

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
 Data File : BF129428.D
 Acq On : 29 Jul 2022 01:48
 Operator : CG\JU
 Sample : N3925-01
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 JC-03-072722-A

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-BF072522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129428.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.516	544	549	552	rBV	4730500	4836857	12.48%	4.252%
2	6.528	715	721	724	rBV	4646237	4723813	12.19%	4.153%
3	6.886	778	782	785	rBV	1290970	1075410	2.77%	0.945%
4	7.451	873	878	881	rBV	3364855	3020342	7.79%	2.655%
5	8.169	996	1000	1003	rBV	1629169	1300913	3.36%	1.144%
6	9.245	1178	1183	1186	rBV	5892501	4902332	12.65%	4.310%
7	9.927	1295	1299	1302	rVB	1434026	1200787	3.10%	1.056%
8	10.722	1429	1434	1437	rBV	2639418	2459030	6.34%	2.162%
9	11.416	1548	1552	1554	rBV	1267592	1030418	2.66%	0.906%
10	11.810	1613	1619	1622	rBV	12564146	13261198	34.21%	11.658%
11	12.521	1730	1740	1741	rBV	16617983	38765969	100.00%	34.080%
12	12.539	1741	1743	1747	rVV2	16737634	20495719	52.87%	18.018%
13	12.568	1747	1748	1750	rVV	669533	476877	1.23%	0.419%
14	12.604	1750	1754	1757	rVB	7403426	6935714	17.89%	6.097%
15	12.639	1757	1760	1762	rBV	507444	502159	1.30%	0.441%
16	12.833	1789	1793	1796	rBV2	413156	467502	1.21%	0.411%
17	12.868	1796	1799	1801	rBV	510449	464363	1.20%	0.408%
18	13.010	1819	1823	1826	rBV	4272550	3901216	10.06%	3.430%
19	13.315	1873	1875	1879	rVB	679059	588517	1.52%	0.517%
20	13.751	1943	1949	1952	rBV4	350374	739794	1.91%	0.650%
21	13.986	1986	1989	1993	rBV	774881	724527	1.87%	0.637%
22	14.068	1998	2003	2005	rBV2	957195	1115488	2.88%	0.981%
23	15.562	2254	2257	2265	rVB	607983	760141	1.96%	0.668%

