

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012725\
 Data File : BF141269.D
 Acq On : 27 Jan 2025 13:45
 Operator : RC/JU
 Sample : Q1183-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VNJ-237

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-BF011025.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141269.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.158	6	11	23	rVB	59931	115267	3.50%	0.492%
2	2.375	30	48	50	rBV2	46052	234219	7.11%	1.000%
3	4.381	383	389	396	rBV	125325	178398	5.42%	0.761%
4	5.022	484	498	504	rBV	1897387	3292201	100.00%	14.049%
5	6.428	732	737	755	rVB	512919	709146	21.54%	3.026%
6	6.804	796	801	806	rBV	594681	731331	22.21%	3.121%
7	7.363	890	896	901	rBV	1086090	1410351	42.84%	6.019%
8	7.622	935	940	951	rBV	50323	71016	2.16%	0.303%
9	8.087	1013	1019	1024	rBV	746017	974424	29.60%	4.158%
10	9.163	1196	1202	1212	rBV	2093223	2791242	84.78%	11.912%
11	9.804	1307	1311	1313	rBV2	28908	36634	1.11%	0.156%
12	9.839	1313	1317	1330	rVB	866672	1102555	33.49%	4.705%
13	10.357	1400	1405	1411	rBV	26139	39603	1.20%	0.169%
14	10.551	1433	1438	1446	rBV	269238	363191	11.03%	1.550%
15	10.634	1447	1452	1459	rVB	37560	69394	2.11%	0.296%
16	11.328	1565	1570	1576	rBV	848910	1054371	32.03%	4.500%
17	11.569	1606	1611	1617	rBV2	25594	52346	1.59%	0.223%
18	11.851	1651	1659	1682	rVB	692635	1382774	42.00%	5.901%
19	12.116	1700	1704	1712	rVB	58546	78862	2.40%	0.337%
20	12.563	1775	1780	1785	rBV2	50187	106605	3.24%	0.455%
21	12.639	1788	1793	1805	rVB2	439659	842504	25.59%	3.595%
22	12.816	1813	1823	1835	rVB	1199401	2804773	85.19%	11.969%
23	12.916	1835	1840	1846	rBV	2077333	2708760	82.28%	11.560%
24	13.827	1990	1995	2004	rBV	81306	170460	5.18%	0.727%
25	13.916	2006	2010	2014	rVV2	27629	52566	1.60%	0.224%
26	13.969	2014	2019	2026	rVB	691288	958327	29.11%	4.090%
27	14.457	2098	2102	2111	rVB	33660	66007	2.00%	0.282%
28	15.439	2263	2269	2280	rVB	567942	899175	27.31%	3.837%
29	16.557	2453	2459	2470	rBV9	42700	136474	4.15%	0.582%

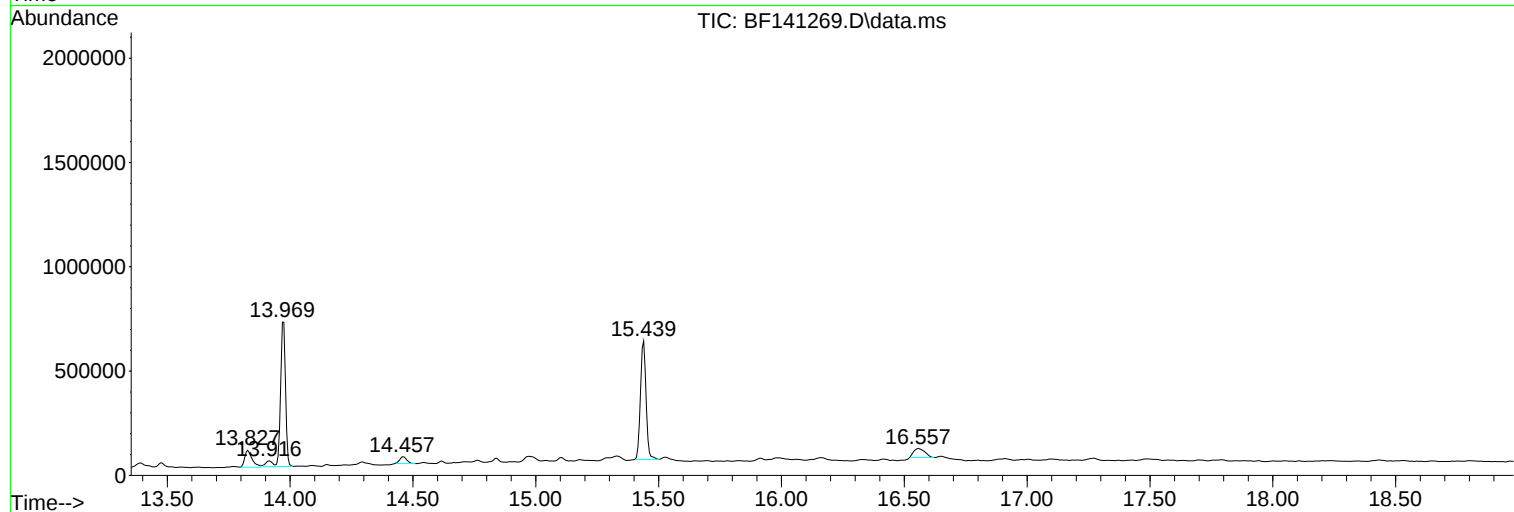
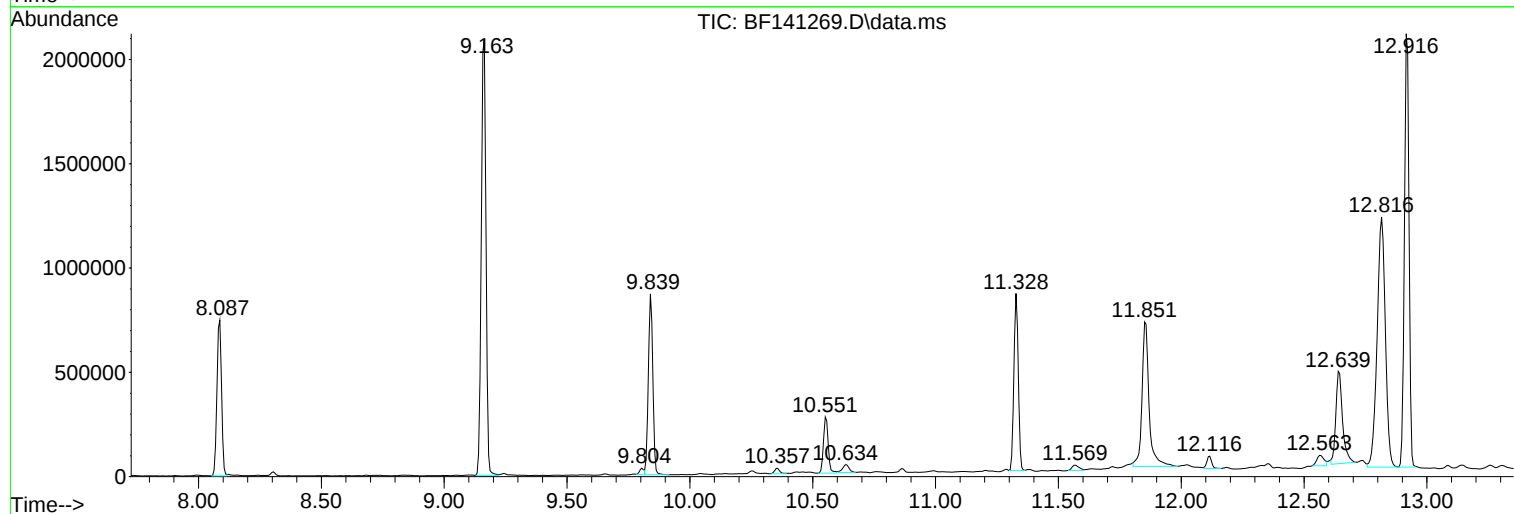
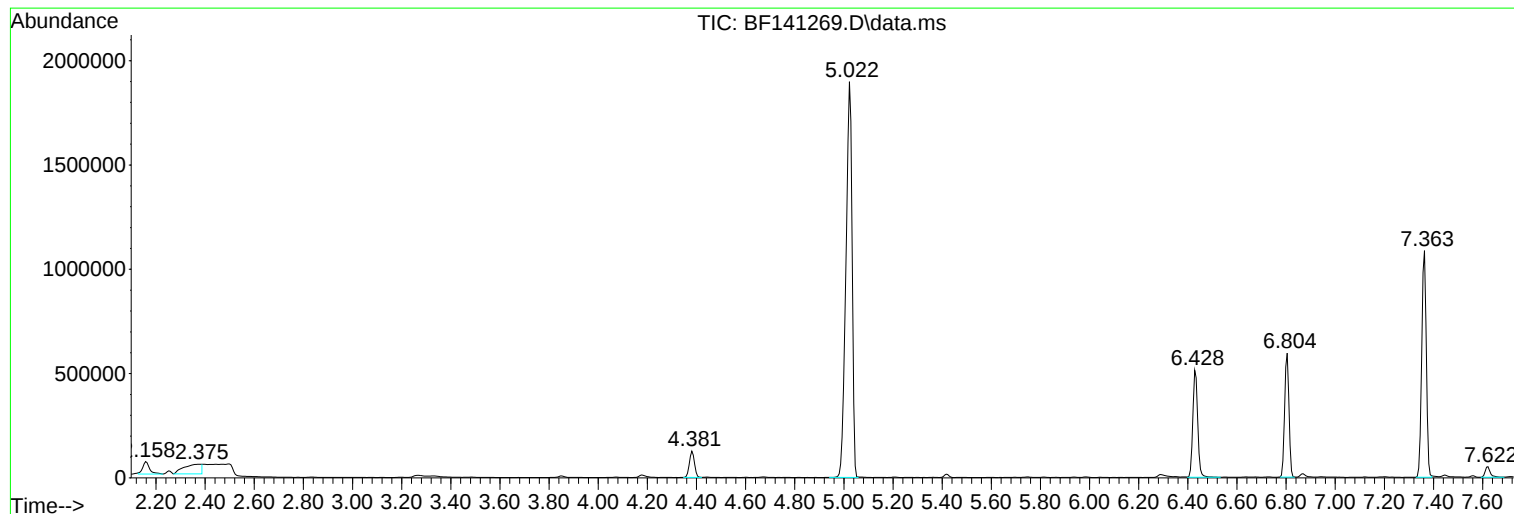
Sum of corrected areas: 23432976

