

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081222\
 Data File : BF129758.D
 Acq On : 12 Aug 2022 22:39
 Operator : CG\JU
 Sample : N4136-03 5X
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-5

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: BF129758.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.116	988	991	994	rVB	909686	706364	1.05%	0.654%
2	9.869	1286	1289	1292	rVB	1013918	799504	1.19%	0.741%
3	10.757	1437	1440	1446	rBV	519149	670441	1.00%	0.621%
4	11.363	1539	1543	1546	rBV	1133235	944499	1.41%	0.875%
5	11.745	1603	1608	1611	rVB	8477385	8179185	12.20%	7.577%
6	11.898	1630	1634	1639	rBV	982984	1117028	1.67%	1.035%
7	12.498	1720	1736	1739	rBV3	18073570	67017808	100.00%	62.083%
8	12.545	1739	1744	1747	rVV	6234606	5042688	7.52%	4.671%
9	12.639	1747	1760	1766	rVV	7385187	16502845	24.62%	15.288%
10	12.692	1766	1769	1780	rVV2	617673	1088877	1.62%	1.009%
11	13.127	1840	1843	1847	rVB3	449282	677513	1.01%	0.628%
12	13.186	1847	1853	1856	rBV	2552290	2273093	3.39%	2.106%
13	13.263	1862	1866	1869	rBV	1436927	1247308	1.86%	1.155%
14	13.927	1976	1979	1983	rBV	941236	868464	1.30%	0.805%
15	14.015	1991	1994	1998	rBV	890806	813358	1.21%	0.753%

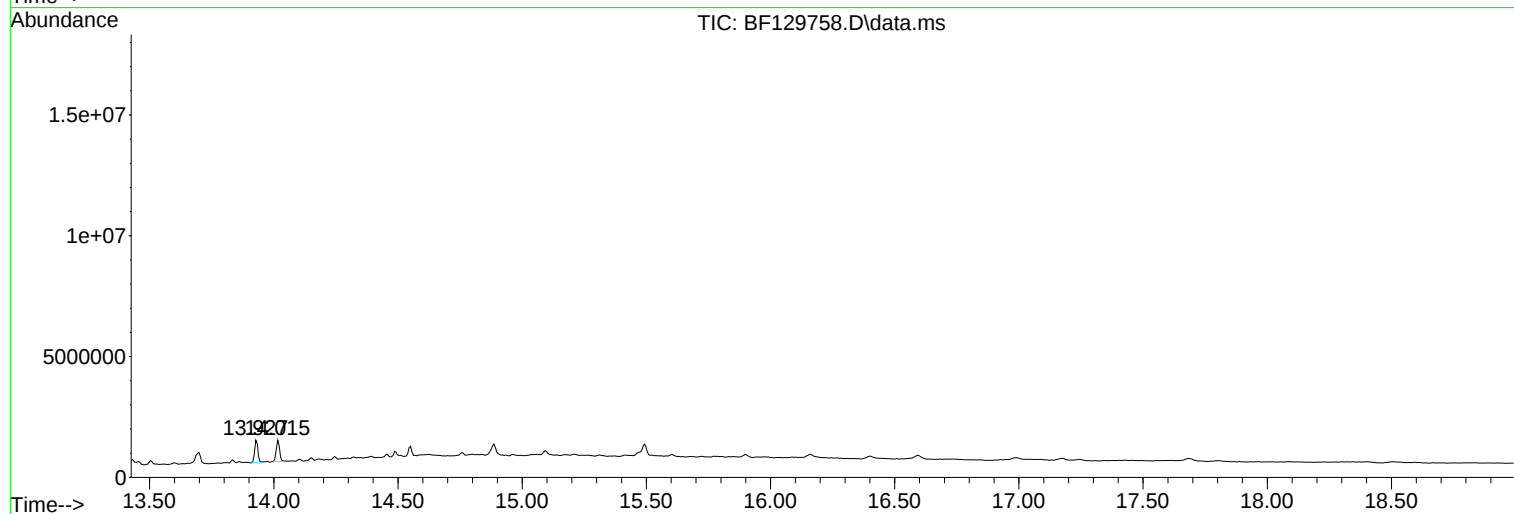
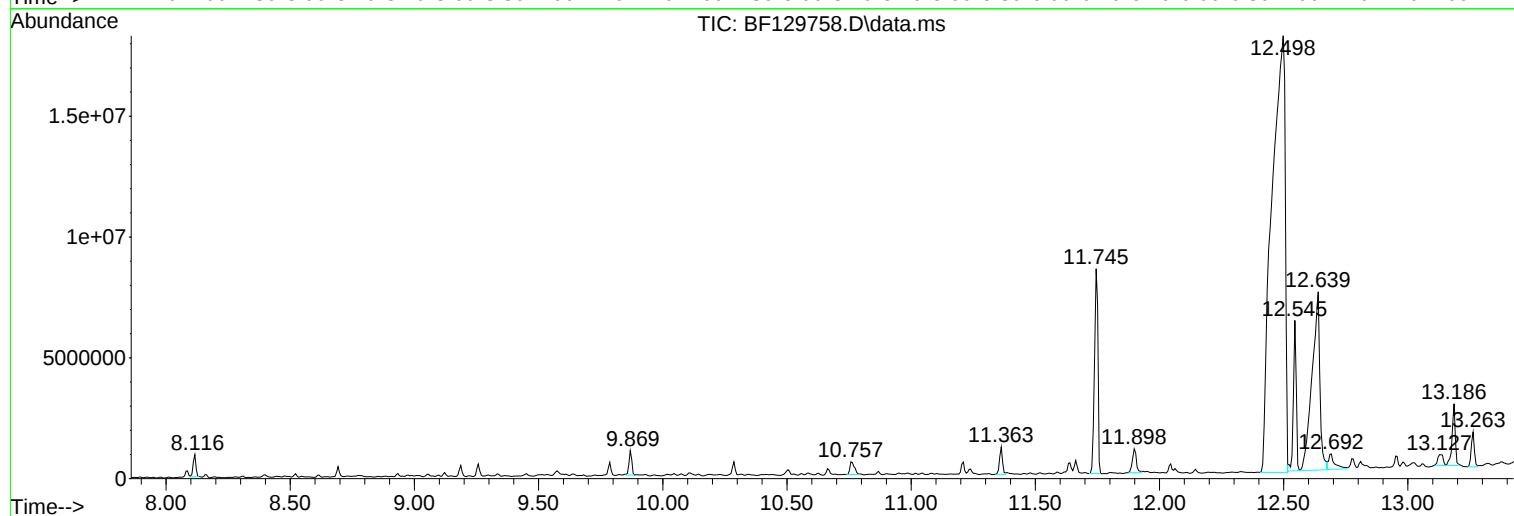
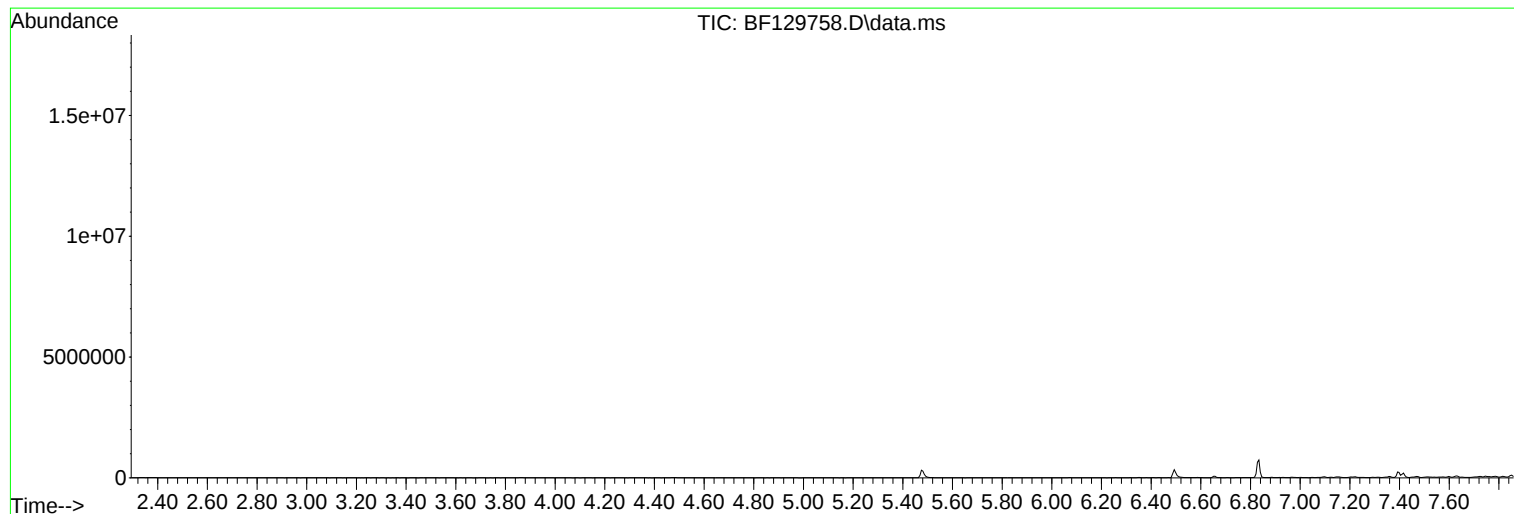
Sum of corrected areas: 107948975

