

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011023\
 Data File : BF132011.D
 Acq On : 10 Jan 2023 23:08
 Operator : CG\JU
 Sample : 01089-03 2X
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PL-2-010923

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: BF132011.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	573	rBV	766205	745670	1.93%	1.217%
2	6.428	734	738	752	rBV	763117	748354	1.94%	1.221%
3	7.351	891	895	898	rBV	571418	447236	1.16%	0.730%
4	8.075	1014	1018	1021	rBV	490328	408344	1.06%	0.666%
5	9.151	1197	1201	1204	rVB	931513	689485	1.78%	1.125%
6	9.833	1313	1317	1320	rVB	538753	410888	1.06%	0.671%
7	11.327	1567	1571	1573	rBV	463533	427640	1.11%	0.698%
8	11.727	1634	1639	1642	rBV	6080246	5972747	15.45%	9.748%
9	11.880	1658	1665	1668	rBV2	500512	571318	1.48%	0.932%
10	12.457	1751	1763	1765	rBV2	12650491	38650322	100.00%	63.082%
11	12.533	1772	1776	1780	rBV2	4654474	4168632	10.79%	6.804%
12	12.598	1780	1787	1796	rVB3	2071234	5107547	13.21%	8.336%
13	12.927	1840	1843	1846	rVB	844005	628120	1.63%	1.025%
14	13.163	1881	1883	1889	rVB2	317969	387931	1.00%	0.633%
15	13.245	1894	1897	1899	rBV	488685	427952	1.11%	0.698%
16	13.916	2007	2011	2016	rVV	505598	476777	1.23%	0.778%
17	13.980	2018	2022	2025	rVV2	475508	559033	1.45%	0.912%
18	15.451	2268	2272	2283	rVB3	265738	442087	1.14%	0.722%

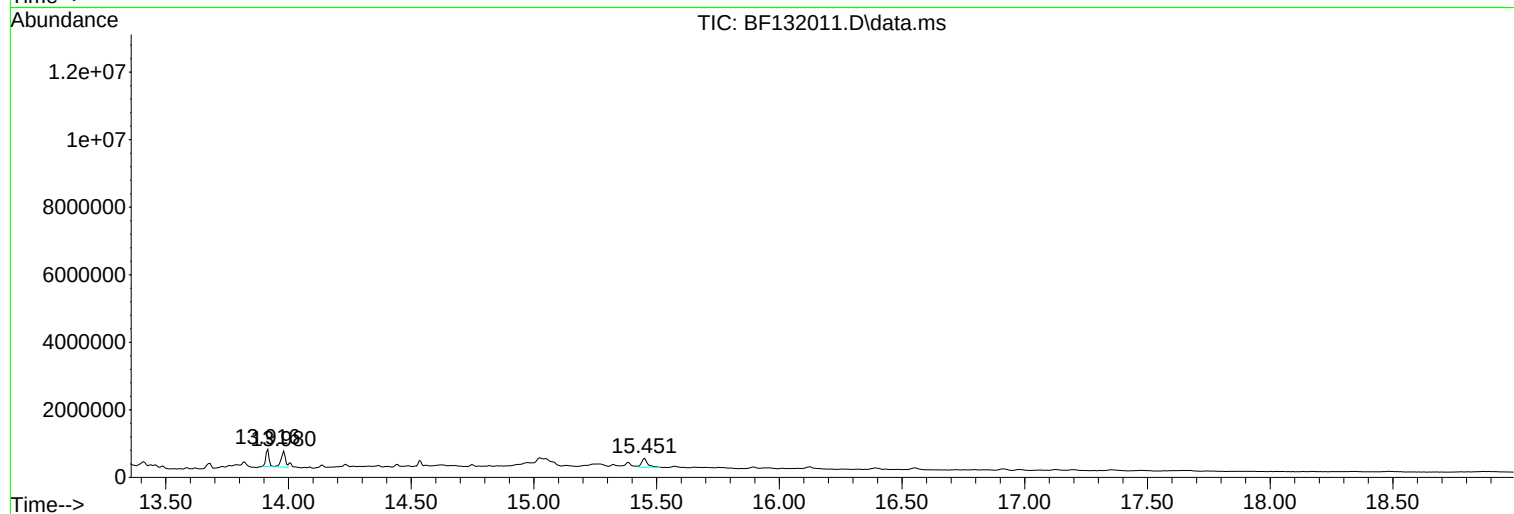
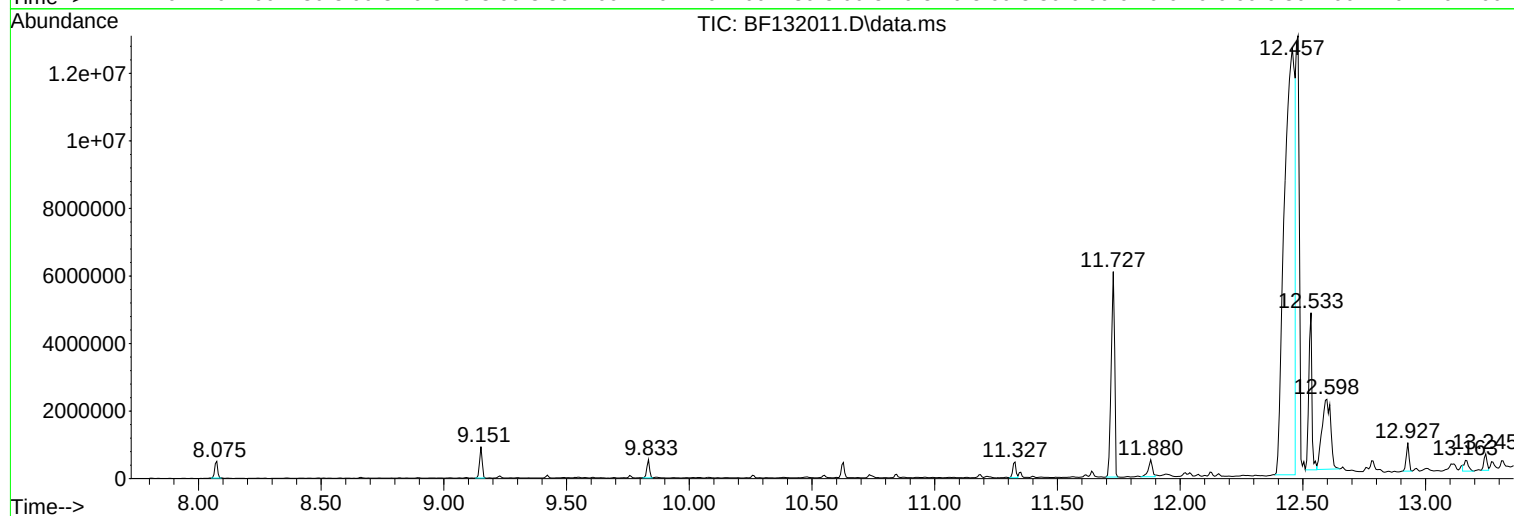
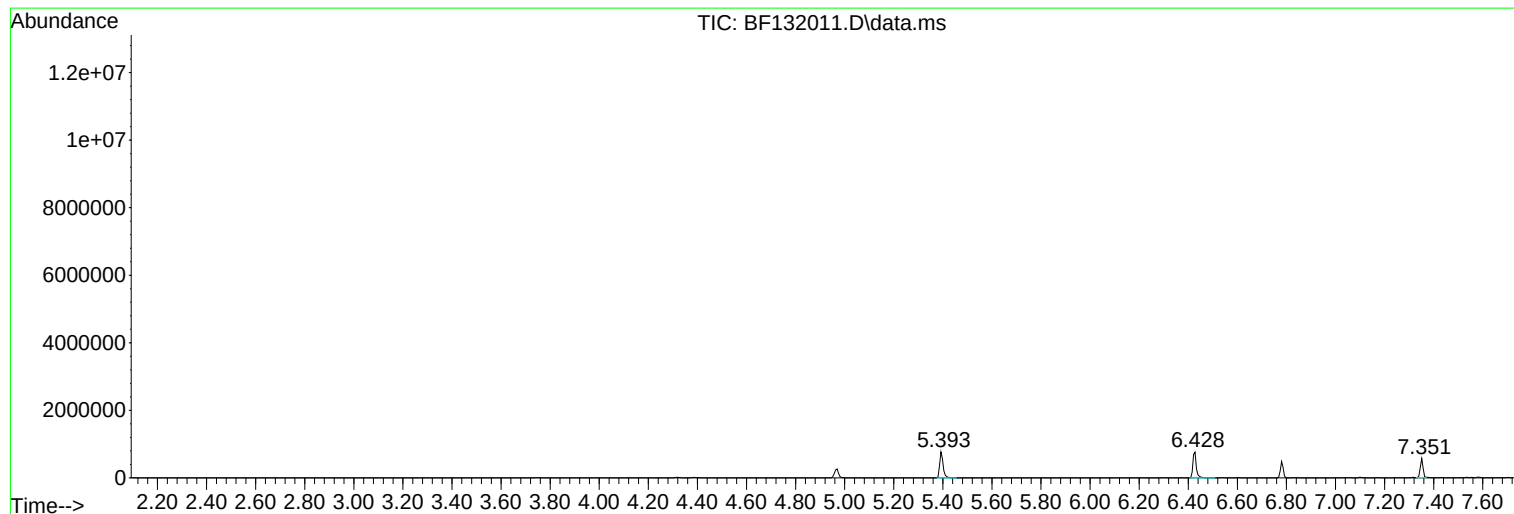
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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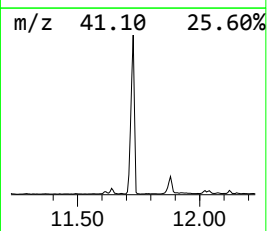
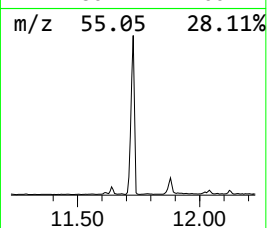
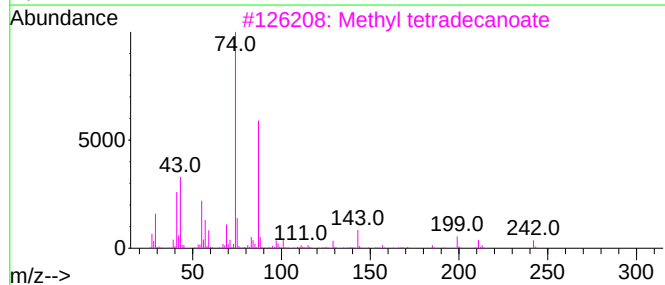
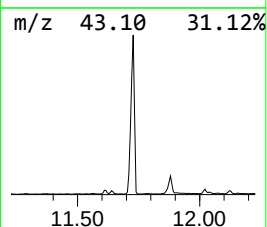
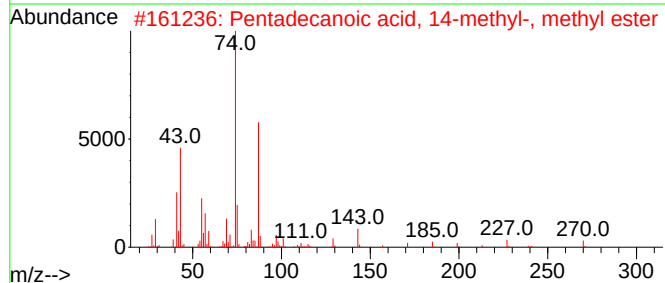
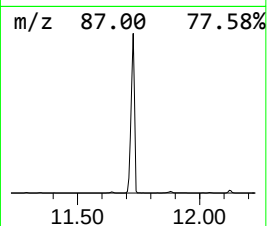