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012725\
Data File : BF141269.D
Acq On : 27 Jan 2025 13:45
Operator : RC/JU
Sample : Q1183-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-237

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.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\BF012725\
Data File : BF141269.D
Acq On : 27 Jan 2025 13:45
Operator : RC/JU
Sample : Q1183-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-237

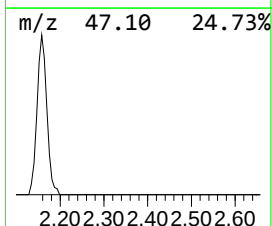
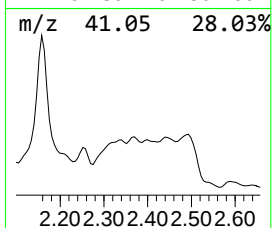
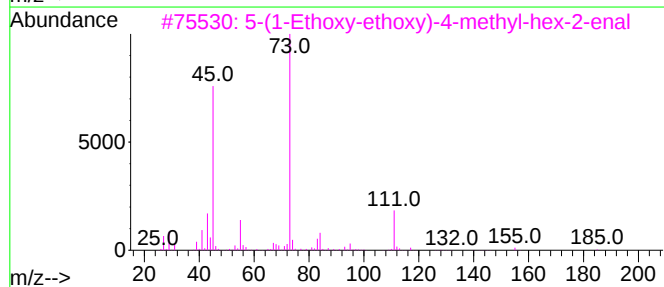
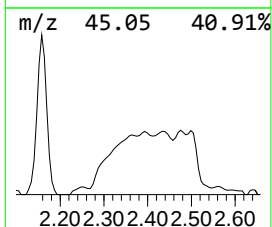
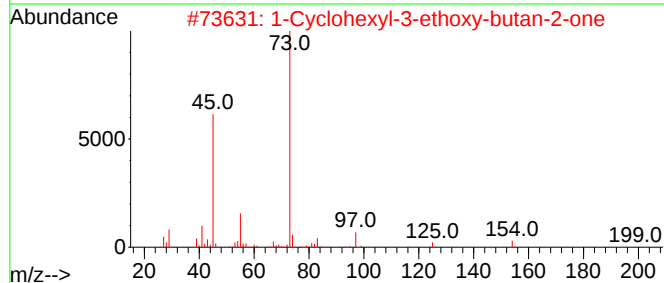
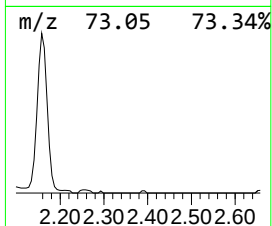
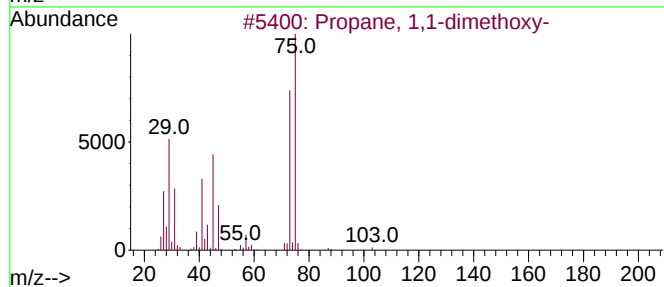
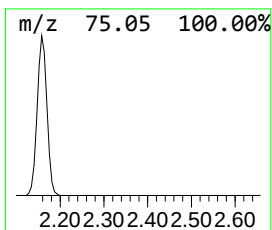
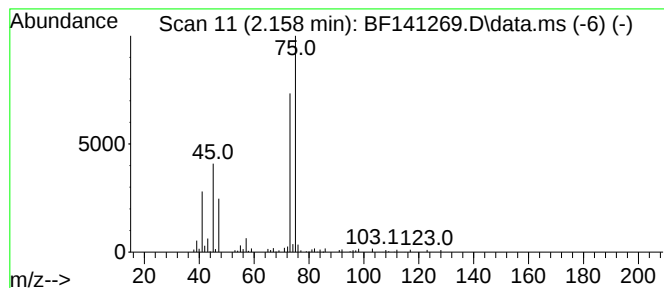
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.158	3.15 ng	115267	1,4-Dichlorobenzene-d4	6.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2			1-Cyclohexyl-3-ethoxy-butan-2-one	198	C12H22O2	074897-69-1	22
3			5-(1-Ethoxy-ethoxy)-4-methyl-hex...	200	C11H20O3	086845-53-6	12
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10
5			2,5-Diethoxy-3-methyl-3-vinylhexane	214	C13H26O2	1000432-70-8	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012725\
Data File : BF141269.D
Acq On : 27 Jan 2025 13:45
Operator : RC/JU
Sample : Q1183-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-237

