



Novel 2-(Adamantan-1-ylamino)Thiazol-4(5H)-One Derivatives and Their Inhibitory Activity towards 11 β -HSD1 – synthesis, Molecular Docking and In Vitro Studies

Renata Studzińska ^{1,*}, Daria Kupczyk ², Wojciech Płaziński ³, Szymon Baumgart ¹, Rafał Bilski ², Renata Paprocka ¹ and Renata Kołodziejska ²

¹ Department of Organic Chemistry, Faculty of Pharmacy, Collegium Medicum in Bydgoszcz, Nicolaus Copernicus University in Toruń, 2 Jurasza Str., 85–089 Bydgoszcz, Poland; sz.baumgart@cm.umk.pl (Sz.B.); renata.bursa@cm.umk.pl (R.P.)

² Department of Medical Biology and Biochemistry, Faculty of Medicine, Collegium Medicum in Bydgoszcz, Nicolaus Copernicus University in Toruń, 24 Karłowicza Str., 85–092 Bydgoszcz, Poland; dariak@cm.umk.pl (D.K.); rafal.bilski@cm.umk.pl (R.B.); renatak@cm.umk.pl (R.K.)

³ J. Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences, 8 Niezapominajek Str., 30-239 Cracow, Poland; wojtek_plazinski@tlen.pl

* Correspondence: rstud@cm.umk.pl

Supplementary information

¹H NMR spectra of compounds 3a–j.

