

Name:	16α-Hydroxyestrone
Lot#:	GR-18-149
Test Date:	05/11/2023 (re-test date: 05/11/2028)
CAS No.:	566-76-7
MF:	C ₁₈ H ₂₂ O ₃
MW:	286.37
Appearance:	White solid
Purity:	97.6% by HPLC (average of two sample preparations)
¹H-NMR:	Conforms (shows a trace of EtOAc)
MS-ESI (+)	Conforms (shows peaks at m/z = 287.2 [M+H] ⁺ and 304.2 [M+NH ₄] ⁺)
Storage	Store at 0-5°C in a dry place away from direct sunlight

Approved by:

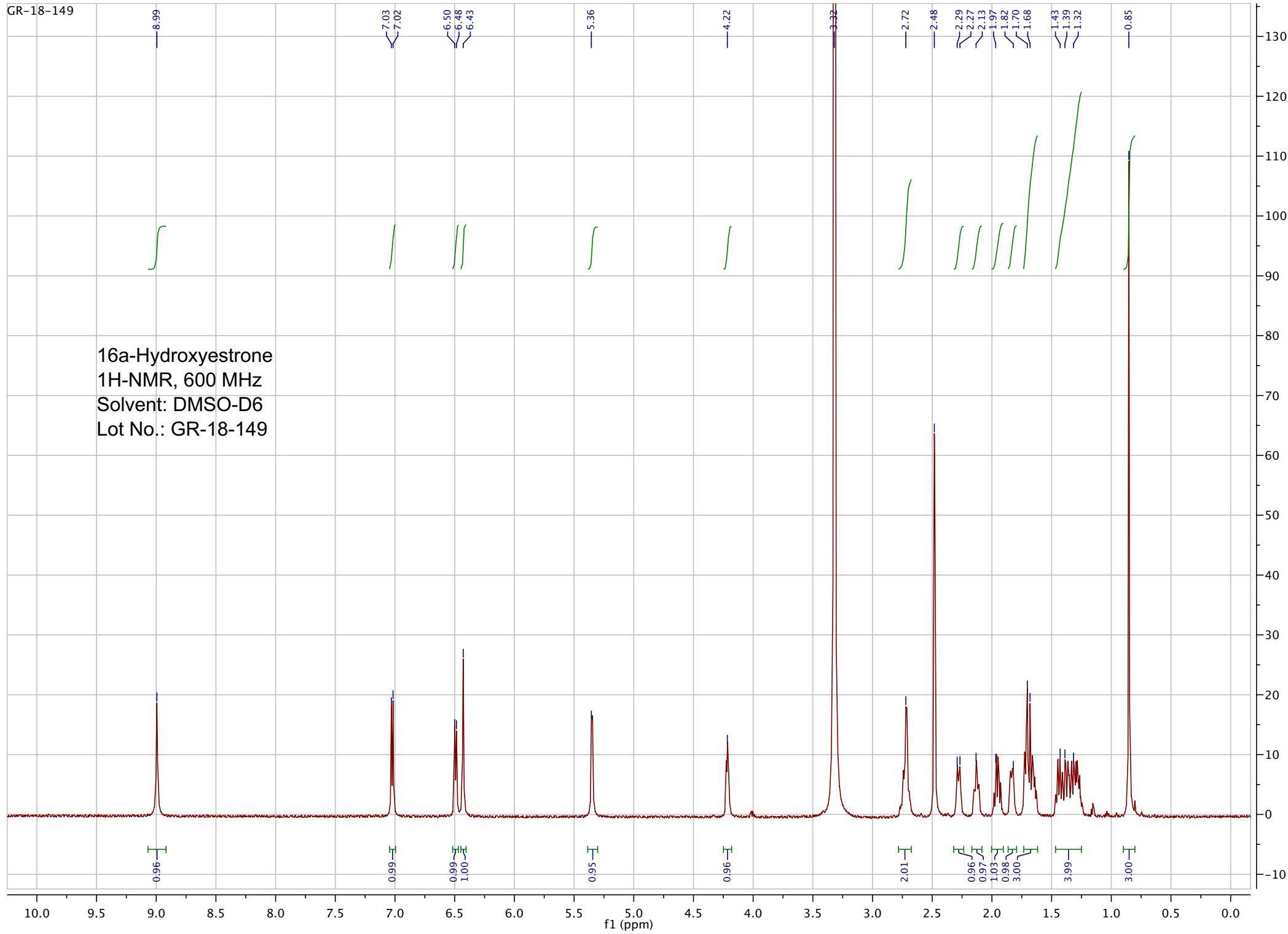
Date: 05/30/2023

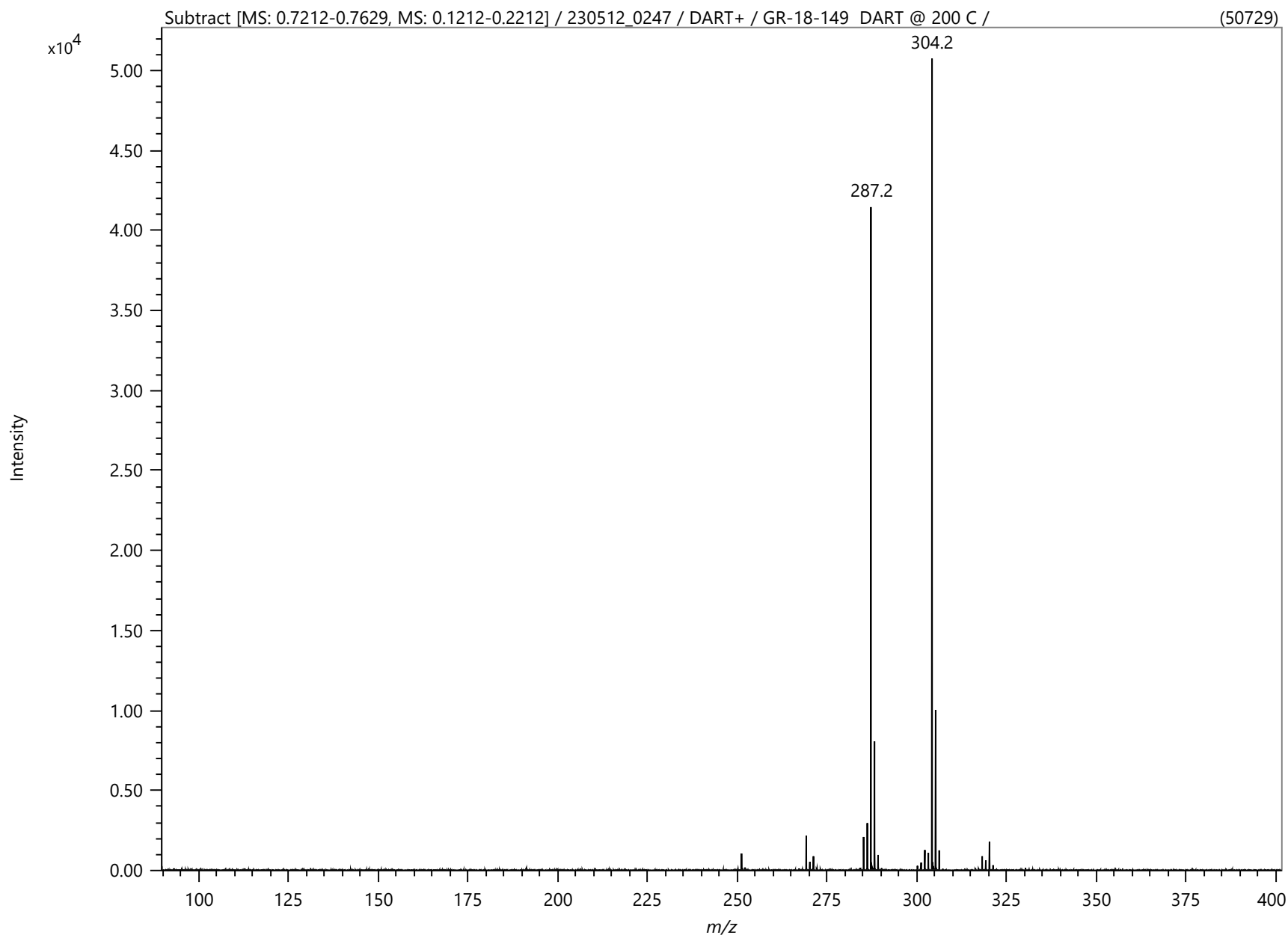


