

Supplementary Material

New aspects of the formation of 2-substituted thiazolidine-4-carboxylic acids and their thiohydantoin derivatives

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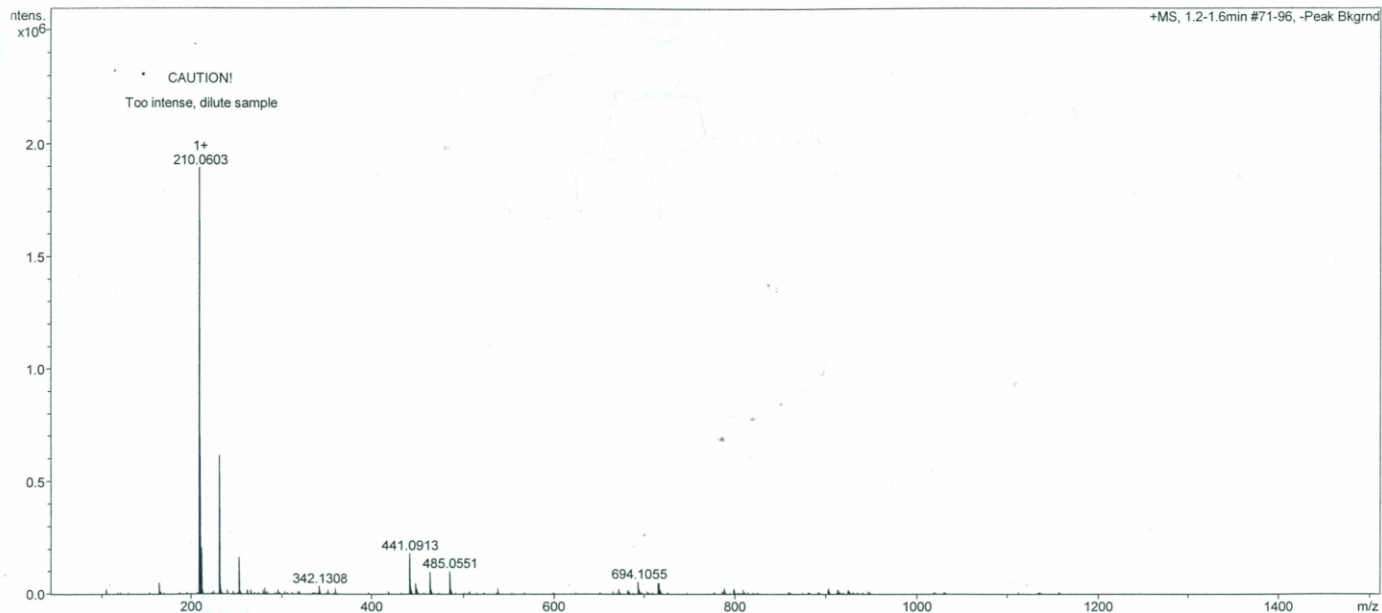
Compound 10c & 11c

School of Chemistry Mass Spectrometry Service

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 Method 3a_AccMass_Loop_Positive.m
 Instrument maXis impact

Source Type ESI
 Ion Polarity Positive

Submitter Elghareeb Elboray
 Supervisor Ron Grigg
 Acquisition Date 05/08/2013 18:53:53
 Scan Begin 50 m/z
 Scan End 1500 m/z



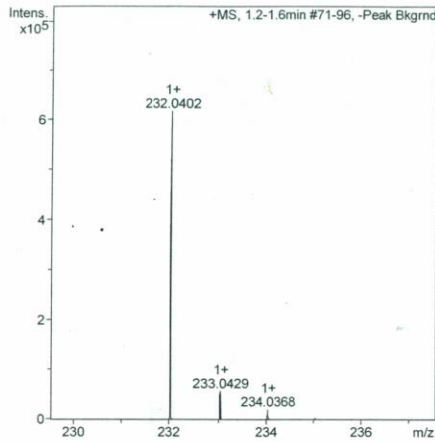
Bruker Compass DataAnalysis 4.1

Analysis Name

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05/08/2013 18:57:05

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Confirm/Find Formula Results

The section below shows the results of formula calculation. If an expected formula was provided and found these are the results that are listed. If no formula was provided or no matches were found the system has attempted to determine the formula constrained by the parameters listed to the left

Concentration too high. Dilute sample!

