

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
 Data File : BF133159.D
 Acq On : 01 May 2023 17:02
 Operator : CG\JU
 Sample : 02558-08
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P001-SS013-1218-01

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-BF042123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133159.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	3	9	37	rVB9	106455	465781	11.60%	1.391%
2	4.916	471	481	488	rBV	45298	71967	1.79%	0.215%
3	5.340	549	553	573	rBV	3364926	3781555	94.21%	11.292%
4	6.375	723	729	732	rBV	3542226	3788965	94.40%	11.314%
5	6.728	786	789	792	rBV	1507327	1128714	28.12%	3.370%
6	7.292	880	885	888	rBV	2867102	2434259	60.65%	7.269%
7	8.010	1004	1007	1011	rBV	1795072	1574066	39.22%	4.700%
8	9.092	1186	1191	1194	rBV	4467963	4013870	100.00%	11.986%
9	9.763	1302	1305	1309	rVB	2206353	1760323	43.86%	5.256%
10	10.475	1423	1426	1430	rVB	354806	274384	6.84%	0.819%
11	10.551	1435	1439	1442	rBV	2715524	2412996	60.12%	7.205%
12	10.692	1461	1463	1470	rVB3	56726	61897	1.54%	0.185%
13	11.245	1553	1557	1561	rBV	2164460	1824976	45.47%	5.450%
14	11.786	1643	1649	1662	rVB2	466543	780207	19.44%	2.330%
15	11.916	1669	1671	1676	rVB4	58983	73953	1.84%	0.221%
16	12.557	1775	1780	1793	rVB	804904	1402797	34.95%	4.189%
17	12.833	1823	1827	1831	rBV	4294389	3989262	99.39%	11.912%
18	12.998	1852	1855	1860	rVB	151274	158080	3.94%	0.472%
19	13.416	1924	1926	1929	rVB	61262	53239	1.33%	0.159%
