

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022023\
 Data File : BF132480.D
 Acq On : 20 Feb 2023 15:18
 Operator : CG\JU
 Sample : 01593-07
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SW-2

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-BF021623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132480.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.231	402	407	408	rBV	104518	101617	1.75%	0.263%
2	5.260	408	412	424	rVB	1425054	1686859	28.99%	4.371%
3	5.648	474	478	482	rBV	3886893	3913838	67.27%	10.141%
4	6.642	642	647	650	rBV	3391616	2998440	51.53%	7.769%
5	7.025	708	712	715	rBV	1654347	1287825	22.13%	3.337%
6	7.589	803	808	811	rVB	3842514	3540934	60.86%	9.175%
7	7.754	832	836	840	rVB	114217	95211	1.64%	0.247%
8	8.313	927	931	934	rBV	1868800	1593887	27.39%	4.130%
9	9.389	1109	1114	1117	rBV	6648740	5818378	100.00%	15.076%
10	9.454	1122	1125	1128	rBV	107243	82249	1.41%	0.213%
11	10.072	1227	1230	1234	rVB	1811217	1560754	26.82%	4.044%
12	10.248	1257	1260	1264	rVB2	70976	69063	1.19%	0.179%
13	10.789	1348	1352	1355	rBV	2193900	1781059	30.61%	4.615%
14	10.872	1361	1366	1369	rBV	2983532	2933260	50.41%	7.600%
15	11.154	1410	1414	1418	rVB2	142624	138215	2.38%	0.358%
16	11.572	1481	1485	1488	rBV	1490357	1319277	22.67%	3.418%
17	12.007	1556	1559	1563	rBV2	56996	74048	1.27%	0.192%
18	12.083	1568	1572	1587	rVV	881275	1054432	18.12%	2.732%
19	12.501	1641	1643	1647	rVB	230789	178413	3.07%	0.462%
20	12.871	1703	1706	1713	rBV	182383	249094	4.28%	0.645%
21	13.160	1751	1755	1759	rBV	4519129	4278483	73.53%	11.086%
22	14.065	1904	1909	1921	rBV2	238252	835576	14.36%	2.165%
23	14.224	1933	1936	1940	rVB	993678	927407	15.94%	2.403%
24	14.318	1949	1952	1956	rVB	388934	353058	6.07%	0.915%
25	15.095	2080	2084	2089	rVB	1016085	1038009	17.84%	2.690%
26	15.789	2198	2202	2207	rVB	521316	684090	11.76%	1.773%

