

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101822\
 Data File : BF130707.D
 Acq On : 18 Oct 2022 19:56
 Operator : CG\JU
 Sample : N5162-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TR-4-101422

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-BF101122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130707.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.181	557	560	577	rBV	1093140	1148658	1.63%	0.843%
2	6.234	735	739	755	rBV	1040850	1095862	1.56%	0.804%
3	8.934	1194	1198	1201	rBV	1544255	1173572	1.67%	0.861%
4	10.398	1441	1447	1450	rBV	932061	808950	1.15%	0.593%
5	11.522	1629	1638	1640	rBV	9856462	15655524	22.23%	11.485%
6	11.698	1656	1668	1671	rBV	2215161	4687915	6.66%	3.439%
7	12.263	1745	1764	1766	rBV2	15309829	70433605	100.00%	51.670%
8	12.327	1771	1775	1777	rVV	10262869	10375818	14.73%	7.612%
9	12.398	1777	1787	1793	rVV2	6689619	21088411	29.94%	15.470%
10	12.457	1795	1797	1805	rVV	1305631	1502041	2.13%	1.102%
11	12.698	1834	1838	1841	rVB	1686863	1318989	1.87%	0.968%
12	12.874	1865	1868	1873	rVB4	485505	821192	1.17%	0.602%
13	12.933	1873	1878	1881	rBV2	915775	1287970	1.83%	0.945%
14	13.016	1888	1892	1895	rBV	1199891	1092476	1.55%	0.801%
15	13.057	1896	1899	1904	rBV3	635279	950813	1.35%	0.698%
16	13.174	1914	1919	1922	rVV2	776604	1105938	1.57%	0.811%
17	13.445	1960	1965	1968	rVB2	570079	712633	1.01%	0.523%
18	13.674	2001	2004	2008	rBV	1093039	1054543	1.50%	0.774%