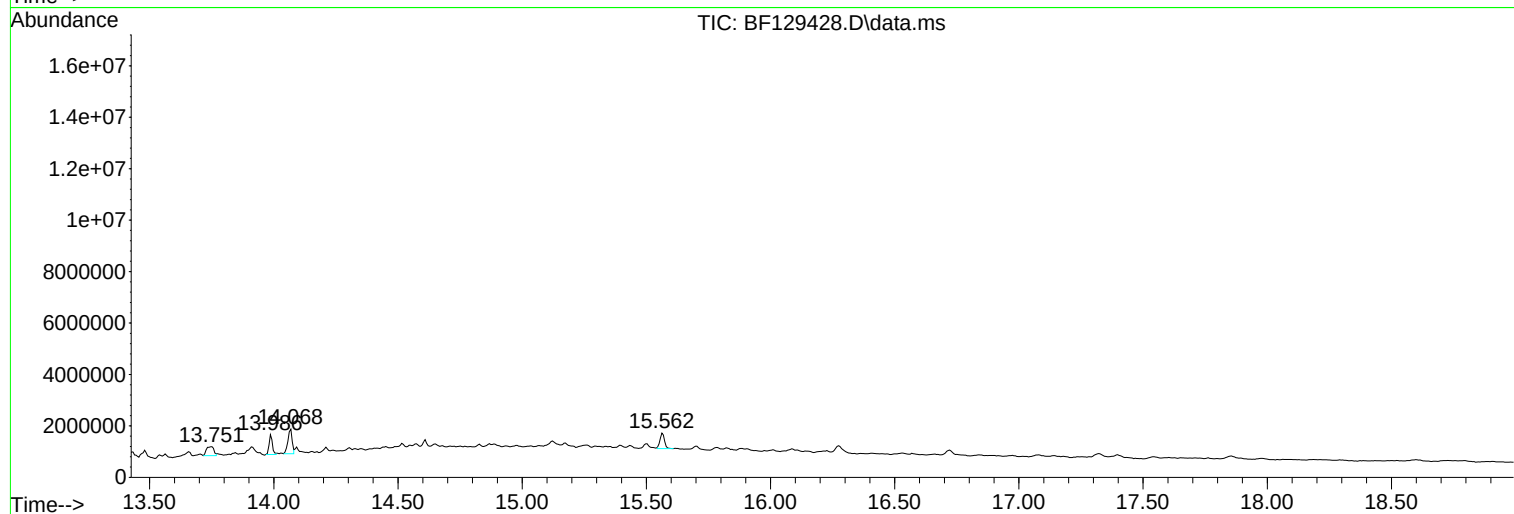
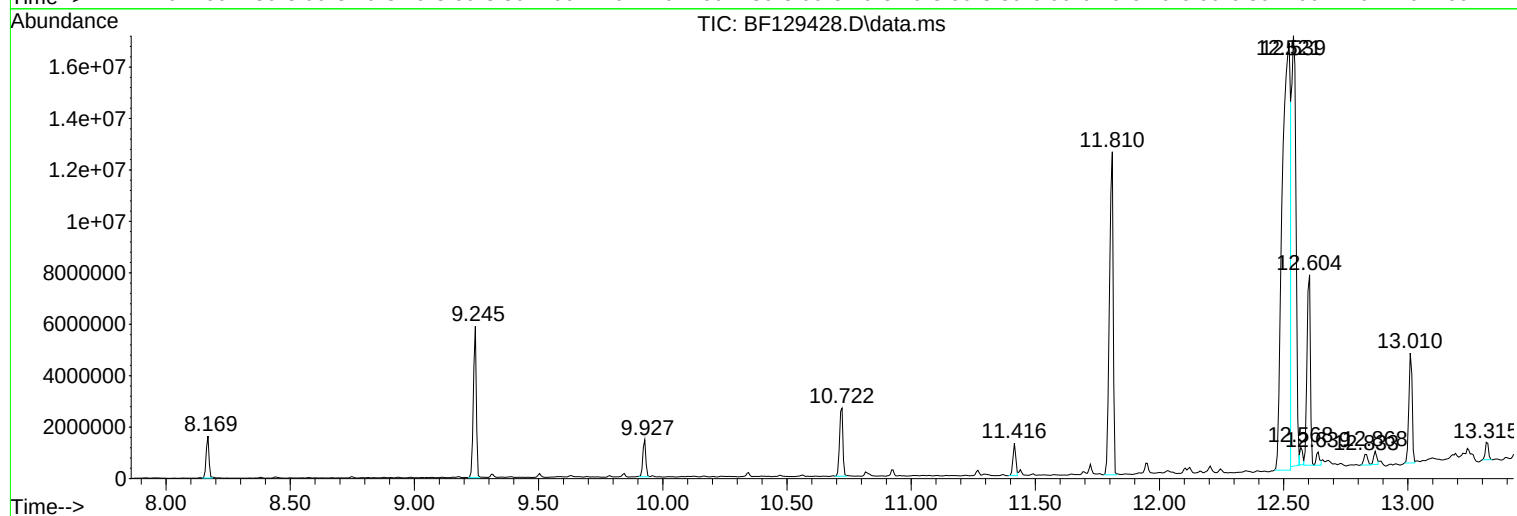
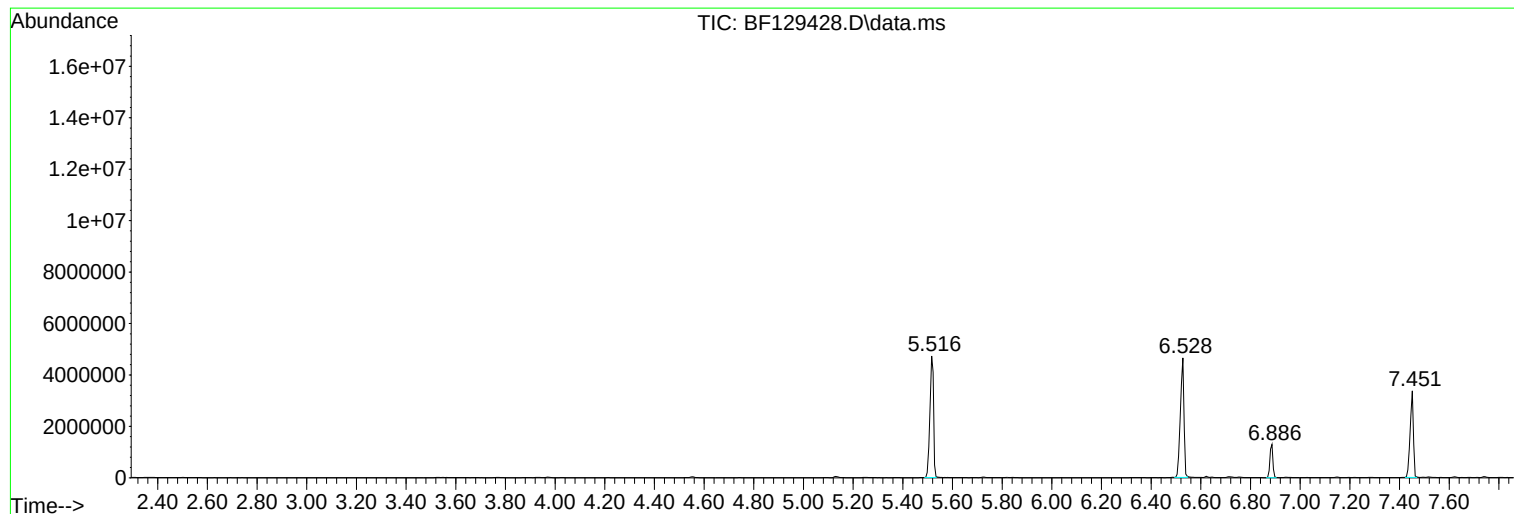
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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
JC-03-072722-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.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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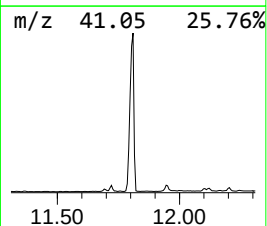
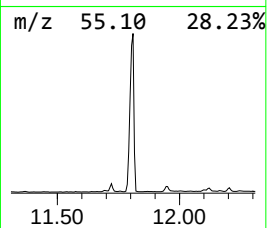
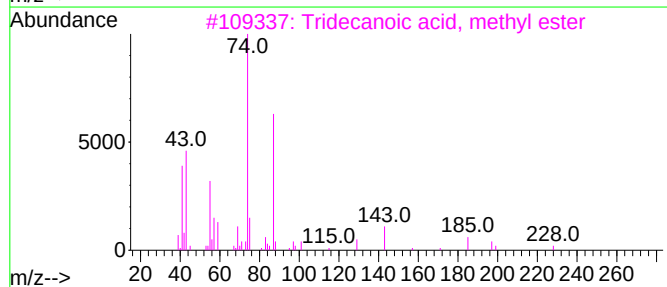
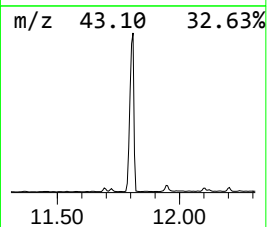
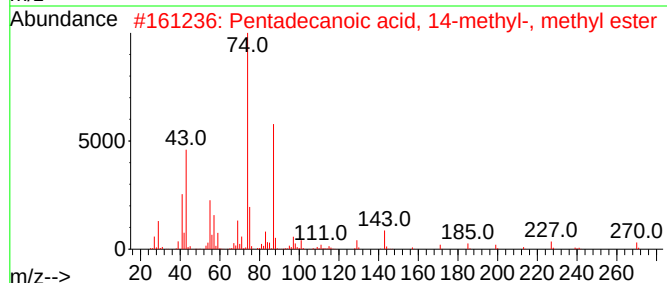
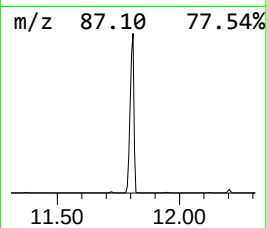
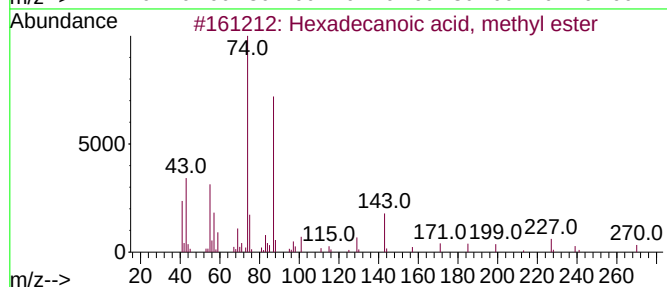
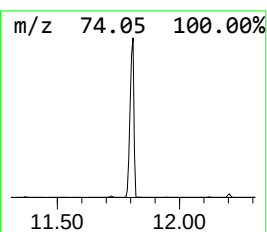
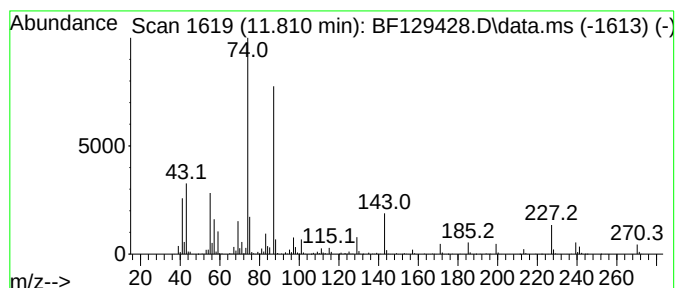
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.	
