (100−200) (hexane: ethyl acetate). The structure and purity of products were confirmed by comparison of their physical and spectral data ($^1$H NMR, $^{13}$C NMR, and HRMS).

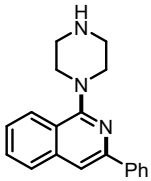



**4-(3-Phenylisoquinolin-1-yl)morpholine (3a).** The crude product was purified by column chromatography (hexane/EtOAc = 90/10) to afford **3a** as white-solid (137.7 mg, 95%): mp 200–201 °C: $^1$H NMR (400 MHz, $CDCl_3$) *δ* 8.20 (d, *J* = 9.5 Hz, 2H), 8.10 (d, *J* = 8.4 Hz, 1H), 7.80 (d, *J* = 8.2 Hz, 1H), 7.74 (s, 1H), 7.62-7.58 (m, 1H), 7.52-7.47 (m, 3H), 7.43-7.39 (m, 1H), 4.02 (t, *J* = 4.7 Hz,

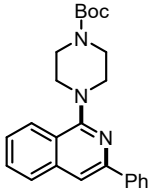
4H), 3.55 (t, $J$ = 4.7 Hz, 4H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 160.7, 148.4, 139.7, 139.2, 129.9, 128.7, 128.5, 127.9, 126.8, 126.1, 125.4, 120.7, 111.7, 67.2, 51.9; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{19}H_{19}N_2O$ 291.1492, found 291.1508.



**4-(3-Phenylisoquinolin-1-yl)thiomorpholine (3b).** The crude product was purified by column chromatography (hexane/EtOAc = 90/10) to afford **3b** as light green-solid (143.8 mg, 94%): mp 177–178 °C: $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.18 (d, $J$ = 8.4 Hz, 2H), 8.03 (d, J = 8.5 Hz, 1H), 7.80 (d, $J$ = 8.1 Hz, 1H), 7.73 (s, 1H), 7.60 (t, $J$ = 8.1 Hz, 1H), 7.52-7.46 (m, 3H), 7.42-7.39 (m, 1H), 3.82 (t, $J$ = 5.1 Hz, 4H), 2.96 (t, $J$ = 5.1 Hz, 4H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 161.1, 148.2, 138.5, 138.0, 128.7, 127.5, 127.3, 126.6, 125.6, 124.9, 124.2, 119.7, 110.5, 52.6, 26.7; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{19}H_{19}N_2S$ 307.1263, found 307.1262.

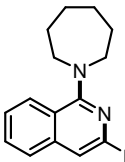


**3-Phenyl-1-(piperazin-1-yl)isoquinoline (3c).** The crude product was purified by column chromatography ($CHCl_3$/MeOH = 90/10) to afford **3c** as white-solid (128.6 mg, 89%): mp 156–157 °C: $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 8.16 (d, $J$ = 7.4 Hz, 2H), 8.10 (d, $J$ = 8.4 Hz, 1H), 8.03 (s, 1H), 7.94 (d, $J$ = 8.2 Hz, 1H), 7.71-7.67 (m, 1H), 7.58-7.54 (m, 1H), 7.47 (t, $J$ = 7.5 Hz, 2H), 7.39-7.36 (m, 1H), 3.56 (t, $J$ = 5.0 Hz, 4H), 3.33 (t, $J$ = 5.0 Hz, 4H); $^{13}$C NMR (100 MHz, DMSO-$d_6$) $\delta$ 160.1, 147.5, 139.3, 130.9, 129.2, 129.1, 128.4, 127.2, 126.8, 125.7, 120.3, 112.3, 49.1, 43.9; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{19}H_{20}N_3$ 290.1652, found 290.1648.

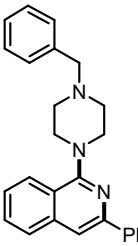


***tert*-Butyl 4-(3-phenylisoquinolin-1-yl)piperazine-1-carboxylate (3d).** The crude product was purified by column chromatography (hexane/EtOAc = 90/10) to afford **3d** as white-solid (188.6 mg, 97%): mp 154–155 °C: $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.16 (d, $J$ = 8.5 Hz, 2H), 8.07 (d, $J$ =

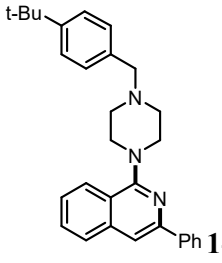
8.4 Hz, 1H), 7.81 (d, $J$ = 8.1 Hz, 1H), 7.73 (s, 1H), 7.62-7.58 (m, 1H), 7.50-7.45 (m, 3H), 7.39-7.35 (m, 1H), 3.73 (t, $J$ = 5.0 Hz, 4H), 3.49 (t, $J$ = 5.1 Hz, 4H), 1.51 (s, 9H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 160.7, 155.1, 148.4, 139.6, 139.2, 129.9, 128.7, 127.8, 126.7, 126.1, 125.3, 120.8, 111.7, 79.9, 51.6, 51.6, 51.5, 51.4, 51.3, 51.2, 51.0, 50.8, 44.5, 44.4, 44.2, 44.0, 43.8, 43.7, 43.6, 43.4, 28.6; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{24}H_{28}N_3O_2$ 390.2176, found 390.2187.



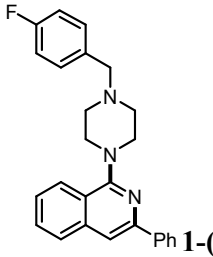
**1-(Azepan-1-yl)-3-phenylisoquinoline (3e).** The crude product was purified by column chromatography (hexane/EtOAc = 95/5) to afford **3e** as white-solid (144.9 mg, 96%): mp 98–99 °C: $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.16 (d, $J$ = 8.5 Hz, 2H), 8.10 (d, $J$ = 8.4 Hz, 1H), 7.75 (d, $J$ = 8.1 Hz, 1H), 7.54 (t, $J$ = 7.3 Hz, 2H), 7.46 (t, $J$ = 7.6 Hz, 2H), 7.41-7.34 (m, 2H), 3.83 (t, $J$ = 5.8 Hz, 4H), 1.98 (s, 4H), 1.78-1.75 (m, 4H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 161.0, 148.0, 140.2, 139.9, 129.3, 128.6, 128.1, 127.5, 126.8, 126.1, 124.8, 120.2, 109.1, 53.2, 29.3, 27.7; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{21}H_{23}N_2$303.1856, found 303.1851.



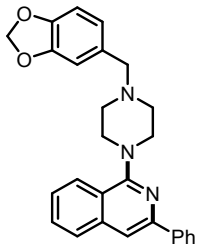
**1-(4-Benzylpiperazin-1-yl)-3-phenylisoquinoline (3f).** The crude product was purified by column chromatography (hexane/EtOAc = 90/10) to afford **3f** as white-solid (191.4 mg, 99%): mp 144–145 °C: $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.17 (d, $J$ = 7.4 Hz, 2H), 8.08 (d, $J$ = 8.2 Hz, 1H), 7.79 (d, $J$ = 8.1 Hz, 1H), 7.70 (s, 1H), 7.58 (t, $J$ = 7.4 Hz, 1H), 7.49-7.44 (m, 3H), 7.41-7.33 (m, 5H), 7.28 (t, $J$ = 7.1 Hz, 1H), 3.66 (s, 2H), 3.57 (s, 4H), 2.77 (s, 4H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 158.7, 148.2, 139.3, 139.2, 131.2, 130.3, 130.2, 129.5, 128.8, 128.7, 128.3, 128.1, 126.7, 124.7, 120.2, 112.5, 60.9, 50.7, 47.8; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{26}H_{26}N_3$ 380.2121, found 380.2111.



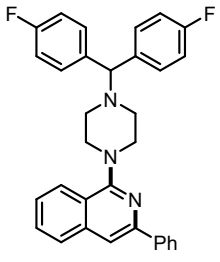
**1-(4-(4-(tert-Butyl)benzyl)piperazin-1-yl)-3-phenylisoquinoline (3g).** The crude product was purified by column chromatography (hexane/EtOAc = 90/10) to afford **3g** as white-solid (211.0 mg, 97%): mp 136–137 °C: $^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.20 (d, $J$ = 7.6 Hz, 2H), 8.10 (d, $J$ = 8.4 Hz, 1H), 7.80 (d, $J$ = 8.1 Hz, 1H), 7.72 (s, 1H), 7.59 (t, $J$ = 7.1 Hz, 1H), 7.51-7.45 (m, 3H), 7.41-7.39 (m, 3H), 7.436-7.34 (m, 2H), 3.65 (s, 2H), 3.60 (t, $J$ = 5.1 Hz, 4H), 2.79 (t, $J$ = 4.3 Hz, 4H), 1.36 (s, 9H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 160.8, 150.0, 148.3, 139.9, 139.2, 135.0, 129.6, 129.0, 128.6, 128.3, 127.7, 126.7, 125.7, 125.6, 125.2, 120.8, 111.1, 62.9, 53.3, 51.3, 34.6, 31.5; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{30}H_{34}N_3$ 436.2747, found 436.2738.



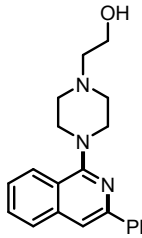
**1-(4-(4-Fluorobenzyl)piperazin-1-yl)-3-phenylisoquinoline (3h).** The crude product was purified by column chromatography (hexane/EtOAc = 90/10) to afford **3h** as white-solid (204.6 mg, 97%): mp 157–158 °C: $^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.22 (d, $J$ = 7.6 Hz, 2H), 8.11 (d, $J$ = 8.2 Hz, 1H), 7.80 (d, $J$ = 8.0 Hz, 1H), 7.73 (s, 1H), 7.59 (t, $J$ = 7.4 Hz, 1H), 7.52-7.46 (m, 3H), 7.42-7.36 (m, 3H), 7.06 (t, $J$ = 8.4 Hz, 2H), 3.60 (d, $J$ = 9.5 Hz, 6H), 2.76 (s, 4H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 162.2 (d, $J$ = 244.7 Hz, 1C), 160.9, 148.4, 139.8, 139.2, 134.0, 130.8, 130.7, 129.8, 128.7, 128.4, 127.8, 126.8, 125.7 (d, $J$ = 24 Hz, 1C), 120.8, 115.2 (d, $J$ = 21.2 Hz, 1C), 111.3, 62.5, 53.3, 51.3; HRMS (ESI-TOF) $[M+H]^+$ Calcd. for $C_{26}H_{25}FN_3$ 398.2027, found 398.2017.



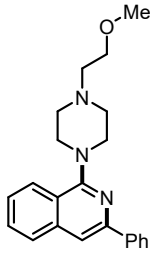
**1-(4-(Benzo[d][1,3]dioxol-5-ylmethyl)piperazin-1-yl)-3-phenylisoquinoline (3i).** The crude product was purified by column chromatography (hexane/EtOAc = 80/20) to afford **3i** as white-solid (198.8 mg, 94%): mp 145–146 °C: $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.17 (d, $J$ = 7.1 Hz, 2H), 8.08 (d, $J$ = 8.2 Hz, 1H), 7.79 (d, $J$ = 8.1 Hz, 1H), 7.70 (s, 1H), 7.58 (t, $J$ = 8.1 Hz, 1H), 7.46 (dd, $J$ = 15.0, 7.1 Hz, 3H), 7.39-7.35 (m, 1H), 6.94 (s, 1H), 6.83-6.77 (m, 2H), 5.96 (s, 2H), 3.56 (s, 6H), 2.74 (t, $J$ = 5.1 Hz, 4H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 160.8, 148.3, 147.8, 146.7, 139.8, 139.2, 132.1, 129.7, 128.7, 128.2, 127.7, 126.7, 125.8, 125.6, 122.4, 120.8, 111.3, 109.7, 108.0, 101.0, 63.0, 53.2, 51.3; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{27}H_{26}N_3O_2$ 424.2020, found 424.2024.



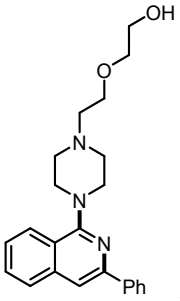
**1-(4-(Bis(4-fluorophenyl)methyl)piperazin-1-yl)-3-phenylisoquinoline (3j).** The crude product was purified by column chromatography (hexane/EtOAc = 90/10) to afford **3j** as white-solid (175.5 mg, 86%): mp 174–175 °C: $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.16 (d, $J$ = 7.6 Hz, 2H), 8.03 (d, $J$ = 8.2 Hz, 1H), 7.78 (d, $J$ = 8.1 Hz, 1H), 7.70 (s, 1H), 7.58-7.54 (m, 1H), 7.48-7.37 (m, 8H), 7.00 (t, $J$ = 8.7 Hz, 4H), 4.36 (s, 1H), 3.54 (s, 4H), 2.67 (s, 4H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 162.0 (d, $J$ = 238.0 Hz, 1C), 160.7, 148.3, 139.8, 139.1, 138.4, 129.7, 129.4, 129.4, 128.7, 128.4, 127.7, 126.7, 125.7 (d, $J$ = 21.0 Hz, 1C), 120.8, 115.6 (d, $J$ = 18.2 Hz, 1C), 111.3, 74.8, 52.1, 51.5; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{32}H_{28}F_2N_3$ 492.2246, found 492.2243.



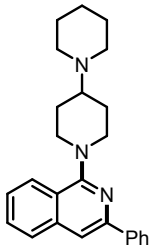
**2-(4-(3-Phenylisoquinolin-1-yl)piperazin-1-yl)ethan-1-ol (3k).** The crude product was purified by column chromatography ($CHCl_3$/MeOH = 95/5) to afford **3k** as white semi-solid (144.8 mg, 87%): mp 132–133 °C: $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.18 (d, $J$ = 8.5 Hz, 2H), 8.06 (d, $J$ = 8.2 Hz, 1H), 7.77 (d, $J$ = 8.1 Hz, 1H), 7.70 (s, 1H), 7.59-7.55 (m, 1H), 7.50-7.44 (m, 3H), 7.40-7.36 (m, 1H), 3.71 (t, $J$ = 5.4 Hz, 2H), 3.57 (s, 4H), 3.28 (s, 1H), 2.81 (t, $J$ = 4.5 Hz, 4H), 2.67 (t, $J$ = 5.4 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 160.7, 148.4, 139.8, 139.2, 129.8, 128.7, 128.4, 127.8, 126.8, 125.9, 125.5, 120.8, 111.4, 59.8, 58.0, 53.2, 51.3; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{21}H_{24}N_3O$ 334.1914, found 334.1907.



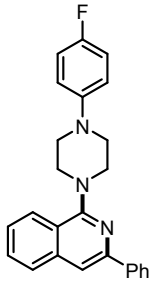
**1-(4-(2-Methoxyethyl)piperazin-1-yl)-3-phenylisoquinoline (3l).** The crude product was purified by column chromatography ($CHCl_3$/MeOH = 95/5) to afford **3l** as white semi-solid (147.2 mg, 90%): mp 128–129 °C: $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.17 (d, $J$ = 9.5 Hz, 2H), 8.06 (d, $J$ = 8.2 Hz, 1H), 7.77 (d, $J$ = 8.1 Hz, 1H), 7.69 (s, 1H), 7.58-7.55 (m, 1H), 7.49-7.43 (m, 3H), 7.39-7.35 (m, 1H), 3.60 (t, $J$ = 5.6 Hz, 6H), 3.39 (s, 3H), 2.85 (d, $J$ = 4.5 Hz, 4H), 2.74 (t, $J$ = 5.6 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$159.5, 147.2, 138.6, 138.0, 128.6, 127.5, 127.2, 126.6, 125.6, 124.7, 124.4, 119.5, 110.1, 69.0, 57.9, 56.9, 52.5, 49.8; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{22}H_{26}N_3O$ 348.2070, found 348.2067.



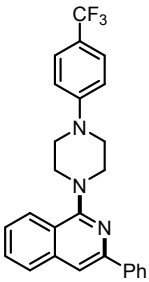

**2-(2-(4-(3-Phenylisoquinolin-1-yl)piperazin-1-yl)ethoxy)ethan-1-ol (3m).** The crude product was purified by column chromatography ($CHCl_3$/MeOH = 95/5) to afford **3m** as white semi-solid (158.4 mg, 84%): mp141–142 °C: $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.15 (d, $J$ = 8.4 Hz, 2H), 8.03 (d, $J$ = 8.3 Hz, 1H), 7.79 (d, $J$ = 8.1 Hz, 1H), 7.70 (s, 1H), 7.58 (t, $J$ = 7.1 Hz, 1H), 7.46 (t, $J$ = 7.5 Hz, 3H), 7.36 (t, $J$ = 7.3 Hz, 1H), 3.81 (s, 1H), 3.73 (dd, $J$ = 9.8, 5.3 Hz, 4H), 3.66 – 3.57 (m, 6H), 2.89 (s, 4H), 2.76 (t, $J$ = 5.2 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 160.4, 148.3, 139.6, 139.2, 129.8, 128.7, 128.4, 127.8, 126.7, 126.0, 125.5, 120.6, 111.4, 72.6, 67.3, 62.0, 58.0, 53.4, 50.6; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{23}H_{28}N_3O_2$ 378.2176,found 378.2181.



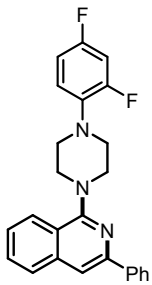

**1-([1,4'-Bipiperidin]-1'-yl)-3-phenylisoquinoline (3n).** The crude product was purified by column chromatography (hexane/EtOAc = 90/10) to afford **3n** as white solid (178.0 mg, 96%): mp 128–129 °C: $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.17 (d, $J$ = 7.3 Hz, 2H), 8.04 (d, $J$ = 8.2 Hz, 1H), 7.74 (d, $J$ = 8.1 Hz, 1H), 7.67 (s, 1H), 7.54 (t, $J$ = 7.1 Hz, 1H), 7.49-7.42 (m, 3H), 7.37 (t, $J$ = 7.3 Hz, 1H), 4.02 (d, $J$ = 12.8 Hz, 2H), 3.02 (t, $J$ = 11.8 Hz, 2H), 2.62-2.52 (m, 5H), 2.02-1.86 (m, 4H), 1.67 (t, $J$ = 5.1 Hz, 4H), 1.49-1.45 (m, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 161.2, 148.3, 139.9, 139.1, 129.7, 128.7, 128.3, 127.7, 126.8, 125.8, 125.7, 120.9, 111.1, 63.3, 51.4, 50.4, 28.4, 26.3, 24.8; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{25}H_{30}N_3$ 372.2434, found 372.2430.



**1-(4-(4-Fluorophenyl)piperazin-1-yl)-3-phenylisoquinoline (3o).** The crude product was purified by column chromatography (hexane/EtOAc = 90/10) to afford **3o** as white-solid (172.4 mg, 90%): mp 166–167 °C: $^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.18 (d, $J$ = 9.2 Hz, 2H), 8.12 (d, $J$ = 8.4 Hz, 1H), 7.82 (d, $J$ = 8.1 Hz, 1H), 7.74 (s, 1H), 7.63-7.59 (m, 1H), 7.51-7.46 (m, 3H), 7.38 (t, $J$ = 7.3 Hz, 1H), 7.03-6.96 (m, 4H), 3.70 (t, $J$ = 4.9 Hz, 4H), 3.42-3.39 (m, 4H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 159.6 (d, $J$ = 212.9 Hz, 1C), 156.1, 148.4, 148.2, 139.7, 139.2, 129.9, 128.7, 128.4, 127.8, 126.8, 125.7 (d, $J$ = 59.9 Hz, 1C), 120.8, 118.0, 117.9, 115.7 (d, $J$ = 22.2 Hz, 1C), 111.6, 51.3, 50.4; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{25}H_{23}FN_3$ 384.1871, found 384.1867.

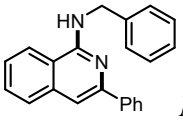


**3-Phenyl-1-(4-(4-(trifluoromethyl)phenyl)piperazin-1-yl)isoquinoline (3p).** The crude product was purified by column chromatography (hexane/EtOAc = 90/10) to afford **3p** as yellow-solid (197.0 mg, 91%): mp 178–178 °C: HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{26}H_{23}F_3N_3$ 434.1839, found 434.1842.

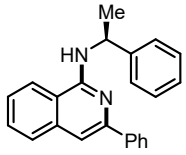


**1-(4-(2,4-Difluorophenyl)piperazin-1-yl)-3-phenylisoquinoline (3q).** The crude product was purified by column chromatography (hexane/EtOAc = 90/10) to afford **3q** as white-solid (180.5 mg, 90%): mp 152–153 °C: $^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.22 (d, $J$ = 8.5 Hz, 2H), 8.14 (d, $J$ =

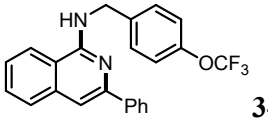
8.4 Hz, 1H), 7.82 (d, $J$ = 8.1 Hz, 1H), 7.75 (s, 1H), 7.63-7.59 (m, 1H), 7.53-7.48 (m, 3H), 7.43-7.39 (m, 1H), 7.03-6.97 (m, 1H), 6.90-6.83 (m, 2H), 3.73 (t, $J$ = 4.8 Hz, 4H), 3.33 (t, $J$ = 4.8 Hz, 4H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 160.6, 159.2 (d, $J$ = 11.5 Hz), 156.9 (dd, $J$ = 26.0, 11.6 Hz), 154.6 (d, $J$ = 11.6 Hz), 148.4, 139.7, 139.2, 136.9 (dd, $J$ = 8.9, 3.4 Hz), 129.8, 128.7, 128.4, 127.8, 126.7, 125.9, 125.4, 120.7, 119.7 (dd, $J$ = 9.3, 4.2 Hz), 111.5, 110.7 (dd, $J$ = 21.4, 3.7 Hz), 105.1, 104.8, 104.6, 51.6, 51.1; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{25}H_{22}F_2N_3$ 402.1776, found 402.1770.



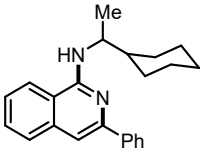

***N*-Benzyl-3-phenylisoquinolin-1-amine (4a).** The crude product was purified by column chromatography (hexane/EtOAc = 95/5) to afford **4a** as pale-yellow-solid (144.2 mg, 93%): mp 147–148 °C: $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.24 (d, $J$ = 7.3 Hz, 2H), 7.78 (d, $J$ = 8.1 Hz, 1H), 7.71 (d, $J$ = 8.2 Hz, 1H), 7.62-7.58 (m, 1H), 7.55-7.50 (m, 5H), 7.44-7.41 (m, 4H), 7.36 (t, $J$ = 7.3 Hz, 1H), 5.55 (s, 1H), 5.02 (d, $J$ = 5.1 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 154.5, 149.1, 140.3, 138.2, 129.9, 128.8, 128.7, 128.3, 127.9, 127.4, 126.9, 125.8, 121.6, 117.5, 107.3, 46.1; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{22}H_{19}N_2$ 311.1543, found 311.1537.



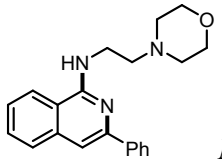

***(S)*-3-Phenyl-N-(1-phenylethyl)isoquinolin-1-amine (4b).** The crude product was purified by column chromatography (hexane/EtOAc = 95/5) to afford **4b** as pale-yellow-solid (151.1 mg, 93%): mp 127–128 °C: $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.04 (d, $J$ = 8.4 Hz, 2H), 7.79 (d, $J$ = 8.2 Hz, 1H), 7.73 (d, $J$ = 8.1 Hz, 1H), 7.59-7.53 (m, 3H), 7.45-7.41 (m, 4H), 7.38-7.33 (m, 3H), 7.27 (d, $J$ = 8.4 Hz, 1H), 5.70-5.63 (m, 1H), 5.51 (d, $J$ = 5.8 Hz, 1H), 1.74 (d, $J$ = 6.9 Hz, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 153.6, 149.0, 145.4, 140.2, 138.1, 129.7, 128.5, 128.4, 128.0, 127.7, 126.9, 126.7, 126.4, 125.6, 121.3, 117.3, 106.9, 50.8, 22.7; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{23}H_{21}N_2$ 325.1699, found 325.1697.




**3-Phenyl-N-(4-(trifluoromethoxy)benzyl)isoquinolin-1-amine (4c).** The crude product was purified by column chromatography (hexane/EtOAc = 95/5) to afford **4c** as white-solid (173.4 mg, 88%): mp 156–157 °C: $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.15 (d, $J$ = 8.5 Hz, 2H), 7.74 (dd, $J$ = 17.1, 8.2 Hz, 2H), 7.62-7.58 (m, 1H), 7.51-7.47 (m, 5H), 7.44-7.38 (m, 2H), 7.22 (d, $J$ = 7.8 Hz, 2H), 5.58 (s, 1H), 4.96 (d, $J$ = 5.4 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 154.2, 149.0, 148.4, 140.1, 139.1, 138.2, 130.0, 129.0 (d, $J$ = 79.0 Hz, 1C), 128.3, 127.9, 126.8, 125.9, 121.4, 121.2, 117.4, 107.5, 45.2; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{23}H_{18}F_3N_2O$ 395.1366, found 395.1363.

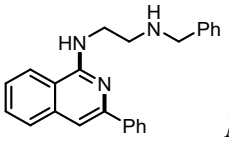



***N*-(1-Cyclohexylethyl)-3-phenylisoquinolin-1-amine (4d).** The crude product was purified by column chromatography (hexane/EtOAc = 95/5) to afford **4d** as white-solid (151.8 mg, 92%): mp 116–117 °C: $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.25 (d, $J$ = 9.5 Hz, 2H), 7.76 (d, $J$ = 8.2 Hz, 2H), 7.61-7.51 (m, 3H), 7.44 (dd, $J$ = 16.0, 8.5 Hz, 3H), 5.18 (d, $J$ = 7.4 Hz, 1H), 4.63 (dd, $J$ = 12.0, 5.7 Hz, 1H), 2.00 (d, $J$ = 12.5 Hz, 1H), 1.88 (t, $J$ = 16.1 Hz, 3H), 1.74 (d, $J$ = 11.5 Hz, 2H), 1.37-1.19 (m, 8H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 154.4, 149.2, 140.6, 138.3, 129.7, 128.6, 128.2, 127.9, 126.8, 125.5, 121.3, 117.5, 106.2, 50.7, 43.5, 29.8, 29.2, 26.8, 26.7, 26.6, 17.9; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{23}H_{27}N_2$ 331.2169, found 331.2163.

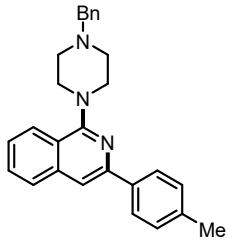



***N*-(2-Morpholinoethyl)-3-phenylisoquinolin-1-amine (4e).** The crude product was purified by column chromatography ($CHCl_3$/MeOH = 98/2) to afford **4e** as white semi-solid (156.5 mg, 94%): mp 112–113 °C: $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.19 (d, $J$ = 8.1 Hz, 2H), 7.86 (d, $J$ = 8.2 Hz, 1H), 7.71 (d, $J$ = 8.1 Hz, 1H), 7.58-7.54 (m, 1H), 7.49-7.36 (m, 5H), 3.85-3.80 (m, 5H), 2.61-2.54 (m, 6H), 1.97-1.91 (m, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 155.3, 149.2, 140.5, 138.1, 129.7, 128.5, 128.2,

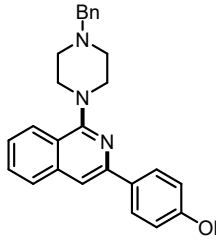
127.7, 126.8, 125.4, 122.0, 117.7, 106.3, 67.1, 58.9, 54.0, 42.2, 24.6; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{21}H_{24}N_3O$ 334.1914, found 334.1907.



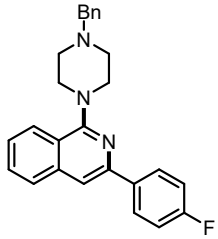
***N*$^1$-Benzyl-*N*$^2$-(3-phenylisoquinolin-1-yl)ethane-1,2-diamine (4f).** The crude product was purified by column chromatography ($CHCl_3$/MeOH = 98/2) to afford **4f** as white semi-solid (144.0 mg, 85%): mp 126–127 °C: $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.14 (d, $J$ = 8.4 Hz, 2H), 7.92 (d, $J$ = 8.3 Hz, 1H), 7.70 (d, $J$ = 8.0 Hz, 1H), 7.55 (t, $J$ = 7.5 Hz, 1H), 7.48 (t, $J$ = 7.5 Hz, 2H), 7.44 – 7.36 (m, 3H), 7.27 (dd, $J$ = 16.0, 7.7 Hz, 5H), 6.43 (s, 1H), 4.91 (s, 1H), 3.90 (s, 2H), 3.84 (s, 2H), 3.10 (t, $J$ = 5.5 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 155.0, 148.8, 140.2, 138.0, 136.5, 130.0, 128.9, 128.7, 128.6, 128.2, 128.0, 127.51, 126.8, 125.9, 122.4, 117.7, 107.1, 52.7, 47.8, 40.3; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{24}H_{24}N_3$ 354.165, found 354.1971.



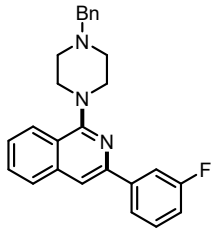
**1-(4-Benzylpiperazin-1-yl)-3-(p-tolyl)isoquinoline (5a)**. The crude product was purified by column chromatography (hexane/EtOAc = 90/10) to afford **5a** as white-solid (182.7 mg, 93%): mp 138–139 °C: $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.06 (d, $J$ = 8.1 Hz, 3H), 7.77 (d, $J$ = 8.1 Hz, 1H), 7.66 (s, 1H), 7.58-7.54 (m, 1H), 7.44 (d, $J$ = 8.2 Hz, 1H), 7.40 (d, $J$ = 8.7 Hz, 2H), 7.36-7.33 (m, 2H), 7.29-7.25 (m, 3H), 3.65 (s, 2H), 3.56 (t, $J$ = 5.1 Hz, 4H), 2.75 (t, $J$ = 4.6 Hz, 4H), 2.40 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 160.8, 148.4, 139.2, 138.3, 138.2, 137.1, 129.6, 129.4, 129.3, 128.4, 127.6, 127.2, 126.6, 125.6, 120.7, 110.6, 63.3, 53.6, 51.5, 21.3; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{27}H_{28}N_3$ 394.2278, found 394.2267.



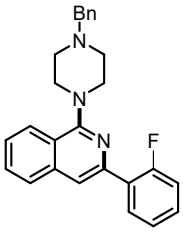

**1-(4-Benzylpiperazin-1-yl)-3-(4-ethoxyphenyl)isoquinoline (5b).** The crude product was purified by column chromatography (hexane/EtOAc = 85/15) to afford **5b** as white-solid (195.0 mg, 92%): mp 129–130 °C: $^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.13 (d, $J$ = 8.8 Hz, 2H), 8.07 (d, $J$ = 8.2 Hz, 1H), 7.75 (d, $J$ = 8.1 Hz, 1H), 7.62 (s, 1H), 7.56 (t, $J$ = 7.1 Hz, 1H), 7.45-7.36 (m, 5H), 7.32-7.29 (m, 1H), 7.01 (d, $J$ = 12.0 Hz, 2H), 4.10 (q, $J$ = 7.0 Hz, 2H), 3.68 (s, 2H), 3.59 (s, 4H), 2.79 (s, 4H), 1.46 (t, $J$ = 6.9 Hz, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 160.7, 159.5, 148.2, 139.4, 138.1, 132.4, 129.7, 129.4, 128.4, 128.0, 127.6, 127.3, 125.6, 125.4, 120.4, 114.6, 110.1, 63.6, 63.3, 53.3, 51.3, 15.0; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{28}H_{30}N_3O$ 424.2383, found 424.2375.



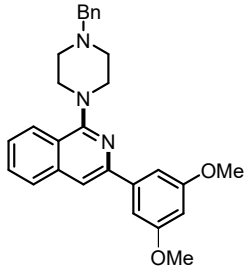

**1-(4-Benzylpiperazin-1-yl)-3-(4-fluorophenyl)isoquinoline (5c).** The crude product was purified by column chromatography (hexane/EtOAc = 90/10) to afford **5c** as white-solid (190.6 mg, 96%): mp 118–119 °C: $^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.10 (dd, $J$ = 8.8, 5.5 Hz, 2H), 8.01 (d, $J$ = 8.4 Hz, 1H), 7.78 (d, $J$ = 8.1 Hz, 1H), 7.65 (s, 1H), 7.59 (t, $J$ = 7.5 Hz, 1H), 7.48-7.44 (m, 1H), 7.42-7.33 (m, 5H), 7.14 (t, $J$ = 8.7 Hz, 2H), 3.88 (s, 2H), 3.68 (s, 4H), 2.99 (s, 4H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 163.2 (d, $J$ = 247.6 Hz, 1C), 160.2, 147.4, 139.2, 135.8, 130.0, 129.9, 128.7, 128.5, 128.4, 128.2, 127.8, 125.7 (d, $J$ = 75.2 Hz, 1C), 120.5, 115.5 (d, $J$ = 21.2 Hz, 1C), 111.3, 62.5, 52.5, 50.2; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{26}H_{25}FN_3$ 398.2027, found 398.2017.




**1-(4-Benzylpiperazin-1-yl)-3-(3-fluorophenyl)isoquinoline (5d).** The crude product was purified by column chromatography (hexane/EtOAc = 90/10) to afford **5d** as white-solid (194.5 mg, 98%): mp 123–124 °C: $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.08 (d, $J$ = 8.4 Hz, 1H), 7.93-7.90 (m, 2H), 7.79 (d, $J$ = 8.1 Hz, 1H), 7.68 (s, 1H), 7.61-7.57 (m, 1H), 7.49-7.33 (m, 6H), 7.28 (t, $J$ = 8.5 Hz, 1H), 7.08-7.04 (m, 1H), 3.66 (s, 2H), 3.58-3.55 (m, 4H), 2.76 (t, $J$ = 4.7 Hz, 4H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 163.5 (d, $J$ = 244.7 Hz, 1C), 160.9, 147.0, 142.4, 142.3, 138.7 (d, $J$ = 75.2 Hz, 1C), 130.0, 129.9, 129.9, 129.3, 128.4, 127.8, 127.2, 125.9 (d, $J$ = 45.3 Hz, 1C), 121.9 (d, $J$ = 103.0 Hz, 1C), 115.1, 114.9, 113.8, 113.5, 111.5, 63.3, 53.4, 51.3; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{26}H_{25}FN_3$ 398.2027,found 398.2017.

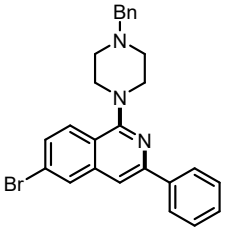



**1-(4-Benzylpiperazin-1-yl)-3-(2-fluorophenyl)isoquinoline (5e).** The crude product was purified by column chromatography (hexane/EtOAc = 90/10) to afford 5e as white-solid (142.9 mg, 72%): mp 117–118 °C: $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.28 (t, $J$ = 8.9 Hz, 1H), 8.08 (d, $J$ = 8.3 Hz, 1H), 7.87 (s, 1H), 7.78 (d, $J$ = 8.1 Hz, 1H), 7.57 (t, $J$ = 8.1 Hz, 1H), 7.50 – 7.44 (m, 1H), 7.32 (ddd, $J$ = 27.9, 16.8, 6.7 Hz, 7H), 7.15 (dd, $J$ = 11.8, 8.0 Hz, 1H), 3.64 (s, 2H), 3.53 (s, 4H), 2.84 – 2.66 (m, 4H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 160.9(d, $J$ = 249.5 Hz, 1C), 160.6, 143.6, 138.9, 138.3, 131.1, 129.7, 129.4, 129.3, (d, $J$ = 8.9 Hz, 1C), 128.4, 128.0, 127.7, 127.5, (d, $J$ = 10.0 Hz, 1C), 126.3, 125.6, 124.4, 120.9, 116.4, 116.0 (d, $J$ = 13.5 Hz, 1C), 63.3, 53.4, 51.3; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{26}H_{25}FN_3$ 398.2027,found 398.2017.

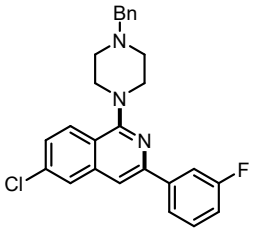



**1-(4-Benzylpiperazin-1-yl)-3-(3, 5-dimethoxyphenyl)isoquinoline (5f).** The crude product was purified by column chromatography (hexane/EtOAc = 90/10) to afford **5f** as white-

solid (197.5 mg, 90%): mp 123–124 °C: $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.07 (d, $J$ = 8.3 Hz, 1H), 7.78 (d, $J$ = 8.1 Hz, 1H), 7.67 (s, 1H), 7.58 (t, $J$ = 8.0 Hz, 1H), 7.46 (t, $J$ = 7.6 Hz, 1H), 7.42 – 7.32 (m, 6H), 7.28 (t, $J$ = 6.6 Hz, 1H), 6.50 (s, 1H), 3.89 (s, 6H), 3.65 (s, 2H), 3.55 (s, 4H), 2.76 (s, 4H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 161.0, 160.7, 147.9, 142.0, 139.0, 138.2, 129.7, 129.3, 128.3, 127.7, 127.1, 125.9, 125.5, 120.9, 111.5, 104.8, 100.5, 63.3, 55.5, 53.3, 51.2; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{28}H_{30}N_3O_2$ 440.2333, found 440.2360.

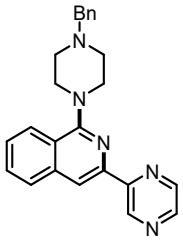



**1-(4-Benzylpiperazin-1-yl)-6-bromo-3-phenylisoquinoline (5g).**The crude product was purified by column chromatography (hexane/EtOAc = 90/10) to afford **5g** as white-solid (150.8 mg, 66%): mp 147–148 °C: $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.17 (d, $J$ = 8.5 Hz, 2H), 8.12 (d, $J$ = 8.3 Hz, 1H), 7.83 (d, $J$ = 8.1 Hz, 1H), 7.76 (s, 1H), 7.62 (t, $J$ = 7.5 Hz, 1H), 7.55 – 7.45 (m, 5H), 7.38 (t, $J$ = 8.4 Hz, 1H), 7.03 (d, $J$ = 8.7 Hz, 1H), 3.74 – 3.66 (m, 4H), 3.61 – 3.53 (m, 4H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 160.27, 153.37, 148.02, 142.54, 139.34, 129.90, 128.56, 128.31, 127.68, 126.50, 126.27, 126.12, 125.14, 114.46, 111.54, 50.71, 47.77, 29.69; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{26}H_{25}Br^{81}N_3$ 460.1206, found 460.1212.

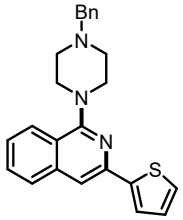



**1-(4-Benzylpiperazin-1-yl)-6-chloro-3-(3-fluorophenyl)isoquinoline (5h).** The crude product was purified by column chromatography (hexane/EtOAc = 90/10) to afford **5h** as white-solid (155.2 mg, 72%): mp 143–144 °C: $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.98 (d, $J$ = 8.9 Hz, 1H), 7.87 (d, $J$ = 11.8 Hz, 2H), 7.75 (d, $J$ = 2.1 Hz, 1H), 7.56 (s, 1H), 7.44-7.33 (m, 6H), 7.28 (t, $J$ = 7.1 Hz, 1H), 7.09-7.05 (m, 1H), 3.65 (s, 2H), 3.54-3.52 (m, 4H), 2.74 (t, $J$ = 4.5 Hz, 4H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 163.4 (d, $J$ = 244.7 Hz, 1C), 162.2, 160.9, 148.2, 141.8, 141.8, 140.1, 138.1, 136.0, 130.1, 130.1, 129.3, 128.4, 127.5, 127.3, 126.6 (d, $J$ = 37.6 Hz, 1C), 122.2, 119.2, 115. (d, $J$ = 22.2 Hz, 1C),,

113.9, 113.6, 110.5, 63.2, 53.2, 51.3; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{26}H_{24}ClFN_3$ 432.1637, found 432.1632.



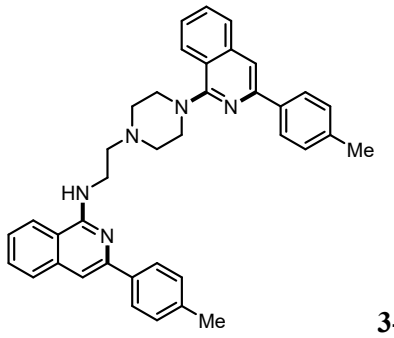
**1-(4-Benzylpiperazin-1-yl)-3-(pyrazin-2-yl)isoquinoline (5i).** The crude product was purified by column chromatography (hexane/EtOAc = 60/40) to afford **5i** as white-solid (139.0 mg, 73%): mp 155–156 °C: $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 9.70 (s, 1H), 8.64 – 8.58 (m, 1H), 8.54 (d, $J$ = 2.5 Hz, 1H), 8.34 (s, 1H), 8.09 (d, $J$ = 8.3 Hz, 1H), 7.87 (d, $J$ = 8.0 Hz, 1H), 7.62 (t, $J$ = 7.5 Hz, 1H), 7.52 (t, $J$ = 8.1 Hz, 1H), 7.41 – 7.32 (m, 4H), 7.28 (t, $J$ = 7.1 Hz, 1H), 3.66 (s, 2H), 3.58 (s, 4H), 2.79 (s, 4H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 160.9, 152.0, 145.2, 143.8, 143.6, 138.8, 137.8, 130.1, 129.4, 128.52, 128.4, 127.3, 127.0, 125.7, 122.0, 113.5, 63.2, 53.2, 51.2; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{24}H_{24}N_5$ 382.2026, found 382.2031.



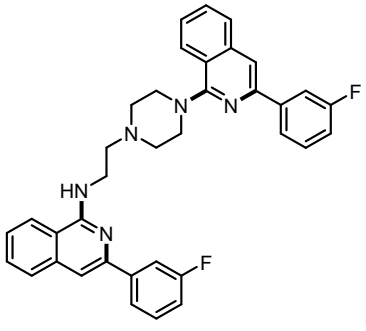
**1-(4-Benzylpiperazin-1-yl)-3-(thiophen-2-yl)isoquinoline (5j).** The crude product was purified by column chromatography (hexane/EtOAc = 90/10) to afford **5j** as white-solid (179.0 mg, 93%): mp 141–142 °C: $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.03 (d, $J$ = 8.1 Hz, 1H), 7.73 (d, $J$ = 8.1 Hz, 1H), 7.64 (d, $J$ = 3.6 Hz, 1H), 7.55 (t, $J$ = 8.1 Hz, 2H), 7.43-7.33 (m, 6H), 7.30-7.26 (m, 1H), 7.12-7.10 (m, 1H), 3.64 (s, 2H), 3.55 (t, $J$ = 5.1 Hz, 4H), 2.74 (t, $J$ = 4.6 Hz, 4H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 160.7, 146.3, 144.1, 139.1, 138.3, 129.9, 129.3, 128.4, 128.0, 127.5, 127.2, 126.5, 125.8, 125.5, 123.4, 120.7, 109.1, 63.3, 53.3, 51.2; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{24}H_{24}N_3S$ 386.1685, found 386.1677.

**General procedure for the synthesis of functionalized 3-aryl-N-(2-(4-(3-phenylisoquinolin-1-yl)piperazin-1-yl)ethyl)isoquinolin-1-amine (6a-d)**

In an oven-dried 10 mL sealed tube, a mixture of 2-(arylethyl)benzonitrile **1** (0.5 mmol) and 2-(piperazin-1-yl)ethan-1-amine **2r** (0.3 mmol) in 2 mL of distilled $H_2O$ was heated at 100 °C for 4h. Progression of the reaction was monitored by TLC analysis; after complete consumption of starting material, the reaction was cooled to room temperature. The reaction mixture was diluted with ethyl acetate (10 mL). The layers were separated, and the organic layer was dried over $Na_2SO_4$. Organic layer was concentrated under reduced pressure. The crude material so obtained was purified by column chromatography on silica gel (100−200) (hexane: ethyl acetate). The structure and purity of products were confirmed by comparison of their physical and spectral data ($^1$H NMR, $^{13}$C NMR, and HRMS).

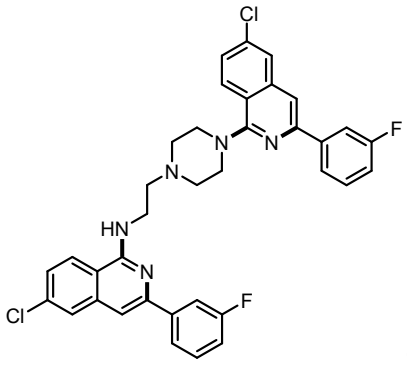



**3-(p-Tolyl)-N-(2-(4-(3-(p-tolyl)isoquinolin-1-yl)piperazin-1-yl)ethyl)isoquinolin-1-amine (6a).** The crude product was purified by column chromatography (hexane/EtOAc = 70/30) to afford **6a** as white-solid (247.7 mg, 88%): mp 162–163 °C: $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.12-8.08 (m, 5H), 7.85-7.81 (m, 2H), 7.73-7.71 (m, 2H), 7.65-7.55 (m, 2H), 7.49-7.41 (m, 3H), 7.39-7.29 (m, 4H), 6.44 (s, 1H), 3.96 (s, 2H), 3.66 (s, 4H), 3.00 (d, $J$ = 19.1 Hz, 6H), 2.41 (s, 6H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 160.5, 154.9, 149.1, 148.5, 139.3, 138.3, 138.1, 137.9, 137.6, 136.9, 129.8, 129.5, 129.3, 127.7, 127.5, 126.6, 125.8, 125.6, 125.5, 122.0, 120.6, 117.6, 111.1, 106.2, 56.8, 53.0, 50.9, 37.8, 21.4; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{38}H_{38}N_5$ 564.3122, found 564.3108.

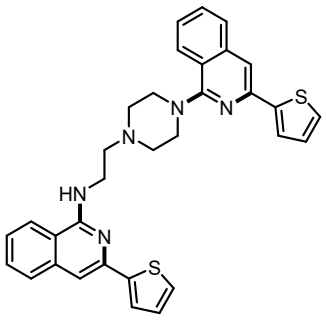



**3-(3-Fluorophenyl)-N-(2-(4-(3-(3-fluorophenyl)isoquinolin-1-yl)piperazin-1-yl)ethyl)isoquinolin-1-amine (6b).** The crude product was purified by column

chromatography (hexane/EtOAc = 70/30) to afford **6b** as white-solid (257.0 mg, 90%): mp 157–158 °C: $^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.97 (dd, $J$ = 12.7, 8.5 Hz, 2H), 7.83 (dd, $J$ = 20.3, 8.3 Hz, 5H), 7.69 (dd, $J$ = 14.7, 7.0 Hz, 3H), 7.59 (dt, $J$ = 21.1, 7.5 Hz, 3H), 7.52 – 7.47 (m, 1H), 7.40 (t, $J$ = 8.0 Hz, 4H), 7.05 (dd, $J$ = 17.9, 9.3 Hz, 3H), 4.17 (s, 2H), 3.80 (s, 4H), 3.41 (d, $J$ = 20.3 Hz, 6H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 163.4 (d, $J$ = 243.7 Hz, 2C), 160.1, 154.8, 147.4, 146.9, 142.8, 142.0, 139.0, 137.8, 130.2, 130.1, 129.9 (d, $J$ = 8.7 Hz, 2C), 128.4, 128.0, 127.6, 127.4, 126.5 (d, $J$ = 21.2 Hz, 2C), 125.3, 122.2, 122.1(d, $J$ = 6.7 Hz, 2C), 120.8, 120.4, 118.0, 115.5, 115.3, 115.3, 115.1, 114.9, 114.7, 113.7, 113.5, 112.2, 107.3, 56.8, 52.8, 50.0, 37.5; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{36}H_{32}F_2N_5$ 572.2620, found 572.2611.



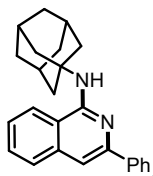

**6-Chloro-N-(2-(4-(6-chloro-3-(3-fluorophenyl)isoquinolin-1-yl)piperazin-1-yl)ethyl)-3-(3-fluorophenyl)isoquinolin-1-amine (6c).** The crude product was purified by column chromatography (hexane/EtOAc = 70/30) to afford **6c** as white-solid (257.0 mg, 90%): mp 171–172 °C: $^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.00 – 7.84 (m, 5H), 7.70 (t, $J$ = 5.7 Hz, 2H), 7.62 (d, $J$ = 1.9 Hz, 1H), 7.52 (s, 1H), 7.45 – 7.32 (m, 4H), 7.23 (s, 1H), 7.07 (td, $J$ = 8.2, 3.9 Hz, 2H), 6.23 (t, $J$ = 3.8 Hz, 1H), 3.89 – 3.81 (m, 2H), 3.56 (s, 4H), 2.88 (dd, $J$ = 13.6, 7.5 Hz, 6H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 163.5 (d, $J$ = 244.7 Hz, 2C), 160.8, 154.7, 148.9, 148.1, 142.4, 142.3, 141.7, 141.6, 140.0, 139.0, 136.1, 136.0, 130.1 (d, $J$ = 22.2 Hz, 2C), 129.9, 127.3, 127.0, 126.5 (d, $J$ = 14.4 Hz, 2C), 123.5, 122.1, 119.1, 116.0, 115.6, 115.4, 115.3, 115.1, 113.8, 113.6, 110.8, 106.0, 56.6, 53.0, 51.4, 38.0; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{36}H_{30}Cl_2F_2N_5$ 640.1841, found 640.1838.



**3-(Thiophen-2-yl)-N-(2-(4-(3-(thiophen-2-yl)isoquinolin-1-yl)piperazin-1-yl)ethyl)isoquinolin-1-amine (6d).** The crude product was purified by column chromatography (hexane/EtOAc = 70/30) to afford **6d** as white-solid (257.1 mg, 94%): mp 147–148 °C: $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.98 (d, $J$ = 8.4 Hz, 1H), 7.91 (d, $J$ = 7.4 Hz, 1H), 7.74 (d, $J$ = 8.1 Hz, 1H), 7.66-7.52 (m, 6H), 7.42 (q, $J$ = 7.7 Hz, 2H), 7.33-7.29 (m, 3H), 7.12-7.08 (m, 2H), 6.66 (s, 1H), 3.99 (s, 2H), 3.76 (s, 4H), 3.10 (s, 6H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 160.2, 154.7, 146.8, 146.0, 144.5, 144.0, 139.0, 137.8, 130.1, 130.0, 128.1, 128.0, 127.6, 127.3, 126.6, 126.0, 125.8, 125.7, 125.6, 123.6, 123.0, 122.2, 120.5, 117.8, 109.6, 104.8, 56.8, 52.8, 50.5, 37.7, 30.2; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{32}H_{30}N_5S_2$ 548.1937, found 548.1927.

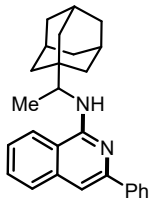
**General procedure for the synthesis of drugs containing isoquinoline (7a-e)**

In an oven-dried 10 mL sealed tube, a mixture of 2-(arylethyl)benzonitrile **1** (0.5 mmol) and corresponding drugs (0.6 mmol) in 2 mL of distilled $H_2O$ was heated at 100 °C for 4h. The progression of the reaction was monitored by TLC analysis; after the complete consumption of starting material, the reaction was cooled to room temperature. The reaction mixture was diluted with ethyl acetate (10 mL). The layers were separated, and the organic layer was dried over $Na_2SO_4$. The organic layer was concentrated under reduced pressure. The crude material so obtained was purified by column chromatography on silica gel (100−200) (hexane: ethyl acetate). The structure and purity of products were confirmed by comparison of their physical and spectral data ($^1$H NMR, $^{13}$C NMR, and HRMS).

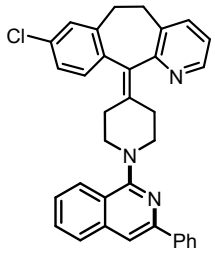


***N*-((3S,5S)-Adamantan-1-yl)-3-phenylisoquinolin-1-amine (7a).** The crude product was purified by column chromatography (hexane/EtOAc = 95/5) to afford **7a** as white-solid (138.0 mg,

78%): mp 109–110 °C: $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.18 (d, $J$ = 7.3 Hz, 2H), 7.68 (q, $J$ = 4.1 Hz, 2H), 7.53 (t, $J$ = 7.4 Hz, 1H), 7.47 (t, $J$ = 7.6 Hz, 2H), 7.41-7.34 (m, 3H), 5.08 (s, 1H), 2.38 (s, 6H), 2.19 (s, 3H), 1.80 (dd, $J$ = 19.8, 12.4 Hz, 6H), 1.25 (s, 3H), 0.89-0.83 (m, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 153.9, 148.7, 140.5, 138.2, 129.4, 128.5, 128.0, 127.9, 126.7, 125.5, 121.4, 117.8, 105.9, 52.5, 42.1, 37.0, 29.9; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{25}H_{27}N_2$ 355.2169, found 355.2170.

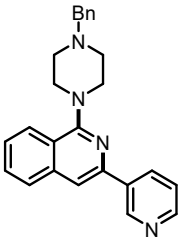



***N*-(1-((3R,5R,7R)-Adamantan-1-yl)ethyl)-3-phenylisoquinolin-1-amine (7b).** The crude product was purified by column chromatography (hexane/EtOAc = 95/5) to afford **7b** as white-solid (160.5 mg, 84%): mp 116–117 °C: $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.17 (d, $J$ = 7.3 Hz, 2H), 7.73 (t, $J$ = 7.6 Hz, 2H), 7.58-7.55 (m, 1H), 7.50-7.41 (m, 3H), 7.39-7.35 (m, 2H), 5.19 (d, $J$ = 8.9 Hz, 1H), 4.55-4.48 (m, 1H), 2.03 (s, 3H), 1.78-1.68 (m, 7H), 1.25 (d, $J$ = 6.7 Hz, 3H), 0.91-0.84 (m, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 154.7, 149.2, 140.6, 138.3, 129.7, 128.5, 128.1, 127.8, 126.8, 125.5, 121.2, 117.4, 106.0, 54.0, 39.0, 37.4, 36.6, 28.6, 14.8; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{27}H_{31}N_2$ 383.2482, found 383.2475.

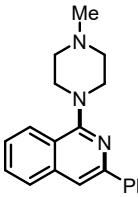



**8-Chloro-11-(1-(3-phenylisoquinolin-1-yl)piperidin-4-ylidene)-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridine (7c).** The crude product was purified by column chromatography (hexane/EtOAc = 80/20) to afford **7c** as white-solid (230.8 mg, 90%): mp 184–185 °C: $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.43 (d, $J$ = 5.9 Hz, 1H), 8.13-8.09 (m, 3H), 7.78 (d, $J$ = 8.1 Hz, 1H), 7.68 (s, 1H), 7.60-7.56 (m, 1H), 7.47-7.42 (m, 4H), 7.34 (t, $J$ = 7.3 Hz, 1H), 7.22 (d, $J$ = 8.2 Hz, 1H), 7.16 (d, $J$ = 7.7 Hz, 2H), 7.12-7.09 (m, 1H), 3.87 (dd, $J$ = 12.2, 3.8 Hz, 2H), 3.48-3.36 (m, 2H), 3.20-3.12 (m, 2H), 2.89-2.59 (m, 6H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 161.0, 157.6, 148.3, 146.7, 139.8, 139.7, 139.2, 139.1, 138.0, 137.6, 133.6, 133.3, 132.9, 131.0, 129.8, 129.1, 128.6, 128.3, 127.7, 126.7,

126.2, 125.9, 125.6, 122.3, 120.9, 111.3, 52.8, 52.7, 31.9, 31.6, 31.4, 31.3; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{34}H_{29}ClN_3$ 514.2045, found 514.2038.



**1-(4-Benzylpiperazin-1-yl)-3-(pyridin-3-yl)isoquinoline (7d).** The crude product was purified by column chromatography (hexane/EtOAc = 60/40) to afford **7d** as white-solid (167.2 mg, 88%): mp 145–146 °C: $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 9.36 (s, 1H), 8.59 (d, $J$ = 4.8 Hz, 1H), 8.41 (d, $J$ = 9.9 Hz, 1H), 8.06 (d, $J$ = 8.3 Hz, 1H), 7.76 (d, $J$ = 8.1 Hz, 1H), 7.67 (s, 1H), 7.58 (t, $J$ = 7.1 Hz, 1H), 7.47 (t, $J$ = 7.6 Hz, 1H), 7.42 – 7.31 (m, 5H), 7.31 – 7.22 (m, 1H), 3.64 (s, 2H), 3.55 (s, 4H), 2.74 (s, 4H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 161.1, 149.1, 148.3, 145.6, 138.9, 138.0, 135.3, 134.0, 130.0, 129.4, 128.4, 127.8, 127.3, 126.4, 125.7, 123.5, 121.0, 111.6, 63.3, 53.3, 51.2; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{25}H_{25}N_4$ 381.2074, found 381.2070.



**1-(4-Methylpiperazin-1-yl)-3-phenylisoquinoline (7e).** The crude product was purified by column chromatography ($CHCl_3$/MeOH = 95/5) to afford **7e** as white semi-solid (148.5 mg, 98%): mp 77–78 °C: $^1$H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, $J$ = 7.2 Hz, 2H), 8.06 (d, $J$ = 8.3 Hz, 1H), 7.77 (d, $J$ = 8.1 Hz, 1H), 7.69 (s, 1H), 7.56 (t, $J$ = 7.5 Hz, 1H), 7.53 – 7.43 (m, 3H), 7.38 (t, $J$ = 7.3 Hz, 1H), 3.61 (s, 4H), 2.75 (s, 4H), 2.43 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 160.6, 148.3, 139.8, 139.2, 129.8, 128.7, 128.4, 127.8, 126.8, 125.9, 125.5, 120.7, 111.4, 55.2, 51.0, 46.2; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $C_{20}H_{22}N_3$ 304.1808, found 304.1802.

**Gram-scale synthesis of 3d**

In an oven-dried 50 mL sealed tube, a mixture of 2-(phenylethyl)benzonitrile **1a** (4.52 mmol) and *tert*-butyl piperazine-1-carboxylate **2d** (5.0 mmol) in 20 mL of distilled $H_2O$ was heated at 100 °C for 4h. The progression of the reaction was monitored by TLC analysis; after the complete consumption of starting

material, the reaction was cooled to room temperature. The reaction mixture was diluted with ethyl acetate (50 mL). The layers were separated, and the organic layer was dried over $Na_2SO_4$. The organic layer was concentrated under reduced pressure. The crude material so obtained was purified by column chromatography on silica gel (100−200) (hexane: ethyl acetate; 90/10). The product was obtained **3d** as a white solid (1.65g, 94%).

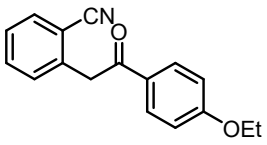
## Reference:


1 L. Tang, S. Jiang, X. Huang, Z. Song, J.- b. Wang, M. Ma, B. Chen, Y. Ma, *Org. Lett.* 2022, **24**, 17, 3232–3237.

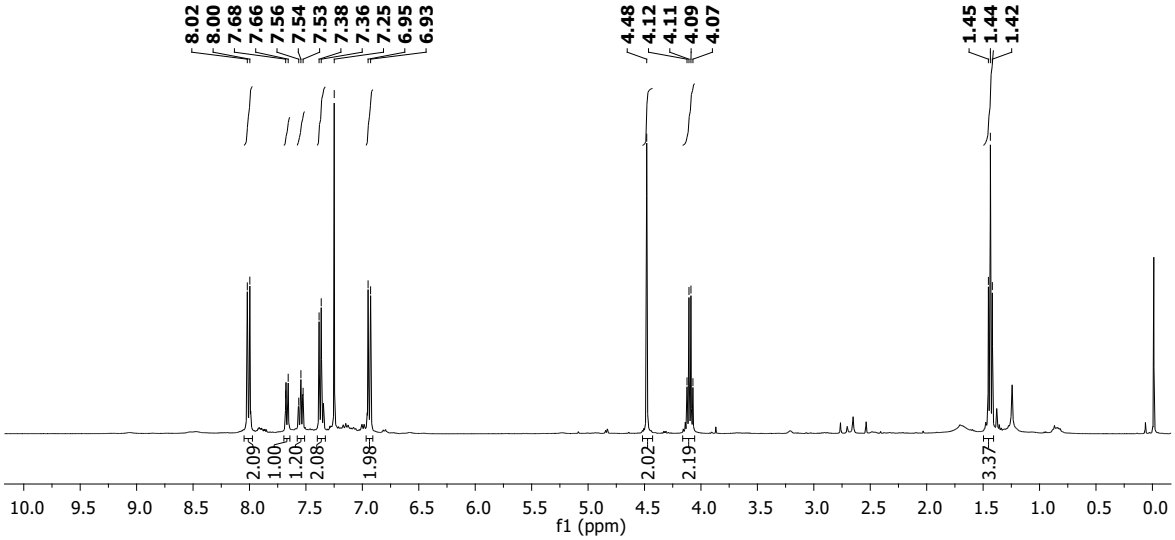
2. K. M.- S. Adusumalli, L. N.- S. Konidena, H.- B. Gandham, K. Kumari, K.- R. Valluru, S. K.- R. Nidasanametla, V. R. Battula, H.- K. Namballa, *Beilstein J. Org. Chem.* 2021, **17,** 2765–2772.

# Copies of $^{1}H$, $^{13}C$ NMR and HRMS

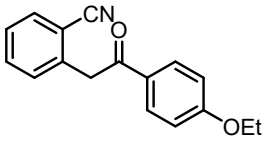
**$^{1}$H NMR** (400 MHz, $CDCl_3$)



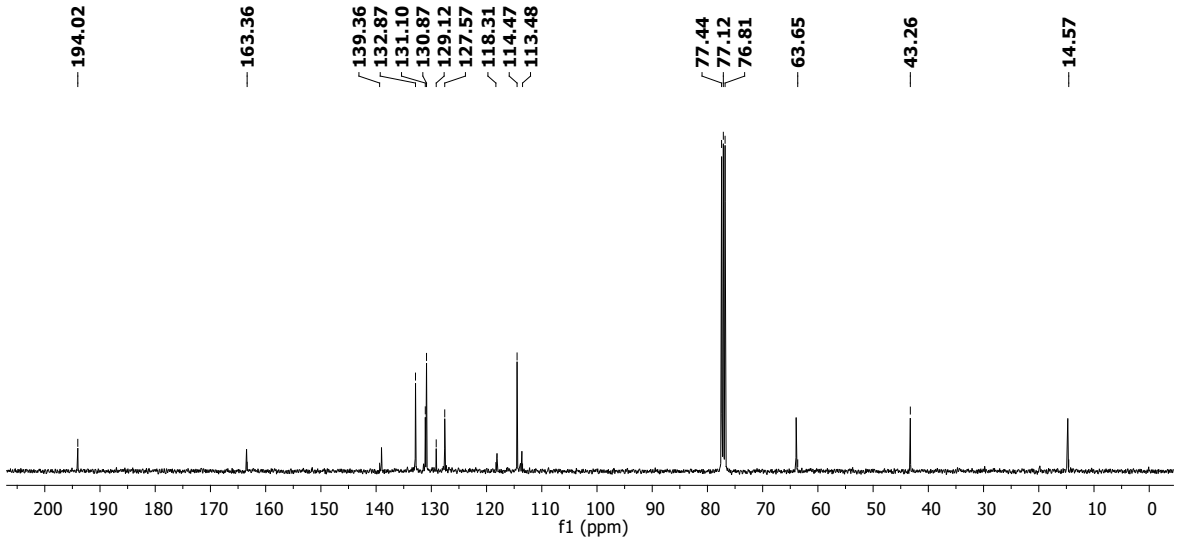

**2-(2-(4-Ethoxyphenyl)-2-oxoethyl)benzonitrile (1c)**



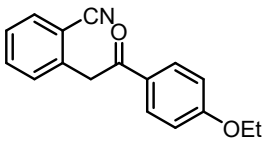

**$^{13}$C NMR** (100 MHz, $CDCl_3$)




**2-(2-(4-Ethoxyphenyl)-2-oxoethyl)benzonitrile (1c)**



## HRMS




## 2-(2-(4-Ethoxyphenyl)-2-oxoethyl)benzonitrile (1c)

### Qualitative Compound Report

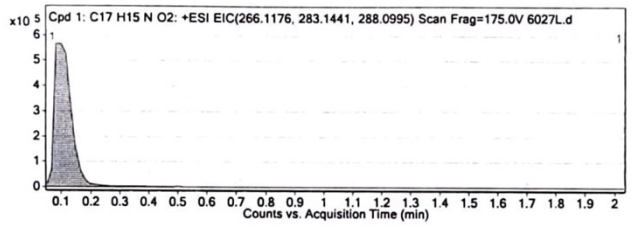
| | | | |
|---|---|---|---|
| **Data File** | 6027L.d | **Sample Name** | 6027L |
| **Sample Type** | Sample | **Position** | P1-A7 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | MS Scan.m | **Acquired Time** | 27-08-2022 12:18:14 |
| **IRM Calibration Status** | [redacted] | **DA Method** | Default.m |
| **Comment** | | | |

| | | | |
|---|---|---|---|
| **Sample Group** | | **Info.** | 3 |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

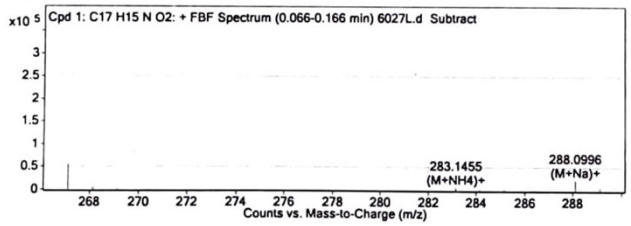
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C17 H15 N O2 | 0.082 | 265.1104 | 303153 | C17 H15 N O2 | 265.1103 | 0.4 | C17 H15 N O2 | C17 H15 N O2 |

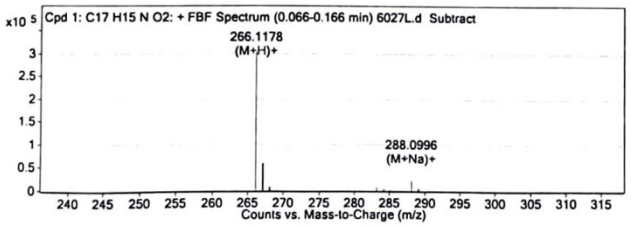
| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C17 H15 N O2 | 266.1178 | 0.082 | Find By Formula | 265.1104 |




MS Spectrum



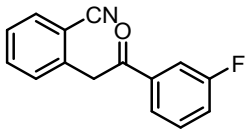

MS Zoomed Spectrum



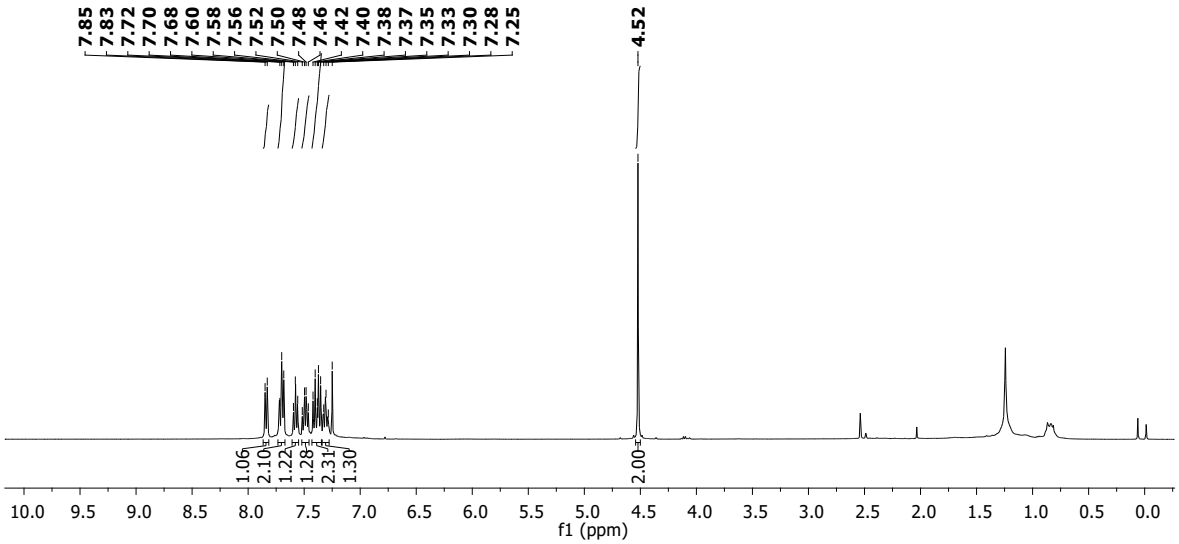

**MS Spectrum Peak List**

| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 266.1178 | 1 | 303153.44 | C17H16NO2 | (M+H)+ |
| 267.1204 | 1 | 56316.19 | C17H16NO2 | (M+H)+ |
| 268.1234 | 1 | 6332.31 | C17H16NO2 | (M+H)+ |
| 269.1301 | 1 | 1022.91 | C17H16NO2 | (M+H)+ |
| 270.1334 | 1 | 191.17 | C17H16NO2 | (M+H)+ |
| 283.1455 | 1 | 4988.18 | C17H19N2O2 | (M+NH4)+ |
| 284.1442 | 1 | 1329.29 | C17H19N2O2 | (M+NH4)+ |
| 285.1441 | 1 | 1537.95 | C17H19N2O2 | (M+NH4)+ |
| 288.0996 | 1 | 21551.84 | C17H15NNaO2 | (M+Na)+ |
| 289.104 | 1 | 4602.46 | C17H15NNaO2 | (M+Na)+ |
| 290.1063 | 1 | 601.08 | C17H15NNaO2 | (M+Na)+ |

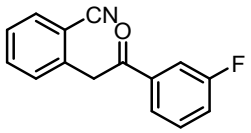
**$^{1}$H NMR** (400 MHz, $CDCl_3$)



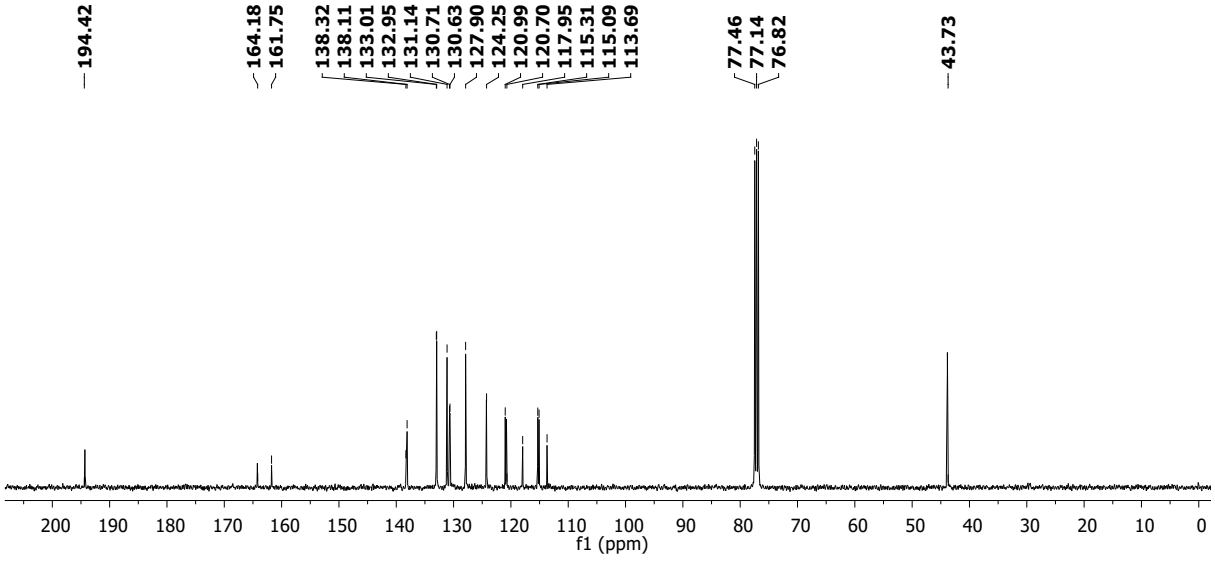

**2-(2-(3-Fluorophenyl)-2-oxoethyl)benzonitrile (1e)**



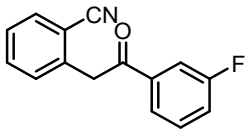

**$^{13}$C NMR** (100 MHz, $CDCl_3$)




**2-(2-(3-Fluorophenyl)-2-oxoethyl)benzonitrile (1e)**



## HRMS




## 2-(2-(3-Fluorophenyl)-2-oxoethyl)benzonitrile (1e)

### Qualitative Compound Report

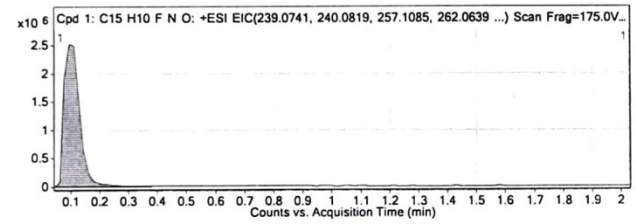
| | | | |
|---|---|---|---|
| **Data File** | 6010.d | **Sample Name** | 6010 |
| **Sample Type** | Sample | **Position** | P1-A5 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | MS Scan.m | **Acquired Time** | 27-08-2022 12:12:45 |
| **IRM Calibration Status** | [redacted] | **DA Method** | Default.m |
| **Comment** | | | |

| | | | |
|---|---|---|---|
| **Sample Group** | | **Info.** | 3 |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

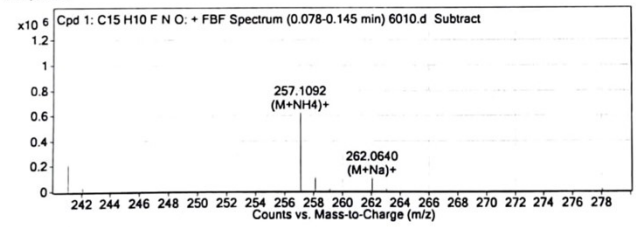
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C15 H10 F N O | 0.095 | 239.0756 | 100495 | C15 H10 F N O | 239.0746 | 3.86 | C15 H10 F N O | C15 H10 F N O |

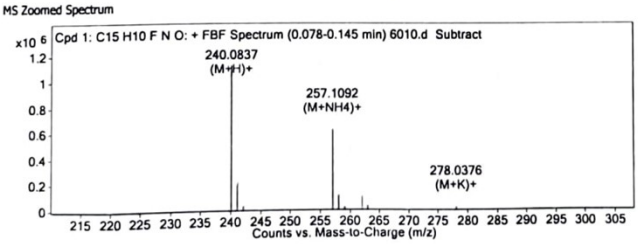
| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C15 H10 F N O | 262.064 | 0.095 | Find By Formula | 239.0756 |




MS Spectrum



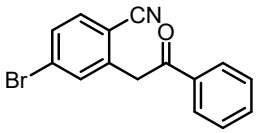

MS Zoomed Spectrum



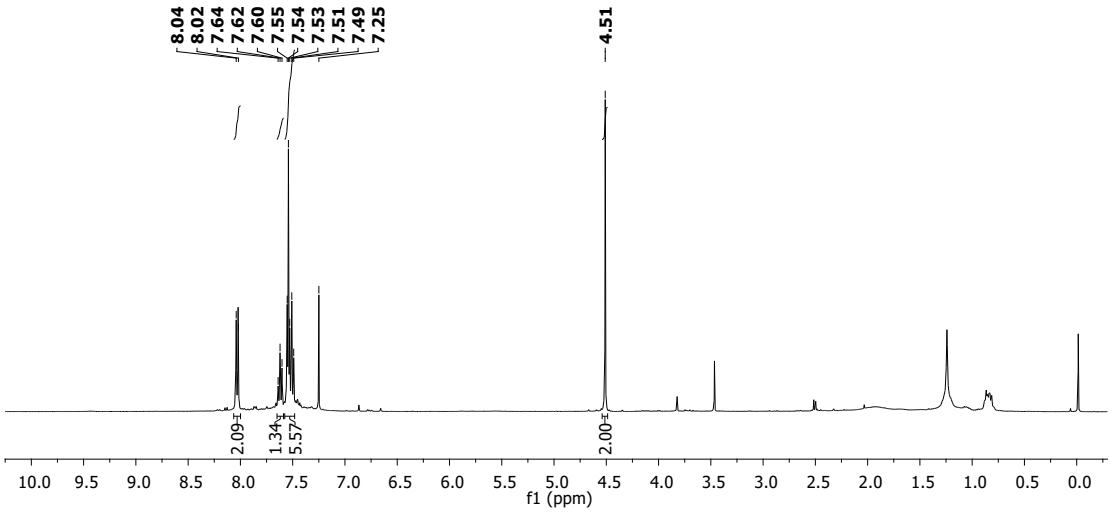

**MS Spectrum Peak List**

| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 240.0837 | 1 | 1092351.25 | C15H11FNO | (M+H)+ |
| 241.0836 | 1 | 207462.53 | C15H11FNO | (M+H)+ |
| 242.0872 | 1 | 24470.77 | C15H11FNO | (M+H)+ |
| 243.093 | 1 | 2564.13 | C15H11FNO | (M+H)+ |
| 244.1044 | 1 | 549.54 | C15H11FNO | (M+H)+ |
| 257.1092 | 1 | 621016 | C15H14FN2O | (M+NH4)+ |
| 258.1111 | 1 | 106529.56 | C15H14FN2O | (M+NH4)+ |
| 259.1129 | 1 | 10674.81 | C15H14FN2O | (M+NH4)+ |
| 260.1173 | 1 | 1663.99 | C15H14FN2O | (M+NH4)+ |
| 262.064 | 1 | 100494.64 | C15H10FNNaO | (M+Na)+ |
| 263.0671 | 1 | 16205.65 | C15H10FNNaO | (M+Na)+ |
| 264.0712 | 1 | 1608.8 | C15H10FNNaO | (M+Na)+ |

