

Supplementary information

Synthesis of novel 2-(isopropylamino)thiazol-4(5*H*)-one derivatives and their inhibitory activity of 11 β -HSD1 and 11 β -HSD2 in aspect of carcinogenesis prevention.

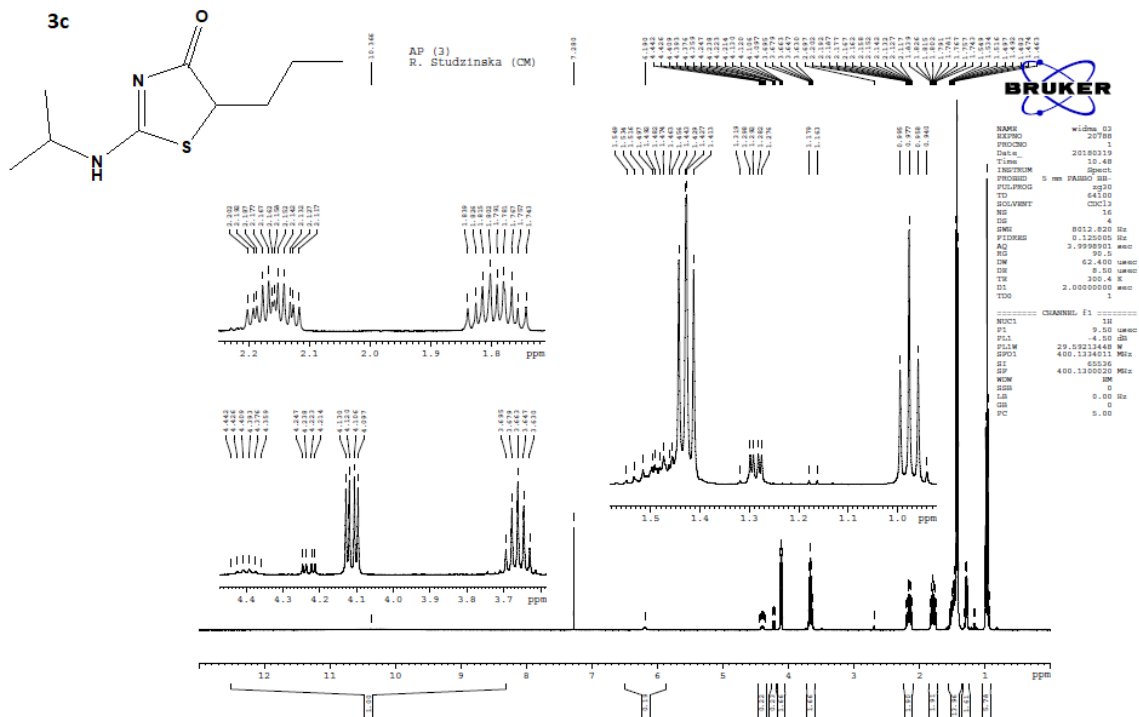
Daria Kupczyk ^{1,*,#}, Renata Studzińska ^{2,*,#}, Rafał Bilski ¹, Szymon Baumgart ², Renata Kołodziejska ¹ and Alina Woźniak¹

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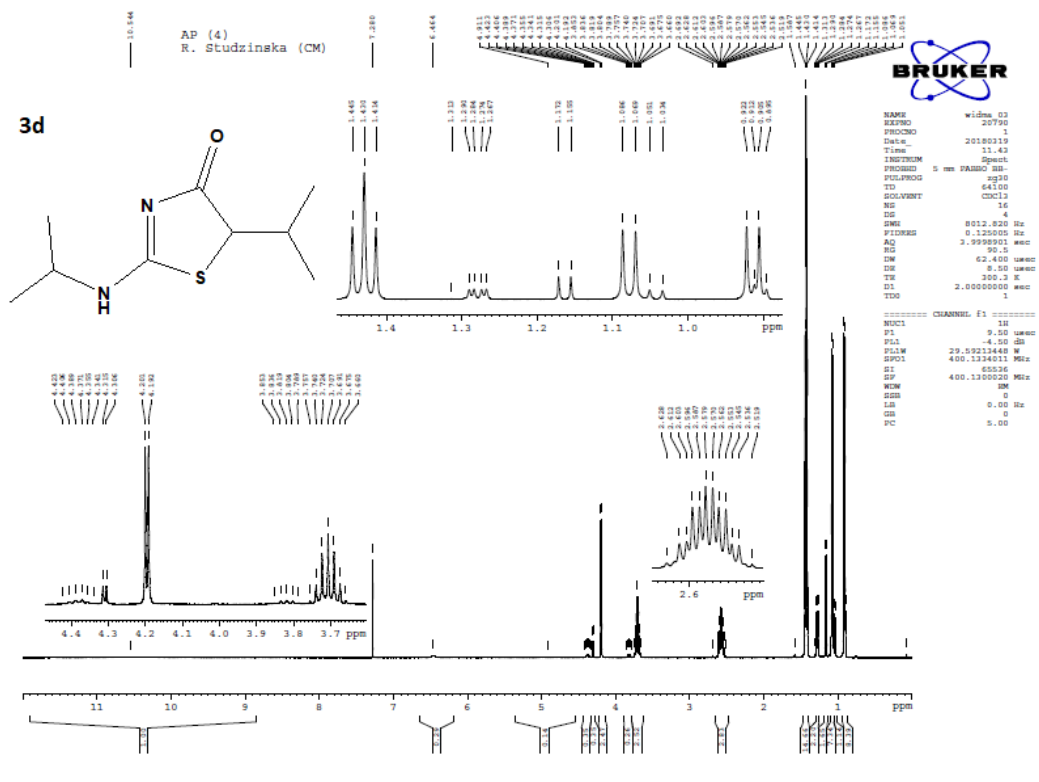
² Nicolaus Copernicus University in Toruń, Collegium Medicum in Bydgoszcz, Faculty of Pharmacy, Department of Organic Chemistry, Jurasza 2, 85–089 Bydgoszcz, Poland; rstud@cm.umk.pl

* Correspondence: dariak@cm.umk.pl (D.K.); rstud@cm.umk.pl (R.S.)