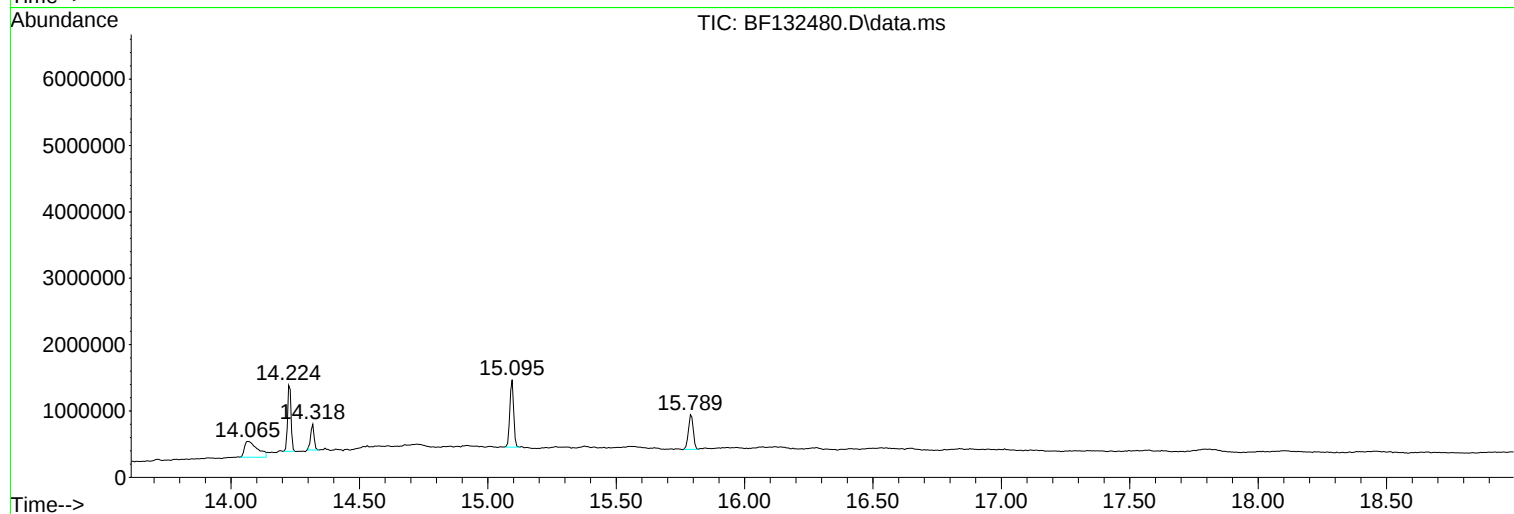
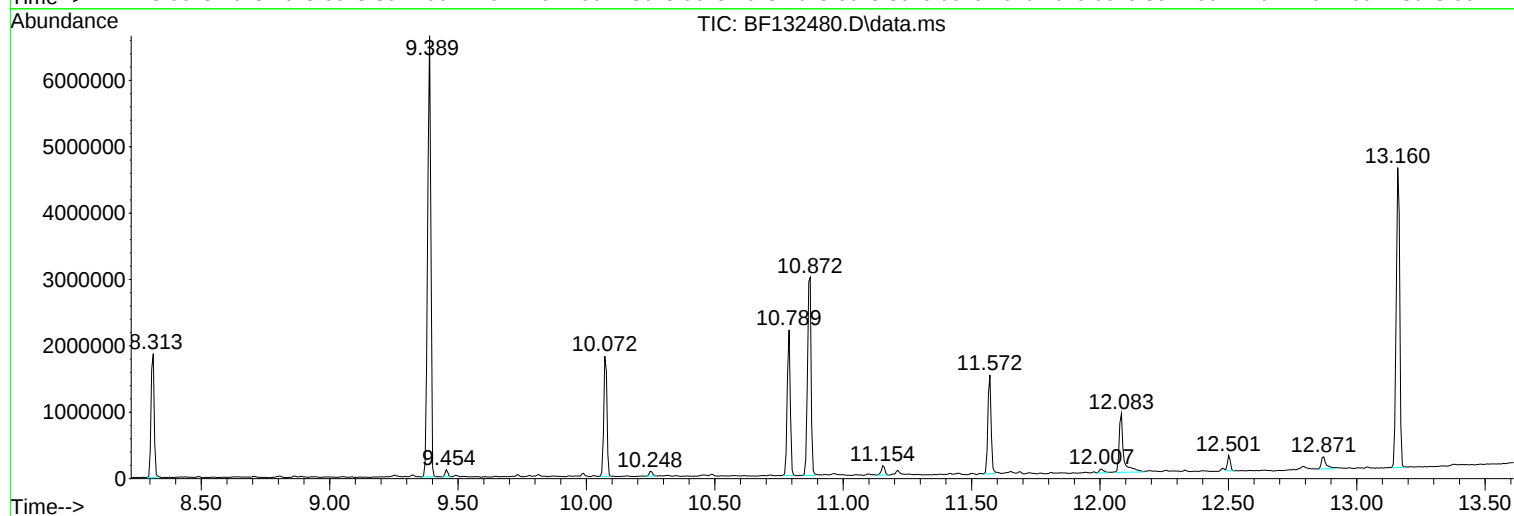
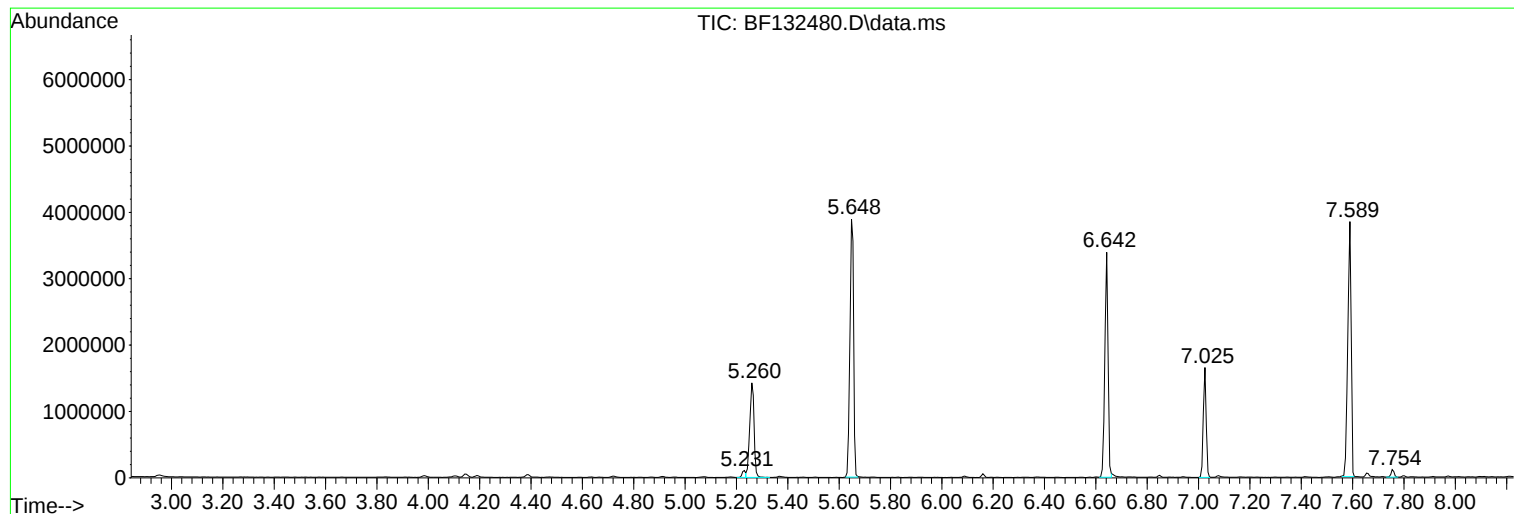
Sum of corrected areas: 38593476

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022023\
Data File : BF132480.D
Acq On : 20 Feb 2023 15:18
Operator : CG\JU
Sample : 01593-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.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\BF022023\
Data File : BF132480.D
Acq On : 20 Feb 2023 15:18
Operator : CG\JU
Sample : 01593-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW-2