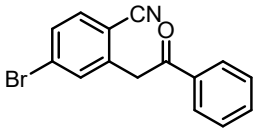
**$^{1}$H NMR** (400 MHz, $CDCl_3$)



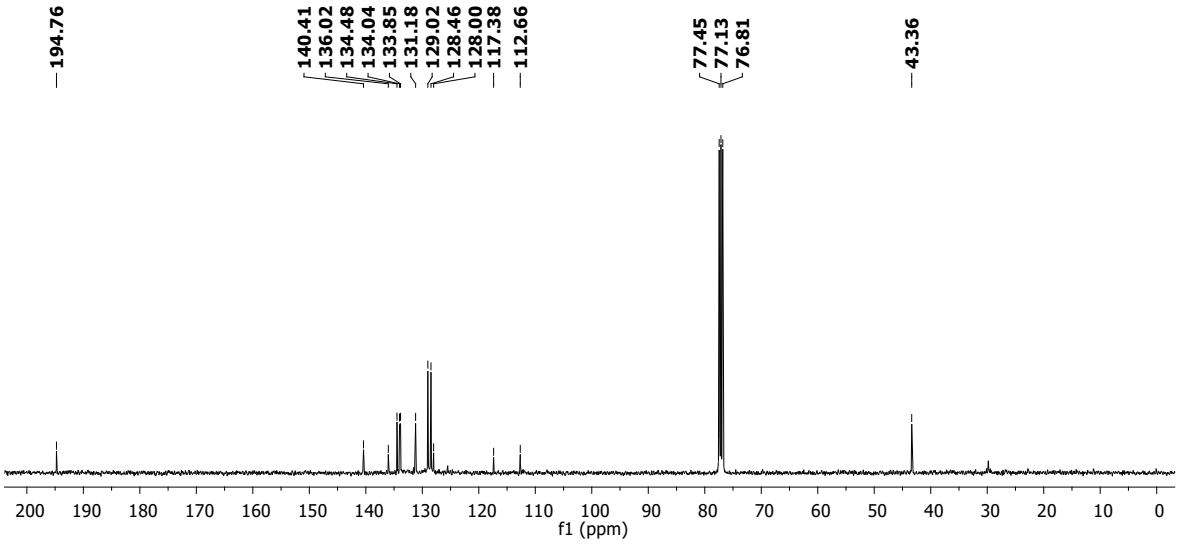

**4-Bromo-2-(2-oxo-2-phenylethyl)benzonitrile (1f)**



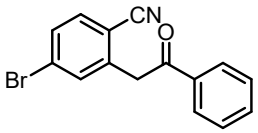

**$^{13}$C NMR** (100 MHz, $CDCl_3$)



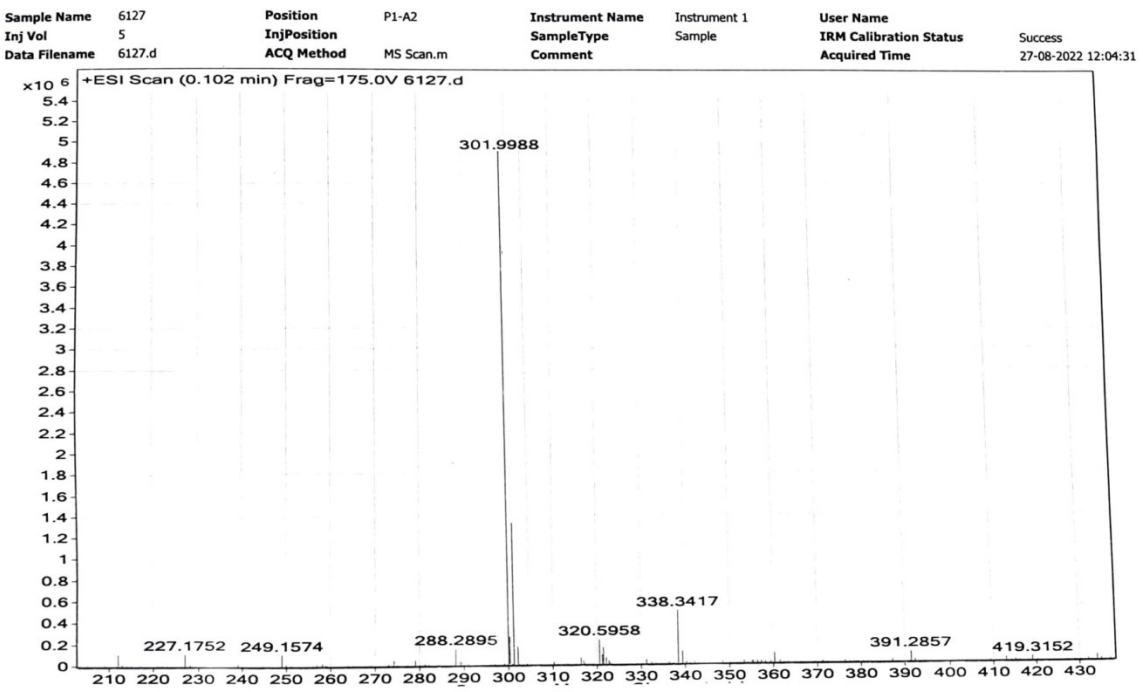

**4-Bromo-2-(2-oxo-2-phenylethyl)benzonitrile (1f)**



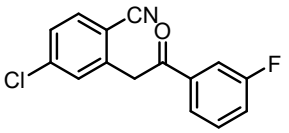
## HRMS



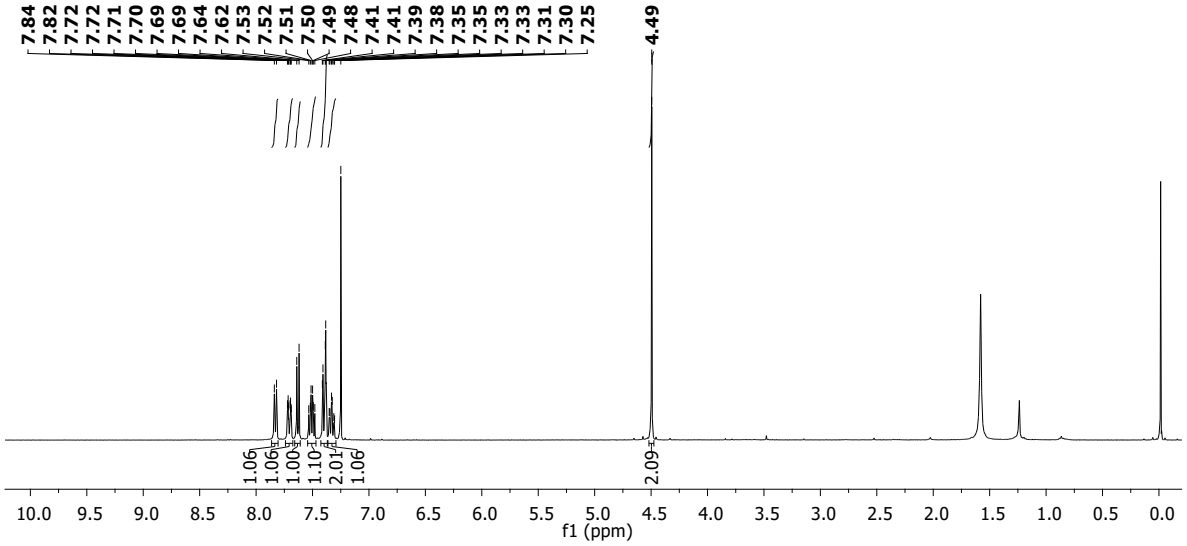

## 4-Bromo-2-(2-oxo-2-phenylethyl)benzonitrile (1f)



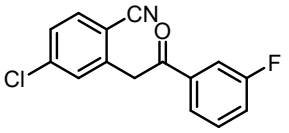
**$^{1}$H NMR** (400 MHz, $CDCl_3$)



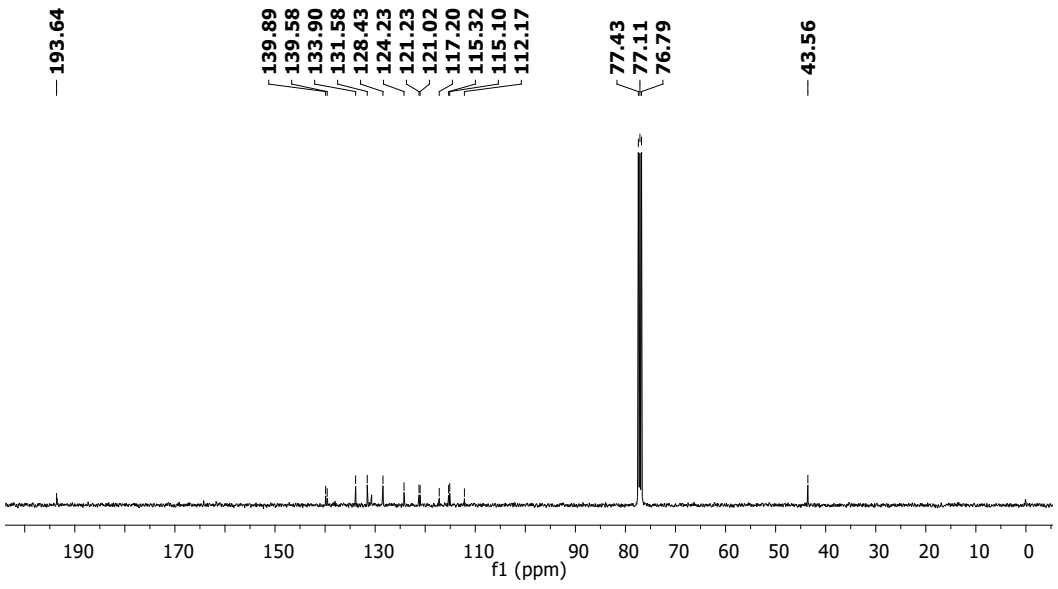

**4-Chloro-2-(2-(3-fluorophenyl)-2-oxoethyl)benzonitrile (1g)**



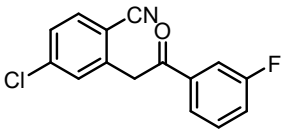

**$^{13}$C NMR** (100 MHz, $CDCl_3$)




**4-Chloro-2-(2-(3-fluorophenyl)-2-oxoethyl)benzonitrile (1g)**



## HRMS




## 4-Chloro-2-(2-(3-fluorophenyl)-2-oxoethyl)benzonitrile (1g)

### Qualitative Compound Report

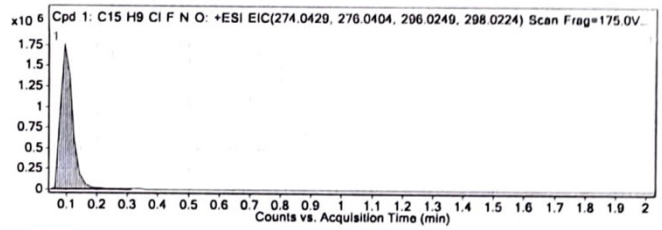
| | | | |
|---|---|---|---|
| **Data File** | 6087.d | **Sample Name** | 6087 |
| **Sample Type** | Sample | **Position** | P1-A1 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | MS Scan.m | **Acquired Time** | 27-08-2022 12:03:43 |
| **IRM Calibration Status** | [redacted] | **DA Method** | Default.m |
| **Comment** | | | |

| | | | |
|---|---|---|---|
| **Sample Group** | | **Info.** | 3 |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

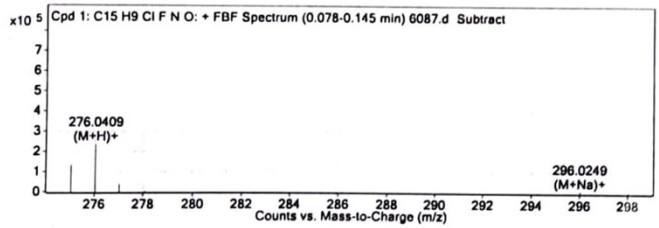
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C15 H9 Cl F N O | 0.095 | 273.0364 | 697232 | C15 H9 Cl F N O | 273.0357 | 2.72 | C15 H9 Cl F N O | C15 H9 Cl F N O |

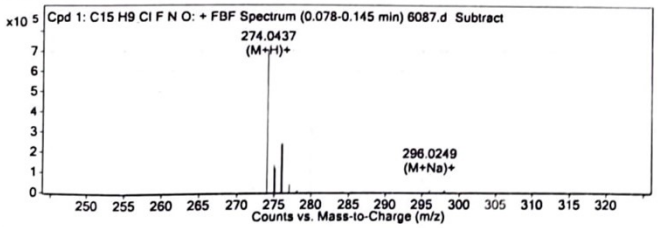
| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C15 H9 Cl F N O | 274.0437 | 0.095 | Find By Formula | 273.0364 |




MS Spectrum



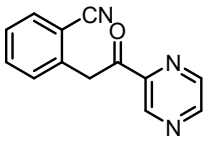

MS Zoomed Spectrum



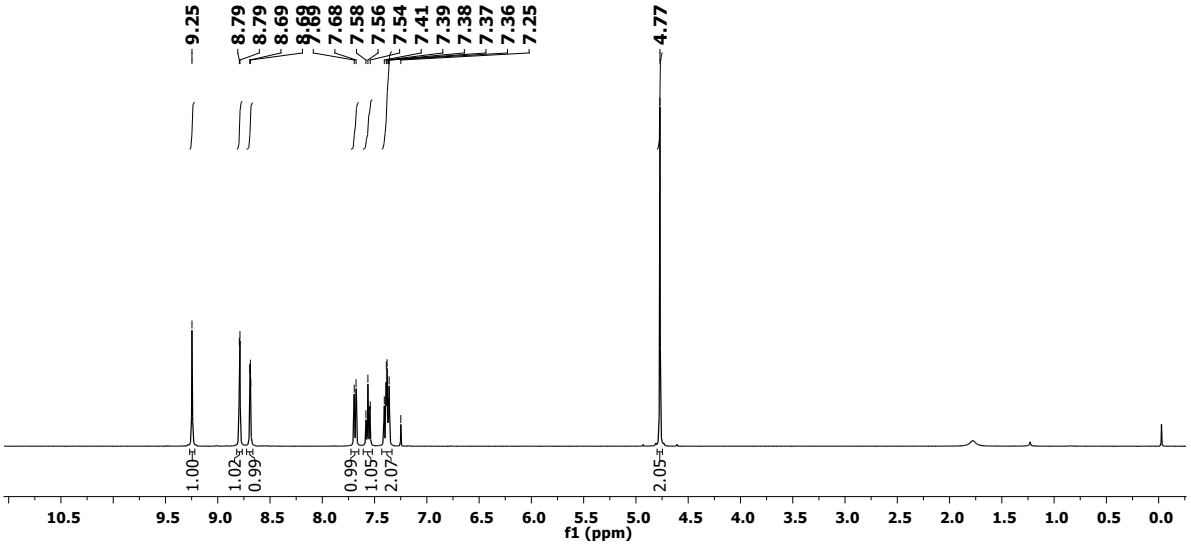

**MS Spectrum Peak List**

| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 274.0437 | 1 | 697232.13 | C15H10ClFNO | (M+H)+ |
| 275.0476 | 1 | 134242.58 | C15H10ClFNO | (M+H)+ |
| 276.0409 | 1 | 234619.55 | C15H10ClFNO | (M+H)+ |
| 277.0428 | 1 | 36483.65 | C15H10ClFNO | (M+H)+ |
| 278.0449 | 1 | 3723.77 | C15H10ClFNO | (M+H)+ |
| 296.0249 | 1 | 7715.33 | C15H9ClFNNaO | (M+Na)+ |
| 297.0319 | 1 | 558.38 | C15H9ClFNNaO | (M+Na)+ |
| 298.0233 | 1 | 2384.09 | C15H9ClFNNaO | (M+Na)+ |
| 299.0249 | 1 | 163.9 | C15H9ClFNNaO | (M+Na)+ |

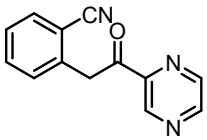
**$^{1}$H NMR** (400 MHz, $CDCl_3$)



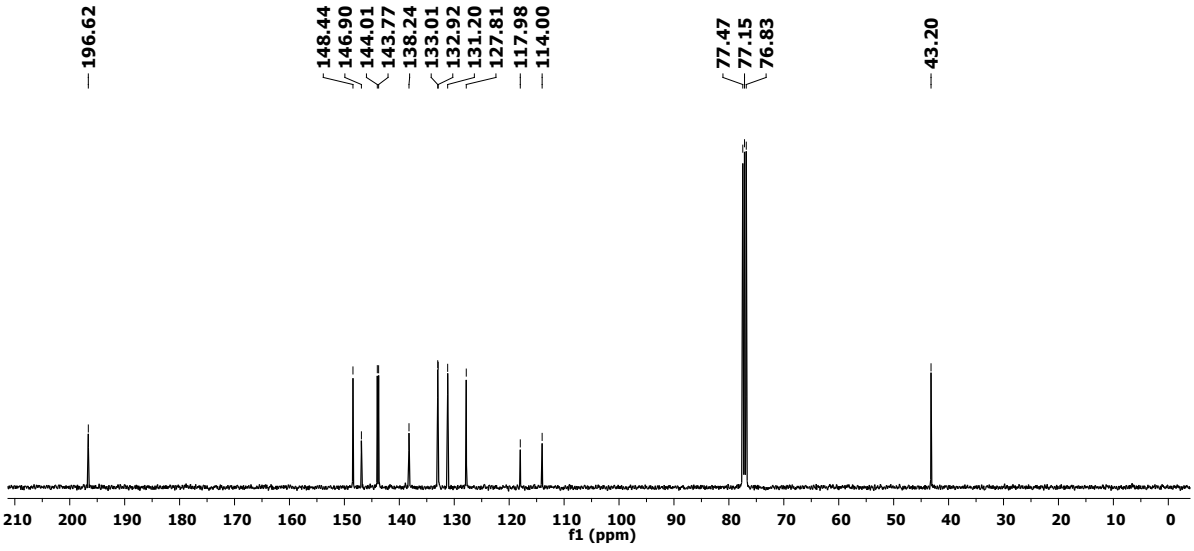

**2-(2-Oxo-2-(pyrazin-2-yl)ethyl)benzonitrile (1i)**



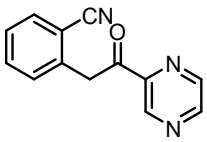

**$^{13}$C NMR** (100 MHz, $CDCl_3$)



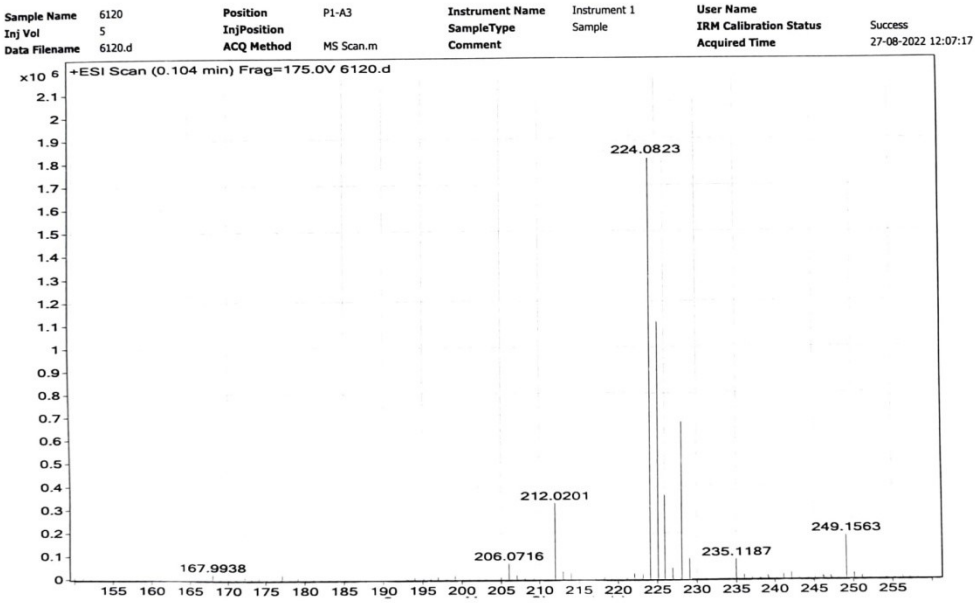

**2-(2-Oxo-2-(pyrazin-2-yl)ethyl)benzonitrile (1i)**



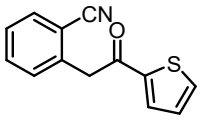
## HRMS



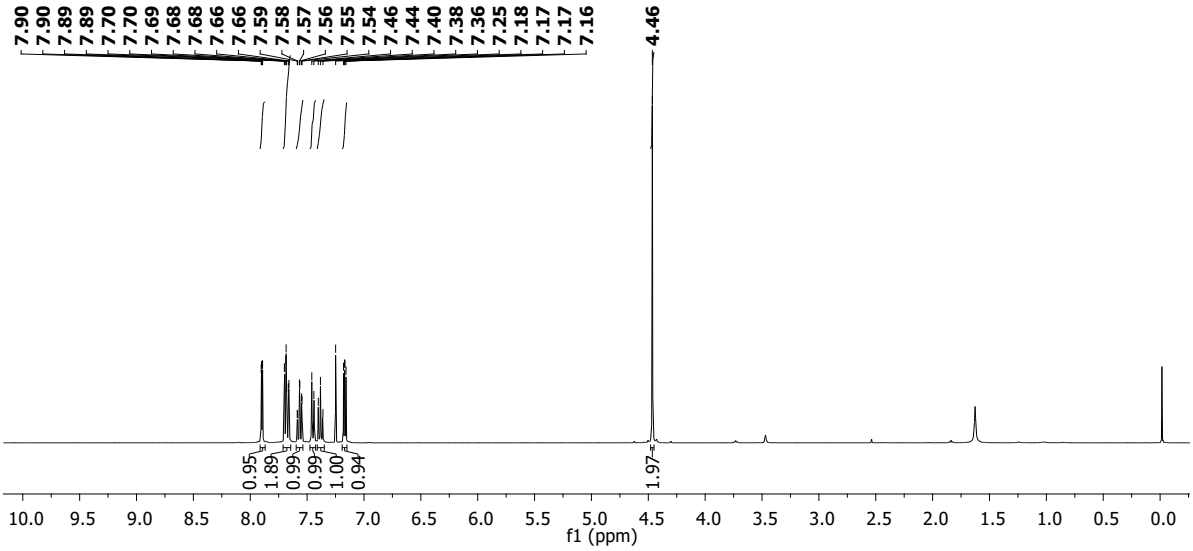

## 2-(2-Oxo-2-(pyrazin-2-yl)ethyl)benzonitrile (1i)



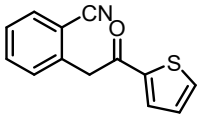
**$^{1}$H NMR** (400 MHz, $CDCl_3$)



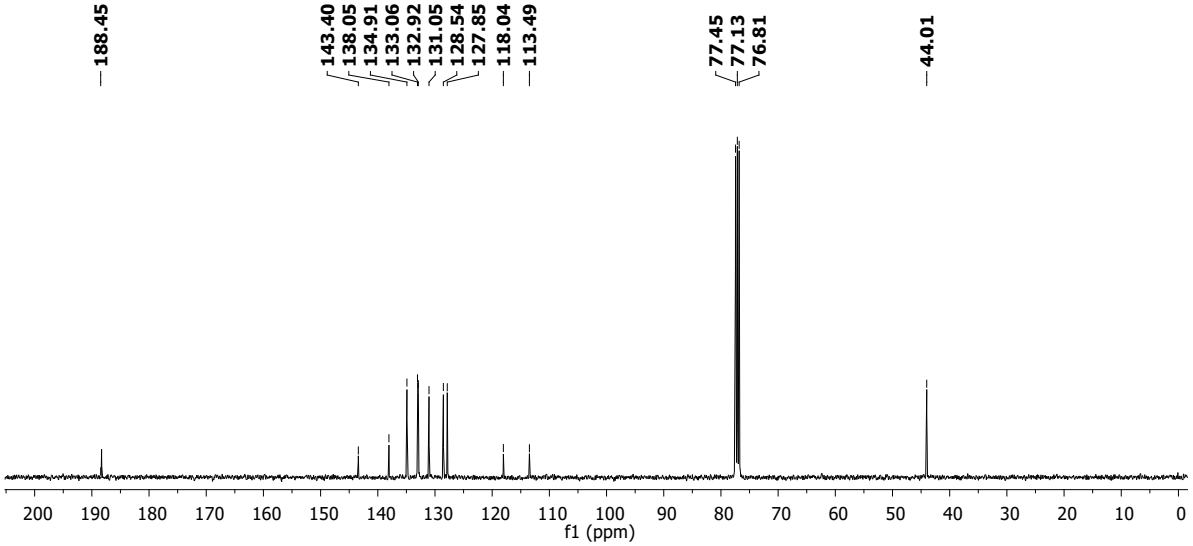

**2-(2-Oxo-2-(thiophen-2-yl)ethyl)benzonitrile (1j)**



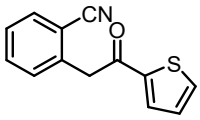

**$^{13}$C NMR** (100 MHz, $CDCl_3$)




**2-(2-Oxo-2-(thiophen-2-yl)ethyl)benzonitrile (1j)**



## HRMS




## 2-(2-Oxo-2-(thiophen-2-yl)ethyl)benzonitrile (1j)

### Qualitative Compound Report

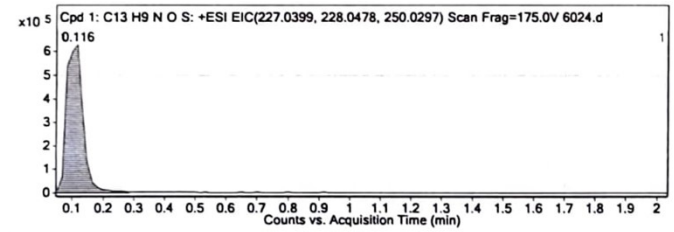
| | | | |
|---|---|---|---|
| **Data File** | 6024.d | **Sample Name** | 6024 |
| **Sample Type** | Sample | **Position** | P1-A6 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | MS Scan.m | **Acquired Time** | 27-08-2022 12:15:29 |
| **IRM Calibration Status** | [redacted] | **DA Method** | Default.m |
| **Comment** | | | |

| | | | |
|---|---|---|---|
| **Sample Group** | | **Info.** | 3 |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

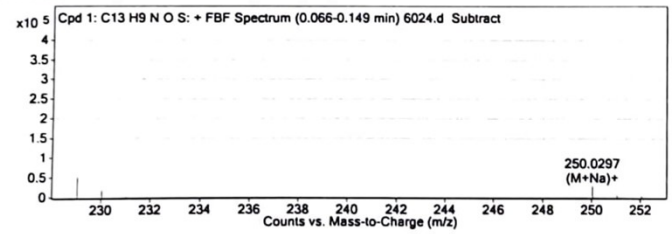
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C13 H9 N O S | 0.116 | 227.0407 | 364630 | C13 H9 N O S | 227.0405 | 0.88 | C13 H9 N O S | C13 H9 N O S |

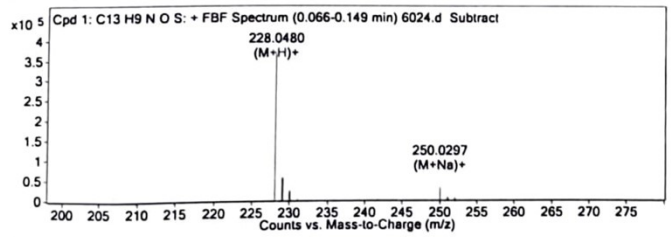
| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C13 H9 N O S | 228.048 | 0.116 | Find By Formula | 227.0407 |




MS Spectrum



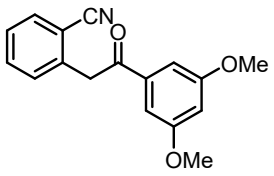

MS Zoomed Spectrum



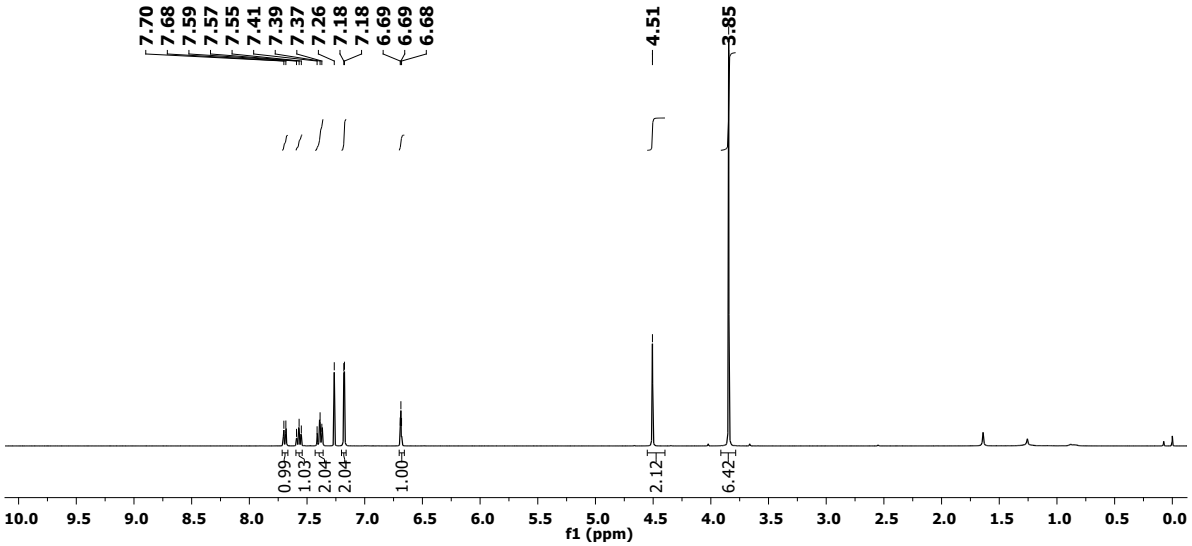

**MS Spectrum Peak List**

| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 228.048 | 1 | 364629.88 | C13H10NOS | (M+H)+ |
| 229.051 | 1 | 51664.19 | C13H10NOS | (M+H)+ |
| 230.046 | 1 | 18223.59 | C13H10NOS | (M+H)+ |
| 231.0485 | 1 | 2601.96 | C13H10NOS | (M+H)+ |
| 232.0485 | 1 | 300.2 | C13H10NOS | (M+H)+ |
| 250.0297 | 1 | 28152.97 | C13H9NNaOS | (M+Na)+ |
| 251.0316 | 1 | 4242.78 | C13H9NNaOS | (M+Na)+ |
| 252.0272 | 1 | 1513.88 | C13H9NNaOS | (M+Na)+ |
| 253.0233 | 1 | 159 | C13H9NNaOS | (M+Na)+ |

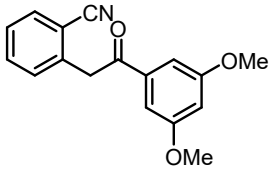
**$^{1}$H NMR** (400 MHz, $CDCl_3$)



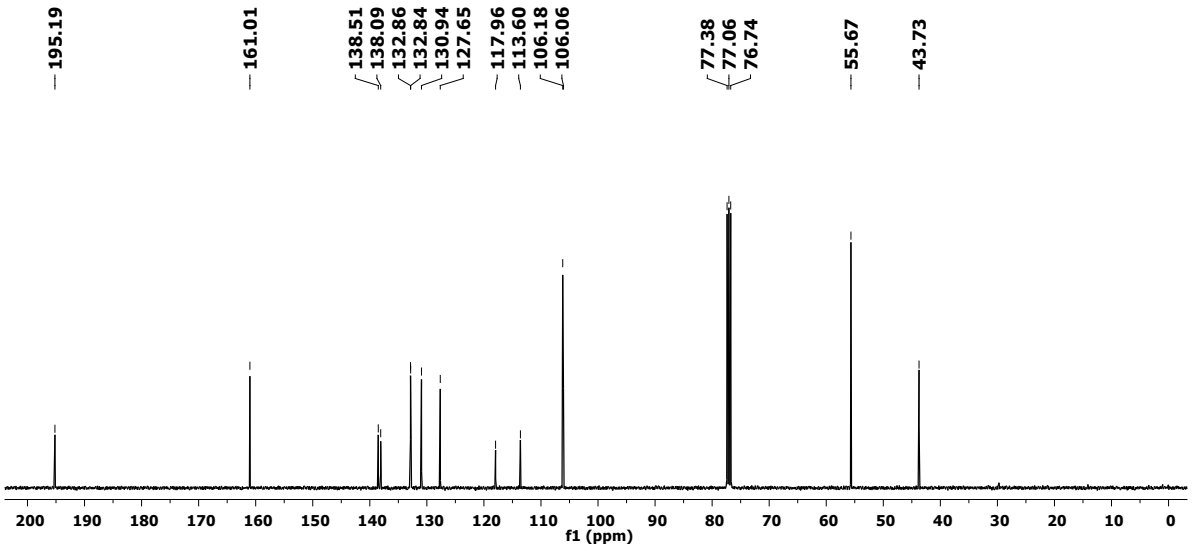

**2-(2-(3,5-Dimethoxyphenyl)-2-oxoethyl)benzonitrile (1k)**



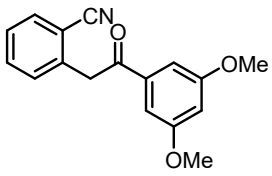

**$^{13}$C NMR** (100 MHz, $CDCl_3$)




**2-(2-(3,5-Dimethoxyphenyl)-2-oxoethyl)benzonitrile (1k)**



## HRMS




## 2-(2-(3,5-Dimethoxyphenyl)-2-oxoethyl)benzonitrile (1k)

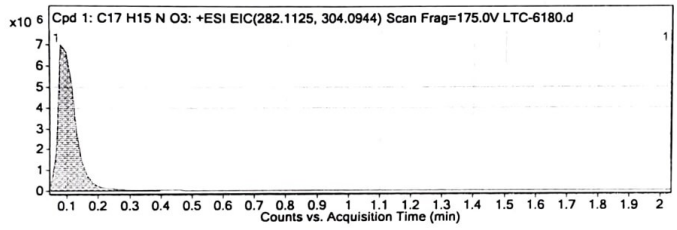
**Qualitative Compound Report**

| | | | |
|---|---|---|---|
| **Data File** | LTC-6180.d | **Sample Name** | LTC-6180 |
| **Sample Type** | Sample | **Position** | P1-A3 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | MS Scan.m | **Acquired Time** | 24-11-2022 15:40:32 |
| **IRM Calibration Status** | [redacted] | **DA Method** | Default.m |
| **Comment** | | | |
| **Sample Group** | | **Info.** | 3 |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

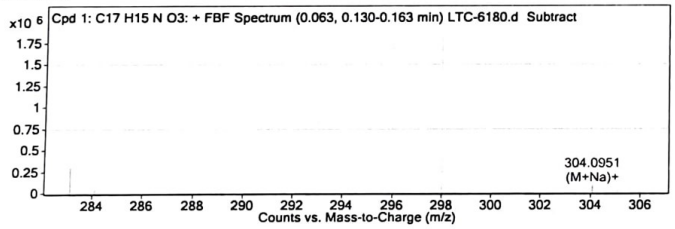
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C17 H15 N O3 | 0.08 | 281.1063 | 1643413 | C17 H15 N O3 | 281.1052 | 3.77 | C17 H15 N O3 | C17 H15 N O3 |

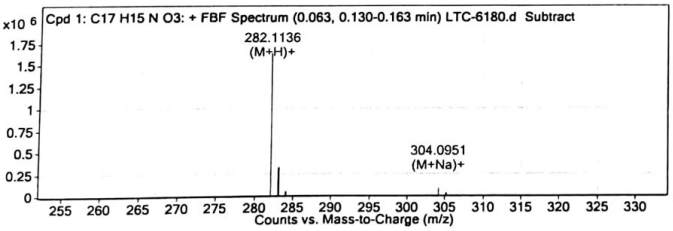
| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C17 H15 N O3 | 282.1136 | 0.08 | Find By Formula | 281.1063 |




MS Spectrum




MS Zoomed Spectrum

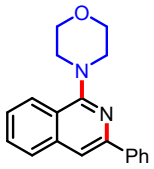



**MS Spectrum Peak List**

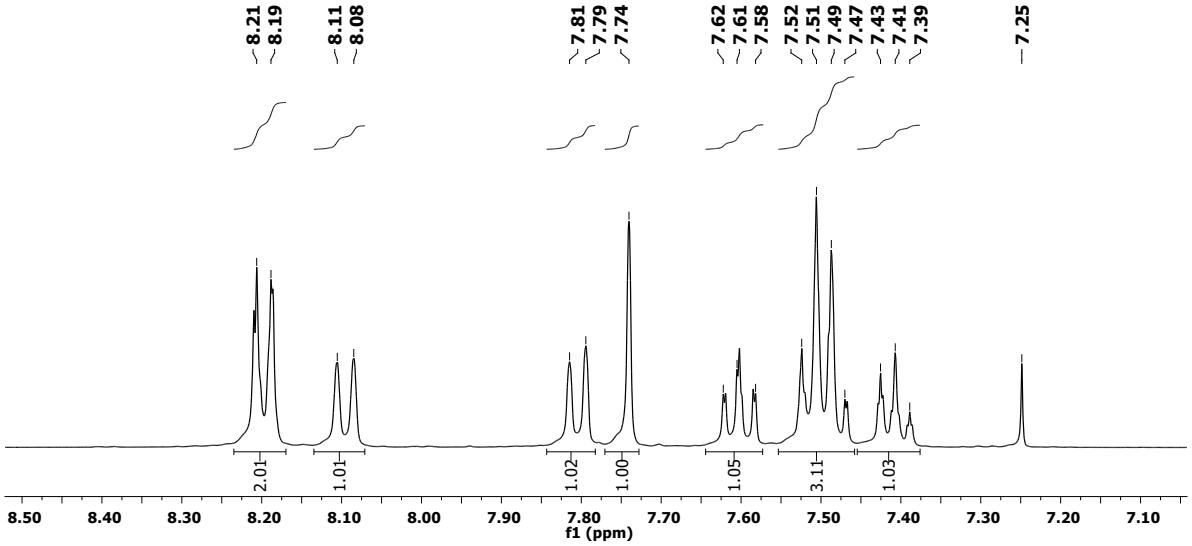
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 282.1136 | 1 | 1643412.5 | C17H16NO3 | (M+H)+ |
| 283.1167 | 1 | 306852.13 | C17H16NO3 | (M+H)+ |
| 284.1193 | 1 | 35890.53 | C17H16NO3 | (M+H)+ |
| 285.1219 | 1 | 3557.73 | C17H16NO3 | (M+H)+ |
| 304.0951 | 1 | 82651.52 | C17H15NNaO3 | (M+Na)+ |
| 305.0998 | 1 | 14885 | C17H15NNaO3 | (M+Na)+ |
| 306.1051 | 1 | 1892.67 | C17H15NNaO3 | (M+Na)+ |
| 307.1097 | 1 | 154.06 | C17H15NNaO3 | (M+Na)+ |

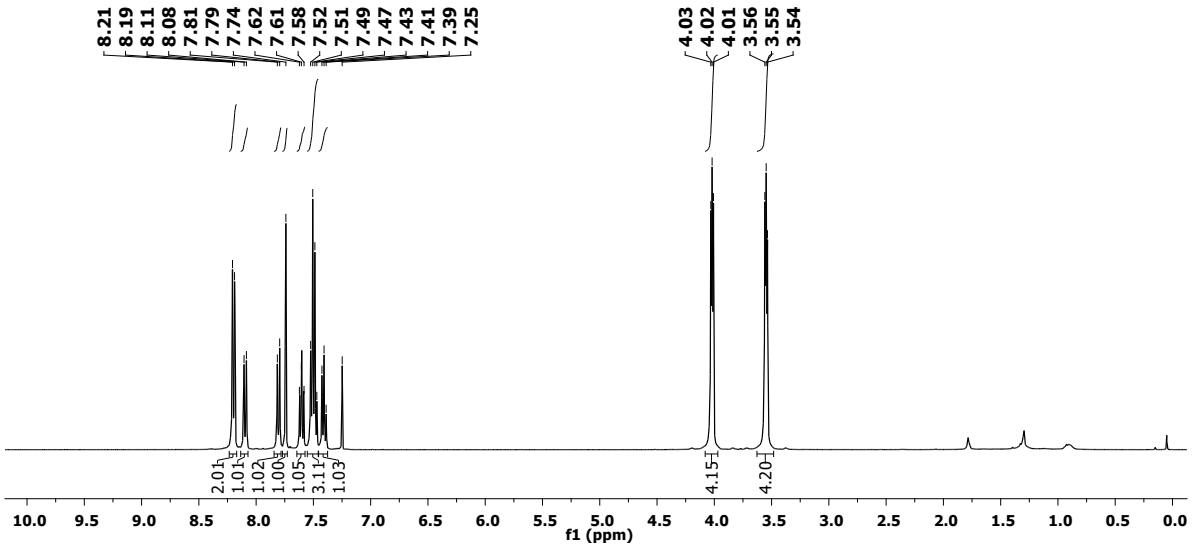
--- End Of Report ---

**$^1$H NMR** (400 MHz, $CDCl_3$)

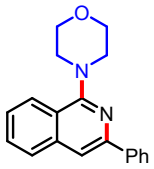



**4-(3-phenylisoquinolin-1-yl)morpholine (3a)**

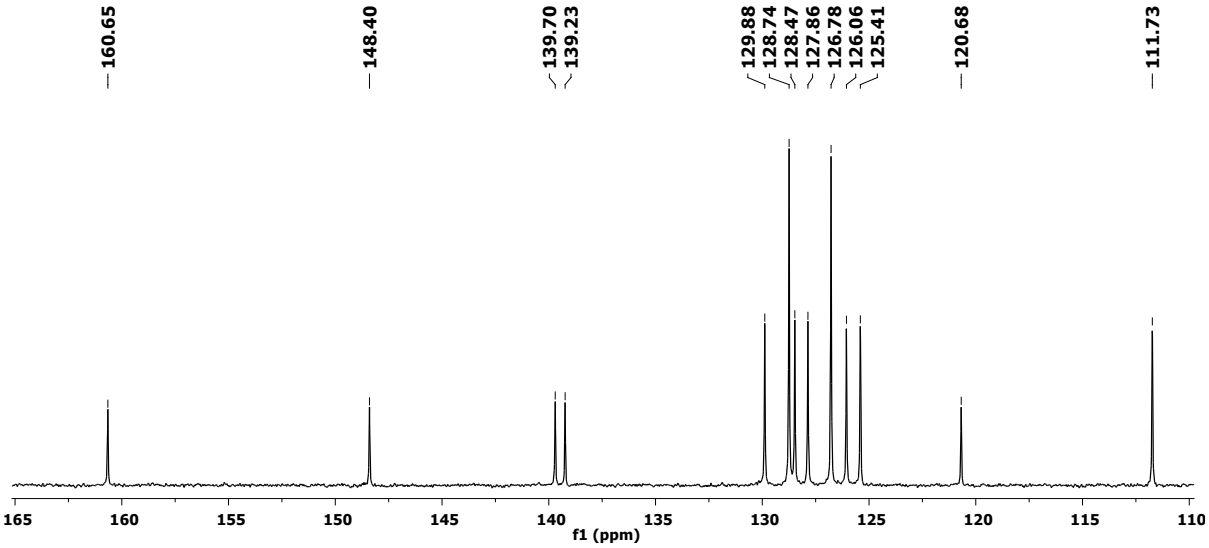


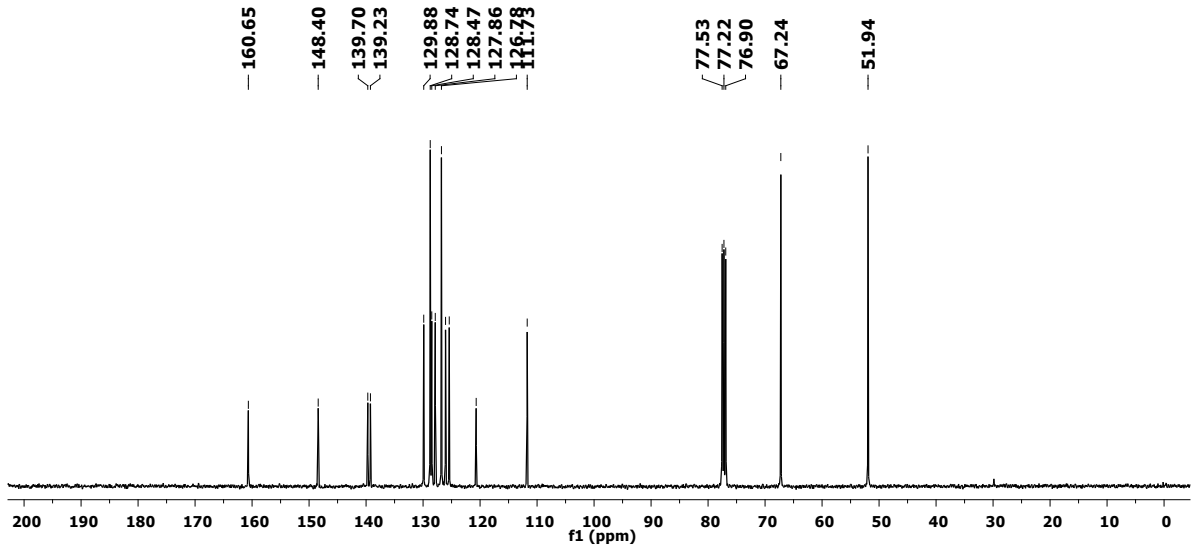



**$^{13}$C NMR** (100 MHz, $CDCl_3$)

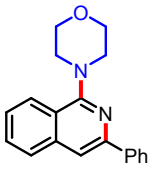



**4-(3-phenylisoquinolin-1-yl)morpholine (3a)**



## HRMS




## 4-(3-phenylisoquinolin-1-yl)morpholine (3a)

### Qualitative Compound Report

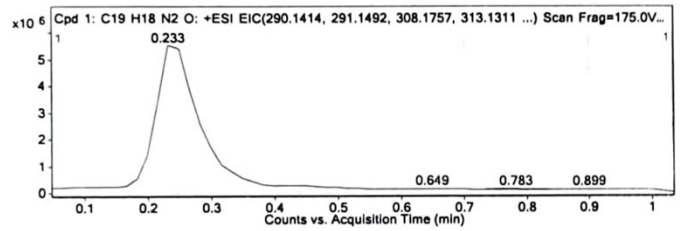
| | | | |
|---|---|---|---|
| **Data File** | H-53D.d | **Sample Name** | H-53D |
| **Sample Type** | Sample | **Position** | P1-A8 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | MS Scan.m | **Acquired Time** | 01-07-2022 12:44:53 |
| **IRM Calibration Status** | [redacted] | **DA Method** | Default.m |
| **Comment** | | | |

| | | | |
|---|---|---|---|
| **Sample Group** | | **Info.** | 3 |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

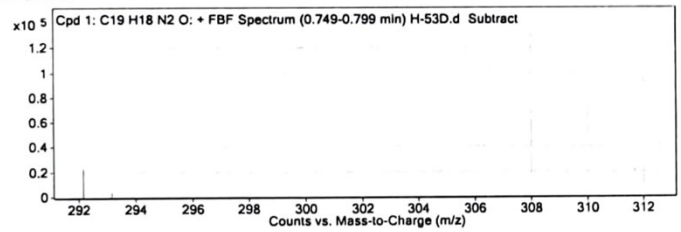
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C19 H18 N2 O | 0.783 | 290.1436 | 114215 | C19 H18 N2 O | 290.1419 | 5.65 | C19 H18 N2 O | C19 H18 N2 O |

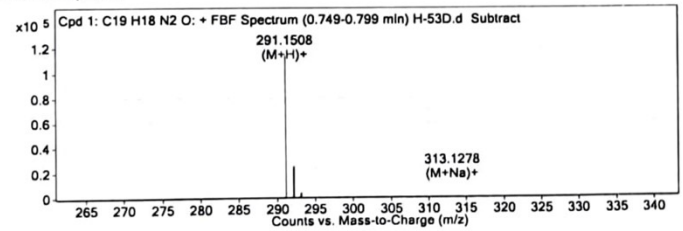
| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C19 H18 N2 O | 291.1508 | 0.783 | Find By Formula | 290.1436 |




MS Spectrum




MS Zoomed Spectrum

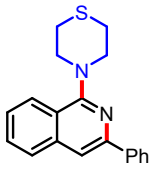



**MS Spectrum Peak List**

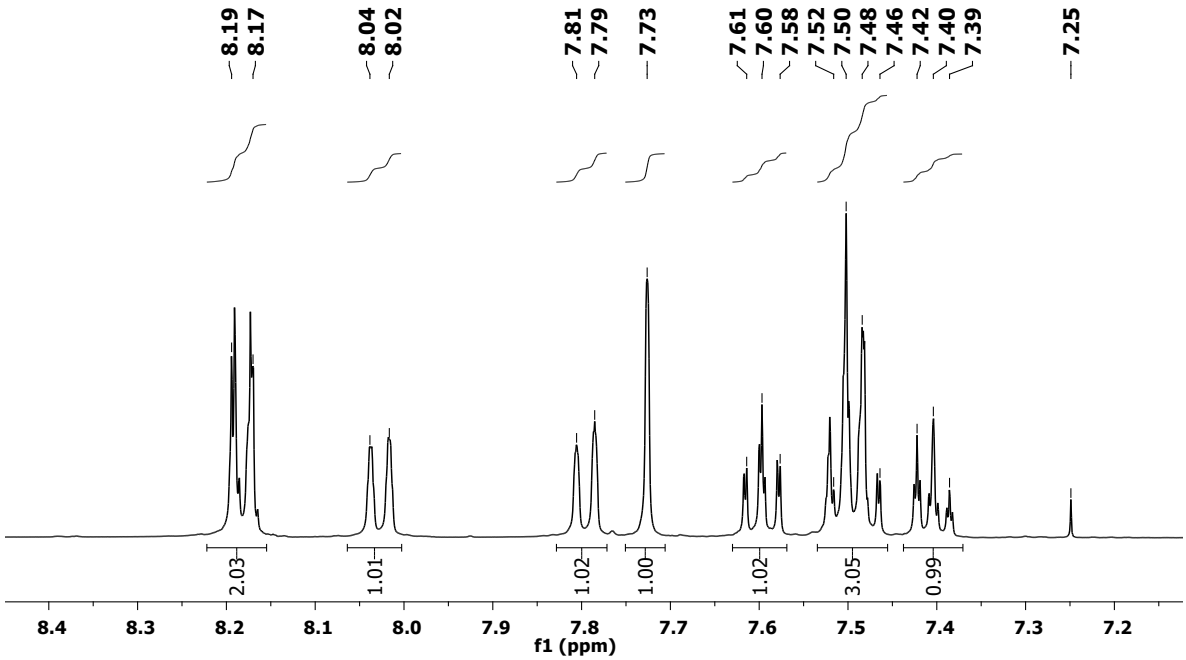
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 291.1508 | 1 | 114215.07 | C19H19N2O | (M+H)+ |
| 292.1529 | 1 | 23036.43 | C19H19N2O | (M+H)+ |
| 293.1647 | 1 | 3558.66 | C19H19N2O | (M+H)+ |
| 313.1278 | 1 | 165.28 | C19H18N2NaO | (M+Na)+ |

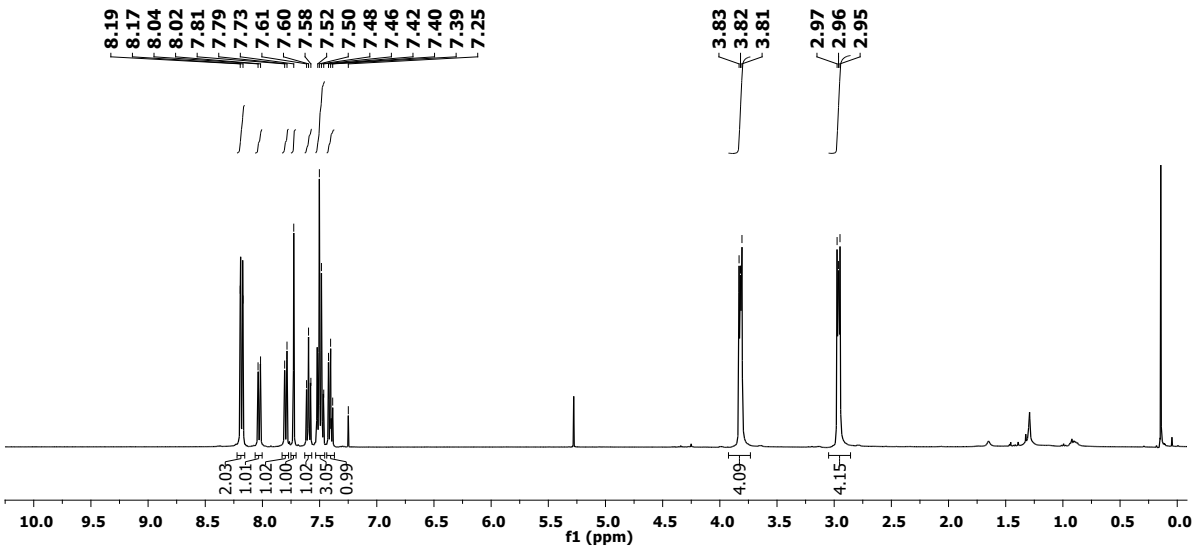
--- End Of Report ---

**$^1$H NMR** (400 MHz, $CDCl_3$)

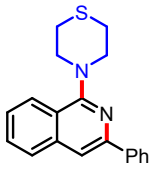



**4-(3-phenylisoquinolin-1-yl)thiomorpholine (3b)**

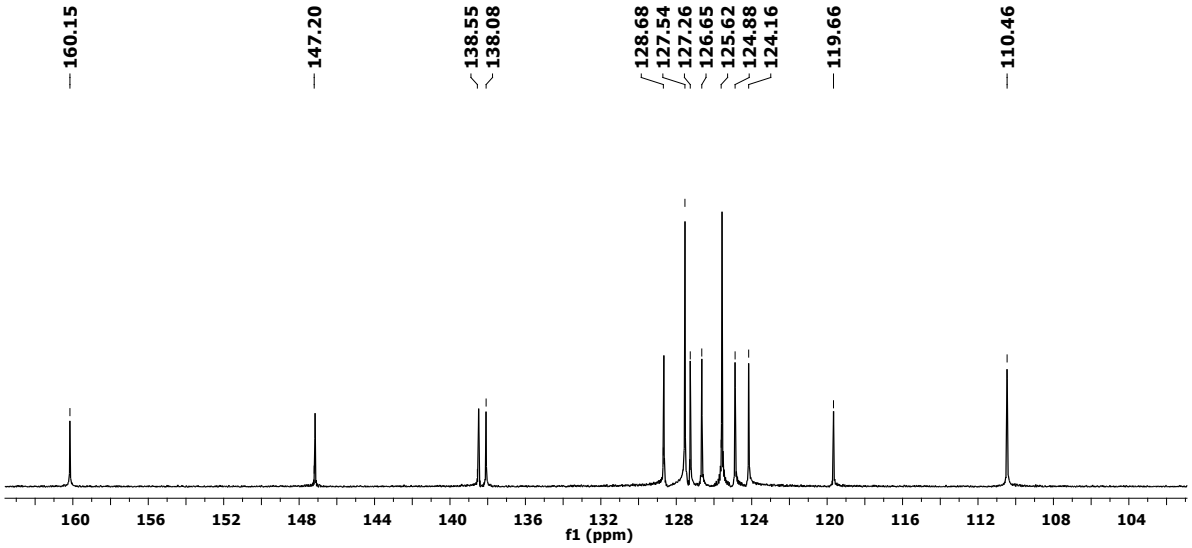


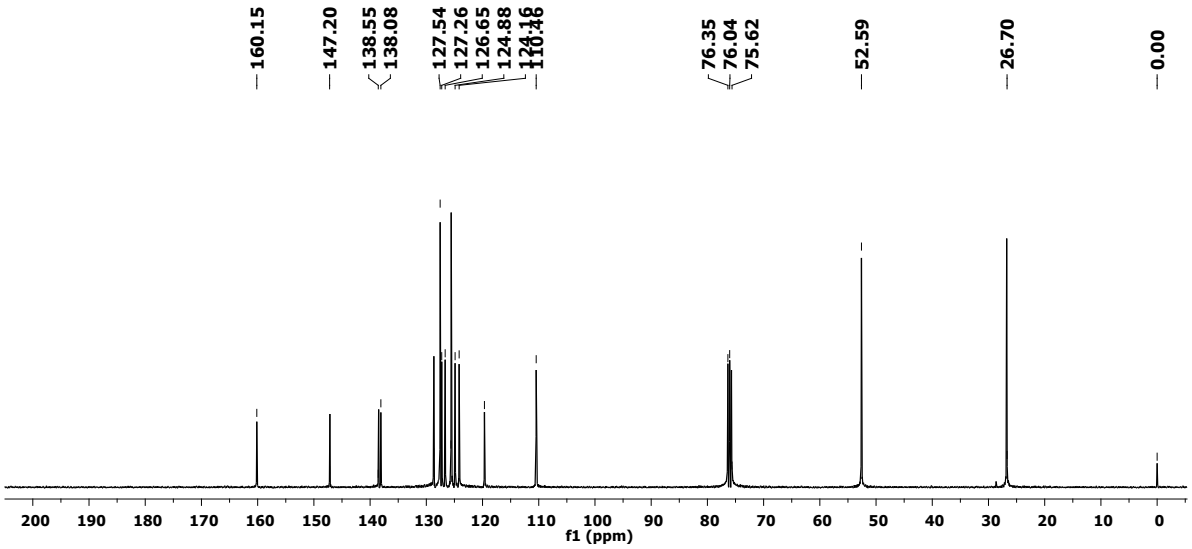



**$^{13}$C NMR** (100 MHz, $CDCl_3$)

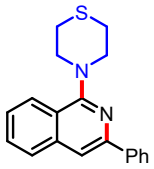



**4-(3-phenylisoquinolin-1-yl)thiomorpholine (3b)**



## HRMS




## 4-(3-phenylisoquinolin-1-yl)thiomorpholine (3b)

### Qualitative Compound Report

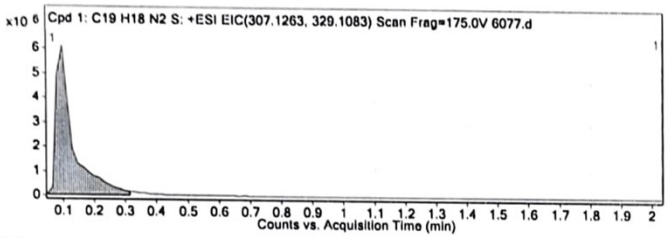
| | | | |
|---|---|---|---|
| Data File | 6077.d | Sample Name | 6077 |
| Sample Type | Sample | Position | P1-C6 |
| Instrument Name | Instrument 1 | User Name | |
| Acq Method | MS Scan.m | Acquired Time | 22-08-2022 14:25:44 |
| IRM Calibration Status | [redacted] | DA Method | Default.m |
| Comment | | | |

| | | | |
|---|---|---|---|
| Sample Group | | Info. | 3 |
| Acquisition SW Version | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

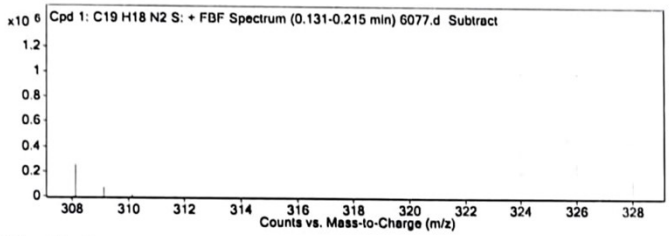
Compound Table

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C19 H18 N2 S | 0.098 | 306.1188 | 1145856 | C19 H18 N2 S | 306.1191 | -0.89 | C19 H18 N2 S | C19 H18 N2 S |

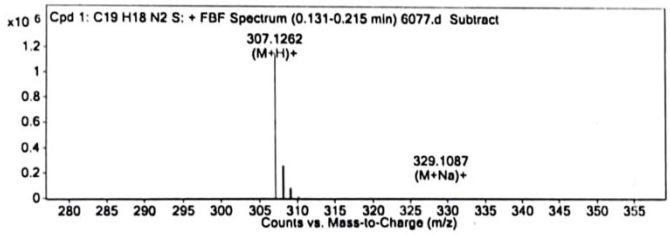
| Compound Label | m/z | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C19 H18 N2 S | 307.1262 | 0.098 | Find By Formula | 306.1188 |




MS Spectrum




MS Zoomed Spectrum

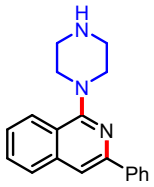



MS Spectrum Peak List

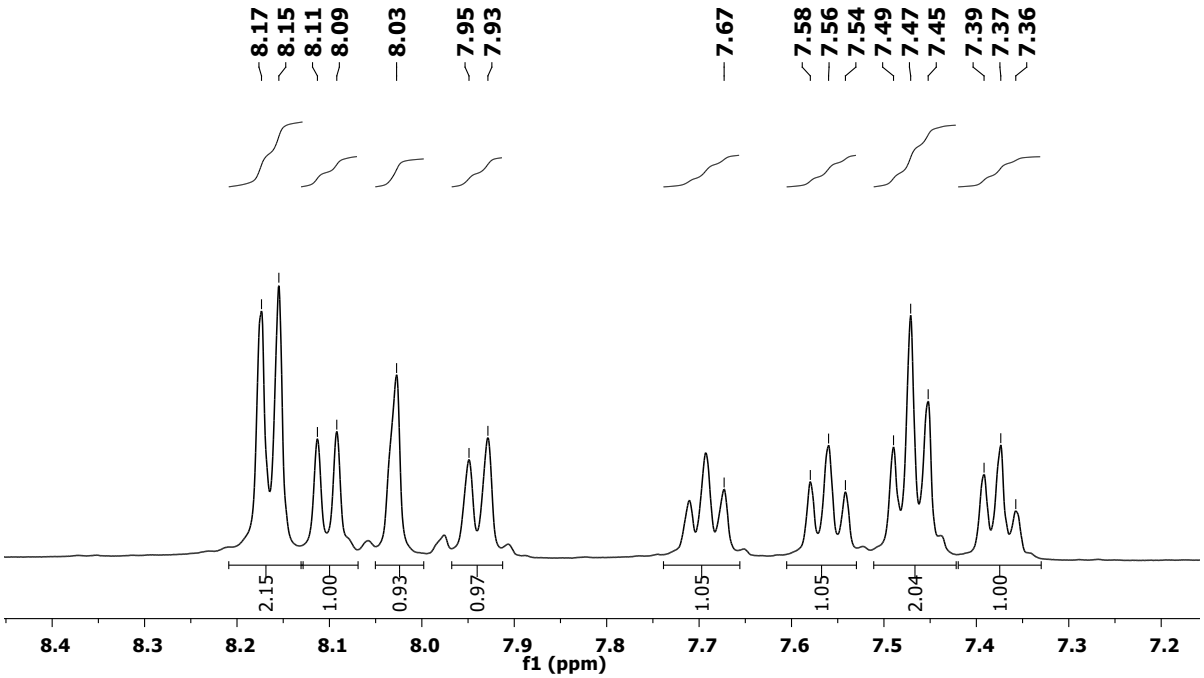
| m/z | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 307.1262 | 1 | 1145856.38 | C19H19N2S | (M+H)+ |
| 308.1288 | 1 | 253236.44 | C19H19N2S | (M+H)+ |
| 309.1253 | 1 | 72100.16 | C19H19N2S | (M+H)+ |
| 310.1256 | 1 | 12318.63 | C19H19N2S | (M+H)+ |
| 311.1237 | 1 | 1586.58 | C19H19N2S | (M+H)+ |
| 329.1087 | 1 | 93.77 | C19H18N2NaS | (M+Na)+ |

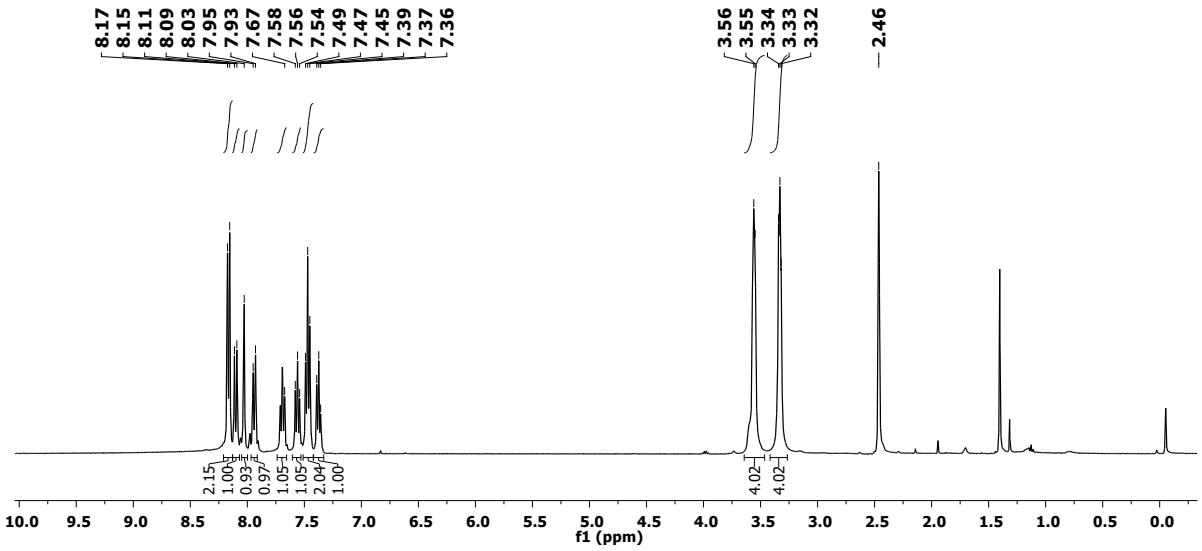
--- End Of Report ---

**$^1$H NMR** (400 MHz, DMSO-$d_6$)

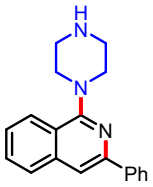



**3-phenyl-1-(piperazin-1-yl)isoquinoline (3c)**

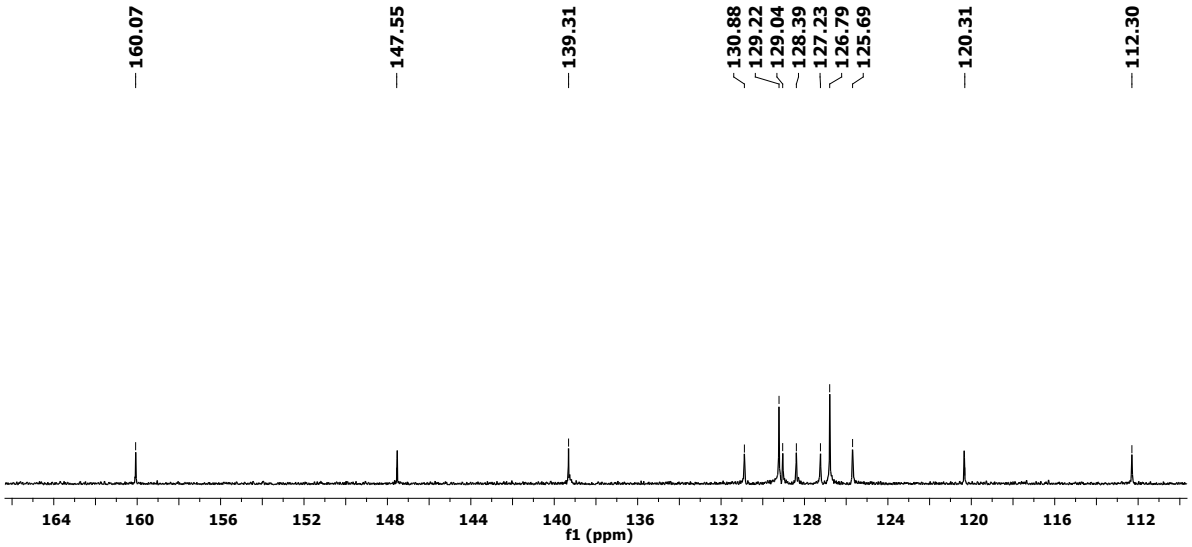


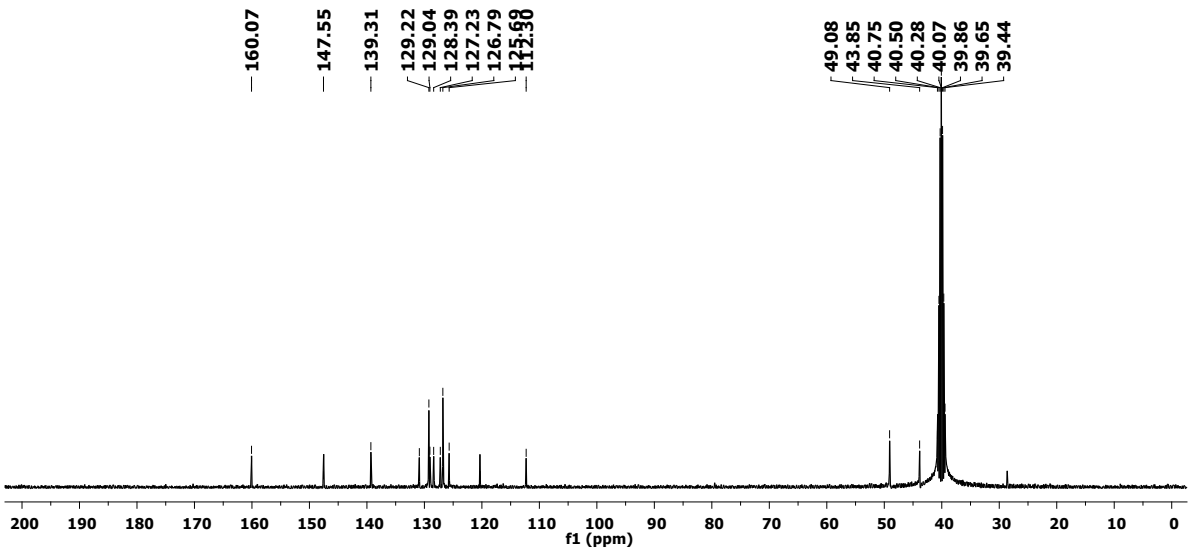



**$^{13}$C NMR** (101 MHz, DMSO-$d_6$)

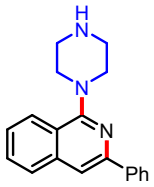



**3-phenyl-1-(piperazin-1-yl)isoquinoline (3c)**



## HRMS



**3-phenyl-1-(piperazin-1-yl)isoquinoline (3c)**

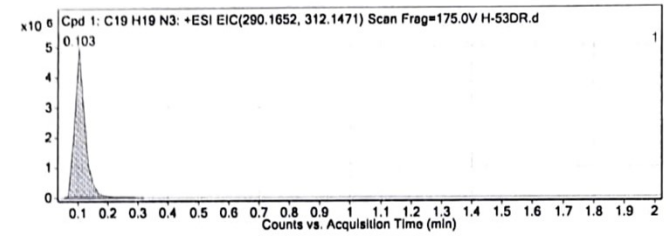
### Qualitative Compound Report

| | | | |
|---|---|---|---|
| Data File | H-53DR.d | Sample Name | H-53DR |
| Sample Type | Sample | Position | P1-B1 |
| Instrument Name | Instrument 1 | User Name | |
| Acq Method | MS Scan.m | Acquired Time | 30-08-2022 16:52:30 |
| IRM Calibration Status | [redacted] | DA Method | Default.m |
| Comment | | | |
| Sample Group | | Info. | 3 |
| Acquisition SW Version | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

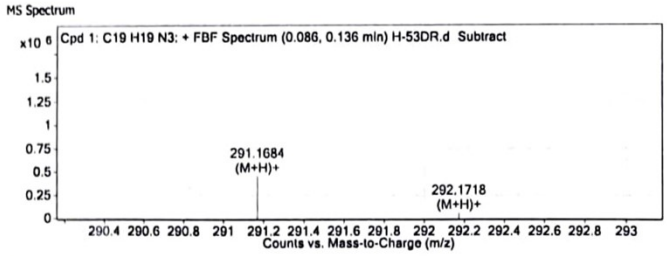
Compound Table

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C19 H19 N3 | 0.103 | 289.1577 | 1544325 | C19 H19 N3 | 289.1579 | -0.78 | C19 H19 N3 | C19 H19 N3 |

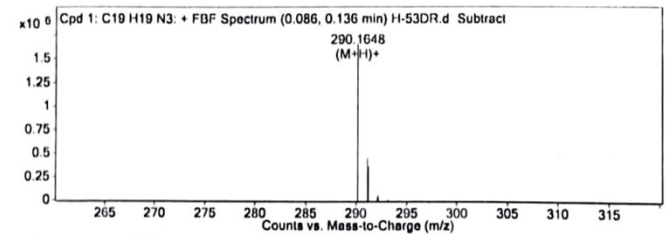
| Compound Label | m/z | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C19 H19 N3 | 290.1648 | 0.103 | Find By Formula | 289.1577 |




MS Spectrum




MS Zoomed Spectrum

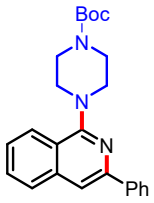



MS Spectrum Peak List

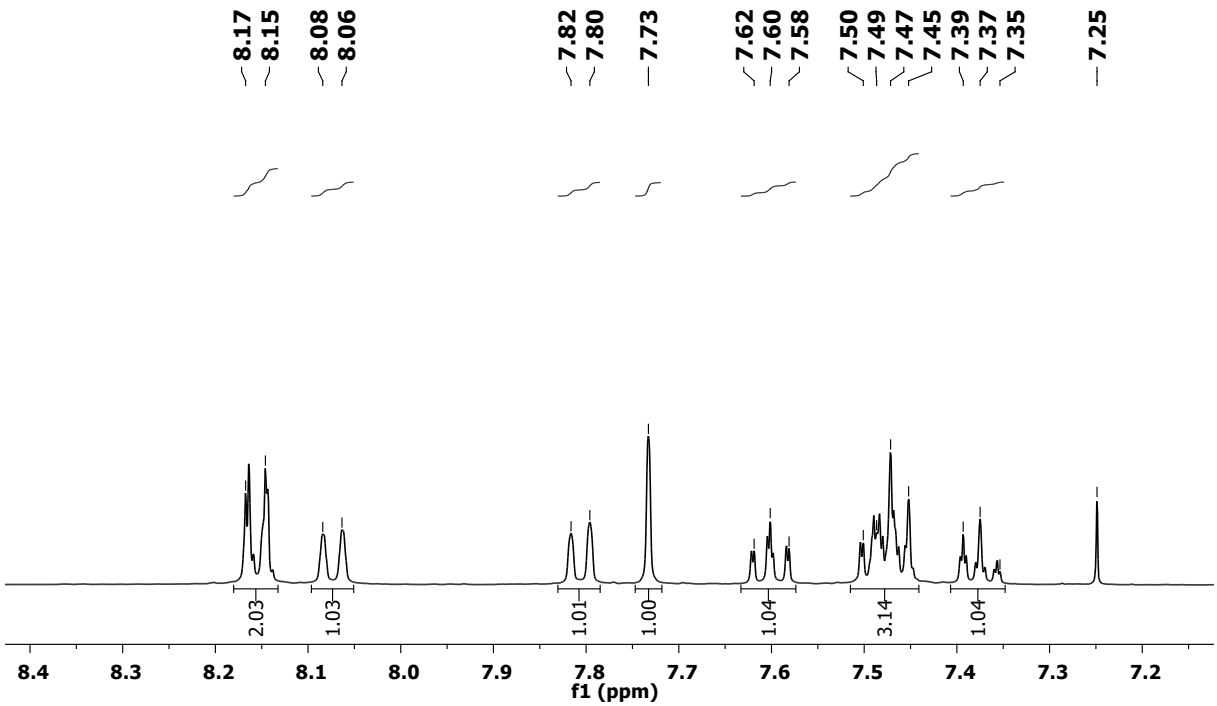
| m/z | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 290.1648 | 1 | 1544325.25 | C19H20N3 | (M+H)+ |
| 291.1684 | 1 | 452446.41 | C19H20N3 | (M+H)+ |
| 292.1718 | 1 | 57022.05 | C19H20N3 | (M+H)+ |
| 293.1753 | 1 | 13059.99 | C19H20N3 | (M+H)+ |

