

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042522\
 Data File : BF127901.D
 Acq On : 26 Apr 2022 01:05
 Operator : CG\JU
 Sample : N2523-01
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SU-01-042122

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127901.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.563	552	557	560	rBV	3428718	3335429	7.55%	3.466%
2	6.563	722	727	730	rBV	3092827	3398317	7.70%	3.531%
3	6.939	788	791	795	rBV	1220472	980068	2.22%	1.018%
4	7.504	883	887	890	rBV	2369809	2208620	5.00%	2.295%
5	8.222	1006	1009	1012	rBV	1261937	1115620	2.53%	1.159%
6	9.298	1188	1192	1195	rBV	3726326	3315740	7.51%	3.445%
7	9.980	1305	1308	1312	rVB	1330483	1096515	2.48%	1.139%
8	10.774	1439	1443	1446	rBV	1813290	1652164	3.74%	1.717%
9	11.474	1558	1562	1565	rBV	1175465	989368	2.24%	1.028%
10	11.874	1623	1630	1633	rBV	11273588	14930607	33.81%	15.514%
11	12.010	1647	1653	1660	rBV	1213637	1479542	3.35%	1.537%
12	12.604	1740	1754	1755	rBV4	11581574	44155499	100.00%	45.880%
13	12.668	1762	1765	1768	rVB	8081690	7606203	17.23%	7.903%
14	12.704	1768	1771	1773	rBV	1892444	1849713	4.19%	1.922%
15	12.892	1800	1803	1807	rVB3	447833	457214	1.04%	0.475%
16	13.074	1830	1834	1836	rBV	2698106	2338308	5.30%	2.430%
17	13.251	1860	1864	1867	rVB4	366494	569160	1.29%	0.591%
18	13.304	1871	1873	1878	rVB2	649458	618958	1.40%	0.643%
19	13.380	1883	1886	1891	rVB	1060237	1033059	2.34%	1.073%
20	13.492	1902	1905	1910	rBV4	359396	451726	1.02%	0.469%
21	14.051	1997	2000	2008	rBV	1080113	1207531	2.73%	1.255%
22	14.127	2010	2013	2018	rVB	795586	763500	1.73%	0.793%
23	15.651	2269	2272	2280	rVB	496324	688942	1.56%	0.716%

