

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042922\
 Data File : BF128010.D
 Acq On : 29 Apr 2022 22:29
 Operator : CG\JU
 Sample : N2605-01 2X
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TR-04-042822

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-BF042222.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128010.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.540	549	553	566	rVB	1249155	1126532	2.38%	1.305%
2	6.545	720	724	739	rVB	1218003	1146605	2.42%	1.328%
3	6.928	785	789	792	rBV	917852	748665	1.58%	0.867%
4	7.486	880	884	887	rBV	861906	727297	1.54%	0.842%
5	8.210	1004	1007	1010	rVB	1072475	818335	1.73%	0.948%
6	9.280	1186	1189	1193	rBV	1229457	1117511	2.36%	1.294%
7	9.969	1301	1306	1309	rVV	1023781	815016	1.72%	0.944%
8	10.757	1437	1440	1450	rBV	699067	600703	1.27%	0.696%
9	11.463	1556	1560	1562	rBV	964654	785682	1.66%	0.910%
10	11.863	1621	1628	1631	rBV	10681623	14476051	30.57%	16.765%
11	11.998	1645	1651	1659	rBV	828628	1053975	2.23%	1.221%
12	12.592	1738	1752	1754	rBV4	11557600	47357205	100.00%	54.845%
13	12.633	1758	1759	1760	rVV	1454252	758377	1.60%	0.878%
14	12.663	1760	1764	1766	rVV	7623636	7536174	15.91%	8.728%
15	12.692	1766	1769	1779	rVV3	1665502	2553070	5.39%	2.957%
16	13.057	1827	1831	1834	rBV	1172538	1044872	2.21%	1.210%
17	13.286	1868	1870	1877	rVB	562979	600829	1.27%	0.696%
18	13.363	1880	1883	1891	rVB	1086828	1009316	2.13%	1.169%
19	14.033	1994	1997	2002	rBV	1049656	939405	1.98%	1.088%
20	14.115	2007	2011	2014	rBV	596574	611875	1.29%	0.709%
21	15.627	2264	2268	2275	rVB	398009	519162	1.10%	0.601%