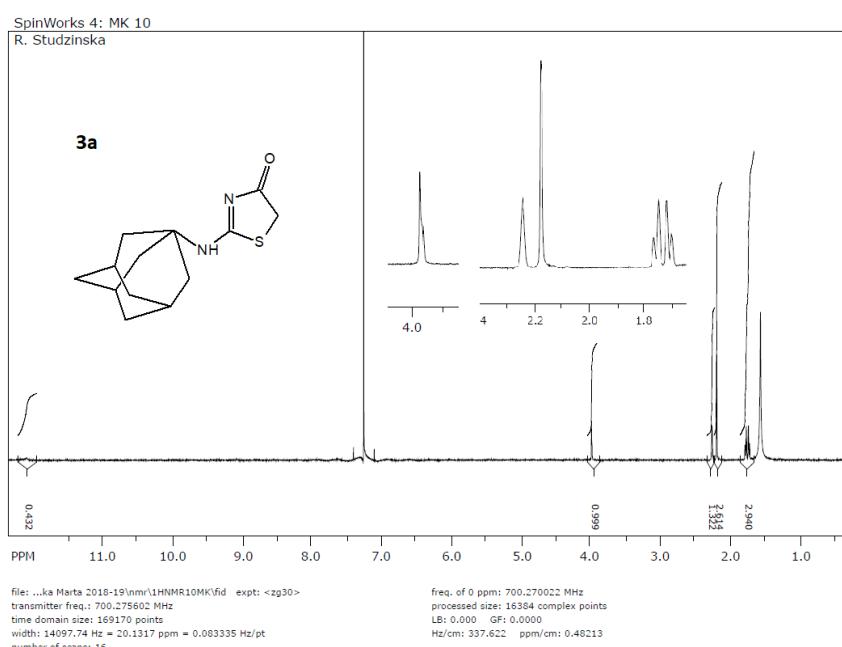
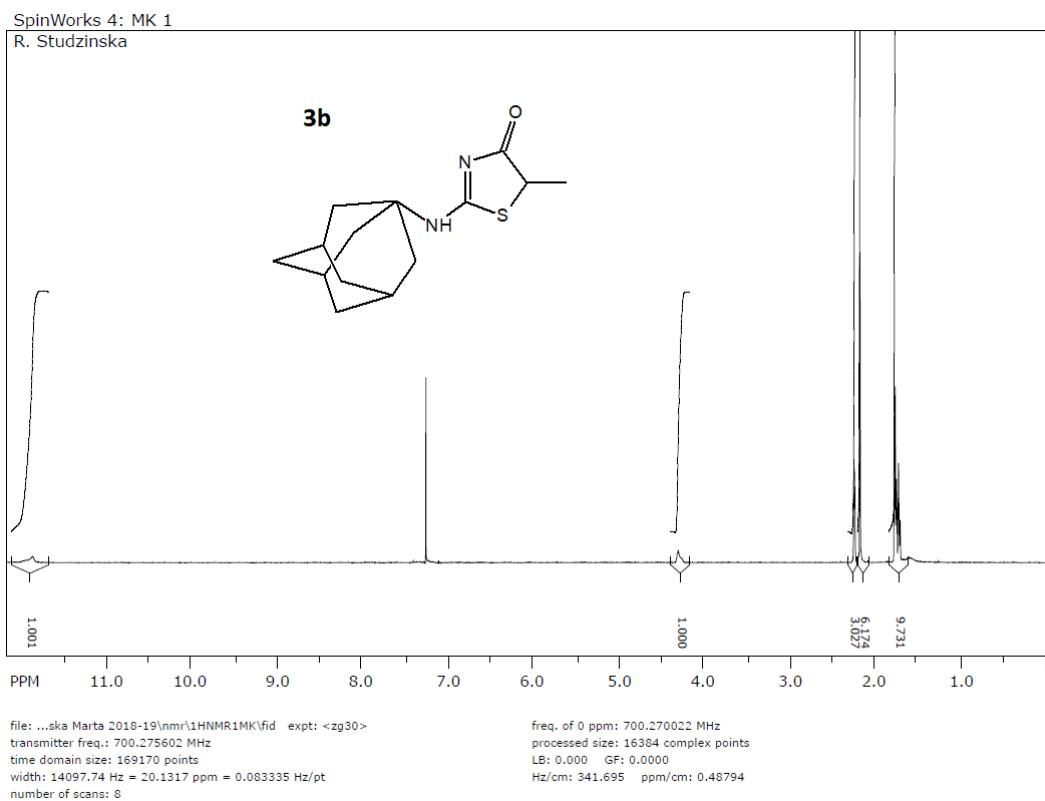
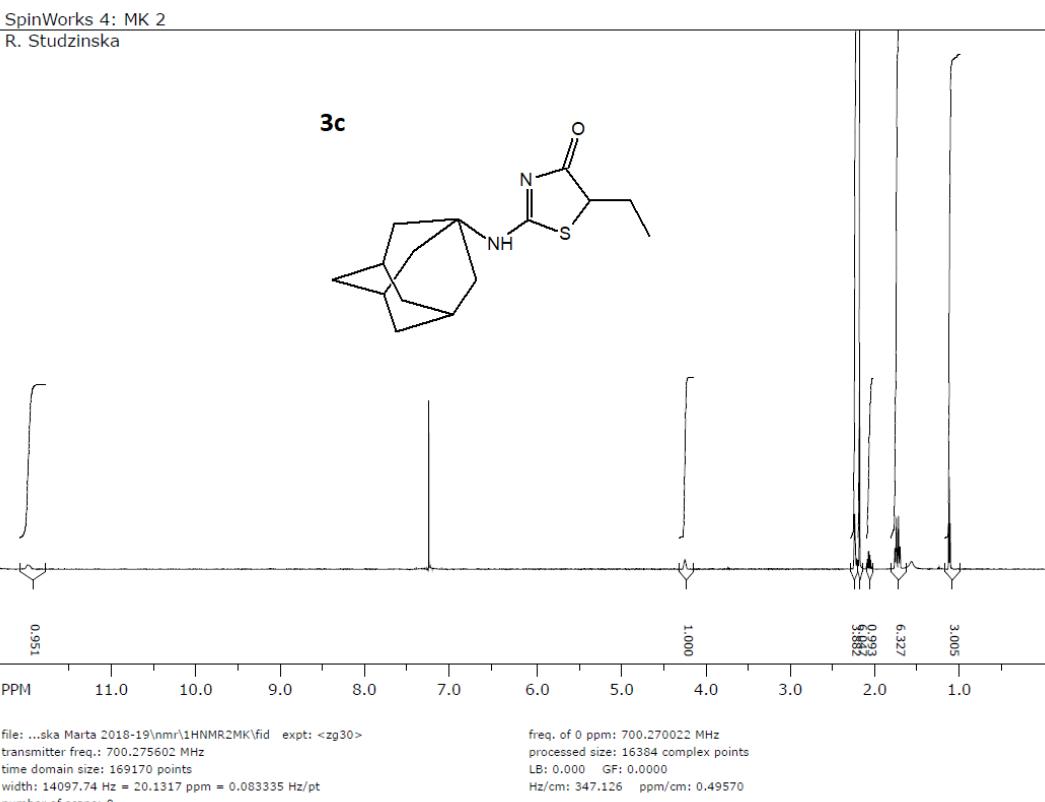
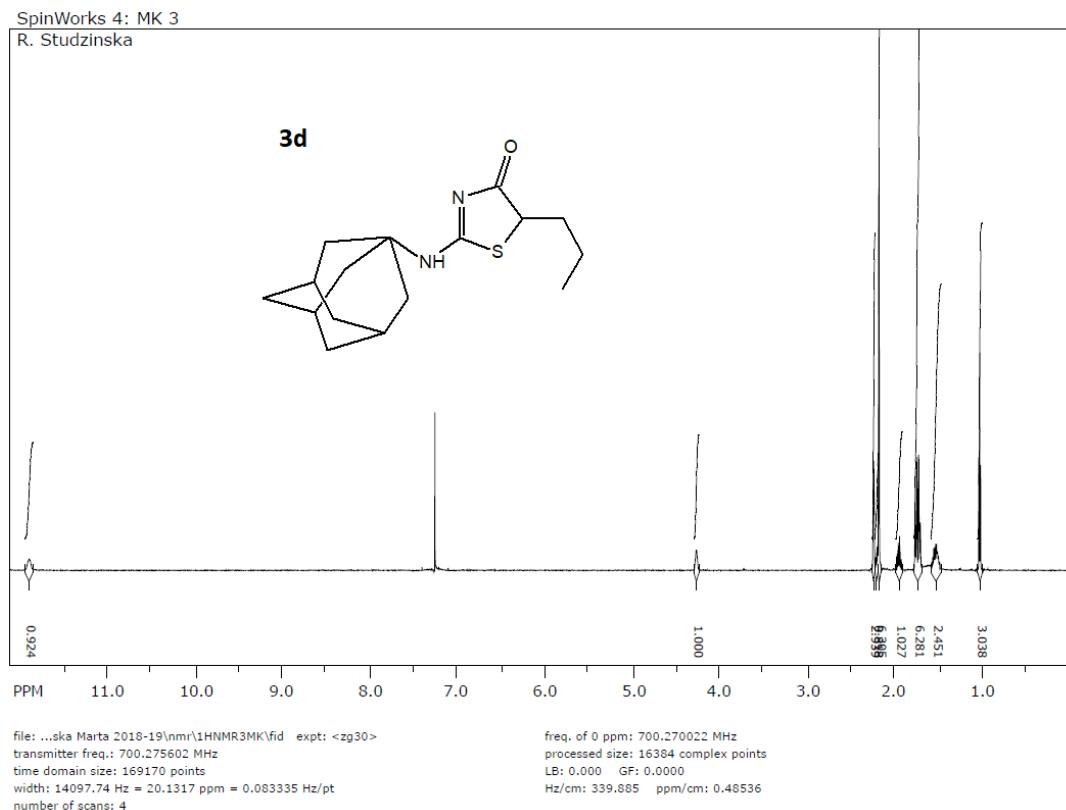
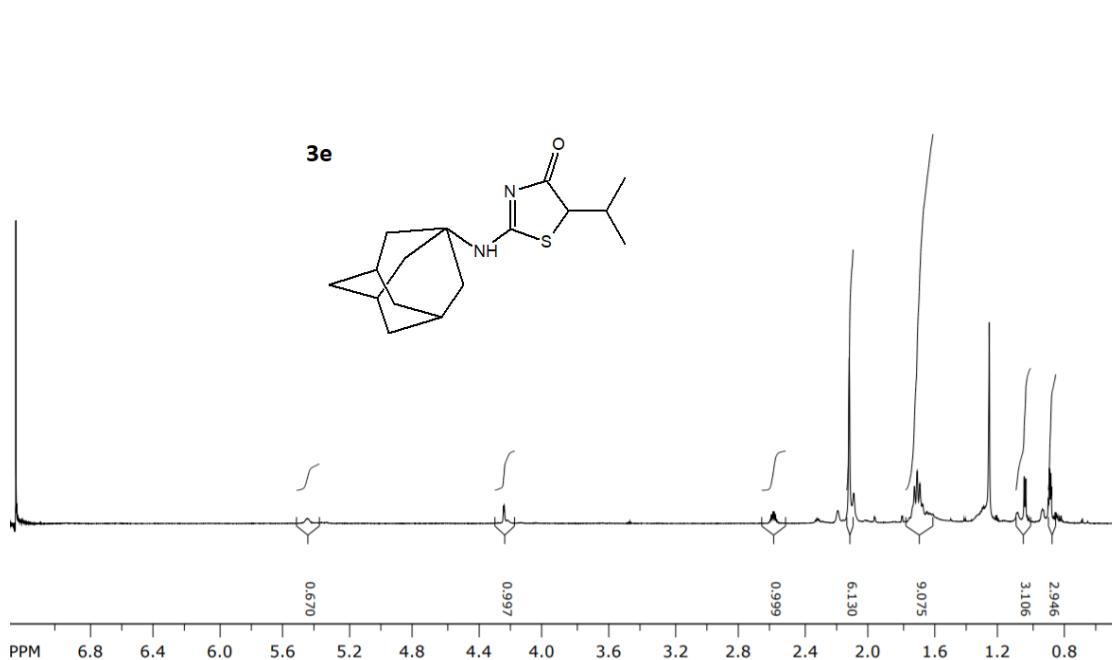
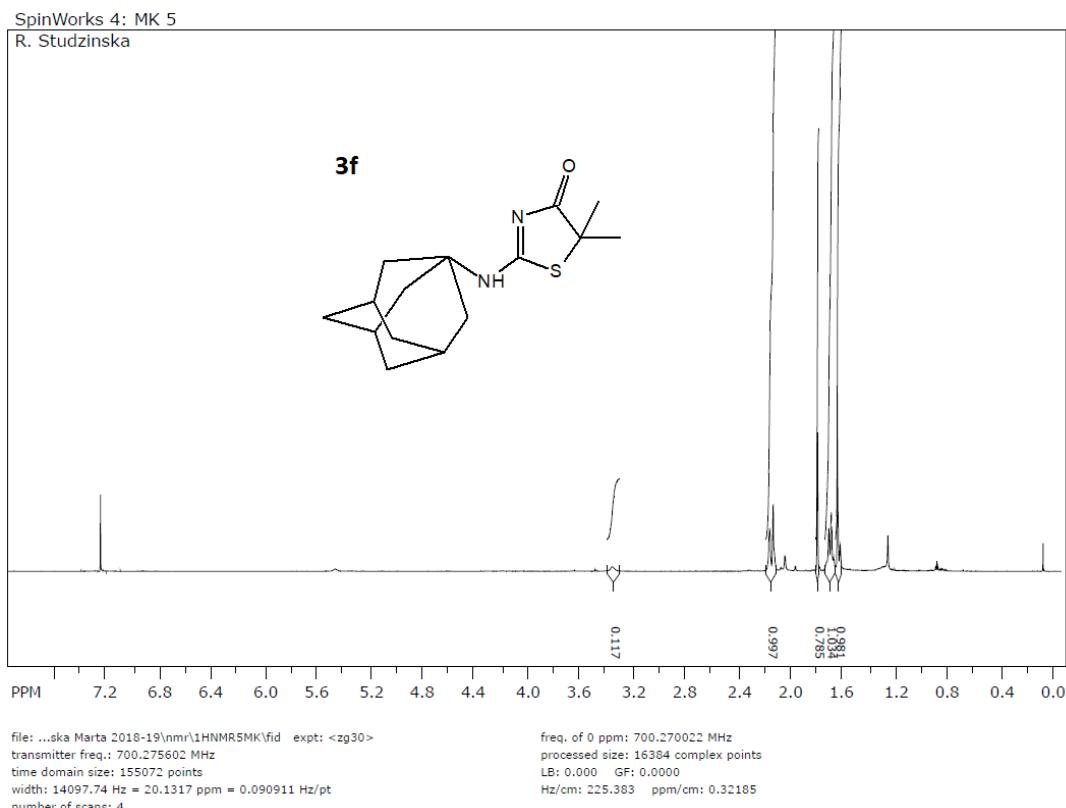
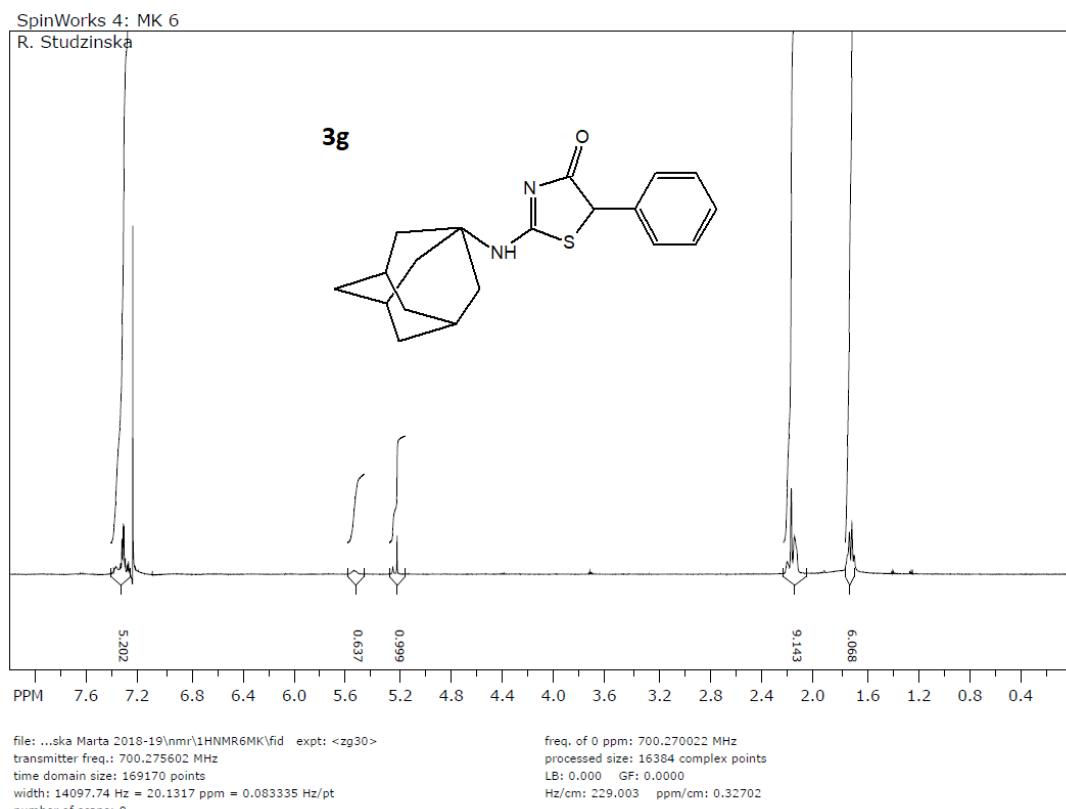
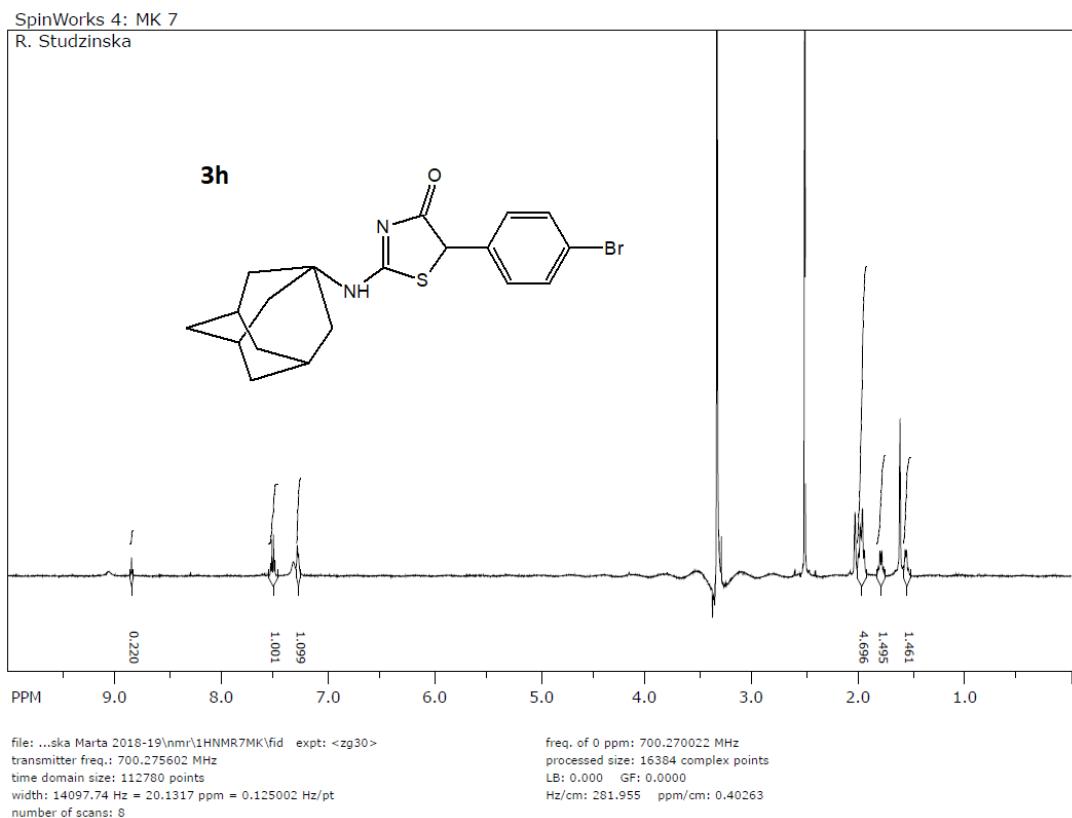
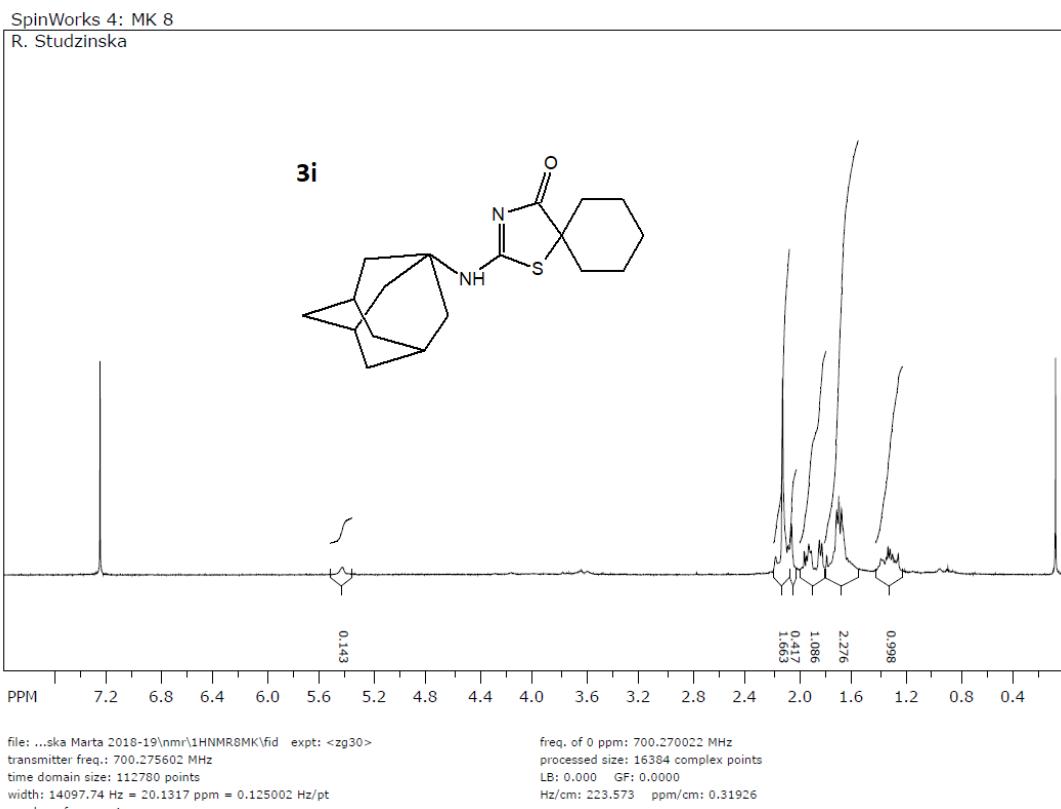