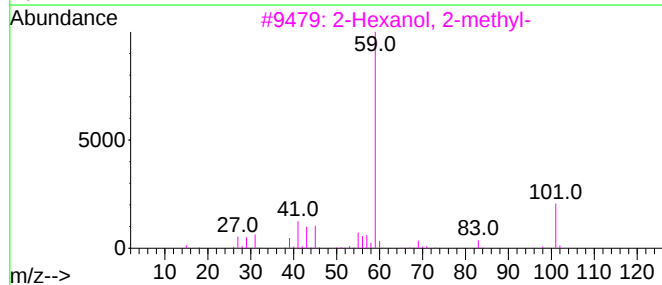
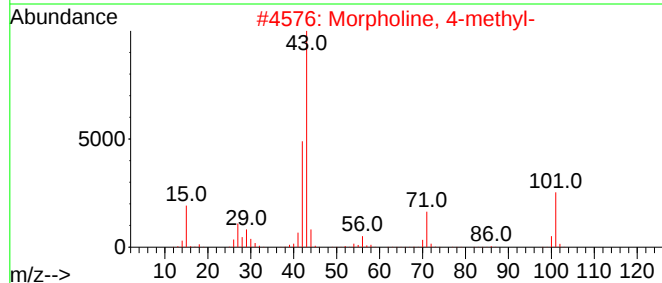
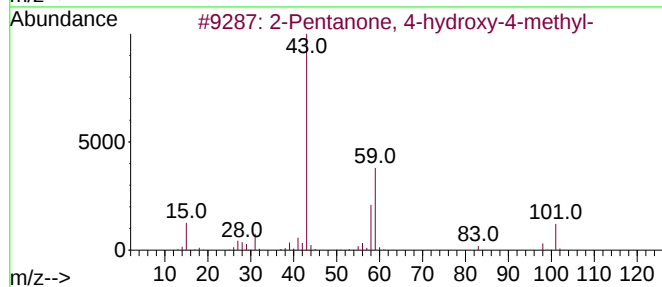
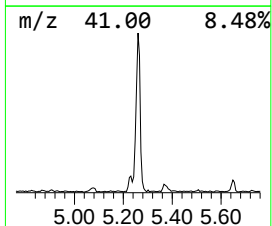
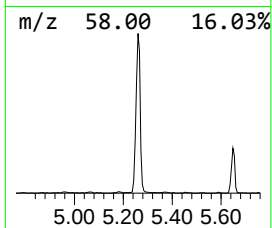
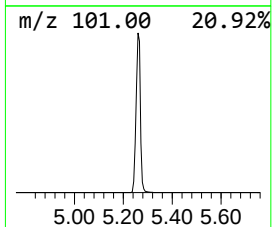
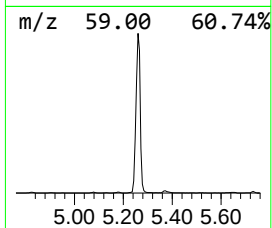
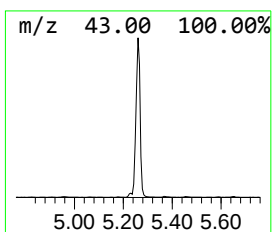
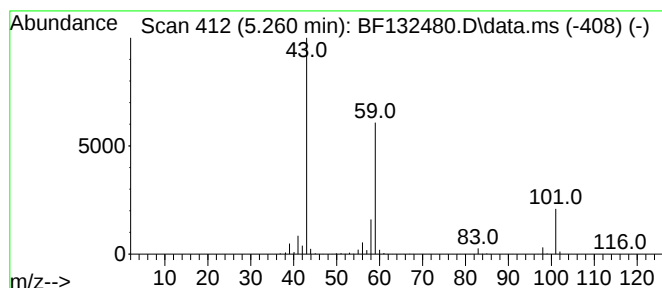
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.260	26.20 ng	1686860	1,4-Dichlorobenzene-d4	7.025

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9		
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022023\
Data File : BF132480.D
Acq On : 20 Feb 2023 15:18
Operator : CG\JU
Sample : 01593-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

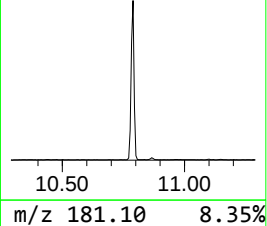
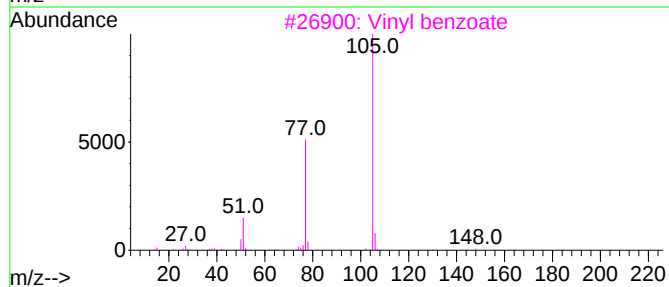
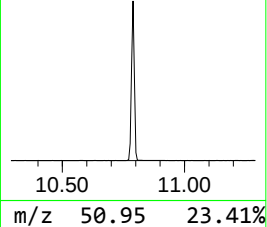
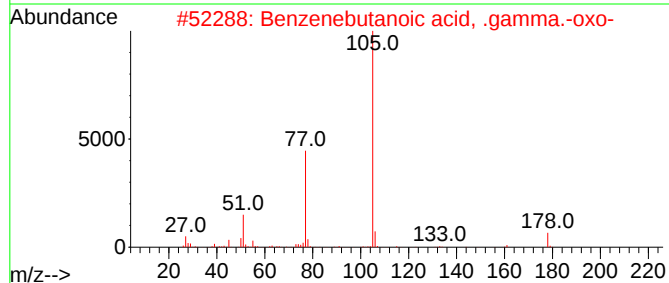
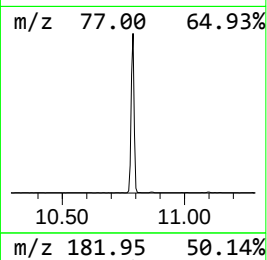
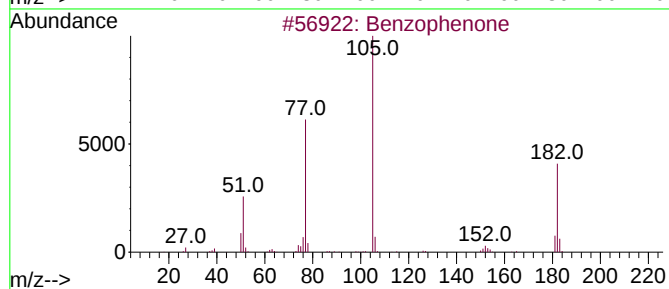
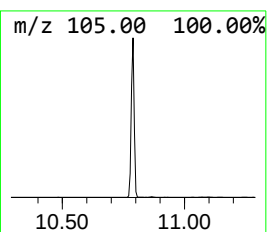
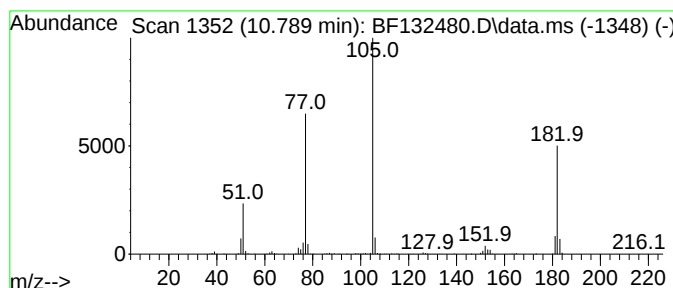
Instrument :
BNA_F
ClientSampleId :
SW-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.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 3

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.789	22.82 ng	1781060	Acenaphthene-d10		10.072
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	49
3	Vinyl benzoate	148	C9H8O2	000769-78-8	47
4	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47
5	N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022023\
Data File : BF132480.D
Acq On : 20 Feb 2023 15:18
Operator : CG\JU
Sample : 01593-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW-2

