Supplementary Material (ESI) for Organic and Biomolecular Chemistry


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

**Scott G. Stewart,* Emilio L. Ghisalberti, Brian W. Skelton and Charles H. Heath**

*The School of Biomedical, Biomolecular & Chemical Sciences, The University of Western Australia, Crawley, WA 6009, Australia; Fax: +61 (8) 6488 1005; E-mail: sgs@cyllene.uwa.edu.au*

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

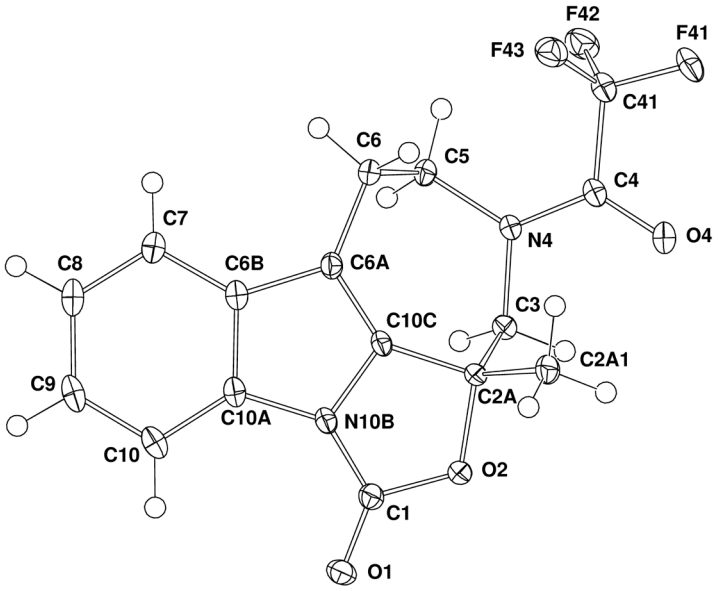



**Figure 1s:** Molecular structure of compound **18**.

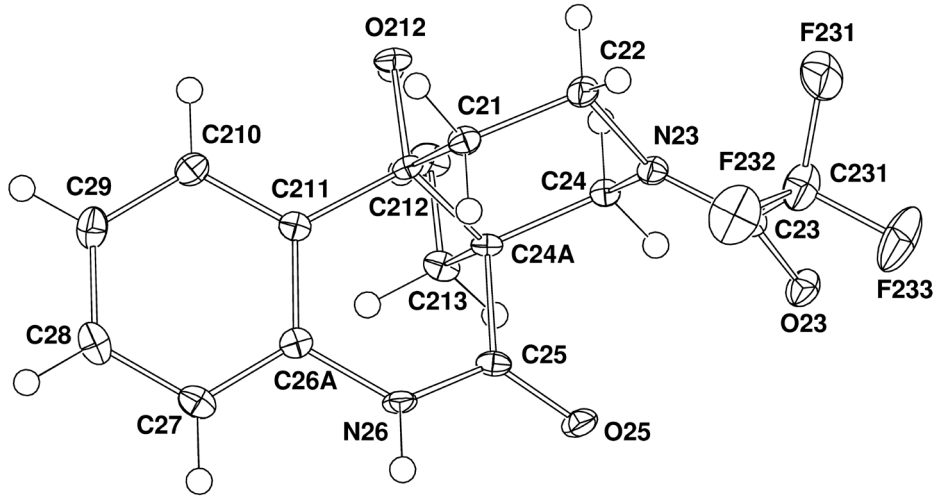



**Figure 2s:** Molecular structure of compound **21.**

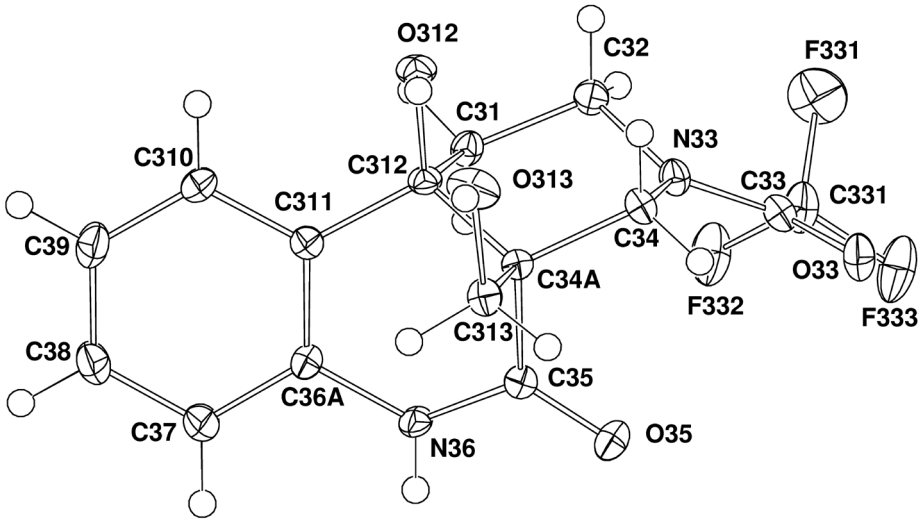