20	13.721	1974	1978	1980	rBV2	69193	103582	2.58%	0.309%
21	13.768	1983	1986	1997	rVB3	176964	379265	9.45%	1.133%
22	13.880	2001	2005	2009	rBV	1270004	1124019	28.00%	3.356%
23	14.063	2033	2036	2039	rVB	83986	73047	1.82%	0.218%
24	14.233	2061	2065	2071	rBV	125773	175363	4.37%	0.524%
25	14.368	2085	2088	2091	rVB	81611	72374	1.80%	0.216%
26	14.663	2136	2138	2141	rBV	46279	44877	1.12%	0.134%
27	14.698	2141	2144	2148	rVB	113504	133236	3.32%	0.398%
28	14.986	2191	2193	2197	rVB2	61871	66928	1.67%	0.200%
29	15.298	2241	2246	2250	rBV	921669	1086164	27.06%	3.243%
30	15.780	2322	2328	2335	rVB4	71808	178359	4.44%	0.533%

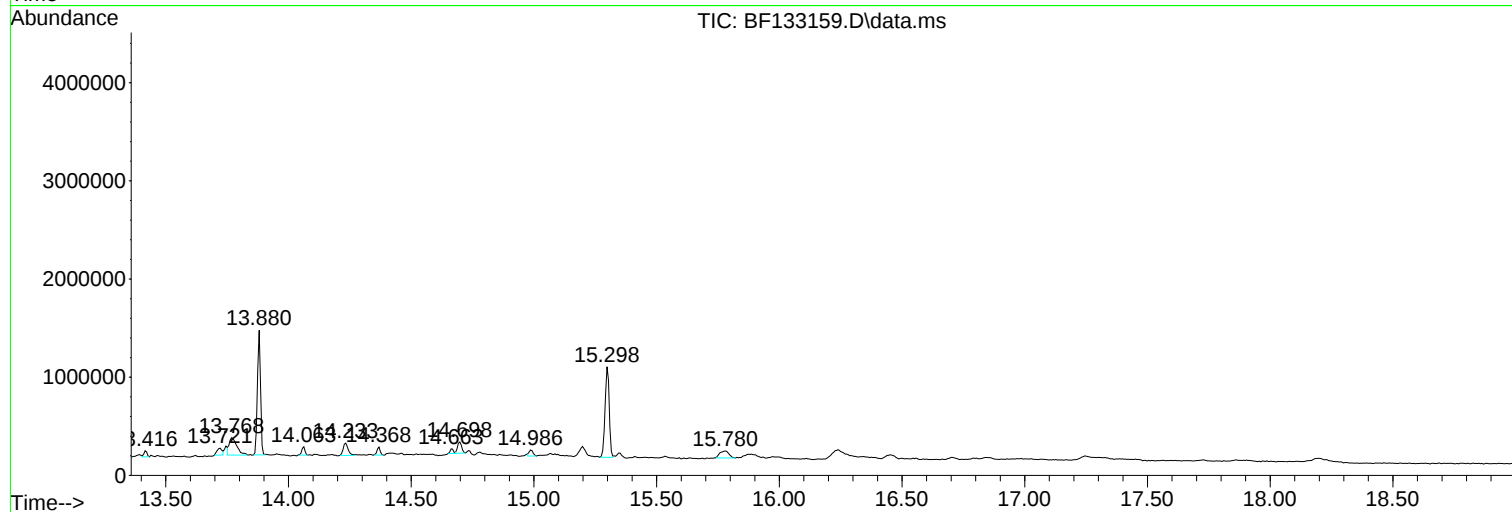
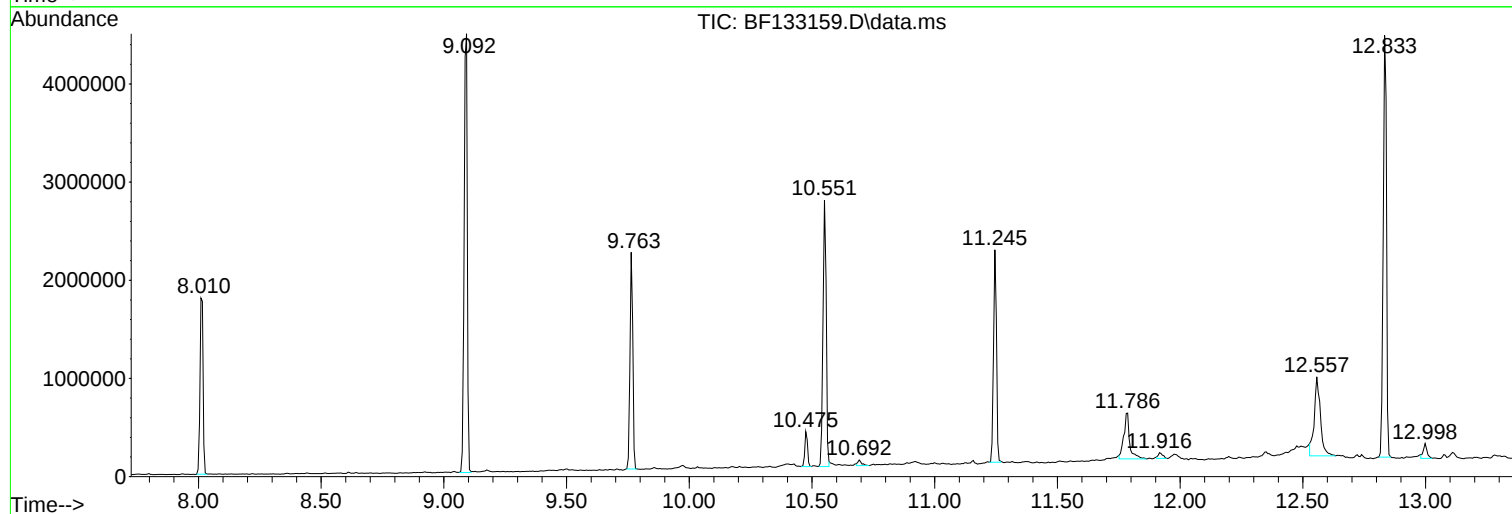
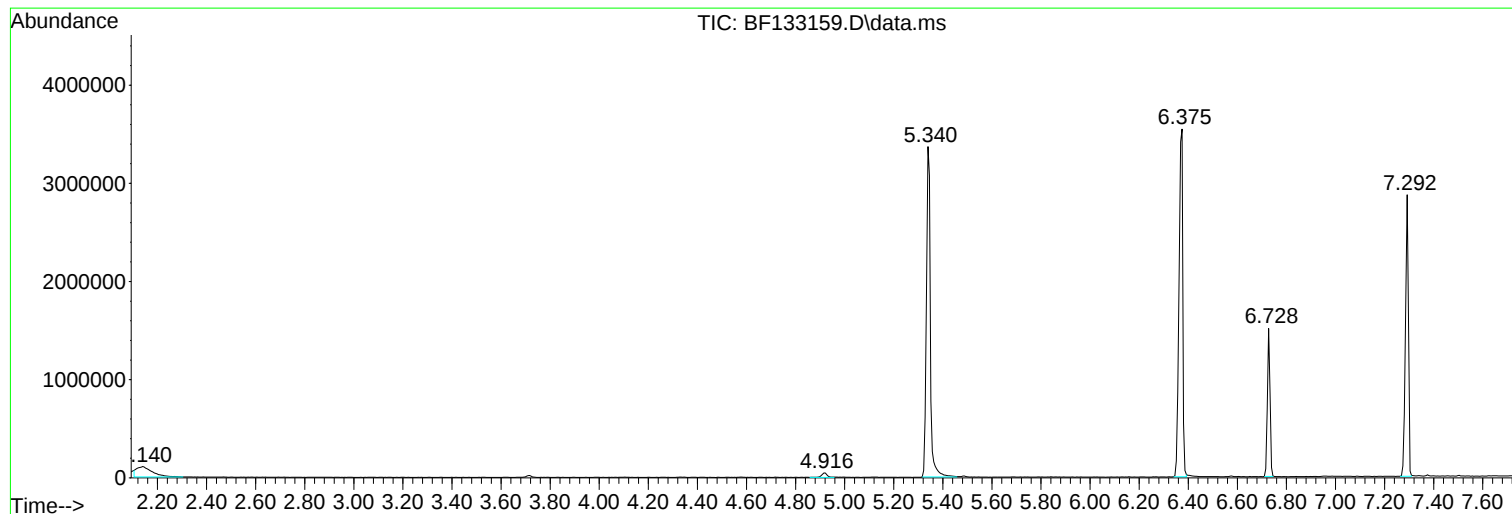
Sum of corrected areas: 33488505

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
Data File : BF133159.D
Acq On : 01 May 2023 17:02
Operator : CG\JU
Sample : 02558-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P001-SS013-1218-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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\BF050123\
Data File : BF133159.D
Acq On : 01 May 2023 17:02
Operator : CG\JU
Sample : 02558-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P001-SS013-1218-01

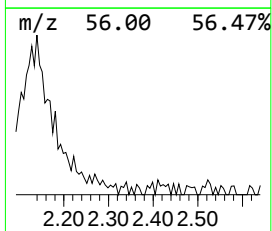
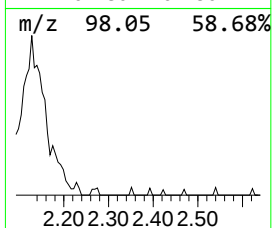
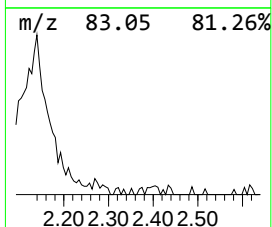
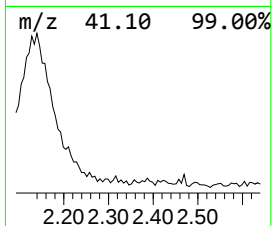
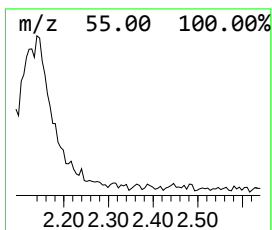