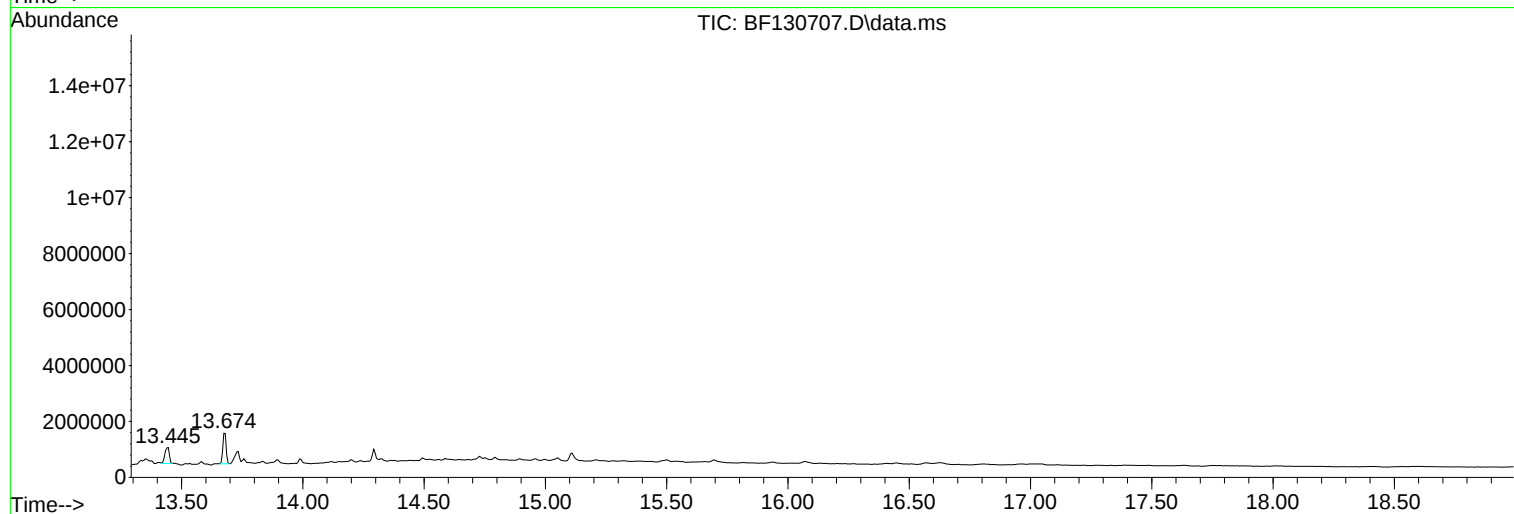
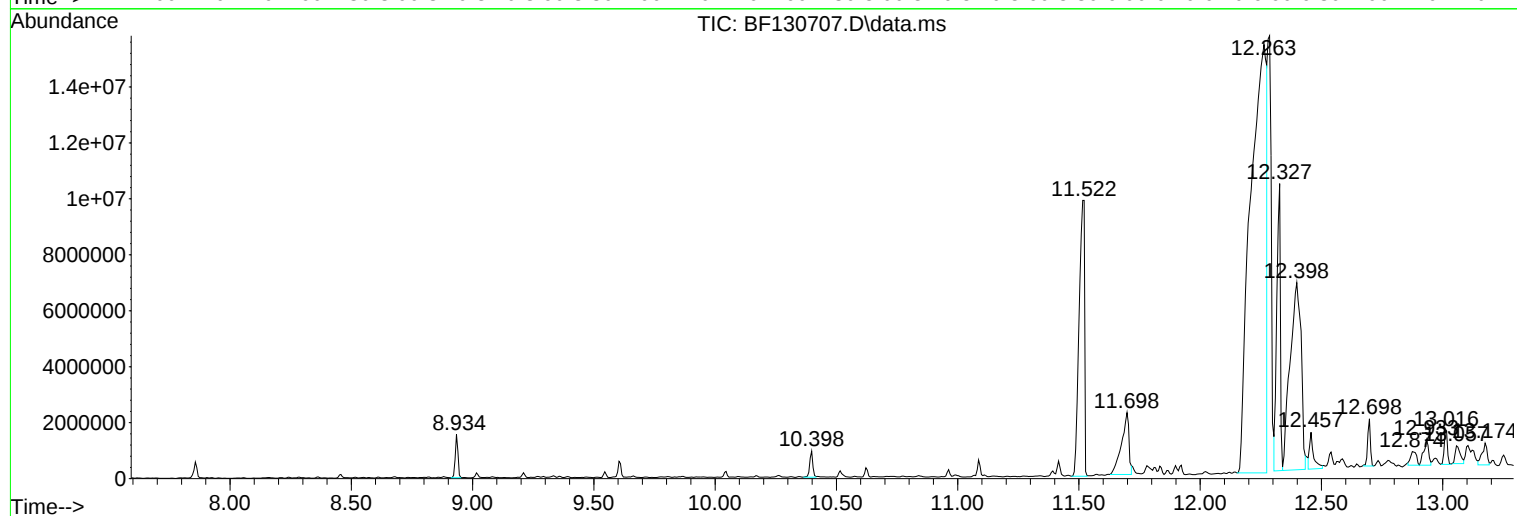
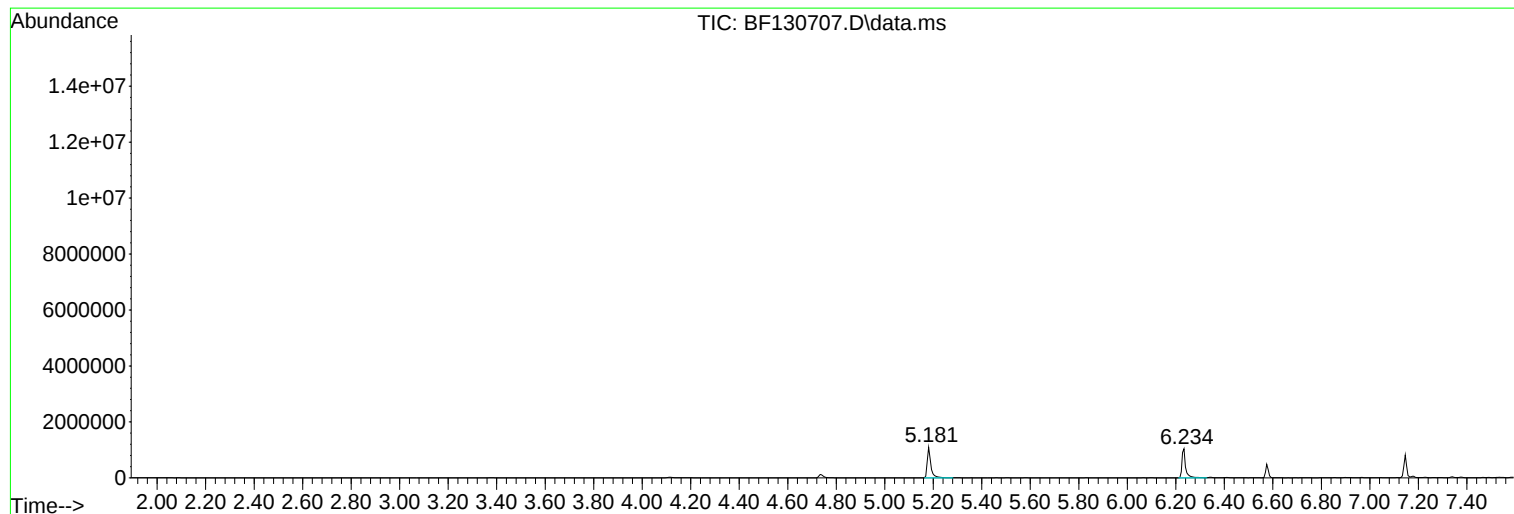
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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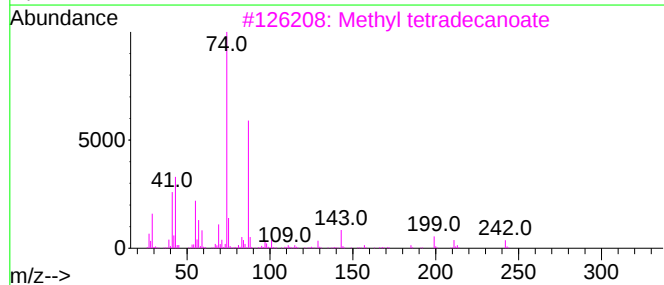
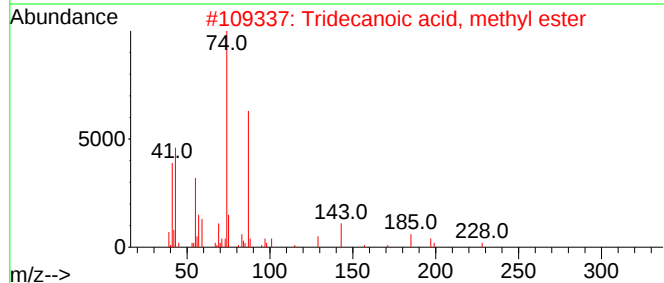
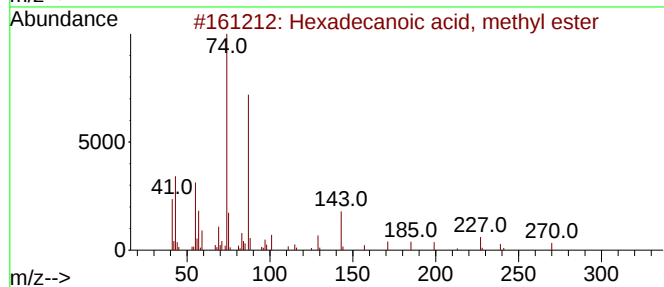
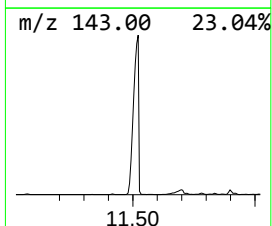
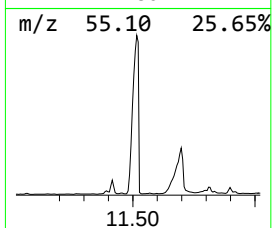
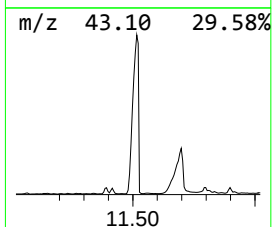
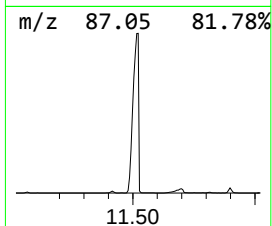
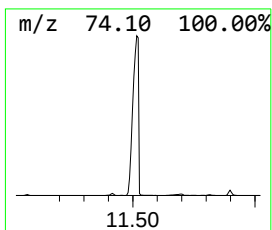
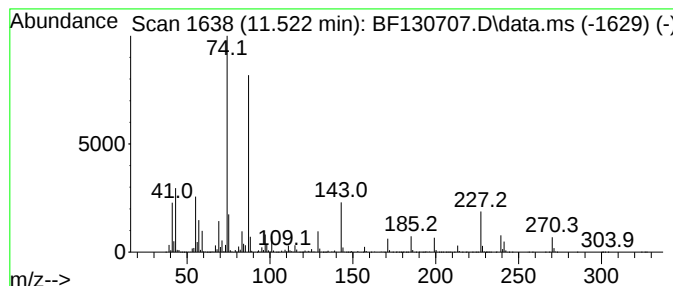
Instrument :
BNA_F
ClientSampleId :
TR-4-101422