Figure S1A ¹H NMR spectra of compound 3a.

**Figure S1B.** ^1H NMR spectra of compound **3b**.**Figure S1C.** ^1H NMR spectra of compound **3c**.

**Figure S1D.** ^1H NMR spectra of compound 3d.**Figure S1E.** ^1H NMR spectra of compounds 3e.

**Figure S1F.** ^1H NMR spectra of compound 3f.**Figure S1G.** ^1H NMR spectra of compound 3g.

**Figure S1H.** ^1H NMR spectra of compound **3h**.**Figure S1I.** ^1H NMR spectra of compound **3i**.

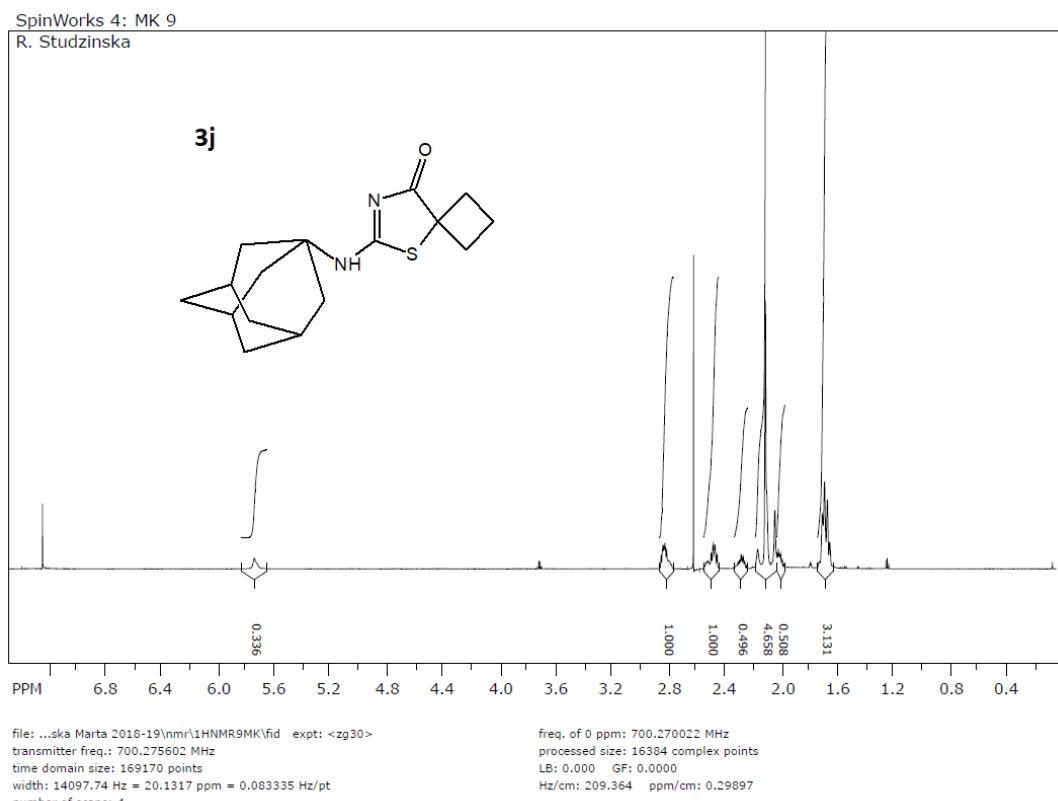


Figure S1J. ^1H NMR spectra of compound 3j.

