

Name:	<i>rac</i> -Cinacalcet-D3 HCl
Lot#:	GR-19-085
Test Date:	02/13/2024 (re-test date: 02/13/2029)
CAS No.:	1185097-33-9
MF:	C ₂₂ H ₂₀ D ₃ ClF ₃ N
MW:	396.89
Appearance:	White solid
Purity:	99.7% CP by HPLC (average of two sample preparations); 99% atom D
¹H-NMR:	Conforms
MS-ESI (+)	Conforms (shows peak at m/z = 361.20 [M _{free base} +H] ⁺)
Storage	Store at -18°C in a dry place away from direct sunlight

Approved by:

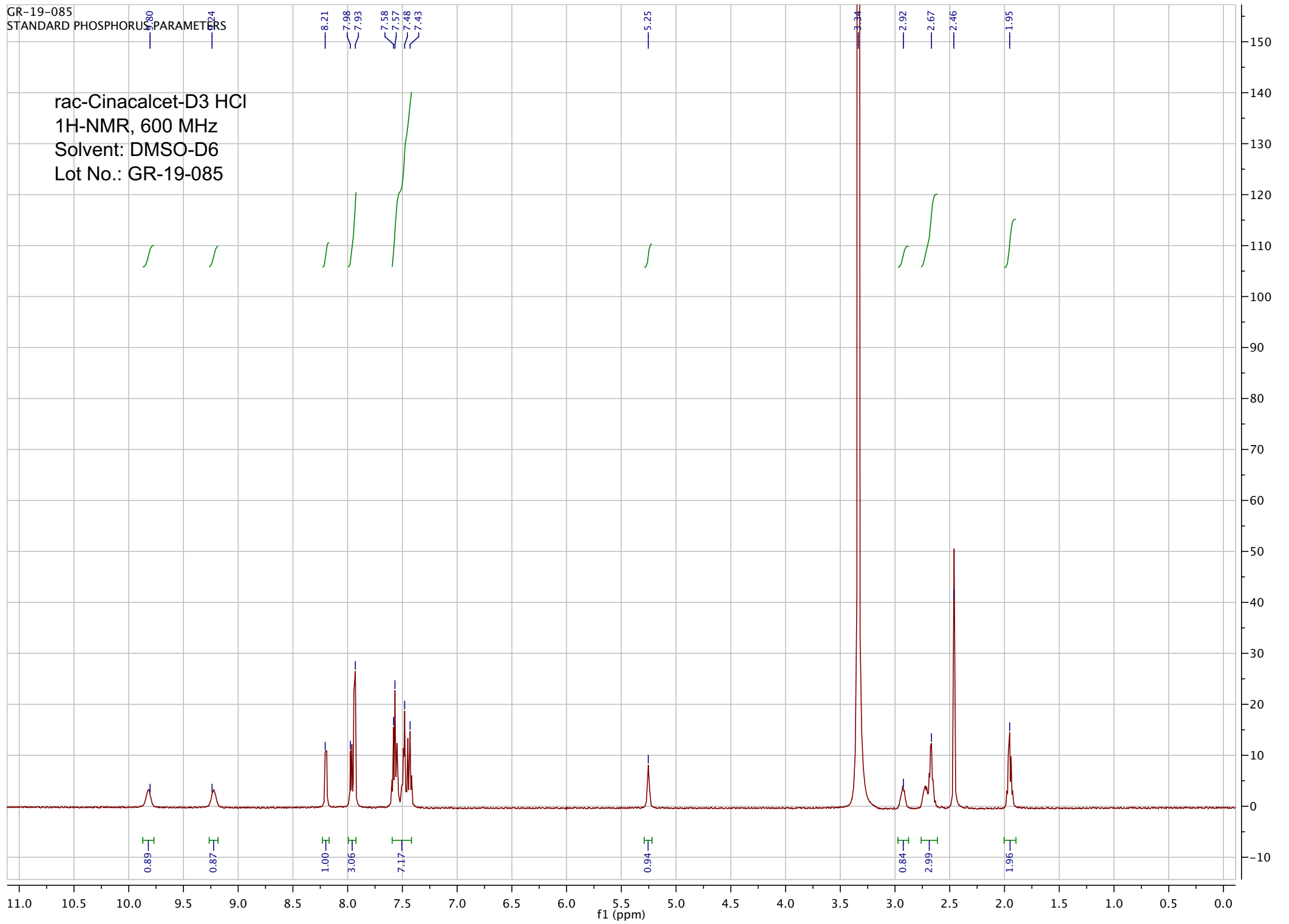
Date: 03/05/2024



Viorica Rusu, QC/QA Manager

GR-19-085
STANDARD PHOSPHORUS PARAMETERS

rac-Cinacalcet-D3 HCl
1H-NMR, 600 MHz
Solvent: DMSO-D6
Lot No.: GR-19-085



24.03.05.4748

MASS SPECTROMETRY

Sample Submission Form 2022-2023

The AIMS Mass Spectrometry Laboratory has no Biocontainment Level designation. All samples of biological origin must therefore be inactivated and free from pathogens.

Is sample of biological origin? Yes No
If yes, has sample been treated to inactivate pathogens? Yes No

Authorized Signature

Chleb

P.I. Name

Expert Synthesis Solutions

Account

Name

Openadic Rusu

Email (Please type)

grusu@esschemco.com

Sample ID

GR-19-085

Molecular Formula

$C_{12}H_{20}D_3ClF_2N$

Molecular Mass

396.89

Solubility:

H₂O

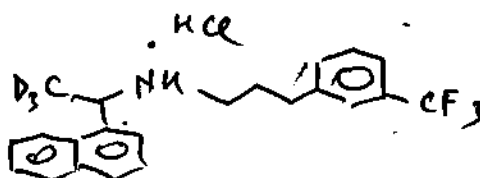
CH₃OH

CH₂CN

CH₂Cl₂

Other

Structure / Sample information:



Please, integrate the peak at $M \pm 10$ Da

Ionization/Analysis:

EI

ESI

DART

MALDI

LC-MS

Polarity:

+

-

GC-MS

Accurate Mass:

AIMS

MASS SPECTROMETRY LABORATORY

uoft.ms/AIMS

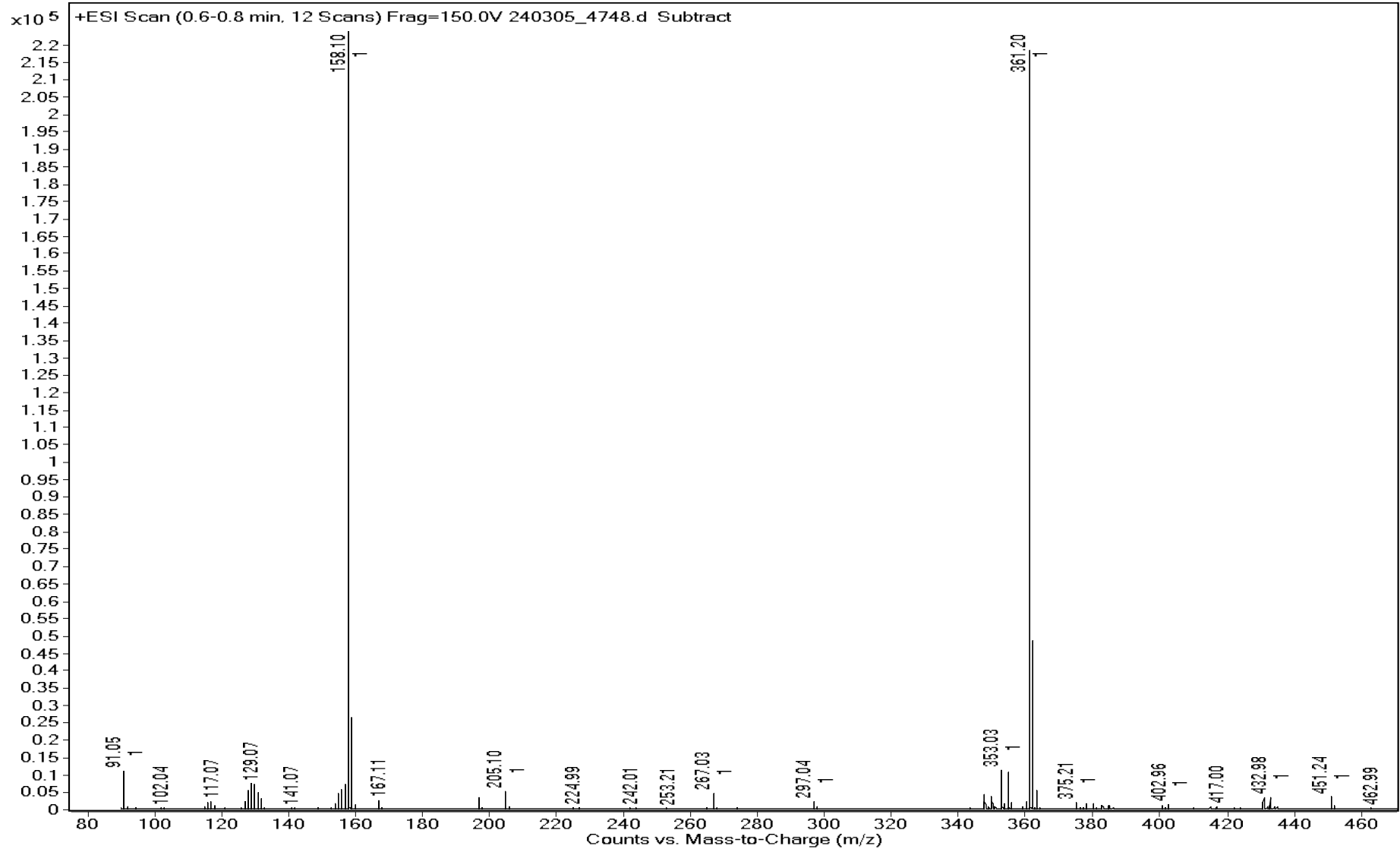
CHEMISTRY
UNIVERSITY OF
TORONTO



Sample Name GR-19-085
DA Method AIMS_Accurate_Mass.m
Comment ESI+

Data File 240305_4748.d
Instrument Agilent 6538 UHD

Acq Method HRMS.m
