

SUPPLEMENTARY INFORMATION

**Synthesis, Characterization and Biological Evaluation of
Carboranylmethylbenzo[*b*]acridones as Novel Agents for Boron
Neutron Capture Therapy**

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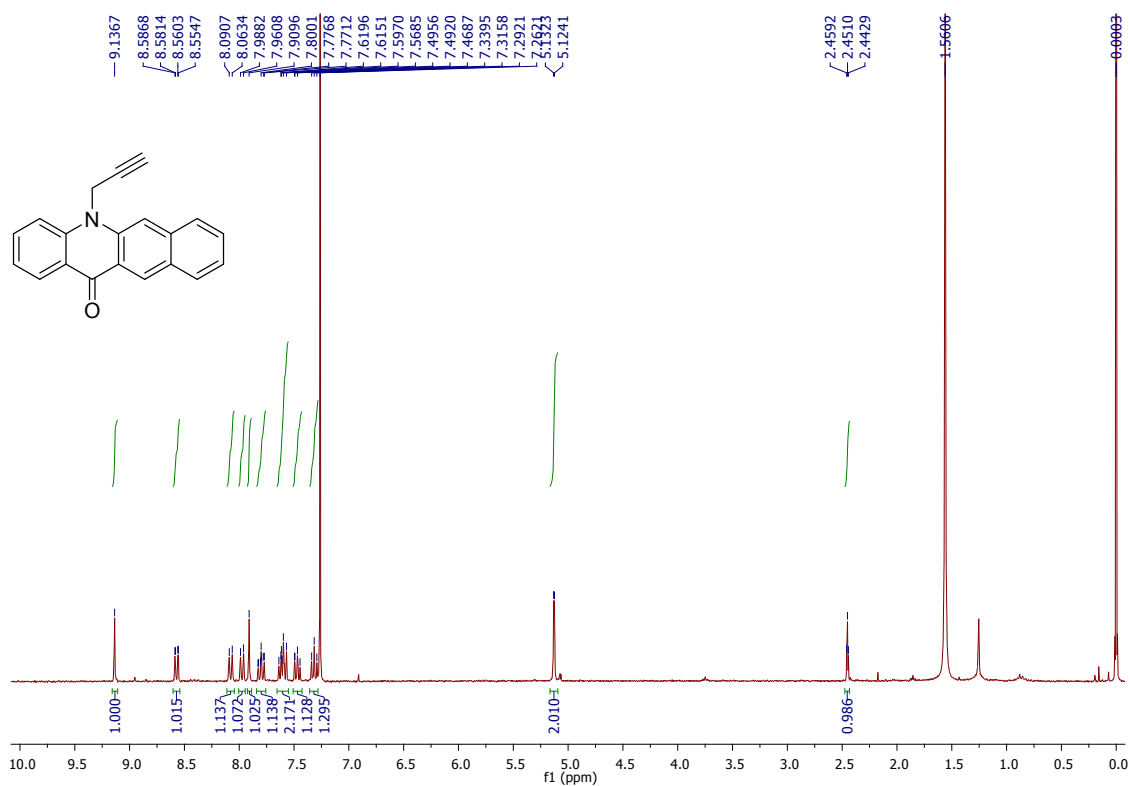
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Técnico, Universidade de Lisboa, Estrada Nacional 10 (km 139.7) 2695-066 Bobadela LRS, Portugal
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Caparica, Portugal and CESAM-Lisboa, Faculdade de Ciências da Universidade de Lisboa, Campo
Grande, 1749-016 Lisboa, Portugal

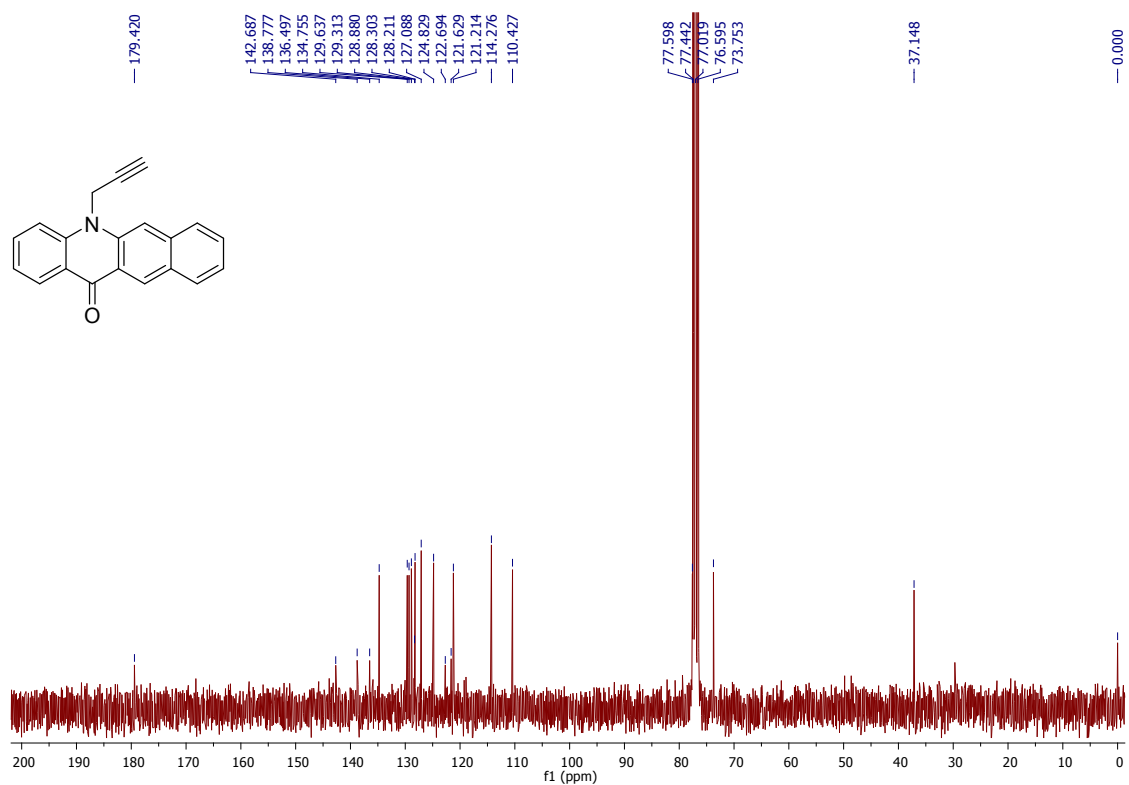
^dFaculdade de Medicina da Universidade de Lisboa, Instituto Medicina Molecular, Av. Prof. Egas Moniz,
1649-028 Lisboa Portugal

^1H and ^{13}C NMR spectra of new synthesized compounds

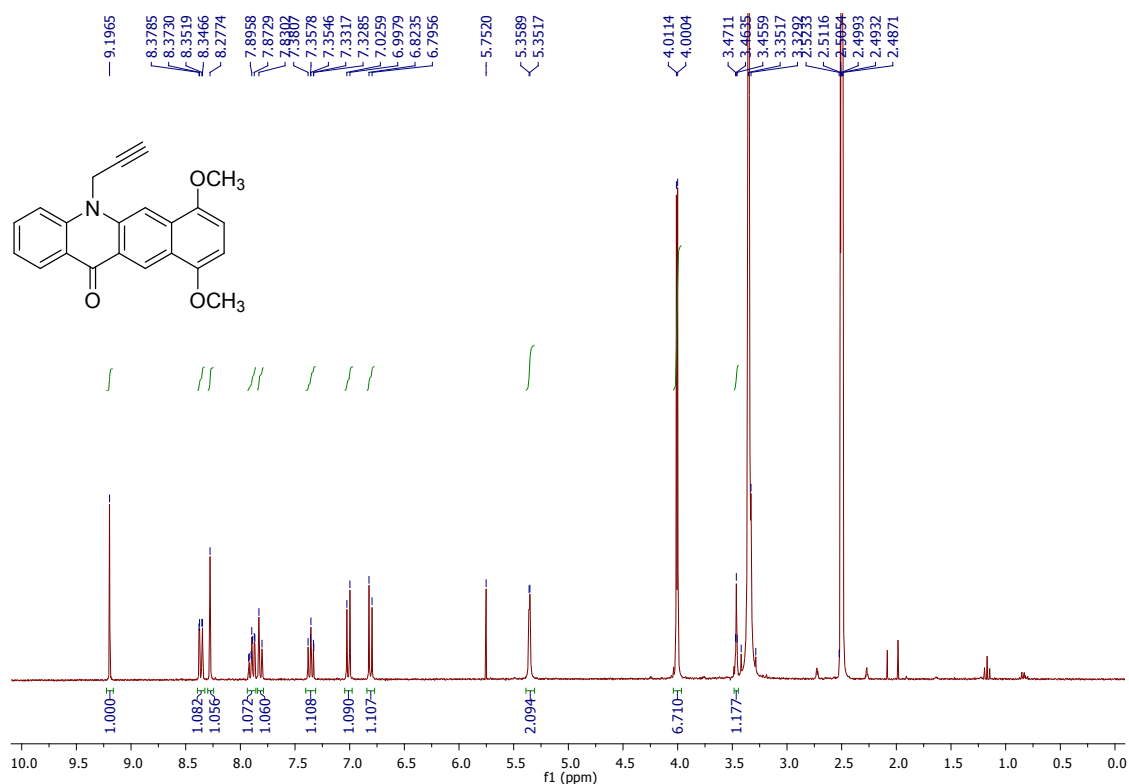
^1H NMR Spectrum of 7-(Prop-2-yn-1-yl)benzo[*b*]acridin-12(7*H*)-one (2a)



