

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011123\
 Data File : BF132033.D
 Acq On : 11 Jan 2023 20:36
 Operator : CG\JU
 Sample : 01090-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SU-3-010923

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-BF010923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132033.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.969	485	490	499	rBV	488941	651916	1.74%	0.994%
2	5.393	558	562	576	rBV	1613621	1500814	4.00%	2.289%
3	6.422	733	737	754	rBV	1548274	1505180	4.01%	2.296%
4	6.775	794	797	801	rBV	507006	449778	1.20%	0.686%
5	7.351	891	895	898	rBV	1205198	975366	2.60%	1.488%
6	8.069	1014	1017	1020	rVB	678205	501029	1.34%	0.764%
7	9.151	1196	1201	1204	rBV	1792072	1579385	4.21%	2.409%
8	9.828	1312	1316	1320	rVB	622619	489873	1.31%	0.747%
9	10.622	1448	1451	1455	rVB	919316	728313	1.94%	1.111%
10	11.322	1566	1570	1573	rBV	537868	440010	1.17%	0.671%
11	11.733	1633	1640	1642	rBV	8744463	10210605	27.22%	15.576%
12	12.457	1750	1763	1764	rBV2	12691204	37511037	100.00%	57.223%
13	12.527	1772	1775	1778	rVV	5261413	4644251	12.38%	7.085%
14	12.569	1778	1782	1783	rVV	642990	585360	1.56%	0.893%
15	12.586	1783	1785	1791	rVB2	486036	540831	1.44%	0.825%
16	12.927	1839	1843	1845	rBV	1295950	1168467	3.11%	1.782%
17	13.163	1877	1883	1890	rVB2	331601	608957	1.62%	0.929%
18	13.239	1893	1896	1899	rBV	548411	465122	1.24%	0.710%
19	13.457	1930	1933	1942	rVB2	361487	513557	1.37%	0.783%
20	13.910	2006	2010	2016	rBV	546641	482912	1.29%	0.737%

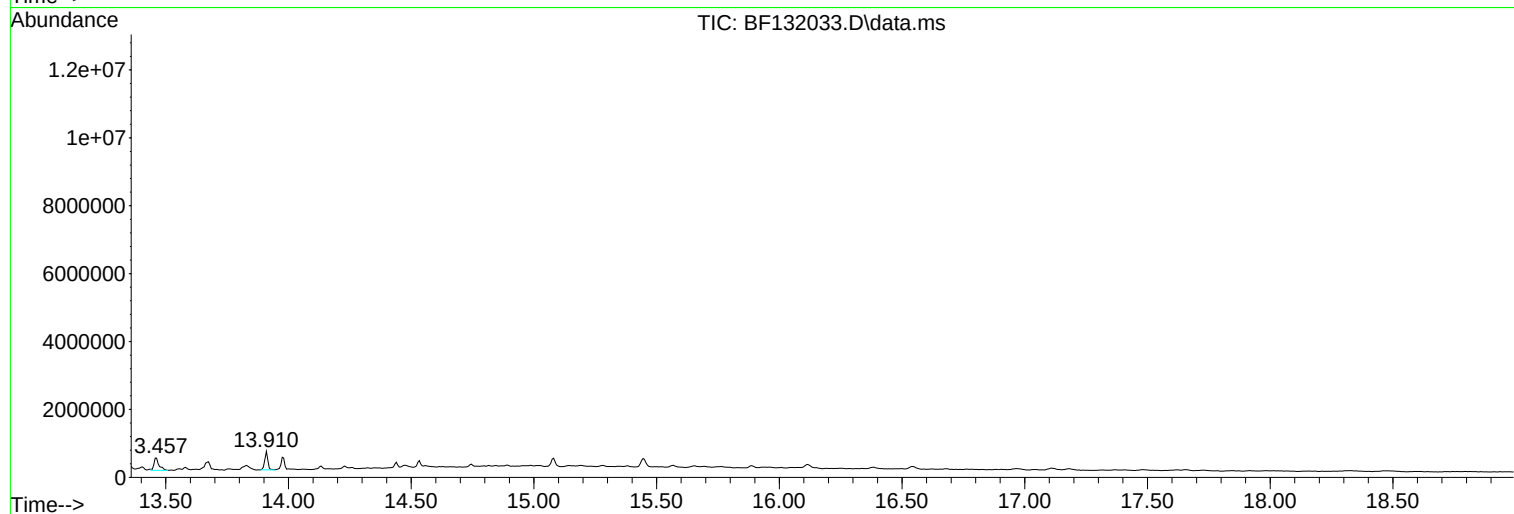
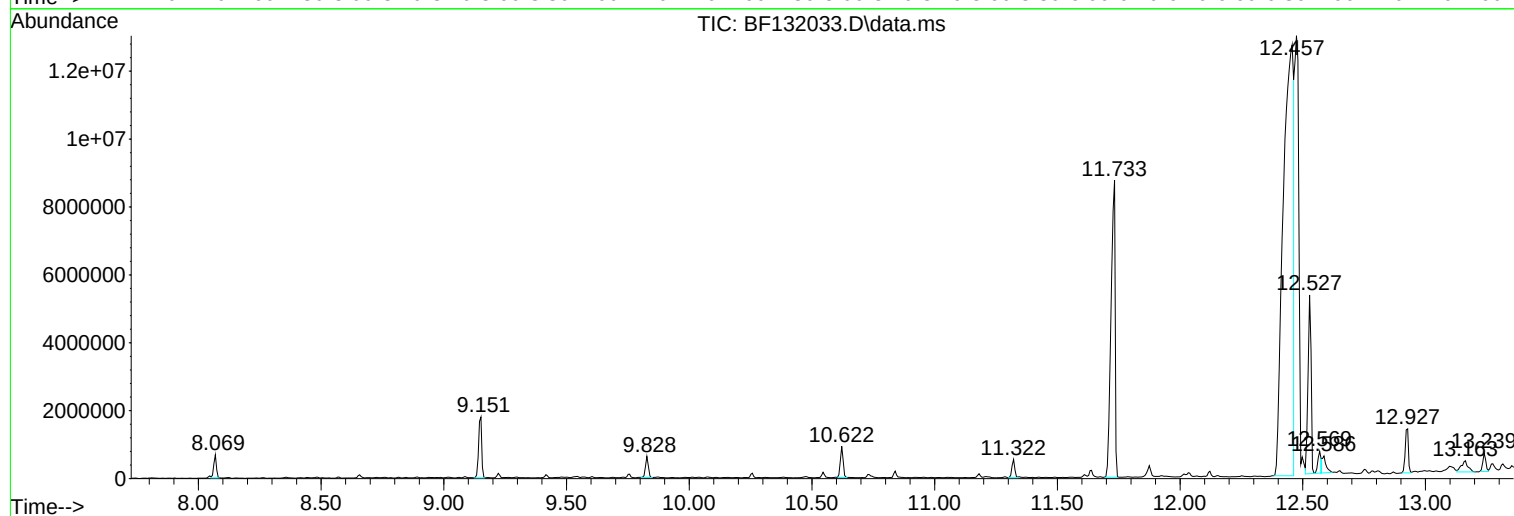
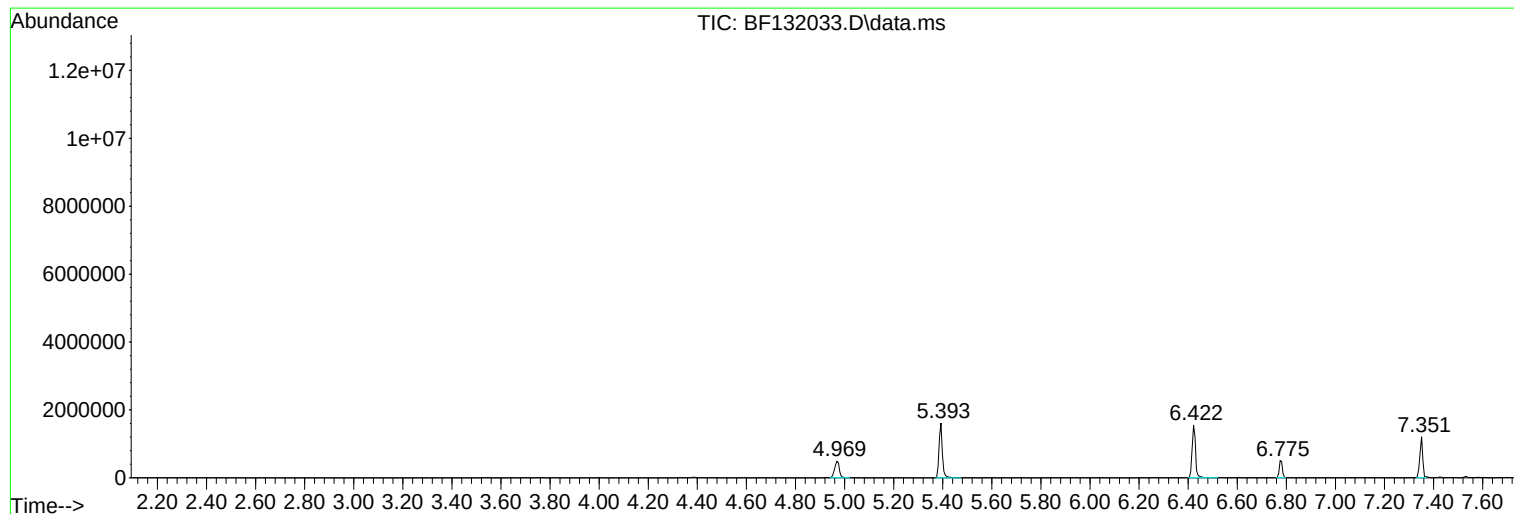
Sum of corrected areas: 65552763