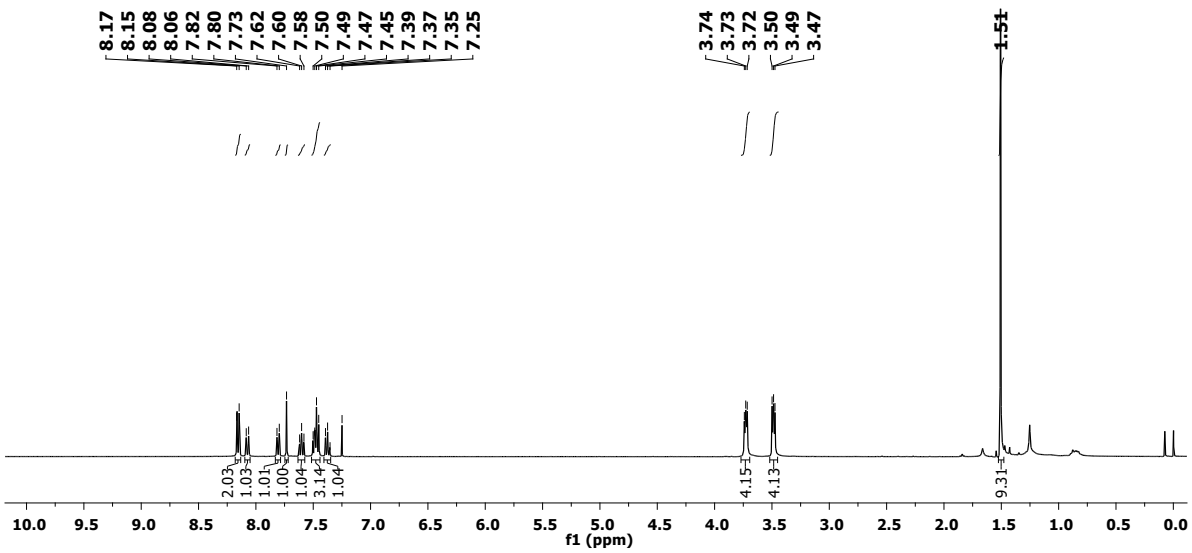
--- End Of Report ---

**$^1$H NMR** (400 MHz, $CDCl_3$)

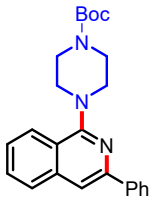



***tert*-butyl 4-(3-phenylisoquinolin-1-yl)piperazine-1-carboxylate (3d)**

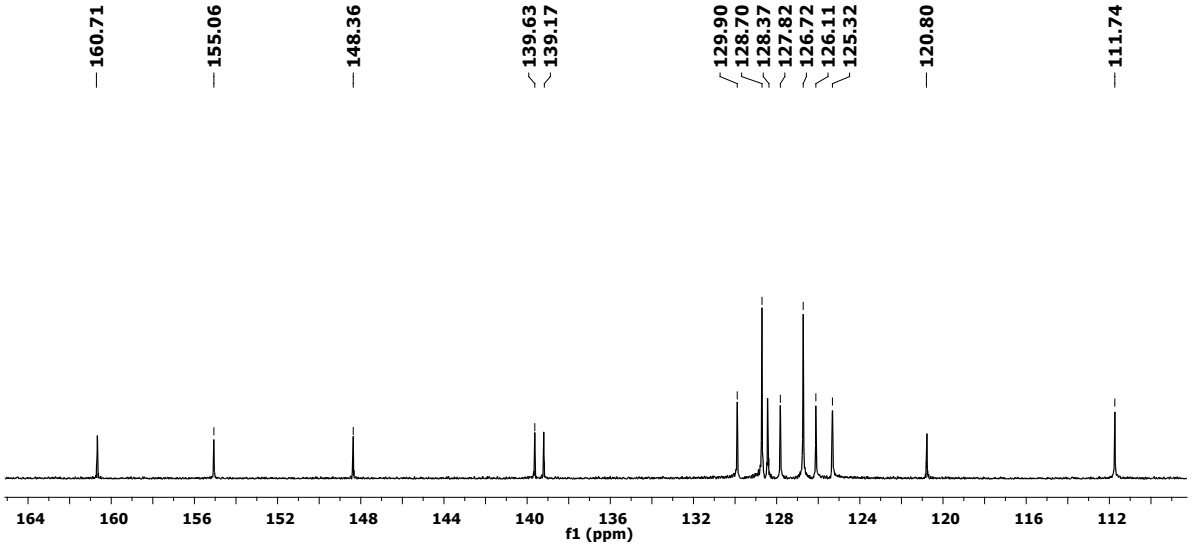


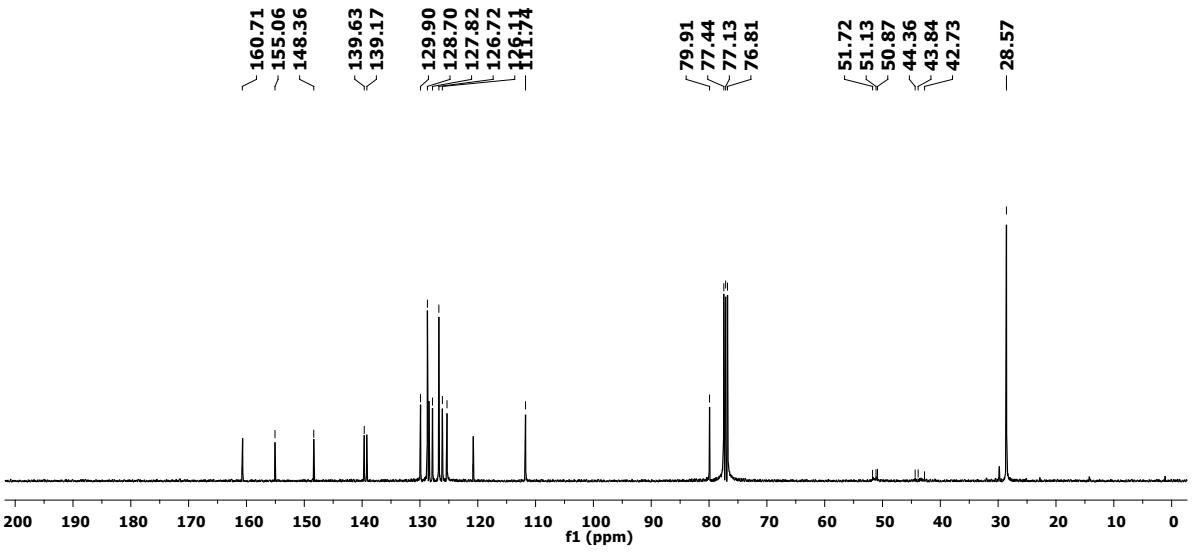



**$^{13}$C NMR** (100 MHz, $CDCl_3$)

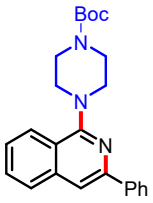



***tert*-butyl 4-(3-phenylisoquinolin-1-yl)piperazine-1-carboxylate (3d)**



## HRMS




### *tert*-butyl 4-(3-phenylisoquinolin-1-yl)piperazine-1-carboxylate (3d)

**Qualitative Compound Report**

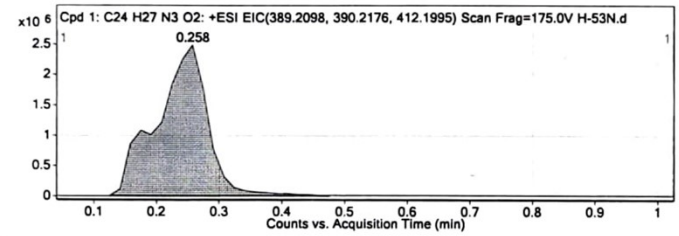
| | | | |
|---|---|---|---|
| **Data File** | H-53N.d | **Sample Name** | H-53N |
| **Sample Type** | Sample | **Position** | P1-A7 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | MS Scan.m | **Acquired Time** | 01-07-2022 12:42:08 |
| **IRM Calibration Status** | [redacted] | **DA Method** | Default.m |
| **Comment** | | | |

| | | | |
|---|---|---|---|
| **Sample Group** | | **Info.** | 3 |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

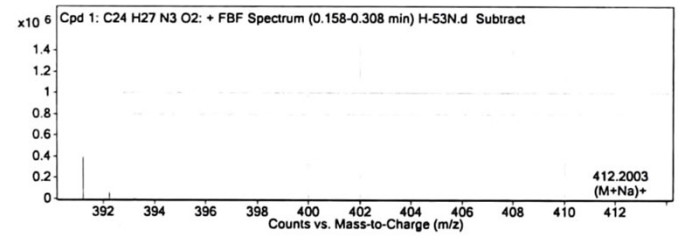
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C24 H27 N3 O2 | 0.258 | 389.2116 | 3831 | C24 H27 N3 O2 | 389.2103 | 3.16 | C24 H27 N3 O2 | C24 H27 N3 O2 |

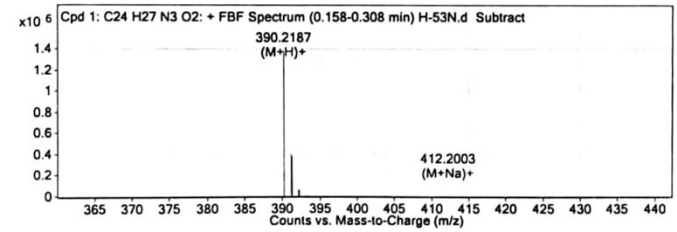
| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C24 H27 N3 O2 | 412.2003 | 0.258 | Find By Formula | 389.2116 |




MS Spectrum




MS Zoomed Spectrum

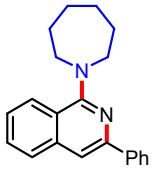



**MS Spectrum Peak List**

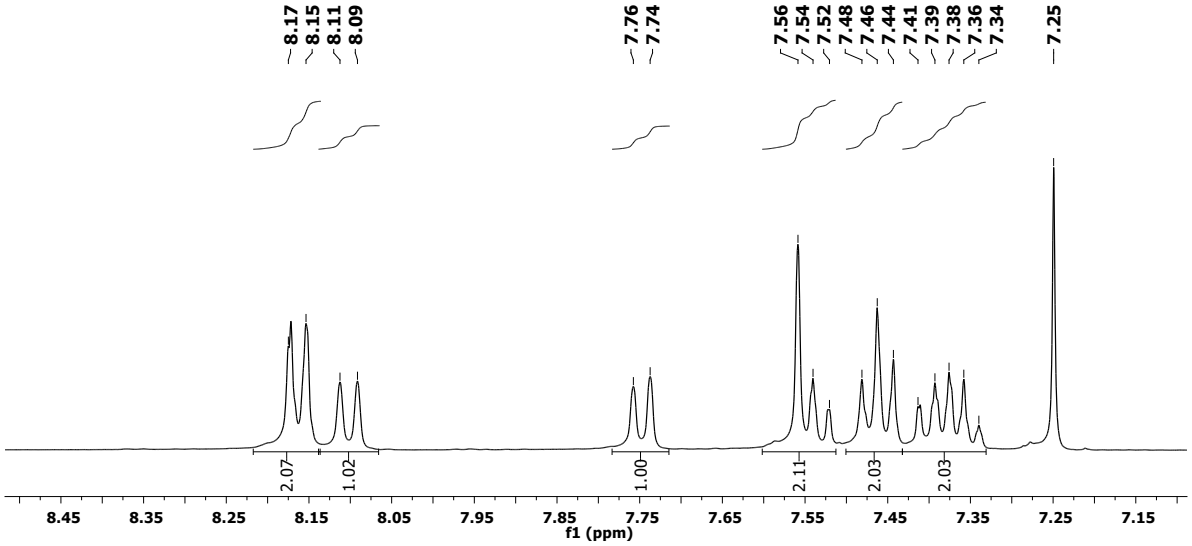
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 390.2187 | 1 | 1361597.75 | C24H28N3O2 | (M+H)+ |
| 391.2224 | 1 | 391633.38 | C24H28N3O2 | (M+H)+ |
| 392.2248 | 1 | 53034.19 | C24H28N3O2 | (M+H)+ |
| 393.2269 | 1 | 5462.49 | C24H28N3O2 | (M+H)+ |
| 412.2003 | 1 | 3831.38 | C24H27N3NaO2 | (M+Na)+ |
| 413.2033 | 1 | 1017.43 | C24H27N3NaO2 | (M+Na)+ |
| 414.2152 | 1 | 39.03 | C24H27N3NaO2 | (M+Na)+ |

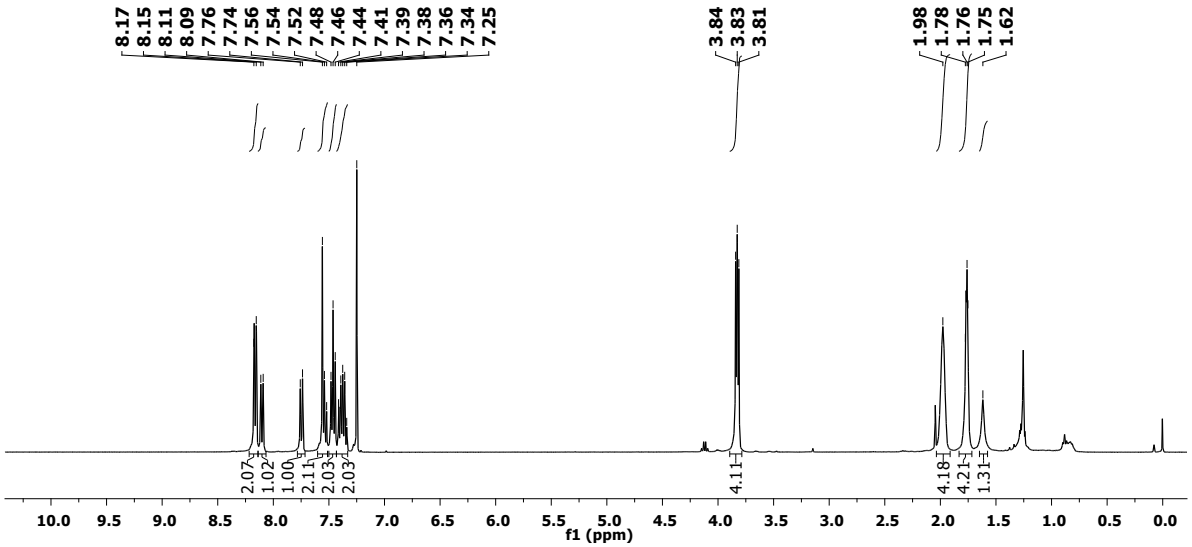
--- End Of Report ---

**$^1$H NMR** (400 MHz, $CDCl_3$)

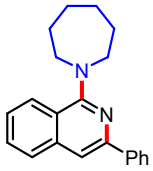



**1-(azepan-1-yl)-3-phenylisoquinoline (3e)**

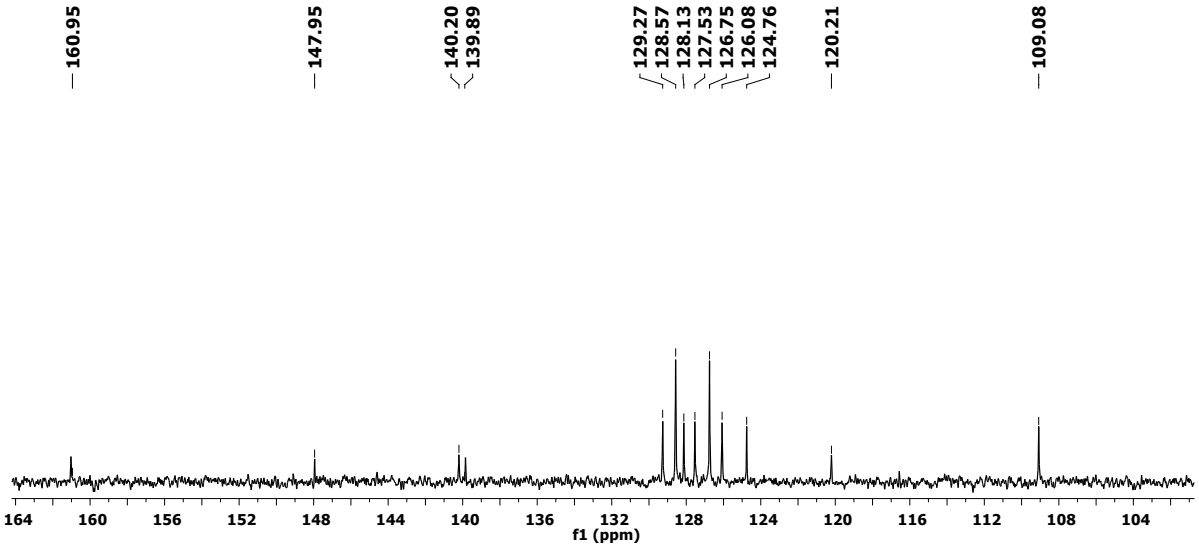


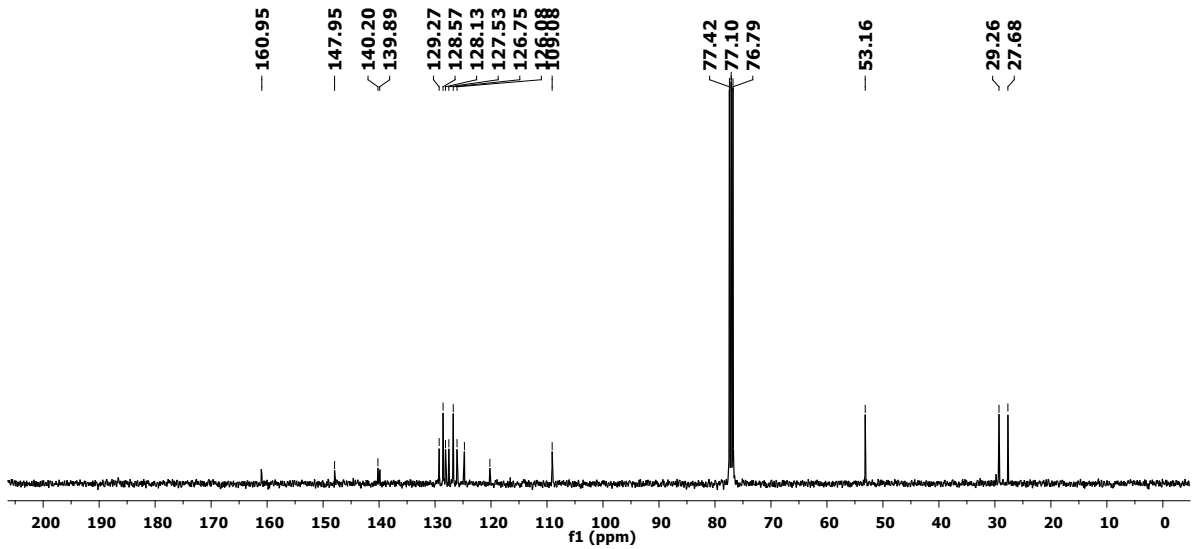



**$^{13}$C NMR** (100 MHz, $CDCl_3$)

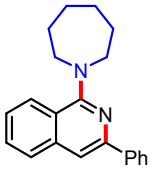



**1-(azepan-1-yl)-3-phenylisoquinoline (3e)**



# HRMS




## 1-(azepan-1-yl)-3-phenylisoquinoline (3e)

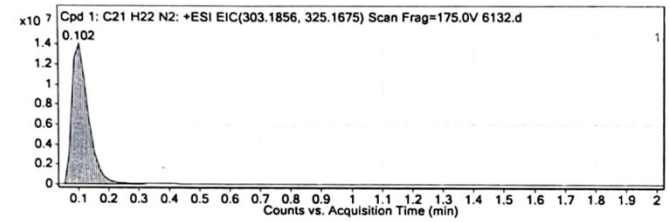
### Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | 6132.d | **Sample Name** | 6132 |
| **Sample Type** | Sample | **Position** | P1-D1 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | MS Scan.m | **Acquired Time** | 22-08-2022 14:36:47 |
| **IRM Calibration Status** | [redacted] | **DA Method** | Default.m |
| **Comment** | | | |
| **Sample Group** | | **Info.** | 3 |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

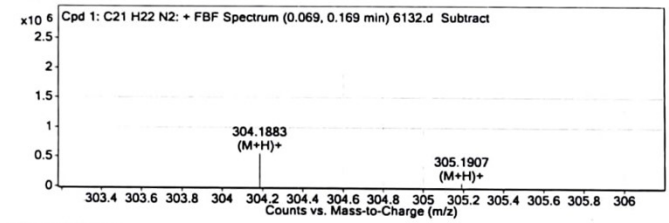
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C21 H22 N2 | 0.102 | 302.1778 | 2284044 | C21 H22 N2 | 302.1783 | -1.6 | C21 H22 N2 | C21 H22 N2 |

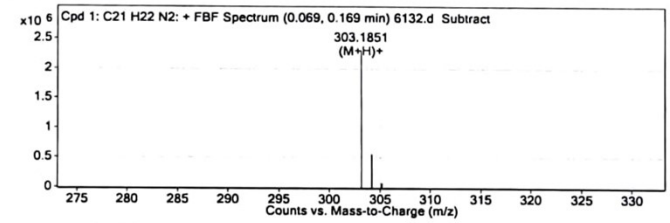
| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C21 H22 N2 | 303.1851 | 0.102 | Find By Formula | 302.1778 |




MS Spectrum




MS Zoomed Spectrum

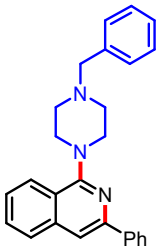



**MS Spectrum Peak List**

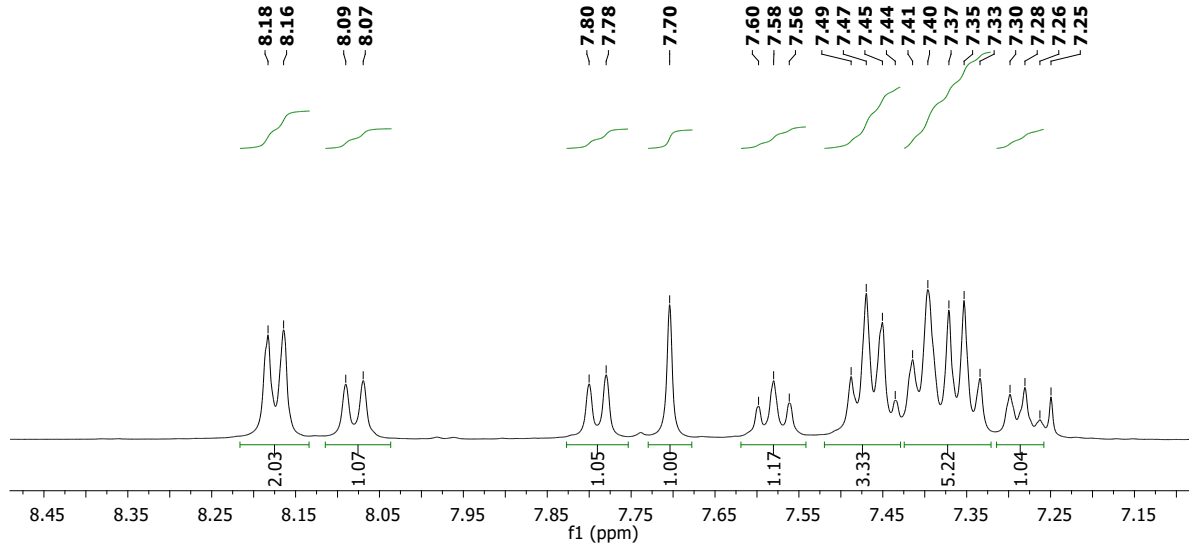
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 303.1851 | 1 | 2284043.75 | C21H23N2 | (M+H)+ |
| 304.1883 | 1 | 560925.31 | C21H23N2 | (M+H)+ |
| 305.1907 | 1 | 65679.25 | C21H23N2 | (M+H)+ |
| 306.1939 | 1 | 4839.15 | C21H23N2 | (M+H)+ |

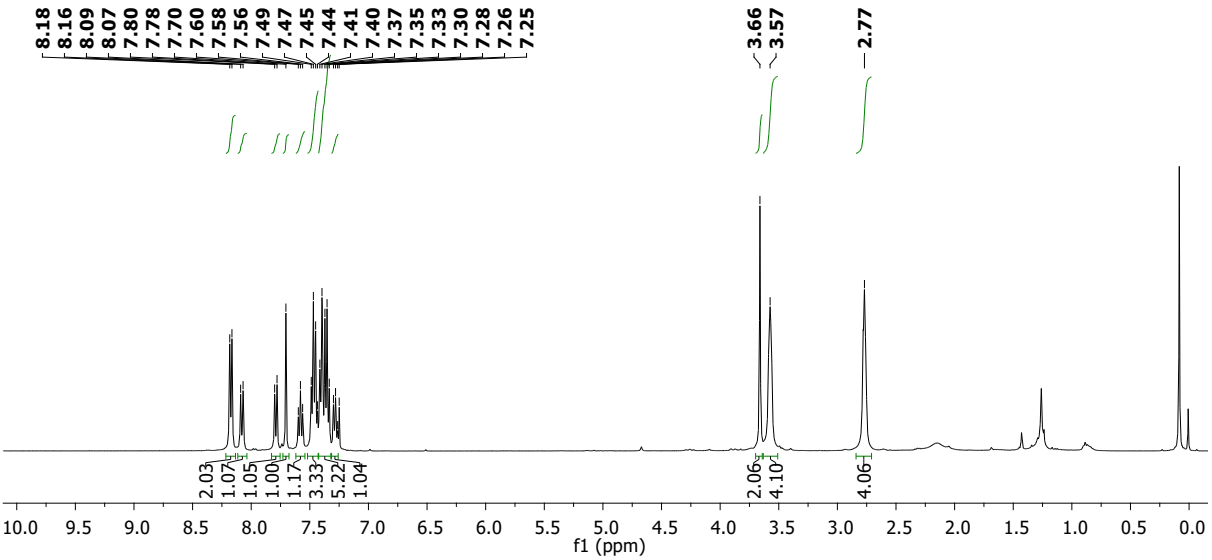
--- End Of Report ---

**$^1$H NMR** (400Hz, $CDCl_3$)

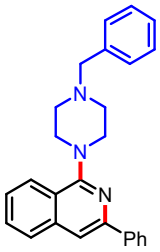



**1-(4-benzylpiperazin-1-yl)-3-phenylisoquinoline (3f)**

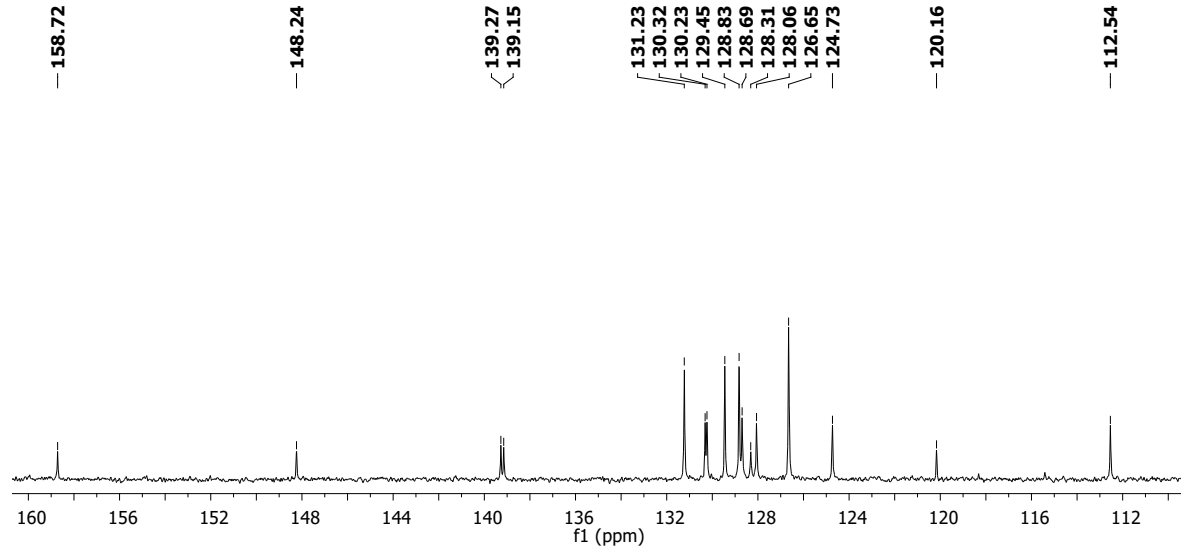


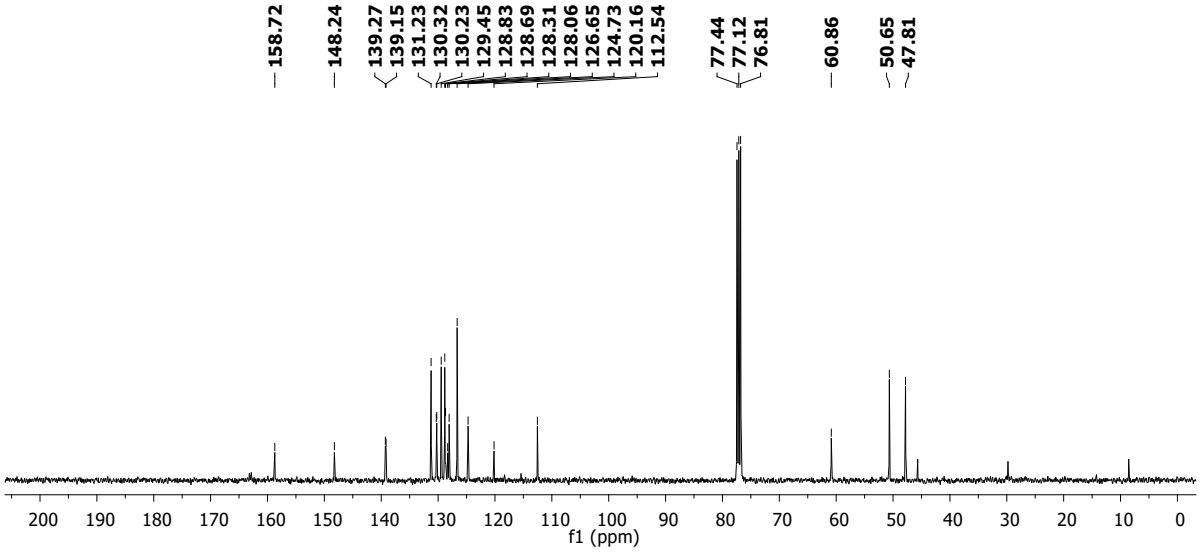



**$^{13}$C NMR** (100 MHz, $CDCl_3$)

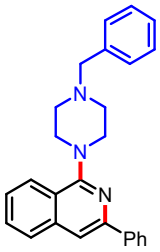



**1-(4-benzylpiperazin-1-yl)-3-phenylisoquinoline (3f)**



## HRMS




### 1-(4-benzylpiperazin-1-yl)-3-phenylisoquinoline (3f)

**Qualitative Compound Report**

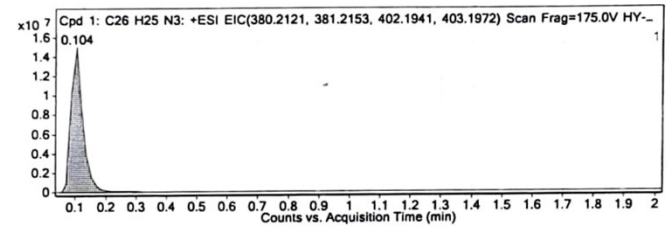
| | | | |
|---|---|---|---|
| **Data File** | HY-36R.d | **Sample Name** | HY-36R |
| **Sample Type** | Sample | **Position** | P1-A9 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | MS Scan.m | **Acquired Time** | 30-08-2022 16:49:41 |
| **IRM Calibration Status** | [redacted] | **DA Method** | Default.m |
| **Comment** | | | |

| | | | |
|---|---|---|---|
| **Sample Group** | | **Info.** | 3 |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

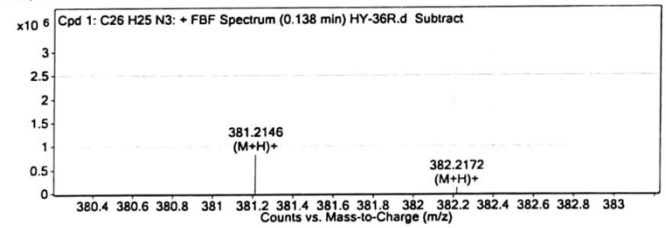
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C26 H25 N3 | 0.104 | 379.2039 | 2948794 | C26 H25 N3 | 379.2048 | -2.58 | C26 H25 N3 | C26 H25 N3 |

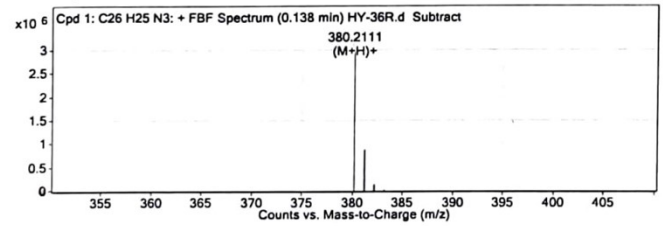
| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C26 H25 N3 | 380.2111 | 0.104 | Find By Formula | 379.2039 |




MS Spectrum




MS Zoomed Spectrum

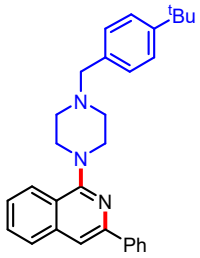



**MS Spectrum Peak List**

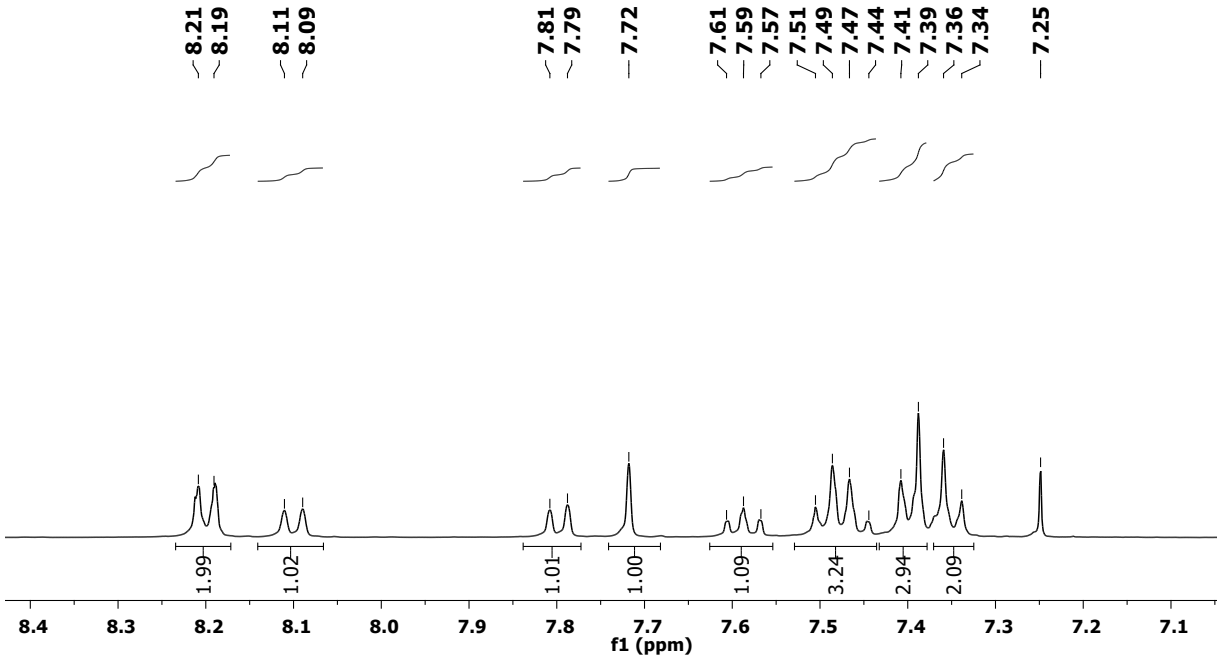
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 380.2111 | 1 | 2948793.5 | C26H26N3 | (M+H)+ |
| 381.2146 | 1 | 831593.75 | C26H26N3 | (M+H)+ |
| 382.2172 | 1 | 120175.98 | C26H26N3 | (M+H)+ |
| 383.2205 | 1 | 10399.29 | C26H26N3 | (M+H)+ |

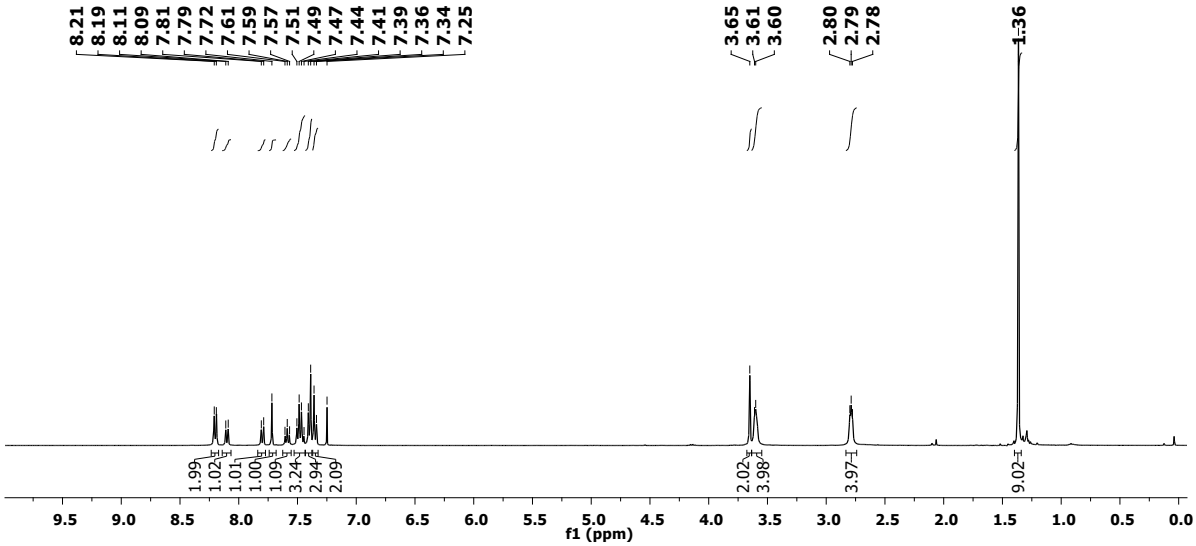
--- End Of Report ---

**$^1$H NMR** (400 MHz, $CDCl_3$)

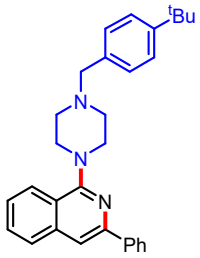



**1-(4-(4-(tert-butyl)benzyl)piperazin-1-yl)-3-phenylisoquinoline (3g)**

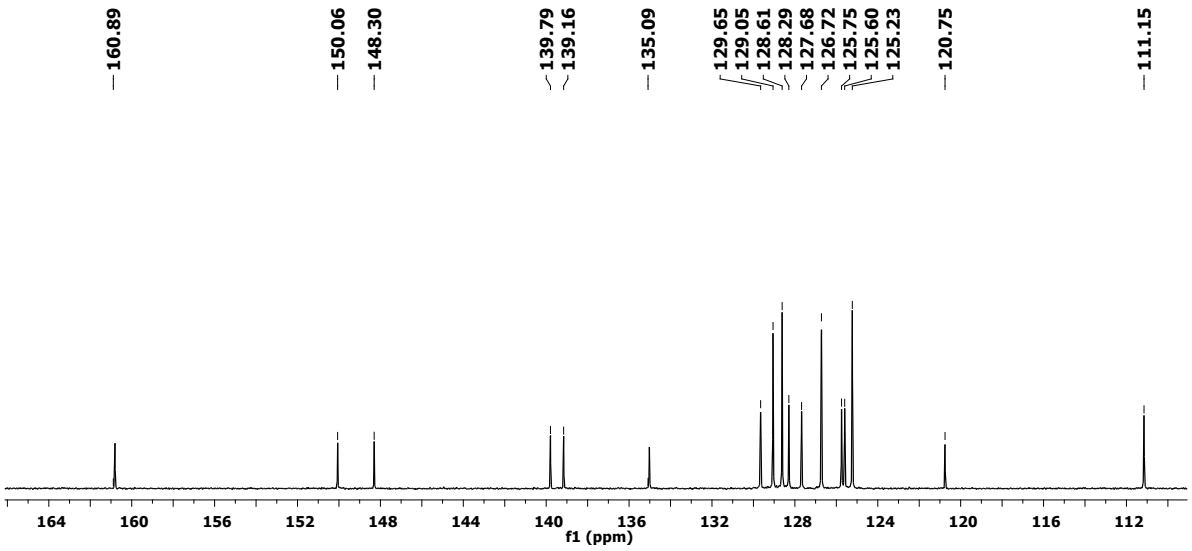


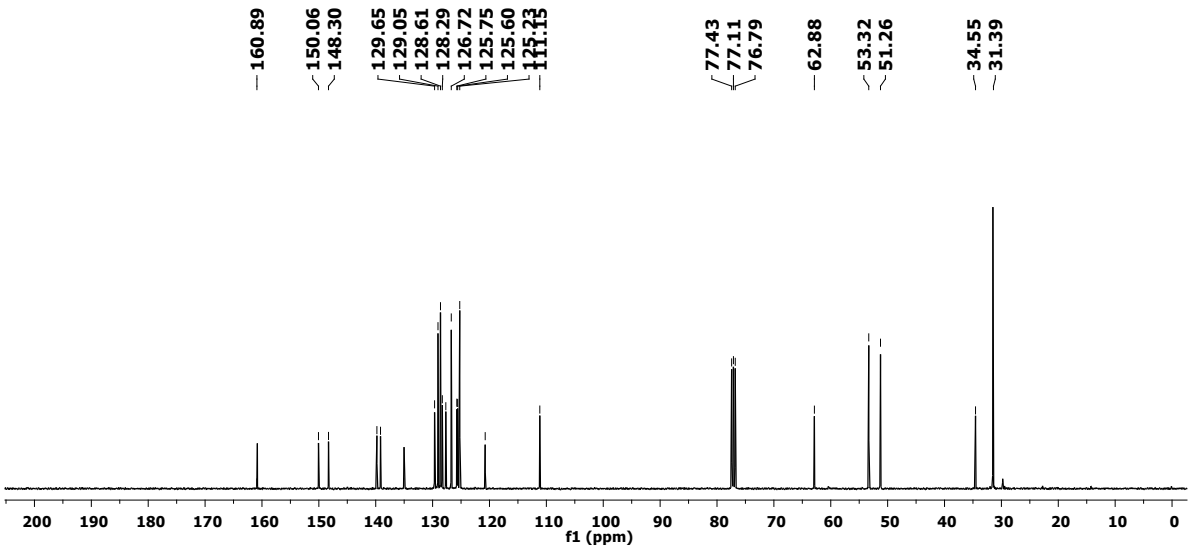



**$^{13}$C NMR** (100 MHz, $CDCl_3$)

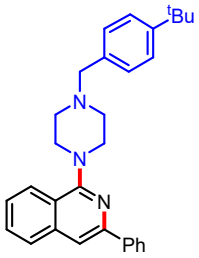



**1-(4-(4-(tert-butyl)benzyl)piperazin-1-yl)-3-phenylisoquinoline (3g)**



## HRMS




**1-(4-(4-(tert-butyl)benzyl)piperazin-1-yl)-3-phenylisoquinoline (3g)**

### Qualitative Compound Report

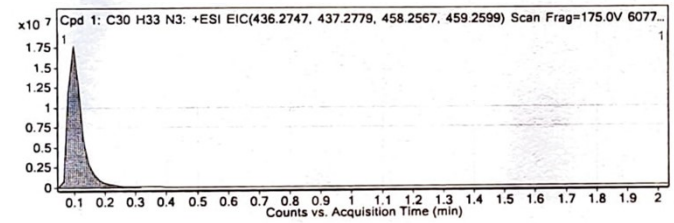
| | | | |
|---|---|---|---|
| **Data File** | 6077.d | **Sample Name** | 6077 |
| **Sample Type** | Sample | **Position** | P1-C6 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | MS Scan.m | **Acquired Time** | 22-08-2022 14:25:44 |
| **IRM Calibration Status** | [redacted] | **DA Method** | Default.m |
| **Comment** | | | |

| | | | |
|---|---|---|---|
| **Sample Group** | | **Info.** | 3 |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

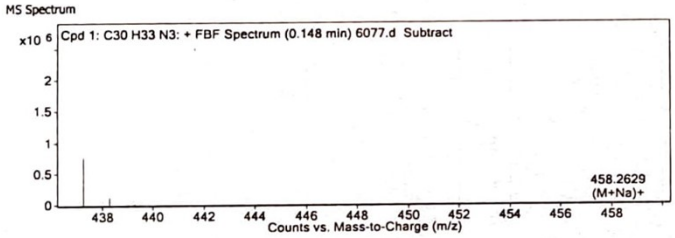
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C30 H33 N3 | 0.098 | 435.2666 | 2188516 | C30 H33 N3 | 435.2674 | -2.05 | C30 H33 N3 | C30 H33 N3 |

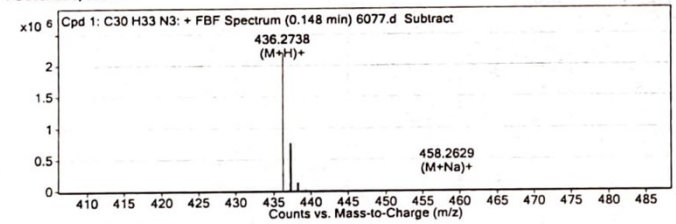
| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C30 H33 N3 | 436.2738 | 0.098 | Find By Formula | 435.2666 |




MS Spectrum




MS Zoomed Spectrum

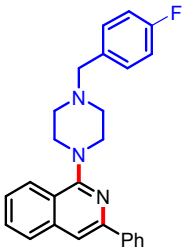



**MS Spectrum Peak List**

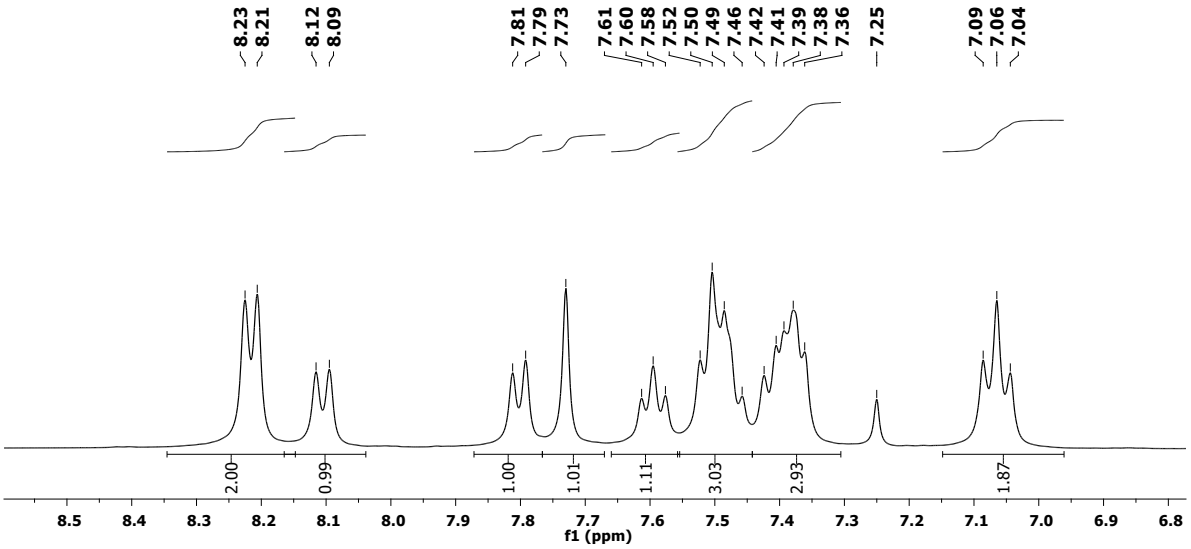
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 436.2738 | 1 | 2188516.25 | C30H34N3 | (M+H)+ |
| 437.2772 | 1 | 760565.63 | C30H34N3 | (M+H)+ |
| 438.2795 | 1 | 118899.78 | C30H34N3 | (M+H)+ |
| 439.2812 | 1 | 11713.95 | C30H34N3 | (M+H)+ |
| 458.2629 | 1 | 1800.7 | C30H33N3Na | (M+Na)+ |
| 459.2656 | 1 | 1020.73 | C30H33N3Na | (M+Na)+ |
| 460.2706 | 1 | 491.23 | C30H33N3Na | (M+Na)+ |

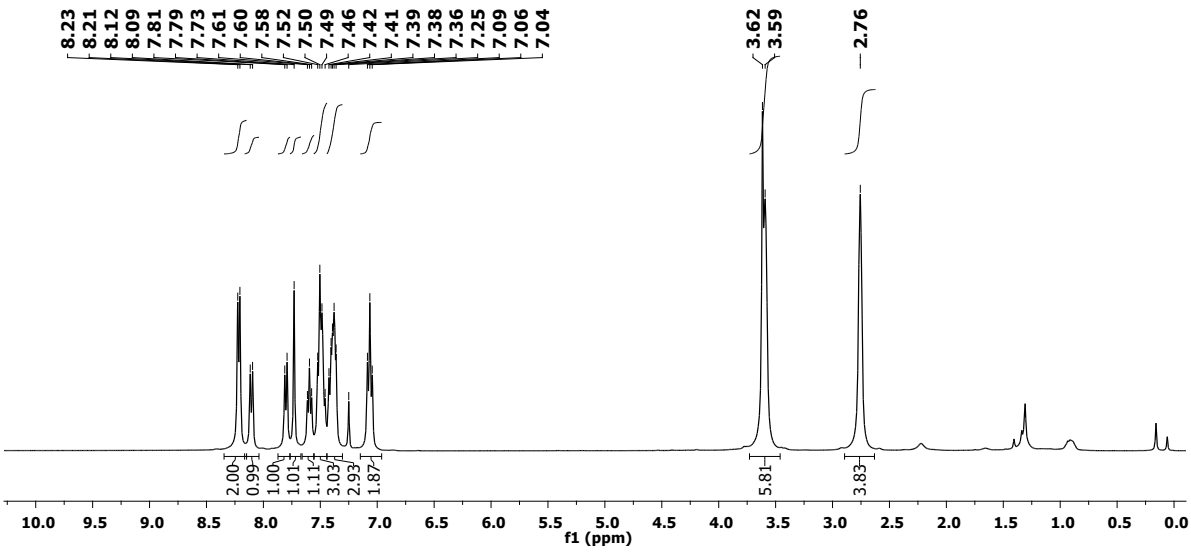
--- End Of Report ---

**$^1$H NMR** (400 MHz, $CDCl_3$)

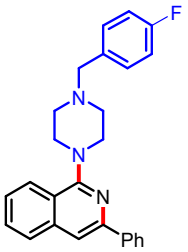



**1-(4-(4-fluorobenzyl)piperazin-1-yl)-3-phenylisoquinoline (3h)**

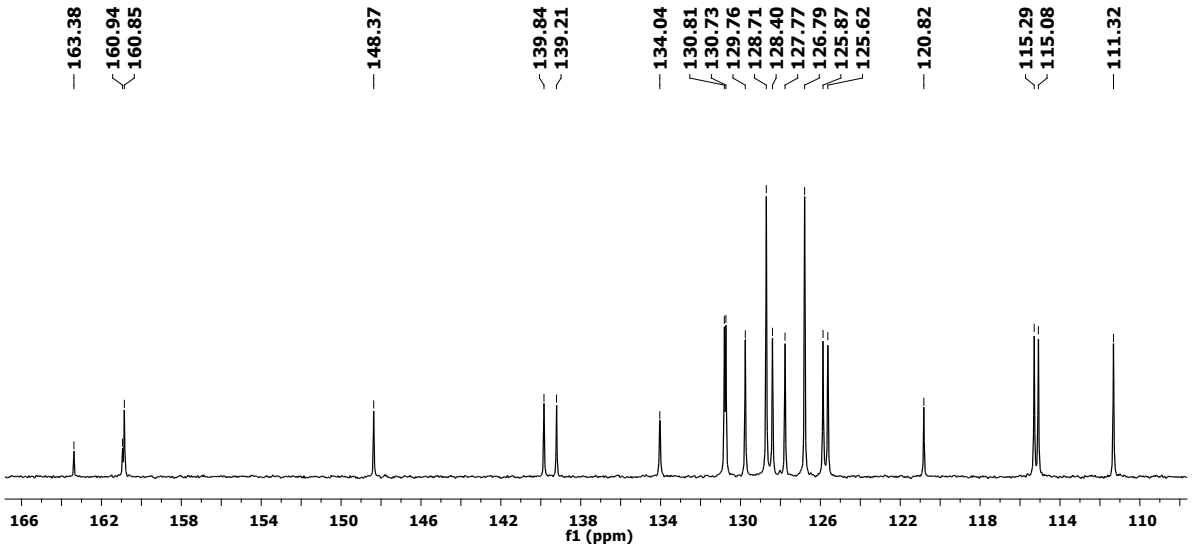


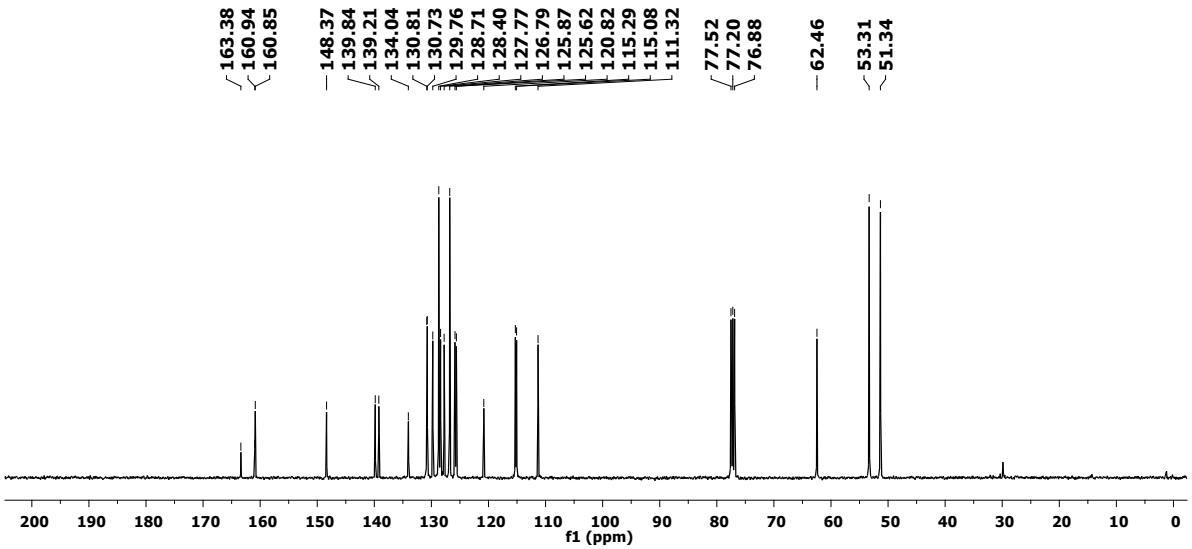



**$^{13}$C NMR** (100 MHz, $CDCl_3$)

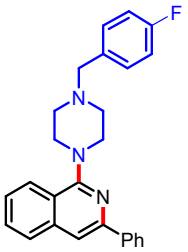



**1-(4-(4-fluorobenzyl)piperazin-1-yl)-3-phenylisoquinoline (3h)**



## HRMS




**1-(4-(4-fluorobenzyl)piperazin-1-yl)-3-phenylisoquinoline (3h)**

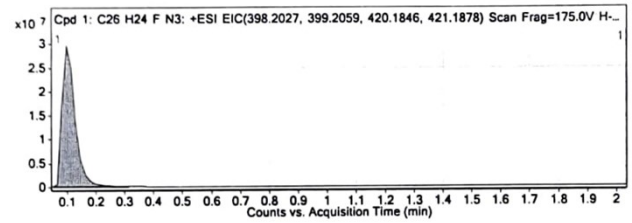
### Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | H-39R.d | **Sample Name** | H-39R |
| **Sample Type** | Sample | **Position** | P1-A8 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | MS Scan.m | **Acquired Time** | 30-08-2022 16:46:59 |
| **IRM Calibration Status** | [redacted] | **DA Method** | Default.m |
| **Comment** | | | |
| **Sample Group** | | **Info.** | 3 |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

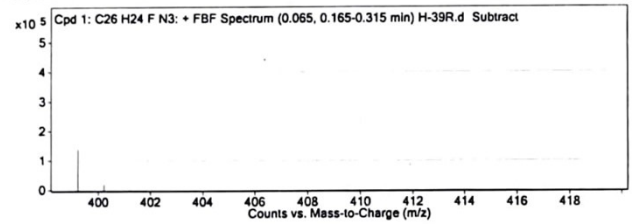
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C26 H24 F N3 | 0.098 | 397.1944 | 463372 | C26 H24 F N3 | 397.1954 | -2.64 | C26 H24 F N3 | C26 H24 F N3 |

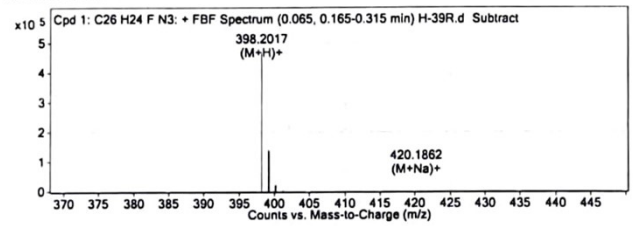
| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C26 H24 F N3 | 398.2017 | 0.098 | Find By Formula | 397.1944 |




MS Spectrum




MS Zoomed Spectrum

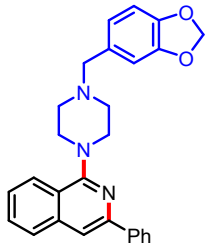



**MS Spectrum Peak List**

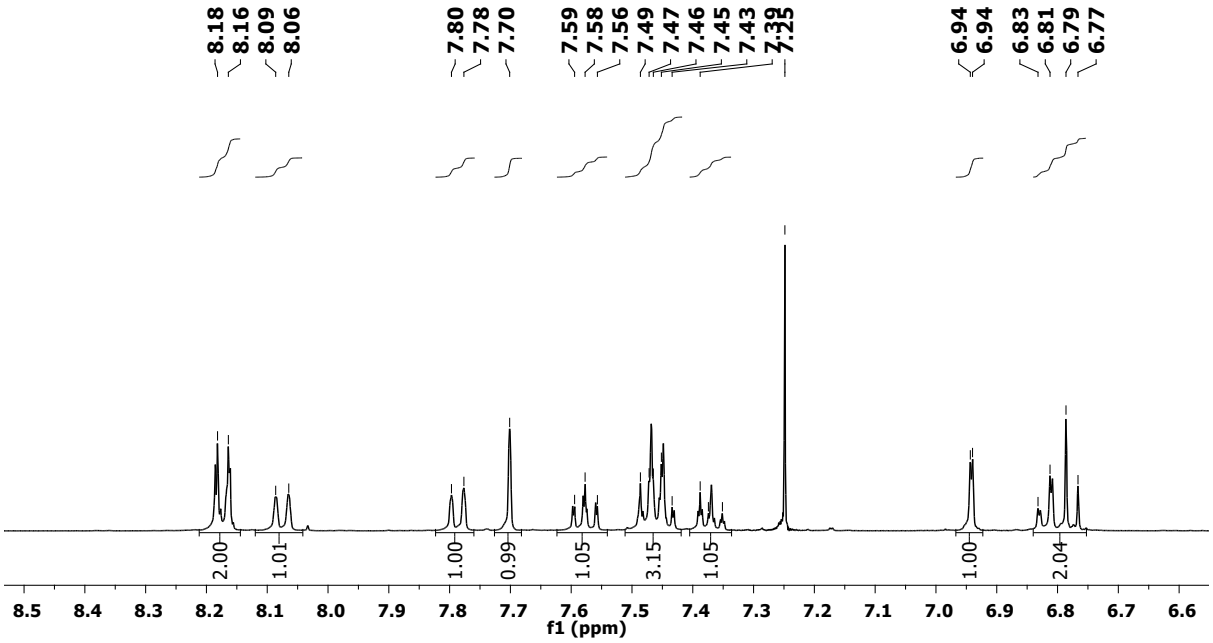
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 398.2017 | 1 | 463371.69 | C26H25FN3 | (M+H)+ |
| 399.2047 | 1 | 138103.36 | C26H25FN3 | (M+H)+ |
| 400.2075 | 1 | 18817.73 | C26H25FN3 | (M+H)+ |
| 401.2123 | 1 | 2120.09 | C26H25FN3 | (M+H)+ |
| 420.1862 | 1 | 295.66 | C26H24FN3Na | (M+Na)+ |

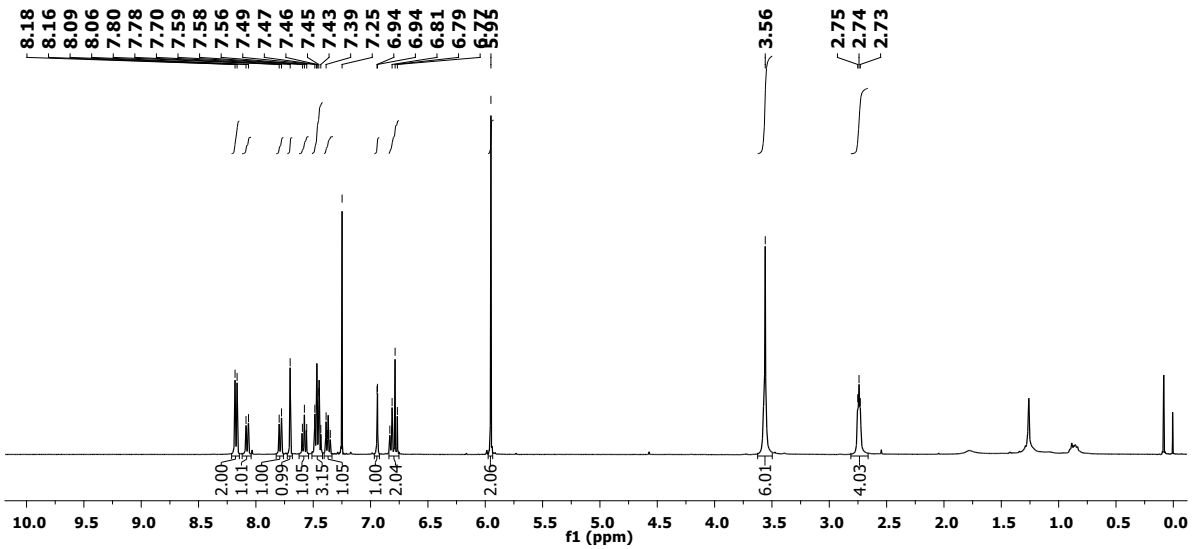
--- End Of Report ---

**$^1$H NMR** (400 MHz, $CDCl_3$)

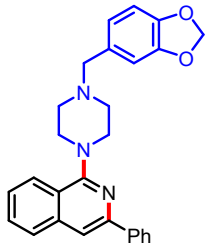



**1-(4-(benzo[d][1,3]dioxol-5-ylmethyl)piperazin-1-yl)-3-phenylisoquinoline(3i)**

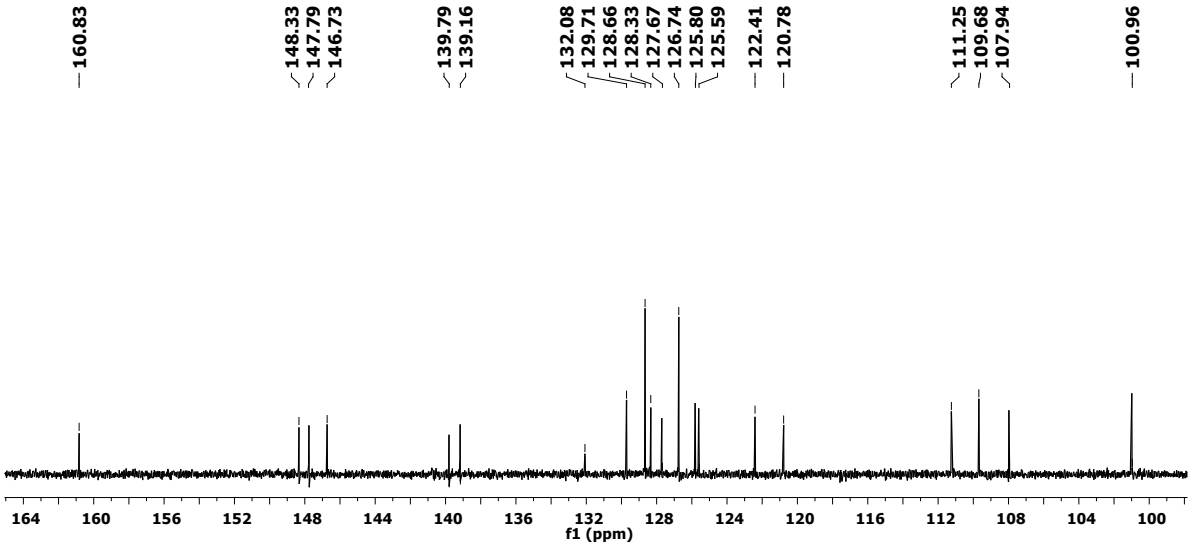


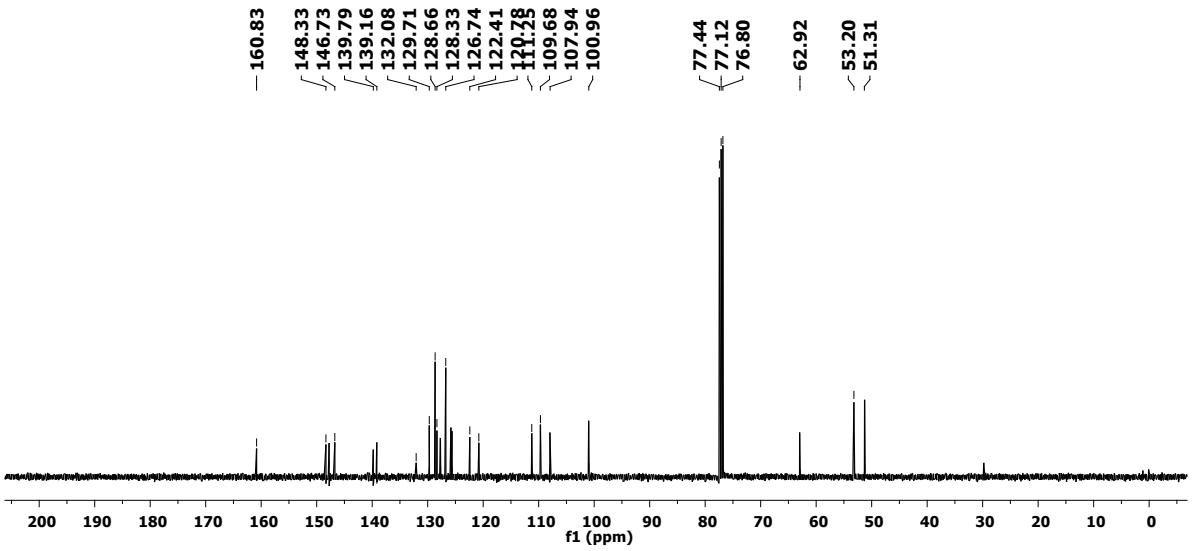



**$^{13}$C NMR** (100 MHz, $CDCl_3$)

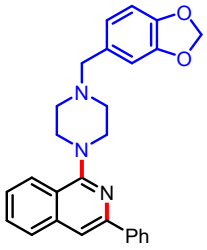



**1-(4-(benzo[d][1,3]dioxol-5-ylmethyl)piperazin-1-yl)-3-phenylisoquinoline(3i)**



## HRMS




**1-(4-(benzo[d][1,3]dioxol-5-ylmethyl)piperazin-1-yl)-3-phenylisoquinoline(3i)**

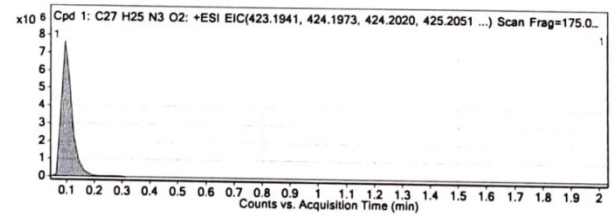
### Qualitative Compound Report

| | | | |
|---|---|---|---|
| Data File | 6010.d | Sample Name | 6010 |
| Sample Type | Sample | Position | P1-A5 |
| Instrument Name | Instrument 1 | User Name | |
| Acq Method | MS Scan.m | Acquired Time | 27-08-2022 12:12:45 |
| IRM Calibration Status | [redacted] | DA Method | Default.m |
| Comment | | | |
| Sample Group | | Info. | 3 |
| Acquisition SW Version | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

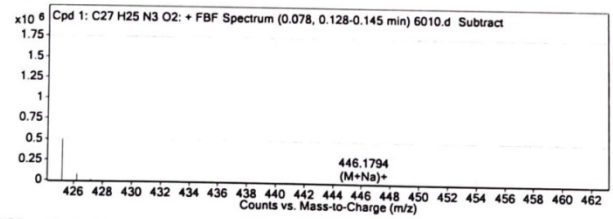
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C27 H25 N3 O2 | 0.095 | 423.1951 | 1594025 | C27 H25 N3 O2 | 423.1947 | 0.95 | C27 H25 N3 O2 | C27 H25 N3 O2 |

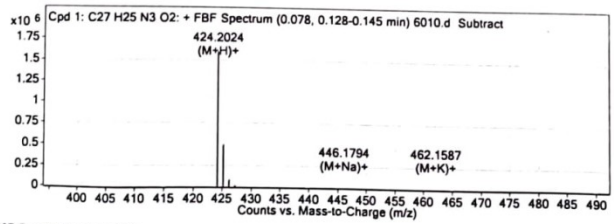
| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C27 H25 N3 O2 | 424.2024 | 0.095 | Find By Formula | 423.1951 |




MS Spectrum



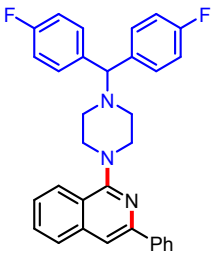

MS Zoomed Spectrum



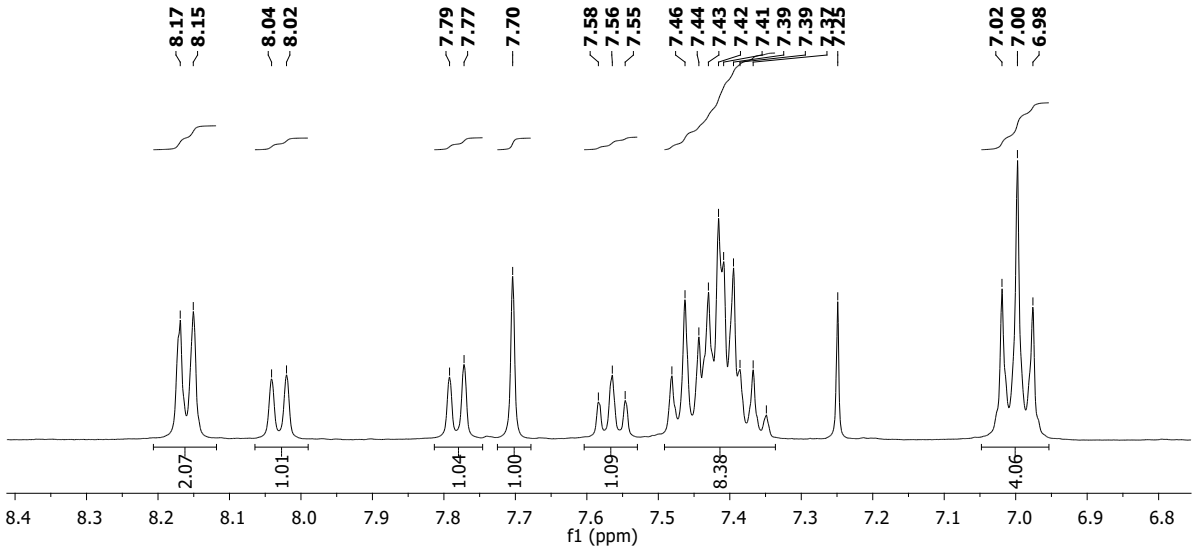

**MS Spectrum Peak List**

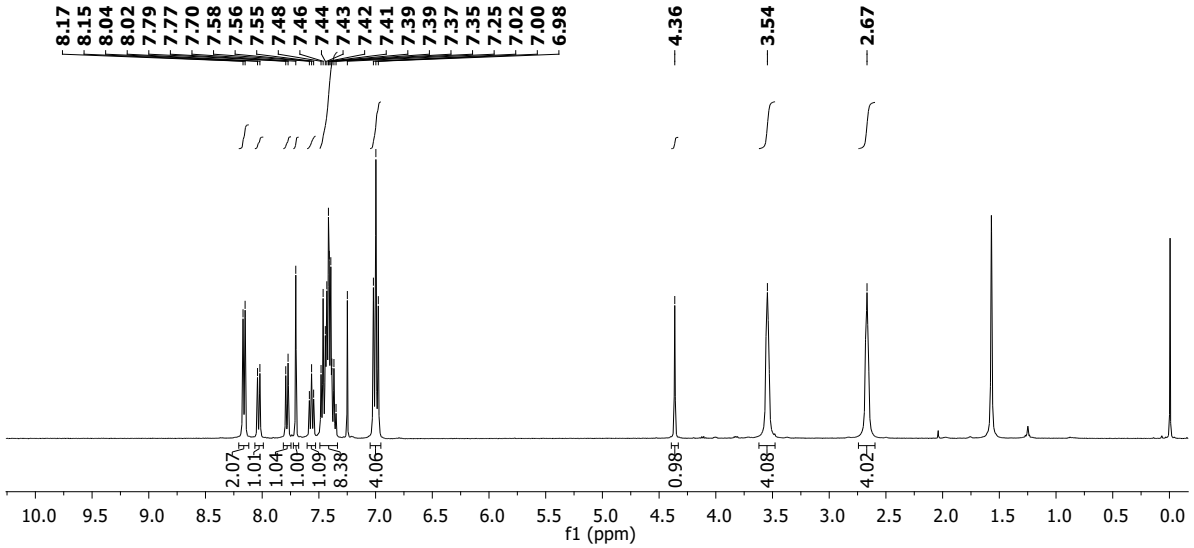
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 424.2024 | 1 | 1594024.63 | C27H26N3O2 | (M+H)+ |
| 425.2056 | 1 | 495776 | C27H26N3O2 | (M+H)+ |
| 426.2077 | 1 | 74889.41 | C27H26N3O2 | (M+H)+ |
| 427.2102 | 1 | 8239.72 | C27H26N3O2 | (M+H)+ |
| 428.2176 | 1 | 1482.33 | C27H26N3O2 | (M+H)+ |
| 446.1794 | 1 | 1443.79 | C27H25N3NaO2 | (M+Na)+ |
| 447.1866 | 1 | 706.86 | C27H25N3NaO2 | (M+Na)+ |
| 448.1936 | 1 | 350.7 | C27H25N3NaO2 | (M+Na)+ |
| 462.1587 | 1 | 3485.6 | C27H25KN3O2 | (M+K)+ |
| 463.1517 | 1 | 1138.13 | C27H25KN3O2 | (M+K)+ |

