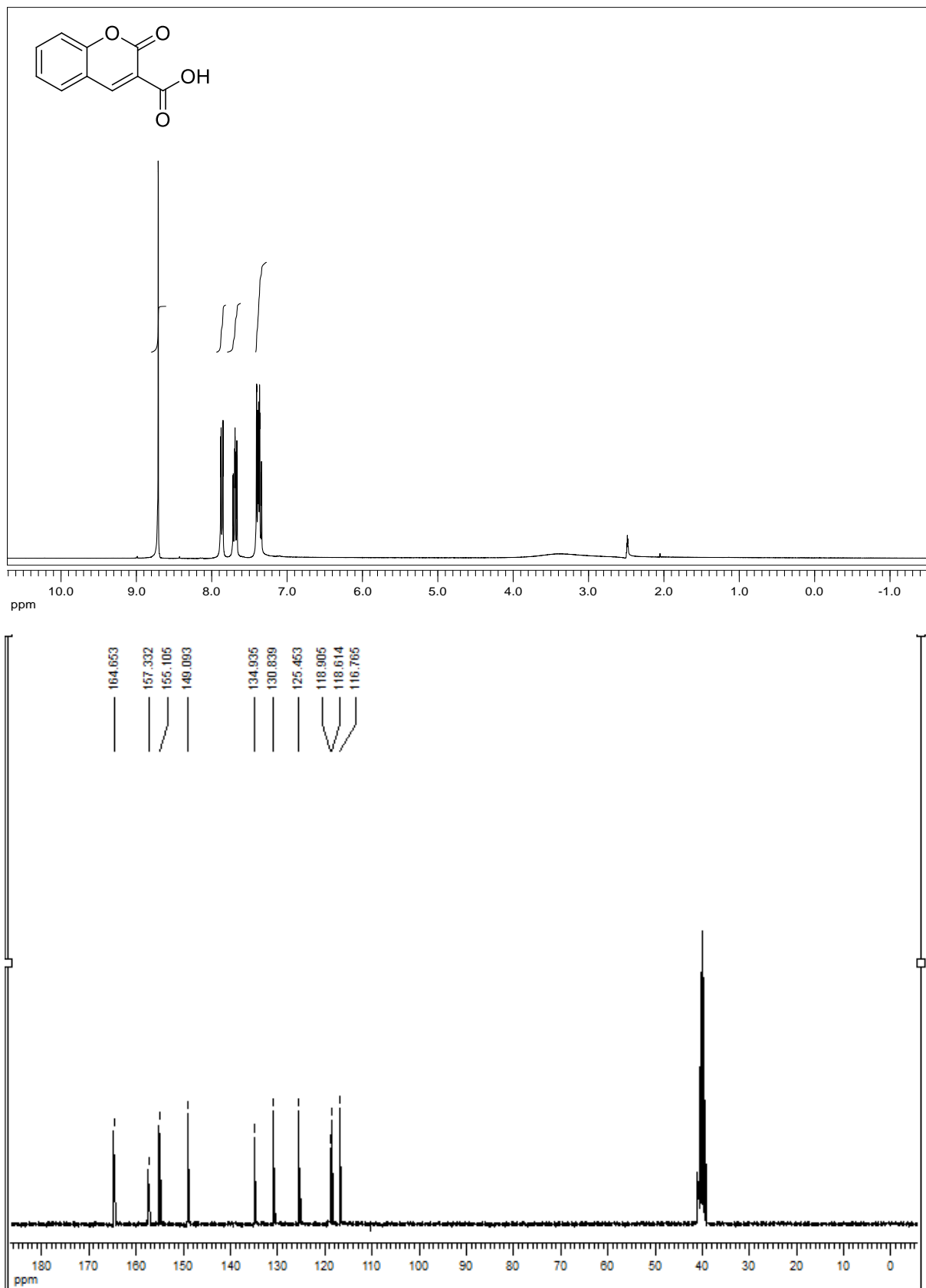


Synthesis, Biological Activity and Multiscale Molecular Modeling Studies for Coumaryl-carboxamid Derivatives as Selective Carbonic Anhydrase IX Inhibitors

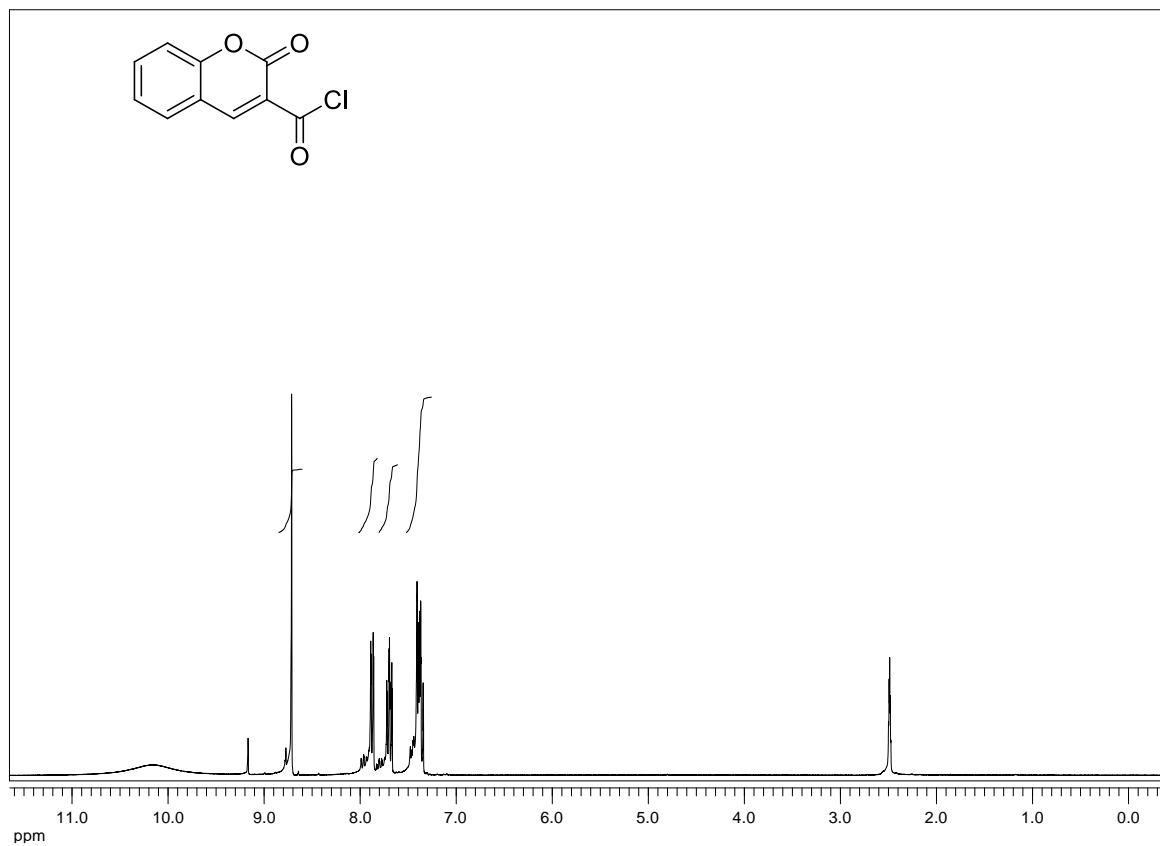
SUPPLEMENTARY MATERIALS

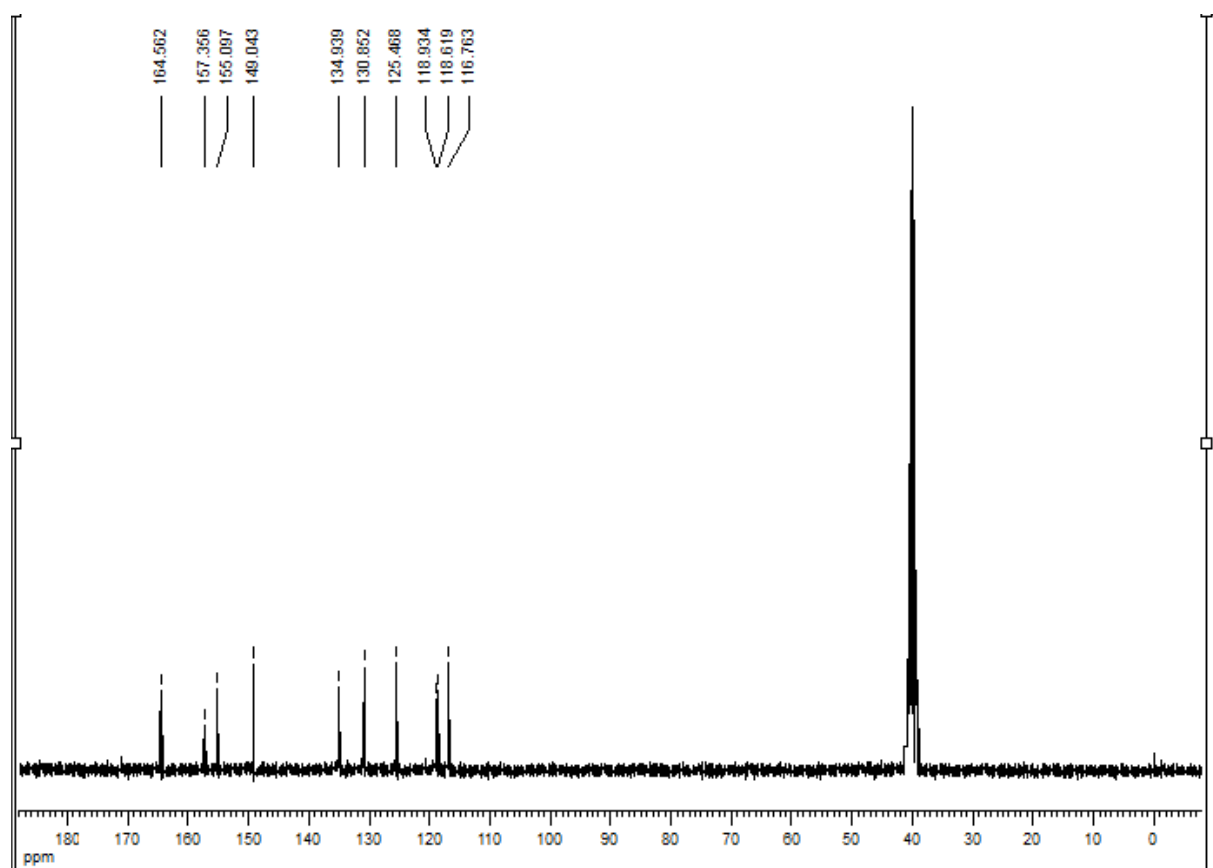
¹ H and ¹³ C NMR and MS spectra of c , d , and e1-e20	2-34
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S1: ^1H NMR (CDCl_3) and ^{13}C NMR ($\text{DMSO-}d_6$) spectra of **c**

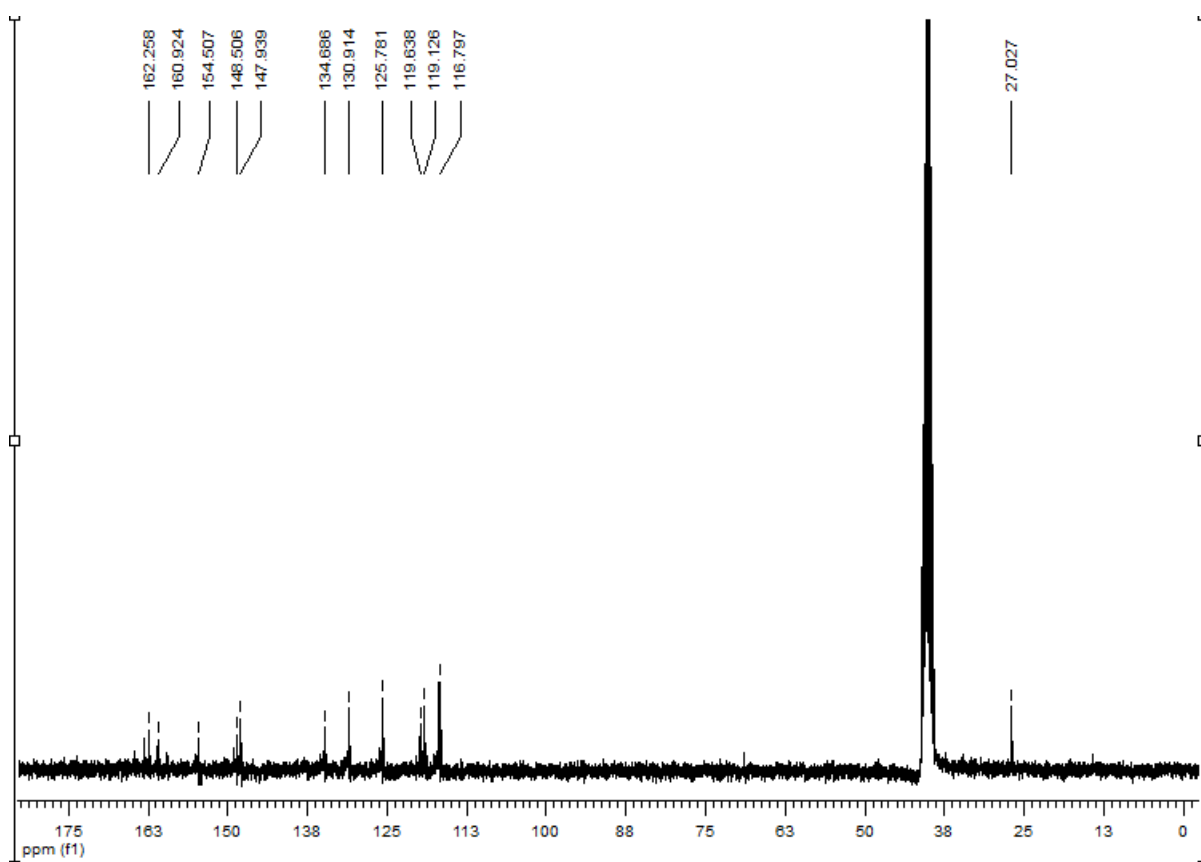
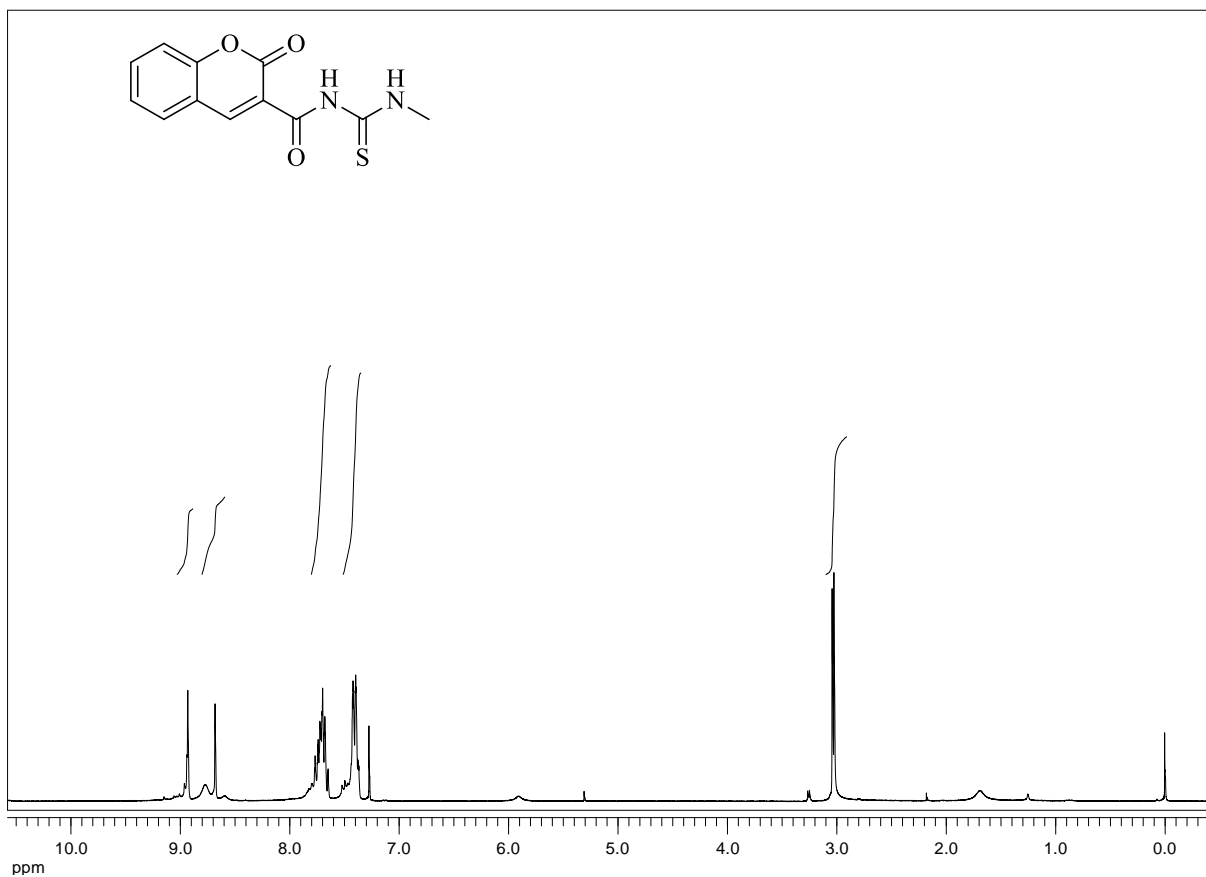


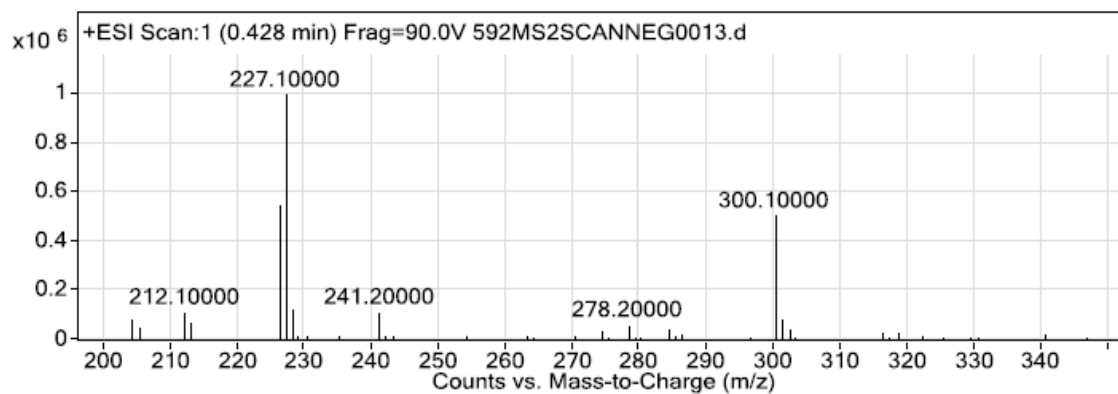
S2: ^1H NMR (CDCl_3) and ^{13}C NMR ($\text{DMSO}-d_6$) spectra of **d**



