

## Supplementary Material

### Versatile Synthesis of Functionalized Tetrahydroisoquinolines by Ring Transformation of 2*H*-Pyranones

Priyanka B. Kole and Fateh V. Singh\*

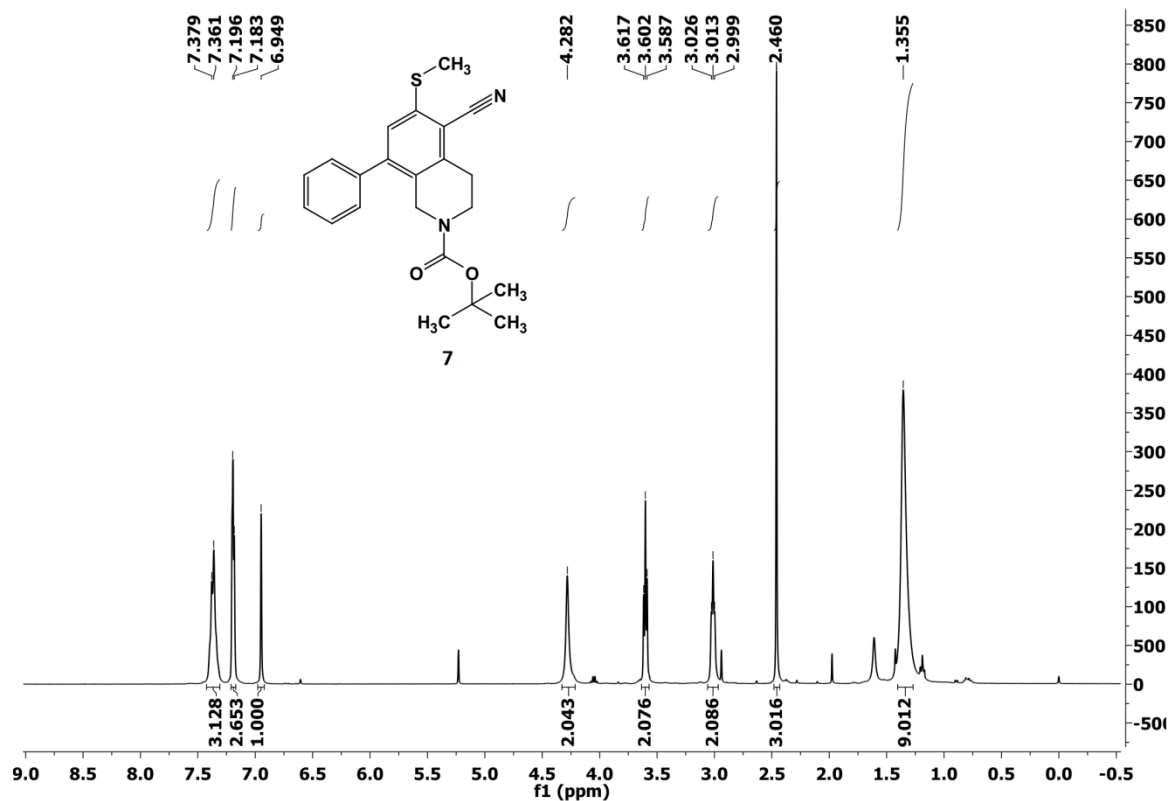
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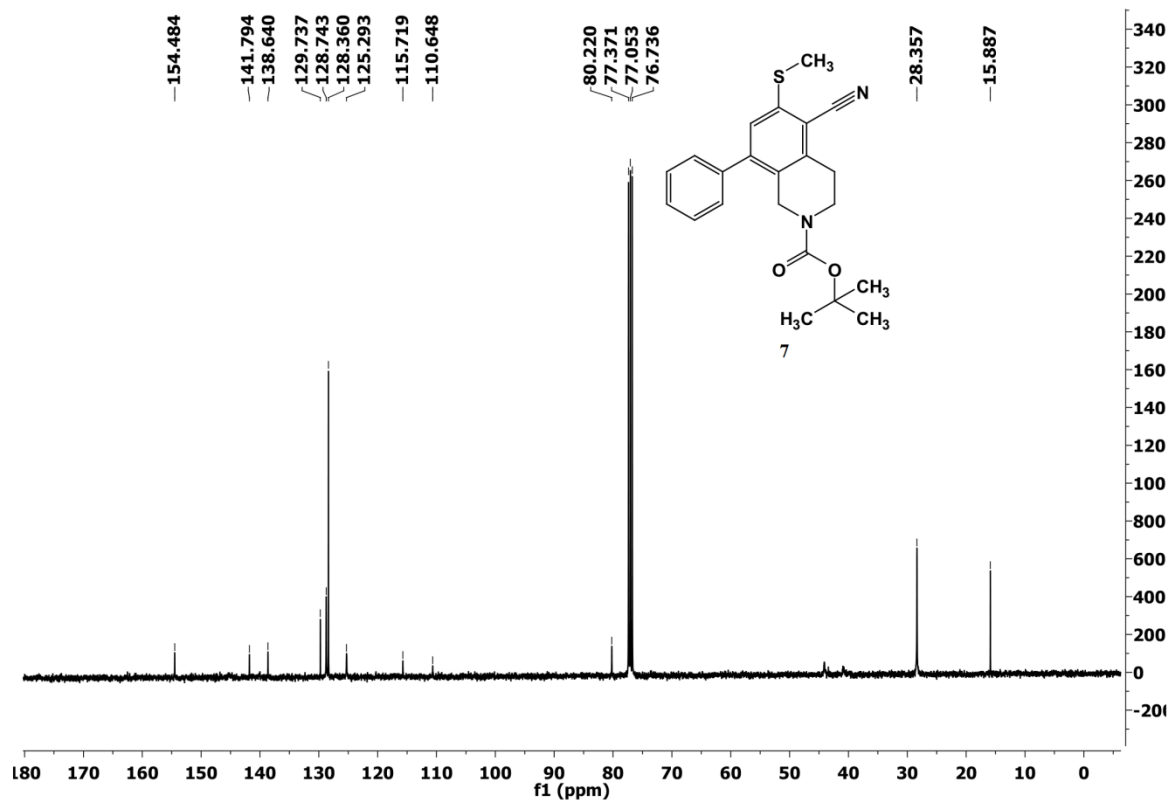
\*E-mail: [fatehveer.singh@vit.ac.in](mailto:fatehveer.singh@vit.ac.in)

<sup>1</sup> H NMR and <sup>13</sup> C NMR spectra of compound <b>7</b>	2
<sup>1</sup> H NMR and <sup>13</sup> C NMR spectra of compounds <b>9a-s</b>	3-21
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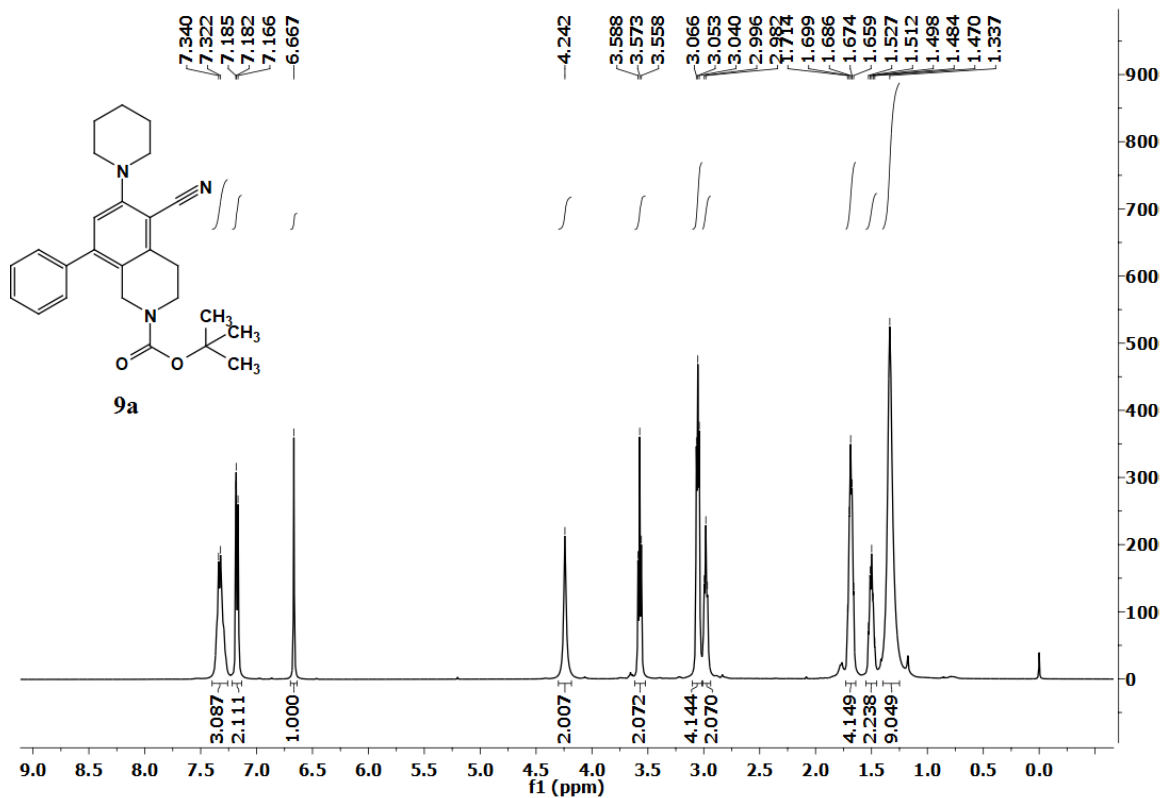
<sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): *tert*-butyl-5-cyano-6-(methylthio)-8-phenyl-3,4-dihydroisoquinoline-2(1H)-carboxylate 7.



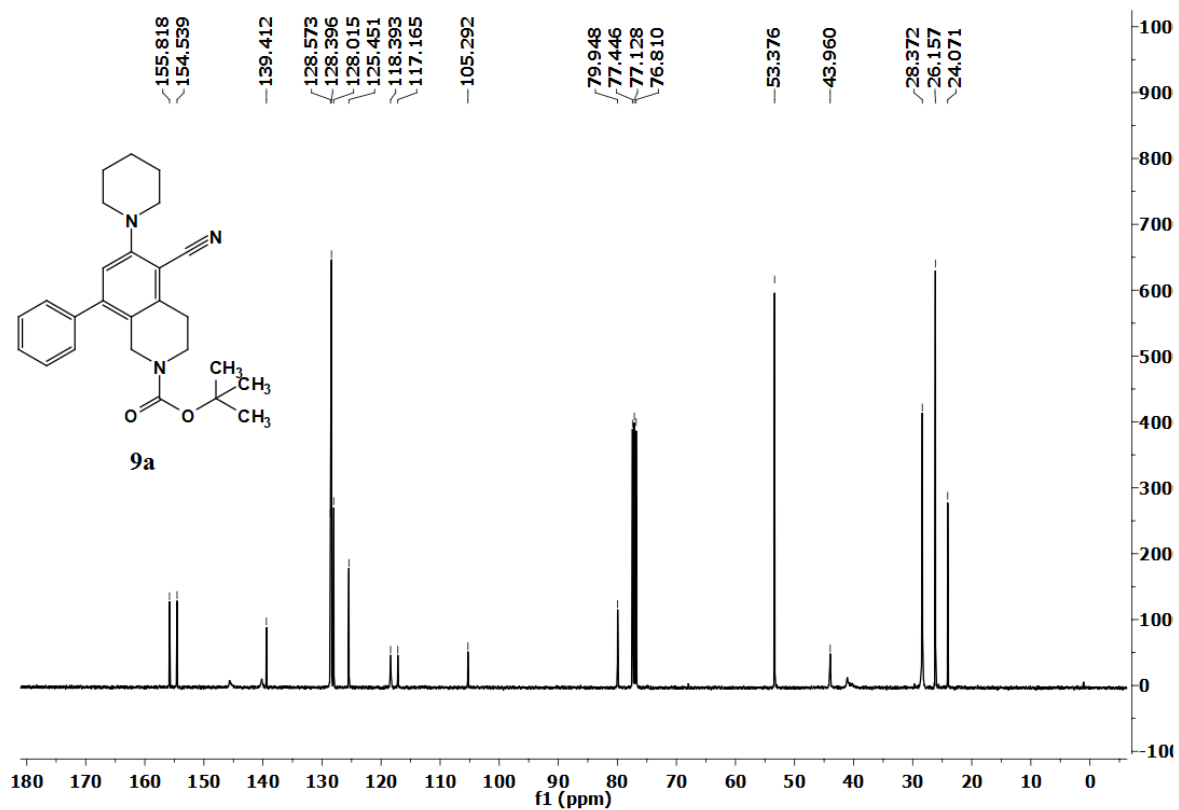
<sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): *tert*-butyl-5-cyano-6-(methylthio)-8-phenyl-3,4-dihydroisoquinoline-2(1H)-carboxylate 7.



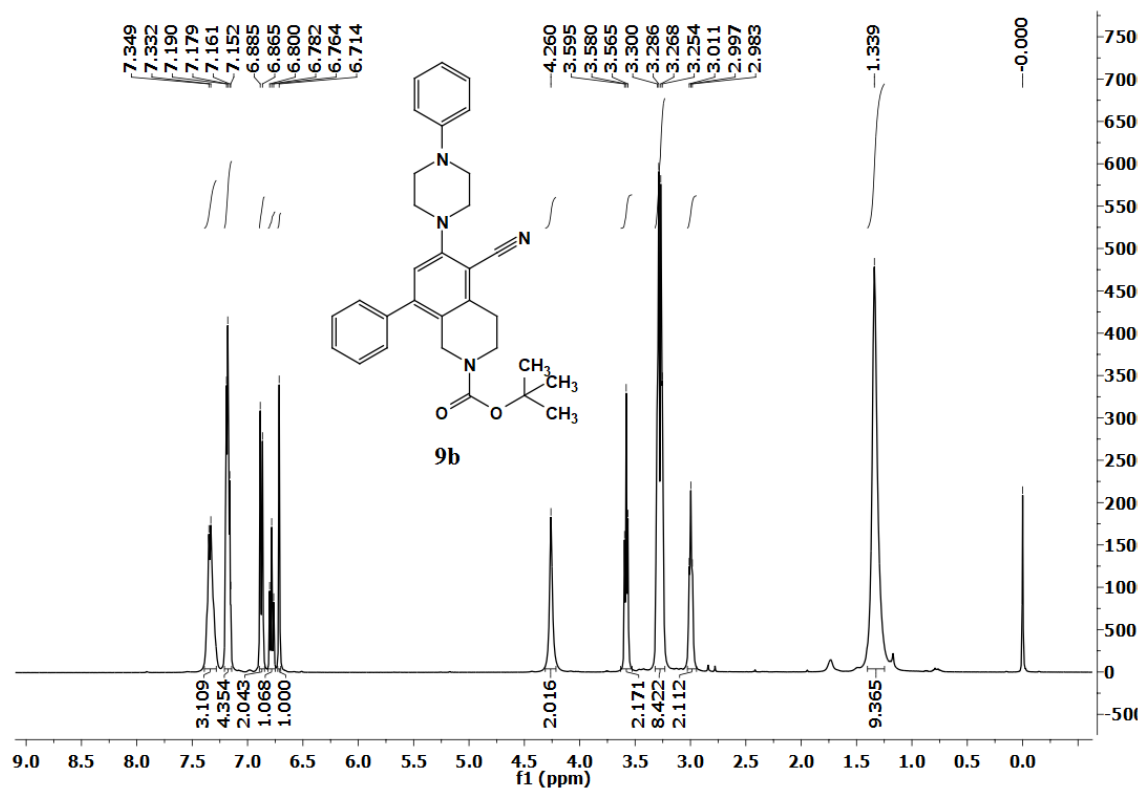
<sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): *tert*-butyl-5-cyano-8-phenyl-6-(piperidin-1-yl)-3,4-dihydroisoquinoline-2(1H)-carboxylate 9a.



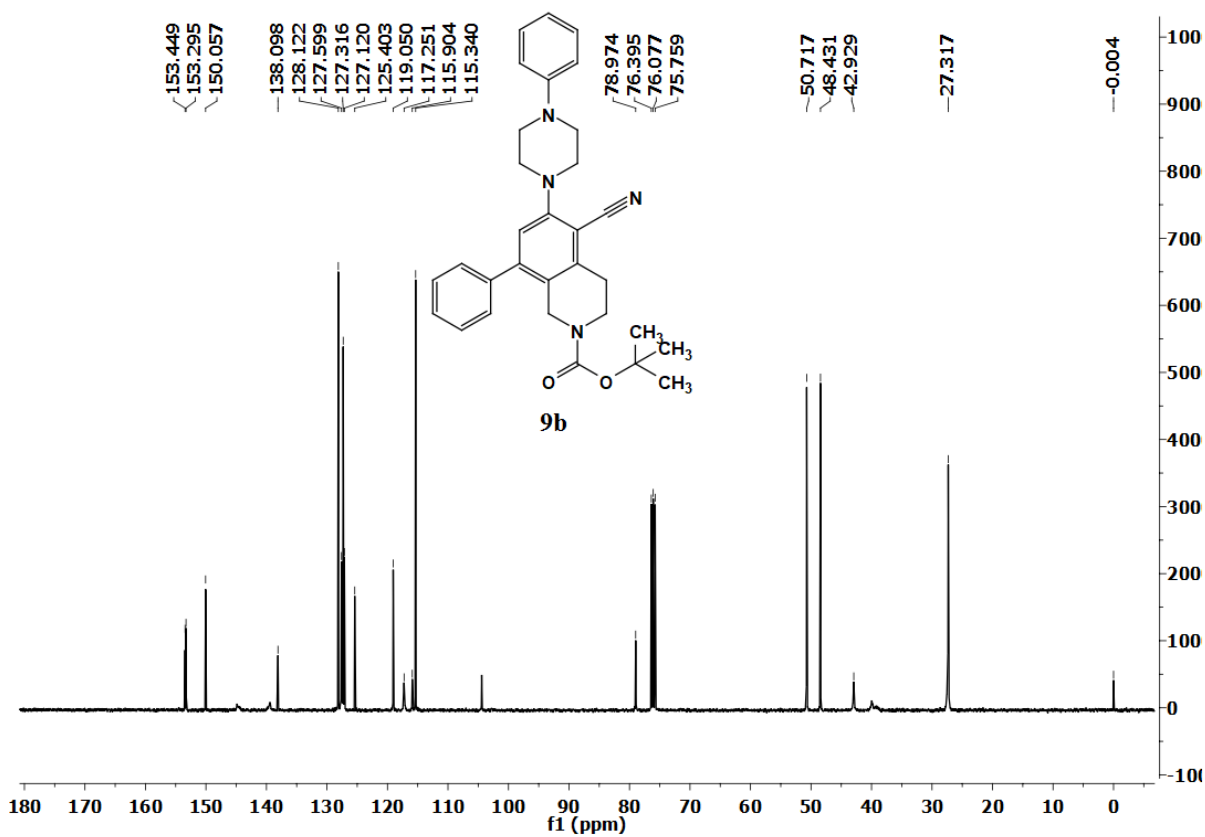
<sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): *tert*-butyl-5-cyano-8-phenyl-6-(piperidin-1-yl)-3,4-dihydroisoquinoline-2(1H)-carboxylate 9a.