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101122.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 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.522	20.00 ng	15655500	Phenanthrene-d10	11.086	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	96
2	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	81
4	Hexadecanoic acid, 2-methyl-	270	C17H34O2	027147-71-3	72
5	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	70



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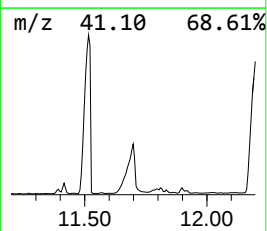
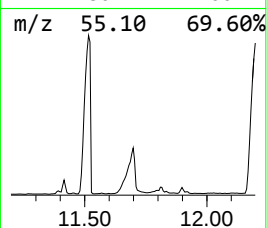
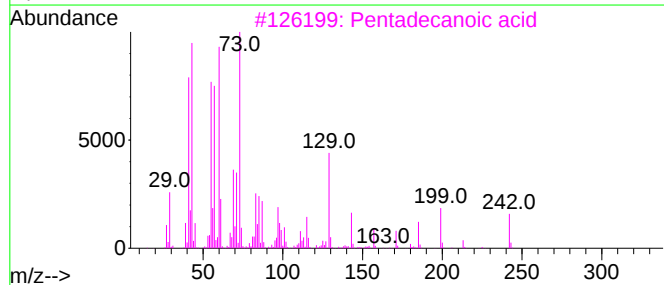
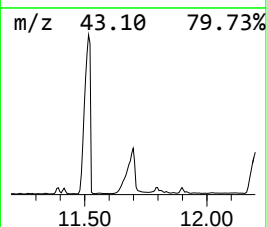
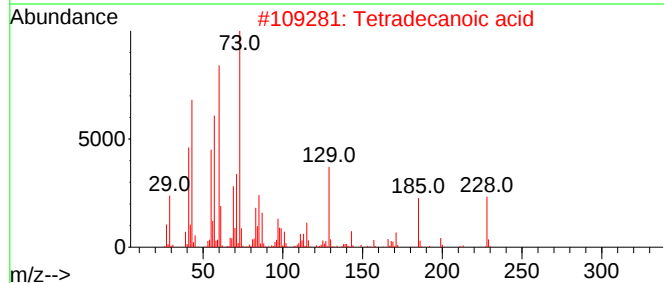
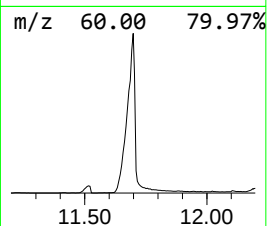
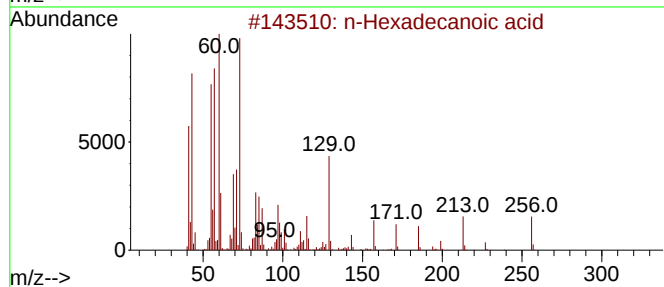
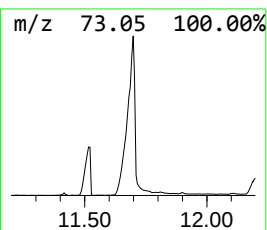
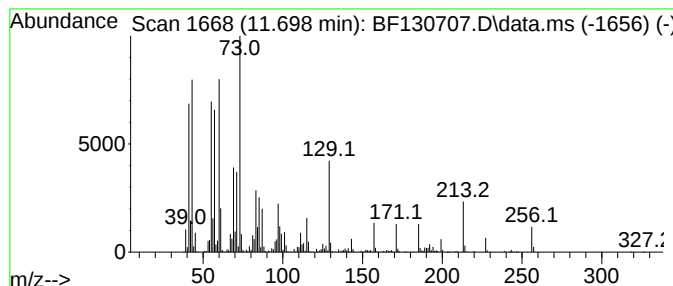
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.698	5.99 ng	4687920	Phenanthrene-d10	11.086

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	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tridecanoic acid	214	C13H26O2	000638-53-9	83
5			Undecanoic acid	186	C11H22O2	000112-37-8	74



