

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122823\
 Data File : BF136792.D
 Acq On : 28 Dec 2023 13:50
 Operator : CG\JU
 Sample : 05897-08
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GHL-SS-33

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-BF122023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136792.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.016	495	498	507	rVB	62019	72642	3.10%	0.549%
2	5.422	563	567	583	rBV	1538729	1366363	58.36%	10.325%
3	6.428	733	738	741	rBV	1552550	1396127	59.63%	10.550%
4	6.781	794	798	801	rBV	482878	375808	16.05%	2.840%
5	7.345	888	894	897	rBV	934138	925256	39.52%	6.991%
6	8.057	1010	1015	1023	rBV	628906	511497	21.85%	3.865%
7	9.133	1193	1198	1202	rBV	1863620	1802745	77.00%	13.622%
8	9.816	1309	1314	1317	rBV	724597	585302	25.00%	4.423%
9	10.610	1445	1449	1452	rBV	1308913	1133230	48.40%	8.563%
10	11.310	1564	1568	1571	rBV	749983	686658	29.33%	5.189%
11	11.380	1577	1580	1585	rVB	27408	26081	1.11%	0.197%
12	11.839	1655	1658	1671	rBV2	175493	178706	7.63%	1.350%
13	12.633	1790	1793	1799	rBV2	33369	43524	1.86%	0.329%
14	12.910	1834	1840	1843	rBV	2312773	2341243	100.00%	17.691%
15	13.857	1995	2001	2015	rBV3	62406	196923	8.41%	1.488%
16	13.963	2015	2019	2026	rVV	718226	628404	26.84%	4.748%
17	14.039	2028	2032	2037	rVB2	28984	35671	1.52%	0.270%
18	14.433	2094	2099	2102	rBV2	66473	82384	3.52%	0.623%
19	14.815	2159	2164	2170	rBV	99321	121621	5.19%	0.919%
20	15.092	2207	2211	2217	rVB3	22159	26555	1.13%	0.201%
21	15.245	2233	2237	2244	rVB2	57460	84168	3.60%	0.636%
22	15.445	2265	2271	2282	rBV	339600	482692	20.62%	3.647%
23	15.751	2318	2323	2333	rVB2	41324	78219	3.34%	0.591%
24	16.357	2421	2426	2433	rVB4	25486	52239	2.23%	0.395%