Acq Date, Time 05/03/2024 4:07:57 PM



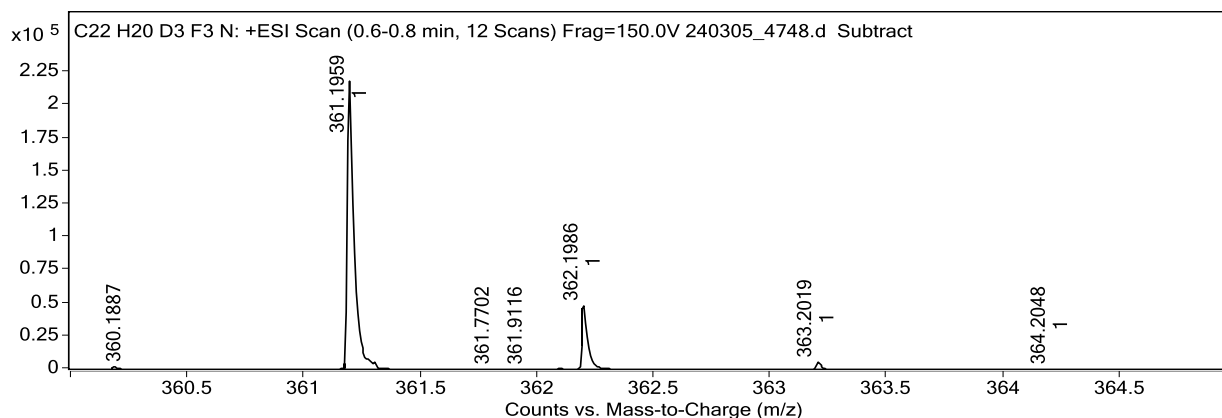
Sample Name	GR-19-085	Data File	240305_4748.d
Acq Method	HRMS.m	DA Method	AIMS_Accurate_Mass.m
Instrument	Agilent 6538 UHD	Acq Date, Time	05/03/2024 4:07:57 PM
Comment	ESI+		

