

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102922\
 Data File : BF130869.D
 Acq On : 29 Oct 2022 21:20
 Operator : CG\JU
 Sample : N5330-01
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TR-5-102722

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-BF102722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130869.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.246	21	27	37	rVB	402769	532402	1.38%	0.744%
2	5.563	586	591	594	rBV	1726745	1545309	4.00%	2.158%
3	6.563	756	761	764	rBV	1573460	1466656	3.80%	2.048%
4	6.945	823	826	830	rBV	468438	391115	1.01%	0.546%
5	7.510	918	922	925	rBV	1018409	852961	2.21%	1.191%
6	8.233	1041	1045	1048	rBV	533796	421320	1.09%	0.588%
7	9.310	1224	1228	1231	rBV	1666365	1364700	3.54%	1.906%
8	9.992	1339	1344	1348	rBV	589315	445978	1.16%	0.623%
9	10.780	1475	1478	1482	rVB	1113095	923198	2.39%	1.289%
10	11.486	1594	1598	1600	rBV	585223	492531	1.28%	0.688%
11	11.886	1660	1666	1669	rBV	9407652	10165238	26.33%	14.196%
12	12.027	1684	1690	1695	rBV2	1067043	1361356	3.53%	1.901%
13	12.610	1777	1789	1791	rBV4	11603702	38603341	100.00%	53.910%
14	12.686	1798	1802	1804	rVV	6700518	5735255	14.86%	8.009%
15	12.721	1804	1808	1818	rVB3	1603071	2931190	7.59%	4.093%
16	13.086	1866	1870	1872	rBV	1562423	1327530	3.44%	1.854%
17	13.268	1894	1901	1903	rBV5	332914	558232	1.45%	0.780%
18	13.315	1907	1909	1911	rVV	457383	445350	1.15%	0.622%
19	13.398	1920	1923	1926	rBV	633770	555783	1.44%	0.776%
20	13.504	1938	1941	1945	rVB2	446553	428184	1.11%	0.598%
21	14.068	2033	2037	2040	rBV	574212	548154	1.42%	0.766%
22	14.133	2044	2048	2051	rVV2	405023	510870	1.32%	0.713%