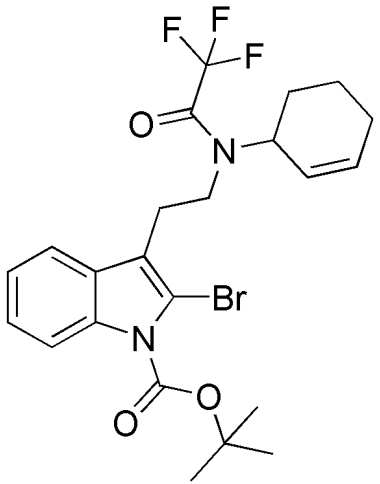

**Figure 3s:** Molecular structure (II) of compound **21.**

**Table1s.** Hydrogen bonds for **21** [Å and °].

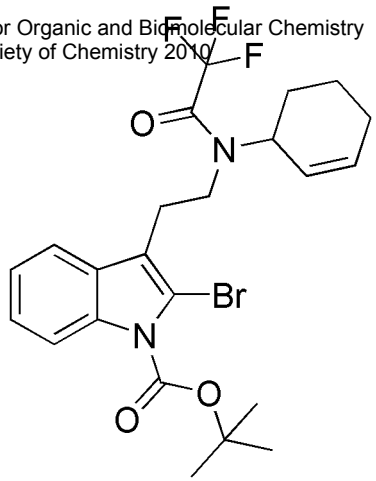
| D-H...A | d(D-H) | d(H...A) | d(D...A) | <(DHA) |
|---|---|---|---|---|
| N(16)-H(16)...O(25) | 0.88 | 2.23 | 3.0866(19) | 165.6 |
| O(112)-H(112)...O(35) | 0.831(17) | 1.928(19) | 2.7143(18) | 158(3) |
| O(113)-H(113)...O(33)[1] | 0.852(17) | 1.944(17) | 2.7936(18) | 175(3) |
| N(26)-H(26)...O(15) | 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:

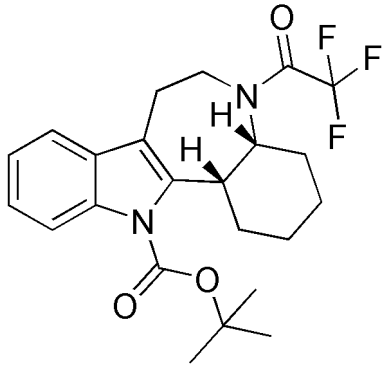
[1] x+1/2,1/2-y,1-z; [2] x-1/2,3/2-y,1-z; [3] 1/2-x,1-y,z-1/2