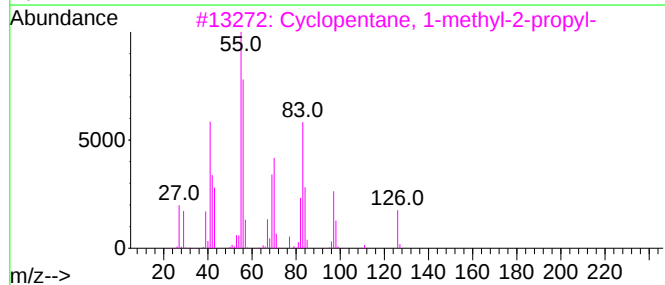
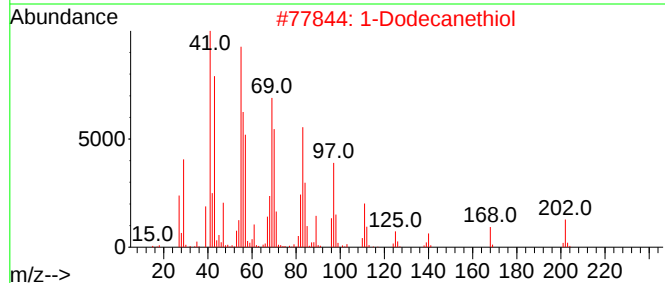
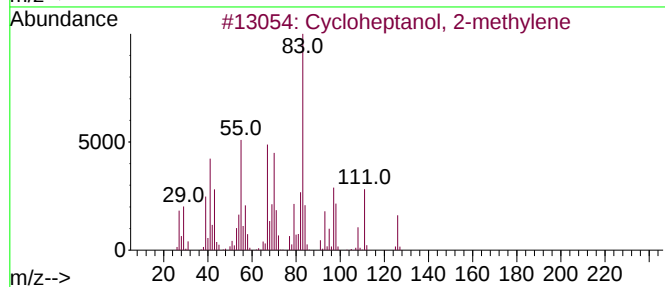
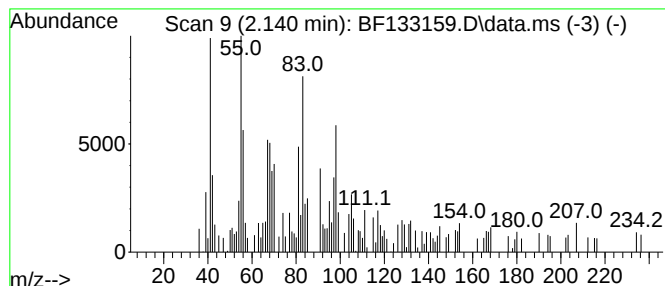
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Cycloheptanol, 2-methylene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.140	8.25 ng	465781	1,4-Dichlorobenzene-d4	6.728

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cycloheptanol, 2-methylene	126	C8H14O	016240-38-3	60
2			1-Dodecanethiol	202	C12H26S	000112-55-0	50
3			Cyclopentane, 1-methyl-2-propyl-	126	C9H18	003728-57-2	46
4			Cyclohexane, (1-methylbutyl)-	154	C11H22	061208-94-4	45
5			Carbonic acid, nonyl 2,2,2-trich...	318	C12H21Cl3O3	1010314-55-5	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
Data File : BF133159.D
Acq On : 01 May 2023 17:02
Operator : CG\JU
Sample : 02558-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P001-SS013-1218-01

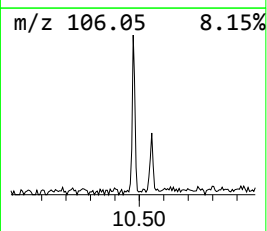
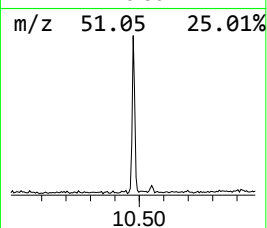
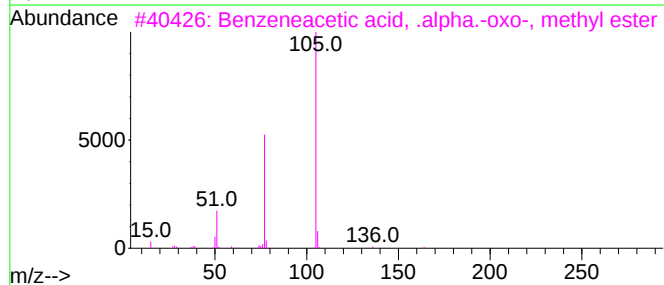
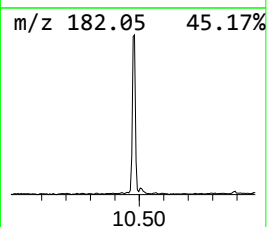
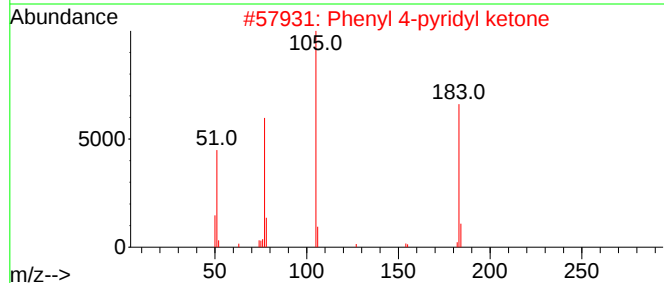
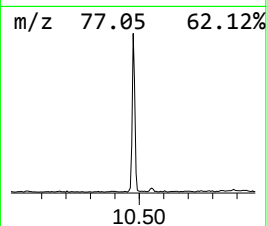
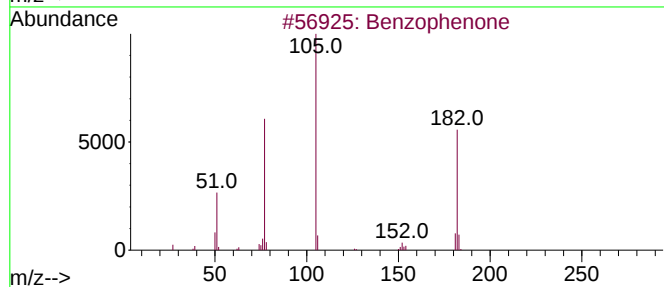
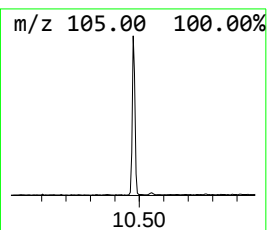
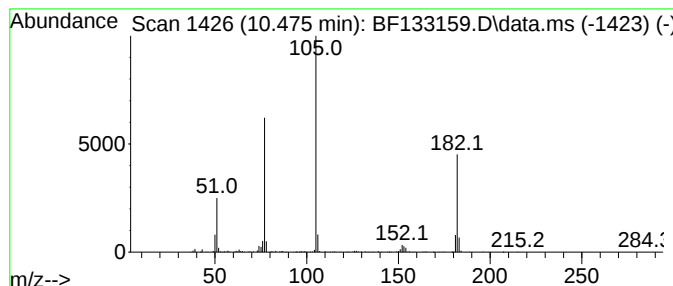
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.475	3.12 ng	274384	Acenaphthene-d10	9.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	50
3			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	49
