

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103024\
 Data File : BF140160.D
 Acq On : 30 Oct 2024 16:26
 Operator : RC/JU
 Sample : P4616-05
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BP-F9-MOVED

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-BF101824.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140160.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	7	14	25	rVB	1166624	1827772	73.01%	9.053%
2	5.498	573	579	584	rBV	1666272	2211390	88.34%	10.953%
3	6.504	743	750	755	rBV	1587177	2283597	91.22%	11.311%
4	6.881	809	814	819	rBV	531798	642802	25.68%	3.184%
5	7.439	903	909	914	rBV	1156719	1493308	59.65%	7.396%
6	7.692	947	952	958	rVB	36822	45887	1.83%	0.227%
7	8.163	1023	1032	1038	rBV	654578	841578	33.62%	4.168%
8	8.375	1062	1068	1073	rBV3	21526	30023	1.20%	0.149%
9	8.751	1127	1132	1136	rBV	25121	30806	1.23%	0.153%
10	9.239	1209	1215	1220	rBV	1987547	2503314	100.00%	12.399%
11	9.322	1224	1229	1234	rBV	38490	52479	2.10%	0.260%
12	9.639	1279	1283	1286	rBV3	18262	29740	1.19%	0.147%
13	9.851	1312	1319	1324	rBV	55953	74041	2.96%	0.367%
14	9.922	1324	1331	1336	rBV	715383	890133	35.56%	4.409%
15	10.351	1397	1404	1408	rBV	60358	81377	3.25%	0.403%
16	10.575	1436	1442	1447	rBV	22284	37072	1.48%	0.184%