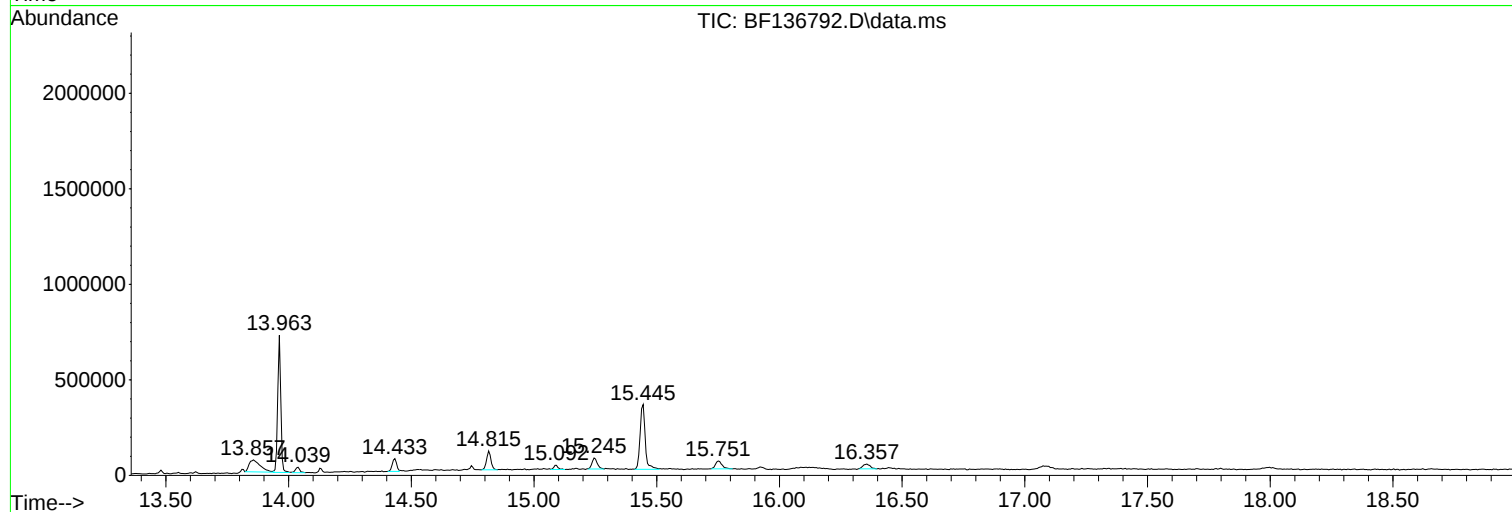
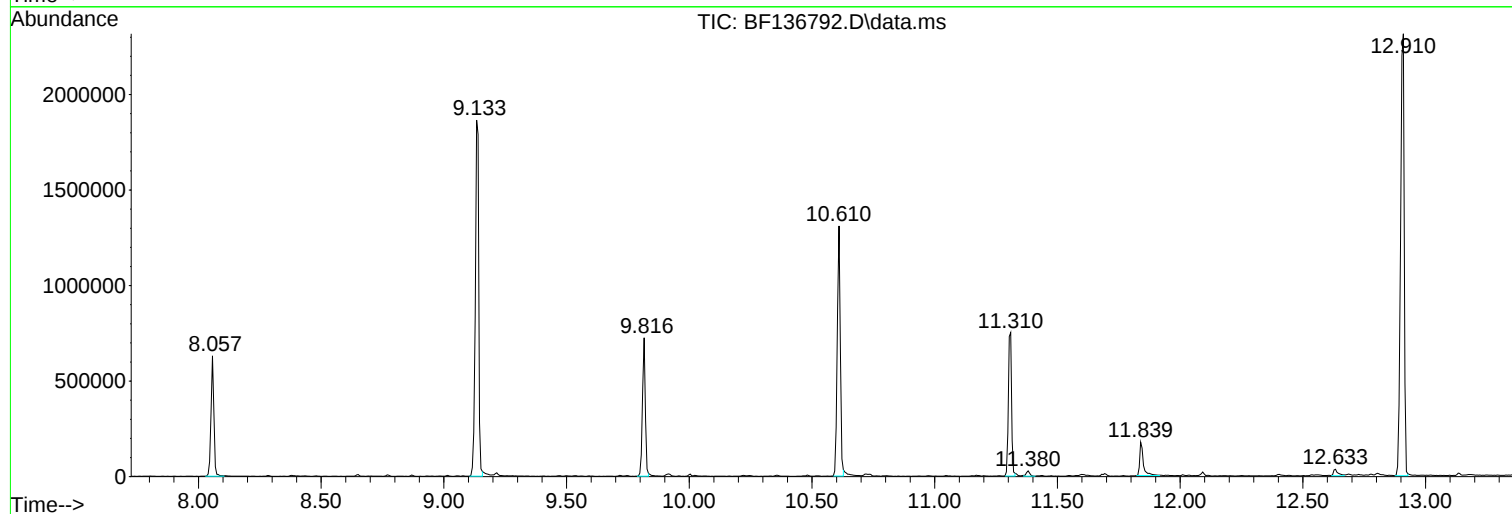
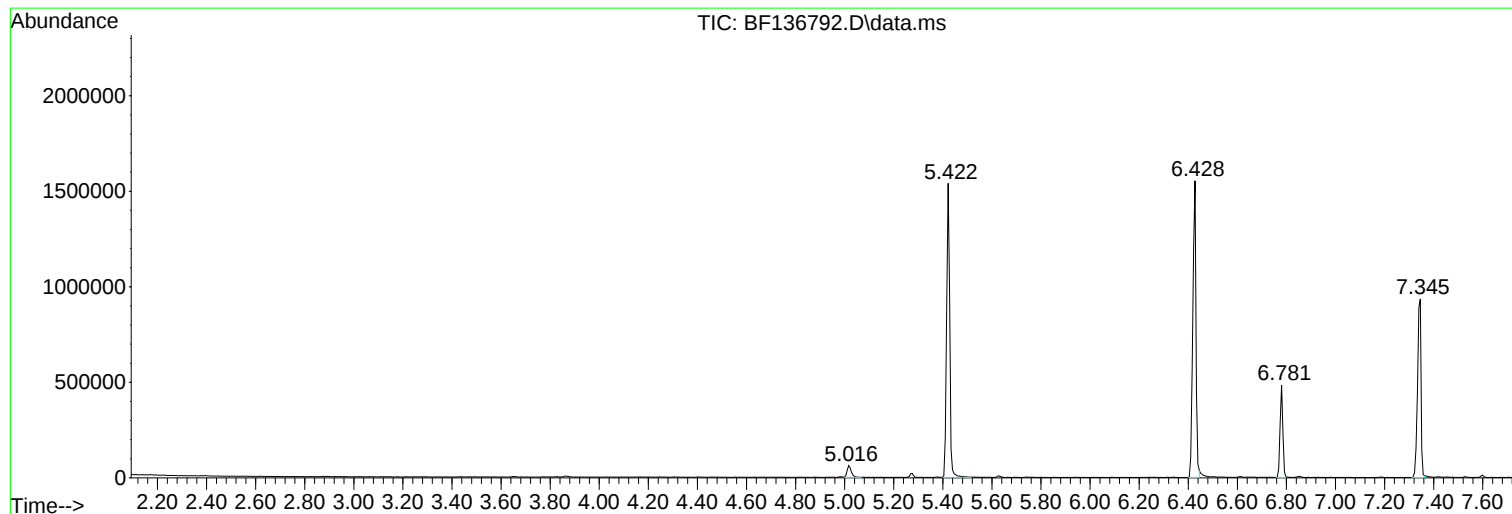
Sum of corrected areas: 13234058

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122823\
Data File : BF136792.D
Acq On : 28 Dec 2023 13:50
Operator : CG\JU
Sample : 05897-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-33

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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\BF122823\
Data File : BF136792.D
Acq On : 28 Dec 2023 13:50
Operator : CG\JU
Sample : 05897-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-33

