

## Supplementary Materials

### Efficient synthesis of 4,8-dibromo derivative of strong electron-deficient benzo[1,2-d:4,5-d']bis([1,2,3]thiadiazole) and its S<sub>N</sub>Ar and cross-coupling reactions

Timofey N. Chmovzh <sup>1,2</sup>, Daria A. Alekhina<sup>1</sup>, Timofey A. Kudryashev <sup>1,3</sup>, and Oleg A. Rakitin <sup>1,\*</sup>

<sup>1</sup> N. D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, 119991 Moscow, Russian Federation

<sup>2</sup> Nanotechnology Education and Research Center, South Ural State University, 454080 Chelyabinsk, Russia

<sup>3</sup> Department of Chemistry, Moscow State University, 119899 Moscow, Russia

\* Correspondence: orakitin@ioc.ac.ru; Tel.: +7 499 135 5327

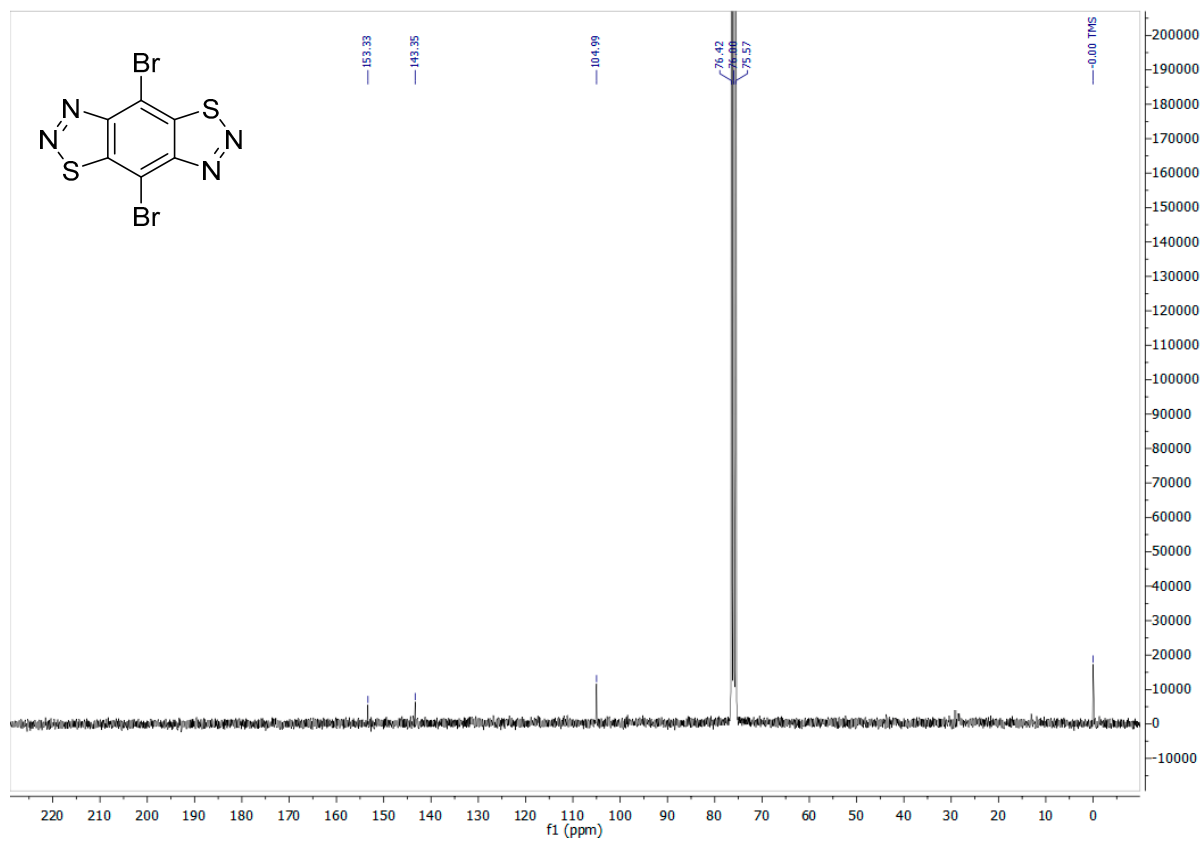
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# $^1\text{H}$ , $^{13}\text{C}$ NMR and HRMS spectra

## 4,8-Dibromobenzo[1,2-d:4,5-d']bis([1,2,3]thiadiazole) (1)

### $^{13}\text{C}$ NMR(75 MHz)



## Display Report

### Analysis Info

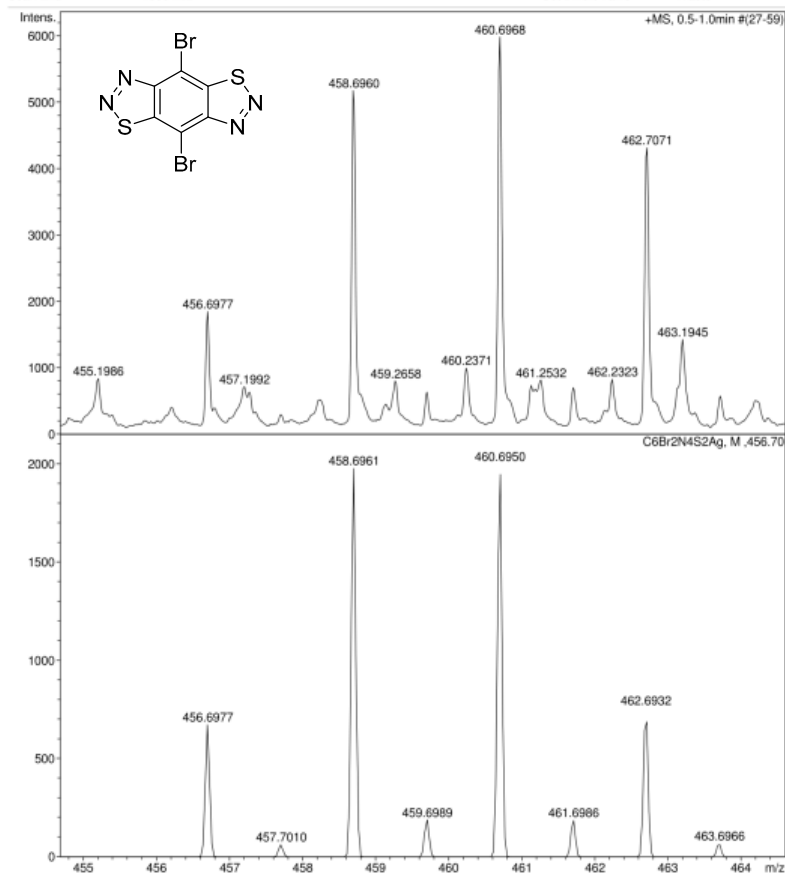
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Acquisition Date 31.08.2021 12:58:20

Operator BDAL@DE  
Instrument / Ser# micrOTOF 10248

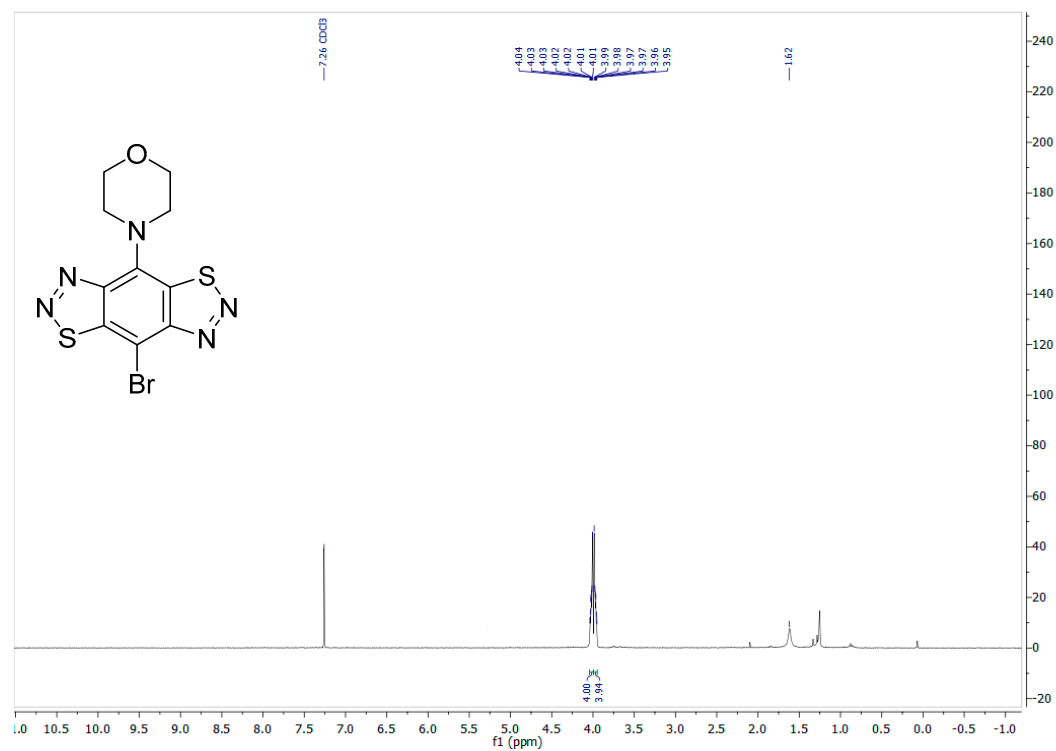
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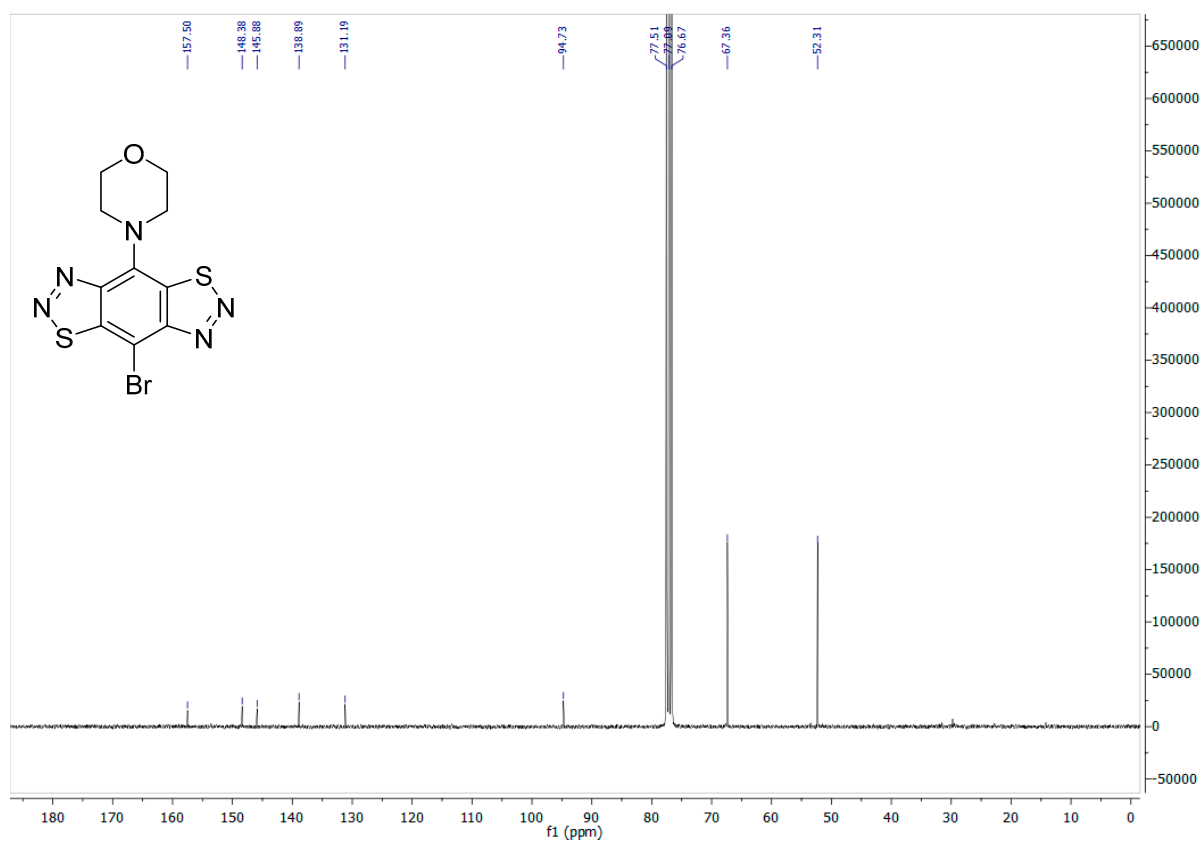


**4-(8-Bromobenzo[1,2-d:4,5-d']bis([1,2,3]thiadiazole)-4-yl)morpholine (12a)**

**<sup>1</sup>H NMR (300 MHz)**



**<sup>13</sup>C NMR (75 MHz)**



## Display Report

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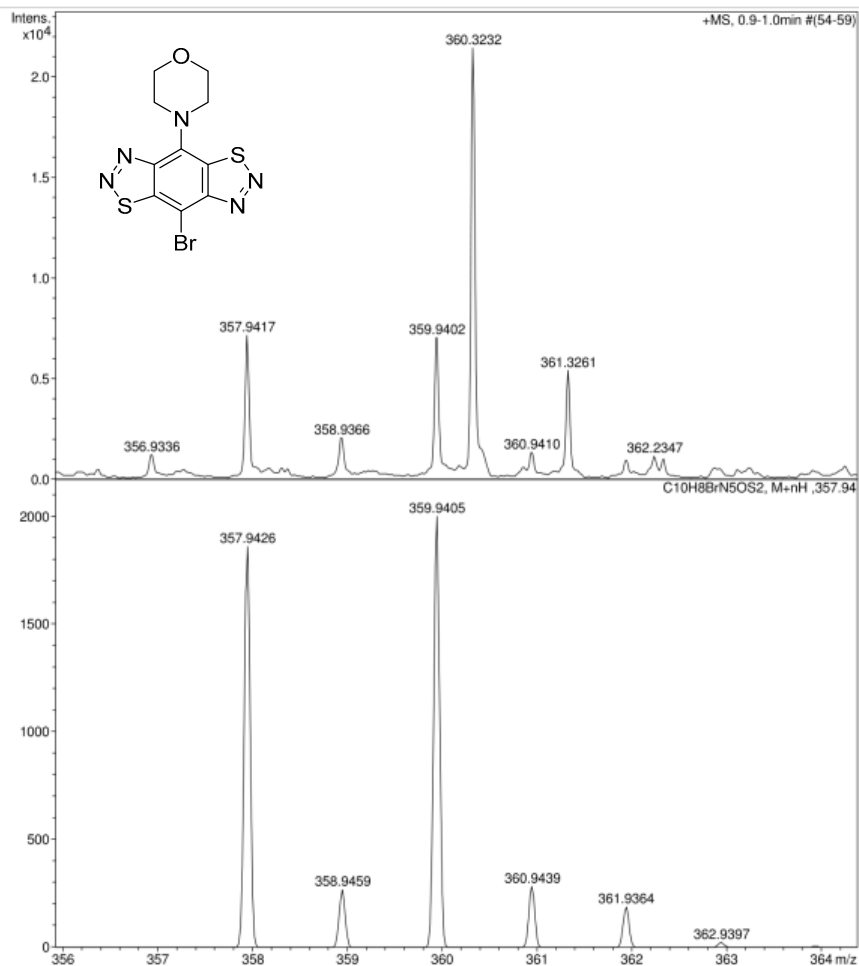
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Acquisition Date 28.09.2021 11:53:23

Operator BDAL@DE  
 Instrument / Ser# microTOF 10248

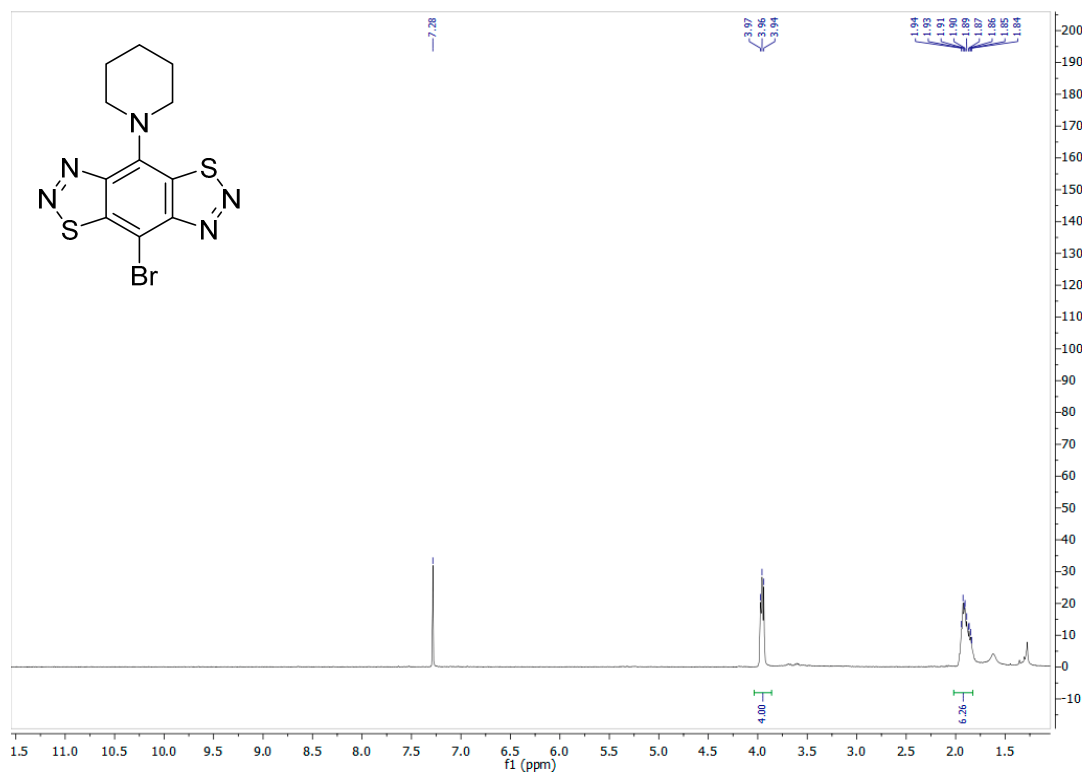
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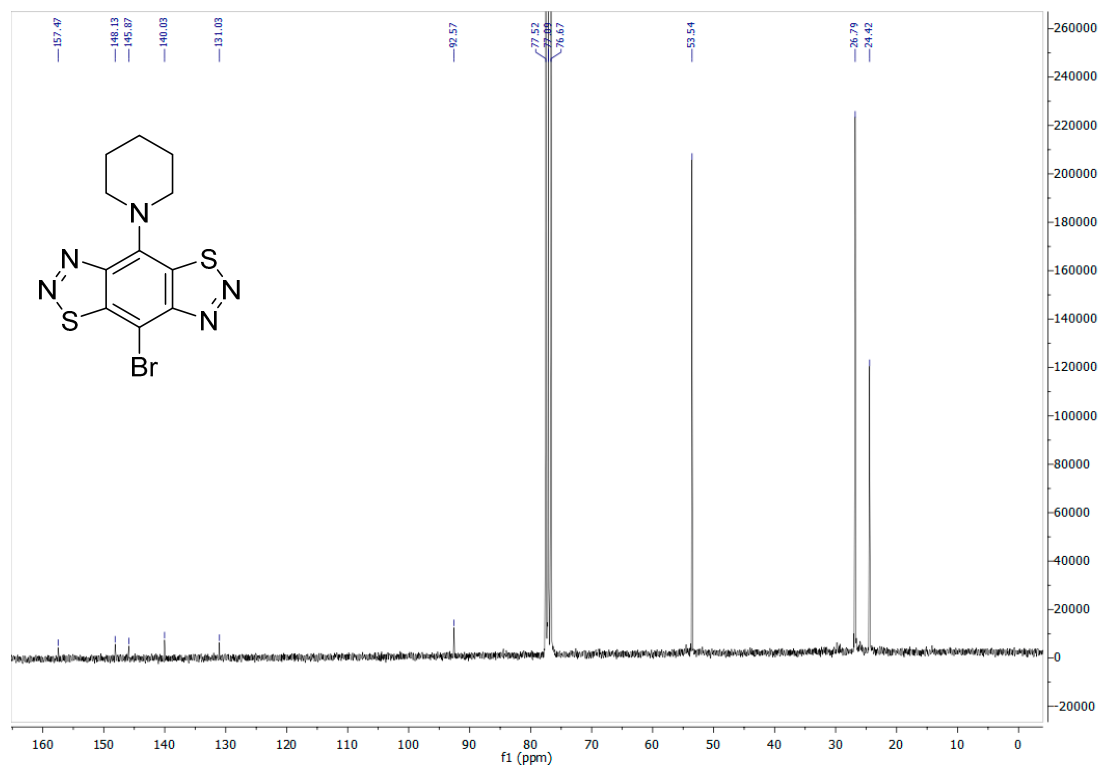


# 4-Bromo-8-(piperidin-1-yl)benzo[1,2-d:4,5-d']bis([1,2,3]thiadiazole) (12b)

$^1\text{H}$  NMR (300 MHz)



$^{13}\text{C}$  NMR (75 MHz)



# Display Report

## Analysis Info

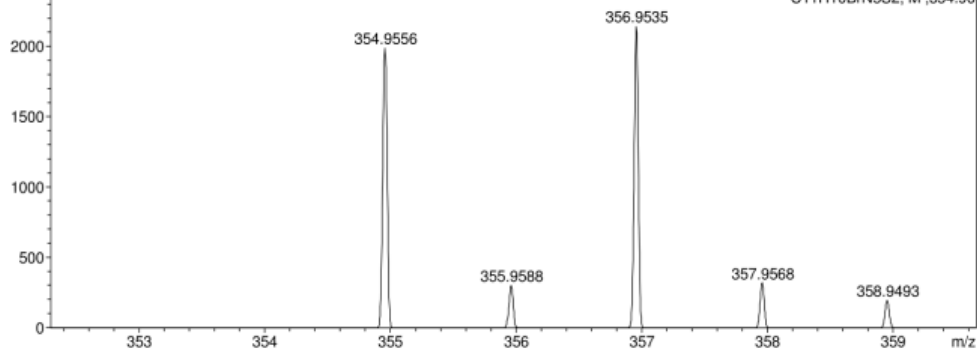
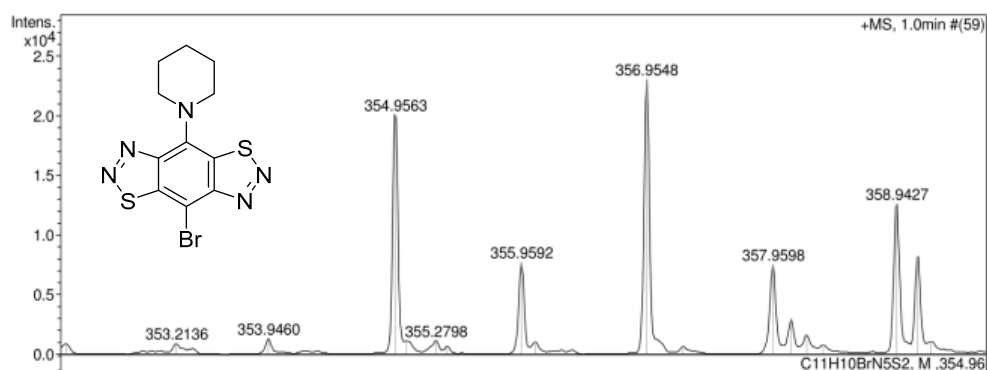
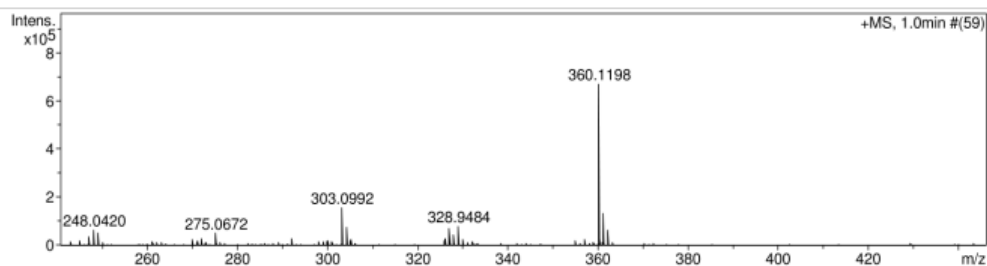
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Operator BDAL@DE  
 Instrument / Ser# micrOTOF 10248

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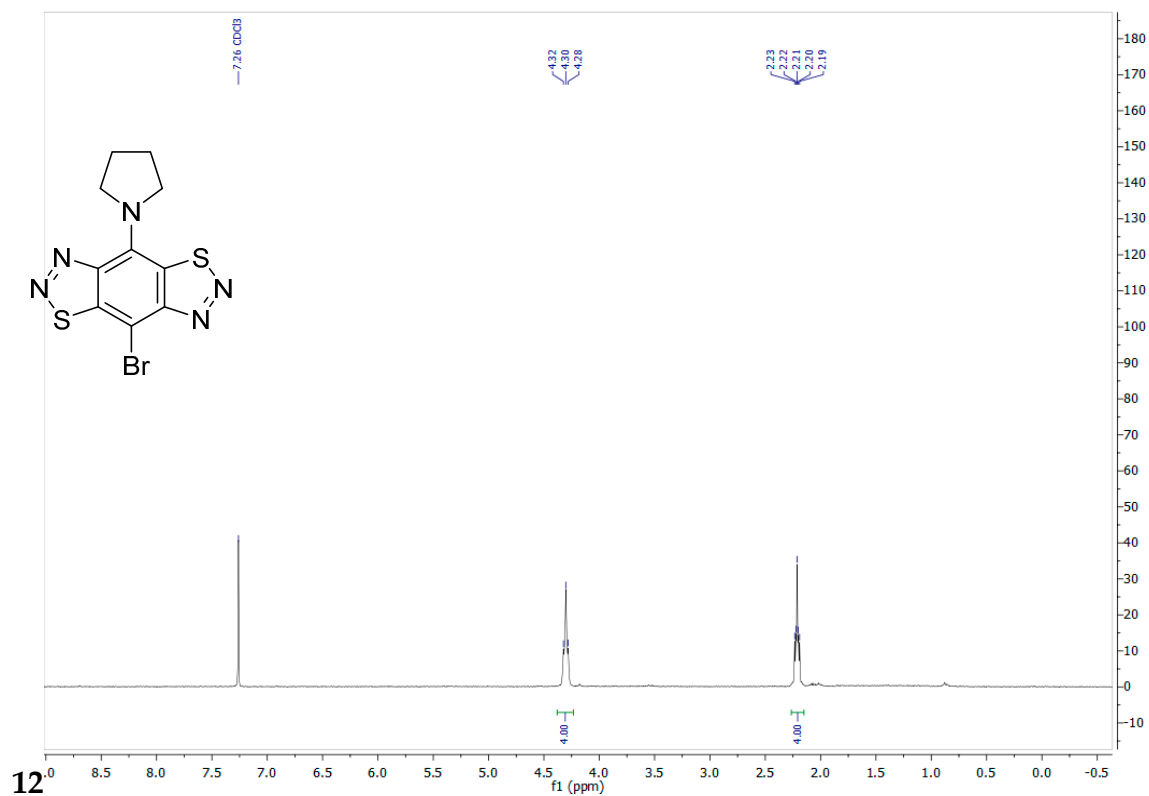
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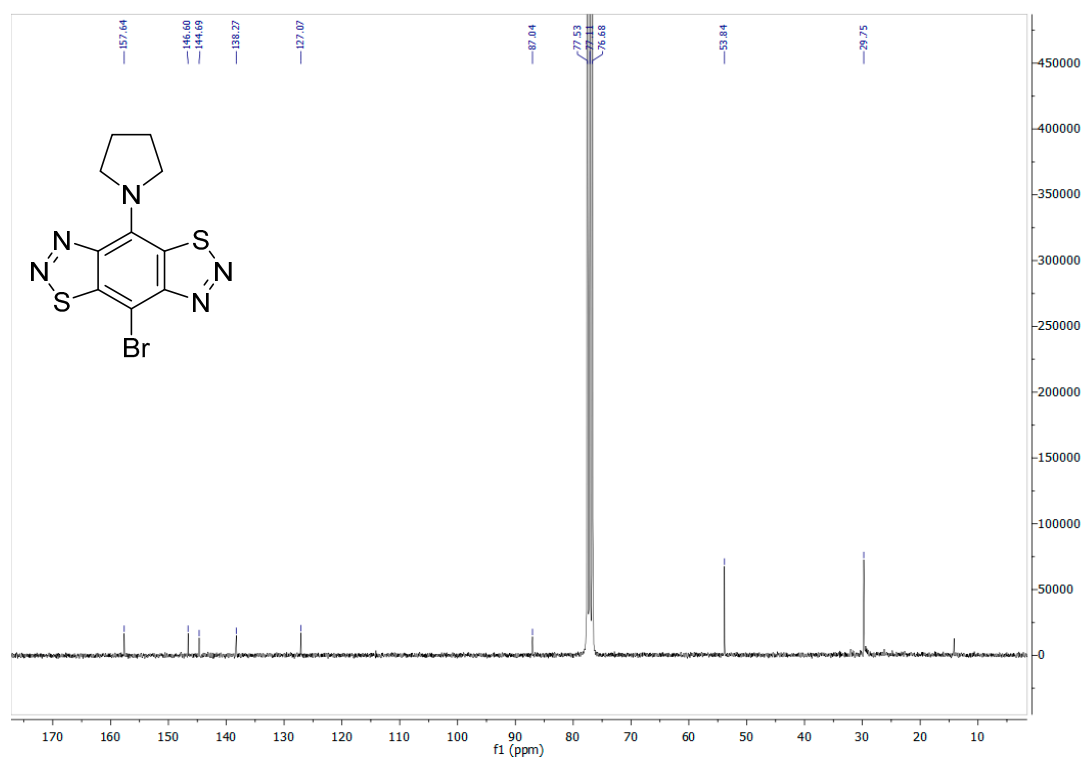


# 4-Bromo-8-(pyrrolidin-1-yl)benzo[1,2-d:4,5-d']bis([1,2,3]thiadiazole) (12c)

<sup>1</sup>H NMR (300 MHz)



<sup>13</sup>C NMR (75 MHz)



