

Name:	Tigecycline-D9
Lot#:	GR-19-033
Test Date:	12/07/2023 (re-test date: 12/07/2028)
CAS No.:	220620-09-7 (unlabeled)
MF:	C ₂₉ H ₃₀ D ₉ N ₅ O ₈
MW:	594.7
Appearance:	Orange Solid
Purity:	97.9% by HPLC; 99% atom D
¹H-NMR:	Conforms (contains some Hexanes)
MS-DART (+)	Conforms (shows peak at m/z = 595.3 [M+H] ⁺)
Storage	Store at -18°C in a dry place away from direct sunlight

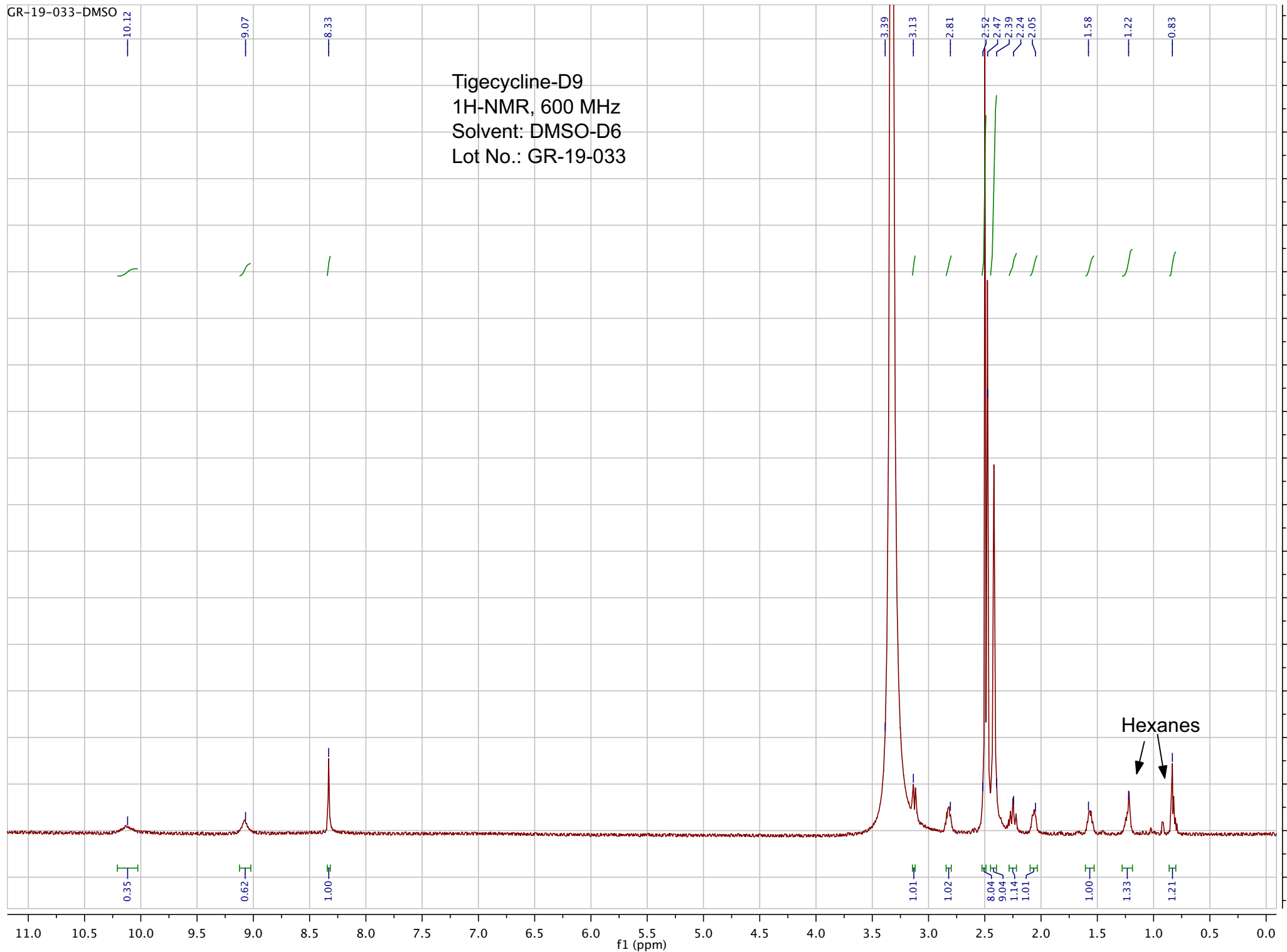
Approved by:

Date: 12/11/2023



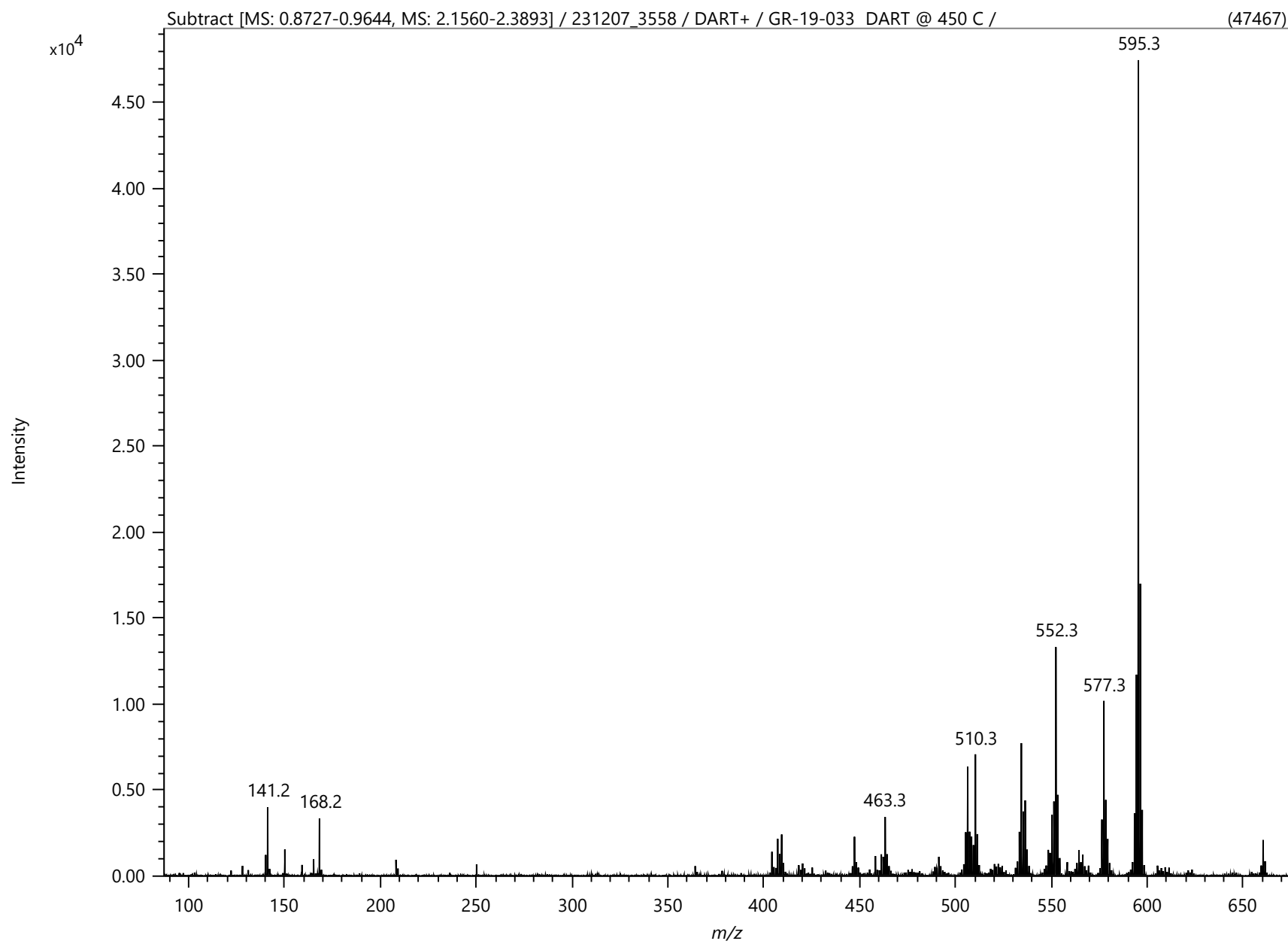
Viorica Rusu, QC/QA Manager

Tigecycline-D9
1H-NMR, 600 MHz
Solvent: DMSO-D6
Lot No.: GR-19-033