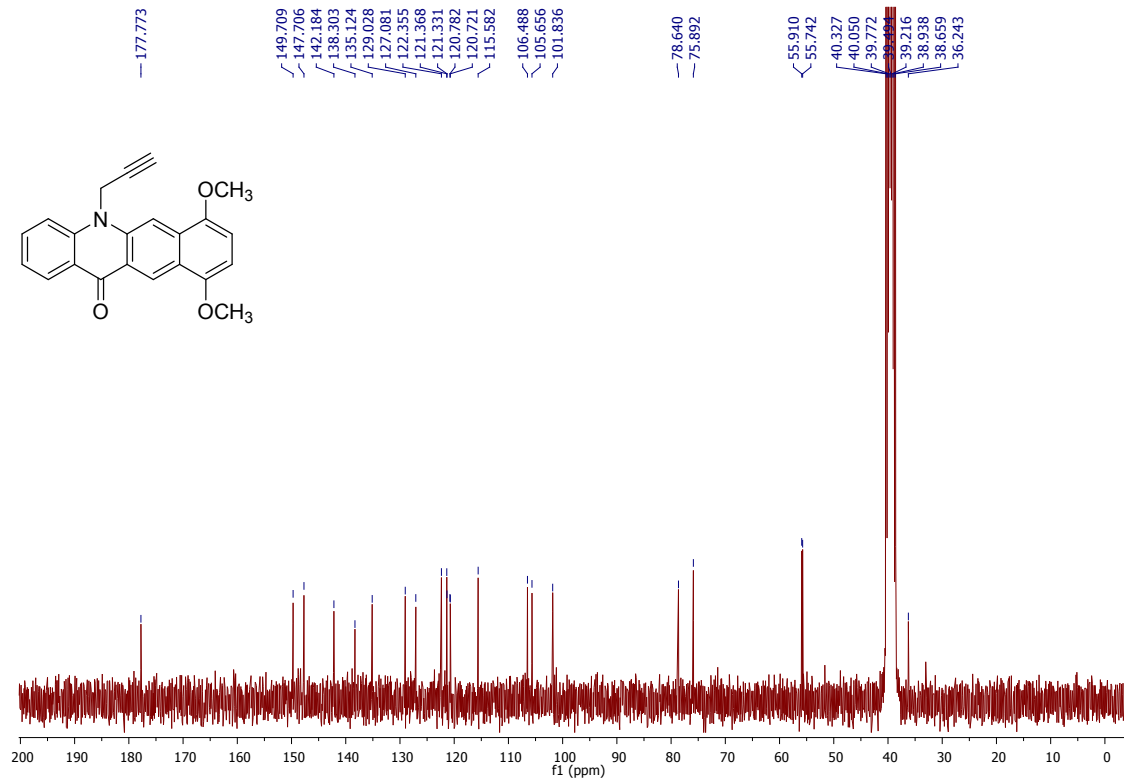
^{13}C NMR Spectrum of 7-(Prop-2-yn-1-yl)benzo[*b*]acridin-12(7*H*)-one (2a)



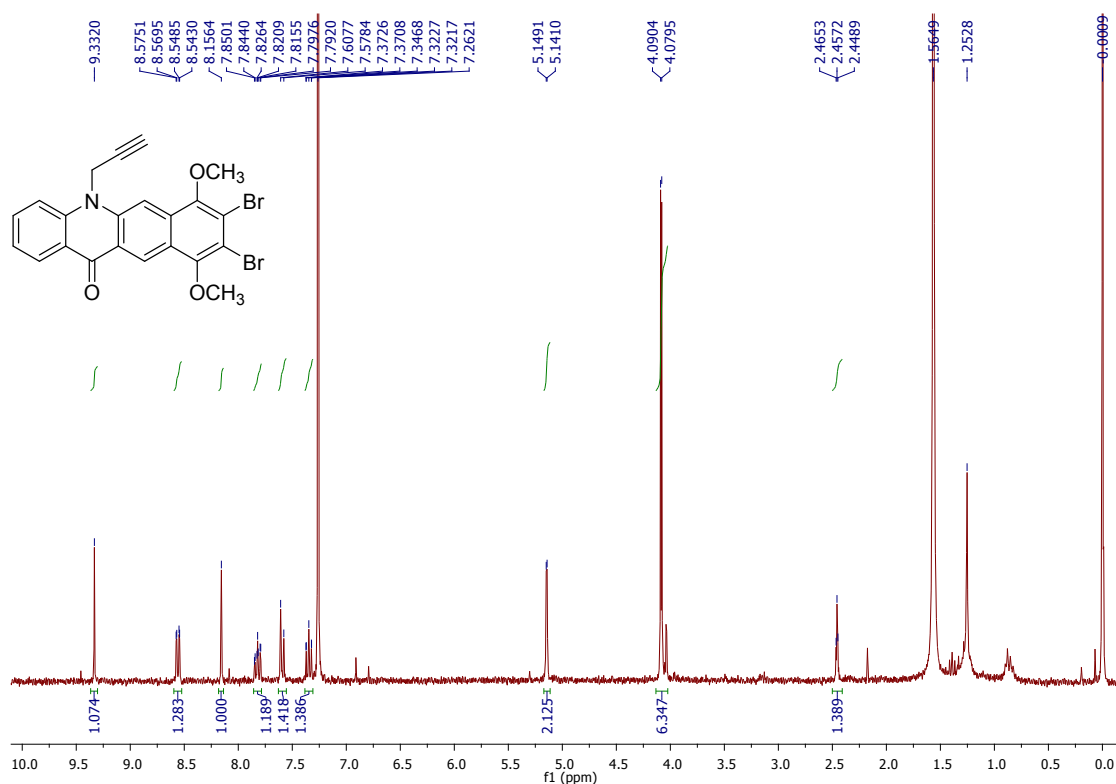
¹H NMR Spectrum of 2,5-Dimethoxy-7-(prop-2-yn-1-yl)benzo[*b*]acridin-12(7*H*)-one (2b)



¹³C NMR Spectrum of 2,5-Dimethoxy-7-(prop-2-yn-1-yl)benzo[*b*]acridin-12(7*H*)-one (2b)

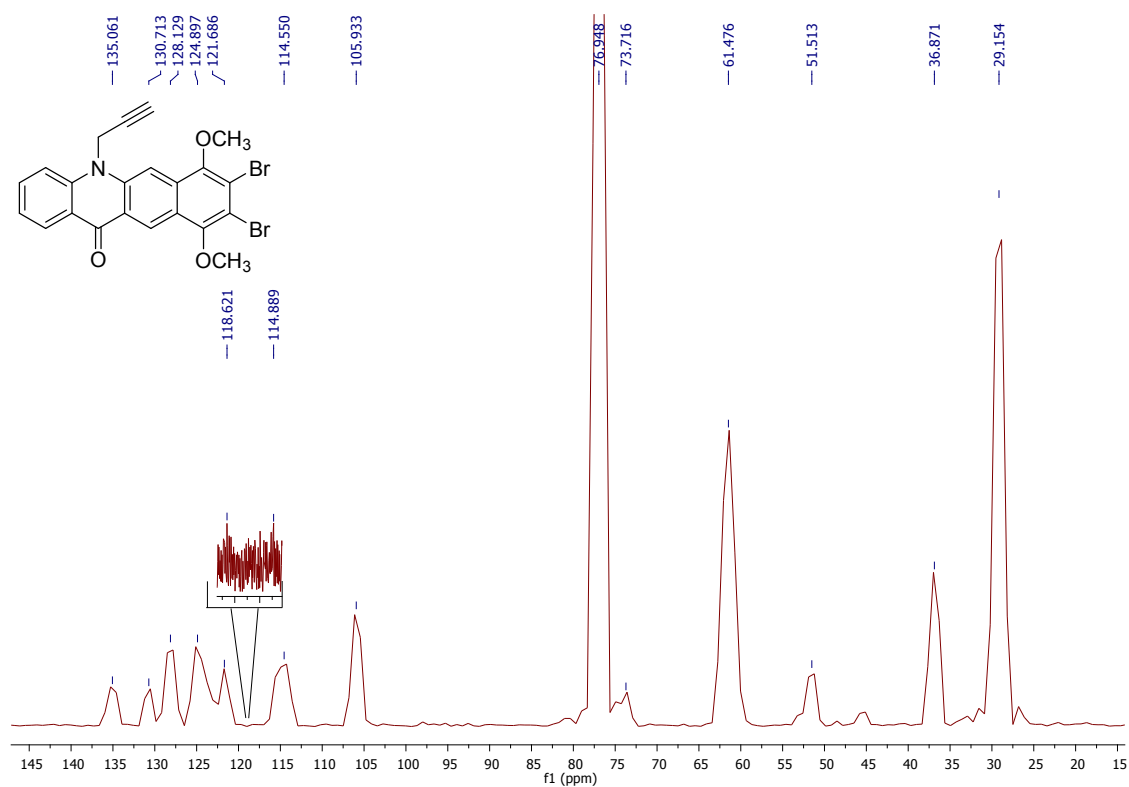


¹H NMR Spectrum of 3,4-Dibromo-2,5-dimethoxy-7-(prop-2-yn-1-yl)benzo[*b*]acridin-12(7*H*)-one (2c)

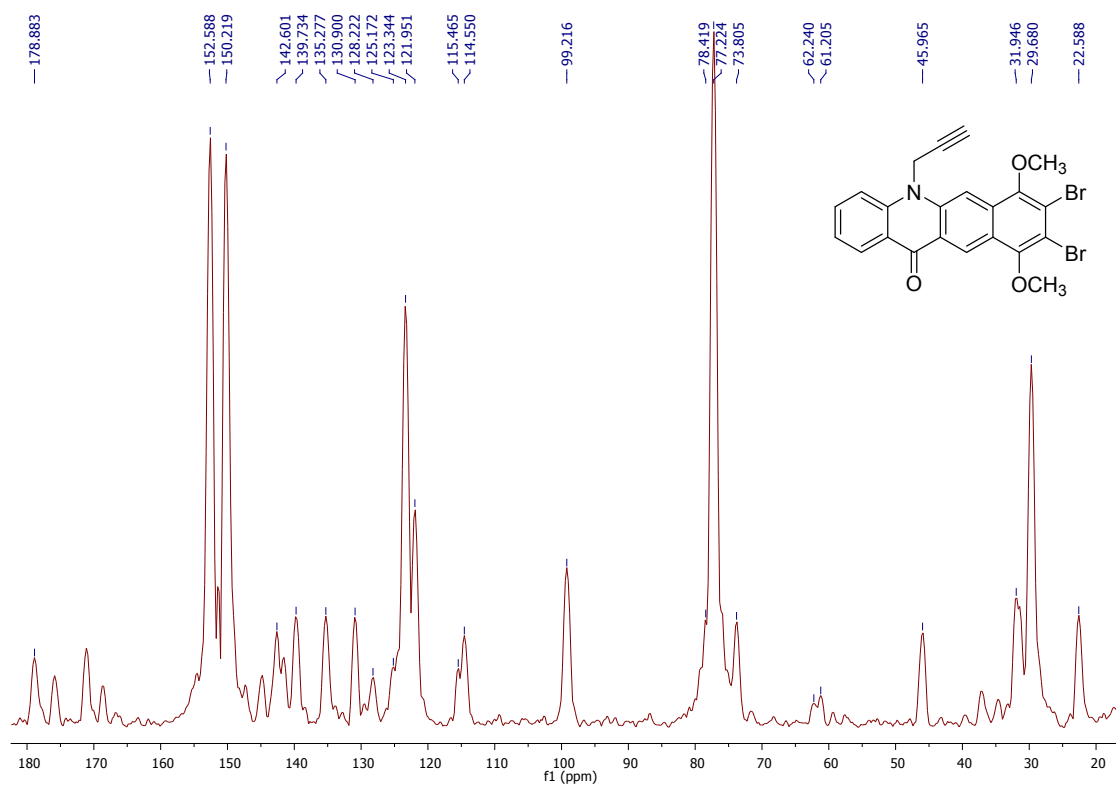


¹³C NMR Spectrum of 3,4-Dibromo-2,5-dimethoxy-7-(prop-2-yn-1-yl)benzo[*b*]acridin-12(7*H*)-one (2c)

