

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012822\
 Data File : BF126717.D
 Acq On : 28 Jan 2022 15:44
 Operator : CG/JU
 Sample : N1319-04
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MH-1D

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-BF011822.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126717.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.287	27	34	44	rVB	553928	755581	15.67%	2.175%
2	5.198	521	529	535	rBV	134081	166203	3.45%	0.479%
3	5.581	588	594	597	rBV	4431068	4644564	96.31%	13.372%
4	6.575	757	763	766	rBV	4388402	4822498	100.00%	13.884%
5	6.957	824	828	831	rBV	1376082	1123946	23.31%	3.236%
6	7.516	918	923	926	rBV	3114937	3169291	65.72%	9.125%
7	8.133	1024	1028	1042	rBV	245820	309503	6.42%	0.891%
8	8.239	1042	1046	1049	rBV	1658924	1465995	30.40%	4.221%
9	9.316	1224	1229	1232	rBV	5326341	4770318	98.92%	13.734%
10	9.422	1243	1247	1251	rBV	193600	172145	3.57%	0.496%
11	9.998	1341	1345	1348	rBV	1937586	1595598	33.09%	4.594%
12	10.786	1475	1479	1482	rBV	2988767	2600125	53.92%	7.486%
13	11.486	1595	1598	1602	rBV	1624874	1426035	29.57%	4.106%
14	11.868	1660	1663	1666	rBV	252476	203817	4.23%	0.587%
15	11.998	1682	1685	1690	rBV	153677	156938	3.25%	0.452%
16	12.580	1781	1784	1787	rVB	292564	216124	4.48%	0.622%
17	12.668	1796	1799	1802	rBV	83622	66329	1.38%	0.191%
18	12.721	1802	1808	1816	rBV3	81788	132825	2.75%	0.382%
19	12.792	1816	1820	1825	rBV	49613	58919	1.22%	0.170%
20	13.080	1864	1869	1872	rBV	4283563	3783896	78.46%	10.894%
21	13.998	2022	2025	2038	rVB2	146654	252197	5.23%	0.726%
22	14.133	2045	2048	2052	rVB	1016452	923439	19.15%	2.659%
23	14.598	2118	2127	2131	rBV4	61002	107544	2.23%	0.310%
24	14.921	2178	2182	2186	rVB	58931	61429	1.27%	0.177%
25	15.004	2192	2196	2200	rVB	109994	114047	2.36%	0.328%
26	15.274	2239	2242	2247	rVB	60231	70960	1.47%	0.204%
27	15.656	2302	2307	2316	rBV	790030	1064017	22.06%	3.063%
28	16.151	2387	2391	2398	rVB2	58547	89064	1.85%	0.256%
29	16.245	2399	2407	2416	rBV2	48076	205598	4.26%	0.592%
30	16.692	2479	2483	2488	rVB2	42908	69207	1.44%	0.199%
31	17.333	2588	2592	2600	rVB3	33530	67341	1.40%	0.194%
32	17.845	2674	2679	2686	rBV8	27022	68182	1.41%	0.196%

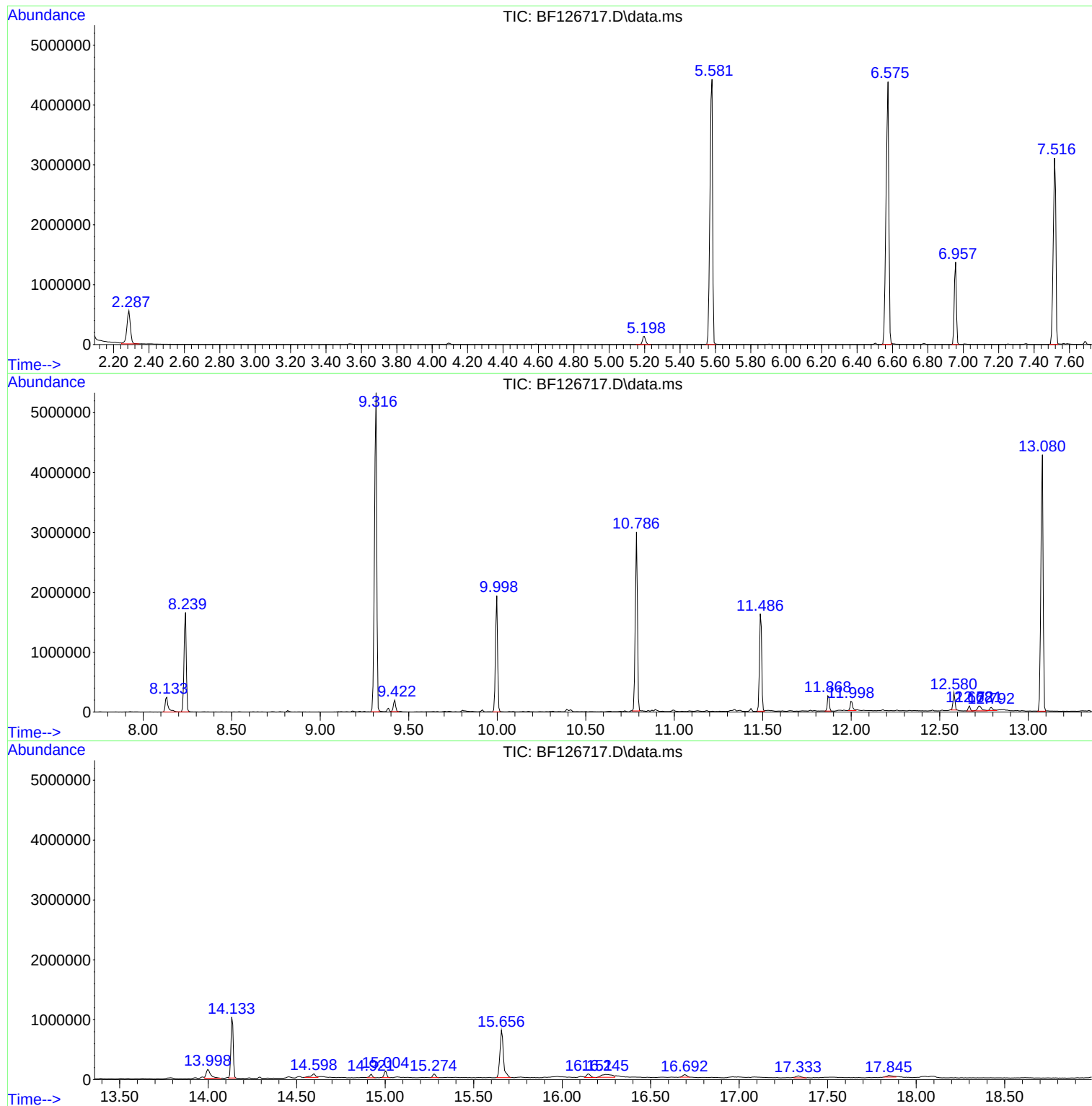
Sum of corrected areas: 34733675

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012822\
Data File : BF126717.D
Acq On : 28 Jan 2022 15:44
Operator : CG/JU
Sample : N1319-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-1D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.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\BF012822\
Data File : BF126717.D
Acq On : 28 Jan 2022 15:44
Operator : CG/JU
Sample : N1319-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-1D