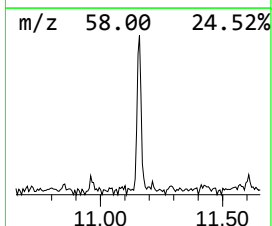
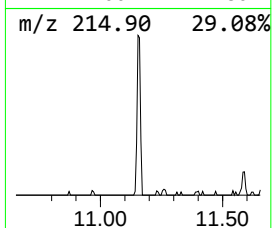
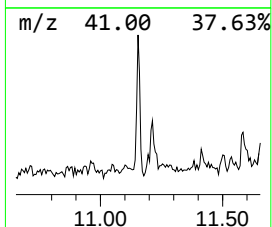
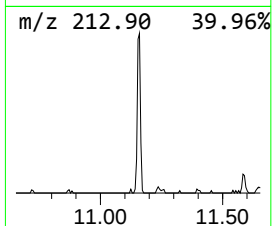
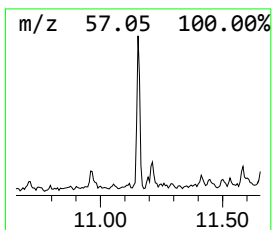
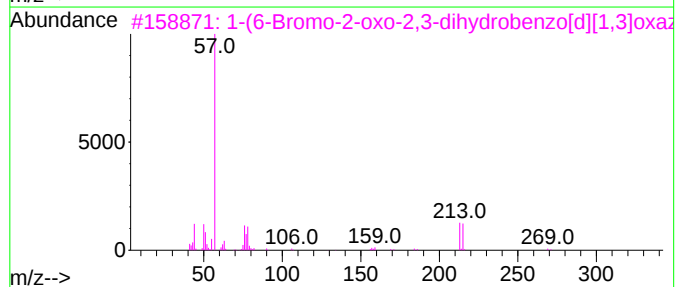
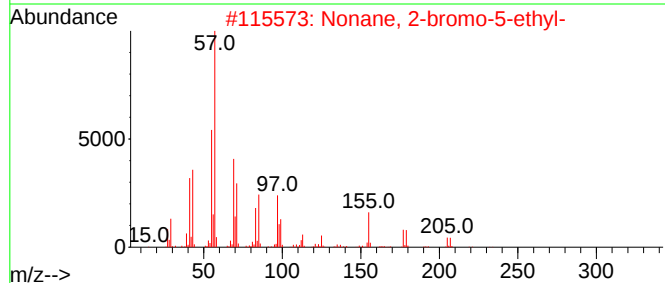
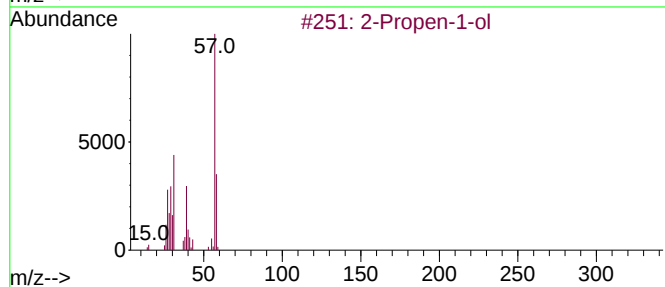
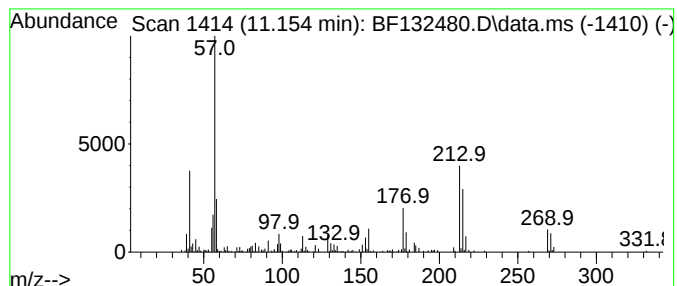
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown11.154 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.154	2.10 ng	138215	Phenanthrene-d10	11.572

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Propen-1-ol	58	C3H6O	000107-18-6	9
2		Nonane, 2-bromo-5-ethyl-	234	C11H23Br	055162-38-4	9
3		1-(6-Bromo-2-oxo-2,3-dihydrobenz...	269	C10H8BrNO3	1000260-89-1	9
4		Formic acid, 2-propenyl ester	86	C4H6O2	001838-59-1	9
5		tert-Butyl 4,4-difluorocyclohexy...	235	C11H19F2NO2	675112-67-1	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022023\
Data File : BF132480.D
Acq On : 20 Feb 2023 15:18
Operator : CG\JU
Sample : 01593-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