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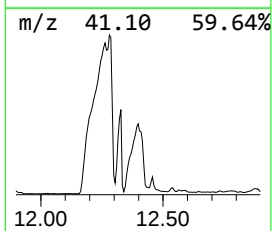
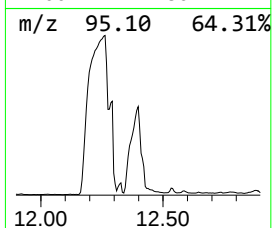
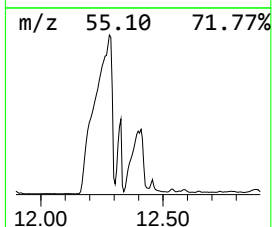
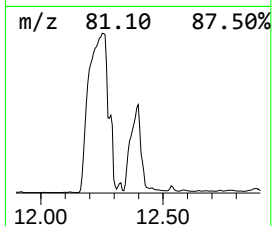
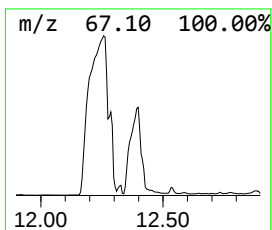
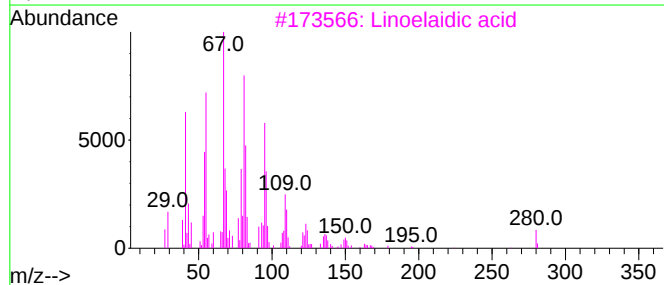
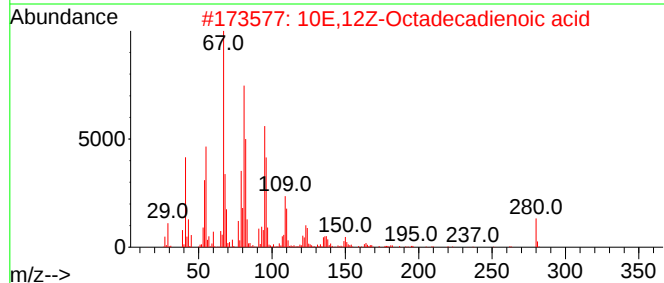
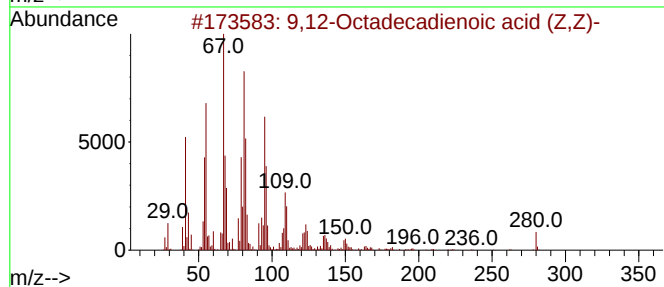
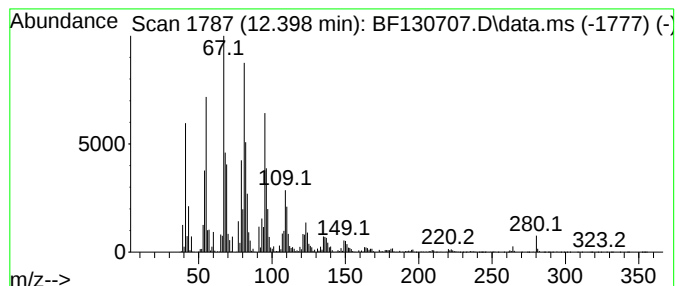
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 9,12-Octadecadienoic acid (... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.398	26.94 ng	21088400	Phenanthrene-d10	11.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	99
2			10E,12Z-Octadecadienoic acid	280	C18H32O2	002420-56-6	99
3			Linoelaidic acid	280	C18H32O2	000506-21-8	98
4			(9E,11E)-Octadecadienoic acid	280	C18H32O2	000544-71-8	98
5			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	91



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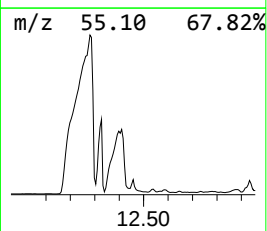
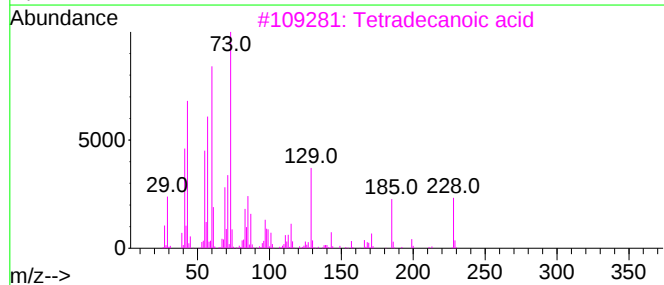
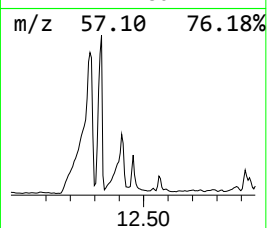
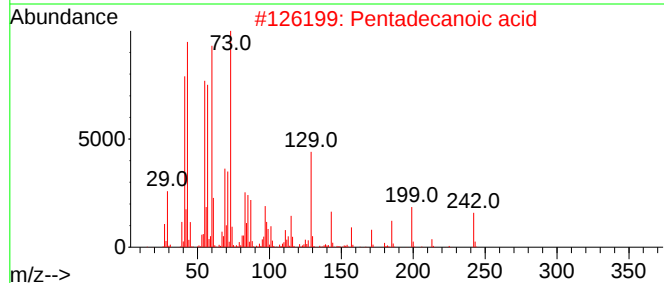
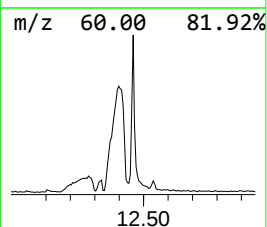
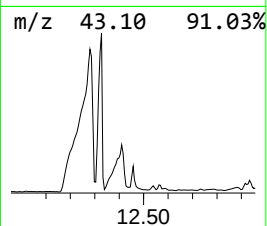
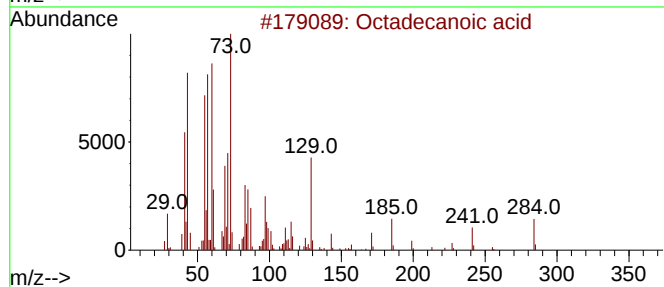
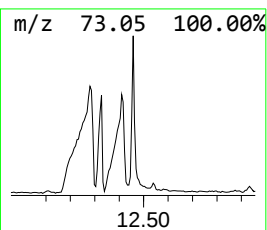
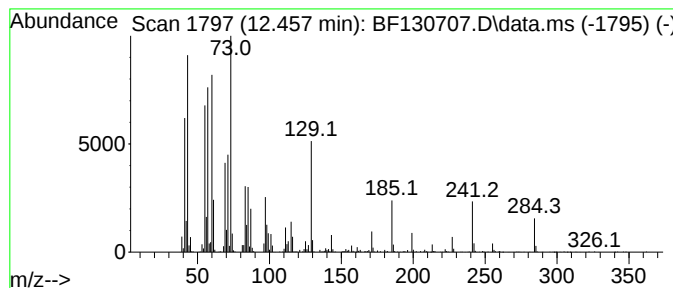
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.457	28.49 ng	1502040	Chrysene-d12	13.733

