

## Supplementary materials

### Exploring the antitubercular activity of anthranilic acid derivatives: from MabA (FabG1) inhibition to intrabacterial acidification

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Figure S1: 1D <sup>19</sup>F NMR spectra of 4 compounds alone and in the presence of MabA

Figure S2: Western blot showing overexpression of MabA in H37Rv\_pMV261-MabA, as compared to the parental control.

Figures S3-S40: <sup>1</sup>H NMR, <sup>13</sup>C NMR and HRMS data of compounds **2-20**

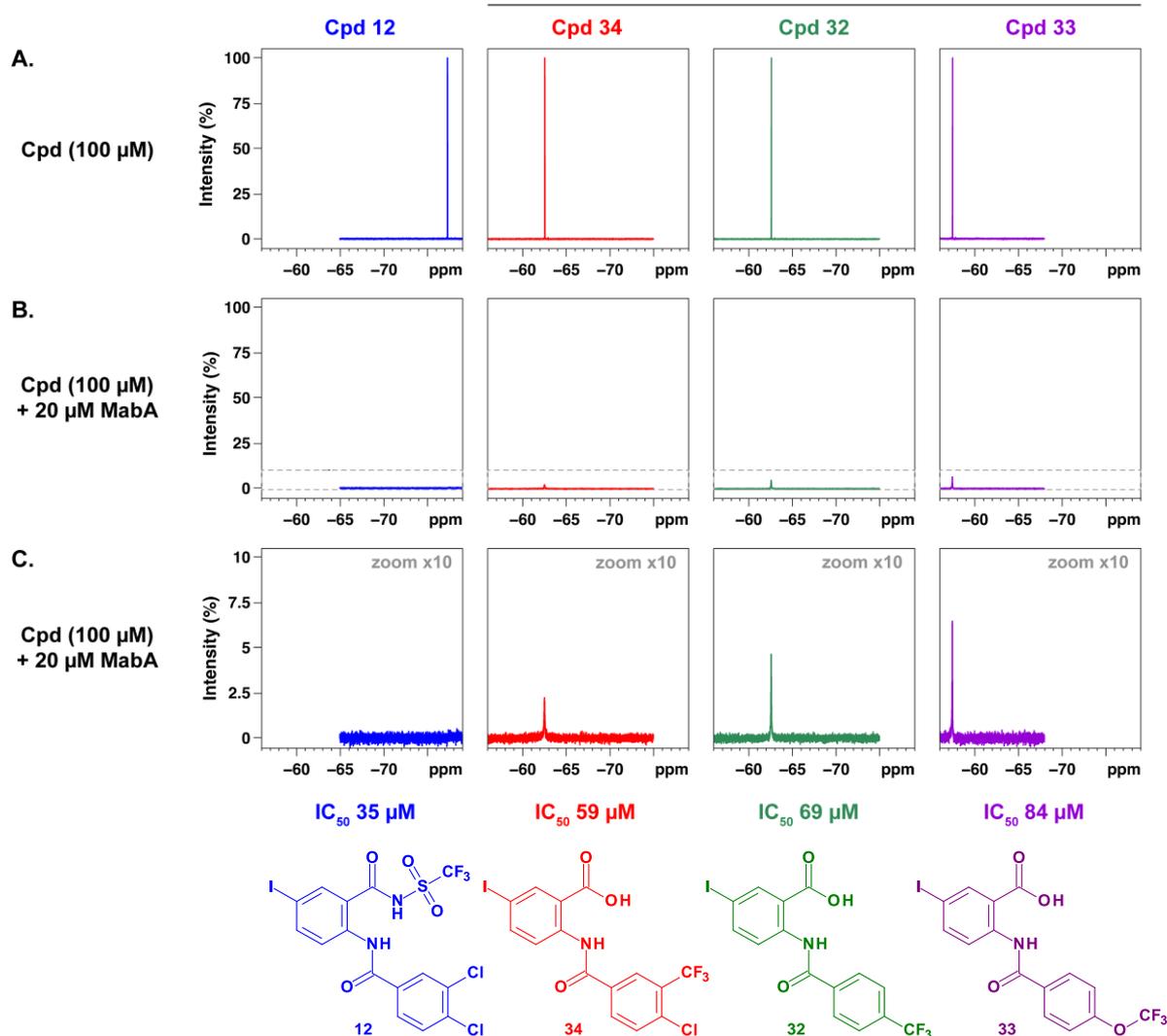


Figure S1: 1D  $^{19}\text{F}$  NMR spectra of compound **12** (this study) and compounds **34**, **32** and **33** from Faion L. *et al.* [20] (in blue, red, green and violet, respectively) at 100  $\mu\text{M}$  alone (**A.**) and in the presence of MabA at 20  $\mu\text{M}$  (**B.** and **C.**). The spectra in **C.** correspond to the ones in **B.** with a 10x magnification of the y-axis. The  $\text{IC}_{50}$  for each compound is indicated at the bottom.

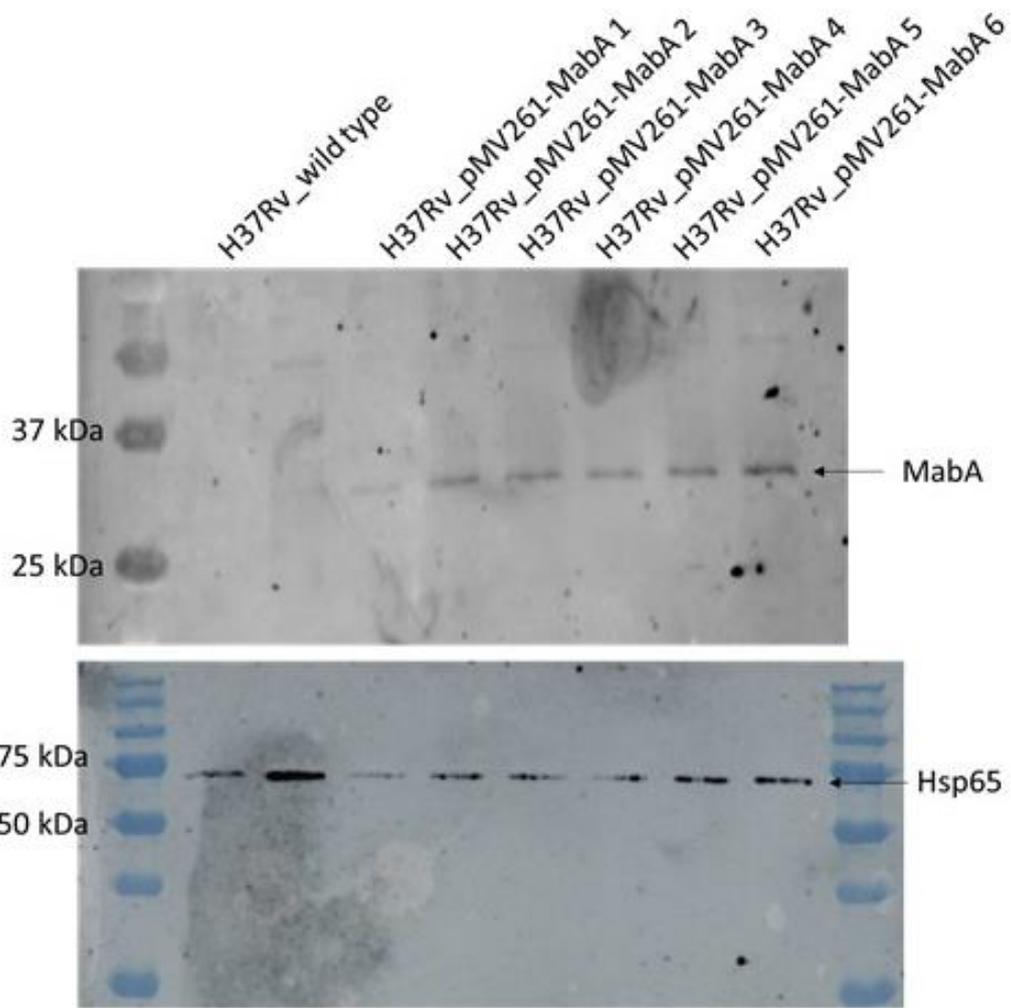
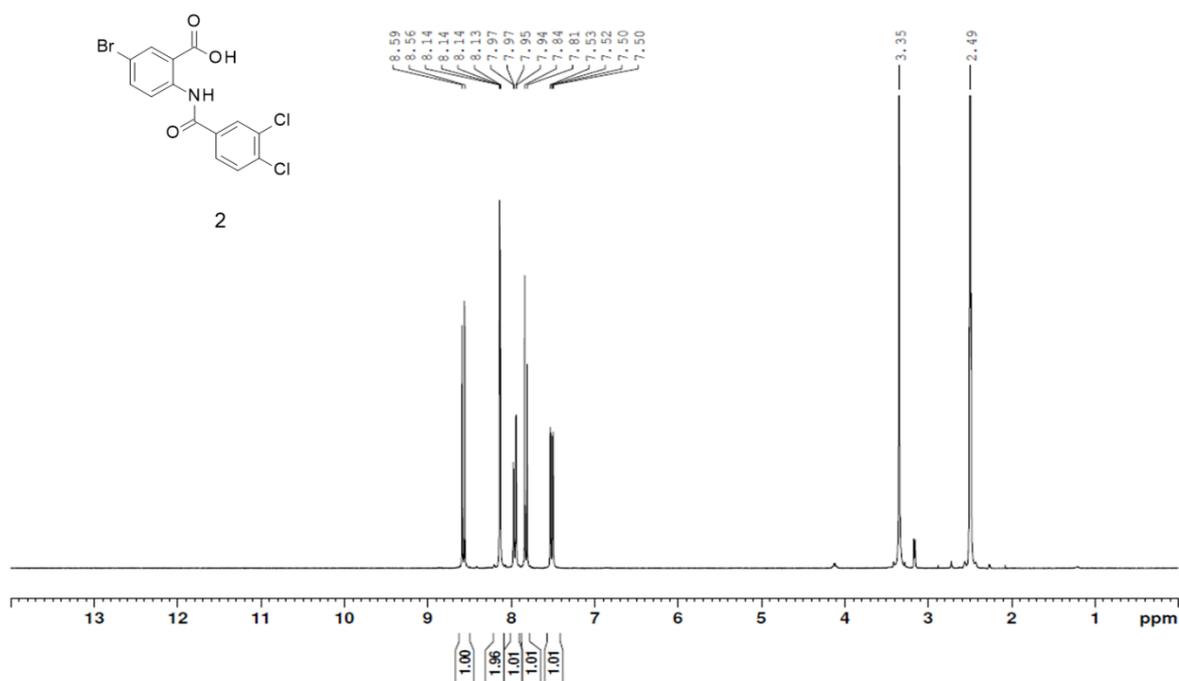


Figure S2: Western blot showing overexpression of MabA in H37Rv\_pMV261-MabA, as compared to the parental control. H37Rv\_pMV261-MabA 1 through 6 correspond to different clones tested.

<sup>1</sup>H NMR of compound 2 (300 MHz, DMSO-d6)



<sup>13</sup>C NMR of compound 2 (75 MHz, DMSO-d6)

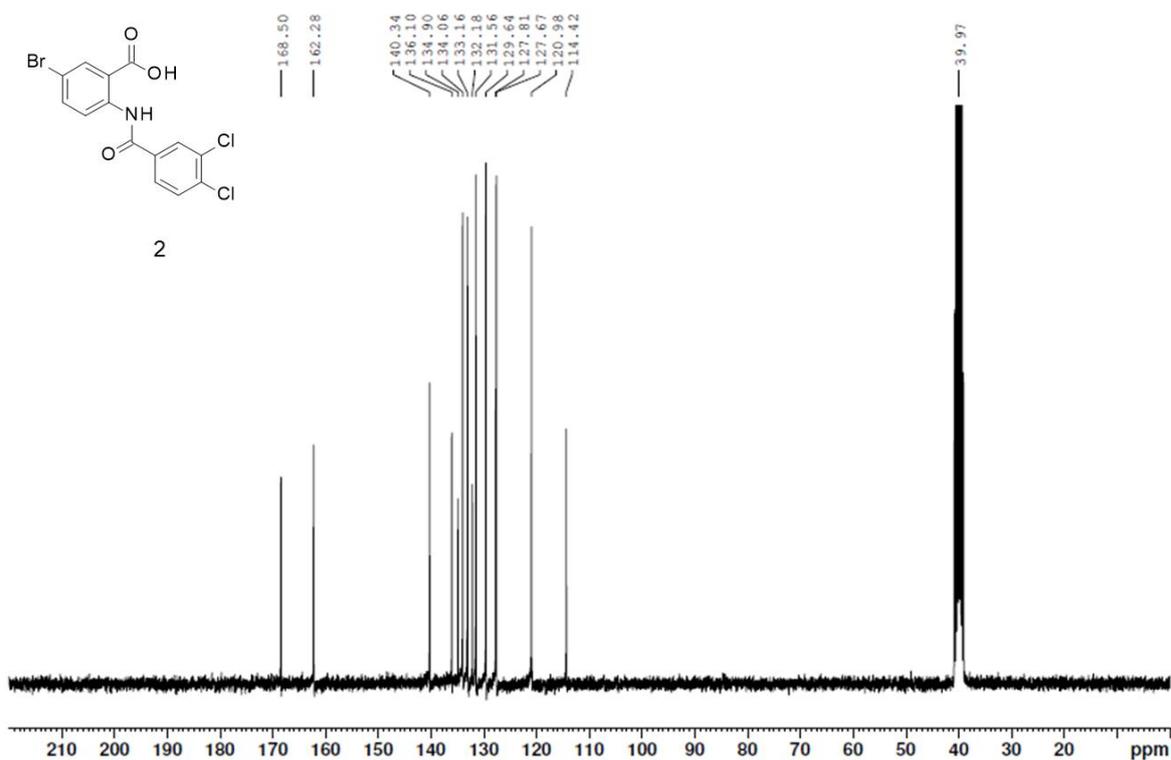
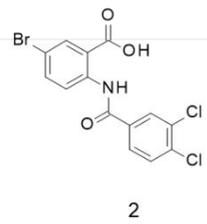


Figure S3: <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 2

Elemental Composition Report



Single Mass Analysis

Tolerance = 100.0 mDa / DBE: min = -1.5, max = 500.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

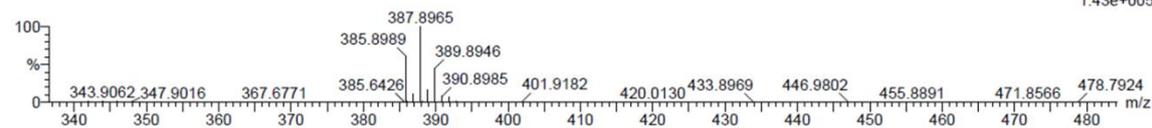
Monoisotopic Mass, Even Electron Ions

337 formula(e) evaluated with 55 results within limits (up to 10 best isotopic matches for each mass)

Elements Used:

C: 0-30 H: 0-40 N: 0-4 O: 0-6 Cl: 0-2 Br: 1-1

1: TOF MS ES-  
1.43e+005

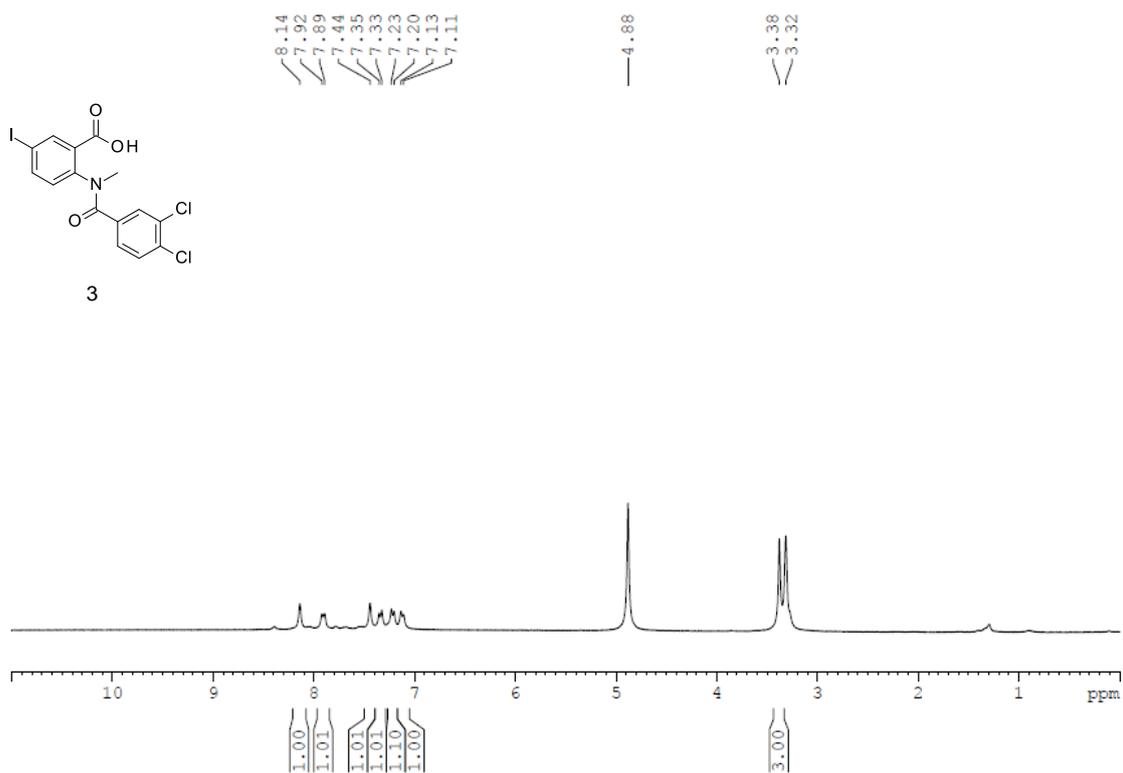


Minimum: 100.0 5.0 -1.5  
Maximum: 100.0 5.0 500.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
385.8989	385.8986	0.3	0.8	10.5	6.7	C14 H7 N O3 Cl2 Br

