

Formation and reactions of azepino[4,5-*b*]indoles: An unprecedented ozone reaction in the formation of novel benzo[*c*]naphthyridinones

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Crystal Structure data for compound **18** and **21**

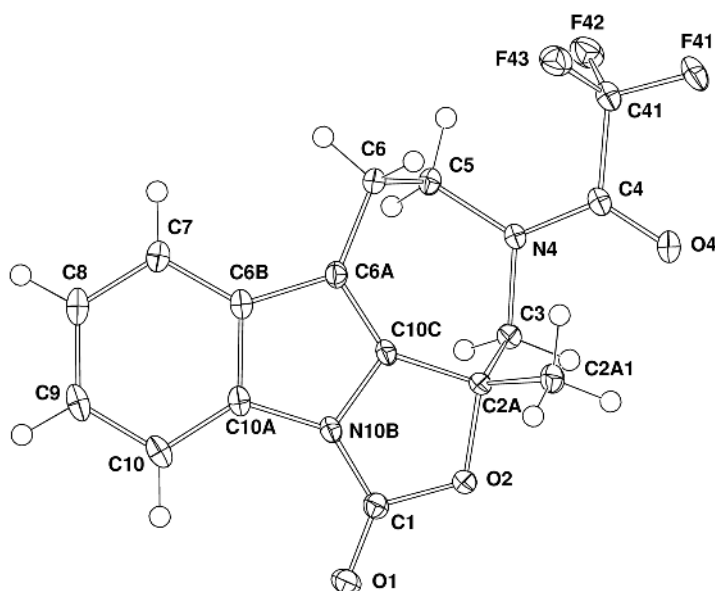


Figure 1s: Molecular structure of compound **18**.

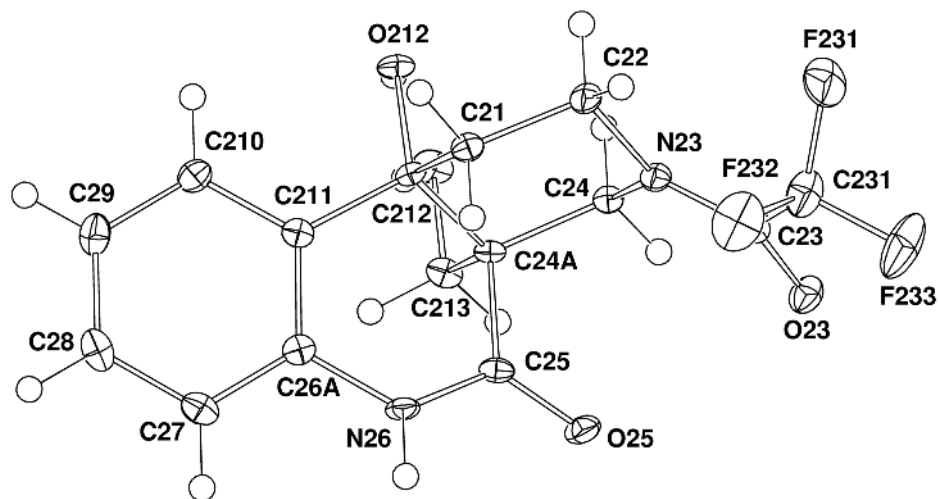


Figure 2s: Molecular structure of compound 21.

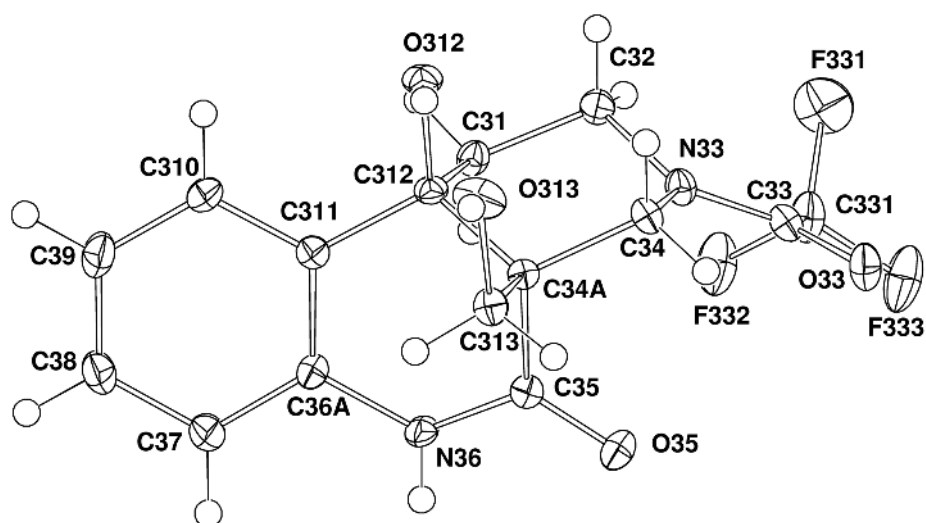


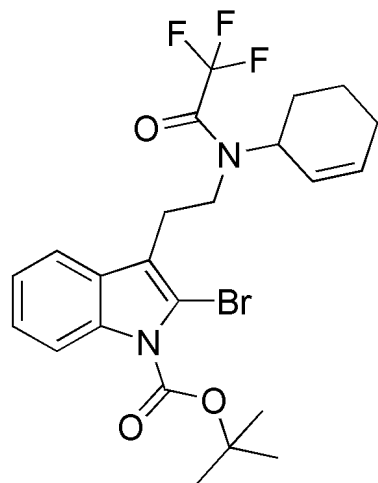
Figure 3s: Molecular structure (II) of compound **21**.

Table 1s. Hydrogen bonds for **21** [Å and °].

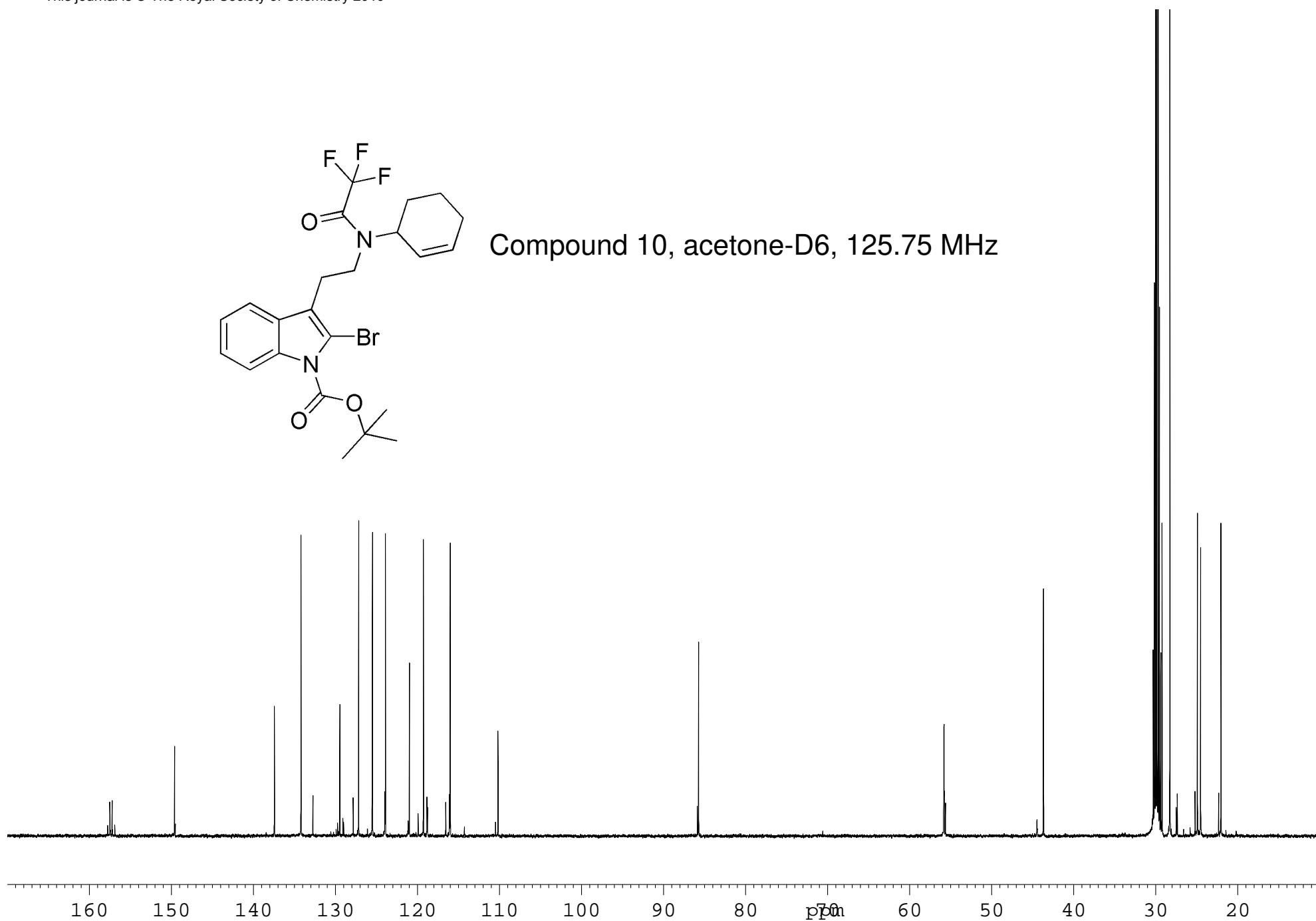
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(16)-H(16)...O(25)	0.88	2.23	3.0866(19)	165.6
O(112)-H(112)...O(35)	0.831(17)	1.928(19)	2.7143(18)	158(3)
O(113)-H(113)...O(33) ¹	0.852(17)	1.944(17)	2.7936(18)	175(3)
N(26)-H(26)...O(15)	0.88	1.88	2.7539(18)	176.3
O(212)-H(212)...O(213)	0.806(16)	1.891(19)	2.6071(18)	147(2)
O(213)-H(213)...O(23) ²	0.774(15)	2.247(18)	2.9006(18)	143(2)
O(213)-H(213)...O(25) ²	0.774(15)	2.252(19)	2.8046(18)	129.0(19)
N(36)-H(36)...O(212) ³	0.88	2.02	2.8621(19)	160.5
O(312)-H(312)...O(313)	0.826(15)	1.852(16)	2.606(2)	151(2)
O(313)-H(313)...O(113) ¹	0.843(17)	1.956(18)	2.7902(19)	170(3)

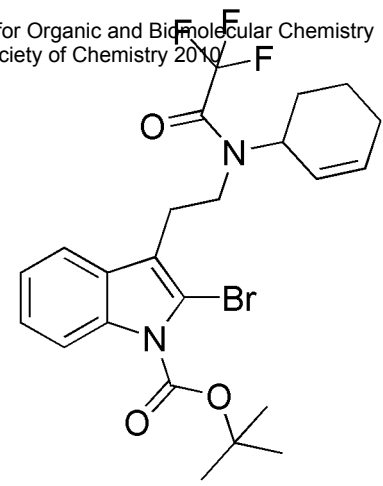
Symmetry transformations used to generate equivalent atoms:

¹ $x+1/2, 1/2-y, 1-z$; ² $x-1/2, 3/2-y, 1-z$; ³ $1/2-x, 1-y, z-1/2$

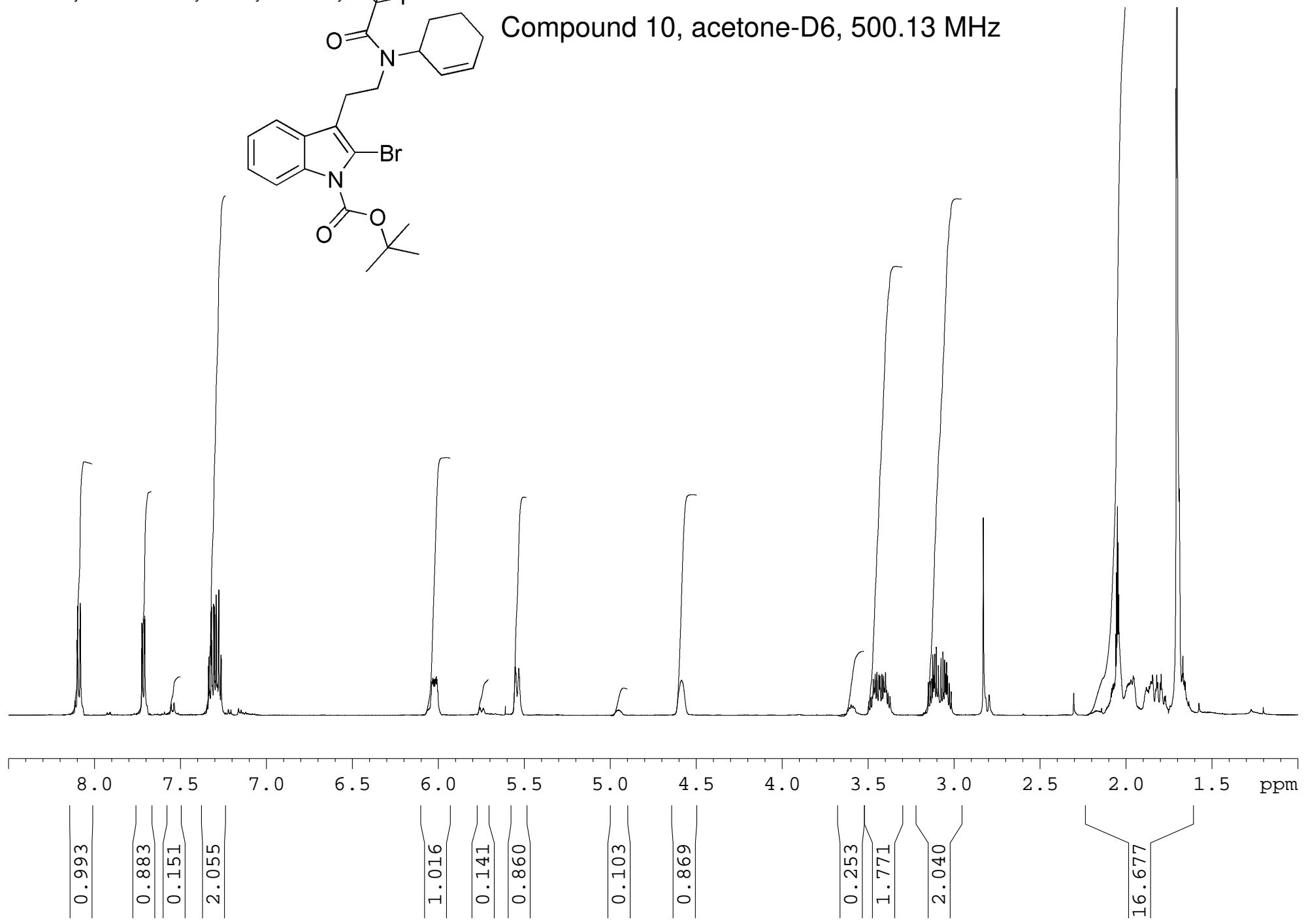


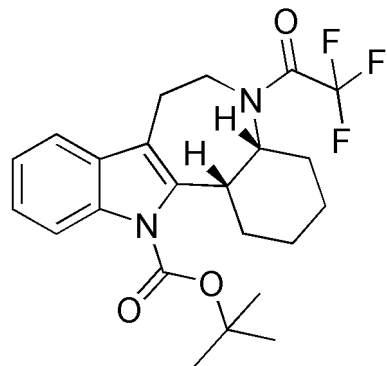
Compound 10, acetone-D₆, 125.75 MHz



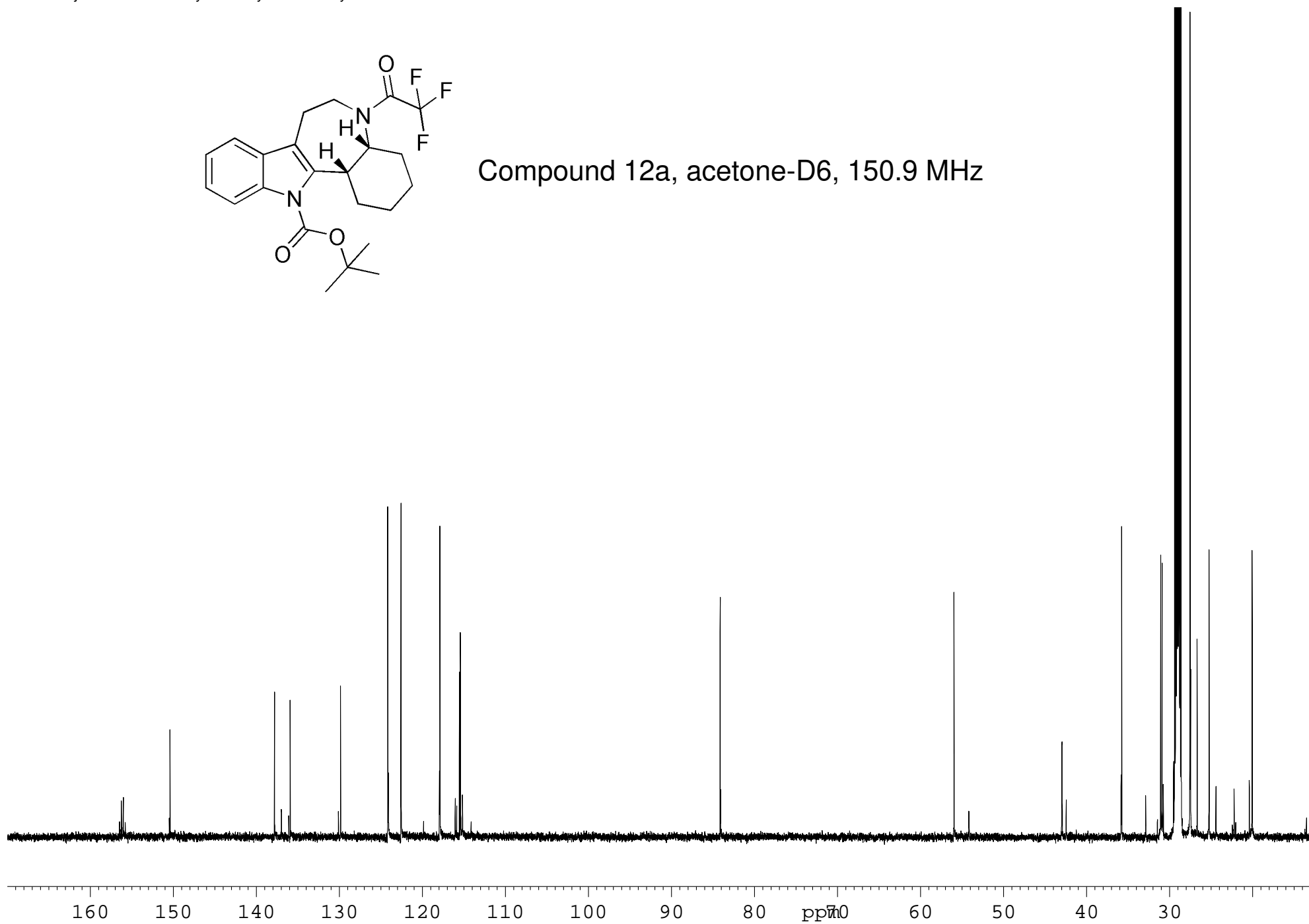


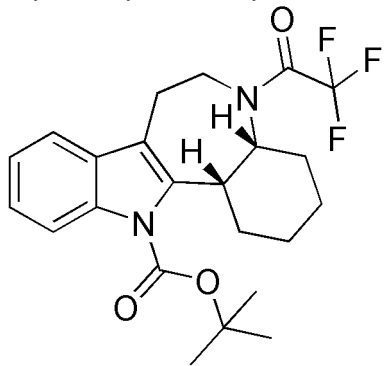
Compound 10, acetone-D6, 500.13 MHz



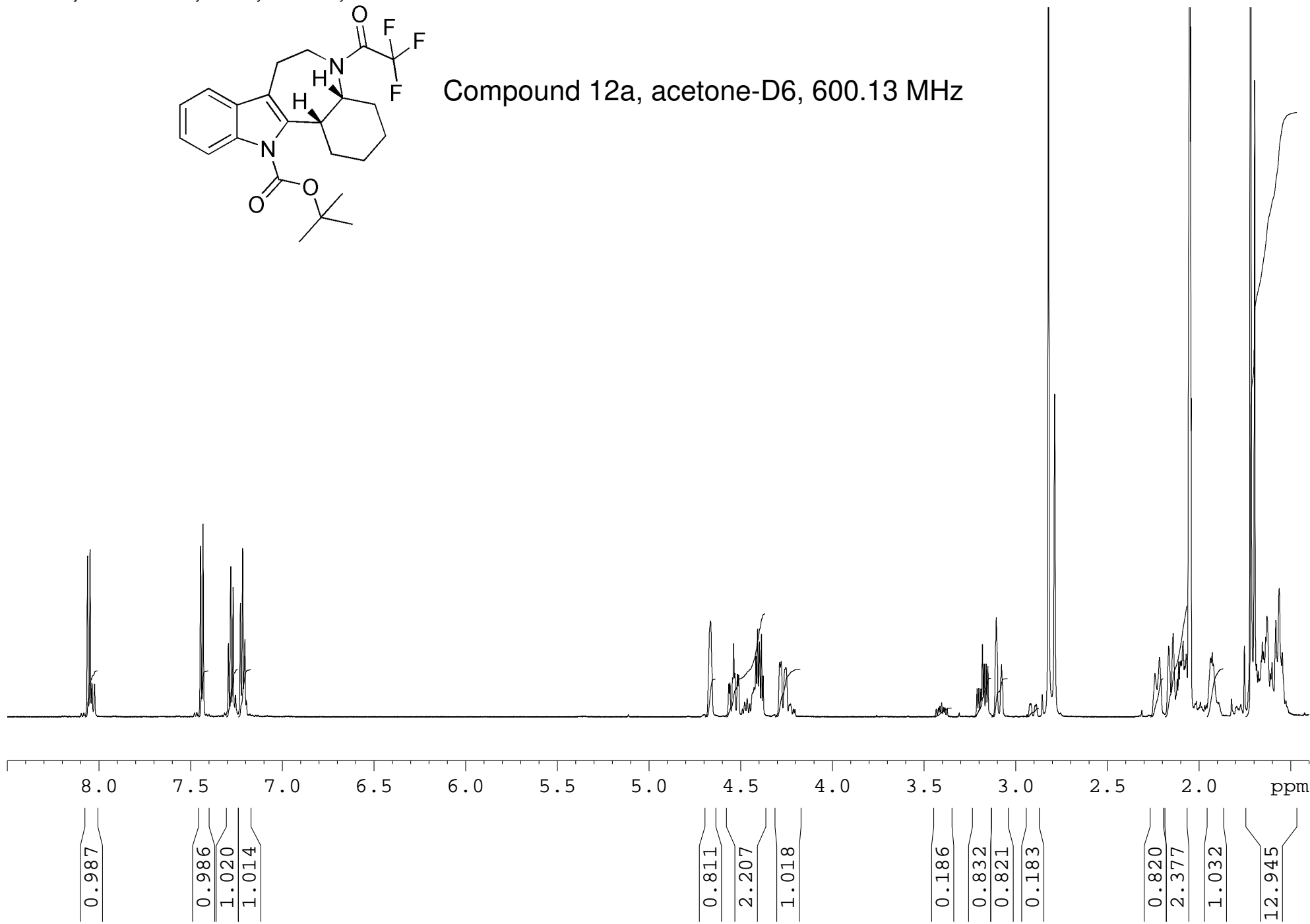