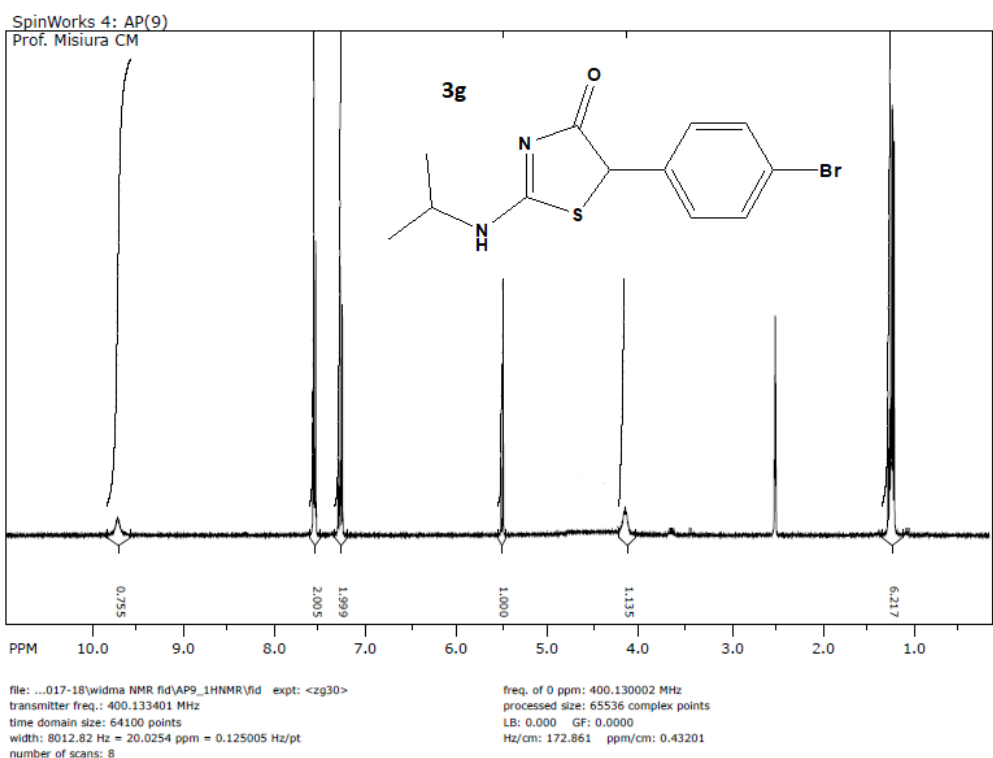
Renata Studzińska and Daria Kupczyk have equally contributed to the present paper and should be considered to be the first authors