4			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
5			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
Data File : BF133159.D
Acq On : 01 May 2023 17:02
Operator : CG\JU
Sample : 02558-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P001-SS013-1218-01

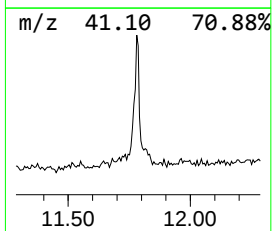
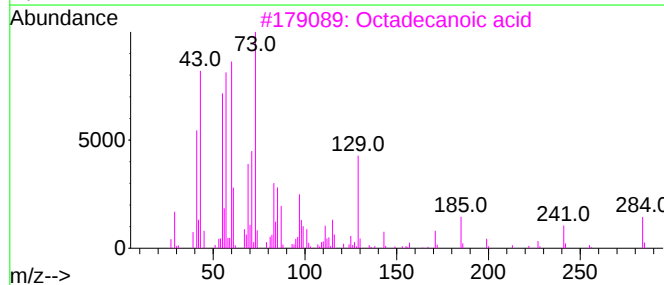
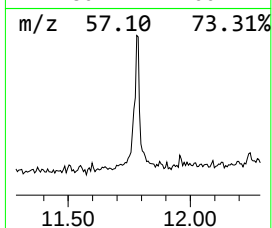
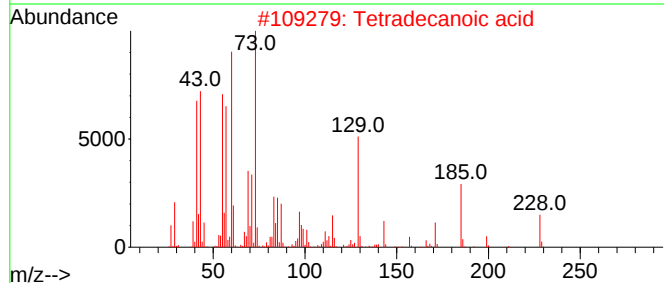
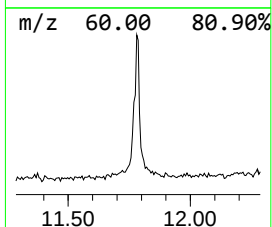
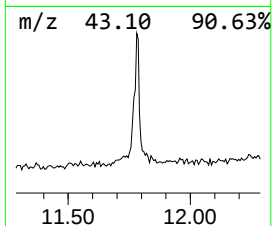
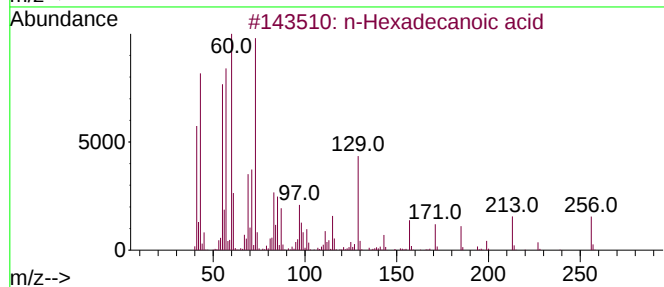
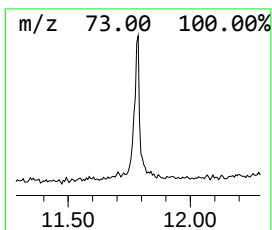
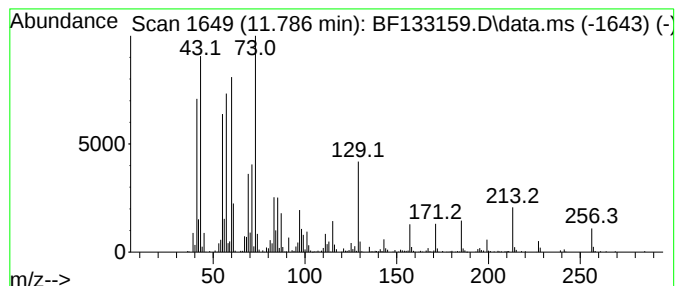
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.786	8.55 ng	780207	Phenanthrene-d10	11.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3			Octadecanoic acid	284	C18H36O2	000057-11-4	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5			Tridecanoic acid	214	C13H26O2	000638-53-9	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
Data File : BF133159.D
Acq On : 01 May 2023 17:02
Operator : CG\JU
Sample : 02558-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P001-SS013-1218-01

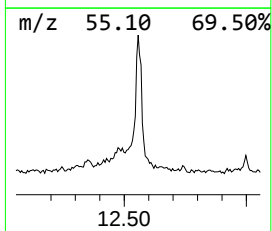
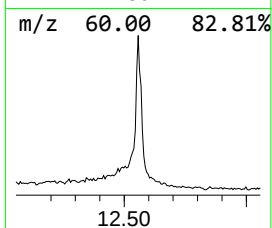
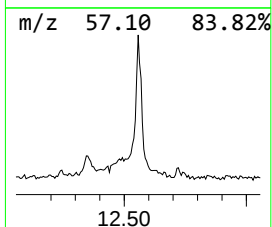
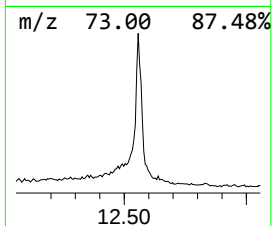
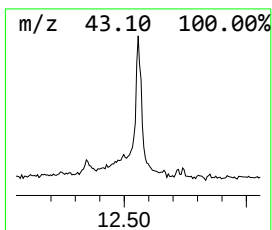
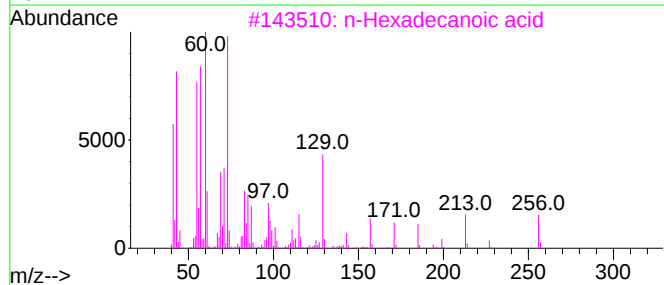
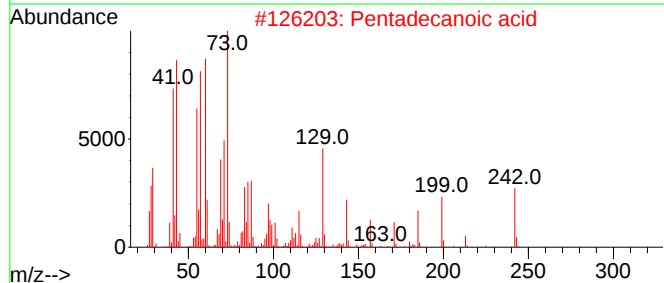