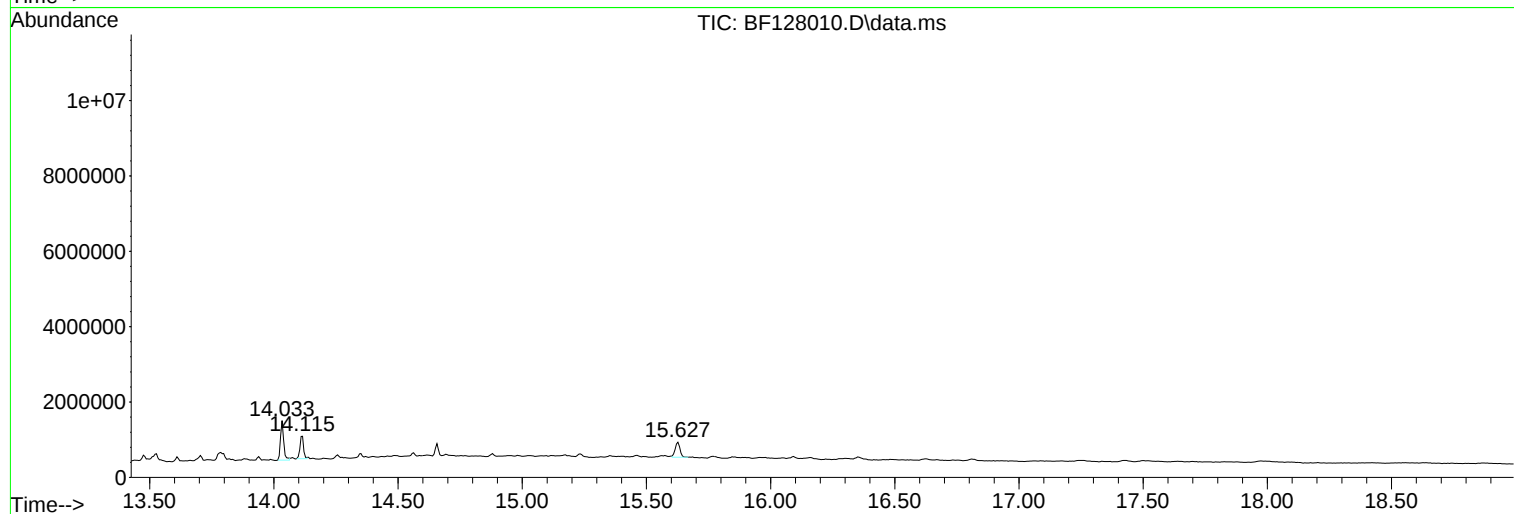
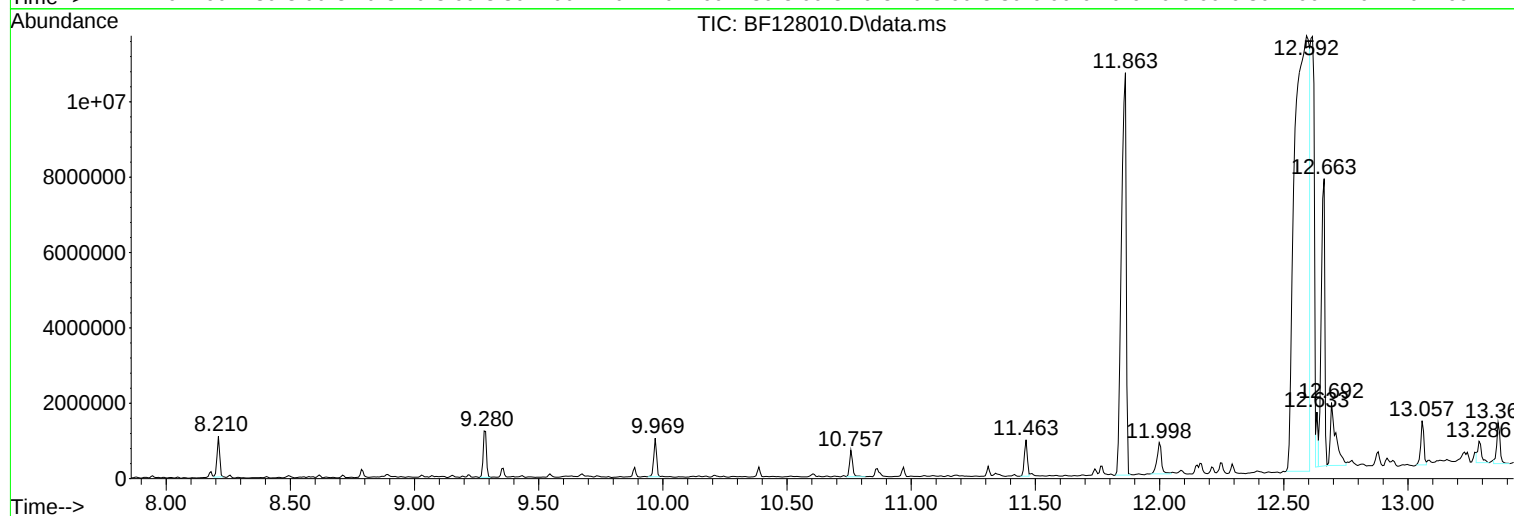
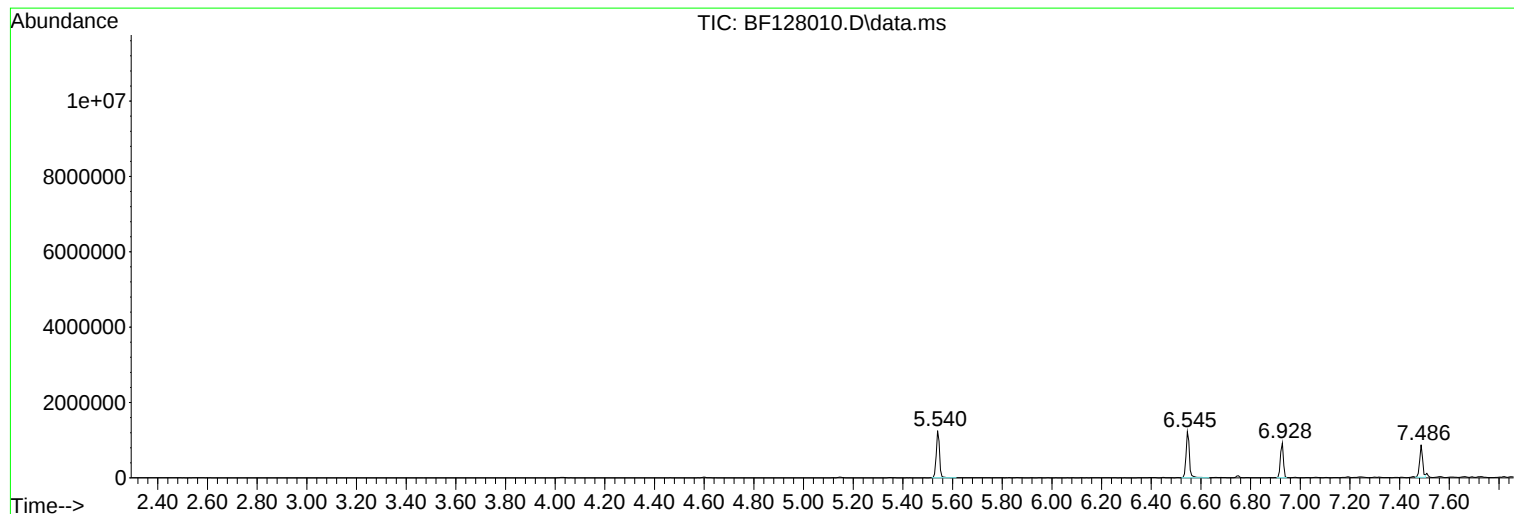
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Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BF128010.D
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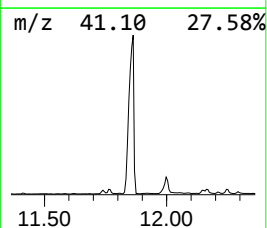
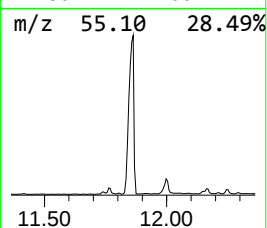
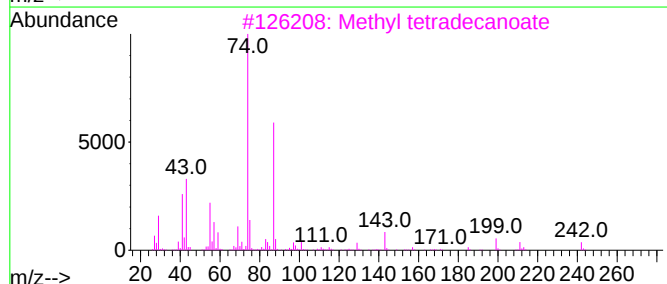
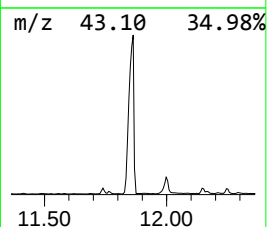
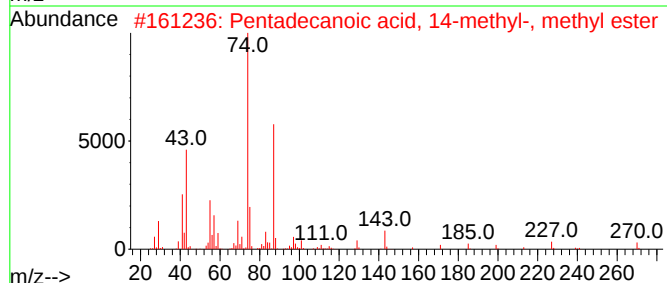
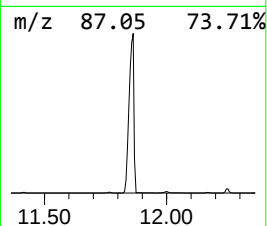
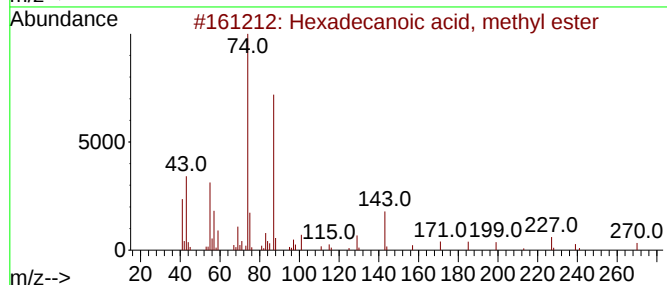
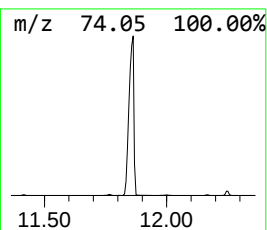
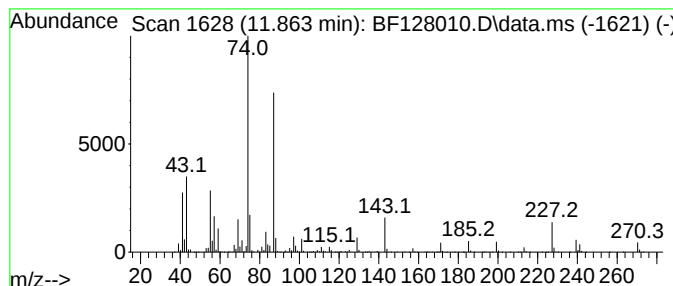
Instrument :
BNA_F
ClientSampleId :
TR-04-042822