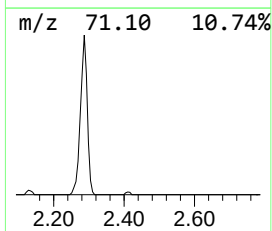
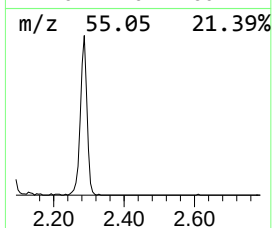
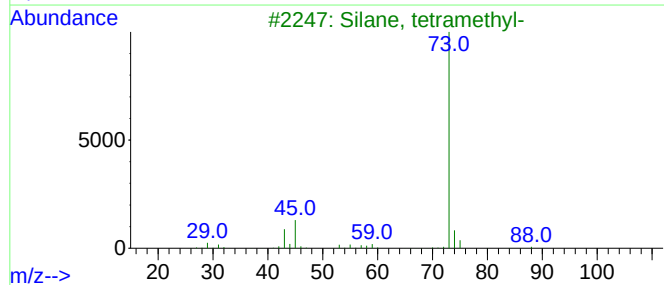
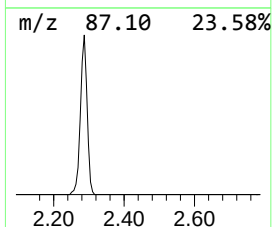
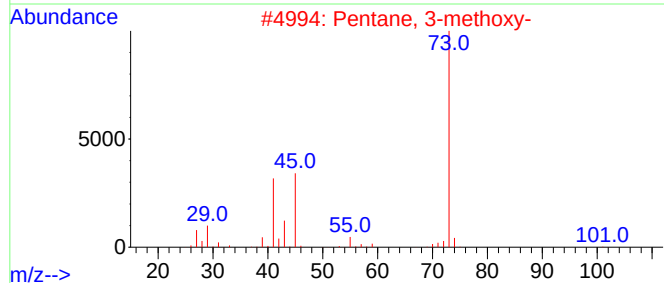
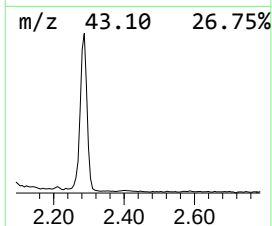
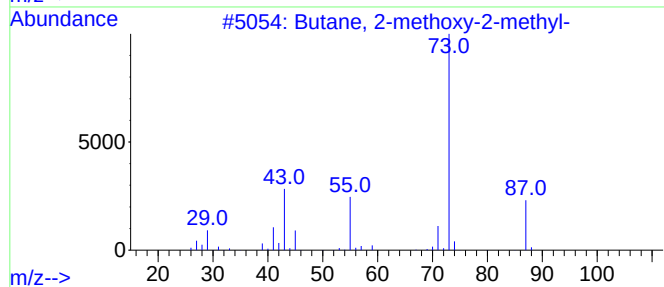
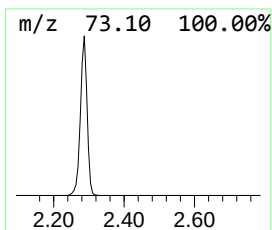
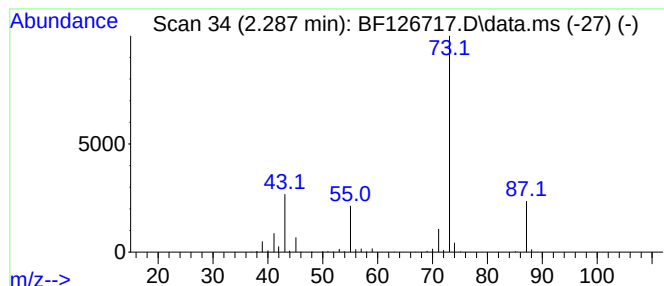
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.287	13.45 ng	755581	1,4-Dichlorobenzene-d4	6.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012822\
Data File : BF126717.D
Acq On : 28 Jan 2022 15:44
Operator : CG/JU
Sample : N1319-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-1D

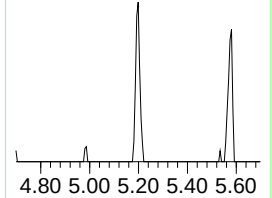
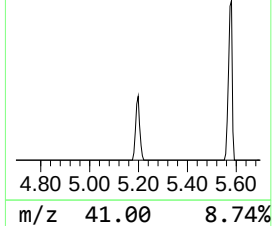
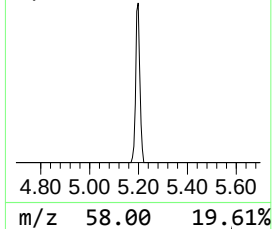
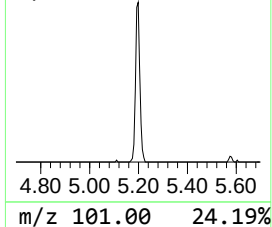
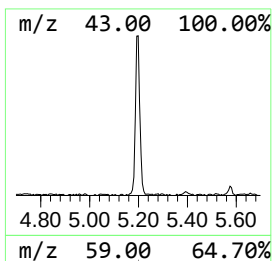
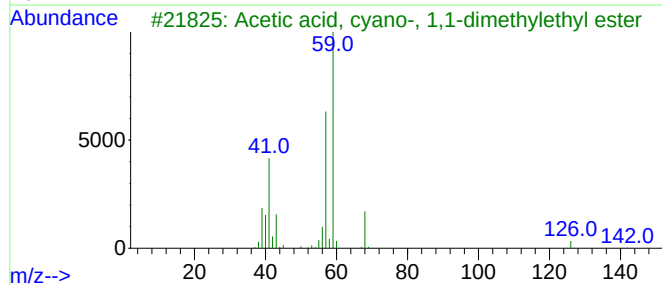
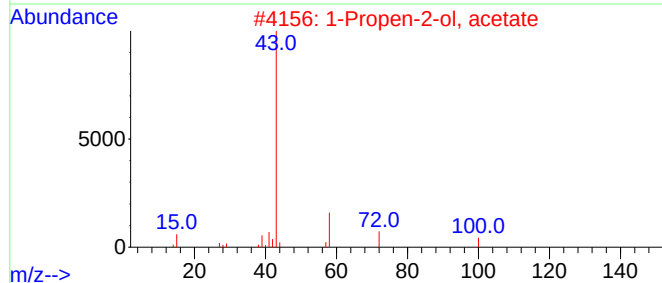
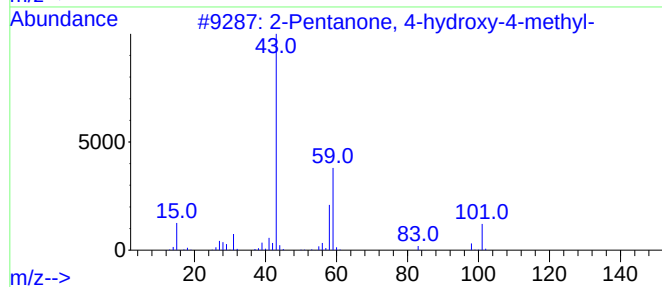
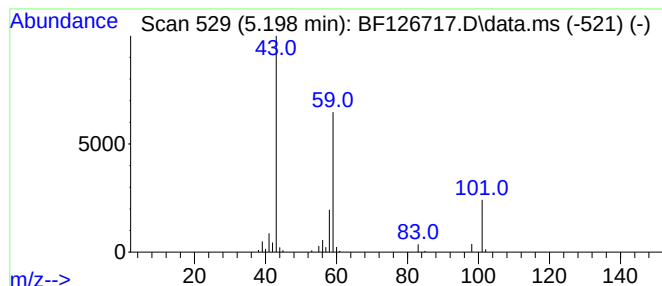
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.198	2.96 ng	166203	1,4-Dichlorobenzene-d4	6.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53		
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	12		
4	Acetone	58	C3H6O	000067-64-1	9		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012822\
Data File : BF126717.D
Acq On : 28 Jan 2022 15:44
Operator : CG/JU
Sample : N1319-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-1D