# Display Report

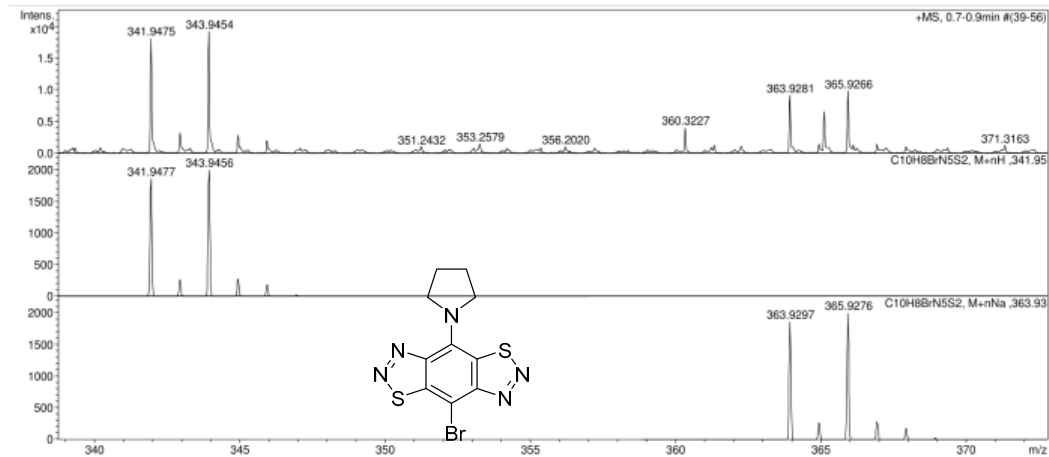
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 Operator BDAL@DE  
 Instrument / Ser# micrOTOF 10248

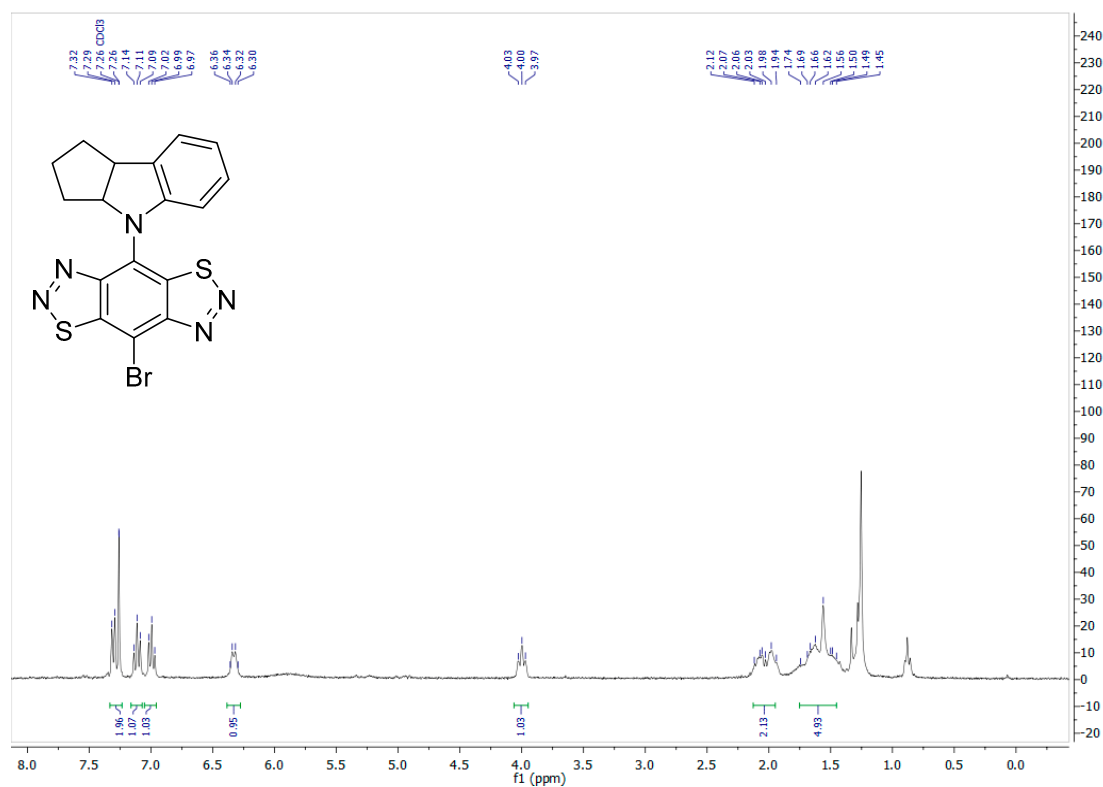
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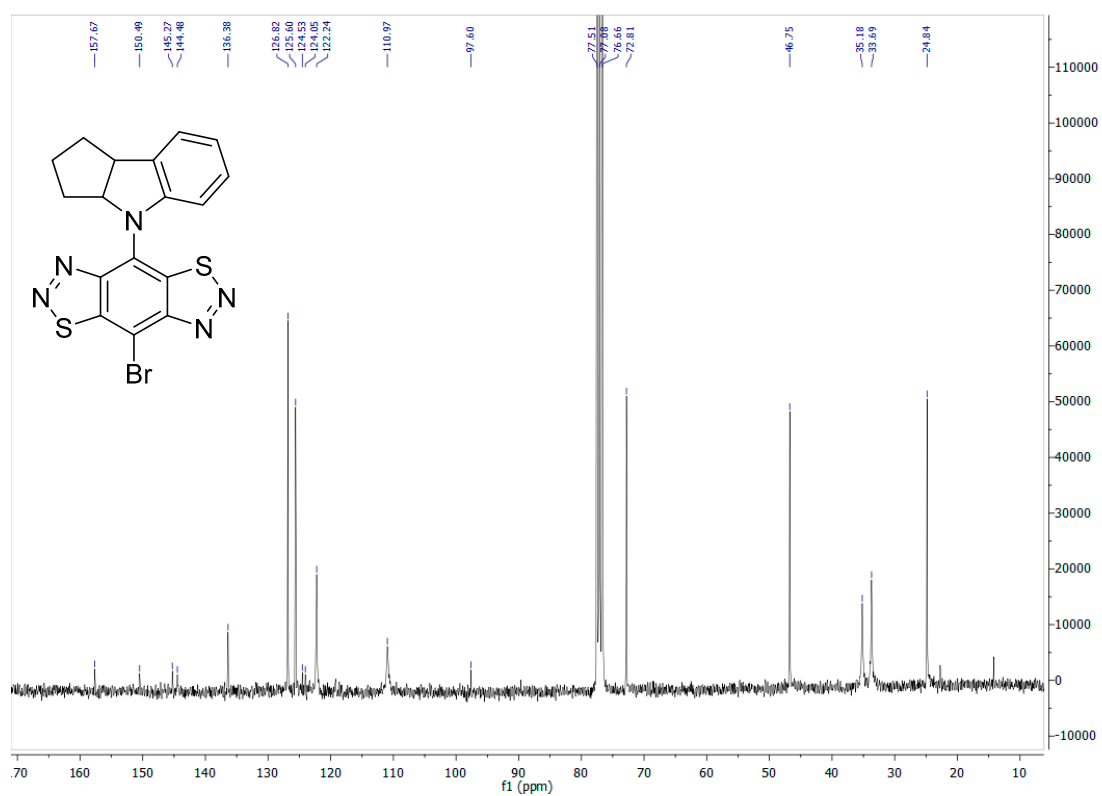


**4-Bromo-8-(2,3,3a,8b-tetrahydrocyclopenta[b]indol-4(1H)-yl)benzo[1,2-d:4,5-d']bis([1,2,3]thiadiazole) (12d)**

**$^1\text{H}$  NMR (300 MHz)**



**$^{13}\text{C}$  NMR(75 MHz)**



# Display Report

## Analysis Info

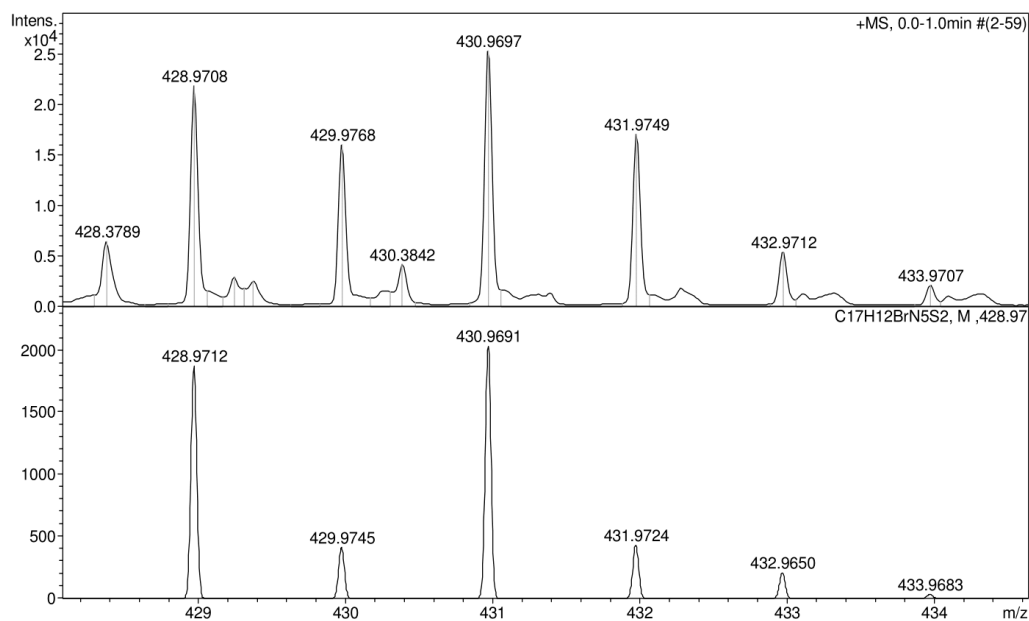
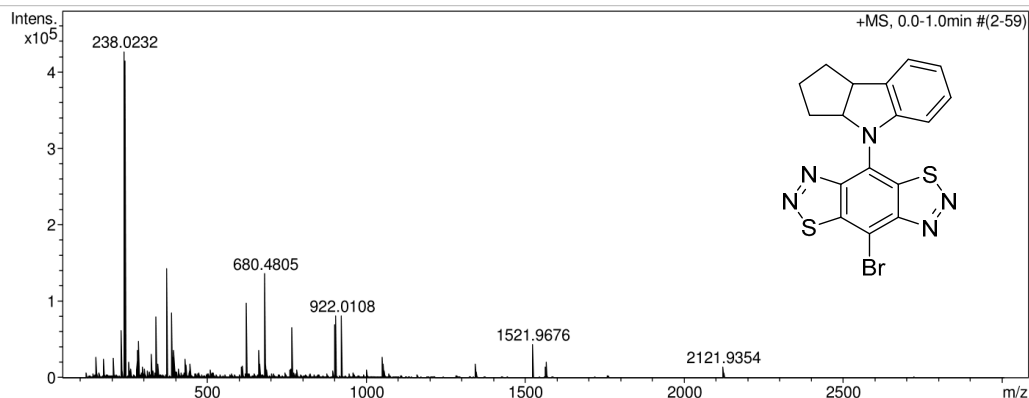
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Acquisition Date 02.09.2022 16:28:34

Operator BDAL@DE  
 Instrument / Ser# micrOTOF 10248

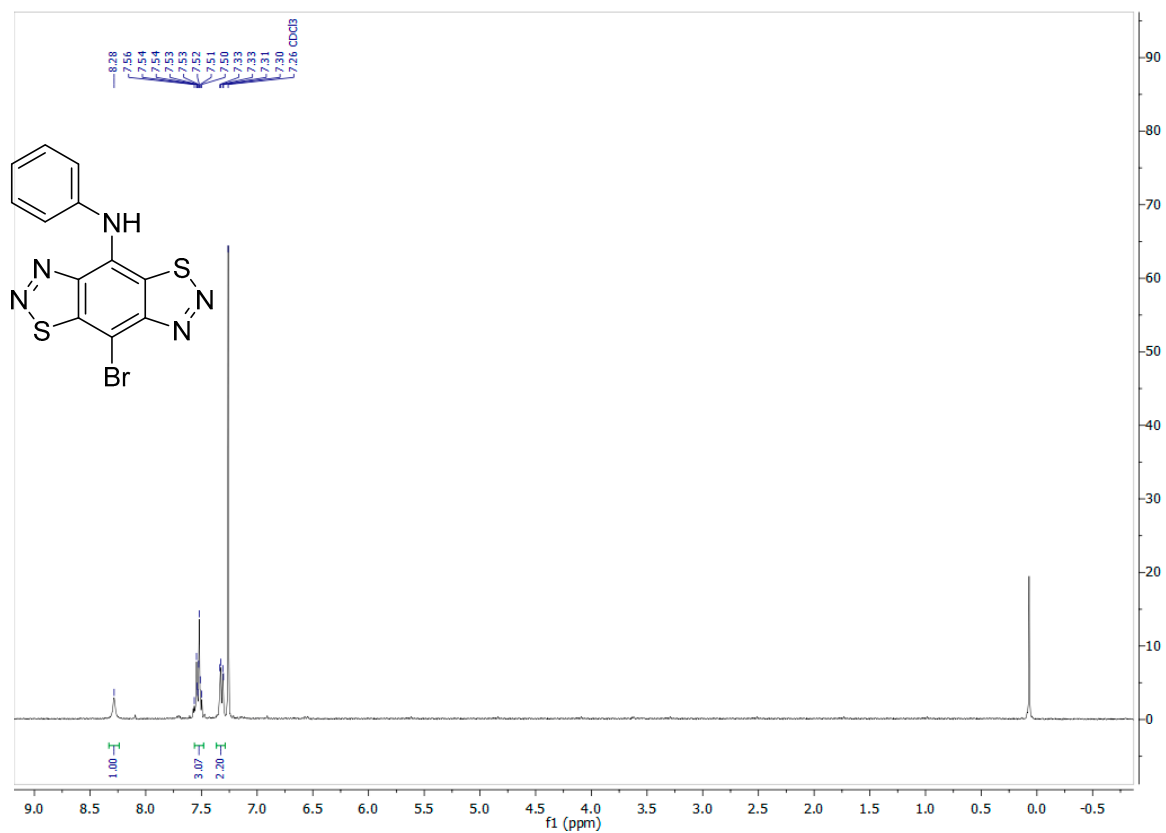
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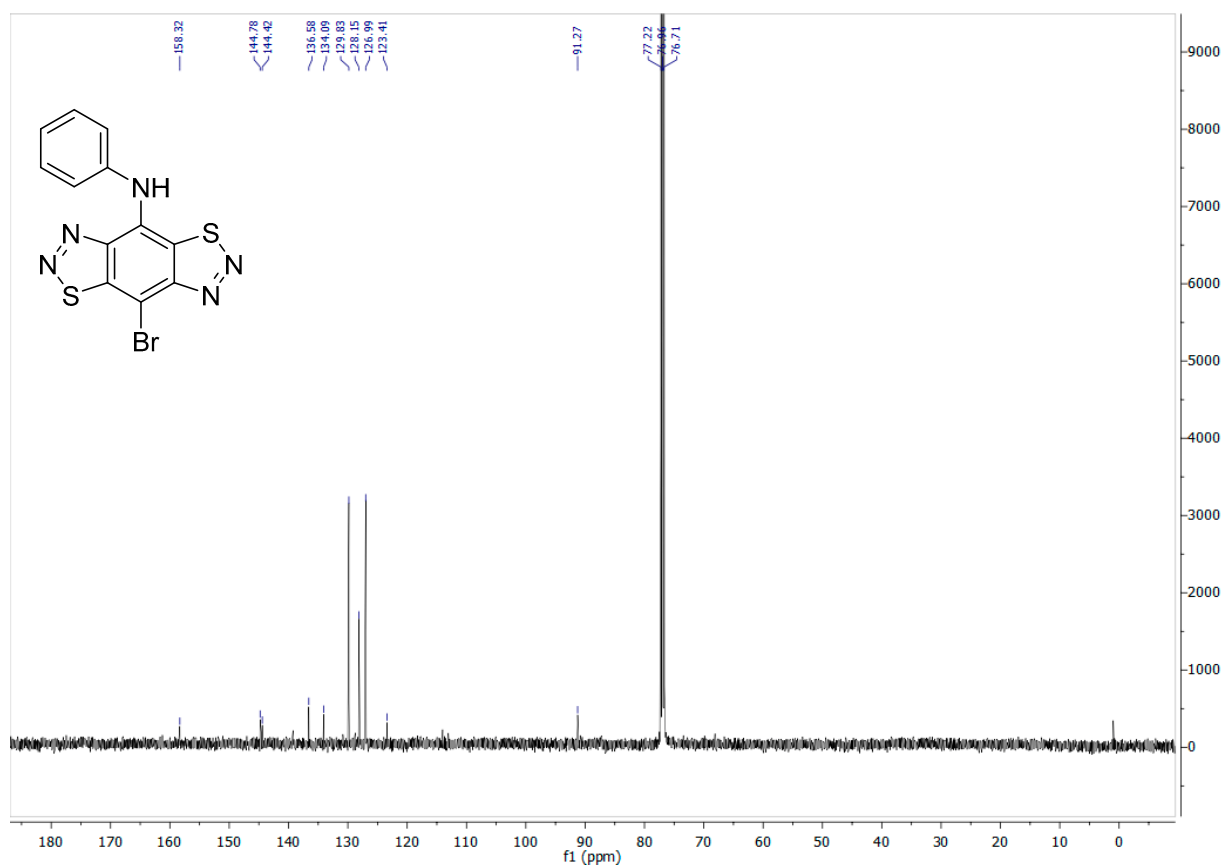


**8-Bromo-N-phenylbenzo[1,2-d:4,5-d']bis([1,2,3]thiadiazole)-4-amine (12e)**

**<sup>1</sup>H NMR (300 MHz)**



**<sup>13</sup>C NMR (75 MHz)**



## Display Report

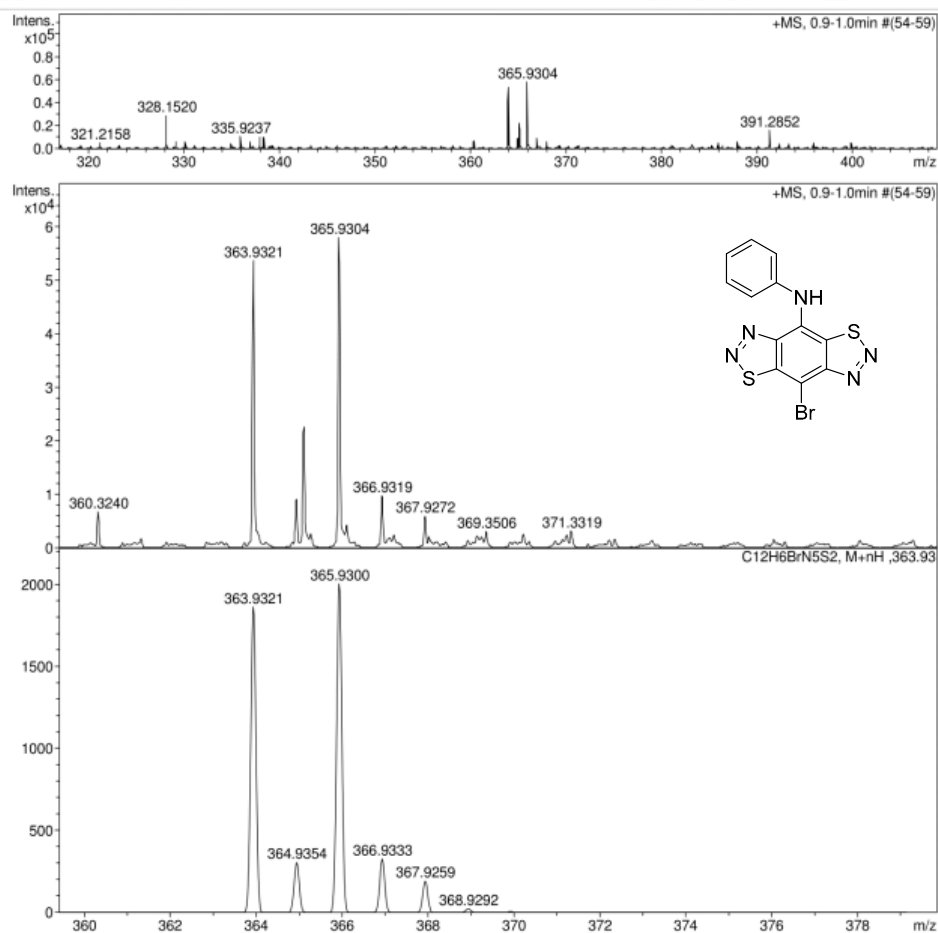
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Operator BDAL@DE  
Instrument / Ser# micrOTOF 10248

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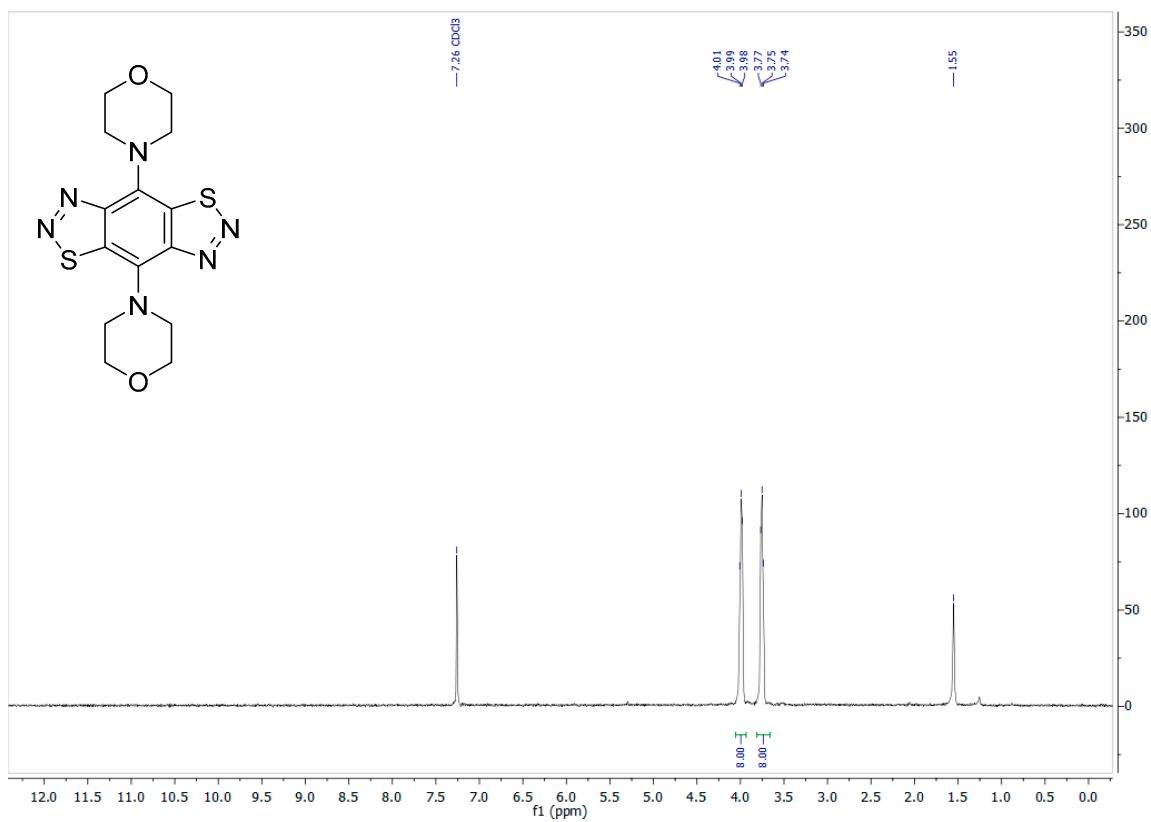
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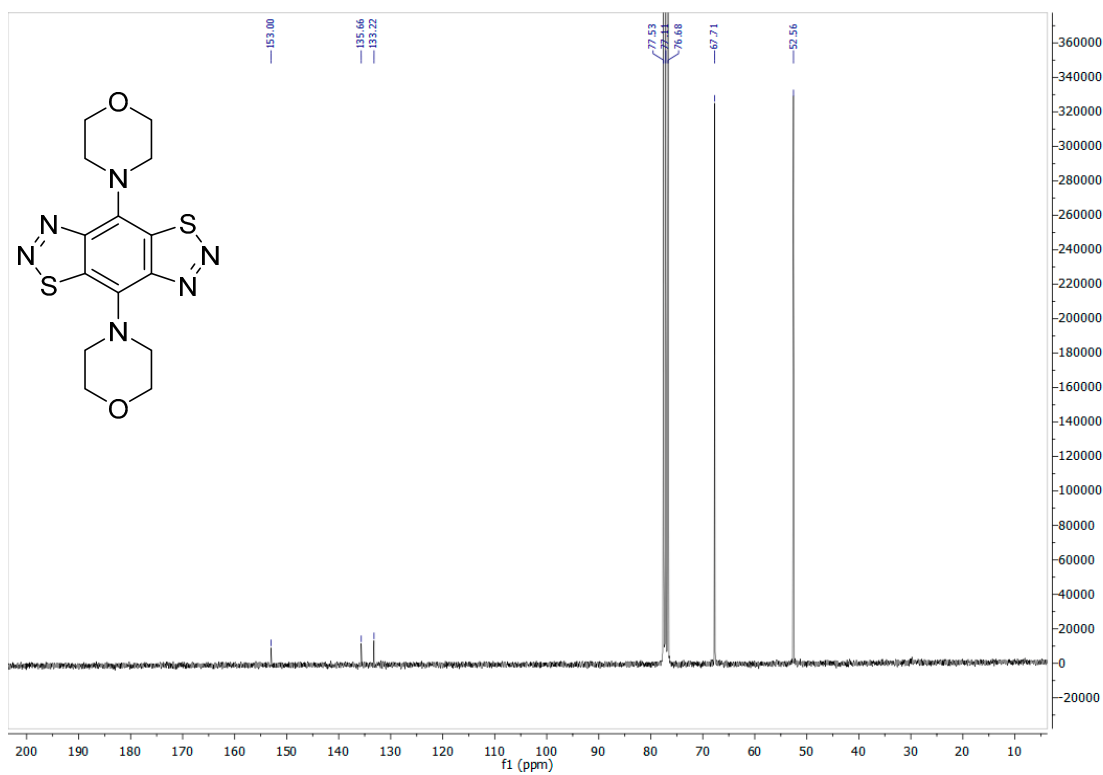


# 4,8-Dimorpholinobenzo[1,2-d:4,5-d']bis([1,2,3]thiadiazole) (13a)

$^1\text{H}$  NMR (300 MHz)



$^{13}\text{C}$  NMR (75 MHz)