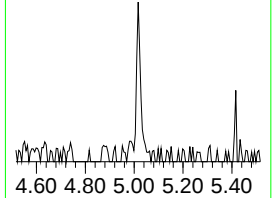
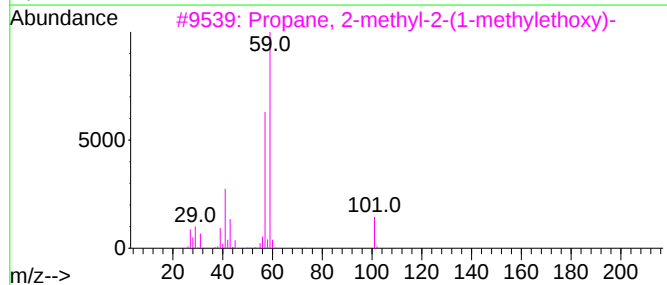
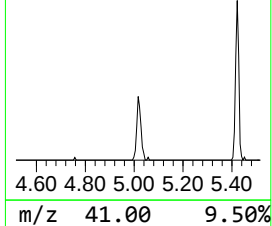
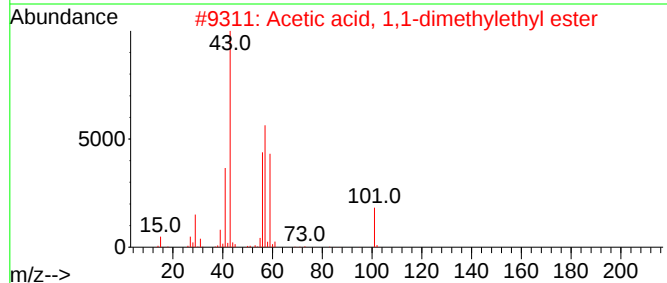
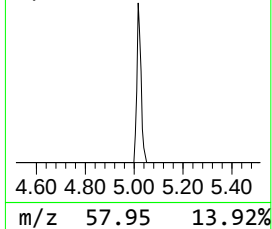
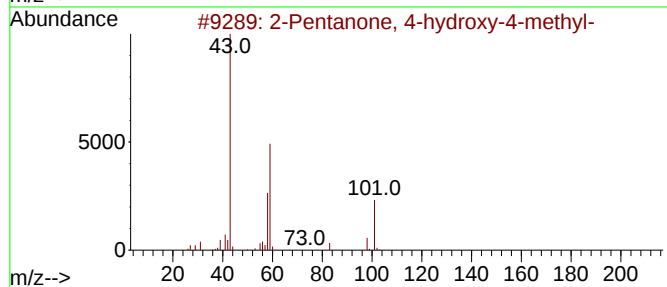
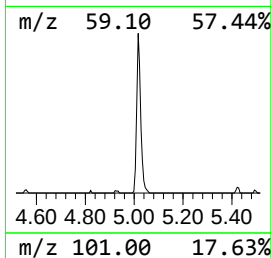
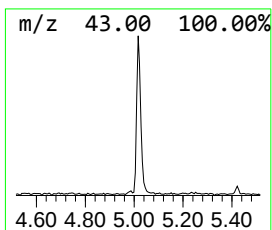
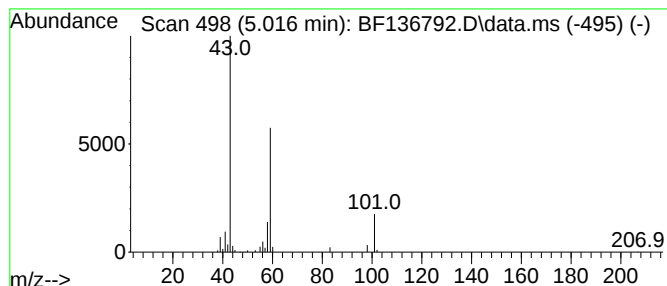
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.016	3.87 ng	72642	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	64		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36		
4	3-Hexanol	102	C6H14O	000623-37-0	33		
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122823\
Data File : BF136792.D
Acq On : 28 Dec 2023 13:50
Operator : CG\JU
Sample : 05897-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-33

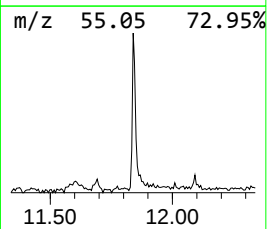
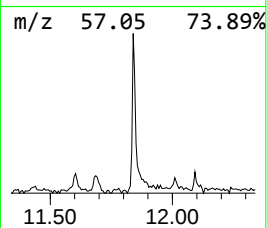
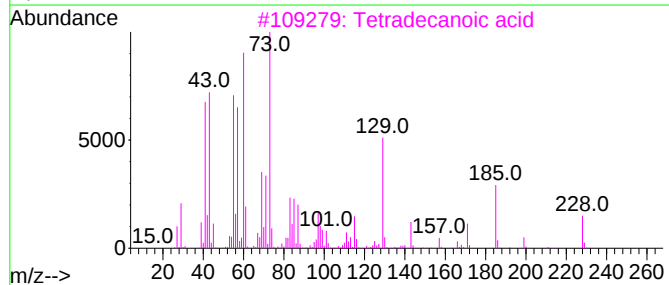
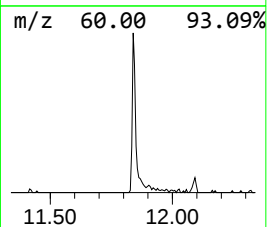
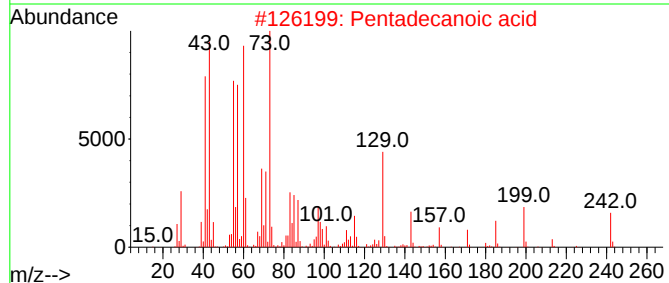
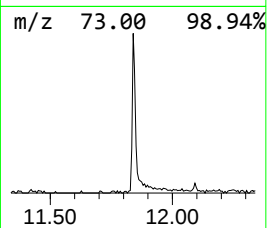
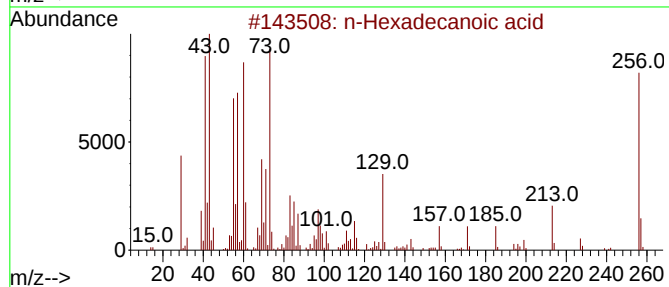
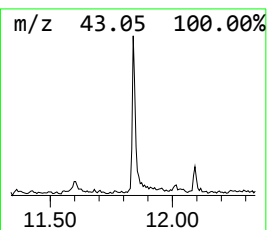
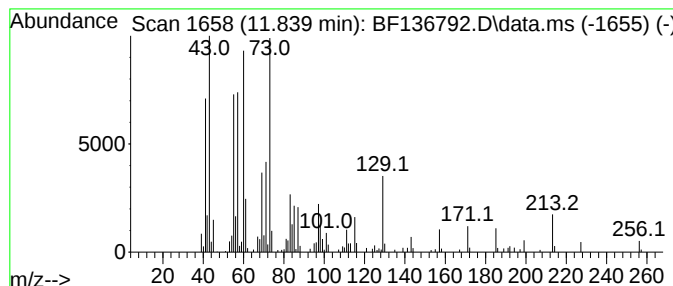
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	5.21 ng	178706	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			Tridecanoic acid	214	C13H26O2	000638-53-9	76
5			Dodecanoic acid	200	C12H24O2	000143-07-7	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122823\
Data File : BF136792.D
Acq On : 28 Dec 2023 13:50
Operator : CG\JU
Sample : 05897-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