Target Ion Species

Ion Species	m/z	Ionic Formula
M+	361.1959	C22 H20 [2H]3 F3 N

MFG Calculator Results

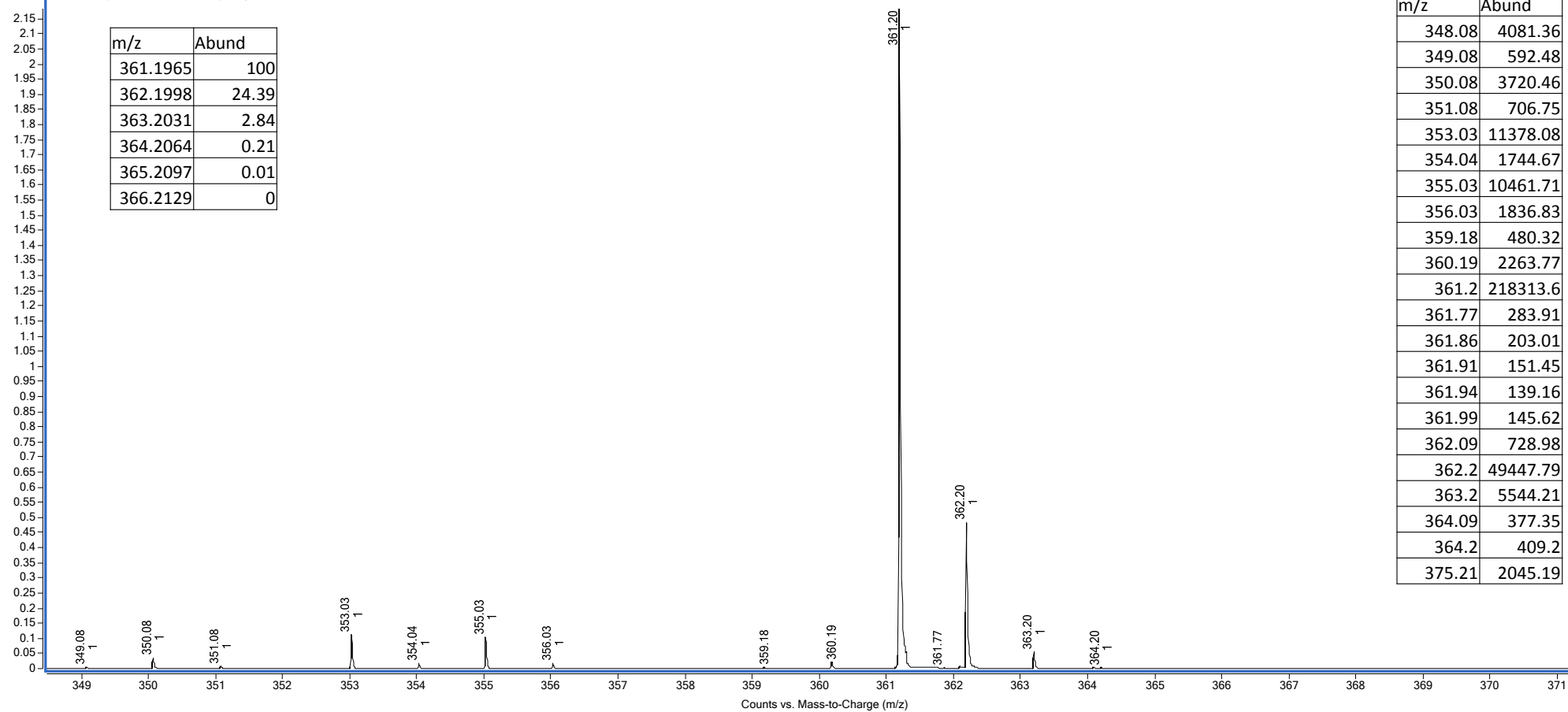
Target m/z	Ionic Formula	Calc m/z	+/- (mDa)	+/- (ppm)	DBE	MFG Score
361.1959	C19 H24 [2H]2 F3 O3	361.1954	0.5	1.4	5.5	98.51
361.1959	C17 H24 [2H] F3 N3 O2	361.1956	0.3	0.8	5.5	98.05
361.1959	C22 H20 [2H]3 F3 N	361.1965	-0.6	-1.7	10.5	97.33
361.1959	C15 H24 F3 N6 O	361.1958	0.1	0.3	5.5	96.64
361.1959	C14 H28 F3 N2 O5	361.1945	1.4	3.9	0.5	86.92
361.1959	C19 H28 F3 O3	361.1985	-2.6	-7.2	4.5	80.89
361.1959	C17 H20 [2H]3 F3 N3 O2	361.1925	3.4	9.4	6.5	74.84
361.1959	C15 H20 [2H]2 F3 N6 O	361.1927	3.2	8.9	6.5	74.53
361.1959	C13 H20 [2H] F3 N9	361.1929	3.0	8.3	6.5	73.16
361.1959	C22 H24 [2H] F3 N	361.1996	-3.7	-10.2	9.5	70.19