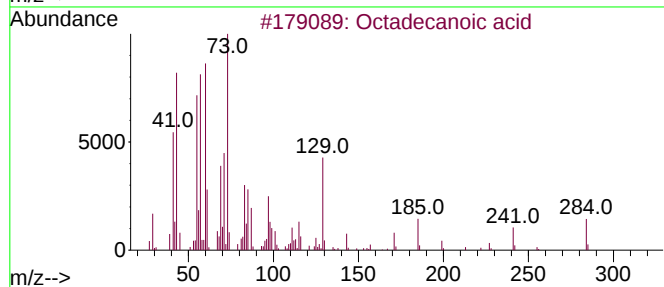
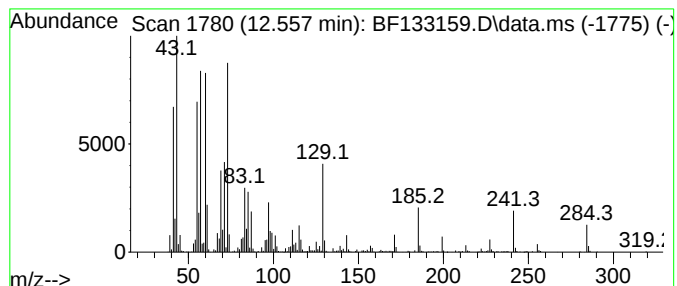
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.557	15.37 ng	1402800	Phenanthrene-d10	11.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Tridecanoic acid	214	C13H26O2	000638-53-9	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
Data File : BF133159.D
Acq On : 01 May 2023 17:02
Operator : CG\JU
Sample : 02558-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P001-SS013-1218-01

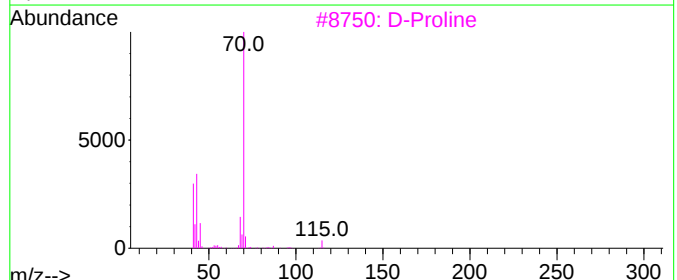
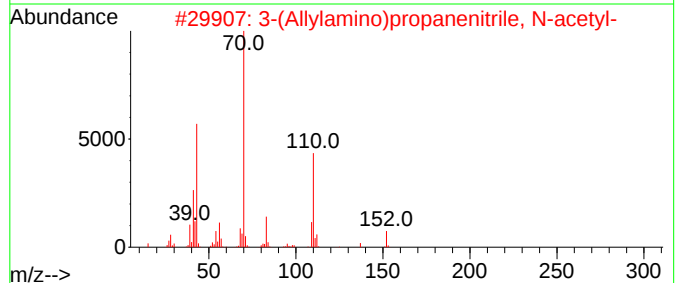
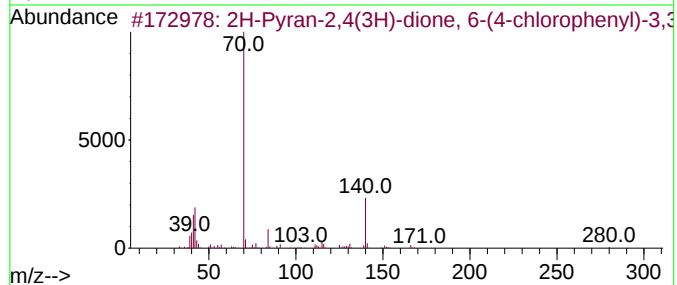
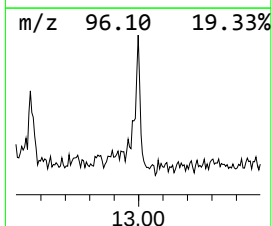
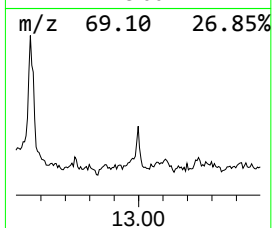
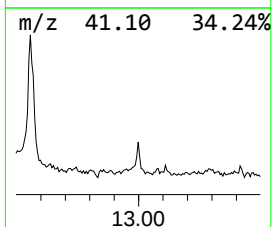
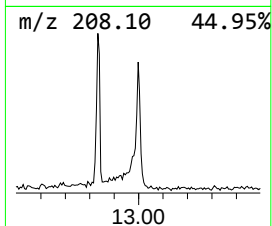
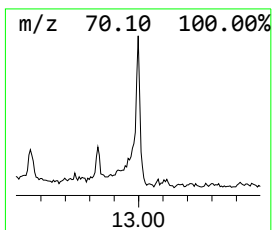
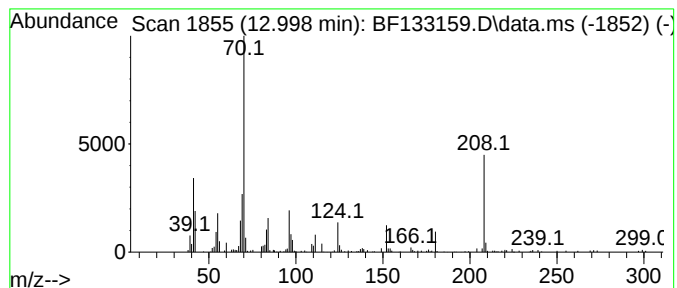
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown12.998 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.998	2.81 ng	158080	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2H-Pyran-2,4(3H)-dione, 6-(4-chl...	280	C15H17C103	075959-47-6	35
2			3-(Allylamino)propanenitrile, N...	152	C8H12N2O	1000475-61-4	35
3			D-Proline	115	C5H9NO2	000344-25-2	27
4			5-Isopropylidene-3,3-dimethyl-di...	154	C9H14O2	1000192-59-3	27
5			2,5-Cyclohexadien-1-one, 3,5-dih...	154	C8H10O3	002065-00-1	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
Data File : BF133159.D
Acq On : 01 May 2023 17:02
Operator : CG\JU