# Display Report

## Analysis Info

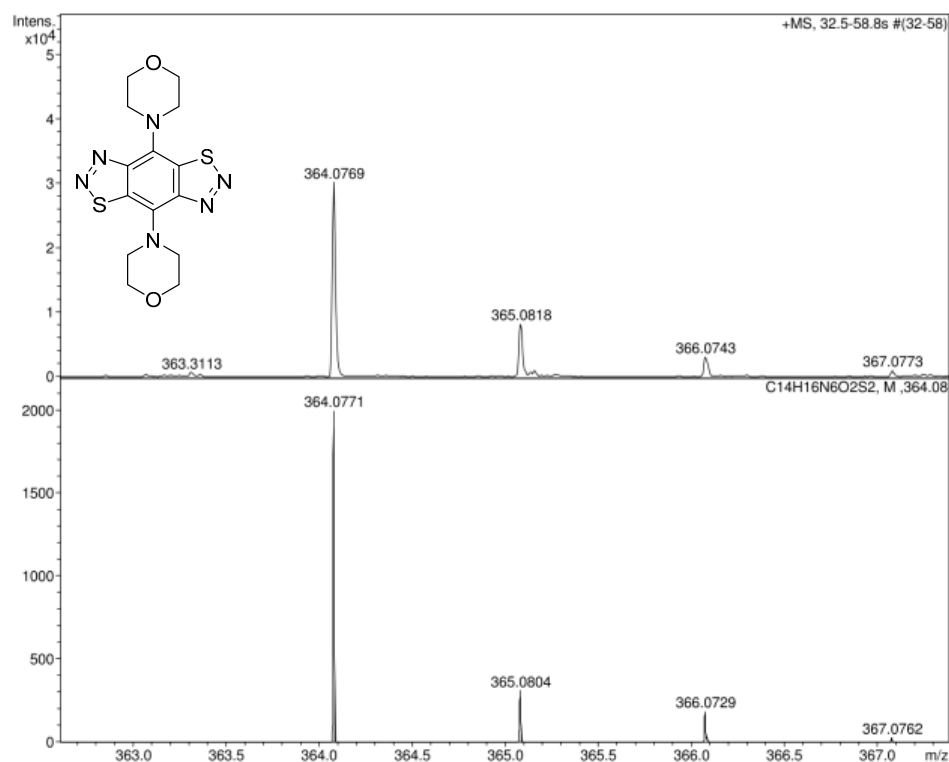
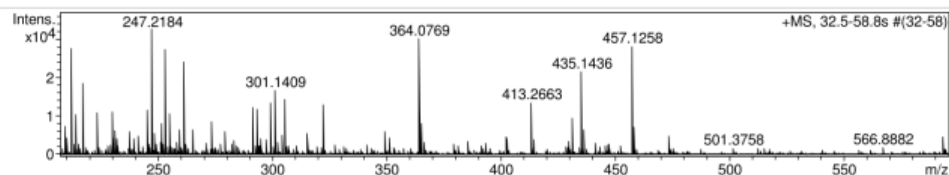
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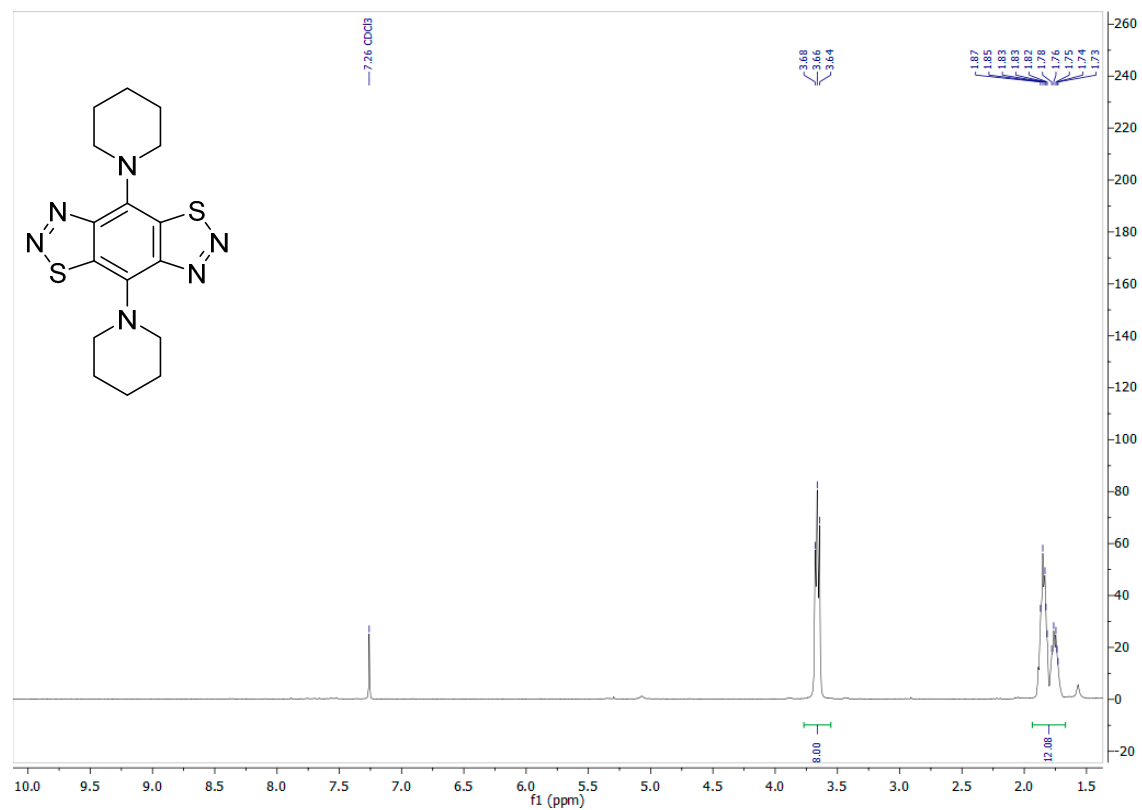
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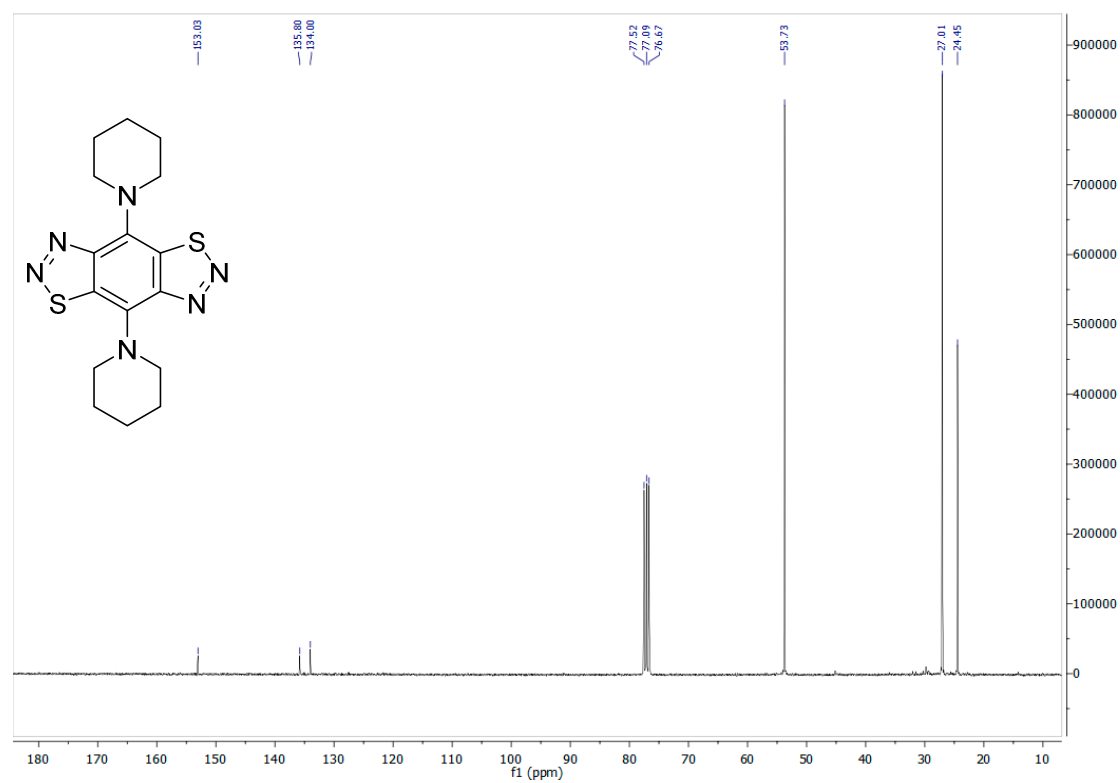


# 4,8-Di(piperidin-1-yl)benzo[1,2-d:4,5-d']bis([1,2,3]thiadiazole) (13b)

$^1\text{H}$  NMR (300 MHz)



$^{13}\text{C}$  NMR (75 MHz)



# Display Report

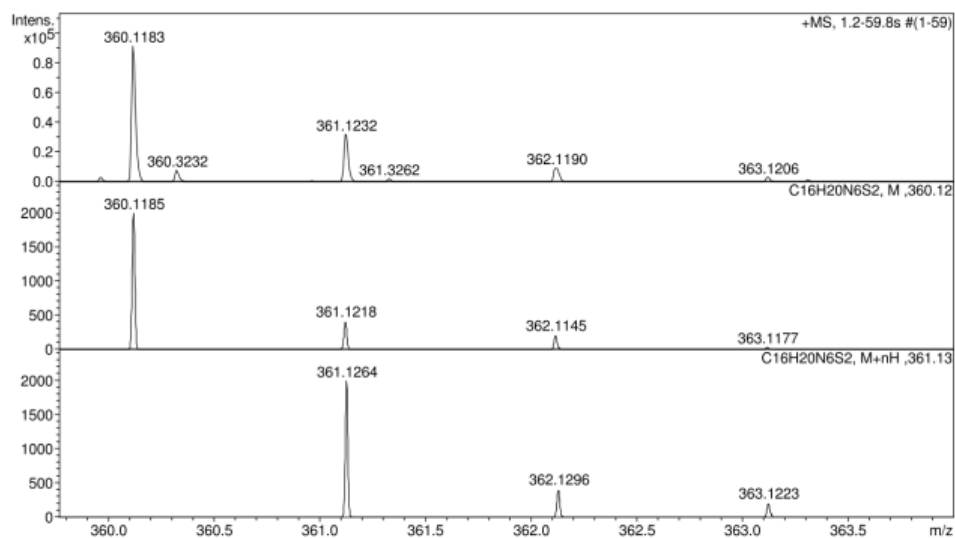
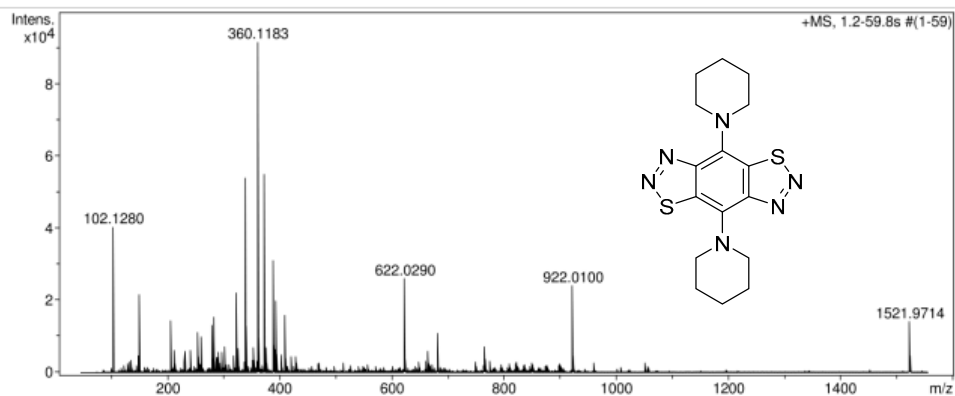
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 Operator BDAL@DE  
 Instrument / Ser# maxis 43

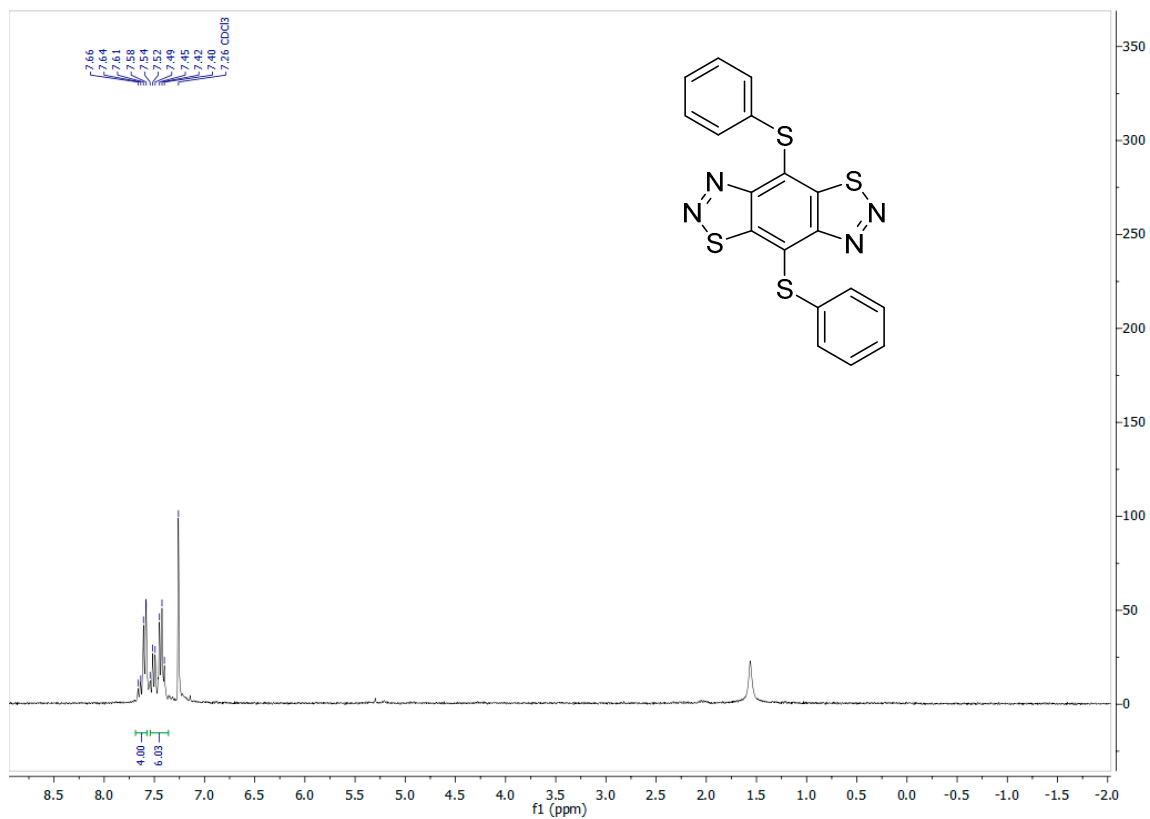
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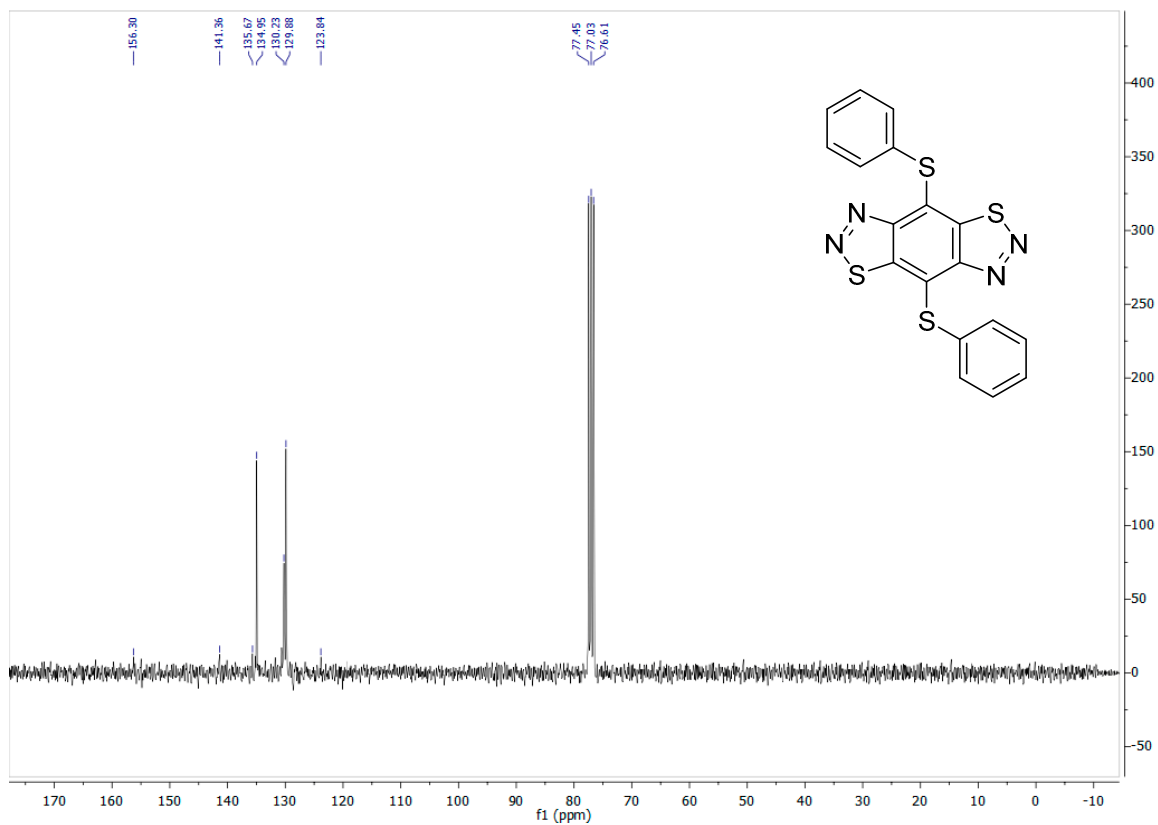


# 4,8-Bis(phenylthio)benzo[1,2-d:4,5-d']bis([1,2,3]thiadiazole) (15a)

$^1\text{H}$  NMR (300 MHz)



$^{13}\text{C}$  NMR(75 MHz)



## Display Report

### Analysis Info

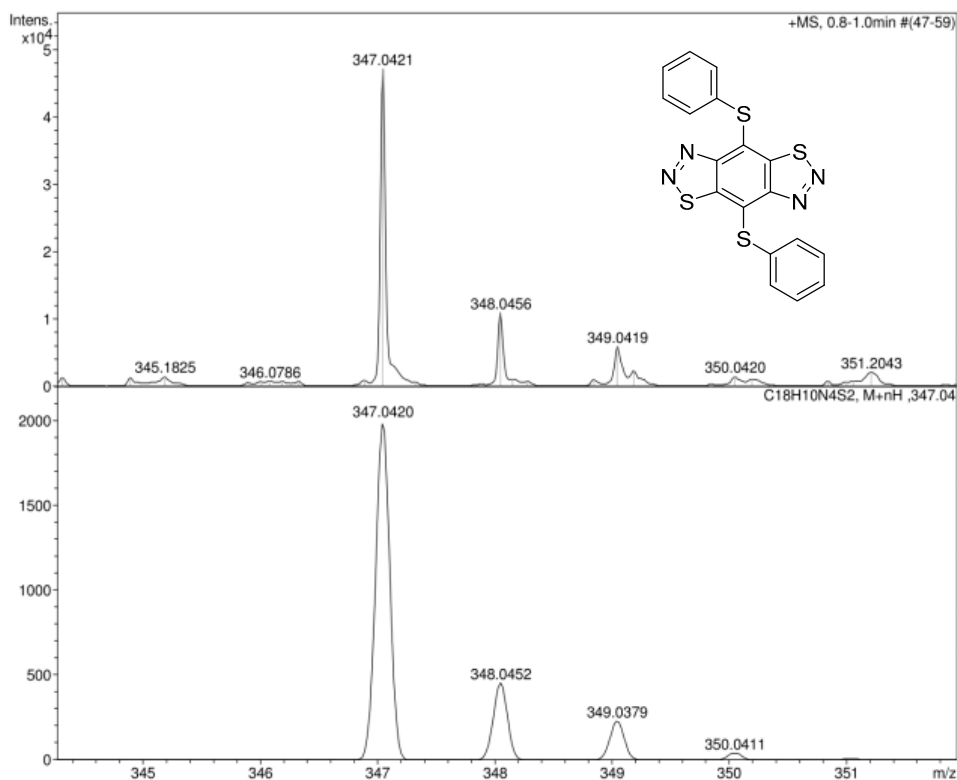
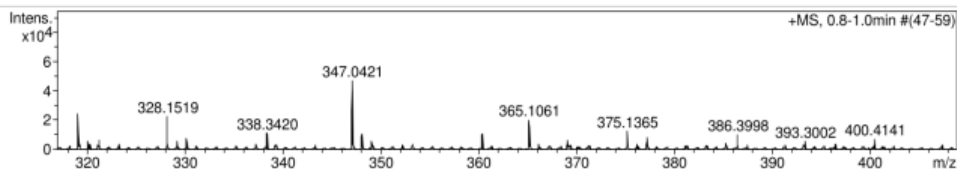
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Operator BDAL@DE  
Instrument / Ser# micrOTOF 10248

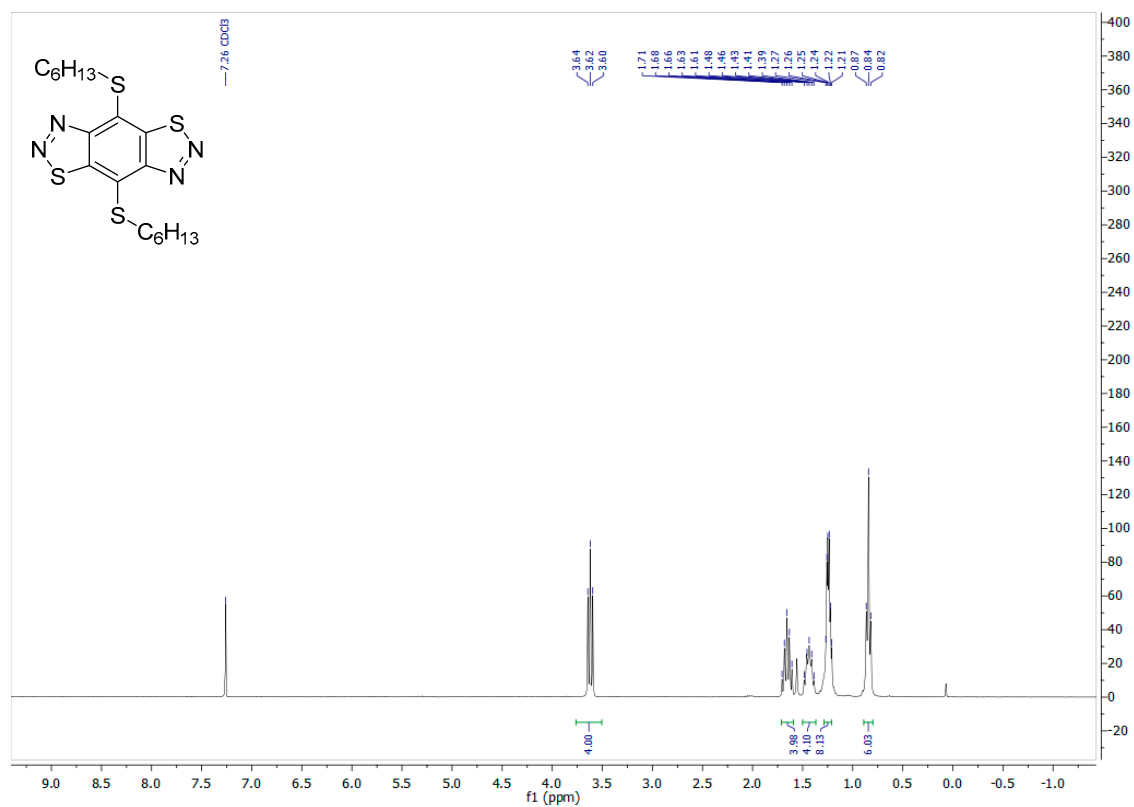
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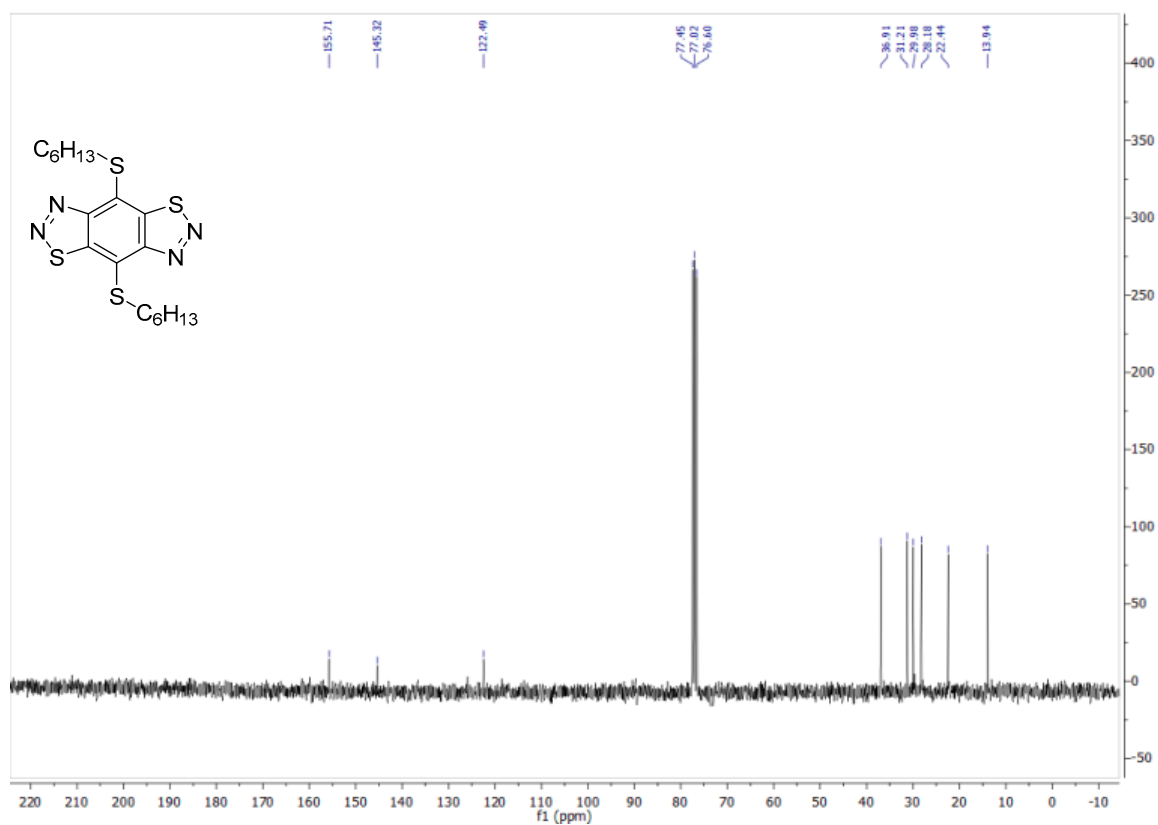


**4,8-Bis(hexylthio)benzo[1,2-d:4,5-d']bis([1,2,3]thiadiazole) (15b)**

**$^1\text{H}$  NMR (300 MHz)**



**$^{13}\text{C}$  NMR(75 MHz)**





# Display Report

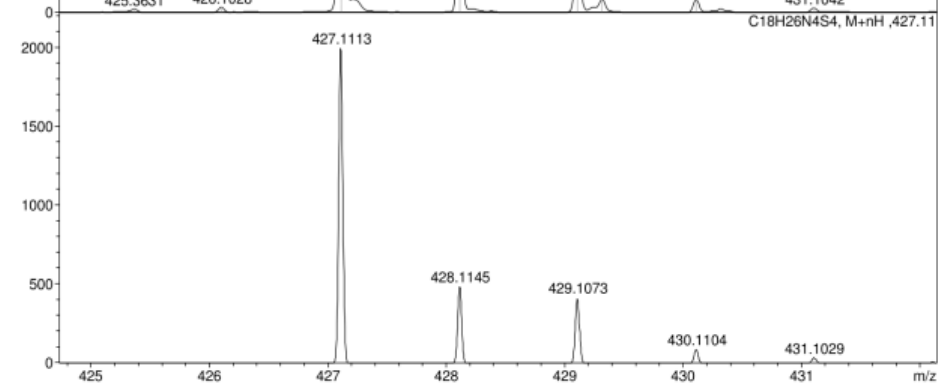
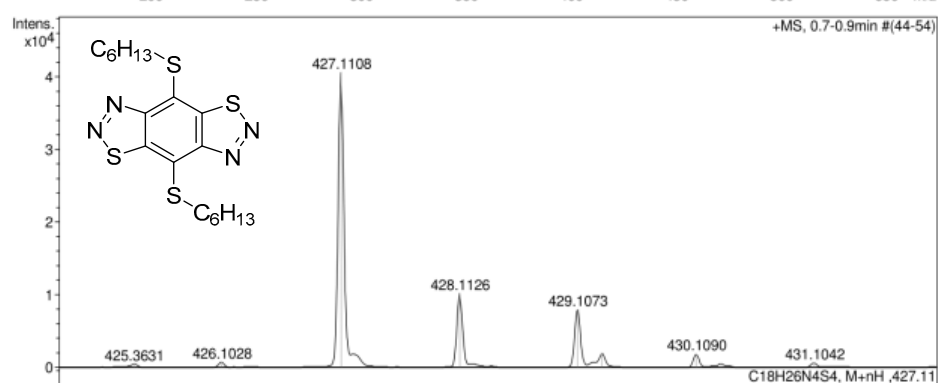
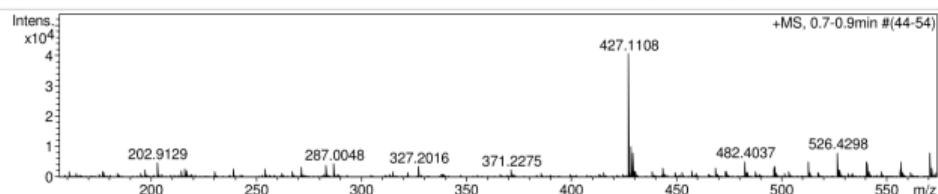
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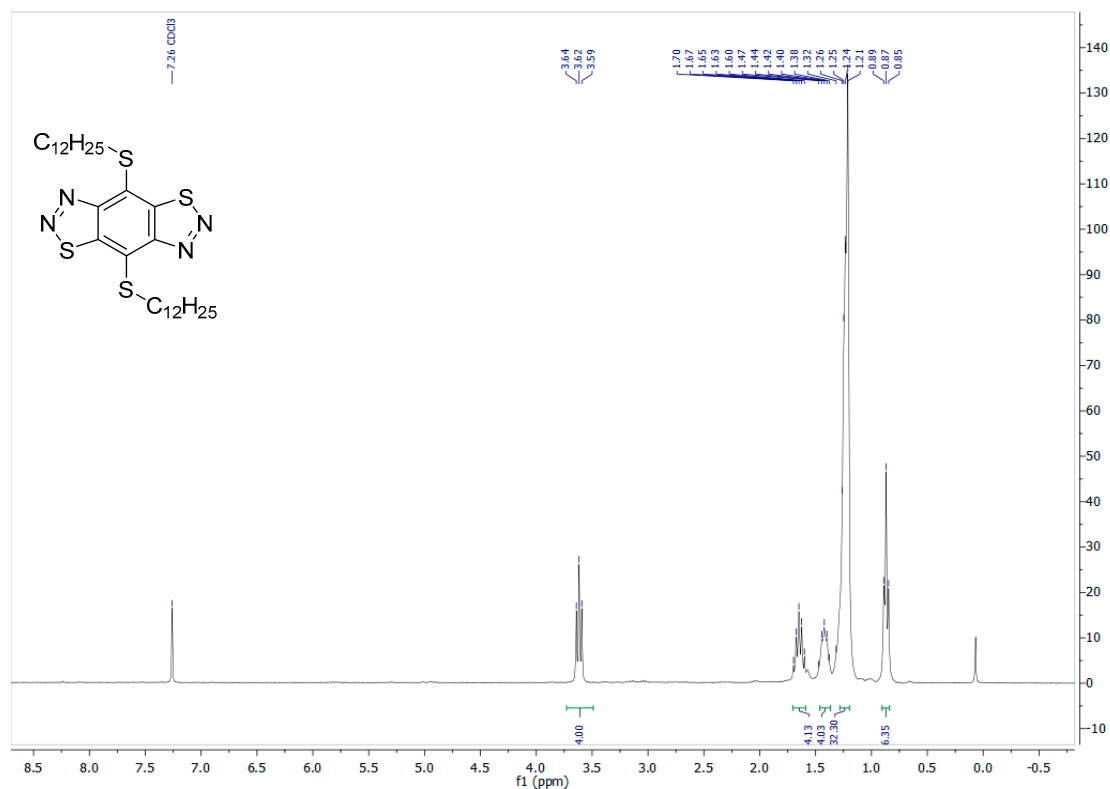
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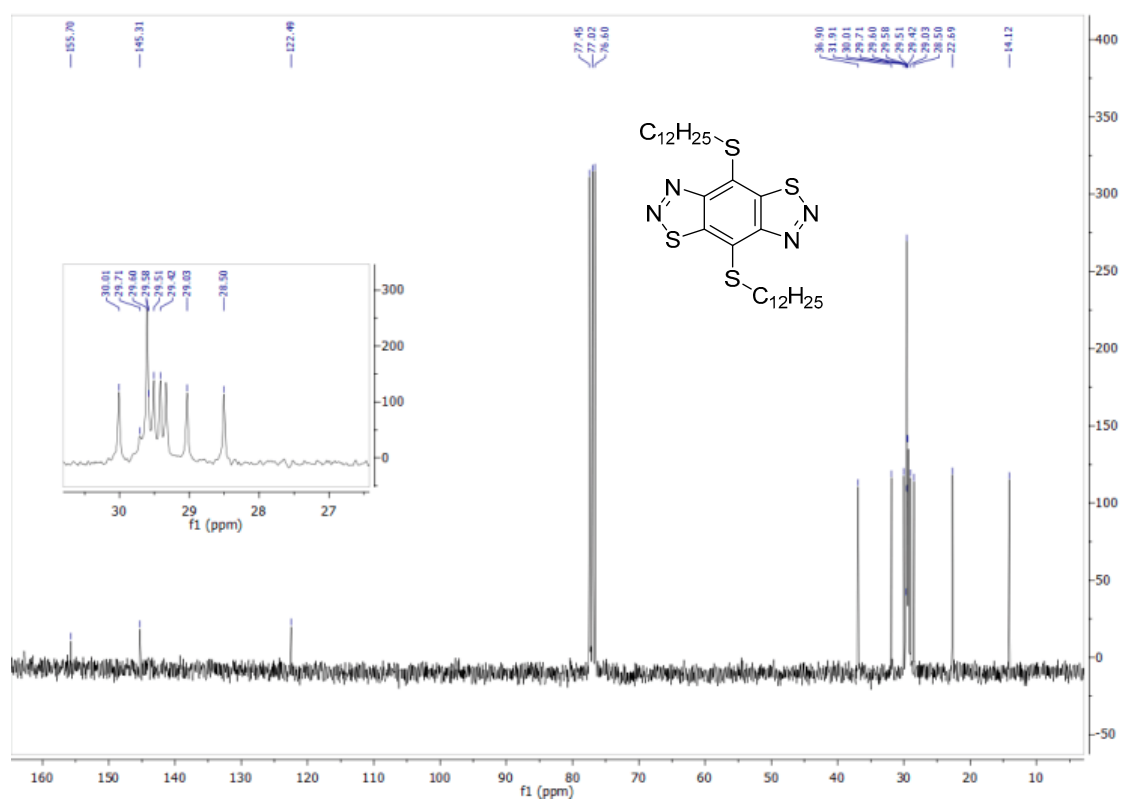