Figure S4: HRMS spectrum of compound 2

**<sup>1</sup>H NMR of compound 3 (300 MHz, MeOD-d4)**



**<sup>13</sup>C NMR of compound 3 (75 MHz, MeOD-d4)**

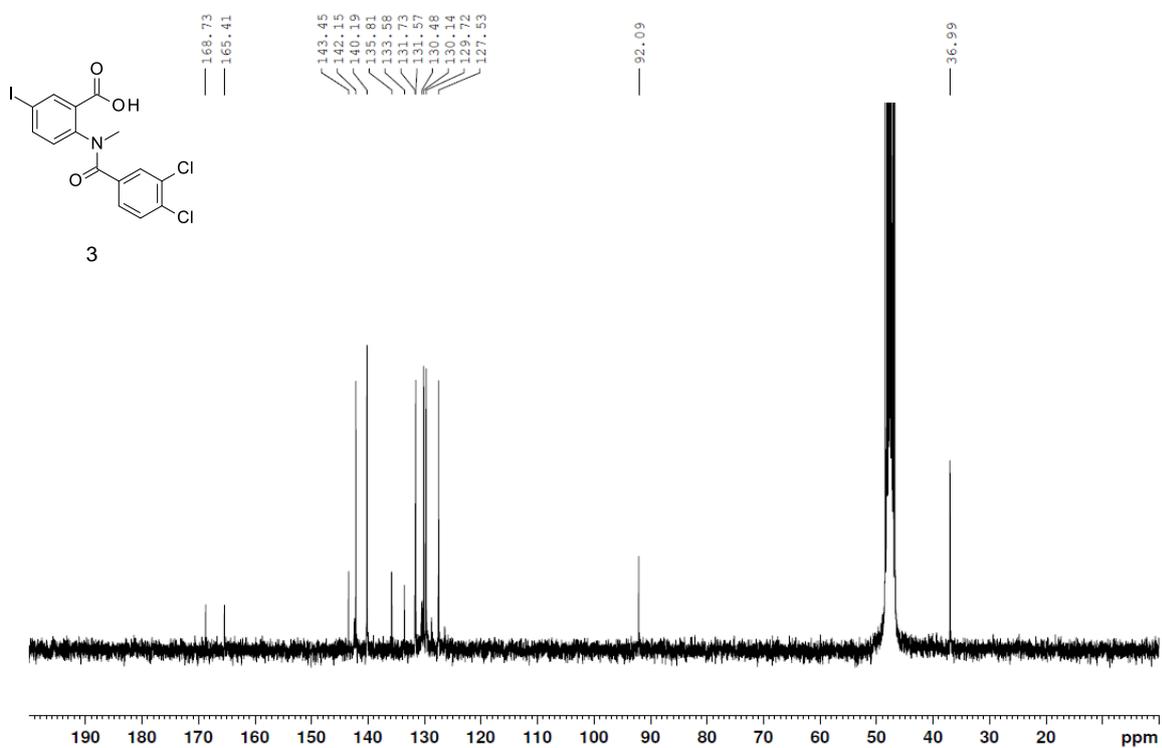
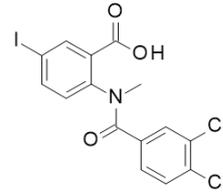


Figure S5: <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 3



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**Elemental Composition Report**

**Single Mass Analysis**

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 80.0

Element prediction: Off

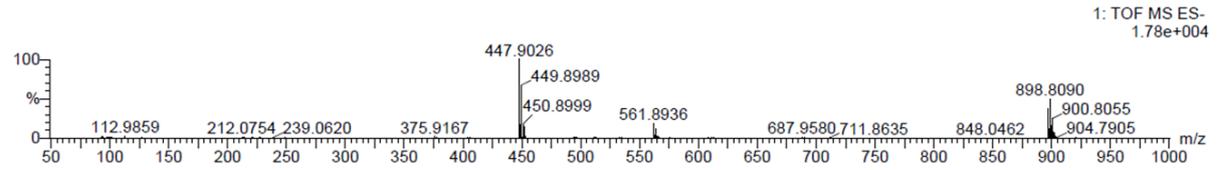
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

768 formula(e) evaluated with 11 results within limits (up to 1 best isotopic matches for each mass)

Elements Used:

C: 6-40 H: 2-36 N: 0-5 O: 0-7 Cl: 1-3 I: 0-1



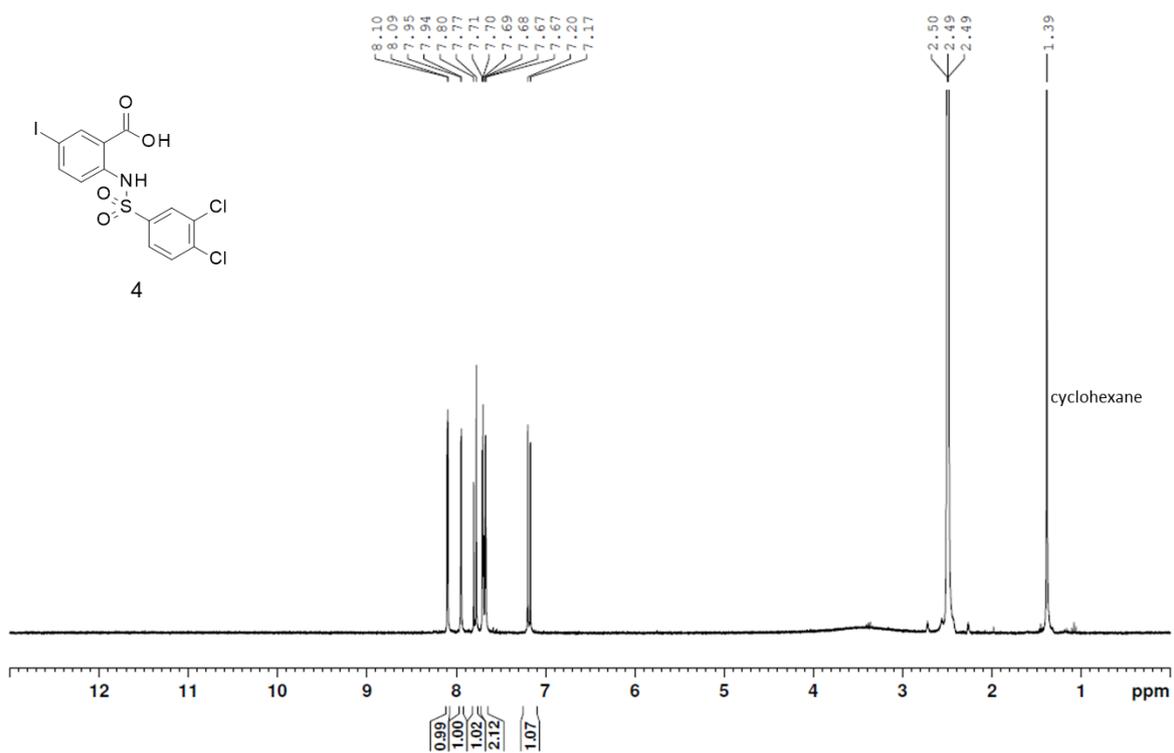
1: TOF MS ES-  
1.78e+04

Minimum: -1.5  
Maximum: 10.0 20.0 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
447.9026	447.9004	2.2	4.9	10.5	2.1	C15 H9 N O3 Cl2 I

Figure S6: HRMS spectrum of compound 3

<sup>1</sup>H NMR of compound 4 (300 MHz, DMSO-d6)



<sup>13</sup>C NMR of compound 4 (75 MHz, DMSO-d6)

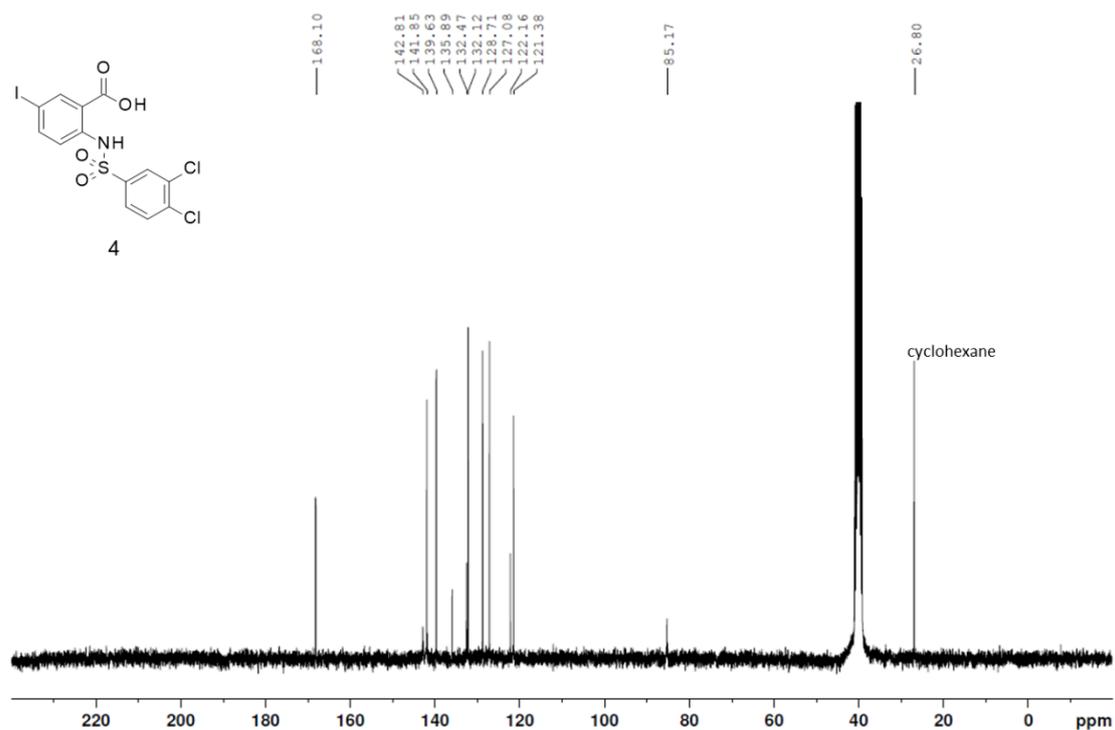
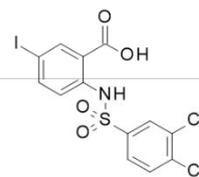


Figure S7: <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 4



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## Elemental Composition Report

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### 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

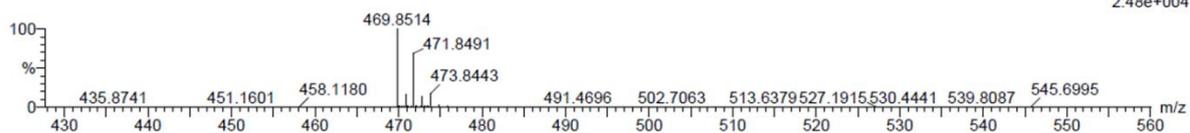
Monoisotopic Mass, Even Electron Ions

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

Elements Used:

C: 1-17 H: 1-17 N: 1-2 O: 0-4 S: 1-1 Cl: 0-2 I: 0-1

1: TOF MS ES-  
2.48e+004

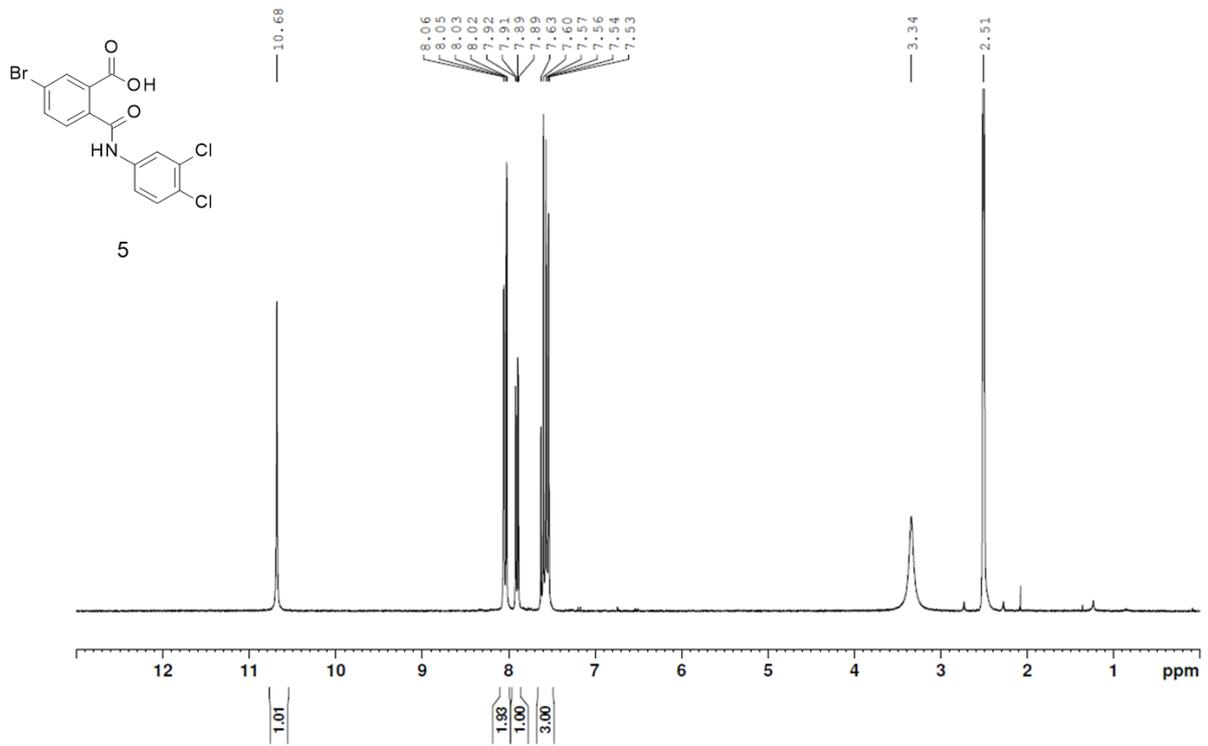


Minimum: -1.5  
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
469.8514	469.8518	-0.4	-0.9	9.5	6.1	C13 H7 N O4 S Cl2 I

Figure S8: HRMS spectrum of compound 4

<sup>1</sup>H NMR of compound 5 (300 MHz, DMSO-d6)



<sup>13</sup>C NMR of compound 5 (75 MHz, DMSO-d6)

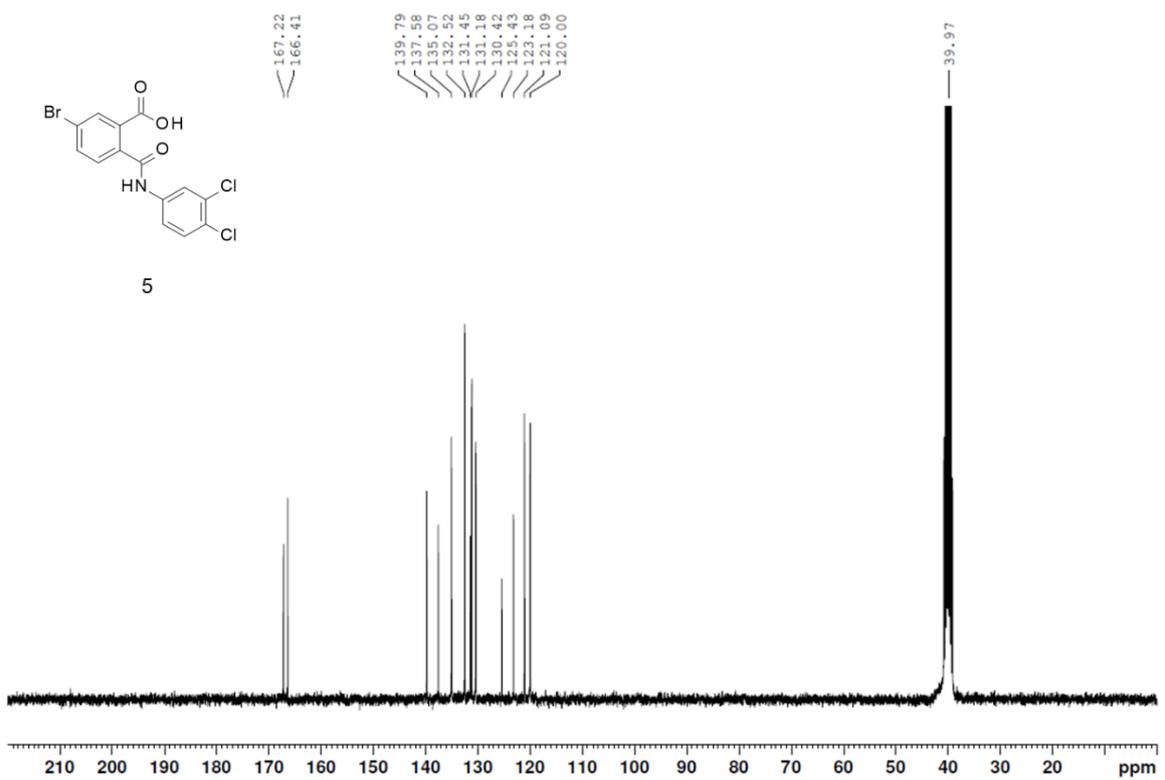
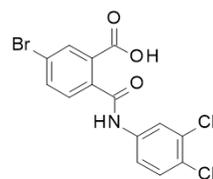


Figure S9: <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 5



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### Elemental Composition Report

#### Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

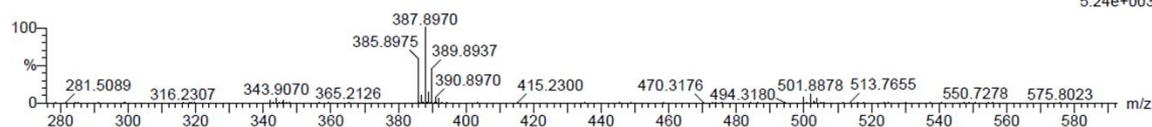
Monoisotopic Mass, Even Electron Ions

335 formula(e) evaluated with 7 results within limits (up to 1 best isotopic matches for each mass)

Elements Used:

C: 2-20 H: 2-36 N: 0-5 O: 0-7 Cl: 1-2 Br: 1-1 I: 0-1

1: TOF MS ES-  
5.24e+003



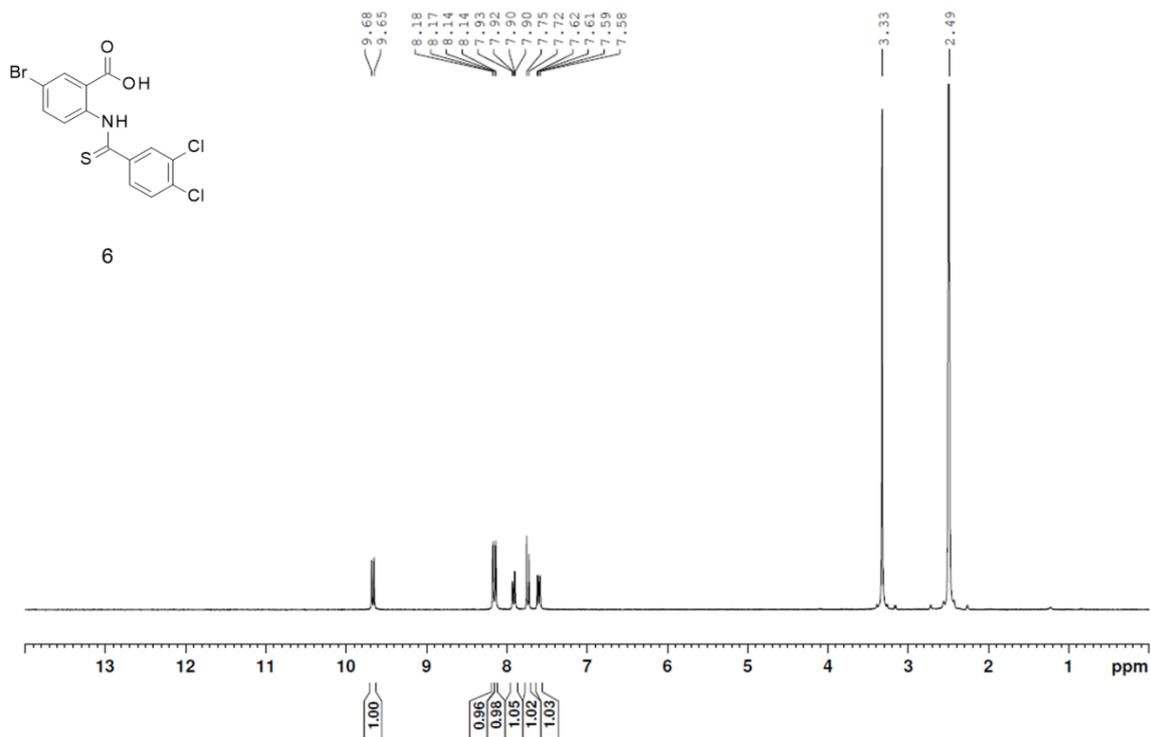
Minimum:

Maximum: 10.0 20.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
385.8975	385.8986	-1.1	-2.9	10.5	0.2	C14 H7 N O3 Cl2 Br

Figure S10: HRMS spectrum of compound 5

<sup>1</sup>H NMR of compound 6 (300 MHz, DMSO-d6)



<sup>13</sup>C NMR of compound 6 (75 MHz, DMSO-d6)

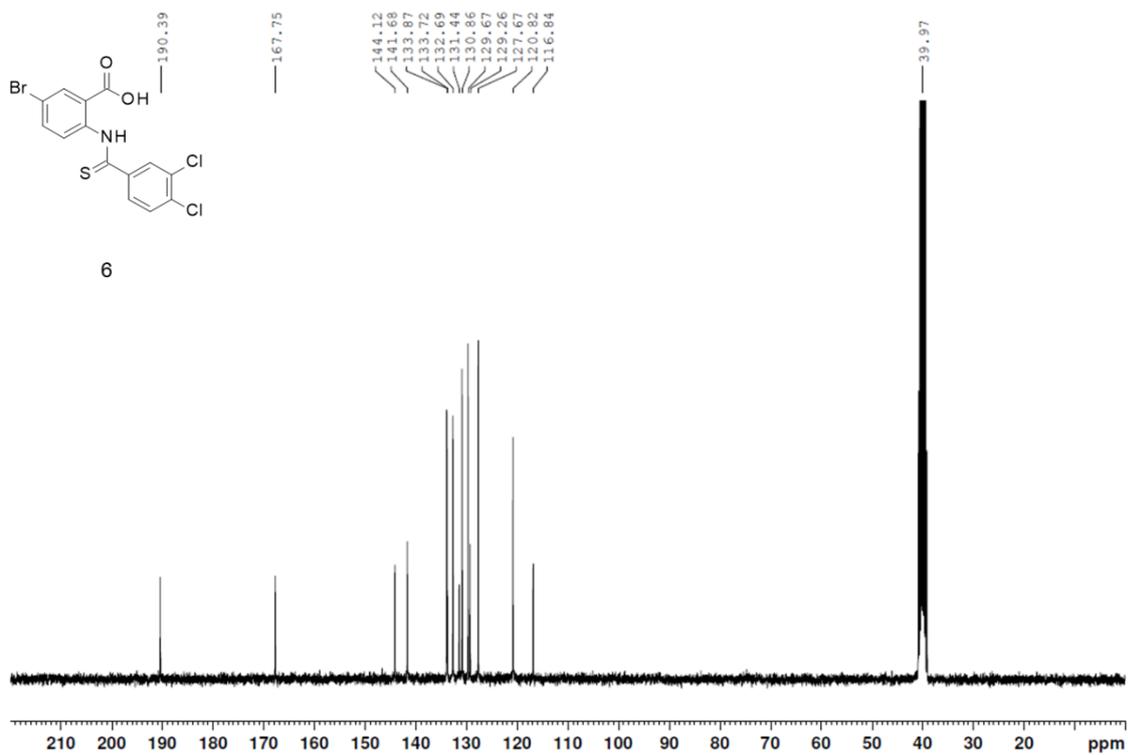
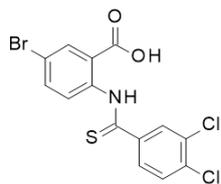


Figure S11: <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 6



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## Elemental Composition Report

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### Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

489 formula(e) evaluated with 16 results within limits (up to 1 best isotopic matches for each mass)

Elements Used:

C: 2-20 H: 2-36 N: 0-5 O: 0-7 S: 0-1 Cl: 1-2 Br: 1-1

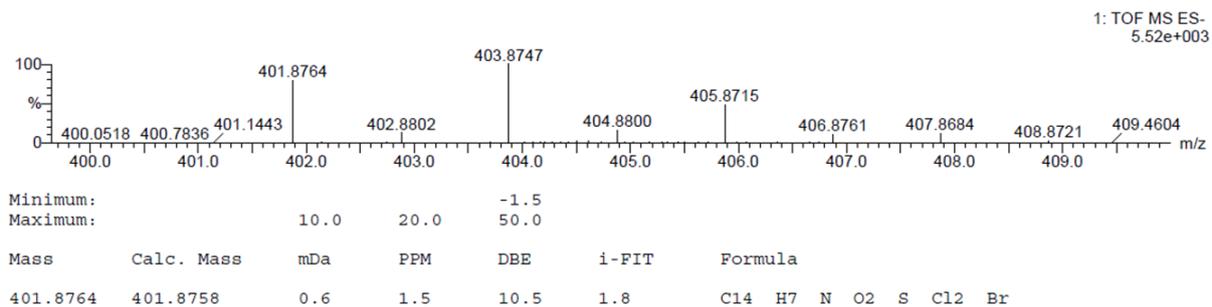
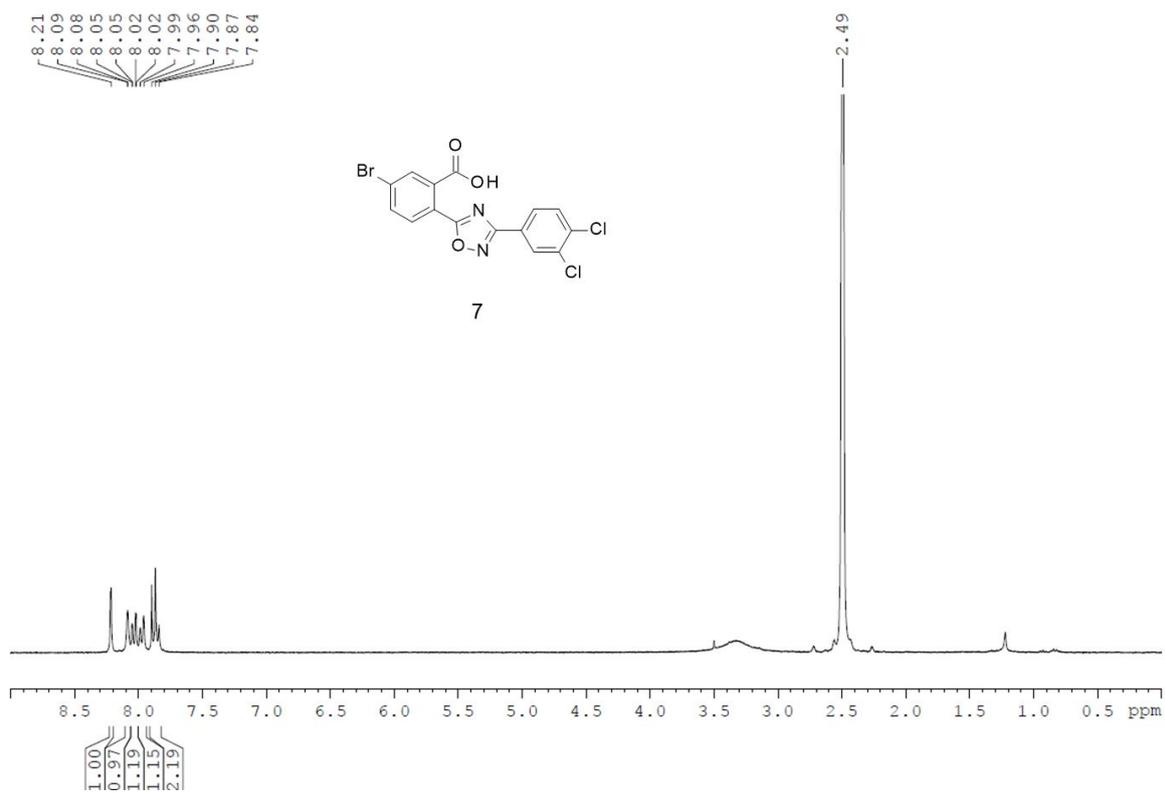


Figure S12: HRMS spectrum of compound 6

<sup>1</sup>H NMR of compound 7 (300 MHz, DMSO-d6)



<sup>13</sup>C NMR of compound 7 (75 MHz, DMSO-d6)

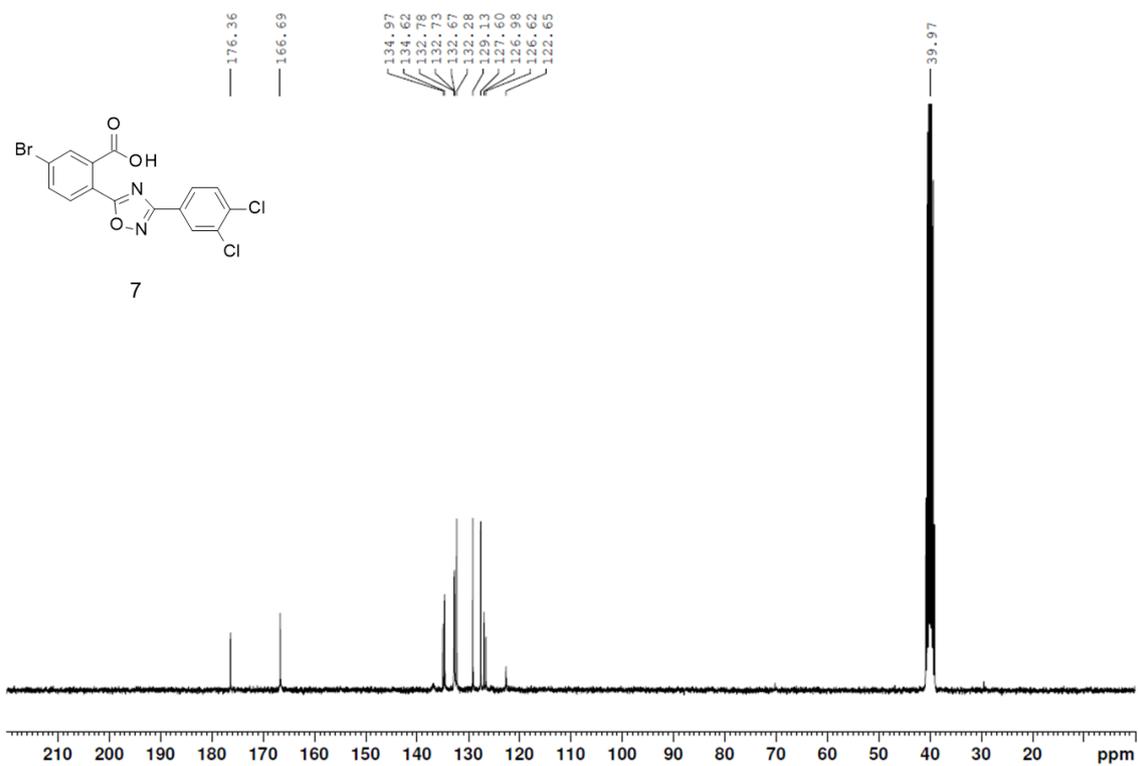


Figure S13: <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 7

## Elemental Composition Report

### Single Mass Analysis

Tolerance = 100.0 mDa / DBE: min = -1.5, max = 500.0

Element prediction: Off

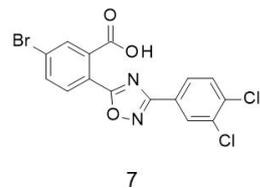
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

562 formula(e) evaluated with 159 results within limits (up to 10 best isotopic matches for each mass)

Elements Used:

C: 0-30 H: 0-40 N: 0-4 O: 0-6 Cl: 0-2 Br: 1-1 I: 0-1



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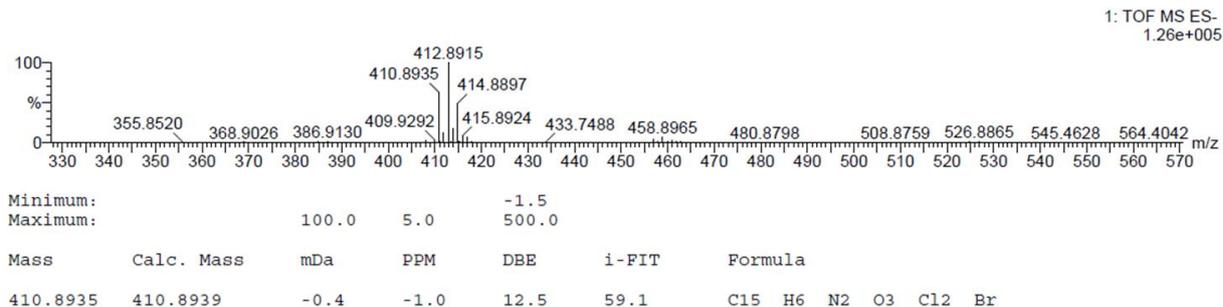
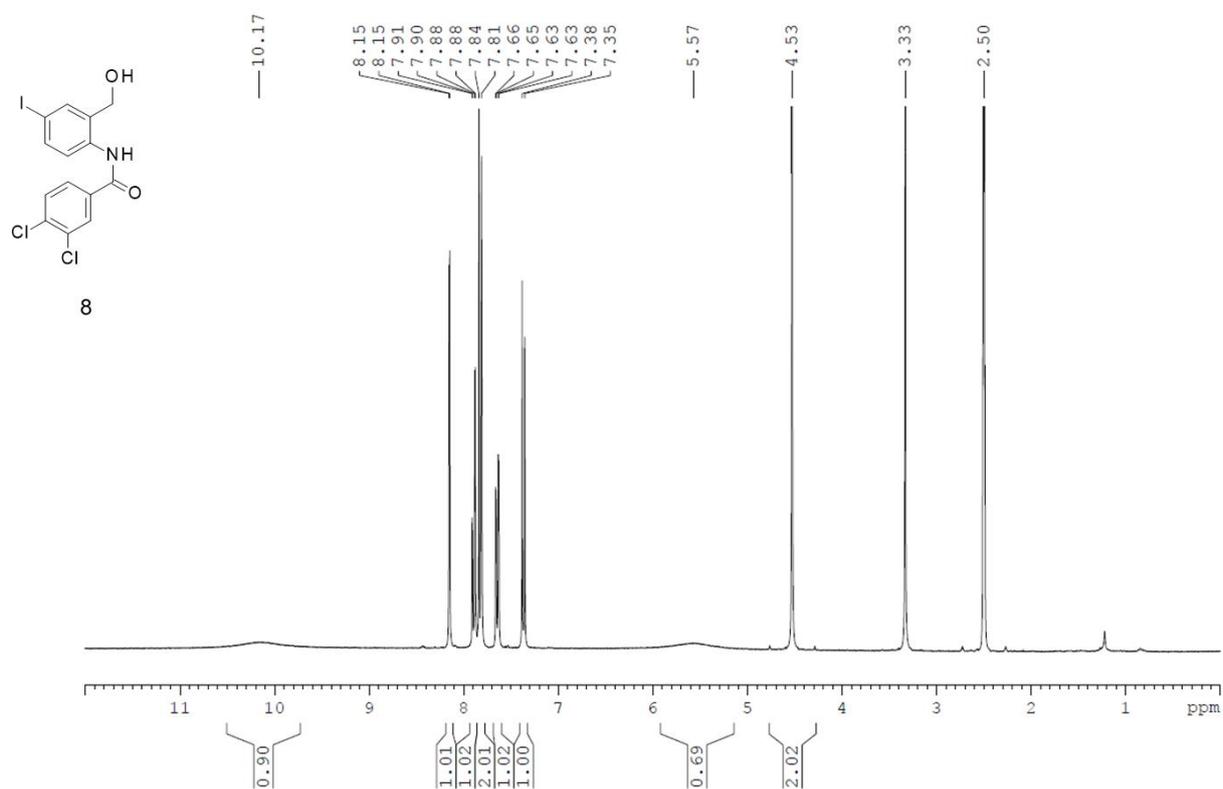