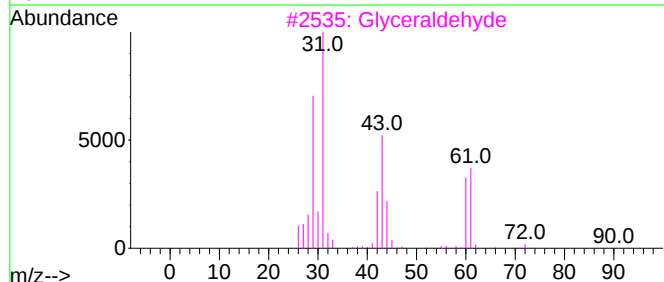
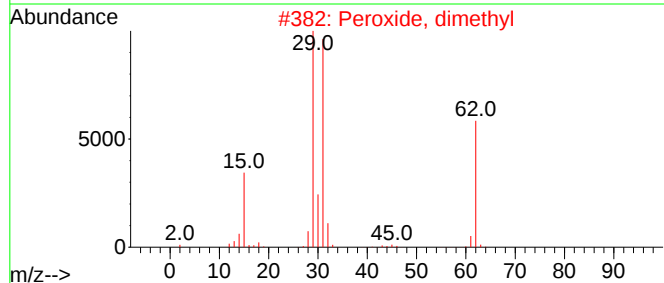
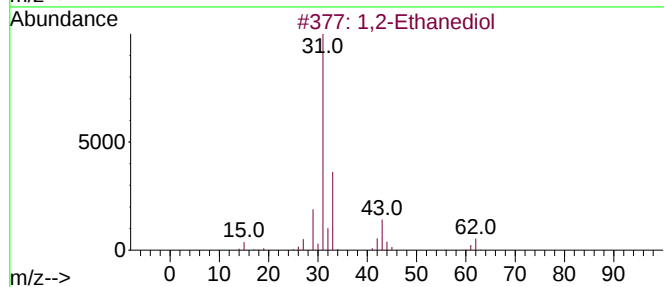
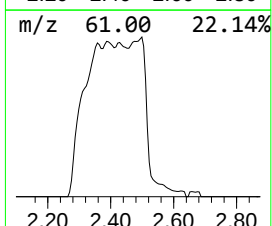
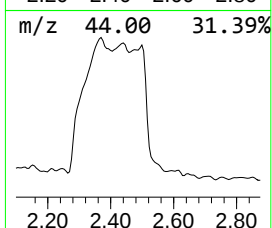
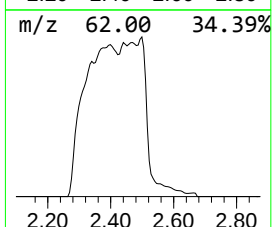
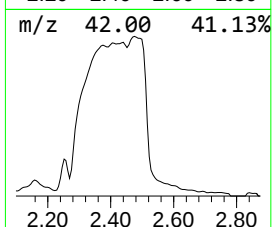
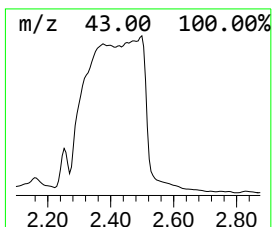
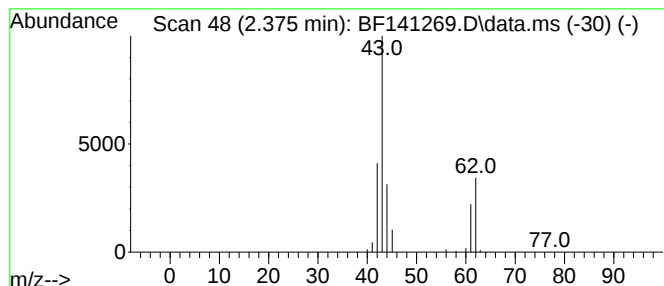
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown2.375 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.375	6.41 ng	234219	1,4-Dichlorobenzene-d4	6.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Ethanediol	62	C2H6O2	000107-21-1	9
2			Peroxide, dimethyl	62	C2H6O2	000690-02-8	4
3			Glyceraldehyde	90	C3H6O3	000056-82-6	4
4			Monoethanolamine	61	C2H7NO	000141-43-5	3
5			Diazirine	42	CH2N2	1000305-84-1	3



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012725\
Data File : BF141269.D
Acq On : 27 Jan 2025 13:45
Operator : RC/JU
Sample : Q1183-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-237

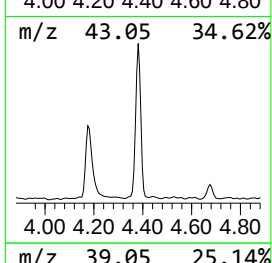
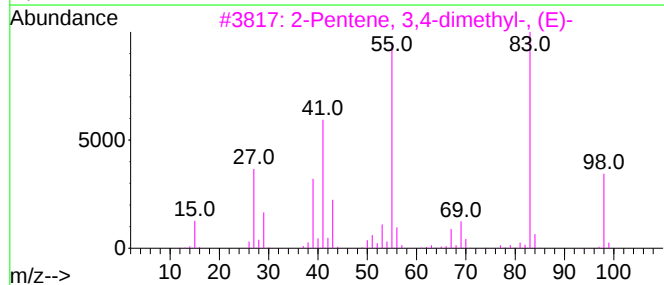
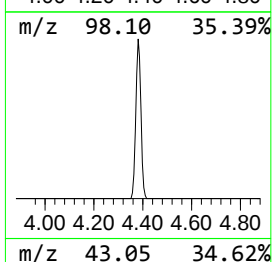
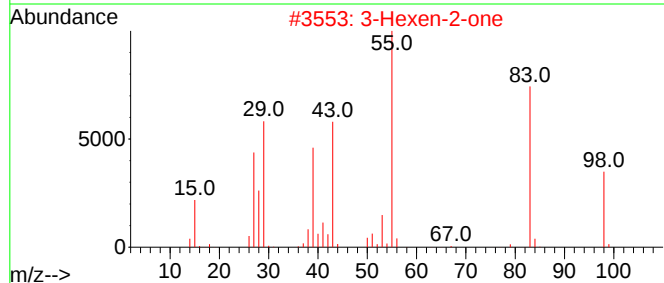
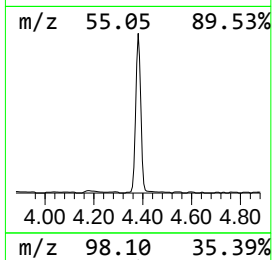
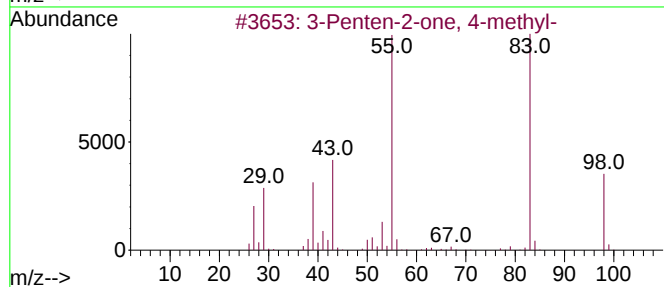
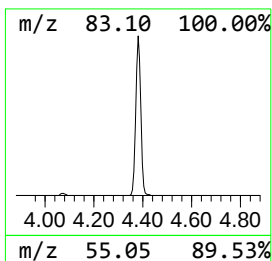
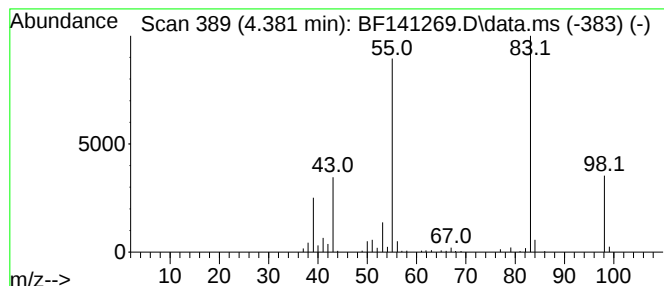
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.381	4.88 ng	178398	1,4-Dichlorobenzene-d4	6.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5			Cyclohexane, methyl-	98	C7H14	000108-87-2	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012725\
Data File : BF141269.D
Acq On : 27 Jan 2025 13:45
Operator : RC/JU
Sample : Q1183-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