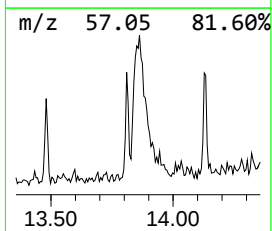
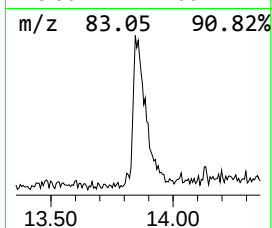
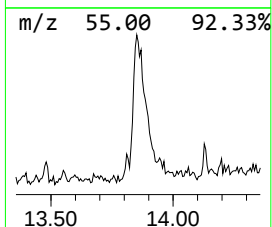
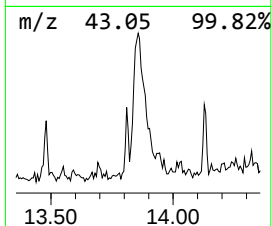
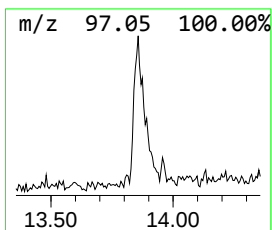
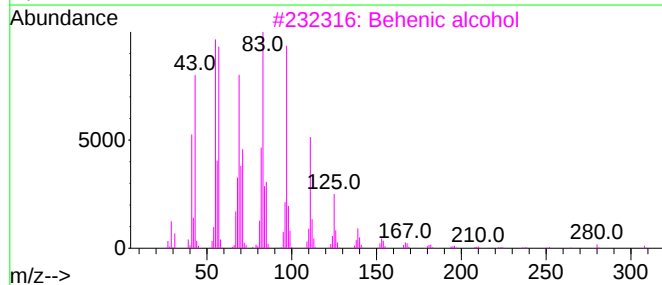
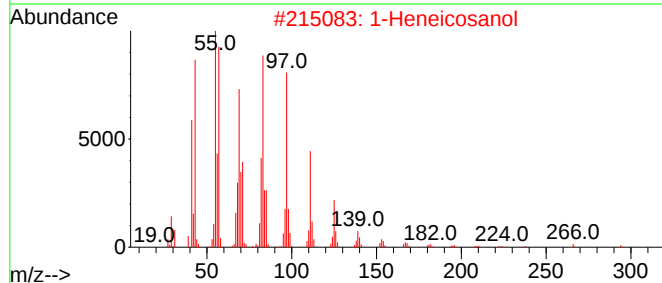
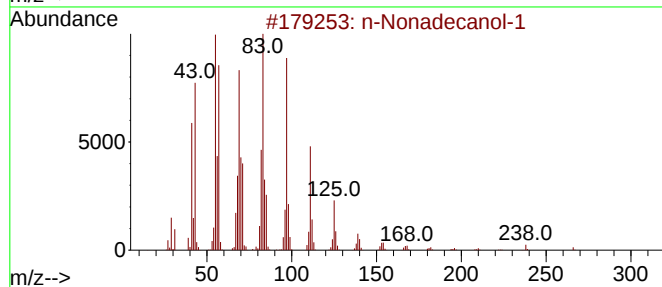
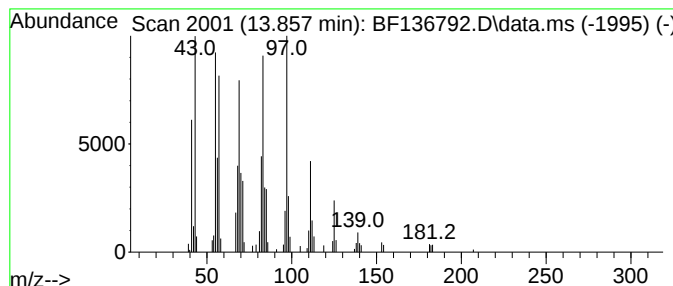
Instrument :
BNA_F
ClientSampleId :
GHL-SS-33