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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



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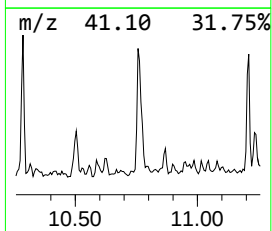
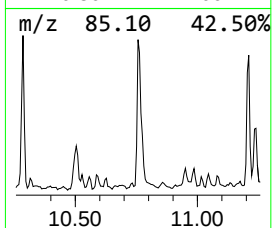
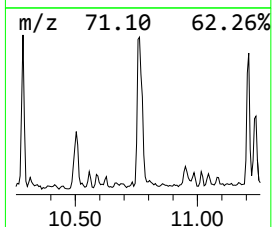
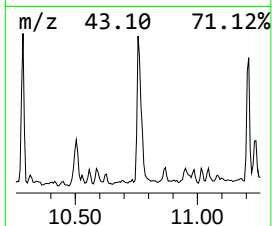
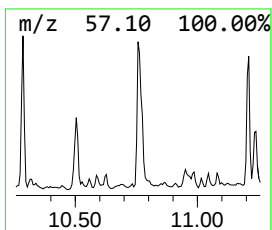
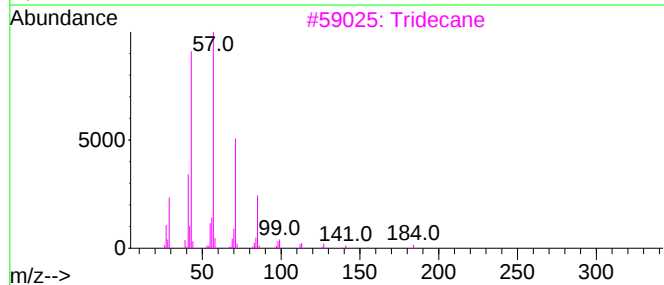
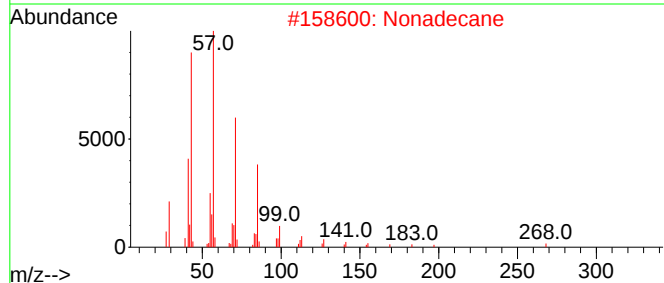
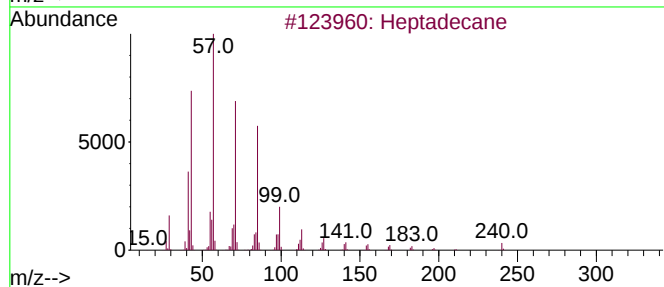
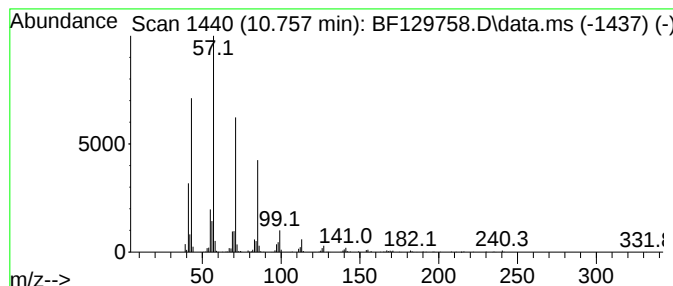
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Heptadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.757	14.20 ng	670441	Phenanthrene-d10	11.363

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane	240	C17H36	000629-78-7	96
2		Nonadecane	268	C19H40	000629-92-5	91
3		Tridecane	184	C13H28	000629-50-5	87
4		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80
5		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	80



