Selenium dioxide mediated benzylic sp$^3$ C–H oxidation in acetic acid: synthesis of lophine derivatives from α-methylene ketones via a domino multicomponent reaction

Vineet Jeena* and Mncedisi Mazibuko

School of Chemistry and Physics, University of KwaZulu-Natal, Scottsville, Pietermaritzburg, 3209, South Africa

Email: jeenav1@ukzn.ac.za

Electronic Supplementary Information
Table of Contents

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>General Information</td>
<td>S1</td>
</tr>
<tr>
<td>Synthetic Procedures and Characterization of Lophine Derivatives</td>
<td>S2</td>
</tr>
<tr>
<td>References</td>
<td>S18</td>
</tr>
<tr>
<td>Spectroscopic data</td>
<td>S19</td>
</tr>
</tbody>
</table>
General information

All $^1$H and $^{13}$C Nuclear Magnetic Resonance (NMR) spectra were recorded on Bruker Avance 400 operating at either 400 or 100 MHz using DMSO-$d_6$ as an internal standard. Chemical shifts are expressed in parts per million (ppm) relative to the residual solvent and coupling constants ($J$ values) were recorded in Hz. High-resolution electron-spray ionization (ESI) mass spectra were recorded on a time-of-flight (TOF) micromass spectrometer. IR spectra were recorded on Perkin Elmer FTIR Spectrometer. Absorption maxima are expressed in wavenumbers (cm$^{-1}$). Melting points were determined using Kofler hot-stage melting apparatus. All reagents that were used are commercially available.

Equipment used for reflux

A specially designed cylindrical tube was charged with the reagents and fitted with a condenser. The mixture was heated to 180 °C and the reaction system monitored. During the course of the reaction (maximum 3 hours) vigorous reflux was observed but no tangible loss of solvent was observed.
2,4,5-Triphenylimidazole (3a)\textsuperscript{1,5,6}

2-Phenylacetophenone (98.12 mg, 0.5 mmol), selenium dioxide (55.48 mg, 0.5 mmol), ammonium acetate (385.4 mg, 5.0 mmol), and benzaldehyde (51.02 µl, 0.5 mmol) were mixed in an elongated tube (equipped with a reflux condenser) with 5.00 ml glacial acetic acid and stirred for 3 hours at 180 °C. After cooling, the reaction mixture was added drop-wise into a 25% ammonia solution at 0 °C to form a white precipitate which was then filtered and dried in oven at 50 °C for 4 hours to afford 2,4,5-triphenylimidazole as a white solid (123.30 mg, 83%). Mp 271 – 273 °C.

IR (KBr, cm\textsuperscript{-1}): 3426, 2855, 1600, 1488;

\textsuperscript{1}H NMR (400 MHz, DMSO-\textit{D}\textsubscript{6}) \( \delta \) 12.72 (s, 1H), 8.12 (d, \( J = 7.84 \) Hz, 2H), 7.62 (d, \( J = 8.08 \) Hz, 2H), 7.55 (d, \( J = 7.25 \) Hz, 2H), 7.51 – 7.44 (m, 4H), 7.39 (t, \( J = 7.46 \) Hz, 2H), 7.32 (t, \( J = 7.46 \) Hz, 2H) 7.24 (t, \( J = 7.66 \) Hz, 1H);

\textsuperscript{13}C (100 MHz, DMSO-\textit{D}\textsubscript{6}) \( \delta \) 146.0, 137.7, 135.7, 131.6, 130.9, 129.1, 128.9, 128.7, 128.7, 127.2, 127.6, 126.9, 125.7;

HRMS (ESI) calcd for \( \text{C}_{21}\text{H}_{18}\text{N}_2 [M + H]^+ \) 297.1392, found 297.1388.
2-(4-Chlorophenyl)-4,5-diphenylimidazole (3b)¹

Prepared by the procedure given for 3a, except using 4-chlorobenzaldehyde (70.28 mg, 0.5 mmol), and obtained as a white solid (127.10 mg, 77%).

Mp 258 – 261 °C.

