

## **The synthesis and antiproliferative activity of isatin-7-sulfonamides**

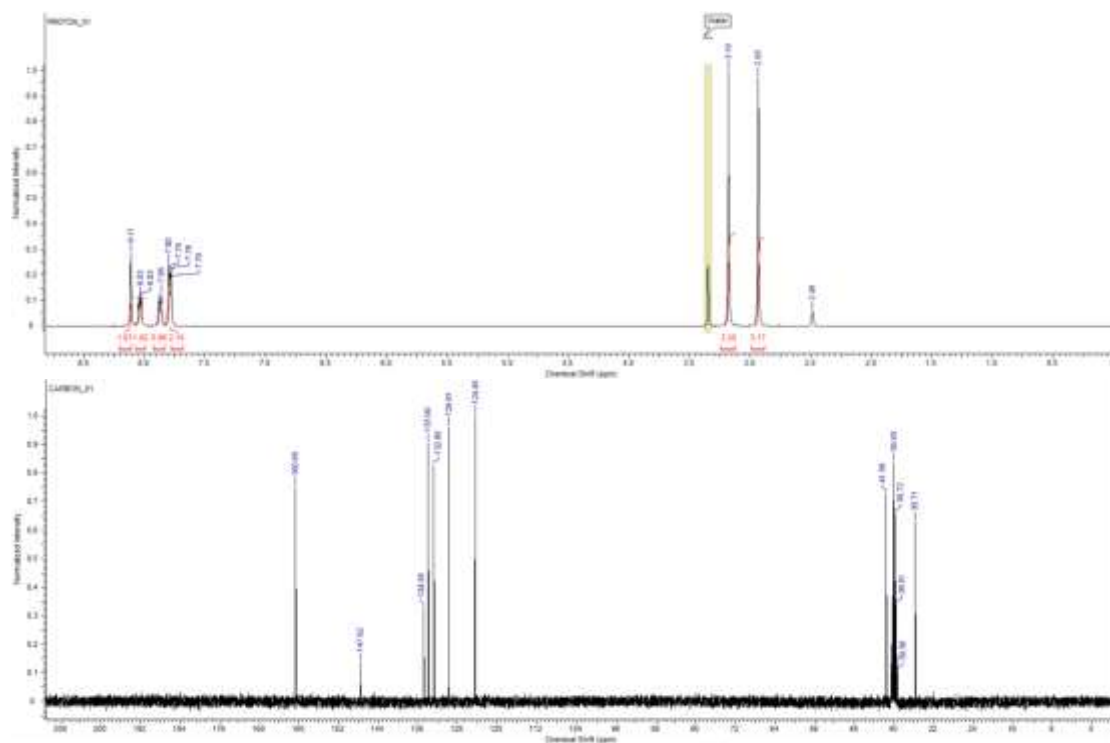
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Fedor B. Bogdanov<sup>2</sup>, Alexander M. Shcherbakov<sup>1,2</sup>, Andrey E. Shchekotikhin<sup>1\*</sup>**

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f.bogdanov.f@ya.ru, alex.scherbakov.2010@ya.ru*

**SUPPLEMENTARY INFORMATION**

***N,N*-Диметил-*N'*-((2-нитрофенил)сульфонил)формимидамид (5)**



## Compound Spectrum List Report

### Analysis Info

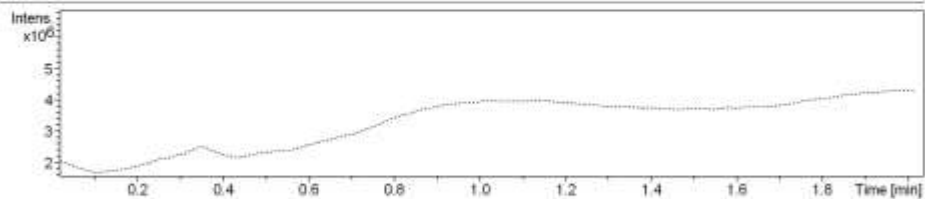
Analysis Name D:\Data\ST\ST-208\_1.d  
Method tune\_low.m  
Sample Name Tune wide  
Comment

Acquisition Date 1/20/2022 3:56:06 PM

Operator Korolev  
Instrument / Ser# micrOTOF-Q II 10225

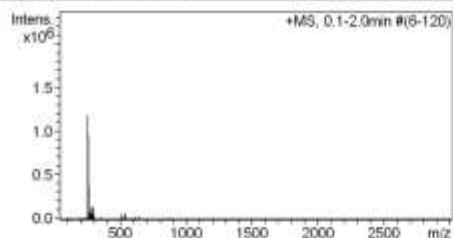
### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source



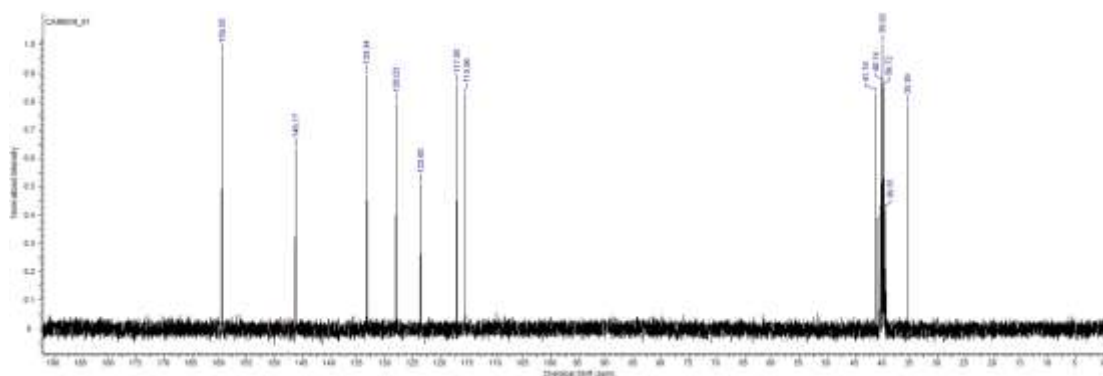
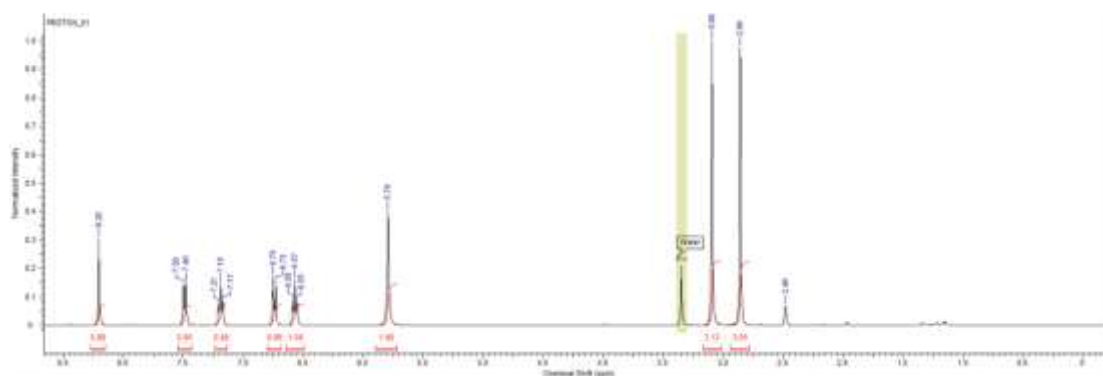
#	RT [min]	Area	Area Frac. %
n.a.	1.1	n.a.	n.a.

### +MS, 0.1-2.0min #(6-120)



#	m/z	I	A %
1	258.0548	1183690	100.0
2	259.0583	189048	19.9
3	260.0533	98907	10.5
4	275.0820	60638	6.1
5	280.0378	138241	15.6
6	281.0396	17422	2.0
7	296.0113	131018	14.0
8	515.1012	52188	10.5
9	537.0833	63181	12.8
10	614.5712	20101	5.1

***N'*-((2-Аминофенил)сульфонил)-*N,N*-диметилформимидамид (6)**



## Compound Spectrum List Report

### Analysis Info

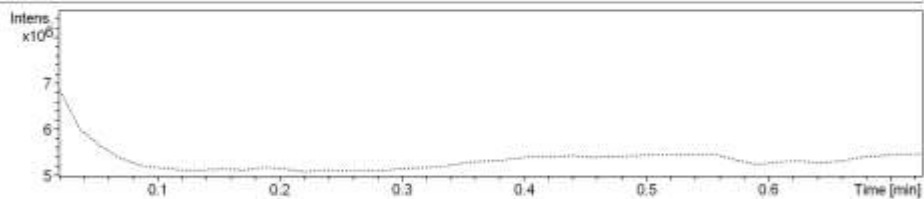
Analysis Name D:\Data\ST\ST-209.d  
Method tune\_low.m  
Sample Name Tune wide  
Comment

Acquisition Date 1/20/2022 10:26:28 AM

Operator Korolev  
Instrument / Ser# micrOTOF-Q II 10225

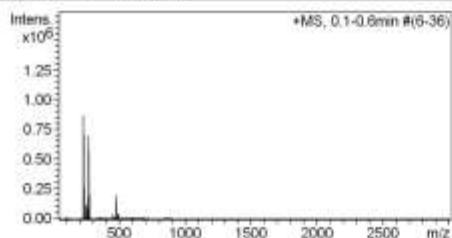
### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source



