

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030921\
 Data File : BM029062.D
 Acq On : 10 Mar 2021 00:58
 Operator : CG/JU
 Sample : M1597-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 AU-06-030821

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-BM022321.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029062.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.246	378	384	396	rBB	179972	269467	2.78%	1.063%
2	6.869	654	660	675	rBB	176480	278389	2.87%	1.098%
3	8.845	989	996	1007	rBB	112236	180851	1.86%	0.713%
4	10.463	1266	1271	1277	rVB	63879	98410	1.01%	0.388%
5	12.951	1688	1694	1701	rBV	255968	356269	3.67%	1.406%
6	14.339	1924	1930	1936	rVB2	86446	124216	1.28%	0.490%
7	15.839	2180	2185	2191	rVB	194299	257917	2.66%	1.018%
8	17.086	2392	2397	2401	rBV	96880	132840	1.37%	0.524%
9	17.762	2505	2512	2516	rBV	1887596	2197890	22.64%	8.671%
10	17.992	2538	2551	2560	rBV2	177006	293079	3.02%	1.156%
11	18.927	2698	2710	2712	rBV	4929792	9707812	100.00%	38.299%
12	18.962	2712	2716	2724	rVB2	5347676	8700549	89.62%	34.325%
13	19.068	2729	2734	2740	rVB	880523	1051851	10.84%	4.150%
14	19.151	2745	2748	2755	rVB2	211736	329443	3.39%	1.300%
15	19.509	2806	2809	2819	rVB	107053	167916	1.73%	0.662%
16	19.715	2840	2844	2849	rVB	355798	452985	4.67%	1.787%
17	20.162	2916	2920	2925	rBV2	108857	127642	1.31%	0.504%
18	20.762	3018	3022	3030	rBV5	56962	100089	1.03%	0.395%
19	20.980	3055	3059	3068	rVB3	86728	133296	1.37%	0.526%
20	21.262	3101	3107	3111	rBV2	147641	266724	2.75%	1.052%
21	23.427	3472	3475	3480	rVB2	78936	119820	1.23%	0.473%