Predicted Isotope Match Table

Isotope	m/z	Calc m/z	Diff (mDa)	Abund (%)	Calc Abund (%)	+/-
1	361.1959	361.1965	-0.6	100.0	100.0	0.0
2	362.1986	362.1998	-1.2	22.6	24.4	1.8
3	363.2019	363.2031	-1.2	2.5	2.8	0.3

+ESI Scan (0.6-0.8 min, 12 Scans) Frag=150.0V 240305_4748.d Subtract



m/z	Abund
361.1965	100
362.1998	24.39
363.2031	2.84
364.2064	0.21
365.2097	0.01
366.2129	0

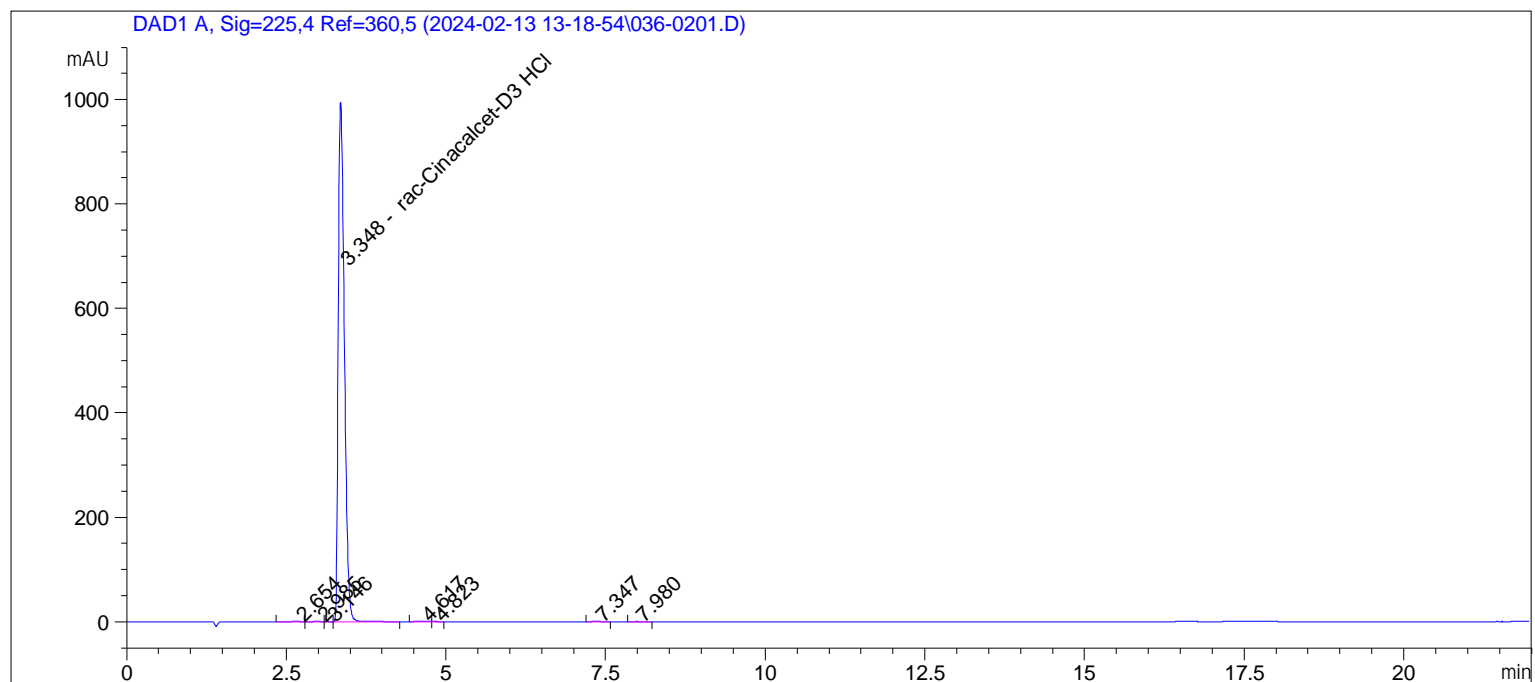
m/z	Abund
348.08	4081.36
349.08	592.48
350.08	3720.46
351.08	706.75
353.03	11378.08
354.04	1744.67
355.03	10461.71
356.03	1836.83
359.18	480.32
360.19	2263.77
361.2	218313.6
361.77	283.91
361.86	203.01
361.91	151.45
361.94	139.16
361.99	145.62
362.09	728.98
362.2	49447.79
363.2	5544.21
364.09	377.35
364.2	409.2
375.21	2045.19