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Nonadecanol-1 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.857	6.27 ng	196923	Chrysene-d12		13.963	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1		284	C19H40O	001454-84-8	95
2	1-Heneicosanol		312	C21H44O	015594-90-8	95
3	Behenic alcohol		326	C22H46O	000661-19-8	94
4	1-Hexadecanol		242	C16H34O	036653-82-4	91
5	Trifluoroacetoxy hexadecane		338	C18H33F3O2	006222-03-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122823\
Data File : BF136792.D
Acq On : 28 Dec 2023 13:50
Operator : CG\JU
Sample : 05897-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-33

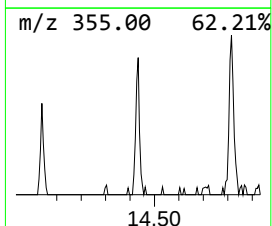
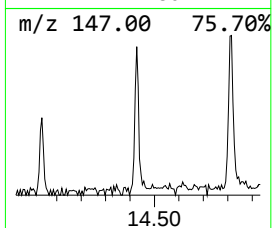
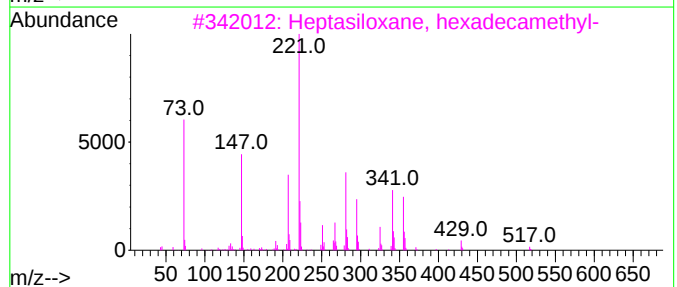
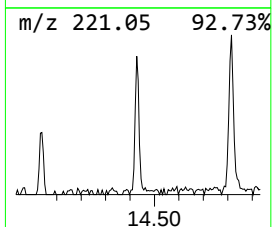
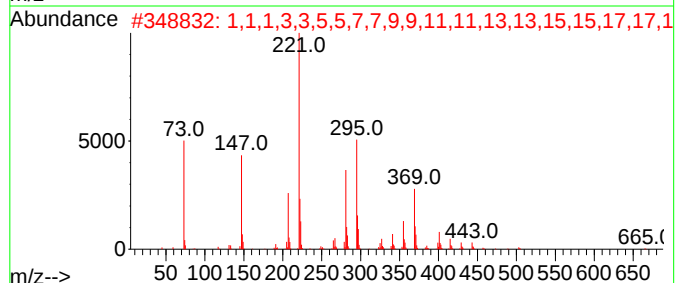
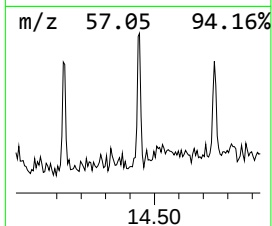
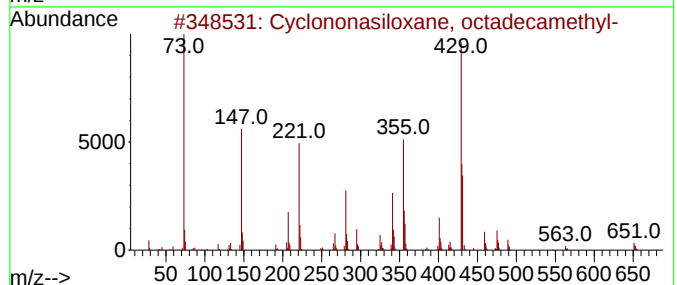
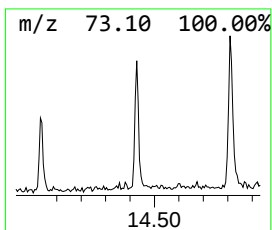
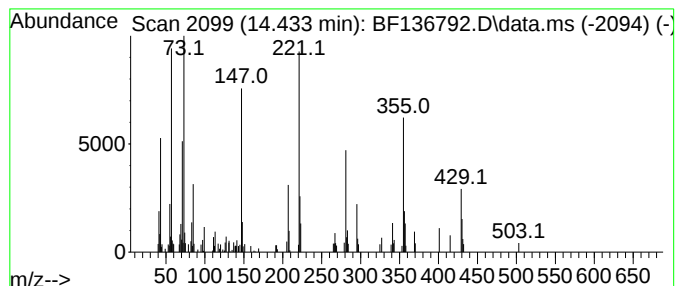
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Cyclononasiloxane, octadeca... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.433	2.62 ng	82384	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	78
2			1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	680	C20H60O8Si9	002652-13-3	47
3			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	47
4			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	42
5			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122823\
Data File : BF136792.D
Acq On : 28 Dec 2023 13:50
Operator : CG\JU
Sample : 05897-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-33

