

# SUPPORTING INFORMATION

## **$\alpha$ -Glucosidase and $\alpha$ -amylase inhibitory potentials of quinoline–1,3,4-oxadiazole conjugates bearing 1,2,3-triazole with antioxidant activity, kinetic studies and computational validation**

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### **Contents**

Table S1: Details of SiteMap analysis to select the putative allosteric site.....	2
Table S2: Induced docking results at the selected allosteric site .....	2
S.3 Synthetic procedures.....	3
S.3.1 General procedure for the synthesis of alkyl azides 6a,b .....	3
S.3.2 General procedure for the synthesis of benzyl azides 8a-h .....	3
S.3.3 General procedure for the synthesis of phenyl azides 10a-j .....	3
S.4 Spectral data.....	4

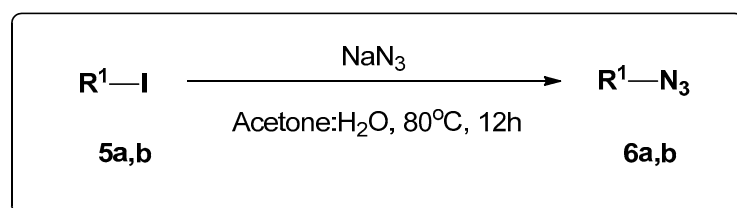
**Table S1: Details of SiteMap analysis to select the putative allosteric site**

Site	SiteScore	DScore	Volume	Balance	Residues
1	1.064	730.247	730.247	0.569	155,156,157,159,160,176,177,215,216,217,218,228,229,231,232,234,235,236,237,239,240,241,242,245,276,277,278,279,280,300,301,304,307,308,309,310,311,312,313,314,349,350,408,412,415,416,419,420,425,426,439
2	1.156	358.435	358.435	1.887	216,217,241,245,246,250,251,254,277,279,280,281,284,285,286,292,293,294,295,296,297,299,329,330,333,339,340
3	0.779	138.915	138.915	0.301	354,365,366,367,370,391,392,474,475,476,480,481,484,486,487,488
4	0.798	116.277	116.277	0.750	15,331,332,334,335,336,337,338,339,340,380,508,509,510,511,512,527
5	0.673	92.267	92.267	0.341	399,403,452,453,454,460,462,463,464,467,468,470,472,473

**Table S2: Induced docking results at the selected allosteric site**

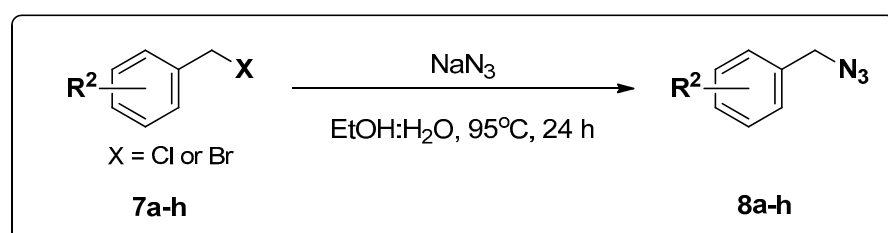
Compound	IC <sub>50</sub> ( $\mu$ M)	Docking Score	Glide energy	Glide Emodel	H-Bond residues
4b	24.87	-5.489	-30.792	-54.445	Arg312 and Glu408
4i	15.85	-6.938	-51.445	-80.251	His245, Asn241, Arg312, Tyr313 and Asn412
4j	26.67	-5.040	-42.085	-59.442	His239 and Arg312
4k	23.69	-6.498	-51.569	-83.536	Phe300 and Arg312
4l	25.23	-5.806	-48.401	-64.485	Lys155 and Gly160 and His239
12k	22.47	-6.757	-51.159	-92.087	His245, Arg312 and Arg439
12m	26.81	-4.961	-51.007	-80.735	His251, Ser281, Tyr286 and Phe333

### S.3 Synthetic procedures



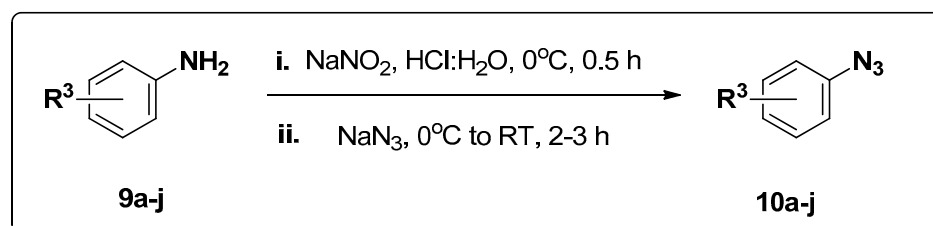
#### S.3.1 General procedure for the synthesis of alkyl azides 6a,b

Appropriate aliphatic halide **5a,b** (20mmol) was dissolved in a mixture of acetone:water (3:1) in a round bottom flask (RBF) and allowed to reflux for 15mins at 80 °C. Subsequently, sodium azide (1.5eq) was added and the mixture refluxed for further 12h. Thereafter, the suspension was poured in water and extracted with ethyl acetate. Dried with anhydrous sodium sulphate and concentrated under reduced pressure to yield yellow oil.



#### S.3.2 General procedure for the synthesis of benzyl azides 8a-h

A solution of relative benzyl halides **7a-h** (8mmol) and sodium azide 0.772g (1.5eq) in a mixture of ethanol:water (8:1) were allowed to stir at 95 °C for 24h. At the end of the reaction after monitoring with TLC, water was added to the suspension and extracted with ethyl acetate. The combined organic layer was dried with anhydrous magnesium sulphate and dried under with a rotavapor at low temperature to obtain a yellow liquid.

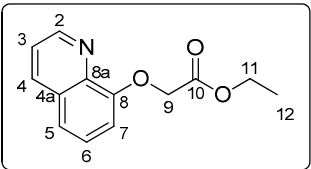


#### S.3.3 General procedure for the synthesis of phenyl azides 10a-j

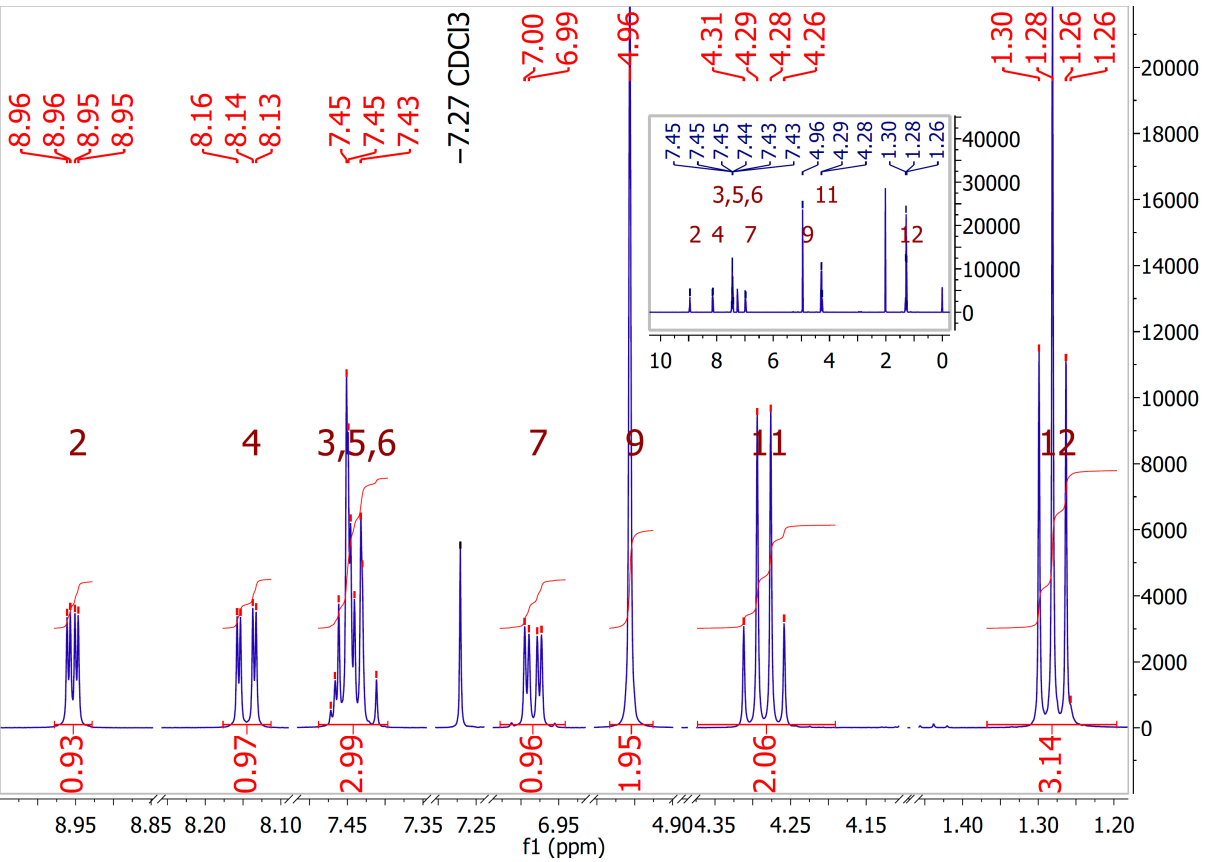
Appropriate aniline 10mmol (1eq) was dissolved to a solution of concentrated HCl:water (1:1) in an RBF and stirred at 0-5 °C. Thereafter, 15.4mmol (1.5eq) of sodium nitrite dissolved in water was added in small portion for 5mins and stirred for a further 30mins. Subsequent amount of sodium azide 19mmol (1.5eq) was added and stirred to rt for further 2-3h. The reaction was diluted with water and extracted with diethyl ether. The combined organic extracts were dried with anhydrous sodium sulphate and concentrated under reduced pressure to obtain crude azides at good yeilds.

S.4 Spectral data

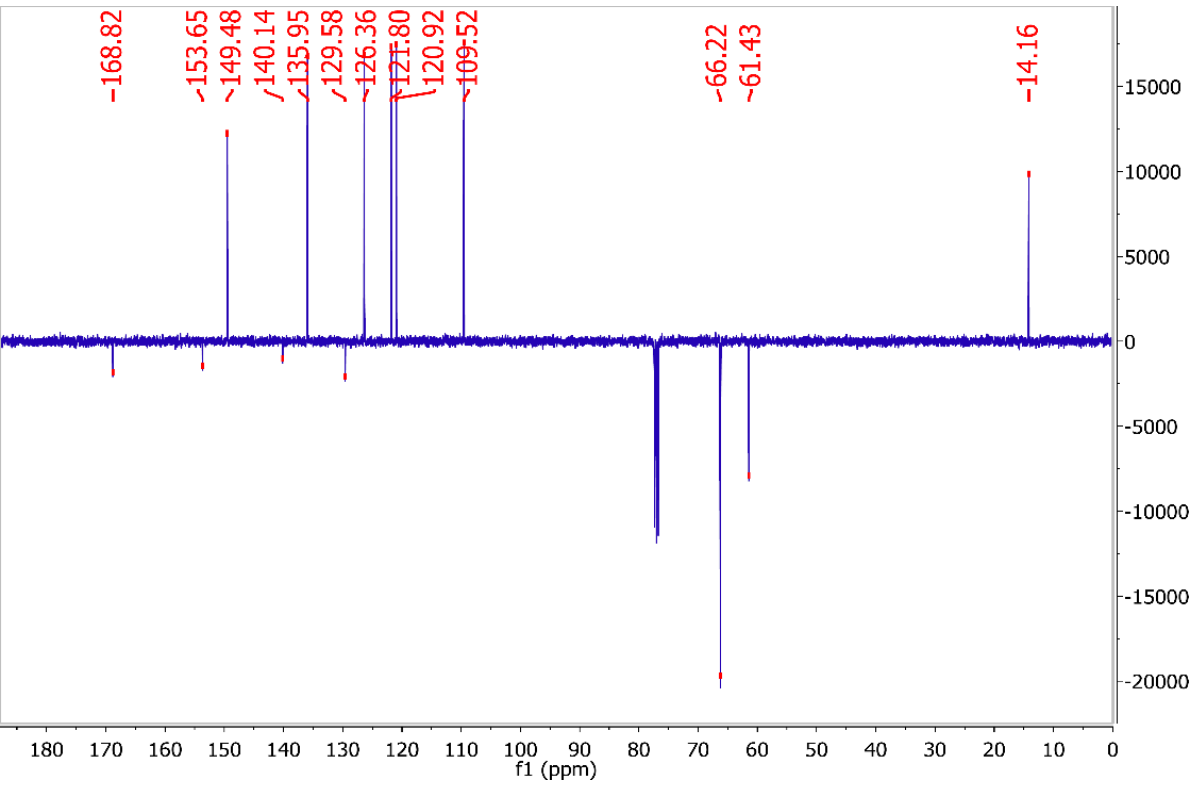
ethyl 2-(quinolin-8-yloxy)acetate (**1**)



<sup>1</sup>H NMR

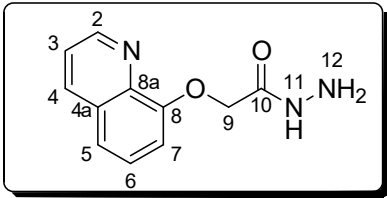


<sup>13</sup>C NMR

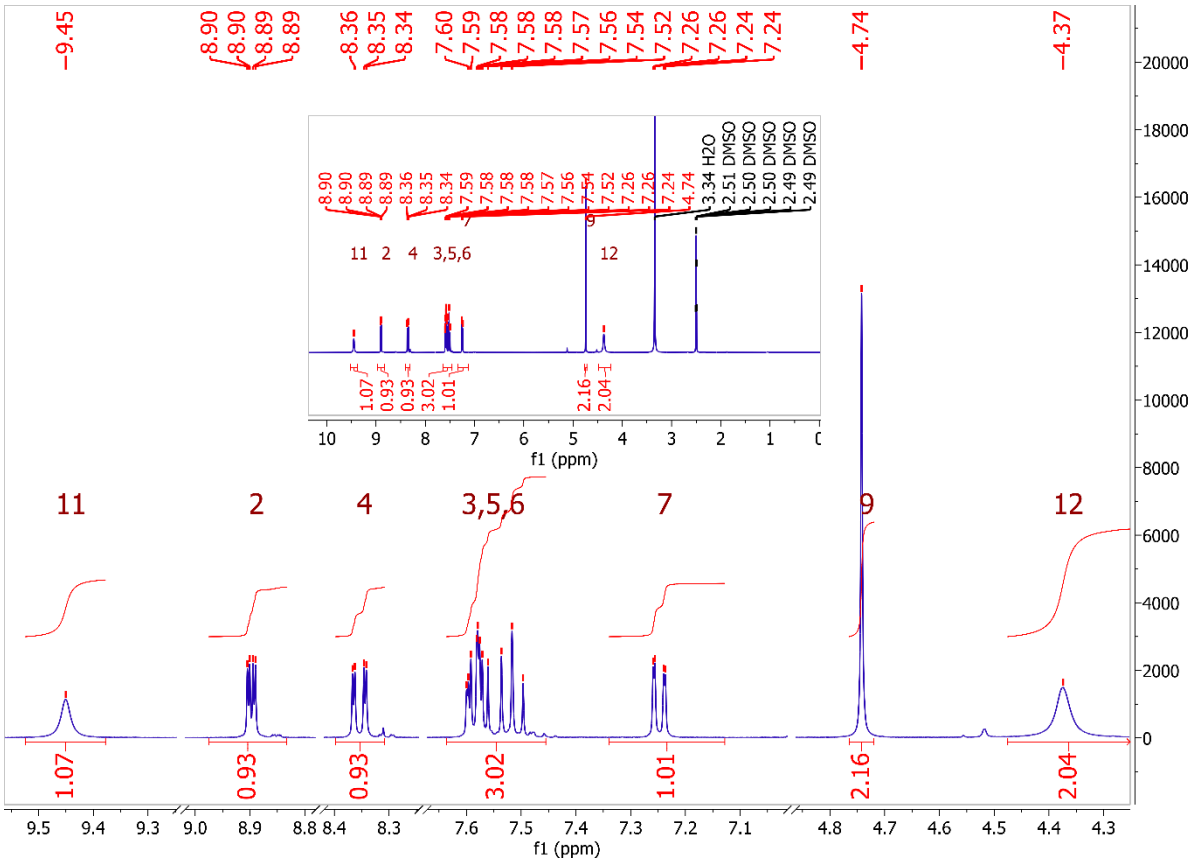




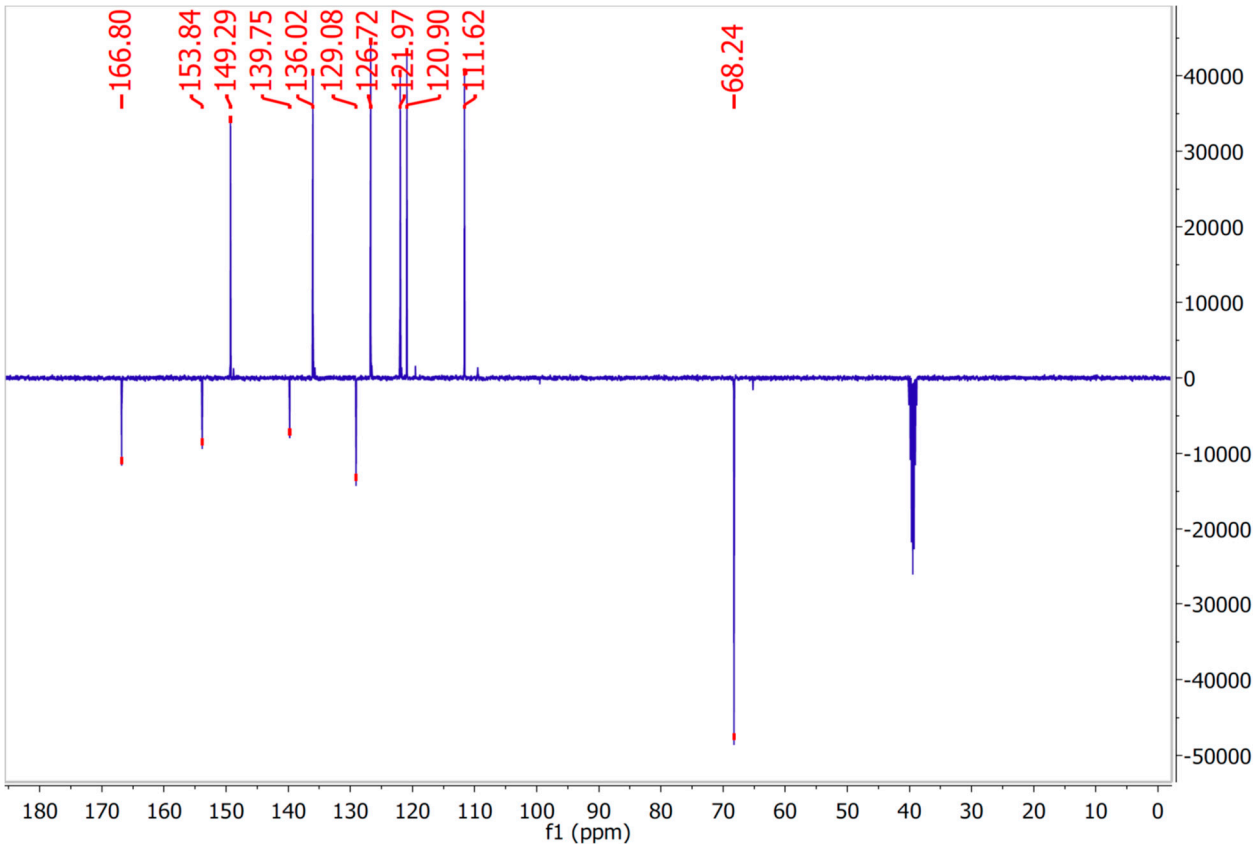
2-(quinolin-8-yloxy)acetohydrazide (2)



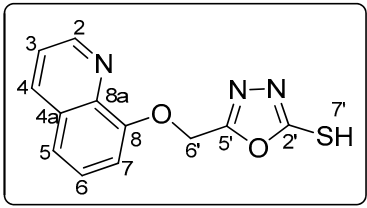
<sup>1</sup>H NMR



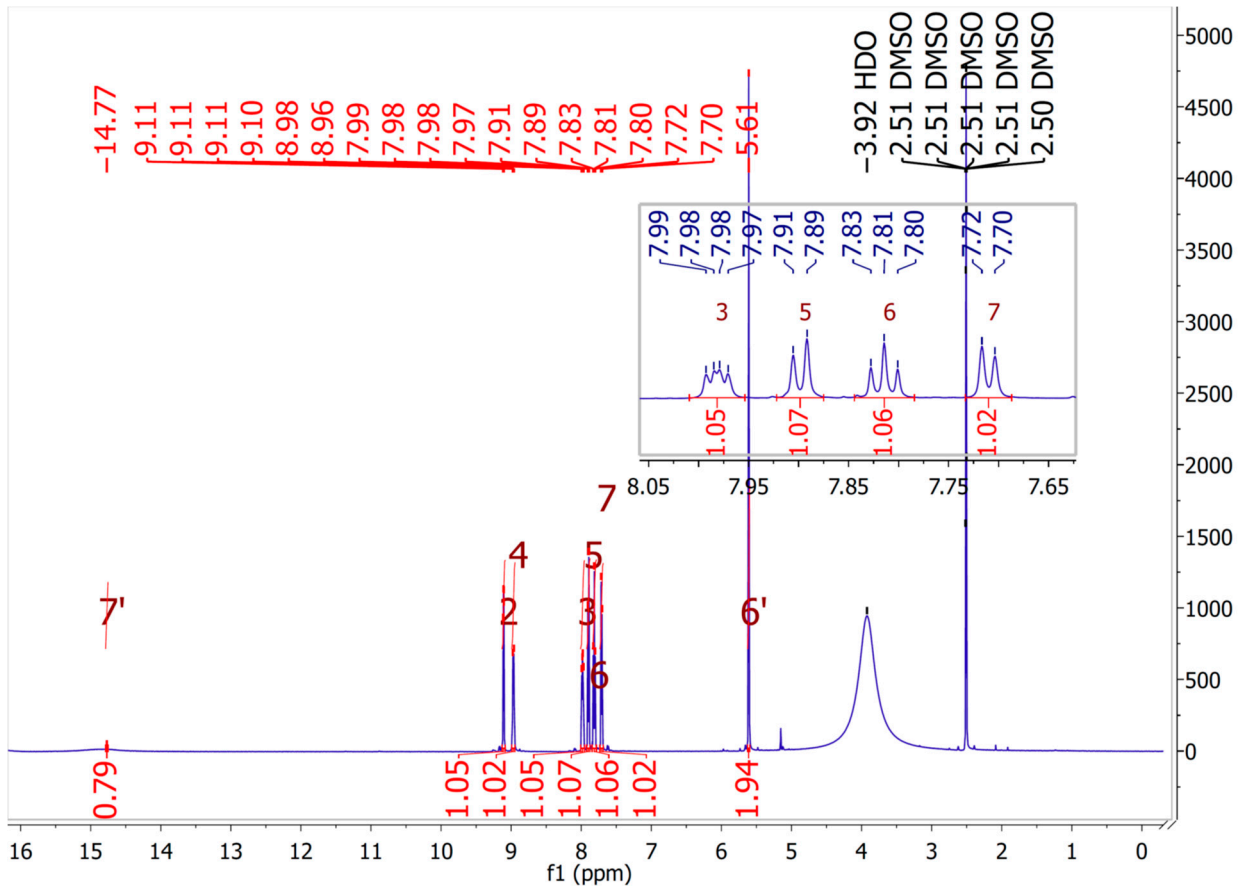
<sup>13</sup>C NMR



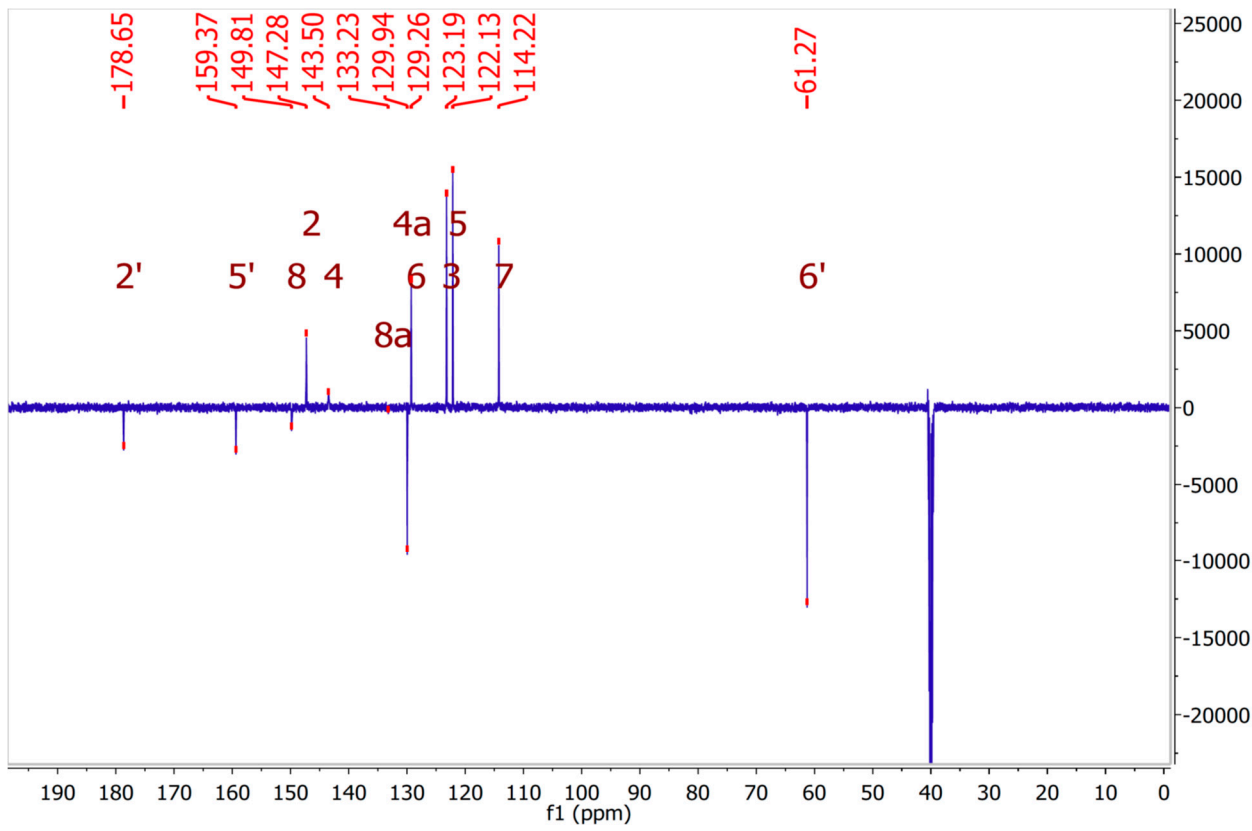
5-[(quinolin-8-yloxy)methyl]-1,3,4-oxadiazole-2-thiol (**3**)



<sup>1</sup>H NMR



<sup>13</sup>C NMR



## HRMS

### Elemental Composition Report \_Compound 3

#### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

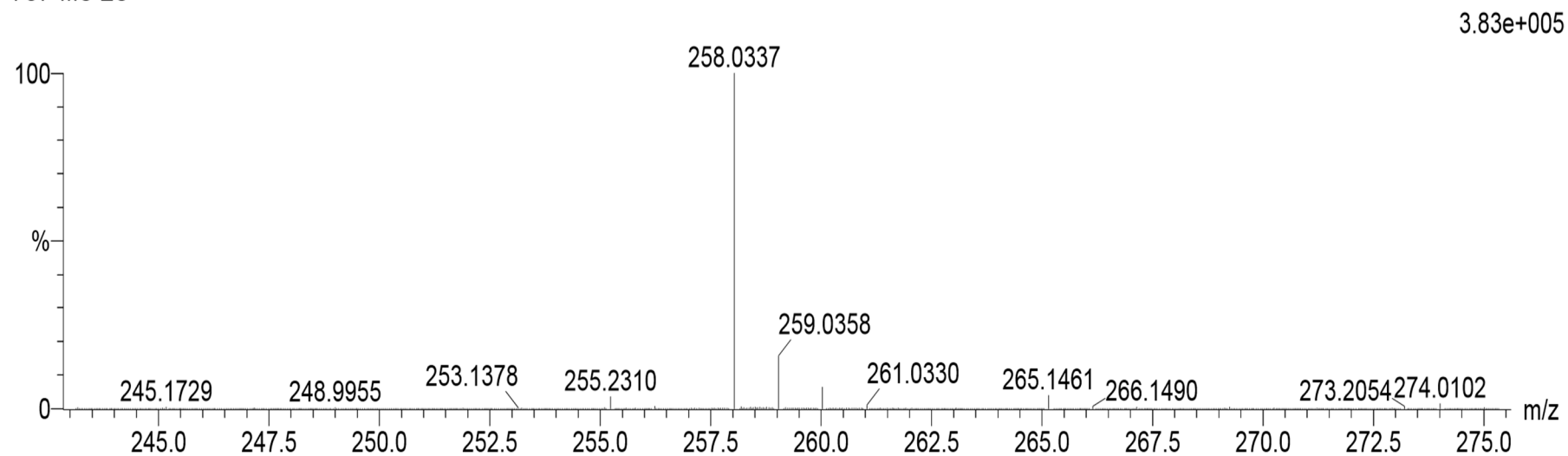
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

33 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) Elements Used:

C: 10-15 H: 5-10 N: 0-5 O: 0-5 S: 0-1

TOF MS ES-

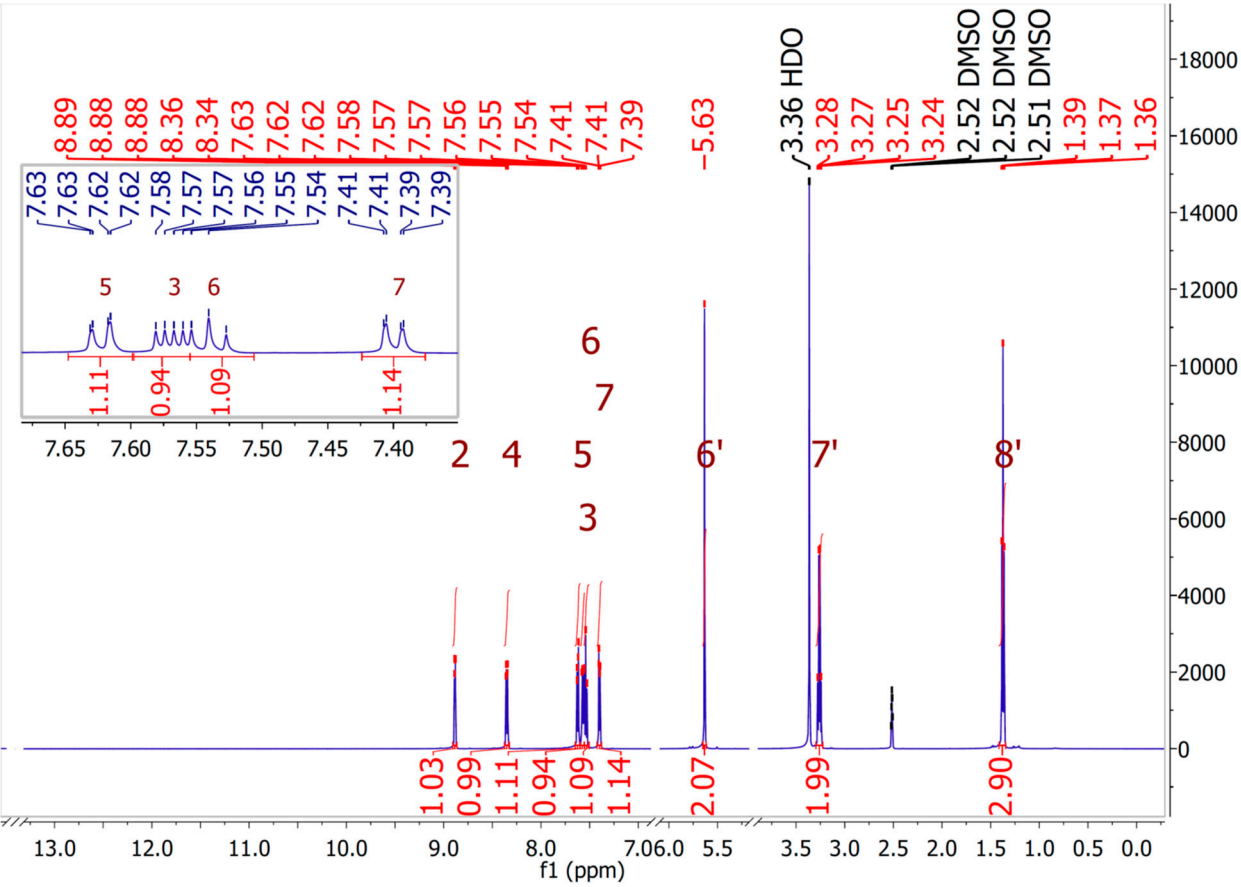


Minimum: -1.5  
Maximum: 5.0 5.0 500.0

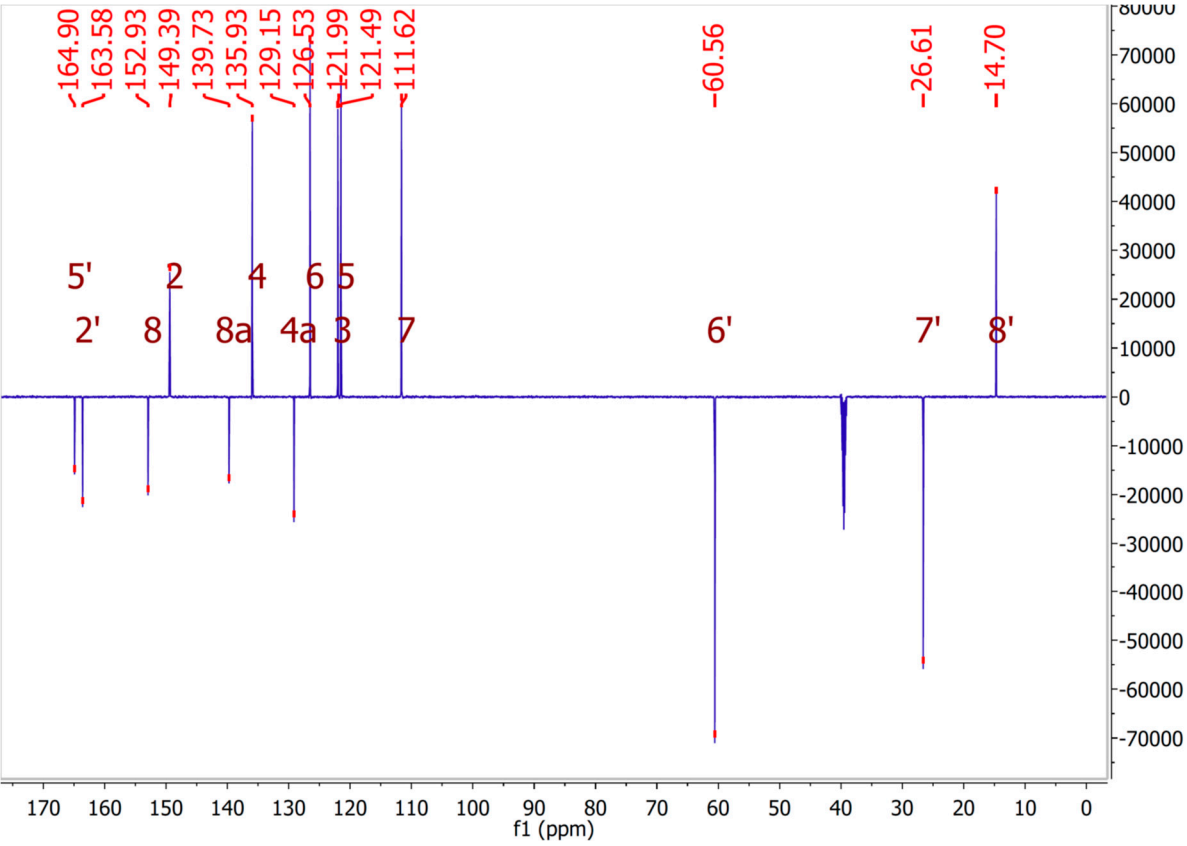
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
258.0337	258.0337	0.0	0.0	10.5	647.6	0.0	C12 H8 N3 O2 S

2-(ethylthio)-5-[(quinolin-8-yloxy)methyl]-1,3,4-oxadiazole (4a)

<sup>1</sup>H NMR



<sup>13</sup>C NMR



# HRMS

## Elemental Composition Report\_ Compound 4a

### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

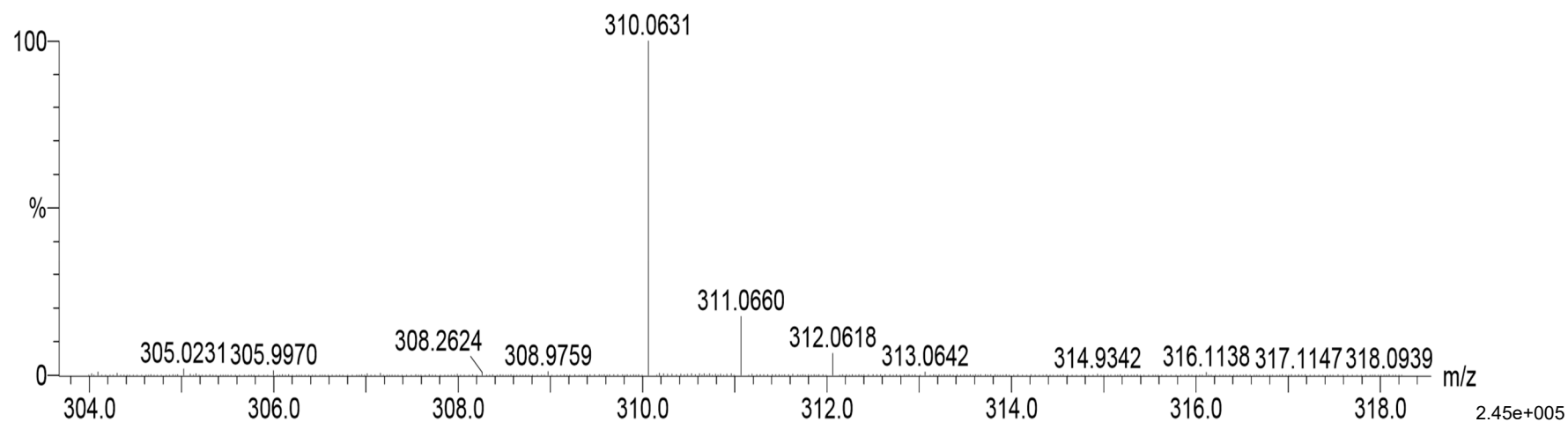
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

74 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) Elements Used:

C: 10-15 H: 10-15 N: 0-5 O: 0-5 S: 0-1 Na: 0-1

TOF MS ES+

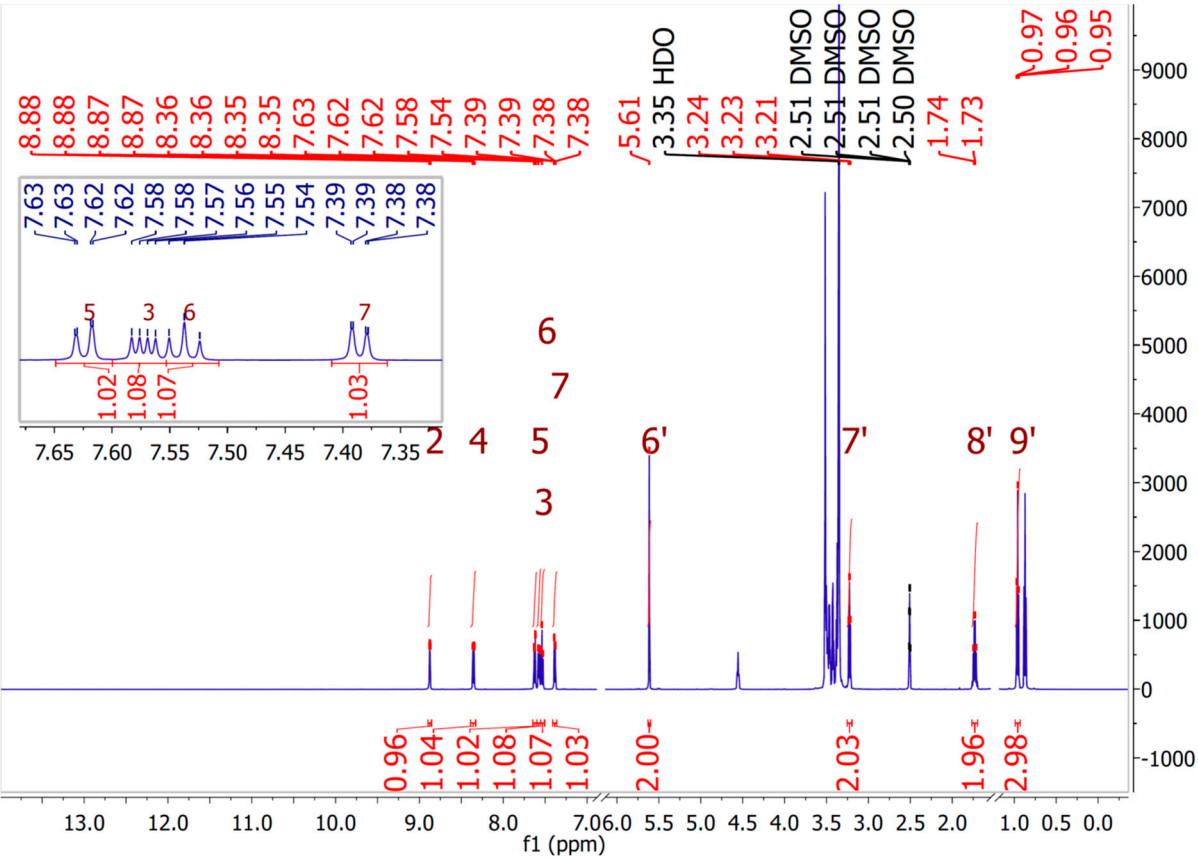


Minimum: -1.5  
Maximum: 5.0 5.0 500.0

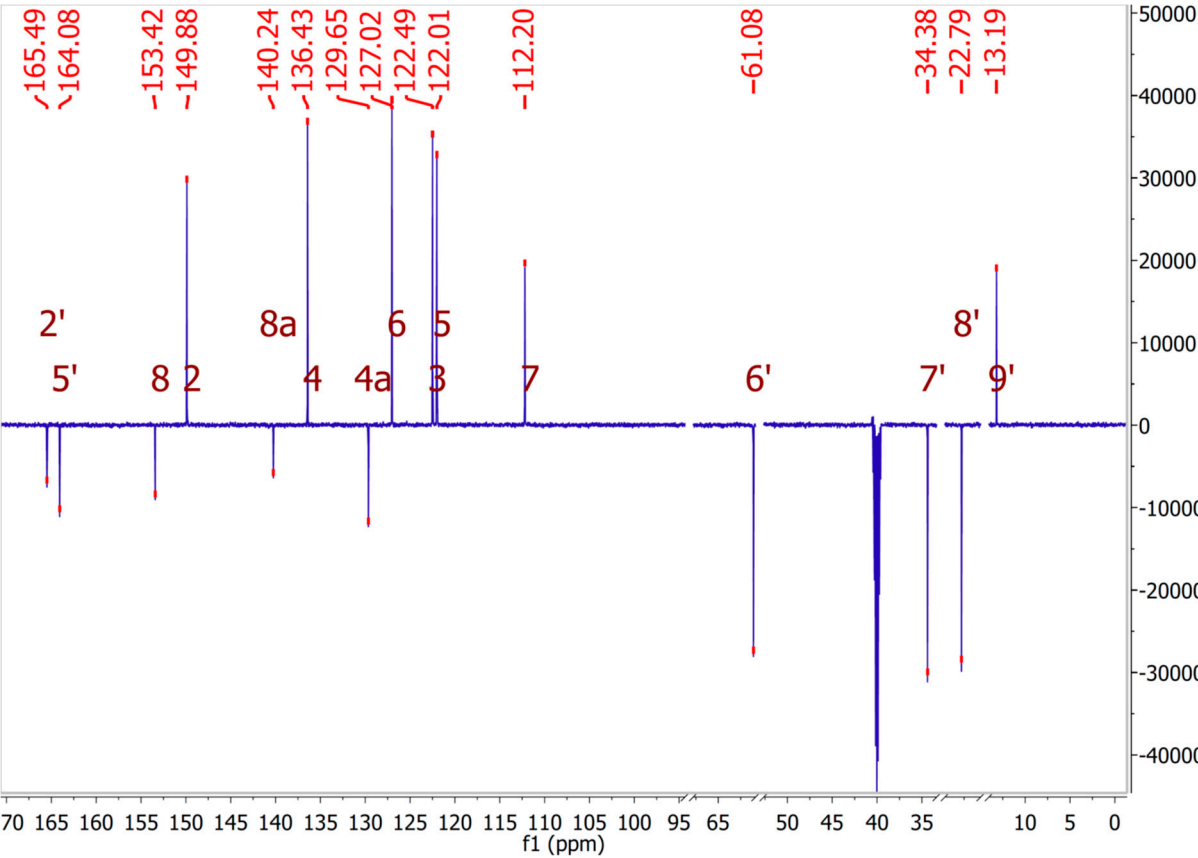
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
310.0631	310.0626	0.5	1.6	9.5	653.9	0.0	C14 H13 N3 O2 S Na

2-(propylthio)-5-[(quinolin-8-yloxy)methyl]-1,3,4-oxadiazole (**4b**)

<sup>1</sup>H NMR



<sup>13</sup>C NMR



## HRMS

### Elemental Composition Report\_Compound 4b

#### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

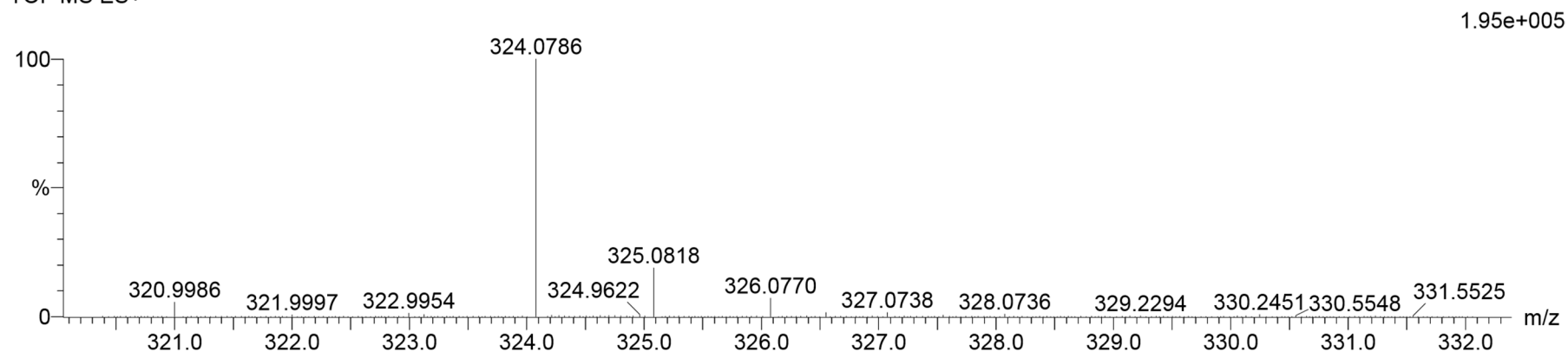
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

86 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) Elements Used:

C: 10-15 H: 10-15 N: 0-5 O: 0-5 Na: 0-1 S: 0-1

TOF MS ES+



Minimum:

Maximum:

-1.5

5.0

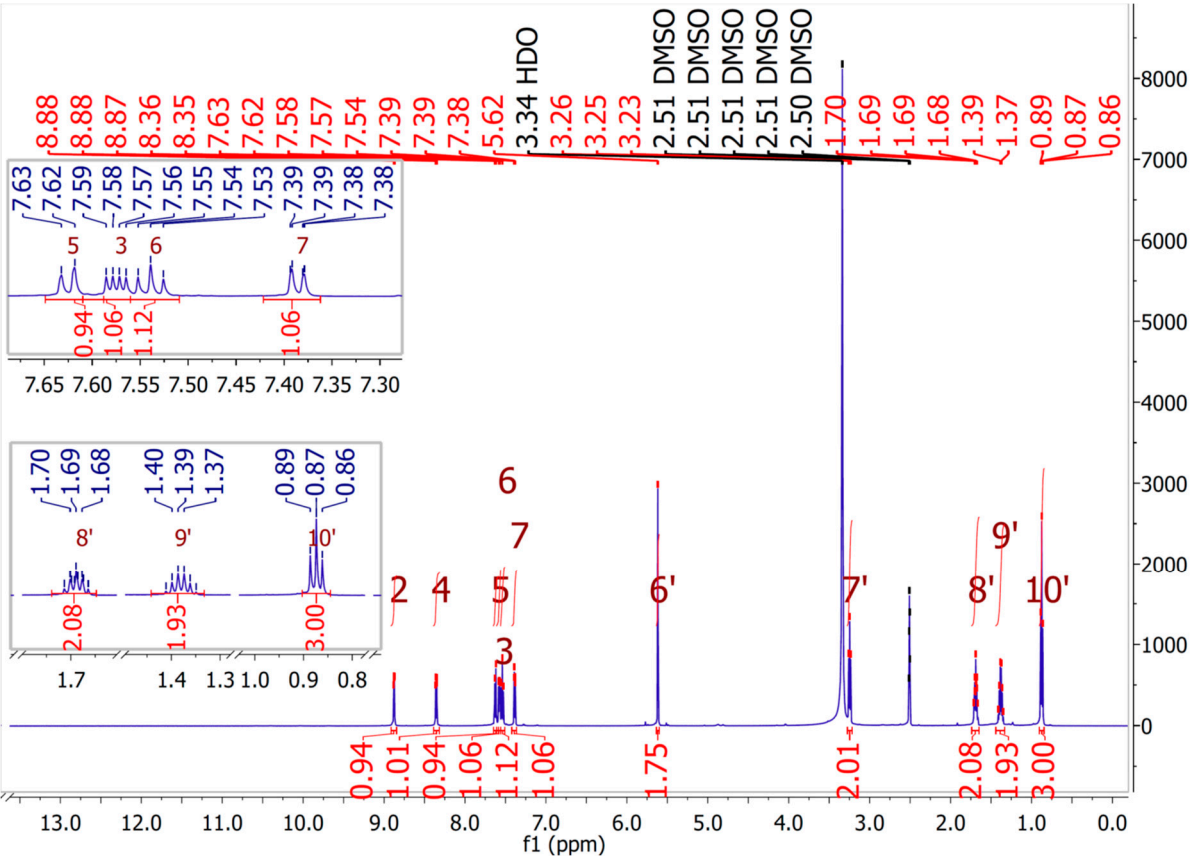
5.0

500.0

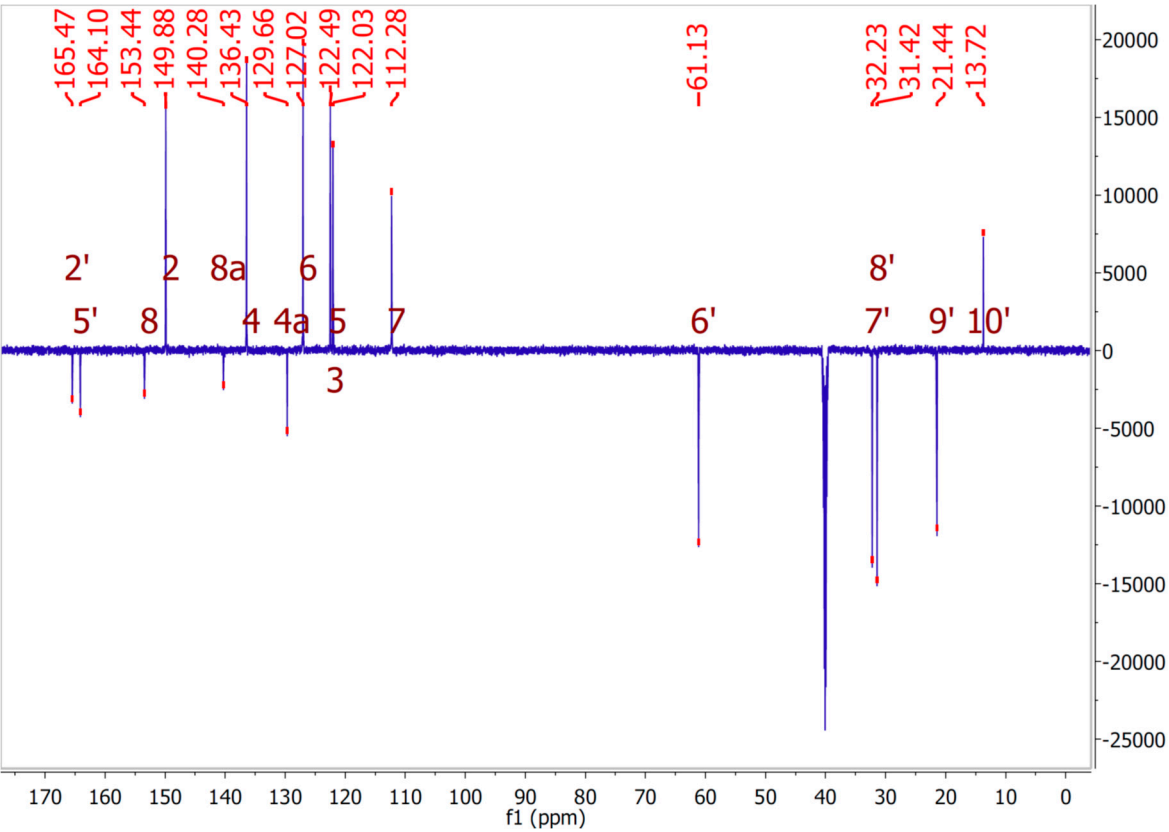
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
324.0786	324.0783	0.3	0.9	9.5	640.5	0.0	C15 H15 N3 O2 Na S

2-(butylthio)-5-[(quinolin-8-yloxy)methyl]-1,3,4-oxadiazole (4c)

<sup>1</sup>H NMR

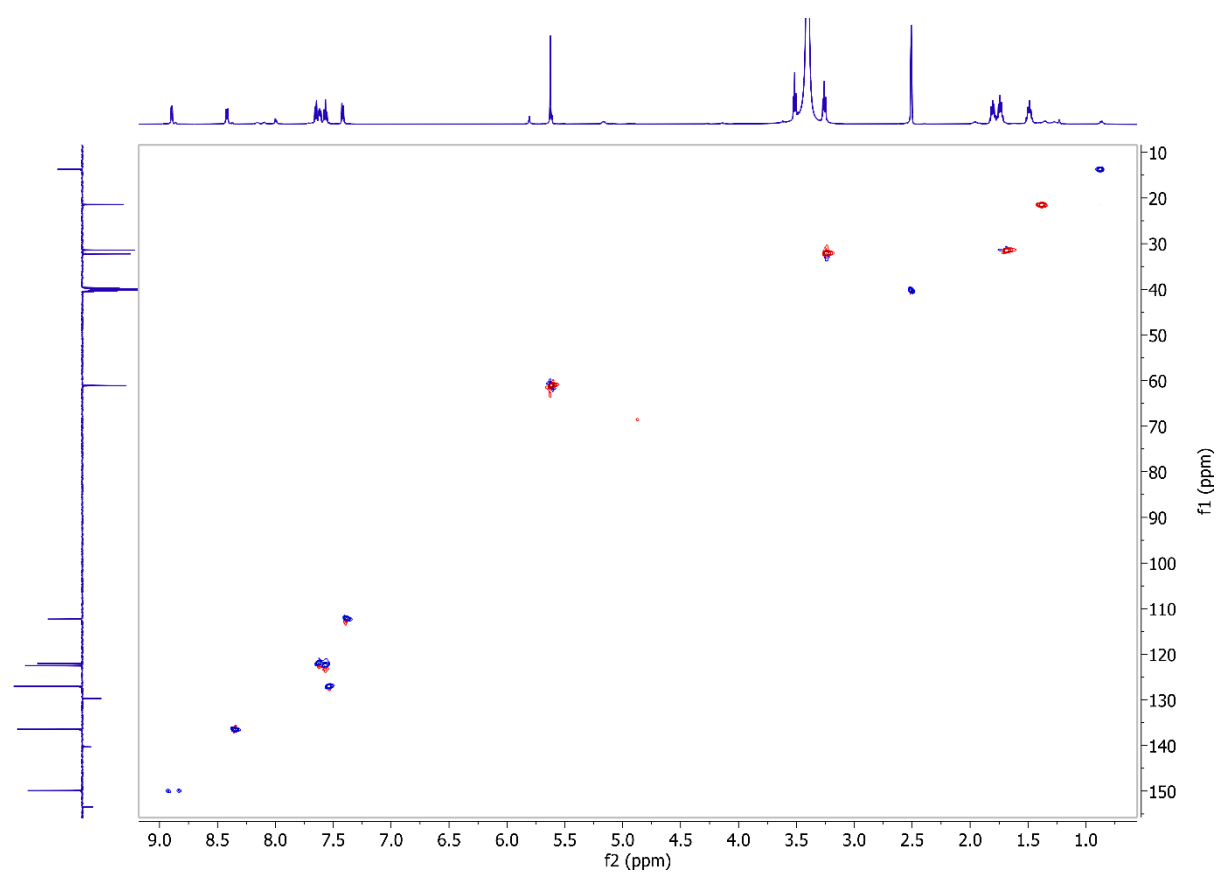


<sup>13</sup>C NMR

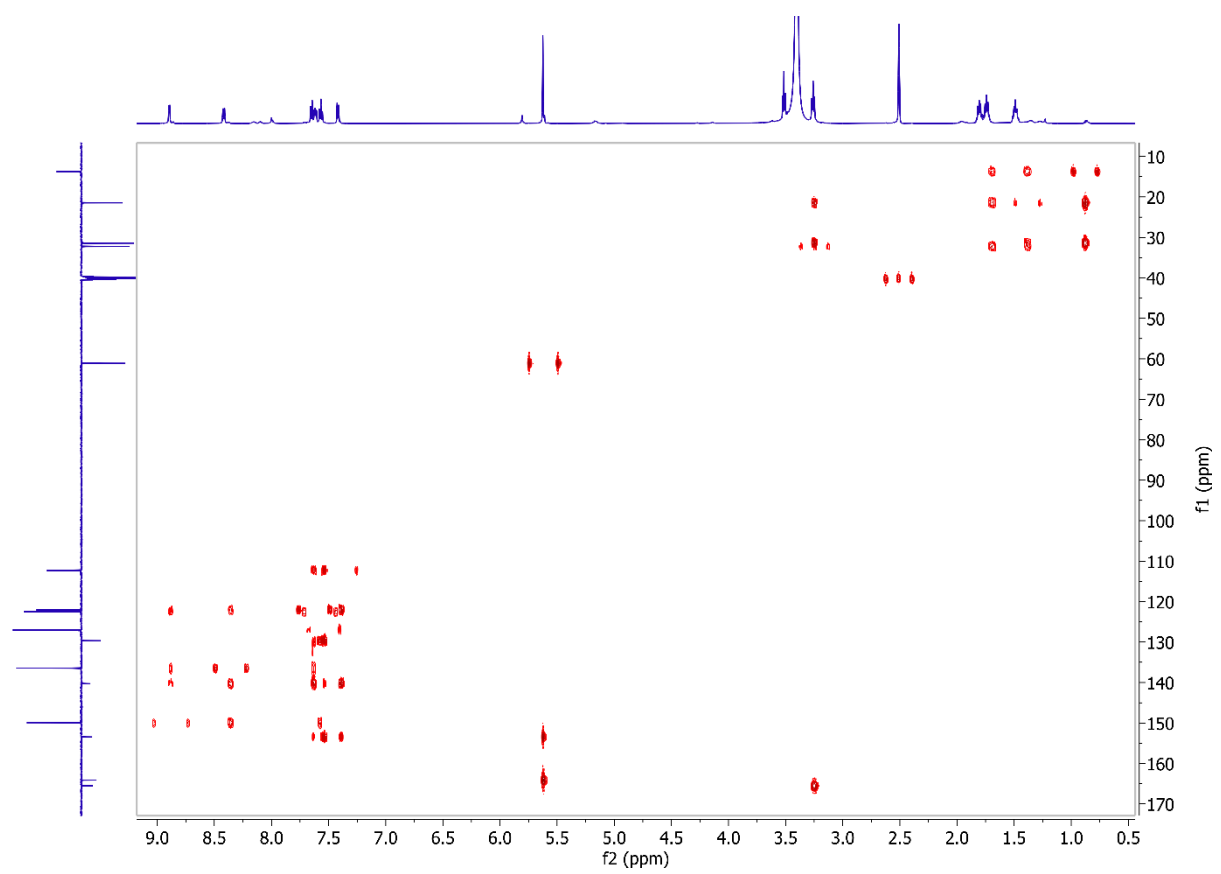




HSQC



HMBC



## HRMS

### Elemental Composition Report\_Comound 4c

#### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

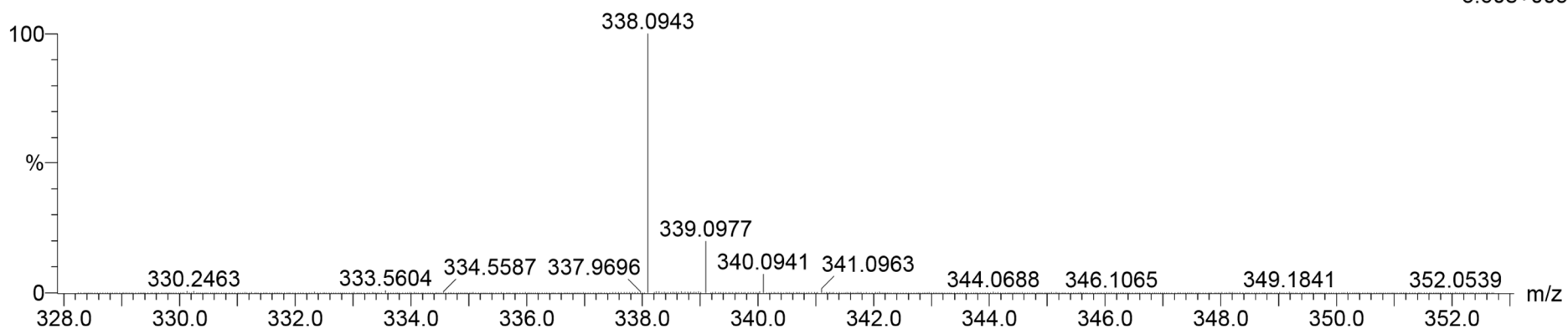
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

62 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) Elements Used:

C: 15-20 H: 15-20 N: 0-5 O: 0-5 Na: 0-1 S: 0-1

TOF MS ES+



Minimum:

Maximum:

-1.5

5.0

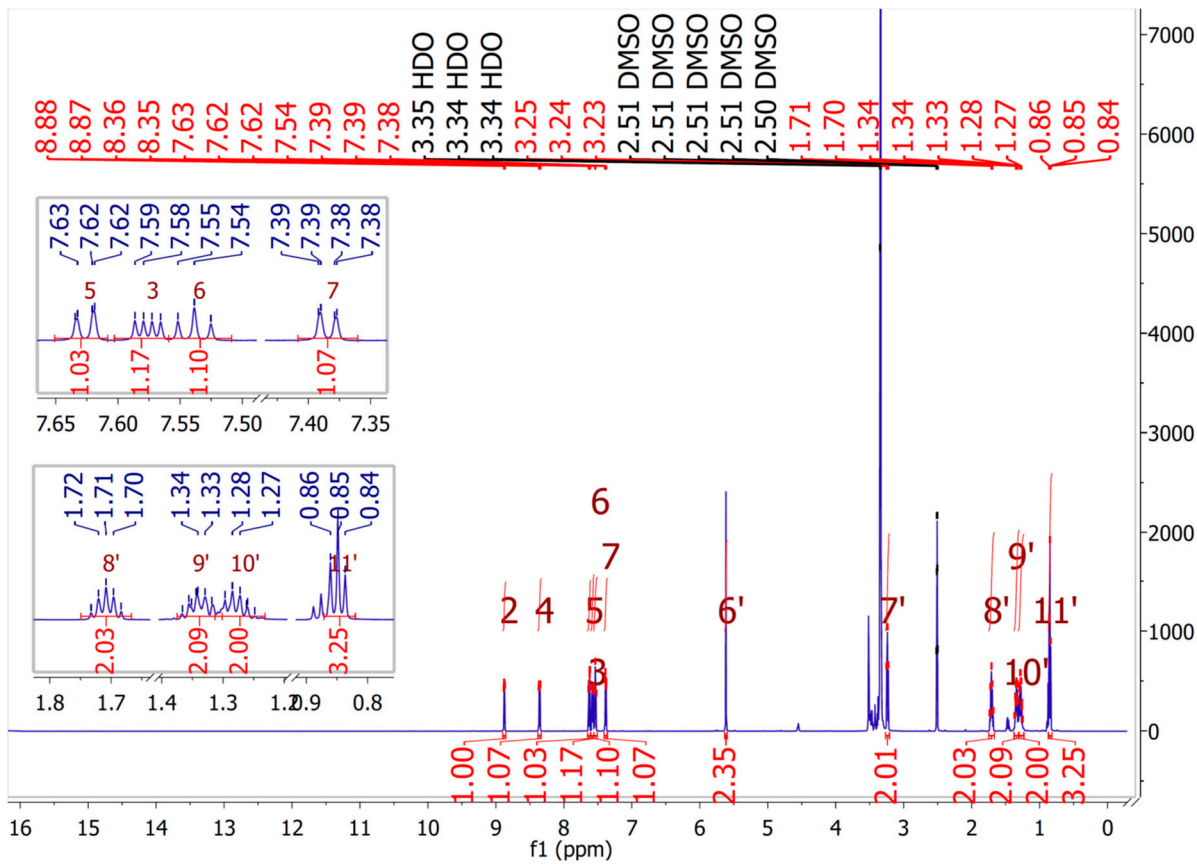
5.0

500.0

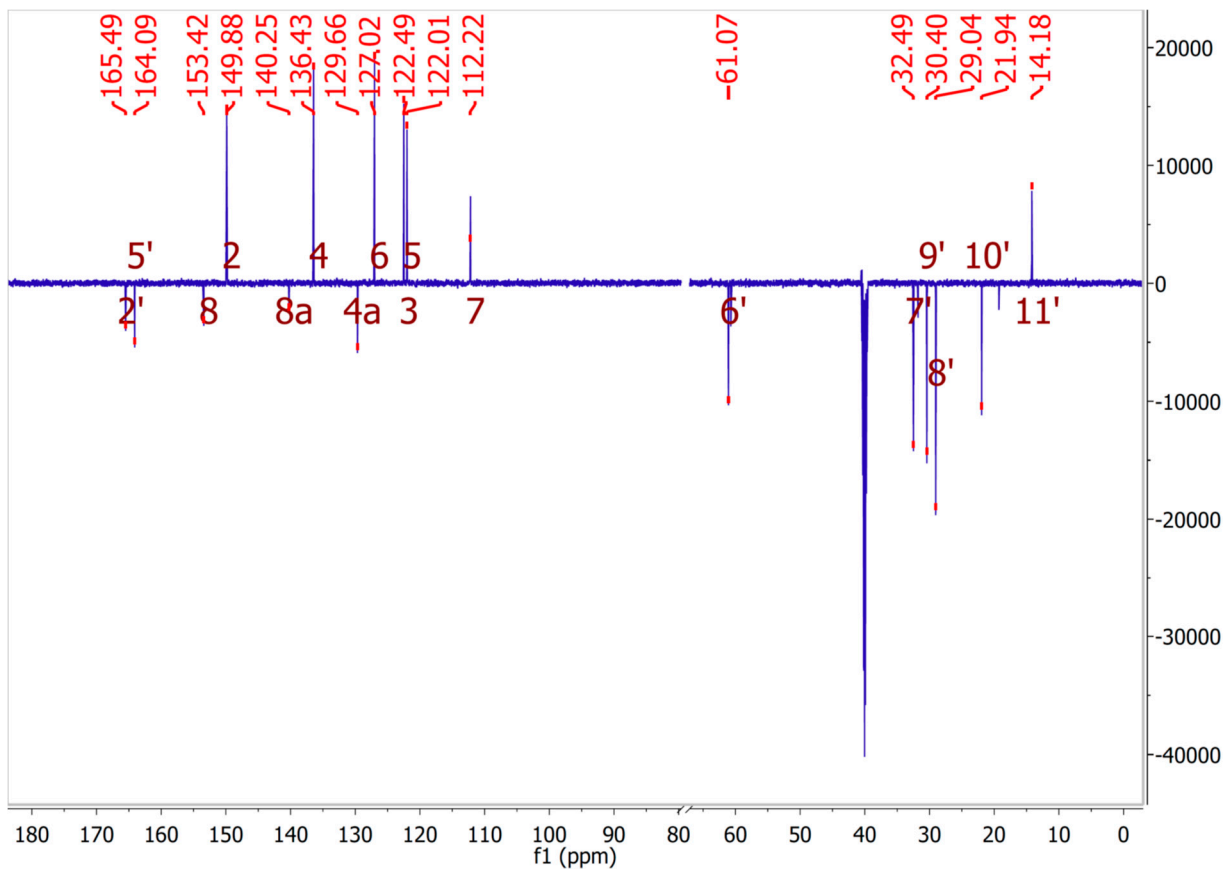
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
338.0943	338.0939	0.4	1.2	9.5	662.4	0.0	C16 H17 N3 O2 Na S

2-(pentylthio)-5-[(quinolin-8-yloxy)methyl]-1,3,4-oxadiazole (**4d**)

<sup>1</sup>H NMR



<sup>13</sup>C NMR



## HRMS

### Elemental Composition Report\_Compound 4d

#### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

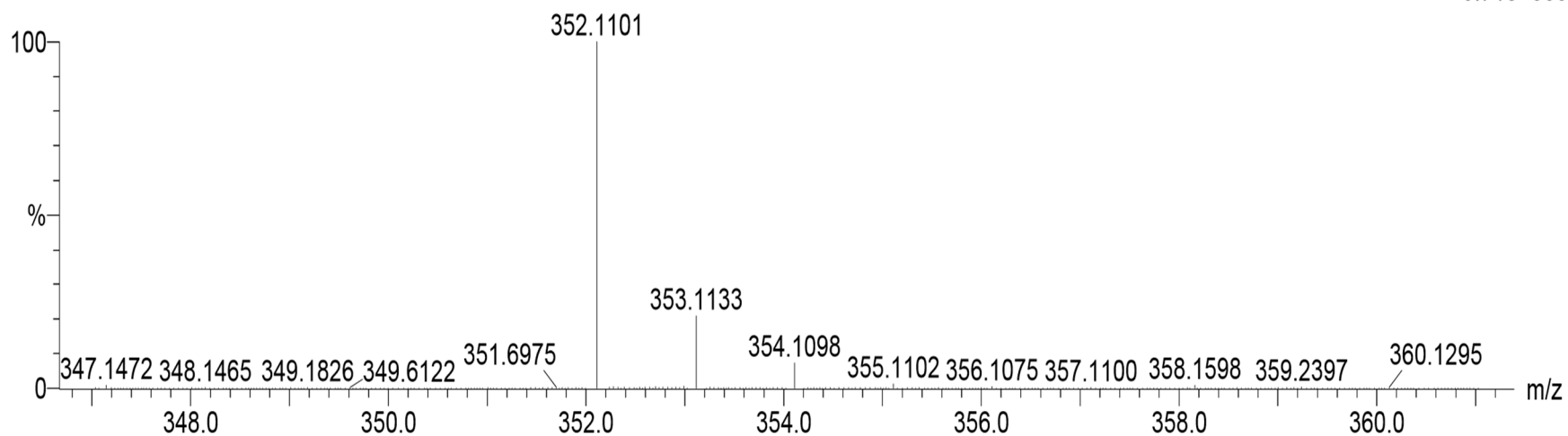
Monoisotopic Mass, Even Electron Ions

59 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) Elements Used:

C: 15-20 H: 15-20 N: 0-5 O: 0-5 Na: 0-1 S: 0-1

TOF MS ES+

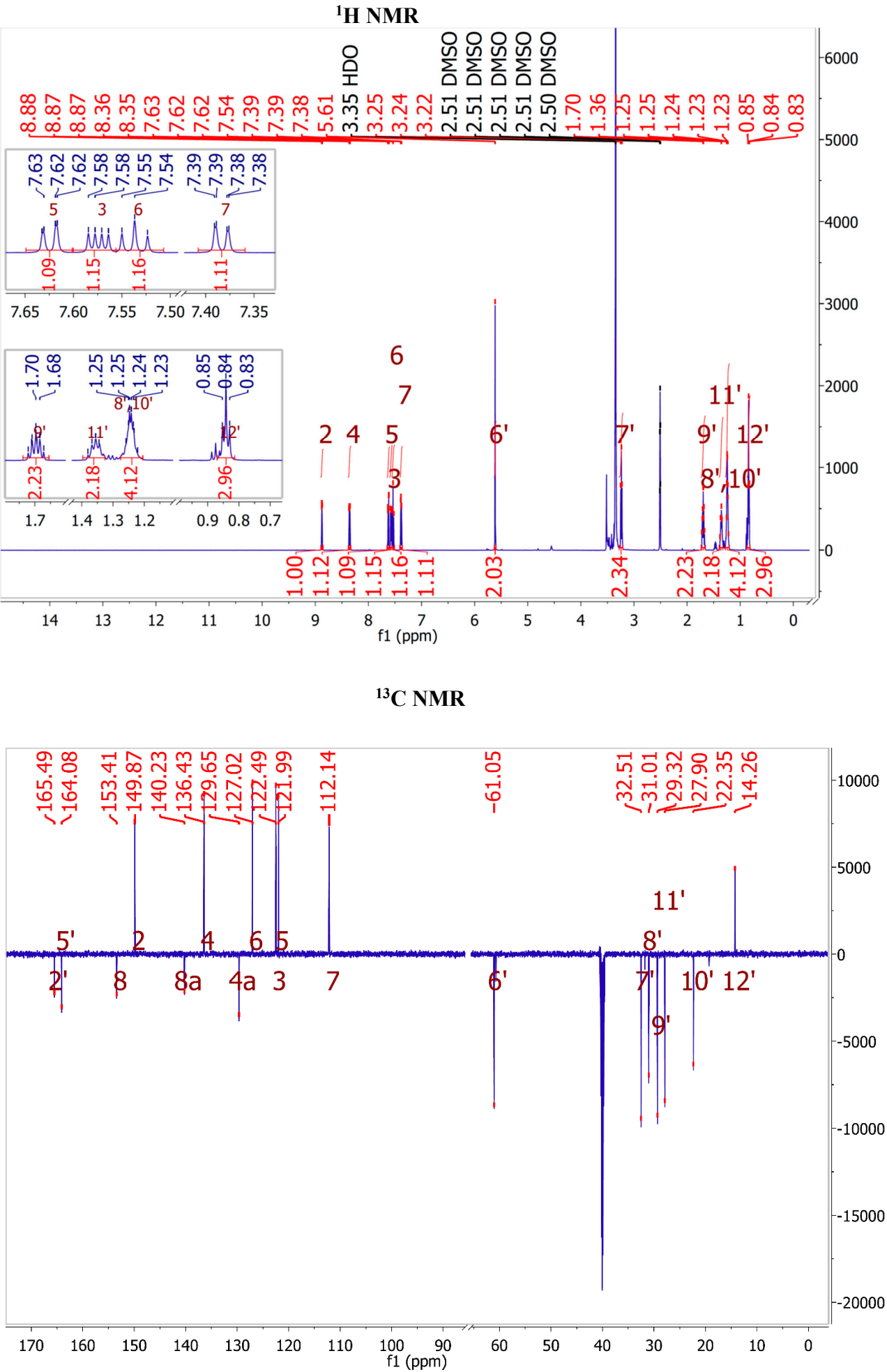
3.71e+005



Minimum: -1.5  
Maximum: 5.0 5.0 500.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
352.1101	352.1096	0.5	1.4	9.5	667.7	0.0	C17 H19 N3 O2 Na

2-(hexylthio)-5-[(quinolin-8-yloxy)methyl]-1,3,4-oxadiazole (4e)



## HRMS

### Elemental Composition Report

#### Single Mass Analysis\_Compound 4e

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

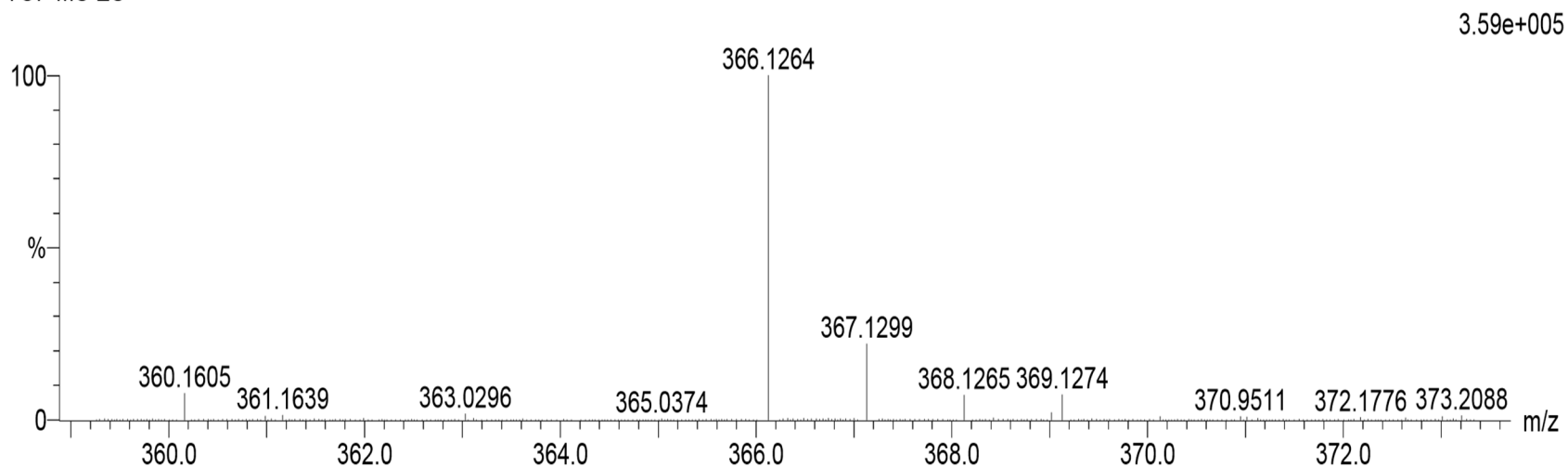
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

29 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) Elements Used:

C: 15-20 H: 20-25 N: 0-5 O: 0-5 Na: 1-1 S: 0-1

TOF MS ES+



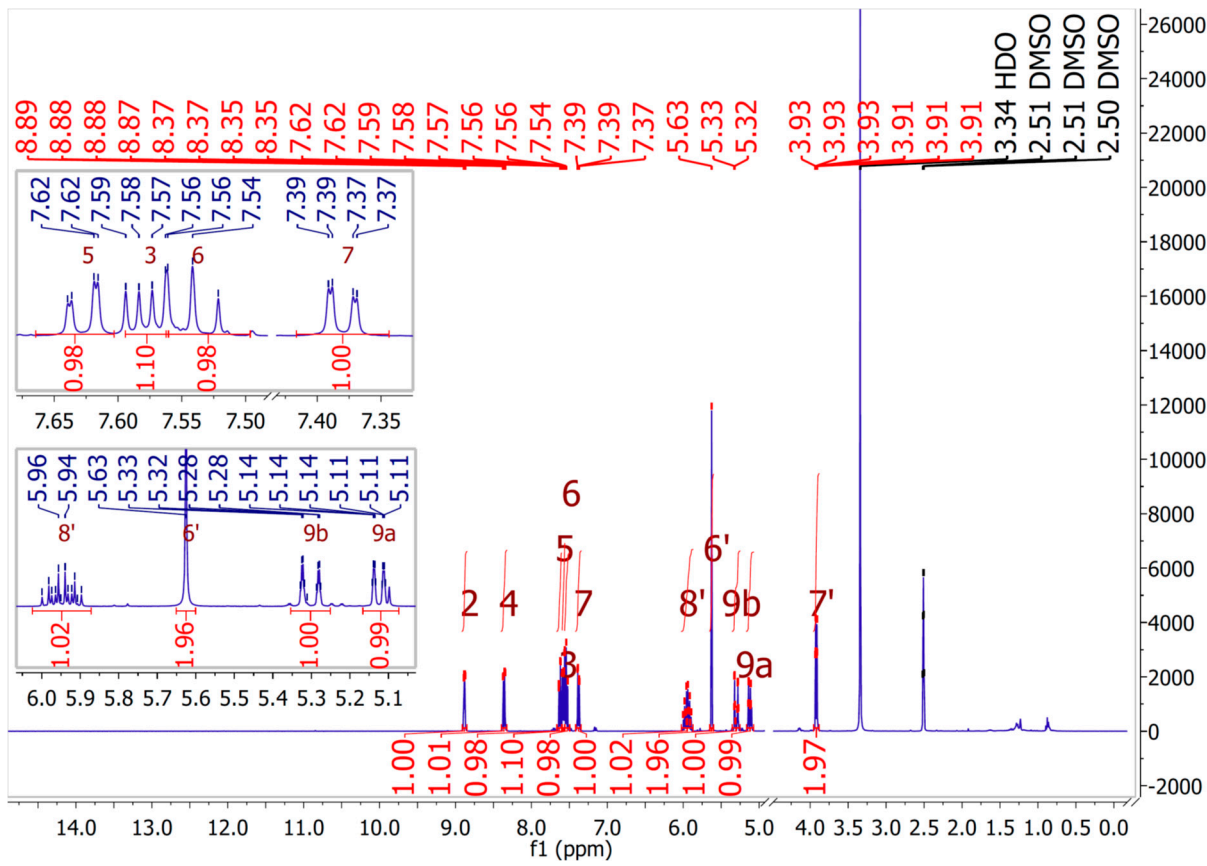
Minimum:

Maximum: 5.0 5.0 -1.5 500.0

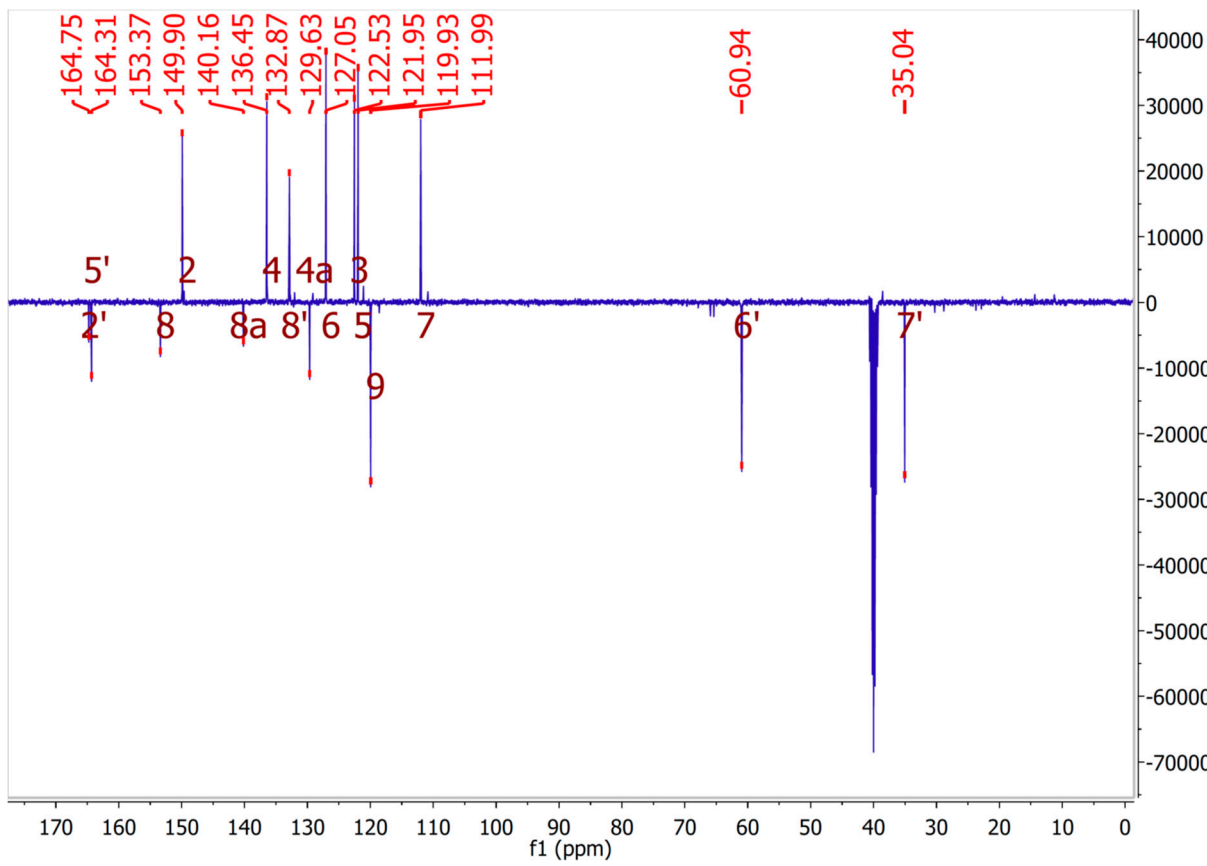
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
366.1252	366.1252	1.2	3.3	9.5	644.4	0.0	C18 H21 N3 O2 Na S

2-(allylthio)-5-[(quinolin-8-yloxy)methyl]-1,3,4-oxadiazole (4f)

<sup>1</sup>H NMR



<sup>13</sup>C NMR



## HRMS

### Elemental Composition Report\_Compound 4f

#### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

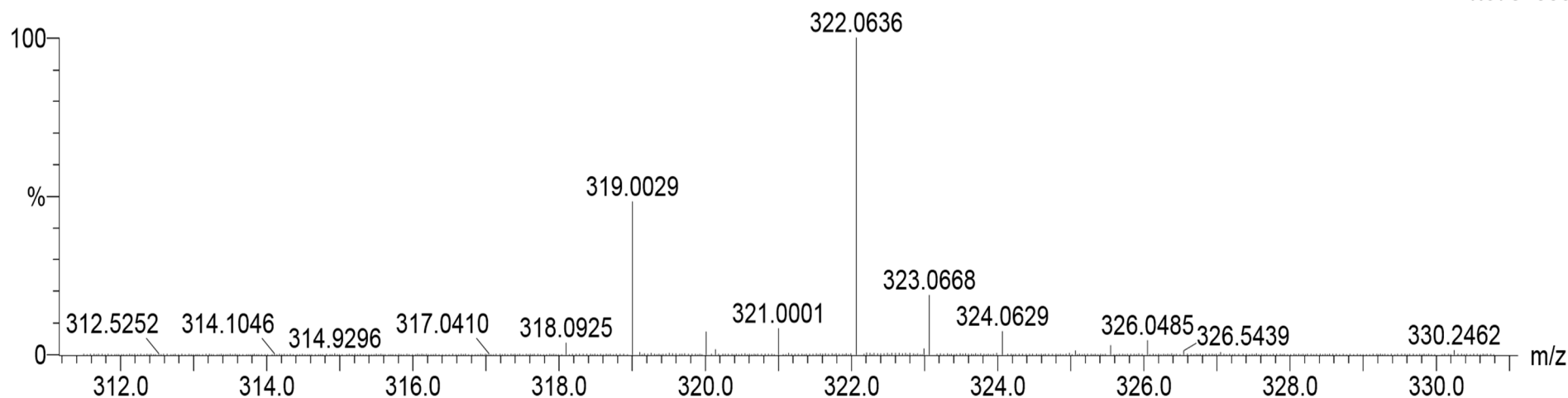
Monoisotopic Mass, Even Electron Ions

39 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) Elements Used:

C: 15-20 H: 10-15 N: 0-5 O: 0-5 Na: 1-1 S: 0-1

TOF MS ES+

1.57e+005



Minimum:

-1.5

Maximum:

5.0

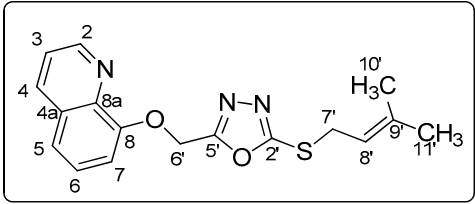
5.0

500.0

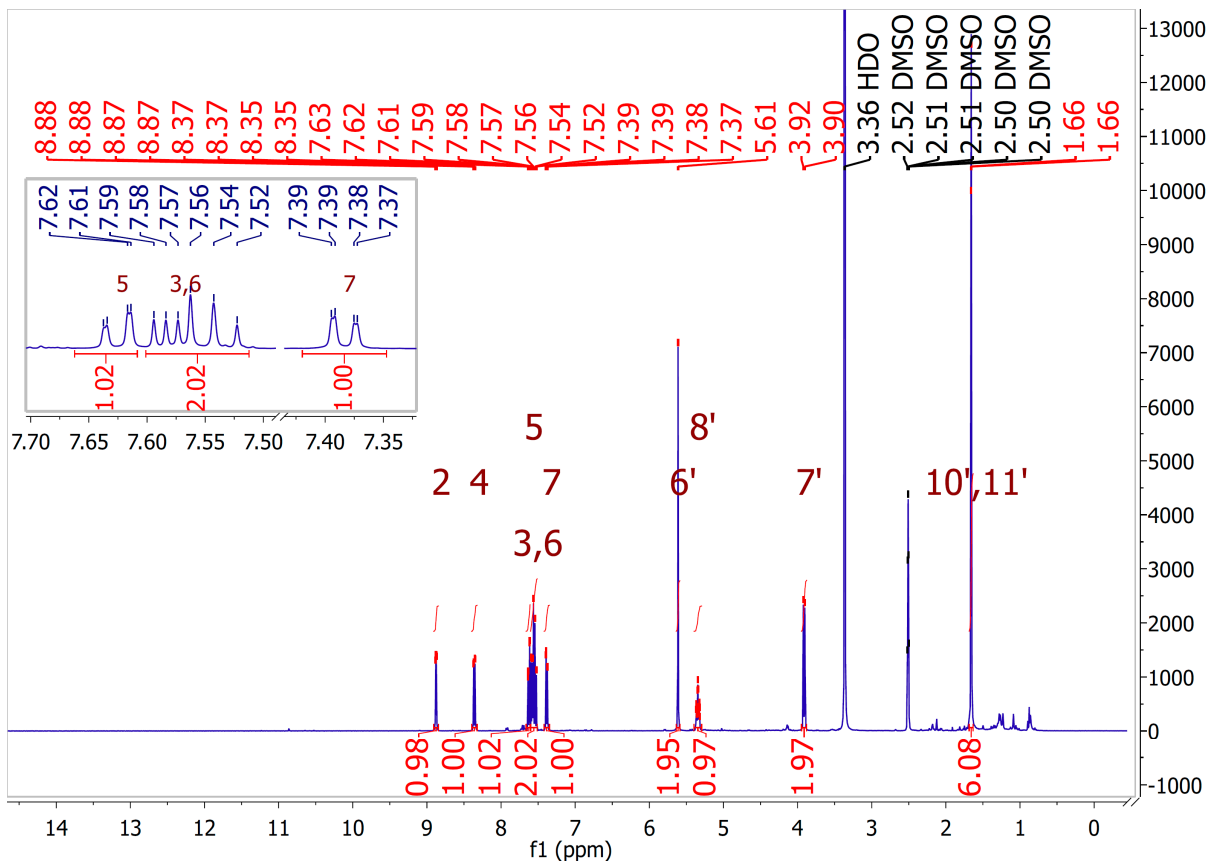
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
322.0636	322.0626	1.0	3.1	10.5	619.2	0.0	C15 H13 N3 O2 Na S



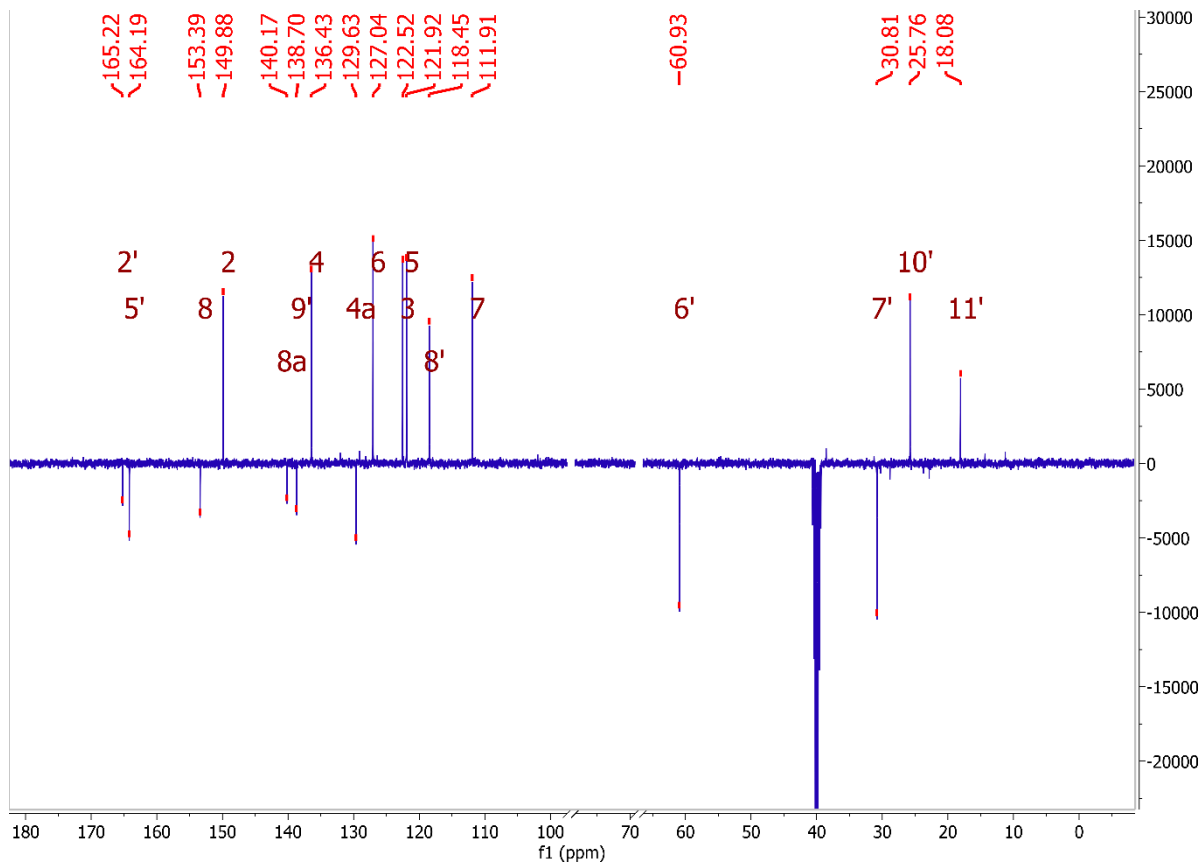
2-[(3-methylbut-2-en-1-yl)thio]-5-[(quinolin-8-yloxy)methyl]-1,3,4-oxadiazole (**4g**)