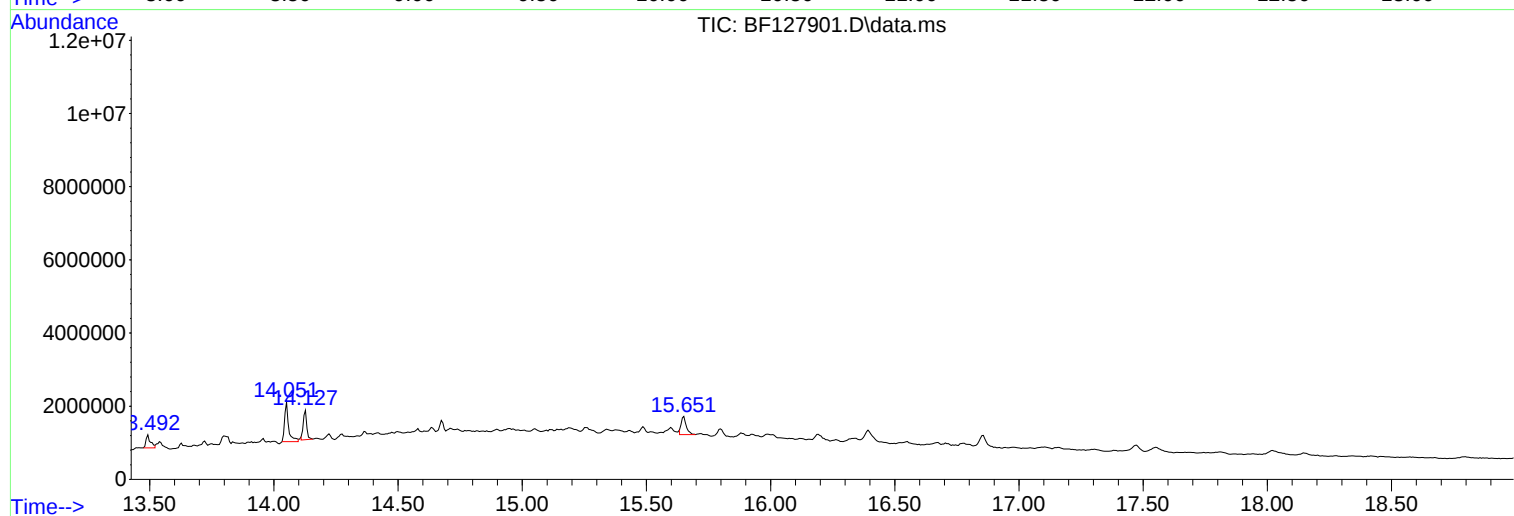
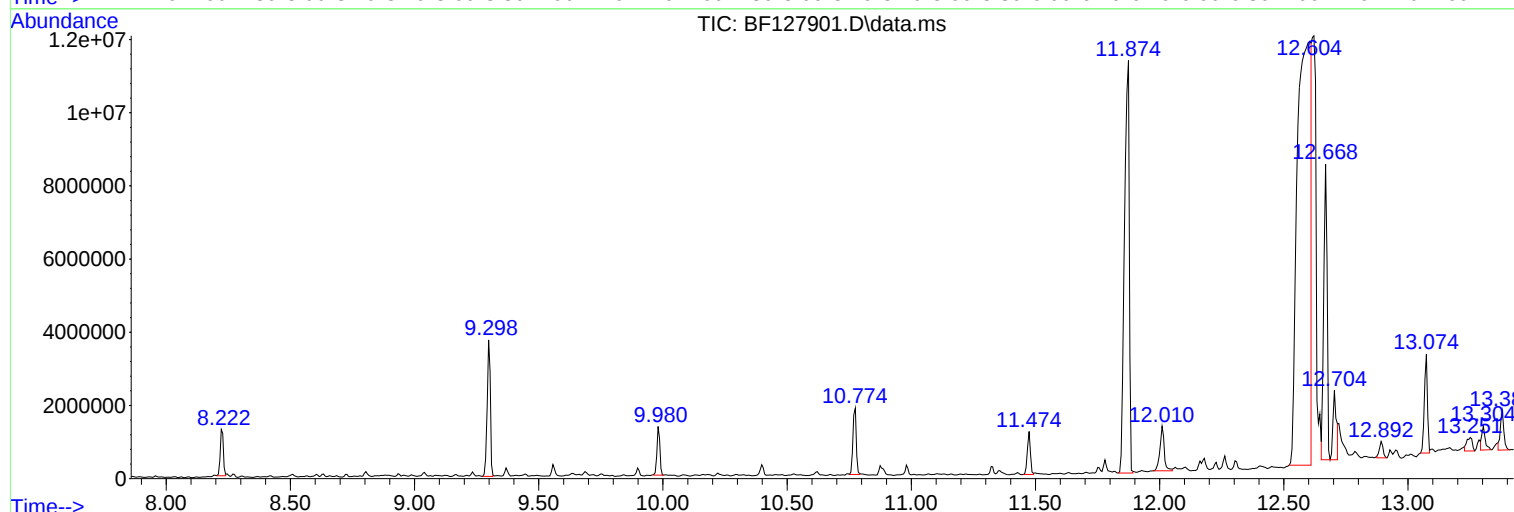
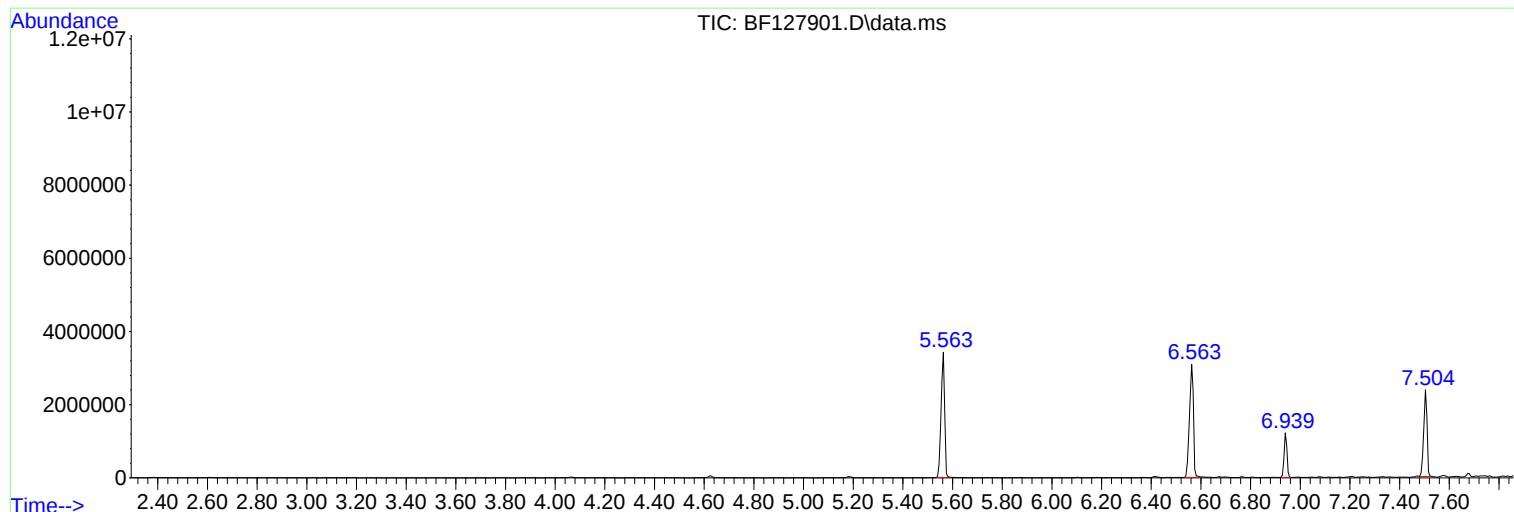
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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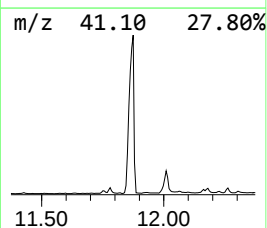
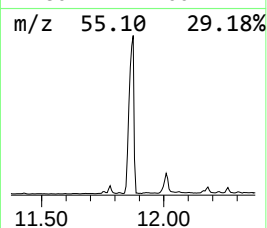
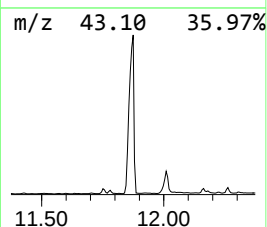
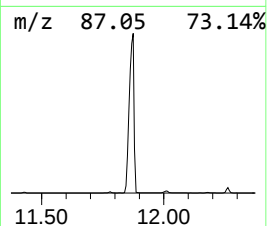
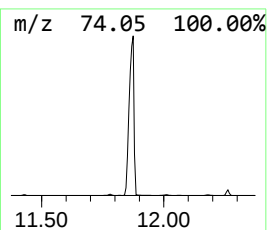
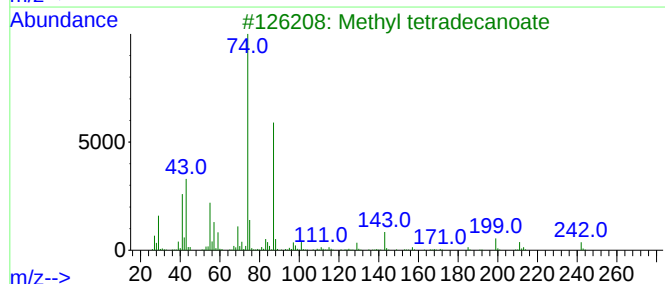
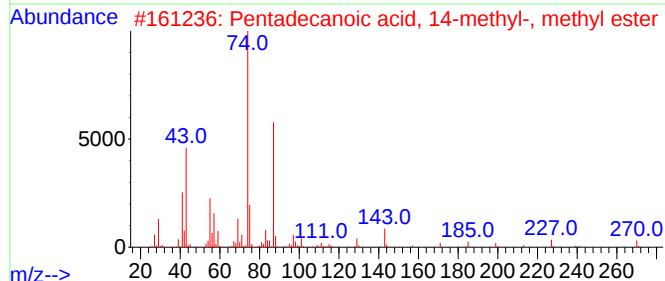
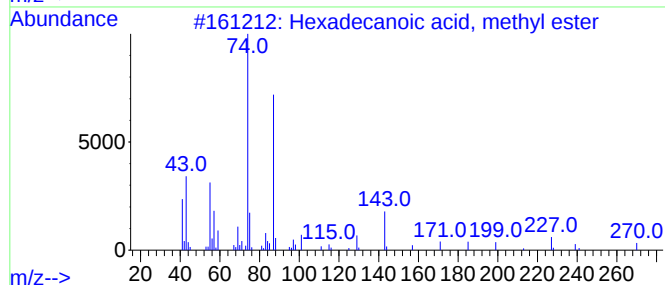
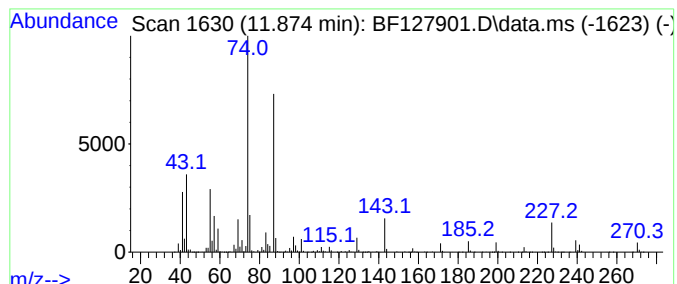
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
11.874	301.82 ng	14930600	Phenanthrene-d10	11.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	96
3			Methyl tetradecanoate	242	C15H30O2	000124-10-7	93
4			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
5			Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	83



