

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121120\
 Data File : BF122672.D
 Acq On : 11 Dec 2020 19:49
 Operator : JU/CG
 Sample : L5015-02 5X
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TR-05-121020

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-BF120520.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122672.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.451	568	572	583	rBV	425261	465853	2.66%	0.957%
2	6.463	741	744	760	rBV	443178	511268	2.92%	1.050%
3	6.839	804	808	815	rBV	1114892	884381	5.05%	1.816%
4	7.398	900	903	908	rBV	311557	288442	1.65%	0.592%
5	8.122	1021	1026	1033	rBV	1230606	1201035	6.86%	2.466%
6	9.198	1205	1209	1214	rBV	816565	681734	3.89%	1.400%
7	9.880	1321	1325	1328	rBV	1387200	1211899	6.92%	2.489%
8	10.669	1453	1459	1470	rVB	276771	319693	1.83%	0.656%
9	11.363	1573	1577	1580	rBV	1257670	1111989	6.35%	2.283%
10	11.763	1640	1645	1648	rBV	6677229	6596938	37.68%	13.547%
11	12.468	1756	1765	1766	rBV	8444364	17509860	100.00%	35.956%
12	12.486	1766	1768	1772	rVV2	8496003	10125839	57.83%	20.793%
13	12.521	1772	1774	1776	rVV2	302448	230256	1.32%	0.473%
14	12.551	1776	1779	1782	rVV	3199183	2987584	17.06%	6.135%
15	12.786	1814	1819	1821	rBV2	238331	264888	1.51%	0.544%
16	12.839	1824	1828	1832	rVB2	257230	387846	2.22%	0.796%
17	12.951	1843	1847	1850	rBV	714207	635747	3.63%	1.305%
18	13.133	1875	1878	1883	rVB4	164878	238413	1.36%	0.490%
19	13.198	1883	1889	1894	rBV4	209113	361133	2.06%	0.742%
20	13.274	1899	1902	1904	rBV	311153	243750	1.39%	0.501%
21	13.939	2013	2015	2021	rVB	262879	234712	1.34%	0.482%
22	14.004	2022	2026	2029	rBV	1162882	1066307	6.09%	2.190%
23	15.474	2271	2276	2289	rVB	786405	1138846	6.50%	2.339%