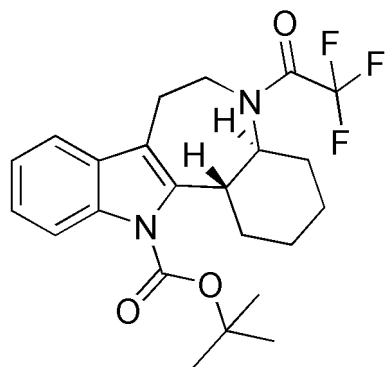
Compound 12a, acetone-D₆, 150.9 MHz



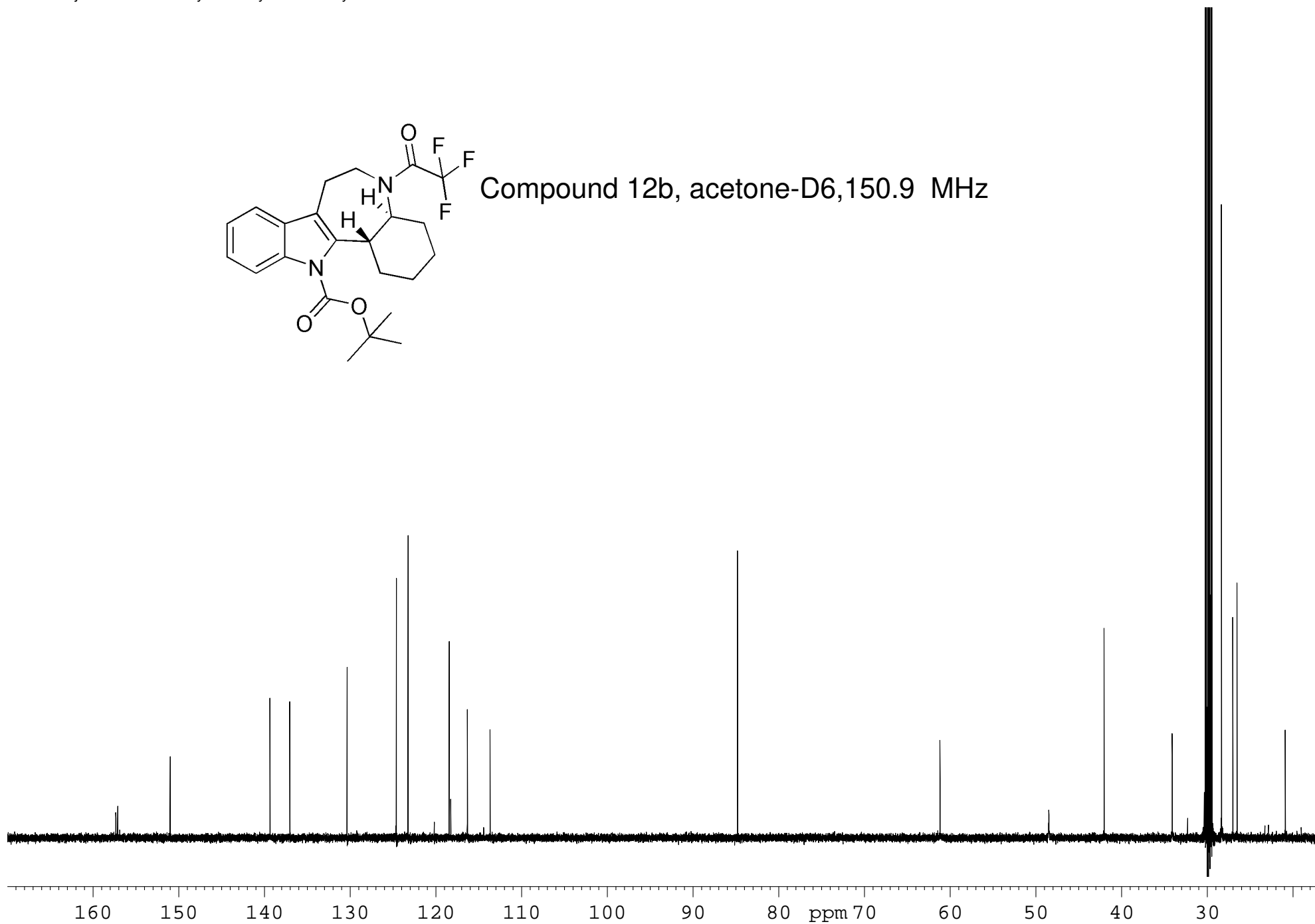


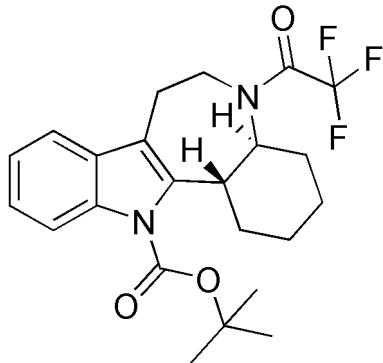
Compound 12a, acetone-D₆, 600.13 MHz



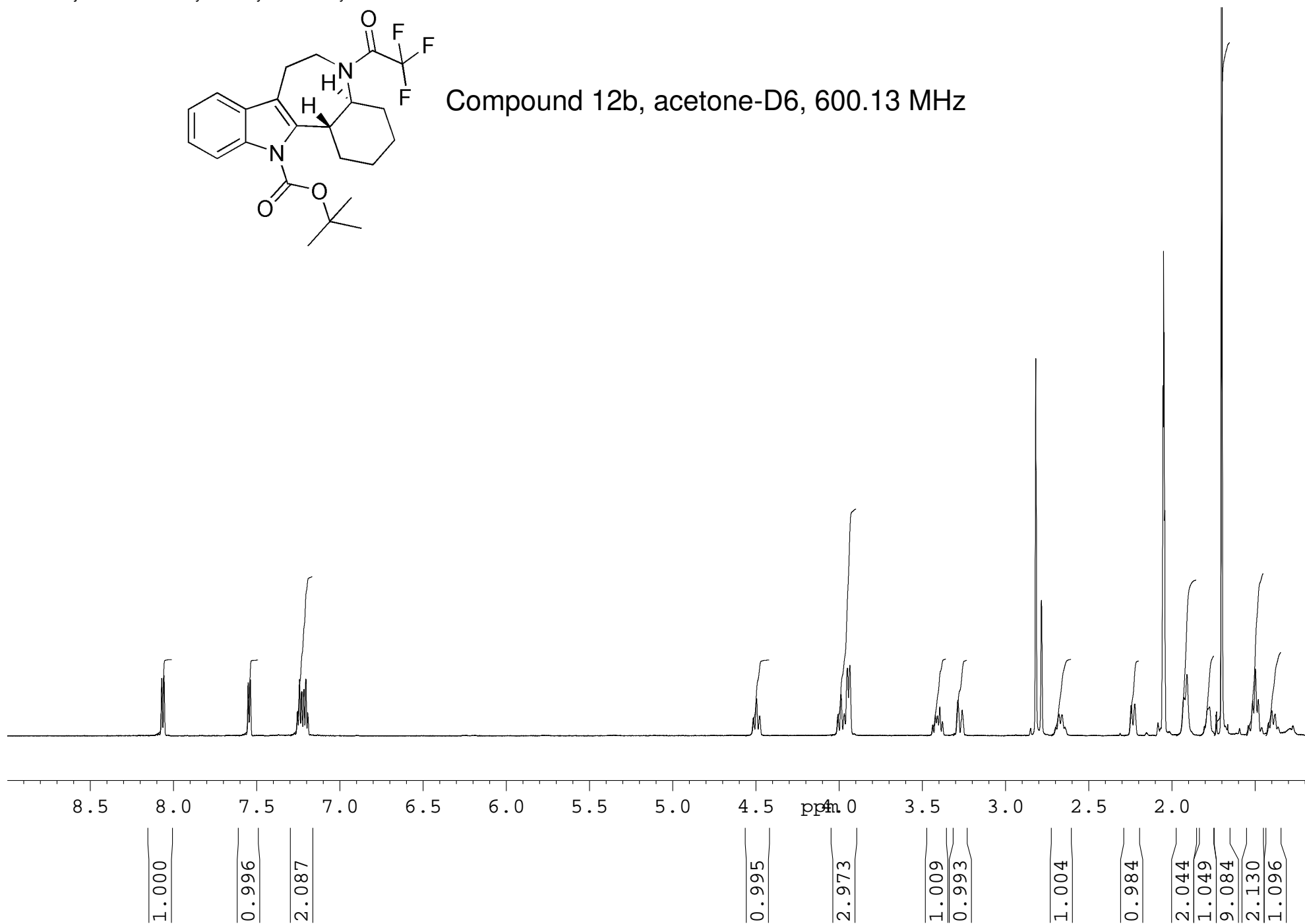


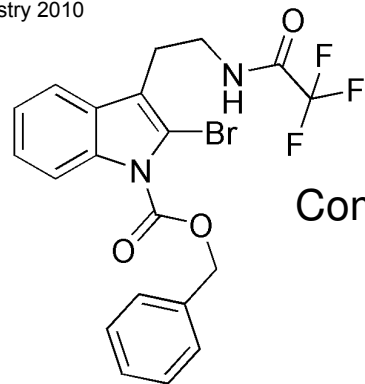
Compound 12b, acetone-D₆, 150.9 MHz



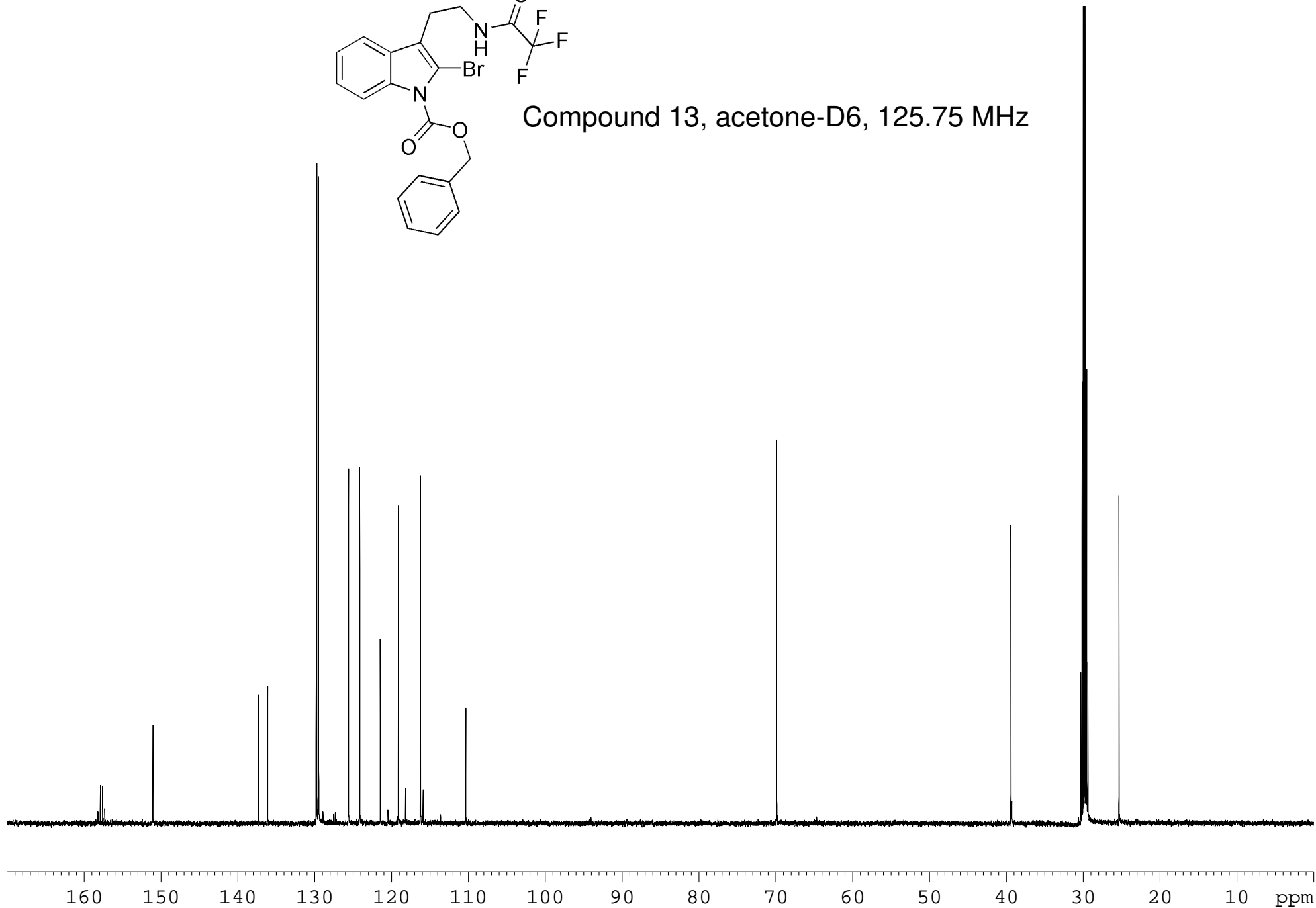