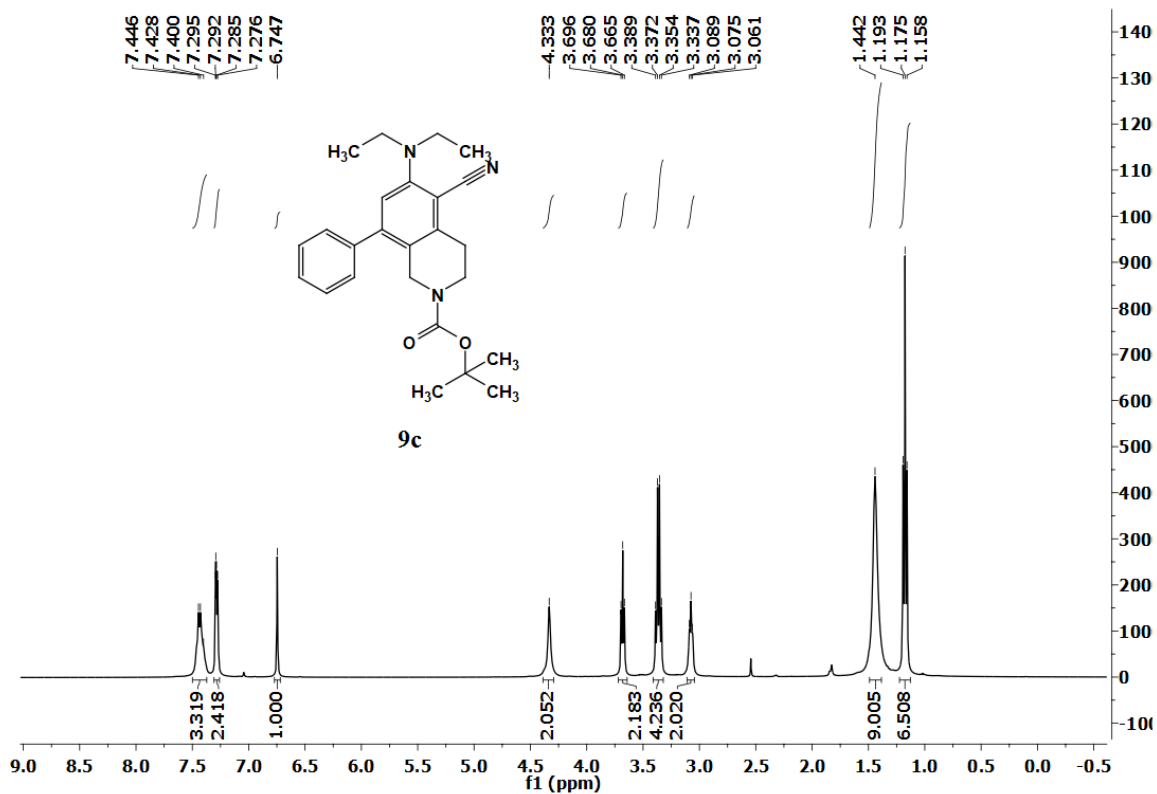
<sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): *tert*-butyl-5-cyano-8-phenyl-6-(4-phenylpiperazin-1-yl)-3,4-dihydroisoquinoline-2(1H)-carboxylate 9b.



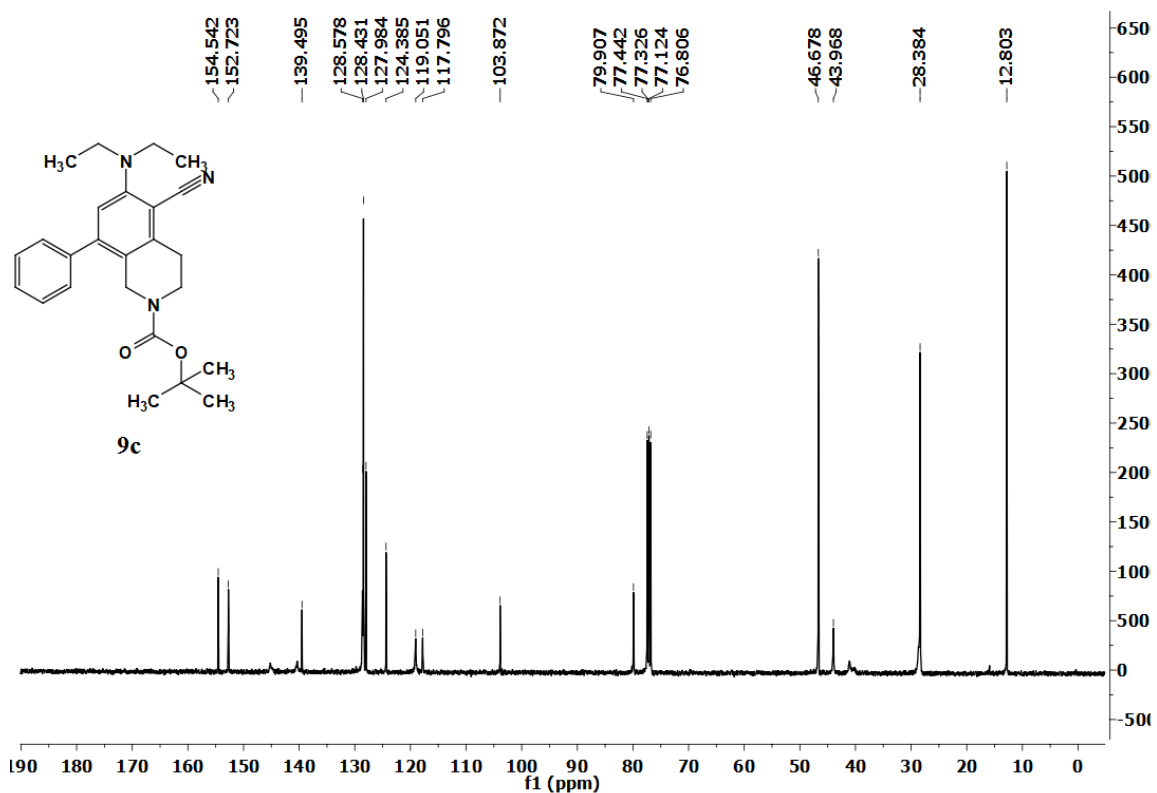
<sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): *tert*-butyl-5-cyano-8-phenyl-6-(4-phenylpiperazin-1-yl)-3,4-dihydroisoquinoline-2(1H)-carboxylate 9b.



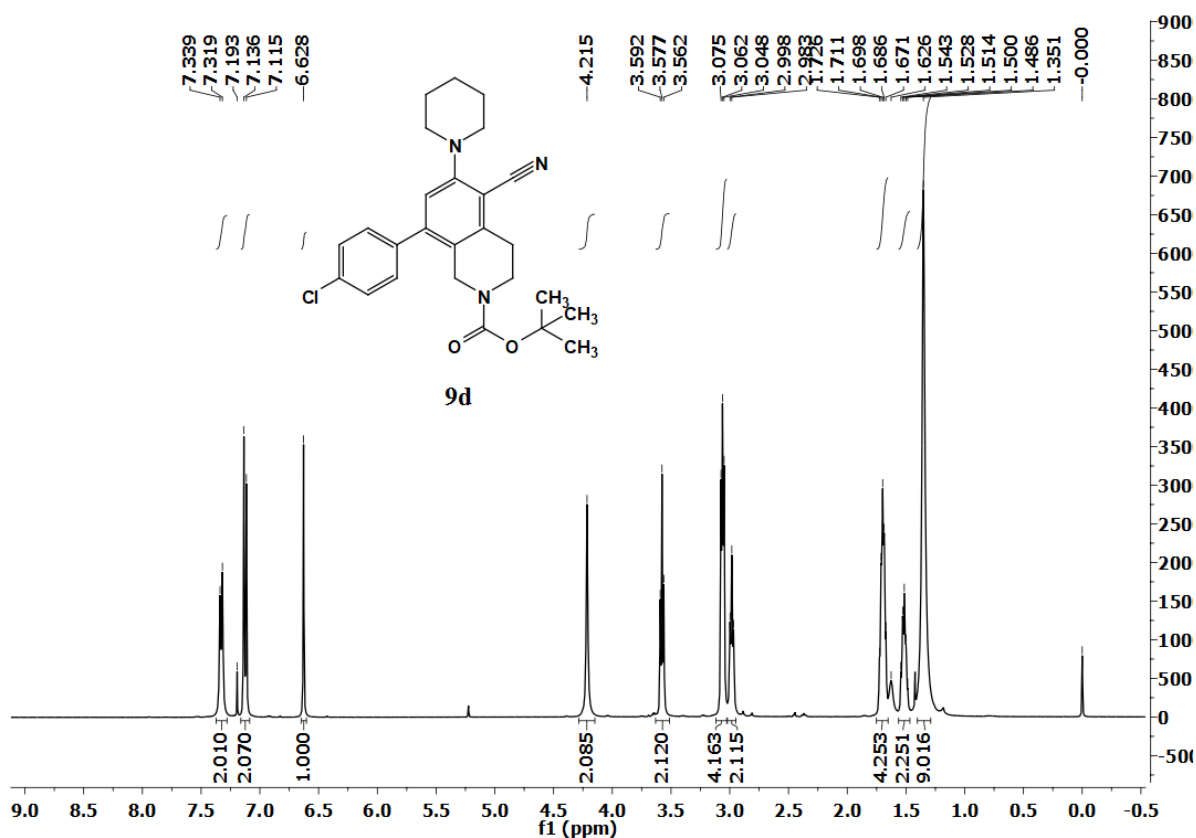
<sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): *tert*-butyl-5-cyano-6-(diethylamino)-8-phenyl-3,4-dihydroisoquinoline-2(1H)-carboxylate 9c.



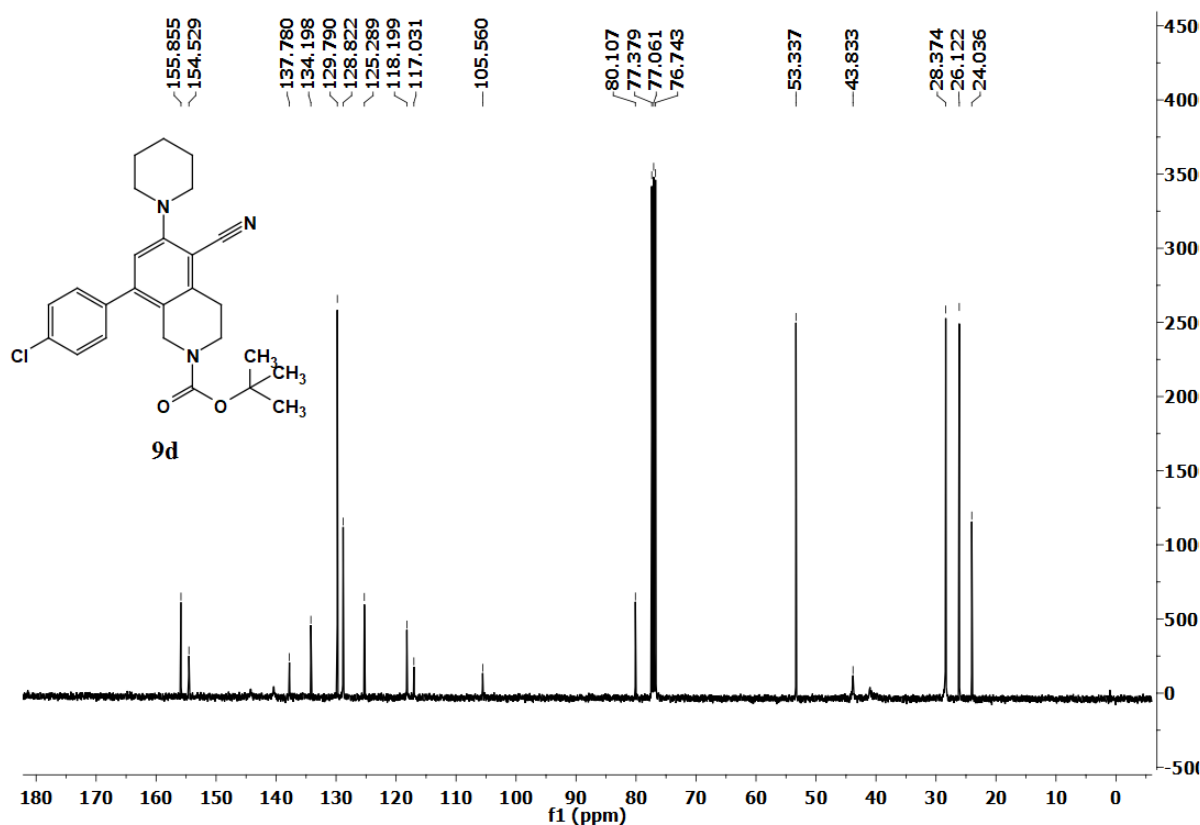
<sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): *tert*-butyl-5-cyano-6-(diethylamino)-8-phenyl-3,4-dihydroisoquinoline-2(1H)-carboxylate 9c.



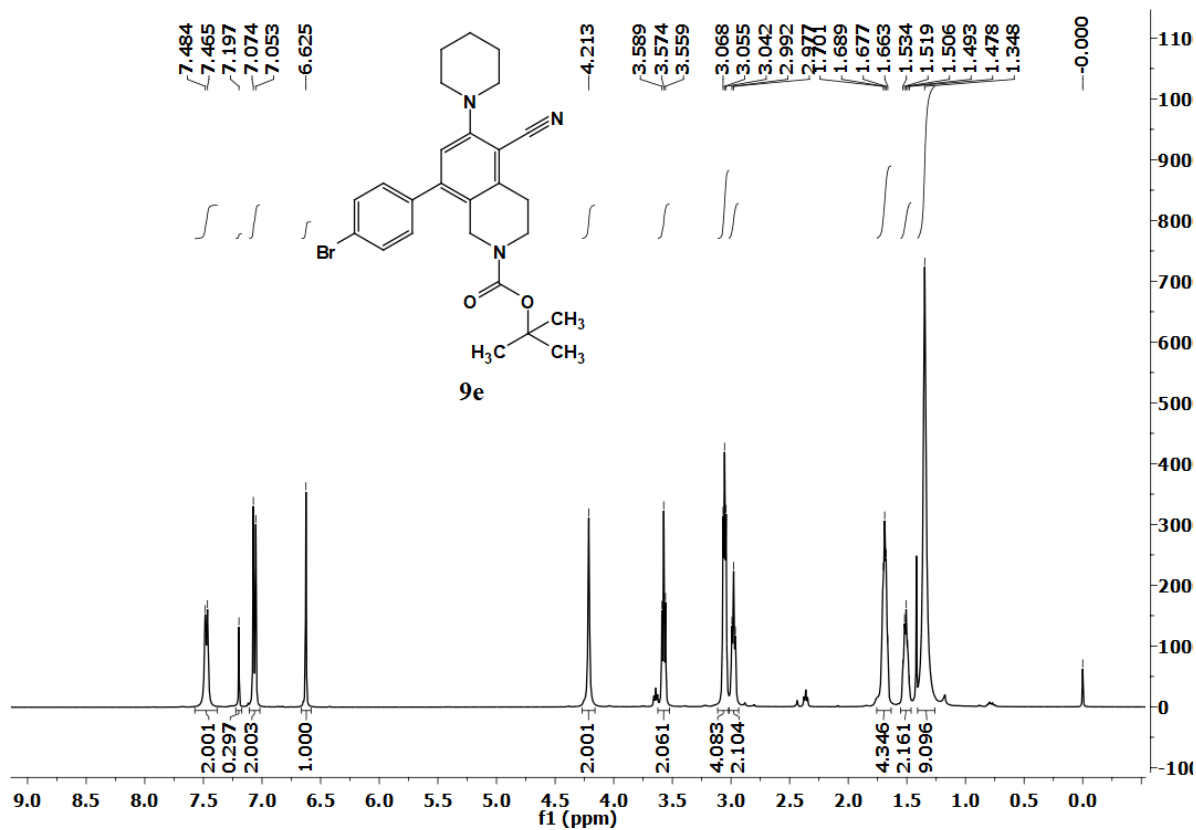
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz): *tert*-butyl-8-(4-chlorophenyl)-5-cyano-6-(piperidin-1-yl)-3,4-dihydroisoquinoline-2(1H)-carboxylate 9d.



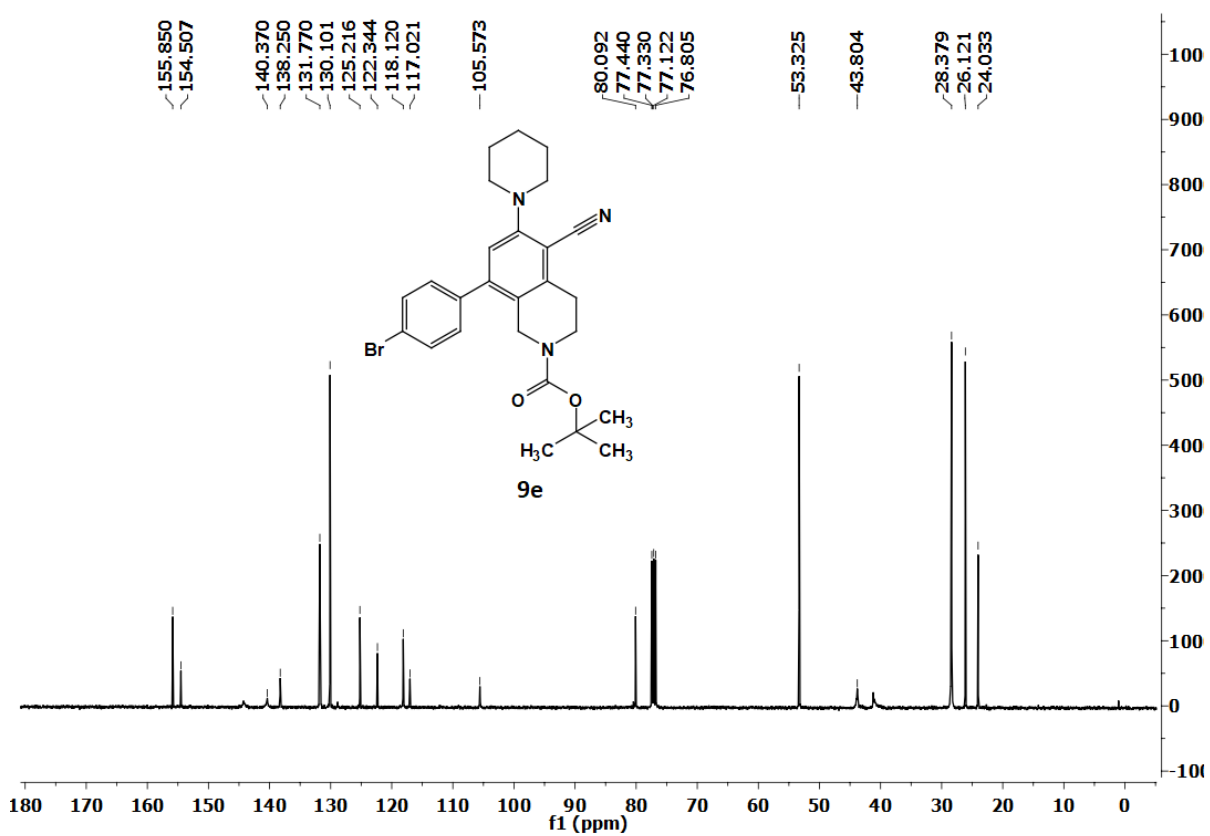
$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz): *tert*-butyl-8-(4-chlorophenyl)-5-cyano-6-(piperidin-1-yl)-3,4-dihydroisoquinoline-2(1H)-carboxylate 9d.