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Hexadecanoic acid, methyl e... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.863	368.50 ng	14476100	Phenanthrene-d10	11.463	
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	96
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	93
4	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
5	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	83



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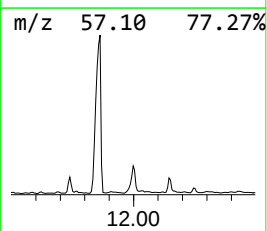
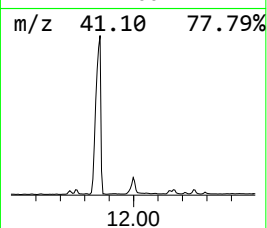
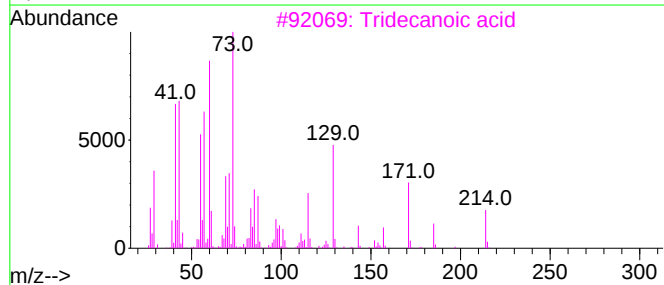
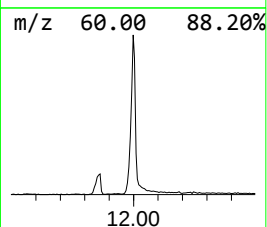
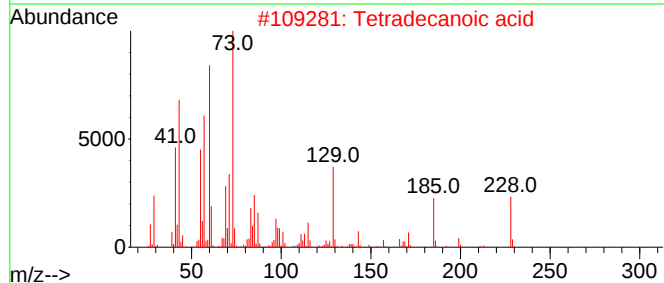
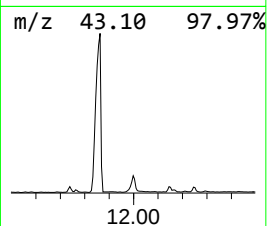
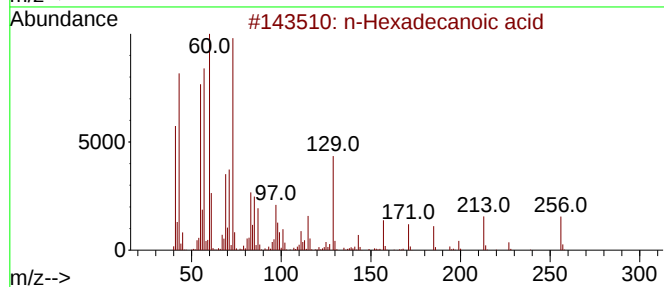
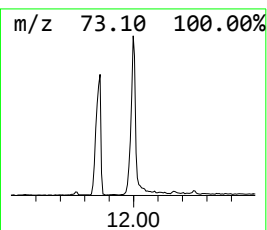
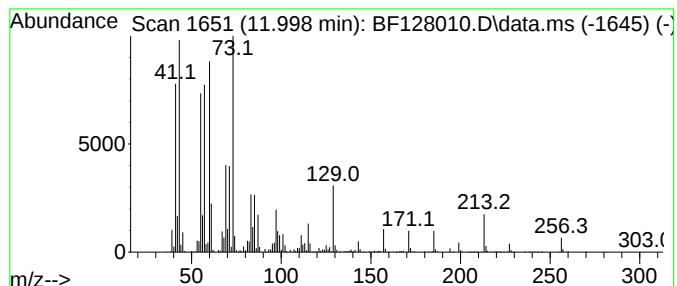
Instrument :
BNA_F
ClientSampleId :
TR-04-042822

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.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 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.998	26.83 ng	1053980	Phenanthrene-d10		11.463	
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	94
3	Tridecanoic acid		214	C13H26O2	000638-53-9	92
4	Pentadecanoic acid		242	C15H30O2	001002-84-2	87
5	Octanoic acid		144	C8H16O2	000124-07-2	45