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
5			Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	55



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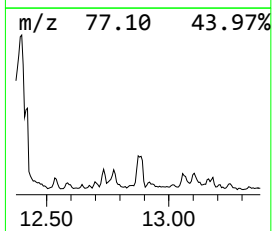
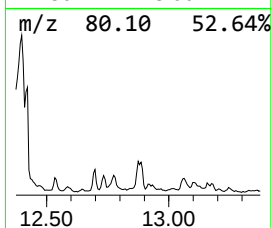
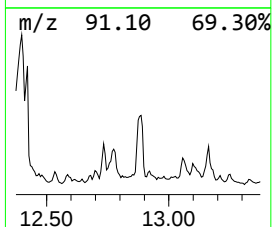
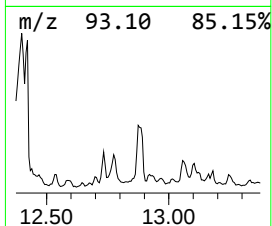
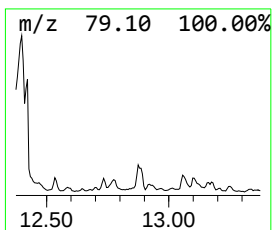
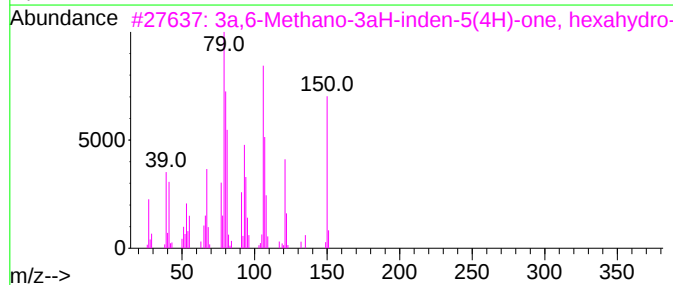
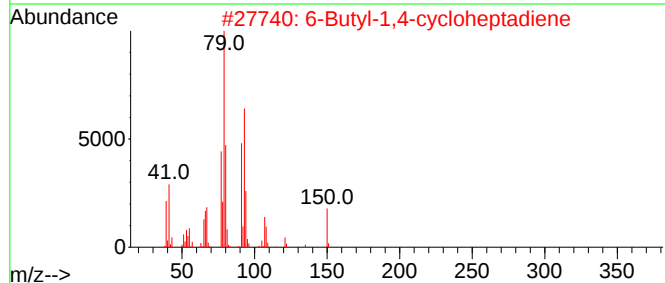
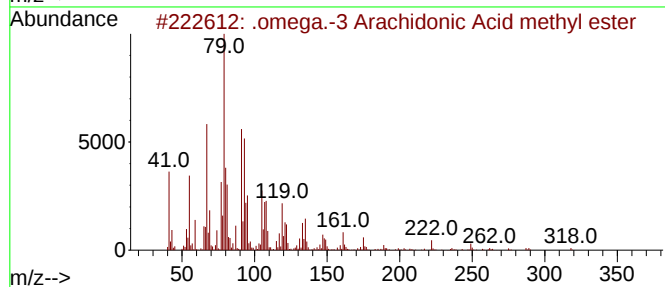
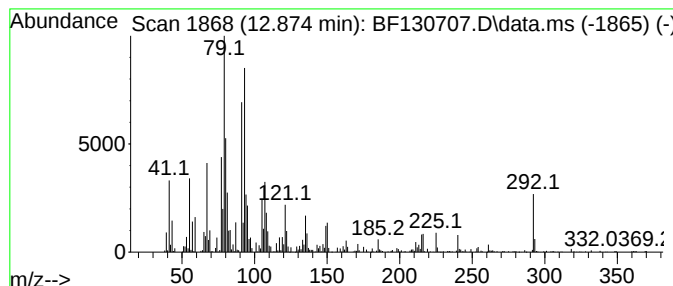
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 .omega.-3 Arachidonic Acid ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.874	15.57 ng	821192	Chrysene-d12	13.733

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.omega.-3 Arachidonic Acid methy...	318	C21H34O2	132712-70-0	78
2			6-Butyl-1,4-cycloheptadiene	150	C11H18	022735-58-6	58
3			3a,6-Methano-3aH-inden-5(4H)-one...	150	C10H14O	016489-26-2	53
4			Santolina triene	136	C10H16	002153-66-4	52
5			5,8,11,14-Eicosatetraenoic acid,...	318	C21H34O2	002566-89-4	49



