

Chemistry & Biodiversity

Supporting Information

Synthesis and *In Vitro* Antileishmanial Efficacy of Novel Ethylene Glycol Analogues of Benzothiadiazine-1,1-dioxide

Nadine Henning, Christina Kannigadu, Janine Aucamp, Helena D. Janse van Rensburg, Frank van der Kooy, and David D. N'Da*

Supplementary Information

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Frank van der Kooy: [0000-0003-2024-0485](https://orcid.org/0000-0003-2024-0485)

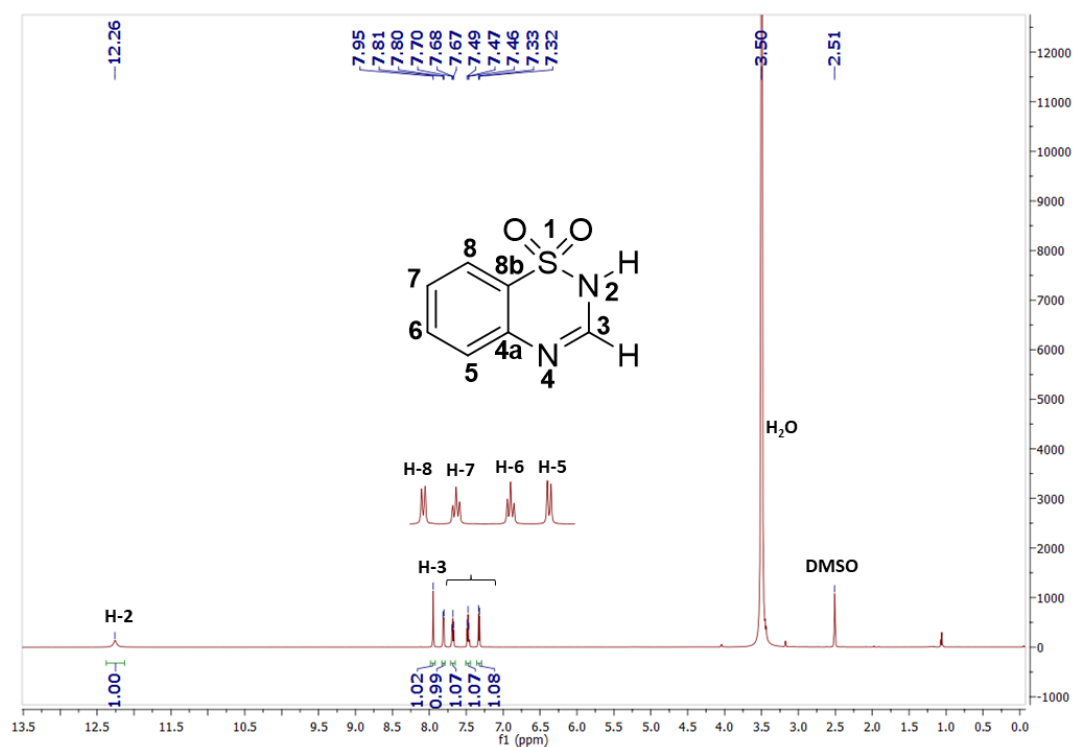
David D. N'Da: [0000-0002-2327-0551](https://orcid.org/0000-0002-2327-0551)

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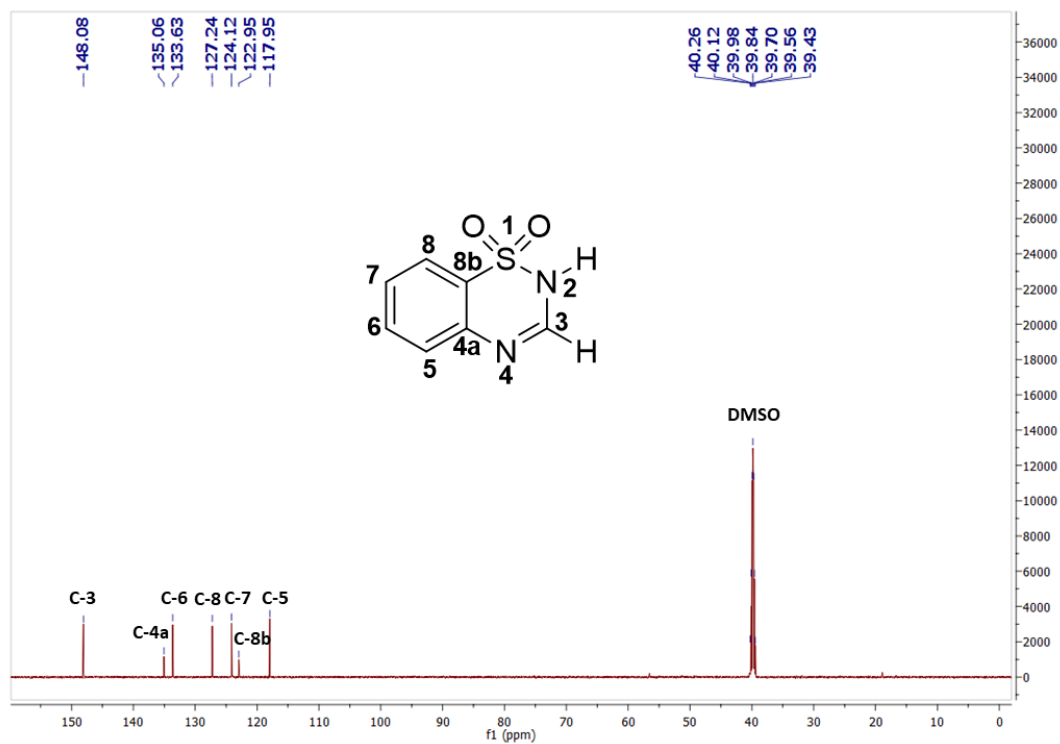
2 <i>H</i> -Benzo[e][1,2,4]thiadiazine-1,1-dioxide (1)	S2
2-(2-Hydroxyethyl)-2 <i>H</i> -benzo[e][1,2,4]thiadiazine-1,1-dioxide (2)	S5
2-(2-Methoxyethyl)-2 <i>H</i> -benzo[e][1,2,4]thiadiazine-1,1-dioxide (3)	S8
2-[2-(2-Methoxyethoxy)ethyl]-2 <i>H</i> -benzo[e][1,2,4]thiadiazine-1,1-dioxide (4)	S11
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2-[2-(4-Bromophenoxy)ethyl]-2 <i>H</i> -benzo[e][1,2,4]thiadiazine-1,1-dioxide (10)	S29
2-[2-(4-Chlorophenoxy)ethyl]-2 <i>H</i> -benzo[e][1,2,4]thiadiazine-1,1-dioxide (11)	S32
2-[2-(4-Nitrophenoxy)ethyl]-2 <i>H</i> -benzo[e][1,2,4]thiadiazine-1,1-dioxide (12)	S35
2-[2-(Allyloxy)ethyl]-2 <i>H</i> -benzo[e][1,2,4]thiadiazine-1,1-dioxide (13)	S38
2-(Prop-2-yn-1-yl)-2 <i>H</i> -benzo[e][1,2,4]thiadiazine-1,1-dioxide (14)	S41

2H-Benzo[e][1,2,4]thiadiazine-1,1-dioxide (1)

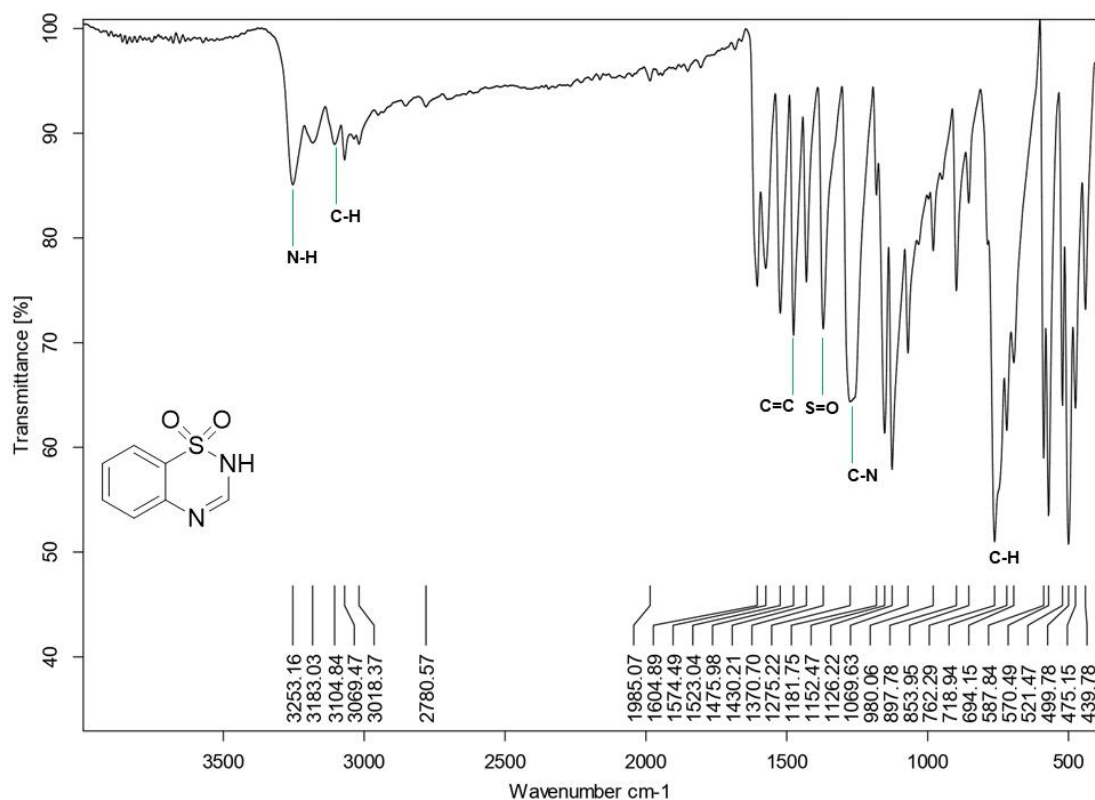
¹H NMR in DMSO



¹³C NMR in DMSO



IR Spectrum



HRMS

Mass Spectrum SmartFormula Report

Analysis Info

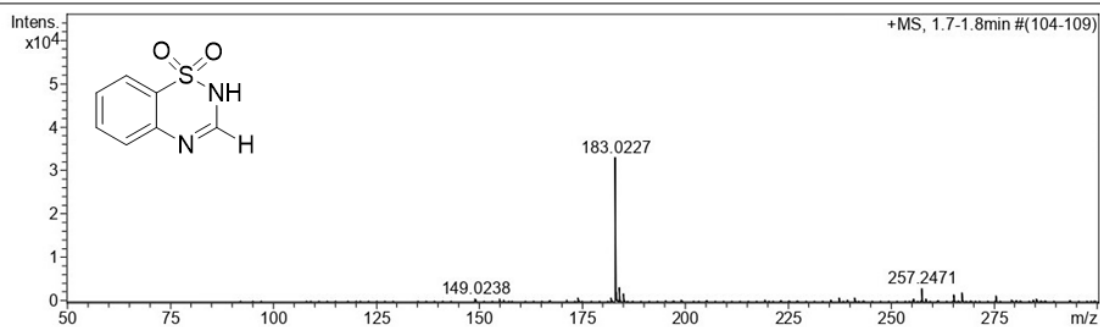
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 Sample Name NH-1
 Comment

Acquisition Date 10/5/2021 2:07:17 PM

Operator Dr JHL Jordaan
 Instrument / Ser# micrOTOF-Q II 2010390

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1600 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
183.0227	1	C7H7N2O2S	100.00	183.0223	-0.4	-2.2	6.0	5.5	even	ok

HPLC Purity



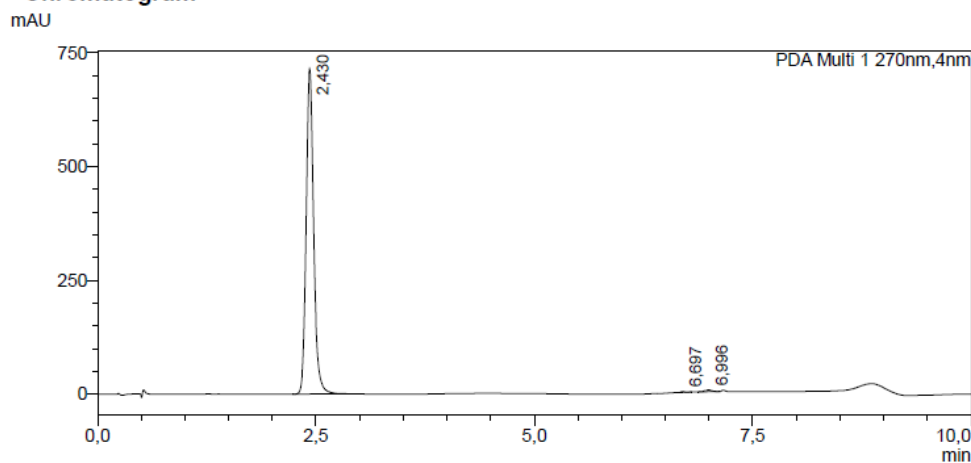
Analysis Report

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Method Filename : screening.lcm
Batch Filename : purity Sept 2024.lcb
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Injection Volume : 0,2 uL
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Date Processed : 16/09/2024 12:55:12

Sample Type : Unknown
Acquired by : System Administrator
Processed by : System Administrator

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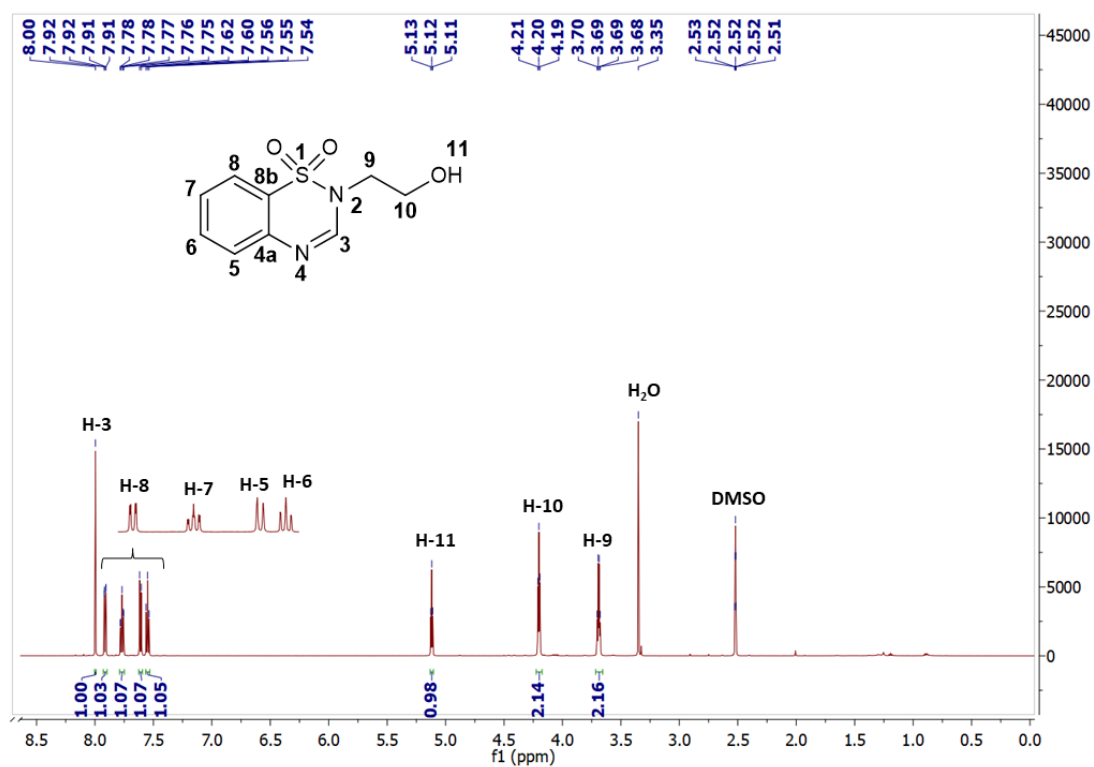
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PDA Ch1 270nm

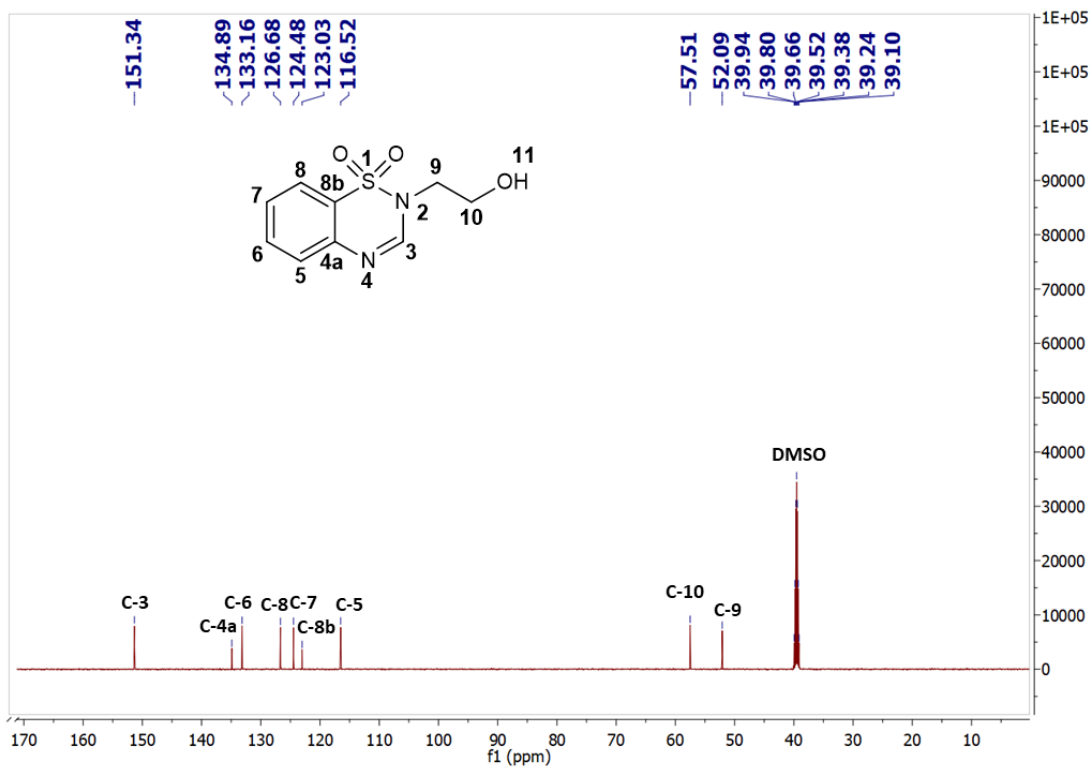
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1	2,430	4275689	99,408
2	6,697	5100	0,119
3	6,996	20361	0,473
Total		4301151	100,000

2-(2-Hydroxyethyl)-2*H*-benzo[e][1,2,4]thiadiazine-1,1-dioxide (2)

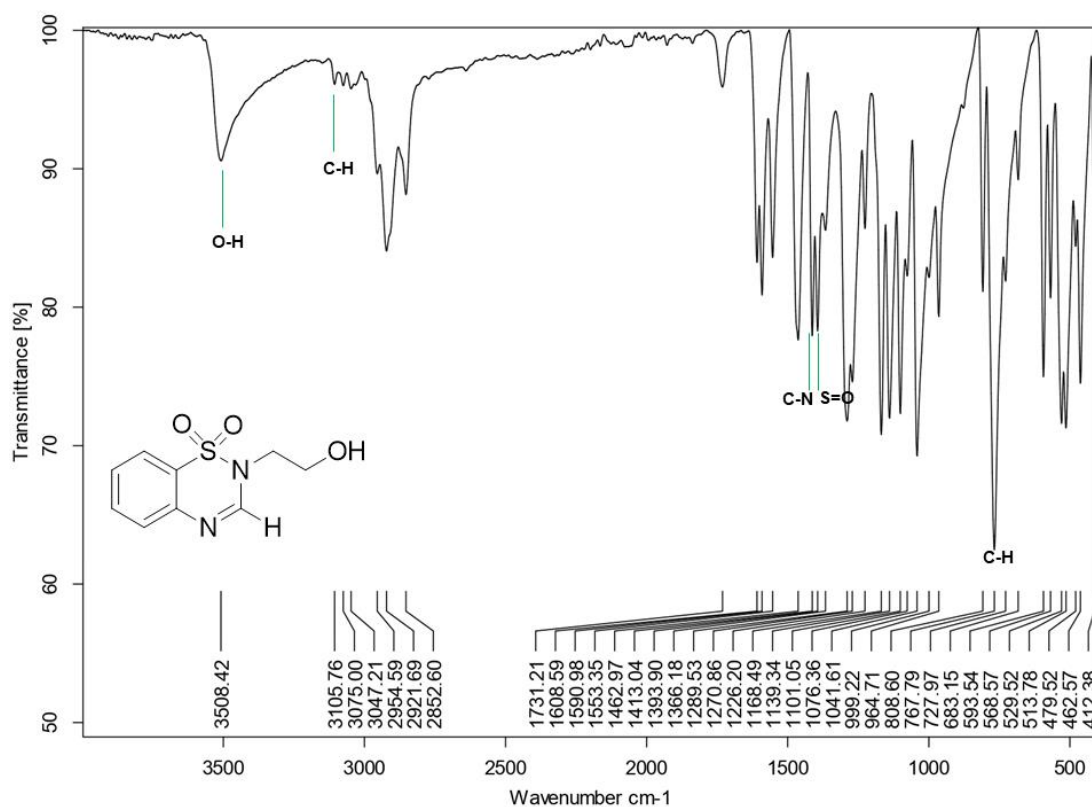
¹H NMR in DMSO



¹³C NMR in DMSO



IR Spectrum



HRMS

Mass Spectrum SmartFormula Report

Analysis Info

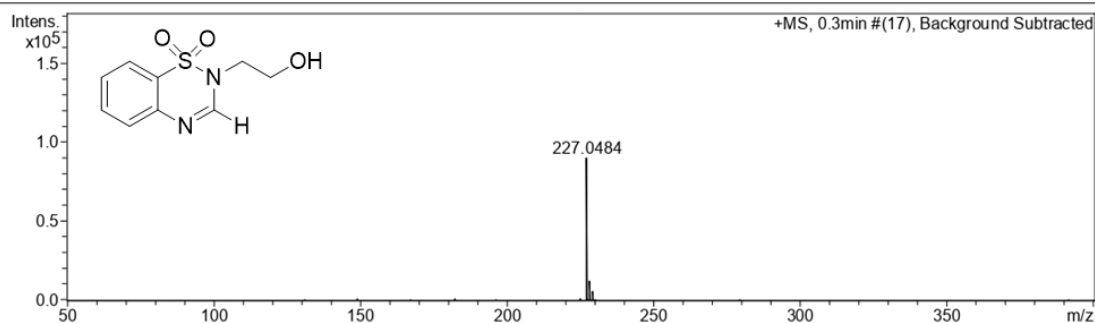
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 Sample Name NH-9
 Comment