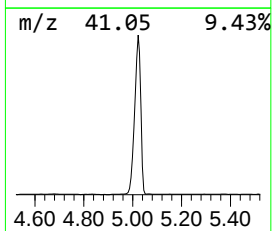
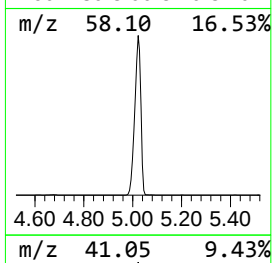
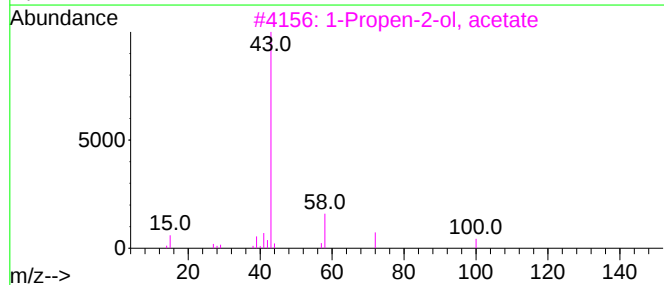
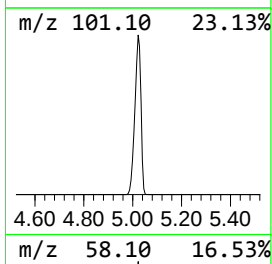
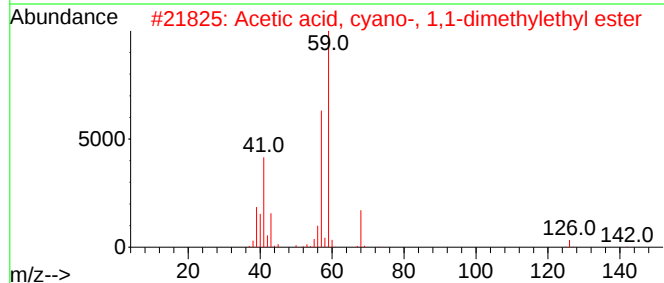
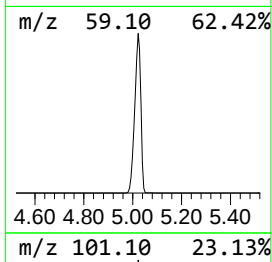
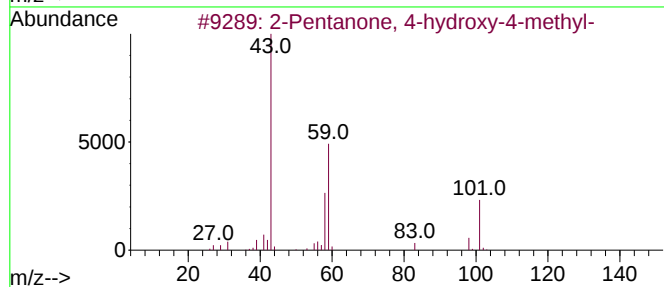
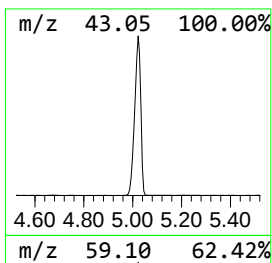
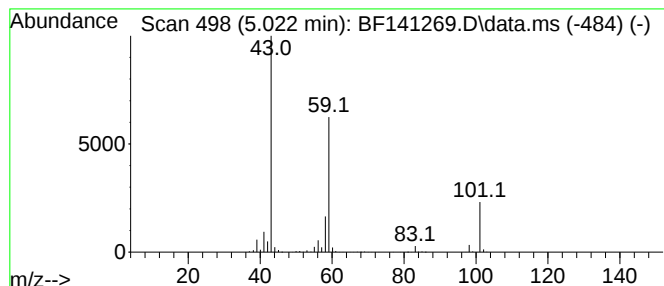
Instrument :
BNA_F
ClientSampleId :
VNJ-237

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.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-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.022	90.03 ng	3292200	1,4-Dichlorobenzene-d4			6.804
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	10
4	Morpholine, 4-methyl-		101	C5H11NO	000109-02-4	9
5	5-Hexen-2-one		98	C6H10O	000109-49-9	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012725\
Data File : BF141269.D
Acq On : 27 Jan 2025 13:45
Operator : RC/JU
Sample : Q1183-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-237