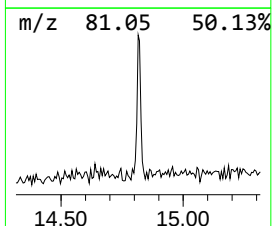
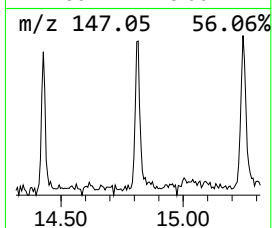
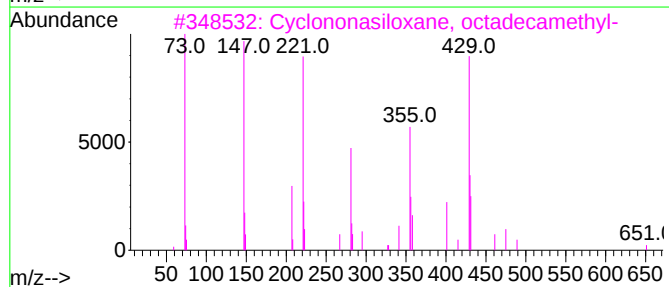
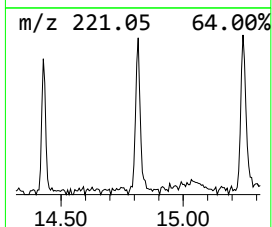
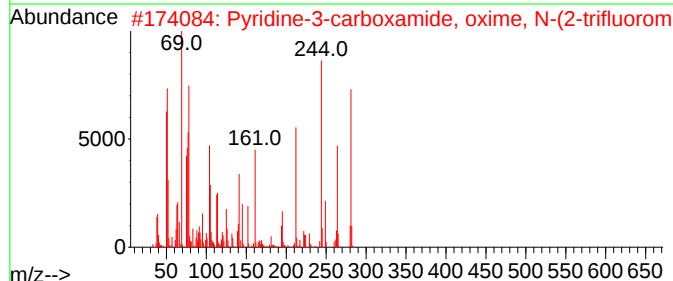
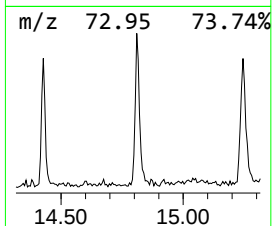
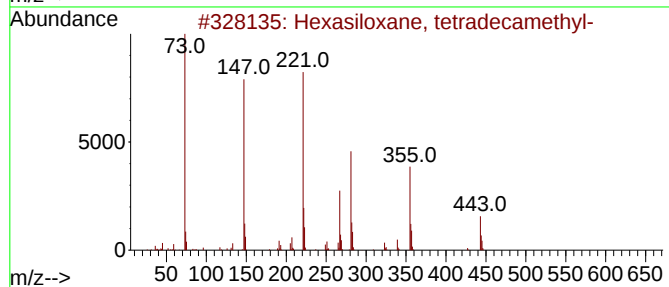
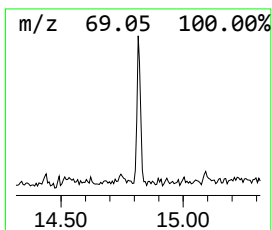
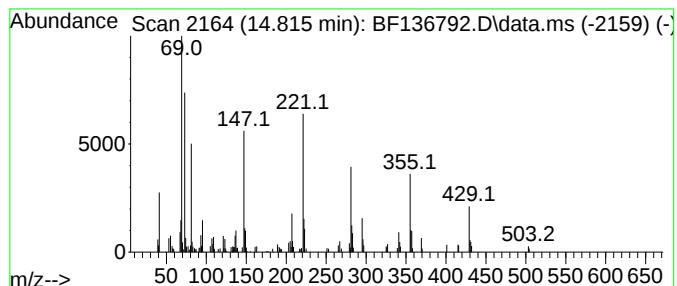
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown14.815 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.815	5.04 ng	121621	Perylene-d12	15.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	49
2			Pyridine-3-carboxamide, oxime, N...	281	C13H10F3N3O	288246-53-7	38
3			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	37
4			5-Methylisoxazol-3-amine bis(tri...	290	C8H4F6N2O3	1000373-35-6	25
5			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122823\
Data File : BF136792.D
Acq On : 28 Dec 2023 13:50
Operator : CG\JU
Sample : 05897-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-33

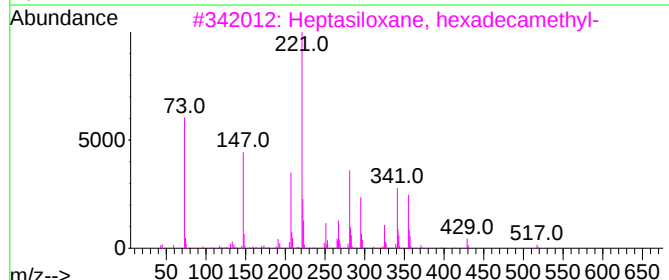
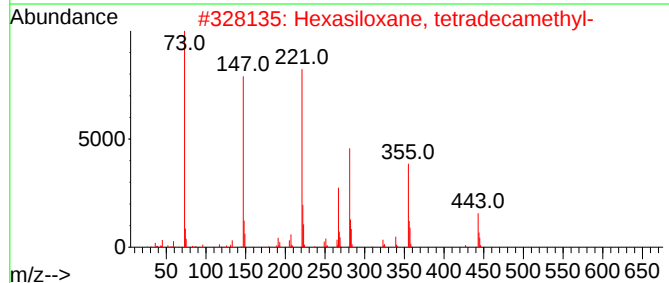
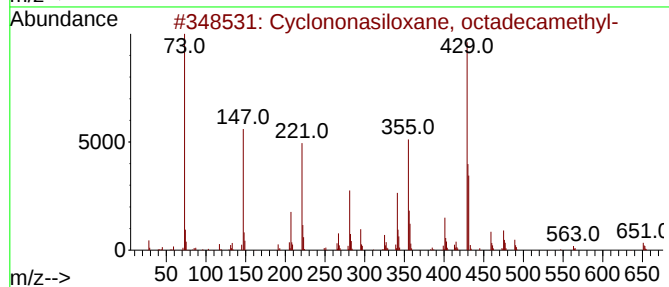
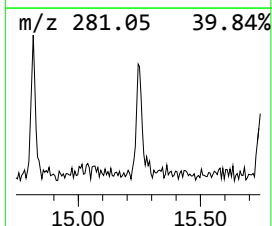
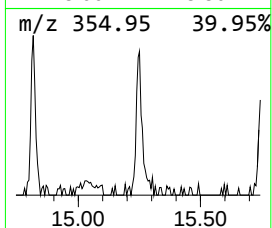
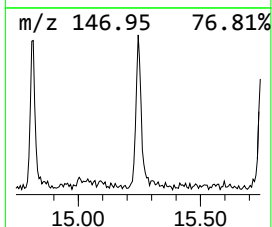
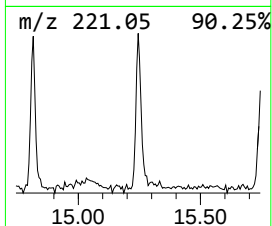
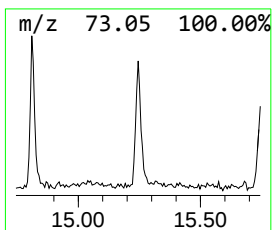
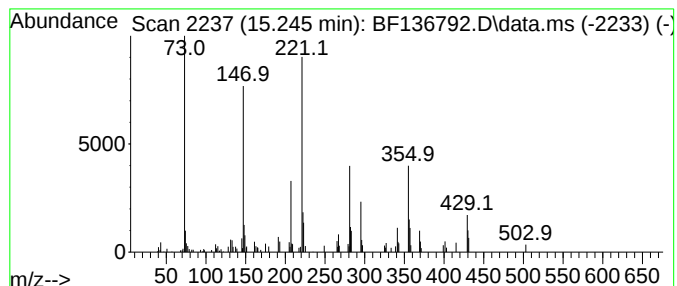
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexasiloxane, tetradecamethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.245	3.49 ng	84168	Perylene-d12	15.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	83
2			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	81
3			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	64
4			Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	30
5			Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122823\
Data File : BF136792.D
Acq On : 28 Dec 2023 13:50
Operator : CG\JU
Sample : 05897-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-33