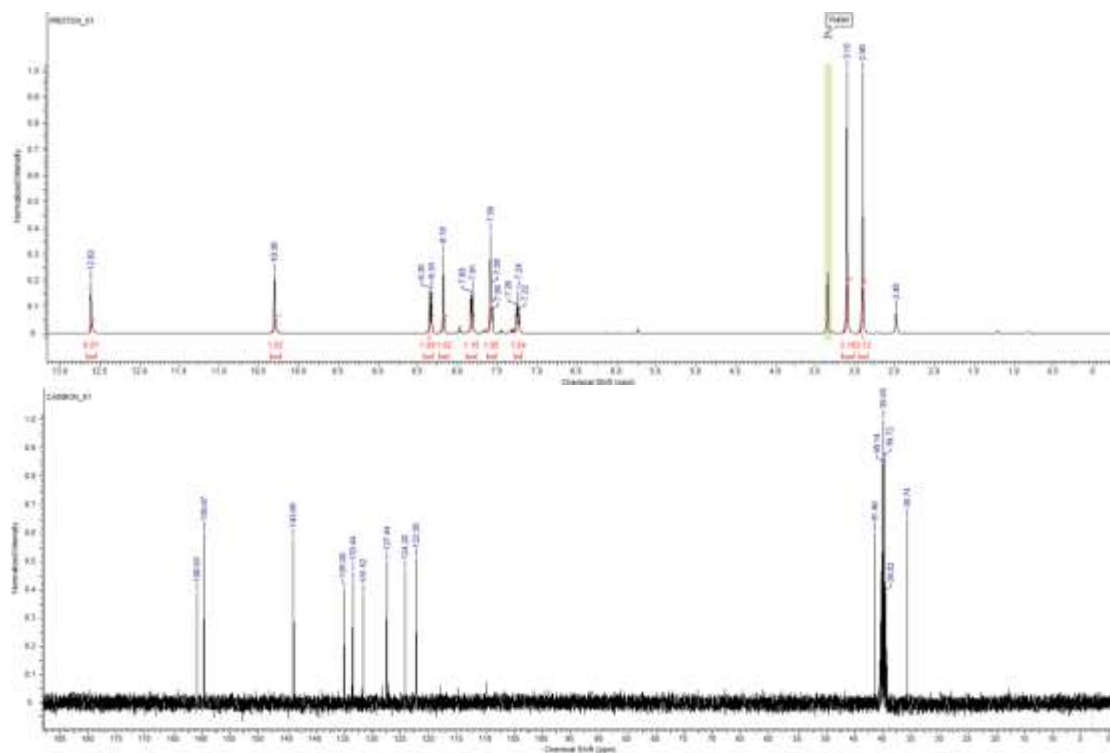
#	RT [min]	Area	Max. m/z
n.a.	0.4	n.a.	228.0795

### +MS, 0.1-0.6min #(6-36)



#	m/z	I	I%
1	228.0795	668060	100.0
2	229.0818	107891	12.4
3	230.0762	51917	6.0
4	250.0608	118694	13.7
5	266.0351	698307	80.4
6	267.0374	90933	10.5
7	268.0324	94780	10.9
8	452.1258	36887	4.2
9	477.1320	196980	22.7
10	478.1338	47412	5.5

***N*-2-(*N*-((Диметиламино)метил)сульфамоил)фенил)-2-(гидроксимино)ацетамид (7a)**



## Compound Spectrum List Report

### Analysis Info

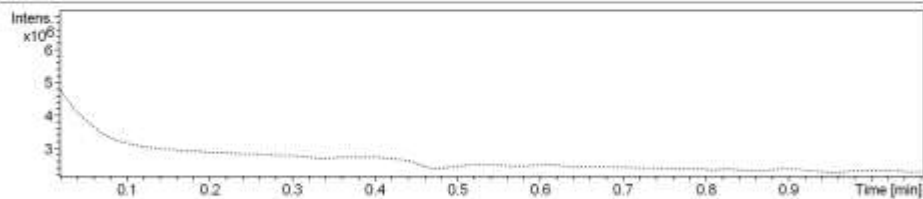
Analysis Name D:\Data\ST\ST-210(2).d  
Method tune\_low.m  
Sample Name Tune wide  
Comment

Acquisition Date 1/21/2022 10:50:31 AM

Operator Korolev  
Instrument / Ser# micrOTOF-Q II 10225

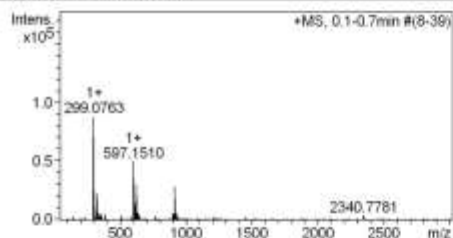
### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source



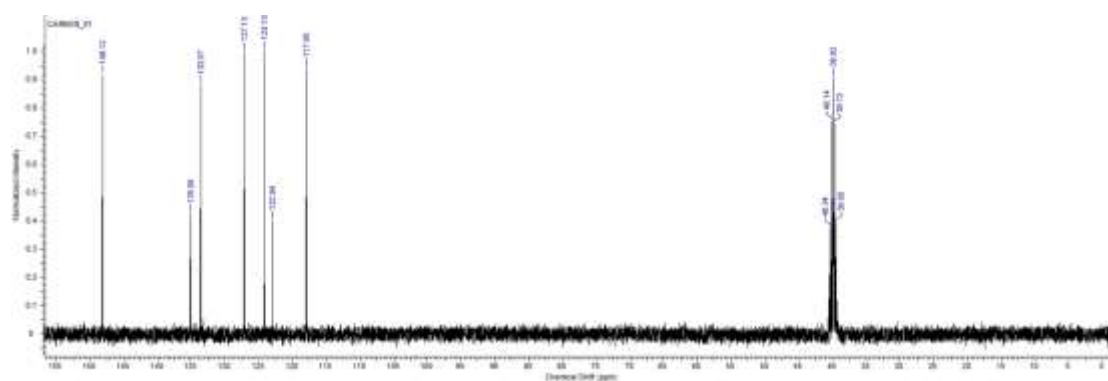
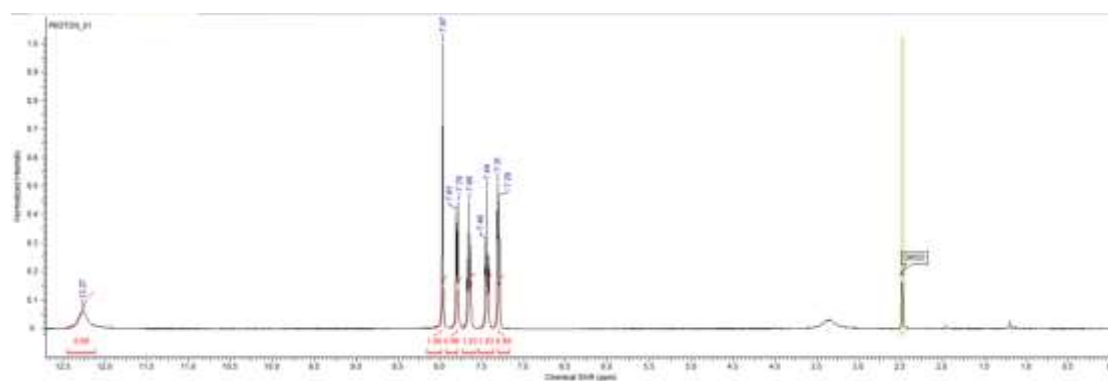
#	RT [min]	Area	Max. m/z
n.a.	0.4	n.a.	299.0763

### +MS, 0.1-0.7min # (8-39)



#	m/z	I	I %
1	299.0763	88067	100.0
2	300.0785	14161	16.1
3	321.0578	22591	25.6
4	597.1510	49375	56.1
5	598.1535	14204	16.1
6	614.1772	14416	16.4
7	619.1331	29677	33.7
8	620.1351	9083	10.3
9	912.2552	28473	32.3
10	913.2568	12600	14.3

**4*H*-бензо[*e*][1,2,4]гиадиазин 1,1-диоксид (7b)**





## Compound Spectrum List Report

### Analysis Info

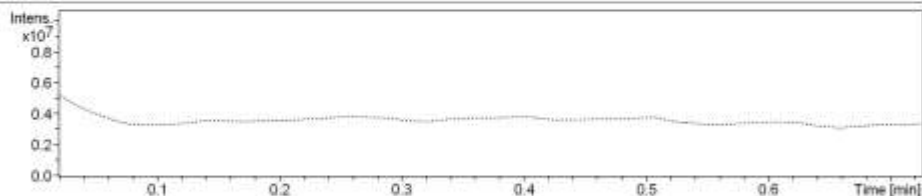
Analysis Name D:\Data\ST\ST-210(1+).d  
Method tune\_low.m  
Sample Name Tune\_wide  
Comment

Acquisition Date 1/21/2022 9:43:17 AM

Operator Korolev  
Instrument / Ser# micrOTOF-Q II 10225

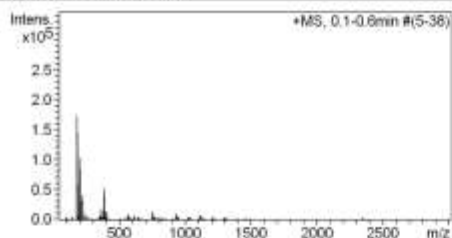
### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source