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Operator Dr JHL Jordaan
 Instrument / Ser# micrOTOF-Q II 2010390

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1600 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
227.0484	1	C ₉ H ₁₁ N ₂ O ₃ S	100.00	227.0485	0.0	0.2	12.6	5.5	even	ok

HPLC Purity



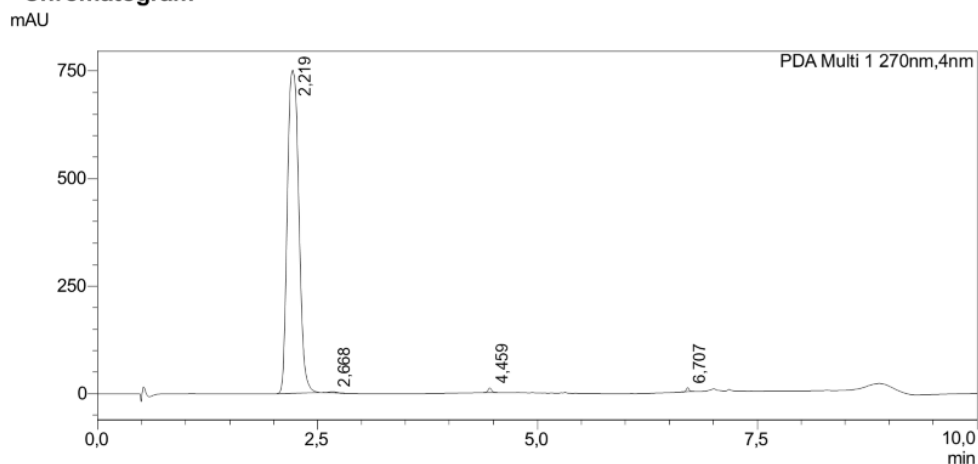
Analysis Report

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Sample ID : NH-02
Data Filename : NH-02_001.lcd
Method Filename : screening.lcm
Batch Filename : purity Sept 2024.lcb
Vial # : 1-3
Injection Volume : 1 uL
Date Acquired : 16/09/2024 13:21:59
Date Processed : 16/09/2024 13:32:02

Sample Type : Unknown
Acquired by : System Administrator
Processed by : System Administrator

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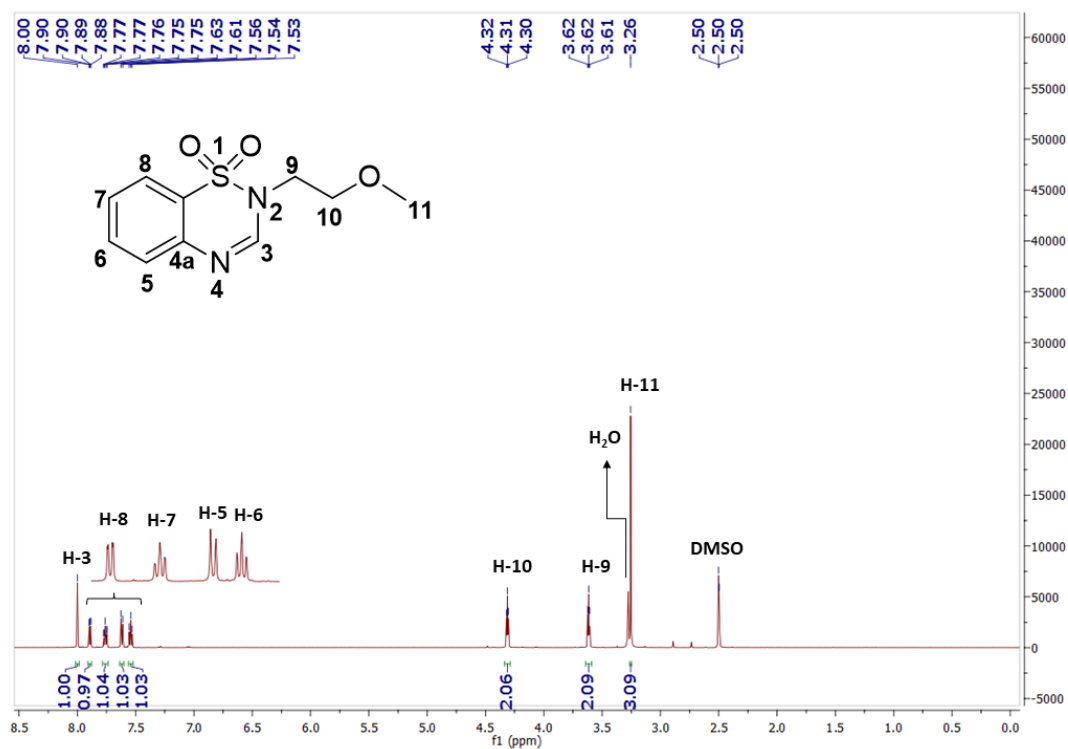
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PDA Ch1 270nm

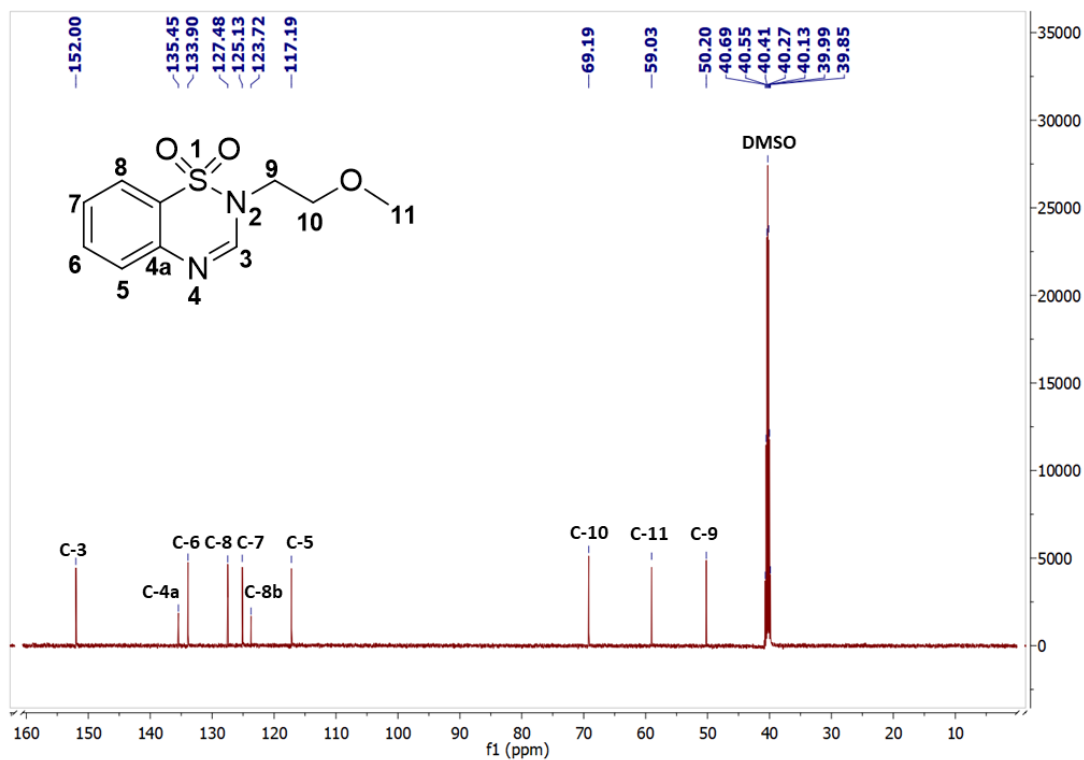
Peak#	Ret. Time	Area	Area%
1	2,219	6825613	98,951
2	2,668	18144	0,263
3	4,459	32850	0,476
4	6,707	21374	0,310
Total		6897981	100,000

2-(2-Methoxyethyl)-2*H*-benzo[*e*][1,2,4]thiadiazine-1,1-dioxide (3)

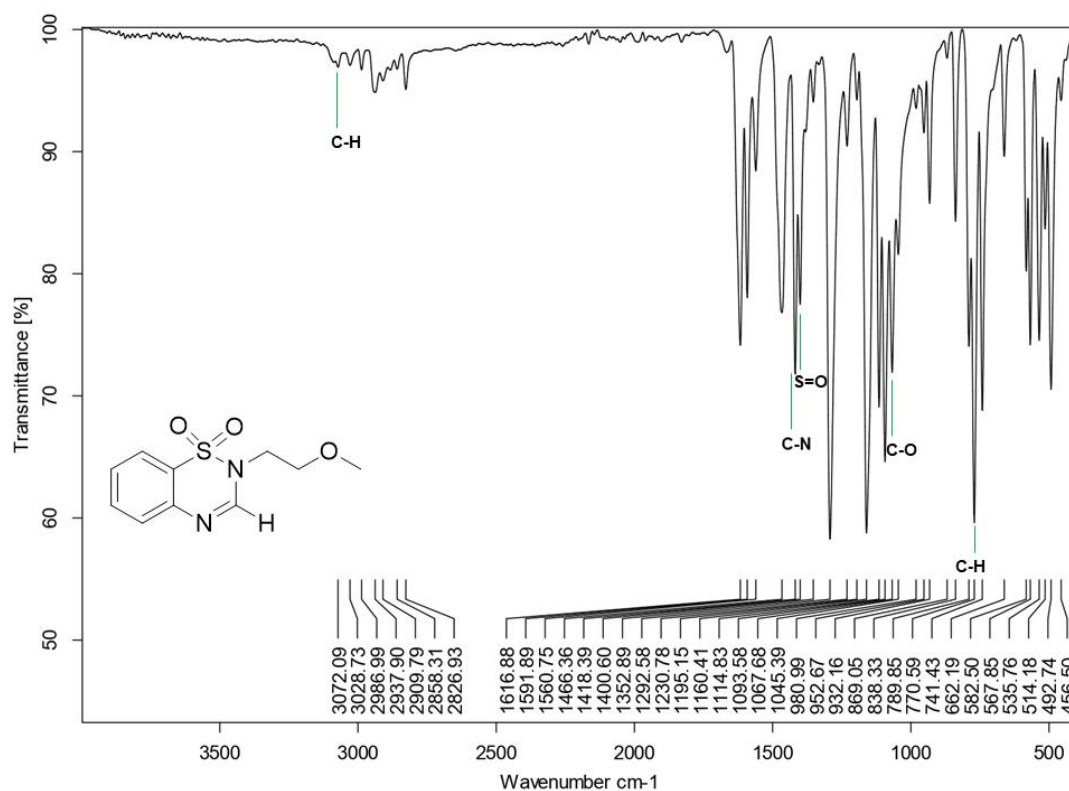
¹H NMR in DMSO



¹³C NMR in DMSO



IR Spectrum



HRMS

Mass Spectrum SmartFormula Report

Analysis Info

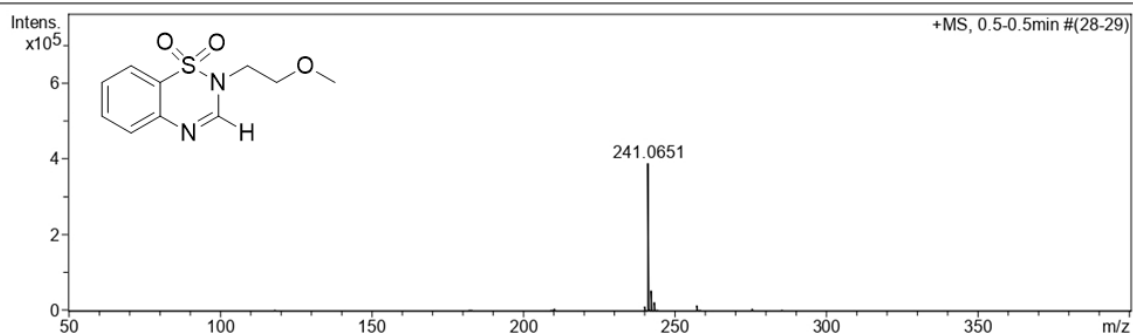
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 Method tune_low no focus50-1600da31052021.m
 Sample Name NH-7
 Comment

Acquisition Date 10/5/2021 1:45:00 PM

Operator Dr JHL Jordaan
 Instrument / Ser# micrOTOF-Q II 2010390

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1600 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
241.0651	1	C 10 H 13 N 2 O 3 S	100.00	241.0641	-1.0	-4.1	5.7	5.5	even	ok

HPLC Purity



Analysis Report

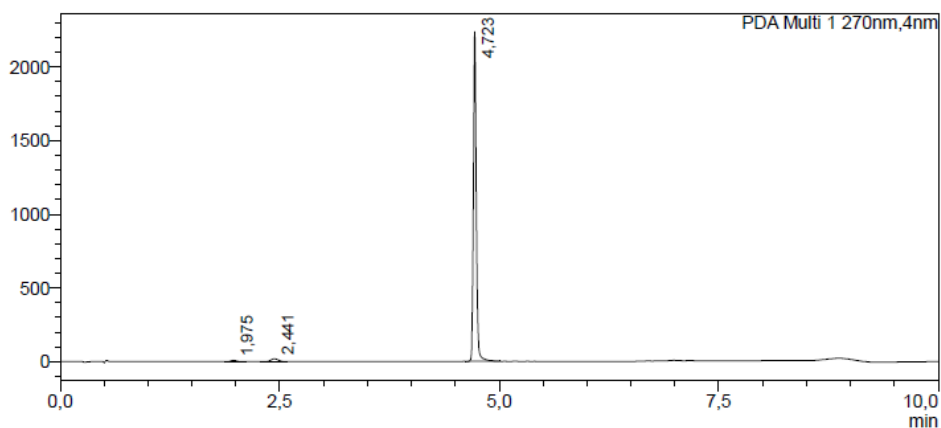
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Sample ID : NH-03
Data Filename : NH-03_005.lcd
Method Filename : screening.lcm
Batch Filename : purity Sept 2024.lcb
Vial # : 1-4
Injection Volume : 0,2 uL
Date Acquired : 16/09/2024 11:12:45
Date Processed : 16/09/2024 12:39:59

Sample Type : Unknown
Acquired by : System Administrator
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mAU



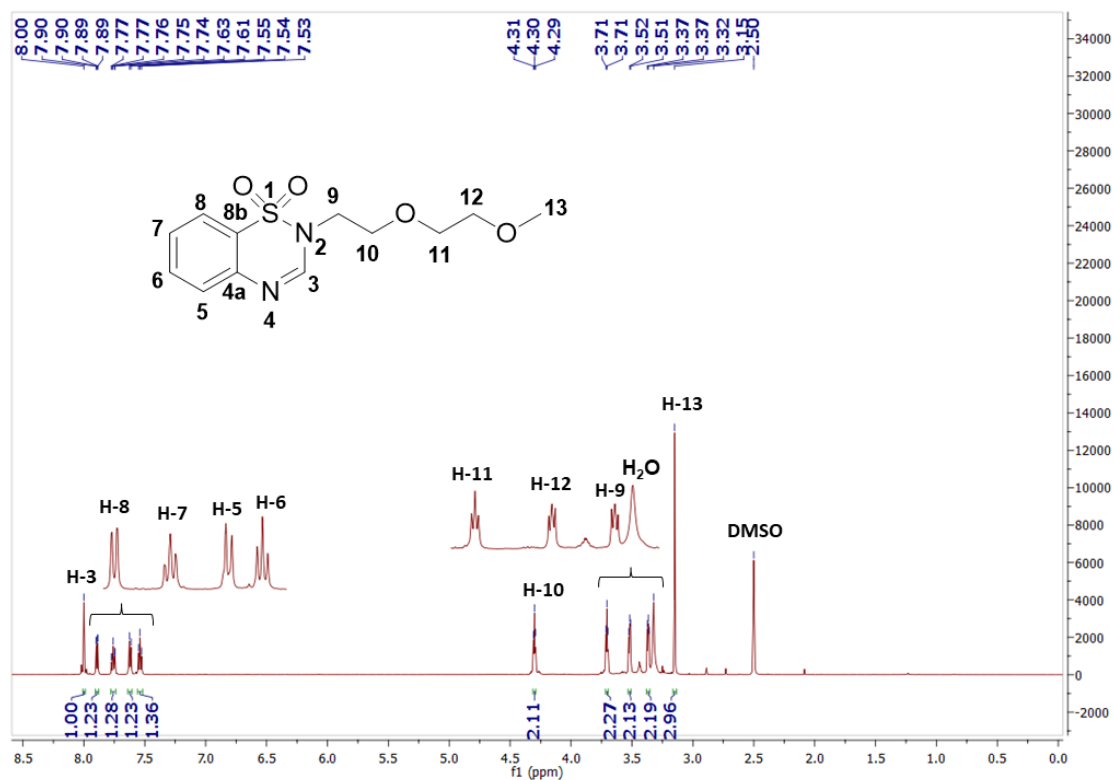
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PDA Ch1 270nm

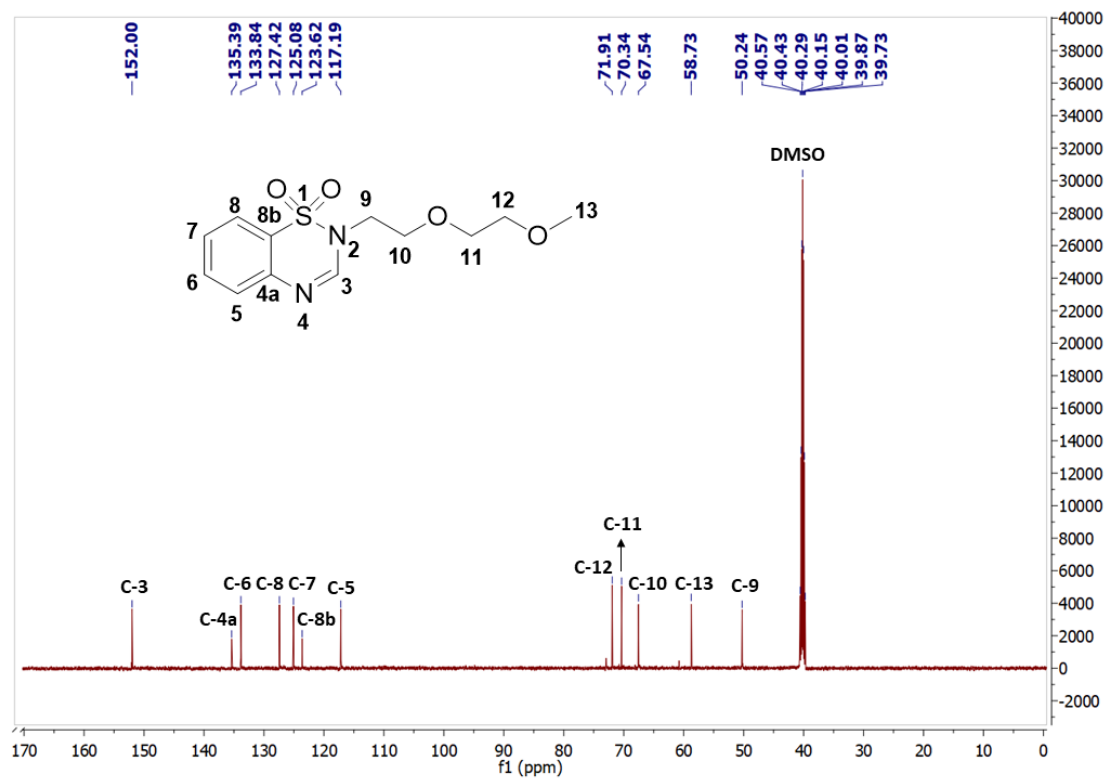
Peak#	Ret. Time	Area	Area%
1	1,975	39267	0,766
2	2,441	110854	2,164
3	4,723	4973145	97,070
Total		5123266	100,000