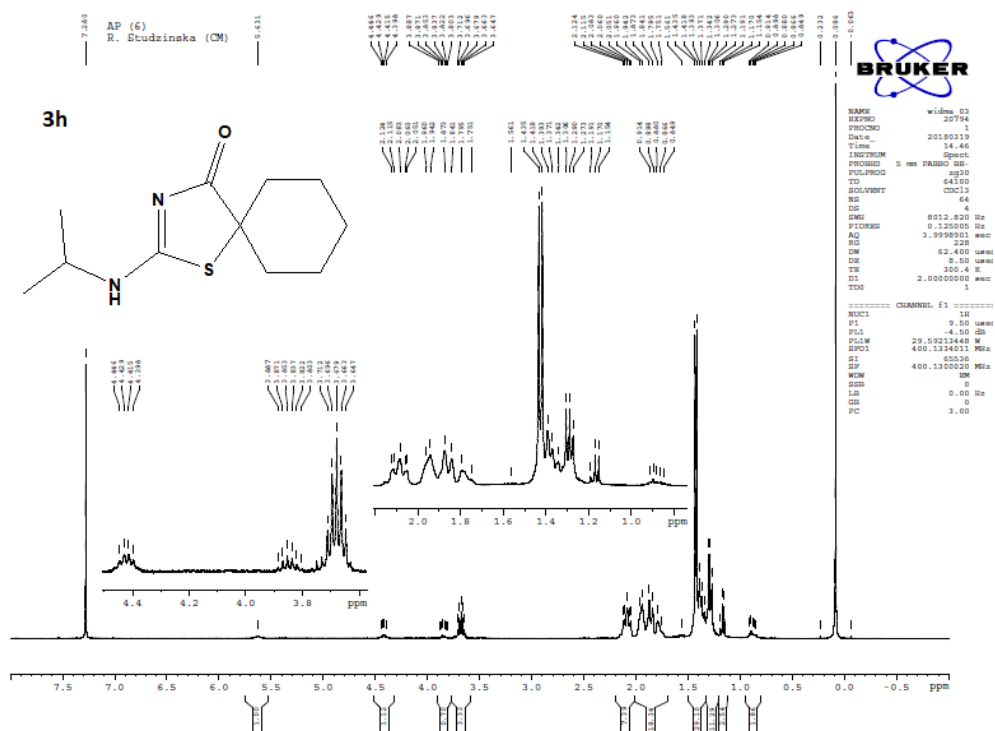
S1.3. ¹H NMR spectra of compound **3c**



S1.4. ¹H NMR spectra of compound **3d**

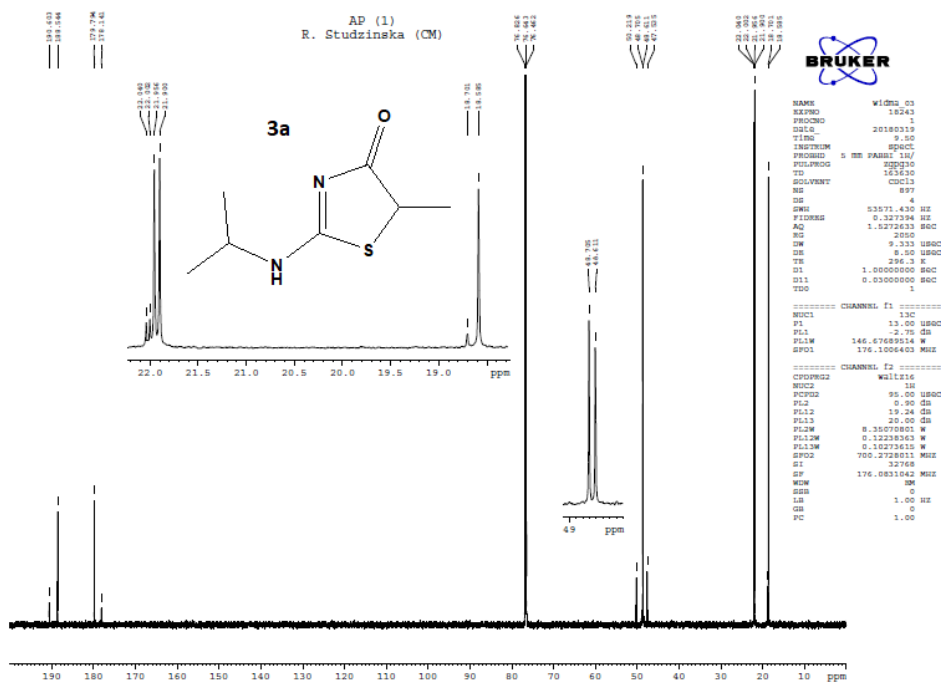


S1.7. ¹H NMR spectra of compound **3g**