17	10.639	1447	1453	1460	rVV	357169	459049	18.34%	2.274%
18	10.710	1460	1465	1477	rVV	1132025	1519484	60.70%	7.526%
19	10.827	1481	1485	1494	rVB	72131	124125	4.96%	0.615%
20	10.945	1501	1505	1510	rBV	38277	47049	1.88%	0.233%
21	11.280	1557	1562	1565	rBV	56497	78187	3.12%	0.387%
22	11.310	1565	1567	1573	rVB	23432	27974	1.12%	0.139%
23	11.416	1579	1585	1590	rBV	643496	825315	32.97%	4.088%
24	11.480	1592	1596	1600	rVB2	21163	28076	1.12%	0.139%
25	11.710	1630	1635	1639	rVB	50807	63827	2.55%	0.316%
26	11.945	1670	1675	1691	rBV	232076	392113	15.66%	1.942%
27	12.116	1700	1704	1709	rVB	49170	62379	2.49%	0.309%
28	12.510	1767	1771	1776	rVB	35842	47033	1.88%	0.233%
29	12.733	1804	1809	1821	rBV	49878	100607	4.02%	0.498%
30	12.880	1831	1834	1846	rVB	28230	41577	1.66%	0.206%
31	13.004	1850	1855	1861	rBV	1383340	1864984	74.50%	9.237%
32	13.239	1891	1895	1899	rBV	26970	37844	1.51%	0.187%
33	13.586	1950	1954	1961	rVB2	24679	33433	1.34%	0.166%
34	13.927	2004	2012	2023	rBV2	56866	156508	6.25%	0.775%
35	14.080	2033	2038	2050	rVB	356556	481540	19.24%	2.385%
36	14.257	2064	2068	2079	rVB	19881	32770	1.31%	0.162%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103024\
Data File : BF140160.D