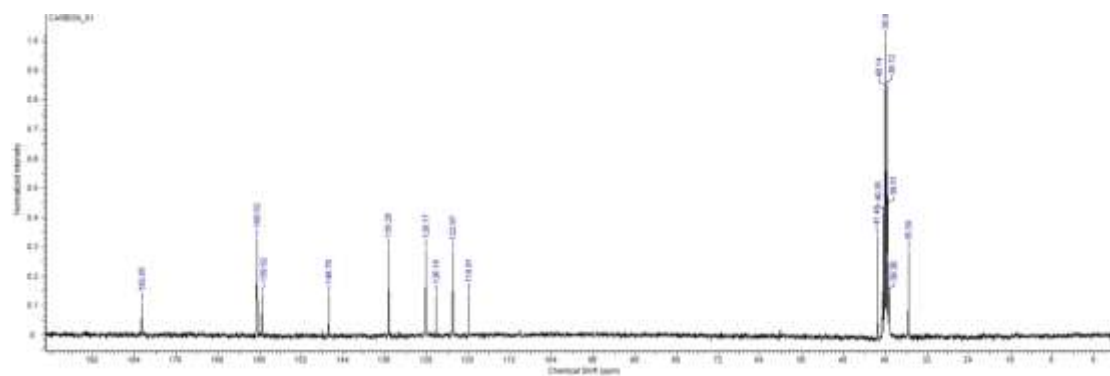
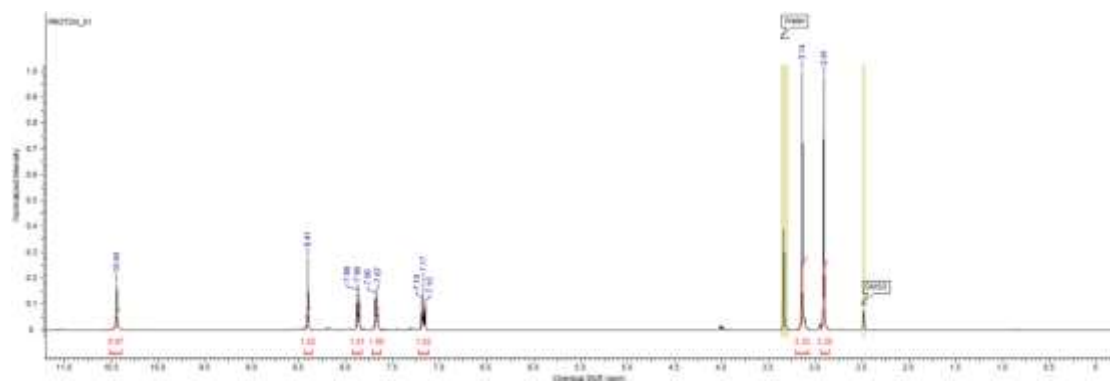
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n.a.	0.4	n.a.	183.0248

### +MS, 0.1-0.6min #(5-38)



#	m/z	I	I%
1	183.0248	172152	100.0
2	184.0270	15773	9.2
3	200.0517	102999	59.8
4	205.0064	27165	15.8
5	220.9817	40955	23.8
6	365.0403	18751	10.9
7	382.0670	52877	30.7
8	387.0237	15833	9.2
9	402.9955	14162	8.2
10	746.0997	13424	7.8

***N'*-((Изатин-7-ил)сульфонил)-*N,N*-диметилформимидамид (8)**



## Compound Spectrum List Report

**Analysis Info**

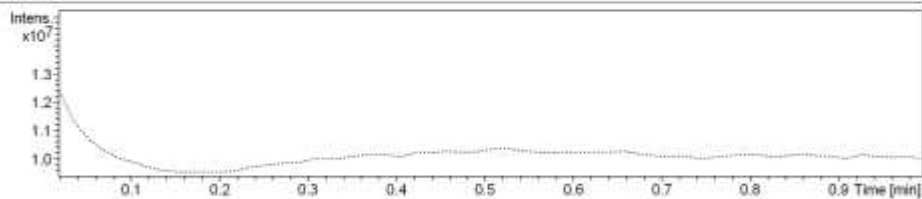
Analysis Name D:\Data\ST\ST-212(1).d  
 Method tune\_low.m  
 Sample Name Tune wide  
 Comment

Acquisition Date 2/8/2022 8:32:48 AM

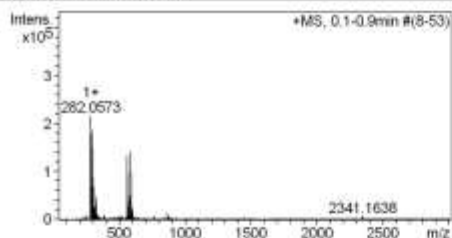
Operator Korolev  
 Instrument / Ser# micrOTOF-Q II 10225

**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	10.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source

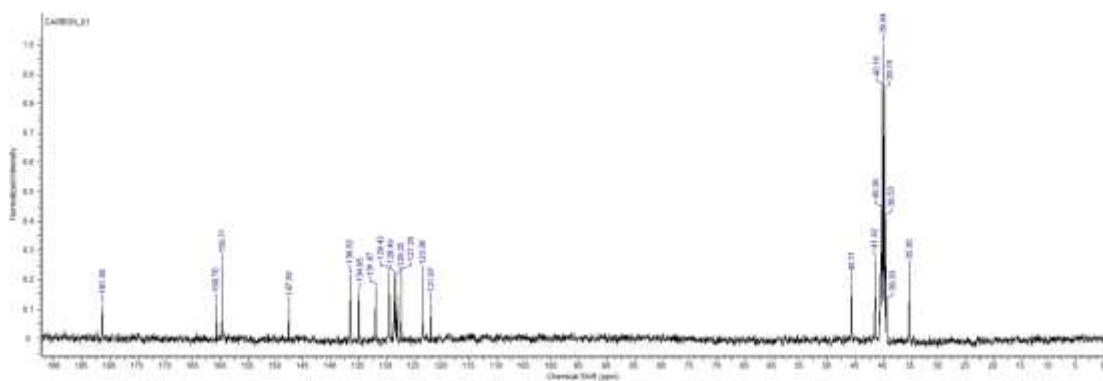
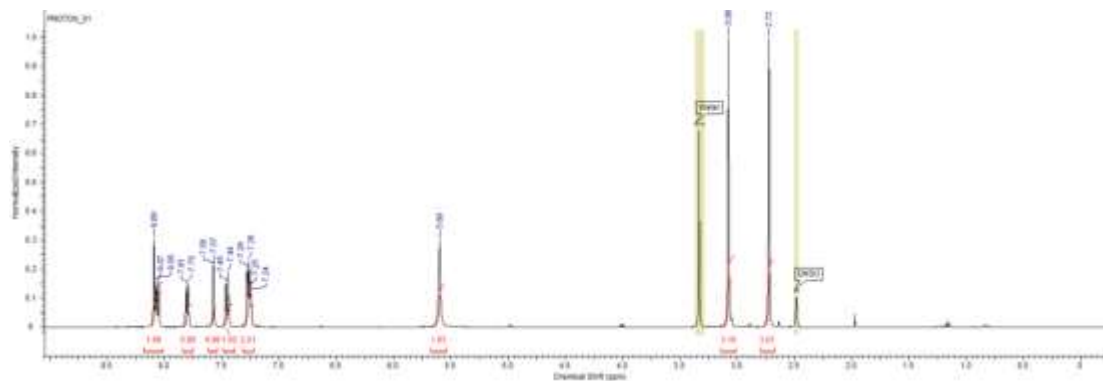


#	RT [min]	Area	Max. m/z
n.a.	0.5	n.a.	282.0573

**+MS, 0.1-0.9min # (8-53)**


#	m/z	I	I%
1	282.0573	215284	100.0
2	283.0608	31145	14.5
3	299.0837	185984	86.4
4	304.0392	90027	41.8
5	321.0643	47917	22.3
6	563.1042	133852	62.2
7	564.1072	40132	18.6
8	580.1308	50738	23.6
9	585.0862	140432	65.2
10	586.0888	40508	18.8

**N'-((1-(2,4-Дихлорбензил)-изатин-7-ил)сульфонил)-N,N-диметилформимидамид (9a)**



## Compound Spectrum List Report

**Analysis Info**

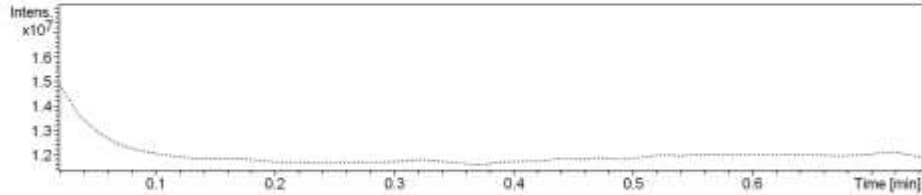
Analysis Name D:\Data\ST\ST-213.d  
 Method nast(2).m  
 Sample Name Tune wide  
 Comment

Acquisition Date 2/8/2022 8:59:01 AM

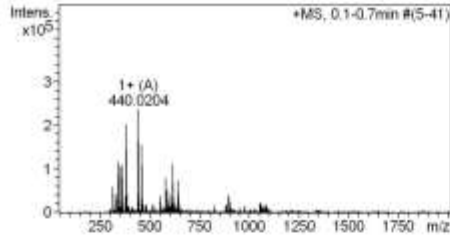
Operator Korolev  
 Instrument / Ser# micrOTOF-Q II 10225

**Acquisition Parameter**

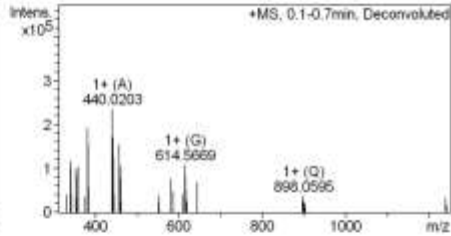
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	550.0 Vpp	Set Divert Valve	Source