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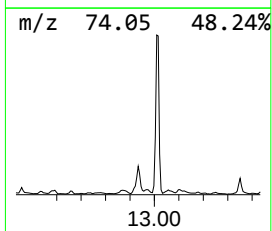
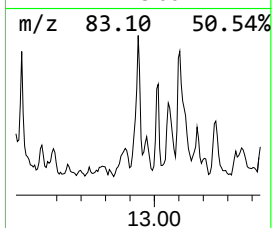
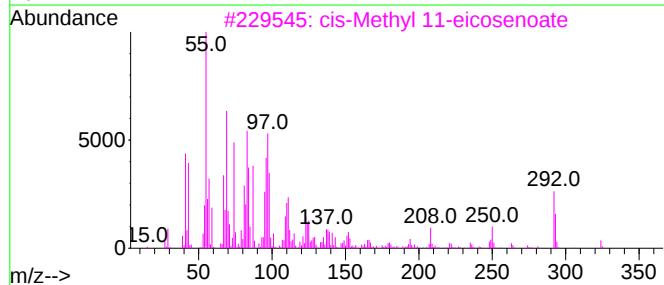
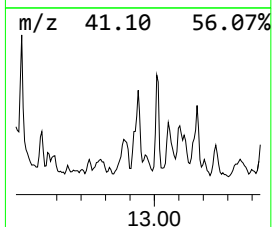
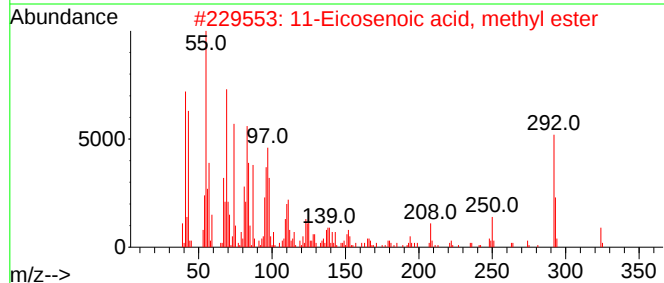
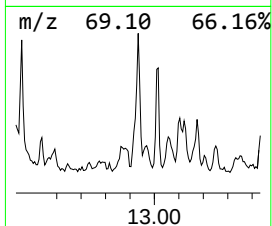
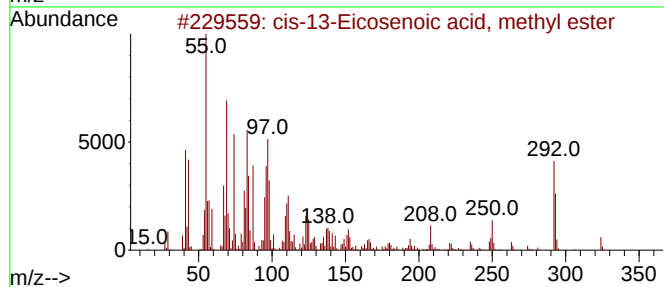
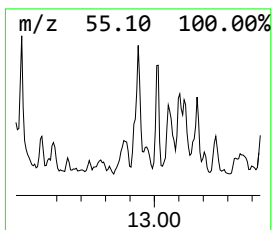
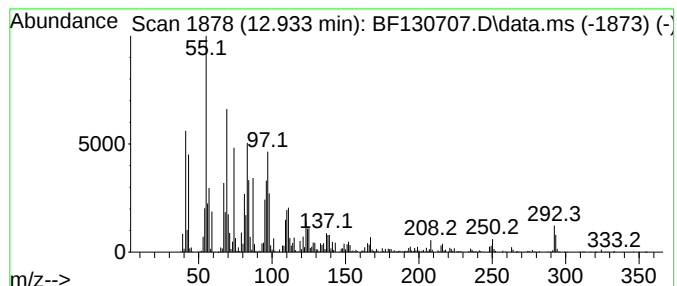
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 cis-13-Eicosenoic acid, met... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.933	24.43 ng	1287970	Chrysene-d12	13.733

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-13-Eicosenoic acid, methyl e...	324	C21H40O2	069120-02-1	99
2			11-Eicosenoic acid, methyl ester	324	C21H40O2	003946-08-5	99
3			cis-Methyl 11-eicosenoate	324	C21H40O2	002390-09-2	99
4			cis-10-Heptadecenoic acid, methy...	282	C18H34O2	1000333-62-1	96
5			9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101822\
Data File : BF130707.D
Acq On : 18 Oct 2022 19:56
Operator : CG\JU
Sample : N5162-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-4-101422