2-[2-(2-Methoxyethoxy)ethyl]-2*H*-benzo[*e*][1,2,4]thiadiazine-1,1-dioxide (4)

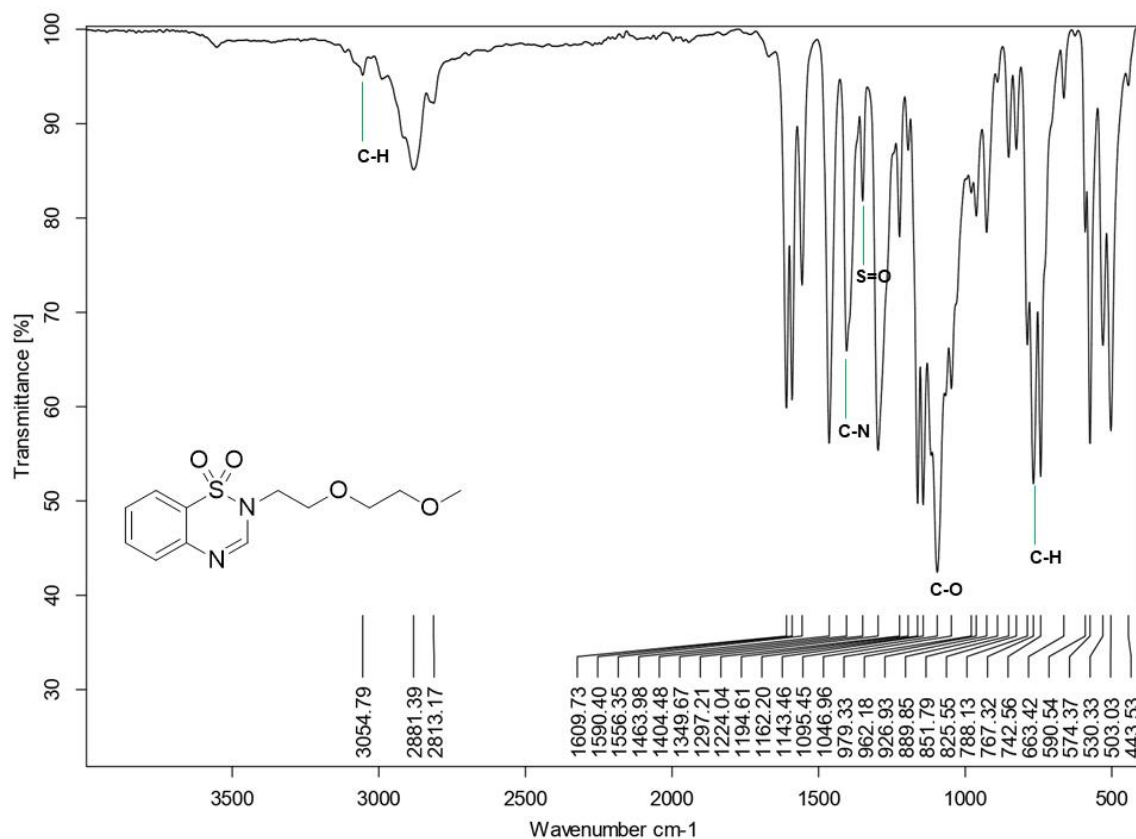
¹H NMR in DMSO



¹³C NMR in DMSO



IR Spectrum



HRMS

Mass Spectrum SmartFormula Report

Analysis Info

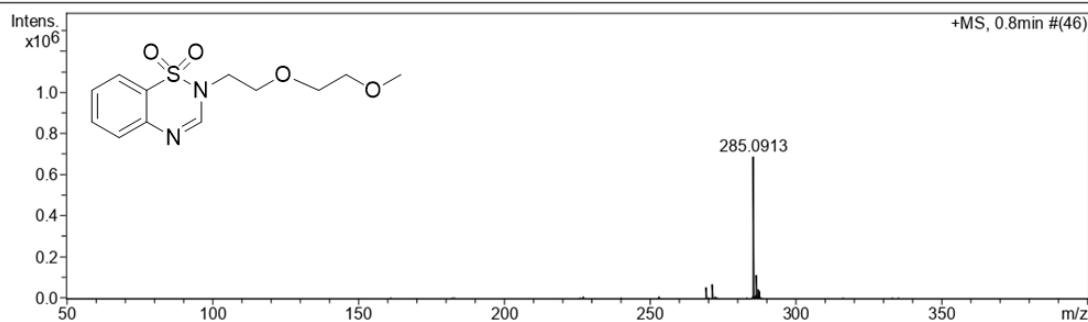
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 Method tune_low no focus50-1600da31052021.m
 Sample Name NH-6
 Comment

Acquisition Date 10/5/2021 1:39:51 PM

Operator Dr JHL Jordaan
 Instrument / Ser# micrOTOF-Q II 2010390

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1600 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSiama	rdb	e ⁻ Conf	N-Rule
285.0913	1	C ₁₂ H ₁₇ N ₂ O ₄ S	100.00	285.0904	-1.0	-3.4	11.2	5.5	even	ok

HPLC Purity



Analysis Report

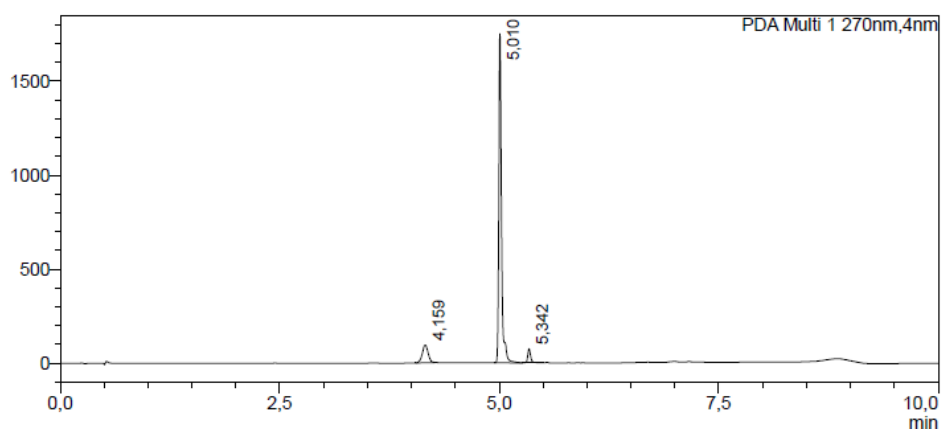
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Sample ID : NH-04
Data Filename : NH-04_006.lcd
Method Filename : screening.lcm
Batch Filename : purity Sept 2024.lcb
Vial # : 1-5
Injection Volume : 0,2 uL
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Date Processed : 16/09/2024 11:58:41

Sample Type : Unknown
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Processed by : System Administrator

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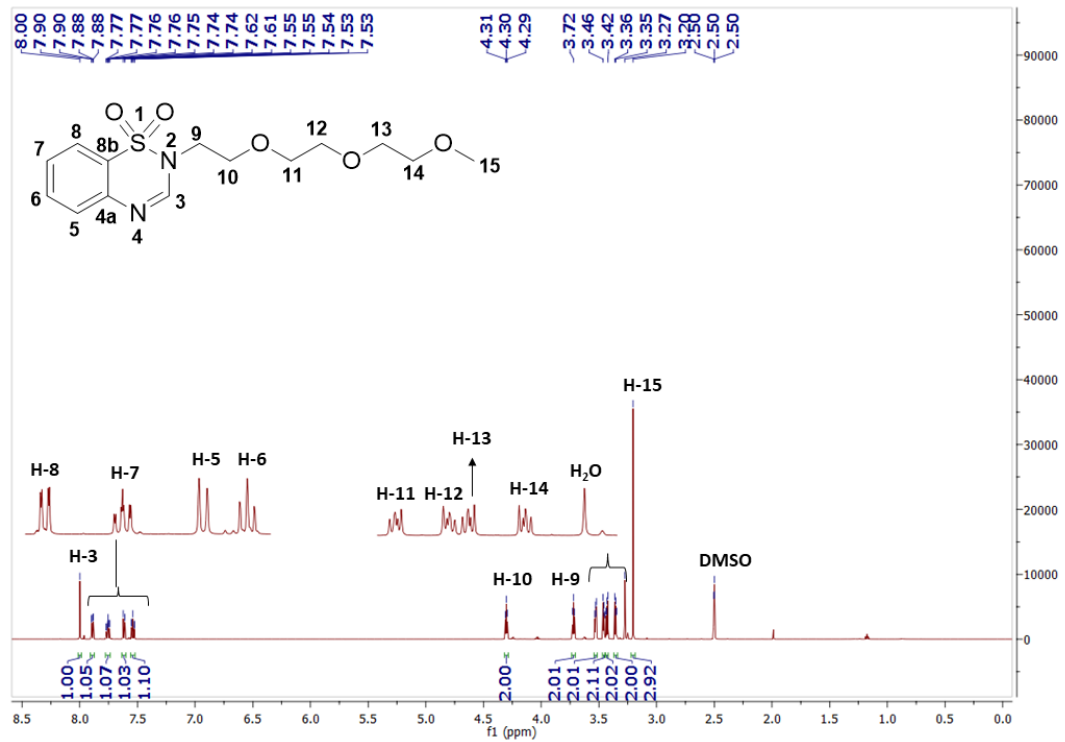
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PDA Ch1 270nm

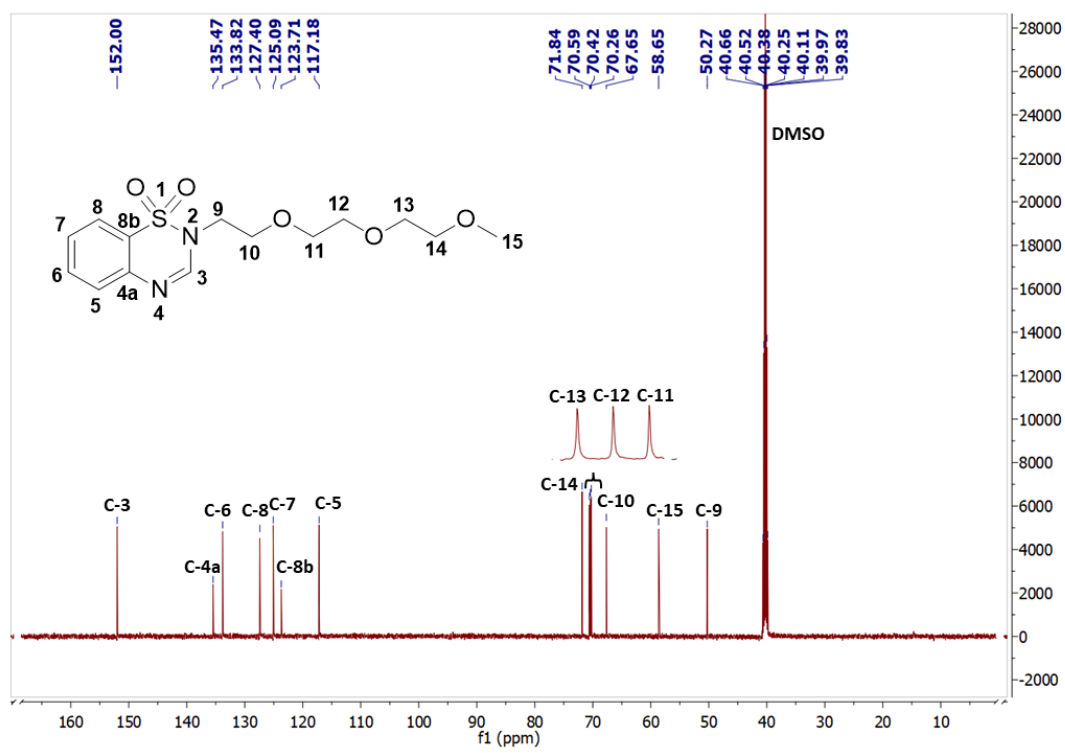
Peak#	Ret. Time	Area	Area%
1	4,159	434961	9,899
2	5,010	3803595	86,559
3	5,342	155646	3,542
Total		4394201	100,000

2-{2-[2-(2-Methoxyethoxy)ethyl]-2H-benzo[e][1,2,4]thiadiazine-1,1-dioxide (5)

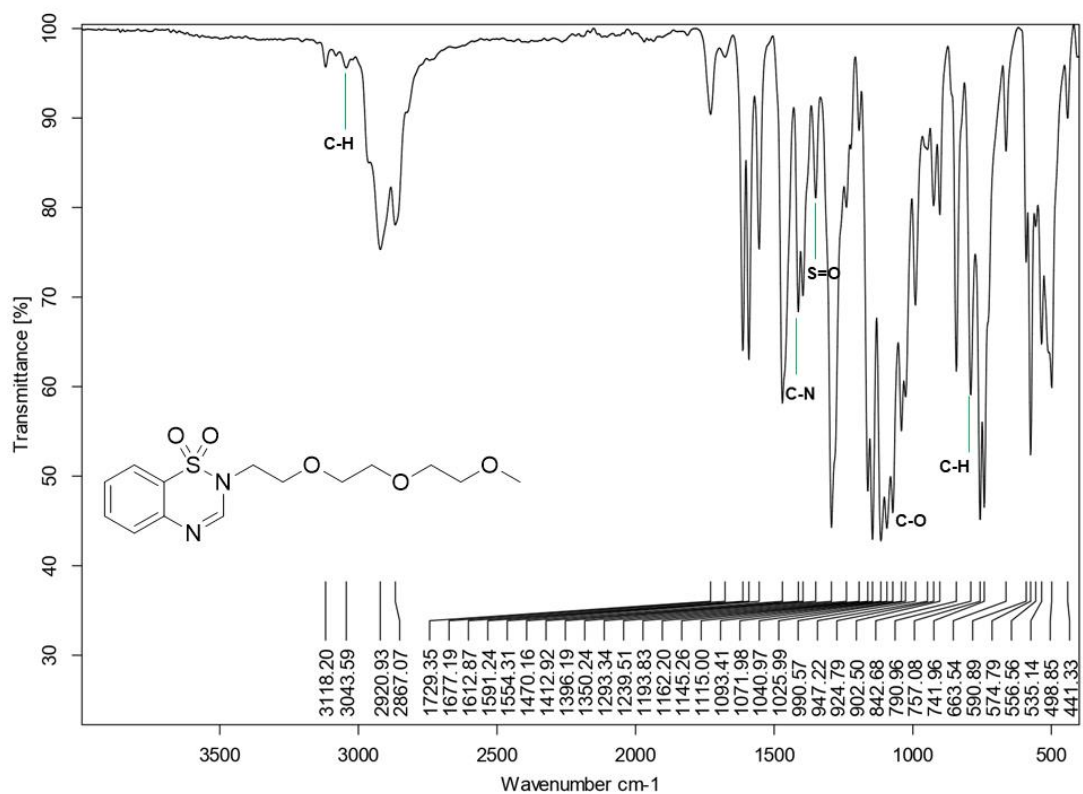
¹H NMR in DMSO



¹³C NMR in DMSO



IR Spectrum



HRMS

Mass Spectrum SmartFormula Report

Analysis Info

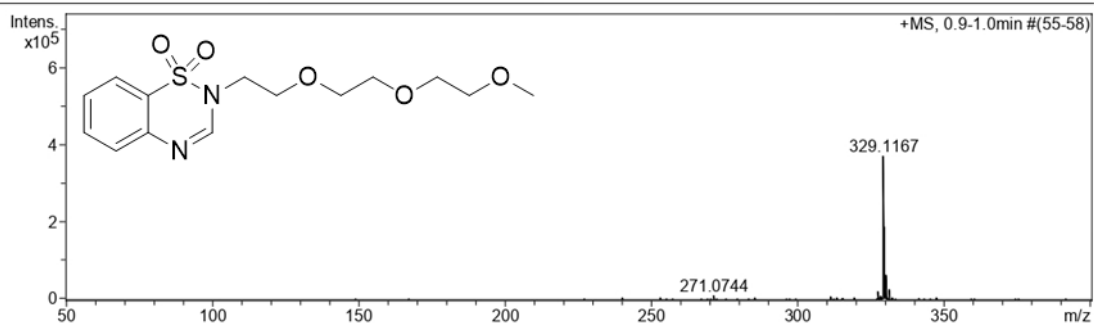
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 Method: tune_low no focus50-1600da31052021.m
 Sample Name: NH-3
 Comment:

Acquisition Date: 10/5/2021 1:33:55 PM

Operator: Dr JHL Jordaan
 Instrument / Ser#: micrOTOF-Q II 2010390

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1600 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
329.1167	1	C ₁₄ H ₂₁ N ₂ O ₅ S	100.00	329.1166	-0.1	-0.4	1.4	5.5	even	ok

HPLC Purity



Analysis Report

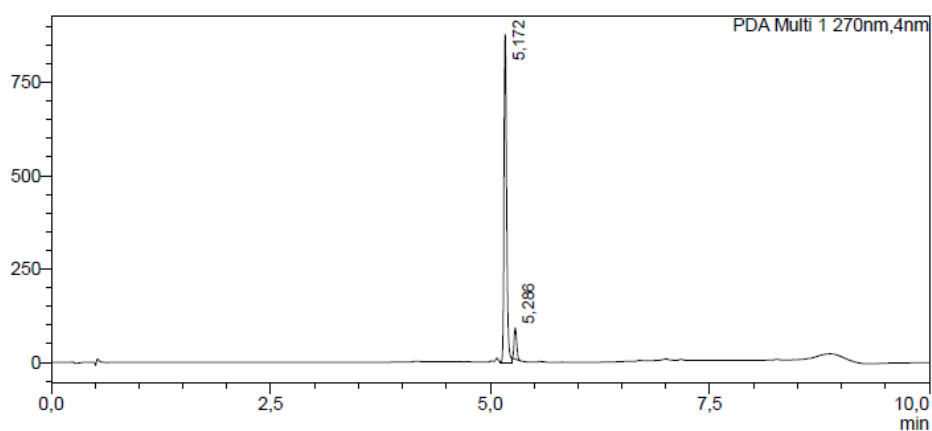
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Method Filename : screening.lcm
Batch Filename : purity Sept 2024.lcb
Vial # : 1-6
Injection Volume : 0,2 uL
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Date Processed : 16/09/2024 11:43:33

Sample Type : Unknown
Acquired by : System Administrator
Processed by : System Administrator

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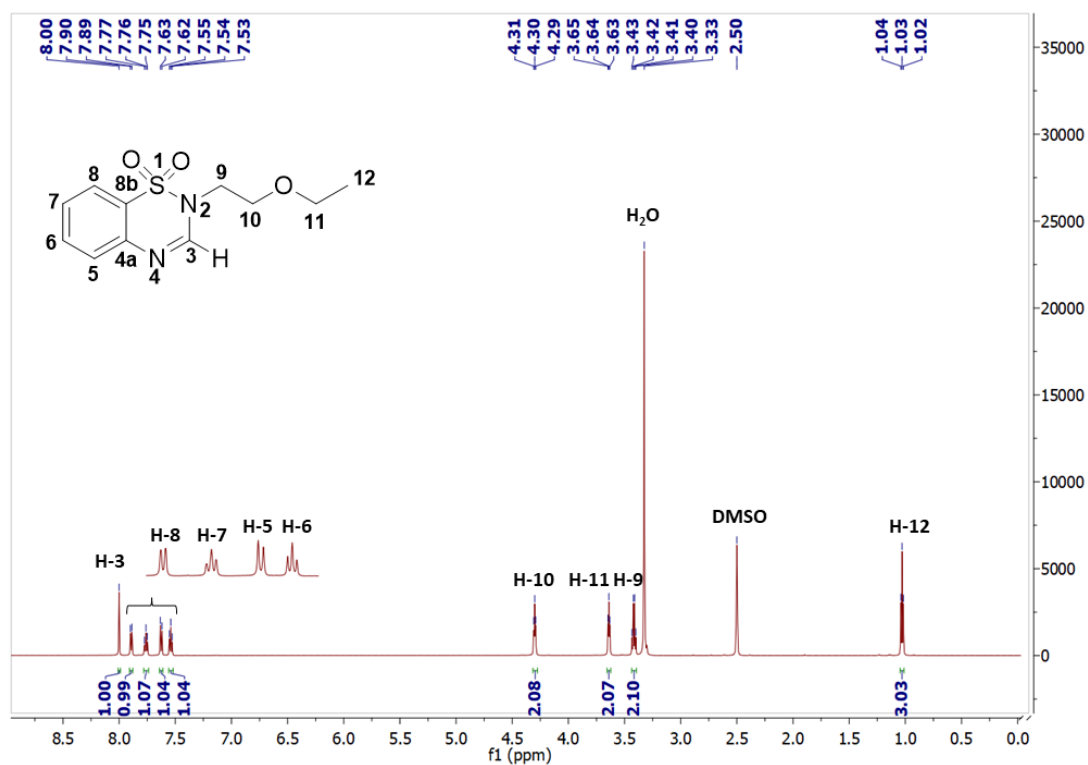
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PDA Ch1 270nm