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011123\
Data File : BF132033.D
Acq On : 11 Jan 2023 20:36
Operator : CG\JU
Sample : 01090-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-3-010923

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011123\
Data File : BF132033.D
Acq On : 11 Jan 2023 20:36
Operator : CG\JU
Sample : 01090-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-3-010923

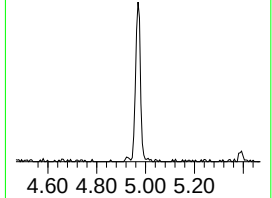
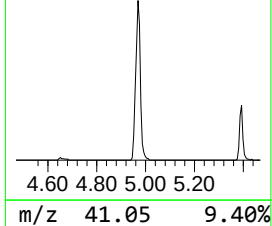
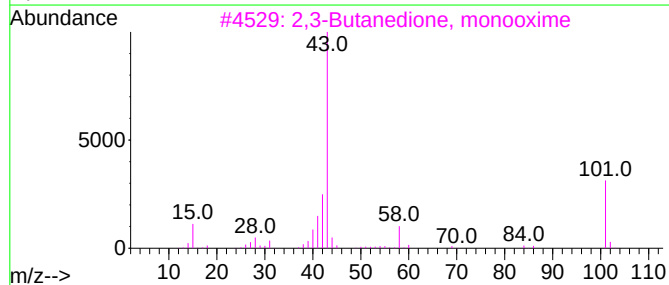
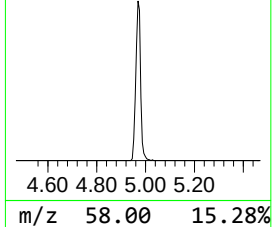
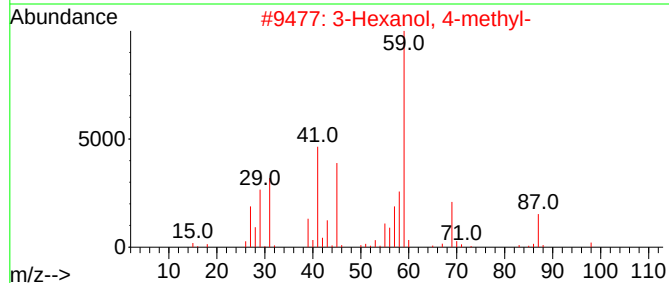
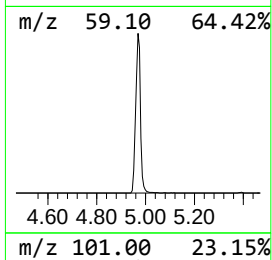
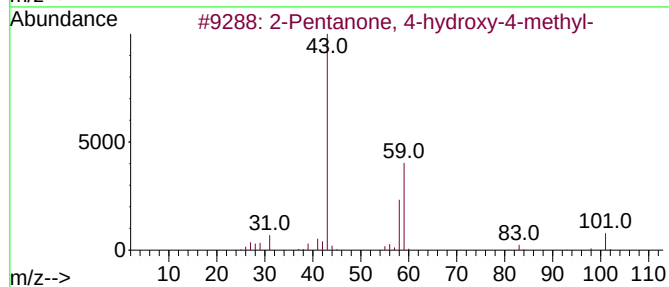
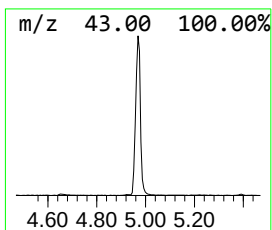
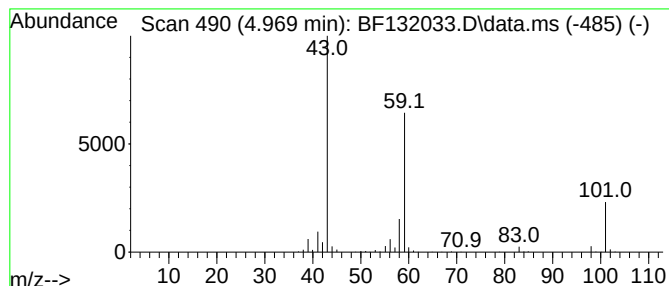
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.969	28.99 ng	651916	1,4-Dichlorobenzene-d4	6.781