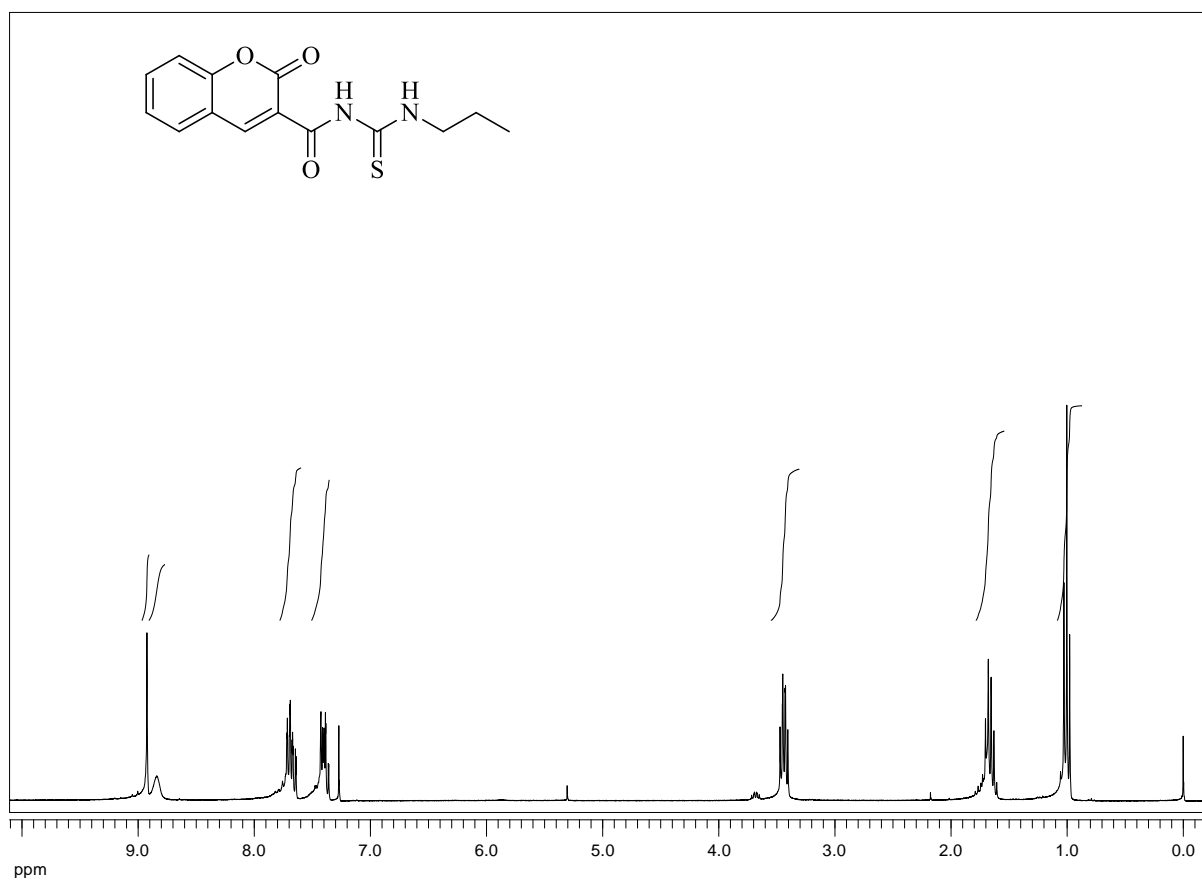


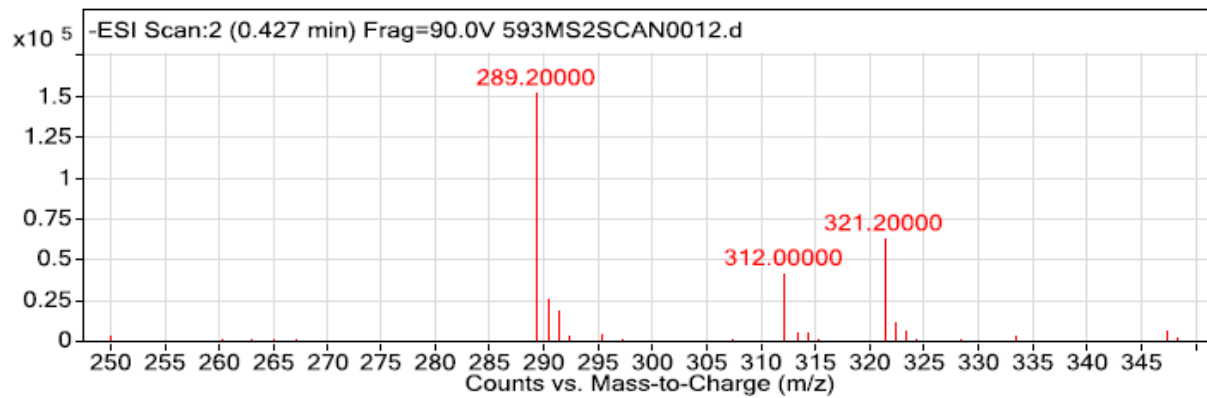
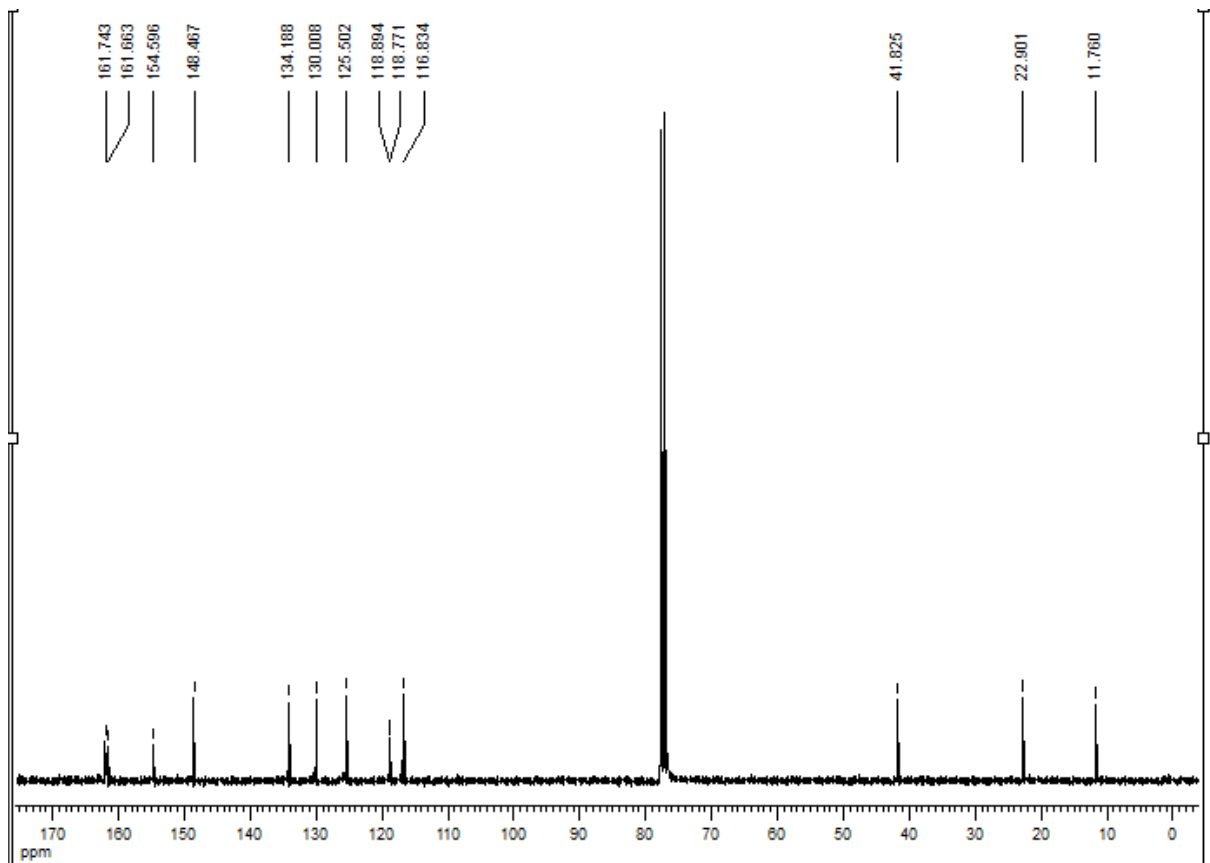
S3: ^1H NMR (CDCl_3), ^{13}C NMR ($\text{DMSO}-d_6$) and MS spectra of **e1**



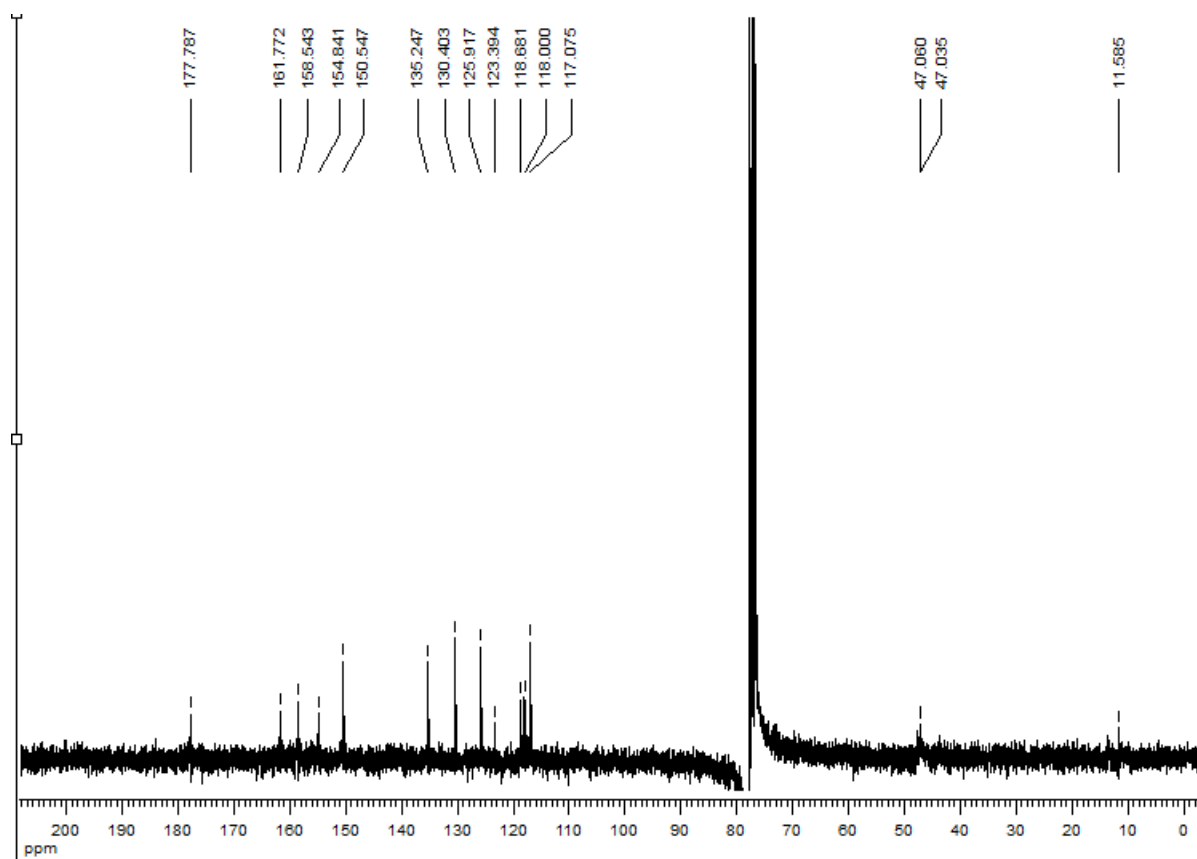
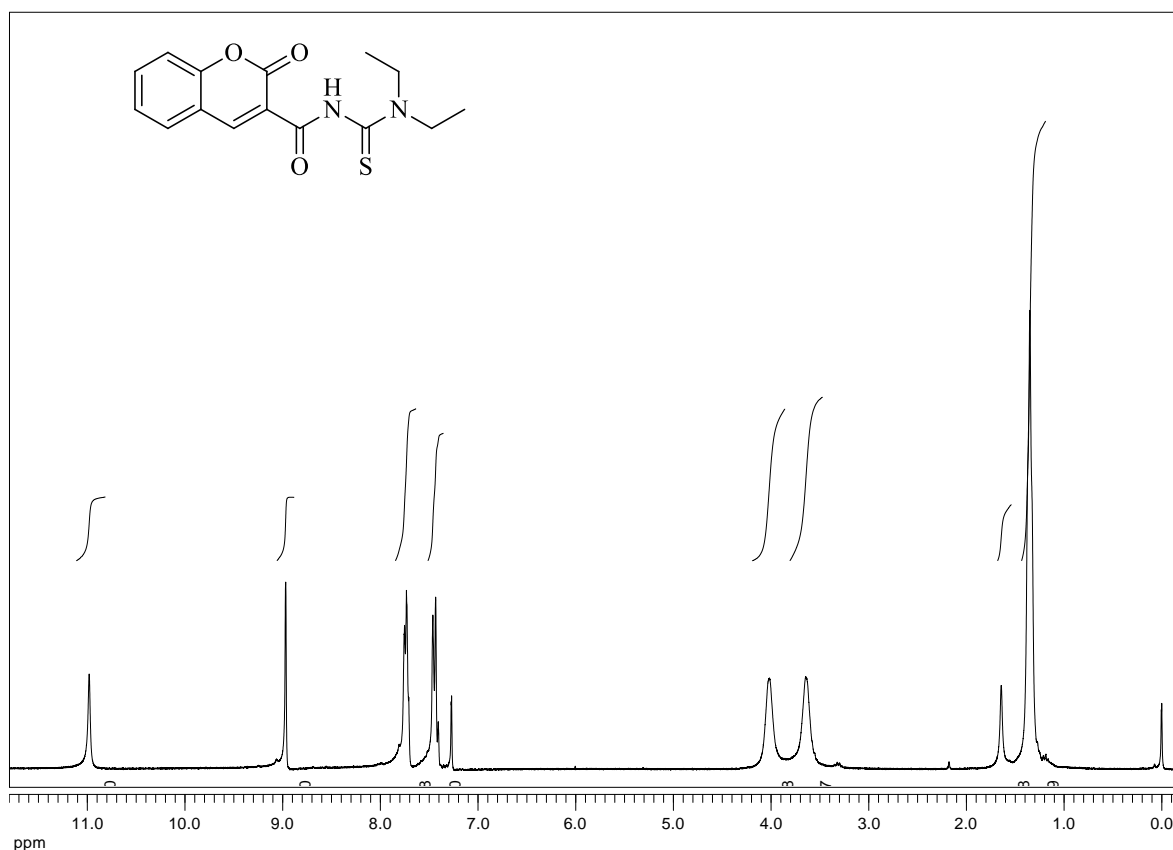


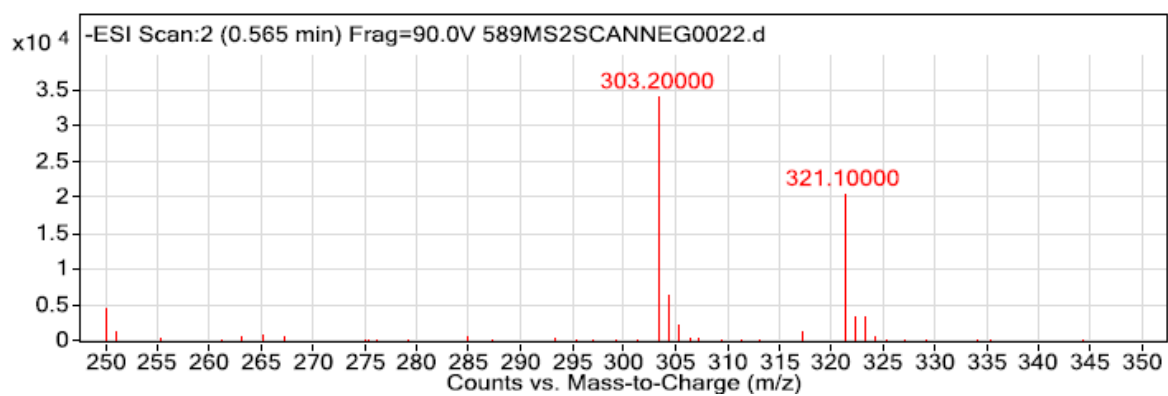
S4: ^1H NMR (CDCl_3), ^{13}C NMR (CDCl_3) and MS spectra of **e2**