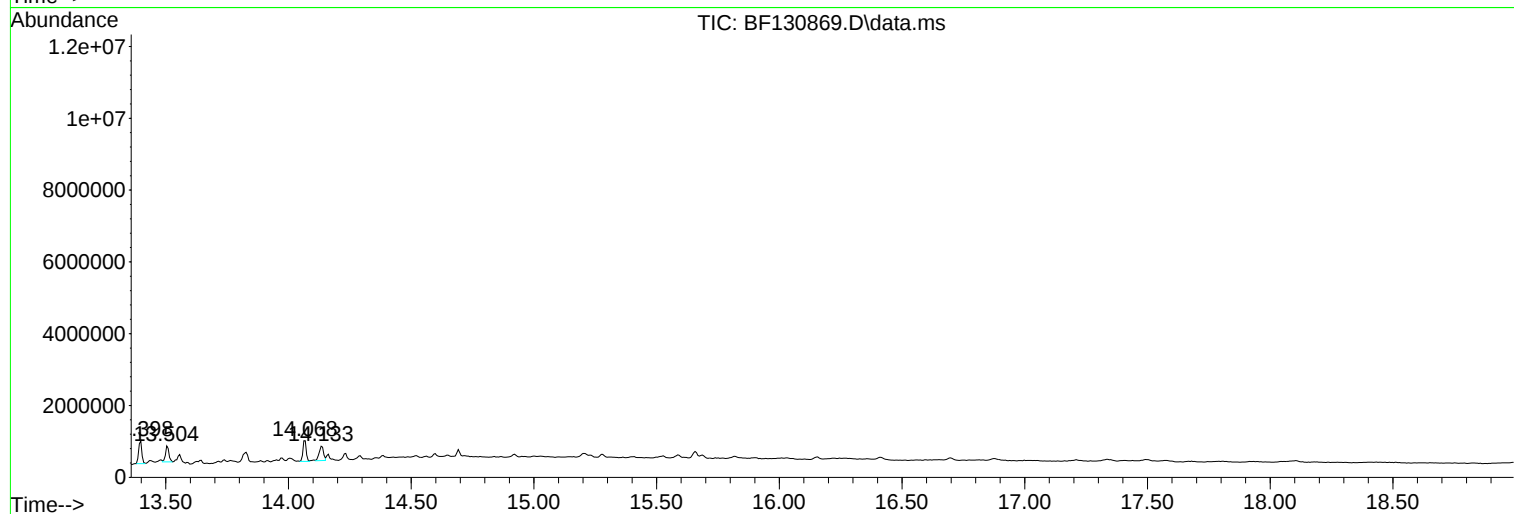
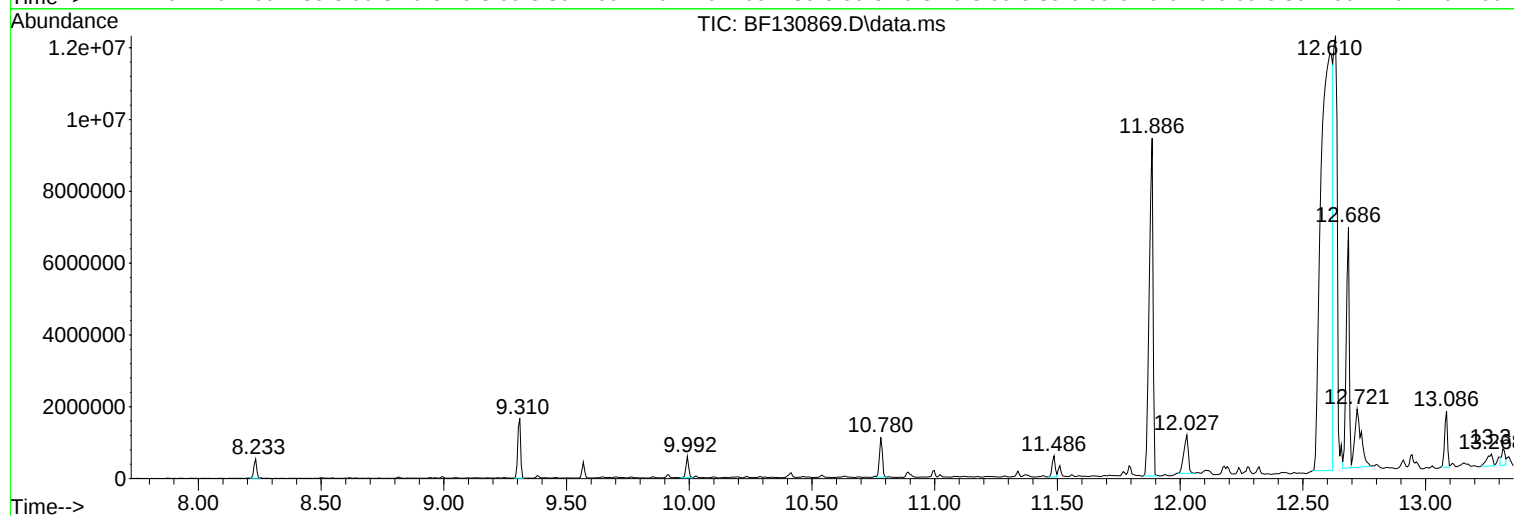
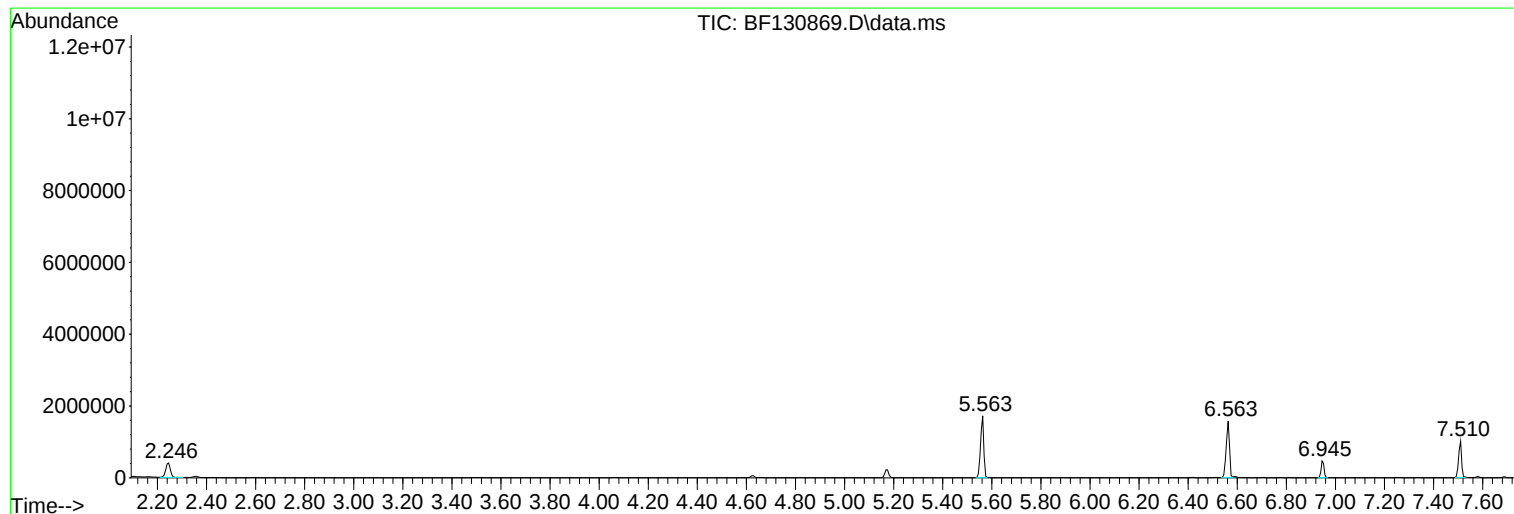
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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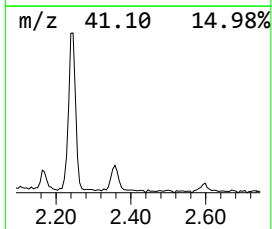
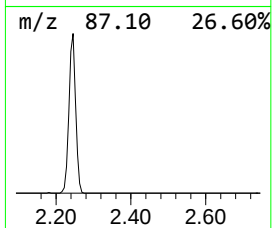
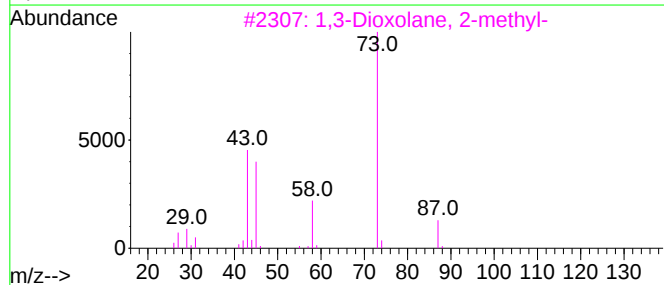
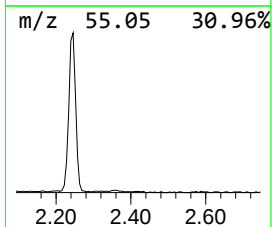
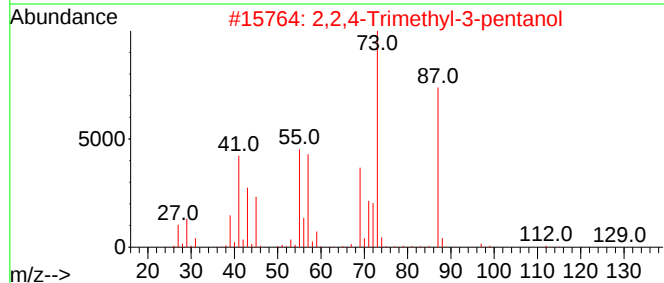
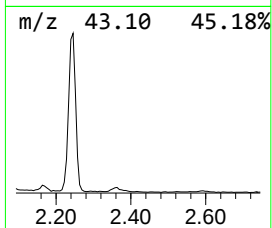
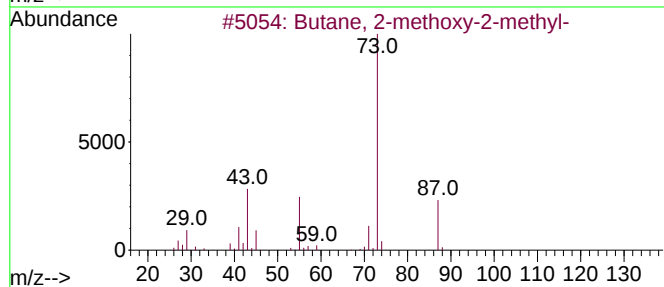
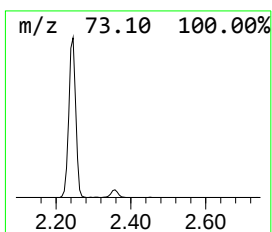
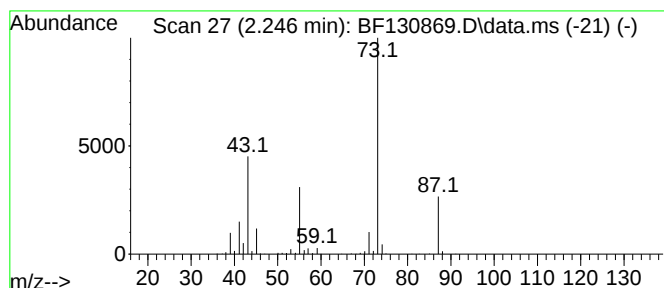
