

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082322\
 Data File : BF129956.D
 Acq On : 23 Aug 2022 16:35
 Operator : CG\JU
 Sample : N4142-03
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 UST-EAST

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129956.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.016	461	464	478	rBV	80642	117917	2.90%	0.451%
2	5.416	529	532	553	rBV	3362300	3211928	78.93%	12.291%
3	6.434	701	705	720	rBV	3452851	3290384	80.86%	12.591%
4	6.775	759	763	772	rBV	1037628	849365	20.87%	3.250%
5	7.345	855	860	863	rBV	2258368	2136712	52.51%	8.176%
6	8.057	976	981	985	rBV	1272769	1161280	28.54%	4.444%
7	9.128	1158	1163	1167	rBV	4064463	4069197	100.00%	15.571%
8	9.810	1274	1279	1282	rBV	1613420	1338320	32.89%	5.121%
9	10.604	1410	1414	1428	rBV	2829015	2626252	64.54%	10.050%
10	10.722	1432	1434	1441	rVB	69438	62811	1.54%	0.240%
11	11.298	1529	1532	1536	rBV	1544676	1305399	32.08%	4.995%
12	11.674	1593	1596	1600	rBV	76097	67253	1.65%	0.257%
13	11.821	1617	1621	1624	rBV	47797	53062	1.30%	0.203%
14	12.380	1708	1716	1719	rBV	102907	118262	2.91%	0.453%
15	12.886	1797	1802	1805	rBV	4280450	3786327	93.05%	14.489%
16	13.780	1948	1954	1966	rBV3	102061	298490	7.34%	1.142%
17	13.945	1979	1982	1987	rBV	1023700	895585	22.01%	3.427%
18	14.033	1992	1997	2002	rBV	53843	56464	1.39%	0.216%
19	14.680	2103	2107	2113	rBV3	52812	64510	1.59%	0.247%
20	15.398	2225	2229	2236	rVB	490672	622924	15.31%	2.384%