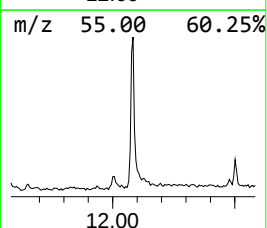
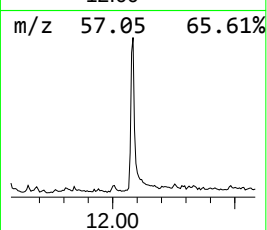
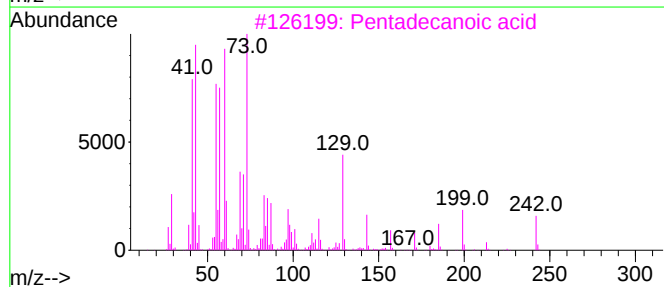
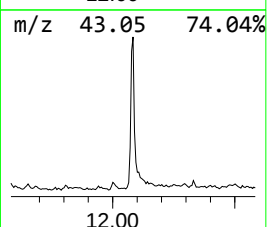
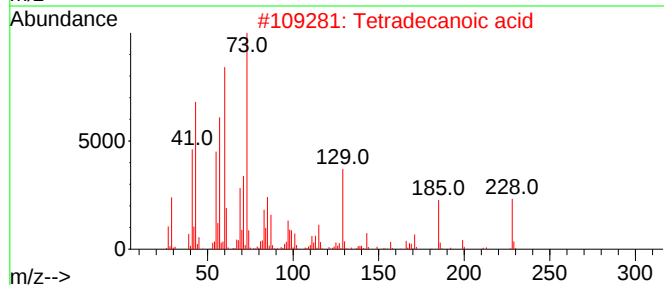
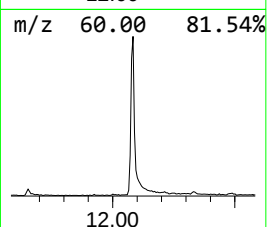
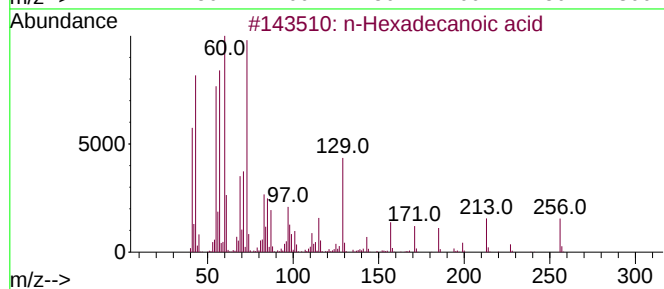
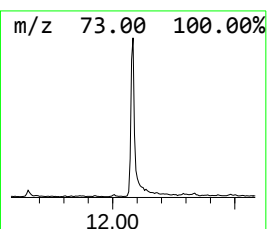
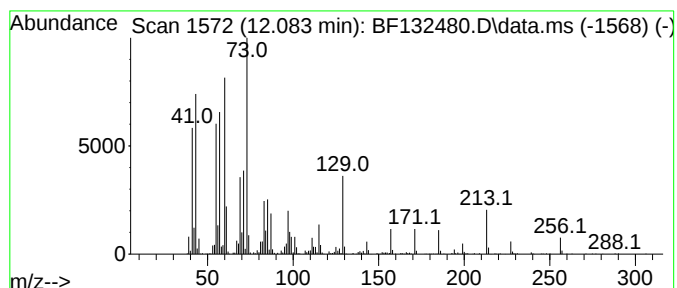
Instrument :
BNA_F
ClientSampleId :
SW-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.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 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.083	15.98 ng	1054430	Phenanthrene-d10	11.572	
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	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Octadecanoic acid	284	C18H36O2	000057-11-4	87
5	Tridecanoic acid	214	C13H26O2	000638-53-9	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022023\
Data File : BF132480.D
Acq On : 20 Feb 2023 15:18
Operator : CG\JU
Sample : 01593-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW-2

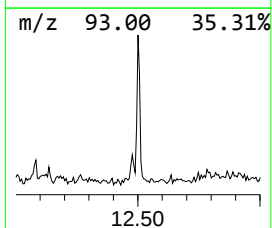
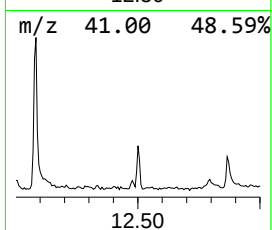
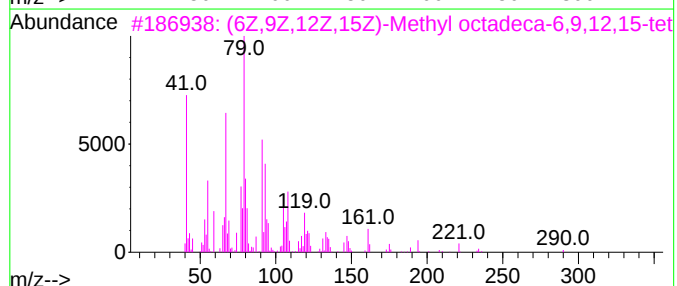
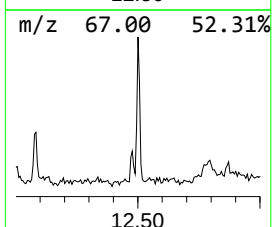
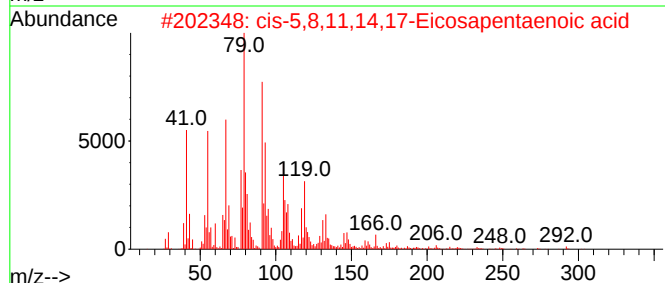
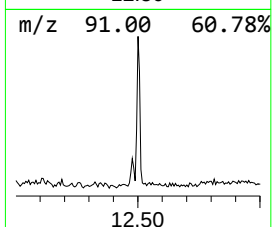
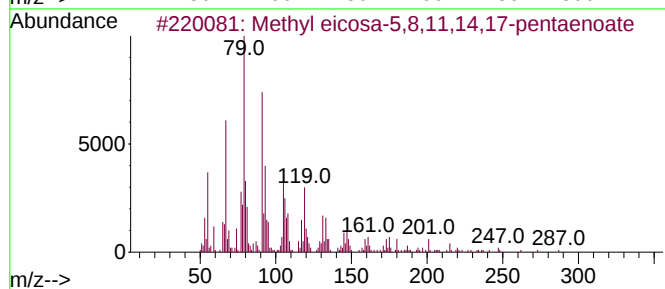
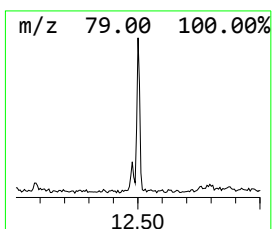
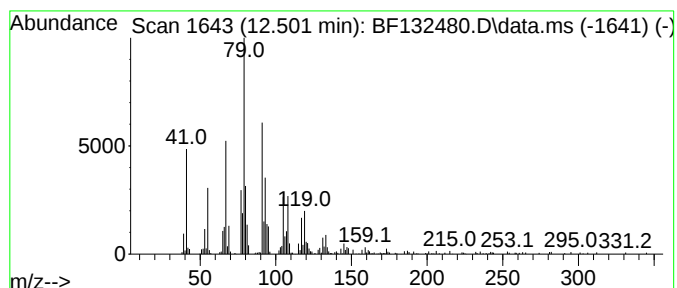
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Methyl eicosa-5,8,11,14,17-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.501	2.70 ng	178413	Phenanthrene-d10	11.572

