

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061821\
 Data File : BF124383.D
 Acq On : 18 Jun 2021 20:10
 Operator : JU/CG
 Sample : M2759-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TR-05-061721

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: BF124383.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.404	561	564	581	rVB	729501	691597	11.65%	3.372%
2	6.428	735	738	748	rBV	759387	712403	12.00%	3.473%
3	6.781	795	798	803	rBB	236078	190072	3.20%	0.927%
4	7.351	891	895	898	rBV	575947	473722	7.98%	2.310%
5	8.069	1013	1017	1019	rBV	281604	243077	4.09%	1.185%
6	9.145	1196	1200	1203	rBV	1171689	889344	14.98%	4.336%
7	9.822	1311	1315	1319	rBV	416238	319551	5.38%	1.558%
8	10.616	1446	1450	1453	rBV	730015	648790	10.93%	3.163%
9	11.310	1565	1568	1571	rBV	410251	314768	5.30%	1.535%
10	11.704	1631	1635	1639	rBV	1651509	1491027	25.11%	7.269%
11	11.845	1656	1659	1668	rBV	93840	100455	1.69%	0.490%
12	12.404	1748	1754	1756	rBV	4465246	5937600	100.00%	28.948%
13	12.427	1756	1758	1764	rVV	5075185	5419876	91.28%	26.424%
14	12.498	1767	1770	1773	rVV	1067780	941612	15.86%	4.591%
15	12.539	1774	1777	1778	rVV2	205758	222791	3.75%	1.086%
16	12.557	1778	1780	1791	rVB	208139	316132	5.32%	1.541%
17	12.898	1831	1838	1842	rBV	885599	836691	14.09%	4.079%
18	13.145	1874	1880	1885	rBV4	66514	88399	1.49%	0.431%
19	13.221	1890	1893	1898	rVB	92525	88698	1.49%	0.432%
20	13.892	2004	2007	2013	rVB	76783	74877	1.26%	0.365%