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
232.040196	C10H11NNaO2S	1+	232.040270	-0.1	-0.3	17.8	100.00	C10 H11 N O2 S	M+Na
254.022041	C10H10NNa2O2S	1+	254.022215	0.2	0.7	12.4	100.00		M+Na2-H
419.109054	C20H23N2O4S2	1+	419.109376	-0.3	-0.8	18.2	100.00		2M+H
441.091256	C20H22N2NaO4S2	1+	441.091320	0.1	0.1	11.6	100.00		2M+Na

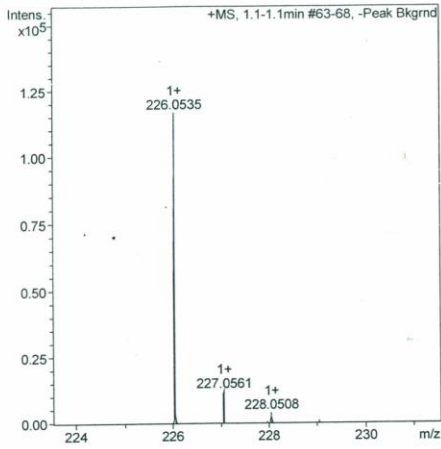
Smart Formula Parameter	Value
Expected Formula	C10H11NO2S
Adducts Considered	;M+H;;M+NH4;;M+Na;;M+K;;M+Na2-H;;2M+H;;2M+Na;

Smart Formula Search Parameters
CHNO and adducts considered implicitly

Formula Search Minimum	S 2
Formula Search Maximum	

Algorithm Parameters	
Tolerance	4 ppm
Match to Isotope Pattern(mSigma)	40
Electron Configuration	even
Estimate No of Carbons	yes
Filter by H/C Ratio	0< H/C < 3
Number of Double Bonds & Rings	0< rings&DB < 80

Compound 10d & 11d



Confirm/Find Formula Results

The section below shows the results of formula calculation. If an expected formula was provided and found these are the results that are listed. If no formula was provided or no matches were found the system has attempted to determine the formula constrained by the parameters listed to the left

Cmpd 1, 1.1 min

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
226.053467	C10H12NO3S	1+	226.053241	-0.2	-1.0	13.6	100.00	C10 H11 N O3 S	M+H
248.034899	C10H11NNaO3S	1+	248.035185	-0.3	-1.2	29.3	100.00		M+Na
270.016638	C10H10NNa2O3S	1+	270.017129	-0.5	-1.8	31.1	100.00		M+Na2-H