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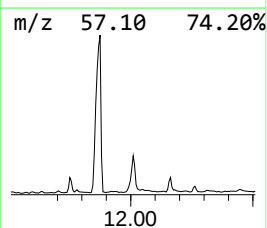
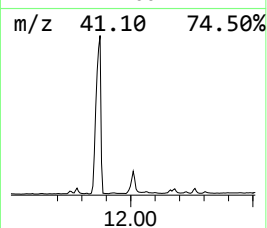
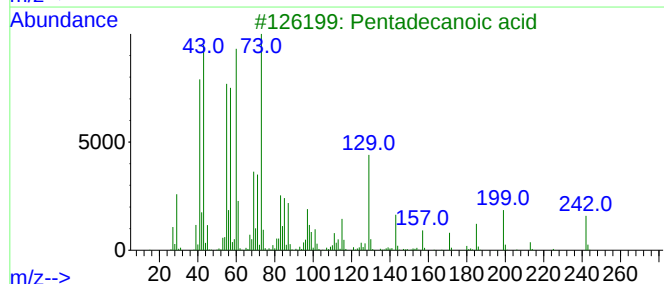
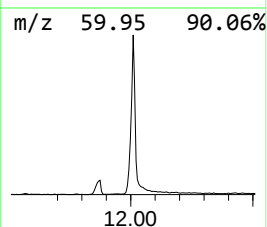
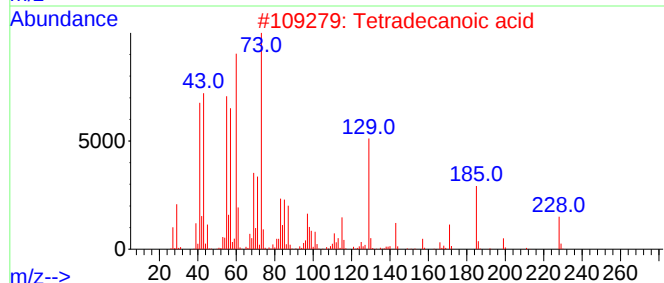
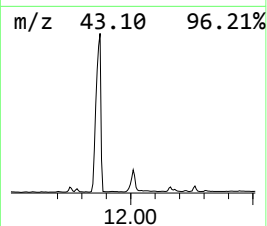
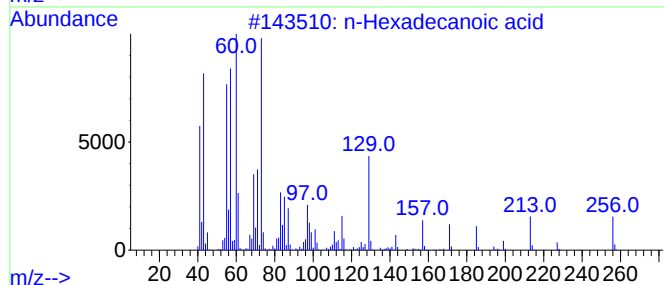
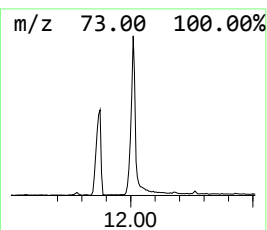
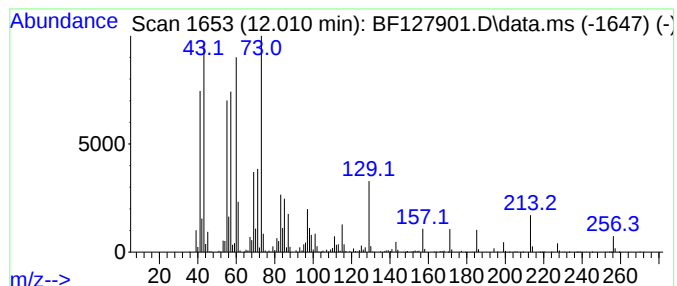
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.010	29.91 ng	1479540	Phenanthrene-d10	11.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tridecanoic acid	214	C13H26O2	000638-53-9	89
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	49



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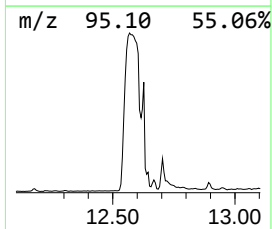
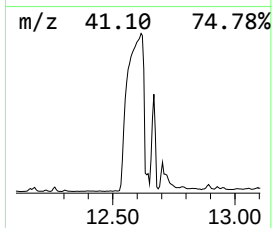
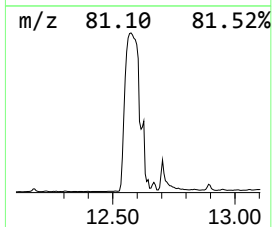
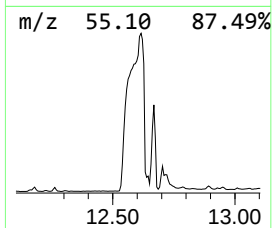
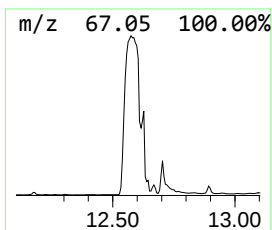
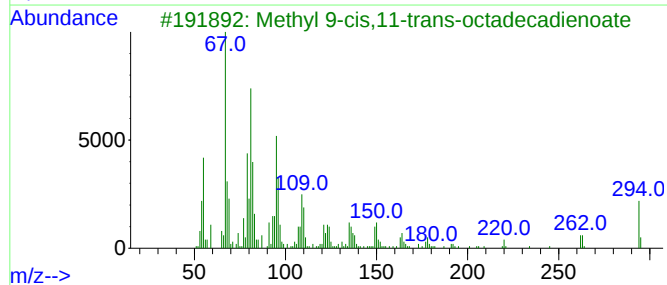
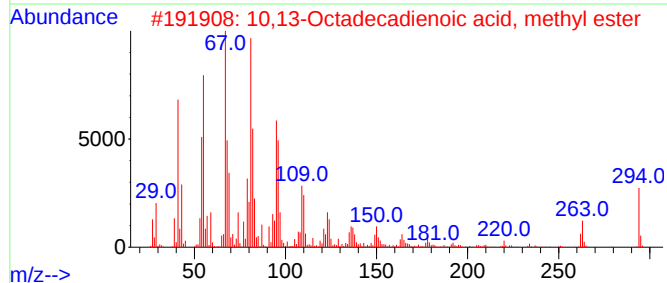
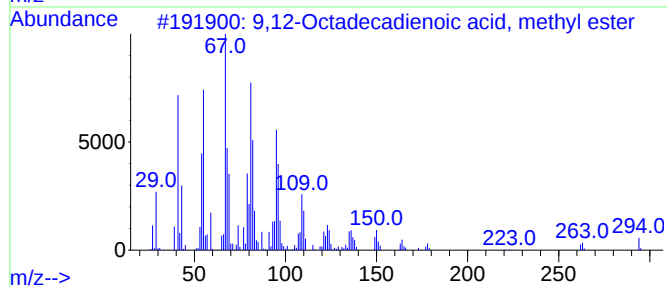
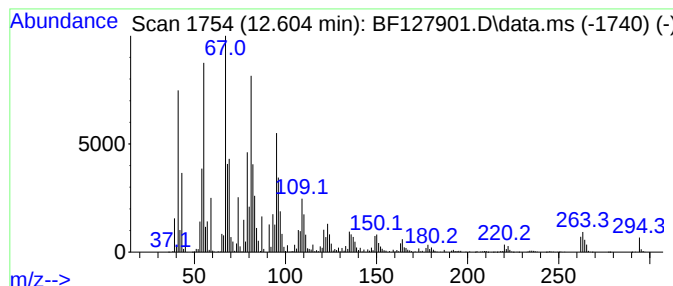
Instrument :
BNA_F
ClientSampleId :
SU-01-042122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.604	892.60 ng	44155500	Phenanthrene-d10	11.474	
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	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	99
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
5	Methyl 7,12-octadecadienoate	294	C19H34O2	1000336-43-8	99