21	13.957	2014	2018	2021	rVB	288879	248721	4.19%	1.213%
22	15.415	2261	2266	2272	rBV	199210	261156	4.40%	1.273%

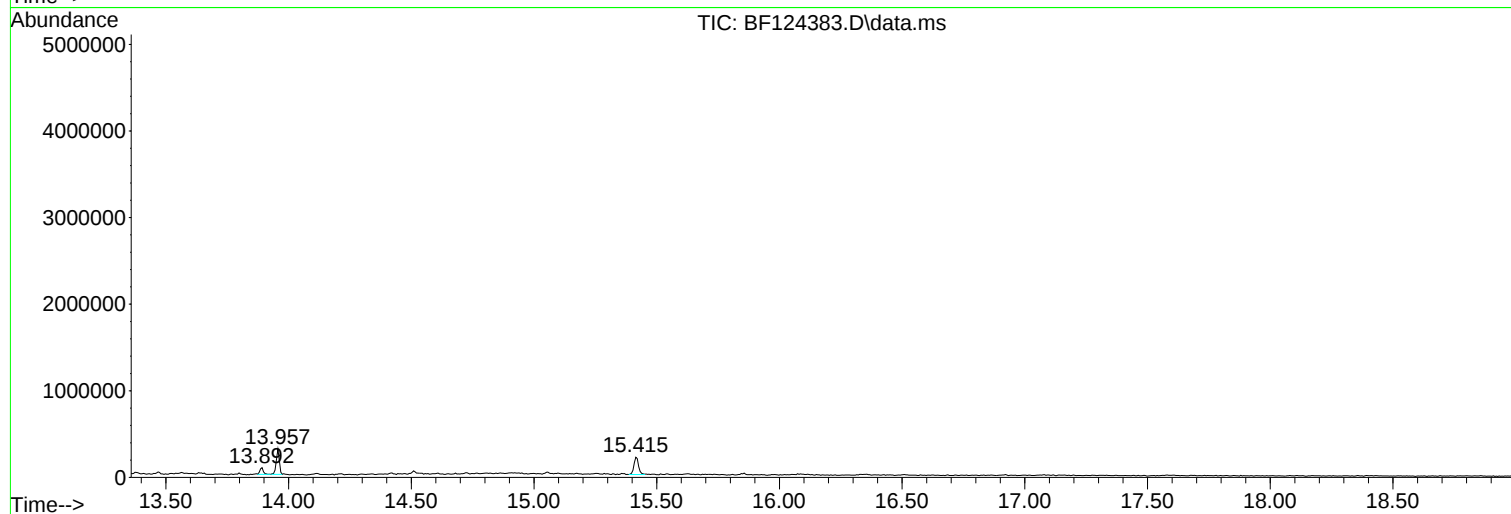
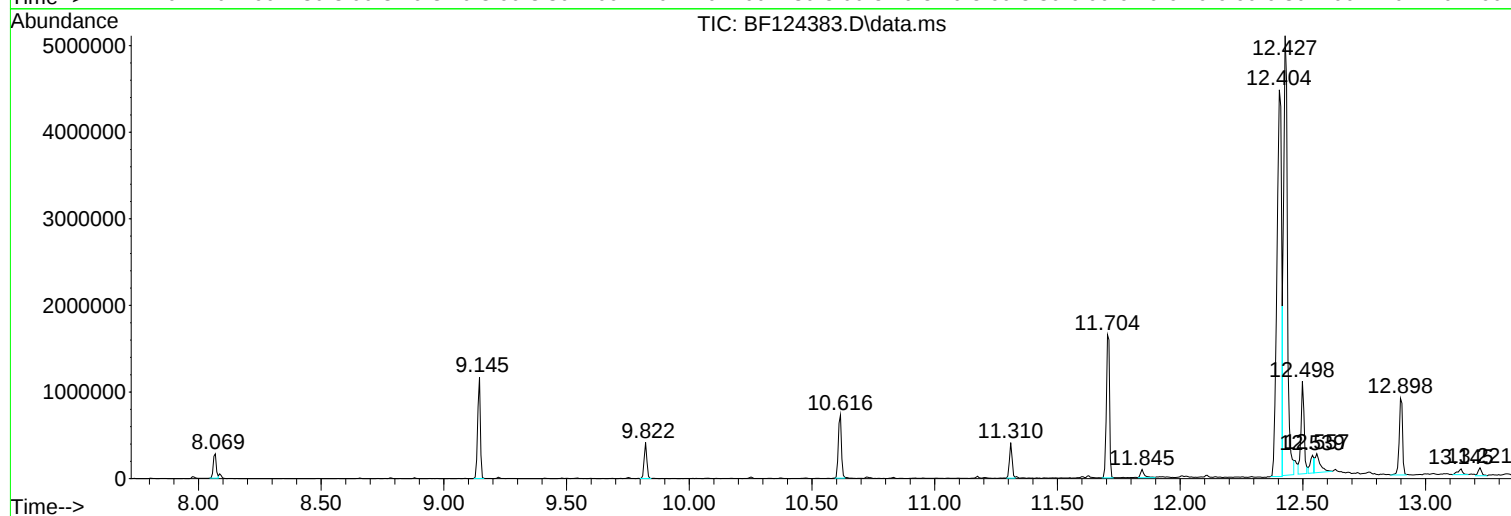
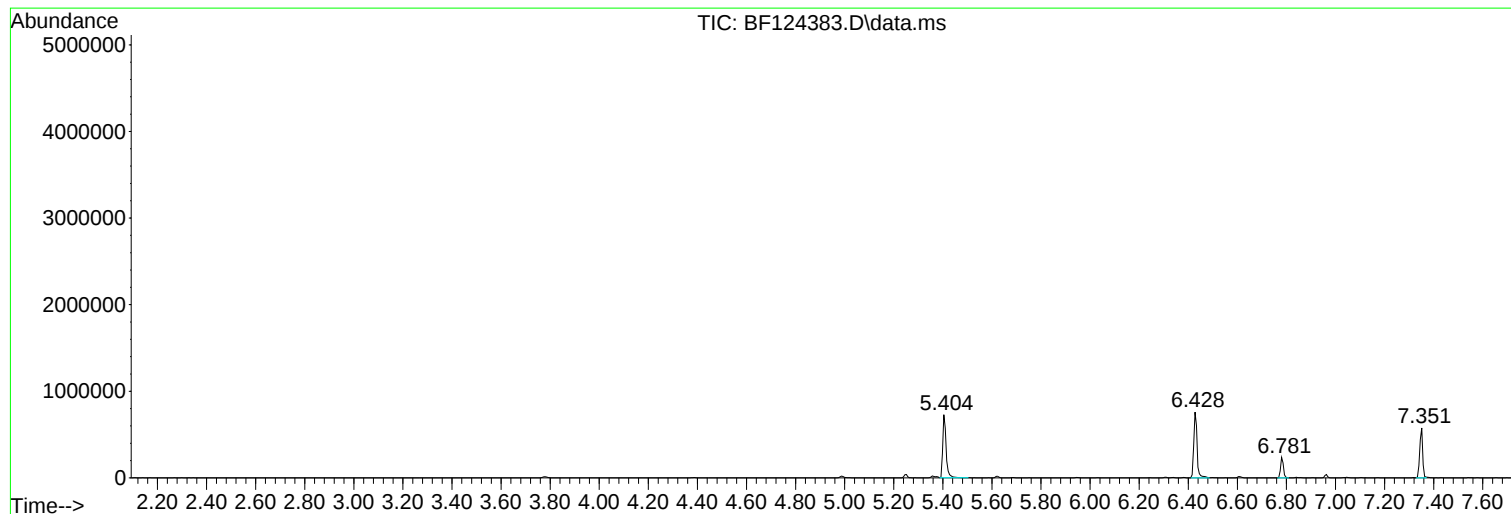
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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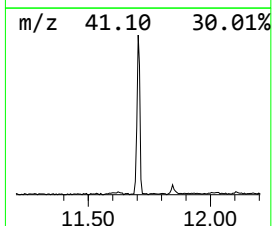
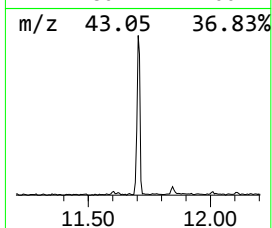
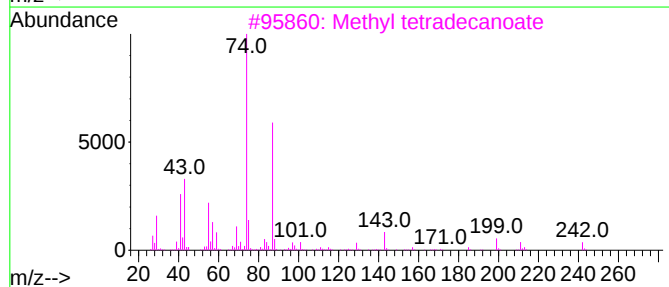
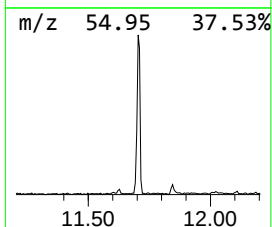
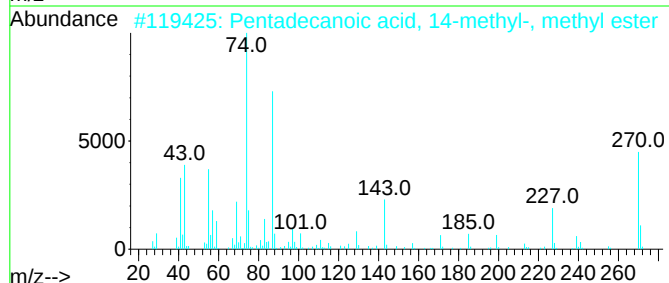
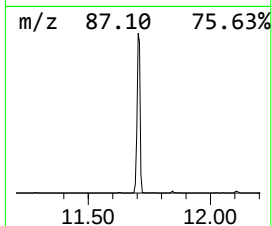
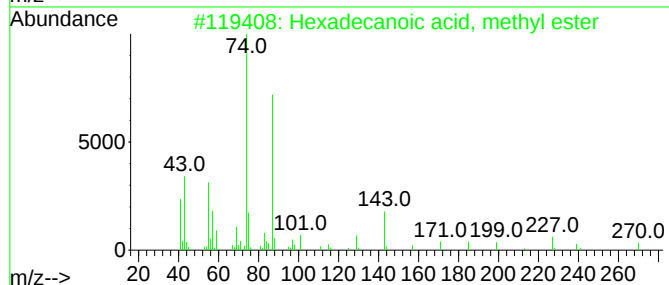
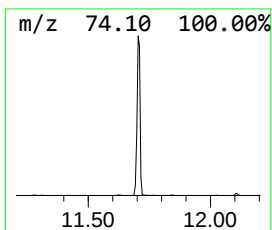
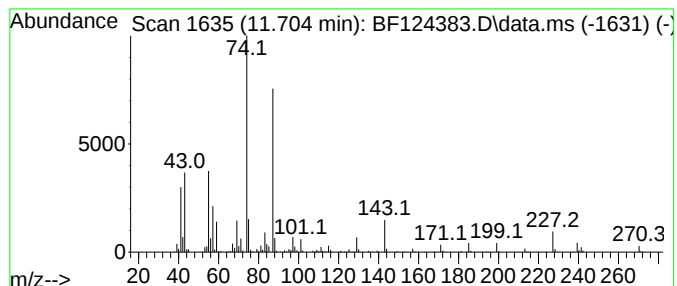
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.704	94.74 ng	1491030	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	95
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	94
3			Methyl tetradecanoate	242	C15H30O2	000124-10-7	93
4			Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	87
5			Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	86



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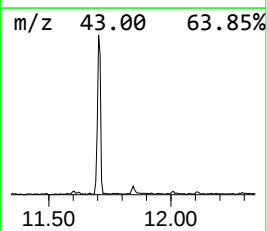
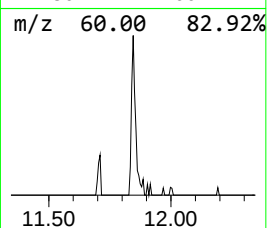
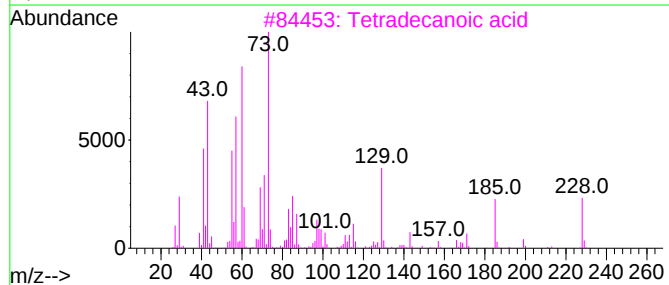
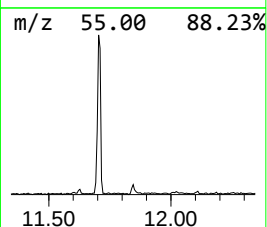
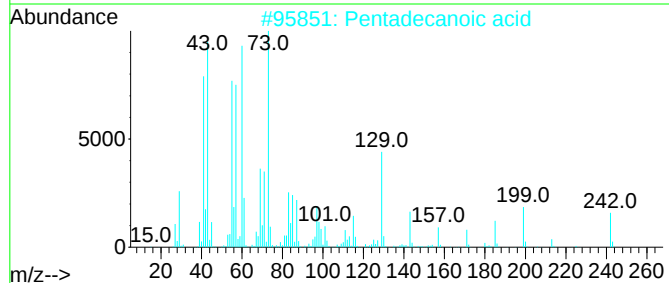
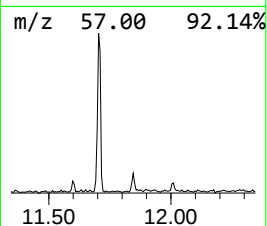