Acq On : 30 Oct 2024 16:26
Operator : RC/JU
Sample : P4616-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F9-MOVED

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-BF101824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.586	2120	2124	2129	rBV	18616	28952	1.16%	0.143%
38	14.886	2170	2175	2186	rBV5	37682	103476	4.13%	0.513%
39	15.610	2292	2298	2304	rBV	352513	558403	22.31%	2.766%

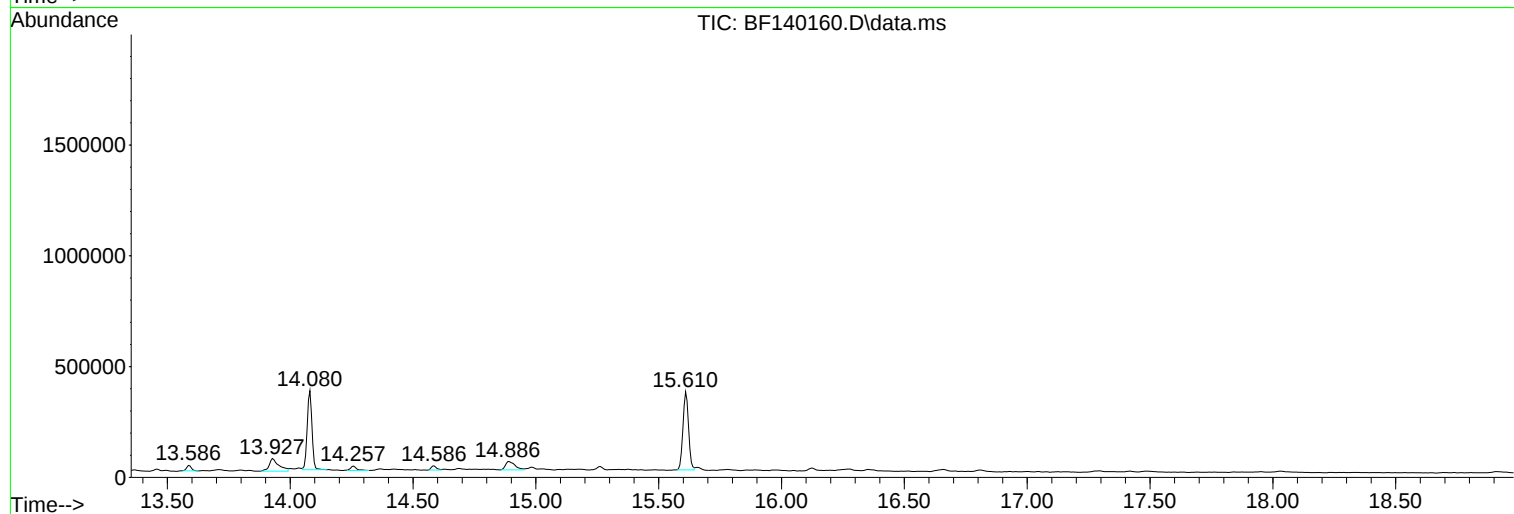
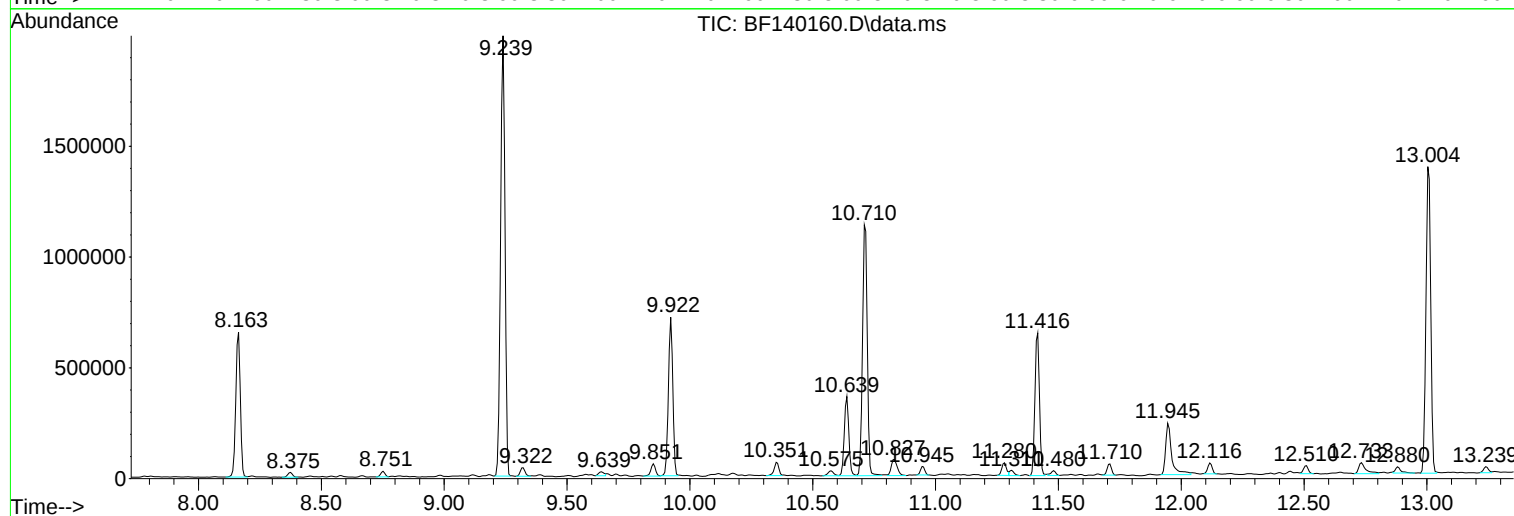
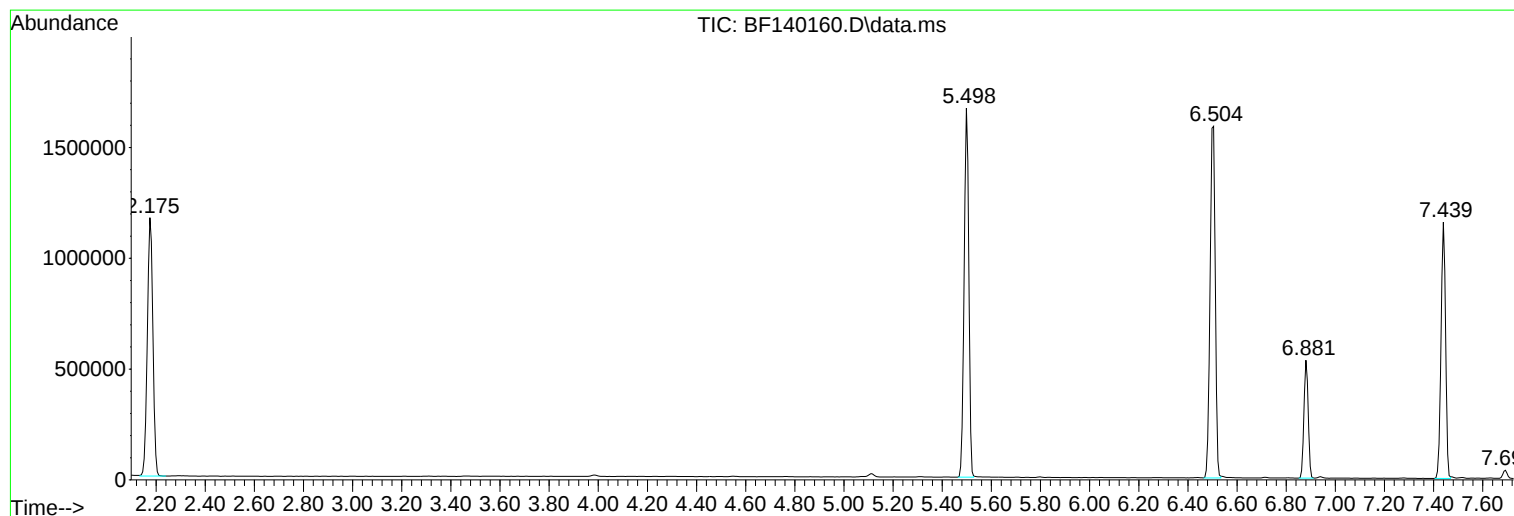
Sum of corrected areas: 20190024

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103024\
Data File : BF140160.D
Acq On : 30 Oct 2024 16:26
Operator : RC/JU
Sample : P4616-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F9-MOVED

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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\BF103024\
Data File : BF140160.D
Acq On : 30 Oct 2024 16:26
Operator : RC/JU
Sample : P4616-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F9-MOVED

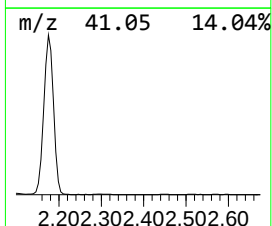
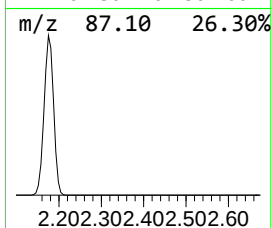
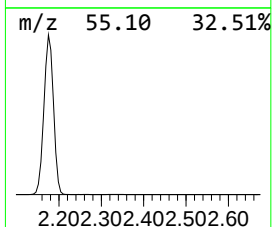
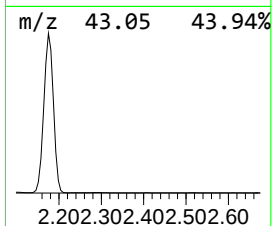
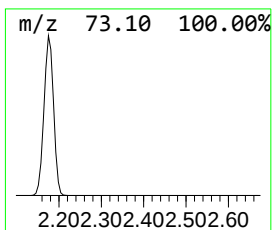