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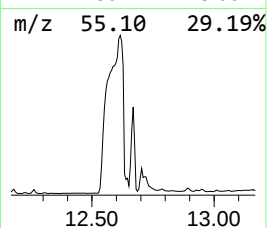
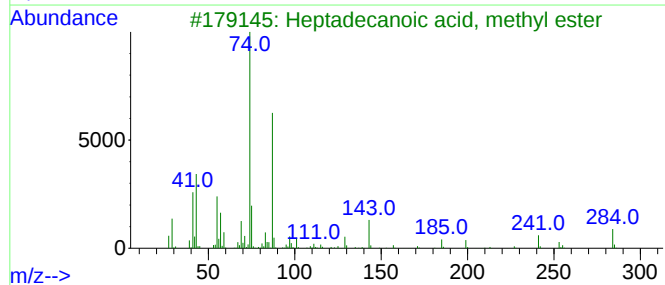
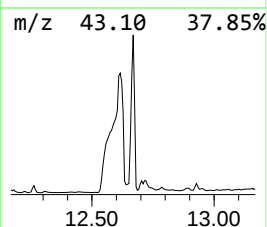
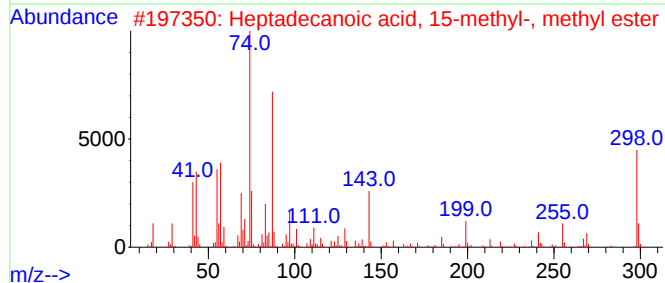
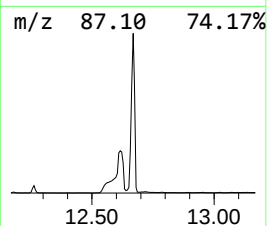
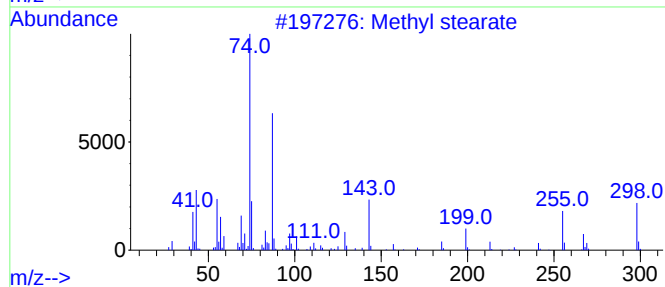
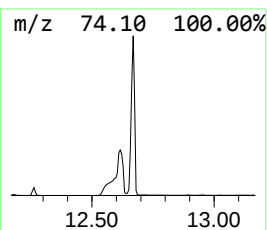
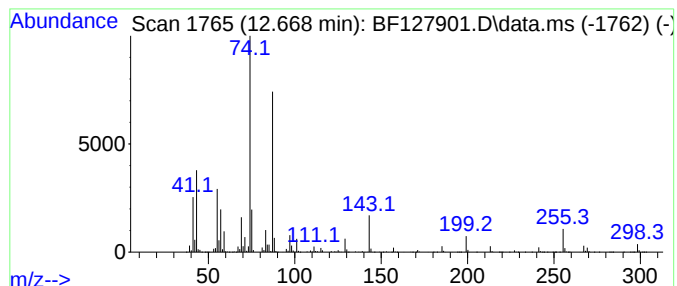
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Methyl stearate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.668	153.76 ng	7606200	Phenanthrene-d10	11.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	97
2			Heptadecanoic acid, 15-methyl-, ...	298	C19H38O2	054833-55-5	93
3			Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	91
4			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
5			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	90



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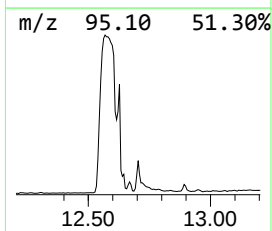
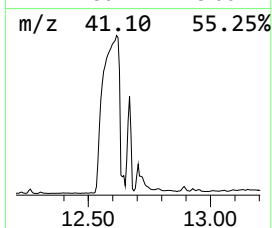
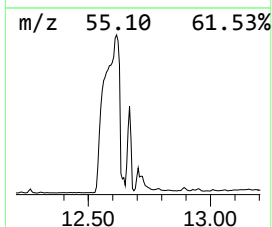
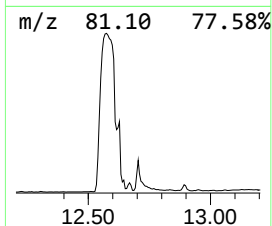
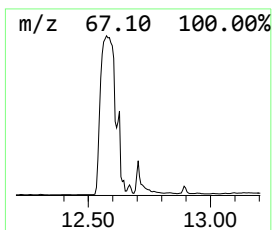
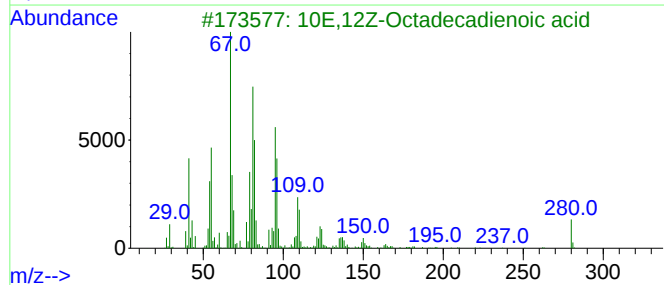
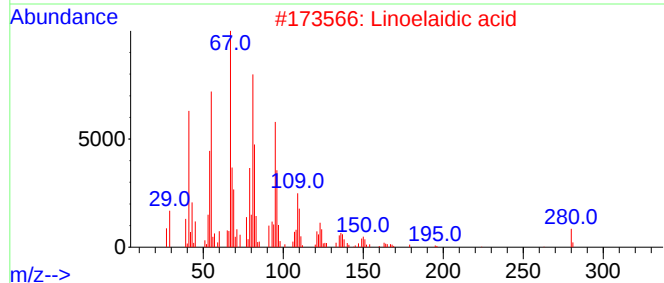
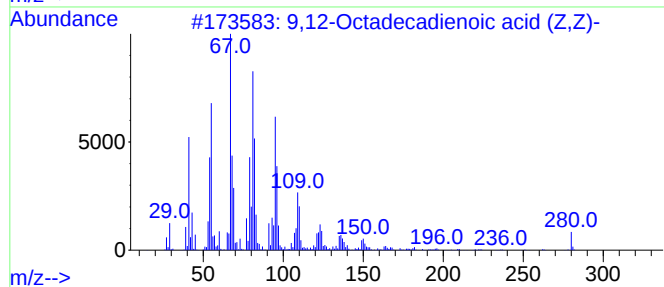
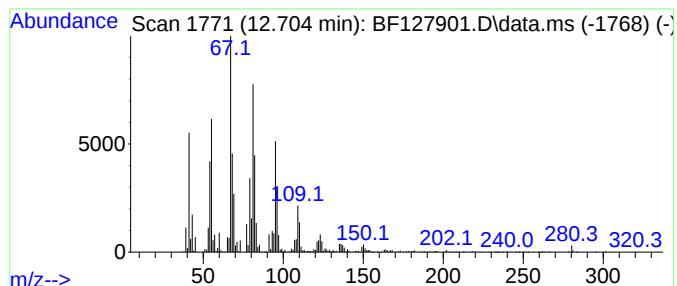
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 9,12-Octadecadienoic acid (... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.704	37.39 ng	1849710	Phenanthrene-d10	11.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	99
2			Linoelaidic acid	280	C18H32O2	000506-21-8	98
3			10E,12Z-Octadecadienoic acid	280	C18H32O2	002420-56-6	98
4			(9E,11E)-Octadecadienoic acid	280	C18H32O2	000544-71-8	97
5			Bicyclo[2.2.2]octane, 2-methyl-	124	C9H16	000766-53-0	91



