

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082522\
 Data File : BM036411.D
 Acq On : 25 Aug 2022 18:04
 Operator : CG/JU
 Sample : N4260-04
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SASP2-T-4-(16-22)

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_M\Methods\8270-BM080122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM036411.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.893	301	307	313	rBV	349969	490011	5.94%	0.946%
2	5.357	379	386	402	rBV	4272033	5912097	71.68%	11.413%
3	6.963	652	659	676	rBV	3882102	6040459	73.23%	11.661%
4	7.781	791	798	807	rBV	937251	1429005	17.32%	2.759%
5	8.951	988	997	1012	rBV	2242728	3735638	45.29%	7.211%
6	10.581	1267	1274	1289	rBV	1179660	1958194	23.74%	3.780%
7	13.051	1687	1694	1710	rBV	5315570	7726218	93.67%	14.915%
8	14.427	1921	1928	1943	rVB	1607937	2274467	27.58%	4.391%
9	15.915	2174	2181	2196	rBV	3783922	5240378	63.53%	10.116%
10	17.168	2388	2394	2405	rBV	1664469	2371126	28.75%	4.577%
11	18.074	2542	2548	2557	rBV	266736	470899	5.71%	0.909%
12	19.233	2738	2745	2753	rBV6	70089	173134	2.10%	0.334%
13	19.351	2761	2765	2775	rBV	145514	254269	3.08%	0.491%
14	19.798	2836	2841	2850	rBV	7129706	8248282	100.00%	15.923%
15	20.562	2968	2971	2975	rBV	167091	199976	2.42%	0.386%
16	21.068	3054	3057	3065	rBV2	226010	366347	4.44%	0.707%
17	21.356	3101	3106	3115	rBV	1717312	2309747	28.00%	4.459%
18	23.674	3494	3500	3510	rVB2	1332325	2600910	31.53%	5.021%

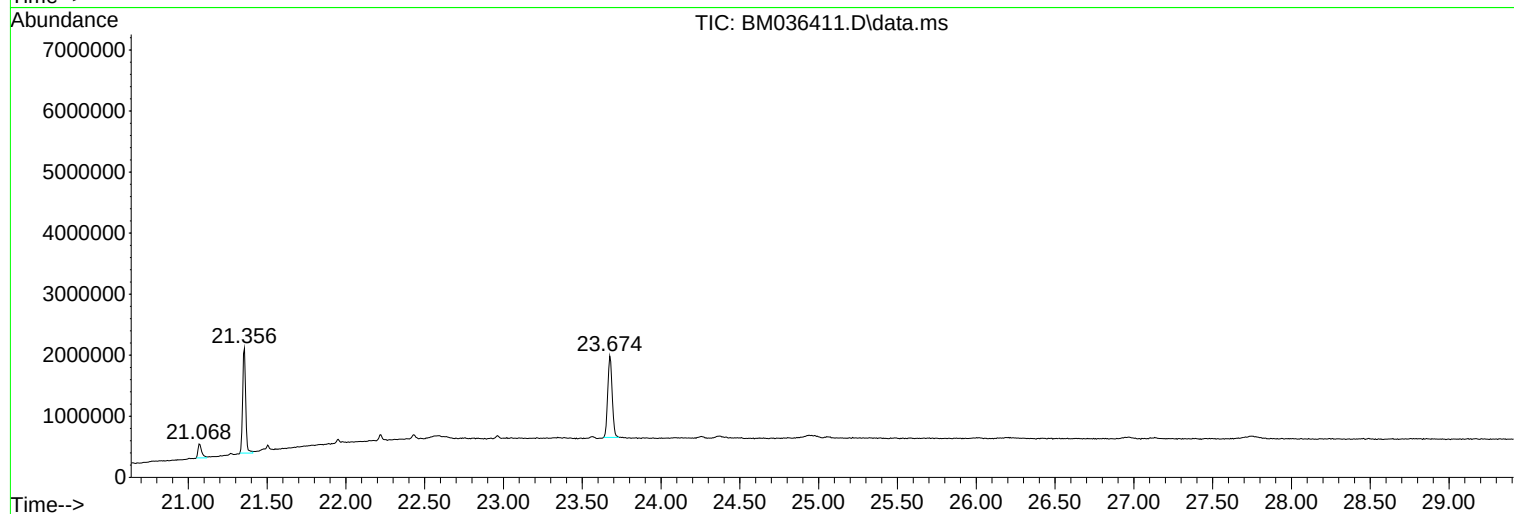
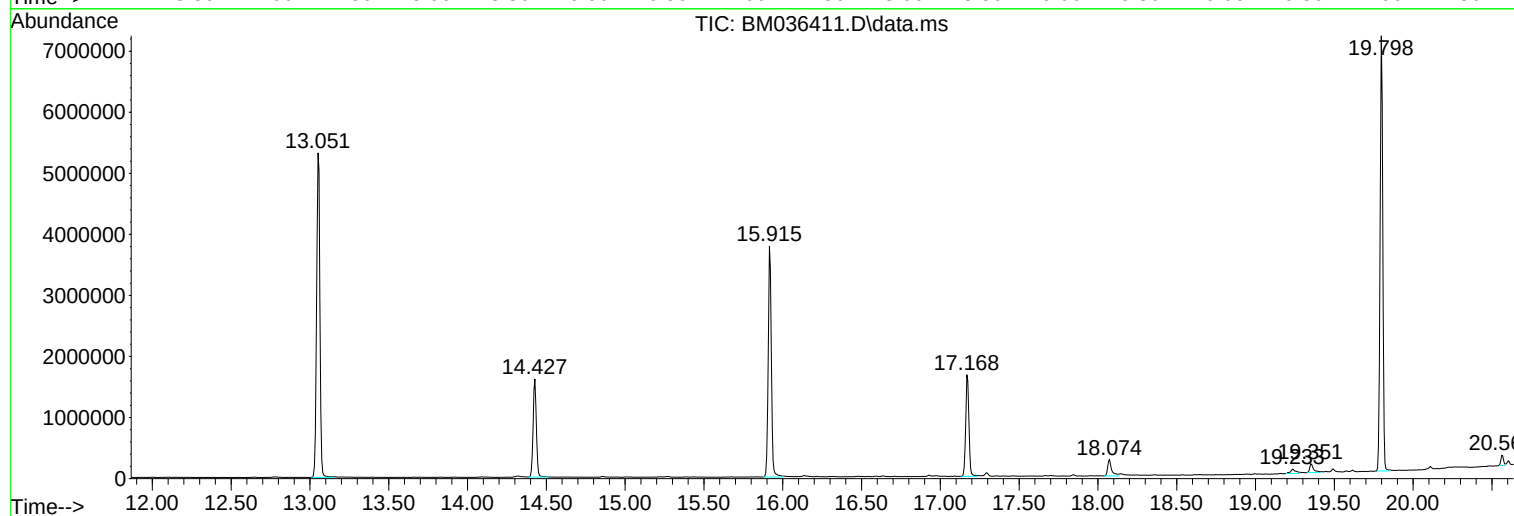
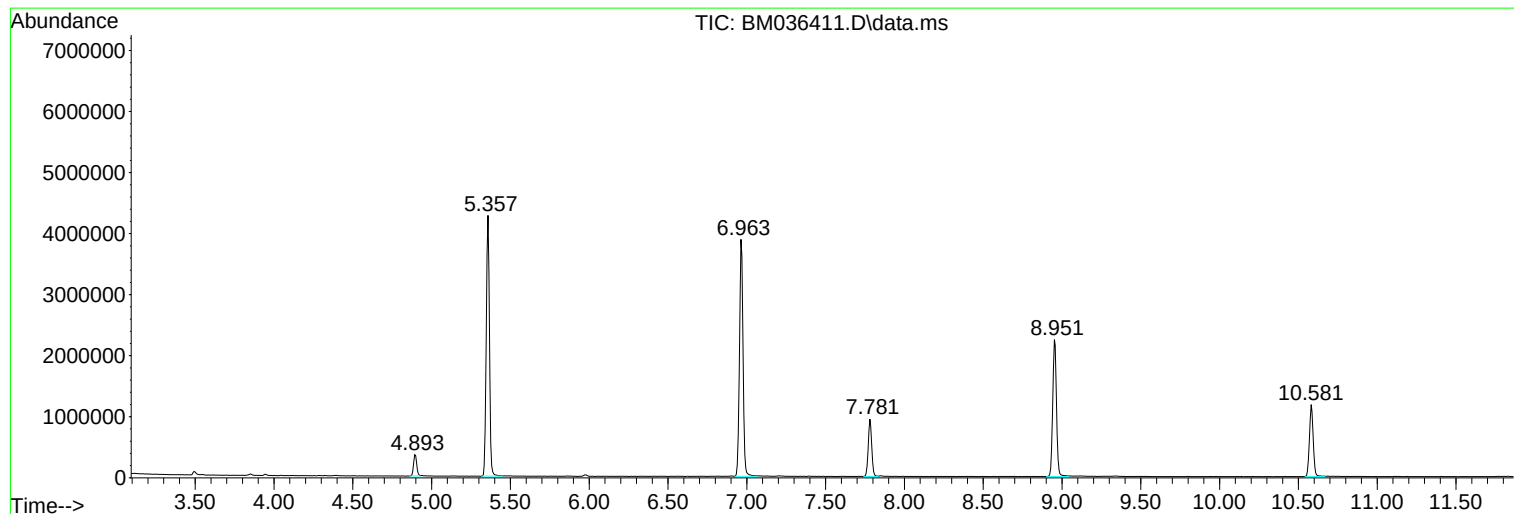
Sum of corrected areas: 51801157

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082522\