**$^1$H NMR** (400 MHz, $CDCl_3$)

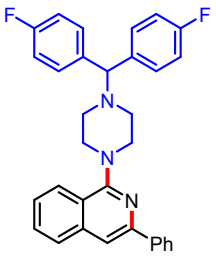



**1-(4-(bis(4-fluorophenyl)methyl)piperazin-1-yl)-3-phenylisoquinoline (3j)**

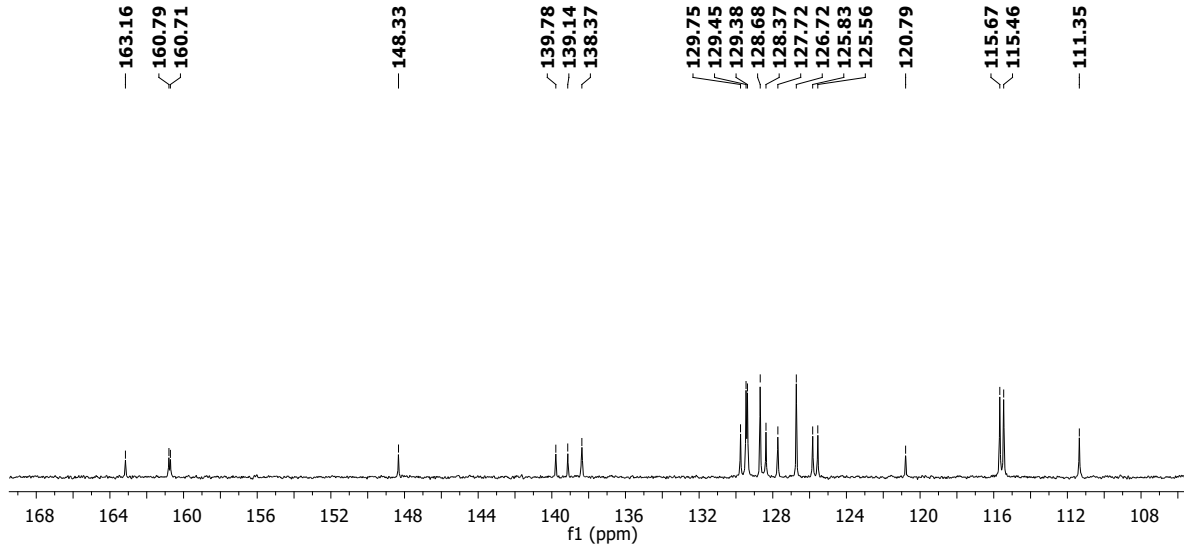


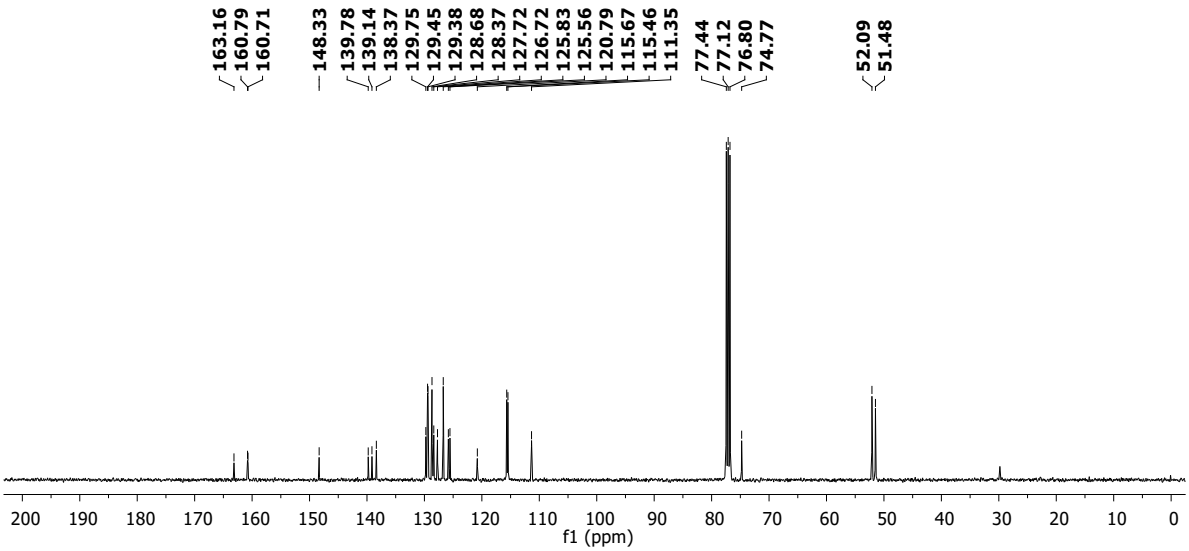



**$^{13}$C NMR** (100 MHz, $CDCl_3$)

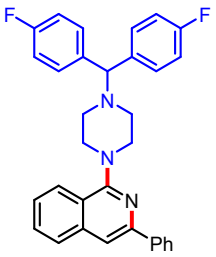



**1-(4-(bis(4-fluorophenyl)methyl)piperazin-1-yl)-3-phenylisoquinoline (3j)**



# HRMS




## 1-(4-(bis(4-fluorophenyl)methyl)piperazin-1-yl)-3-phenylisoquinoline (3j)

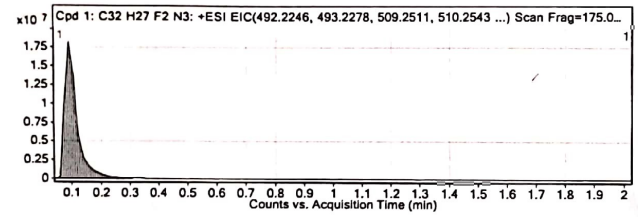
### Qualitative Compound Report

| | | | |
|---|---|---|---|
| Data File | 6131.d | Sample Name | 6131 |
| Sample Type | Sample | Position | P1-A7 |
| Instrument Name | Instrument 1 | User Name | |
| Acq Method | MS Scan.m | Acquired Time | 16-08-2022 15:07:10 |
| IRM Calibration Status | Success | DA Method | Default.m |
| Comment | | | |
| Sample Group | | Info. | 3 |
| Acquisition SW Version | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

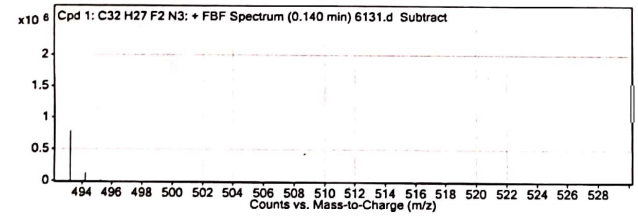
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C32 H27 F2 N3 | 0.09 | 491.217 | 2094277 | C32 H27 F2 N3 | 491.2173 | -0.53 | C32 H27 F2 N3 | C32 H27 F2 N3 |

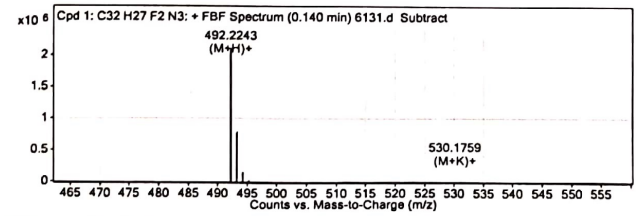
| Compound Label | m/z | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C32 H27 F2 N3 | 492.2243 | 0.09 | Find By Formula | 491.217 |




MS Spectrum




MS Zoomed Spectrum

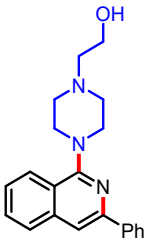



**MS Spectrum Peak List**

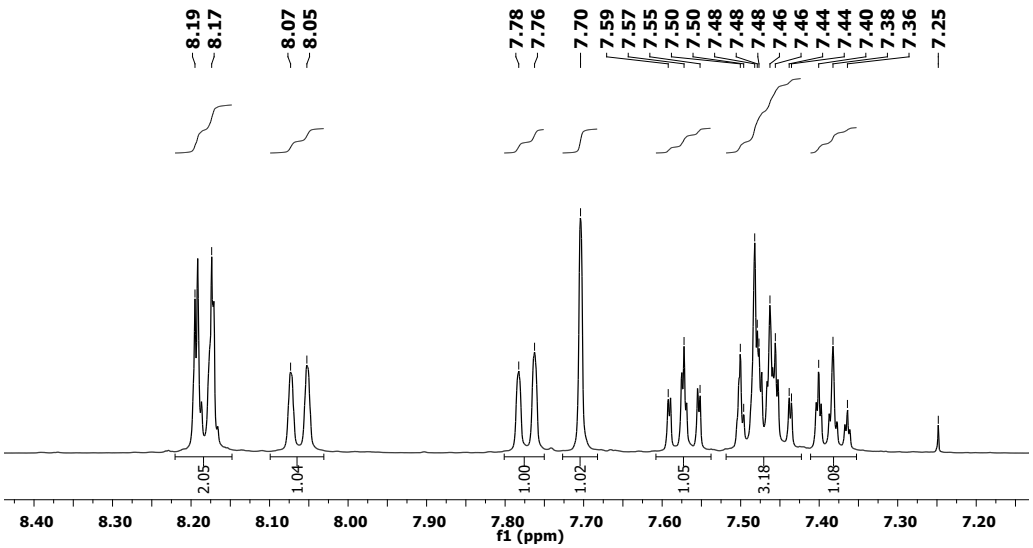
| m/z | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 492.2243 | 1 | 2094277.13 | C32H28F2N3 | (M+H)+ |
| 493.2277 | 1 | 792727.81 | C32H28F2N3 | (M+H)+ |
| 494.2304 | 1 | 127369.35 | C32H28F2N3 | (M+H)+ |
| 495.2326 | 1 | 15063.14 | C32H28F2N3 | (M+H)+ |
| 496.2368 | 1 | 1404.23 | C32H28F2N3 | (M+H)+ |
| 530.1759 | 1 | 346.01 | C32H27F2KN3 | (M+K)+ |

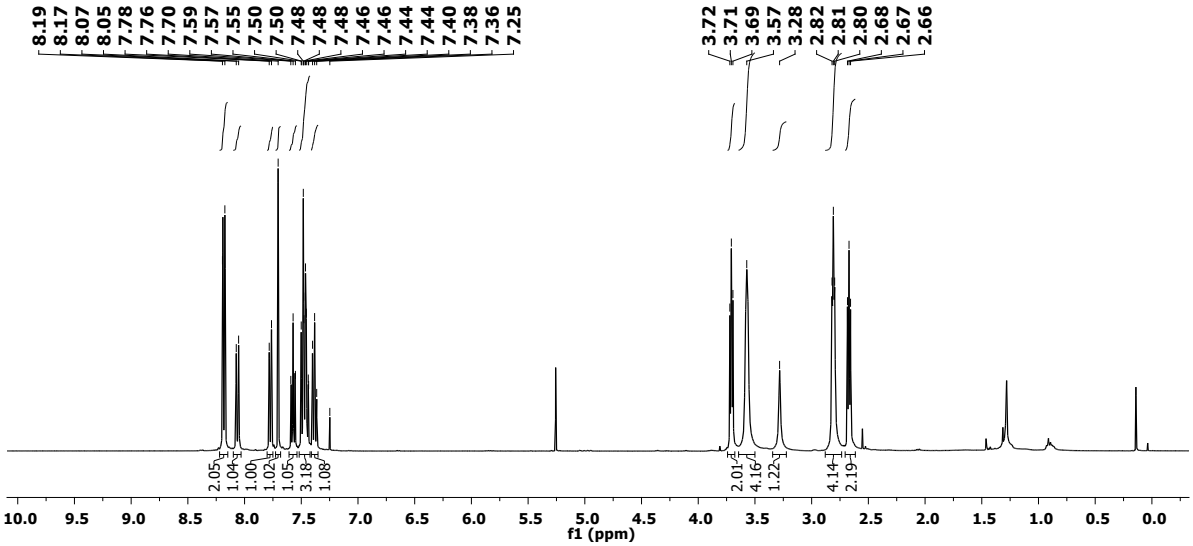
--- End Of Report ---

**$^1$H NMR** (400 MHz, $CDCl_3$)

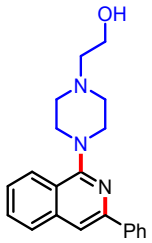



**2-(4-(3-phenylisoquinolin-1-yl)piperazin-1-yl)ethan-1-ol (3k)**

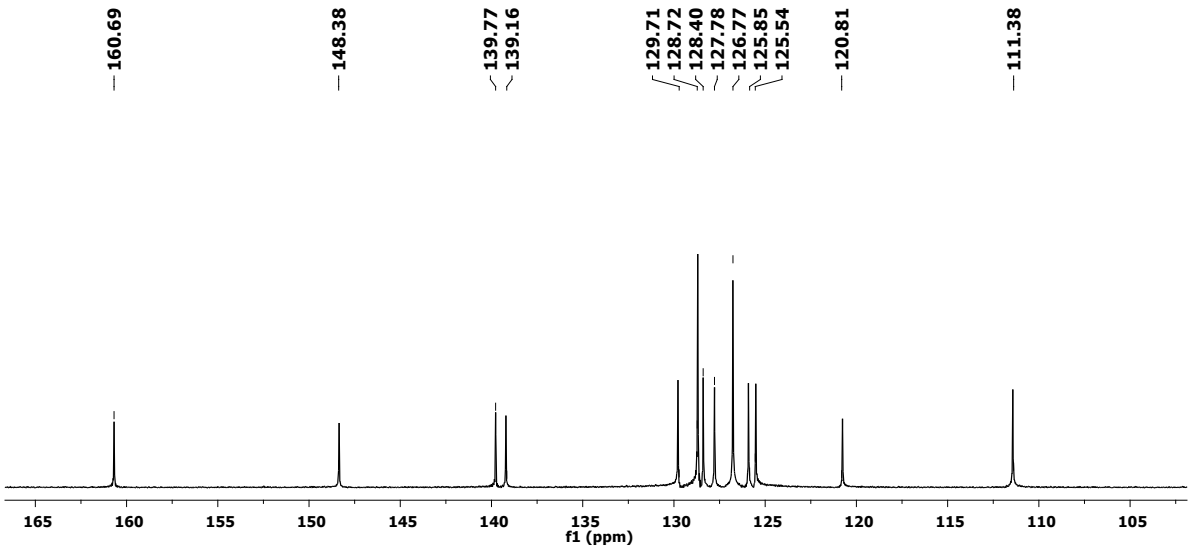


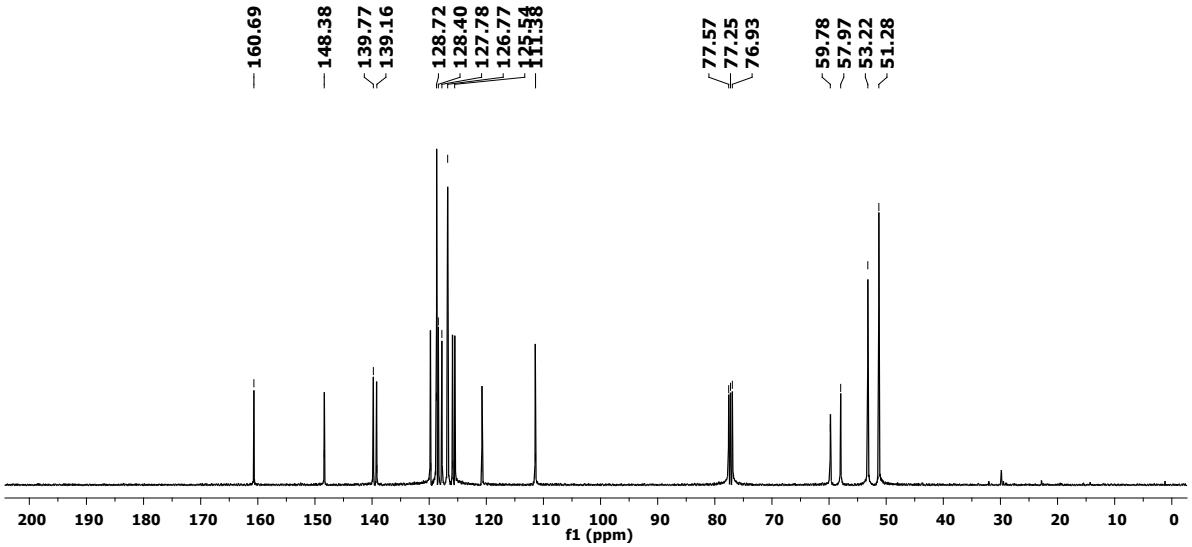



**$^{13}$C NMR** (100 MHz, $CDCl_3$)

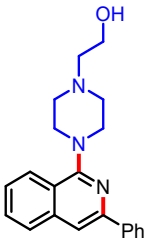



**2-(4-(3-phenylisoquinolin-1-yl)piperazin-1-yl)ethan-1-ol (3k)**



# HRMS




**2-(4-(3-phenylisoquinolin-1-yl)piperazin-1-yl)ethan-1-ol (3k)**

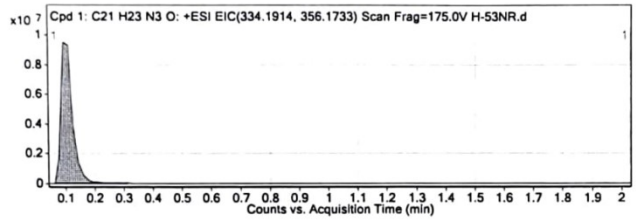
## Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | H-53NR.d | **Sample Name** | H-53NR |
| **Sample Type** | Sample | **Position** | P1-A7 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | MS Scan.m | **Acquired Time** | 30-08-2022 16:46:11 |
| **IRM Calibration Status** | [redacted] | **DA Method** | Default.m |
| **Comment** | | | |
| **Sample Group** | | **Info.** | 3 |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

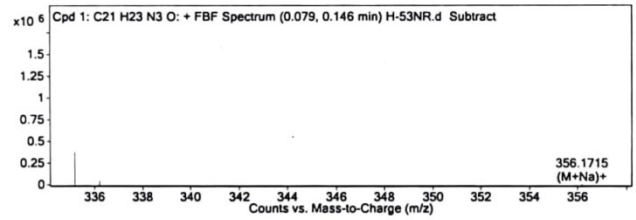
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C21 H23 N3 O | 0.096 | 333.1833 | 1550251 | C21 H23 N3 O | 333.1841 | -2.3 | C21 H23 N3 O | C21 H23 N3 O |

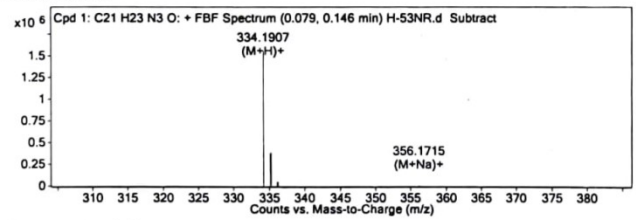
| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C21 H23 N3 O | 334.1907 | 0.096 | Find By Formula | 333.1833 |




MS Spectrum




MS Zoomed Spectrum

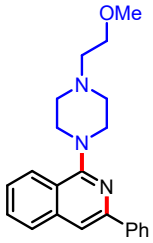



**MS Spectrum Peak List**

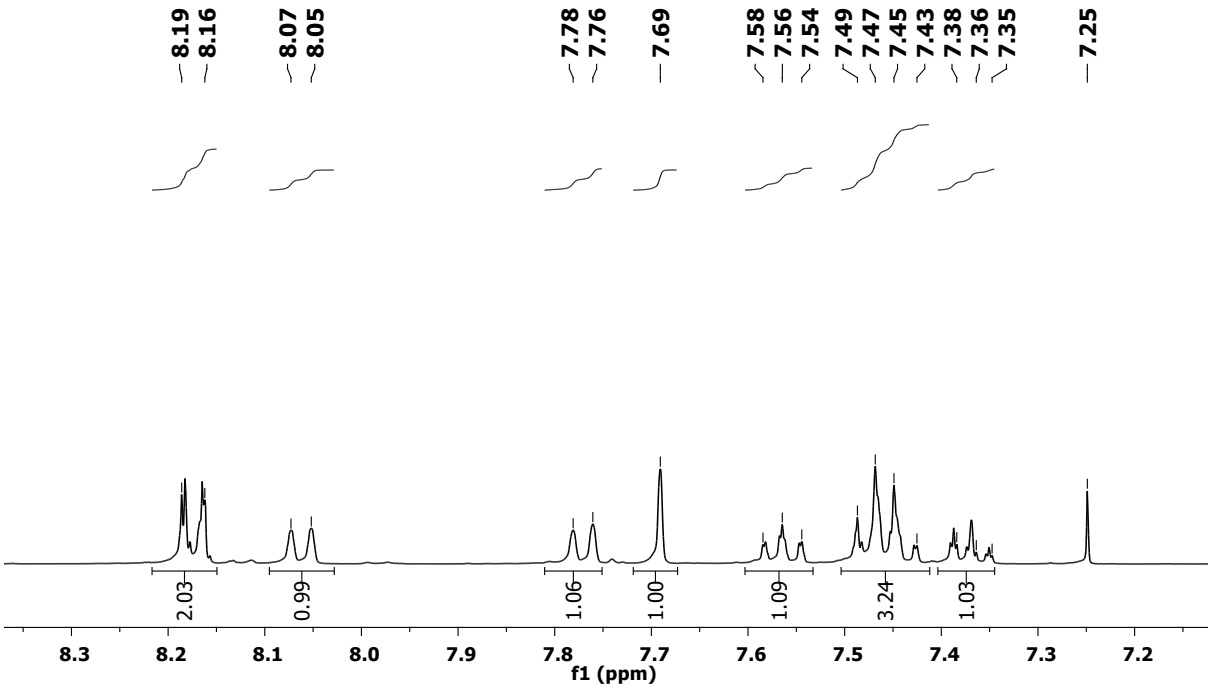
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 334.1907 | 1 | 1550251.38 | C21H24N3O | (M+H)+ |
| 335.1938 | 1 | 382346.13 | C21H24N3O | (M+H)+ |
| 336.1954 | 1 | 46585.23 | C21H24N3O | (M+H)+ |
| 337.1965 | 1 | 4537.2 | C21H24N3O | (M+H)+ |
| 356.1715 | 1 | 5052.91 | C21H23N3NaO | (M+Na)+ |
| 357.1737 | 1 | 1270.61 | C21H23N3NaO | (M+Na)+ |
| 358.1853 | 1 | 126.17 | C21H23N3NaO | (M+Na)+ |

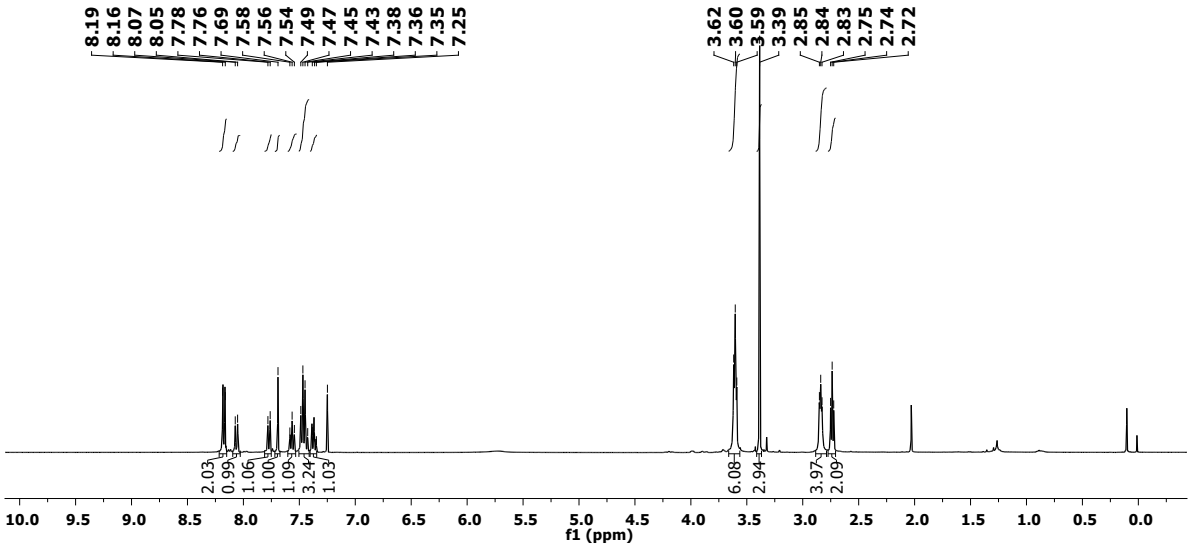
--- End Of Report ---

**$^1$H NMR** (400 MHz, $CDCl_3$)

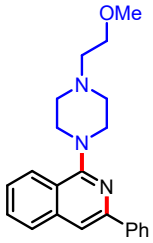



**1-(4-(2-methoxyethyl)piperazin-1-yl)-3-phenylisoquinoline (3l)**

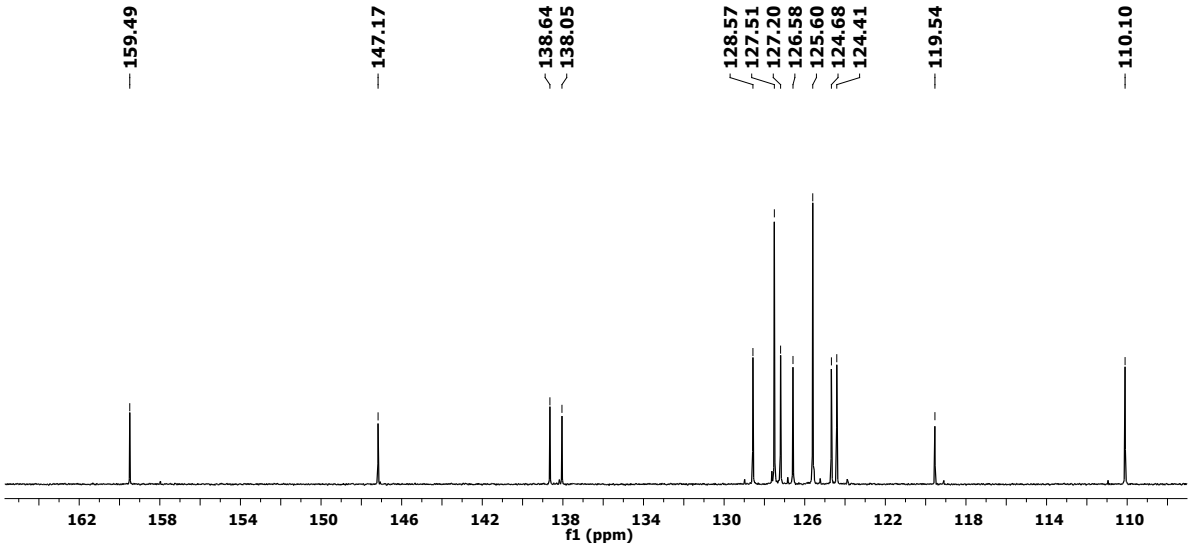


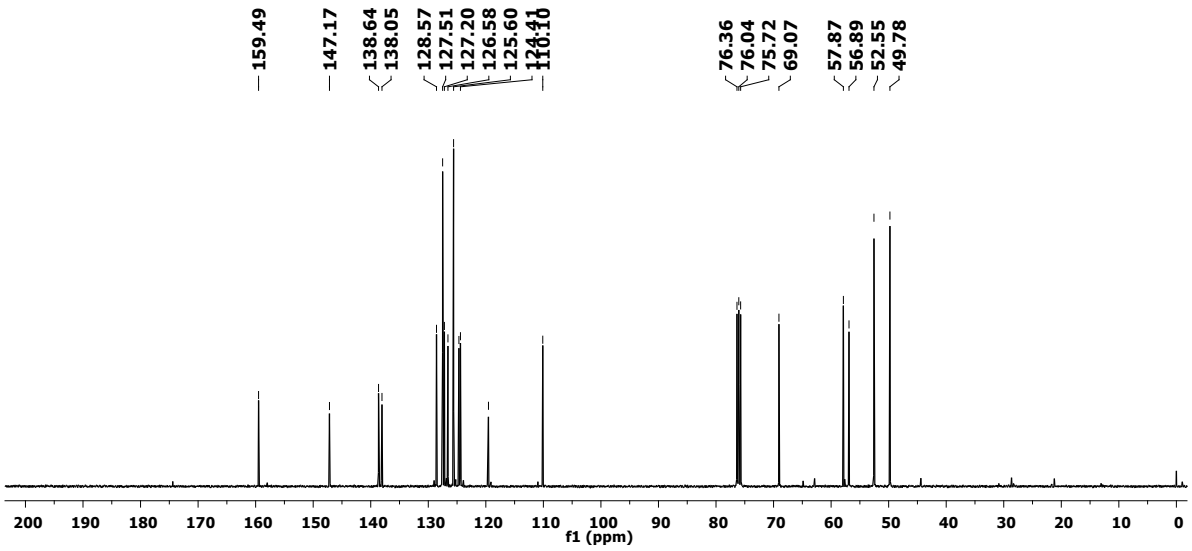



**$^{13}$C NMR** (100 MHz, $CDCl_3$)

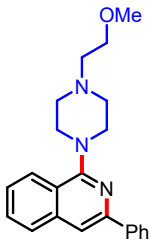



**1-(4-(2-methoxyethyl)piperazin-1-yl)-3-phenylisoquinoline (3l)**



## HRMS




**1-(4-(2-methoxyethyl)piperazin-1-yl)-3-phenylisoquinoline (3l)**

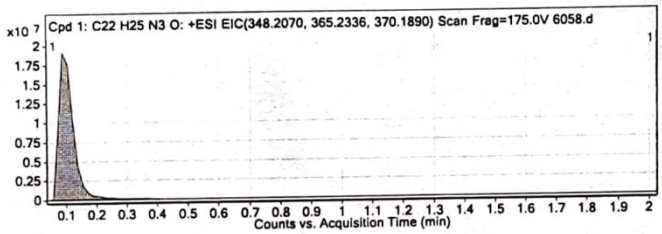
### Qualitative Compound Report

| | | | |
|---|---|---|---|
| Data File | 6058.d | Sample Name | 6058 |
| Sample Type | Sample | Position | P1-C3 |
| Instrument Name | Instrument 1 | User Name | |
| Acq Method | MS Scan.m | Acquired Time | 22-08-2022 14:19:28 |
| IRM Calibration Status | [redacted] | DA Method | Default.m |
| Comment | | | |
| Sample Group | | Info. | 3 |
| Acquisition SW Version | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

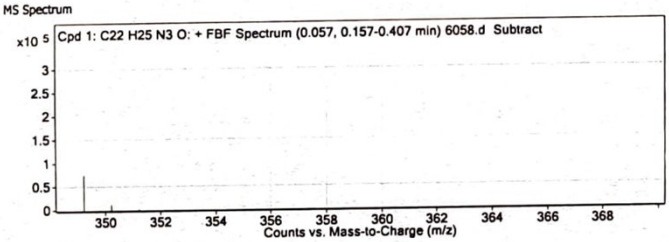
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C22 H25 N3 O | 0.09 | 347.1993 | 298896 | C22 H25 N3 O | 347.1998 | -1.26 | C22 H25 N3 O | C22 H25 N3 O |

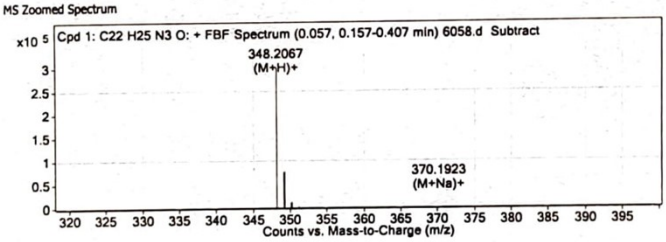
| Compound Label | m/z | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C22 H25 N3 O | 348.2067 | 0.09 | Find By Formula | 347.1993 |




MS Spectrum




MS Zoomed Spectrum

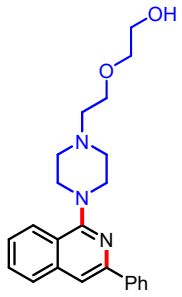



**MS Spectrum Peak List**

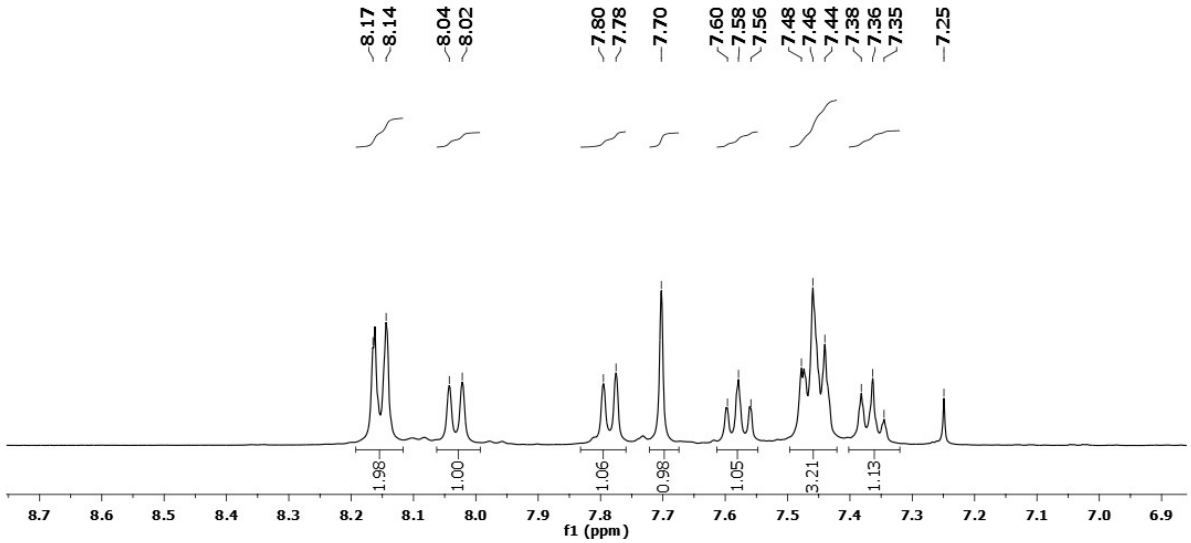
| m/z | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 348.2067 | 1 | 298896.19 | C22H26N3O | (M+H)+ |
| 349.2096 | 1 | 75754.75 | C22H26N3O | (M+H)+ |
| 350.2111 | 1 | 9930.89 | C22H26N3O | (M+H)+ |
| 351.2121 | 1 | 1141.47 | C22H26N3O | (M+H)+ |
| 370.1923 | 1 | 421.57 | C22H25N3NaO | (M+Na)+ |

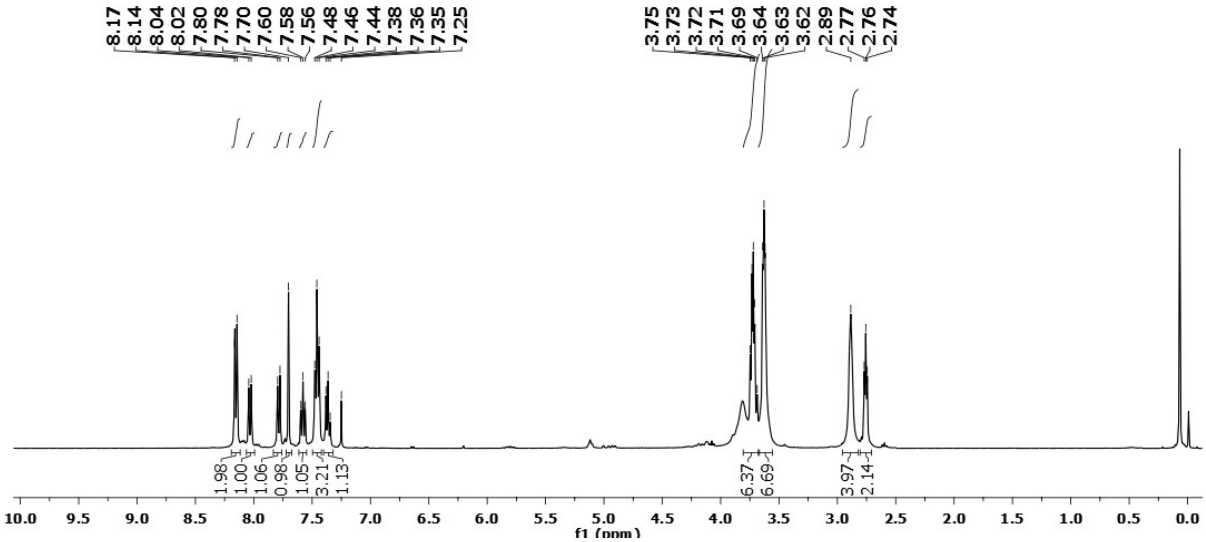
--- End Of Report ---

**$^1$H NMR** (400 MHz, $CDCl_3$)

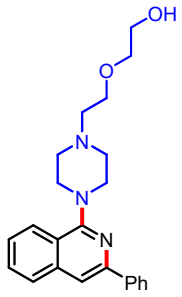



**2-(2-(4-(3-phenylisoquinolin-1-yl)piperazin-1-yl)ethoxy)ethan-1-ol (3m)**

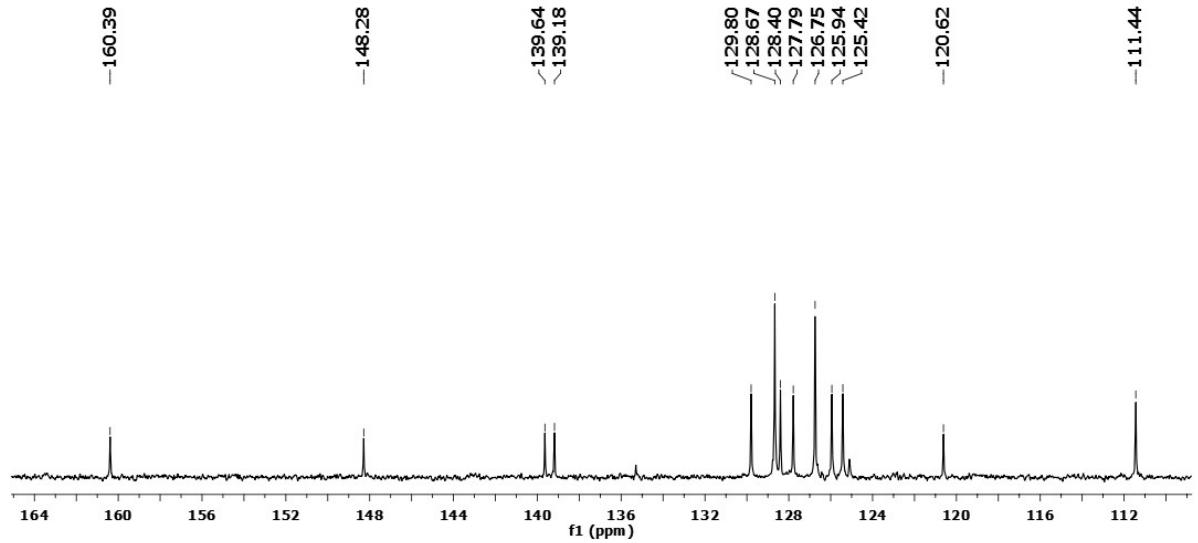


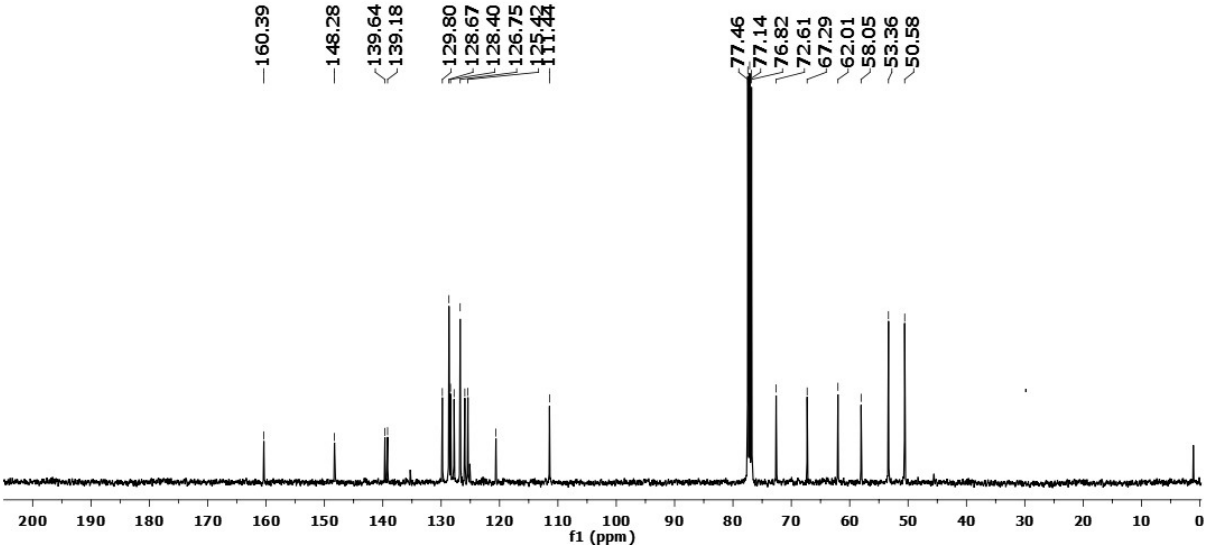



**$^{13}$C NMR** (100 MHz, $CDCl_3$)

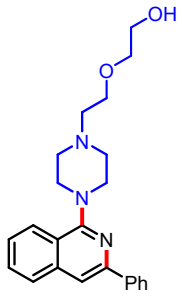



**2-(2-(4-(3-phenylisoquinolin-1-yl)piperazin-1-yl)ethoxy)ethan-1-ol (3m)**



## HRMS




**2-(2-(4-(3-phenylisoquinolin-1-yl)piperazin-1-yl)ethoxy)ethan-1-ol (3m)**

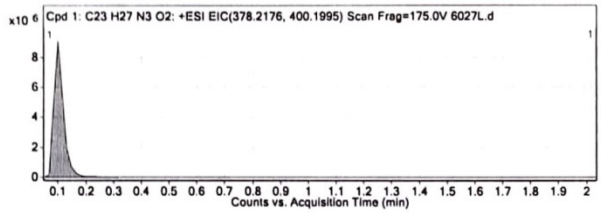
### Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | 6027L.d | **Sample Name** | 6027L |
| **Sample Type** | Sample | **Position** | P1-A7 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | MS Scan.m | **Acquired Time** | 27-08-2022 12:18:14 |
| **IRM Calibration Status** | [redacted] | **DA Method** | Default.m |
| **Comment** | | | |
| **Sample Group** | | **Info.** | 3 |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

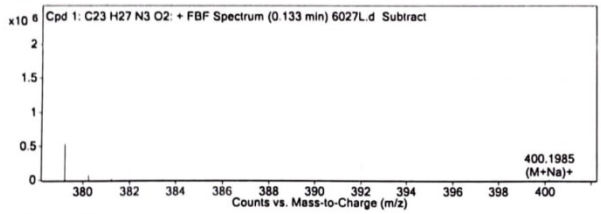
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C23 H27 N3 O2 | 0.099 | 377.2107 | 1934284 | C23 H27 N3 O2 | 377.2103 | 1 | C23 H27 N3 O2 | C23 H27 N3 O2 |

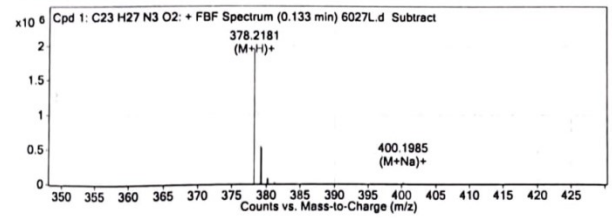
| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C23 H27 N3 O2 | 378.2181 | 0.099 | Find By Formula | 377.2107 |




MS Spectrum



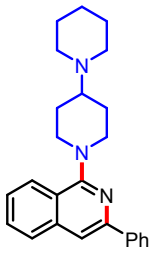

MS Zoomed Spectrum



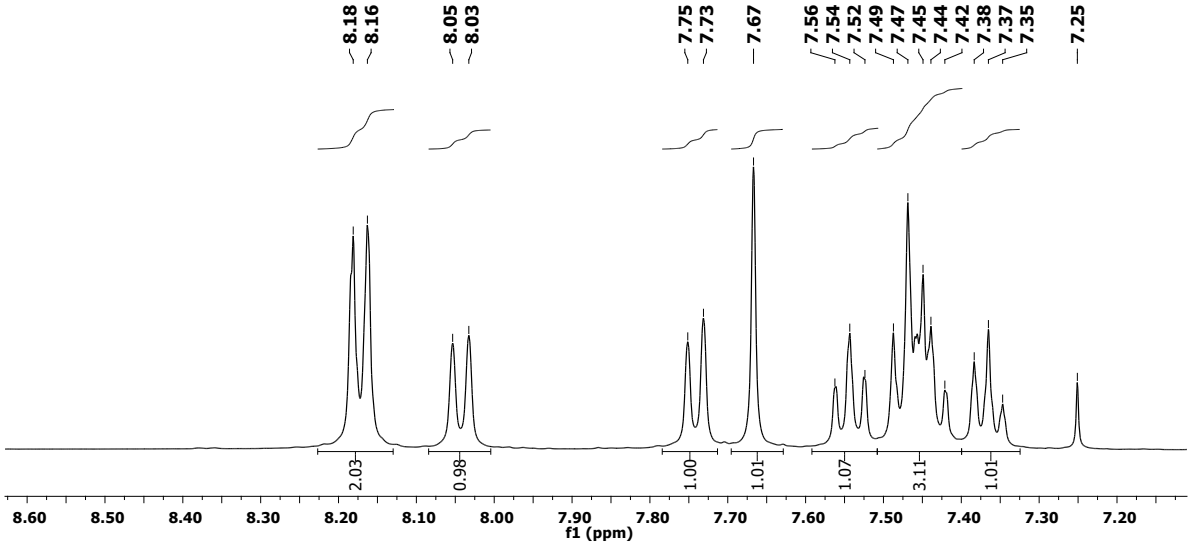

**MS Spectrum Peak List**

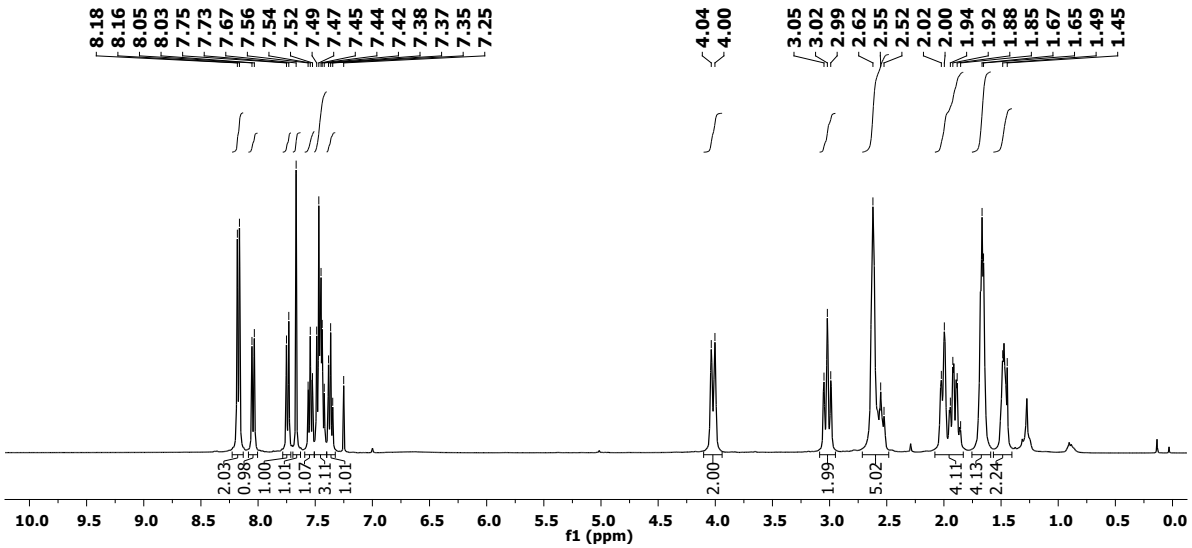
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 378.2181 | 1 | 1934283.88 | C23H28N3O2 | (M+H)+ |
| 379.221 | 1 | 531813 | C23H28N3O2 | (M+H)+ |
| 380.2232 | 1 | 69661.97 | C23H28N3O2 | (M+H)+ |
| 381.2235 | 1 | 9666.9 | C23H28N3O2 | (M+H)+ |
| 400.1985 | 1 | 8020.65 | C23H27N3NaO2 | (M+Na)+ |
| 401.2062 | 1 | 2466.63 | C23H27N3NaO2 | (M+Na)+ |
| 402.1993 | 1 | 845.64 | C23H27N3NaO2 | (M+Na)+ |

**$^1$H NMR** (400 MHz, $CDCl_3$)

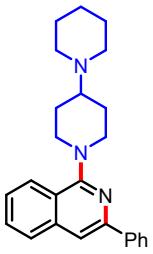



**1-([1,4'-bipiperidin]-1'-yl)-3-phenylisoquinoline (3n)**

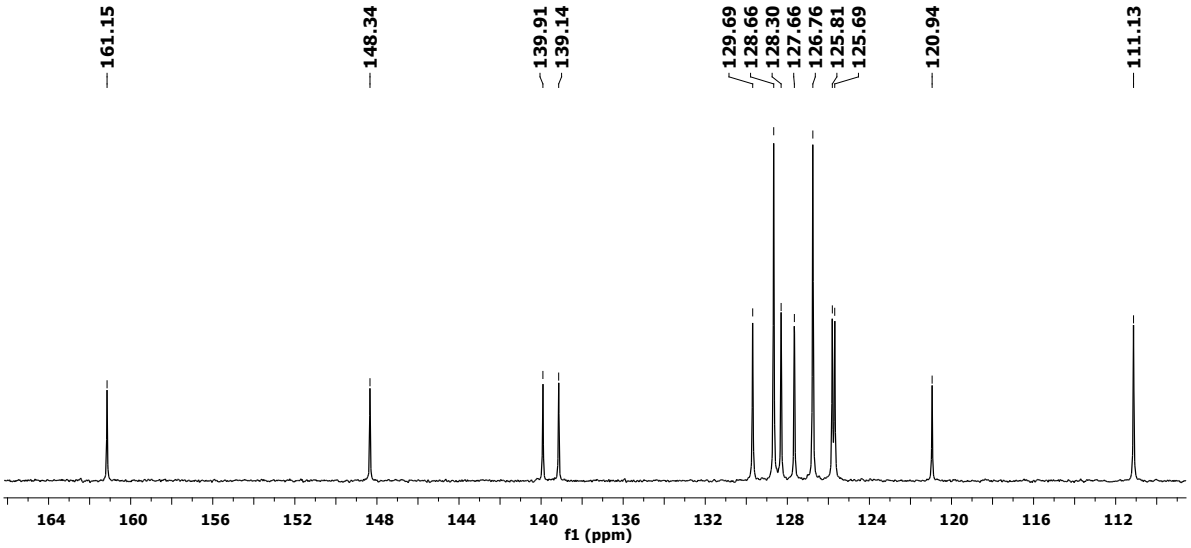


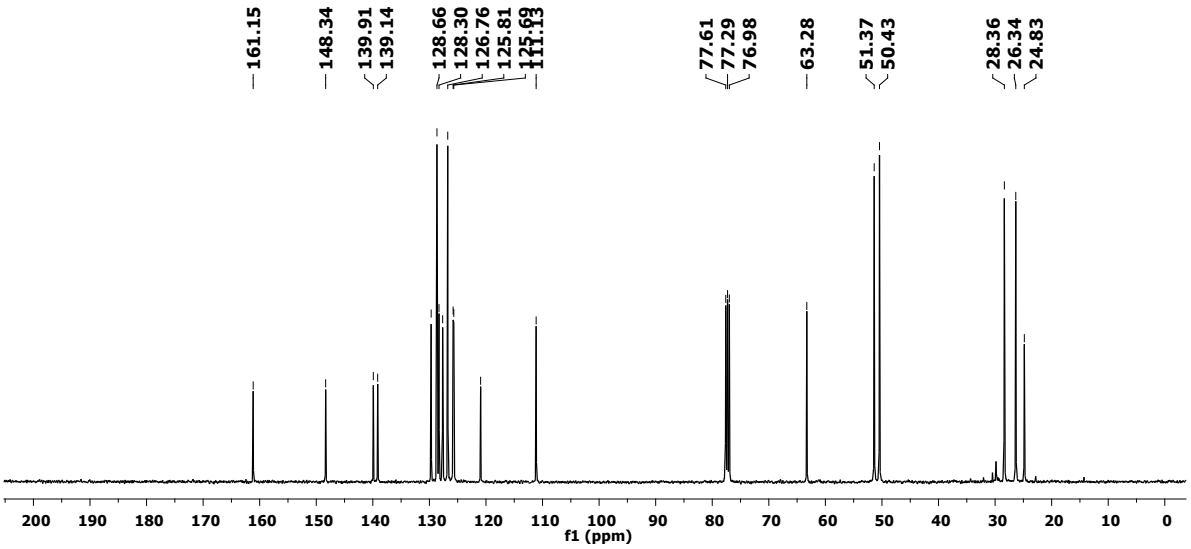



**$^{13}$C NMR** (100 MHz, $CDCl_3$)

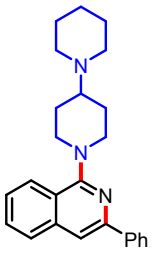



**1-([1,4'-bipiperidin]-1'-yl)-3-phenylisoquinoline (3n)**



## HRMS



**1-([1,4'-bipiperidin]-1'-yl)-3-phenylisoquinoline (3n)**

### Qualitative Compound Report

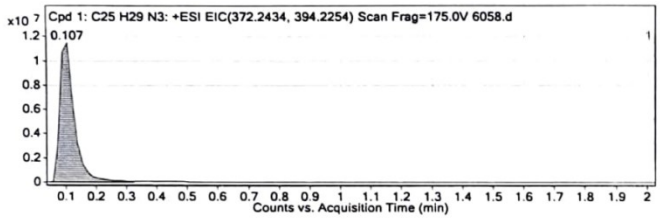
| | | | |
|---|---|---|---|
| **Data File** | 6058.d | **Sample Name** | 6058 |
| **Sample Type** | Sample | **Position** | P1-C3 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | MS Scan.m | **Acquired Time** | 22-08-2022 14:19:28 |
| **IRM Calibration Status** | [redacted] | **DA Method** | Default.m |
| **Comment** | | | |

| | | | |
|---|---|---|---|
| **Sample Group** | | **Info.** | 3 |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

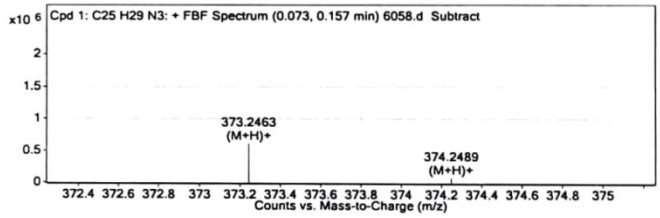
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C25 H29 N3 | 0.107 | 371.2358 | 2083256 | C25 H29 N3 | 371.2361 | -1.06 | C25 H29 N3 | C25 H29 N3 |

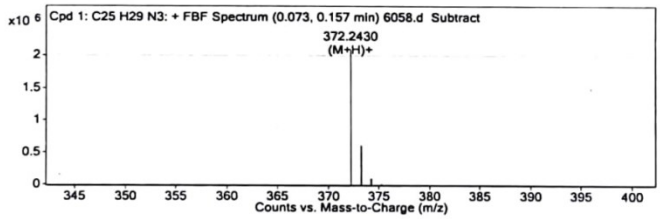
| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C25 H29 N3 | 372.243 | 0.107 | Find By Formula | 371.2358 |




MS Spectrum




MS Zoomed Spectrum

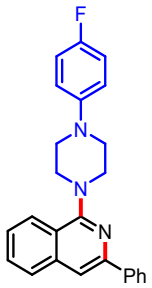



**MS Spectrum Peak List**

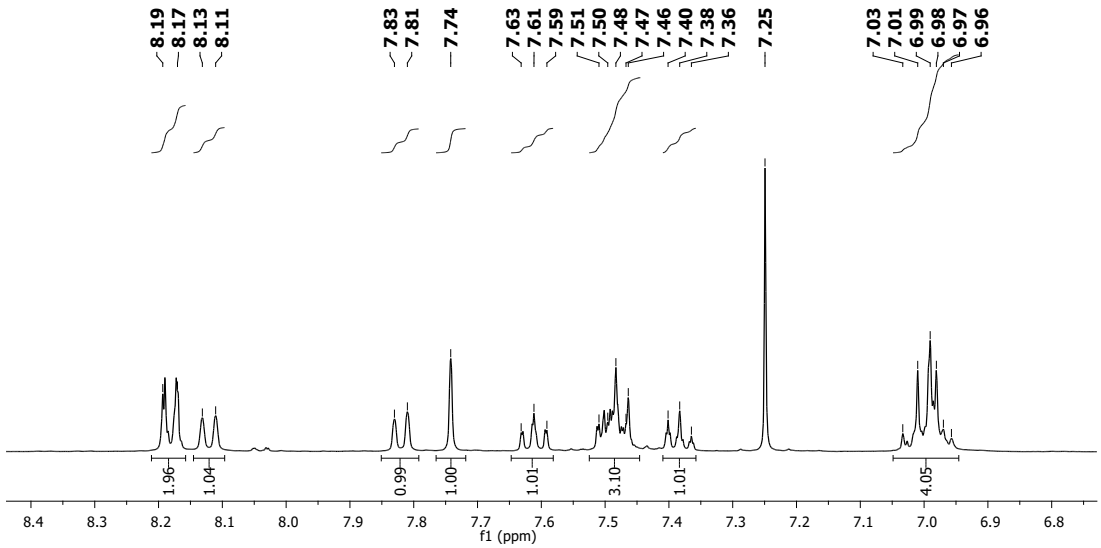
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 372.243 | 1 | 2083256.25 | C25H30N3 | (M+H)+ |
| 373.2463 | 1 | 609266.38 | C25H30N3 | (M+H)+ |
| 374.2489 | 1 | 79538.83 | C25H30N3 | (M+H)+ |
| 375.2529 | 1 | 6962.61 | C25H30N3 | (M+H)+ |

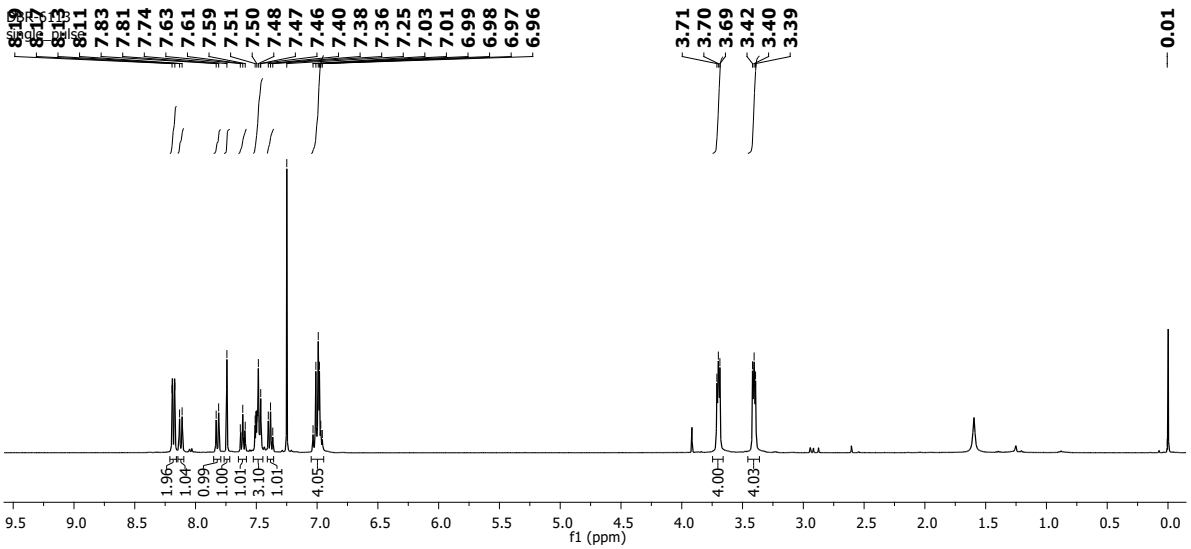
--- End Of Report ---

**$^1$H NMR** (400 MHz, $CDCl_3$)

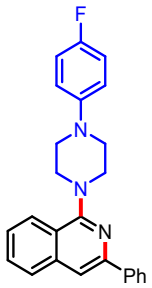



**1-(4-(4-fluorophenyl)piperazin-1-yl)-3-phenylisoquinoline (3o)**

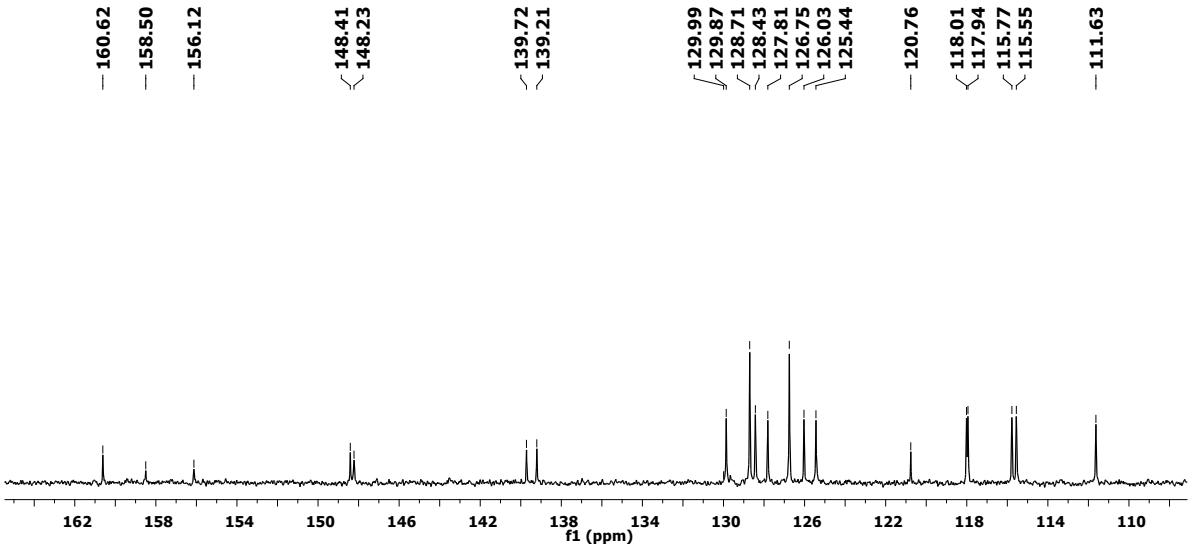


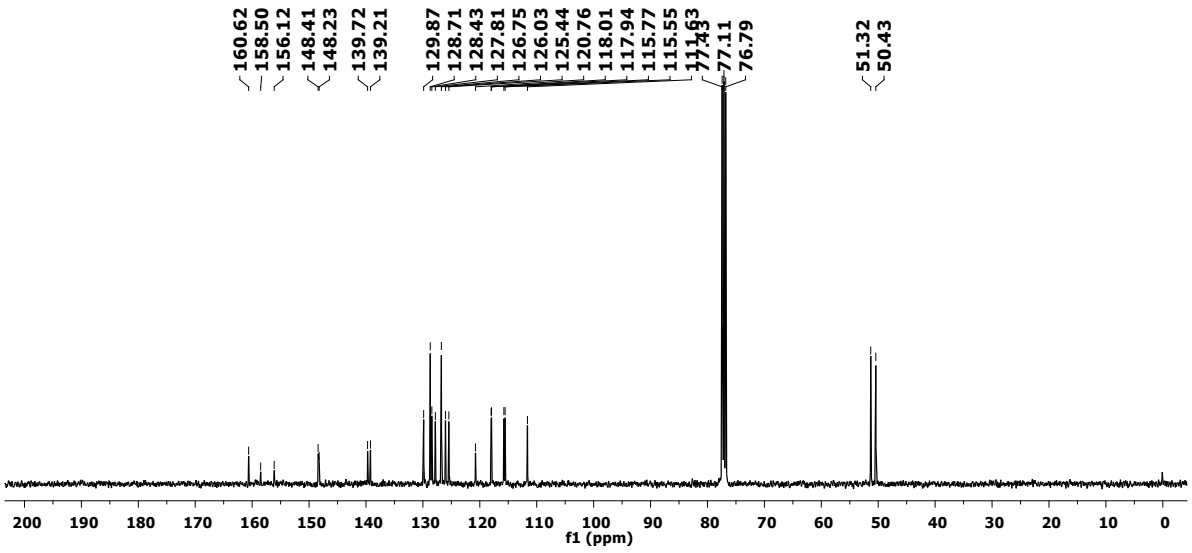



**$^{13}$C NMR** (100 MHz, $CDCl_3$)

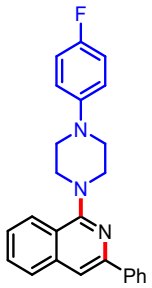



**1-(4-(4-fluorophenyl)piperazin-1-yl)-3-phenylisoquinoline (3o)**



## HRMS




**1-(4-(4-fluorophenyl)piperazin-1-yl)-3-phenylisoquinoline (3o)**

### Qualitative Compound Report

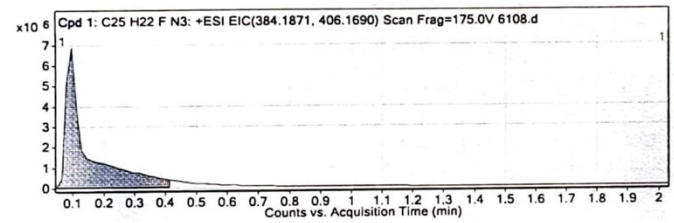
| | | | |
|---|---|---|---|
| **Data File** | 6108.d | **Sample Name** | 6108 |
| **Sample Type** | Sample | **Position** | P1-C9 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | MS Scan.m | **Acquired Time** | 22-08-2022 14:33:59 |
| **IRM Calibration Status** | Success [redacted] | **DA Method** | Default.m |
| **Comment** | | | |

| | | | |
|---|---|---|---|
| **Sample Group** | | **Info.** | 3 |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

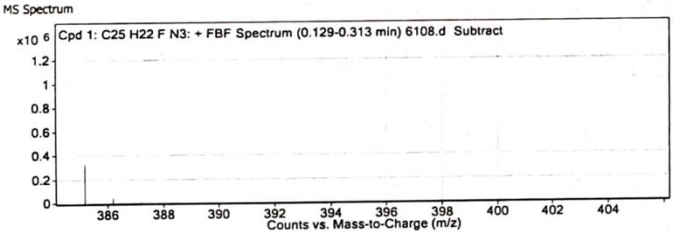
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C25 H22 F N3 | 0.096 | 383.1793 | 1134601 | C25 H22 F N3 | 383.1798 | -1.35 | C25 H22 F N3 | C25 H22 F N3 |

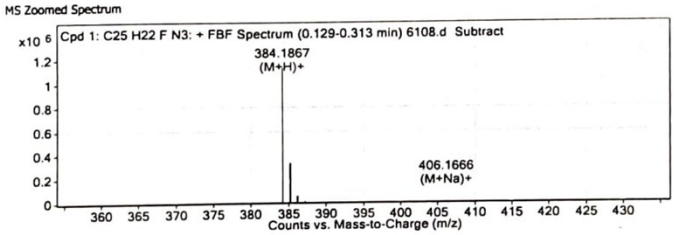
| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C25 H22 F N3 | 384.1867 | 0.096 | Find By Formula | 383.1793 |




MS Spectrum




MS Zoomed Spectrum

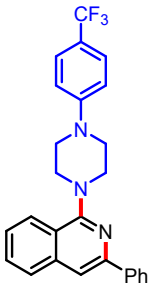



**MS Spectrum Peak List**

| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 384.1867 | 1 | 1134601.13 | C25H23FN3 | (M+H)+ |
| 385.1894 | 1 | 327934.5 | C25H23FN3 | (M+H)+ |
| 386.192 | 1 | 40999.23 | C25H23FN3 | (M+H)+ |
| 387.1943 | 1 | 4051.82 | C25H23FN3 | (M+H)+ |
| 406.1666 | 1 | 547.93 | C25H22FN3Na | (M+Na)+ |

--- End Of Report ---

## HRMS




**3-phenyl-1-(4-(4-(trifluoromethyl)phenyl)piperazin-1-yl)isoquinoline (3p)**

### Qualitative Compound Report

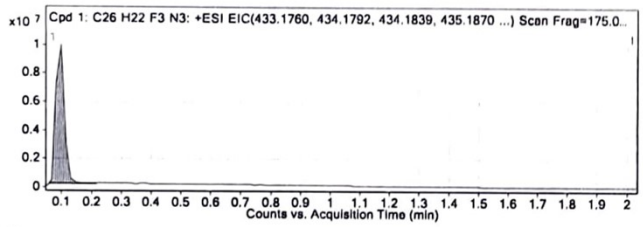
| | | | |
|---|---|---|---|
| Data File | 6024.d | Sample Name | 6024 |
| Sample Type | Sample | Position | P1-A6 |
| Instrument Name | Instrument 1 | User Name | |
| Acq Method | MS Scan.m | Acquired Time | 27-08-2022 12:15:29 |
| IRM Calibration Status | [redacted] | DA Method | Default.m |
| Comment | | | |

| | | | |
|---|---|---|---|
| Sample Group | | Info. | 3 |
| Acquisition SW Version | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

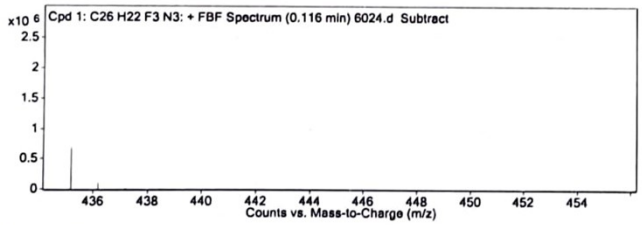
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C26 H22 F3 N3 | 0.099 | 433.177 | 2274990 | C26 H22 F3 N3 | 433.1766 | 0.9 | C26 H22 F3 N3 | C26 H22 F3 N3 |

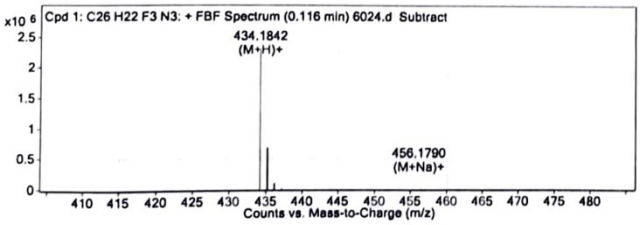
| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C26 H22 F3 N3 | 434.1842 | 0.099 | Find By Formula | 433.177 |




MS Spectrum



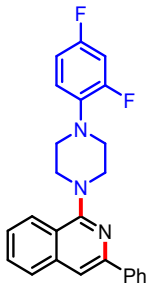

MS Zoomed Spectrum



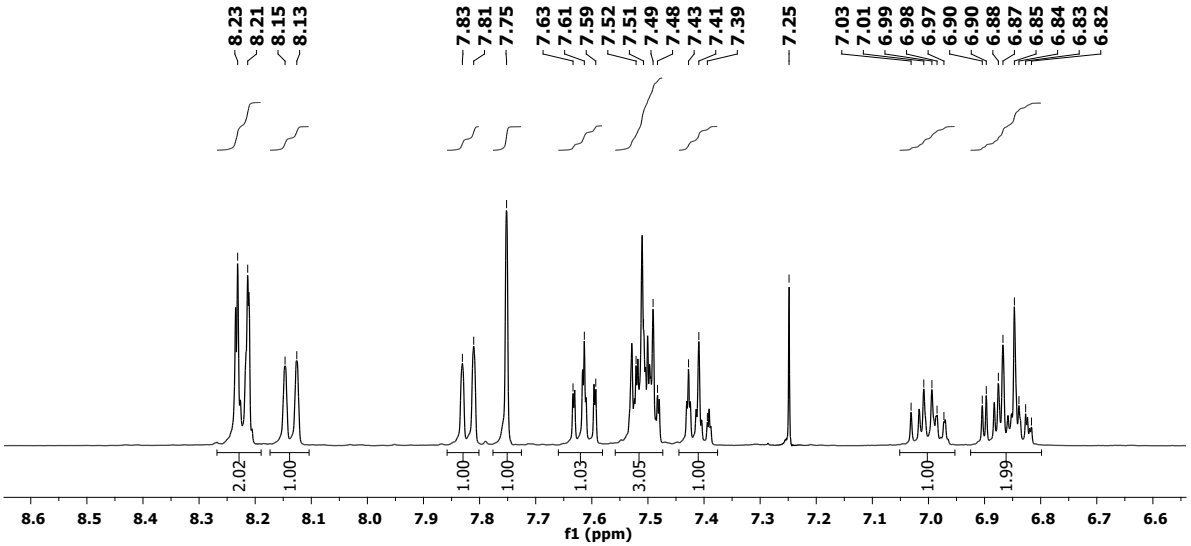

**MS Spectrum Peak List**

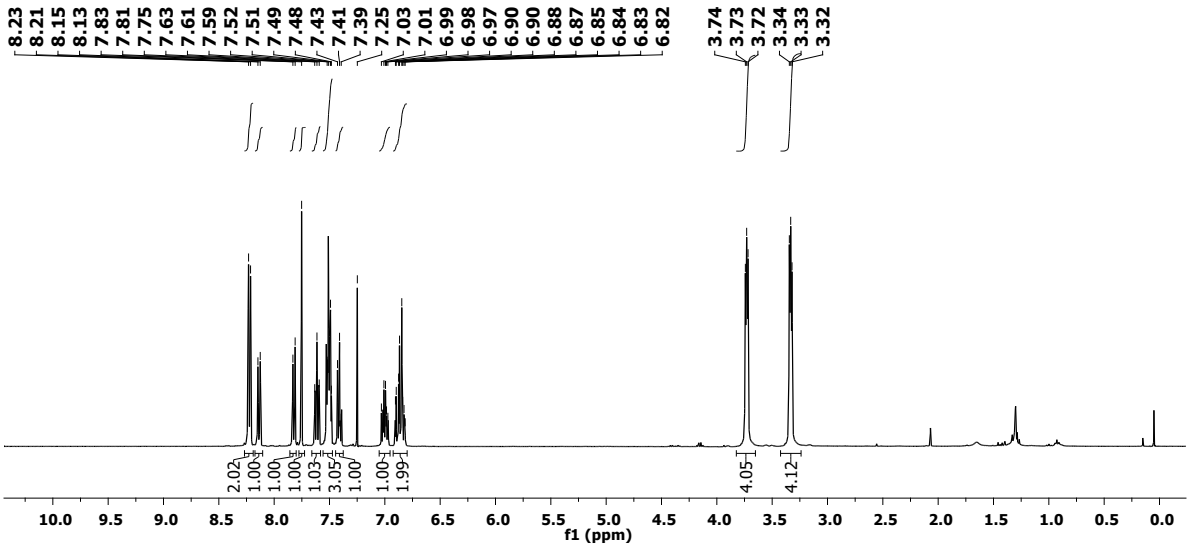
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 434.1842 | 1 | 2274990.25 | C26H23F3N3 | (M+H)+ |
| 435.1876 | 1 | 685033.25 | C26H23F3N3 | (M+H)+ |
| 436.19 | 1 | 92855.79 | C26H23F3N3 | (M+H)+ |
| 437.1935 | 1 | 17526.18 | C26H23F3N3 | (M+H)+ |
| 438.1977 | 1 | 3477.65 | C26H23F3N3 | (M+H)+ |
| 456.179 | 1 | 289.95 | C26H22F3N3Na | (M+Na)+ |

**$^1$H NMR** (400 MHz, $CDCl_3$)

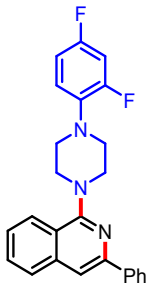



**1-(4-(2,4-difluorophenyl)piperazin-1-yl)-3-phenylisoquinoline (3q)**

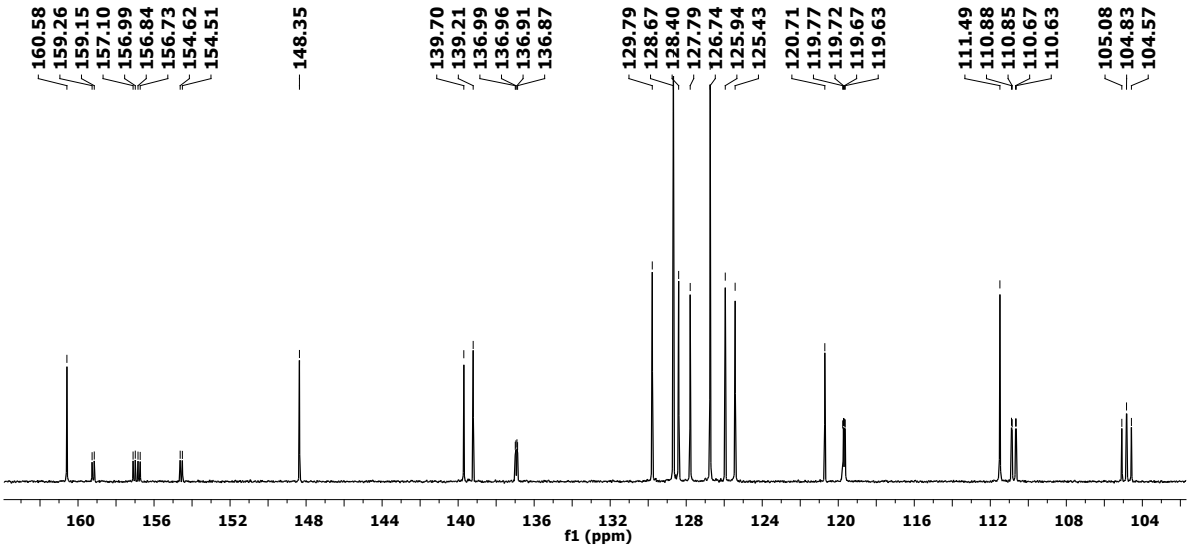


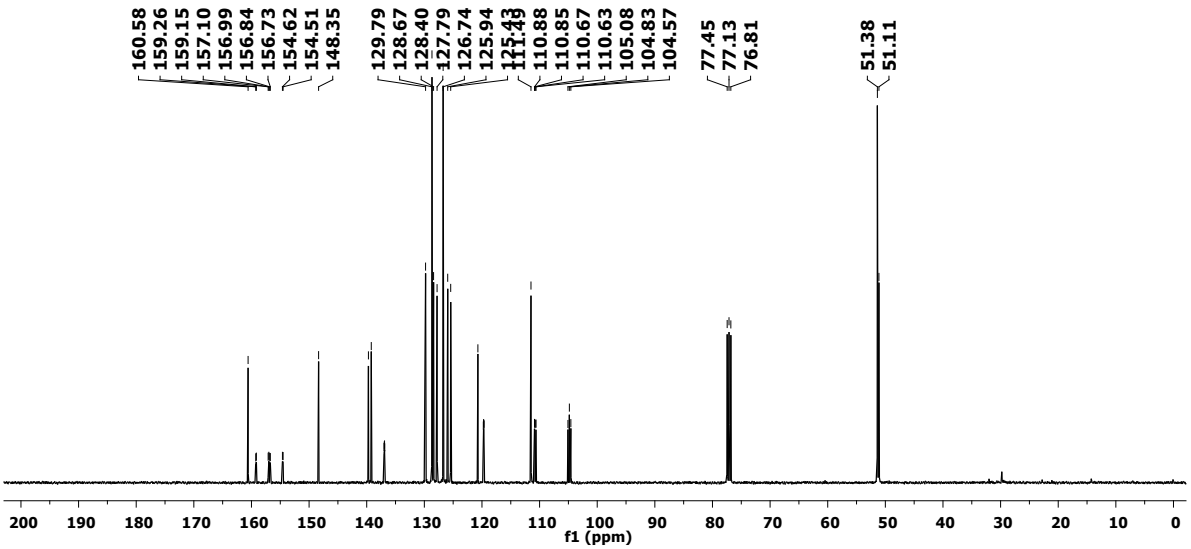



**$^{13}$C NMR** (100 MHz, $CDCl_3$)

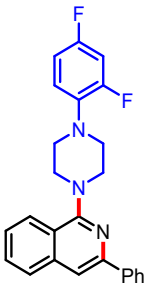



**1-(4-(2,4-difluorophenyl)piperazin-1-yl)-3-phenylisoquinoline (3q)**



## HRMS




**1-(4-(2,4-difluorophenyl)piperazin-1-yl)-3-phenylisoquinoline (3q)**

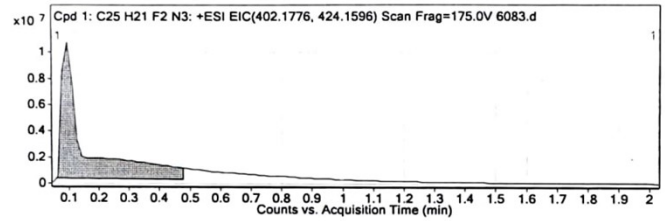
### Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | 6083.d | **Sample Name** | 6083 |
| **Sample Type** | Sample | **Position** | P1-C7 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | MS Scan.m | **Acquired Time** | 22-08-2022 14:30:30 |
| **IRM Calibration Status** | [redacted] | **DA Method** | Default.m |
| **Comment** | | | |
| **Sample Group** | | **Info.** | 3 |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