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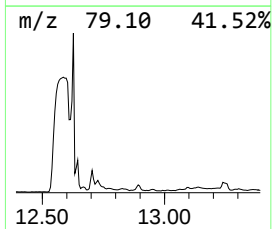
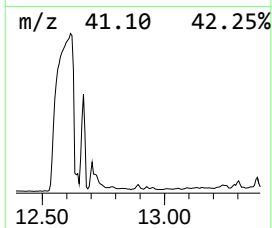
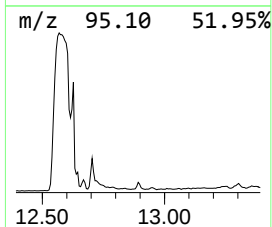
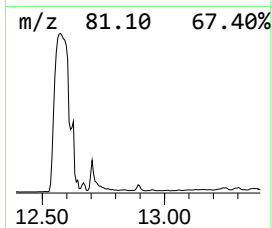
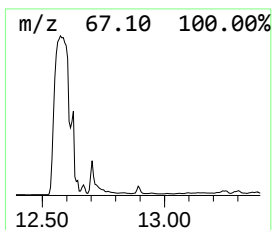
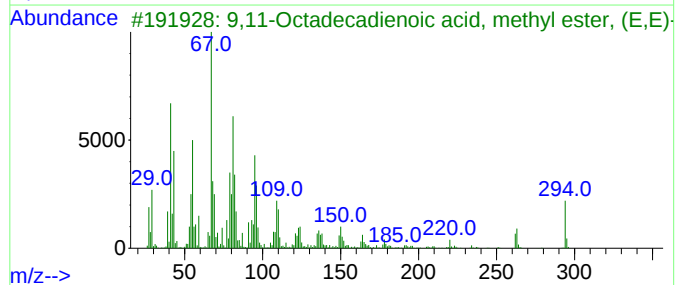
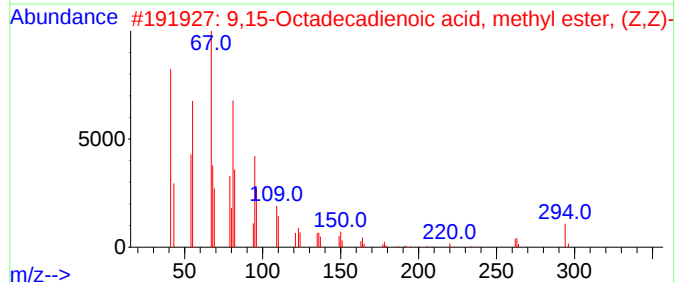
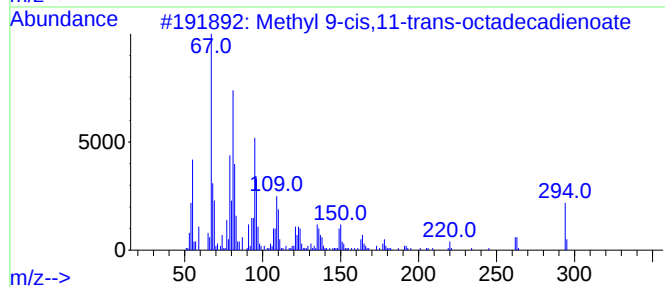
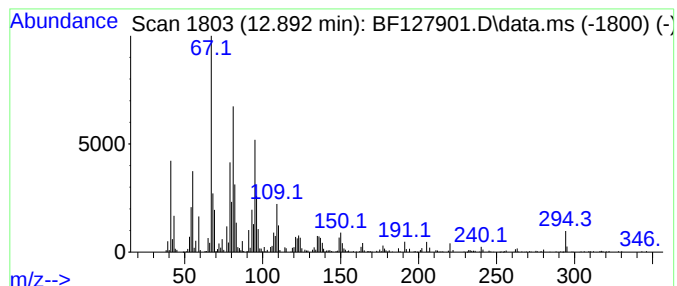
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Methyl 9-cis,11-trans-octad... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.892	11.98 ng	457214	Chrysene-d12	14.127

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	95
2			9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	95
3			9,11-Octadecadienoic acid, methy...	294	C19H34O2	013038-47-6	94
4			Methyl 9,12-heptadecadienoate	280	C18H32O2	1000336-36-2	93
5			Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042522\
Data File : BF127901.D
Acq On : 26 Apr 2022 01:05
Operator : CG\JU
Sample : N2523-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-01-042122