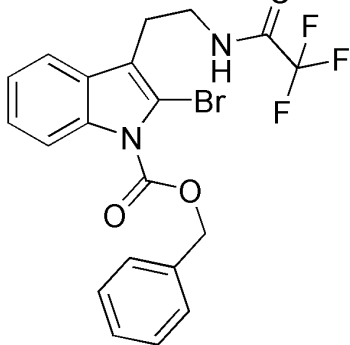
Compound 12b, acetone-D₆, 600.13 MHz



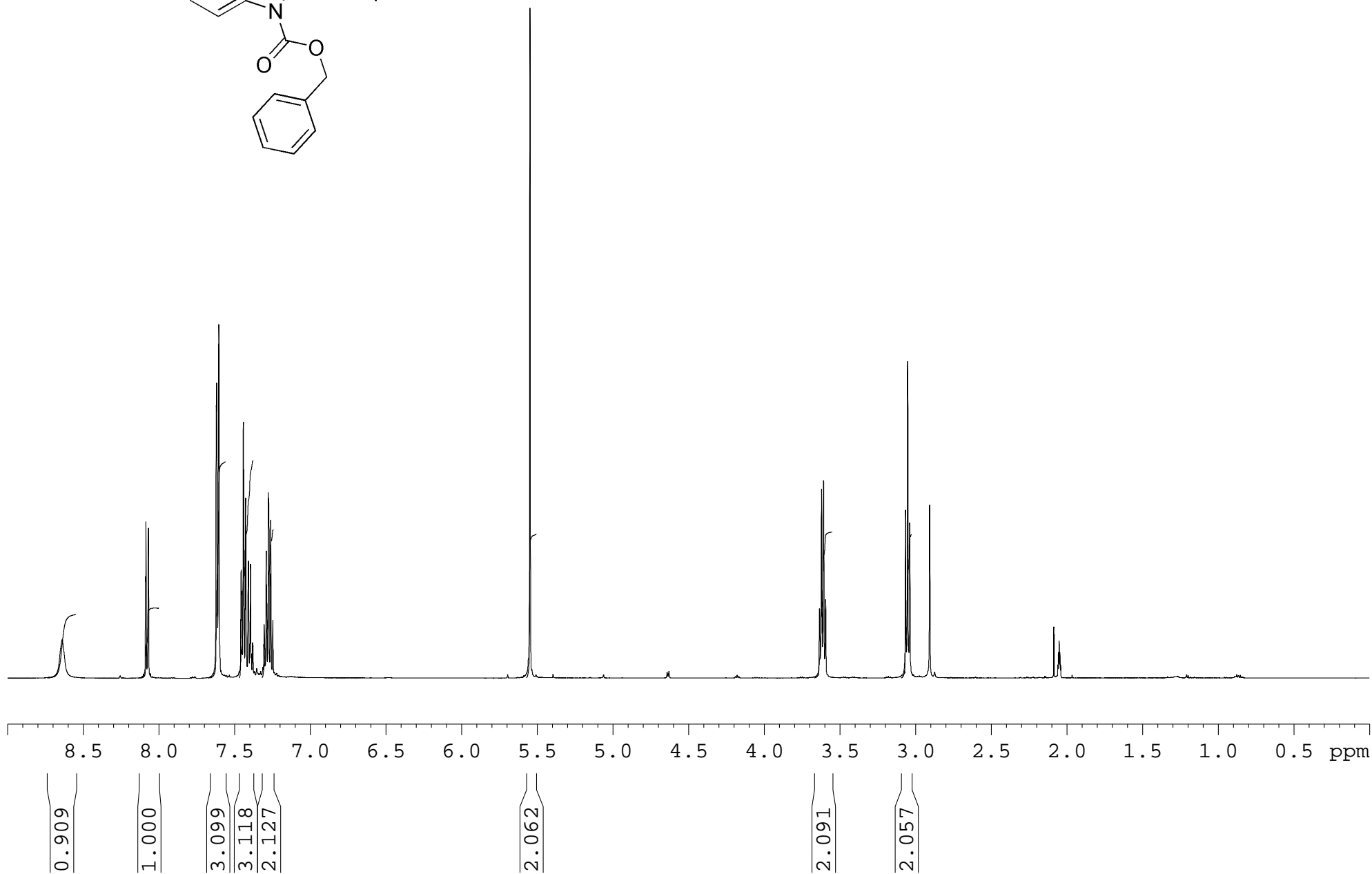


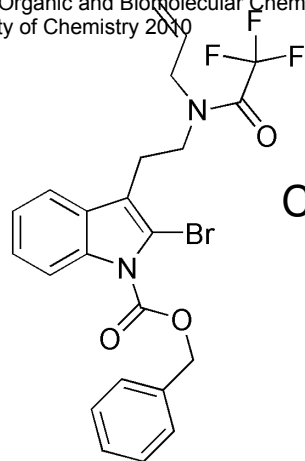
Compound 13, acetone-D₆, 125.75 MHz



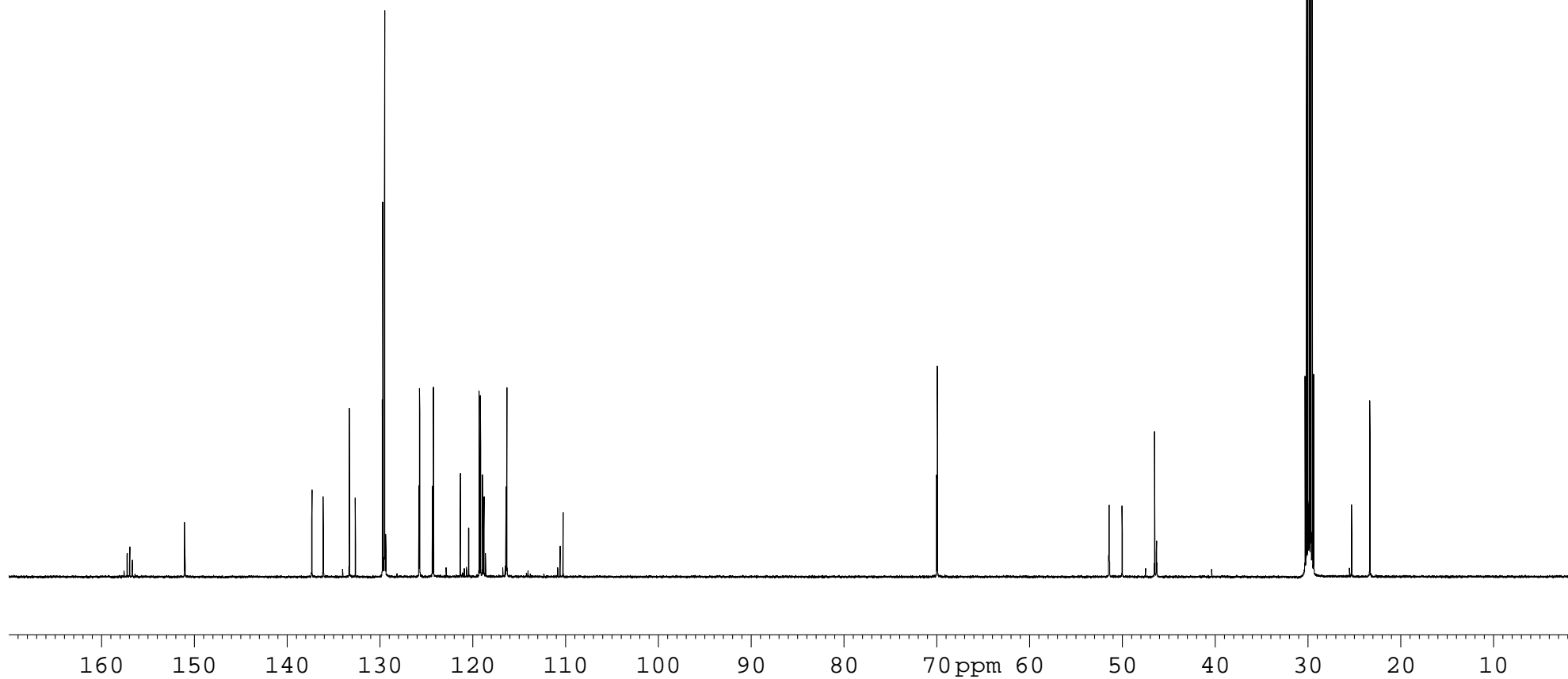


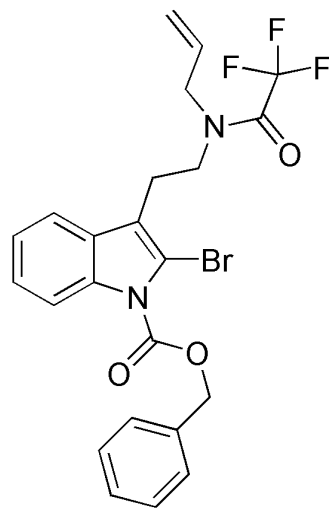
Compound 13, acetone-D6, 500.13 MHz



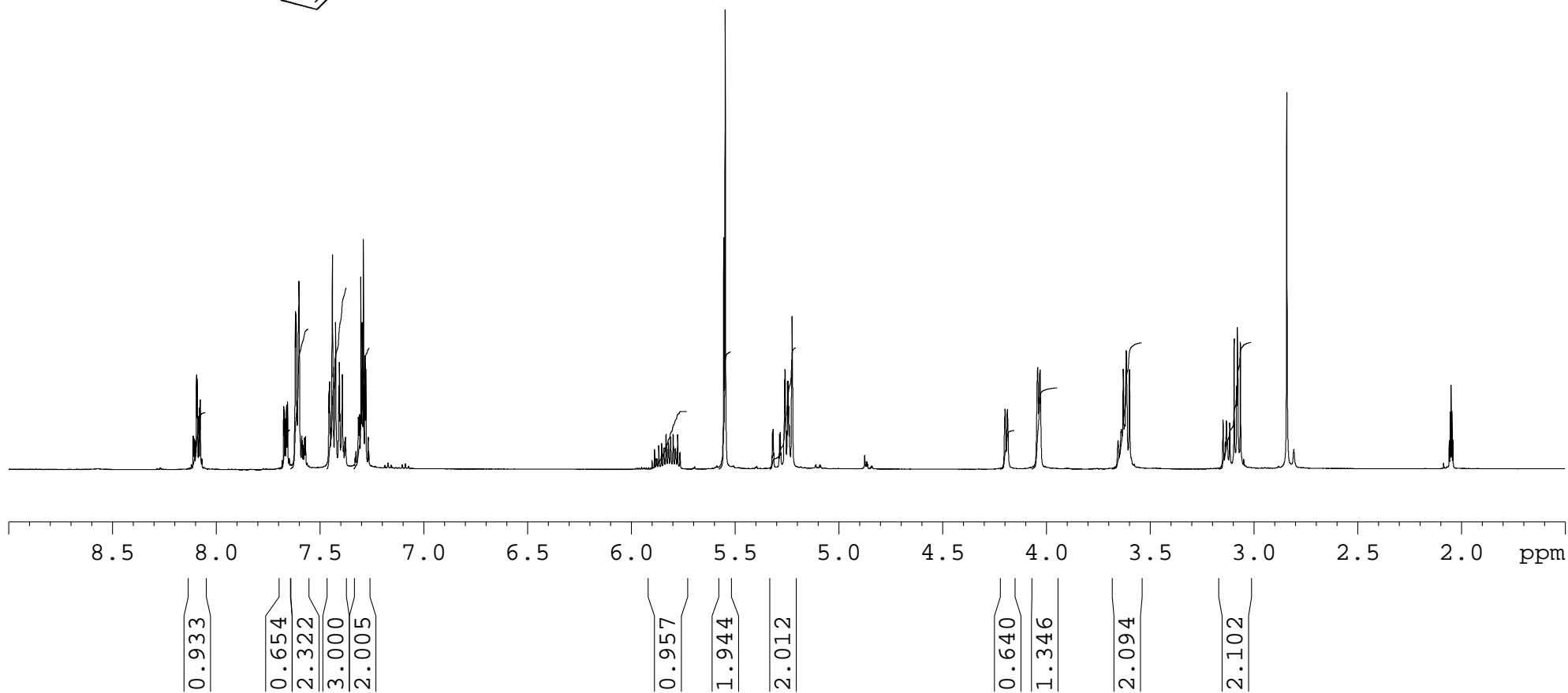