11.810	257.39 ng	13261200	Phenanthrene-d10	11.416	
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	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	83
5	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	81



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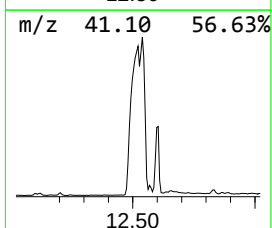
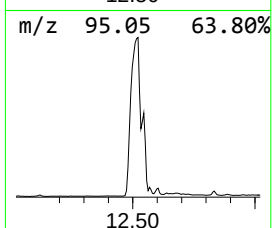
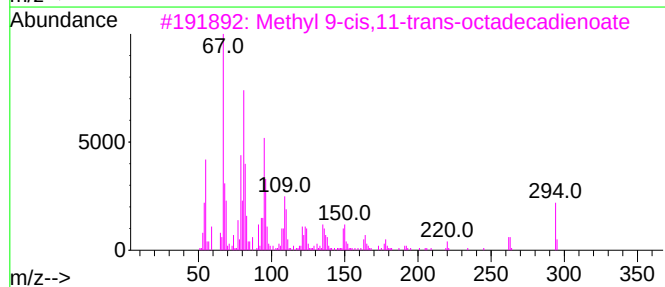
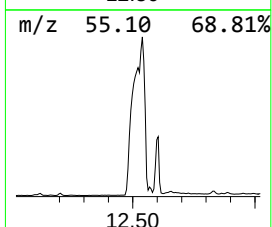
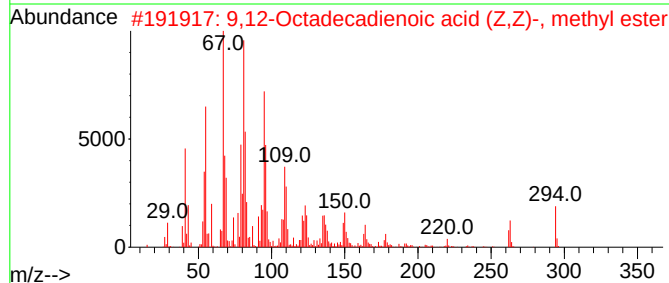
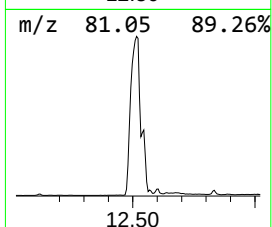
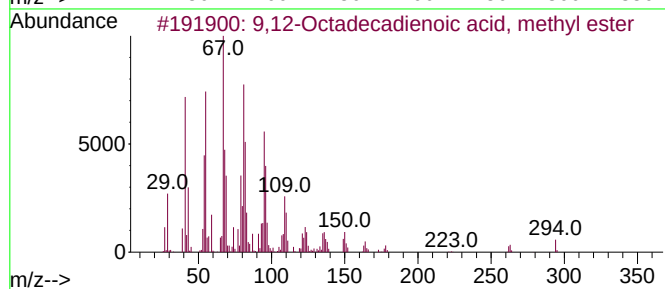
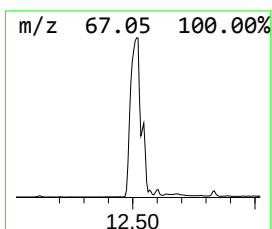
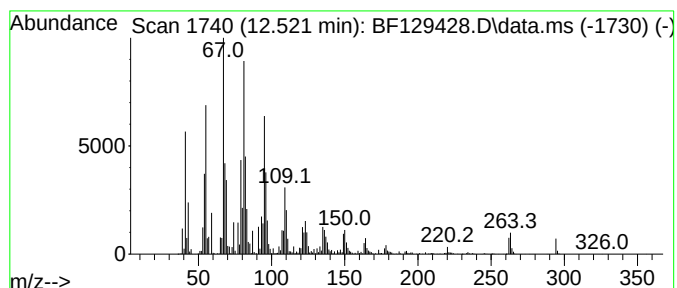
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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.521	752.43 ng	38766000	Phenanthrene-d10	11.416		
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 (Z,Z)-...	294	C19H34O2	000112-63-0	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		10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99



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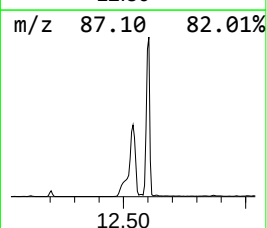
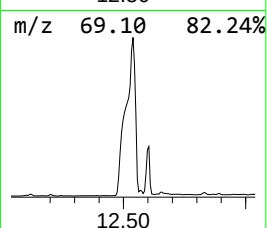
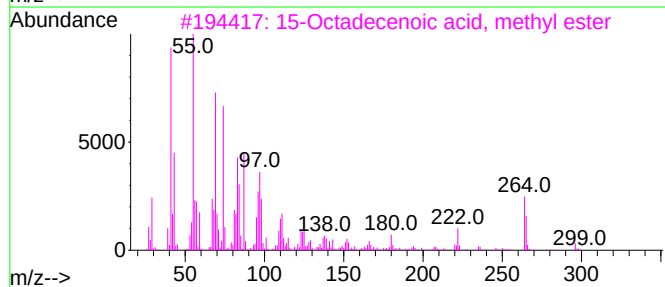
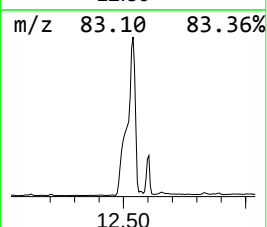
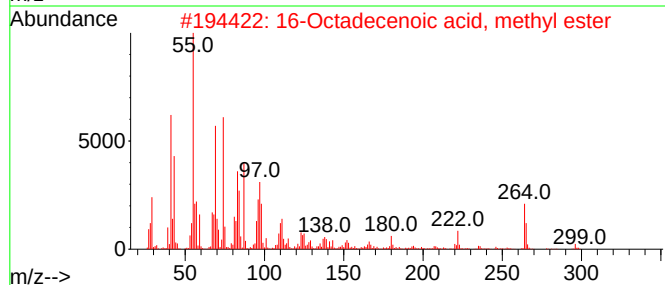
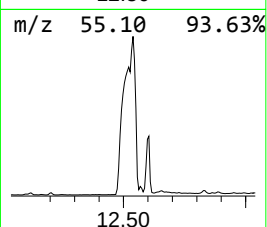