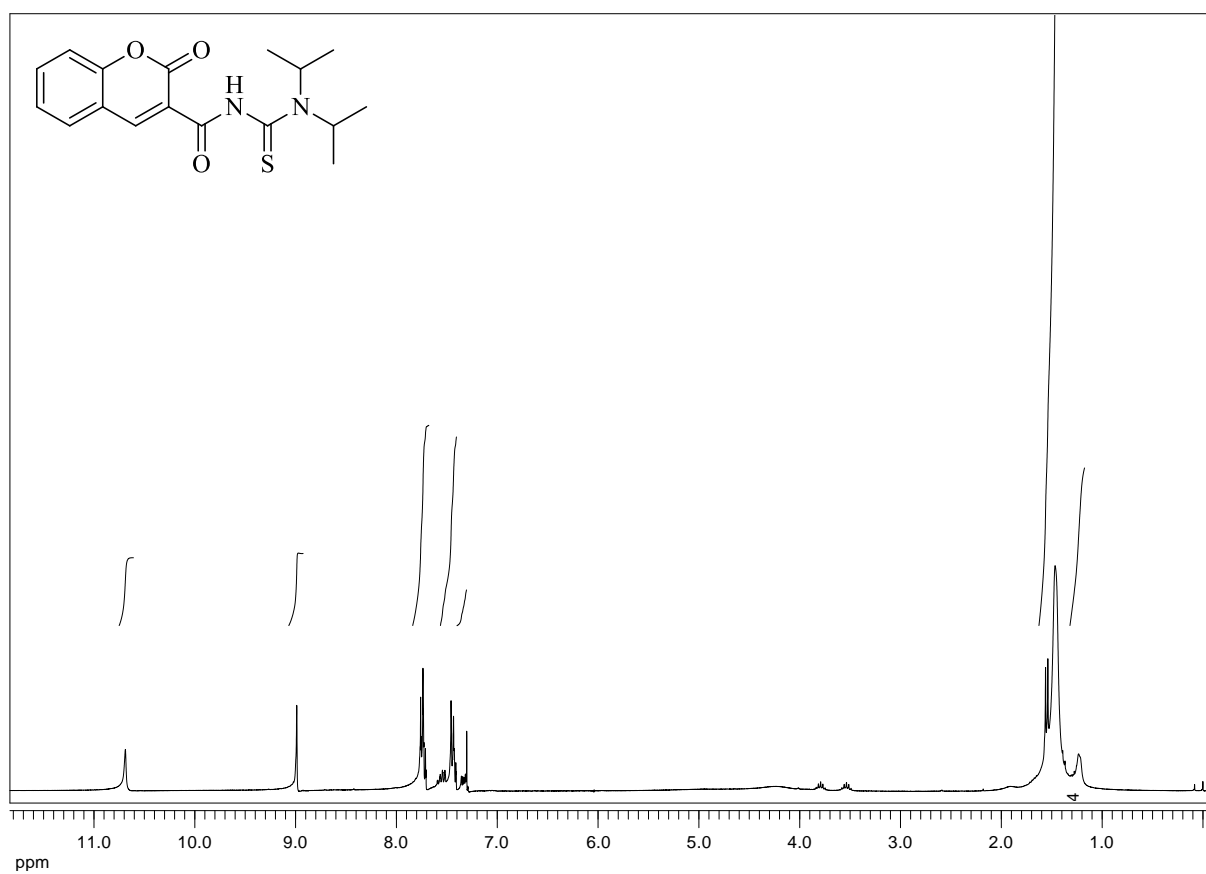


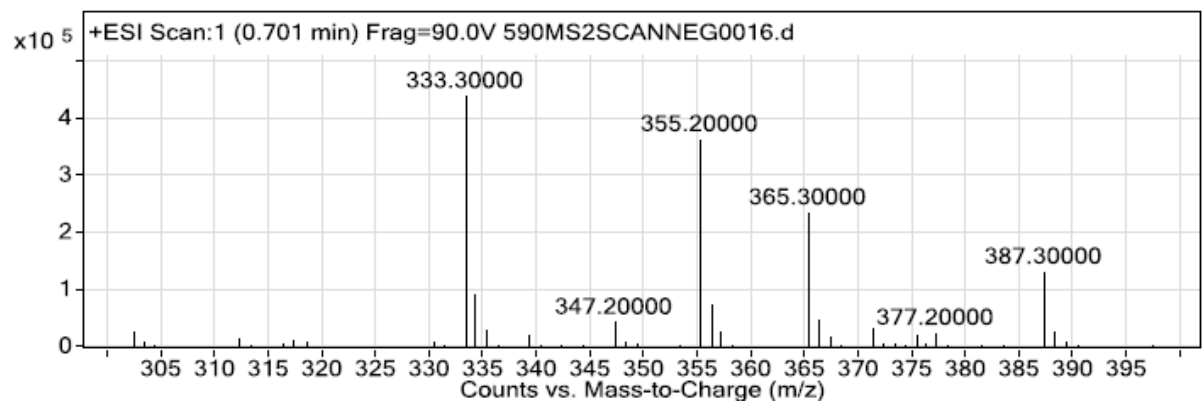
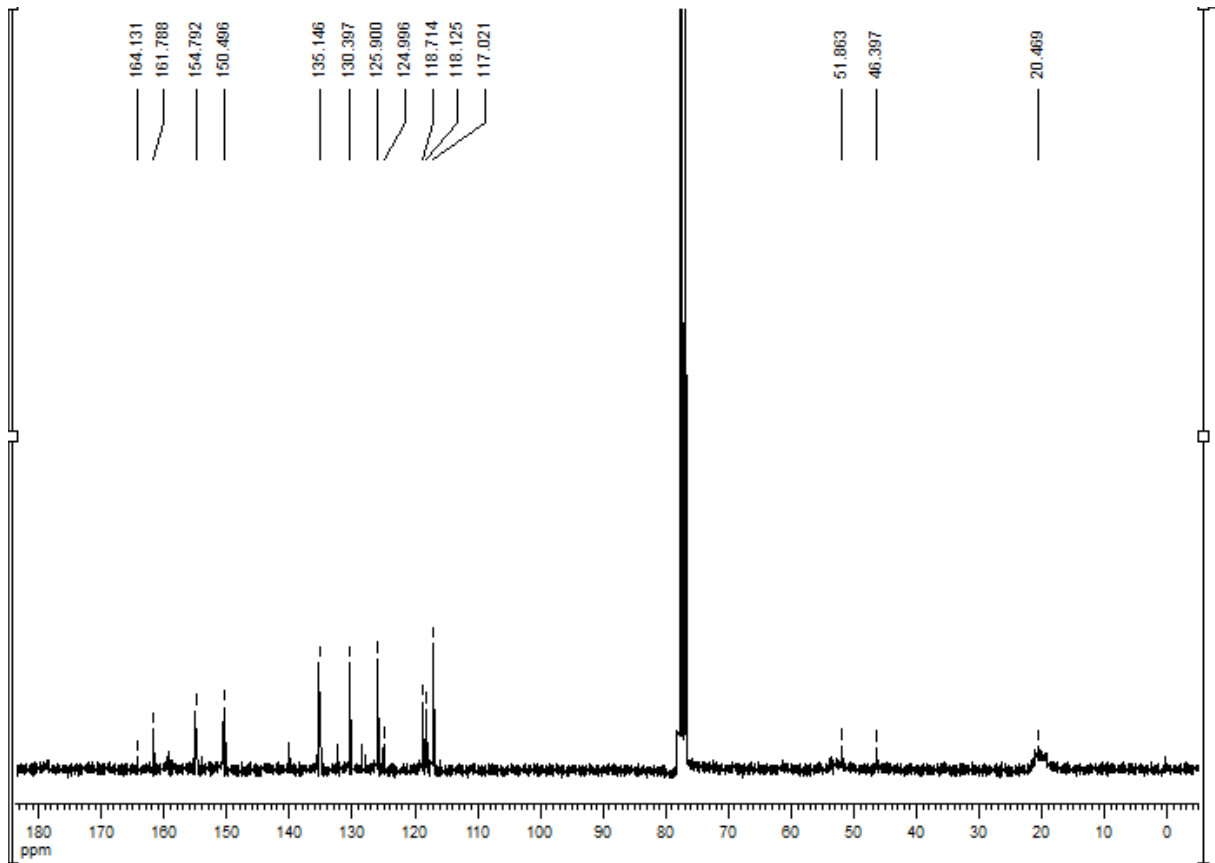
S5: ^1H NMR (CDCl_3), ^{13}C NMR (CDCl_3) and MS spectra of **e3**



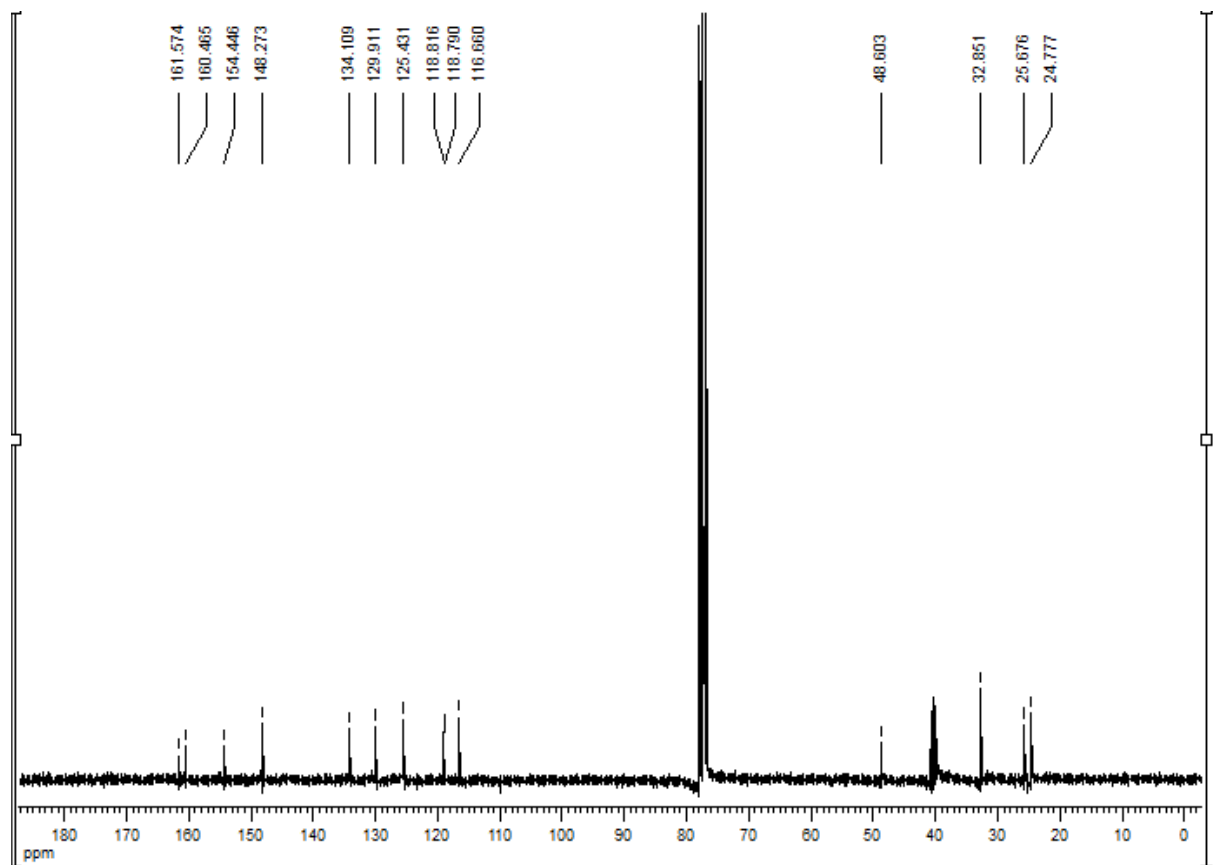
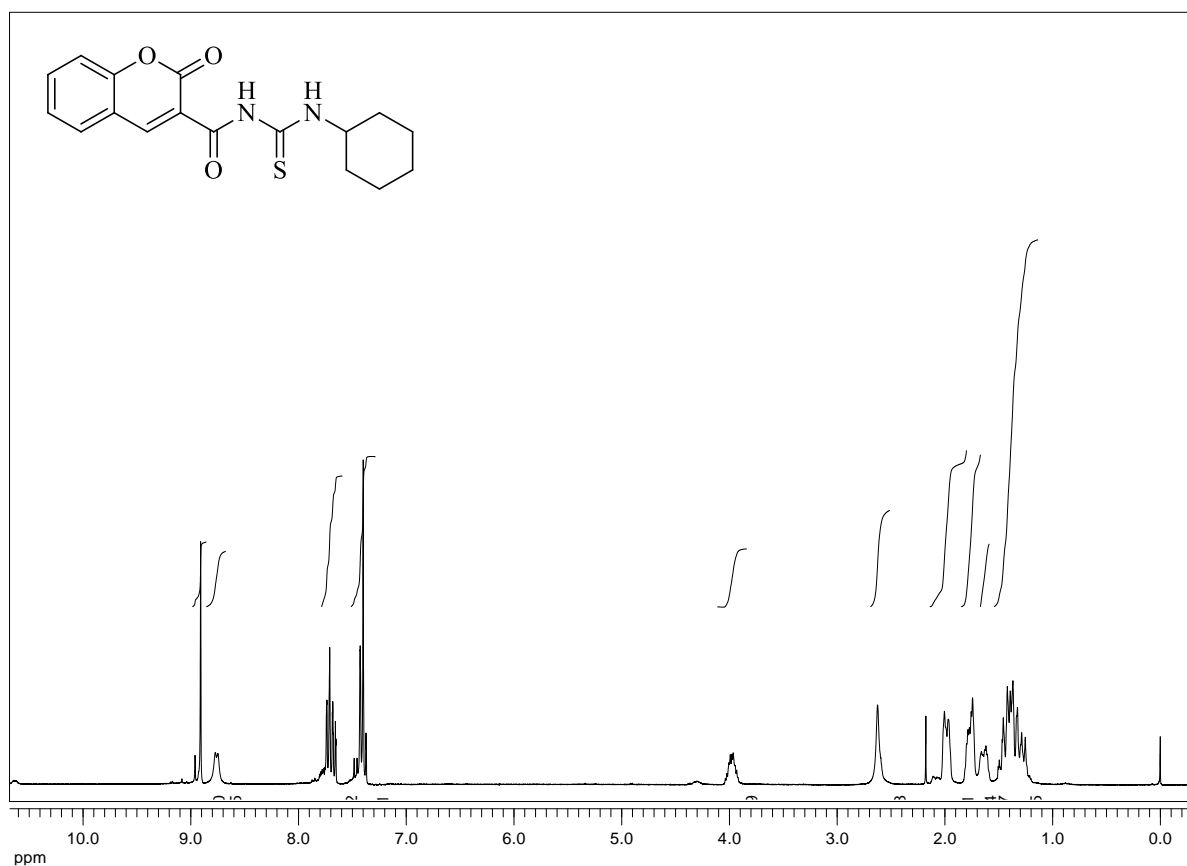


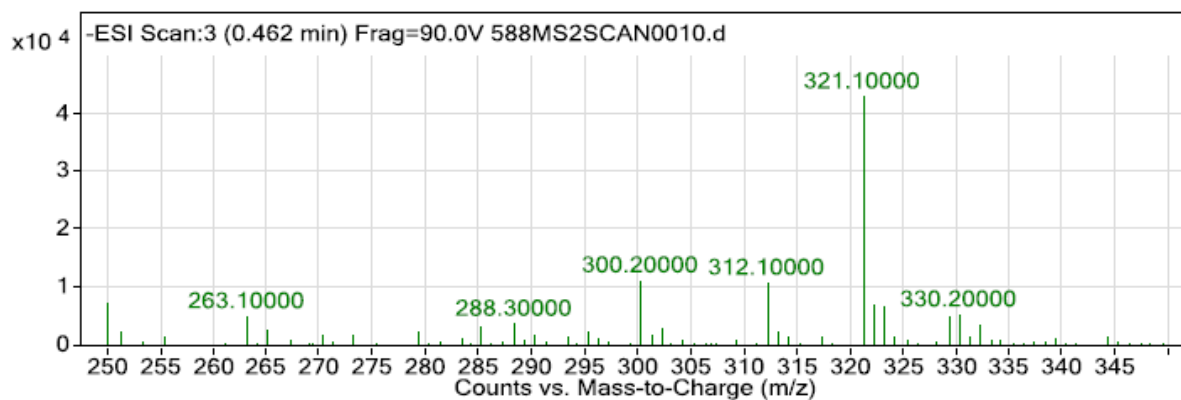
S6: ¹H NMR (CDCl₃), ¹³C NMR (CDCl₃) and MS spectra of **e4**



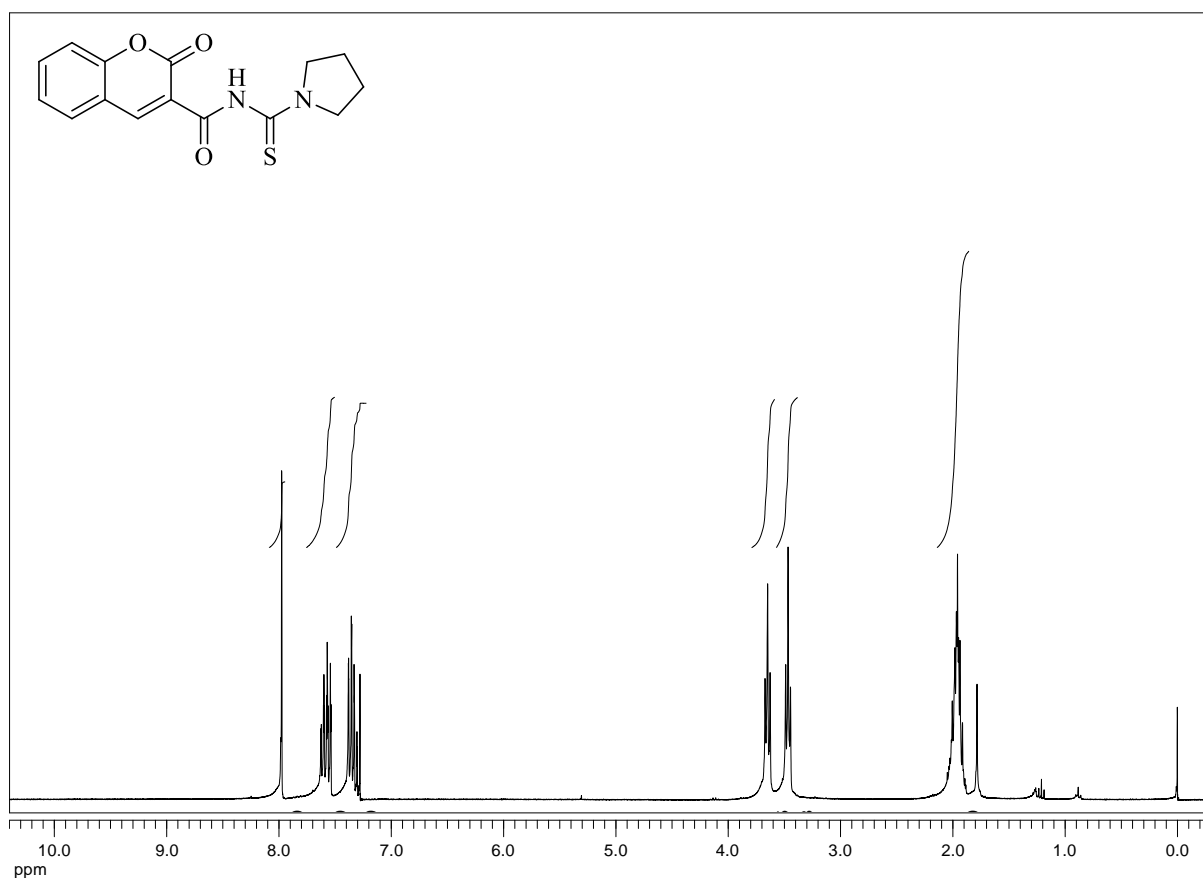


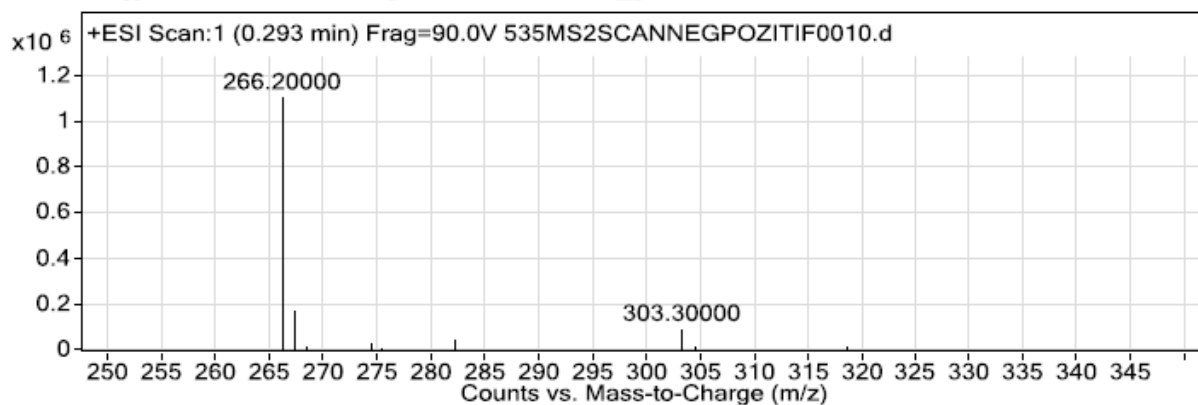
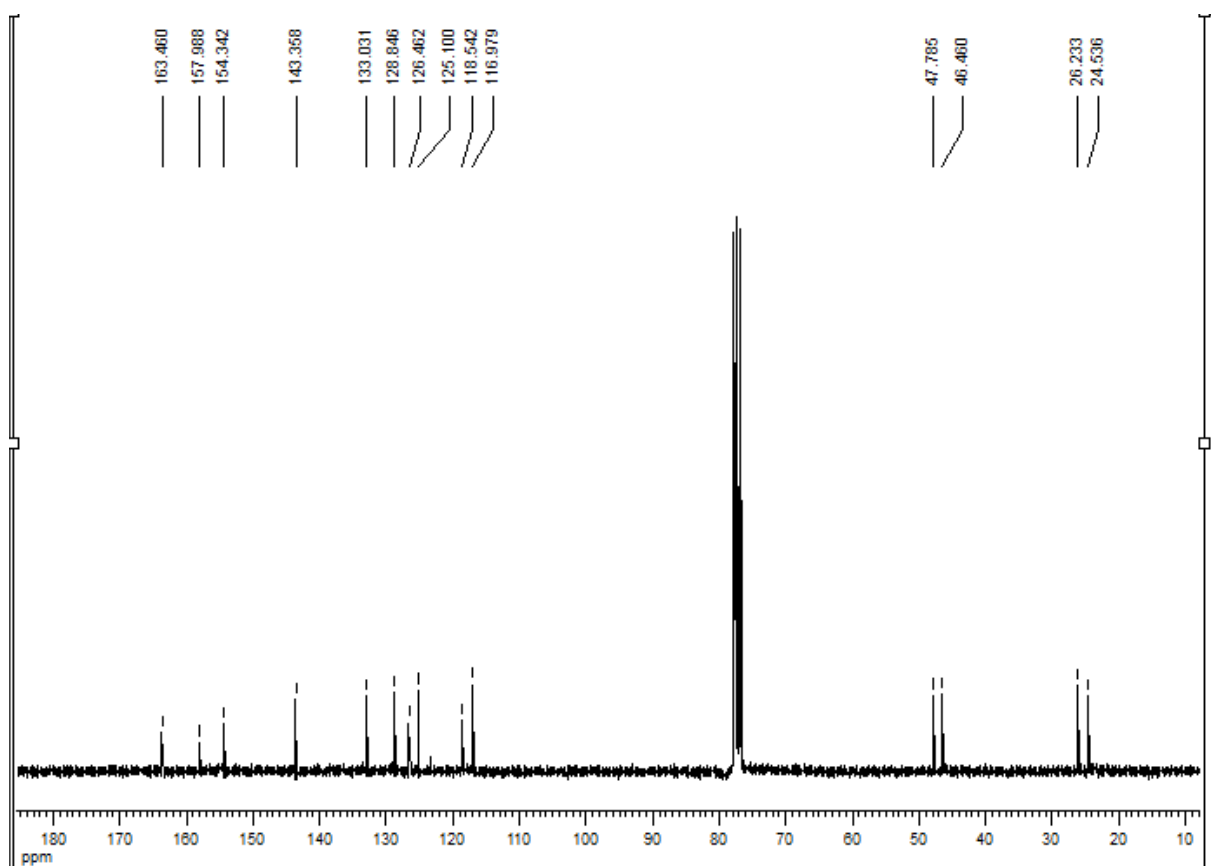
S7: ^1H NMR (CDCl_3), ^{13}C NMR (CDCl_3) and MS spectra of e5