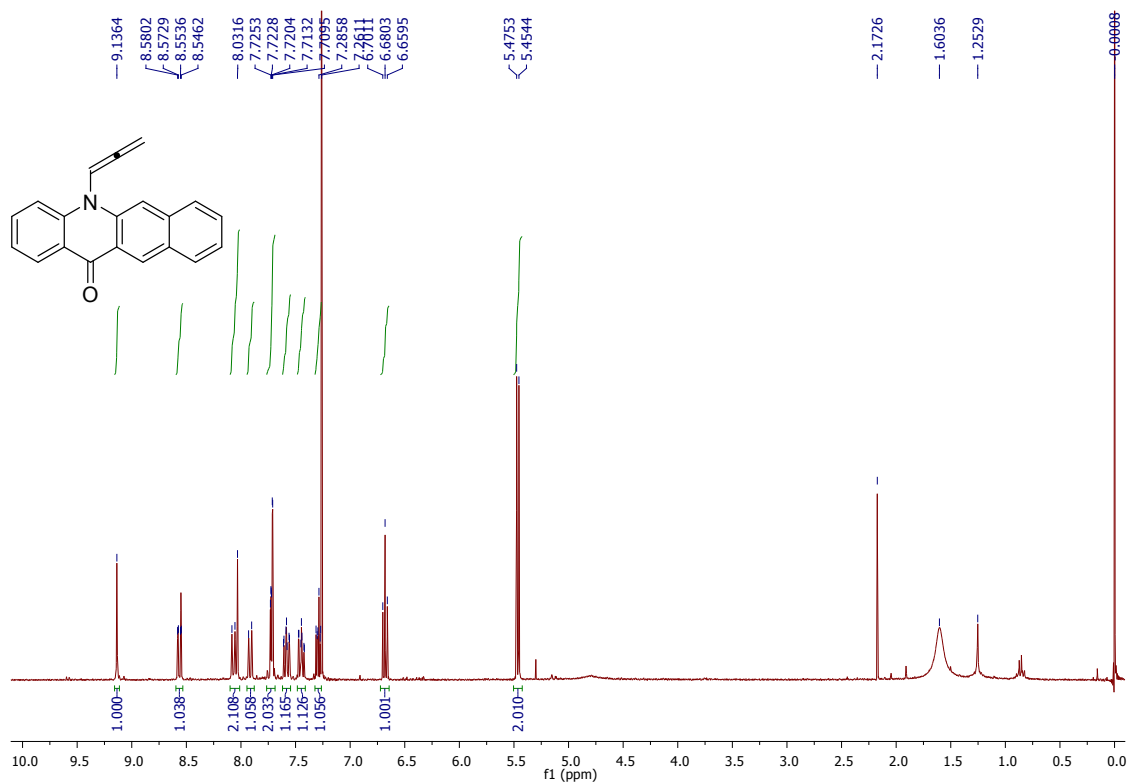
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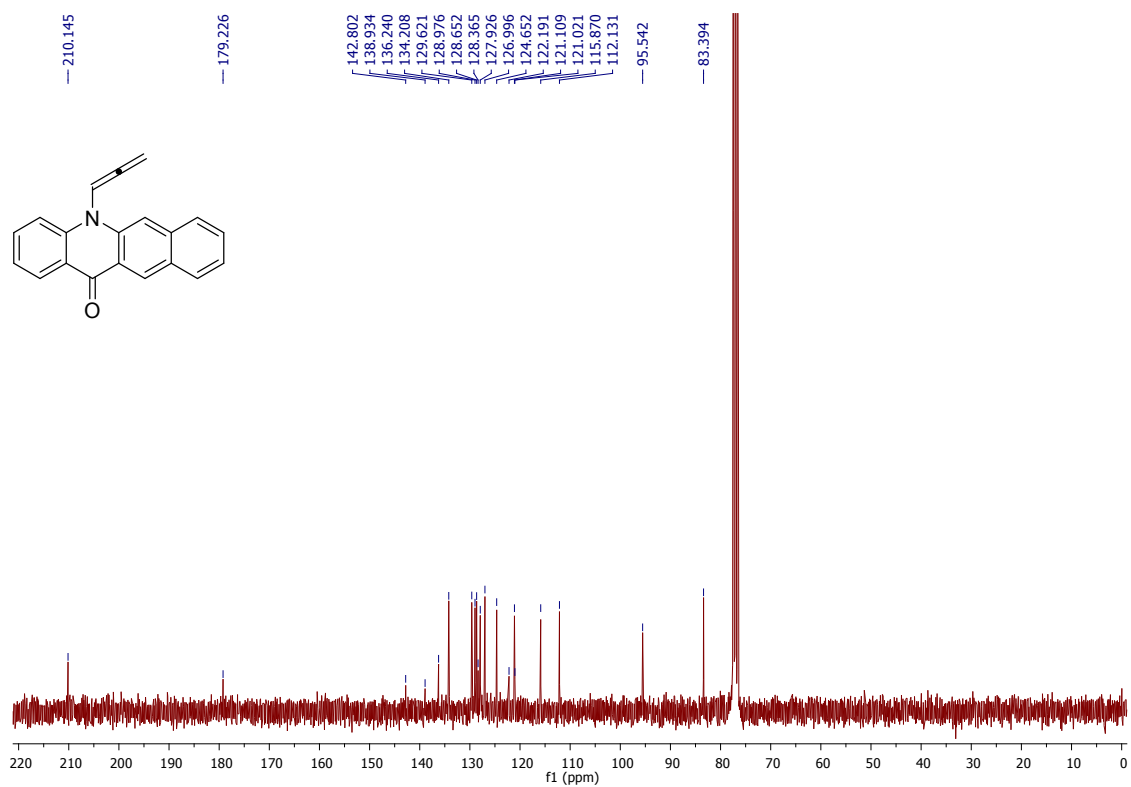
HMBC Projection



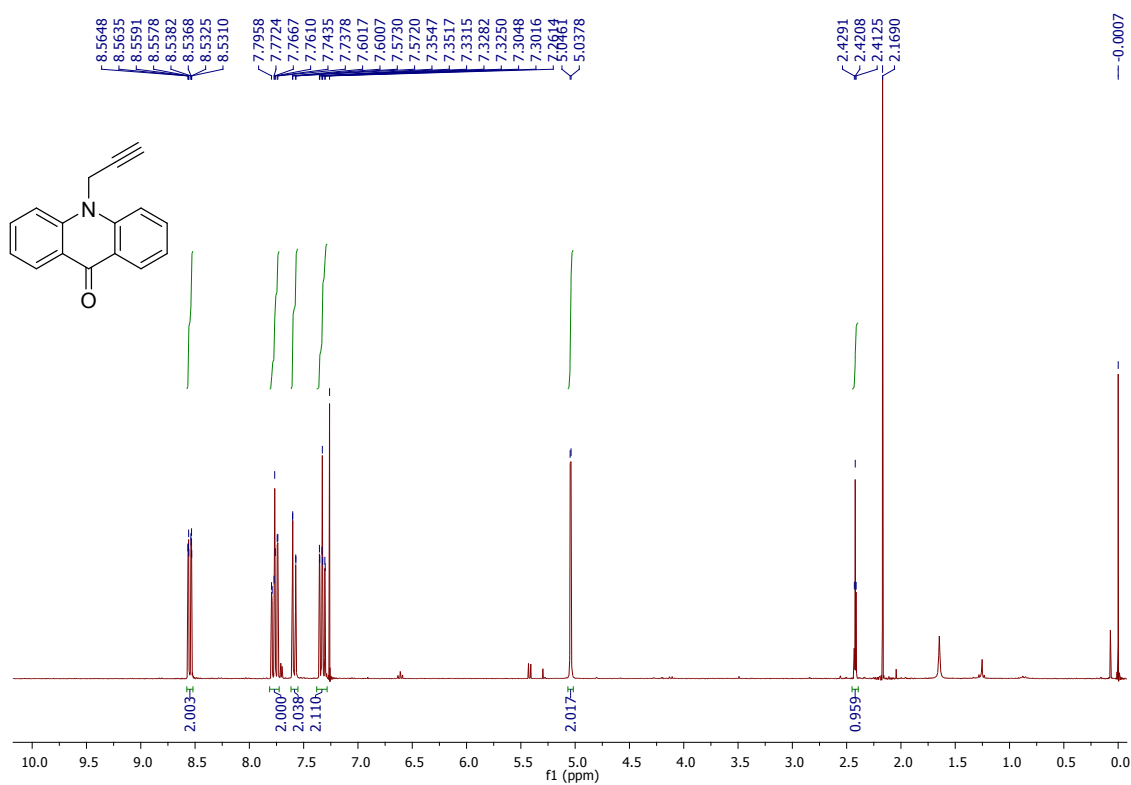
¹H NMR Spectrum of 7-(Propa-2-dien-1-yl)benzo[*b*]acridin-12(7*H*)-one (3)