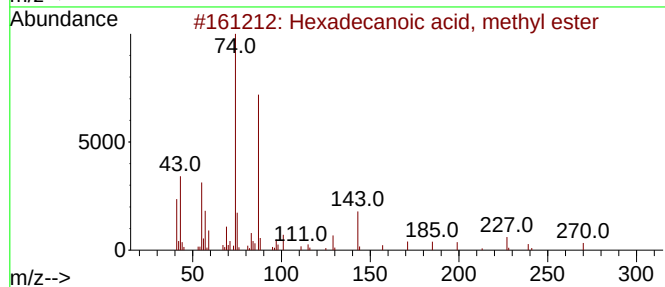
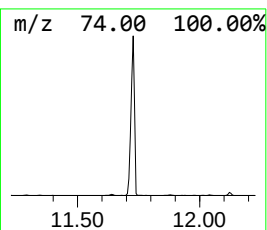
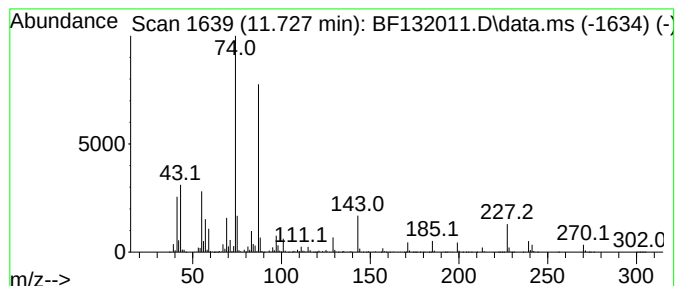
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.727	279.33 ng	5972750	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			Methyl tetradecanoate	242	C15H30O2	000124-10-7	83
4			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	81
5			Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	81



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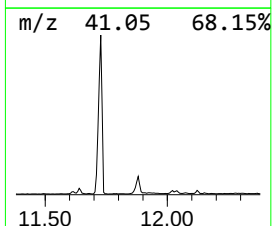
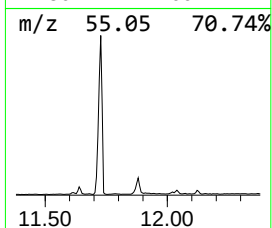
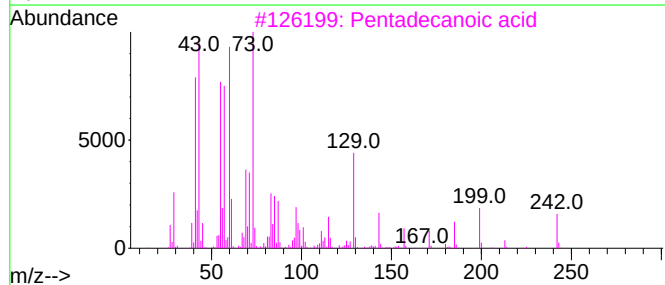
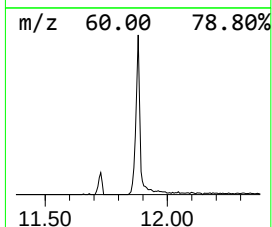
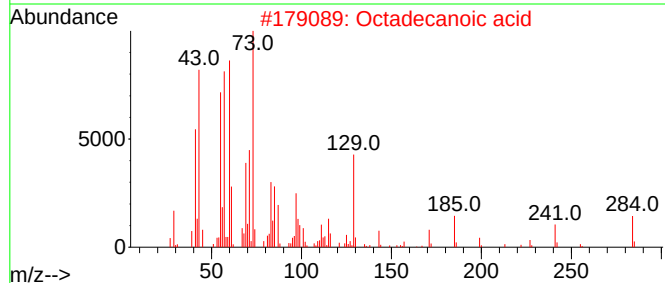
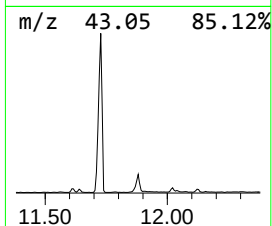
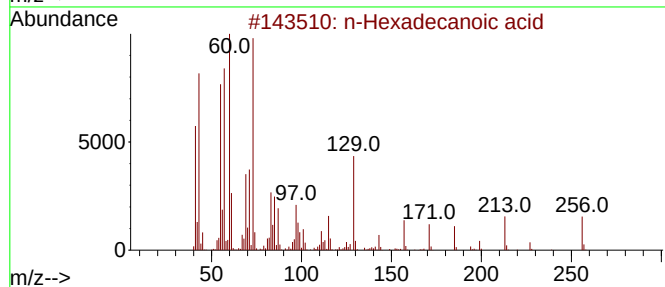
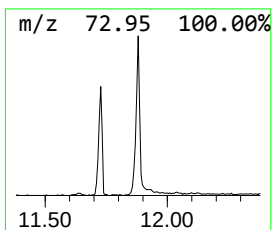
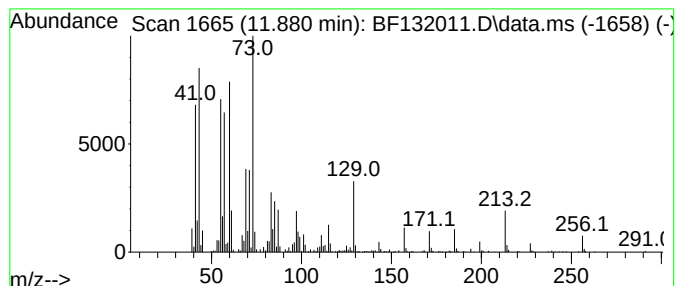