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.246	27.22 ng	532402	1,4-Dichlorobenzene-d4	6.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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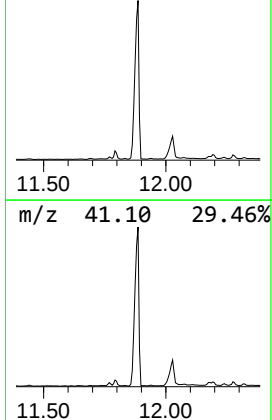
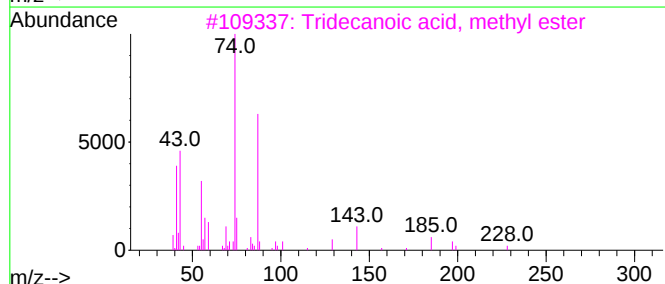
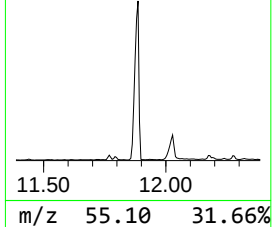
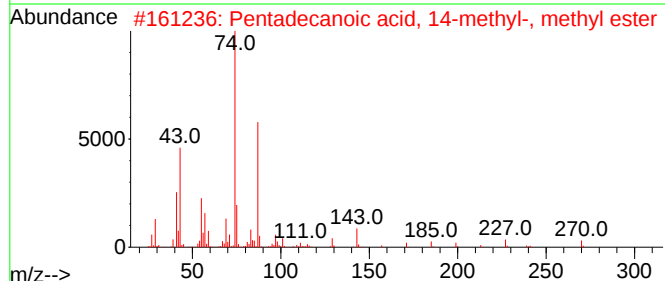
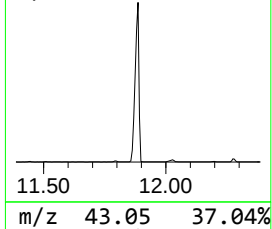
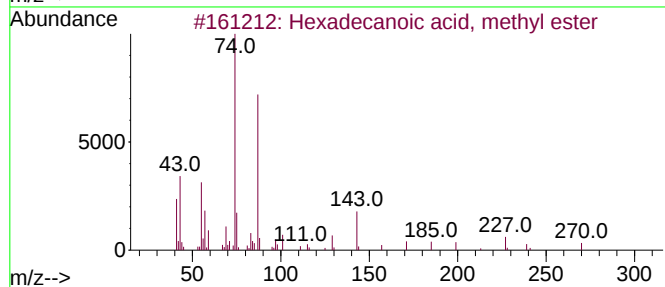
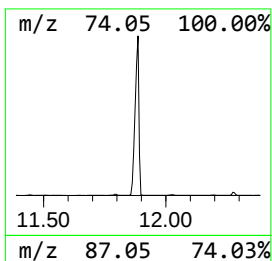
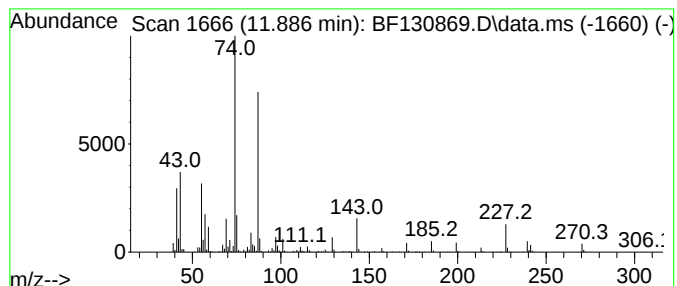
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	412.78 ng	10165200	Phenanthrene-d10	11.486