#	RT [min]	Area	Int. Type	Intens.	S/N	Chromatogram	Max. m/z
n.a.	0.4	n.a.	Average spectrum	n.a.	n.a.	n.a.	440.0204

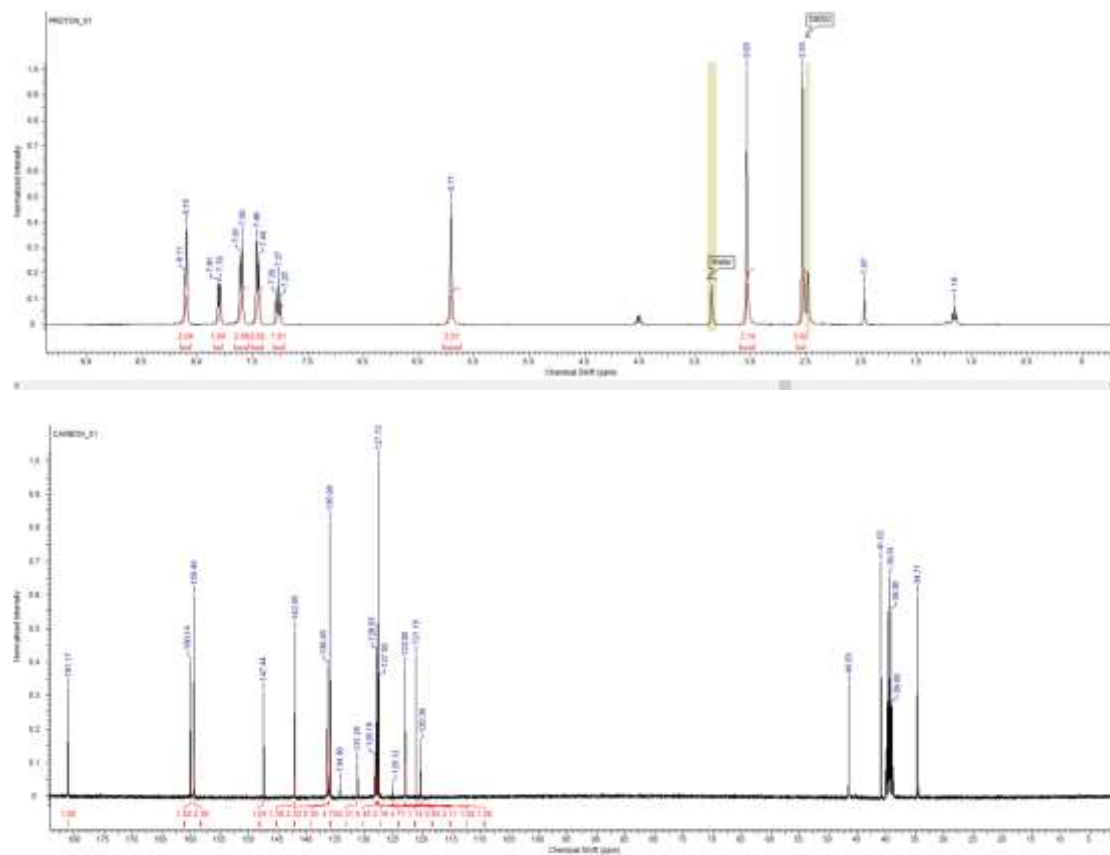
**+MS, 0.1-0.7min # (5-41)**


#	m/z	Res.	S/N	I	I %
1	341.3024	8786	166.2	117874	49.7
2	353.2638	9654	139.1	103850	43.7
3	359.3127	8585	143.1	109492	46.1
4	381.2952	9267	252.5	202990	85.5
5	440.0204	9333	289.9	237387	100.0
6	442.0173	9178	212.8	174498	73.5
7	457.0458	9440	189.4	156048	65.7
8	459.0438	9239	142.1	117237	49.4
9	579.5308	8883	88.5	79490	33.5
10	614.5668	8907	120.0	110808	46.7



#	m/z	Res.	S/N	I	I %
1	341.3024			117873	49.7
2	353.2644			103849	43.7
3	359.3129			109492	46.1
4	381.2951			202989	85.5
5	440.0203			237386	100.0
6	442.0158			174498	73.5
7	457.0458			156048	65.7
8	459.0367			117236	49.4
9	579.5308			79490	33.5
10	614.5668			110807	46.7

**N'-1-(4-((Трифторметил)тио)бензил)изатин-7-ил)сульфонил)-N,N-диметилформимид амид (9b)**



## Compound Spectrum List Report

**Analysis Info**

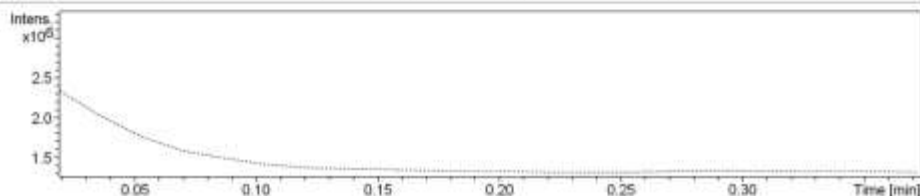
Analysis Name D:\Data\ST\ST-228.d  
 Method tune\_norm.m  
 Sample Name Tune wide  
 Comment

Acquisition Date 5/29/2022 10:34:12 PM

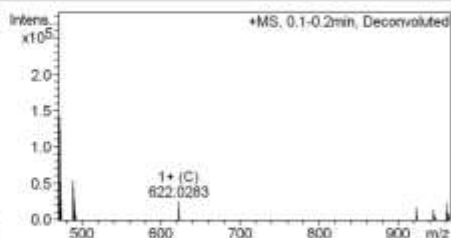
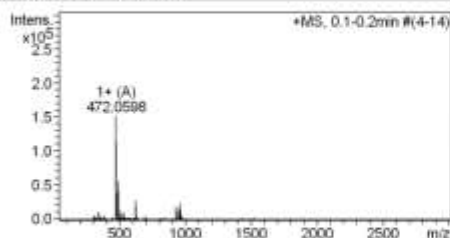
Operator Korolev  
 Instrument / Ser# micrOTOF-Q II 10225

**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	550.0 Vpp	Set Divert Valve	Source



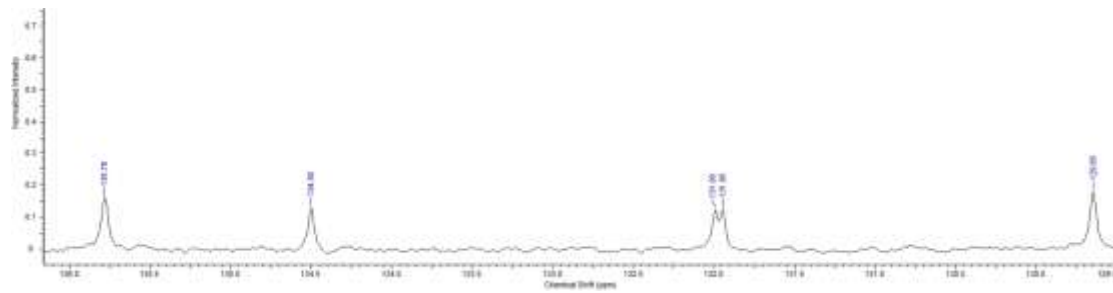
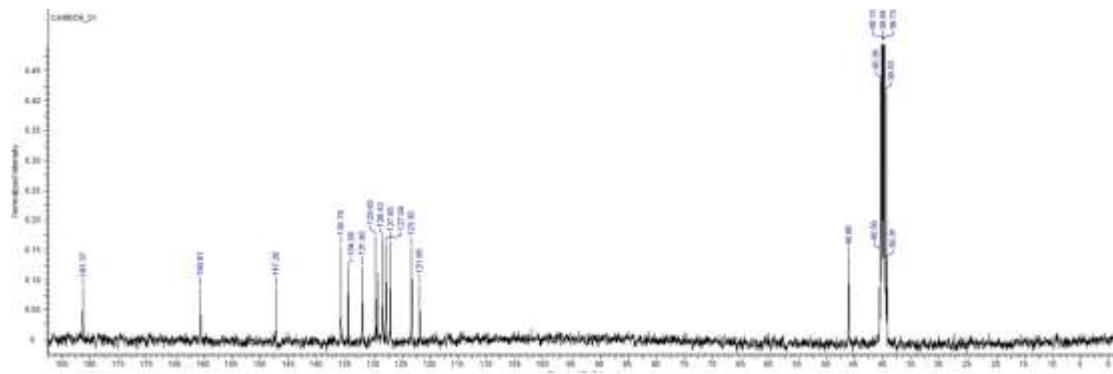
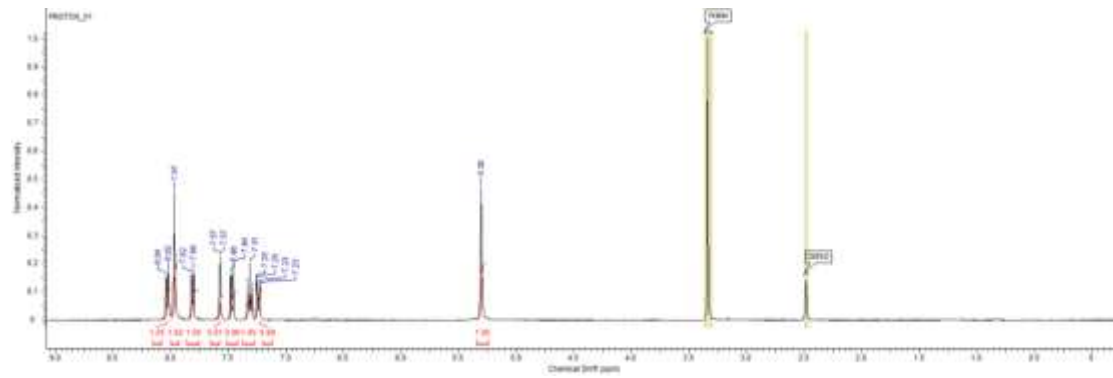
#	RT [min]	Area	Int. Type	Intens.	S/N	Chromatogram	Max. m/z
n.a.	0.2	n.a.	Average spectrum	n.a.	n.a.	n.a.	472.0598