<sup>1</sup>H NMR



<sup>13</sup>C NMR



## HRMS

### Elemental Composition Report\_Compound 4g

#### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

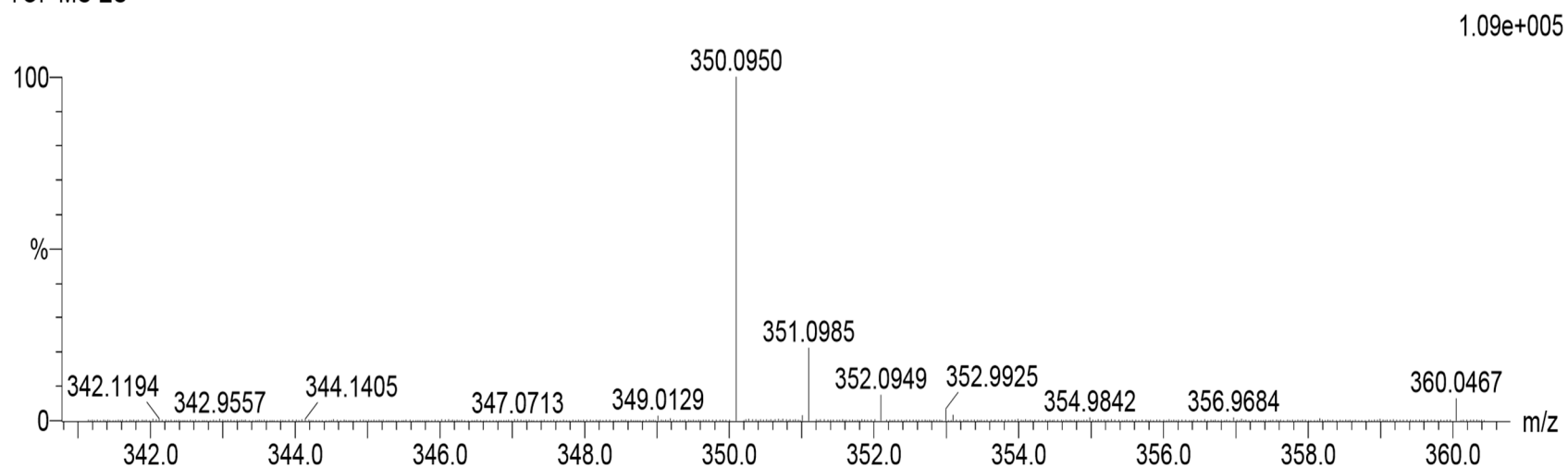
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

26 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) Elements Used:

C: 15-20 H: 15-20 N: 0-5 O: 0-5 Na: 1-1 S: 0-1

TOF MS ES+



Minimum:

-1.5

Maximum:

5.0

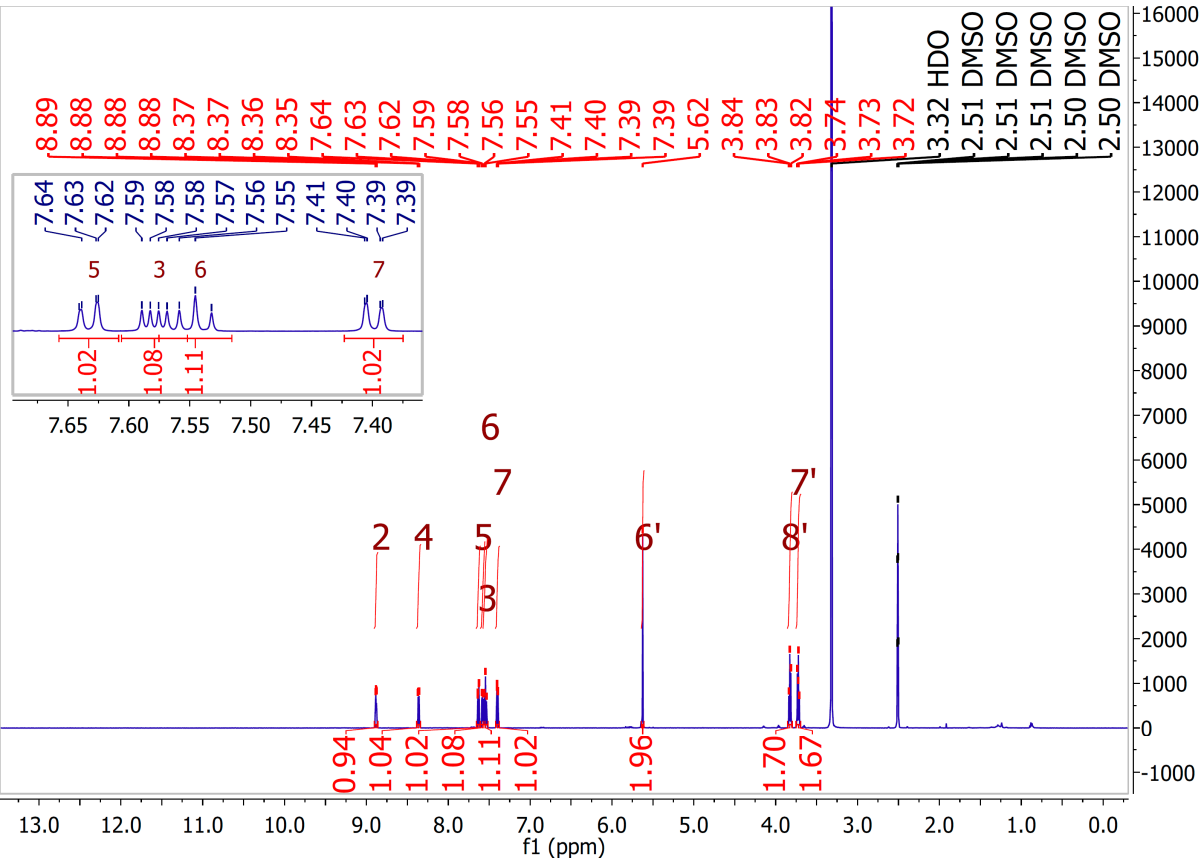
5.0

500.0

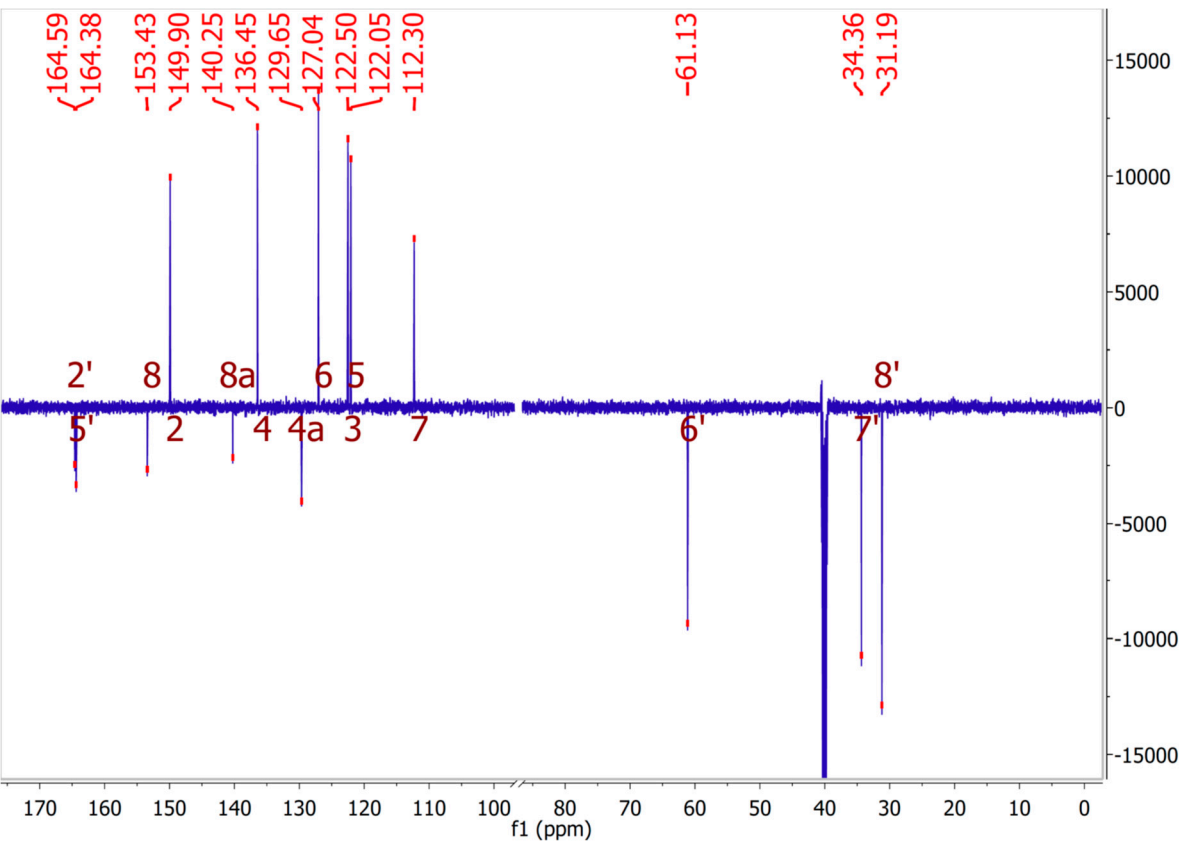
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
350.0950	350.0939	1.1	3.1	10.5	558.3	0.0	C17 H17 N3 O2 Na S

2-[(2-bromoethyl)thio]-5-[(quinolin-8-yloxy)methyl]-1,3,4-oxadiazole (**4h**)

<sup>1</sup>H NMR



<sup>13</sup>C NMR



## HRMS

### Elemental Composition Report\_Compound 4h

#### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

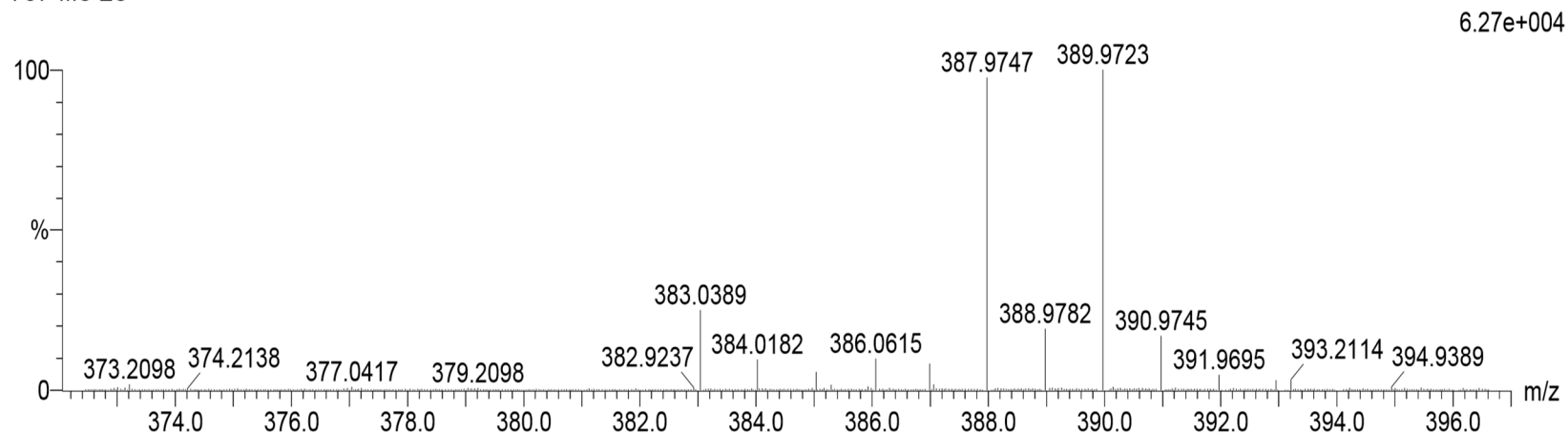
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

98 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) Elements Used:

C: 10-15 H: 10-15 N: 0-5 O: 0-5 Na: 1-1 S: 0-1 Br: 0-1

TOF MS ES+



Minimum:

-1.5

Maximum:

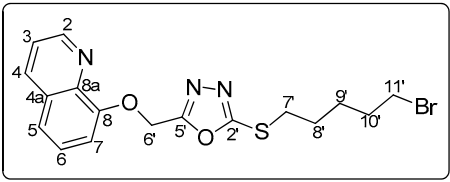
5.0

5.0

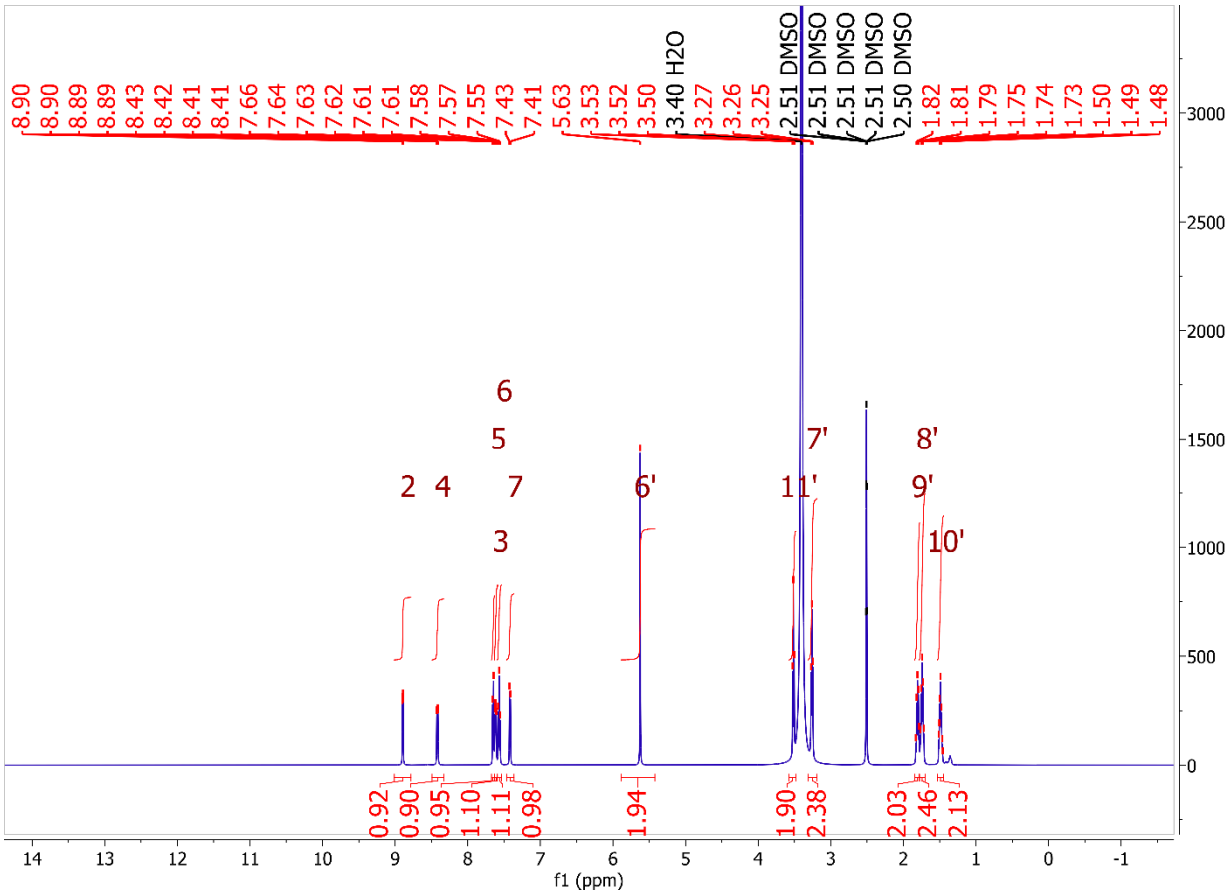
500.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)				Formula			
387.9747	387.9731	1.6	4.1	9.5	553.1	0.0	C14	H12	N3	O2	Na	S	Br

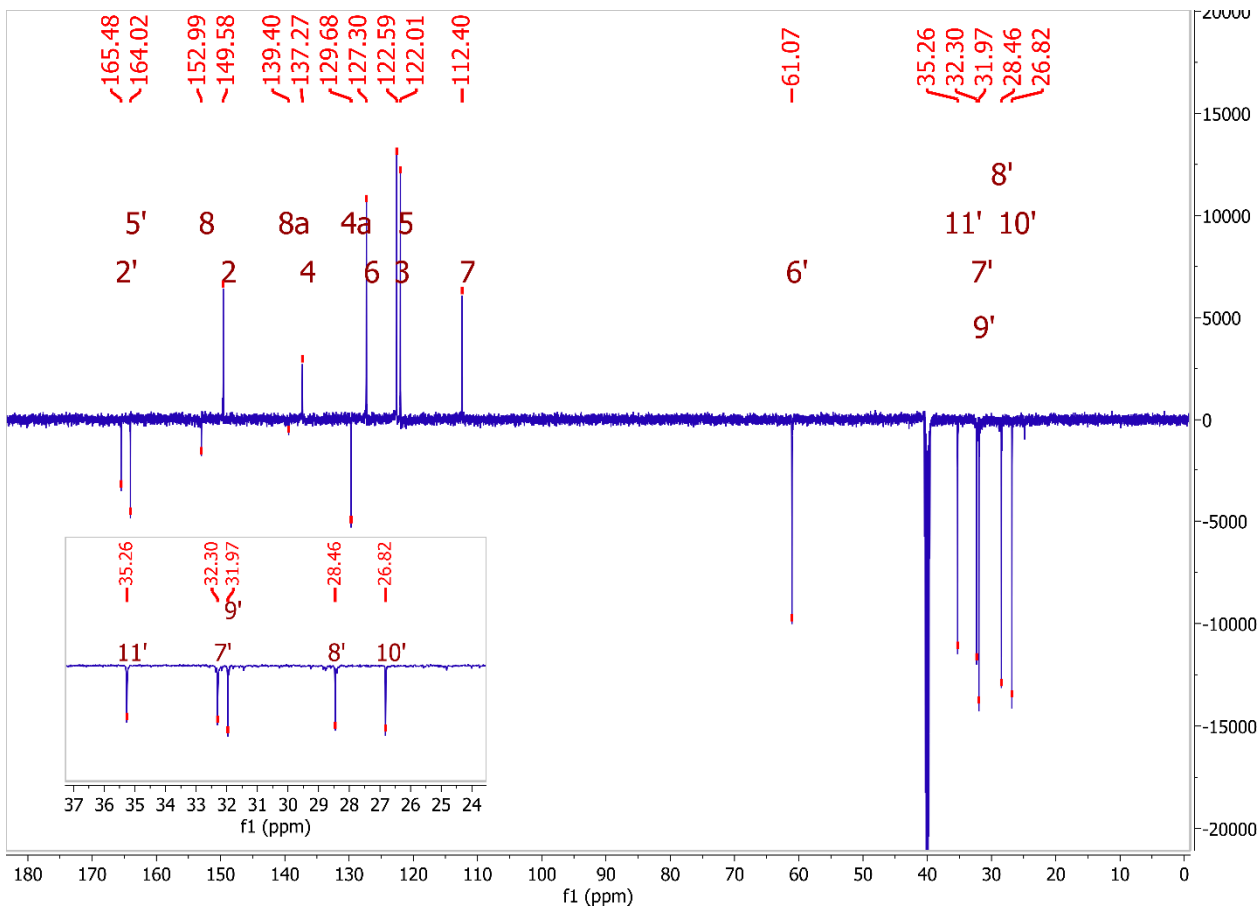
2-[(5-bromopentyl)thio]-5-[(quinolin-8-yloxy)methyl]-1,3,4-oxadiazole (4i)



<sup>1</sup>H NMR



<sup>13</sup>C NMR



## HRMS

### Elemental Composition Report\_Compound 4i

#### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

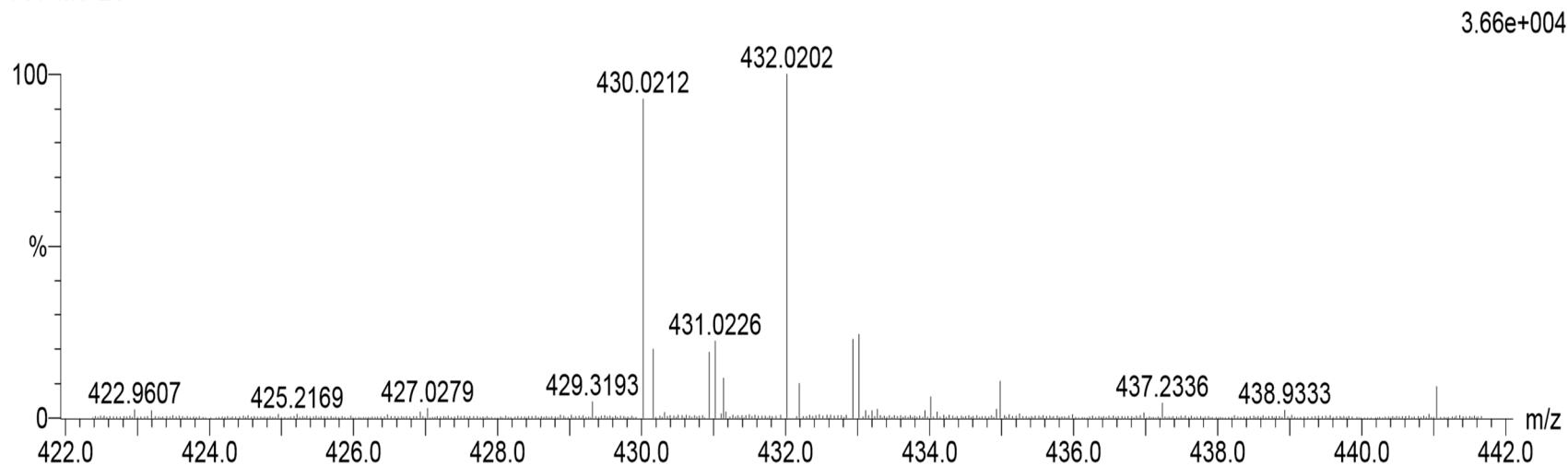
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

73 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) Elements Used:

C: 15-20 H: 15-20 N: 0-5 O: 0-5 Na: 1-1 S: 0-1 Br: 0-1

TOF MS ES+

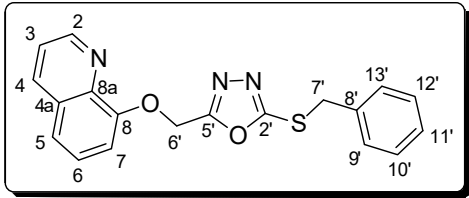


Minimum:

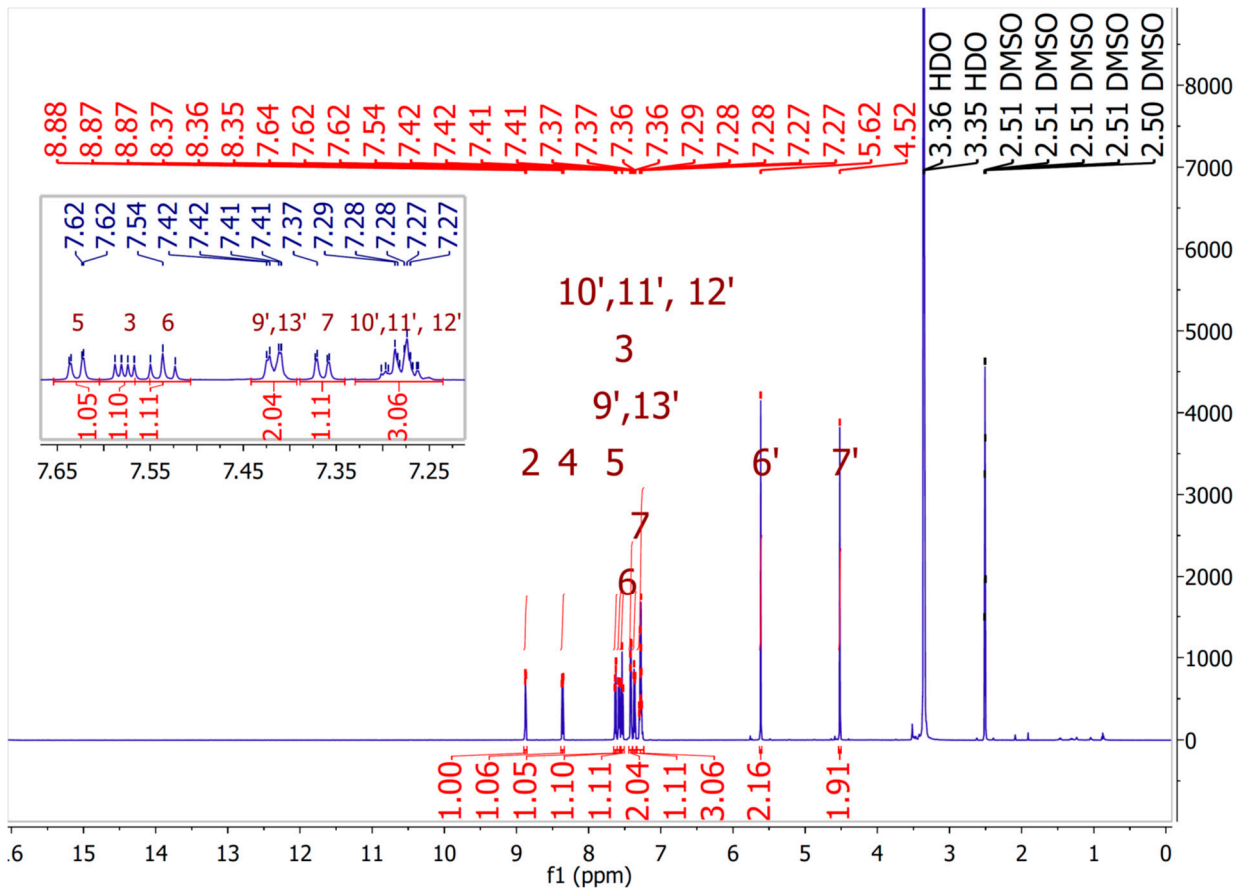
Maximum: 5.0 5.0 -1.5 500.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
430.0212	430.0201	1.1	2.6	9.5	560.0	0.0	C17 H18 N3 O2 Na S Br

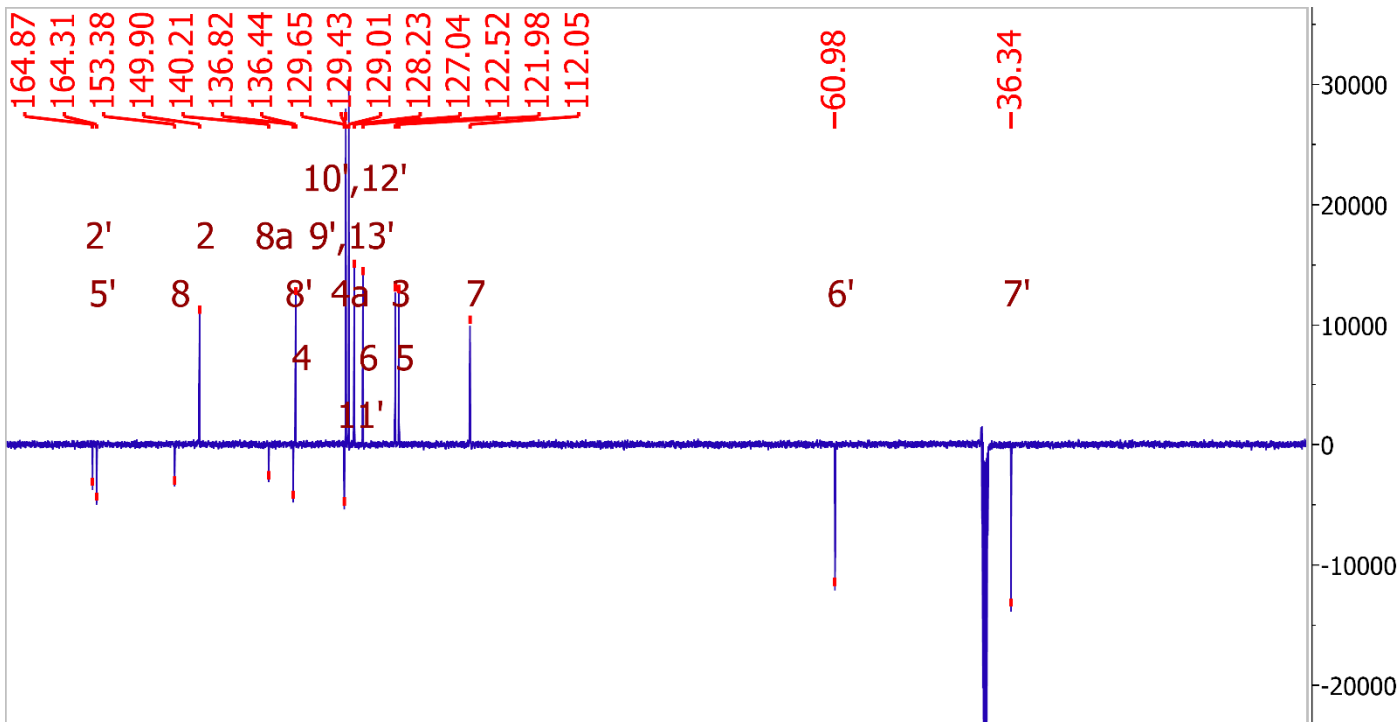
2-(benzylthio)-5-[(quinolin-8-yloxy)methyl]-1,3,4-oxadiazole (**4j**)



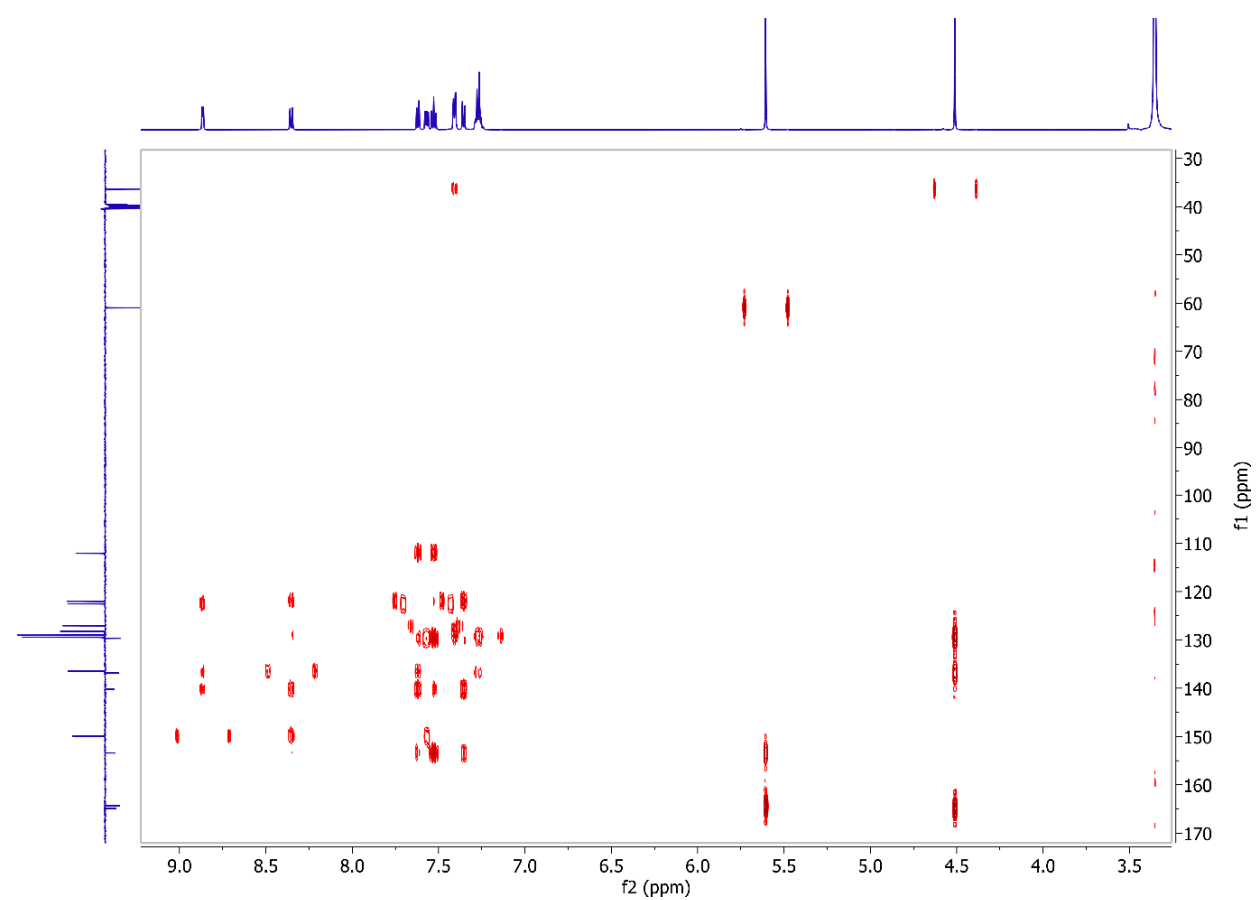
<sup>1</sup>H NMR



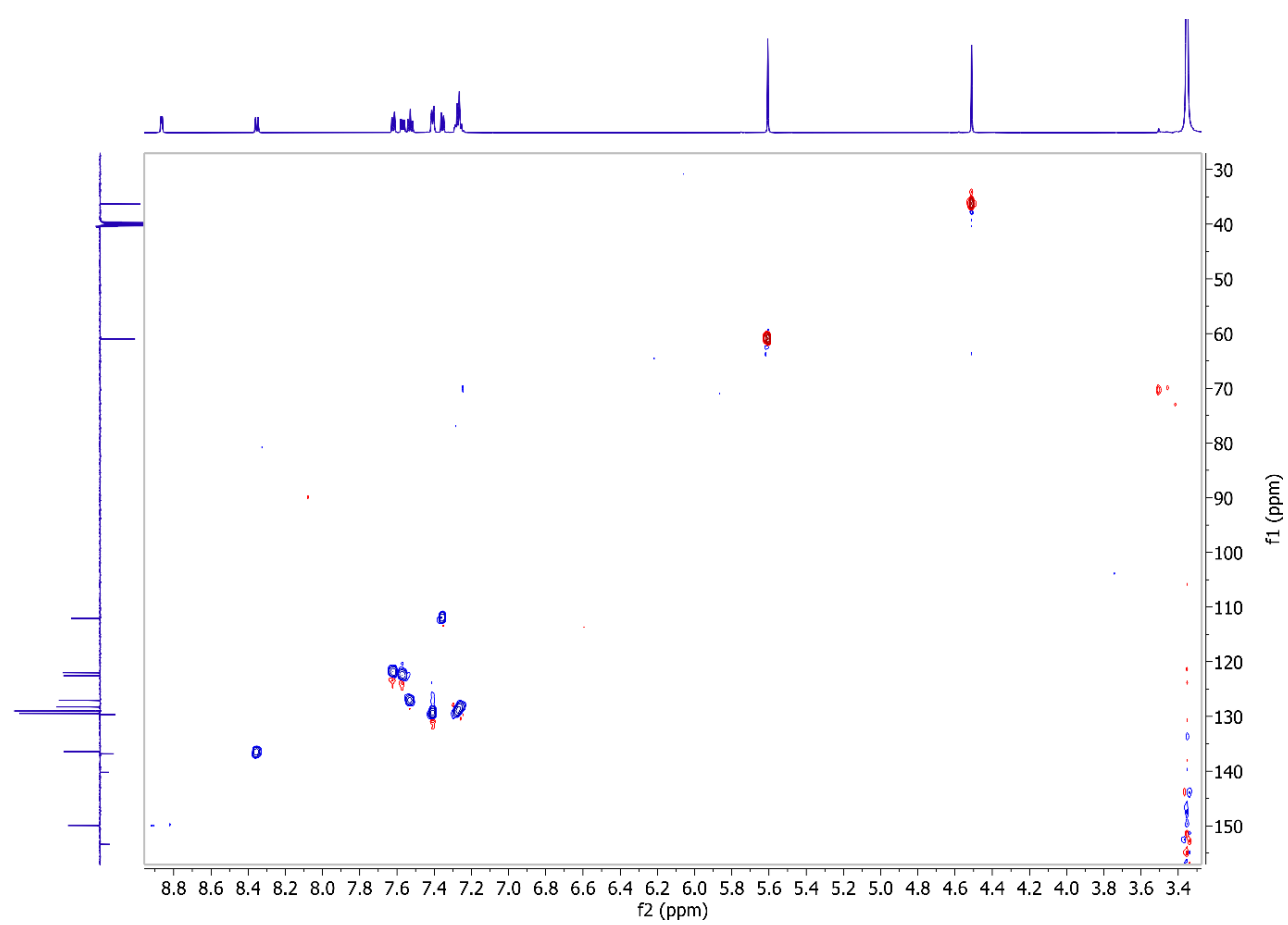
<sup>13</sup>C NMR



# HMBC



# HSQC





## HRMS

### Elemental Composition Report\_Compound 4j

#### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

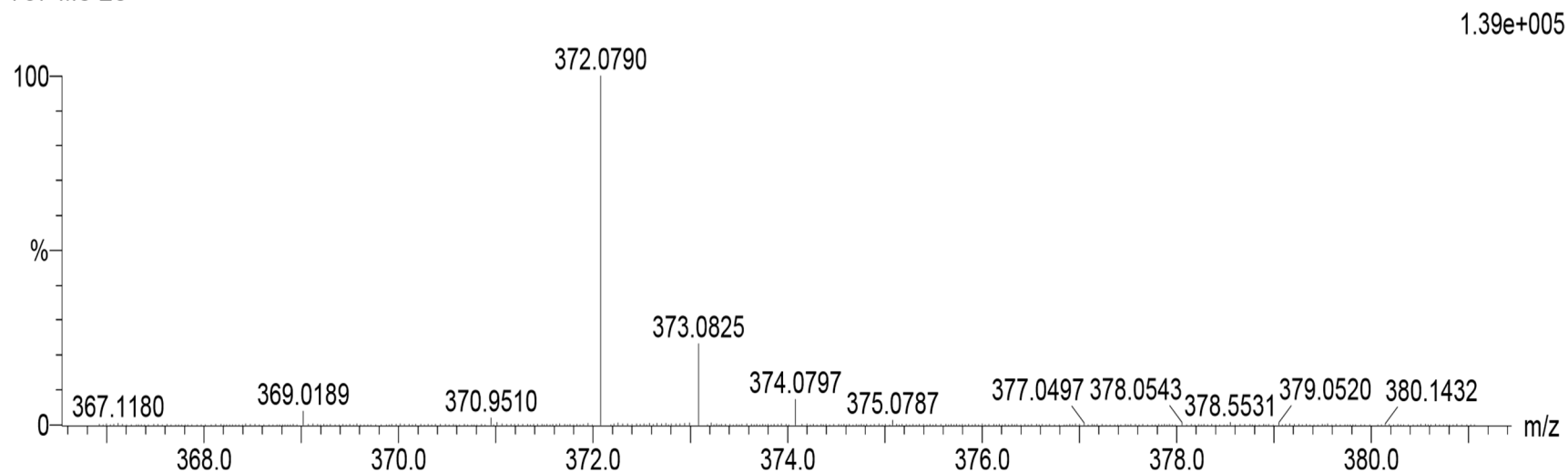
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

33 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) Elements Used:

C: 15-20 H: 15-20 N: 0-5 O: 0-5 Na: 1-1 S: 0-1

TOF MS ES+

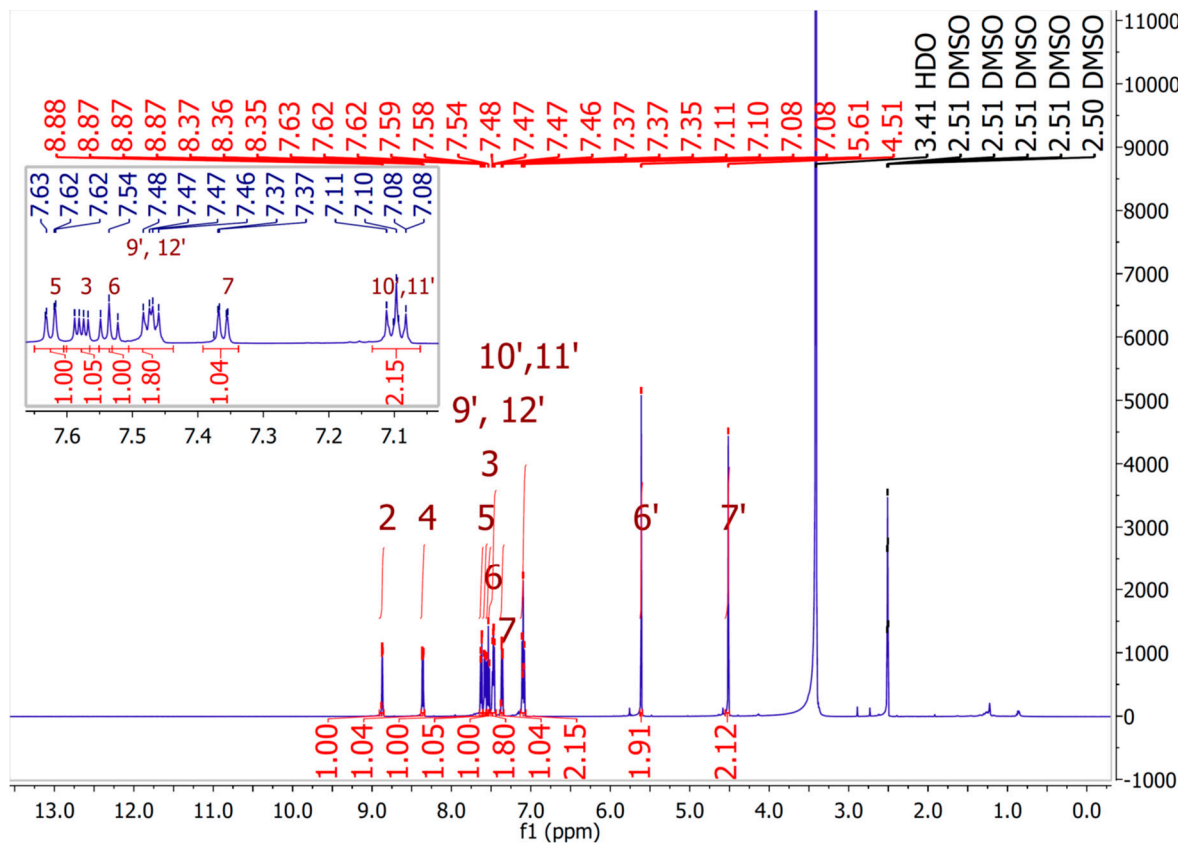
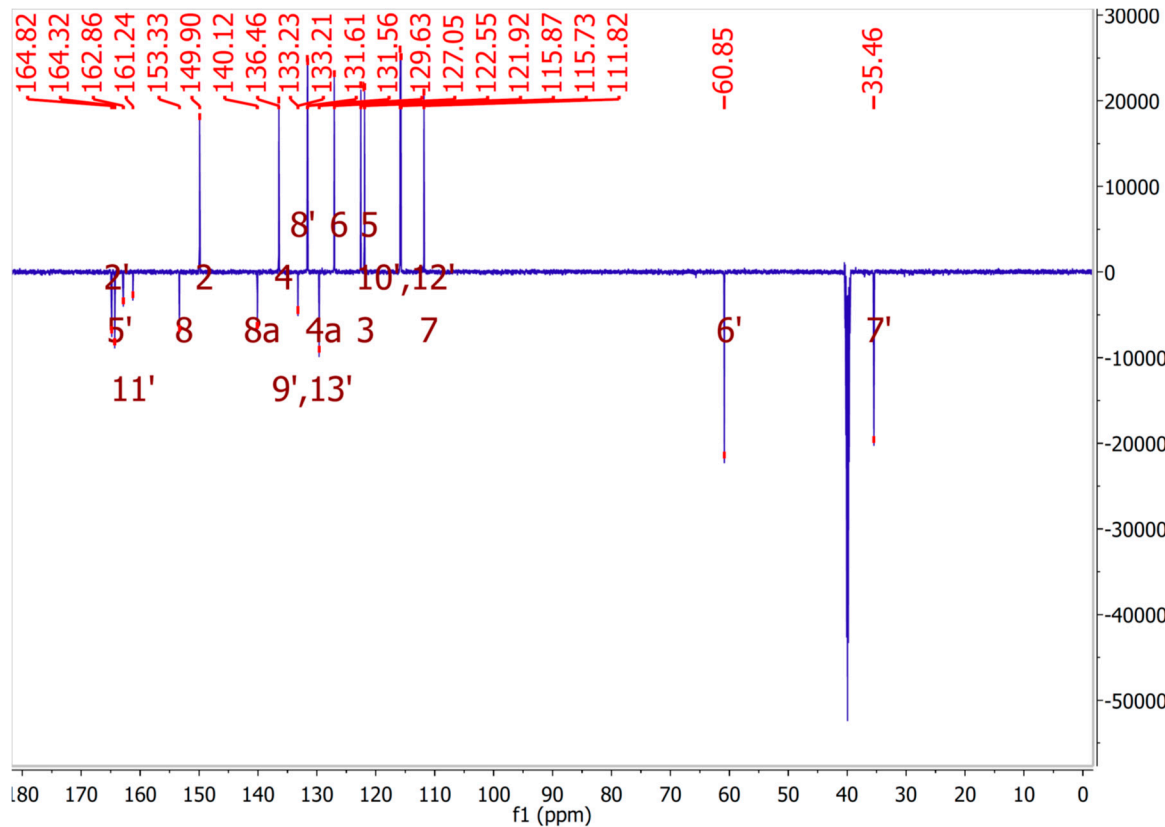


Minimum: -1.5  
Maximum: 5.0 5.0 500.0

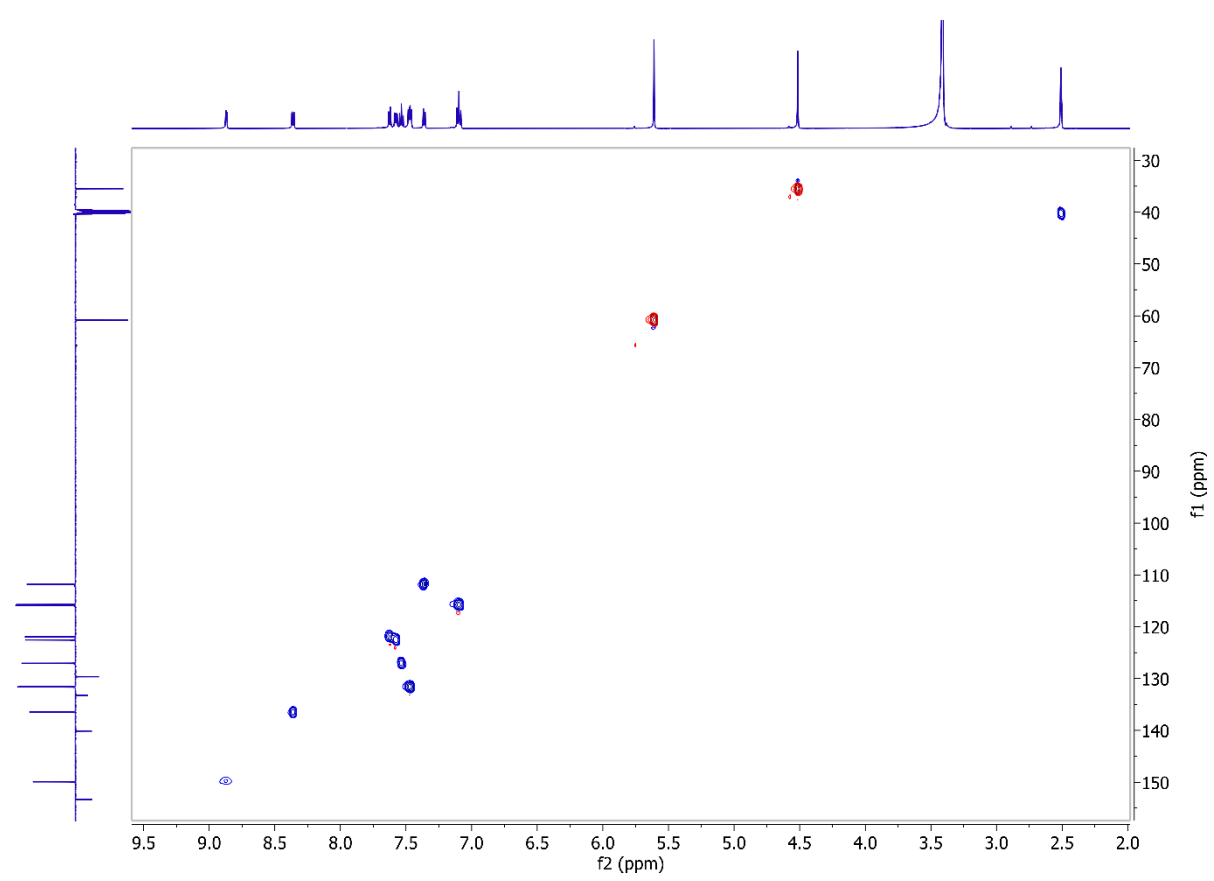
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
372.0790	372.0783	0.7	1.9	13.5	585.5	0.0	C19 H15 N3 O2 Na