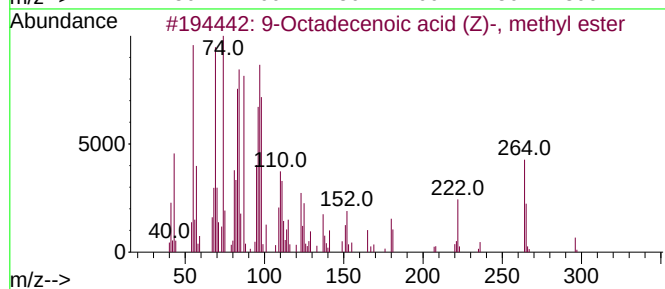
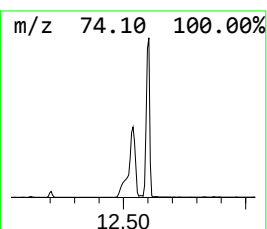
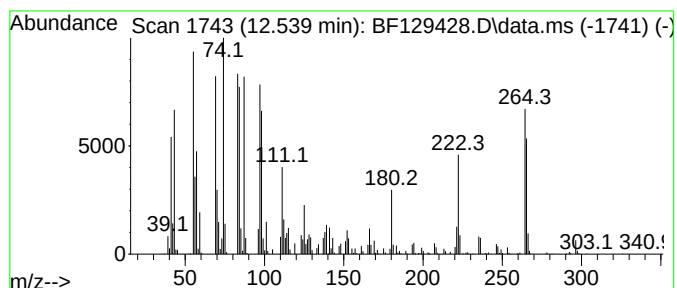
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.539	397.81 ng	20495700	Phenanthrene-d10	11.416	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	94
2	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	93
3	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	93
4	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	91
5	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	91



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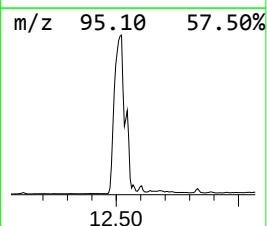
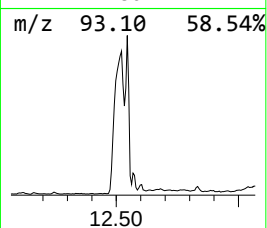
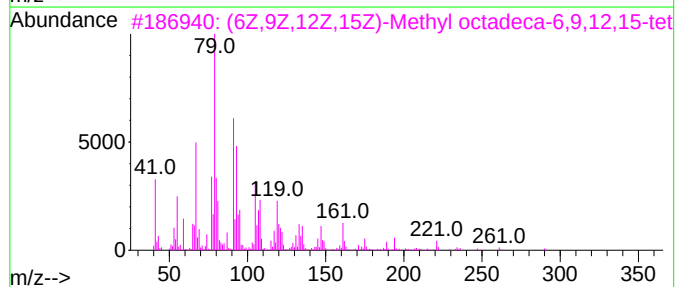
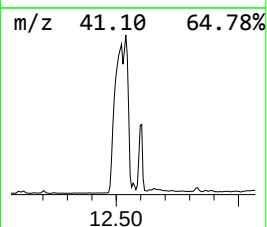
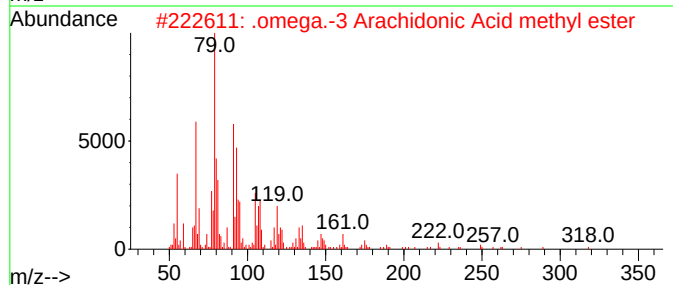
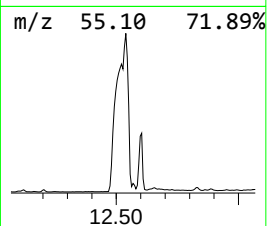
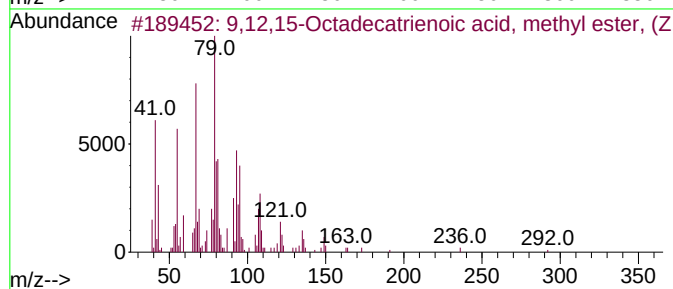
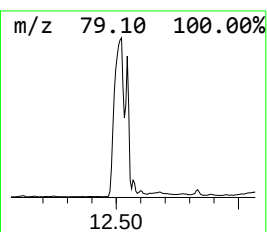
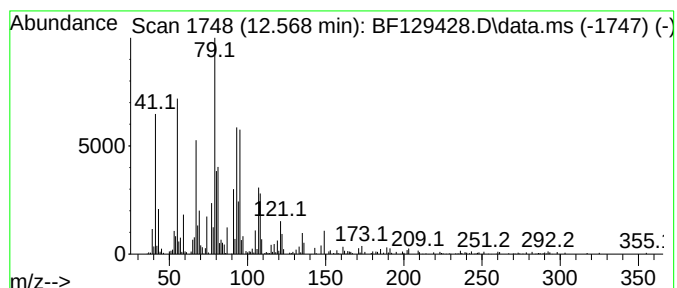
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 9,12,15-Octadecatrienoic ac... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.569	9.26 ng	476877	Phenanthrene-d10	11.416	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12,15-Octadecatrienoic acid, m...	292	C19H32O2	000301-00-8	93
2	.omega.-3 Arachidonic Acid methy...	318	C21H34O2	132712-70-0	80