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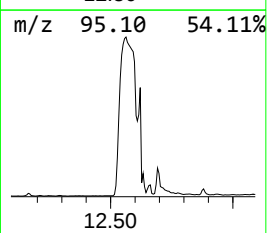
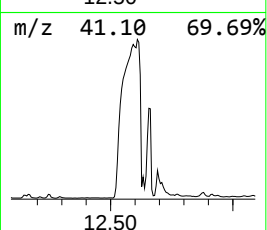
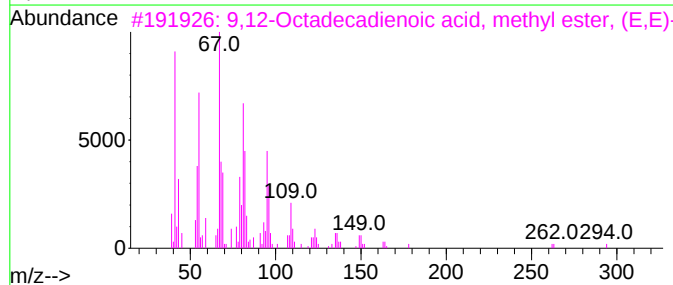
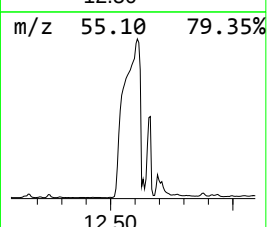
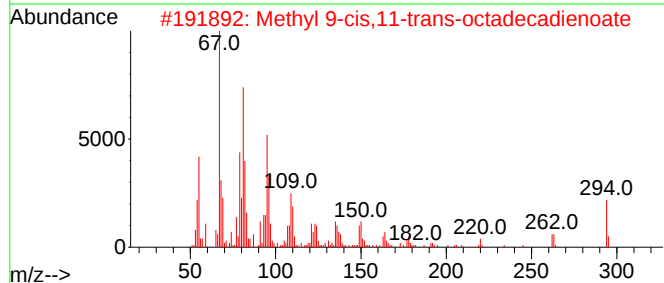
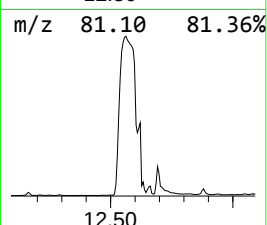
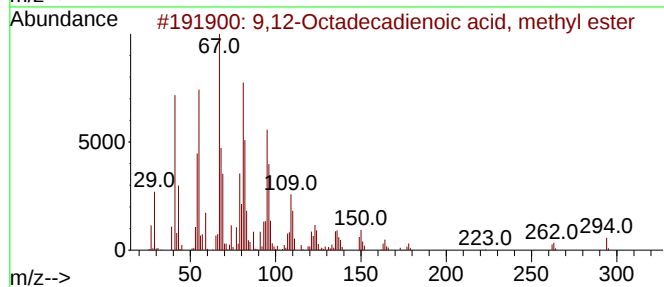
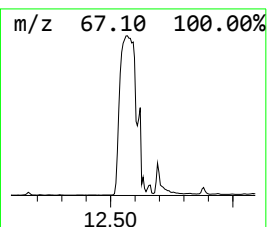
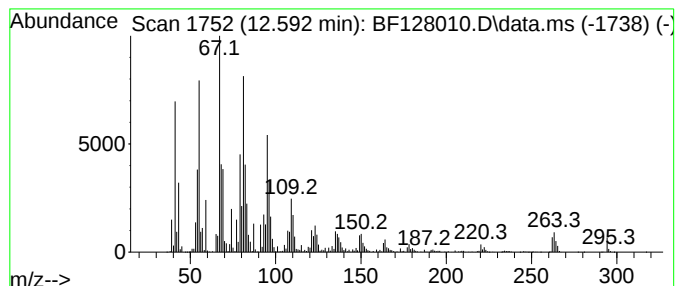
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.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.
12.592	1205.51 ng	47357200	Phenanthrene-d10			11.463
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...		294	C19H34O2	002462-85-3	99
2	Methyl 9-cis,11-trans-octadecadi...		294	C19H34O2	013058-52-1	99
3	9,12-Octadecadienoic acid, methy...		294	C19H34O2	002566-97-4	99
4	10,13-Octadecadienoic acid, meth...		294	C19H34O2	056554-62-2	99
5	Methyl 7,12-octadecadienoate		294	C19H34O2	1000336-43-8	99



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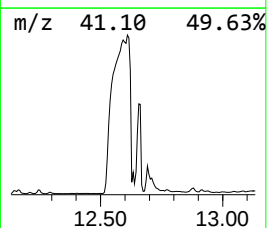
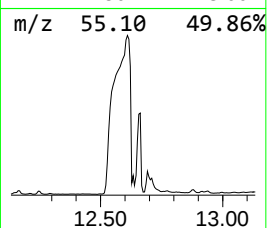
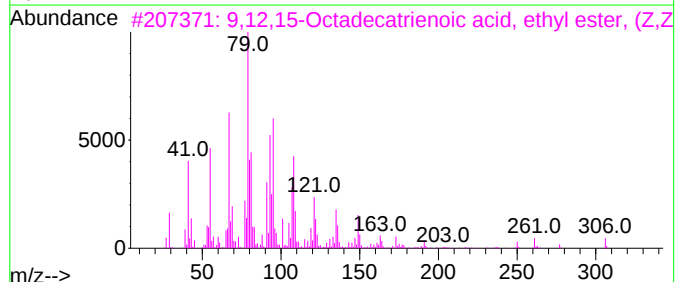
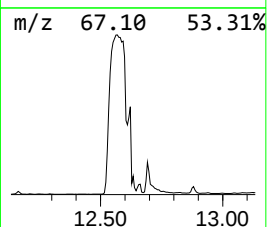
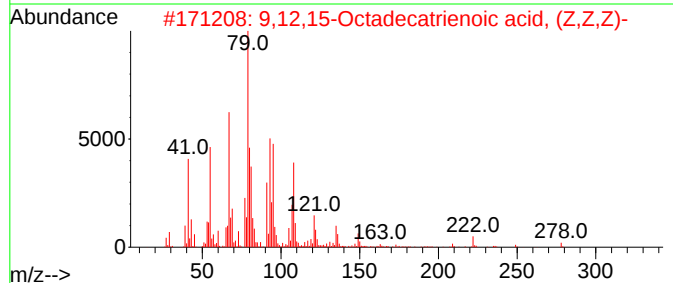
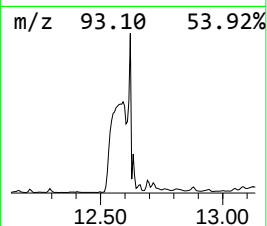
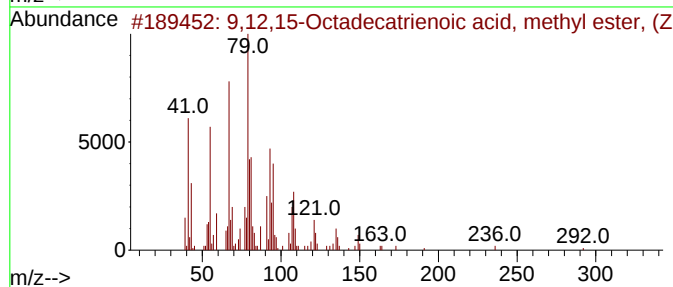
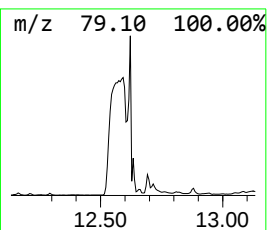
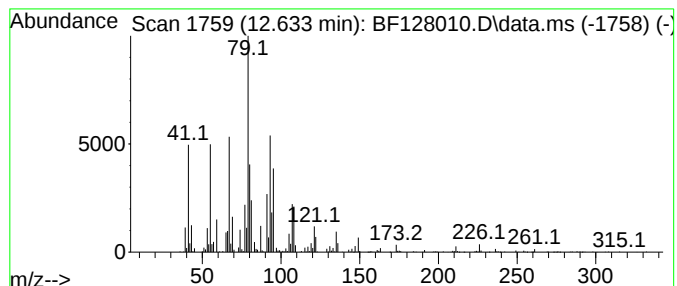
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 9,12,15-Octadecatrienoic ac... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.633	19.30 ng	758377	Phenanthrene-d10	11.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12,15-Octadecatrienoic acid, m...	292	C19H32O2	000301-00-8	90		
2	9,12,15-Octadecatrienoic acid, (...	278	C18H30O2	000463-40-1	78		
3	9,12,15-Octadecatrienoic acid, e...	306	C20H34O2	001191-41-9	72		
4	Methyl 2-hydroxy-octadeca-9,12,1...	308	C19H32O3	1000336-39-1	70		
5	1-Undecen-3-yne	150	C11H18	074744-28-8	64		