IR (KBr, cm⁻¹): 3423, 3059, 1602, 1324;

¹H NMR (400 MHz, DMSO-D₆) δ 12.78 (s, 1H), 8.12 (d, J = 8.57 Hz, 2H), 7.56 (d, J = 8.57 Hz, 6H), 7.38 (s, 6H);

¹³C (100 MHz, DMSO-D₆) δ 144.9, 133.3, 129.9, 129.8, 129.7, 129.3, 129.2, 129.0, 128.8, 128.3, 127.6, 127.3;

HRMS (ESI) calcd for C₂₁H₁₅N₂Cl [M + H]^+ 331.1002, found 331.1009.
2-(4-Bromophenyl)-4,5-diphenylimidazole (3c)\(^1\)

![Chemical Structure](image)

Prepared by the procedure given for 3a, except using 4-bromobenzaldehyde (92.51 mg, 0.5 mmol), and obtained as a white solid (137.20, 73%).

Mp 255 – 258 °C.

IR (KBr, cm\(^{-1}\)): 3408, 3060, 1601, 1323;

\(^1\)H NMR (400 MHz, DMSO-D\(_6\)) \(\delta\) 12.80 (s, 1H), 8.06 (d, \(J = 8.42\) Hz, 2H), 7.70 (d, \(J = 8.61\) Hz, 2H), 7.55 (d, \(J = 7.14\) Hz, 4H), 7.38 (s, 6H);

\(^{13}\)C (100 MHz, DMSO-D\(_6\)) \(\delta\) 144.9, 137.8, 135.5, 132.1, 131.5, 130.0, 129.8, 129.4, 128.9, 127.6, 121.9;

HRMS (ESI) calcd for C\(_{21}\)H\(_{15}\)BrN\(_2\) [M + H]\(^+\) 375.0497, found 375.0500.
2-(4-Fluorophenyl)-4,5-diphenyl-1H-imidazole (d)\textsuperscript{2,3}

Prepared by the procedure given for 3a, except using 4-fluorobenzaldehyde (53.63 µl, 0.5 mmol), and obtained as a fawn solid (131.30 mg, 84%).

Mp 249 – 253 °C.

IR (KBr, cm\textsuperscript{-1}): 3408, 3029, 1608, 1492, 1221, 1159, 1131, 694;

\textsuperscript{1}H NMR (400 MHz, DMSO-D\textsubscript{6}) \textit{δ} 12.70 (s, 1H), 8.14 (q, \textit{J} = 5.59 Hz, 2H), 7.55 (d, \textit{J} = 6.88 Hz, 4H), 7.36 – 7.31 (m, 8H);

\textsuperscript{13}C (100 MHz, DMSO-D\textsubscript{6}) \textit{δ} 163.8, 161.4, 145.2, 137.6, 135.6, 131.5, 129.1, 128.9, 128.7, 128.3, 127.8, 127.8, 127.5, 127.5, 127.0, 116.2, 116.0;

HRMS (ESI) calcd for C\textsubscript{21}H\textsubscript{15}FN\textsubscript{2} [M + H]\textsuperscript{+} 315.1298, found 315.1307.
2-(4-Methoxyphenyl)-4,5-diphenyl-1H-imidazole (3e)\textsuperscript{1,2}

Prepared by the procedure given for 3a, except using 4-methoxybenzaldehyde (60.83 µl, 0.5 mmol), and obtained as a pale-white solid (141.30 mg, 87%).

Mp 226 – 229 °C.

IR (KBr, cm\textsuperscript{-1}): 3400, 3027, 1613, 1492, 1174;

\textsuperscript{1}H NMR (400 MHz, DMSO-D\textsubscript{6}) \( \delta \) 12.52 (s, 1H), 8.03 (d, \( J = 9.13 \) Hz, 2H), 7.56 – 7.51 (d, \( J = 13.52 \), 4H) 7.44 – 7.23 (m, 6H), 7.07 (d, \( J = 8.73 \) Hz, 2H), 3.83 (s, 3H);

\textsuperscript{13}C (100 MHz, DMSO-D\textsubscript{6}) \( \delta \) 159.9, 146.1, 137.3, 135.8, 131.7, 129.1, 128.8, 128.6, 128.1, 128.1, 127.5, 127.2, 126.9, 123.7, 114.6, 55.7;

HRMS (ESI) calcd for C\textsubscript{22}H\textsubscript{18}N\textsubscript{2}O [M + H]\textsuperscript{+} 327.1497, found 327.1494.
4,5-Diphenyl-2-(p-tolyl)-1H-imidazole (3f)\textsuperscript{1,3}

![Chemical structure](image)

Prepared by the procedure given for 3a, except using p-tolualdehyde (58.95 µl, 0.5 mmol), and obtained as a pale-white solid (129.00 mg, 83%).