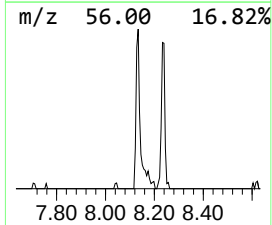
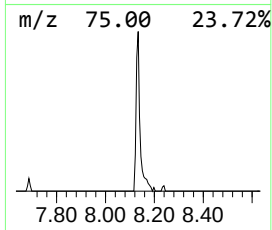
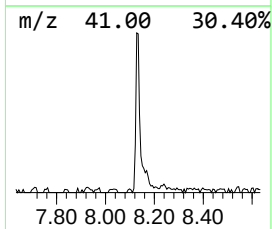
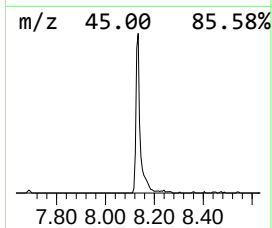
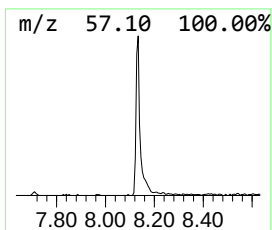
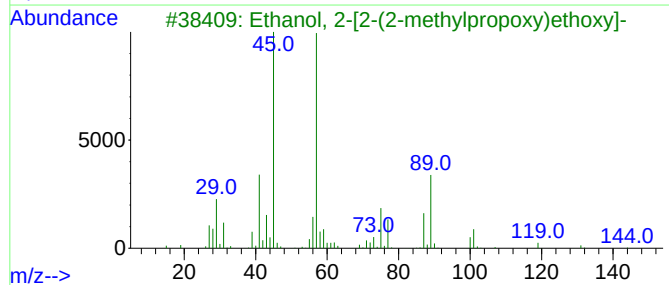
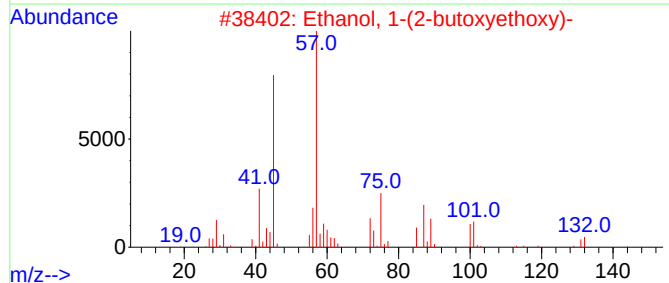
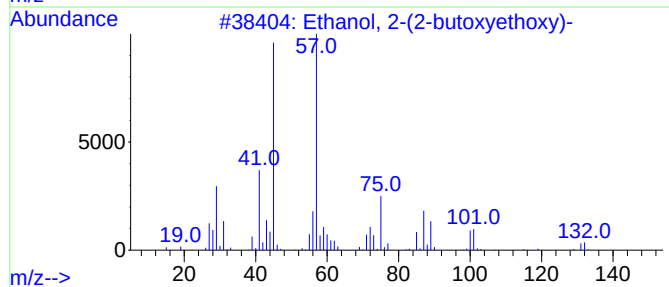
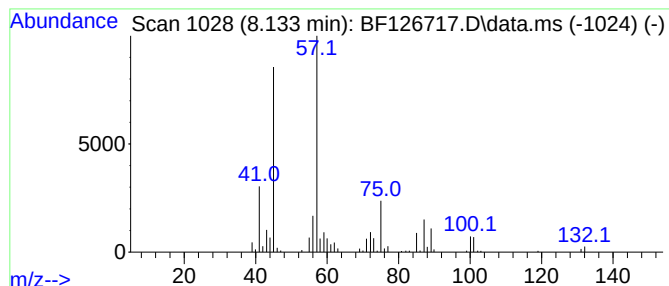
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.133	4.22 ng	309503	Naphthalene-d8	8.239

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	91
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
5			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012822\
Data File : BF126717.D
Acq On : 28 Jan 2022 15:44
Operator : CG/JU
Sample : N1319-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-1D