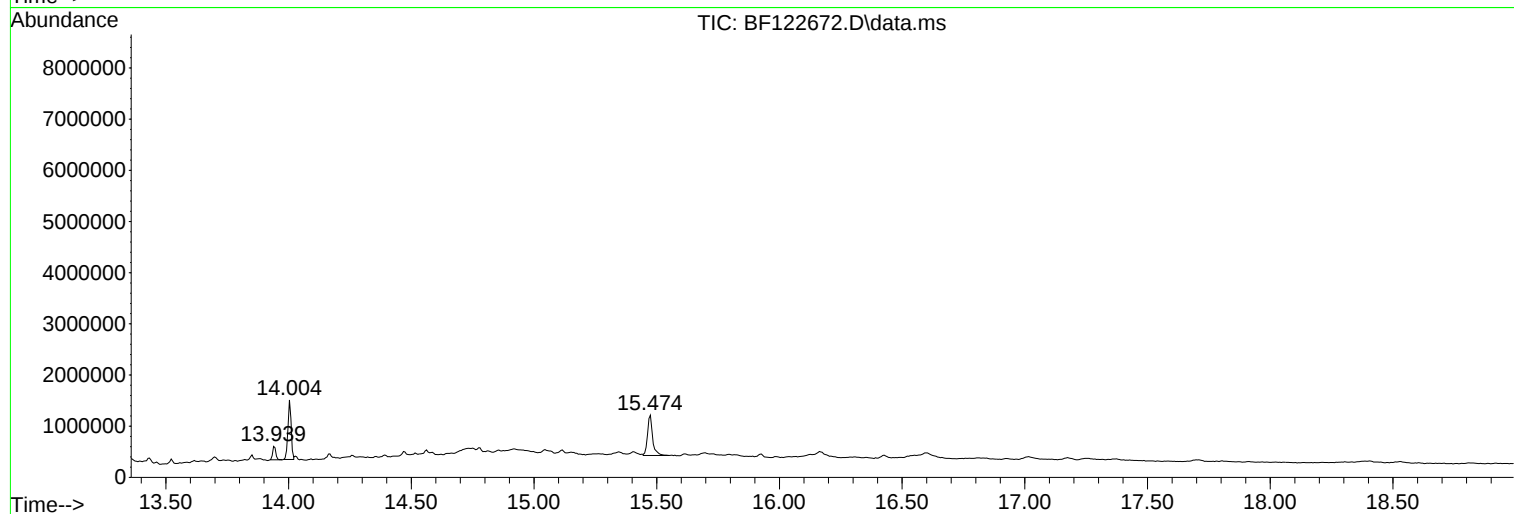
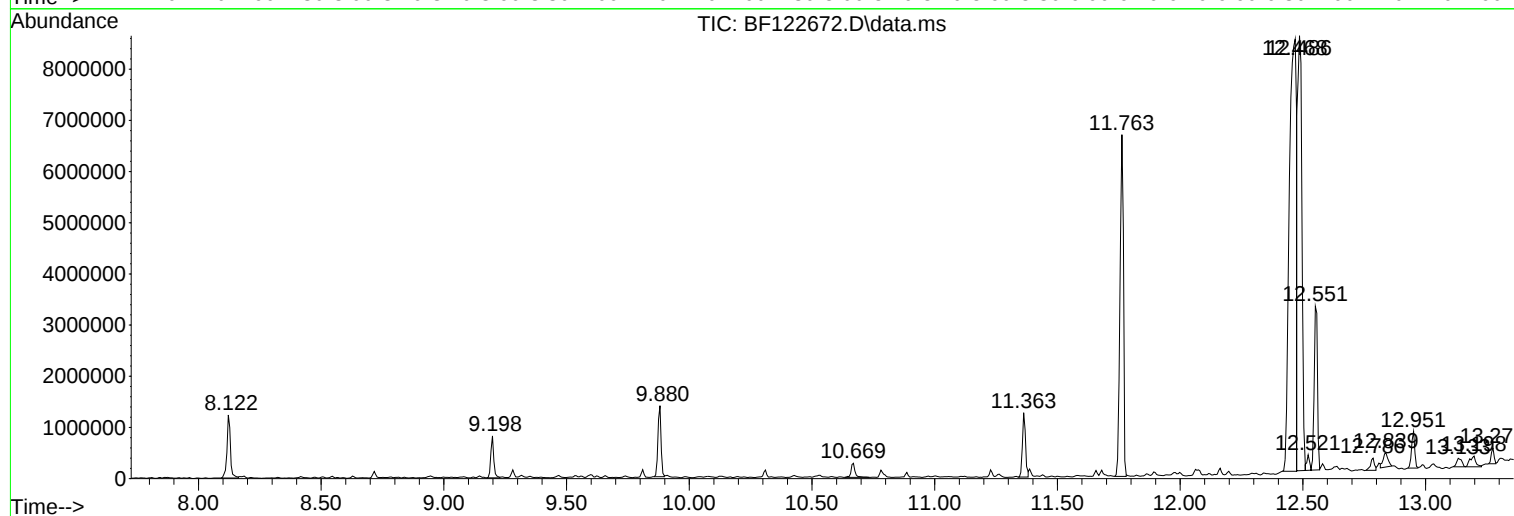
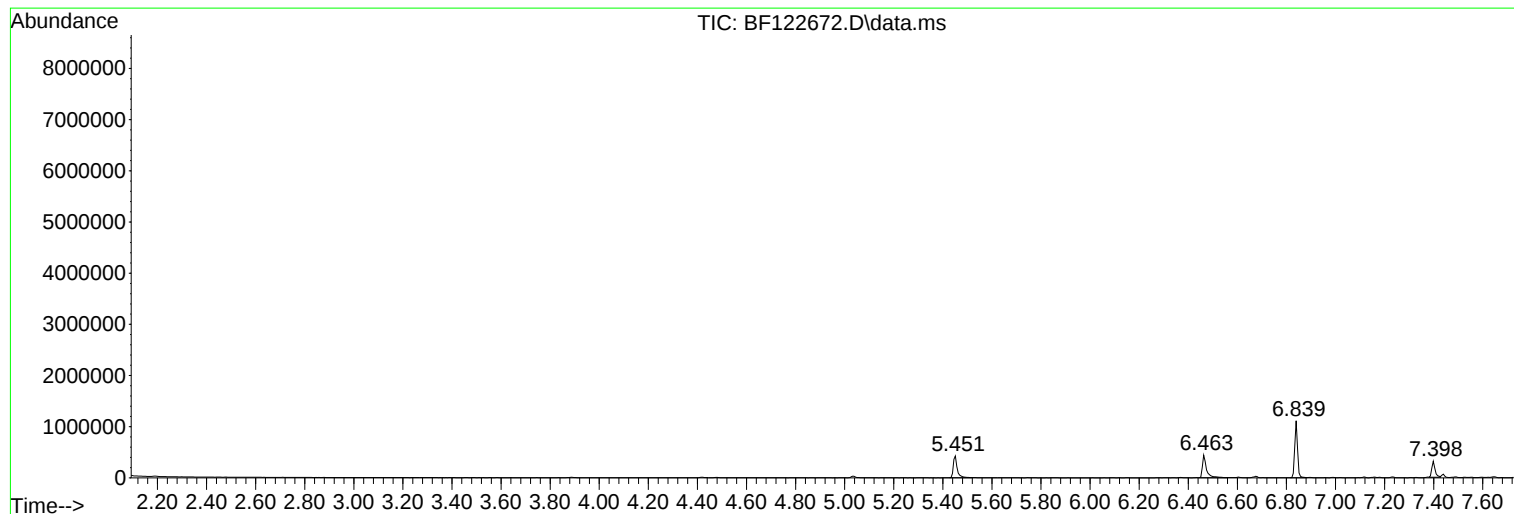
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Instrument :
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ClientSampleId :
TR-05-121020

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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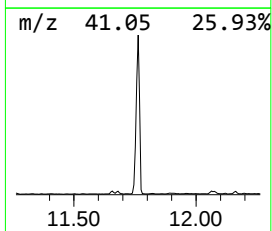
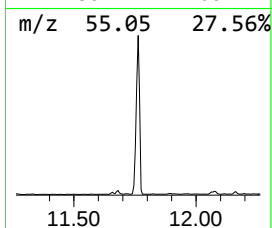
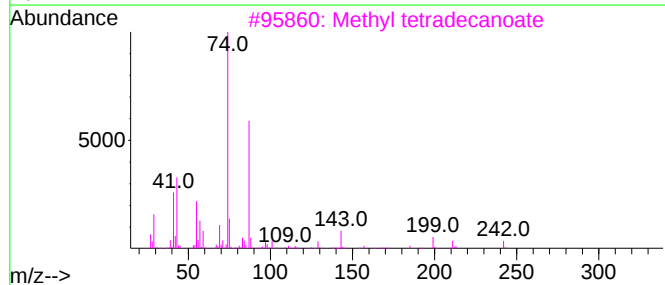
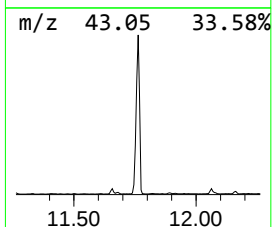
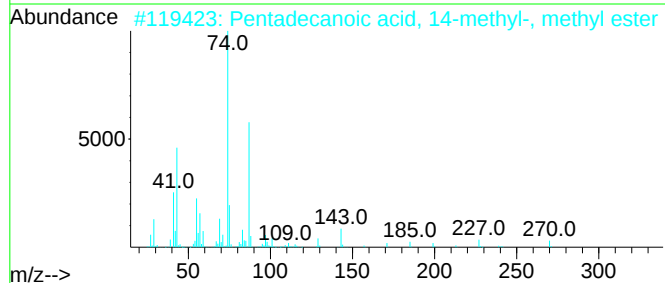
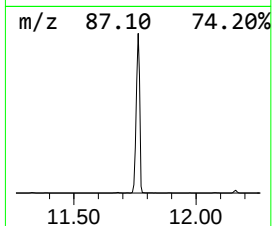
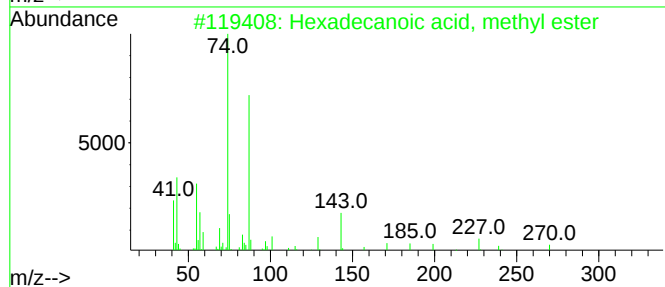
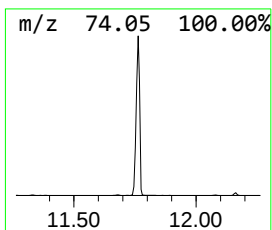
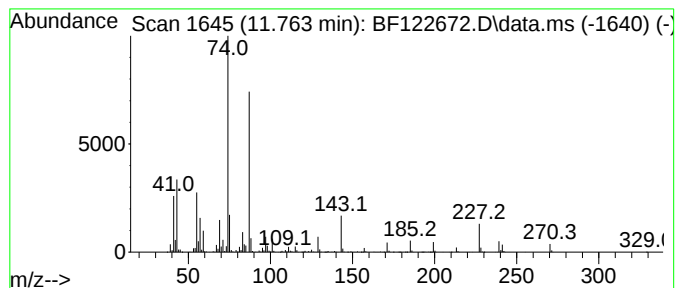
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
11.763	118.65 ng	6596940	Phenanthrene-d10	11.363