2-([4-fluorobenzyl)thio]-5-[(quinolin-8-yloxy)methyl]-1,3,4-oxadiazole (**4k**)

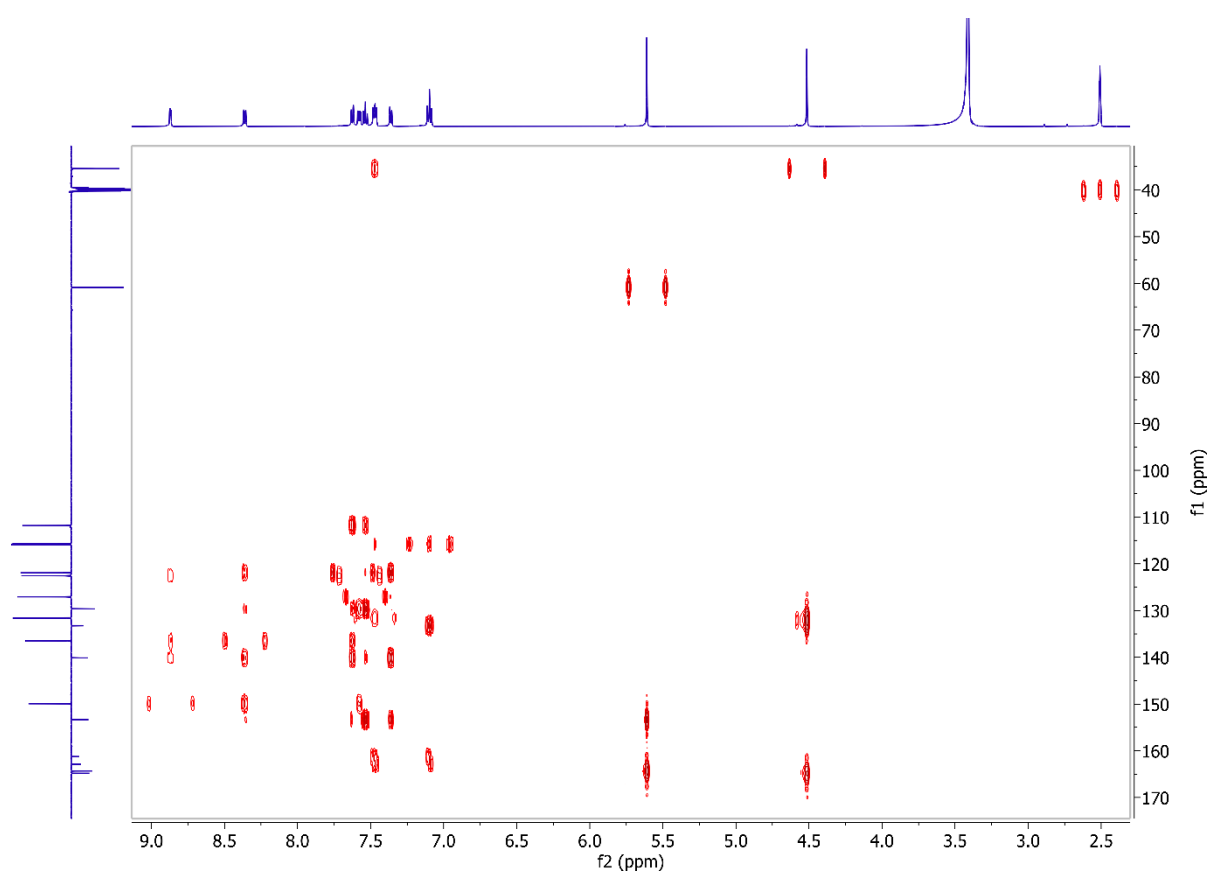
## <sup>1</sup>H NMR

<sup>13</sup>C NMR

# HSQC



# HMBC



# HRMS

## Elemental Composition Report\_Compound 4k

### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

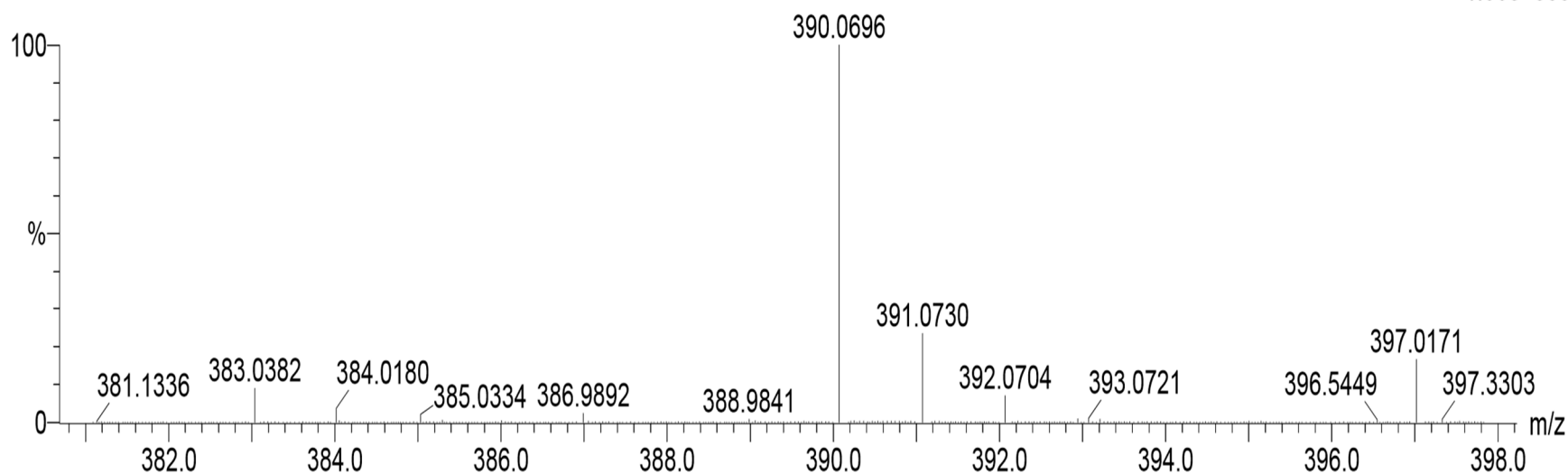
Monoisotopic Mass, Even Electron Ions

62 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) Elements Used:

C: 15-20 H: 10-15 N: 0-5 O: 0-5 Na: 1-1 S: 0-1 F: 0-1

TOF MS ES+

1.66e+005



Minimum:

-1.5

Maximum:

5.0

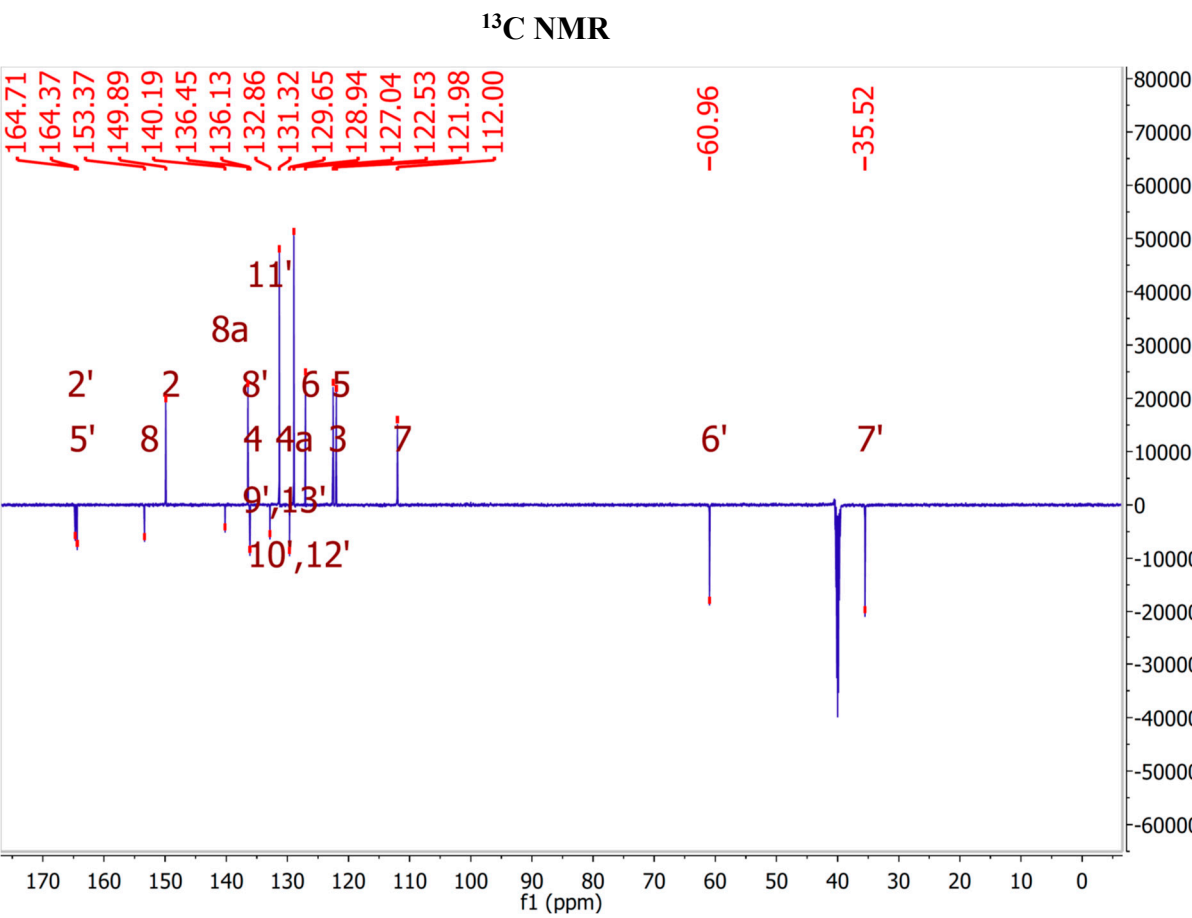
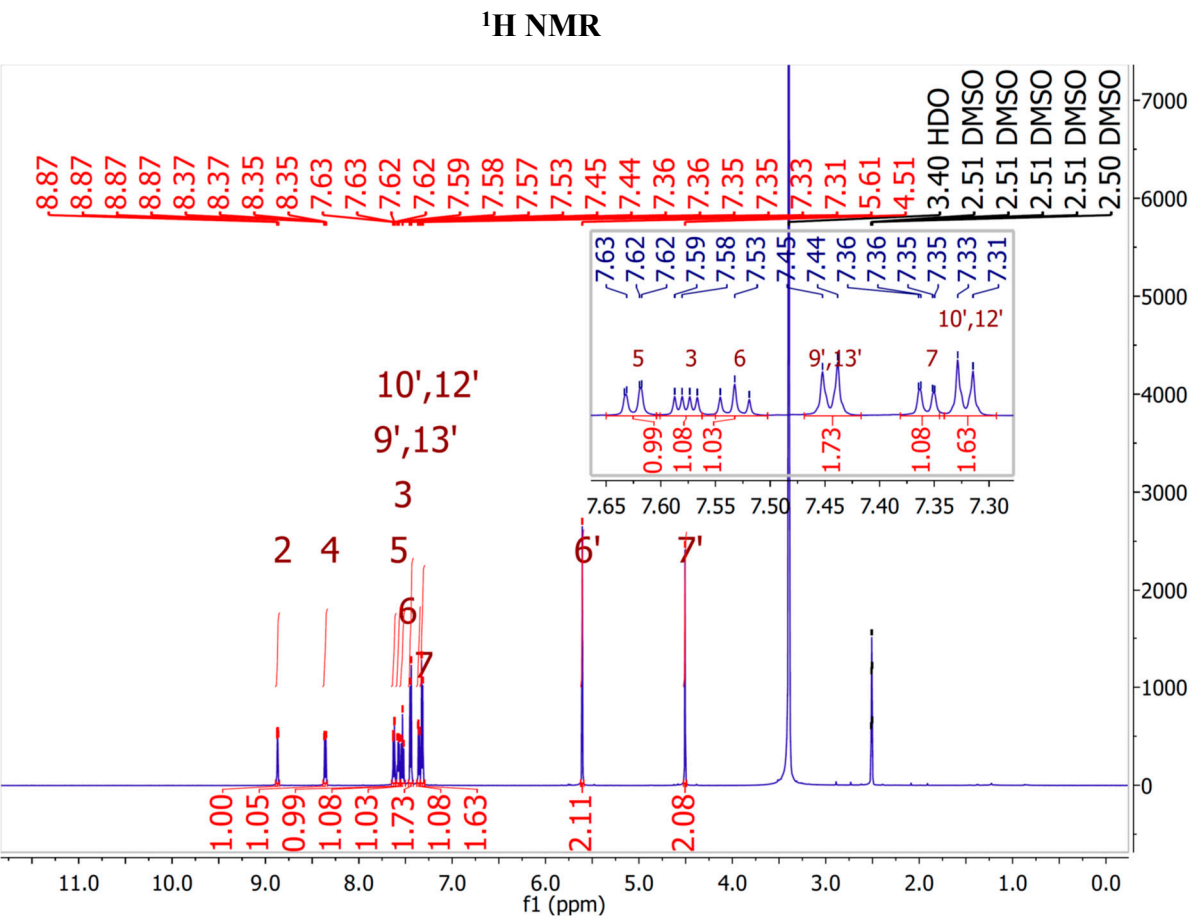
5.0

500.0

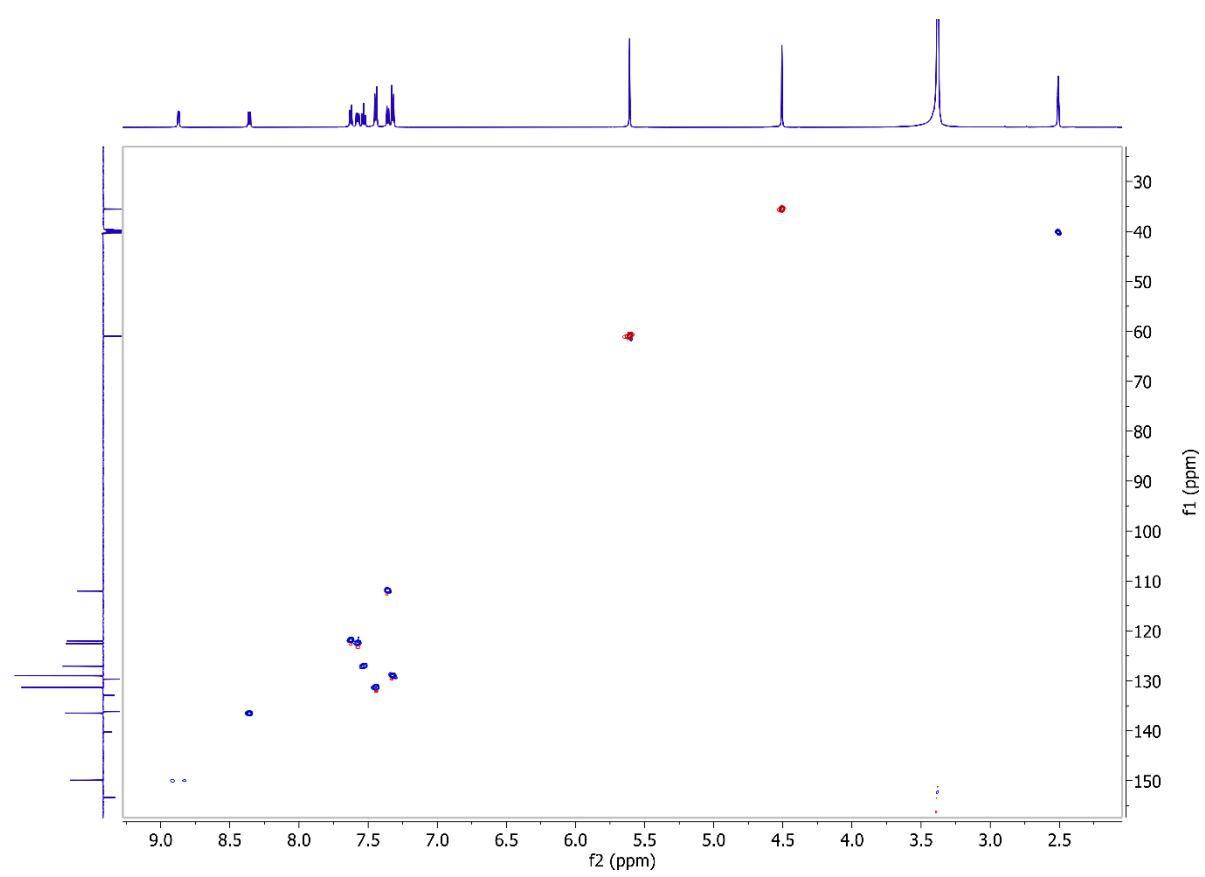
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
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390.0696	390.0688	0.8	2.1	13.5	582.5	0.0	C19 H14 N3 O2 Na S F
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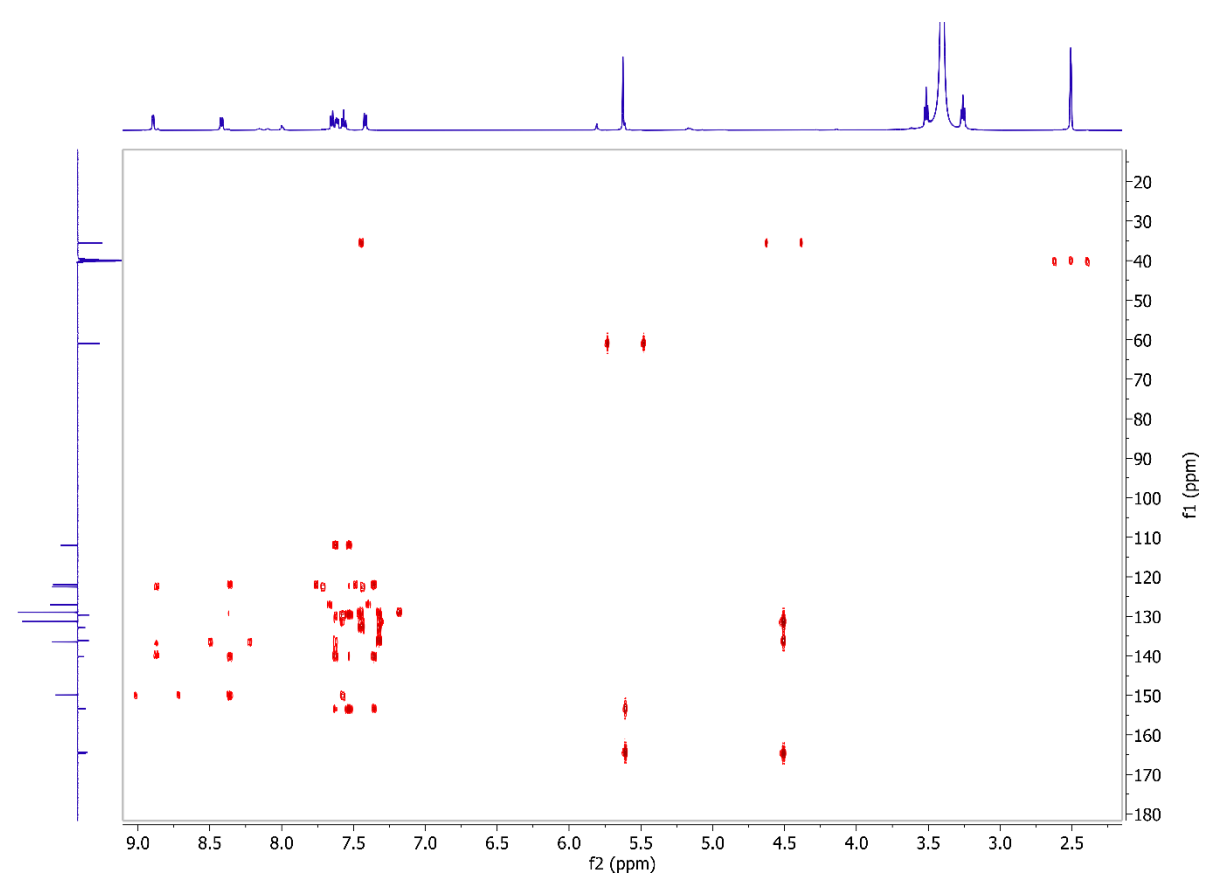
2-[(4-chlorobenzyl)thio]-5-[(quinolin-8-yloxy)methyl]-1,3,4-oxadiazole (41)



HSQC



HMBC



## HRMS

### Elemental Composition Report\_Compound 4l

#### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

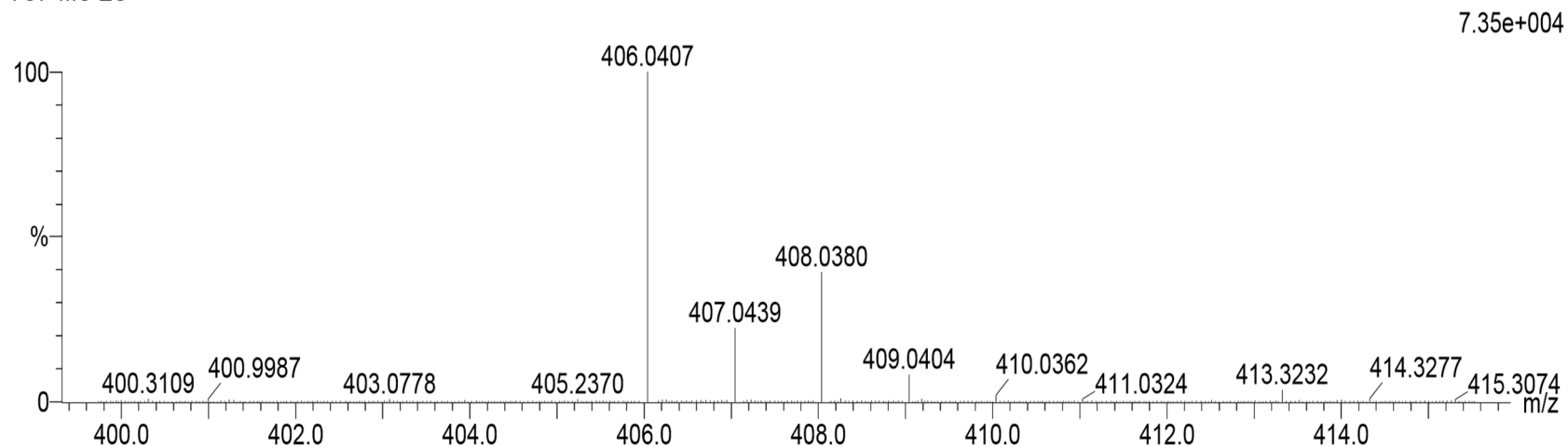
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

67 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) Elements Used:

C: 15-20 H: 10-15 N: 0-5 O: 0-5 Na: 1-1 S: 0-1 Cl: 0-1

TOF MS ES+



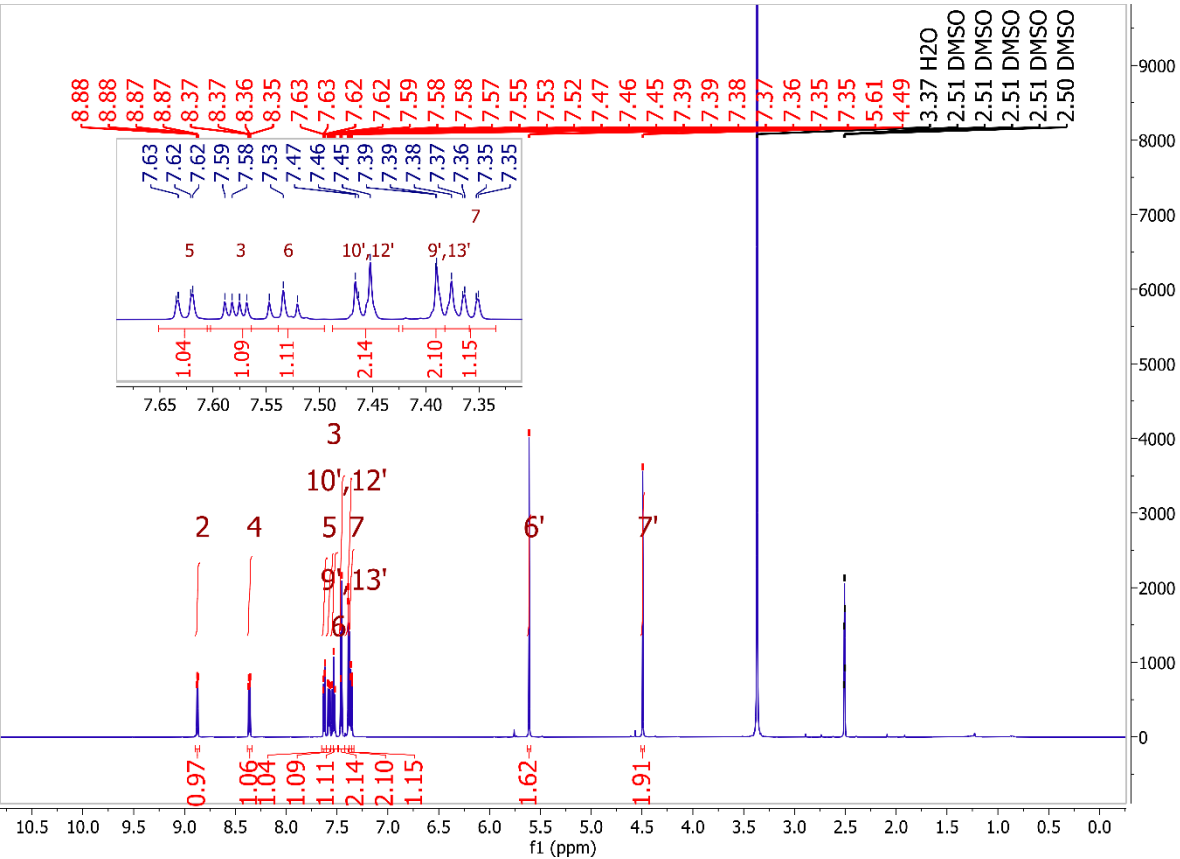
Minimum: -1.5

Maximum: 5.0 5.0 500.0

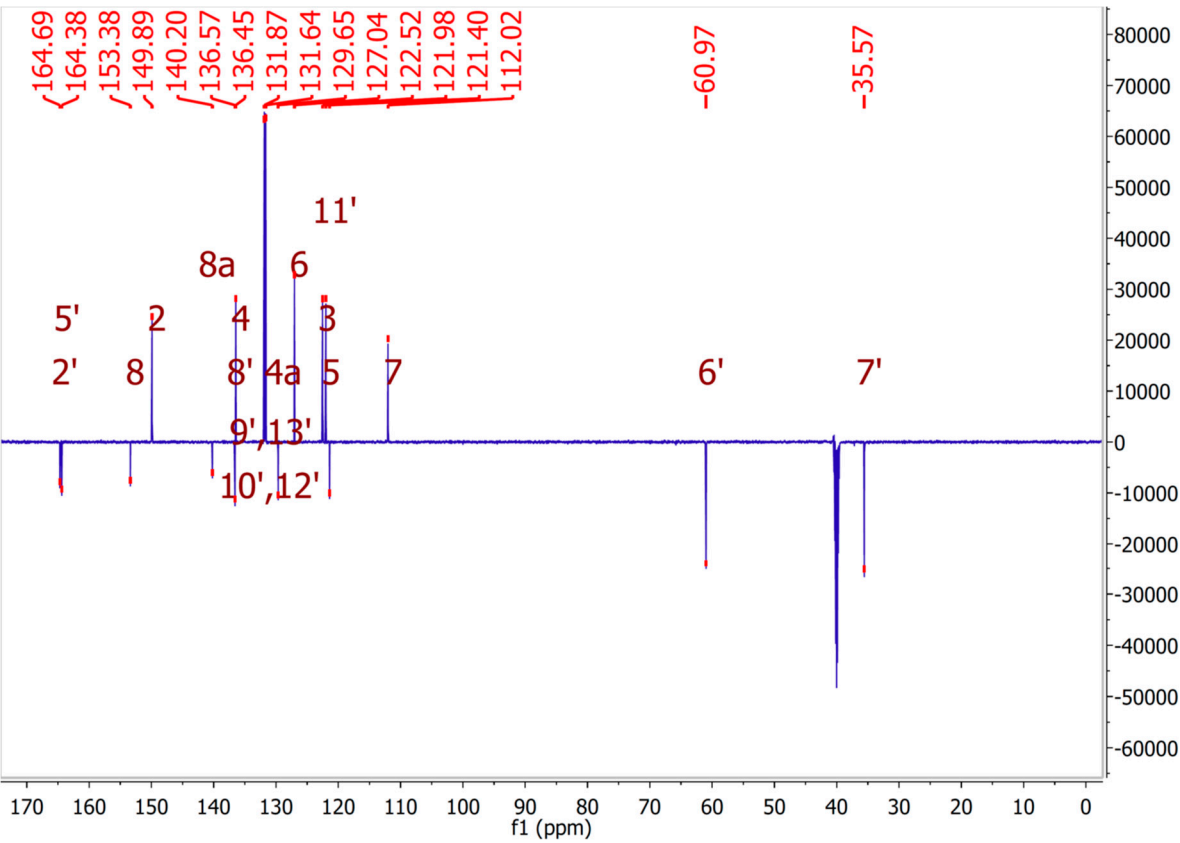
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
406.0407	406.0393	1.4	3.4	13.5	525.4	0.0	C19 H14 N3 O2 Na S Cl

2-[(4-bromobenzyl)thio]-5-[(quinolin-8-yloxy)methyl]-1,3,4-oxadiazole (**4m**)

<sup>1</sup>H NMR



<sup>13</sup>C NMR





## HRMS

### Elemental Composition Report\_Compound 4m

#### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

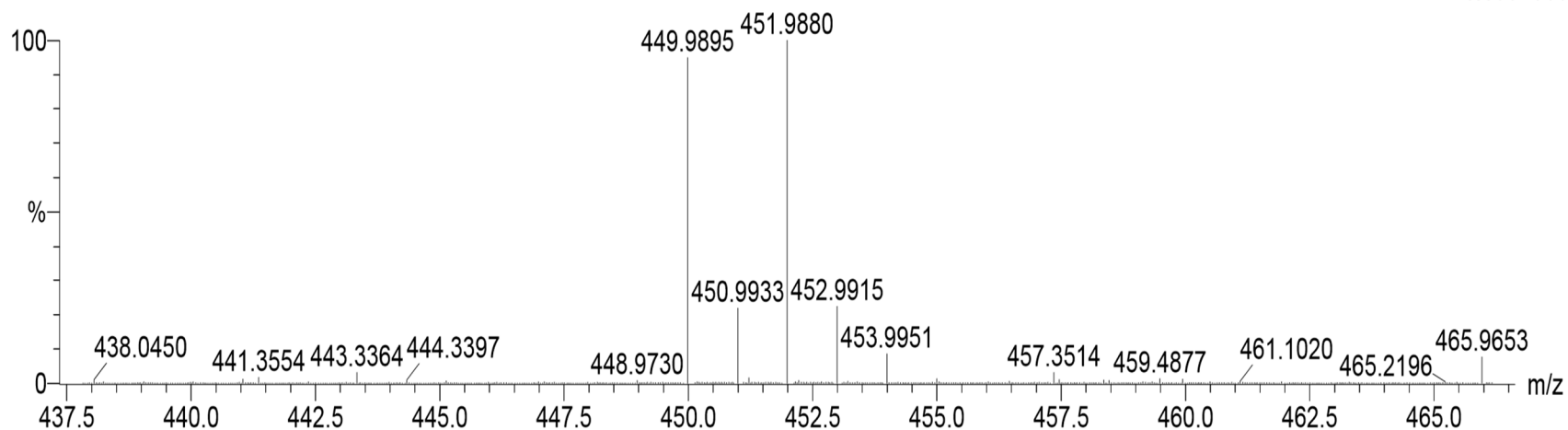
Monoisotopic Mass, Even Electron Ions

90 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) Elements Used:

C: 15-20 H: 10-15 N: 0-5 O: 0-5 Na: 1-1 S: 0-1 Br: 0-1

TOF MS ES+

1.15e+005



Minimum:

-1.5

Maximum:

5.0

5.0

500.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
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449.9895	449.9888	0.7	1.6	13.5	541.5	0.0	C19 H14 N3 O2 Na S Br
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## HRMS

### Elemental Composition Report\_Compound 4n

#### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

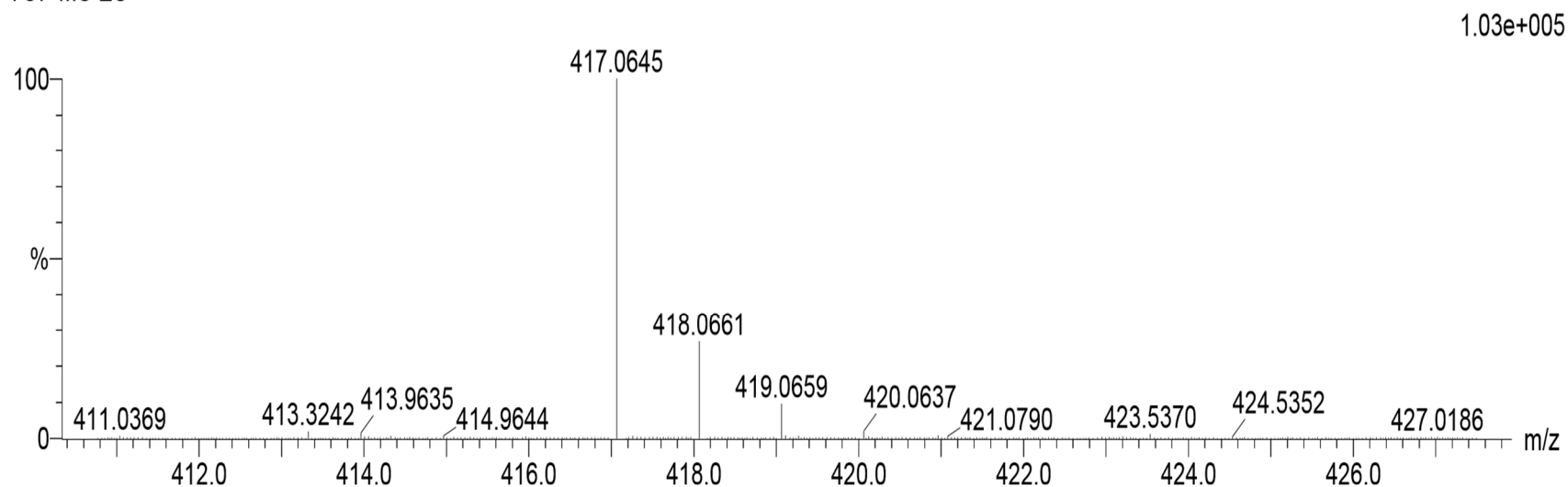
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

46 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) Elements Used:

C: 15-20 H: 10-15 N: 0-5 O: 0-5 Na: 1-1 S: 0-1

TOF MS ES+



Minimum:

-1.5

Maximum:

5.0

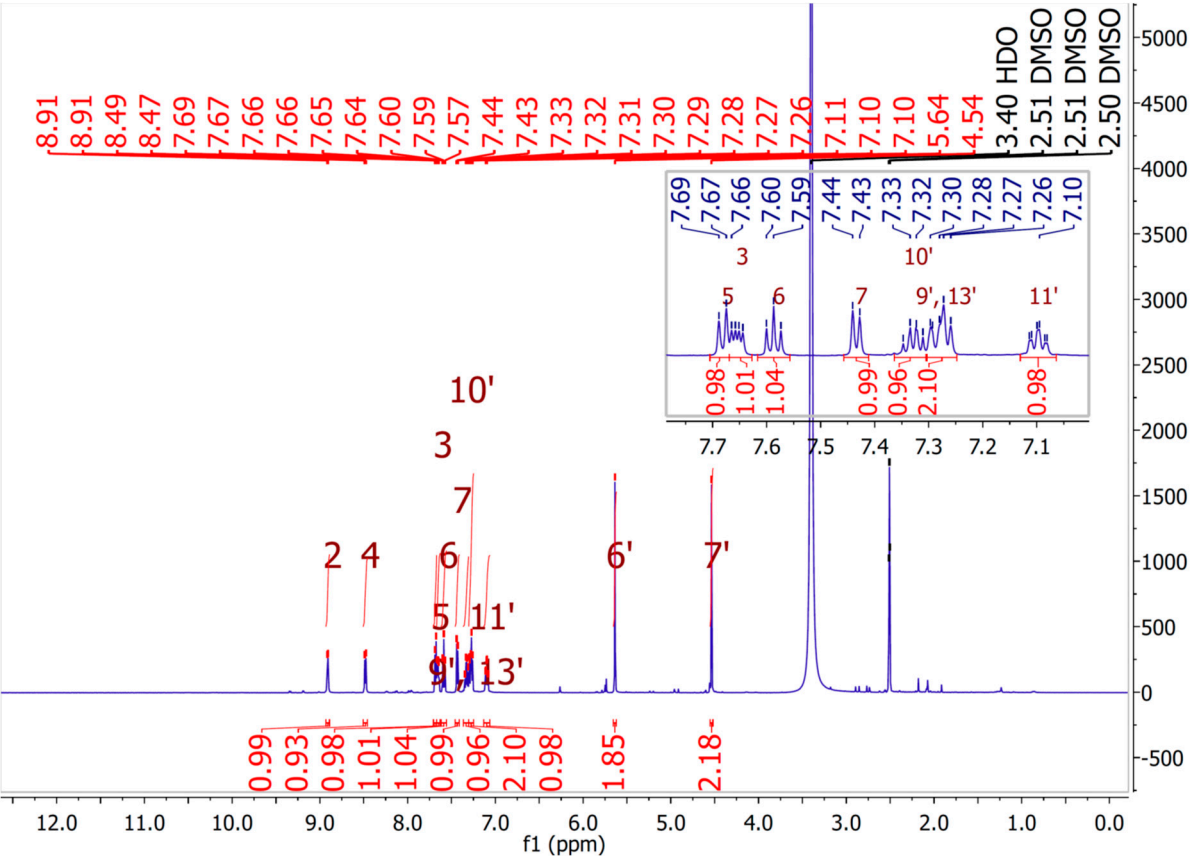
5.0

500.0

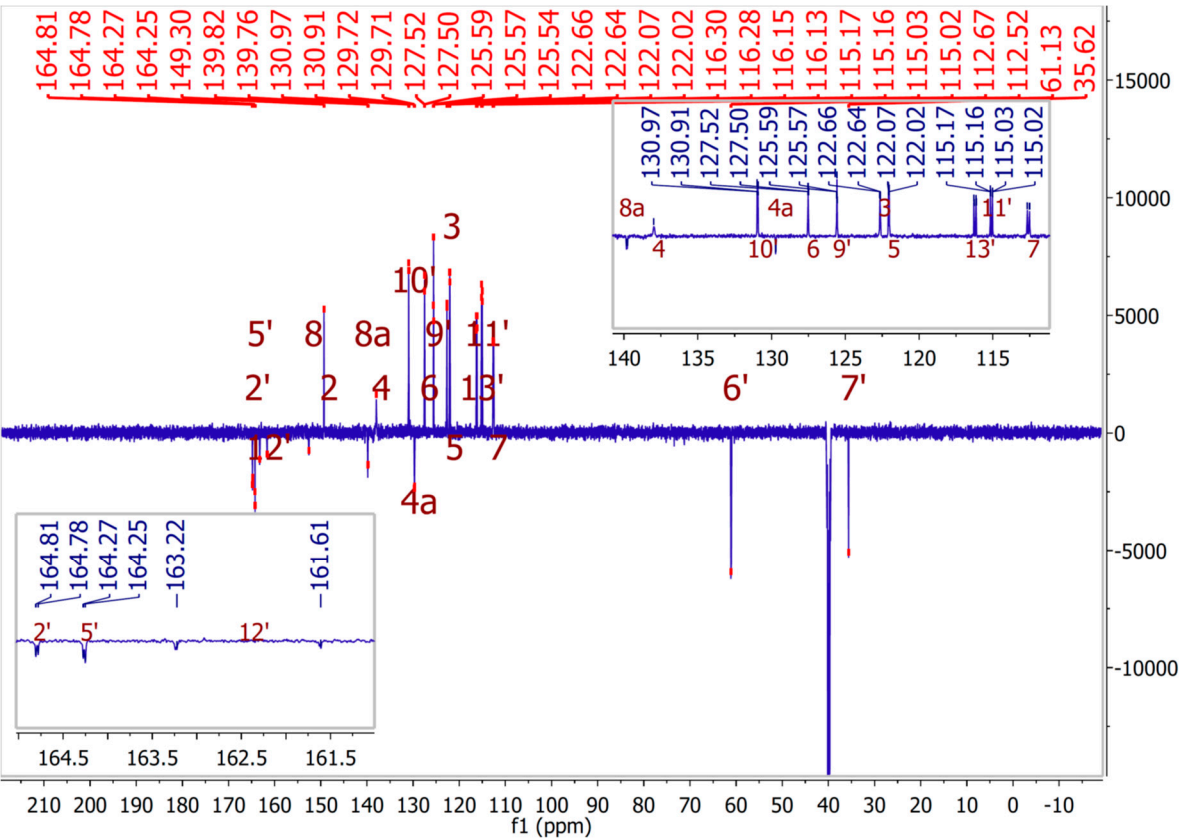
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
417.0645	417.0633	1.2	2.9	14.5	557.5	0.0	C19 H14 N4 O4 Na S

2-[(3-fluorobenzyl)thio]-5-[(quinolin-8-yloxy)methyl]-1,3,4-oxadiazole (4o)

<sup>1</sup>H NMR



<sup>13</sup>C NMR



# HRMS

## Elemental Composition Report\_Compound 4o

### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

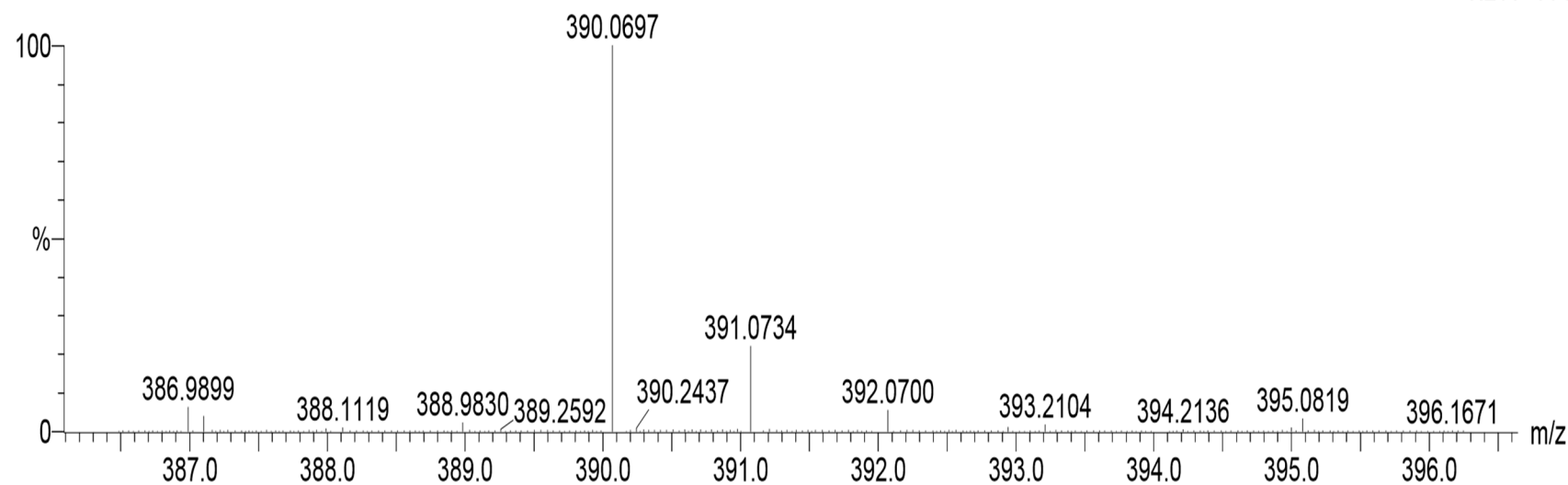
Monoisotopic Mass, Even Electron Ions

62 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) Elements Used:

C: 15-20 H: 10-15 N: 0-5 O: 0-5 Na: 1-1 S: 0-1 F: 0-1

TOF MS ES+

8.26e+004



Minimum:

-1.5

Maximum:

5.0

5.0

500.0

Mass

Calc. Mass

mDa

PPM

DBE

i-FIT

i-FIT (Norm)