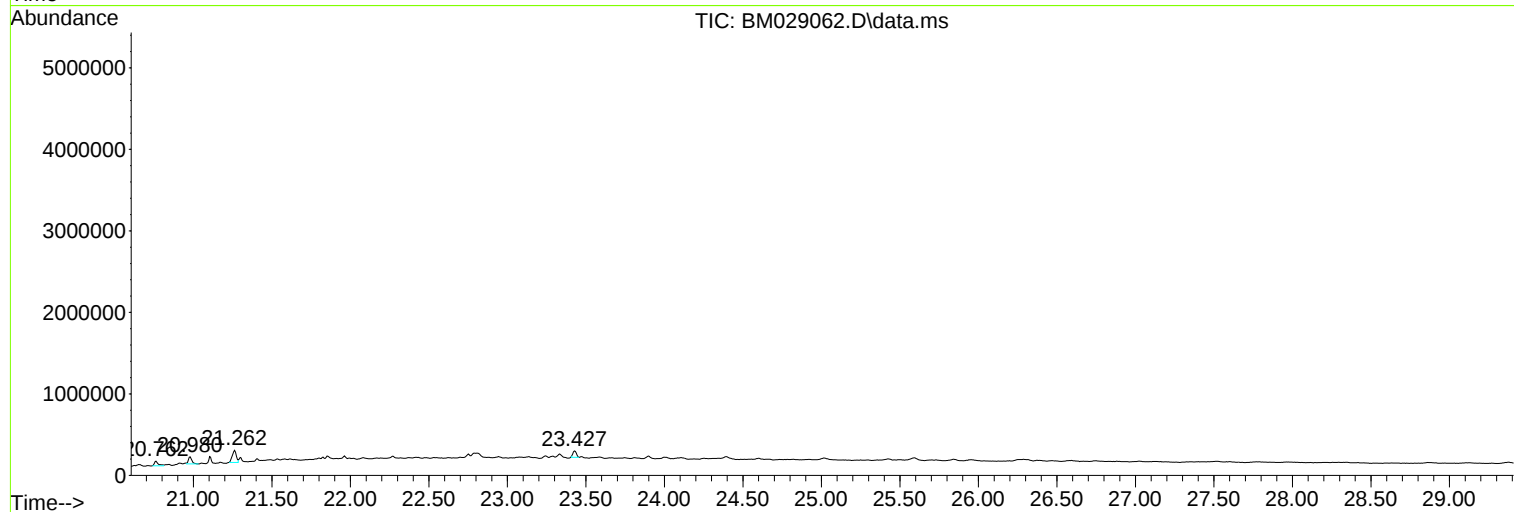
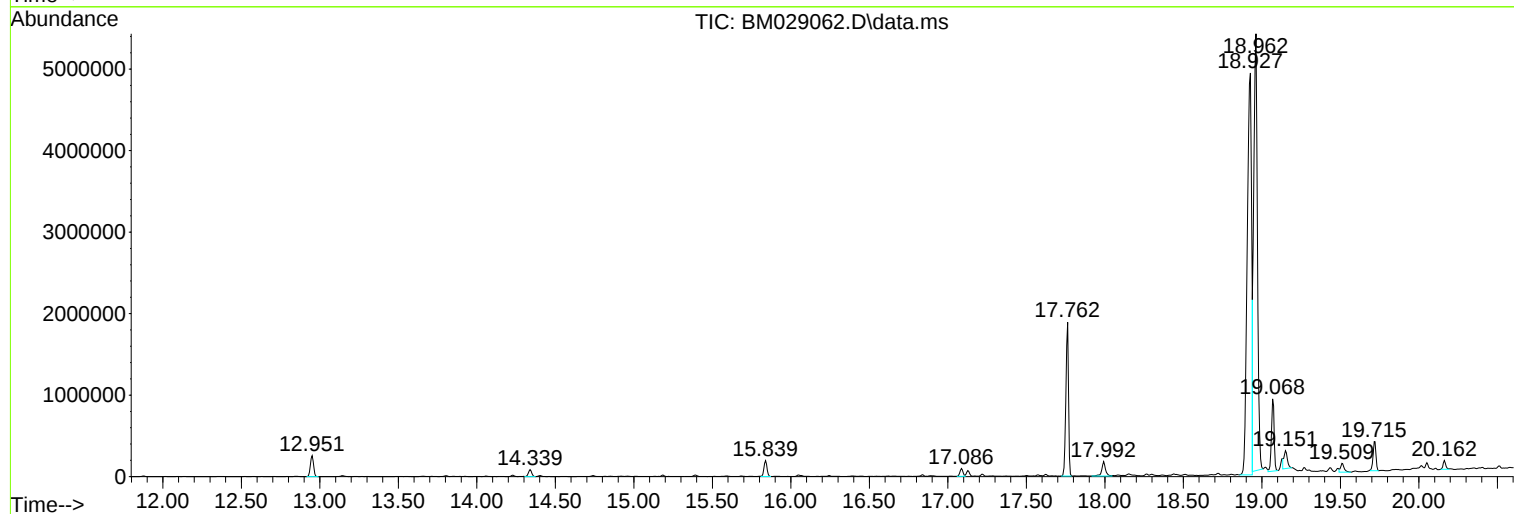
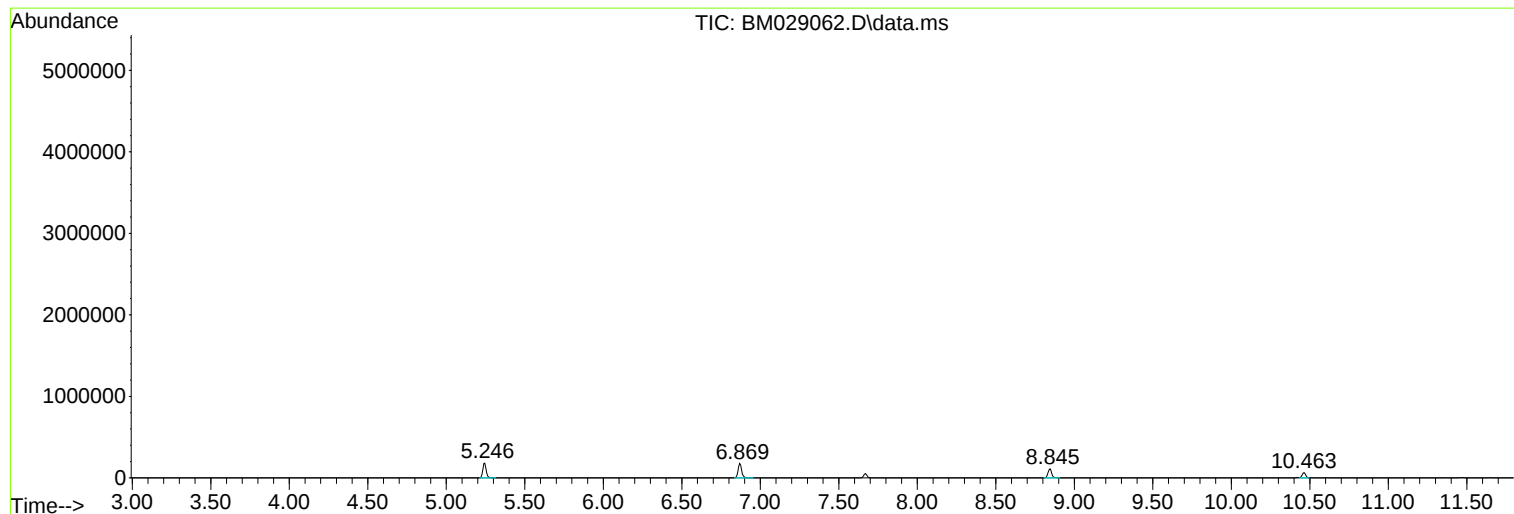
Sum of corrected areas: 25347455

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030921\
Data File : BM029062.D
Acq On : 10 Mar 2021 00:58
Operator : CG/JU
Sample : M1597-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
AU-06-030821

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.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_M\Data\BM030921\
Data File : BM029062.D
Acq On : 10 Mar 2021 00:58
Operator : CG/JU
Sample : M1597-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
AU-06-030821