Sample : 02558-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P001-SS013-1218-01

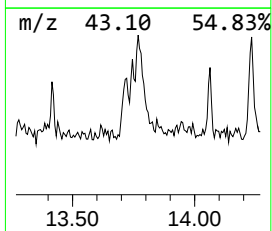
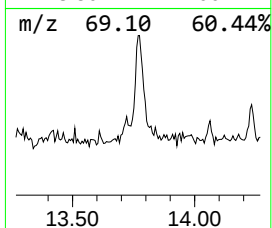
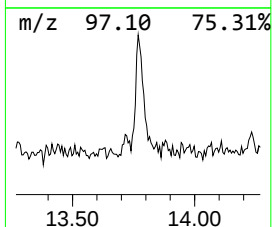
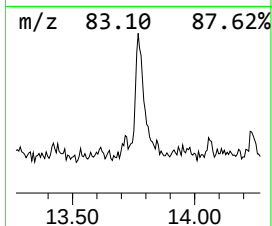
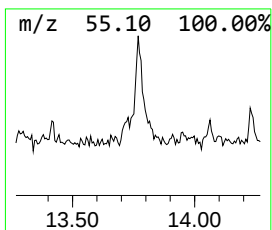
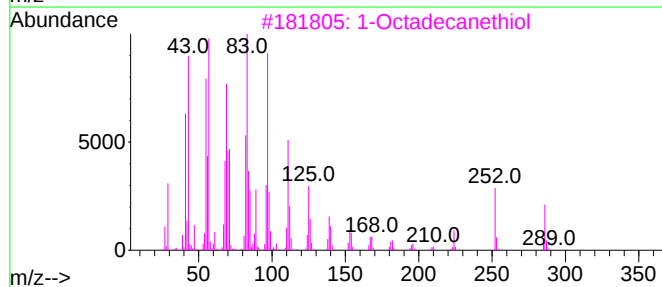
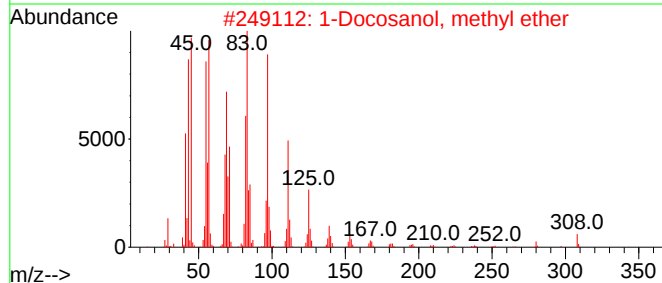
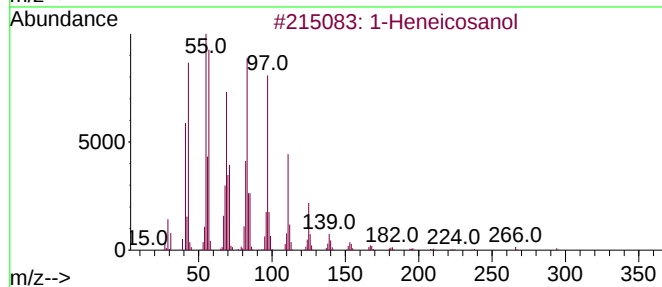
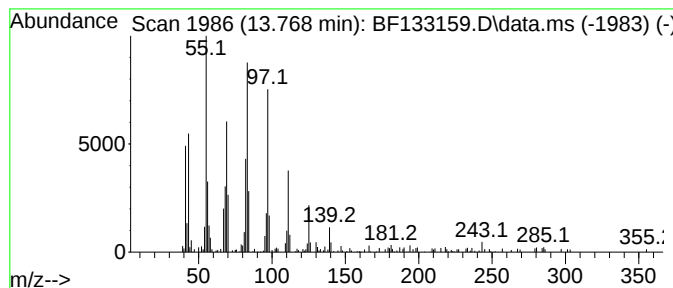
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.769	6.75 ng	379265	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	90
2			1-Docosanol, methyl ether	340	C23H48O	1000333-91-9	87
3			1-Octadecanethiol	286	C18H38S	002885-00-9	86
4			Propyl triacontyl ether	481	C33H68O	1000406-28-6	83
5			Octacosyl propyl ether	452	C31H64O	1000406-28-5	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
Data File : BF133159.D
Acq On : 01 May 2023 17:02
Operator : CG\JU
Sample : 02558-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P001-SS013-1218-01

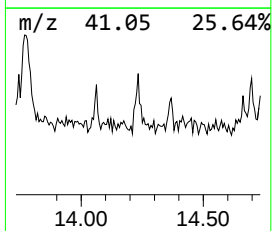
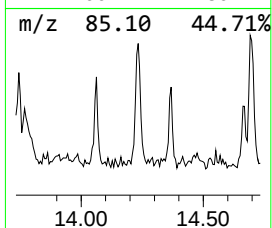
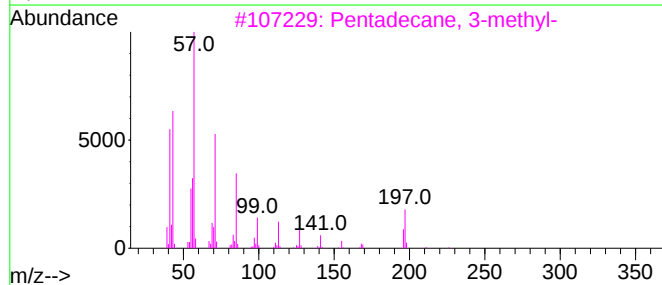
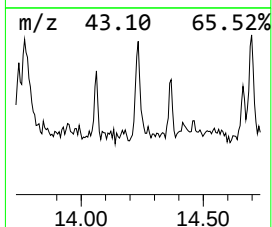
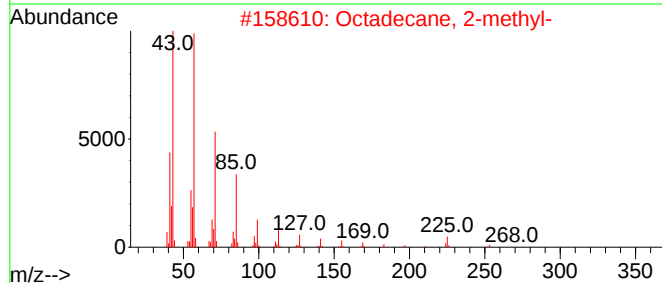
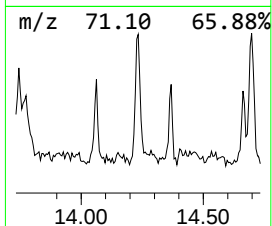
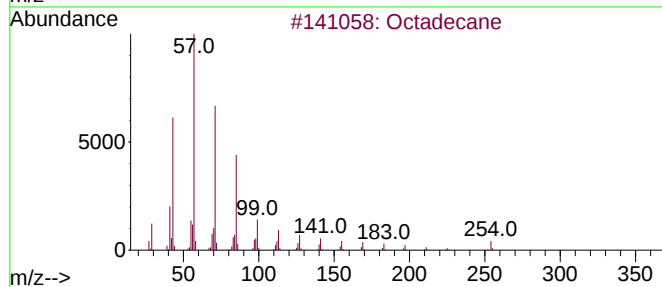
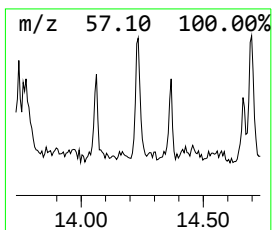
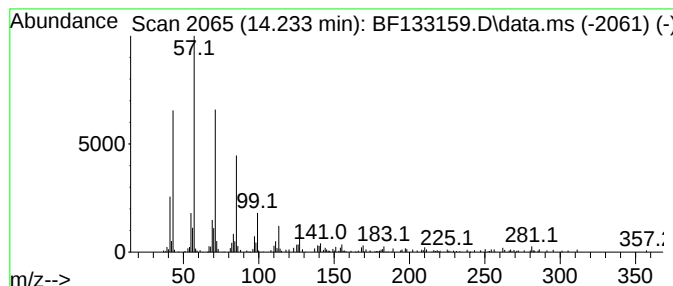
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.233	3.12 ng	175363	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	93