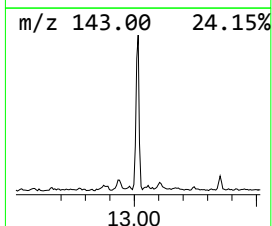
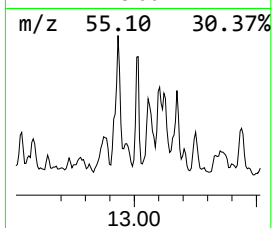
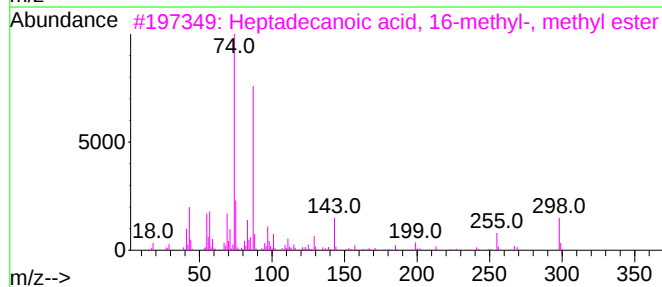
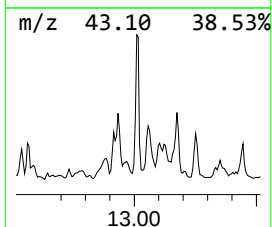
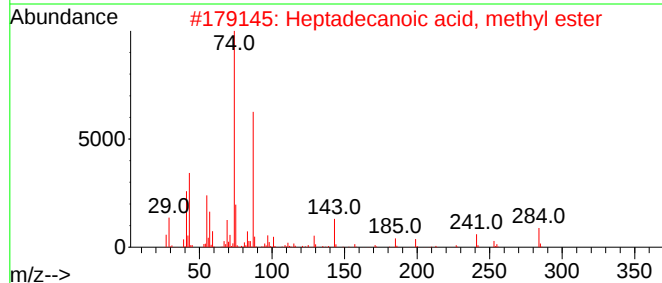
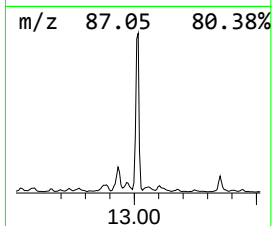
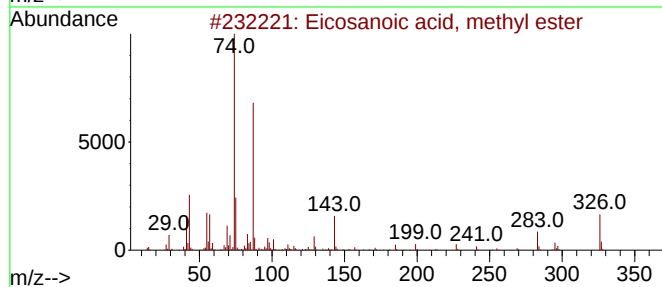
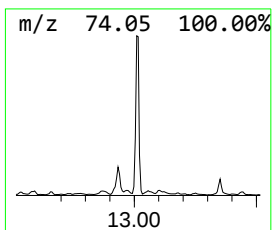
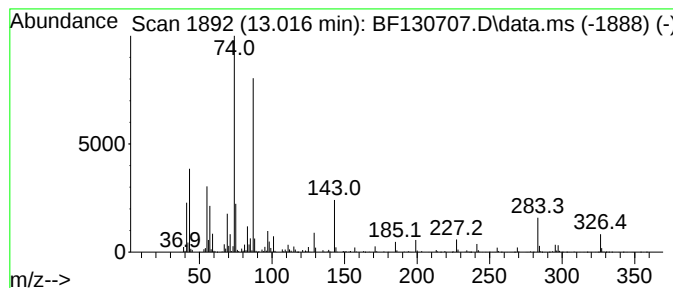
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosanoic acid, methyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.016	20.72 ng	1092480	Chrysene-d12	13.733

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	99
2			Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	93
3			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	91
4			Methyl 18-methylnonadecanoate	326	C21H42O2	1000424-52-4	90
5			Methyl stearate	298	C19H38O2	000112-61-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101822\
Data File : BF130707.D
Acq On : 18 Oct 2022 19:56
Operator : CG\JU
Sample : N5162-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-4-101422

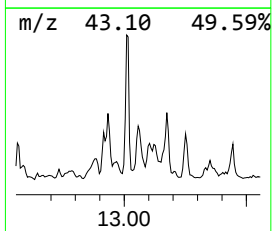
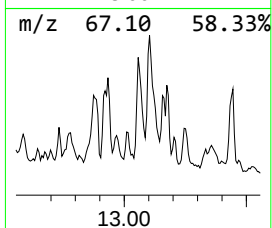
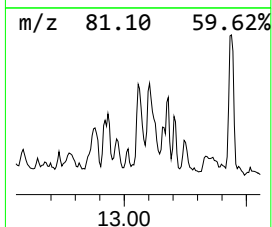
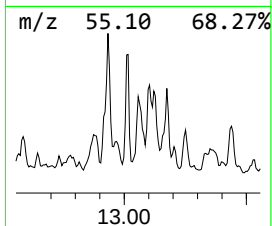
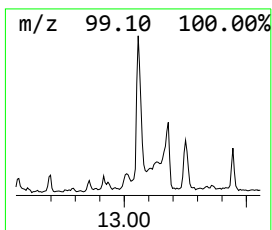
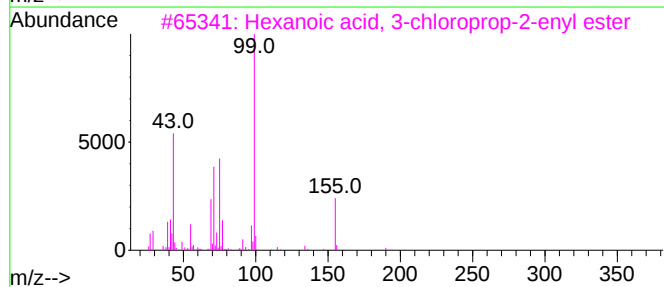
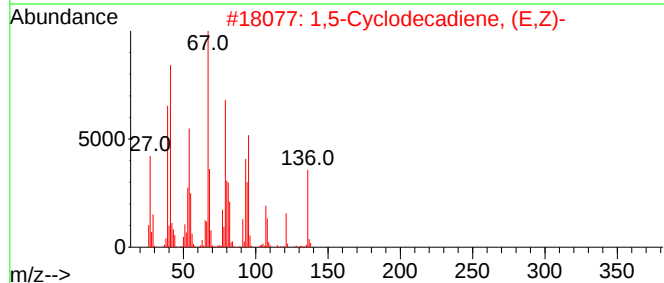
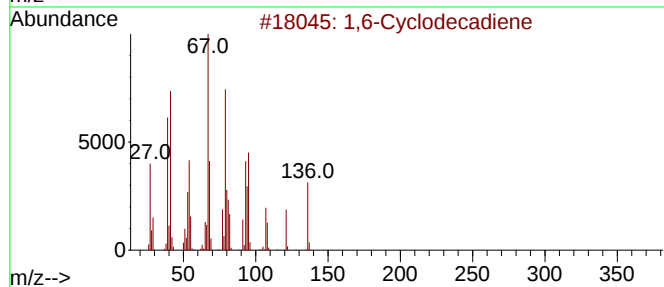
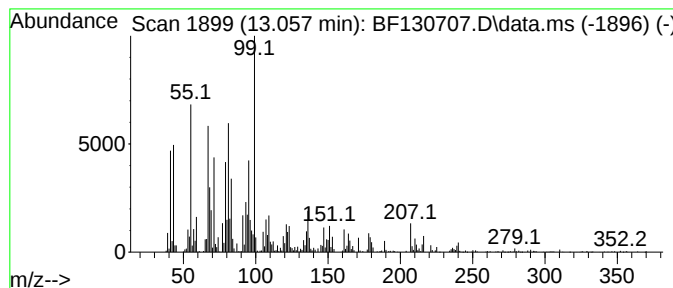
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown13.057 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.057	18.03 ng	950813	Chrysene-d12	13.733