Data File : BM036411.D
Acq On : 25 Aug 2022 18:04
Operator : CG/JU
Sample : N4260-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SASP2-T-4-(16-22)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.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_M\Data\BM082522\
Data File : BM036411.D
Acq On : 25 Aug 2022 18:04
Operator : CG/JU
Sample : N4260-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SASP2-T-4-(16-22)

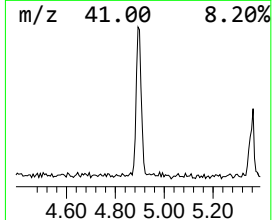
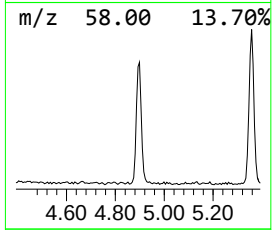
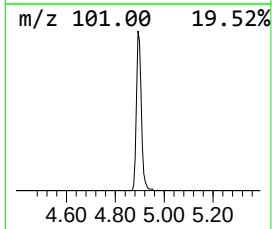
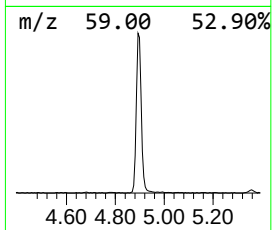
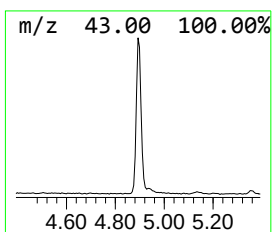
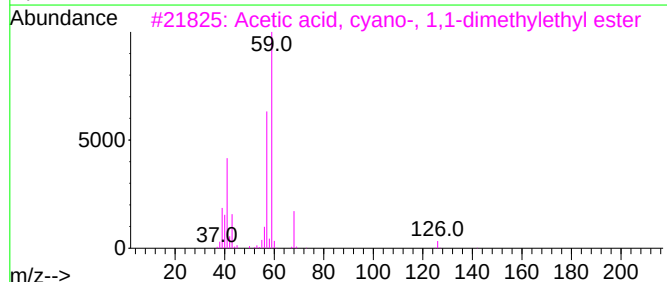
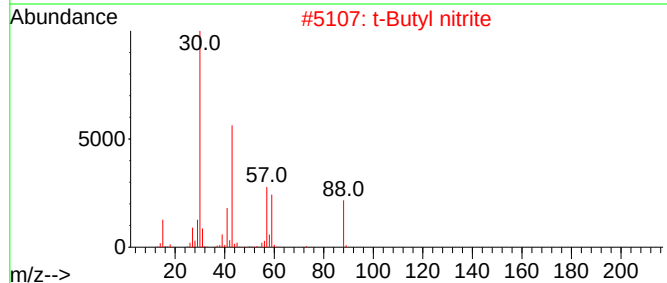
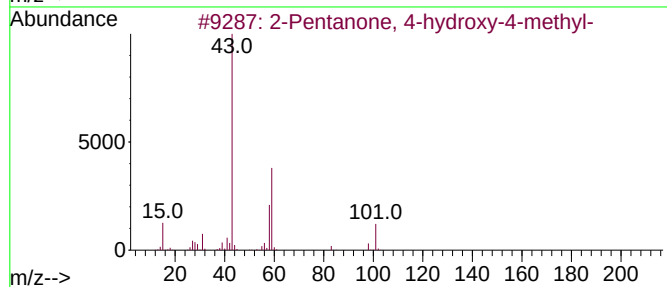
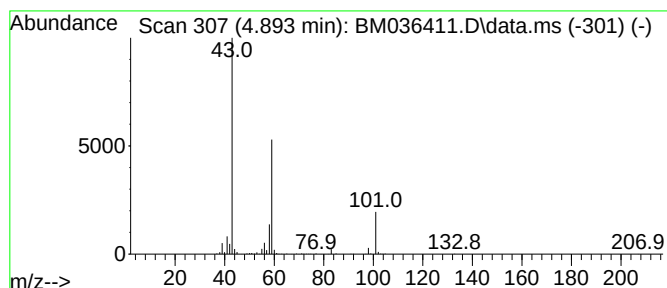