^{13}C NMR spectra of compounds 3a–j

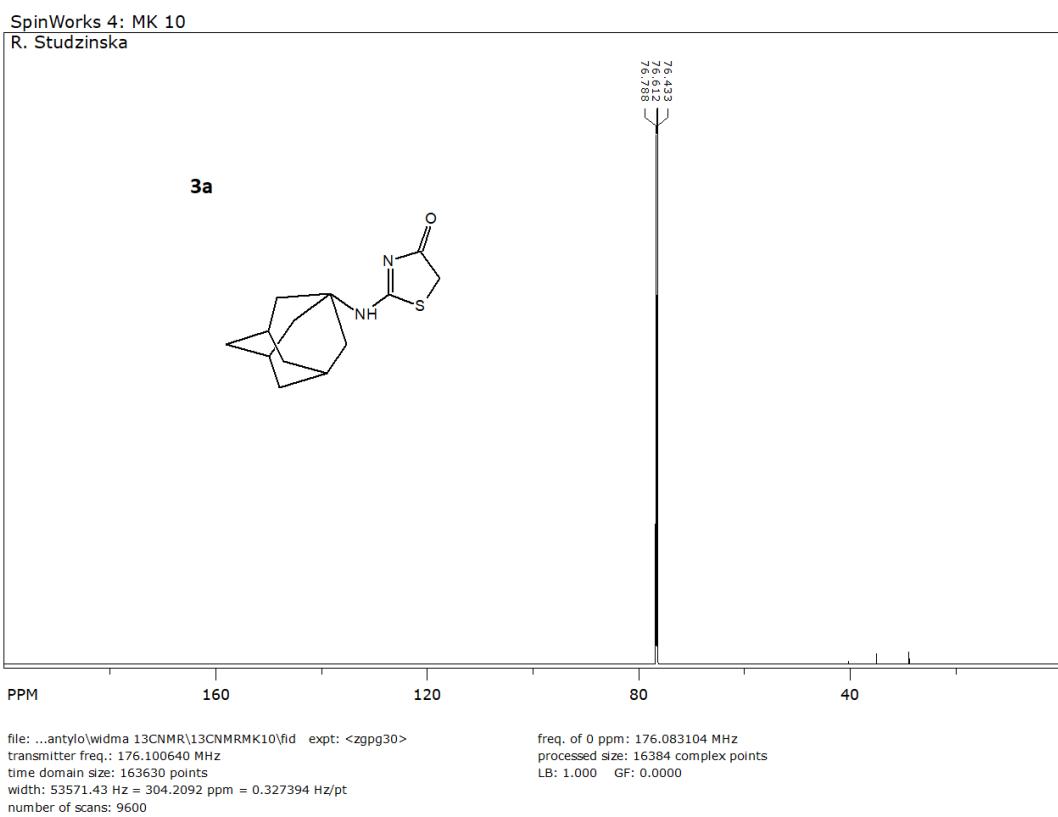
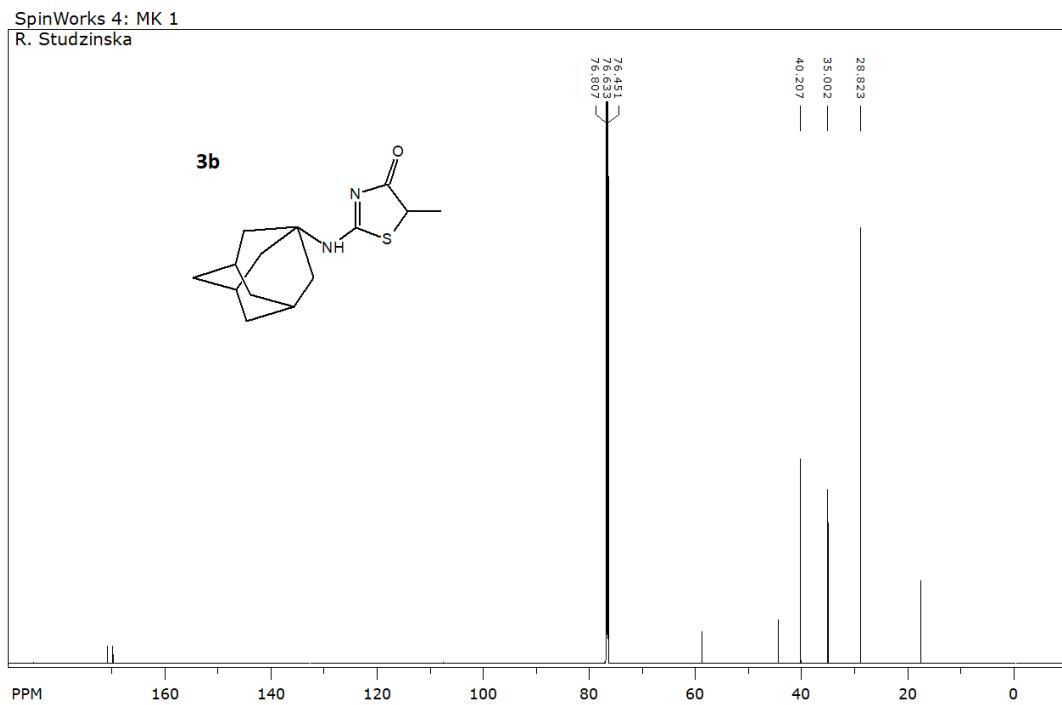
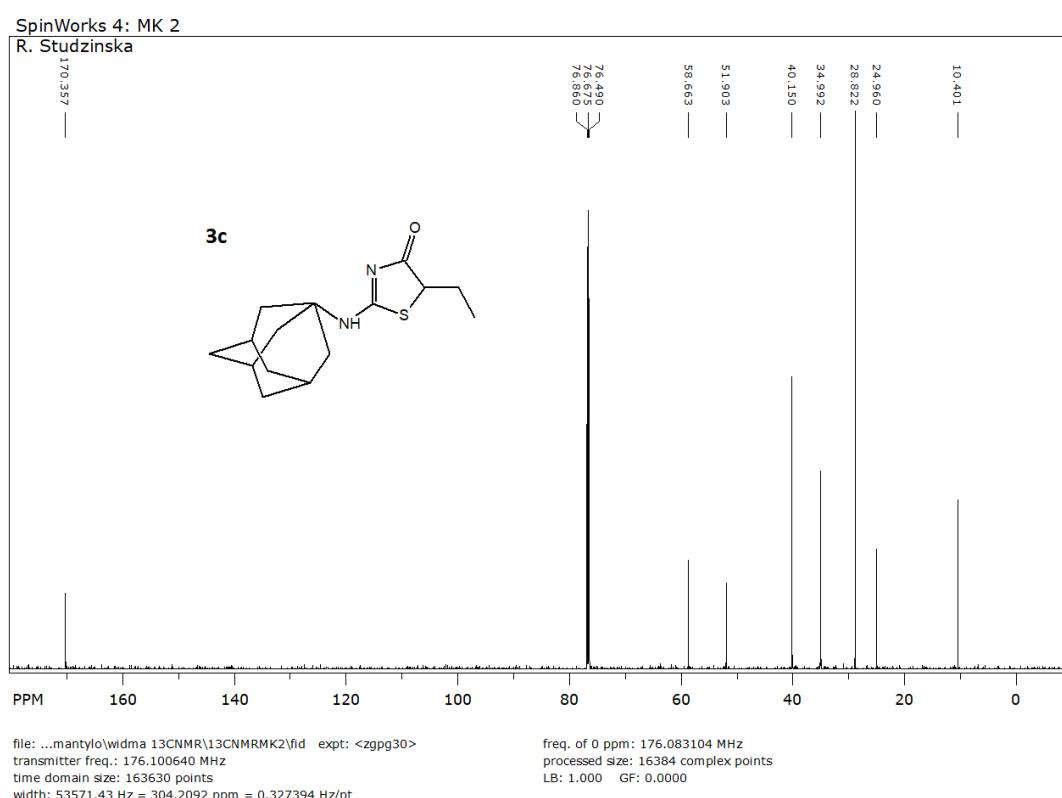
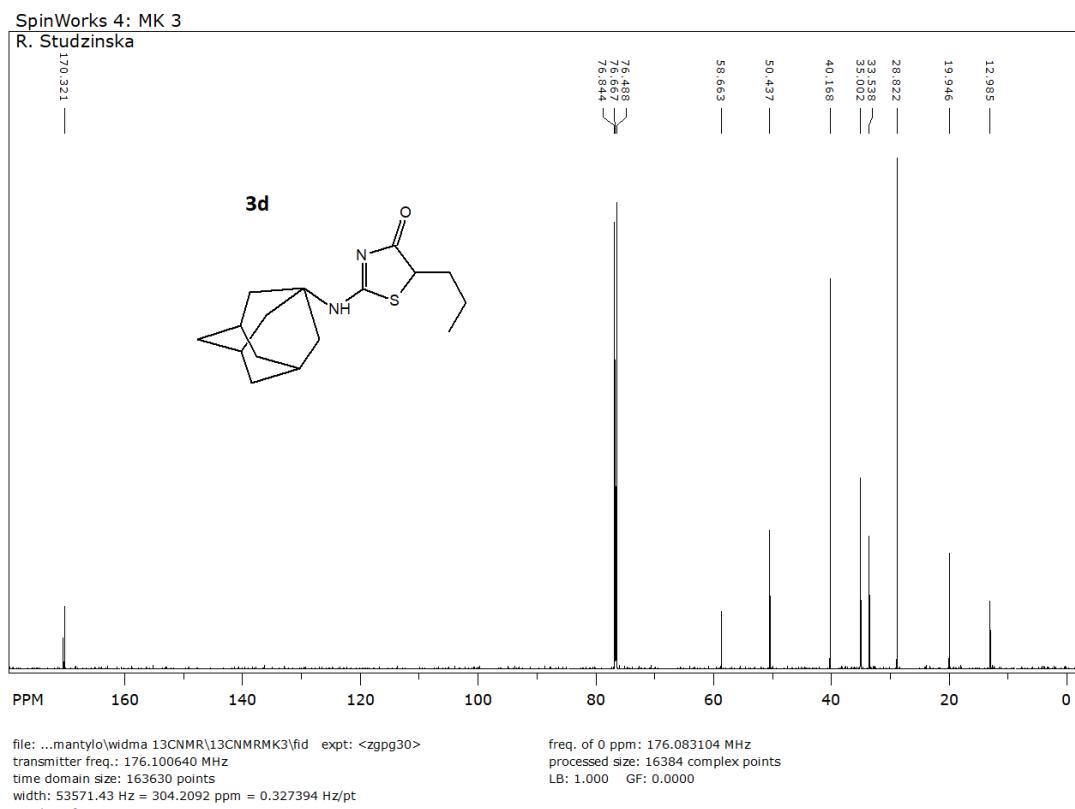