Mp 230 – 232 °C.

IR (KBr, cm\textsuperscript{-1}): 3394, 3029, 1603, 1486, 1321;

\textsuperscript{1}H NMR (400 MHz, DMSO-D6) \(\delta\) 12.48 (s, 1H), 7.74 (t, \(J = 4.23\) Hz, 1H), 7.59 – 7.52 (q, \(J = 7.40\) Hz, 4H), 7.46 – 7.42 (t, \(J = 7.16\) Hz, 2H), 7.34 – 7.29 (m, 6H), 7.24 – 7.22 (d, \(J = 7.24\) Hz, 1H), 2.66 (s, 3H);

\textsuperscript{13}C (100 MHz, DMSO-D6) \(\delta\) 146.6, 137.1, 136.8, 135.9, 131.7, 131.6, 130.5, 129.2, 129.1, 128.8, 128.7, 128.6, 128.1, 127.9, 127.5, 126.9, 126.2, 21.6;

HRMS (ESI) calcd for C\textsubscript{22}H\textsubscript{18}N\textsubscript{2} [M + H]\textsuperscript{+} 311.1548, found 311.1554.
5-(4-Chlorophenyl)-2,4-diphenyl-1H-imidazole (3g)\(^4\)

![Chemical Structure](image)

Prepared by the procedure given for 3a, using 4-chloro-2-phenylacetophenone (115.30 mg, 0.5 mmol), and obtained as a white solid (130.20 mg, 82%).

Mp 241 – 245 °C.

IR (KBr, cm\(^{-1}\)): 3415, 3055, 1600, 1322; \(^1\)H NMR (400 MHz, DMSO-D\(_6\)) \(\delta\) 12.73 (s, 1H), 8.10 (d, \(J = 7.79\) Hz, 2H), 7.55 – 7.38, (m, 12H);

\(^{13}\)C (100 MHz, DMSO-D\(_6\)) \(\delta\) 146.4, 146.2, 138.2, 136.3, 135.5, 134.5, 132.7, 131.5, 131.3, 130.7, 130.5, 130.3, 129.2, 129.1, 129.0, 128.8, 128.7, 128.5, 127.7, 127.4, 127.2, 125.7;

HRMS (ESI) calcd for C\(_{21}\)H\(_{15}\)ClN\(_2\) [M + H]\(^+\) 331.1002, found 331.1007.
2,5-Bis(4-chlorophenyl)-4-phenyl-1H-imidazole (3h)

Prepared by the procedure given for 3a, using 4-chloro-2-phenylacetophenone (115.30 mg, 0.5 mmol) and 4-chlorobenzaldehyde (70.30 mg, 0.5 mmol), and obtained as a white solid (135.60 mg, 74%).

Mp 249 – 252 °C.

IR (KBr, cm⁻¹): 3419, 3063, 1600, 1311;

¹H NMR (400 MHz, DMSO-D₆) δ 12.83 (s, 1H), 8.10 (d, J = 8.66 Hz, 2H), 7.56 – 7.37 (m, 11H);

¹³C (100 MHz, DMSO-D₆) δ 145.2, 133.4, 129.5, 129.3, 129.1, 128.8, 127.4;

2-(4-Bromophenyl)-5-(4-chlorophenyl)-4-phenyl-1H-imidazole (3i)

Prepared by the procedure given for 3a, using 4-chloro-2-phenylacetophenone (115.30 mg, 0.5 mmol) and 4-bromobenzaldehyde (92.50 mg, 0.5 mmol), and obtained as a white solid (135.60 mg, 87%).

Mp 248 – 250 °C.

IR (KBr, cm\(^{-1}\)): 3416, 3064, 1600, 1323;

\(^1\)H NMR (400 MHz, DMSO-D\(_6\)) \(\delta\) 12.84 (s, 1H), 8.04 (d, \(J = 9.00\) Hz, 2H), 7.69 (d, \(J = 8.53\) Hz, 2H), 7.54 – 7.36 (m, 9H);

\(^13\)C (100 MHz, DMSO-D\(_6\)) \(\delta\) 145.2, 132.2, 129.9, 129.1, 128.9, 127.6, 122.0;

HRMS (ESI) calcd for C\(_{21}\)H\(_{14}\)BrClN\(_2\) [M + H]+ 409.0107, found 409.0117.
5-(4-Chlorophenyl)-2-(4-methoxyphenyl)-4-phenyl-1H-imidazole (3j)

Prepared by the procedure given for 3a, except using 4-chloro-2-phenylacetophenone (115.30 mg, 0.5 mmol) and 4-methoxybenzaldehyde (60.83 µl, 0.5 mmol), and obtained as a white solid (109.80 mg, 61%).