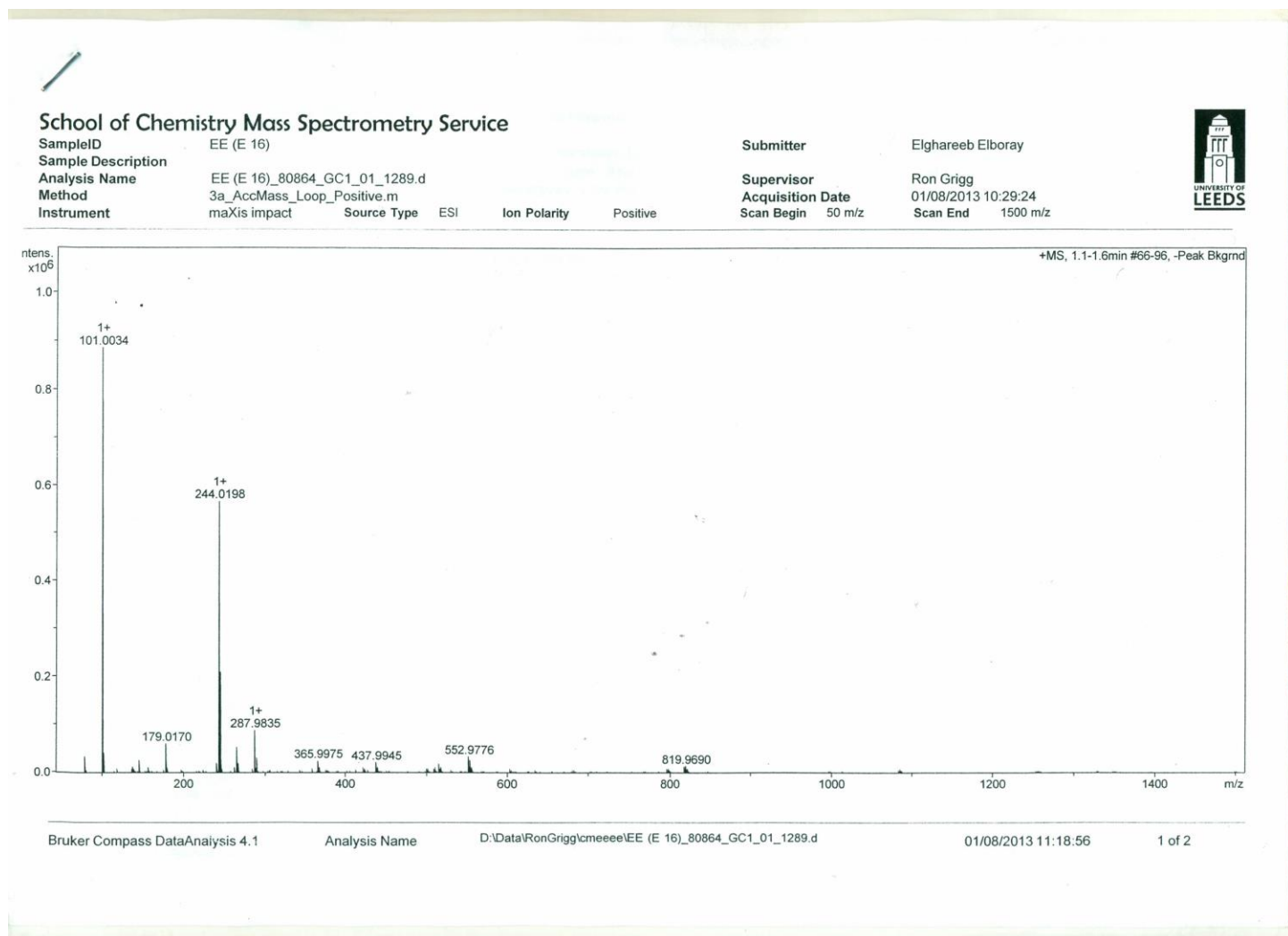
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 Expected Formula C10H11NO3S
 Adducts Considered ;M+H;;M+NH4;;M+Na;;M+K;;M+Na
 2-H;;2M+H;;2M+Na;

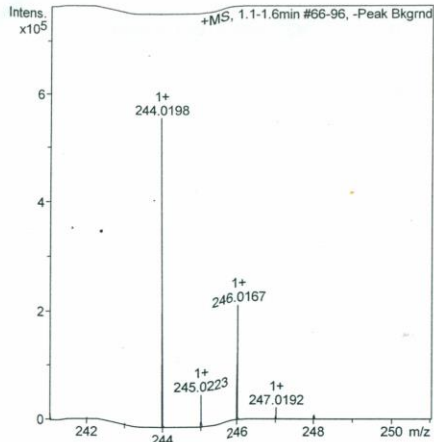
Smart Formula Search Parameters
 CHNO and adducts considered implicitly

Formula Search Minimum S 2
 Formula Search Maximum

Algorithm Parameters
 Tolerance 4 ppm
 Match to Isotope Pattern(mSigma) 40
 Electron Configuration even
 Estimate No of Carbons yes
 Filter by H/C Ratio 0< H/C < 3
 Number of Double Bonds & Rings 0< rings&DB < 80

Compound 10f & 11f





Confirm/Find Formula Results

The section below shows the results of formula calculation. If an expected formula was provided and found these are the results that are listed. If no formula was provided or no matches were found the system has attempted to determine the formula constrained by the parameters listed to the left

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
244.019803	C10H11ClNO2S	1+	244.019354	-0.4	-1.8	8.3	100.00	C10 H10 Cl N O2 S	M+H
266.001261	C10H10ClNNaO2S	1+	266.001298	-0.0	-0.1	6.8	100.00		M+Na
287.983475	C10H9ClNNa2O2S	1+	287.983242	-0.2	-0.8	15.5	100.00		M+Na2-H
509.013514	C20H20Cl2N2NaO4S2	1+	509.013375	-0.1	-0.3	23.2	100.00		2M+Na