Viorica Rusu, QC/QA Manager

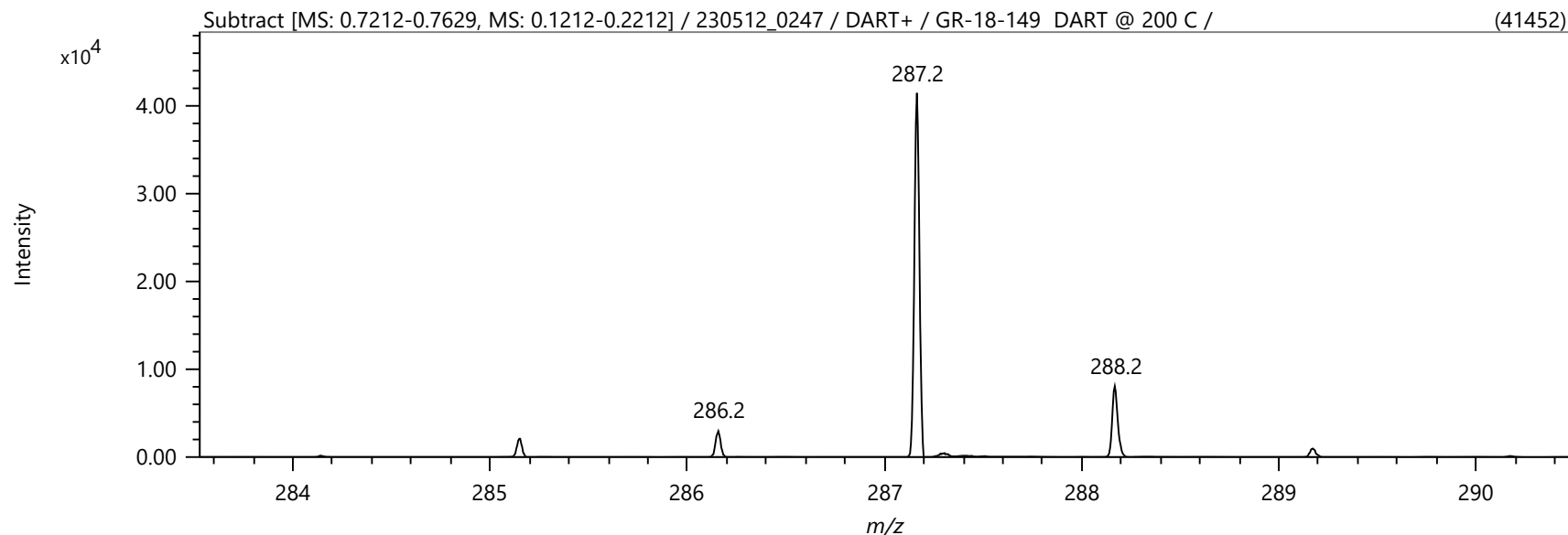
GR-18-149

16a-Hydroxyestrone
1H-NMR, 600 MHz
Solvent: DMSO-D6
Lot No.: GR-18-149





Spectrum



Elemental Composition

Parameters

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

Elements Set 1:

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

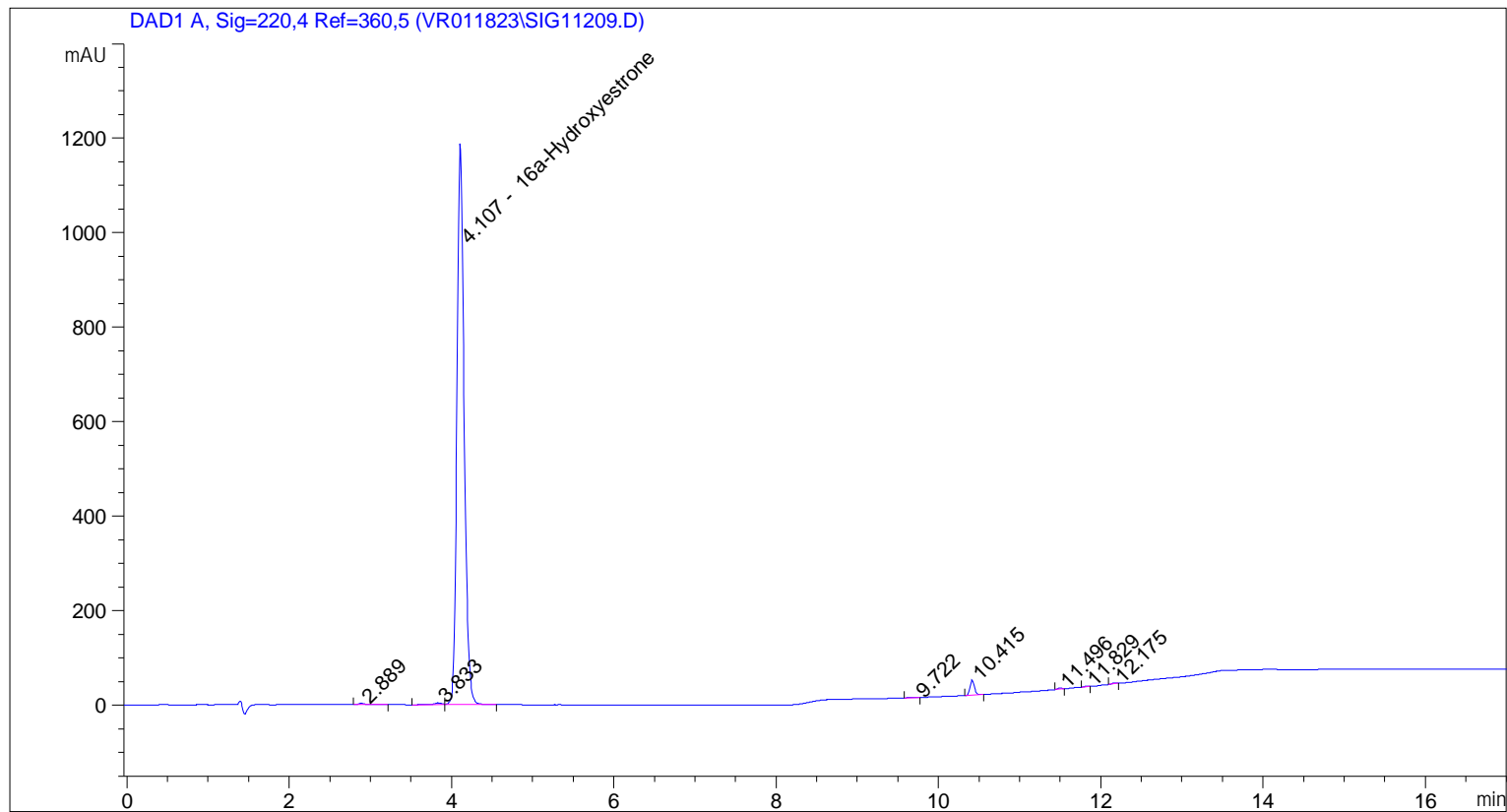
Results

Mass	Intensity	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
287.16411	41451.75	C18 H23 O3	287.16417	-0.06	-0.22	7.5
		C14 H19 N6 O	287.16149	2.62	9.13	8.5
		C7 H23 N6 O6	287.16736	-3.25	-11.33	-0.5
		C13 H23 N2 O5	287.16015	3.96	13.78	3.5
		C8 H19 N10 O2	287.16870	-4.59	-15.98	4.5
		C11 H27 O8	287.17004	-5.94	-20.68	-1.5