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56	
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28	
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25	
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23	
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011123\
Data File : BF132033.D
Acq On : 11 Jan 2023 20:36
Operator : CG\JU
Sample : 01090-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

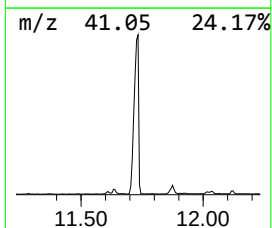
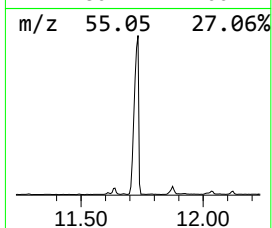
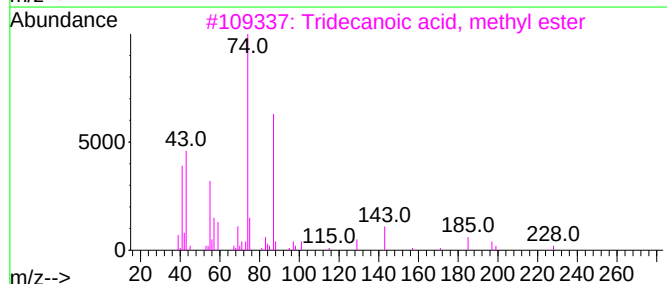
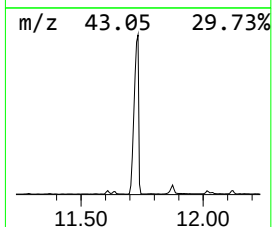
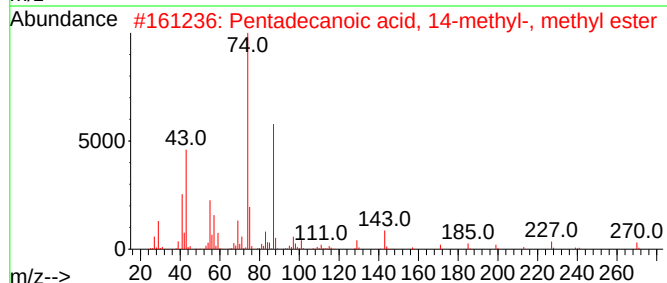
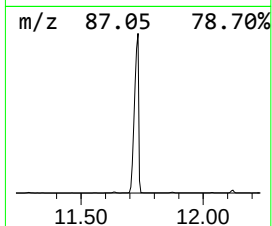
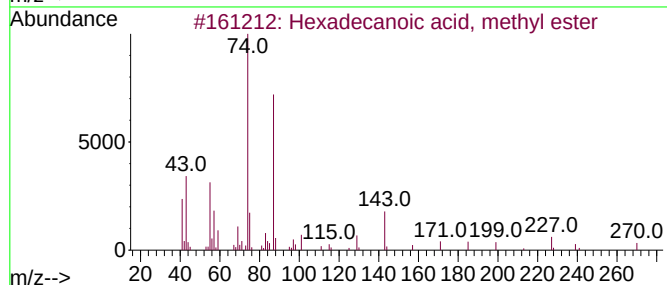
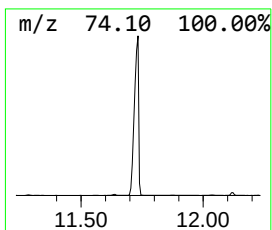
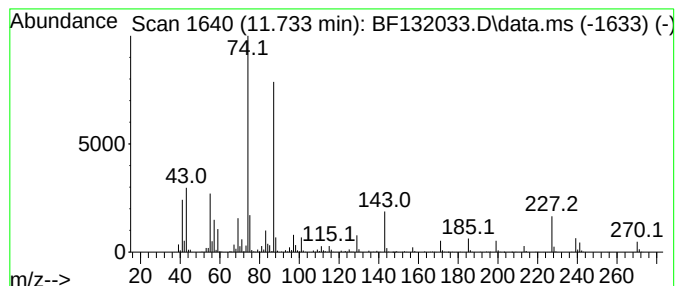
Instrument :
BNA_F
ClientSampleId :
SU-3-010923

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
11.733	464.11 ng	10210600	Phenanthrene-d10			11.322
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	Decanoic acid, methyl ester		186	C11H22O2	000110-42-9	87
5	Methyl 9-methyltetradecanoate		256	C16H32O2	213617-69-7	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011123\
Data File : BF132033.D
Acq On : 11 Jan 2023 20:36
Operator : CG\JU
Sample : 01090-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

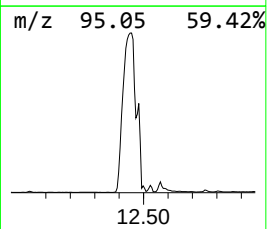
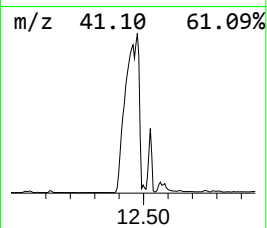
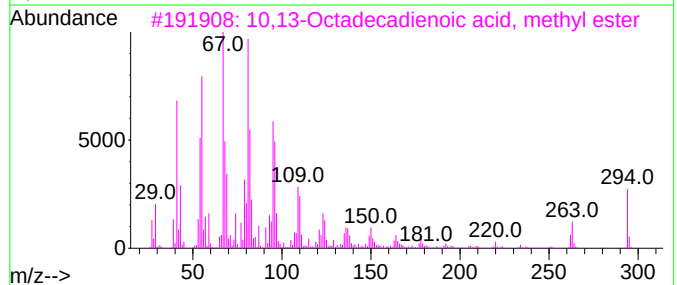
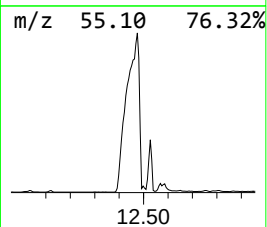
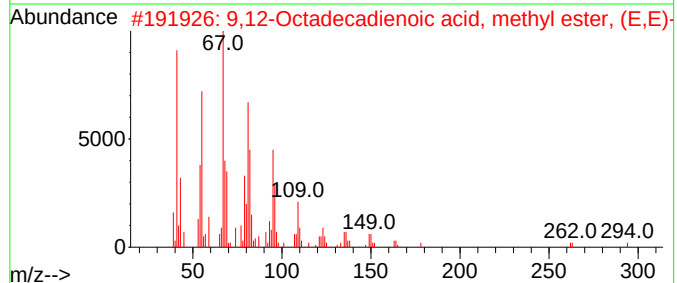
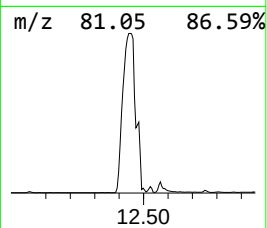
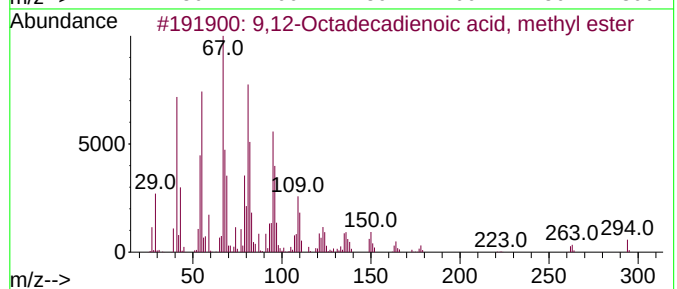
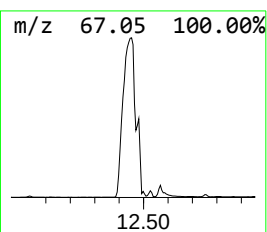
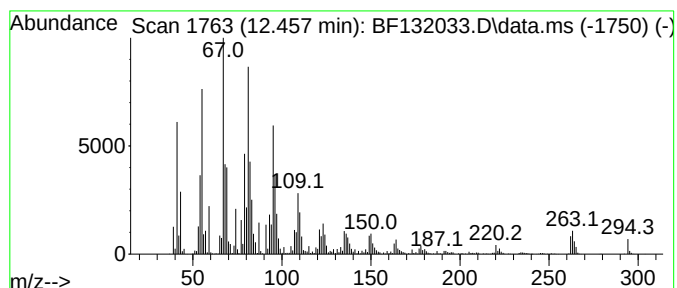
Instrument :
BNA_F
ClientSampleId :
SU-3-010923