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.893	6.86 ng	490011	1,4-Dichlorobenzene-d4	7.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	t-Butyl nitrite	103	C4H9NO2	000540-80-7	38		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082522\
Data File : BM036411.D
Acq On : 25 Aug 2022 18:04
Operator : CG/JU
Sample : N4260-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SASP2-T-4-(16-22)

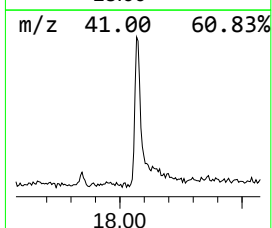
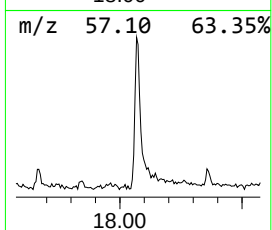
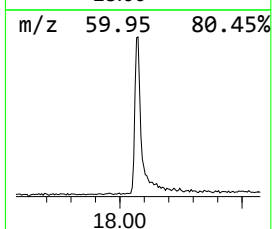
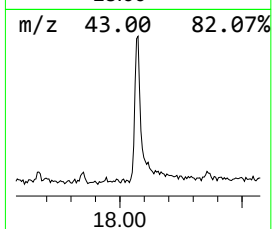
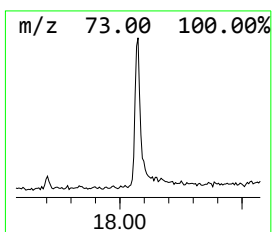
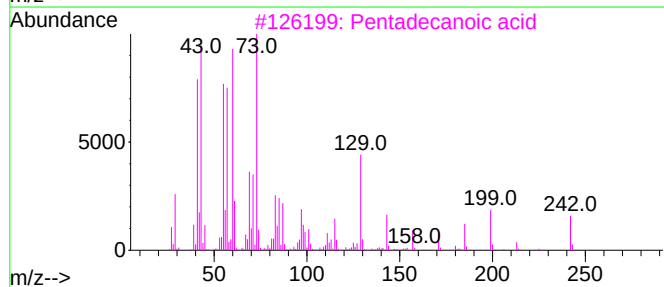
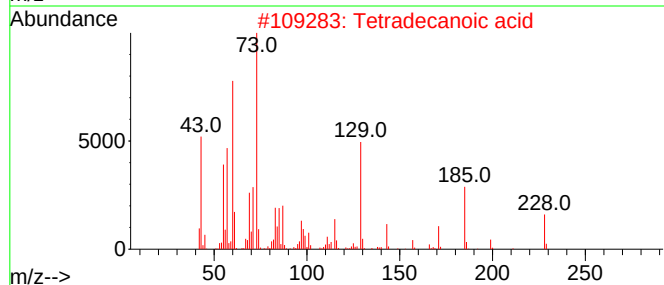
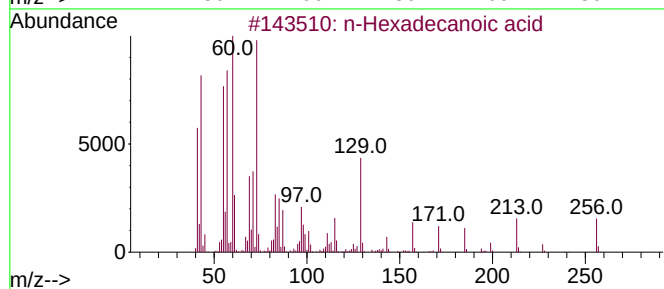
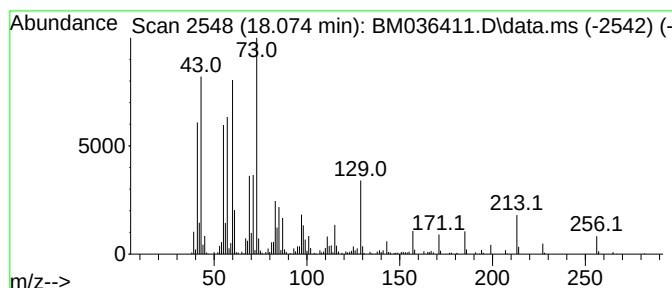
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.074	3.97 ng	470899	Phenanthrene-d10	17.168