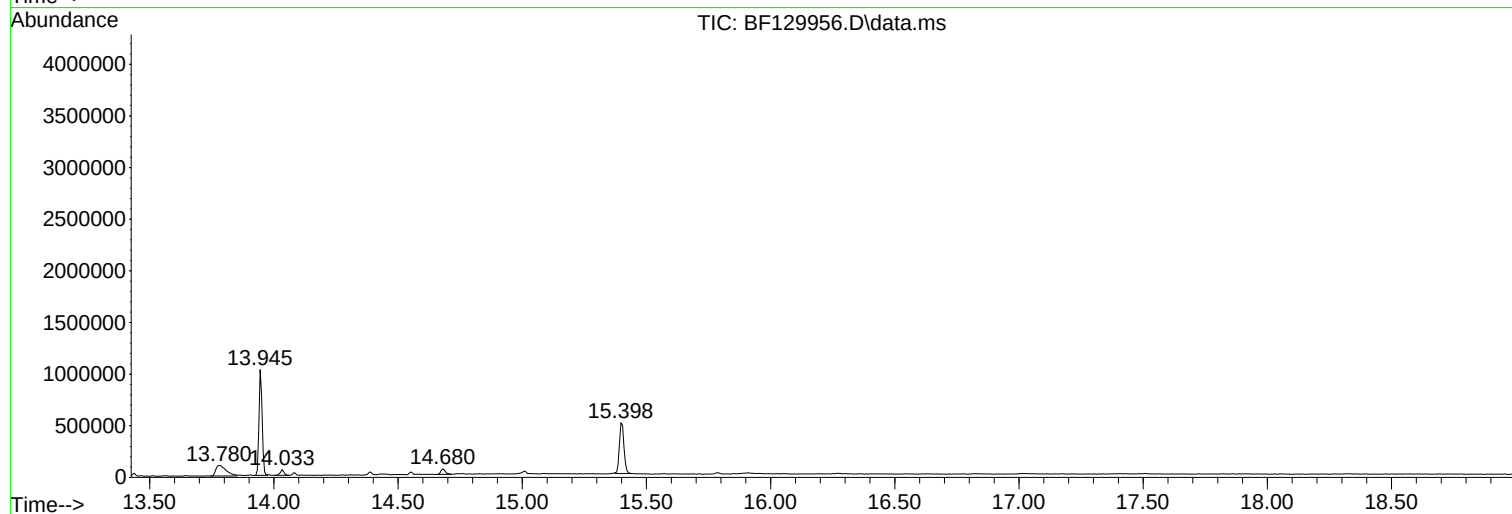
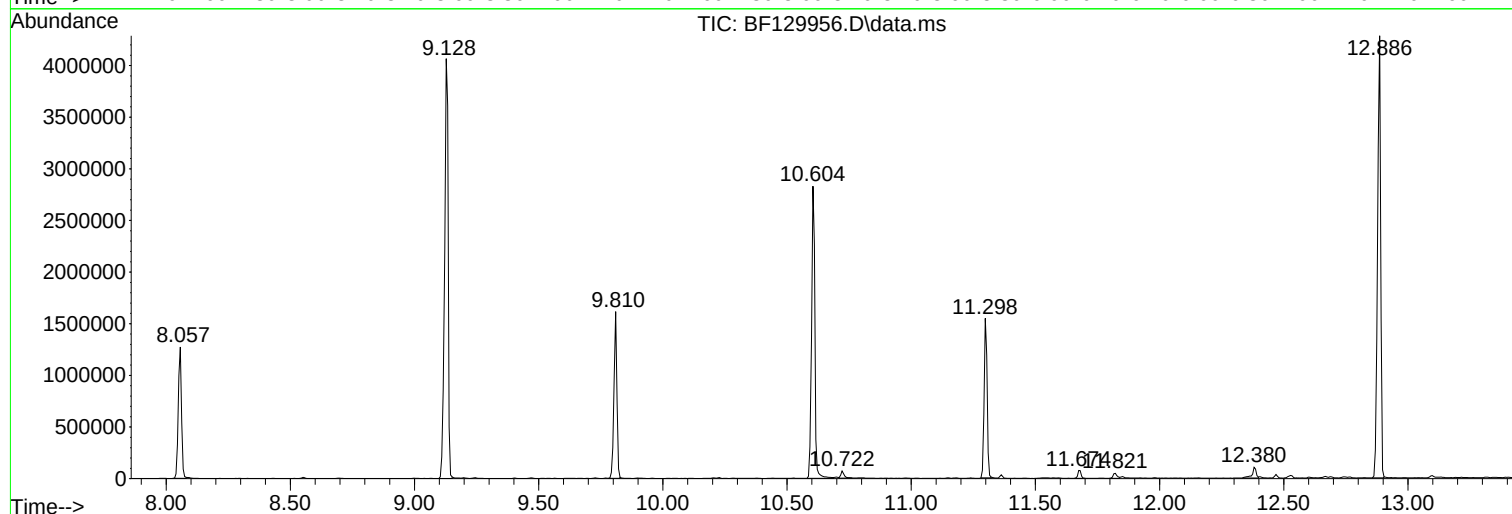
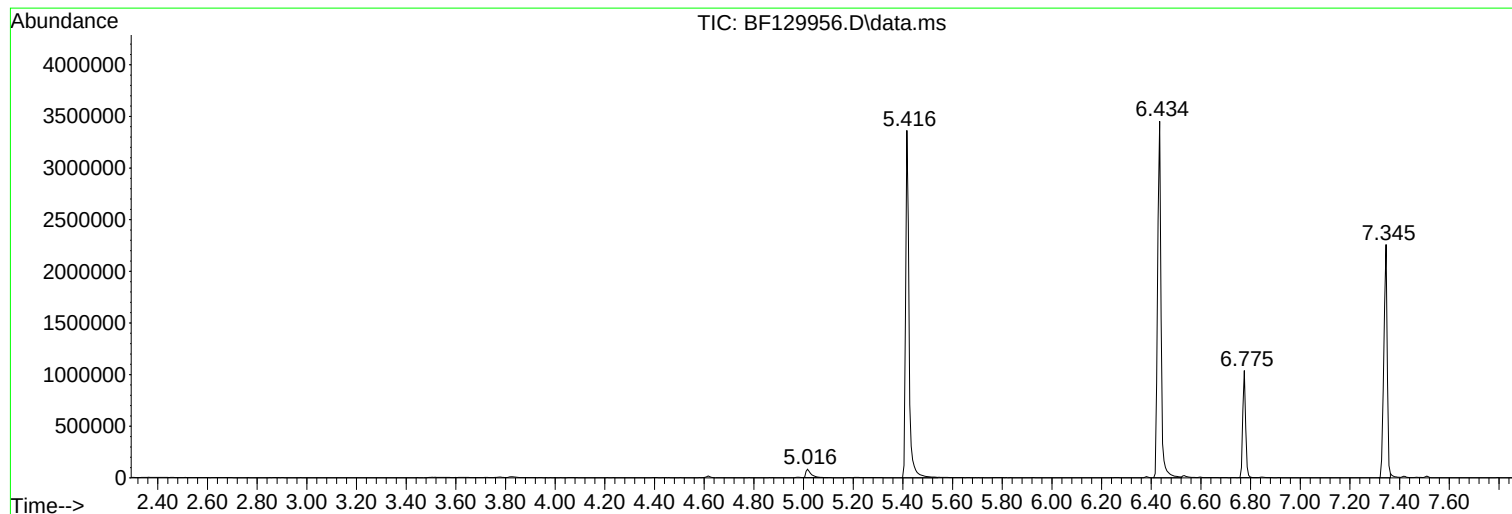
Sum of corrected areas: 26132442