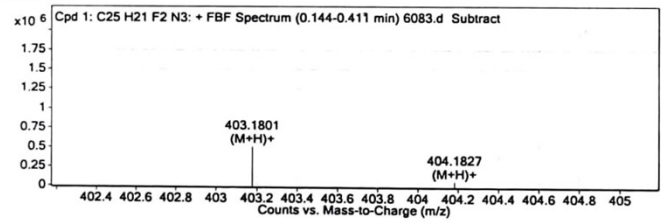
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C25 H21 F2 N3 | 0.094 | 401.1697 | 1734701 | C25 H21 F2 N3 | 401.1704 | -1.68 | C25 H21 F2 N3 | C25 H21 F2 N3 |

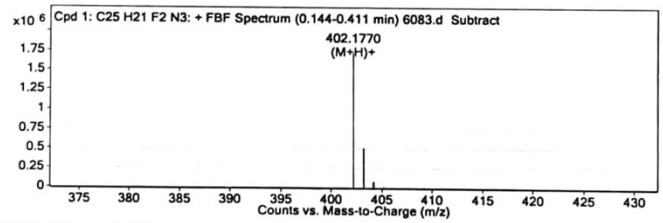
| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C25 H21 F2 N3 | 402.177 | 0.094 | Find By Formula | 401.1697 |




MS Spectrum




MS Zoomed Spectrum

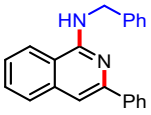



**MS Spectrum Peak List**

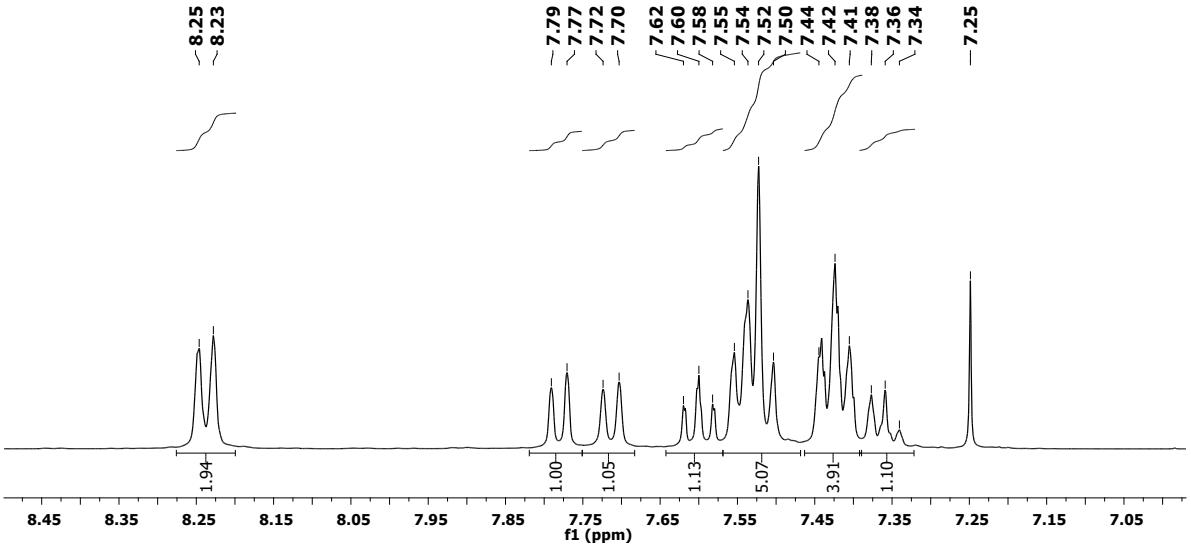
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 402.177 | 1 | 1734701.38 | C25H22F2N3 | (M+H)+ |
| 403.1801 | 1 | 506079.47 | C25H22F2N3 | (M+H)+ |
| 404.1827 | 1 | 62908.66 | C25H22F2N3 | (M+H)+ |
| 405.1858 | 1 | 5362.37 | C25H22F2N3 | (M+H)+ |

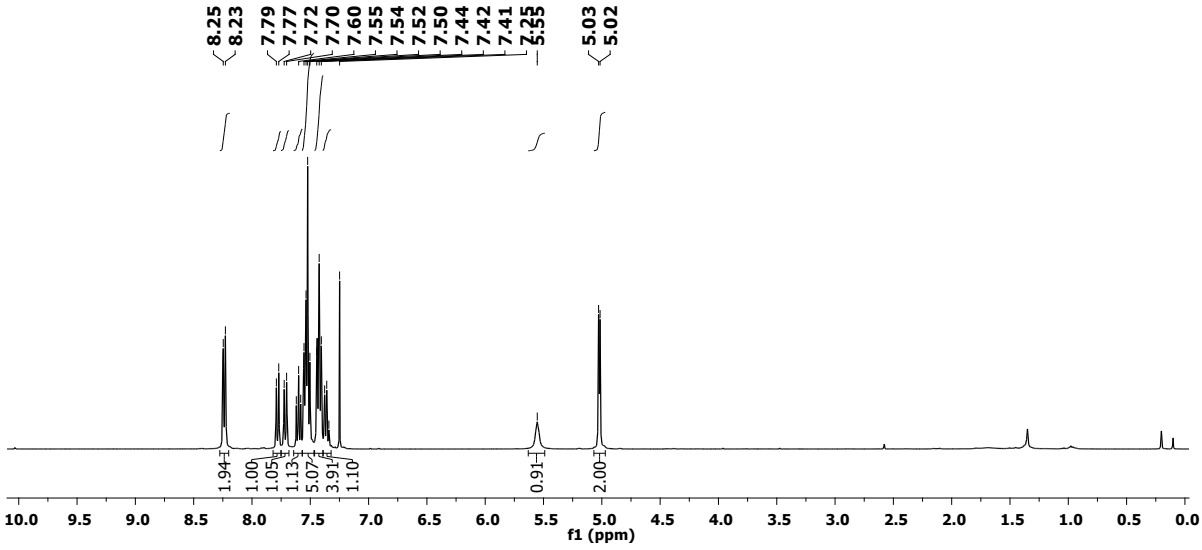
--- End Of Report ---

**$^1$H NMR** (400 MHz, $CDCl_3$)

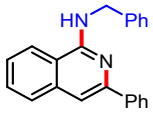



**11-(2-Bromo-5-methylphenyl)-11,12-dihydrobenzo[*c*]phenanthridin-6-amine (4a)**

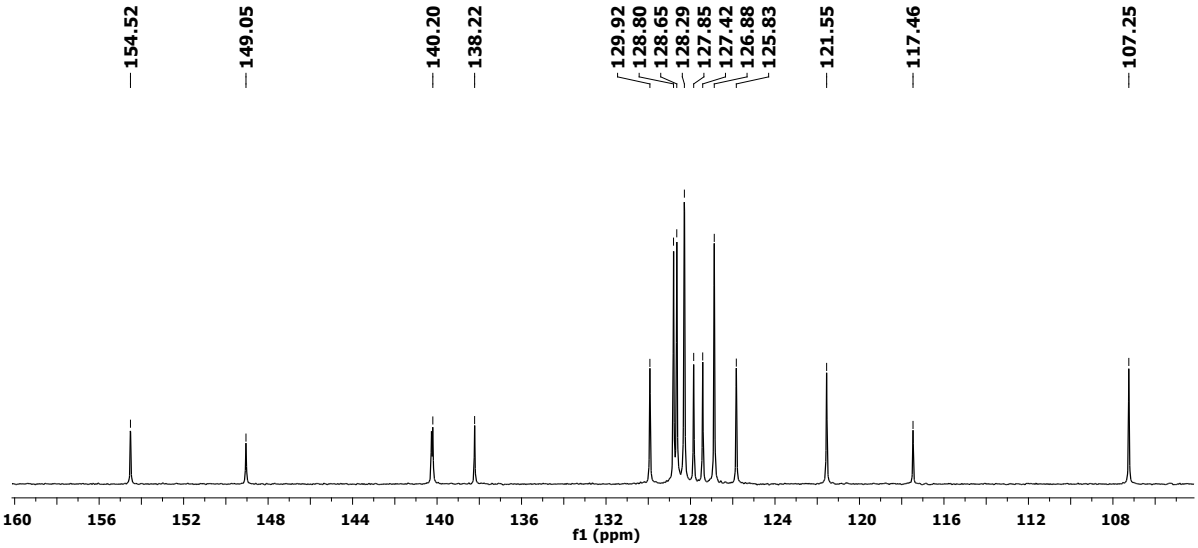


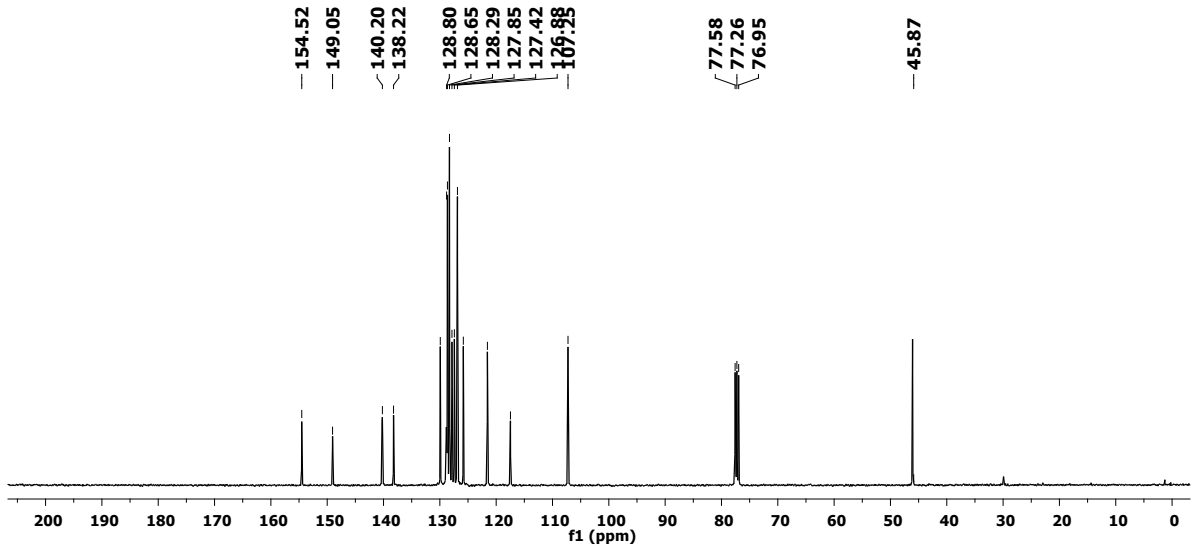



**$^{13}$C NMR** (100 MHz, $CDCl_3$)

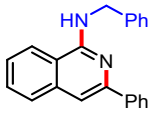



**11-(2-Bromo-5-methylphenyl)-11,12-dihydrobenzo[*c*]phenanthridin-6-amine (4a)**



## HRMS




## 11-(2-Bromo-5-methylphenyl)-11,12-dihydrobenzo[*c*]phenanthridin-6-amine (4a)

### Qualitative Compound Report

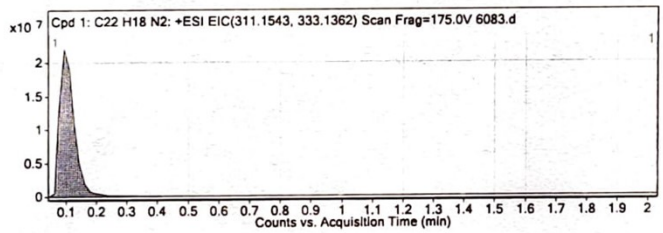
| | | | |
|---|---|---|---|
| **Data File** | 6083.d | **Sample Name** | 6083 |
| **Sample Type** | Sample | **Position** | P1-C7 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | MS Scan.m | **Acquired Time** | 22-08-2022 14:30:30 |
| **IRM Calibration Status** | Success | **DA Method** | Default.m |
| **Comment** | | | |

| | | | |
|---|---|---|---|
| **Sample Group** | | **Info.** | 3 |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

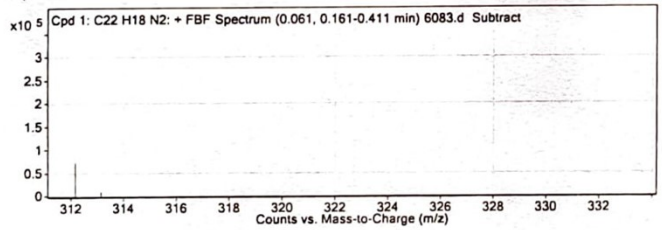
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C22 H18 N2 | 0.094 | 310.1464 | 304089 | C22 H18 N2 | 310.147 | -1.94 | C22 H18 N2 | C22 H18 N2 |

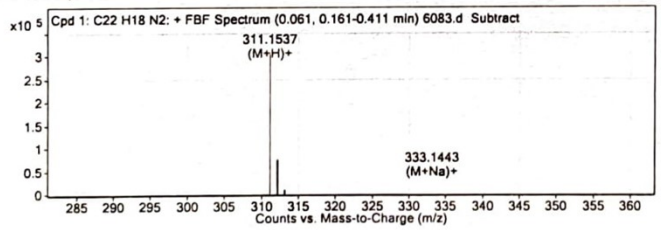
| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C22 H18 N2 | 311.1537 | 0.094 | Find By Formula | 310.1464 |




MS Spectrum




MS Zoomed Spectrum

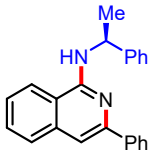



**MS Spectrum Peak List**

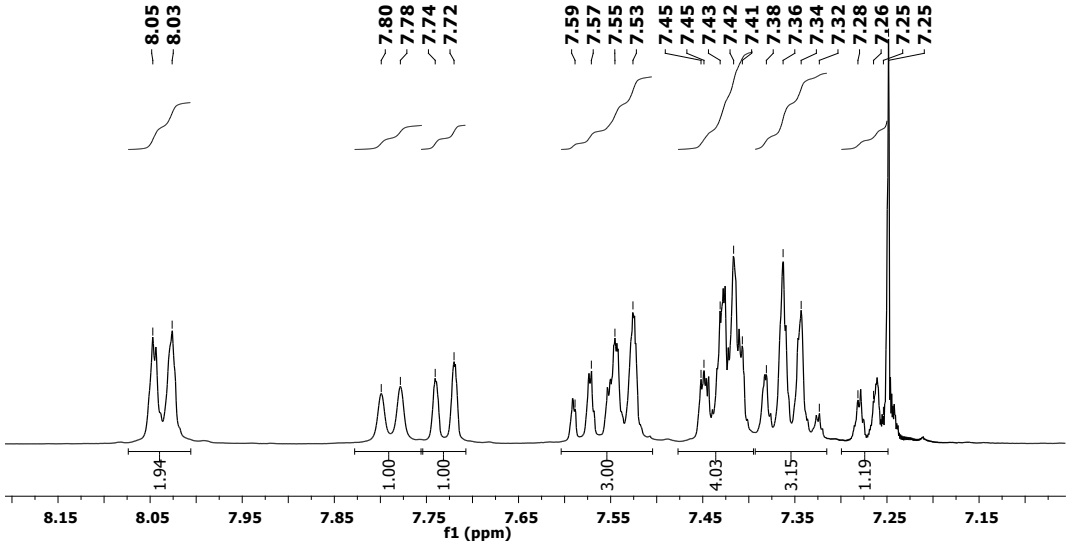
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 311.1537 | 1 | 304088.69 | C22H19N2 | (M+H)+ |
| 312.1568 | 1 | 73609.42 | C22H19N2 | (M+H)+ |
| 313.1597 | 1 | 8796.37 | C22H19N2 | (M+H)+ |
| 314.1633 | 1 | 691.07 | C22H19N2 | (M+H)+ |
| 333.1443 | 1 | 332.95 | C22H18N2Na | (M+Na)+ |
| 334.1482 | 1 | 73.88 | C22H18N2Na | (M+Na)+ |

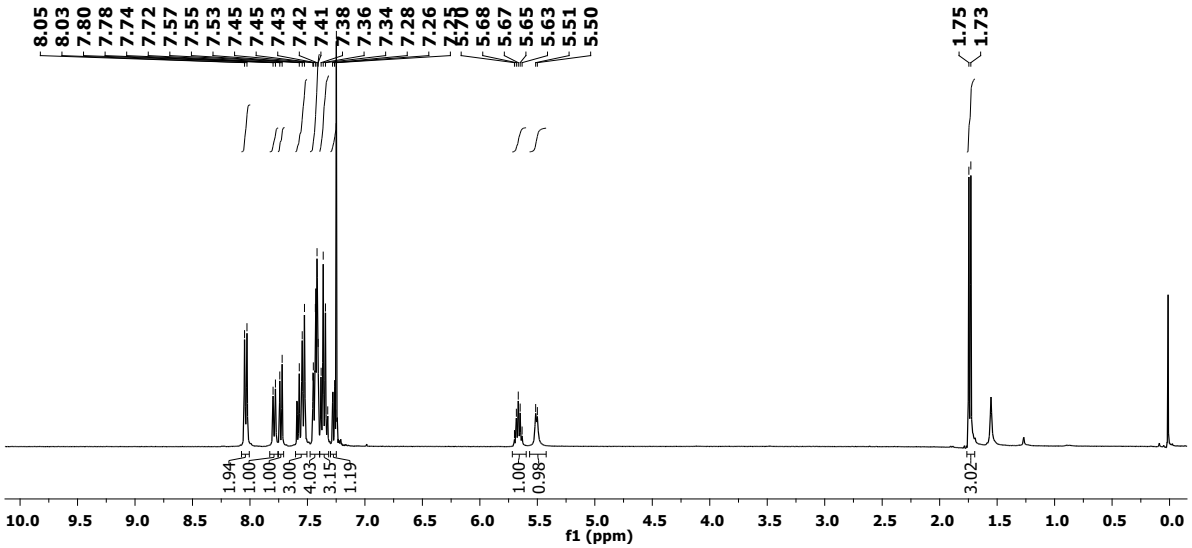
--- End Of Report ---

**$^1$H NMR** (400 MHz, $CDCl_3$)

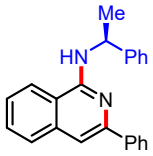



**(*S*)-3-phenyl-N-(1-phenylethyl)isoquinolin-1-amine (4b)**

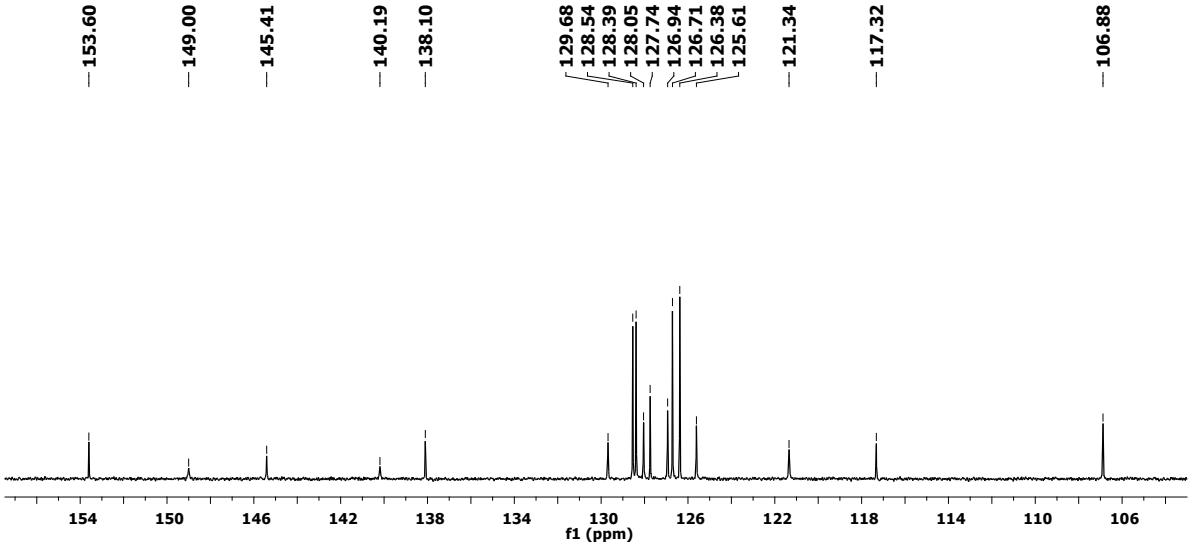


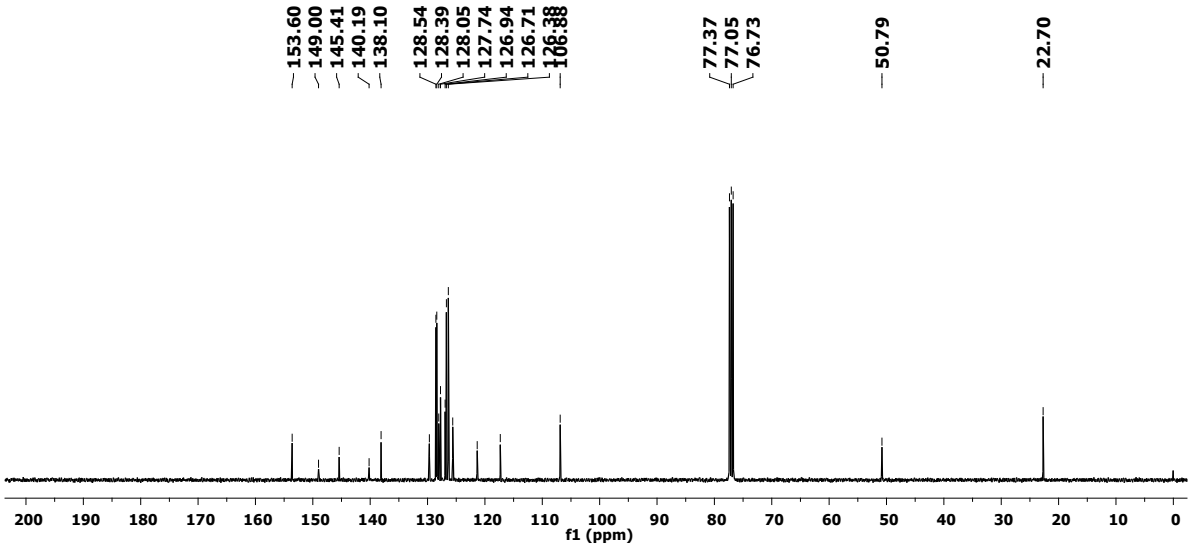



**$^{13}$C NMR** (100 MHz, $CDCl_3$)

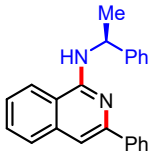



**(*S*)-3-phenyl-N-(1-phenylethyl)isoquinolin-1-amine (4b)**



## HRMS




**(*S*)-3-phenyl-N-(1-phenylethyl)isoquinolin-1-amine (4b)**

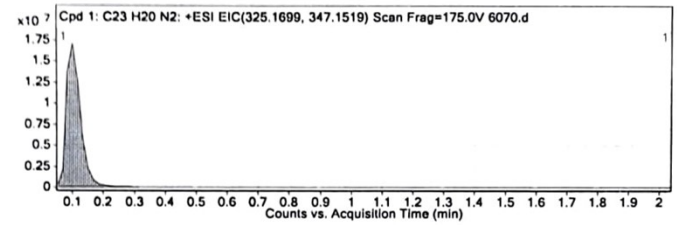
### Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | 6070.d | **Sample Name** | 6070 |
| **Sample Type** | Sample | **Position** | P1-C4 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | MS Scan.m | **Acquired Time** | 22-08-2022 14:22:11 |
| **IRM Calibration Status** | [redacted] | **DA Method** | Default.m |
| **Comment** | | | |
| **Sample Group** | | **Info.** | 3 |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (05125) | | |

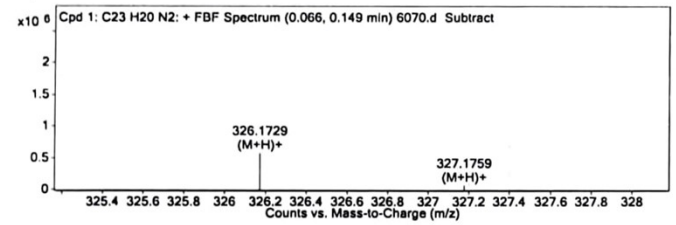
Compound Table

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C23 H20 N2 | 0.099 | 324.1624 | 2172303 | C23 H20 N2 | 324.1626 | -0.74 | C23 H20 N2 | C23 H20 N2 |

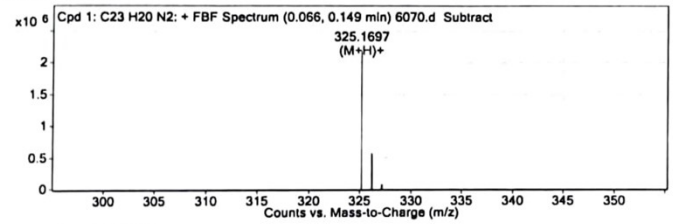
| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C23 H20 N2 | 325.1697 | 0.099 | Find By Formula | 324.1624 |




MS Spectrum




MS Zoomed Spectrum

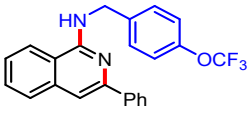



MS Spectrum Peak List

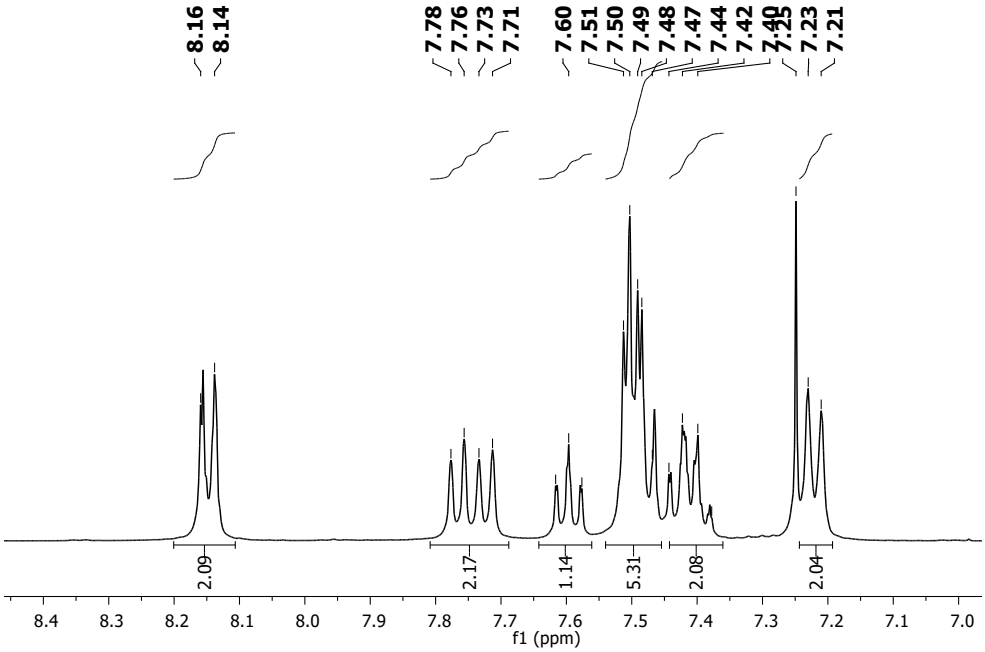
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 325.1697 | 1 | 2172303 | C23H21N2 | (M+H)+ |
| 326.1729 | 1 | 577834.81 | C23H21N2 | (M+H)+ |
| 327.1759 | 1 | 69264.16 | C23H21N2 | (M+H)+ |
| 328.179 | 1 | 4495.24 | C23H21N2 | (M+H)+ |

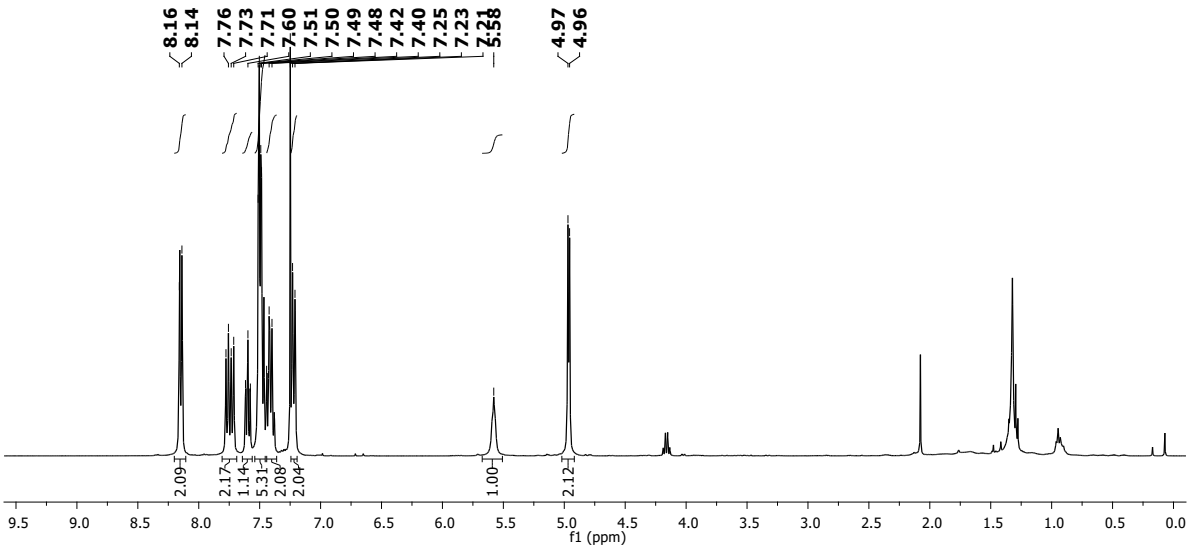
--- End Of Report ---

**$^1$H NMR** (400 MHz, $CDCl_3$,)

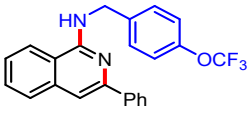



**3-phenyl-N-(4-(trifluoromethoxy)benzyl)isoquinolin-1-amine (4c)**

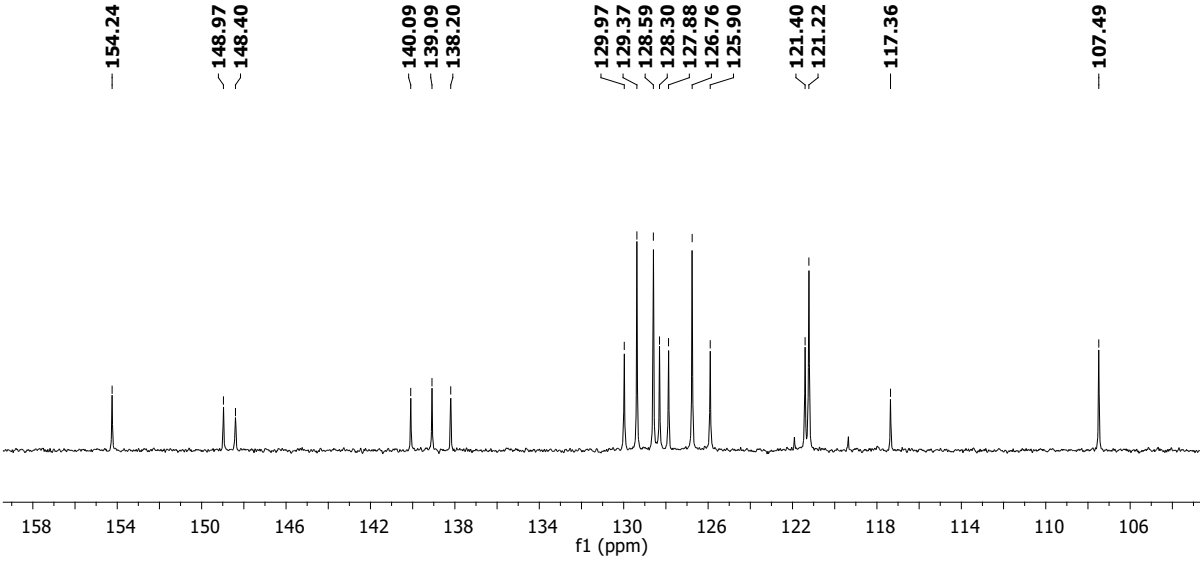


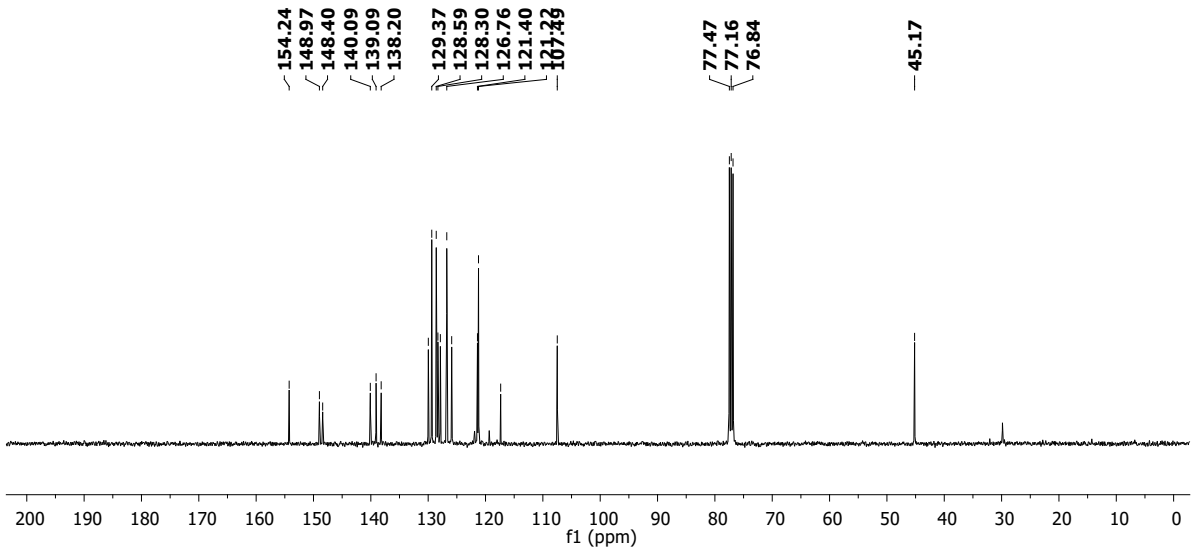



**$^{13}$C NMR** (100 MHz, $CDCl_3$)

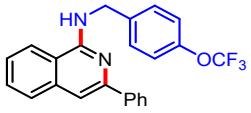



**3-phenyl-N-(4-(trifluoromethoxy)benzyl)isoquinolin-1-amine (4c)**



## HRMS




### 3-phenyl-N-(4-(trifluoromethoxy)benzyl)isoquinolin-1-amine (4c)

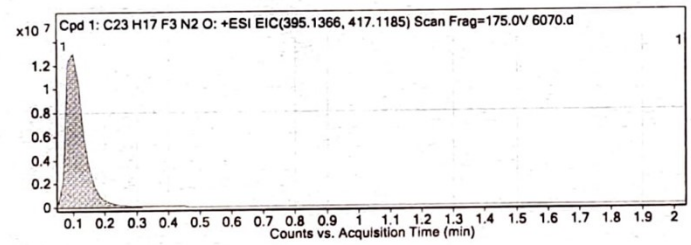
**Qualitative Compound Report**

| | | | |
|---|---|---|---|
| Data File | 6070.d | Sample Name | 6070 |
| Sample Type | Sample | Position | P1-C4 |
| Instrument Name | Instrument 1 | User Name | |
| Acq Method | MS Scan.m | Acquired Time | 22-08-2022 14:22:11 |
| IRM Calibration Status | [redacted] | DA Method | Default.m |
| Comment | | | |
| Sample Group | | Info. | 3 |
| Acquisition SW Version | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

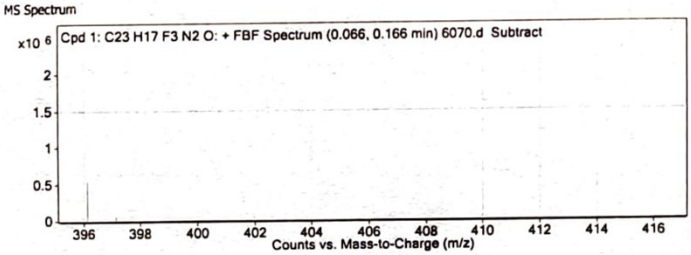
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C23 H17 F3 N2 O | 0.099 | 394.129 | 2014655 | C23 H17 F3 N2 O | 394.1293 | -0.68 | C23 H17 F3 N2 O | C23 H17 F3 N2 O |

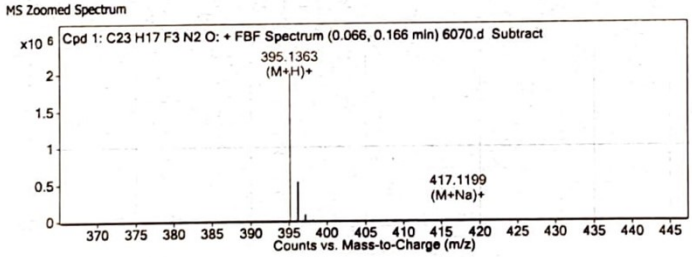
| Compound Label | m/z | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C23 H17 F3 N2 O | 395.1363 | 0.099 | Find By Formula | 394.129 |




MS Spectrum




MS Zoomed Spectrum

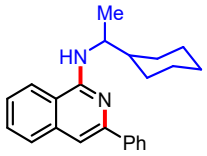



**MS Spectrum Peak List**

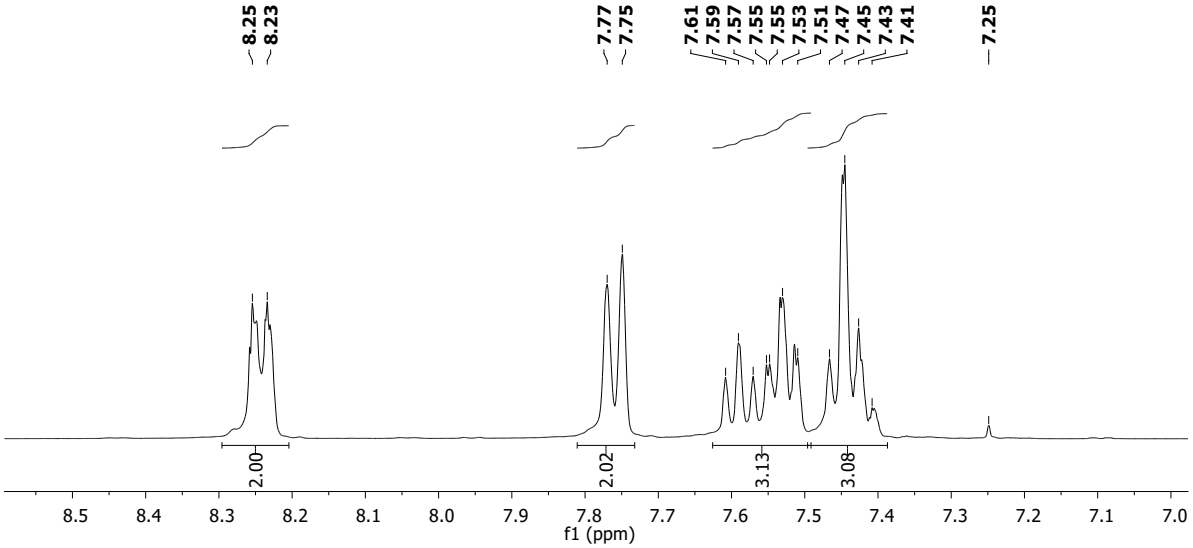
| m/z | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 395.1363 | 1 | 2014654.5 | C23H18F3N2O | (M+H)+ |
| 396.1396 | 1 | 526486.44 | C23H18F3N2O | (M+H)+ |
| 397.1419 | 1 | 65863.29 | C23H18F3N2O | (M+H)+ |
| 398.1454 | 1 | 4963.21 | C23H18F3N2O | (M+H)+ |
| 417.1199 | 1 | 503.01 | C23H17F3N2NaO | (M+Na)+ |

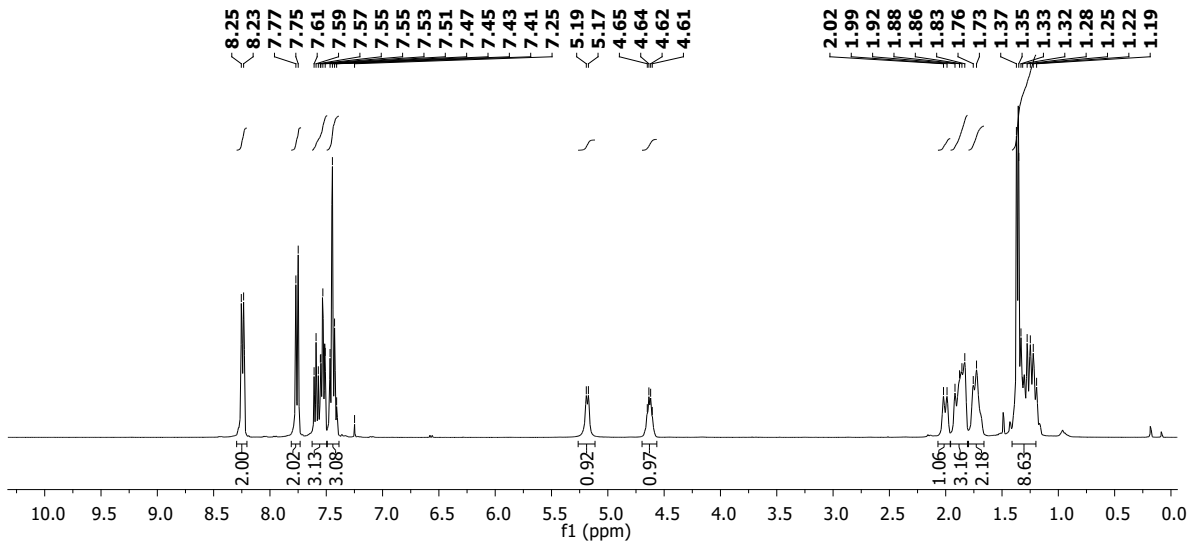
--- End Of Report ---

**$^1$H NMR** (400 MHz, $CDCl_3$)

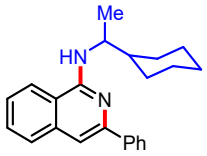



***N*-(1-cyclohexylethyl)-3-phenylisoquinolin-1-amine (4d)**

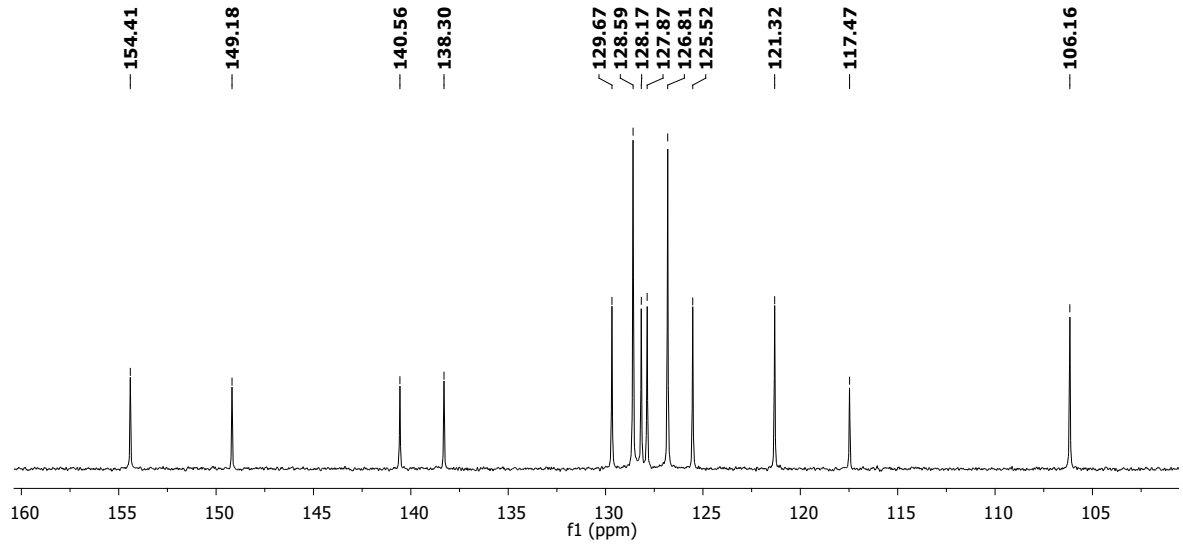


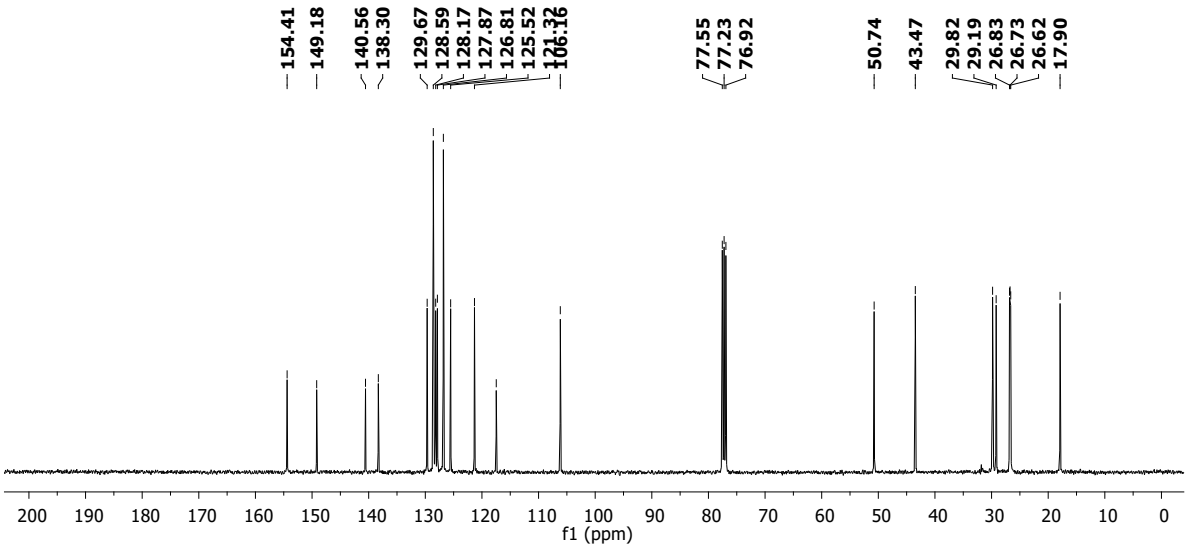



**$^{13}$C NMR** (100 MHz, $CDCl_3$)

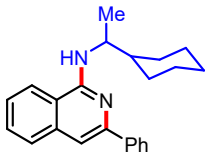



***N*-(1-cyclohexylethyl)-3-phenylisoquinolin-1-amine (4d)**



## HRMS




### *N*-(1-cyclohexylethyl)-3-phenylisoquinolin-1-amine (4d)

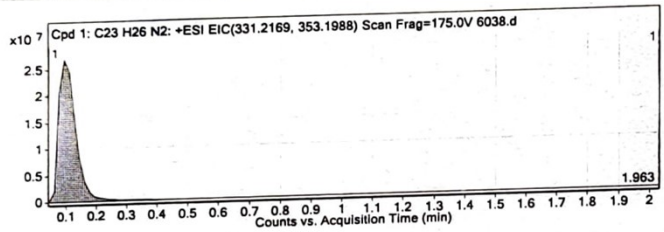
**Qualitative Compound Report**

| | | | |
|---|---|---|---|
| Data File | 6038.d | Sample Name | 6038 |
| Sample Type | Sample | Position | P1-C2 |
| Instrument Name | Instrument 1 | User Name | |
| Acq Method | MS Scan.m | Acquired Time | 22-08-2022 14:14:43 |
| IRM Calibration Status | [redacted] | DA Method | Default.m |
| Comment | | | |
| Sample Group | Info. | 3 | |
| Acquisition SW Version | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

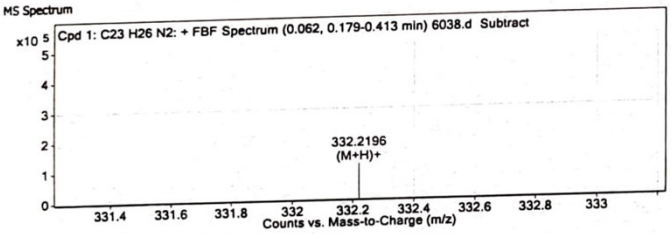
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C23 H26 N2 | 0.096 | 330.2091 | 454781 | C23 H26 N2 | 330.2096 | -1.66 | C23 H26 N2 | C23 H26 N2 |

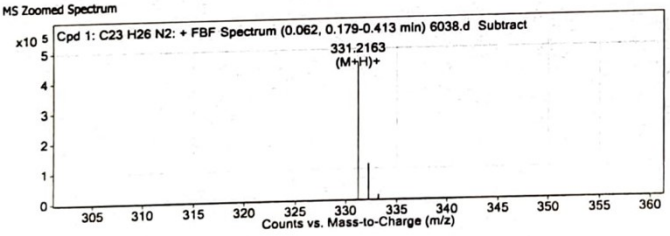
| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C23 H26 N2 | 331.2163 | 0.096 | Find By Formula | 330.2091 |




MS Spectrum




MS Zoomed Spectrum

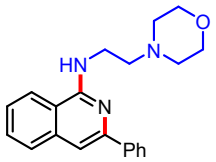



**MS Spectrum Peak List**

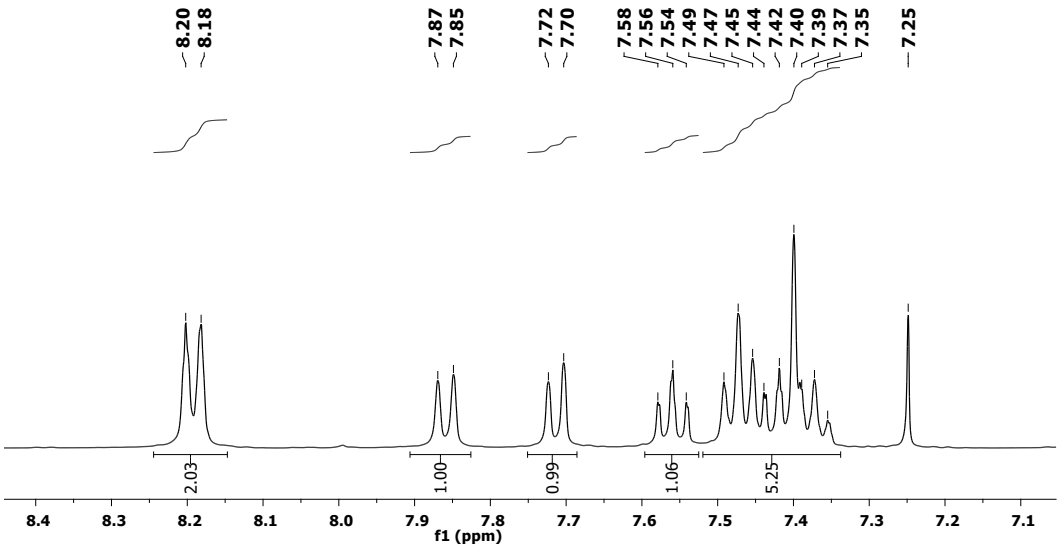
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 331.2163 | 1 | 454781.16 | C23H27N2 | (M+H)+ |
| 332.2196 | 1 | 115788.58 | C23H27N2 | (M+H)+ |
| 333.2225 | 1 | 14064.04 | C23H27N2 | (M+H)+ |

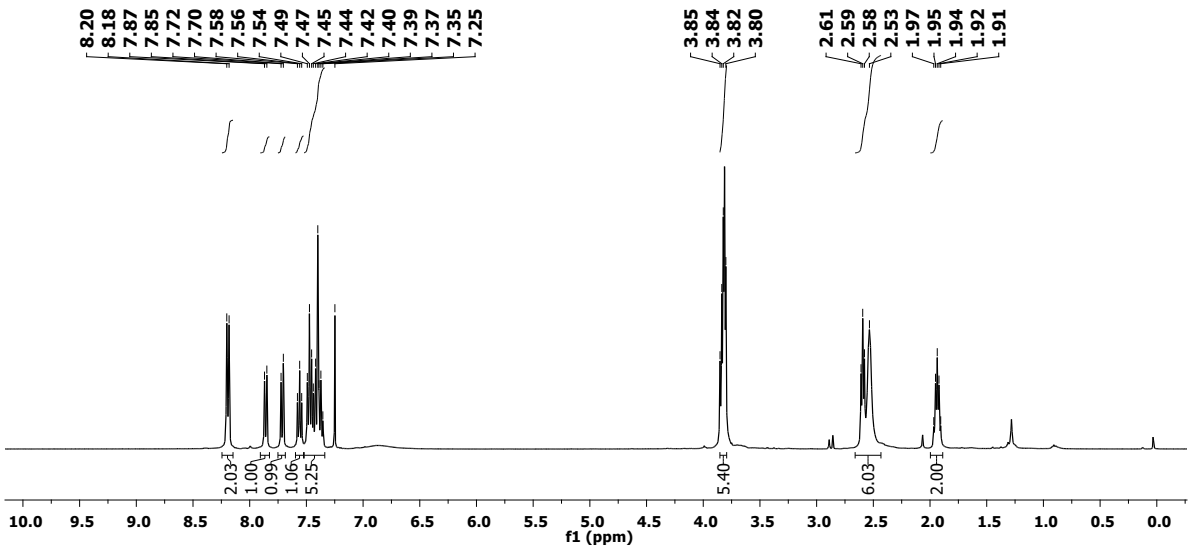
--- End Of Report ---

**$^1$H NMR** (400 MHz, $CDCl_3$)

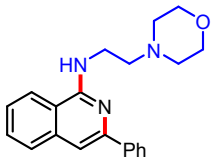



***N*-(2-morpholinoethyl)-3-phenylisoquinolin-1-amine (4e)**

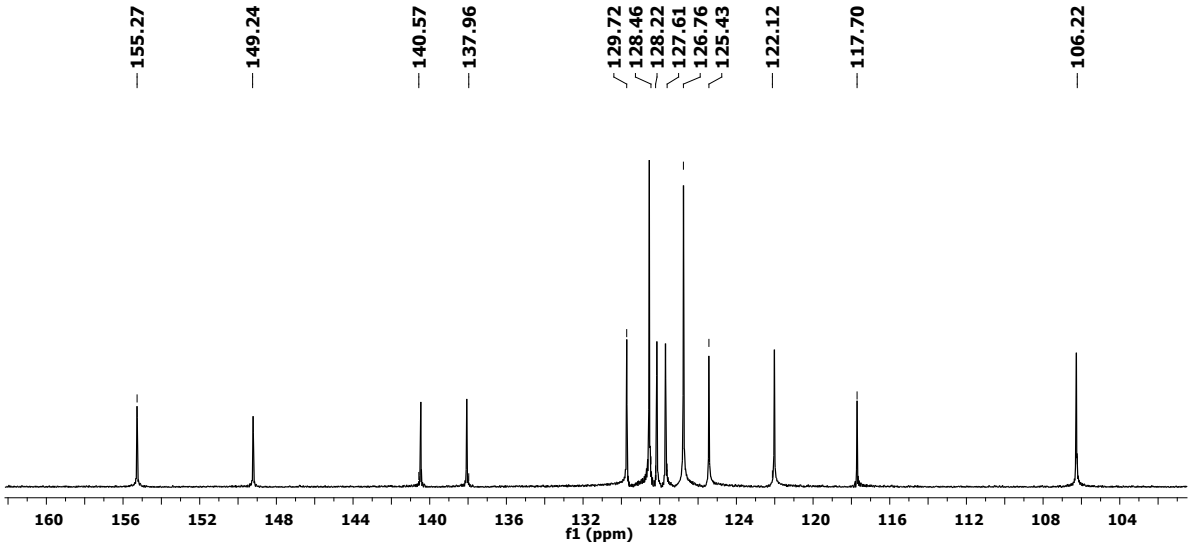


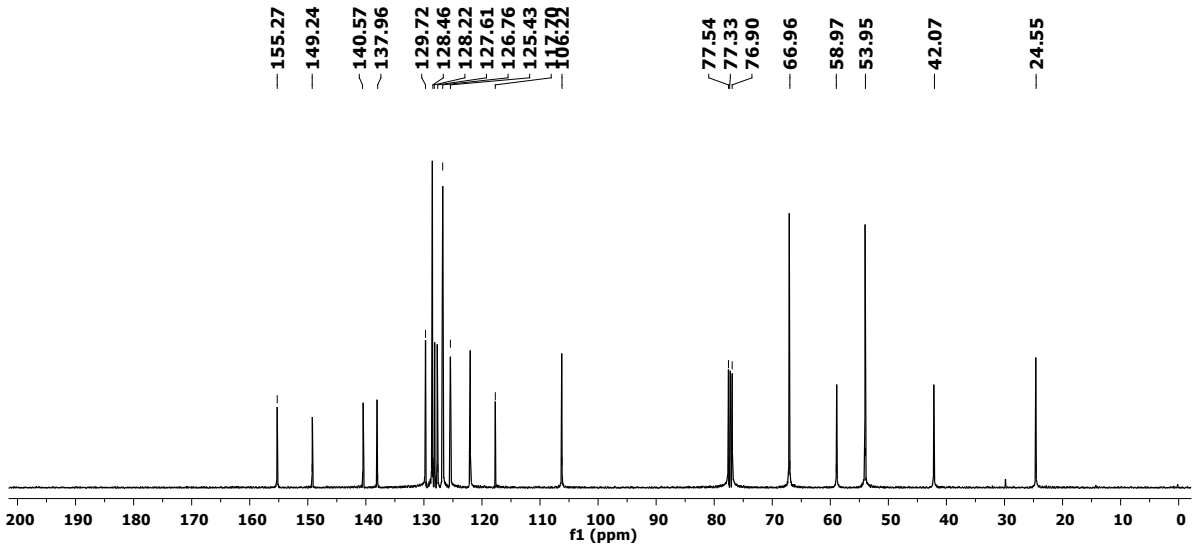



**$^{13}$C NMR** (100 MHz, $CDCl_3$)

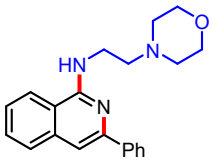



***N*-(2-morpholinoethyl)-3-phenylisoquinolin-1-amine (4e)**



# HRMS




## *N*-(2-morpholinoethyl)-3-phenylisoquinolin-1-amine (4e)

### Qualitative Compound Report

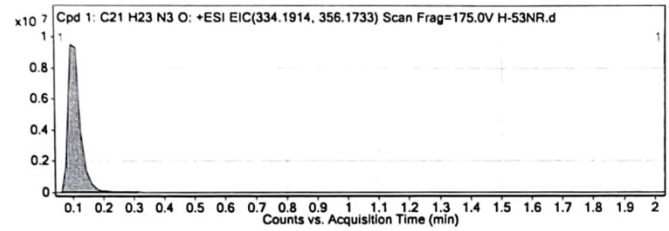
| | | | |
|---|---|---|---|
| **Data File** | H-53NR.d | **Sample Name** | H-53NR |
| **Sample Type** | Sample | **Position** | P1-A7 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | MS Scan.m | **Acquired Time** | 30-08-2022 16:46:11 |
| **IRM Calibration Status** | [redacted] | **DA Method** | Default.m |
| **Comment** | | | |

| | | | |
|---|---|---|---|
| **Sample Group** | | **Info.** | 3 |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

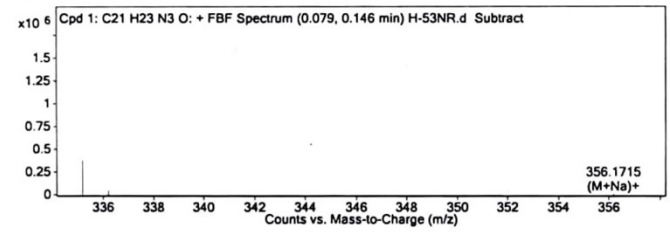
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C21 H23 N3 O | 0.096 | 333.1833 | 1550251 | C21 H23 N3 O | 333.1841 | -2.3 | C21 H23 N3 O | C21 H23 N3 O |

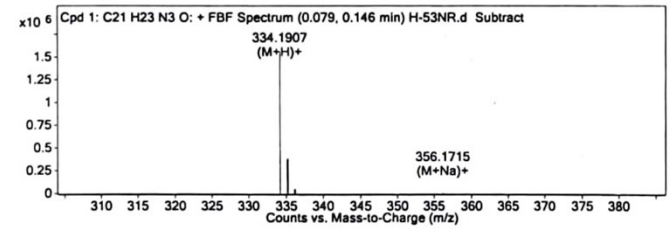
| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C21 H23 N3 O | 334.1907 | 0.096 | Find By Formula | 333.1833 |




MS Spectrum




MS Zoomed Spectrum

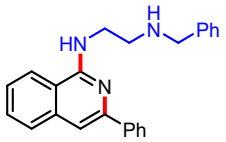



**MS Spectrum Peak List**

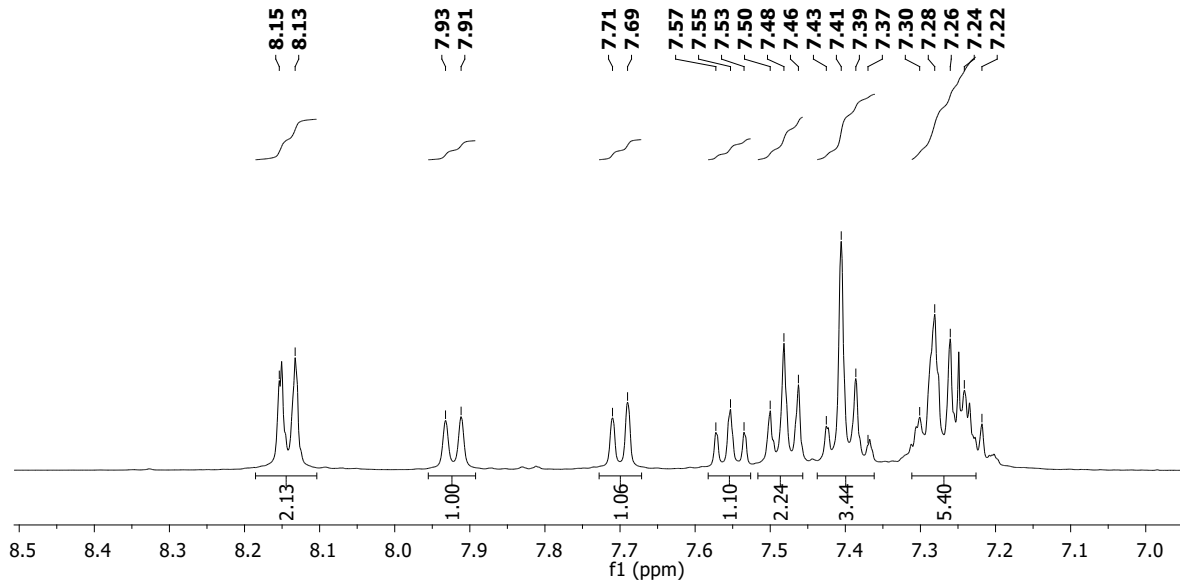
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 334.1907 | 1 | 1550251.38 | C21H24N3O | (M+H)+ |
| 335.1938 | 1 | 382346.13 | C21H24N3O | (M+H)+ |
| 336.1954 | 1 | 46585.23 | C21H24N3O | (M+H)+ |
| 337.1965 | 1 | 4537.2 | C21H24N3O | (M+H)+ |
| 356.1715 | 1 | 5052.91 | C21H23N3NaO | (M+Na)+ |
| 357.1737 | 1 | 1270.61 | C21H23N3NaO | (M+Na)+ |
| 358.1853 | 1 | 126.17 | C21H23N3NaO | (M+Na)+ |

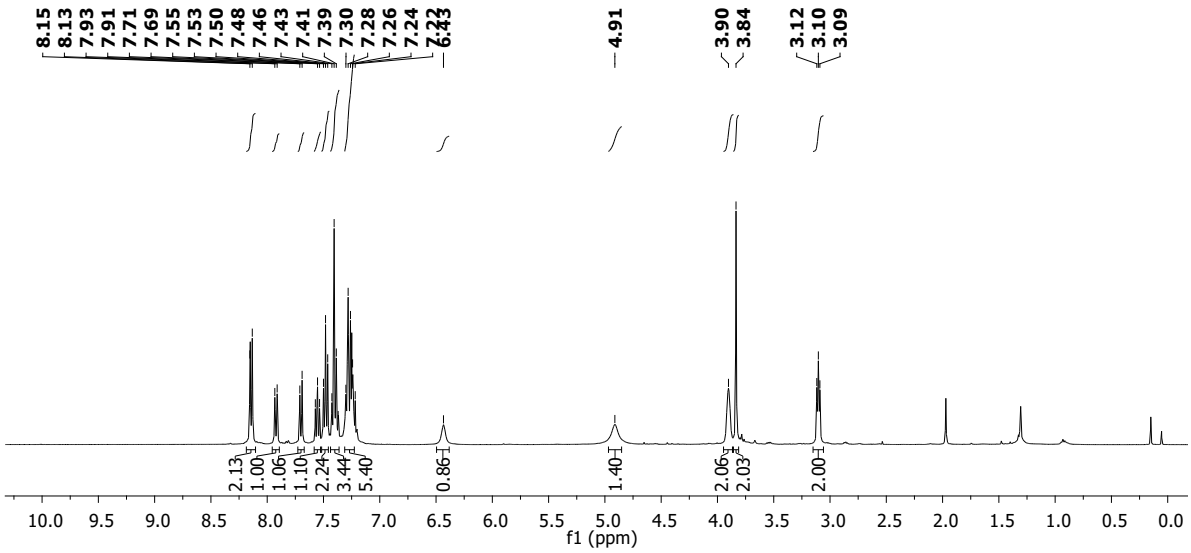
--- End Of Report ---

**$^1$H NMR** (400 MHz, $CDCl_3$)

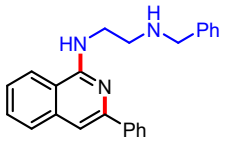



***N*$^1$-benzyl-*N*$^2$-(3-phenylisoquinolin-1-yl)ethane-1,2-diamine (4f)**

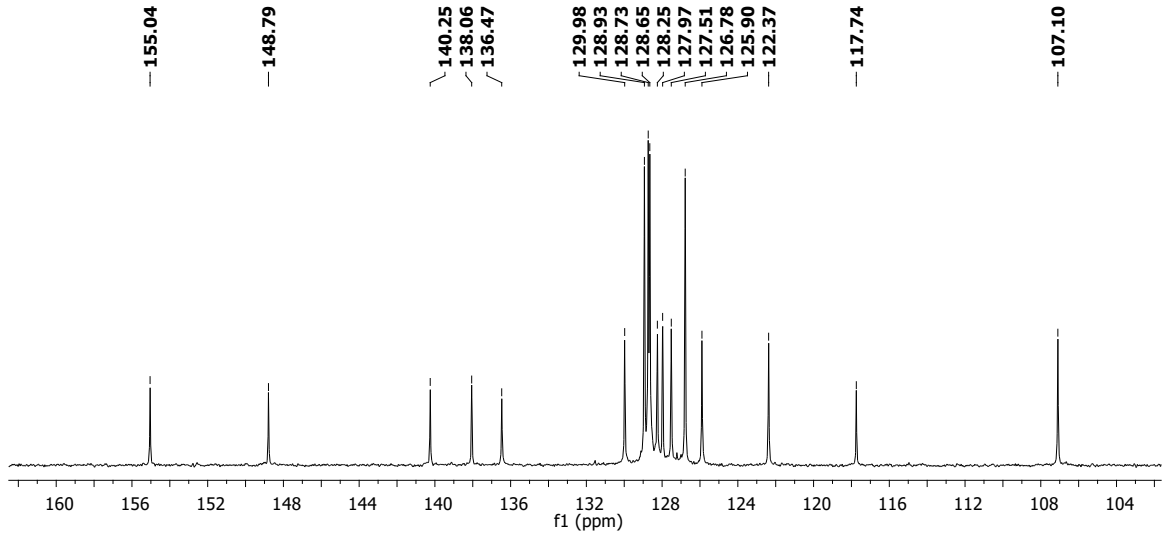


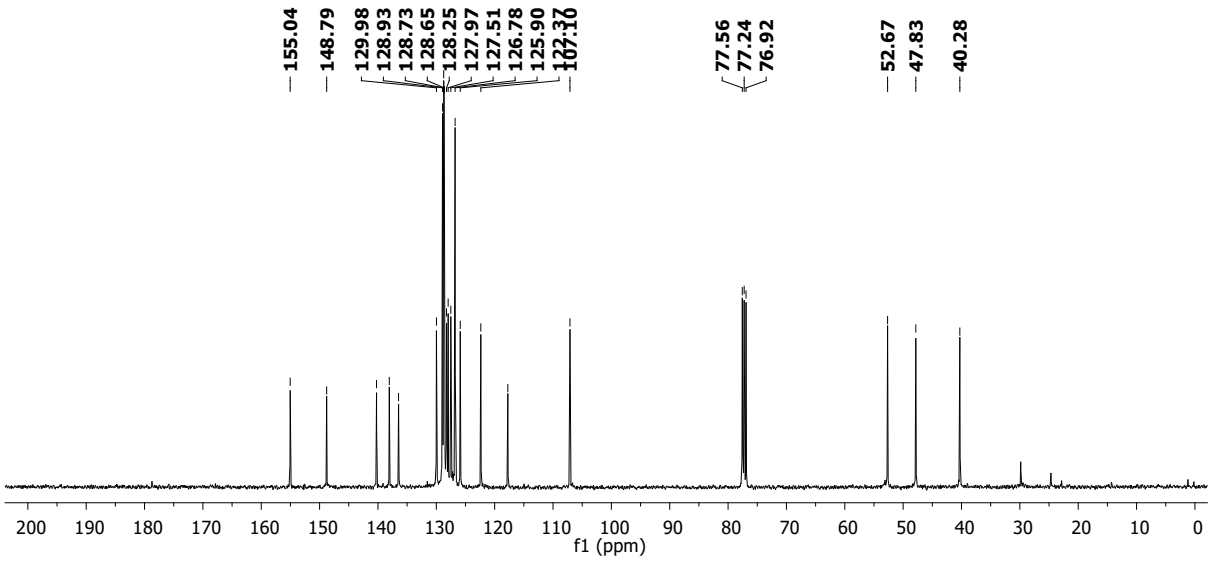



**$^{13}$C NMR** (100 MHz, $CDCl_3$)

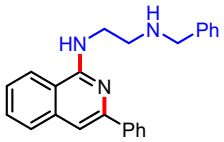



***N*$^1$-benzyl-*N*$^2$-(3-phenylisoquinolin-1-yl)ethane-1,2-diamine (4f)**



## HRMS




### $N^1$-benzyl-$N^2$-(3-phenylisoquinolin-1-yl)ethane-1,2-diamine (4f)

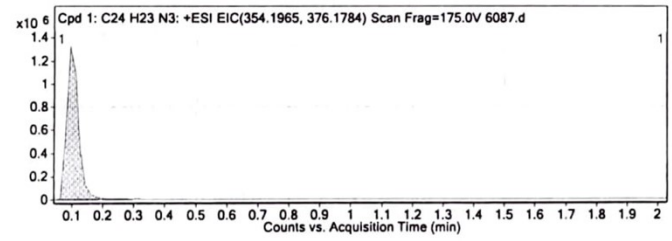
**Qualitative Compound Report**

| | | | |
|---|---|---|---|
| **Data File** | 6087.d | **Sample Name** | 6087 |
| **Sample Type** | Sample | **Position** | P1-A1 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | MS Scan.m | **Acquired Time** | 27-08-2022 12:03:43 |
| **IRM Calibration Status** | [redacted] | **DA Method** | Default.m |
| **Comment** | | | |
| **Sample Group** | | **Info.** | 3 |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

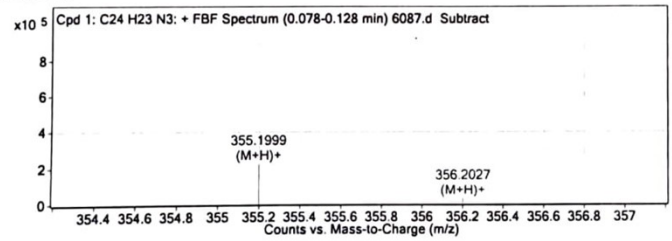
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C24 H23 N3 | 0.095 | 353.1898 | 828849 | C24 H23 N3 | 353.1892 | 1.62 | C24 H23 N3 | C24 H23 N3 |

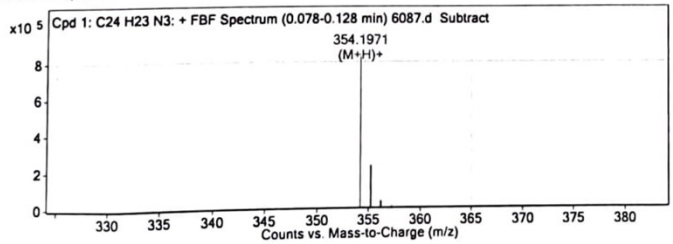
| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C24 H23 N3 | 354.1971 | 0.095 | Find By Formula | 353.1898 |




MS Spectrum




MS Zoomed Spectrum

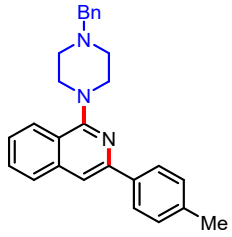



**MS Spectrum Peak List**

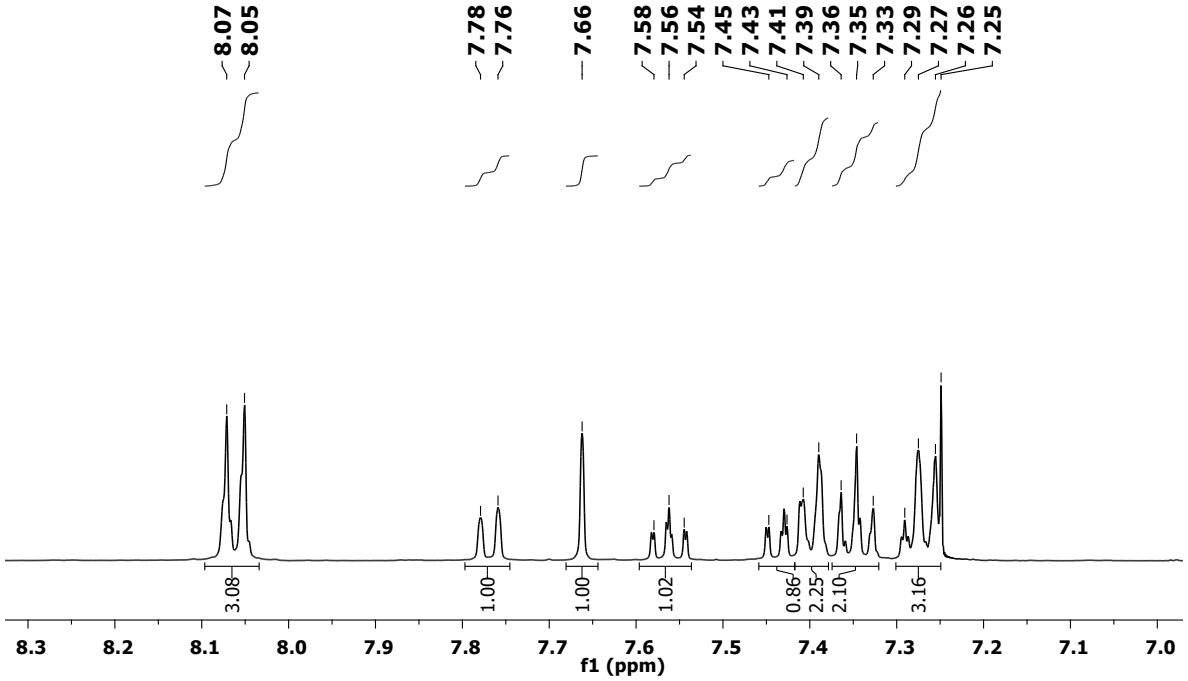
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 354.1971 | 1 | 828848.81 | C24H24N3 | (M+H)+ |
| 355.1999 | 1 | 221484.63 | C24H24N3 | (M+H)+ |
| 356.2027 | 1 | 27831 | C24H24N3 | (M+H)+ |
| 357.2089 | 1 | 2425.44 | C24H24N3 | (M+H)+ |