Formula

390.0697

390.0688

0.9

2.3

13.5

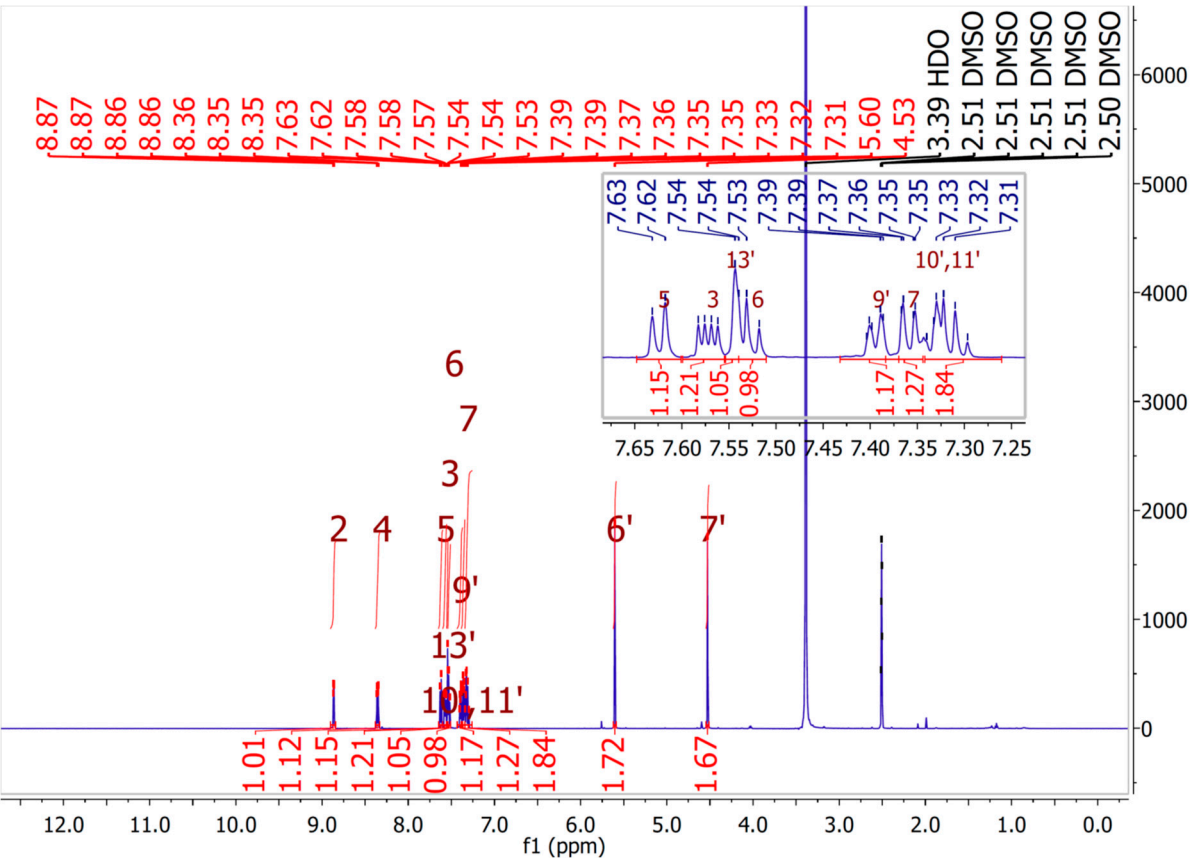
550.7

0.0

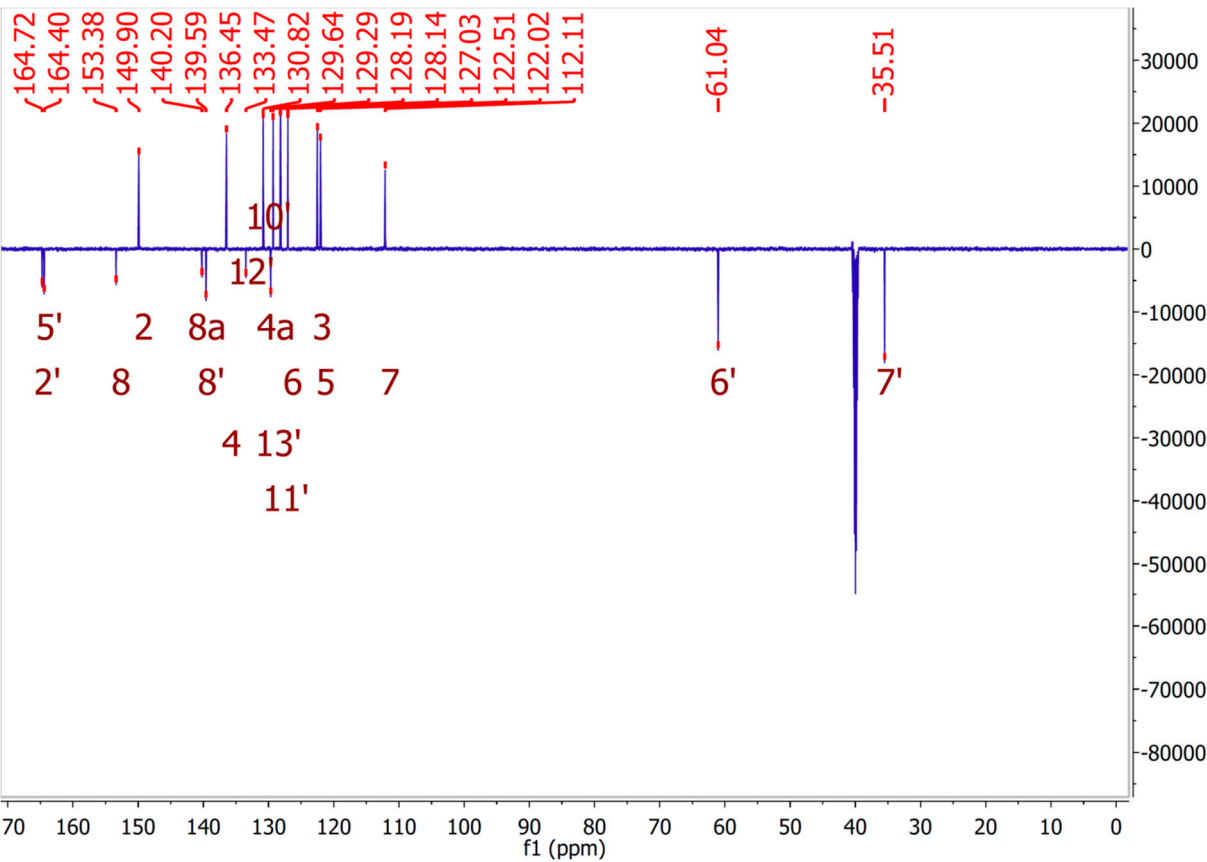
C19 H14 N3 O2 Na S F

2-[(3-chlorobenzyl)thio]-5-[(quinolin-8-yloxy)methyl]-1,3,4-oxadiazole (4p)

<sup>1</sup>H NMR



<sup>13</sup>C NMR



# HRMS

## Elemental Composition Report\_Compound 4p

### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

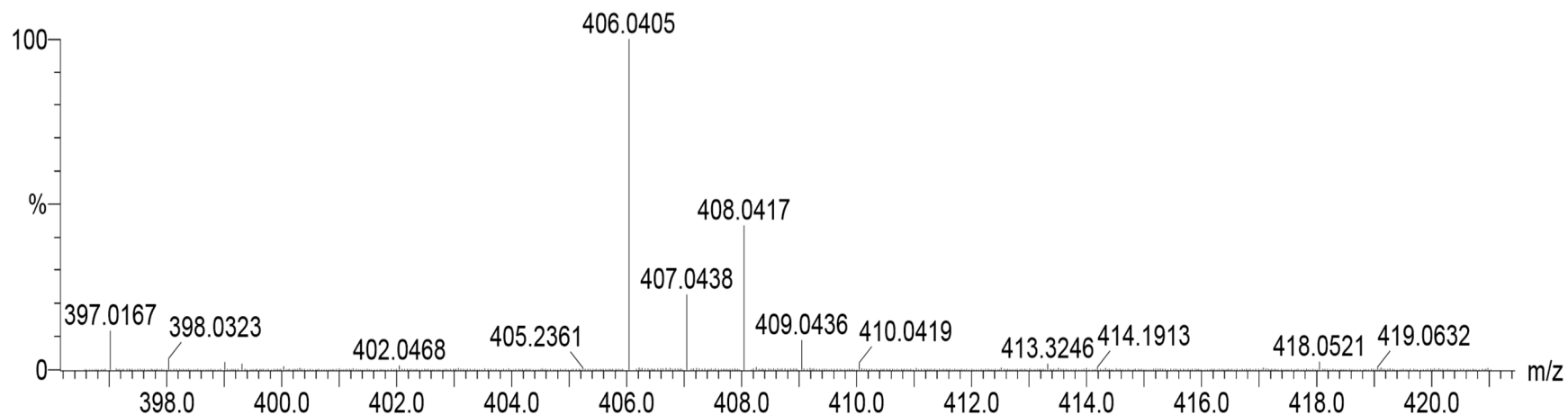
Monoisotopic Mass, Even Electron Ions

67 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) Elements Used:

C: 15-20 H: 10-15 N: 0-5 O: 0-5 Na: 1-1 S: 0-1 Cl: 0-1

9.87e+004

TOF MS ES+



Minimum:

Maximum:

5.0

5.0

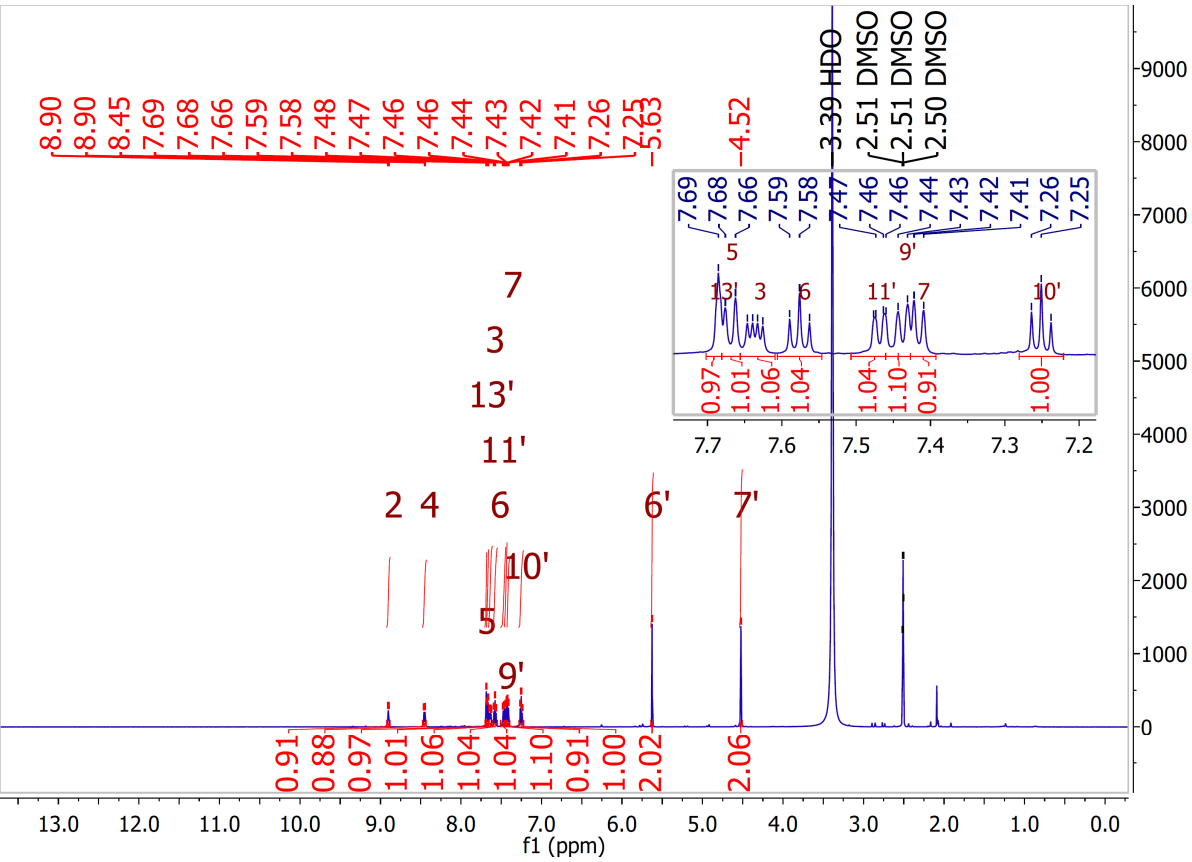
-1.5

500.0

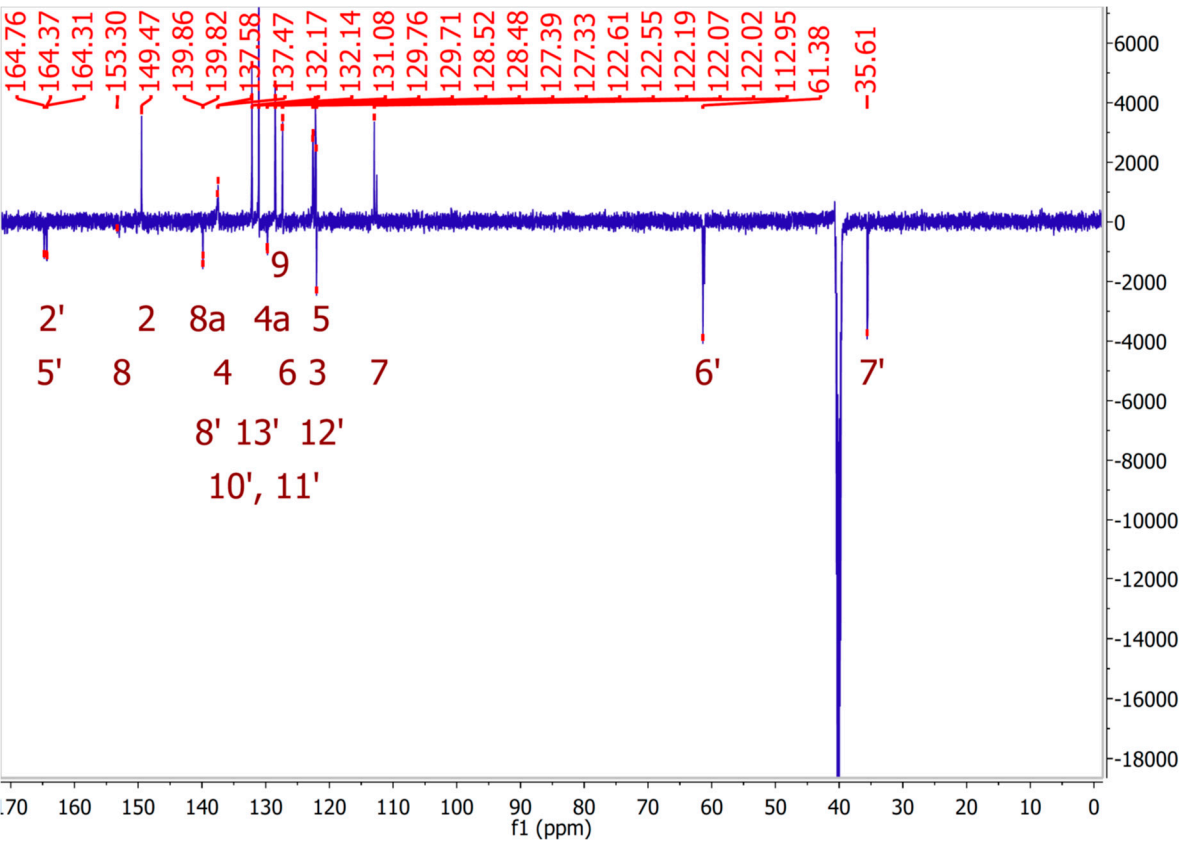
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
406.0405	406.0393	1.2	3.0	13.5	538.1	0.0	C19 H14 N3 O2 Na S Cl

2-[(3-bromobenzyl)thio]-5-[(quinolin-8-yloxy)methyl]-1,3,4-oxadiazole (**4q**)

<sup>1</sup>H NMR



<sup>13</sup>C NMR





## HRMS

### Elemental Composition Report\_Compound 4q

#### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

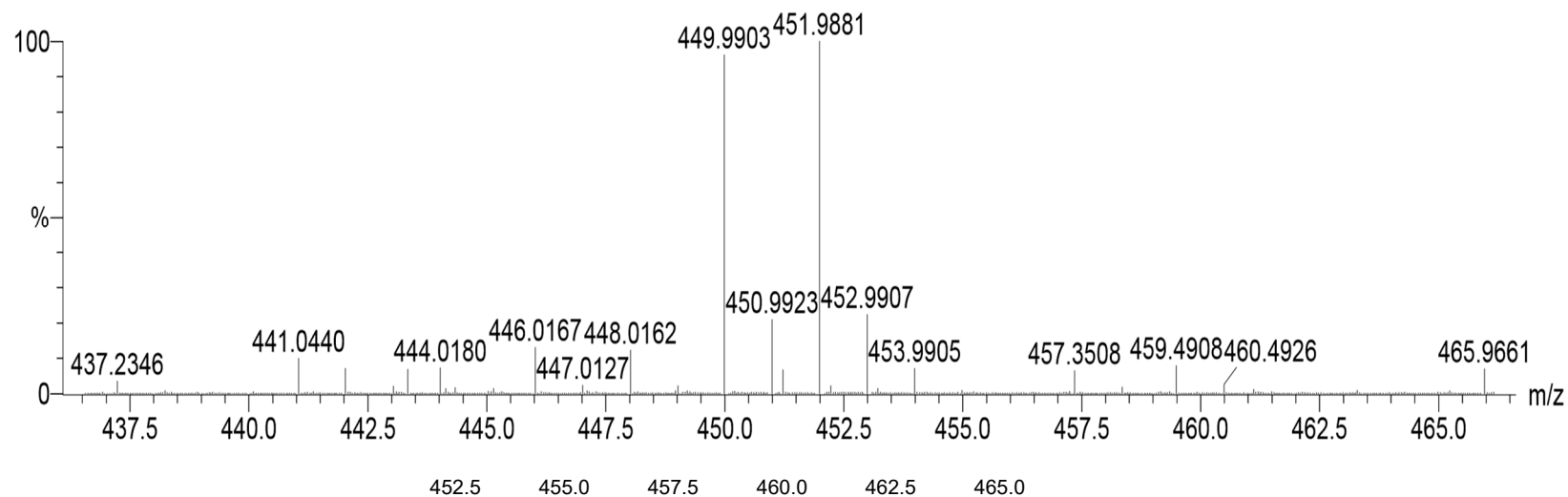
Monoisotopic Mass, Even Electron Ions

90 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) Elements Used:

C: 15-20 H: 10-15 N: 0-5 O: 0-5 Na: 1-1 S: 0-1 Br: 0-1

TOF MS ES+

5.21e+004



Minimum:

-1.5

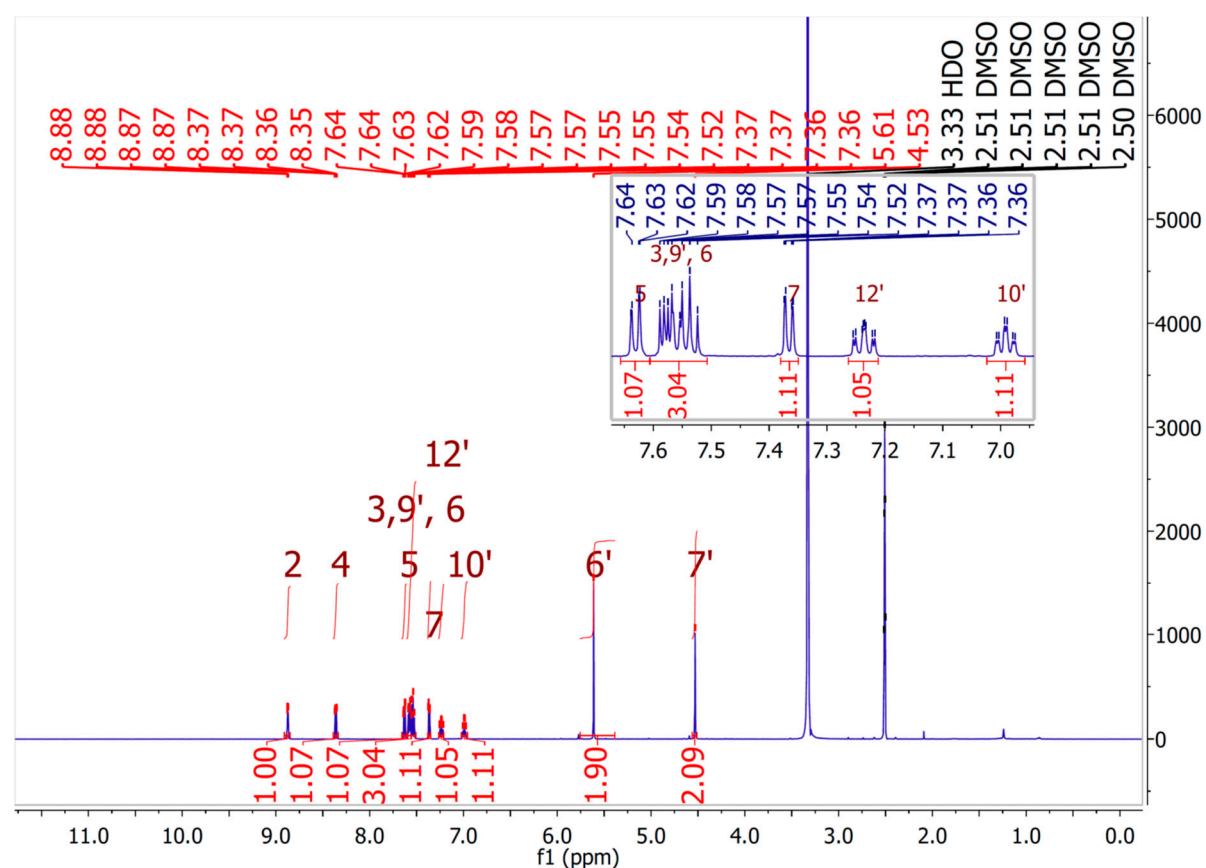
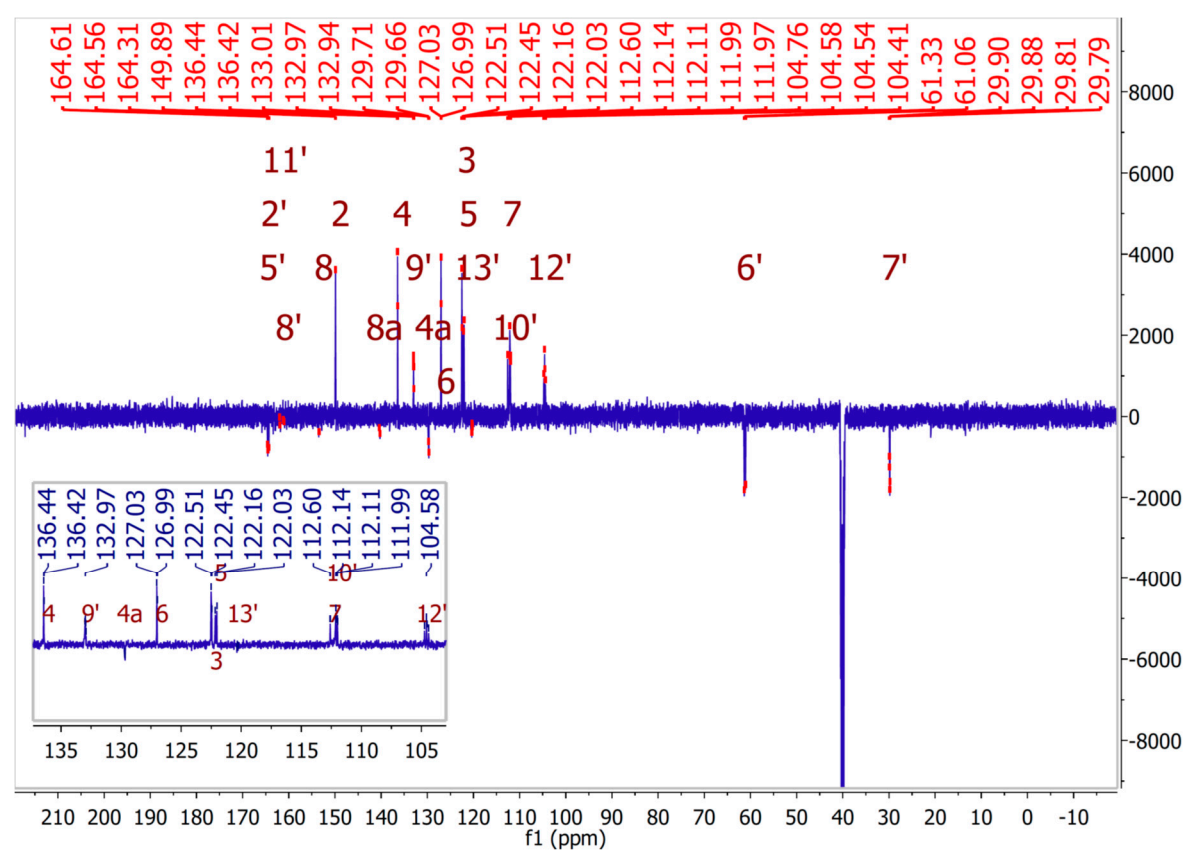
Maximum:

5.0

5.0

500.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
449.9903	449.9888	1.5	3.3	13.5	492.1	0.0	C19 H14 N3 O2 Na S Br

<sup>1</sup>H NMR<sup>13</sup>C NMR

## HRMS

### Elemental Composition Report\_Compound 4r

#### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

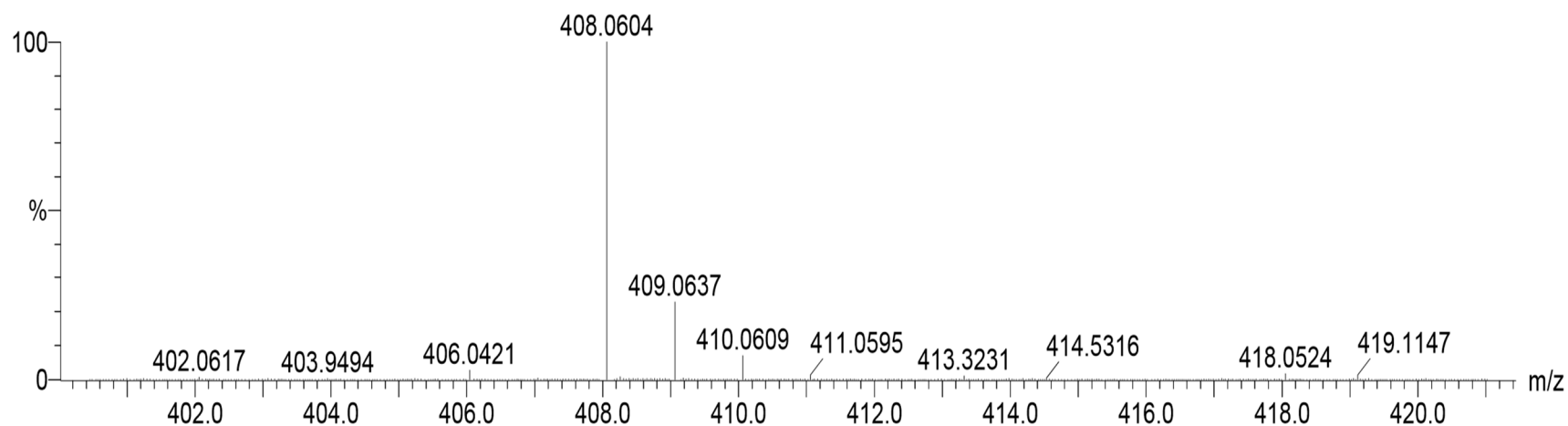
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

101 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) Elements Used:

C: 15-20 H: 10-15 N: 0-5 O: 0-5 Na: 1-1 S: 0-1 F: 0-2

TOF MS ES+



1.25e+005

Minimum:

Maximum:

5.0

5.0

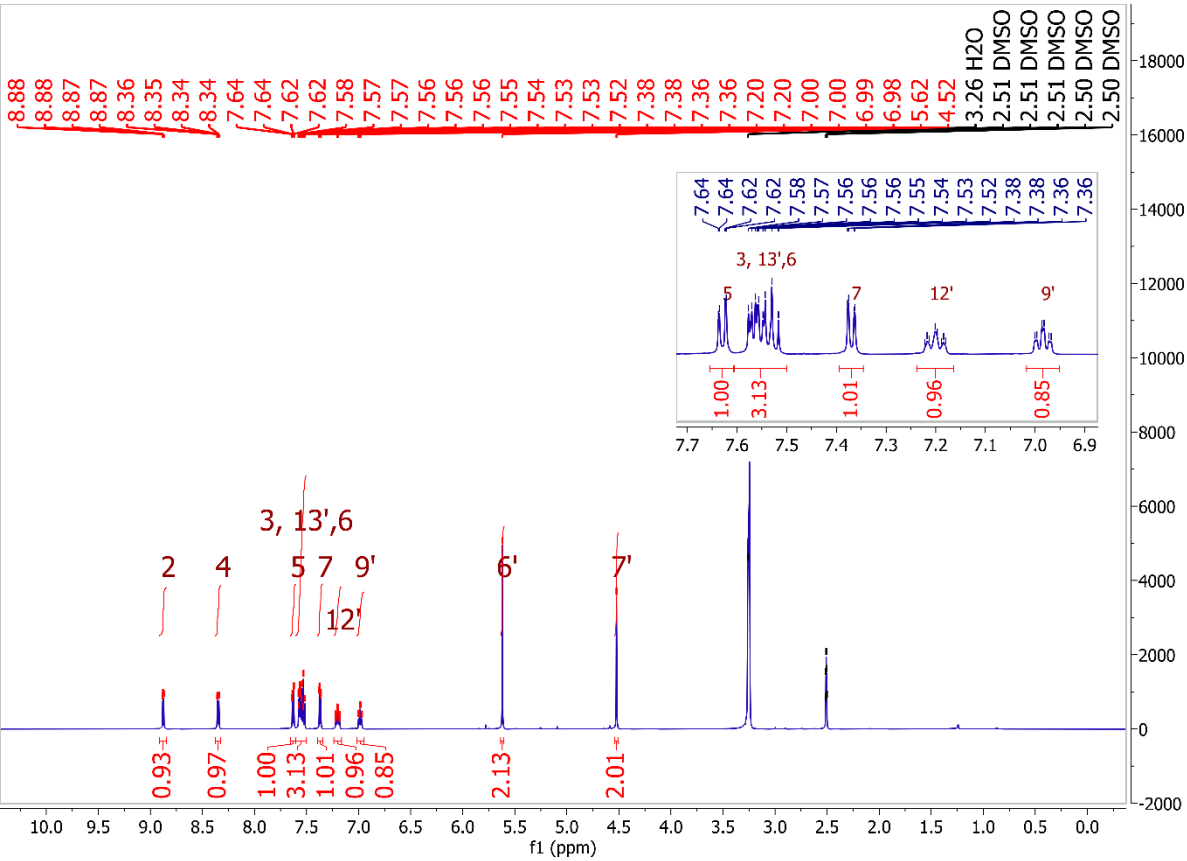
-1.5

500.0

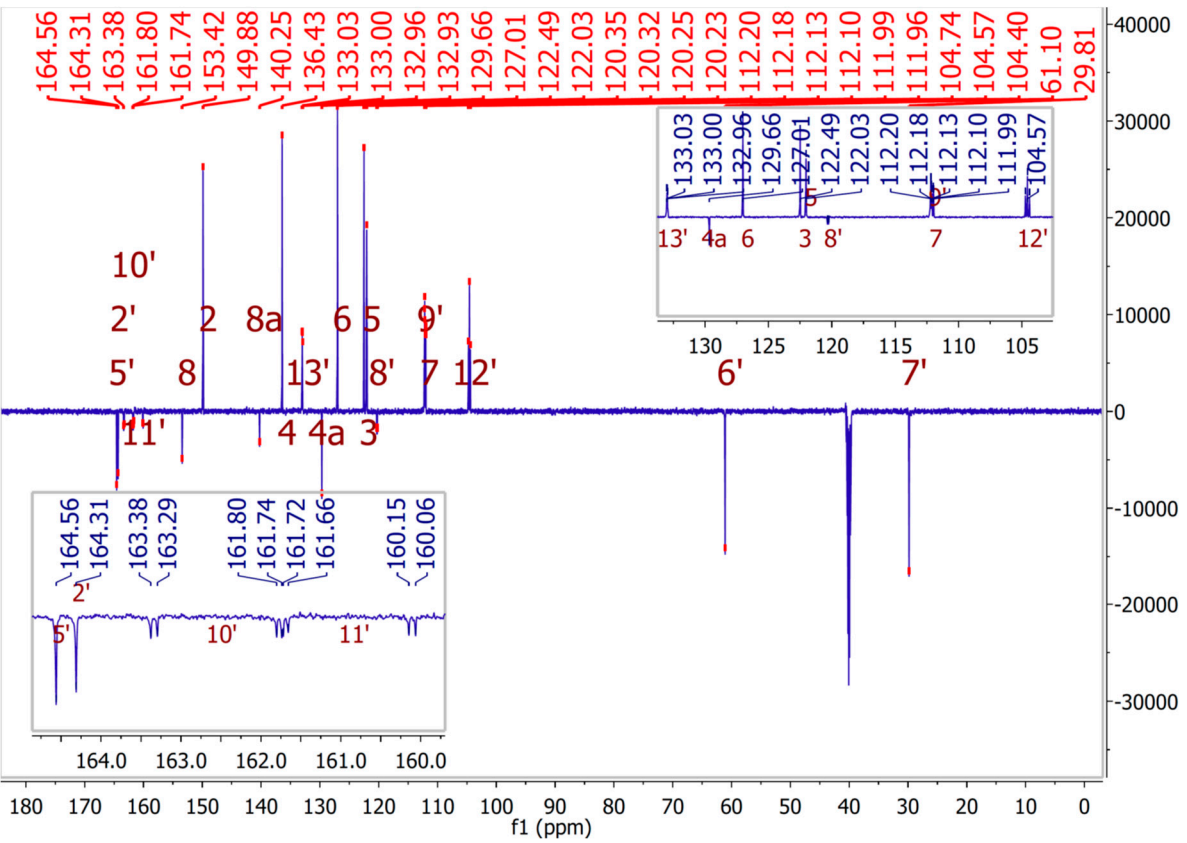
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
408.0604	408.0594	1.0	2.5	13.5	569.4	0.0	C19 H13 N3 O2 Na S F2

2-[(3,4-difluorobenzyl)thio]-5-[(quinolin-8-yloxy)methyl]-1,3,4-oxadiazole (4s)

<sup>1</sup>H NMR



<sup>13</sup>C NMR



# HRMS

## Elemental Composition Report\_Compound 4s

### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

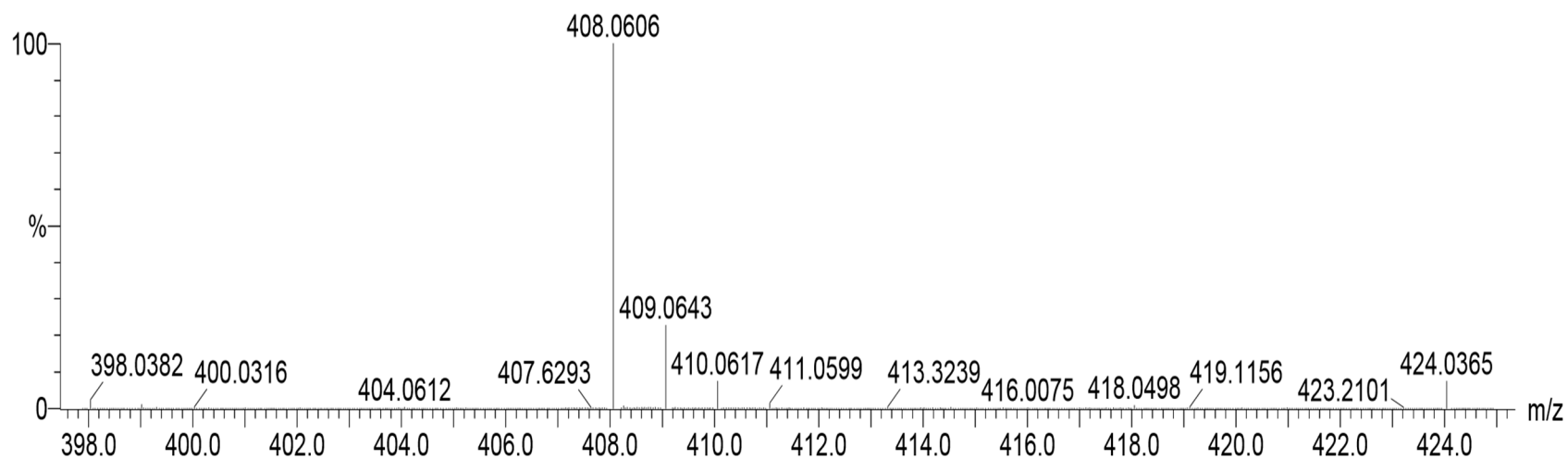
Monoisotopic Mass, Even Electron Ions

101 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) Elements Used:

C: 15-20 H: 10-15 N: 0-5 O: 0-5 F: 0-2 Na: 1-1 S: 0-1

3.07e+005

TOF MS ES+



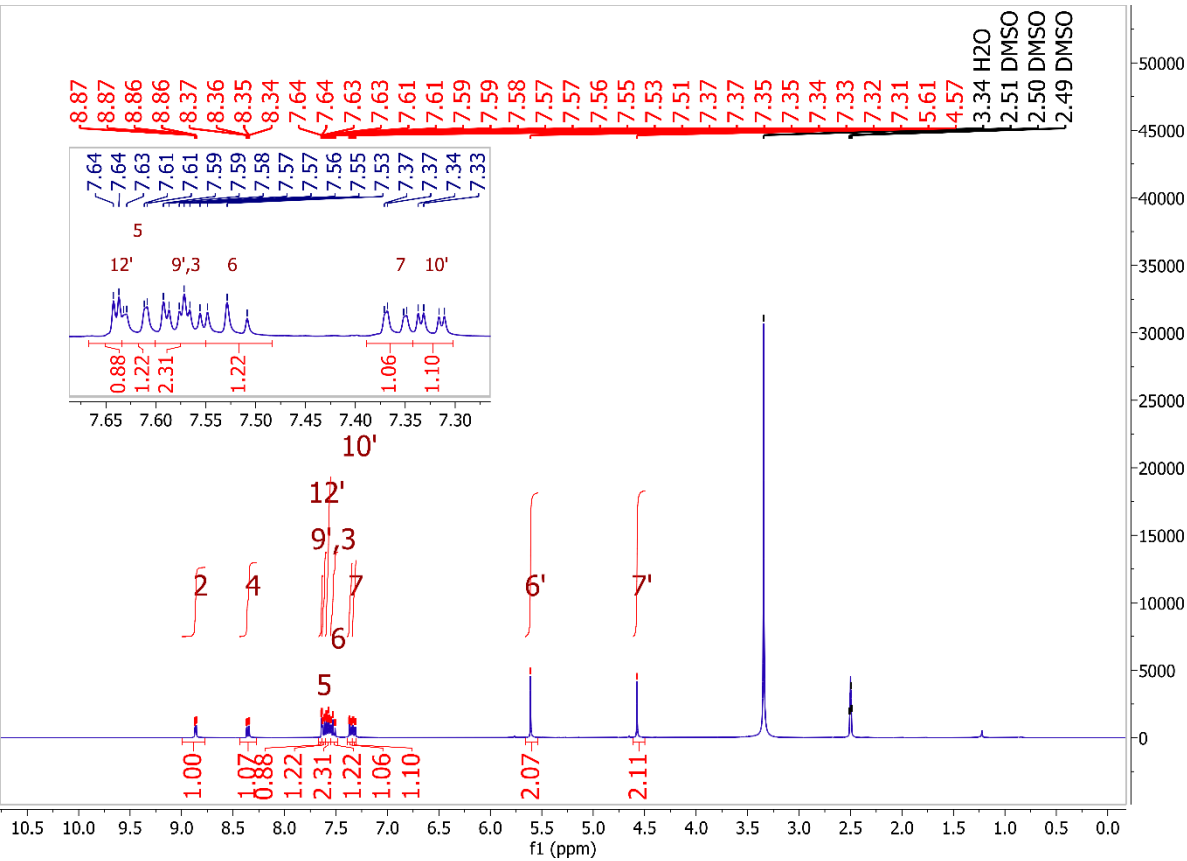
Minimum:

Maximum: 5.0 5.0 -1.5 500.0

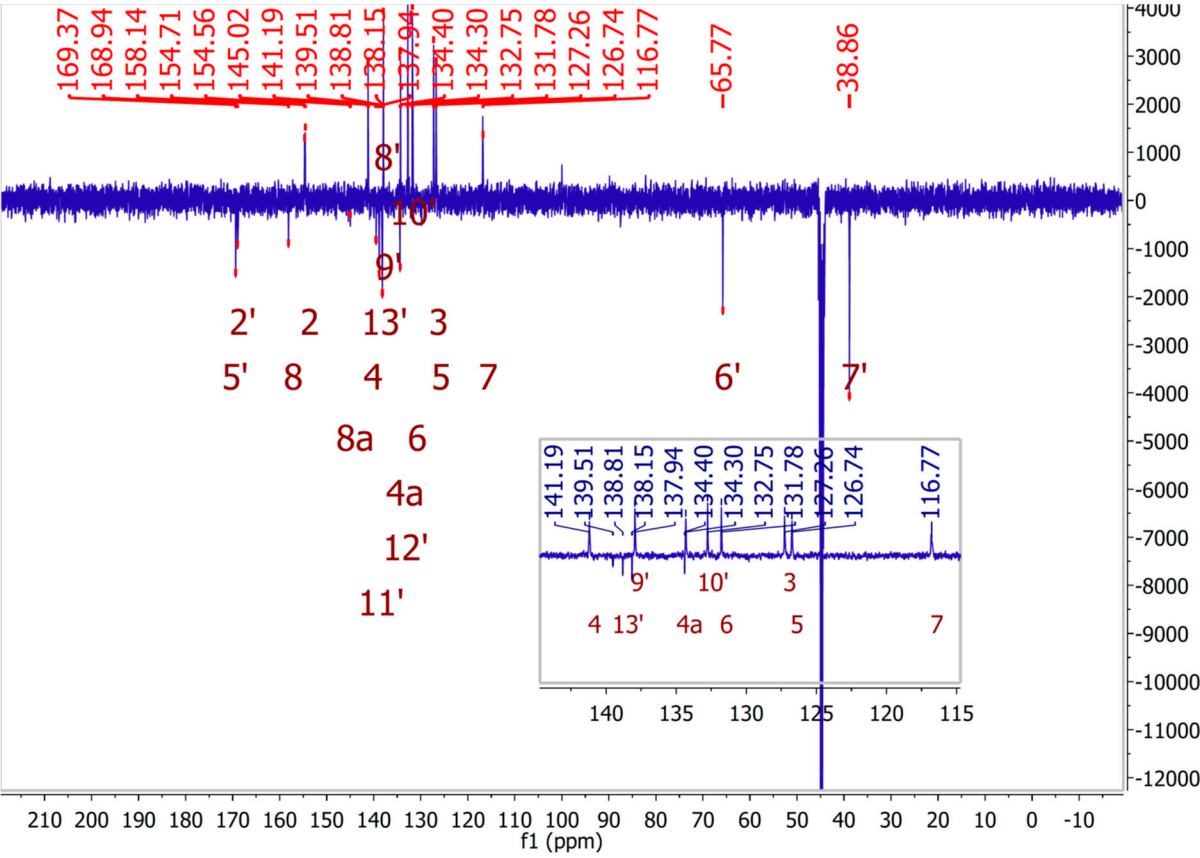
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
408.0606	408.0594	1.2	2.9	13.5	597.7	0.0	C19 H13 N3 O2 F2 Na S

2-[(2,4-dichlorobenzyl)thio]-5-[(quinolin-8-yloxy)methyl]-1,3,4-oxadiazole (4t)

<sup>1</sup>H NMR



<sup>13</sup>C NMR



## HRMS

### Elemental Composition Report\_Compound 4t

#### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

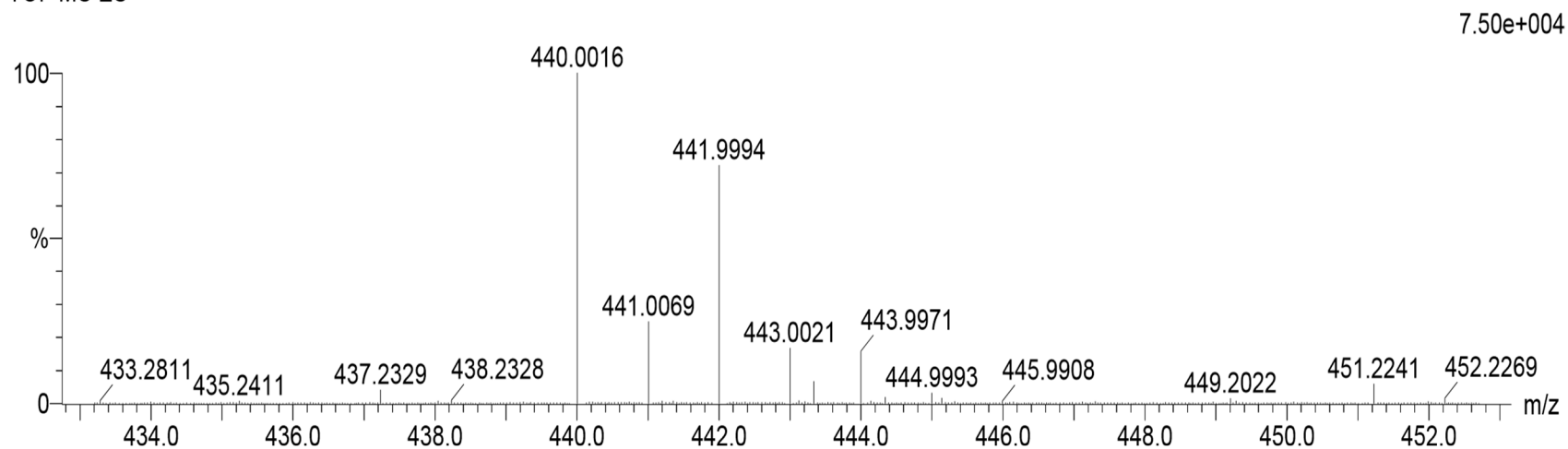
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

122 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) Elements Used:

C: 15-20 H: 10-15 N: 0-5 O: 0-5 Na: 1-1 S: 0-1 Cl: 0-2

TOF MS ES+



Minimum:

-1.5

Maximum:

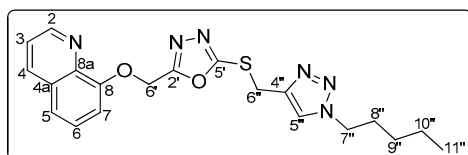
5.0

5.0

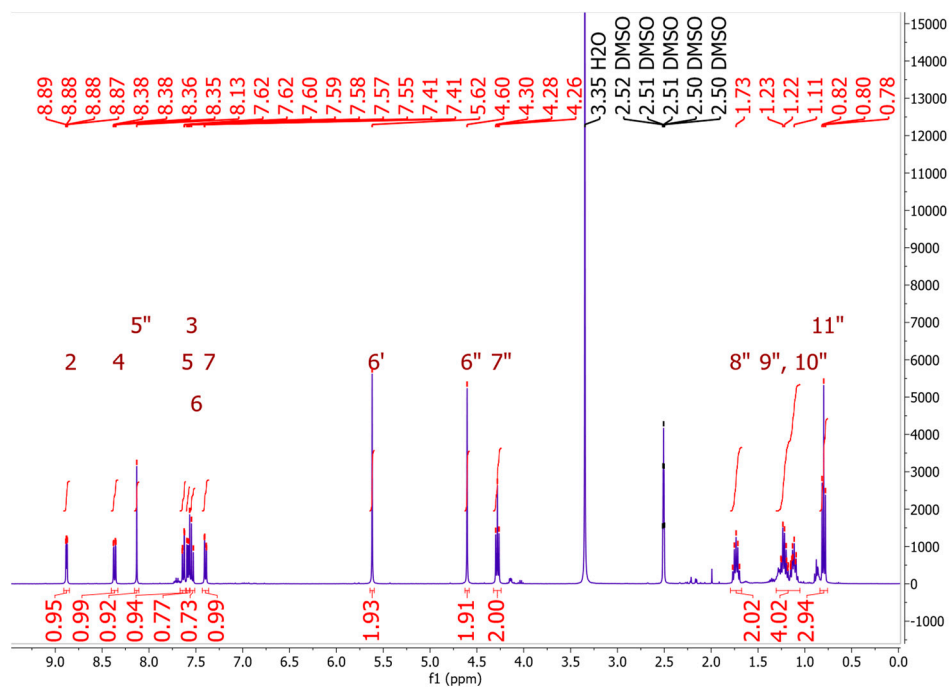
500.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula				
440.0016	440.0003	1.3	3.0	13.5	531.6	0.0	C19	H13	N3	O2	Na S Cl2