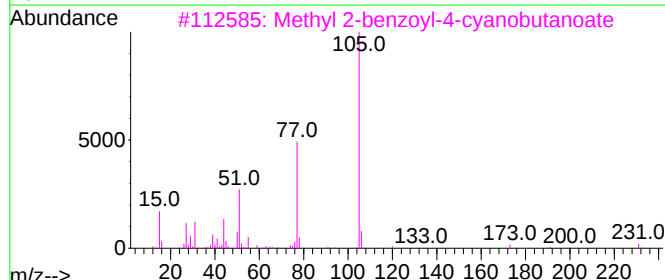
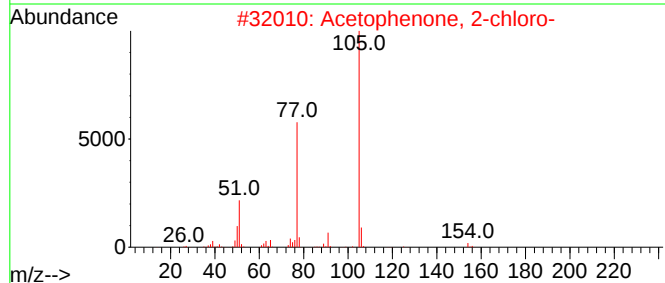
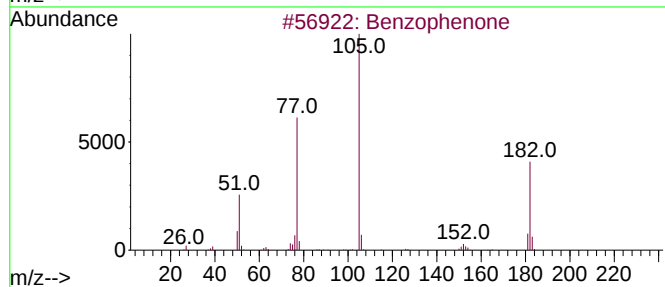
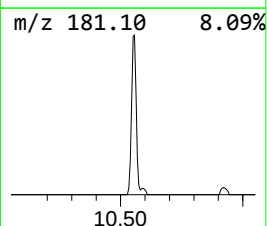
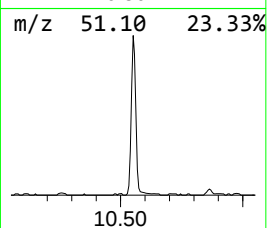
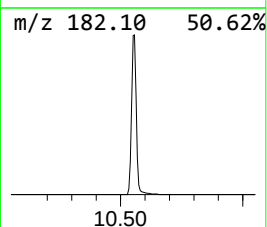
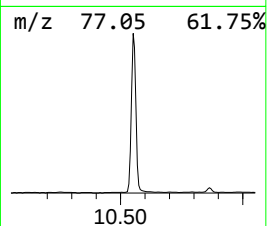
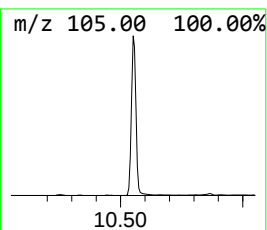
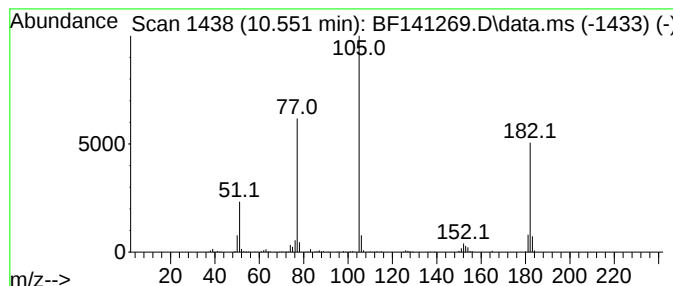
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.551	6.59 ng	363191	Acenaphthene-d10	9.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3			Methyl 2-benzoyl-4-cyanobutanoate	231	C13H13NO3	1010486-83-8	47
4			Benzeneacetic acid, .alpha.-oxo-...	178	C10H10O3	001603-79-8	47
5			Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012725\
Data File : BF141269.D
Acq On : 27 Jan 2025 13:45
Operator : RC/JU
Sample : Q1183-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

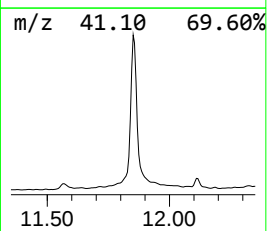
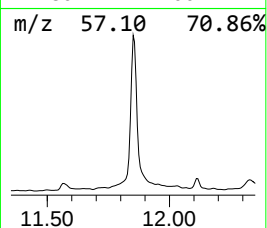
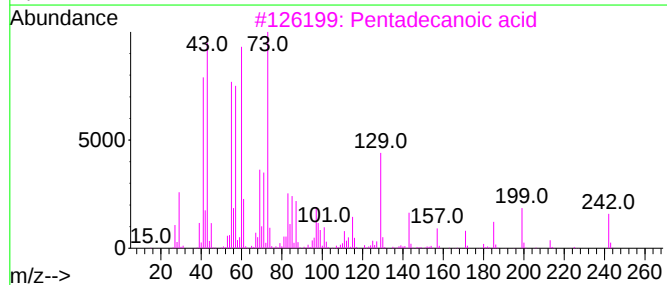
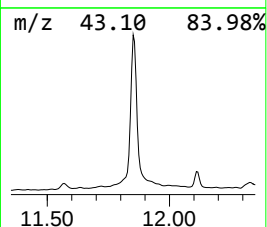
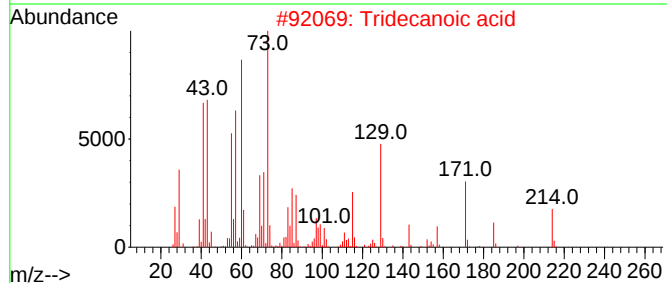
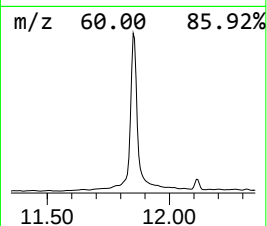
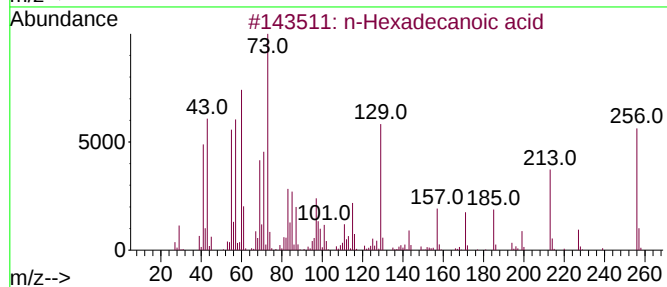
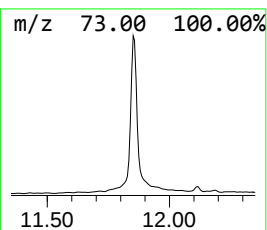
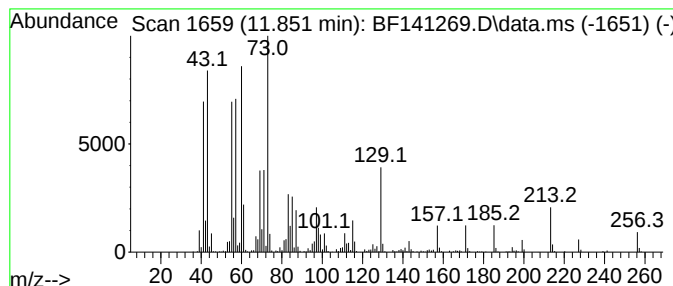
Instrument :
BNA_F
ClientSampleId :
VNJ-237

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.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 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.851	26.23 ng	1382770	Phenanthrene-d10		11.328	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Tridecanoic acid		214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	76
5	n-Decanoic acid		172	C10H20O2	000334-48-5	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012725\
Data File : BF141269.D
Acq On : 27 Jan 2025 13:45
Operator : RC/JU
Sample : Q1183-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