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082322\
Data File : BF129956.D
Acq On : 23 Aug 2022 16:35
Operator : CG\JU
Sample : N4142-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UST-EAST

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082322\
Data File : BF129956.D
Acq On : 23 Aug 2022 16:35
Operator : CG\JU
Sample : N4142-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UST-EAST

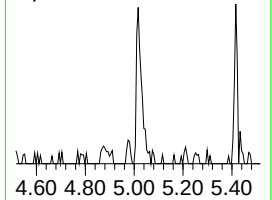
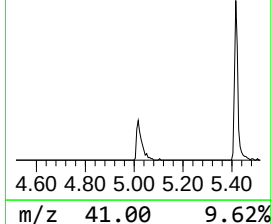
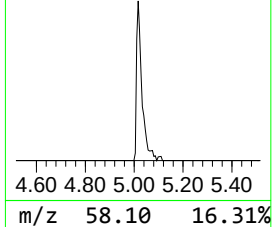
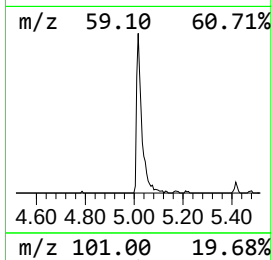
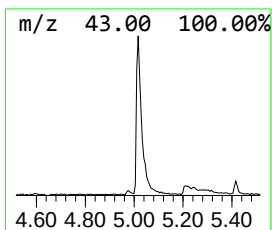
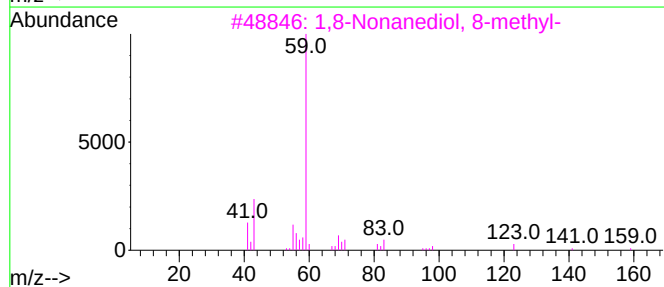
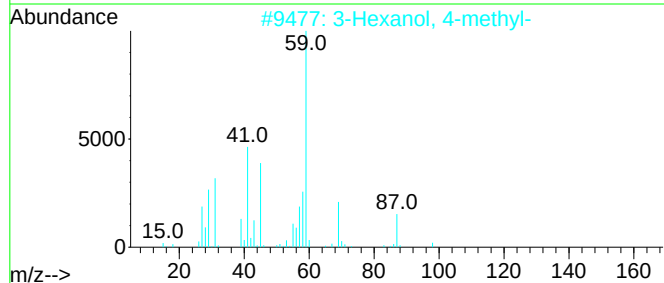
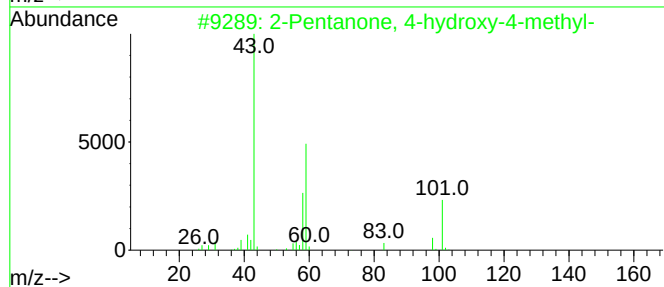
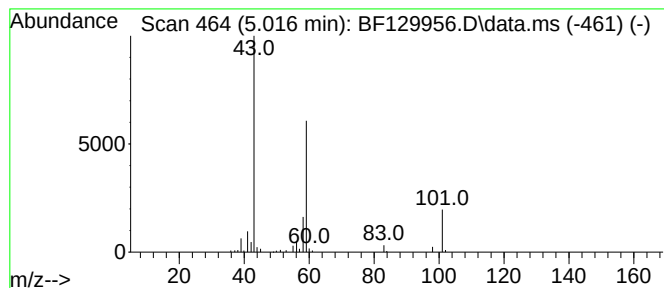
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	2.78 ng	117917	1,4-Dichlorobenzene-d4	6.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28		
3	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082322\
Data File : BF129956.D
Acq On : 23 Aug 2022 16:35
Operator : CG\JU
Sample : N4142-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UST-EAST