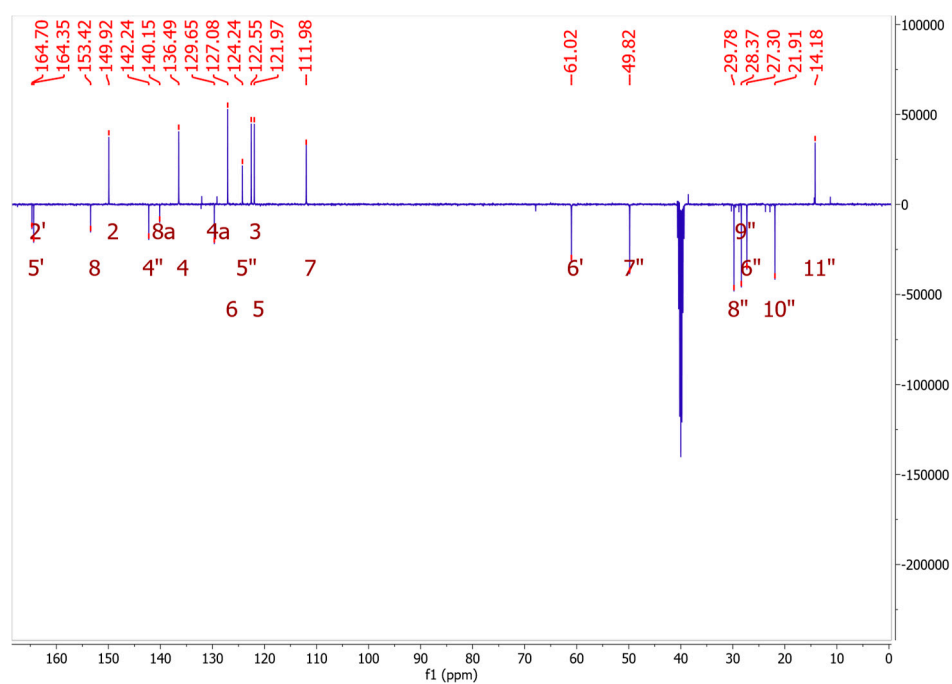
2-{[(1-pentyl-1H-1,2,3-triazol-4-yl)methyl]thio}-5-[(quinolin-8-yloxy)methyl]-1,3,4-oxadiazole (**12a**)



<sup>1</sup>H NMR



<sup>13</sup>C NMR





## Elemental Composition Report \_Compound 12a

Page 1

### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

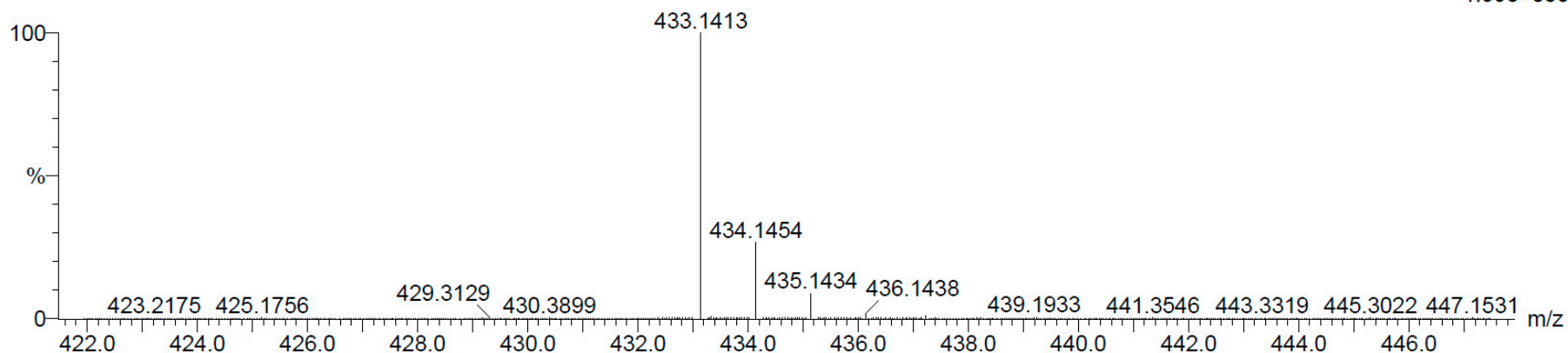
72 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 20-25 H: 20-25 N: 5-10 O: 0-5 S: 0-1 Na: 0-1

NC-5a 16 (0.507) Cm (1:61)

TOF MS ES+  
1.99e+005



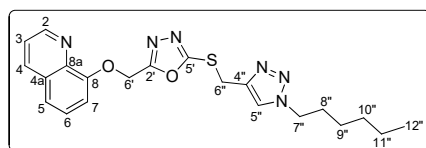
Minimum: -1.5

Maximum: 5.0 5.0 500.0

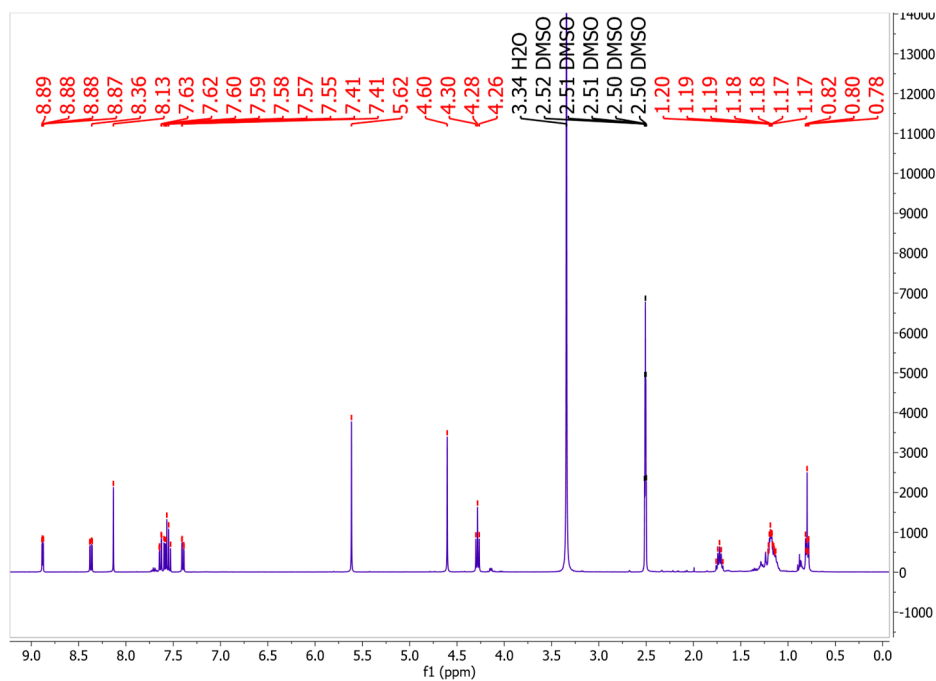
Mass Calc. Mass mDa PPM DBE i-FIT i-FIT (Norm) Formula

433.1413 433.1423 -1.0 -2.3 12.5 544.5 0.0 C20 H22 N6 O2 S Na

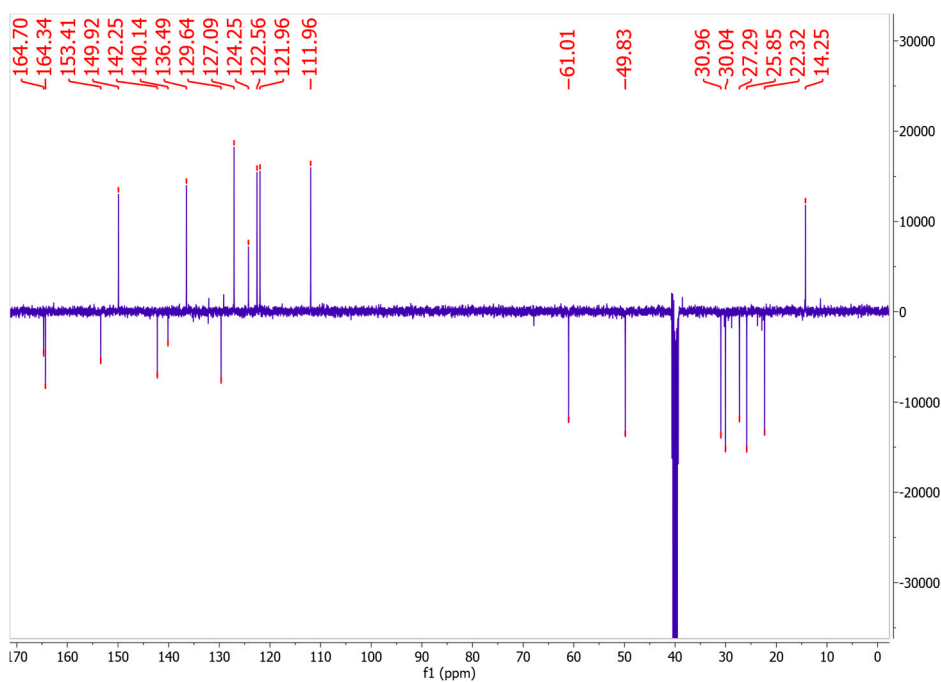
2-{[(1-hexyl-1H-1,2,3-triazol-4-yl)methyl]thio}-5-[(quinolin-8-yloxy)methyl]-1,3,4-oxadiazole (**12b**)



<sup>1</sup>H NMR



<sup>13</sup>C NMR



**Single Mass Analysis**

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

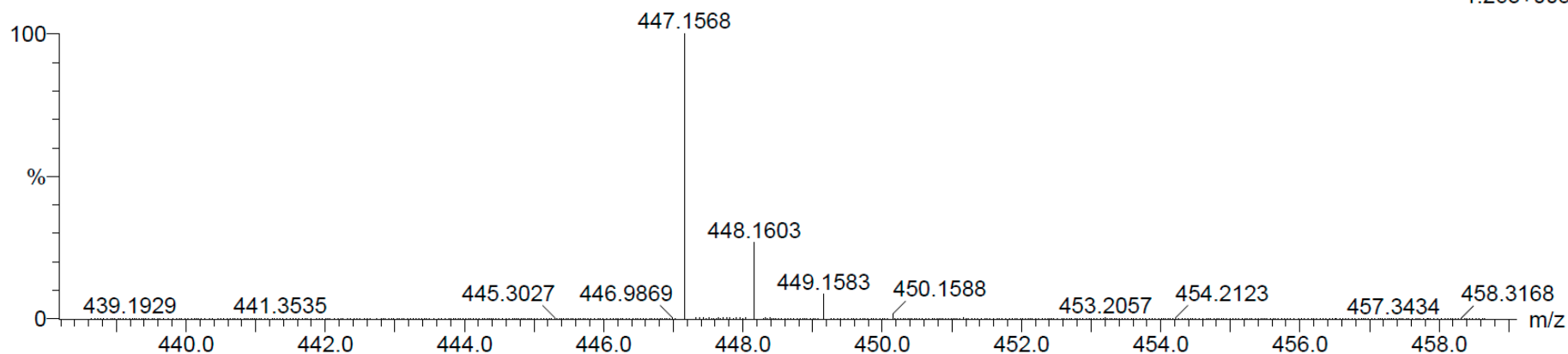
Monoisotopic Mass, Even Electron Ions

64 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 20-25 H: 20-25 N: 5-10 O: 0-5 Na: 0-1 S: 0-1

NC-5b 50 (1.653) Cm (1:61)

TOF MS ES+  
1.26e+005

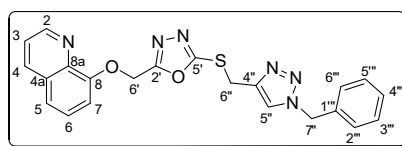
Minimum: -1.5

Maximum: 5.0 5.0 500.0

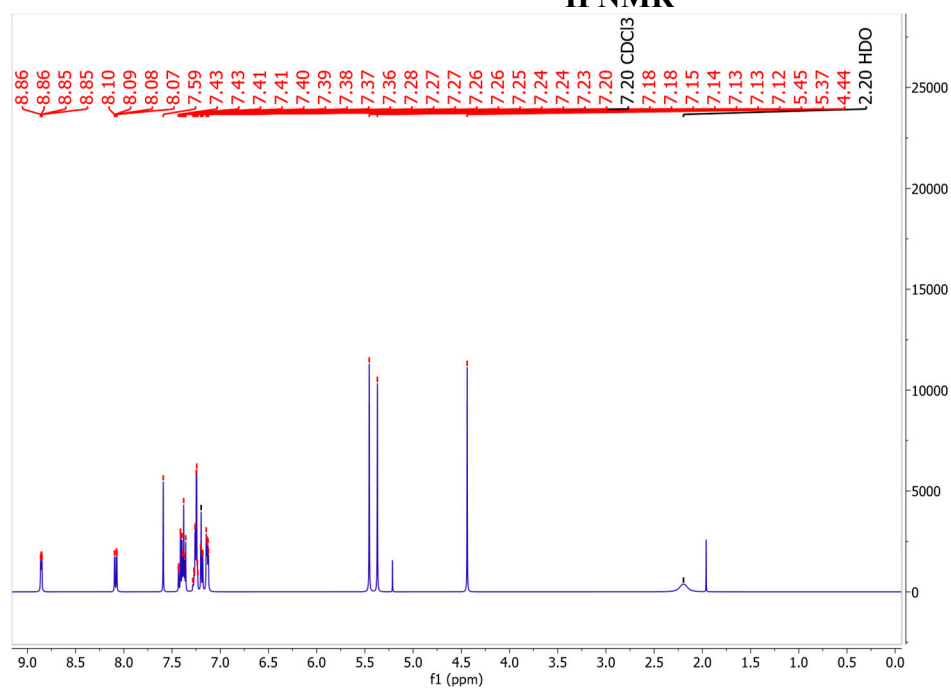
Mass Calc. Mass mDa PPM DBE i-FIT i-FIT (Norm) Formula

447.1568 447.1579 -1.1 -2.5 12.5 472.2 0.0 C21 H24 N6 O2 Na

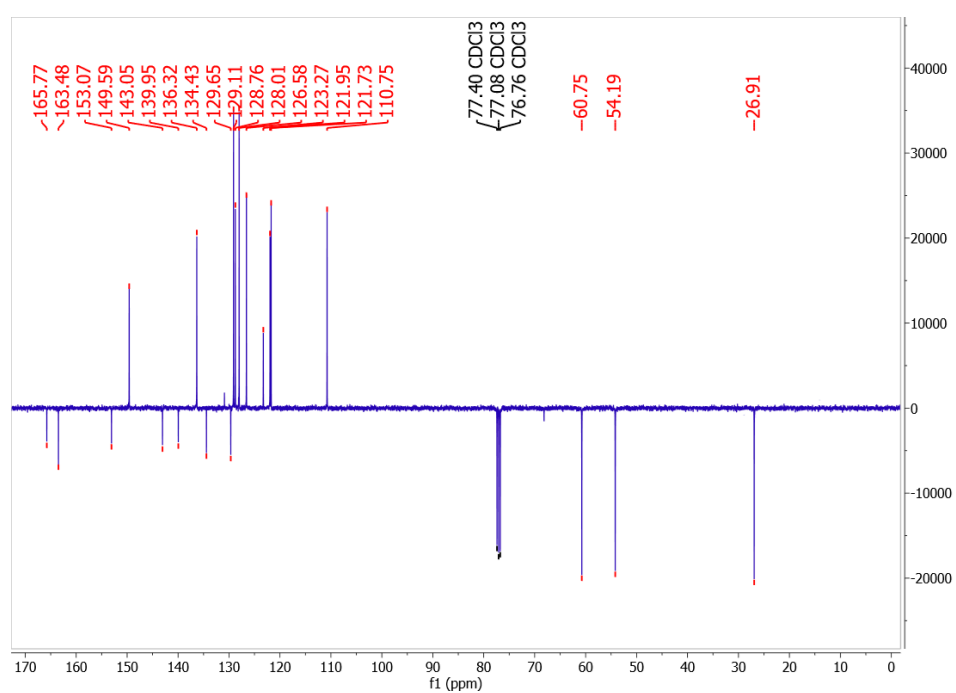
2-{[(1-benzyl-1H-1,2,3-triazol-4-yl)methyl]thio}-5-[(quinolin-8-yloxy)methyl]-1,3,4-oxadiazole (**12c**)



<sup>1</sup>H NMR



<sup>13</sup>C NMR



## Elemental Composition Report \_Compound 12c

Page 1

### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

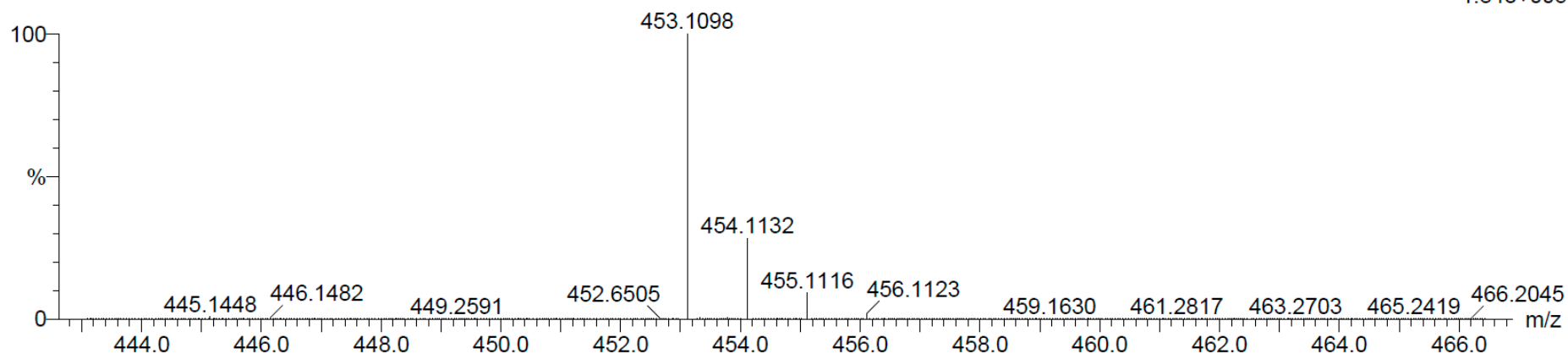
63 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 20-25 H: 15-20 N: 5-10 O: 0-5 Na: 0-1 S: 0-1

NC-5c 13 (0.405) Cm (1:61)

TOF MS ES+  
1.84e+005



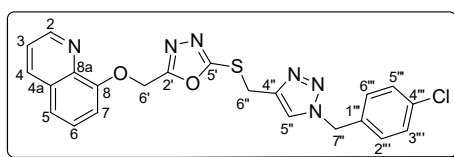
Minimum: -1.5

Maximum: 5.0 5.0 500.0

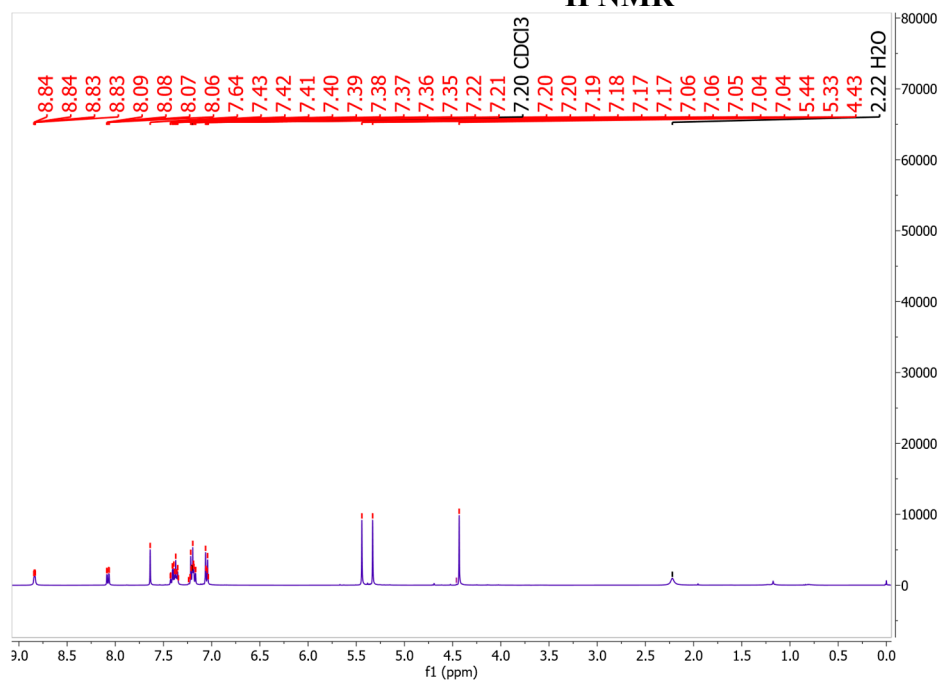
Mass Calc. Mass mDa PPM DBE i-FIT i-FIT (Norm) Formula

453.1098 453.1110 -1.2 -2.6 16.5 530.5 0.0 C22 H18 N6 O2 Na S

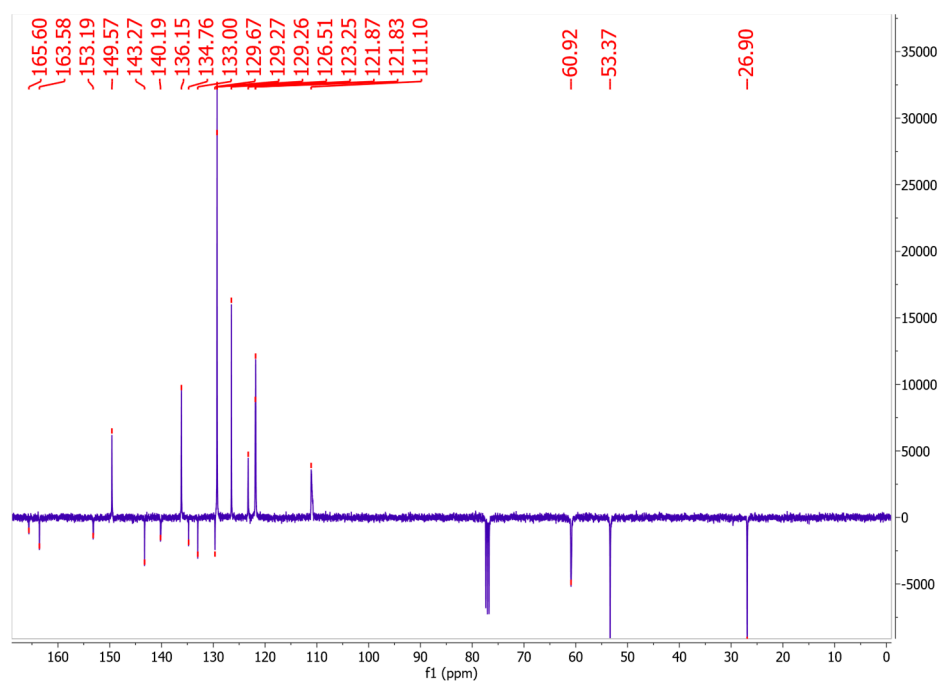
2-[[1-(4-chlorobenzyl)-1H-1,2,3-triazol-4-yl)methyl]thio}-5-[(quinolin-8-yloxy)methyl]-  
1,3,4-oxadiazole (**12d**)



<sup>1</sup>H NMR



<sup>13</sup>C NMR



**Single Mass Analysis**

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

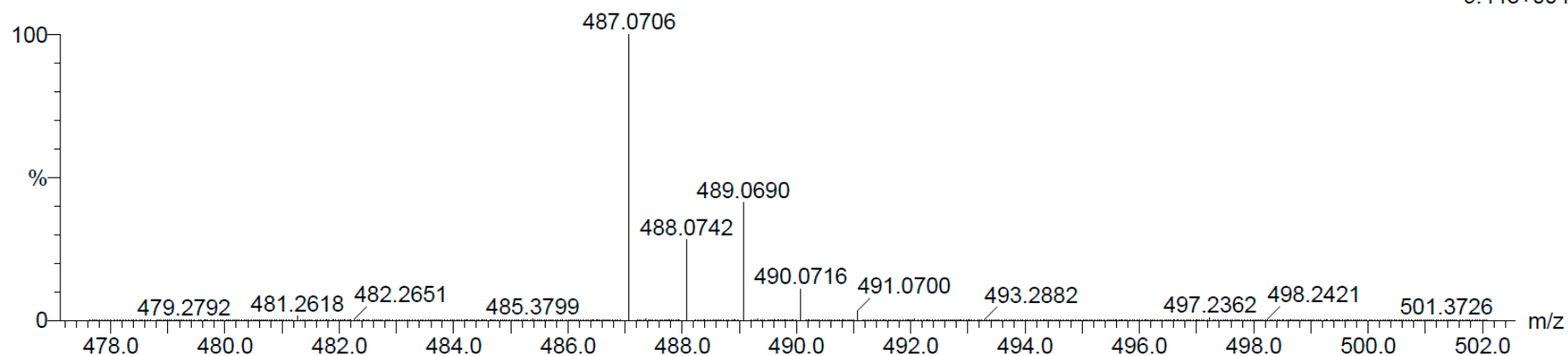
Monoisotopic Mass, Even Electron Ions

120 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 20-25 H: 15-20 N: 5-10 O: 0-5 Na: 0-1 S: 0-1 Cl: 0-1

NC-5d 61 (2.022) Cm (1:61)

TOF MS ES+  
9.44e+004

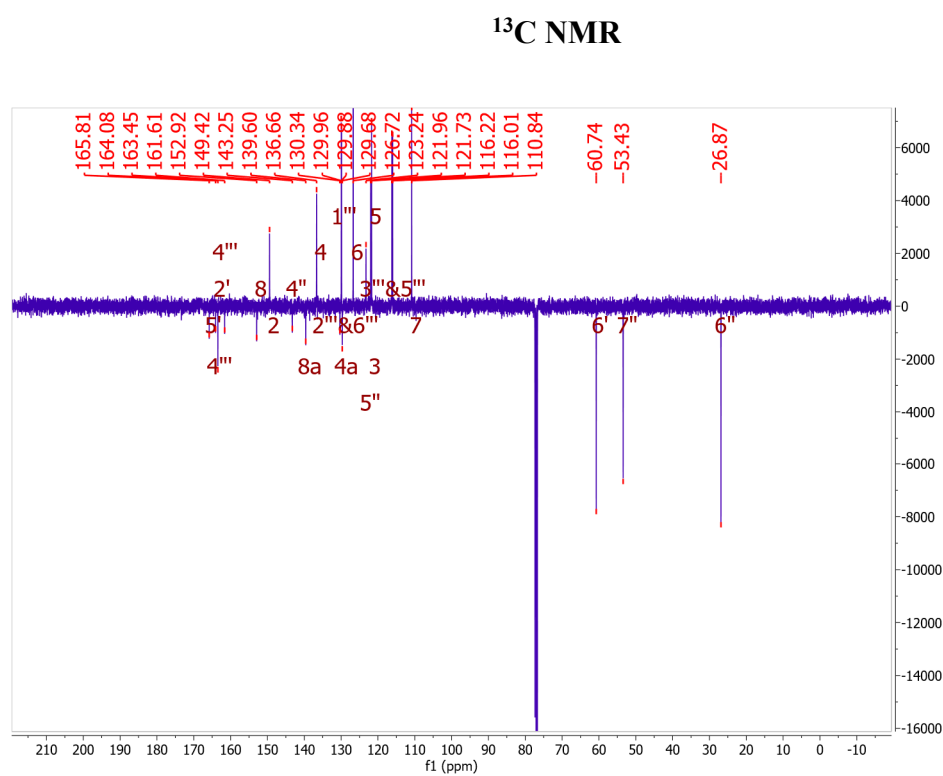
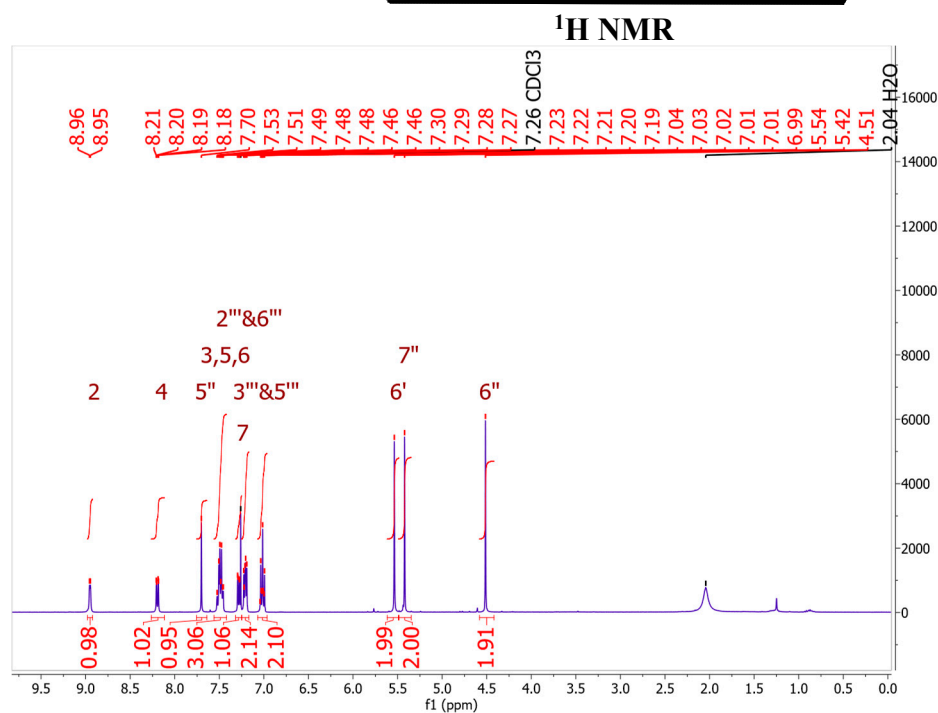
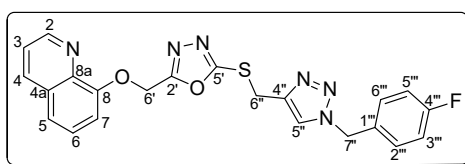
Minimum: -1.5

Maximum: 5.0 5.0 500.0

Mass Calc. Mass mDa PPM DBE i-FIT i-FIT (Norm) Formula

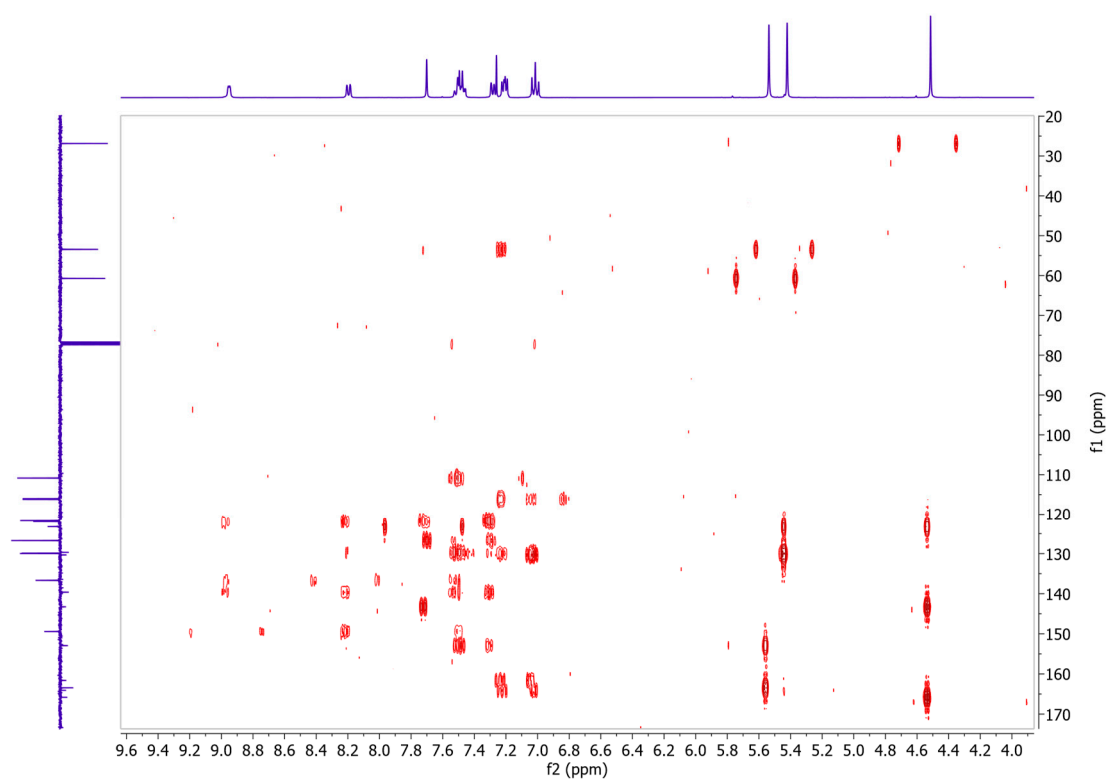
487.0706 487.0720 -1.4 -2.9 16.5 458.7 0.0 C22 H17 N6 O2 Na Cl

2-{[(1-(4-fluorobenzyl)-1H-1,2,3-triazol-4-yl)methyl]thio}-5-[(quinolin-8-yloxy)methyl]-  
1,3,4-oxadiazole (**12e**)

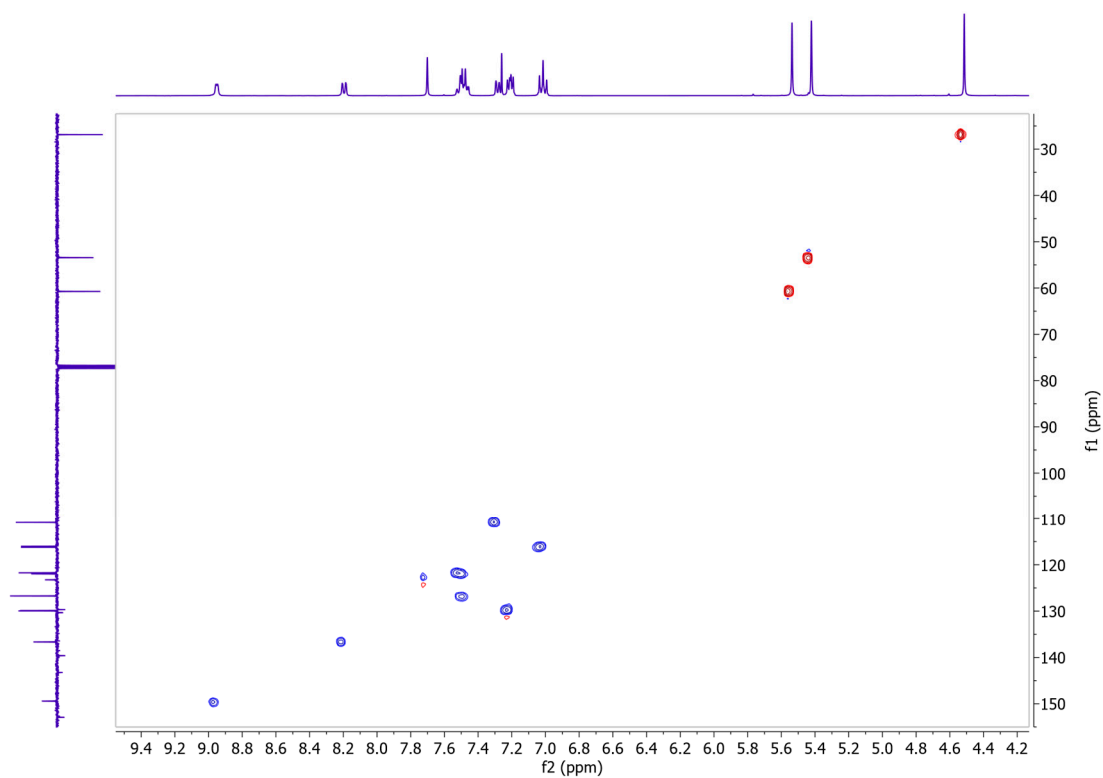




## HMBC NMR



## HSQC NMR



## Elemental Composition Report \_Compound 12e

Page 1

### Single Mass Analysis

Tolerance = 4.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

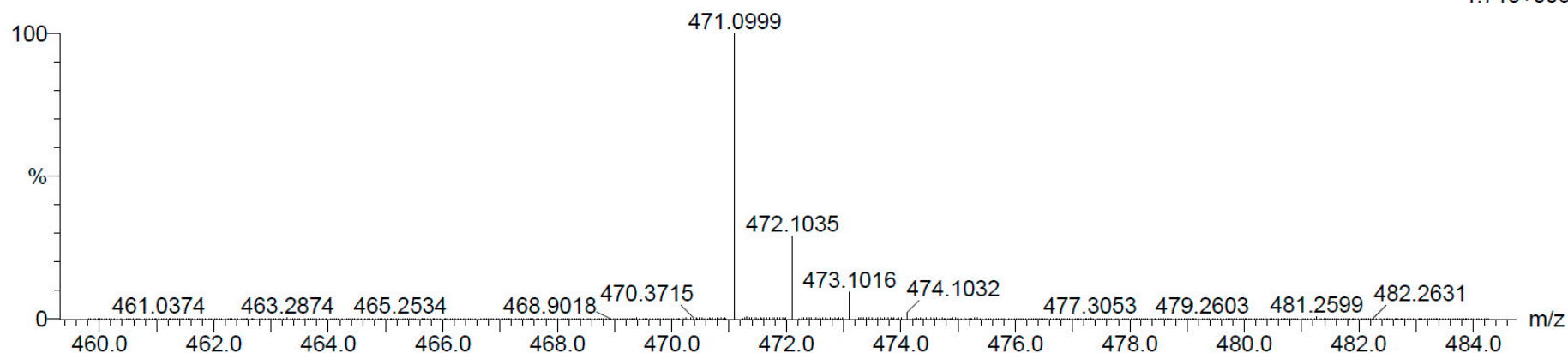
90 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 20-25 H: 15-20 N: 5-10 O: 0-5 Na: 1-1 S: 0-1 Br: 0-1

NC-5r 4 (0.101) Cm (1:61)

TOF MS ES+  
1.71e+005



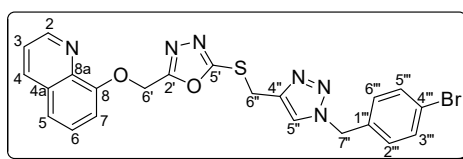
Minimum: -1.5

Maximum: 5.0 4.0 500.0

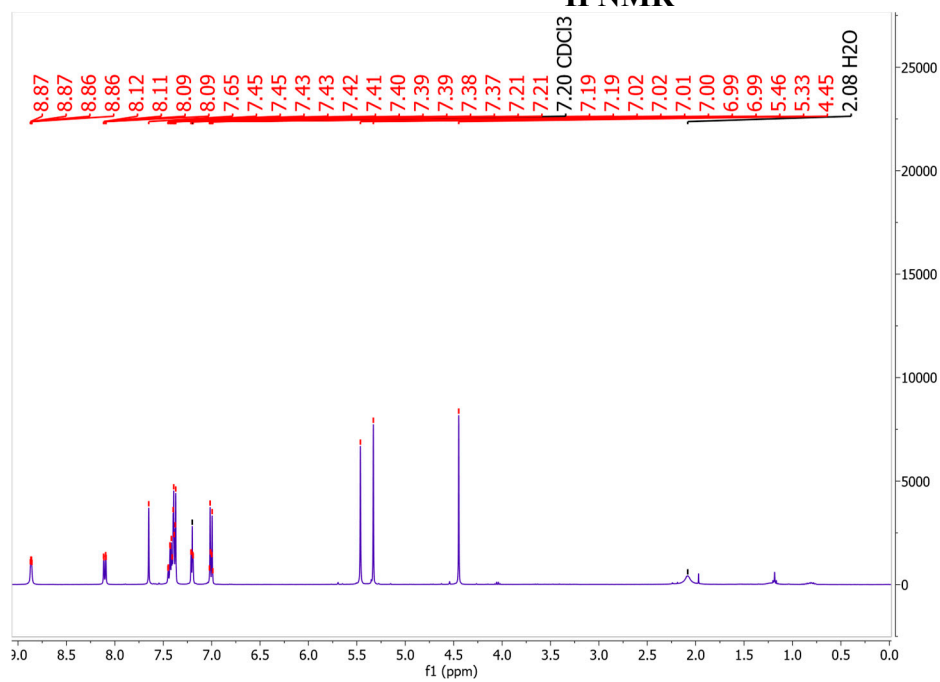
Mass Calc. Mass mDa PPM DBE i-FIT i-FIT (Norm) Formula

471.0999 471.1004 -0.5 -1.1 20.5 514.7 0.0 C25 H16 N6 O Na S F

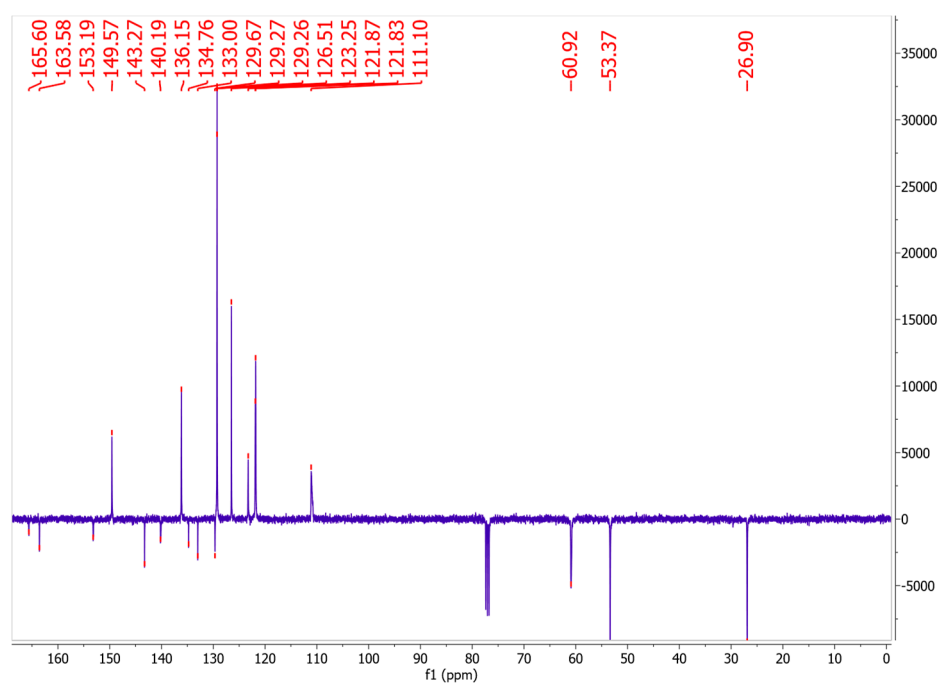
2-{[(1-(4-bromobenzyl)-1H-1,2,3-triazol-4-yl)methyl]thio}-5-[(quinolin-8-yloxy)methyl]-  
1,3,4-oxadiazole (**12f**)



<sup>1</sup>H NMR



<sup>13</sup>C NMR



**Single Mass Analysis**

Tolerance = 4.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

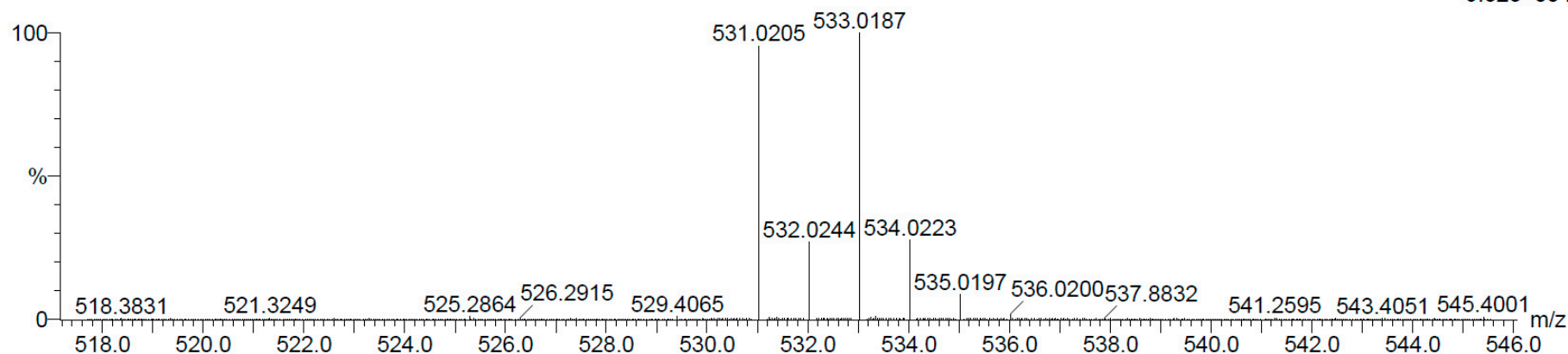
Monoisotopic Mass, Even Electron Ions

68 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 20-25 H: 15-20 N: 5-10 O: 0-5 Na: 1-1 S: 0-1 Br: 0-1

NC-5s 43 (1.416) Cm (1:61)