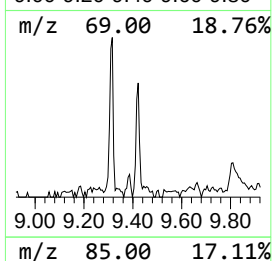
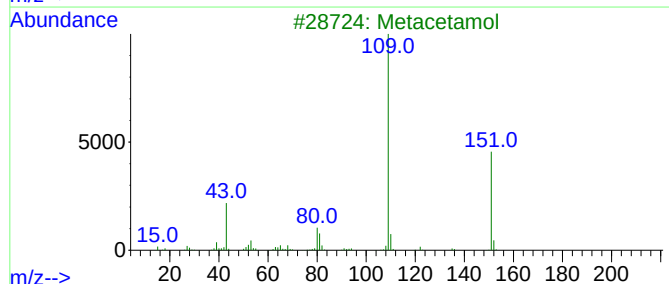
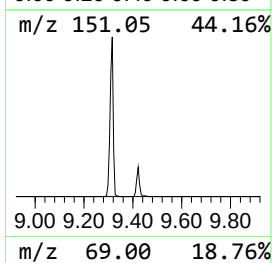
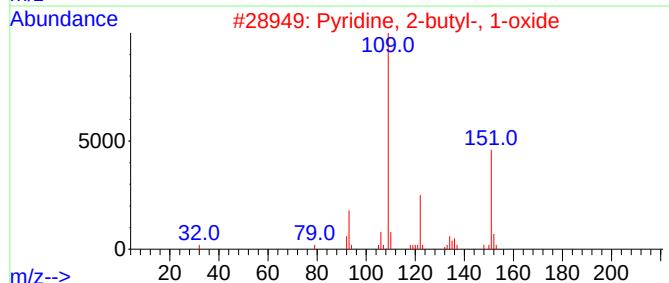
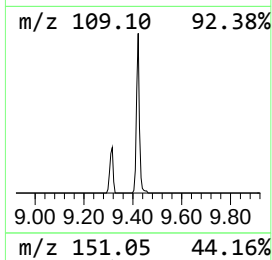
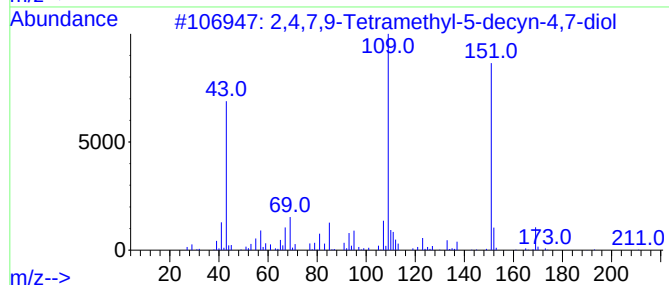
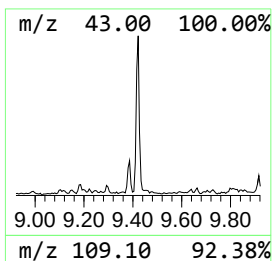
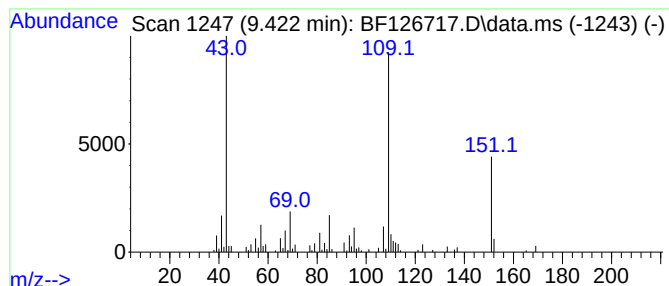
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.422	2.16 ng	172145	Acenaphthene-d10	9.998

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	90	
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	53	
3	Metacetamol	151	C8H9NO2	000621-42-1	53	
4	Acetaminophen	151	C8H9NO2	000103-90-2	53	
5	Acetamide, N-(2-hydroxyphenyl)-	151	C8H9NO2	000614-80-2	42	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012822\
Data File : BF126717.D
Acq On : 28 Jan 2022 15:44
Operator : CG/JU
Sample : N1319-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

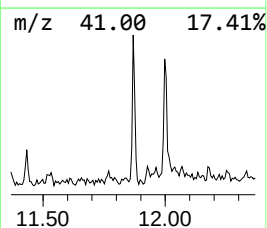
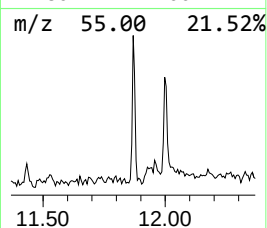
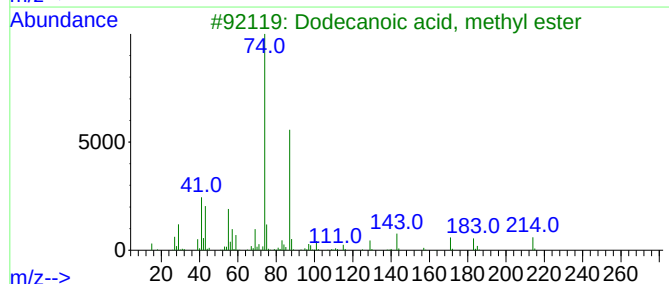
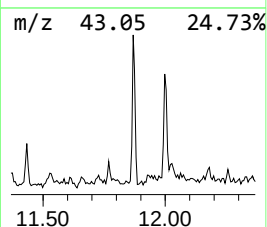
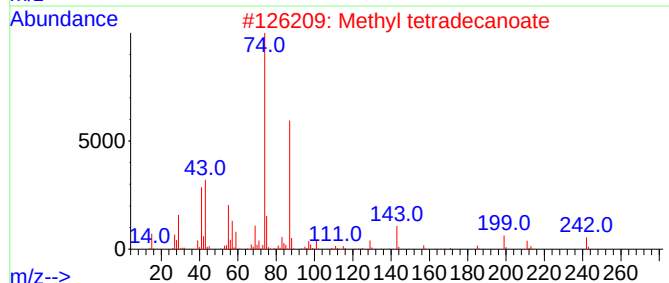
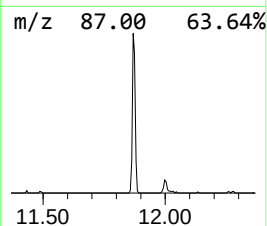
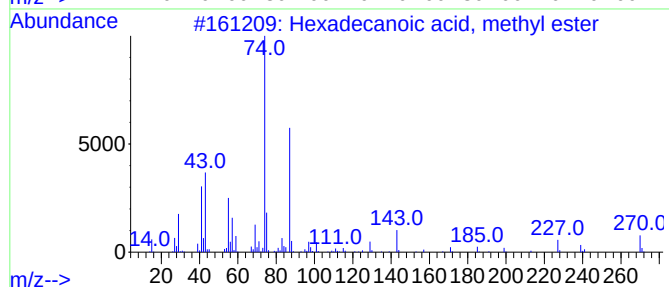
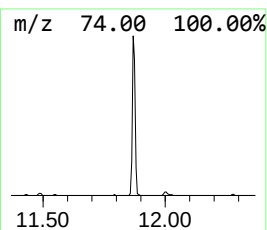
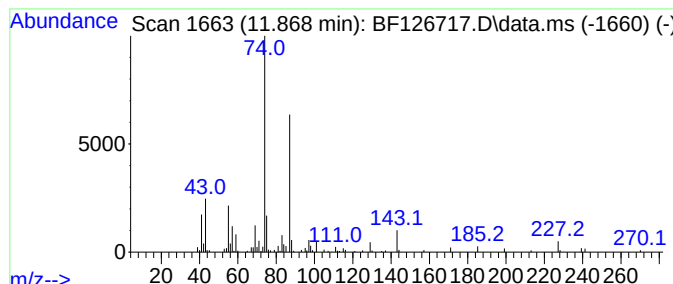
Instrument :
BNA_F
ClientSampleId :
MH-1D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Hexadecanoic acid, methyl e... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.868	2.86 ng	203817	Phenanthrene-d10		11.486	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester		270	C17H34O2	000112-39-0	97
2	Methyl tetradecanoate		242	C15H30O2	000124-10-7	90
3	Dodecanoic acid, methyl ester		214	C13H26O2	000111-82-0	90
4	Tridecanoic acid, methyl ester		228	C14H28O2	001731-88-0	90
5	Pentadecanoic acid, methyl ester		256	C16H32O2	007132-64-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012822\
Data File : BF126717.D
Acq On : 28 Jan 2022 15:44
Operator : CG/JU
Sample : N1319-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