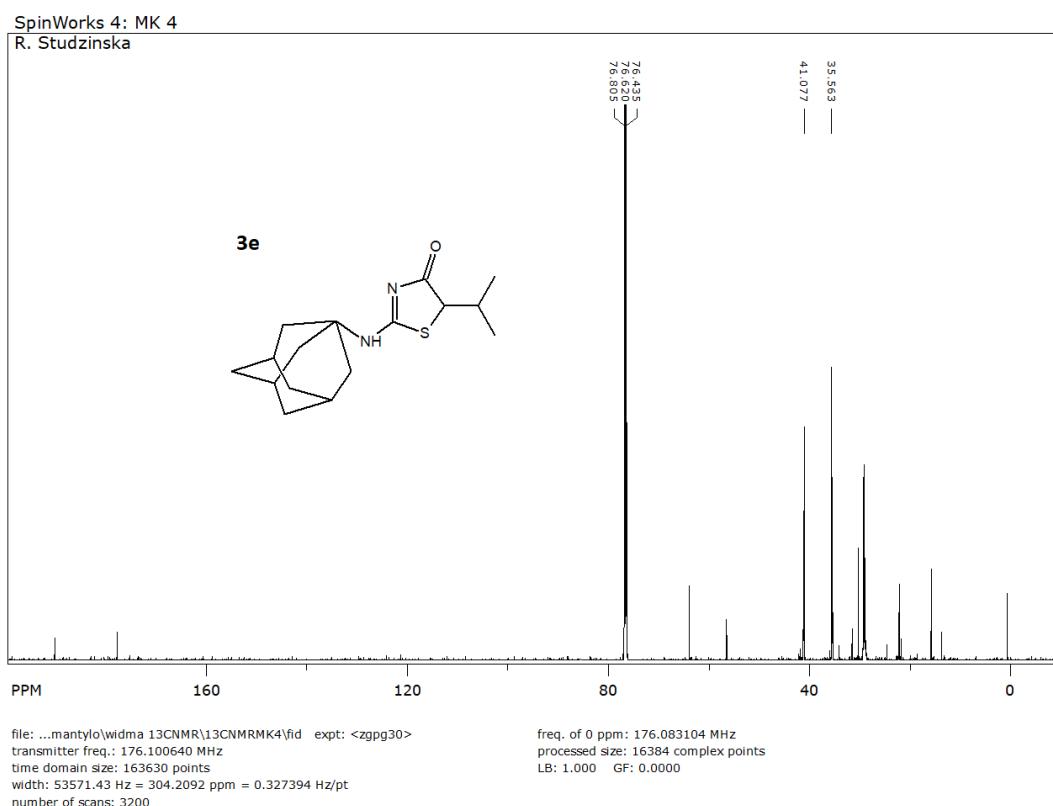
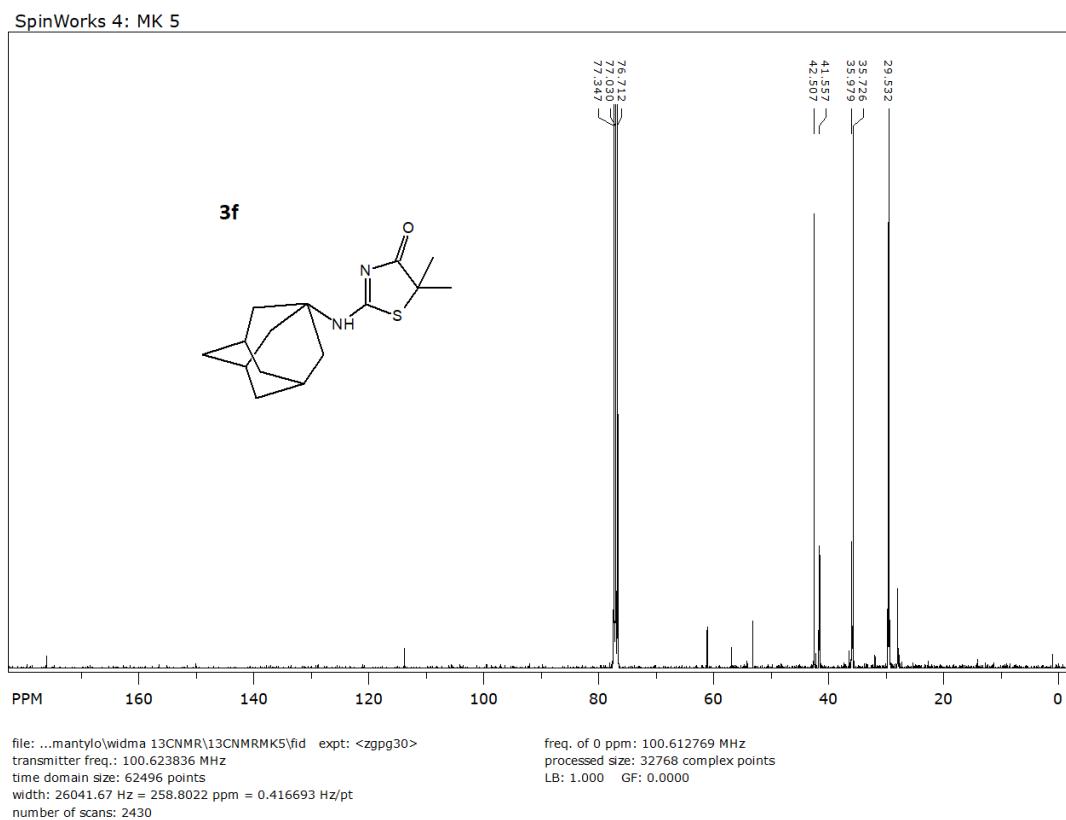
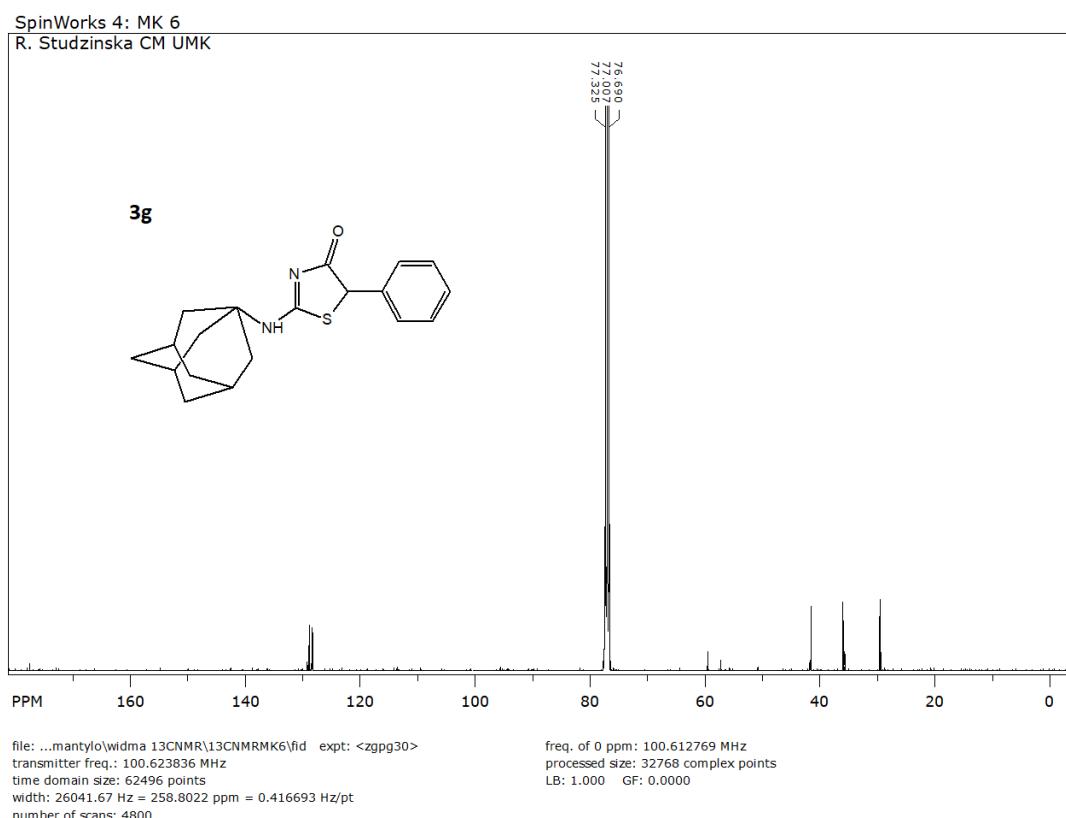
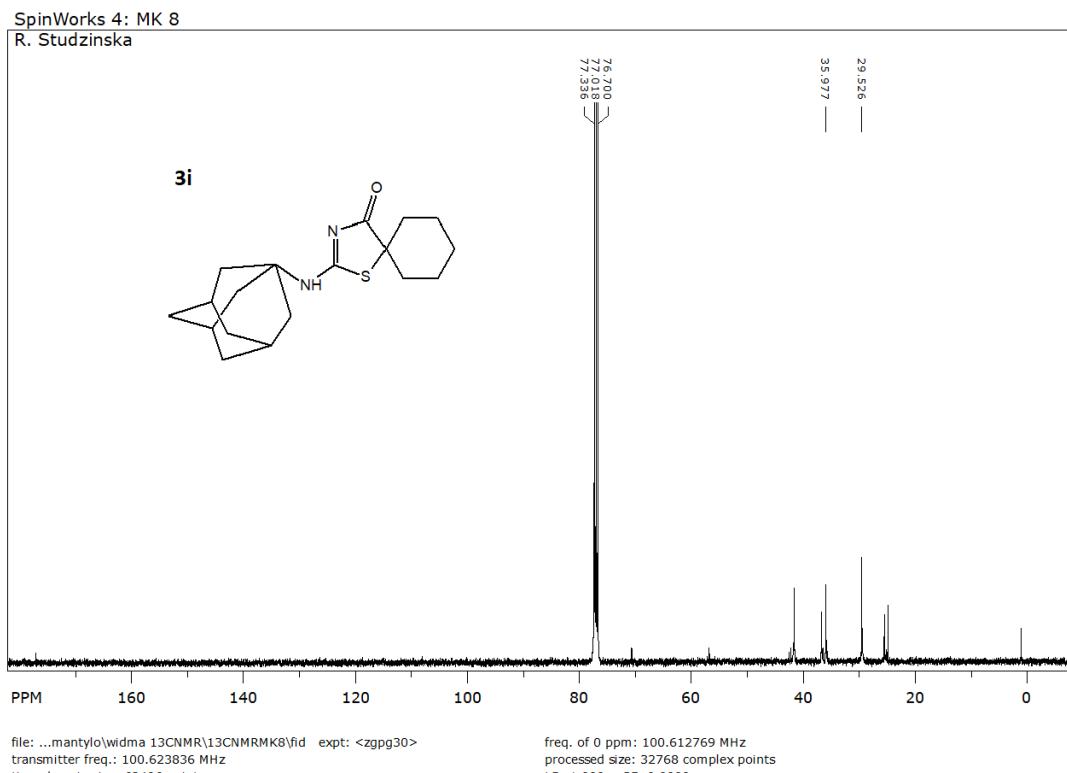
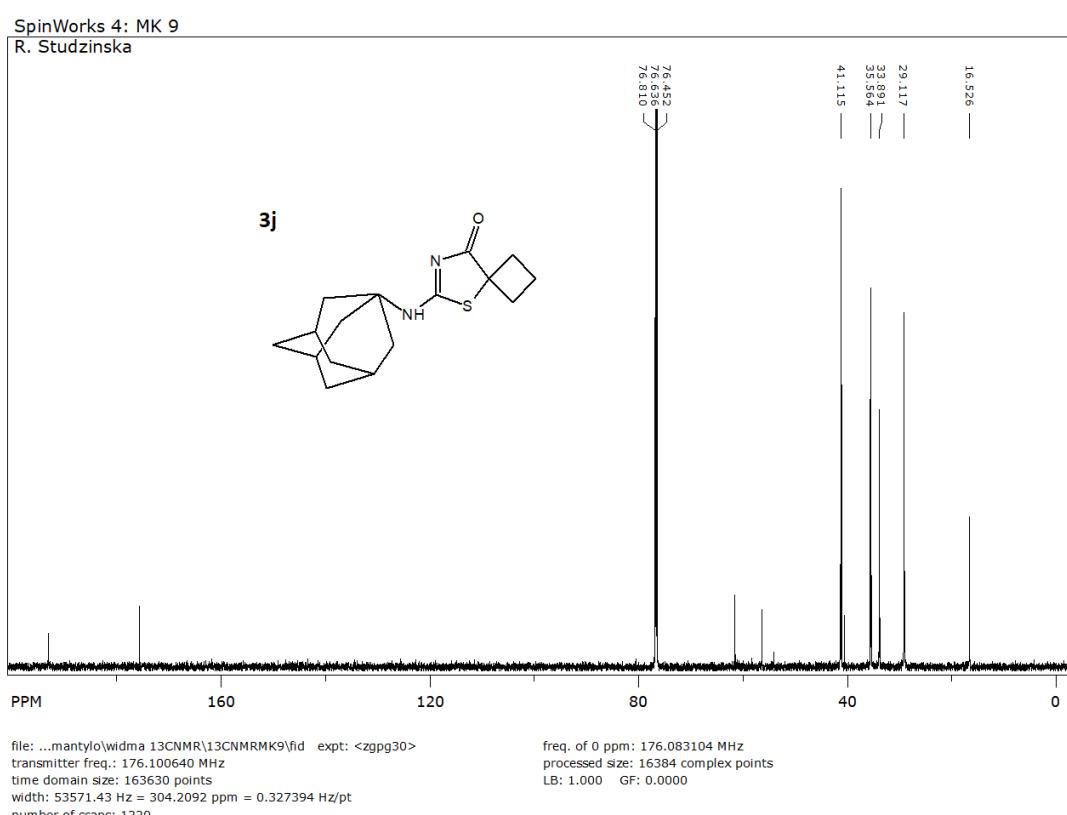