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.457	1705.01 ng	37511000	Phenanthrene-d10	11.322	
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, methy...	294	C19H34O2	002566-97-4	99
3	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
4	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	99
5	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	98



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011123\
Data File : BF132033.D
Acq On : 11 Jan 2023 20:36
Operator : CG\JU
Sample : 01090-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-3-010923

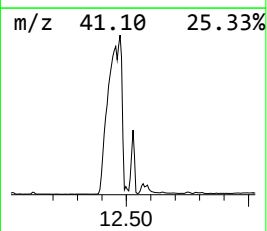
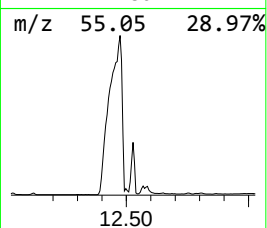
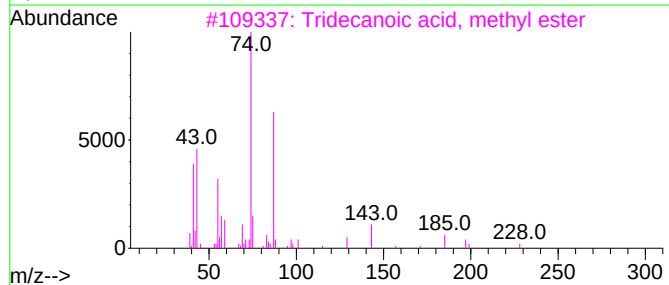
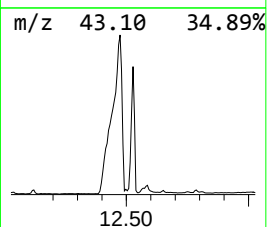
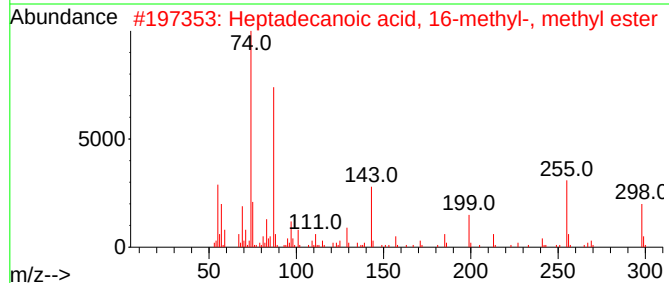
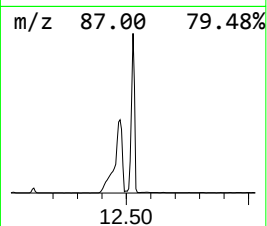
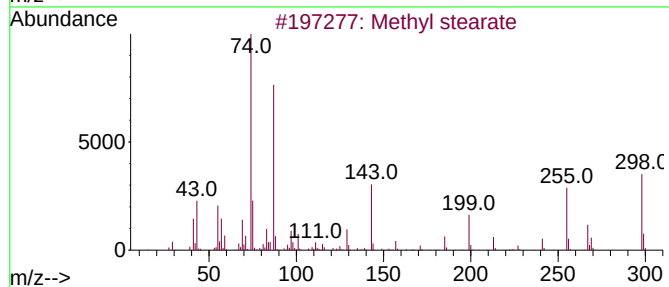
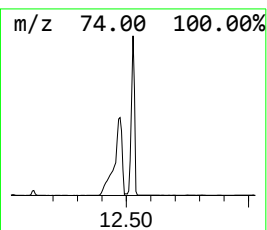
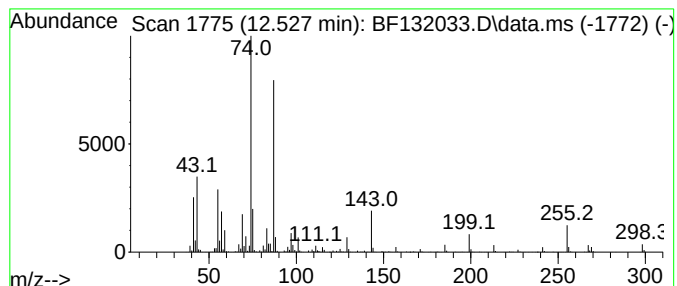
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Methyl stearate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.527	211.10 ng	4644250	Phenanthrene-d10	11.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	98
2			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	94
3			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
4			Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	90
5			Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011123\
Data File : BF132033.D
Acq On : 11 Jan 2023 20:36
Operator : CG\JU
Sample : 01090-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