Mp 233 – 237 °C.

IR (KBr, cm\(^{-1}\)): 3408, 3060, 2289, 1601, 1220;

\(^1\)H NMR (400 MHz, DMSO-D\(_6\)) \(\delta\) 12.58 (s, 1H), 8.01 (d, \(J = 8.21\) Hz, 2H), 7.57 – 7.44 (m, 6H), 7.41 – 7.27 (m, 3H), 7.07 (d, \(J = 8.21\) Hz, 2H), 3.83 (s, 3H);

\(^1^3\)C (100 MHz, DMSO-D\(_6\)) \(\delta\) 160.0, 146.3, 137.9, 135.9, 135.6, 134.7, 132.5, 131.5, 131.3, 130.3, 129.2, 129.0, 128.9, 128.7, 128.3, 127.8, 127.3, 123.5, 114.6, 55.7;

HRMS (ESI) calcd for C\(_{22}\)H\(_{17}\)ClN\(_2\)O [M + H]\(^+\) 361.1108, found 361.1097.
5-(4-Chlorophenyl)-2-(4-fluorophenyl)-4-phenyl-1\textit{H}-imidazole (3k)

![Chemical structure](image)

Prepared by the procedure given for 3\textit{a}, except using 4-chloro-2-phenylacetophenone (115.30 mg, 0.5 mmol) and 4-fluorobenzaldehyde (53.63 µl, 0.5 mmol), and obtained as a cream-white solid (132.40 mg, 76%).

Mp 245 – 249 °C.

IR (KBr, cm\textsuperscript{-1}): 3431, 3062, 1488, 1222, 1159, 1129, 698;

\textsuperscript{1}H NMR (400 MHz, DMSO-D\textsubscript{6}) \( \delta \) 12.75 (s, 1H), 8.13 (q, \( J = 5.58 \) Hz, 2H), 7.56 – 7.52 (t, \( J = 8.30 \) Hz, 4H), 7.39 – 7.31 (m, 7H);

\textsuperscript{13}C (100 MHz, DMSO-D\textsubscript{6}) \( \delta \) 163.9, 161.4, 145.4, 129.0, 127.9, 127.8, 127.4, 127.3, 116.2, 116.0;

HRMS (ESI) cacld for C\textsubscript{21}H\textsubscript{14}ClFN\textsubscript{2} [M + H]\textsuperscript{+} 349.0912, found 349.0912.
2-(2-Methoxyphenyl)-4,5-diphenyl-1H-imidazole (3l)\(^5\)

![Chemical Structure](image)

Prepared by the procedure given for 3a, except using 2-methoxybenzaldehyde (60.40 µl, 0.5 mmol), and obtained as a white solid (145.20 mg, 88%).

Mp 230 – 233 °C.

IR (KBr, cm\(^{-1}\)): 3429, 3032, 2940, 1601, 1481;

\(^1\)H NMR (400 MHz, DMSO-D\(_6\)) \(\delta\) 11.89 (s, 1H), 8.07 (d, \(J = 5.91\) Hz, 2H), 7.55 (d, \(J = 7.14\) Hz, 2H), 7.48 (d, \(J = 7.14\) Hz, 2H), 7.44 – 7.37 (m, 4H), 7.31 (t, \(J = 7.45\) Hz, 2H), 7.22 – 7.18 (m, 2H), 7.08 (t, \(J = 7.45\) Hz, 1H), 3.93 (s, 3H);

\(^1^3\)C (100 MHz, DMSO-D\(_6\)) \(\delta\) 156.5, 143.7, 136.9, 135.8, 131.7, 130.2, 129.3, 129.1, 129.0, 128.6, 128.1, 127.9, 127.6, 126.9, 121.1, 119.4, 112.1, 56.0;

HRMS (ESI) calcd for C\(_{22}\)H\(_{18}\)N\(_2\)O [M + H]\(^+\) 325.1341, found 325.1345.
2-(2-Fluorophenyl)-4,5-diphenyl-1H-imidazole (3m)²

Prepared by the procedure given for 3a, except using 2-fluorobenzaldehyde (52.69 µl, 0.5 mmol), and obtained as a white solid (130.80 mg, 83%).