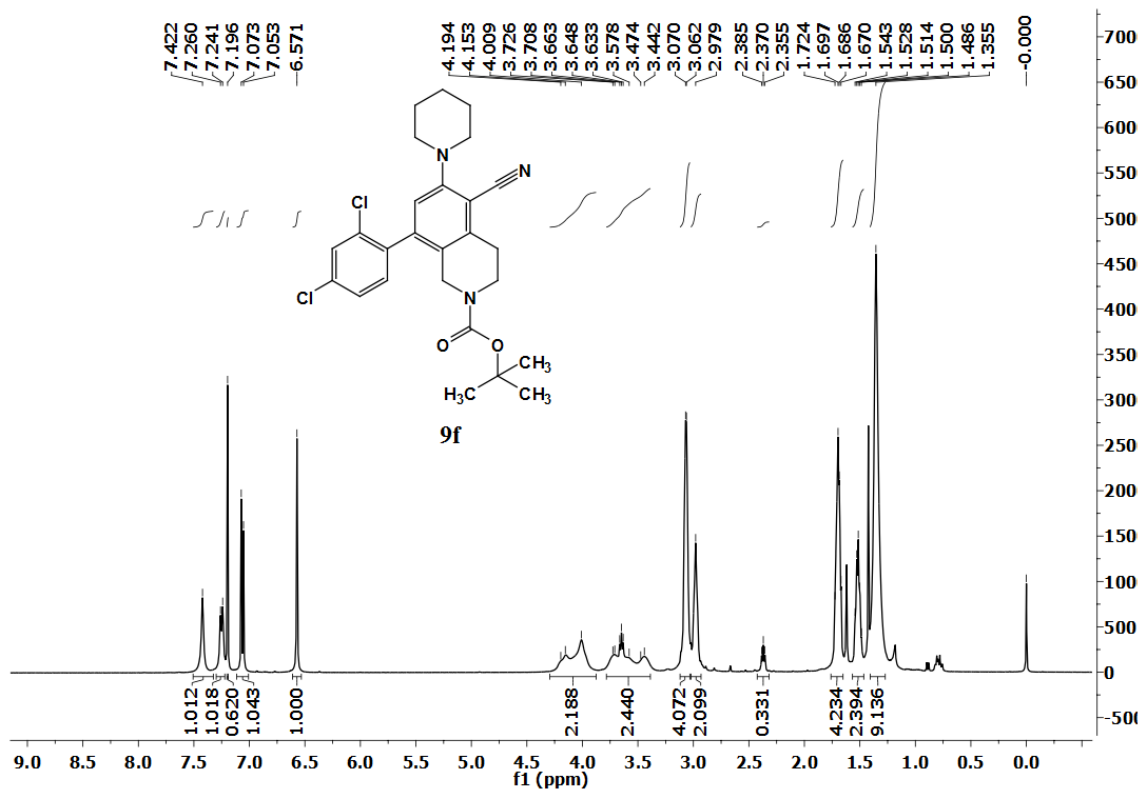
<sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): *tert*-butyl-8-(4-bromophenyl)-5-cyano-6-(piperidin-1-yl)-3,4-dihydroisoquinoline-2(1H)-carboxylate **9e**.



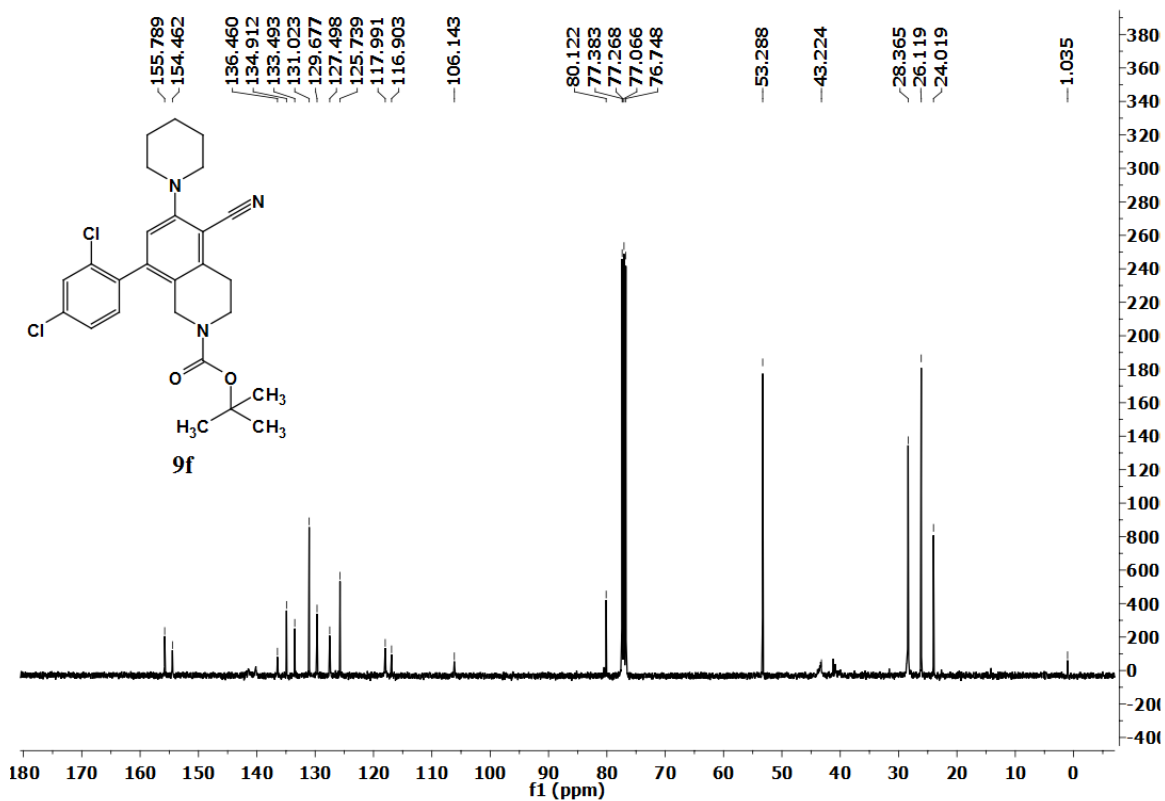
<sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): *tert*-butyl-8-(4-bromophenyl)-5-cyano-6-(piperidin-1-yl)-3,4-dihydroisoquinoline-2(1H)-carboxylate **9e**.



$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz): *tert*-butyl-5-cyano-8-(2,4-dichlorophenyl)-6-(piperidin-1-yl)-3,4-dihydroisoquinoline-2(1H)-carboxylate 9f.

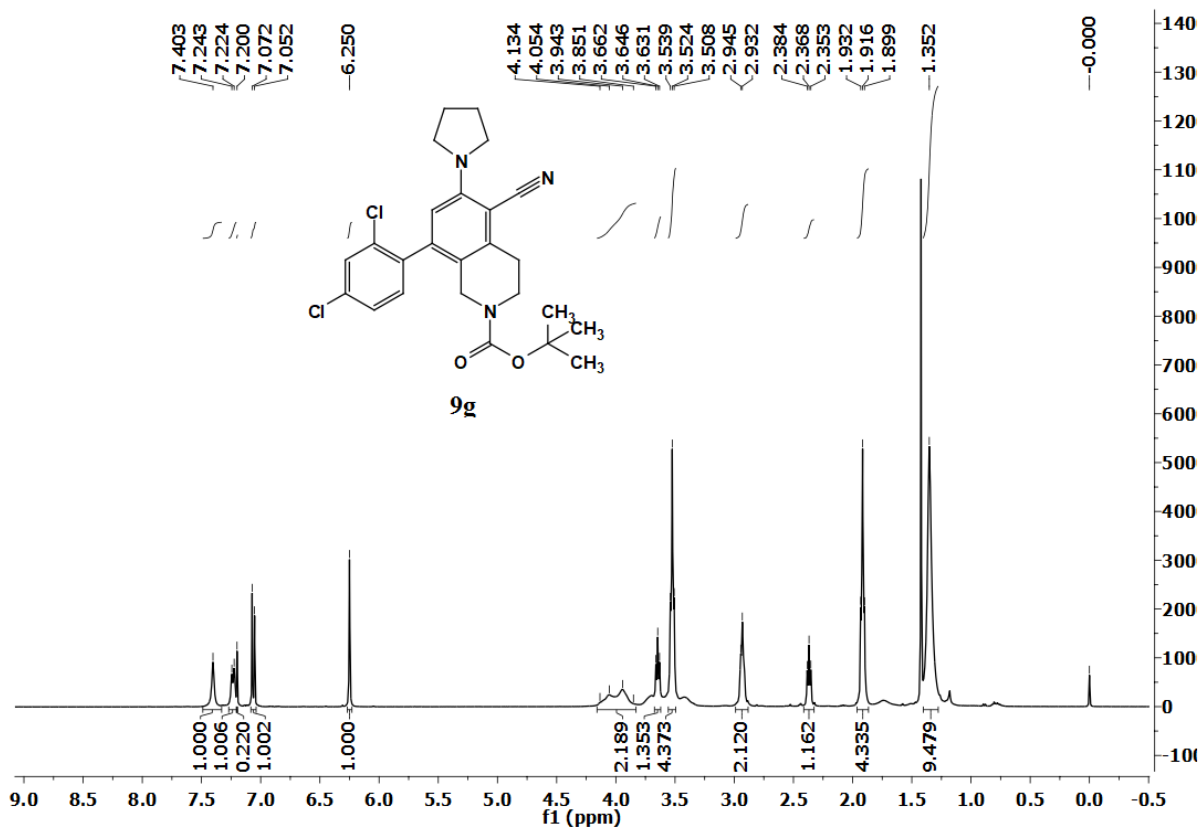


$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz): *tert*-butyl-5-cyano-8-(2,4-dichlorophenyl)-6-(piperidin-1-yl)-3,4-dihydroisoquinoline-2(1H)-carboxylate 9f.

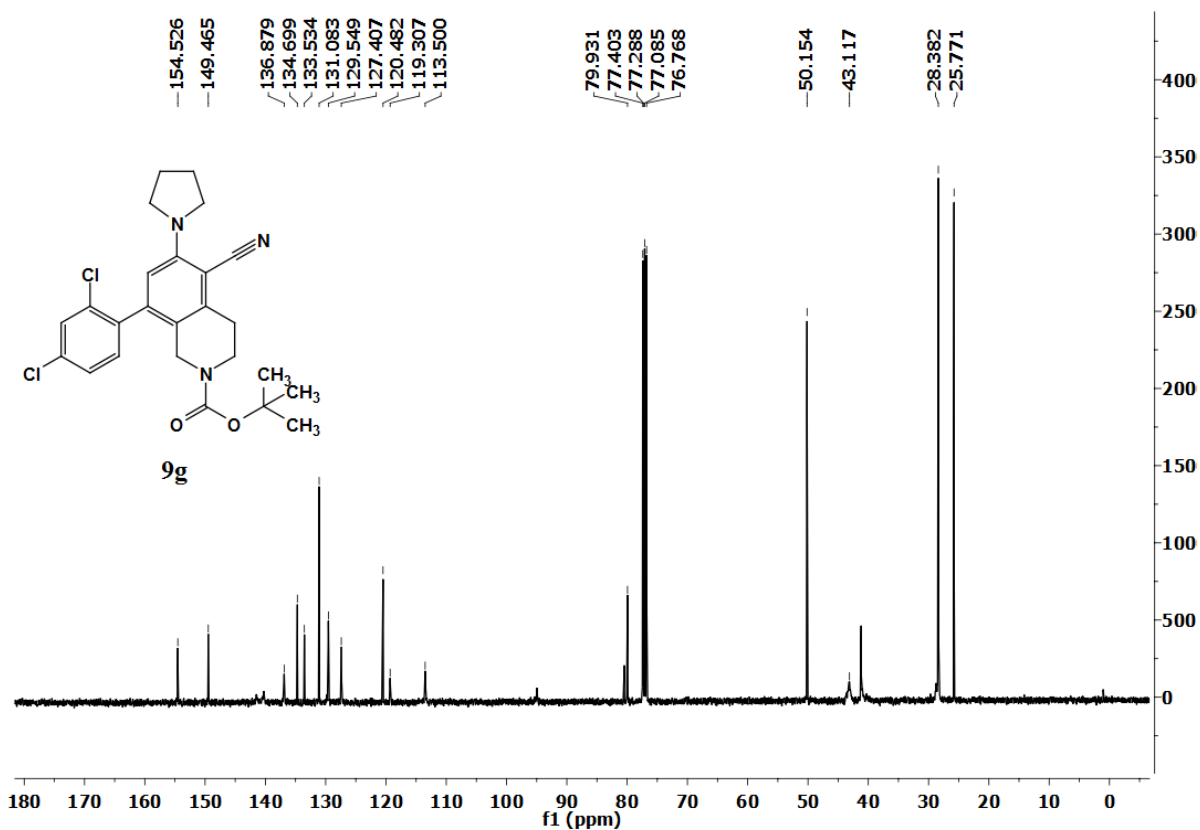




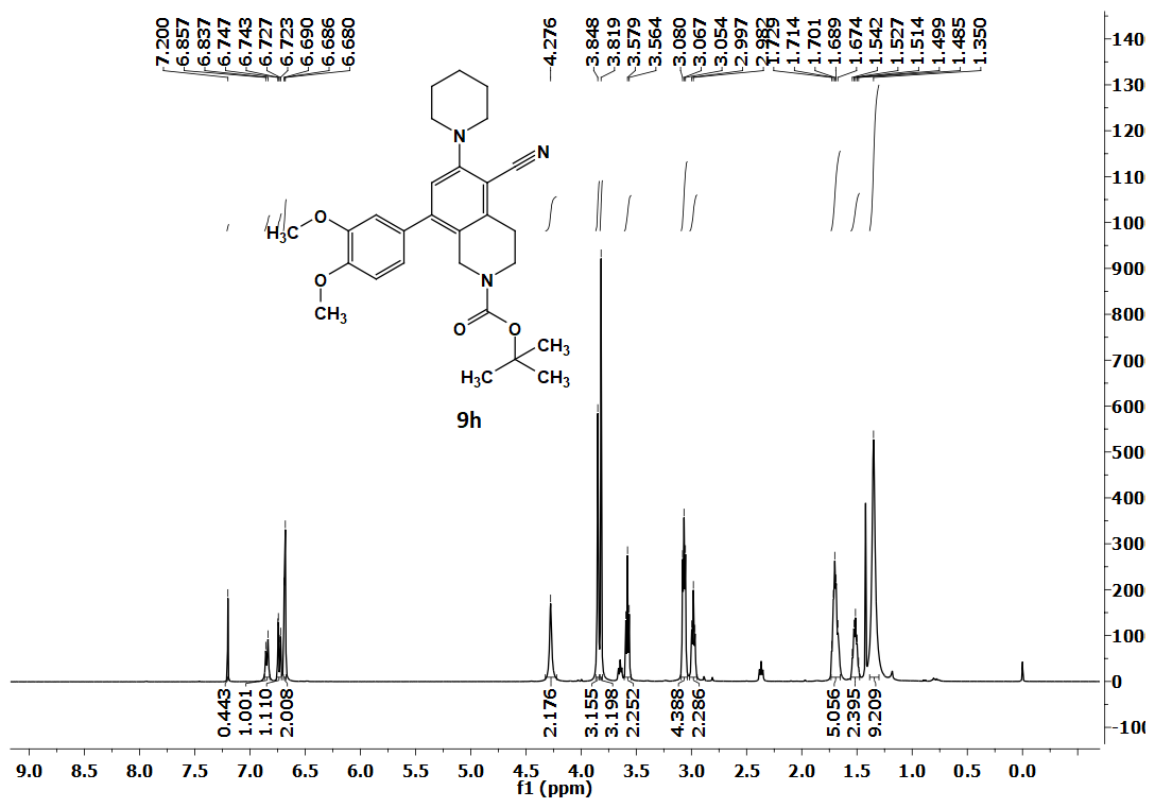
<sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): *tert*-butyl-5-cyano-8-(2,4-dichlorophenyl)-6-(pyrrolidin-1-yl)-3,4-dihydroisoquinoline-2(1H)-carboxylate 9g.



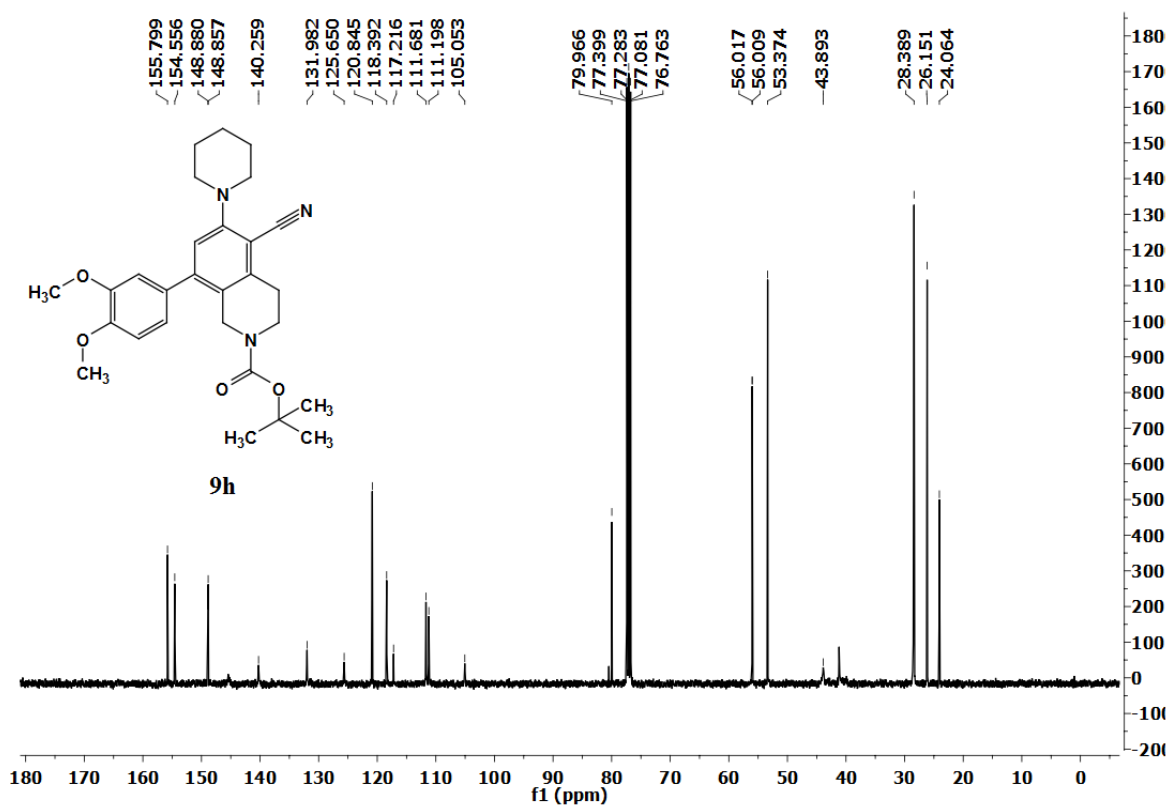
<sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): *tert*-butyl-5-cyano-8-(2,4-dichlorophenyl)-6-(pyrrolidin-1-yl)-3,4-dihydroisoquinoline-2(1H)-carboxylate 9g.