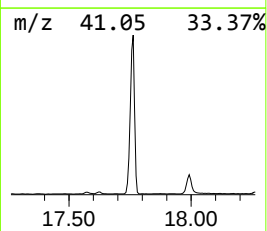
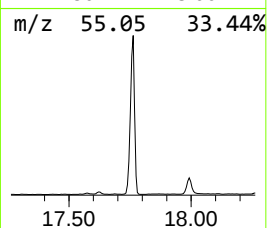
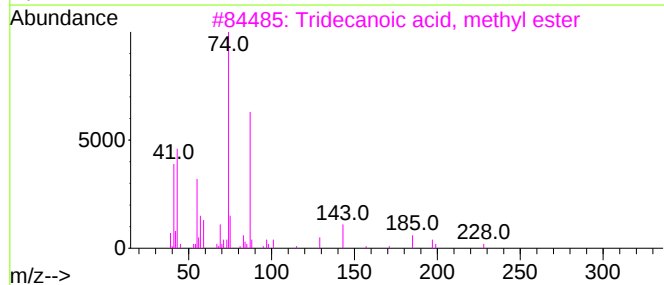
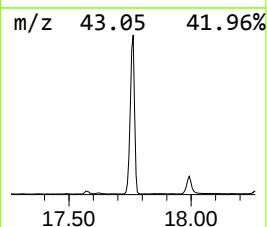
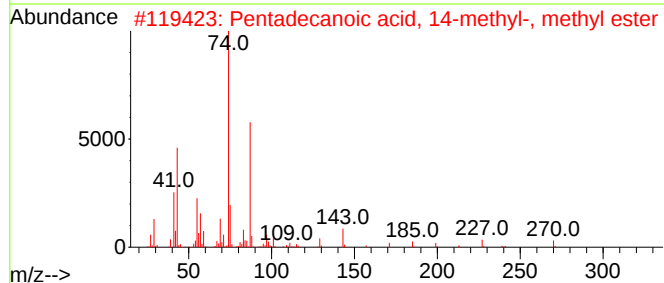
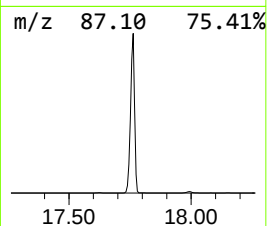
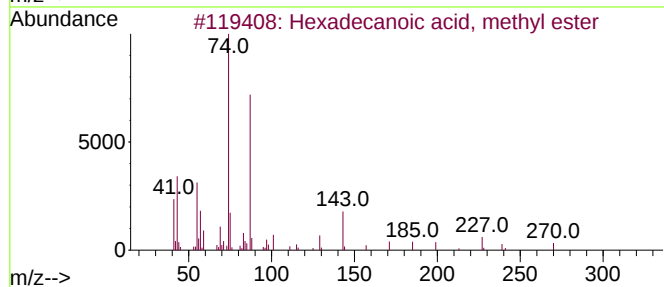
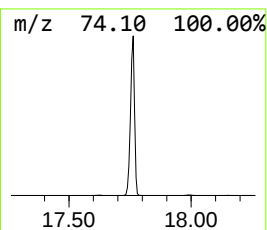
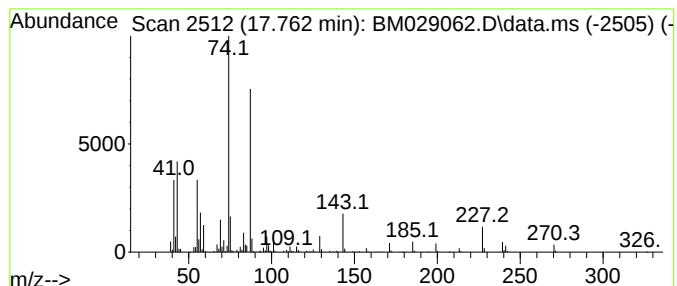
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.762	330.91 ng	2197890	Phenanthrene-d10	17.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	95
3			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	92
4			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
5			Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030921\
Data File : BM029062.D
Acq On : 10 Mar 2021 00:58
Operator : CG/JU
Sample : M1597-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
AU-06-030821

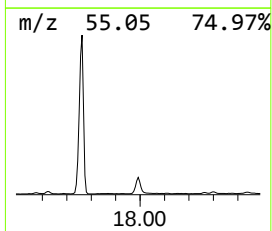
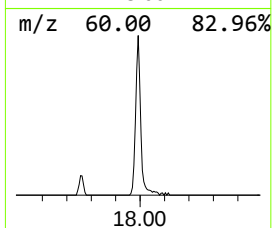
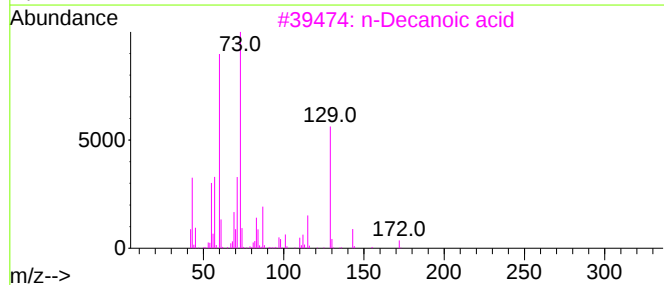
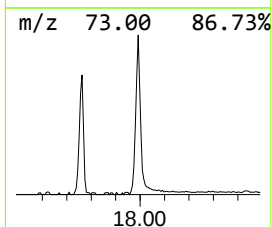
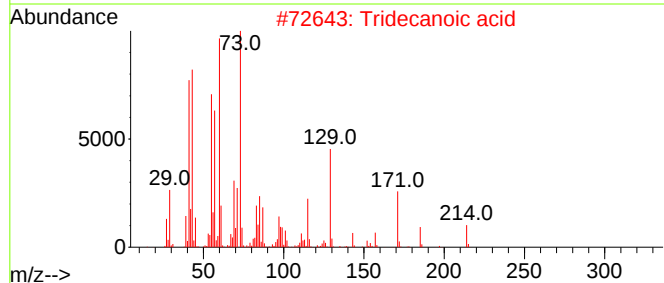
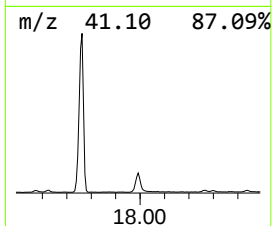
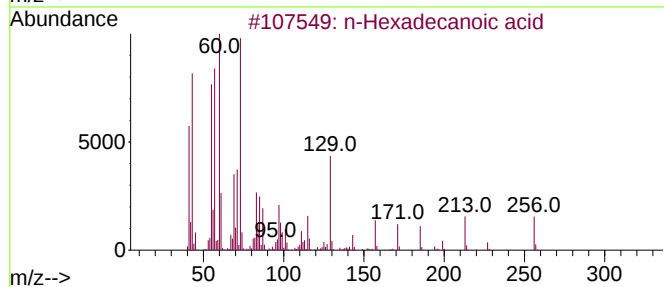
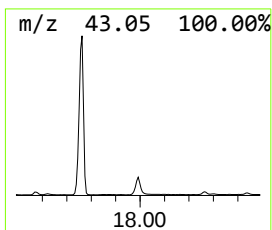
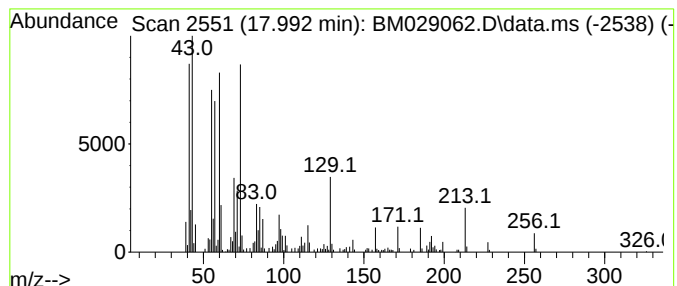
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.992	44.13 ng	293079	Phenanthrene-d10	17.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			n-Decanoic acid	172	C10H20O2	000334-48-5	87
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5			Octadecanoic acid	284	C18H36O2	000057-11-4	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030921\
Data File : BM029062.D
Acq On : 10 Mar 2021 00:58
Operator : CG/JU
Sample : M1597-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