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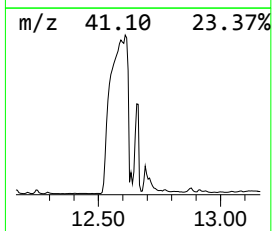
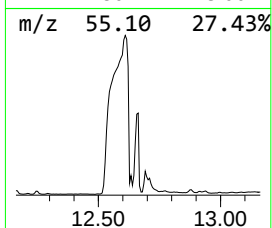
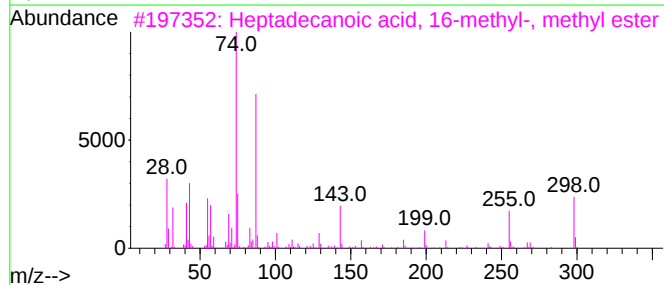
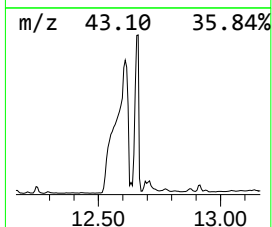
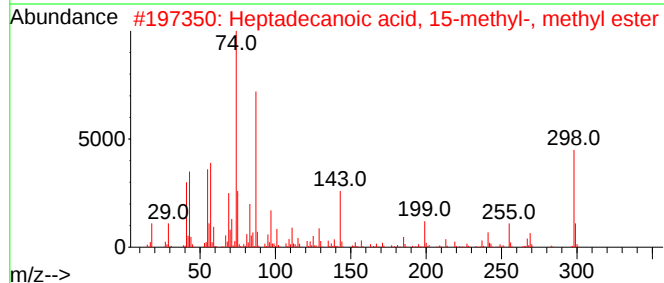
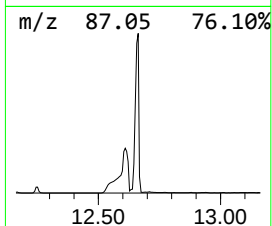
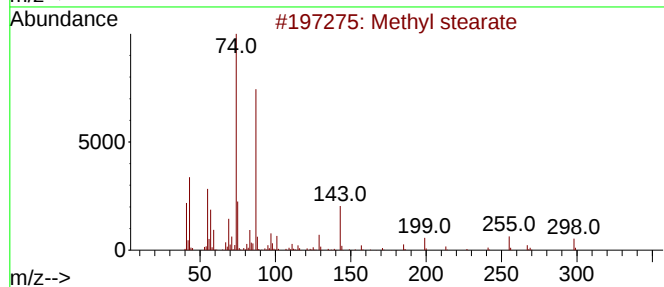
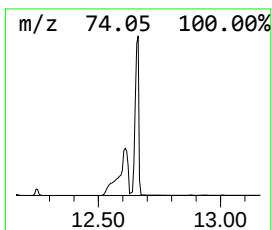
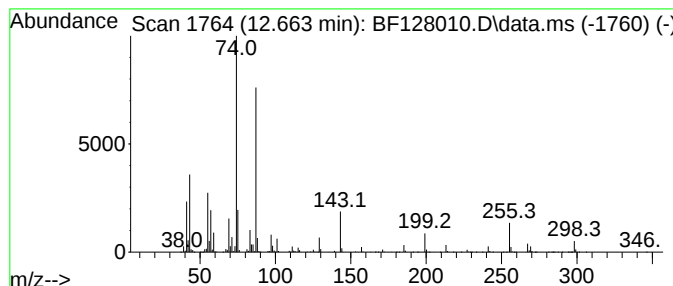
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Methyl stearate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.663	191.84 ng	7536170	Phenanthrene-d10	11.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	98
2			Heptadecanoic acid, 15-methyl-, ...	298	C19H38O2	054833-55-5	93
3			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	91
4			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
5			Methyl tetradecanoate	242	C15H30O2	000124-10-7	86



