

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061121\
 Data File : BF124267.D
 Acq On : 11 Jun 2021 18:33
 Operator : JU/CG
 Sample : M2625-03
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 18-B12(146-150)

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-BF060321.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124267.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	13	17	22	rBB	16176	20815	1.87%	0.290%
2	5.051	500	504	511	rVB	69948	84021	7.55%	1.170%
3	5.469	571	575	582	rBV	987069	840799	75.55%	11.713%
4	5.851	636	640	643	rBB	16710	14461	1.30%	0.201%
5	6.481	743	747	750	rBV	983389	828865	74.48%	11.547%
6	6.840	805	808	811	rBV	274683	212935	19.13%	2.966%
7	7.404	899	904	907	rBV	650733	567812	51.02%	7.910%
8	8.028	1007	1010	1020	rBB	21249	26301	2.36%	0.366%
9	8.122	1022	1026	1029	rBV	341172	264059	23.73%	3.679%
10	9.198	1205	1209	1212	rBV	1408440	1084890	97.49%	15.113%
11	9.881	1321	1325	1328	rBV	389215	331553	29.79%	4.619%
12	10.669	1455	1459	1462	rBV	937244	774719	69.61%	10.792%
13	11.369	1574	1578	1581	rBV	392198	352054	31.63%	4.904%
14	11.892	1664	1667	1672	rVB2	32210	30616	2.75%	0.427%
15	12.951	1843	1847	1851	rBV	1178280	1112872	100.00%	15.503%
16	13.874	1997	2004	2014	rBV8	23604	58923	5.29%	0.821%
17	14.010	2023	2027	2031	rBV	292865	244963	22.01%	3.413%
18	14.763	2151	2155	2160	rBV2	48054	57970	5.21%	0.808%
19	15.486	2273	2278	2283	rBV	201320	256304	23.03%	3.570%
20	17.039	2539	2542	2547	rVB5	7877	13467	1.21%	0.188%

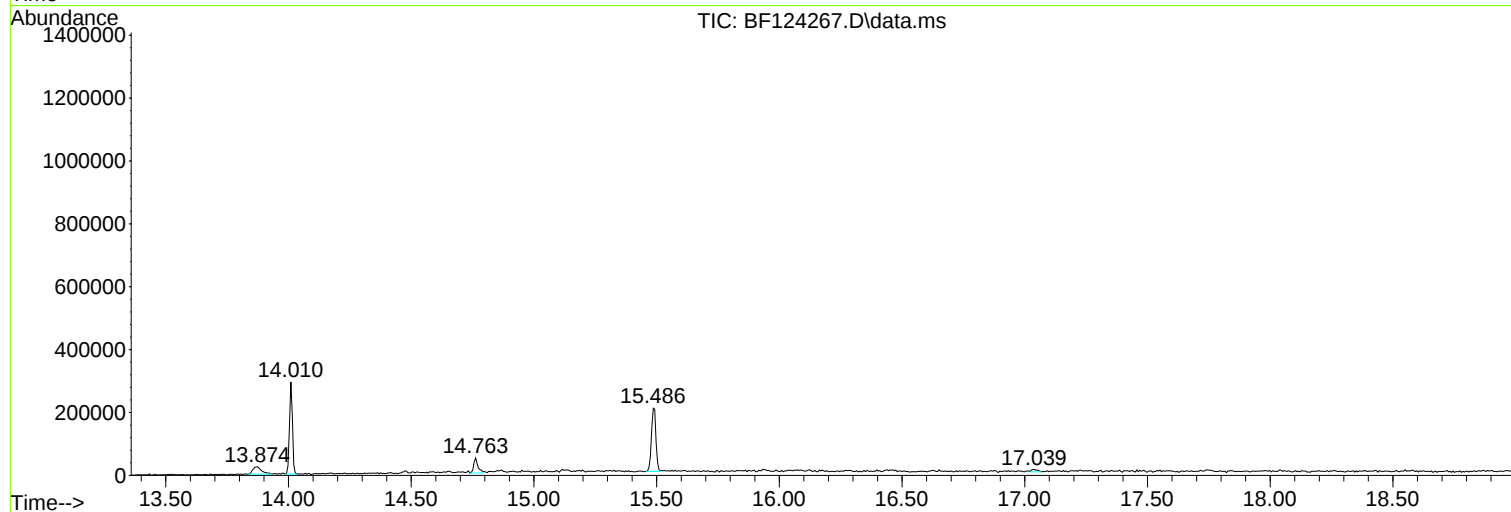
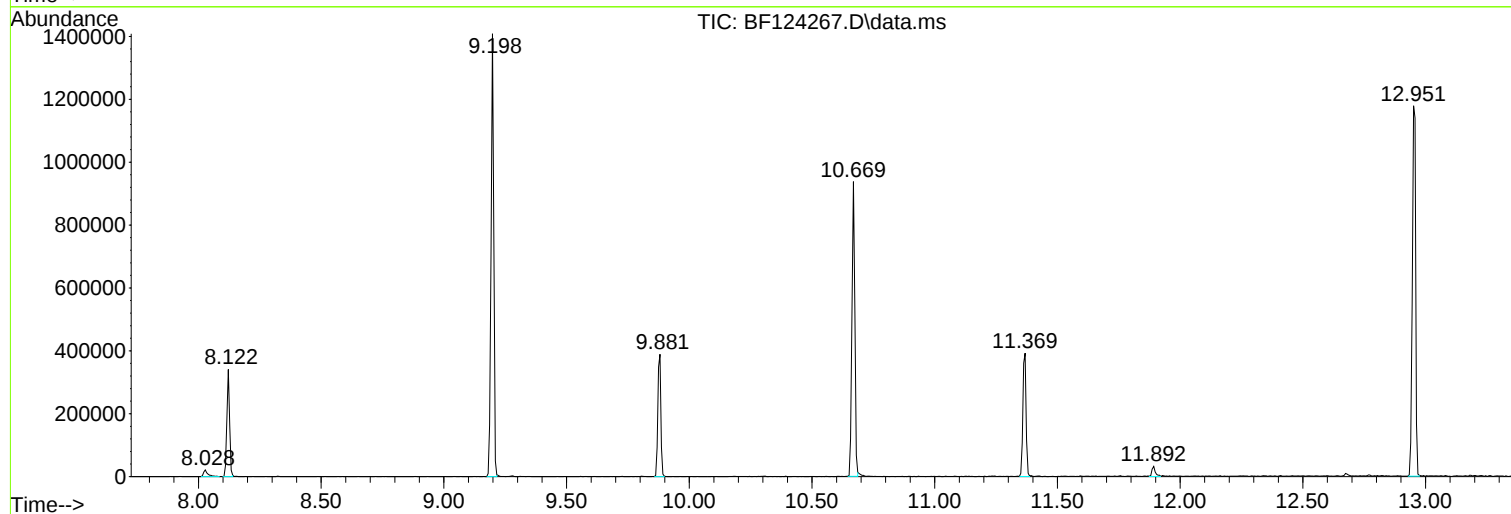
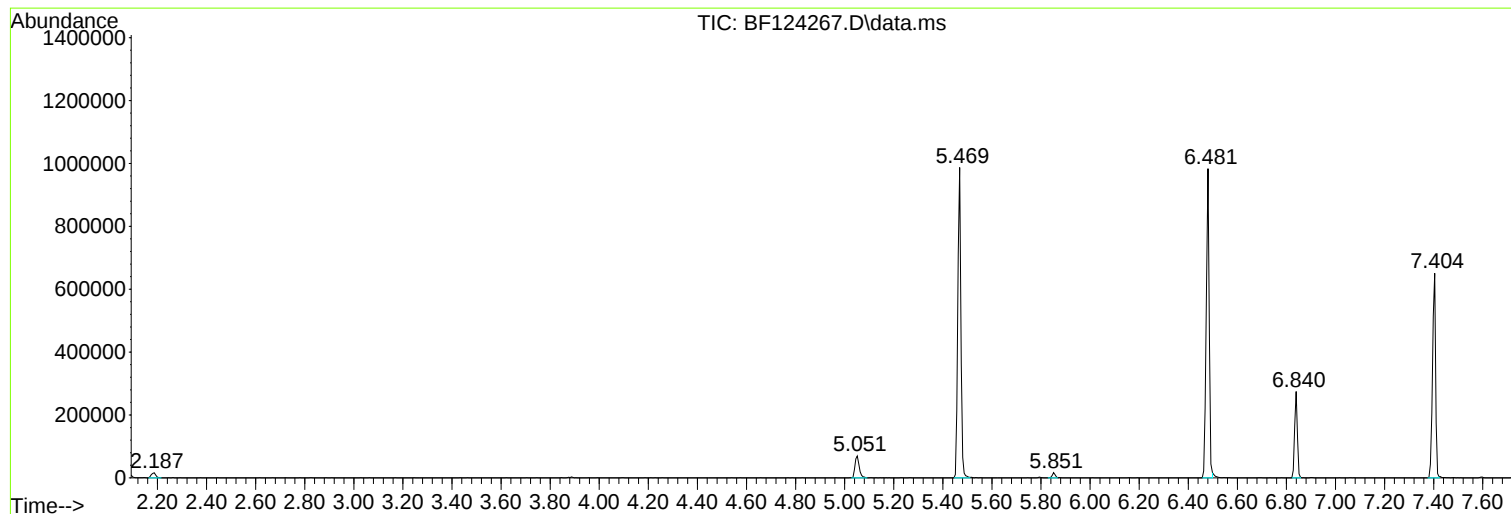
Sum of corrected areas: 7178399

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061121\
Data File : BF124267.D
Acq On : 11 Jun 2021 18:33