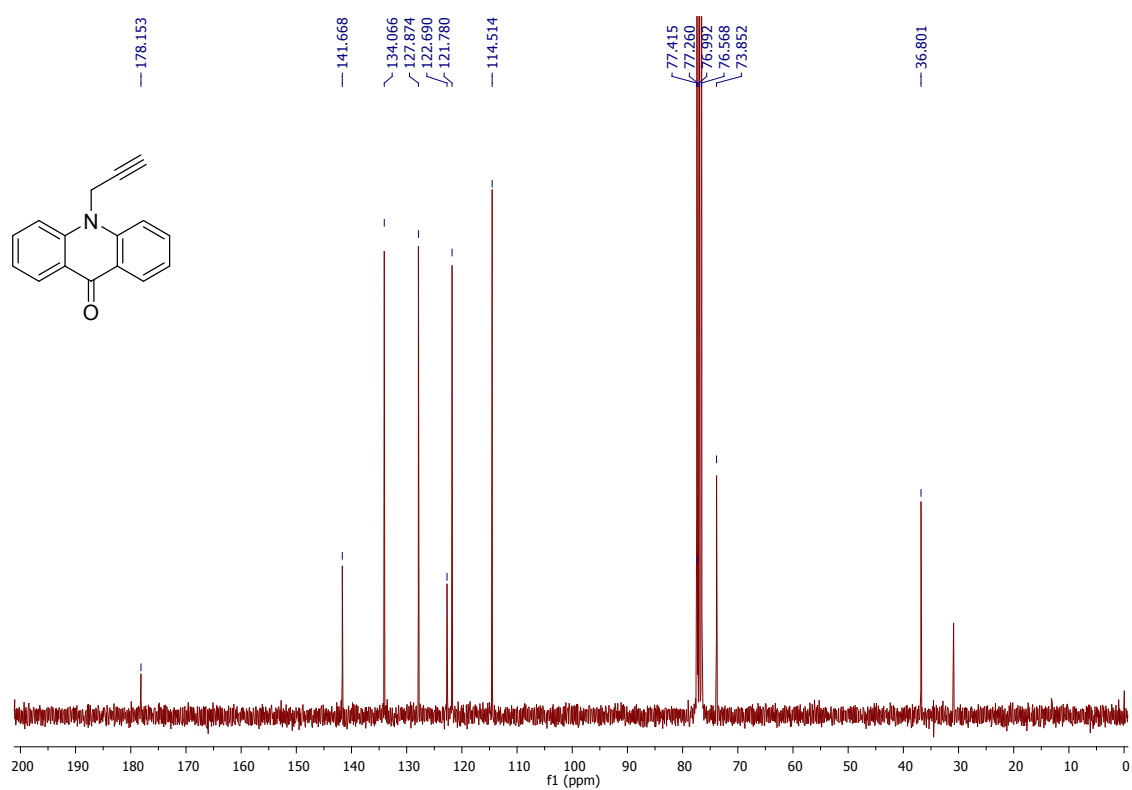
¹³C NMR Spectrum of 7-(Propa-2-dien-1-yl)benzo[*b*]acridin-12(7*H*)-one (3)



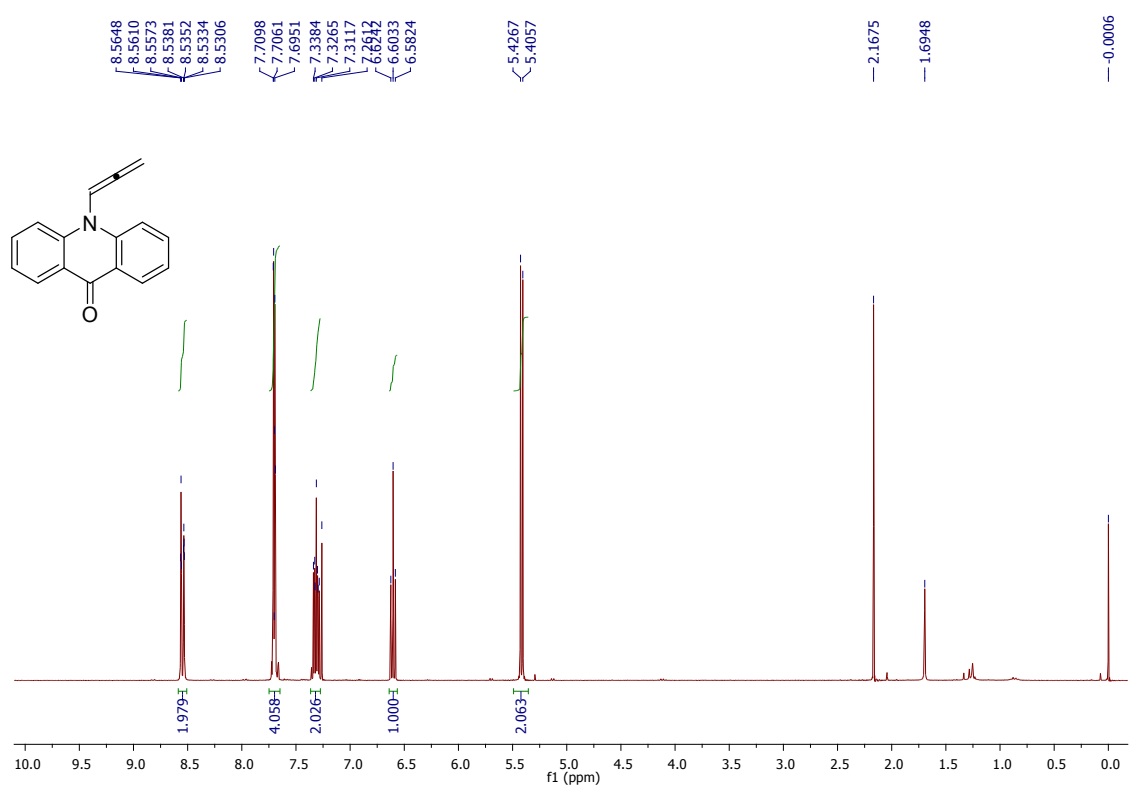
¹H NMR Spectrum of 10-(Prop-2-yn-1-yl)acridin-9(10*H*)-one (7)



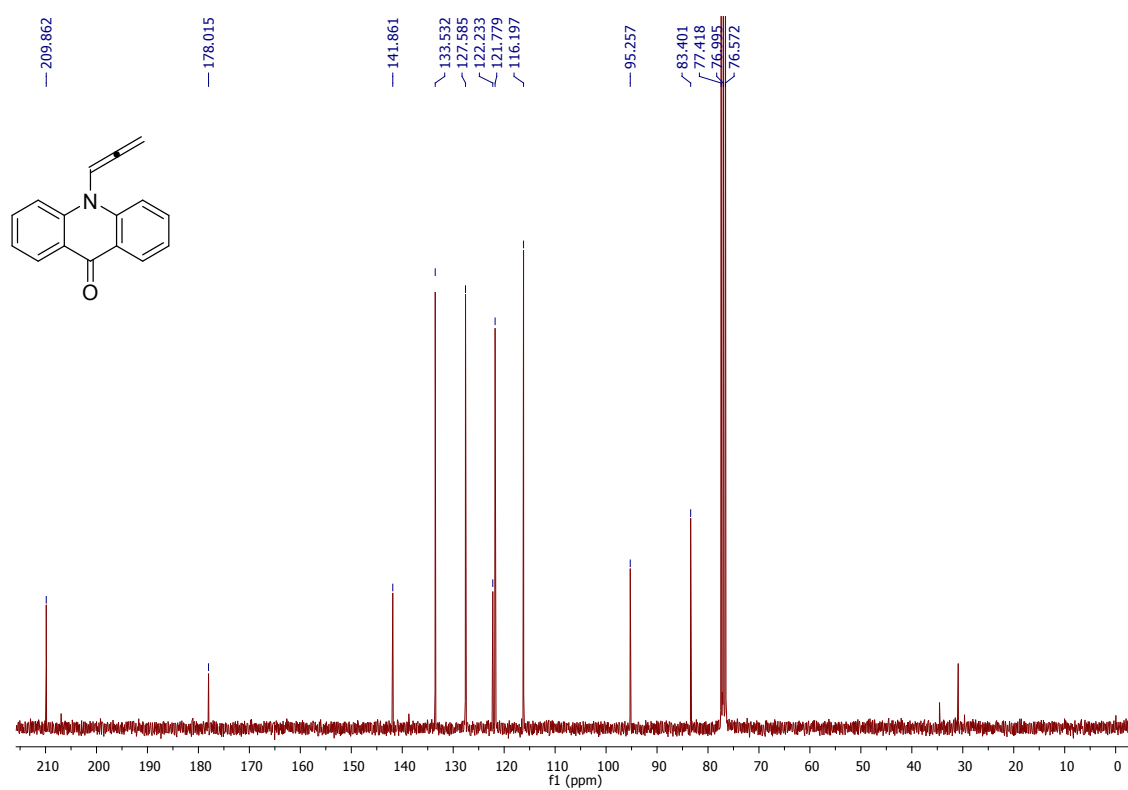
¹³C NMR Spectrum of 10-(Prop-2-yn-1-yl)acridin-9(10*H*)-one (7)



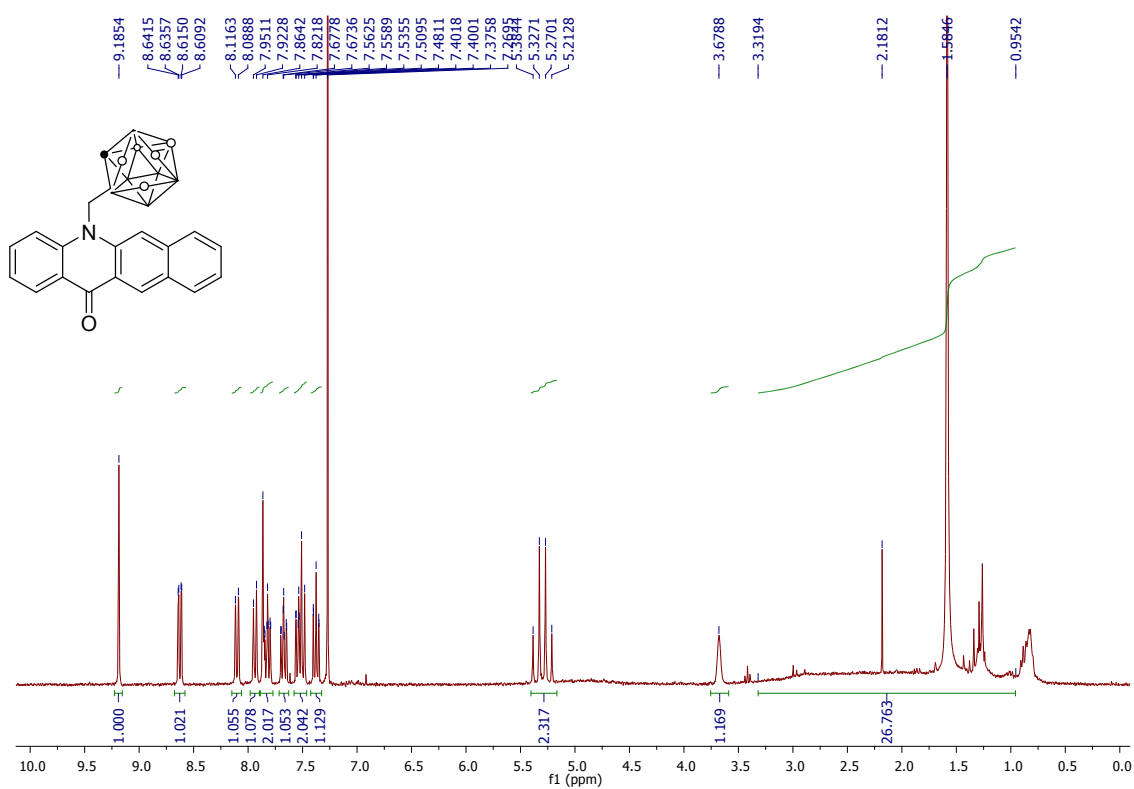
¹H NMR Spectrum of 10-(Propa-1,2-dien-1-yl)acridin-9(10*H*)-one (8)