**\*MS, 0.1-0.2min # (4-14)**


#	m/z	Res.	S/N	I	I%
1	472.0598	10024	1310.9	151948	100.0
2	473.0621	8873	279.7	32590	21.4
3	474.0573	8580	146.3	17142	11.3
4	489.0859	8801	447.7	55448	36.5
5	490.0791	8222	245.5	30547	20.1
6	494.0402	9927	106.6	13496	8.9
7	622.0286	8855	189.6	27065	17.8
8	922.0125	10016	137.8	17948	11.8
9	943.1147	9585	120.7	15340	10.1
10	960.1431	9891	193.2	23585	15.5

#	m/z	Res.	S/N	I	I%
1	472.0587			151947	100.0
2	489.0806			55447	36.5
3	622.0283			27065	17.8
4	922.0119			17948	11.8
5	943.1130			15339	10.1
6	960.1387			23584	15.5

### 1-(2,4-Дихлорбензил)-изатин-7-сульфонамид (2a)





## Compound Spectrum List Report

**Analysis Info**

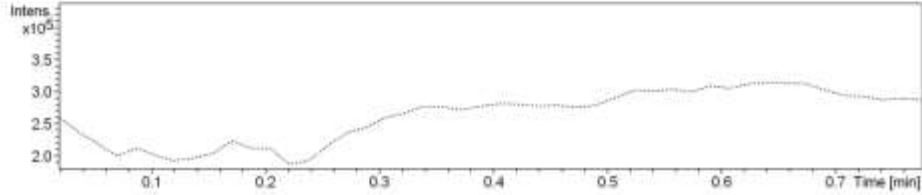
Analysis Name D:\Data\ST\ST-215(-).d  
 Method proba.m  
 Sample Name Tune wide  
 Comment

Acquisition Date 4/10/2022 5:17:04 PM

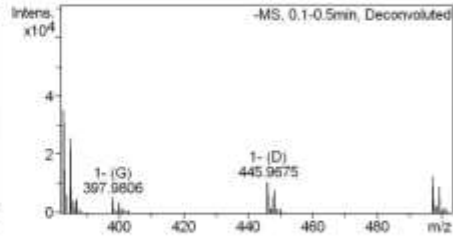
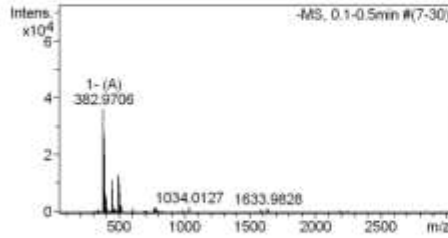
Operator Korolev  
 Instrument / Ser# micrOTOF-Q II 10225

**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	3000 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	550.0 Vpp	Set Divert Valve	Source

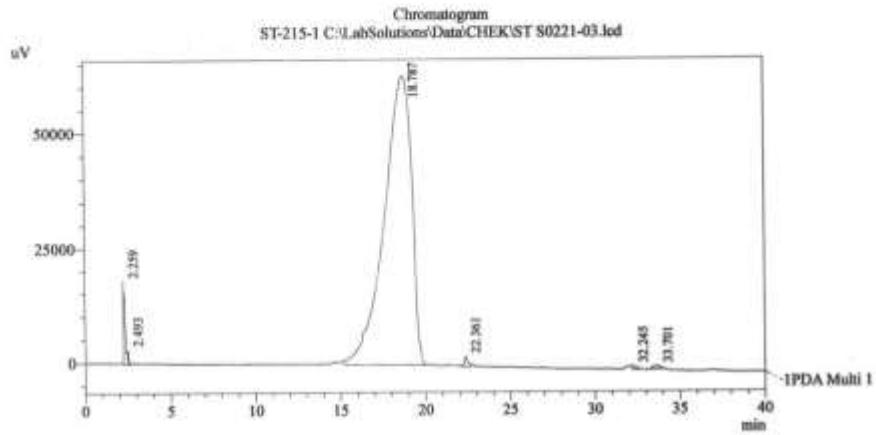


#	RT [min]	Area	Int. Type	Intens.	S/N	Chromatogram	Max. m/z
n.a.	0.3	n.a.	Average spectrum	n.a.	n.a.	n.a.	382.9706

**-MS, 0.1-0.5min # (7-30)**


#	m/z	Res.	S/N	I	I%
1	382.9706	6432	8044.2	36236	100.0
2	383.9734	6156	1420.7	6403	17.7
3	384.9676	6341	5776.3	26039	71.9
4	385.9704	6179	1009.5	4554	12.6
5	386.9654	6443	1145.9	5171	14.3
6	397.9804	6572	1239.8	5616	15.5
7	445.9673	6528	2413.7	11121	30.7
8	447.9651	6557	1772.2	8172	22.6
9	496.9662	6720	2772.1	13001	35.9
10	498.9642	6749	2027.1	9514	26.3

#	m/z	Res.	S/N	I	I%
1	382.9706			36235	100.0
2	384.9660			26039	71.9
3	397.9806			5616	15.5
4	399.9765			3855	10.6
5	445.9675			11120	30.7
6	447.9635			8171	22.6
7	496.9663			13001	35.9
8	498.9625			9514	26.3



1 PDA Multi 1 / 254nm 4nm

PDA Ch1 254nm 4nm

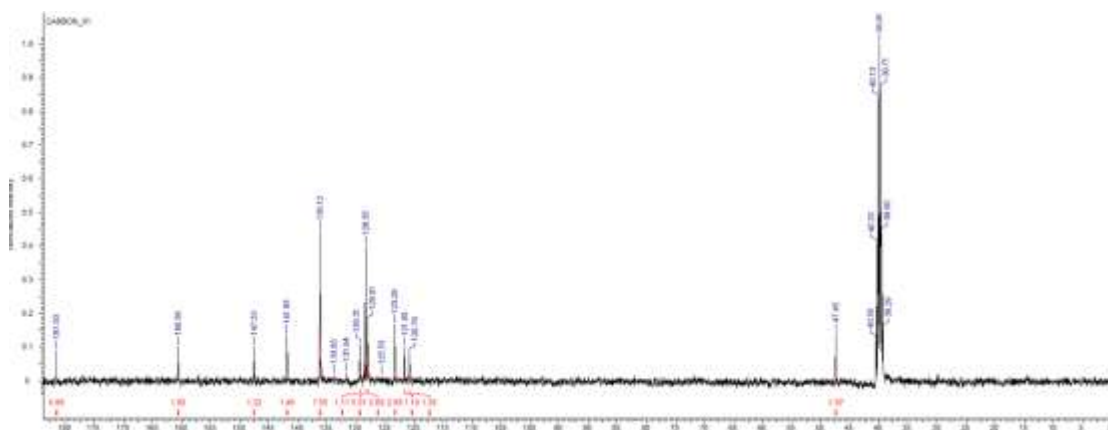
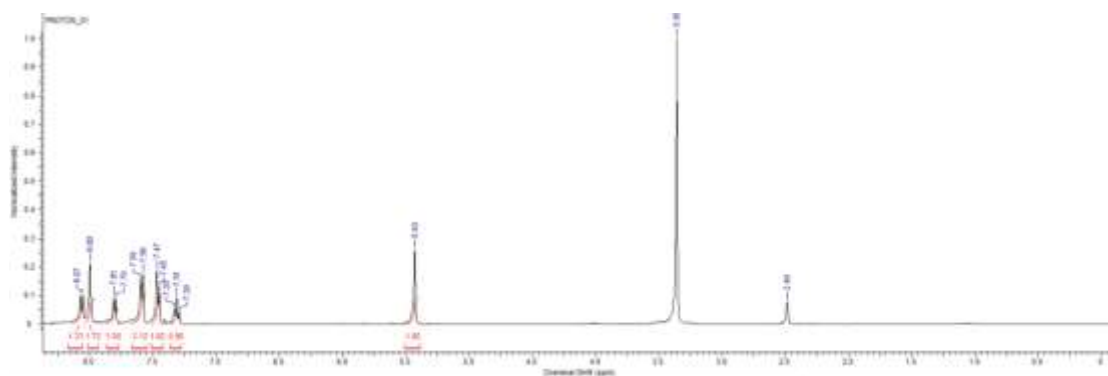
Peak#	Ret. Time	Area	Height	Area %
1	2.259	127254	17986	1.753
2	2.493	16179	3142	0.223
3	18.787	7057484	62994	97.203
4	22.361	30367	2167	0.418
5	32.245	10963	785	0.151
6	33.701	18348	652	0.253
Total		7260596	87727	100.000