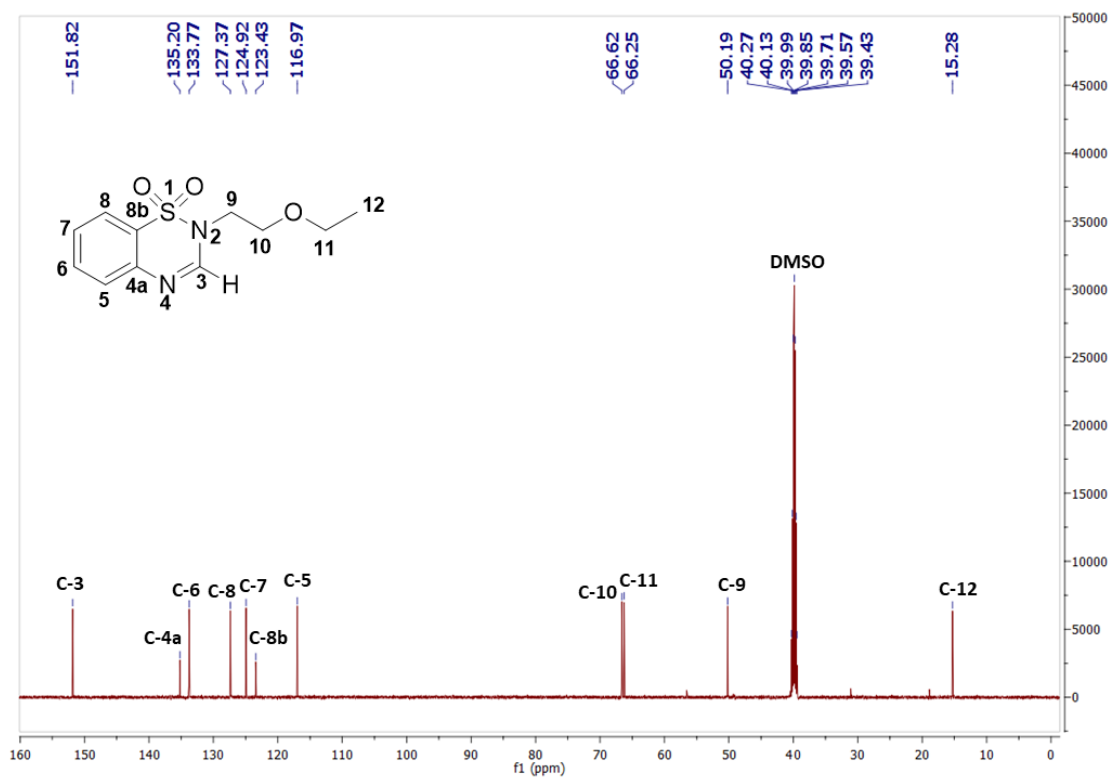
Peak#	Ret. Time	Area	Area%
1	5,172	1836155	91,825
2	5,286	163466	8,175
Total		1999621	100,000

2-(2-Ethoxyethyl)-2H-benzo[e][1,2,4]thiadiazine-1,1-dioxide (6)

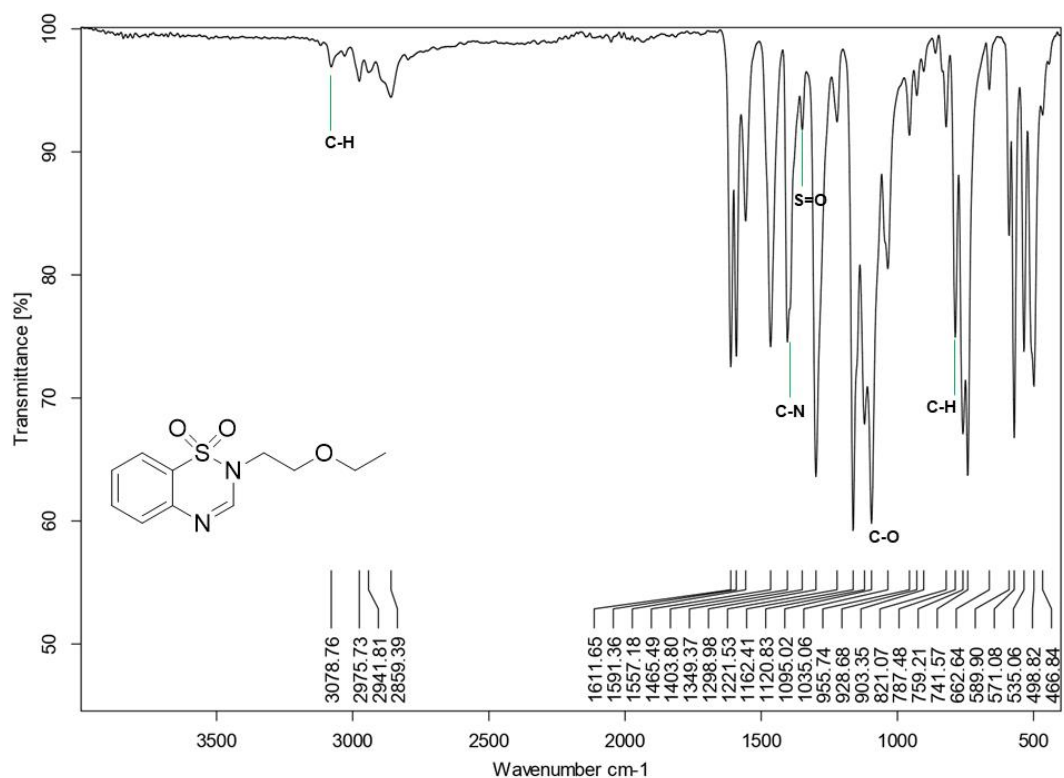
¹H NMR in DMSO



¹³C NMR in DMSO



IR Spectrum



HRMS

Mass Spectrum SmartFormula Report

Analysis Info

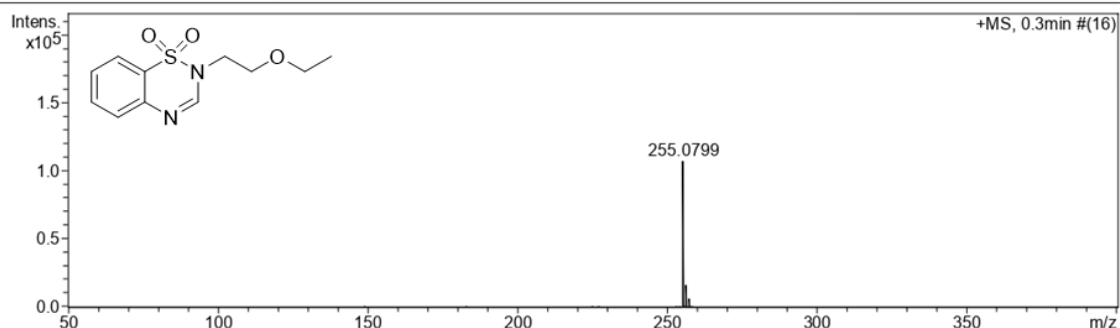
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 Method tune_low no focus50-1600da31052021.m
 Sample Name NH-4
 Comment

Acquisition Date 10/5/2021 1:36:45 PM

Operator Dr JHL Jordaan
 Instrument / Ser# micrOTOF-Q II 2010390

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1600 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
255.0799	1	C 11 H 15 N 2 O 3 S	100.00	255.0798	-0.1	-0.3	8.0	5.5	even	ok

HPLC Purity



Analysis Report

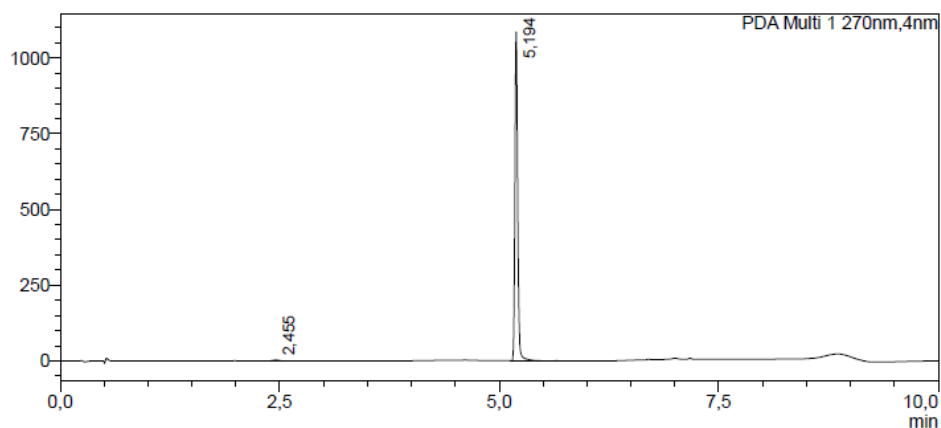
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Sample ID : NH-06
Data Filename : NH-06_008.lcd
Method Filename : screening.lcm
Batch Filename : purity Sept 2024.lcb
Vial # : 1-7
Injection Volume : 0,2 uL
Date Acquired : 16/09/2024 11:43:56
Date Processed : 16/09/2024 11:53:57

Sample Type : Unknown
Acquired by : System Administrator
Processed by : System Administrator

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mAU



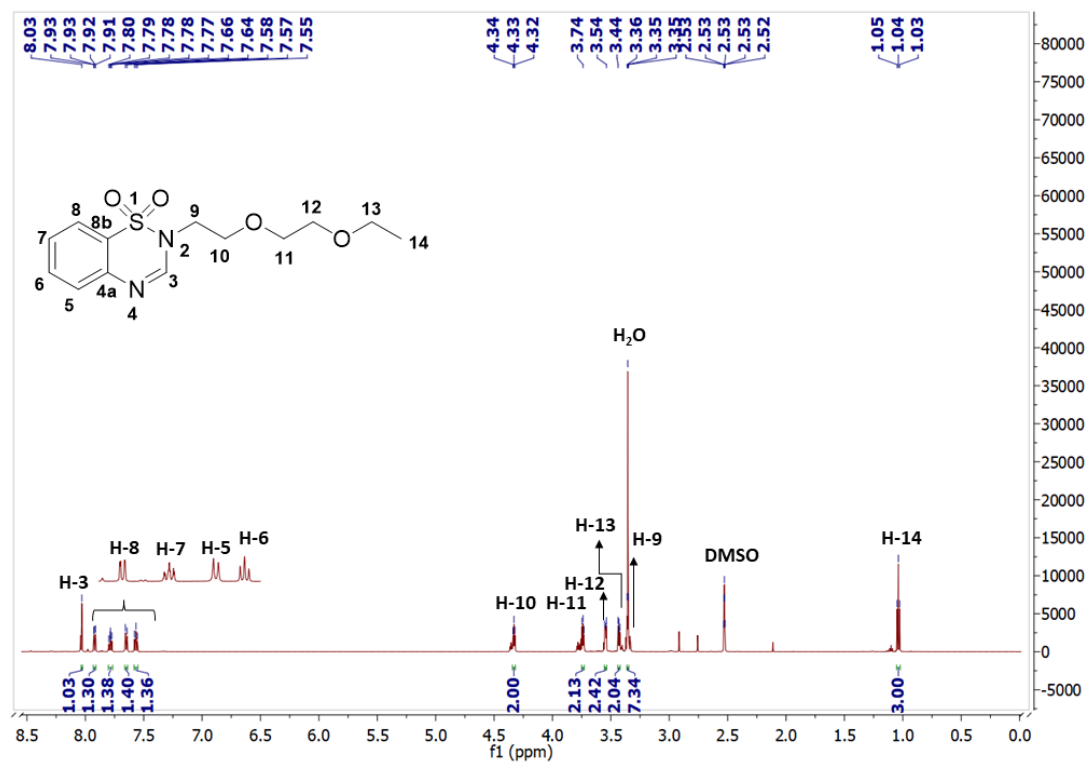
<Peak Table>

PDA Ch1 270nm

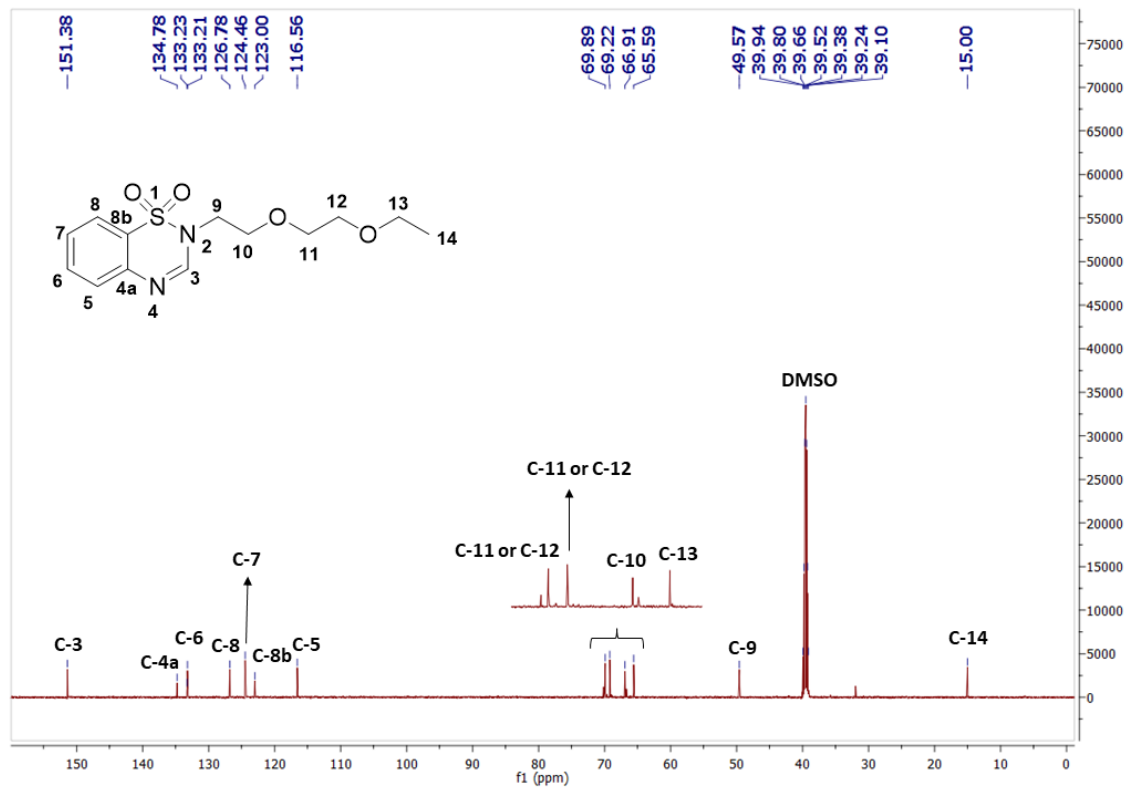
Peak#	Ret. Time	Area	Area%
1	2,455	13802	0,587
2	5,194	2337494	99,413
Total		2351296	100,000

2-[2-(2-Ethoxyethoxy)ethyl]-2H-benzo[e][1,2,4]thiadiazine-1,1-dioxide (7)

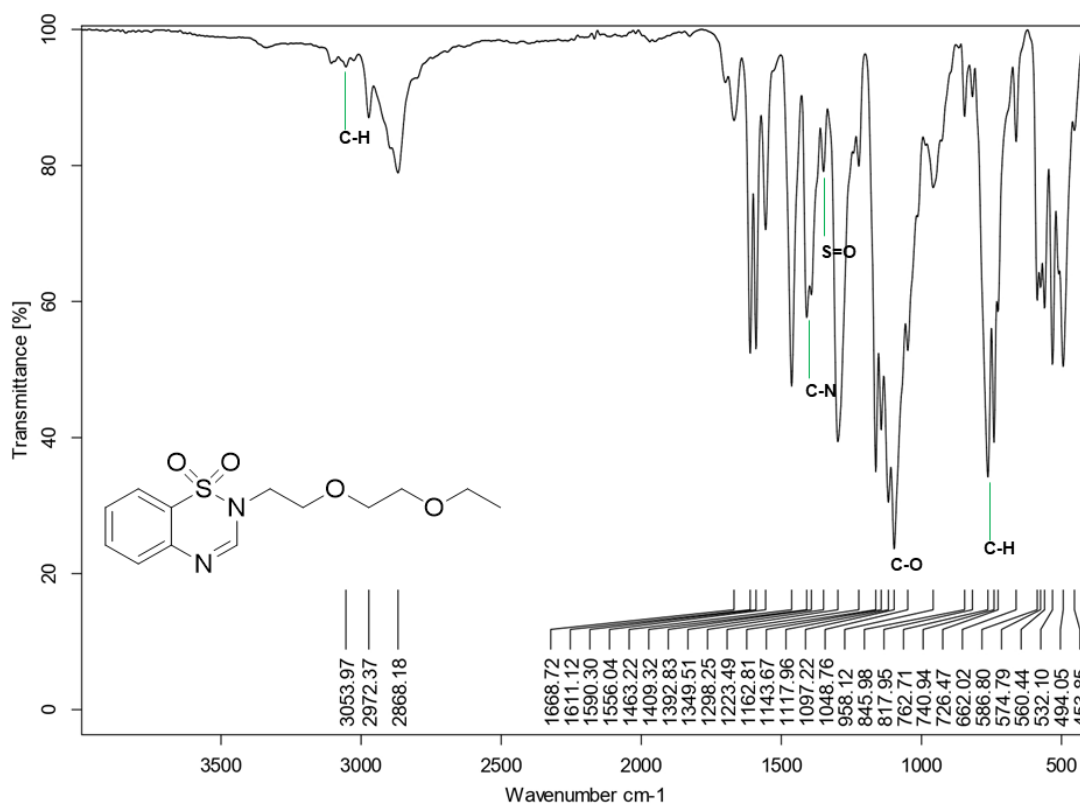
¹H NMR in DMSO



¹³C NMR in DMSO



IR Spectrum



HRMS

Mass Spectrum SmartFormula Report

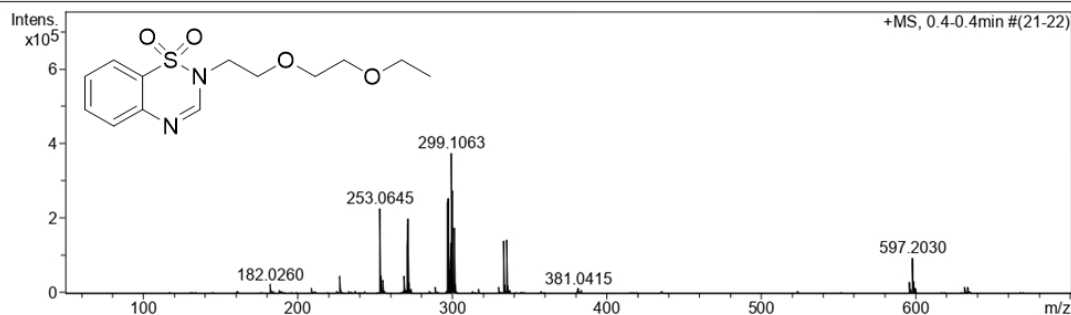
Analysis Info

Analysis Name D:\Data\18112021\LADMS000002.d
 Method tune_low no focus50-1600da31052021.m
 Sample Name NH-11
 Comment

Acquisition Date 11/18/2021 8:41:28 AM
 Operator Dr JHL Jordaan
 Instrument / Ser# micrOTOF-Q II 2010390

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
299.1063	1	C ₁₃ H ₁₉ N ₂ O ₄ S	100.00	299.1060	-0.3	-0.9	355.0	5.5	even	ok

HPLC Purity



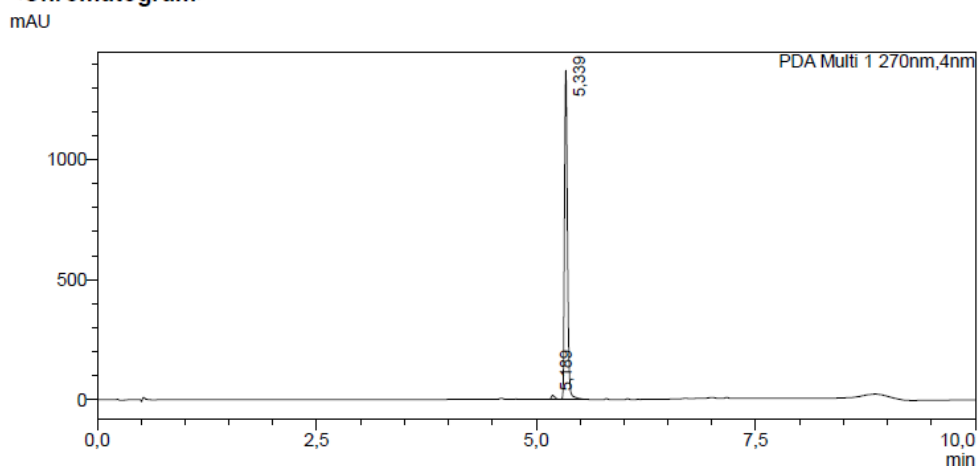
Analysis Report

<Sample Information>

Sample Name : NH-07
Sample ID : NH-07
Data Filename : NH-07_009.lcd
Method Filename : screening.lcm
Batch Filename : purity Sept 2024.lcb
Vial # : 1-8
Injection Volume : 0,2 uL
Date Acquired : 16/09/2024 11:54:20
Date Processed : 16/09/2024 12:48:13

Sample Type : Unknown
Acquired by : System Administrator
Processed by : System Administrator