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl eicosa-5,8,11,14,17-penta...	316	C21H32O2	001191-65-7	91
2			cis-5,8,11,14,17-Eicosapentaenoi...	302	C20H30O2	010417-94-4	87
3			(6Z,9Z,12Z,15Z)-Methyl octadeca...	290	C19H30O2	073097-00-4	86
4			4,7,10,13,16,19-Docosahexaenoic ...	342	C23H34O2	002566-90-7	83
5			5,8,11,14,17-Eicosapentaenoic ac...	316	C21H32O2	002734-47-6	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022023\
Data File : BF132480.D
Acq On : 20 Feb 2023 15:18
Operator : CG\JU
Sample : 01593-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW-2

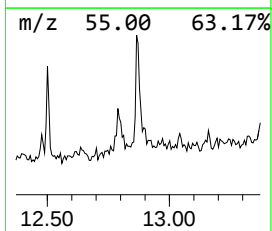
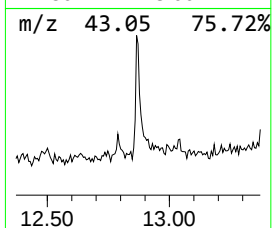
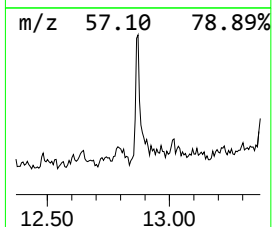
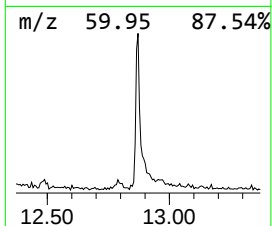
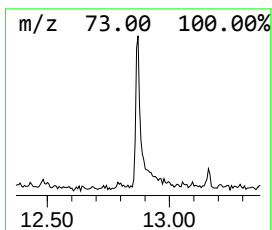
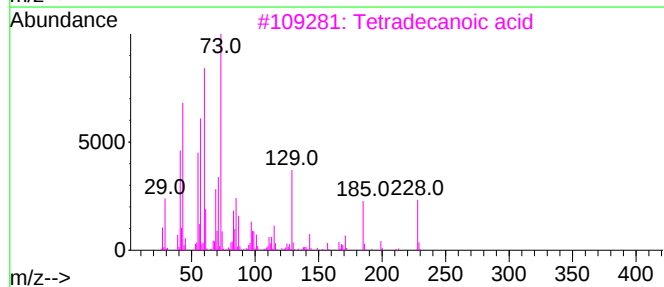
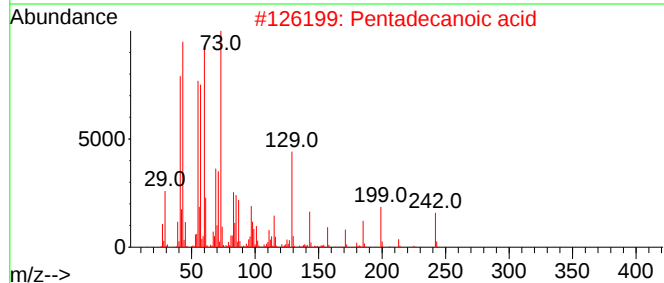
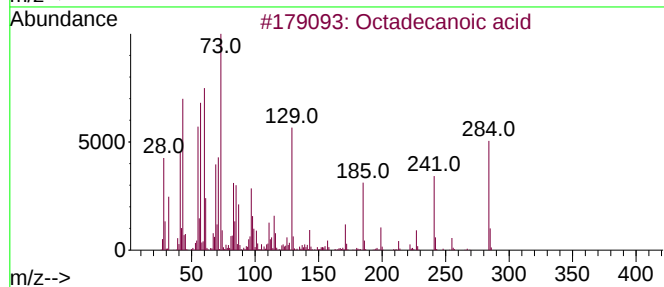
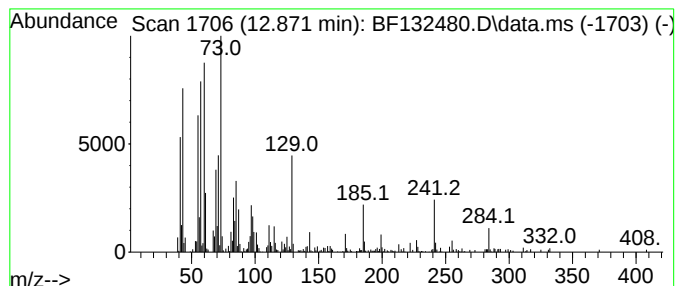
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.871	3.78 ng	249094	Phenanthrene-d10	11.572

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	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
5			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022023\
Data File : BF132480.D
Acq On : 20 Feb 2023 15:18
Operator : CG\JU
Sample : 01593-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