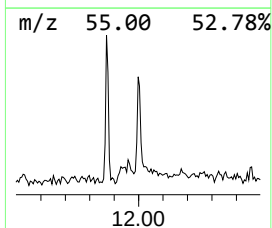
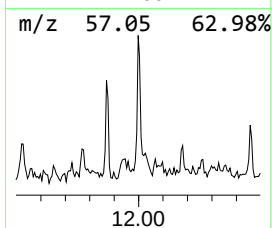
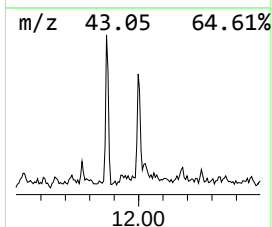
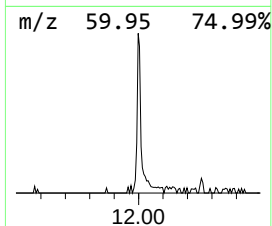
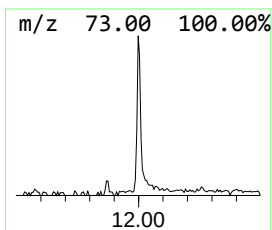
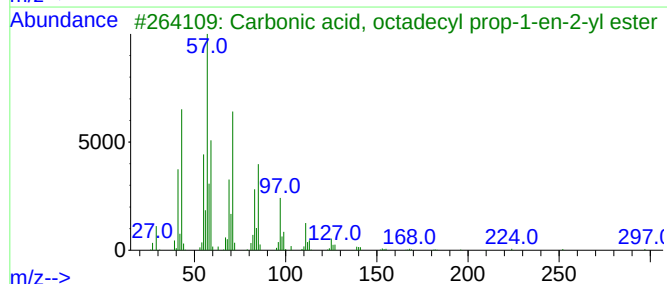
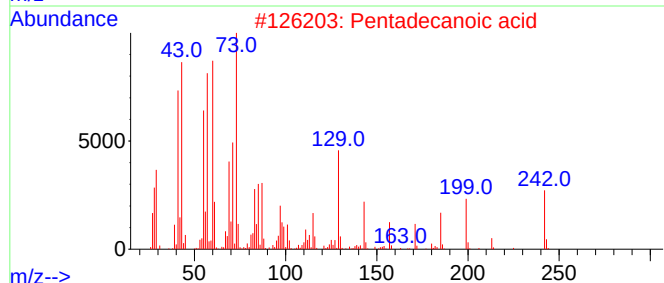
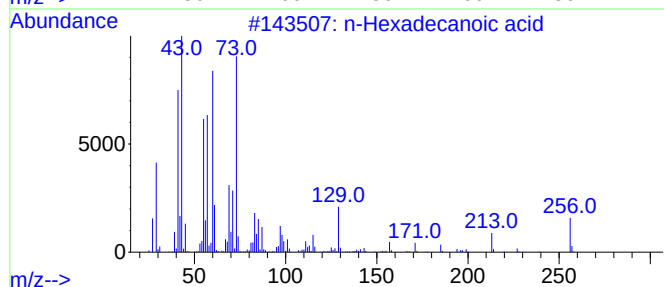
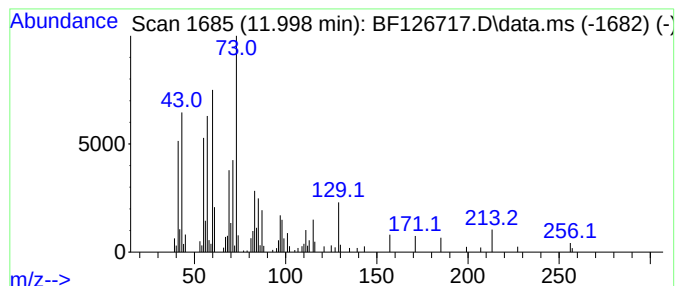
Instrument :
BNA_F
ClientSampleId :
MH-1D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.998	2.20 ng	156938	Phenanthrene-d10		11.486	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	94
2	Pentadecanoic acid		242	C15H30O2	001002-84-2	90
3	Carbonic acid, octadecyl prop-1-...		354	C22H42O3	1000383-11-5	20
4	Carbonic acid, hexadecyl prop-1-...		326	C20H38O3	1000382-90-3	18
5	Carbonic acid, dodecyl vinyl ester		256	C15H28O3	1000382-54-8	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012822\
Data File : BF126717.D
Acq On : 28 Jan 2022 15:44
Operator : CG/JU
Sample : N1319-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