<Chromatogram>

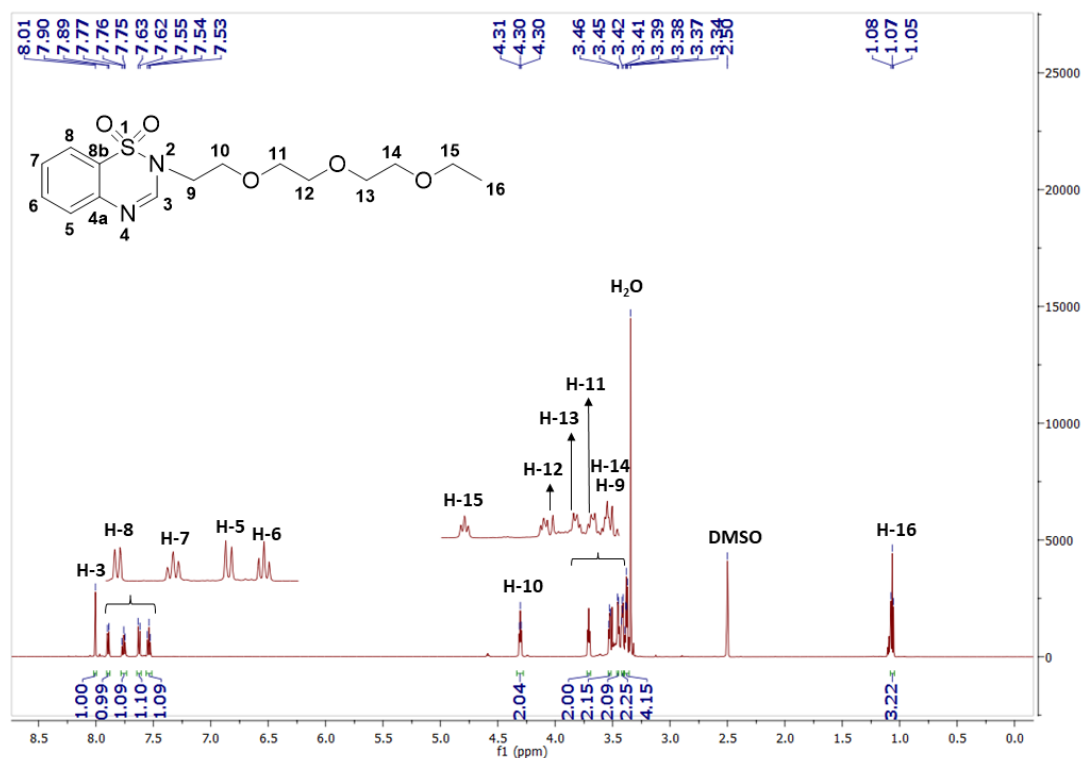


<Peak Table>

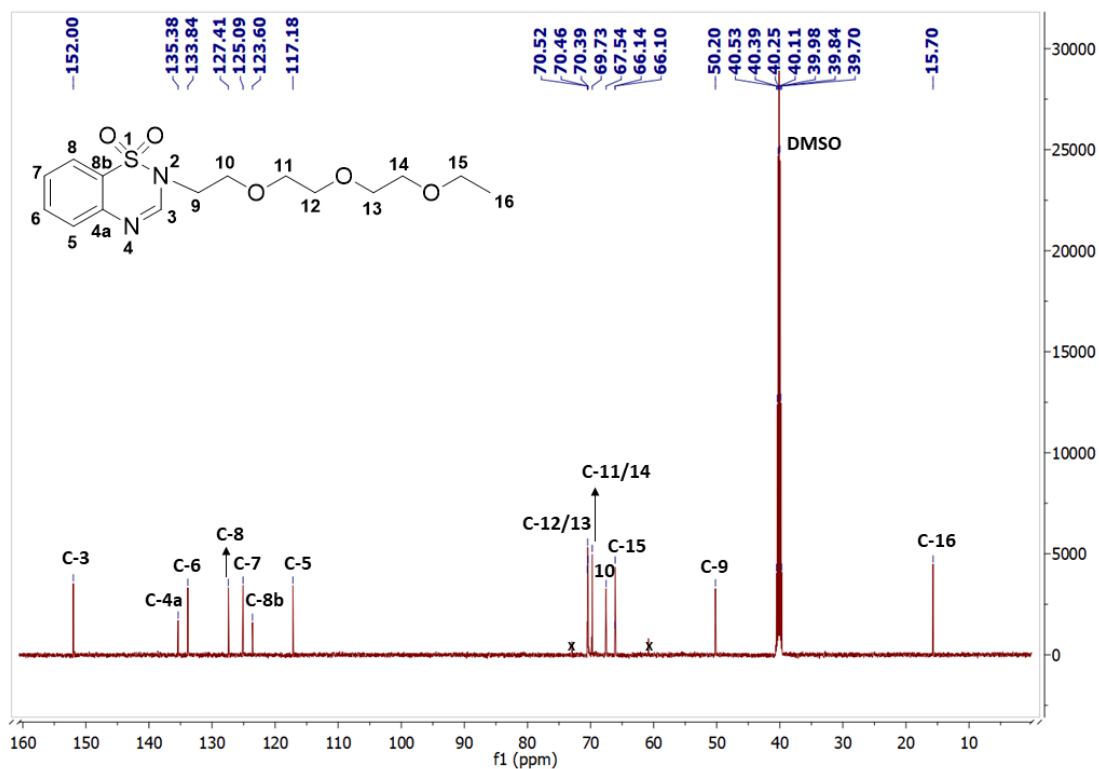
PDA Ch1 270nm			
Peak#	Ret. Time	Area	Area%
1	5,189	48583	1,529
2	5,339	3128918	98,471
Total		3177501	100,000

2-{2-[2-(2-Ethoxyethoxy)ethyl]-2H-benzo[e][1,2,4]thiadiazine-1,1-dioxide (8)

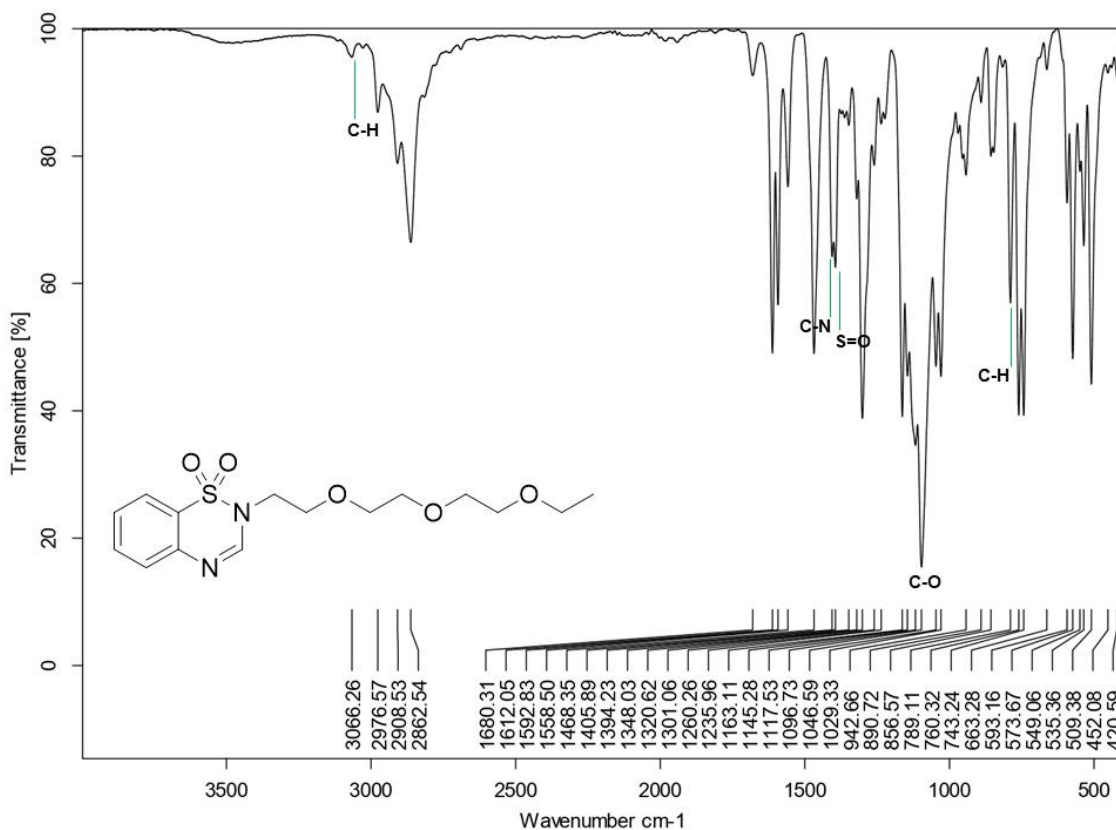
¹H NMR in DMSO



¹³C NMR in DMSO



IR Spectrum



HRMS

Mass Spectrum SmartFormula Report

Analysis Info

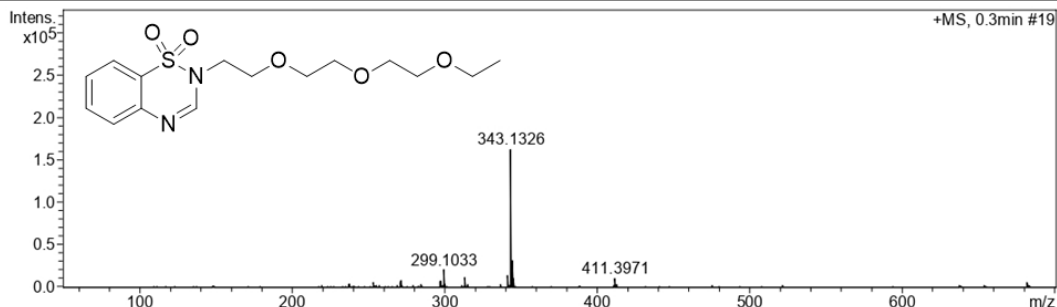
Analysis Name D:\Data\18112021\LADMS000005.d
 Method tune_low no focus50-1600da31052021.m
 Sample Name NH-13
 Comment

Acquisition Date 11/18/2021 8:49:09 AM

Operator Dr JHL Jordaan
 Instrument / Ser# micrOTOF-Q II 2010390

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1600 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdB	e ⁻ Conf	N-Rule
343.1326	1	C ₁₅ H ₂₃ N ₂ O ₅ S	100.00	343.1322	-0.3	-1.0	8.0	5.5	even	ok

HPLC Purity



Analysis Report

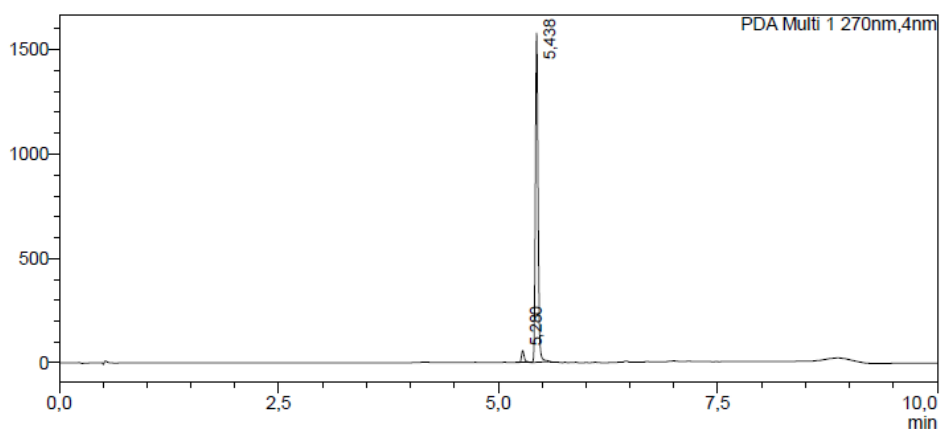
<Sample Information>

Sample Name : NH-08
Sample ID : NH-08
Data Filename : NH-08_010.lcd
Method Filename : screening.lcm
Batch Filename : purity Sept 2024.lcb
Vial # : 1-9
Injection Volume : 0,2 uL
Date Acquired : 16/09/2024 12:04:44
Date Processed : 16/09/2024 12:49:40

Sample Type : Unknown
Acquired by : System Administrator
Processed by : System Administrator

<Chromatogram>

mAU



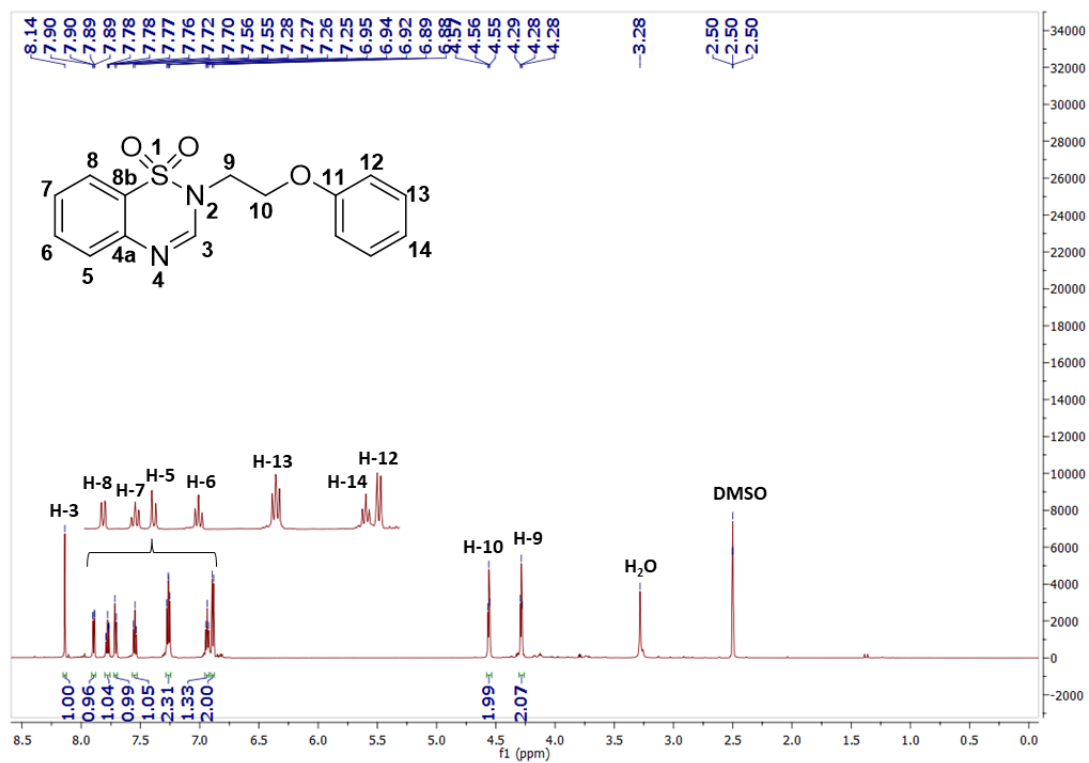
<Peak Table>

PDA Ch1 270nm

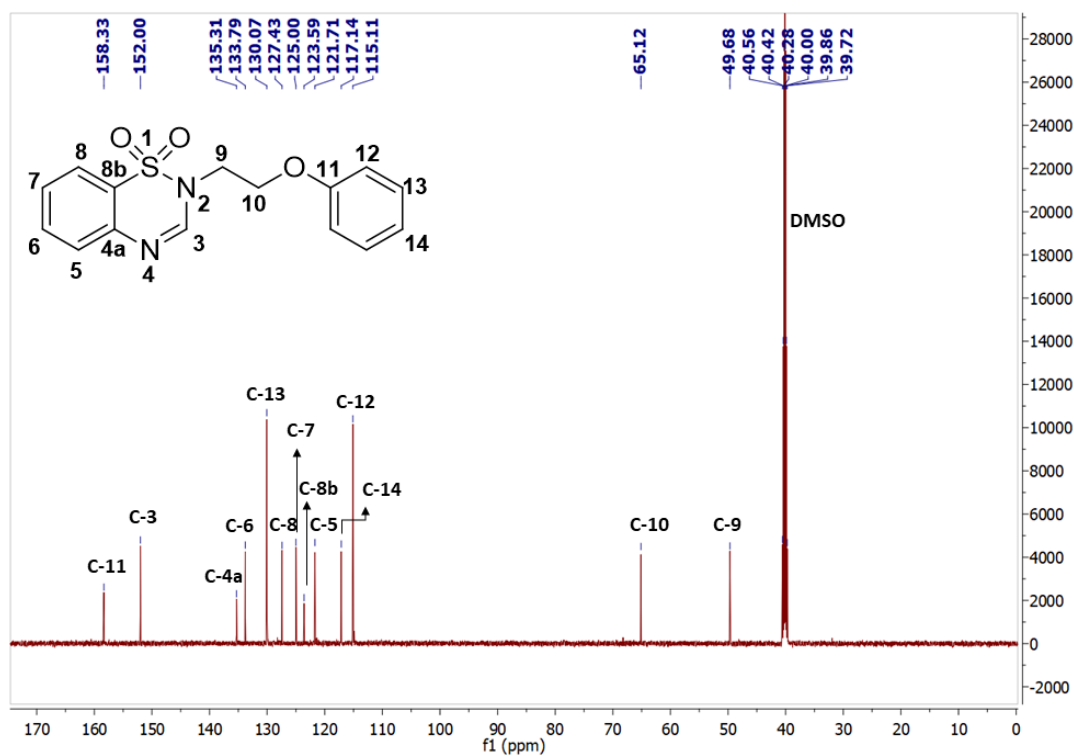
Peak#	Ret. Time	Area	Area%
1	5,280	126266	3,732
2	5,438	3256746	96,268
Total		3383012	100,000

2-(2-Phenoxyethyl)-2*H*-benzo[e][1,2,4]thiadiazine-1,1-dioxide (9)

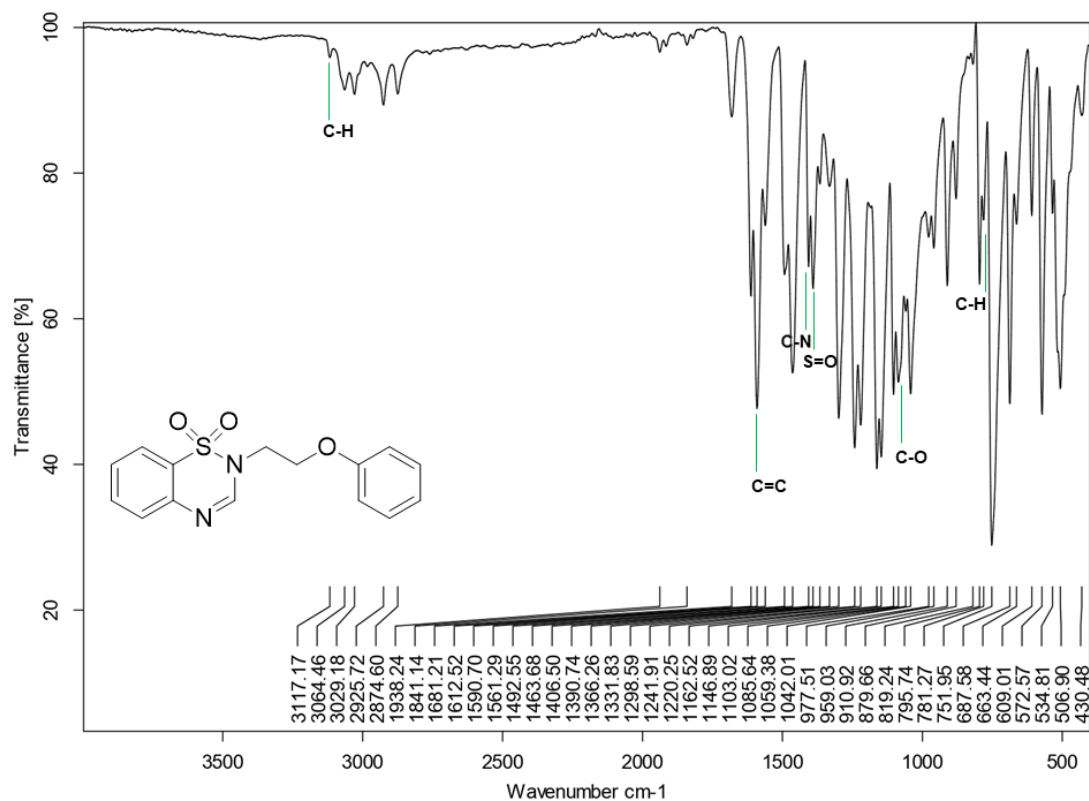
¹H NMR in DMSO



¹³C NMR in DMSO



IR Spectrum



HRMS

Mass Spectrum SmartFormula Report

Analysis Info

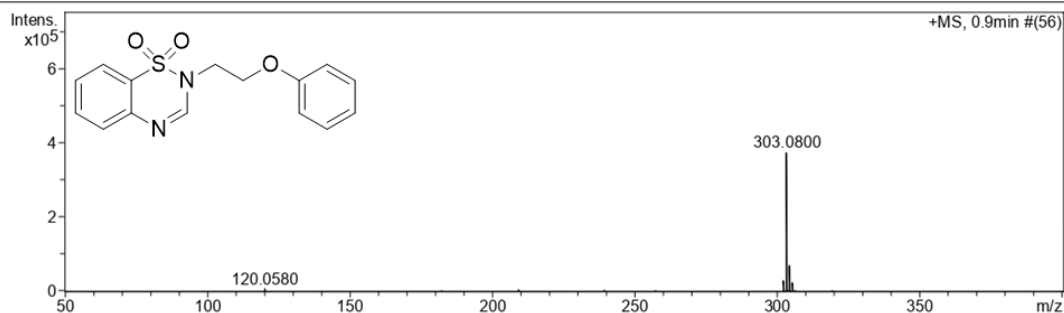
Analysis Name D:\Data\05102021\LADMS000009.d
 Method tune_low no focus50-1600da31052021.m
 Sample Name NH-5
 Comment