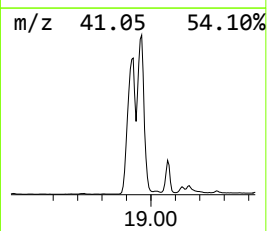
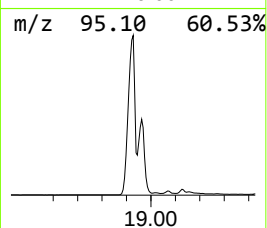
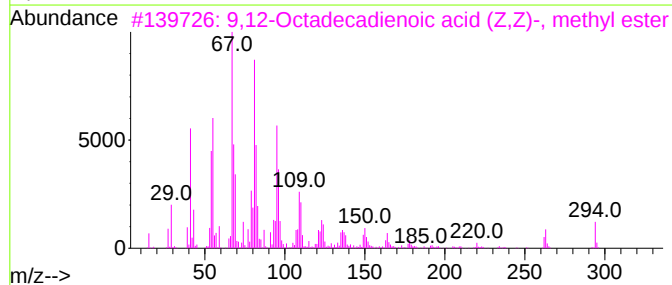
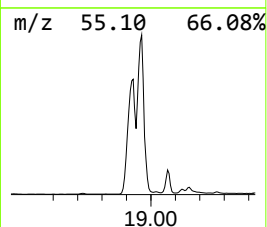
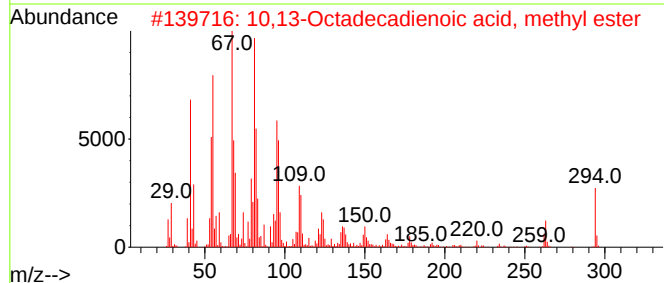
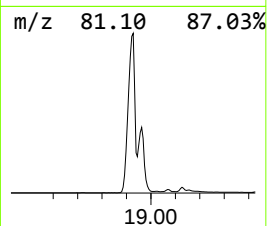
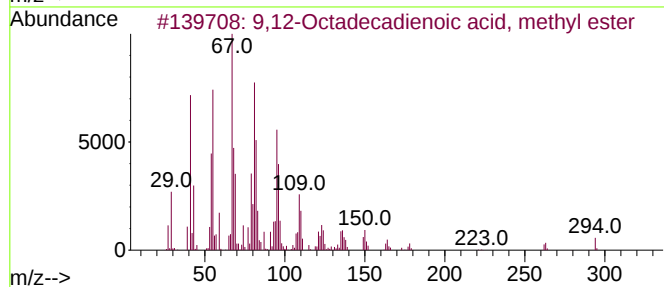
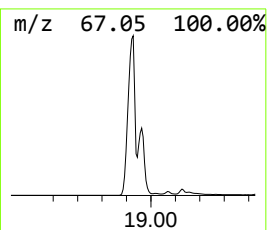
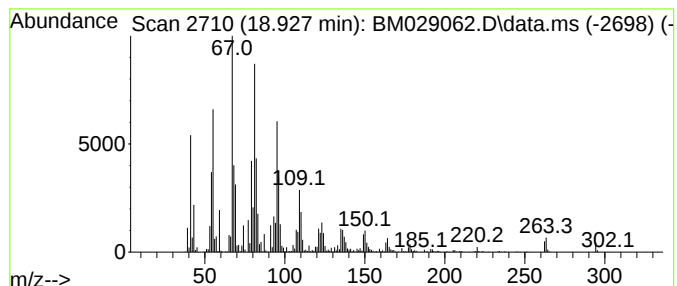
Instrument :
BNA_M
ClientSampleId :
AU-06-030821