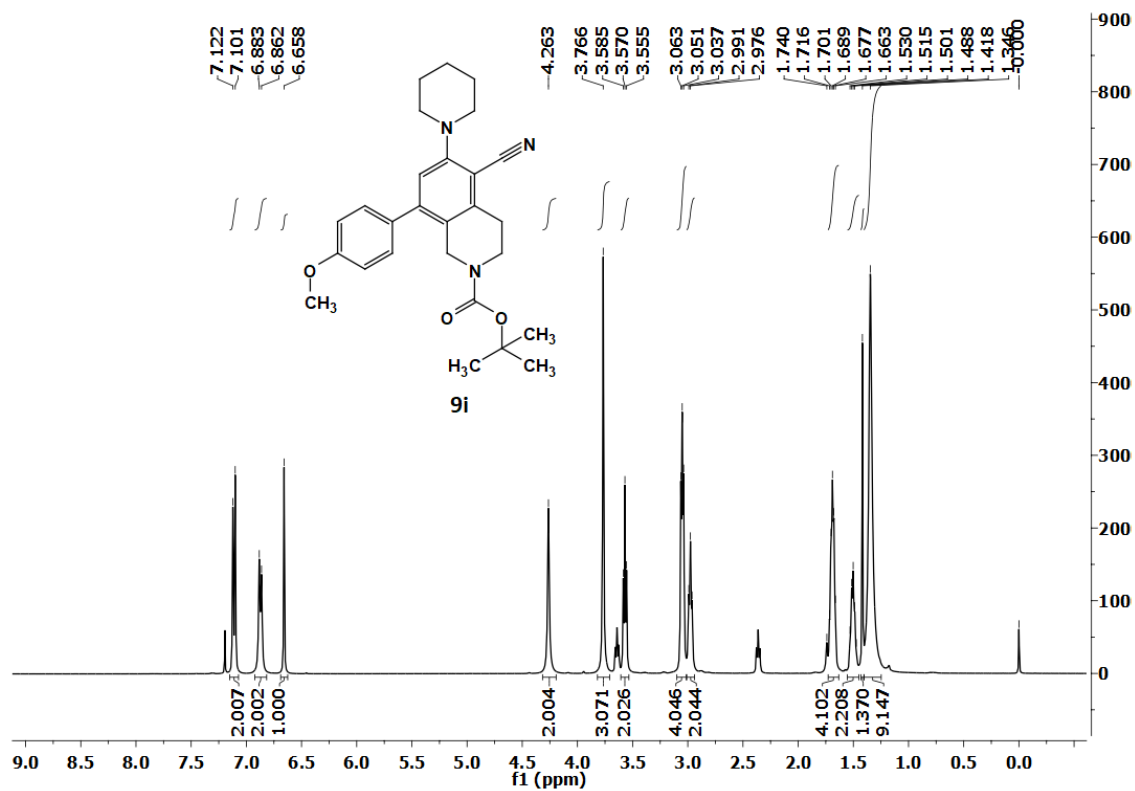
<sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): *tert*-butyl-5-cyano-8-(3,4-dimethoxyphenyl)-6-(piperidin-1-yl)-3,4-dihydroisoquinoline-2(1H)-carboxylate 9h.



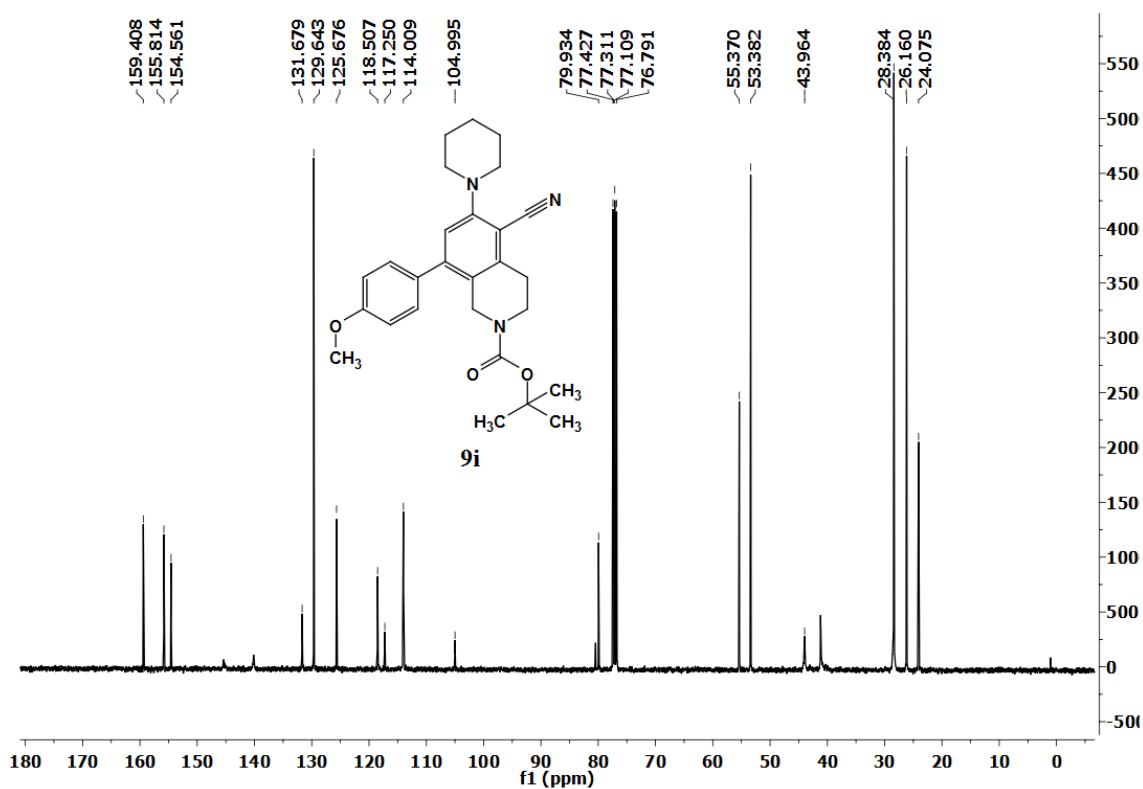
<sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): *tert*-butyl-5-cyano-8-(3,4-dimethoxyphenyl)-6-(piperidin-1-yl)-3,4-dihydroisoquinoline-2(1H)-carboxylate 9h.



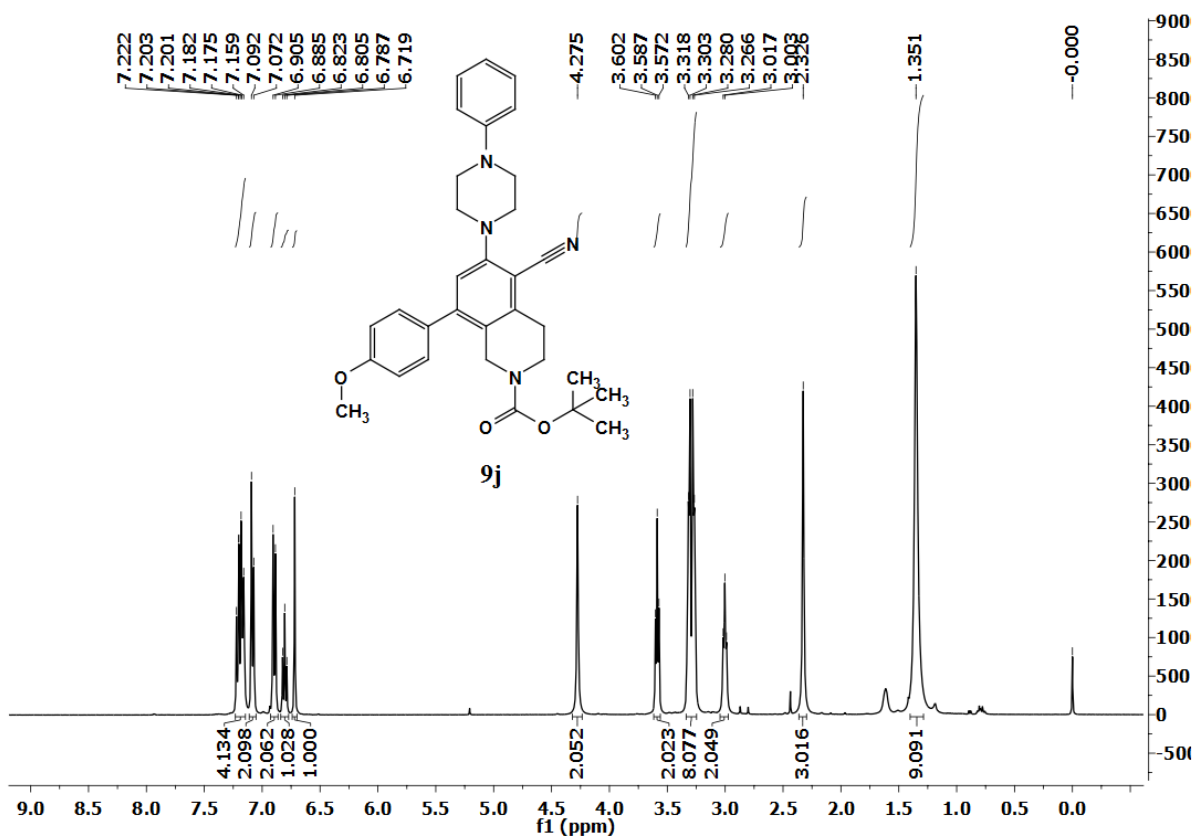
<sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): *tert*-butyl-5-cyano-8-(4-methoxyphenyl)-6-(piperidin-1-yl)-3,4-dihydroisoquinoline-2(1H)-carboxylate 9i.



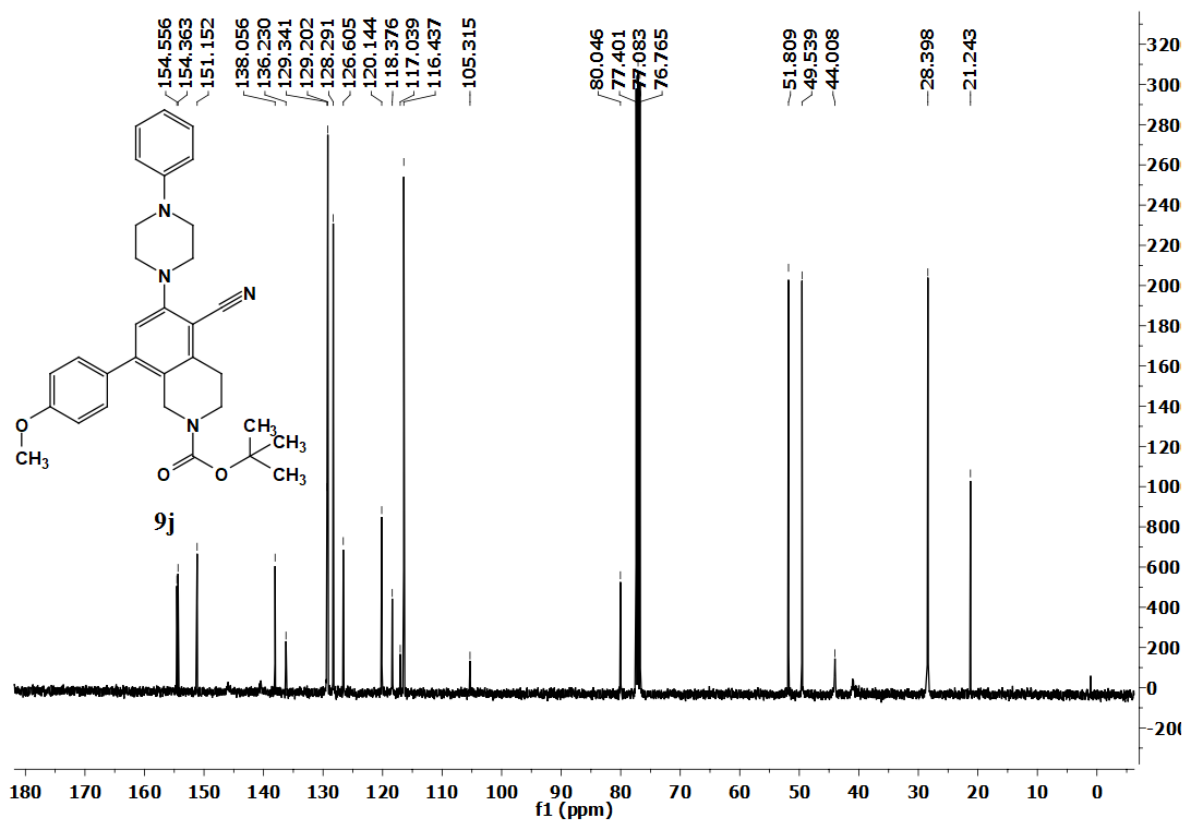
<sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): *tert*-butyl-5-cyano-8-(4-methoxyphenyl)-6-(piperidin-1-yl)-3,4-dihydroisoquinoline-2(1H)-carboxylate 9i.



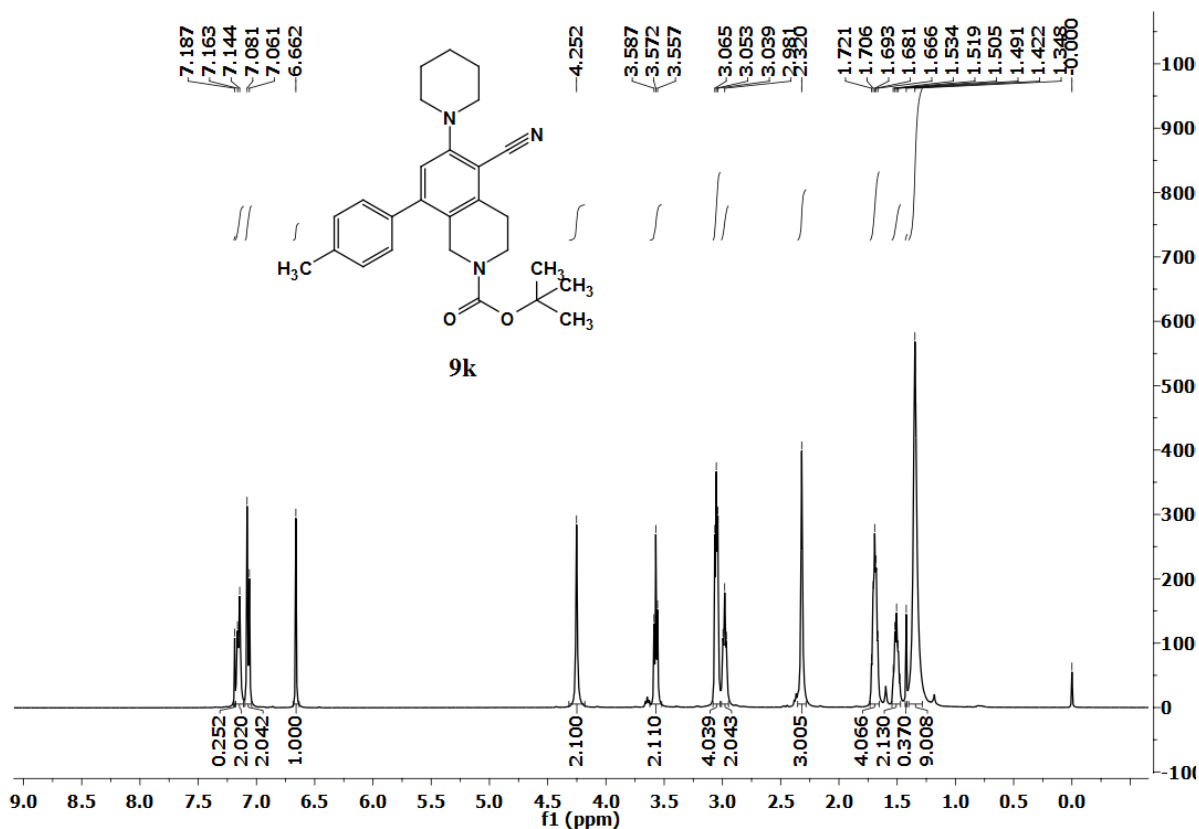
<sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): *tert*-butyl-5-cyano-8-(4-methoxyphenyl)-6-(4-phenylpiperazin-1-yl)-3,4-dihydroisoquinoline-2(1H)-carboxylate 9j.



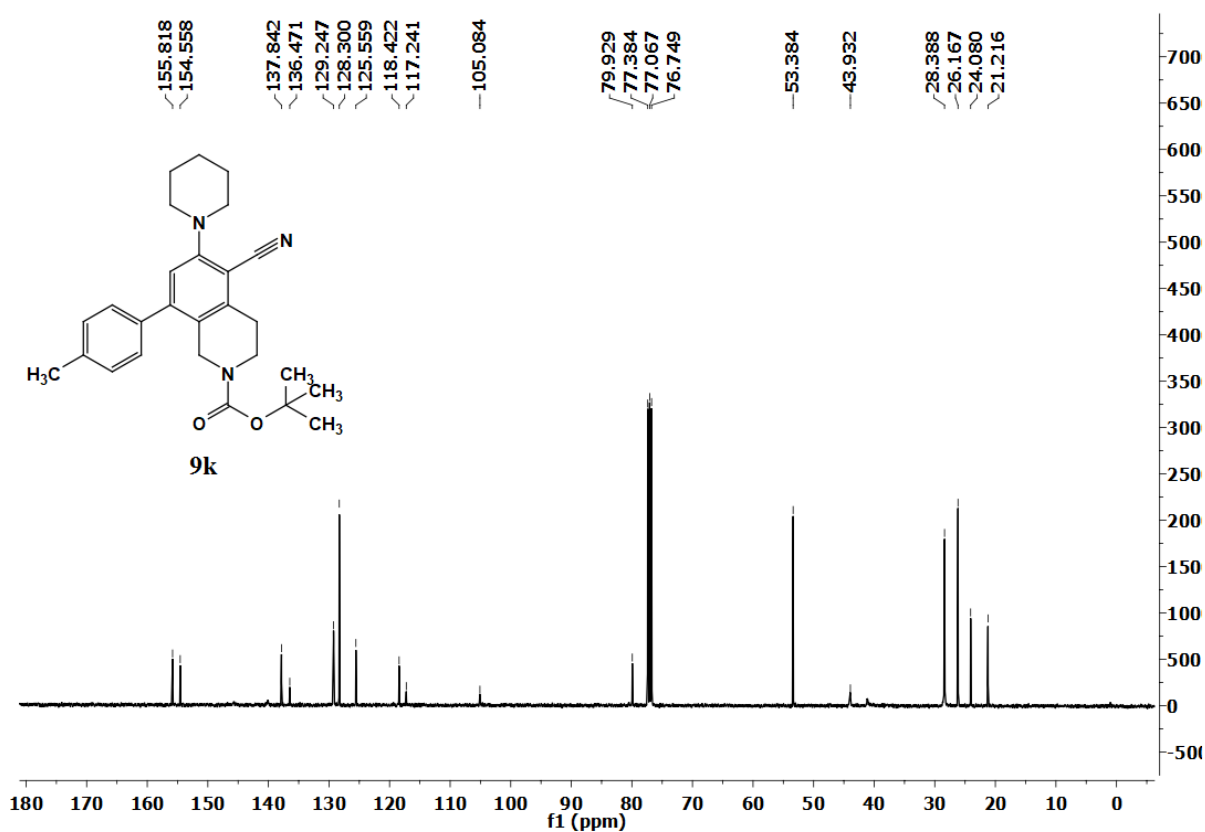
<sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): *tert*-butyl-5-cyano-8-(4-methoxyphenyl)-6-(4-phenylpiperazin-1-yl)-3,4-dihydroisoquinoline-2(1H)-carboxylate 9j.