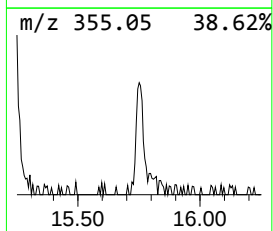
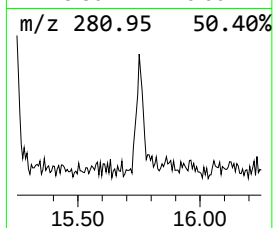
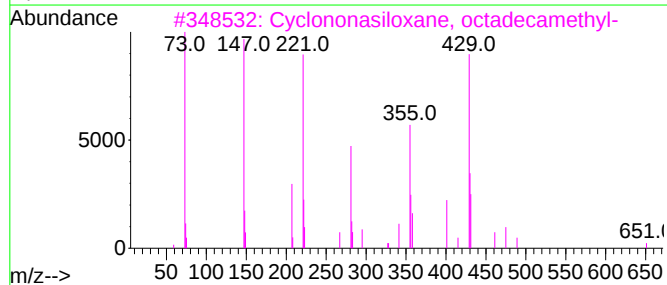
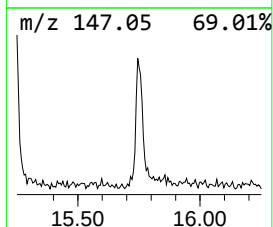
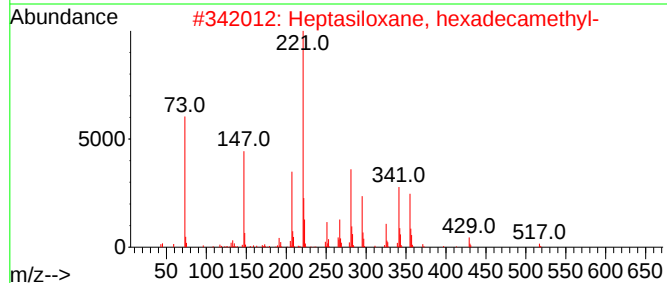
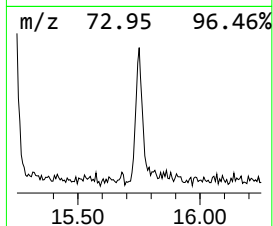
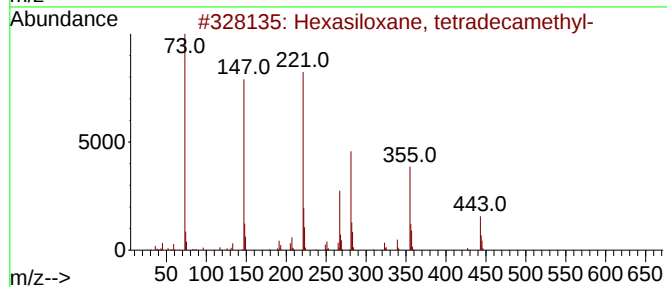
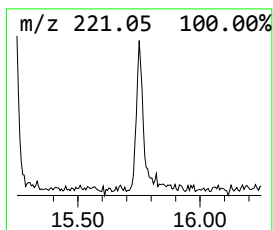
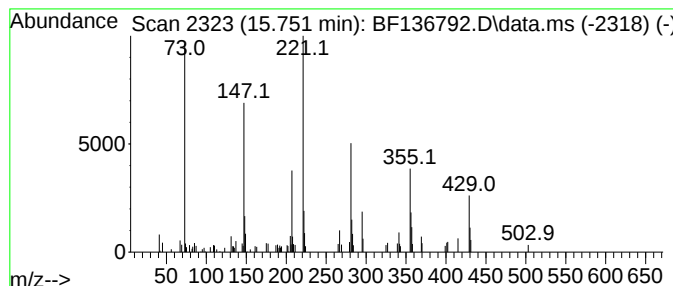
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptasiloxane, hexadecamethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.751	3.24 ng	78219	Perylene-d12	15.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	74
2			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	53
3			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	49
4			2-Methyl-6-tert-butylphenol, TBD...	278	C17H30O5Si	1000467-05-0	27
5			Indole, 5-(4-methylphenyl)-N-met...	221	C16H15N	1000380-54-7	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122823\
Data File : BF136792.D
Acq On : 28 Dec 2023 13:50
Operator : CG\JU
Sample : 05897-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-33

