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Supplementary information to:

Original article:

NOVEL 1,2,4-OXADIAZOLE DERIVATIVES AS SELECTIVE BUTYRYLCHOLINESTERASE INHIBITORS: DESIGN, SYNTHESIS, AND BIOLOGICAL EVALUATION

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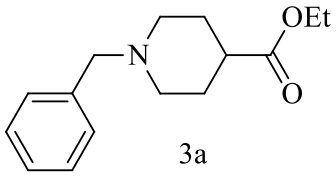
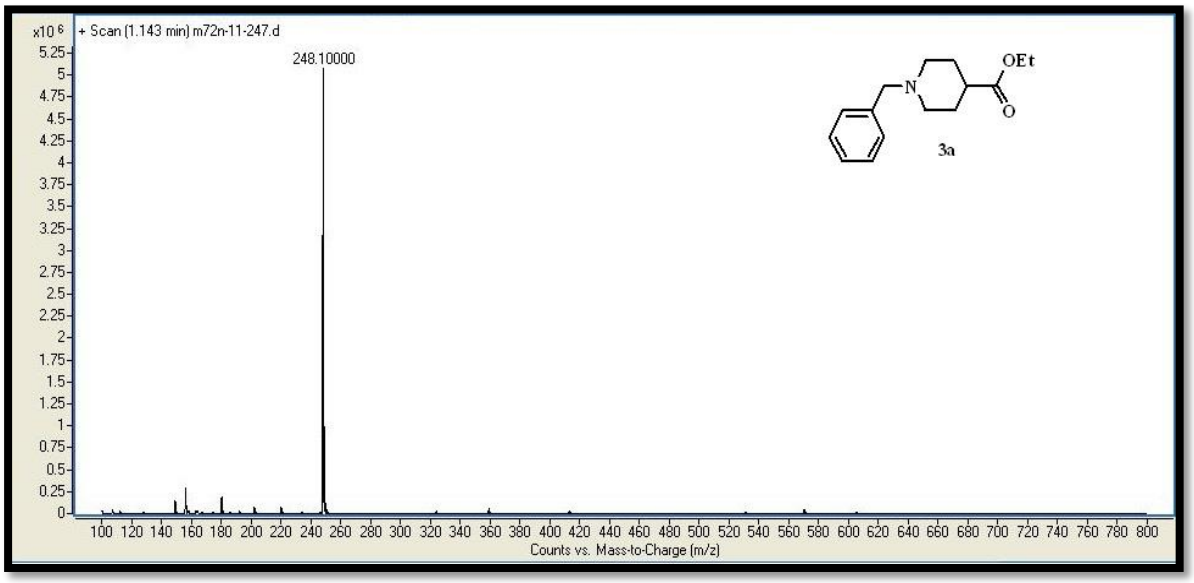
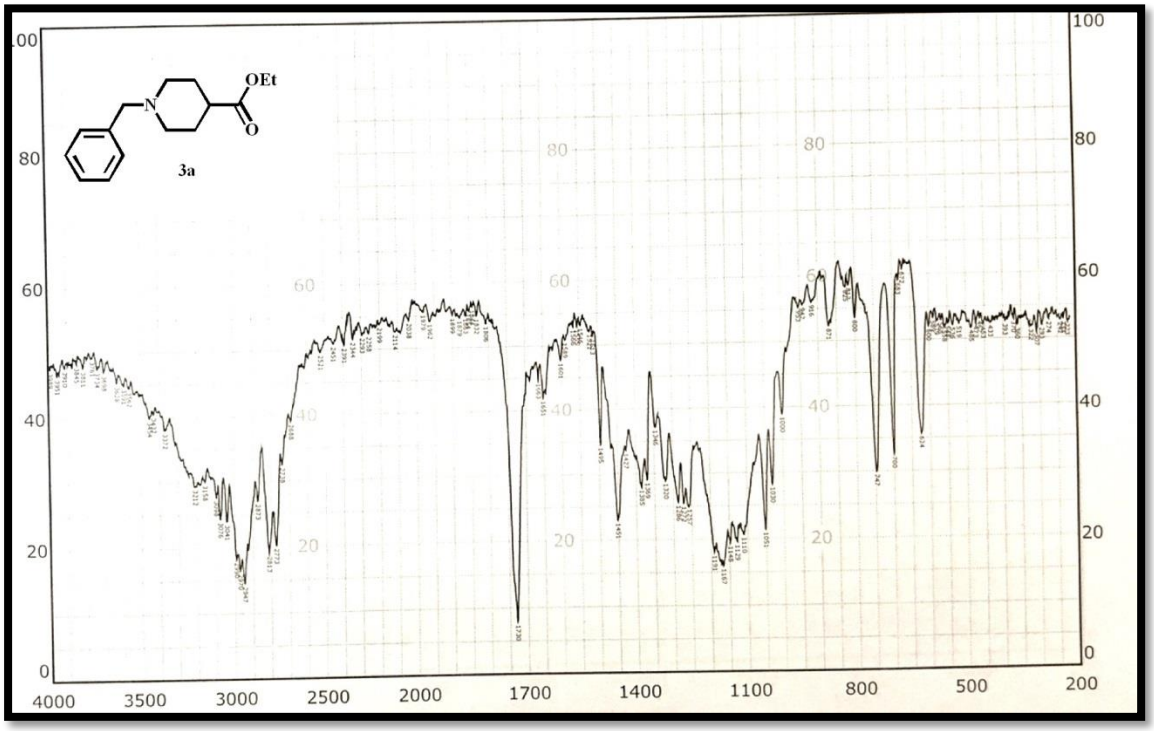


3a

Ethyl 1-benzylpiperidine-4-carboxylate (3a)
Yellow oily liquid (59.7 % yield); IR (KBr, cm^{-1}): 1733 (C=O); LC-MS $[M + 1]^+$: m/z 248.





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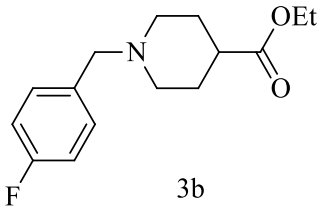
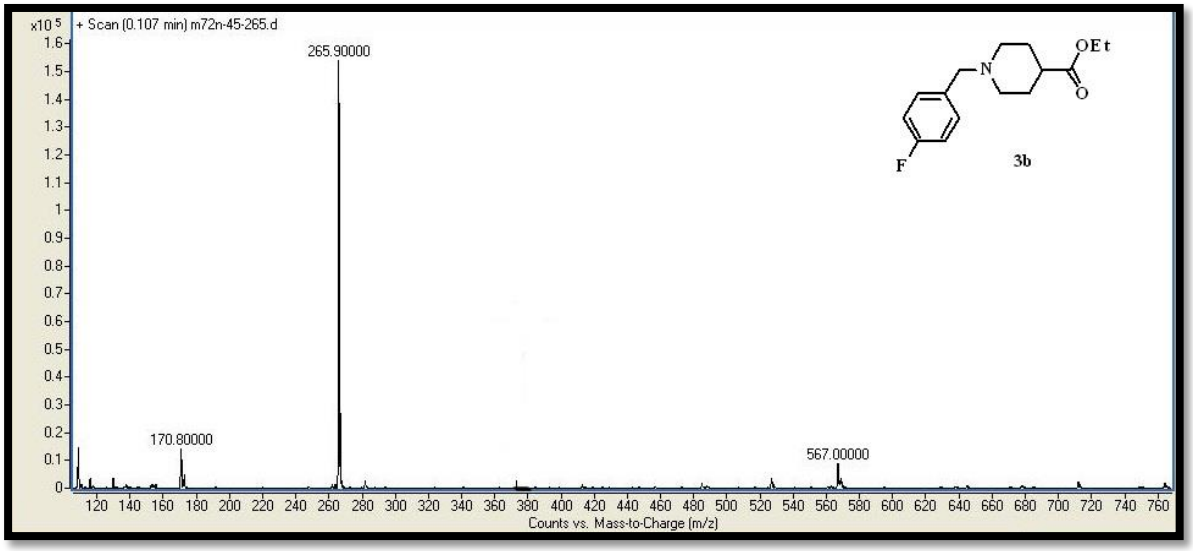
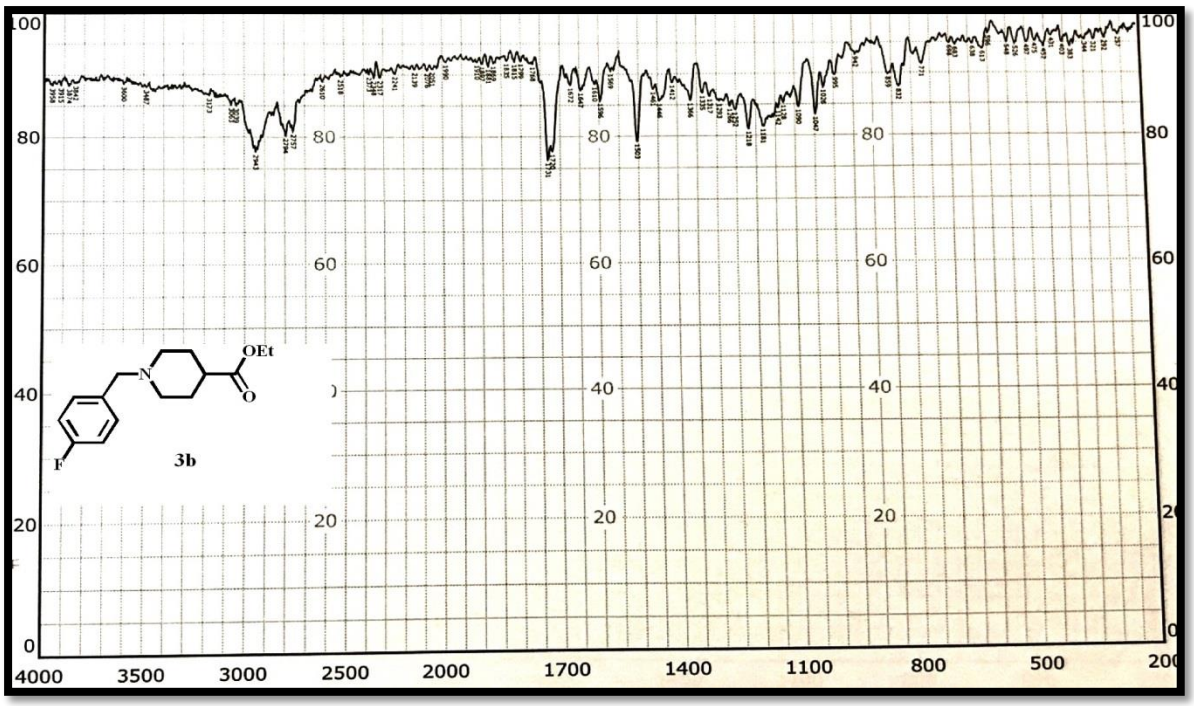
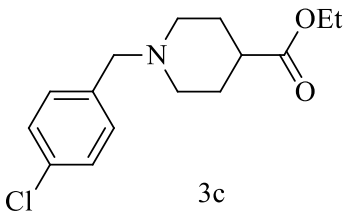


3b

Ethyl 1-(4-fluorobenzyl)piperidine-4-carboxylate (3b)
Yellow oily liquid (73.5 % yield); IR (KBr, cm^{-1}): 1732 (C=O); LC-MS $[M + 1]^+$: m/z 265.9.

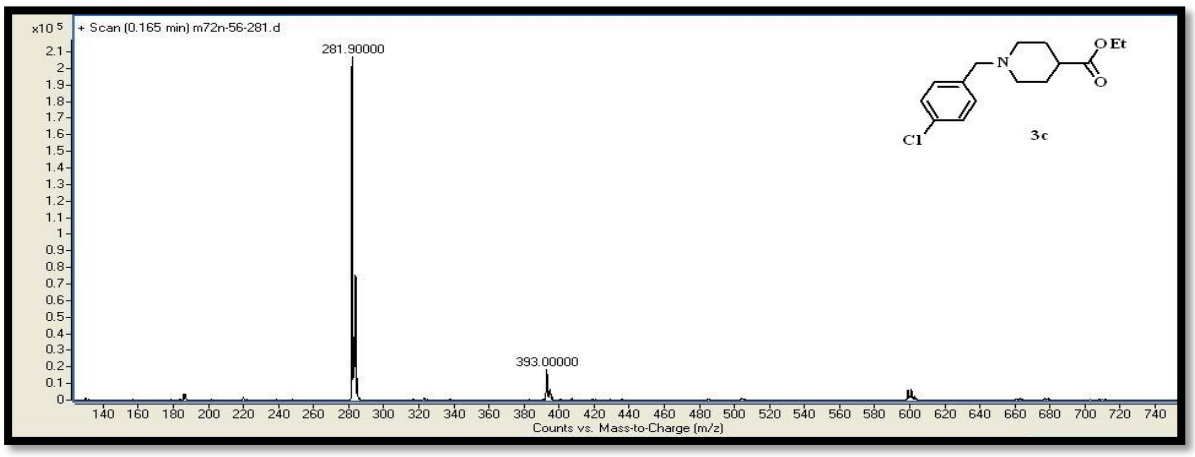


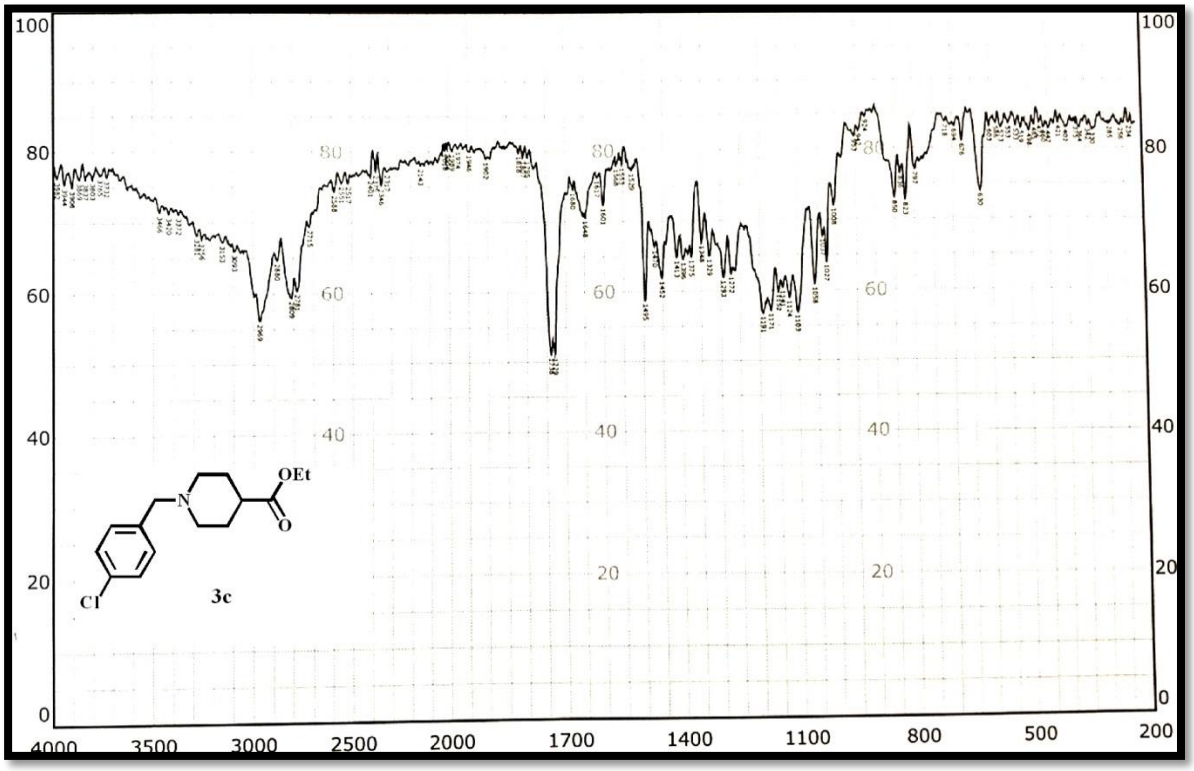




3c

Ethyl 1-(4-chlorobenzyl)piperidine-4-carboxylate (3c)
Yellow oily liquid (68.9 % yield); IR (KBr, cm^{-1}): 1738 (C=O); LC-MS $[M + 1]^+$: m/z 281.9.





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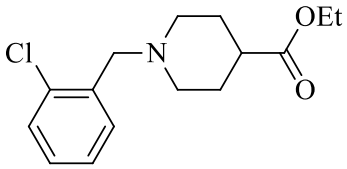
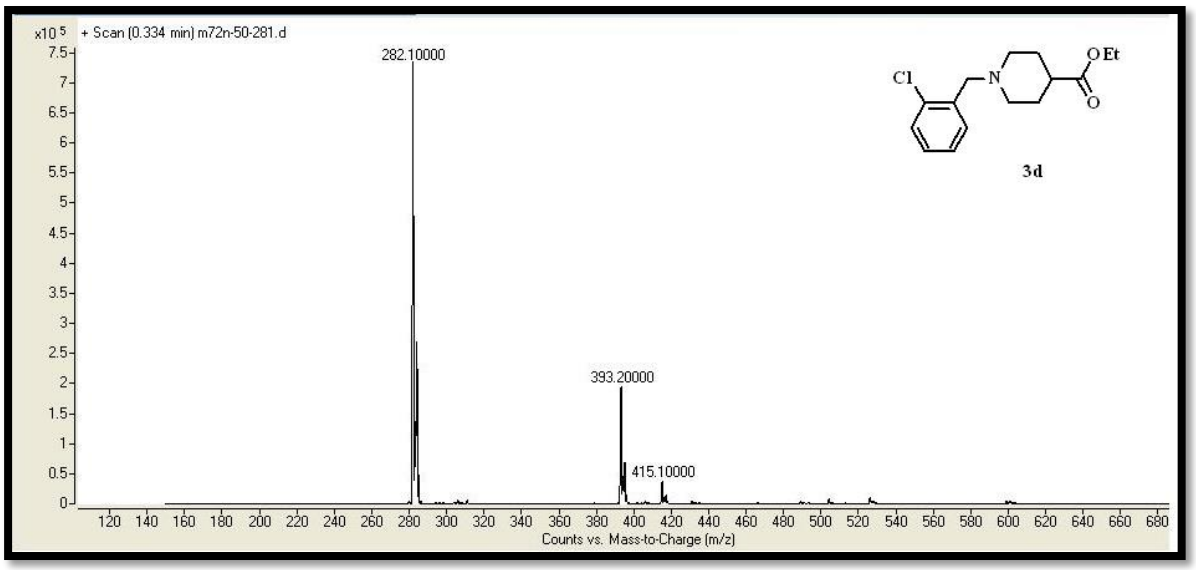
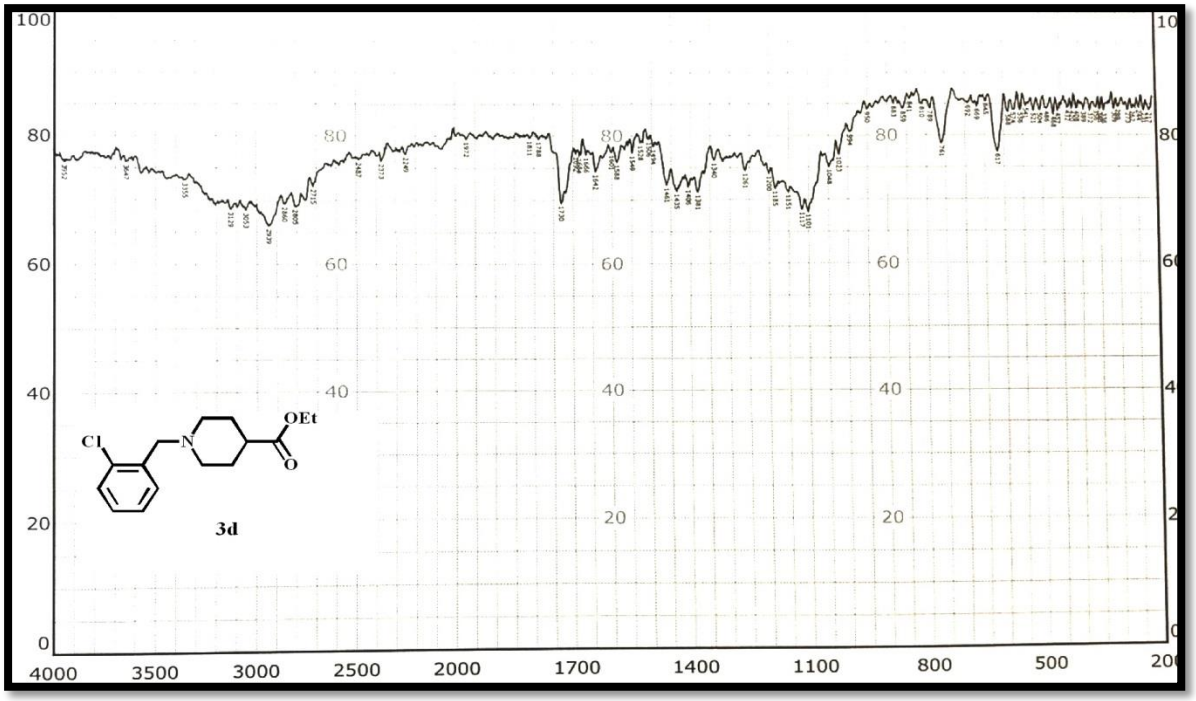


3d

Ethyl 1-(2-chlorobenzyl)piperidine-4-carboxylate (3d)
Yellow oily liquid (60.6 % yield); IR (KBr, cm^{-1}): 1738 (C=O); LC-MS $[M + 1]^+$: m/z 282.





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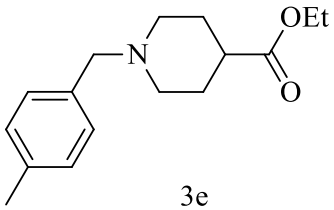
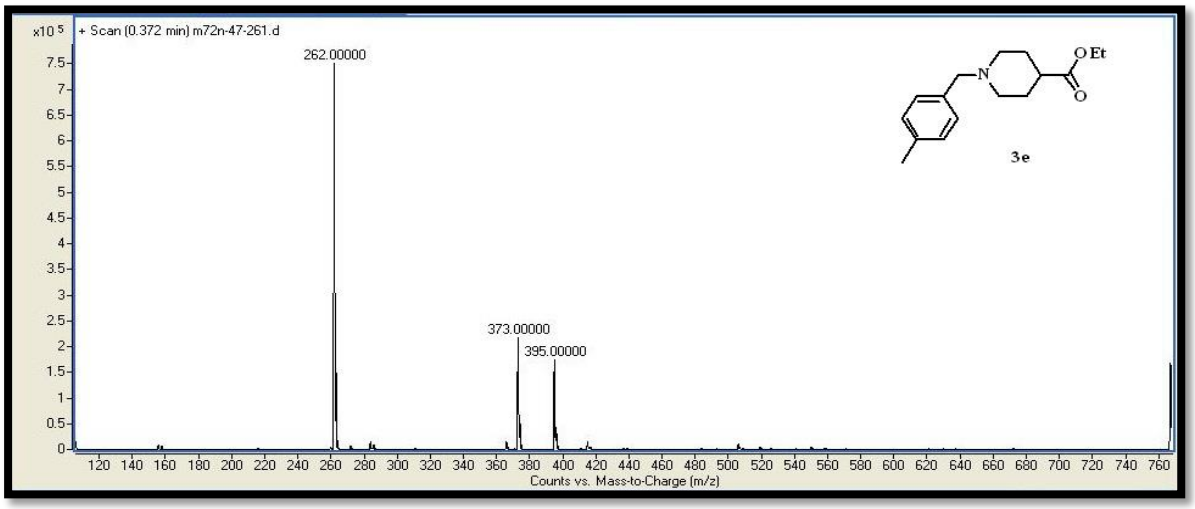
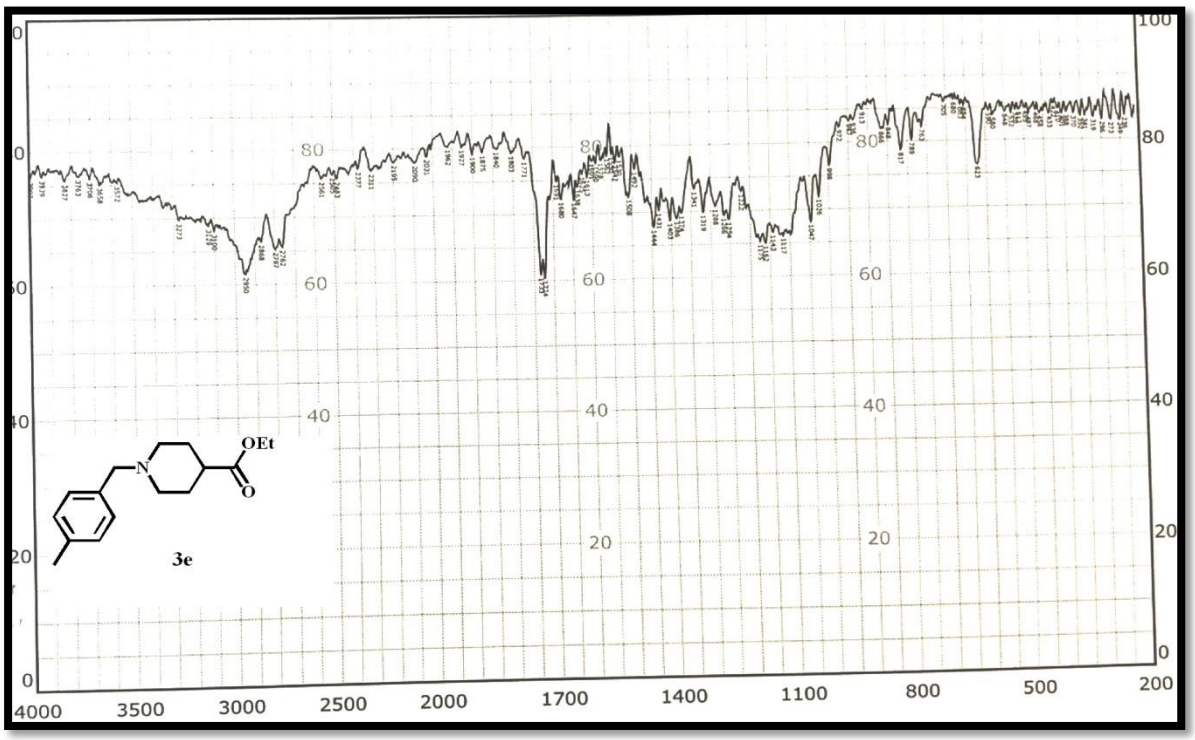


3e

Ethyl 1-(4-methylbenzyl)piperidine-4-carboxylate (3e)
Yellow oily liquid (76.6 % yield); IR (KBr, cm^{-1}): 1733 (C=O); LC-MS $[M + 1]^+$: m/z 262.





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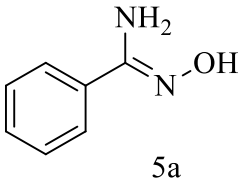
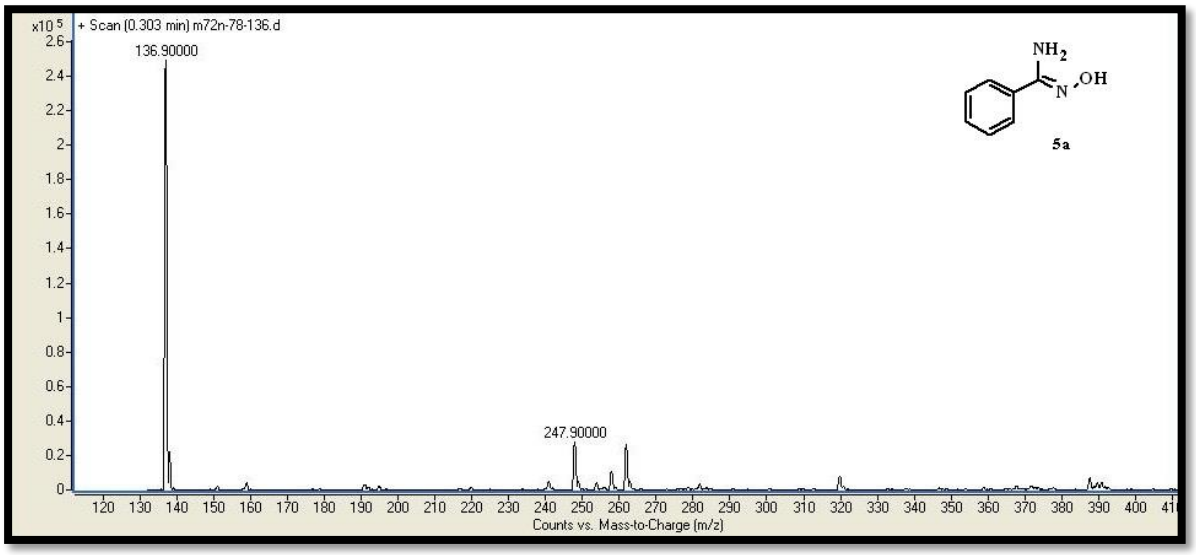
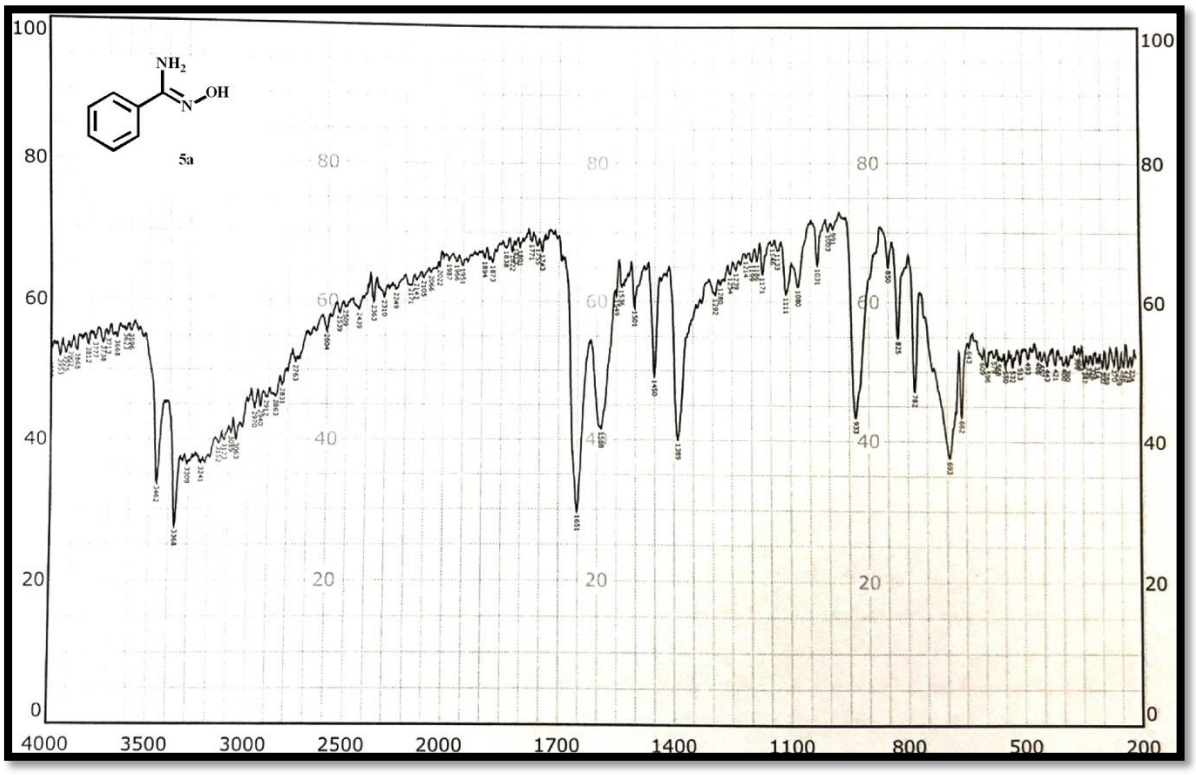


5a

N'-hydroxybenzamidine (5a)
Light yellow powder (96.5 % yield); mp: 68-70 °C; IR (KBr, cm^{-1}): 1657 (C=N), 3349, 3468 (NH_2); LC-MS $[M + 1]^+$: m/z 136.9.





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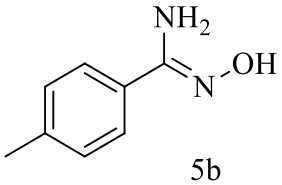
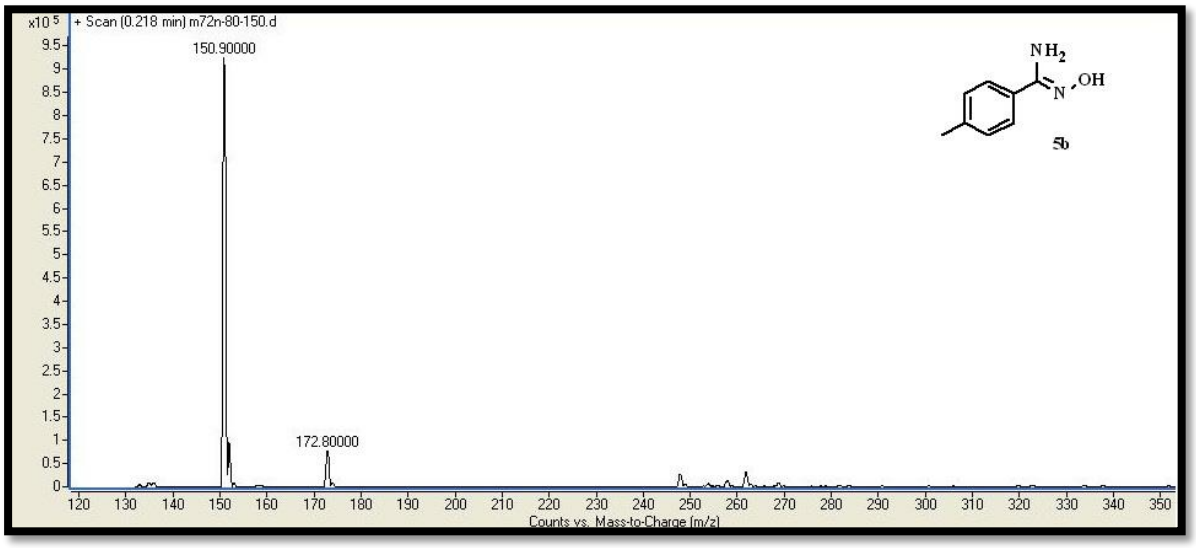
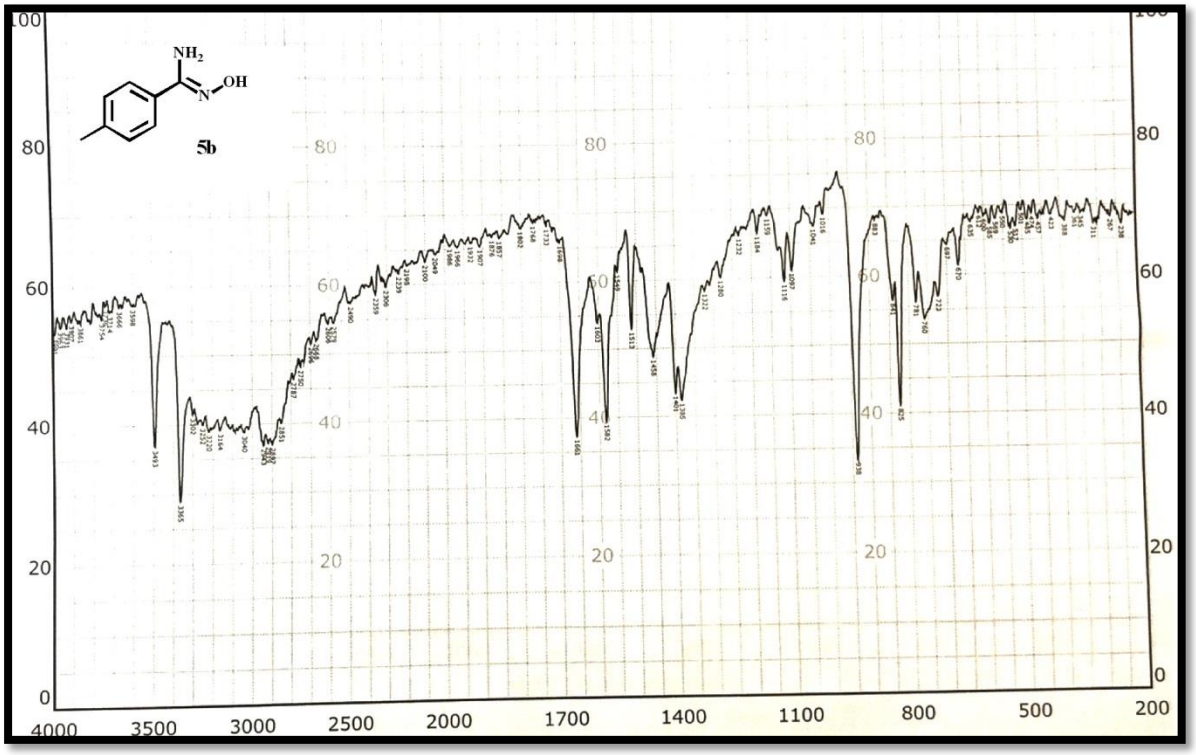


5b

N'-hydroxy-4-methylbenzamidine (5b)
Light yellow powder (81.9 % yield); mp: 145.8-148 °C; IR (KBr, cm^{-1}): 1661 (C=N), 3365, 3493 (NH_2); LC-MS $[M + 1]^+$: m/z 150.9.