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			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
4			Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
5			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86



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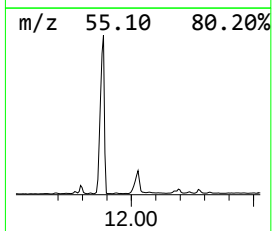
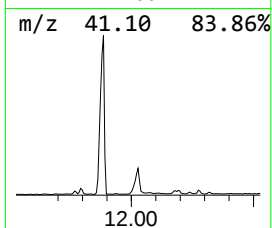
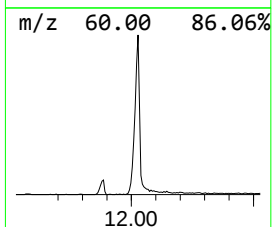
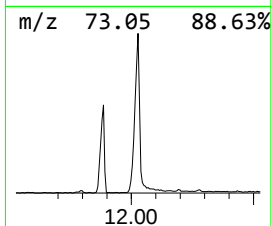
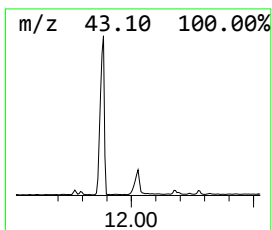
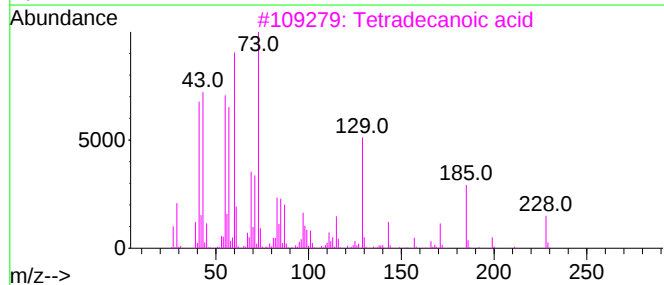
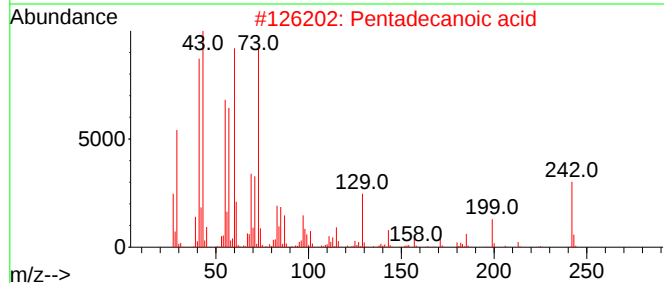
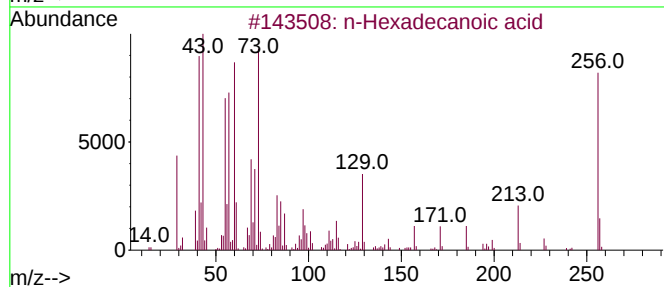
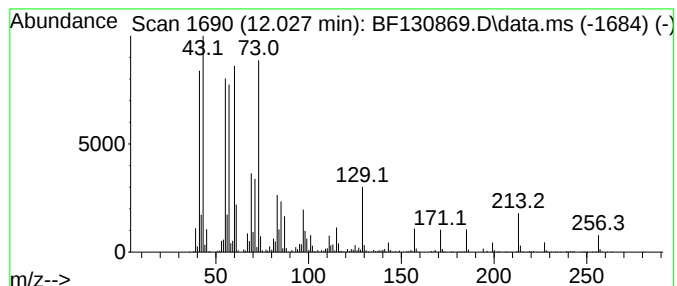
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.027	55.28 ng	1361360	Phenanthrene-d10	11.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4			Tridecanoic acid	214	C13H26O2	000638-53-9	76
5			Dodecanoic acid	200	C12H24O2	000143-07-7	53



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ALS Vial : 20 Sample Multiplier: 1

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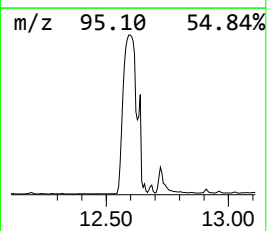
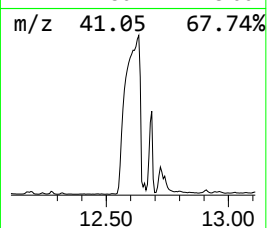
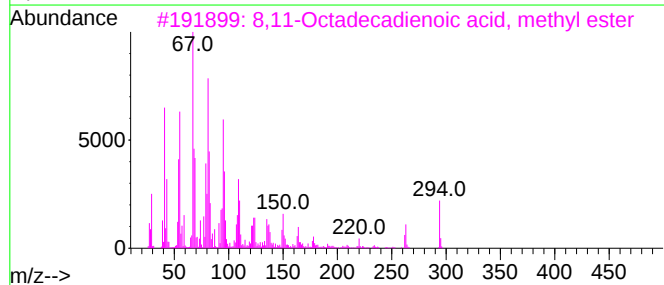
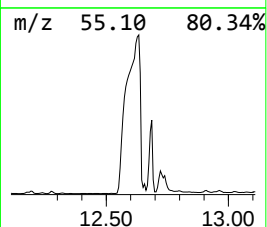
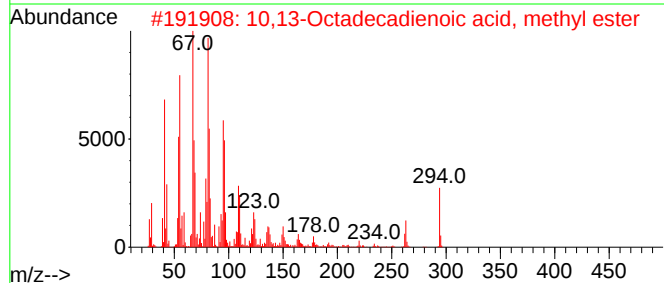
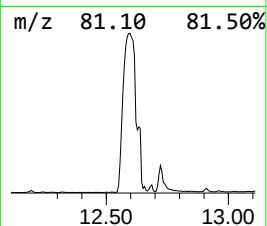
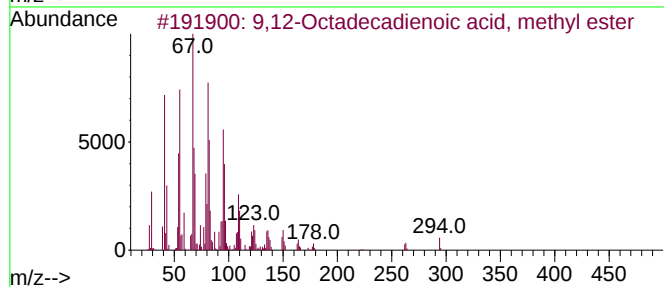
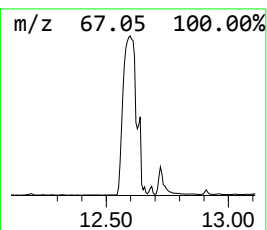
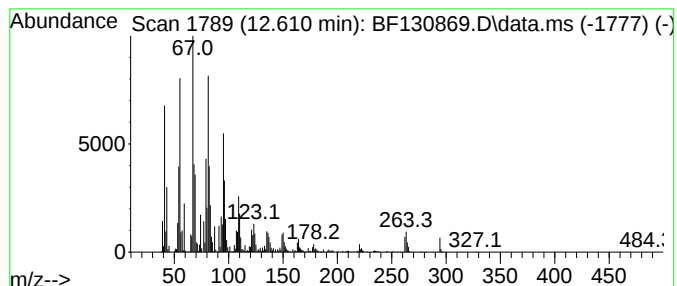
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Peak Number 4 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.610	1567.55 ng	38603300	Phenanthrene-d10	11.486