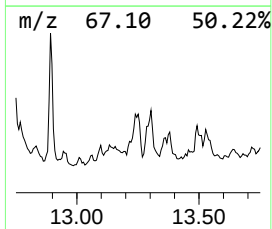
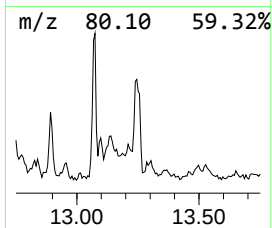
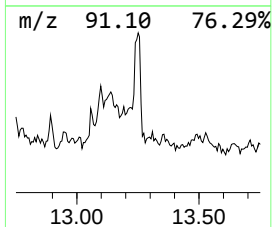
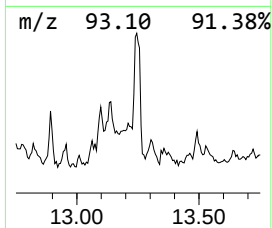
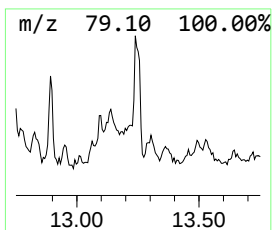
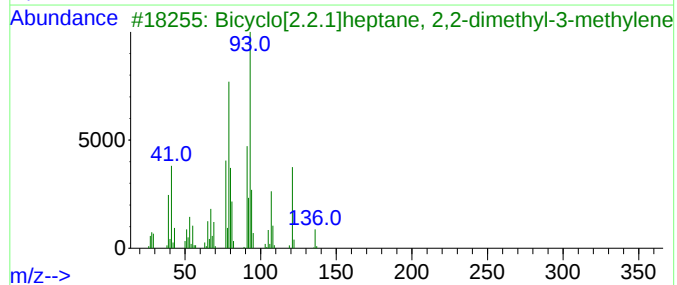
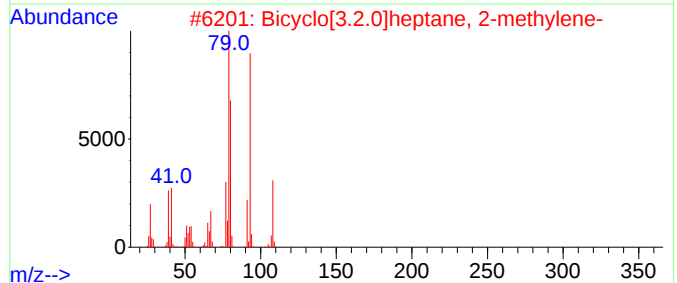
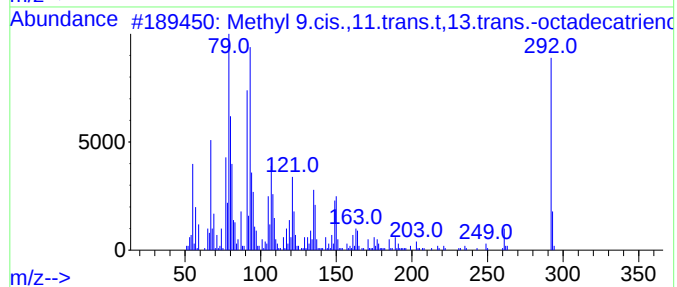
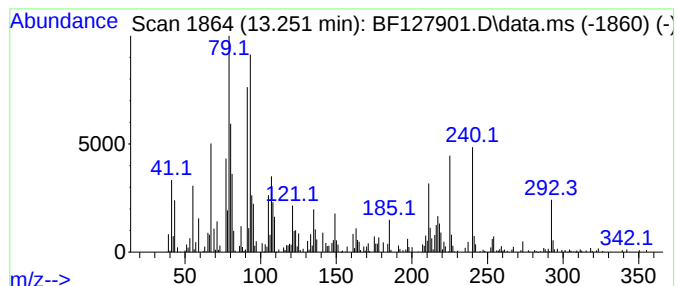
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Methyl 9.cis.,11.trans.t,13... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.251	14.91 ng	569160	Chrysene-d12	14.127

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl 9.cis.,11.trans.t,13.tran...	292	C19H32O2	1000336-42-6	83
2			Bicyclo[3.2.0]heptane, 2-methylene-	108	C8H12	089243-94-7	46
3			Bicyclo[2.2.1]heptane, 2,2-dimet...	136	C10H16	005794-03-6	43
4			Methyl 6-cis,9-cis,11-trans-octa...	292	C19H32O2	1010336-37-7	43
5			1-Methylene-2-vinylcyclopentane	108	C8H12	006196-78-7	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042522\
Data File : BF127901.D
Acq On : 26 Apr 2022 01:05
Operator : CG\JU
Sample : N2523-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-01-042122

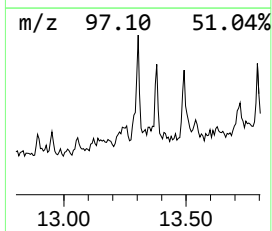
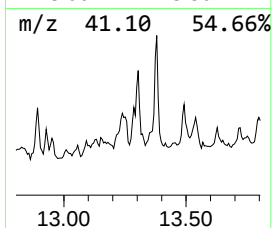
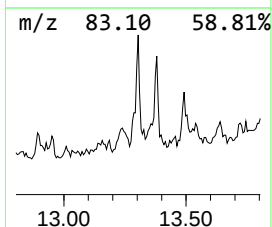
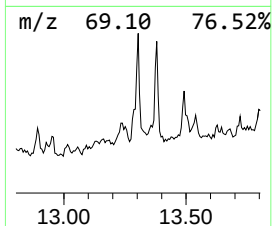
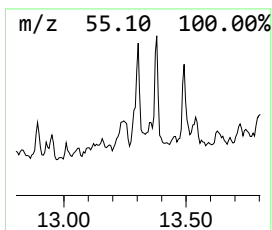
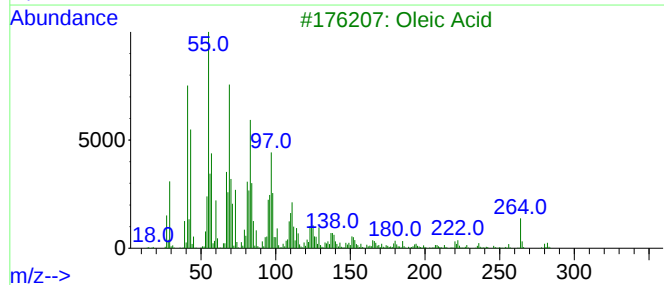
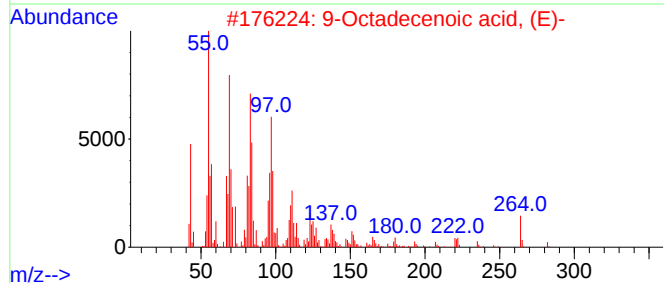
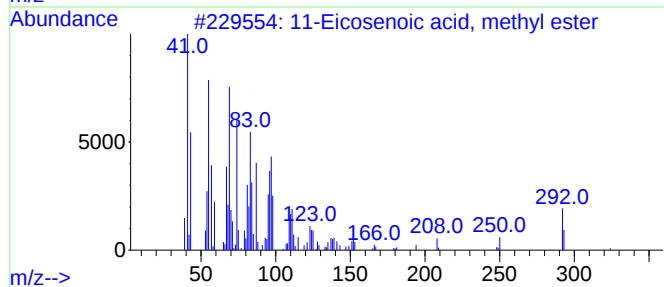
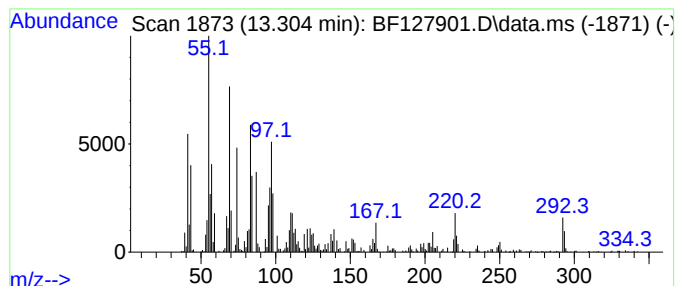
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.304	16.21 ng	618958	Chrysene-d12	14.127