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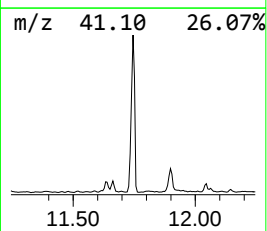
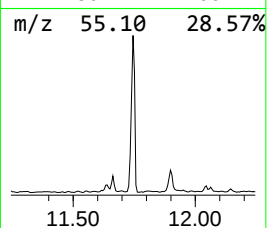
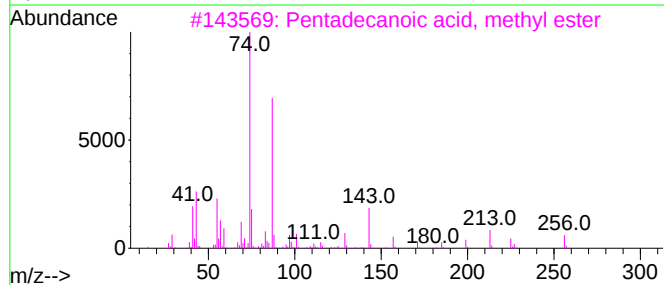
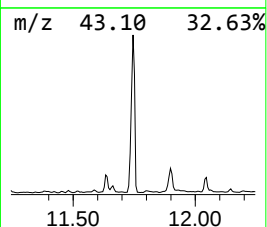
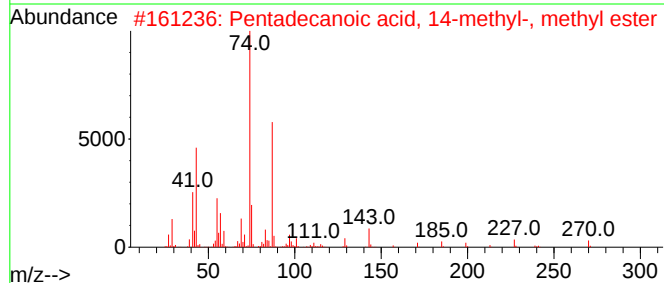
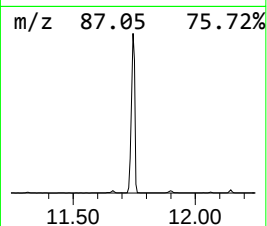
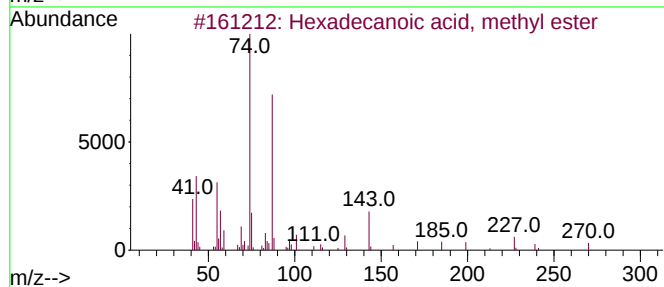
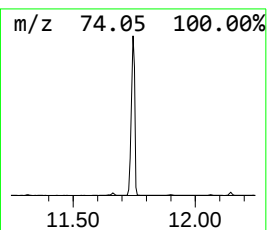
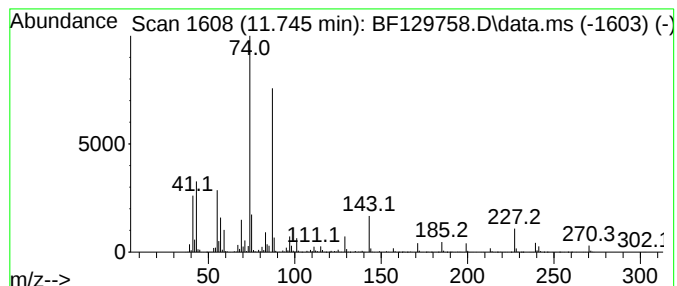
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.745	173.20 ng	8179190	Phenanthrene-d10	11.363

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			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
4			Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	87
5			Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	80



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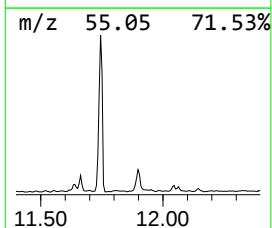
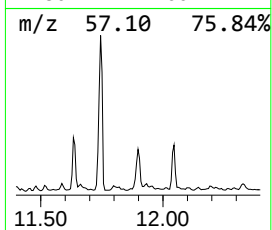
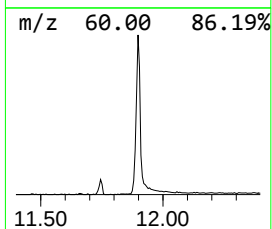
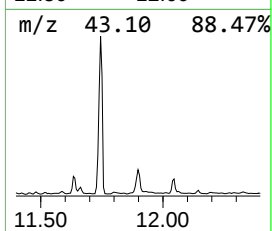
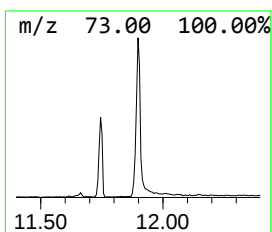
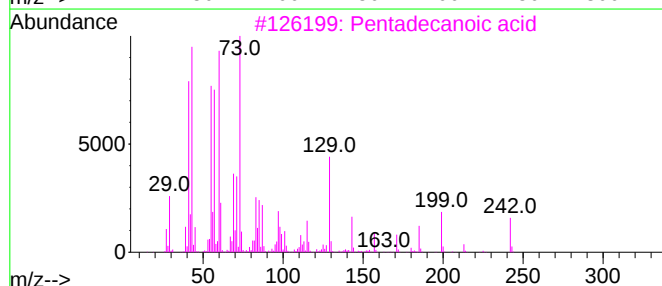
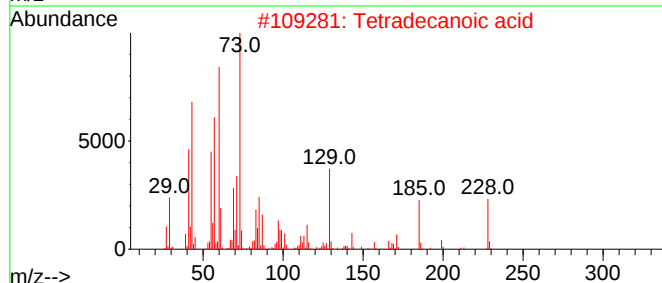
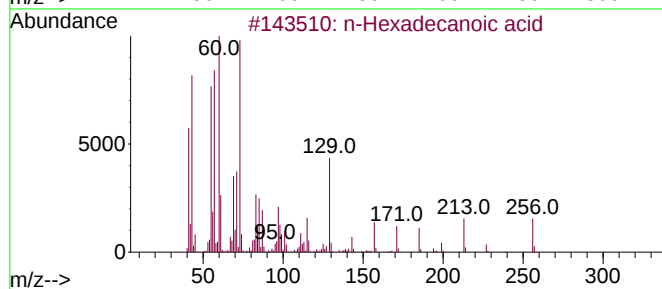
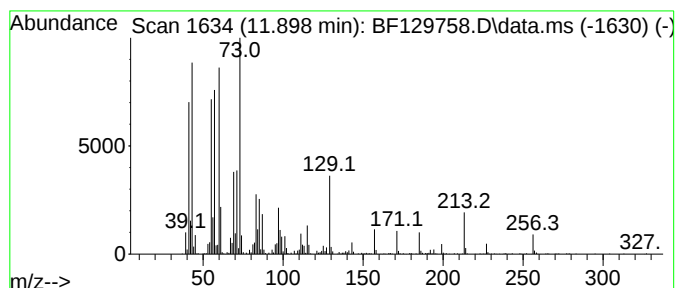
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.898	23.65 ng	1117030	Phenanthrene-d10	11.363	
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	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Octadecanoic acid	284	C18H36O2	000057-11-4	87
5	Tridecanoic acid	214	C13H26O2	000638-53-9	74