Figure S2A. ^{13}C NMR spectra of compound 3a.**Figure S2B.** ^{13}C NMR spectra of compound 3b.**Figure S2C.** ^{13}C NMR spectra of compound 3c.

**Figure S2D.** ^{13}C NMR spectra of compound 3d.**Figure S2E.** ^{13}C NMR spectra of compound 3e.

**Figure S2F.** ^{13}C NMR spectra of compound 3f.**Figure S2G.** ^{13}C NMR spectra of compound 3g.

**Figure S2H.** ^{13}C NMR spectra of compound 3i.**Figure S2I.** ^{13}C NMR spectra of compound 3j.Mass spectrum of compounds 3a–j

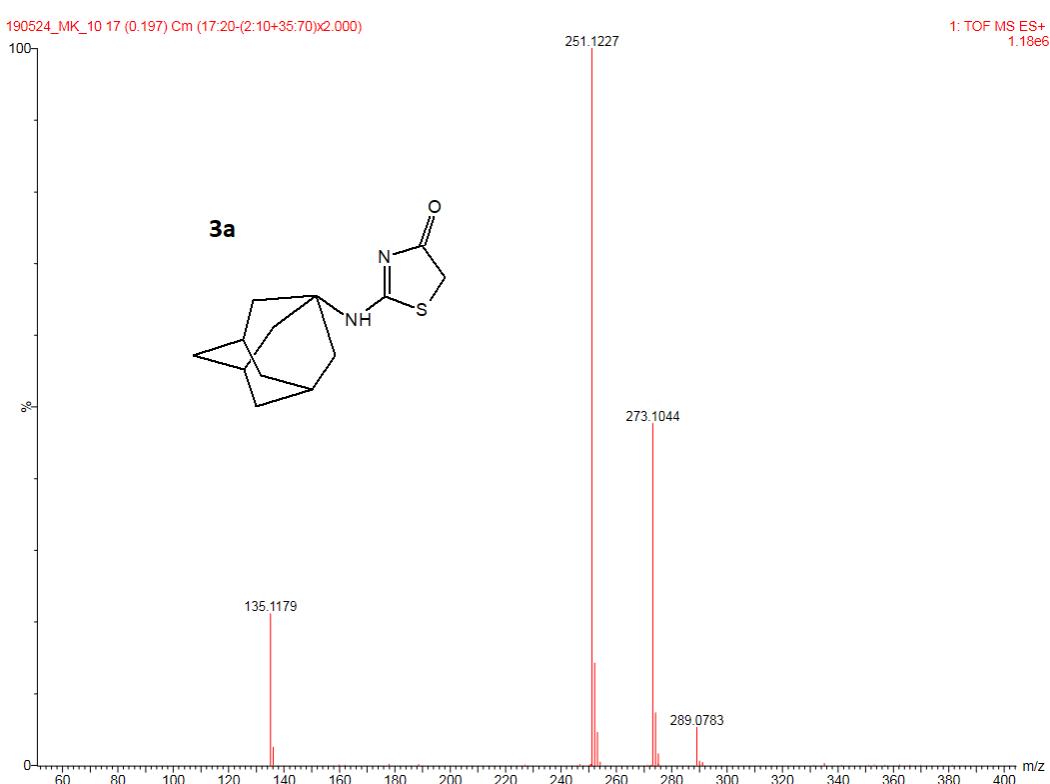


Figure S3A. Mass spectrum of compound **3a**.

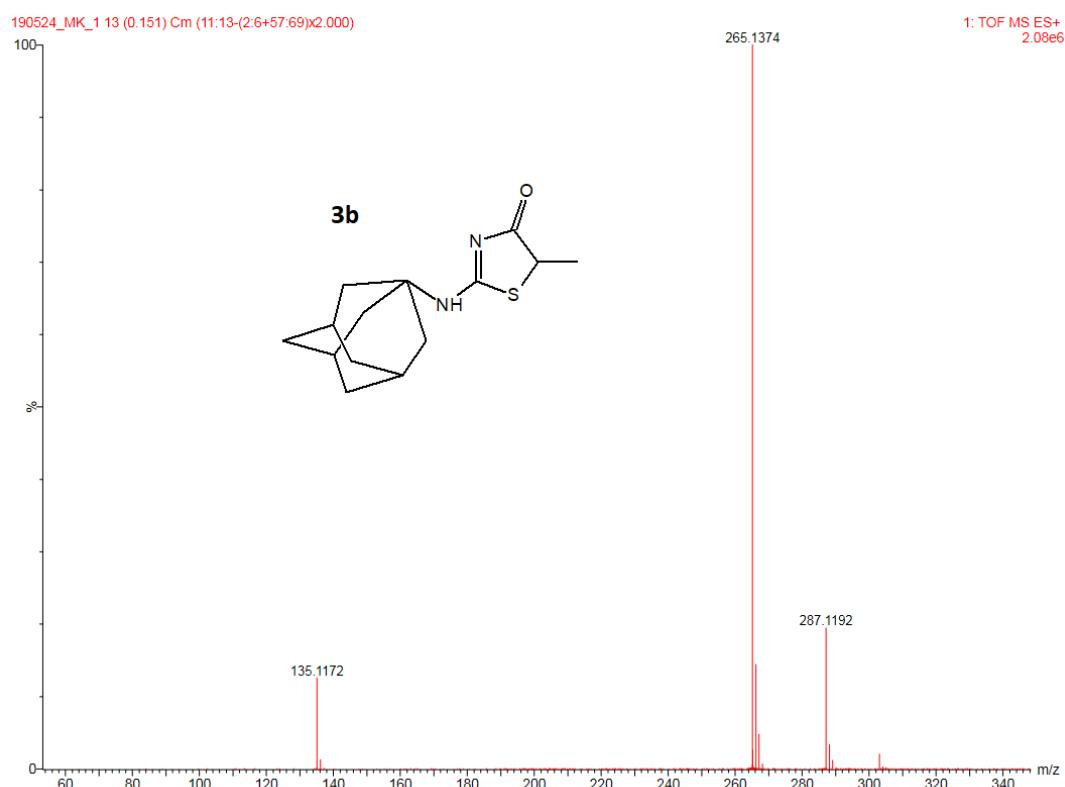


Figure S3B. Mass spectrum of compound **3b**.

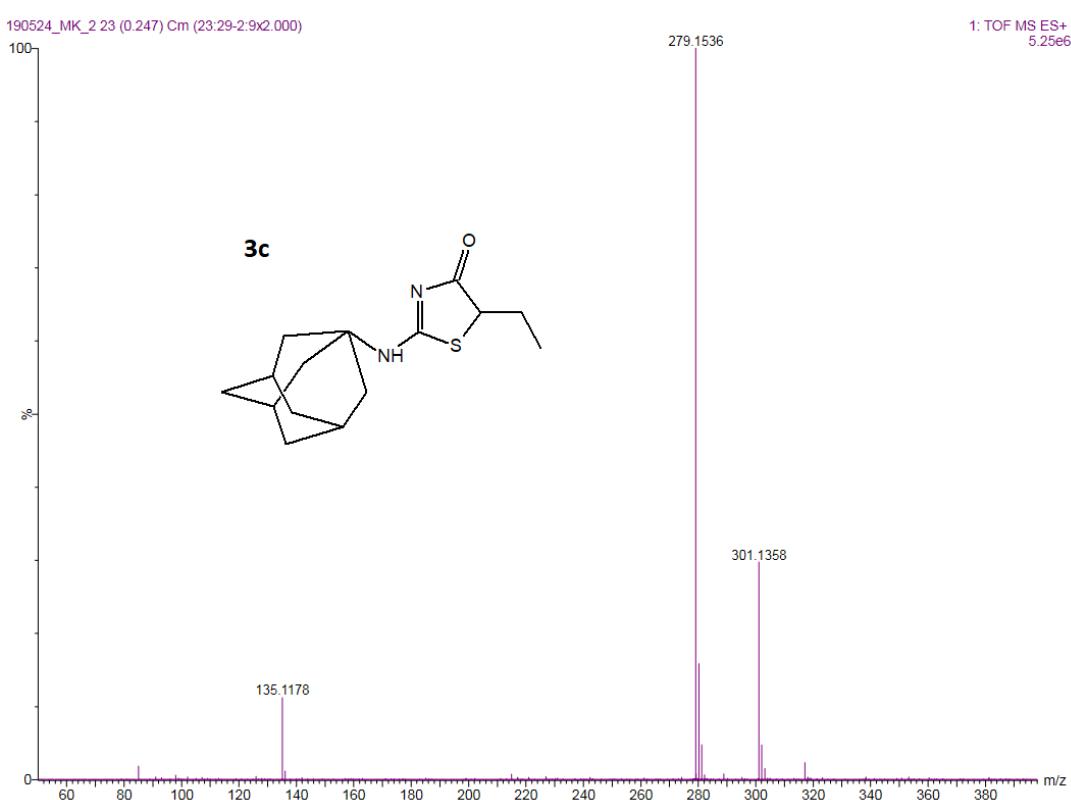


Figure S3C. Mass spectrum of compound **3c**.