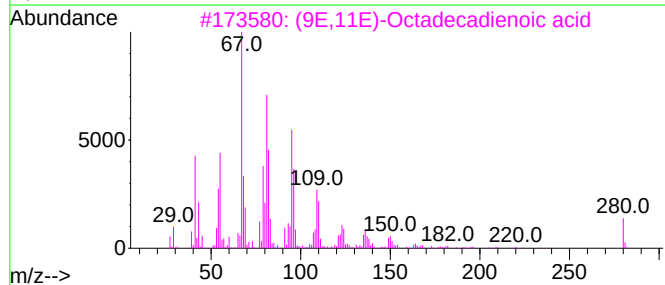
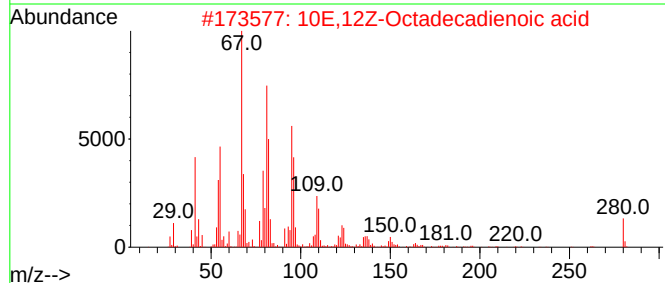
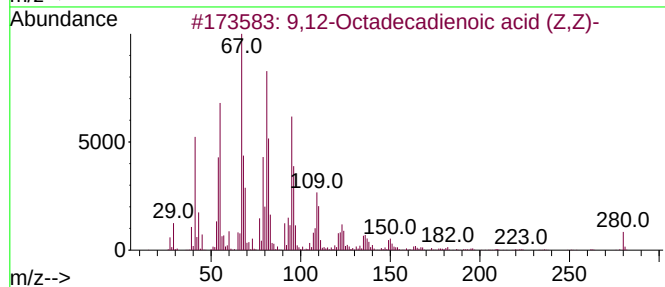
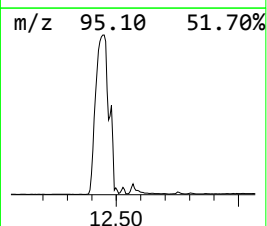
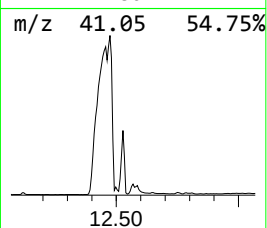
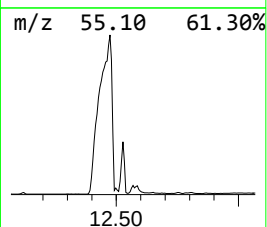
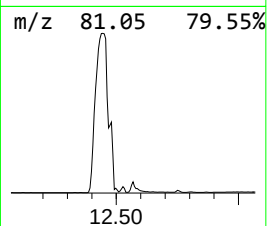
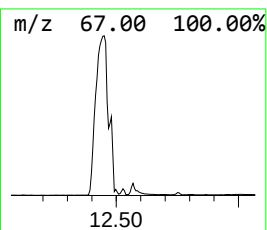
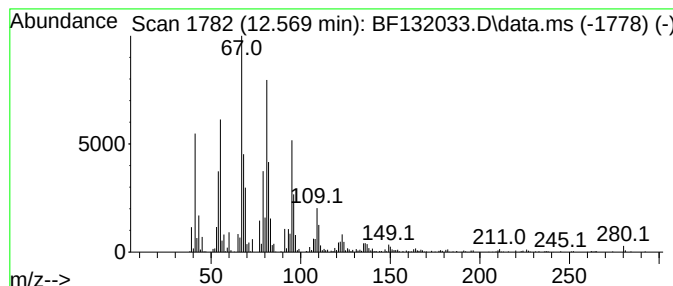
Instrument :
BNA_F
ClientSampleId :
SU-3-010923

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 9,12-Octadecadienoic acid (... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.569	26.61 ng	585360	Phenanthrene-d10	11.322	
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	98
3	(9E,11E)-Octadecadienoic acid	280	C18H32O2	000544-71-8	96
4	Linoleaidic acid	280	C18H32O2	000506-21-8	95
5	3,4-Octadiene, 7-methyl-	124	C9H16	037050-05-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011123\
Data File : BF132033.D
Acq On : 11 Jan 2023 20:36
Operator : CG\JU
Sample : 01090-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

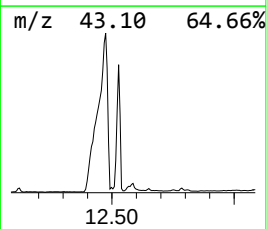
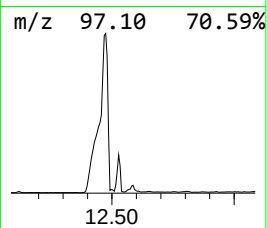
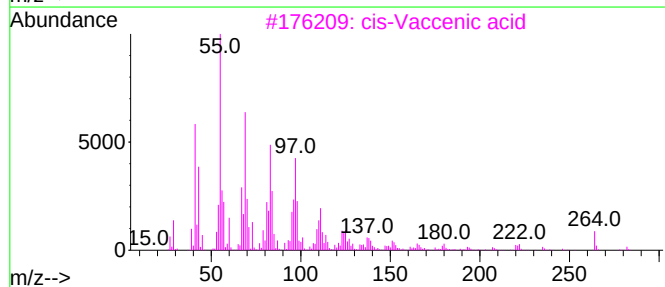
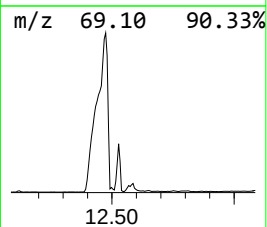
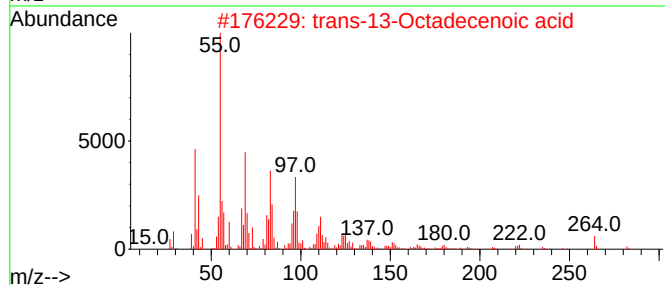
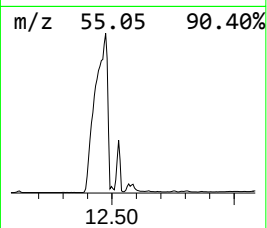
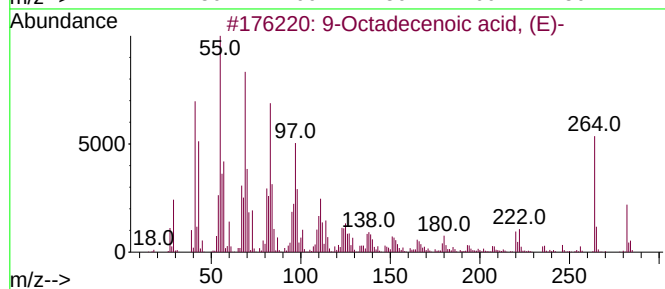
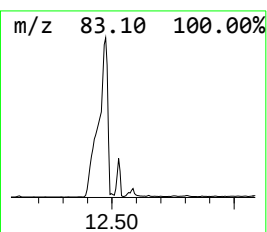
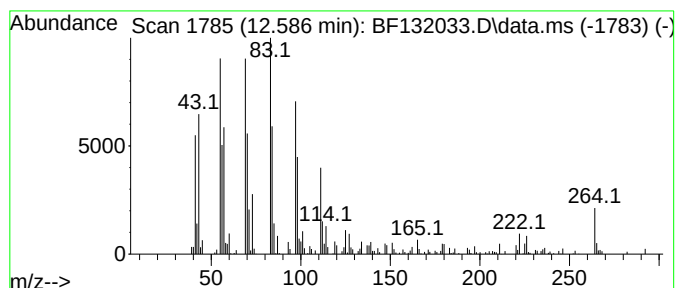
Instrument :
BNA_F
ClientSampleId :
SU-3-010923