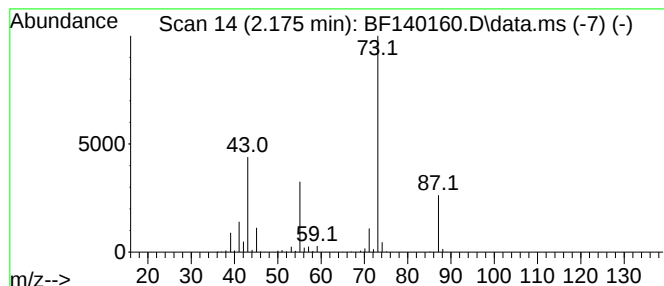
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.175	56.87 ng	1827770	1,4-Dichlorobenzene-d4	6.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103024\
Data File : BF140160.D
Acq On : 30 Oct 2024 16:26
Operator : RC/JU
Sample : P4616-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F9-MOVED

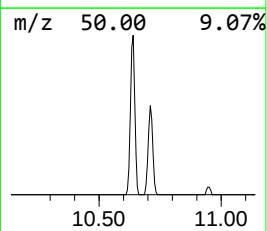
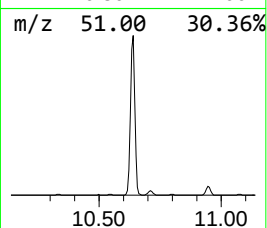
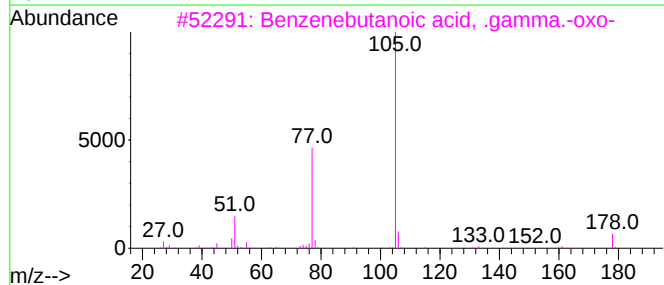
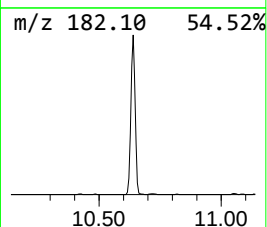
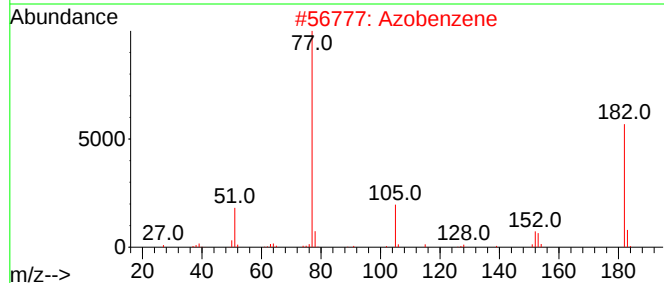
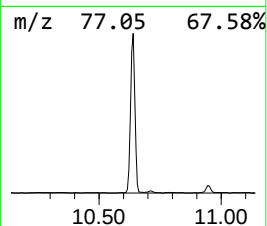
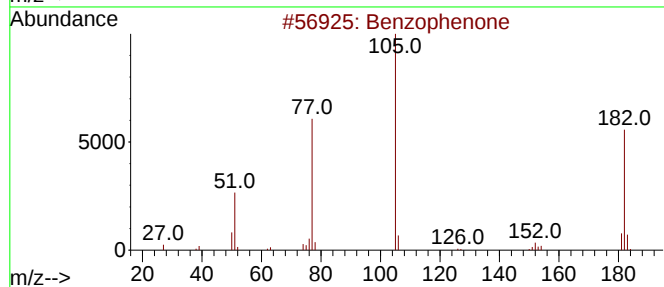
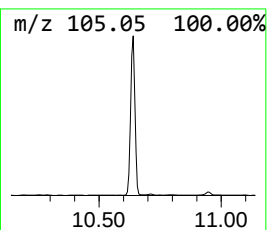
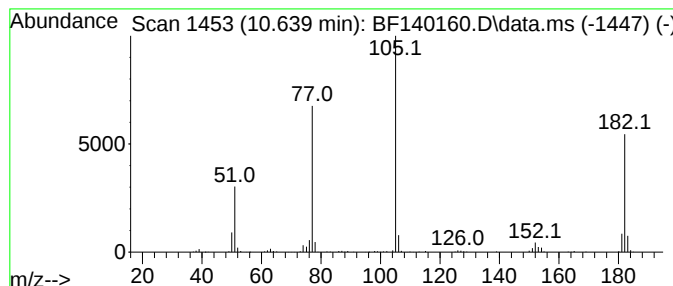
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.639	10.31 ng	459049	Acenaphthene-d10	9.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	58
3			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	50
4			N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	50
5			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103024\
Data File : BF140160.D
Acq On : 30 Oct 2024 16:26
Operator : RC/JU
Sample : P4616-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F9-MOVED