Operator : JU/CG
Sample : M2625-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
18-B12(146-150)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061121\
Data File : BF124267.D
Acq On : 11 Jun 2021 18:33
Operator : JU/CG
Sample : M2625-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
18-B12(146-150)

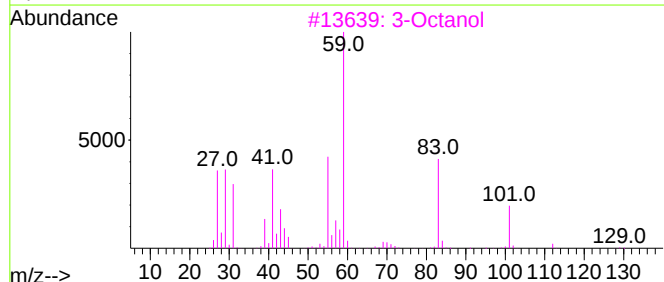
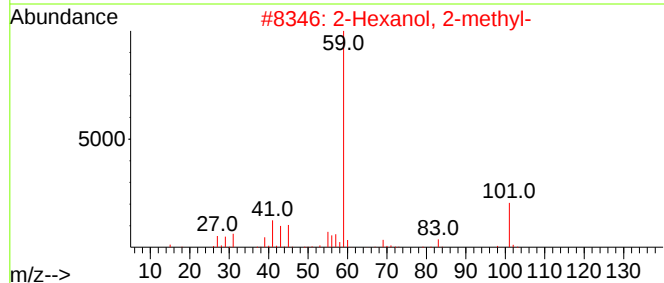
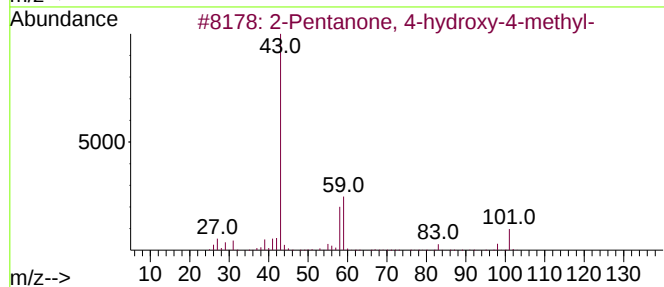
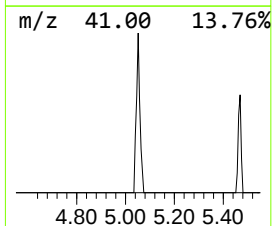
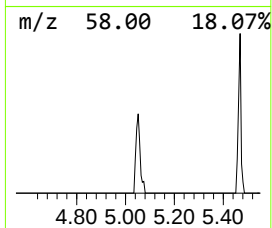
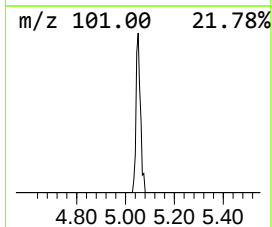
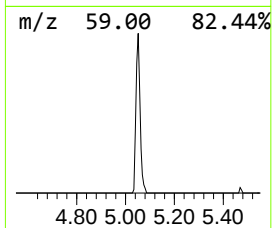
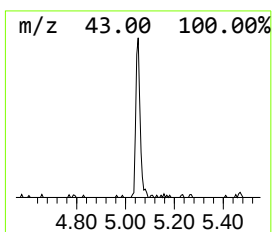
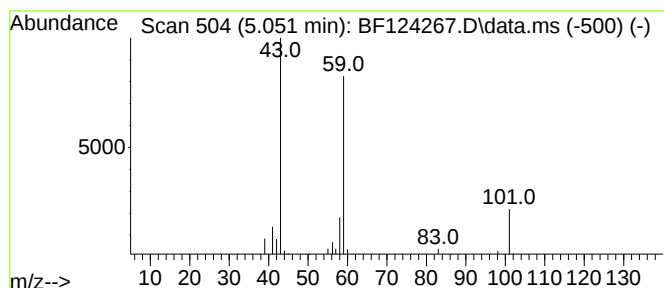
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.051	7.89 ng	84021	1,4-Dichlorobenzene-d4	6.840

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	64		
3	3-Octanol	130	C8H18O	000589-98-0	38		