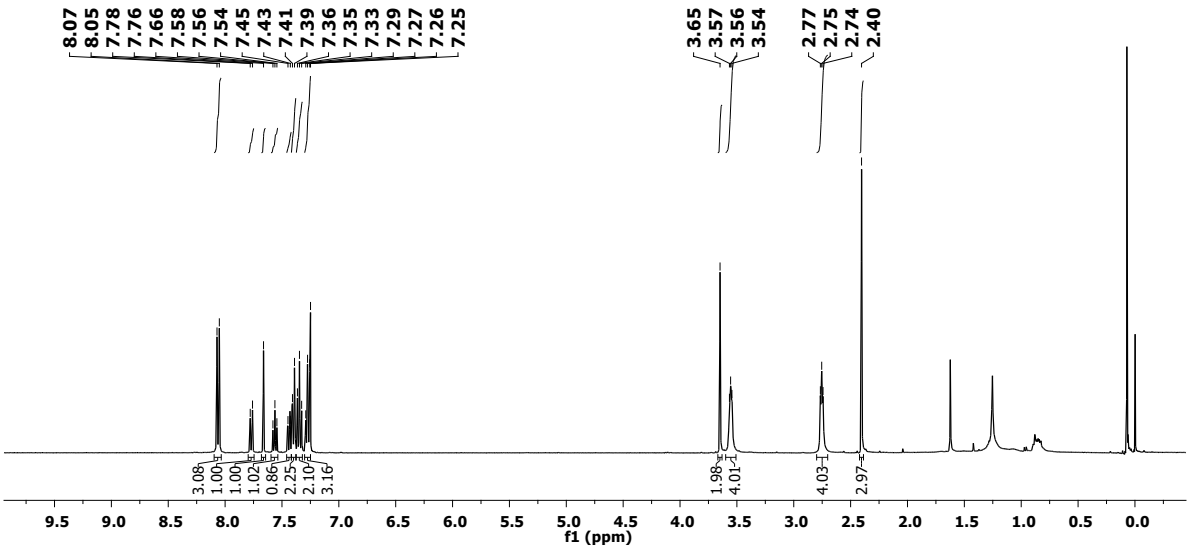
--- End Of Report ---

**$^1$H NMR** (400 MHz, $CDCl_3$)

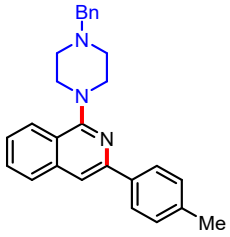



**1-(4-benzylpiperazin-1-yl)-3-(p-tolyl)isoquinoline (5a)**

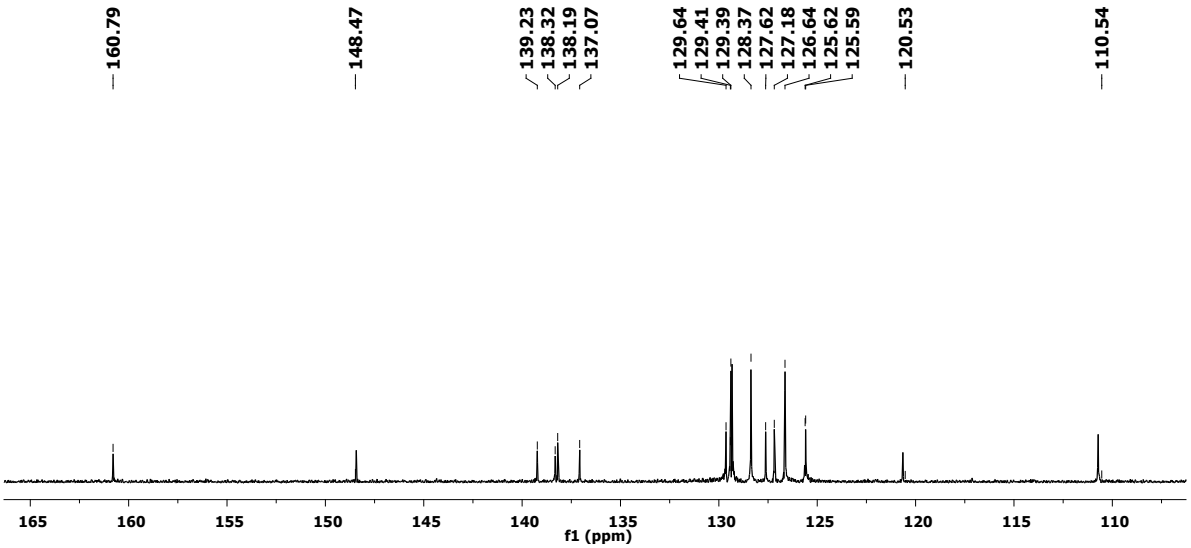


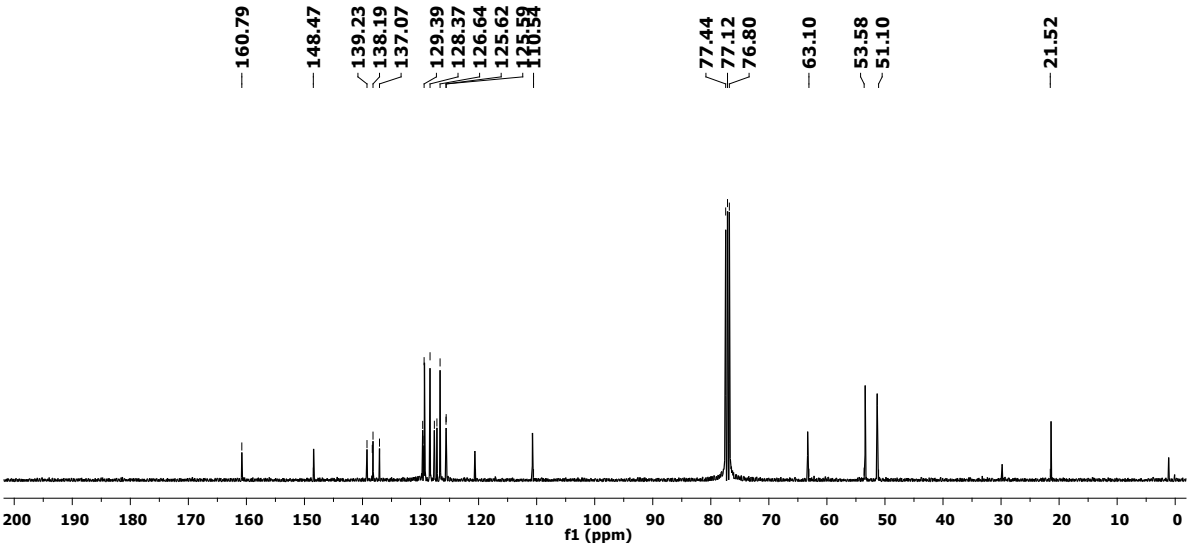



**$^{13}$C NMR** (100 MHz, $CDCl_3$)

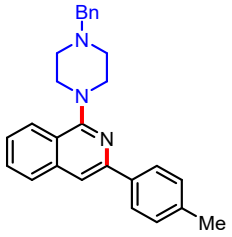



**1-(4-benzylpiperazin-1-yl)-3-(p-tolyl)isoquinoline (5a)**



# HRMS




## 1-(4-benzylpiperazin-1-yl)-3-(p-tolyl)isoquinoline (5a)

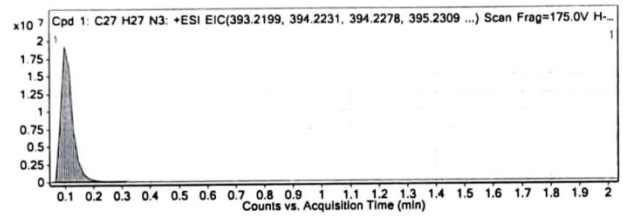
### Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | H-22BR.d | **Sample Name** | H-22BR |
| **Sample Type** | Sample | **Position** | P1-A6 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | MS Scan.m | **Acquired Time** | 30-08-2022 16:43:27 |
| **IRM Calibration Status** | [redacted] | **DA Method** | Default.m |
| **Comment** | | | |
| **Sample Group** | | **Info.** | 3 |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

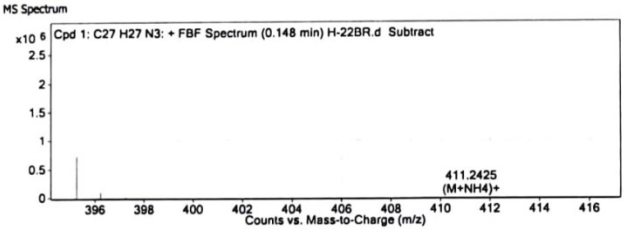
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C27 H27 N3 | 0.098 | 393.2195 | 2301118 | C27 H27 N3 | 393.2205 | -2.48 | C27 H27 N3 | C27 H27 N3 |

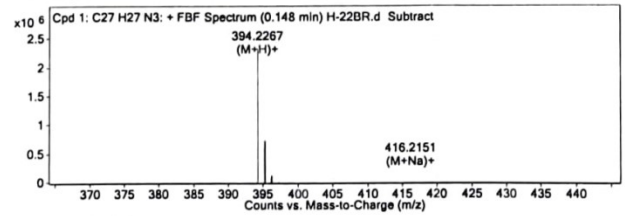
| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C27 H27 N3 | 394.2267 | 0.098 | Find By Formula | 393.2195 |




MS Spectrum




MS Zoomed Spectrum

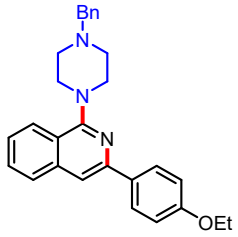



**MS Spectrum Peak List**

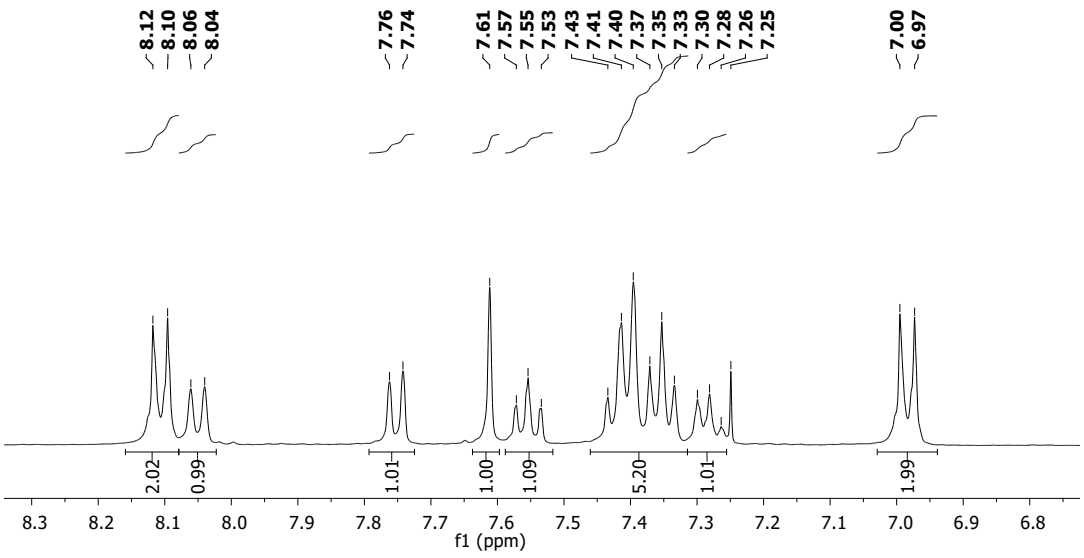
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 394.2267 | 1 | 2301117.5 | C27H28N3 | (M+H)+ |
| 395.2301 | 1 | 735334.69 | C27H28N3 | (M+H)+ |
| 396.2332 | 1 | 101582.48 | C27H28N3 | (M+H)+ |
| 397.2361 | 1 | 8996.79 | C27H28N3 | (M+H)+ |
| 411.2425 | 1 | 847.5 | C27H31N4 | (M+NH4)+ |
| 412.2406 | 1 | 434.63 | C27H31N4 | (M+NH4)+ |
| 416.2151 | 1 | 3233.88 | C27H27N3Na | (M+Na)+ |
| 417.2143 | 1 | 772.43 | C27H27N3Na | (M+Na)+ |

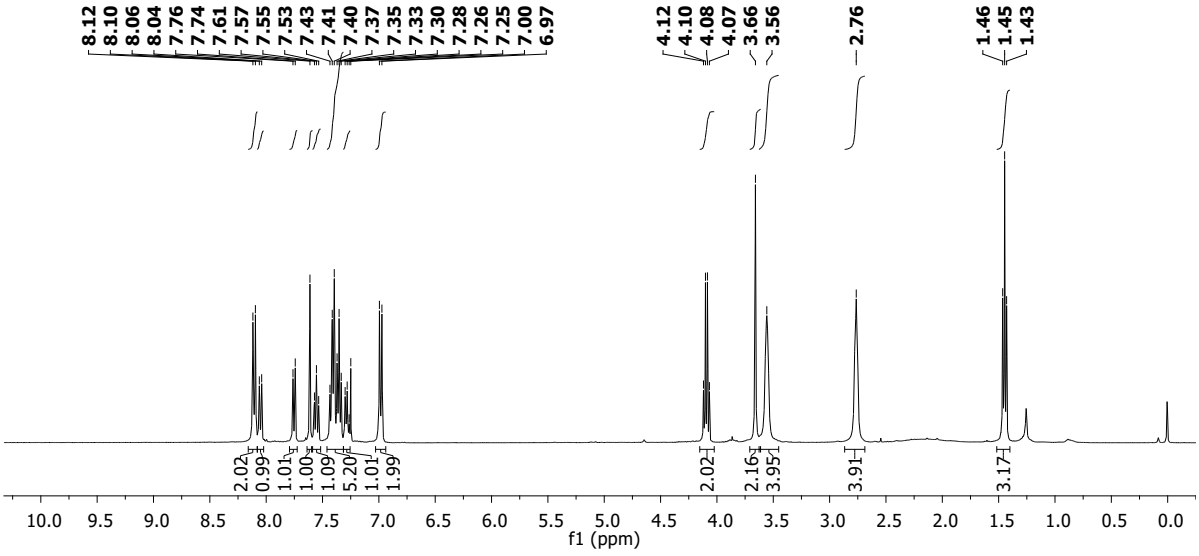
--- End Of Report ---

**$^1$H NMR** (400 MHz, $CDCl_3$)

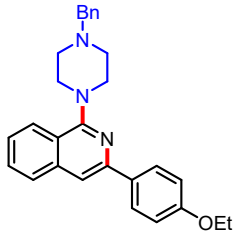



**1-(4-benzylpiperazin-1-yl)-3-(4-ethoxyphenyl)isoquinoline (5b)**

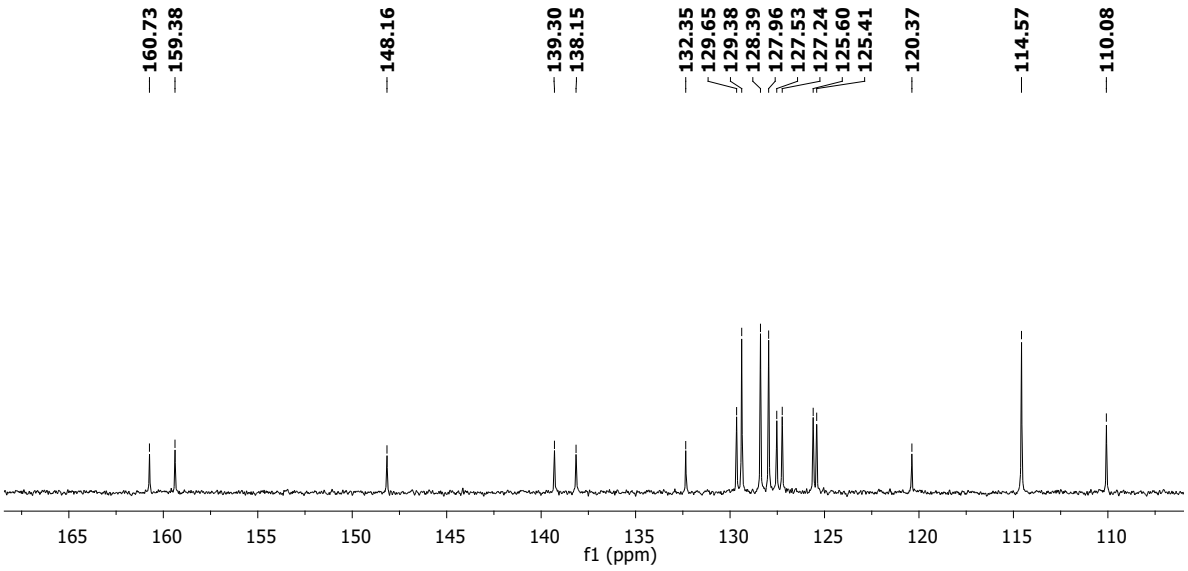


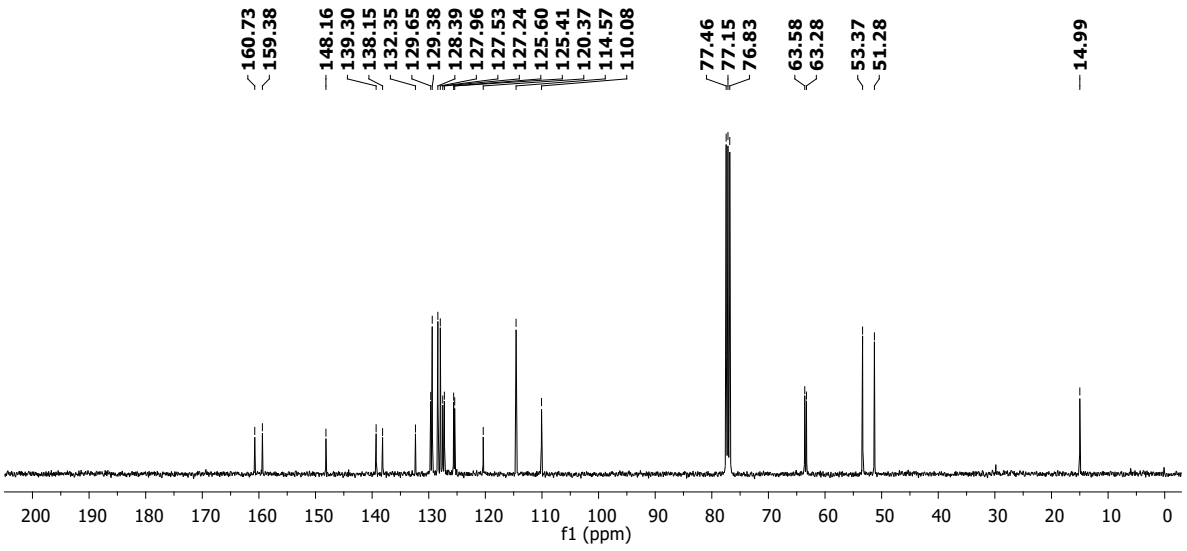



**$^{13}$C NMR** (100 MHz, $CDCl_3$)

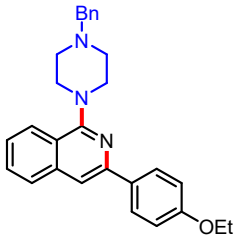



**1-(4-benzylpiperazin-1-yl)-3-(4-ethoxyphenyl)isoquinoline (5b)**



# HRMS




## 1-(4-benzylpiperazin-1-yl)-3-(4-ethoxyphenyl)isoquinoline (5b)

### Qualitative Compound Report

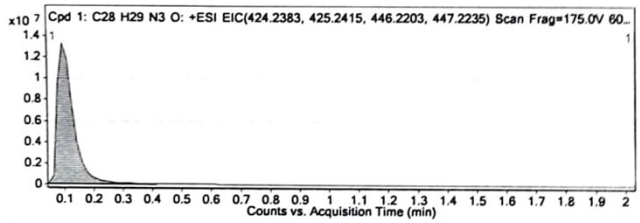
| | | | |
|---|---|---|---|
| **Data File** | 6038.d | **Sample Name** | 6038 |
| **Sample Type** | Sample | **Position** | P1-C2 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | MS Scan.m | **Acquired Time** | 22-08-2022 14:14:43 |
| **IRM Calibration Status** | [redacted] | **DA Method** | Default.m |
| **Comment** | | | |

| | | | |
|---|---|---|---|
| **Sample Group** | | **Info.** | 3 |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

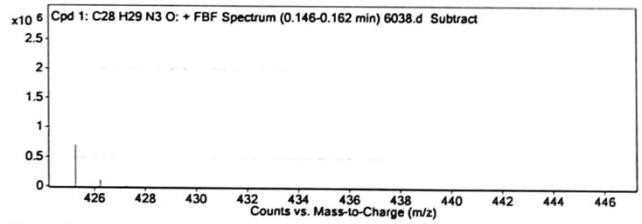
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C28 H29 N3 O | 0.096 | 423.2304 | 2303110 | C28 H29 N3 O | 423.2311 | -1.67 | C28 H29 N3 O | C28 H29 N3 O |

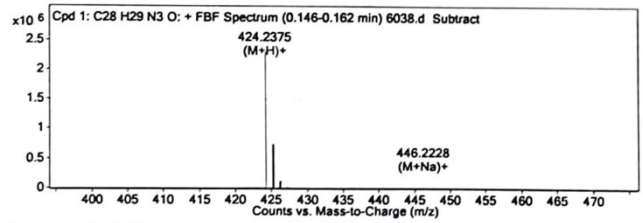
| Compound Label | m/z | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C28 H29 N3 O | 424.2375 | 0.096 | Find By Formula | 423.2304 |




MS Spectrum




MS Zoomed Spectrum

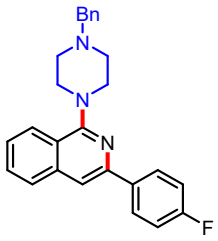



**MS Spectrum Peak List**

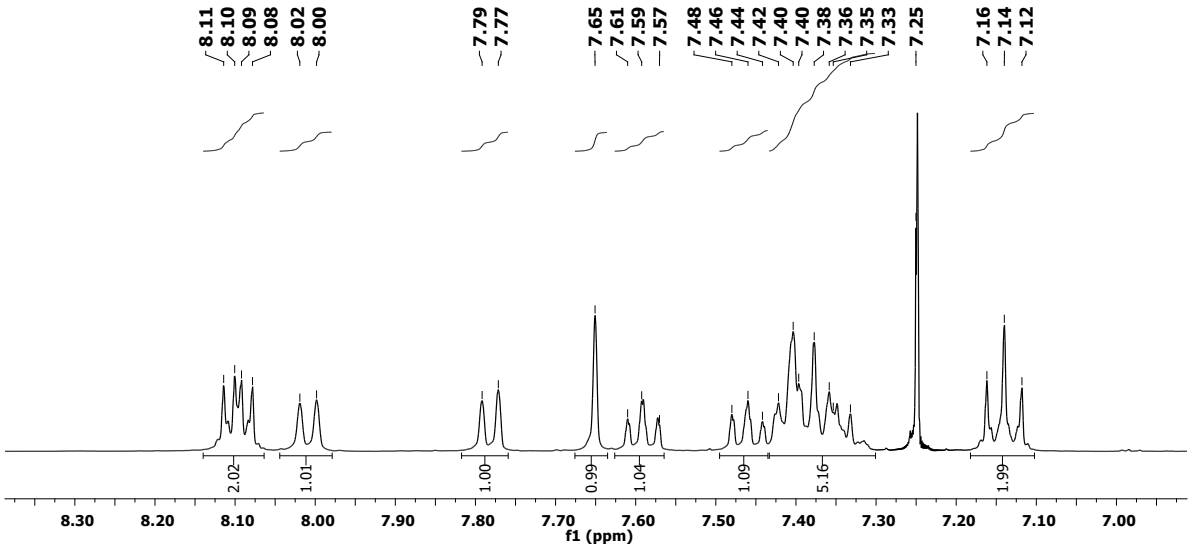
| m/z | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 424.2375 | 1 | 2303109.5 | C28H30N3O | (M+H)+ |
| 425.2412 | 1 | 700857.5 | C28H30N3O | (M+H)+ |
| 426.2433 | 1 | 116324.69 | C28H30N3O | (M+H)+ |
| 427.2461 | 1 | 12653.43 | C28H30N3O | (M+H)+ |
| 428.2462 | 1 | 1169.12 | C28H30N3O | (M+H)+ |
| 446.2228 | 1 | 2561.41 | C28H29N3NaO | (M+Na)+ |
| 447.2221 | 1 | 958.18 | C28H29N3NaO | (M+Na)+ |

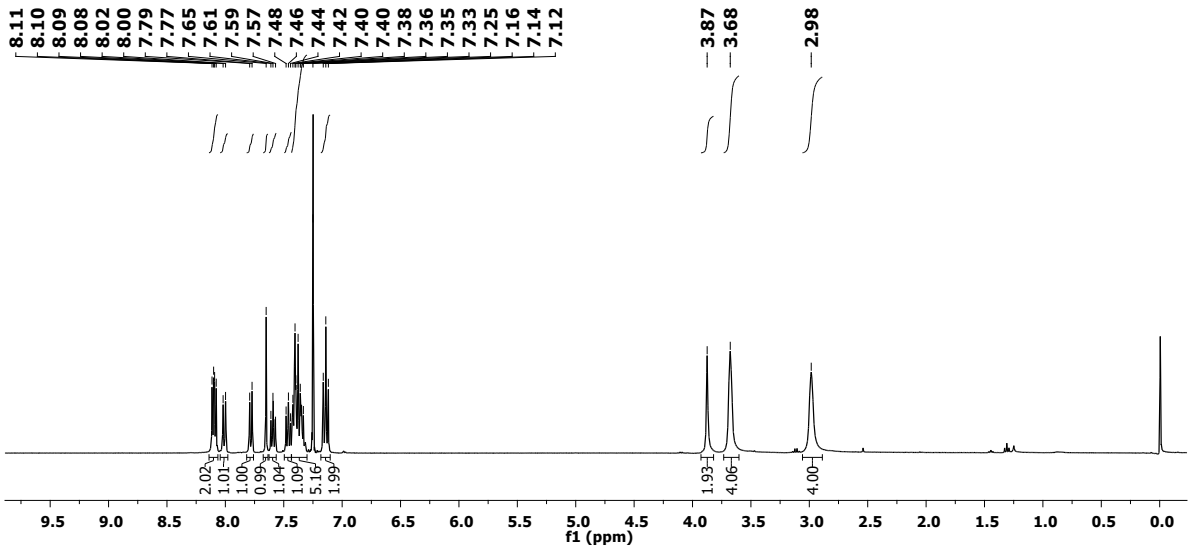
--- End Of Report ---

**$^1$H NMR** (400 MHz, $CDCl_3$)

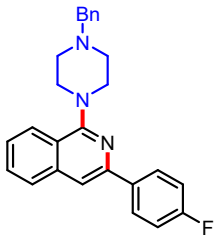



**1-(4-benzylpiperazin-1-yl)-3-(4-fluorophenyl)isoquinoline (5c)**

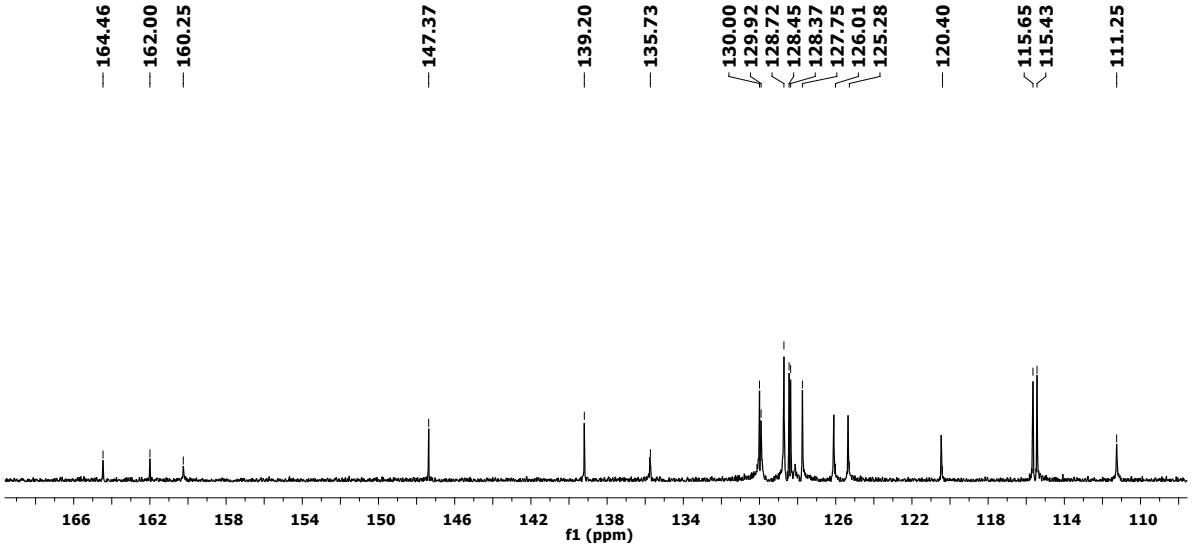


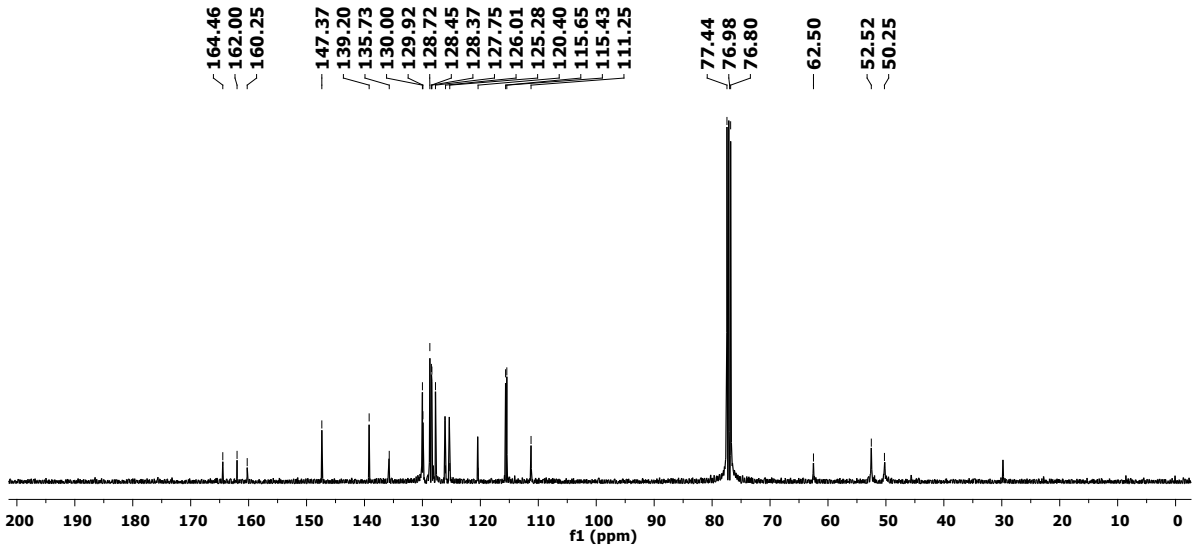



**$^{13}$C NMR** (100 MHz, $CDCl_3$)

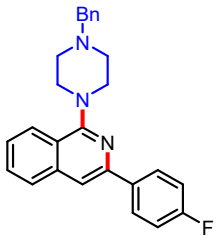



**1-(4-benzylpiperazin-1-yl)-3-(4-fluorophenyl)isoquinoline (5c)**



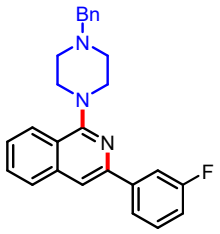



**HRMS**

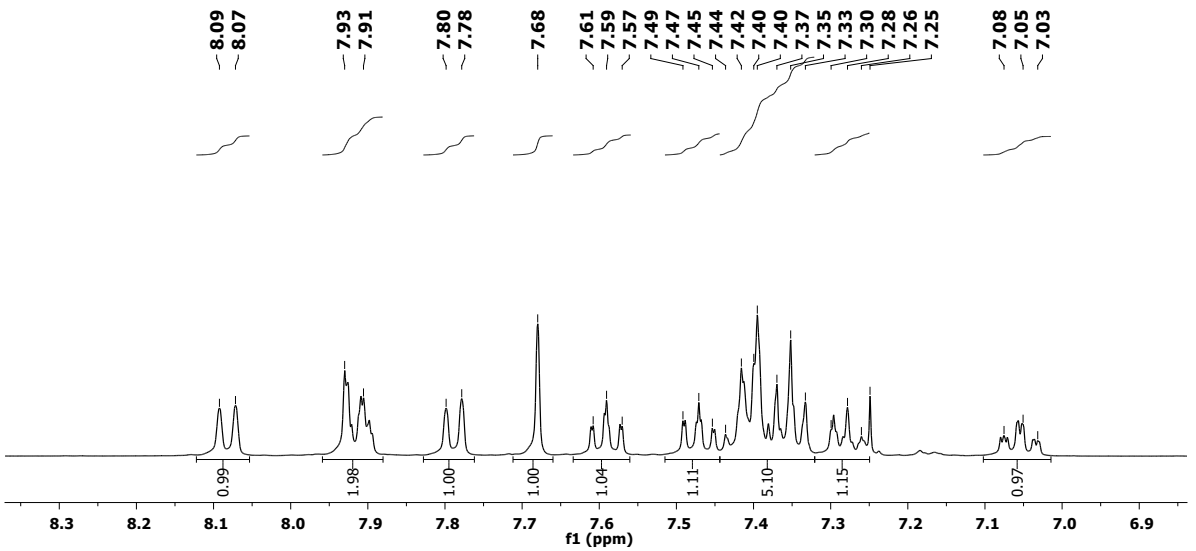


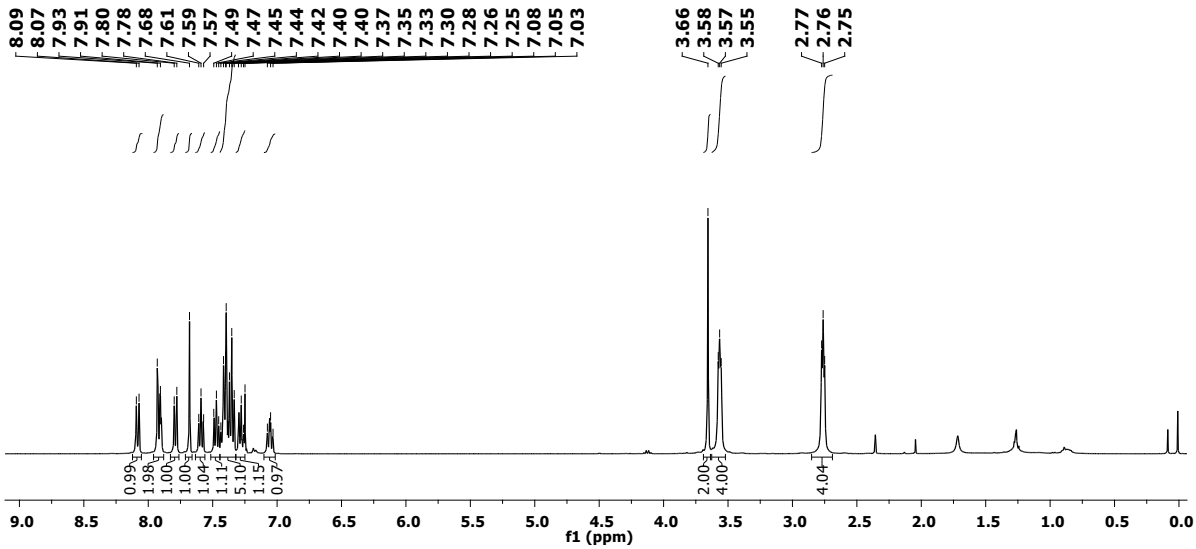

**1-(4-benzylpiperazin-1-yl)-3-(4-fluorophenyl)isoquinoline (5c)**

**$^1$H NMR** (400 MHz, $CDCl_3$)

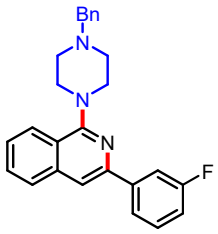



**1-(4-benzylpiperazin-1-yl)-3-(3-fluorophenyl)isoquinoline (5d)**

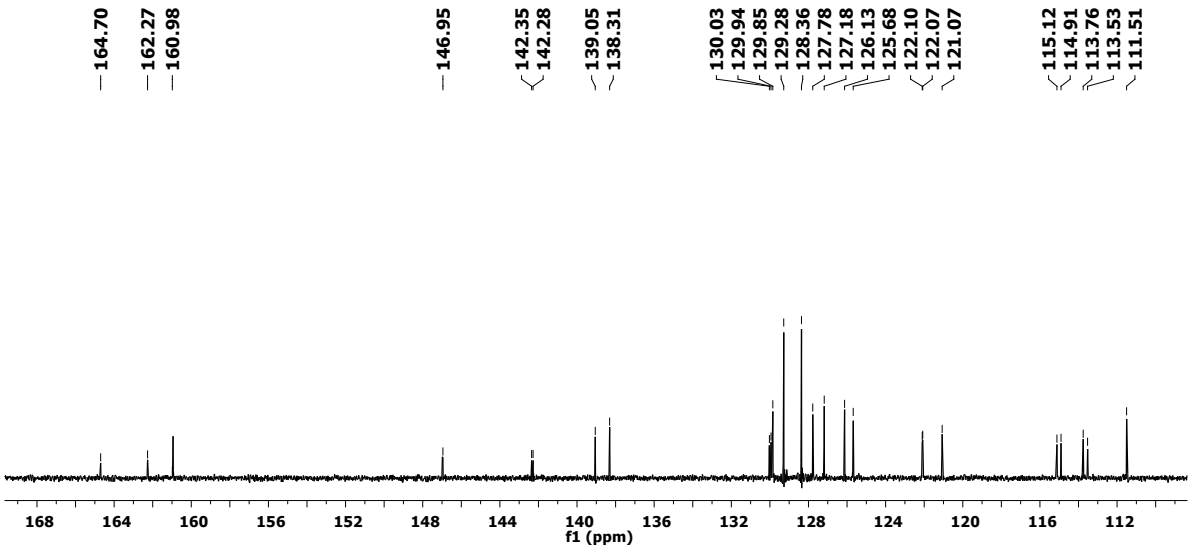


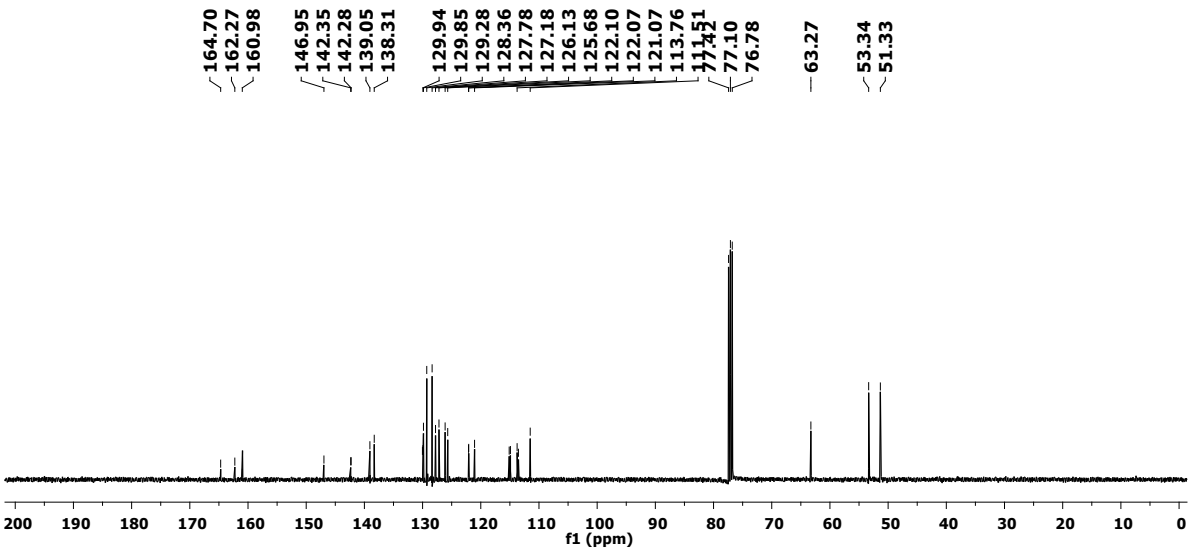



**$^{13}$C NMR** (100 MHz, $CDCl_3$)

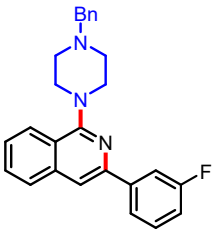



**1-(4-benzylpiperazin-1-yl)-3-(3-fluorophenyl)isoquinoline (5d)**



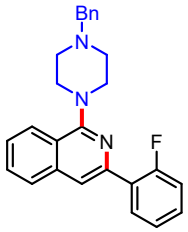



**HRMS**

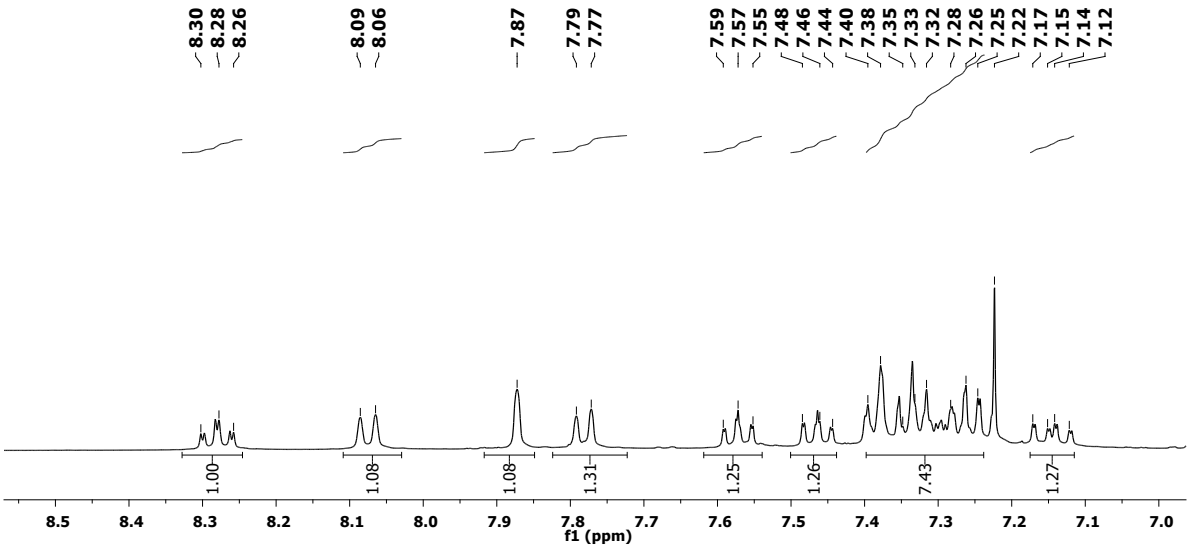


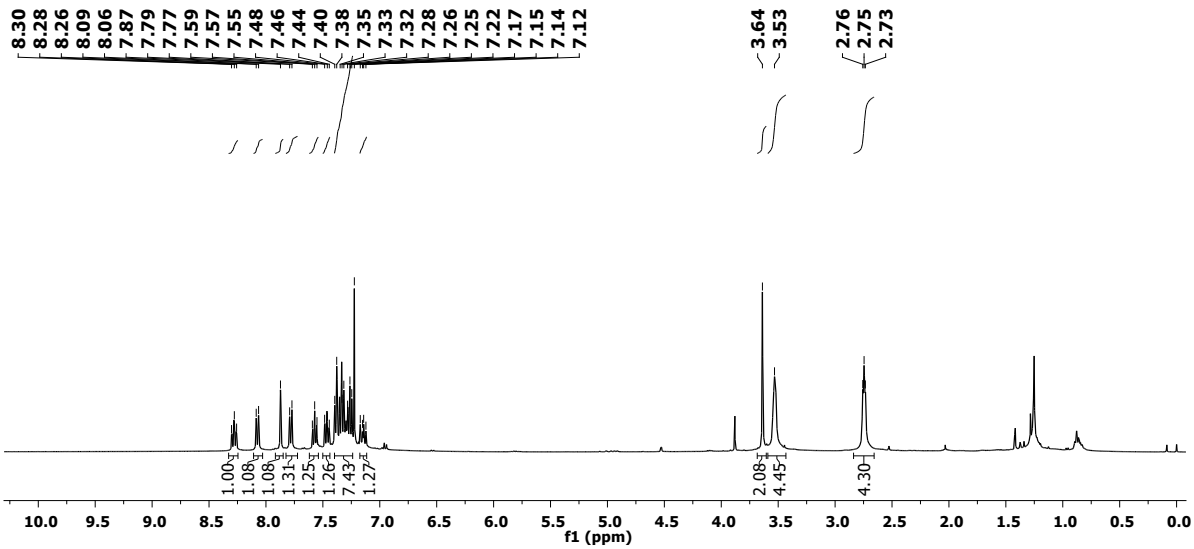

**1-(4-benzylpiperazin-1-yl)-3-(3-fluorophenyl)isoquinoline (5d)**

**$^1$H NMR** (400 MHz, $CDCl_3$)

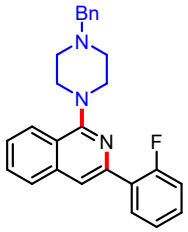



**1-(4-Benzylpiperazin-1-yl)-3-(2-fluorophenyl)isoquinoline (5e)**

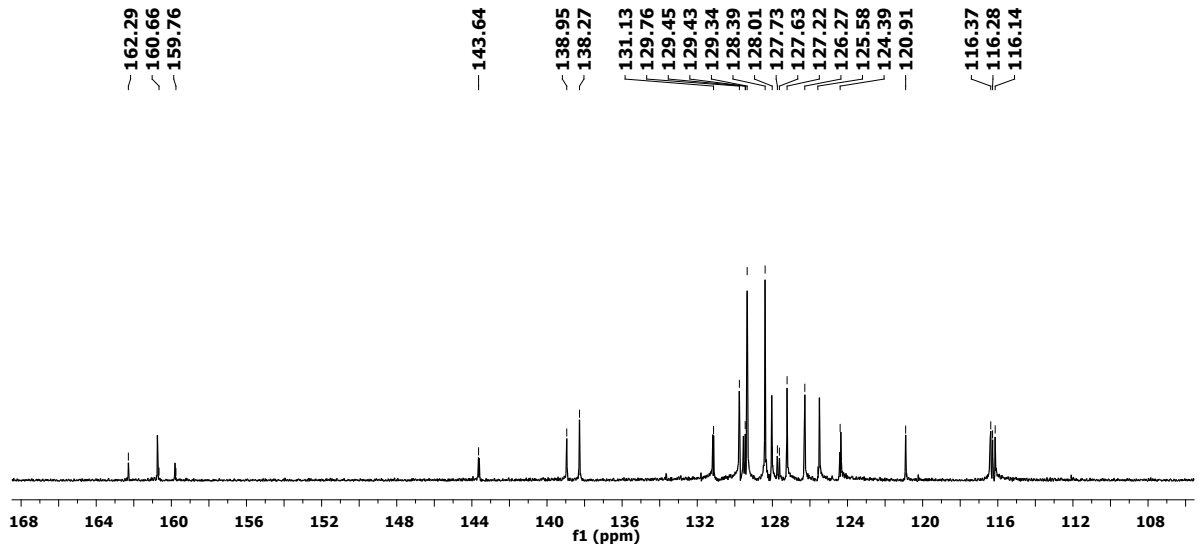


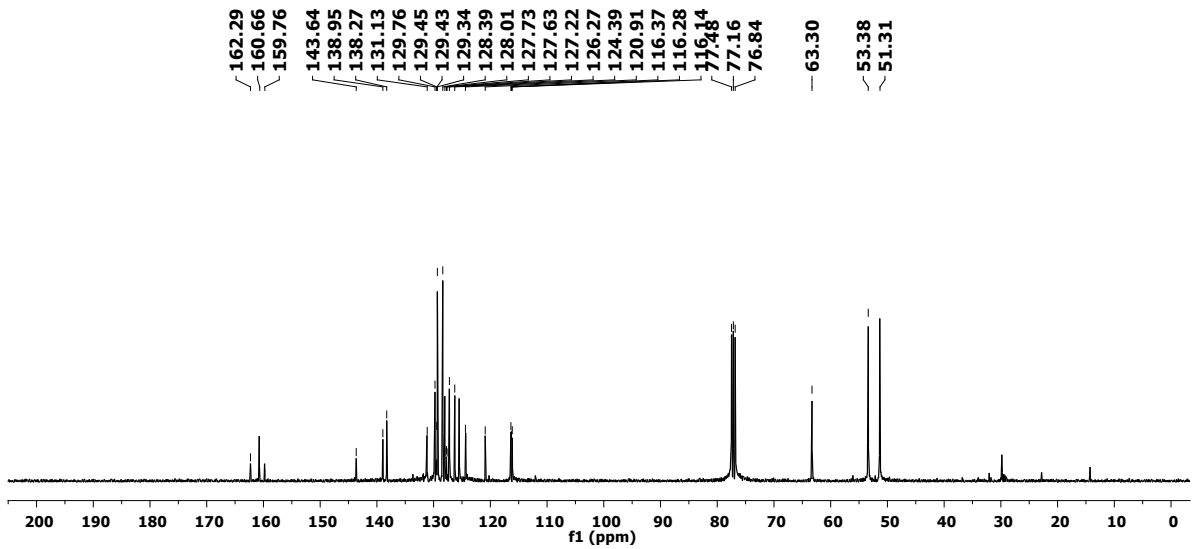



**$^{13}$C NMR** (100 MHz, $CDCl_3$)

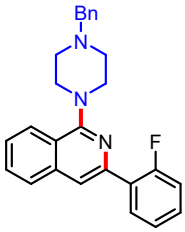



**1-(4-Benzylpiperazin-1-yl)-3-(2-fluorophenyl)isoquinoline (5e)**



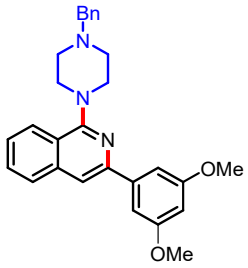



**HRMS**

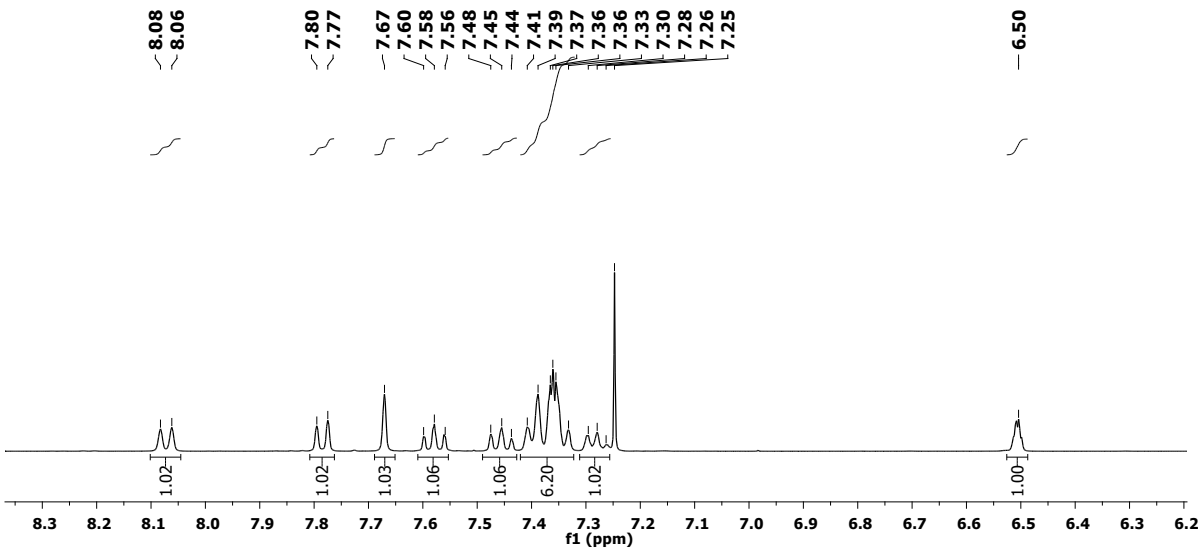


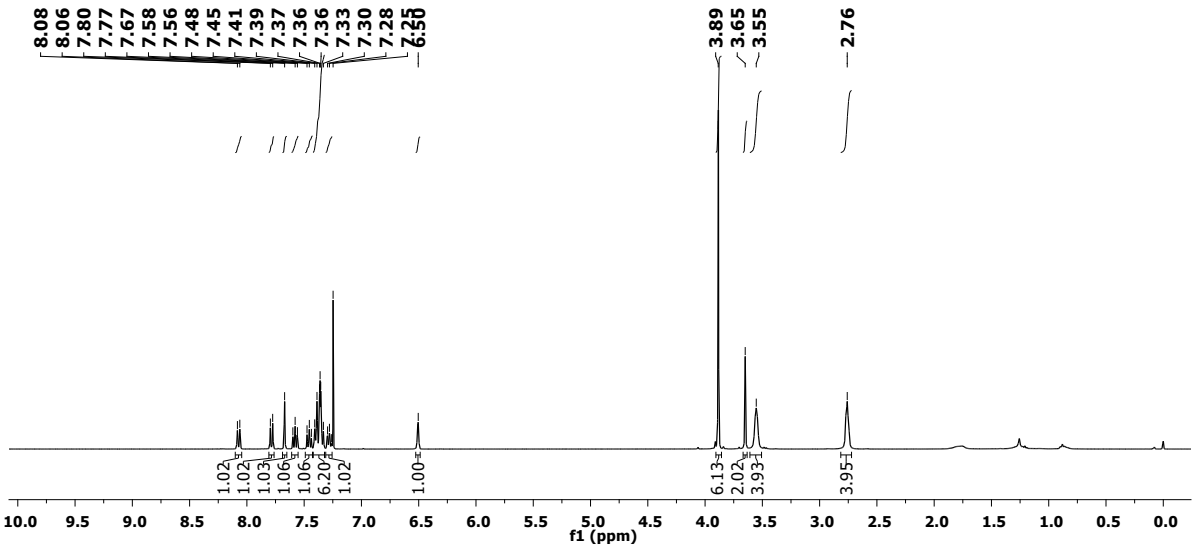

**1-(4-Benzylpiperazin-1-yl)-3-(2-fluorophenyl)isoquinoline (5e)**

**$^1$H NMR** (400 MHz, $CDCl_3$)

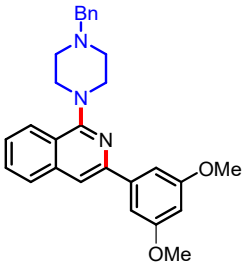



**1-(4-Benzylpiperazin-1-yl)-3-(3,5-dimethoxyphenyl)isoquinoline (5f)**

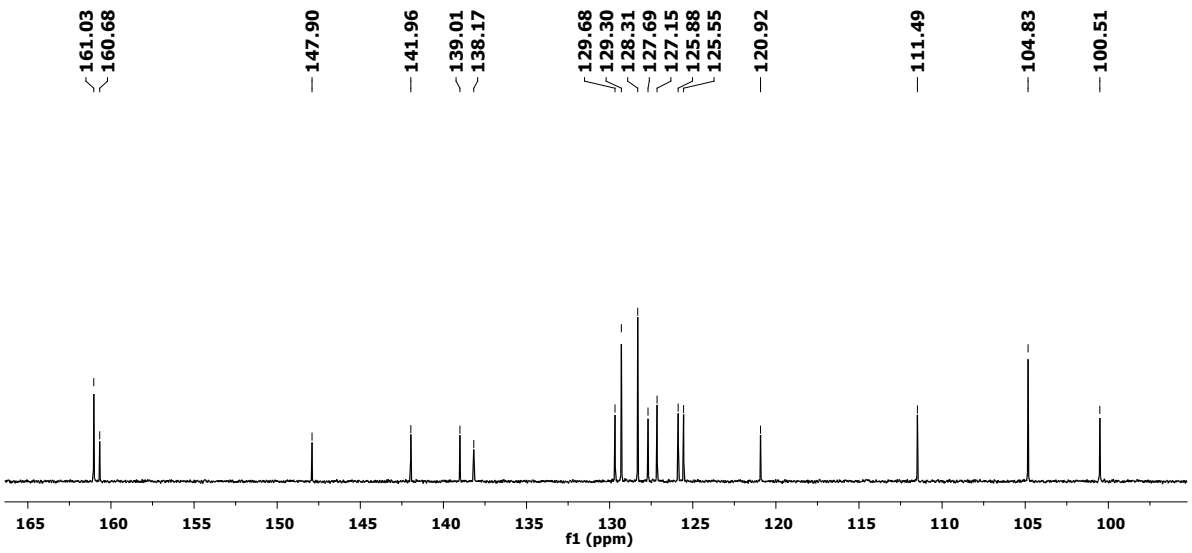


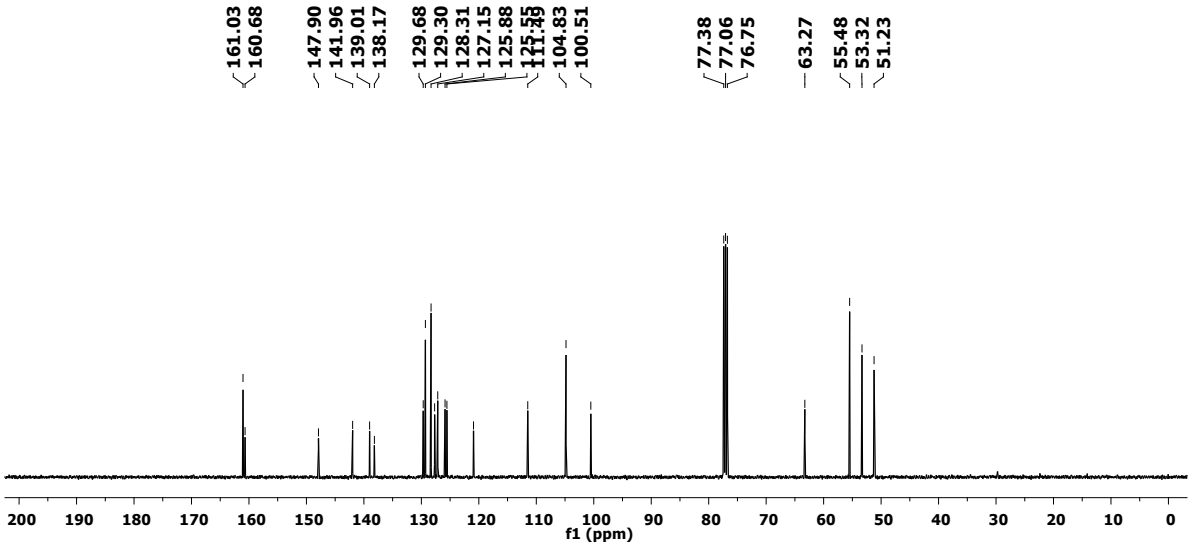



**$^{13}$C NMR** (100 MHz, $CDCl_3$)

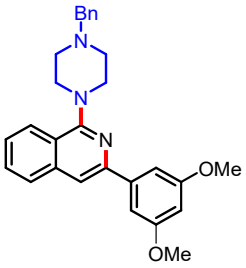



**1-(4-Benzylpiperazin-1-yl)-3-(3, 5-dimethoxyphenyl)isoquinoline (5f)**



# HRMS




## 1-(4-Benzylpiperazin-1-yl)-3-(3, 5-dimethoxyphenyl)isoquinoline (5f)

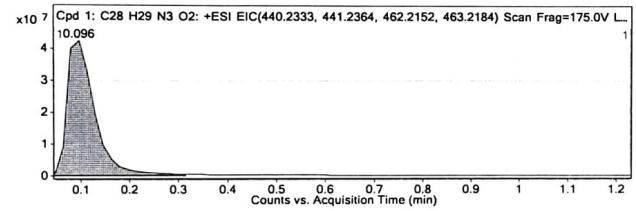
### Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | LTC-6182.d | **Sample Name** | LTC-6182 |
| **Sample Type** | Sample | **Position** | P1-A4 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | MS Scan.m | **Acquired Time** | 24-11-2022 13:23:40 |
| **IRM Calibration Status** | Success | **DA Method** | Default.m |
| **Comment** | | | |
| **Sample Group** | | **Info.** | 3 |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

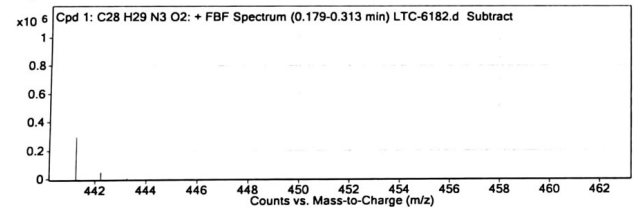
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C28 H29 N3 O2 | 0.096 | 439.2287 | 918977 | C28 H29 N3 O2 | 439.226 | 6.09 | C28 H29 N3 O2 | C28 H29 N3 O2 |

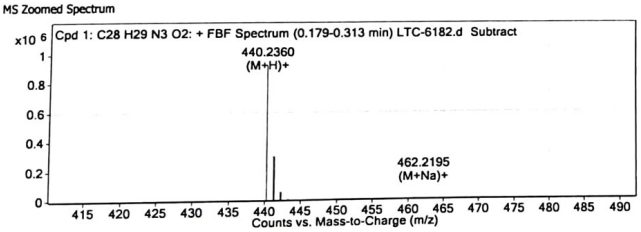
| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C28 H29 N3 O2 | 440.236 | 0.096 | Find By Formula | 439.2287 |




MS Spectrum




MS Zoomed Spectrum

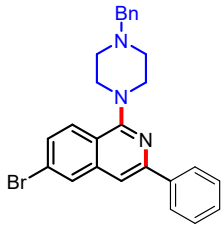



**MS Spectrum Peak List**

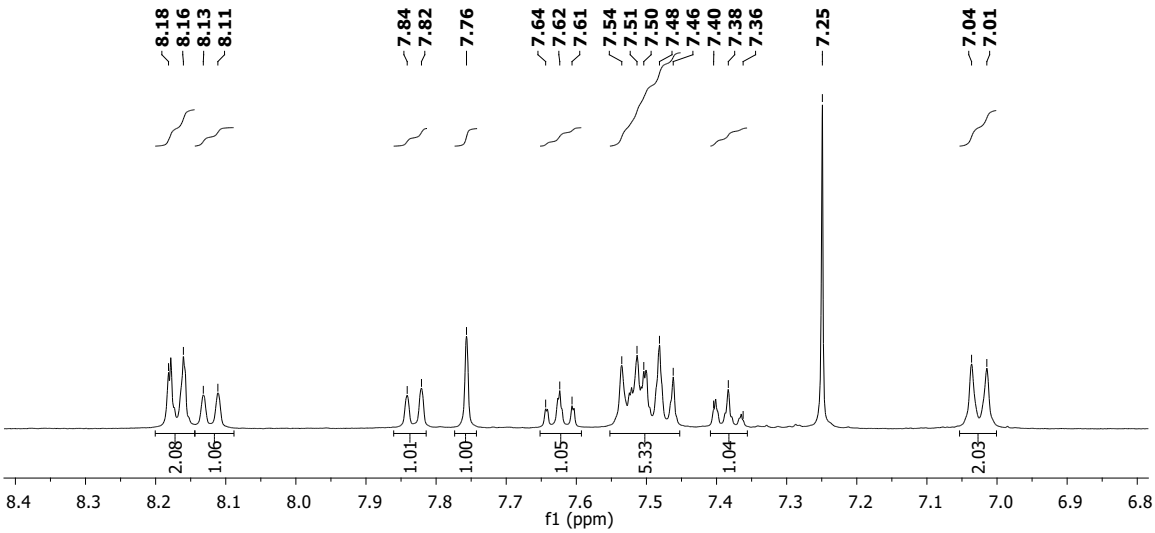
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 440.236 | 1 | 918976.94 | C28H30N3O2 | (M+H)+ |
| 441.239 | 1 | 296866.38 | C28H30N3O2 | (M+H)+ |
| 442.2412 | 1 | 46774.33 | C28H30N3O2 | (M+H)+ |
| 443.247 | 1 | 5889.57 | C28H30N3O2 | (M+H)+ |
| 444.2545 | 1 | 584.87 | C28H30N3O2 | (M+H)+ |
| 462.2195 | 1 | 1059.59 | C28H29N3NaO2 | (M+Na)+ |
| 463.2273 | 1 | 204.18 | C28H29N3NaO2 | (M+Na)+ |

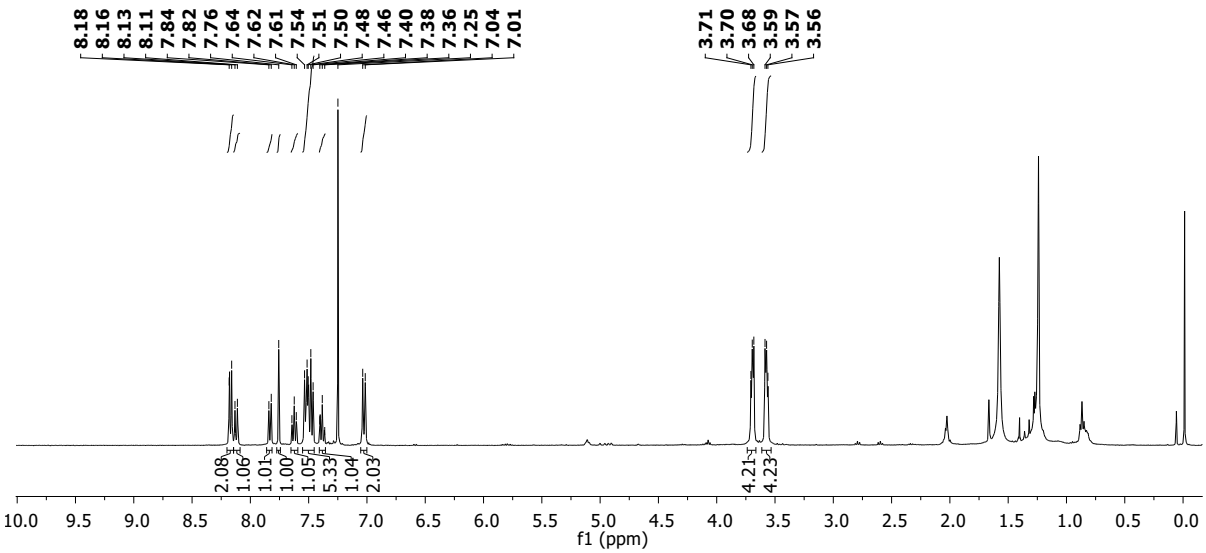
--- End Of Report ---

**$^1$H NMR** (400 MHz, $CDCl_3$)

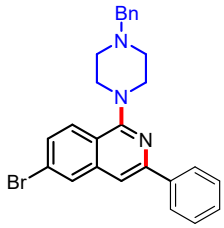



**1-(4-benzylpiperazin-1-yl)-6-bromo-3-phenylisoquinoline (5g)**

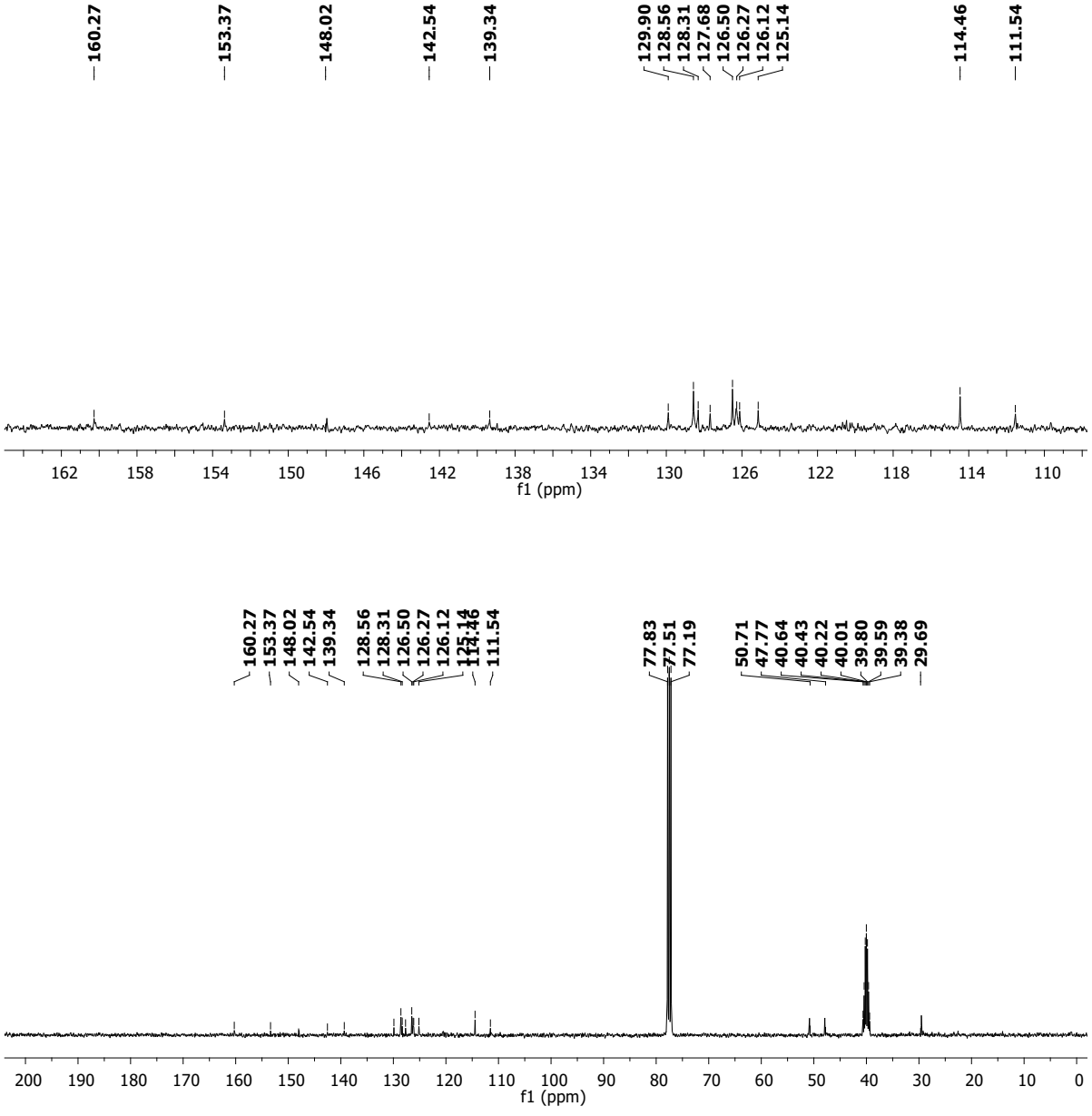


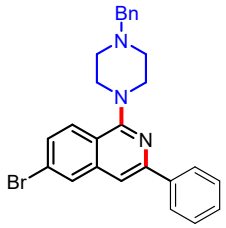
**$^{13}$C NMR** (100 MHz, $CDCl_3$/DMSO-$d_6$)




**1-(4-benzylpiperazin-1-yl)-6-bromo-3-phenylisoquinoline (5g)**



# HRMS




## 1-(4-benzylpiperazin-1-yl)-6-bromo-3-phenylisoquinoline (5g)

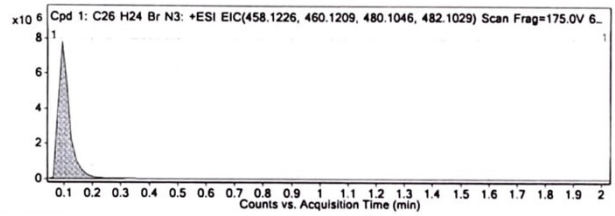
### Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | 6119.d | **Sample Name** | 6119 |
| **Sample Type** | Sample | **Position** | P1-A4 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | MS Scan.m | **Acquired Time** | 27-08-2022 12:10:01 |
| **IRM Calibration Status** | [redacted] | **DA Method** | Default.m |
| **Comment** | | | |
| **Sample Group** | | **Info.** | 3 |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

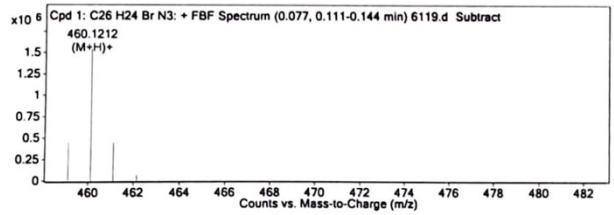
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C26 H24 Br N3 | 0.094 | 457.1158 | 1550701 | C26 H24 Br N3 | 457.1154 | 0.94 | C26 H24 Br N3 | C26 H24 Br N3 |

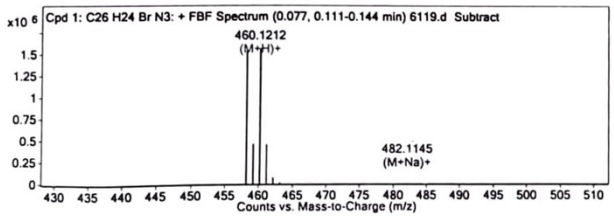
| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C26 H24 Br N3 | 460.1212 | 0.094 | Find By Formula | 457.1158 |




MS Spectrum




MS Zoomed Spectrum

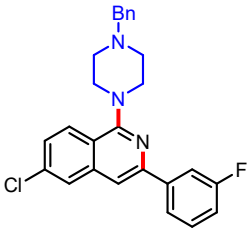



**MS Spectrum Peak List**

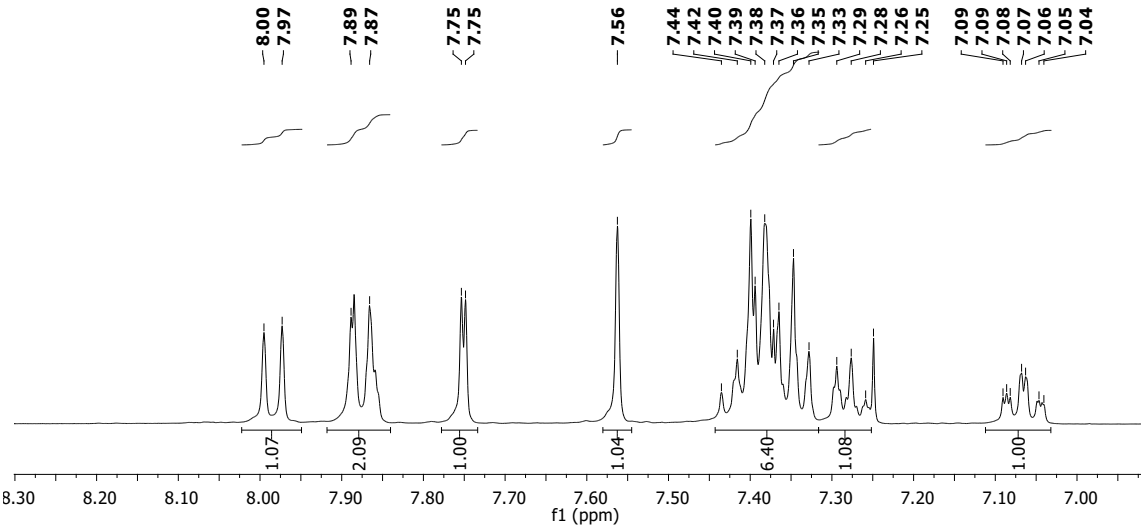
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 458.1232 | 1 | 1534943 | C26H25BrN3 | (M+H)+ |
| 459.1267 | 1 | 458370.59 | C26H25BrN3 | (M+H)+ |
| 460.1212 | 1 | 1550700.63 | C26H25BrN3 | (M+H)+ |
| 461.1242 | 1 | 458310.06 | C26H25BrN3 | (M+H)+ |
| 462.1263 | 1 | 62931.36 | C26H25BrN3 | (M+H)+ |
| 463.1381 | 1 | 6454.58 | C26H25BrN3 | (M+H)+ |
| 482.1145 | 1 | 279.63 | C26H24BrN3Na | (M+Na)+ |
| 483.1038 | 1 | 129.75 | C26H24BrN3Na | (M+Na)+ |