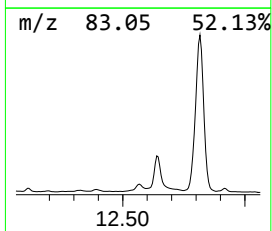
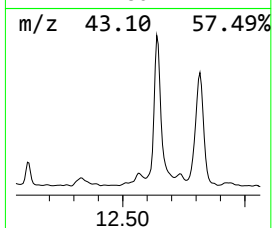
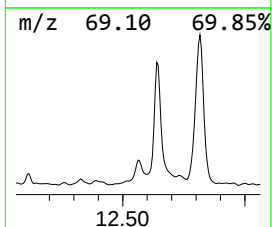
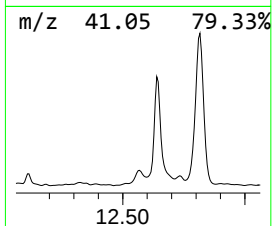
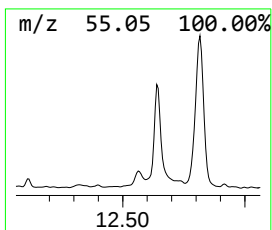
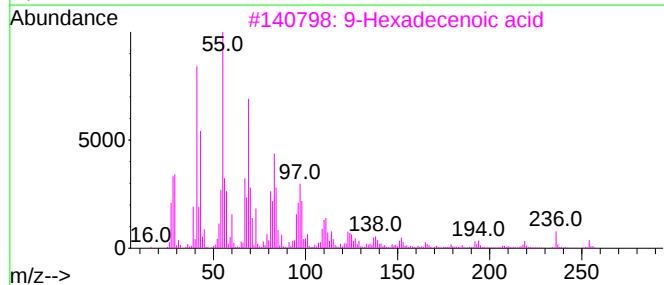
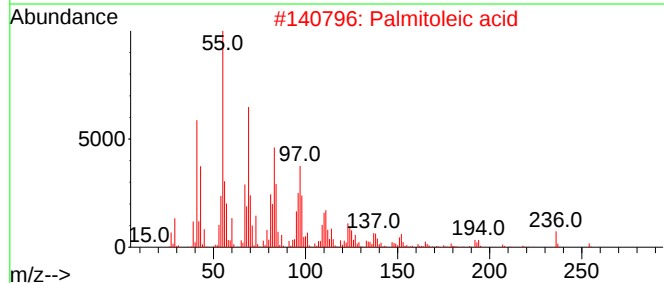
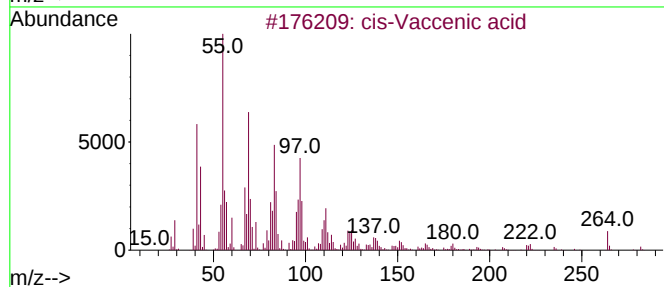
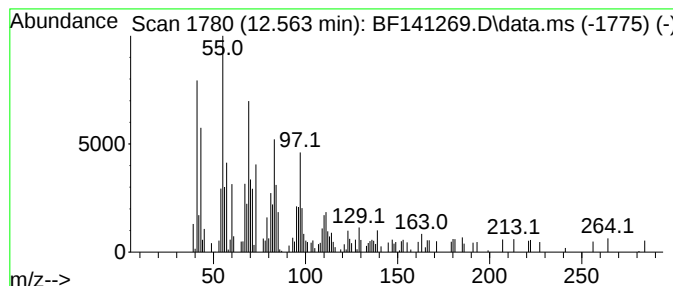
Instrument :
BNA_F
ClientSampleId :
VNJ-237

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 cis-Vaccenic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.563	2.02 ng	106605	Phenanthrene-d10		11.328	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	cis-Vaccenic acid		282	C18H34O2	000506-17-2	83
2	Palmitoleic acid		254	C16H30O2	000373-49-9	81
3	9-Hexadecenoic acid		254	C16H30O2	002091-29-4	76
4	9-octadecanoic acid, 2,2,3,3,4,4...		464	C22H35F7O2	1000376-61-4	76
5	Oleic Acid		282	C18H34O2	000112-80-1	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012725\
Data File : BF141269.D
Acq On : 27 Jan 2025 13:45
Operator : RC/JU
Sample : Q1183-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

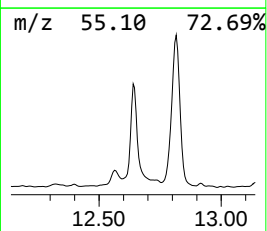
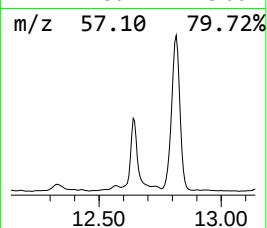
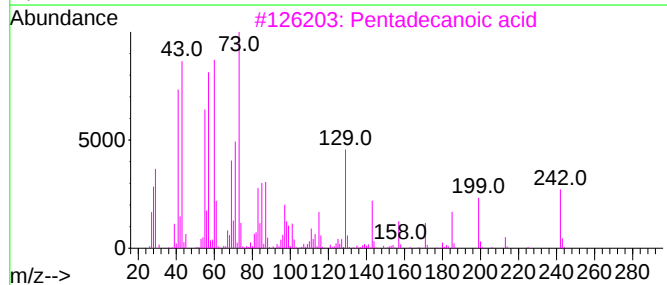
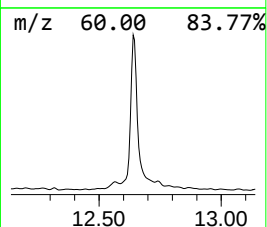
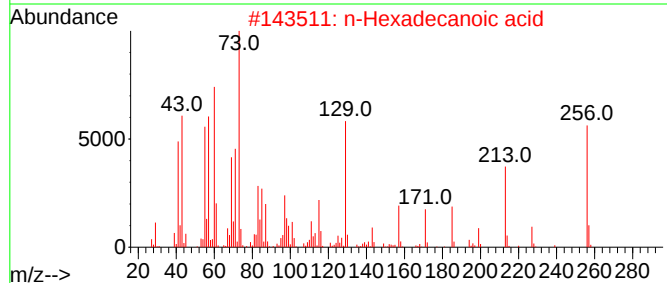
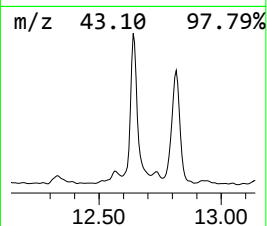
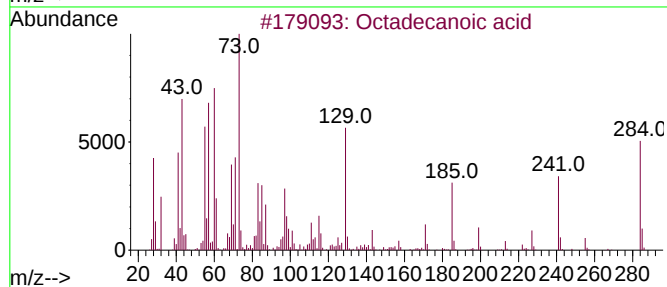
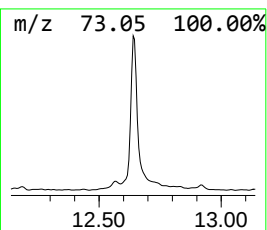
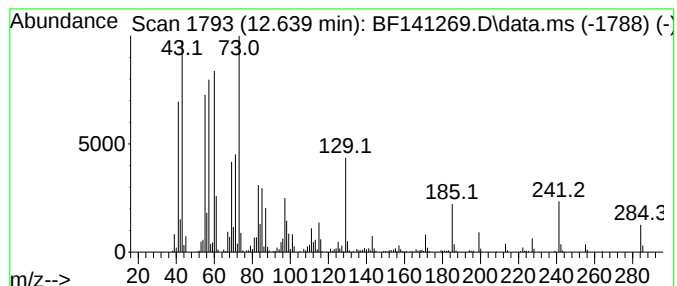
Instrument :
BNA_F
ClientSampleId :
VNJ-237