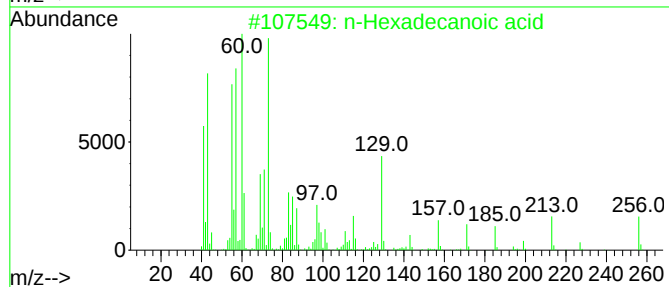
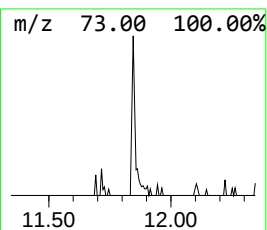
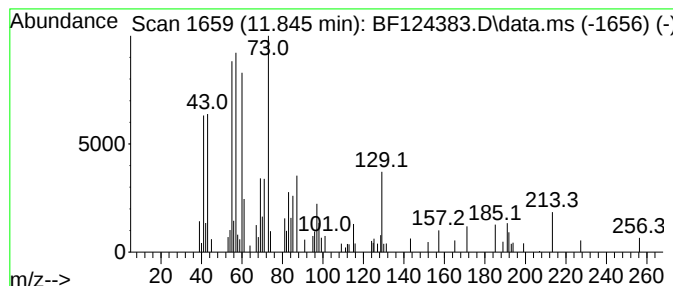
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.845	6.38 ng	100455	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4			n-Decanoic acid	172	C10H20O2	000334-48-5	50
5			Lactose	342	C12H22O11	000063-42-3	50



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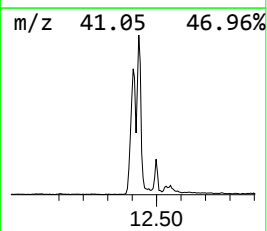
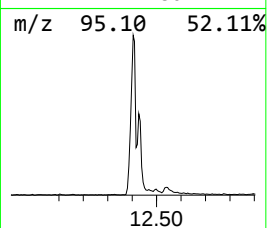
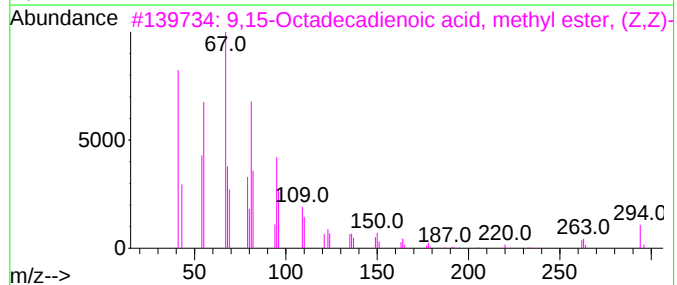
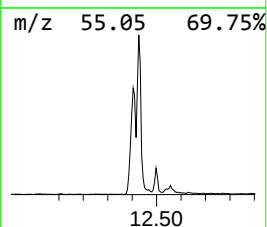
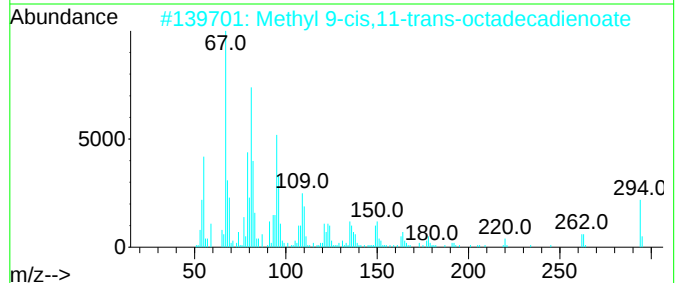
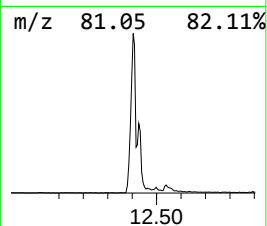
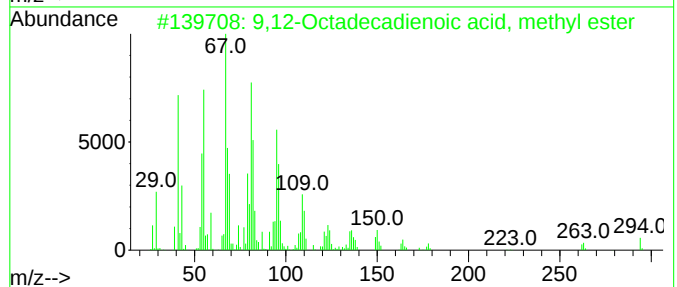
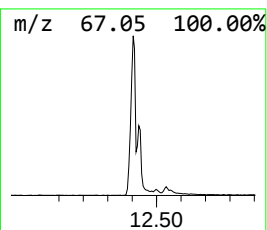
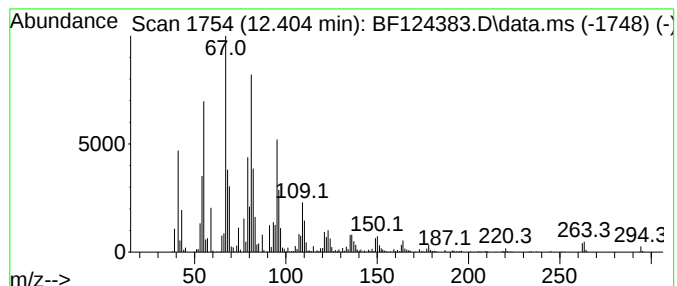
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.404	377.27 ng	5937600	Phenanthrene-d10	11.310	
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	1000336-44-0	99
3	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	98
5	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	97



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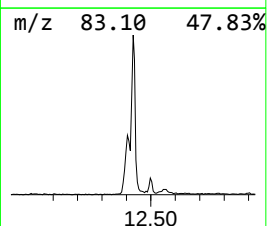
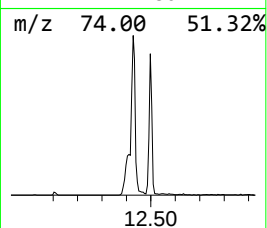
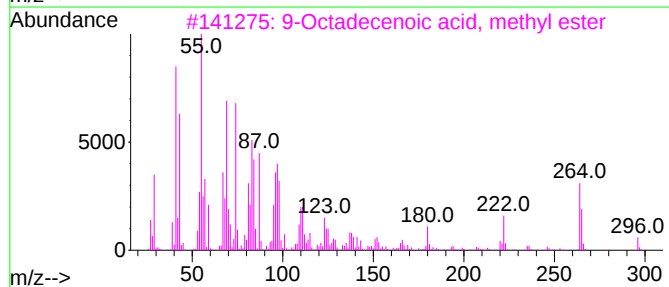
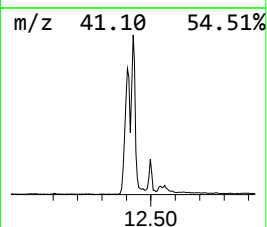
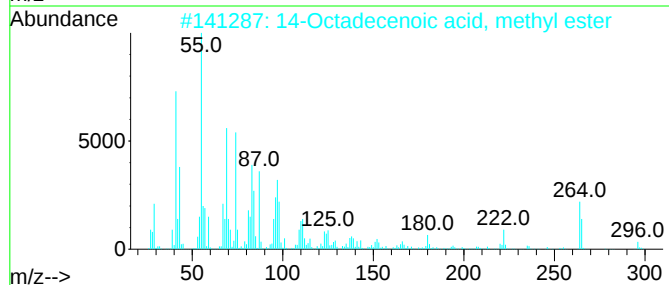
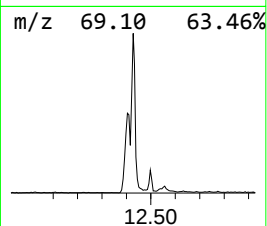
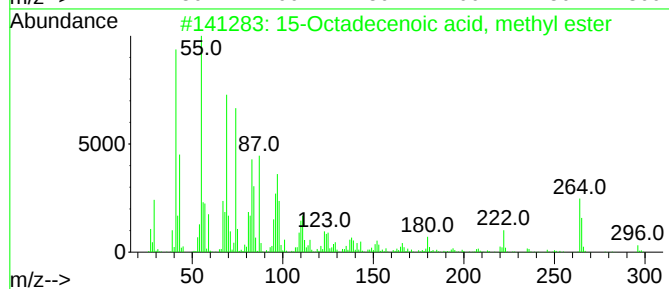
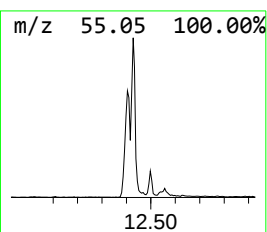