Acquisition Date 10/5/2021 1:37:45 PM

Operator Dr JHL Jordaan
 Instrument / Ser# micrOTOF-Q II 2010390

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1600 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
303.0800	1	C ₁₅ H ₁₅ N ₂ O ₃ S	100.00	303.0798	-0.2	-0.6	5.1	9.5	even	ok

HPLC Purity



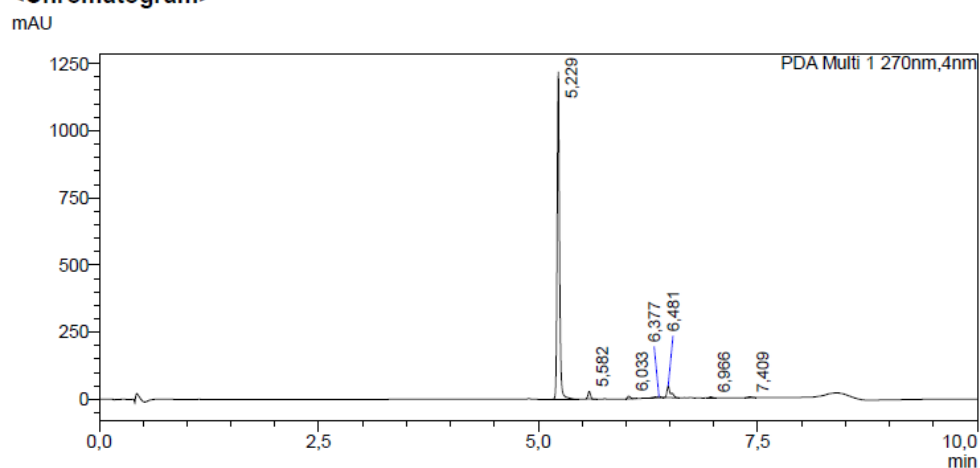
Analysis Report

<Sample Information>

Sample Name : NH-09 HPLC grade001
Sample ID : NH-09 HPLC grade001
Data Filename : NH-09 HPLC grade001_006.lcd
Method Filename : screening.lcm
Batch Filename : purity Sept 2024.lcb
Vial # : 1-17
Injection Volume : 3 uL
Date Acquired : 17/09/2024 10:00:43
Date Processed : 17/09/2024 10:10:44

Sample Type : Unknown
Acquired by : System Administrator
Processed by : System Administrator

<Chromatogram>

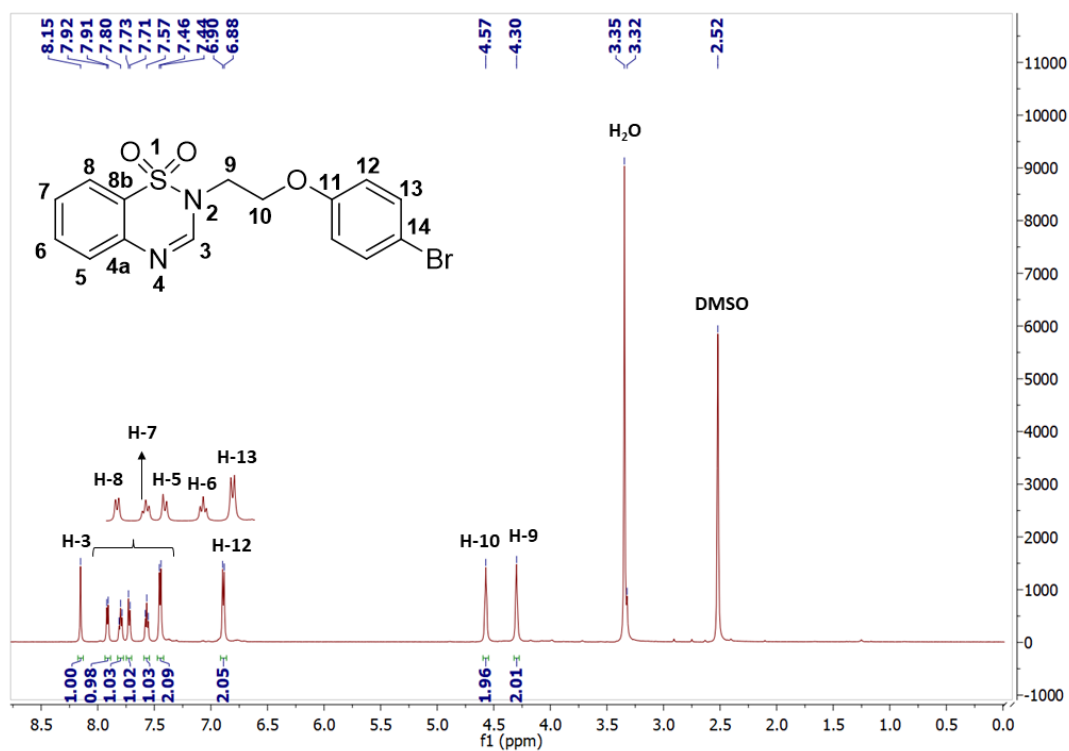


<Peak Table>

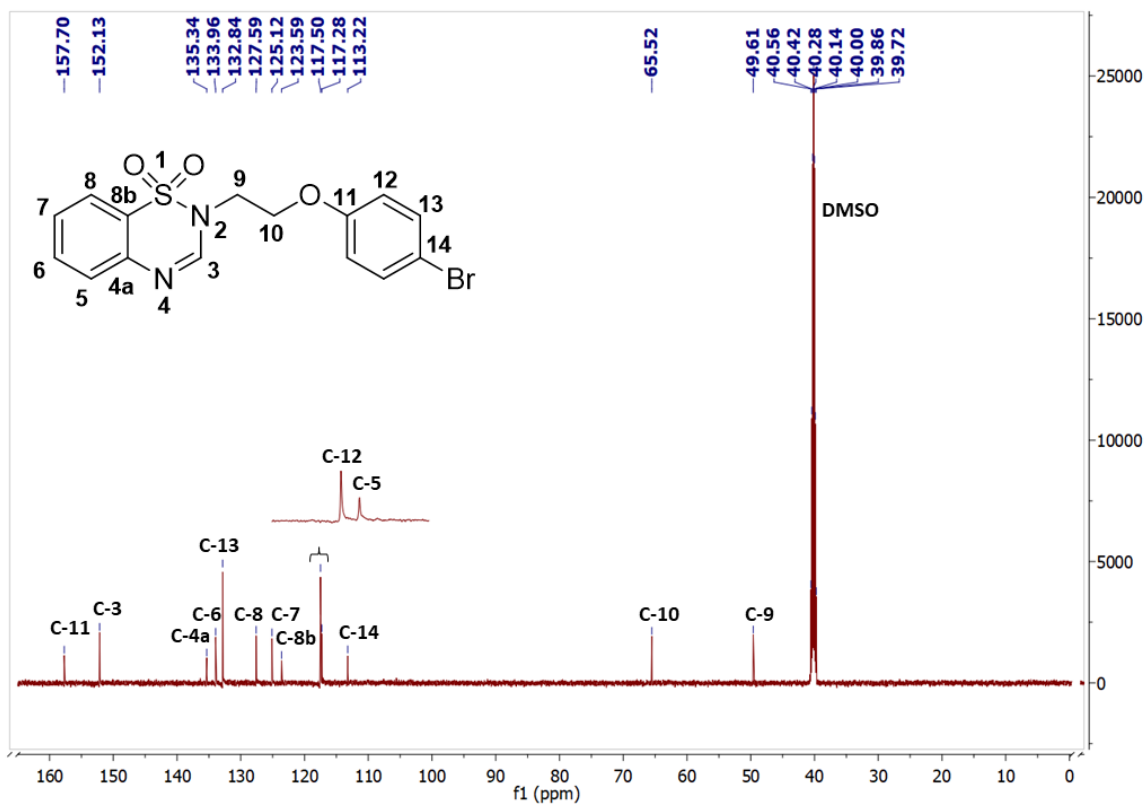
Peak#	Ret. Time	Area	Area%
1	5,229	2409992	90,460
2	5,582	53477	2,007
3	6,033	22499	0,845
4	6,377	27885	1,047
5	6,481	131514	4,936
6	6,966	9057	0,340
7	7,409	9723	0,365
Total		2664147	100,000

2-[2-(4-Bromophenoxy)ethyl]-2H-benzo[e][1,2,4]thiadiazine-1,1-dioxide (10)

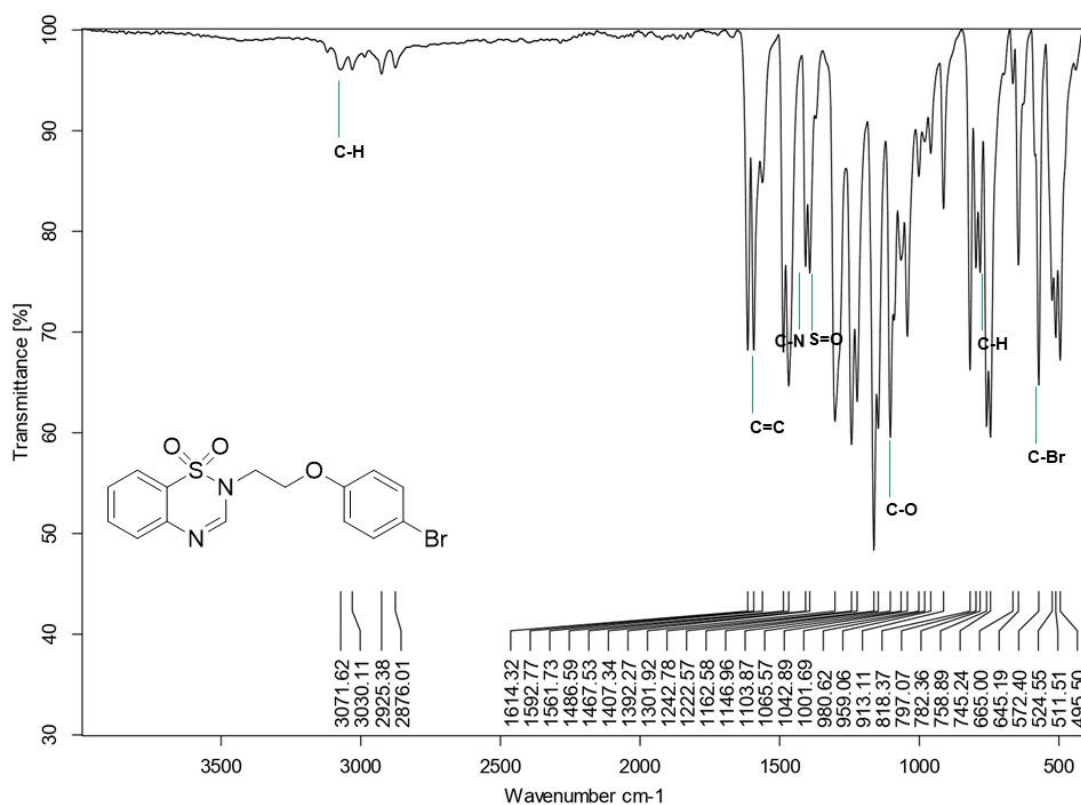
¹H NMR in DMSO



¹³C NMR in DMSO



IR Spectrum



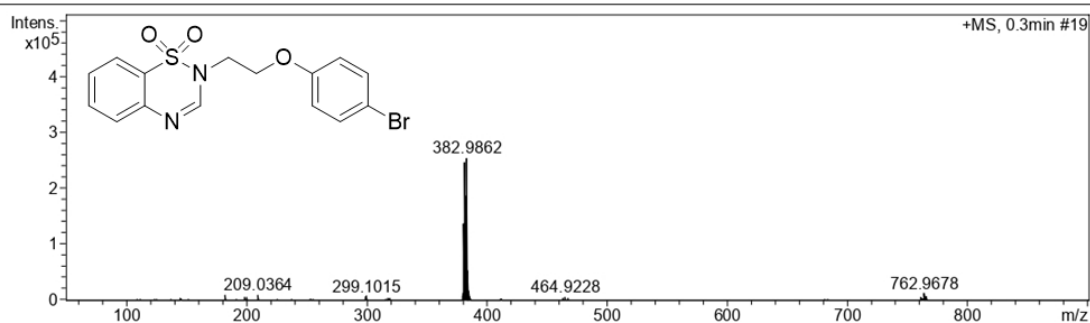
HRMS

Mass Spectrum SmartFormula Report

Analysis Info		Acquisition Date	
Analysis Name	D:\Data\18112021\LADMS000003.d	11/18/2021 8:42:22 AM	
Method	tune_low no focus50-1600da31052021.m	Operator	Dr JHL Jordaan
Sample Name	NH-12	Instrument / Ser#	micrOTOF-Q II 2010390
Comment			

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdB	e ⁻ Conf	N-Rule
380.9884	1	C ₁₅ H ₁₄ BrN ₂ O ₃ S	100.00	380.9903	1.9	5.0	229.5	9.5	even	ok

HPLC Purity



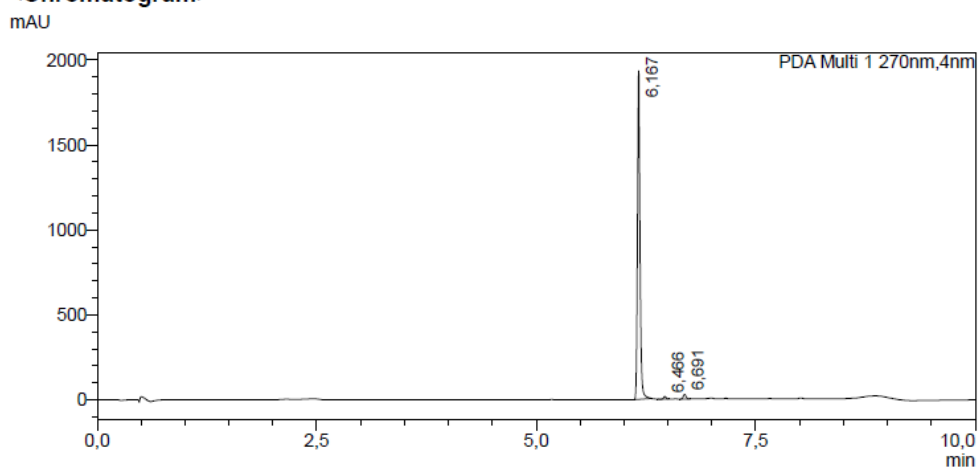
Analysis Report

<Sample Information>

Sample Name : NH-10
Sample ID : NH-10
Data Filename : NH-10_003.lcd
Method Filename : screening.lcm
Batch Filename : purity Sept 2024.lcb
Vial # : 1-11
Injection Volume : 3 uL
Date Acquired : 16/09/2024 13:42:48
Date Processed : 16/09/2024 13:52:49

Sample Type : Unknown
Acquired by : System Administrator
Processed by : System Administrator

<Chromatogram>



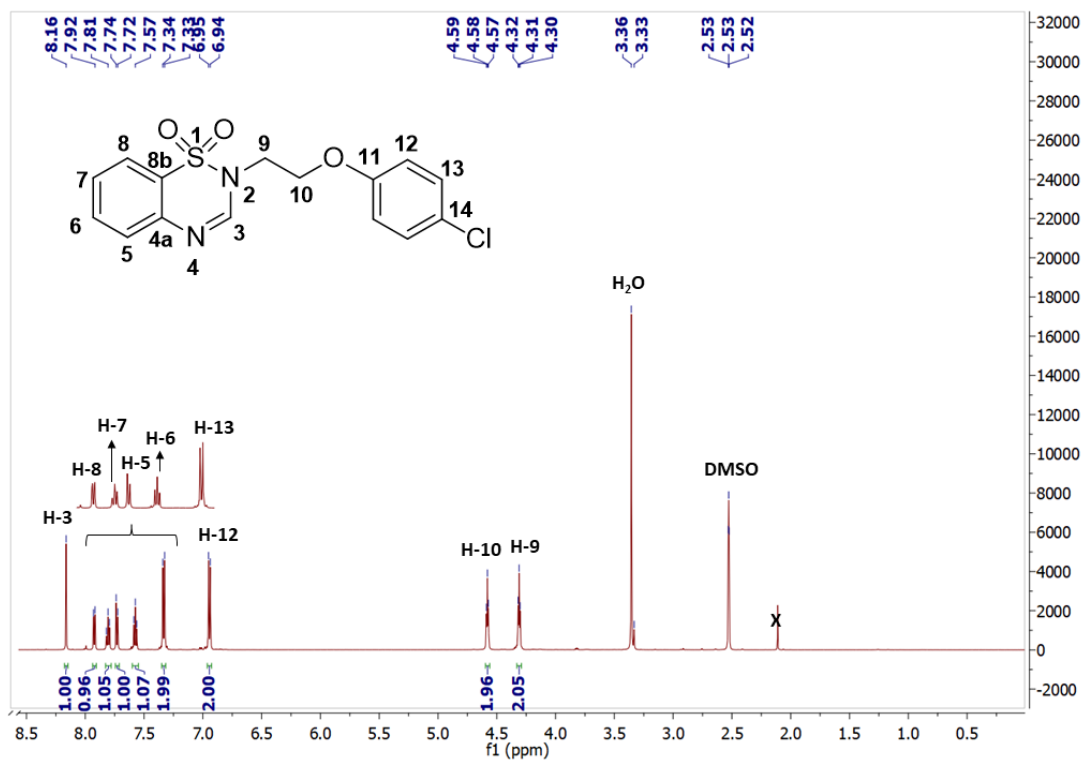
<Peak Table>

PDA Ch1 270nm

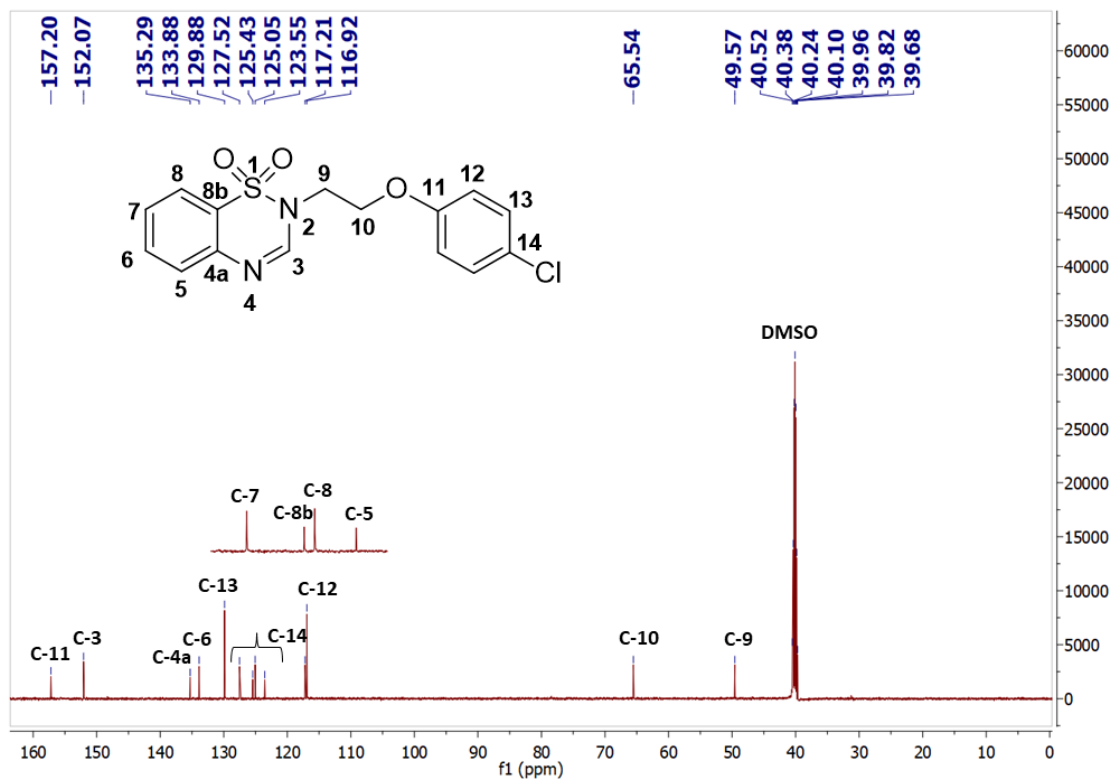
Peak#	Ret. Time	Area	Area%
1	6,167	3994275	97,813
2	6,466	27591	0,676
3	6,691	61733	1,512
Total		4083598	100,000

2-[2-(4-Chlorophenoxy)ethyl]-2H-benzo[e][1,2,4]thiadiazine-1,1-dioxide (11)