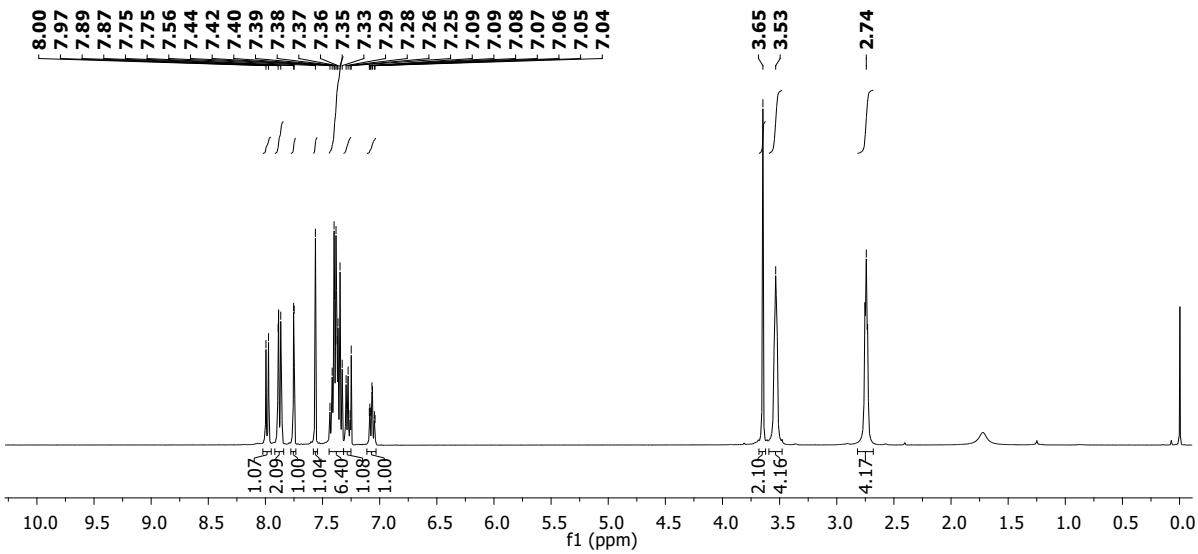
--- End Of Report ---

**$^1$H NMR** (400 MHz, $CDCl_3$)

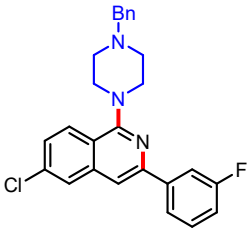



**1-(4-benzylpiperazin-1-yl)-6-chloro-3-(3-fluorophenyl)isoquinoline (5h)**

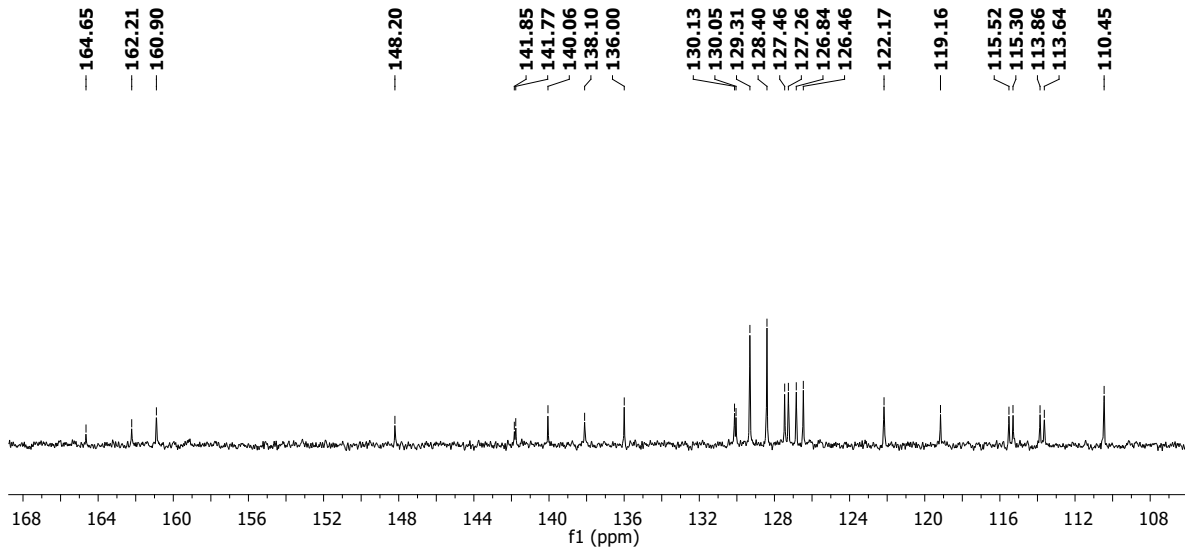


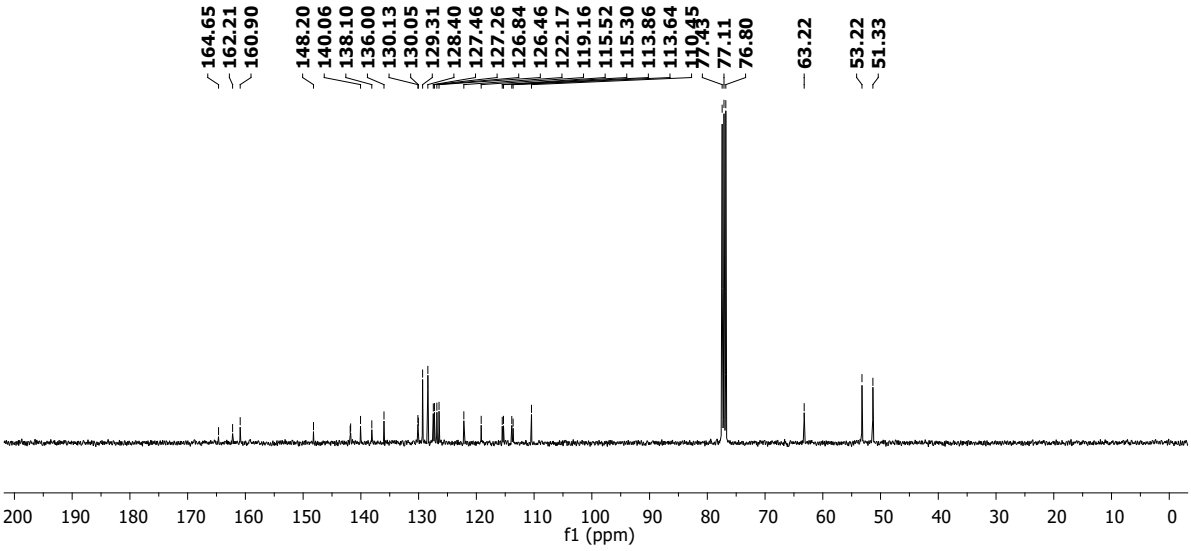



**$^{13}$C NMR** (100 MHz, $CDCl_3$)

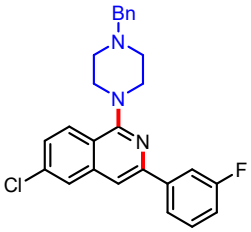



**1-(4-benzylpiperazin-1-yl)-6-chloro-3-(3-fluorophenyl)isoquinoline (5h)**



## HRMS




**1-(4-benzylpiperazin-1-yl)-6-chloro-3-(3-fluorophenyl)isoquinoline (5h)**

### Qualitative Compound Report

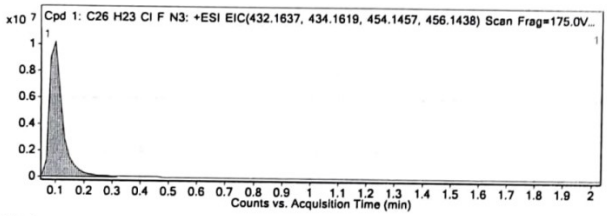
| | | | |
|---|---|---|---|
| **Data File** | 6106.d | **Sample Name** | 6106 |
| **Sample Type** | Sample | **Position** | P1-C8 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | MS Scan.m | **Acquired Time** | 22-08-2022 14:31:14 |
| **IRM Calibration Status** | [redacted] | **DA Method** | Default.m |
| **Comment** | | | |

| | | | |
|---|---|---|---|
| **Sample Group** | | **Info.** | 3 |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

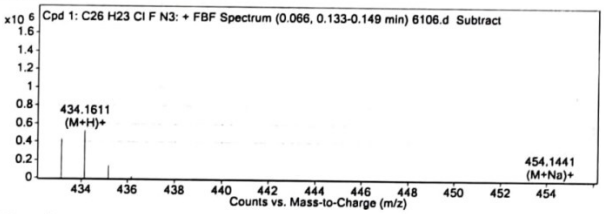
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C26 H23 Cl F N3 | 0.099 | 431.1558 | 1423418 | C26 H23 Cl F N3 | 431.1565 | -1.6 | C26 H23 Cl F N3 | C26 H23 Cl F N3 |

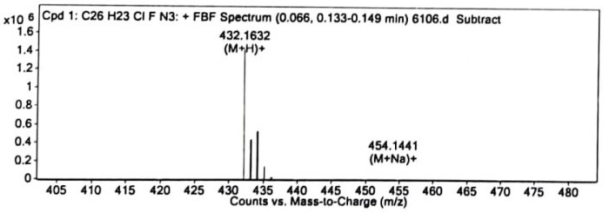
| Compound Label | m/z | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C26 H23 Cl F N3 | 432.1632 | 0.099 | Find By Formula | 431.1558 |




MS Spectrum




MS Zoomed Spectrum

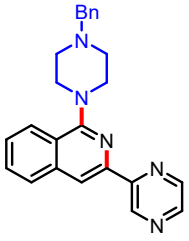



**MS Spectrum Peak List**

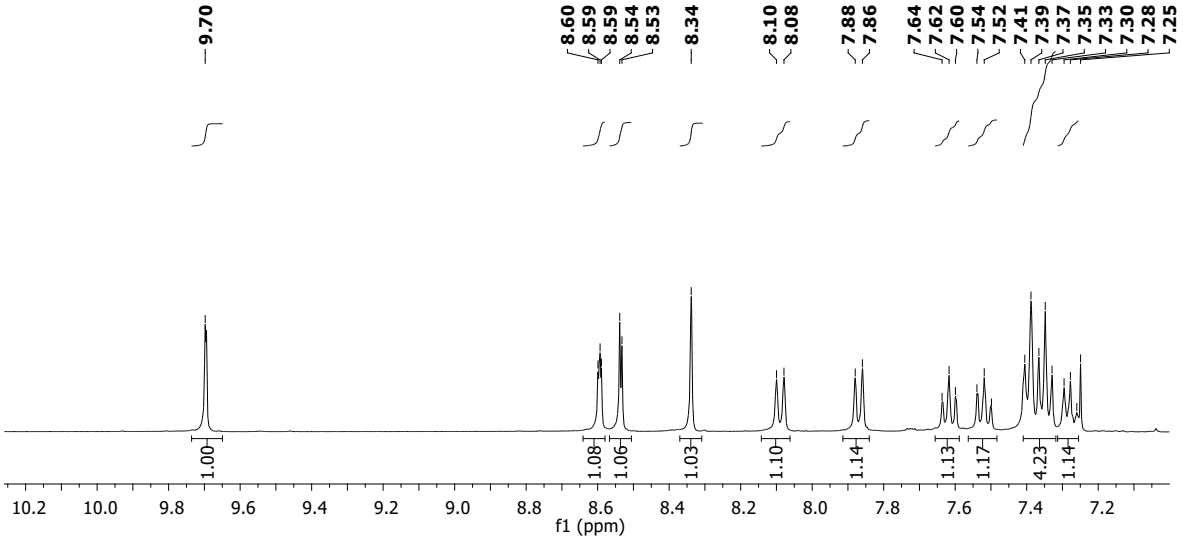
| m/z | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 432.1632 | 1 | 1423418.13 | C26H24ClFN3 | (M+H)+ |
| 433.166 | 1 | 428891.25 | C26H24ClFN3 | (M+H)+ |
| 434.1611 | 1 | 522343.78 | C26H24ClFN3 | (M+H)+ |
| 435.1632 | 1 | 137243.33 | C26H24ClFN3 | (M+H)+ |
| 436.1657 | 1 | 18225.63 | C26H24ClFN3 | (M+H)+ |
| 437.1745 | 1 | 1795.43 | C26H24ClFN3 | (M+H)+ |
| 454.1441 | 1 | 756.52 | C26H23ClFN3Na | (M+Na)+ |
| 455.1553 | 1 | 261.44 | C26H23ClFN3Na | (M+Na)+ |
| 456.1424 | 1 | 223.39 | C26H23ClFN3Na | (M+Na)+ |

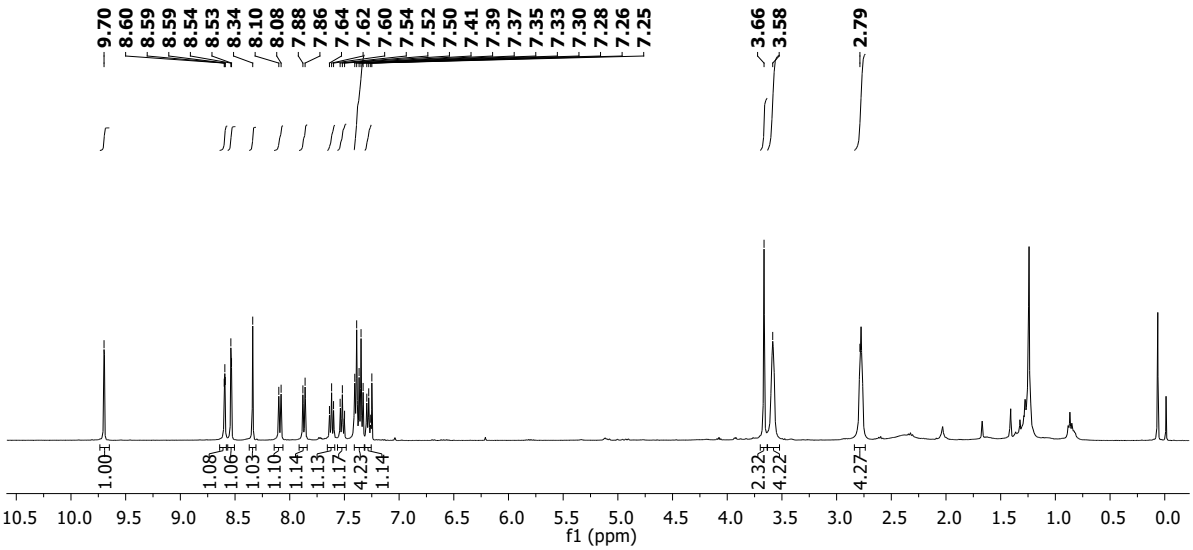
--- End Of Report ---

**$^1$H NMR** (400 MHz, $CDCl_3$)

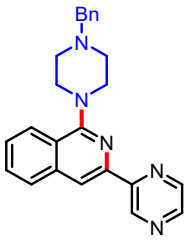



**1-(4-benzylpiperazin-1-yl)-3-(pyrazin-2-yl)isoquinoline (5i)**

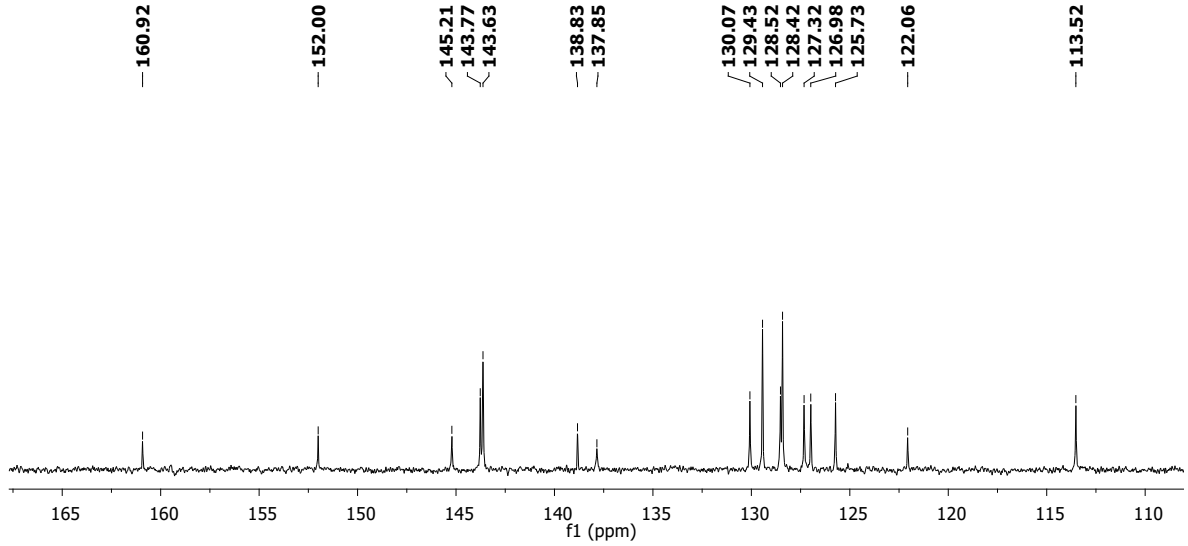


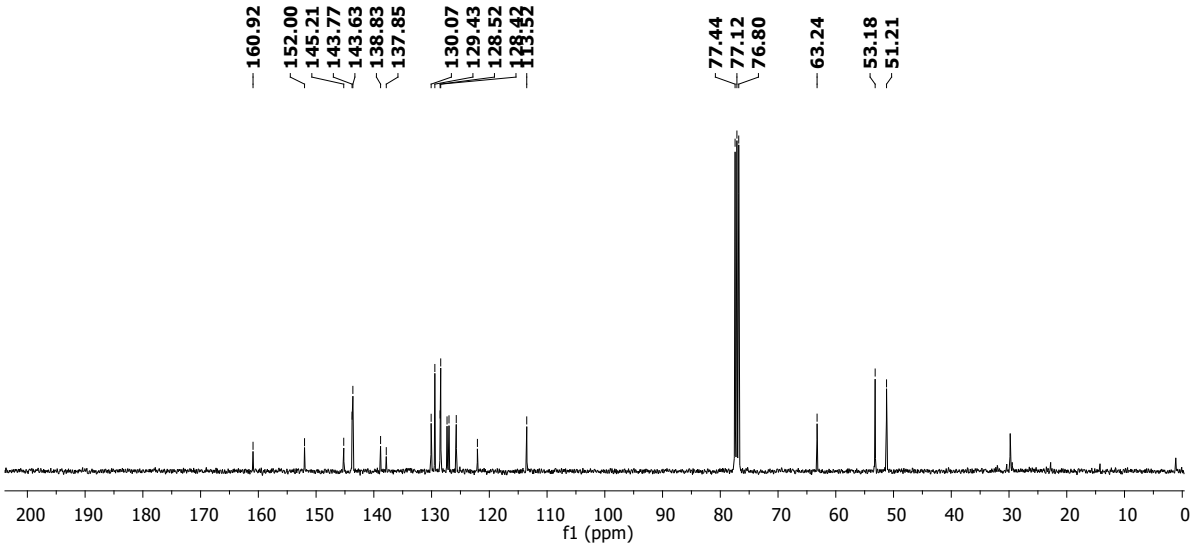



**$^{13}$C NMR** (100 MHz, $CDCl_3$)

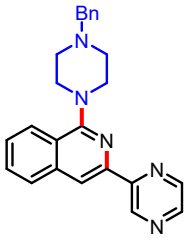



**1-(4-benzylpiperazin-1-yl)-3-(pyrazin-2-yl)isoquinoline (5i)**



# HRMS




## 1-(4-benzylpiperazin-1-yl)-3-(pyrazin-2-yl)isoquinoline (5i)

### Qualitative Compound Report

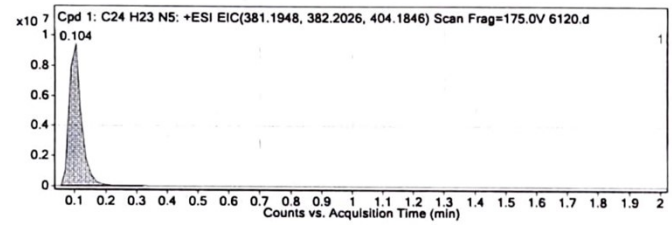
| | | | |
|---|---|---|---|
| **Data File** | 6120.d | **Sample Name** | 6120 |
| **Sample Type** | Sample | **Position** | P1-A3 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | MS Scan.m | **Acquired Time** | 27-08-2022 12:07:17 |
| **IRM Calibration Status** | [redacted] | **DA Method** | Default.m |
| **Comment** | | | |

| | | | |
|---|---|---|---|
| **Sample Group** | | **Info.** | 3 |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

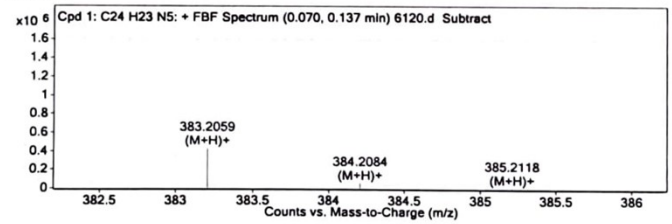
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C24 H23 N5 | 0.104 | 381.1958 | 1473696 | C24 H23 N5 | 381.1953 | 1.21 | C24 H23 N5 | C24 H23 N5 |

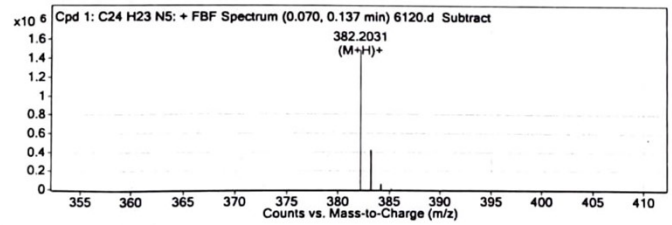
| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C24 H23 N5 | 382.2031 | 0.104 | Find By Formula | 381.1958 |




MS Spectrum




MS Zoomed Spectrum

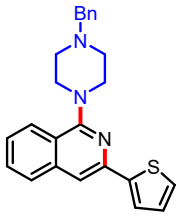



**MS Spectrum Peak List**

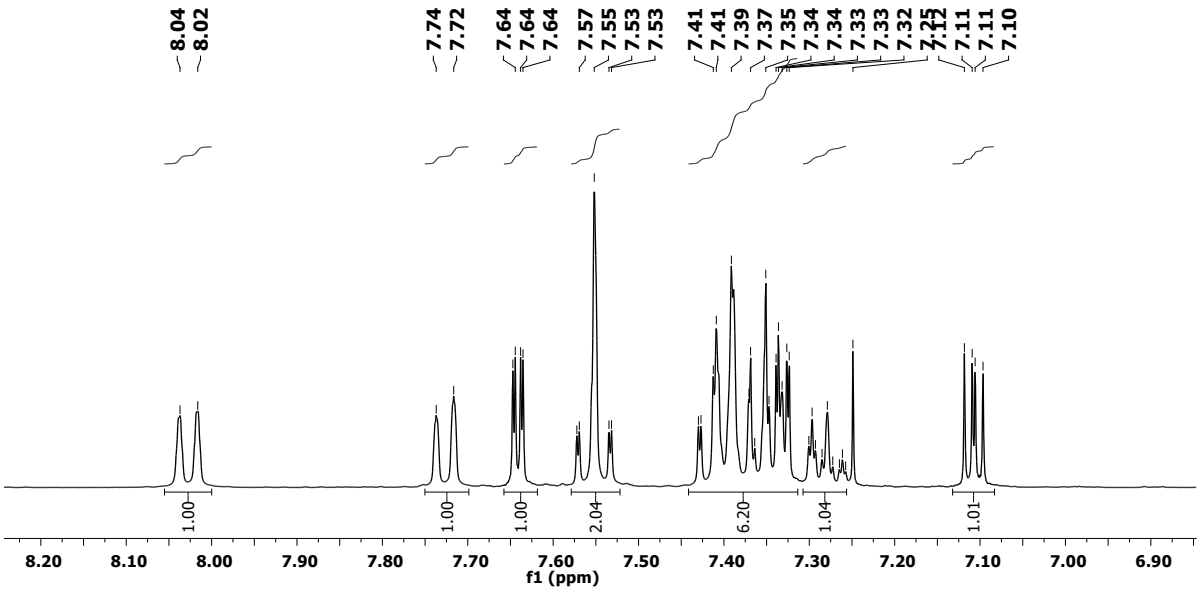
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 382.2031 | 1 | 1473695.5 | C24H24N5 | (M+H)+ |
| 383.2059 | 1 | 425375.34 | C24H24N5 | (M+H)+ |
| 384.2084 | 1 | 52959.84 | C24H24N5 | (M+H)+ |
| 385.2118 | 1 | 4647.96 | C24H24N5 | (M+H)+ |
| 386.2231 | 1 | 753.6 | C24H24N5 | (M+H)+ |

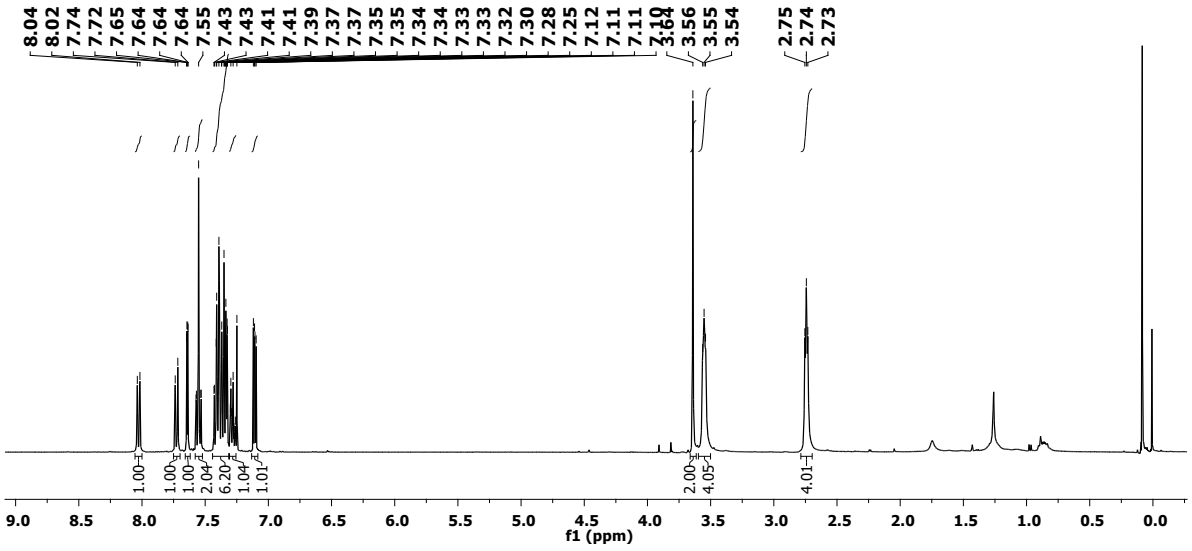
--- End Of Report ---

**$^1$H NMR** (400 MHz, $CDCl_3$)

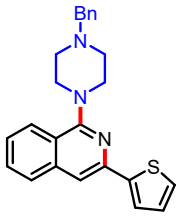



**1-(4-benzylpiperazin-1-yl)-3-(thiophen-2-yl)isoquinoline (5j)**

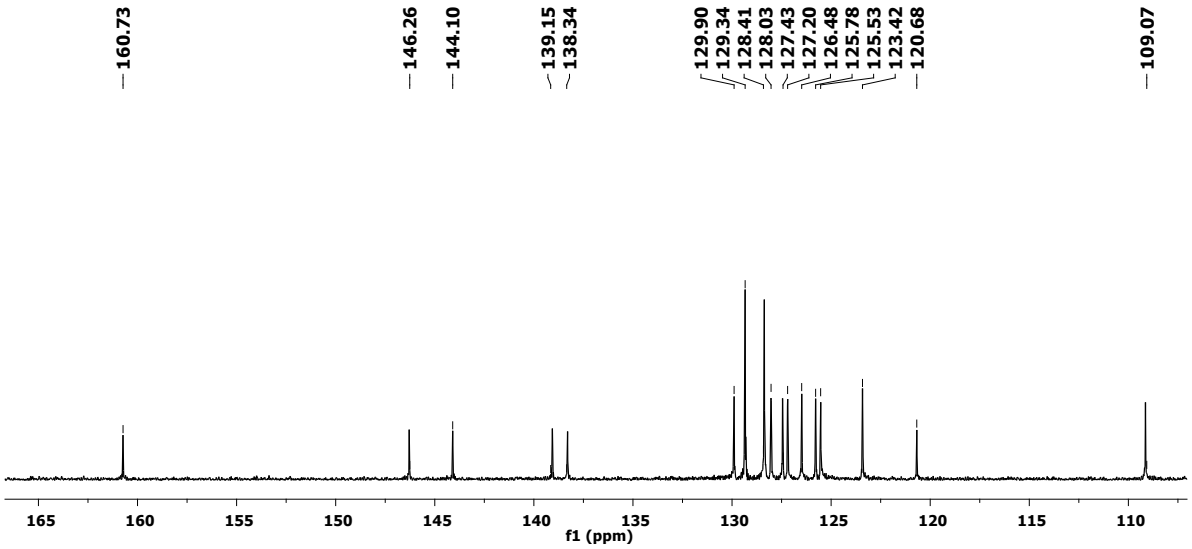


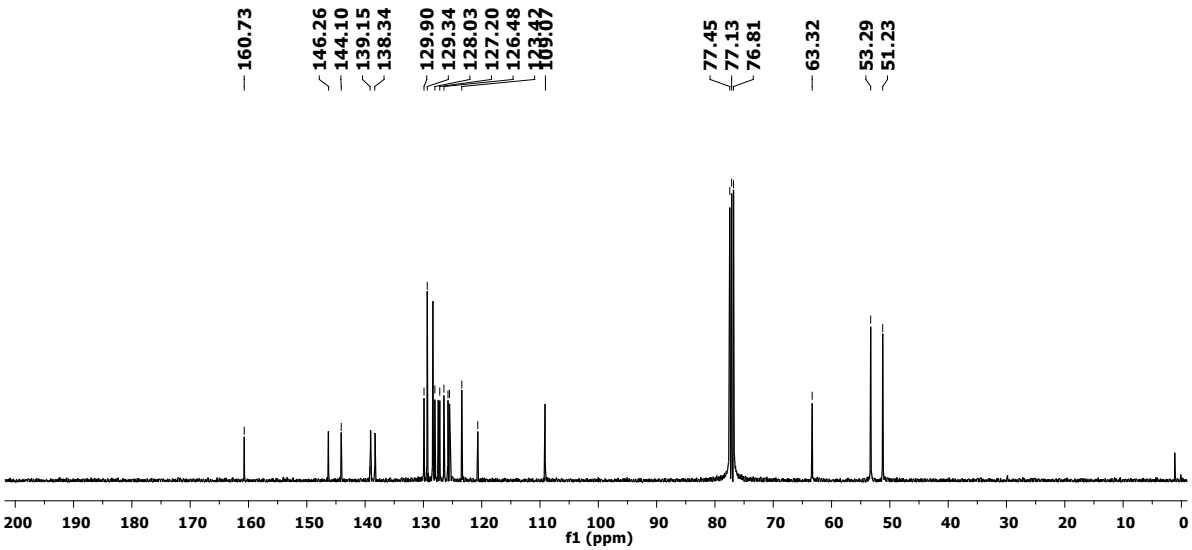



**$^{13}$C NMR** (100 MHz, $CDCl_3$)

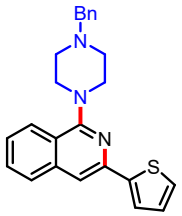



**1-(4-benzylpiperazin-1-yl)-3-(thiophen-2-yl)isoquinoline (5j)**



# HRMS




## 1-(4-benzylpiperazin-1-yl)-3-(thiophen-2-yl)isoquinoline (5j)

### Qualitative Compound Report

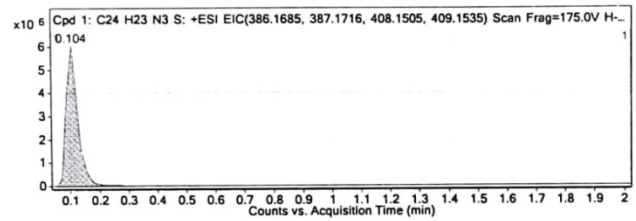
| | | | |
|---|---|---|---|
| **Data File** | H-30R.d | **Sample Name** | H-30R |
| **Sample Type** | Sample | **Position** | P1-A5 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | MS Scan.m | **Acquired Time** | 30-08-2022 16:40:42 |
| **IRM Calibration Status** | [redacted] | **DA Method** | Default.m |
| **Comment** | | | |

| | | | |
|---|---|---|---|
| **Sample Group** | | **Info.** | 3 |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

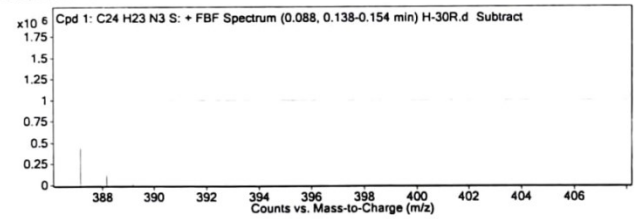
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C24 H23 N3 S | 0.104 | 385.1605 | 1576653 | C24 H23 N3 S | 385.1613 | -1.88 | C24 H23 N3 S | C24 H23 N3 S |

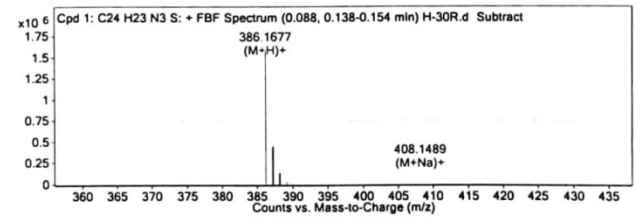
| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C24 H23 N3 S | 386.1677 | 0.104 | Find By Formula | 385.1605 |




MS Spectrum




MS Zoomed Spectrum

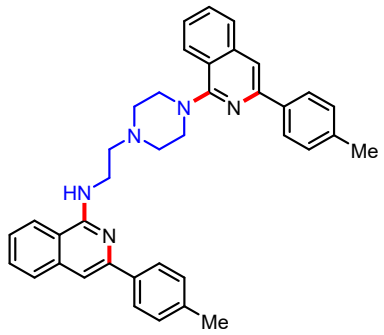



**MS Spectrum Peak List**

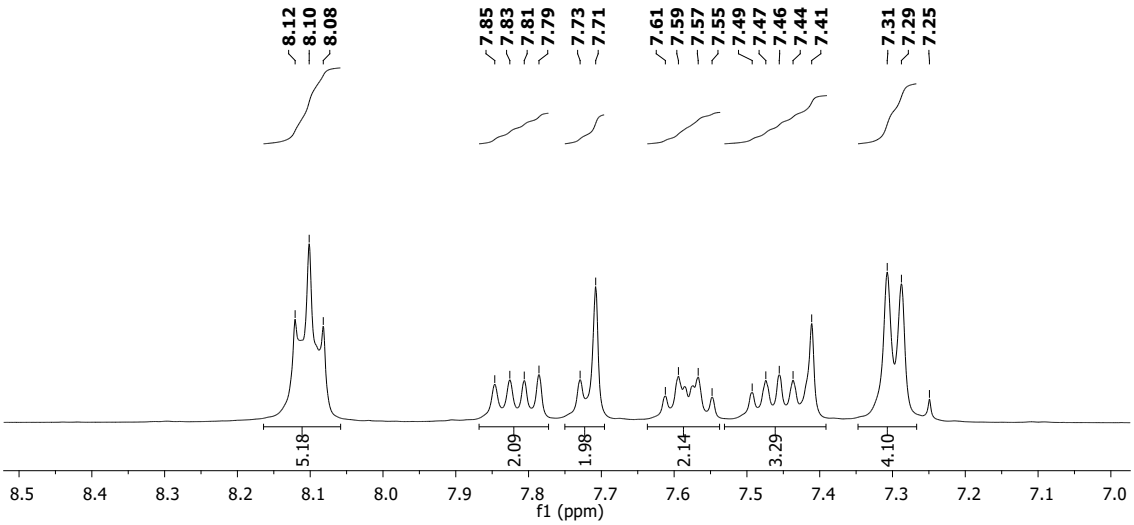
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 386.1677 | 1 | 1576652.5 | C24H24N3S | (M+H)+ |
| 387.171 | 1 | 439205.53 | C24H24N3S | (M+H)+ |
| 388.1688 | 1 | 122517.7 | C24H24N3S | (M+H)+ |
| 389.1686 | 1 | 22567.92 | C24H24N3S | (M+H)+ |
| 390.1704 | 1 | 2803.85 | C24H24N3S | (M+H)+ |
| 408.1489 | 1 | 343.33 | C24H23N3NaS | (M+Na)+ |

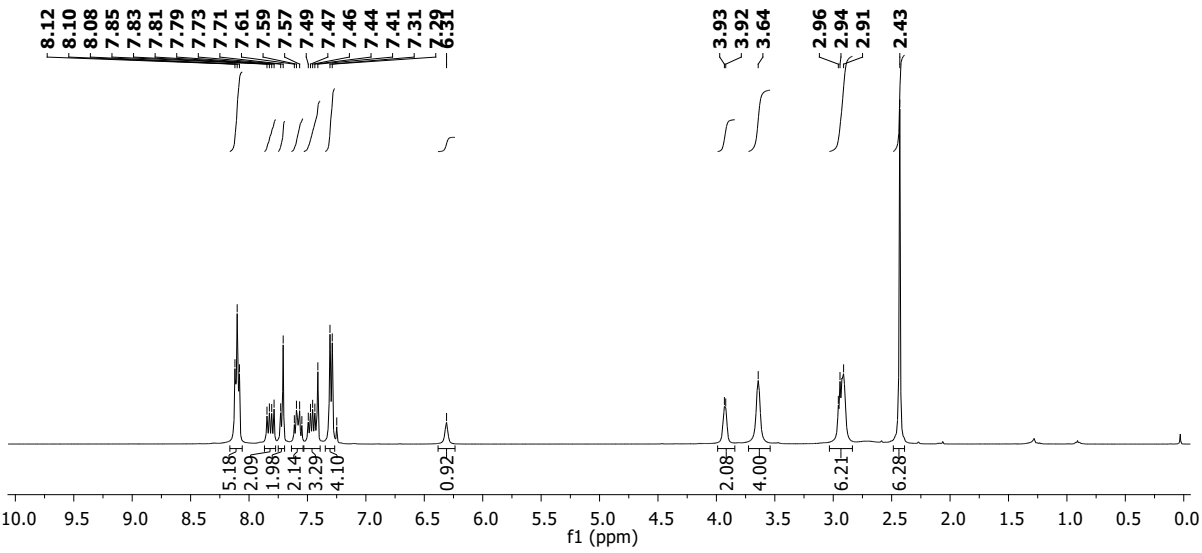
--- End Of Report ---

**$^1$H NMR** (400MHz, $CDCl_3$)

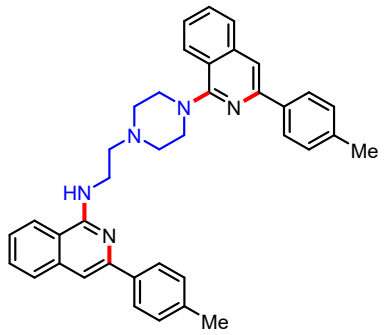



**3-(p-tolyl)-N-(2-(4-(3-(p-tolyl)isoquinolin-1-yl)piperazin-1-yl)ethyl)isoquinolin-1-amine (6a)**

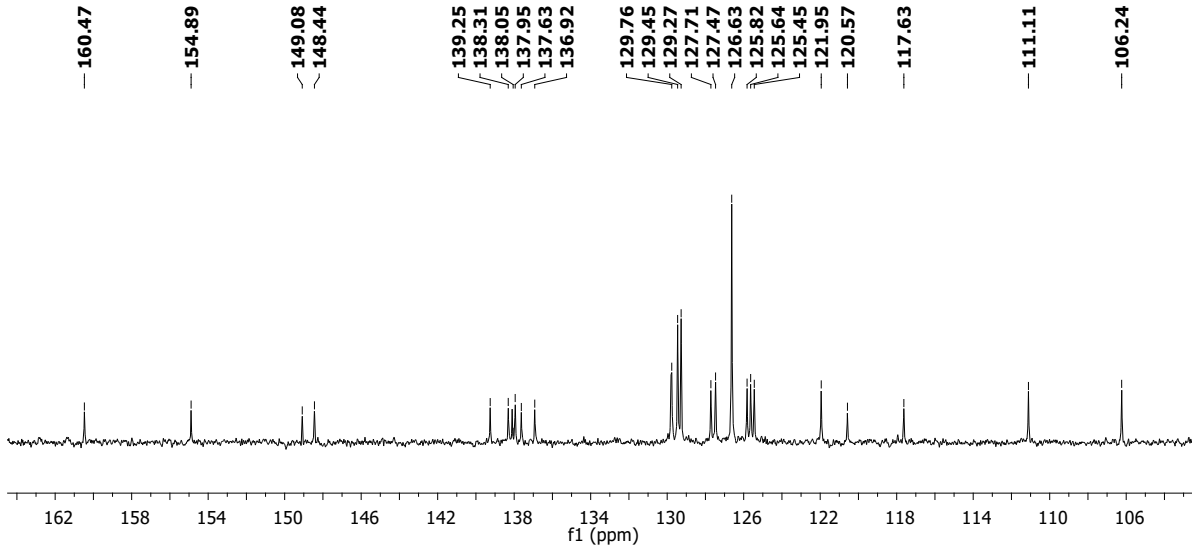


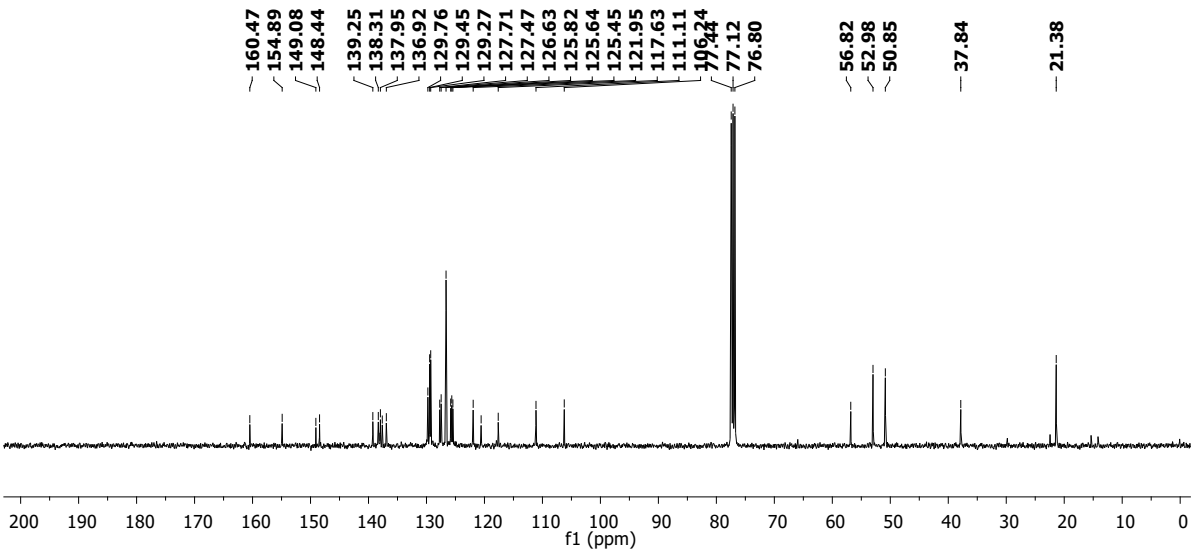



**$^{13}$C NMR** (100MHz, $CDCl_3$)

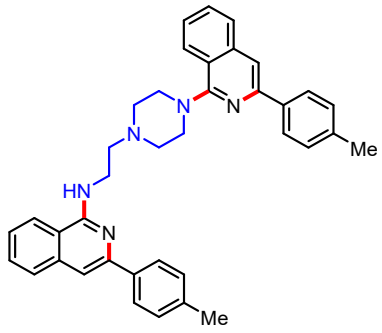



**3-(p-tolyl)-N-(2-(4-(3-(p-tolyl)isoquinolin-1-yl)piperazin-1-yl)ethyl)isoquinolin-1-amine (6a)**



## HRMS




**3-(p-tolyl)-N-(2-(4-(3-(p-tolyl)isoquinolin-1-yl)piperazin-1-yl)ethyl)isoquinolin-1-amine (6a)**

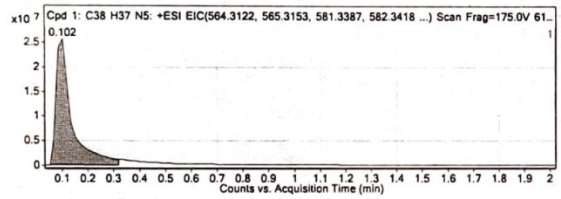
### Qualitative Compound Report

| | | | |
|---|---|---|---|
| Data File | 6132.d | Sample Name | 6132 |
| Sample Type | Sample | Position | P1-D1 |
| Instrument Name | Instrument 1 | User Name | |
| Acq Method | MS Scan.m | Acquired Time | 22-08-2022 14:36:47 |
| IRM Calibration Status | [redacted] | DA Method | Default.m |
| Comment | | | |
| Sample Group | | Info. | 3 |
| Acquisition SW Version | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

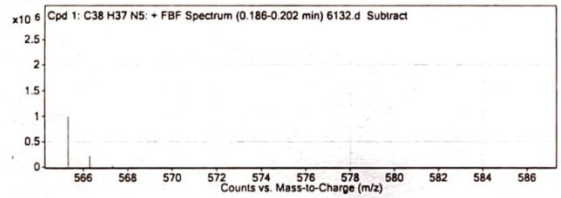
Compound Table

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C38 H37 N5 | 0.102 | 563.3036 | 2377080 | C38 H37 N5 | 563.3049 | -2.27 | C38 H37 N5 | C38 H37 N5 |

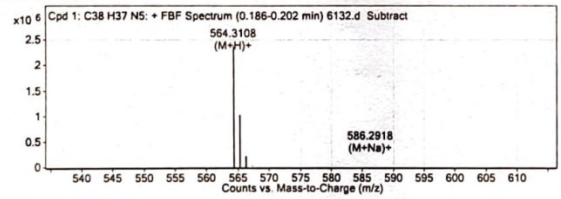
| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C38 H37 N5 | 564.3108 | 0.102 | Find By Formula | 563.3036 |




MS Spectrum




MS Zoomed Spectrum

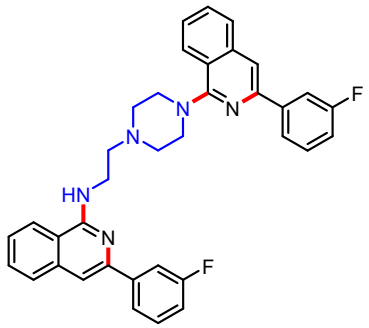



MS Spectrum Peak List

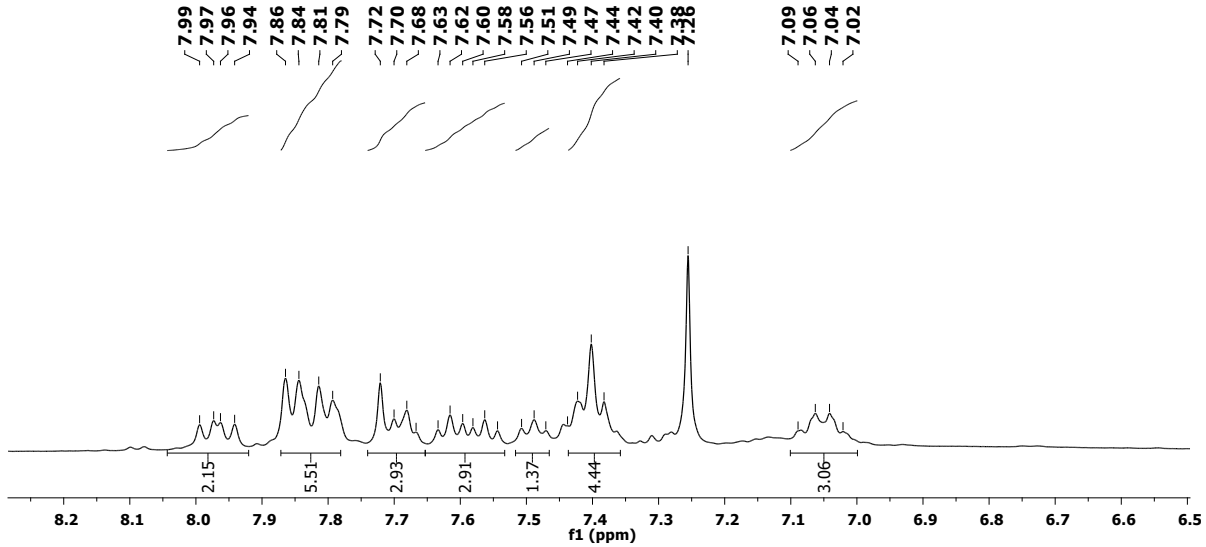
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 564.3108 | 1 | 2377079.5 | C38H38N5 | (M+H)+ |
| 565.3144 | 1 | 1000293.81 | C38H38N5 | (M+H)+ |
| 566.3169 | 1 | 213664.19 | C38H38N5 | (M+H)+ |
| 567.3192 | 1 | 29510.3 | C38H38N5 | (M+H)+ |
| 568.3183 | 1 | 2893.23 | C38H38N5 | (M+H)+ |
| 586.2918 | 1 | 1832.8 | C38H37N5Na | (M+Na)+ |
| 587.2953 | 1 | 693.91 | C38H37N5Na | (M+Na)+ |

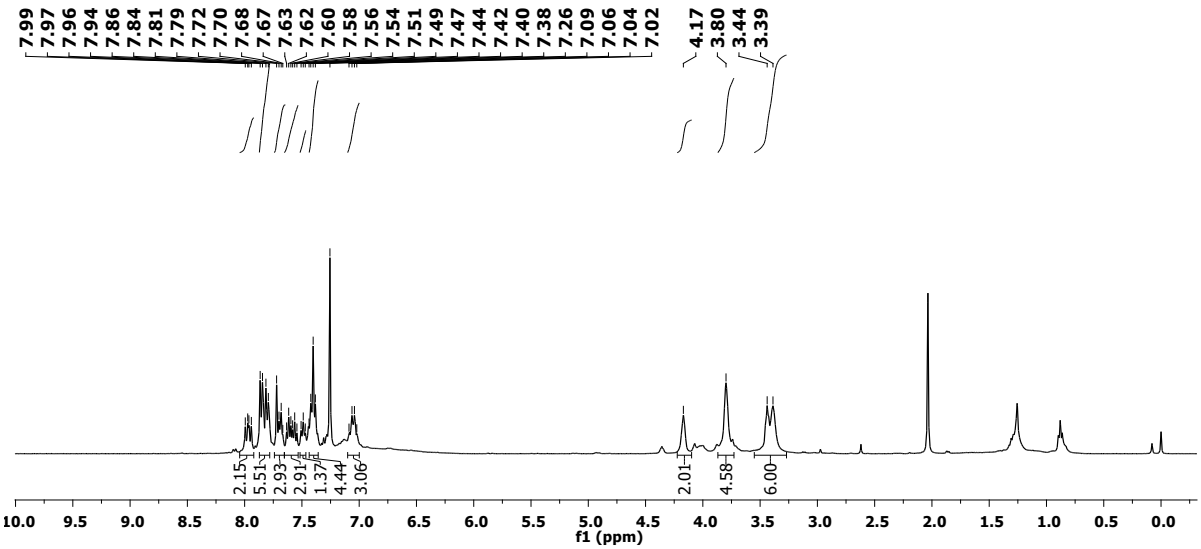
--- End Of Report ---

**$^1$H NMR** (400MHz, $CDCl_3$)

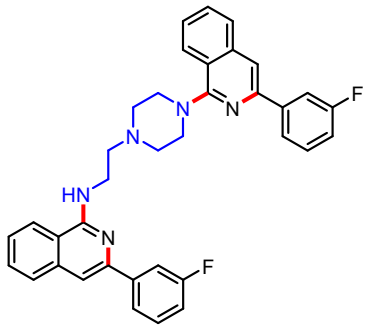



**3-(3-fluorophenyl)-N-(2-(4-(3-(3-fluorophenyl)isoquinolin-1-yl)piperazin-1-yl)ethyl)isoquinolin-1-amine (6b)**

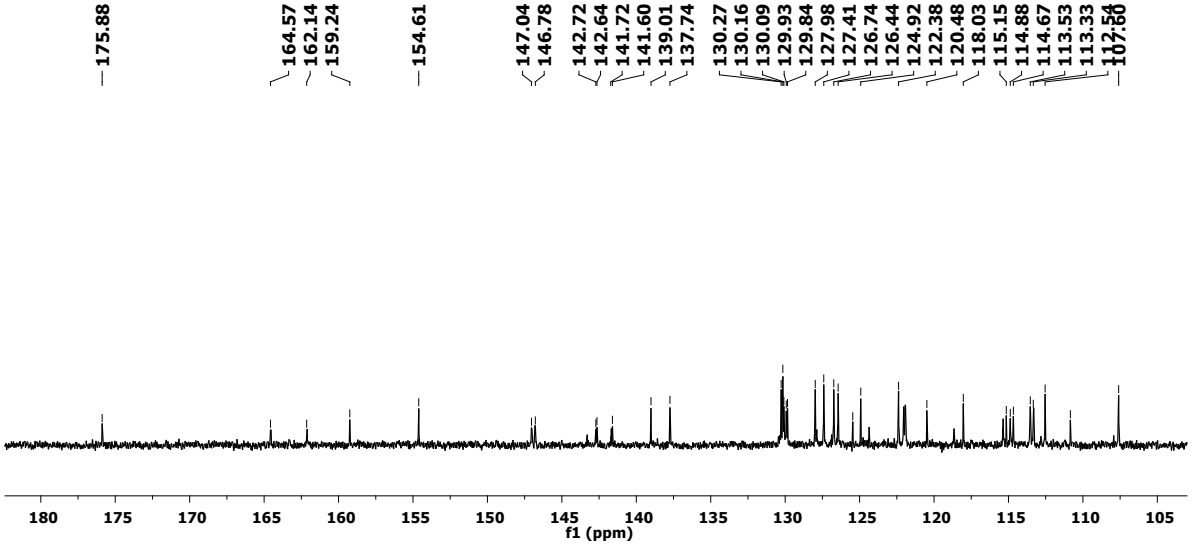


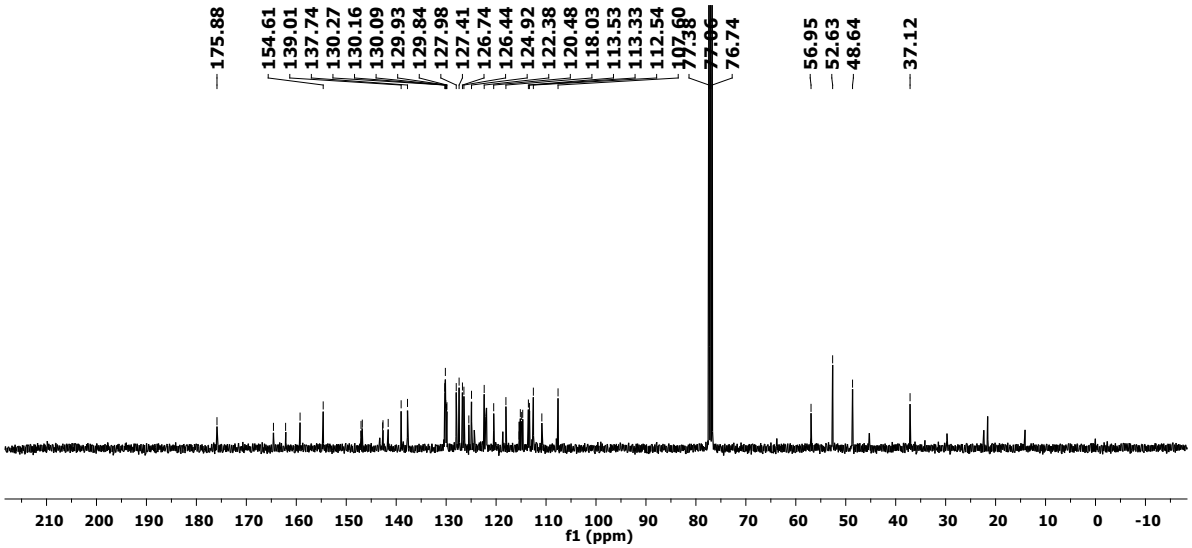



**$^{13}$C NMR** (100MHz, $CDCl_3$)

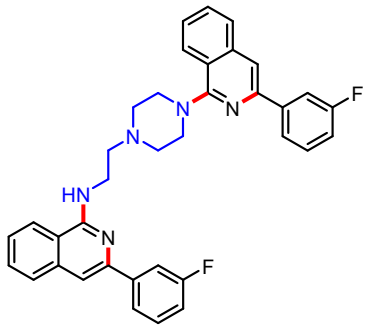



**3-(3-fluorophenyl)-N-(2-(4-(3-(3-fluorophenyl)isoquinolin-1-yl)piperazin-1-yl)ethyl)isoquinolin-1-amine (6b)**



## HRMS



**3-(3-fluorophenyl)-N-(2-(4-(3-(3-fluorophenyl)isoquinolin-1-yl)piperazin-1-yl)ethyl)isoquinolin-1-amine (6b)**

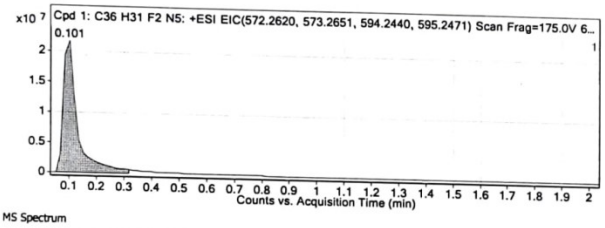
### Qualitative Compound Report

| | | | |
|---|---|---|---|
| Data File | 6135.d | Sample Name | 6135 |
| Sample Type | Sample | Position | P1-D2 |
| Instrument Name | Instrument 1 | User Name | |
| Acq Method | MS Scan.m | Acquired Time | 22-08-2022 14:41:36 |
| IRM Calibration Status | [redacted] | DA Method | Default.m |
| Comment | | | |
| Sample Group | | Info. | 3 |
| Acquisition SW Version | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

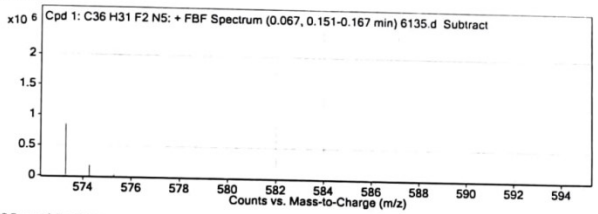
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C36 H31 F2 N5 | 0.101 | 571.254 | 2088570 | C36 H31 F2 N5 | 571.2548 | -1.4 | C36 H31 F2 N5 | C36 H31 F2 N5 |

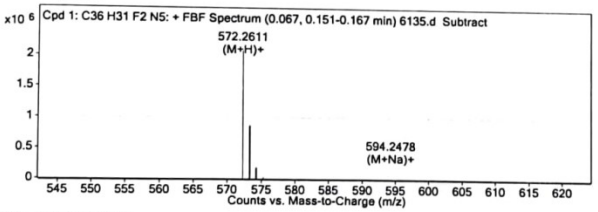
| Compound Label | m/z | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C36 H31 F2 N5 | 572.2611 | 0.101 | Find By Formula | 571.254 |




MS Spectrum




MS Zoomed Spectrum

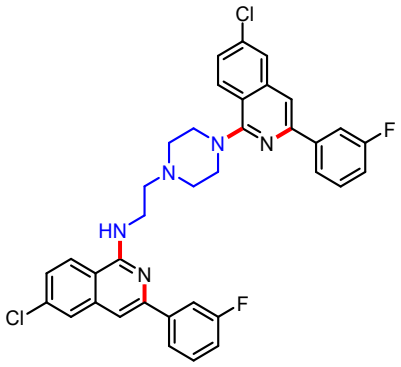



**MS Spectrum Peak List**

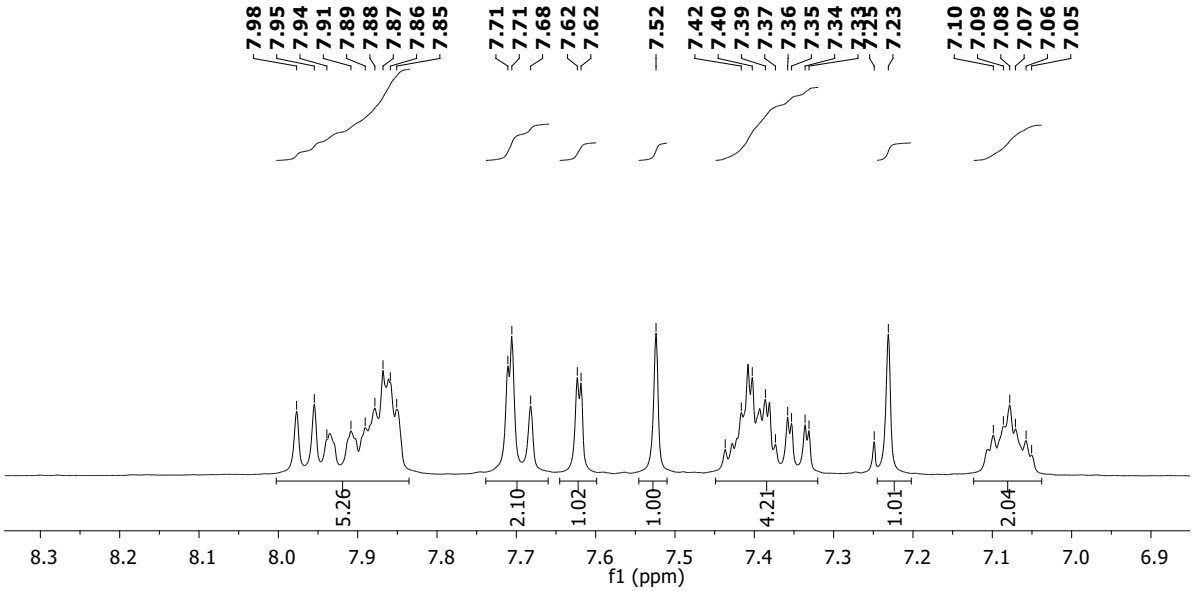
| m/z | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 572.2611 | 1 | 2088570.38 | C36H32F2N5 | (M+H)+ |
| 573.2649 | 1 | 843501.94 | C36H32F2N5 | (M+H)+ |
| 574.2665 | 1 | 175412.33 | C36H32F2N5 | (M+H)+ |
| 575.2688 | 1 | 22947.63 | C36H32F2N5 | (M+H)+ |
| 576.2708 | 1 | 2352.36 | C36H32F2N5 | (M+H)+ |
| 594.2478 | 1 | 2102.71 | C36H31F2N5Na | (M+Na)+ |
| 595.2489 | 1 | 794.67 | C36H31F2N5Na | (M+Na)+ |

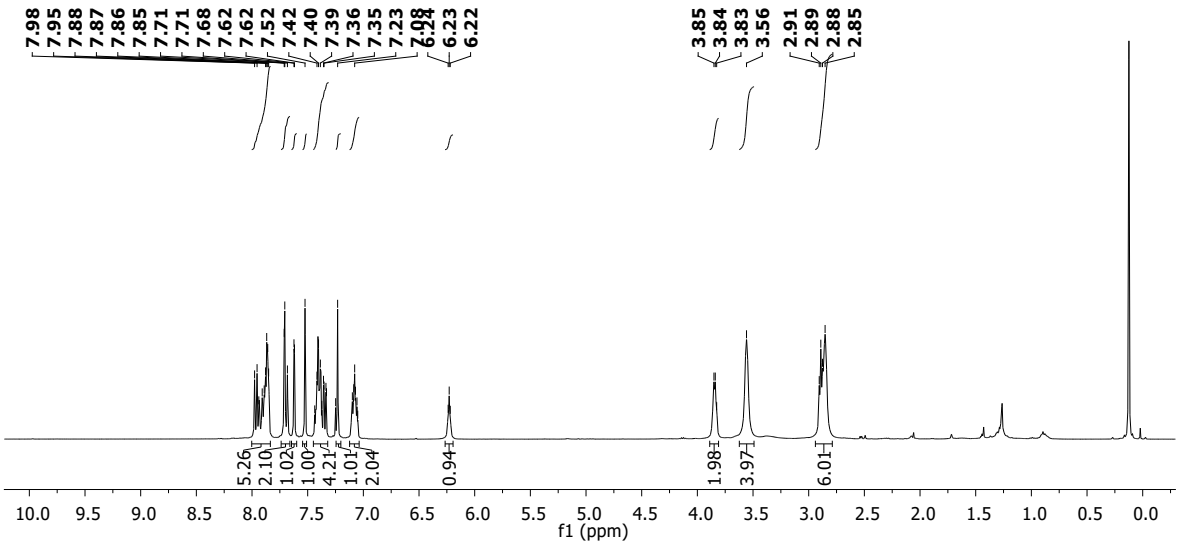
--- End Of Report ---

**$^1$H NMR** (400 MHz, $CDCl_3$)

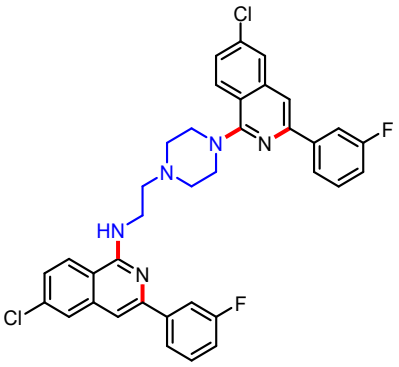



**6-chloro-N-(2-(4-(6-chloro-3-(3-fluorophenyl)isoquinolin-1-yl)piperazin-1-yl)ethyl)-3-(3-fluorophenyl)isoquinolin-1-amine (6c)**

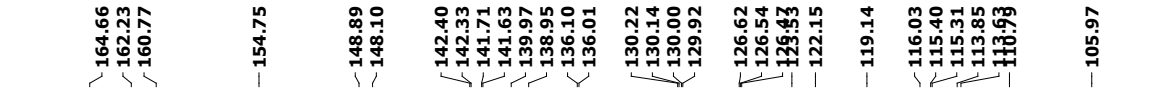


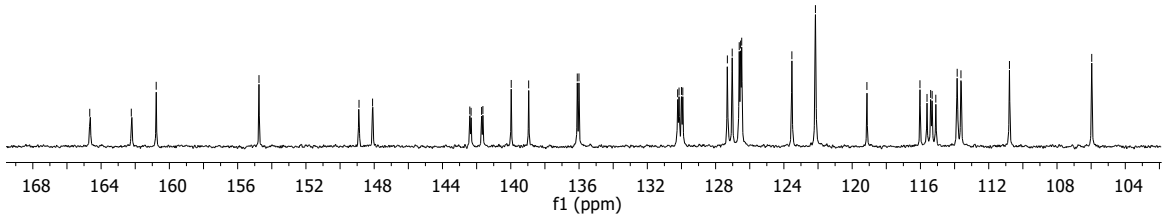



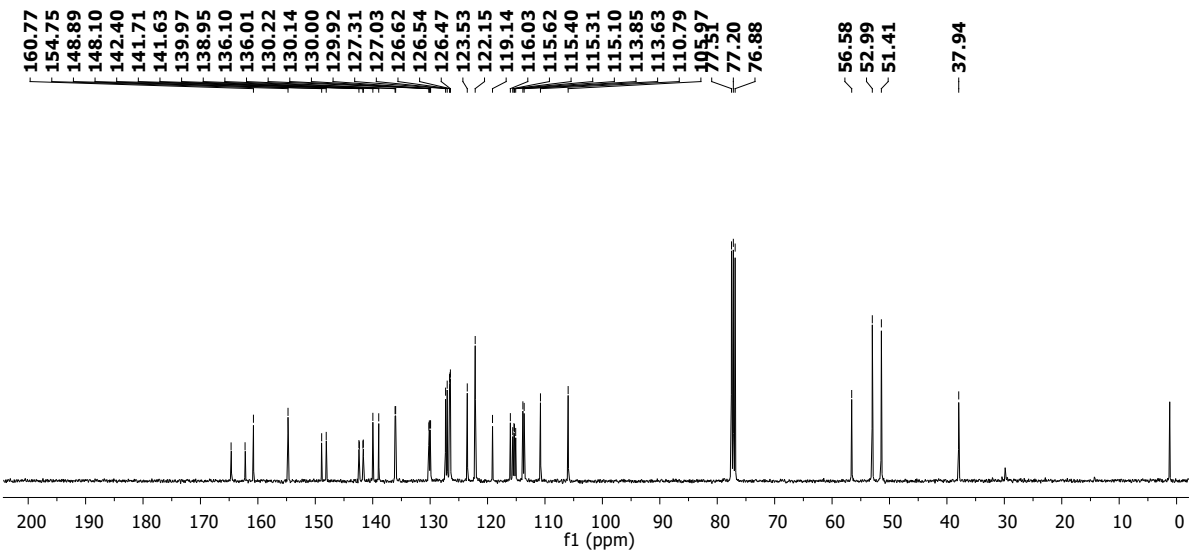
**$^{13}$C NMR** (100 MHz, $CDCl_3$)



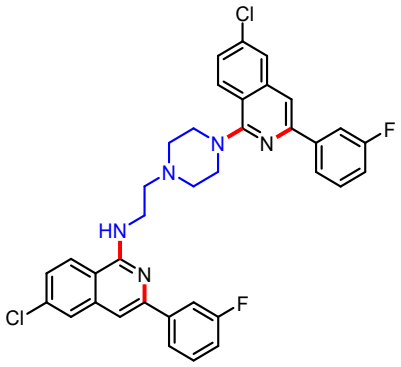

**6-chloro-N-(2-(4-(6-chloro-3-(3-fluorophenyl)isoquinolin-1-yl)piperazin-1-yl)ethyl)-3-(3-fluorophenyl)isoquinolin-1-amine (6c)**



## HRMS




**6-chloro-N-(2-(4-(6-chloro-3-(3-fluorophenyl)isoquinolin-1-yl)piperazin-1-yl)ethyl)-3-(3-fluorophenyl)isoquinolin-1-amine (6c)**

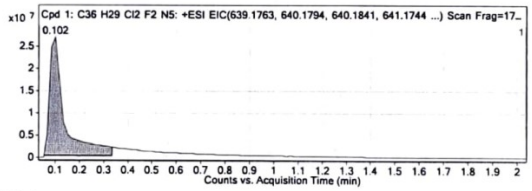
### Qualitative Compound Report

| | | | |
|---|---|---|---|
| Data File | 6127.d | Sample Name | 6127 |
| Sample Type | Sample | Position | P1-A2 |
| Instrument Name | Instrument 1 | User Name | |
| Acq Method | MS Scan.m | Acquired Time | 27-08-2022 12:04:31 |
| IRM Calibration Status | [redacted] | DA Method | Default.m |
| Comment | | | |
| Sample Group | | Info. | 3 |
| Acquisition SW Version | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

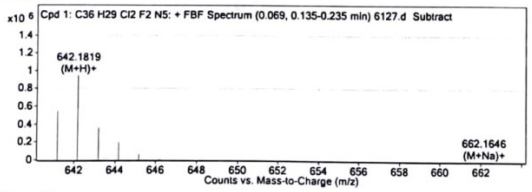
Compound Table

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C36 H29 Cl2 F2 N5 | 0.102 | 639.1764 | 1304191 | C36 H29 Cl2 F2 N5 | 639.1768 | -0.57 | C36 H29 Cl2 F2 N5 | C36 H29 Cl2 F2 N5 |

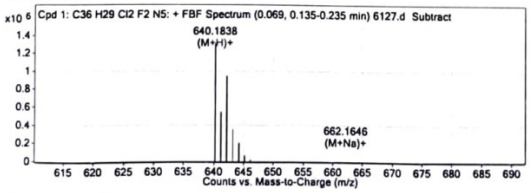
| Compound Label | m/z | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C36 H29 Cl2 F2 N5 | 640.1838 | 0.102 | Find By Formula | 639.1764 |




MS Spectrum



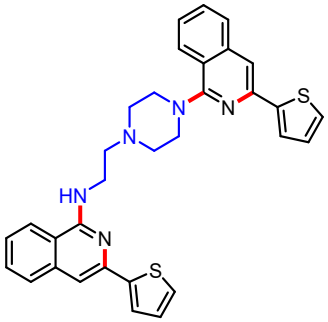

MS Zoomed Spectrum



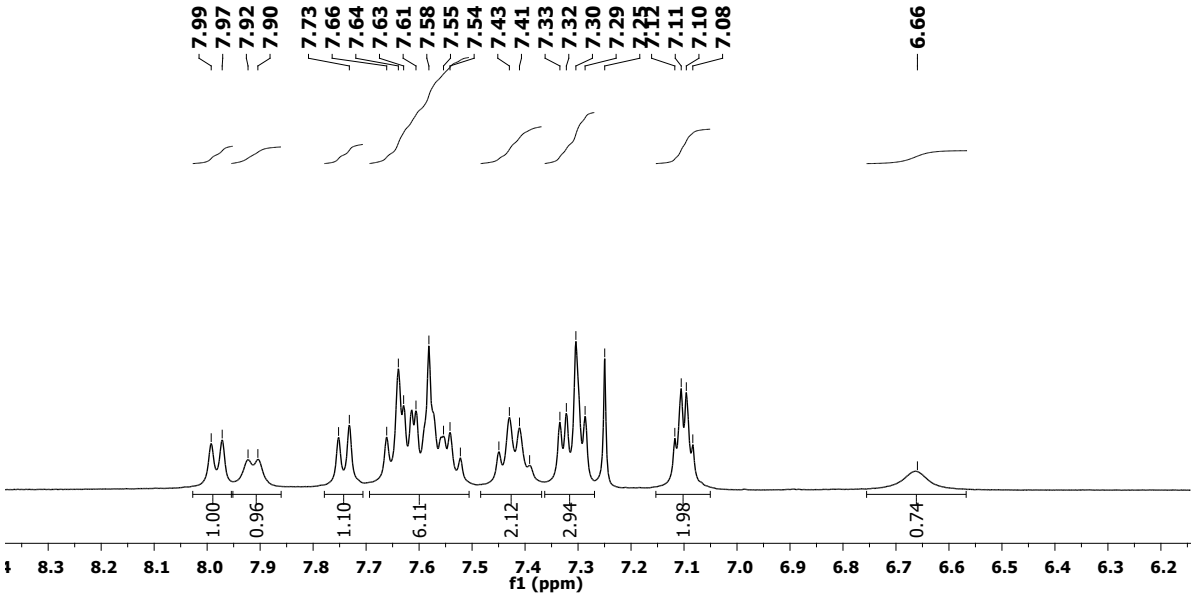

MS Spectrum Peak List

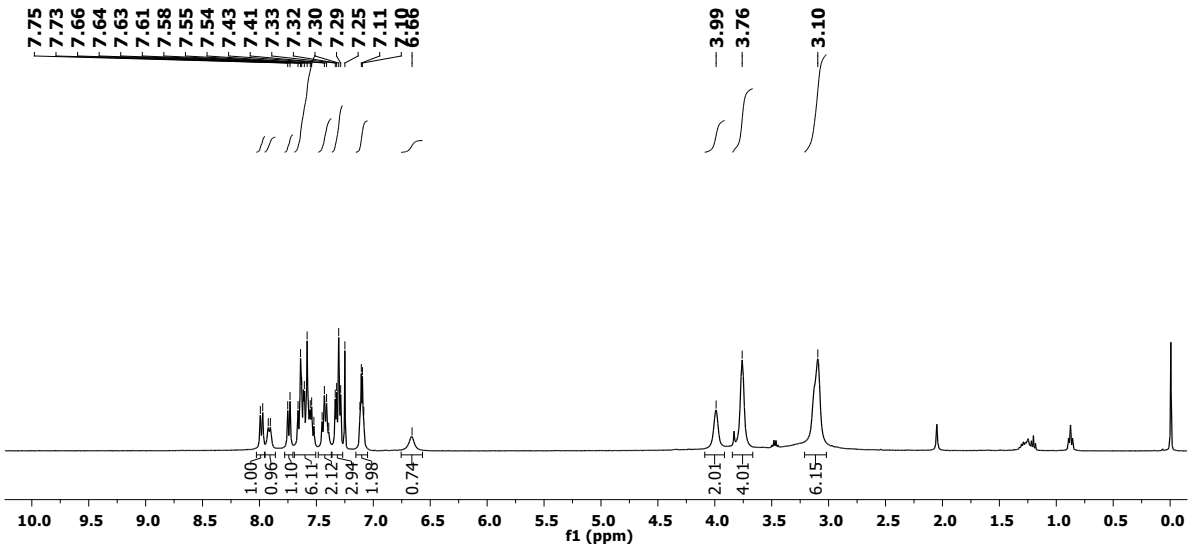
| m/z | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 640.1838 | 1 | 1304191.25 | C36H30Cl2F2N5 | (M+H)+ |
| 641.1869 | 1 | 544455.44 | C36H30Cl2F2N5 | (M+H)+ |
| 642.1819 | 1 | 944997.94 | C36H30Cl2F2N5 | (M+H)+ |
| 643.184 | 1 | 356752.56 | C36H30Cl2F2N5 | (M+H)+ |
| 644.1806 | 1 | 196923.97 | C36H30Cl2F2N5 | (M+H)+ |
| 645.1812 | 1 | 59258.64 | C36H30Cl2F2N5 | (M+H)+ |
| 646.1835 | 1 | 11020.03 | C36H30Cl2F2N5 | (M+H)+ |
| 647.1873 | 1 | 1373.56 | C36H30Cl2F2N5 | (M+H)+ |
| 662.1646 | 1 | 1273.61 | C36H29Cl2F2N5Na | (M+Na)+ |
| 663.1665 | 1 | 559.96 | C36H29Cl2F2N5Na | (M+Na)+ |
| 664.1643 | 1 | 857.61 | C36H29Cl2F2N5Na | (M+Na)+ |