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.927	1461.58 ng	9707810	Phenanthrene-d10		17.086	
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
2		10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
3		9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
4		9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
5		9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030921\
Data File : BM029062.D
Acq On : 10 Mar 2021 00:58
Operator : CG/JU
Sample : M1597-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

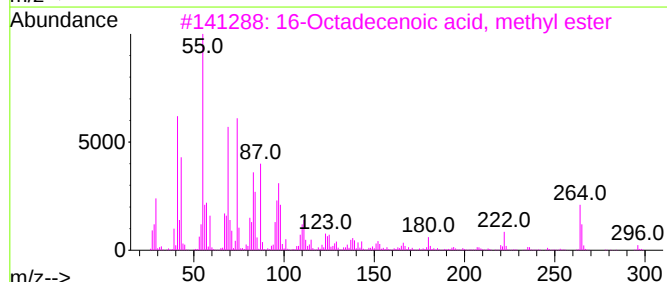
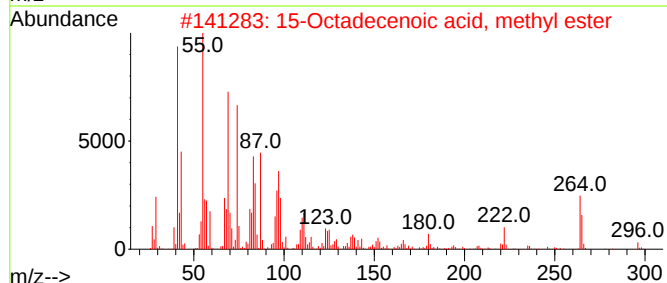
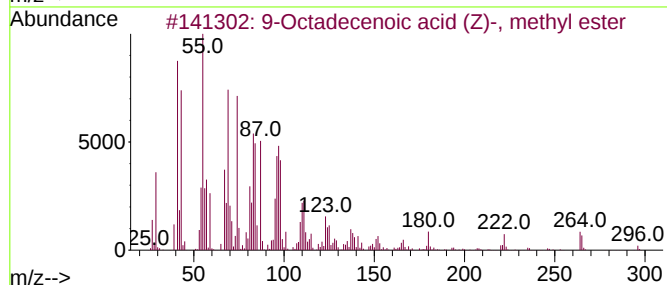
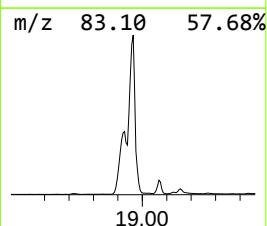
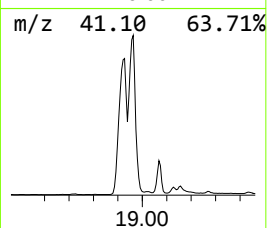
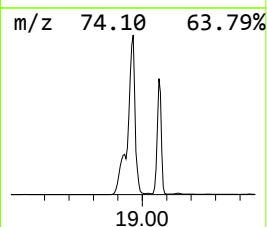
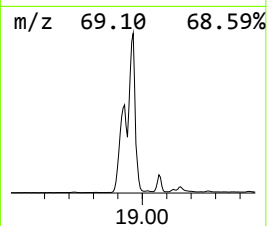
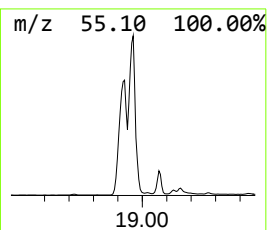
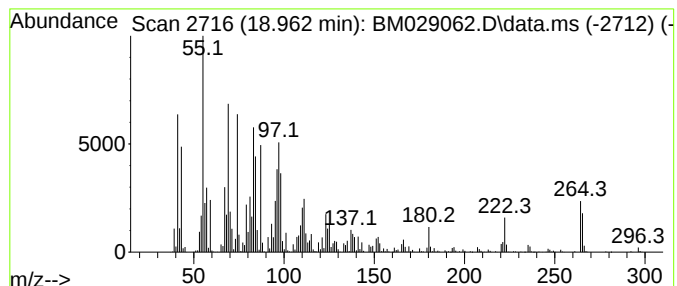
Instrument :
BNA_M
ClientSampleId :
AU-06-030821

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.962	1309.93 ng	8700550	Phenanthrene-d10	17.086	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99
3	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	99
4	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
5	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030921\
Data File : BM029062.D
Acq On : 10 Mar 2021 00:58
Operator : CG/JU
Sample : M1597-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
AU-06-030821