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11-Eicosenoic acid, methyl ester	324	C21H40O2	003946-08-5	91
2			9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	90
3			Oleic Acid	282	C18H34O2	000112-80-1	74
4			14-Pentadecenoic acid	240	C15H28O2	017351-34-7	70
5			cis-Methyl 11-eicosenoate	324	C21H40O2	002390-09-2	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042522\
Data File : BF127901.D
Acq On : 26 Apr 2022 01:05
Operator : CG\JU
Sample : N2523-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-01-042122

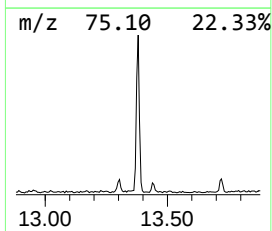
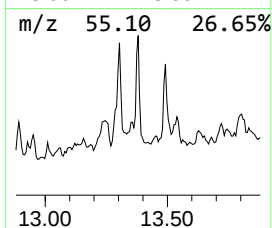
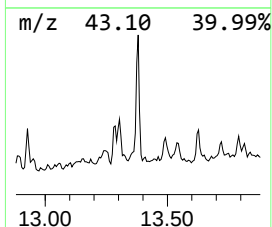
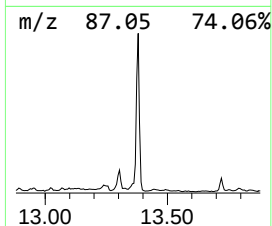
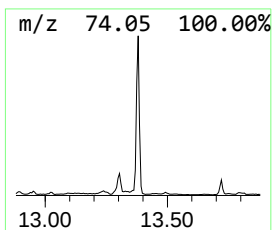
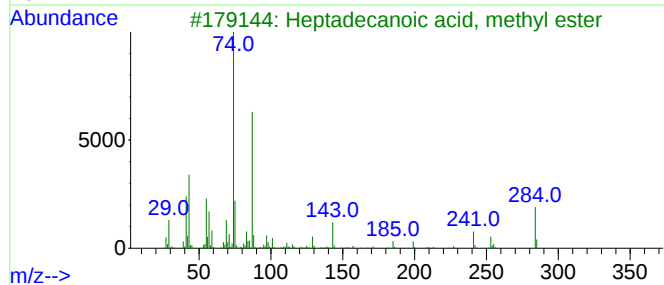
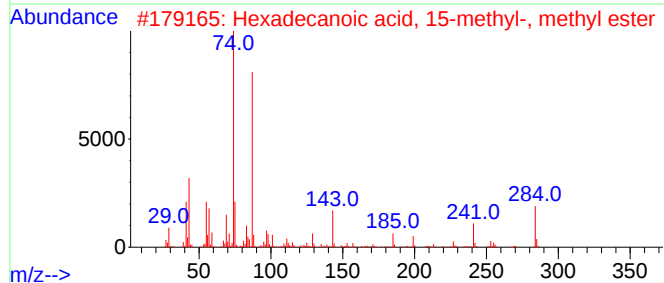
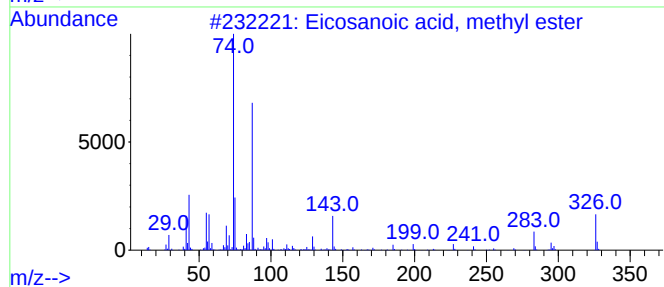
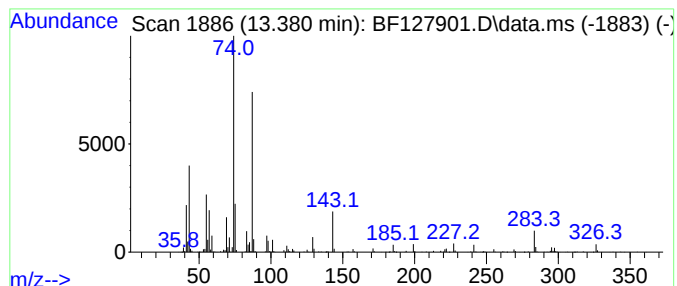
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosanoic acid, methyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.380	27.06 ng	1033060	Chrysene-d12	14.127

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	97
2			Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	93
3			Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	91
4			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	91
5			Hexadecanoic acid, 14-methyl-, m...	284	C18H36O2	002490-49-5	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042522\
Data File : BF127901.D
Acq On : 26 Apr 2022 01:05
Operator : CG\JU
Sample : N2523-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SU-01-042122

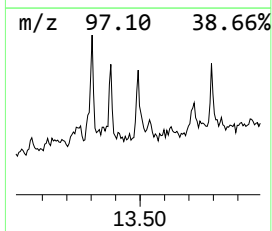
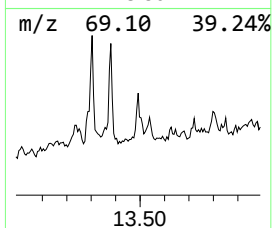
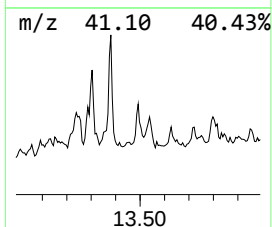
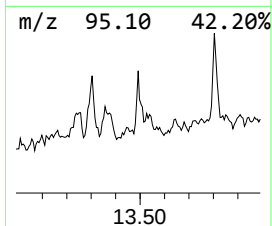
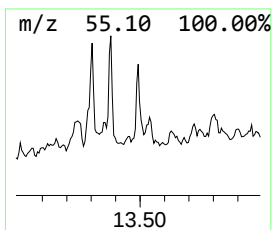
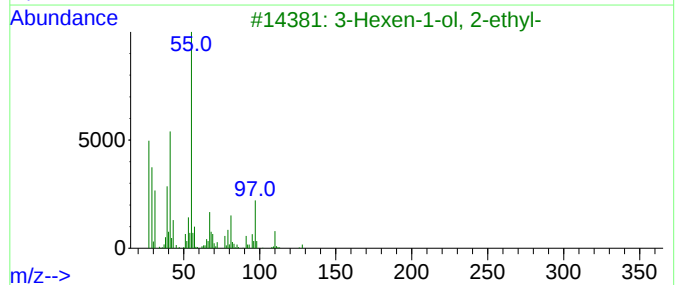
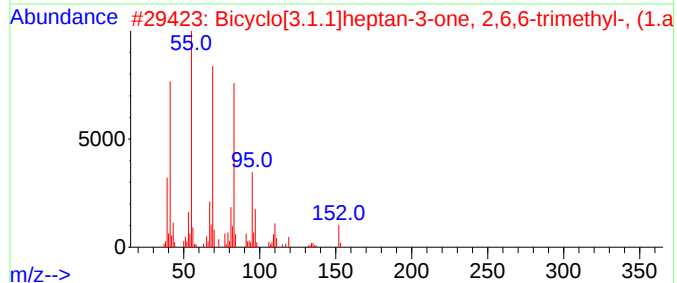
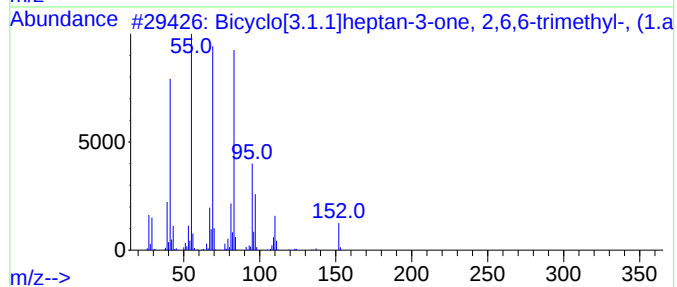
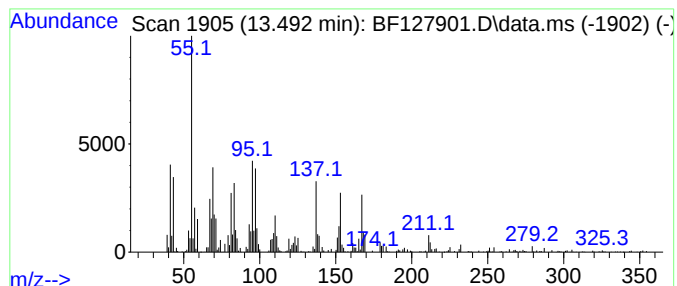
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown13.492 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.492	11.83 ng	451726	Chrysene-d12	14.127