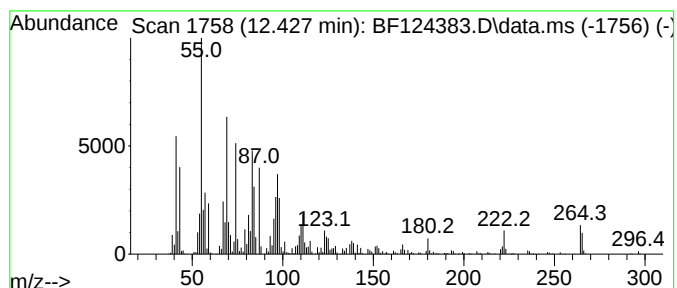
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 15-Octadecenoic acid, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.427	344.37 ng	5419880	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99
2			14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	99
3			9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99
4			13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
5			16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	99



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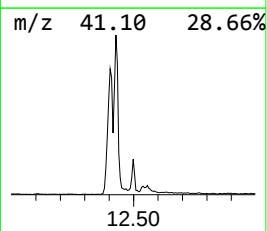
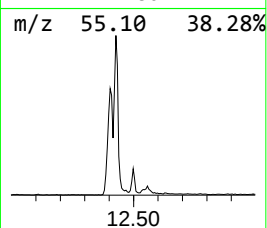
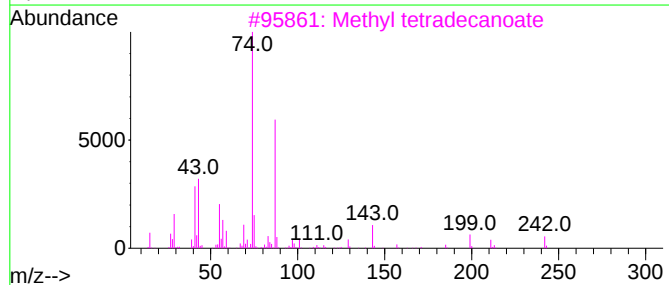
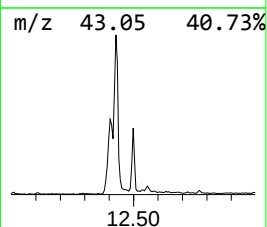
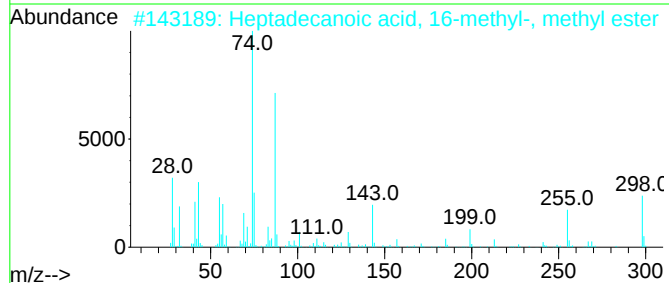
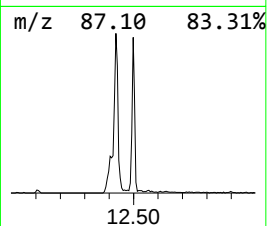
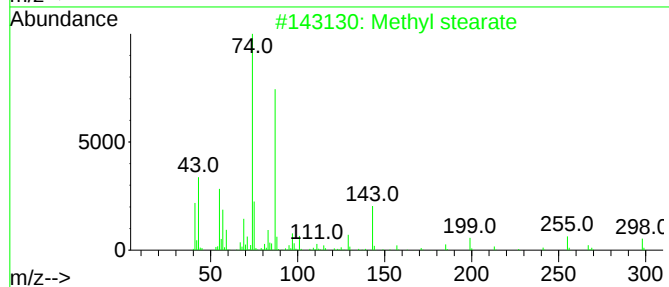
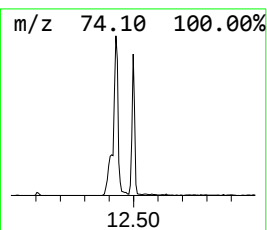
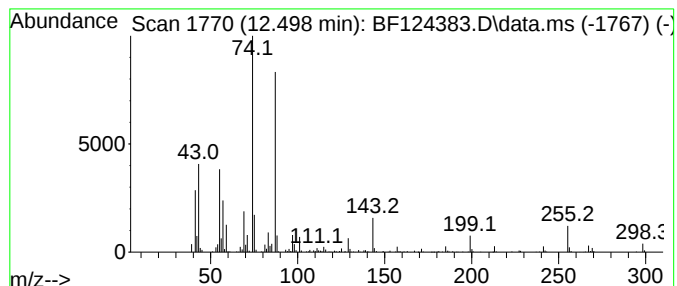
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Methyl stearate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.498	59.83 ng	941612	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	96
2			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	89
3			Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
4			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	86
5			Undecanoic acid, 10-methyl-, met...	214	C13H26O2	005129-56-6	80