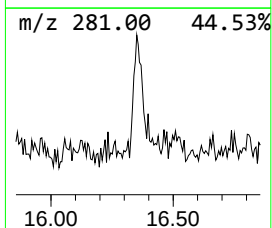
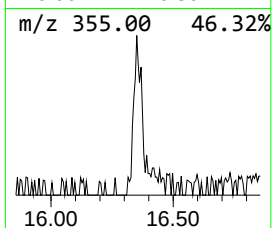
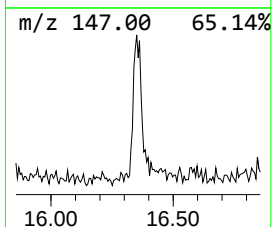
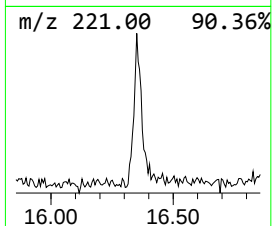
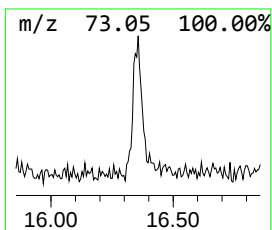
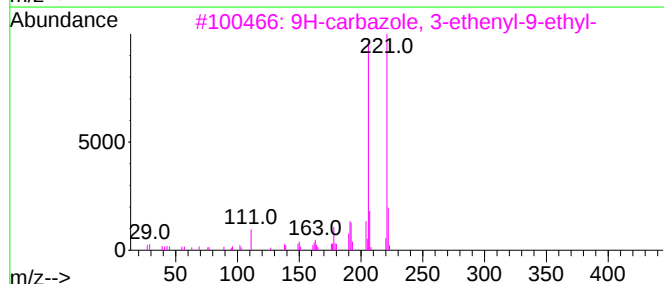
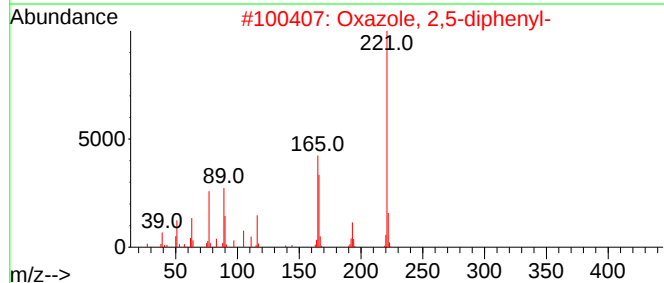
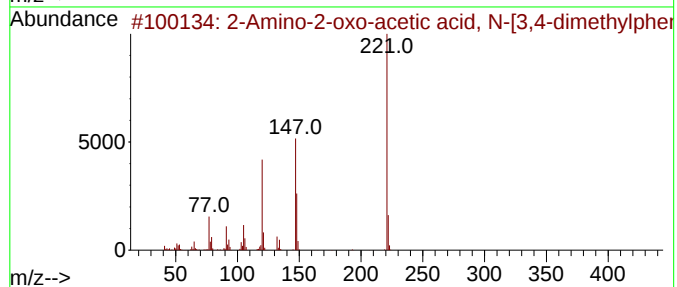
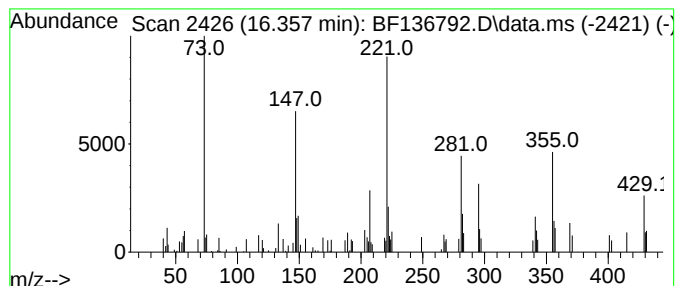
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown16.357 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.357	2.16 ng	52239	Perylene-d12	15.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15NO3	024451-17-0	35		
2	Oxazole, 2,5-diphenyl-	221	C15H11NO	000092-71-7	25		
3	9H-carbazole, 3-ethenyl-9-ethyl-	221	C16H15N	1000400-80-8	22		
4	1H-Indole, 1-ethyl-2-phenyl-	221	C16H15N	013228-39-2	22		
5	(S,S)-(-)-Hydrobenzoin, tert-but...	328	C20H28O2Si	537658-24-5	22		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122823\
Data File : BF136792.D
Acq On : 28 Dec 2023 13:50
Operator : CG\JU
Sample : 05897-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-33

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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-...	5.016	3.9	ng	72642	1	6.781	375808	20.0
n-Hexadecanoic ...	11.839	5.2	ng	178706	4	11.310	686658	20.0
n-Nonadecanol-1	13.857	6.3	ng	196923	5	13.963	628404	20.0
Cyclononasiloxa...	14.433	2.6	ng	82384	5	13.963	628404	20.0
unknown14.815	14.815	5.0	ng	121621	6	15.445	482692	20.0
Hexasiloxane, t...	15.245	3.5	ng	84168	6	15.445	482692	20.0
Heptasiloxane, ...	15.751	3.2	ng	78219	6	15.445	482692	20.0
unknown16.357	16.357	2.2	ng	52239	6	15.445	482692	20.0