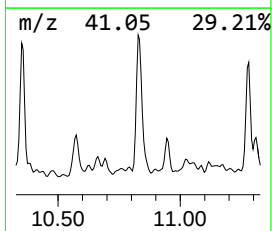
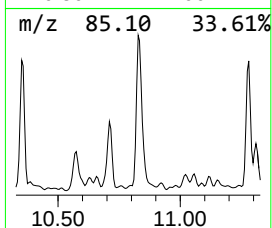
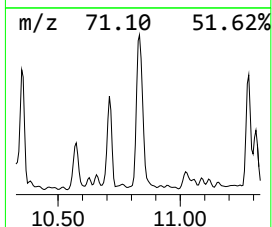
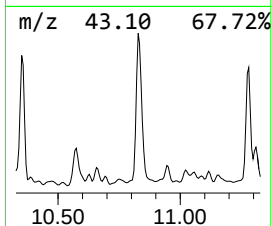
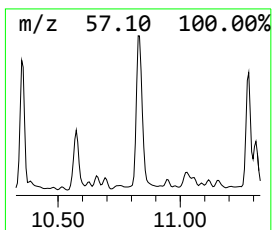
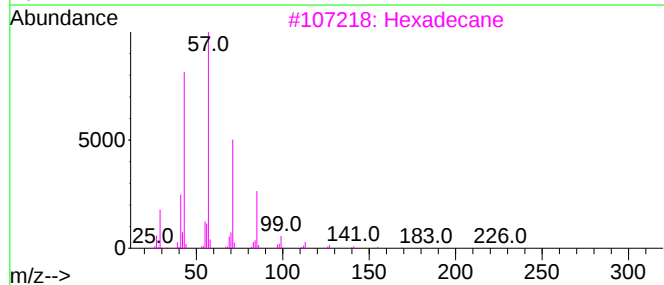
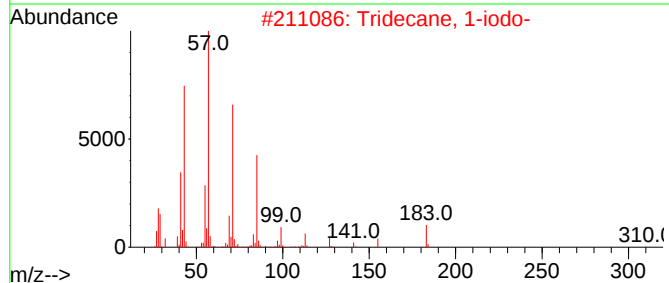
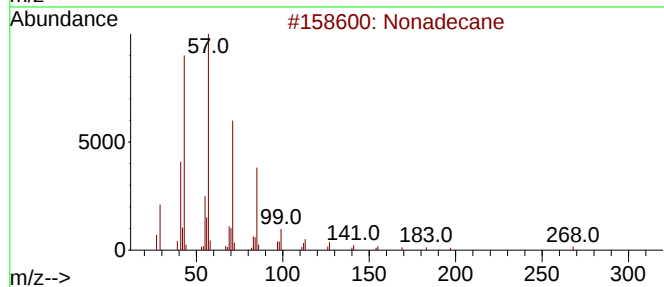
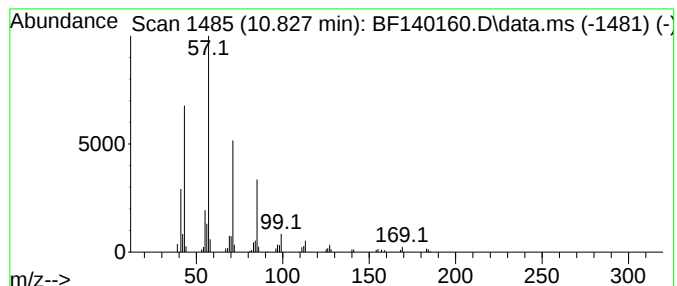
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.828	3.01 ng	124125	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	91
2			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	90
3			Hexadecane	226	C16H34	000544-76-3	90
4			Eicosane	282	C20H42	000112-95-8	87
5			Octacosane	394	C28H58	000630-02-4	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103024\
Data File : BF140160.D
Acq On : 30 Oct 2024 16:26
Operator : RC/JU
Sample : P4616-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F9-MOVED

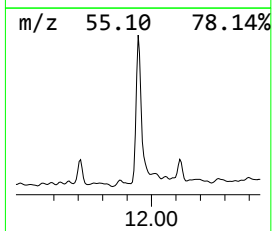
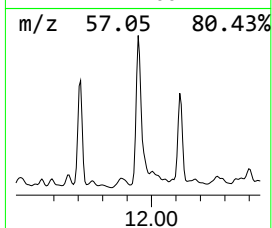
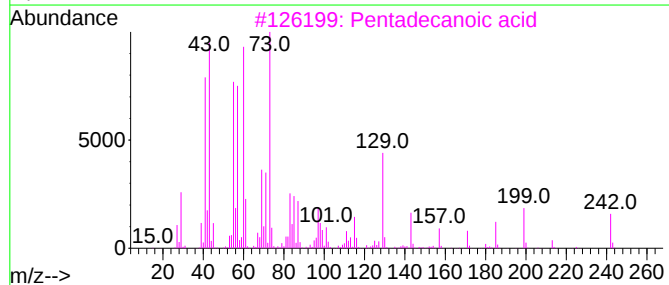
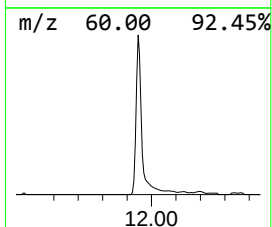
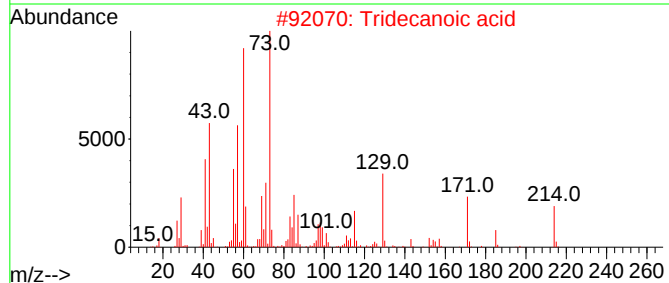
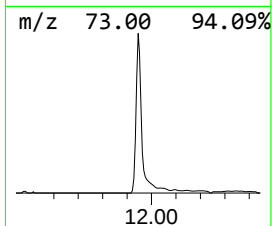
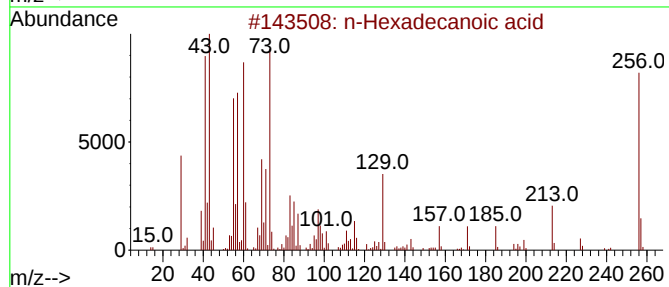
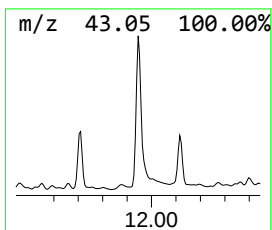