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
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, (E)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.586	24.58 ng	540831	Phenanthrene-d10	11.322	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	90
2	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	64
3	cis-Vaccenic acid	282	C18H34O2	000506-17-2	64
4	1-Hexyl-1-nitrocyclohexane	213	C12H23NO2	118252-09-8	47
5	n-Pentadecanol	228	C15H32O	000629-76-5	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011123\
Data File : BF132033.D
Acq On : 11 Jan 2023 20:36
Operator : CG\JU
Sample : 01090-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

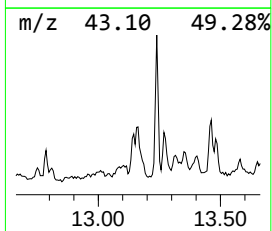
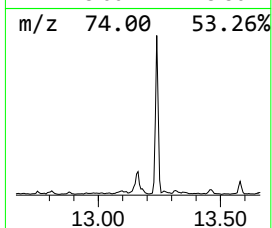
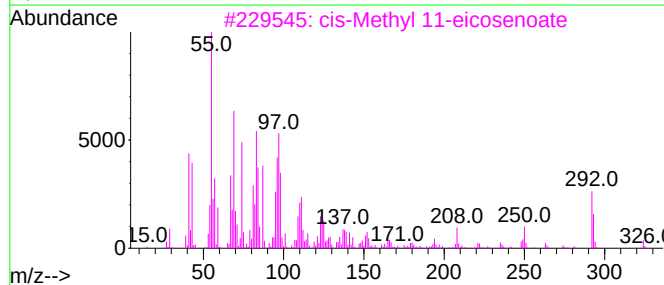
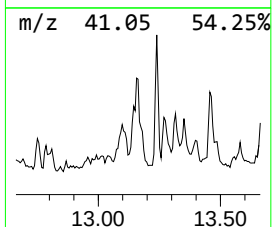
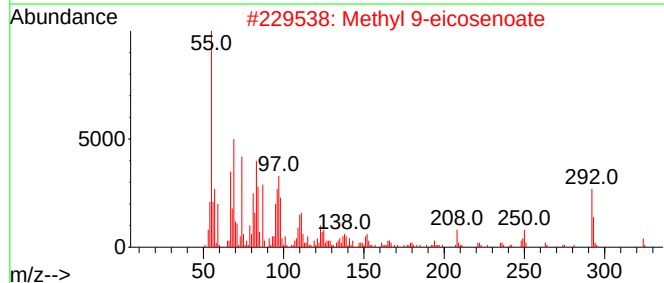
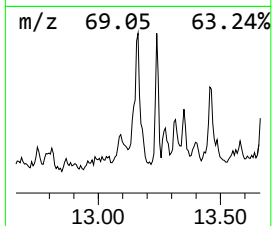
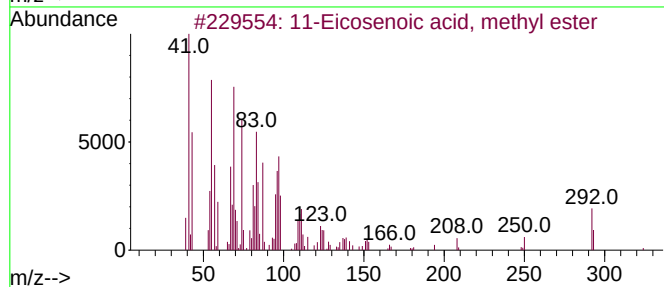
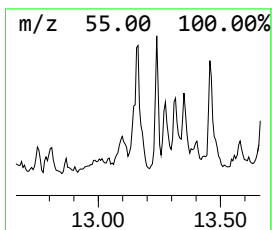
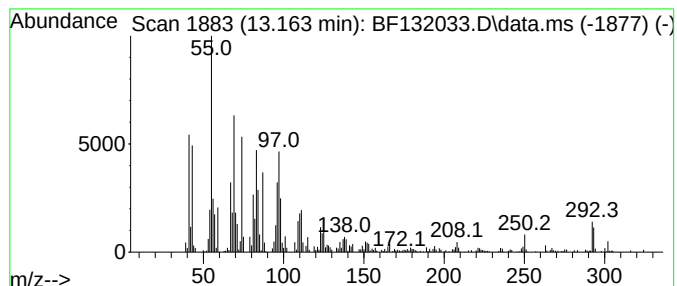
Instrument :
BNA_F
ClientSampleId :
SU-3-010923

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 11-Eicosenoic acid, methyl ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.163	25.22 ng	608957	Chrysene-d12	13.974	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Eicosenoic acid, methyl ester	324	C21H40O2	003946-08-5	97
2	Methyl 9-eicosenoate	324	C21H40O2	1000336-50-5	94
3	cis-Methyl 11-eicosenoate	324	C21H40O2	002390-09-2	91
4	cis-13-Eicosenoic acid, methyl e...	324	C21H40O2	069120-02-1	91
5	Methyl 9-heptadecenoate or 9-17:1	282	C18H34O2	1000336-38-0	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011123\
Data File : BF132033.D
Acq On : 11 Jan 2023 20:36
Operator : CG\JU
Sample : 01090-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-3-010923