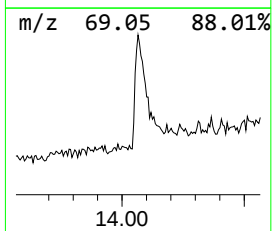
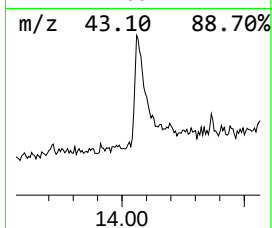
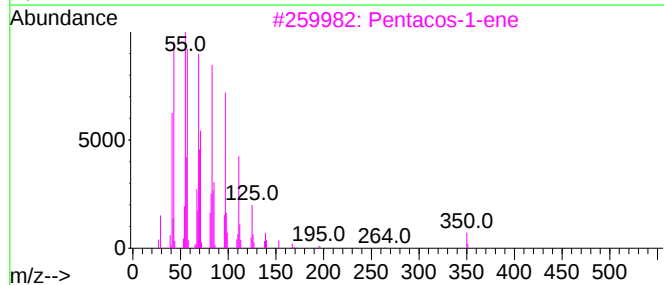
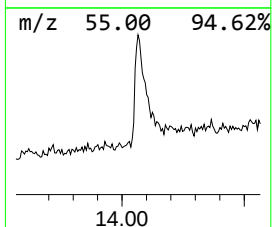
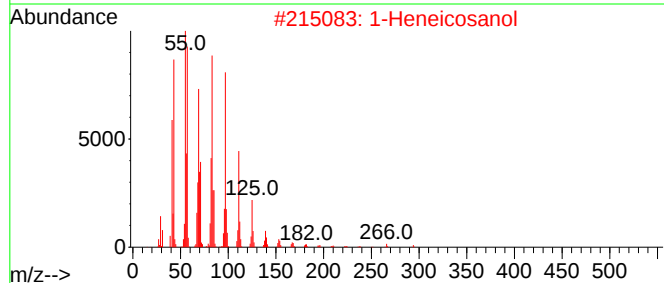
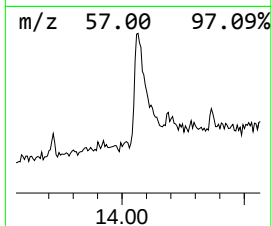
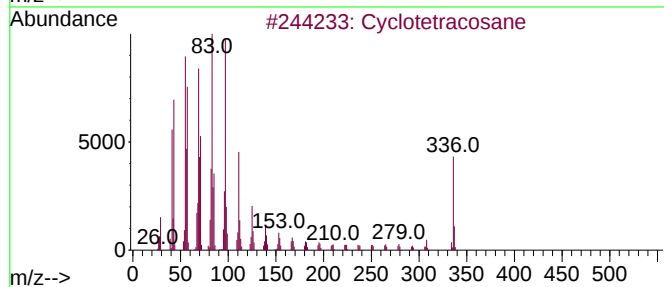
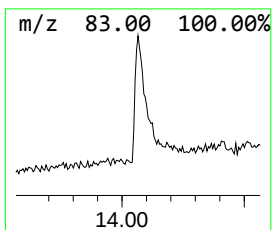
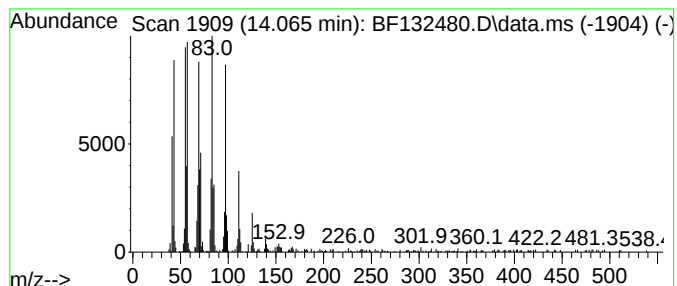
Instrument :
BNA_F
ClientSampleId :
SW-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclotetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.066	18.02 ng	835576	Chrysene-d12	14.224	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	97
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	Pentacos-1-ene	350	C25H50	016980-85-1	94
4	Behenic alcohol	326	C22H46O	000661-19-8	94
5	1-Heptacosanol	396	C27H56O	002004-39-9	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022023\
Data File : BF132480.D
Acq On : 20 Feb 2023 15:18
Operator : CG\JU
Sample : 01593-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW-2

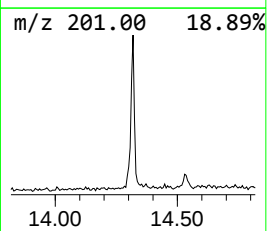
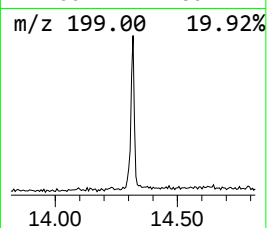
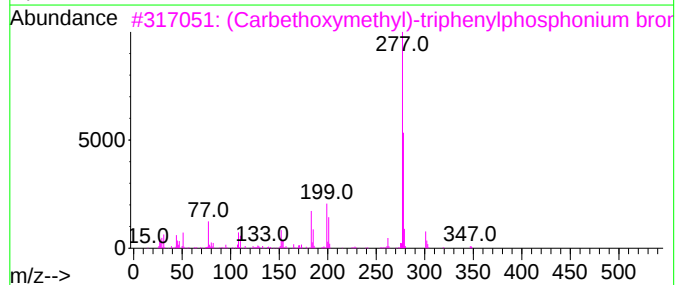
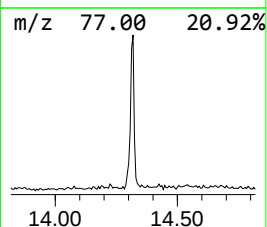
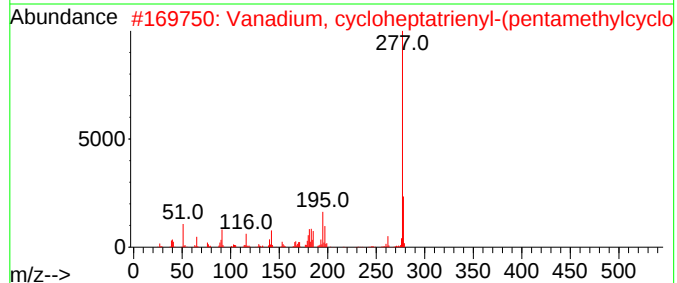
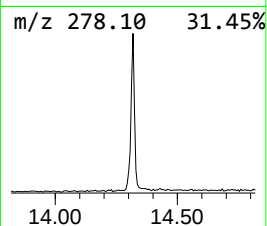
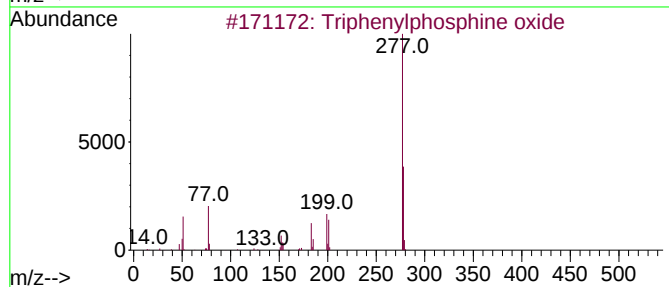
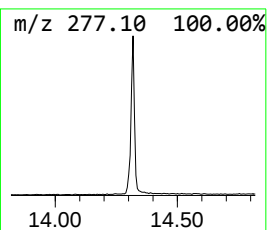
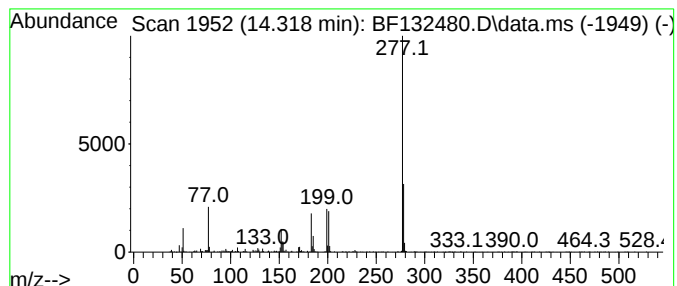
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Triphenylphosphine oxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.318	7.61 ng	353058	Chrysene-d12	14.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	94
2			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	50
3			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	50
4			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45
5			Dimethoxymethyl-hydroxy-tripheny...	354	C21H23O3P	1000132-00-1	33