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,6-Cyclodecadiene	136	C10H16	007049-13-0	42
2			1,5-Cyclodecadiene, (E,Z)-	136	C10H16	001124-78-3	42
3			Hexanoic acid, 3-chloroprop-2-en...	190	C9H15ClO2	1000299-36-1	38
4			Cyclohexanol, 1-(1,2-propadienyl)-	138	C9H14O	034761-56-3	38
5			3-Methyl-cis-3a,4,7,7a-tetrahydr...	136	C10H16	1000144-04-4	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101822\
Data File : BF130707.D
Acq On : 18 Oct 2022 19:56
Operator : CG\JU
Sample : N5162-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-4-101422

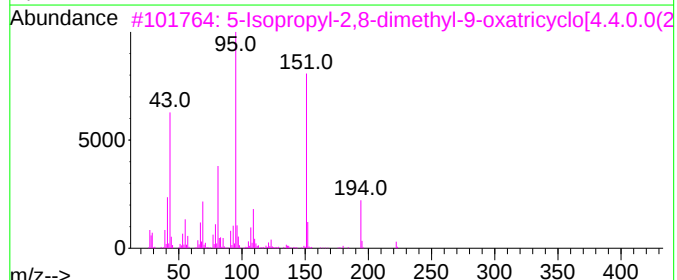
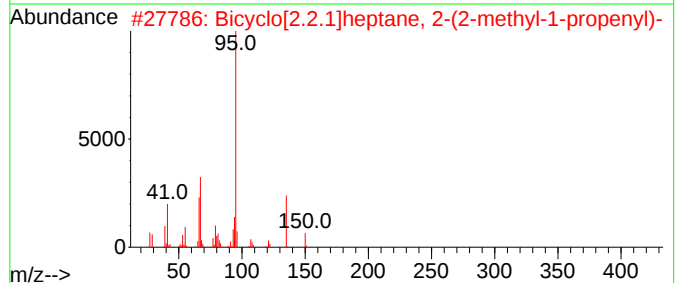
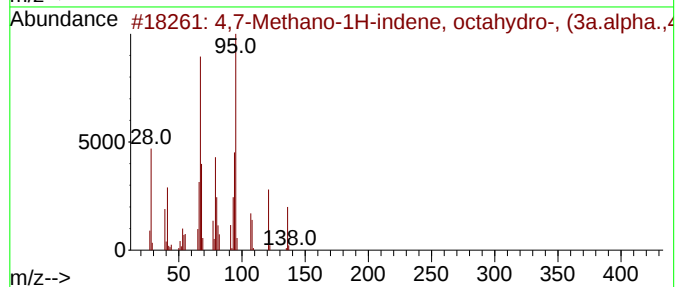
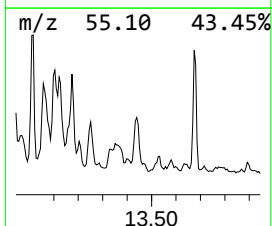
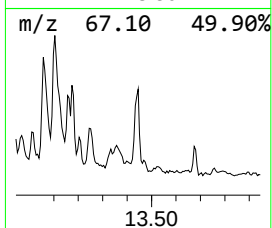
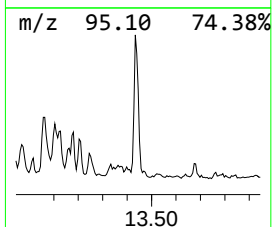
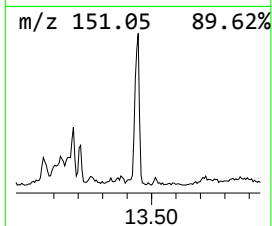
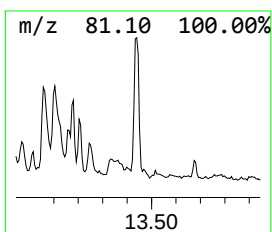
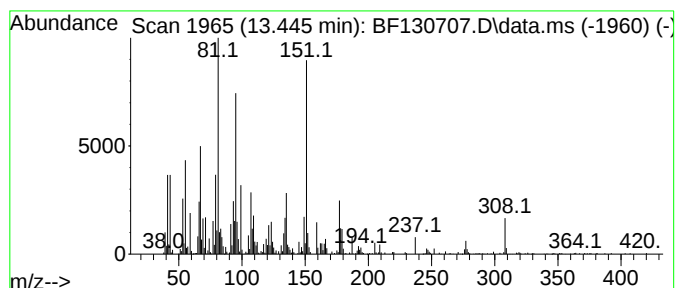
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown13.445 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.445	13.52 ng	712633	Chrysene-d12	13.733

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4,7-Methano-1H-indene, octahydro...	136	C10H16	002825-83-4	38
2			Bicyclo[2.2.1]heptane, 2-(2-meth...	150	C11H18	061142-27-6	27
3			5-Isopropyl-2,8-dimethyl-9-oxatr...	222	C14H22O2	1010185-23-8	22
4			Naphthalene, decahydro-2,2-dimet...	166	C12H22	031124-85-3	14
5			2-Cyanomethyl-hexahydro-pyrimidi...	175	C8H9N5	1000185-88-3	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101822\
Data File : BF130707.D
Acq On : 18 Oct 2022 19:56
Operator : CG\JU
Sample : N5162-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-4-101422

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101122.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 ...	11.698	6.0	ng	4687920	4	11.086	15655500	20.0
9,12-Octadecadi...	12.398	26.9	ng	21088400	4	11.086	15655500	20.0
Octadecanoic acid	12.457	28.5	ng	1502040	5	13.733	1054540	20.0
.omega.-3 Arach...	12.874	15.6	ng	821192	5	13.733	1054540	20.0
cis-13-Eicoseno...	12.933	24.4	ng	1287970	5	13.733	1054540	20.0
Eicosanoic acid...	13.016	20.7	ng	1092480	5	13.733	1054540	20.0
unknown13.057	13.057	18.0	ng	950813	5	13.733	1054540	20.0
unknown13.445	13.445	13.5	ng	712633	5	13.733	1054540	20.0