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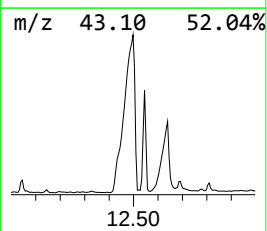
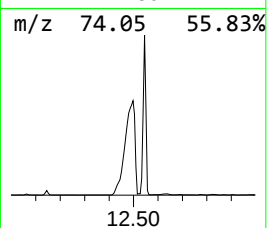
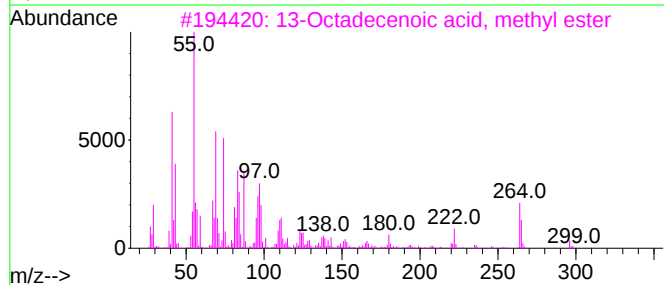
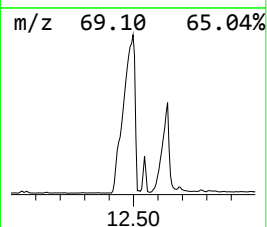
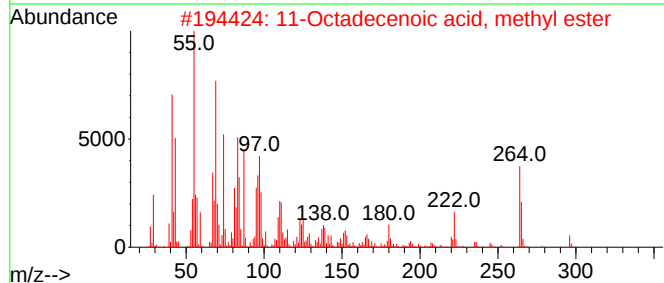
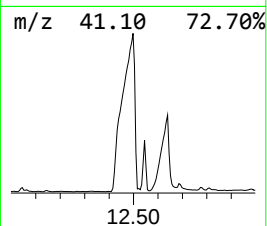
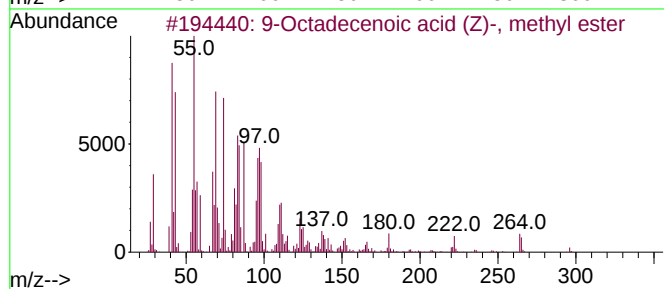
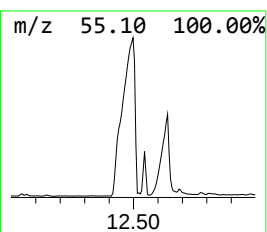
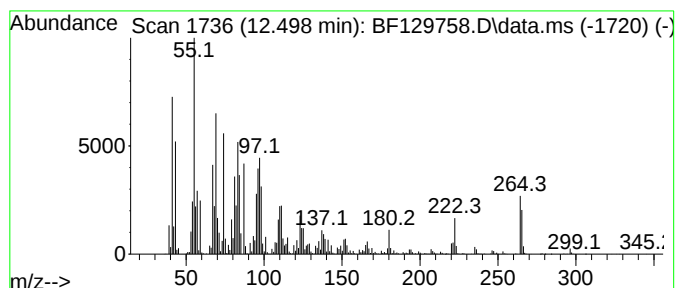
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TIC Integration Parameters: LSCINT.P

Peak Number 4 9-Octadecenoic acid (Z)-, m... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.498	1419.12 ng	67017800	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2			11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	99
3			13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
4			6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	98
5			14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	98



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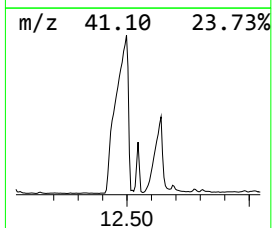
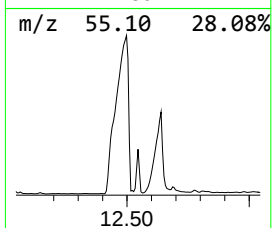
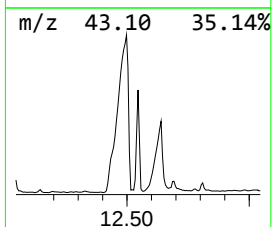
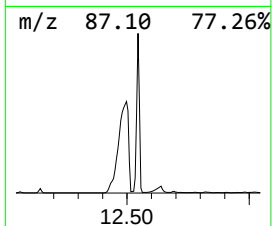
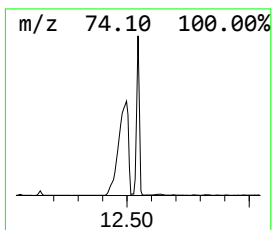
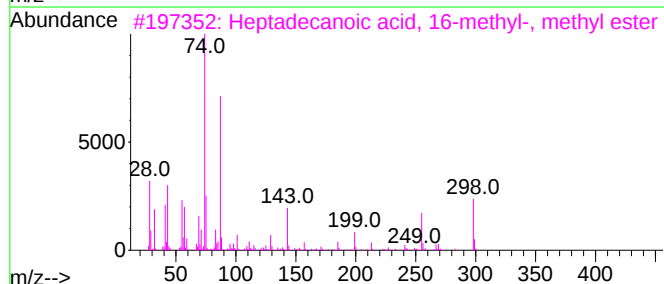
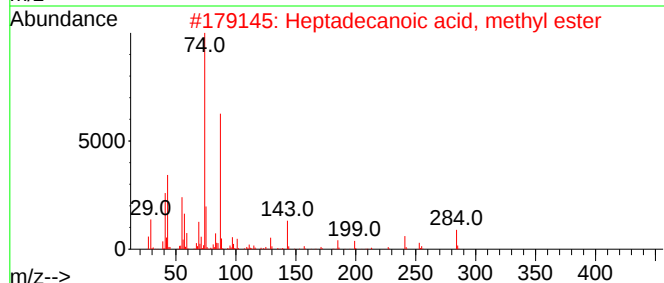
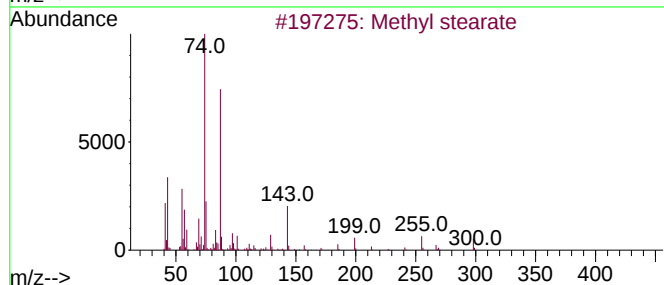
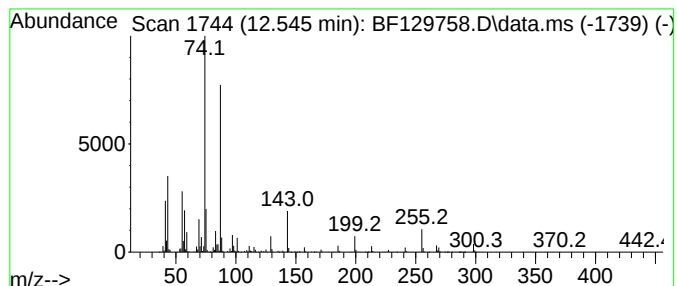
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Methyl stearate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.545	106.78 ng	5042690	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	98
2			Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	91
3			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	90
4			Methyl tetradecanoate	242	C15H30O2	000124-10-7	90
5			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	90