Mass	Intensity	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
		C9 H19 N8 O3	287.15746	6.64	23.13	4.5
		C12 H23 N4 O4	287.17138	-7.28	-25.33	3.5
		C8 H23 N4 O7	287.15613	7.98	27.79	-0.5
		C13 H19 N8	287.17272	-8.61	-29.99	8.5
		C20 H19 N2	287.15428	9.83	34.24	12.5

```

=====
Acq. Operator   : vrusu
Acq. Instrument : Instrument 1                Location : Vial 60
Injection Date  : 5/11/2023 9:00:17 AM
                                           Inj Volume : 5.0 µl
Acq. Method    : C:\CHEM32\1\METHODS\VR051123_149.M
Last changed   : 5/11/2023 8:59:07 AM by vrusu
Analysis Method : C:\CHEM32\1\METHODS\VR051123_149PM.M
Last changed   : 5/11/2023 9:52:29 AM by vrusu
  
```



=====
 Area Percent Report
 =====

```

Sorted By      : Signal
Calib. Data Modified : 5/11/2023 9:51:28 AM
Multiplier:    : 1.0000
Dilution:      : 1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 1: DAD1 A, Sig=220,4 Ref=360,5

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	2.889	BB	0.0899	17.45137	0.2318	?
2	3.833	BV	0.1062	29.35920	0.3899	?
3	4.107	VB	0.0941	7339.13623	97.4661	16a-Hydroxyestrone
4	9.722	BB	0.0883	3.21810	0.0427	?
5	10.415	BB	0.0587	122.72327	1.6298	?
6	11.496	BB	0.0513	7.92650	0.1053	?
7	11.829	BB	0.0571	3.52882	0.0469	?
8	12.175	BB	0.0576	6.59002	0.0875	?

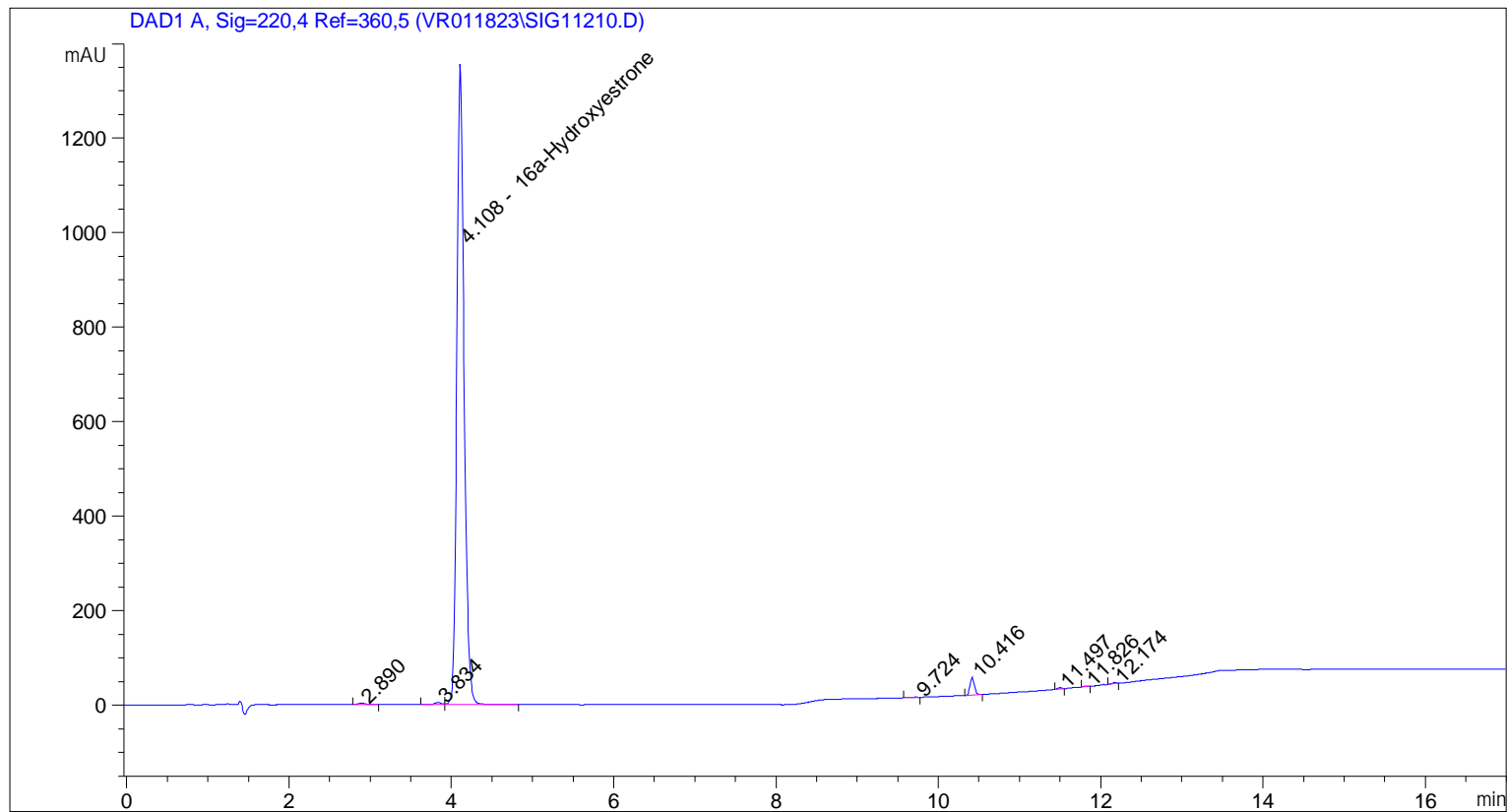