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tridecanoic acid	214	C13H26O2	000638-53-9	59
5			Isopropyl palmitate	298	C19H38O2	000142-91-6	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082522\
Data File : BM036411.D
Acq On : 25 Aug 2022 18:04
Operator : CG/JU
Sample : N4260-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

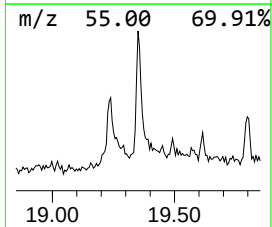
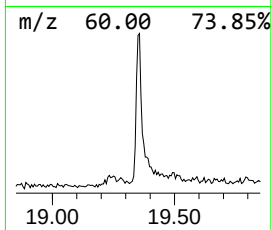
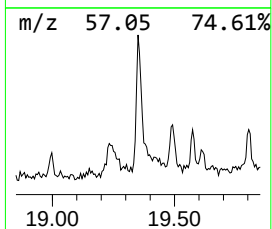
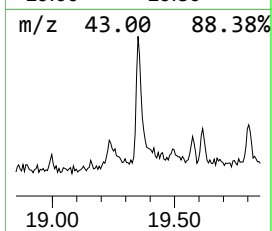
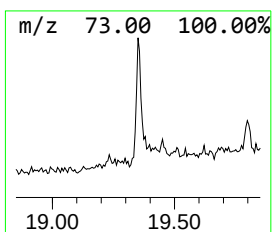
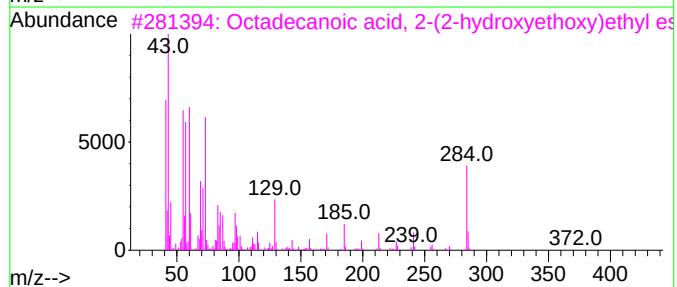
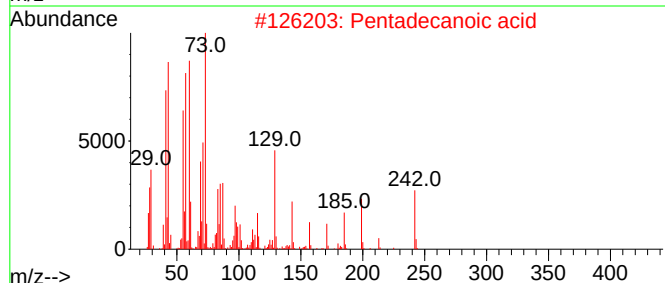
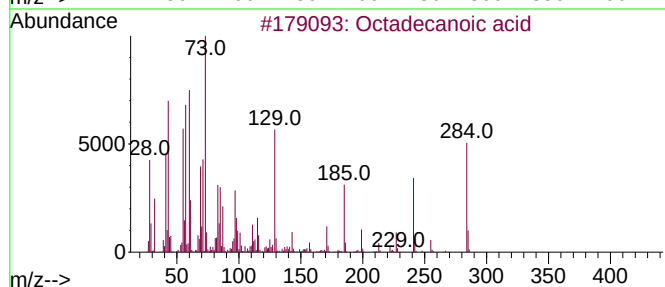
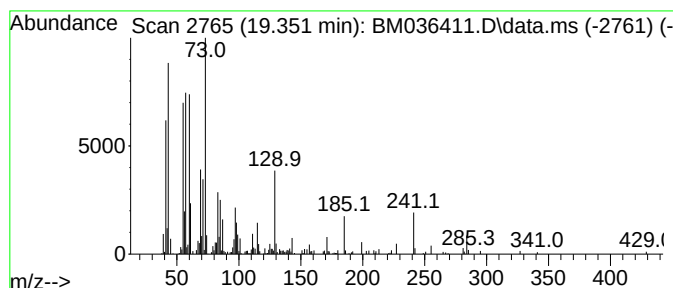
Instrument :
BNA_M
ClientSampleId :