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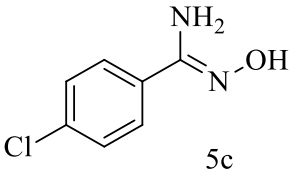
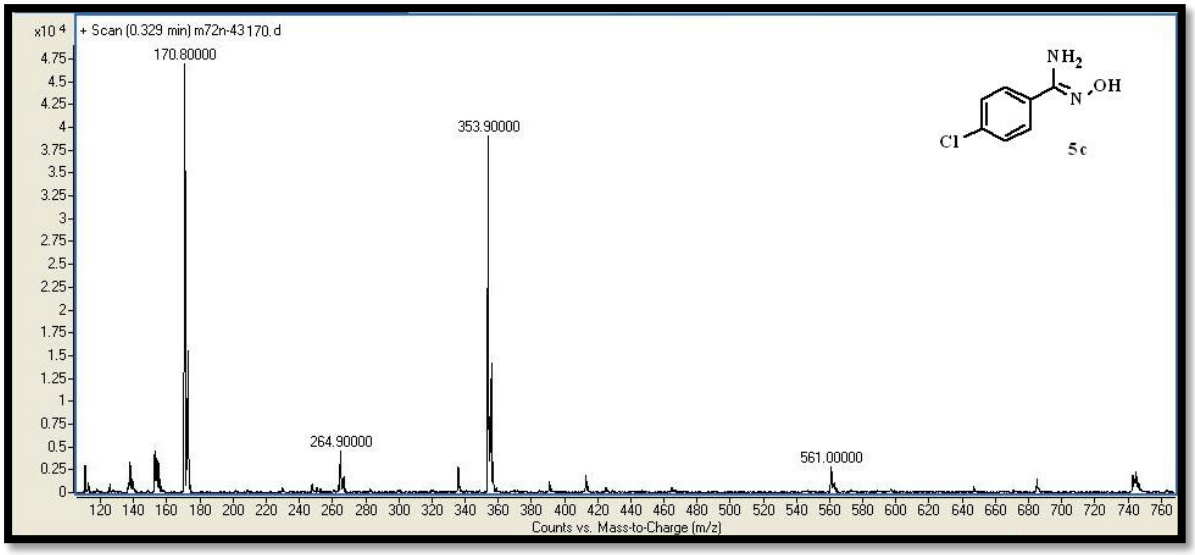
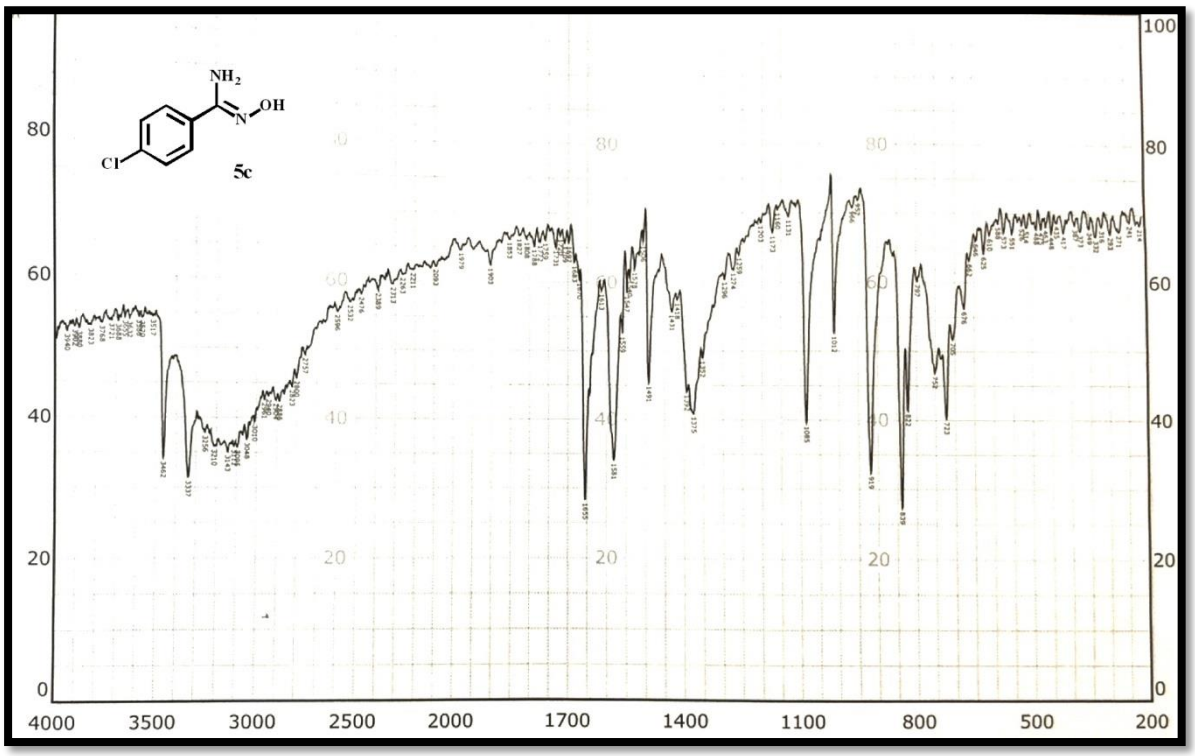


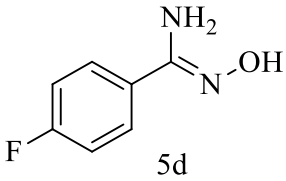
5c

4-Chloro-N′-hydroxy benzamidine (5c)

Light yellow powder (87.5 % yield); mp: 125.8-128 °C; IR (KBr, cm^{-1}): 1655 (C=N), 3337, 3462 (NH_2); LC-MS $[M + 1]^+$: m/z 170.8.



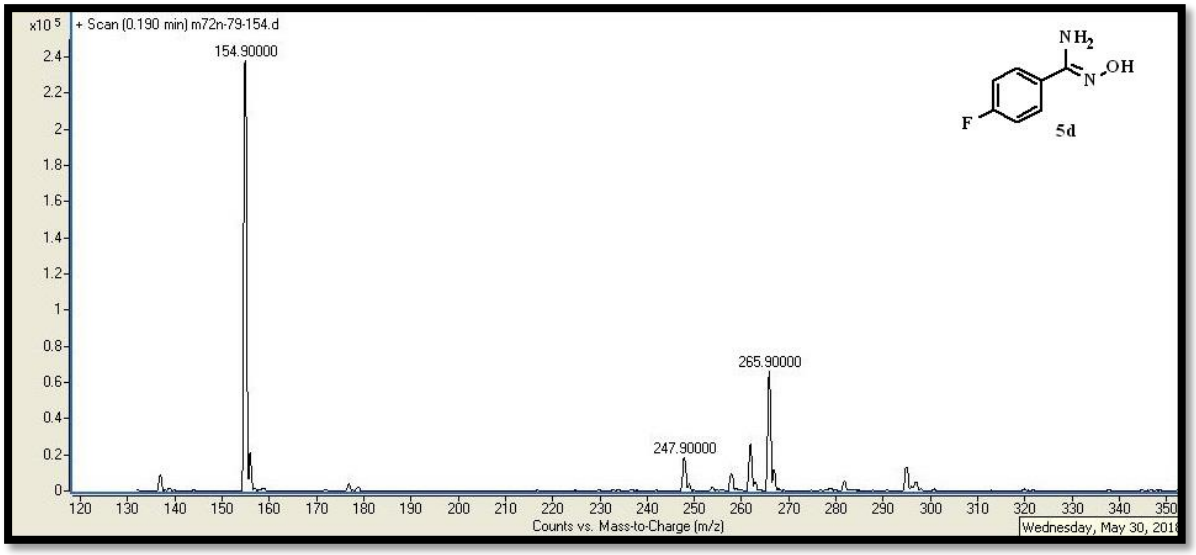


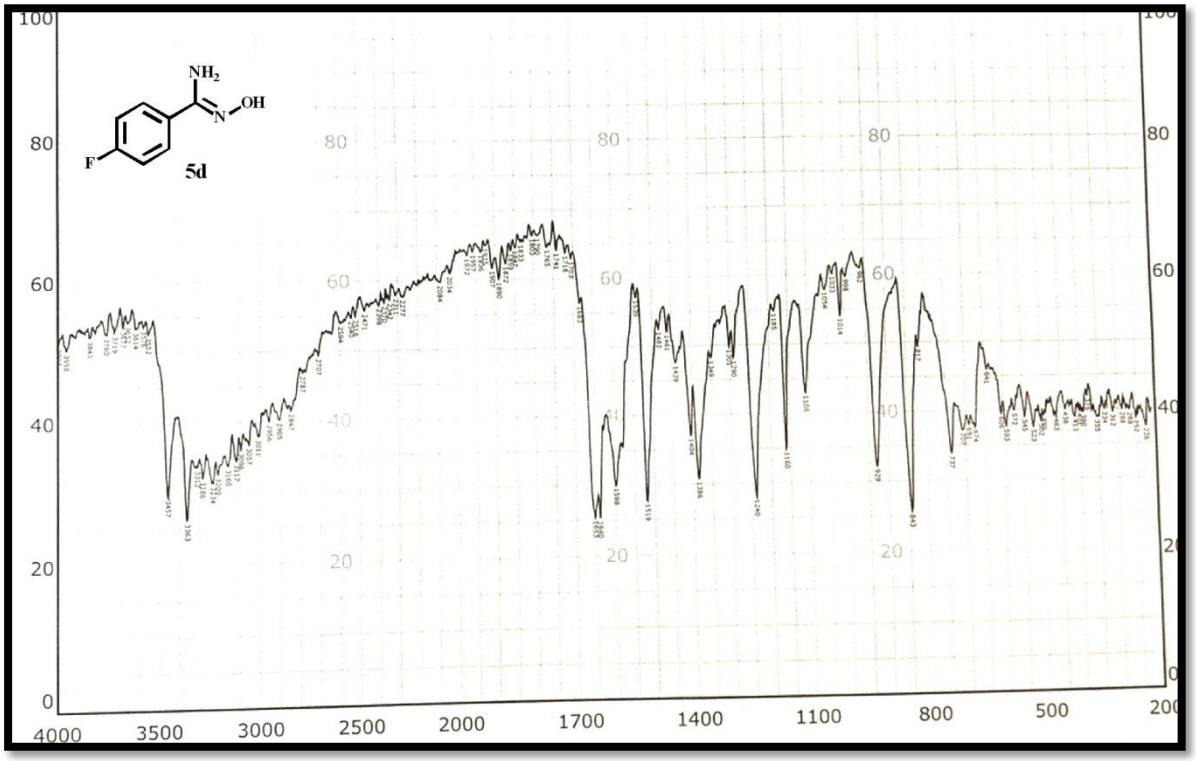


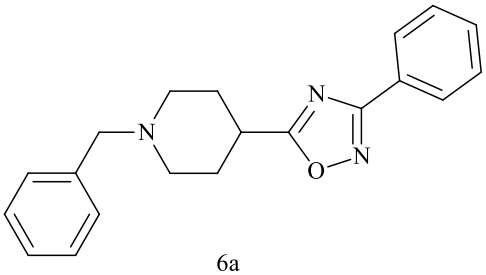
5d

4-Fluoro-N′-hydroxy benzamidine (5d)

Light yellow powder (68.2 % yield); mp: 94.5-99.5 °C; IR (KBr, cm^{-1}): 1653 (C=N), 3363, 3457 (NH_2); LC-MS $[M + 1]^+$: m/z 154.9.







6a

5-(1-benzylpiperidin-4-yl)-3-phenyl-1,2,4-oxadiazole (6a)

Light yellow powder; yield: 54.4 %; mp: 70.8-71.2 °C; IR (KBr, cm^{-1}): 1587 (C=N), 1142 (C-O); LC-MS $[M + 1]^+$: m/z 320; ^1H NMR ($CDCl_3$, 400 MHz) δ: 2.02-2.20 (m, 6H, H-piperidine), 2.94-3.03 (m, 3H, H-piperidine), 3.54 (s, 2H, CH_2-benzyl), 7.25-7.34 (m, 5H, H_2, H_3, H_4, H_5, H_6-benzyl), 7.47-7.48 (m, 3H, H_3, H_4, H_5-phenyl), 8.07-8.08 (m, 2H, H_2, H_6-phenyl); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 29.56 ($2CH_2$), 34.64 (CH), 52.75 ($2CH_2$), 63.20 (CH_2), 126.99 (C), 127.07 (CH), 127.42 (2CH), 128.25 (2CH), 128.80 (2CH), 129.04 (2CH), 131.05 (CH), 138.29 (C), 168.19 (C), 182.07 (C); Anal. calcd for $C_{20}H_{21}N_3O$: C, 75.21; H, 6.63; N, 13.16, found: C, 75.43; H, 6.61; N, 13.13.

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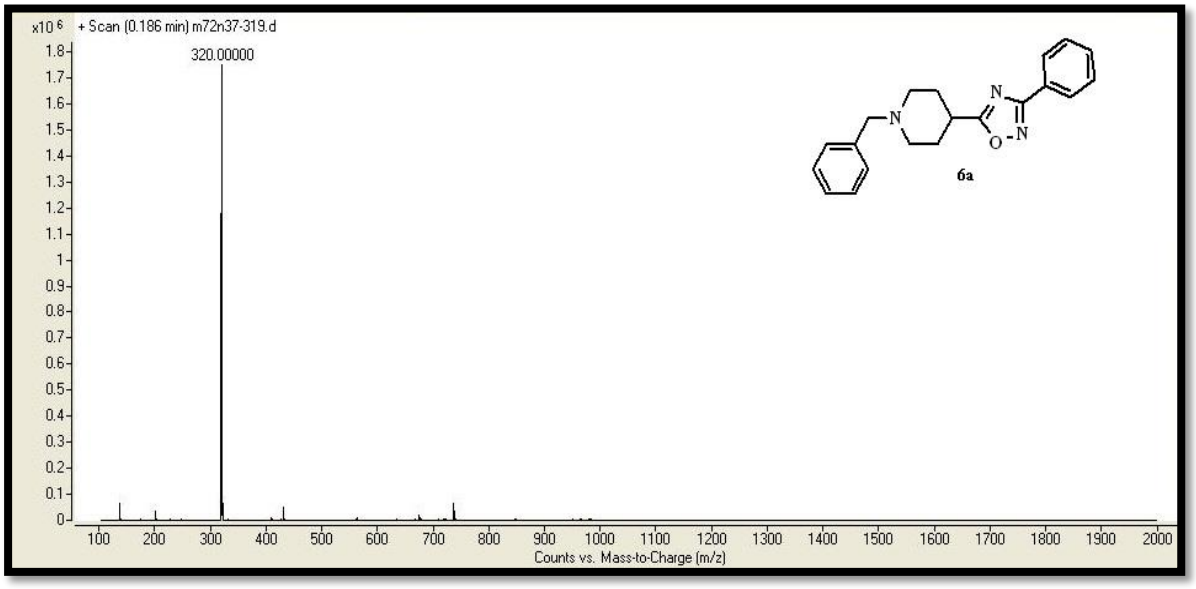

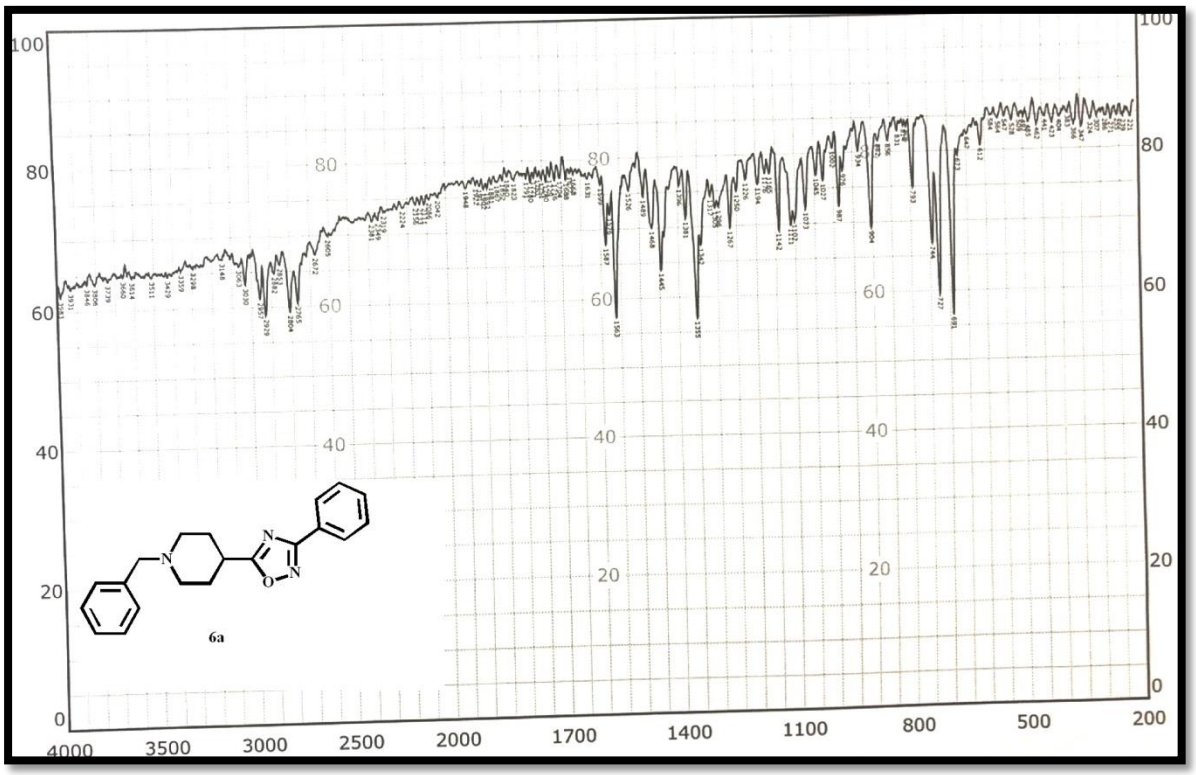

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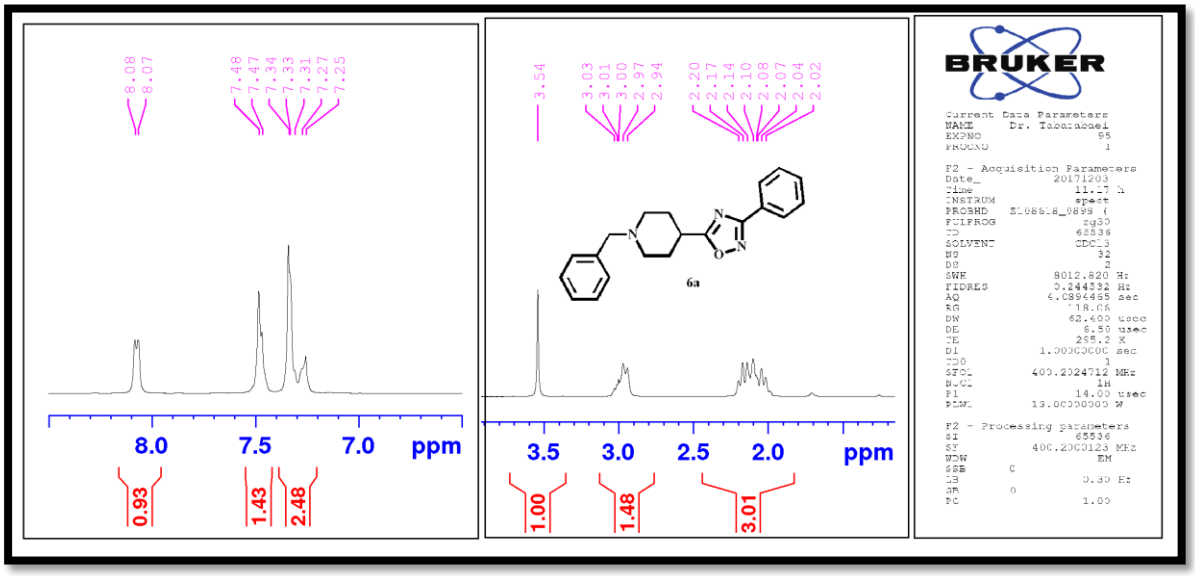
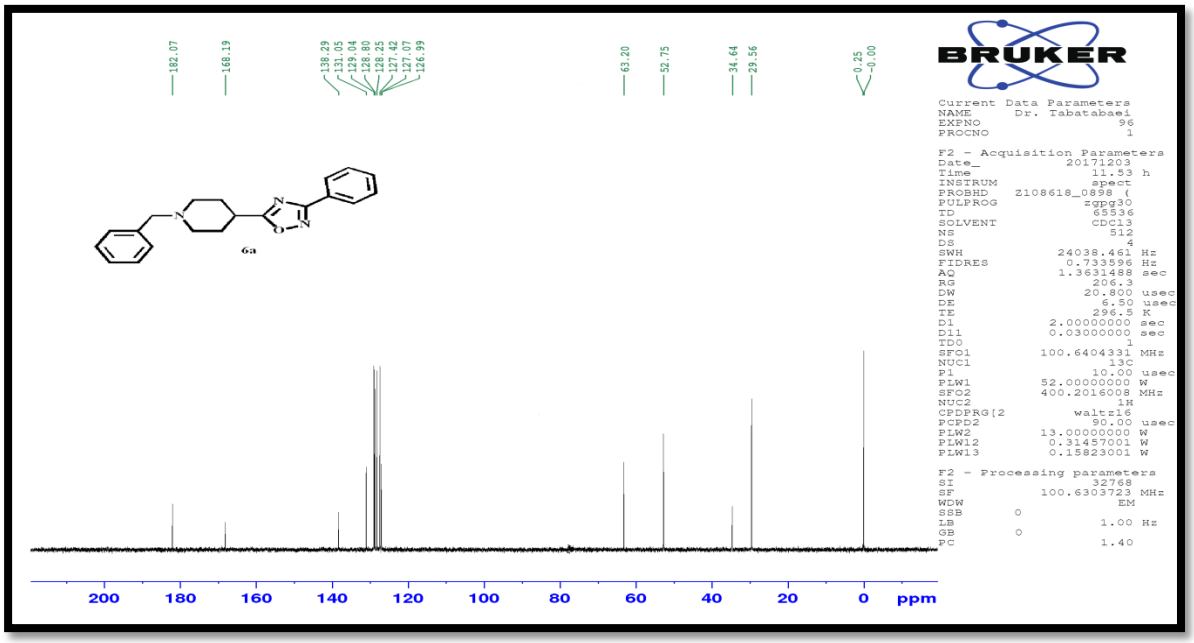
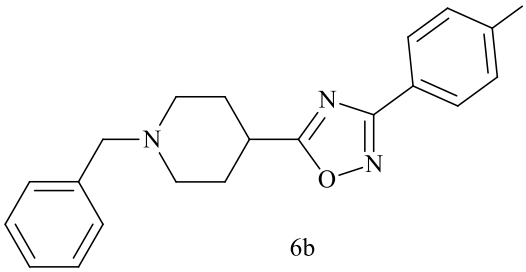


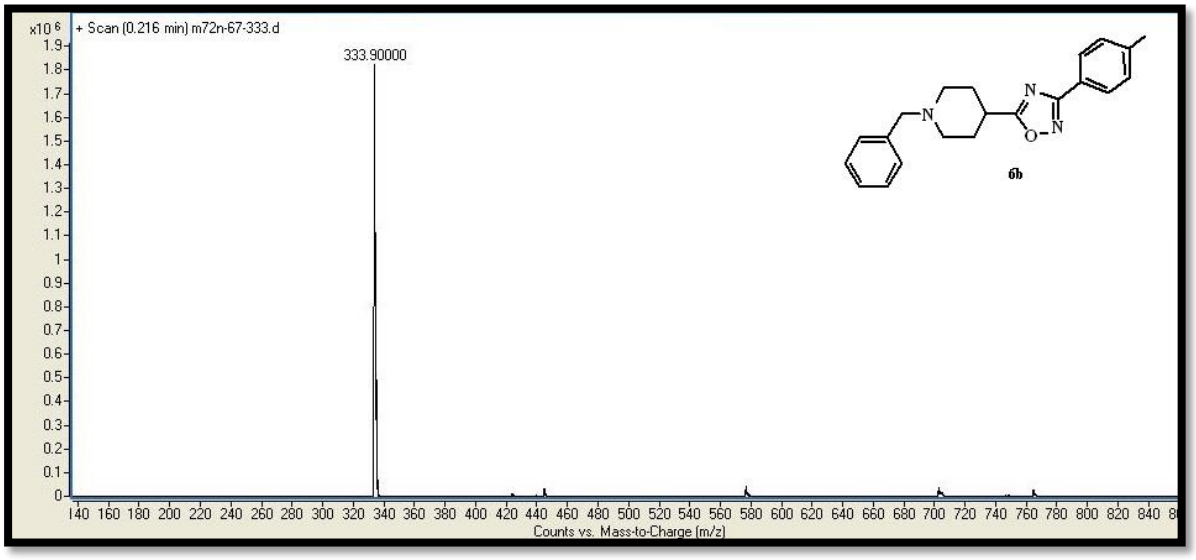




6b

5-(1-benzylpiperidin-4-yl)-3-(p-tolyl)-1,2,4-oxadiazole (6b)

Light yellow powder; yield: 32.9 %; mp: 88.5-89.8 °C; IR (KBr, cm^{-1}): 1582 (C=N), 1145 (C-O), 1346,1440 (CH_3); LC-MS $[M + 1]^+$: m/z 333.9; ^1H NMR ($CDCl_3$, 400 MHz) δ: 2.00-2.18 (m, 6H, H-piperidine), 2.40 (s, 3H, CH_3), 2.93-3.01 (m, 3H, H-piperidine), 3.53 (s, 2H, CH_2-benzyl), 7.26-7.28 (m, 2H, H_3, H_5-phenyl), 7.32-7.33 (m, 5H, H_2, H_3, H_4, H_5, H_6-benzyl), 7.95-7.97 (m, 2H, H_2, H_6-phenyl); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 21.55 (CH_3), 29.54 ($2CH_2$), 34.62 (CH), 52.74 ($2CH_2$), 63.18 (CH_2), 124.13 (C), 127.04 (2CH), 127.31 (CH), 128.23 (2CH), 129.02 (2CH), 129.49 (2CH), 138.28 (C), 141.31 (C), 168.15 (C), 181.86 (C); Anal. calcd for $C_{21}H_{23}N_3O$: C, 75.65; H, 6.95; N, 12.60, found: C, 75.87; H, 6.92; N, 12.56.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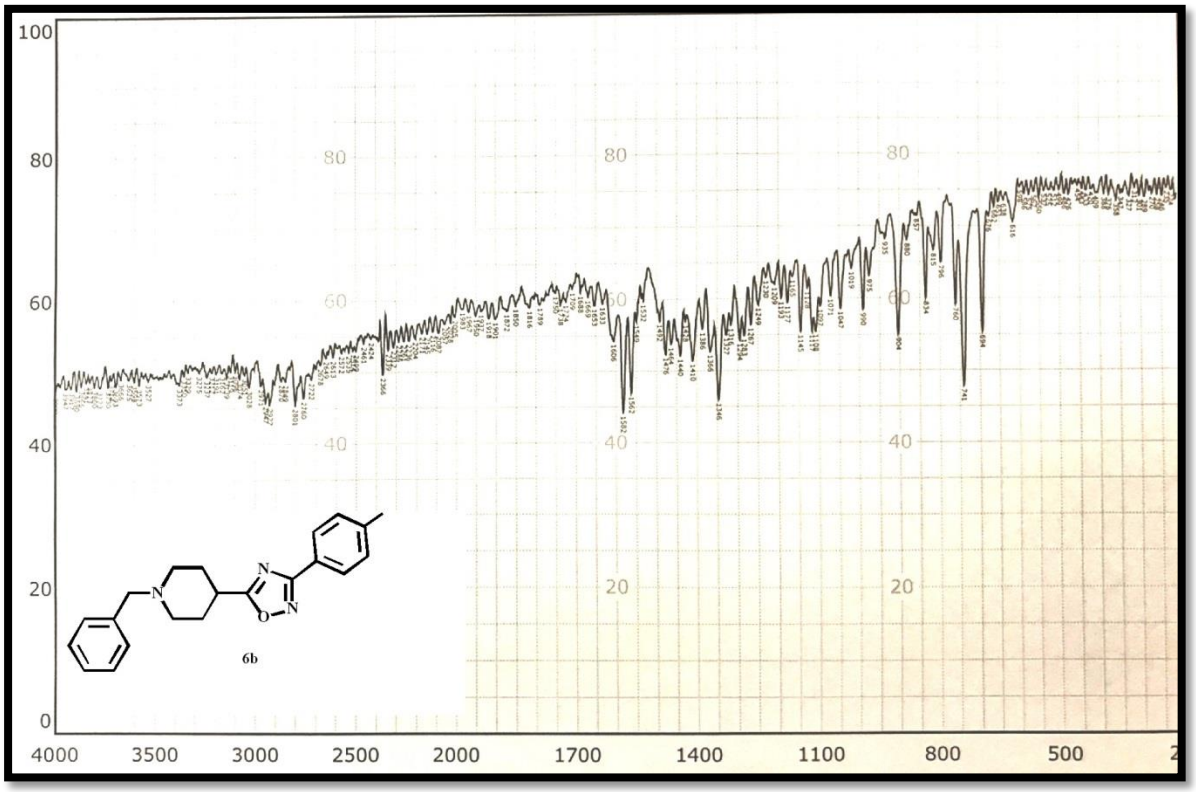
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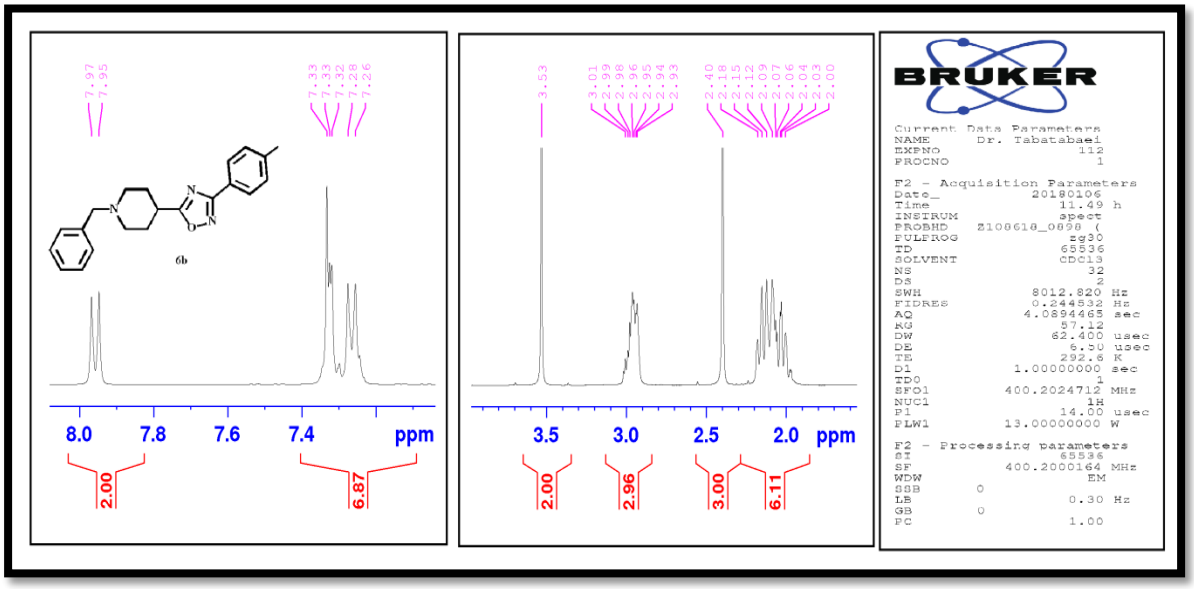
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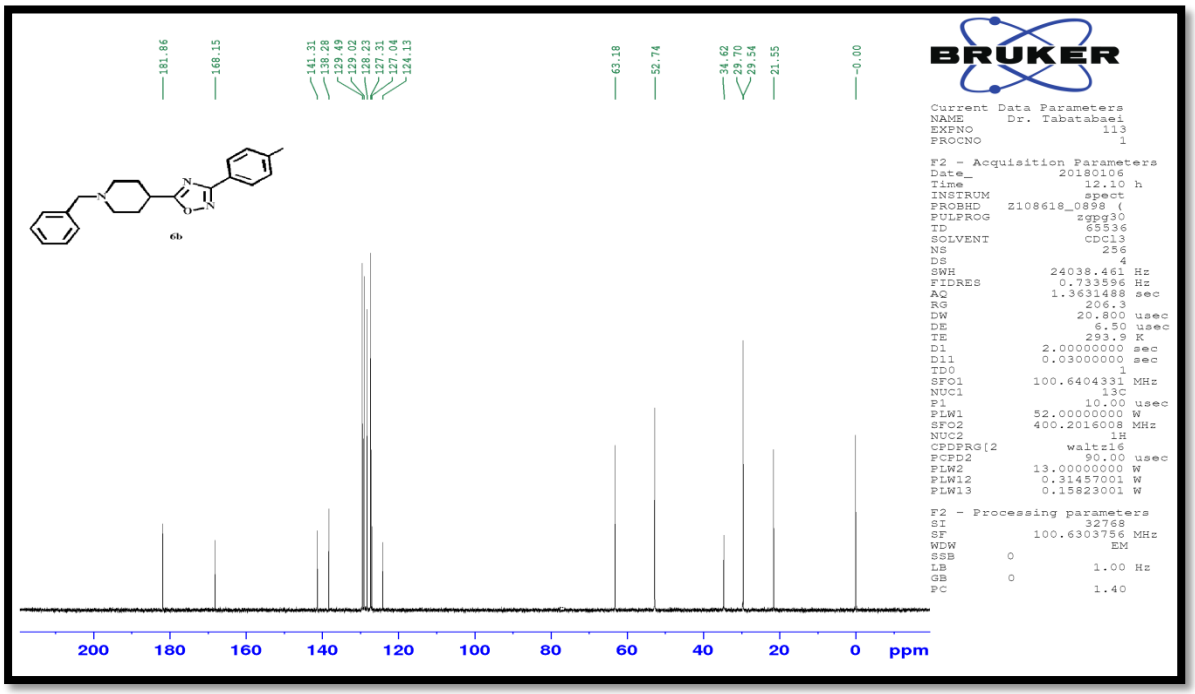
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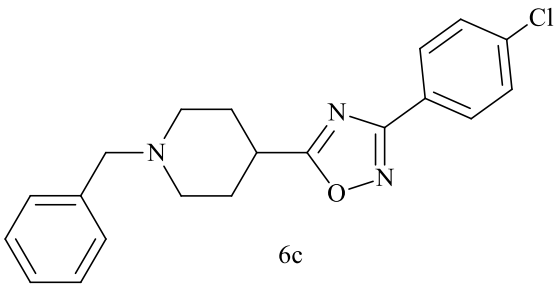

6c

5-(1-benzylpiperidin-4-yl)-3-(4-chlorophenyl)-1,2,4-oxadiazole (6c)

Light yellow powder; yield: 32.1 %; mp: 106-108 °C; IR (KBr, cm^{-1}): 1592 (C=N), 1139 (C-O); LC-MS $[M + 1]^+$: m/z 354; ^1H NMR ($CDCl_3$, 400 MHz) δ: 2.00-2.19 (m, 6H, H-piperidine), 2.94-3.02 (m, 3H, H-piperidine), 3.54 (s, 2H, CH_2-benzyl), 7.26-7.34 (m, 5H, H_2, H_3, H_4, H_5, H_6-benzyl), 7.44-7.46 (m, 2H, H_3, H_5-phenyl), 8.00-8.02 (m, 2H, H_2, H_6-phenyl); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 29.53 ($2CH_2$), 34.61 (CH), 52.71 ($2CH_2$), 63.18 (CH_2), 125.47 (C), 127.08 (2CH), 128.75 (CH), 128.72 (2CH), 129.04 (2CH), 129.12 (2CH), 137.17 (C), 138.23 (C), 167.39 (C), 182.30 (C); Anal. calcd for $C_{20}H_{20}ClN_3O$: C, 67.89; H, 5.70; N, 11.88, found: C, 68.12; H, 5.69; N, 11.82.