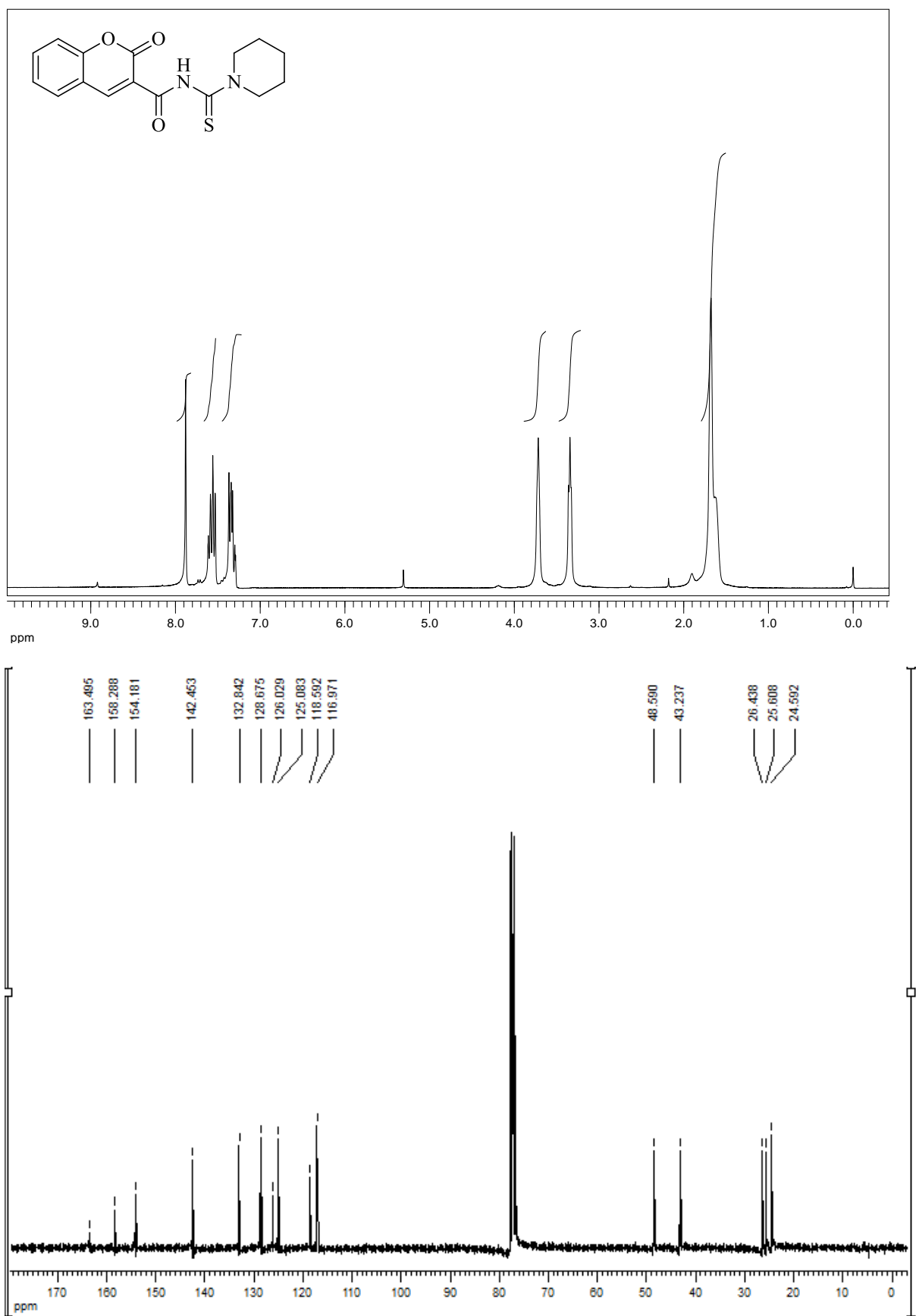


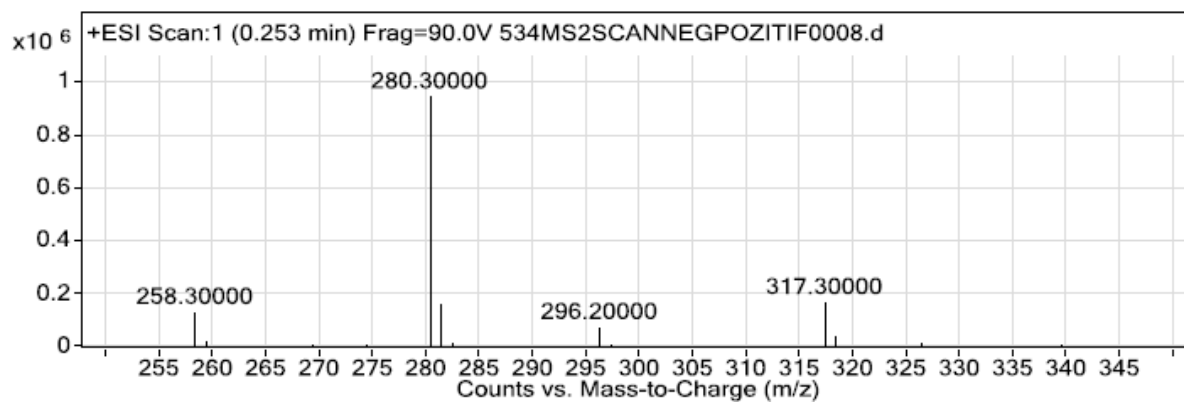
S8: ¹H NMR (CDCl₃), ¹³C NMR (CDCl₃) and MS spectra of **e6**



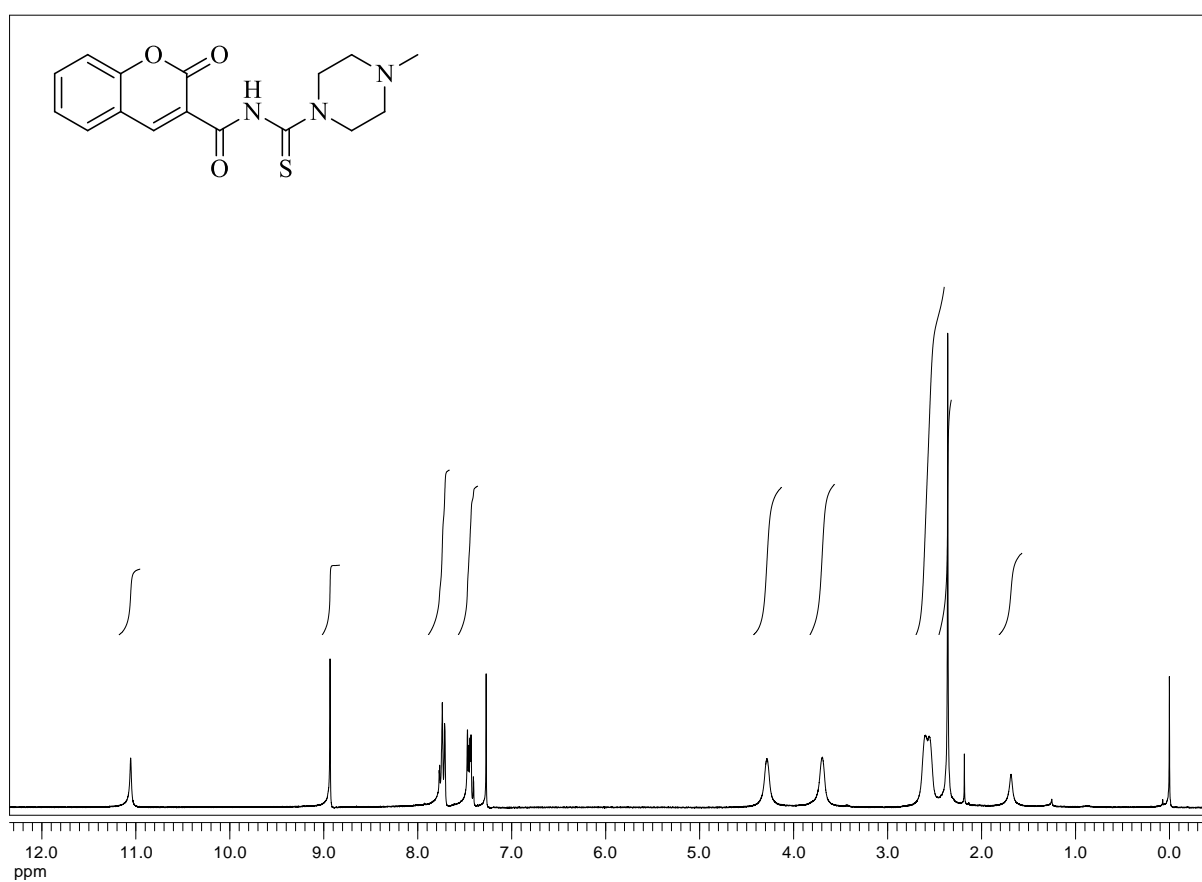


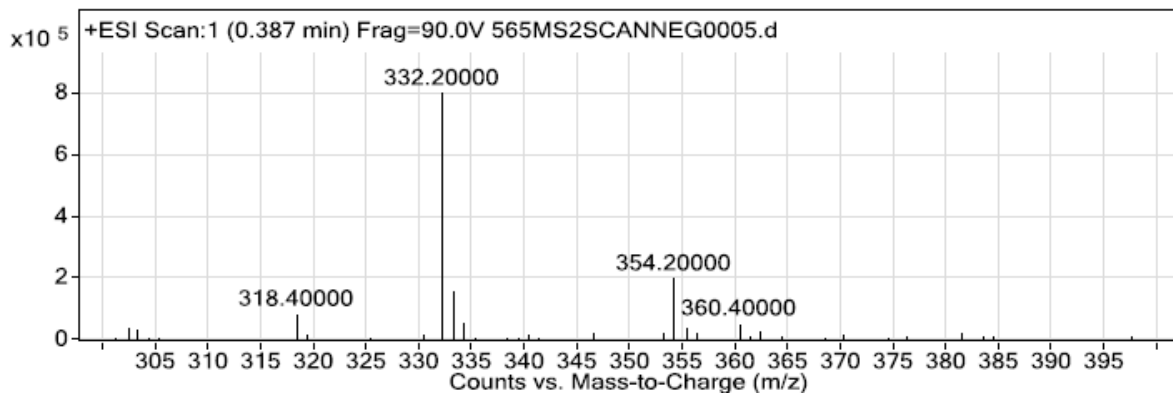
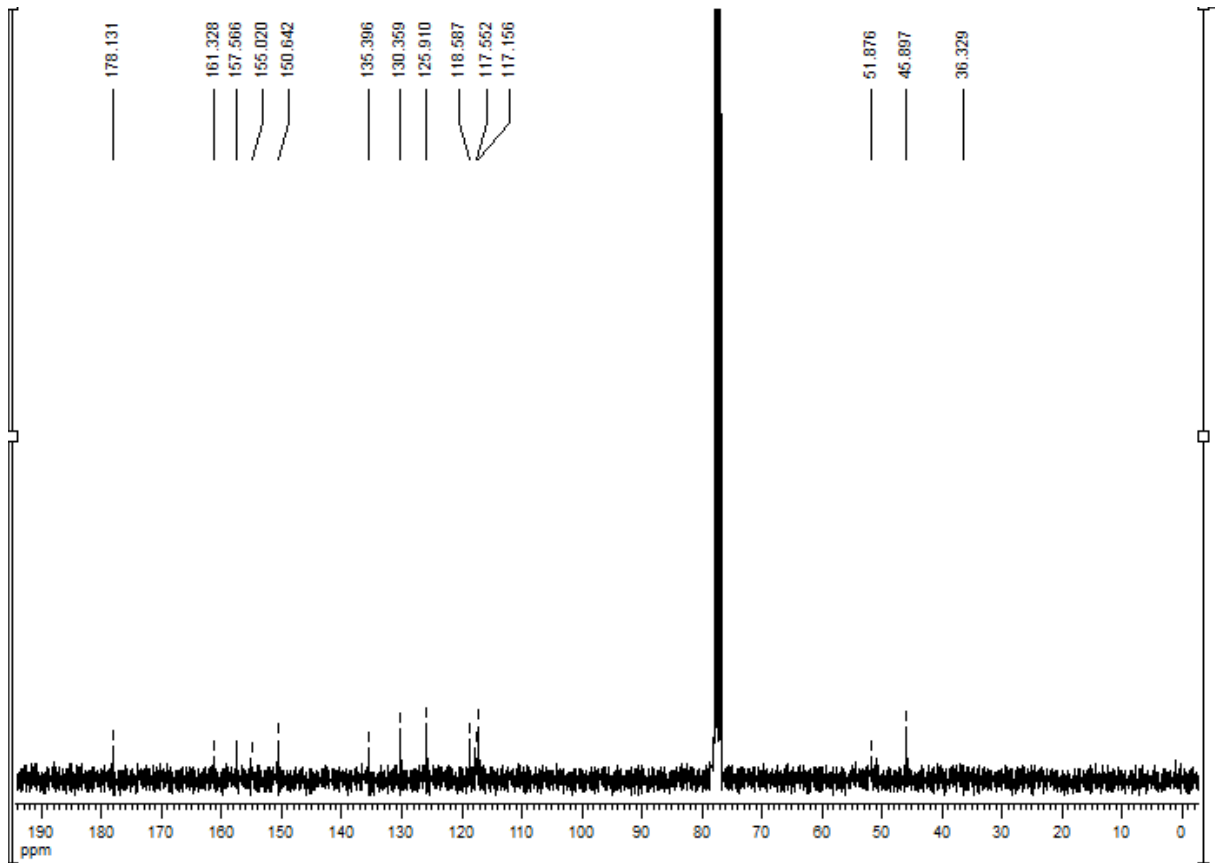
S9: ^1H NMR (CDCl_3), ^{13}C NMR (CDCl_3) and MS spectra of e7



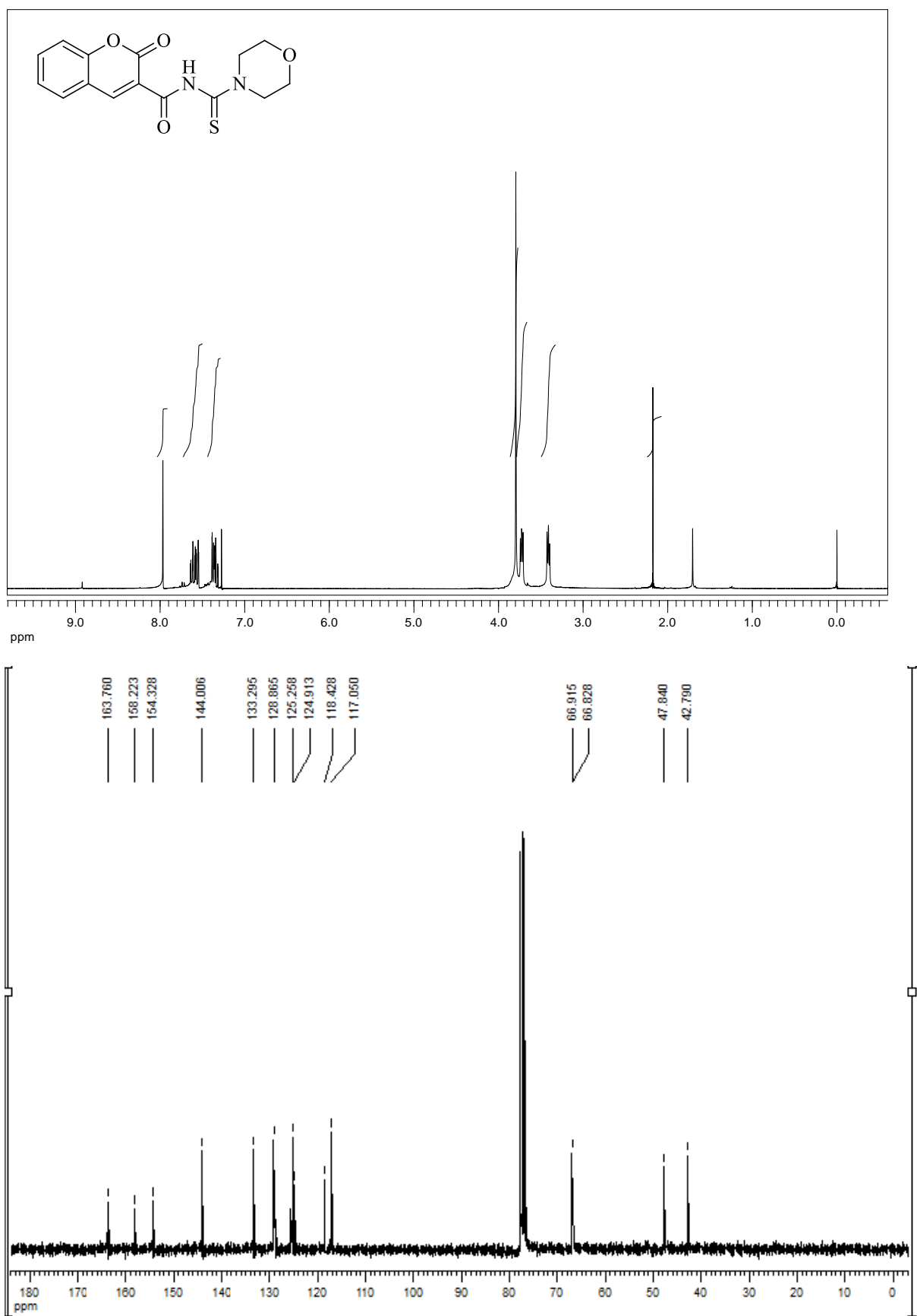


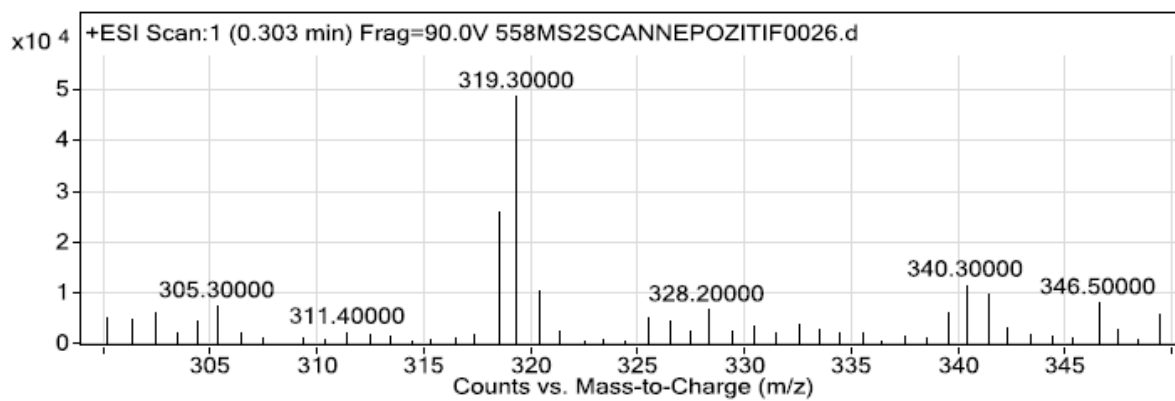
S10: ¹H NMR (CDCl₃), ¹³C NMR (CDCl₃) and MS spectra of **e8**