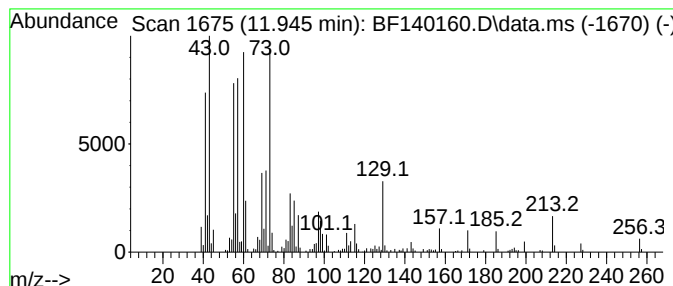
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	9.50 ng	392113	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103024\
Data File : BF140160.D
Acq On : 30 Oct 2024 16:26
Operator : RC/JU
Sample : P4616-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F9-MOVED

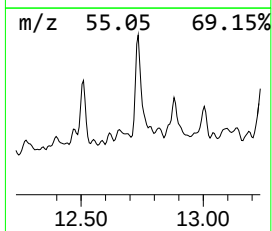
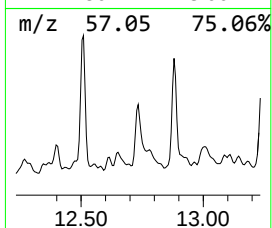
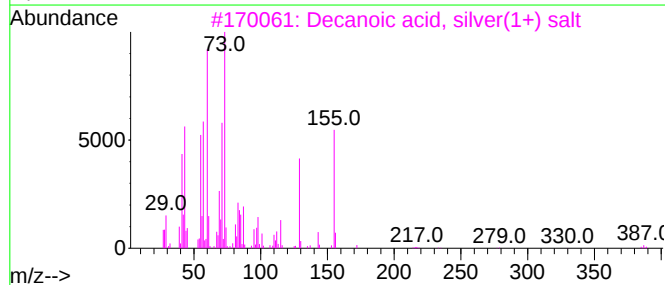
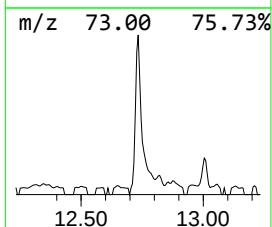
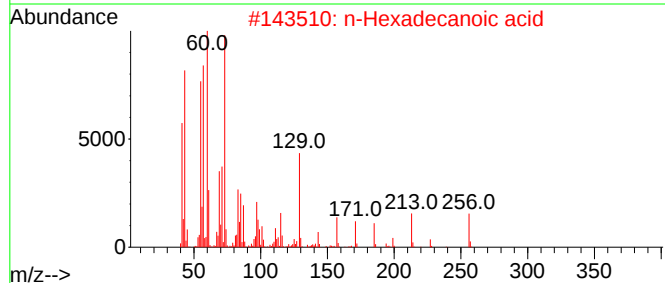
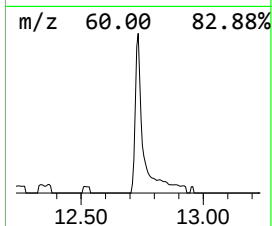
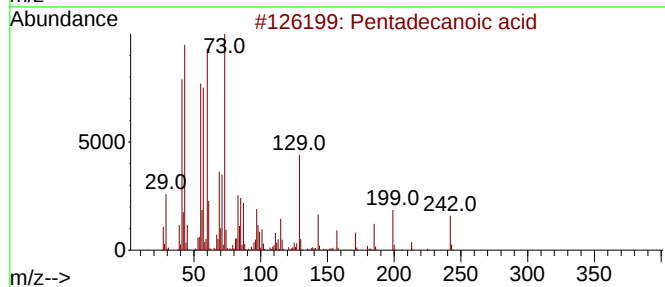
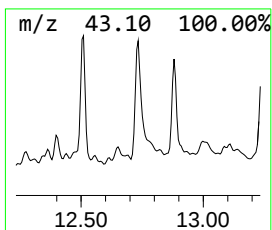
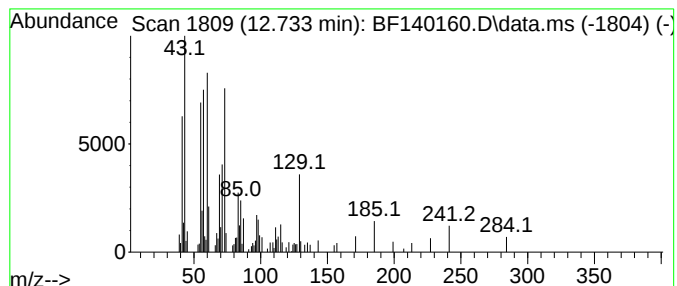
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Pentadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.733	2.44 ng	100607	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
3			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	64
4			Tridecanoic acid	214	C13H26O2	000638-53-9	64
5			Octadecanoic acid	284	C18H36O2	000057-11-4	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103024\
Data File : BF140160.D
Acq On : 30 Oct 2024 16:26
Operator : RC/JU
Sample : P4616-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F9-MOVED