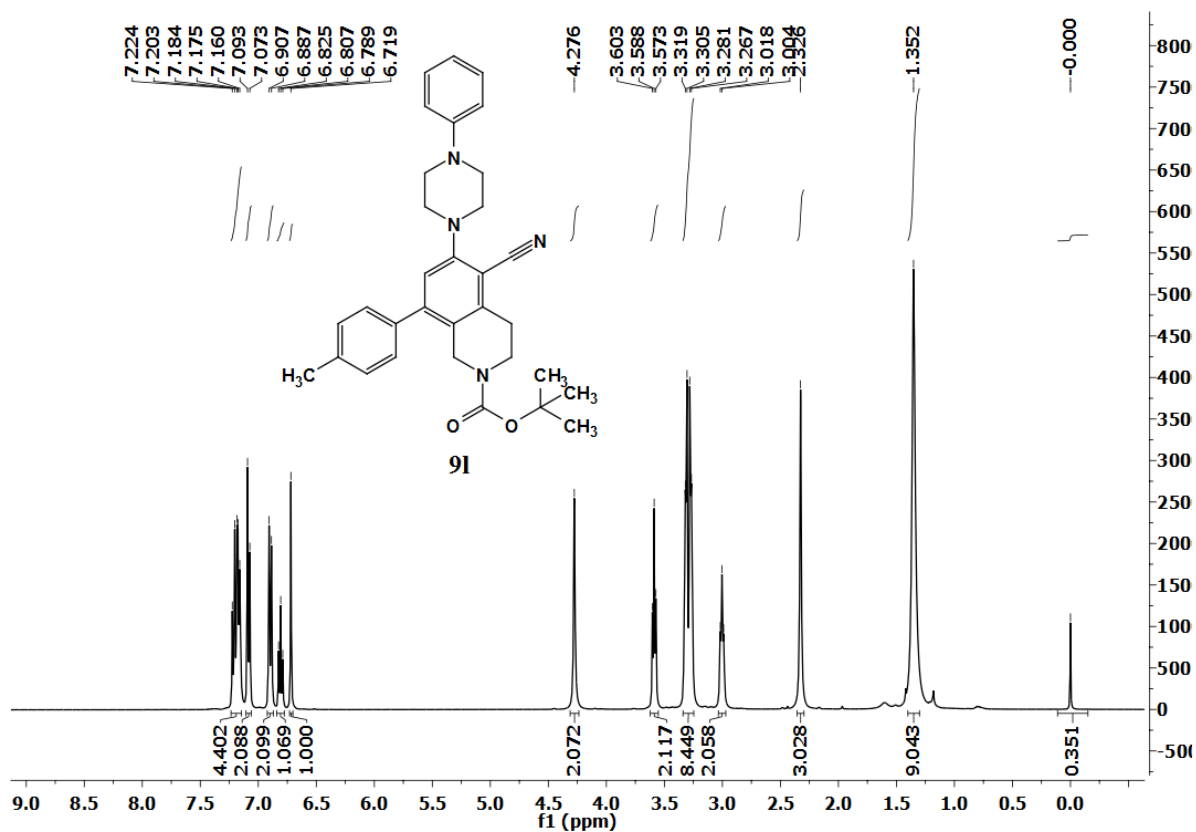
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz): *tert*-butyl-5-cyano-6-(piperidin-1-yl)-8-(*p*-tolyl)-3,4-dihydroisoquinoline-2(1H)-carboxylate 9k.



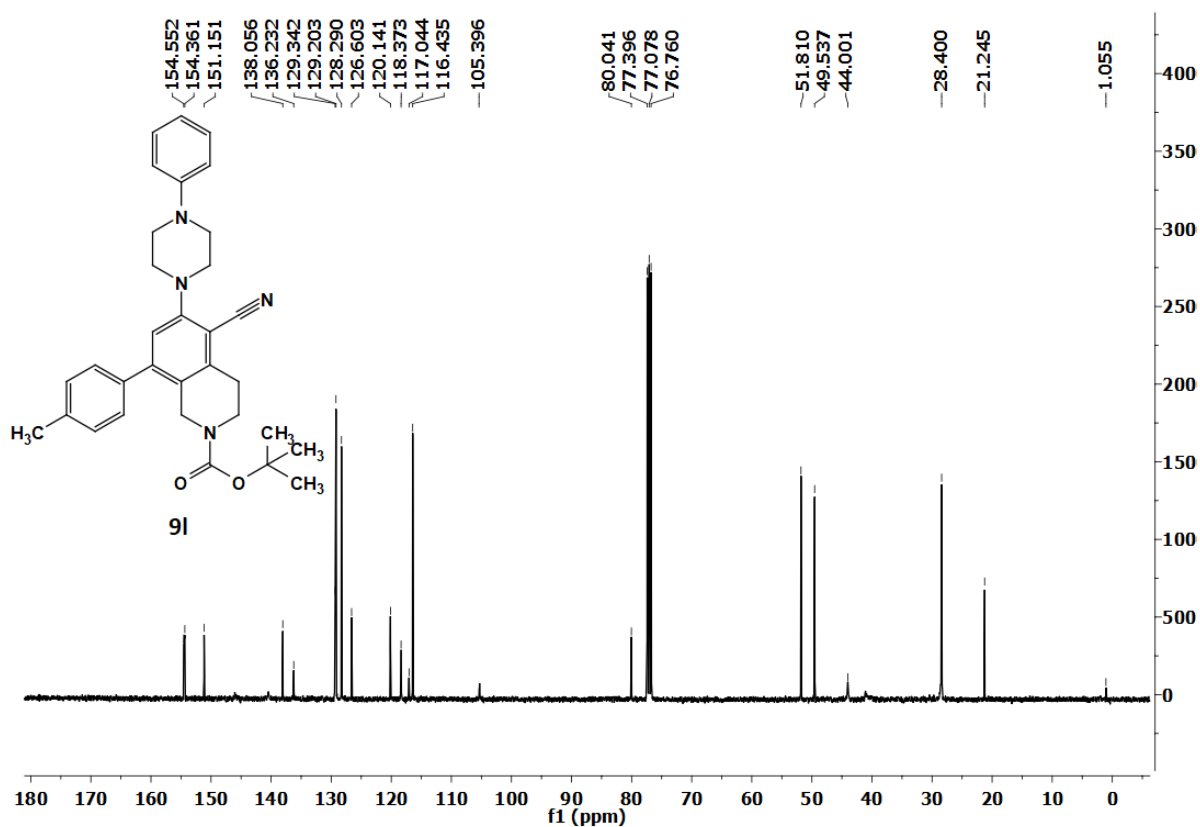
$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz): *tert*-butyl-5-cyano-6-(piperidin-1-yl)-8-(*p*-tolyl)-3,4-dihydroisoquinoline-2(1H)-carboxylate 9k.



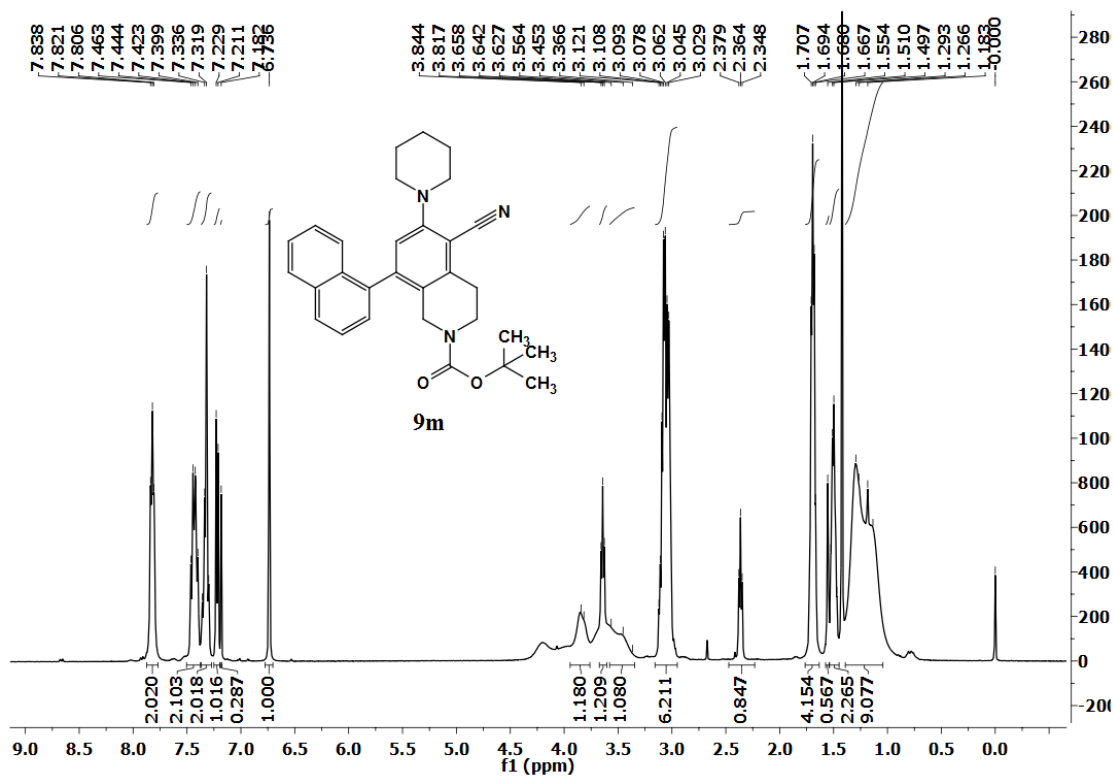
<sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): *tert*-butyl-5-cyano-6-(4-phenylpiperazin-1-yl)-8-(*p*-tolyl)-3,4-dihydroisoquinoline-2(1H)-carboxylate 9l.



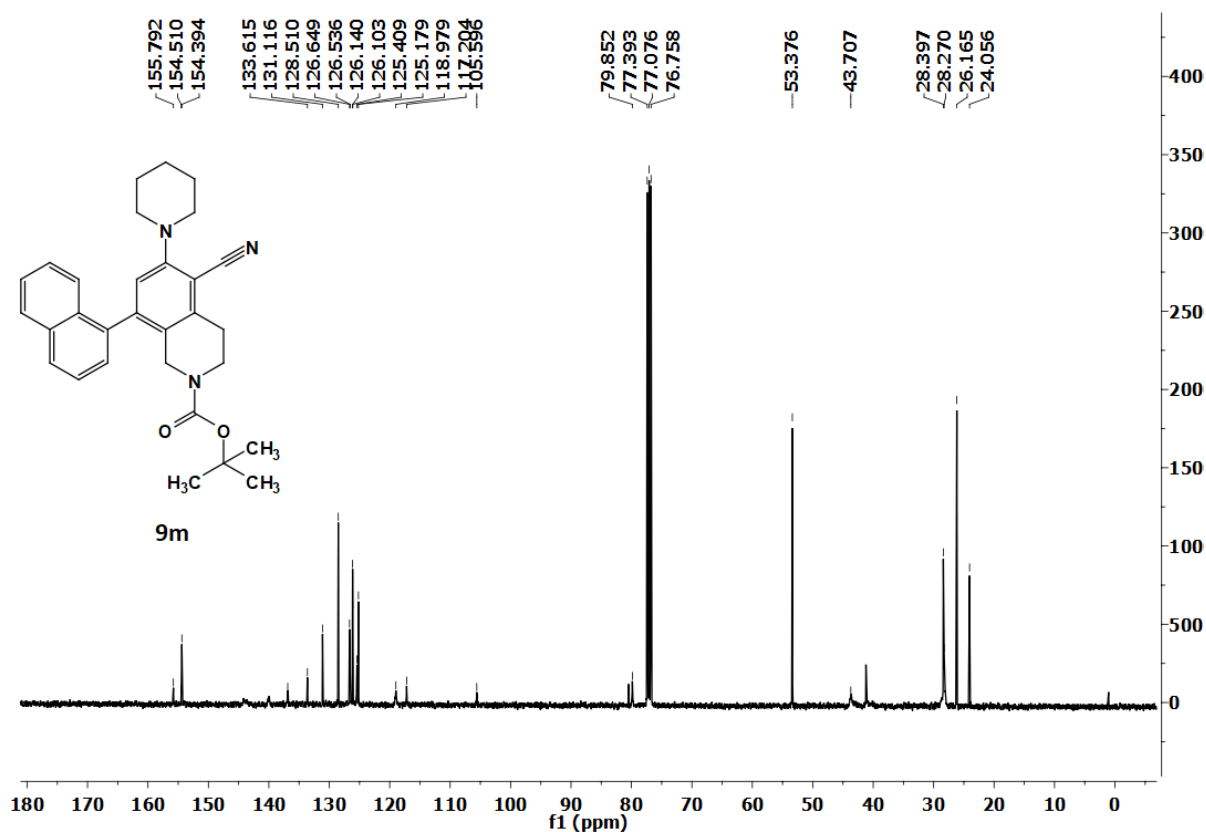
<sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): *tert*-butyl-5-cyano-6-(4-phenylpiperazin-1-yl)-8-(*p*-tolyl)-3,4-dihydroisoquinoline-2(1H)-carboxylate 9l.



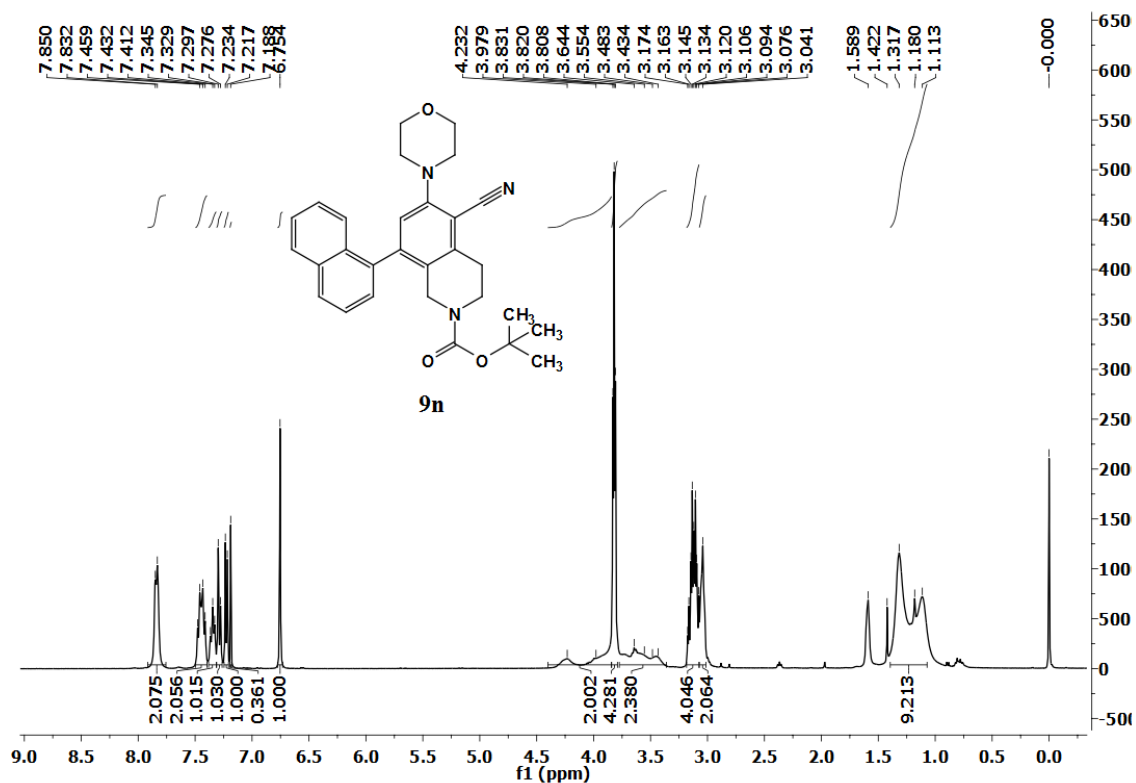
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz): *tert*-butyl-5-cyano-8-(naphthalen-1-yl)-6-(piperidin-1-yl)-3,4-dihydroisoquinoline-2(1H)-carboxylate 9m.



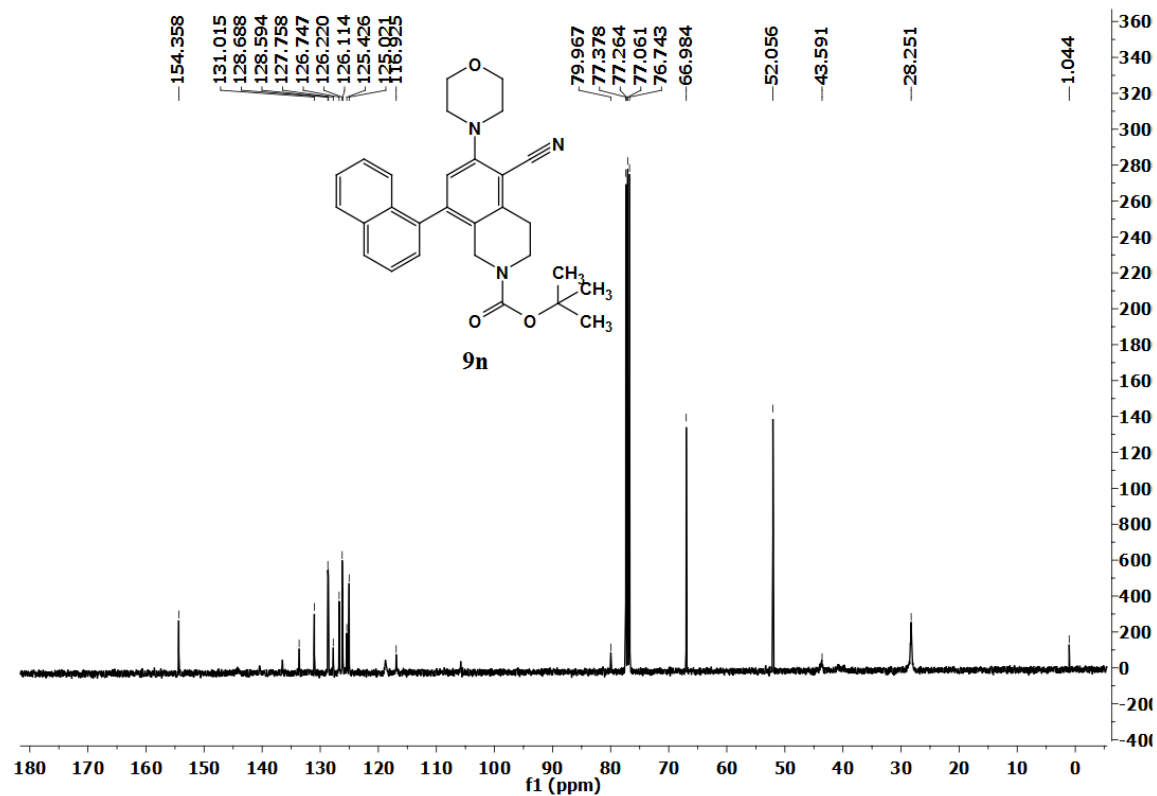
$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz): *tert*-butyl-5-cyano-8-(naphthalen-1-yl)-6-(piperidin-1-yl)-3,4-dihydroisoquinoline-2(1H)-carboxylate 9m.



<sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): *tert*-butyl-5-cyano-6-morpholino-8-(naphthalen-1-yl)-3,4-dihydroisoquinoline-2(1H)-carboxylate **9n**.

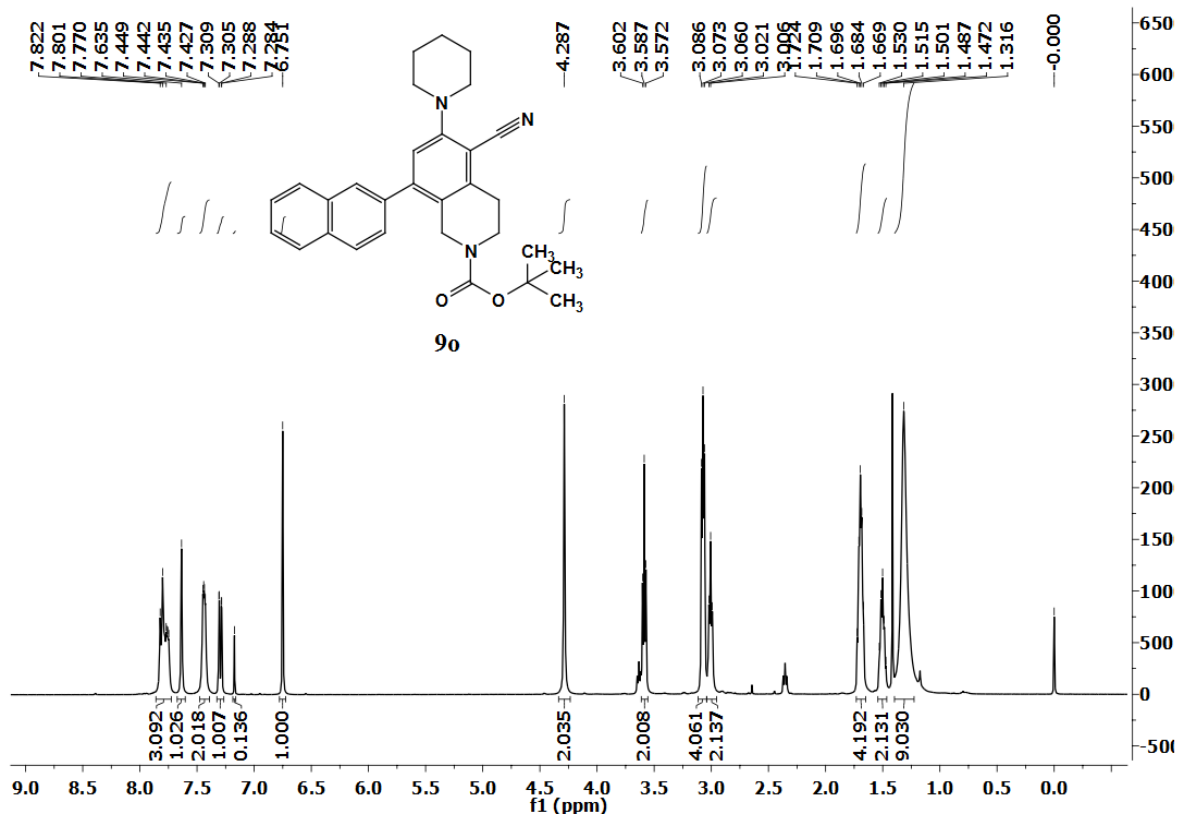


<sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): *tert*-butyl-5-cyano-6-morpholino-8-(naphthalen-1-yl)-3,4-dihydroisoquinoline-2(1H)-carboxylate **9n**.

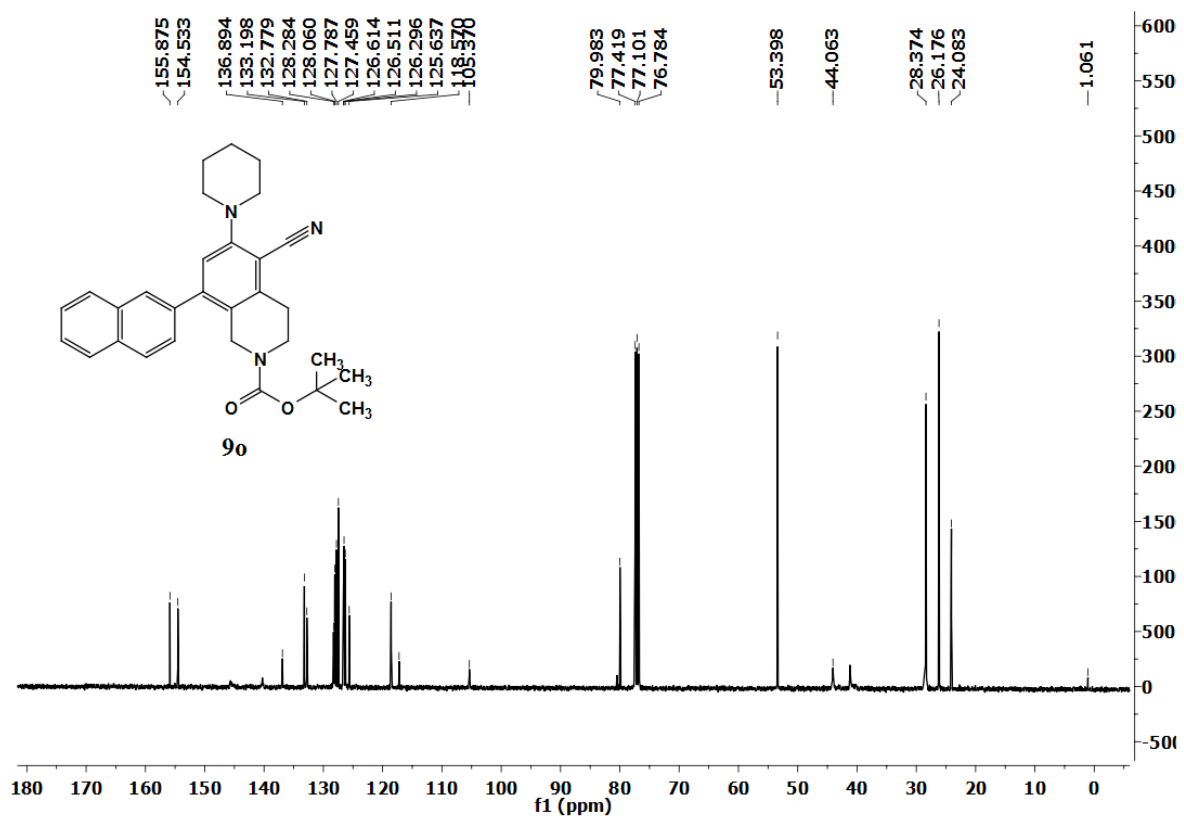




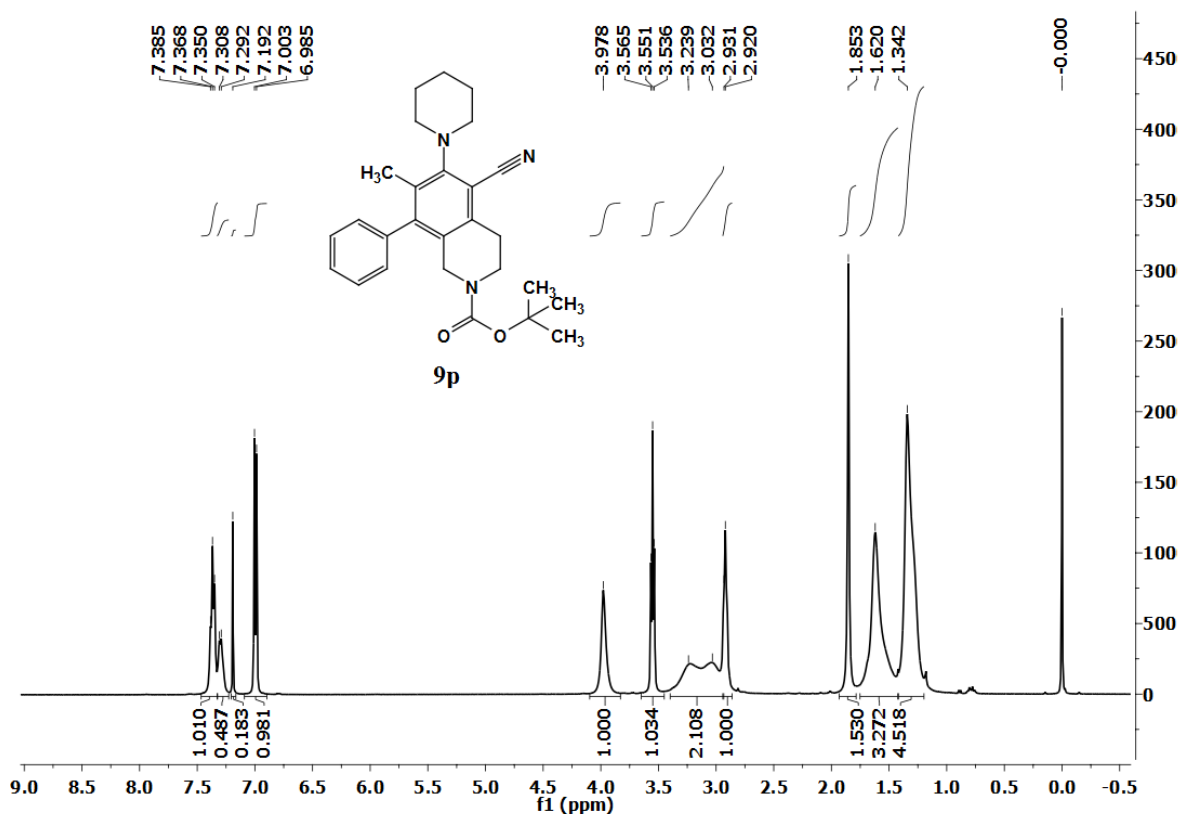
<sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): *tert*-butyl-5-cyano-8-(naphthalen-2-yl)-6-(piperidin-1-yl)-3,4-dihydroisoquinoline-2(1H)-carboxylate 9o.



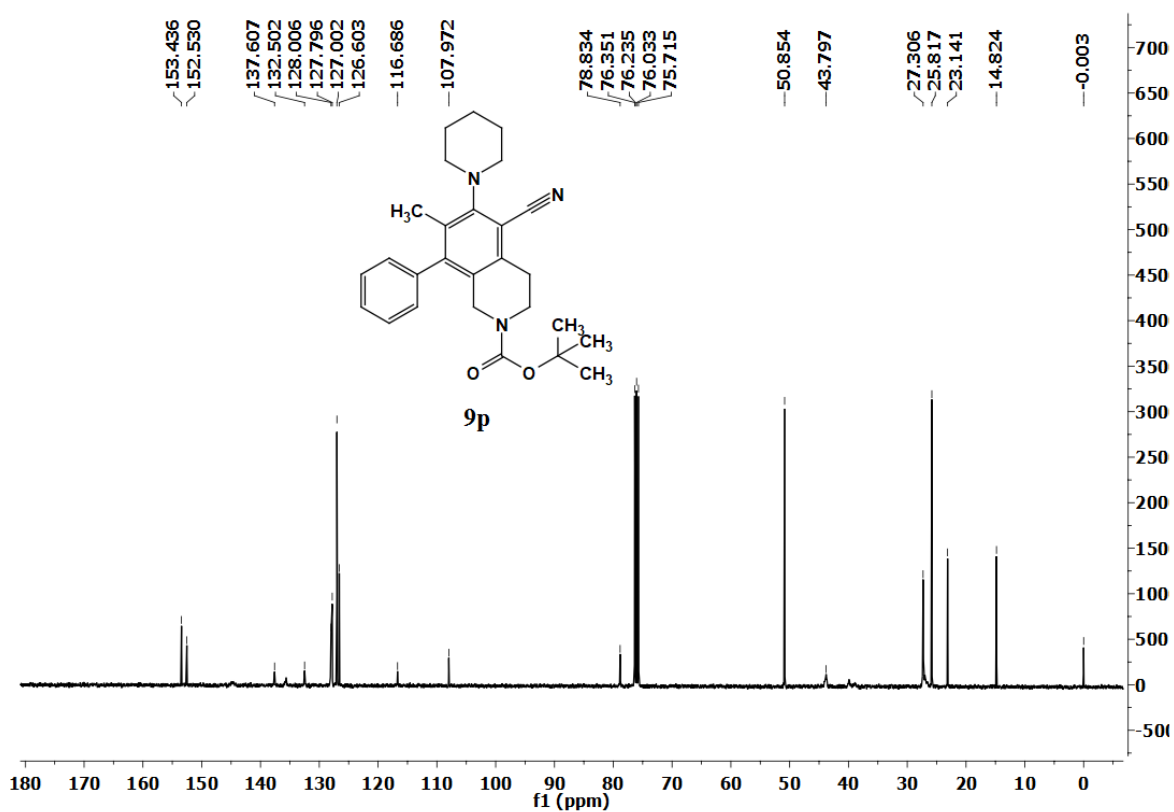
<sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): *tert*-butyl-5-cyano-8-(naphthalen-2-yl)-6-(piperidin-1-yl)-3,4-dihydroisoquinoline-2(1H)-carboxylate 9o.



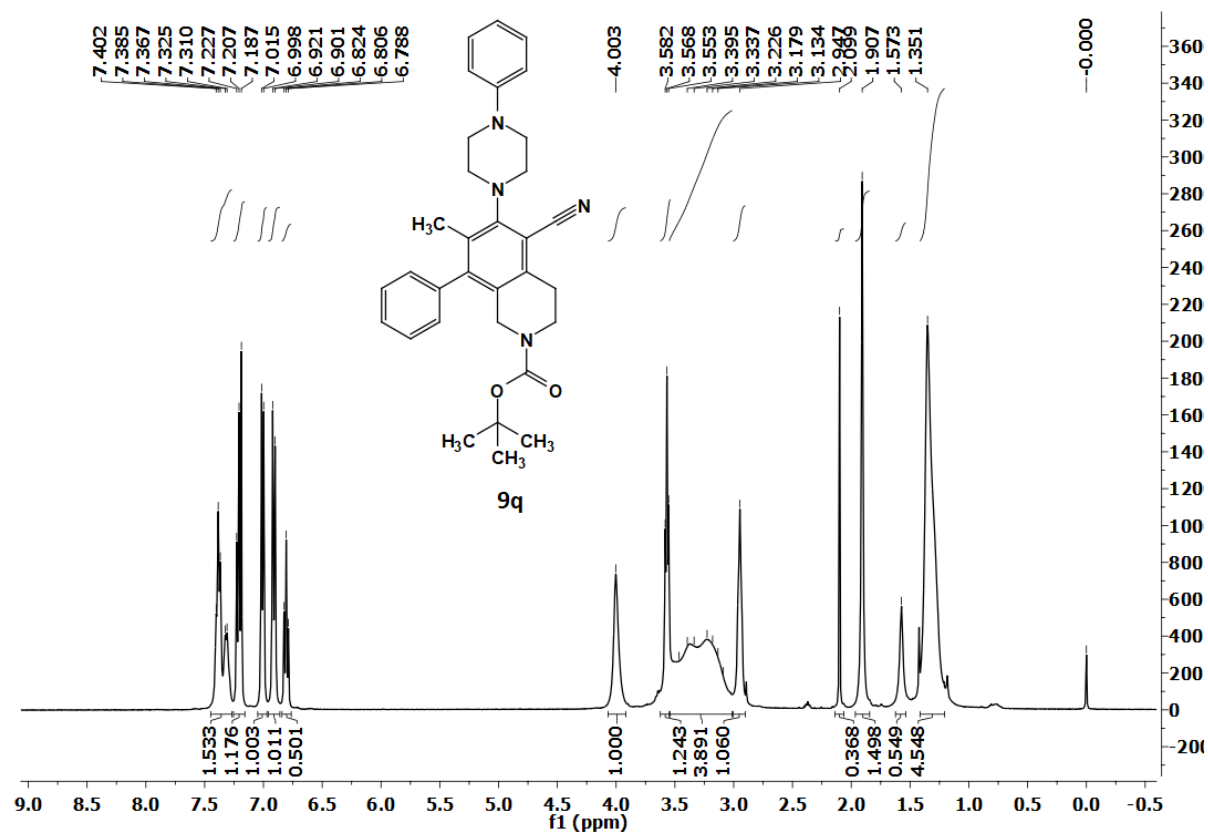
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz): *tert*-butyl-5-cyano-7-methyl-8-phenyl-6-(piperidin-1-yl)-3,4-dihydroisoquinoline-2(1H)-carboxylate **9p**.



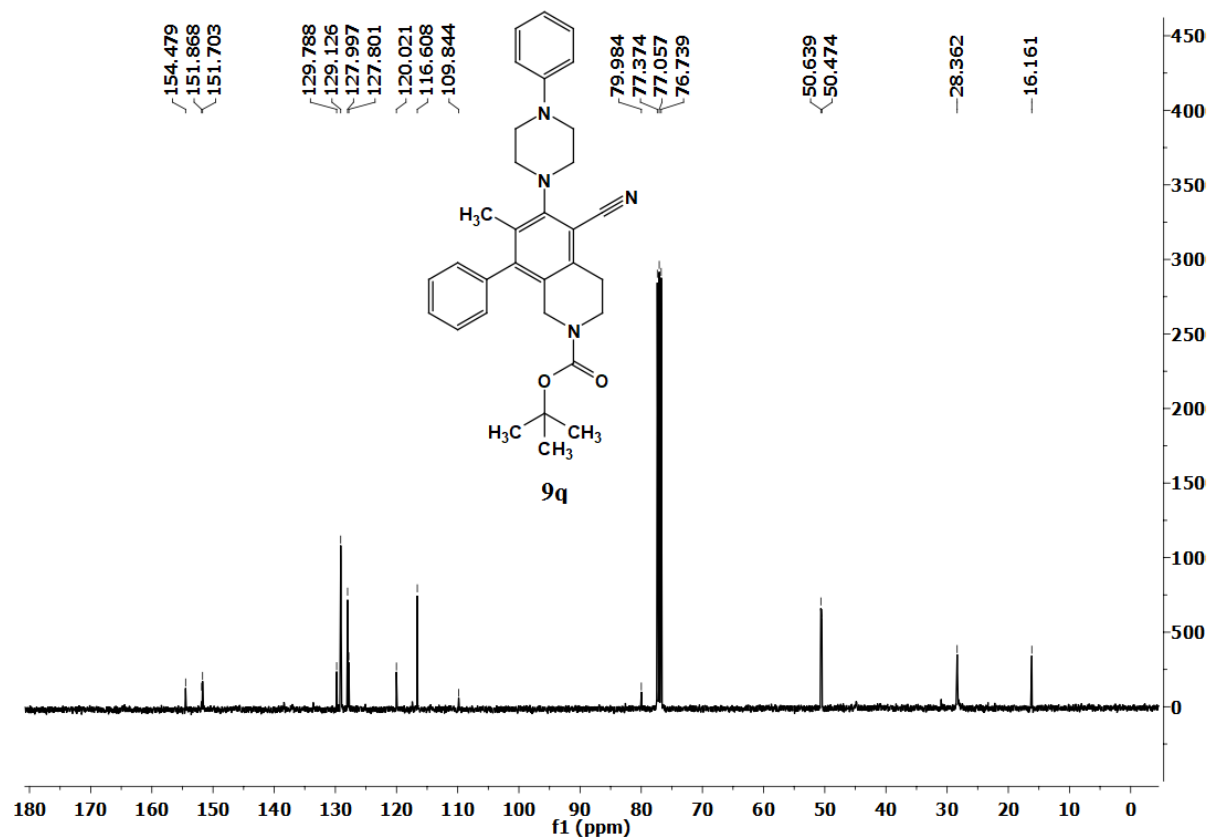
$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz): *tert*-butyl-5-cyano-7-methyl-8-phenyl-6-(piperidin-1-yl)-3,4-dihydroisoquinoline-2(1H)-carboxylate **9p**.