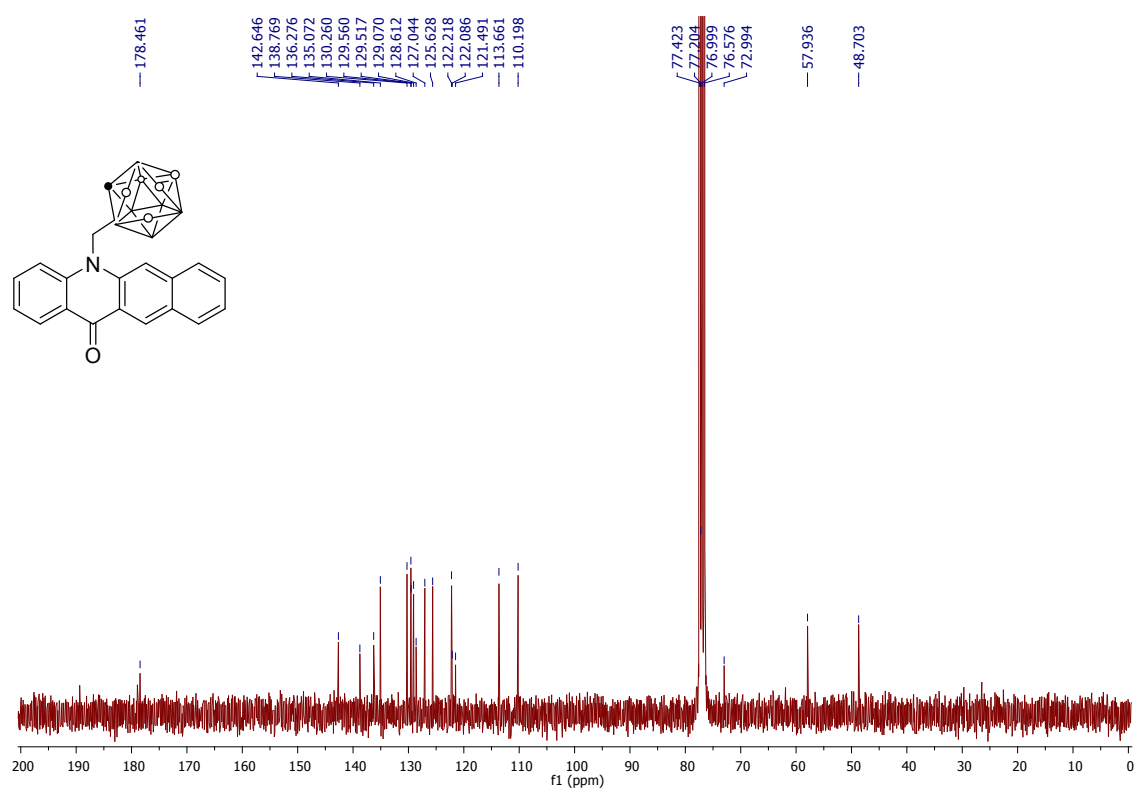
^{13}C NMR Spectrum of 10-(Propa-1,2-dien-1-yl)acridin-9(10*H*)-one (8)



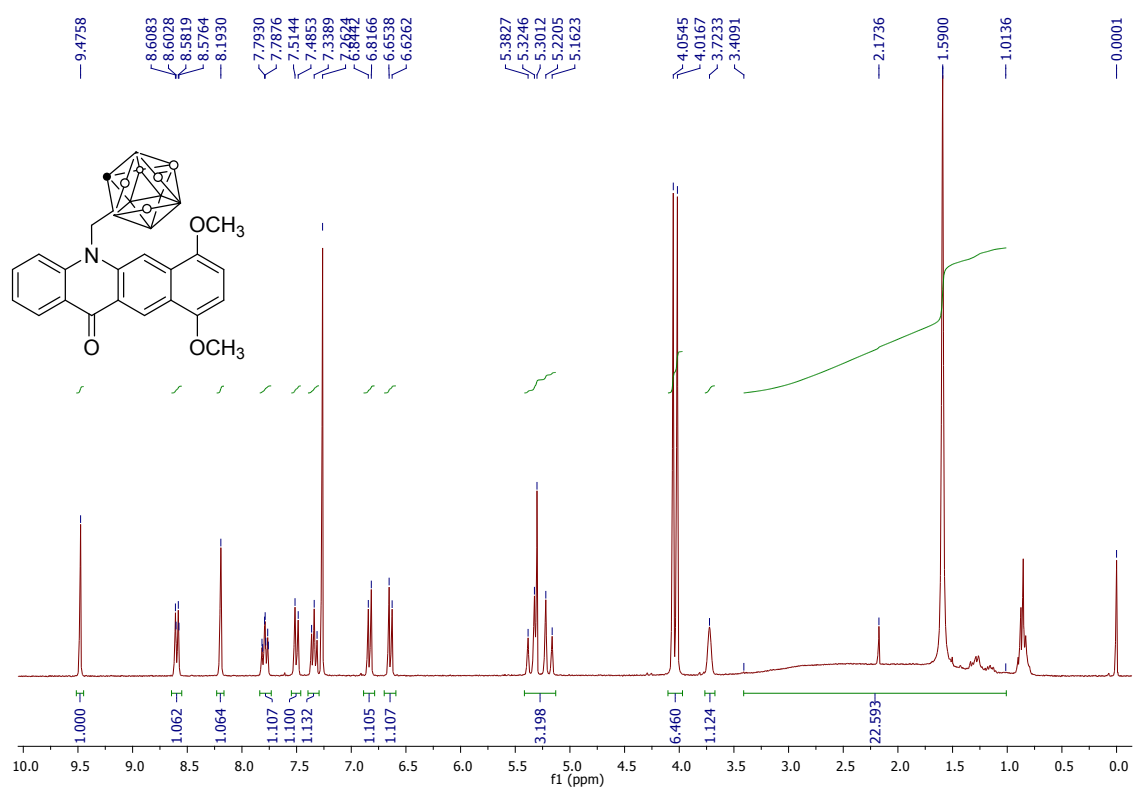
^1H NMR Spectrum of 7-Carboranylmethylbenzo[*b*]acridin-12(7*H*)-one (4a)



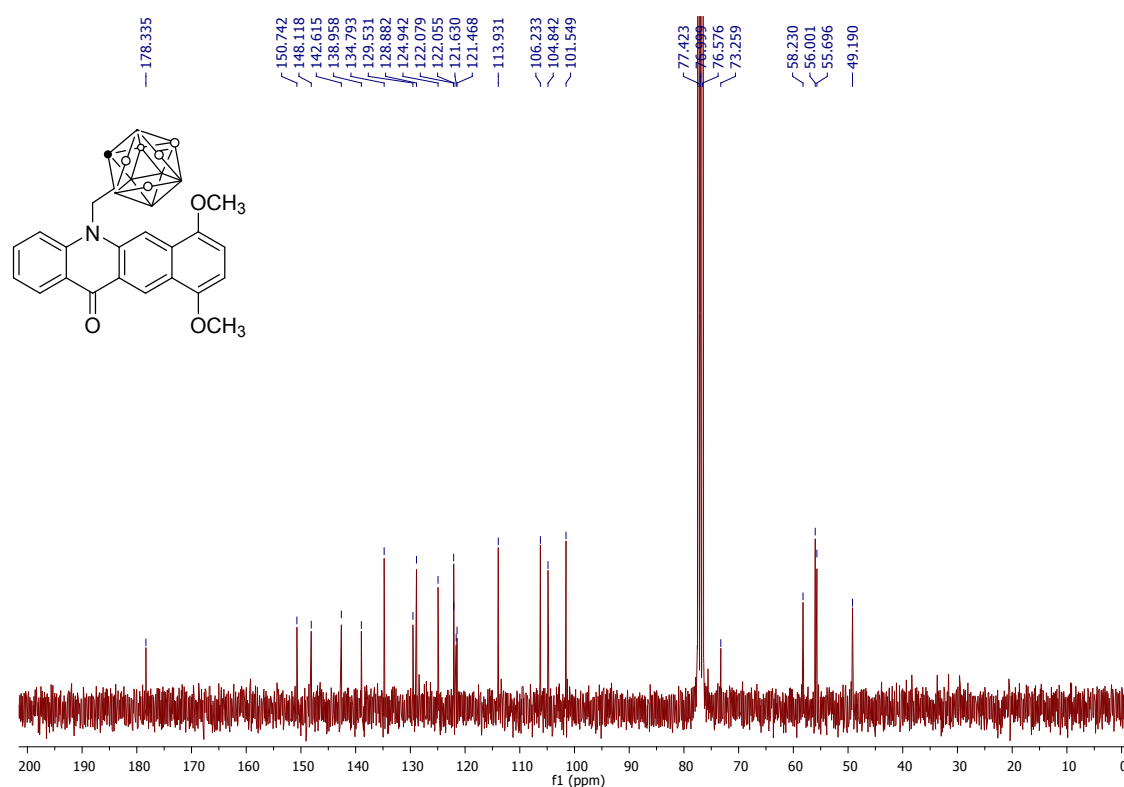
¹³C NMR Spectrum of 7-Carboranylmethylbenzo[*b*]acridin-12(7*H*)-one (4a)