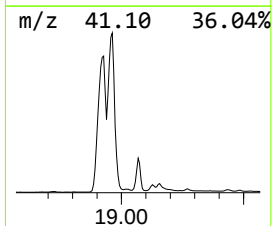
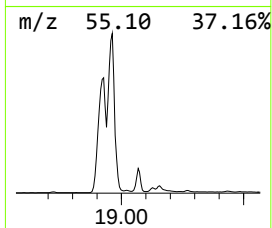
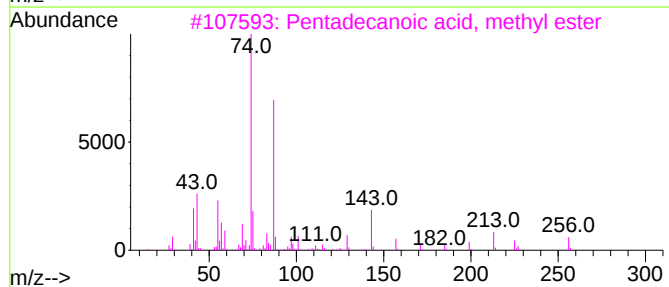
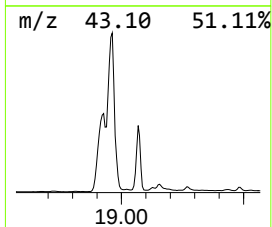
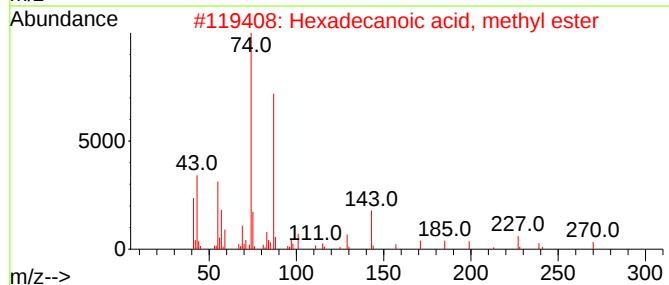
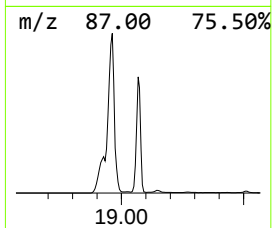
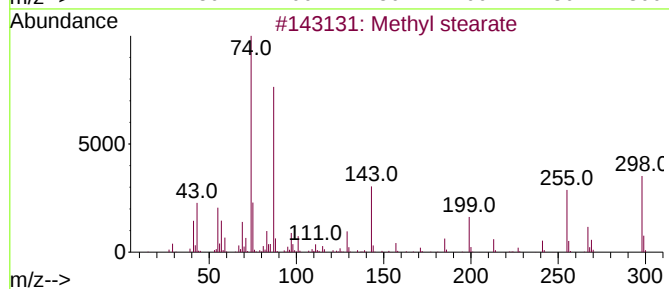
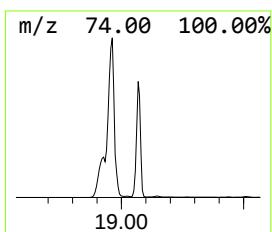
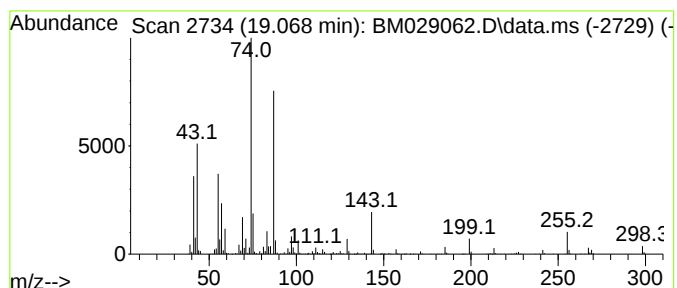
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Methyl stearate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.068	158.36 ng	1051850	Phenanthrene-d10	17.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	98
2			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	90
3			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
4			Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	90
5			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030921\
Data File : BM029062.D
Acq On : 10 Mar 2021 00:58
Operator : CG/JU
Sample : M1597-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

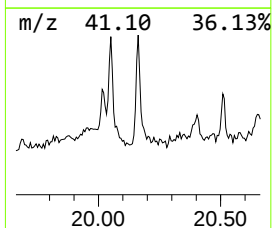
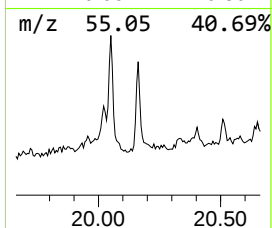
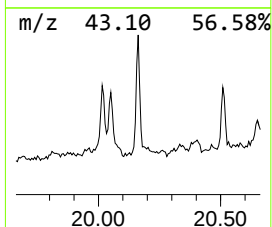
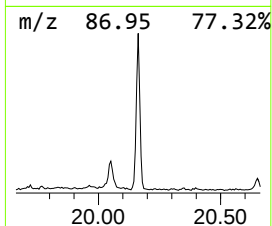
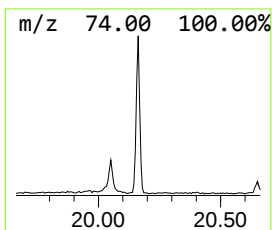
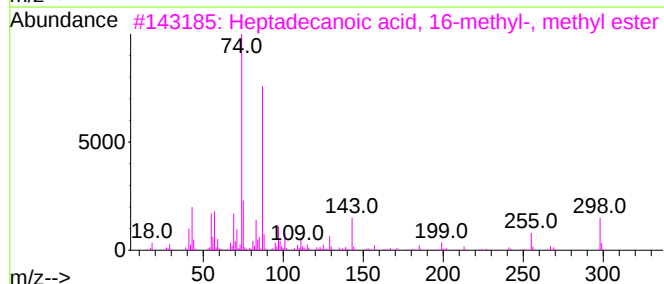
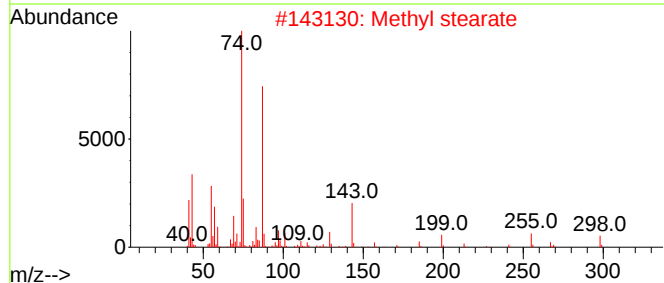
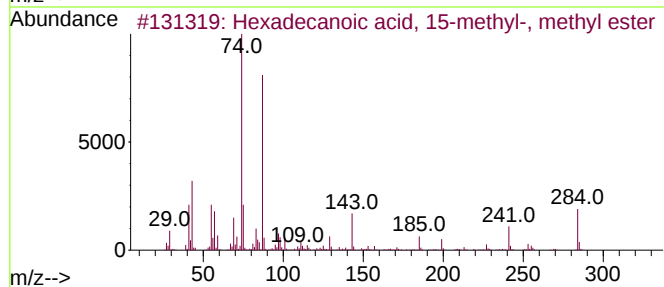
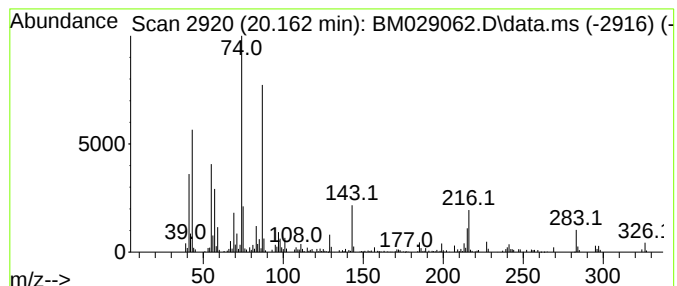
Instrument :
BNA_M
ClientSampleId :
AU-06-030821