Figure S14: HRMS spectrum of compound 7

<sup>1</sup>H NMR of compound 8 (300 MHz, DMSO-d6)



<sup>13</sup>C NMR of compound 8 (75 MHz, DMSO-d6)

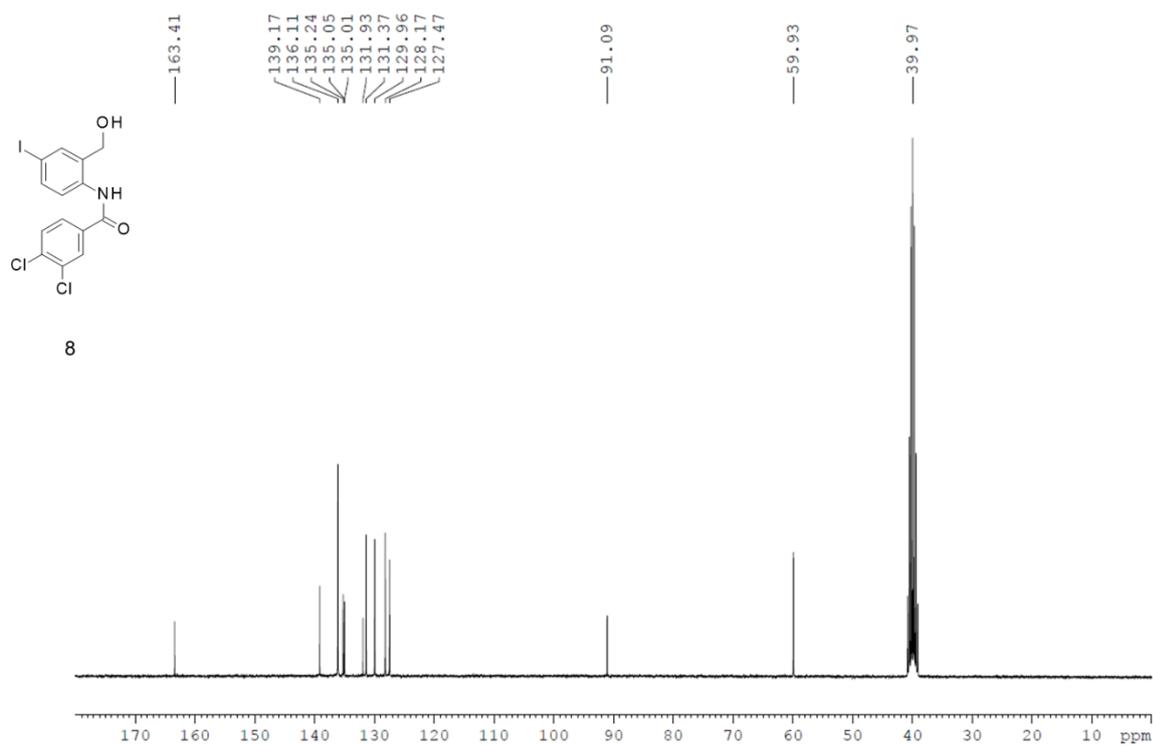
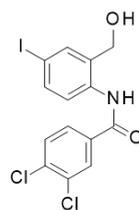


Figure S15: <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 8



## Elemental Composition Report

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### Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

8

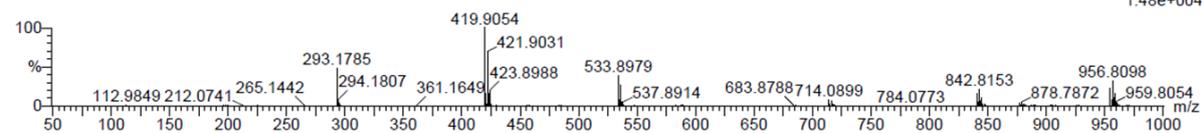
Monoisotopic Mass, Even Electron Ions

391 formula(e) evaluated with 10 results within limits (up to 1 best isotopic matches for each mass)

Elements Used:

C: 2-20 H: 2-36 N: 0-5 O: 0-7 Cl: 1-2 I: 0-1

1: TOF MS ES-  
1.48e+004

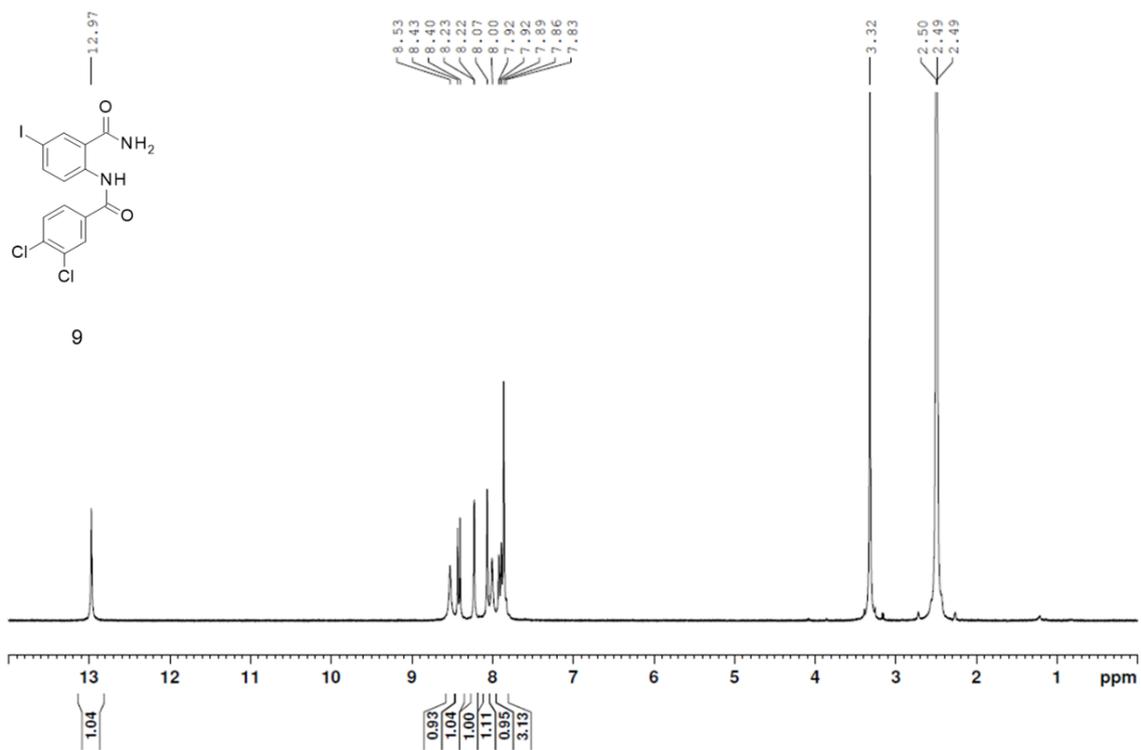


Minimum: -1.5  
Maximum: 10.0 20.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
419.9054	419.9055	-0.1	-0.2	9.5	0.2	C14 H9 N O2 Cl2 I

Figure S16: HRMS spectrum of compound 8

<sup>1</sup>H NMR of compound 9 (300 MHz, DMSO-d6)



<sup>13</sup>C NMR of compound 9 (75 MHz, DMSO-d6)

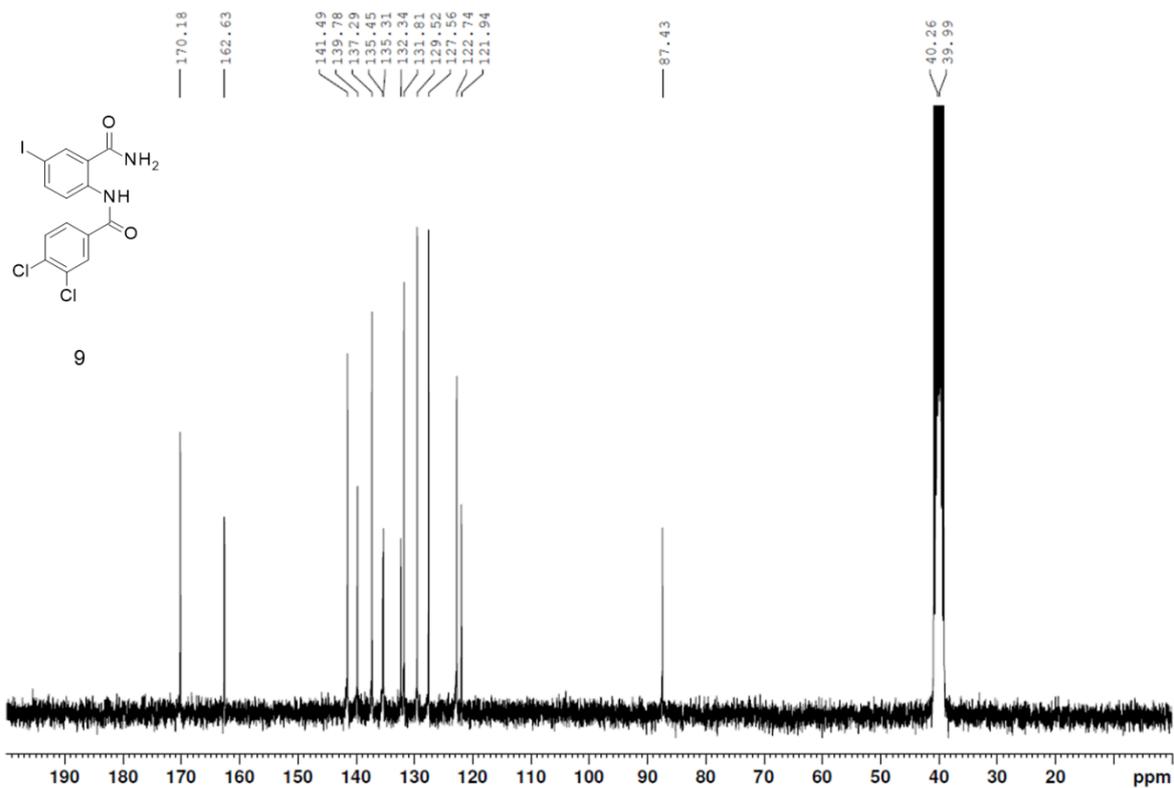


Figure S17: <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 9

## Elemental Composition Report

### Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 80.0

Element prediction: Off

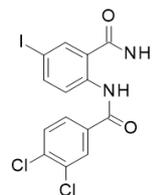
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

635 formula(e) evaluated with 12 results within limits (up to 1 closest results for each mass)

Elements Used:

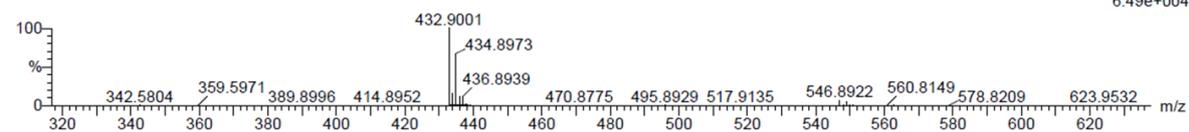
C: 6-40 H: 2-36 N: 0-4 O: 0-7 Cl: 1-3 I: 0-1



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1: TOF MS ES-  
6.49e+004

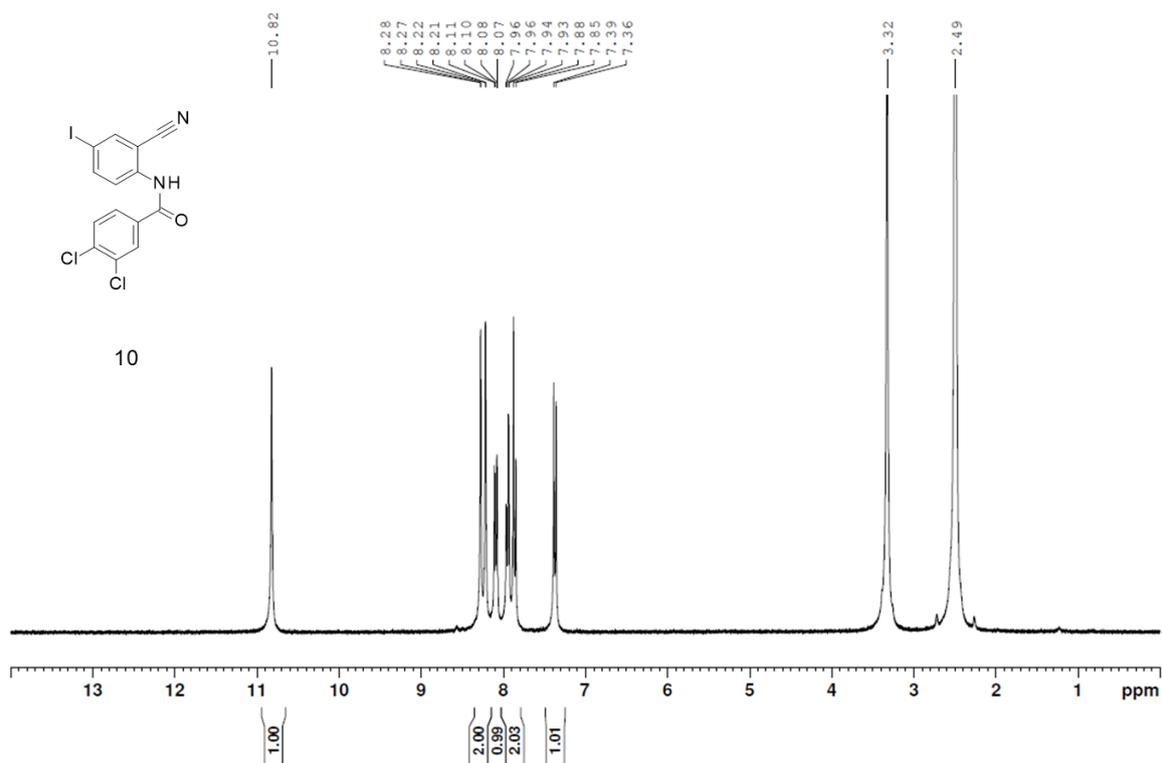


Minimum: -1.5  
Maximum: 10.0 20.0 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
432.9001	432.9008	-0.7	-1.6	10.5	5.6	C14 H8 N2 O2 Cl2 I

Figure S18: HRMS spectrum of compound 9

<sup>1</sup>H NMR of compound 10 (300 MHz, DMSO-d6)



<sup>13</sup>C NMR of compound 10 (75 MHz, DMSO-d6)

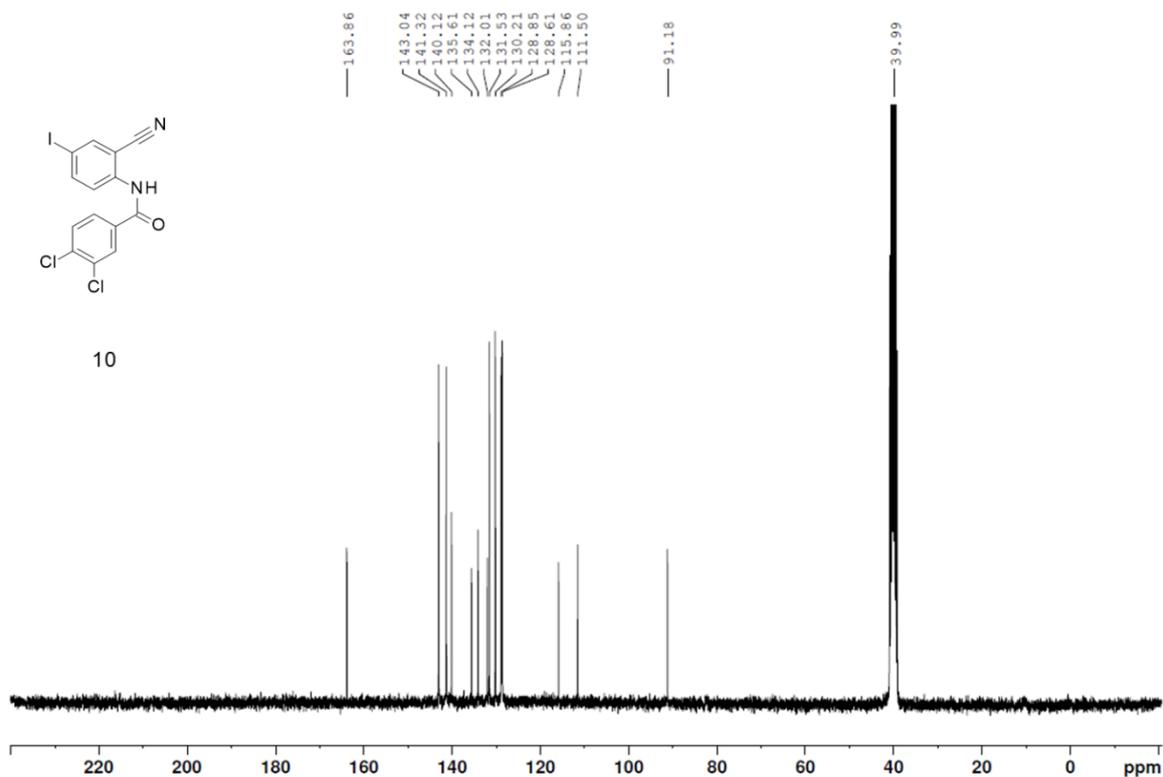
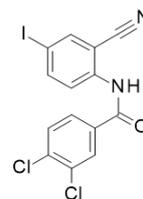


Figure S19: <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 10



Elemental Composition Report

Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

10

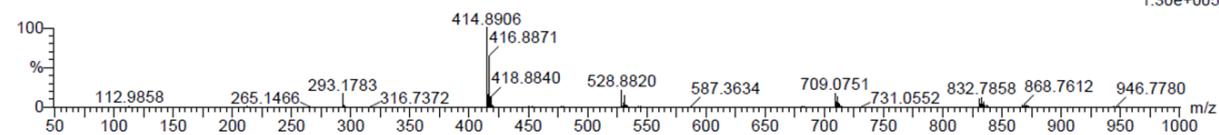
Monoisotopic Mass, Even Electron Ions

603 formula(e) evaluated with 12 results within limits (up to 1 closest results for each mass)