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	33		
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	28		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061121\
Data File : BF124267.D
Acq On : 11 Jun 2021 18:33
Operator : JU/CG
Sample : M2625-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

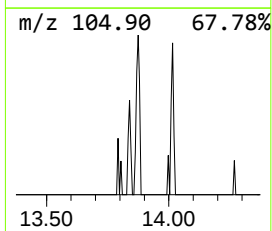
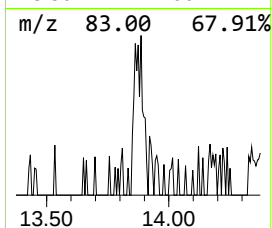
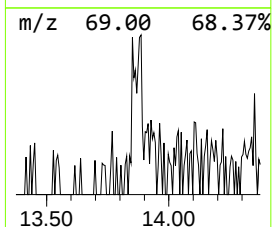
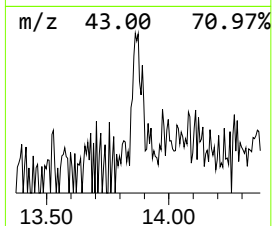
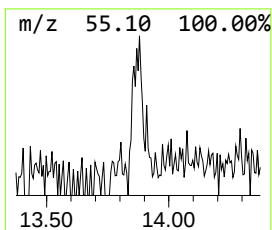
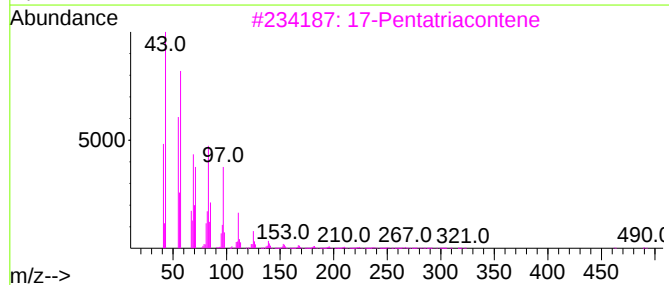
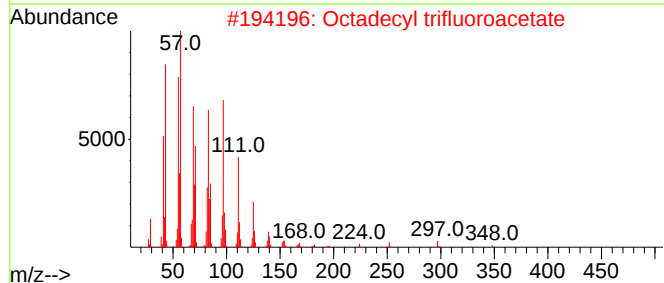
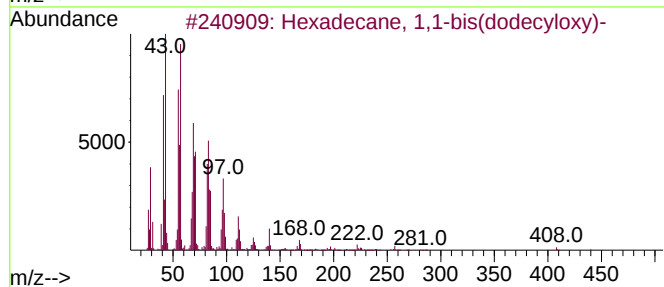
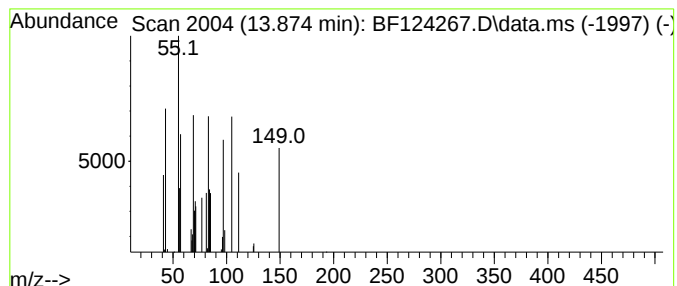
Instrument :
BNA_F
ClientSampleId :
18-B12(146-150)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Hexadecane, 1,1-bis(dodecyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.874	