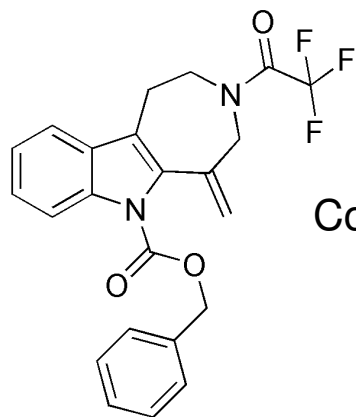
Compound 14, acetone-D6, 125.75 MHz



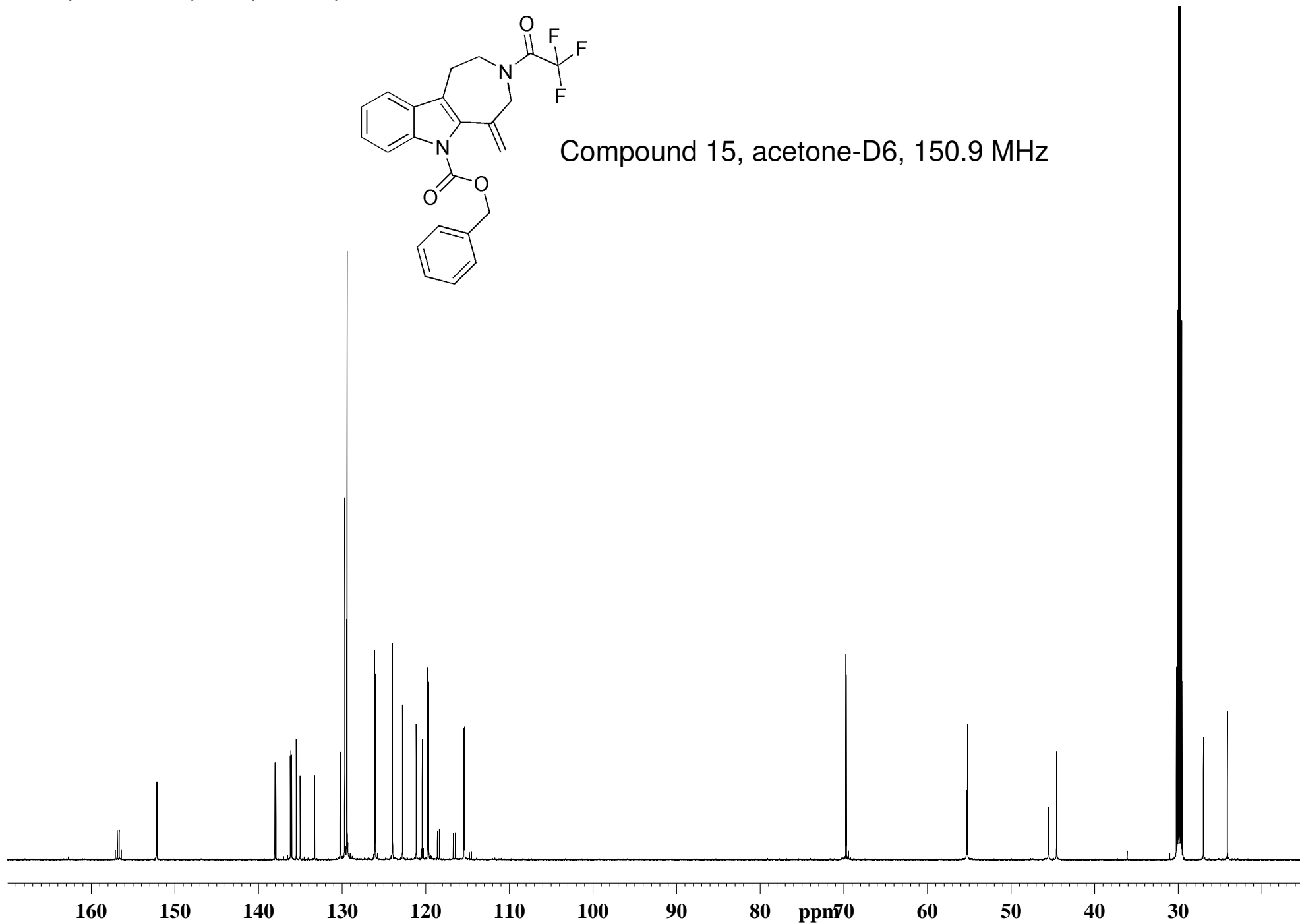


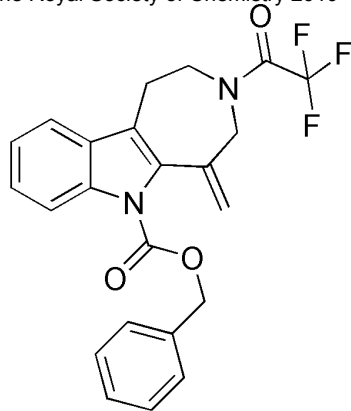
Compound 14, acetone-D₆, 500.13 MHz



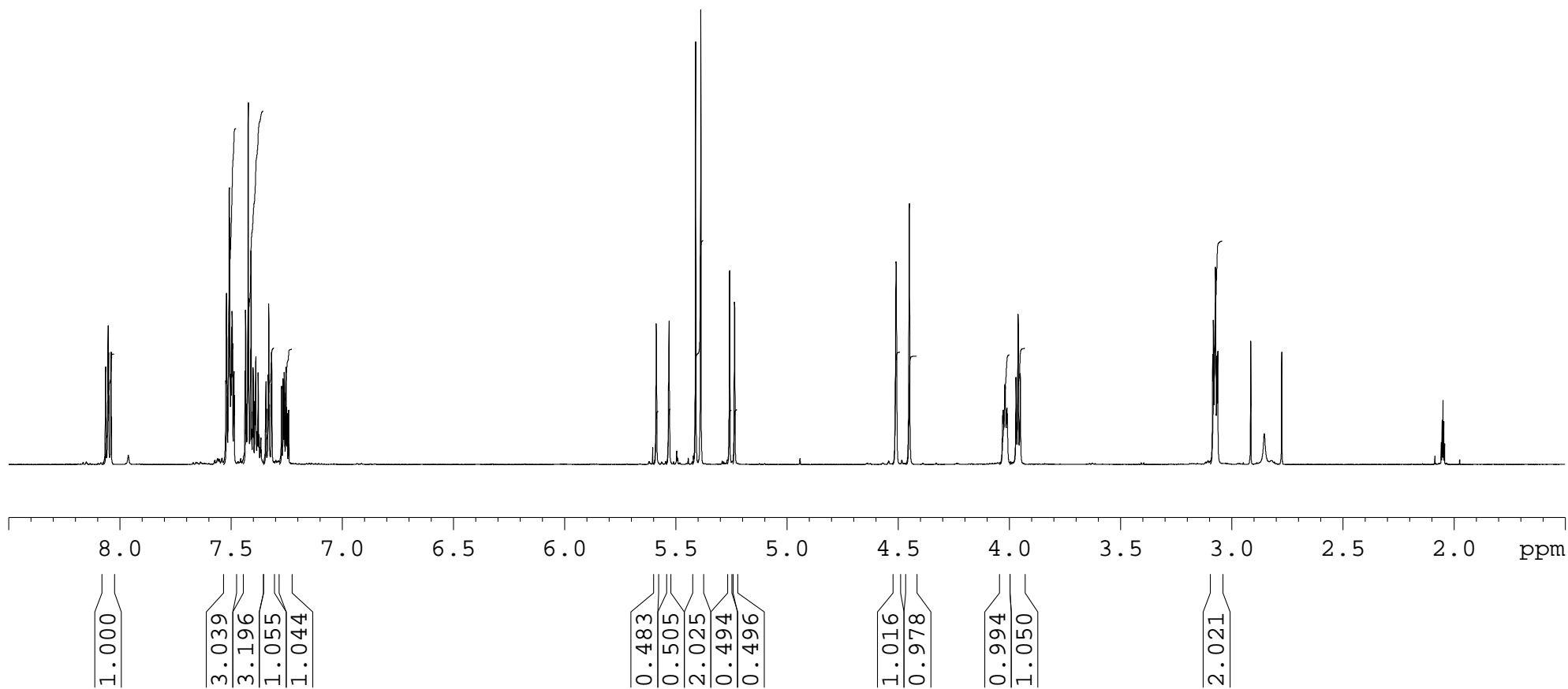


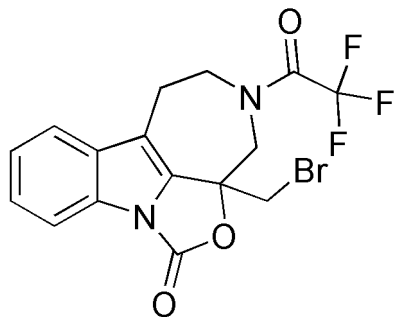
Compound 15, acetone-D6, 150.9 MHz



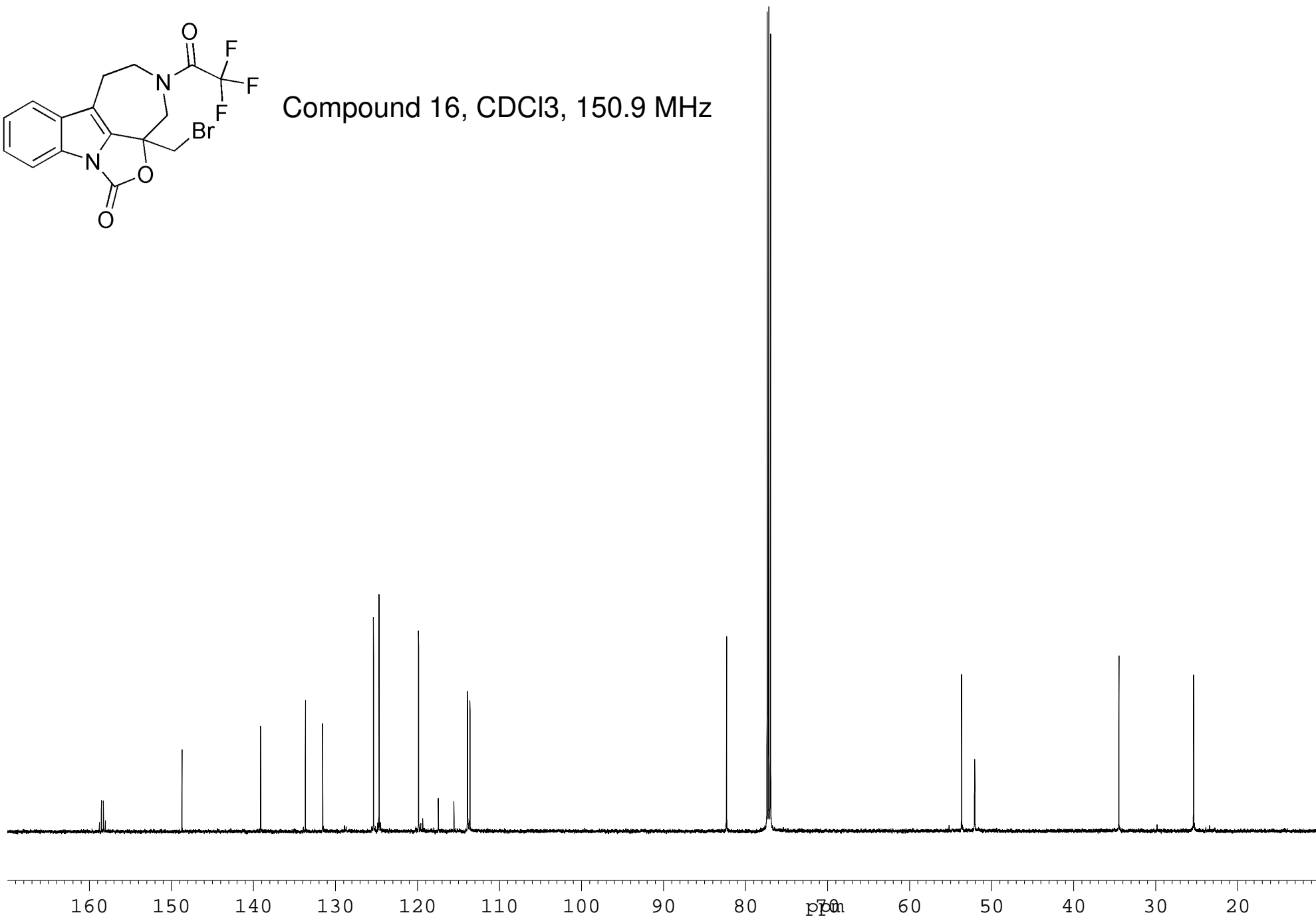