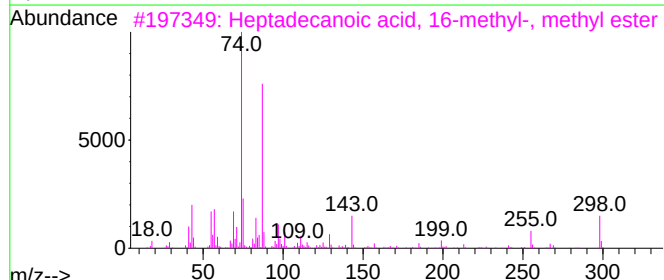
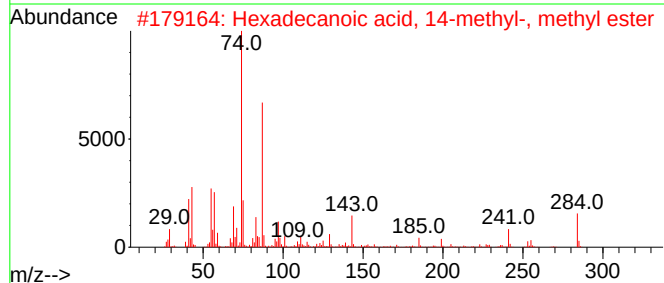
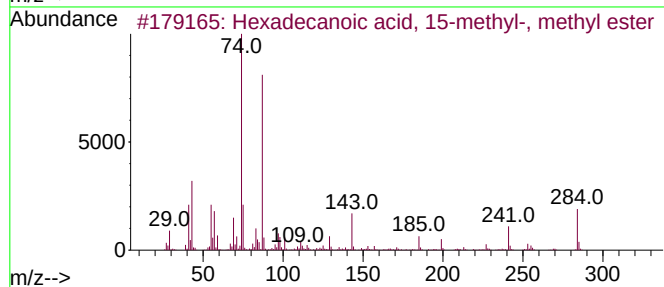
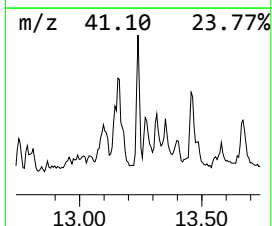
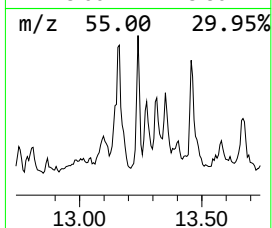
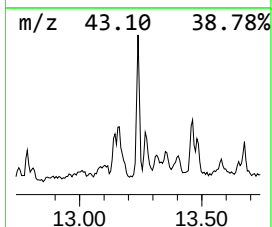
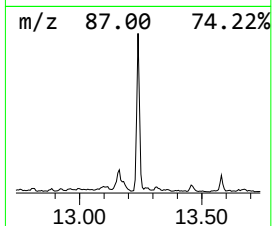
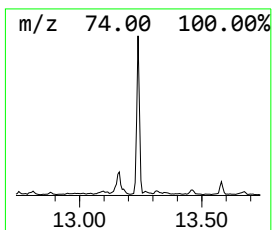
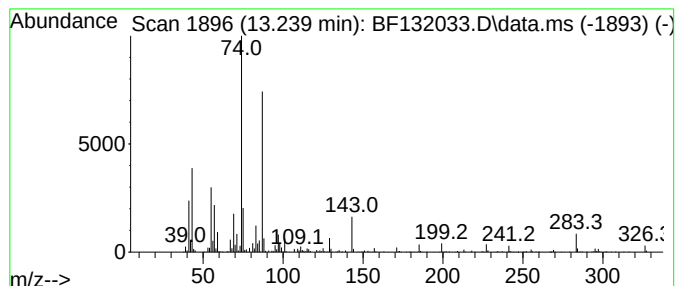
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexadecanoic acid, 15-methy... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.239	19.26 ng	465122	Chrysene-d12	13.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	95
2			Hexadecanoic acid, 14-methyl-, m...	284	C18H36O2	002490-49-5	94
3			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	93
4			Methyl 18-methylnonadecanoate	326	C21H42O2	1000424-52-4	91
5			Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011123\
Data File : BF132033.D
Acq On : 11 Jan 2023 20:36
Operator : CG\JU
Sample : 01090-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-3-010923

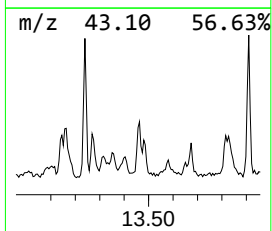
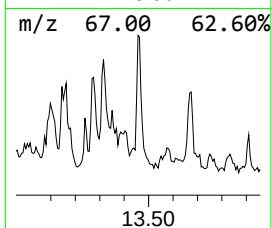
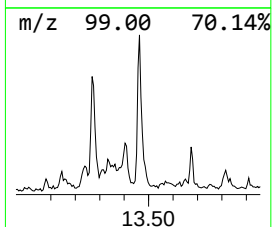
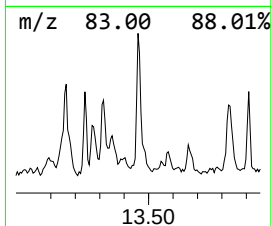
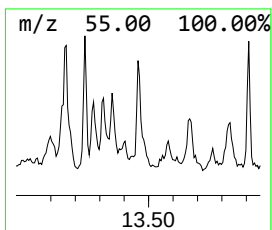
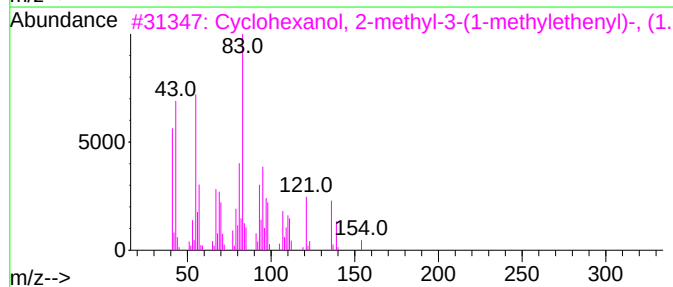
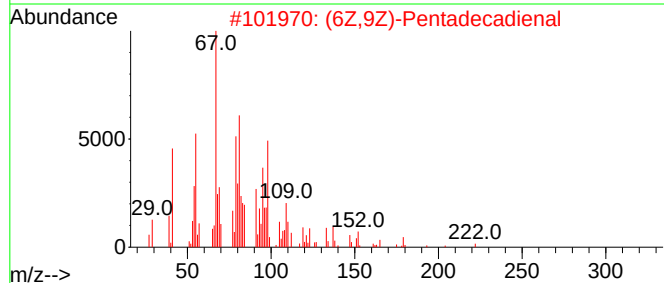
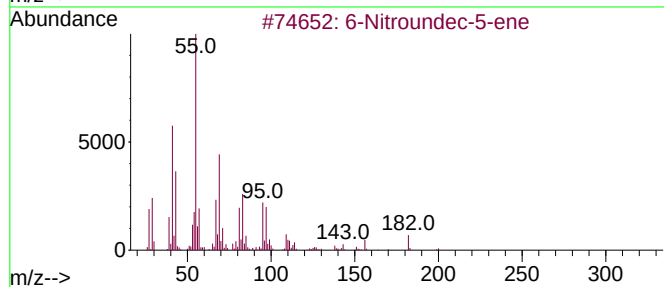
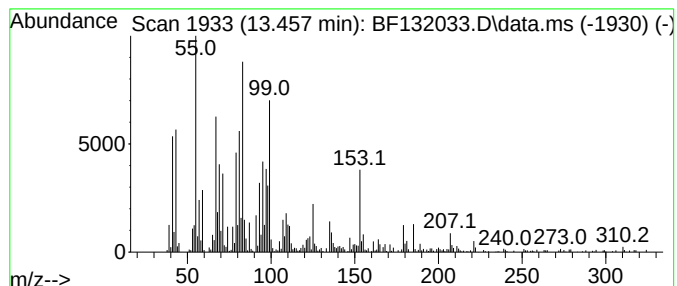
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown13.457 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.457	21.27 ng	513557	Chrysene-d12	13.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Nitroundec-5-ene			199	C11H21NO2	1000192-40-3	38
2	(6Z,9Z)-Pentadecadienal			222	C15H26O	121781-63-3	38
3	Cyclohexanol, 2-methyl-3-(1-meth...			154	C10H18O	054244-81-4	30
4	4-Chloro-3-n-hexyltetrahydropyran			204	C11H21ClO	066555-66-6	30
5	2-Pentene, 3,4-dimethyl-, (Z)-			98	C7H14	004914-91-4	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011123\
Data File : BF132033.D
Acq On : 11 Jan 2023 20:36
Operator : CG\JU
Sample : 01090-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