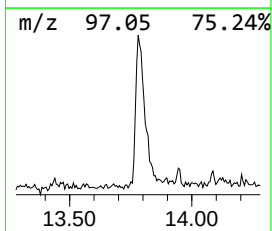
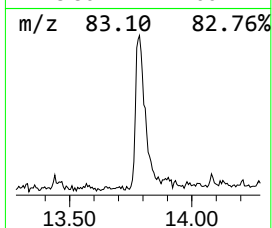
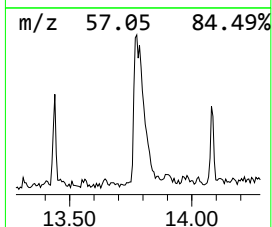
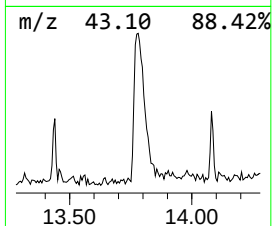
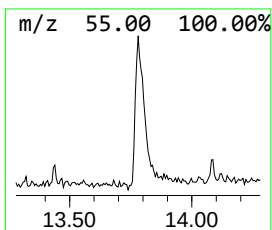
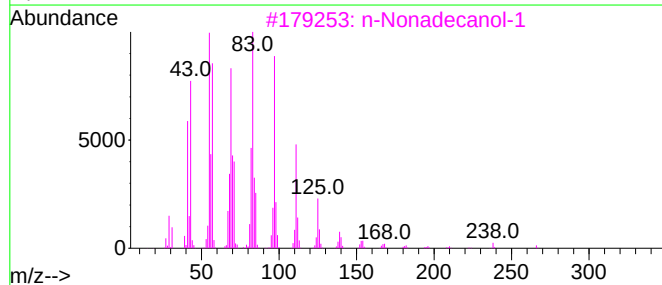
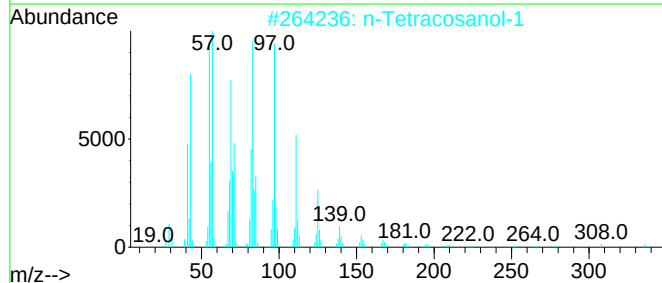
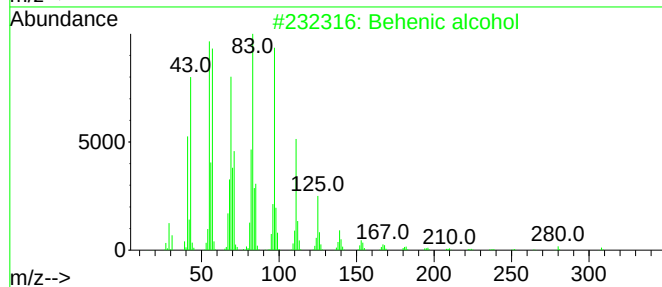
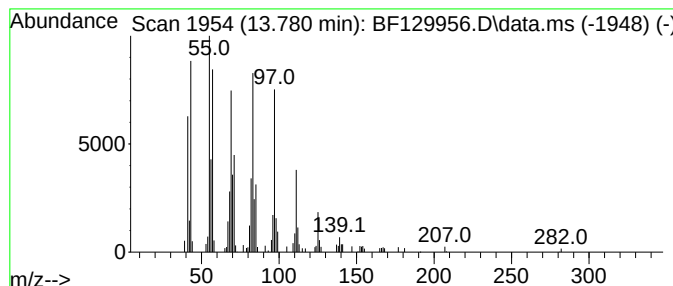
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Behenic alcohol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.780	6.67 ng	298490	Chrysene-d12	13.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	95
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	93
4			1-Heneicosanol	312	C21H44O	015594-90-8	93
5			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082322\
Data File : BF129956.D
Acq On : 23 Aug 2022 16:35
Operator : CG\JU
Sample : N4142-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UST-EAST