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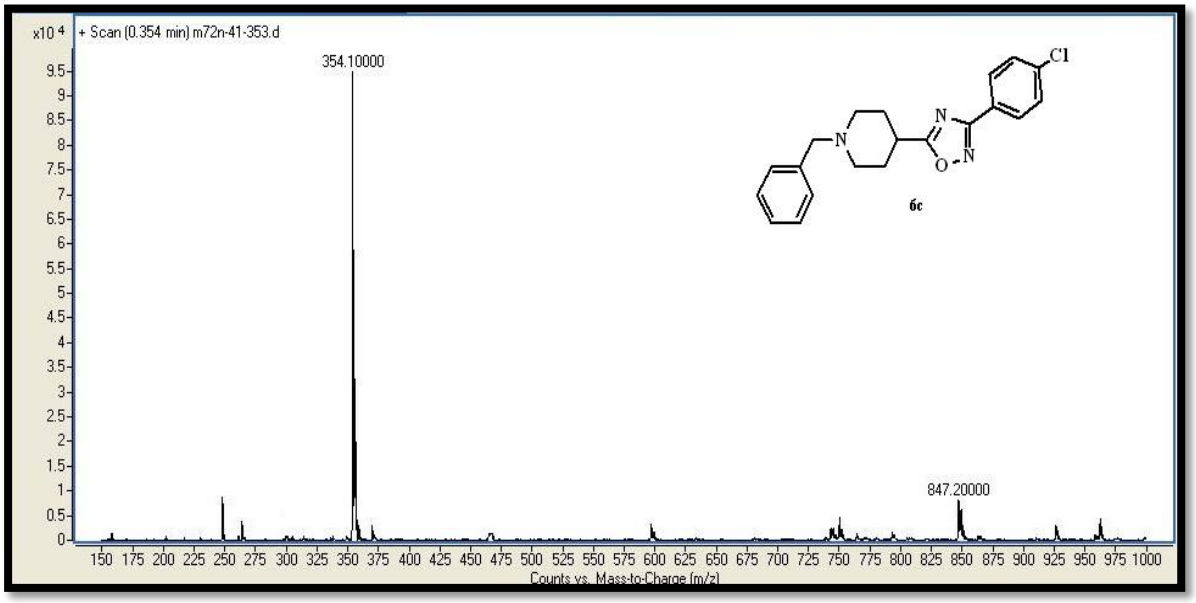

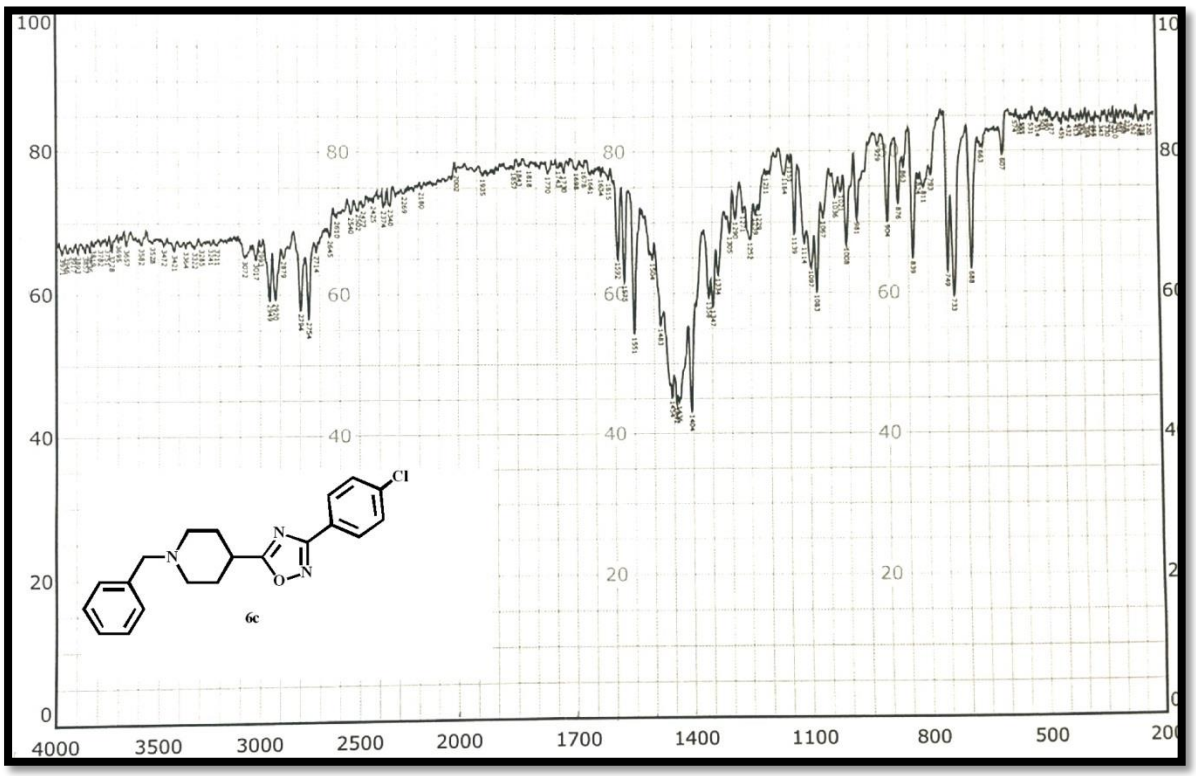

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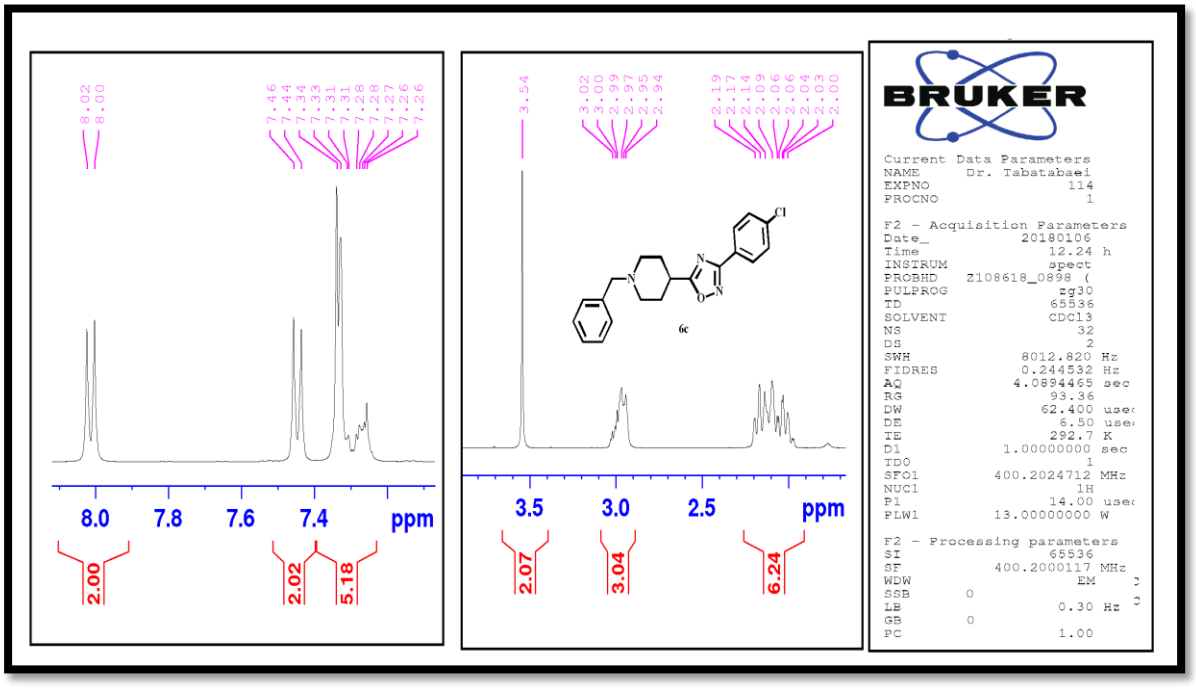
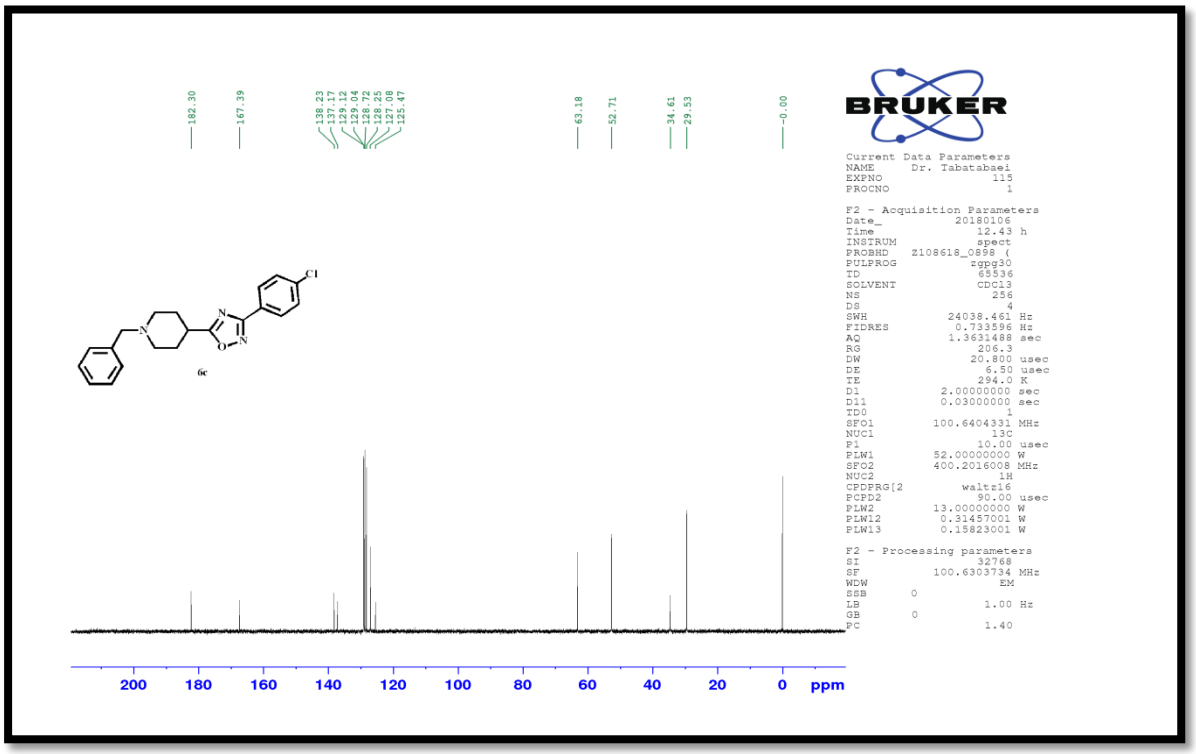
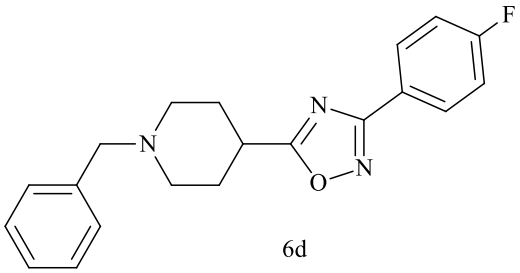


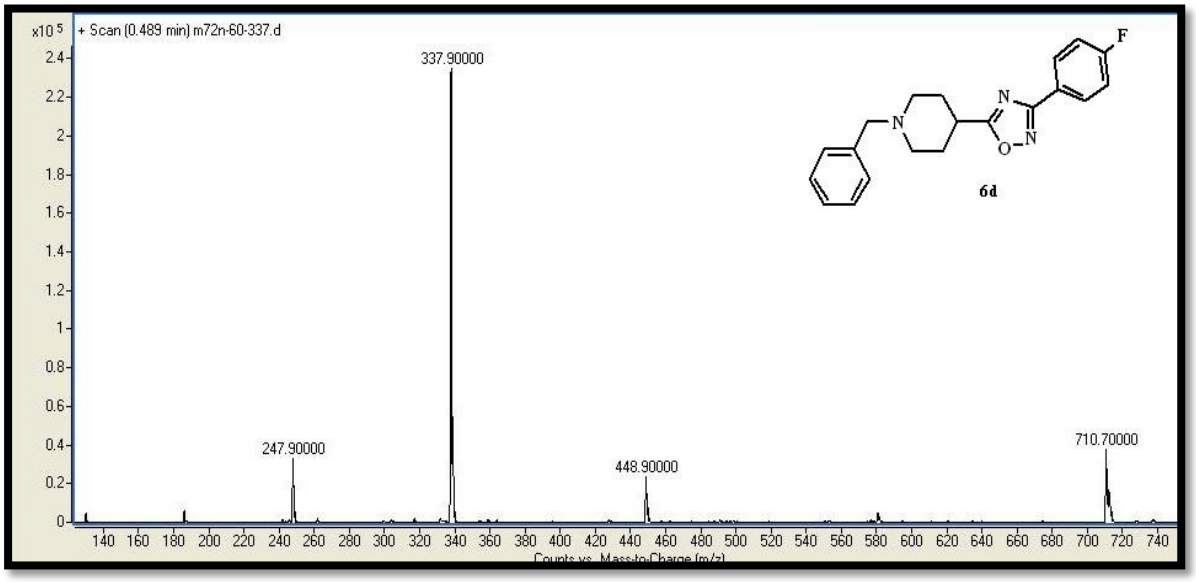




6d

5-(1-benzylpiperidin-4-yl)-3-(4-fluorophenyl)-1,2,4-oxadiazole (6d)

Light yellow powder; yield: 40.7 %; mp: 92.7-93.6 °C; IR (KBr, cm^{-1}): 1571 (C=N), 1130 (C-O); LC-MS $[M + 1]^+$: m/z 337.9; ^1H NMR ($CDCl_3$, 400 MHz) δ: 1.93-2.12 (m, 6H, H-piperidine), 2.87-2.93 (m, 3H, H-piperidine), 3.47 (s, 2H, CH_2-benzyl), 7.06-7.10 (m, 2H, H_3, H_5-phenyl), 7.18-7.26 (m, 5H, H_2, H_3, H_4, H_5, H_6-benzyl), 7.98-8.01 (m, 2H, H_2, H_6-phenyl); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 29.55 ($2CH_2$), 34.61 (CH), 52.73 ($2CH_2$), 63.20 (CH_2), 115.90 (C), 123.23 (2CH), 127.12 (CH), 128.28 (2CH), 129.08 (2CH), 129.54 (2CH), 129.62 (C), 138.24 (C), 165.67 (C), 182.21 (C); Anal. calcd for $C_{20}H_{20}FN_3O$: C, 71.20; H, 5.97; N, 12.45, found: C, 71.41; H, 5.99; N, 12.40.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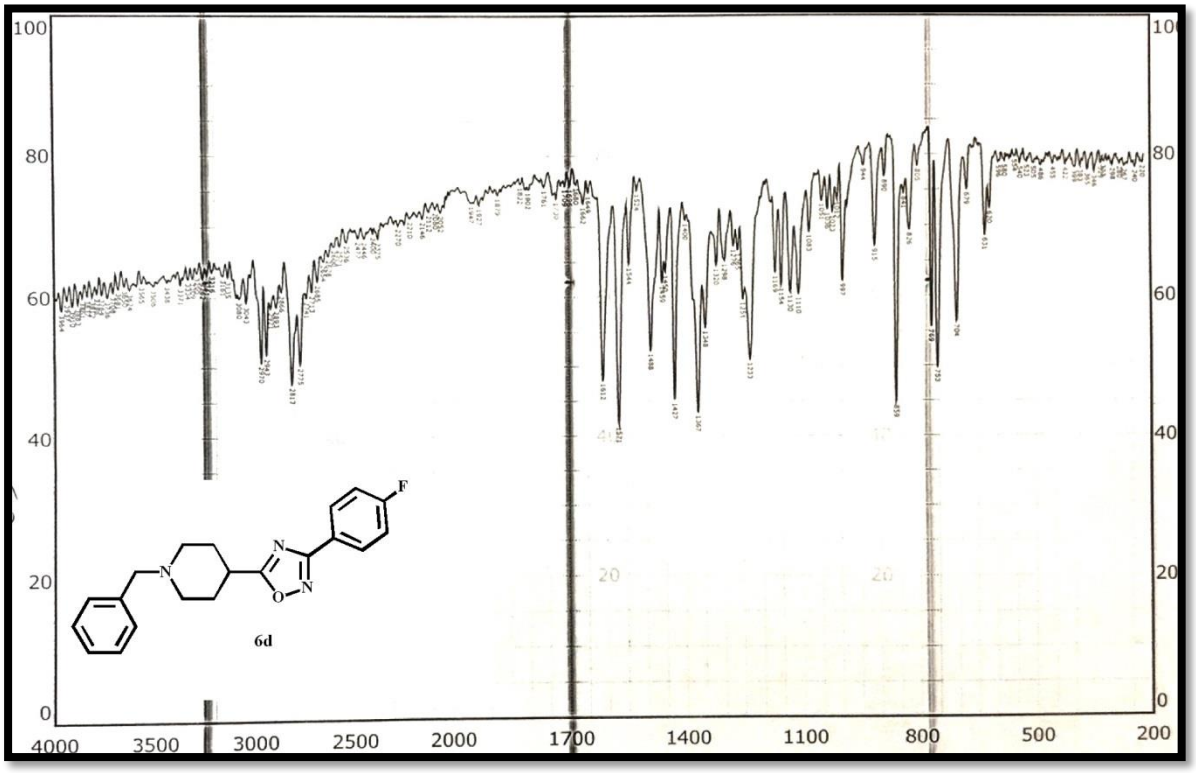
6d

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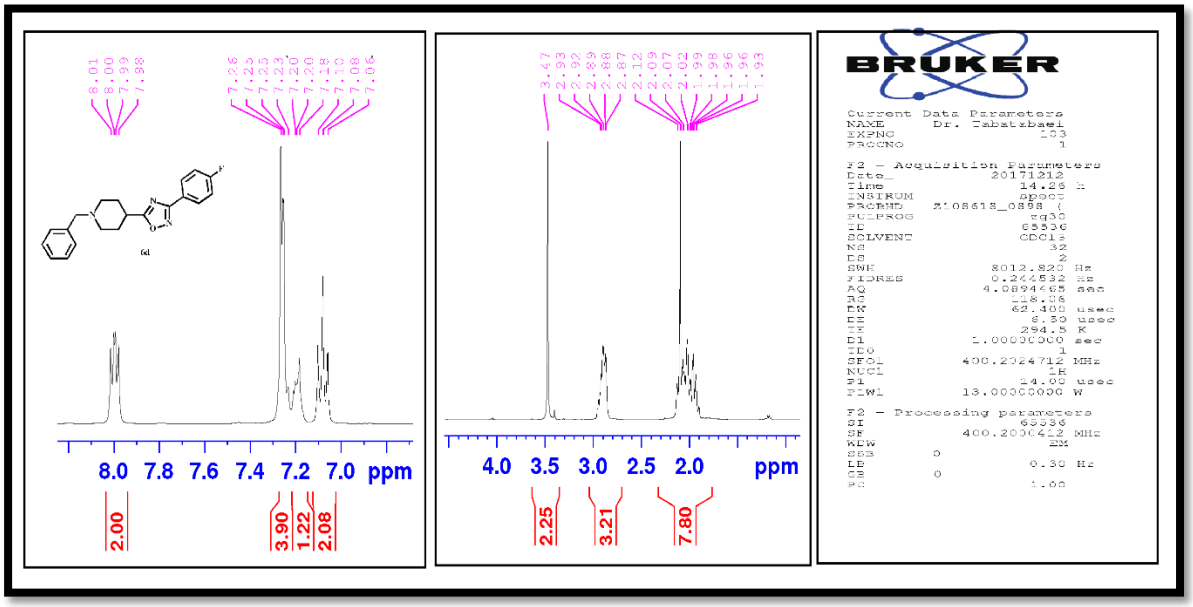

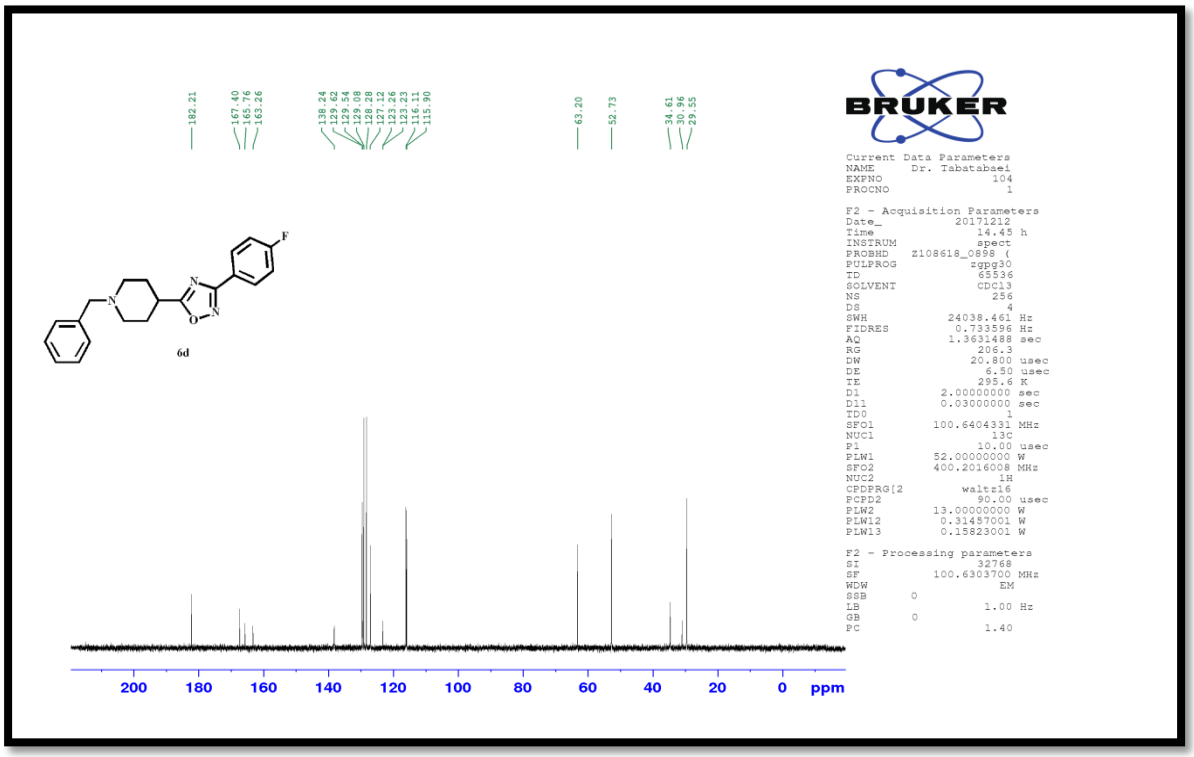

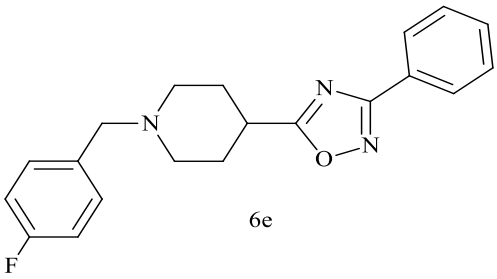

6e

5-(1-(4-fluorobenzyl)piperidin-4-yl)-3-phenyl-1,2,4-oxadiazole (6e)

Light yellow powder; yield: 20.9 %; mp: 93.4-94.5 °C; IR (KBr, cm^{-1}): 1596 (C=N), 1214 (C-O); LC-MS $[M + 1]^+$: m/z 338; ^1H NMR ($CDCl_3$, 400 MHz) δ: 1.97-2.07 (m, 4H, H-piperidine), 2.11-2.19 (m, 4H, H-piperidine), 2.92-3.05 (m, 1H, H-piperidine), 3.50 (s, 2H, CH_2-benzyl), 7.01 (t, 2H, *J* = 8 Hz, H_3, H_5-benzyl), 7.26-7.32 (m, 2H, H_2, H_6-benzyl), 7.45-7.50 (m, 3H, H_3, H_4, H_5-phenyl), 8.08 (d, 2H, *J* = 8 Hz, H_2, H_6-phenyl); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 29.53 ($2CH_2$), 34.60 (CH), 52.65 ($2CH_2$), 62.35 (CH_2), 115.15 (2CH), 126.95 (C), 127.42 (2CH), 128.81 (2CH), 130.40 (2CH), 131.08 (CH), 133.98 (C), 160.79 (C), 168.20 (C), 182.00 (C); Anal. calcd for $C_{20}H_{20}FN_3O$: C, 71.20; H, 5.97; N, 12.45, found: C, 71.40; H, 5.94; N, 12.48.

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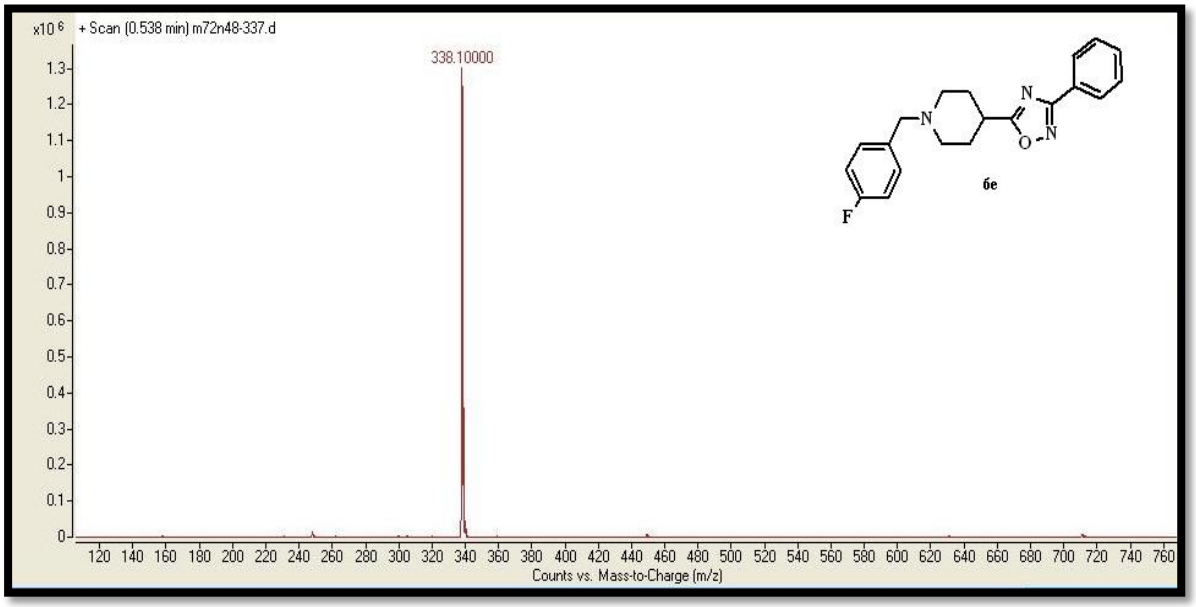

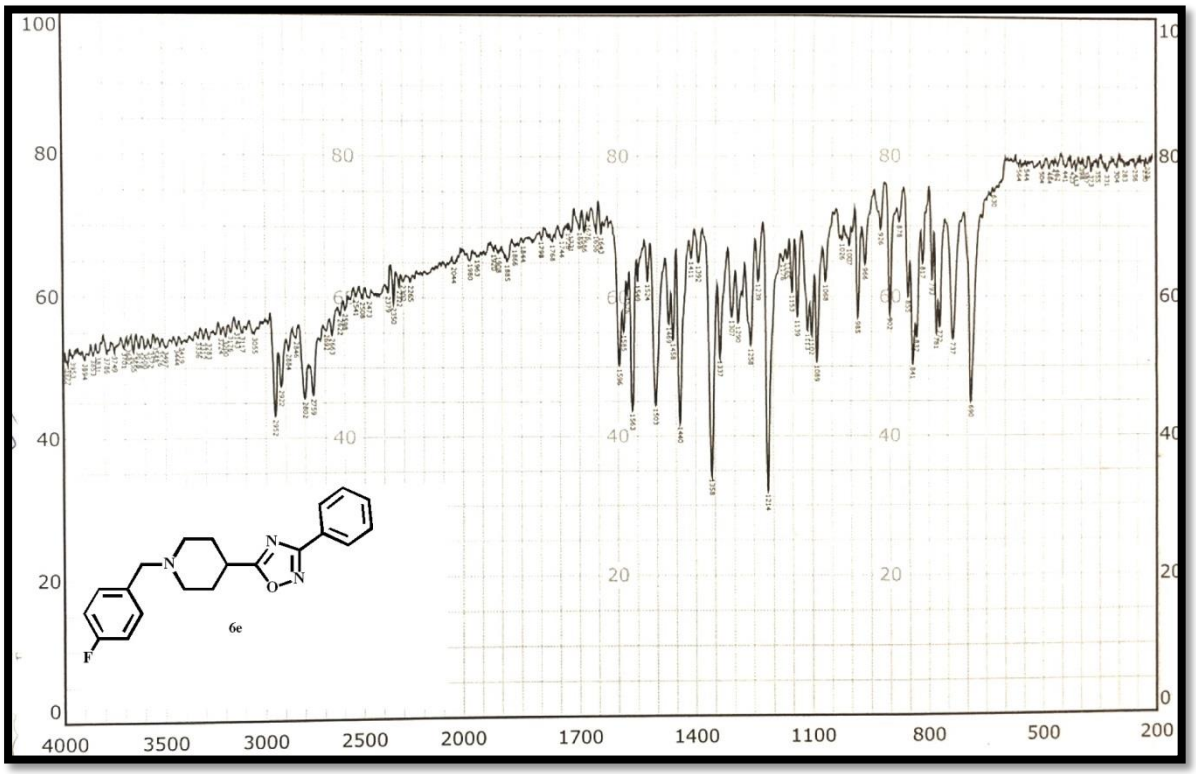

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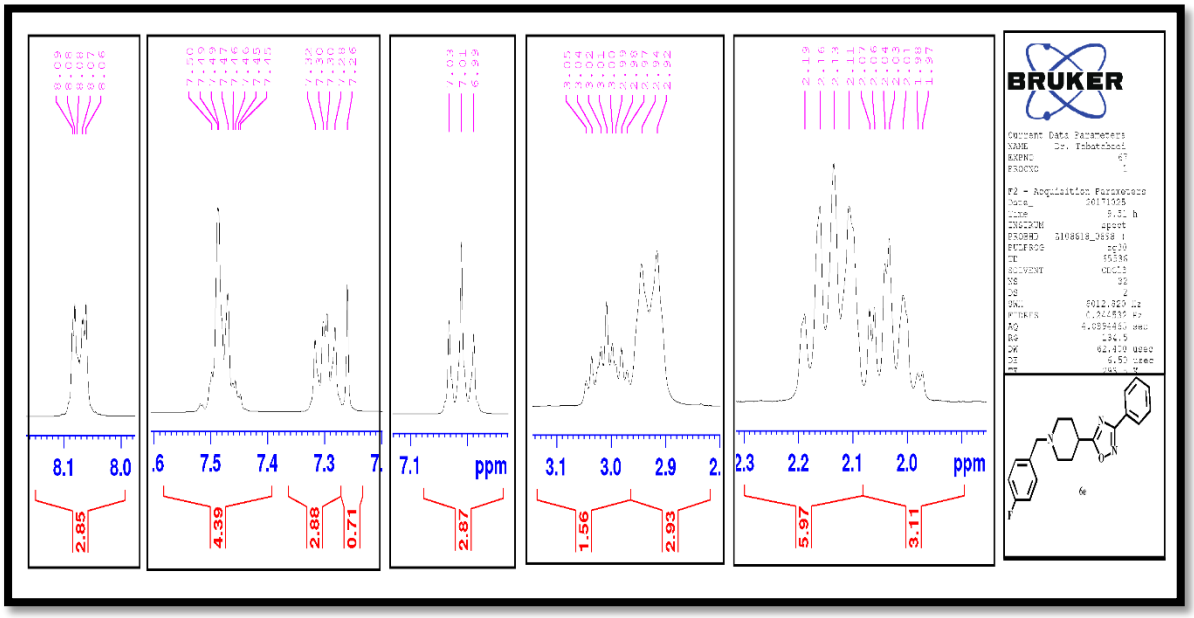

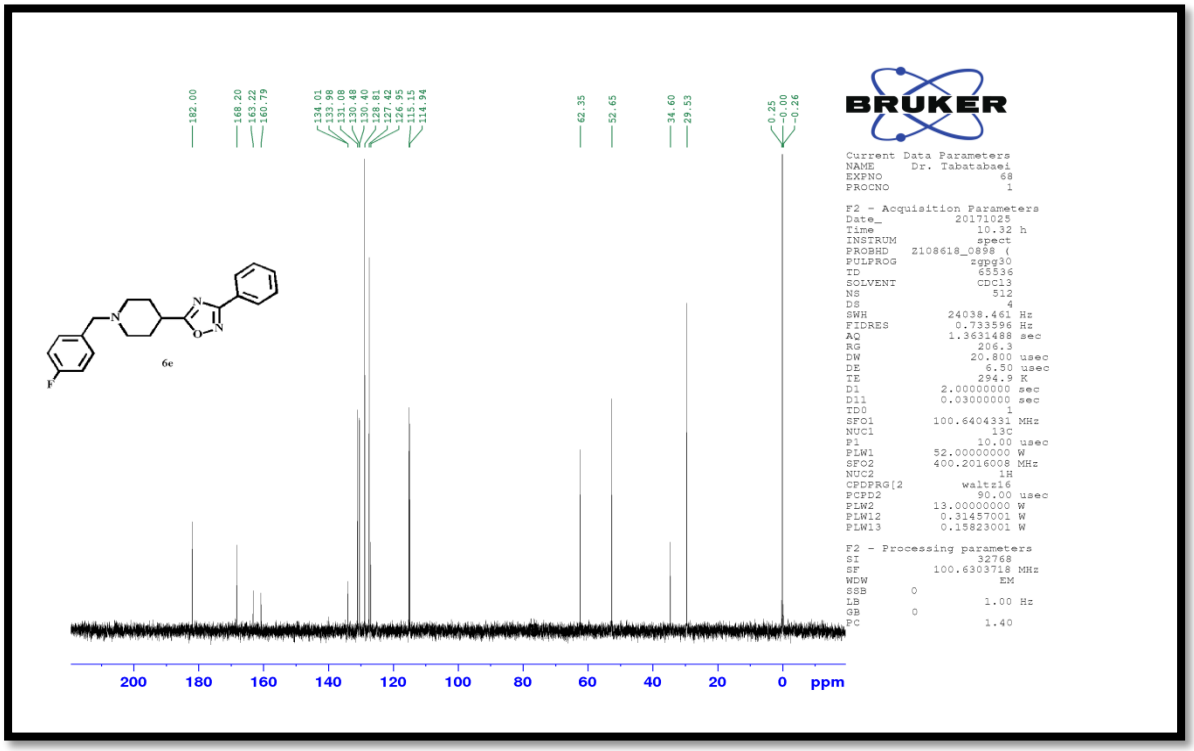

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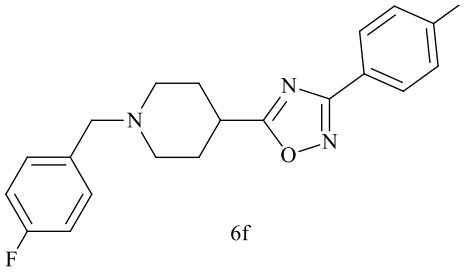

6f

5-(1-(4-fluorobenzyl)piperidin-4-yl)-3-(p-tolyl)-1,2,4-oxadiazole (6f)

White powder; yield: 56.3 %; mp: 90-90.8 °C; IR (KBr, cm^{-1}): 1582 (C=N), 1223 (C-O), 1344,1440 (CH_3); LC-MS $[M + 1]^+$: m/z 351.9; ^1H NMR ($CDCl_3$, 400 MHz) δ: 2.02-2.17 (m, 6H, H-piperidine), 2.40 (s, 3H, CH_3), 2.90-3.01 (m, 3H, H-piperidine), 3.49 (s, 2H, CH_2-benzyl), 6.98-7.03 (m, 2H, H_3, H_5-benzyl), 7.26-7.31 (m, 4H, H_2, H_6-benzyl, H_3, H_5-phenyl), 7.95 (d, 2H, J = 8 Hz, H_2, H_6-phenyl); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 21.55 (CH_3), 29.53 ($2CH_2$), 34.59 (CH), 52.65 ($2CH_2$), 62.34 (CH_2), 115.13 (2CH), 124.13 (C), 127.33 (2CH), 129.51 (2CH), 130.46 (2CH), 134.04 (CH), 141.35 (C), 160.77 (C), 168.18 (C), 181.81 (C); Anal. calcd for $C_{21}H_{22}FN_3O$: C, 71.77; H, 6.31; N, 11.96, found: C, 72.01; H, 6.32; N, 11.91.