# 4,8-Bis(dodecylthio)benzo[1,2-d:4,5-d']bis([1,2,3]thiadiazole) (15c)

$^1\text{H}$  NMR (300 MHz)



$^{13}\text{C}$  NMR (75 MHz)



## Display Report

### Analysis Info

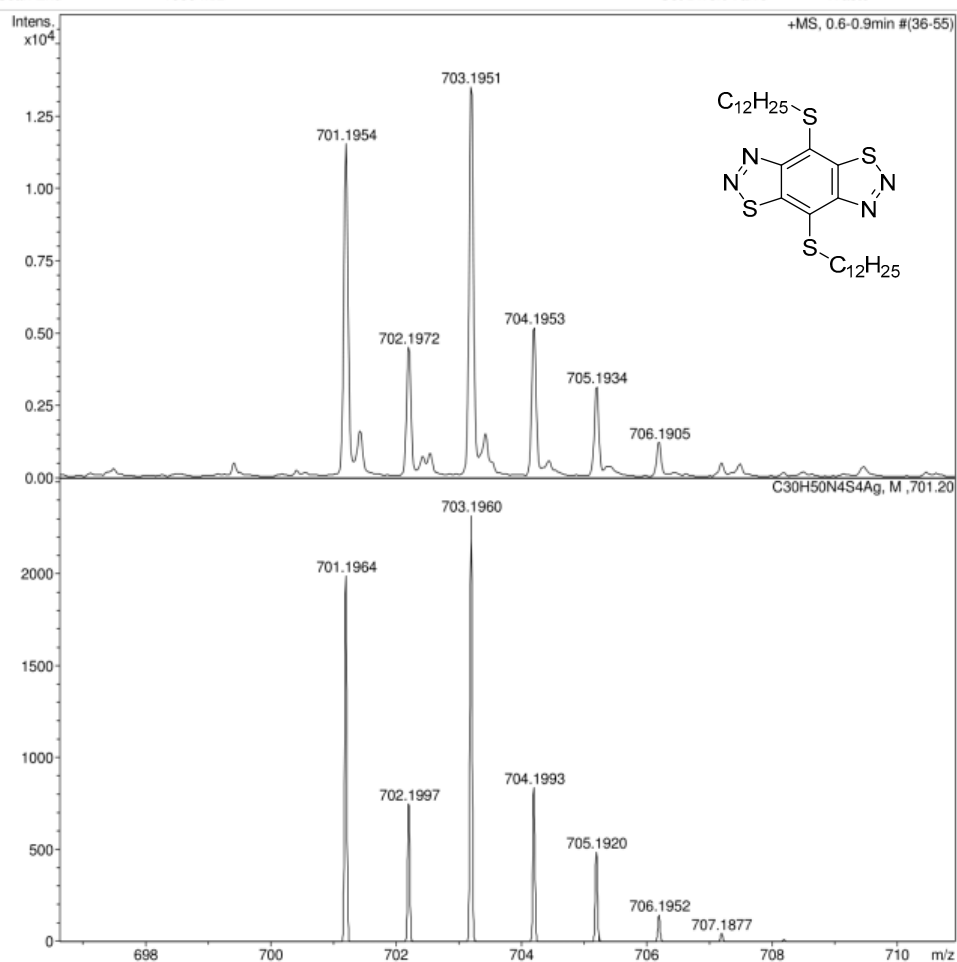
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Instrument / Ser# micrOTOF 10248

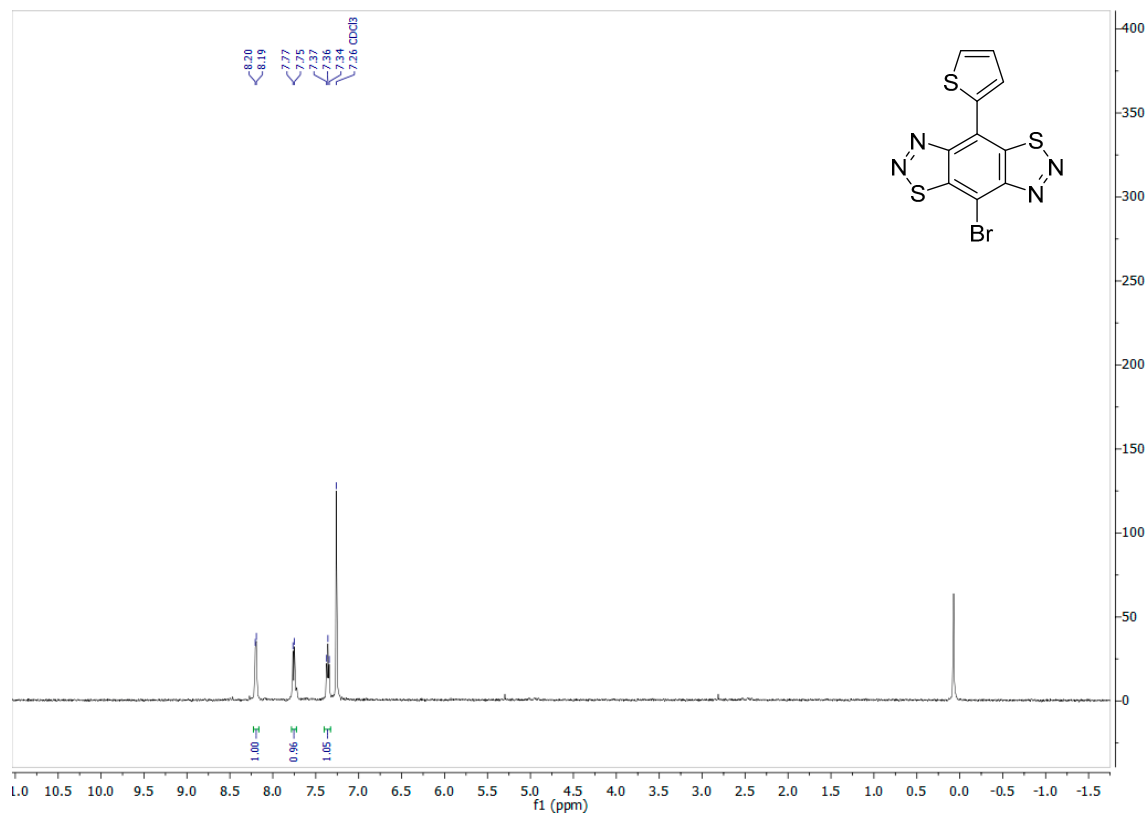
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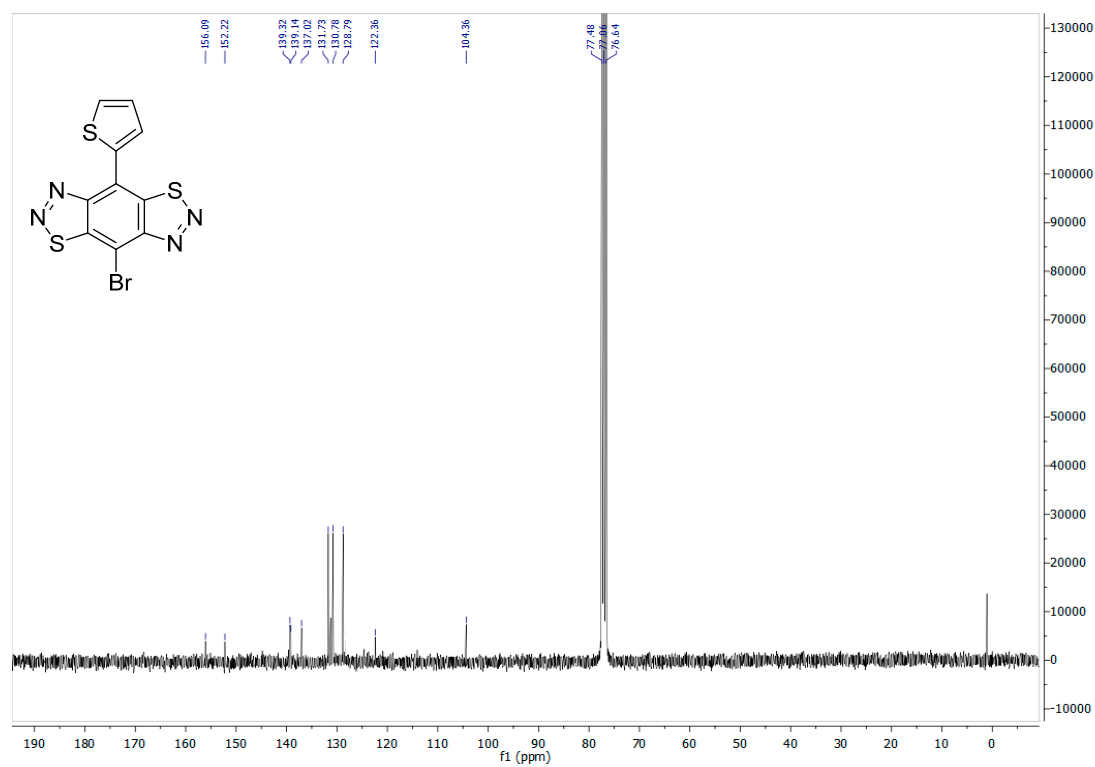


# 4-Bromo-8-(thiophen-2-yl)benzo[1,2-d:4,5-d']bis([1,2,3]thiadiazole) (18a)

$^1\text{H}$  NMR (300 MHz)



$^{13}\text{C}$  NMR (75 MHz)



## Display Report

### Analysis Info

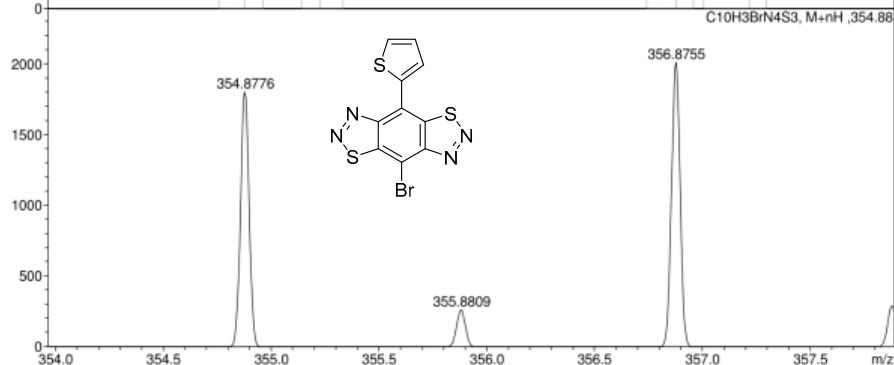
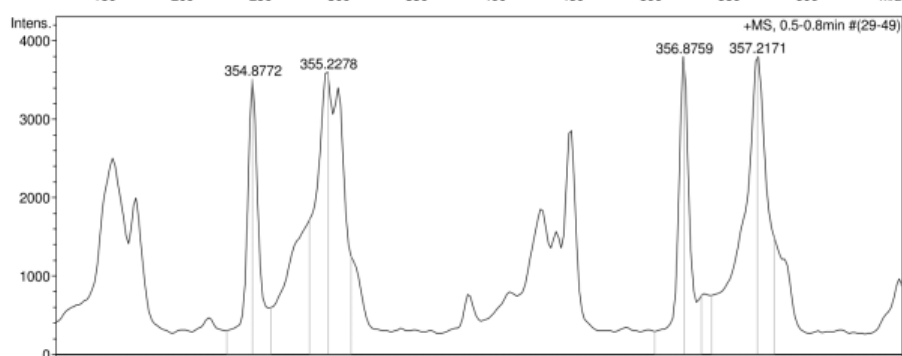
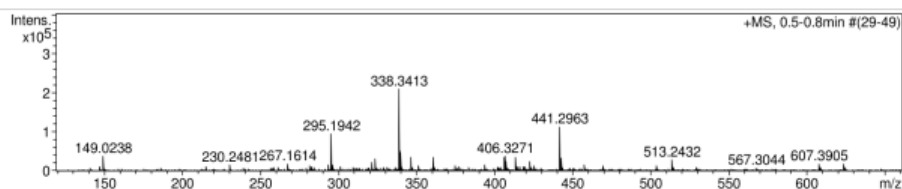
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Acquisition Date 20.09.2022 11:28:31

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 Instrument / Ser# micrOTOF 10248

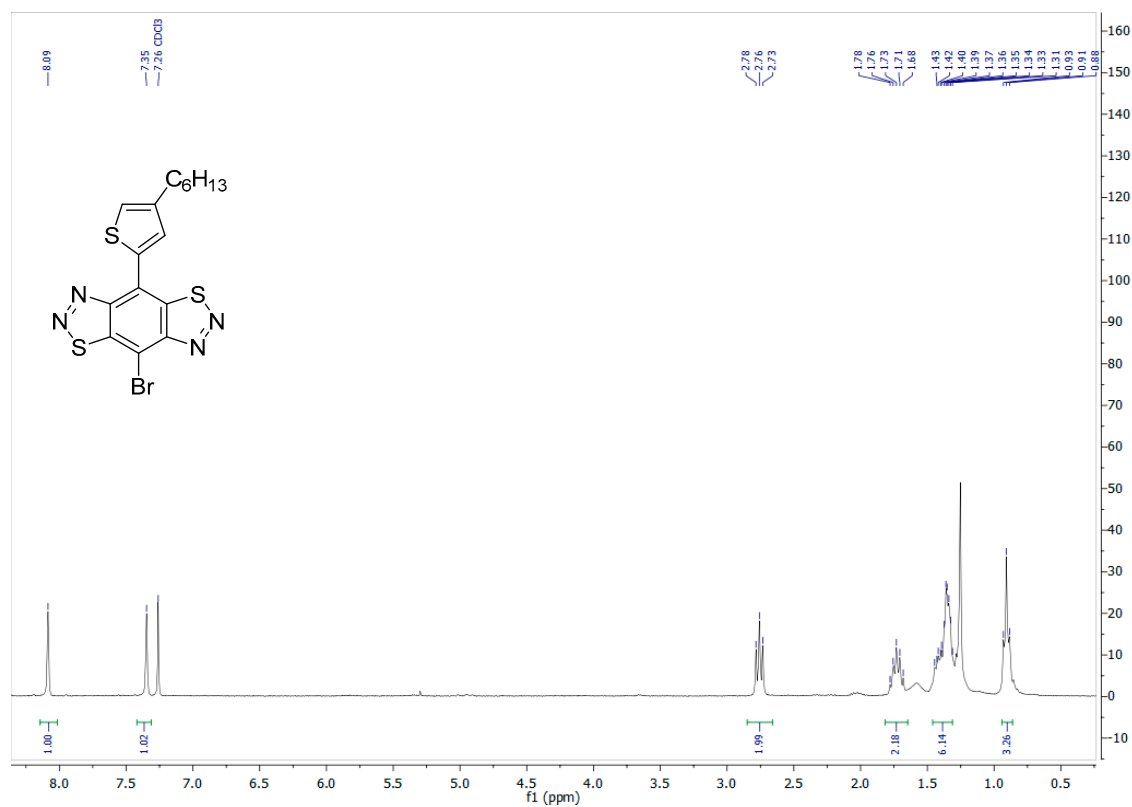
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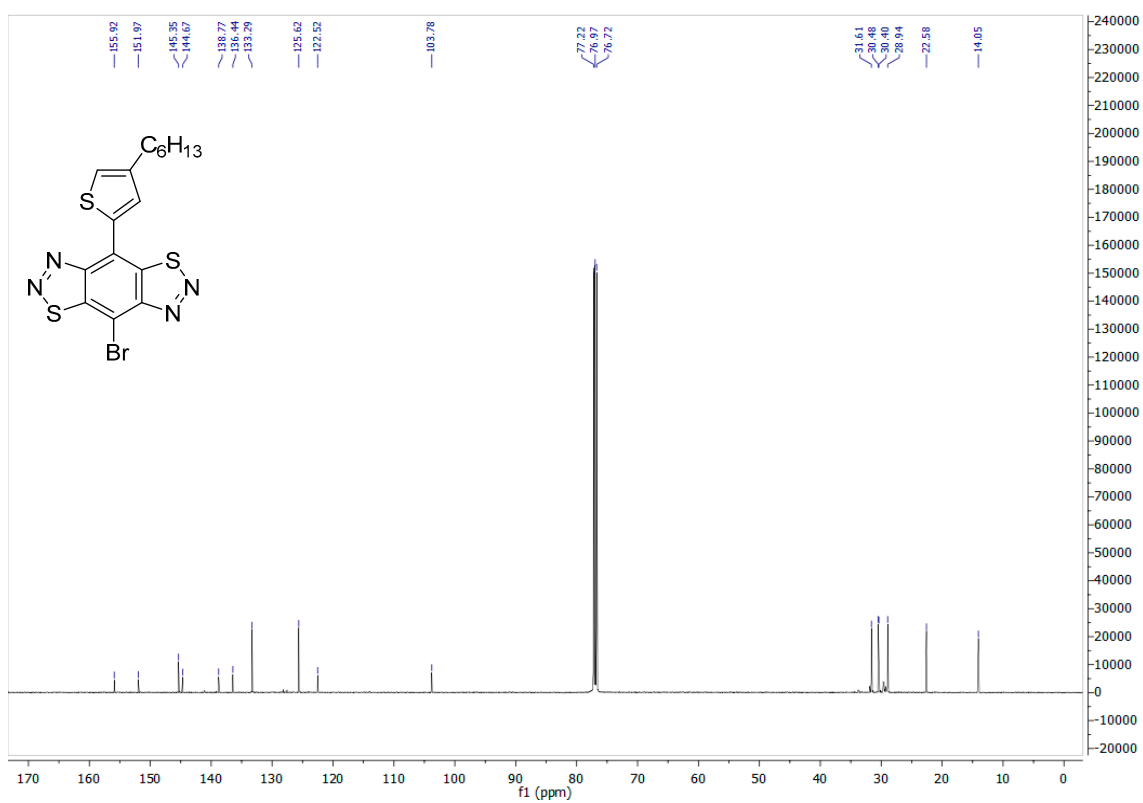


**4-Bromo-8-(4-hexylthiophen-2-yl)benzo[1,2-d:4,5-d']bis([1,2,3]thiadiazole) (18b)**

**<sup>1</sup>H NMR (300 MHz)**



**<sup>13</sup>C NMR(75 MHz)**



# Display Report

## Analysis Info

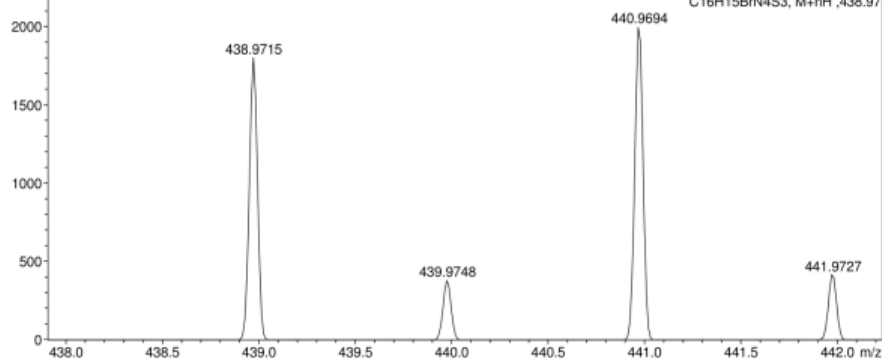
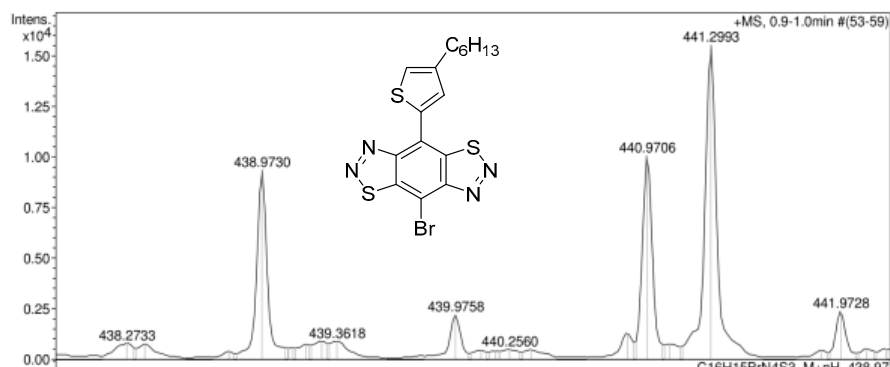
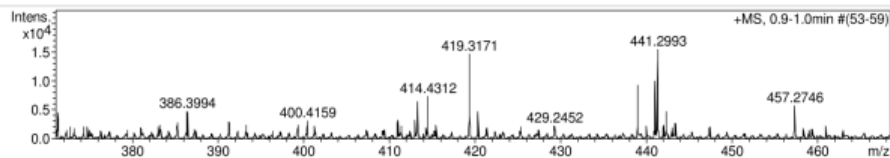
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 Sample Name /SUSU Tim-537  
 Comment C16H15BrN4S3 mH 438.9714 calibrant added CH3CN

Acquisition Date 07.07.2022 16:59:13

Operator BDAL@DE  
 Instrument / Ser# micrOTOF 10248

## Acquisition Parameter

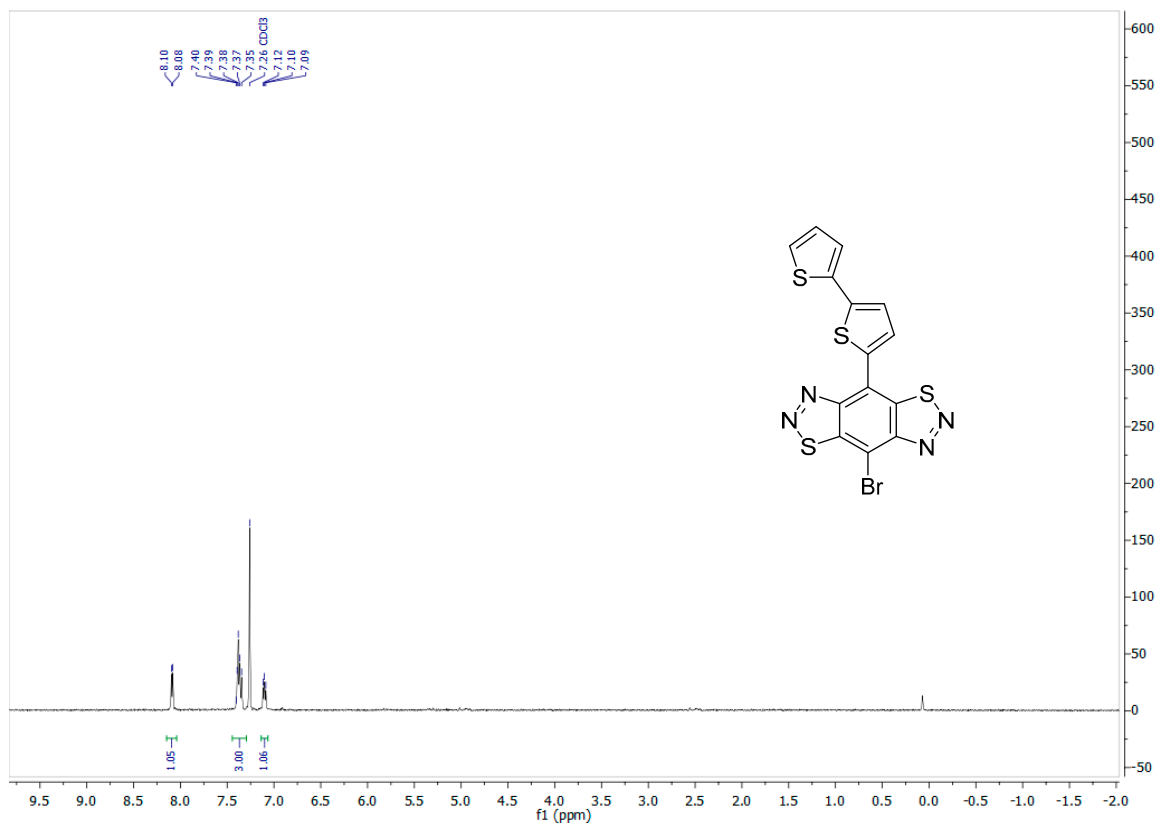
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



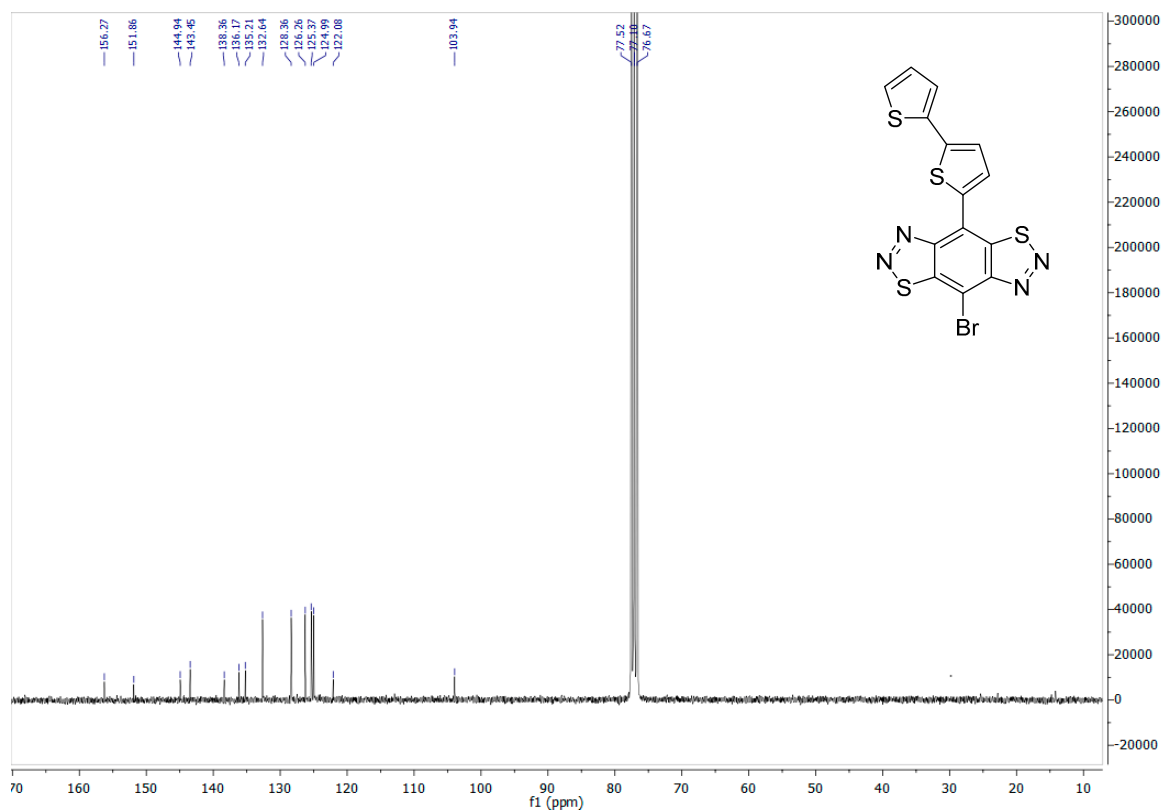


4-([2,2'-Bithiophen]-5-yl)-8-bromobenzo[1,2-d:4,5-d']bis([1,2,3]thiadiazole) (18c)

$^1\text{H}$  NMR (300 MHz)



$^{13}\text{C}$  NMR (75 MHz)



# Display Report

## Analysis Info

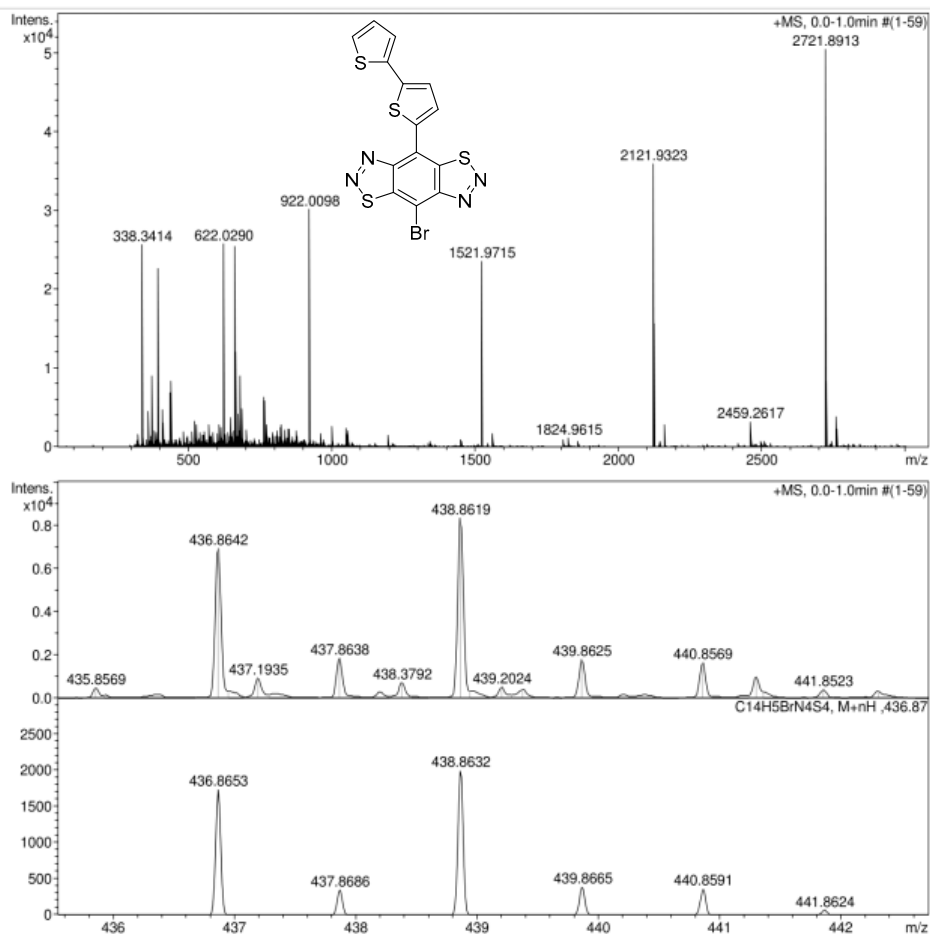
Analysis Name D:\Data\Chizhov\Rakitin\Chmovzh\tim-535\_&clb.d  
 Method tune\_wide.m  
 Sample Name /SUSU Tim-535  
 Comment CH3CN 100 %, dil. 20, calibrant added