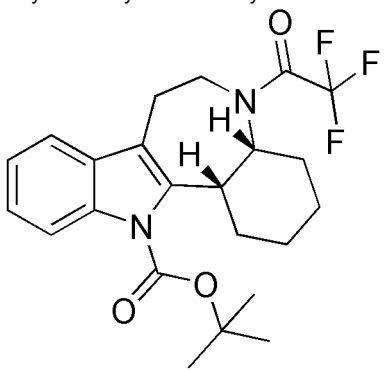

Compound 10, acetone-D6, 125.75 MHz



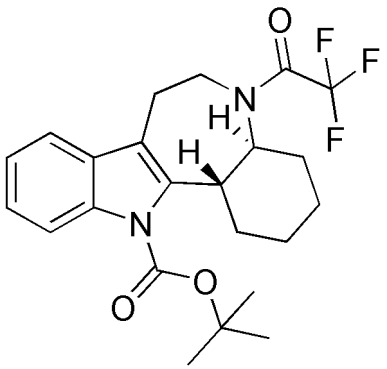

Compound 10, acetone-D6, 500.13 MHz



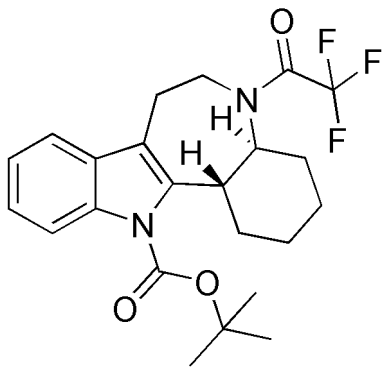

Compound 12a, acetone-D6, 150.9 MHz



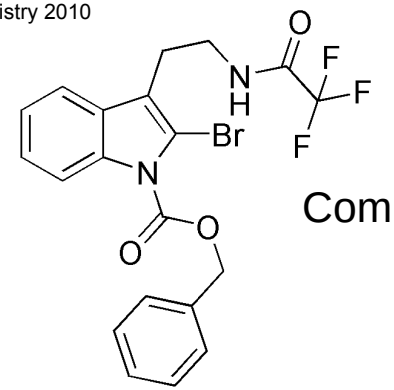

Compound 12a, acetone-D6, 600.13 MHz