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			8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	99
4			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
5			Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	99



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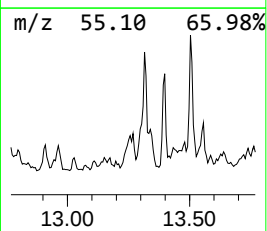
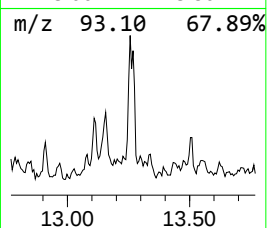
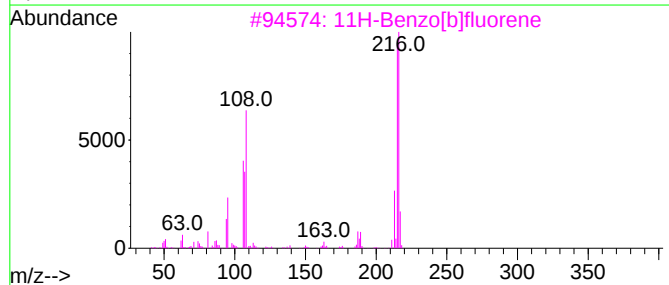
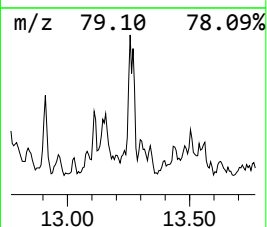
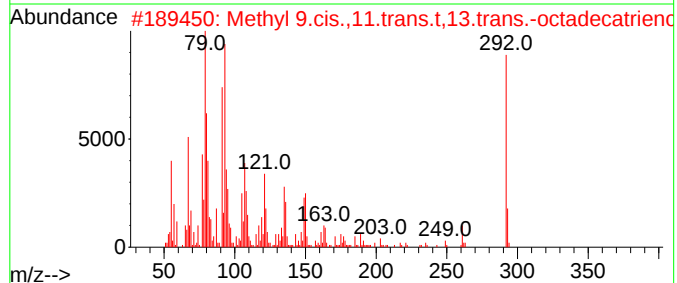
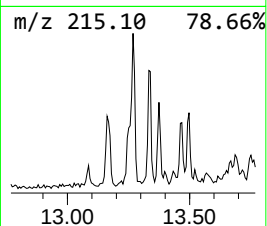
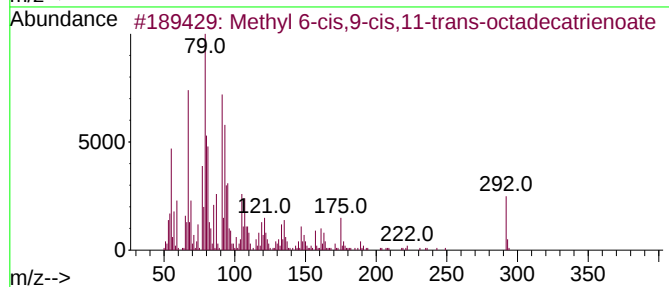
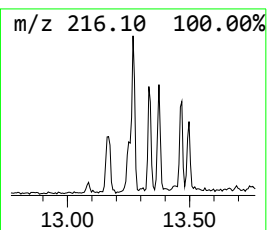
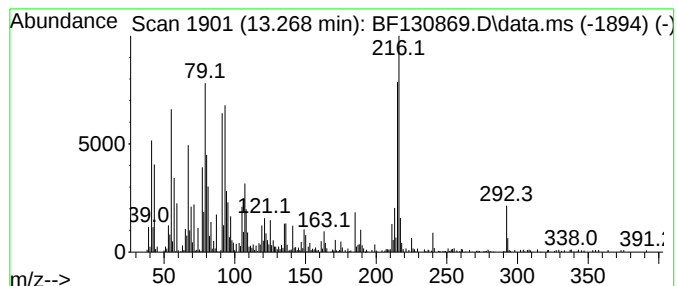
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Peak Number 5 Methyl 6-cis,9-cis,11-trans... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.268	21.85 ng	558232	Chrysene-d12	14.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl 6-cis,9-cis,11-trans-octa...	292	C19H32O2	1010336-37-7	83
2			Methyl 9.cis.,11.trans.t,13.tran...	292	C19H32O2	1000336-42-6	70
3			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	64
4			7H-Benzo[c]fluorene	216	C17H12	000205-12-9	64
5			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	50