3	(6Z,9Z,12Z,15Z)-Methyl octadeca...	290	C19H30O2	073097-00-4	72
4	9-Octadecen-12-ynoic acid, methy...	292	C19H32O2	056847-05-3	64
5	3-Dodecen-1-yne, (Z)-	164	C12H20	025091-24-1	64



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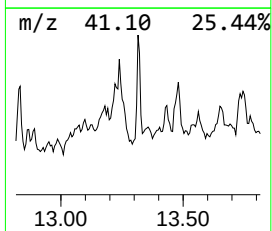
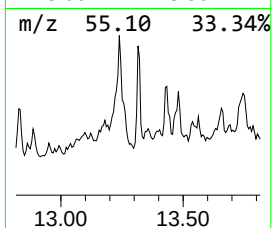
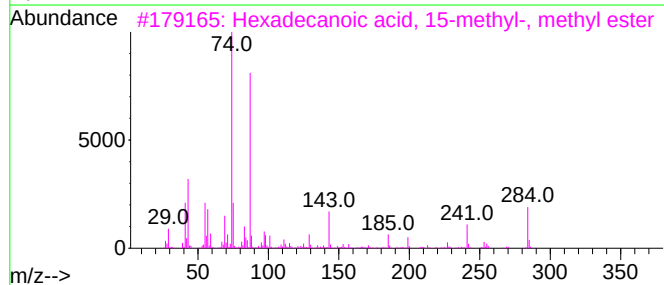
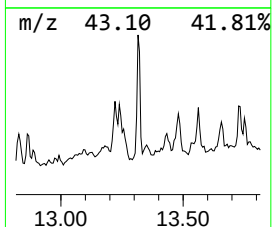
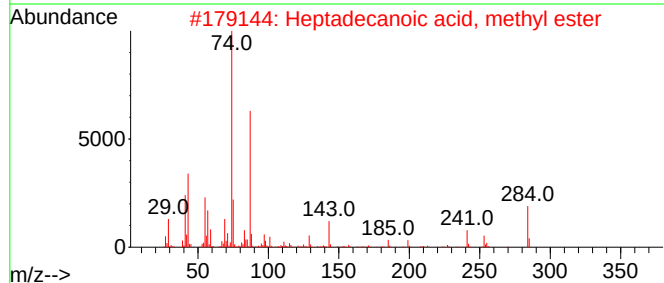
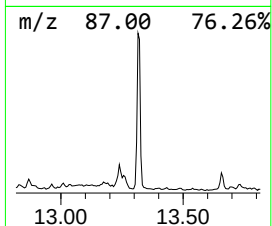
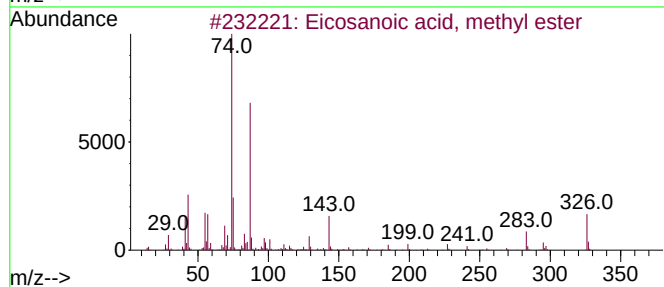
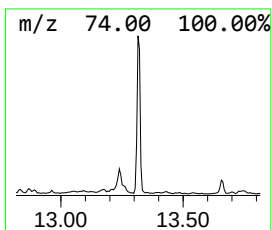
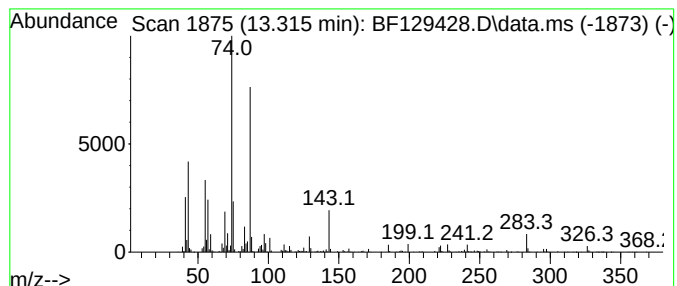
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Eicosanoic acid, methyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.316	10.55 ng	588517	Chrysene-d12	14.068

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	97
2			Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	93
3			Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	91
4			Methyl stearate	298	C19H38O2	000112-61-8	90
5			Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	90



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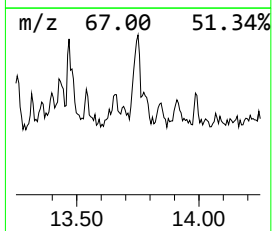
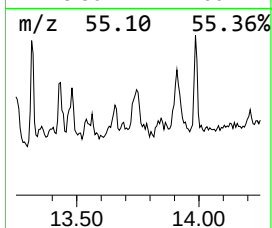
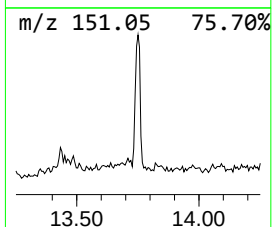
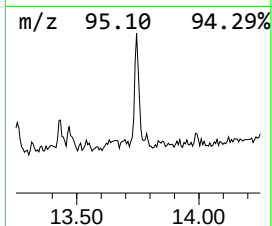