Method Filename : FRA02CvA.lcm 28.02.2022 12:28:52

Time	Unit	Command	Value
0.01	Pumps	B.Conc	30
30.00	Pumps	B.Conc	80
40.00	Pumps	B.Conc	90
45.00	Pumps	B.Conc	30
55.00	Controller	Stop	

Shimadzu LC-20 AD; System - FRA 02 vA; Colon- Kromasil C-18, 4.6x250 mm, 5 µm, N 59967  
Elution: A - COOHNH4 0.2% pH 4.5; B - MeCN, fl - 1 ml/min, loop 20 µl

**(4-((Трифторметил)тио)бензил)-изатин-7-сульфонамид (2b)**



## Compound Spectrum List Report

**Analysis Info**

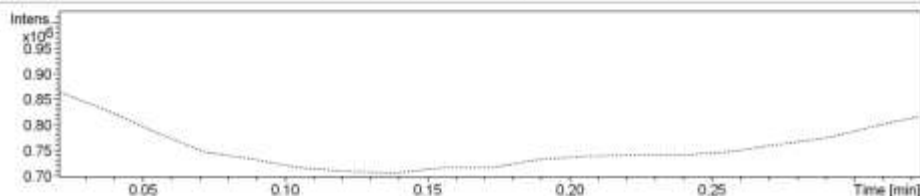
Analysis Name D:\Data\ST\ST-230(-).d  
 Method tune\_norm.m  
 Sample Name Tune wide  
 Comment

Acquisition Date 5/29/2022 11:00:37 PM

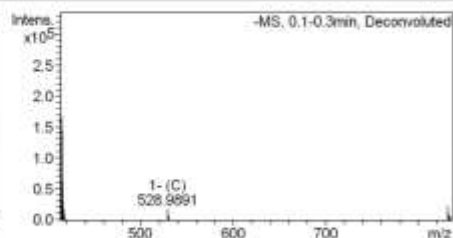
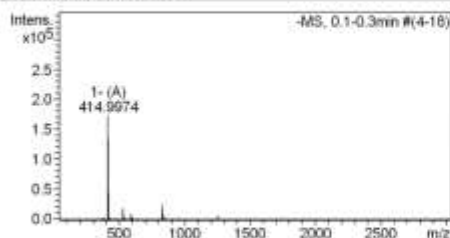
Operator Korolev  
 Instrument / Ser# micrOTOF-Q II 10225

**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	550.0 Vpp	Set Divert Valve	Source

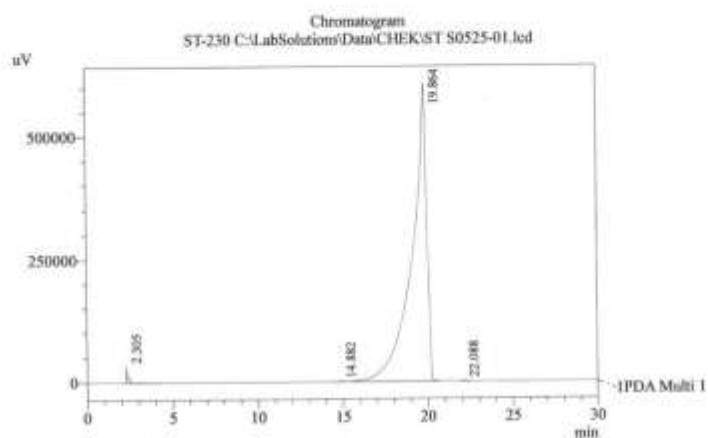


#	RT [min]	Area	Int. Type	Intens.	S/N	Chromatogram	Max. m/z
n.a.	0.2	n.a.	Average spectrum	n.a.	n.a.	n.a.	414.9974

**-MS, 0.1-0.3min # (4-18)**


#	m/z	Res.	S/N	I	I%
1	414.9974	8951	9031.7	172576	100.0
2	415.9986	9155	1987.4	37983	22.0
3	416.9951	8293	1061.5	20292	11.8
4	528.9903	7762	931.5	18201	10.5
5	529.9927	8419	213.3	4168	2.4
6	589.0503	7720	508.6	9516	5.5
7	831.0107	8125	1426.7	23761	13.8
8	832.0107	8150	580.1	9667	5.6
9	833.0098	9206	496.2	8272	4.8
10	1247.0132	8473	337.7	5837	3.4

#	m/z	Res.	S/N	I	I%
1	414.9961			172576	100.0
2	528.9891			18200	10.5
3	831.0081			23761	13.8



1 PDA Multi 1 / 254nm 4nm

PDA Ch1 254nm 4nm

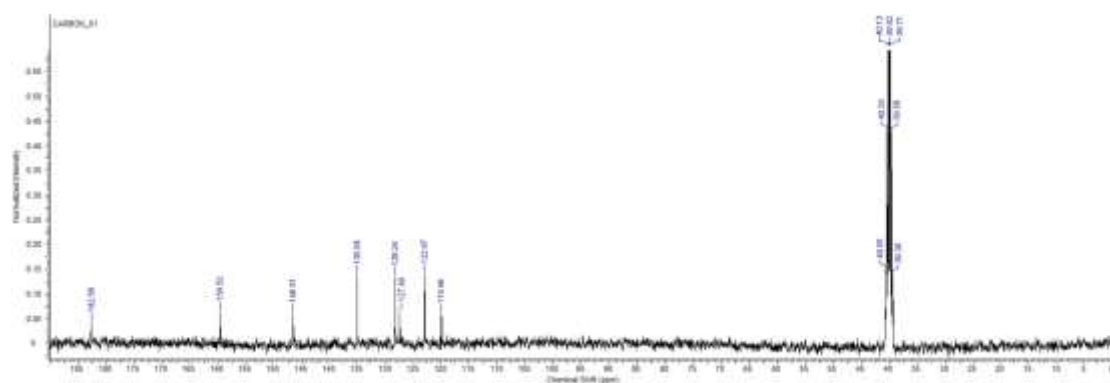
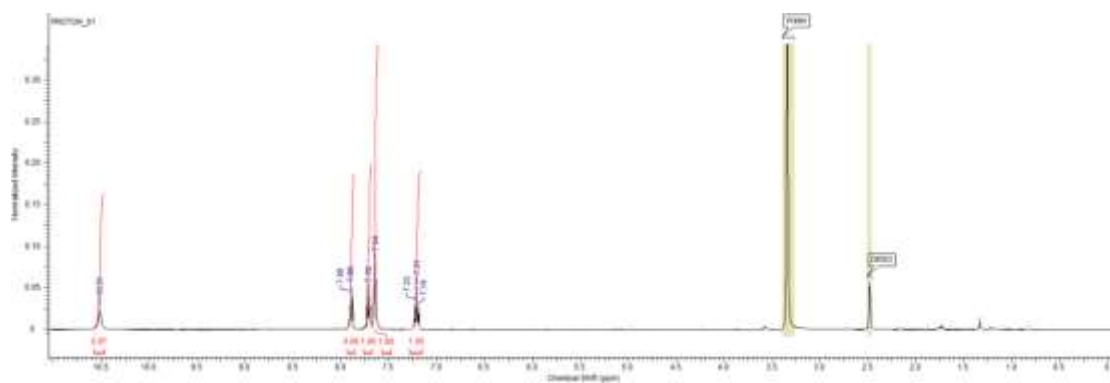
Peak#	Ret. Time	Area	Height	Area %
1	2.305	181409	33701	0.502
2	14.882	10657	884	0.029
3	19.864	35959981	609041	99.425
4	22.088	15989	1206	0.044
Total		36168036	644832	100.000

Method Filename : FOS v.lcm 25.05.2022 14:22:28

Time	Unit	Command	Value
0.01	Pumps	B.Conc	30
30.00	Pumps	B.Conc	90
33.00	Pumps	B.Conc	30
45.00	Controller	Stop	

Shimadzu LC-20 AD; System - FOS Colon-Kromasil-100-5µm. C-18, 4,6x250 mm, N 62511  
Elution: A - H<sub>3</sub>PO<sub>4</sub> 0,01M pH 2,6; B - MeCN,  $\beta$  - 1.0 ml/min, loop 20 µl

## 2,3-диоксииндолин-7-сульфонамид 10



# Compound Spectrum List Report

## Analysis Info

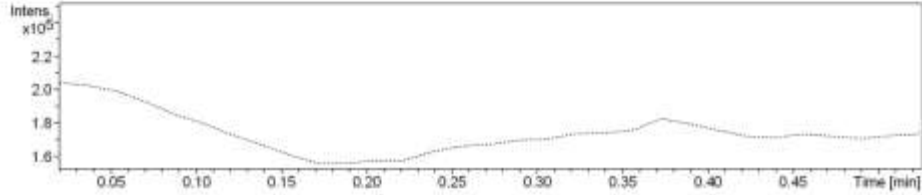
Analysis Name D:\Data\ST\ST-225.d  
Method tune\_low.m  
Sample Name Tune wide  
Comment

Acquisition Date 4/23/2022 6:13:01 PM

Operator Korolev  
Instrument / Ser# micrOTOF-Q II 10225

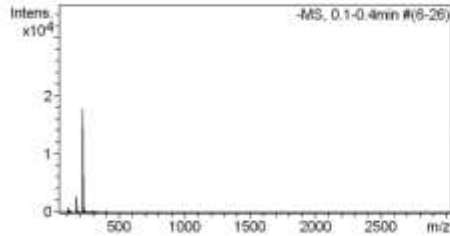
## Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source