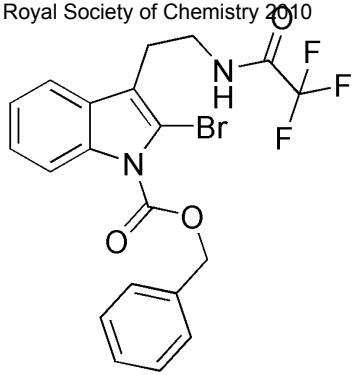

Compound 12b, acetone-D6,150.9 MHz



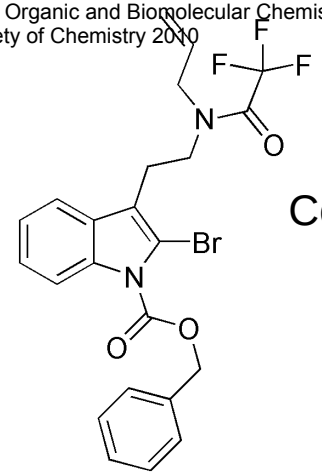

Compound 12b, acetone-D6, 600.13 MHz



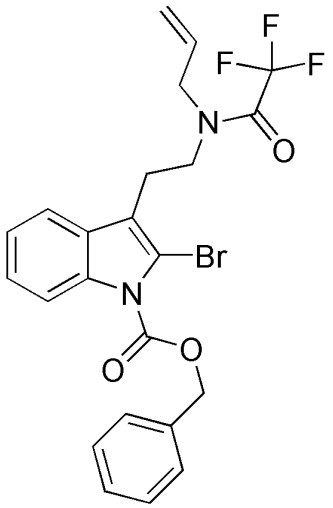

Compound 13, acetone-D6, 125.75 MHz



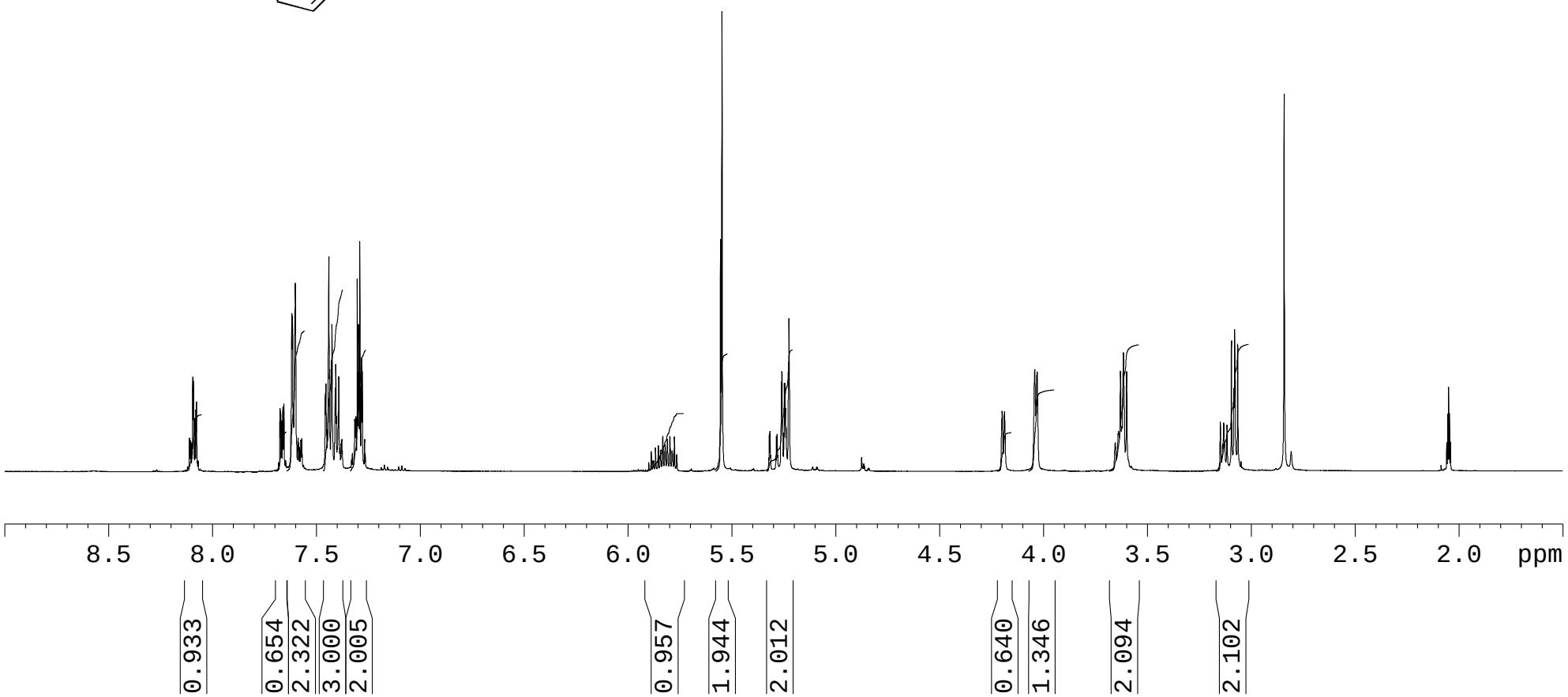