Sample Name: GR-18-149

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
Totals :				7529.93350		

=====
*** End of Report ***

```

=====
Acq. Operator   : vrusu
Acq. Instrument : Instrument 1                Location : Vial 61
Injection Date  : 5/11/2023 9:21:42 AM
                                           Inj Volume : 5.0 µl
Acq. Method     : C:\CHEM32\1\METHODS\VR051123_149.M
Last changed    : 5/11/2023 9:20:34 AM by vrusu
Analysis Method : C:\CHEM32\1\METHODS\VR051123_149PM.M
Last changed    : 5/11/2023 9:52:29 AM by vrusu
  
```



=====
 Area Percent Report
 =====

```

Sorted By           :      Signal
Calib. Data Modified :      5/11/2023 9:51:28 AM
Multiplier:         :      1.0000
Dilution:           :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 1: DAD1 A, Sig=220,4 Ref=360,5

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	2.890	BB	0.0816	17.84267	0.2066	?
2	3.834	BV	0.0933	27.66681	0.3204	?
3	4.108	VB	0.0945	8425.64355	97.5669	16a-Hydroxyestrone
4	9.724	BB	0.0841	3.13315	0.0363	?
5	10.416	BB	0.0583	140.34227	1.6251	?
6	11.497	BB	0.0515	8.82978	0.1022	?
7	11.826	BB	0.0555	4.44827	0.0515	?
8	12.174	BB	0.0568	7.85300	0.0909	?

Sample Name: GR-18-149 spl-2

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
Totals :				8635.75951		

=====
*** End of Report ***