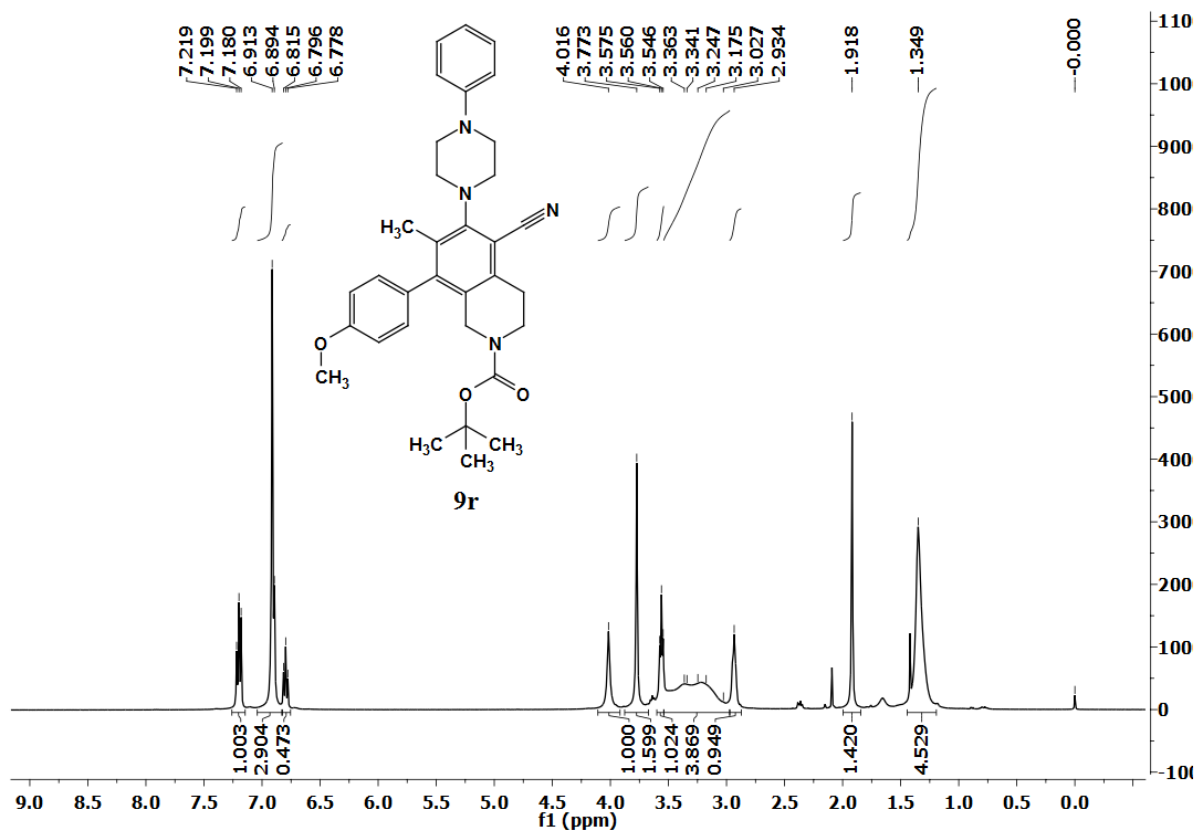
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz): *tert*-butyl-5-cyano-7-methyl-8-phenyl-6-(4-phenylpiperazin-1-yl)-3,4-dihydroisoquinoline-2(1H)-carboxylate 9q.



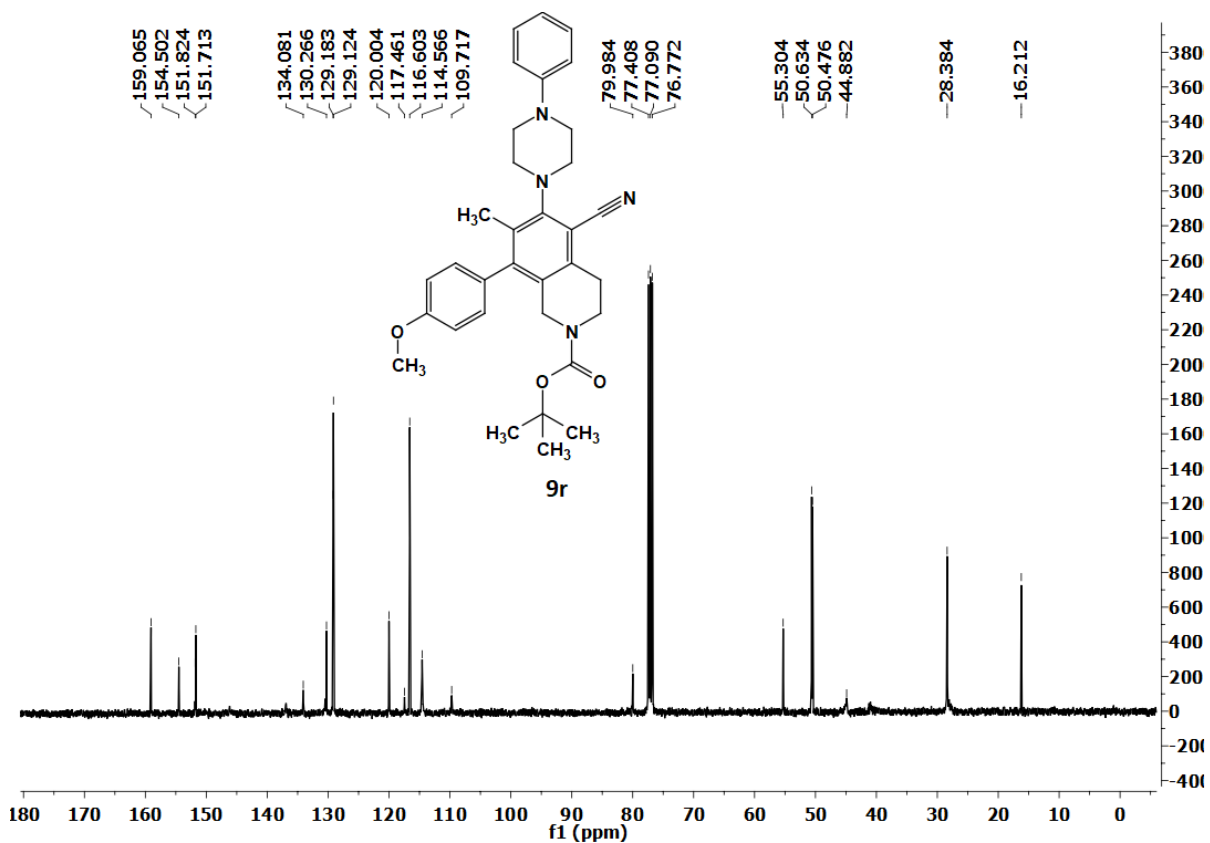
$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz): *tert*-butyl-5-cyano-7-methyl-8-phenyl-6-(4-phenylpiperazin-1-yl)-3,4-dihydroisoquinoline-2(1H)-carboxylate 9q.



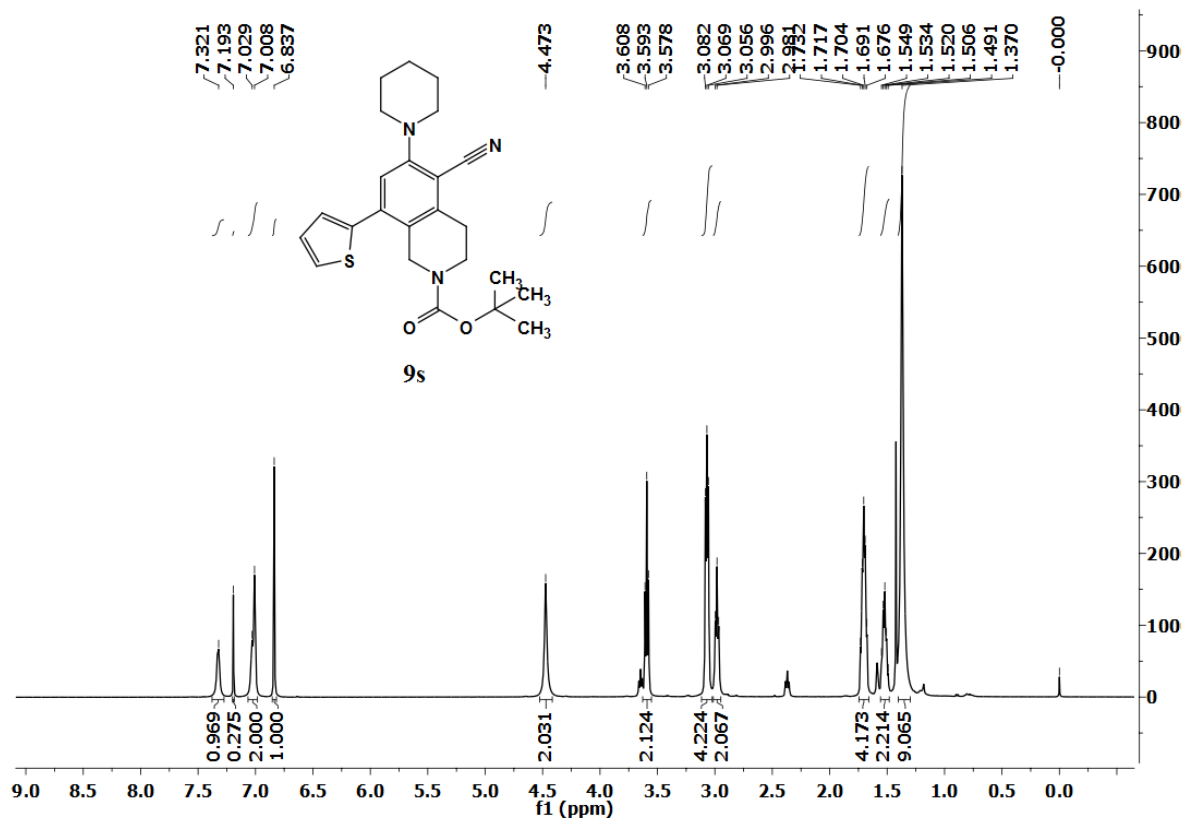
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz): *tert*-butyl-5-cyano-8-(4-methoxyphenyl)-7-methyl-6-(4-phenylpiperazin-1-yl)-3,4-dihydroisoquinoline-2(1H)-carboxylate 9r.



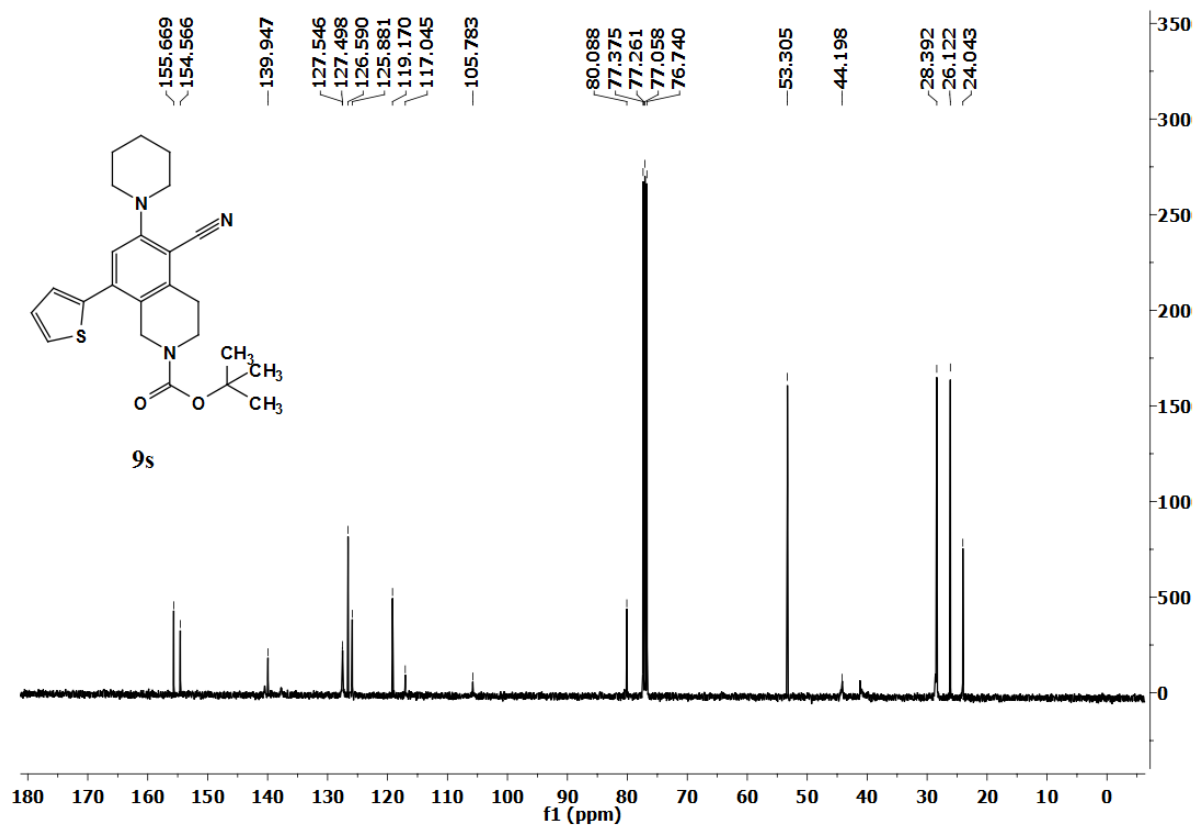
$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz): *tert*-butyl-5-cyano-8-(4-methoxyphenyl)-7-methyl-6-(4-phenylpiperazin-1-yl)-3,4-dihydroisoquinoline-2(1H)-carboxylate 9r.



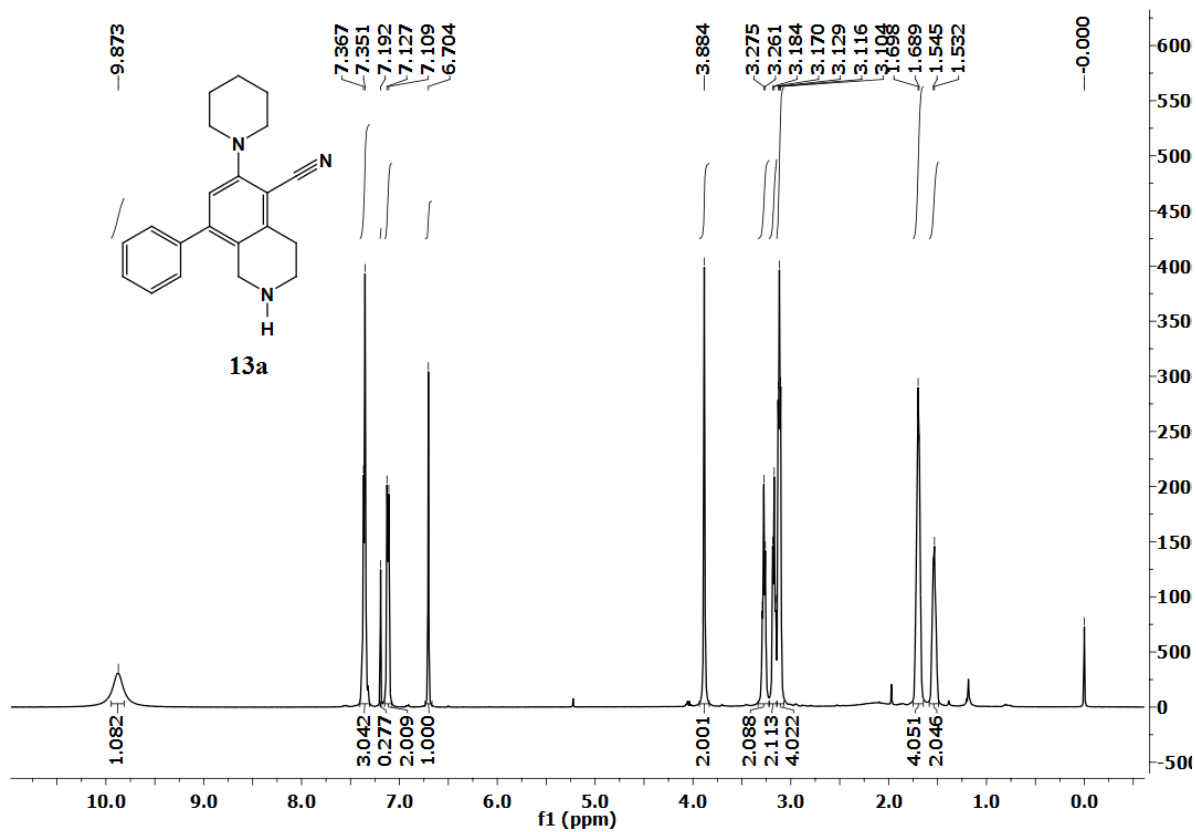
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz): *tert*-butyl-5-cyano-6-(piperidin-1-yl)-8-(thiophen-2-yl)-3,4-dihydroisoquinoline-2(1H)-carboxylate 9s.