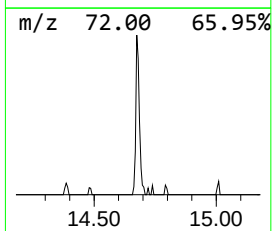
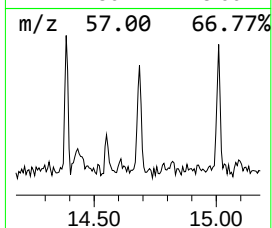
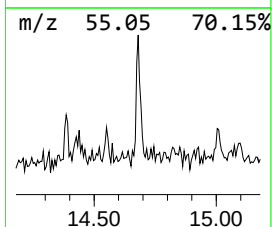
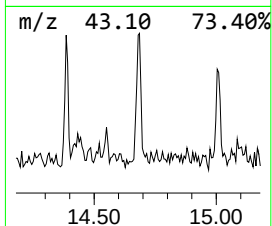
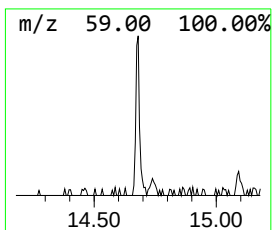
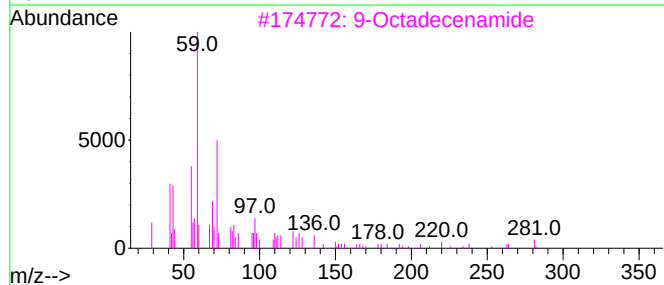
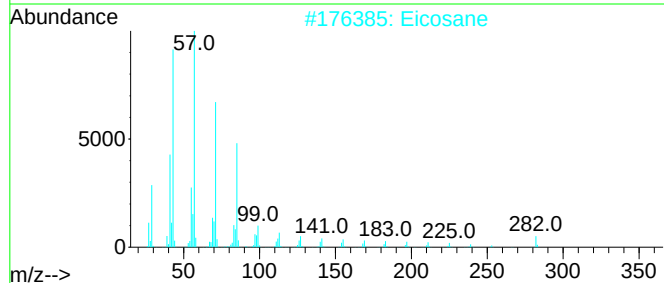
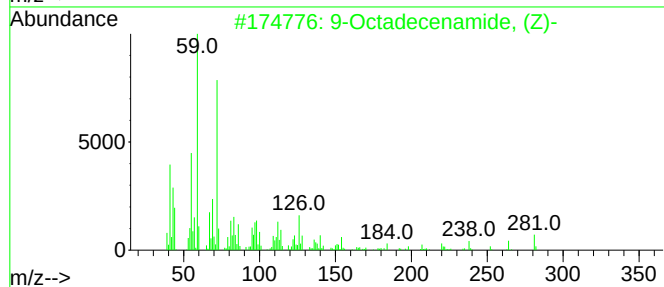
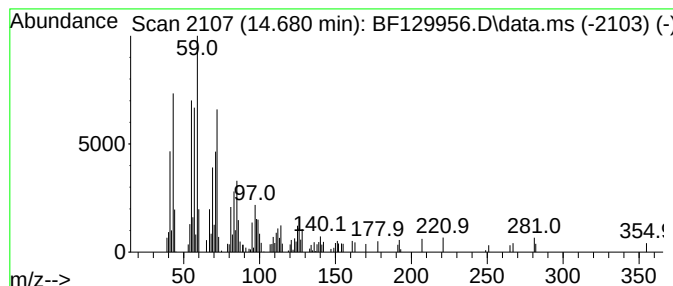
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.680	2.07 ng	64510	Perylene-d12	15.398

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2		Eicosane	282	C20H42	000112-95-8	60
3		9-Octadecenamide	281	C18H35NO	003322-62-1	53
4		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	49
5		Cyclohexanecarboxamide	127	C7H13NO	001122-56-1	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082322\
Data File : BF129956.D
Acq On : 23 Aug 2022 16:35
Operator : CG\JU
Sample : N4142-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UST-EAST

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.016	2.8	ng	117917	1	6.775	849365	20.0
Behenic alcohol	13.780	6.7	ng	298490	5	13.945	895585	20.0
9-Octadecenamid...	14.680	2.1	ng	64510	6	15.398	622924	20.0