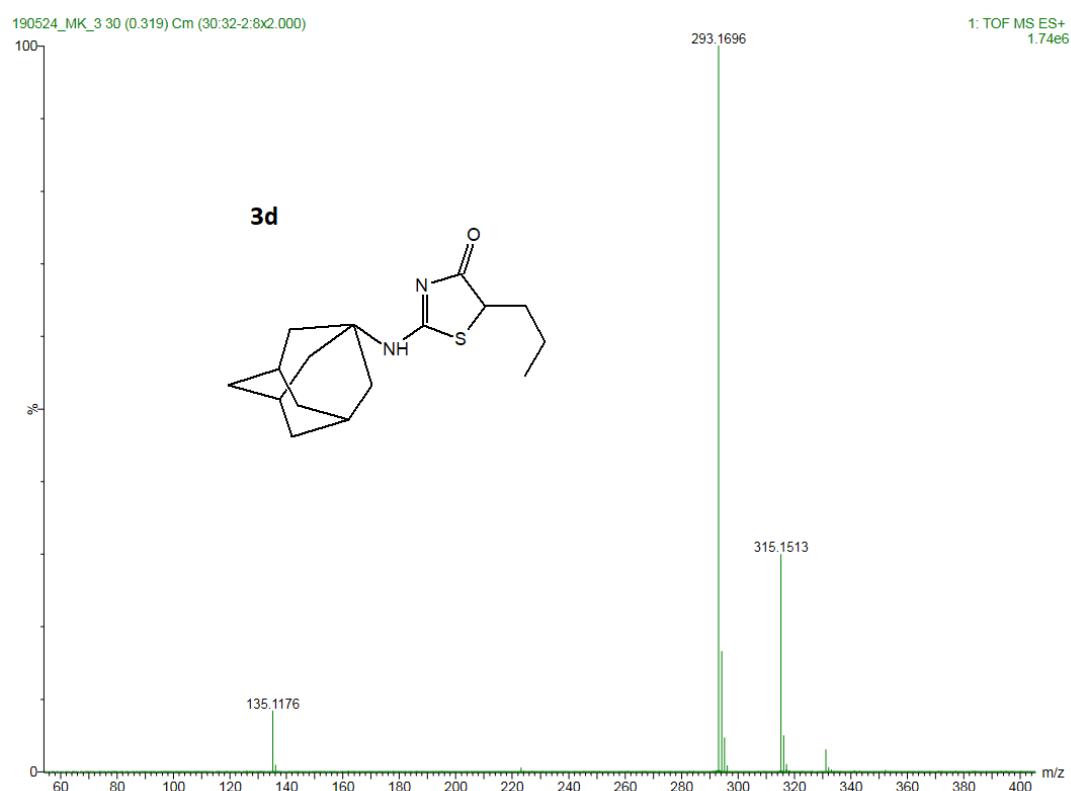


Figure S3D. Mass spectrum of compound **3d**.

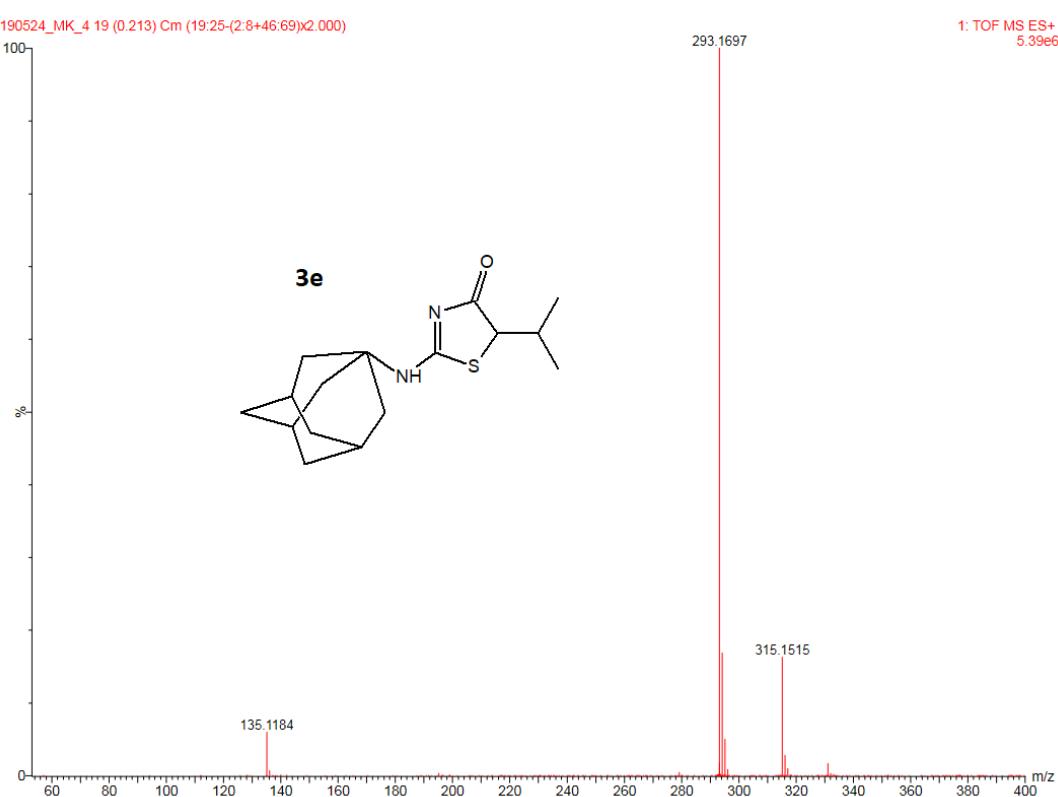


Figure S3E. Mass spectrum of compound 3e.

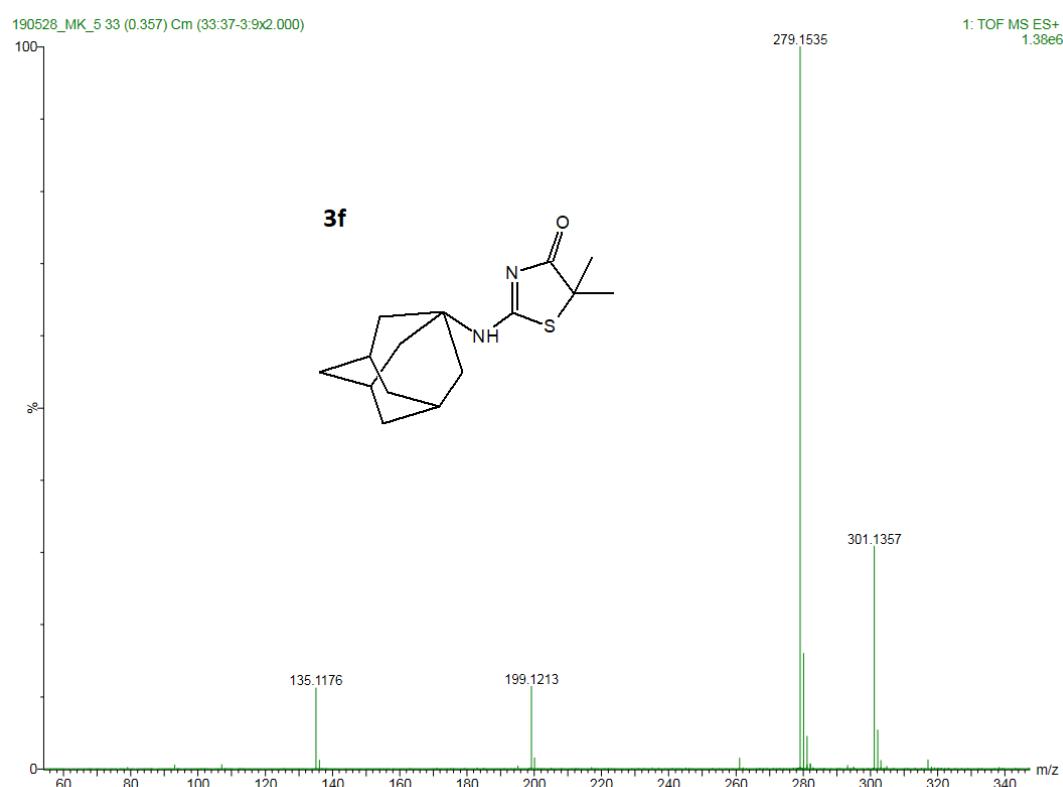


Figure S3F Mass spectrum of compound 3f.