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			Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
4			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
5			Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	87



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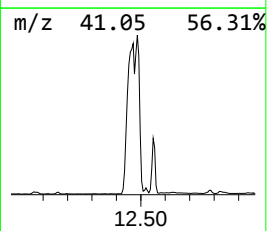
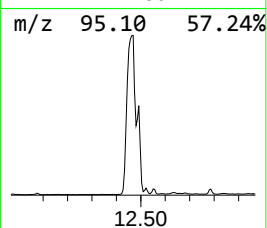
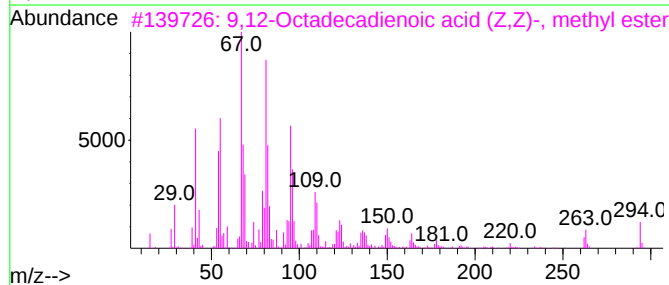
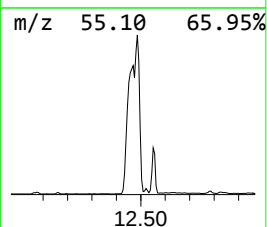
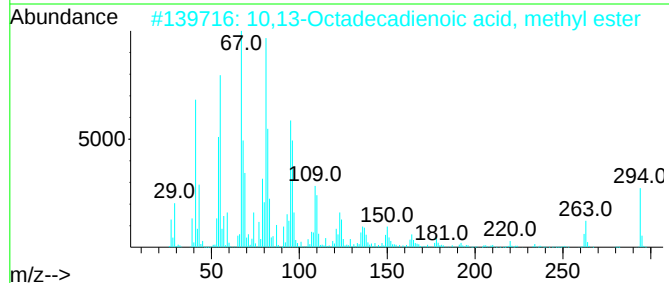
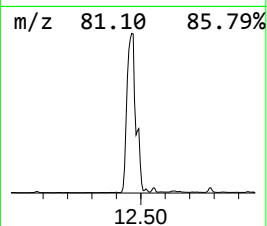
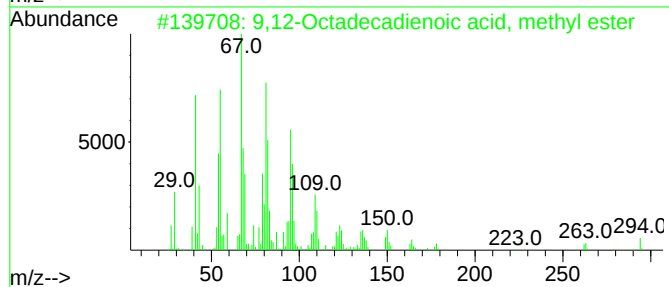
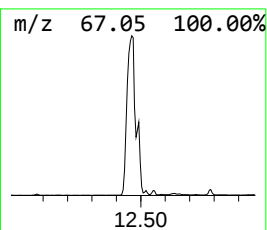
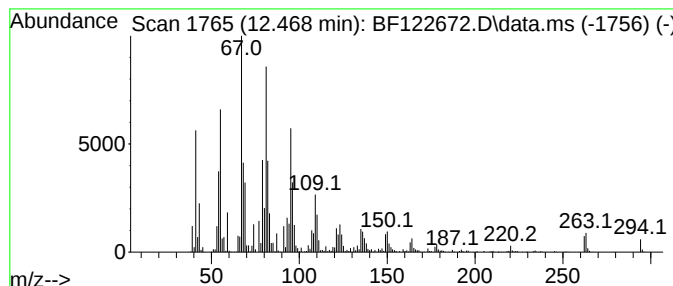
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.469	314.93 ng	17509900	Phenanthrene-d10	11.363

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	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99		
5	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	99		