Sample Name: VR-19-085

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=====
Acq. Operator   : vrusu                               Seq. Line :    2
Acq. Instrument : Instrument 1                       Location  : Vial 36
Injection Date  : 2/13/2024 1:43:13 PM              Inj       :    1
                                                    Inj Volume: 3.0 µl

Acq. Method    : C:\CHEM32\1\DATA\2024-02-13 13-18-54\VR021324_085.M
Last changed   : 2/13/2024 1:18:34 PM by vrusu
Analysis Method: C:\CHEM32\1\METHODS\VR021324_085PM.M
Last changed   : 2/13/2024 2:49:24 PM by vrusu
=====
    
```



Area Percent Report

```

Sorted By           :      Signal
Calib. Data Modified :      2/13/2024 2:48:44 PM
Multiplier          :      1.0000
Dilution            :      1.0000
Use Multiplier & Dilution Factor with ISTDs
    
```

Signal 1: DAD1 A, Sig=225,4 Ref=360,5

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	2.654	BV	0.1340	5.28166	0.0798	?
2	2.985	VV	0.1051	4.00920	0.0606	?
3	3.146	VV	0.0774	1.49480	0.0226	?
4	3.348	VB	0.1052	6594.46582	99.6421	rac-Cinacalcet-D3 HCl
5	4.617	BV	0.1823	5.43225	0.0821	?
6	4.823	VV	0.0811	1.74215	0.0263	?
7	7.347	VV	0.1491	3.97420	0.0600	?
8	7.980	BB	0.1216	1.75126	0.0265	?

Totals : 6618.15133

Sample Name: VR-19-085

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=====
Acq. Operator   : vrusu                               Seq. Line :    2
Acq. Instrument : Instrument 1                         Location  : Vial 36
Injection Date  : 2/13/2024 1:43:13 PM                Inj       :    1
                                                    Inj Volume: 3.0 µl
Acq. Method     : C:\CHEM32\1\DATA\2024-02-13 13-18-54\VR021324_085.M
Last changed    : 2/13/2024 1:18:34 PM by vrusu
Analysis Method : C:\CHEM32\1\METHODS\VR021324_085PM.M
Last changed    : 2/13/2024 2:49:24 PM by vrusu
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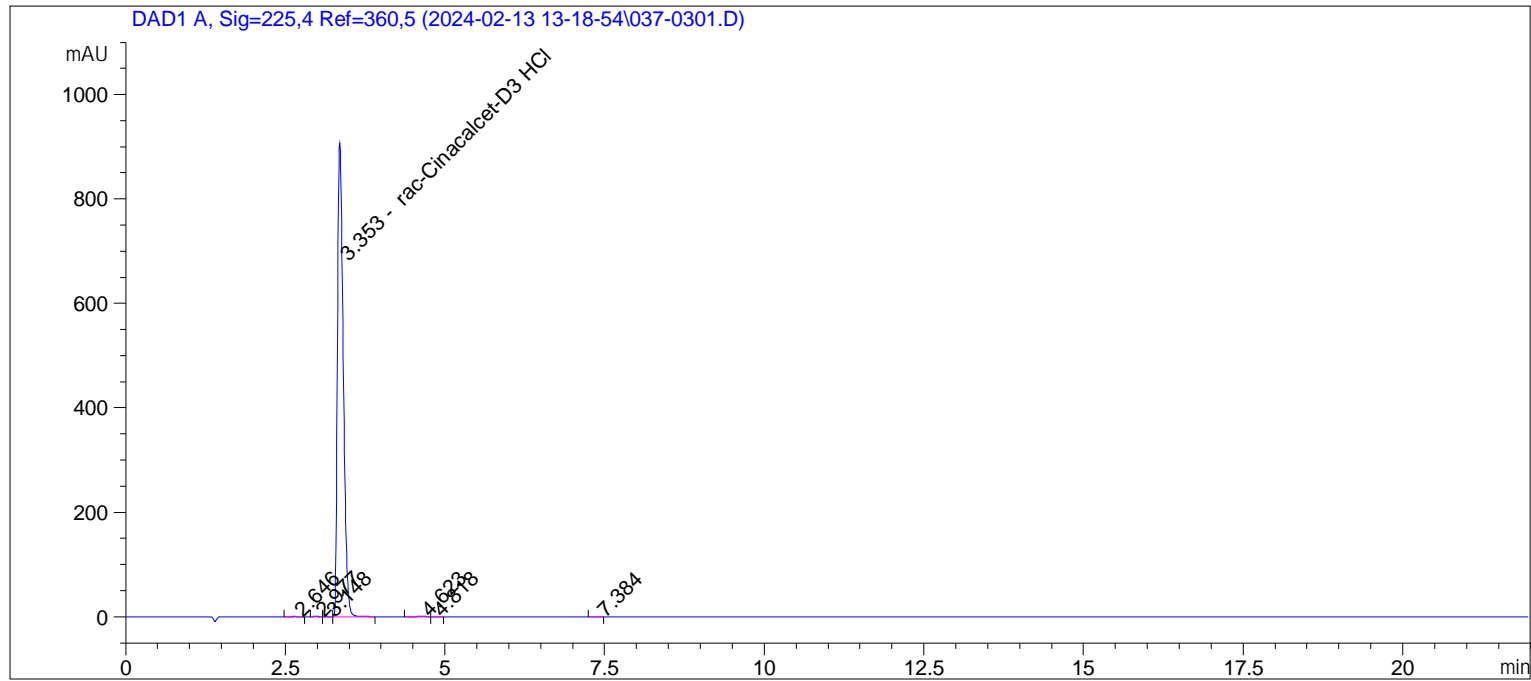
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*** End of Report ***
```