Compound 13, acetone-D6, 500.13 MHz

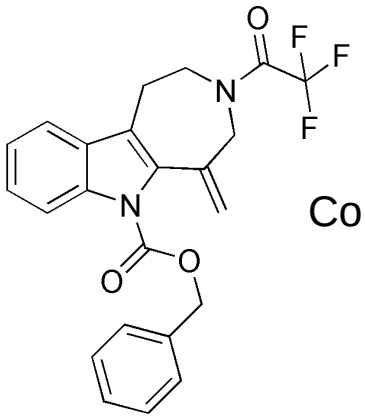



Compound 14, acetone-D6, 125.75 MHz

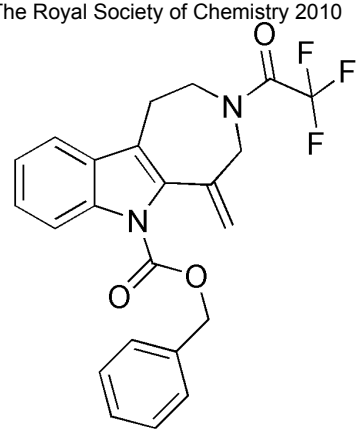



Compound 14, acetone-D6, 500.13 MHz

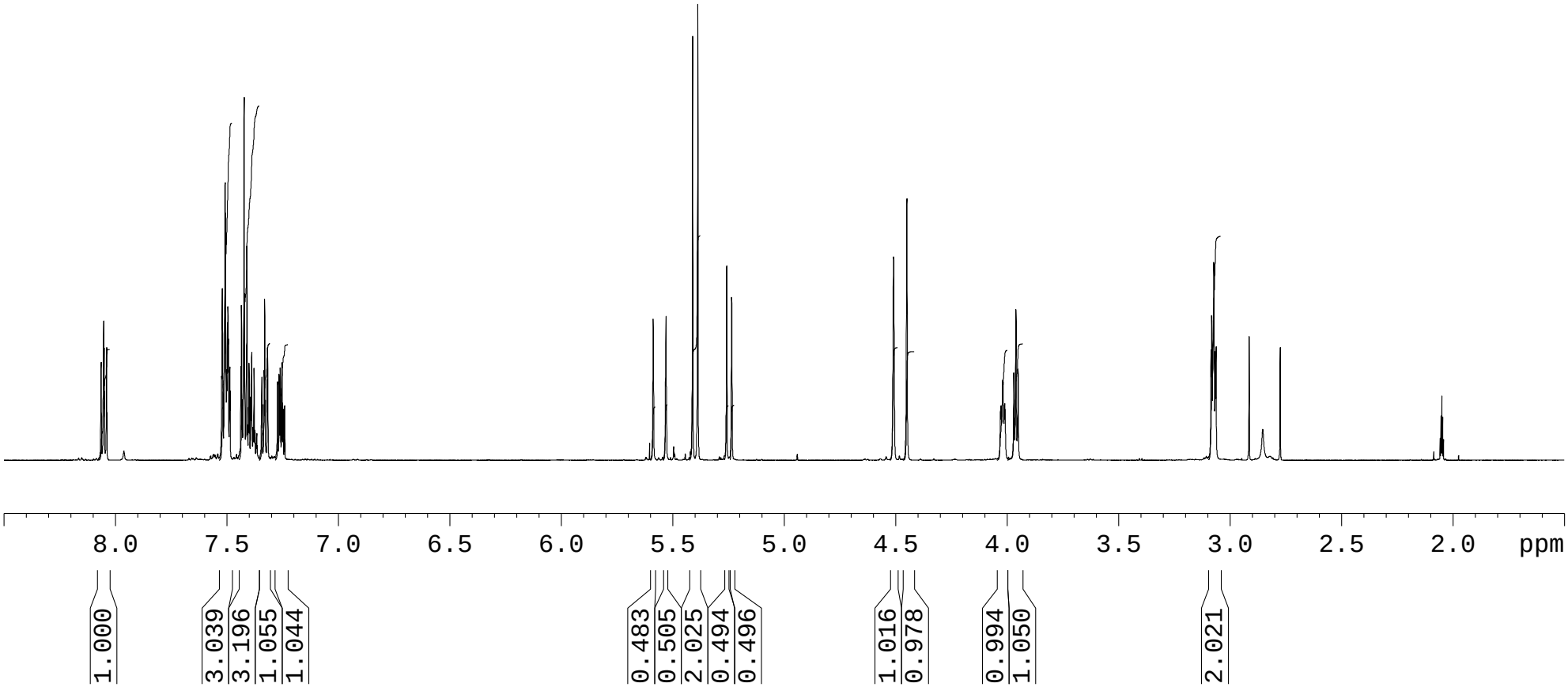


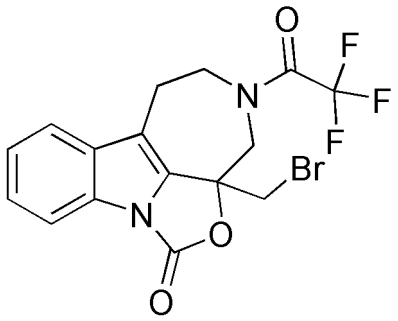



Compound 15, acetone-D6, 150.9 MHz