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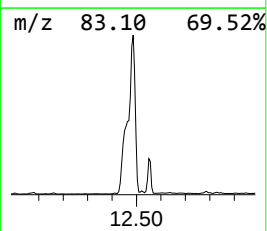
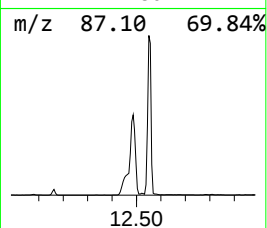
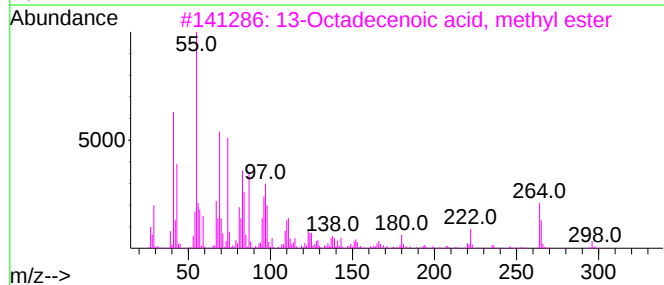
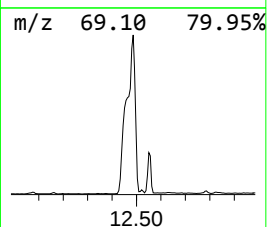
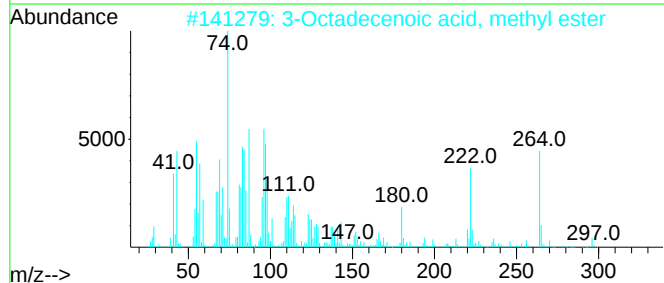
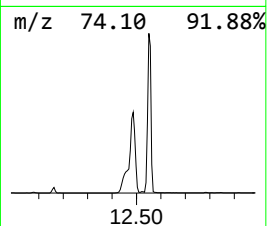
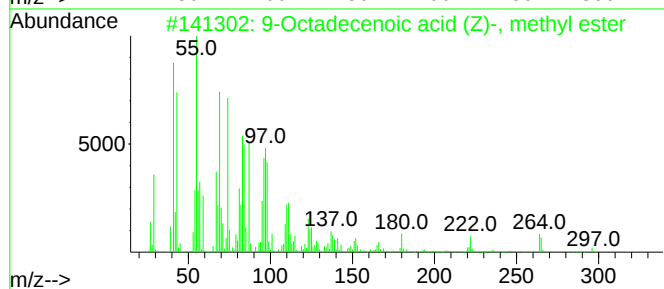
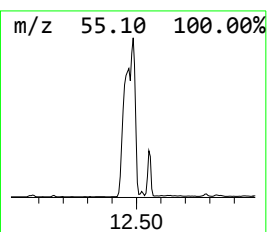
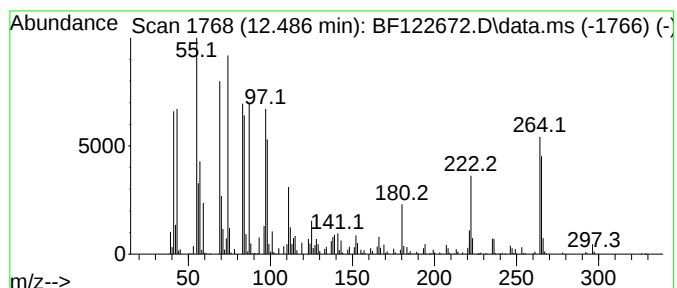
Instrument :
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ClientSampleId :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.486	182.12 ng	10125800	Phenanthrene-d10	11.363	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	89
2	3-Octadecenoic acid, methyl ester	296	C19H36O2	056599-33-8	70
3	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	59
4	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	55
5	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	53



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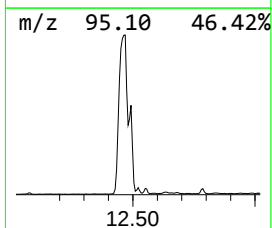
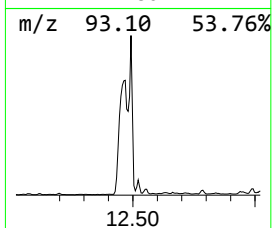
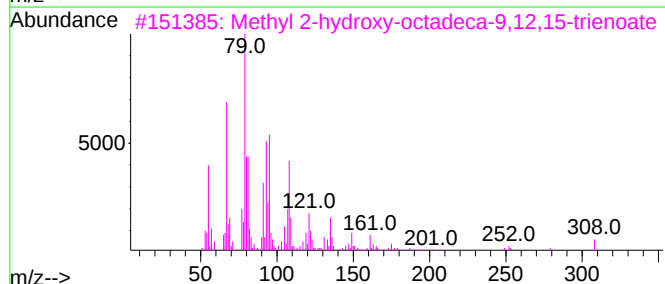
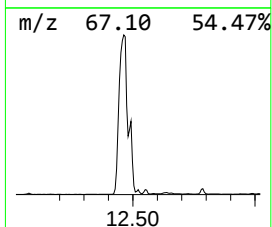
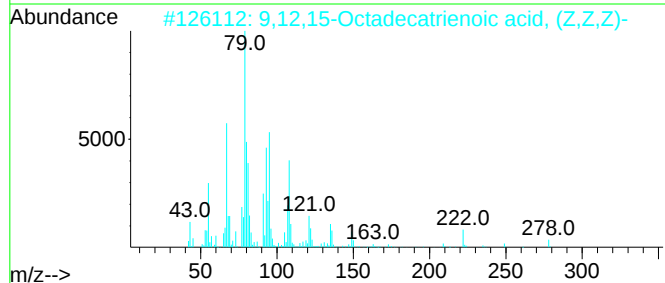
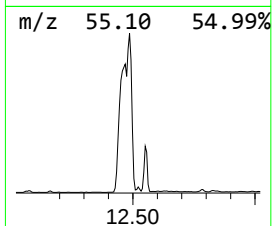
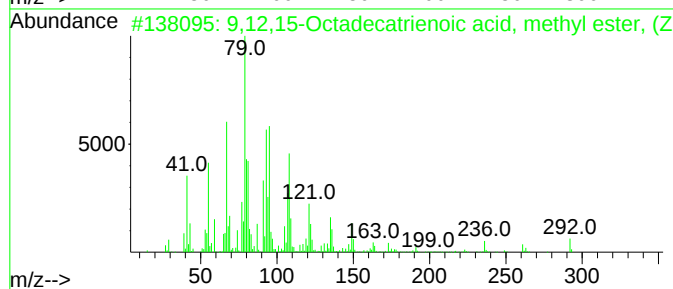
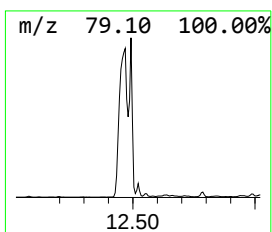
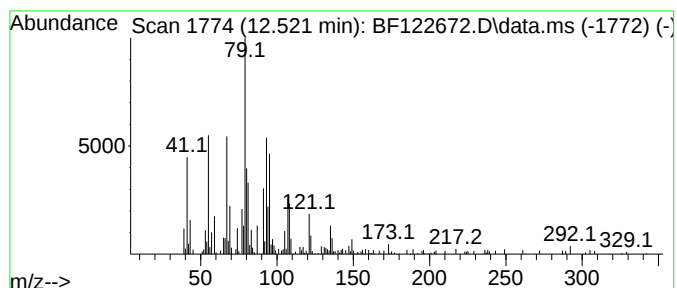
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.521	4.14 ng	230256	Phenanthrene-d10	11.363	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12,15-Octadecatrienoic acid, m...	292	C19H32O2	000301-00-8	93
2	9,12,15-Octadecatrienoic acid, (...	278	C18H30O2	000463-40-1	80
3	Methyl 2-hydroxy-octadeca-9,12,1...	308	C19H32O3	1000336-39-1	72
4	3-Undecen-1-yne, (Z)-	150	C11H18	074744-32-4	64
5	Spiro[2.4]heptane, 1,5-dimethyl-...	136	C10H16	062238-24-8	53