Acquisition Date 29.06.2022 11:45:24

Operator BDAL@DE  
 Instrument / Ser# micrOTOF 10248

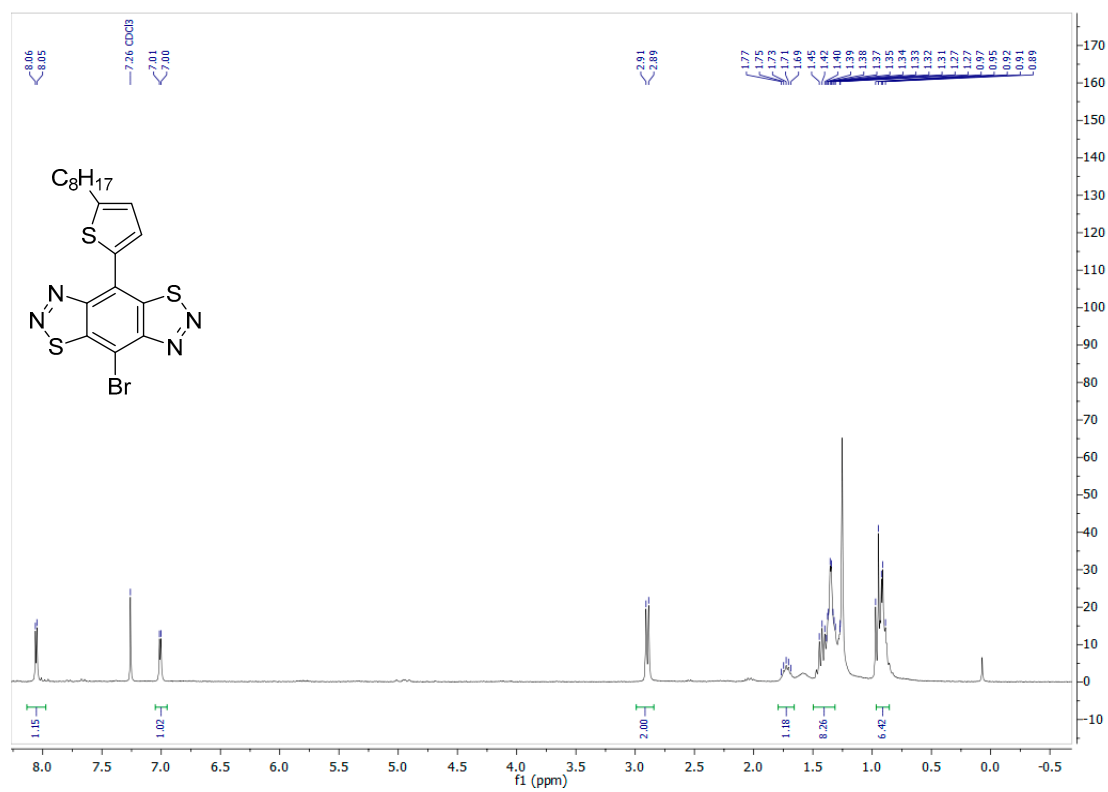
## Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

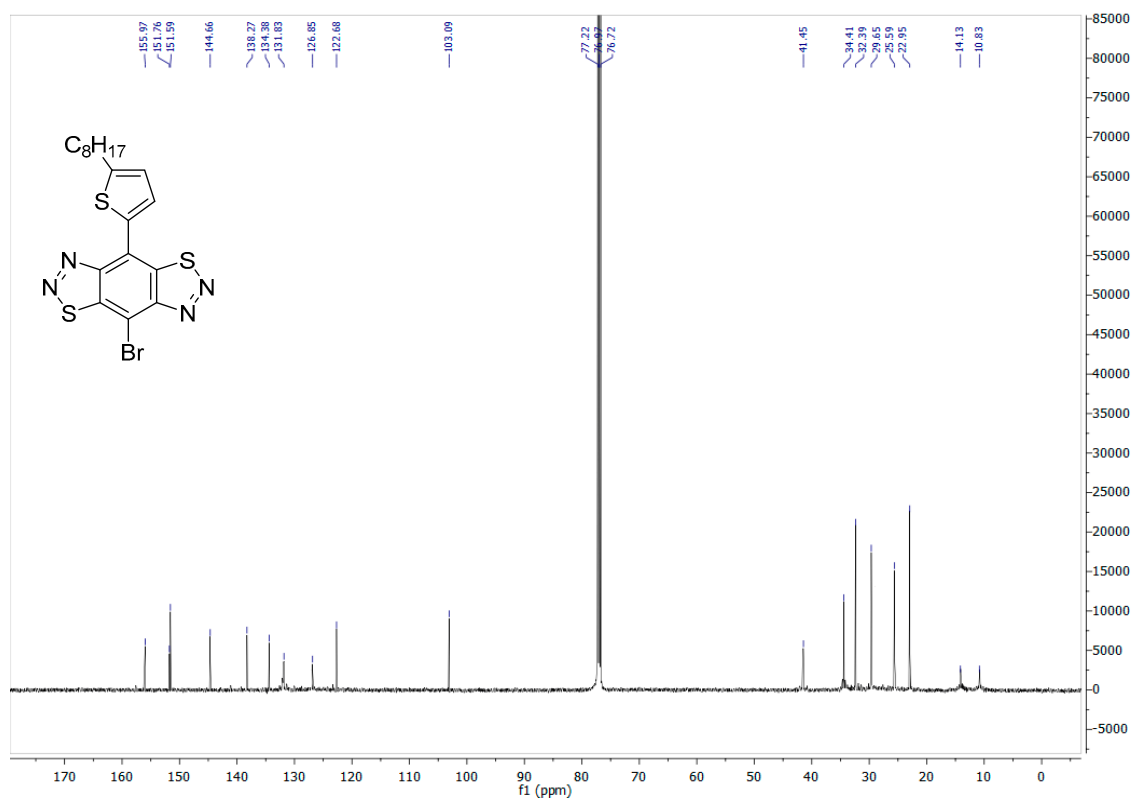


**4-Bromo-8-(5-(2-ethylhexyl)thiophen-2-yl)benzo[1,2-d:4,5-d']bis([1,2,3]thiadiazole)  
(18d)**

**<sup>1</sup>H NMR (300 MHz)**



**<sup>13</sup>C NMR(75 MHz)**



# Display Report

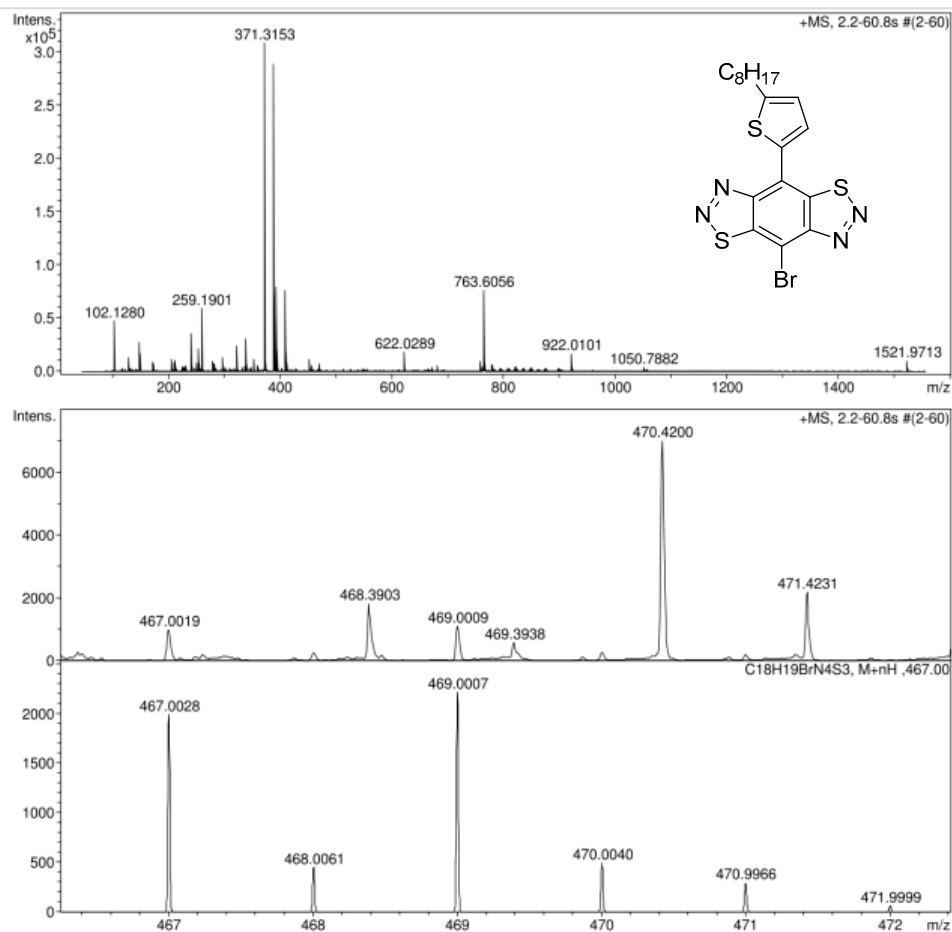
## Analysis Info

Analysis Name D:\Data\Chizhov\Miscellaneous\Rakitin\Chmovzh\tim-549\_&clblow.d  
 Method tune\_low\_1550.m  
 Sample Name /SUSU Tim-549  
 Comment CH3CN 100 %, dil. 20, calibrant added

Acquisition Date 25.08.2022 15:40:33  
 Operator BDAL@DE  
 Instrument / Ser# maXis 43

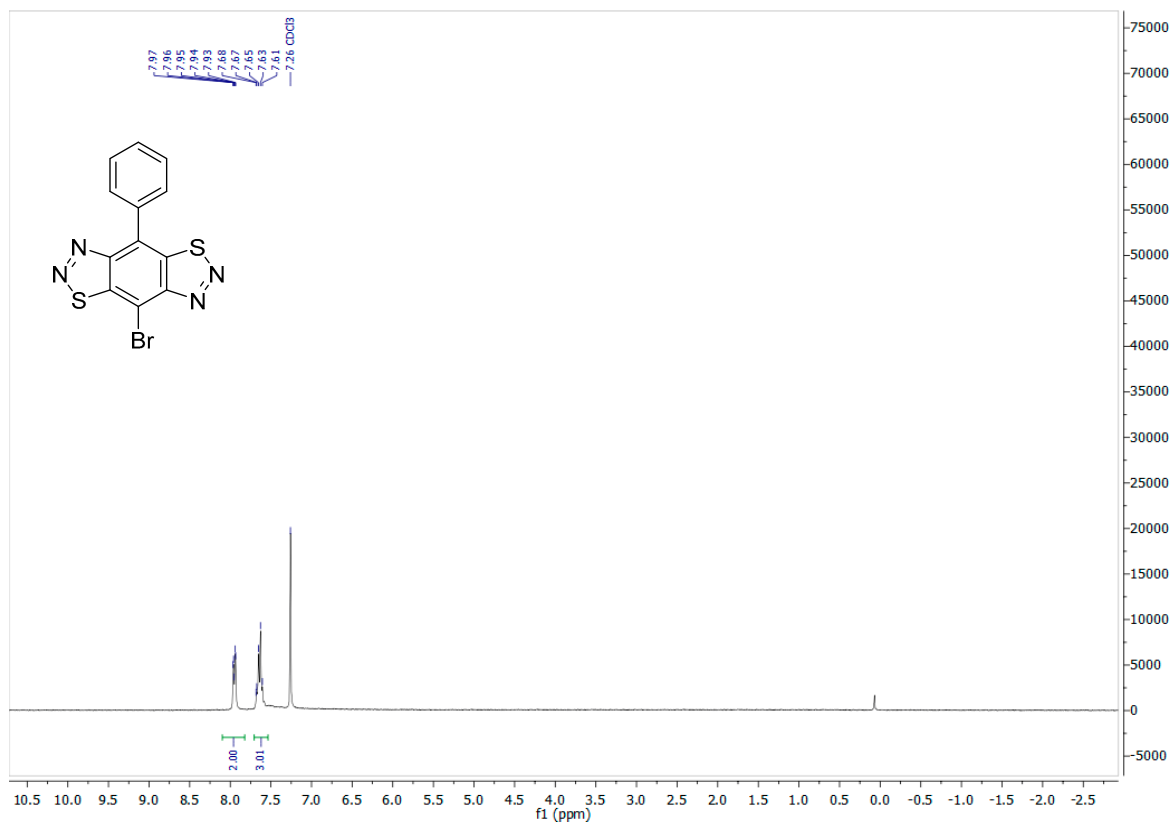
## Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1550 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

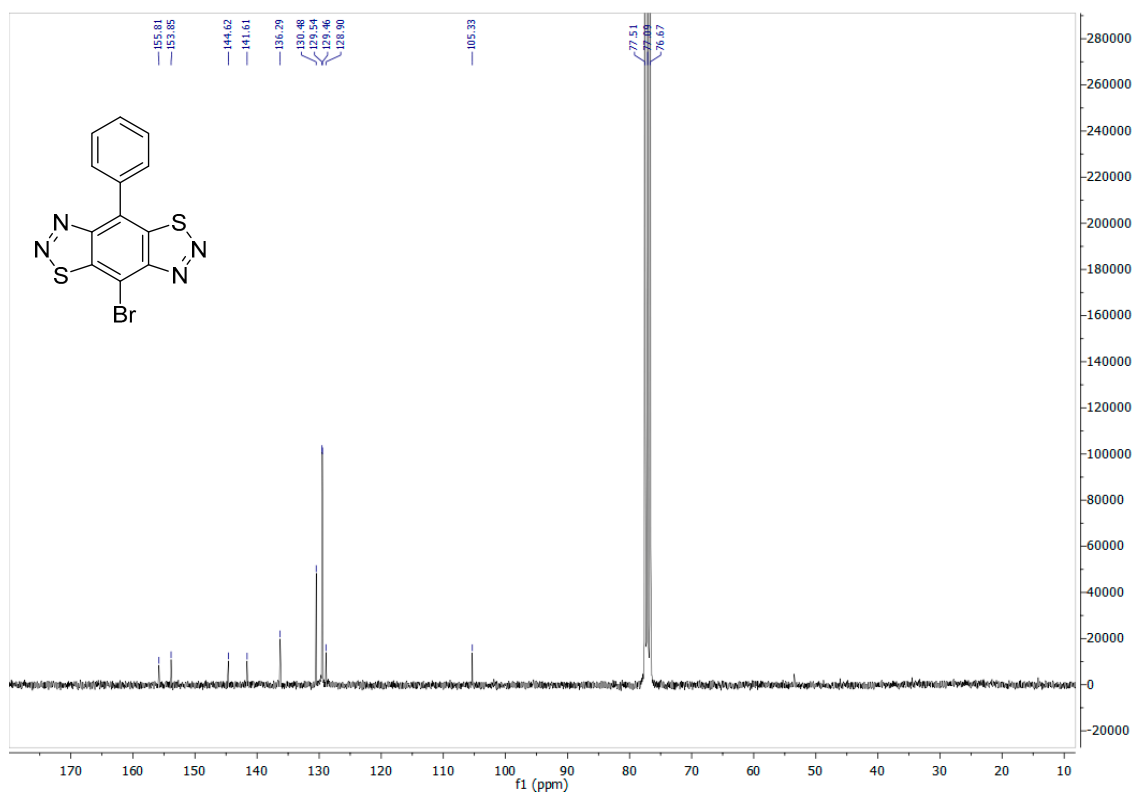


**4-Bromo-8-phenylbenzo[1,2-d:4,5-d']bis([1,2,3]thiadiazole) (18e)**

**$^1\text{H}$  NMR (300 MHz)**



**$^{13}\text{C}$  NMR (75 MHz)**



# Display Report

## Analysis Info

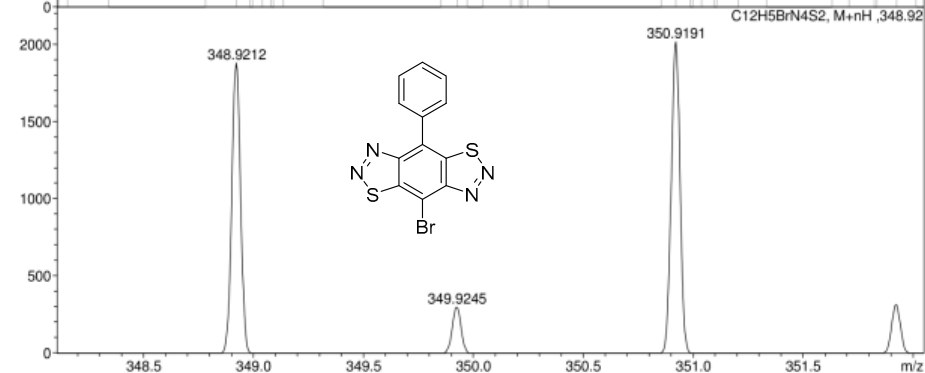
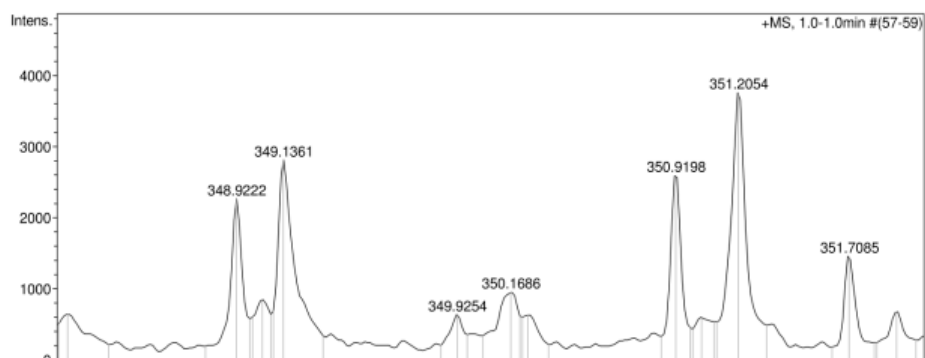
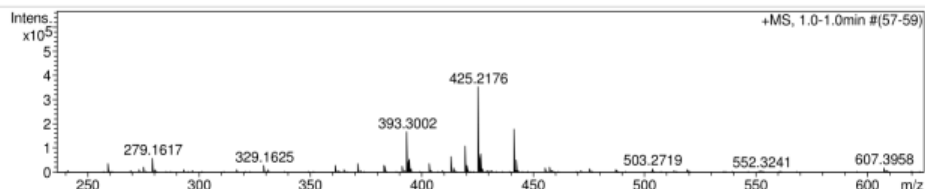
Analysis Name D:\Data\Kolotyrykina\2022\Chmovsh\0921004.d  
 Method tune\_50-1600\_pos\_15\_12.m  
 Sample Name /SUSU Tim-556  
 Comment C12H5BrN4S2 mH 348.9211 calibrant added CH3OH

Acquisition Date 21.09.2022 10:25:32

Operator BDAL@DE  
 Instrument / Ser# micrOTOF 10248

## Acquisition Parameter

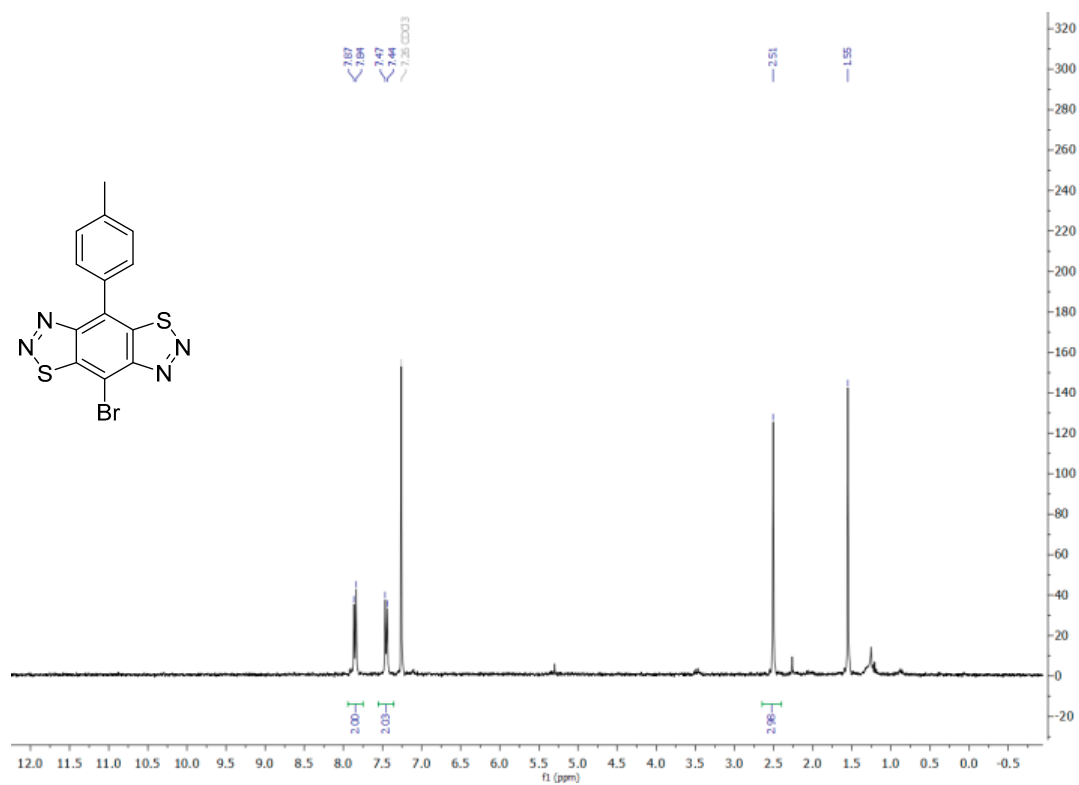
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



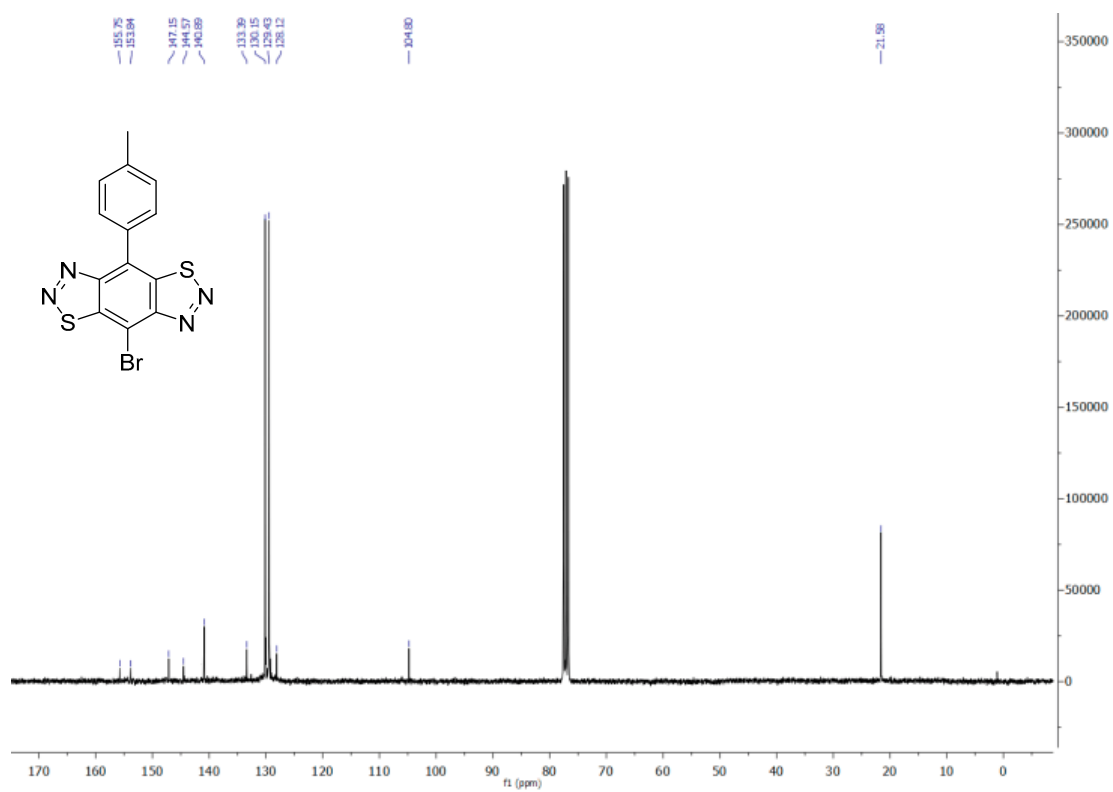


**8-Bromo-4-(p-tolyl)benzo[1,2-d:5,4-d']bis([1,2,3]thiadiazole) (18f)**

**$^1\text{H}$  NMR (300 MHz)**



**$^{13}\text{C}$  NMR (75 MHz)**



## Display Report

### Analysis Info

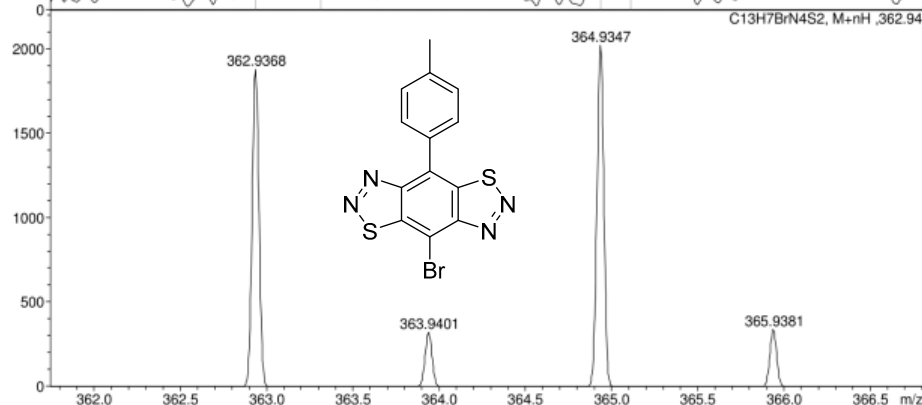
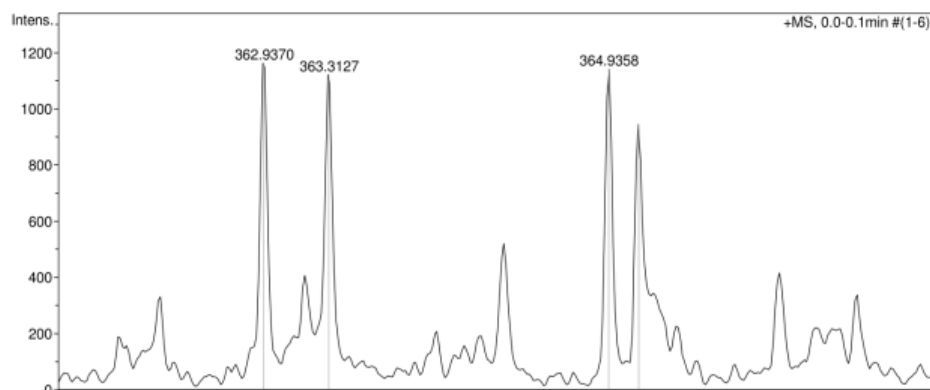
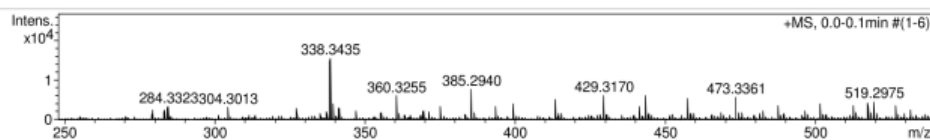
Analysis Name D:\Data\Kolotyrkina\2022\Chmovsh\0915007.d  
Method tune\_50-1600\_pos\_15\_12.m  
Sample Name /SUSU Tim-553  
Comment C13H7BrN4S2 mH 362.9368 calibrant added CH3CN

Acquisition Date 15.09.2022 13:26:12

Operator BDAL@DE  
Instrument / Ser# micrOTOF 10248

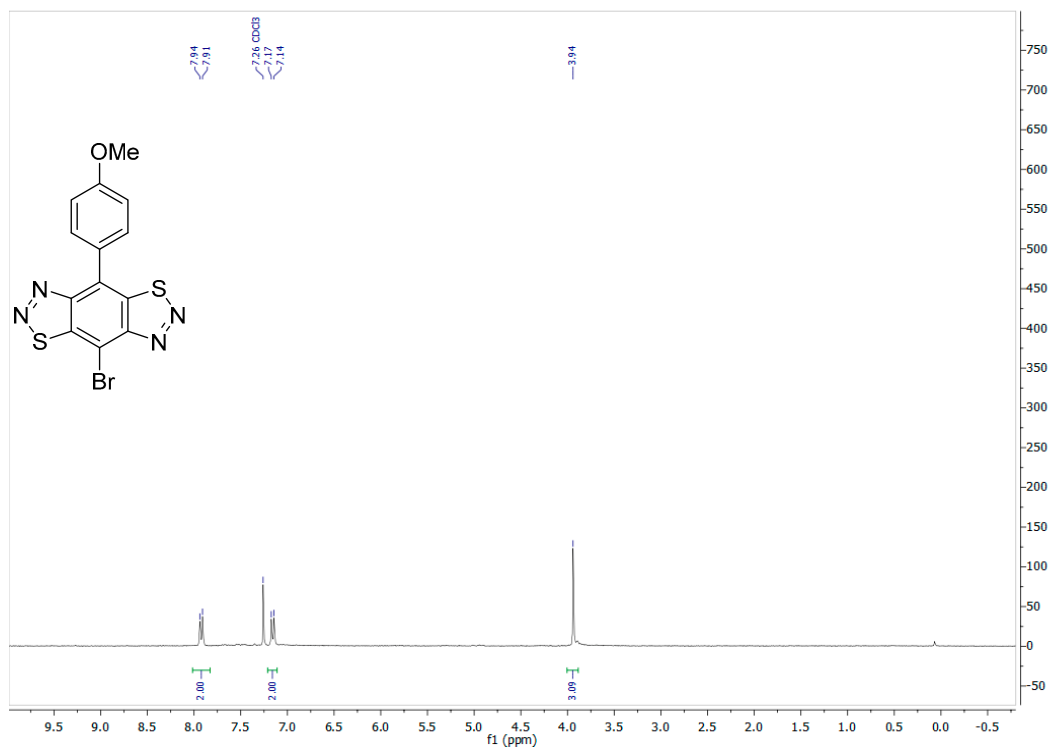
### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