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.880	26.72 ng	571318	Phenanthrene-d10	11.328

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Octadecanoic acid	284	C18H36O2	000057-11-4	87
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tridecanoic acid	214	C13H26O2	000638-53-9	81
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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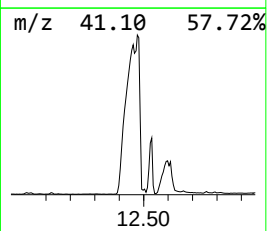
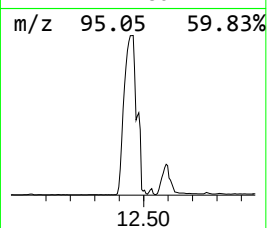
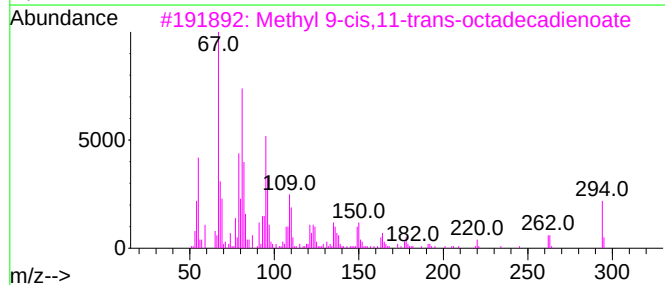
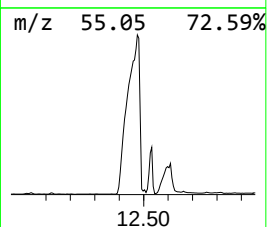
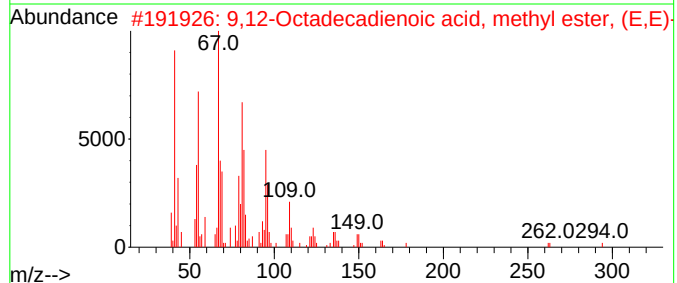
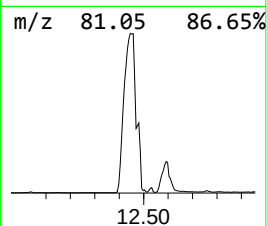
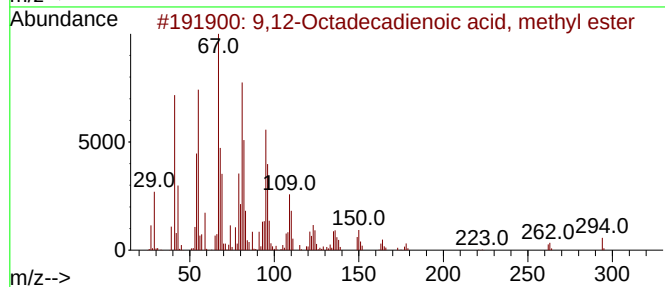
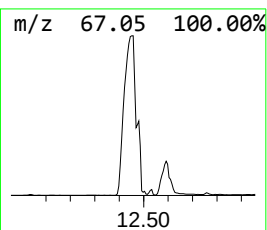
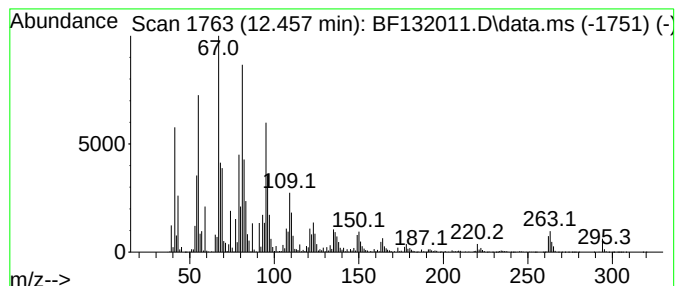
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Peak Number 3 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.457	1807.61 ng	38650300	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		9,12-Octadecadienoic acid, methy...	294 C19H34O2	002566-97-4 99