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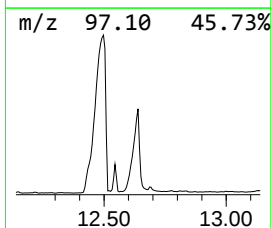
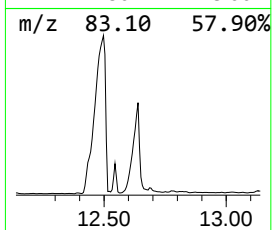
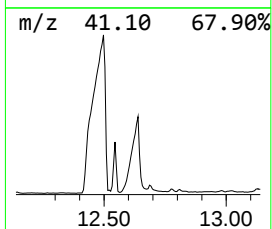
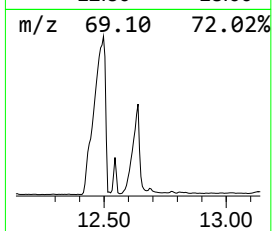
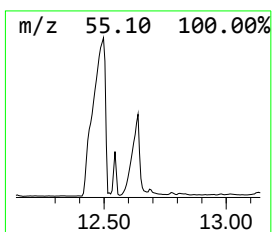
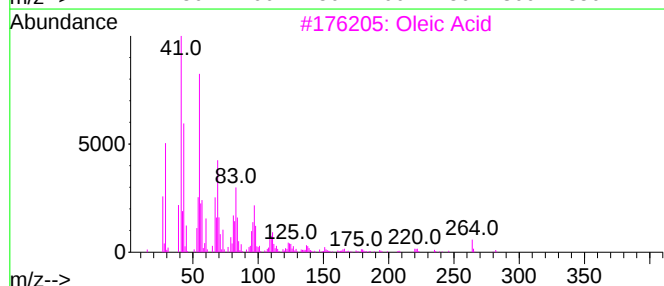
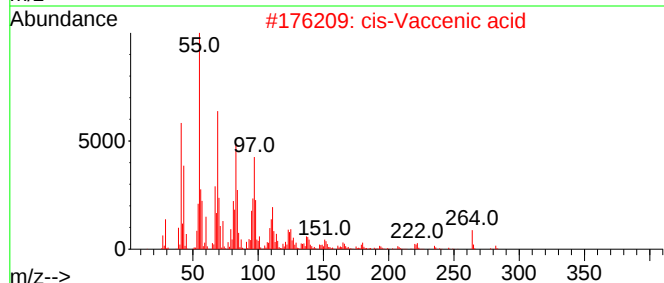
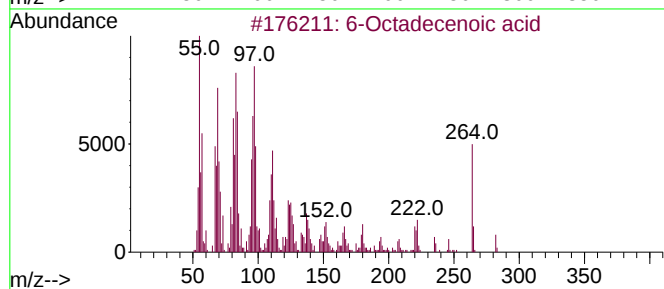
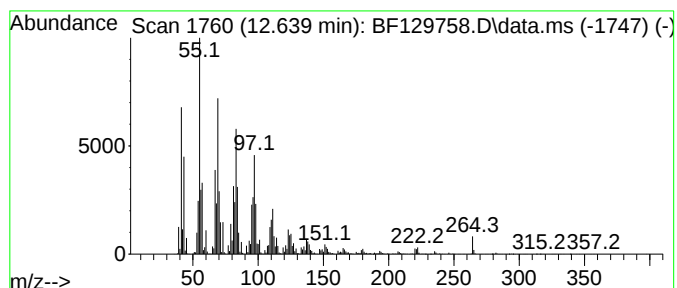
Instrument :
BNA_F
ClientSampleId :
WC-5

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 6 6-Octadecenoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.639	349.45 ng	16502800	Phenanthrene-d10	11.363	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Octadecenoic acid	282	C18H34O2	1000336-66-8	98
2	cis-Vaccenic acid	282	C18H34O2	000506-17-2	94
3	Oleic Acid	282	C18H34O2	000112-80-1	94
4	6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	91
5	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081222\
Data File : BF129758.D
Acq On : 12 Aug 2022 22:39
Operator : CG\JU
Sample : N4136-03 5X
Misc :
ALS Vial : 21 Sample Multiplier: 1