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022023\
Data File : BF132480.D
Acq On : 20 Feb 2023 15:18
Operator : CG\JU
Sample : 01593-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW-2

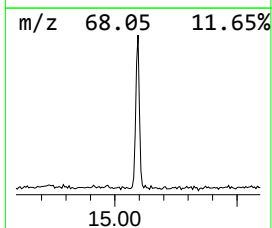
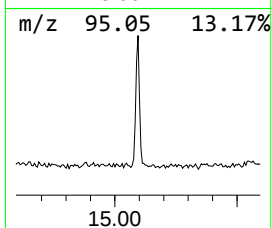
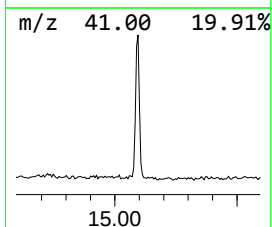
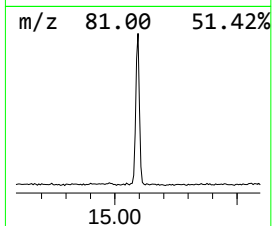
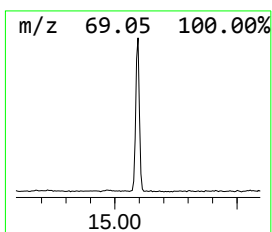
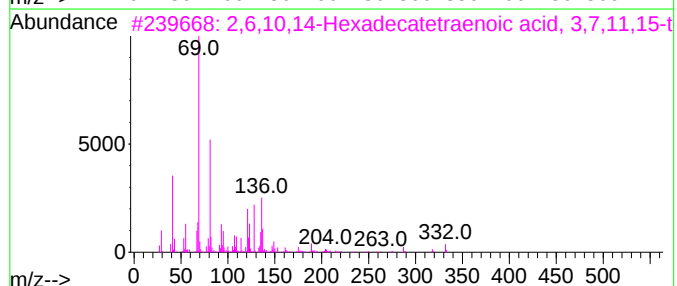
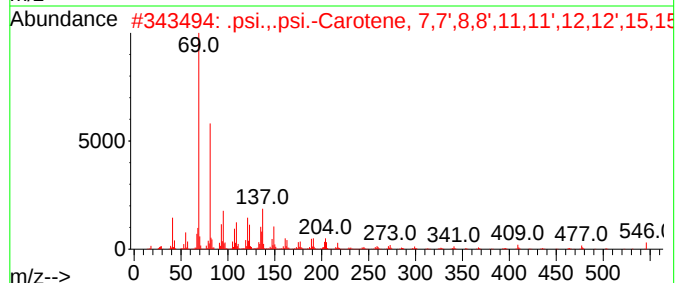
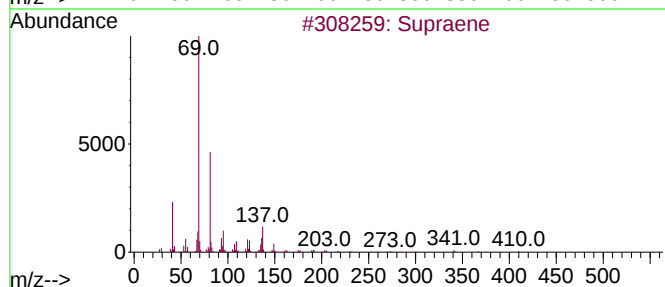
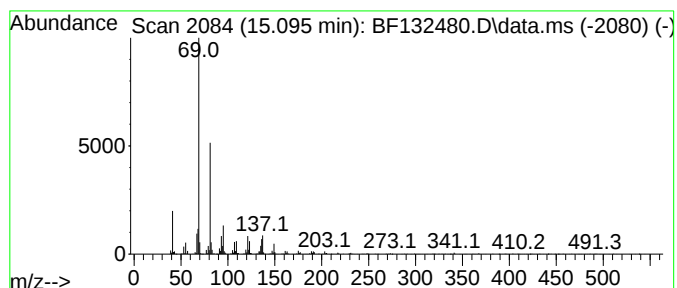
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Supraene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.095	30.35 ng	1038010	Perylene-d12	15.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
3			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
4			Trideca-1,3,7,11-tetraene-1,1-di...	268	C18H24N2	1000159-88-9	53
5			1,5-Heptadiene, 2,6-dimethyl-	124	C9H16	006709-39-3	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022023\
Data File : BF132480.D
Acq On : 20 Feb 2023 15:18
Operator : CG\JU
Sample : 01593-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.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-...	5.260	26.2	ng	1686860	1	7.025	1287830	20.0
Benzophenone	10.789	22.8	ng	1781060	3	10.072	1560750	20.0
unknown11.154	11.154	2.1	ng	138215	4	11.572	1319280	20.0
n-Hexadecanoic ...	12.083	16.0	ng	1054430	4	11.572	1319280	20.0
Methyl eicosa-5...	12.501	2.7	ng	178413	4	11.572	1319280	20.0
Octadecanoic acid	12.871	3.8	ng	249094	4	11.572	1319280	20.0
Cyclotetracosane	14.066	18.0	ng	835576	5	14.224	927407	20.0
Triphenylphosph...	14.318	7.6	ng	353058	5	14.224	927407	20.0
Supraene	15.095	30.4	ng	1038010	6	15.789	684090	20.0