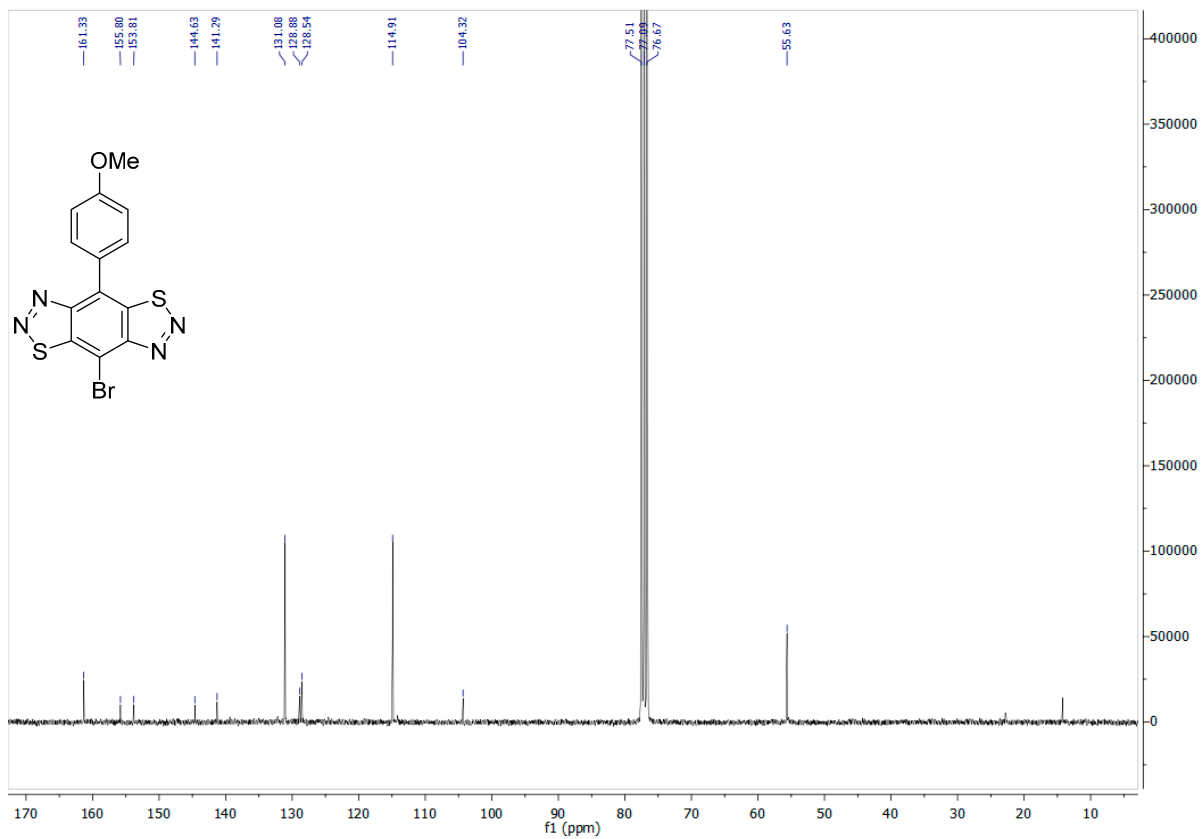


# 4-Bromo-8-(4-methoxyphenyl)benzo[1,2-d:4,5-d']bis([1,2,3]thiadiazole) (18g)

$^1\text{H}$  NMR (300 MHz)



$^{13}\text{C}$  NMR (75 MHz)



## Display Report

### Analysis Info

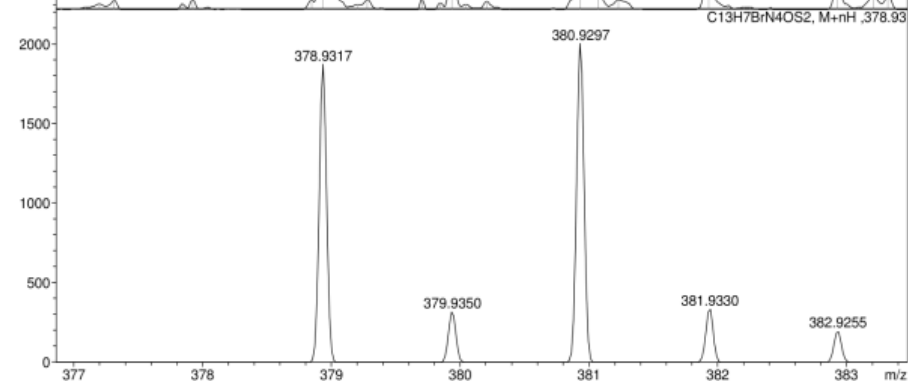
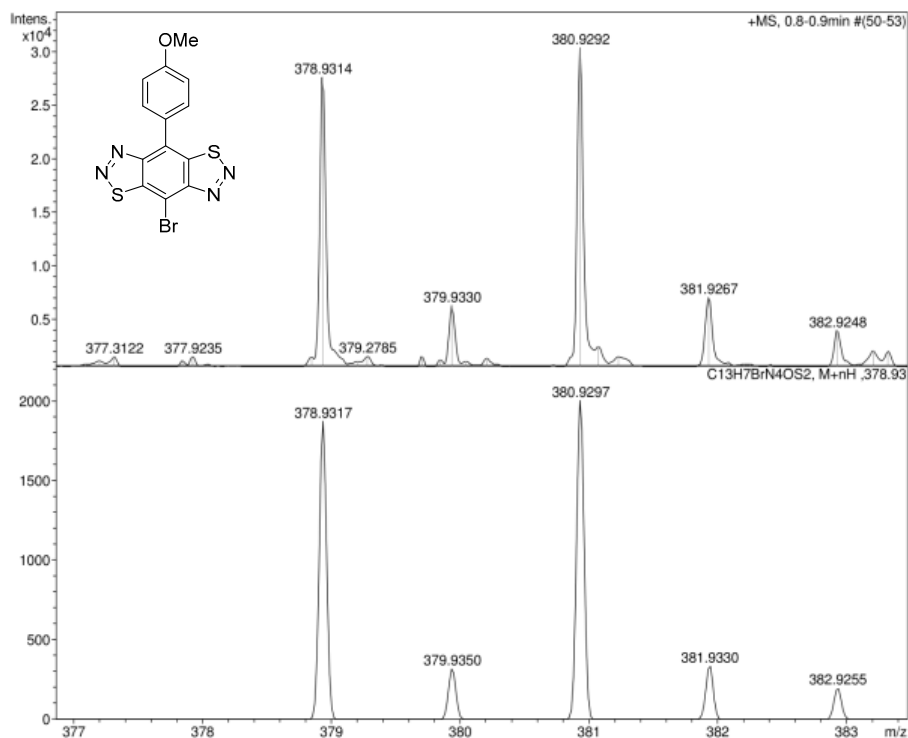
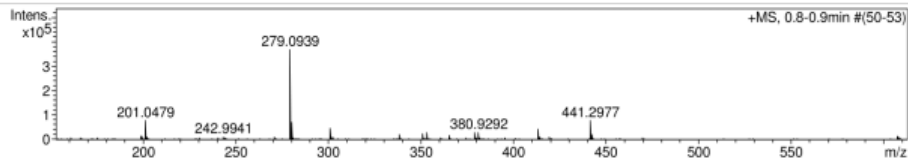
Analysis Name D:\Data\Kolotyrkina\2022\Chmovsh\1004026.d  
Method tune\_50-1600\_pos\_15\_12.m  
Sample Name /SUSU Tim-558  
Comment C13H7BrN4OS2 mH 378.9317 clb added CH3CN

Acquisition Date 04.10.2022 19:31:48

Operator BDAL@DE  
Instrument / Ser# micrOTOF 10248

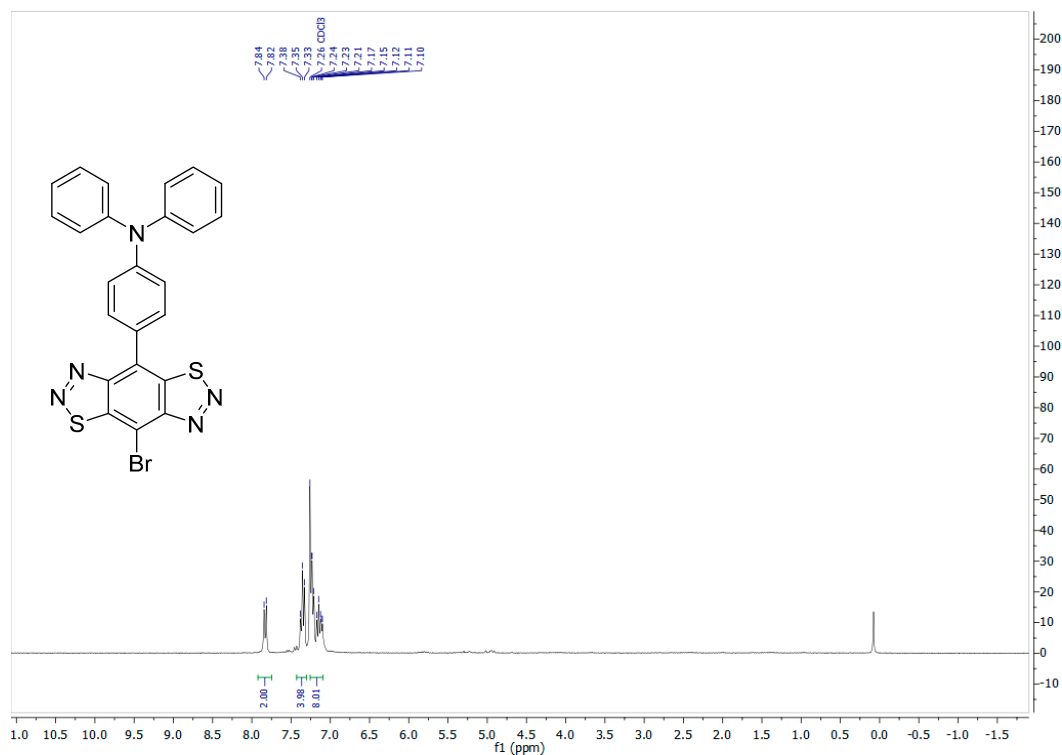
### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

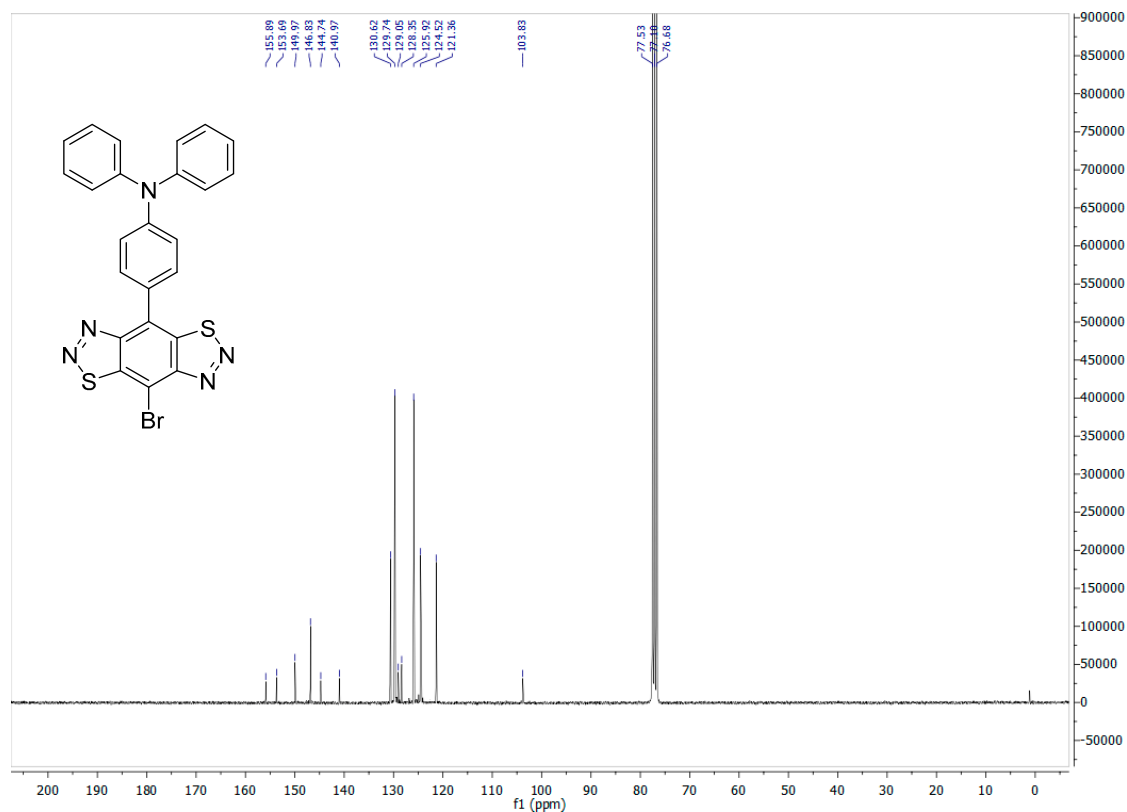


# 4-(8-Bromobenzo[1,2-d:4,5-d']bis([1,2,3]thiadiazole)-4-yl)-N,N-diphenylaniline (18h)

<sup>1</sup>H NMR (300 MHz)



<sup>13</sup>C NMR (75 MHz)



## Display Report

### Analysis Info

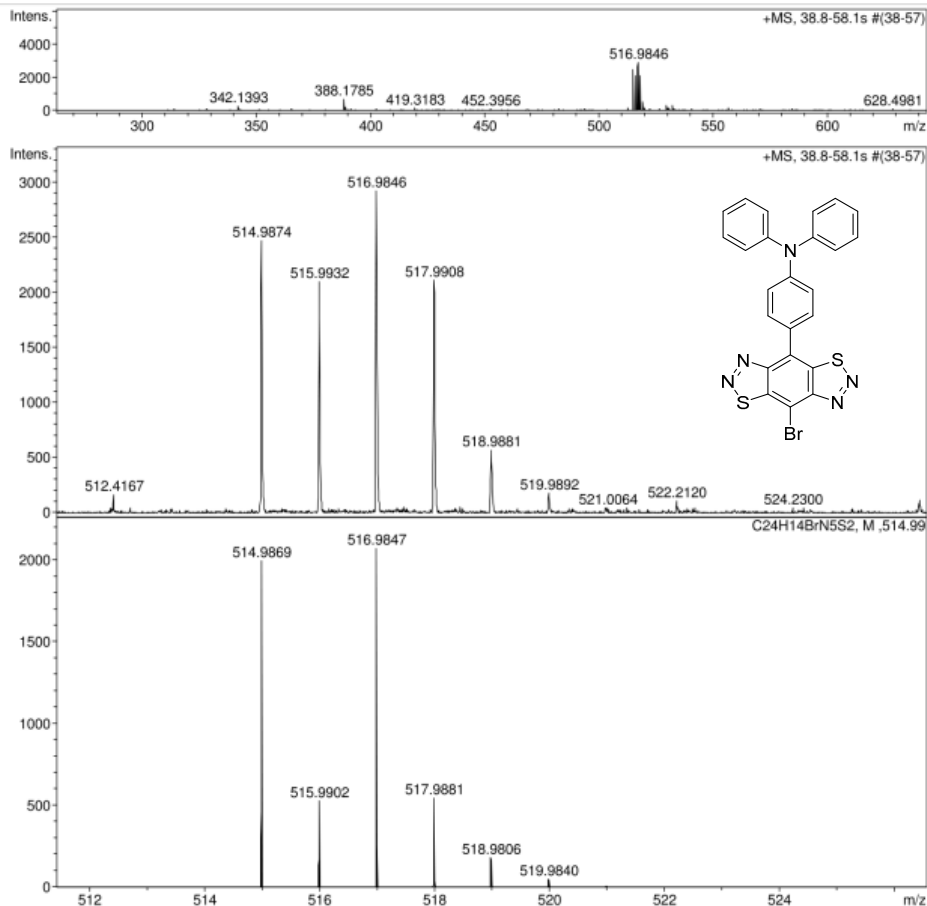
Analysis Name D:\Data\Kolotyorkina\2022\Chmovsh\0728022.d  
 Method tune\_wide.m  
 Sample Name /SUSU Tim-546  
 Comment C24H14BrN5S2 mH 515.9946 clb added CH3CN

Acquisition Date 28.07.2022 15:44:25

Operator BDAL@DE  
 Instrument / Ser# maXis 43

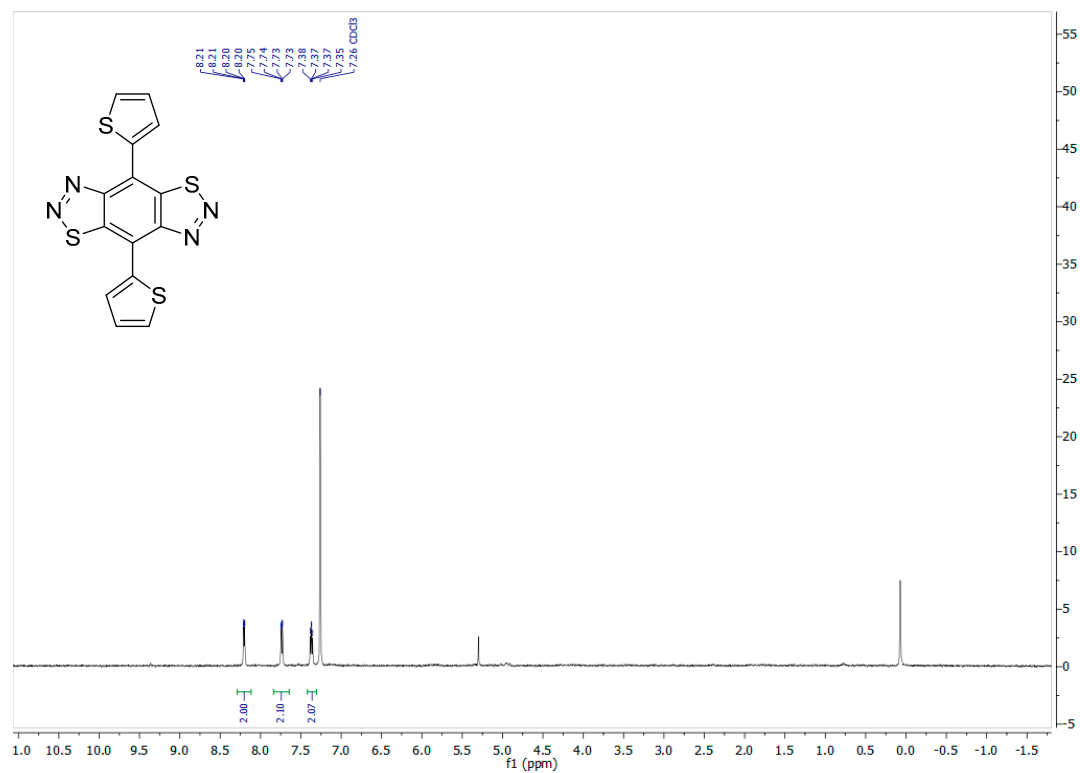
### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



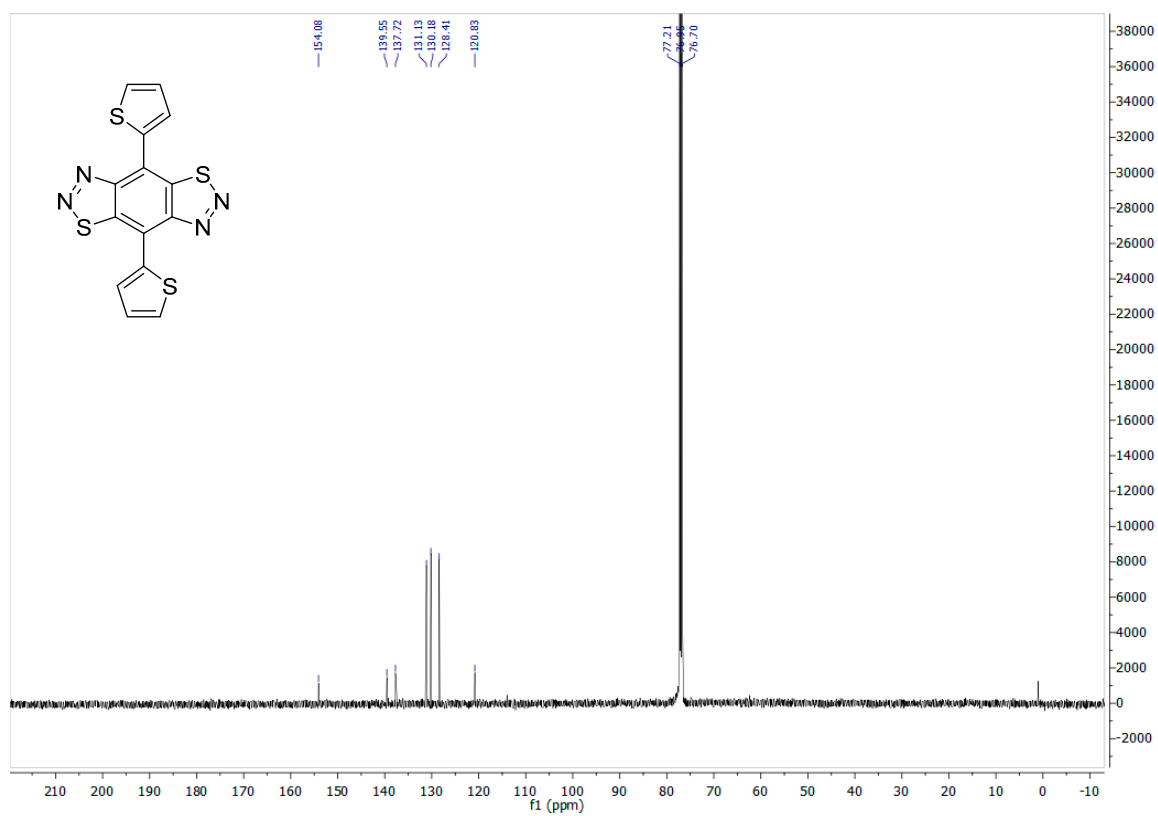
**4,8-Di(thiophen-2-yl)benzo[1,2-d:4,5-d']bis([1,2,3]thiadiazole) (19a)**

**$^1\text{H}$  NMR (300 MHz)**



**$^{13}\text{C}$  NMR(75 MHz)**





## Display Report

### Analysis Info

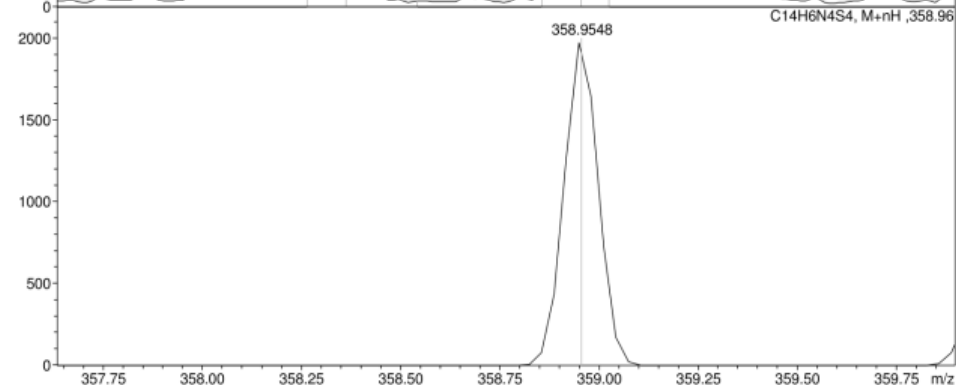
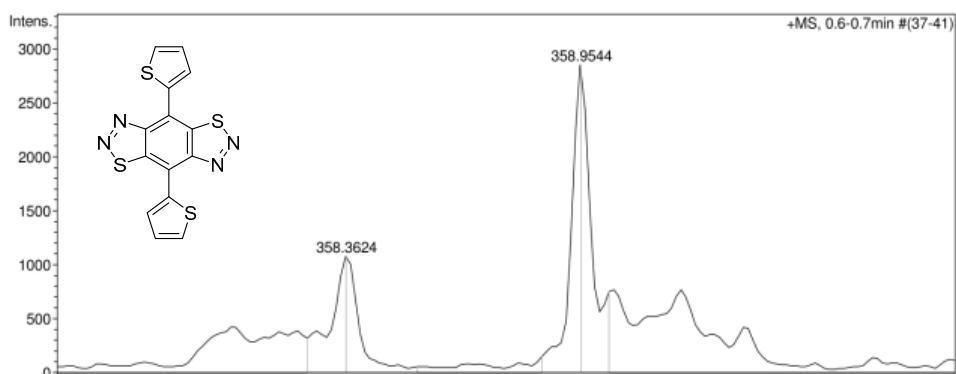
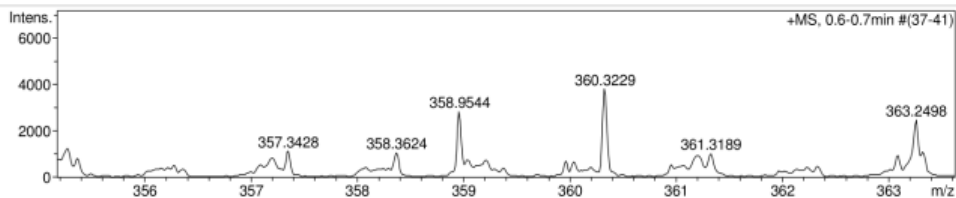
Analysis Name D:\Data\Kolotyrkina\2022\Chmovsh\0413003.d  
Method tune\_50-1600\_pos\_15\_12.m  
Sample Name /SUSU Tim-519  
Comment C14H6N4S4 mH 358.9548 clb added CH3CN

Acquisition Date 13.04.2022 10:32:53

Operator BDAL@DE  
Instrument / Ser# micrOTOF 10248

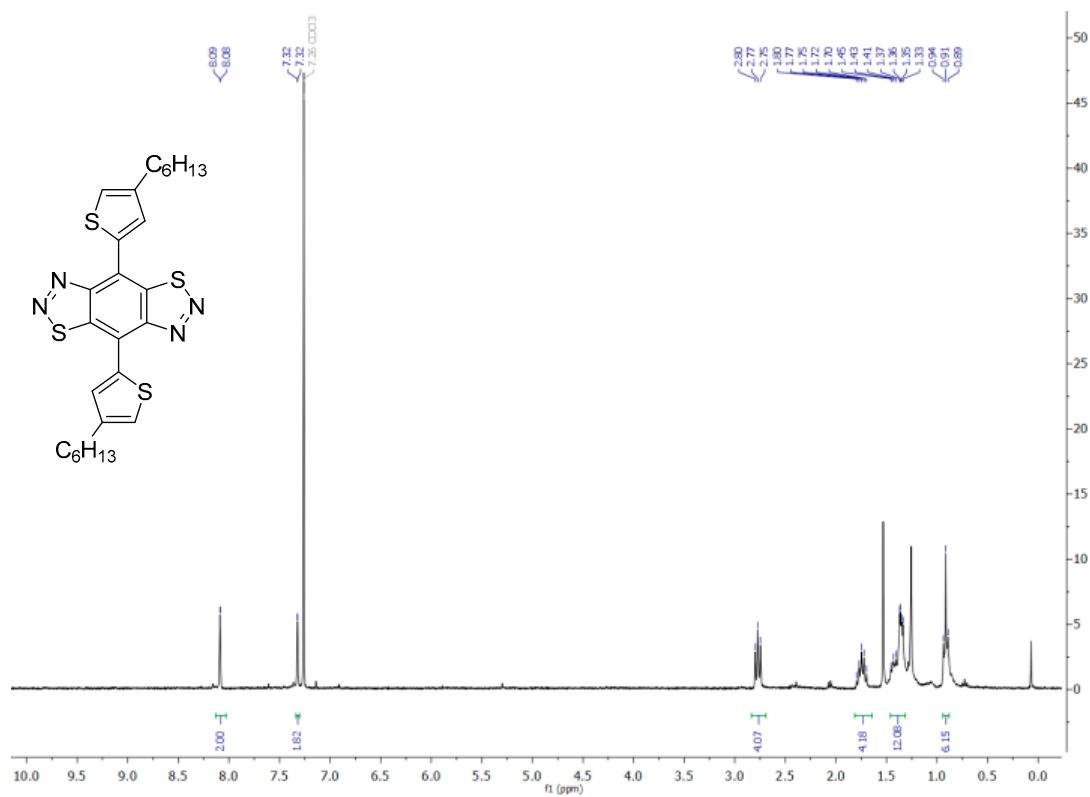
### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