4.81 ng	58923	Chrysene-d12		14.010	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexadecane, 1,1-bis(dodecyloxy)-		595	C40H82O2	056554-64-4	53
2	Octadecyl trifluoroacetate		366	C20H37F3O2	079392-43-1	50
3	17-Pentatriacontene		491	C35H70	006971-40-0	50
4	Carbonochloridic acid, decyl ester		220	C11H21ClO2	055488-51-2	50
5	Nonadecyl pentafluoropropionate		430	C22H39F5O2	1000351-88-8	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061121\
Data File : BF124267.D
Acq On : 11 Jun 2021 18:33
Operator : JU/CG
Sample : M2625-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
18-B12(146-150)

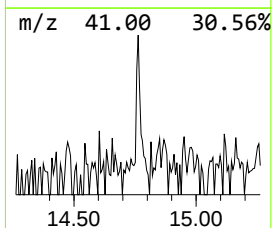
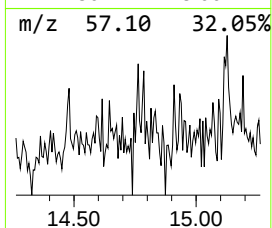
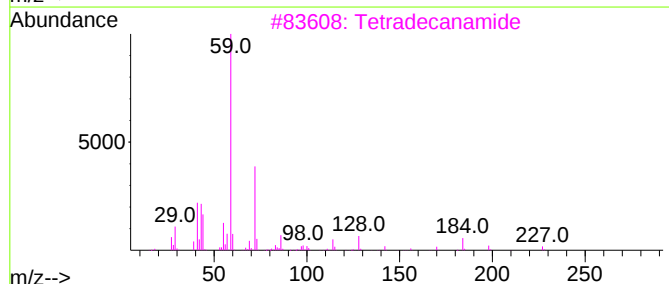
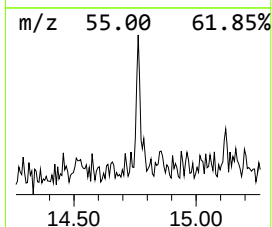
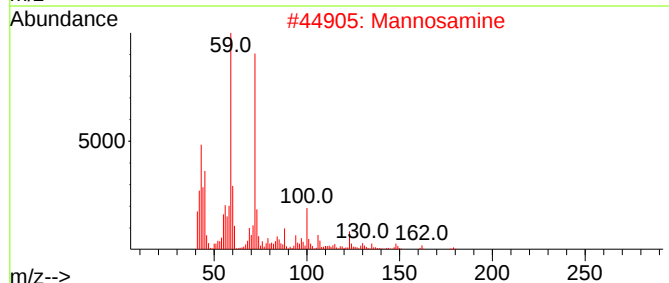
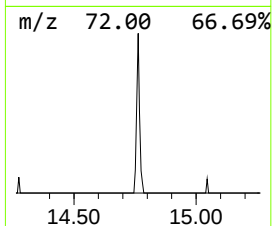