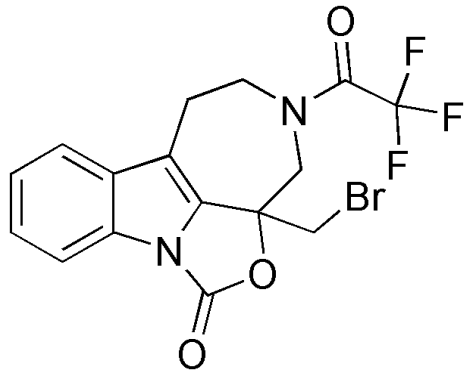



Compound 15, acetone-D6, 600.13 MHz

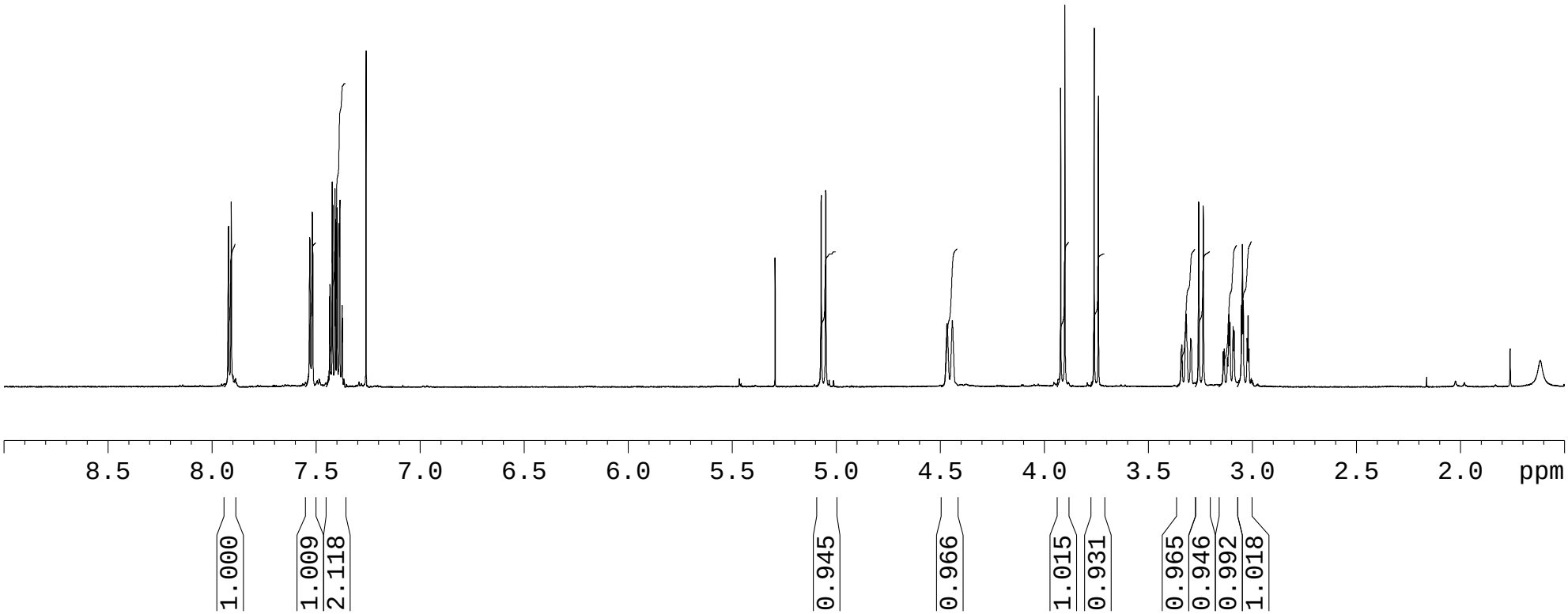


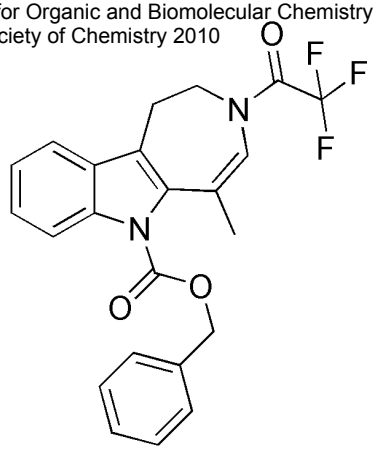



Compound 16, CDCl3, 150.9 MHz

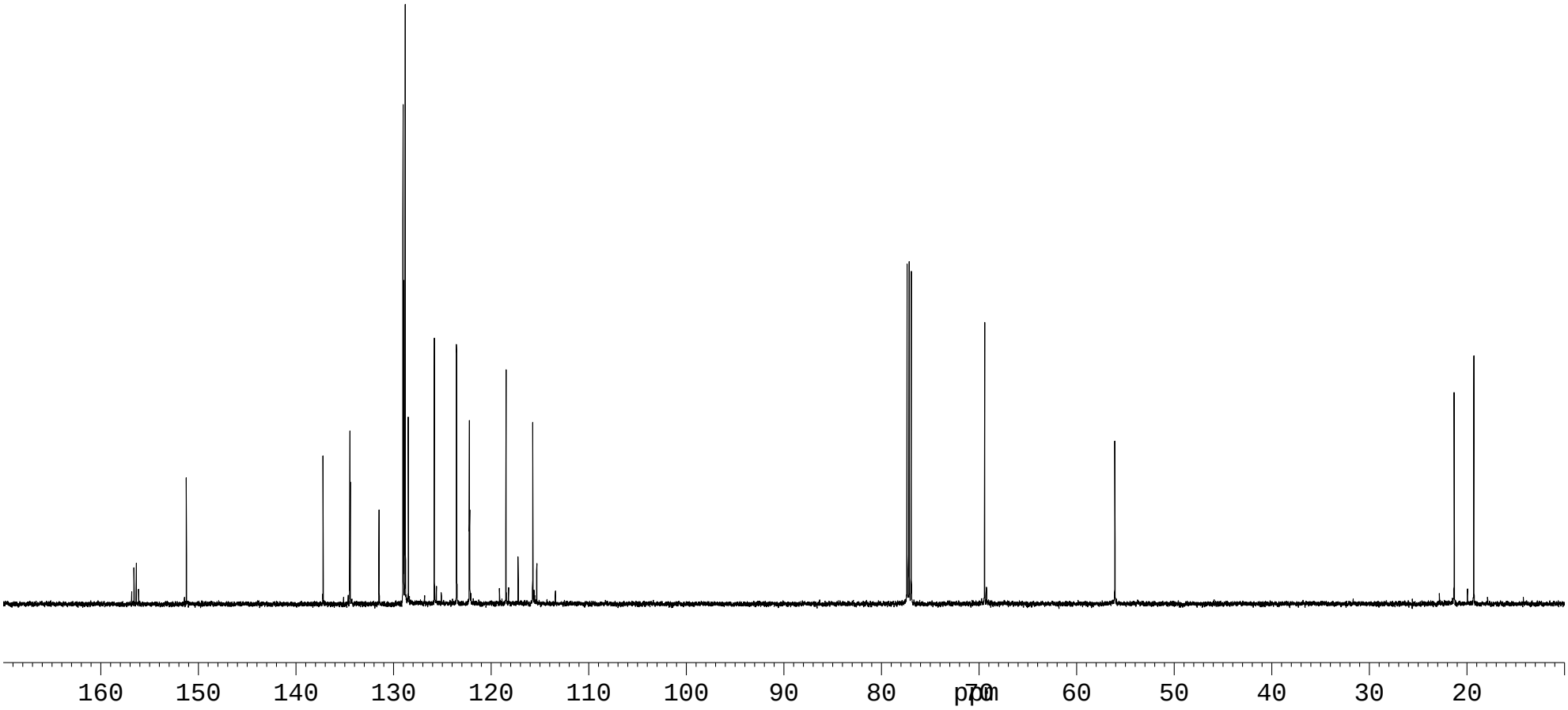


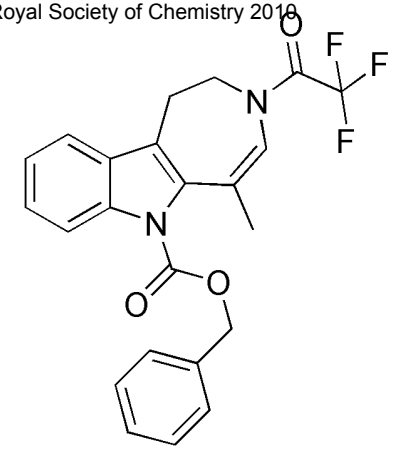

Compound 16, CDCl3, 600.13 MHz