2			Octadecane, 2-methyl-	268	C19H40	001560-88-9	93
3			Pentadecane, 3-methyl-	226	C16H34	002882-96-4	93
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
5			Tetracosane	338	C24H50	000646-31-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
Data File : BF133159.D
Acq On : 01 May 2023 17:02
Operator : CG\JU
Sample : 02558-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

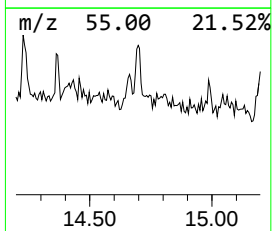
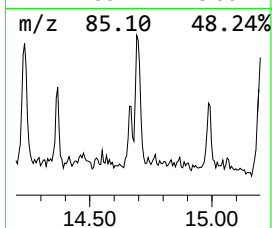
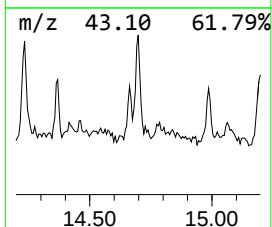
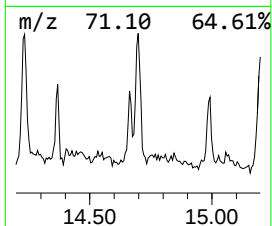
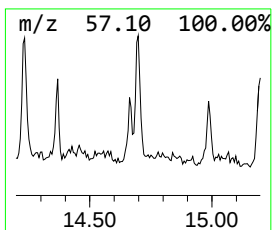
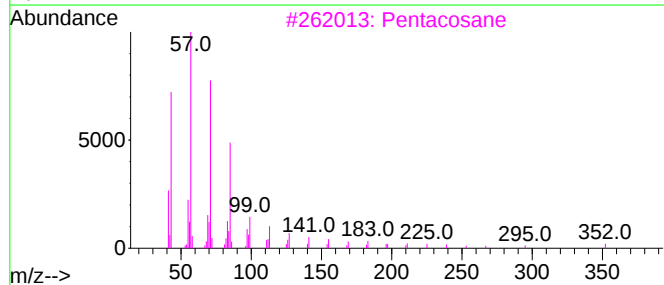
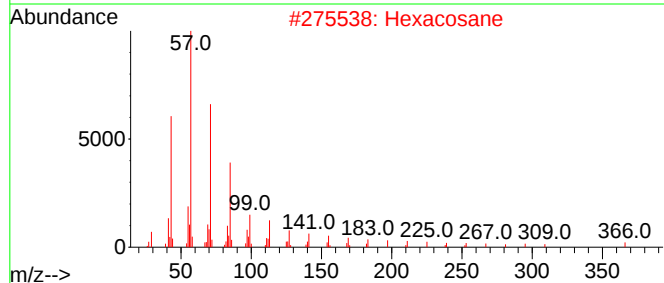
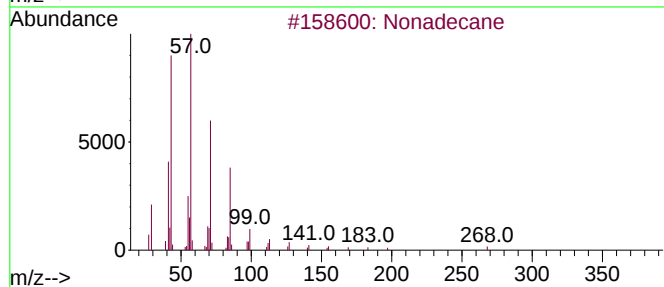
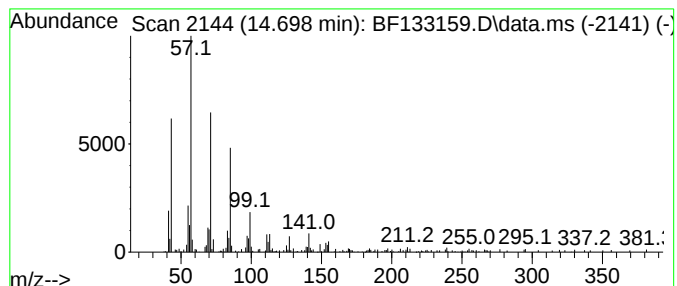
Instrument :
BNA_F
ClientSampleId :
P001-SS013-1218-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.698	2.45 ng	133236	Perylene-d12		15.298	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Nonadecane		268	C19H40	000629-92-5	91
2	Hexacosane		366	C26H54	000630-01-3	87
3	Pentacosane		352	C25H52	000629-99-2	87
4	Heptadecane		240	C17H36	000629-78-7	83
5	Octadecane		254	C18H38	000593-45-3	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
Data File : BF133159.D
Acq On : 01 May 2023 17:02
Operator : CG\JU
Sample : 02558-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P001-SS013-1218-01

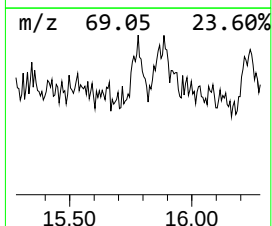