3		Methyl 9-cis,11-trans-octadecadi...	294 C19H34O2	013058-52-1 99
4		Linoleic acid	280 C18H32O2	000506-21-8 98
5		9,15-Octadecadienoic acid, methy...	294 C19H34O2	017309-05-6 98



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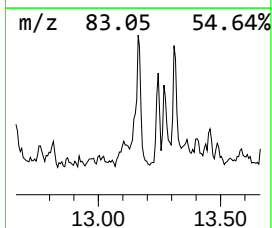
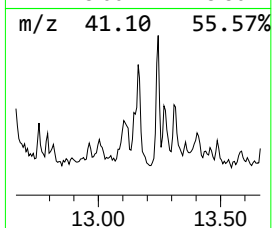
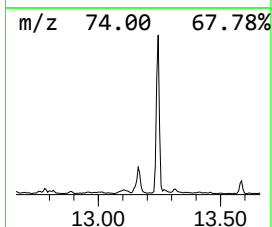
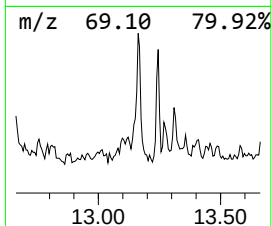
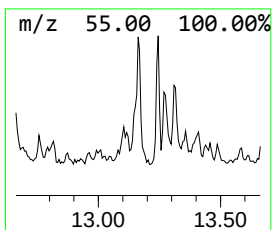
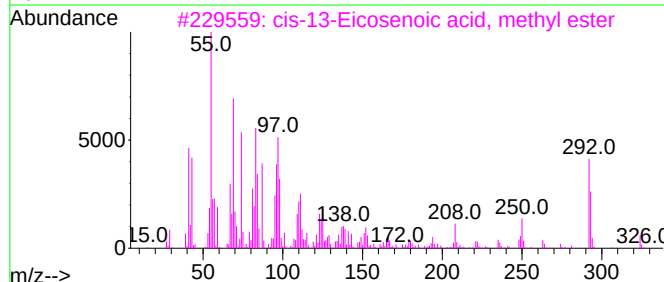
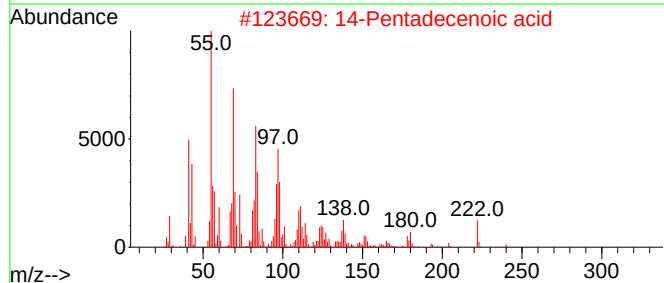
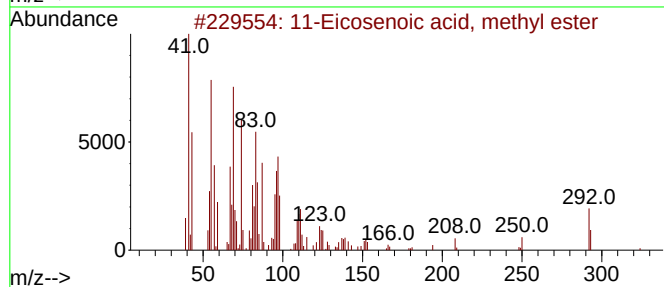
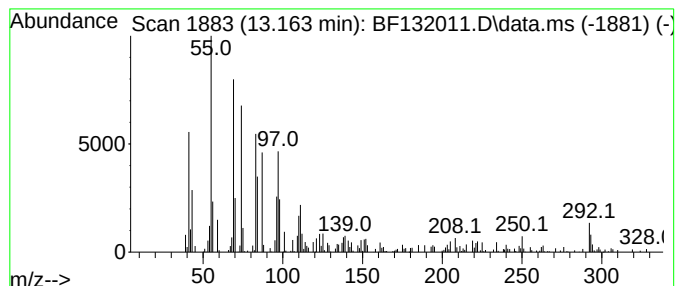
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 11-Eicosenoic acid, methyl ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.163	13.88 ng	387931	Chrysene-d12	13.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11-Eicosenoic acid, methyl ester	324	C21H40O2	003946-08-5	83