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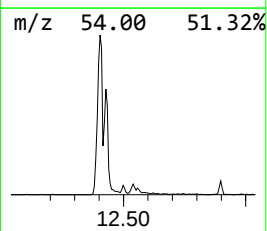
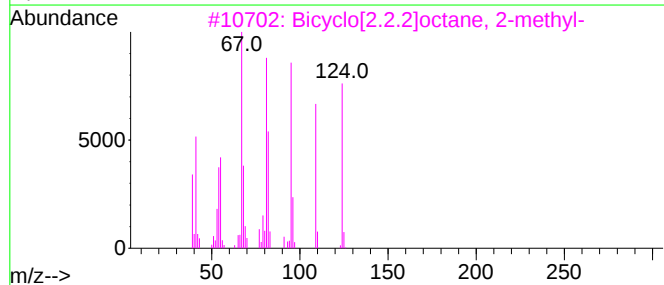
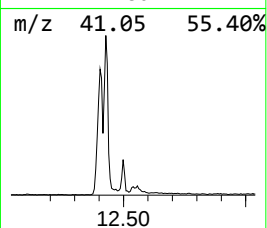
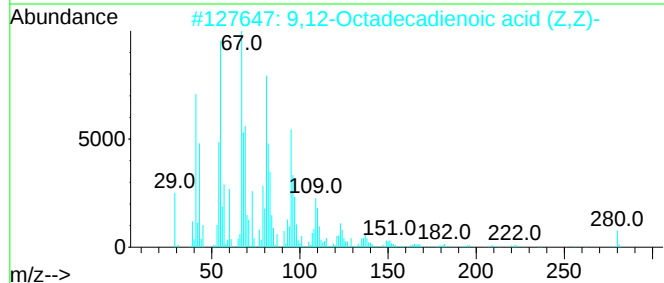
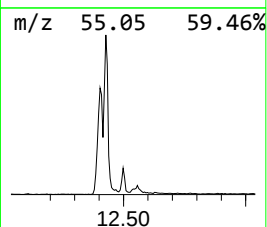
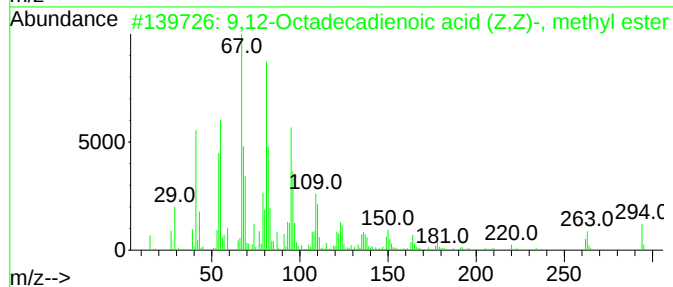
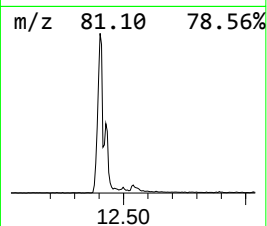
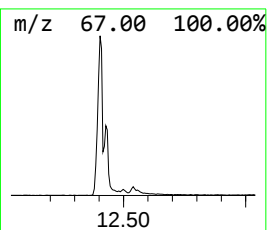
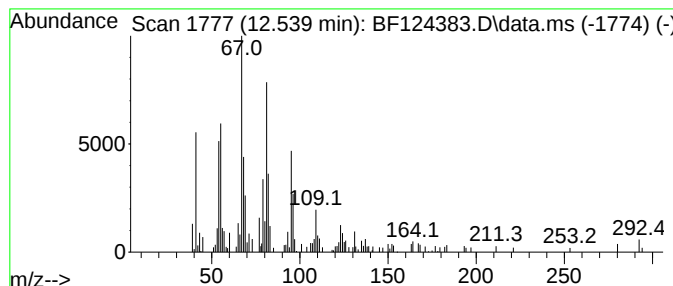
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.539	14.16 ng	222791	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	94		
2	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	91		
3	Bicyclo[2.2.2]octane, 2-methyl-	124	C9H16	000766-53-0	87		
4	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	86		
5	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	86		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061821\
Data File : BF124383.D
Acq On : 18 Jun 2021 20:10
Operator : JU/CG
Sample : M2759-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

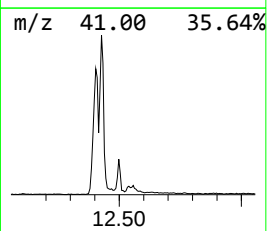
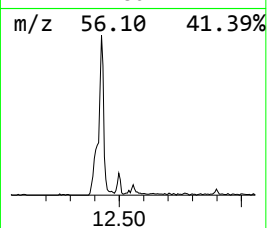
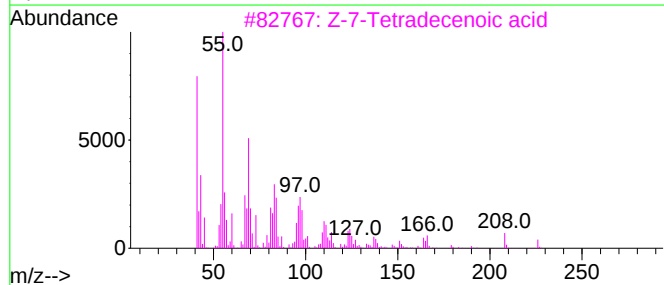
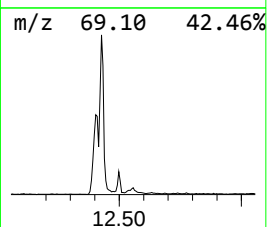
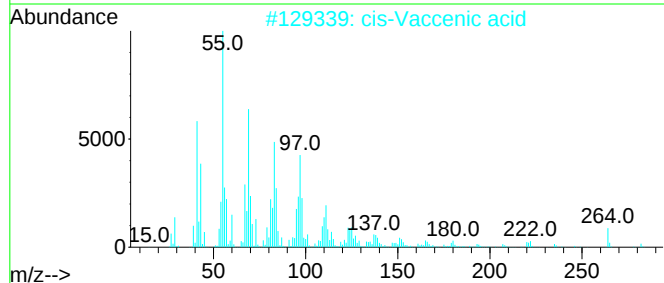
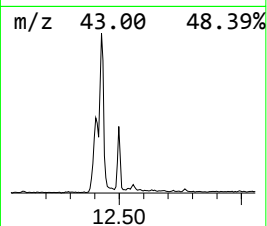
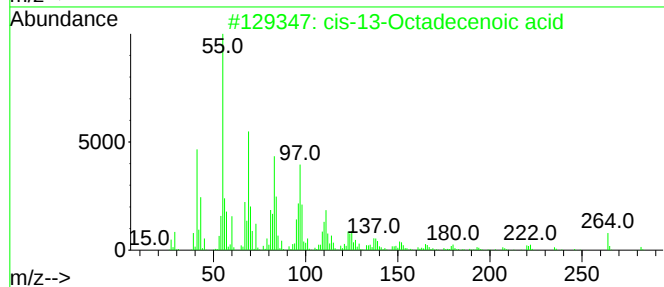
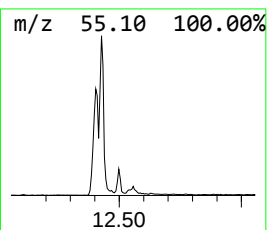
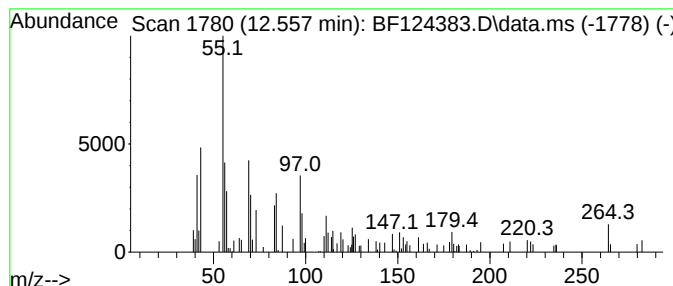
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ClientSampleId :
TR-05-061721