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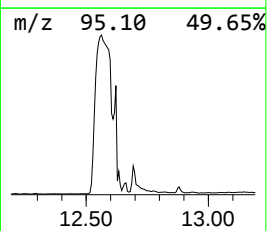
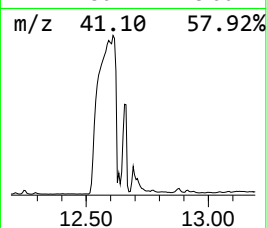
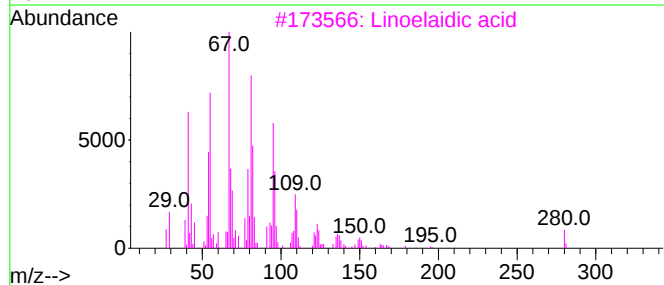
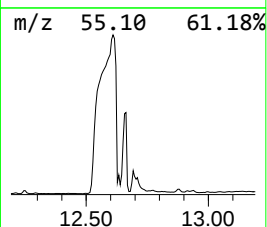
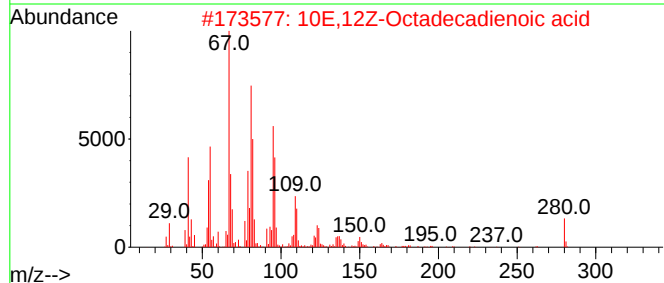
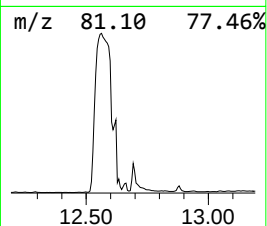
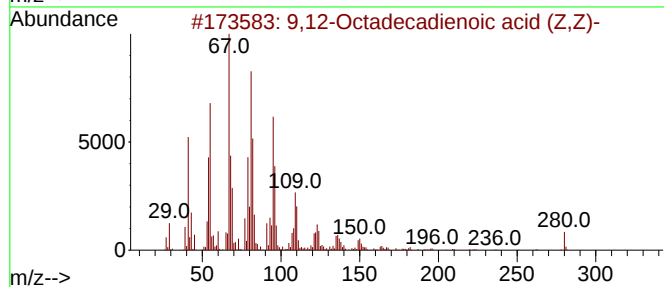
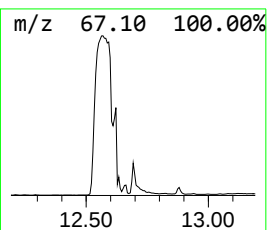
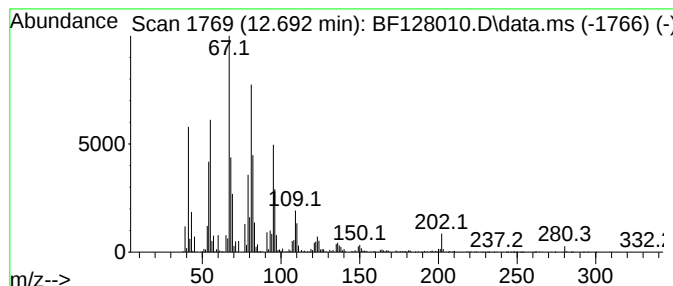
Instrument :
BNA_F
ClientSampleId :
TR-04-042822

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9,12-Octadecadienoic acid (... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.692	64.99 ng	2553070	Phenanthrene-d10	11.463	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	99
2	10E,12Z-Octadecadienoic acid	280	C18H32O2	002420-56-6	98
3	Linoelaidic acid	280	C18H32O2	000506-21-8	98
4	(9E,11E)-Octadecadienoic acid	280	C18H32O2	000544-71-8	98
5	Cyclodecene	138	C10H18	003618-12-0	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042922\
Data File : BF128010.D
Acq On : 29 Apr 2022 22:29
Operator : CG\JU
Sample : N2605-01 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