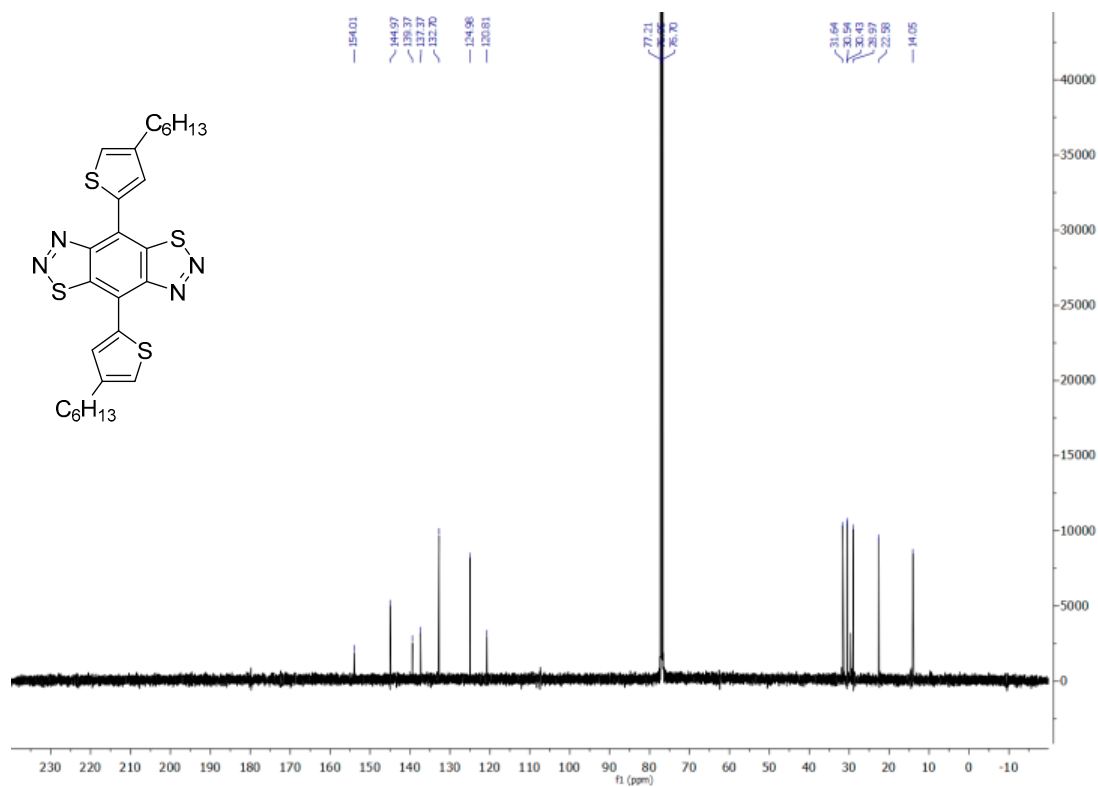


**4,8-Bis(4-hexylthiophen-2-yl)benzo[1,2-d:4,5-d']bis([1,2,3]thiadiazole) (19b)**

**<sup>1</sup>H NMR (300 MHz)**



**<sup>13</sup>C NMR (75 MHz)**



# Display Report

## Analysis Info

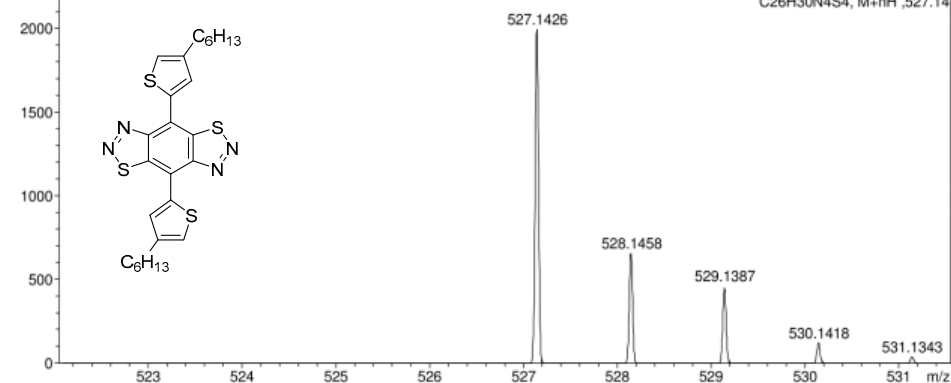
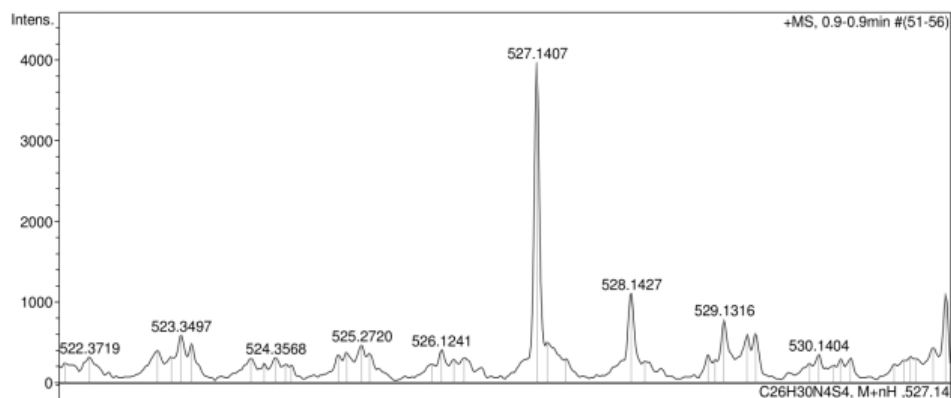
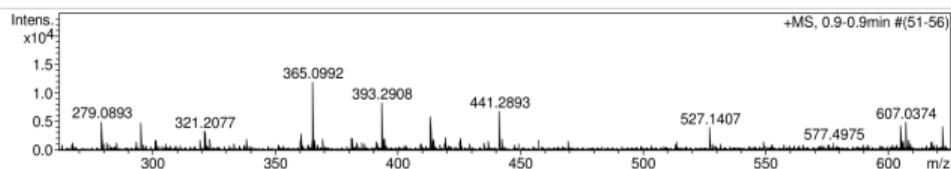
Analysis Name D:\Data\Kolotyrkina\2022\Chmovsh\0324040.d  
 Method tune\_50-1600\_pos\_15\_12.m  
 Sample Name /SUSU Tim-517  
 Comment C26H30N4S4 mH 527.1426 calibrant added CN3CN

Acquisition Date 24.03.2022 19:08:23

Operator BDAL@DE  
 Instrument / Ser# microTOF 10248

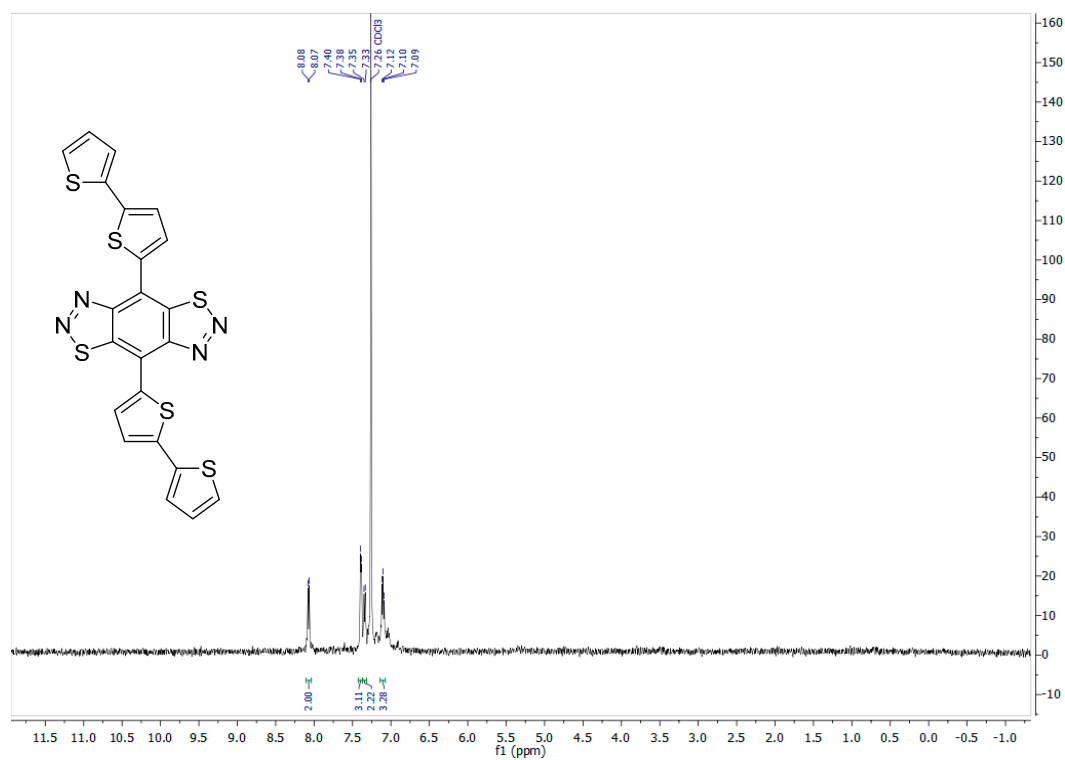
## Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

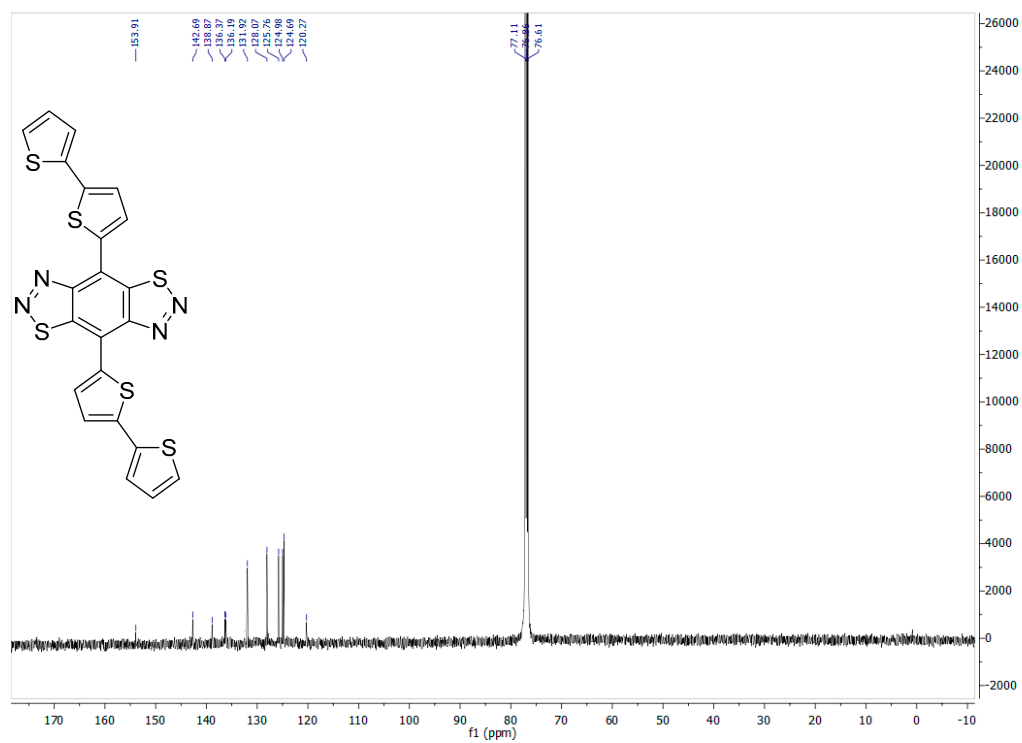


# 4,8-Di([2,2'-bithiophen]-5-yl)benzo[1,2-d:4,5-d']bis([1,2,3]thiadiazole) (19c)

<sup>1</sup>H NMR (300 MHz)



<sup>13</sup>C NMR (75 MHz)



## Display Report

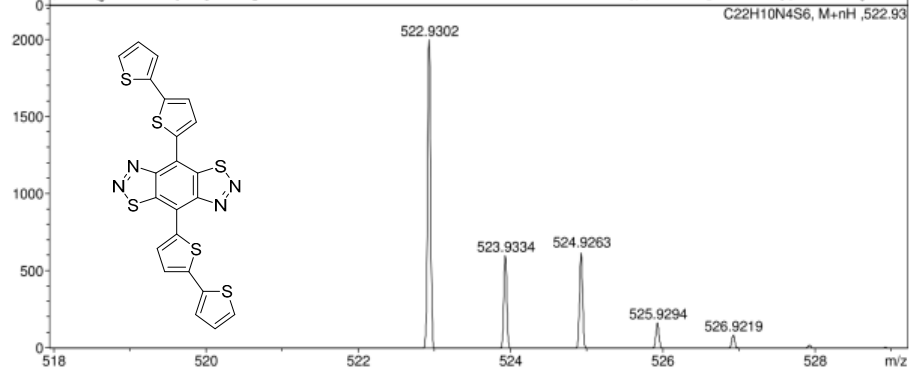
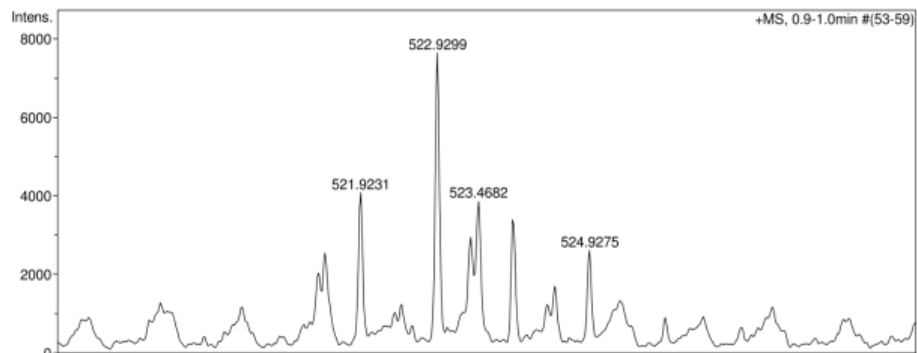
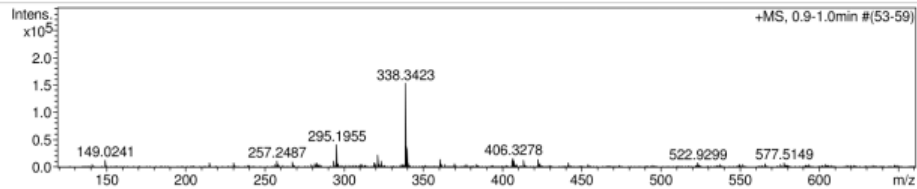
### Analysis Info

Analysis Name D:\Data\Kolotyrkina\2022\Chmovsh\0920003.d  
Method tune\_50-1600\_pos\_15\_12.m  
Sample Name /SUSU Tim-555  
Comment C22H10N4S6 mH 522.9302 calibrant added CH3CN

Acquisition Date 20.09.2022 11:35:18  
Operator BDAL@DE  
Instrument / Ser# micrOTOF 10248

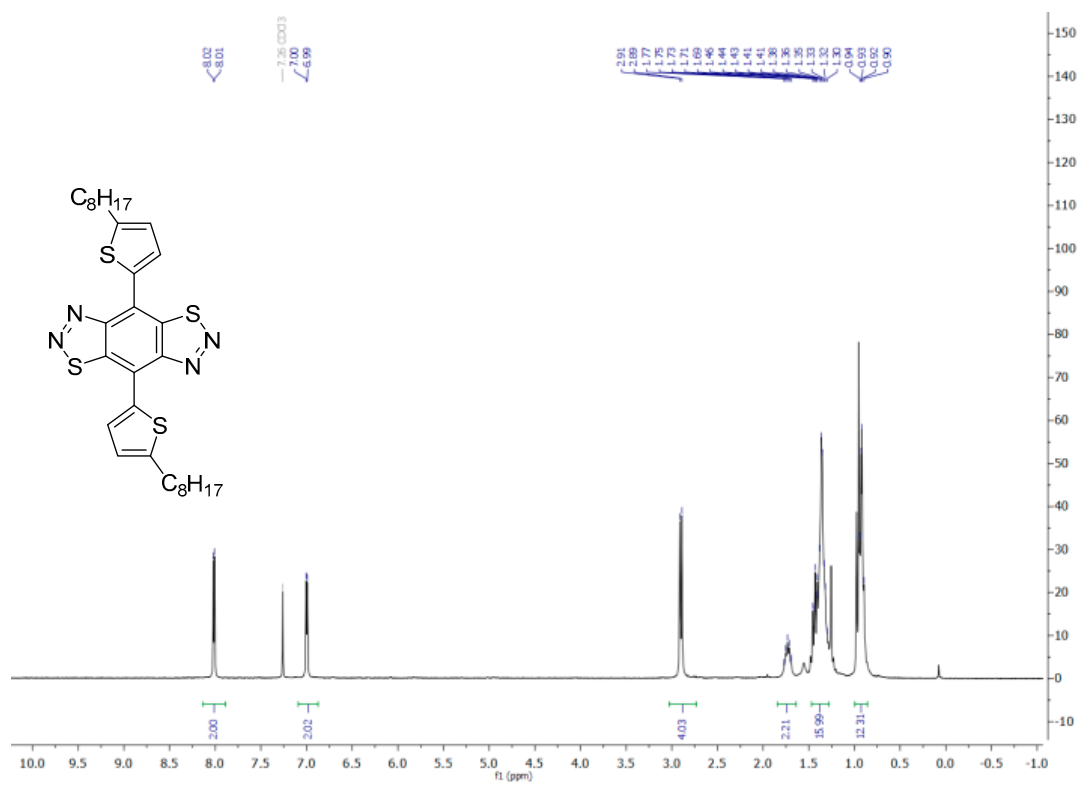
### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

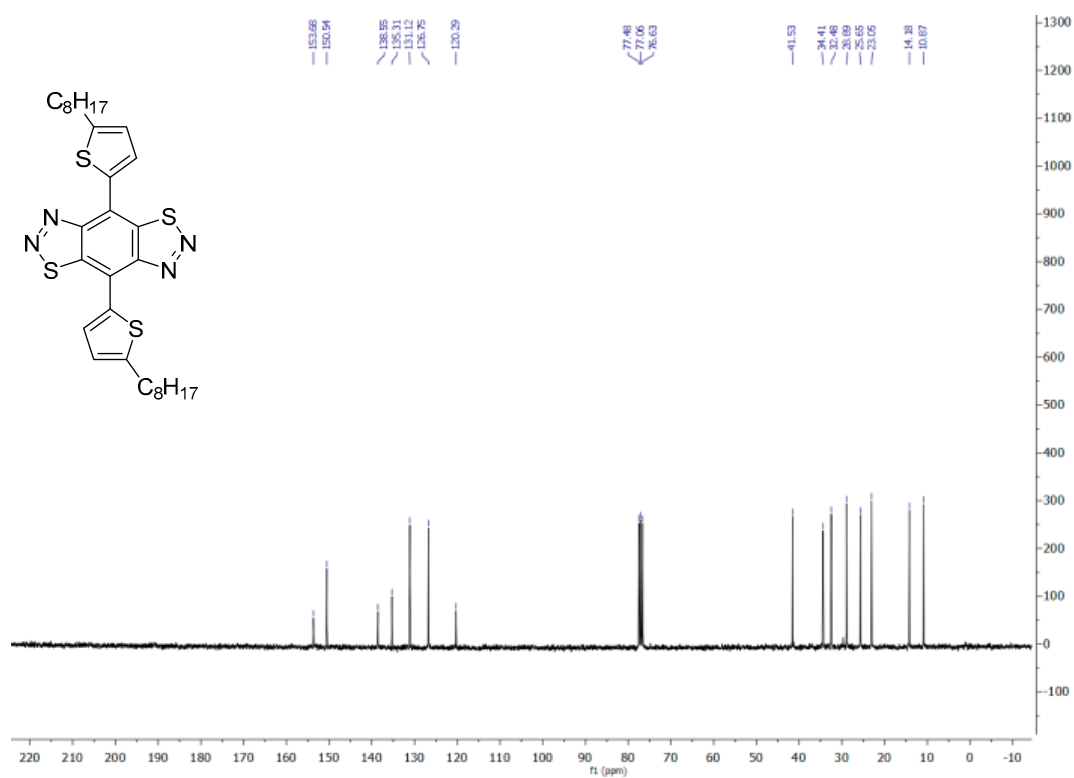


4,8-Bis(5-(2-ethylhexyl)thiophen-2-yl)benzo[1,2-d:4,5-d']bis([1,2,3]thiadiazole) (19d)

$^1\text{H}$  NMR (300 MHz)



$^{13}\text{C}$  NMR (75 MHz)





# Display Report

## Analysis Info

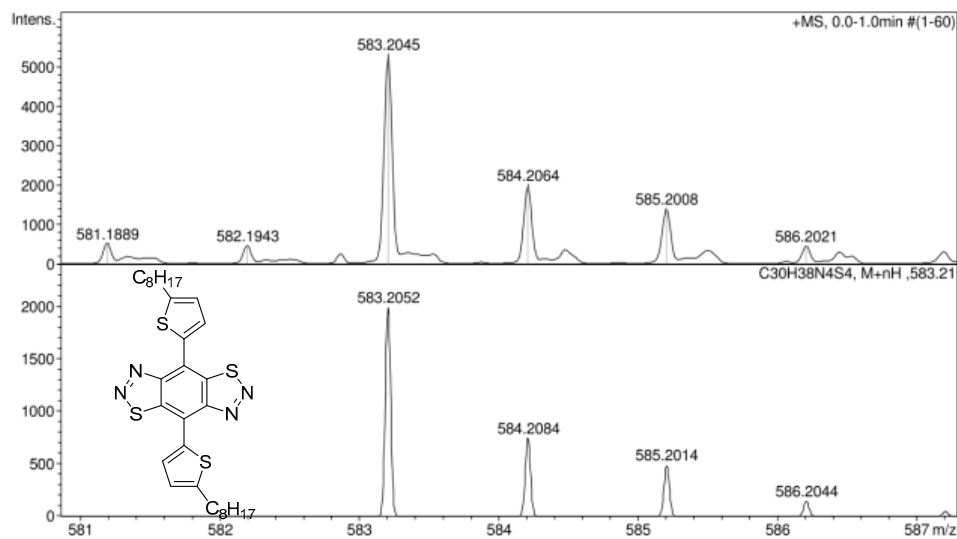
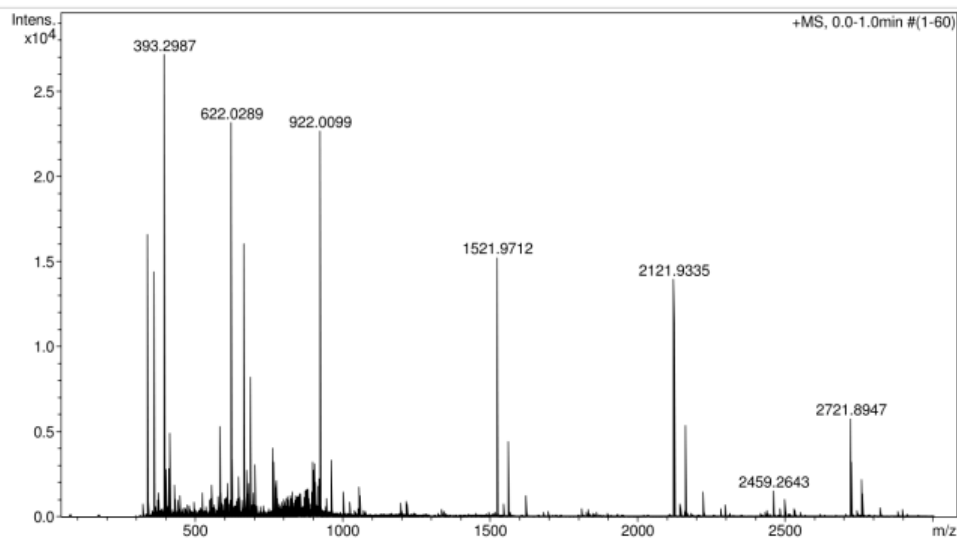
Analysis Name D:\Data\Chizhov\Rakitin\Chmovzh\tim-507\_&clb.d  
 Method tune\_wide.m  
 Sample Name /SUSU Tim-507  
 Comment CH3CN 100 %, dil. 200, calibrant added

Acquisition Date 01.02.2022 16:28:52

Operator BDAL@DE  
 Instrument / Ser# micrOTOF 10248

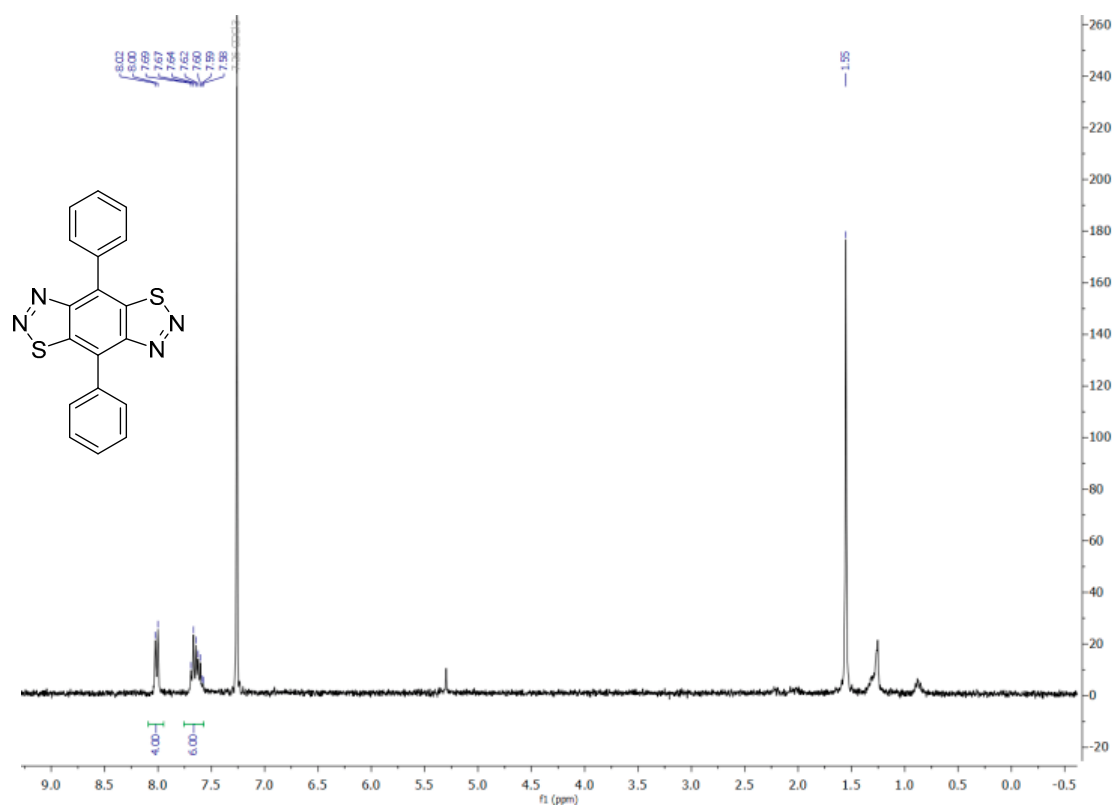
## Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

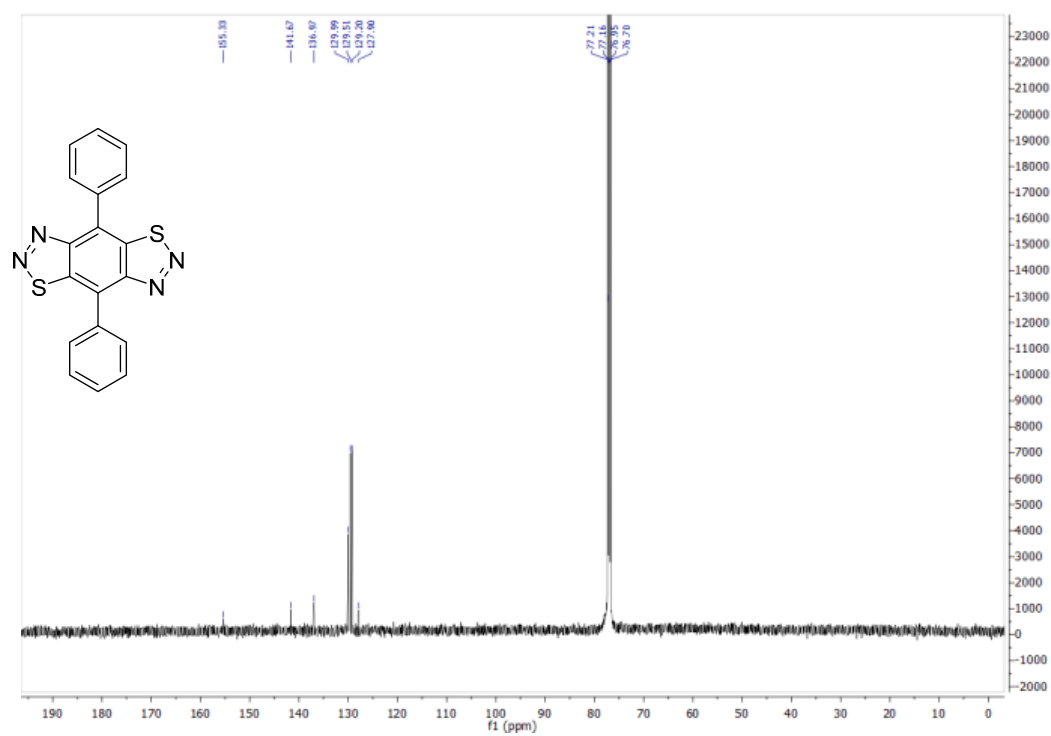


# 4,8-Diphenylbenzo[1,2-d:4,5-d']bis([1,2,3]thiadiazole) (19e)

<sup>1</sup>H NMR (300 MHz)



<sup>13</sup>C NMR(75 MHz)



# Display Report

## Analysis Info

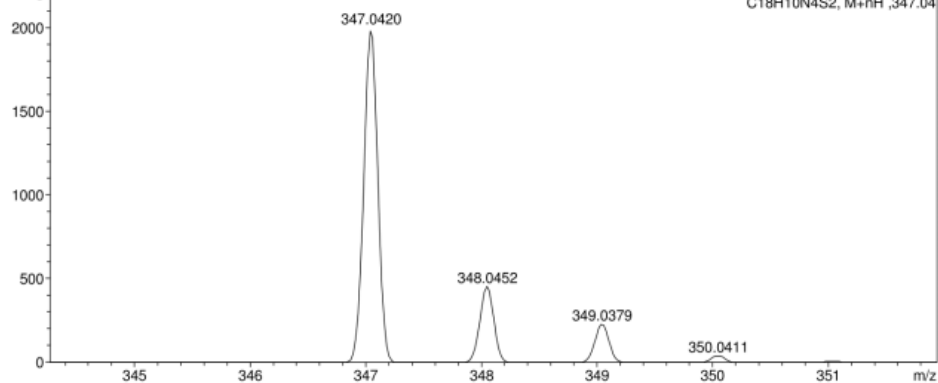
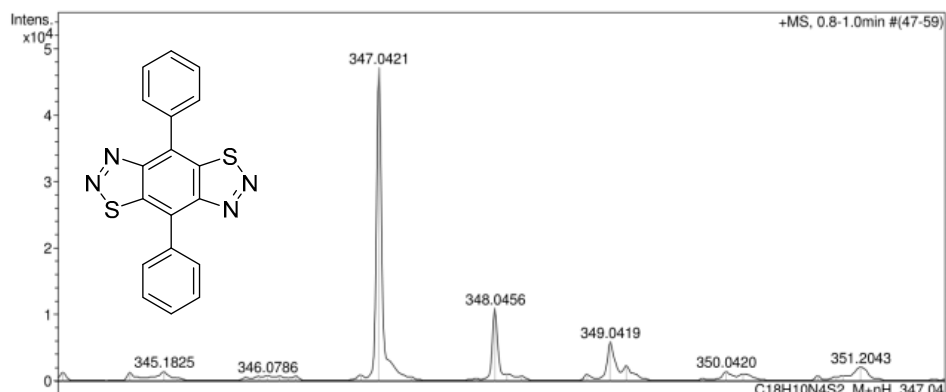
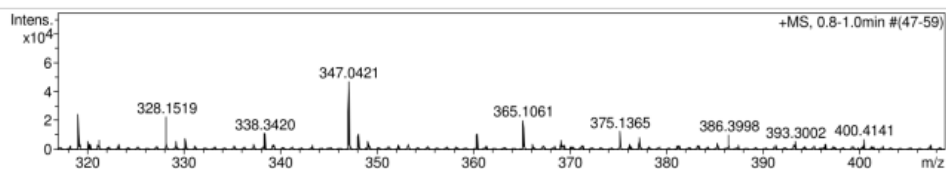
Analysis Name D:\Data\Kolotyrkina\2022\Chmovsh\0608028.d  
 Method tune\_50-1600\_pos\_15\_12.m  
 Sample Name /SUSU Tim-533  
 Comment C18H10N4S2 mH 347.0419 clb added CH3CN