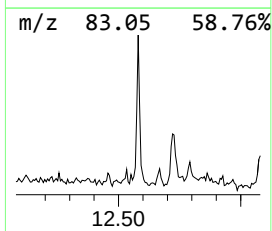
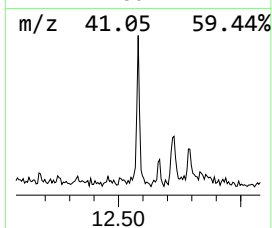
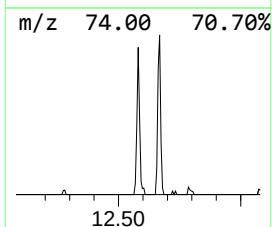
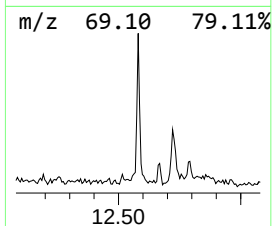
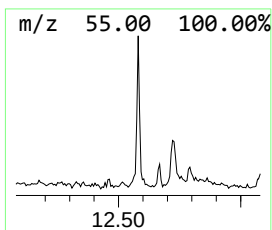
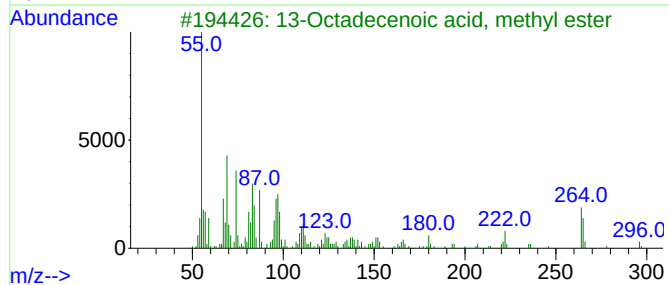
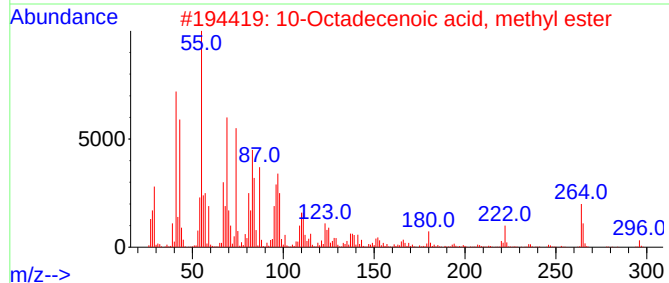
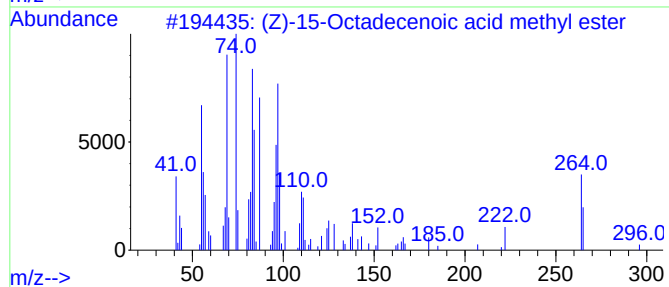
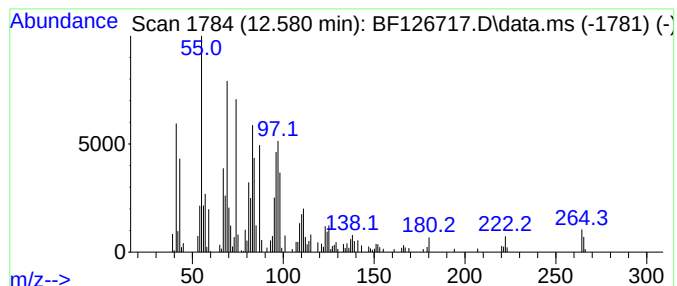
Instrument :
BNA_F
ClientSampleId :
MH-1D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 (Z)-15-Octadecenoic acid me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.580	3.03 ng	216124	Phenanthrene-d10		11.486	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	(Z)-15-Octadecenoic acid methyl ...		296	C19H36O2	1000427-69-3	91
2	10-Octadecenoic acid, methyl ester		296	C19H36O2	013481-95-3	68
3	13-Octadecenoic acid, methyl ester		296	C19H36O2	056554-47-3	64
4	Oleic Acid		282	C18H34O2	000112-80-1	64
5	14-Pentadecenoic acid		240	C15H28O2	017351-34-7	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012822\
Data File : BF126717.D
Acq On : 28 Jan 2022 15:44
Operator : CG/JU
Sample : N1319-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-1D

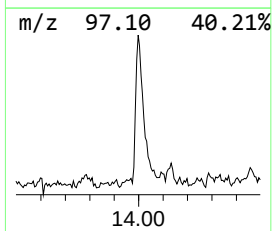
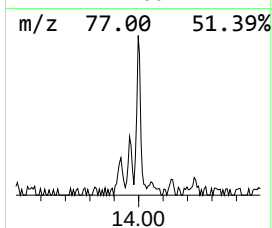
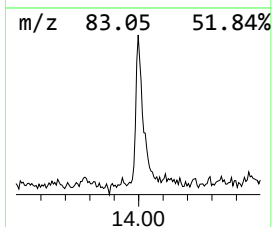
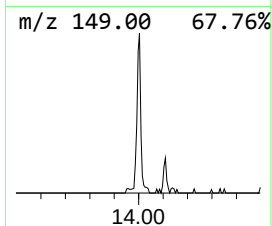
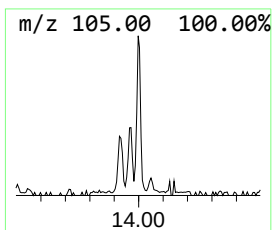
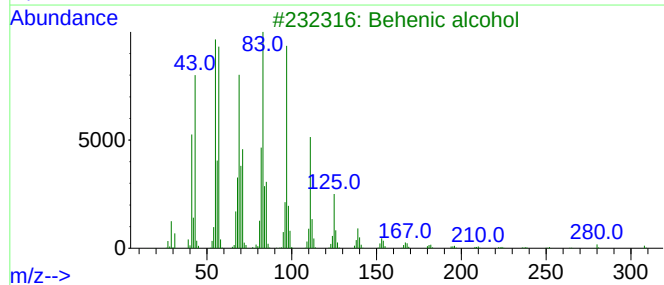
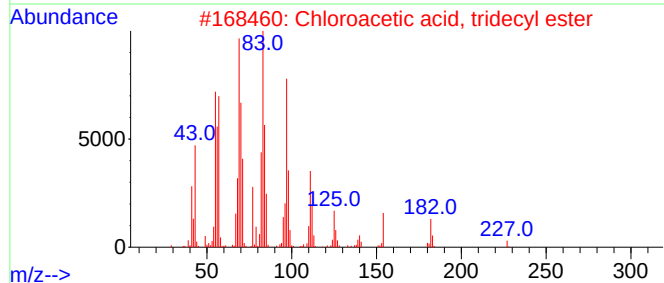
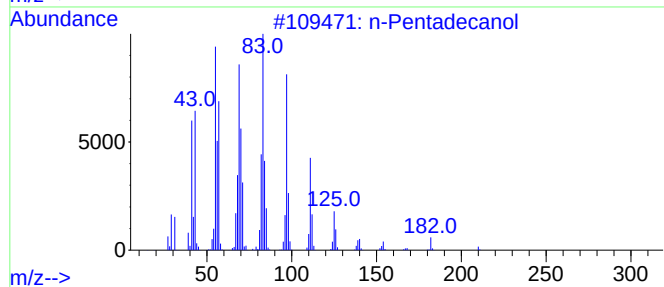
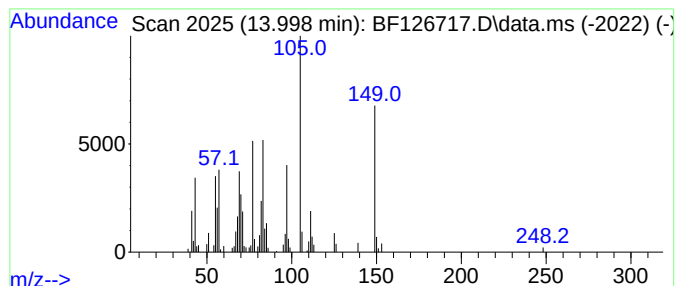
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown13.998 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.998	5.46 ng	252197	Chrysene-d12	14.133

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Pentadecanol	228	C15H32O	000629-76-5	43
2			Chloroacetic acid, tridecyl ester	276	C15H29ClO2	018277-85-5	43
3			Behenic alcohol	326	C22H46O	000661-19-8	38
4			1-Tetradecanol	214	C14H30O	000112-72-1	38
5			Phenyl(2-phenyl-1,3-dioxolan-2-y...	270	C17H18O3	1000507-07-6	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012822\
Data File : BF126717.D
Acq On : 28 Jan 2022 15:44
Operator : CG/JU
Sample : N1319-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