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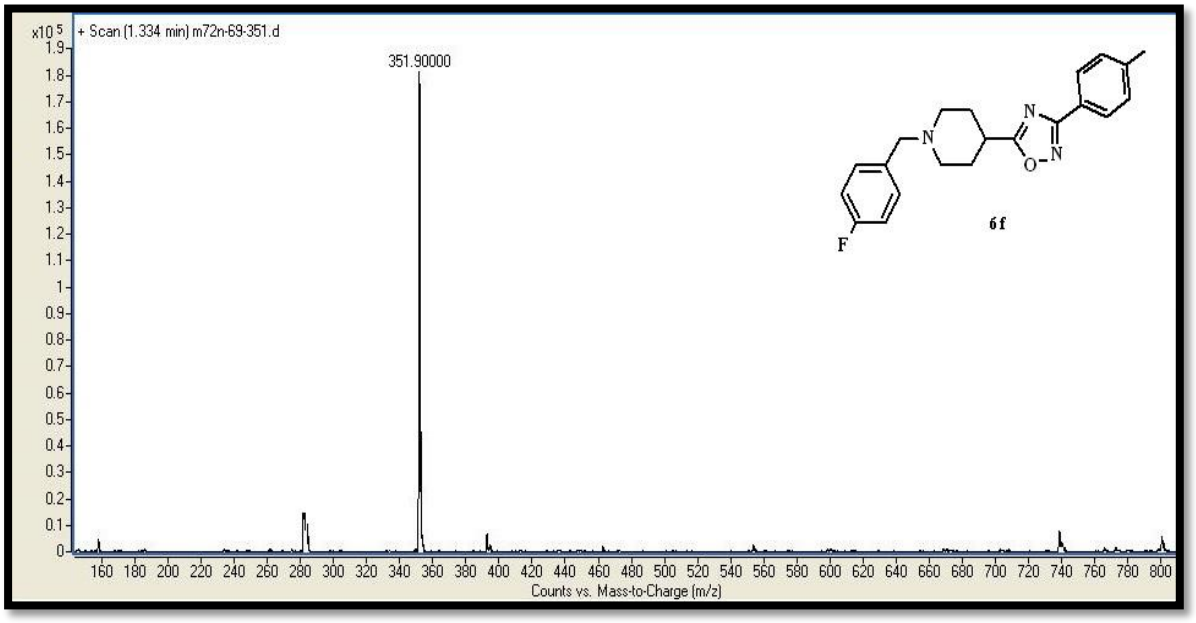

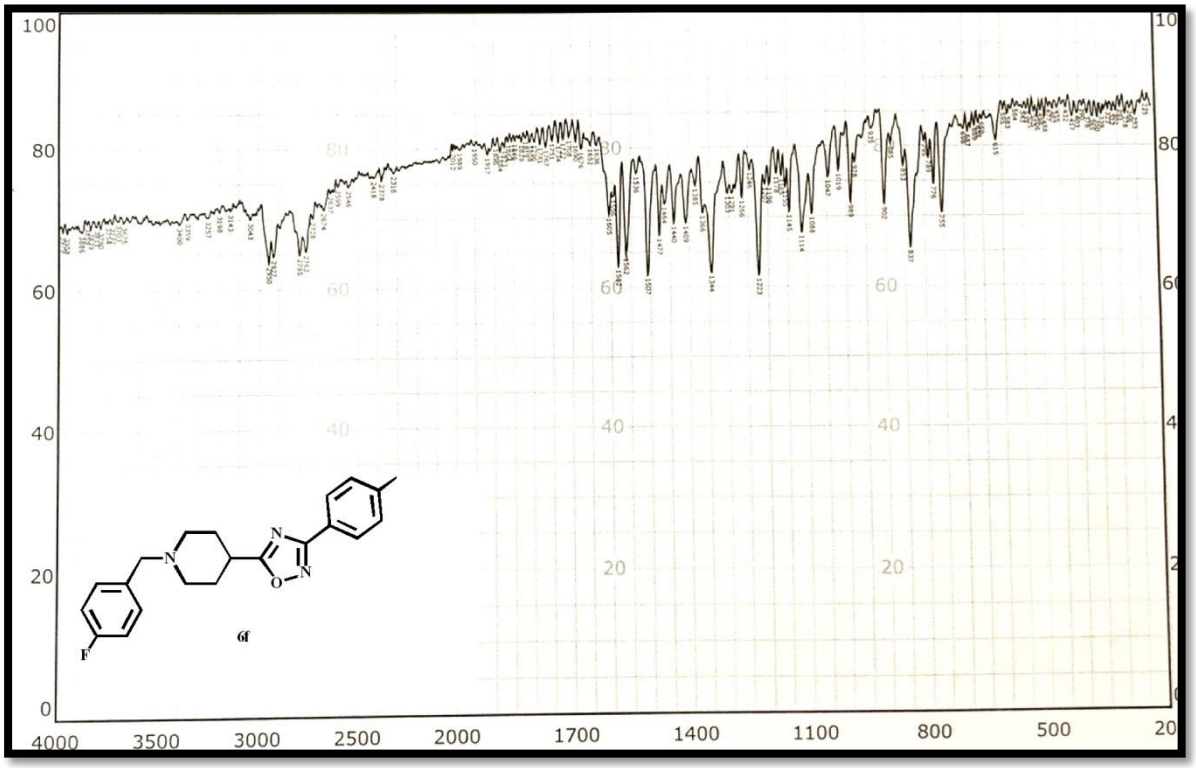

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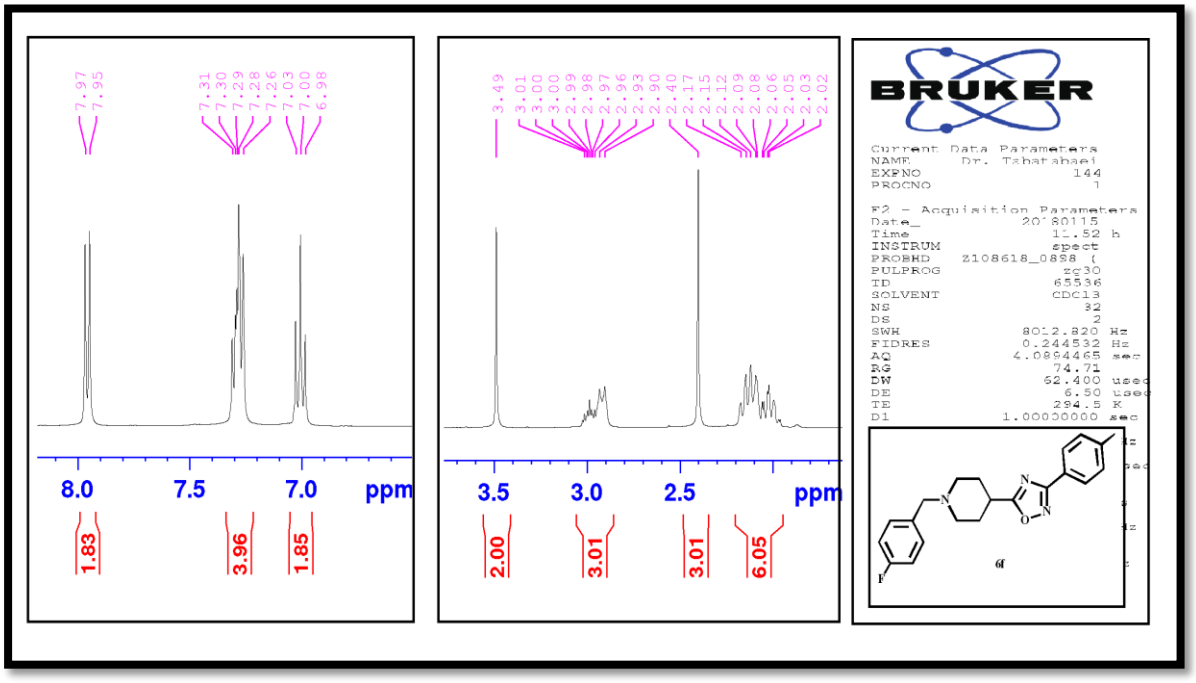

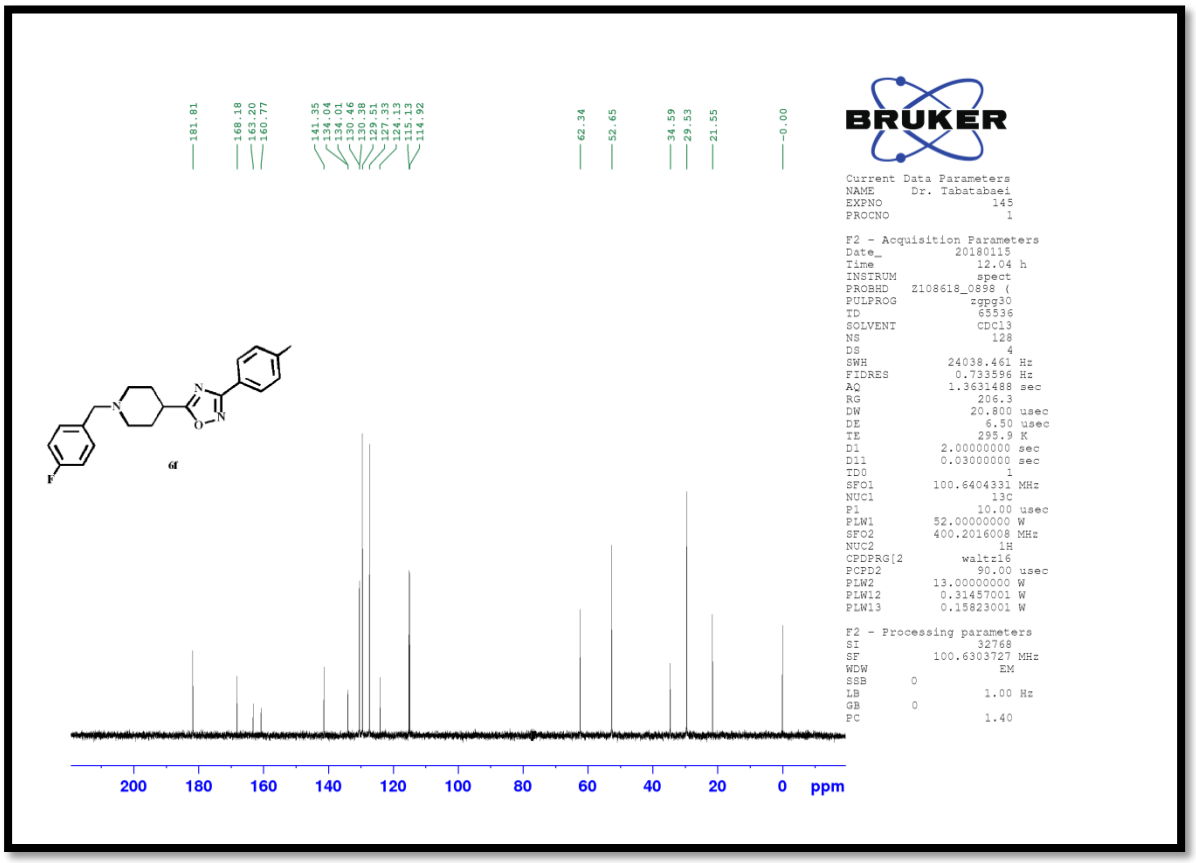

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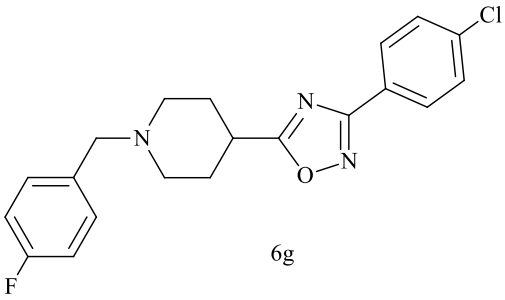

6g

3-(4-chlorophenyl)-5-(1-(4-fluorobenzyl)piperidin-4-yl)-1,2,4-oxadiazole (6g)

Light yellow powder; yield: 36.0 %; mp: 106.7-107.7 °C; IR (KBr, cm^{-1}): 1596 (C=N), 1153 (C-O); LC-MS $[M + 1]^+$: m/z 372; ^1H NMR ($CDCl_3$, 400 MHz) δ: 1.96-2.06 (m, 4H, H-piperidine), 2.10-2.19 (m, 4H, H-piperidine), 2.91-3.02 (m, 1H, H-piperidine), 3.50 (s, 2H, CH_2-benzyl), 7.01 (t, 2H, *J* = 8 Hz, H_3, H_5-benzyl), 7.26-7.31 (m, 2H, H_2, H_6-benzyl), 7.44 (d, 2H, *J* = 8 Hz, H_3, H_5-phenyl), 8.02 (d, 2H, *J* = 8 Hz, H_2, H_6-phenyl); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 29.52 ($2CH_2$), 34.59 (CH), 52.62 ($2CH_2$), 62.34 (CH_2), 115.16 (2CH), 125.48 (C), 128.73 (2CH), 130.39 (2CH), 133.96 (2CH), 137.21 (C), 160.80 (C), 163.23 (C), 167.42 (C), 182.24 (C); Anal. calcd for $C_{20}H_{19}ClFN_3O$: C, 64.60; H, 5.15; N, 11.30, found: C, 64.84; H, 5.14; N, 11.23.

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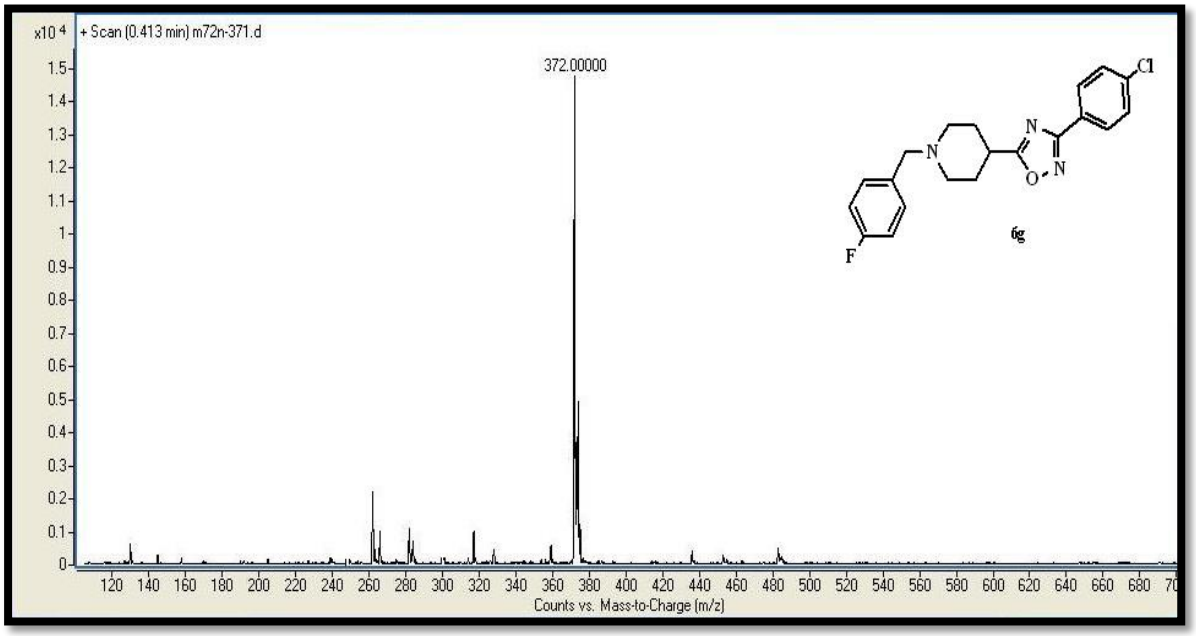

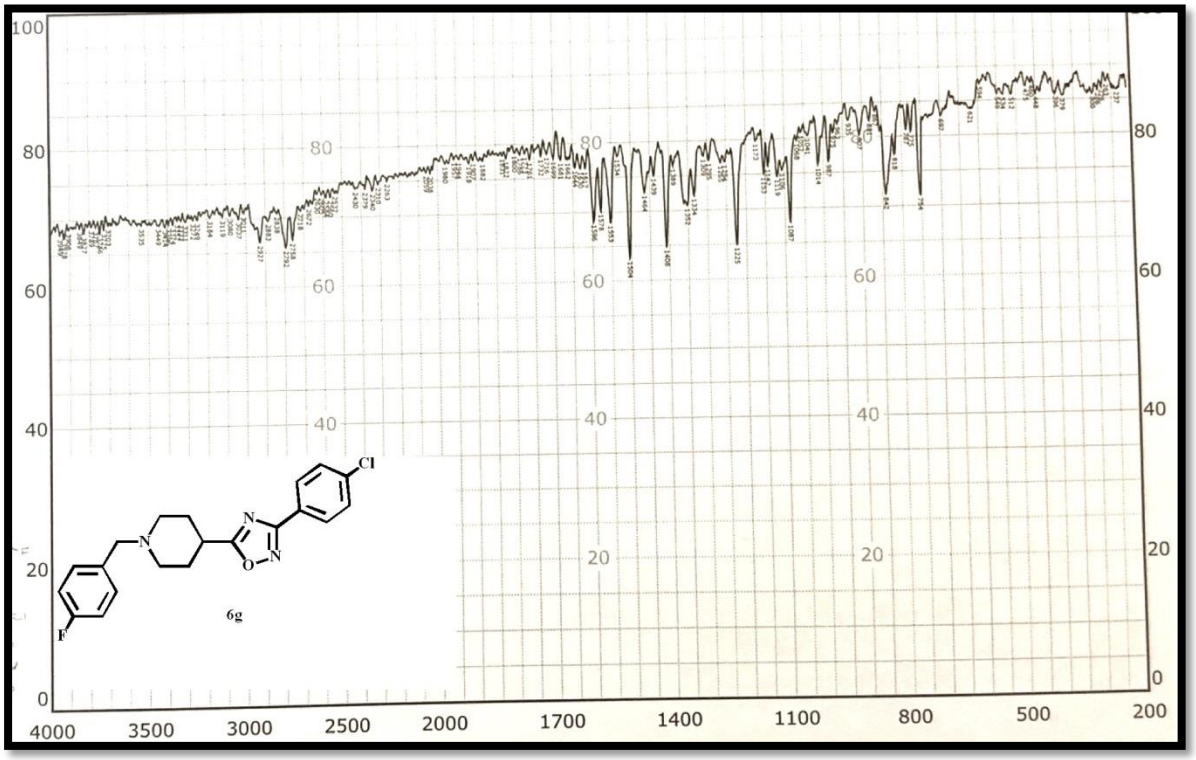

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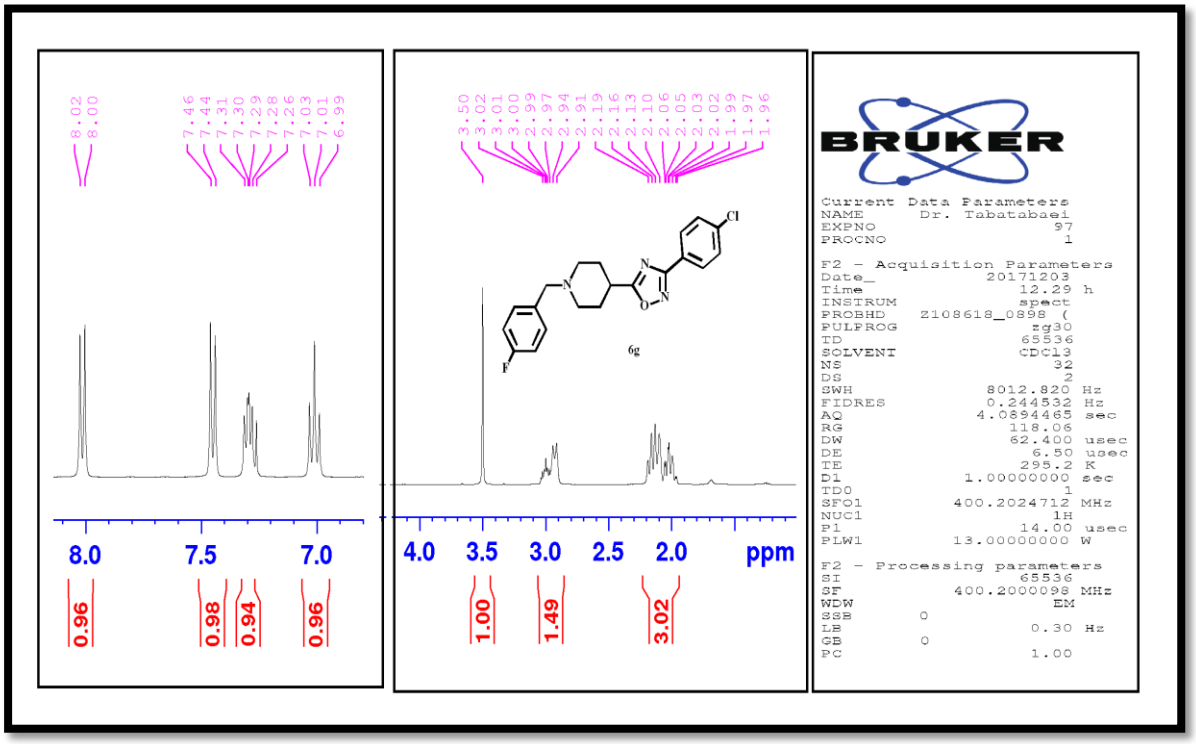

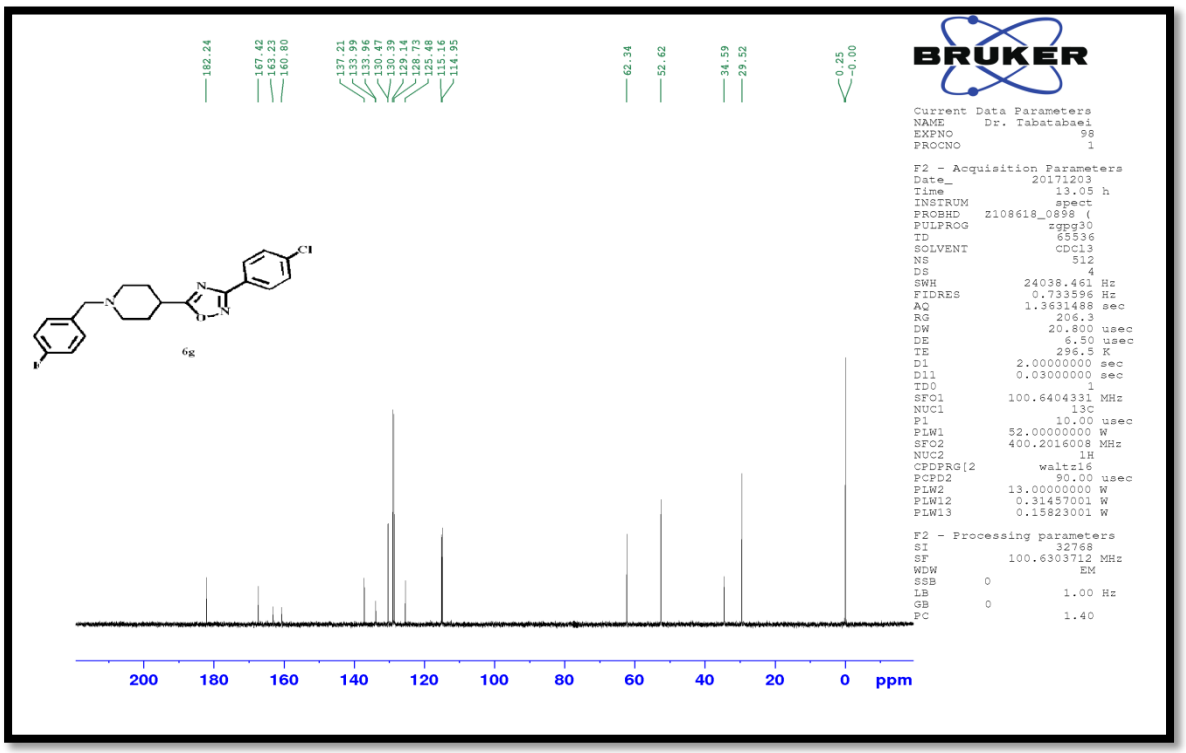

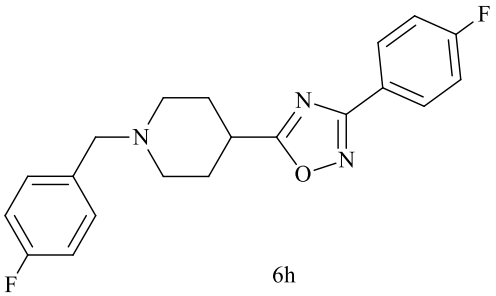

6h

5-(1-(4-fluorobenzyl)piperidin-4-yl)-3-(4-fluorophenyl)-1,2,4-oxadiazole (6h)

Light yellow powder; yield: 31.6 %; mp: 115.7-117.7 °C; IR (KBr, cm^{-1}): 1609 (C=N), 1230 (C-O); LC-MS $[M + 1]^+$: m/z 355.8; ^1H NMR ($CDCl_3$, 400 MHz) δ: 1.90-2.11 (m, 6H, H-piperidine), 2.84-2.95 (m, 3H, H-piperidine), 3.43 (s, 2H, CH_2-benzyl), 6.91-6.96 (m, 2H, H_3, H_5-benzyl), 7.08 (t, 2H, J = 8 Hz, H_3, H_5-phenyl), 7.19-7.24 (m, 2H, H_2, H_6-benzyl), 7.98-8.02 (m, 2H, H_2, H_6-phenyl); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 29.52 ($2CH_2$), 34.57 (CH), 52.63 ($2CH_2$), 62.35 (CH_2), 115.90 (2CH), 123.20 (2CH), 129.53 (C), 130.43 (2CH), 133.97 (2CH), 160.81 (C), 163.27 (C), 165.77 (C), 167.41 (C), 182.13 (C); Anal. calcd for $C_{20}H_{19}F_2N_3O$: C, 67.59; H, 5.39; N, 11.82, found: C, 67.82; H, 5.36; N, 11.76.

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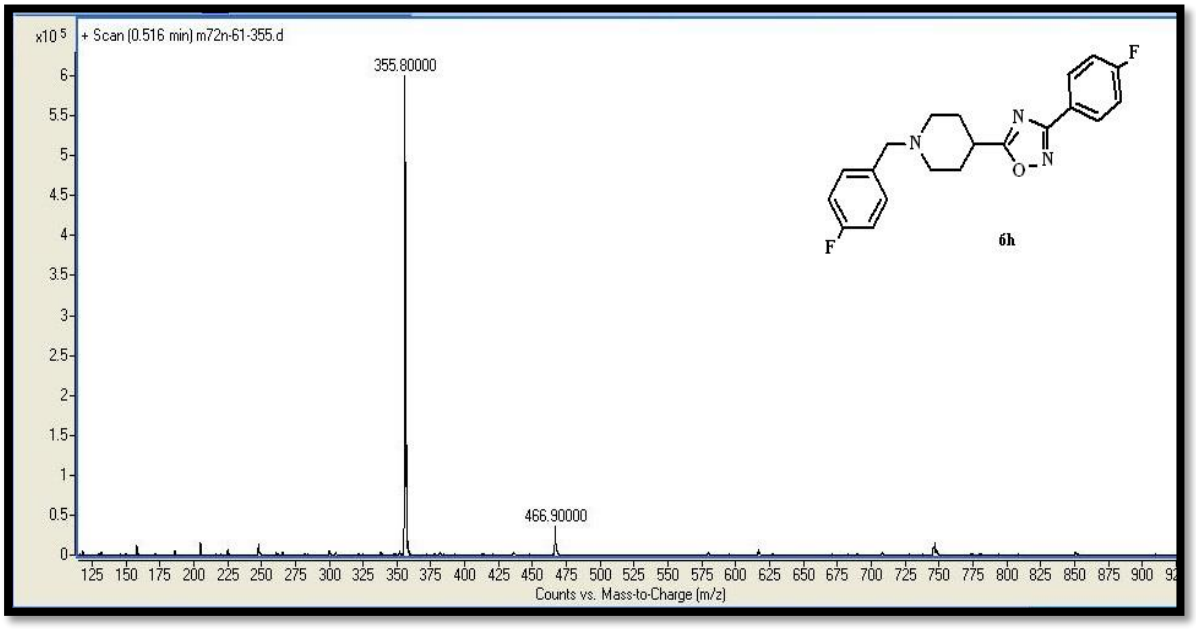

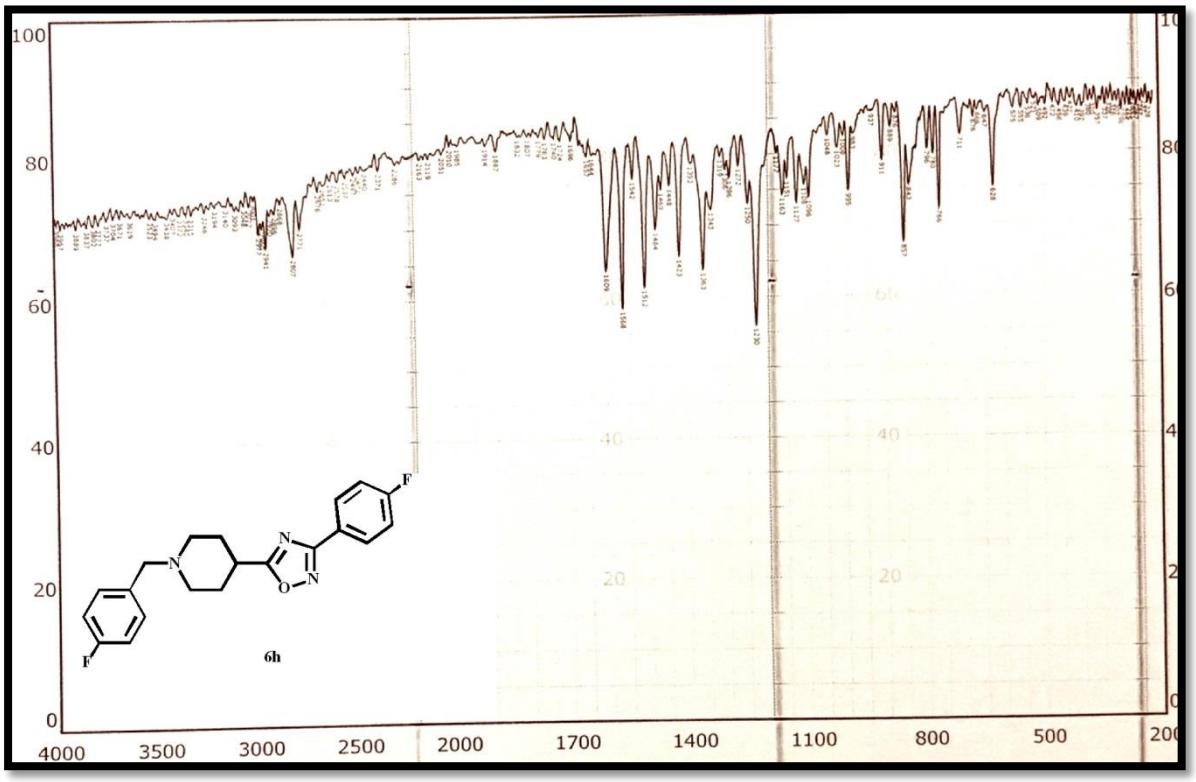

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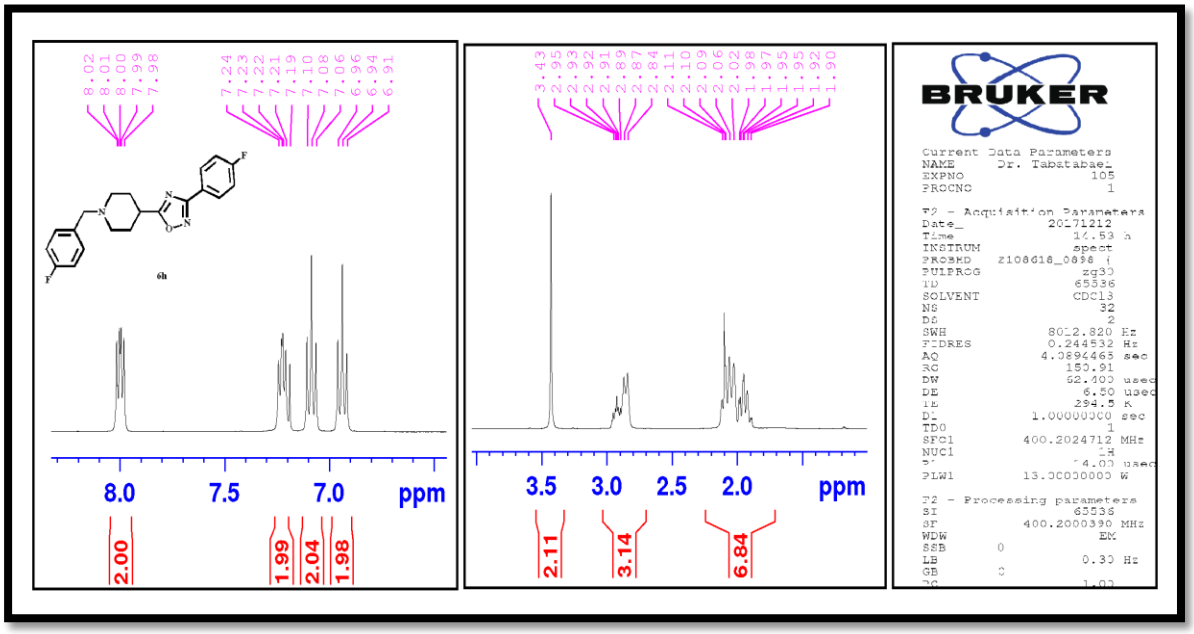

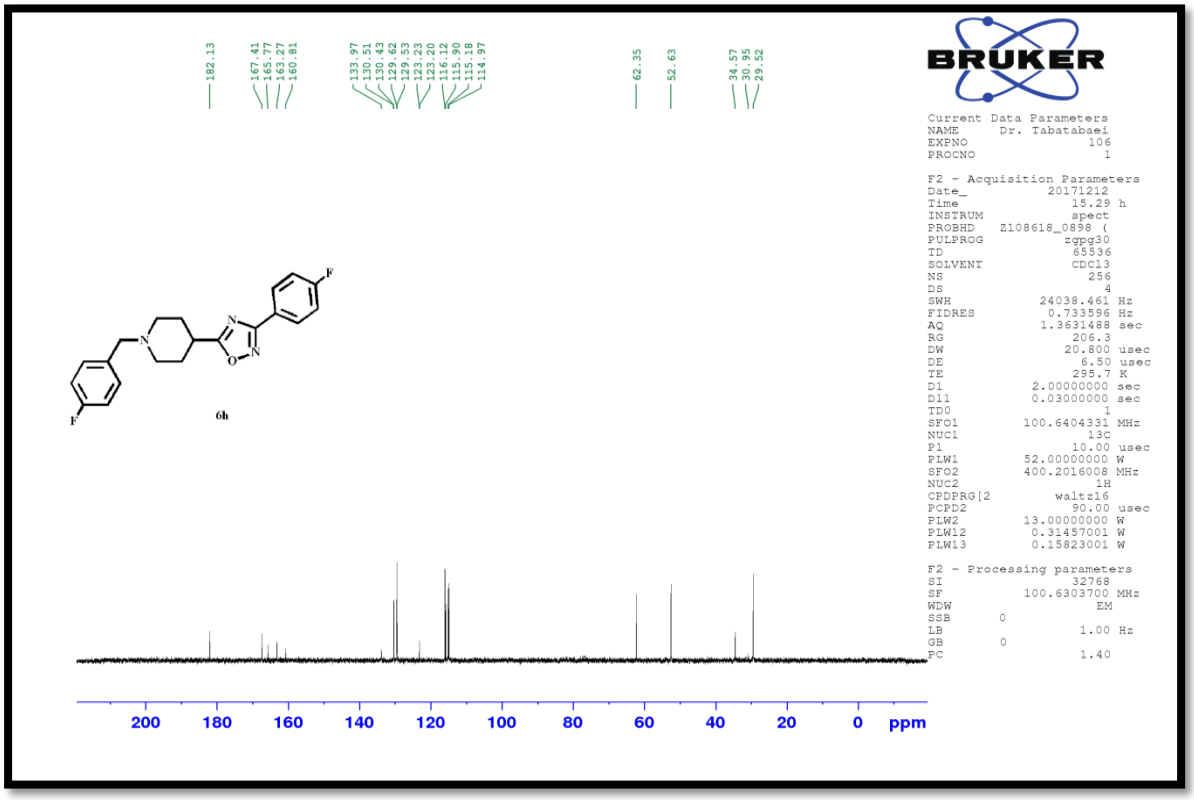

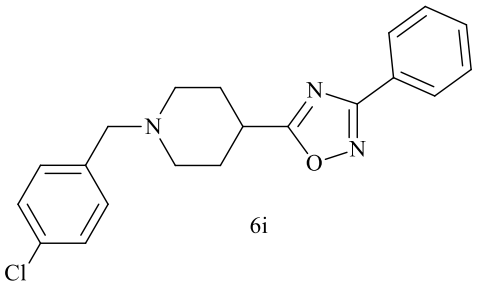

6i

5-(1-(4-chlorobenzyl)piperidin-4-yl)-3-phenyl-1,2,4-oxadiazole (6i)

Light yellow powder; yield: 39.4 %; mp: 95.6-96.7 °C; IR (KBr, cm^{-1}): 1586 (C=N), 1110 (C-O); LC-MS $[M + 1]^+$: m/z 353.8; ^1H NMR ($CDCl_3$, 400 MHz) δ: 1.96-2.18 (m, 6H, H-piperidine), 2.89-3.02 (m, 3H, H-piperidine), 3.48 (s, 2H, CH_2-benzyl), 7.25-7.30 (m, 4H, H_2, H_3, H_5, H_6-benzyl), 7.46-7.48 (m, 3H, H_3, H_4, H_5-phenyl), 8.06-8.08 (m, 2H, H_2, H_6-phenyl); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 29.50 ($2CH_2$), 34.51 (CH), 52.65 ($2CH_2$), 62.33 (CH_2), 126.93 (C), 127.33 (2CH), 127.42 (2CH), 128.37 (2CH), 130.22 (2CH), 131.05 (CH), 132.70 (C), 136.89 (C), 168.16 (C), 181.94 (C); Anal. calcd for $C_{20}H_{20}ClN_3O$: C, 67.89; H, 5.70; N, 11.88, found: C, 68.12; H, 5.68; N, 11.93.