Acquisition Date 08.06.2022 16:45:25

Operator BDAL@DE  
 Instrument / Ser# micrOTOF 10248

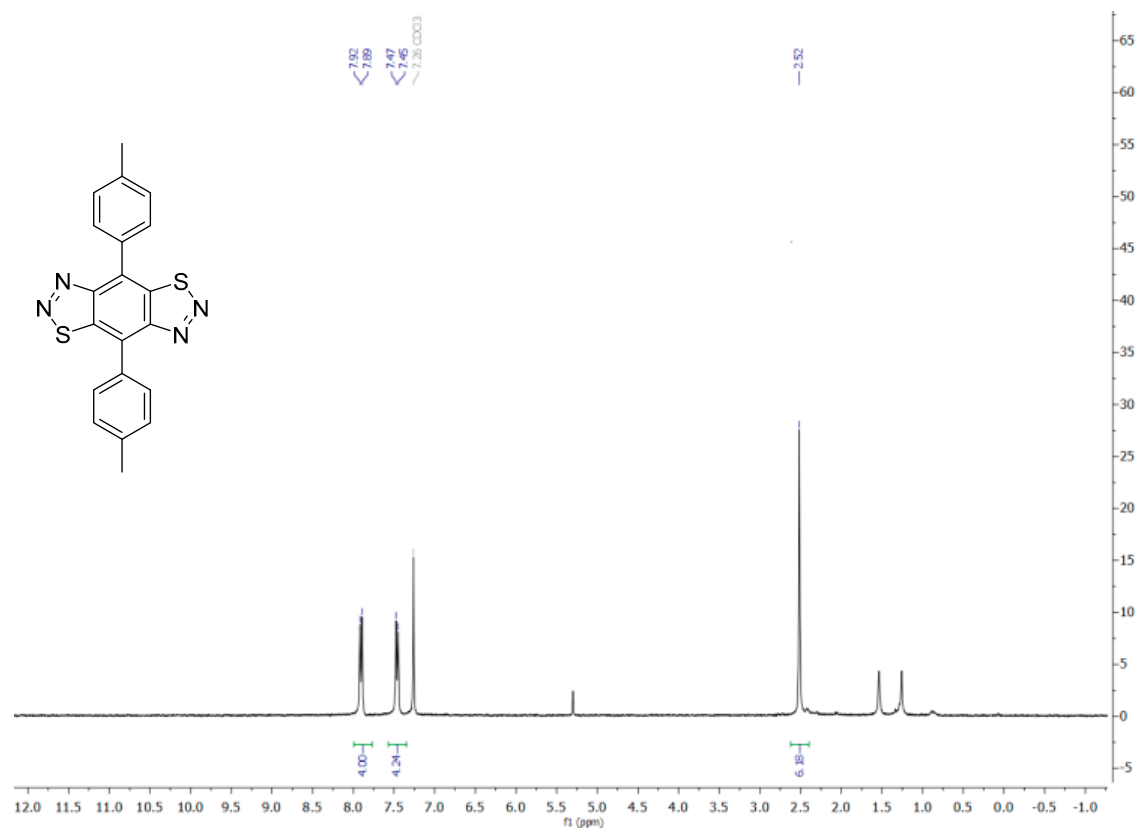
## Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

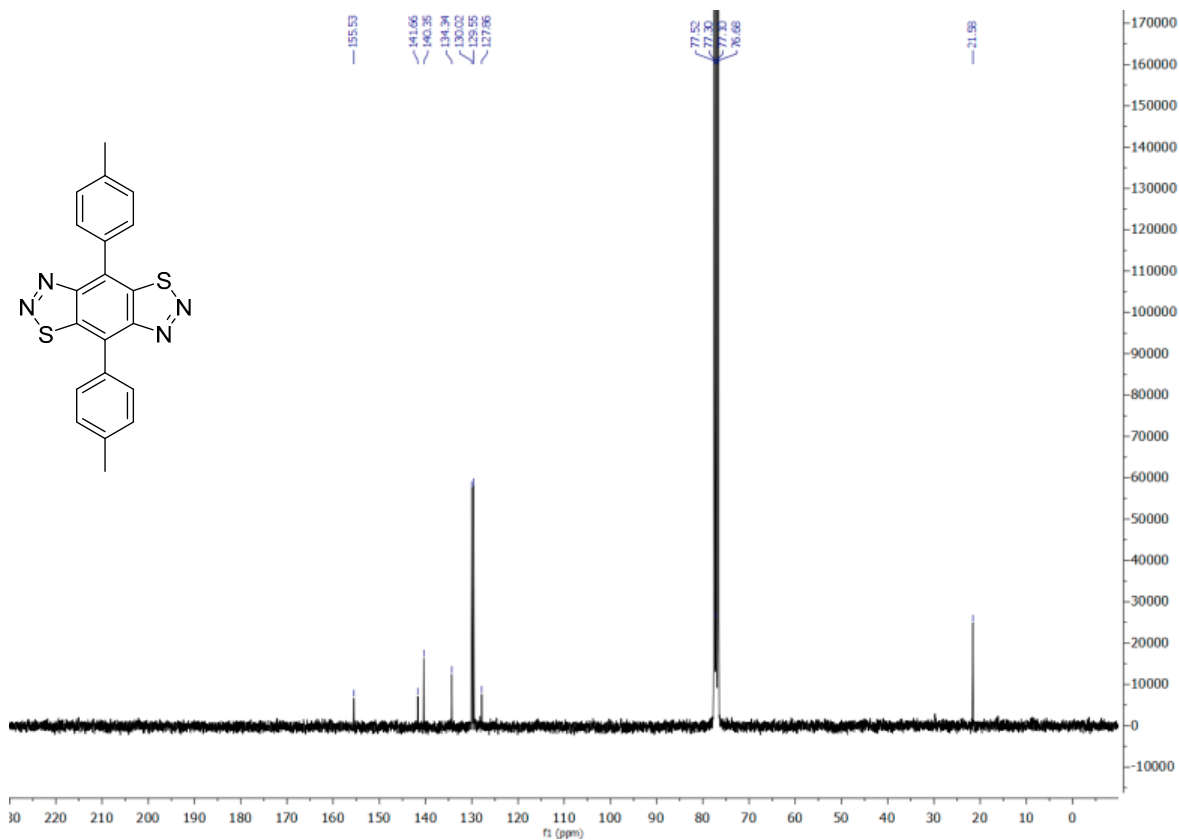


**4,8-Di-p-tolylbenzo[1,2-d:4,5-d']bis([1,2,3]thiadiazole) (19f)**

**$^1\text{H}$  NMR (300 MHz)**



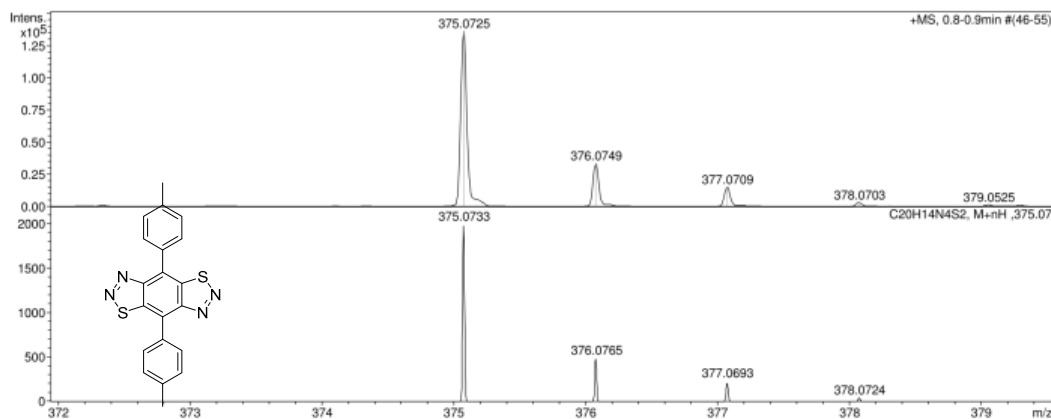
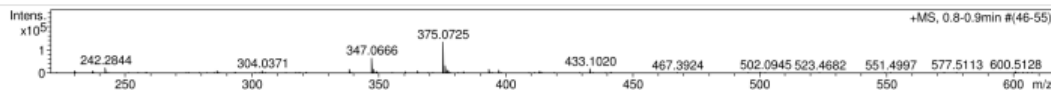
**$^{13}\text{C}$  NMR (75 MHz)**



## Display Report

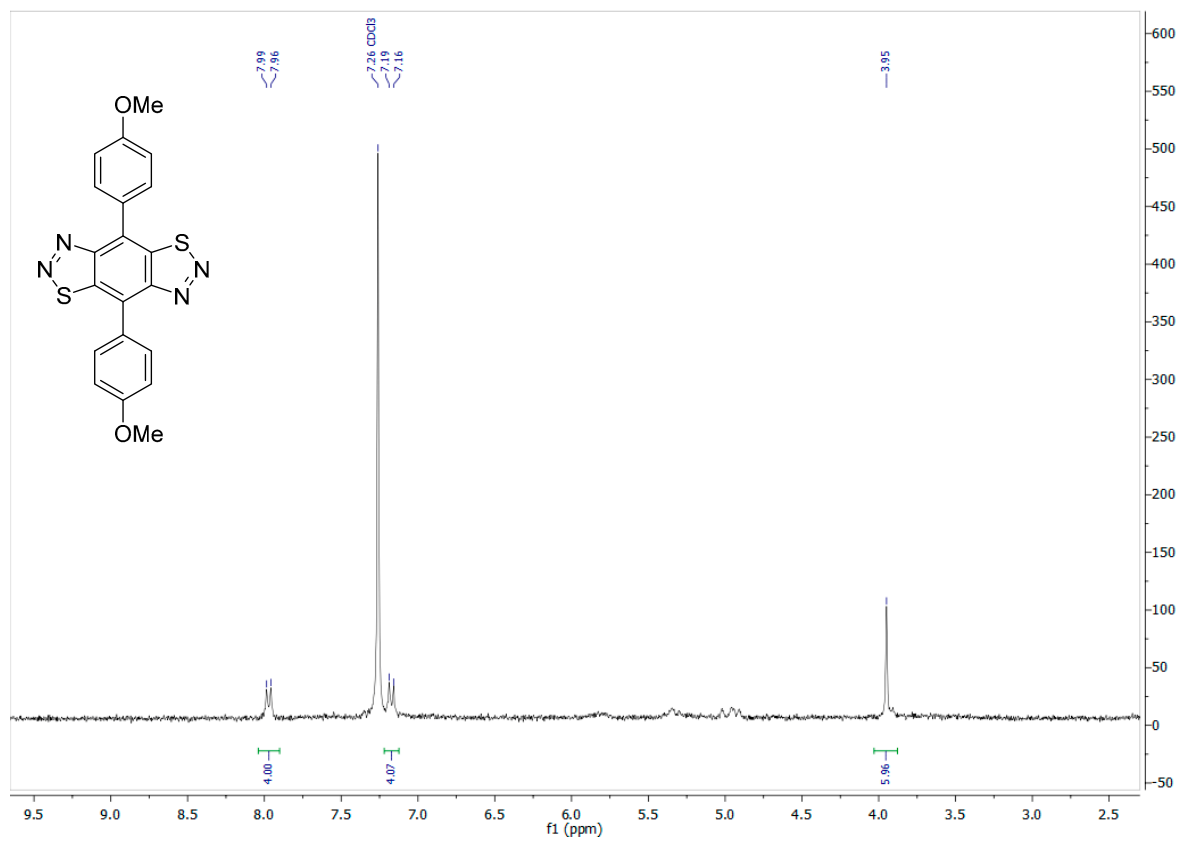
<b>Analysis Info</b>		Acquisition Date	30.03.2022 10:00:29
Analysis Name	D:\Data\Kolotyarkina\2022\Chmovsh\0330001.d	Operator	BDAL@DE
Method	tune_50-1600_pos_15_12.m	Instrument / Ser#	micrOTOF 10248
Sample Name	/SUSU Tim-518		
Comment	C20H14N4S2 mH 375.0732 calibrant added CH3CN		

<b>Acquisition Parameter</b>					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



**4,8-Bis(4-methoxyphenyl)benzo[1,2-d:4,5-d']bis([1,2,3]thiadiazole) (19g)**

**<sup>1</sup>H NMR (300 MHz)**



# Display Report

## Analysis Info

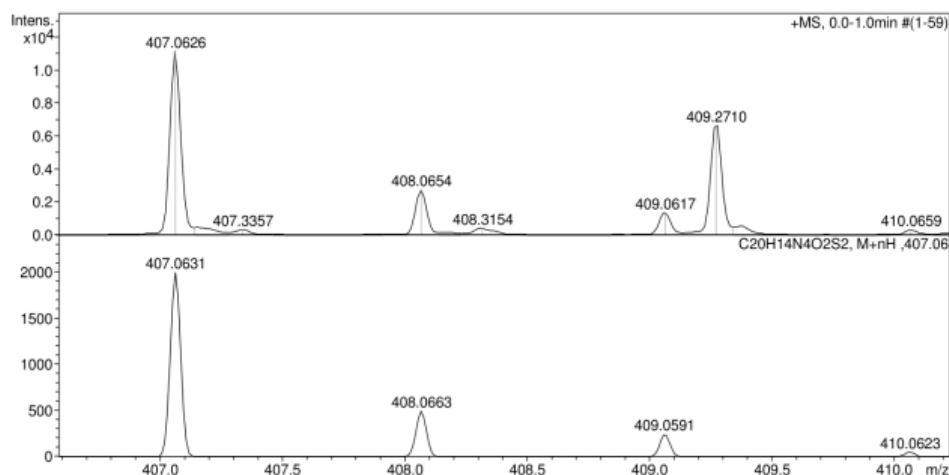
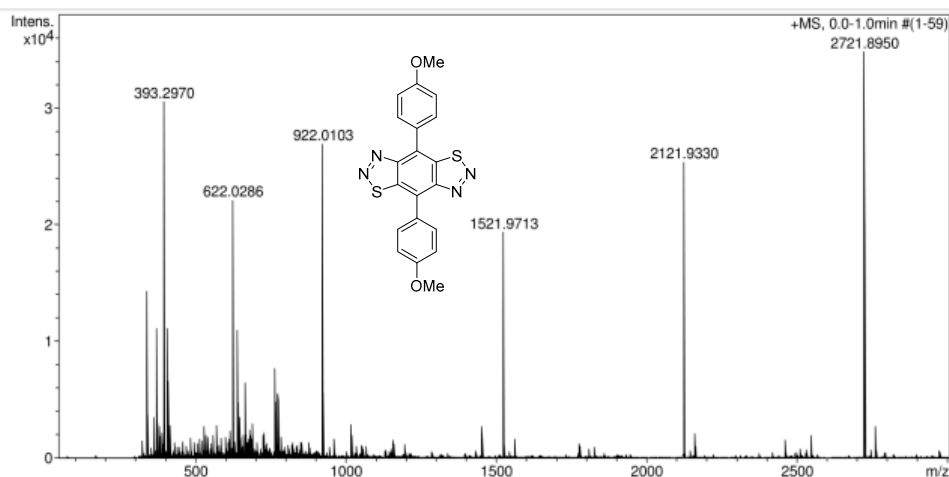
Analysis Name D:\Data\Chizhov\Rakitin\Chmovzh\tim-534\_&clb.d  
 Method tune\_wide.m  
 Sample Name /SUSU Tim-534  
 Comment CH3CN 100 %, dil. 20, calibrant added

Acquisition Date 28.06.2022 17:07:17

Operator BDAL@DE  
 Instrument / Ser# microTOF 10248

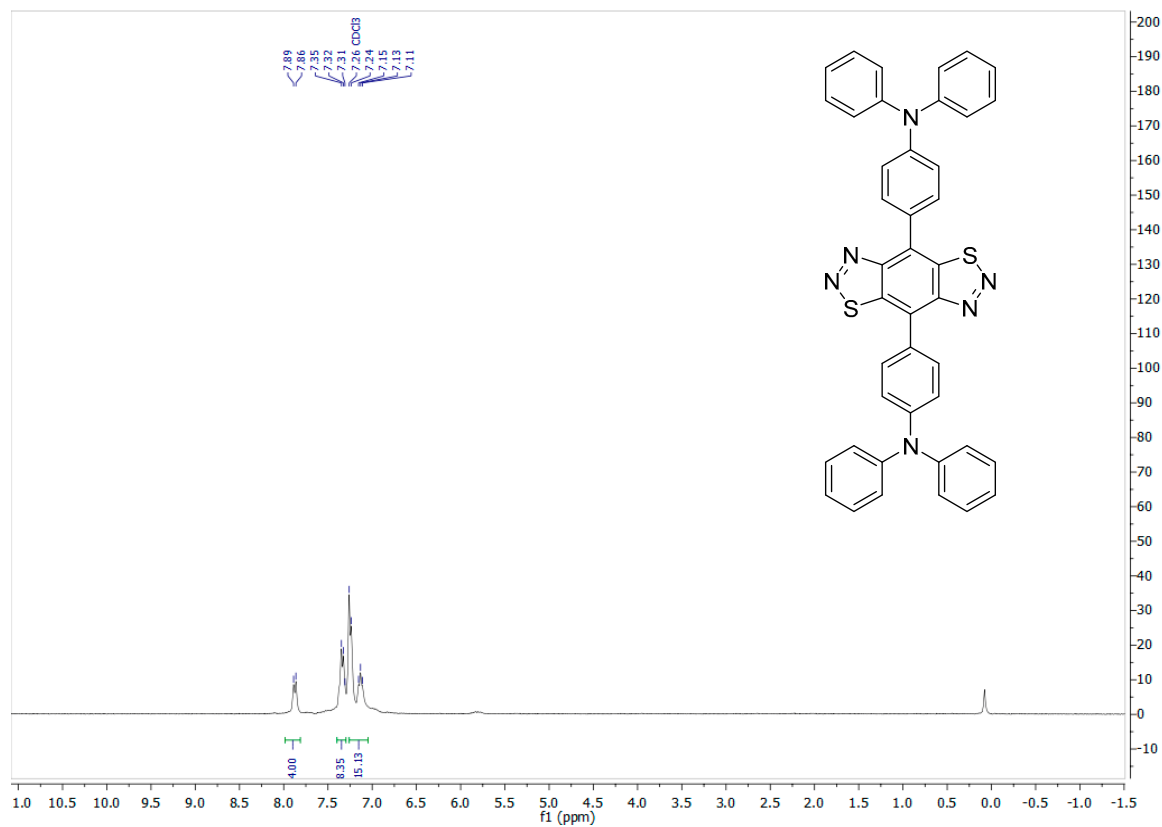
## Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
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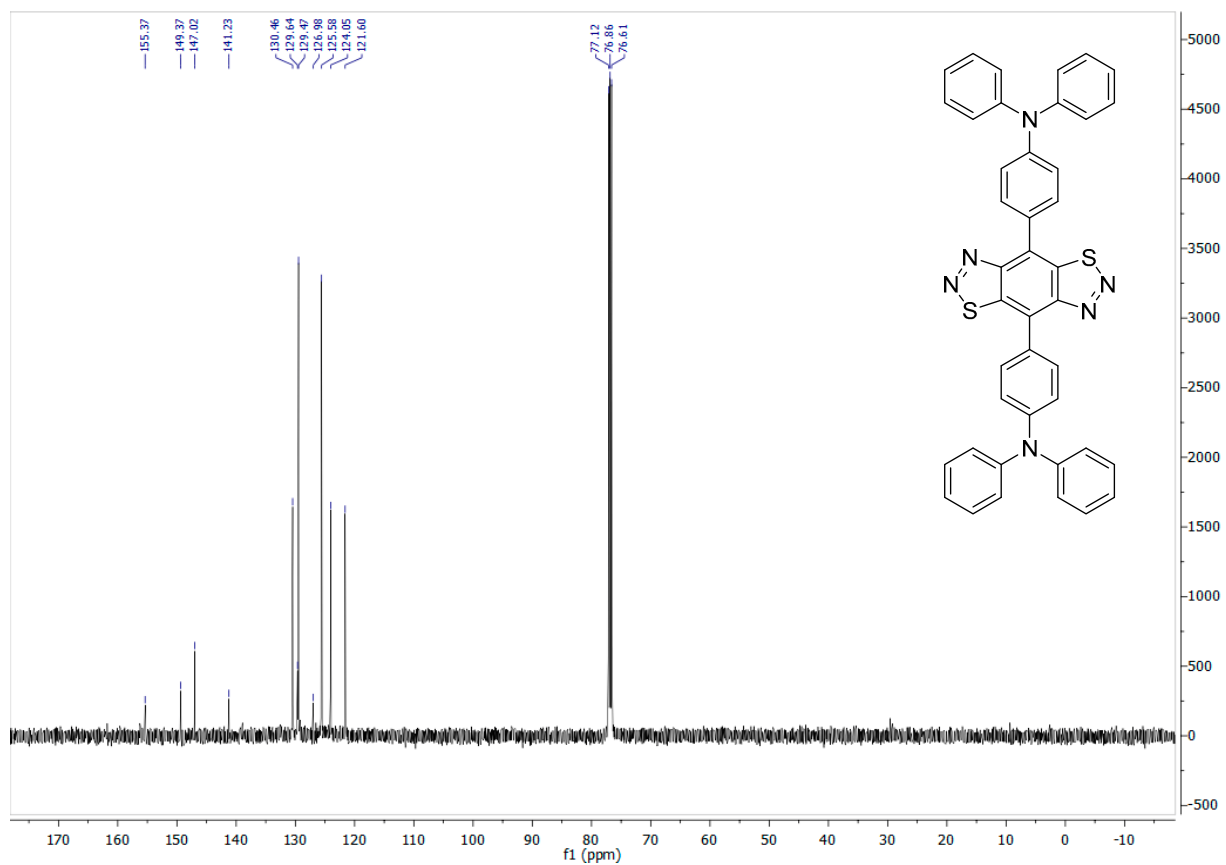
**4,4'-(Benzo[1,2-d:4,5-d']bis([1,2,3]thiadiazole)-4,8-diyl)bis(N,N-diphenylaniline) (19h)**

**<sup>1</sup>H NMR (300 MHz)**



**<sup>13</sup>C NMR(75 MHz)**





# Display Report

## Analysis Info

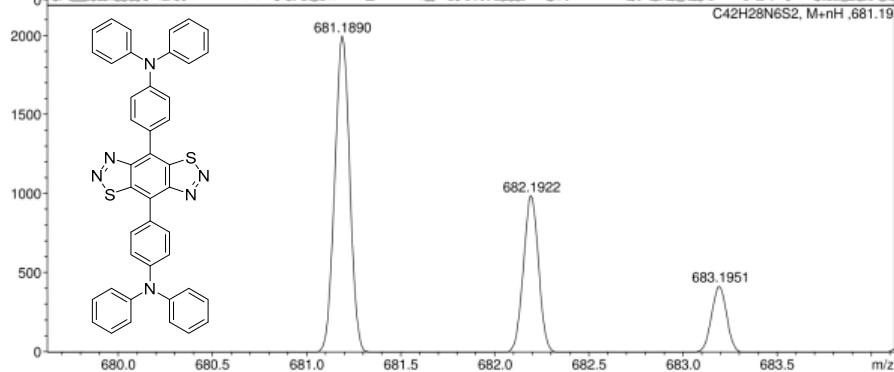
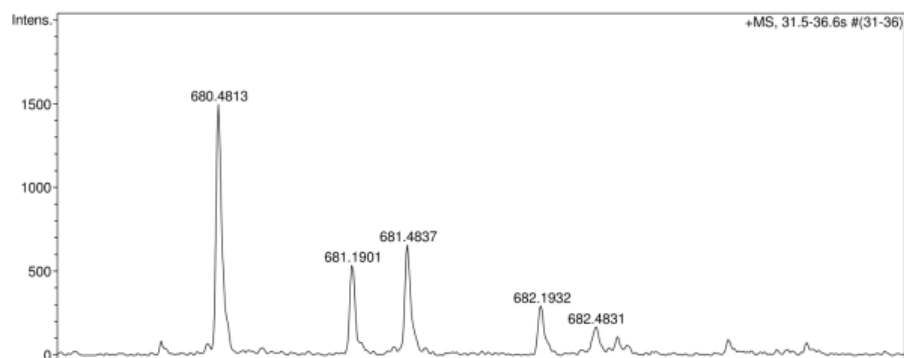
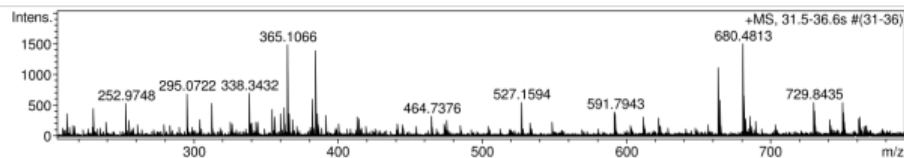
Analysis Name D:\Data\Kolotyrkina\2022\Chmovsh\0713009.d  
 Method tune\_low.m  
 Sample Name /SUSU Tim-539  
 Comment C42H28N6S2 mH 681.1890clb added CH3CN

Acquisition Date 13.07.2022 14:03:45

Operator BDAL@DE  
 Instrument / Ser# maXis 43

## Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

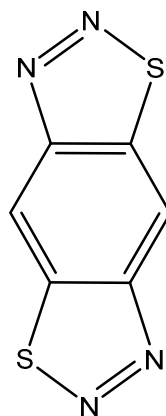
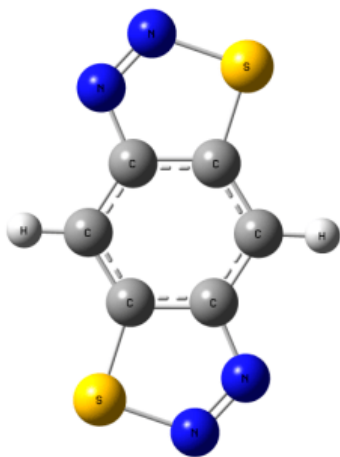


### Quantum-chemical calculations

DFT calculations were performed with the Gaussian 16 Rev C.01.<sup>1</sup> DFT calculations were performed with the Gaussian 16 Rev C.01. M11 DFT functional with 6-31+g(d) basis set was used for all calculations. Calculations were performed in dichloromethane (PCM model). Data from X-ray diffraction experiments were used as starting points for geometry optimization. Cartesian coordinates are given in angstroms; absolute energies for all substances are given in hartrees. Analysis of vibrational frequencies was performed for the optimized structure. The compound was characterized by only real vibrational frequencies. Wavefunction stability, using *stable* keyword, was also checked for the molecule.

For calculations of optimized geometries, frequencies, thermodynamics, HOMO and LUMO energies following keywords were used:

*# opt freq 6-31+g(d) scrf=(solvent=dichloromethane) nosymm m11 test*



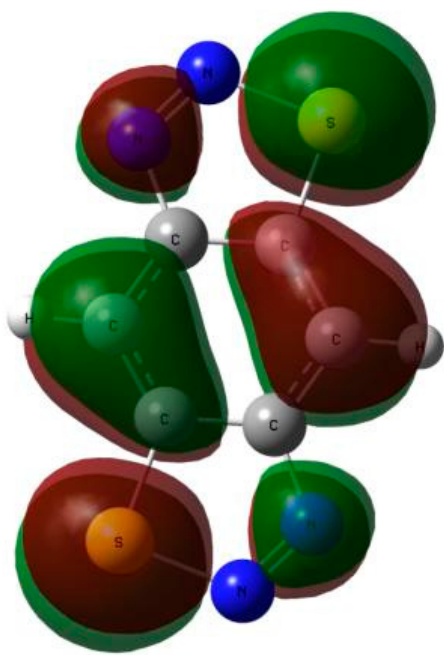
Charge 0; multiplicity 1

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S	6.50031800	2.71554400	5.46659000
N	4.44929700	3.60408300	4.33387400
N	5.56231600	3.07917600	4.07791200
C	2.98324600	4.44144200	7.59676800
C	3.04398300	4.34416300	6.21269500
C	4.20732800	3.78281500	5.69345300
S	1.75621700	5.05904400	8.64216800
N	3.80724800	4.17051900	9.77488200
N	2.69423600	4.69543800	10.03084600
C	5.27329500	3.33315800	6.51198800
C	5.21255800	3.43043700	7.89606200
C	4.04921600	3.99178500	8.41530400
H	6.01272100	3.09520200	8.55422700
H	2.24382100	4.67939500	5.55453000

DFT M11 / 6-31+g(d) solvent dichloromethane, PCM model		
Total electronic energy=	-1244.877827	E <sub>0</sub>
Sum of electronic and zero-point Energies=	-1244.797330	E <sub>0</sub> + E <sub>ZPE</sub>
Sum of electronic and thermal Energies=	-1244.789137	E <sub>0</sub> + E <sub>tot</sub>
Sum of electronic and thermal Enthalpies=	-1244.788193	E <sub>0</sub> + H <sub>corr</sub>
Sum of electronic and thermal Free Energies=	-1244.831394	E <sub>0</sub> + G <sub>corr</sub>
Zero-point correction ( <i>unscaled</i> ) =	0.080497	
Number of imaginary vibrational frequencies = 0		
E HOMO = -9.23 eV		
E LUMO = -1.04 eV		
E gap = 8.19 eV		

HOMO:



LUMO:

