

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011023\
 Data File : BF132013.D
 Acq On : 11 Jan 2023 00:11
 Operator : CG\JU
 Sample : 01089-01 5X
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PL-1-010923

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-BF010923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132013.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.393	559	562	575	rBV	310268	306163	1.97%	0.848%
2	6.428	734	738	749	rBV	300770	310276	2.00%	0.859%
3	6.781	795	798	802	rBV	490775	383216	2.47%	1.061%
4	7.351	891	895	898	rBV	220920	186134	1.20%	0.515%
5	8.075	1014	1018	1021	rVB	493572	429945	2.77%	1.190%
6	9.151	1197	1201	1204	rVB	419356	310906	2.00%	0.861%
7	9.833	1313	1317	1320	rBV	566261	441271	2.84%	1.222%
8	10.628	1449	1452	1455	rVB	183737	164556	1.06%	0.456%
9	11.328	1567	1571	1573	rBV	530506	468399	3.01%	1.297%
10	11.727	1634	1639	1642	rBV	4970872	4385480	28.21%	12.140%
11	12.433	1751	1759	1760	rBV	9817181	15545925	100.00%	43.035%
12	12.451	1760	1762	1767	rVV	8772433	9289899	59.76%	25.717%
13	12.522	1770	1774	1777	rVB	2404998	2005318	12.90%	5.551%
14	12.922	1838	1842	1845	rBV	371326	310253	2.00%	0.859%
15	13.116	1867	1875	1878	rBV3	111825	223799	1.44%	0.620%
16	13.163	1878	1883	1891	rVB3	175553	268642	1.73%	0.744%
17	13.239	1893	1896	1899	rBV	216620	206642	1.33%	0.572%
18	13.910	2007	2010	2013	rBV	190283	176064	1.13%	0.487%
19	13.980	2018	2022	2025	rVV	446105	384336	2.47%	1.064%
20	15.445	2268	2271	2278	rVB	257205	326318	2.10%	0.903%

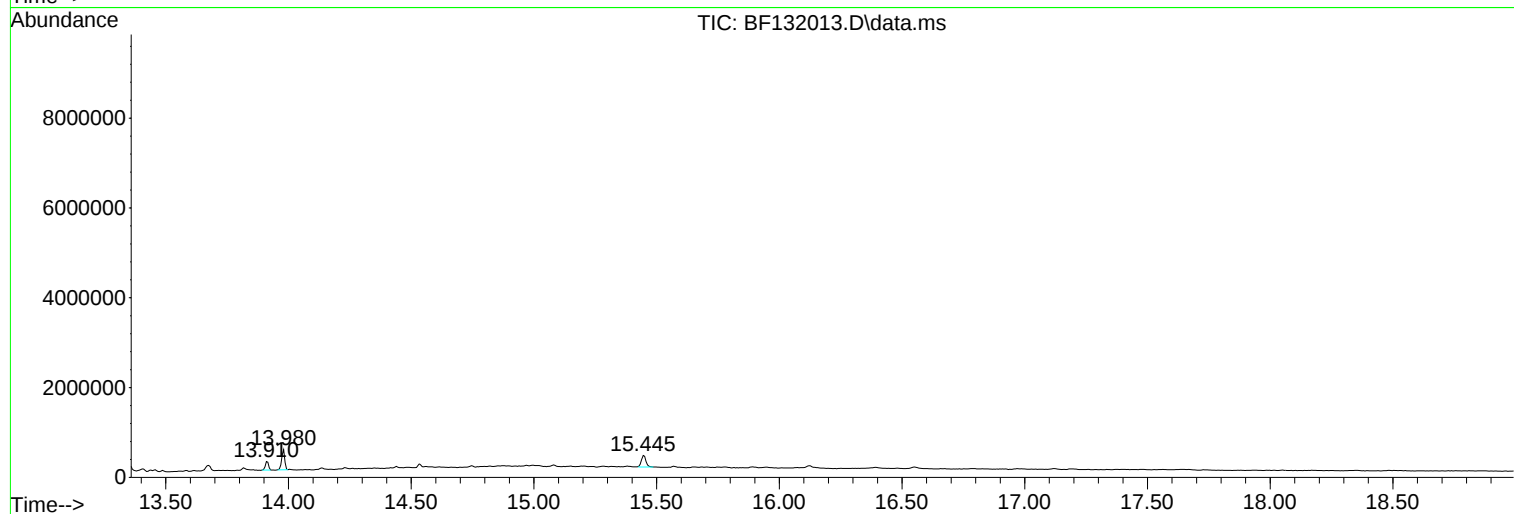
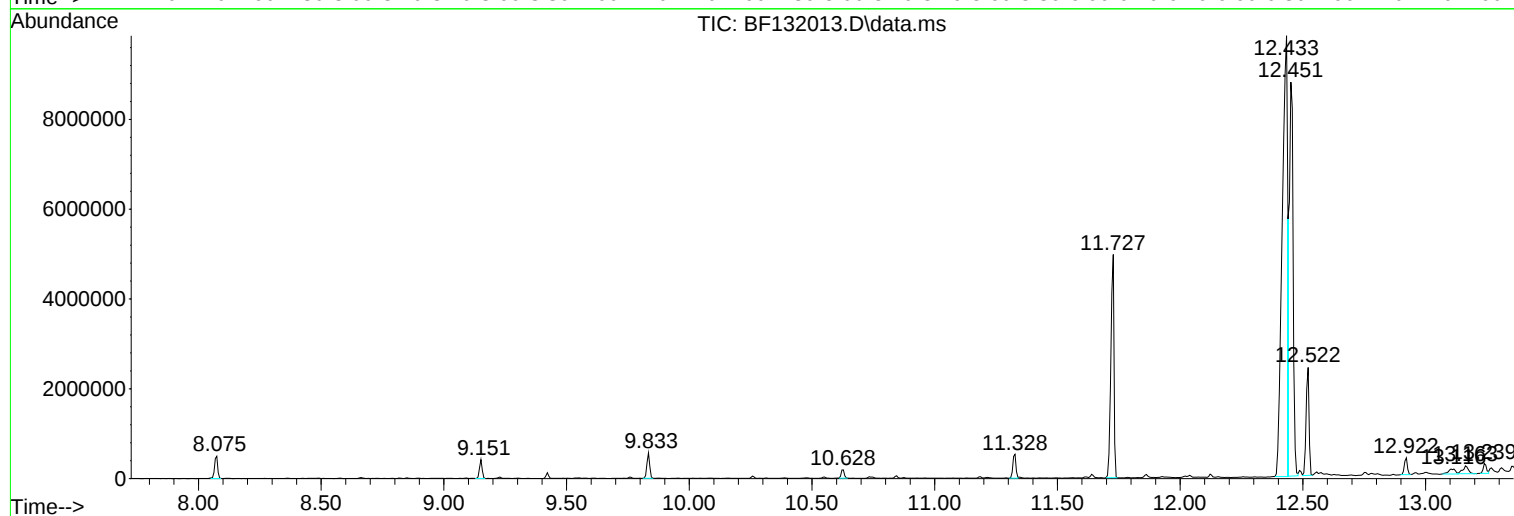
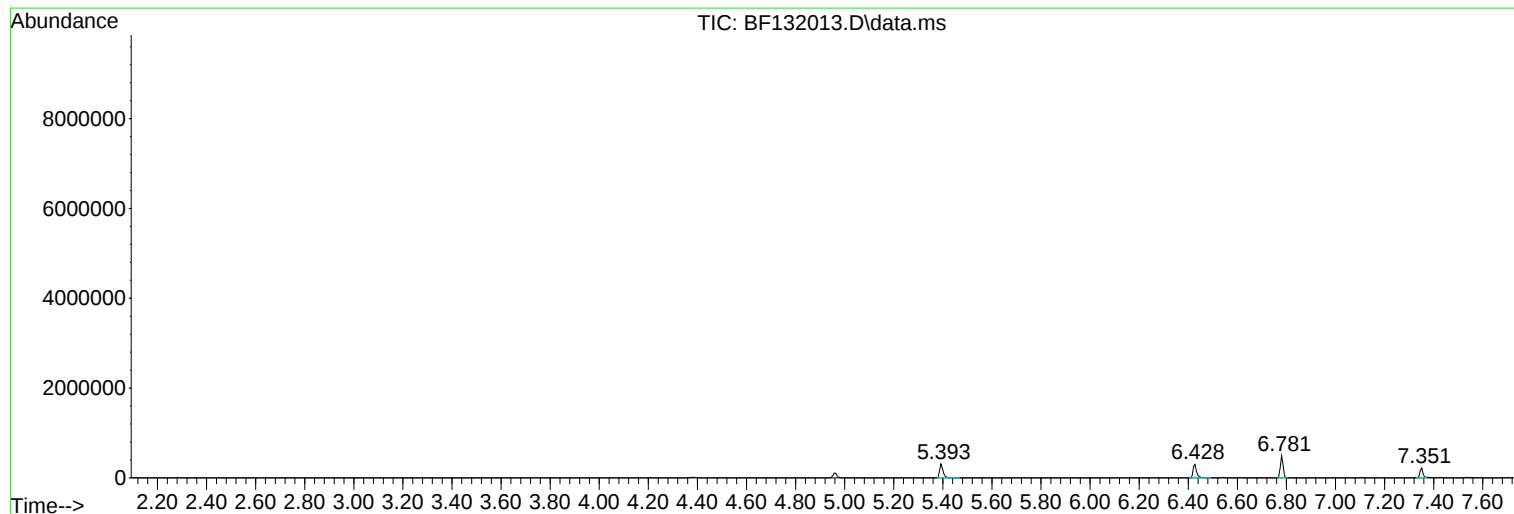
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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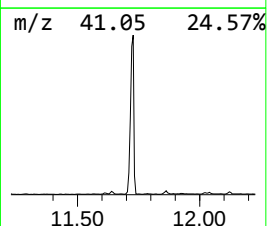
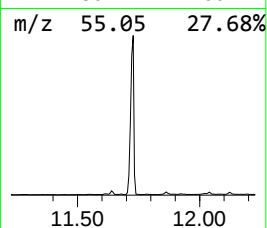
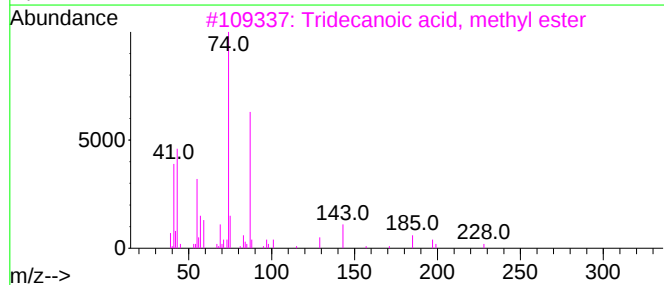
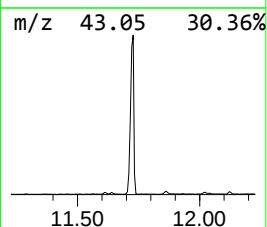
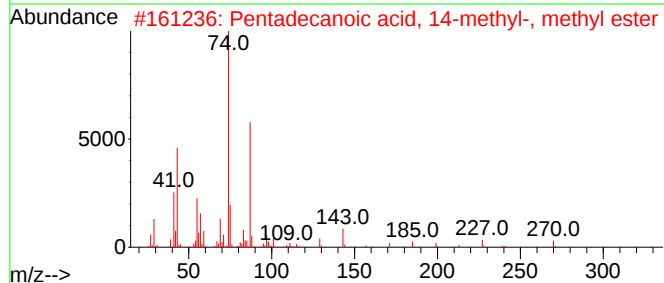
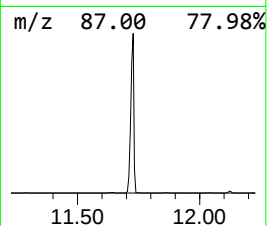
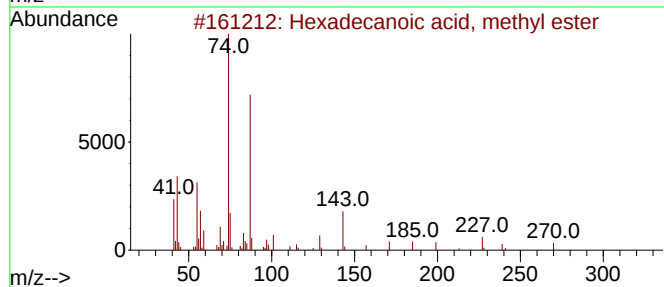
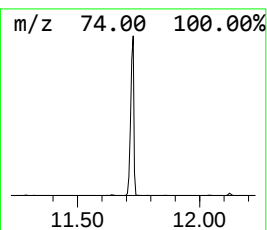
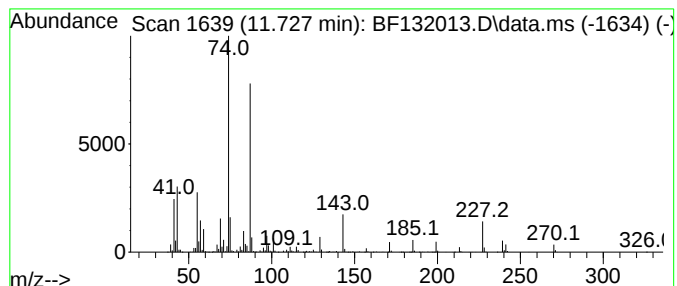
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.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.
11.727	187.25 ng	4385480	Phenanthrene-d10	11.328

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	91
3			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
4			Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	81
5			Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	80



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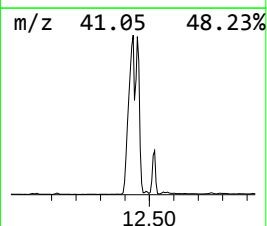
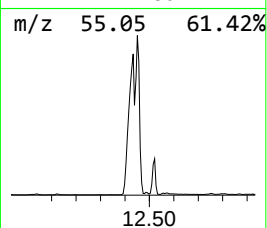
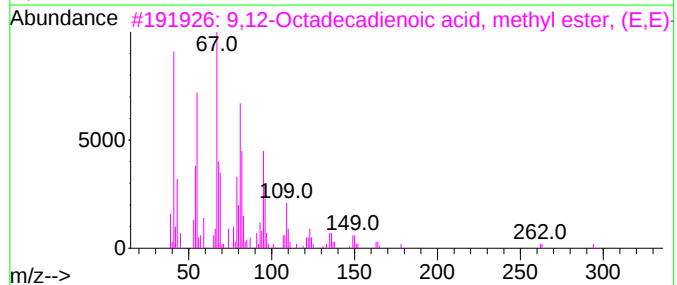
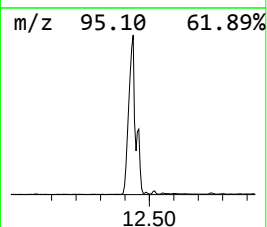
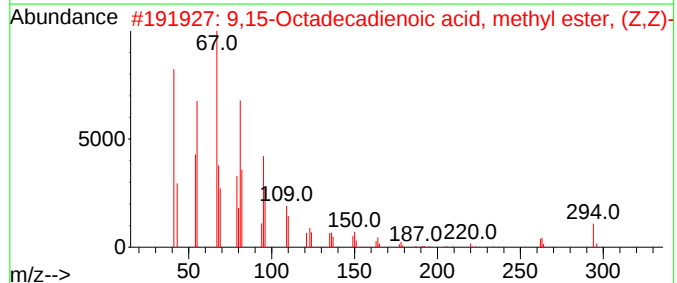
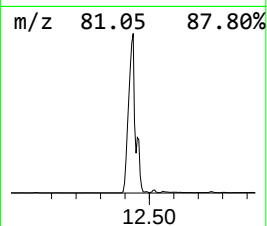
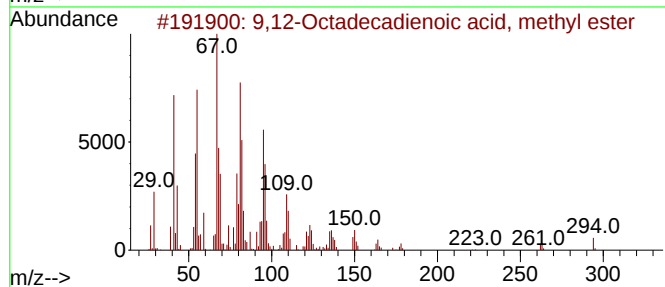
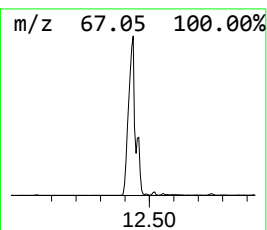
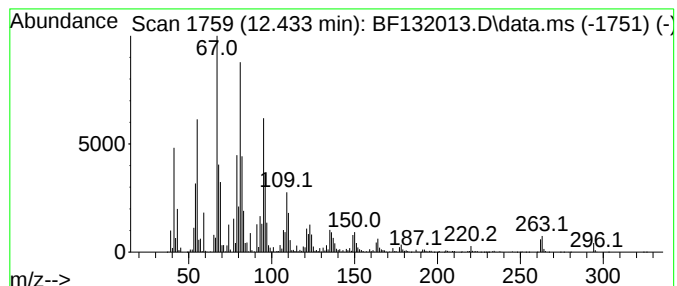
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Peak Number 2 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.433	663.79 ng	15545900	Phenanthrene-d10	11.328

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
2			9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
3			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	98
4			Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	98
5			9,11-Octadecadienoic acid, methy...	294	C19H34O2	013038-47-6	97



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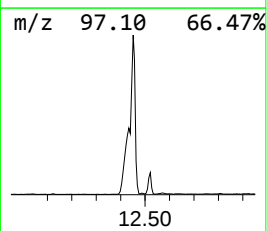
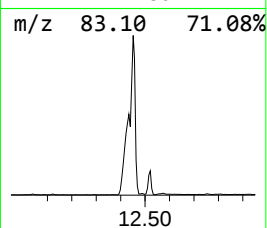
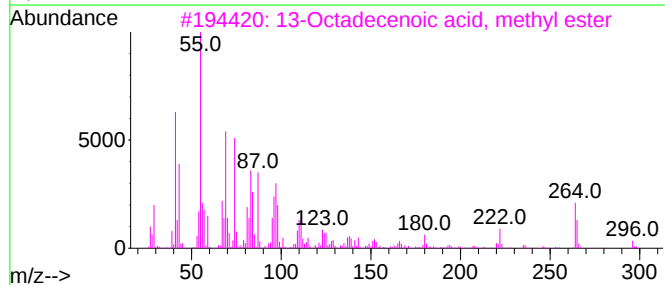
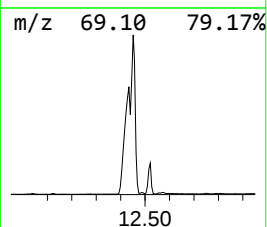
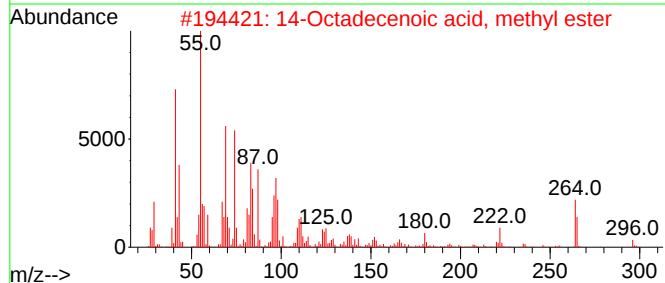
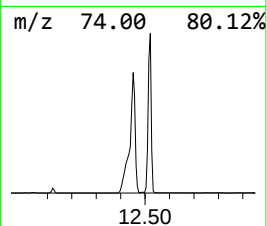
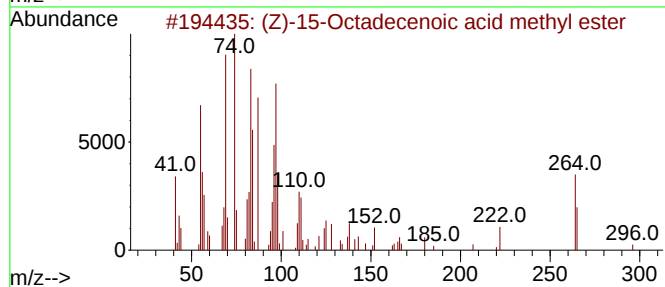
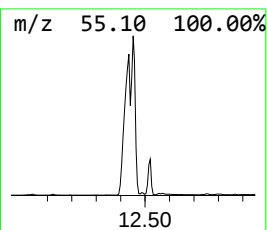
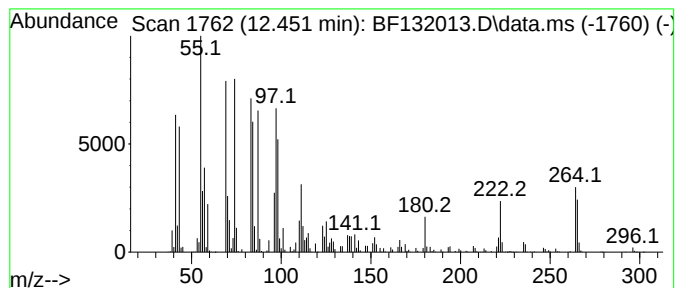
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 (Z)-15-Octadecenoic acid me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.451	396.67 ng	9289900	Phenanthrene-d10	11.328	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(Z)-15-Octadecenoic acid methyl ...	296	C19H36O2	1000427-69-3	94
2	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	90
3	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	90
4	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	90
5	cis-13-Octadecenoic acid, methyl...	296	C19H36O2	1010333-58-3	74



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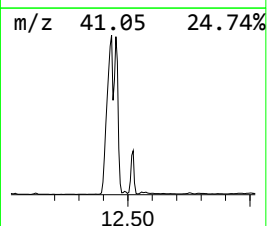
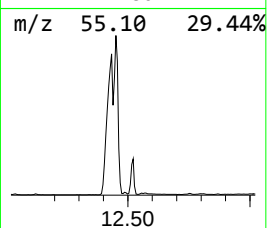
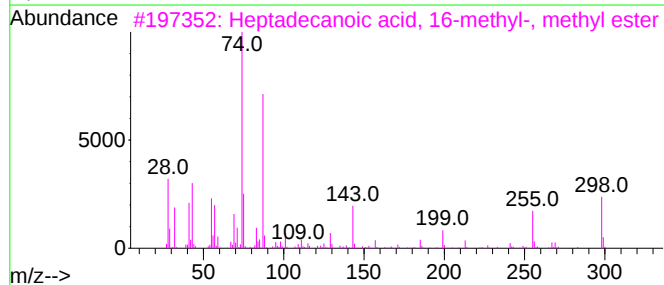
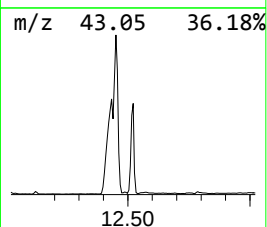
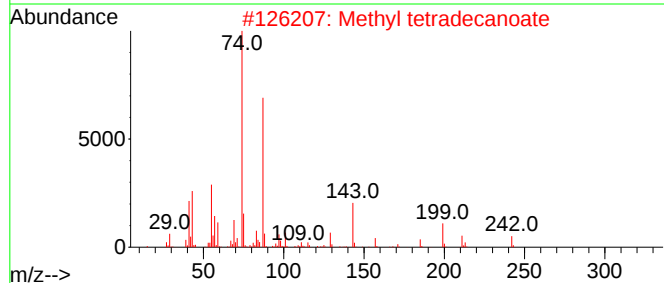
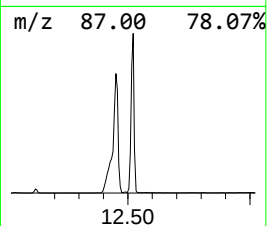
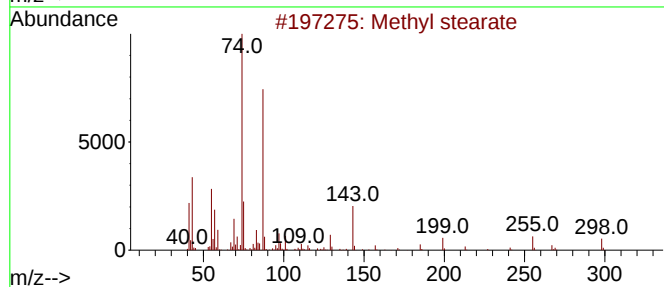
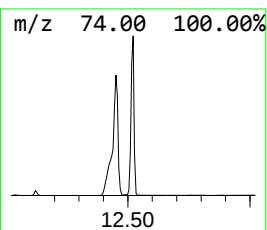
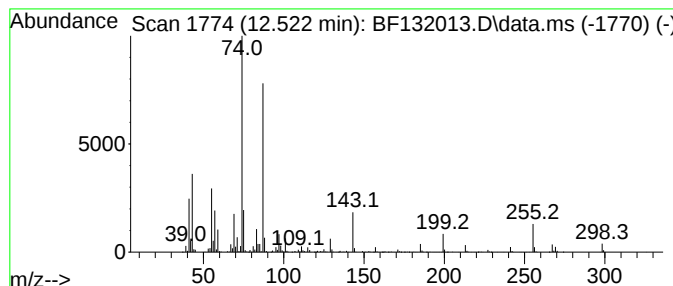
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Peak Number 4 Methyl stearate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.522	85.62 ng	2005320	Phenanthrene-d10	11.328

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	98
2			Methyl tetradecanoate	242	C15H30O2	000124-10-7	90
3			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	89
4			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	86
5			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	83



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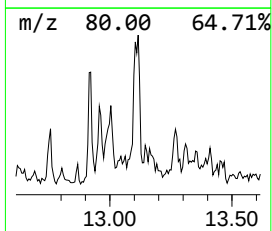
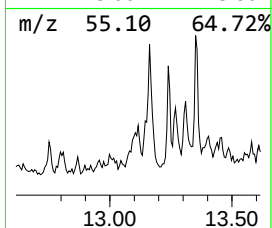
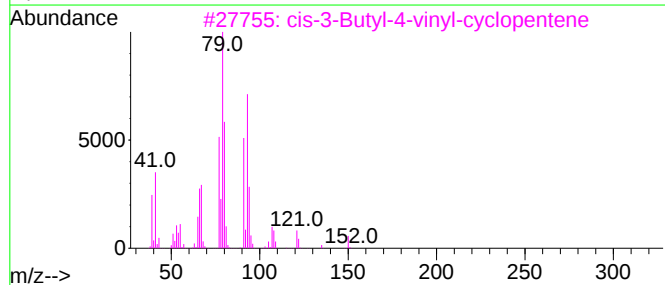
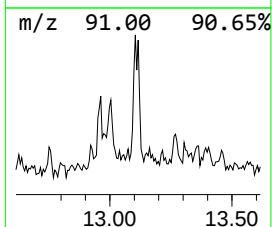
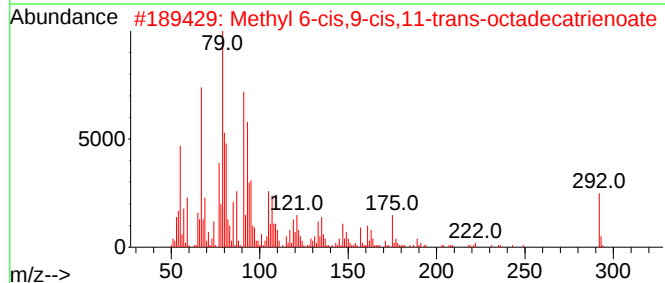
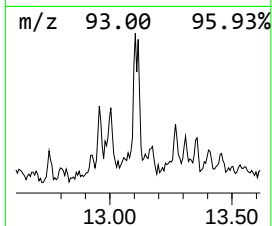
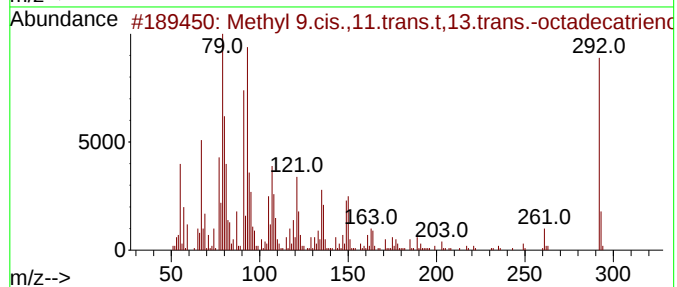
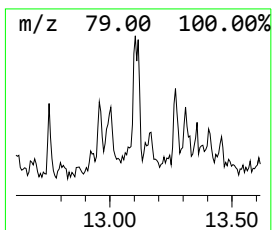
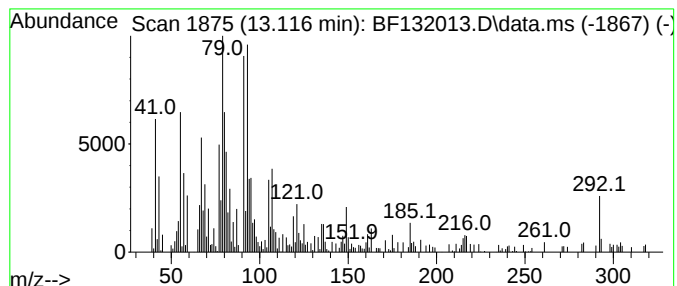
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Peak Number 5 Methyl 9.cis.,11.trans.t,13... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.116	11.65 ng	223799	Chrysene-d12	13.980	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 9.cis.,11.trans.t,13.tran...	292	C19H32O2	1000336-42-6	86
2	Methyl 6-cis,9-cis,11-trans-octa...	292	C19H32O2	1010336-37-7	70
3	cis-3-Butyl-4-vinyl-cyclopentene	150	C11H18	093779-52-3	55
4	9,12,15-Octadecatrienoic acid, m...	292	C19H32O2	000301-00-8	49
5	Tricyclo[4.2.1.0(2,5)]nonane	122	C9H14	1000195-06-2	49



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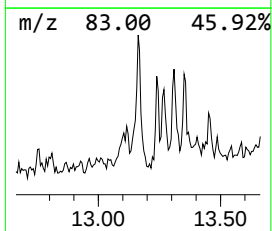
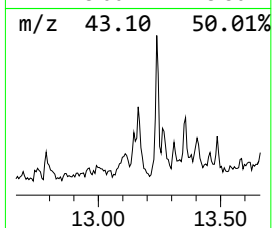
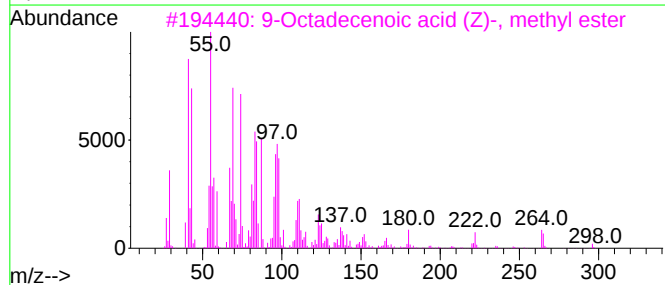
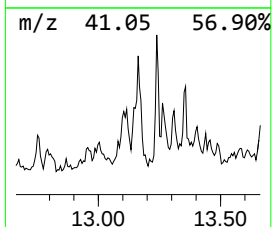
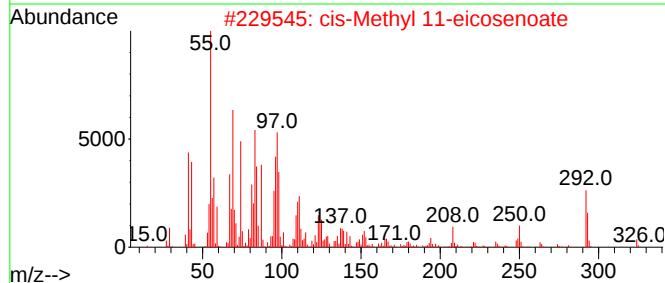
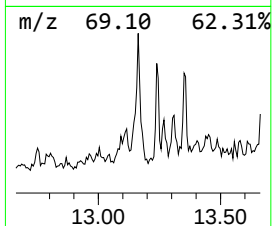
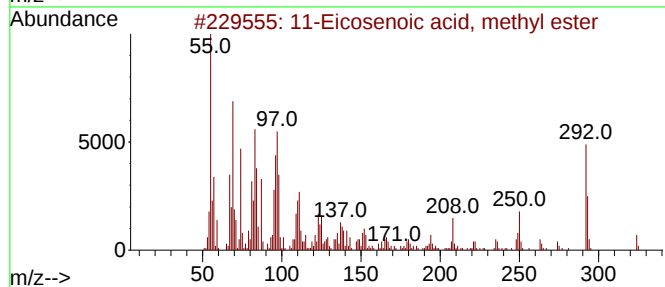
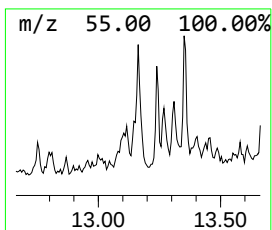
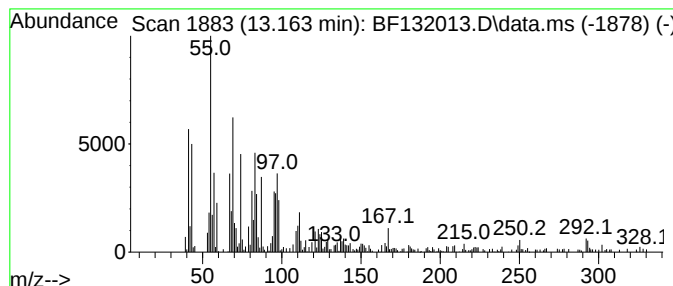
Instrument :
BNA_F
ClientSampleId :
PL-1-010923

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 11-Eicosenoic acid, methyl ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.163	13.98 ng	268642	Chrysene-d12	13.980	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Eicosenoic acid, methyl ester	324	C21H40O2	003946-08-5	95
2	cis-Methyl 11-eicosenoate	324	C21H40O2	002390-09-2	94
3	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	94
4	cis-13-Eicosenoic acid, methyl e...	324	C21H40O2	069120-02-1	93
5	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011023\
Data File : BF132013.D
Acq On : 11 Jan 2023 00:11
Operator : CG\JU
Sample : 01089-01 5X
Misc :
ALS Vial : 19 Sample Multiplier: 1

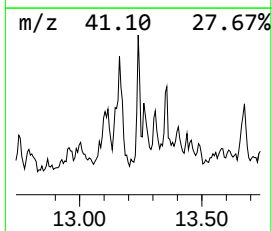
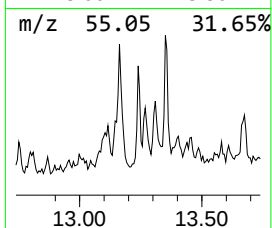
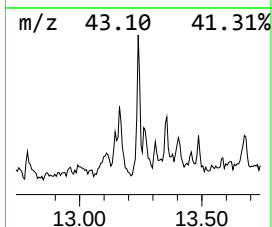
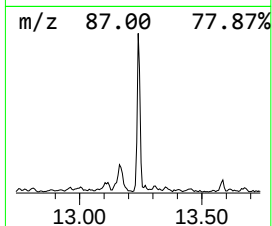
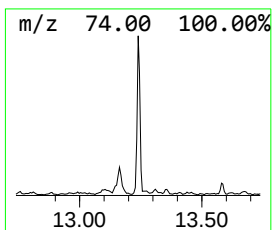
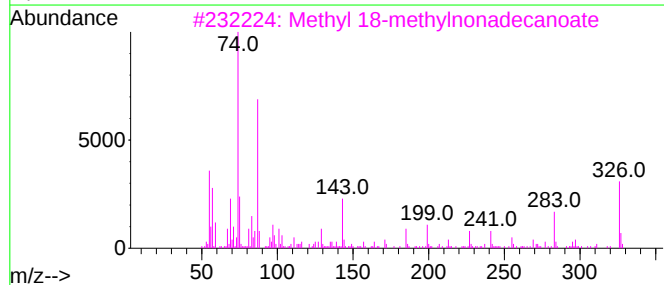
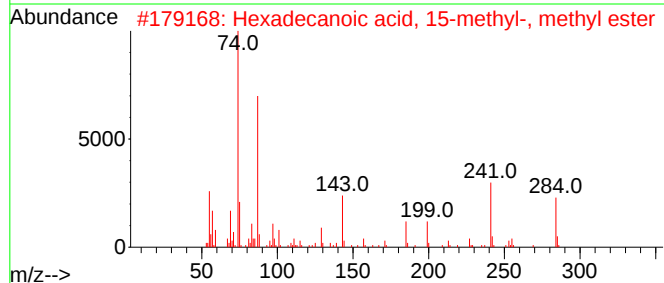
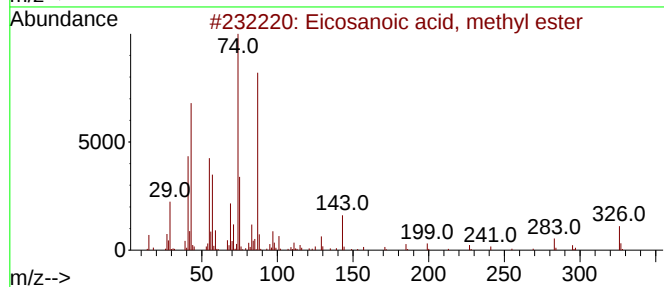
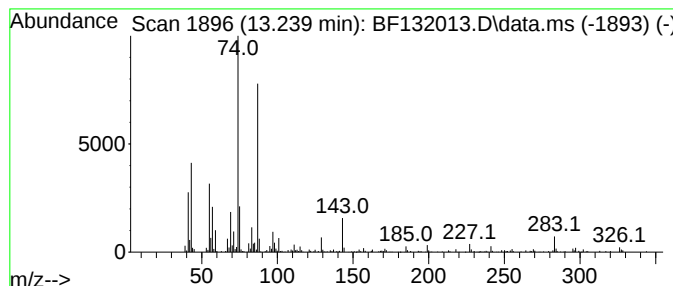
Instrument :
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ClientSampleId :
PL-1-010923

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosanoic acid, methyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.239	10.75 ng	206642	Chrysene-d12	13.980	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	96
2	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	93
3	Methyl 18-methylnonadecanoate	326	C21H42O2	1000424-52-4	91
4	Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	91
5	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011023\
Data File : BF132013.D
Acq On : 11 Jan 2023 00:11
Operator : CG\JU
Sample : 01089-01 5X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PL-1-010923

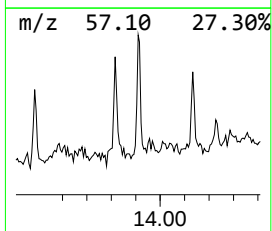
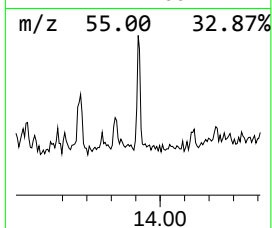
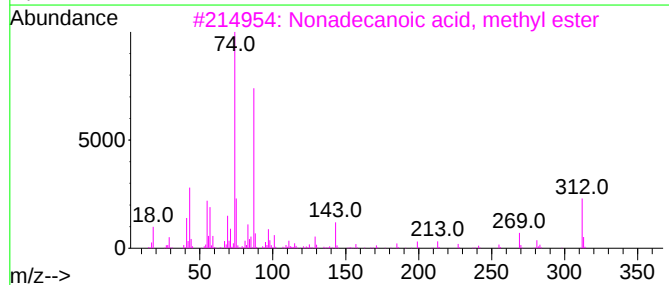
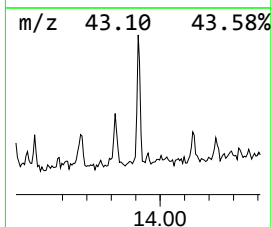
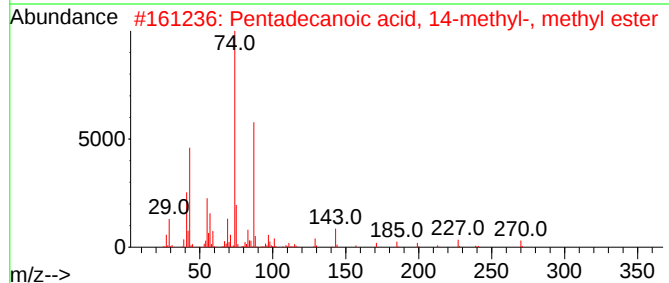
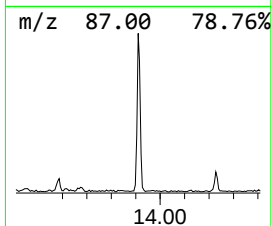
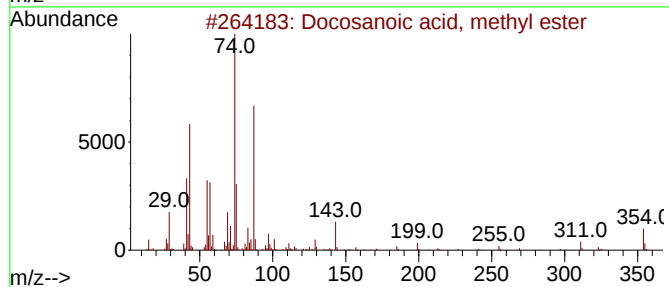
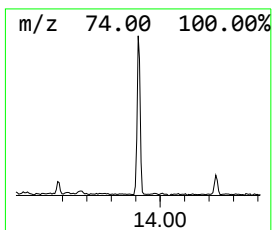
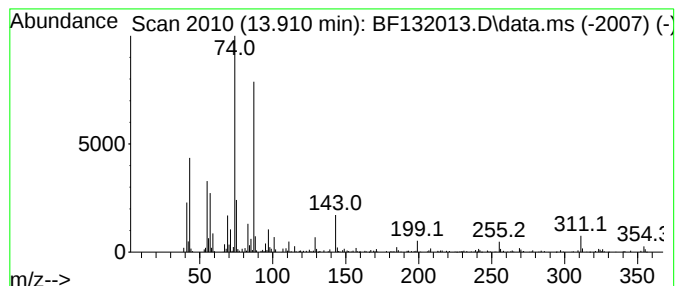
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Docosanoic acid, methyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	9.16 ng	176064	Chrysene-d12	13.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosanoic acid, methyl ester	354	C23H46O2	000929-77-1	98
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	93
3			Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	93
4			Methyl 20-methyl-heneicosanoate	354	C23H46O2	1000336-47-4	91
5			Octadecanoic acid, 10-methyl-, m...	312	C20H40O2	002490-19-9	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011023\
Data File : BF132013.D
Acq On : 11 Jan 2023 00:11
Operator : CG\JU
Sample : 01089-01 5X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PL-1-010923

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.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...	11.727	187.3	ng	4385480	4	11.328	468399	20.0
9,12-Octadecadi...	12.433	663.8	ng	15545900	4	11.328	468399	20.0
(Z)-15-Octadece...	12.451	396.7	ng	9289900	4	11.328	468399	20.0
Methyl stearate	12.522	85.6	ng	2005320	4	11.328	468399	20.0
Methyl 9.cis.,1...	13.116	11.7	ng	223799	5	13.980	384336	20.0
11-Eicosenoic a...	13.163	14.0	ng	268642	5	13.980	384336	20.0
Eicosanoic acid...	13.239	10.8	ng	206642	5	13.980	384336	20.0
Docosanoic acid...	13.910	9.2	ng	176064	5	13.980	384336	20.0