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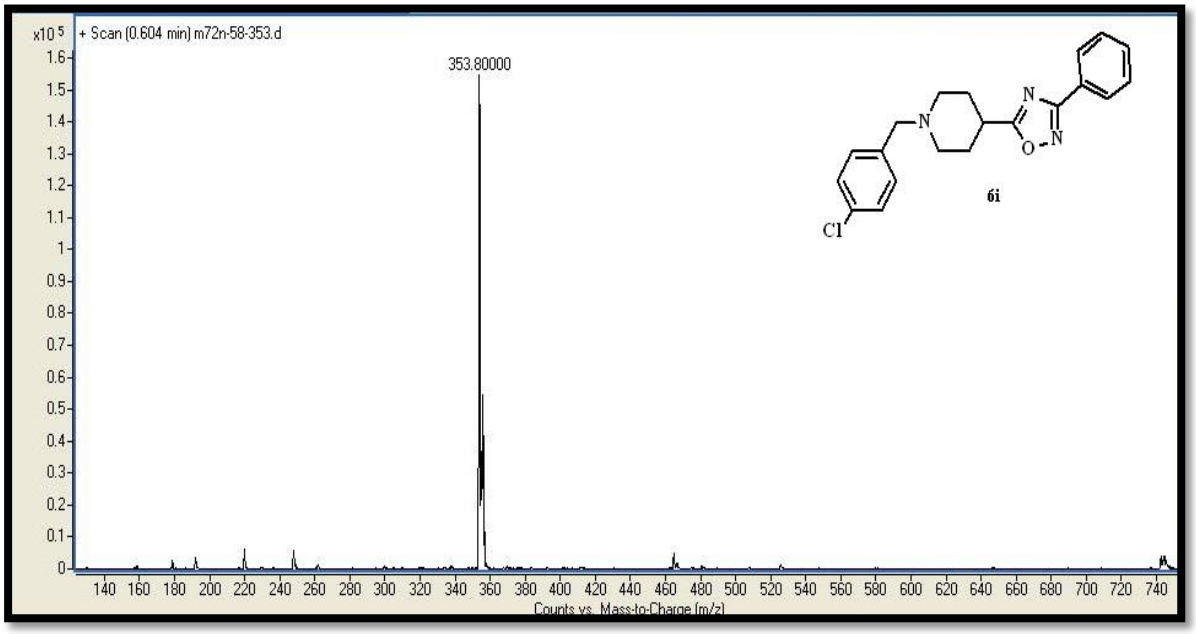

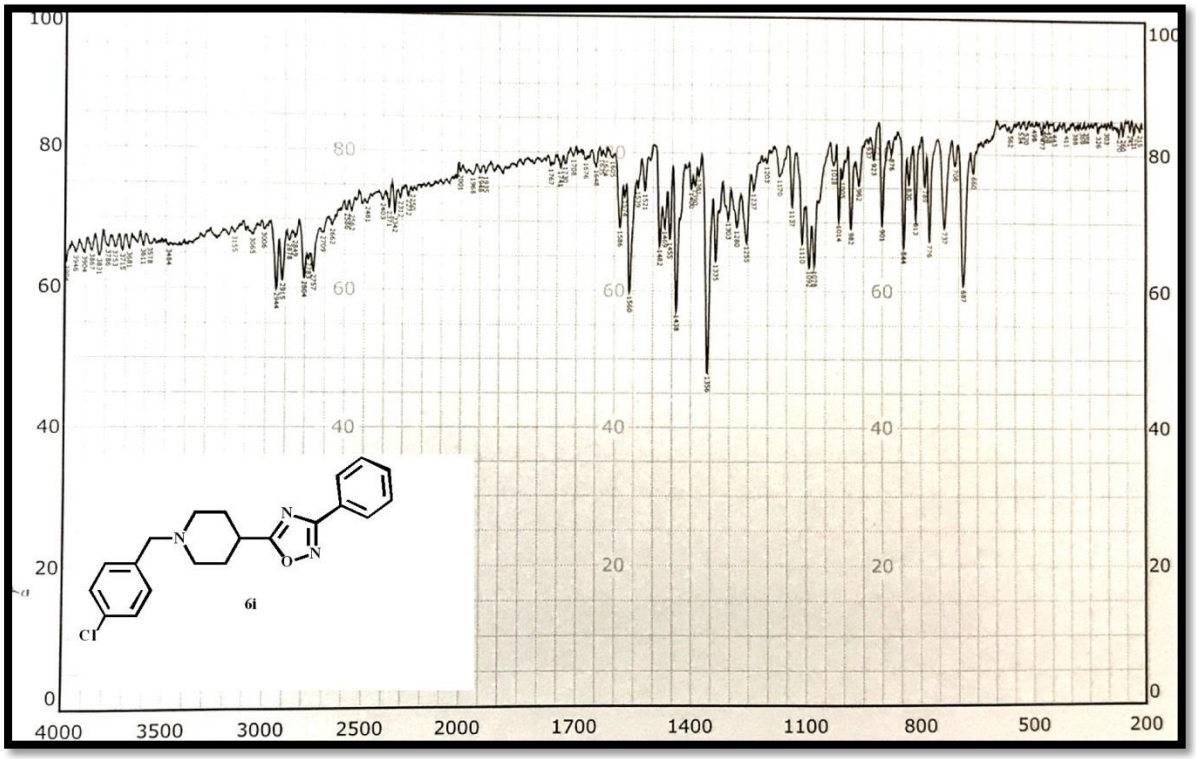

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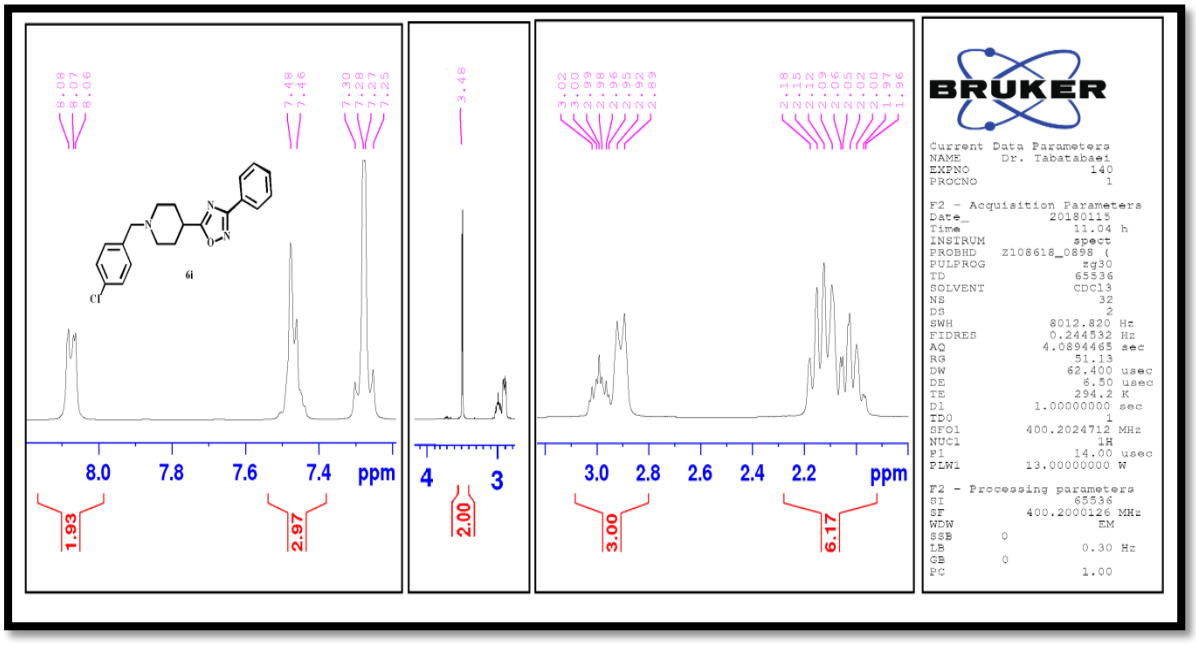

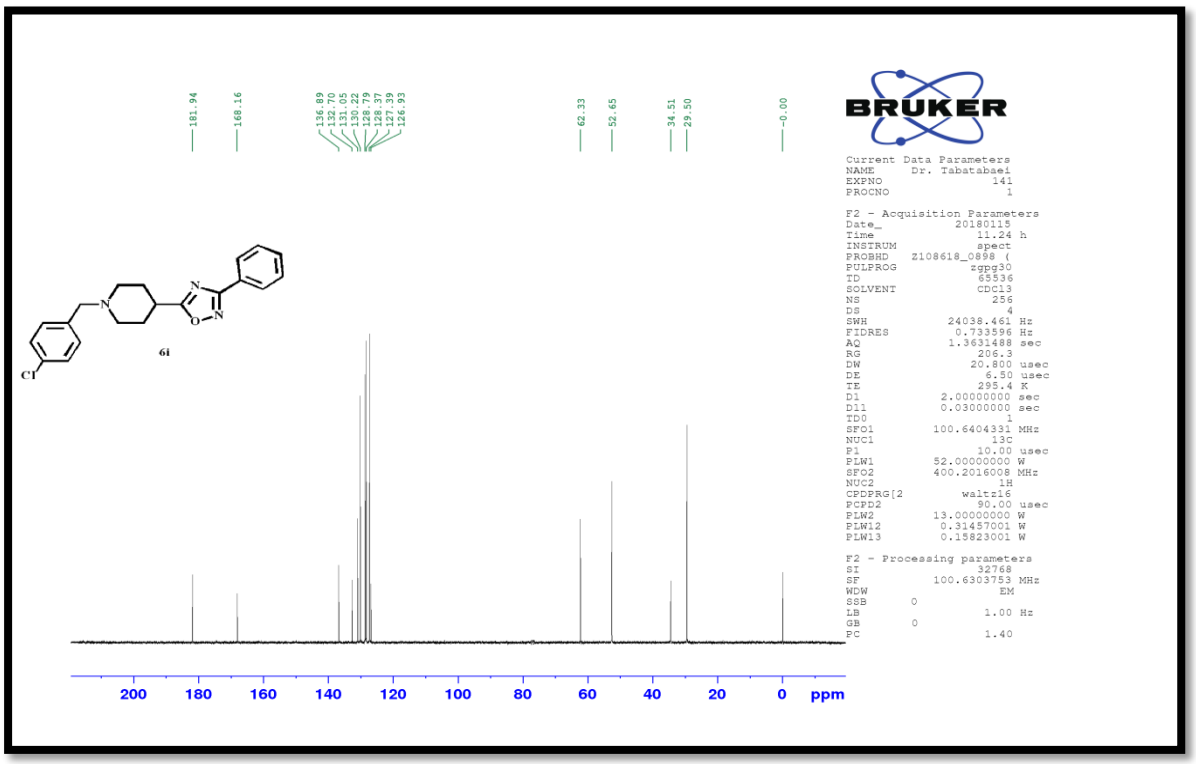

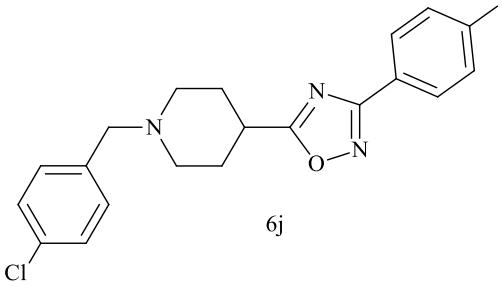

6j

5-(1-(4-chlorobenzyl)piperidin-4-yl)-3-(p-tolyl)-1,2,4-oxadiazole (6j)

Light yellow powder; yield: 40.3 %; mp: 103.5-104.7 °C; IR (KBr, cm^{-1}): 1582 (C=N), 1213 (C-O), 1358,1486 (CH_3); LC-MS $[M + 1]^+$: m/z 367.8; ^1H NMR ($CDCl_3$, 400 MHz) δ: 1.89-2.11 (m, 6H, H-piperidine), 2.33 (s, 3H, CH_3), 2.82-2.94 (m, 3H, H-piperidine), 3.42 (s, 2H, CH_2-benzyl), 7.18-7.23 (m, 6H, H_2, H_3, H_5, H_6-benzyl, H_3, H_5-phenyl), 7.87 (d, 2H, *J* = 8 Hz, H_2, H_6-phenyl); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 21.59 (CH_3), 29.52 ($2CH_2$), 34.55 (CH), 52.70 ($2CH_2$), 62.37 (CH_2), 124.13 (C), 127.35 (2CH), 128.43 (2CH), 129.54 (2CH), 130.28 (2CH), 132.78 (C), 136.89 (C), 141.39 (C), 168.22 (C), 181.78 (C); Anal. calcd for $C_{21}H_{22}ClN_3O$: C, 68.56; H, 6.03; N, 11.42, found: C, 68.79; H, 6.01; N, 11.37.

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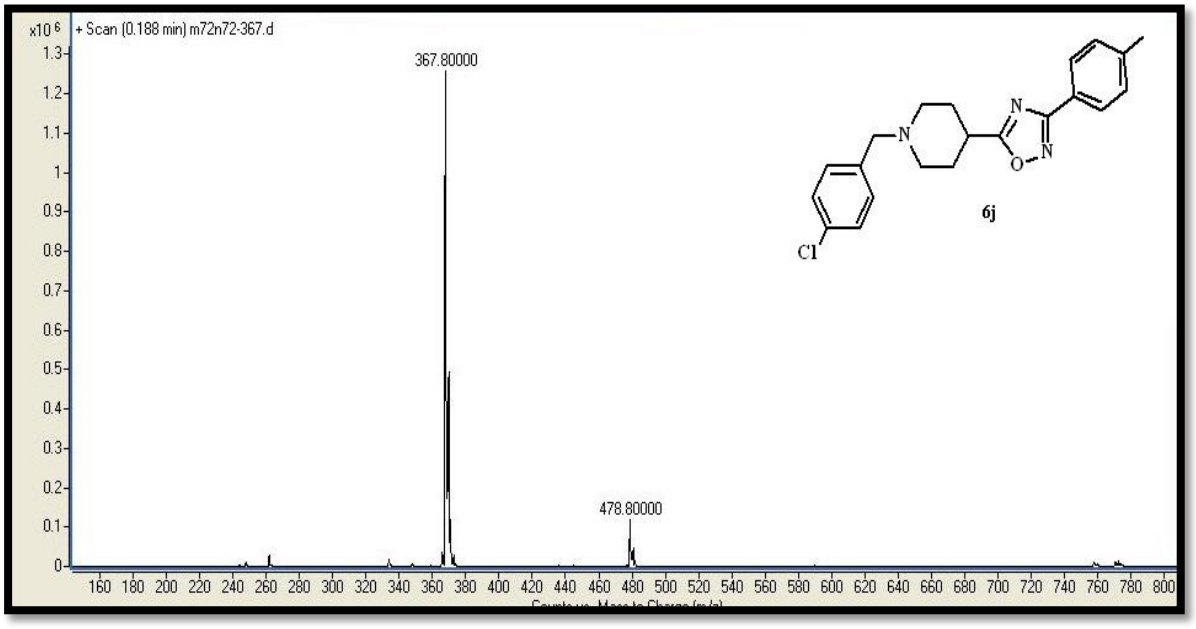

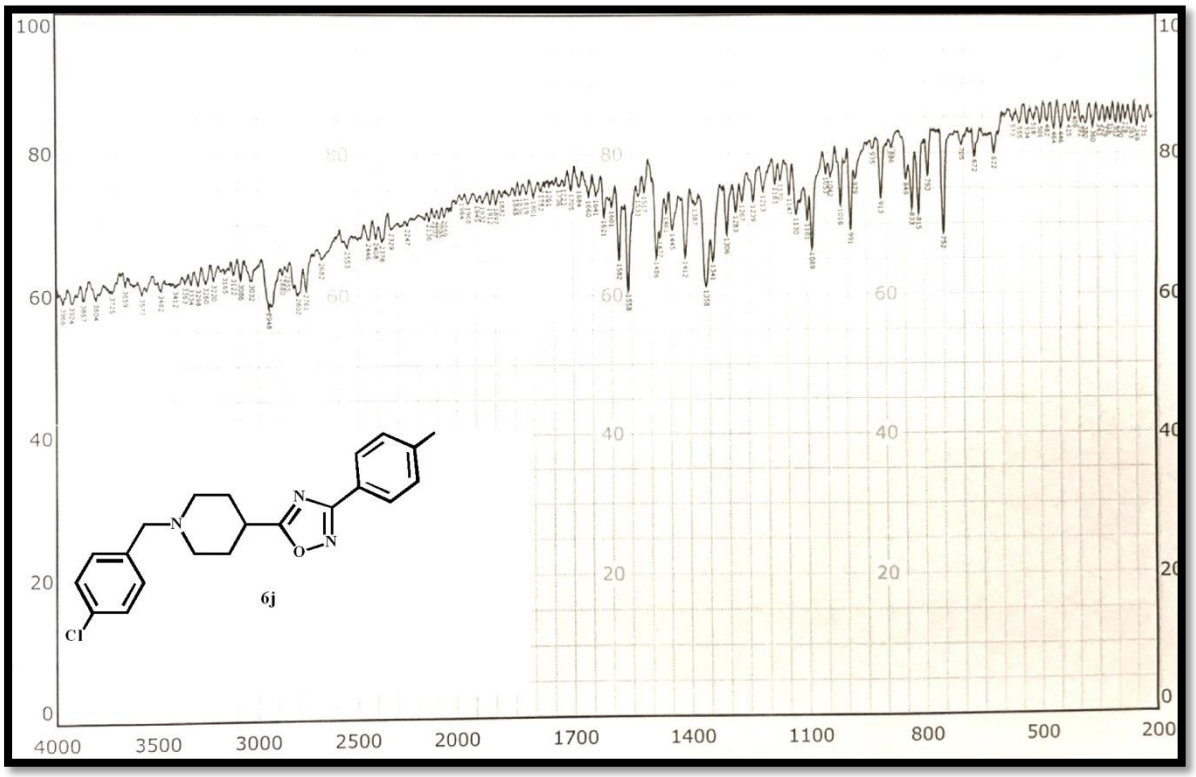

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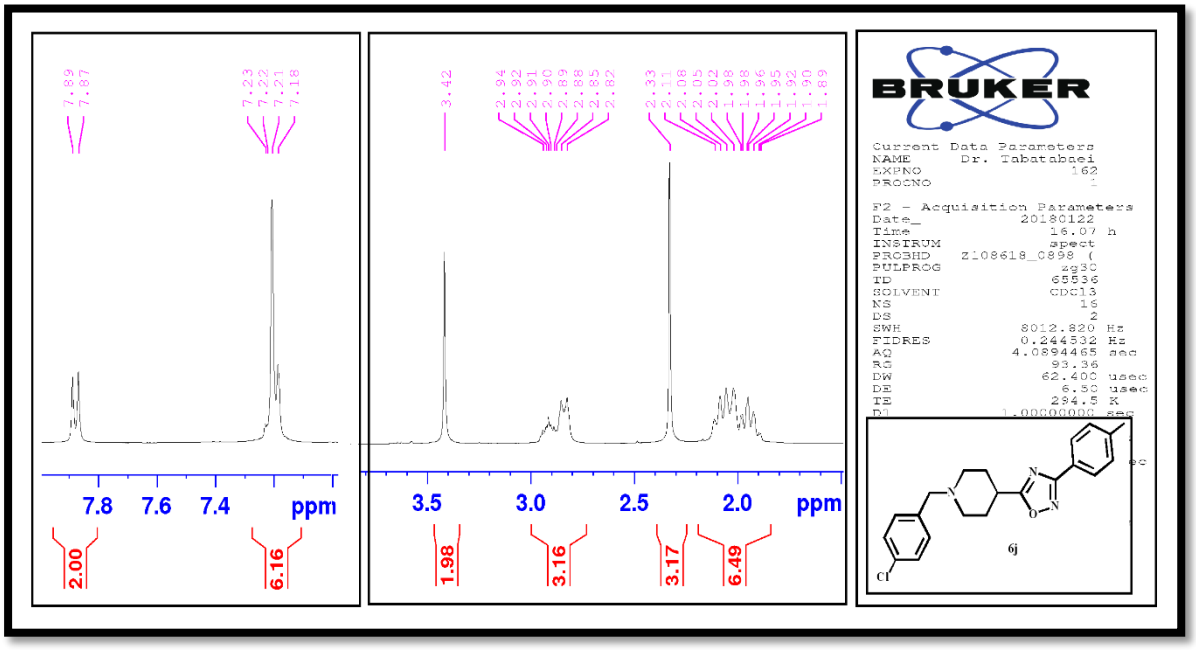

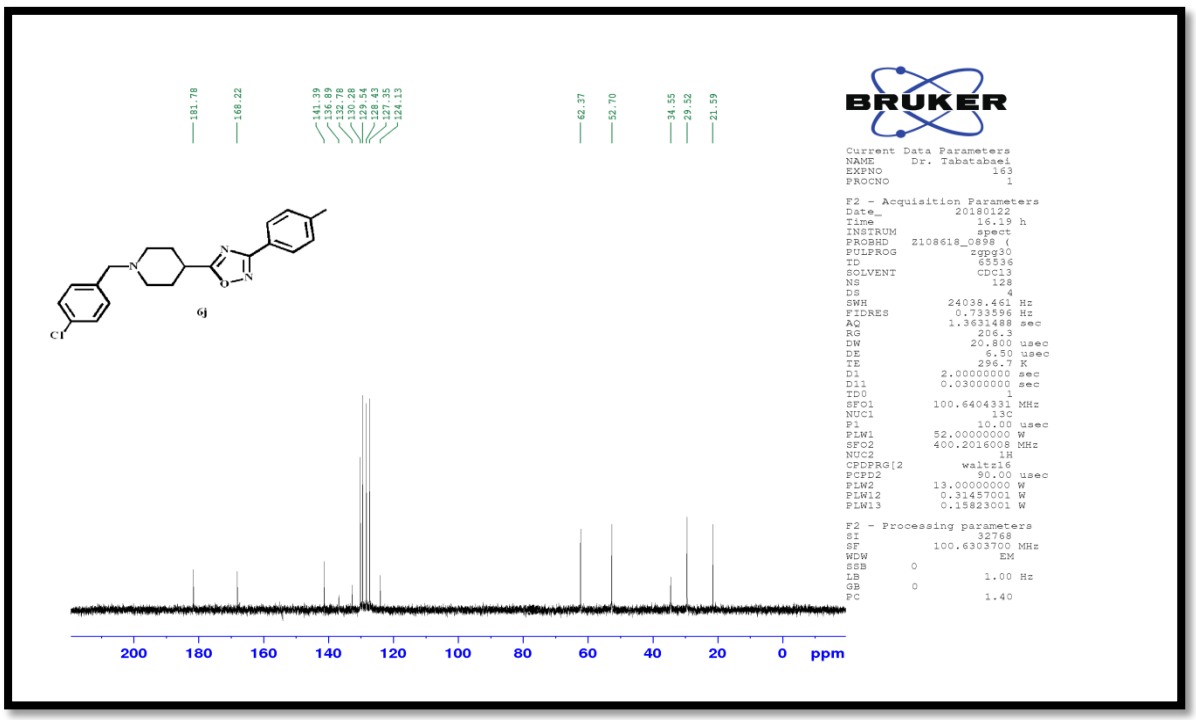

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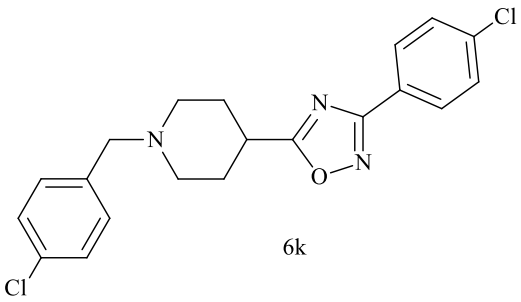

6k

5-(1-(4-chlorobenzyl)piperidin-4-yl)-3-(4-chlorophenyl)-1,2,4-oxadiazole (6k)

Light yellow powder; yield: 51.7 %; mp: 110.7-113.7 °C; IR (KBr, cm^{-1}): 1582 (C=N), 1213 (C-O); LC-MS $[M + 1]^+$: m/z 387.8; ^1H NMR ($CDCl_3$, 400 MHz) δ: 1.88-2.11 (m, 6H, H-piperidine), 2.82-2.95 (m, 3H, H-piperidine), 3.41 (s, 2H, CH_2-benzyl), 7.18-7.22 (m, 4H, H_2, H_3, H_5, H_6-benzyl), 7.35 (d, 2H, J = 8 Hz, H_3, H_5-phenyl), 7.92 (d, 2H, J = 8 Hz, H_2, H_6-phenyl); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 29.47 ($2CH_2$), 34.50 (CH), 52.63 ($2CH_2$), 62.36 (CH_2), 125.45 (C), 128.75 (2CH), 129.16 (2CH), 129.46 (2CH), 130.32 (2CH), 132.82 (C), 136.73 (C), 137.23 (C), 167.41 (C), 182.19 (C); Anal. calcd for $C_{20}H_{19}Cl_2N_3O$: C, 61.86; H, 4.93; N, 10.82, found: C, 62.09; H, 4.91; N, 10.78.

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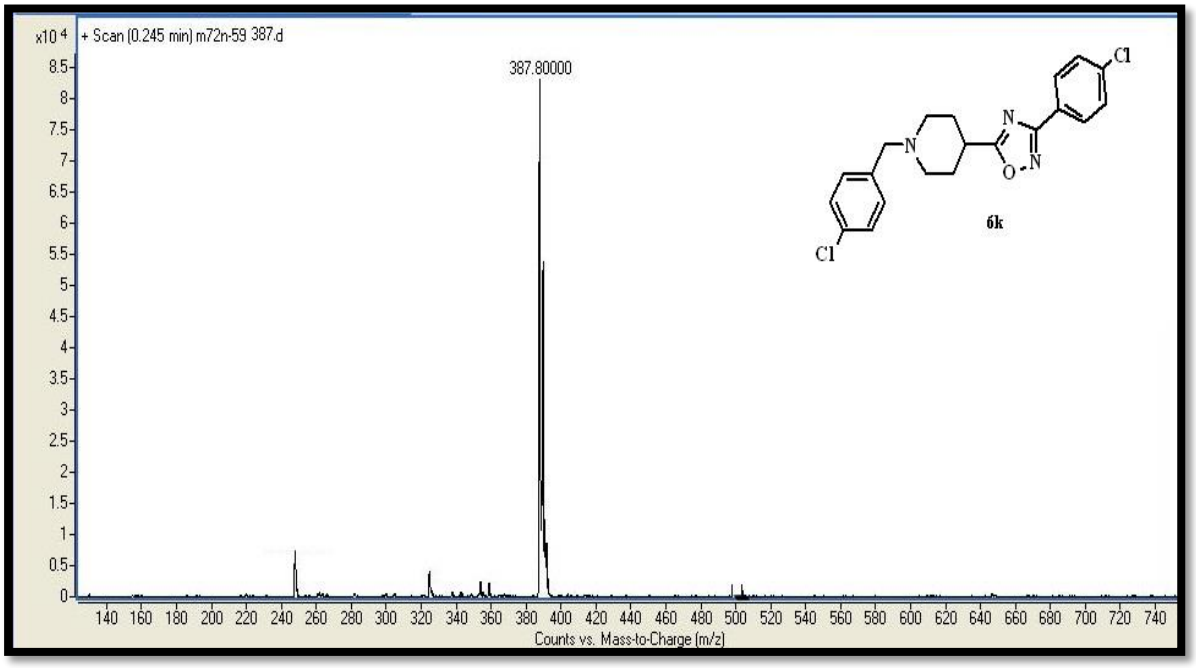

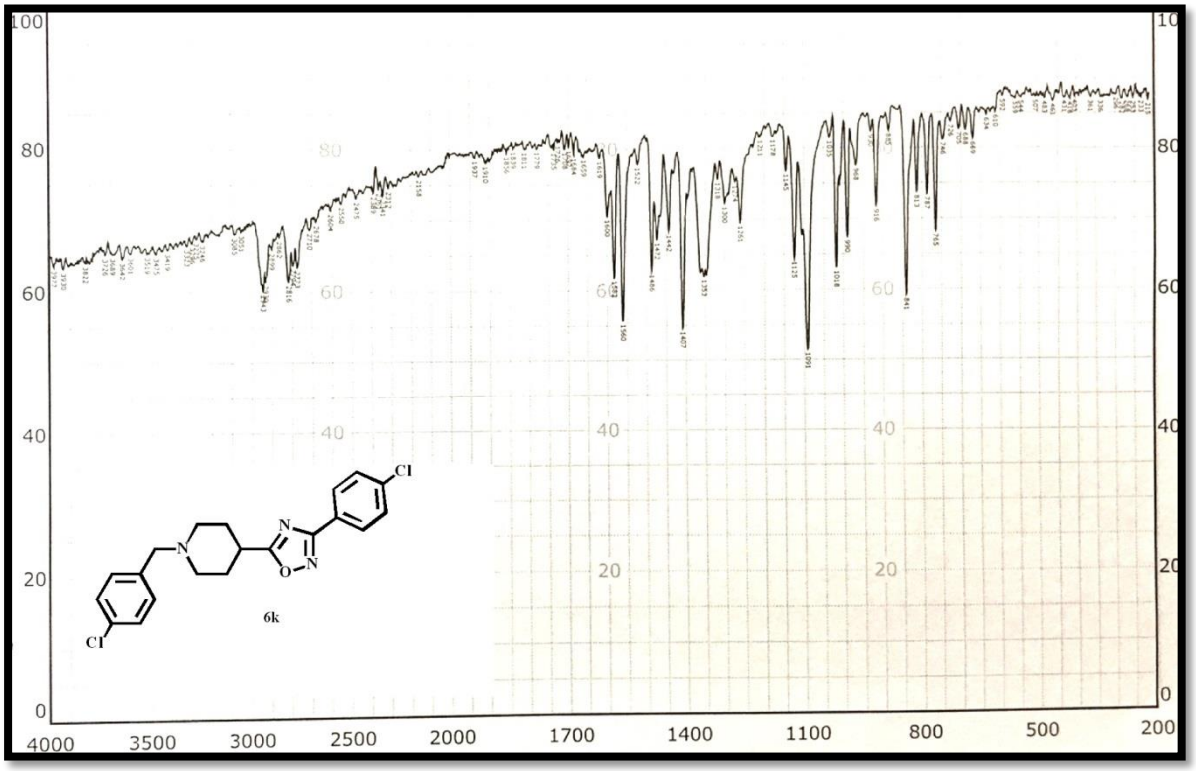

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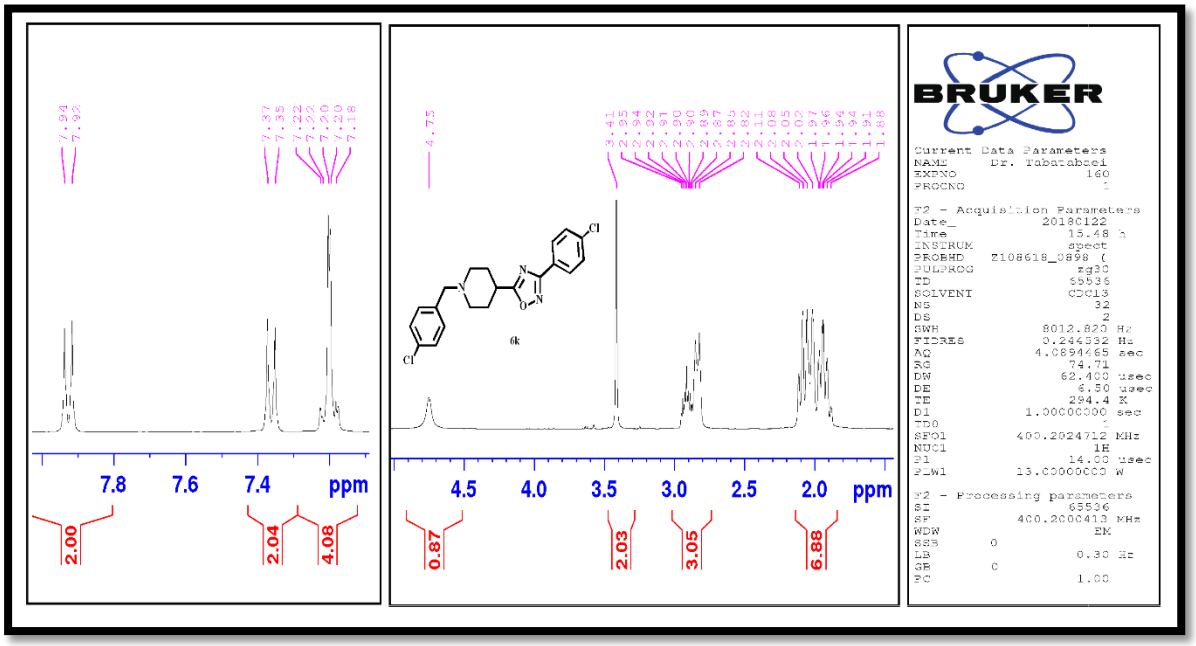

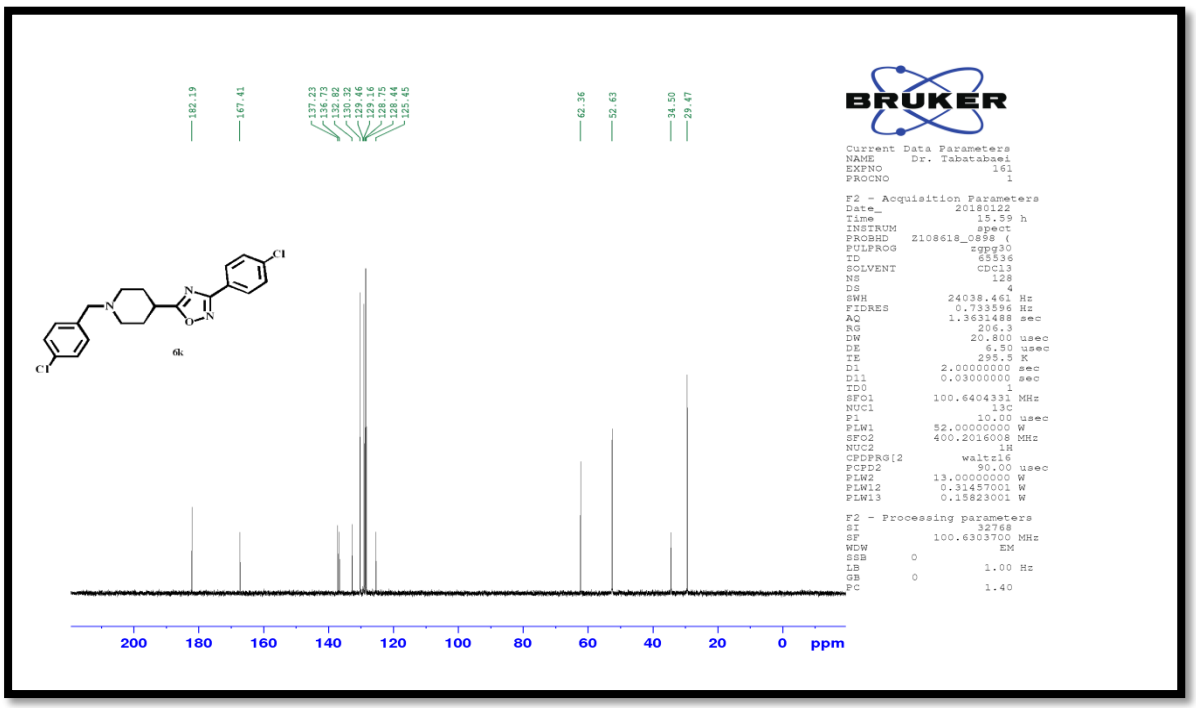

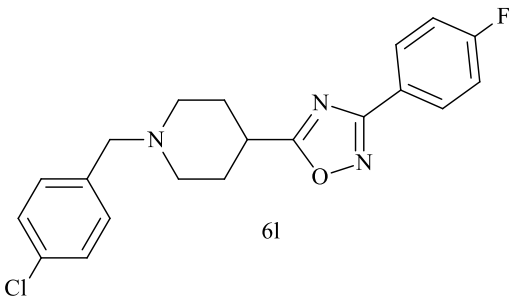

6l

5-(1-(4-chlorobenzyl)piperidin-4-yl)-3-(4-fluorophenyl)-1,2,4-oxadiazole (6l)

Light yellow powder; yield: 40.7 %; mp: 89.9-90.4 °C; IR (KBr, cm^{-1}): 1600 (C=N), 1221 (C-O); LC-MS $[M + 1]^+$: m/z 371.8; ^1H NMR ($CDCl_3$, 400 MHz) δ: 1.99-2.19 (m, 6H, H-piperidine), 2.90-3.02 (m, 3H, H-piperidine), 3.49 (s, 2H, CH_2-benzyl), 7.13-7.18 (m, 2H, H_3, H_5-phenyl), 7.26-7.29 (m, 4H, H_2, H_3, H_5, H_6-benzyl), 8.05-8.09 (m, 2H, H_2, H_6-phenyl); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 29.51 ($2CH_2$), 34.51 (CH), 52.66 ($2CH_2$), 62.35 (CH_2), 115.88 (2CH), 123.16 (C), 129.51 (2CH), 130.23 (2CH), 132.74 (2CH), 136.86 (C), 163.24 (C), 165.73 (C), 167.37 (C), 182.09 (C); Anal. calcd for $C_{20}H_{19}ClFN_3O$: C, 64.60; H, 5.15; N, 11.30, found: C, 64.81; H, 5.12; N, 11.37.