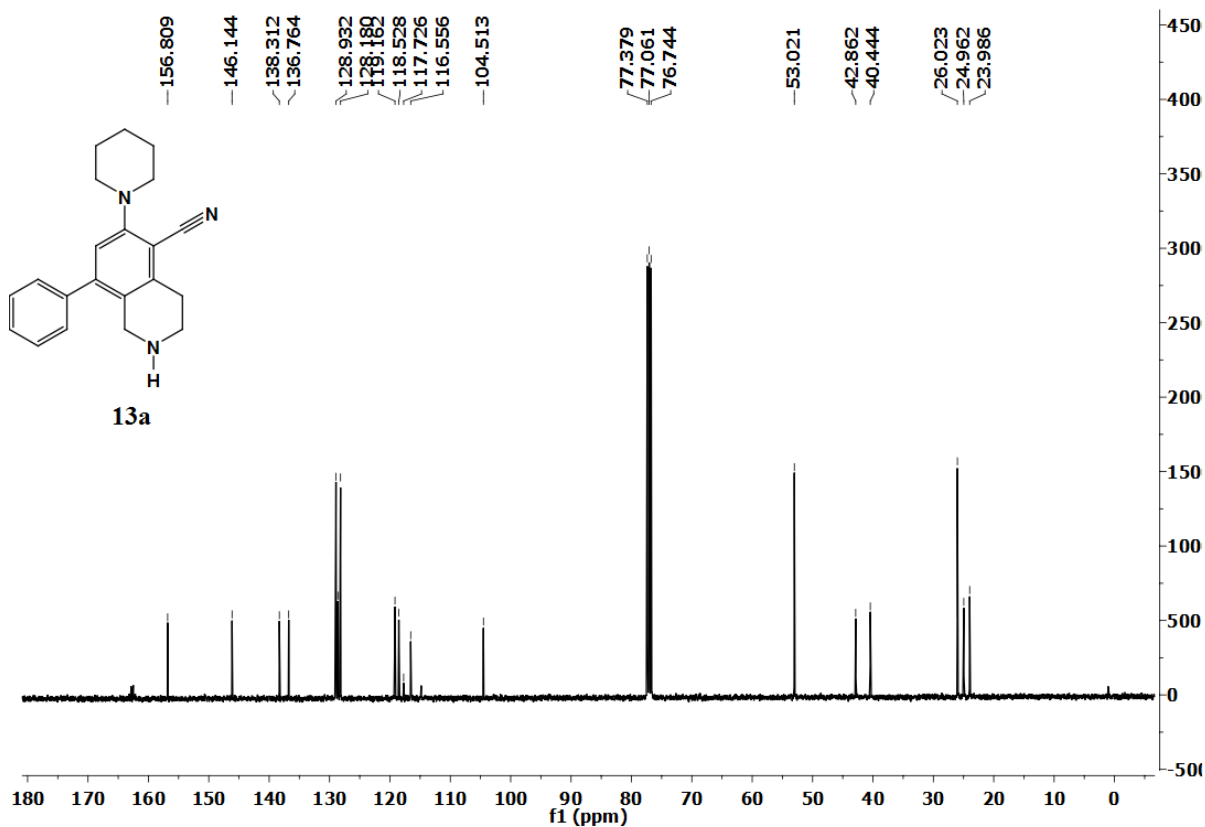
$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz): *tert*-butyl-5-cyano-6-(piperidin-1-yl)-8-(thiophen-2-yl)-3,4-dihydroisoquinoline-2(1H)-carboxylate 9s.



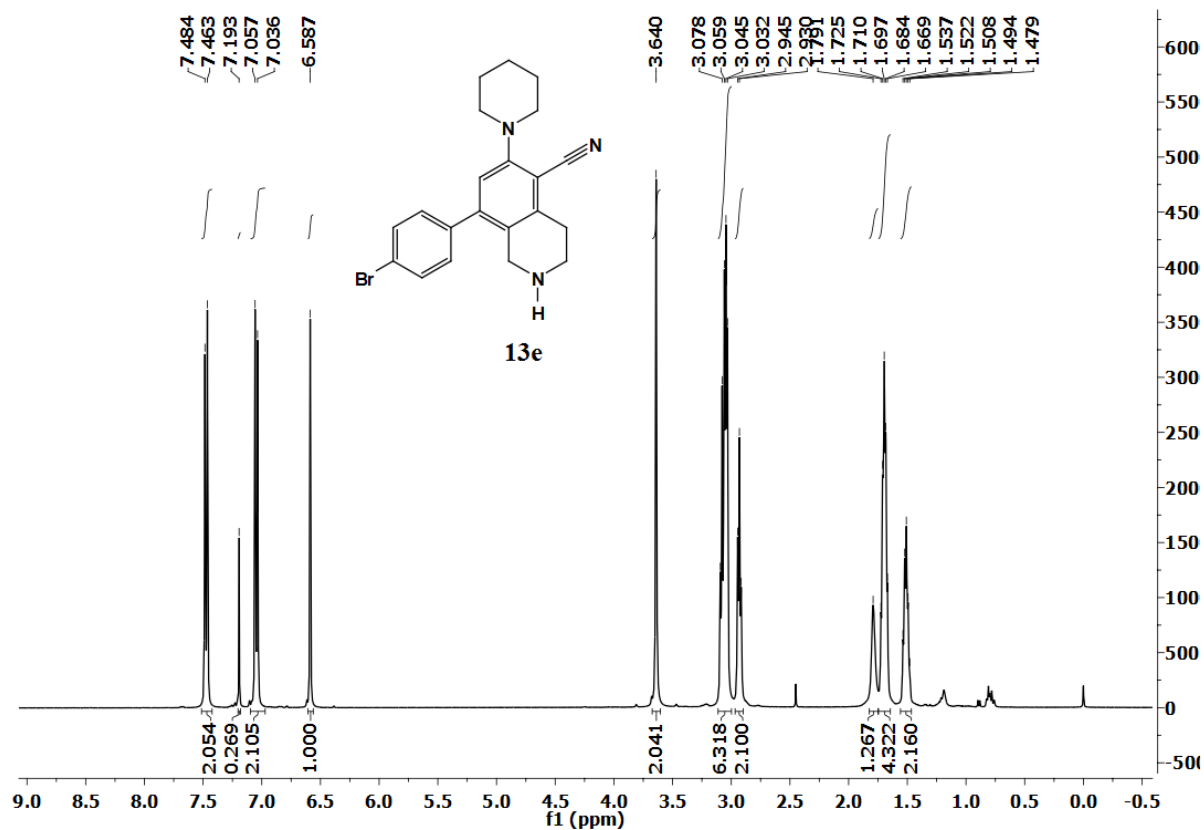
<sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): 8-Phenyl-6-(piperidin-1-yl)-1,2,3,4-tetrahydroisoquinoline-5-carbonitrile 13a.



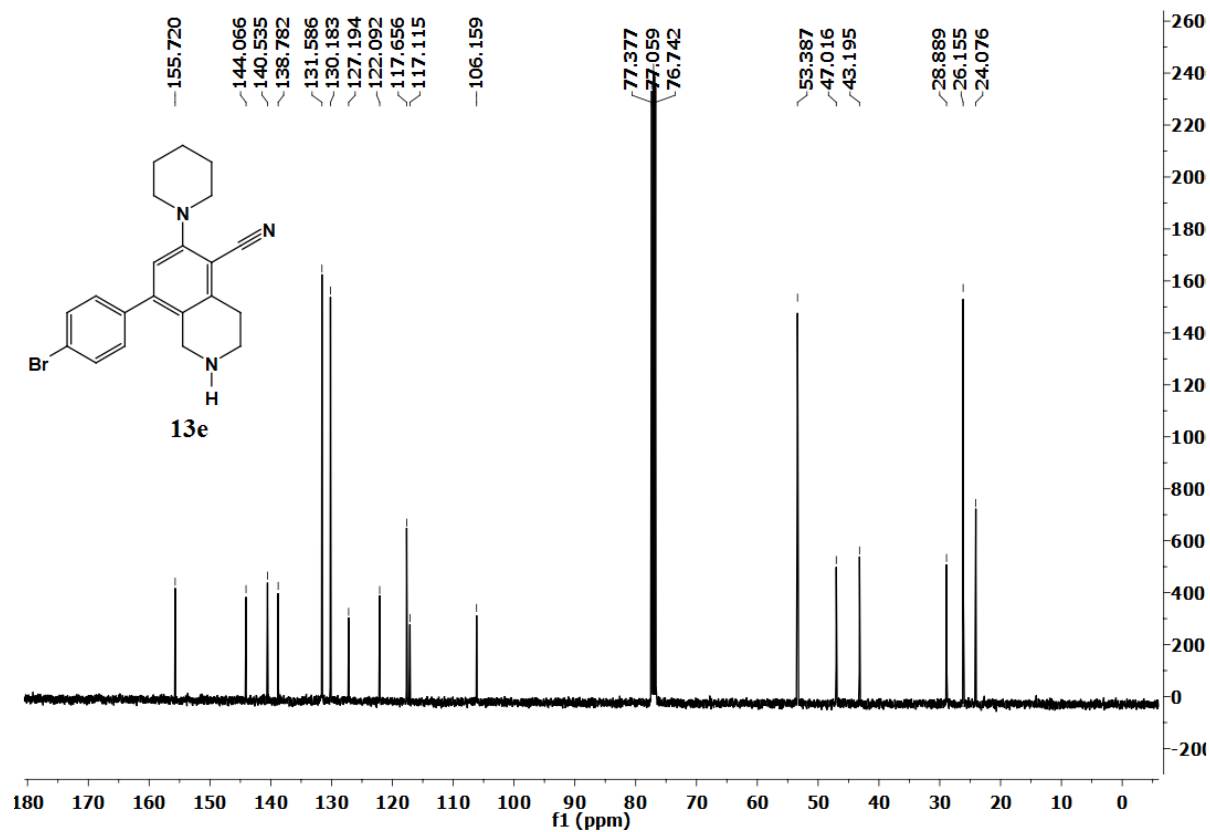
<sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): 8-Phenyl-6-(piperidin-1-yl)-1,2,3,4-tetrahydroisoquinoline-5-carbonitrile 13a.



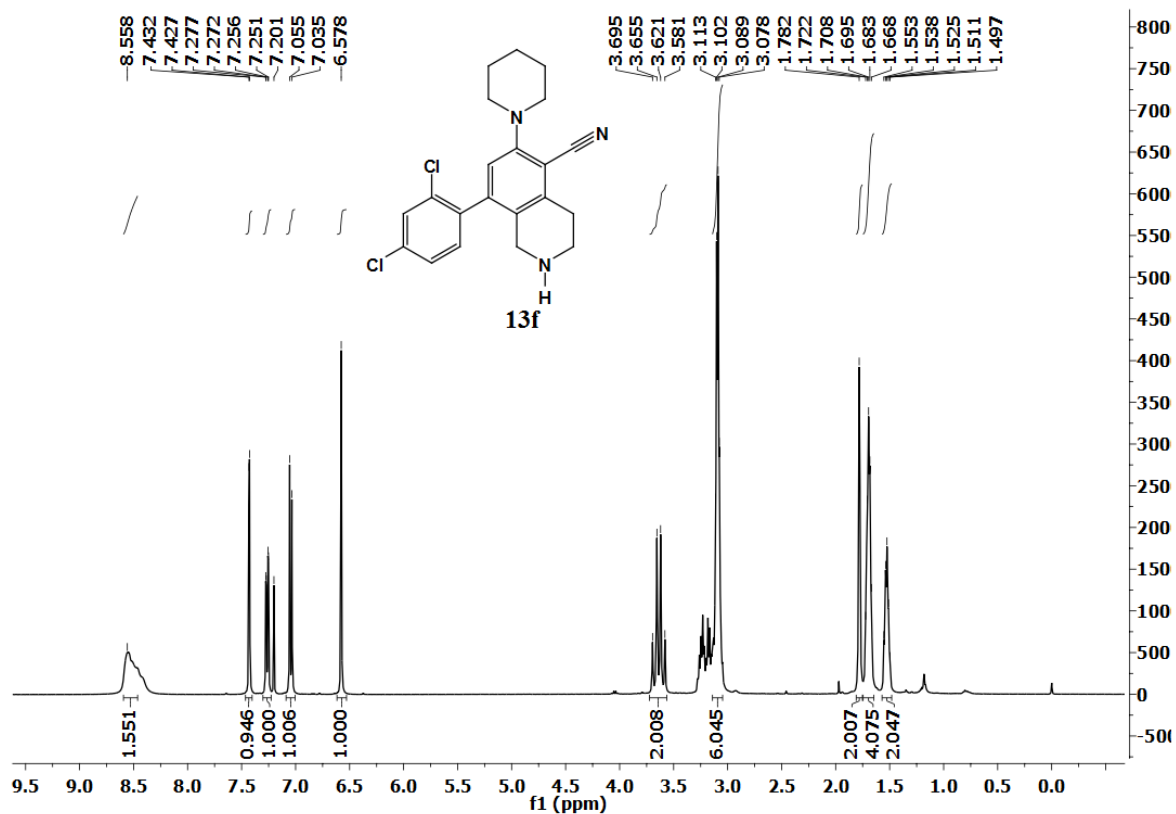
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz): 8-(4-bromophenyl)-6-(piperidin-1-yl)-1,2,3,4-tetrahydroisoquinoline-5-carbonitrile **13e**.



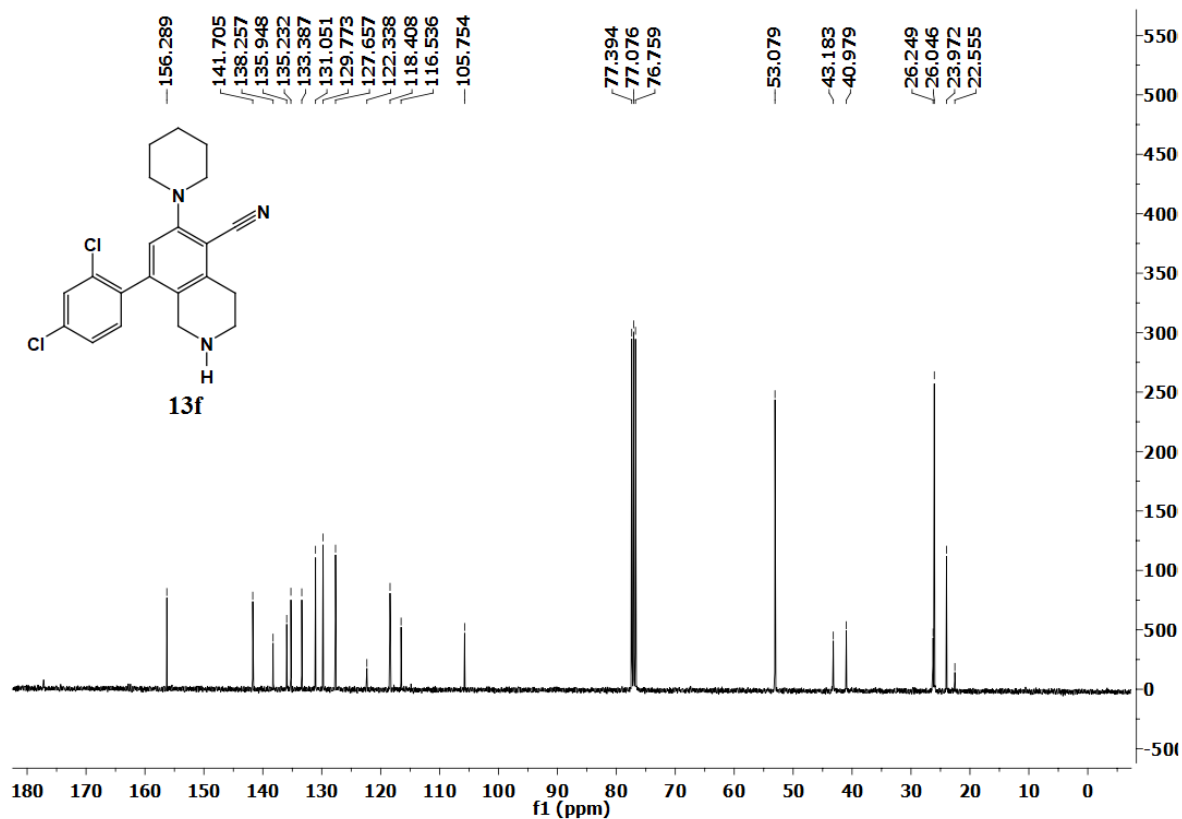
$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz): 8-(4-bromophenyl)-6-(piperidin-1-yl)-1,2,3,4-tetrahydroisoquinoline-5-carbonitrile **13e**.



<sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): 8-(2,4-dichlorophenyl)-6-(piperidin-1-yl)-1,2,3,4-tetrahydroisoquinoline-5-carbonitrile **13f**.



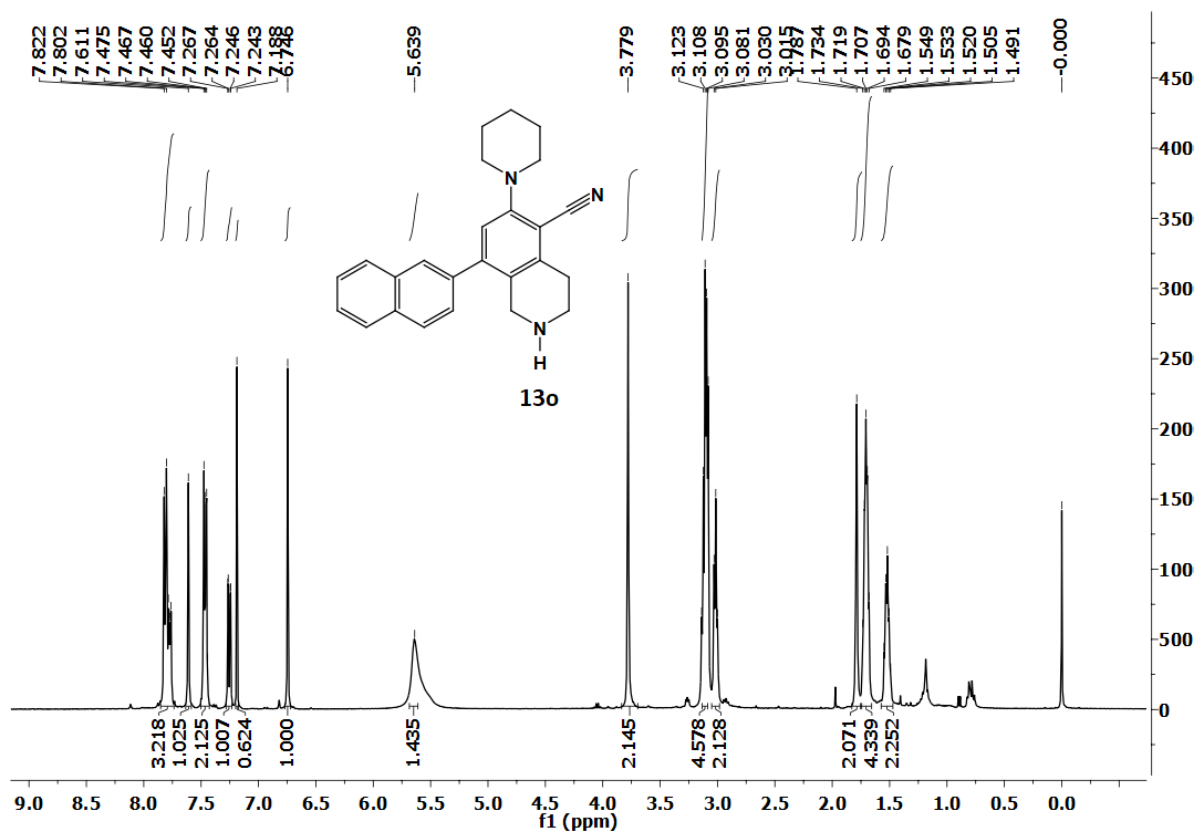
<sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): 8-(2,4-dichlorophenyl)-6-(piperidin-1-yl)-1,2,3,4-tetrahydroisoquinoline-5-carbonitrile **13f**.







<sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): 8-(naphthalen-2-yl)-6-(piperidin-1-yl)-1,2,3,4-tetrahydroisoquinoline-5-carbonitrile 13o.



<sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): 8-(naphthalen-2-yl)-6-(piperidin-1-yl)-1,2,3,4-tetrahydroisoquinoline-5-carbonitrile 13o.