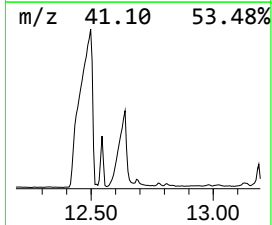
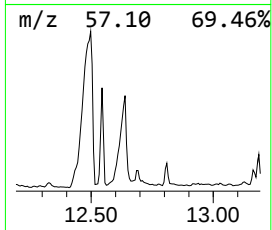
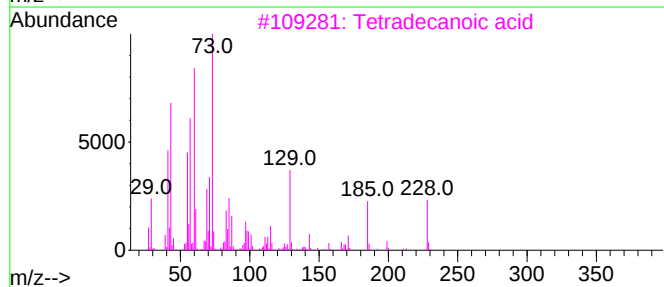
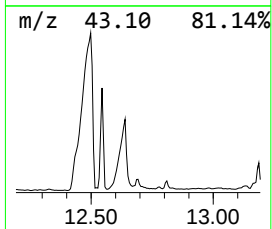
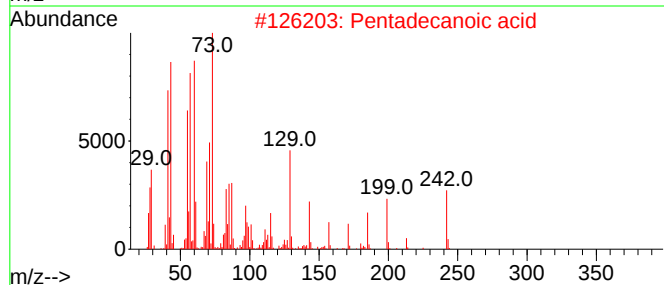
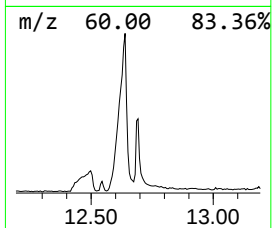
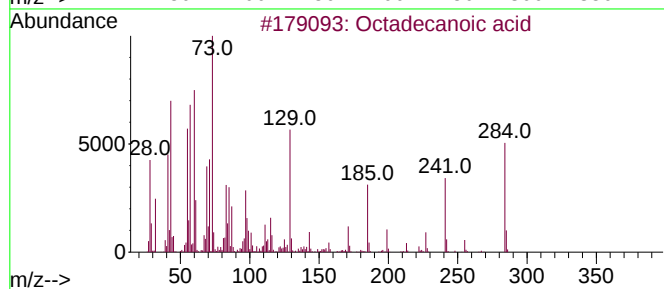
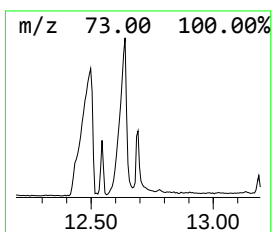
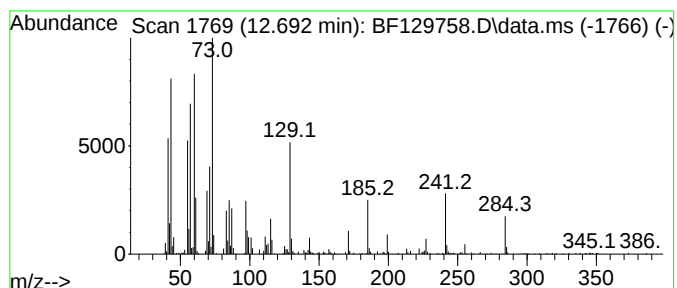
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.692	26.77 ng	1088880	Chrysene-d12	14.015	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	n-Decanoic acid	172	C10H20O2	000334-48-5	62
5	n-Decyl .alpha.-d-2-deoxyglucoside	304	C16H32O5	1000211-42-8	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081222\
Data File : BF129758.D
Acq On : 12 Aug 2022 22:39
Operator : CG\JU
Sample : N4136-03 5X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-5

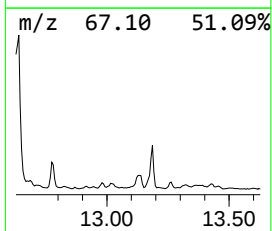
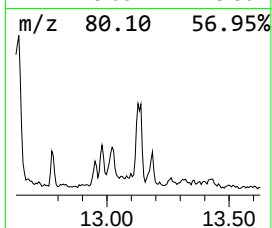
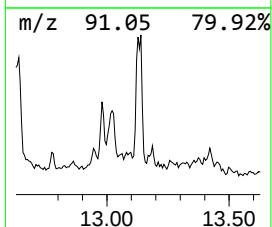
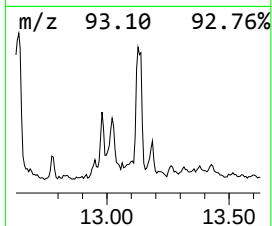
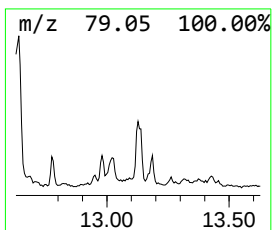
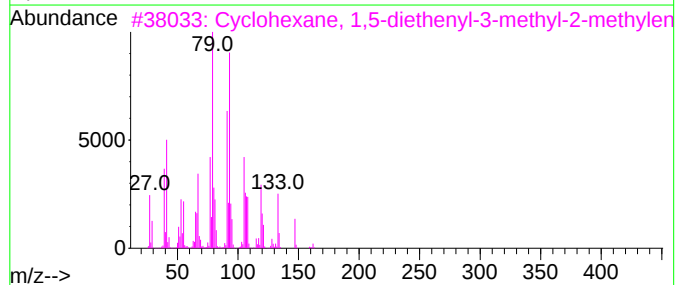
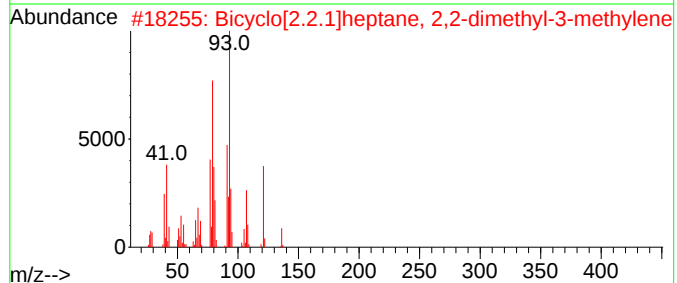
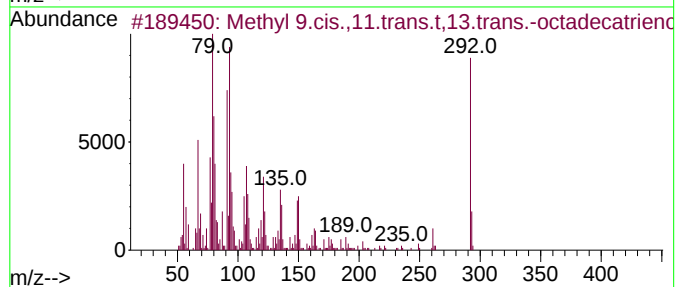
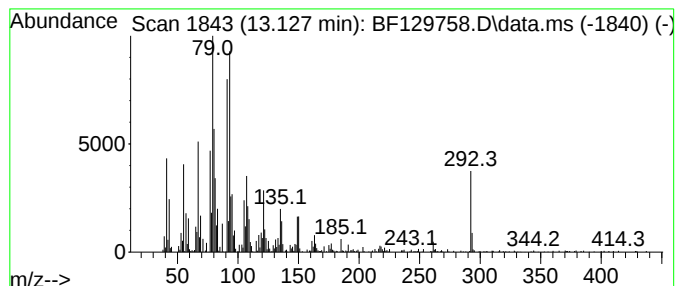
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Methyl 9.cis.,11.trans.t,13... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.127	16.66 ng	677513	Chrysene-d12	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl 9.cis.,11.trans.t,13.tran...	292	C19H32O2	1000336-42-6	99
2			Bicyclo[2.2.1]heptane, 2,2-dimet...	136	C10H16	005794-03-6	68
3			Cyclohexane, 1,5-diethenyl-3-met...	162	C12H18	074742-35-1	64
4			6-Butyl-1,4-cycloheptadiene	150	C11H18	022735-58-6	58
5			Cyclopentane, 1-ethenyl-3-methyl...	108	C8H12	029668-63-1	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081222\
Data File : BF129758.D
Acq On : 12 Aug 2022 22:39
Operator : CG\JU
Sample : N4136-03 5X
Misc :
ALS Vial : 21 Sample Multiplier: 1