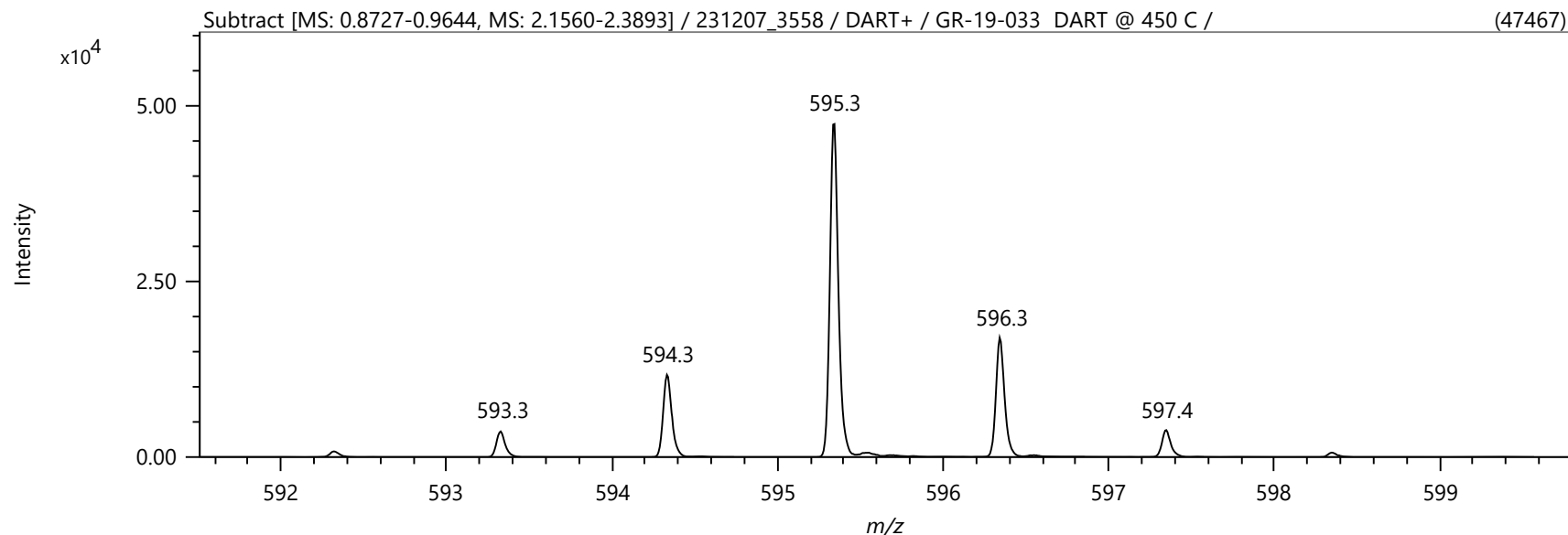


Hexanes





Spectrum



Elemental Composition

Parameters

Tolerance: ±10.00 ppm
 Electron: Even
 Charge: +1
 DBE: -1.5 - 100.0

Elements Set 1:

Symbol	C	H	O	N	D
Min	0	0	0	0	9
Max	100	200	20	10	9

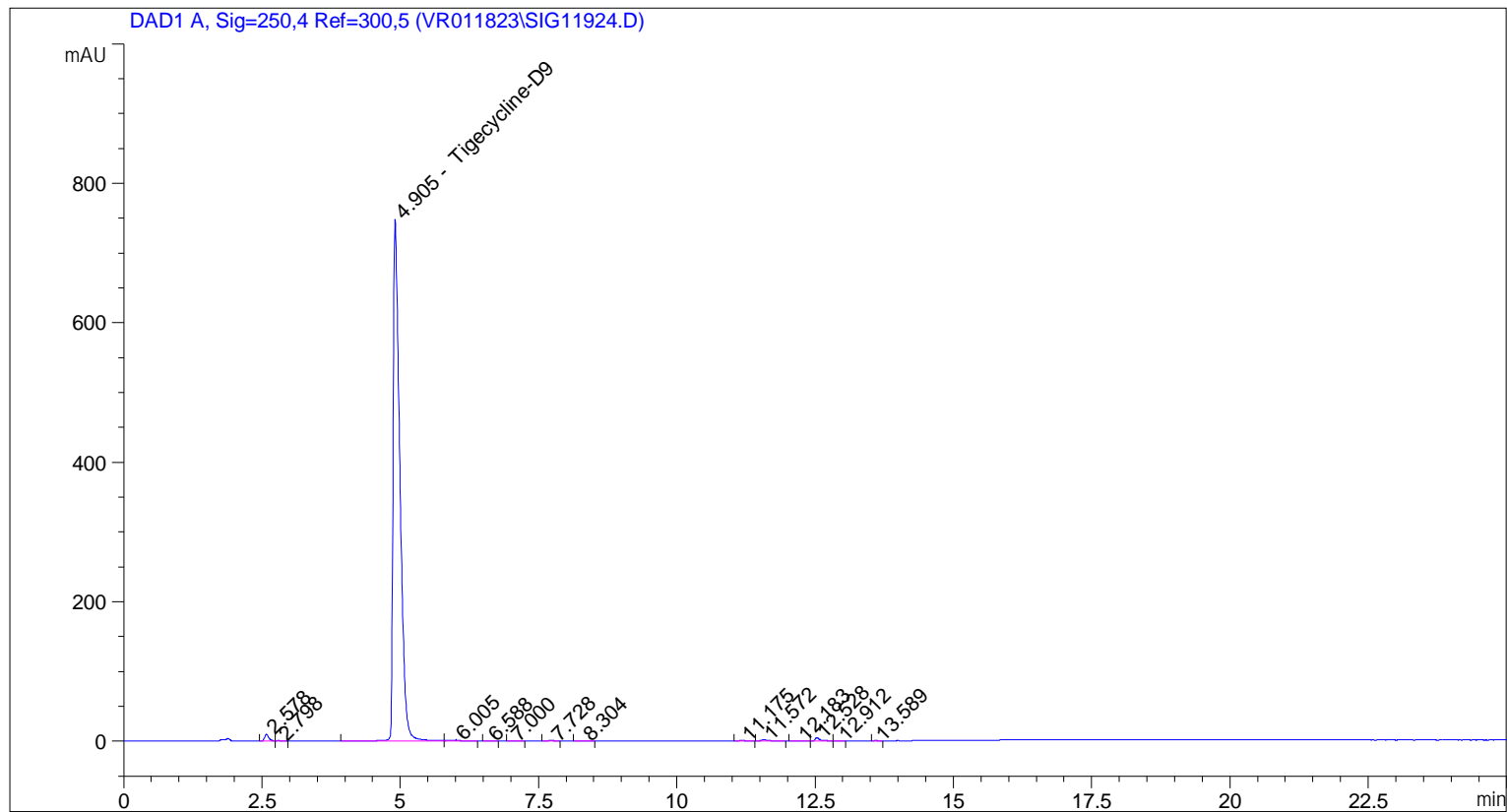
Results

Mass	Intensity	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
595.34344	47466.53	C29 H31 N5 O8 D9	595.34363	-0.19	-0.31	12.5
		C28 H35 N O12 D9	595.34229	1.15	1.93	7.5
		C30 H27 N9 O4 D9	595.34497	-1.52	-2.56	17.5
		C41 H27 N3 O D9	595.34178	1.66	2.79	25.5
		C17 H35 N7 O15 D9	595.34548	-2.04	-3.42	-0.5
		C24 H31 N7 O10 D9	595.33961	3.84	6.44	8.5