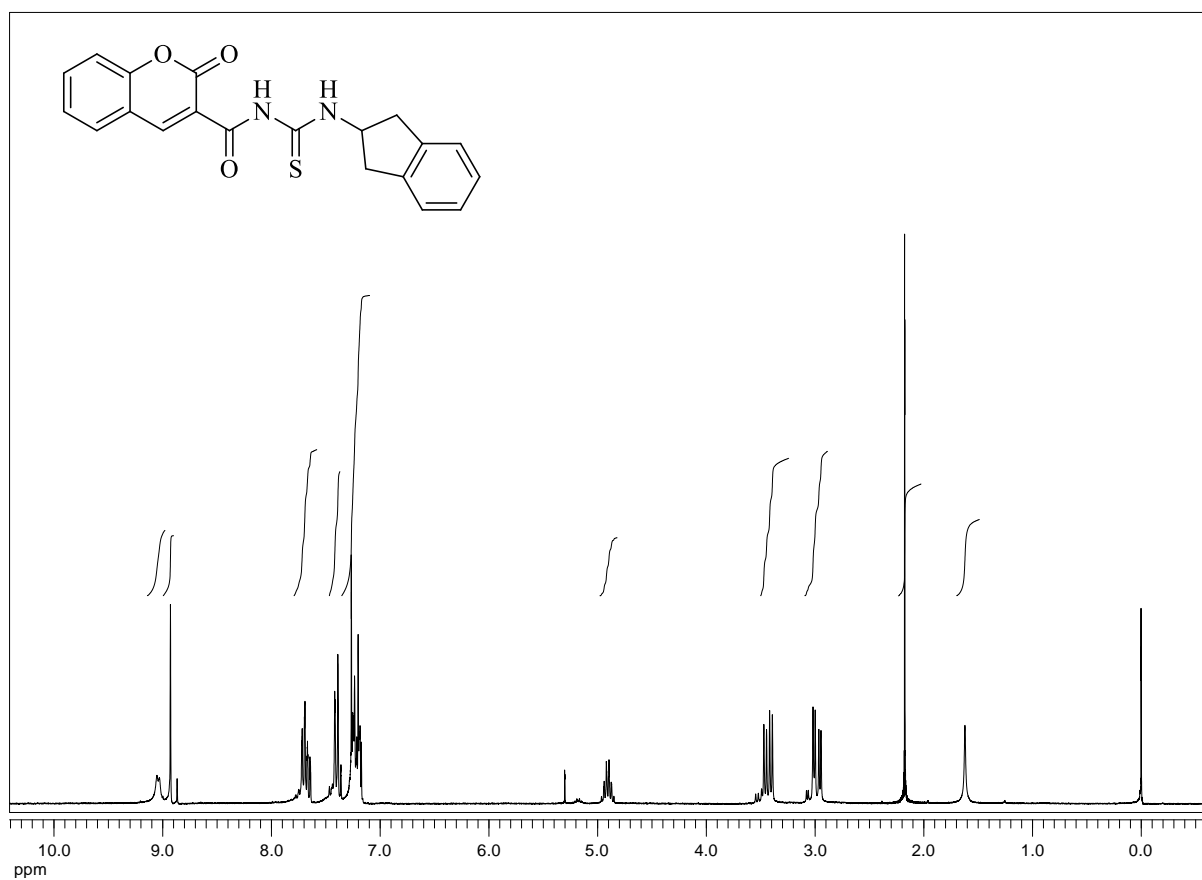


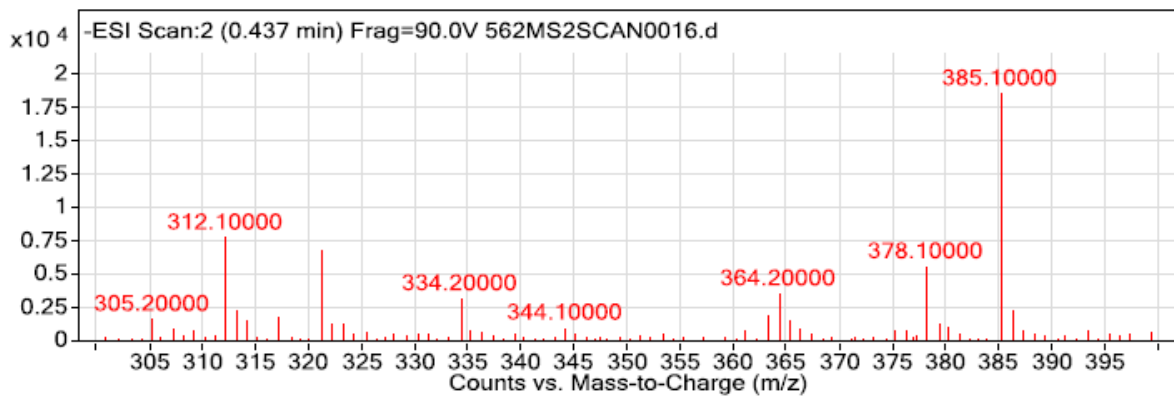
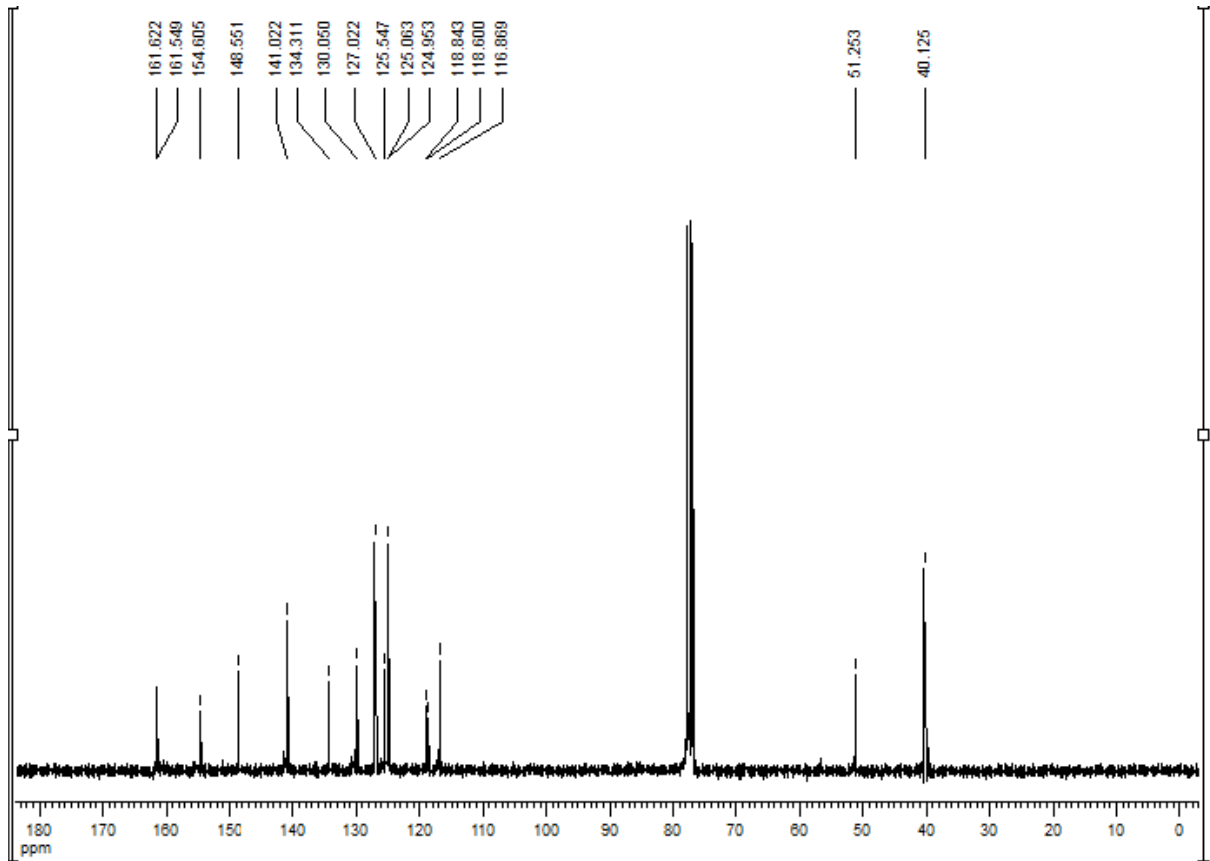
S11: ^1H NMR (CDCl_3), ^{13}C NMR (CDCl_3) and MS spectra of **e9**



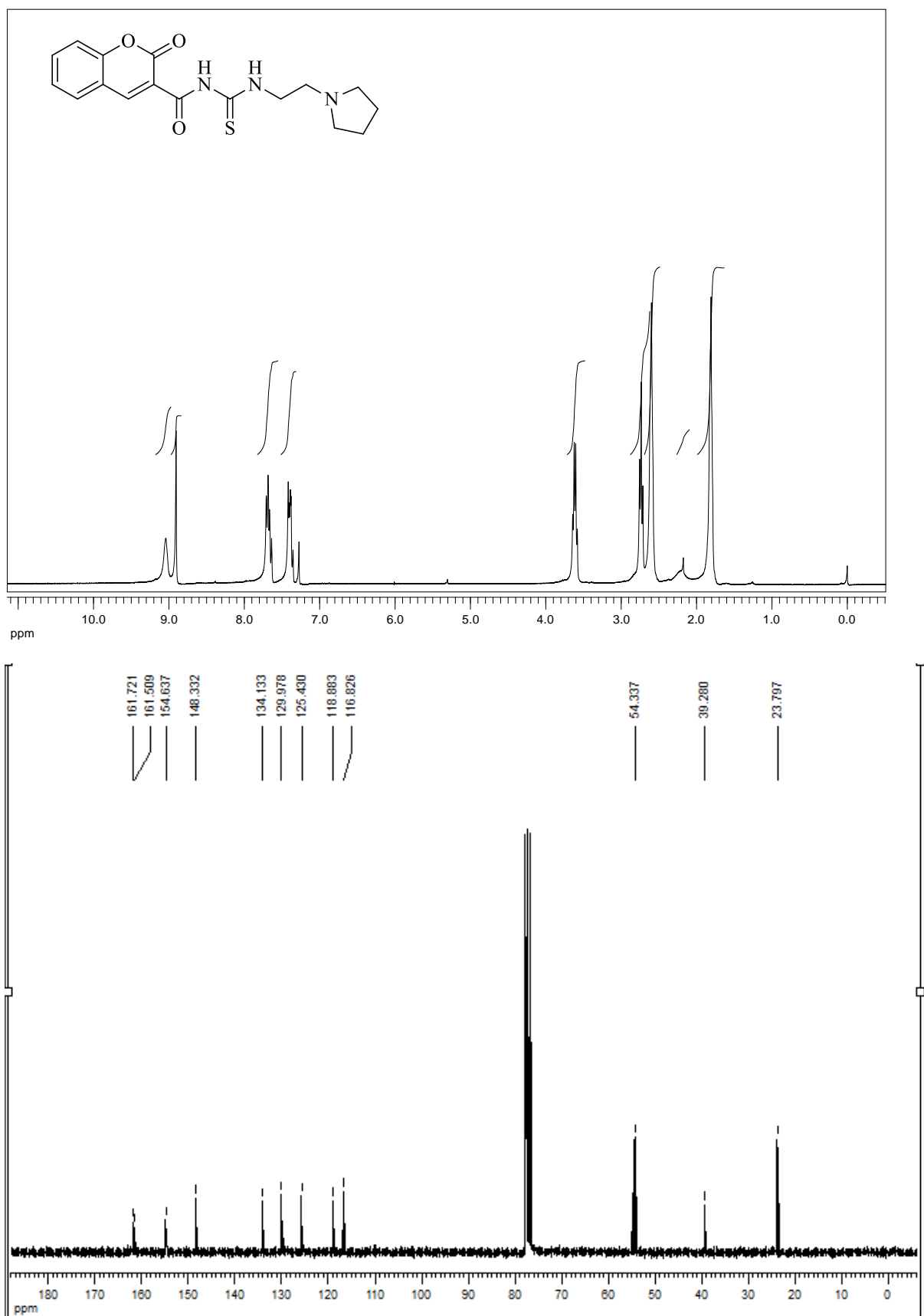


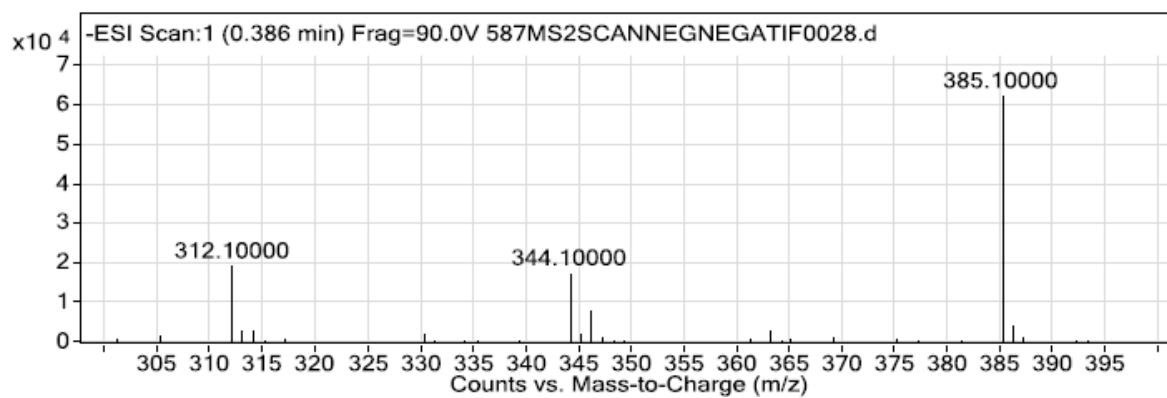
S12: ¹H NMR (CDCl₃), ¹³C NMR (CDCl₃) and MS spectra of **e10**