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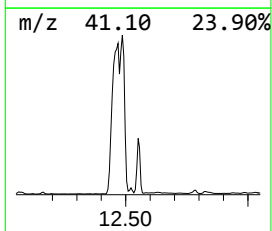
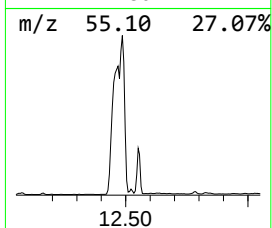
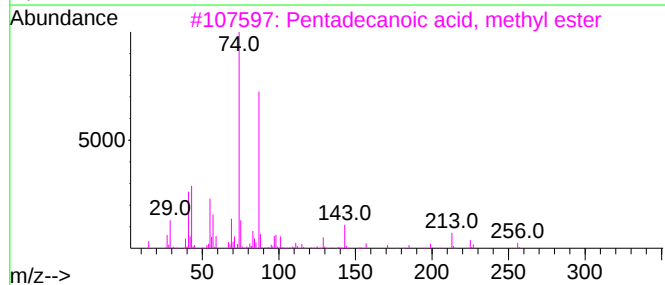
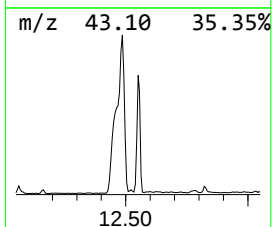
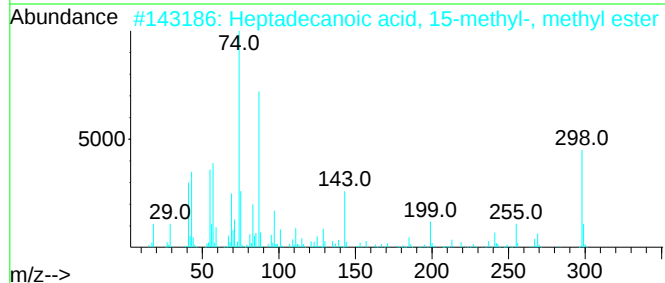
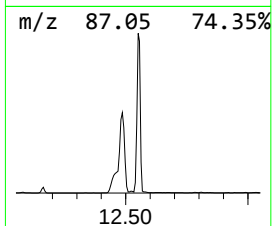
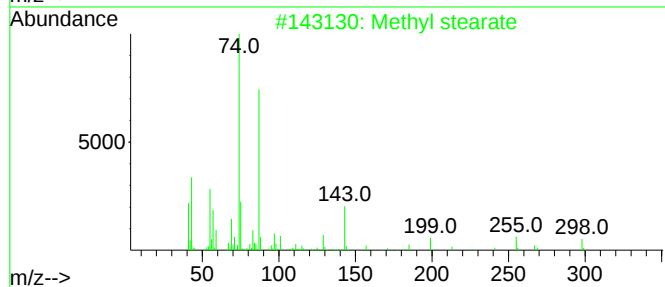
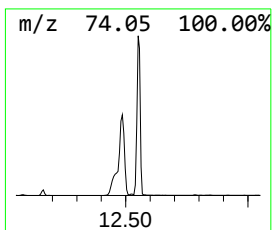
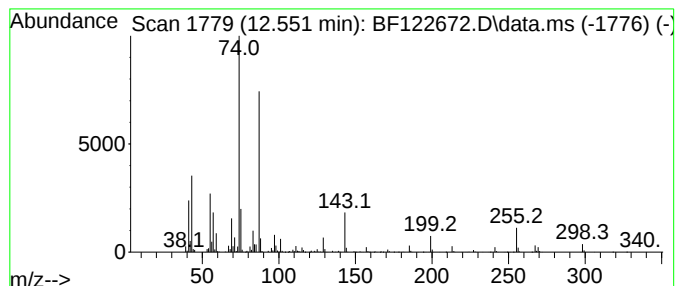
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Methyl stearate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.551	53.73 ng	2987580	Phenanthrene-d10	11.363

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			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	91
4			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	91
5			Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	91