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexadecanoic acid, 15-methy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.162	9.57 ng	127642	Chrysene-d12	21.262	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	96
2	Methyl stearate	298	C19H38O2	000112-61-8	94
3	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	94
4	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	90
5	Methyl 18-methylnonadecanoate	326	C21H42O2	1000352-20-6	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030921\
Data File : BM029062.D
Acq On : 10 Mar 2021 00:58
Operator : CG/JU
Sample : M1597-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
AU-06-030821

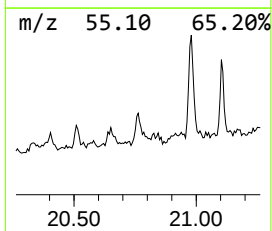
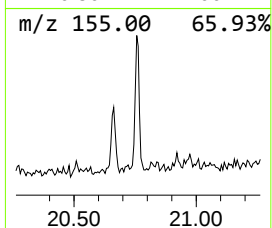
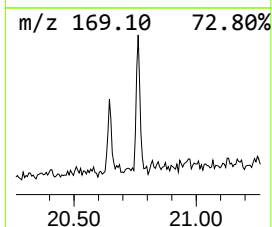
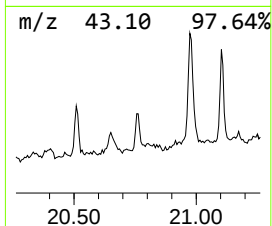
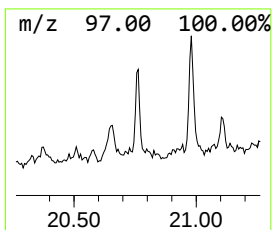
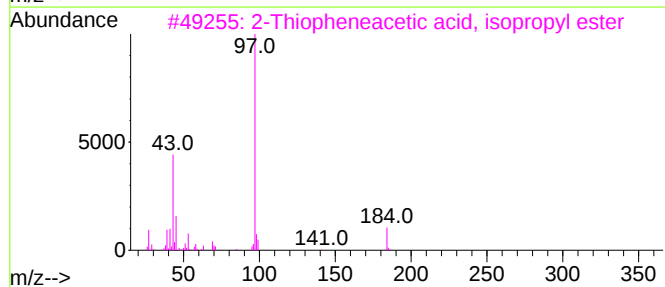
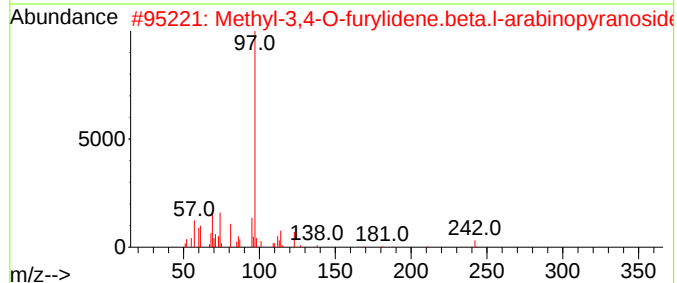
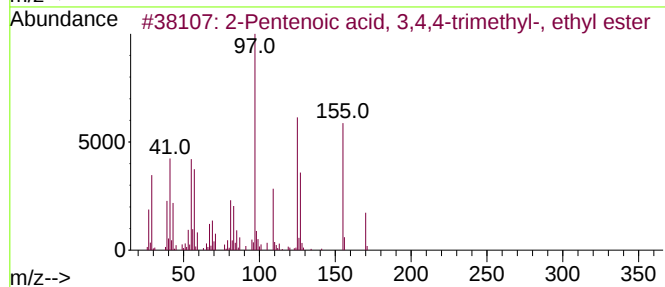
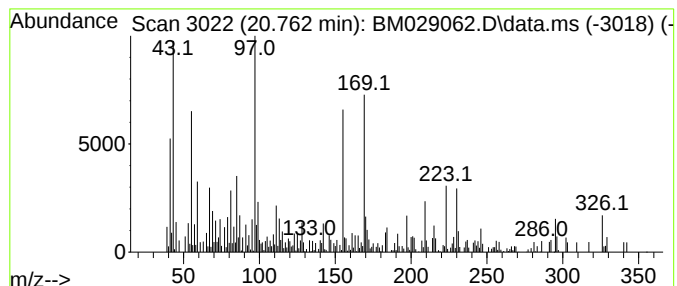
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown20.762 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.762	7.51 ng	100089	Chrysene-d12	21.262