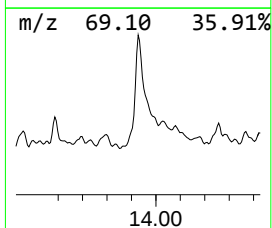
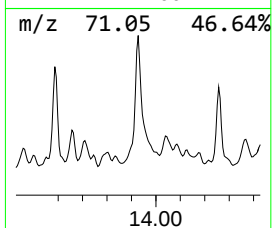
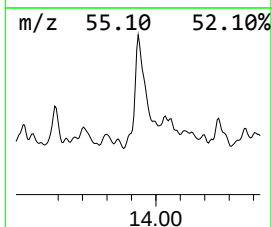
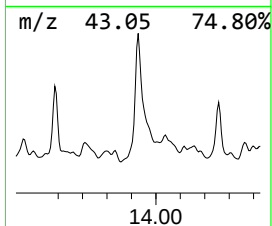
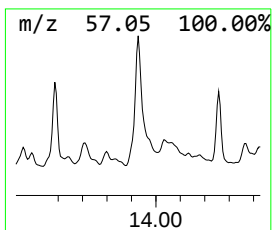
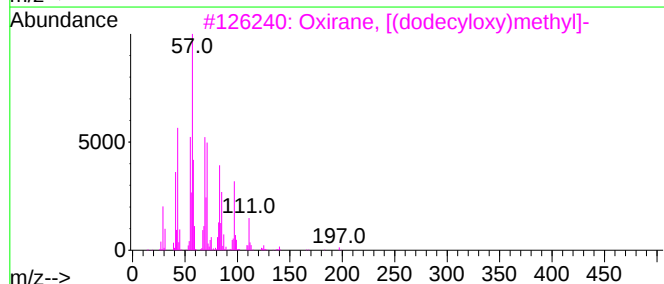
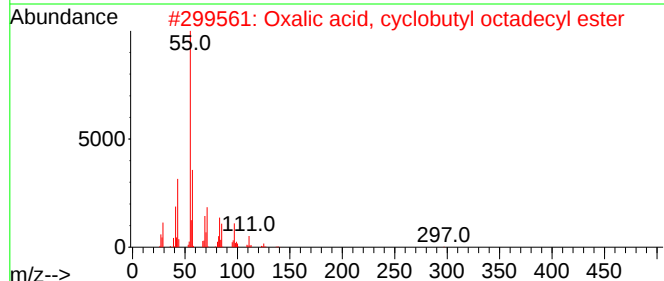
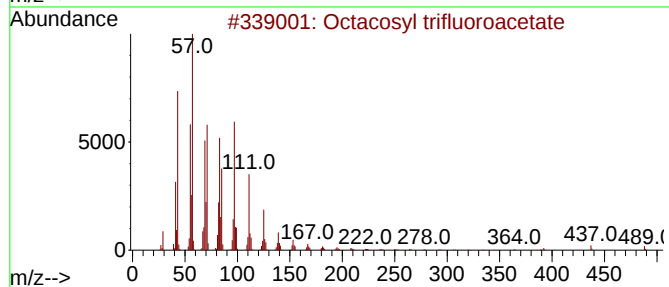
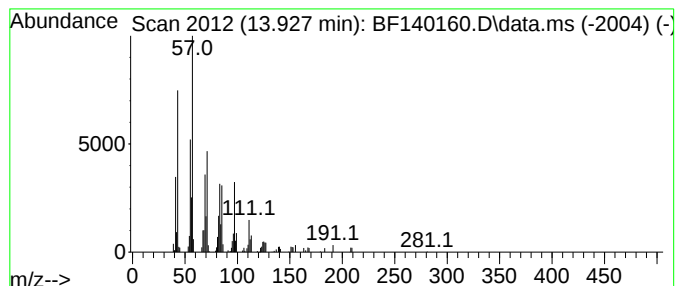
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octacosyl trifluoroacetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.927	6.50 ng	156508	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
2			Oxalic acid, cyclobutyl octadecy...	396	C24H44O4	1000309-70-8	91
3			Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	87
4			Oxalic acid, cyclobutyl heptadec...	382	C23H42O4	1000309-70-7	74
5			Pentadecane, 1-bromo-	290	C15H31Br	000629-72-1	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103024\
Data File : BF140160.D
Acq On : 30 Oct 2024 16:26
Operator : RC/JU
Sample : P4616-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F9-MOVED

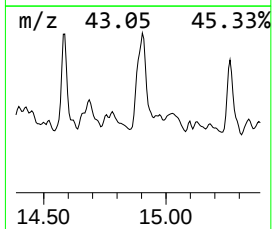
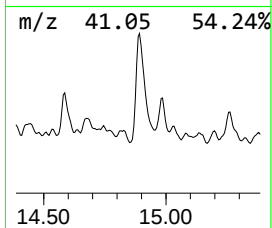
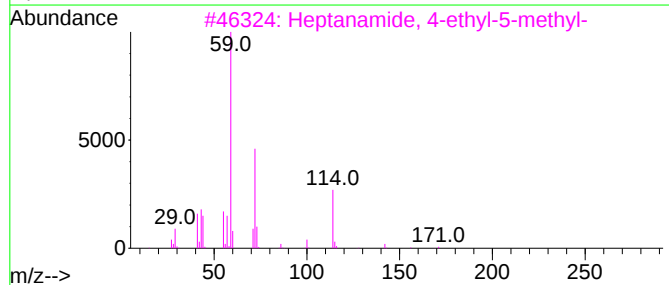
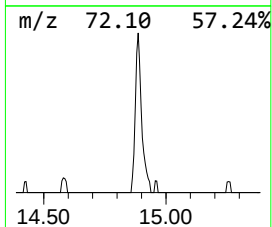
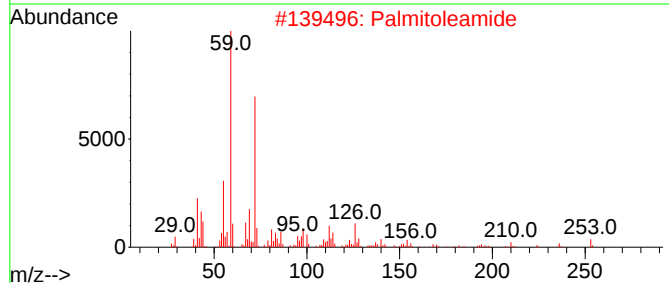