Mp 238 – 241 °C.

IR (KBr, cm⁻¹): 3453, 3058, 1602, 1484, 1220, 1101, 695;

¹H NMR (400 MHz, DMSO-D₆) δ 12.55 (s, 1H), 8.02 (t, J = 7.80 Hz, 1H), 7.54 – 7.33, (m, 13H);

¹³C (100 MHz, DMSO-D₆) δ 160.6, 158.1, 141.3, 141.3, 131.4, 130.9, 130.8, 130.1, 130.1, 129.6, 129.0, 128.3, 127.6, 127.1, 125.1, 125.1, 119.2, 119.1, 116.8, 116.6;

HRMS (ESI) calcd for C₂₁H₁₅FN₂ [M + Na]^+ 337.1117, found 337.1114.
2-(2-Nitrophenyl)-4,5-diphenyl-1H-imidazole (3n)\textsuperscript{2,5}

Prepared by the procedure given for 3a, except using 2-nitrobenzaldehyde (75.60 mg, 0.5 mmol), and obtained as a yellow solid (142.00 mg, 83%).

Mp 229 – 232 °C.

IR (KBr, cm\textsuperscript{-1}): 3397, 3031, 1601, 1524, 1351, 1143, 693;

\textsuperscript{1}H NMR (400 MHz, DMSO-D\textsubscript{6}) δ 12.95 (s, 1H), 8.00 (d, J = 8.51 Hz, 1H), 7.93 (d, J = 7.09 Hz, 1H), 7.79 (t, J = 7.44 Hz, 1H), 7.65 (t, J = 7.80 Hz, 1H), 7.51 (d, J = 7.80 Hz, 4H), 7.39 – 7.25 (m, 6H);

\textsuperscript{13}C (100 MHz, DMSO-D\textsubscript{6}) δ 148.8, 141.5, 132.6, 130.3, 129.9, 129.4, 129.2, 128.9, 128.8, 127.6, 124.5, 123.9;

HRMS (ESI) calcd for C\textsubscript{21}H\textsubscript{15}N\textsubscript{3}O [M + H]\textsuperscript{+} 342.1243, found 342.1248.
2-(3-Nitrophenyl)-4,5-diphenyl-1H-imidazole (3o)

Prepared by the procedure given for 3a, except using 2-nitrobenzaldehyde (75.60 mg, 0.5 mmol), and obtained as a yellow solid (87.40 mg, 51%).

Mp 281 – 285 °C.

IR (KBr, cm⁻¹): 3394, 3057, 1520, 1347;

¹H NMR (400 MHz, DMSO-D₆) δ 13.08 (s, 1H), 8.97 (s, 1H), 8.51 (d, J = 8.01 Hz, 1H), 8.20 (d, J = 8.35 Hz, 1H), 7.77 (t, J = 8.02 Hz, 1H), 7.55 (d, J = 7.47 Hz, 4H), 7.40 (brs, 6H);

¹³C (100 MHz, DMSO-D₆) δ 148.8, 143.9, 132.3, 131.6, 130.8, 129.4, 128.9, 128.7, 128.2, 123.0, 119.9;

2-(2-Furyl)-4,5-diphenyl-1H-imidazole (3p)³

Prepared by the procedure given for 3a, except using furfural (41.42 µl, 0.5 mmol), and obtained as a brown solid (95.30 mg, 67%).

Mp 237 – 239 ºC.

IR (KBr, cm⁻¹): 3023, 1601, 1500, 1485, 739, 695;

¹H NMR (400 MHz, DMSO-D₆) δ 12.81 (s, 1H), 8.06 (d, 2H), 7.81, (s, 1H), 7.54 – 7.48 (dd, J = 7.16 Hz, 4H), 7.43 (t, J = 7.78 Hz, 2H), 7.37 (t, J = 7.37 Hz, 1H), 7.31 (t, J = 7.37 Hz, 2H), 7.23 (t, J = 7.37 Hz, 1H), 6.98 (d, J = 3.41 Hz, 1H), 6.66 (s, 1H);

¹³C (100 MHz, DMSO-D₆) δ 146.2, 143.5, 139.1, 137.5, 135.4, 131.3, 129.1, 128.8, 128.7, 128.3, 128.0, 127.6, 127.1, 112.3, 107.9;