2			14-Pentadecenoic acid	240	C15H28O2	017351-34-7	58
3			cis-13-Eicosenoic acid, methyl e...	324	C21H40O2	069120-02-1	58
4			Cyclopropaneoctanoic acid, 2-hex...	282	C18H34O2	010152-61-1	45
5			2-Hexenal	98	C6H10O	000505-57-7	38



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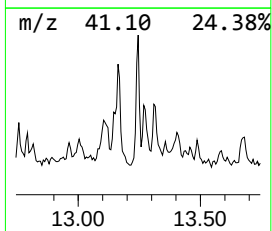
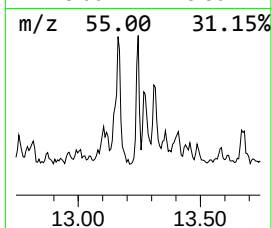
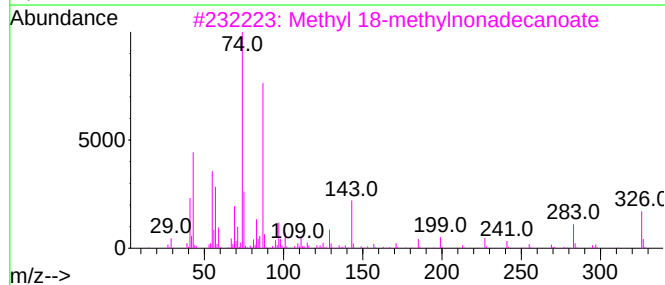
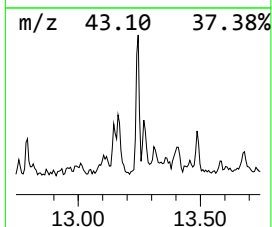
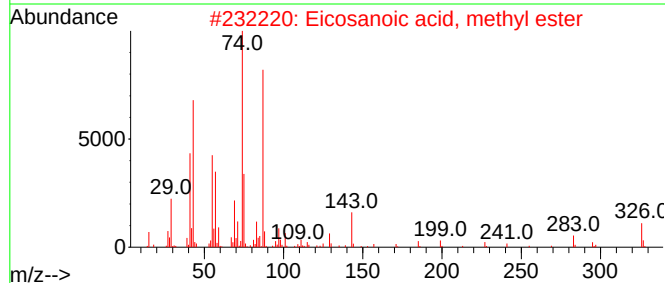
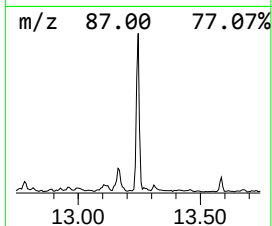
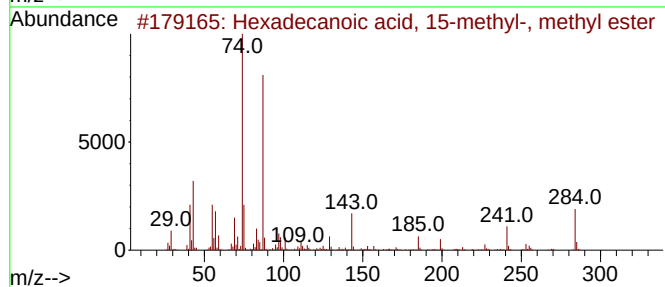
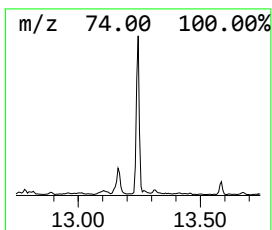
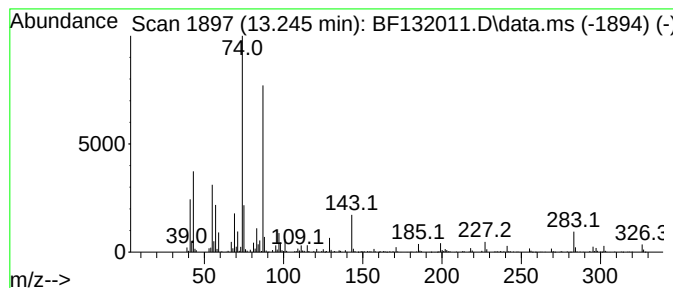
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecanoic acid, 15-methy... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.245	15.31 ng	427952	Chrysene-d12	13.980	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	97