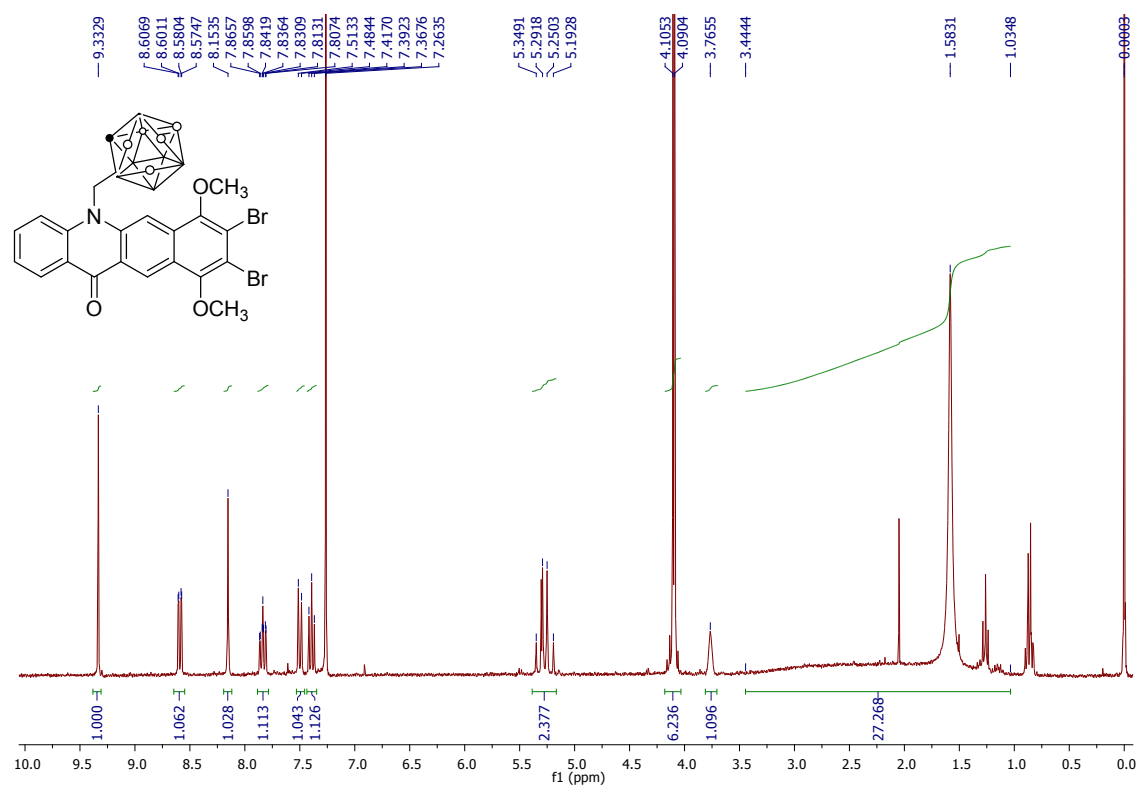
¹H NMR Spectrum of 2,5-Dimethoxy-7-carboranylmethylbenzo[*b*]acridin-12(7*H*)-one (4b)



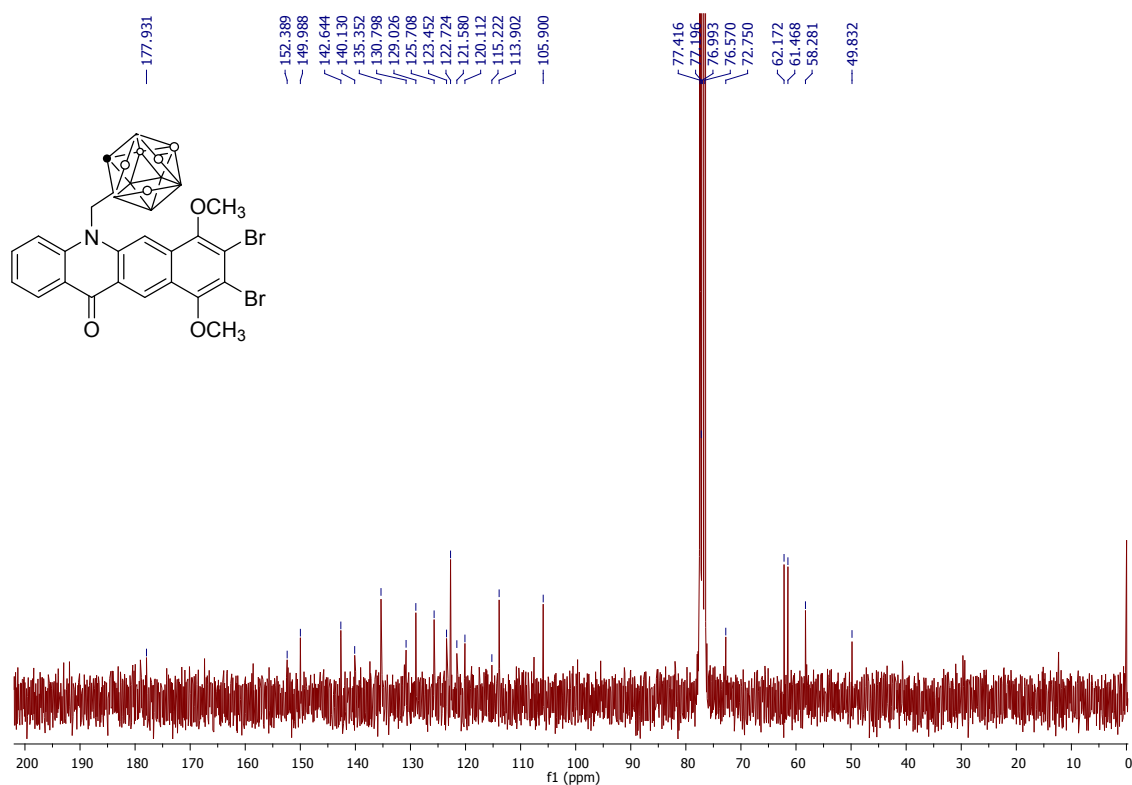
¹³C NMR Spectrum of 2,5-Dimethoxy-7-carboranylmethylbenzo[*b*]acridin-12(7*H*)-one (4b)



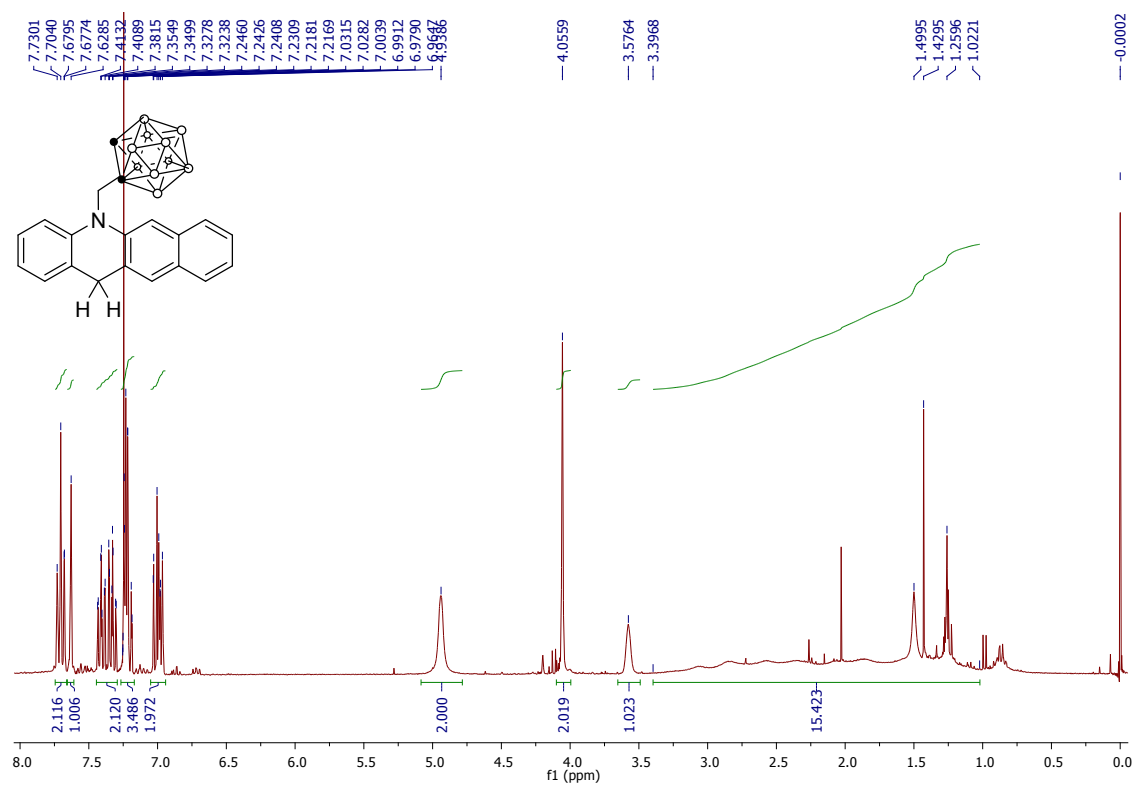
¹H NMR Spectrum of 3,4-Dibromo-2,5-dimethoxy-7-carboranylmethylbenzo[*b*]acridin-12(7*H*)-one (4c)