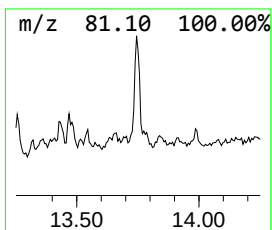
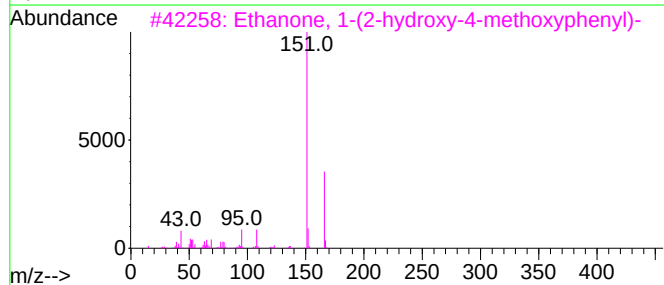
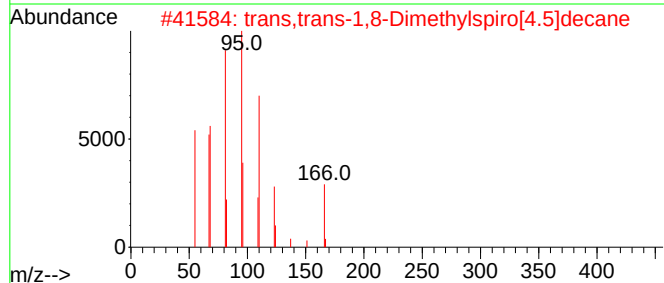
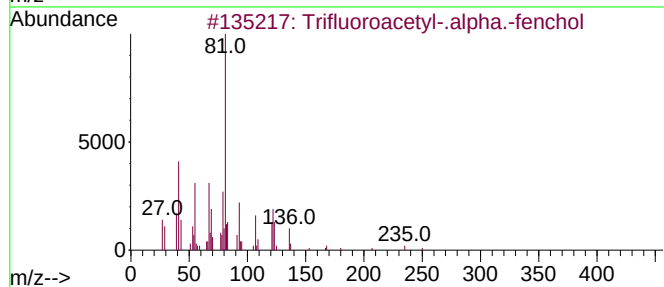
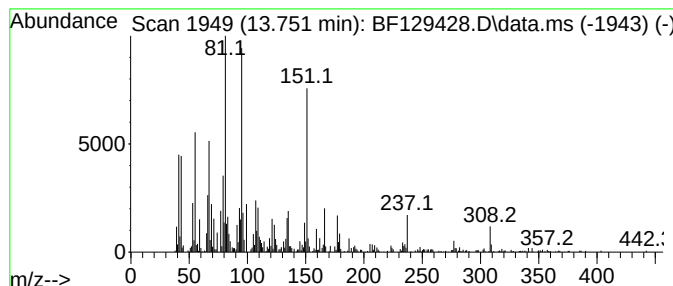
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown13.751 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.751	13.26 ng	739794	Chrysene-d12	14.068

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetyl-.alpha.-fenchol	250	C12H17F3O2	031076-73-0	44
2			trans,trans-1,8-Dimethylspiro[4.5]undecane	166	C12H22	1000111-72-8	35
3			Ethanone, 1-(2-hydroxy-4-methoxyphenyl)-	166	C9H10O3	000552-41-0	30
4			2,8-Bornanediol, stereoisomer	170	C10H18O2	013429-50-0	27
5			Methyl 2-octylcyclopropene-1-octanoate	308	C20H36O2	003220-60-8	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
Data File : BF129428.D
Acq On : 29 Jul 2022 01:48
Operator : CG\JU
Sample : N3925-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

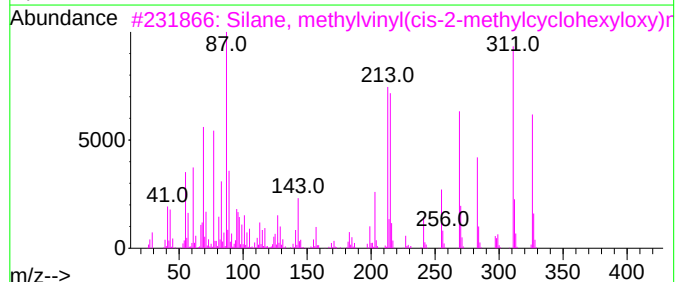
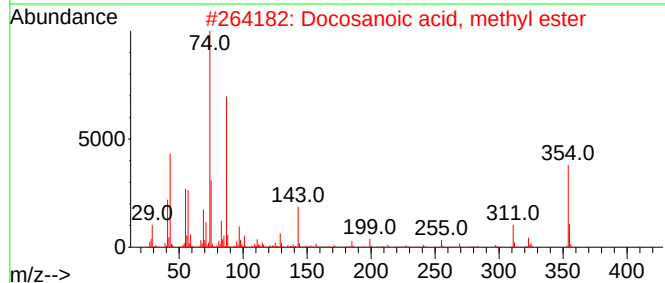
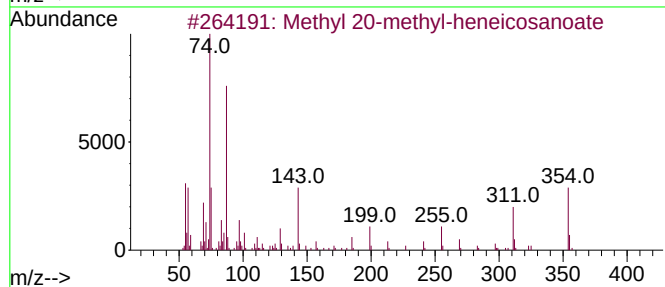
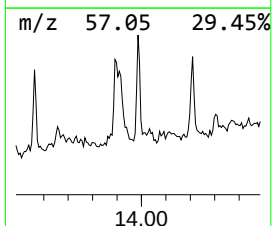
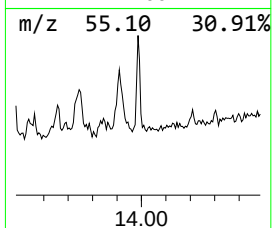
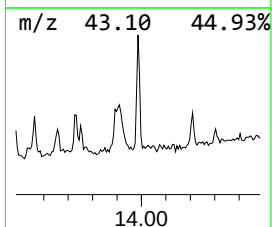
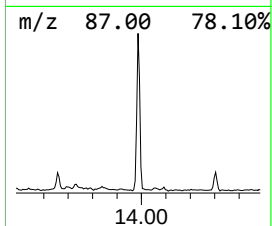
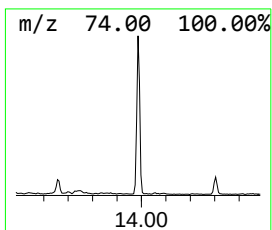