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.639	15.98 ng	842504	Phenanthrene-d10		11.328	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octadecanoic acid		284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	91
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	89
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	83
5	n-Decanoic acid		172	C10H20O2	000334-48-5	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012725\
Data File : BF141269.D
Acq On : 27 Jan 2025 13:45
Operator : RC/JU
Sample : Q1183-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-237

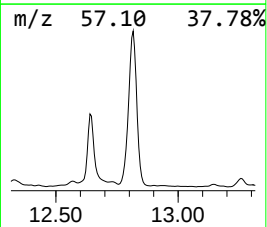
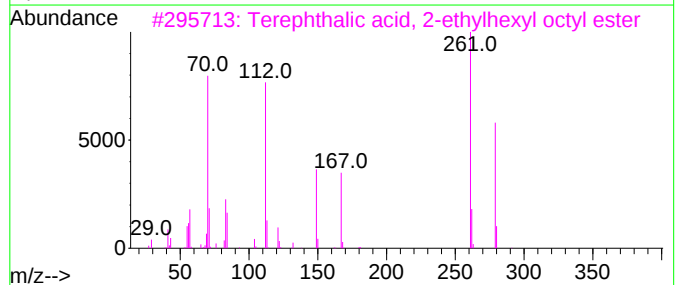
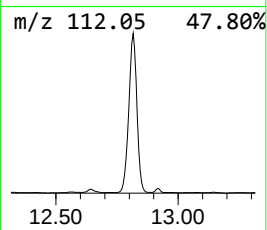
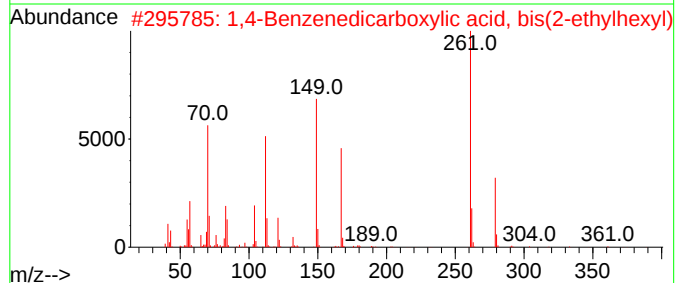
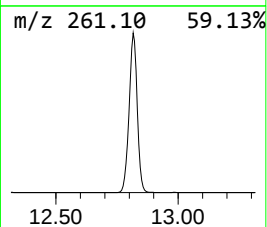
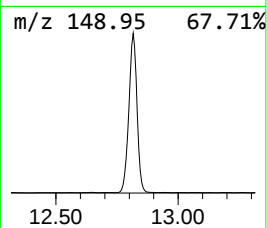
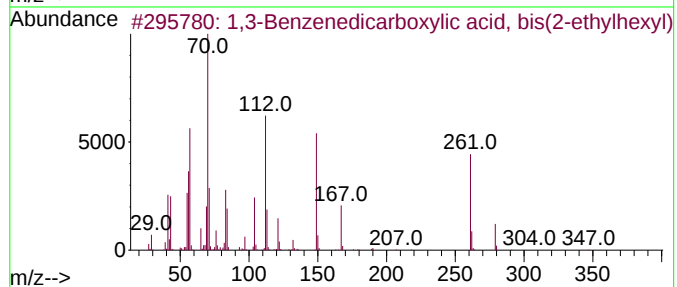
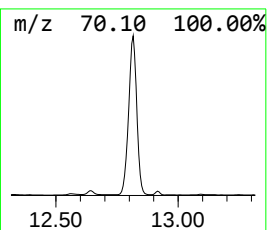
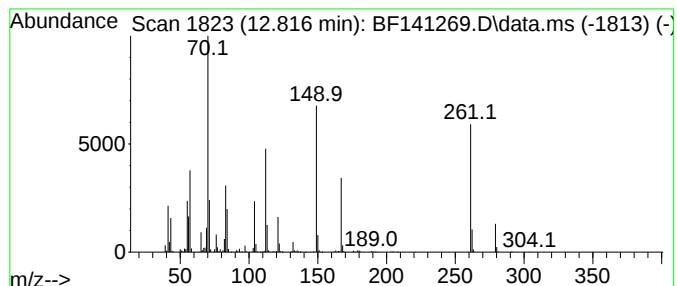
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1,3-Benzenedicarboxylic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.816	58.53 ng	2804770	Chrysene-d12	13.975

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	78
2			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	74
3			Terephthalic acid, 2-ethylhexyl ...	390	C24H38O4	1000324-00-5	58
4			Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	49
5			Terephthalic acid, monochloride,...	296	C16H21ClO3	1000324-22-9	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012725\
Data File : BF141269.D
Acq On : 27 Jan 2025 13:45
Operator : RC/JU
Sample : Q1183-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-237

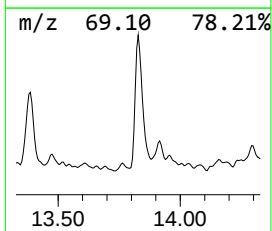
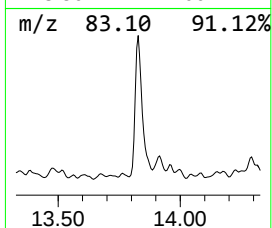
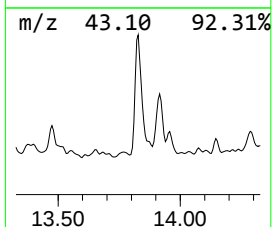
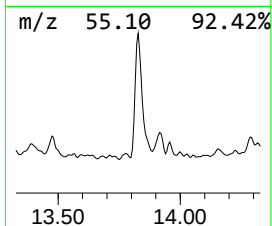
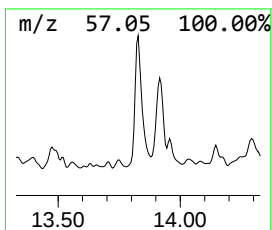
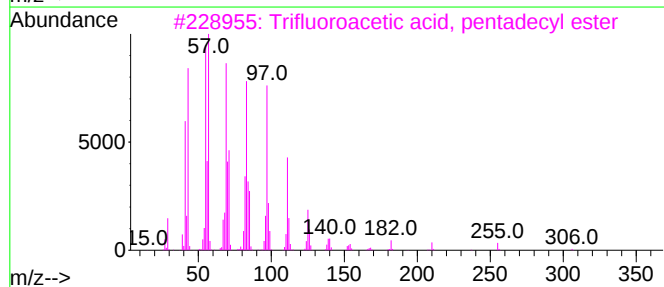
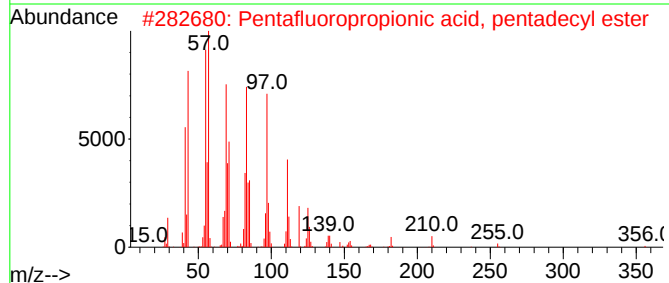
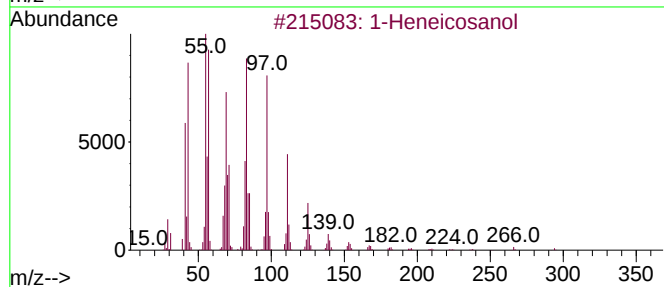
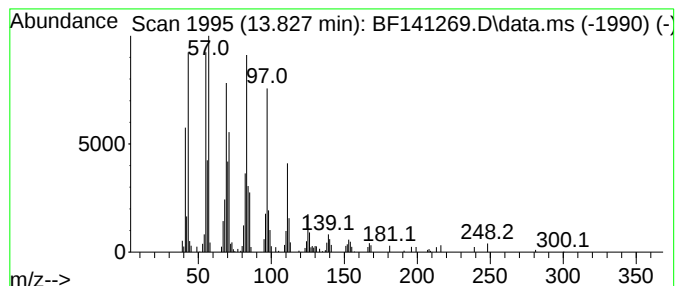
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Heneicosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	3.56 ng	170460	Chrysene-d12	13.975