Elements Used:

C: 6-40 H: 2-36 N: 0-4 O: 0-7 Cl: 1-3 I: 0-1

1: TOF MS ES-  
1.30e+005

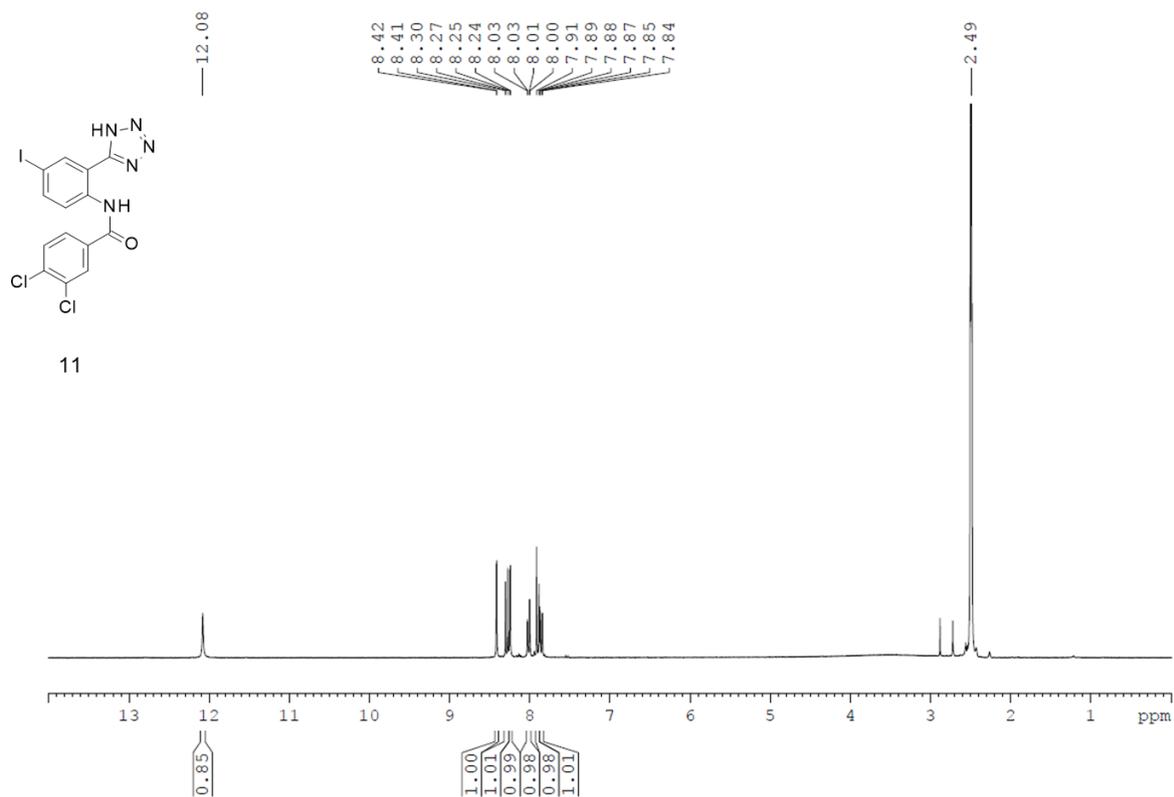


Minimum: -1.5  
Maximum: 10.0 20.0 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
414.8906	414.8902	0.4	1.0	11.5	1.1	C14 H6 N2 O Cl2 I

Figure S20: HRMS spectrum of compound 10

<sup>1</sup>H NMR of compound 11 (300 MHz, DMSO-d6)



<sup>13</sup>C NMR of compound 11 (75 MHz, DMSO-d6)

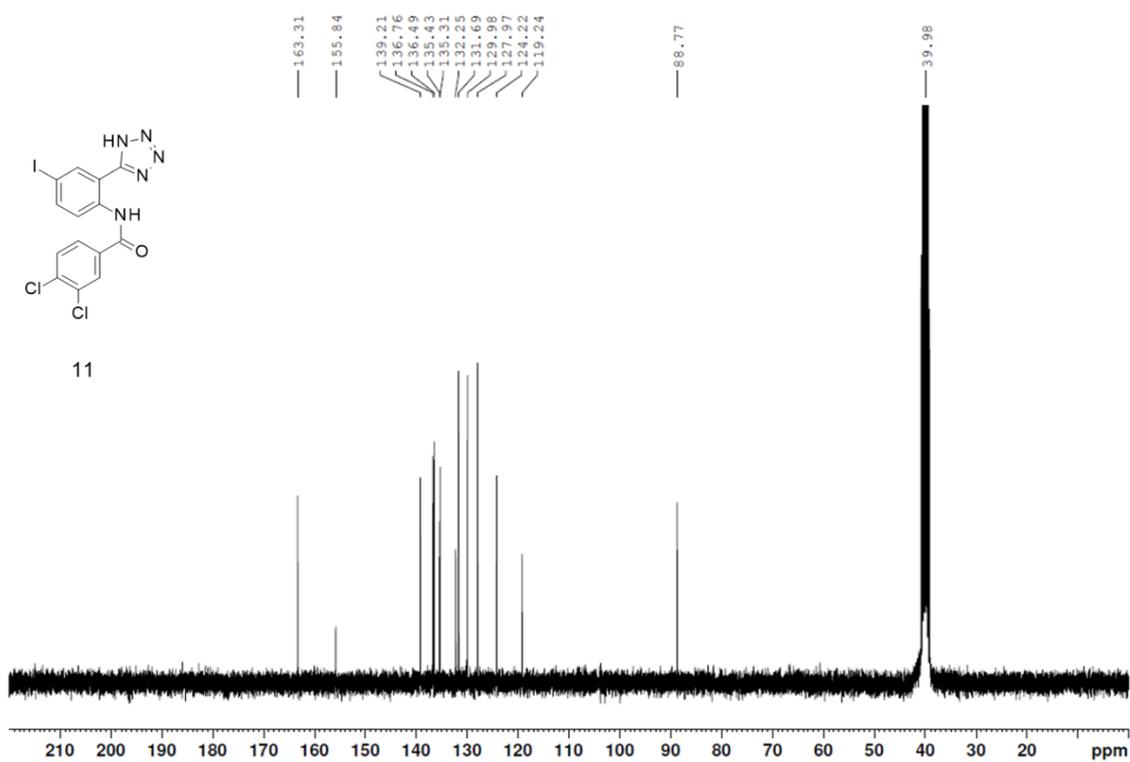


Figure S21: <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 11

## Elemental Composition Report

### Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 80.0

Element prediction: Off

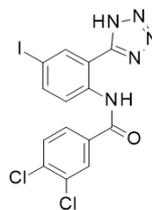
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

783 formula(e) evaluated with 17 results within limits (up to 1 closest results for each mass)

Elements Used:

C: 6-40 H: 2-36 N: 0-5 O: 0-7 Cl: 1-3 I: 0-1



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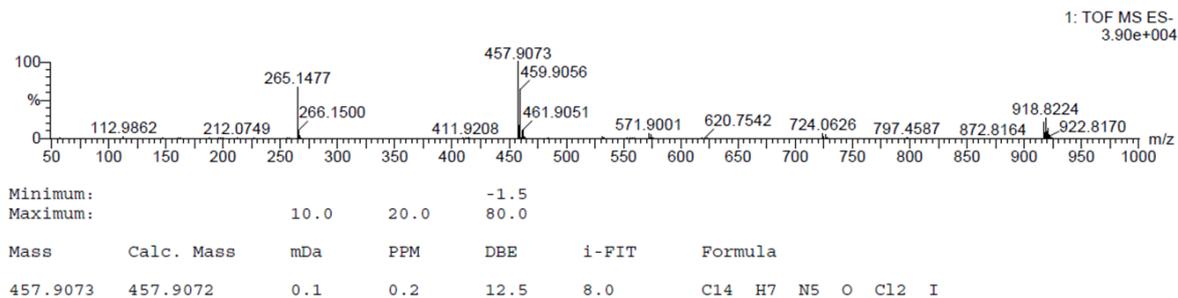
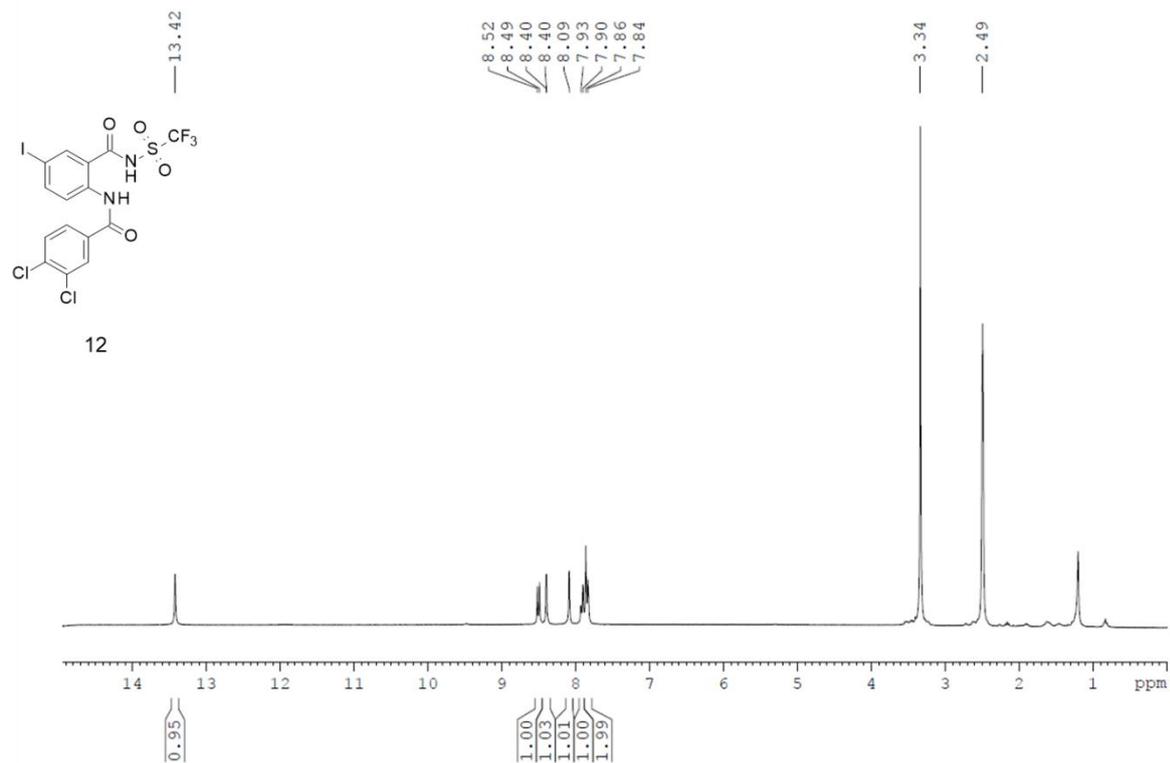


Figure S22: HRMS spectrum of compound 11

<sup>1</sup>H NMR of compound 12 (300 MHz, DMSO-d6)



<sup>13</sup>C NMR of compound 12 (75 MHz, DMSO-d6)

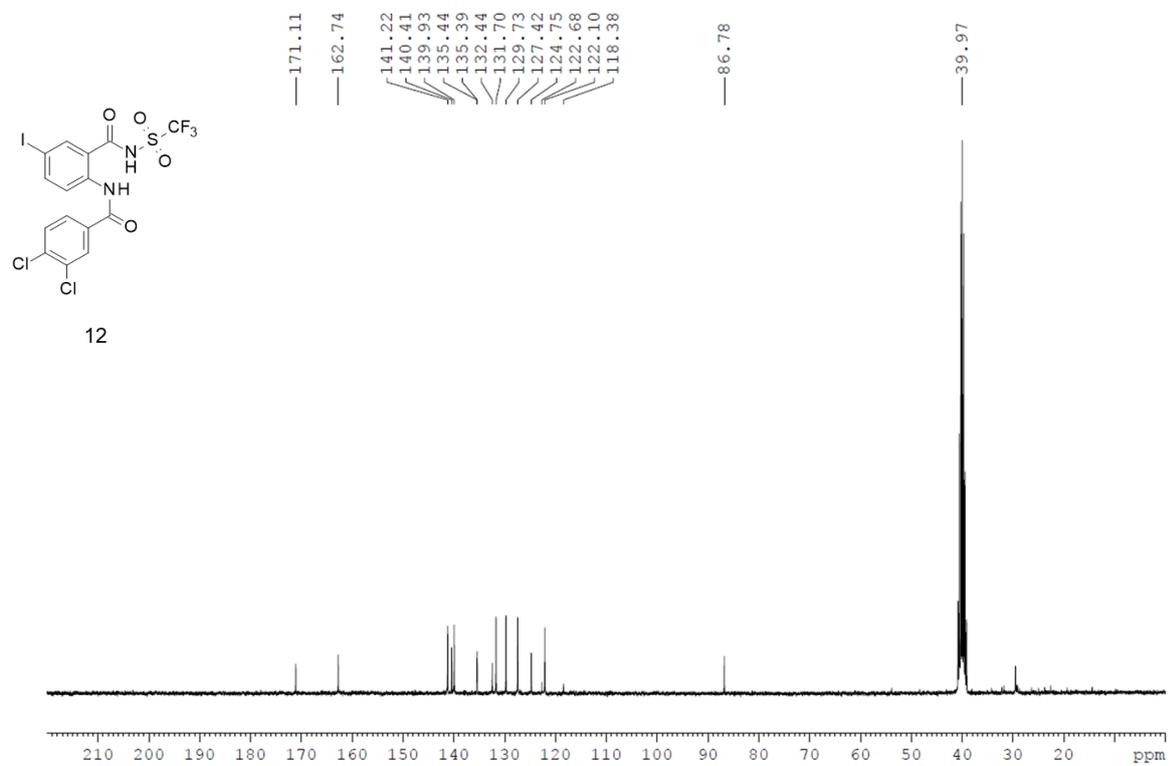


Figure S23: <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 12

## Elemental Composition Report

### Single Mass Analysis

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

Element prediction: Off

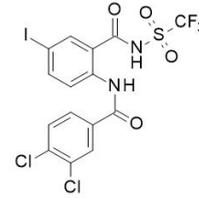
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

11796 formula(e) evaluated with 19 results within limits (up to 5 closest results for each mass)

Elements Used:

C: 15-15 H: 0-60 N: 0-10 O: 0-15 F: 1-3 S: 0-3 Cl: 0-2 I: 0-1



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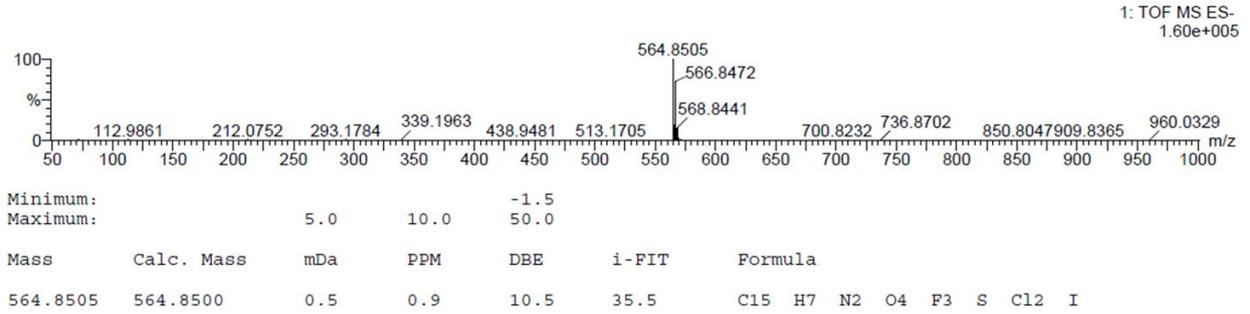
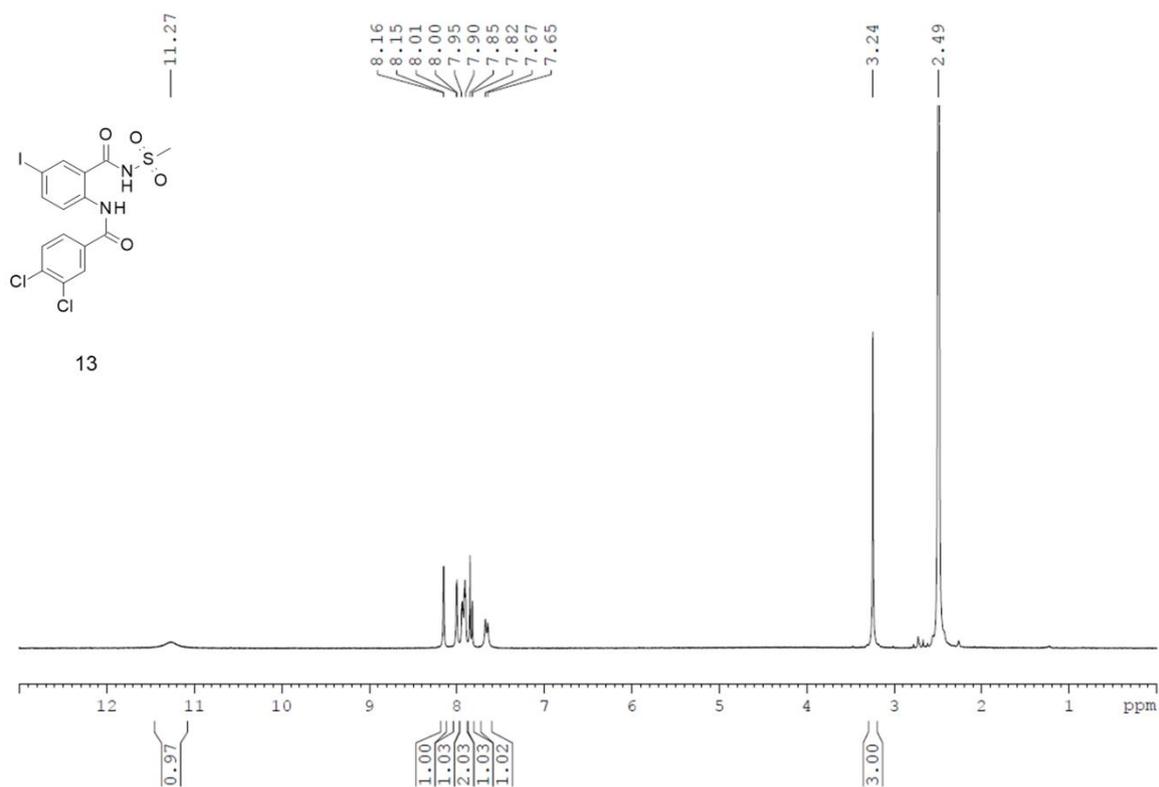