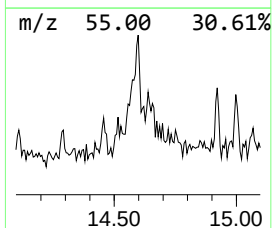
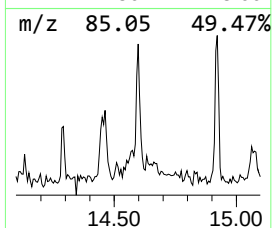
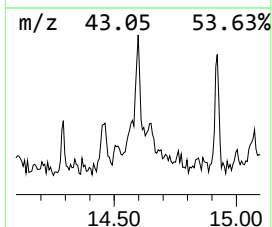
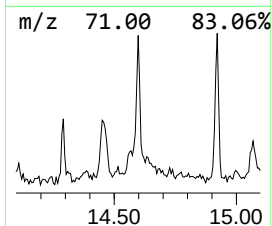
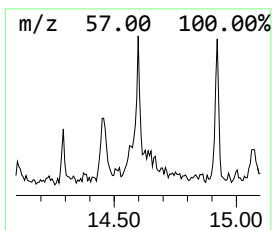
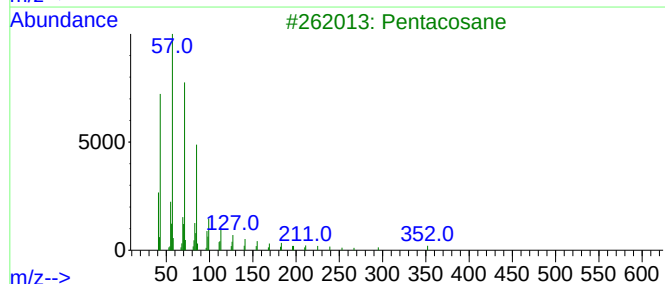
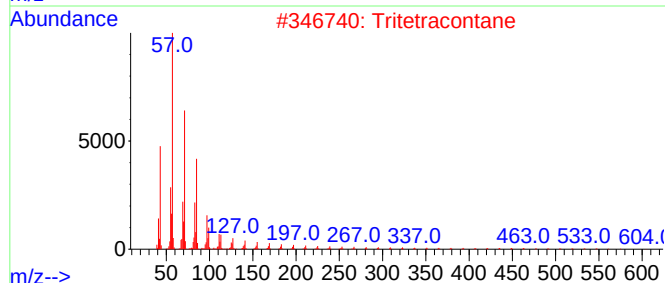
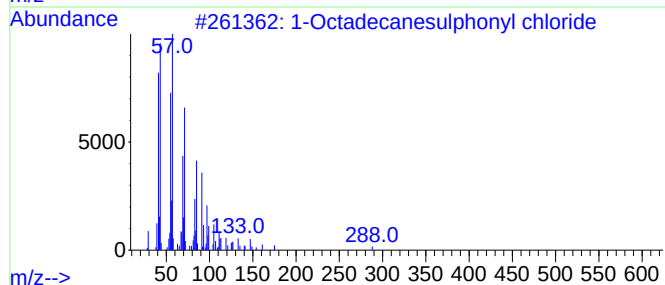
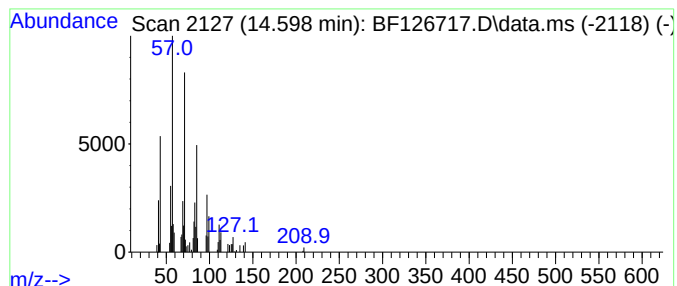
Instrument :
BNA_F
ClientSampleId :
MH-1D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Octadecanesulphonyl chloride Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.598	2.33 ng	107544	Chrysene-d12	14.133	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	90
2	Tritetracontane	605	C43H88	007098-21-7	86
3	Pentacosane	352	C25H52	000629-99-2	74
4	Heneicosane	296	C21H44	000629-94-7	72
5	Hexacosane	366	C26H54	000630-01-3	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012822\
Data File : BF126717.D
Acq On : 28 Jan 2022 15:44
Operator : CG/JU
Sample : N1319-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-1D

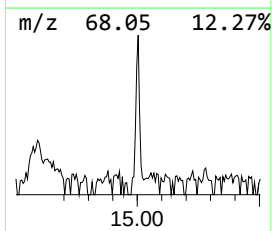
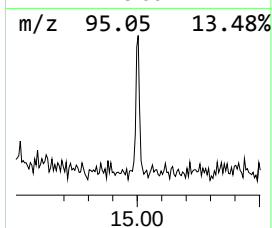
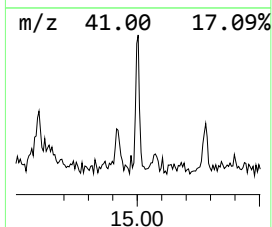
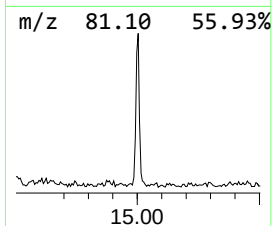
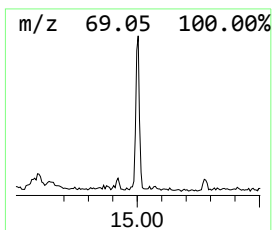
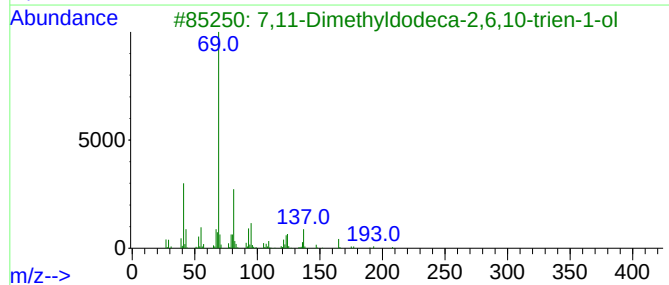
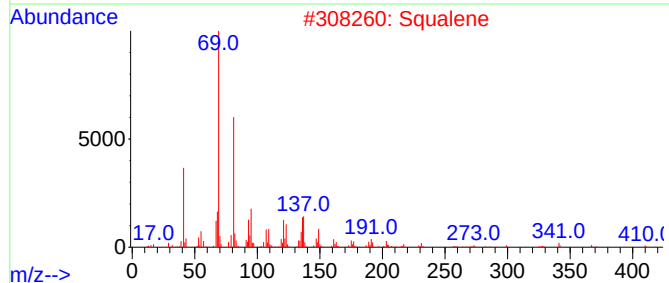
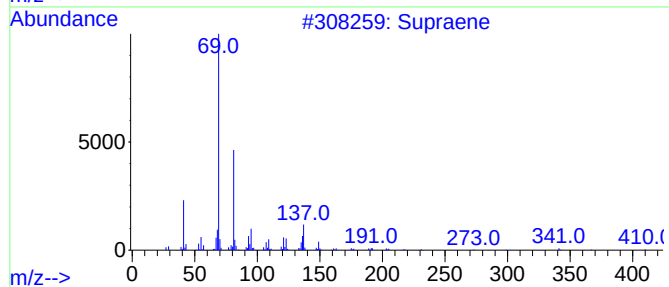
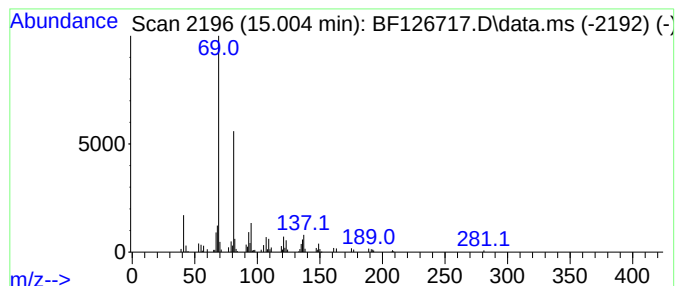
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Supraene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.004	2.14 ng	114047	Perylene-d12	15.656