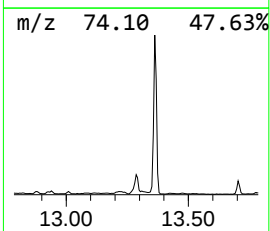
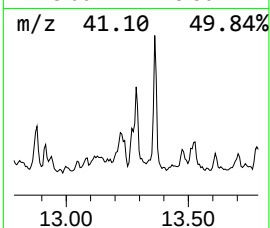
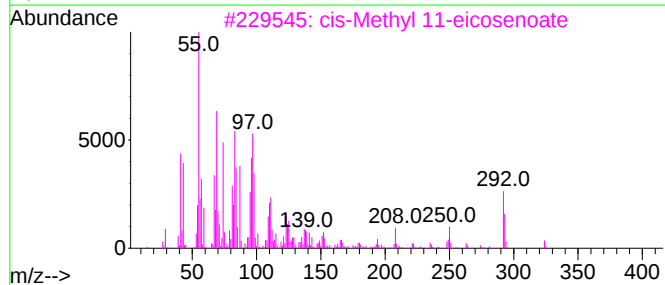
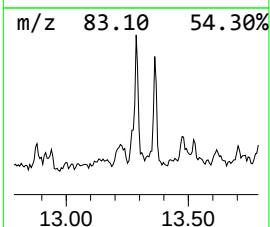
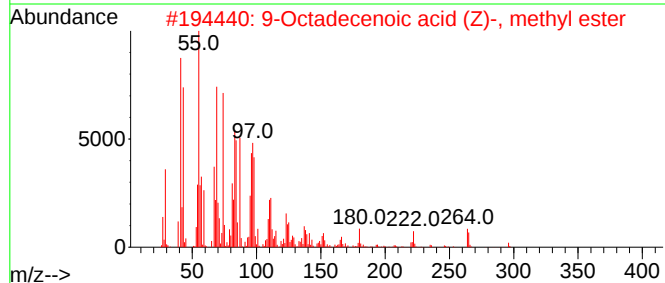
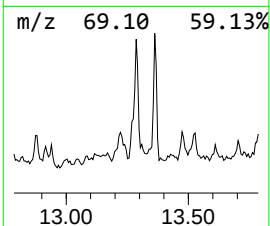
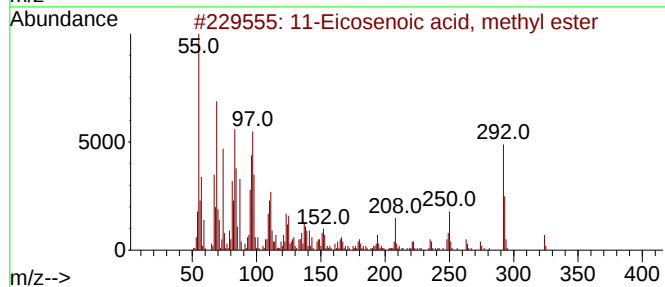
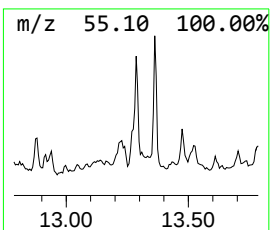
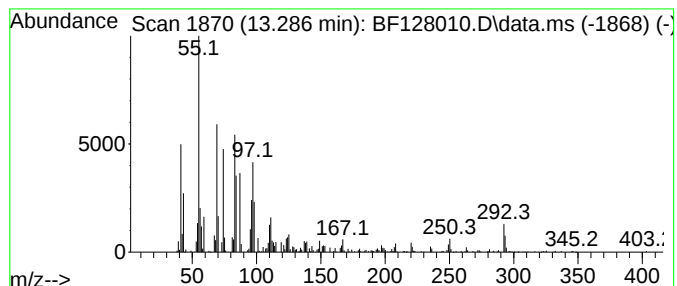
Instrument :
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ClientSampleId :
TR-04-042822

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 11-Eicosenoic acid, methyl ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.286	19.64 ng	600829	Chrysene-d12	14.115	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Eicosenoic acid, methyl ester	324	C21H40O2	003946-08-5	78
2	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	70
3	cis-Methyl 11-eicosenoate	324	C21H40O2	002390-09-2	49
4	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	38
5	1-Hexadecene, 16-bromo-	302	C16H31Br	118625-56-2	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042922\
Data File : BF128010.D
Acq On : 29 Apr 2022 22:29
Operator : CG\JU
Sample : N2605-01 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-04-042822

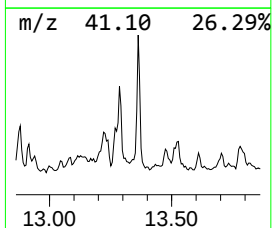
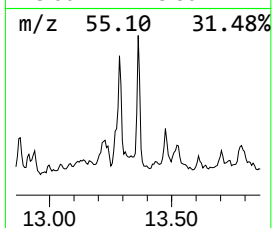
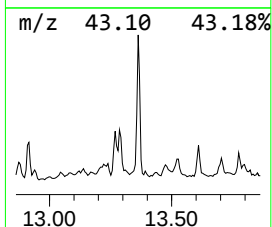
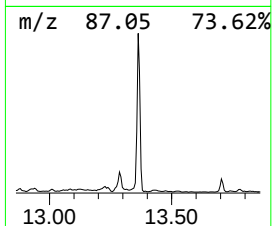
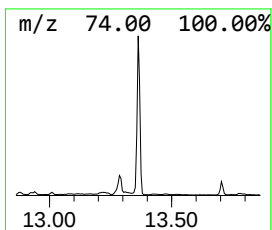
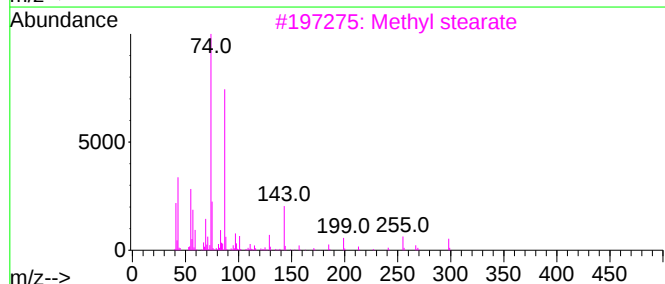
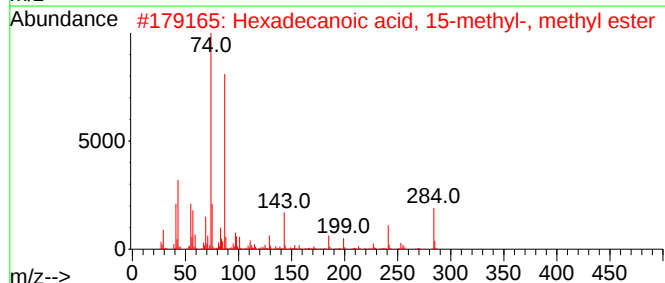
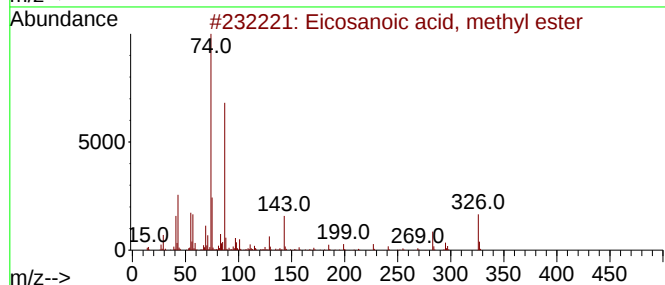
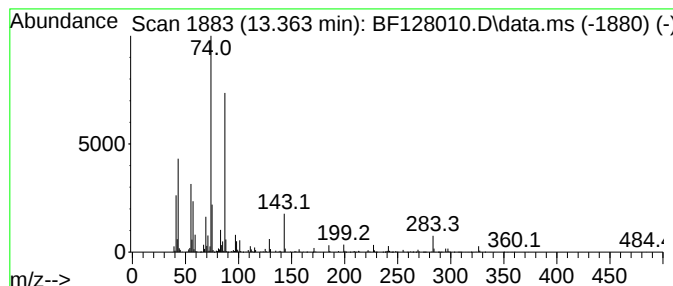
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosanoic acid, methyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.363	32.99 ng	1009320	Chrysene-d12	14.115