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	000547-60-4	46
2			Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	38
3			3-Hexen-1-ol, 2-ethyl-	128	C8H16O	053907-73-6	14
4			2,4-Pentadien-1-ol, 3-propyl-, (...)	126	C8H14O	1000142-17-9	10
5			Ethyl 2-(bromomethyl)acrylate	192	C6H9BrO2	017435-72-2	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042522\
Data File : BF127901.D
Acq On : 26 Apr 2022 01:05
Operator : CG\JU
Sample : N2523-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-01-042122

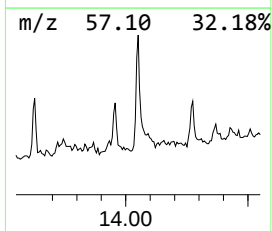
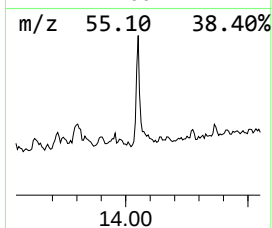
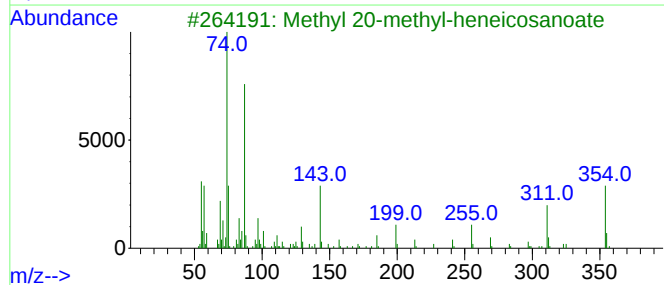
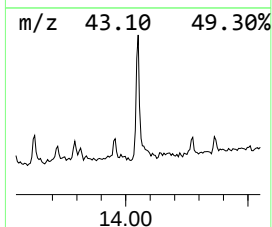
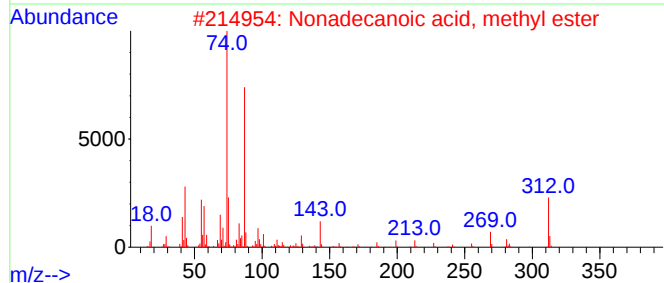
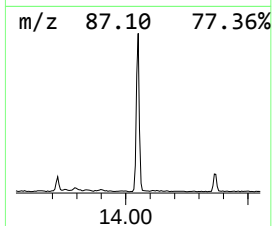
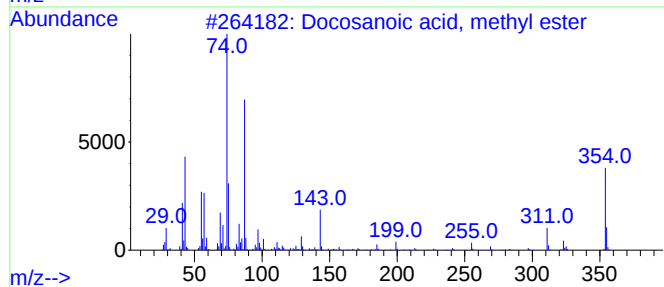
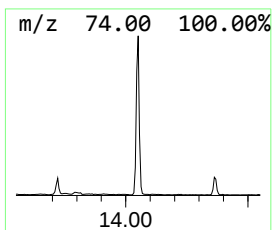
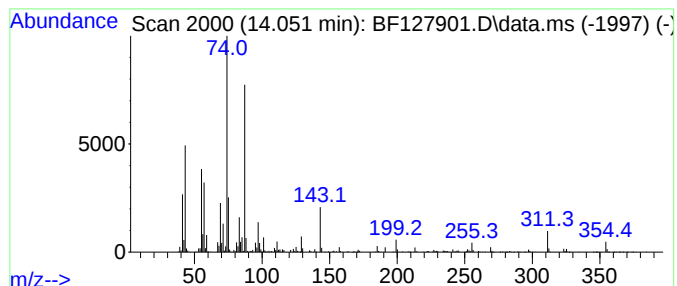
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Docosanoic acid, methyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.051	31.63 ng	1207530	Chrysene-d12	14.127

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosanoic acid, methyl ester	354	C23H46O2	000929-77-1	98
2			Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	94
3			Methyl 20-methyl-heneicosanoate	354	C23H46O2	1000336-47-4	92
4			Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	87
5			Methyl 18-methylnonadecanoate	326	C21H42O2	1000424-52-4	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042522\
Data File : BF127901.D
Acq On : 26 Apr 2022 01:05
Operator : CG\JU
Sample : N2523-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-01-042122

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

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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n-Hexadecanoic ...	12.010	29.9	ng	1479540	4	11.474	989368	20.0
9,12-Octadecadi...	12.604	892.6	ng	44155500	4	11.474	989368	20.0
Methyl stearate	12.668	153.8	ng	7606200	4	11.474	989368	20.0
9,12-Octadecadi...	12.704	37.4	ng	1849710	4	11.474	989368	20.0
Methyl 9-cis,11...	12.892	12.0	ng	457214	5	14.127	763500	20.0
Methyl 9.cis.,1...	13.251	14.9	ng	569160	5	14.127	763500	20.0
11-Eicosenoic a...	13.304	16.2	ng	618958	5	14.127	763500	20.0
Eicosanoic acid...	13.380	27.1	ng	1033060	5	14.127	763500	20.0
unknown13.492	13.492	11.8	ng	451726	5	14.127	763500	20.0
Docosanoic acid...	14.051	31.6	ng	1207530	5	14.127	763500	20.0