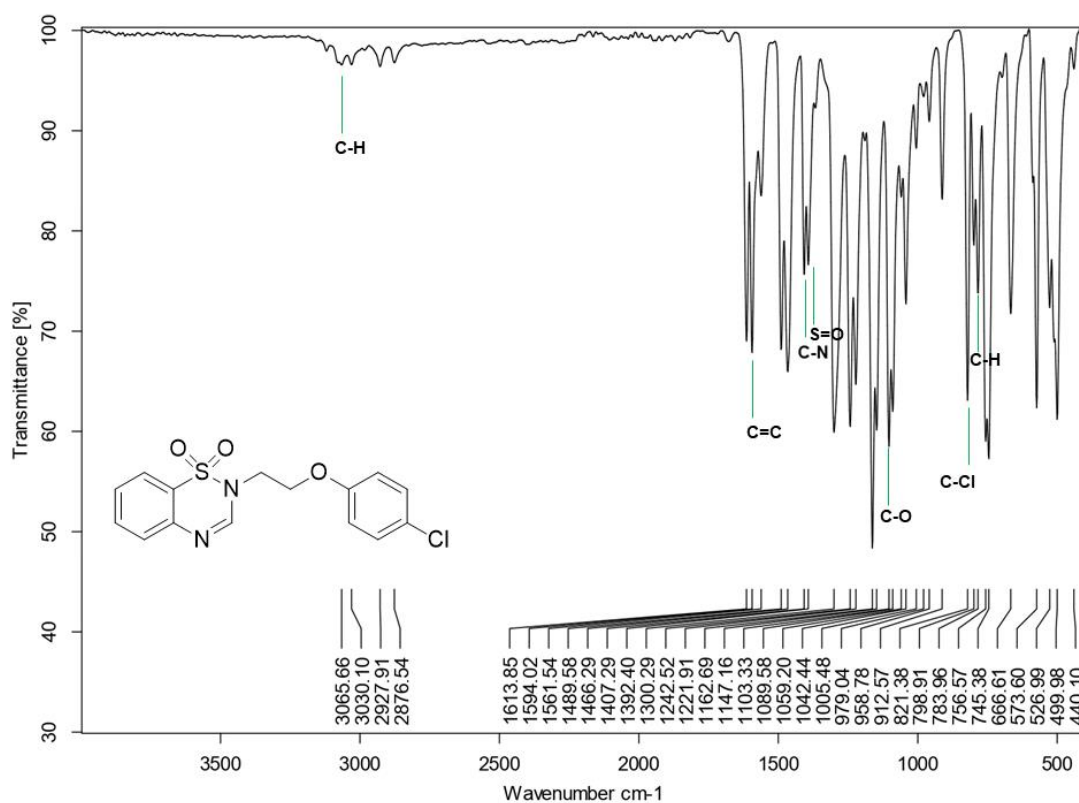
¹H NMR in DMSO



¹³C NMR in DMSO



IR Spectrum



HRMS

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\Data\18112021\LADMS000007.d
 Method tune_low no focus50-1600da31052021.m
 Sample Name NH-14
 Comment

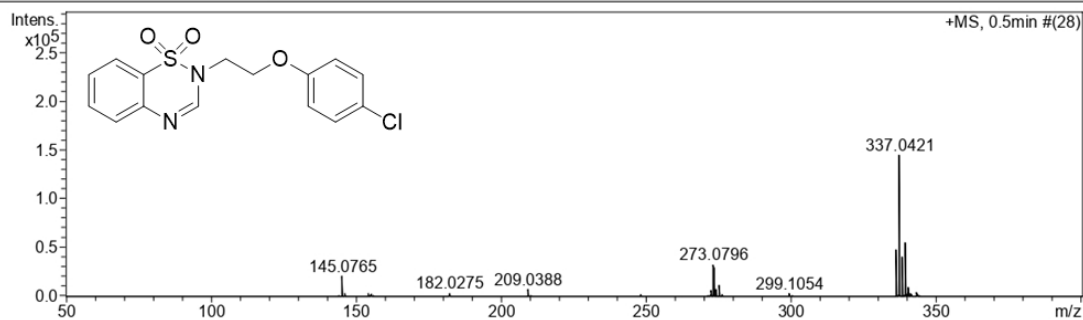
Acquisition Date 11/18/2021 9:01:39 AM

Operator Dr JHL Jordaan

Instrument / Ser# micrOTOF-Q II 2010390

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1600 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
337.0421	1	C 15 H 14 Cl N 2 O 3 S	100.00	337.0408	-1.3	-3.9	47.0	9.5	even	ok

HPLC Purity



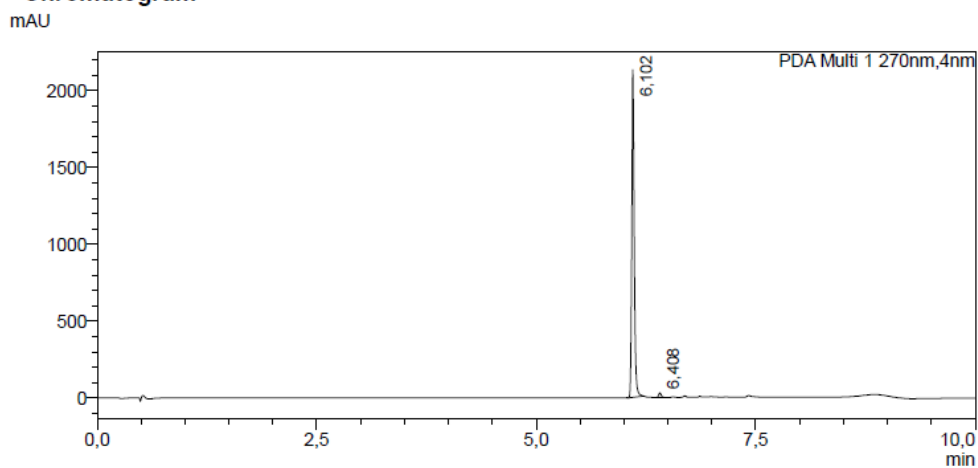
Analysis Report

<Sample Information>

Sample Name : NH-11
Sample ID : NH-11
Data Filename : NH-11_004.lcd
Method Filename : screening.lcm
Batch Filename : purity Sept 2024.lcb
Vial # : 1-12
Injection Volume : 1 uL
Date Acquired : 16/09/2024 13:53:10
Date Processed : 16/09/2024 14:03:11

Sample Type : Unknown
Acquired by : System Administrator
Processed by : System Administrator

<Chromatogram>

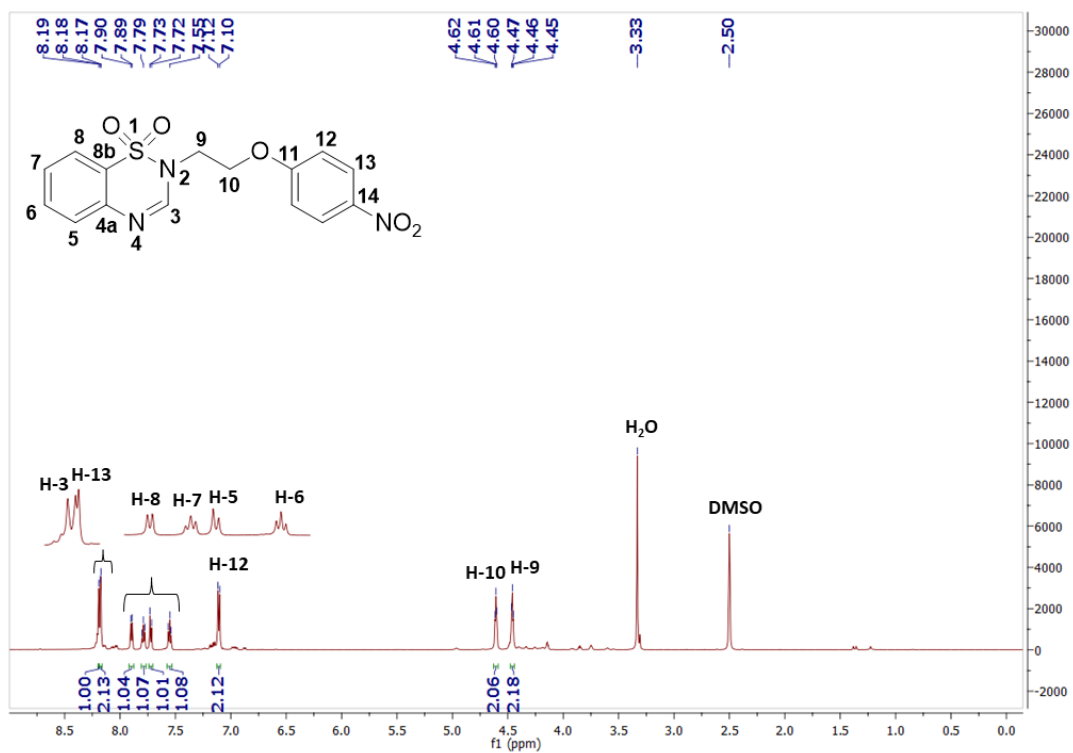


<Peak Table>

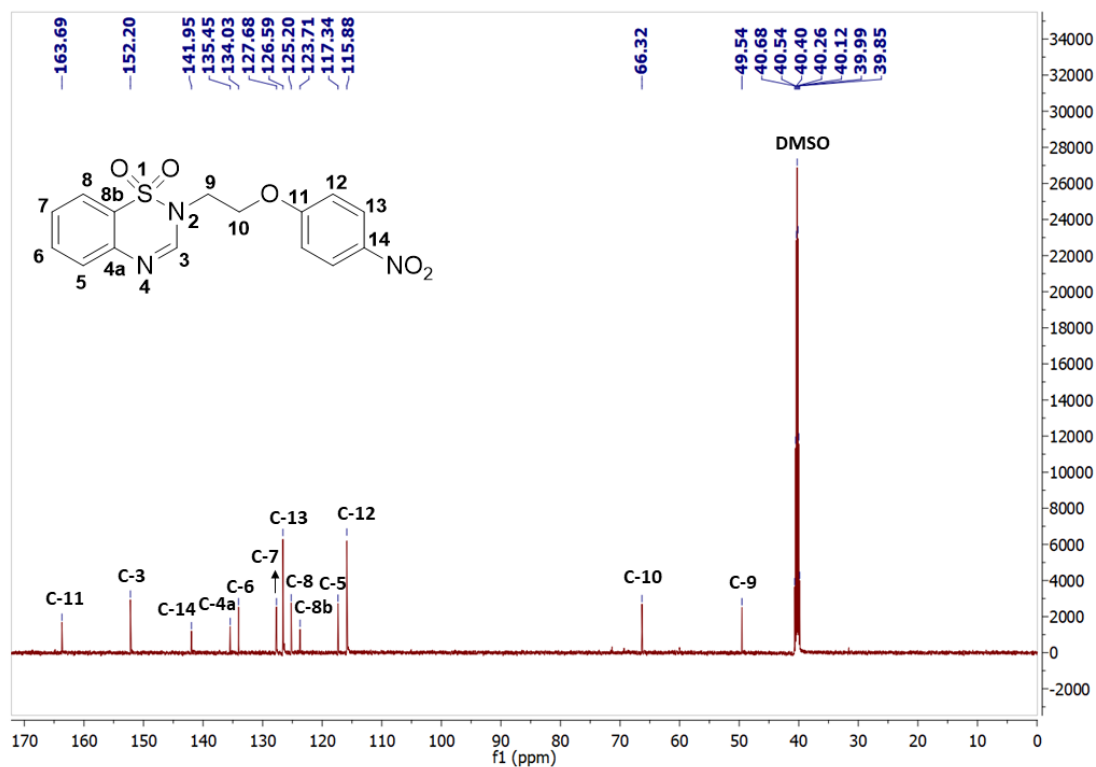
PDA Ch1 270nm			
Peak#	Ret. Time	Area	Area%
1	6,102	4273371	98,540
2	6,408	63308	1,460
Total		4336678	100,000

2-[2-(4-Nitrophenoxy)ethyl]-2H-benzo[e][1,2,4]thiadiazine-1,1-dioxide (12)

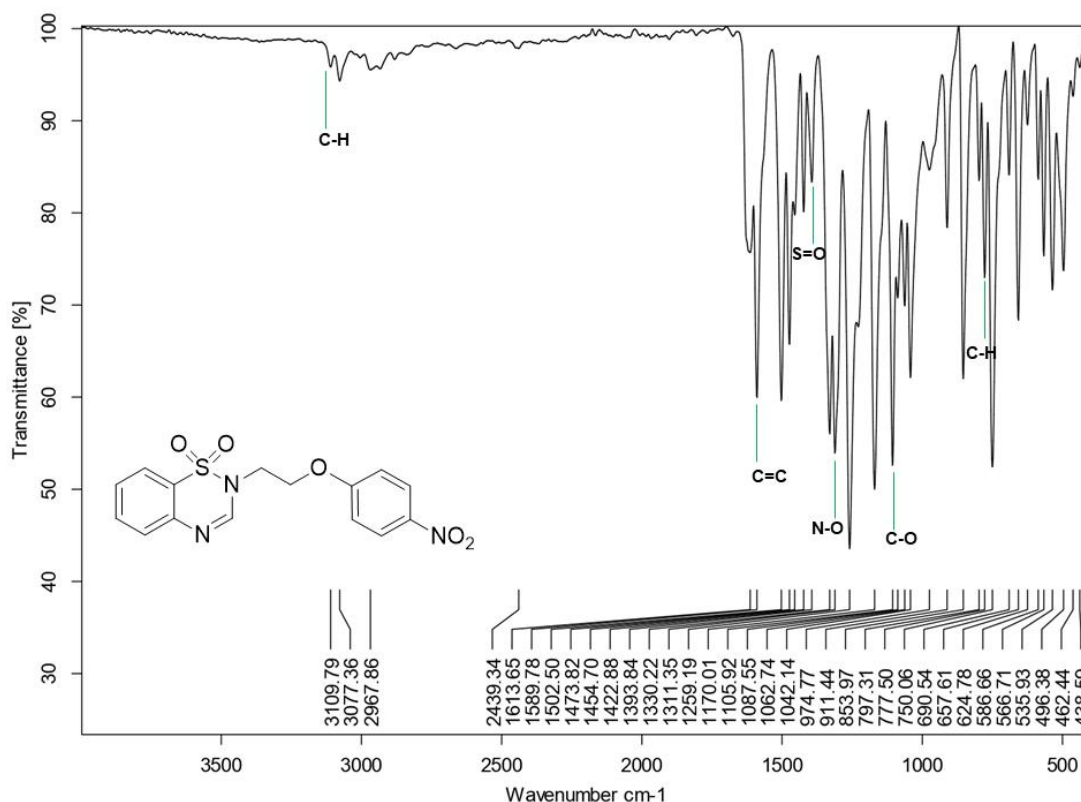
¹H NMR in DMSO



¹³C NMR in DMSO



IR Spectrum



HRMS

Mass Spectrum SmartFormula Report

Analysis Info

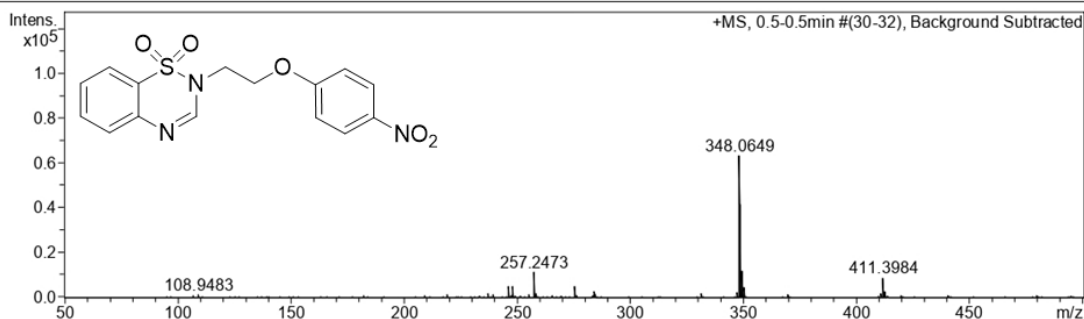
Analysis Name D:\Data\05102021\LADMS000014.d
 Method tune_low no focus50-1600da31052021.m
 Sample Name NH-10
 Comment

Acquisition Date 10/5/2021 2:04:04 PM

Operator Dr JHL Jordaan
 Instrument / Ser# micrOTOF-Q II 2010390

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1600 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
348.0649	1	C ₁₅ H ₁₄ N ₃ O ₅ S	100.00	348.0649	-0.0	-0.0	4.4	10.5	even	ok

HPLC Purity



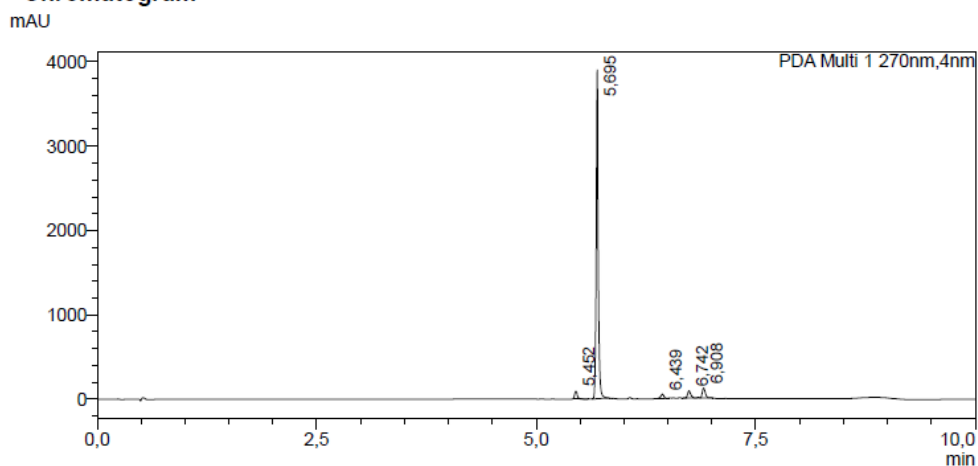
Analysis Report

<Sample Information>

Sample Name : NH-12
Sample ID : NH-12
Data Filename : NH-12_005.lcd
Method Filename : screening.lcm
Batch Filename : purity Sept 2024.lcb
Vial # : 1-13
Injection Volume : 1 uL
Date Acquired : 16/09/2024 14:03:31
Date Processed : 16/09/2024 14:13:32

Sample Type : Unknown
Acquired by : System Administrator
Processed by : System Administrator

<Chromatogram>

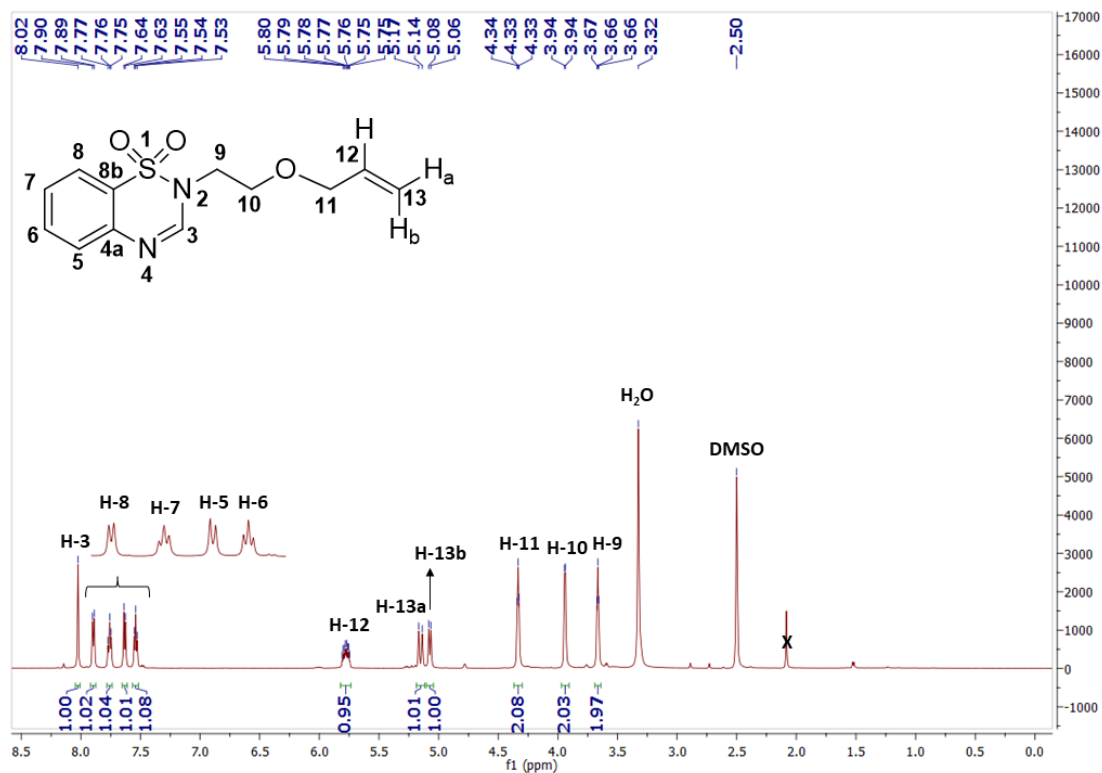


<Peak Table>

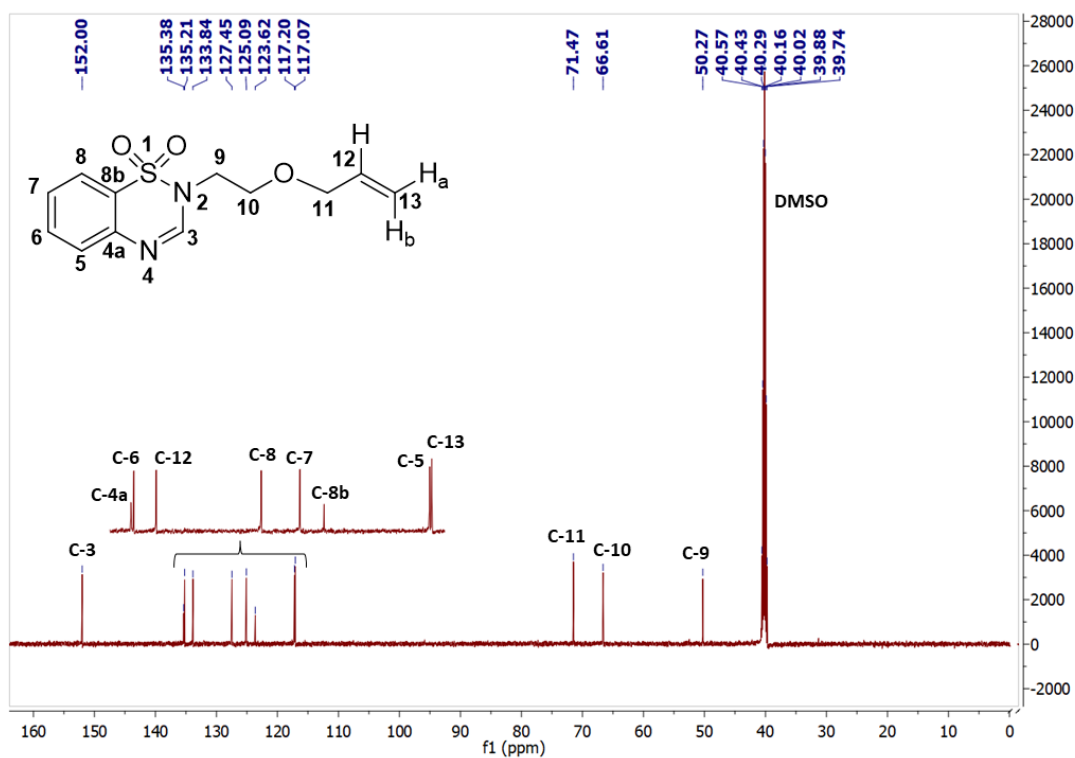
Peak#	Ret. Time	Area	Area%
1	5.452	170079	2,350
2	5.695	6465636	89,348
3	6.439	119276	1,648
4	6.742	207209	2,863
5	6.908	274300	3,791
Total		7236498	100,000