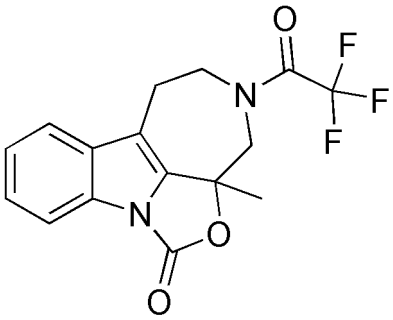



Compound 17, CDCL3, 150.9 MHz

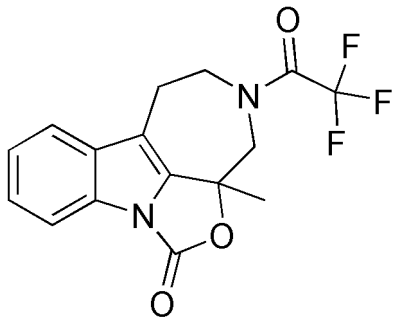




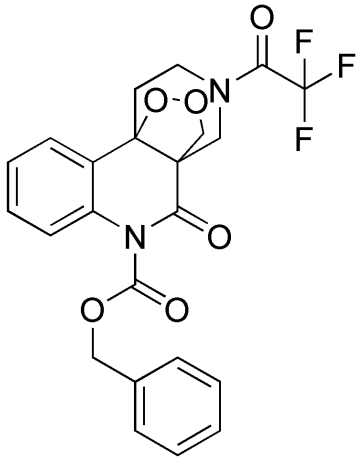

Compound 17, CDCl3, 600.13 MHz



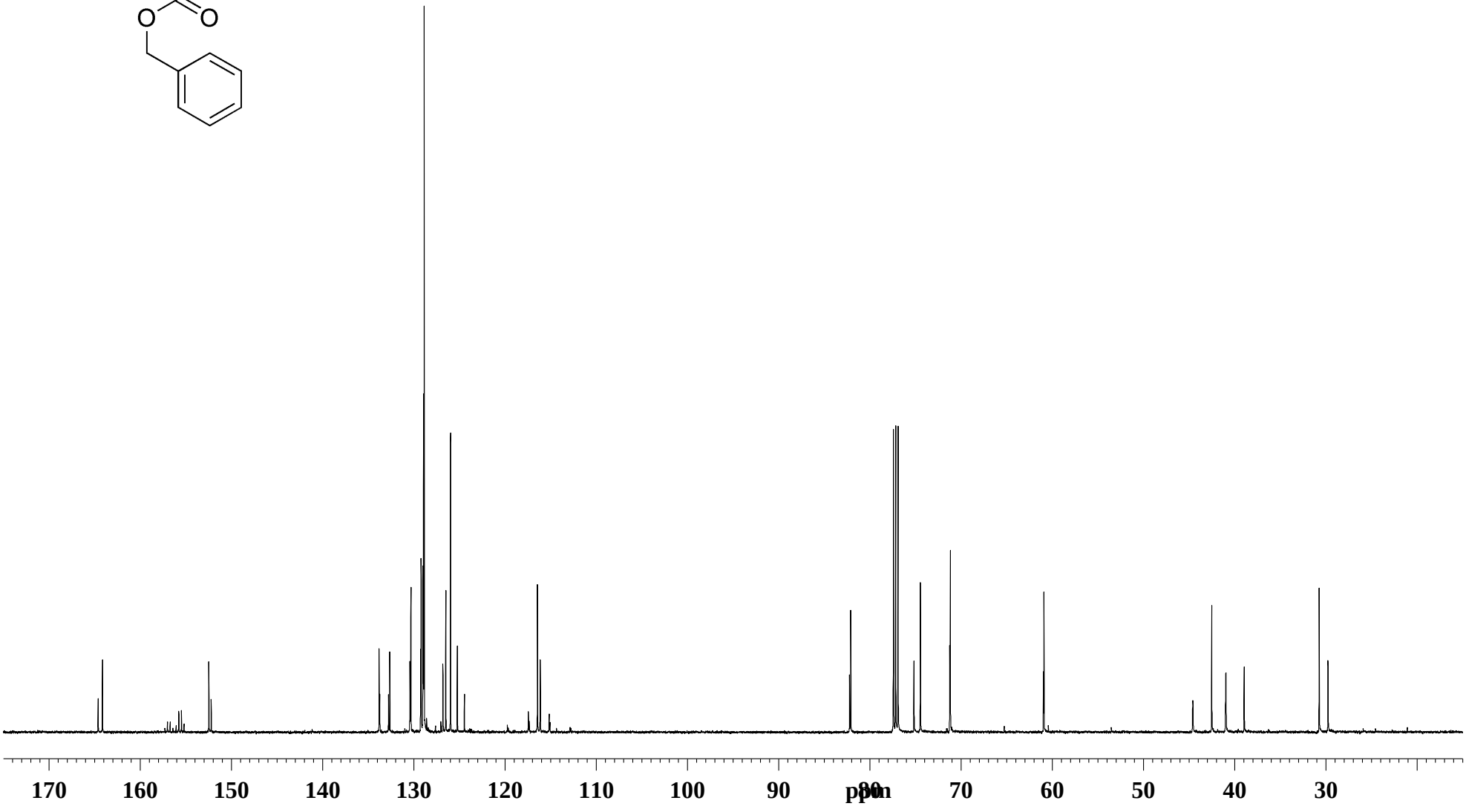

Compound 18, CDCl3, 150.9 MHz

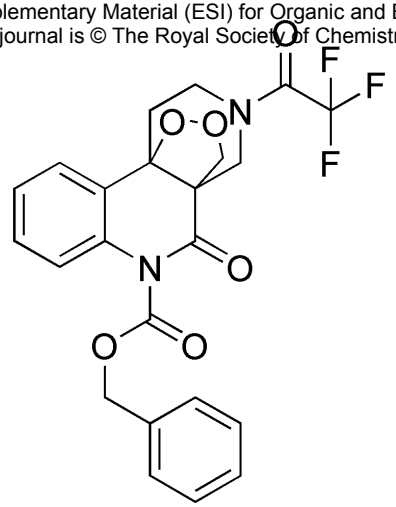