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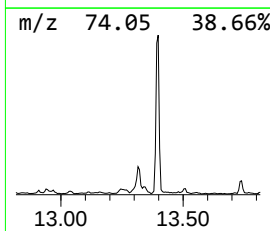
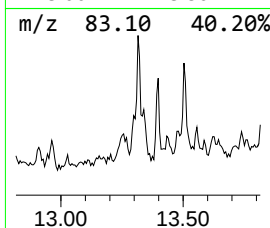
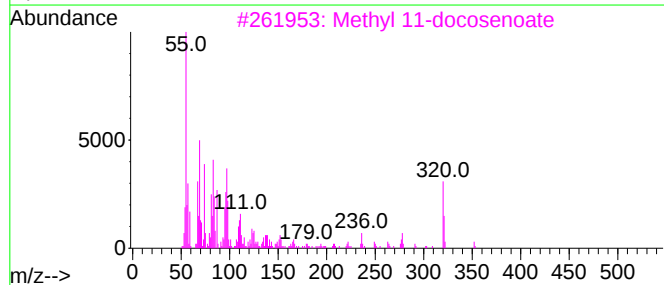
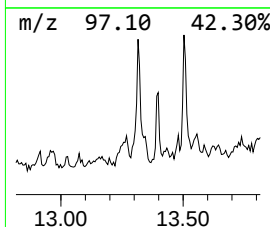
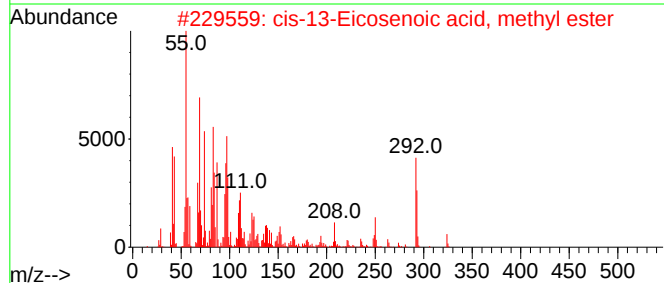
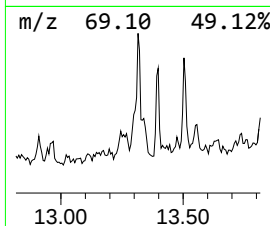
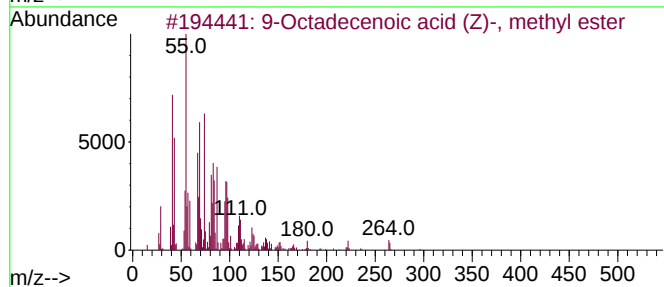
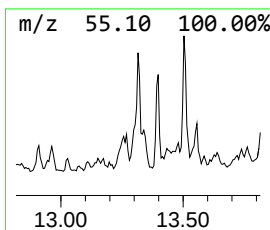
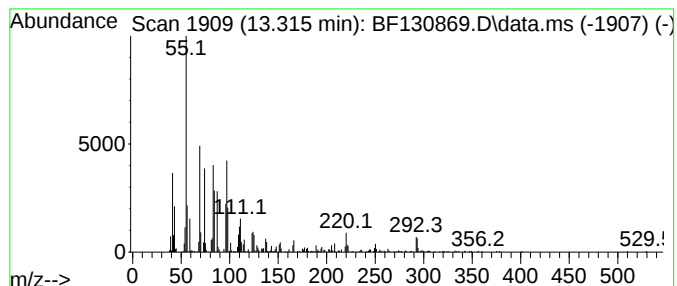
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9-Octadecenoic acid (Z)-, m... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.315	17.43 ng	445350	Chrysene-d12	14.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	93
2			cis-13-Eicosenoic acid, methyl e...	324	C21H40O2	069120-02-1	91
3			Methyl 11-docosenoate	352	C23H44O2	1000336-23-0	91
4			cis-Methyl 11-eicosenoate	324	C21H40O2	002390-09-2	87
5			12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102922\
Data File : BF130869.D
Acq On : 29 Oct 2022 21:20
Operator : CG\JU
Sample : N5330-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-5-102722