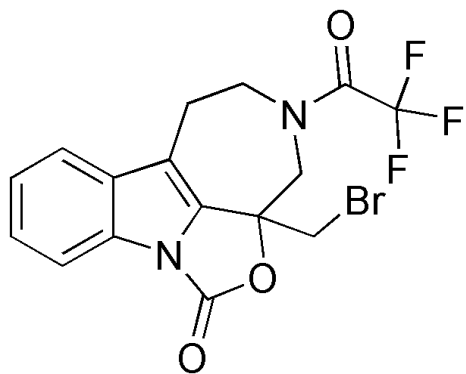
Compound 15, acetone-D₆, 600.13 MHz



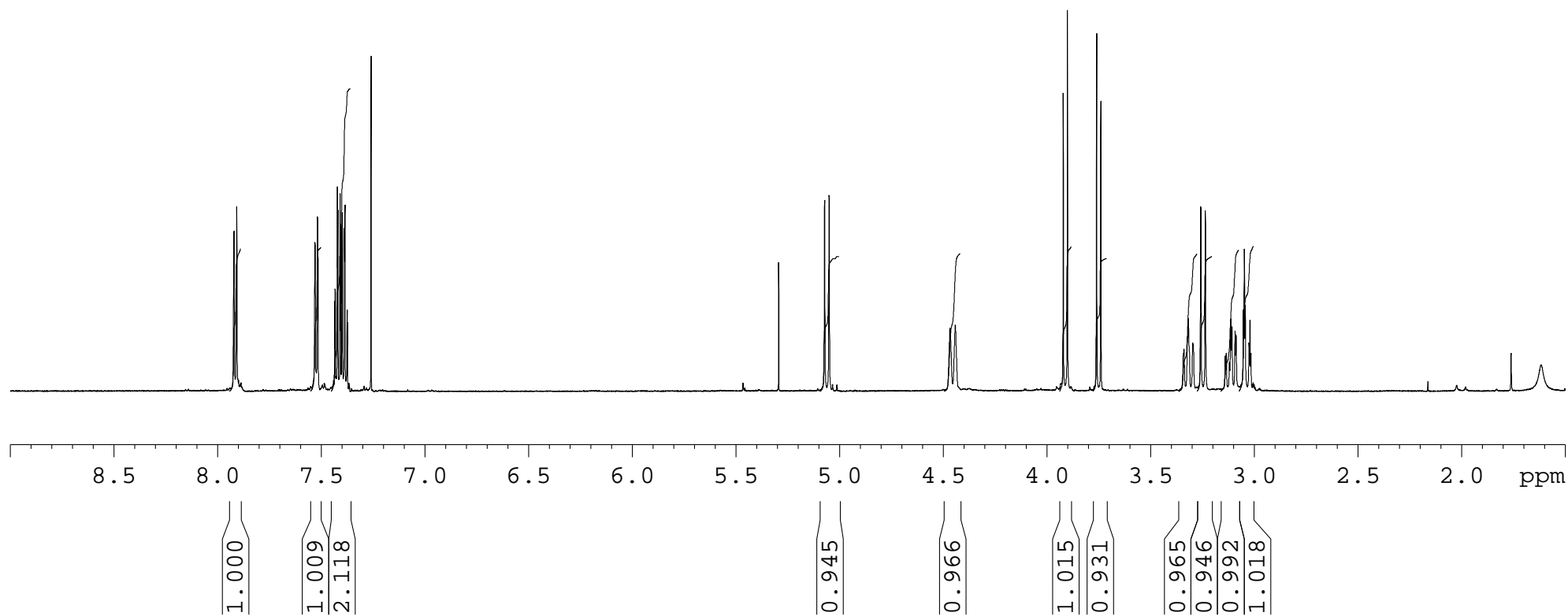


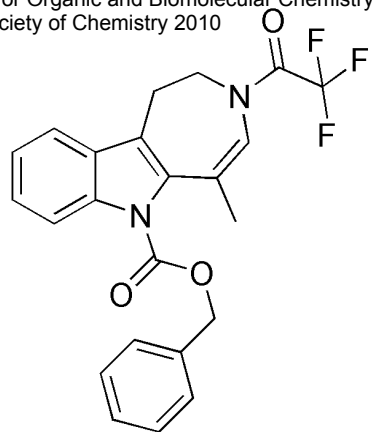
Compound 16, CDCl₃, 150.9 MHz



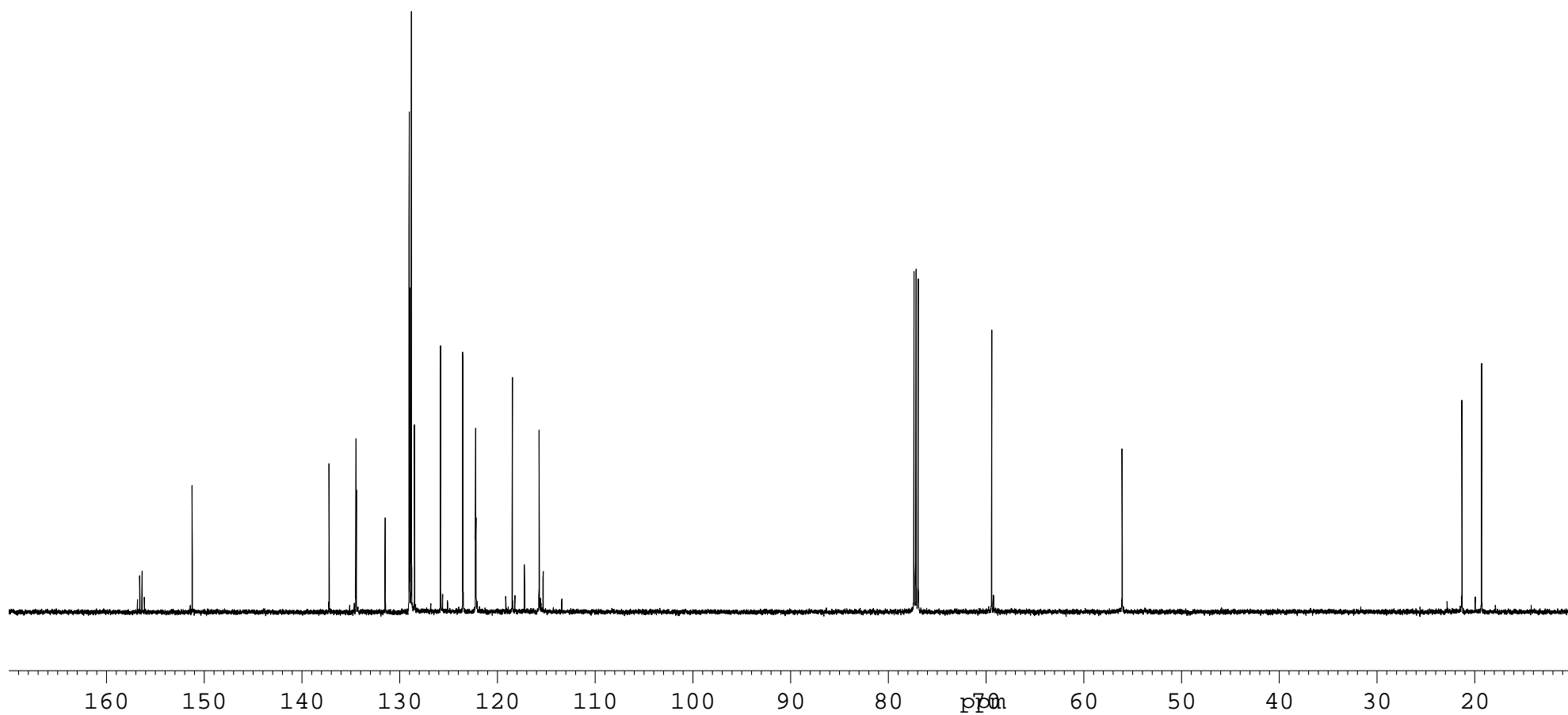


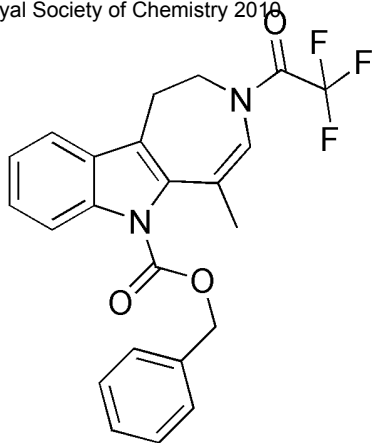
Compound 16, CDCl₃, 600.13 MHz



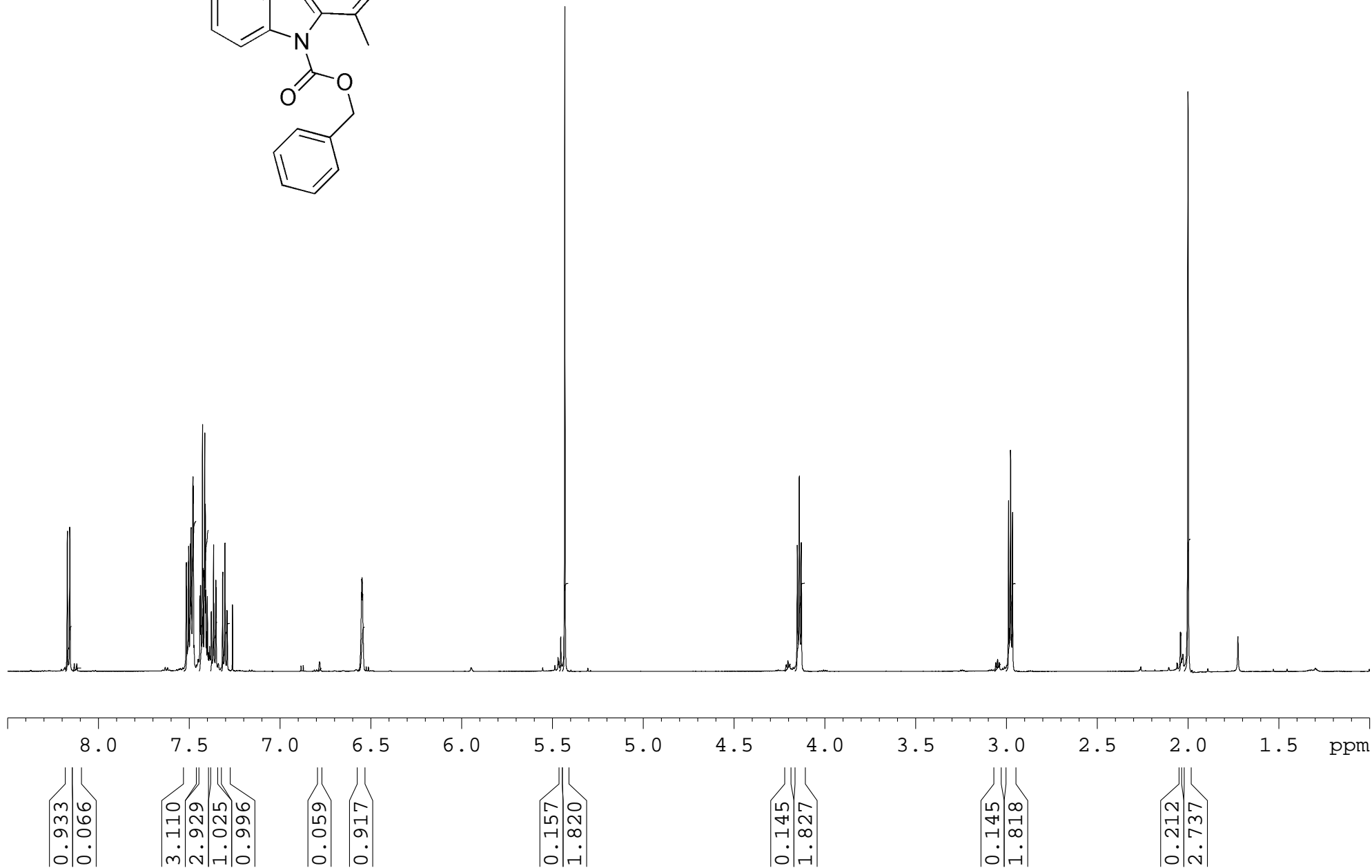