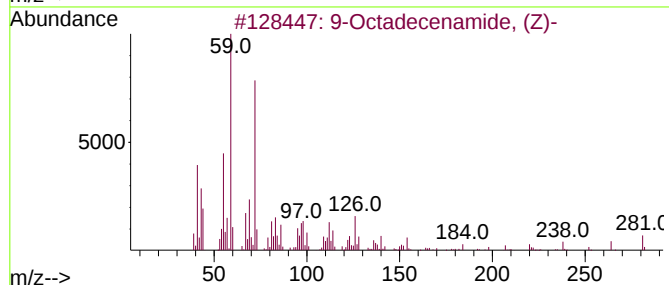
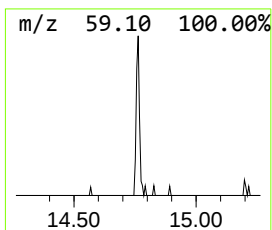
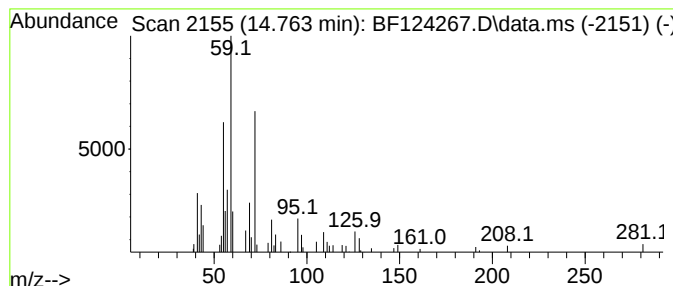
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.763	4.52 ng	57970	Perylene-d12	15.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	70
2			Mannosamine	179	C6H13NO5	1000127-68-8	50
3			Tetradecanamide	227	C14H29NO	000638-58-4	50
4			8-Methyl-6-nonenamide	169	C10H19NO	1000293-20-9	45
5			d-Glucosamine	179	C6H13NO5	000090-77-7	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061121\
Data File : BF124267.D
Acq On : 11 Jun 2021 18:33
Operator : JU/CG
Sample : M2625-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
18-B12(146-150)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.051	7.9	ng	84021	1	6.840	212935	20.0
Hexadecane, 1,1...	13.874	4.8	ng	58923	5	14.010	244963	20.0
9-Octadecenamid...	14.763	4.5	ng	57970	6	15.486	256304	20.0