**$^1$H NMR** (400MHz, $CDCl_3$)

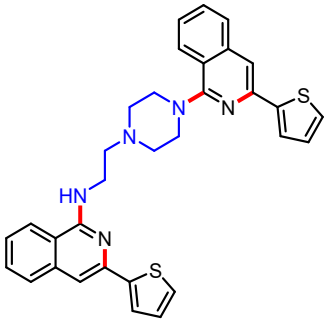



**3-(thiophen-2-yl)-N-(2-(4-(3-(thiophen-2-yl)isoquinolin-1-yl)piperazin-1-yl)ethyl)isoquinolin-1-amine (6d)**

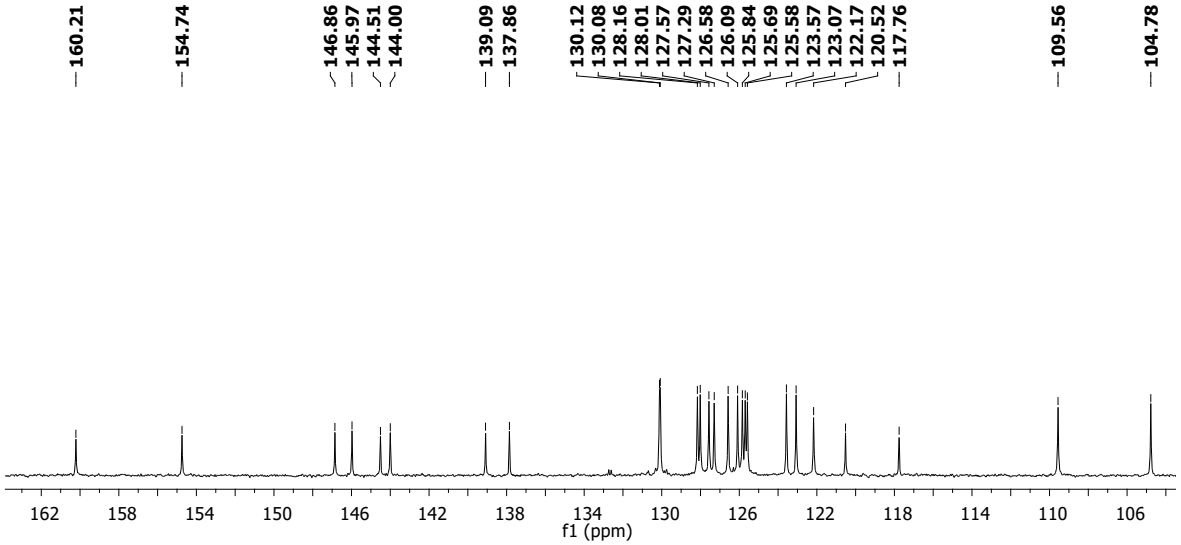


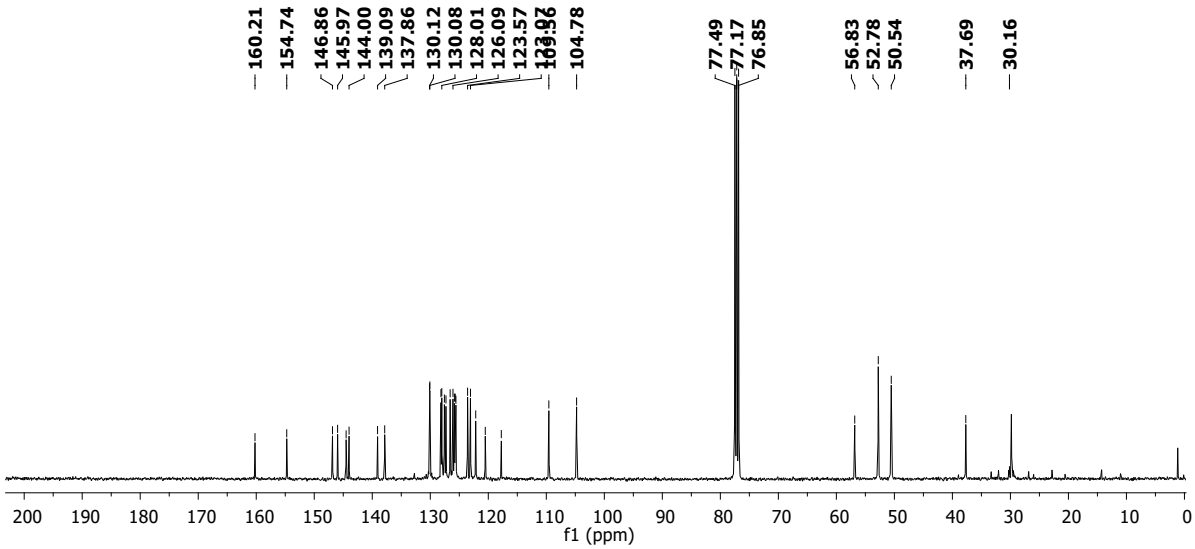



**$^{13}$C NMR** (100MHz, $CDCl_3$)

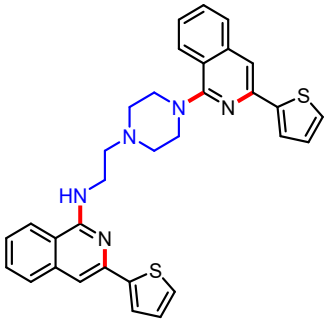



**3-(thiophen-2-yl)-N-(2-(4-(3-(thiophen-2-yl)isoquinolin-1-yl)piperazin-1-yl)ethyl)isoquinolin-1-amine (6d)**



## HRMS



**3-(thiophen-2-yl)-N-(2-(4-(3-(thiophen-2-yl)isoquinolin-1-yl)piperazin-1-yl)ethyl)isoquinolin-1-amine (6d)**

### Qualitative Compound Report

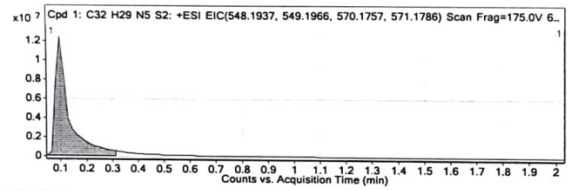
| | | | |
|---|---|---|---|
| **Data File** | 6108.d | **Sample Name** | 6108 |
| **Sample Type** | Sample | **Position** | P1-C9 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | MS Scan.m | **Acquired Time** | 22-08-2022 14:33:59 |
| **IRM Calibration Status** | [redacted] | **DA Method** | Default.m |
| **Comment** | | | |

| | | | |
|---|---|---|---|
| **Sample Group** | | **Info.** | 3 |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

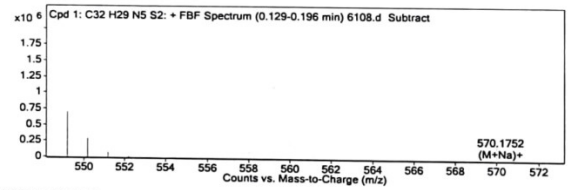
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C32 H29 N5 S2 | 0.096 | 547.1854 | 1765410 | C32 H29 N5 S2 | 547.1864 | -1.92 | C32 H29 N5 S2 | C32 H29 N5 S2 |

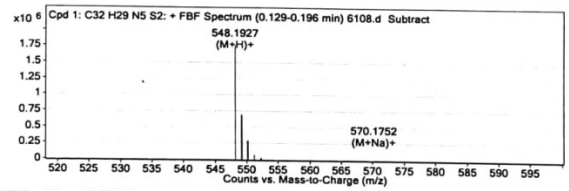
| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C32 H29 N5 S2 | 548.1927 | 0.096 | Find By Formula | 547.1854 |




MS Spectrum




MS Zoomed Spectrum

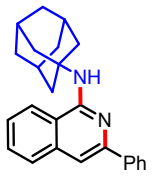



**MS Spectrum Peak List**

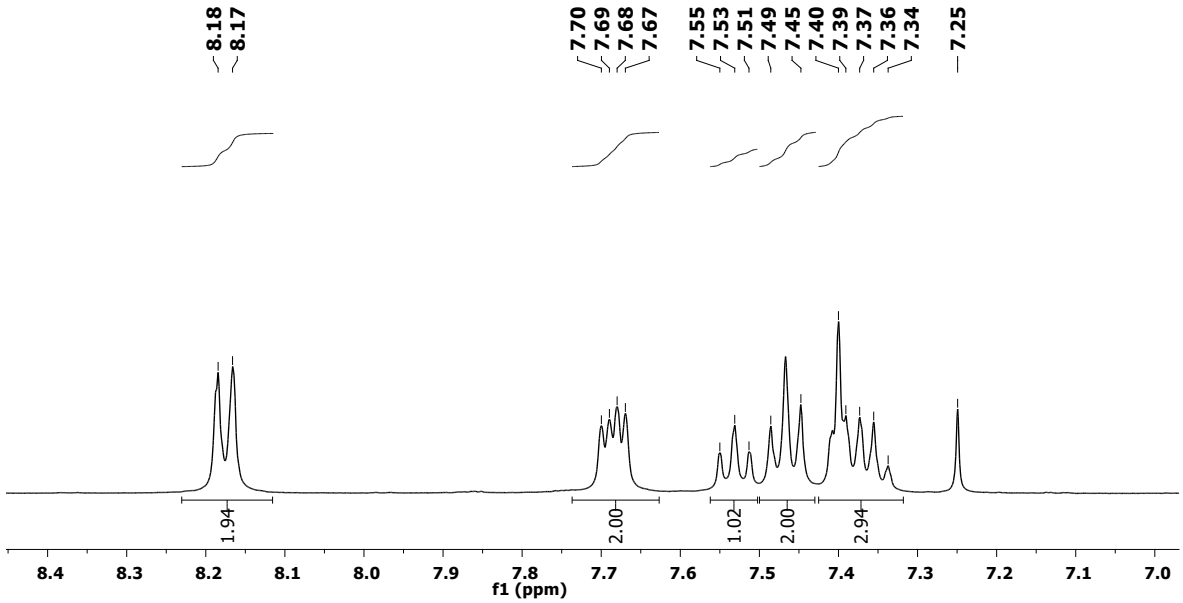
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 548.1927 | 1 | 1765409.63 | C32H30N5S2 | (M+H)+ |
| 549.1958 | 1 | 697886.5 | C32H30N5S2 | (M+H)+ |
| 550.1928 | 1 | 283527.34 | C32H30N5S2 | (M+H)+ |
| 551.1926 | 1 | 70663.61 | C32H30N5S2 | (M+H)+ |
| 552.1921 | 1 | 14966.3 | C32H30N5S2 | (M+H)+ |
| 553.1925 | 1 | 2919.04 | C32H30N5S2 | (M+H)+ |
| 570.1752 | 1 | 1268.2 | C32H29N5NaS2 | (M+Na)+ |
| 571.1733 | 1 | 594.27 | C32H29N5NaS2 | (M+Na)+ |
| 572.1742 | 1 | 198.91 | C32H29N5NaS2 | (M+Na)+ |
| 573.1926 | 1 | 64 | C32H29N5NaS2 | (M+Na)+ |

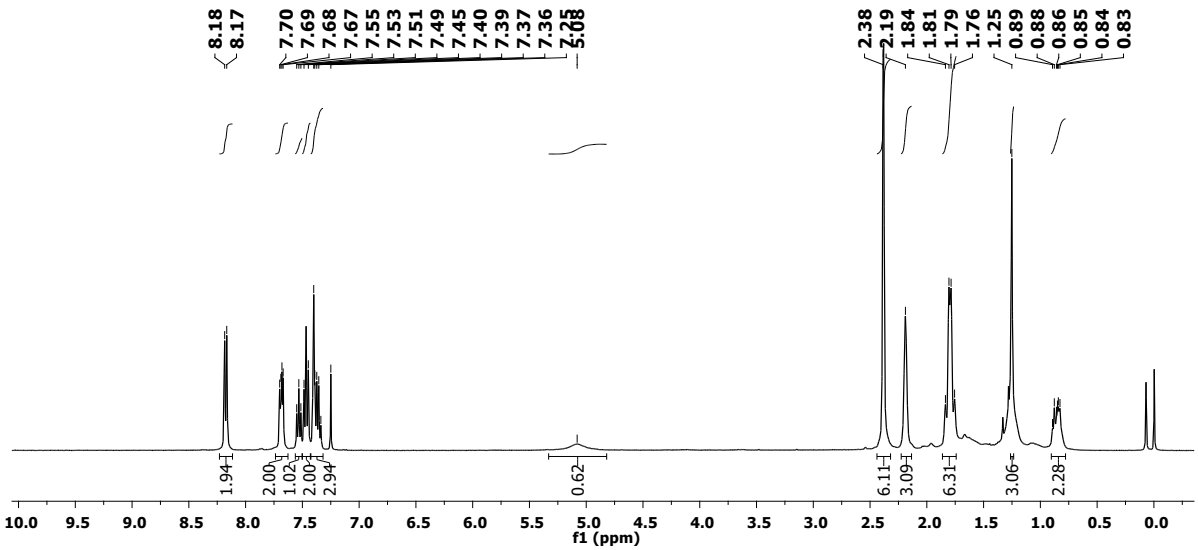
--- End Of Report ---

**$^1$H NMR** (400MHz, $CDCl_3$)

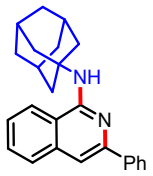



***N*-((3S,5S)-adamantan-1-yl)-3-phenylisoquinolin-1-amine (7a)**

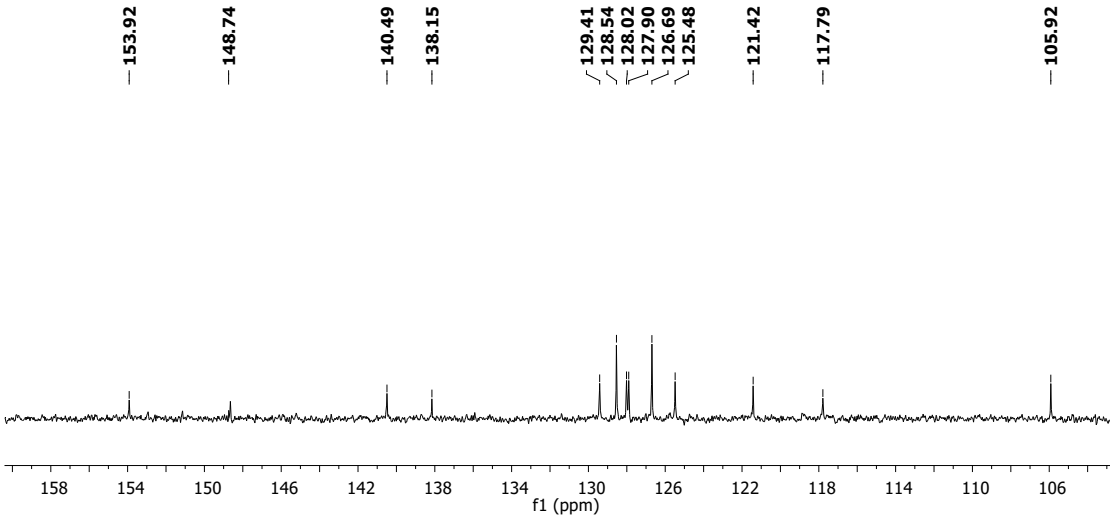


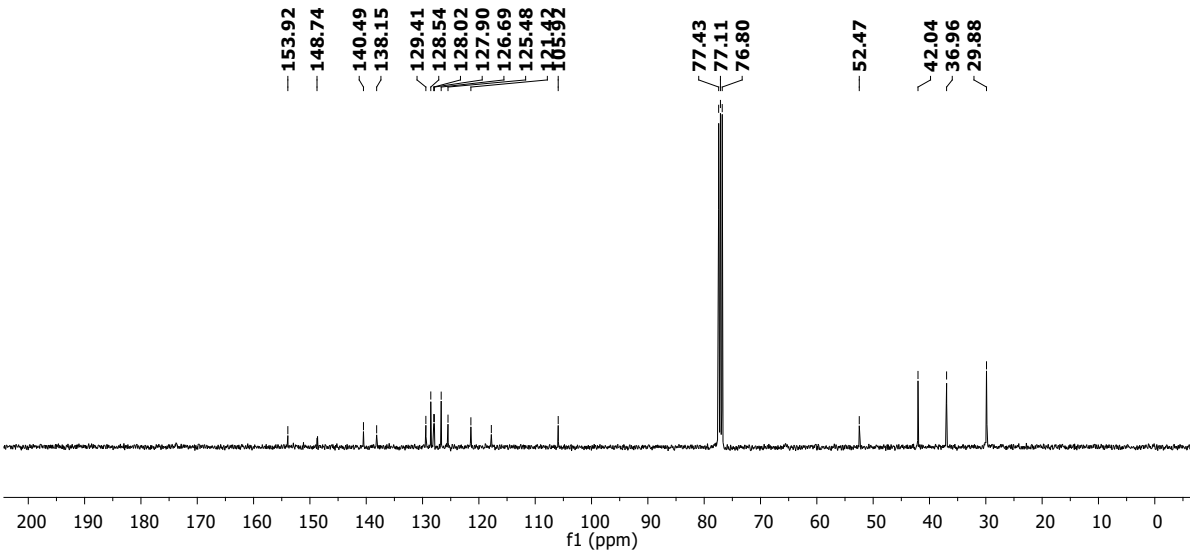



**$^{13}$C NMR** (100MHz, $CDCl_3$)

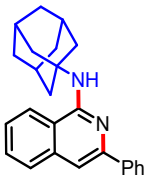



***N*-((3S,5S)-adamantan-1-yl)-3-phenylisoquinolin-1-amine (7a)**



## HRMS




***N*-((3S,5S)-adamantan-1-yl)-3-phenylisoquinolin-1-amine (7a)**

### Qualitative Compound Report

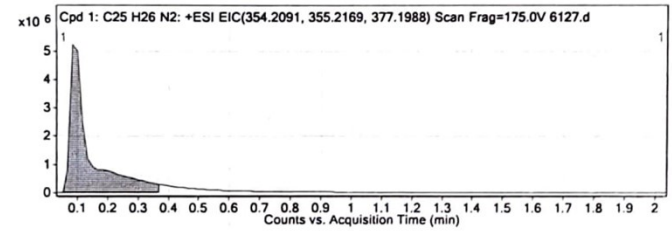
| | | | |
|---|---|---|---|
| **Data File** | 6127.d | **Sample Name** | 6127 |
| **Sample Type** | Sample | **Position** | P1-A2 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | MS Scan.m | **Acquired Time** | 27-08-2022 12:04:31 |
| **IRM Calibration Status** | [redacted] | **DA Method** | Default.m |
| **Comment** | | | |

| | | | |
|---|---|---|---|
| **Sample Group** | | **Info.** | 3 |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

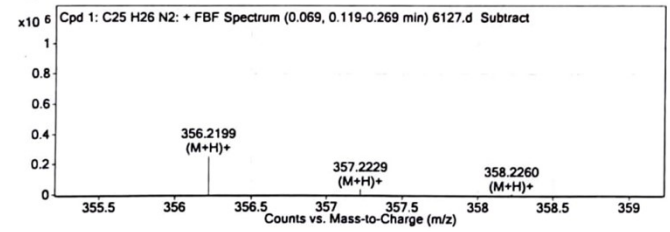
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C25 H26 N2 | 0.085 | 354.2096 | 938132 | C25 H26 N2 | 354.2096 | 0.05 | C25 H26 N2 | C25 H26 N2 |

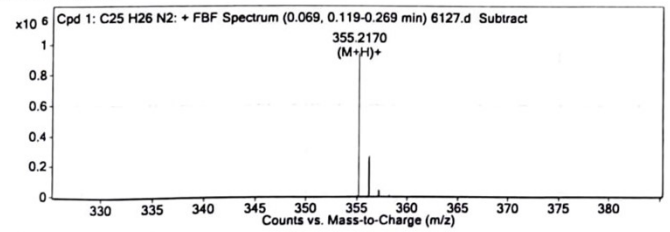
| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C25 H26 N2 | 355.217 | 0.085 | Find By Formula | 354.2096 |




MS Spectrum




MS Zoomed Spectrum

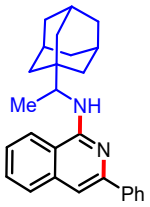



**MS Spectrum Peak List**

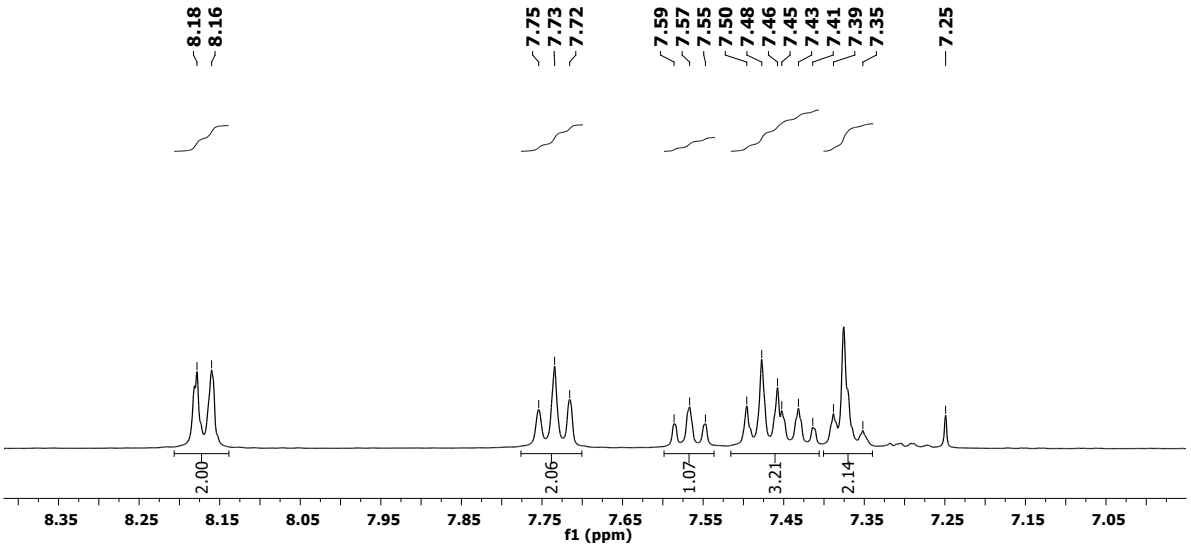
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 355.217 | 1 | 938131.63 | C25H27N2 | (M+H)+ |
| 356.2199 | 1 | 254303.81 | C25H27N2 | (M+H)+ |
| 357.2229 | 1 | 32521.18 | C25H27N2 | (M+H)+ |
| 358.226 | 1 | 2945.39 | C25H27N2 | (M+H)+ |
| 359.2274 | 1 | 508.19 | C25H27N2 | (M+H)+ |

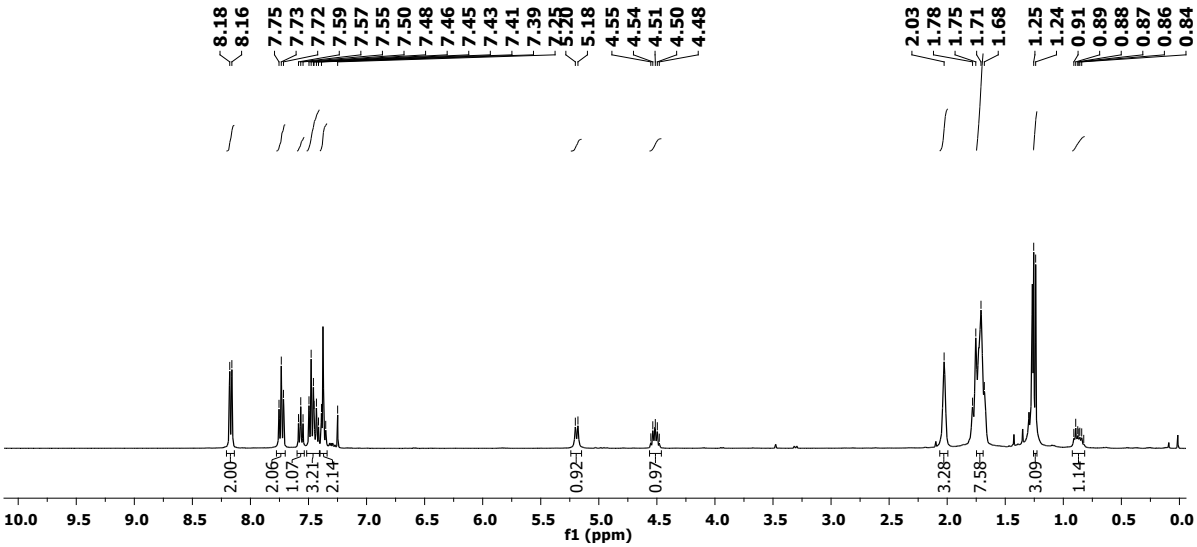
--- End Of Report ---

**$^1$H NMR** (400MHz, $CDCl_3$)

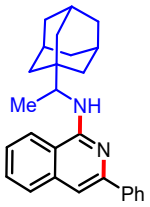



***N*-(1-((3r,5r,7r)-adamantan-1-yl)ethyl)-3-phenylisoquinolin-1-amine (7b)**

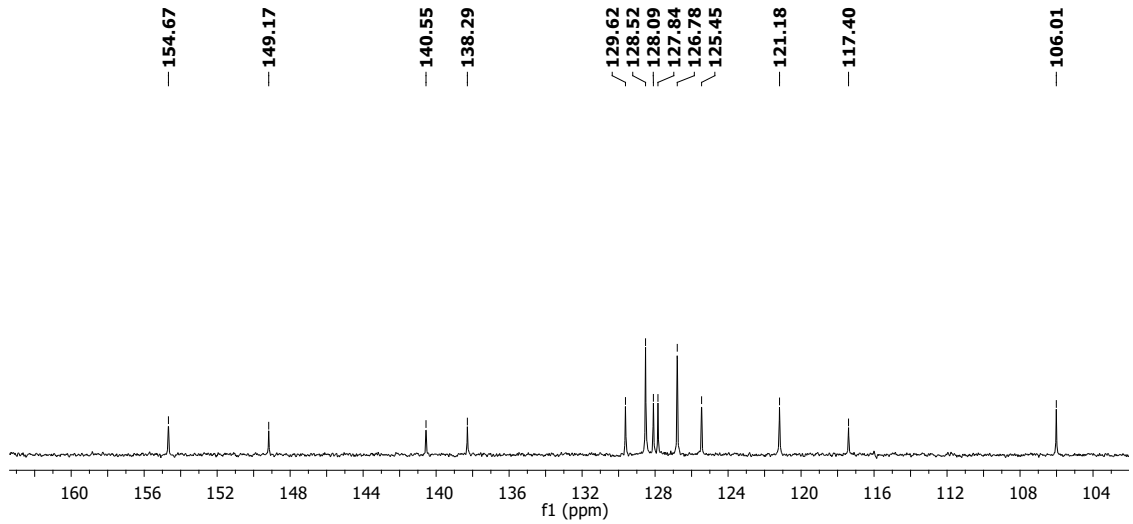


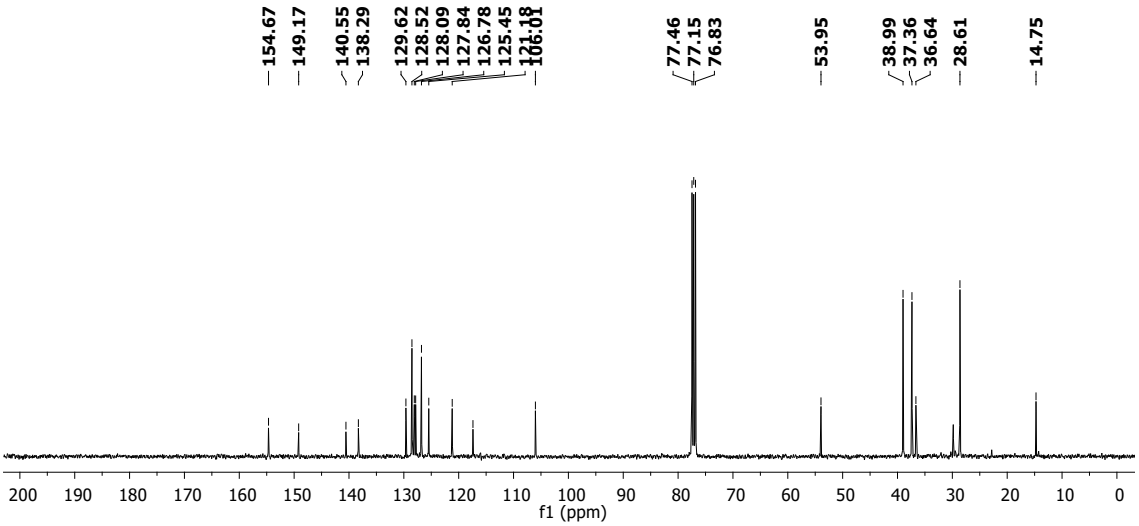



**$^{13}$C NMR** (100MHz, $CDCl_3$)

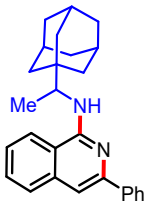



***N*-(1-((3r,5r,7r)-adamantan-1-yl)ethyl)-3-phenylisoquinolin-1-amine (7b)**



## HRMS




***N*-(1-((3r,5r,7r)-adamantan-1-yl)ethyl)-3-phenylisoquinolin-1-amine (7b)**

### Qualitative Compound Report

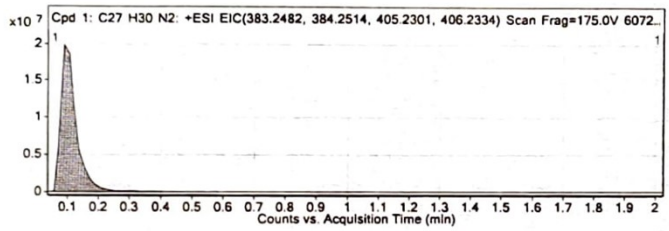
| | | | |
|---|---|---|---|
| Data File | 6072.d | Sample Name | 6072 |
| Sample Type | Sample | Position | P1-C5 |
| Instrument Name | Instrument 1 | User Name | |
| Acq Method | MS Scan.m | Acquired Time | 22-08-2022 14:22:58 |
| IRM Calibration Status | [redacted] | DA Method | Default.m |
| Comment | | | |

| | | | |
|---|---|---|---|
| Sample Group | | Info. | 3 |
| Acquisition SW Version | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

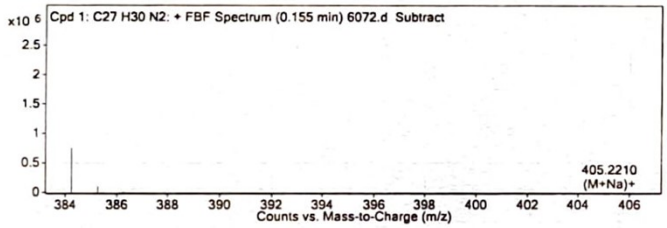
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C27 H30 N2 | 0.089 | 382.2403 | 2391152 | C27 H30 N2 | 382.2409 | -1.6 | C27 H30 N2 | C27 H30 N2 |

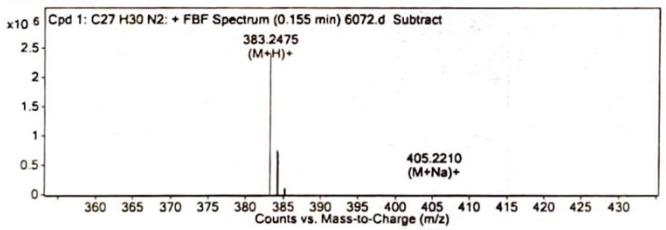
| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C27 H30 N2 | 383.2475 | 0.089 | Find By Formula | 382.2403 |




MS Spectrum




MS Zoomed Spectrum

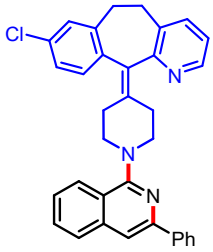



**MS Spectrum Peak List**

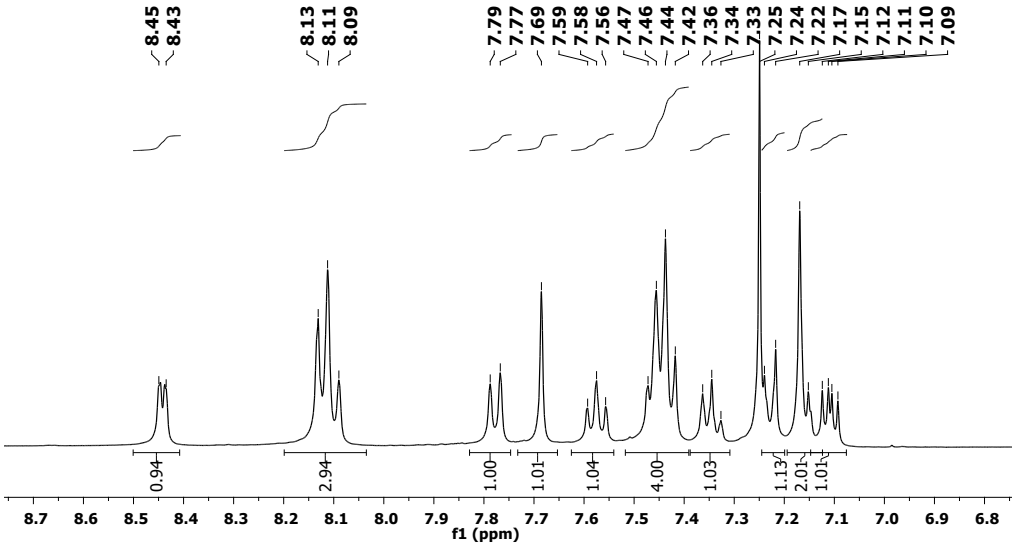
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 383.2475 | 1 | 2391152 | C27H31N2 | (M+H)+ |
| 384.251 | 1 | 757584.25 | C27H31N2 | (M+H)+ |
| 385.2537 | 1 | 100404.1 | C27H31N2 | (M+H)+ |
| 386.2568 | 1 | 10762.69 | C27H31N2 | (M+H)+ |
| 405.221 | 1 | 982.4 | C27H30N2Na | (M+Na)+ |
| 406.2177 | 1 | 320.13 | C27H30N2Na | (M+Na)+ |
| 407.2076 | 1 | 600.23 | C27H30N2Na | (M+Na)+ |

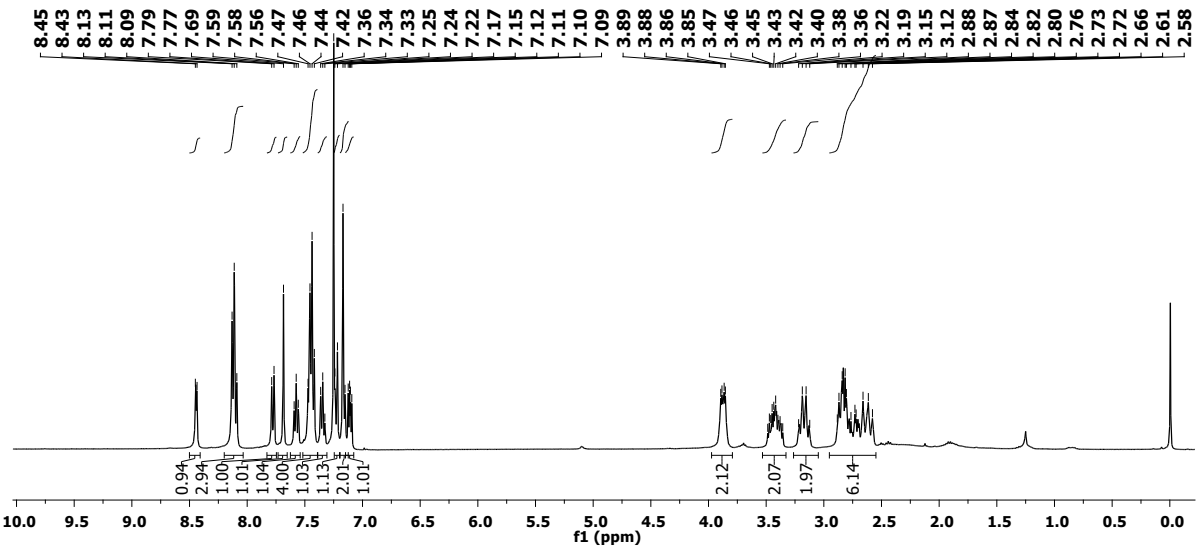
--- End Of Report ---

**$^1$H NMR** (400MHz, $CDCl_3$)

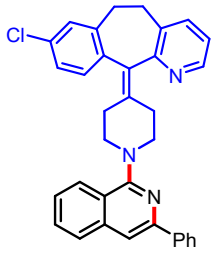



**8-chloro-11-(1-(3-phenylisoquinolin-1-yl)piperidin-4-ylidene)-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridine (7c)**

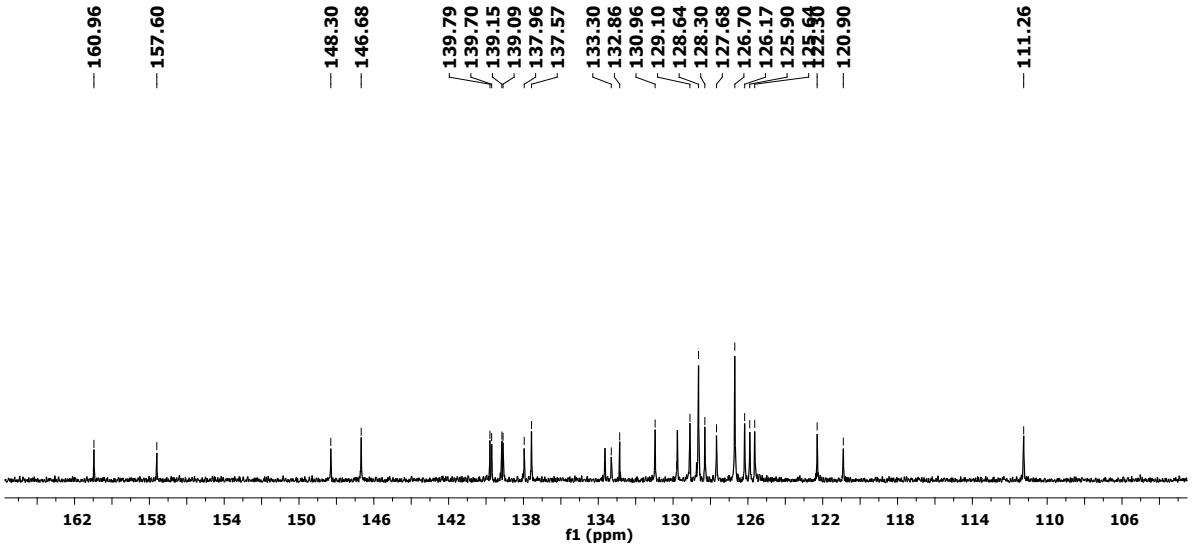


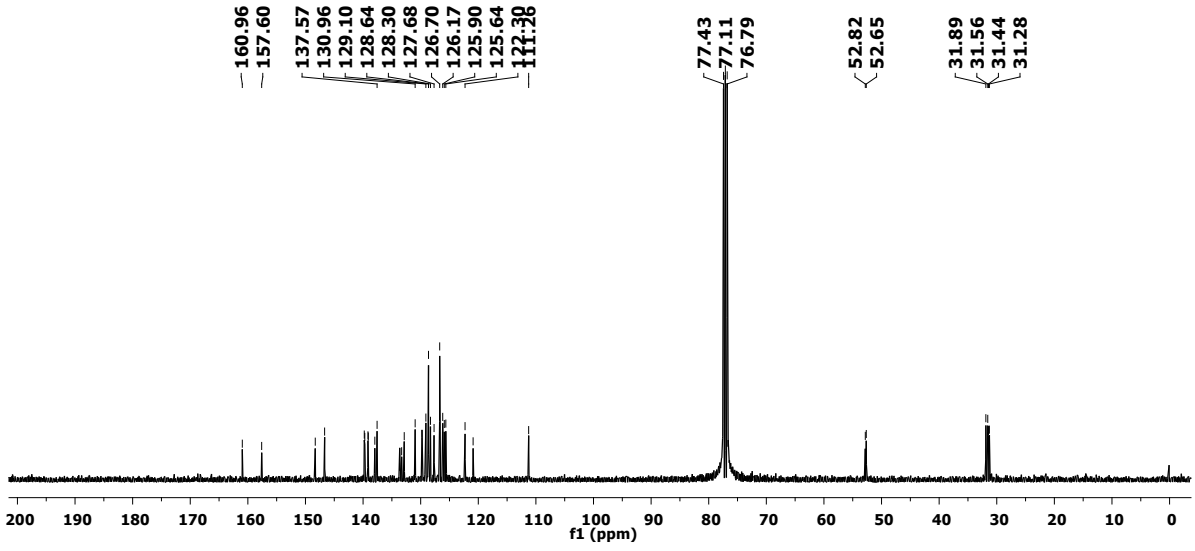



**$^{13}$C NMR** (100MHz, $CDCl_3$)

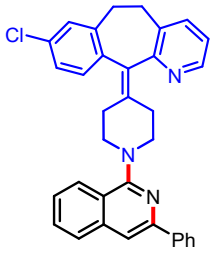



**8-chloro-11-(1-(3-phenylisoquinolin-1-yl)piperidin-4-ylidene)-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridine (7c)**



## HRMS




**8-chloro-11-(1-(3-phenylisoquinolin-1-yl)piperidin-4-ylidene)-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridine (7c)**

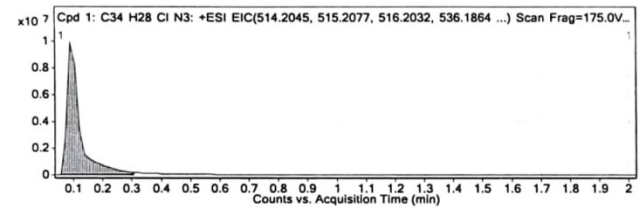
### Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | 6072.d | **Sample Name** | 6072 |
| **Sample Type** | Sample | **Position** | P1-C5 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | MS Scan.m | **Acquired Time** | 22-08-2022 14:22:58 |
| **IRM Calibration Status** | [redacted] | **DA Method** | Default.m |
| **Comment** | | | |
| **Sample Group** | | **Info.** | 3 |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

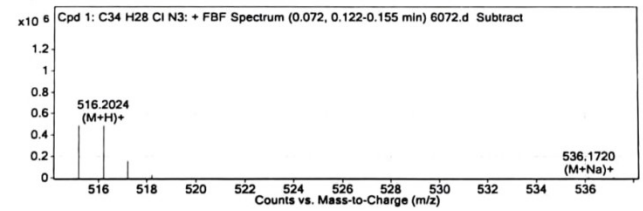
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C34 H28 Cl N3 | 0.089 | 513.1963 | 1201101 | C34 H28 Cl N3 | 513.1972 | -1.62 | C34 H28 Cl N3 | C34 H28 Cl N3 |

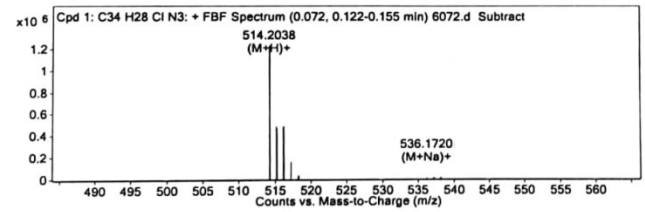
| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C34 H28 Cl N3 | 514.2038 | 0.089 | Find By Formula | 513.1963 |




MS Spectrum




MS Zoomed Spectrum

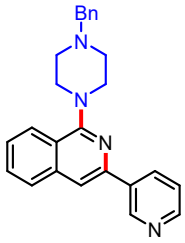



**MS Spectrum Peak List**

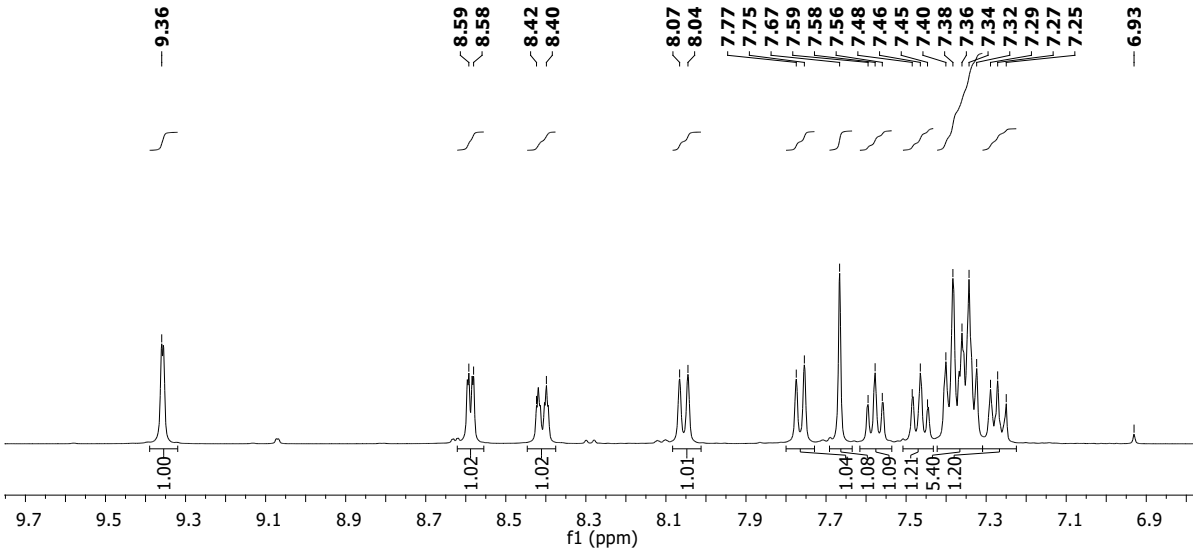
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 514.2038 | 1 | 1201101.38 | C34H29ClN3 | (M+H)+ |
| 515.2069 | 1 | 486156.59 | C34H29ClN3 | (M+H)+ |
| 516.2024 | 1 | 491078.34 | C34H29ClN3 | (M+H)+ |
| 517.2043 | 1 | 157501.08 | C34H29ClN3 | (M+H)+ |
| 518.2068 | 1 | 27348.97 | C34H29ClN3 | (M+H)+ |
| 519.2097 | 1 | 3369.94 | C34H29ClN3 | (M+H)+ |
| 536.172 | 1 | 9902.57 | C34H28ClN3Na | (M+Na)+ |
| 537.1727 | 1 | 4986.8 | C34H28ClN3Na | (M+Na)+ |
| 538.1704 | 1 | 3869.37 | C34H28ClN3Na | (M+Na)+ |

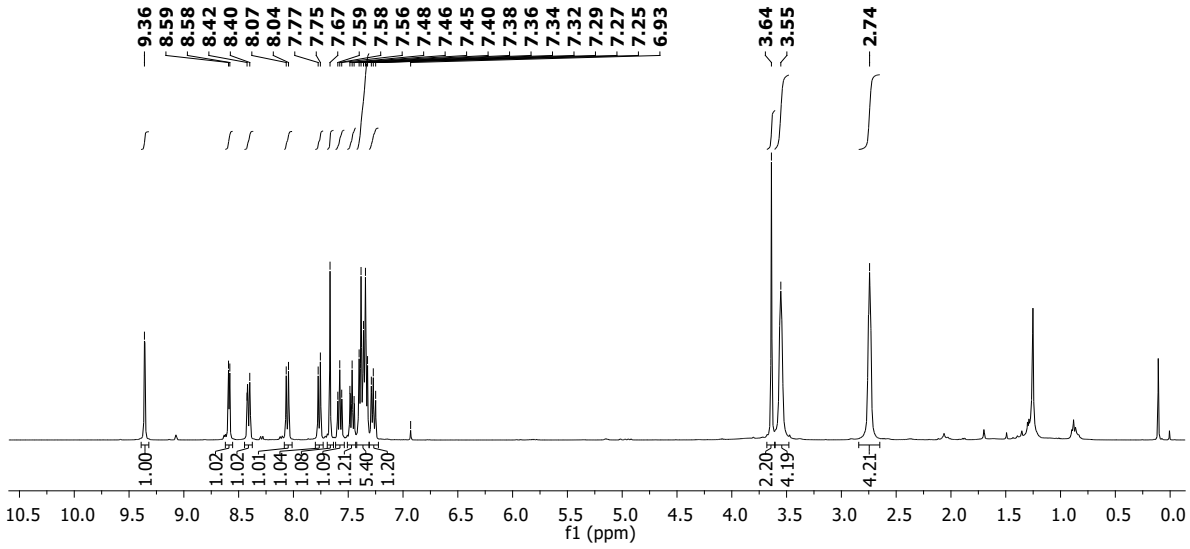
--- End Of Report ---

**$^1$H NMR** (400 MHz, $CDCl_3$)

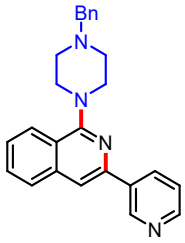



**1-(4-benzylpiperazin-1-yl)-3-(pyridin-3-yl)isoquinoline (7d)**

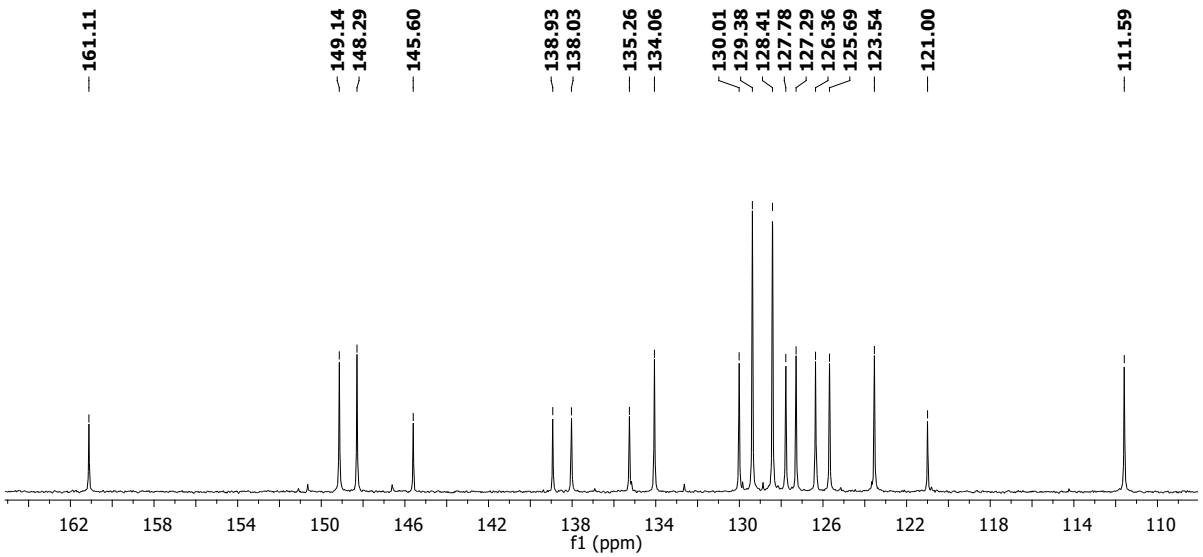


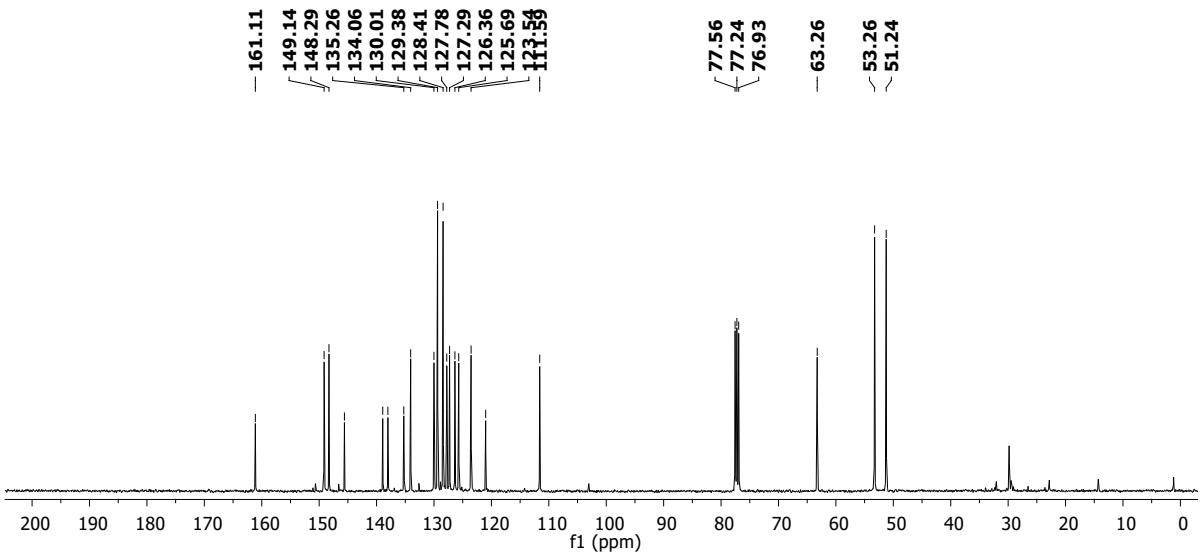



**$^{13}$C NMR** (100 MHz, $CDCl_3$)

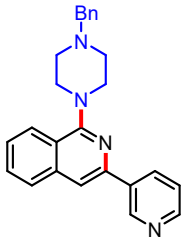



**1-(4-benzylpiperazin-1-yl)-3-(pyridin-3-yl)isoquinoline (7d)**



## HRMS




**1-(4-benzylpiperazin-1-yl)-3-(pyridin-3-yl)isoquinoline (7d)**

### Qualitative Compound Report

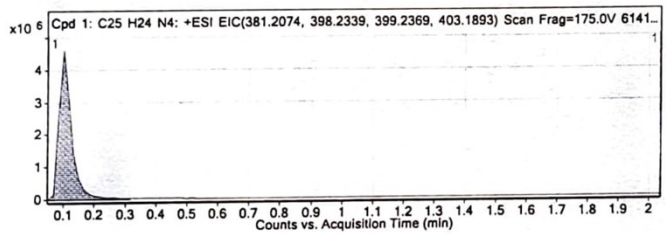
| | | | |
|---|---|---|---|
| **Data File** | 6141.d | **Sample Name** | 6141 |
| **Sample Type** | Sample | **Position** | P1-D3 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | MS Scan.m | **Acquired Time** | 22-08-2022 14:44:24 |
| **IRM Calibration Status** | Success | **DA Method** | Default.m |
| **Comment** | | | |

| | | | |
|---|---|---|---|
| **Sample Group** | | **Info.** | 3 |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

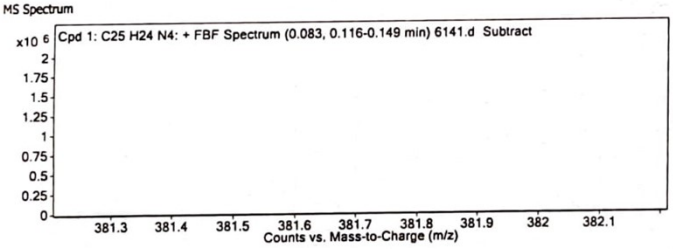
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C25 H24 N4 | 0.099 | 380.1998 | 1881189 | C25 H24 N4 | 380.2001 | -0.8 | C25 H24 N4 | C25 H24 N4 |

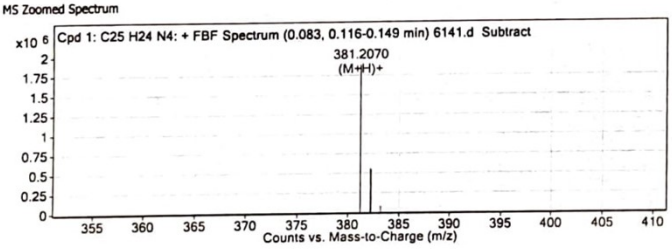
| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C25 H24 N4 | 381.207 | 0.099 | Find By Formula | 380.1998 |




MS Spectrum




MS Zoomed Spectrum

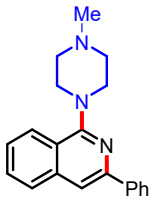



**MS Spectrum Peak List**

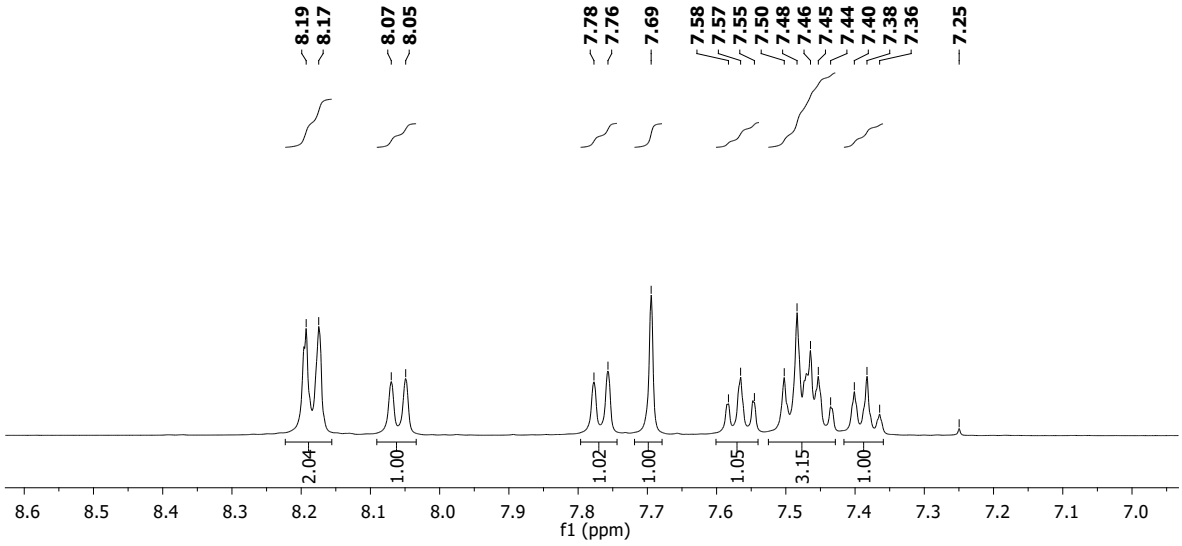
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 381.207 | 1 | 1881189.13 | C25H25N4 | (M+H)+ |
| 382.2102 | 1 | 550599.81 | C25H25N4 | (M+H)+ |

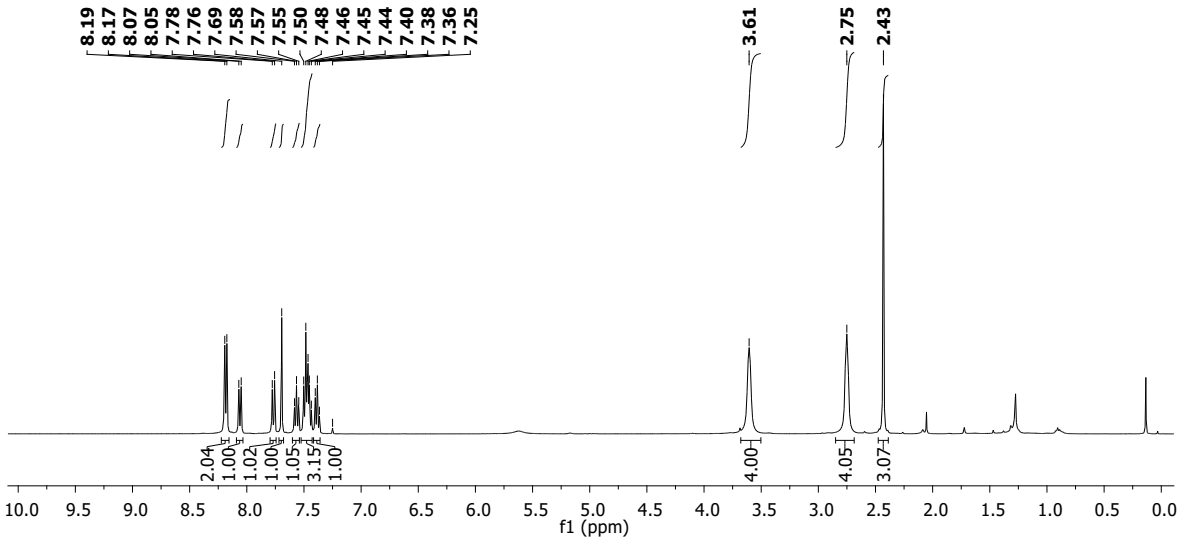
--- End Of Report ---

**$^1$H NMR** (400 MHz, $CDCl_3$)

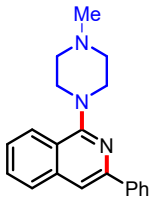



**1-(4-methylpiperazin-1-yl)-3-phenylisoquinoline (7e)**

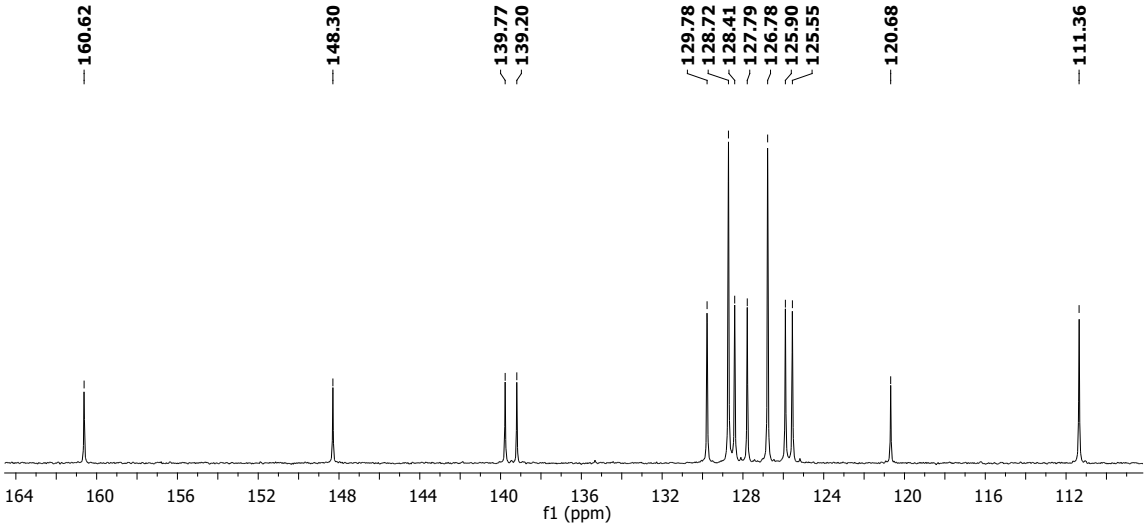


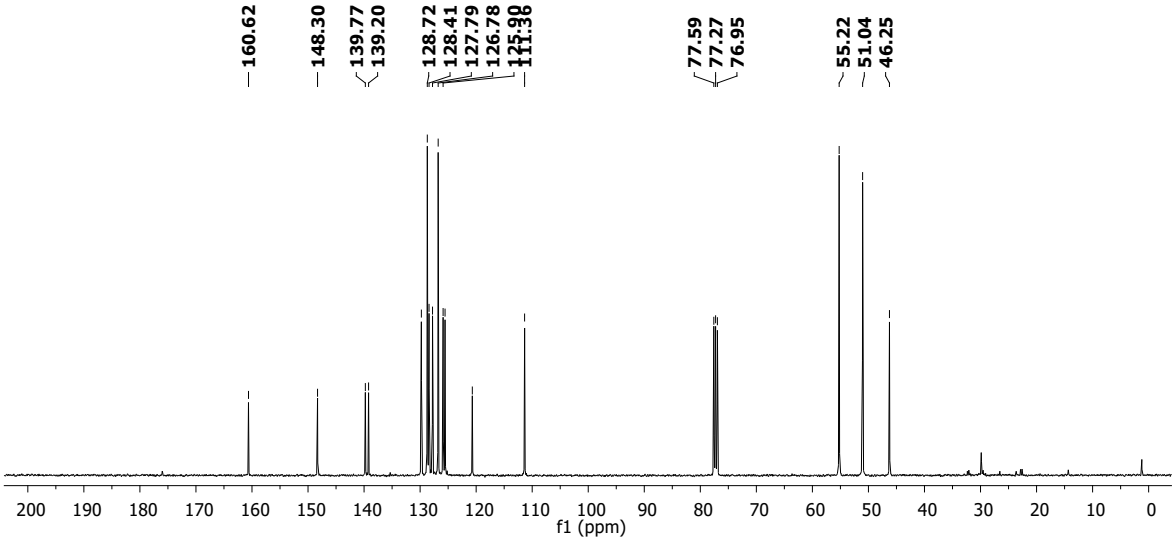



**$^{13}$C NMR** (100 MHz, $CDCl_3$)

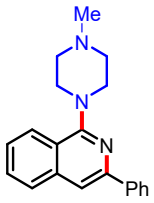



**1-(4-methylpiperazin-1-yl)-3-phenylisoquinoline (7e)**



## HRMS




**1-(4-methylpiperazin-1-yl)-3-phenylisoquinoline (7e)**

### Qualitative Compound Report

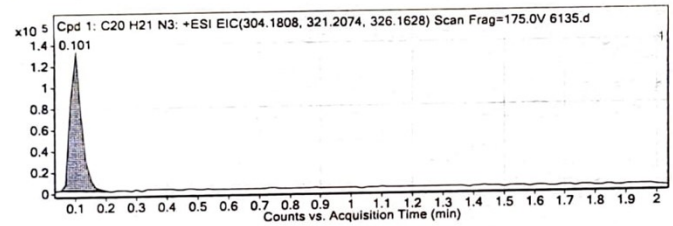
| | | | |
|---|---|---|---|
| Data File | 6135.d | Sample Name | 6135 |
| Sample Type | Sample | Position | P1-D2 |
| Instrument Name | Instrument 1 | User Name | |
| Acq Method | MS Scan.m | Acquired Time | 22-08-2022 14:41:36 |
| IRM Calibration Status | Success | DA Method | Default.m |
| Comment | | | |

| | | | |
|---|---|---|---|
| Sample Group | | Info. | 3 |
| Acquisition SW | 6200 series TOF/6500 series | | |
| Version | Q-TOF B.05.01 (B5125) | | |

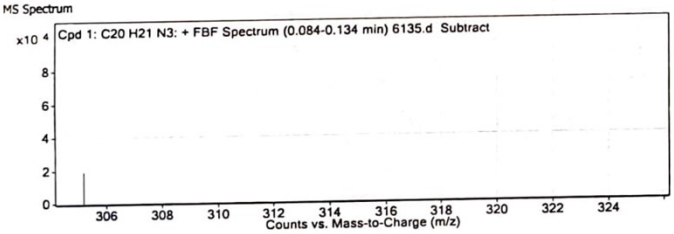
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C20 H21 N3 | 0.101 | 303.1729 | 82674 | C20 H21 N3 | 303.1735 | -2.07 | C20 H21 N3 | C20 H21 N3 |

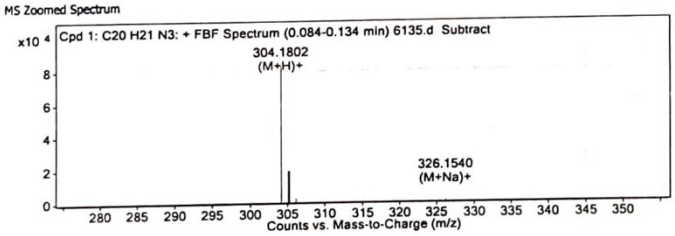
| Compound Label | m/z | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C20 H21 N3 | 304.1802 | 0.101 | Find By Formula | 303.1729 |




MS Spectrum




MS Zoomed Spectrum

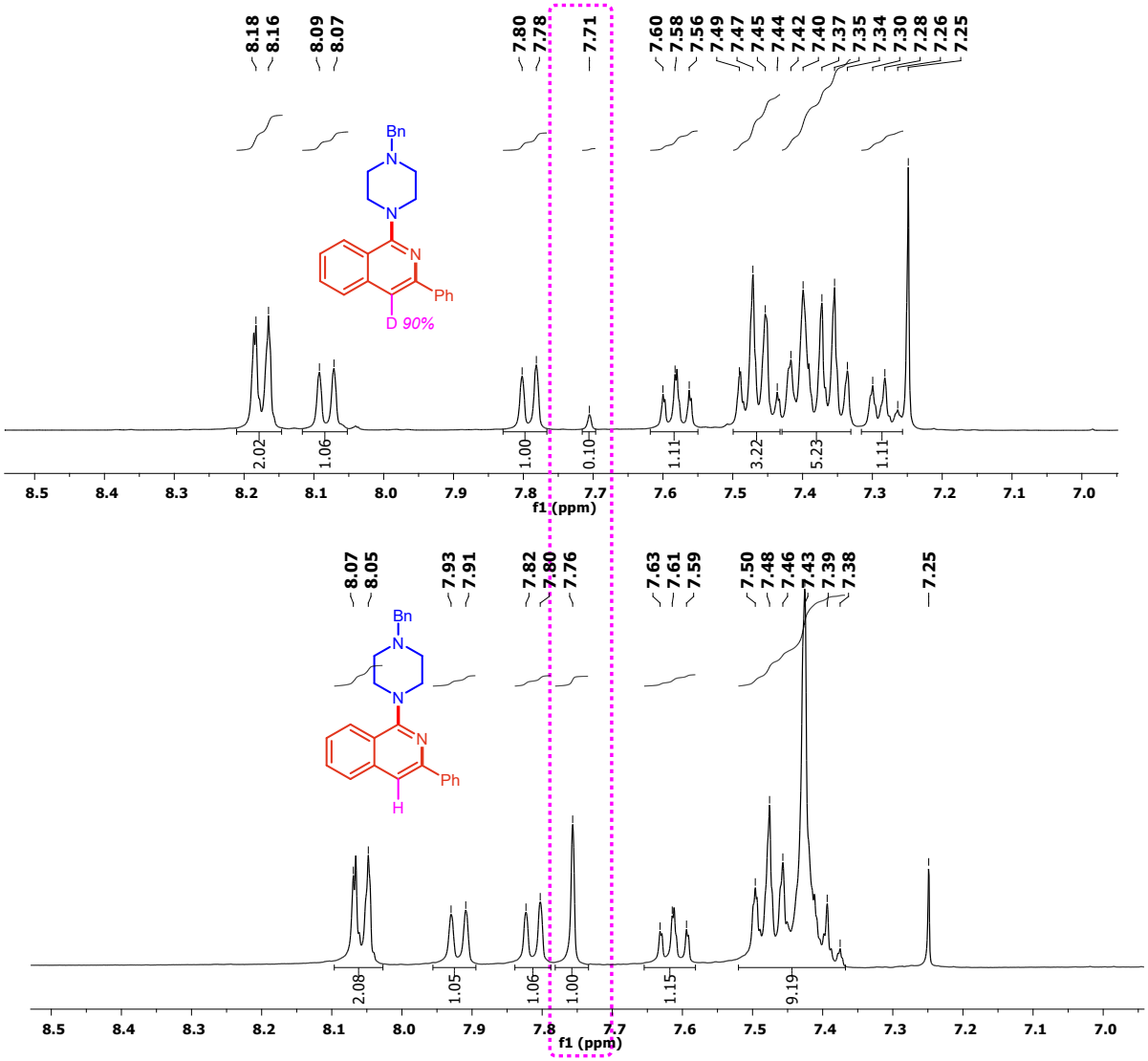



**MS Spectrum Peak List**

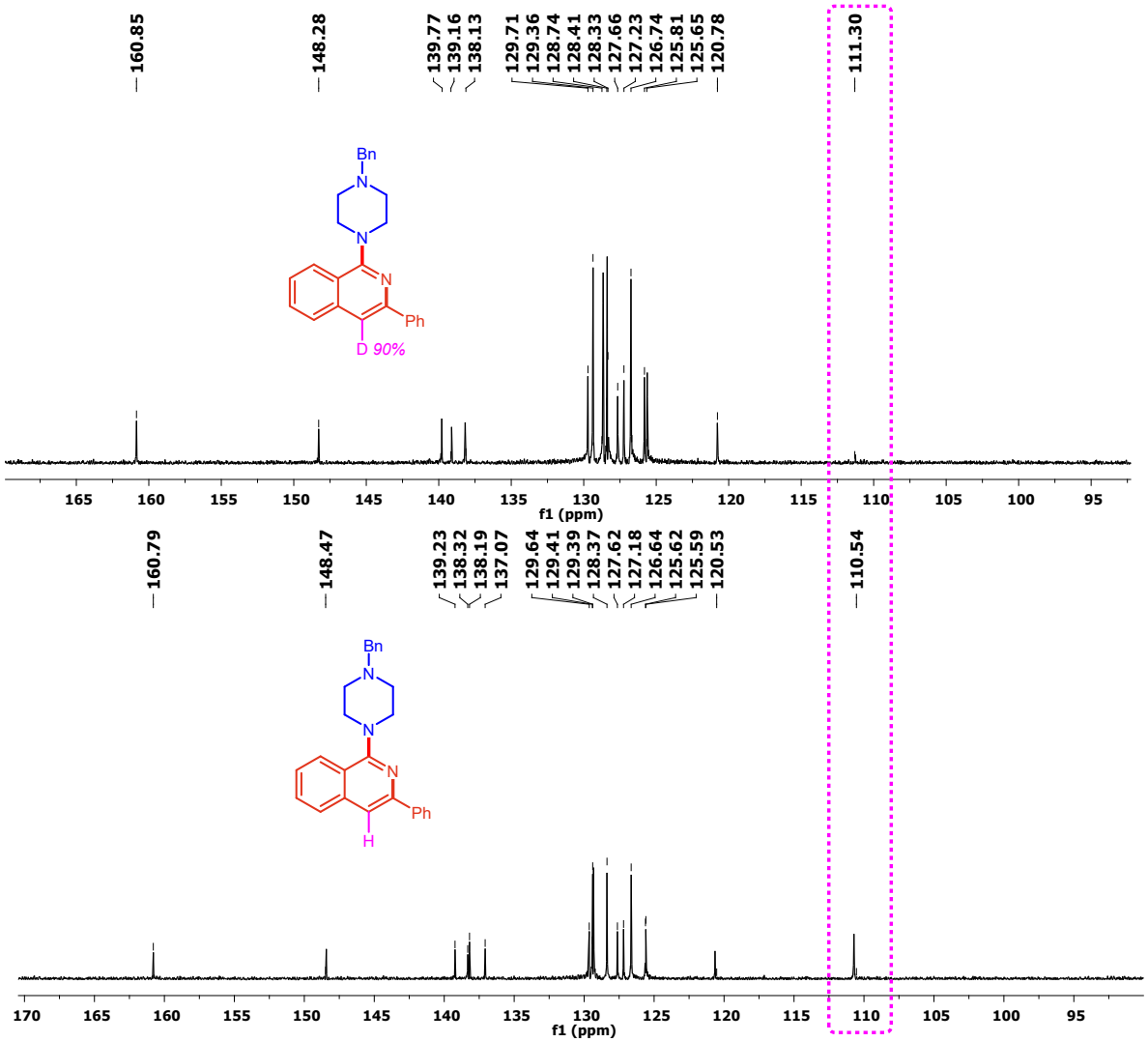
| m/z | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 304.1802 | 1 | 82673.52 | C20H22N3 | (M+H)+ |
| 305.1834 | 1 | 18822.01 | C20H22N3 | (M+H)+ |
| 326.154 | 1 | 608.51 | C20H21N3Na | (M+Na)+ |

--- End Of Report ---

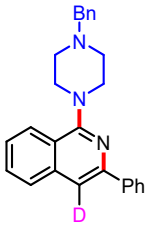
**$^1$H NMR** (400MHz, $CDCl_3$)



**$^{13}$C NMR** (100MHz, $CDCl_3$)



## HRMS




## 1-(4-benzylpiperazin-1-yl)-3-phenylisoquinoline-4-d (3f-D)

### Qualitative Compound Report

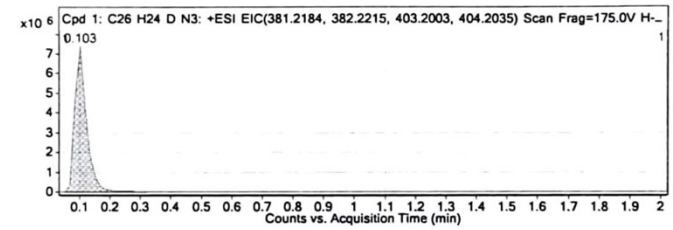
| | | | |
|---|---|---|---|
| **Data File** | H-53DR.d | **Sample Name** | H-53DR |
| **Sample Type** | Sample | **Position** | P1-B1 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | MS Scan.m | **Acquired Time** | 30-08-2022 16:52:30 |
| **IRM Calibration Status** | [redacted] | **DA Method** | Default.m |
| **Comment** | | | |

| | | | |
|---|---|---|---|
| **Sample Group** | | **Info.** | 3 |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

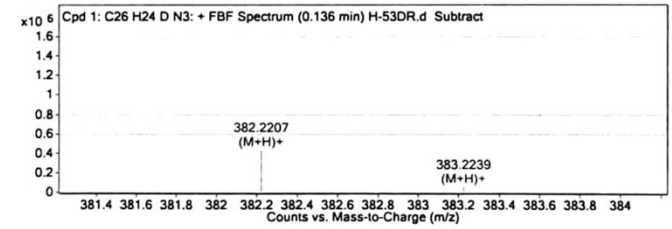
**Compound Table**

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C26 H24 D N3 | 0.103 | 380.2103 | 1446683 | C26 H24 D N3 | 380.2111 | -2.14 | C26 H24 D N3 | C26 H24 D N3 |

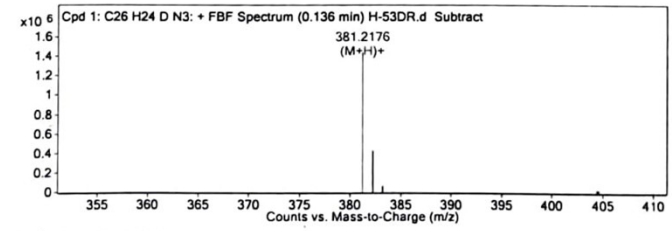
| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C26 H24 D N3 | 381.2176 | 0.103 | Find By Formula | 380.2103 |




MS Spectrum




MS Zoomed Spectrum




**MS Spectrum Peak List**

| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 381.2176 | 1 | 1446683.13 | C26H25DN3 | (M+H)+ |
| 382.2207 | 1 | 433069.34 | C26H25DN3 | (M+H)+ |
| 383.2239 | 1 | 56594.17 | C26H25DN3 | (M+H)+ |
| 384.2279 | 1 | 5304.43 | C26H25DN3 | (M+H)+ |

--- End Of Report ---