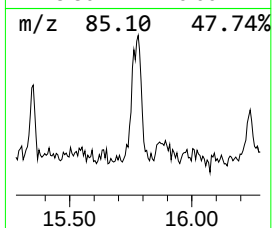
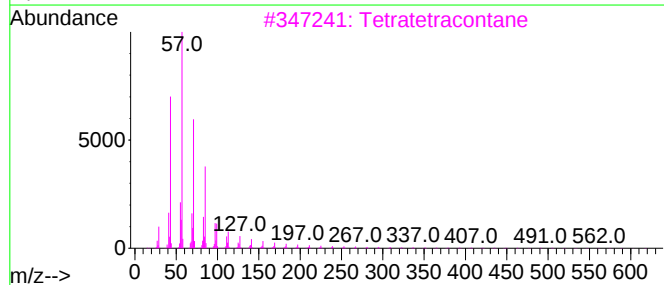
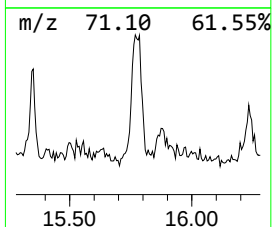
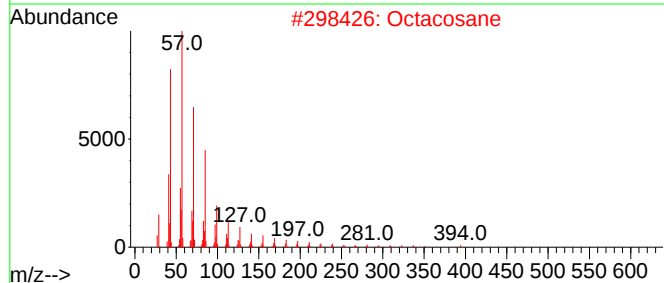
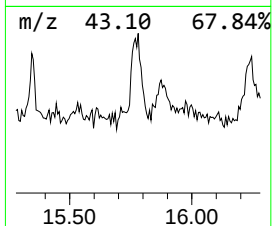
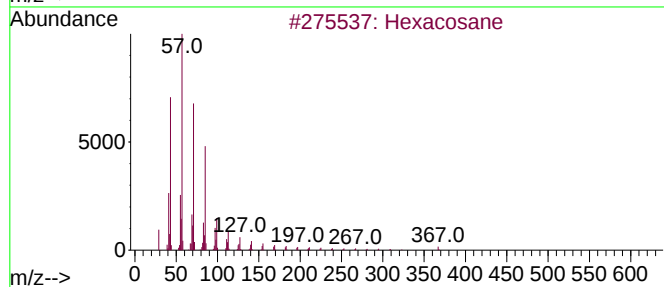
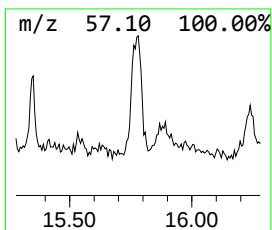
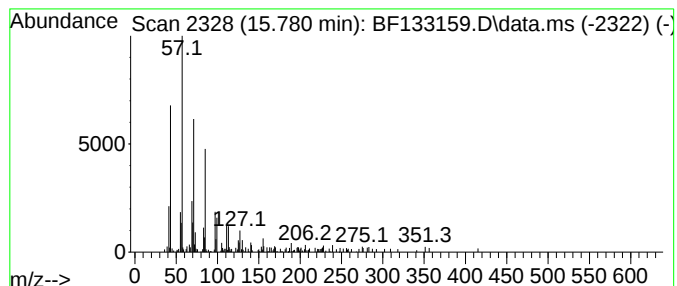
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.780	3.28 ng	178359	Perylene-d12	15.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	87
2			Octacosane	394	C28H58	000630-02-4	87
3			Tetratetracontane	619	C44H90	007098-22-8	87
4			Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	87
5			Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
Data File : BF133159.D
Acq On : 01 May 2023 17:02
Operator : CG\JU
Sample : 02558-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P001-SS013-1218-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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
Cycloheptanol, ...	2.140	8.3	ng	465781	1	6.728	1128710	20.0
Benzophenone	10.475	3.1	ng	274384	3	9.763	1760320	20.0
n-Hexadecanoic ...	11.786	8.6	ng	780207	4	11.245	1824980	20.0
Octadecanoic acid	12.557	15.4	ng	1402800	4	11.245	1824980	20.0
unknown12.998	12.998	2.8	ng	158080	5	13.880	1124020	20.0
1-Heneicosanol	13.769	6.8	ng	379265	5	13.880	1124020	20.0
Octadecane	14.233	3.1	ng	175363	5	13.880	1124020	20.0
Nonadecane	14.698	2.5	ng	133236	6	15.298	1086160	20.0
Hexacosane	15.780	3.3	ng	178359	6	15.298	1086160	20.0