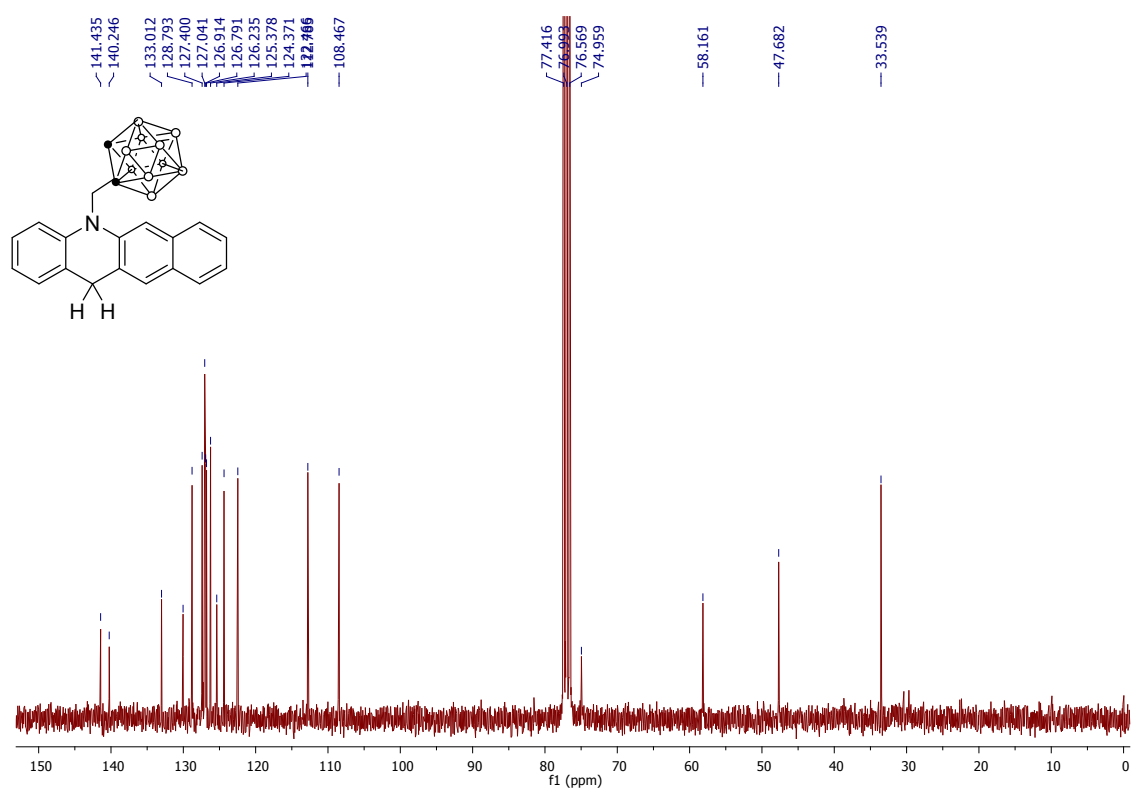
^{13}C NMR Spectrum of 3,4-Dibromo-2,5-dimethoxy-7-carboranylmethylbenzo[*b*]acridin-12(7*H*)-one (4c)



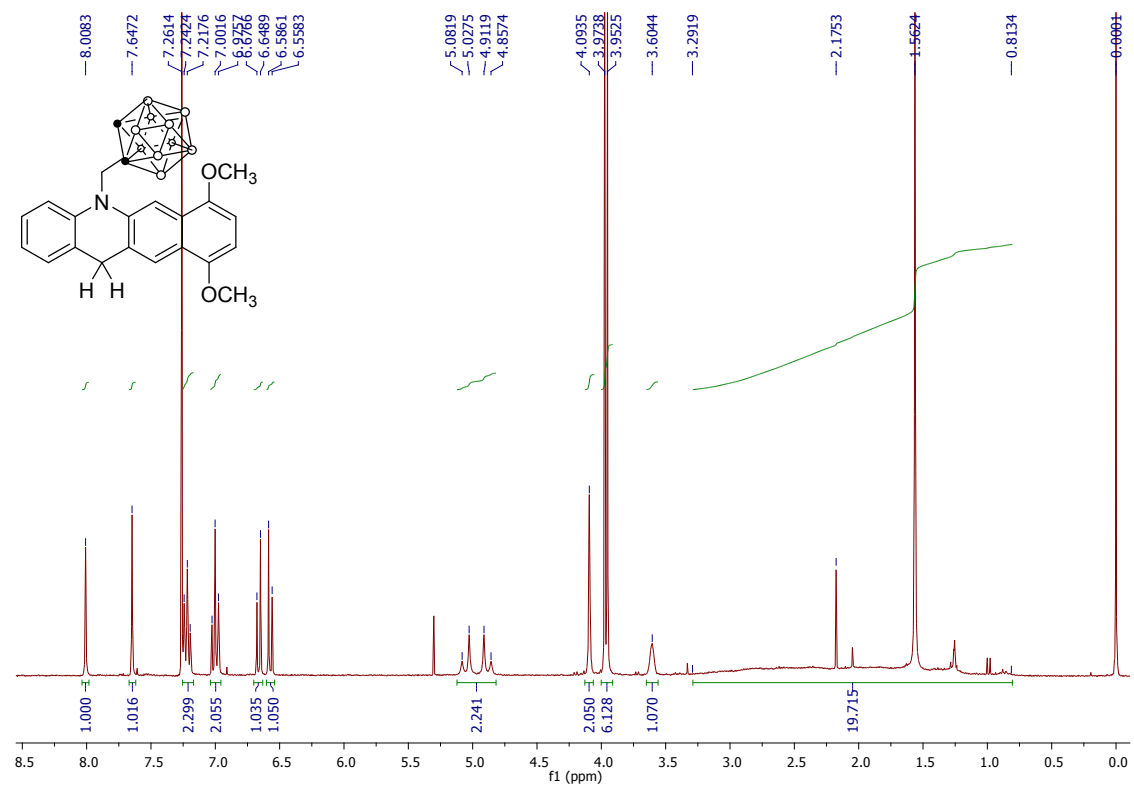
^1H NMR Spectrum of 7-Carboranylmethyl-7,12-dihydrobenzo[*b*]acridine (5a)



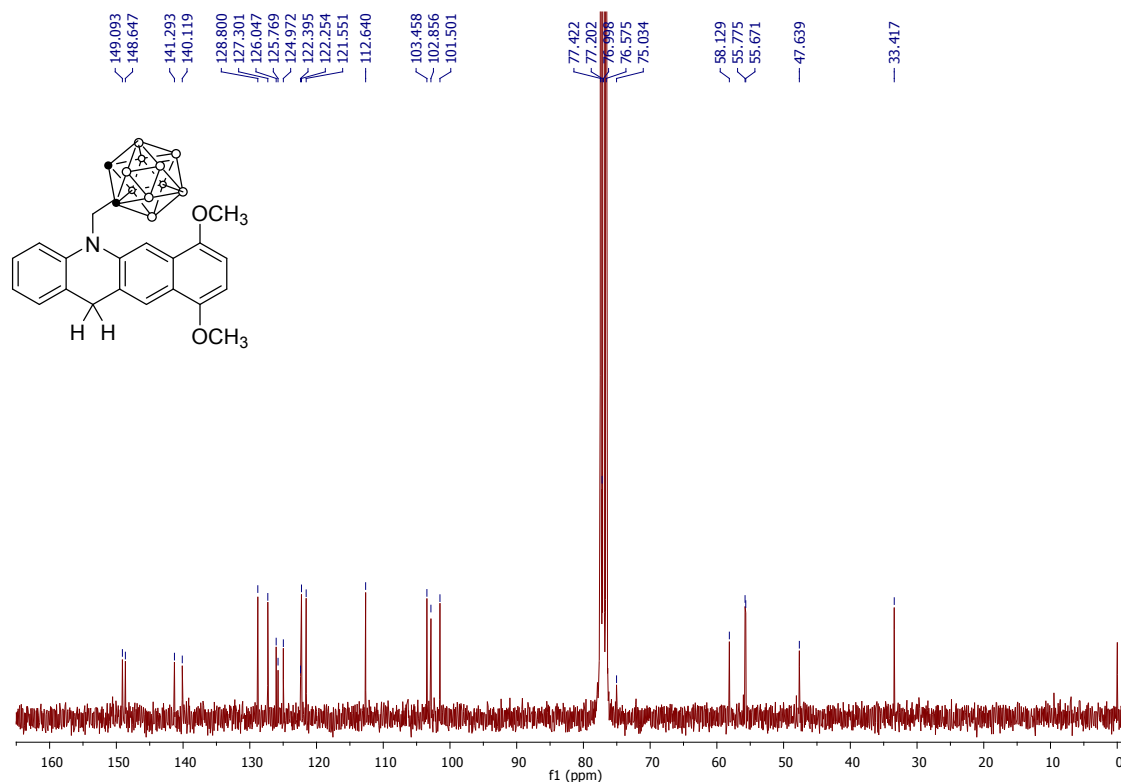
¹³C NMR Spectrum of 7-Carboranylmethyl-7,12-dihydrobenzo[*b*]acridine (5a)



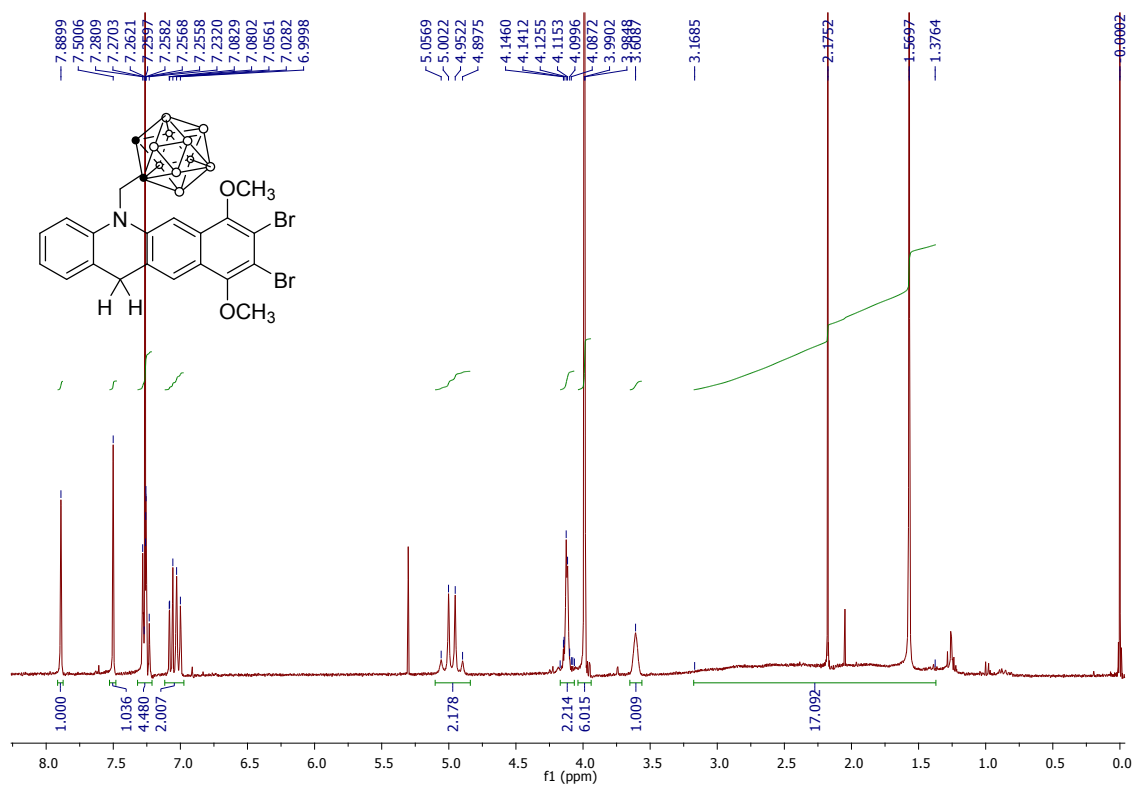
¹H NMR Spectrum of 2,5-Dimethoxy-7-carboranylmethyl-7,12-dihydrobenzo[*b*]acridine (5b)