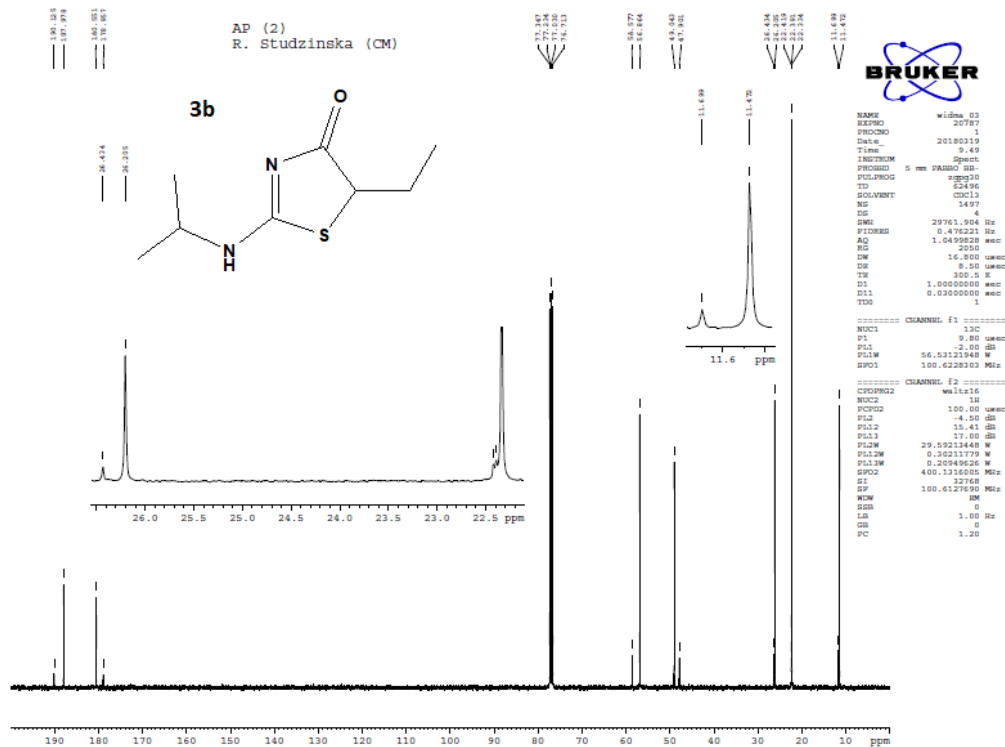


S1.8. ¹H NMR spectra of compound **3h**

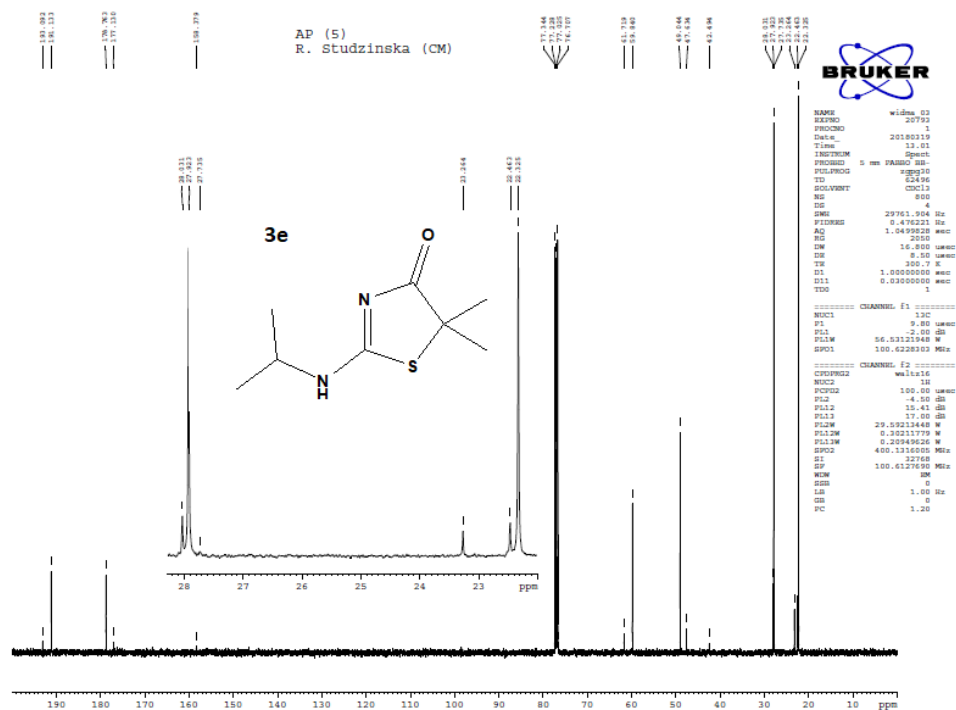
S2. ¹³C NMR spectra of compounds **3a** – **3i**