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	98
2			Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	95
3			Methyl stearate	298	C19H38O2	000112-61-8	93
4			Hexadecanoic acid, 14-methyl-, m...	284	C18H36O2	002490-49-5	91
5			Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042922\
Data File : BF128010.D
Acq On : 29 Apr 2022 22:29
Operator : CG\JU
Sample : N2605-01 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

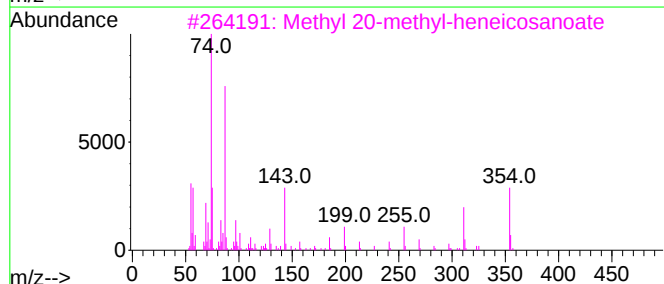
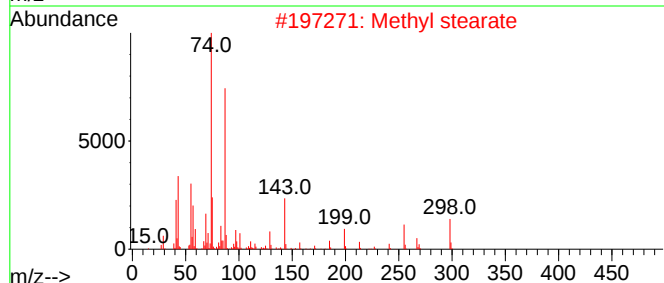
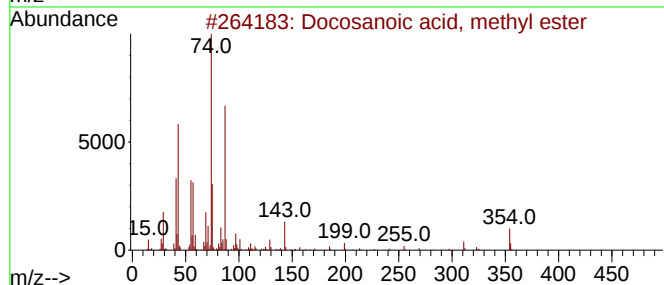
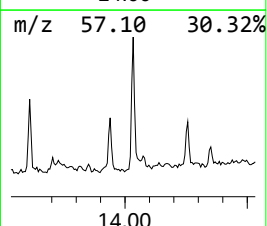
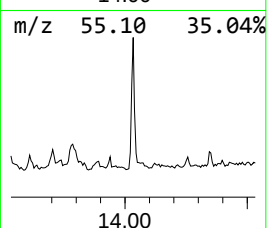
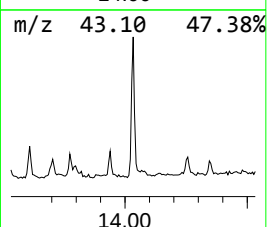
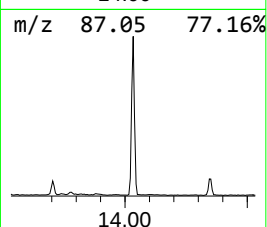
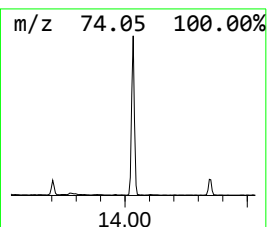
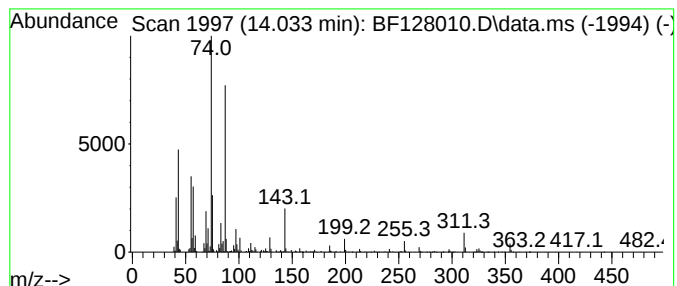
Instrument :
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ClientSampleId :
TR-04-042822

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Docosanoic acid, methyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.033	30.71 ng	939405	Chrysene-d12		14.115	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Docosanoic acid, methyl ester		354	C23H46O2	000929-77-1	99
2	Methyl stearate		298	C19H38O2	000112-61-8	97
3	Methyl 20-methyl-heneicosanoate		354	C23H46O2	1000336-47-4	91
4	Nonadecanoic acid, methyl ester		312	C20H40O2	001731-94-8	90
5	Hexadecanoic acid, 15-methyl-, m...		284	C18H36O2	006929-04-0	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042922\
Data File : BF128010.D
Acq On : 29 Apr 2022 22:29
Operator : CG\JU
Sample : N2605-01 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-04-042822

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexadecanoic ac...	11.863	368.5	ng	14476100	4	11.463	785682	20.0
n-Hexadecanoic ...	11.998	26.8	ng	1053980	4	11.463	785682	20.0
9,12-Octadecadi...	12.592	1205.5	ng	47357200	4	11.463	785682	20.0
9,12,15-Octadec...	12.633	19.3	ng	758377	4	11.463	785682	20.0
Methyl stearate	12.663	191.8	ng	7536170	4	11.463	785682	20.0
9,12-Octadecadi...	12.692	65.0	ng	2553070	4	11.463	785682	20.0
11-Eicosenoic a...	13.286	19.6	ng	600829	5	14.115	611875	20.0
Eicosanoic acid...	13.363	33.0	ng	1009320	5	14.115	611875	20.0
Docosanoic acid...	14.033	30.7	ng	939405	5	14.115	611875	20.0