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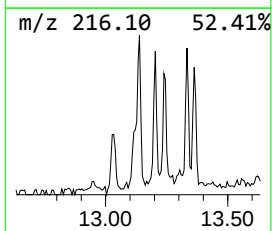
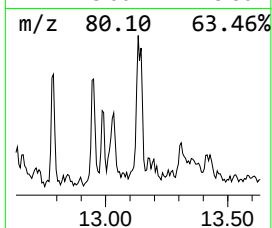
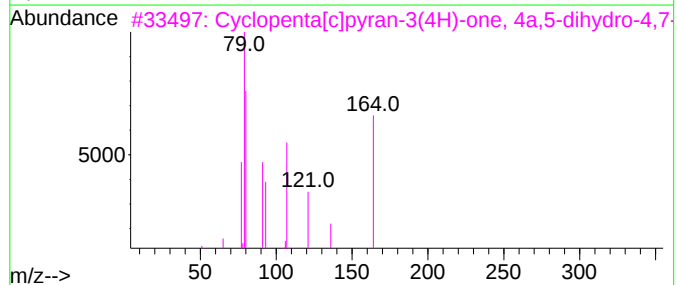
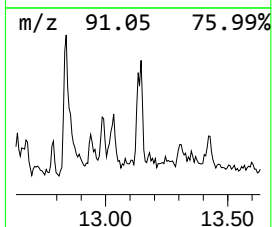
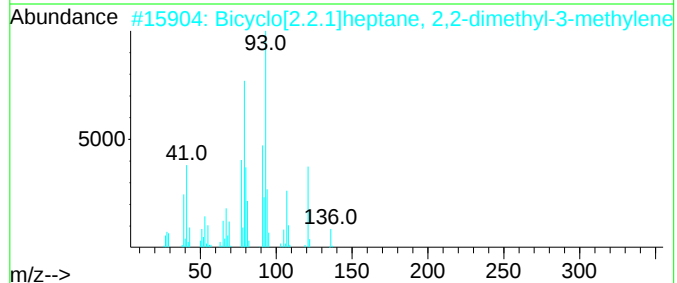
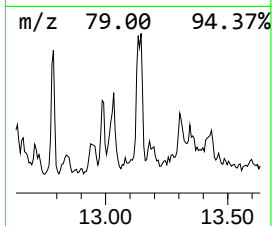
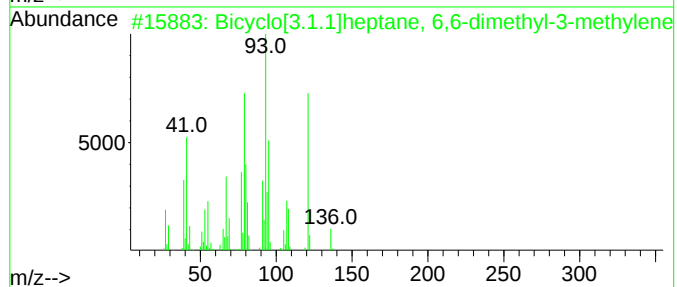
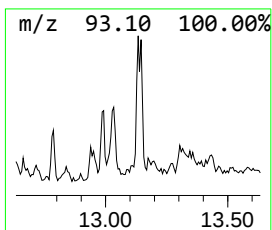
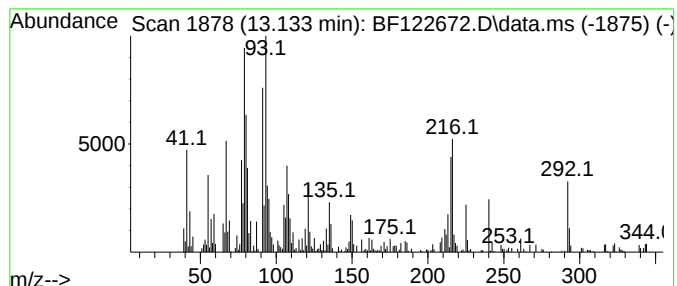
Instrument :
BNA_F
ClientSampleId :
TR-05-121020

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Bicyclo[3.1.1]heptane, 6,6-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.133	4.47 ng	238413	Chrysene-d12	14.004	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.1]heptane, 6,6-dimet...	136	C10H16	016022-04-1	55
2	Bicyclo[2.2.1]heptane, 2,2-dimet...	136	C10H16	005794-03-6	43
3	Cyclopenta[c]pyran-3(4H)-one, 4a...	164	C10H12O2	075364-51-1	41
4	Cyclopentane, 1-ethenyl-3-methyl...	108	C8H12	029668-63-1	38
5	1-Methylene-2-vinylcyclopentane	108	C8H12	006196-78-7	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121120\
Data File : BF122672.D
Acq On : 11 Dec 2020 19:49
Operator : JU/CG
Sample : L5015-02 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