Figure S24: HRMS spectrum of compound 12

<sup>1</sup>H NMR of compound 13 (300 MHz, DMSO-d6)



<sup>13</sup>C NMR of compound 13 (75 MHz, DMSO-d6)

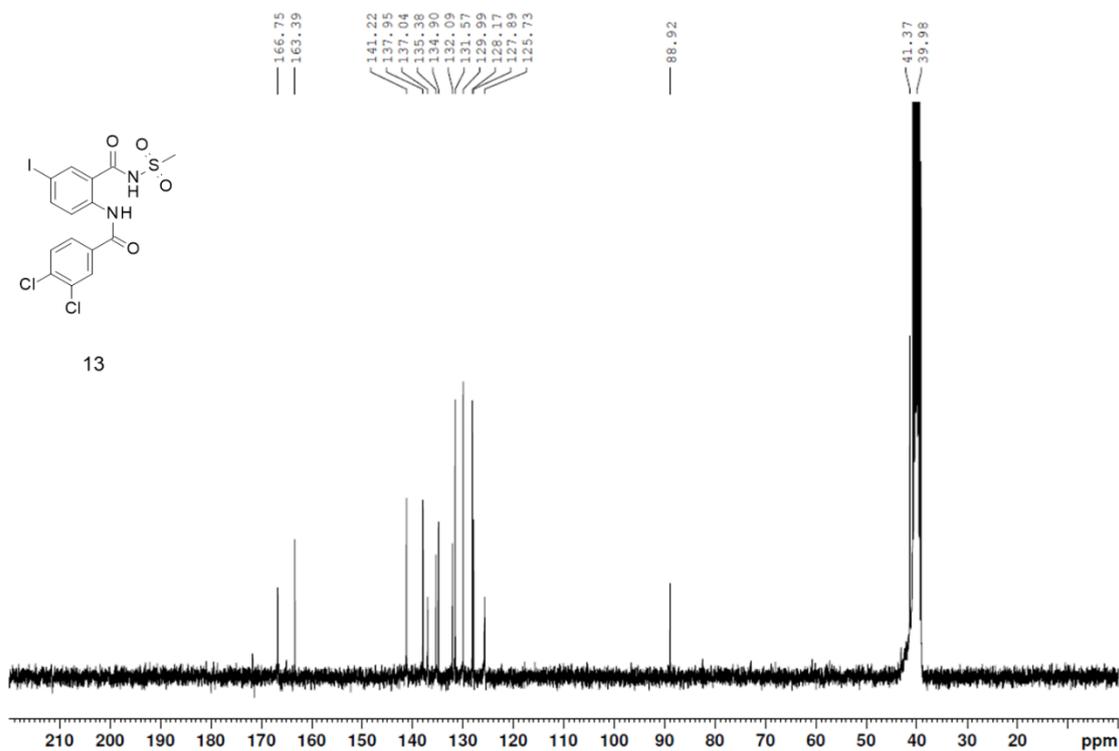
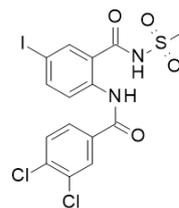


Figure S25: <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 13



13

**Elemental Composition Report**

**Single Mass Analysis**

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

1636 formula(e) evaluated with 30 results within limits (up to 1 best isotopic matches for each mass)

Elements Used:

C: 6-40 H: 2-36 N: 0-5 O: 0-7 S: 0-1 Cl: 1-3 I: 0-1

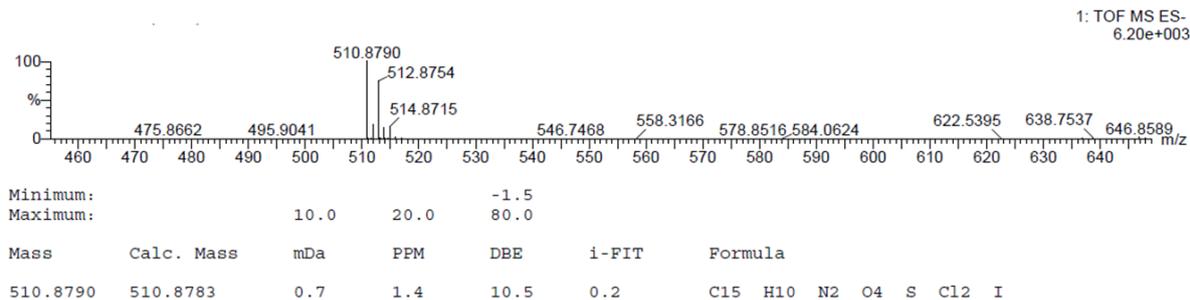
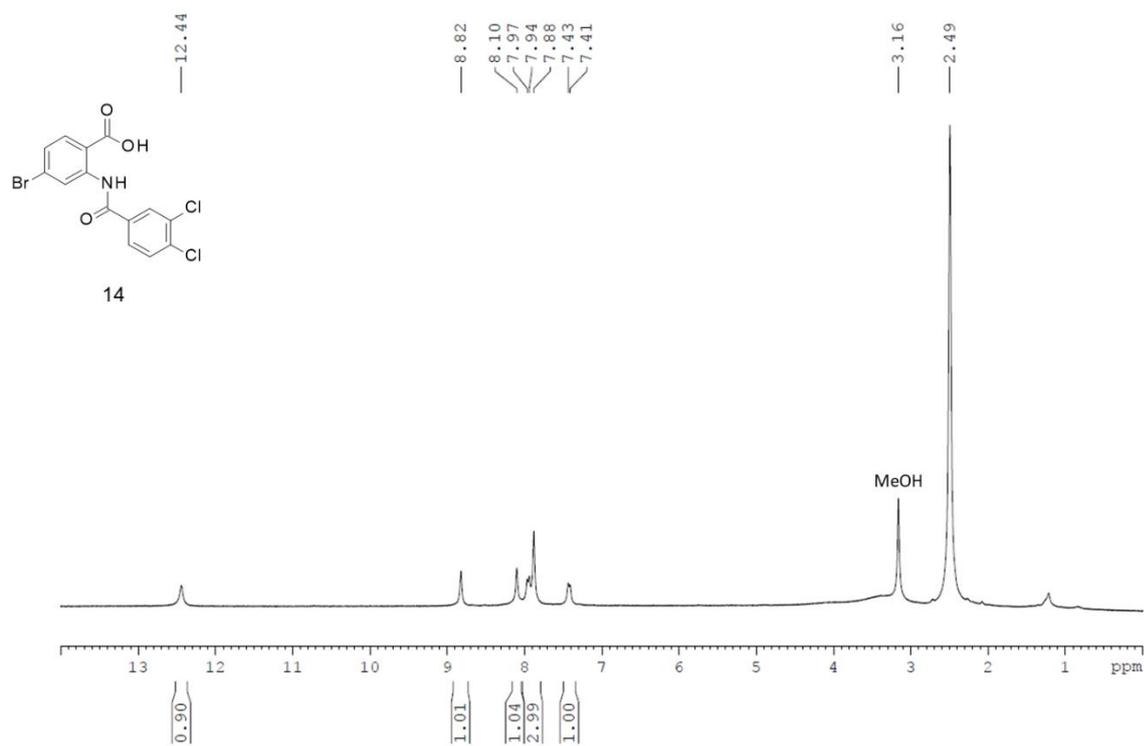


Figure S26: HRMS spectrum of compound 13

<sup>1</sup>H NMR of compound 14 (300 MHz, DMSO-d6)



<sup>13</sup>C JMOD NMR of compound 14 (75 MHz, DMSO-d6)

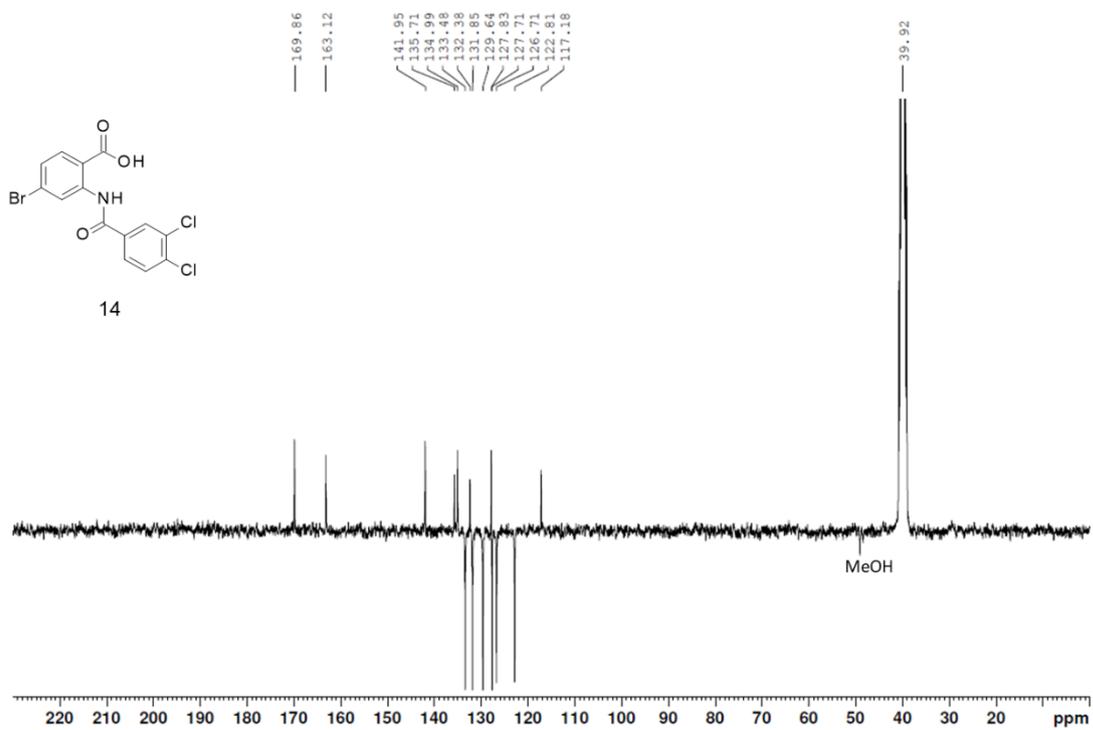


Figure S27: <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 14

## Elemental Composition Report

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### Single Mass Analysis

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

Element prediction: Off

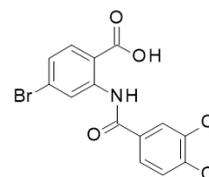
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

2876 formula(e) evaluated with 6 results within limits (up to 5 closest results for each mass)

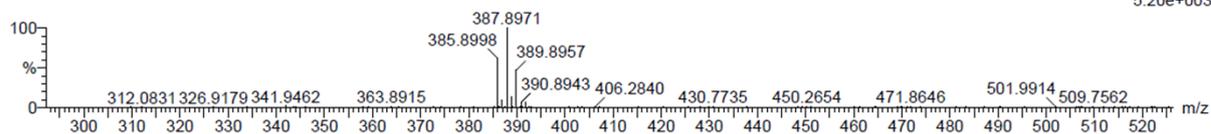
Elements Used:

C: 10-50 H: 0-60 N: 0-10 O: 0-15 Cl: 0-2 Br: 0-1 I: 0-1



14

1: TOF MS ES-  
5.20e+003

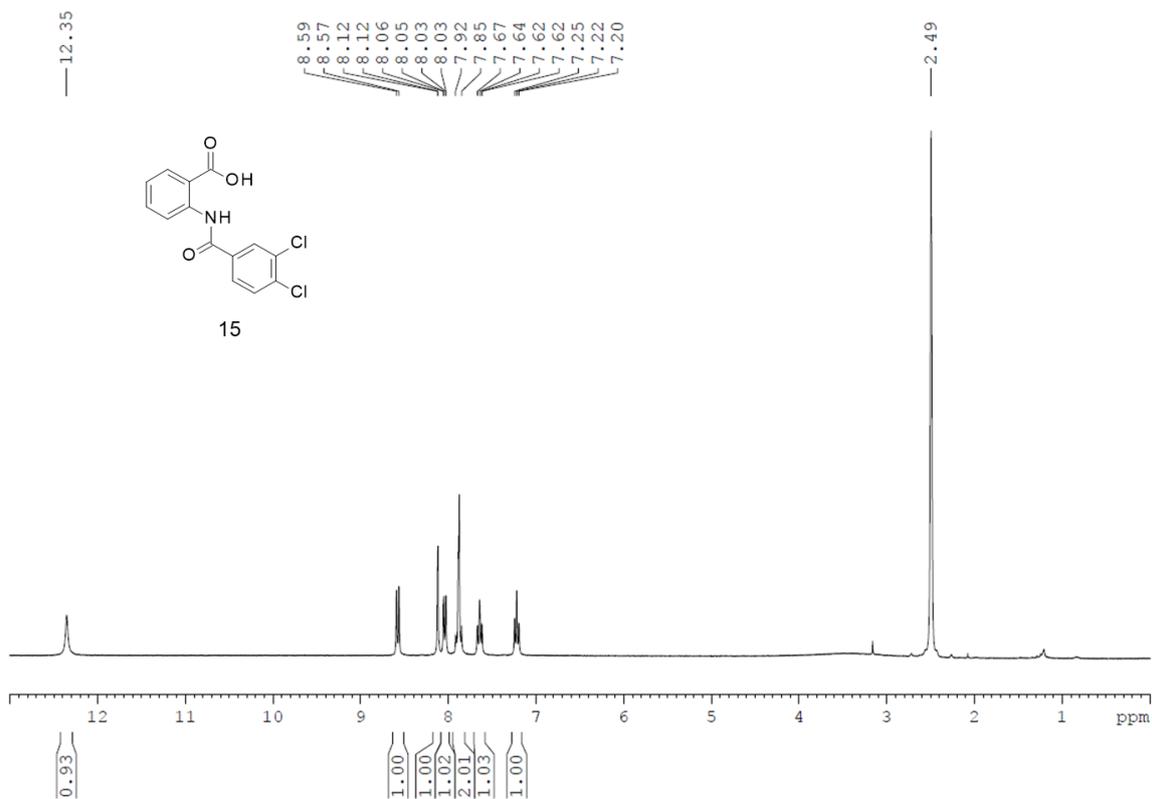


Minimum: -1.5  
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
385.8998	385.8986	1.2	3.1	10.5	1.8	C14 H7 N O3 Cl2 Br

Figure S28: HRMS spectrum of compound 14

**<sup>1</sup>H NMR of compound 15 (300 MHz, DMSO-d6)**



**<sup>13</sup>C JMOD NMR of compound 15 (75 MHz, DMSO-d6)**

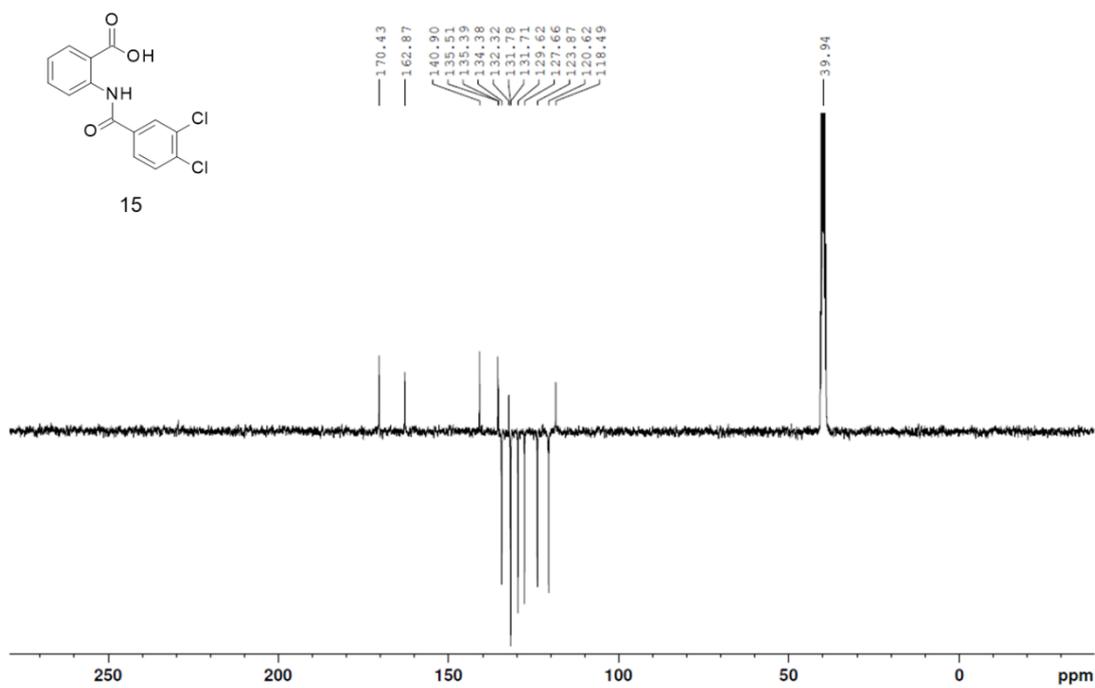
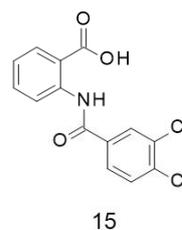


Figure S29: <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 15



Elemental Composition Report

Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

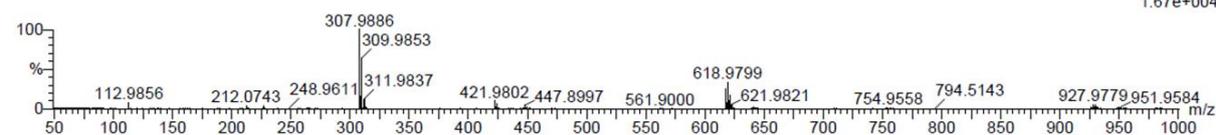
Monoisotopic Mass, Even Electron Ions

343 formula(e) evaluated with 5 results within limits (up to 1 best isotopic matches for each mass)

Elements Used:

C: 2-20 H: 2-36 N: 0-5 O: 0-7 Cl: 1-2 I: 0-1

1: TOF MS ES-  
1.67e+004

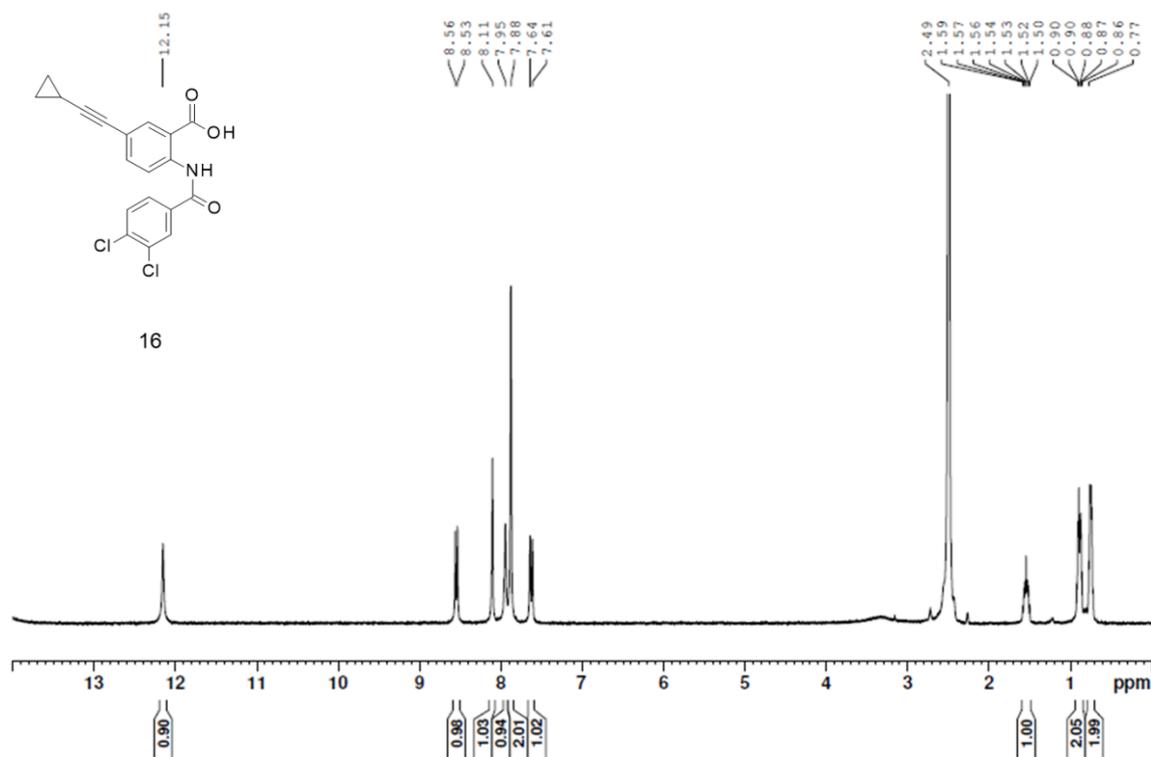


Minimum: -1.5  
Maximum: 10.0 20.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
307.9886	307.9881	0.5	1.6	10.5	1.1	C14 H8 N O3 Cl2

Figure S30: HRMS spectrum of compound 15

<sup>1</sup>H NMR of compound 16 (300 MHz, DMSO-d6)



<sup>13</sup>C NMR of compound 16 (75 MHz, DMSO-d6)

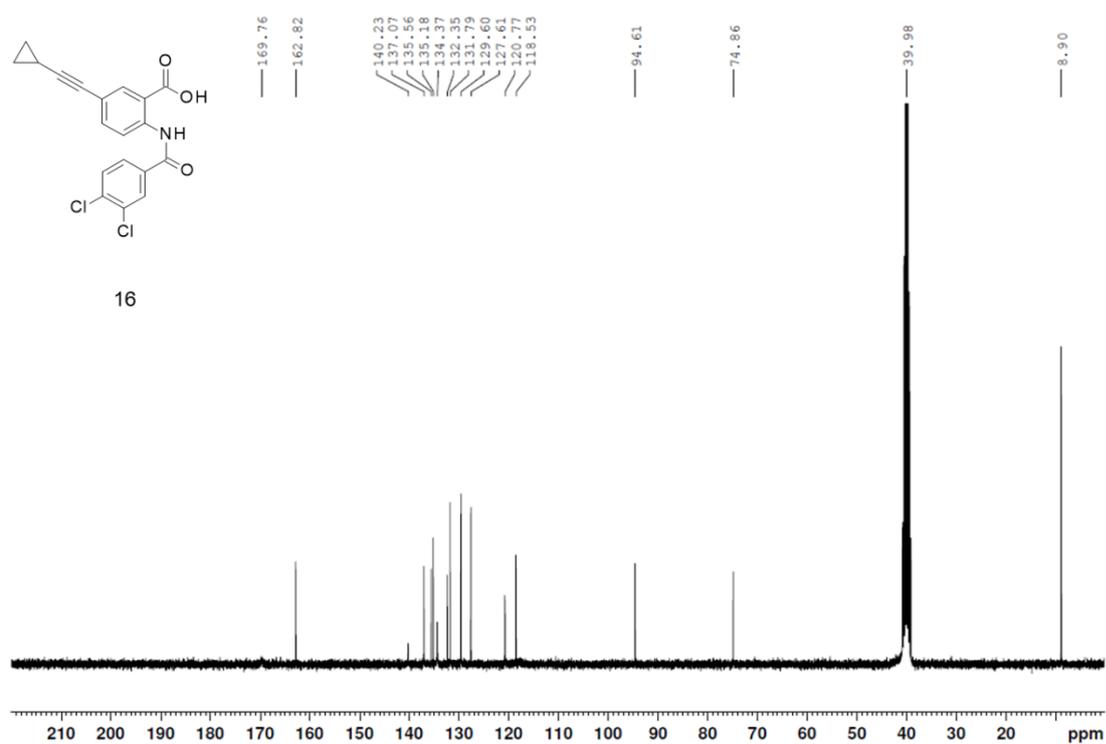
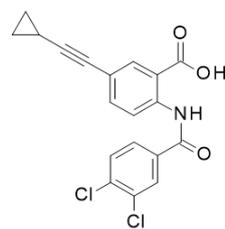


Figure S31: <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 16



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### Elemental Composition Report

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#### Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

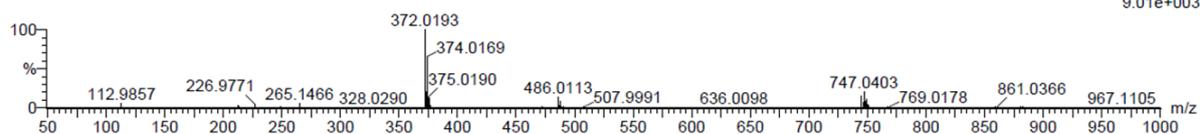
Monoisotopic Mass, Even Electron Ions

221 formula(e) evaluated with 5 results within limits (up to 1 best isotopic matches for each mass)

Elements Used:

C: 2-20 H: 2-36 N: 0-5 O: 0-7 Cl: 1-2

1: TOF MS ES-  
9.01e+003

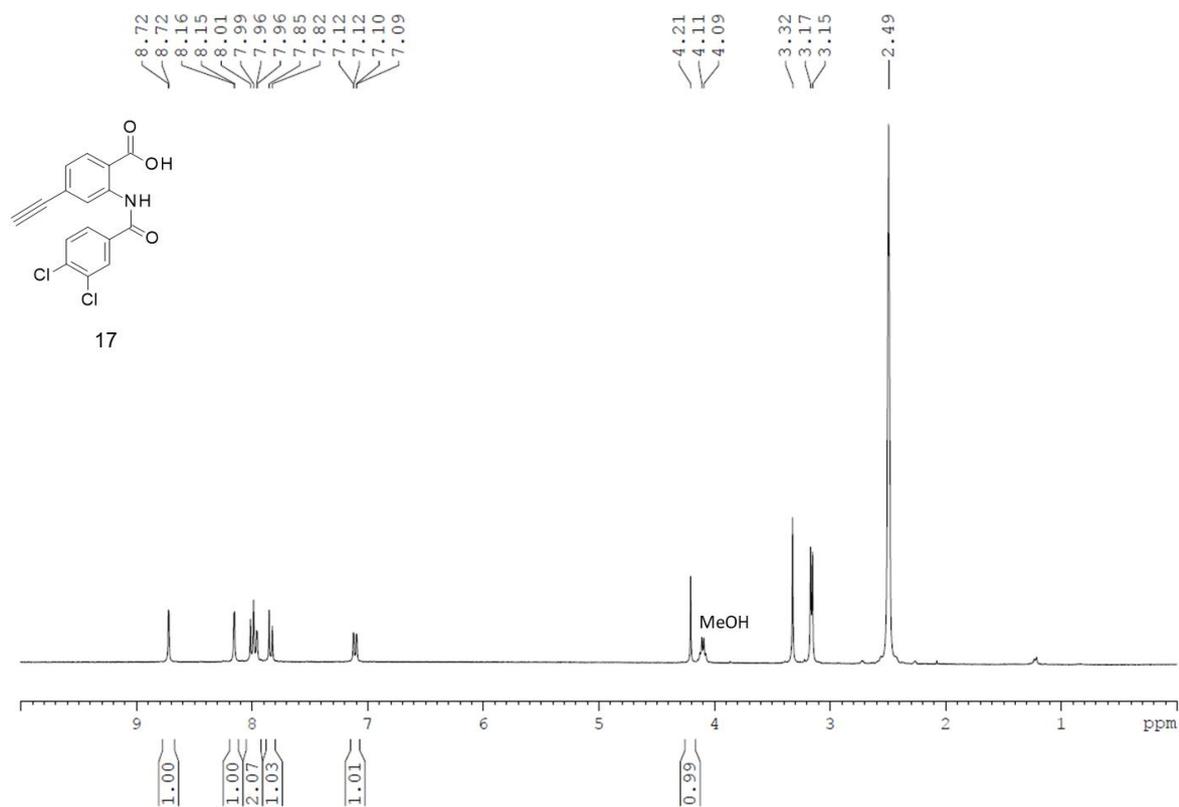


Minimum: -1.5  
Maximum: 10.0 20.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
372.0193	372.0194	-0.1	-0.3	13.5	1.1	C19 H12 N O3 Cl2

Figure S32: HRMS spectrum of compound 16

<sup>1</sup>H NMR of compound 17 (300 MHz, DMSO-d6)



<sup>13</sup>C NMR of compound 17 (75 MHz, DMSO-d6)

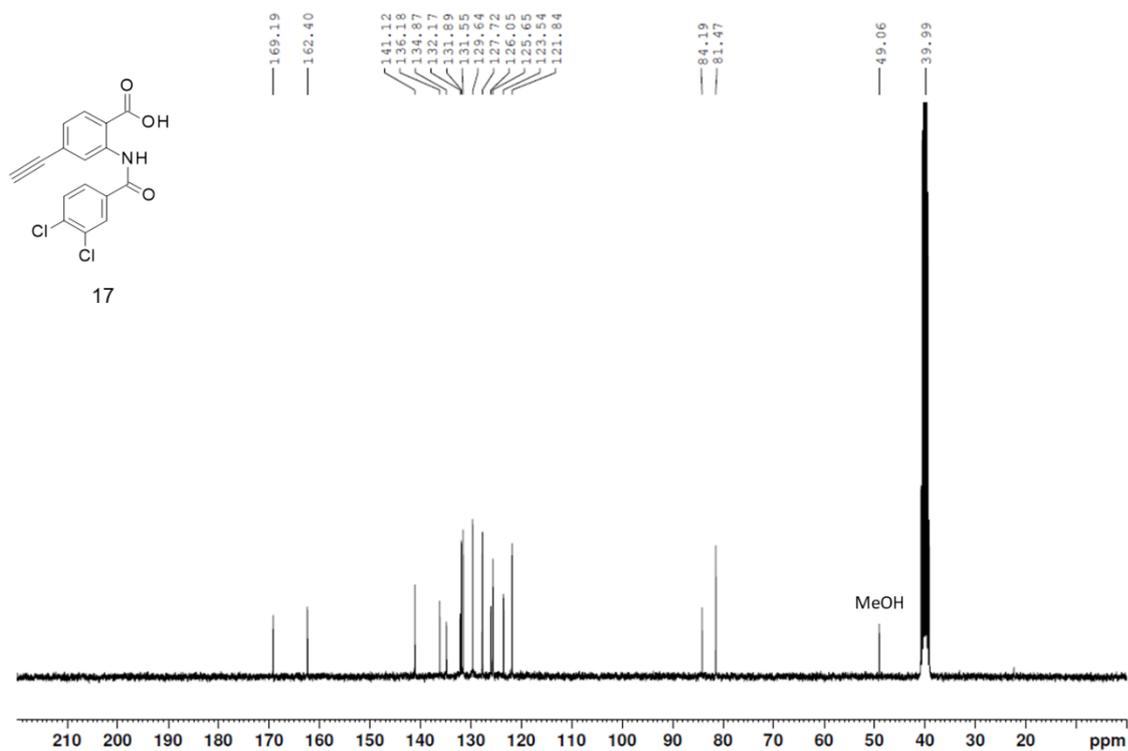


Figure S33: <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 17

## Elemental Composition Report

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### Single Mass Analysis

Tolerance = 100.0 mDa / DBE: min = -1.5, max = 500.0

Element prediction: Off

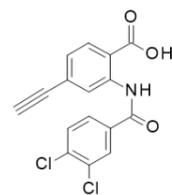
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

350 formula(e) evaluated with 59 results within limits (up to 10 best isotopic matches for each mass)

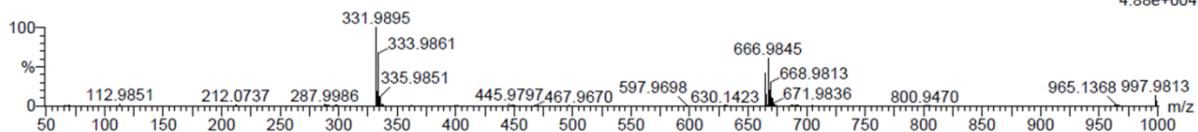
Elements Used:

C: 0-30 H: 0-40 N: 0-4 O: 0-6 Cl: 0-2



17

1: TOF MS ES-  
4.88e+004



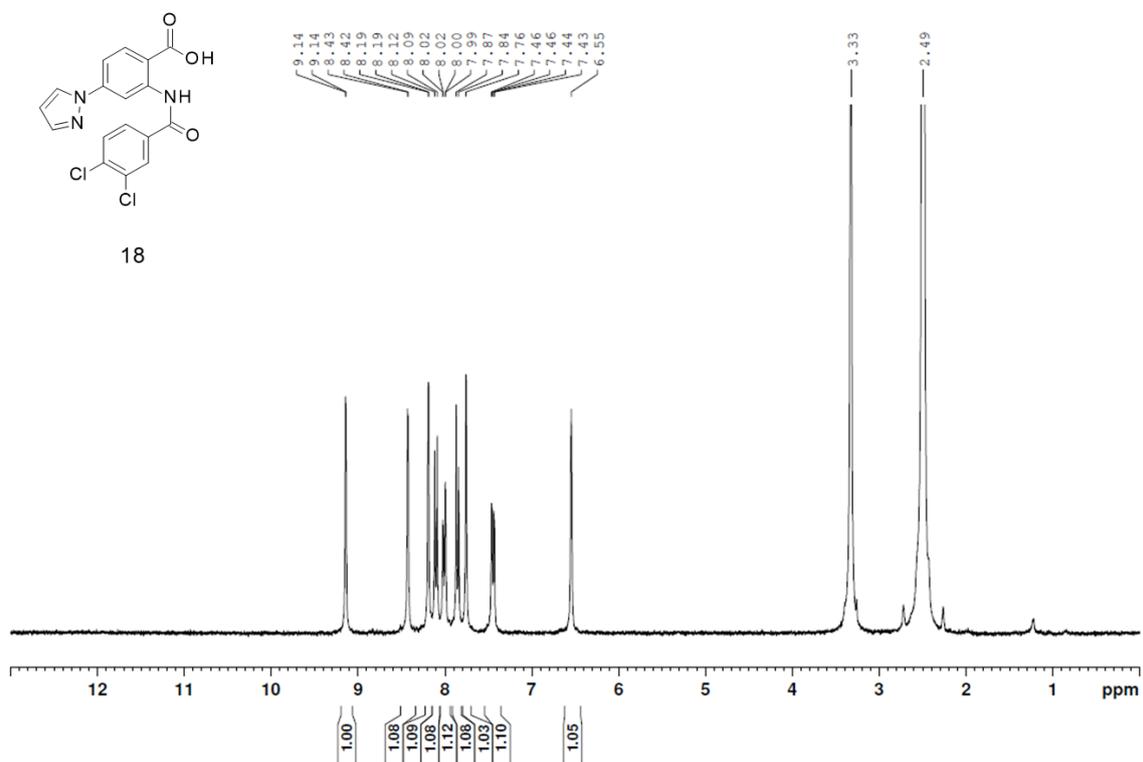
Minimum:

Maximum: 100.0 5.0 -1.5 500.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
331.9895	331.9881	1.4	4.2	12.5	9.8	C16 H8 N O3 Cl2

Figure S34: HRMS spectrum of compound 17

<sup>1</sup>H NMR of compound 18 (300 MHz, DMSO-d6)



<sup>13</sup>C JMOD NMR of compound 18 (75 MHz, DMSO-d6)