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Supraene	410	C30H50	007683-64-9	91
2		Squalene	410	C30H50	000111-02-4	90
3		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	83
4		.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
5		trans-Farnesol	222	C15H26O	000106-28-5	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012822\
Data File : BF126717.D
Acq On : 28 Jan 2022 15:44
Operator : CG/JU
Sample : N1319-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-1D

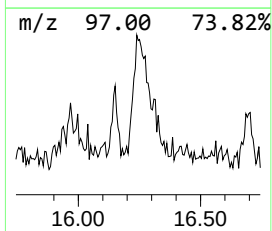
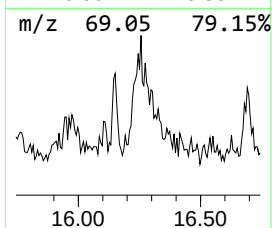
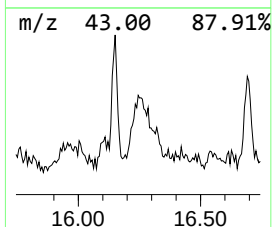
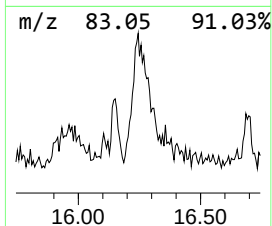
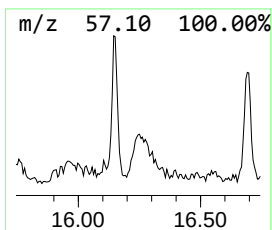
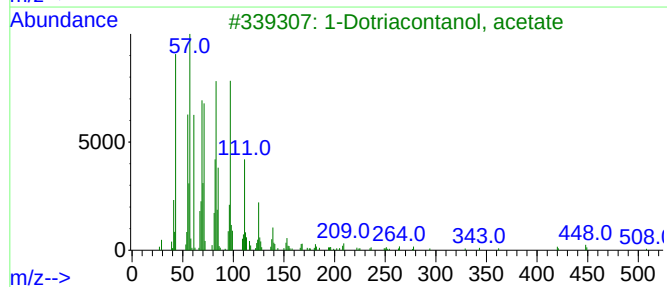
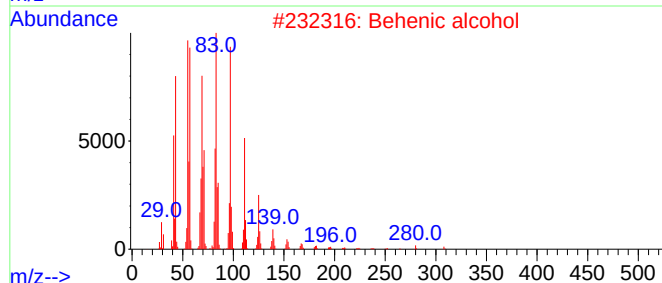
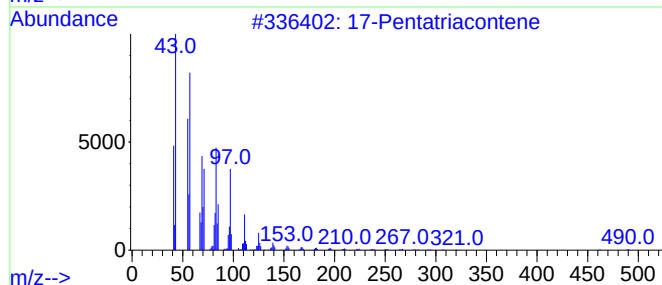
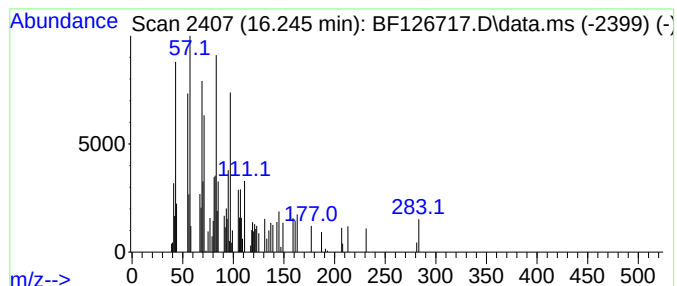
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 17-Pentatriacontene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.245	3.86 ng	205598	Perylene-d12	15.656

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17-Pentatriacontene	491	C35H70	006971-40-0	87
2			Behenic alcohol	326	C22H46O	000661-19-8	52
3			1-Dotriacontanol, acetate	509	C34H68O2	023811-94-1	52
4			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	46
5			4-Methyl-dodec-3-en-1-ol	198	C13H26O	156992-84-6	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012822\
Data File : BF126717.D
Acq On : 28 Jan 2022 15:44
Operator : CG/JU
Sample : N1319-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-1D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.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...	2.287	13.4	ng	755581	1	6.957	1123950	20.0
2-Pentanone, 4-...	5.198	3.0	ng	166203	1	6.957	1123950	20.0
Ethanol, 2-(2-b...	8.133	4.2	ng	309503	2	8.239	1466000	20.0
2,4,7,9-Tetrame...	9.422	2.2	ng	172145	3	9.998	1595600	20.0
Hexadecanoic ac...	11.868	2.9	ng	203817	4	11.486	1426040	20.0
n-Hexadecanoic ...	11.998	2.2	ng	156938	4	11.486	1426040	20.0
(Z)-15-Octadece...	12.580	3.0	ng	216124	4	11.486	1426040	20.0
unknown13.998	13.998	5.5	ng	252197	5	14.133	923439	20.0
1-Octadecanesul...	14.598	2.3	ng	107544	5	14.133	923439	20.0
Supraene	15.004	2.1	ng	114047	6	15.656	1064020	20.0
17-Pentatriacon...	16.245	3.9	ng	205598	6	15.656	1064020	20.0