S2.1. ¹³C NMR spectra of compounds **3a**

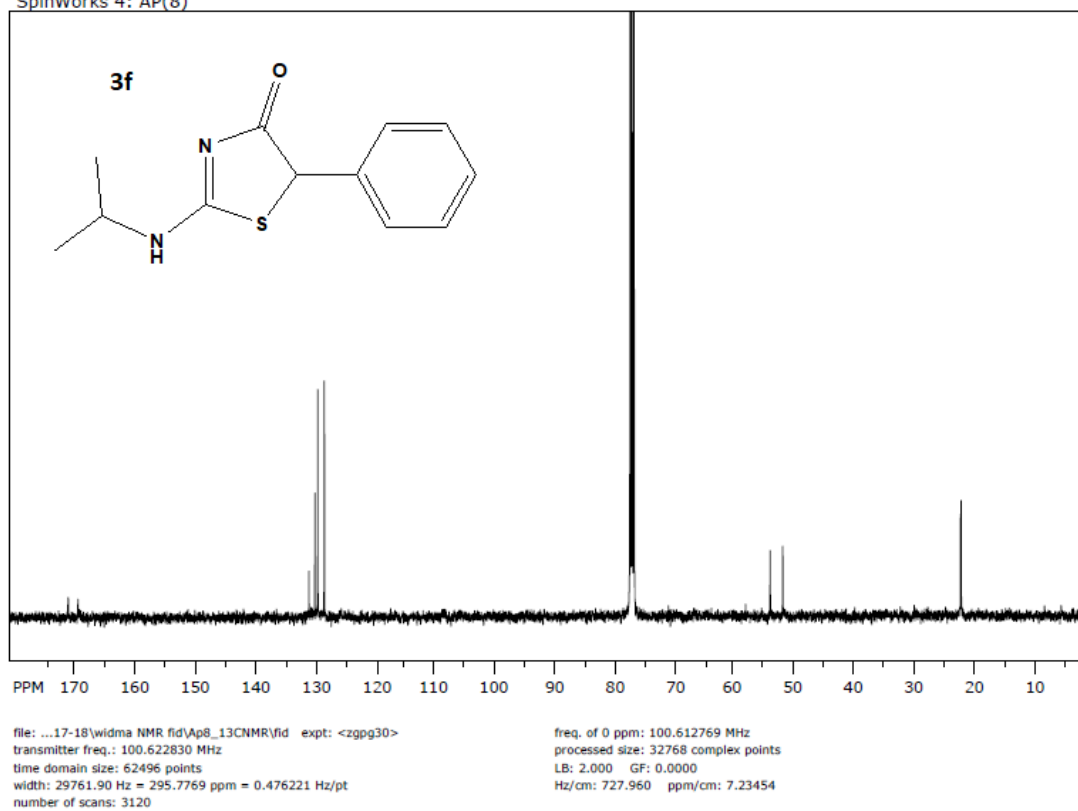


S2.2. ¹³C NMR spectra of compounds **3b**



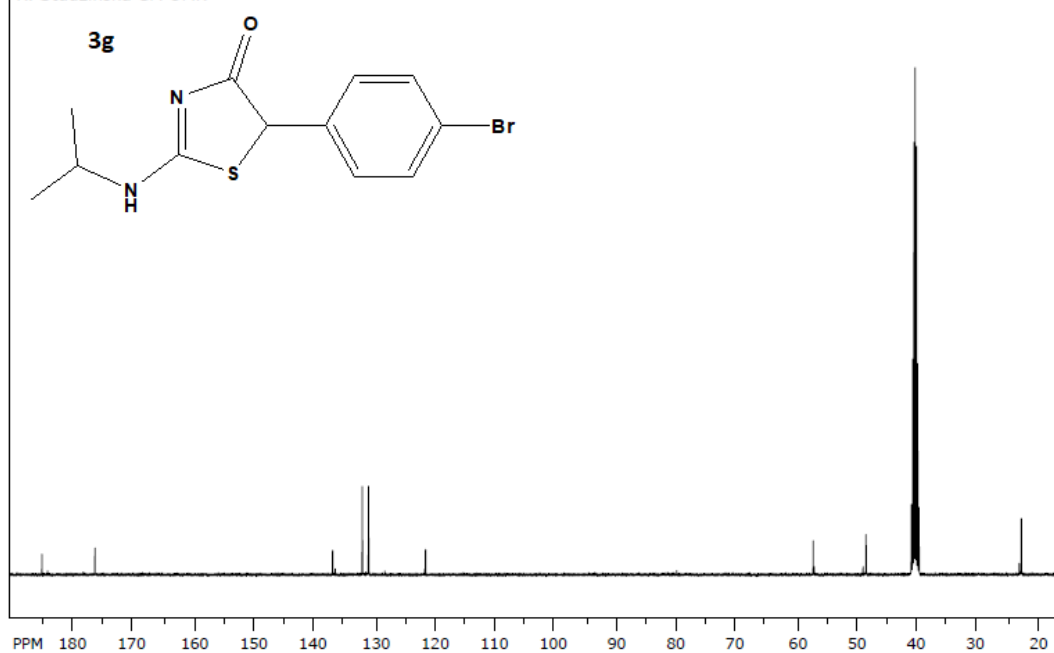
S2.5. ¹³C NMR spectra of compounds **3e**

SpinWorks 4: AP(8)