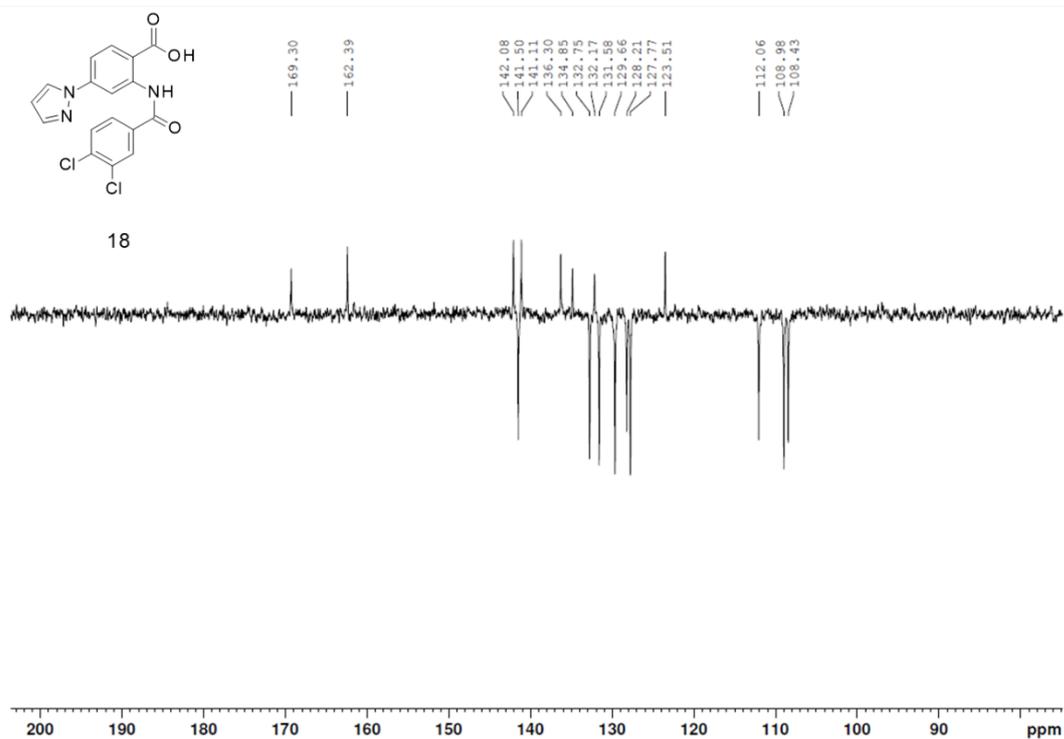


Figure S35: <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 18

## Elemental Composition Report

### Single Mass Analysis

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

Element prediction: Off

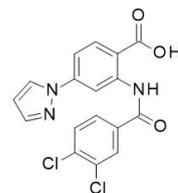
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

2596 formula(e) evaluated with 22 results within limits (up to 5 closest results for each mass)

Elements Used:

C: 10-50 H: 0-60 N: 0-10 O: 0-15 Cl: 0-2 Br: 0-1 I: 0-1



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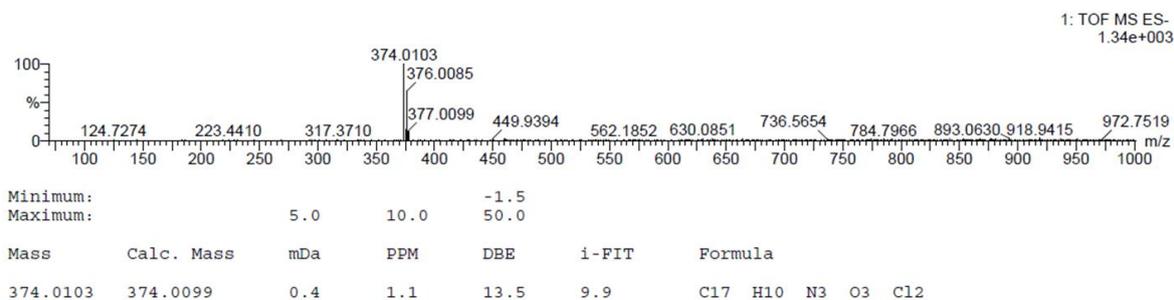
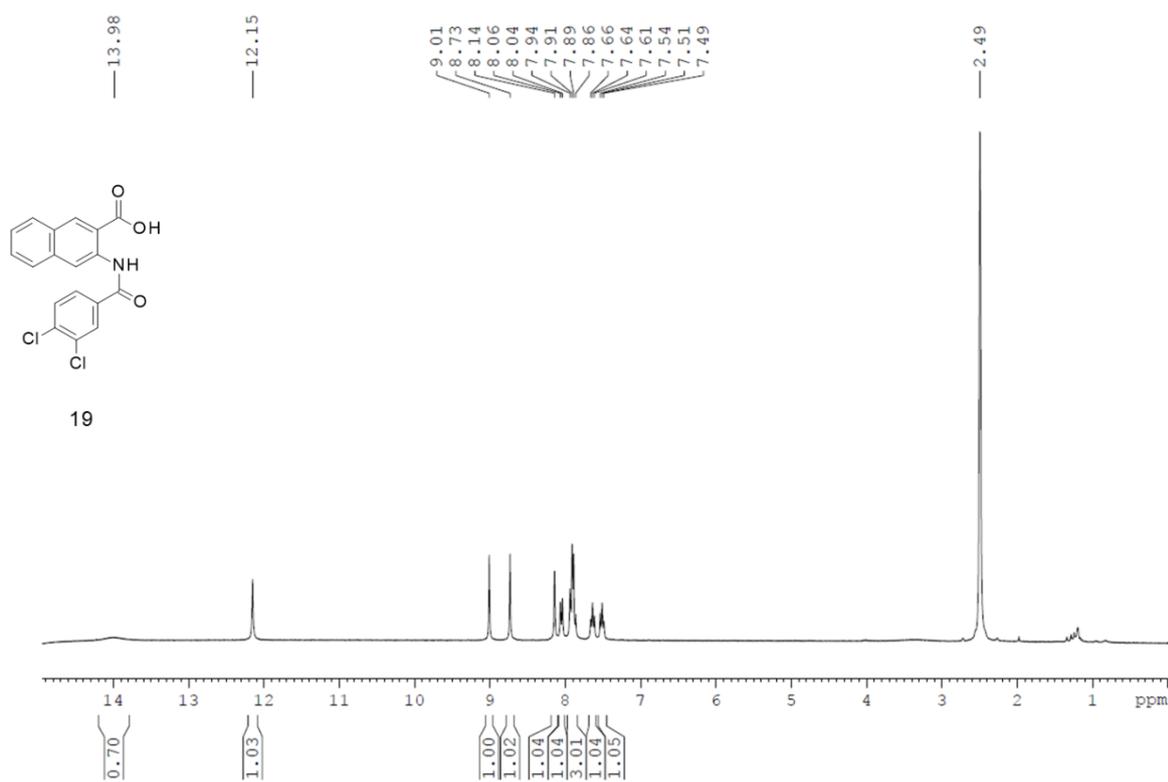


Figure S36: HRMS spectrum of compound 18

<sup>1</sup>H NMR of compound 19 (300 MHz, DMSO-d6)



<sup>13</sup>C NMR of compound 19 (75 MHz, DMSO-d6)

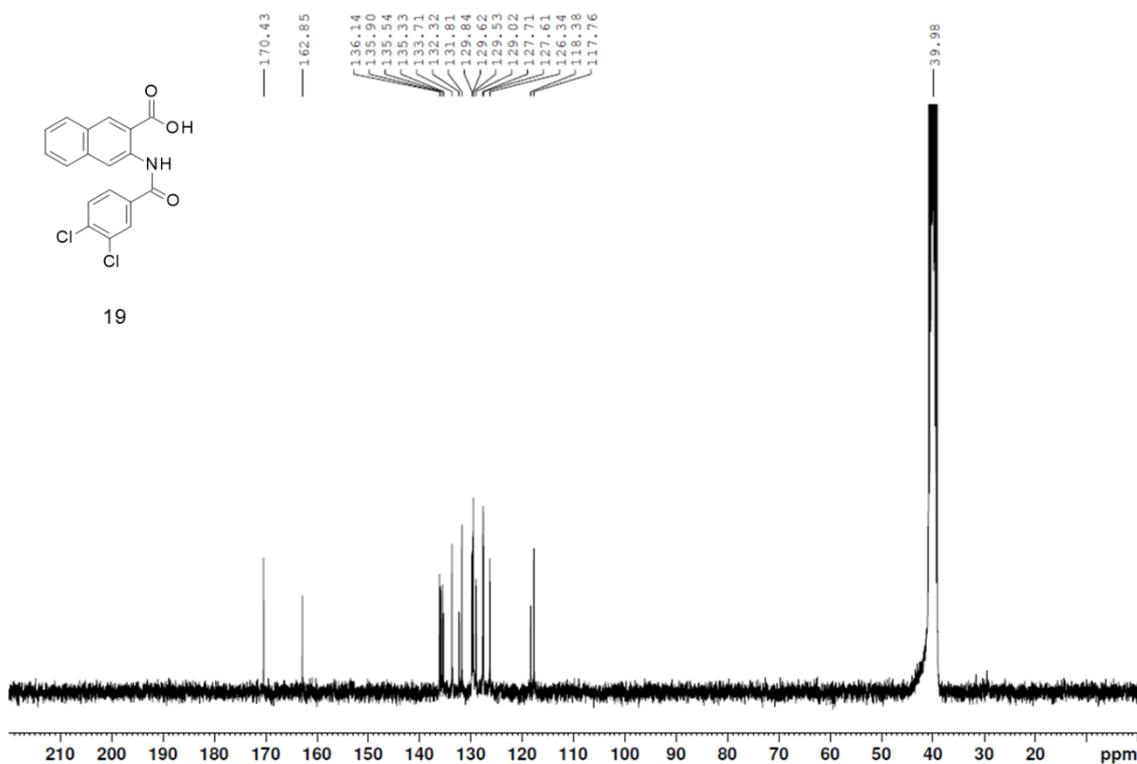
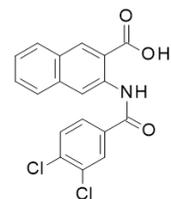


Figure S37: <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 19



19

### Elemental Composition Report

#### Single Mass Analysis

Tolerance = 100.0 mDa / DBE: min = -1.5, max = 500.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

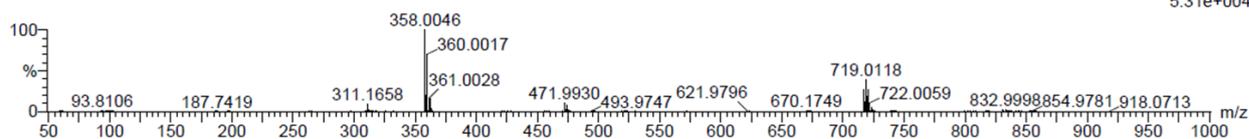
Monoisotopic Mass, Even Electron Ions

360 formula(e) evaluated with 67 results within limits (up to 10 best isotopic matches for each mass)

Elements Used:

C: 0-30 H: 0-40 N: 0-4 O: 0-6 Cl: 0-2

1: TOF MS ES-  
5.31e+004

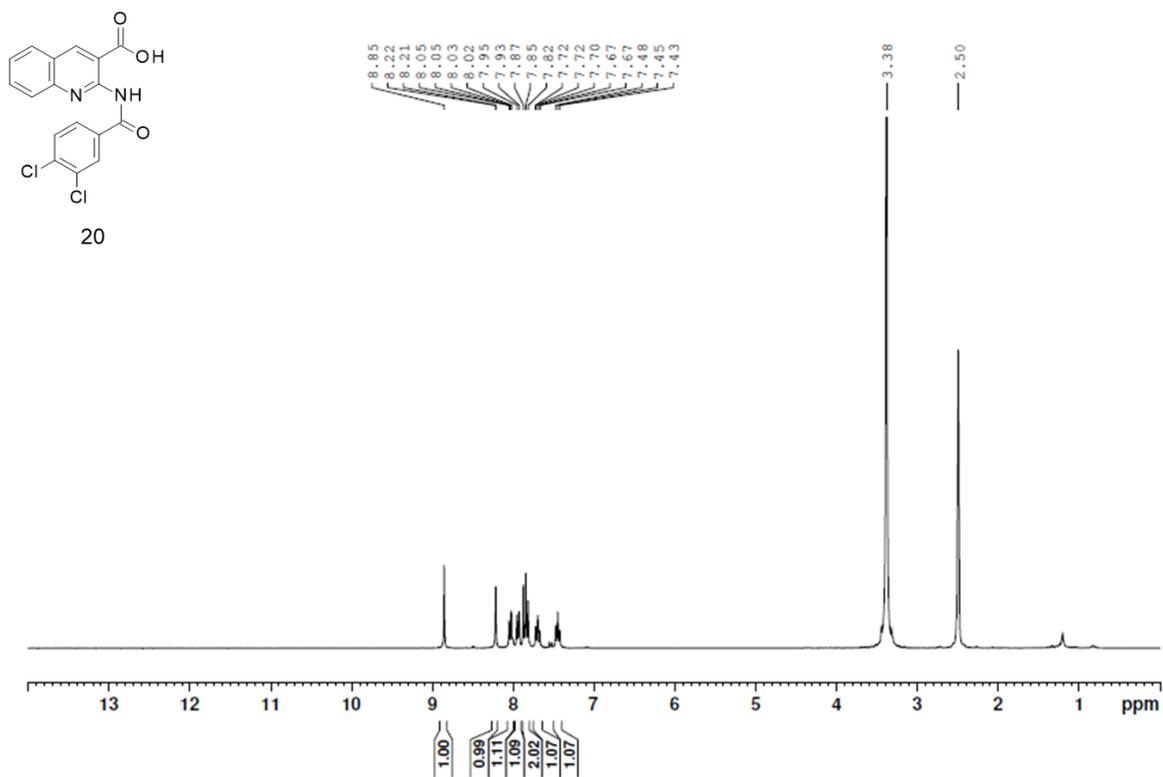


Minimum: -1.5  
Maximum: 100.0 5.0 500.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
358.0046	358.0038	0.8	2.2	13.5	54.2	C18 H10 N O3 Cl2

Figure S38: HRMS spectrum of compound 19

<sup>1</sup>H NMR of compound 20 (300 MHz, DMSO-d6)



<sup>13</sup>C NMR of compound 20 (75 MHz, DMSO-d6)

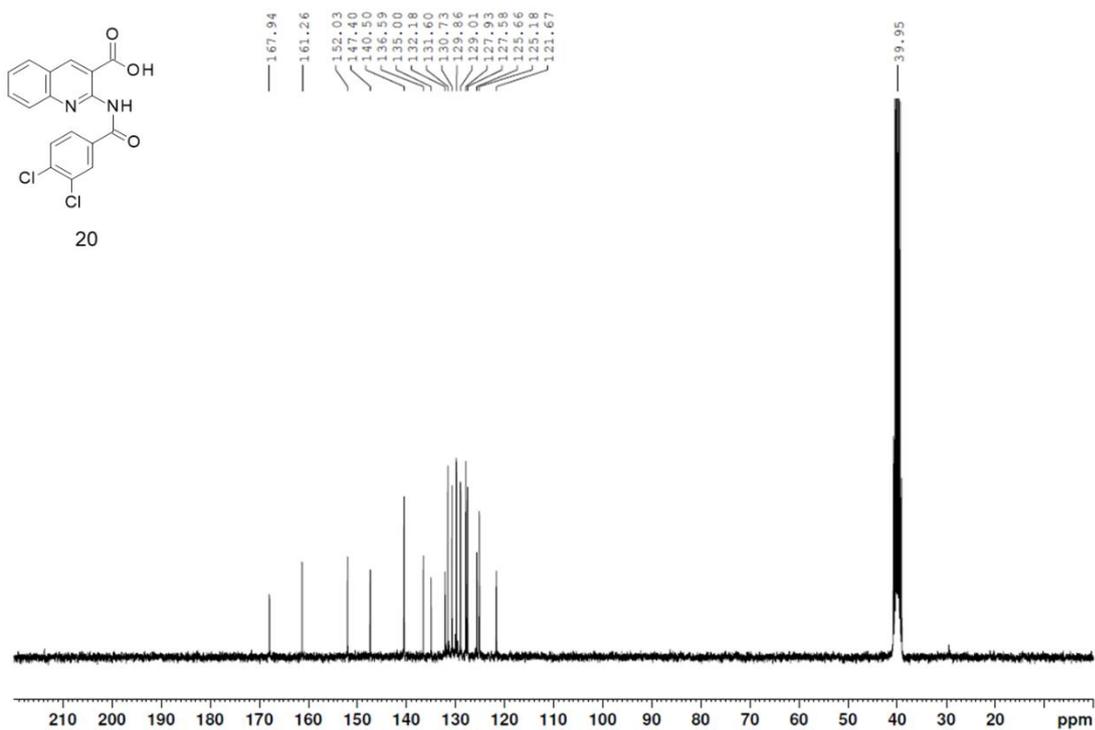
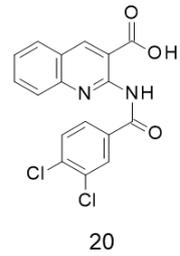


Figure S39: <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 20



**Elemental Composition Report**

**Single Mass Analysis**

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

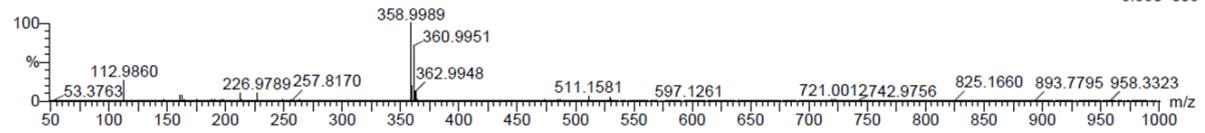
Monoisotopic Mass, Even Electron Ions

403 formula(e) evaluated with 6 results within limits (up to 1 best isotopic matches for each mass)

Elements Used:

C: 2-20 H: 2-36 N: 0-5 O: 0-7 Cl: 1-2 I: 0-1

1: TOF MS ES-  
3.83e+003



Minimum: -1.5  
Maximum: 10.0 20.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
358.9989	358.9990	-0.1	-0.3	13.5	0.0	C17 H9 N2 O3 Cl2

Figure S40: HRMS spectrum of compound 20