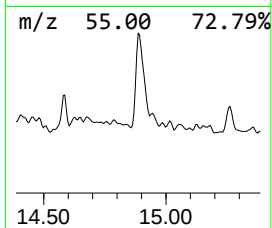
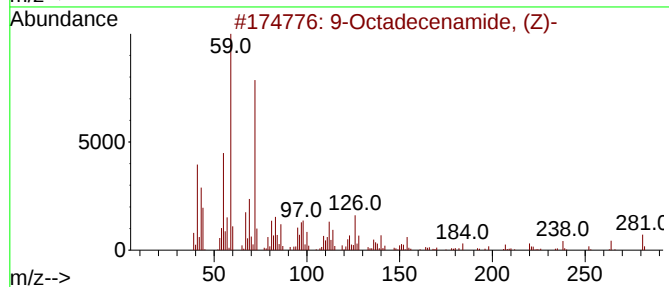
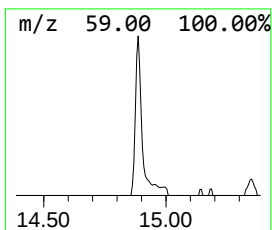
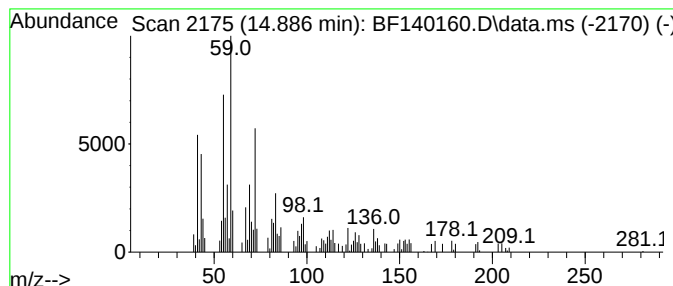
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.886	3.71 ng	103476	Perylene-d12	15.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	68
2			Palmitoleamide	253	C16H31NO	106010-22-4	64
3			Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	50
4			Octanamide	143	C8H17NO	000629-01-6	46
5			Tetradecanamide	227	C14H29NO	000638-58-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103024\
Data File : BF140160.D
Acq On : 30 Oct 2024 16:26
Operator : RC/JU
Sample : P4616-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F9-MOVED

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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...	2.175	56.9	ng	1827770	1	6.881	642802	20.0
Benzophenone	10.639	10.3	ng	459049	3	9.922	890133	20.0
Nonadecane	10.828	3.0	ng	124125	4	11.416	825315	20.0
n-Hexadecanoic ...	11.945	9.5	ng	392113	4	11.416	825315	20.0
Pentadecanoic acid	12.733	2.4	ng	100607	4	11.416	825315	20.0
Octacosyl trifl...	13.927	6.5	ng	156508	5	14.080	481540	20.0
9-Octadecenamid...	14.886	3.7	ng	103476	6	15.610	558403	20.0