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 7 cis-13-Octadecenoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.557	20.09 ng	316132	Phenanthrene-d10	11.310	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	81
2	cis-Vaccenic acid	282	C18H34O2	000506-17-2	64
3	Z-7-Tetradecenoic acid	226	C14H26O2	1000130-98-4	59
4	Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	59
5	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061821\
Data File : BF124383.D
Acq On : 18 Jun 2021 20:10
Operator : JU/CG
Sample : M2759-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-05-061721

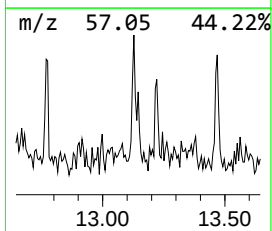
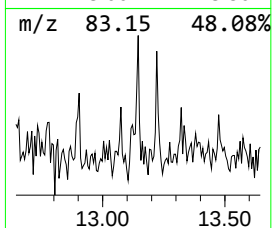
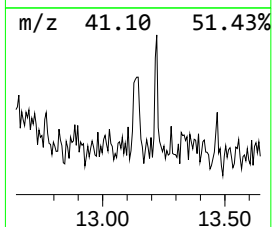
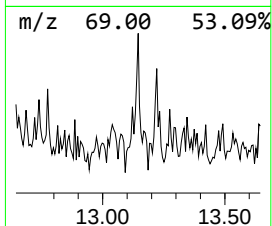
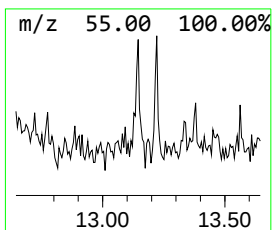
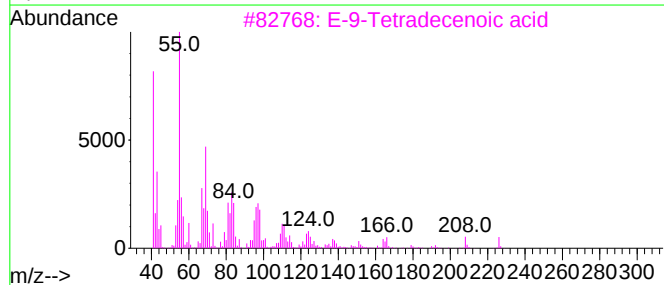
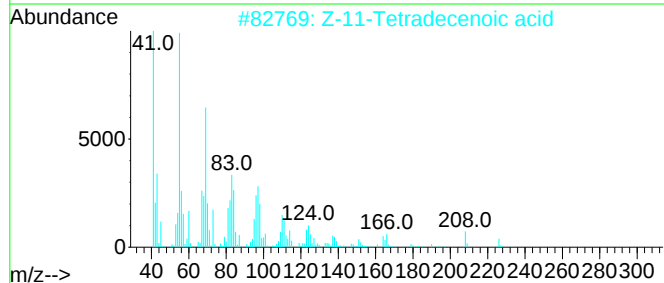
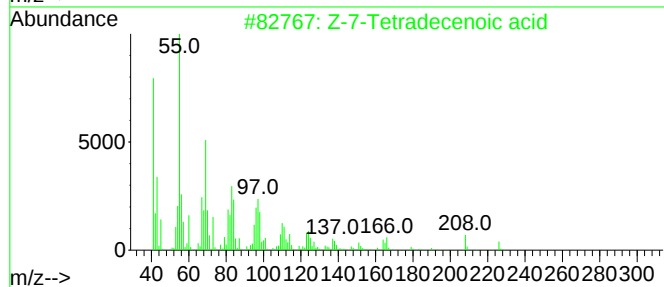
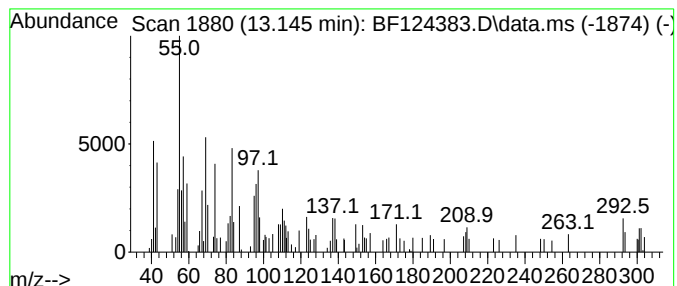
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Z-7-Tetradecenoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.145	7.11 ng	88399	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Z-7-Tetradecenoic acid	226	C14H26O2	1000130-98-4	70
2			Z-11-Tetradecenoic acid	226	C14H26O2	1000130-83-3	49
3			E-9-Tetradecenoic acid	226	C14H26O2	1000131-35-8	46
4			Myristoleic acid	226	C14H26O2	000544-64-9	43