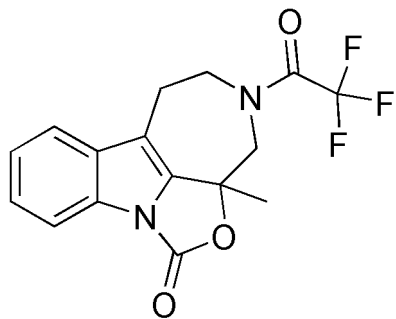
Compound 17, CDCl₃, 150.9 MHz



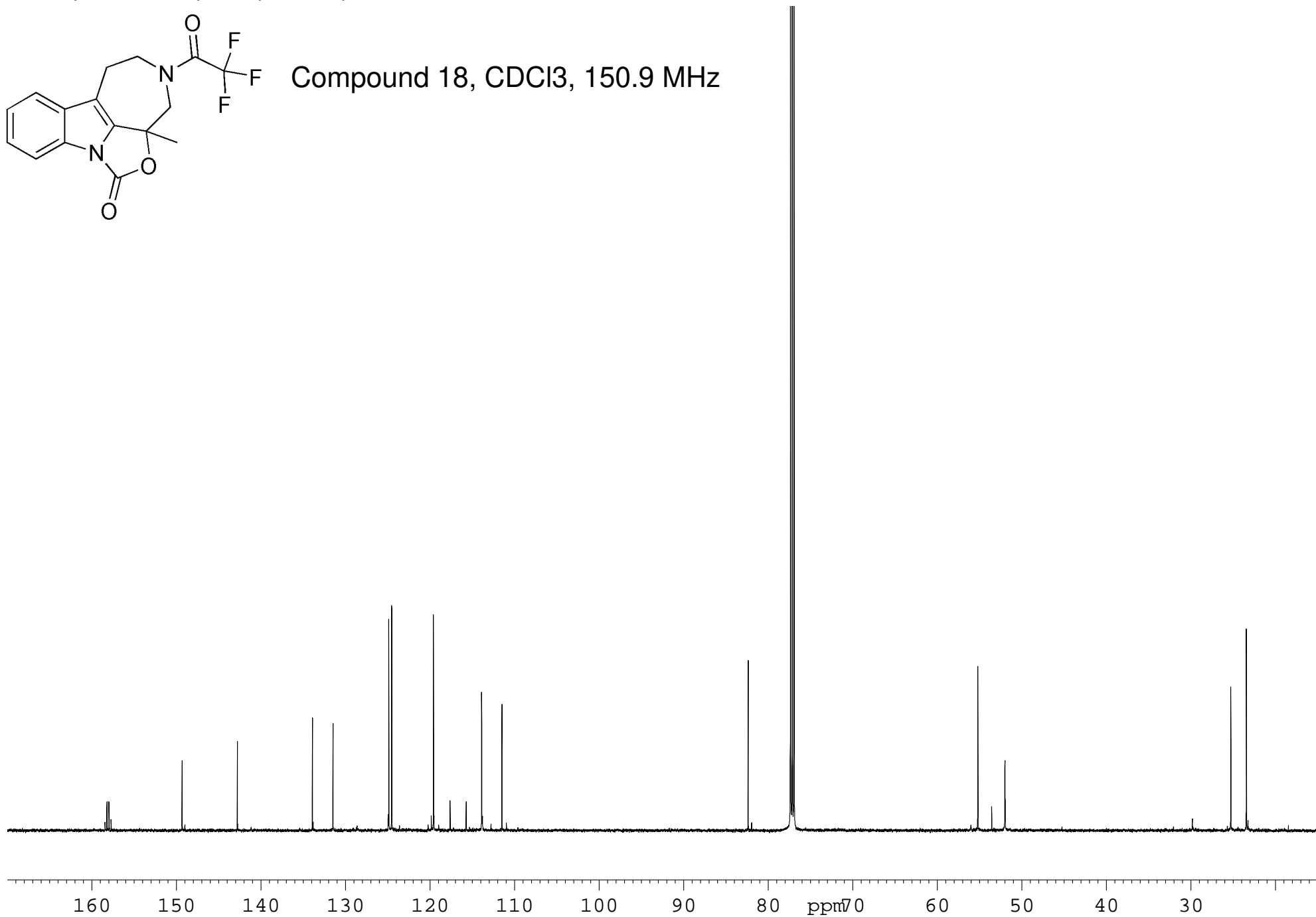


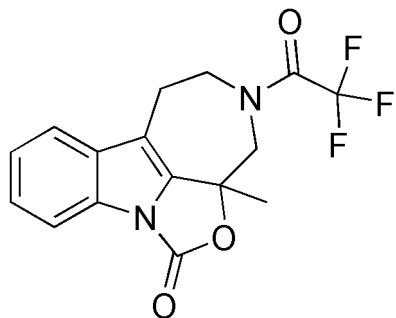
Compound 17, CDCl₃, 600.13 MHz



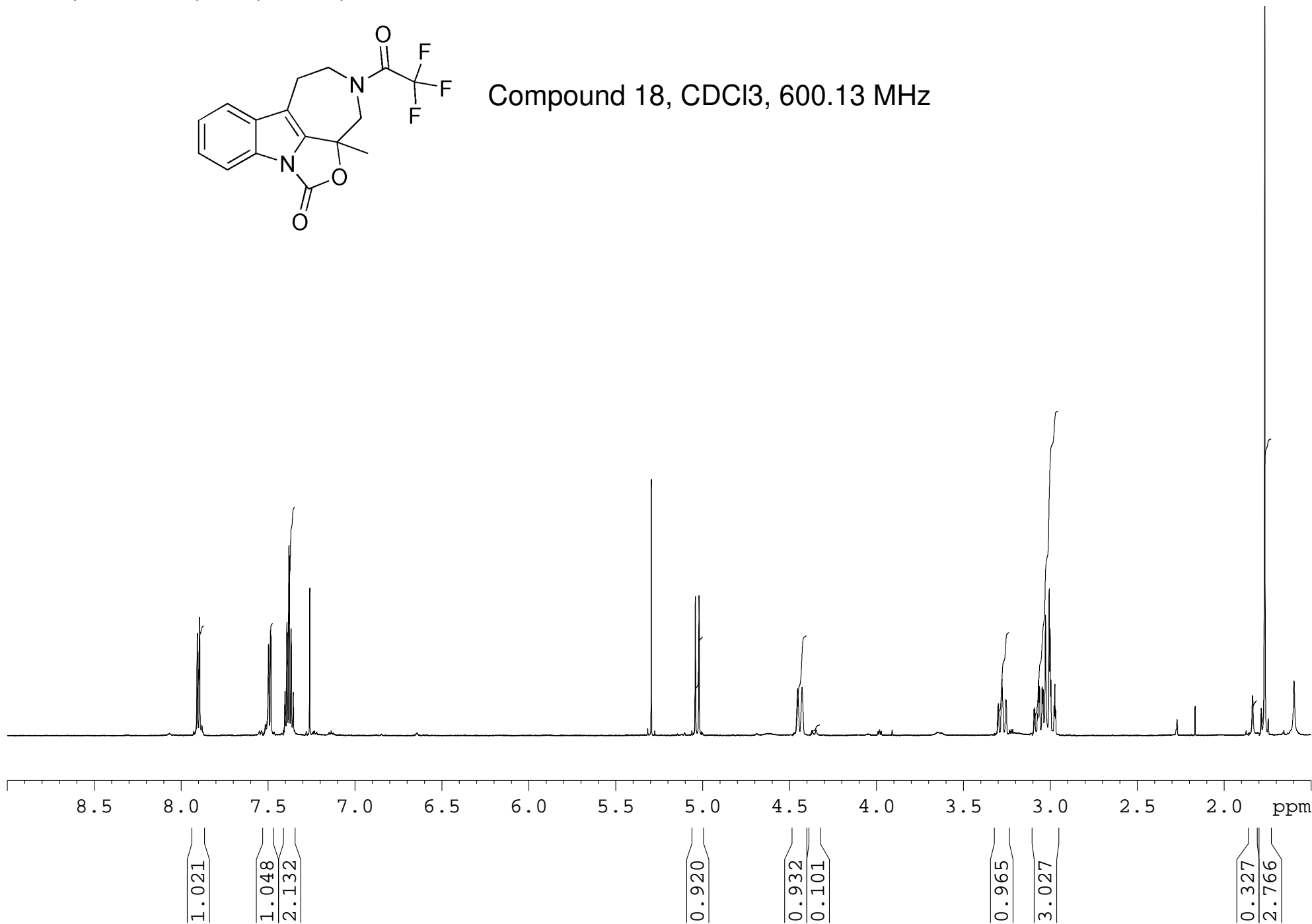


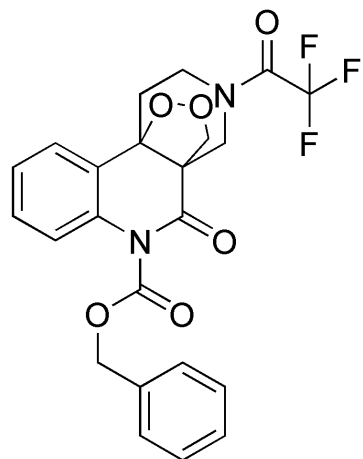
Compound 18, CDCl₃, 150.9 MHz



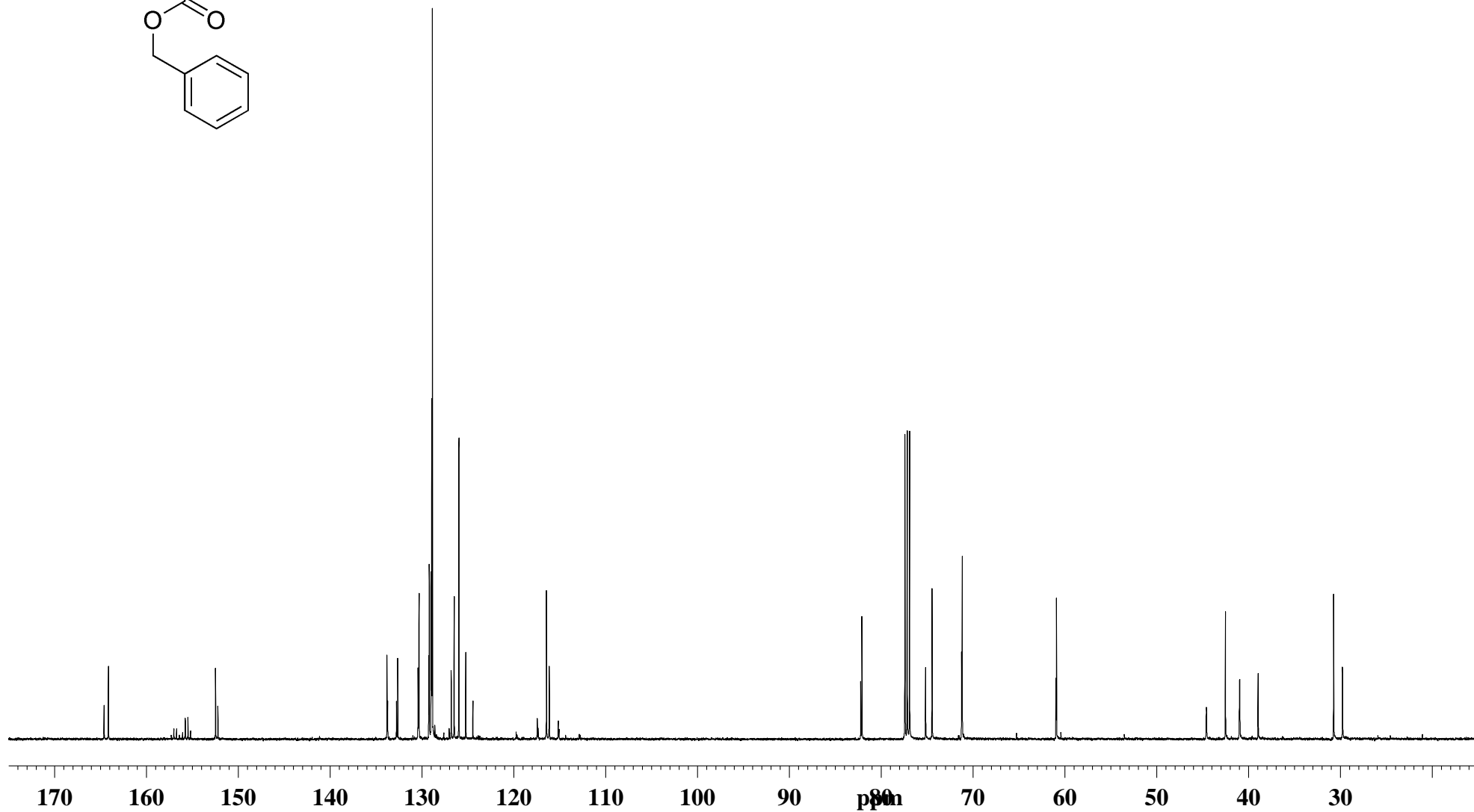


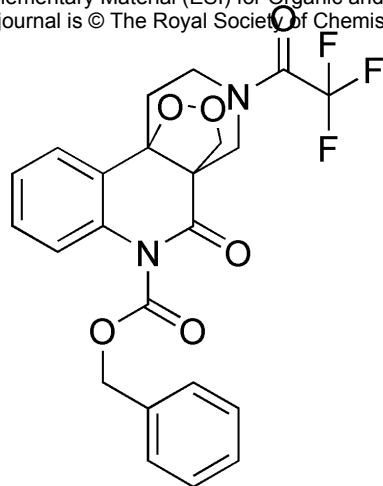