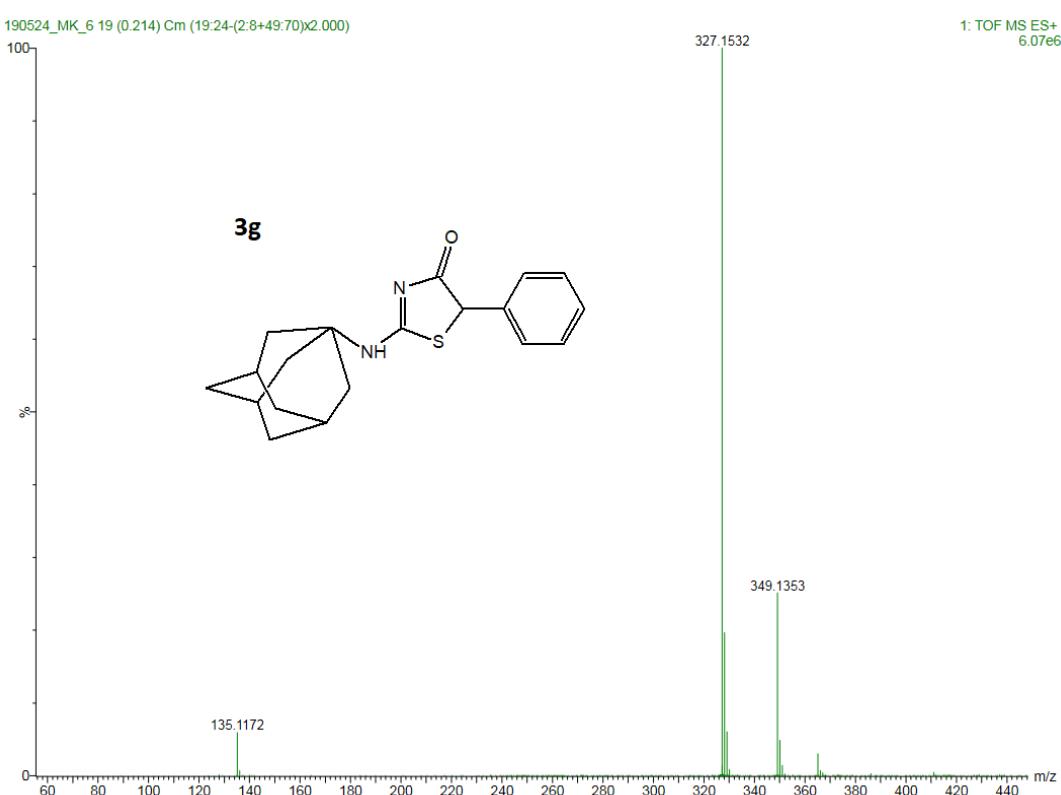


Figure S3G. Mass spectrum of compound **3g**.

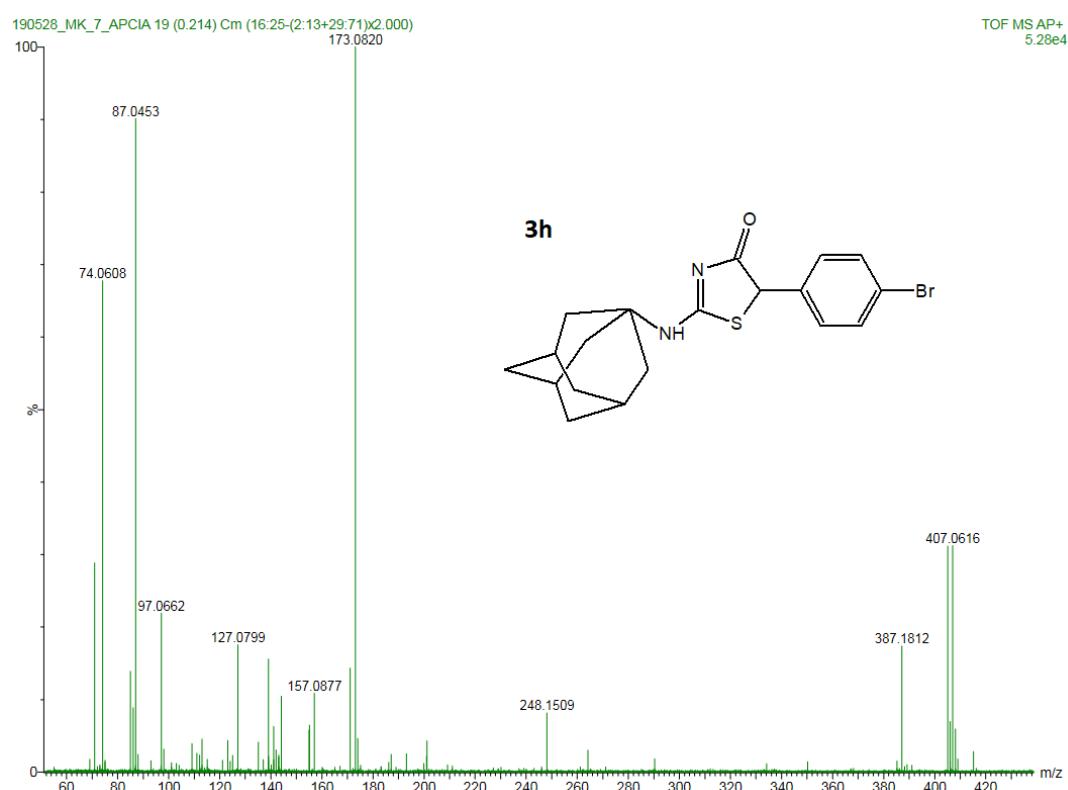


Figure S3H Mass spectrum of compound **3h**.

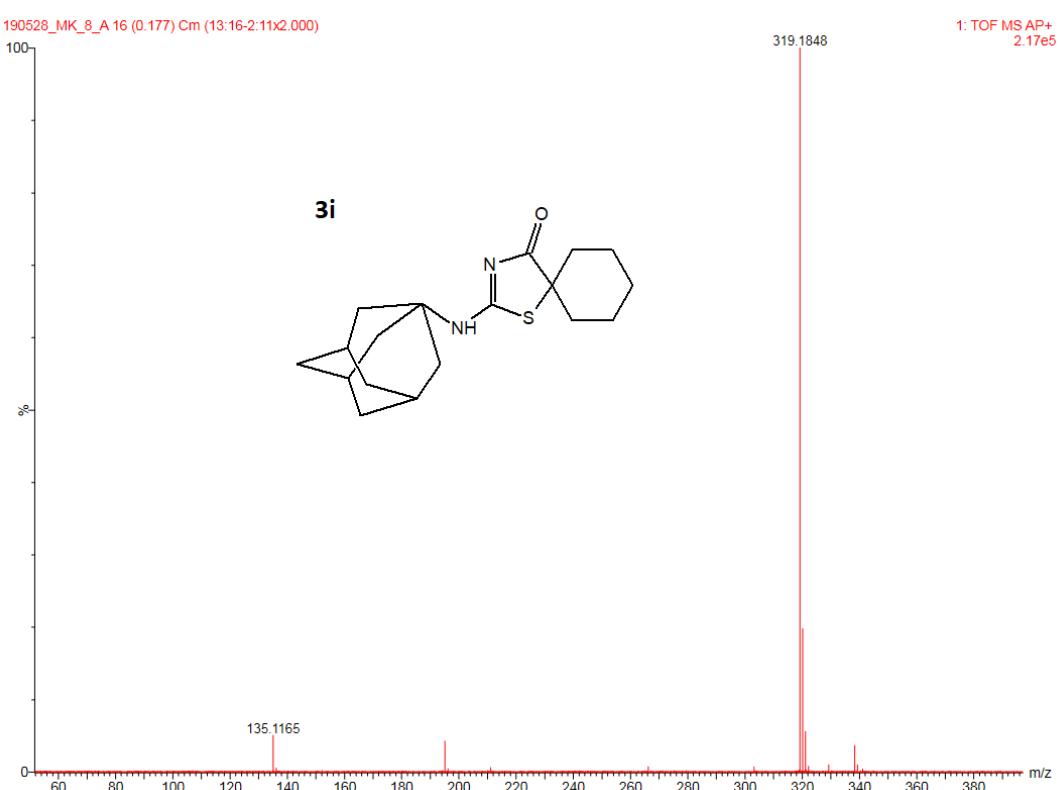


Figure S3I. Mass spectrum of compound 3i.

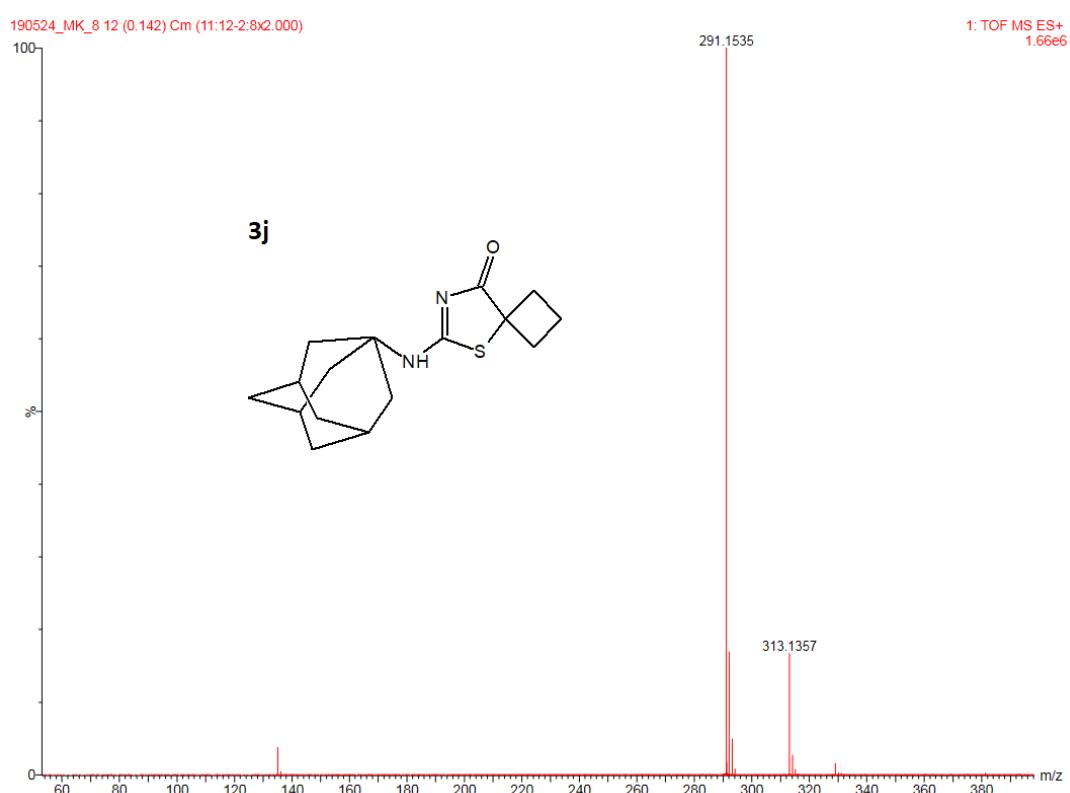


Figure S3J. Mass spectrum of compound 3j.