TOF MS ES+  
9.32e+004

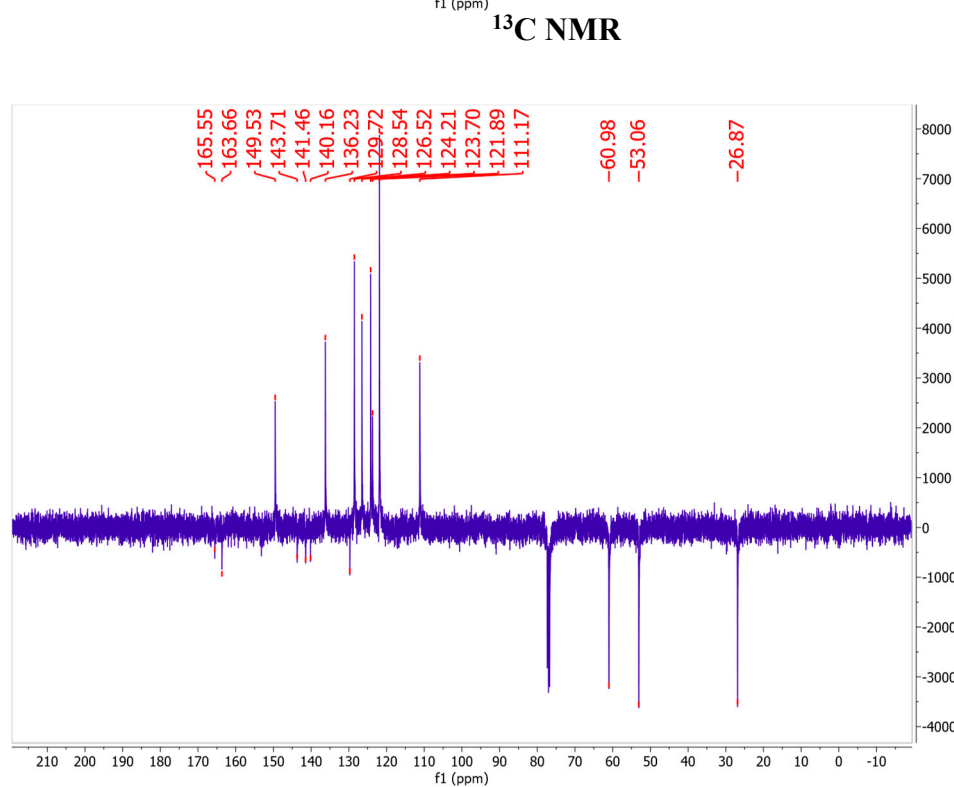
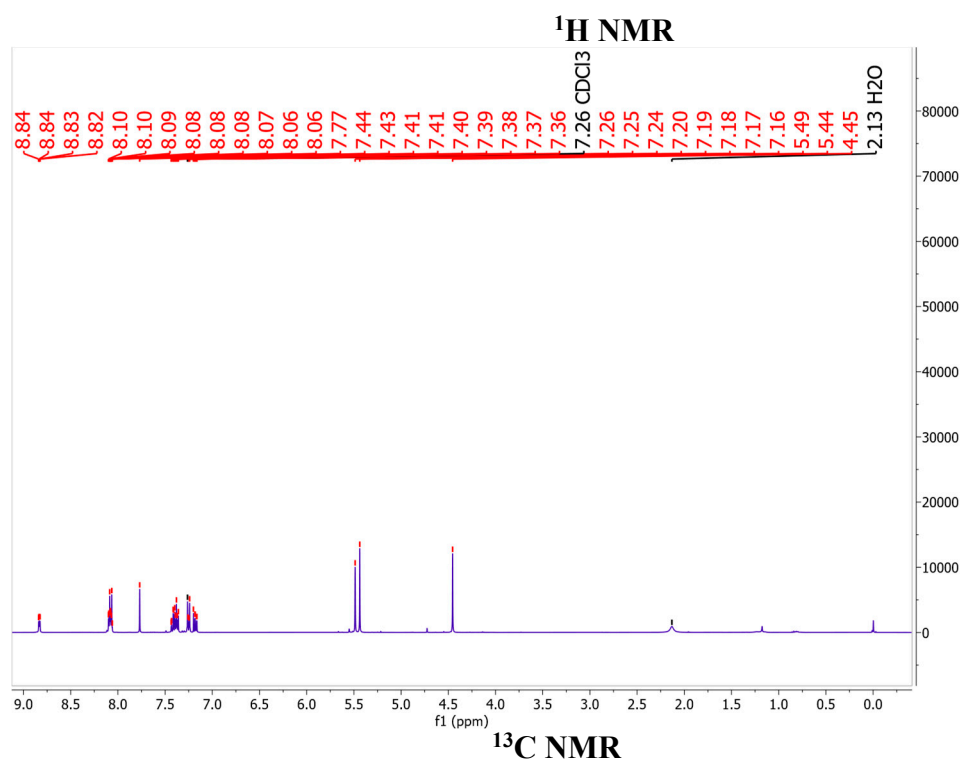
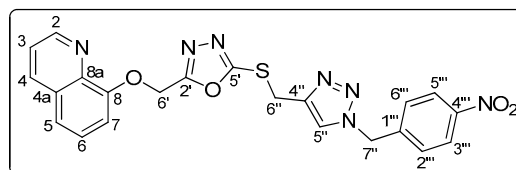
Minimum: -1.5

Maximum: 5.0 4.0 500.0

Mass Calc. Mass mDa PPM DBE i-FIT i-FIT (Norm) Formula

531.0205 531.0215 -1.0 -1.9 16.5 468.4 0.0 C22 H17 N6 O2 Na S Br

2-{[(1-(4-nitrobenzyl)-1H-1,2,3-triazol-4-yl)methyl]thio}-5-[(quinolin-8-yloxy)methyl]-  
1,3,4-oxadiazole (**12g**)



**Single Mass Analysis**

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

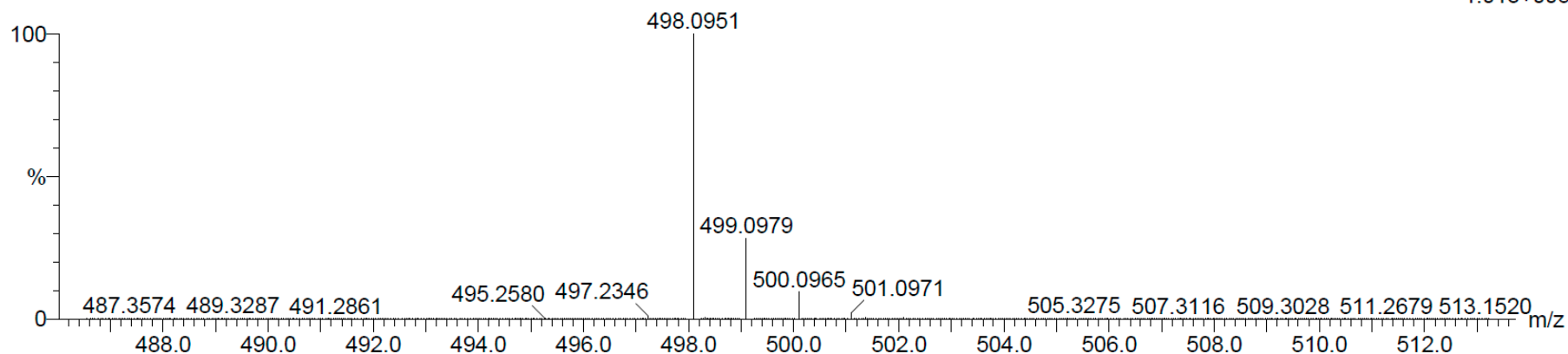
Monoisotopic Mass, Even Electron Ions

55 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 20-25 H: 15-20 N: 5-10 O: 0-5 Na: 0-1 S: 0-1

NC-5e 9 (0.270) Cm (1:61)

TOF MS ES+  
1.01e+005

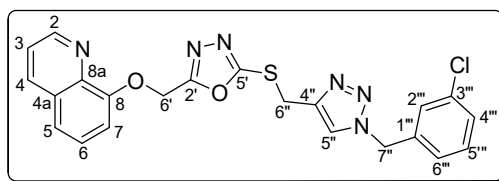
Minimum: -1.5

Maximum: 5.0 5.0 500.0

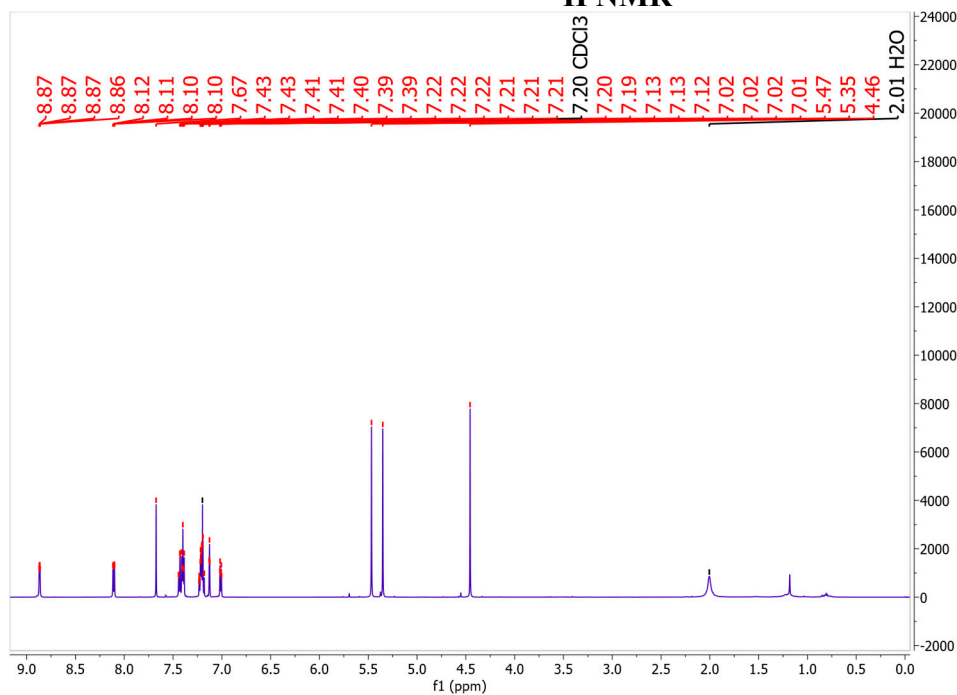
Mass Calc. Mass mDa PPM DBE i-FIT i-FIT (Norm) Formula

498.0951 498.0960 -0.9 -1.8 17.5 478.2 0.0 C22 H17 N7 O4 Na S

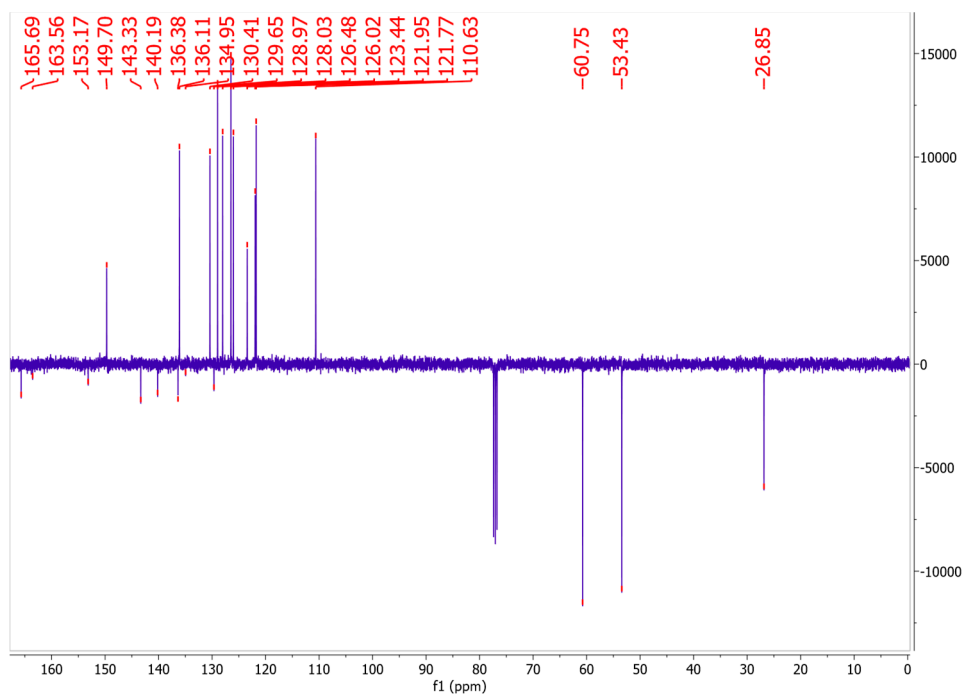
2-{[(1-(3-chlorobenzyl)-1H-1,2,3-triazol-4-yl)methyl]thio}-5-[(quinolin-8-yloxy)methyl]-  
1,3,4-oxadiazole (**12h**)



<sup>1</sup>H NMR



<sup>13</sup>C NMR



## Elemental Composition Report\_Compound 12h

Page 1

### Single Mass Analysis

Tolerance = 4.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

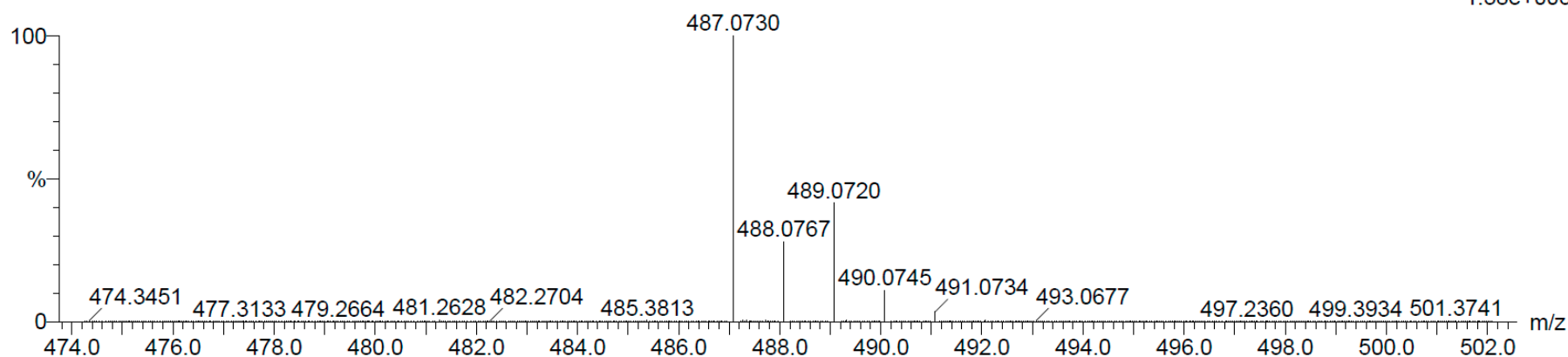
65 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 20-25 H: 15-20 N: 5-10 O: 0-5 Na: 1-1 S: 0-1 Cl: 0-1

NC-5q 11 (0.338) Cm (1:61)

TOF MS ES+  
1.38e+005



Minimum: -1.5

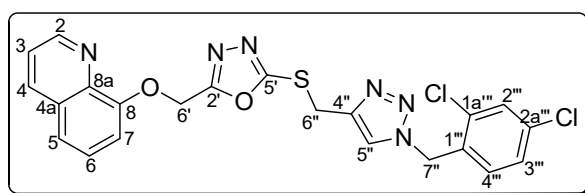
Maximum: 5.0 4.0 500.0

Mass Calc. Mass mDa PPM DBE i-FIT i-FIT (Norm) Formula

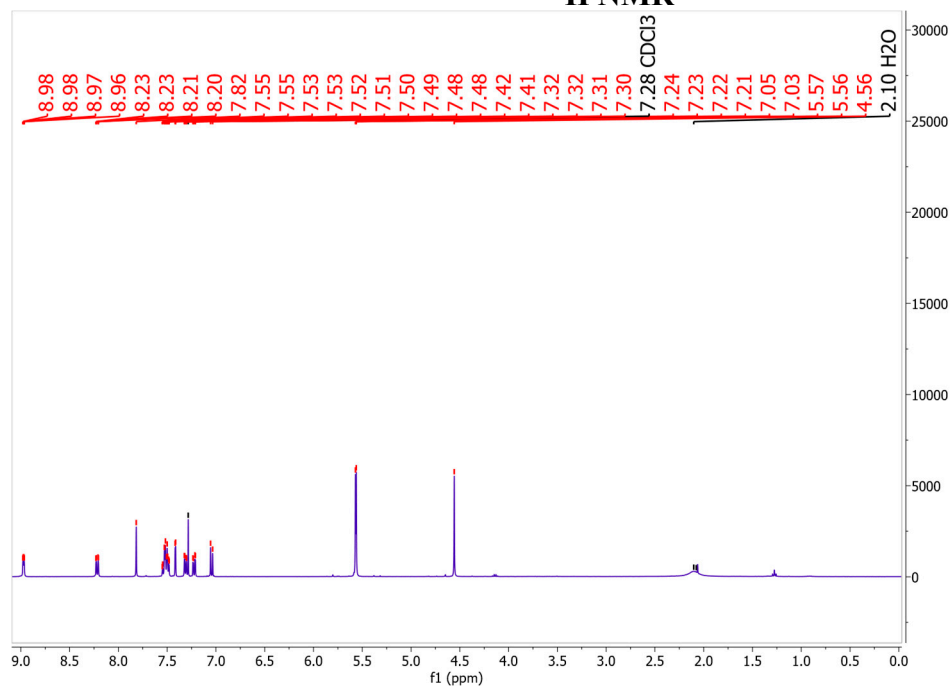
487.0730 487.0720 1.0 2.1 16.5 508.7 0.0 C22 H17 N6 O2 Na S Cl



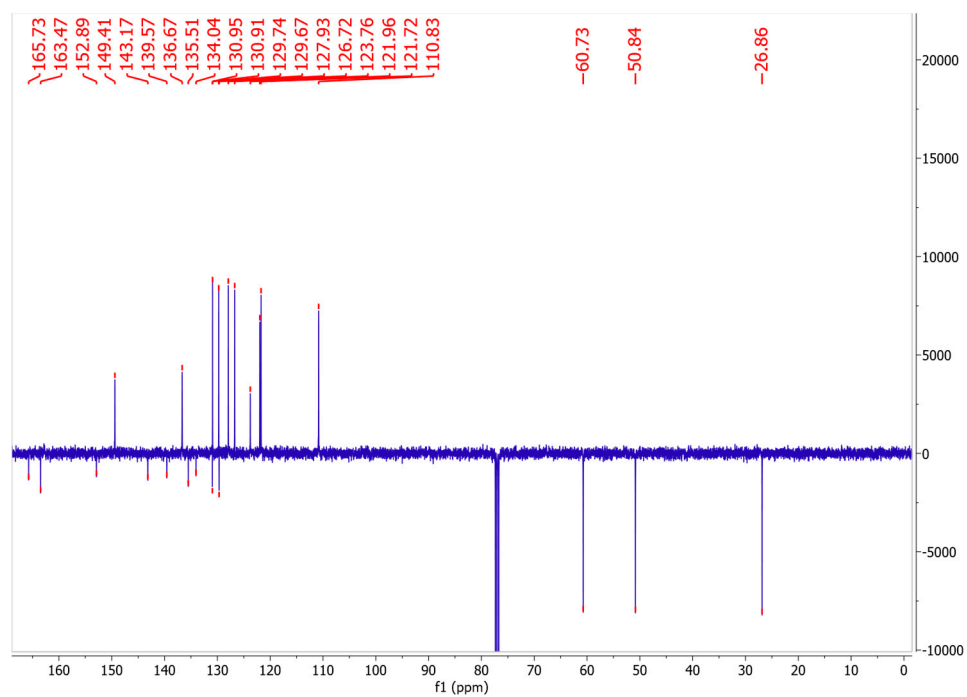
2-{[(1-(2,4-dichlorobenzyl)-1H-1,2,3-triazol-4-yl)methyl]thio}-5-[(quinolin-8-yloxy)methyl]-1,3,4-oxadiazole (**12i**)



<sup>1</sup>H NMR



<sup>13</sup>C NMR



## Elemental Composition Report\_Compound 12i

Page 1

### Single Mass Analysis

Tolerance = 4.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

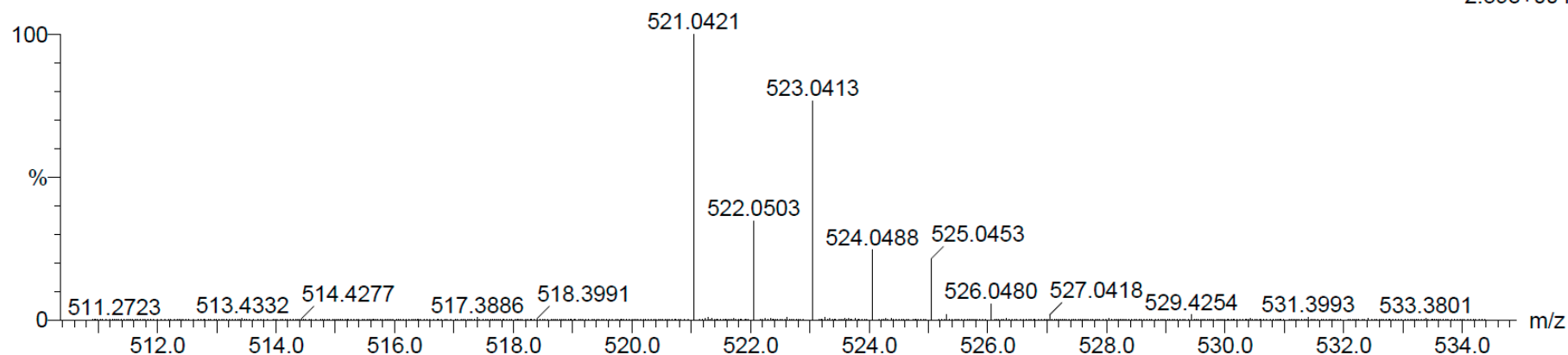
89 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 20-25 H: 15-20 N: 5-10 O: 0-5 Na: 1-1 S: 0-1 Cl: 0-2

NC-5t 31 (1.011) Cm (1:61)

TOF MS ES+  
2.39e+004



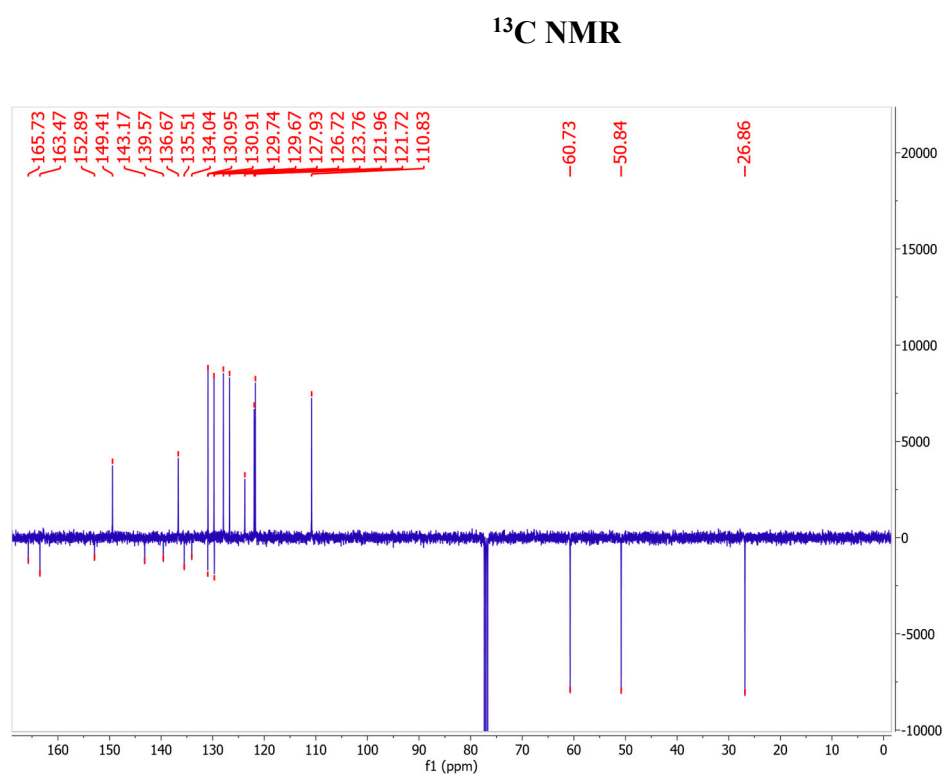
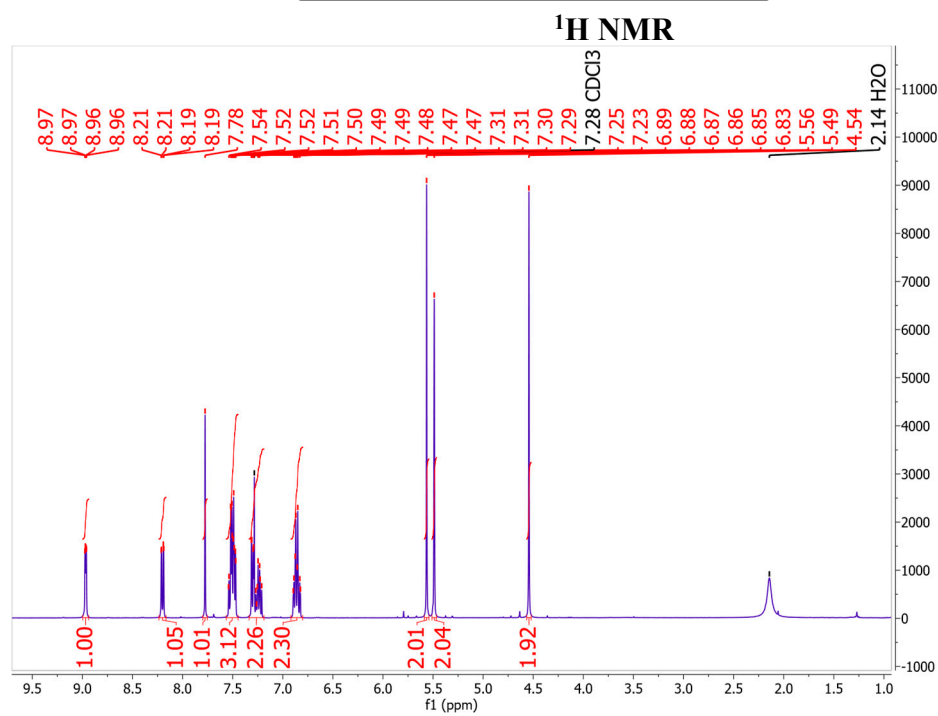
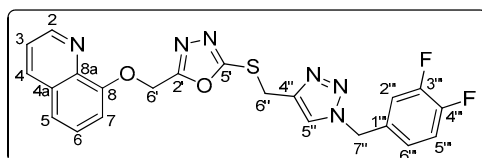
Minimum: -1.5

Maximum: 5.0 4.0 500.0

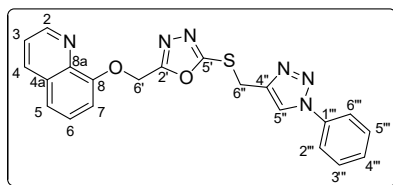
Mass Calc. Mass mDa PPM DBE i-FIT i-FIT (Norm) Formula

521.0421 521.0411 1.0 1.9 16.5 392.9 0.0 C<sub>21</sub> H<sub>15</sub> N<sub>6</sub> O<sub>5</sub> Na S Cl

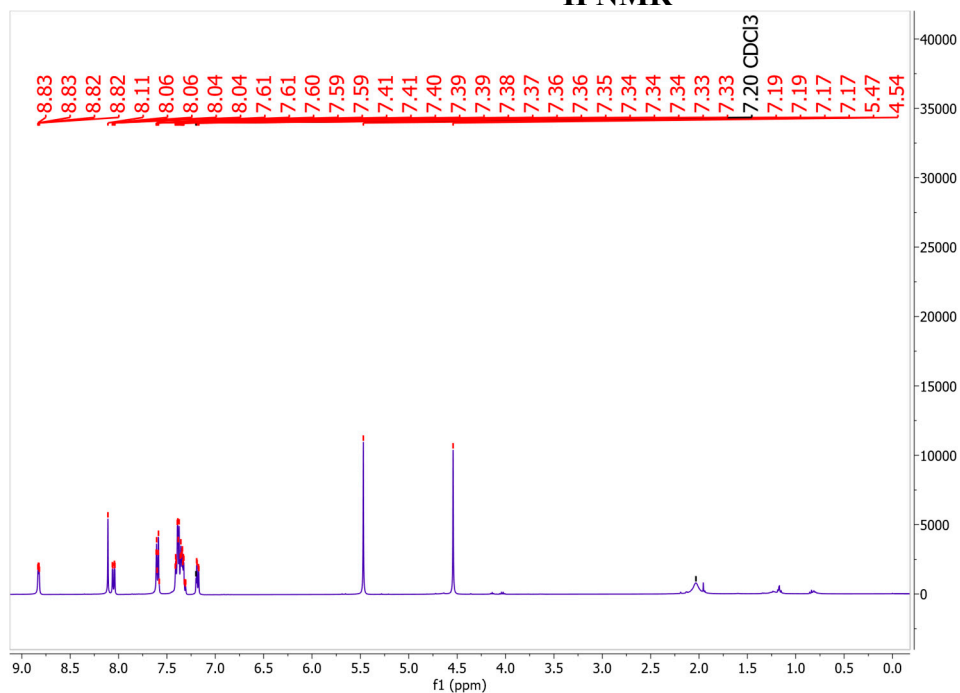
2-{[(1-(3,4-difluorobenzyl)-1H-1,2,3-triazol-4-yl)methyl]thio}-5-[(quinolin-8-yloxy)methyl]-  
1,3,4-oxadiazole (**12j**)



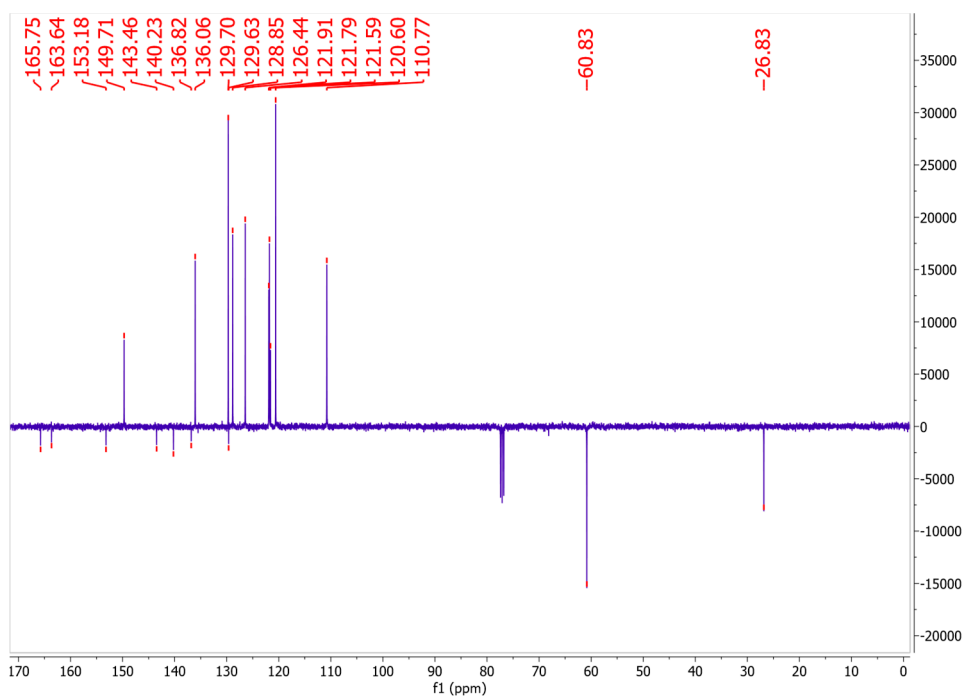
2-[[[(1-phenyl-1H-1,2,3-triazol-4-yl)methyl]thio]-5-[(quinolin-8-yloxy)methyl]-1,3,4-oxadiazole (**12k**)



<sup>1</sup>H NMR



<sup>13</sup>C NMR



**Single Mass Analysis**

Tolerance = 4.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

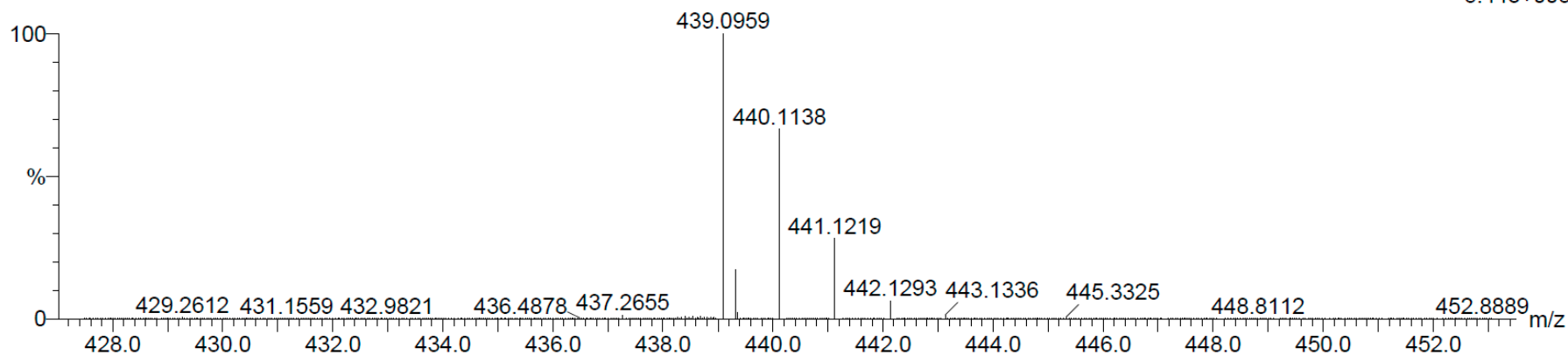
Monoisotopic Mass, Even Electron Ions

69 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 20-25 H: 15-20 N: 5-10 O: 0-5 Na: 0-1 S: 0-1

NC-5f 55 (1.853) Cm (1:60)

TOF MS ES+  
5.44e+005

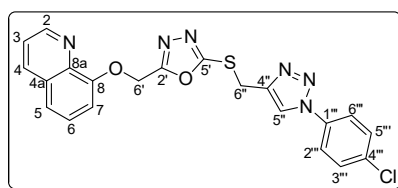
Minimum: -1.5

Maximum: 5.0 4.0 500.0

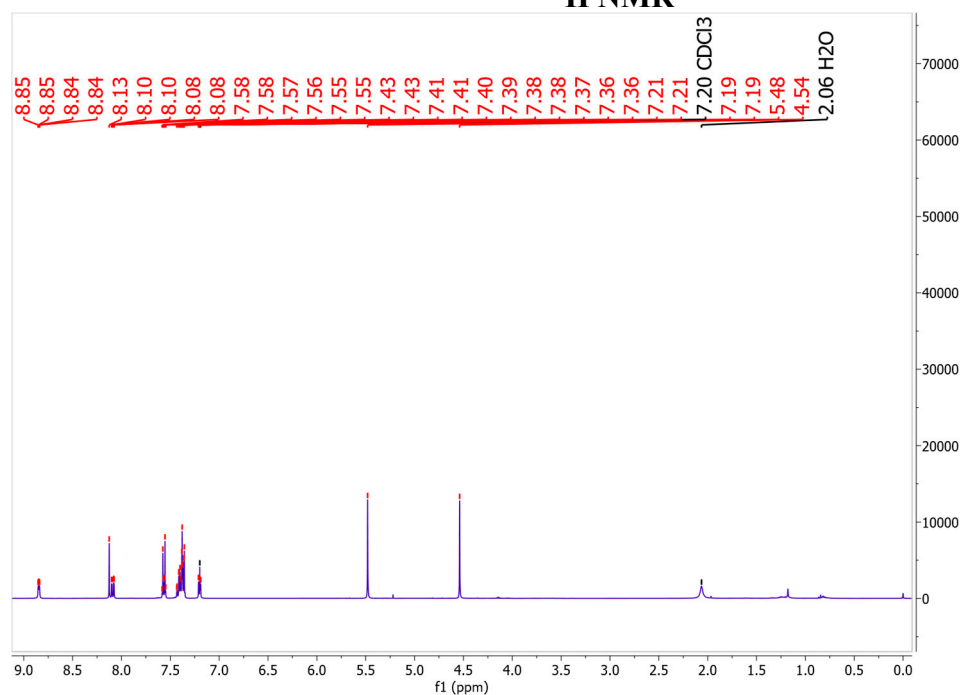
Mass Calc. Mass mDa PPM DBE i-FIT i-FIT (Norm) Formula

439.0959 439.0953 0.6 1.4 16.5 515.7 0.0 C21 H16 N6 O2 Na S

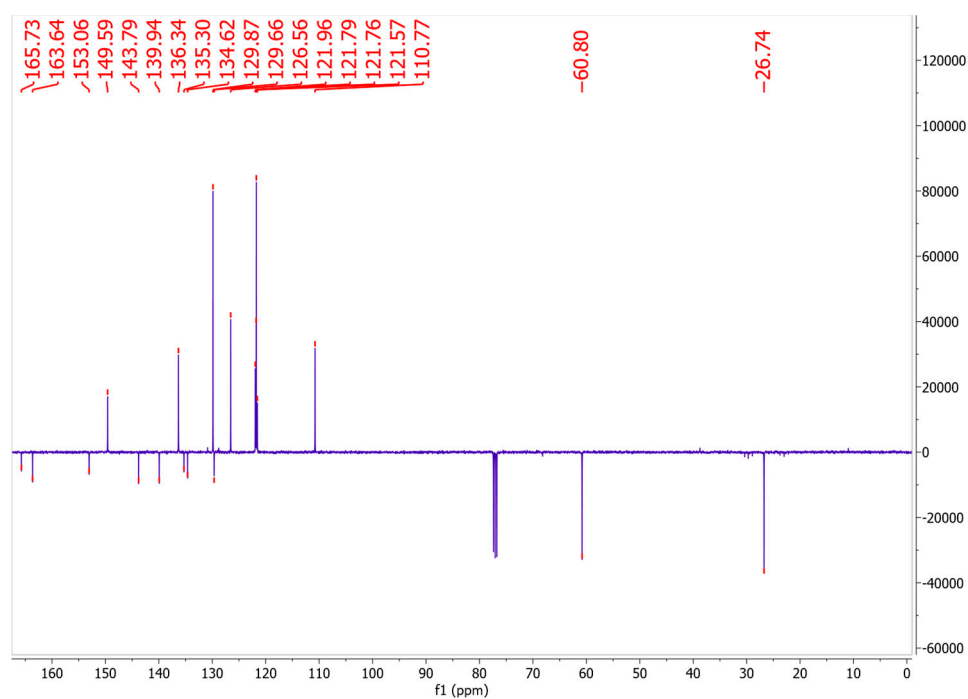
2-{[(1-(4-chlorophenyl)-1H-1,2,3-triazol-4-yl)methyl]thio}-5-[(quinolin-8-yloxy)methyl]-  
1,3,4-oxadiazole (**12l**)



<sup>1</sup>H NMR



<sup>13</sup>C NMR



**Single Mass Analysis**

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

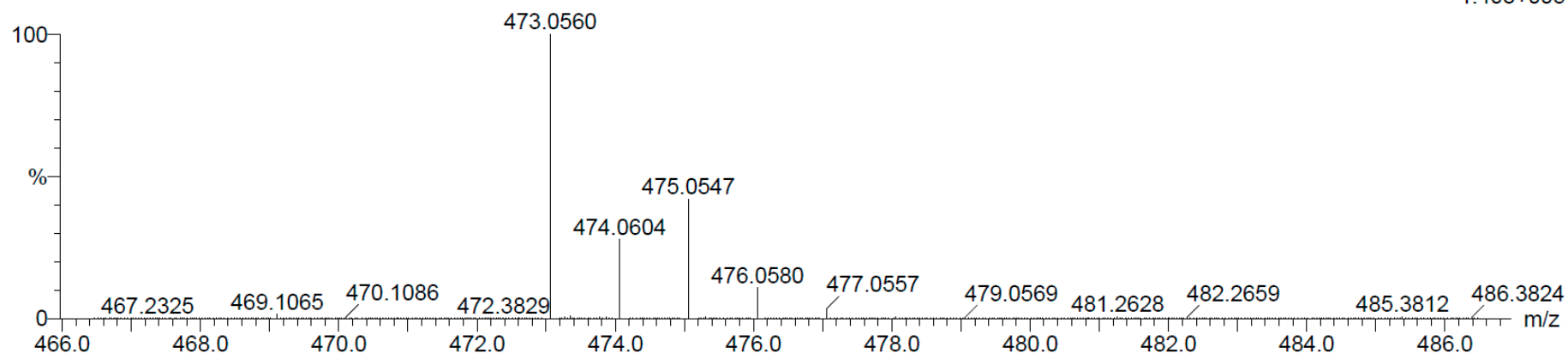
Monoisotopic Mass, Even Electron Ions

127 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 20-25 H: 15-20 N: 5-10 O: 0-5 Na: 0-1 S: 0-1 Cl: 0-1

NC-5g 3 (0.068) Cm (1:61)

TOF MS ES+  
1.40e+005

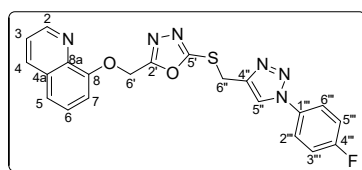
Minimum: -1.5

Maximum: 5.0 5.0 500.0

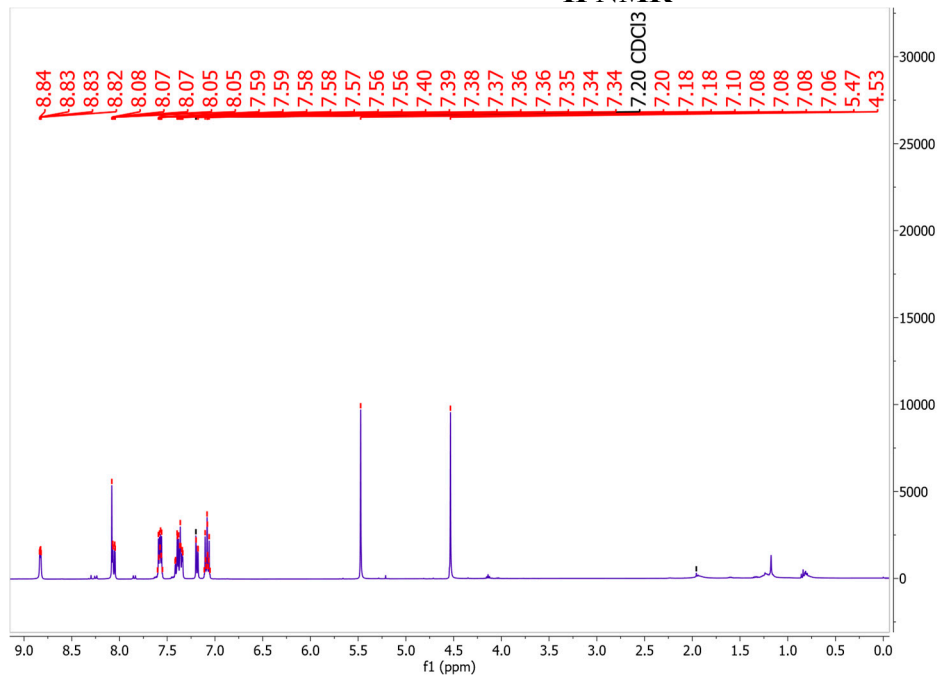
Mass Calc. Mass mDa PPM DBE i-FIT i-FIT (Norm) Formula

473.0560 473.0563 -0.3 -0.6 16.5 504.3 0.0 C21 H15 N6 O2 Na S Cl

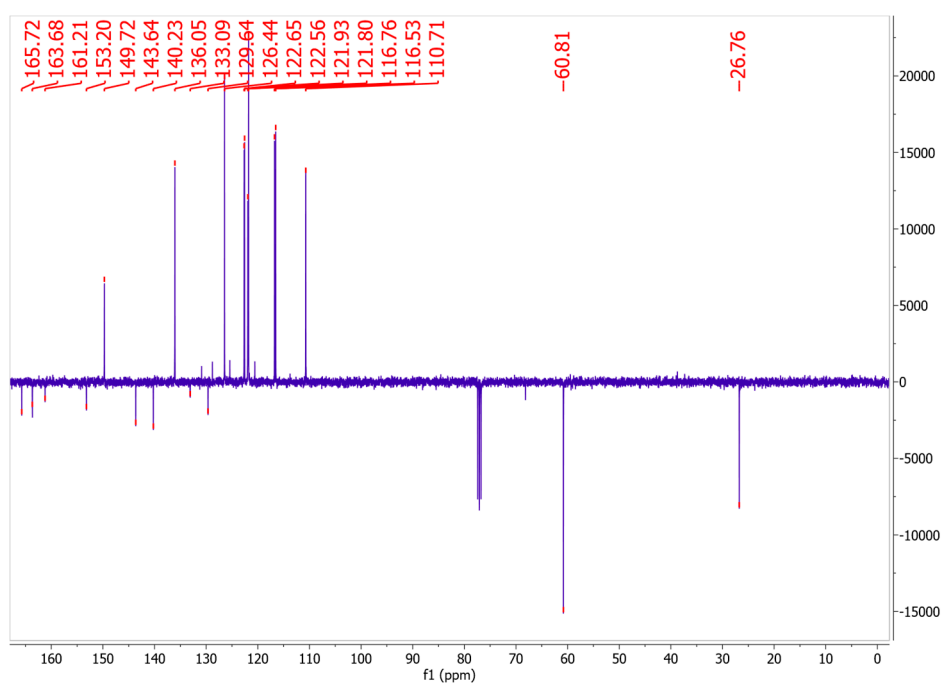
2-{[(1-(4-fluorophenyl)-1H-1,2,3-triazol-4-yl)methyl]thio}-5-[(quinolin-8-yloxy)methyl]-1,3,4-oxadiazole (**12m**)



<sup>1</sup>H NMR



<sup>13</sup>C NMR





**Single Mass Analysis**

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

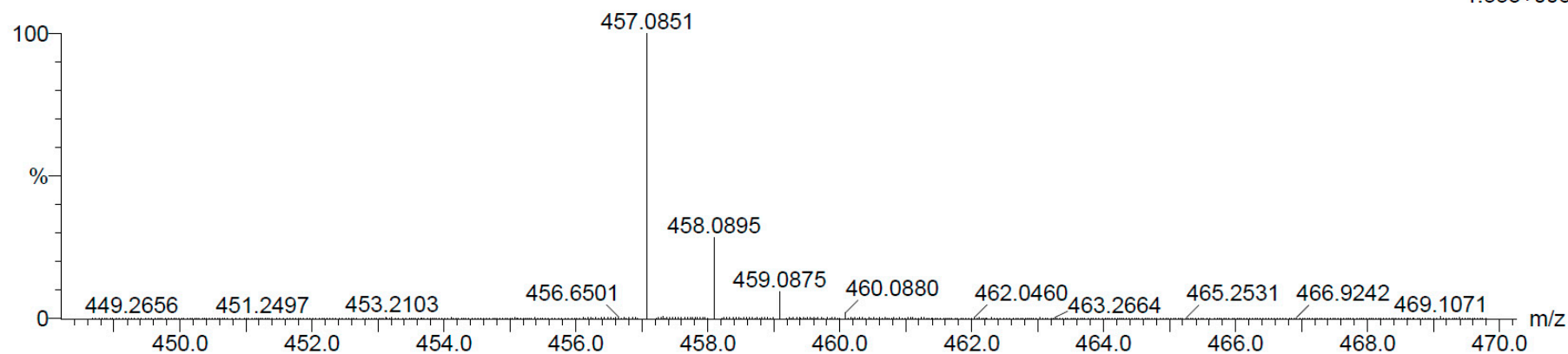
Monoisotopic Mass, Even Electron Ions

134 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 20-25 H: 15-20 N: 5-10 O: 0-5 Na: 0-1 S: 0-1 F: 0-1

NC-5h 38 (1.247) Cm (1:61)

TOF MS ES+  
1.33e+005

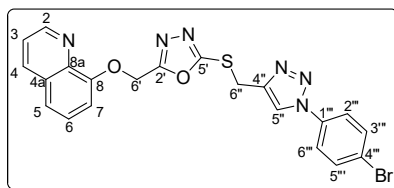
Minimum: -1.5

Maximum: 5.0 5.0 500.0

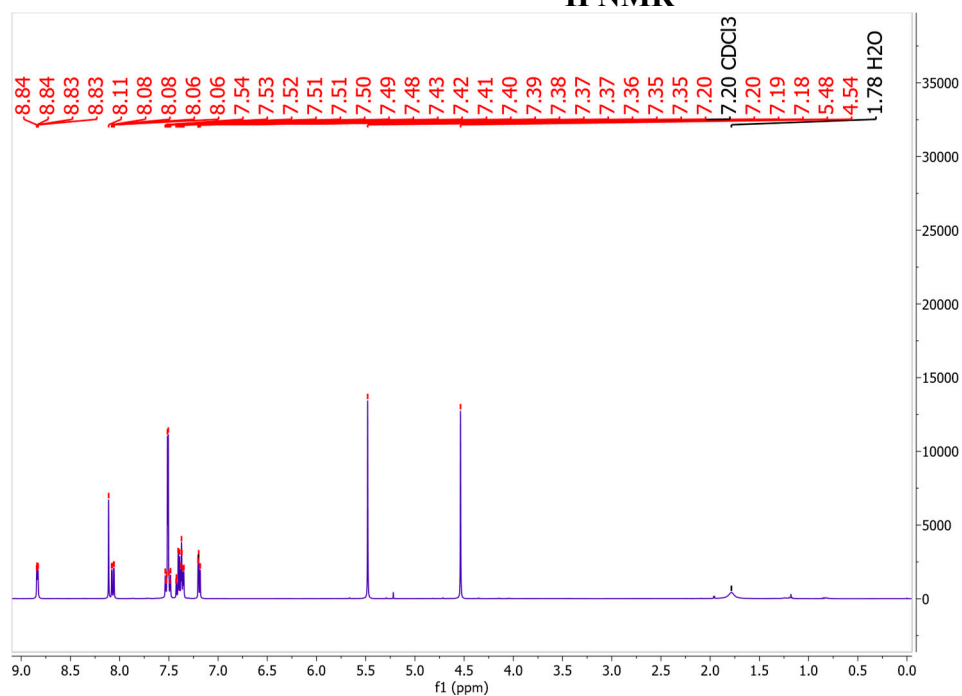
Mass Calc. Mass mDa PPM DBE i-FIT i-FIT (Norm) Formula