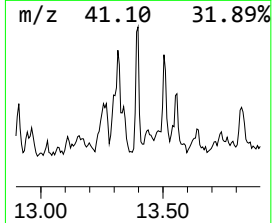
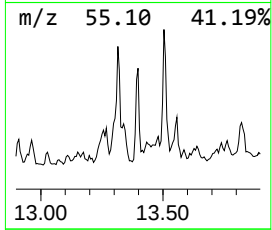
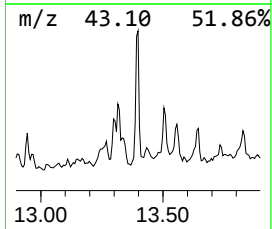
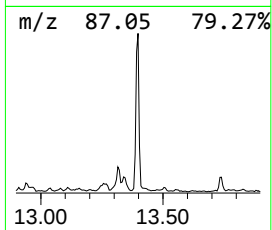
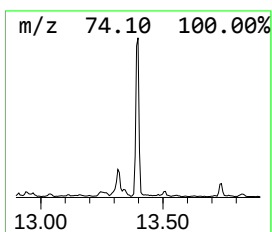
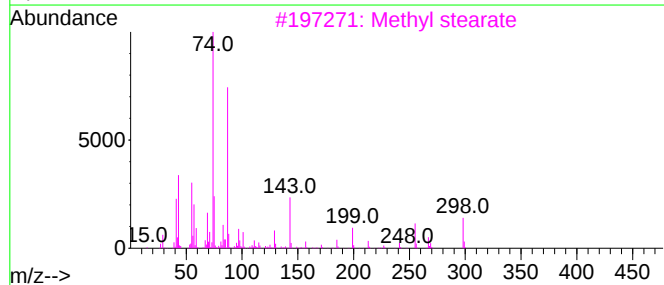
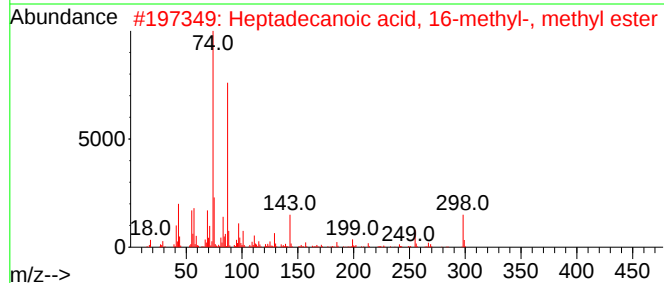
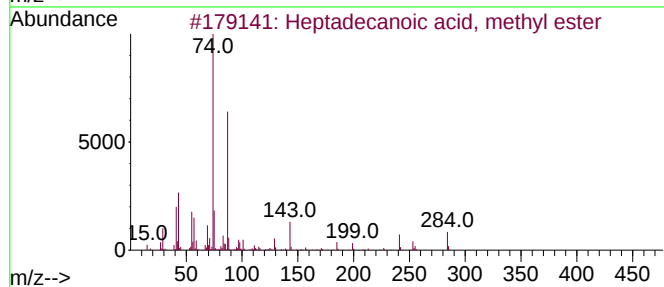
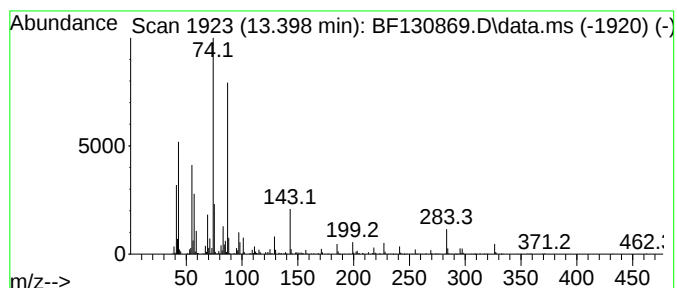
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 7 Heptadecanoic acid, methyl ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.398	21.76 ng	555783	Chrysene-d12	14.139	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	93
2	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	91
3	Methyl stearate	298	C19H38O2	000112-61-8	90
4	Hexadecanoic acid, 14-methyl-, m...	284	C18H36O2	002490-49-5	87
5	Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102922\
Data File : BF130869.D
Acq On : 29 Oct 2022 21:20
Operator : CG\JU
Sample : N5330-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-5-102722

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

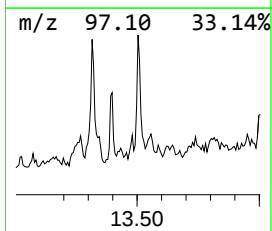
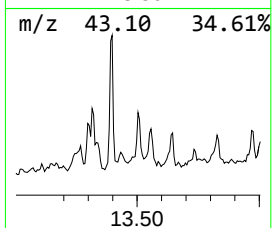
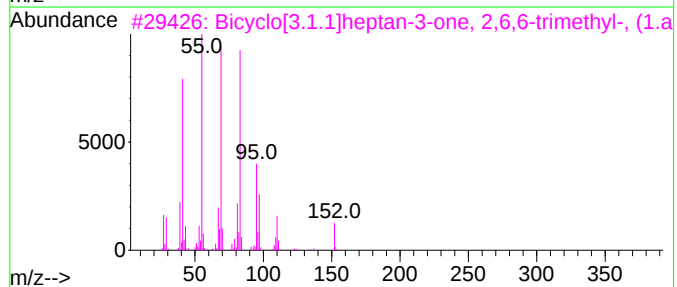
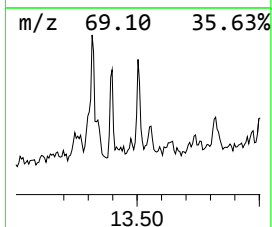
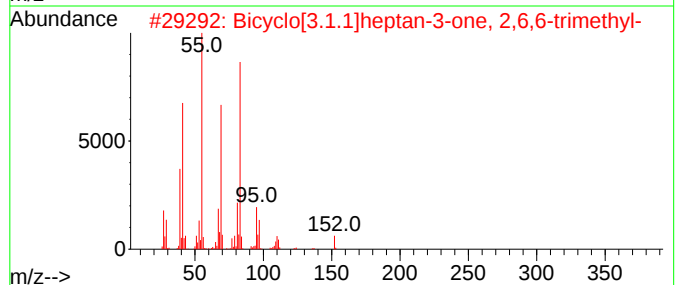
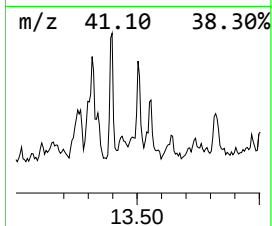
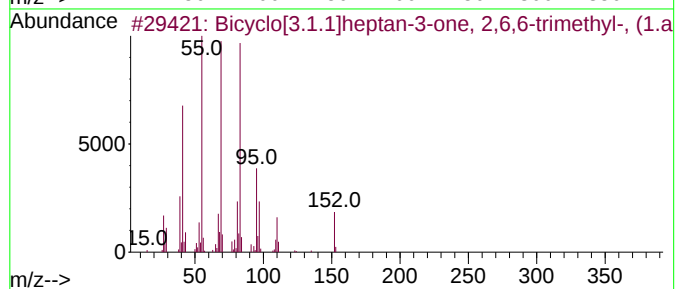
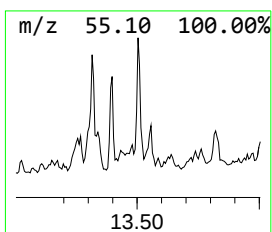
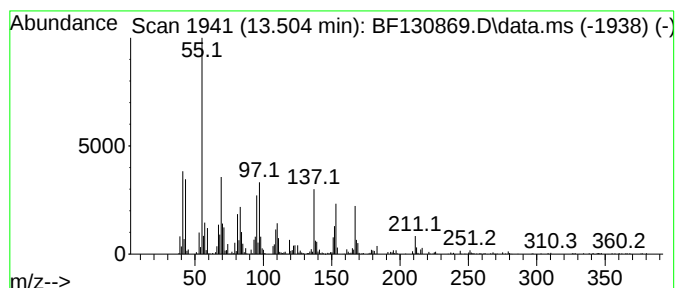
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown13.504 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.504	16.76 ng	428184	Chrysene-d12	14.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	38
2			Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	018358-53-7	27
3			Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	000547-60-4	25
4			3-n-Hexylthiane, S,S-dioxide	218	C11H20S2	061639-18-7	22
5			Erucic acid	338	C22H42O2	000112-86-7	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102922\
Data File : BF130869.D
Acq On : 29 Oct 2022 21:20
Operator : CG\JU
Sample : N5330-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