SASP2-T-4-(16-22)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.351	2.20 ng	254269	Chrysene-d12	21.356	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Tridecanoic acid	214	C13H26O2	000638-53-9	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082522\
Data File : BM036411.D
Acq On : 25 Aug 2022 18:04
Operator : CG/JU
Sample : N4260-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SASP2-T-4-(16-22)

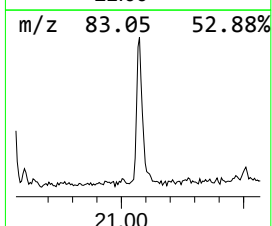
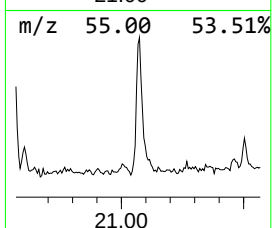
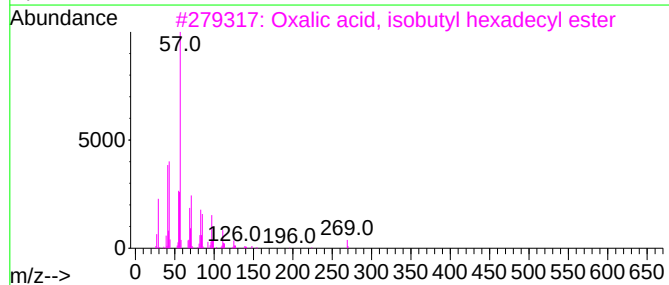
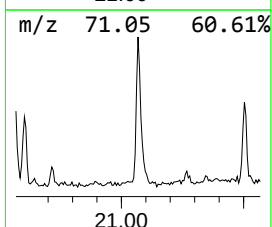
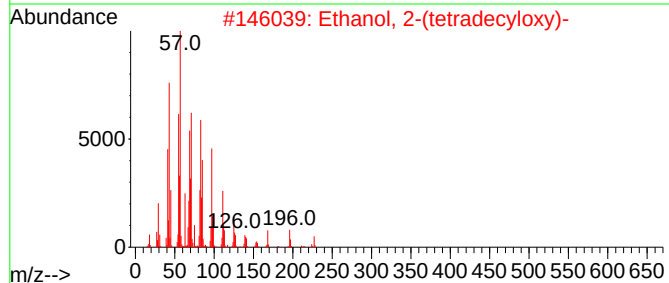
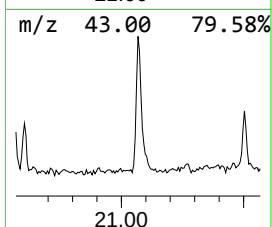
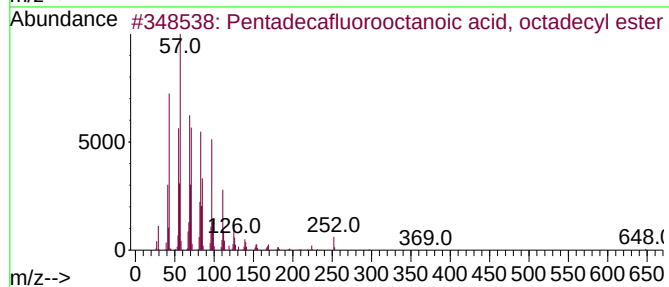
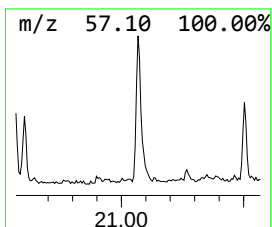
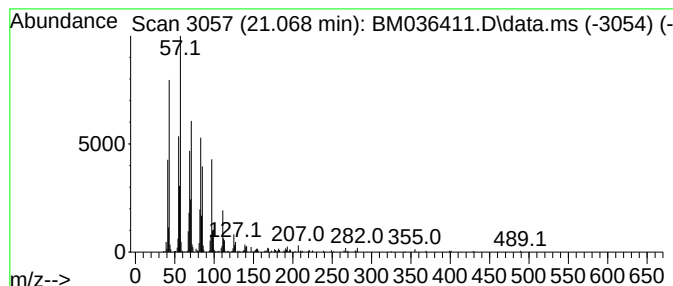
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Pentadecafluorooctanoic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.068	3.17 ng	366347	Chrysene-d12	21.356

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
2			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
3			Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
4			Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	90
5			Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082522\
Data File : BM036411.D
Acq On : 25 Aug 2022 18:04
Operator : CG/JU
Sample : N4260-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SASP2-T-4-(16-22)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.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-...	4.893	6.9	ng	490011	1	7.781	1429010	20.0
n-Hexadecanoic ...	18.074	4.0	ng	470899	4	17.168	2371130	20.0
Octadecanoic acid	19.351	2.2	ng	254269	5	21.356	2309750	20.0
Pentadecafluoro...	21.068	3.2	ng	366347	5	21.356	2309750	20.0