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
3			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	95
4			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	95
5			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012725\
Data File : BF141269.D
Acq On : 27 Jan 2025 13:45
Operator : RC/JU
Sample : Q1183-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-237

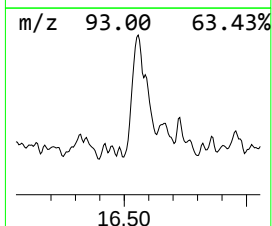
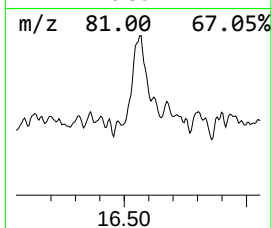
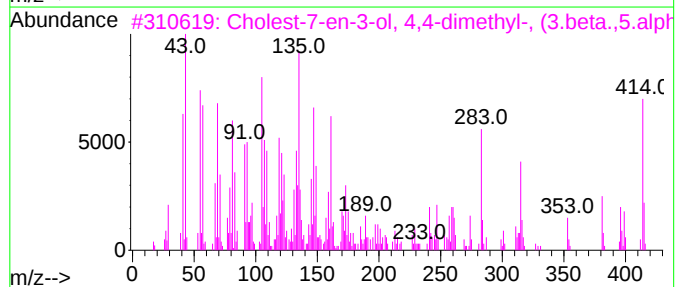
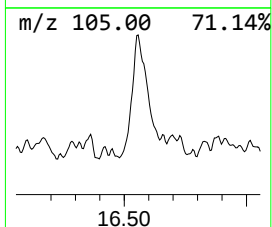
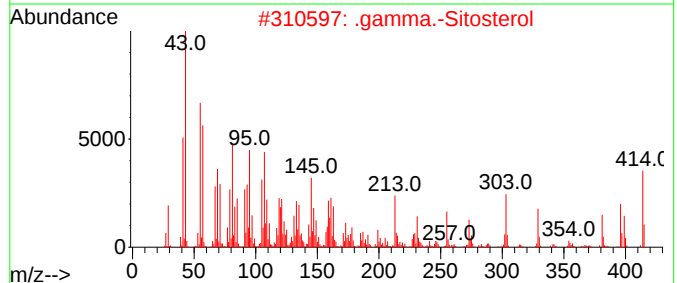
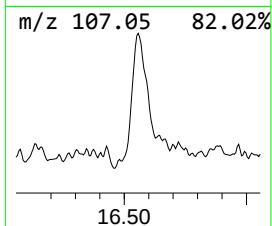
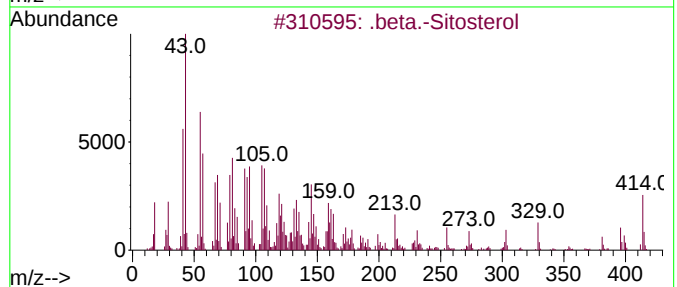
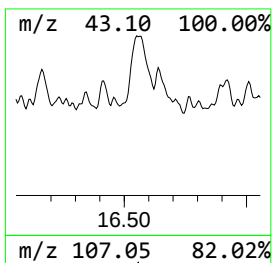
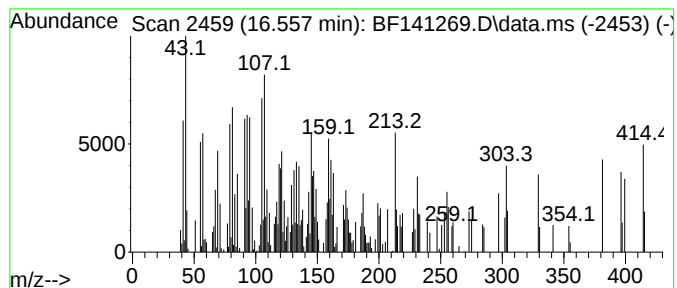
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 .beta.-Sitosterol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.557	3.04 ng	136474	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.beta.-Sitosterol	414	C29H50O	000083-46-5	97
2			.gamma.-Sitosterol	414	C29H50O	000083-47-6	95
3			Cholest-7-en-3-ol, 4,4-dimethyl-...	414	C29H50O	006384-28-7	35
4			Cholest-5-ene, 3-ethoxy-, (3.beta...)	414	C29H50O	000986-19-6	30
5			17-(1,5-Dimethylhexyl)-10,13-dim...	414	C29H50O	1000210-86-9	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012725\
Data File : BF141269.D
Acq On : 27 Jan 2025 13:45
Operator : RC/JU
Sample : Q1183-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-237

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.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
Propane, 1,1-di...	2.158	3.1	ng	115267	1	6.804	731331	20.0
unknown2.375	2.375	6.4	ng	234219	1	6.804	731331	20.0
3-Penten-2-one,...	4.381	4.9	ng	178398	1	6.804	731331	20.0
2-Pentanone, 4-...	5.022	90.0	ng	3292200	1	6.804	731331	20.0
Benzophenone	10.551	6.6	ng	363191	3	9.839	1102560	20.0
n-Hexadecanoic ...	11.851	26.2	ng	1382770	4	11.328	1054370	20.0
cis-Vaccenic acid	12.563	2.0	ng	106605	4	11.328	1054370	20.0
Octadecanoic acid	12.639	16.0	ng	842504	4	11.328	1054370	20.0
1,3-Benzenedica...	12.816	58.5	ng	2804770	5	13.975	958327	20.0
1-Heneicosanol	13.827	3.6	ng	170460	5	13.975	958327	20.0
.beta.-Sitosterol	16.557	3.0	ng	136474	6	15.439	899175	20.0