5			Ethyl 9-heptadecenoate	296	C19H36O2	1000336-70-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061821\
Data File : BF124383.D
Acq On : 18 Jun 2021 20:10
Operator : JU/CG
Sample : M2759-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

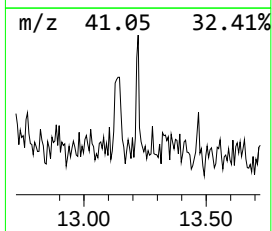
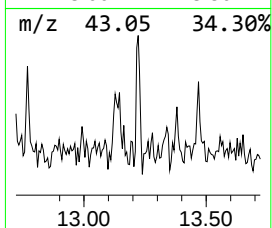
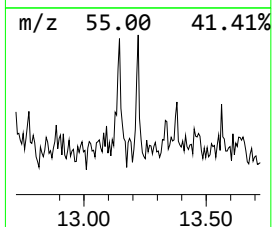
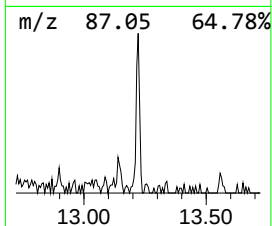
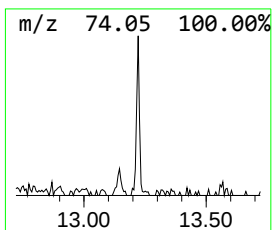
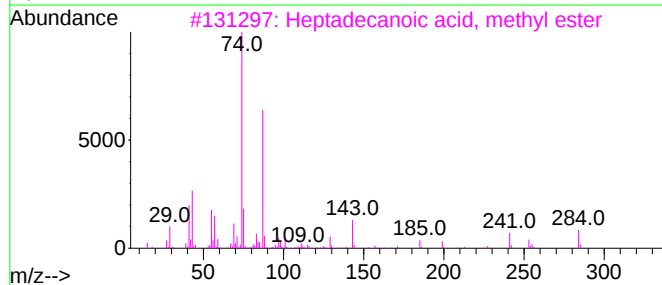
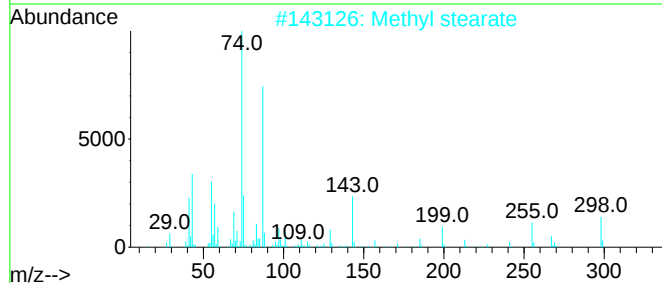
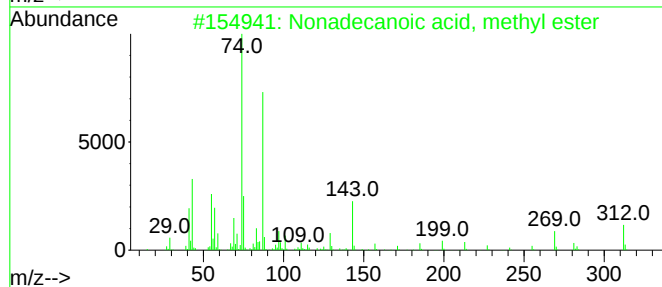
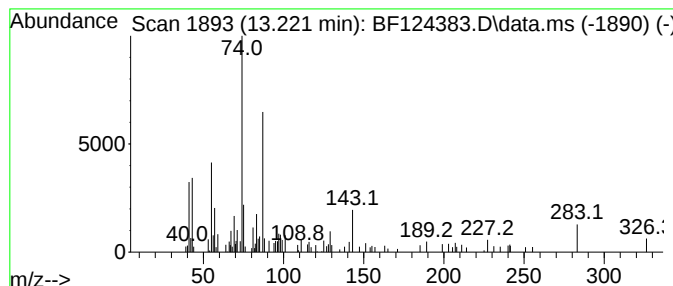
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Nonadecanoic acid, methyl e... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.221	7.13 ng	88698	Chrysene-d12	13.957	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	83
2	Methyl stearate	298	C19H38O2	000112-61-8	83
3	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	80
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	80
5	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061821\
Data File : BF124383.D
Acq On : 18 Jun 2021 20:10
Operator : JU/CG
Sample : M2759-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-05-061721

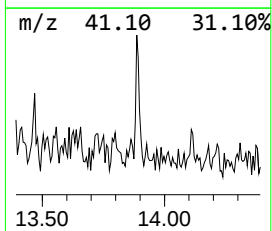
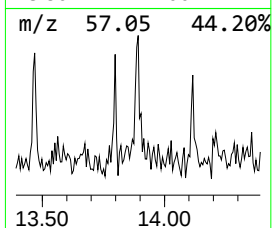
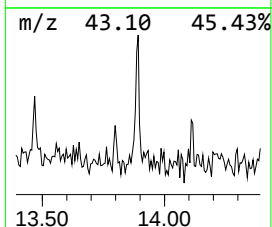
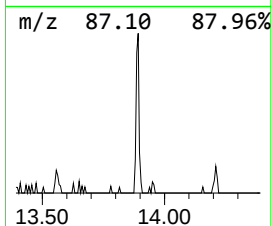
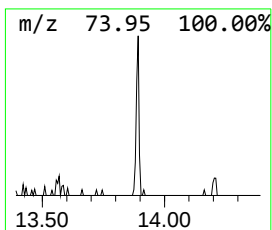
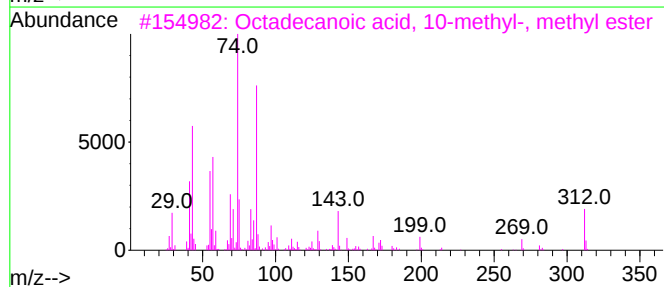
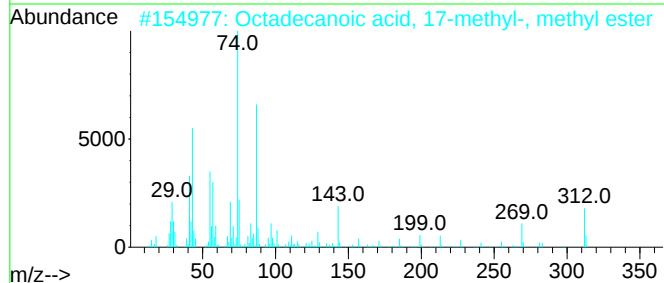
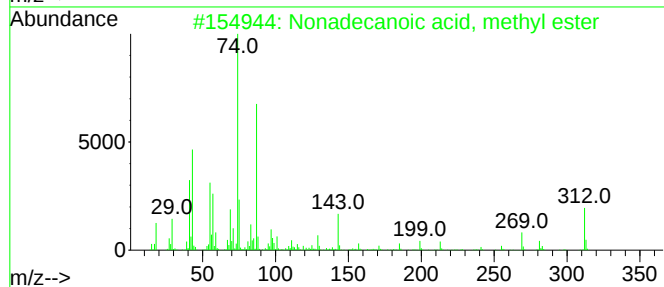
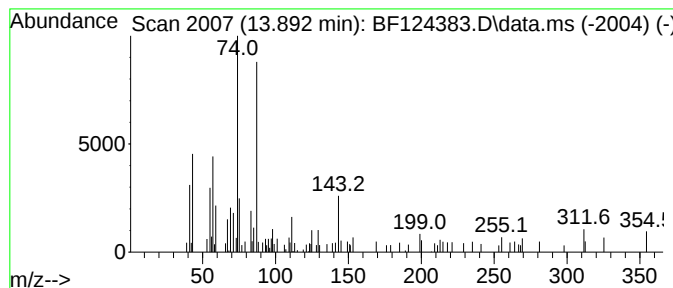
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecanoic acid, 17-methy... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	6.02 ng	74877	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	74
2			Octadecanoic acid, 17-methyl-, m...	312	C20H40O2	055124-97-5	64
3			Octadecanoic acid, 10-methyl-, m...	312	C20H40O2	002490-19-9	64
4			Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	53
5			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061821\
Data File : BF124383.D
Acq On : 18 Jun 2021 20:10
Operator : JU/CG
Sample : M2759-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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
Hexadecanoic ac...	11.704	94.7	ng	1491030	4	11.310	314768	20.0
n-Hexadecanoic ...	11.845	6.4	ng	100455	4	11.310	314768	20.0
9,12-Octadecadi...	12.404	377.3	ng	5937600	4	11.310	314768	20.0
15-Octadecenoic...	12.427	344.4	ng	5419880	4	11.310	314768	20.0
Methyl stearate	12.498	59.8	ng	941612	4	11.310	314768	20.0
9,12-Octadecadi...	12.539	14.2	ng	222791	4	11.310	314768	20.0
cis-13-Octadece...	12.557	20.1	ng	316132	4	11.310	314768	20.0
Z-7-Tetradeceno...	13.145	7.1	ng	88399	5	13.957	248721	20.0
Nonadecanoic ac...	13.221	7.1	ng	88698	5	13.957	248721	20.0
Octadecanoic ac...	13.892	6.0	ng	74877	5	13.957	248721	20.0