S2.6. ¹³C NMR spectra of compounds **3f**

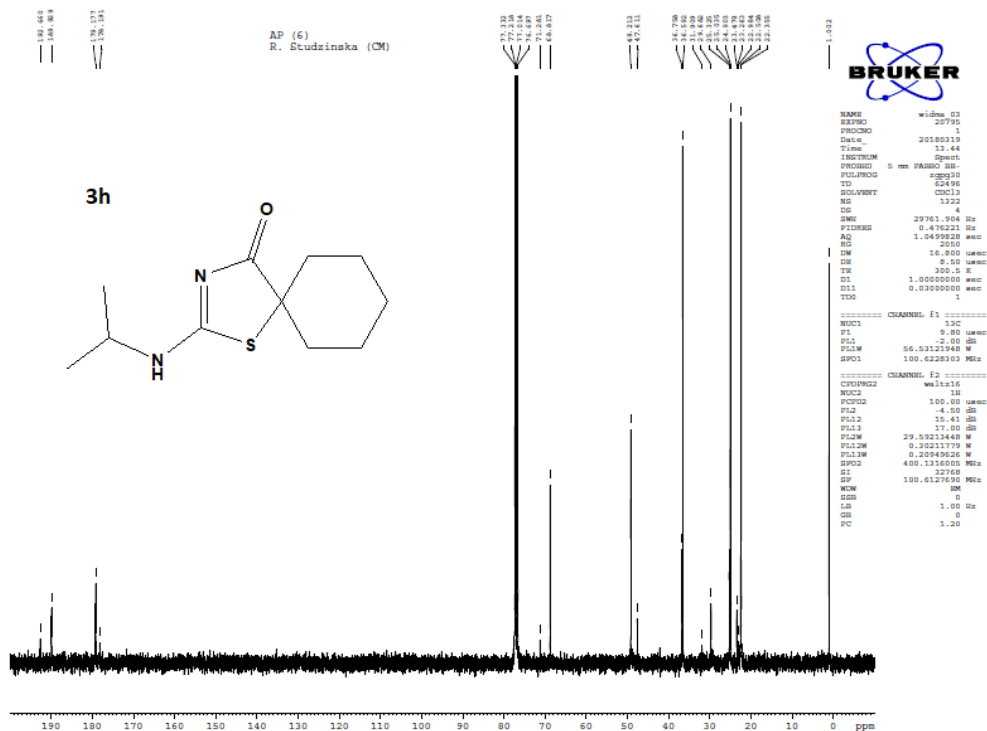
SpinWorks 4: AP(9)
R. Studzinska CM UMK

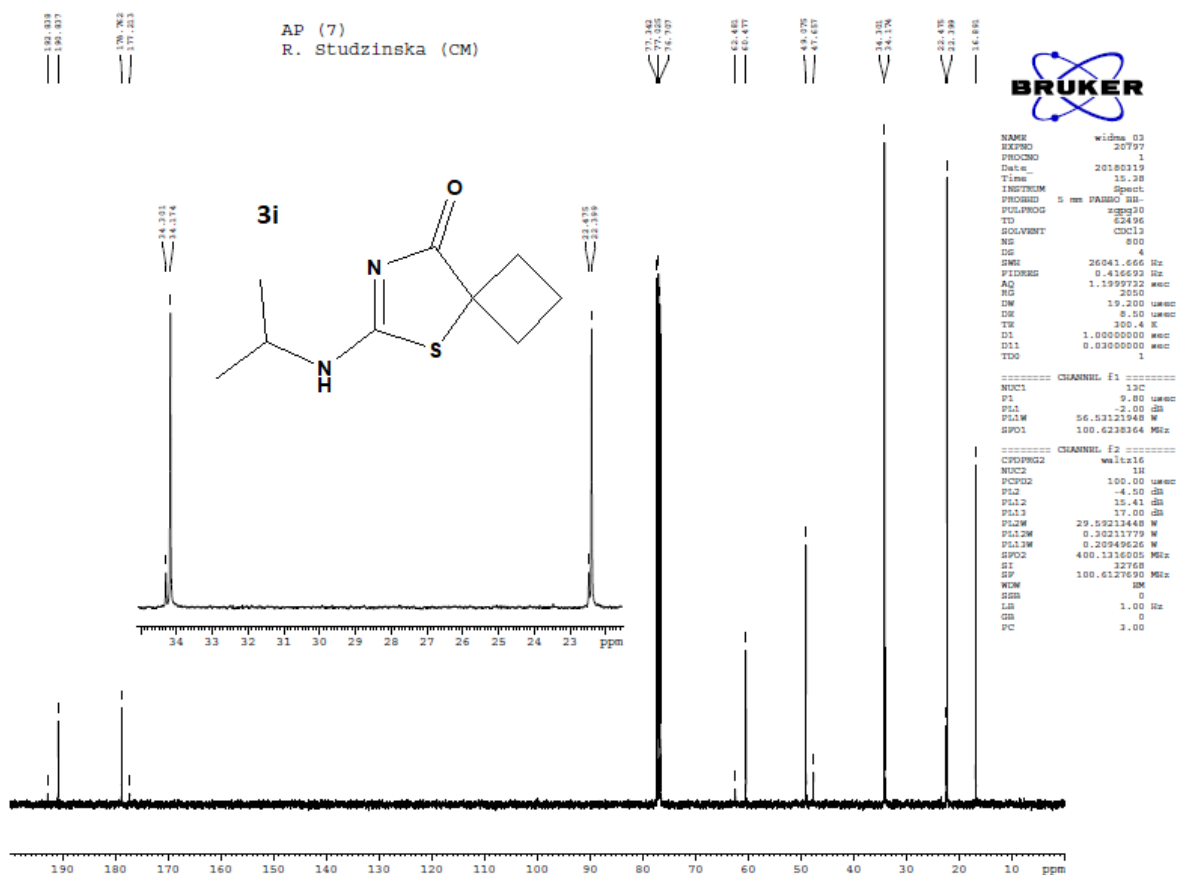


file: ...17-18\widma NMR fid\AP9_13CNMR\fid exp: <zpgg30>
transmitter freq.: 100.622830 MHz
time domain size: 62496 points
width: 29761.90 Hz = 295.7769 ppm = 0.476221 Hz/pt
number of scans: 1600

freq. of 0 ppm: 100.612769 MHz
processed size: 32768 complex points
LB: 1.000 GF: 0.0000
Hz/cm: 704.305 ppm/cm: 6.99945

S2.7. ¹³C NMR spectra of compounds **3g**





S2.9. ^{13}C NMR spectra of compounds **3i**

S3. HRMS spectra of compounds **3a – 3i**

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

62 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

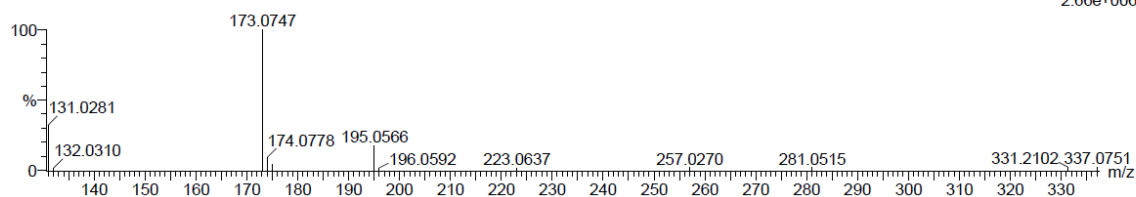
Elements Used:

C: 0-12 H: 0-20 N: 0-3 O: 0-2 S: 0-2

R.Studzinska

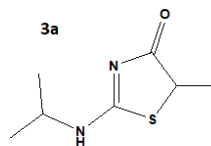
180515_AP_17 (0.194) Cm (7:8-16:29)

1: TOF MS ES+
2.66e+006



Minimum: -1.5
Maximum: 15.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
173.0747	173.0749	-0.2	-1.2	2.5	27.1	n/a	n/a	C7 H13 N2 O S



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S3.1. HRMS spectra of compounds **3a**

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

52 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

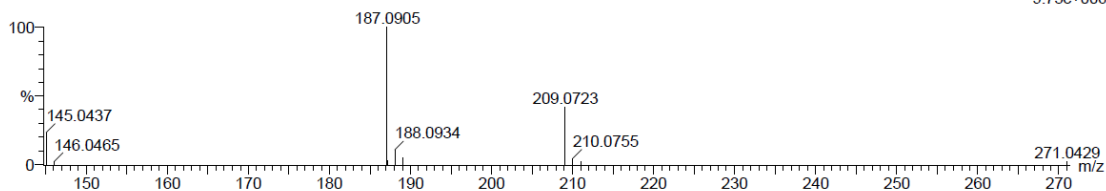
Elements Used:

C: 0-10 H: 0-20 N: 0-3 O: 0-2 S: 0-2

R.Studzinska

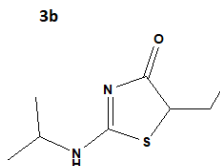
180515_AP_27 (0.194) Cm (7:9-18:29)