2	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	95
3	Methyl 18-methylnonadecanoate	326	C21H42O2	1000424-52-4	90
4	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	90
5	Methyl stearate	298	C19H38O2	000112-61-8	90



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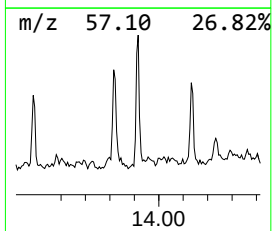
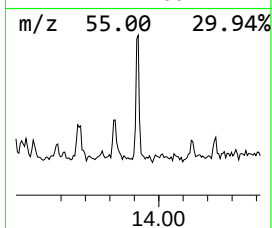
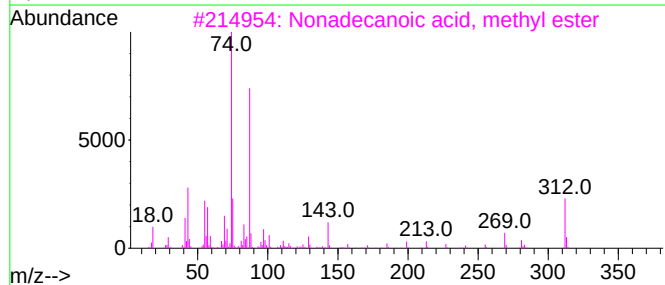
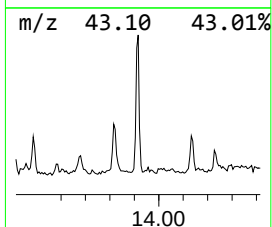
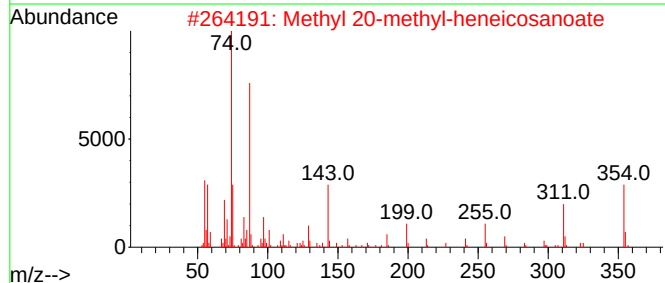
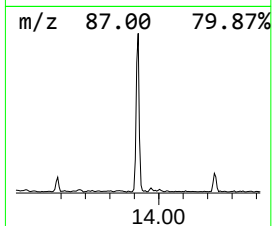
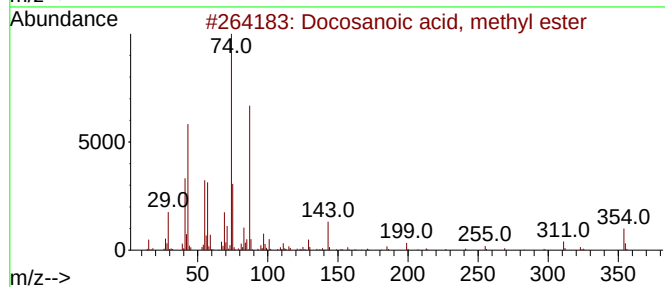
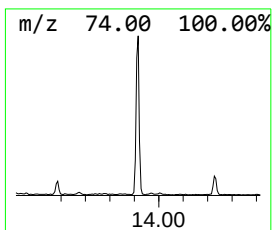
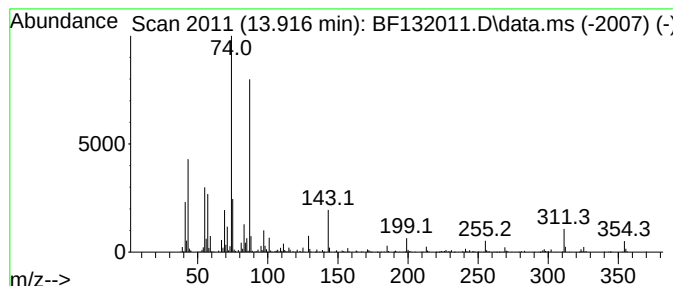
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Docosanoic acid, methyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.916	17.06 ng	476777	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			Methyl 20-methyl-heneicosanoate	354	C23H46O2	1000336-47-4	95
3			Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	91
4			Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	90
5			Methyl stearate	298	C19H38O2	000112-61-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011023\
Data File : BF132011.D
Acq On : 10 Jan 2023 23:08
Operator : CG\JU
Sample : 01089-03 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PL-2-010923

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	279.3	ng	5972750	4	11.328	427640	20.0
n-Hexadecanoic ...	11.880	26.7	ng	571318	4	11.328	427640	20.0
9,12-Octadecadi...	12.457	1807.6	ng	38650300	4	11.328	427640	20.0
11-Eicosenoic a...	13.163	13.9	ng	387931	5	13.980	559033	20.0
Hexadecanoic ac...	13.245	15.3	ng	427952	5	13.980	559033	20.0
Docosanoic acid...	13.916	17.1	ng	476777	5	13.980	559033	20.0