457.0851 457.0859 -0.8 -1.8 16.5 521.4 0.0 C21 H15 N6 O2 Na S F

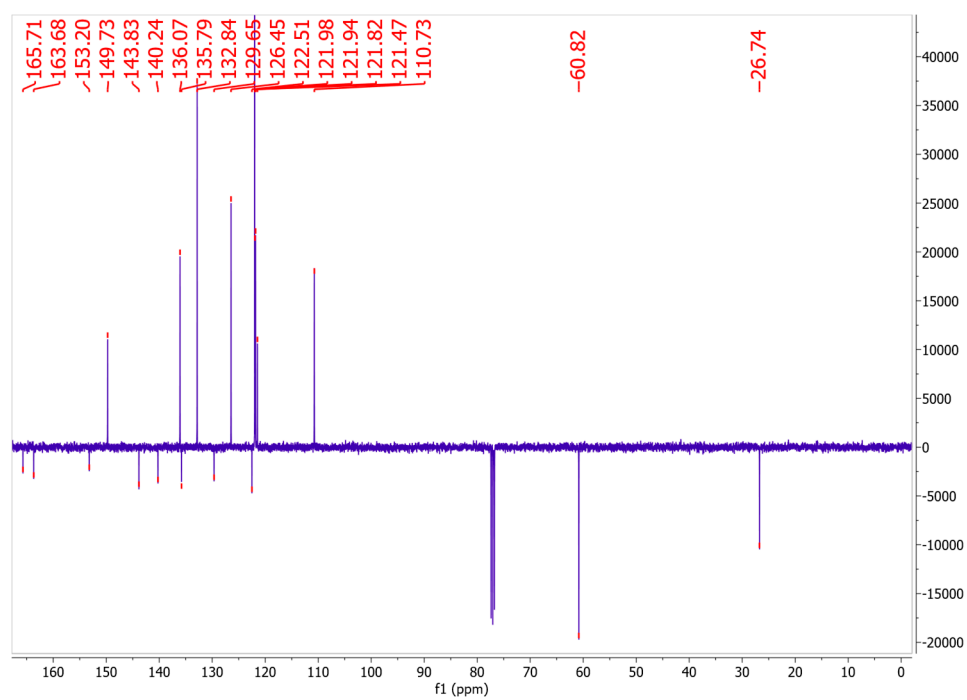
2-{[(1-(4-bromophenyl)-1H-1,2,3-triazol-4-yl)methyl]thio}-5-[(quinolin-8-yloxy)methyl]-  
1,3,4-oxadiazole (**12n**)



<sup>1</sup>H NMR



<sup>13</sup>C NMR



## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

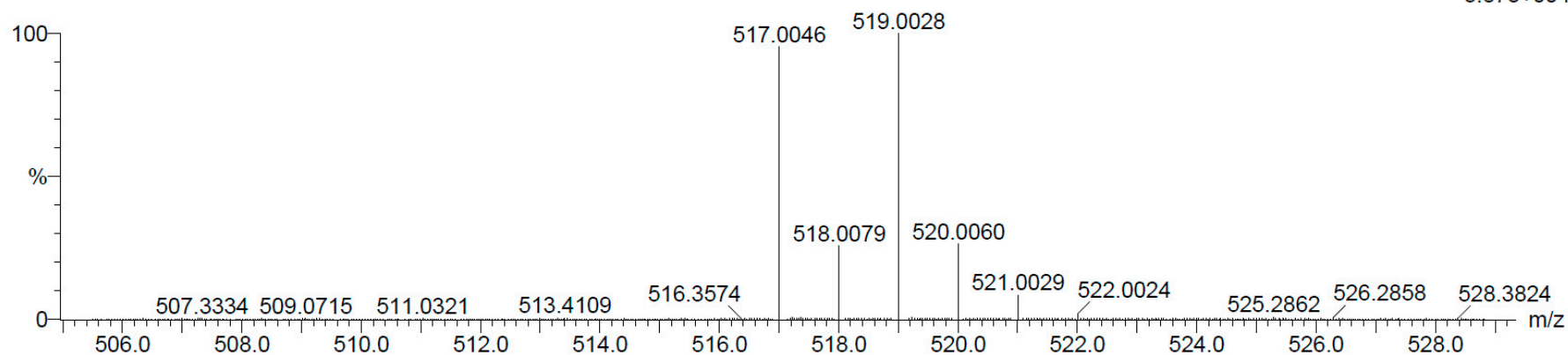
130 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 20-25 H: 15-20 N: 5-10 O: 0-5 Na: 0-1 S: 0-1 Br: 0-1

NC-5i 37 (1.215) Cm (1:61)

TOF MS ES+  
3.87e+004



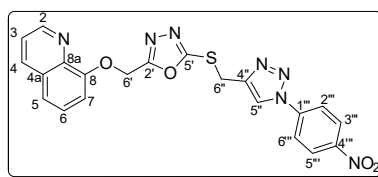
Minimum: -1.5

Maximum: 5.0 5.0 500.0

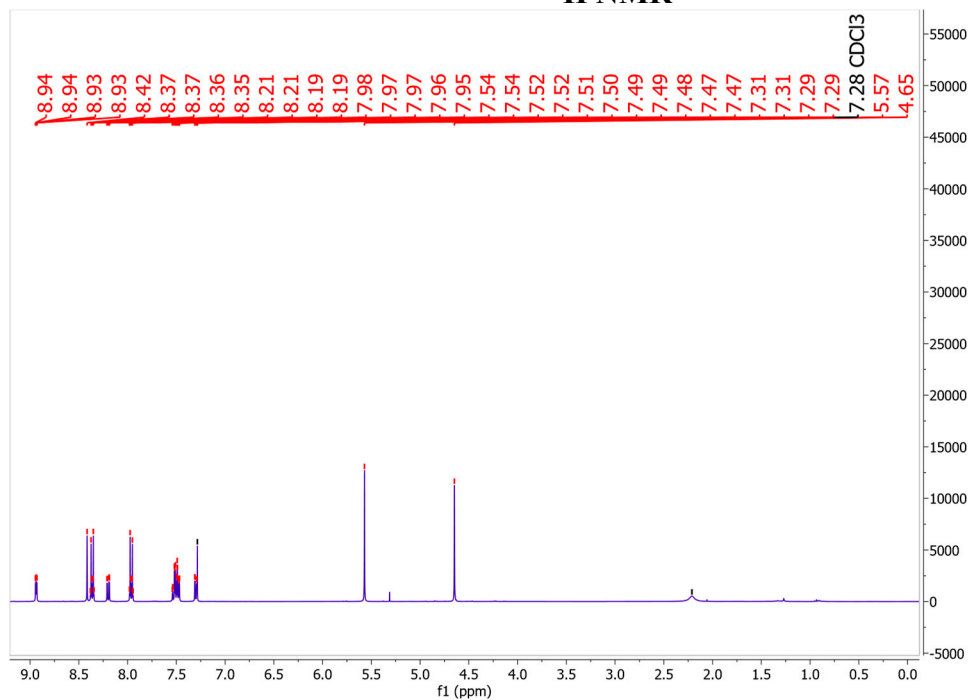
Mass Calc. Mass mDa PPM DBE i-FIT i-FIT (Norm) Formula

517.0046 517.0058 -1.2 -2.3 16.5 404.1 0.0 C21 H15 N6 O2 Na S Br

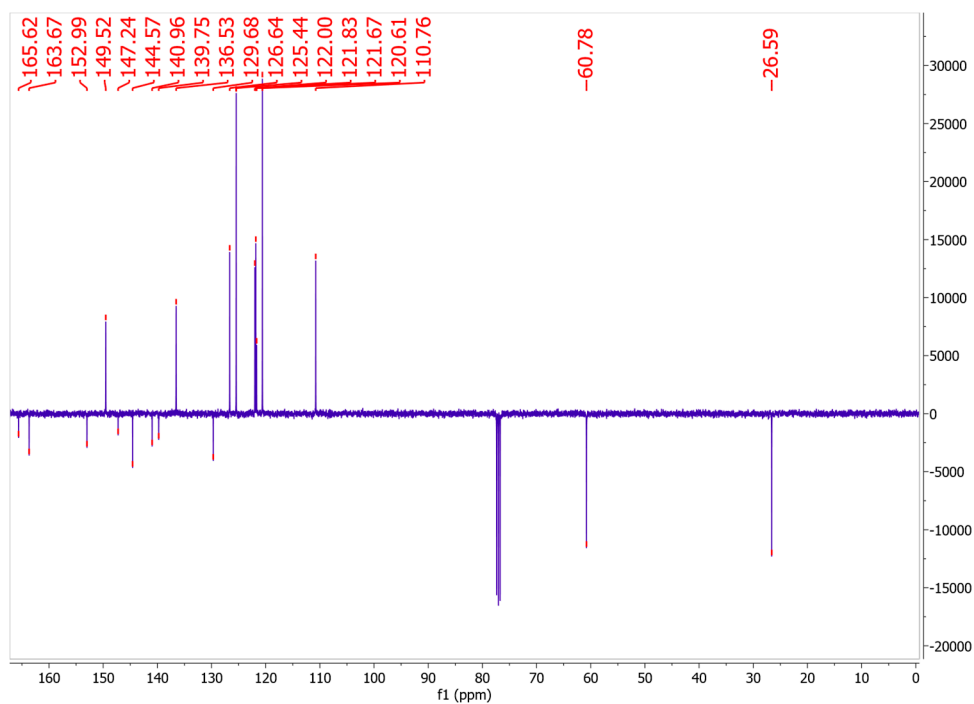
2-{[(1-(4-nitrophenyl)-1H-1,2,3-triazol-4-yl)methyl]thio}-5-[(quinolin-8-yloxy)methyl]-  
1,3,4-oxadiazole (**12o**)



<sup>1</sup>H NMR



<sup>13</sup>C NMR



**Single Mass Analysis**

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

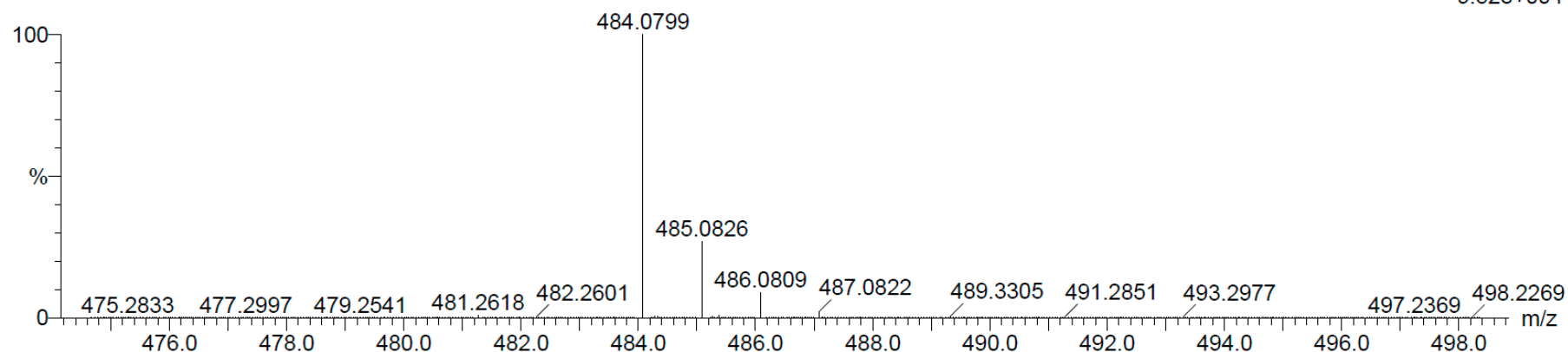
Monoisotopic Mass, Even Electron Ions

53 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 20-25 H: 15-20 N: 5-10 O: 0-5 Na: 0-1 S: 0-1

NC-5I 43 (1.416) Cm (1:61)

TOF MS ES+  
9.52e+004

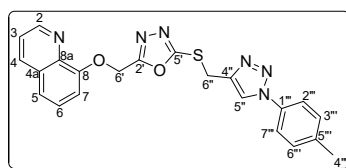
Minimum: -1.5

Maximum: 5.0 5.0 500.0

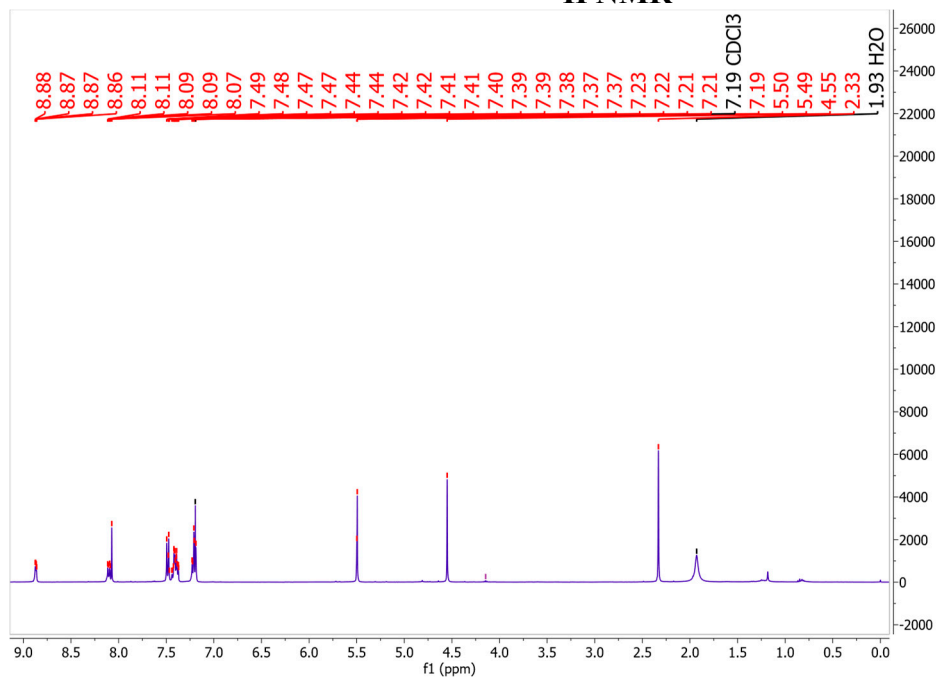
Mass Calc. Mass mDa PPM DBE i-FIT i-FIT (Norm) Formula

484.0799 484.0804 -0.5 -1.0 17.5 465.6 0.0 C21 H15 N7 O4 Na S

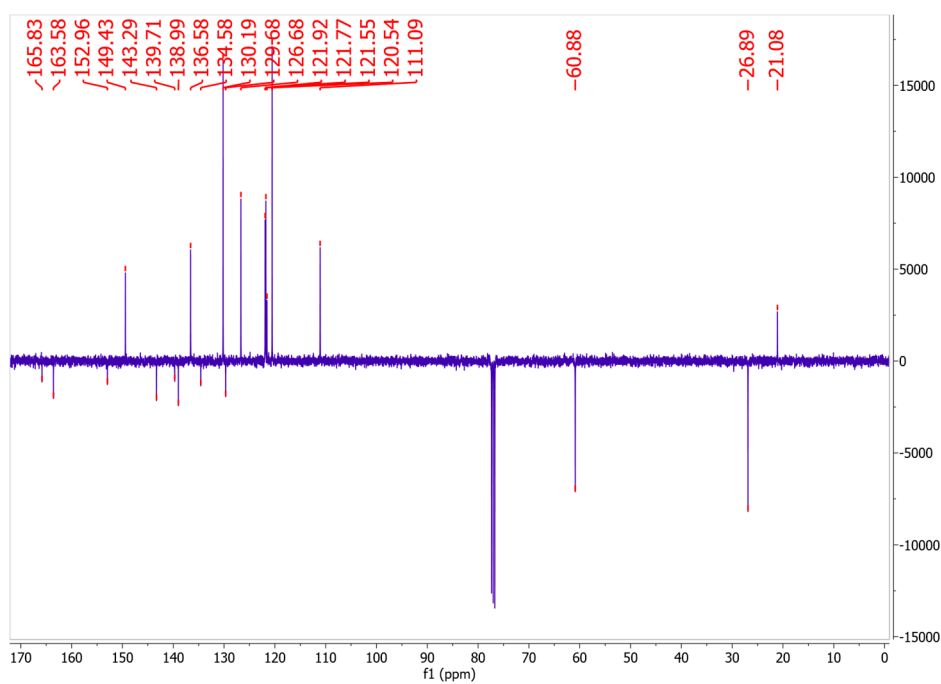
2-[(quinolin-8-yloxy)methyl]-5-{[(1-(p-tolyl)-1H-1,2,3-triazol-4-yl)methyl]thio}-1,3,4-oxadiazole (**12p**)



<sup>1</sup>H NMR



<sup>13</sup>C NMR



## Elemental Composition Report\_Compound 12p

Page 1

### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

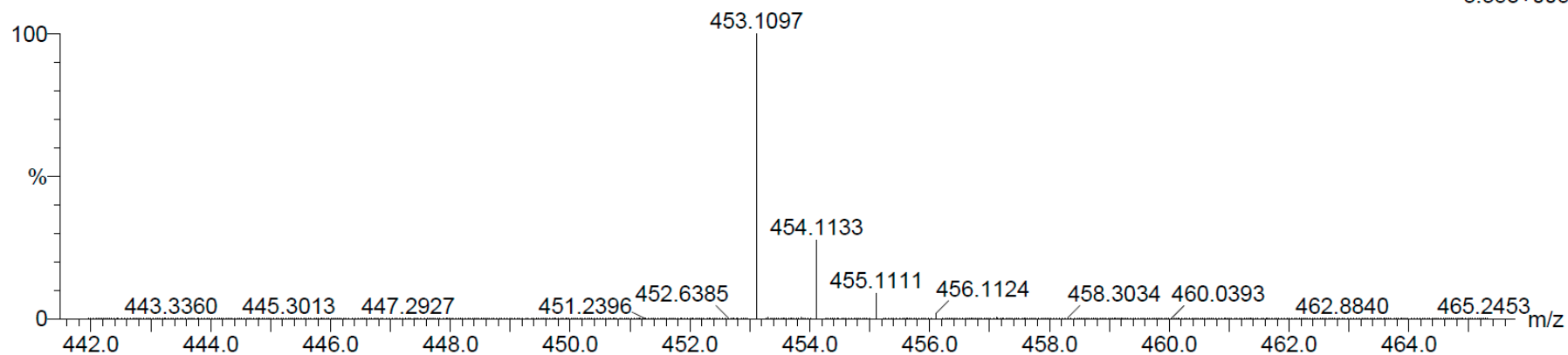
63 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 20-25 H: 15-20 N: 5-10 O: 0-5 Na: 0-1 S: 0-1

NC-5j 45 (1.482) Cm (1:61)

TOF MS ES+  
3.35e+005



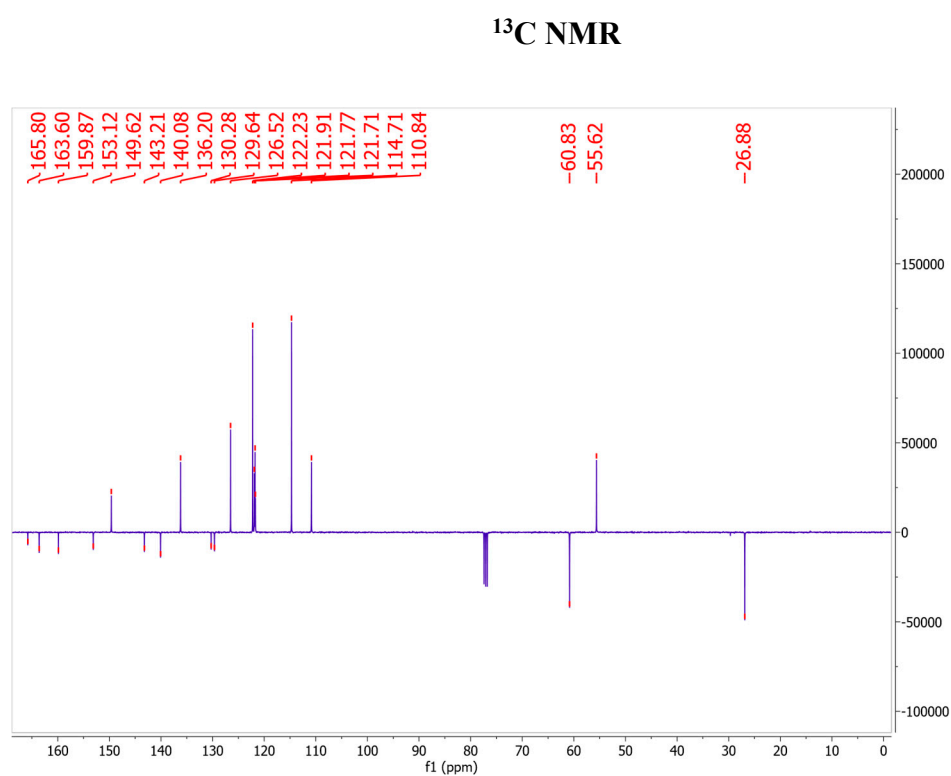
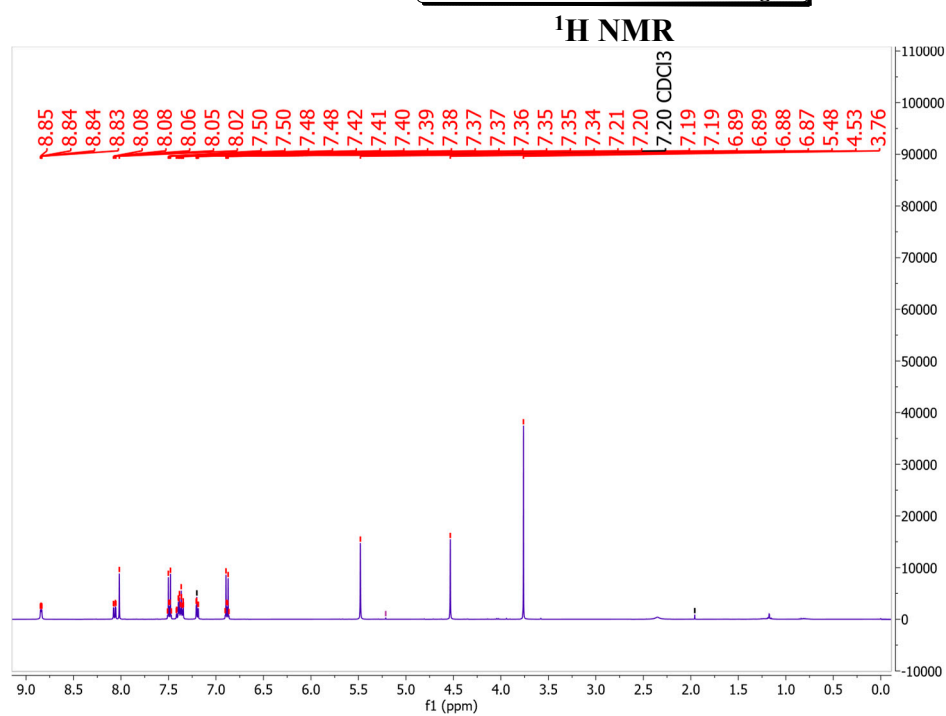
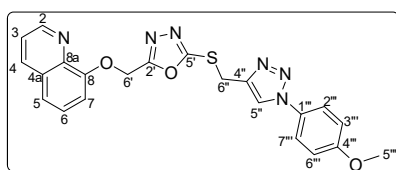
Minimum: -1.5

Maximum: 5.0 5.0 500.0

Mass Calc. Mass mDa PPM DBE i-FIT i-FIT (Norm) Formula

453.1097 453.1110 -1.3 -2.9 16.5 588.2 0.0 C22 H18 N6 O2 Na S

2-{[(1-(4-methoxyphenyl)-1H-1,2,3-triazol-4-yl)methyl]thio}-5-[(quinolin-8-yloxy)methyl]-  
1,3,4-oxadiazole (**12q**)





**Single Mass Analysis**

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

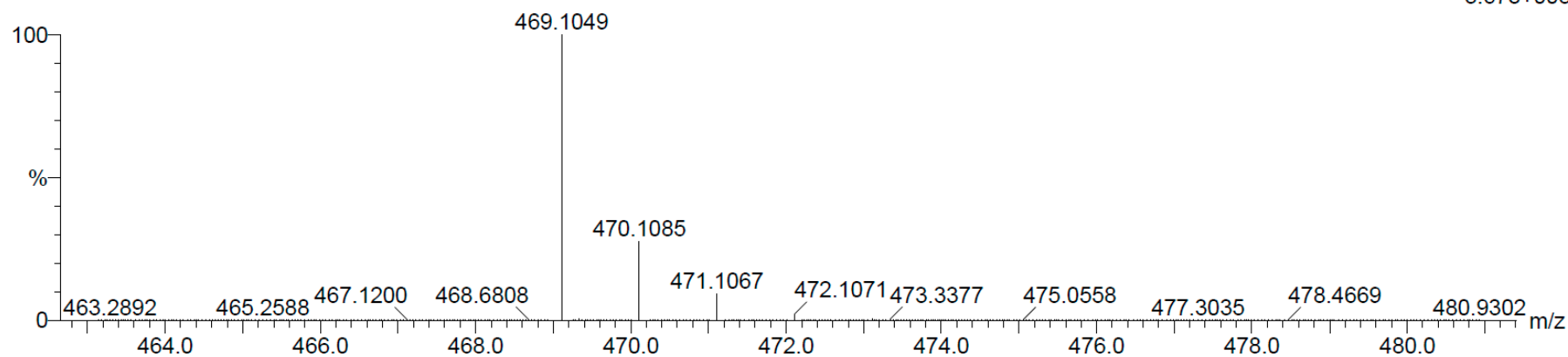
Monoisotopic Mass, Even Electron Ions

55 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 20-25 H: 15-20 N: 5-10 O: 0-5 Na: 0-1 S: 0-1

NC-5k 25 (0.809) Cm (1:61)

TOF MS ES+  
3.67e+005

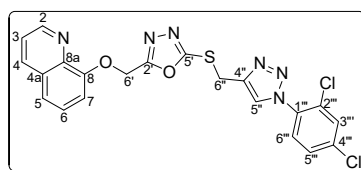
Minimum: -1.5

Maximum: 5.0 5.0 500.0

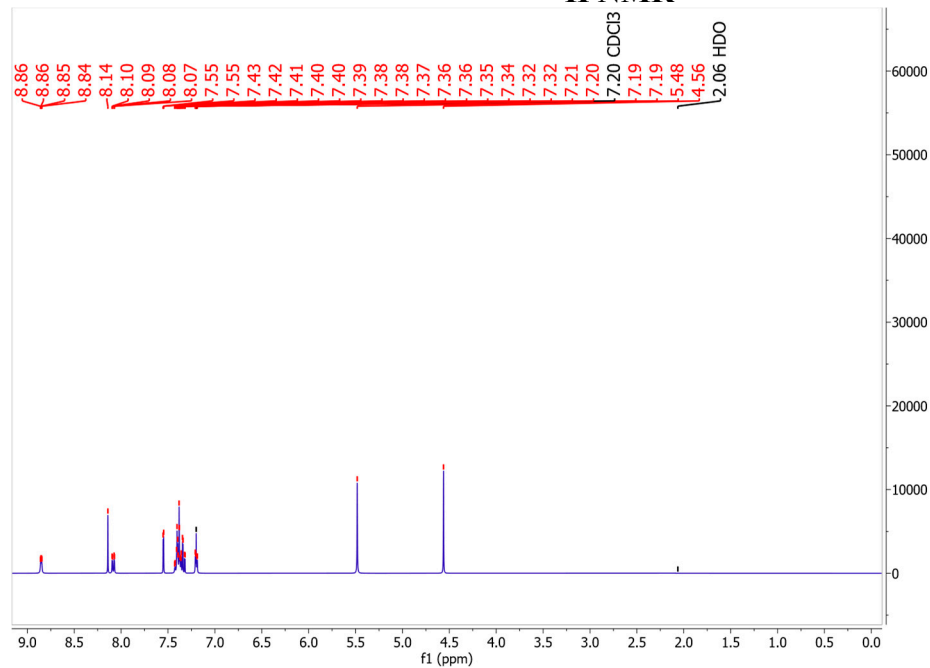
Mass Calc. Mass mDa PPM DBE i-FIT i-FIT (Norm) Formula

469.1049 469.1059 -1.0 -2.1 16.5 587.7 0.0 C22 H18 N6 O3 Na S

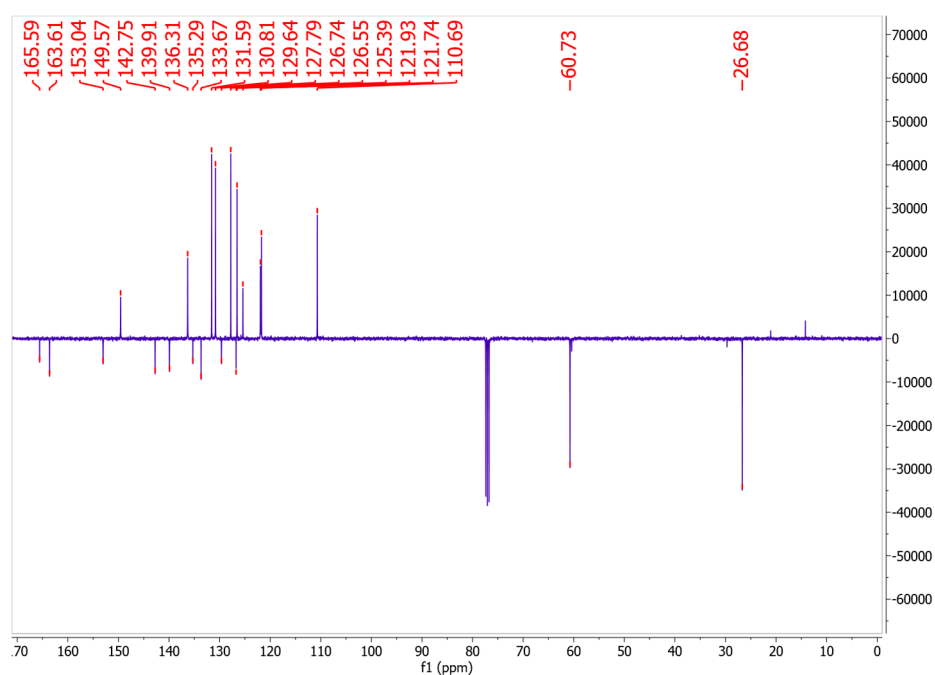
2-[[1-(2,4-dichlorophenyl)-1H-1,2,3-triazol-4-yl)methyl]thio}-5-[(quinolin-8-yloxy)methyl]-1,3,4-oxadiazole (**12r**)



<sup>1</sup>H NMR



<sup>13</sup>C NMR



## Elemental Composition Report\_Compound 12r

Page 1

### Single Mass Analysis

Tolerance = 4.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

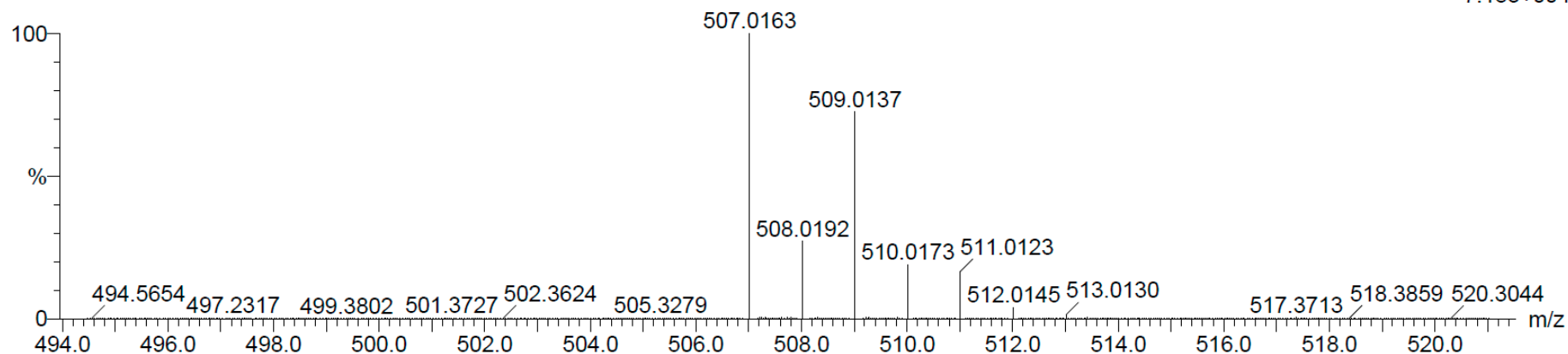
191 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 20-25 H: 10-15 N: 5-10 O: 0-5 Na: 0-1 S: 0-1 Cl: 0-2

NC-5m 11 (0.337) Cm (1:61)

TOF MS ES+  
7.18e+004



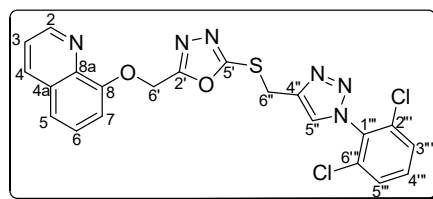
Minimum: -1.5

Maximum: 5.0 4.0 500.0

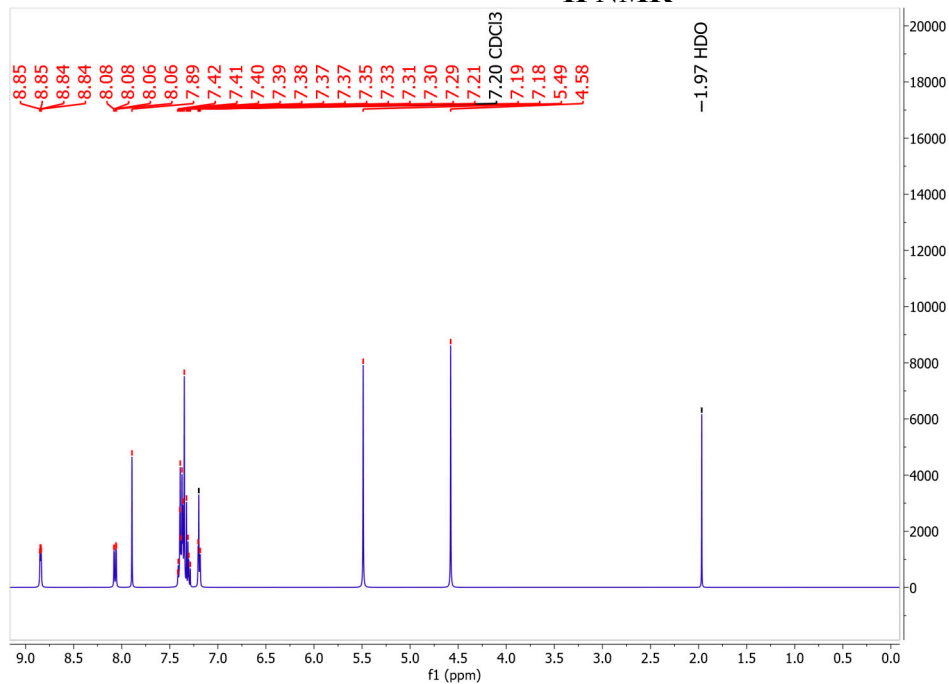
Mass Calc. Mass mDa PPM DBE i-FIT i-FIT (Norm) Formula

507.0163 507.0174 -1.1 -2.2 16.5 470.1 0.0 C21 H14 N6 O2 Na S Cl2

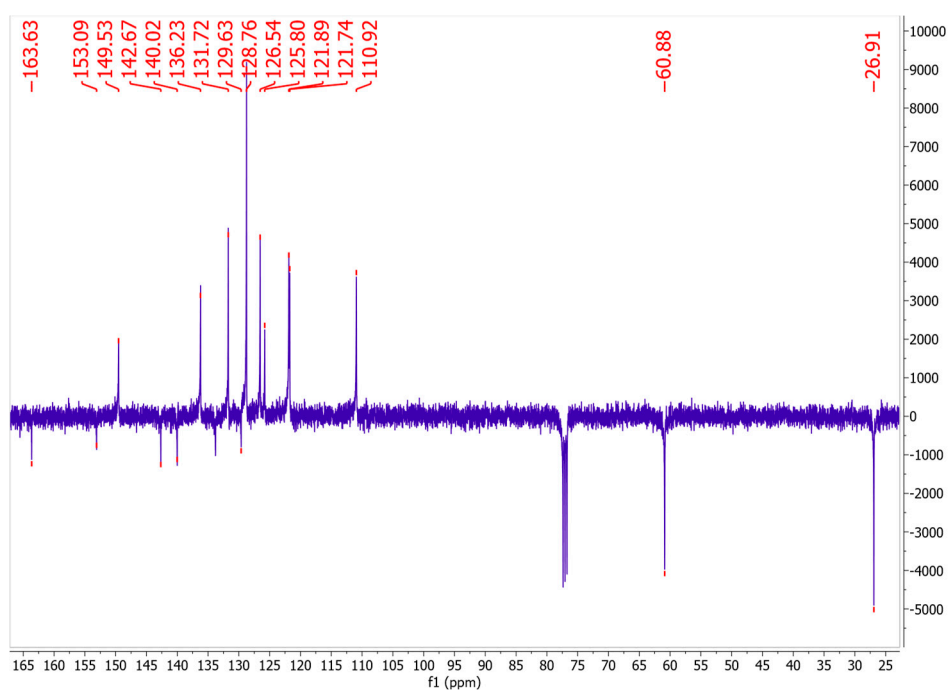
2-{[(1-(2,6-dichlorophenyl)-1H-1,2,3-triazol-4-yl)methyl]thio}-5-[(quinolin-8-yloxy)methyl]-1,3,4-oxadiazole (**12s**)



<sup>1</sup>H NMR



<sup>13</sup>C NMR



## Elemental Composition Report\_Compound 12s

Page 1

### Single Mass Analysis

Tolerance = 4.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

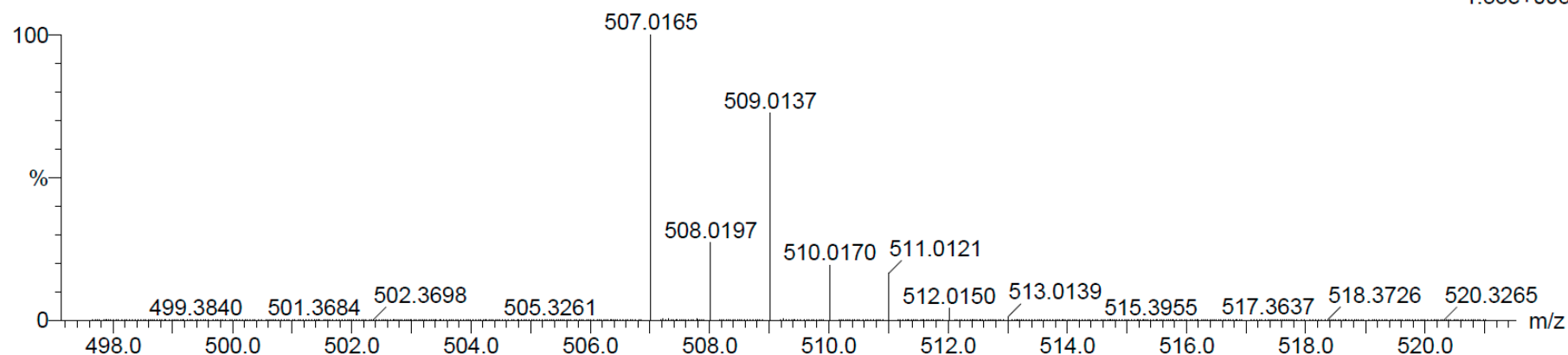
191 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 20-25 H: 10-15 N: 5-10 O: 0-5 Na: 0-1 S: 0-1 Cl: 0-2

NC-5n 22 (0.709) Cm (1:61)

TOF MS ES+  
1.33e+005



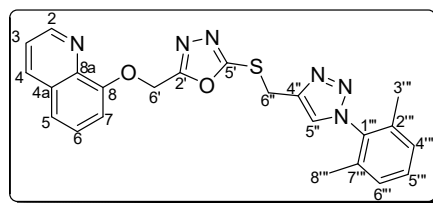
Minimum: -1.5

Maximum: 5.0 4.0 500.0

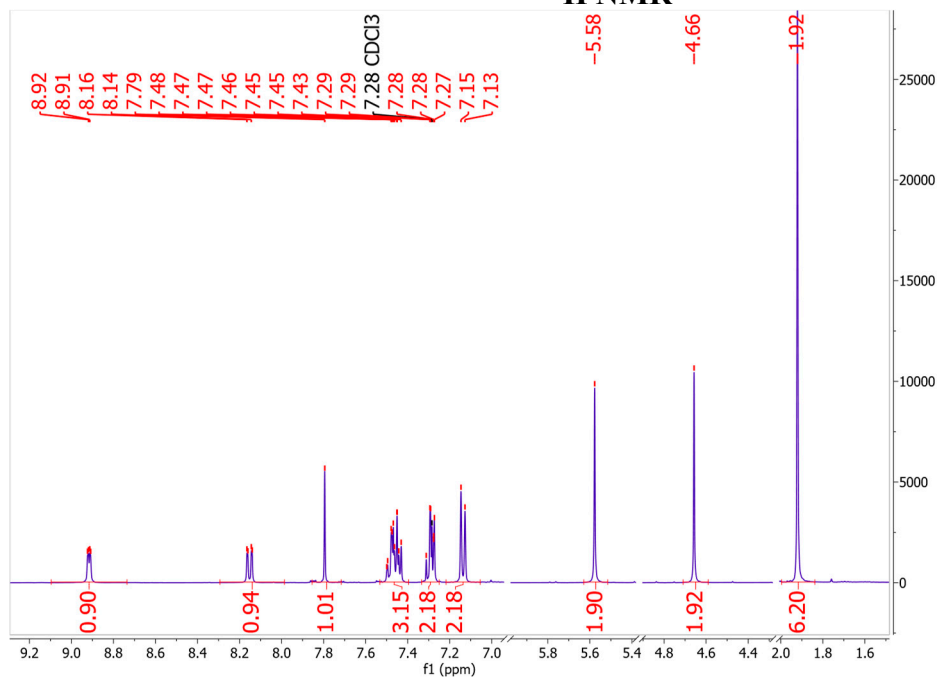
Mass Calc. Mass mDa PPM DBE i-FIT i-FIT (Norm) Formula

507.0165 507.0174 -0.9 -1.8 16.5 476.7 0.0 C21 H14 N6 O2 Na S Cl2

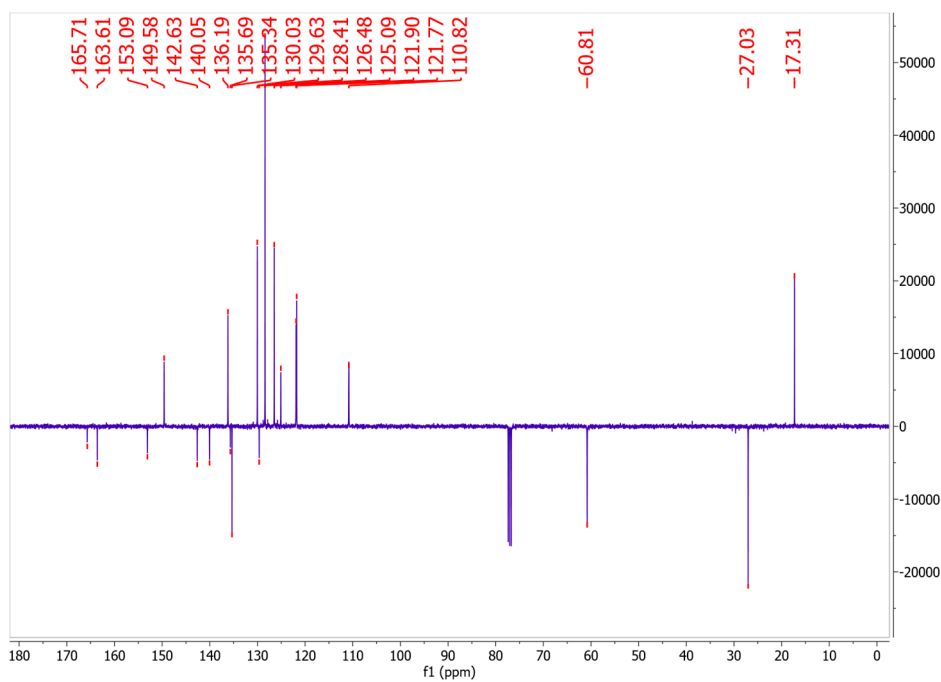
2-{[(1-(2,6-dimethylphenyl)-1H-1,2,3-triazol-4-yl)methyl]thio}-5-[(quinolin-8-yloxy)methyl]-1,3,4-oxadiazole (**12t**)



<sup>1</sup>H NMR



<sup>13</sup>C NMR



## Elemental Composition Report\_Compound 12t

Page 1

### Single Mass Analysis

Tolerance = 4.0 PPM / DBE: min = -1.5, max = 500.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

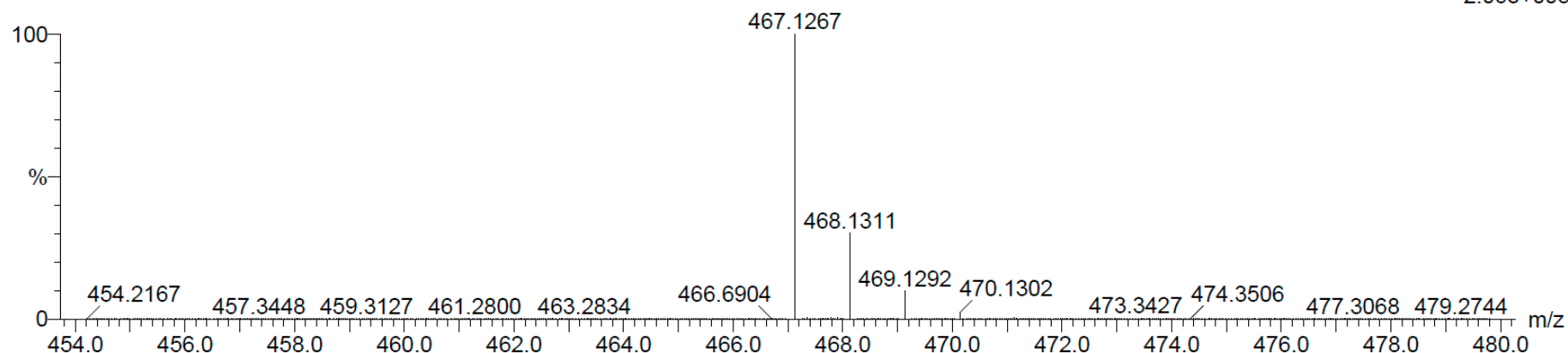
29 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 20-25 H: 15-20 N: 5-10 O: 0-5 Na: 1-1 S: 0-1

NC-5p 18 (0.574) Cm (1:61)

TOF MS ES+  
2.06e+005



Minimum: -1.5

Maximum: 5.0 4.0 500.0

Mass Calc. Mass mDa PPM DBE i-FIT i-FIT (Norm) Formula

467.1267 467.1266 0.1 0.2 16.5 537.3 0.0 C23 H20 N6 O2 Na S