1: TOF MS ES+
9.75e+006



Minimum: -1.5
Maximum: 15.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
187.0905	187.0905	0.0	0.0	2.5	54.1	n/a	n/a	C8 H15 N2 O S



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S3.2. HRMS spectra of compounds **3b**

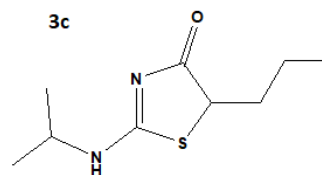
Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3



Monoisotopic Mass, Even Electron Ions

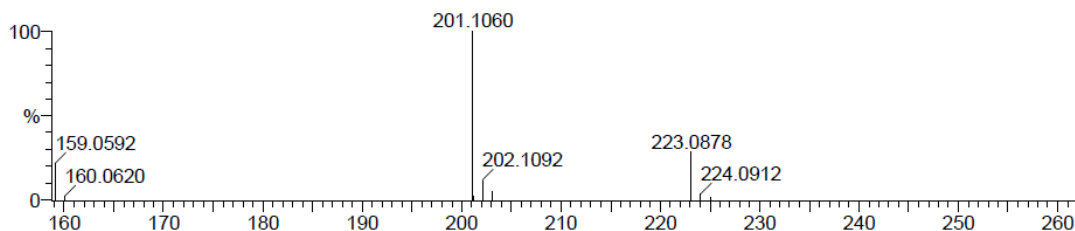
65 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-15 H: 0-20 N: 0-3 O: 0-2 S: 0-2

R.Studzinska

180515_AP_3 7 (0.194) Cm (6:9-15:30)



Minimum: -1.5
Maximum: 15.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
201.1060	201.1062	-0.2	-1.0	2.5	56.2	n/a	n/a	C9 H17 N2 O S

S3.3. HRMS spectra of compounds **3c**

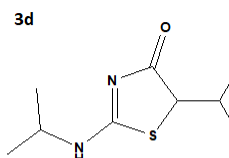
Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3



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Monoisotopic Mass, Even Electron Ions

65 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

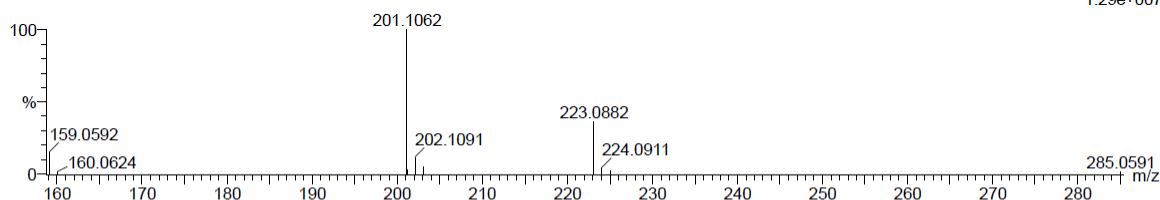
Elements Used:

C: 0-15 H: 0-20 N: 0-3 O: 0-2 S: 0-2

R.Studzinska

180515_AP_4 7 (0.194) Cm (6:9-15:30)

1: TOF MS ES+
1.29e+007



Minimum: -1.5
Maximum: 15.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
201.1062	201.1062	0.0	0.0	2.5	54.4	n/a	n/a	C9 H17 N2 O S

S3.4. HRMS spectra of compounds **3d**

Elemental Composition Report

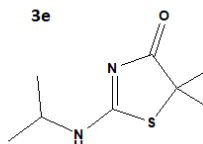
Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3



Monoisotopic Mass, Even Electron Ions

66 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

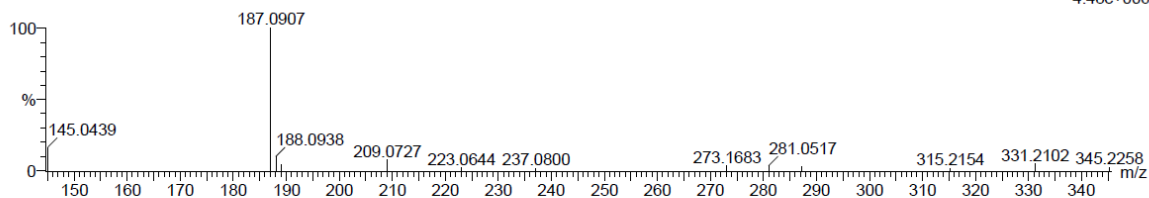
Elements Used:

C: 0-15 H: 0-20 N: 0-3 O: 0-2 S: 0-2

R.Studzinska

180515_AP_5 7 (0.194) Cm (7:8-(1:4+14:29))

1: TOF MS ES+
4.48e+006



Minimum: -1.5
Maximum: 15.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
187.0907	187.0905	0.2	1.1	2.5	30.7	n/a	n/a	C8 H15 N2 O S

S3.5. HRMS spectra of compounds **3e**

Elemental Composition Report

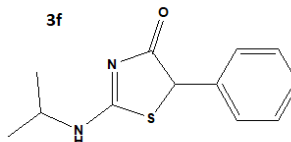
Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3