Compound 18, CDCl₃, 600.13 MHz



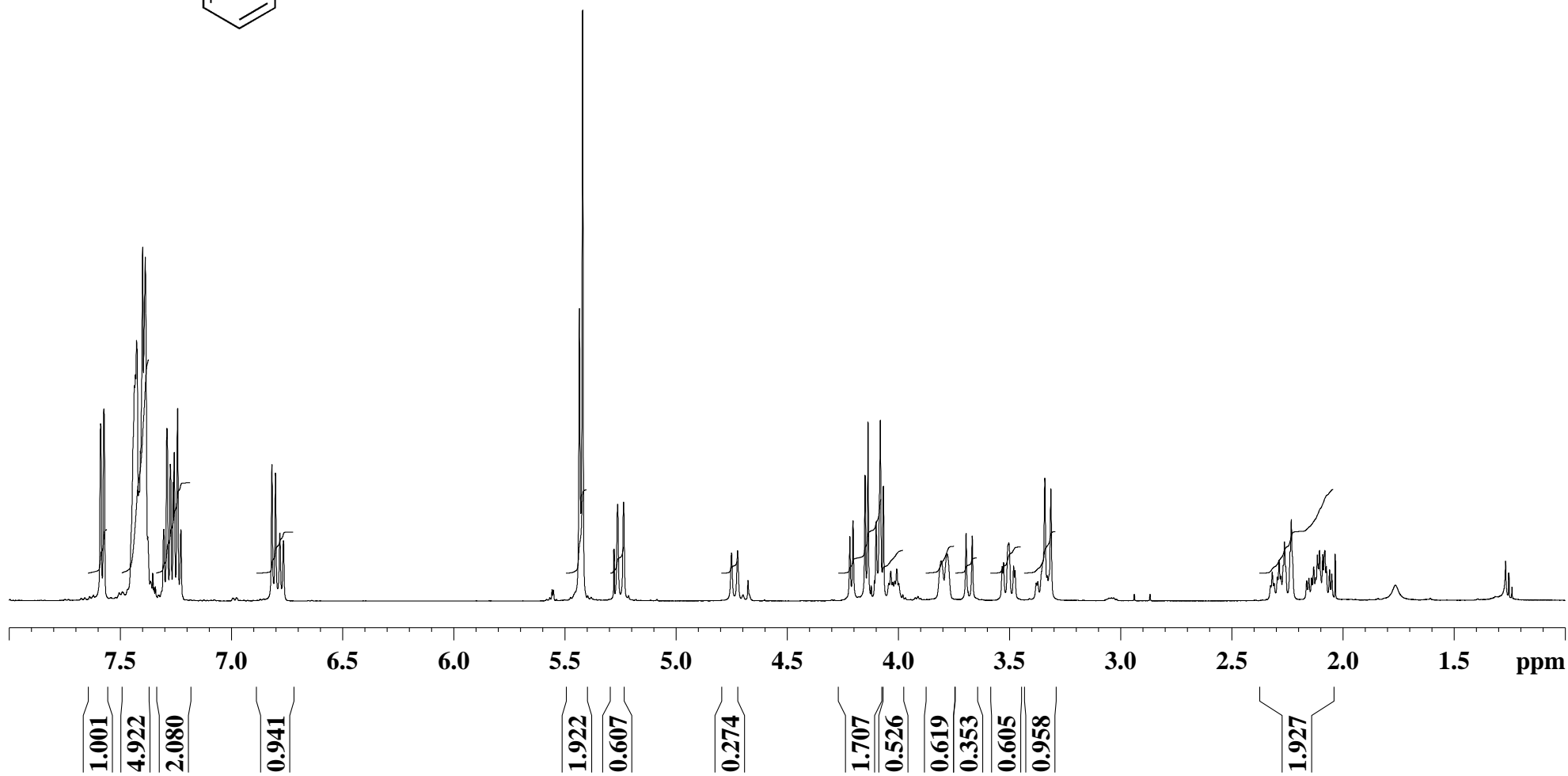


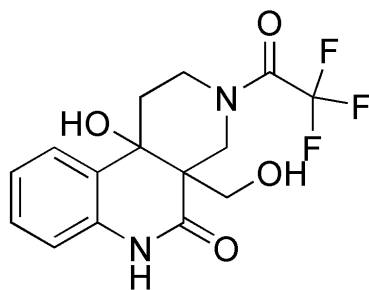
Compound 20, CDCl₃, 125.75 MHz



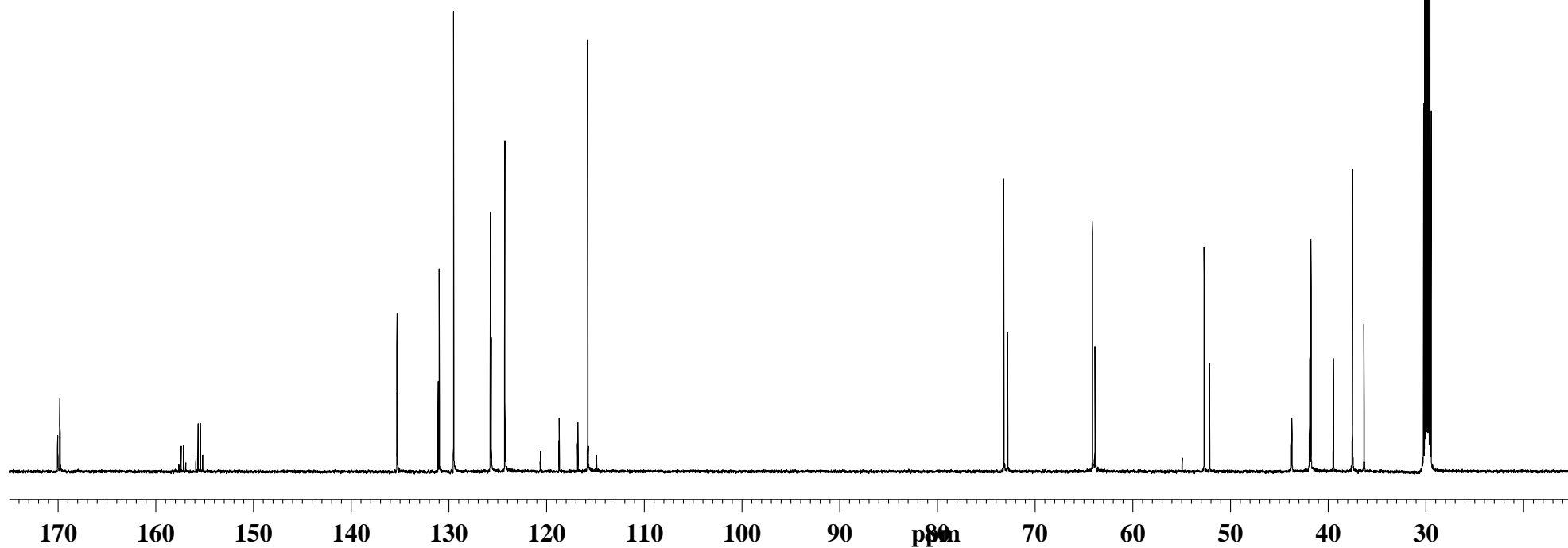


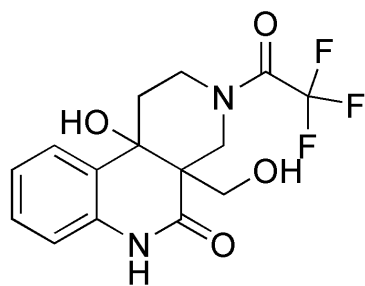
Compound 20, CDCL₃, 500.13 MHz





Compound 21, acetone-D₆, 150.9 MHz





Compound 21, acetone-D₆, 600.13 MHz