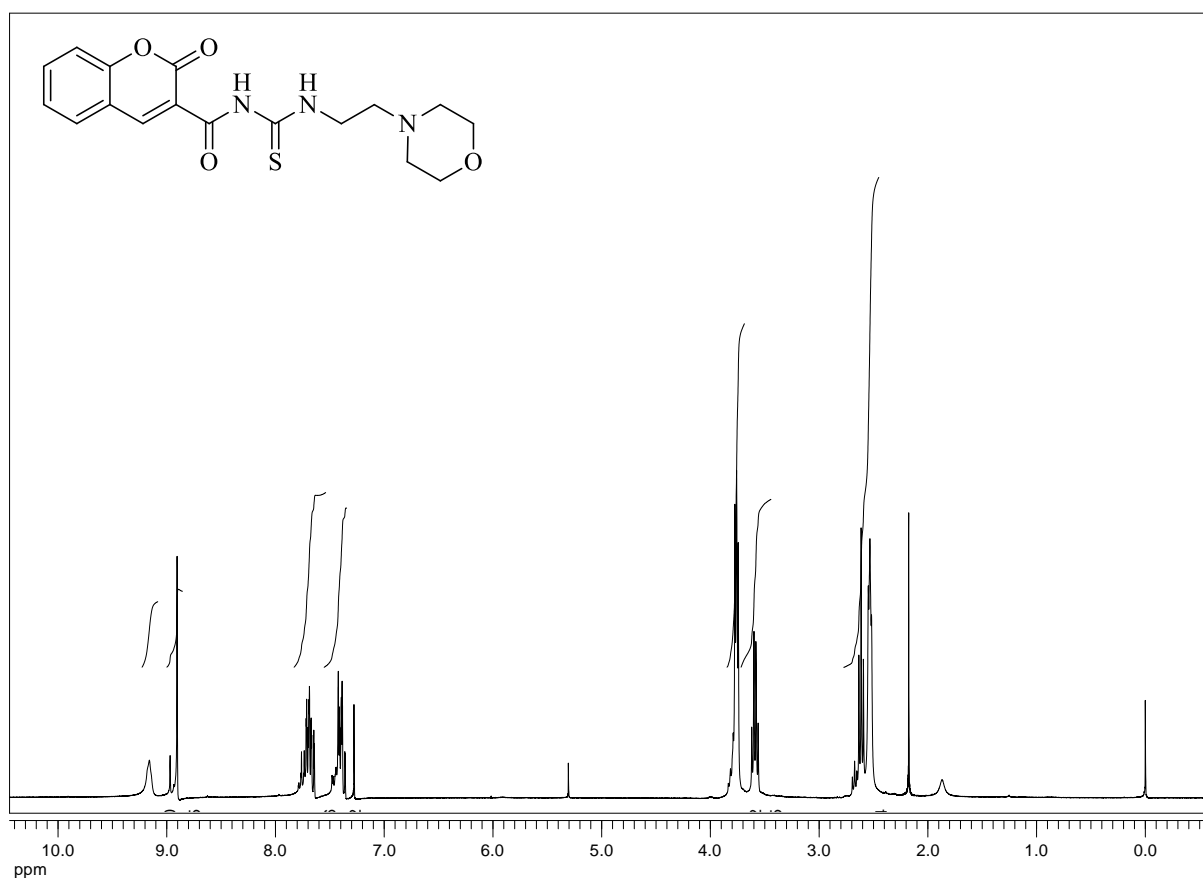


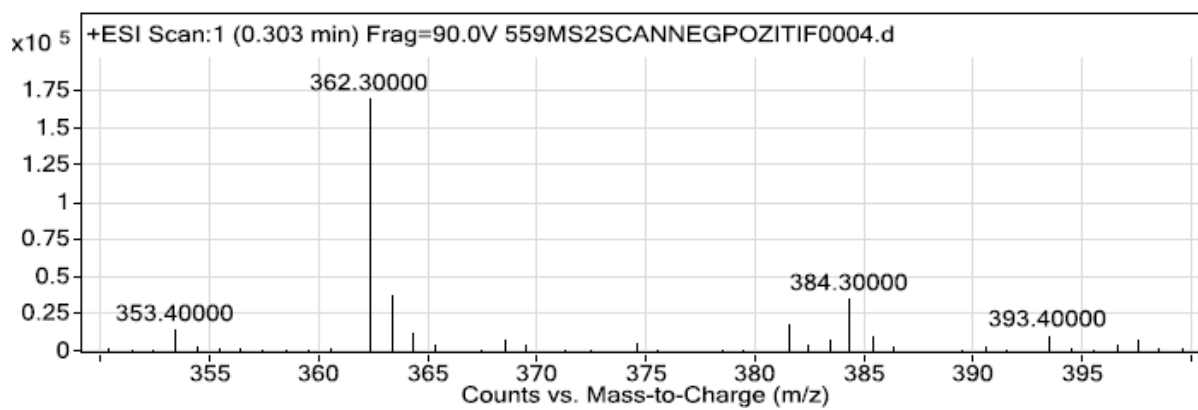
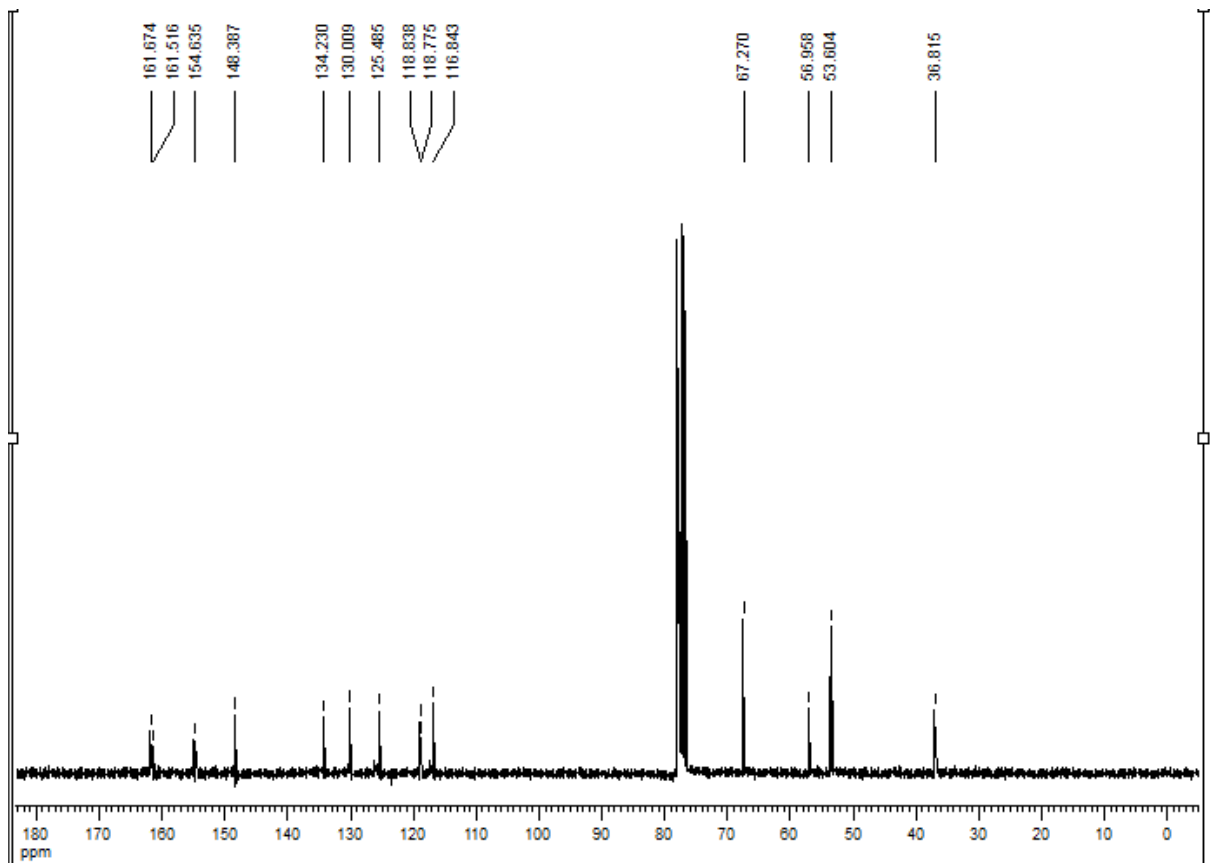
S13: ^1H NMR (CDCl_3), ^{13}C NMR (CDCl_3) and MS spectra of **e11**



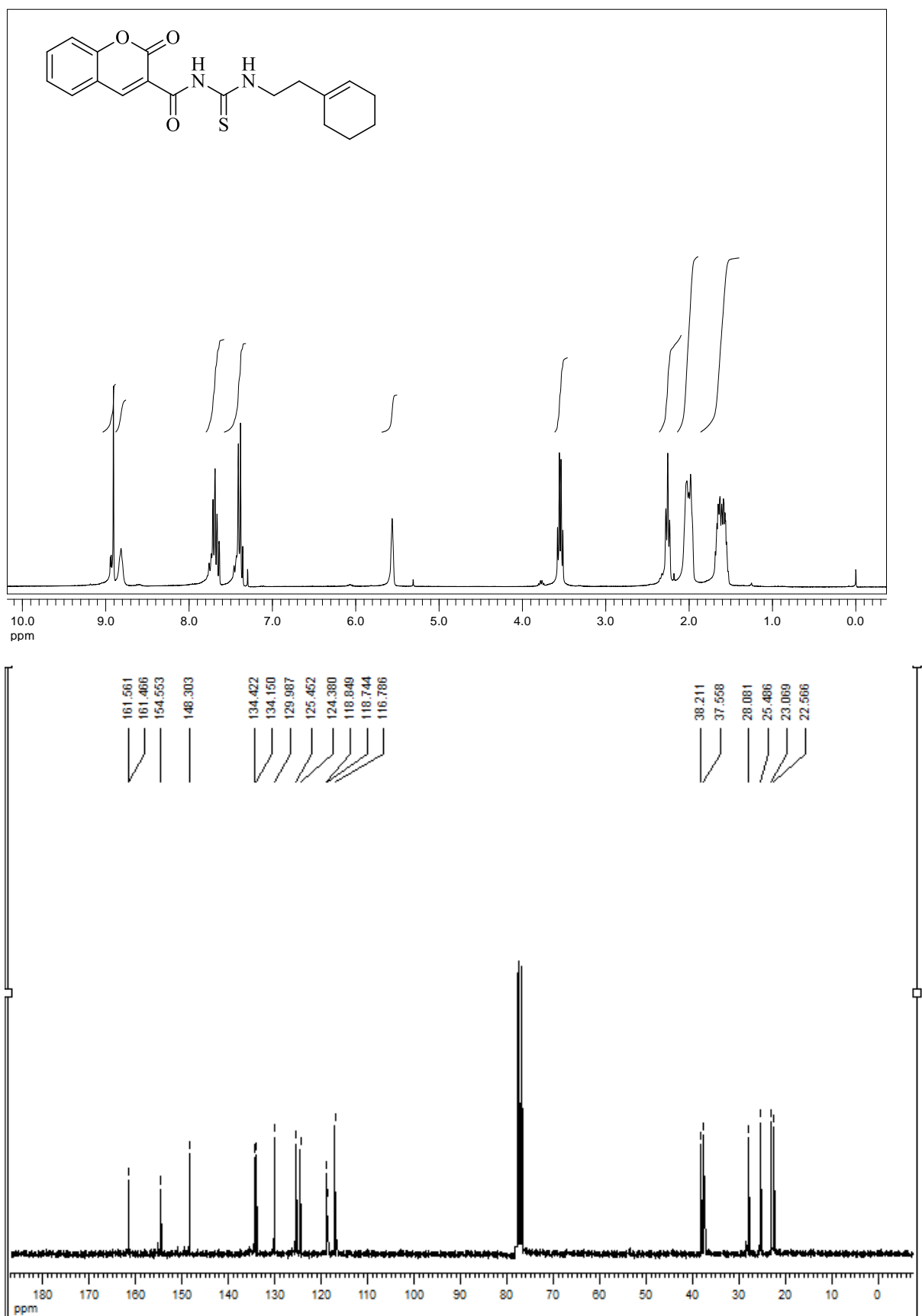


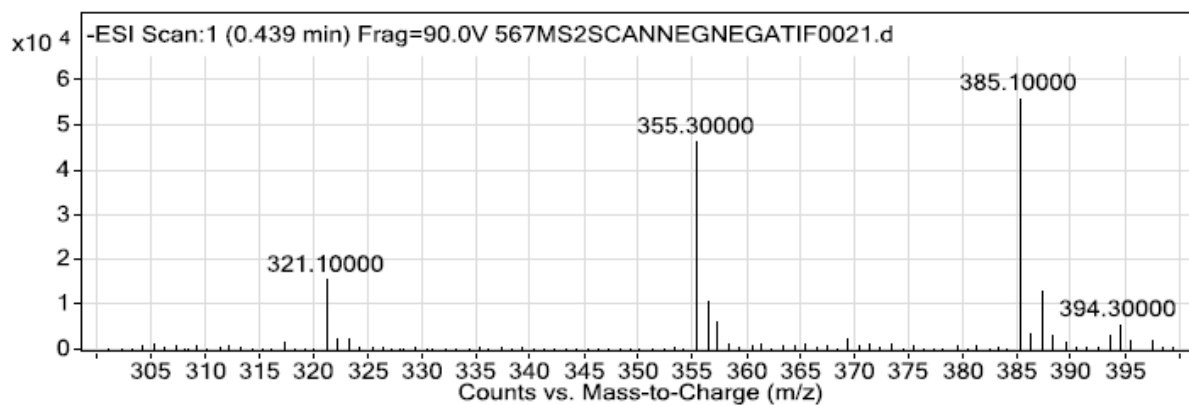
S14: ¹H NMR (CDCl₃), ¹³C NMR (CDCl₃) and MS spectra of **e12**



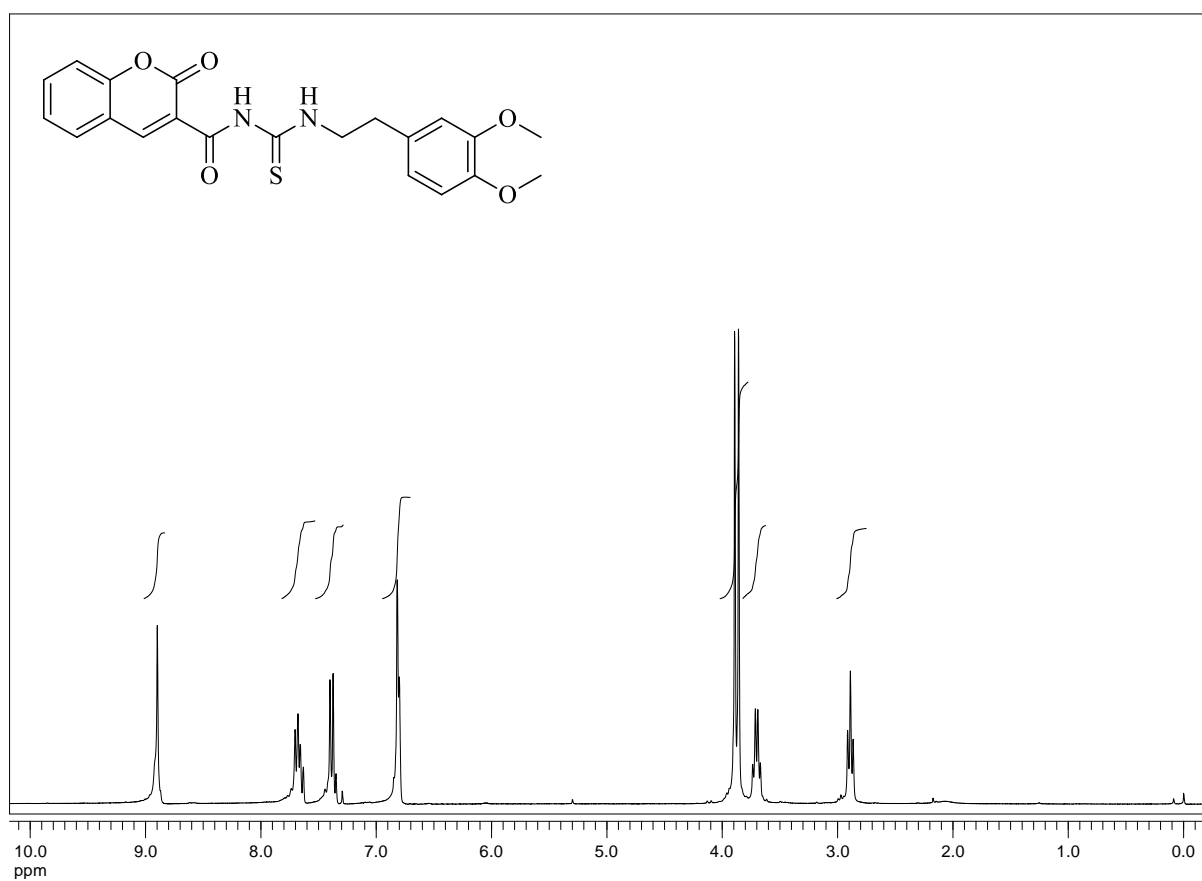


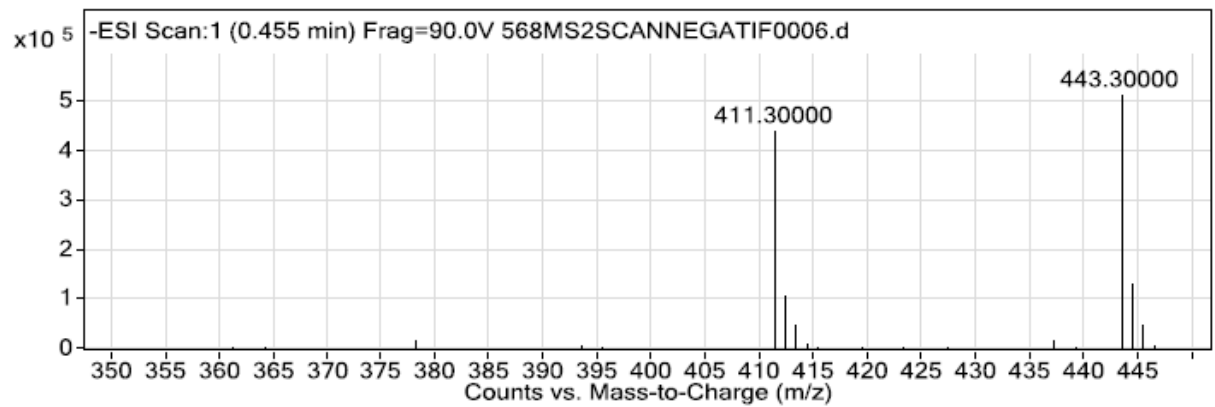
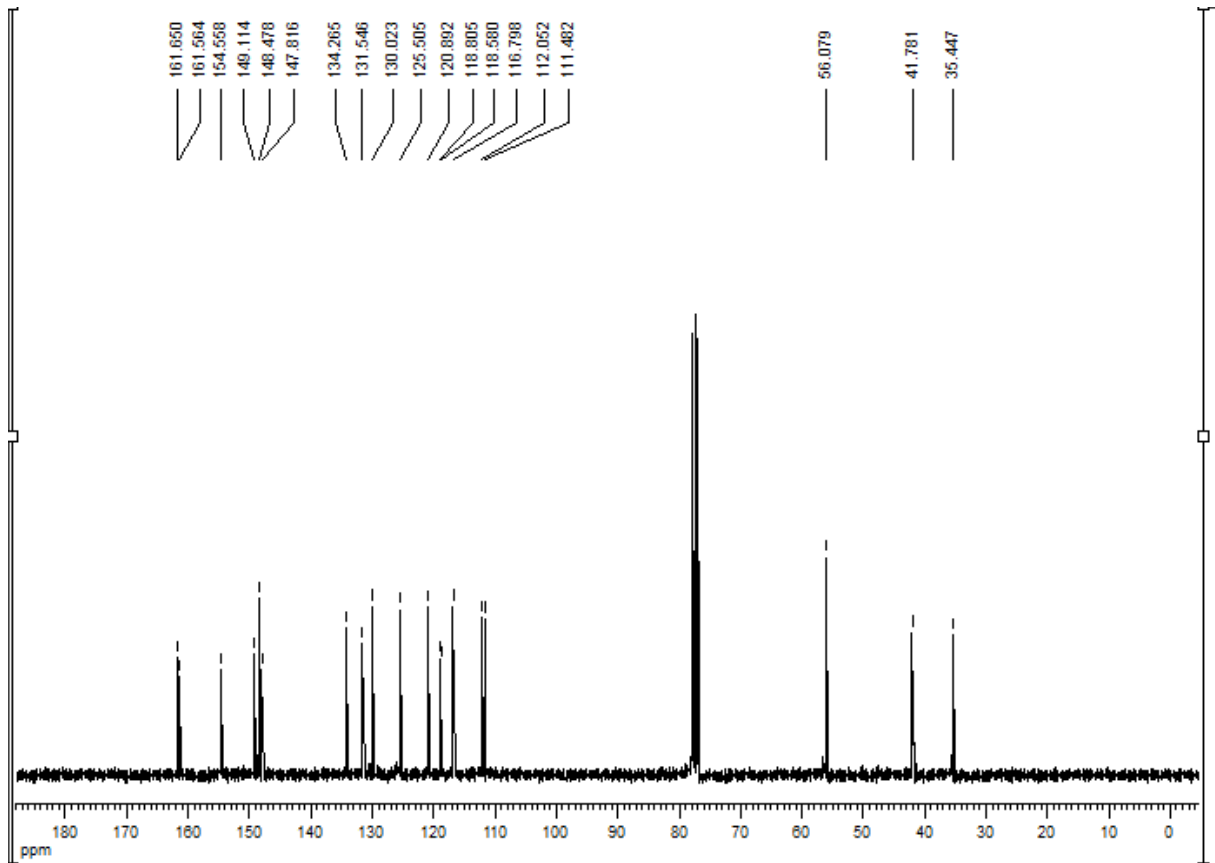
S15: ^1H NMR (CDCl_3), ^{13}C NMR (CDCl_3) and MS spectra of **e13**