Monoisotopic Mass, Even Electron Ions

51 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

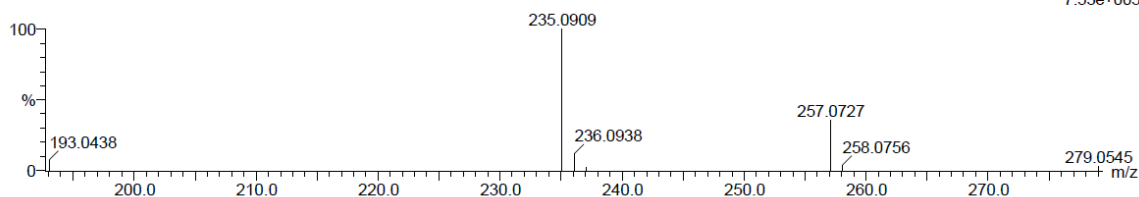
Elements Used:

C: 0-15 H: 0-20 N: 0-3 O: 0-2 S: 0-2

R.Studzinska

180515_AP_8 7 (0.194) Cm (6:9-(1:3+12:30))

1: TOF MS ES+
7.53e+005



Minimum: -1.5
Maximum: 15.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
235.0909	235.0905	0.4	1.7	6.5	34.2	n/a	n/a	C12 H15 N2 O S

S3.6. HRMS spectra of compounds **3f**

Elemental Composition Report

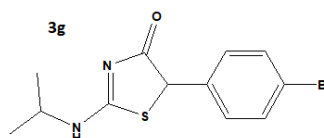
Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3



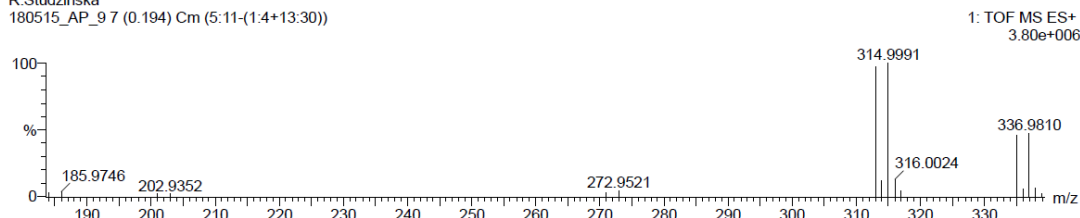
Monoisotopic Mass, Even Electron Ions

171 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-15 H: 0-20 N: 0-3 O: 0-2 S: 0-2 Br: 0-8

R.Studzinska
180515_AP_9 7 (0.194) Cm (5:11-(1:4+13:30))



Minimum: -1.5
Maximum: 15.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
313.0011	313.0010	0.1	0.3	6.5	28.9	n/a	n/a	C12 H14 N2 O S Br

S3.7. HRMS spectra of compounds 3g

Elemental Composition Report

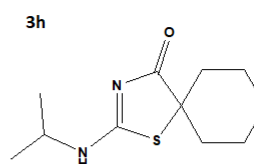
Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3



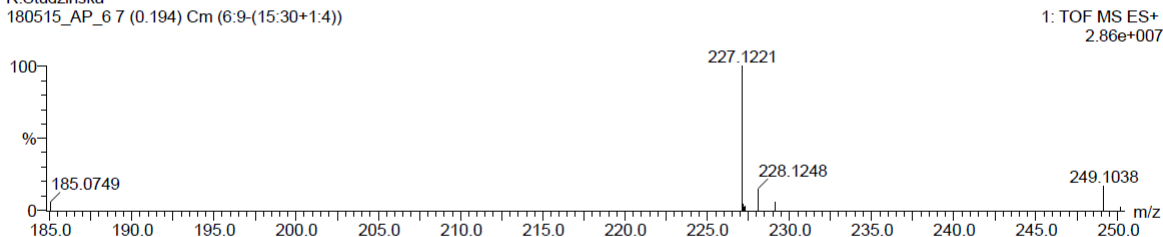
Monoisotopic Mass, Even Electron Ions

58 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-15 H: 0-20 N: 0-3 O: 0-2 S: 0-2

R.Studzinska
180515_AP_6 7 (0.194) Cm (6:9-(15:30+1:4))



Minimum: -1.5
Maximum: 15.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
227.1221	227.1218	0.3	1.3	3.5	138.6	n/a	n/a	C11 H19 N2 O S

S3.8. HRMS spectra of compounds 3h

Elemental Composition Report

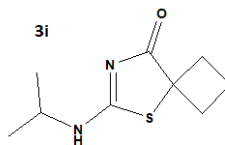
Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3



Monoisotopic Mass, Even Electron Ions

65 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

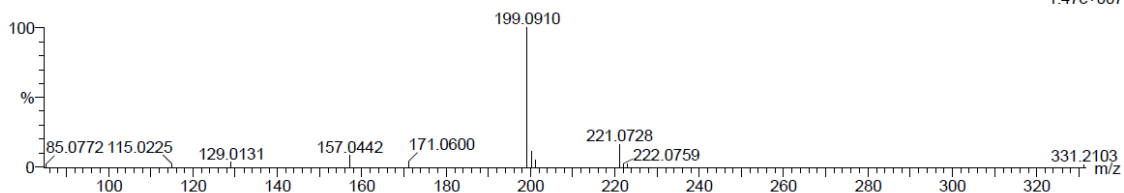
Elements Used:

C: 0-15 H: 0-20 N: 0-3 O: 0-2 S: 0-2

R.Studzinska

180515_AP_7 7 (0.194) Cm (6:9-(1:3+16:30))

1: TOF MS ES+
1.47e+007



Minimum:

Maximum: 15.0 10.0 -1.5

Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
199.0910	199.0905	0.5	2.5	3.5	56.7	n/a	n/a	C9 H15 N2 O S

S3.9. HRMS spectra of compounds 3i