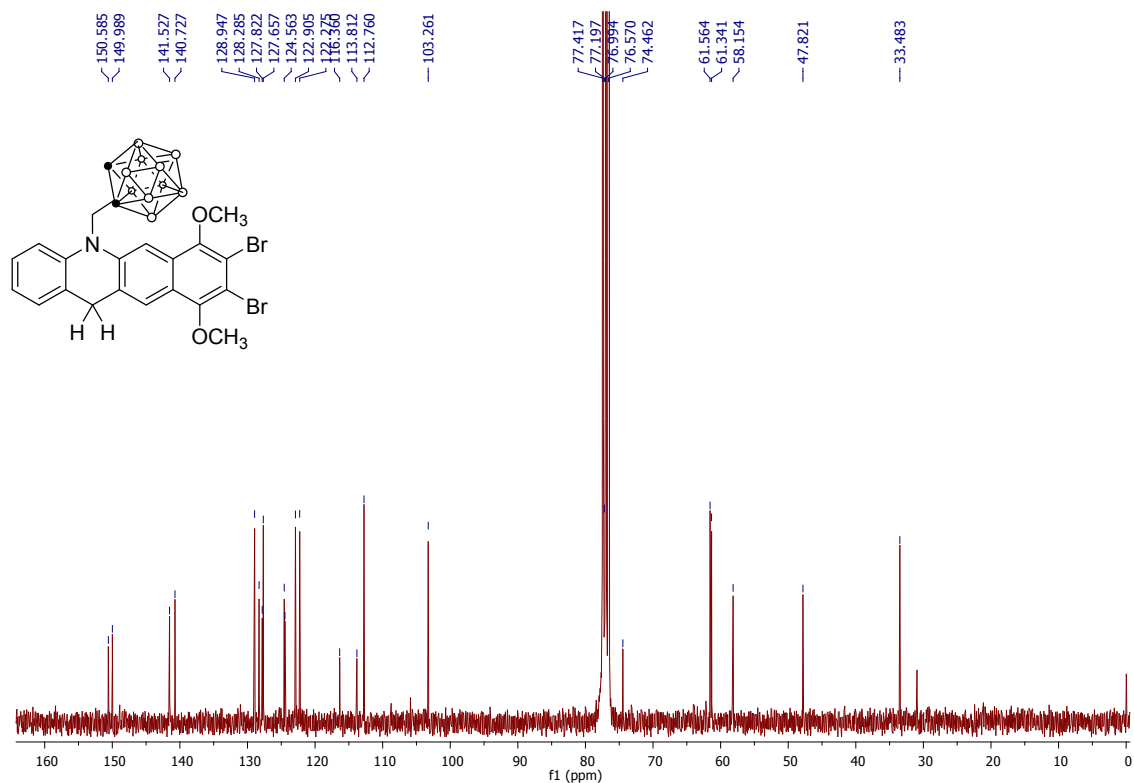
¹³C NMR Spectrum of 2,5-Dimethoxy-7-carboranylmethyl-7,12-dihydrobenzo[*b*]acridine (5b)



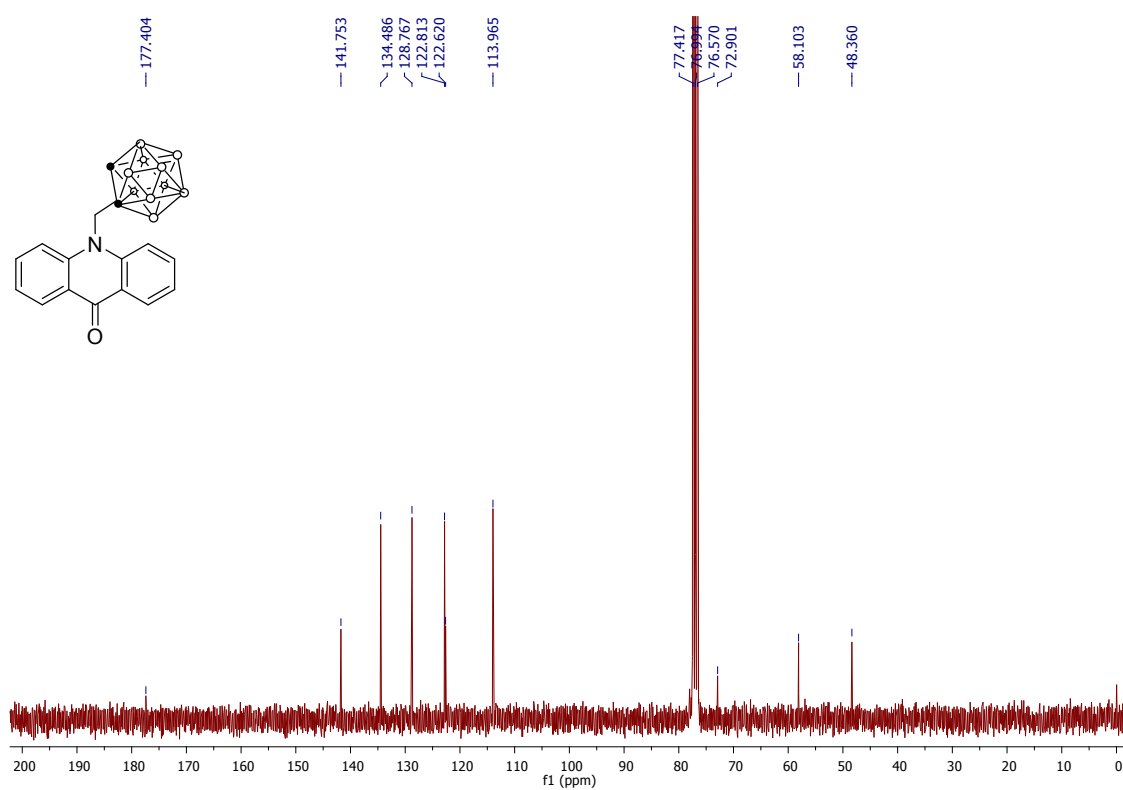
¹H NMR Spectrum of 3,4-Dibromo-2,5-dimethoxy-7-carboranylmethyl-7,12-dihydrobenzo[*b*]acridine (5c)



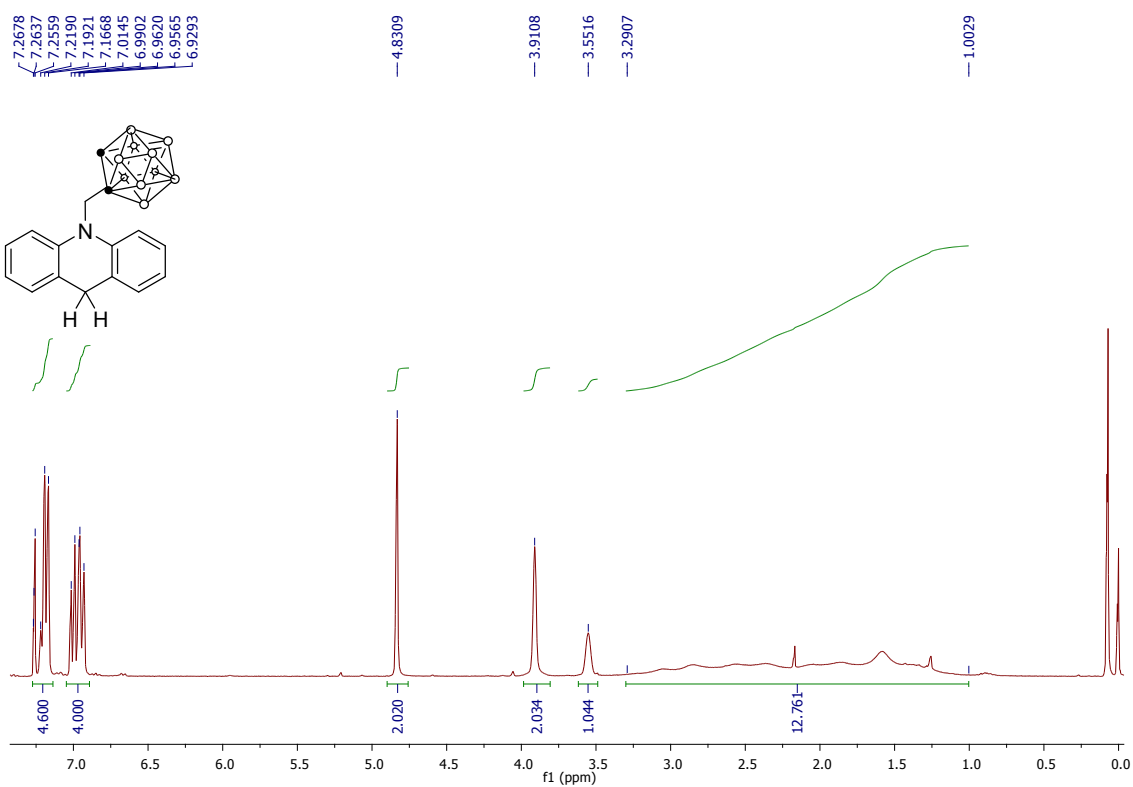
^{13}C NMR Spectrum of 3,4-Dibromo-2,5-dimethoxy-7-carboranylmethyl-7,12-dihydrobenzo[*b*]acridine (5c)



¹³C NMR Spectrum of 10-Carboranylmethylacridin-9(10*H*)-one (9)



¹H NMR Spectrum of 10-Carboranylmethyl-9,10-dihydroacridine (10)



¹³C NMR Spectrum of 10-Carboranylmethyl-9,10-dihydroacridine (10)