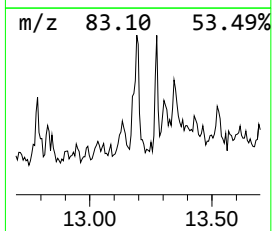
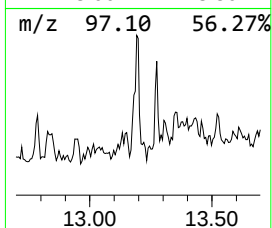
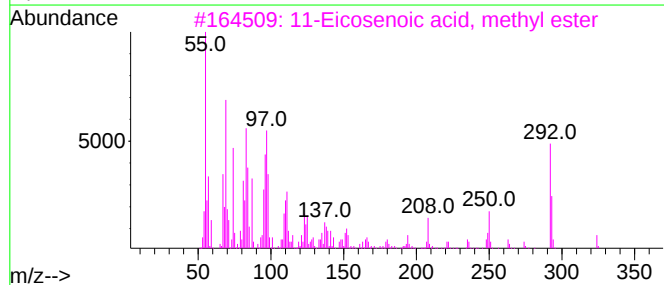
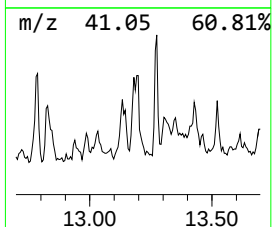
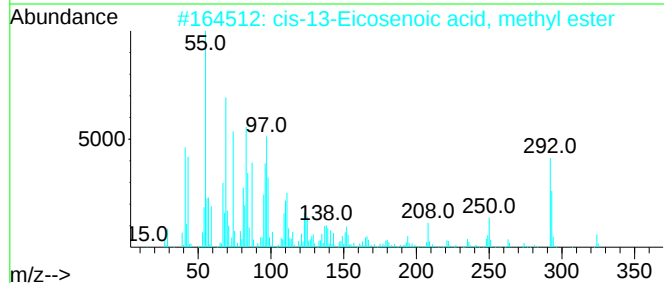
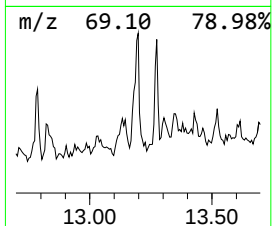
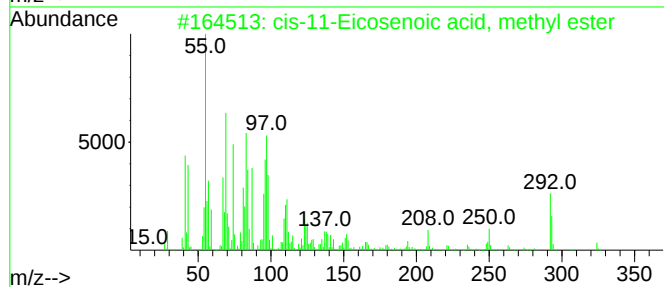
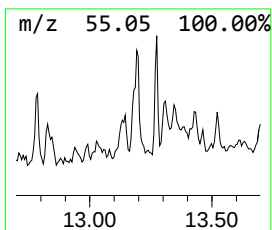
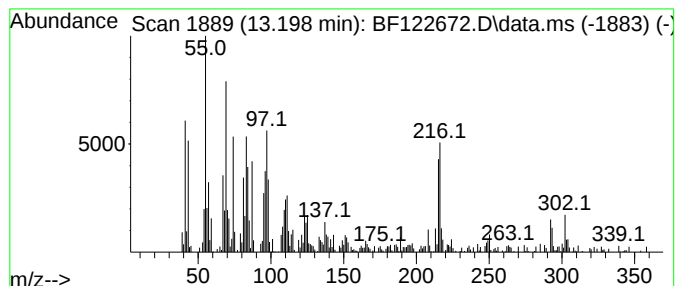
Instrument :
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ClientSampleId :
TR-05-121020

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 cis-11-Eicosenoic acid, met... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.198	6.77 ng	361133	Chrysene-d12	14.004	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-11-Eicosenoic acid, methyl e...	324	C21H40O2	1000333-63-8	96
2	cis-13-Eicosenoic acid, methyl e...	324	C21H40O2	1000333-52-1	87
3	11-Eicosenoic acid, methyl ester	324	C21H40O2	003946-08-5	84
4	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	44
5	Cyclopentadecanone, 2-hydroxy-	240	C15H28O2	004727-18-8	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121120\
Data File : BF122672.D
Acq On : 11 Dec 2020 19:49
Operator : JU/CG
Sample : L5015-02 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-05-121020

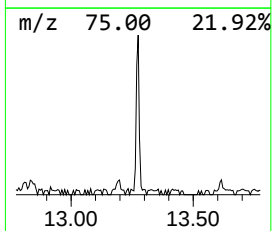
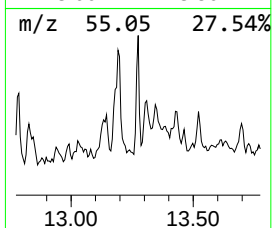
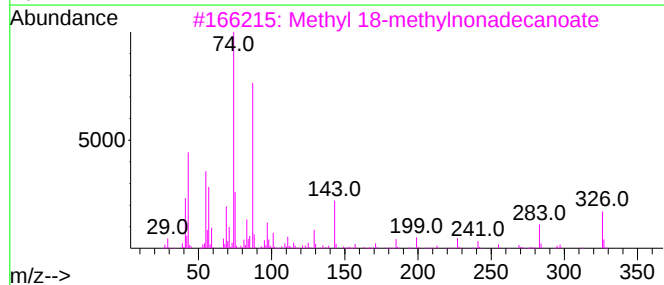
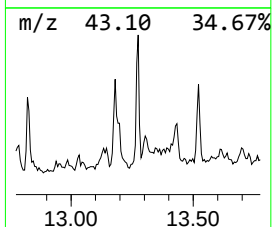
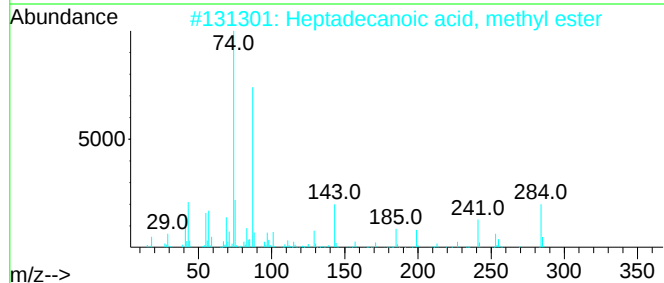
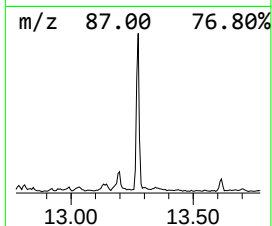
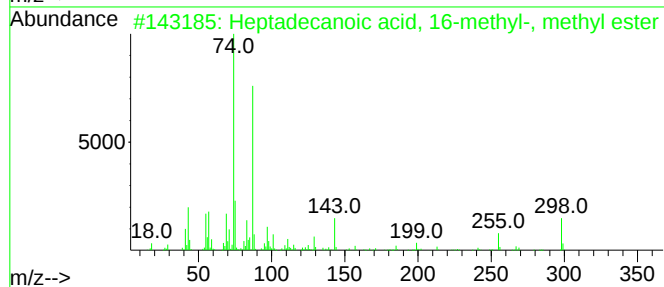
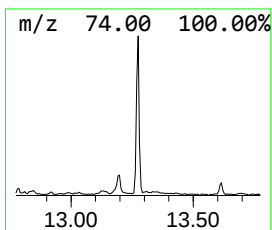
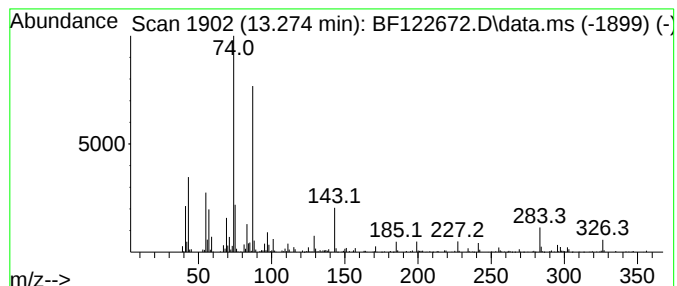
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptadecanoic acid, 16-meth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.274	4.57 ng	243750	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	96
2			Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	95
3			Methyl 18-methylnonadecanoate	326	C21H42O2	1000352-20-6	94
4			Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	91
5			Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121120\
Data File : BF122672.D
Acq On : 11 Dec 2020 19:49
Operator : JU/CG
Sample : L5015-02 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TR-05-121020