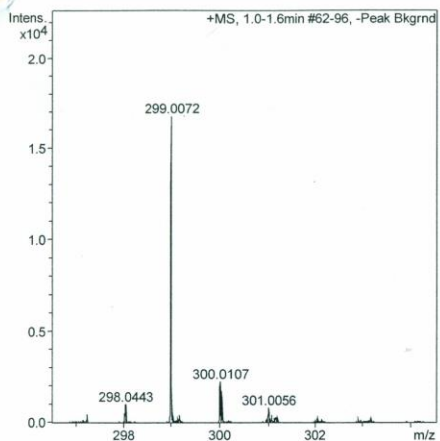
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 Expected Formula C10H10ClNO2S
 Adducts Considered ;M+H;;M+NH4;;M+Na;;M+K;;M+Na
 2-H;;2M+H;;2M+Na;

Smart Formula Search Parameters
 CHNO and adducts considered
 implicitly

Formula Search Minimum Cl 2 S 2
 Formula Search Maximum

Algorithm Parameters 4 ppm
 Tolerance 40
 Match to Isotope Pattern(mSigma) even
 Electron Configuration yes
 Estimate No of Carbons 0 < H/C < 3
 Filter by H/C Ratio 0 < rings&DB < 80
 Number of Double Bonds & Rings

Compound 10h



Confirm/Find Formula Results

The section below shows the results of formula calculation. If an expected formula was provided and found these are the results that are listed. If no formula was provided or no matches were found the system has attempted to determine the formula constrained by the parameters listed to the left

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
255.042980	C10H11N2O4S	1+	255.043404	0.4	1.7	32.7	100.00	C10 H10 N2 O4 S	M+H
299.007241	C10H9N2Na2O4S	1+	299.007293	-0.1	-0.2	7.9	100.00		M+Na2-H

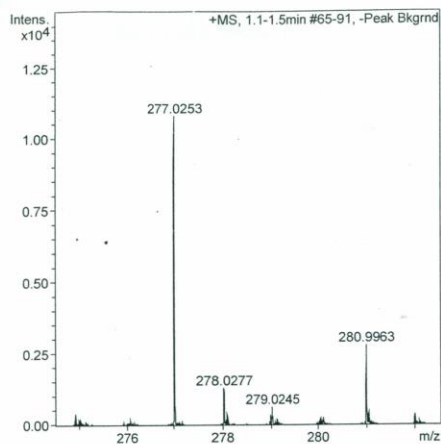
Smart Formula Parameter	Value
Expected Formula	C10H10N2O4S
Adducts Considered	;M+H ₂ ;M+NH ₄ ⁺ ;M+Na ₂ ⁺ ;M+K ₂ ⁺ ;M+Na ₂ H ₂ ⁺ ;2M+H ₂ ⁺ ;2M+Na ₂ ⁺

Smart Formula Search Parameters
CHNO and adducts considered implicitly

Formula Search Minimum	
Formula Search Maximum	S 2

Algorithm Parameters	
Tolerance	4 ppm
Match to Isotope Pattern(mSigma)	40
Electron Configuration	even
Estimate No of Carbons	yes
Filter by H/C Ratio	0 < H/C < 3
Number of Double Bonds & Rings	0 < rings&DB < 80

Compound 12



Confirm/Find Formula Results

The section below shows the results of formula calculation. If an expected formula was provided and found these are the results that are listed. If no formula was provided or no matches were found the system has attempted to determine the formula constrained by the parameters listed to the left

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
255.043122	C10H11N2O4S	1+	255.043404	0.3	1.1	30.8	100.00	C10 H10 N2 O4 S	M+H
277.025302	C10H10N2NaO4S	1+	277.025349	-0.0	-0.2	4.7	100.00		M+Na
299.007874	C10H9N2Na2O4S	1+	299.007293	-0.6	-1.9	30.6	100.00		M+Na2-H

Smart Formula Parameter	Value
Expected Formula	C10H10N2O4S
Adducts Considered	;M+H;;M+NH4;;M+Na;;M+K;;M+Na 2-H;;2M+H;;2M+Na;