Sample Name: VR-19-085 spl-2

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=====
Acq. Operator   : vrusu                               Seq. Line :    3
Acq. Instrument : Instrument 1                         Location  : Vial 37
Injection Date  : 2/13/2024 2:06:30 PM                Inj       :    1
                                                    Inj Volume: 3.0 µl

Acq. Method     : C:\CHEM32\1\DATA\2024-02-13 13-18-54\VR021324_085.M
Last changed    : 2/13/2024 1:18:34 PM by vrusu
Analysis Method : C:\CHEM32\1\METHODS\VR021324_085PM.M
Last changed    : 2/13/2024 2:49:24 PM by vrusu
=====
    
```



Area Percent Report

```

Sorted By           :      Signal
Calib. Data Modified :      2/13/2024 2:48:44 PM
Multiplier          :      1.0000
Dilution            :      1.0000
Use Multiplier & Dilution Factor with ISTDs
    
```

Signal 1: DAD1 A, Sig=225,4 Ref=360,5

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	2.646	VV	0.1084	2.12487	0.0371	?
2	2.977	VB	0.0896	2.19175	0.0382	?
3	3.148	BV	0.0691	1.02696	0.0179	?
4	3.353	VB	0.0976	5723.03760	99.7906	rac-Cinacalcet-D3 HCl
5	4.623	BV	0.1864	4.22351	0.0736	?
6	4.818	VB	0.0857	1.26146	0.0220	?
7	7.384	BB	0.0957	1.18179	0.0206	?

Totals : 5735.04794

Sample Name: VR-19-085 spl-2

```
=====
Acq. Operator   : vrusu                               Seq. Line :    3
Acq. Instrument : Instrument 1                         Location  : Vial 37
Injection Date  : 2/13/2024 2:06:30 PM                Inj       :    1
                                                    Inj Volume: 3.0 µl
Acq. Method     : C:\CHEM32\1\DATA\2024-02-13 13-18-54\VR021324_085.M
Last changed    : 2/13/2024 1:18:34 PM by vrusu
Analysis Method : C:\CHEM32\1\METHODS\VR021324_085PM.M
Last changed    : 2/13/2024 2:49:24 PM by vrusu
=====
```

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