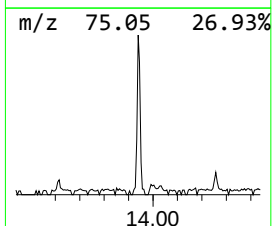
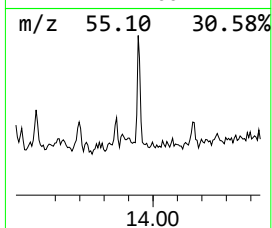
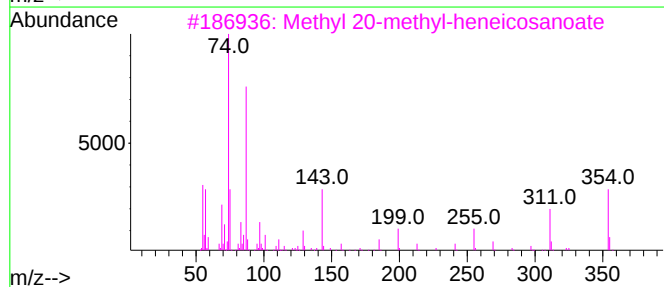
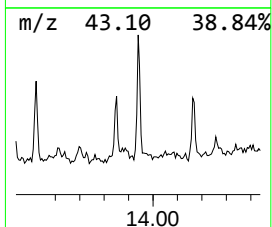
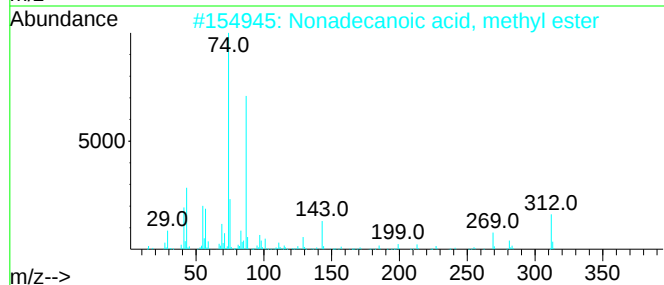
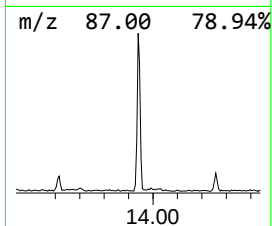
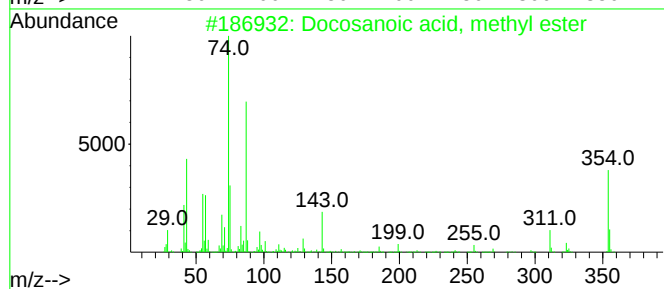
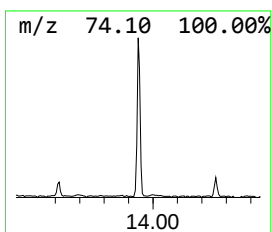
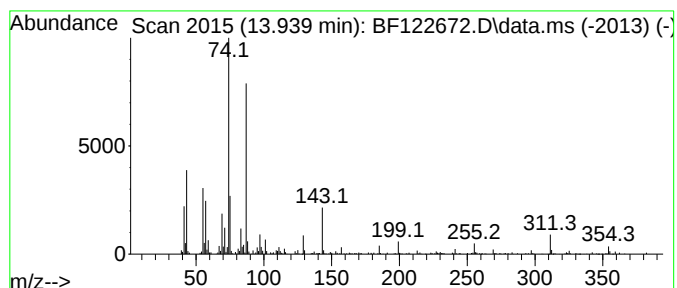
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Docosanoic acid, methyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.939	4.40 ng	234712	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosanoic acid, methyl ester	354	C23H46O2	000929-77-1	95
2			Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	91
3			Methyl 20-methyl-heneicosanoate	354	C23H46O2	1000336-47-4	90
4			Methyl stearate	298	C19H38O2	000112-61-8	87
5			Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121120\
Data File : BF122672.D
Acq On : 11 Dec 2020 19:49
Operator : JU/CG
Sample : L5015-02 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-05-121020

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.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...	11.763	118.7	ng	6596940	4	11.363	1111990	20.0
9,12-Octadecadi...	12.469	314.9	ng	17509900	4	11.363	1111990	20.0
9-Octadecenoic ...	12.486	182.1	ng	10125800	4	11.363	1111990	20.0
9,12,15-Octadec...	12.521	4.1	ng	230256	4	11.363	1111990	20.0
Methyl stearate	12.551	53.7	ng	2987580	4	11.363	1111990	20.0
Bicyclo[3.1.1]h...	13.133	4.5	ng	238413	5	14.004	1066310	20.0
cis-11-Eicoseno...	13.198	6.8	ng	361133	5	14.004	1066310	20.0
Heptadecanoic a...	13.274	4.6	ng	243750	5	14.004	1066310	20.0
Docosanoic acid...	13.939	4.4	ng	234712	5	14.004	1066310	20.0