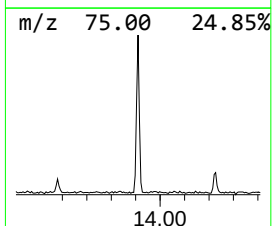
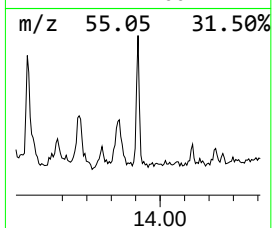
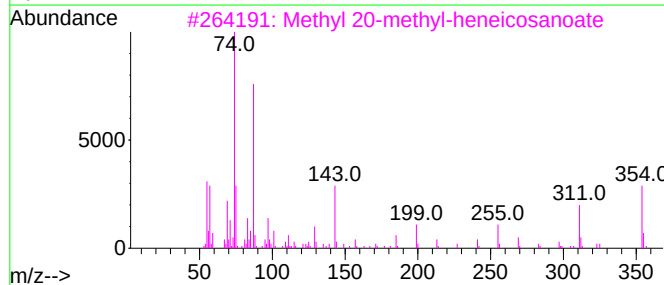
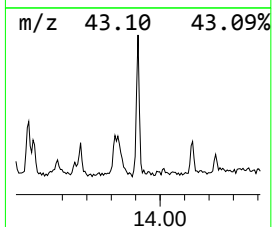
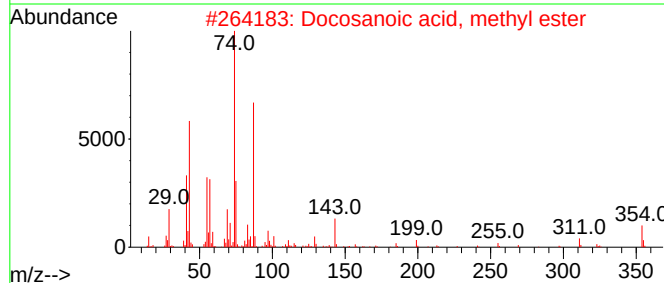
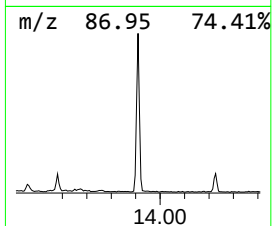
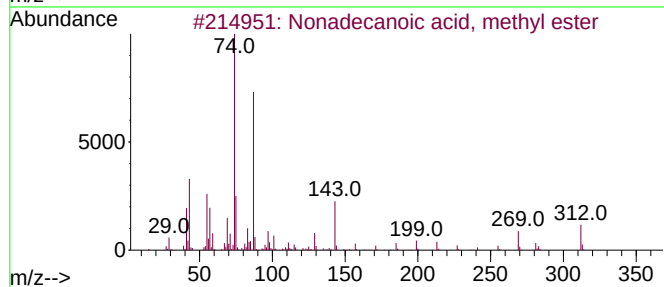
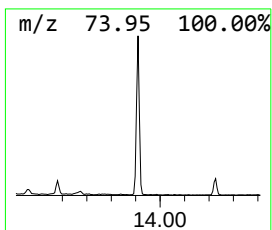
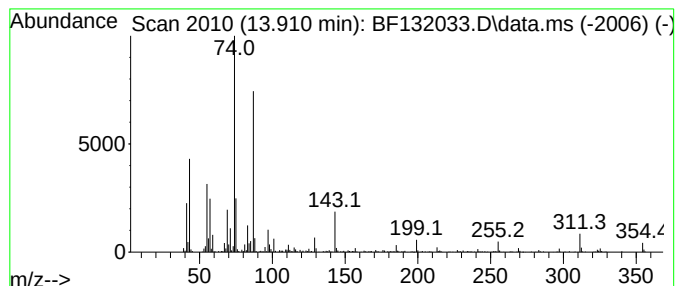
Instrument :
BNA_F
ClientSampleId :
SU-3-010923

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Nonadecanoic acid, methyl e... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.910	20.00 ng	482912	Chrysene-d12		13.974	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Nonadecanoic acid, methyl ester		312	C20H40O2	001731-94-8	98
2	Docosanoic acid, methyl ester		354	C23H46O2	000929-77-1	97
3	Methyl 20-methyl-heneicosanoate		354	C23H46O2	1000336-47-4	95
4	Hexadecanoic acid, 15-methyl-, m...		284	C18H36O2	006929-04-0	93
5	Eicosanoic acid, methyl ester		326	C21H42O2	001120-28-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011123\
Data File : BF132033.D
Acq On : 11 Jan 2023 20:36
Operator : CG\JU
Sample : 01090-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-3-010923

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.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
2-Pentanone, 4-...	4.969	29.0	ng	651916	1	6.781	449778	20.0
Hexadecanoic ac...	11.733	464.1	ng	10210600	4	11.322	440010	20.0
9,12-Octadecadi...	12.457	1705.0	ng	37511000	4	11.322	440010	20.0
Methyl stearate	12.527	211.1	ng	4644250	4	11.322	440010	20.0
9,12-Octadecadi...	12.569	26.6	ng	585360	4	11.322	440010	20.0
9-Octadecenoic ...	12.586	24.6	ng	540831	4	11.322	440010	20.0
11-Eicosenoic a...	13.163	25.2	ng	608957	5	13.974	482912	20.0
Hexadecanoic ac...	13.239	19.3	ng	465122	5	13.974	482912	20.0
unknown13.457	13.457	21.3	ng	513557	5	13.974	482912	20.0
Nonadecanoic ac...	13.910	20.0	ng	482912	5	13.974	482912	20.0