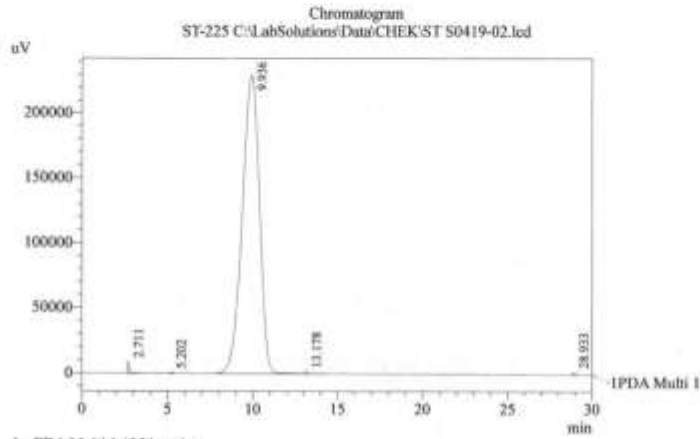


#	RT [min]	Area	Max. m/z
n.a.	0.3	n.a.	224.9972

## -MS, 0.1-0.4min #(6-26)



#	m/z	I	I %
1	112.9813	736	4.1
2	129.0419	261	1.5
3	173.0442	2831	15.9
4	224.9972	17779	100.0
5	226.0012	2111	11.9
6	226.9964	1182	6.6
7	227.2045	203	1.1
8	255.2382	226	1.3
9	287.9989	229	1.3
10	399.0564	315	1.8



1 PDA Multi 1 / 254nm 4nm

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %
1	2.711	58660	9299	0.358
2	5.202	10666	1094	0.065
3	9.936	16251574	229942	99.343
4	13.178	14749	1829	0.090
5	28.933	23409	2540	0.143
Total		16359038	244704	100.000

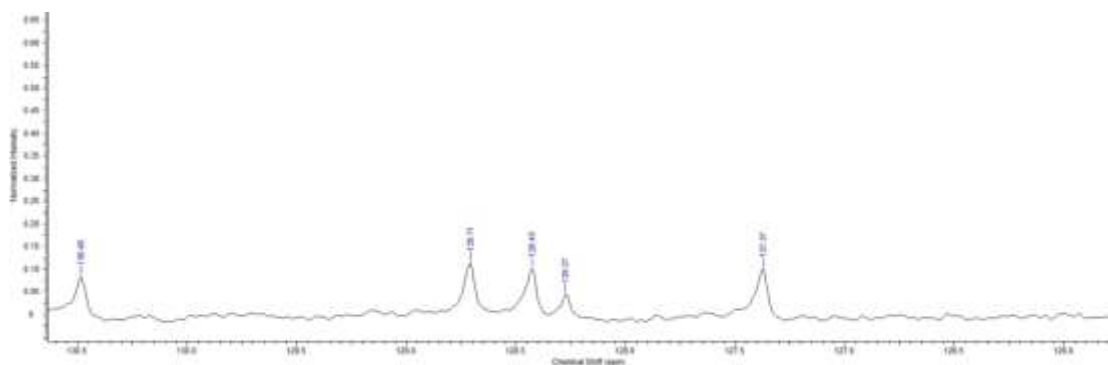
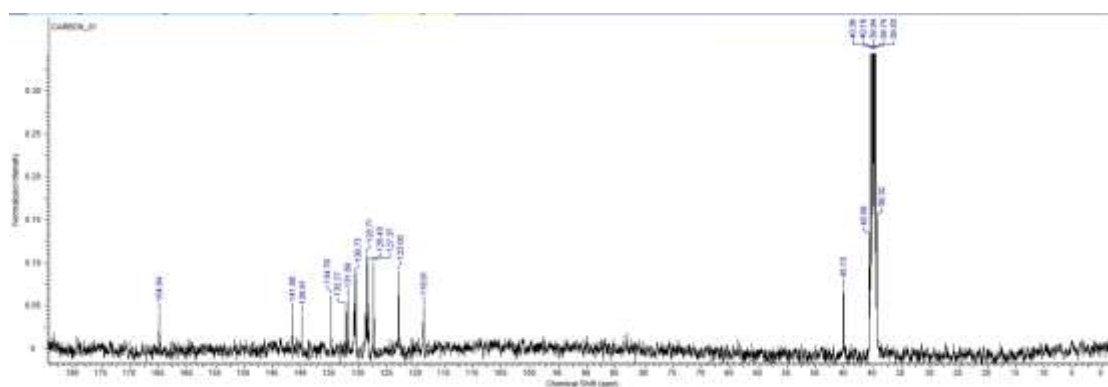
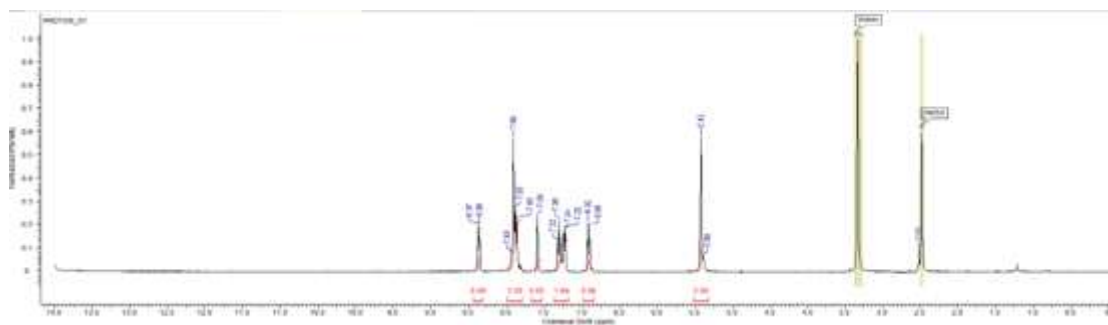
Method Filename : FOS Av.lcm 19.04.2022 12:17:25

Time	Unit	Command	Value
0.01	Pumps	B,Conc	10
30.00	Pumps	B,Conc	50
35.00	Pumps	B,Conc	10
45.00	Controller	Stop	

Shimadzu LC-20 AD; System - FOS Colon- Kromasil-100-5µm. C-18, 4,6x250 mm. N 62511  
Elution: A - H<sub>3</sub>PO<sub>4</sub> 0,01M pH 2,6; B - MeCN,  $\phi$  - 1.0 ml/min, loop 20 µl



**(Z)-1-(2,4-Дихлорбензил)-3-(гидроксиимино)-2-оксоиндолин-7-сульфонамид (11a)**



## Compound Spectrum List Report

**Analysis Info**

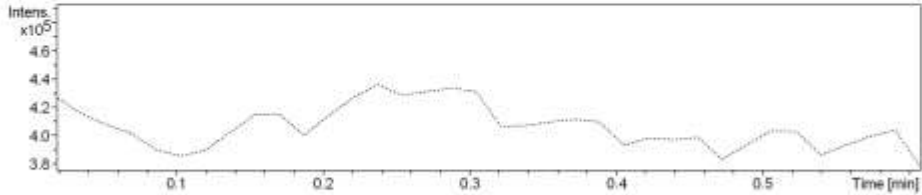
Analysis Name D:\Data\ST\ST-220(-).d  
 Method proba.m  
 Sample Name Tune wide  
 Comment

Acquisition Date 4/10/2022 4:56:28 PM

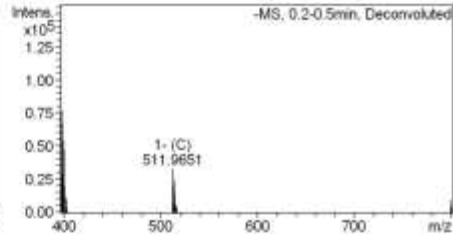
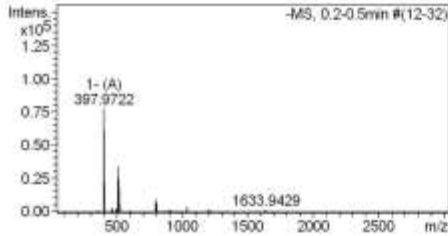
Operator Korolev  
 Instrument / Ser# microTOF-Q II 10225

**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	3000 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	550.0 Vpp	Set Divert Valve	Source



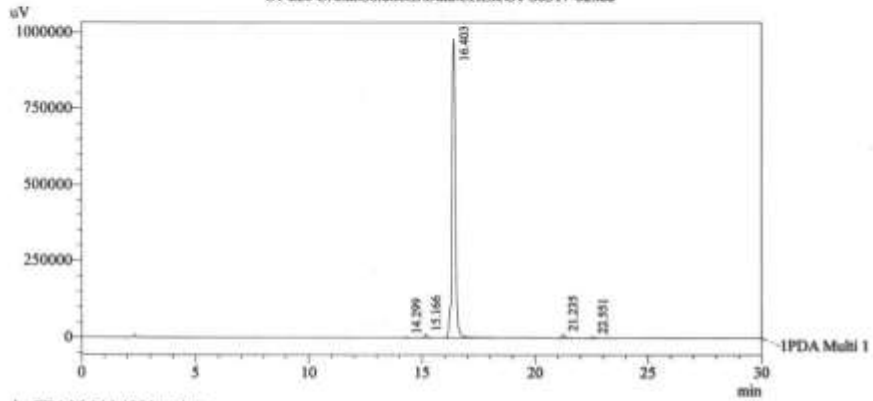
#	RT [min]	Area	Int. Type	Intens.	S/N	Chromatogram	Max. m/z
n.a.	0.4	n.a.	Average spectrum	n.a.	n.a.	n.a.	397.9722