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentenoic acid, 3,4,4-trimethyl...	170	C10H18O2	091140-23-7	35
2			Methyl-3,4-O-furylidene.beta.l-a...	242	C11H14O6	053547-58-3	35
3			2-Thiopheneacetic acid, isopropyl...	184	C9H12O2S	068100-13-0	22
4			3-Butene-1,2-diol, 1-(2-furanyl)...	168	C9H12O3	021141-71-9	20
5			2-Thiopheneacetic acid, 4-methyl...	226	C12H18O2S	1000278-95-6	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030921\
Data File : BM029062.D
Acq On : 10 Mar 2021 00:58
Operator : CG/JU
Sample : M1597-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
AU-06-030821

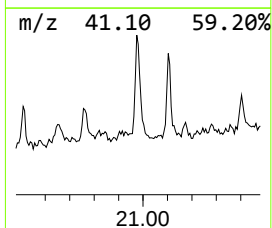
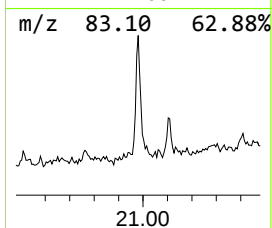
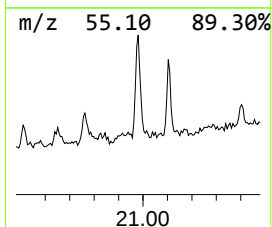
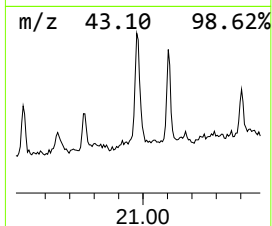
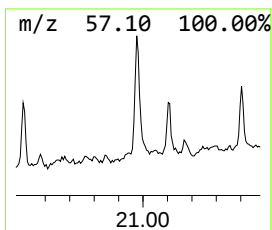
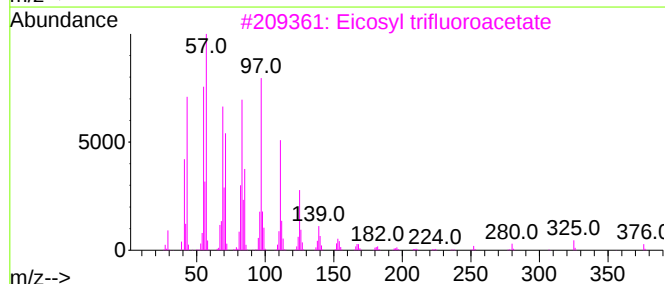
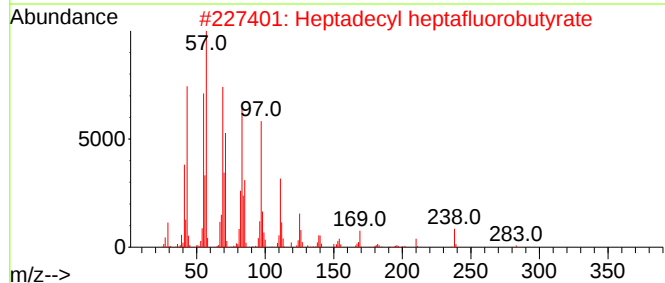
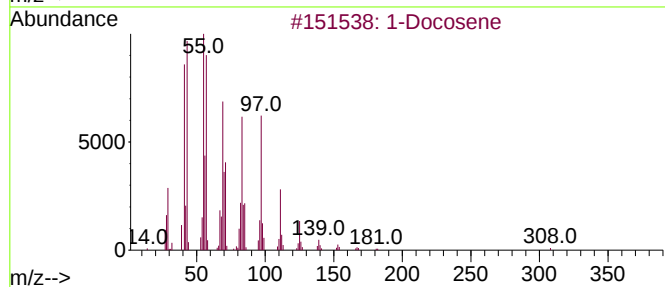
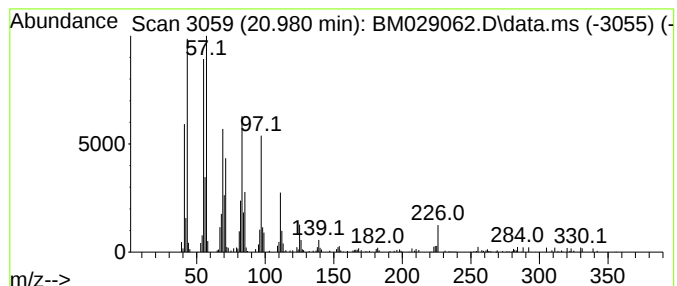
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Docosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.980	10.00 ng	133296	Chrysene-d12	21.262

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Docosene	308	C22H44	001599-67-3	93
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
3			Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	91
4			Carbonic acid, heptadecyl isobut...	356	C22H44O3	1000314-61-4	91
5			Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030921\
Data File : BM029062.D
Acq On : 10 Mar 2021 00:58
Operator : CG/JU
Sample : M1597-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
AU-06-030821

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.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
Hexadecanoic ac...	17.762	330.9	ng	2197890	4	17.086	132840	20.0
n-Hexadecanoic ...	17.992	44.1	ng	293079	4	17.086	132840	20.0
9,12-Octadecadi...	18.927	1461.6	ng	9707810	4	17.086	132840	20.0
9-Octadecenoic ...	18.962	1309.9	ng	8700550	4	17.086	132840	20.0
Methyl stearate	19.068	158.4	ng	1051850	4	17.086	132840	20.0
Hexadecanoic ac...	20.162	9.6	ng	127642	5	21.262	266724	20.0
unknown20.762	20.762	7.5	ng	100089	5	21.262	266724	20.0
1-Docosene	20.980	10.0	ng	133296	5	21.262	266724	20.0