2-[2-(Allyloxy)ethyl]-2*H*-benzo[*e*][1,2,4]thiadiazine-1,1-dioxide (13)

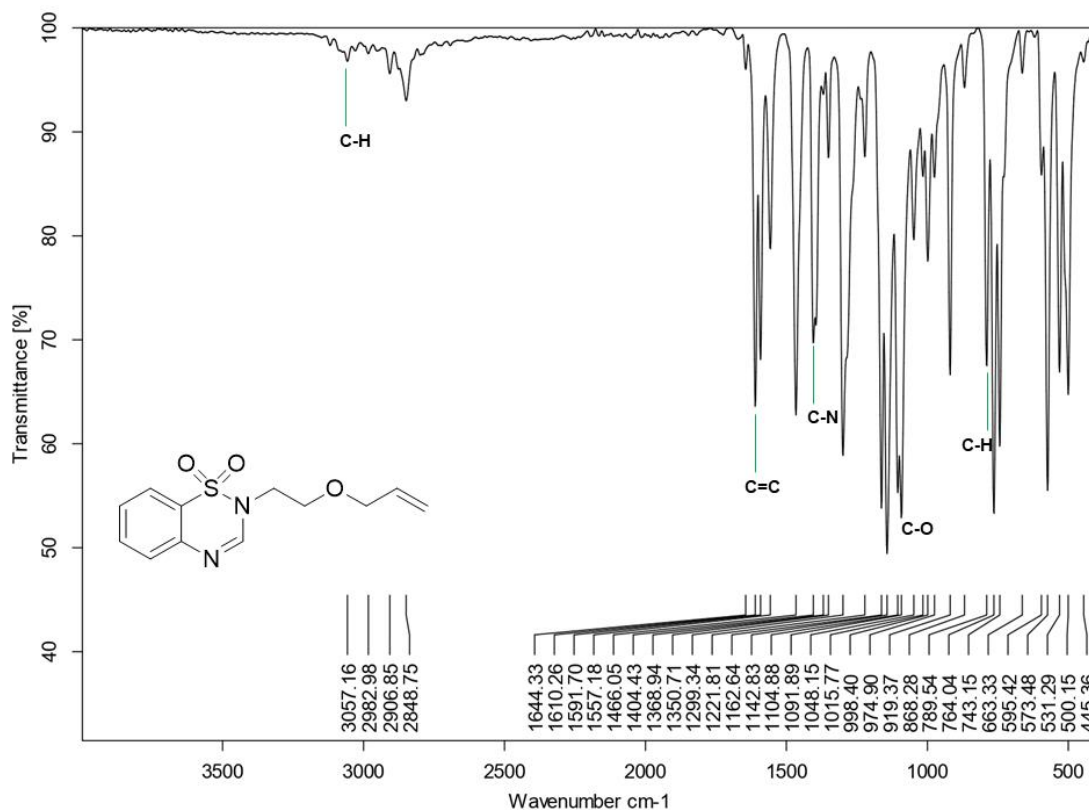
¹H NMR in DMSO



¹³C NMR in DMSO



IR Spectrum



HRMS

Mass Spectrum SmartFormula Report

Analysis Info

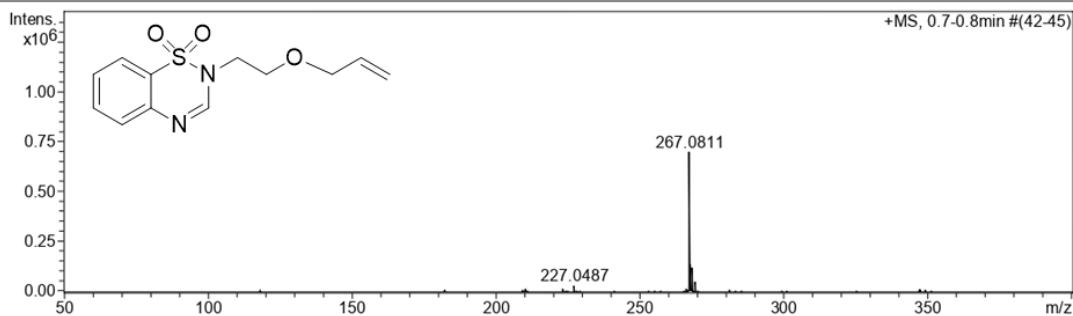
Analysis Name D:\Data\05102021\LADMS000012.d
 Method tune_low no focus50-1600da31052021.m
 Sample Name NH-8
 Comment

Acquisition Date 10/5/2021 1:51:22 PM

Operator Dr JHL Jordaan
 Instrument / Ser# micrOTOF-Q II 2010390

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1600 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
267.0811	1	C ₁₂ H ₁₅ N ₂ O ₃ S	100.00	267.0798	-1.3	-4.9	13.4	6.5	even	ok

HPLC Purity



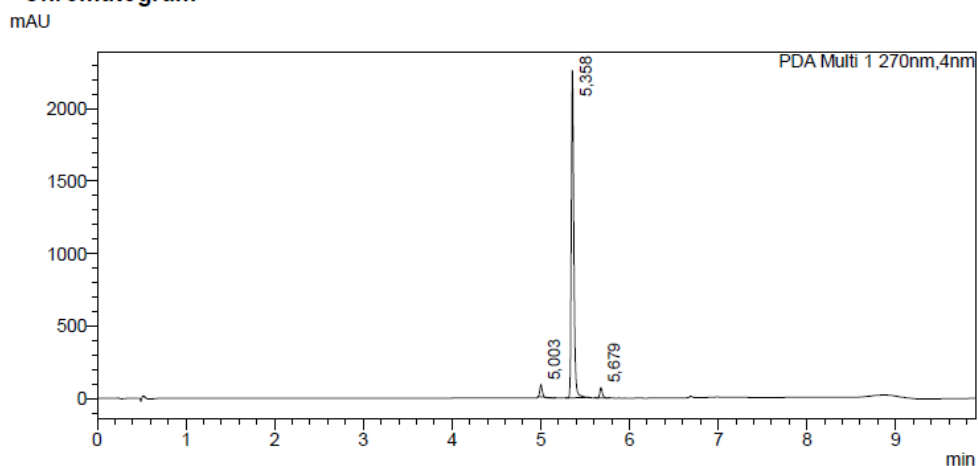
Analysis Report

<Sample Information>

Sample Name : NH-013
Sample ID : NH-013
Data Filename : NH-013_006.lcd
Method Filename : screening.lcm
Batch Filename : purity Sept 2024.lcb
Vial # : 1-14
Injection Volume : 1 uL
Date Acquired : 16/09/2024 14:13:54
Date Processed : 16/09/2024 14:23:55

Sample Type : Unknown
Acquired by : System Administrator
Processed by : System Administrator

<Chromatogram>



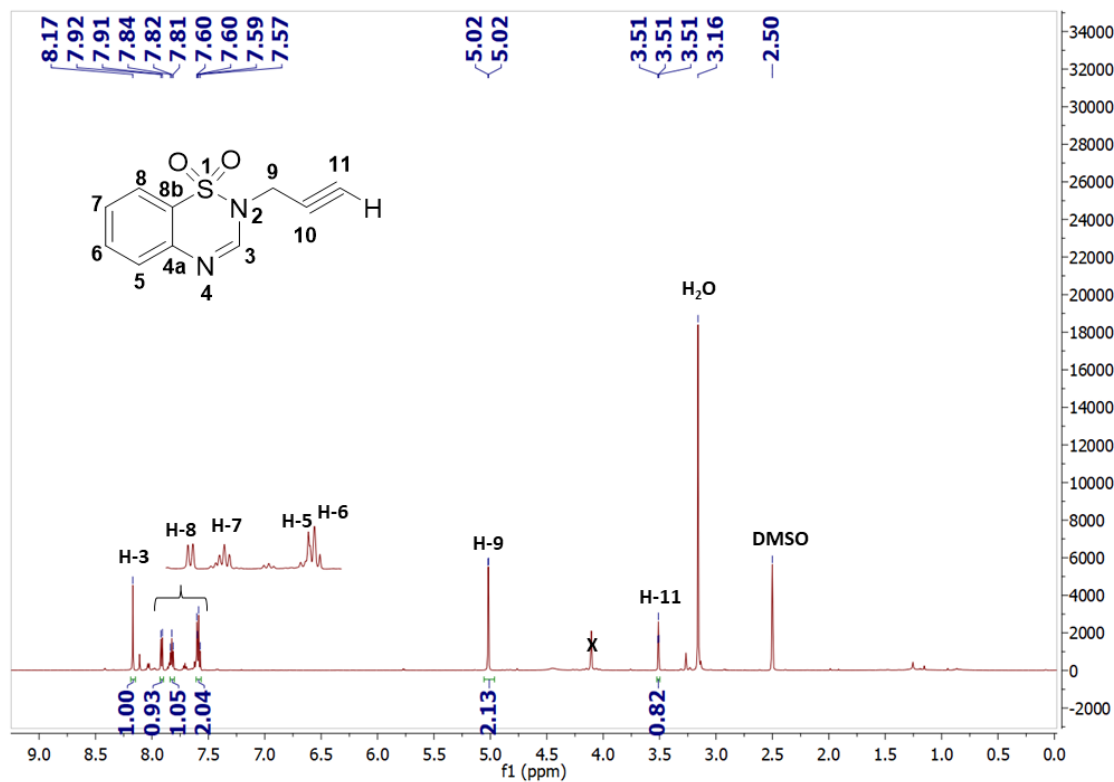
<Peak Table>

PDA Ch1 270nm

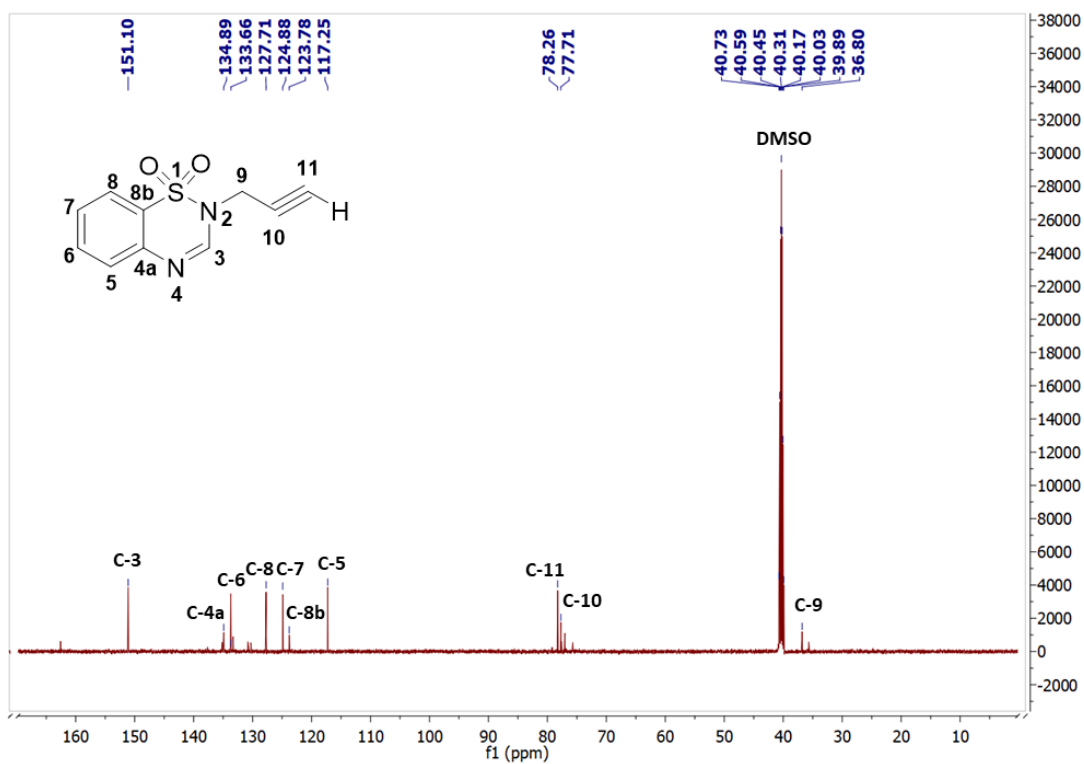
Peak#	Ret. Time	Area	Area%
1	5,003	142715	3,006
2	5,358	4455758	93,841
3	5,679	149739	3,154
Total		4748211	100,000

2-(Prop-2-yn-1-yl)-2H-benzo[e][1,2,4]thiadiazine-1,1-dioxide (14)

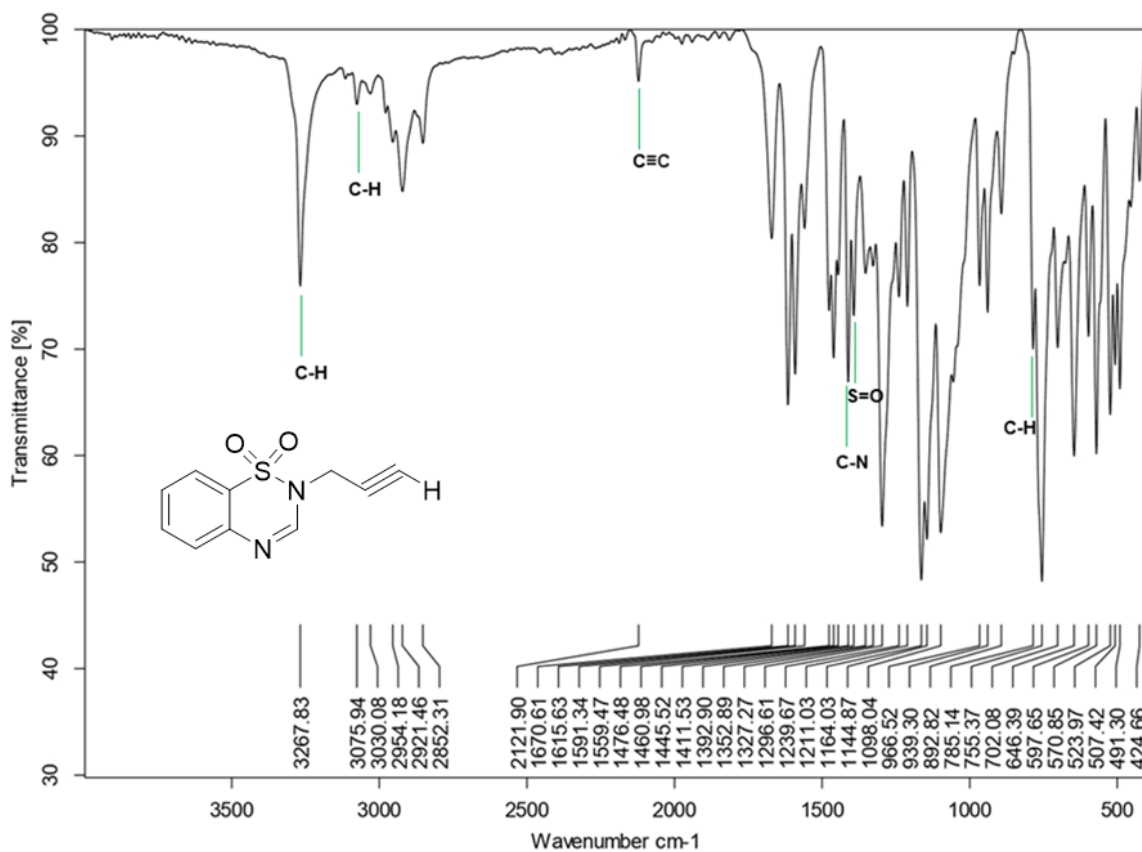
¹H NMR in DMSO



¹³C NMR in DMSO



IR Spectrum

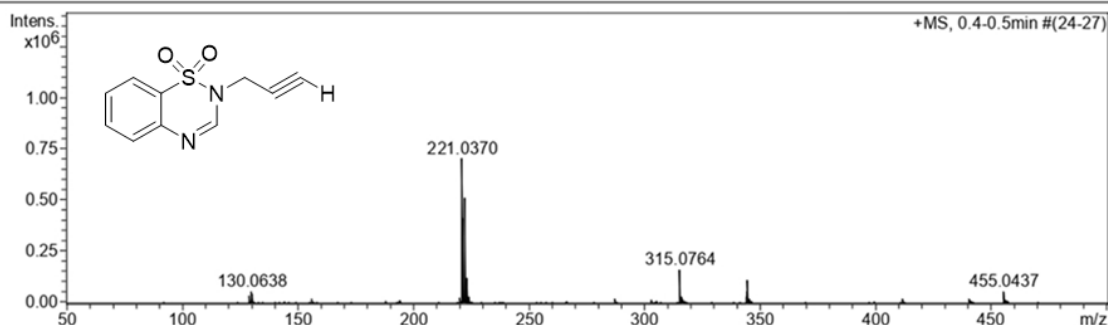


HRMS

Mass Spectrum SmartFormula Report

Analysis Info		Acquisition Date	
Analysis Name	D:\Data\11022022\LADMS000005.d	2/11/2022 10:38:38 AM	
Method	tune_low no focus50-1600da27012022HPLC.m	Operator	Dr JHL Jordan
Sample Name	NH-18	Instrument / Ser#	micrOTOF-Q II 2010390
Comment			

Acquisition Parameter					
Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	1.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
221.0370	1	C ₁₀ H ₉ N ₂ O ₂ S	100.00	221.0379	1.0	4.3	308.6	7.5	even	ok

HPLC Purity



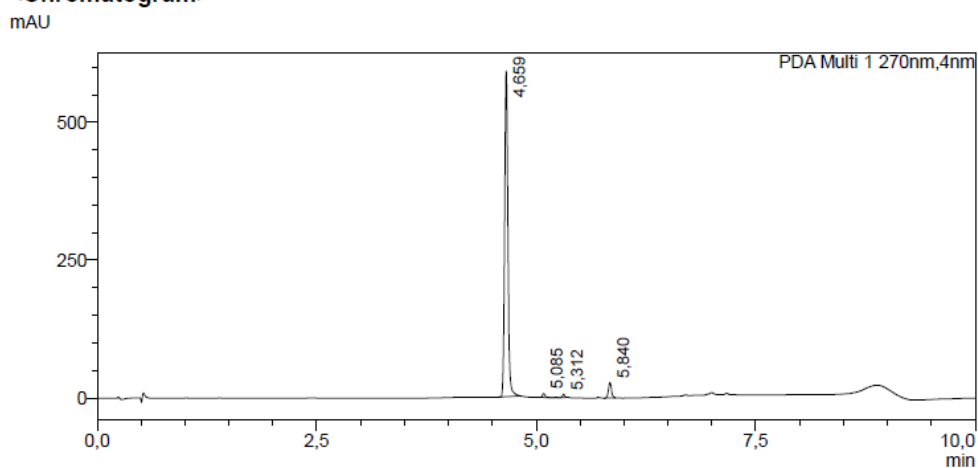
Analysis Report

<Sample Information>

Sample Name : NH-014
Sample ID : NH-014
Data Filename : NH-014_016.lcd
Method Filename : screening.lcm
Batch Filename : purity Sept 2024.lcb
Vial # : 1-15
Injection Volume : 0,2 uL
Date Acquired : 16/09/2024 13:07:13
Date Processed : 16/09/2024 13:17:15

Sample Type : Unknown
Acquired by : System Administrator
Processed by : System Administrator

<Chromatogram>



<Peak Table>

PDA Ch1 270nm

Peak#	Ret. Time	Area	Area%
1	4,659	1505872	94,232
2	5,085	15311	0,958
3	5,312	10261	0,642
4	5,840	66605	4,168
Total		1598050	100,000