Mass	Intensity	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
		C34 H31 N3 O6 D9	595.34765	-4.21	-7.07	16.5
		C21 H39 N O17 D9	595.34817	-4.72	-7.93	-1.5
		C23 H35 N3 O14 D9	595.33827	5.17	8.69	3.5
		C35 H27 N7 O2 D9	595.34899	-5.55	-9.32	21.5
		C36 H27 N5 O3 D9	595.33776	5.69	9.55	21.5

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Acq. Operator   : vrusu
Acq. Instrument : Instrument 1                Location : Vial 9
Injection Date  : 12/7/2023 7:53:51 AM
                                           Inj Volume : 5.0 µl
Acq. Method     : C:\CHEM32\1\METHODS\VR120723_033.M
Last changed    : 12/7/2023 7:53:01 AM by vrusu
Analysis Method : C:\CHEM32\1\METHODS\VR120723_033PM.M
Last changed    : 12/7/2023 9:11:45 AM by vrusu
  
```



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 Area Percent Report
 =====

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Sorted By           :      Signal
Calib. Data Modified :      12/7/2023 9:07:47 AM
Multiplier:         :      1.0000
Dilution:           :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 1: DAD1 A, Sig=250,4 Ref=300,5

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	2.578	BV	0.0797	51.29694	0.7903	?
2	2.798	VB	0.0755	2.98935	0.0461	?
3	4.905	BV	0.1271	6357.38379	97.9427	Tigecycline-D9
4	6.005	VV	0.1525	13.95866	0.2150	?
5	6.588	BB	0.0875	1.43299	0.0221	?
6	7.000	BB	0.1191	1.23444	0.0190	?
7	7.728	BB	0.1116	5.68259	0.0875	?
8	8.304	BB	0.1149	2.30508	0.0355	?

Sample Name: GR-19-033

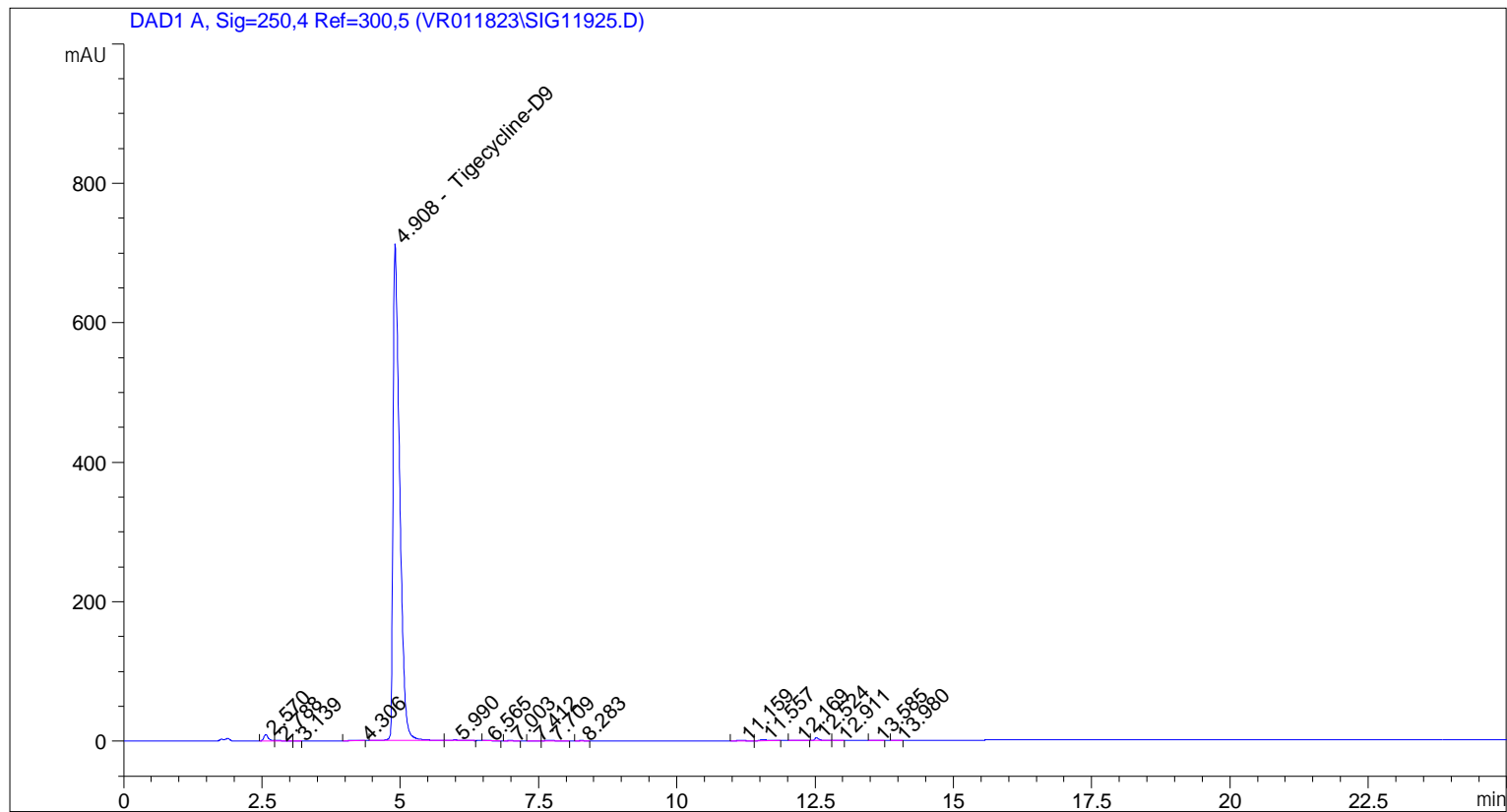
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
9	11.175	BB	0.1074	7.06053	0.1088	?
10	11.572	BB	0.1444	15.58628	0.2401	?
11	12.183	BB	0.1536	2.26030	0.0348	?
12	12.528	BV	0.0829	26.63395	0.4103	?
13	12.912	VV	0.1071	1.54632	0.0238	?
14	13.589	BB	0.0681	1.55339	0.0239	?

Totals : 6490.92461

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*** End of Report ***

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Acq. Operator   : vrusu
Acq. Instrument : Instrument 1                Location : Vial 10
Injection Date  : 12/7/2023 8:25:12 AM
                                           Inj Volume : 5.0 µl
Acq. Method     : C:\CHEM32\1\METHODS\VR120723_033.M
Last changed    : 12/7/2023 8:21:43 AM by vrusu
Analysis Method : C:\CHEM32\1\METHODS\VR120723_033PM.M
Last changed    : 12/7/2023 9:11:45 AM by vrusu
  