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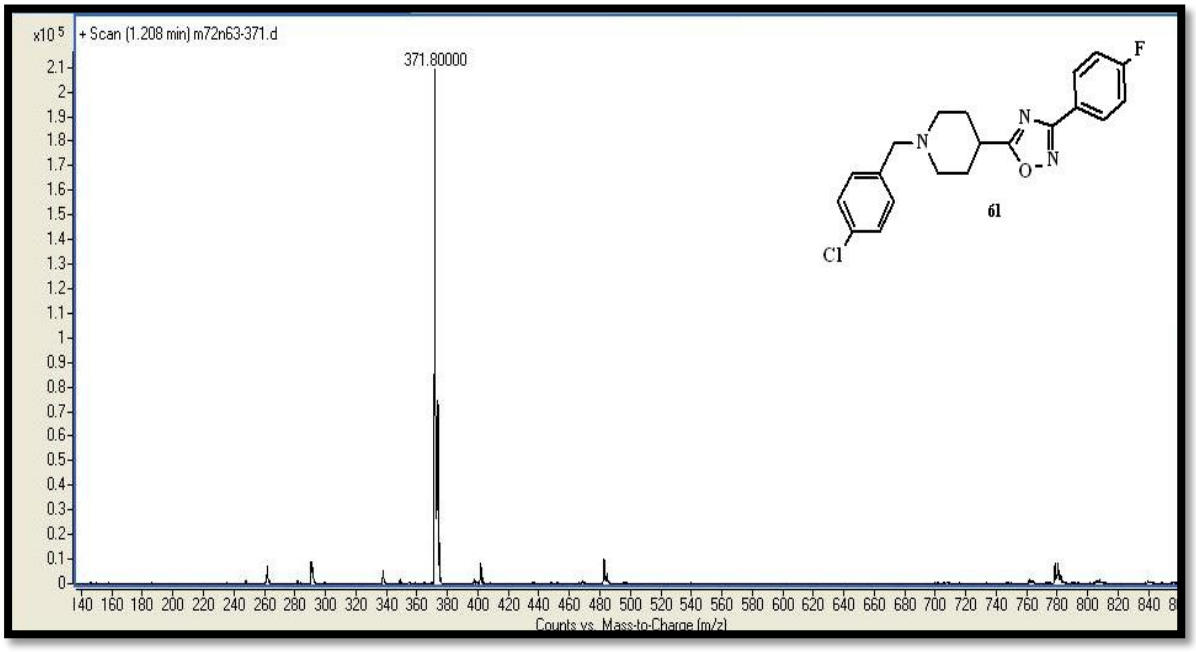

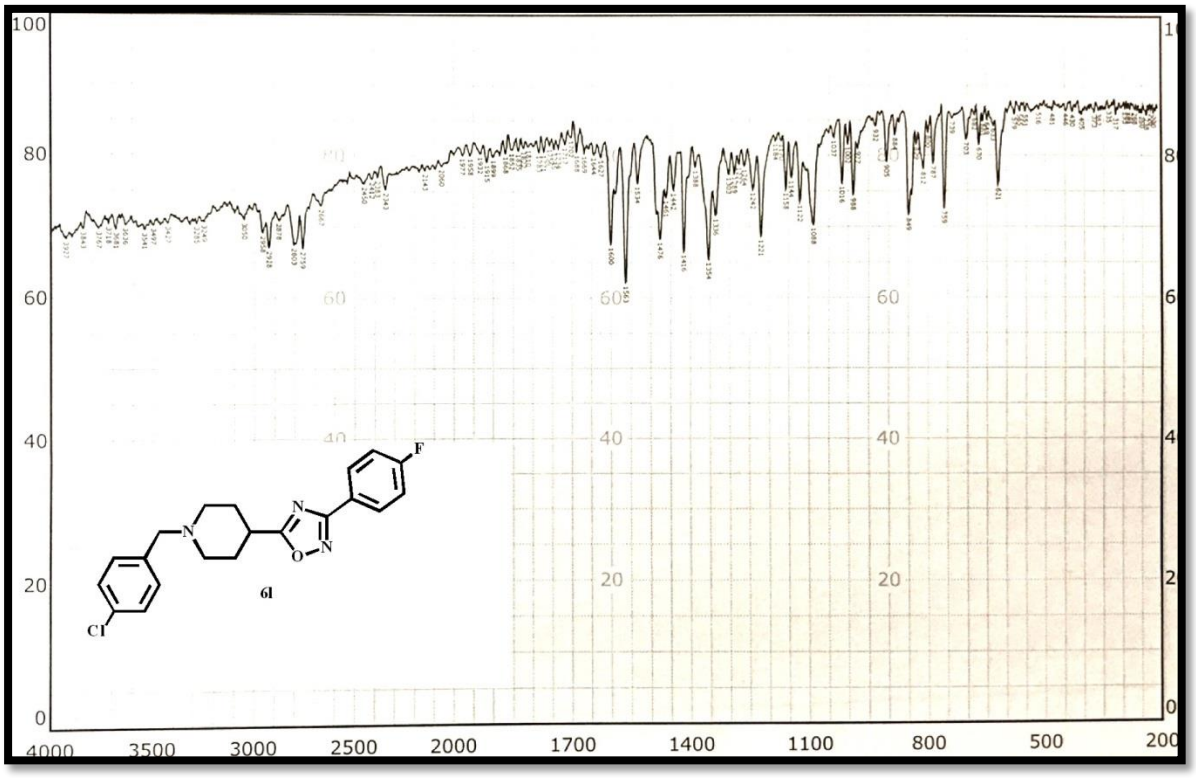

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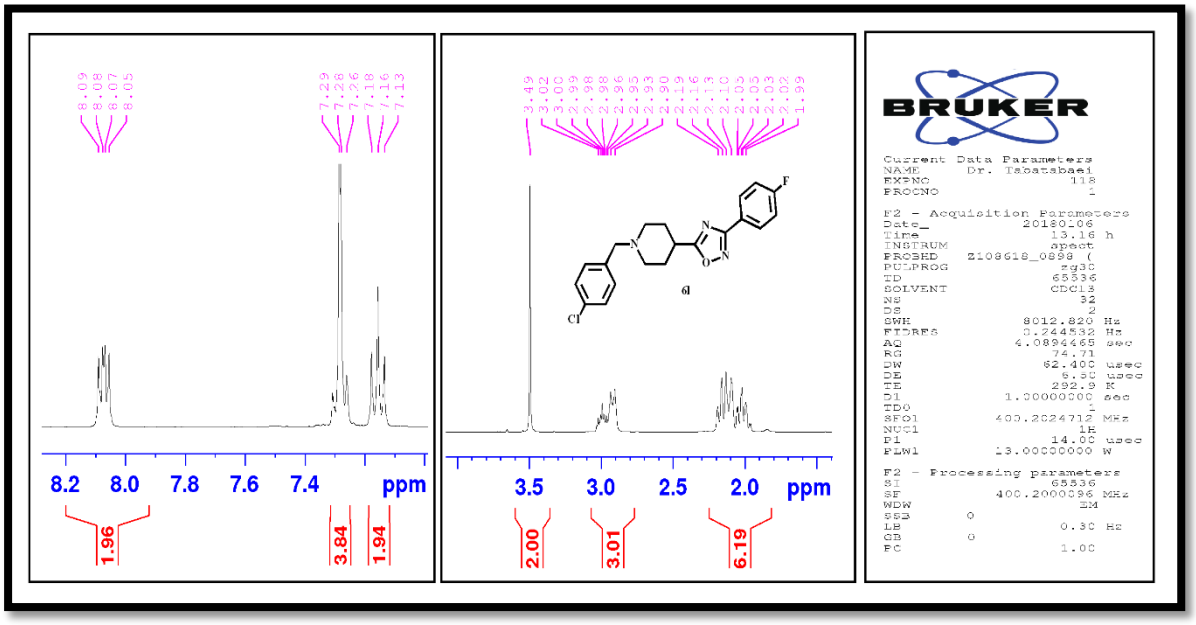

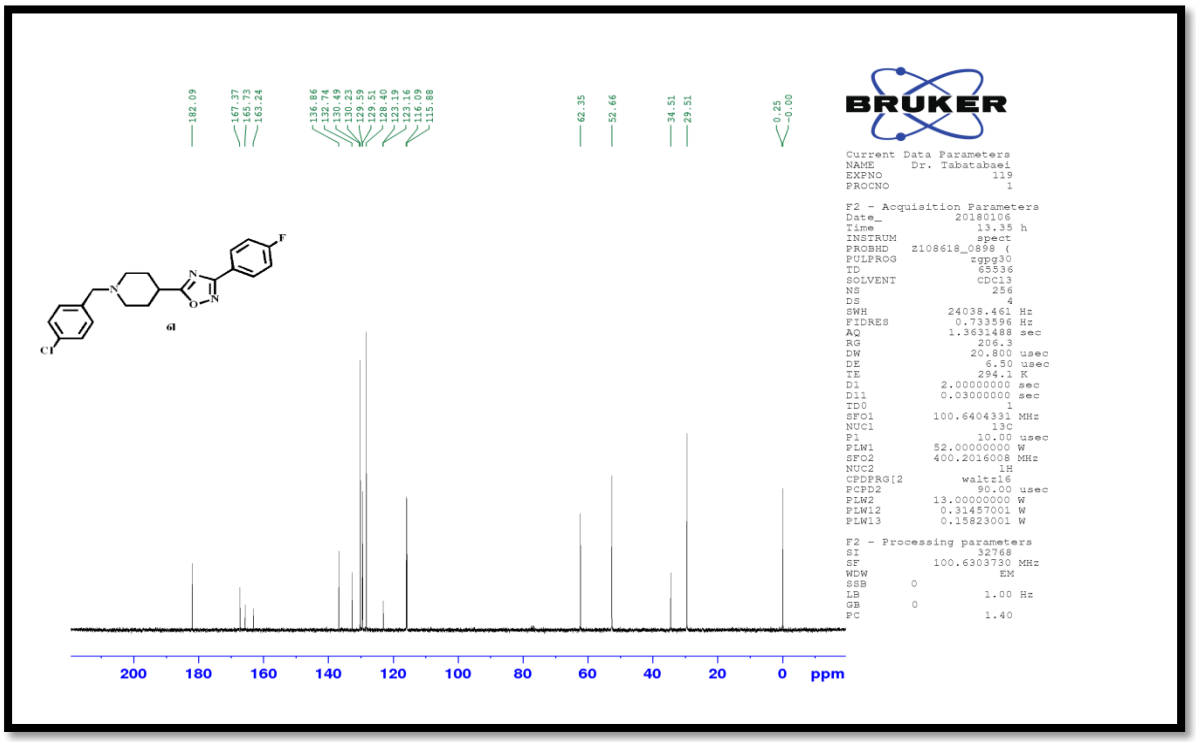

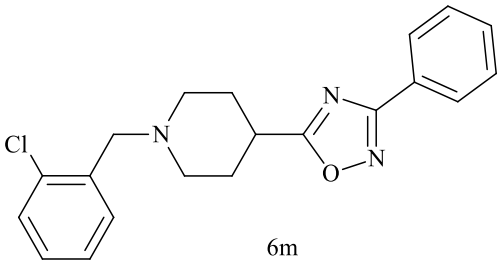

6m

5-(1-(2-chlorobenzyl)piperidin-4-yl)-3-phenyl-1,2,4-oxadiazole (6m)

Light yellow powder; yield: 28.6 %; mp: 61.5-62.2 °C; IR (KBr, cm^{-1}): 1583 (C=N), 1134 (C-O); LC-MS $[M + 1]^+$: m/z 354; ^1H NMR ($CDCl_3$, 400 MHz) δ: 2.01-2.18 (m, 6H, H-piperidine), 2.93-3.02 (m, 3H, H-piperidine), 3.50 (s, 2H, CH_2-benzyl), 7.13-7.15 (m, 3H, H_4, H_5, H_6-benzyl), 7.21-7.25 (m, 3H, H_3, H_4, H_5-phenyl), 7.44-7.49 (m, 1H, H_3-benzyl), 8.06 (d, 2H, J = 8 Hz, H_2, H_6-phenyl); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 29.56 ($2CH_2$), 34.67 (CH), 52.69 ($2CH_2$), 62.92 (CH_2), 126.89 (C), 127.00 (CH), 127.42 (2CH), 128.79 (2CH), 128.93 (2CH), 129.04 (CH), 131.04 (CH), 135.14 (C), 136.66 (C), 168.18 (C), 182.09 (C); Anal. calcd for $C_{20}H_{20}ClN_3O$: C, 67.89; H, 5.70; N, 11.88, found: C, 68.13; H, 5.67; N, 11.80.

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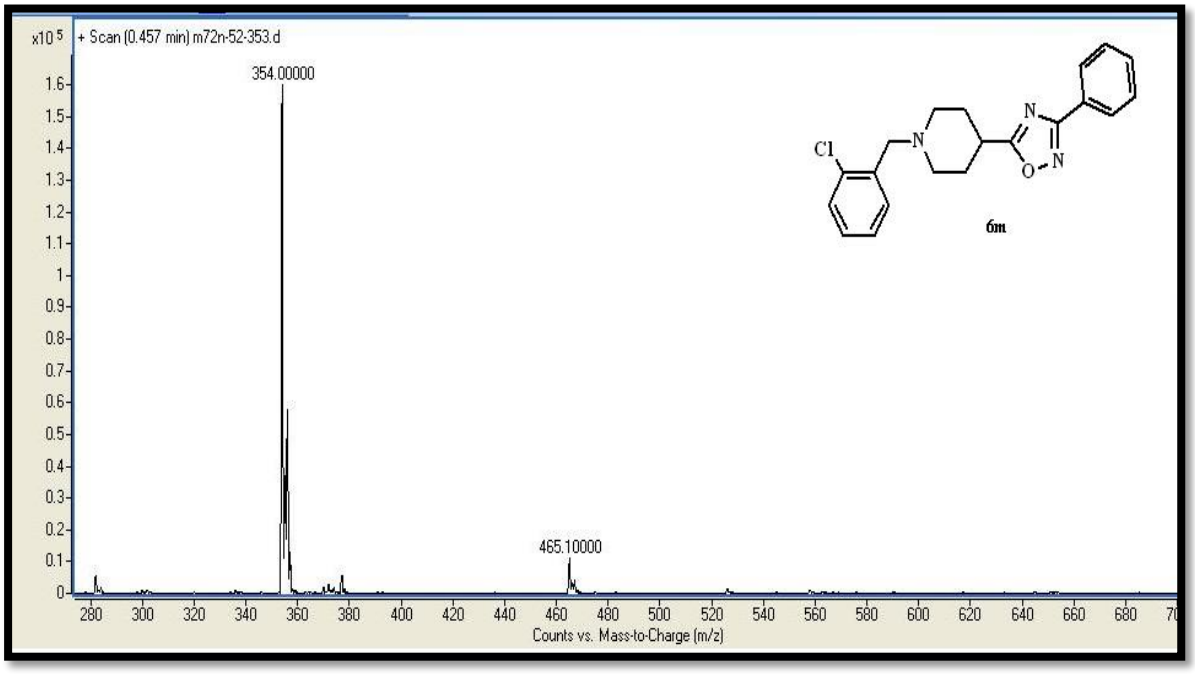

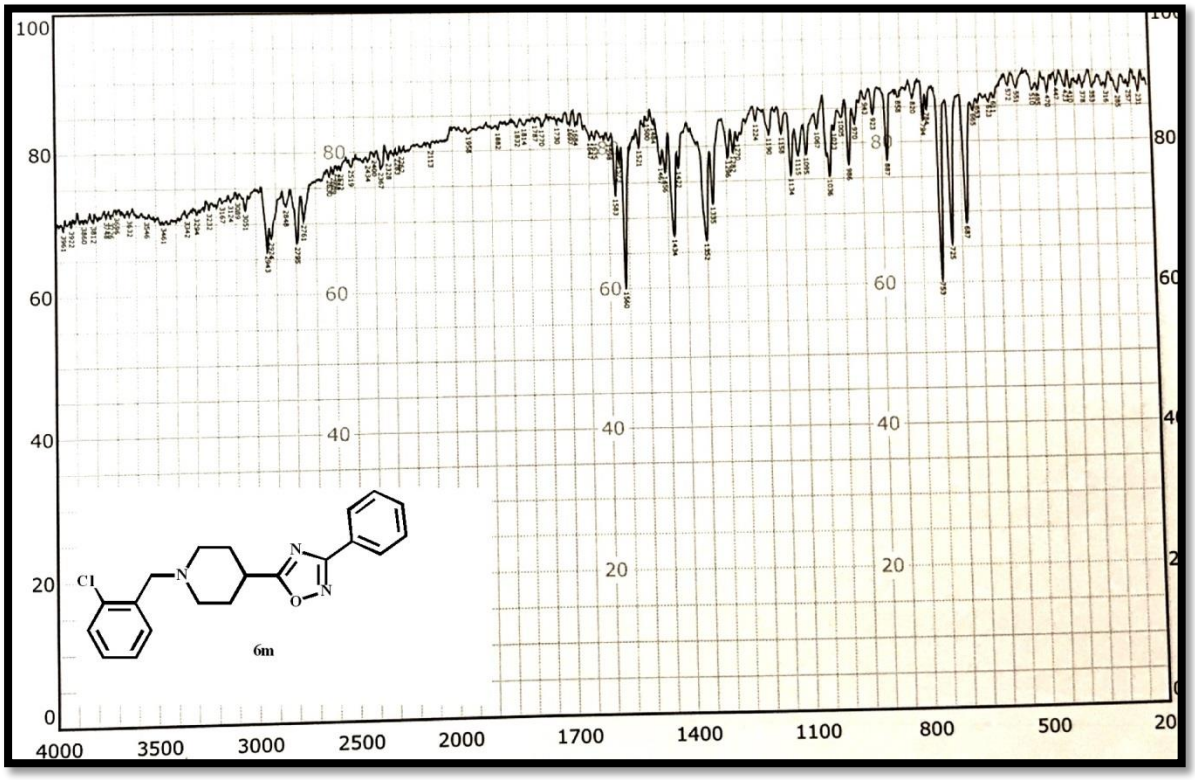

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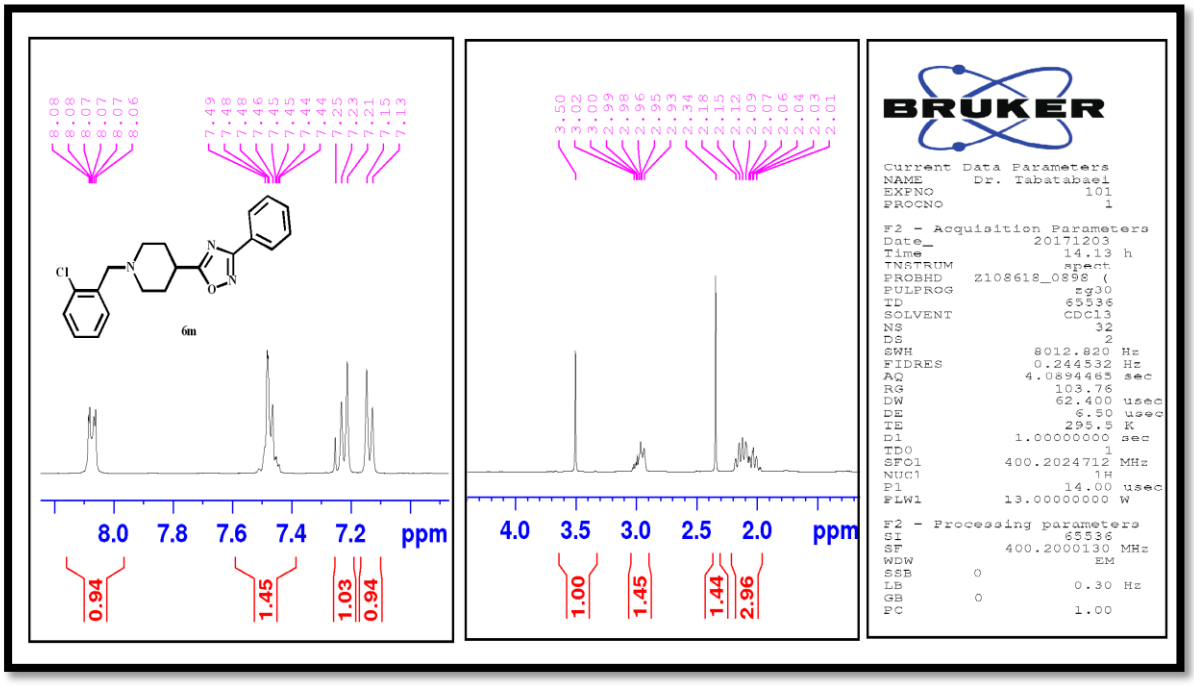

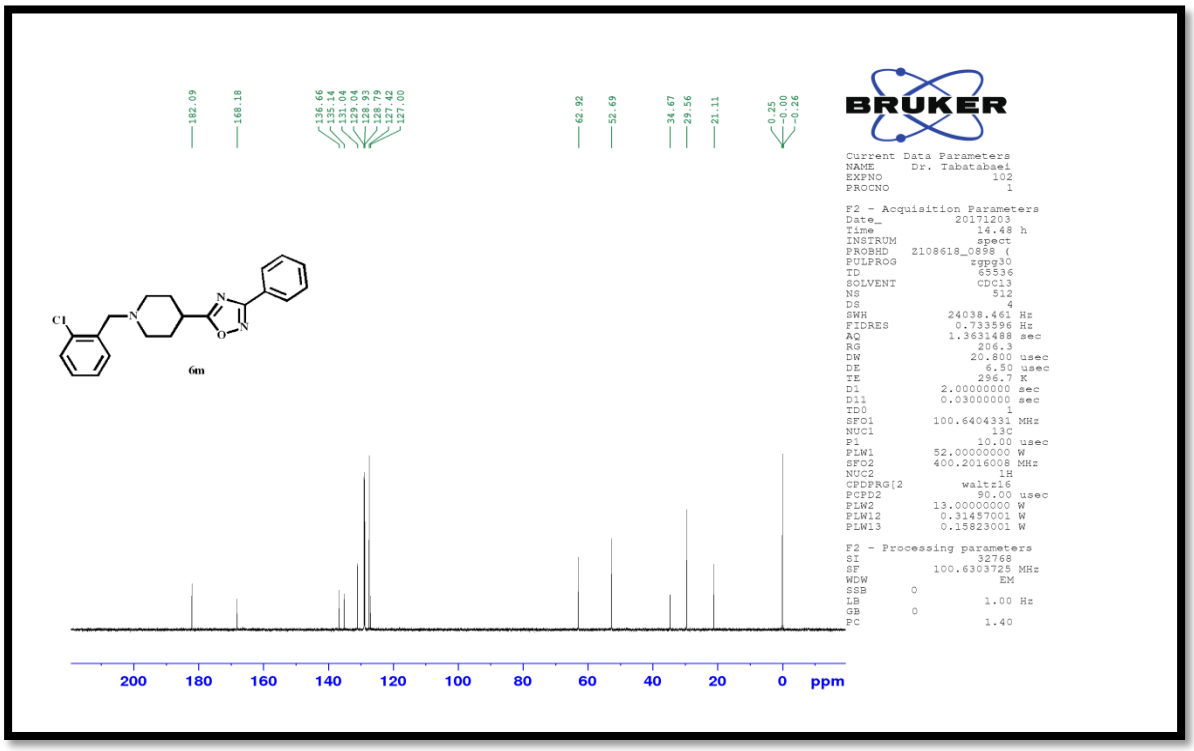

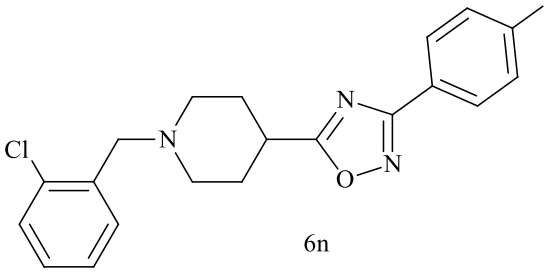

6n

5-(1-(2-chlorobenzyl)piperidin-4-yl)-3-(p-tolyl)-1,2,4-oxadiazole (6n)

White powder; yield: 33.8 %; mp: 121.8-124.7 °C; IR (KBr, cm^{-1}): 1582 (C=N), 1146 (C-O), 1442,1350 (CH_3); LC-MS $[M + 1]^+$: m/z 367.9; ^1H NMR ($CDCl_3$, 400 MHz) δ: 2.09-2.14 (m, 4H, H-piperidine), 2.24-2.31 (m, 2H, H-piperidine), 2.40 (s, 3H, CH_3), 2.97-3.04 (m, 3H, H-piperidine), 3.65 (s, 2H, CH_2-benzyl), 7.17-7.28 (m, 3H, H_4, H_5, H_6-benzyl), 7.34 (d, 2H, J = 8 Hz, H_3, H_5-phenyl), 7.50-7.51 (m, 1H, H_3-benzyl), 7.95 (d, 2H, J = 8 Hz, H_2, H_6-phenyl); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 21.56 (CH_3), 29.62 ($2CH_2$), 34.56 (CH), 52.85 ($2CH_2$), 59.34 (CH_2), 124.14 (C), 126.62 (2CH), 127.33 (CH), 128.07 (2CH), 129.51 (2CH), 130.48 (CH), 134.19 (C), 136.05 (C), 141.33 (C), 168.18 (C), 181.85 (C); Anal. calcd for $C_{21}H_{22}ClN_3O$: C, 68.56; H, 6.03; N, 11.42, found: C, 68.75; H, 5.99; N, 11.38.

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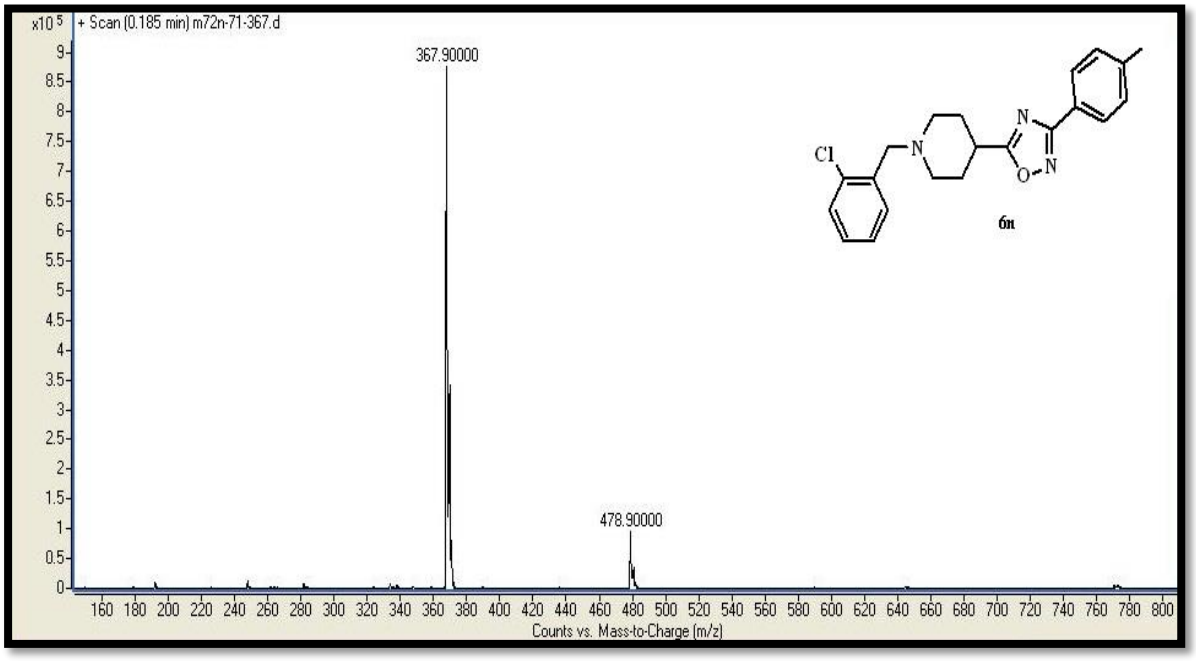

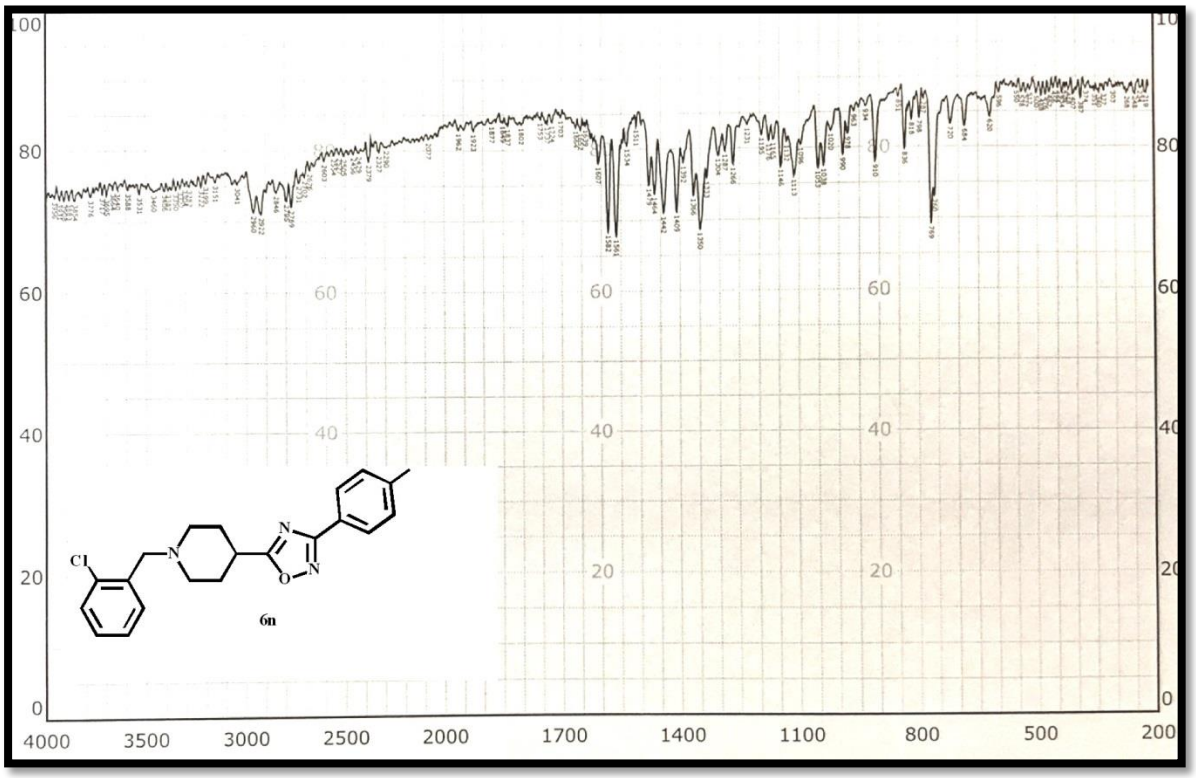

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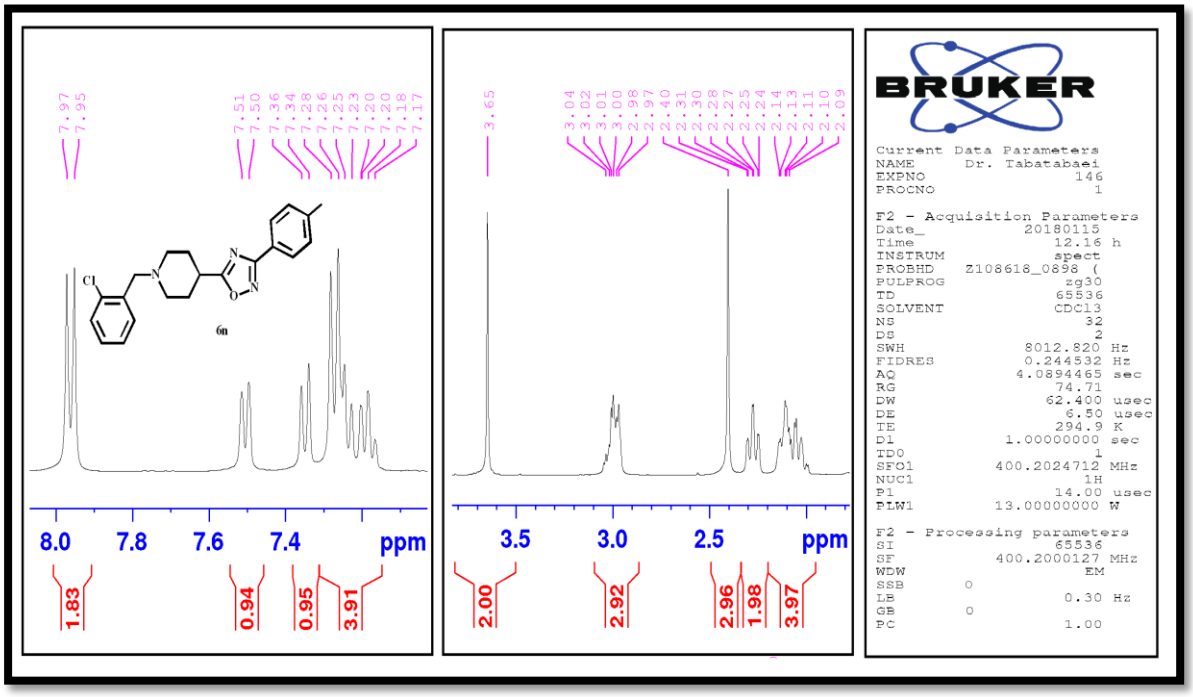

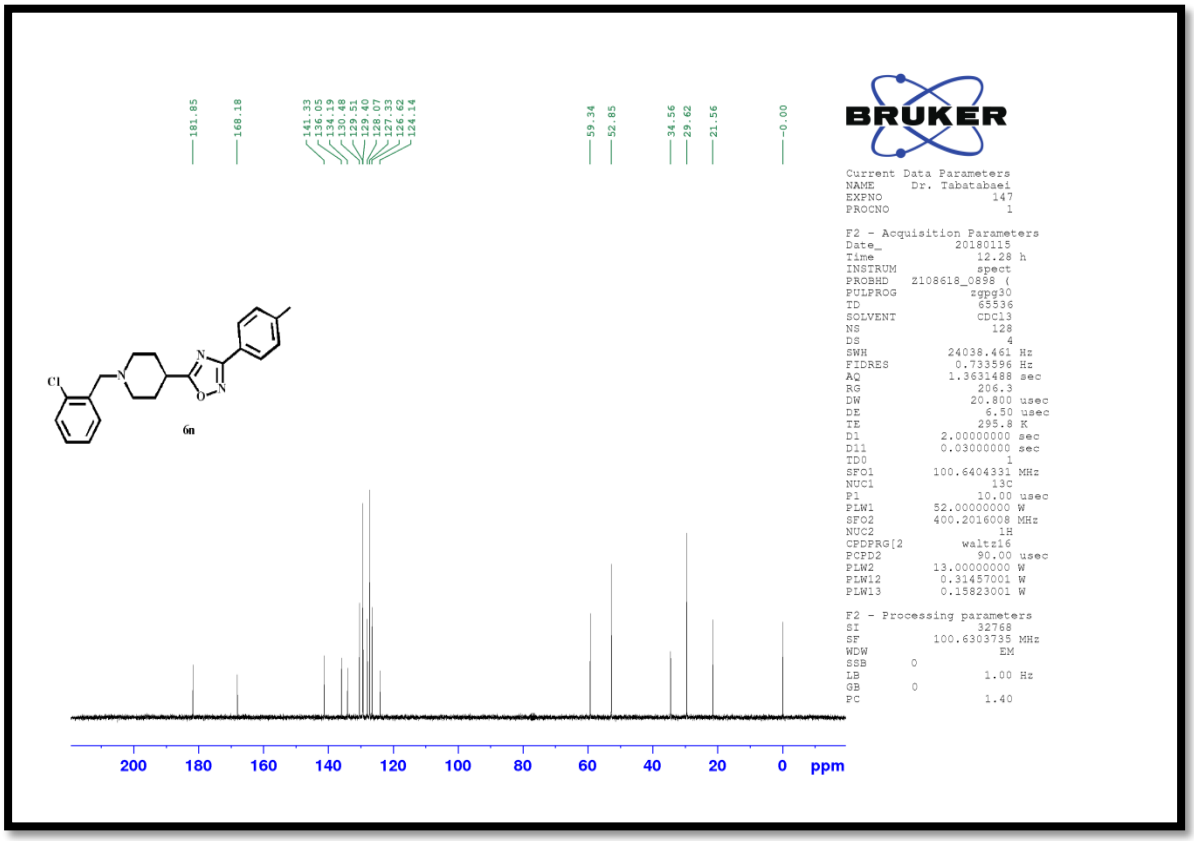

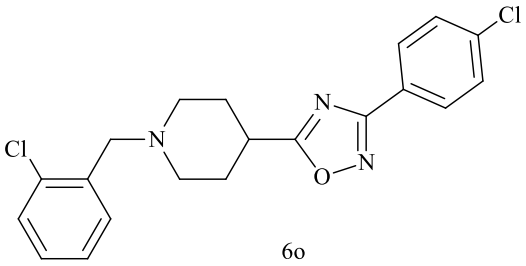

6o

5-(1-(2-chlorobenzyl)piperidin-4-yl)-3-(4-chlorophenyl)-1,2,4-oxadiazole (6o)

White powder; yield: 33.8 %; mp: 85.5-87 °C; IR (KBr, cm^{-1}): 1597 (C=N), 1141 (C-O); LC-MS $[M + 1]^+$: m/z 387.8; ^1H NMR ($CDCl_3$, 400 MHz) δ: 1.95-2.07 (m, 4H, H-piperidine), 2.19-2.24 (m, 2H, H-piperidine), 2.90-2.97 (m, 3H, H-piperidine), 3.58 (s, 2H, CH_2-benzyl), 7.14-7.19 (m, 2H, H_4, H_5-benzyl), 7.27 (d, 1H, *J* = 8 Hz ,H_3-benzyl), 7.36 (d, 2H, *J* = 8 Hz, H_3, H_5-phenyl), 7.42 (d, 1H, *J* = 8 Hz ,H_6-benzyl), 7.93 (d, 2H, *J* = 8 Hz, H_2, H_6-phenyl); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 29.60 ($2CH_2$), 34.55 (CH), 52.81 ($2CH_2$), 59.35 (CH_2), 125.50 (C), 126.67 (CH), 128.16 (2CH), 129.16 (2CH), 129.45 (2CH), 130.54 (CH), 134.25 (C), 135.99 (C), 137.21 (C), 167.43 (C), 182.28 (C); Anal. calcd for $C_{20}H_{19}Cl_2N_3O$: C, 61.86; H, 4.93; N, 10.82, found: C, 62.09; H, 4.92; N, 10.75.