Smart Formula Search Parameters
CHNO and adducts considered
implicitly

Formula Search Minimum
Formula Search Maximum S 2

Algorithm Parameters
Tolerance 4 ppm
Match to Isotope Pattern(mSigma) 40
Electron Configuration even
Estimate No of Carbons yes
Filter by H/C Ratio 0 < H/C < 3
Number of Double Bonds & Rings 0 < rings&DB < 80

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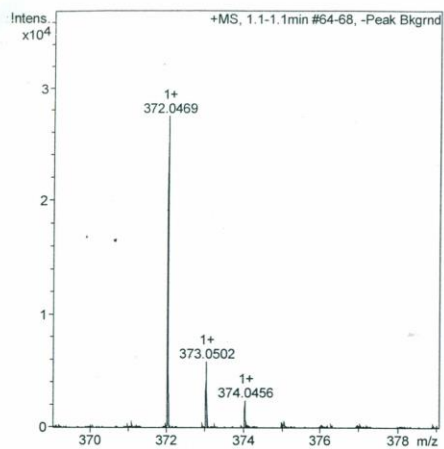
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Compound 15h



Confirm/Find Formula Results

The section below shows the results of formula calculation. If an expected formula was provided and found these are the results that are listed. If no formula was provided or no matches were found the system has attempted to determine the formula constrained by the parameters listed to the left

Cmpd 1, 1.1 min

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
372.046864	C17H14N3O3S2	1+	372.047110	0.2	0.7	15.6	100.00	C17 H13 N3 O3 S2	M+H
394.029116	C17H13N3NaO3S2	1+	394.029054	-0.1	-0.2	29.8	100.00		M+Na

Smart Formula Parameter Value
 Expected Formula C17H13N3O3S2
 Adducts Considered ;M+H₂;M+NH4₊;M+Na₊;M+K₊;M+Na₊
 2-H₂;2M+H₂;2M+Na₊

Smart Formula Search Parameters
 CHNO and adducts considered implicitly

Formula Search Minimum S 4
 Formula Search Maximum

Algorithm Parameters
 Tolerance 4 ppm
 Match to Isotope Pattern(mSigma) 40
 Electron Configuration even
 Estimate No of Carbons yes
 Filter by H/C Ratio 0 < H/C < 3
 Number of Double Bonds & Rings 0 < rings&DB < 80

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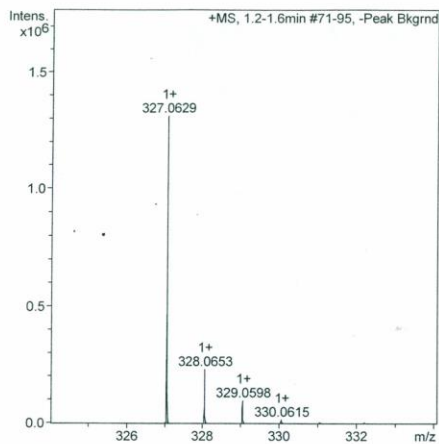
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Compound 15c



Confirm/Find Formula Results

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Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
327.062930	C17H15N2O52	1+	327.062032	-0.9	-2.7	21.4	100.00	C17 H14 N2 O S2	M+H
349.044324	C17H14N2NaOS2	1+	349.043976	-0.3	-1.0	16.8	100.00		M+Na
365.018738	C17H14KN2O52	1+	365.017913	0.8	2.3	12.4	100.00		M+K
675.099032	C34H28N4NaO254	1+	675.098731	-0.3	-0.4	10.9	100.00		2M+Na

Smart Formula Parameter	Value
Expected Formula	C17H14N2O52
Adducts Considered	;M+H ₊ ;M+NH ₄ ⁺ ;M+Na ₊ ;M+K ₊ ;M+Na ₂ H ₊ ;2M+H ₊ ;2M+Na ₊

Smart Formula Search Parameters
CHNO and adducts considered implicitly

Formula Search Minimum	S 4
Formula Search Maximum	

Algorithm Parameters	Value
Tolerance	4 ppm
Match to Isotope Pattern(mSigma)	40
Electron Configuration	even
Estimate No of Carbons	yes
Filter by H/C Ratio	0 < H/C < 3
Number of Double Bonds & Rings	0 < rings&DB < 80

Bruker Compass DataAnalysis 4.1

Analysis Name

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