```



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 Area Percent Report
 =====

```

Sorted By           :      Signal
Calib. Data Modified :      12/7/2023 9:07:47 AM
Multiplier:         :      1.0000
Dilution:           :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 1: DAD1 A, Sig=250,4 Ref=300,5

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	2.570	BV	0.0802	47.94440	0.7918	?
2	2.788	VV	0.0999	4.06619	0.0672	?
3	3.139	VV	0.0929	8.44801e-1	0.0140	?
4	4.306	BB	0.2270	1.60456	0.0265	?
5	4.908	BV	0.1251	5927.28467	97.8873	Tigecycline-D9
6	5.990	VB	0.1354	11.28639	0.1864	?
7	6.565	BB	0.0955	1.39294	0.0230	?
8	7.003	BB	0.1148	1.15509	0.0191	?

Sample Name: GR-19-033 spl-2

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
9	7.412	BV	0.1301	1.24705	0.0206	?
10	7.709	VB	0.1263	6.42234	0.1061	?
11	8.283	BB	0.0935	1.79873	0.0297	?
12	11.159	BB	0.1091	6.92883	0.1144	?
13	11.557	BB	0.1417	13.67468	0.2258	?
14	12.169	BB	0.1412	2.28448	0.0377	?
15	12.524	BB	0.0824	23.85138	0.3939	?
16	12.911	BB	0.0788	8.40282e-1	0.0139	?
17	13.585	BB	0.0776	1.75608	0.0290	?
18	13.980	BB	0.0836	8.29315e-1	0.0137	?

Totals : 6055.21219

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*** End of Report ***