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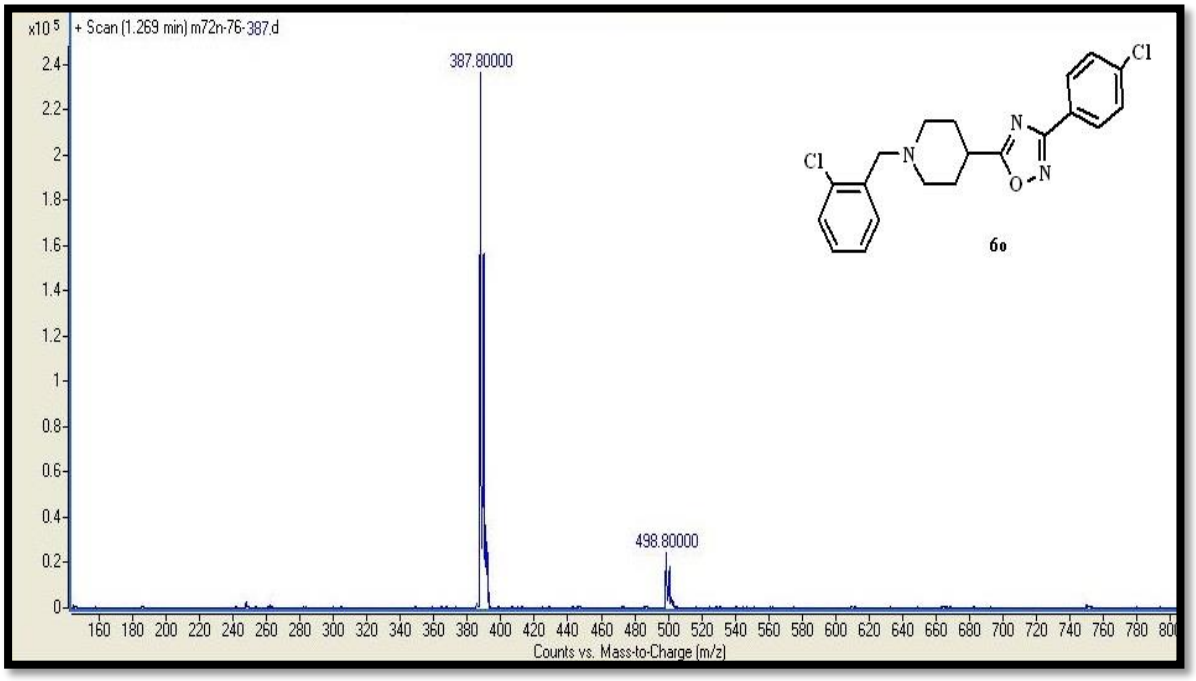

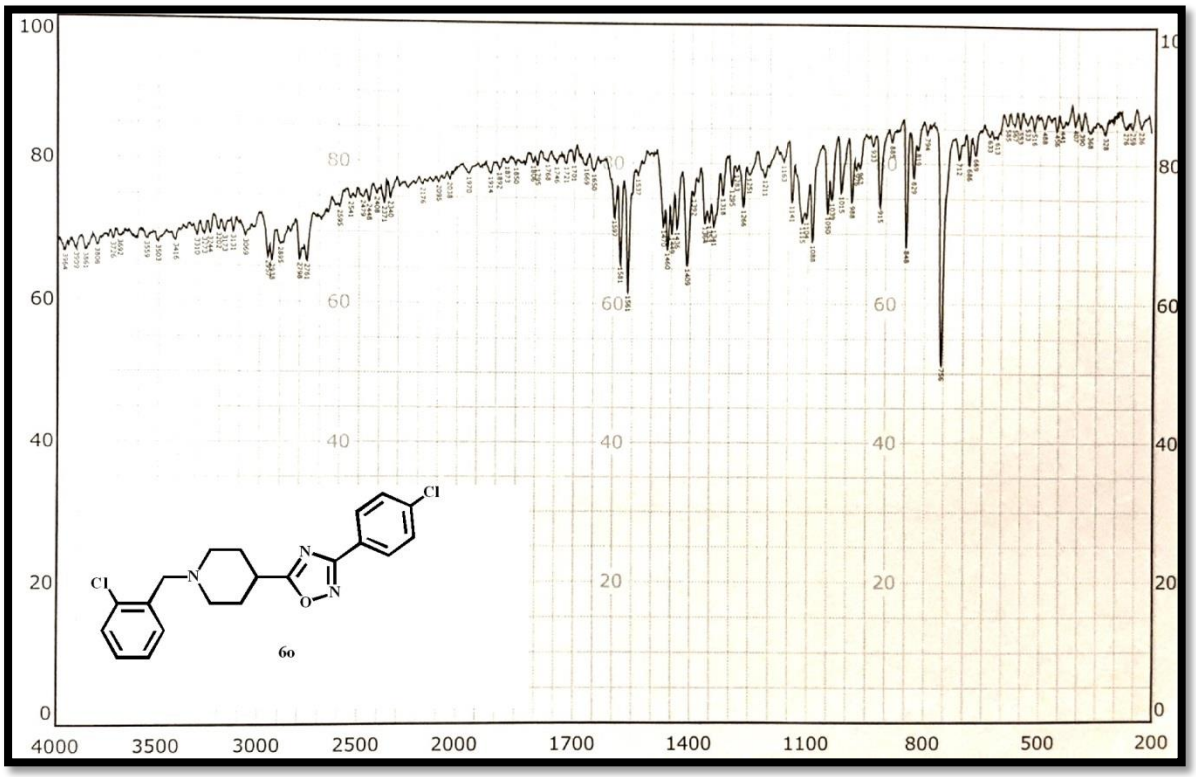

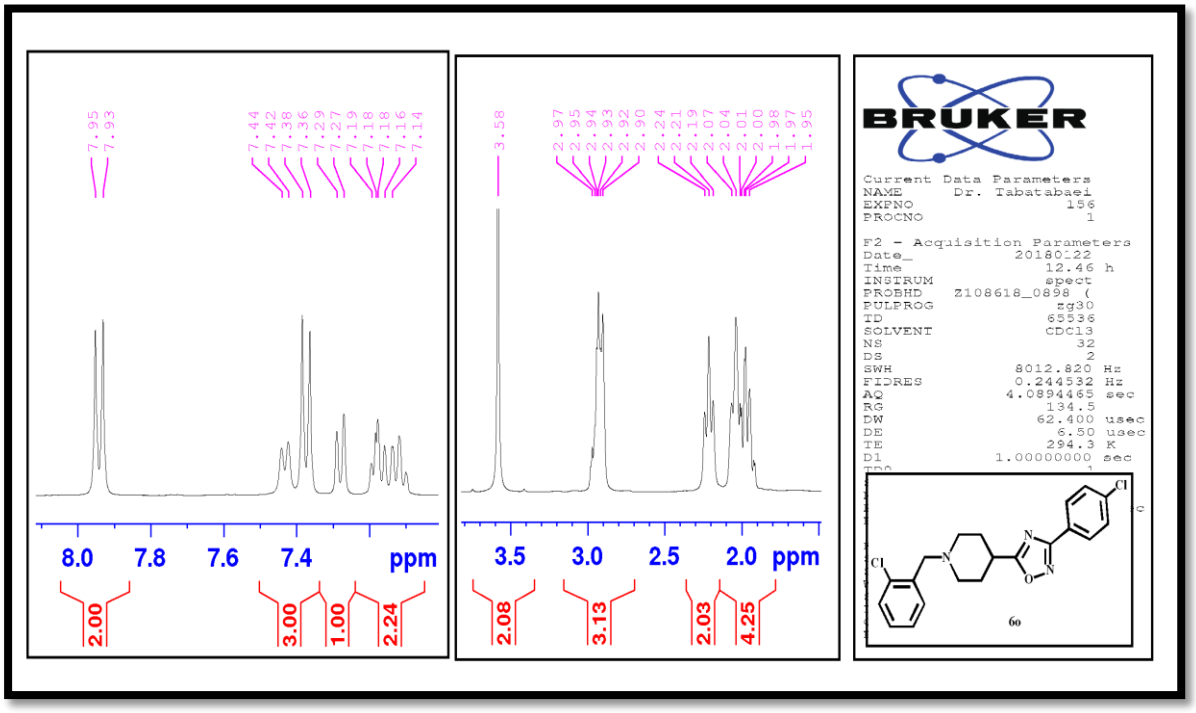
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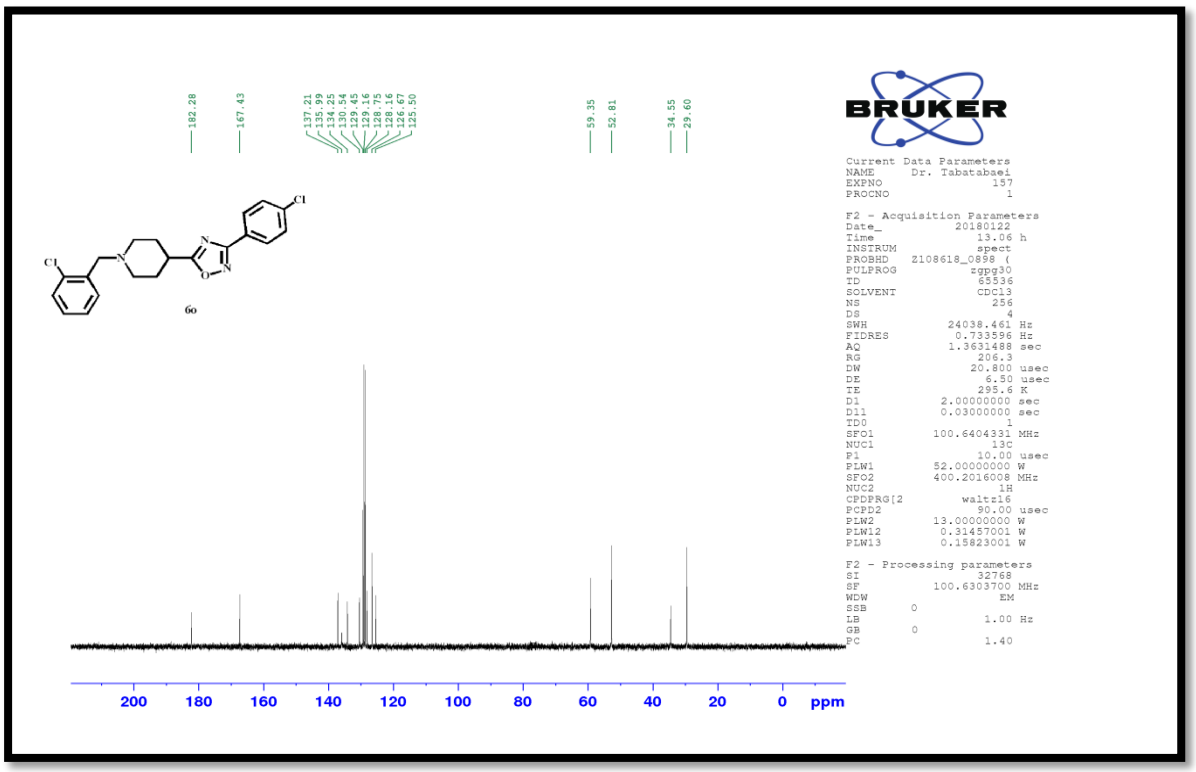
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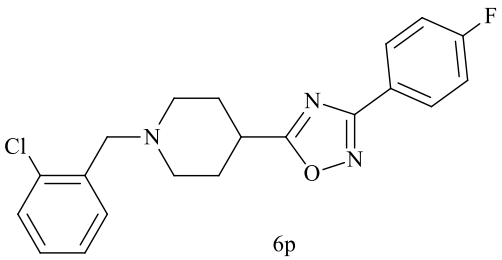

6p

5-(1-(2-chlorobenzyl)piperidin-4-yl)-3-(4-fluorophenyl)-1,2,4-oxadiazole (6p)

Light yellow powder; yield: 30.5 %; mp: 69.5-70 °C; IR (KBr, cm^{-1}): 1600 (C=N), 1212 (C-O); LC-MS $[M + 1]^+$: m/z 371.8; ^1H NMR ($CDCl_3$, 400 MHz) δ: 2.05-2.17 (m, 4H, H-piperidine), 2.29-2.34 (m, 2H, H-piperidine), 3.00-3.03 (m, 3H, H-piperidine), 3.68 (s, 2H, CH_2-benzyl), 7.20-7.29 (m, 3H, H_4, H_5, H_6-benzyl), 7.37 (d, 2H, J = 8 Hz, H_3, H_5-phenyl), 7.53-7.54 (m, 1H, H_3-benzyl), 8.08-8.12 (m, 2H, H_2, H_6-phenyl); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 29.61 ($2CH_2$), 34.54 (CH), 52.82 ($2CH_2$), 59.35 (CH_2), 115.90 (C), 123.22 (CH), 126.66 (2CH), 128.15 (2CH), 129.45 (2CH), 130.54 (CH), 134.24 (C), 136.00 (C), 163.27 (C), 167.41 (C), 182.18 (C); Anal. calcd for $C_{20}H_{19}ClFN_3O$: C, 64.60; H, 5.15; N, 11.30, found: C, 64.79; H, 5.13; N, 11.23.

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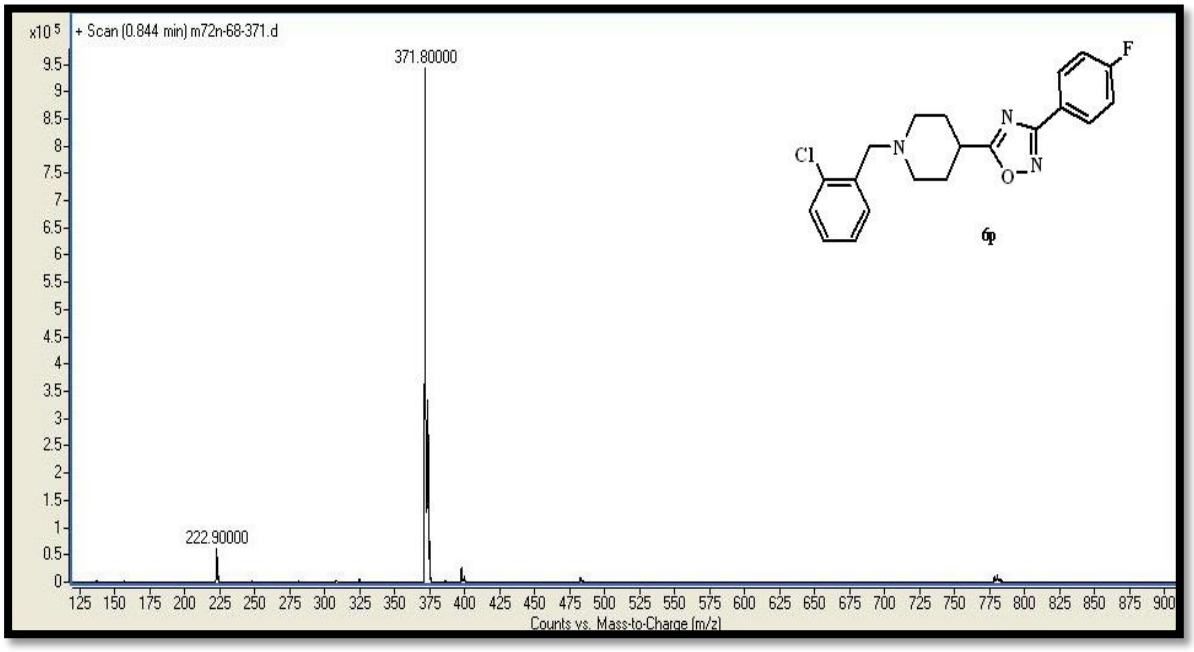

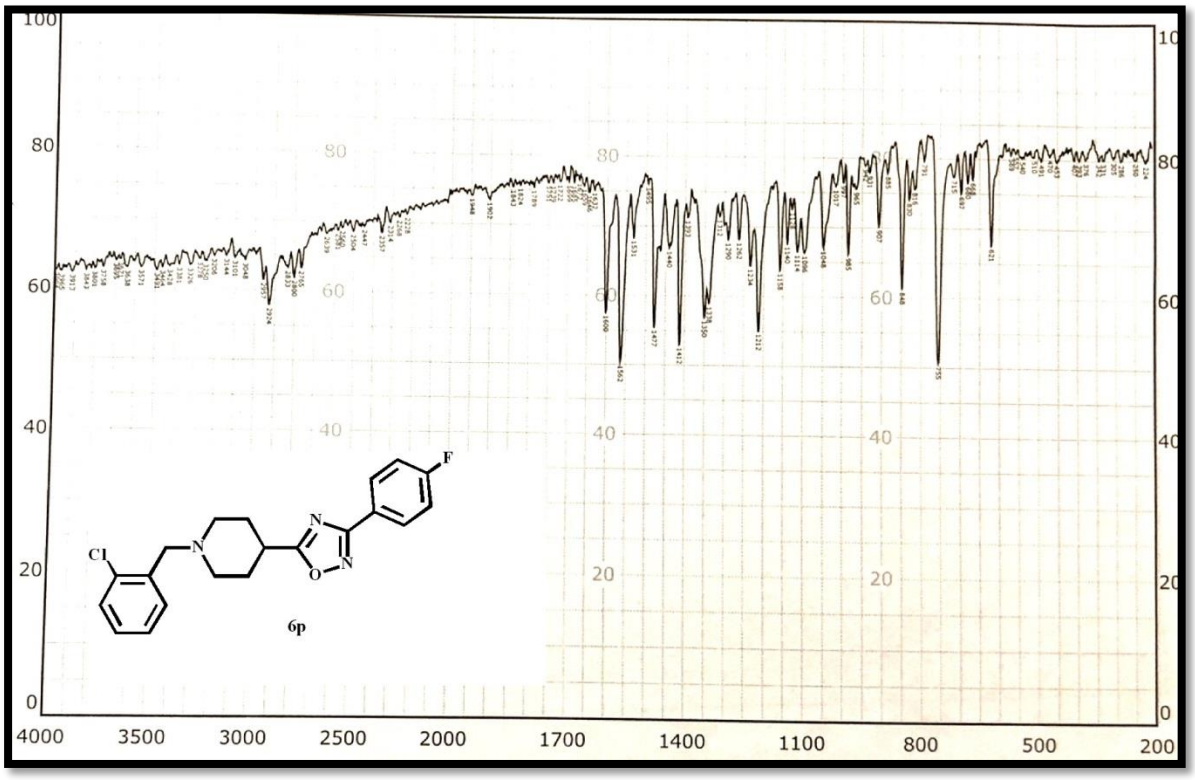

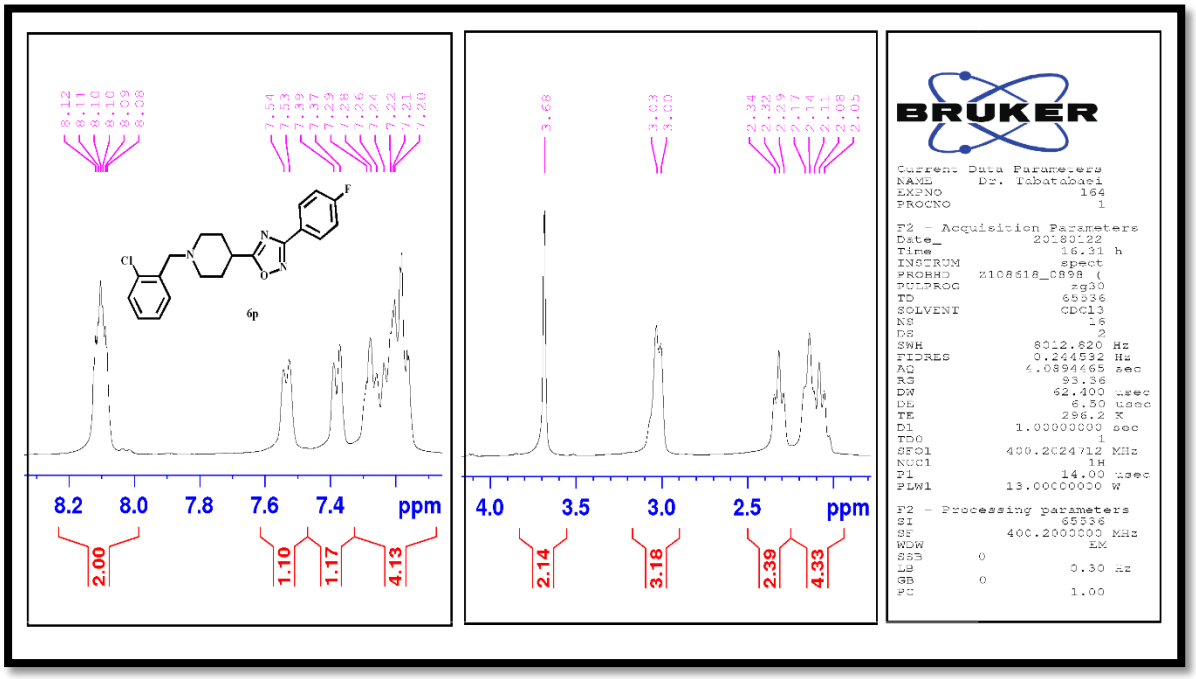
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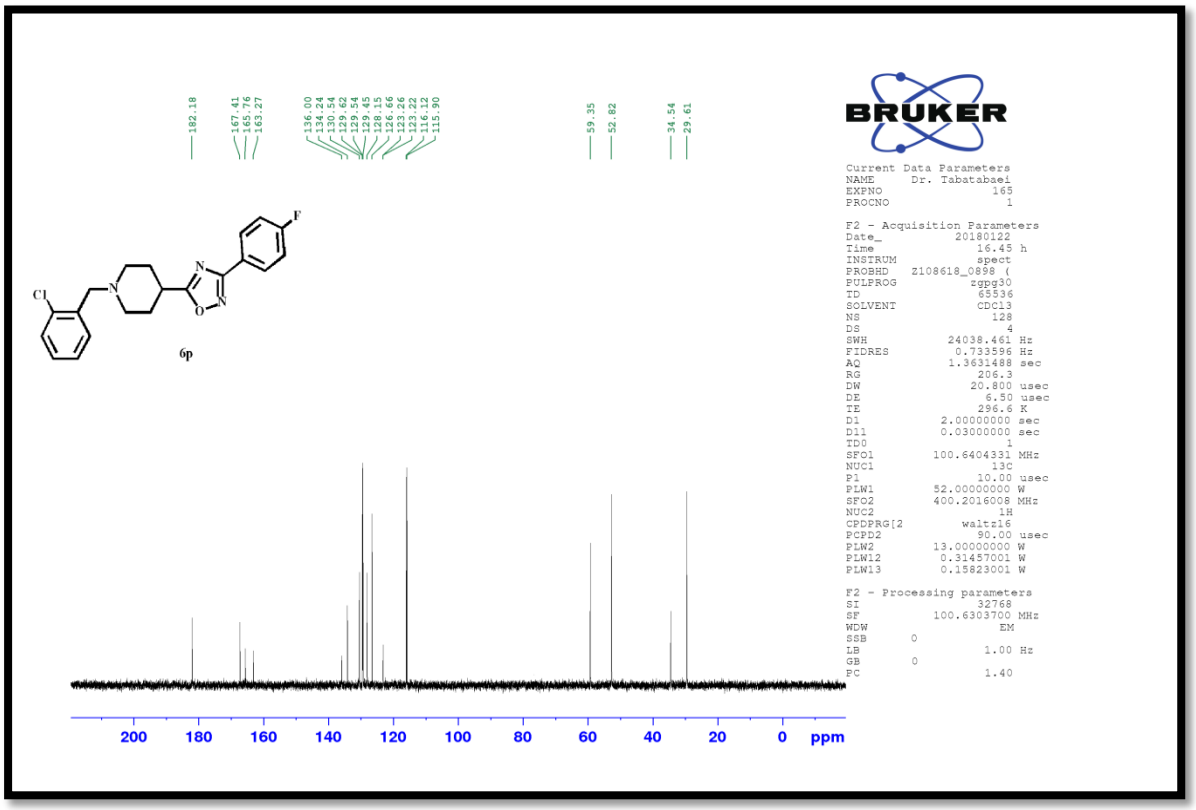
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NUC2 1H
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PLW2 13.00000000 W
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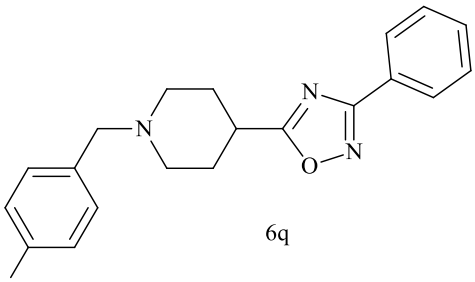

6q

5-(1-(4-methylbenzyl)piperidin-4-yl)-3-phenyl-1,2,4-oxadiazole (6q)

Light yellow powder; yield: 32.8 %; mp: 90.3-91.4 °C; IR (KBr, cm^{-1}): 1589 (C=N), 1145 (C-O), 1363,1440 (CH_3); LC-MS $[M + 1]^+$: m/z 334; ^1H NMR ($CDCl_3$, 400 MHz) δ: 2.09-2.14 (m, 6H, H-piperidine), 2.26-2.31 (m, 3H, CH_3), 2.98-3.05 (m, 3H, H-piperidine), 3.65 (s, 2H, CH_2-benzyl), 7.17-7.27 (m, 2H, H_3, H_5-benzyl), 7.34 (d, 2H, J = 8 Hz, H_2, H_6-benzyl),7.47-7.52 (m, 3H, H_3, H_4, H_5-phenyl), 8.07 (d, 2H, J = 8 Hz, H_2, H_6-phenyl); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 21.55 (CH_3), 29.62 ($2CH_2$), 34.56 (CH), 52.84 ($2CH_2$), 59.35 (CH_2), 126.63 (C), 127.42 (2CH), 128.80 (2CH), 129.41 (2CH), 130.50 (2CH), 131.06 (CH), 134.21 (C), 136.04 (C), 168.20 (C), 182.04 (C); Anal. calcd for $C_{21}H_{23}N_3O$: C, 75.65; H, 6.95; N, 12.60, found: C, 75.86; H, 6.94; N, 12.55.

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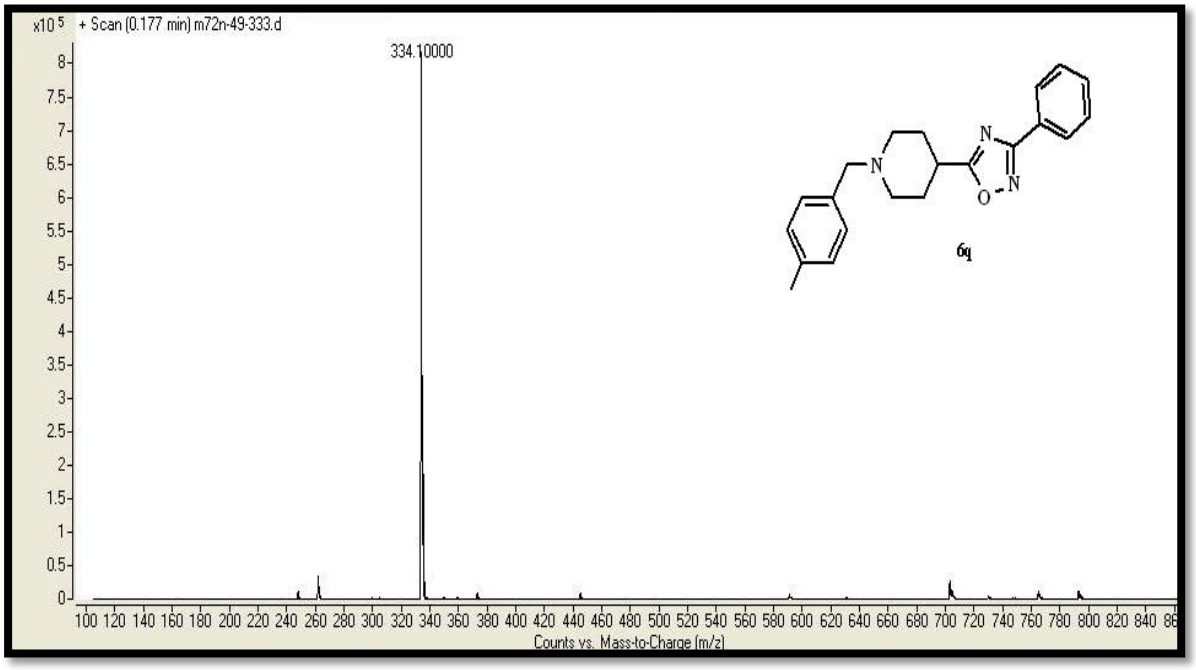

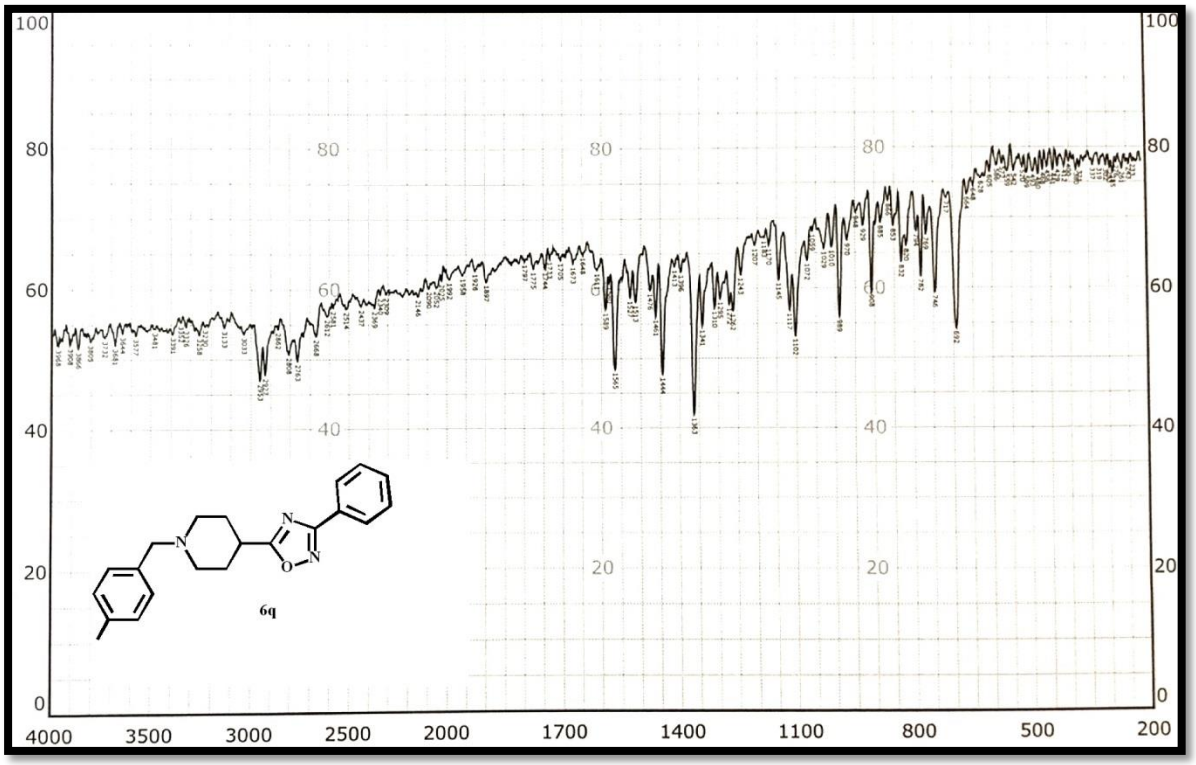

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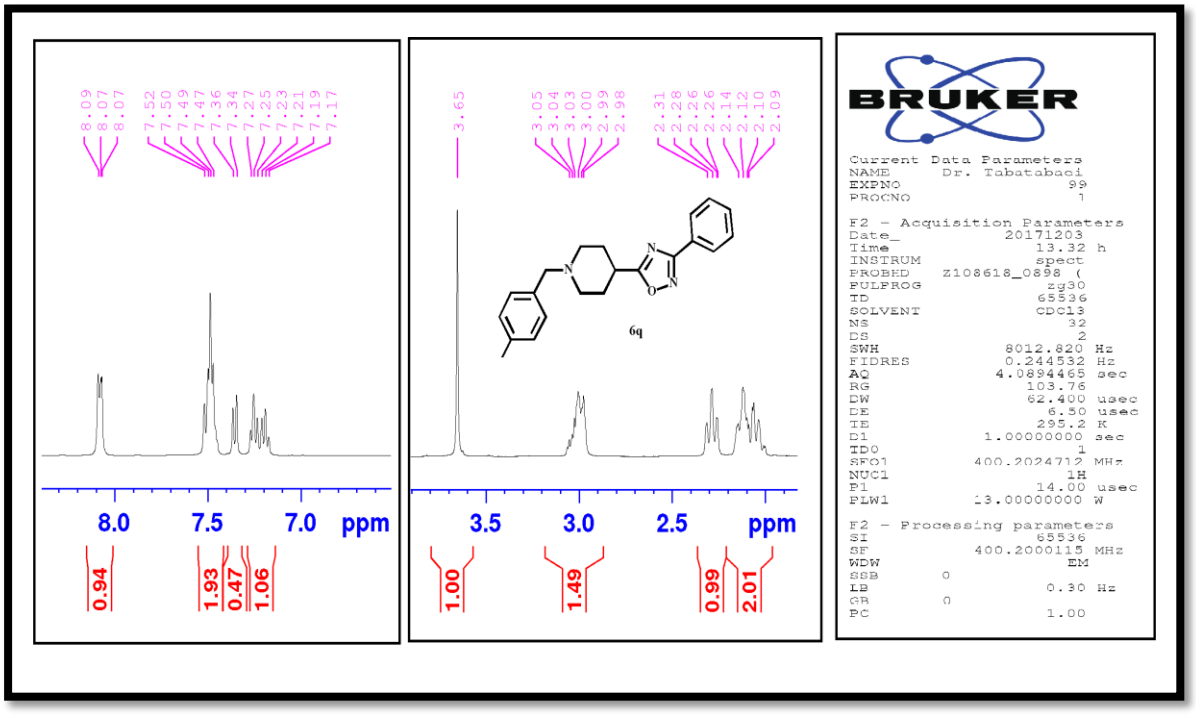