2-Cyclohexyl-4,5-diphenyl-1H-imidazole (3q)\(^4\)

![Chemical Structure](image)

2-phenylacetophenone (98.12 mg, 0.5 mmol) and selenium dioxide (55.48 mg, 0.5 mmol) were reacted under glacial acetic acid (5.00 ml) in an elongated tube equipped with a reflux condenser and a stirrer bar magnet for 3 hours at 180 °C. Subsequently, cyclohexane carboxaldehyde (60.57 µl, 0.5 mmol) and ammonium acetate (385.4 mg, mmol, 5.0 mmol) were directly added into the reaction mixture and allowed to react for another 3 hours at 180 °C. After cooling, the ultimate reaction mixture was added dropwise into a 25% ammonia solution at 0 °C to form a white precipitate which was then filtered and dried in oven at 50 °C for 4 hours to afford 2-cyclohexyl-4,5-diphenyl-1H-imidazole as a brown solid (133.30 mg, 83%).

Mp 243 – 245 °C.

IR (KBr, cm\(^{-1}\)): 3031, 1603;

\(^1\)H NMR (400 MHz, DMSO-D\(_6\)) \(\delta\) 11.92 (s, 1H), 7.50 (d, \(J = 7.94\) Hz, 2H), 7.42 (q, \(J = 7.19\) Hz, 4H), 7.26 (m, 3H), 7.17 (t, \(J = 6.95\) Hz, 1H), 2.71 (m, 1H), 1.97 (d, \(J = 11.61\) Hz, 2H), 1.79 (d, \(J = 12.44\) Hz, 2H), 1.68 – 1.56 (m, 3H), 1.42 – 1.23 (m, 3H);

\(^13\)C (100 MHz, DMSO-D\(_6\)) \(\delta\) 152.9, 136.3, 135.5, 132.1, 129.0, 128.5, 128.3, 127.6, 127.5, 126.5, 126.2, 37.7, 32.0, 26.2;
HRMS (ESI) calcd for C$_{21}$H$_{15}$N$_3$O [M + H]$^+$ 303.1861, found 303.1869.

References

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
6 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)
Elements Used:
217mxn22 9 (0.269) Cm (1:61)
TOF MS ES+

Minimum:
Maximum:
Mass  Calc. Mass  mDa  PPM  DBE  i-FIT  i-FIT (Norm)  Formula
365.0615  365.0612  0.3  0.8  14.5  62.2  0.0  C21 H15 N2 Cl2

S27
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
10 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)
Elements Used:

217xxn23 4 (0.101) Cm (1.81)
TOF MS ES+

Minimum: 1.5
Maximum: 5.0 5.0 100.0

Mass  Calc. Mass  mDa  PPM  DBE  i-FIT  i-FIT (Norm)  Formula
409.0117 409.0107 1.0  2.4  14.5  9.5  0.0  C21 H15 N2 Cl Br
**Elemental Composition Report**

**Single Mass Analysis**

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
29 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)

Elements Used:

217rxn37 29 (0.944) Cm (1.61)
TOF MS ES+

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>i-FIT (Norm)</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>361.1097</td>
<td>361.1108</td>
<td>-1.1</td>
<td>-3.0</td>
<td>14.5</td>
<td>77.2</td>
<td>0.0</td>
<td>C22 H18 N2 O Cl</td>
</tr>
</tbody>
</table>

Minimum:  5.0  5.0  -1.5
Maximum:  5.0  100.0

---

**IR Spectrum**

### Elemental Composition Report

#### Single Mass Analysis
- **Tolerance**: 5.0 PPM / DBE: min = -1.5, max = 100.0
- **Element prediction**: Off
- **Number of isotope peaks used for i-FIT**: 2

**Monoisotopic Mass, Even Electron Ions**

10 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)

**Elements Used**:
- C: 20-25
- H: 10-15
- N: 0-5
- F: 0-1
- Cl: 0-1

**217mz384 (0.138) Cm (1:90)**

TOF MS ES+

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>i-FIT (Norm)</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>349.0912</td>
<td>349.0908</td>
<td>0.4</td>
<td>1.1</td>
<td>14.5</td>
<td>57.6</td>
<td>0.0</td>
<td>C21 H15 N2 F Cl</td>
</tr>
</tbody>
</table>

**Minimum**:

-5.0

**Maximum**:

5.0 5.0 100.0

---

[Diagram of mass spectra with peaks labeled]