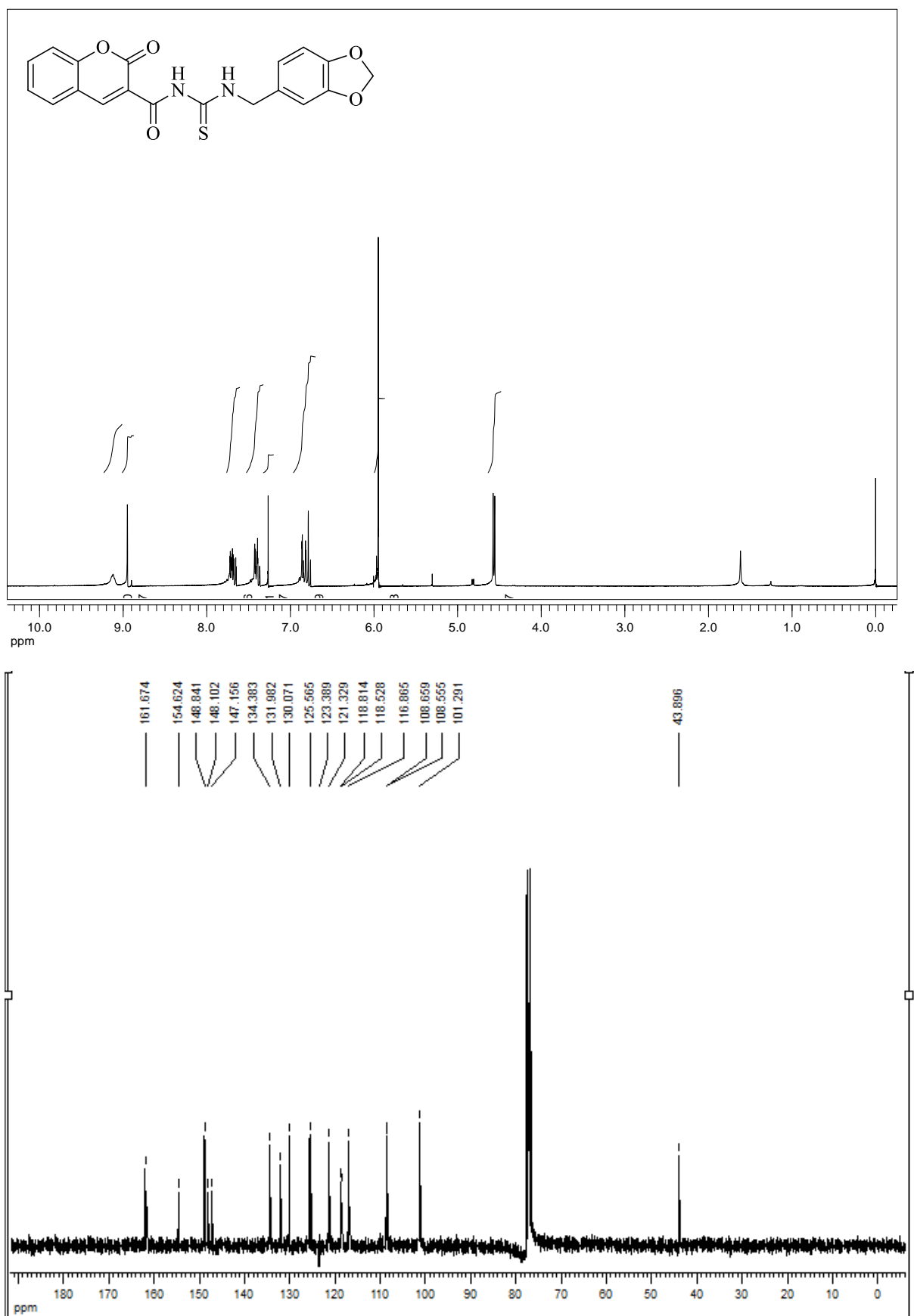


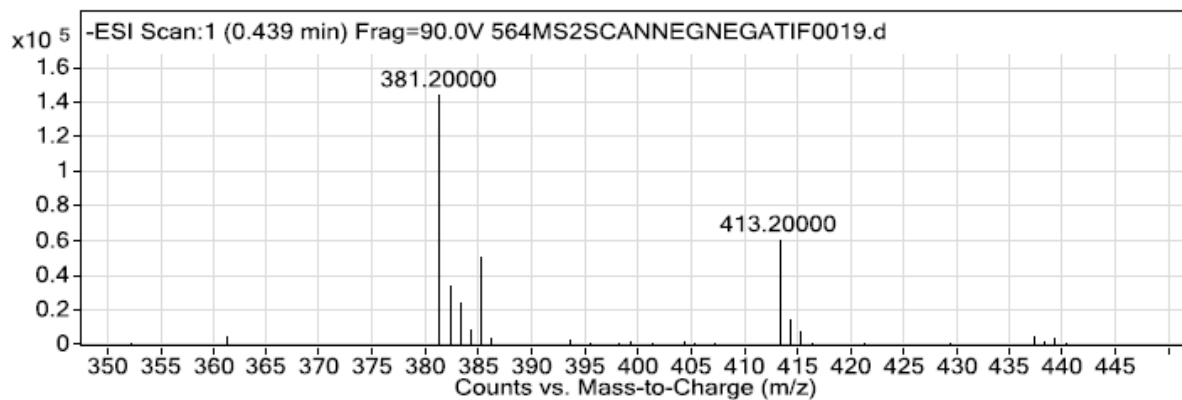
S16: ¹H NMR (CDCl₃), ¹³C NMR (CDCl₃) and MS spectra of **e14**



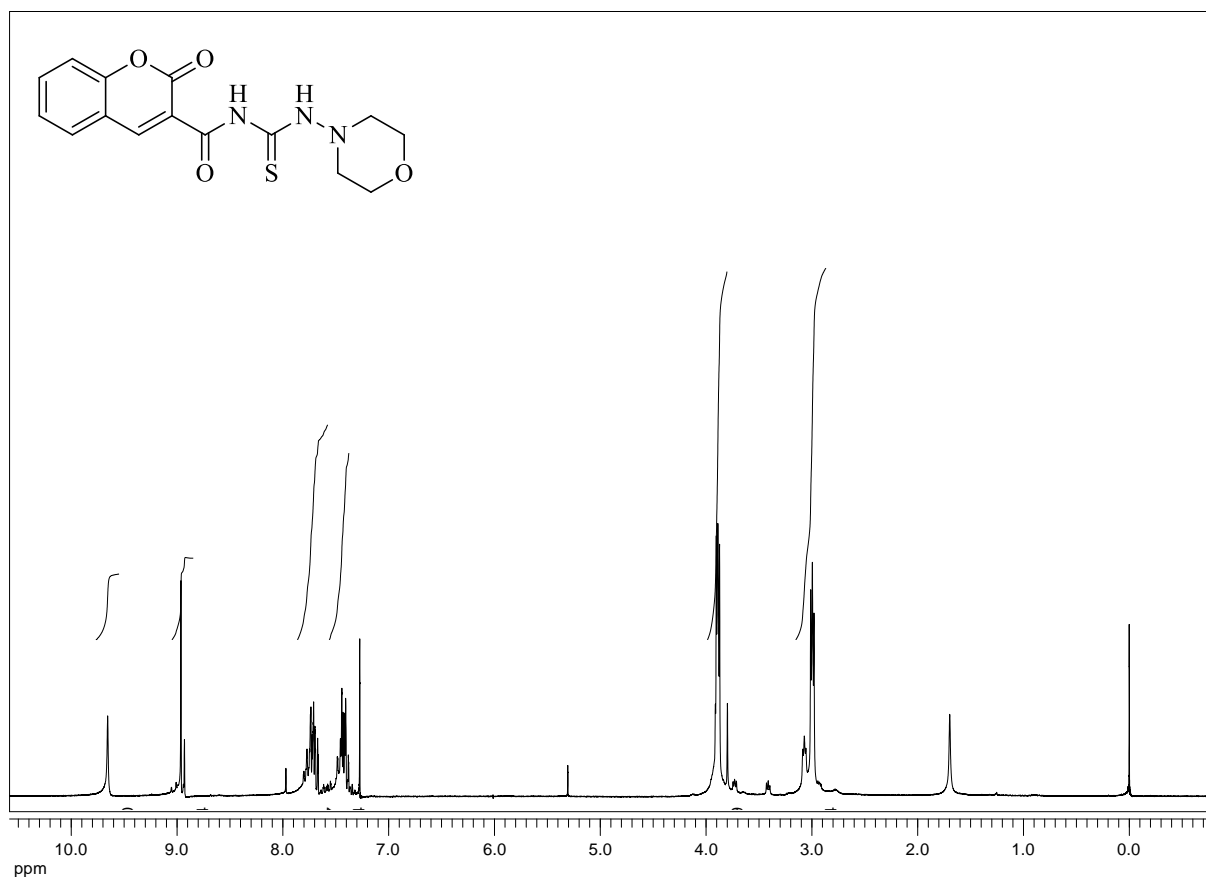


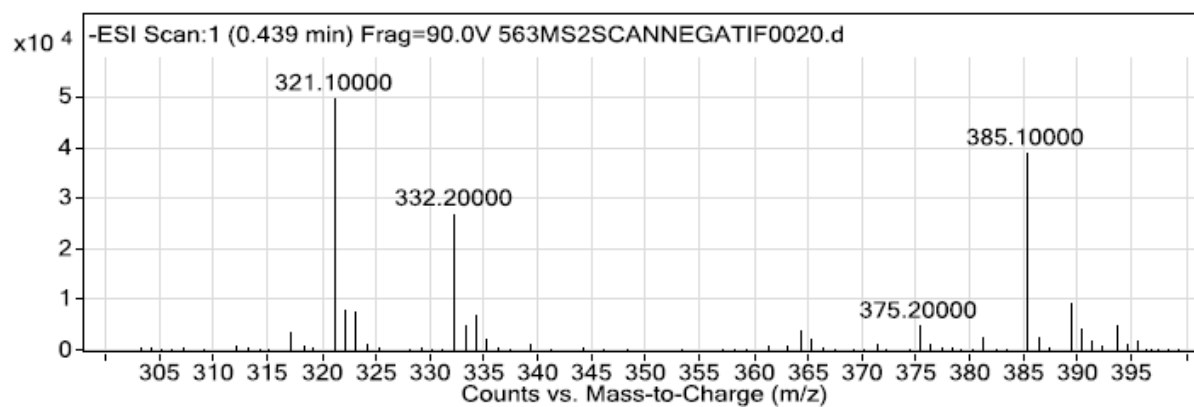
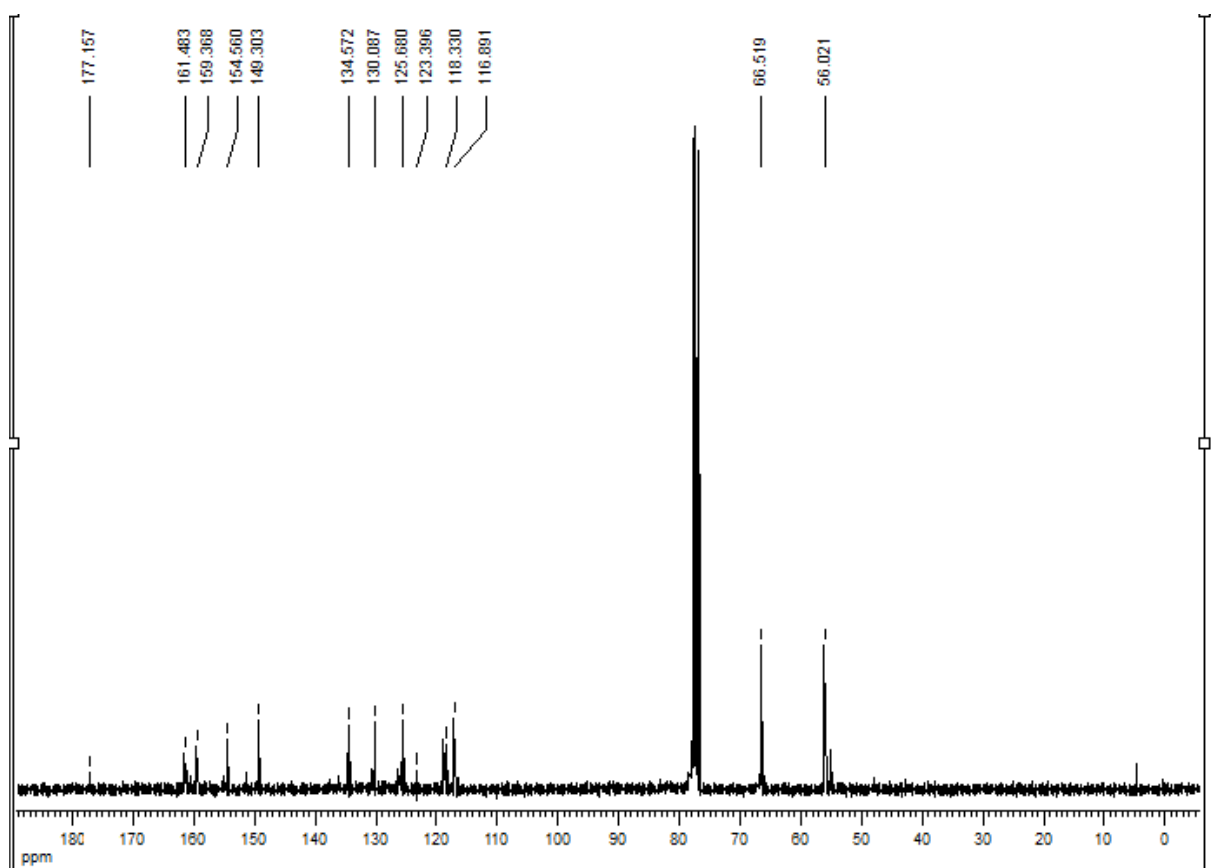
S17: ^1H NMR (CDCl_3), ^{13}C NMR (CDCl_3) and MS spectra of **e15**



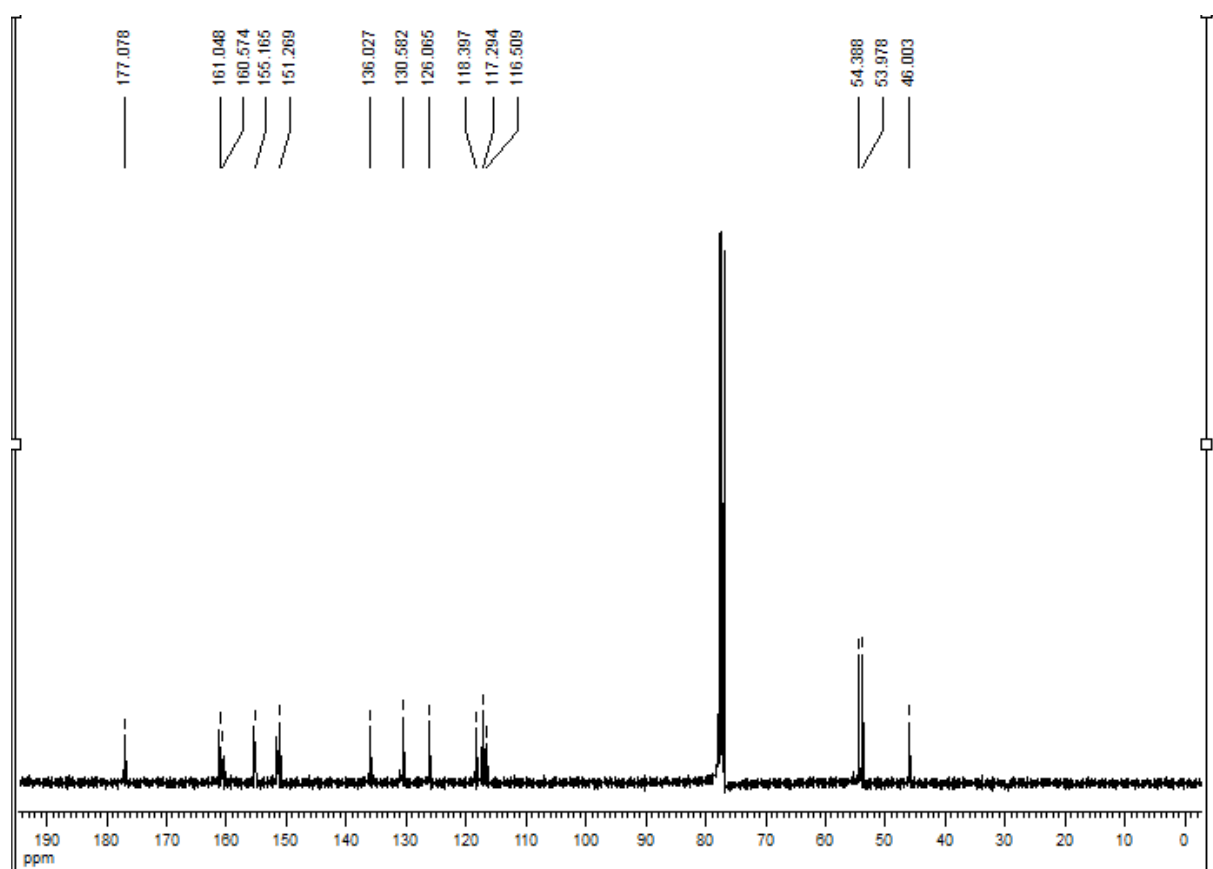
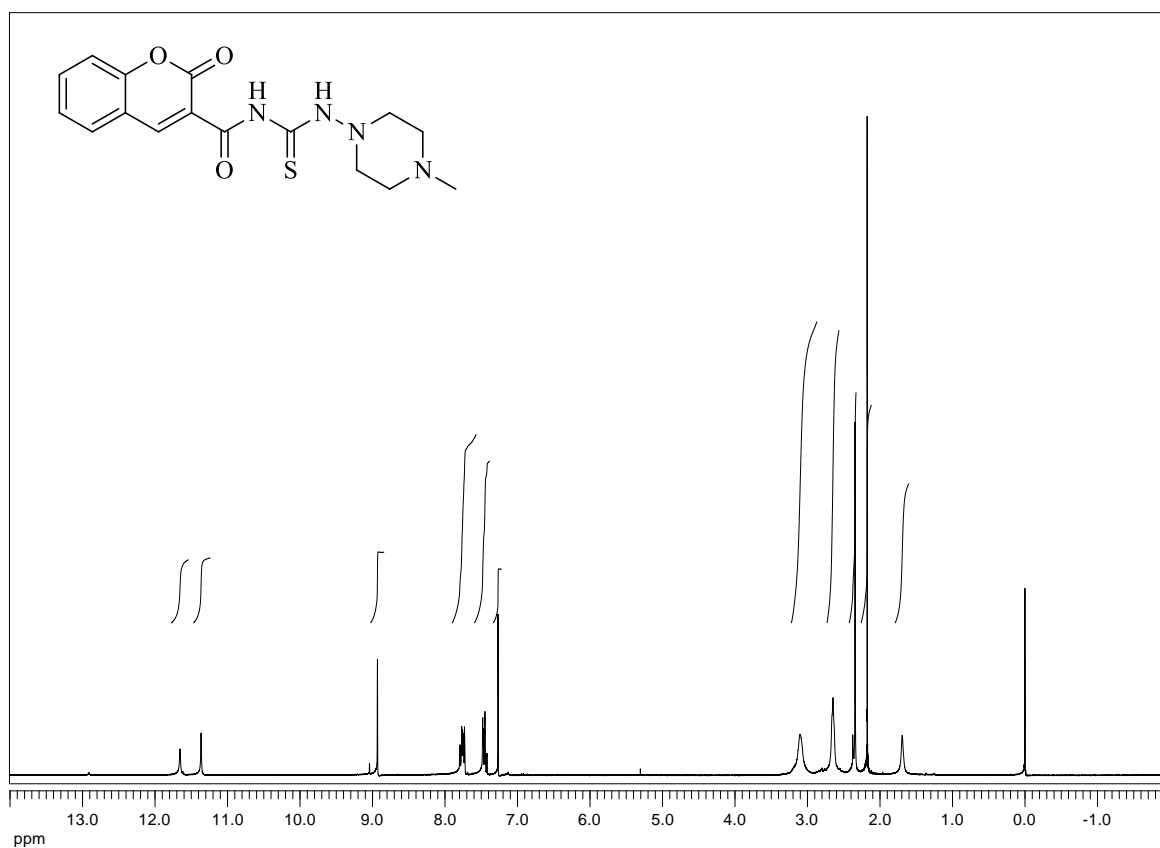