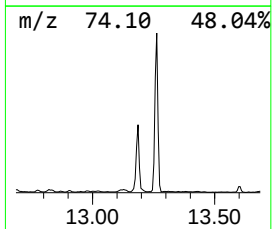
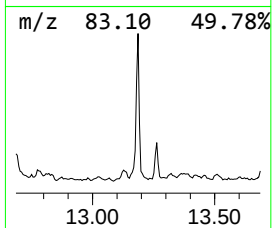
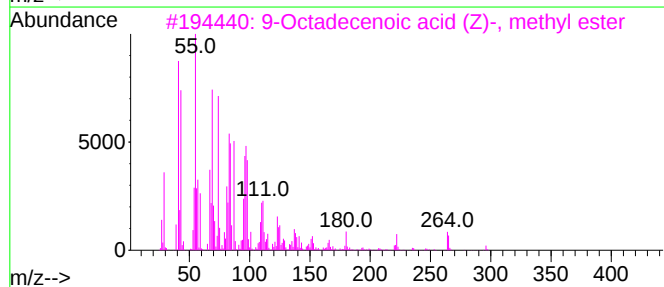
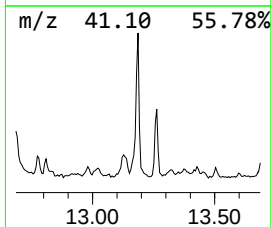
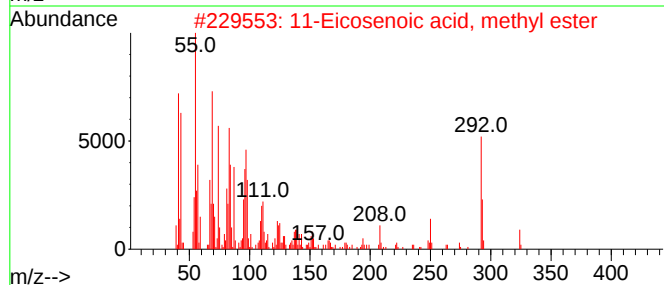
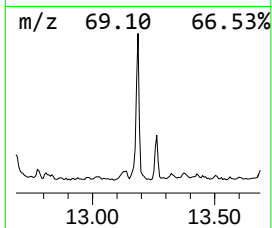
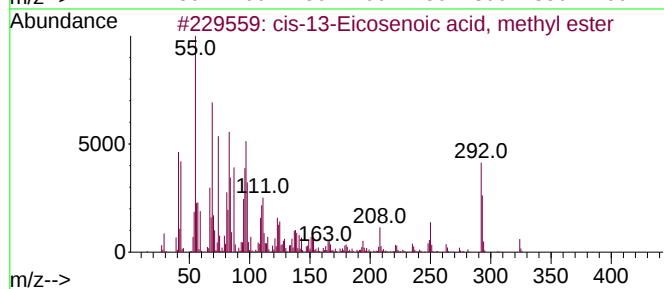
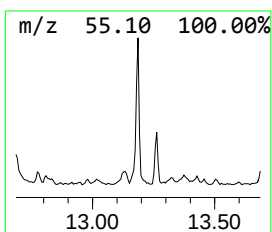
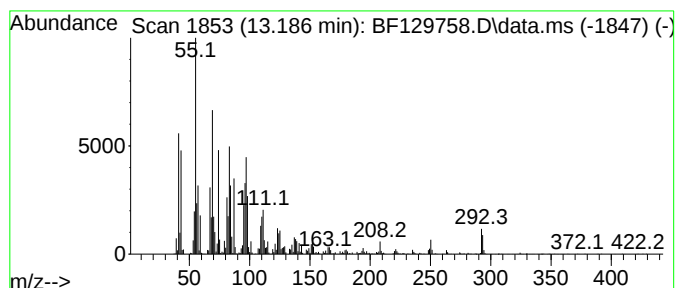
Instrument :
BNA_F
ClientSampleId :
WC-5

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 9 cis-13-Eicosenoic acid, met... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.186	55.89 ng	2273090	Chrysene-d12	14.015	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-13-Eicosenoic acid, methyl e...	324	C21H40O2	069120-02-1	94
2	11-Eicosenoic acid, methyl ester	324	C21H40O2	003946-08-5	94
3	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	94
4	cis-Methyl 11-eicosenoate	324	C21H40O2	002390-09-2	91
5	Methyl 9-eicosenoate	324	C21H40O2	1000336-50-5	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081222\
Data File : BF129758.D
Acq On : 12 Aug 2022 22:39
Operator : CG\JU
Sample : N4136-03 5X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-5

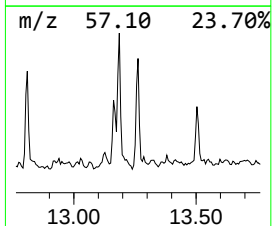
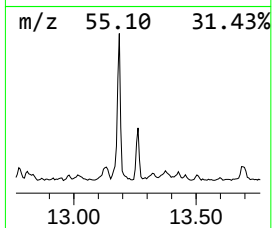
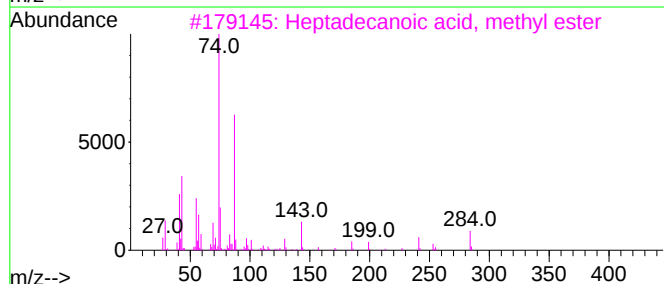
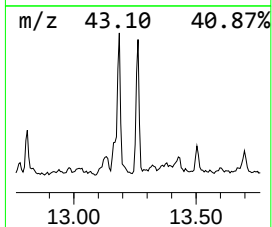
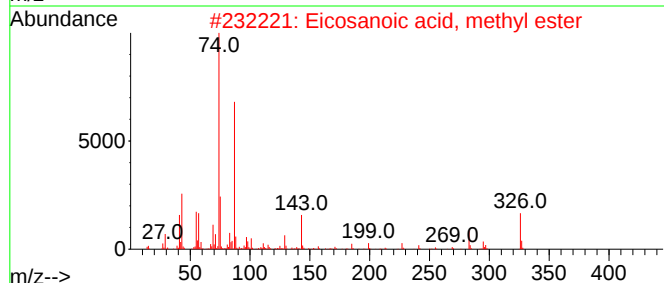
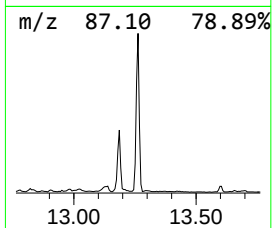
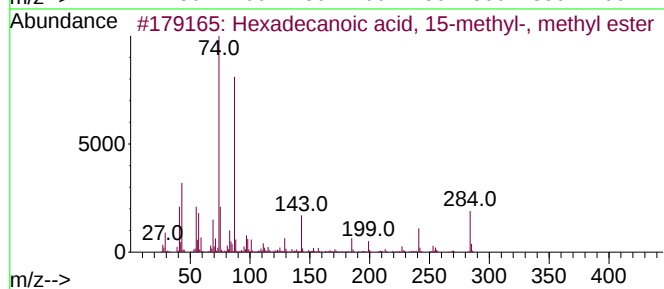
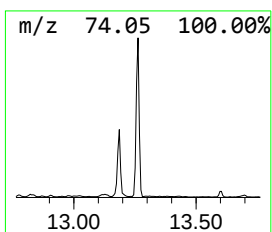
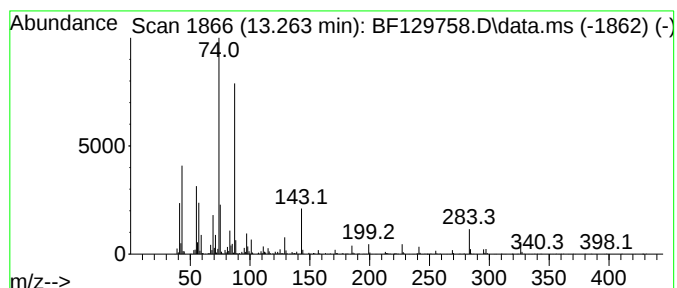
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexadecanoic acid, 15-methy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.263	30.67 ng	1247310	Chrysene-d12	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	93
2			Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	91
3			Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	90
4			Methyl stearate	298	C19H38O2	000112-61-8	90
5			Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081222\
Data File : BF129758.D
Acq On : 12 Aug 2022 22:39
Operator : CG\JU
Sample : N4136-03 5X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-5