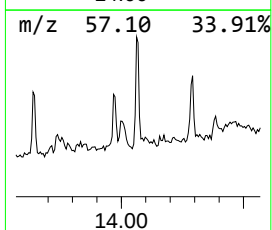
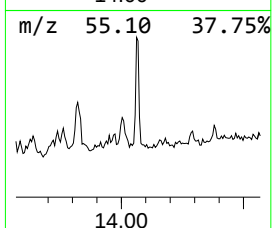
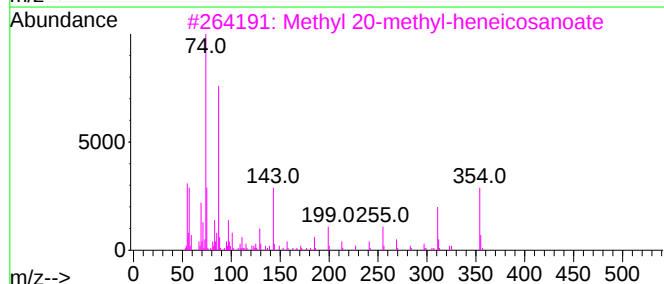
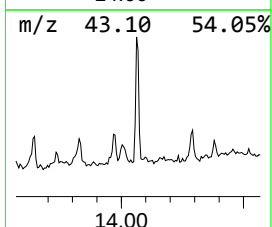
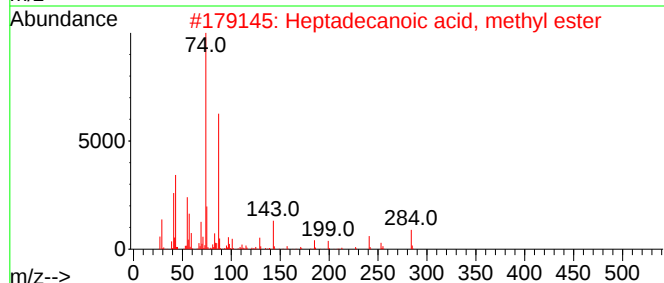
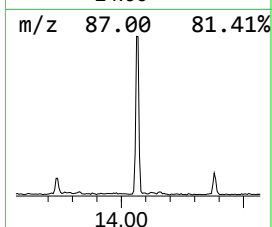
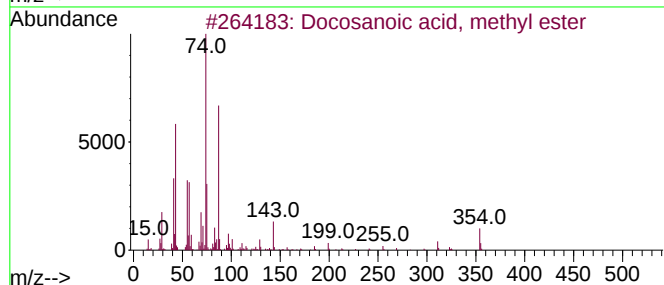
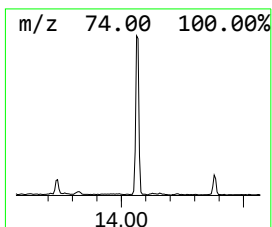
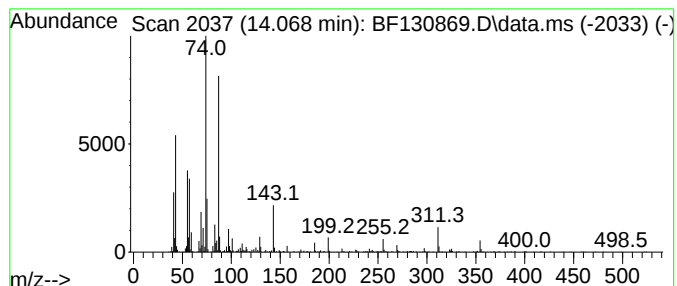
Instrument :
BNA_F
ClientSampleId :
TR-5-102722

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Docosanoic acid, methyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.068	21.46 ng	548154	Chrysene-d12	14.139	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosanoic acid, methyl ester	354	C23H46O2	000929-77-1	99
2	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	93
3	Methyl 20-methyl-heneicosanoate	354	C23H46O2	1000336-47-4	91
4	Methyl stearate	298	C19H38O2	000112-61-8	87
5	Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102922\
Data File : BF130869.D
Acq On : 29 Oct 2022 21:20
Operator : CG\JU
Sample : N5330-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-5-102722

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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
Butane, 2-metho...	2.246	27.2	ng	532402	1	6.945	391115	20.0
Hexadecanoic ac...	11.886	412.8	ng	10165200	4	11.486	492531	20.0
n-Hexadecanoic ...	12.027	55.3	ng	1361360	4	11.486	492531	20.0
9,12-Octadecadi...	12.610	1567.6	ng	38603300	4	11.486	492531	20.0
Methyl 6-cis,9-...	13.268	21.9	ng	558232	5	14.139	510870	20.0
9-Octadecenoic ...	13.315	17.4	ng	445350	5	14.139	510870	20.0
Heptadecanoic a...	13.398	21.8	ng	555783	5	14.139	510870	20.0
unknown13.504	13.504	16.8	ng	428184	5	14.139	510870	20.0
Docosanoic acid...	14.068	21.5	ng	548154	5	14.139	510870	20.0