Compound 18, CDCl3, 600.13 MHz

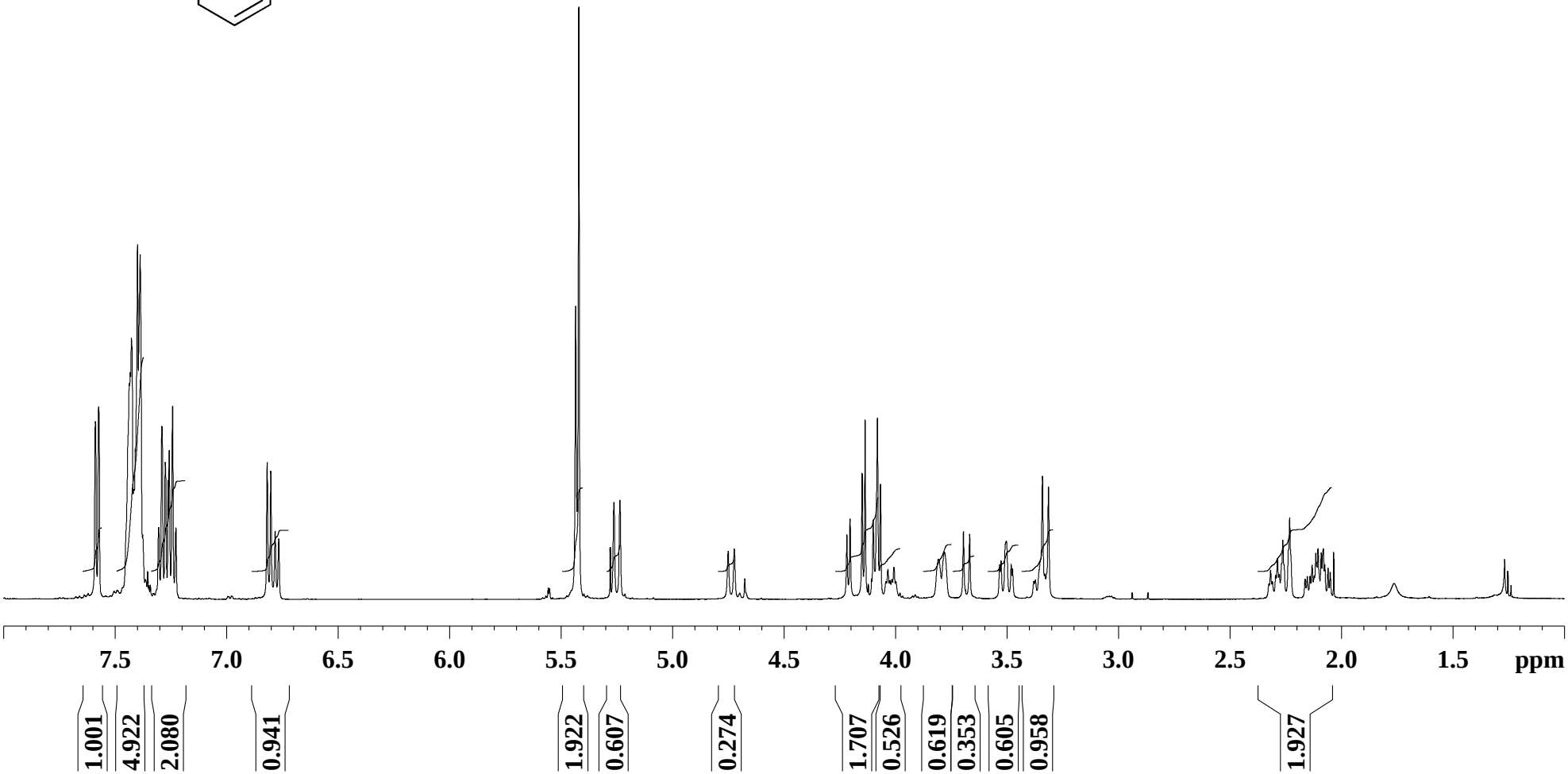


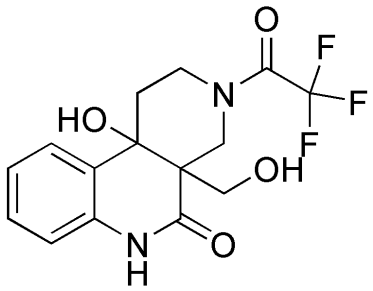

Compound 20, CDCl3, 125.75 MHz



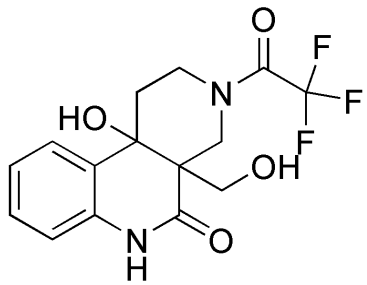



Compound 20, CDCL3, 500.13 MHz






Compound 21, acetone-D6, 150.9 MHz




Compound 21,acetone-D6, 600.13 MHz