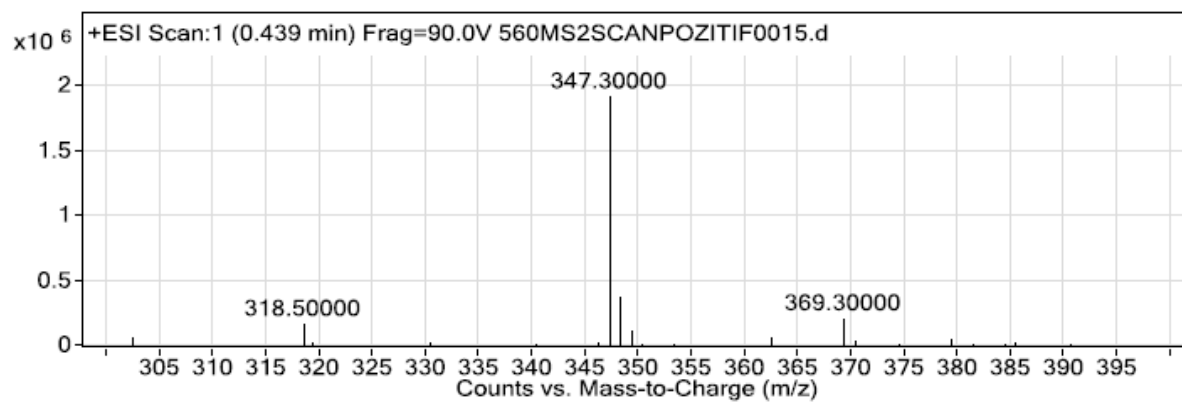
S18: ¹H NMR (CDCl₃), ¹³C NMR (CDCl₃) and MS spectra of **e16**



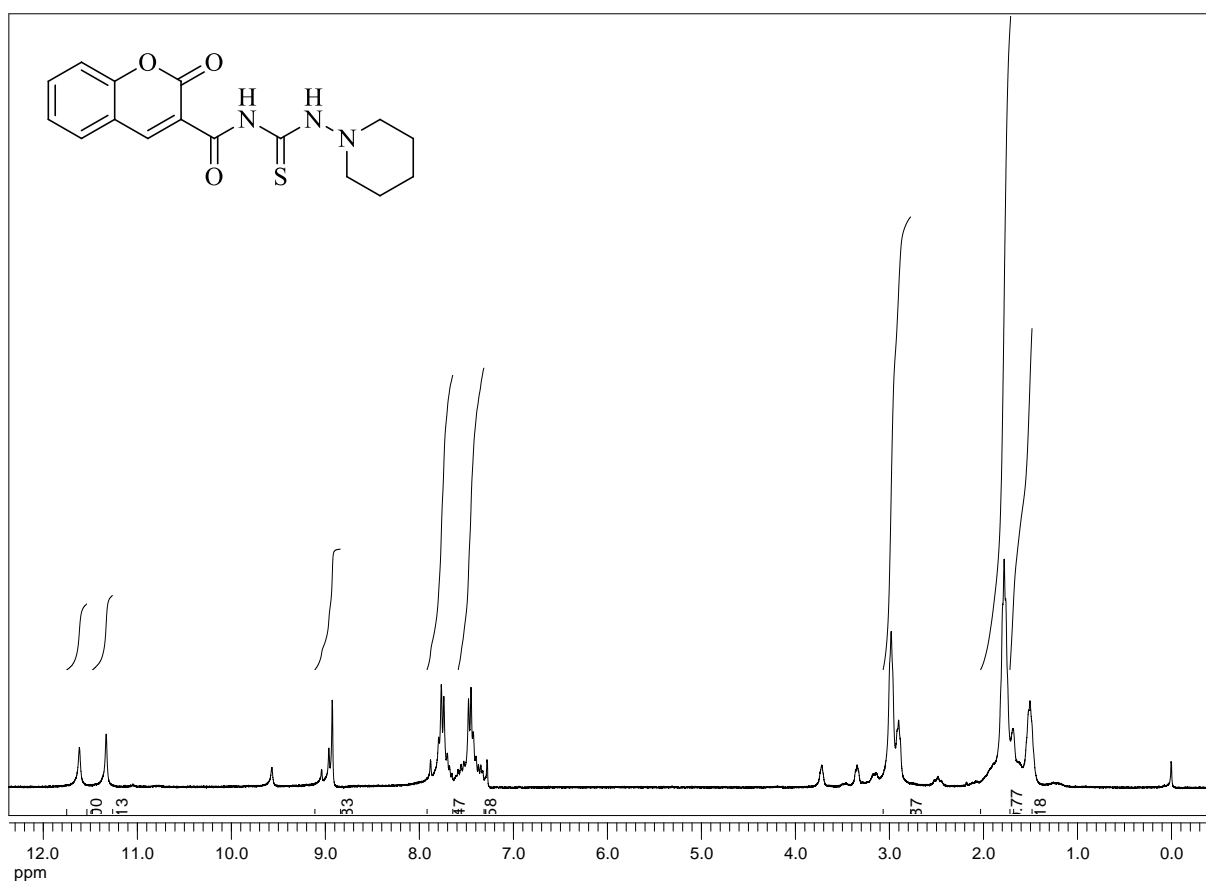


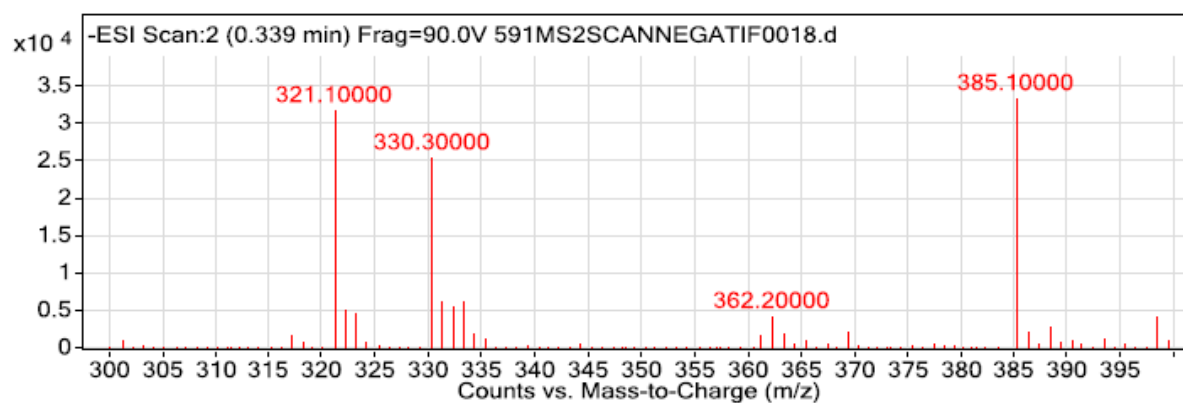
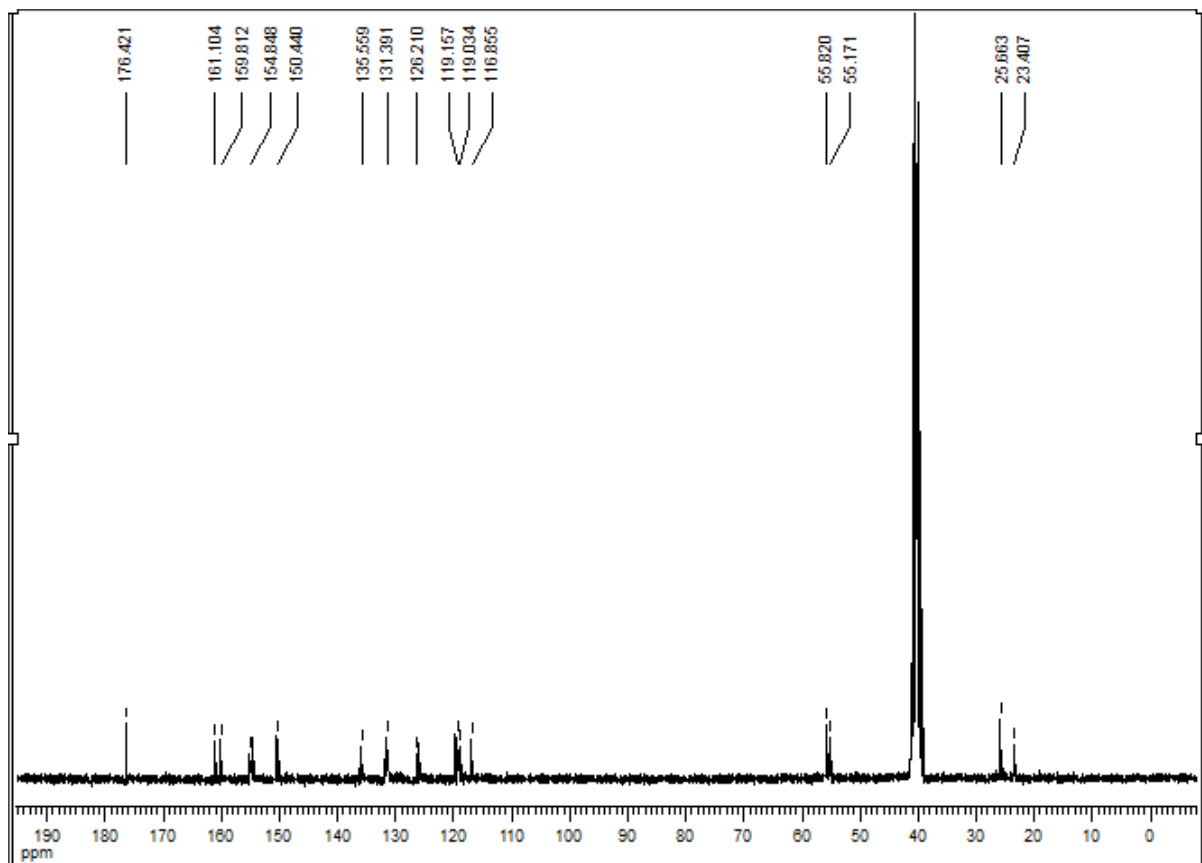
S19: ^1H NMR (CDCl_3), ^{13}C NMR (CDCl_3) and MS spectra of **e17**



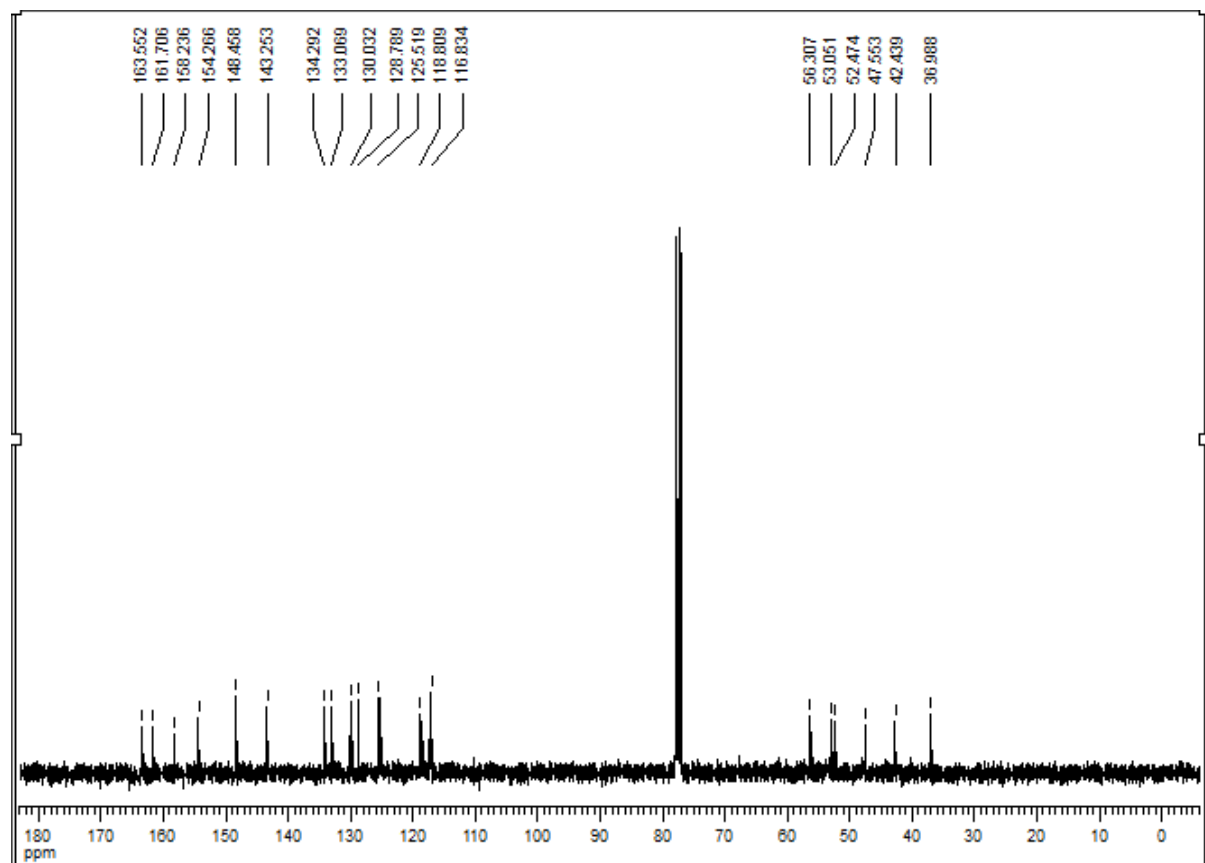
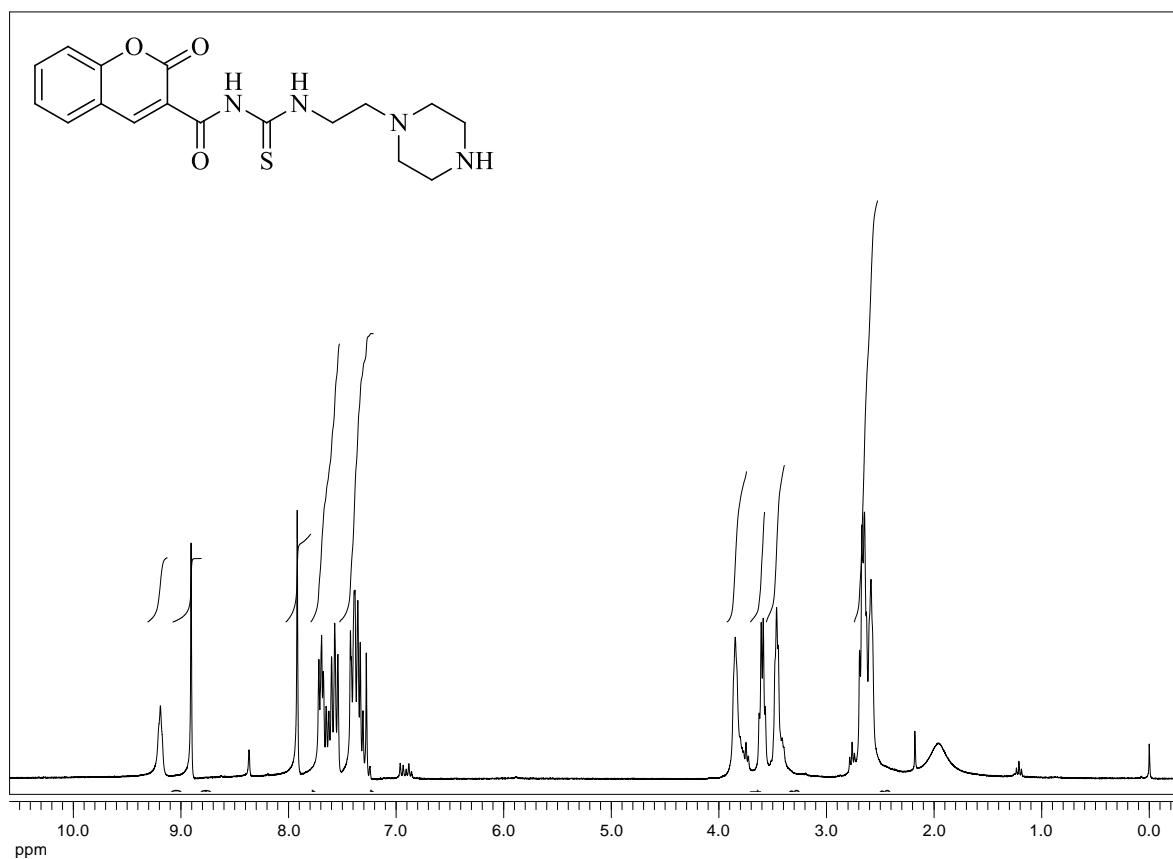


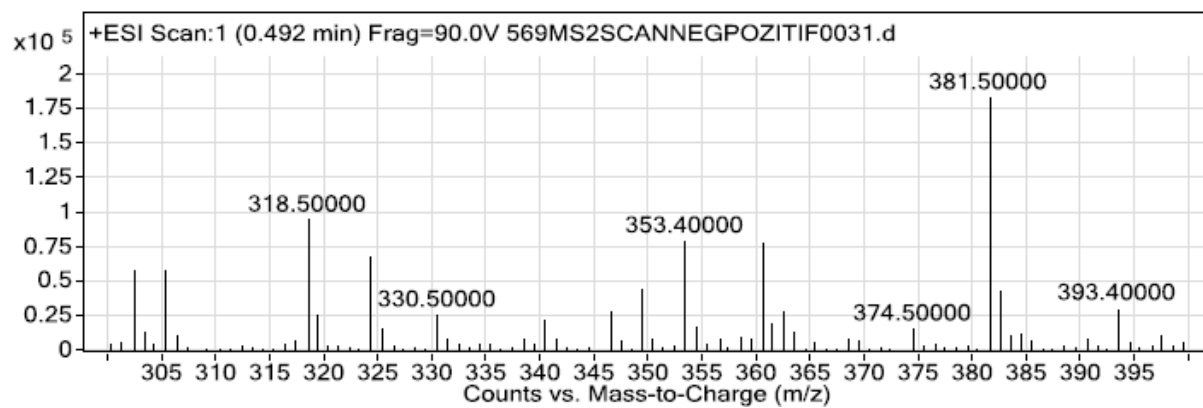
S20: ¹H NMR (CDCl₃), ¹³C NMR (CDCl₃) and MS spectra of **e18**





S21: ^1H NMR (CDCl_3), ^{13}C NMR (CDCl_3) and MS spectra of **e19**





S22: ¹H NMR (CDCl₃), ¹³C NMR (CDCl₃) and MS spectra of **e20**