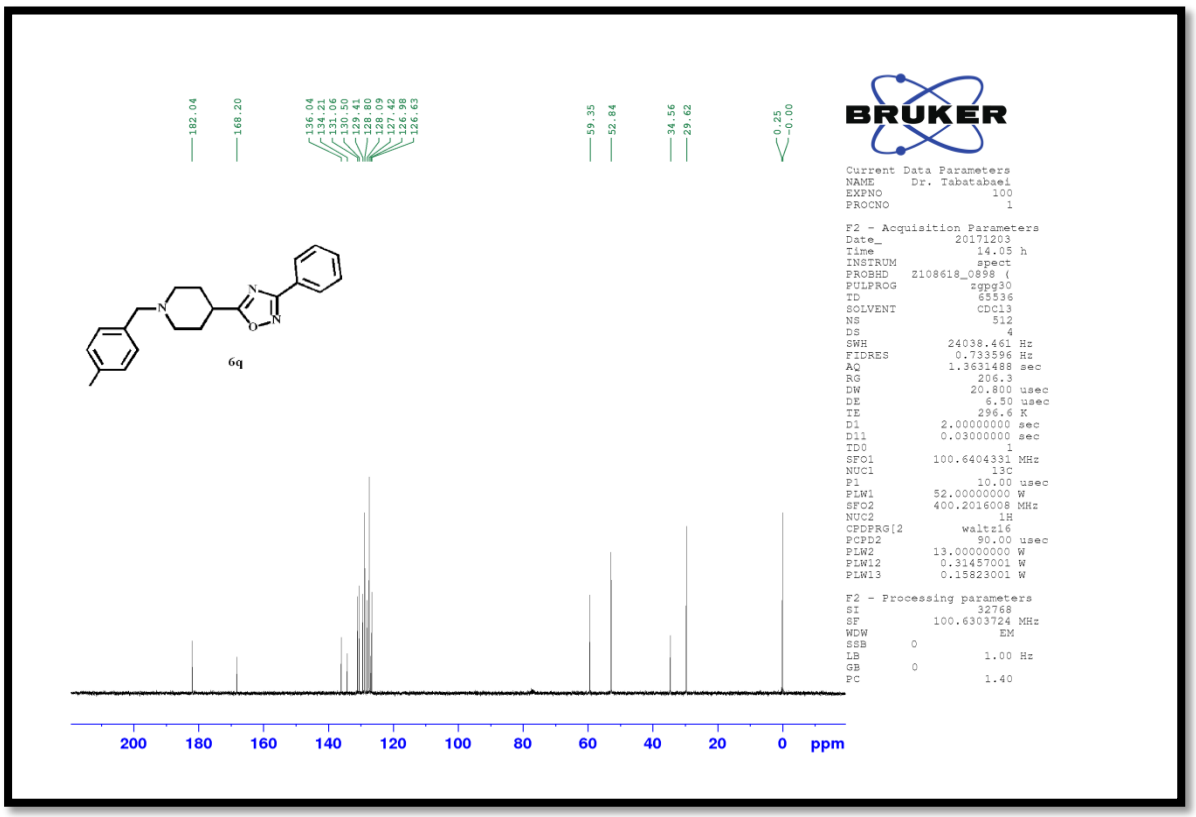

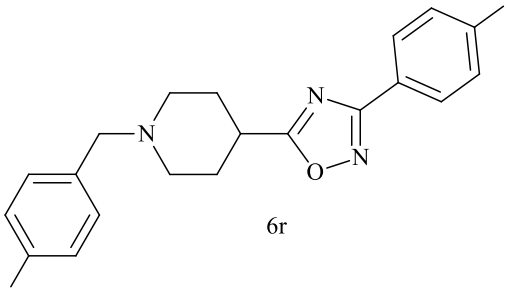

6r

5-(1-(4-methylbenzyl)piperidin-4-yl)-3-(p-tolyl)-1,2,4-oxadiazole (6r)

Light yellow powder; yield: 47.2 %; mp: 84.5-85.3 °C; IR (KBr, cm^{-1}): 1579 (C=N), 1117 (C-O), 1358,1410 (CH_3); LC-MS $[M + 1]^+$: m/z 347.9; ^1H NMR ($CDCl_3$, 400 MHz) δ: 2.02-2.15 (m, 6H, H-piperidine), 2.33 (s , 3H , CH_3-benzyl), 2.39 (s , 3H , CH_3-phenyl), 2.92-2.96 (m, 3H, H-piperidine), 3.49 (s, 2H, CH_2-benzyl), 7.12 (d, 2H, *J* = 8 Hz, H_3, H_5-benzyl), 7.20 (d, 2H, *J* = 8 Hz, H_2, H_6-benzyl), 7.25 (d, 2H, *J* = 8 Hz, H_3, H_5-phenyl), 7.95 (d, 2H, *J* = 8 Hz, H_2, H_6-phenyl); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 21.10 (CH_3), 21.54 (CH_3), 29.54 ($2CH_2$), 34.64 (CH), 52.68 ($2CH_2$), 62.90 (CH_2), 124.15 (C), 127.31 (2CH), 128.91 (2CH), 129.00 (2CH), 129.48 (2CH), 135.15 (C), 136.60 (C), 141.28 (C), 168.14 (C), 181.88 (C); Anal. calcd for $C_{22}H_{25}N_3O$: C, 76.05; H, 7.25; N, 12.09, found: C, 76.28; H, 7.23; N, 12.02.

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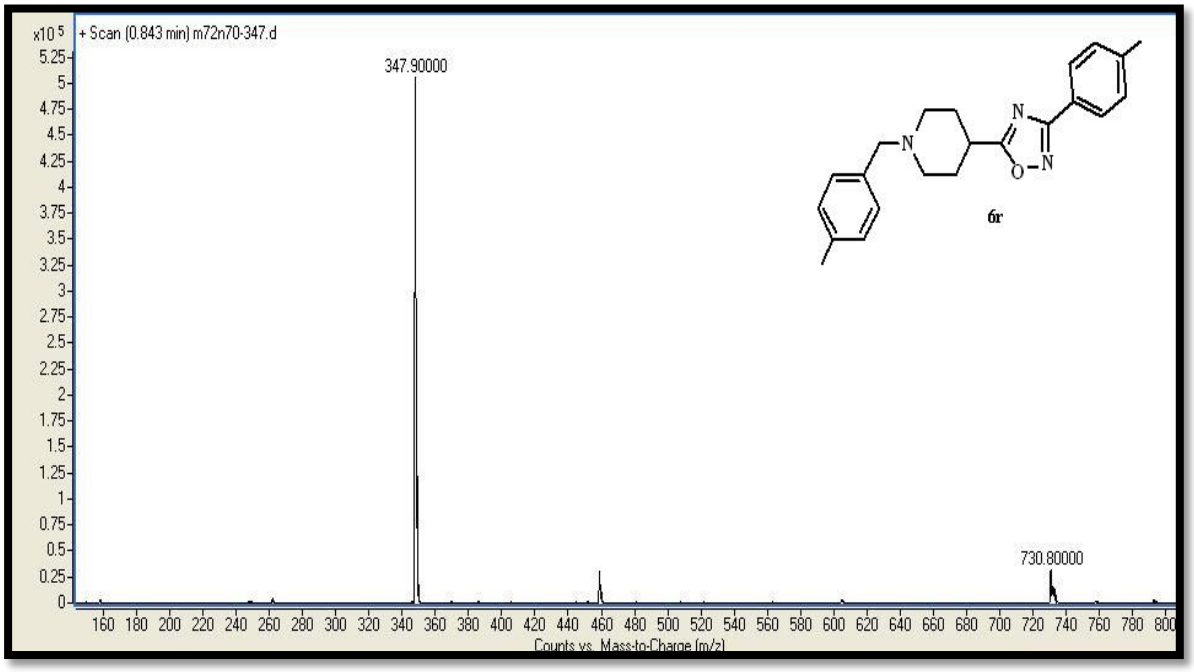

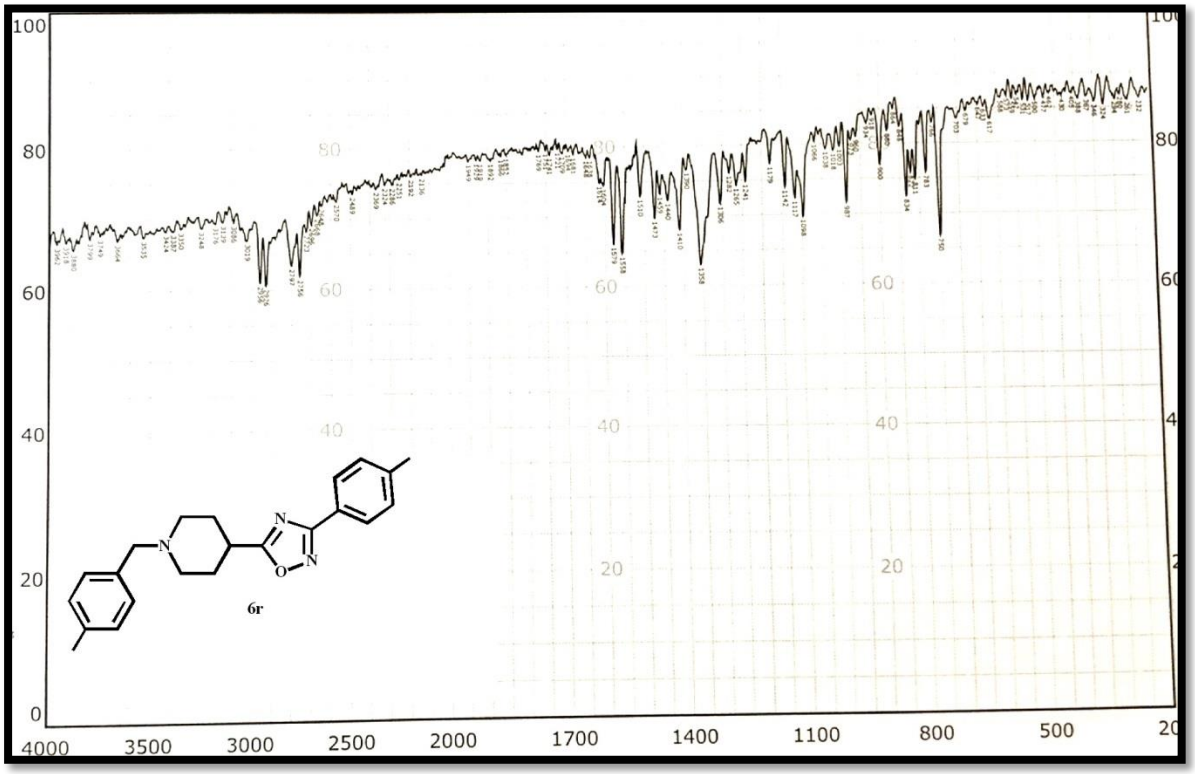

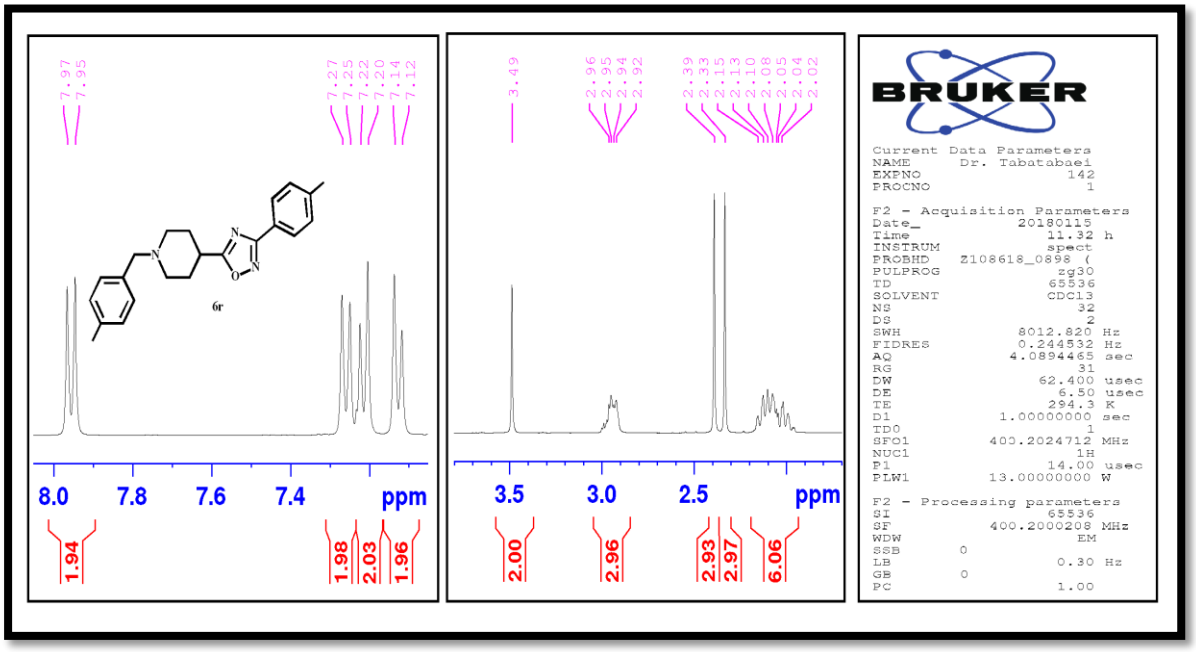
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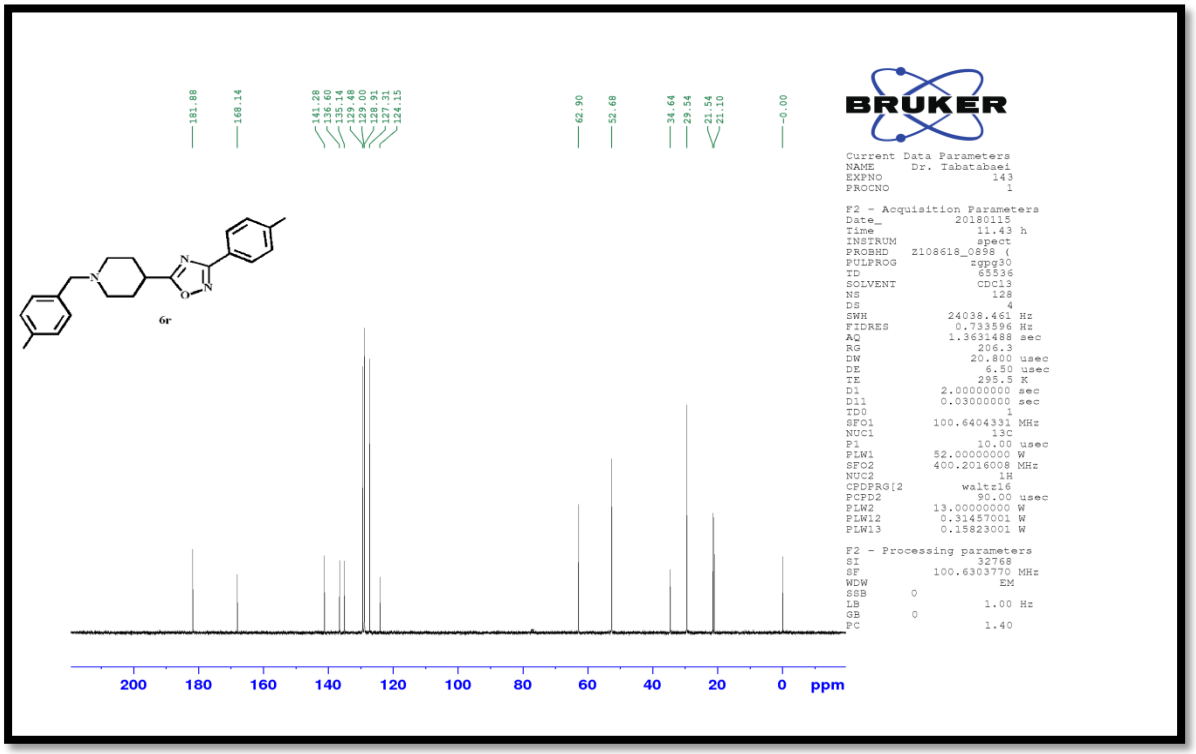
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D11 0.03000000 sec
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NUC1 13C
P1 10.00 usec
PLW1 52.00000000 W
SFO2 400.2016008 MHz
NUC2 1H
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PCPD2 90.00 usec
PLW2 13.00000000 W
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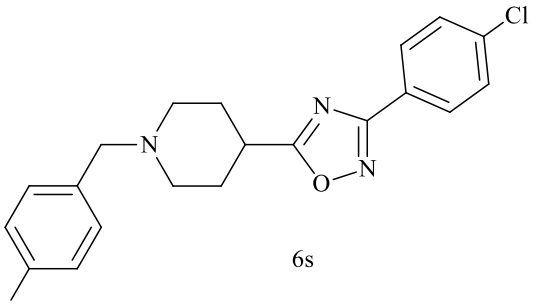

6s

3-(4-chlorophenyl)-5-(1-(4-methylbenzyl)piperidin-4-yl)-1,2,4-oxadiazole (6s)

Light yellow powder; yield: 47.3 %; mp: 111.4-112.5 °C; IR (KBr, cm^{-1}): 1585 (C=N), 1128 (C-O), 1361,1446 (CH_3); LC-MS $[M + 1]^+$: m/z 367.8; ^1H NMR ($CDCl_3$, 400 MHz) δ: 1.95-2.10 (m, 6H, H-piperidine), 2.26 (s, 3H, CH_3), 2.86-2.91 (m, 3H, H-piperidine), 3.43 (s, 2H, CH_2-benzyl), 7.05 (d, 2H, *J* = 8 Hz, H_3, H_5-benzyl), 7.15 (d, 2H, *J* = 8 Hz, H_2, H_6-benzyl), 7.35 (d, 2H, *J* = 8 Hz, H_3, H_5-phenyl), 7.92 (d, 2H, *J* = 8 Hz, H_2, H_6-phenyl); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 21.15 (CH_3), 29.55 ($2CH_2$), 34.66 (CH), 52.68 ($2CH_2$), 62.93 (CH_2), 125.53 (C), 128.76 (2CH), 128.97 (2CH), 129.07 (2CH), 129.15 (2CH), 135.09 (C), 136.72 (C), 137.19 (C), 167.42 (C), 182.35 (C); Anal. calcd for $C_{21}H_{22}ClN_3O$: C, 68.56; H, 6.03; N, 11.42, found: C, 68.79; H, 6.01; N, 11.38.

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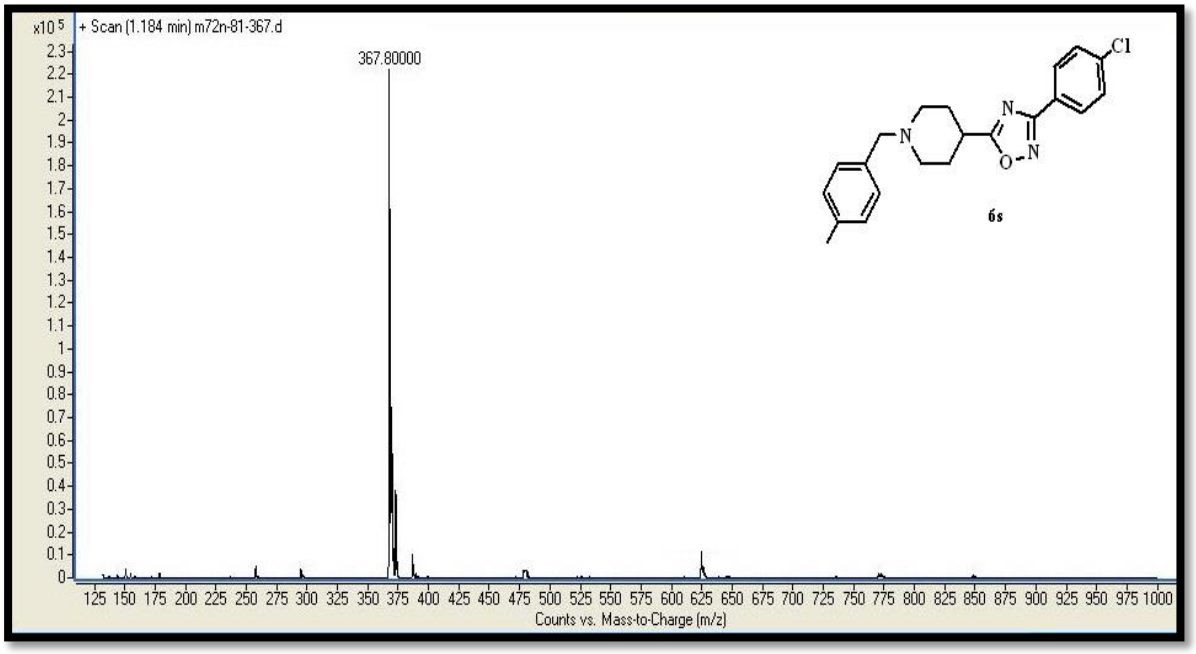

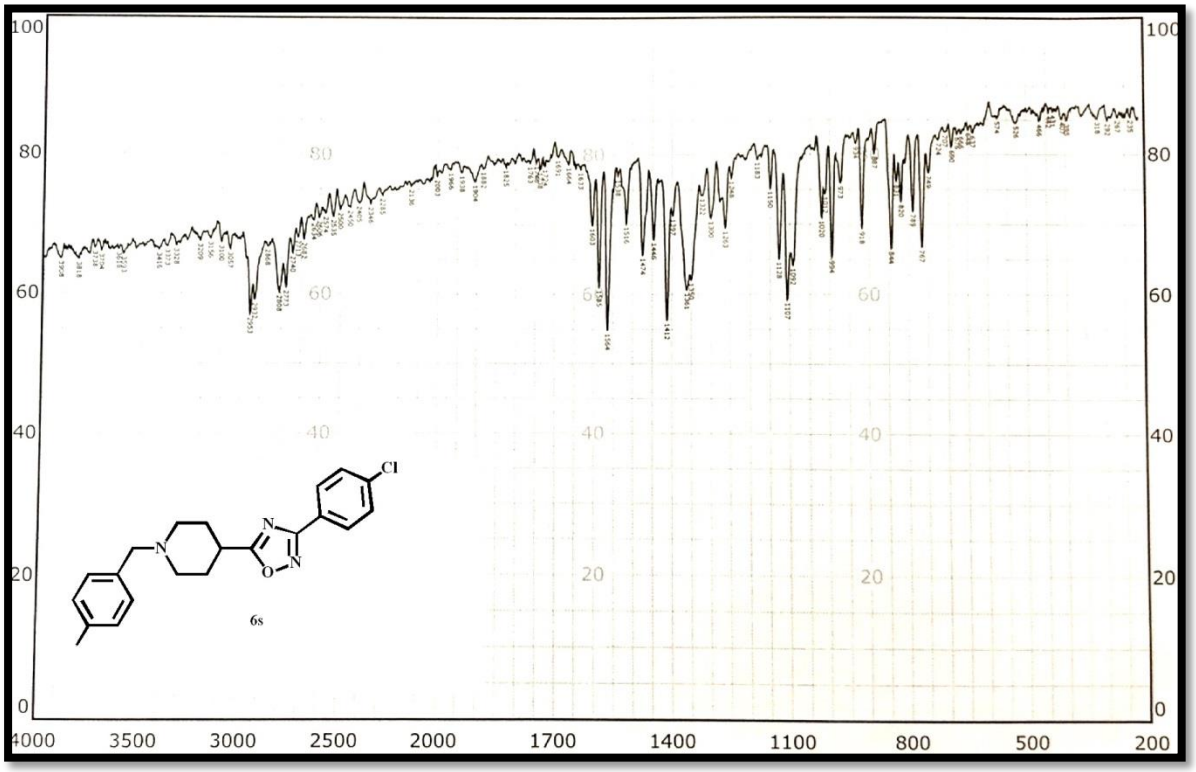

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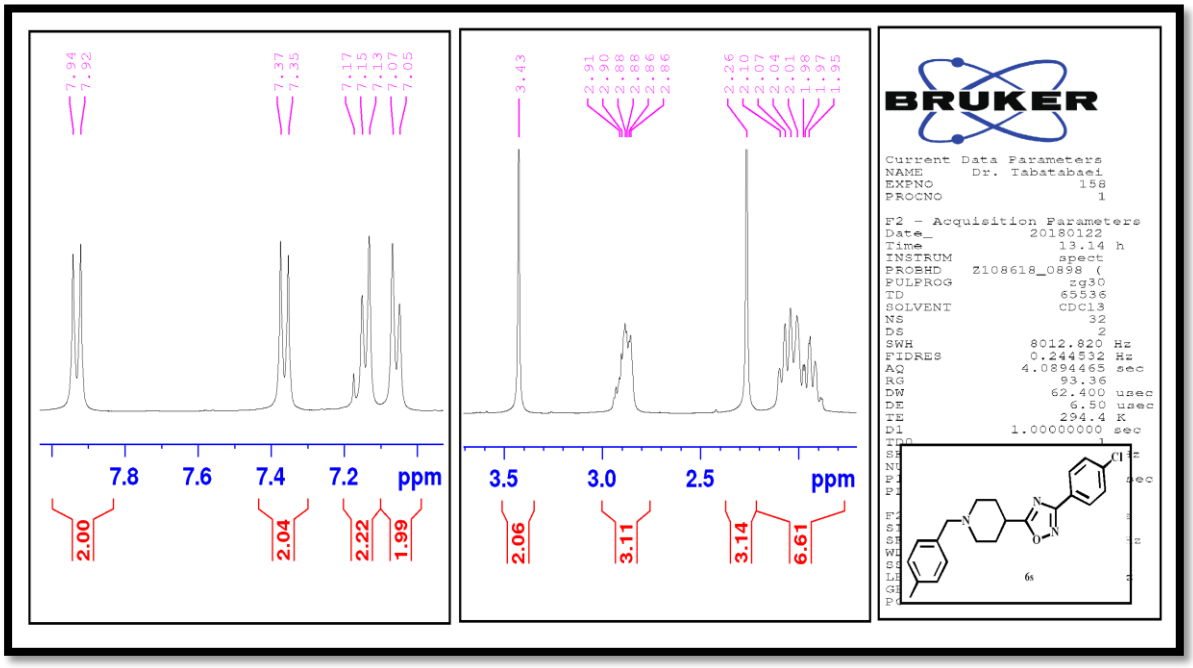

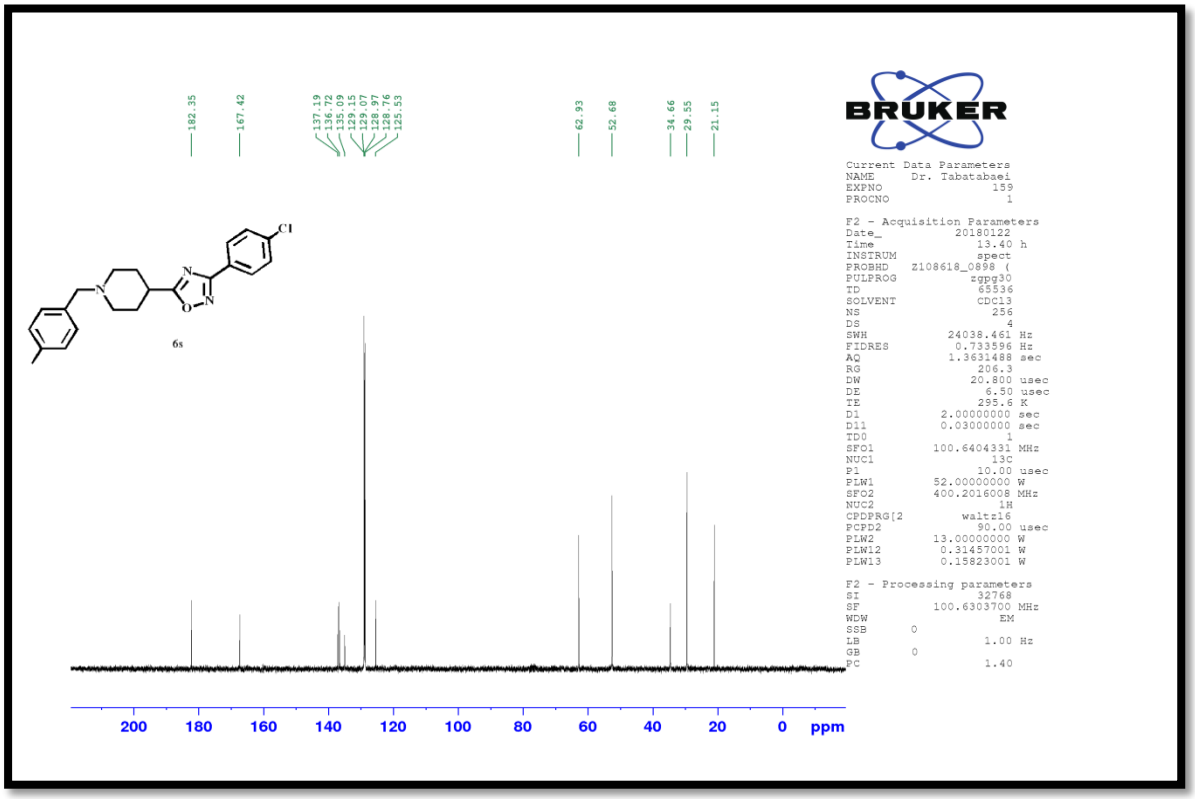

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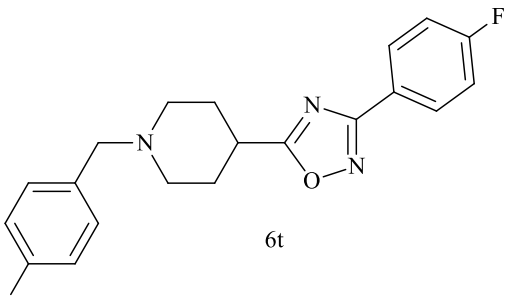

6t

3-(4-fluorophenyl)-5-(1-(4-methylbenzyl)piperidin-4-yl)-1,2,4-oxadiazole (6t)

Light yellow powder; yield: 48.2 %; mp: 96.5-97.2 °C; IR (KBr, cm^{-1}): 1600 (C=N), 1223 (C-O), 1352,1444 (CH_3); LC-MS $[M + 1]^+$: m/z 351.7; ^1H NMR ($CDCl_3$, 400 MHz) δ: 1.99-2.17 (m, 6H, H-piperidine), 2.34 (s, 3H, CH_3), 2.94-2.98 (m, 3H, H-piperidine), 3.50 (s, 2H, CH_2-benzyl), 7.13-7.17 (m, 4H, H_2, H_3, H_5, H_6-benzyl), 7.23 (t, 2H, J = 8 Hz, H_3, H_5-phenyl), 8.05-8.09 (m, 2H, H_2, H_6-phenyl); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 21.11 (CH_3), 29.54 ($2CH_2$), 34.64 (CH), 52.67 ($2CH_2$), 62.92 (CH_2), 115.86 (2CH), 123.20 (C), 128.93 (2CH), 129.51 (2CH), 135.09 (2CH), 136.68 (C), 163.23 (C), 165.72 (C), 167.36 (C), 182.22 (C); Anal. calcd for $C_{21}H_{22}FN_3O$: C, 71.77; H, 6.31; N, 11.96, found: C, 72.02; H, 6.30; N, 11.87.

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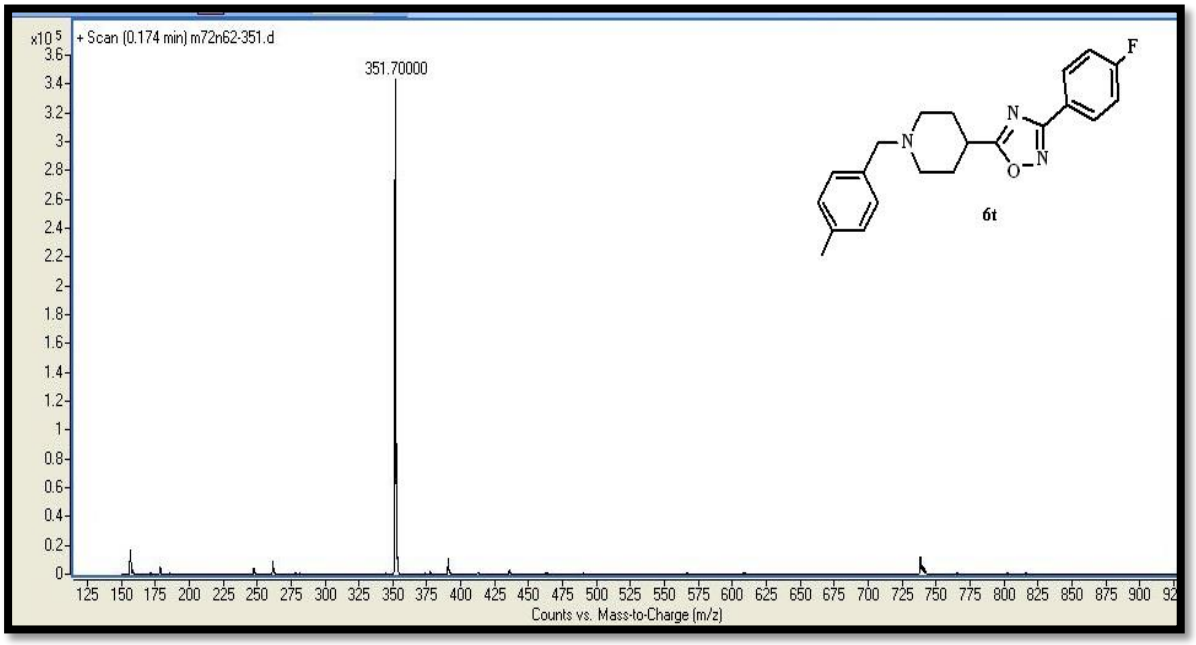

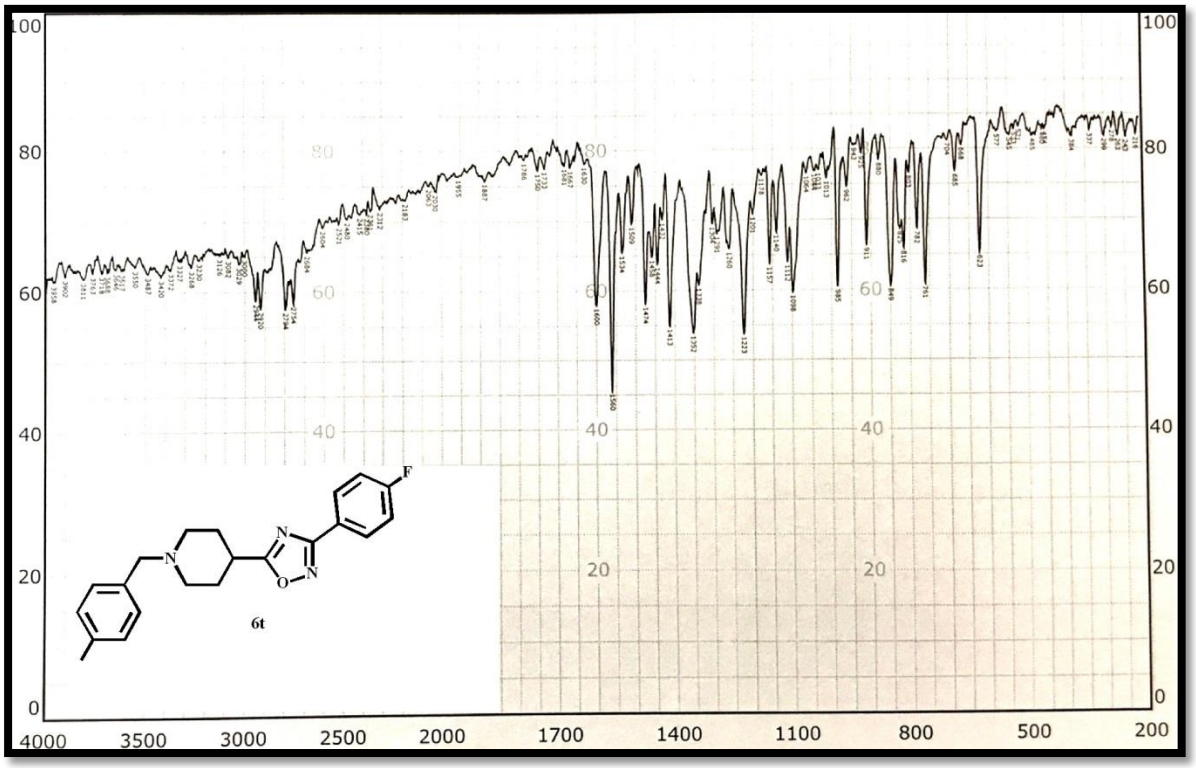

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