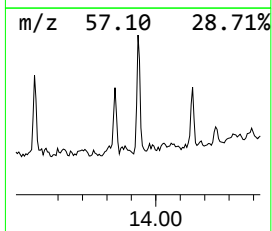
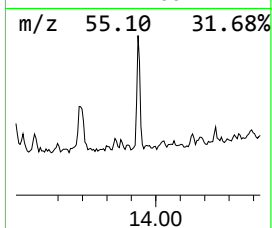
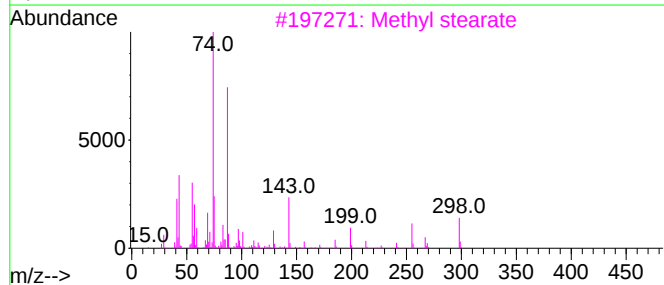
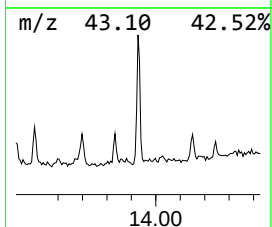
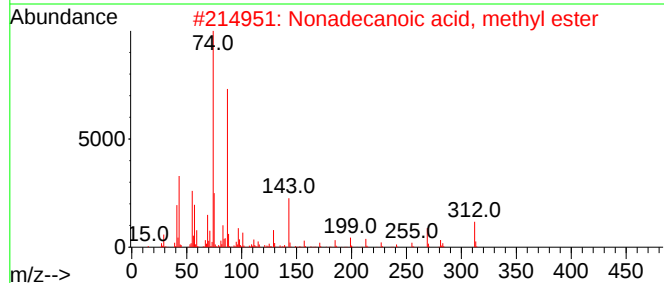
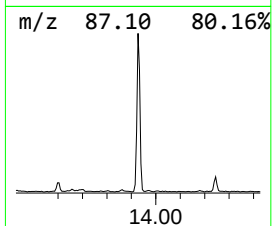
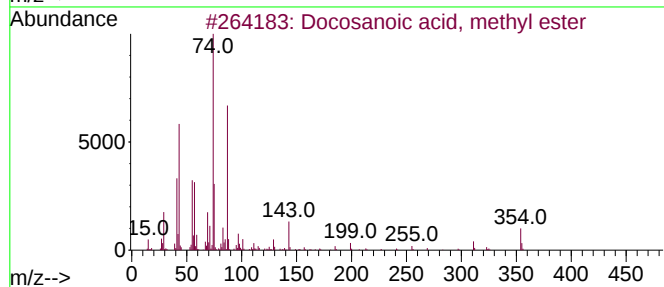
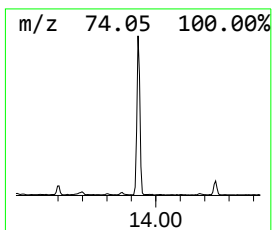
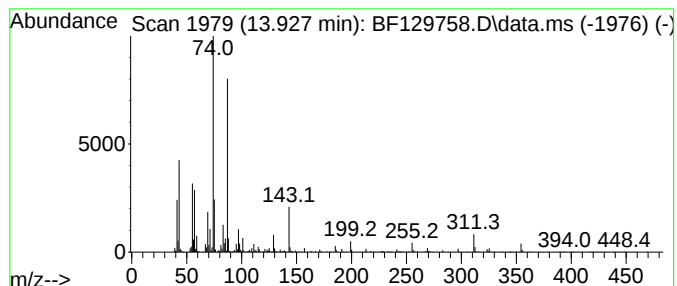
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Docosanoic acid, methyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.927	21.36 ng	868464	Chrysene-d12	14.015

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	90
3			Methyl stearate	298	C19H38O2	000112-61-8	86
4			Methyl tetradecanoate	242	C15H30O2	000124-10-7	83
5			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081222\
Data File : BF129758.D
Acq On : 12 Aug 2022 22:39
Operator : CG\JU
Sample : N4136-03 5X
Misc :
ALS Vial : 21 Sample Multiplier: 1

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\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Hexadecanoic ac...	11.745	173.2	ng	8179190	4	11.363	944499	20.0
n-Hexadecanoic ...	11.898	23.6	ng	1117030	4	11.363	944499	20.0
9-Octadecenoic ...	12.498	1419.1	ng	67017800	4	11.363	944499	20.0
Methyl stearate	12.545	106.8	ng	5042690	4	11.363	944499	20.0
6-Octadecenoic ...	12.639	349.4	ng	16502800	4	11.363	944499	20.0
Octadecanoic acid	12.692	26.8	ng	1088880	5	14.015	813358	20.0
Methyl 9.cis.,1...	13.127	16.7	ng	677513	5	14.015	813358	20.0
cis-13-Eicoseno...	13.186	55.9	ng	2273090	5	14.015	813358	20.0
Hexadecanoic ac...	13.263	30.7	ng	1247310	5	14.015	813358	20.0
Docosanoic acid...	13.927	21.4	ng	868464	5	14.015	813358	20.0