**-MS, 0.2-0.5min #(12-32)**


#	m/z	Res.	S/N	I	I%
1	397.9722	6259	14609.4	77672	100.0
2	398.9750	6270	2656.9	14153	18.2
3	399.9696	6241	10324.5	55091	70.9
4	400.9718	6225	1899.4	10155	13.1
5	401.9664	6252	2133.4	11427	14.7
6	511.9651	6787	5197.3	33371	43.0
7	512.9686	6706	1080.5	6950	8.9
8	513.9625	6659	3784.6	24375	31.4
9	796.9574	7340	1194.5	6502	8.4
10	798.9536	7414	1788.2	9745	12.5

#	m/z	Res.	S/N	I	I%
1	397.9722			77671	100.0
2	399.9676			55091	70.9
3	511.9651			33371	43.0
4	513.9606			24374	31.4
5	798.9534			9745	12.5

Chromatogram  
ST-220 C:\LabSolutions\Data\CHEKST S0317-02.lcd



1 PDA Multi 1 / 254nm 4nm

PDA Ch1 254nm 4nm

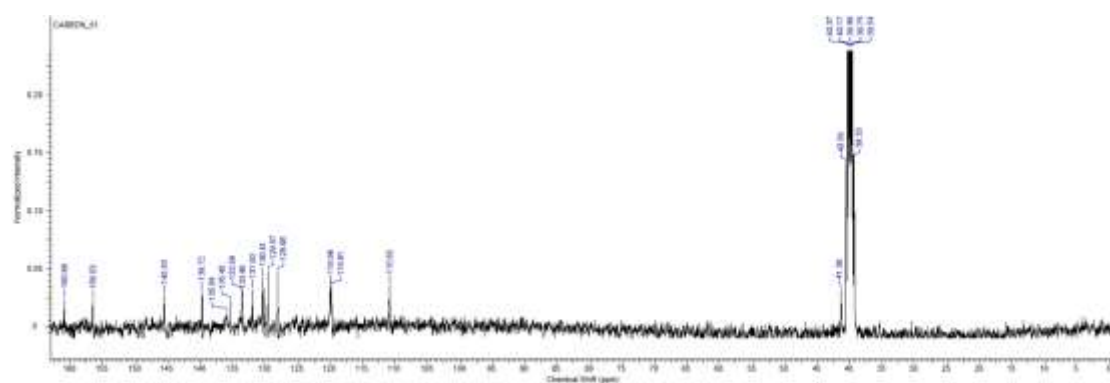
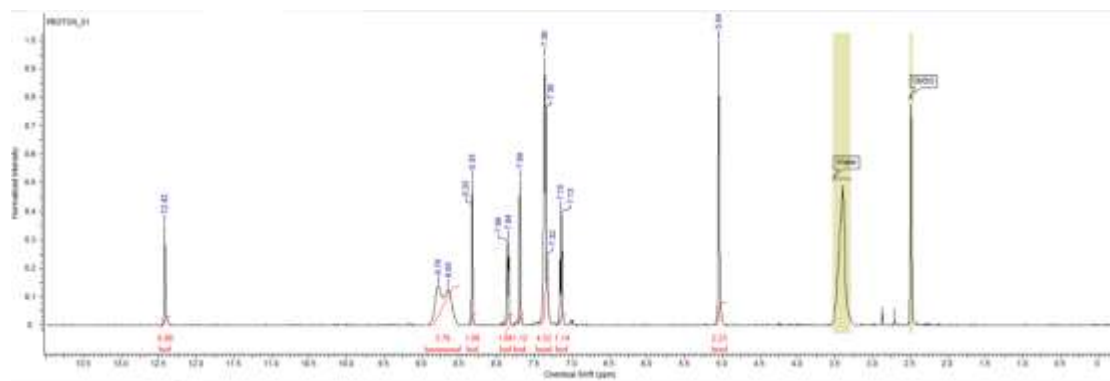
Peak#	Ret. Time	Area	Height	Area %
1	14.299	13713	1900	0.125
2	15.166	91278	10901	0.830
3	16.403	10785342	978937	98.059
4	21.235	90710	11020	0.825
5	22.551	17788	2419	0.162
Total		10998831	1005177	100.000

Method Filename : FRA02CvA.lcm 17.03.2022 13:06:30

Time	Unit	Command	Value
0.01	Pumps	B.Conc	30
30.00	Pumps	B.Conc	80
40.00	Pumps	B.Conc	90
45.00	Pumps	B.Conc	30
55.00	Controller	Stop	

Shimadzu LC-20 AD; System - FRA 02 vA, Column- Knimaasil C-18, 4.6x250 mm, 5 µm, N 59967  
Elution: A - COOHINH4 0.2% pH 4.5; B - MeCN, F - 1 ml/min, loop 20 nkl

**(Z)-2-(1-(2,4-Дихлорбензил)-2-оксо-7-сульфамолиндолин-3-иминогуанидин гидрохлорид (11b)**



## Compound Spectrum List Report

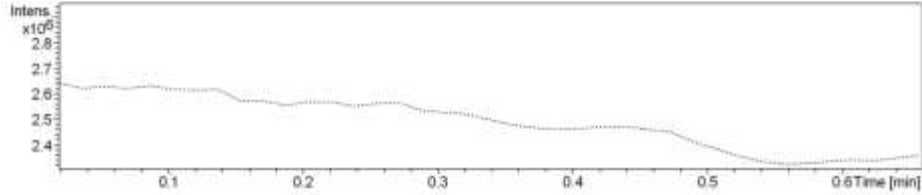
**Analysis Info**

Analysis Name D:\Data\ST\ST-223.d  
 Method tune\_wide.m  
 Sample Name Tune wide  
 Comment

Acquisition Date 4/10/2022 3:13:36 PM  
 Operator Korolev  
 Instrument / Ser# micrOTOF-Q II 10225

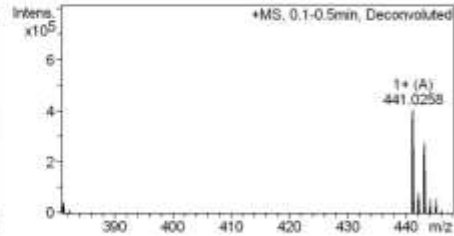
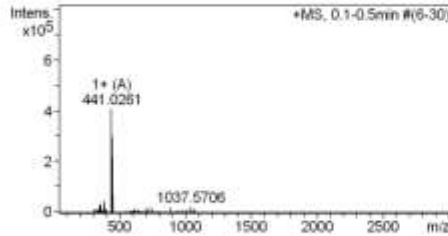
**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	550.0 Vpp	Set Divert Valve	Source



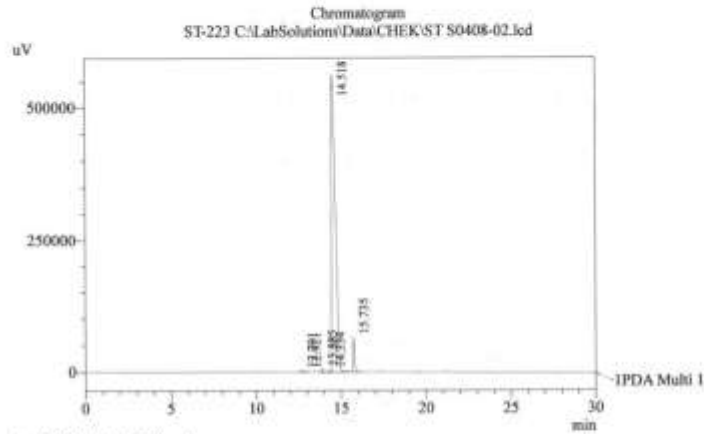
#	RT [min]	Area	Int. Type	Intens.	S/N	Chromatogram	Max. m/z
n.a.	0.3	n.a.	Average spectrum	n.a.	n.a.	n.a.	441.0261

**+MS, 0.1-0.5min # (6-30)**



#	m/z	Res.	S/N	I	I%
1	353.2621	6331	1195.9	29527	7.2
2	359.3115	6281	1198.1	31154	7.6
3	381.2933	6363	1456.2	44805	11.0
4	441.0261	6464	9342.7	408296	100.0
5	442.0280	6779	1858.6	81663	20.0
6	443.0234	6526	6542.1	288728	70.7
7	444.0252	6918	1295.4	57491	14.1
8	445.0207	6617	1288.8	57478	14.1
9	711.5730	7542	299.6	19622	4.8
10	1037.5706	7863	336.5	21576	5.3

#	m/z	Res.	S/N	I	I%
1	381.2932			44805	11.0
2	441.0258			408265	100.0
3	443.0215			288728	70.7



1 PDA Multi 1 / 270nm 4nm

PDA Ch1 270nm 4nm

Peak#	Ret. Time	Area	Height	Area %
1	12.701	15778	2242	0.162
2	12.921	11165	1911	0.115
3	13.885	36803	6574	0.379
4	14.334	19736	2654	0.203
5	14.518	9194422	563754	94.670
6	15.735	434170	65970	4.470
Total		9712074	643106	100.000

Method Filename : FOS Av.lcm 08.04.2022 13:25:10

Time	Unit	Command	Valu
0.01	Pumps	B.Conc	20
30.00	Pumps	B.Conc	80
35.00	Pumps	B.Conc	20
45.00	Controller	Stop	

Shimadzu LC-20 AD; System - FOS Colon- Kromasil-100-5µm, C-18, 4,6x250 mm, N 62511  
Elution: A - H<sub>3</sub>PO<sub>4</sub> 0,01M pH 2,6; B - MeCN, fl - 1.0 ml/min, loop 20 µl