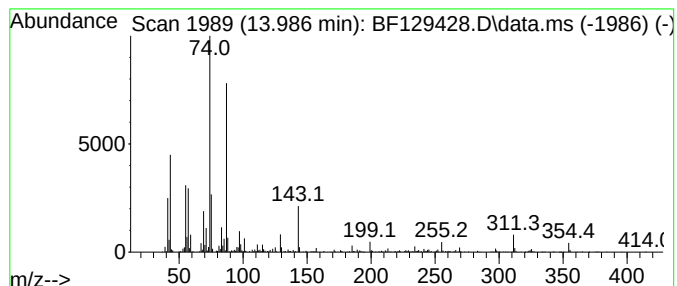
Instrument :
BNA_F
ClientSampleId :
JC-03-072722-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Methyl 20-methyl-heneicosan... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.986	12.99 ng	724527	Chrysene-d12	14.068	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 20-methyl-heneicosanoate	354	C23H46O2	1000336-47-4	97
2	Docosanoic acid, methyl ester	354	C23H46O2	000929-77-1	96
3	Silane, methylvinyl(cis-2-methyl...	326	C19H38O2Si	1000421-05-3	95
4	Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	90
5	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072822\
Data File : BF129428.D
Acq On : 29 Jul 2022 01:48
Operator : CG\JU
Sample : N3925-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
JC-03-072722-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.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...	11.810	257.4	ng	13261200	4	11.416	1030420	20.0
9,12-Octadecadi...	12.521	752.4	ng	38766000	4	11.416	1030420	20.0
9-Octadecenoic ...	12.539	397.8	ng	20495700	4	11.416	1030420	20.0
9,12,15-Octadec...	12.569	9.3	ng	476877	4	11.416	1030420	20.0
Eicosanoic acid...	13.316	10.6	ng	588517	5	14.068	1115490	20.0
unknown13.751	13.751	13.3	ng	739794	5	14.068	1115490	20.0
Methyl 20-methy...	13.986	13.0	ng	724527	5	14.068	1115490	20.0