

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102922\
 Data File : BF130860.D
 Acq On : 29 Oct 2022 16:46
 Operator : CG\JU
 Sample : N5284-04
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MH-3-WC

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-BF102722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130860.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.269	24	31	37	rVB	1169126	1500827	96.82%	11.938%
2	5.169	519	524	535	rVB	369696	398440	25.70%	3.169%
3	5.557	585	590	593	rBV	1661629	1456624	93.97%	11.587%
4	6.557	755	760	763	rBV	1638662	1492770	96.30%	11.874%
5	6.945	822	826	829	rVB	624915	514789	33.21%	4.095%
6	7.504	916	921	924	rBV	1124840	931094	60.07%	7.406%
7	8.228	1040	1044	1047	rBV	772976	594386	38.35%	4.728%
8	9.304	1223	1227	1230	rBV	2047170	1550088	100.00%	12.330%
9	9.986	1339	1343	1347	rVB	694386	544244	35.11%	4.329%
10	10.775	1473	1477	1480	rBV	872368	678003	43.74%	5.393%
11	11.480	1593	1597	1600	rBV	556538	478862	30.89%	3.809%
12	11.992	1679	1684	1689	rBV4	33153	38527	2.49%	0.306%
13	12.575	1778	1783	1788	rBV3	39743	50579	3.26%	0.402%
14	12.692	1800	1803	1807	rBV	28637	27828	1.80%	0.221%
15	12.792	1815	1820	1822	rBV5	12965	20327	1.31%	0.162%
16	12.922	1837	1842	1849	rBV3	34631	74002	4.77%	0.589%
17	13.069	1863	1867	1870	rBV	1528131	1239472	79.96%	9.859%
18	14.122	2043	2046	2049	rBV	460553	422982	27.29%	3.365%
19	14.221	2059	2063	2067	rBV	172183	179565	11.58%	1.428%
20	14.898	2175	2178	2179	rBV	48242	53617	3.46%	0.426%
21	15.639	2300	2304	2308	rBV2	244064	324501	20.93%	2.581%

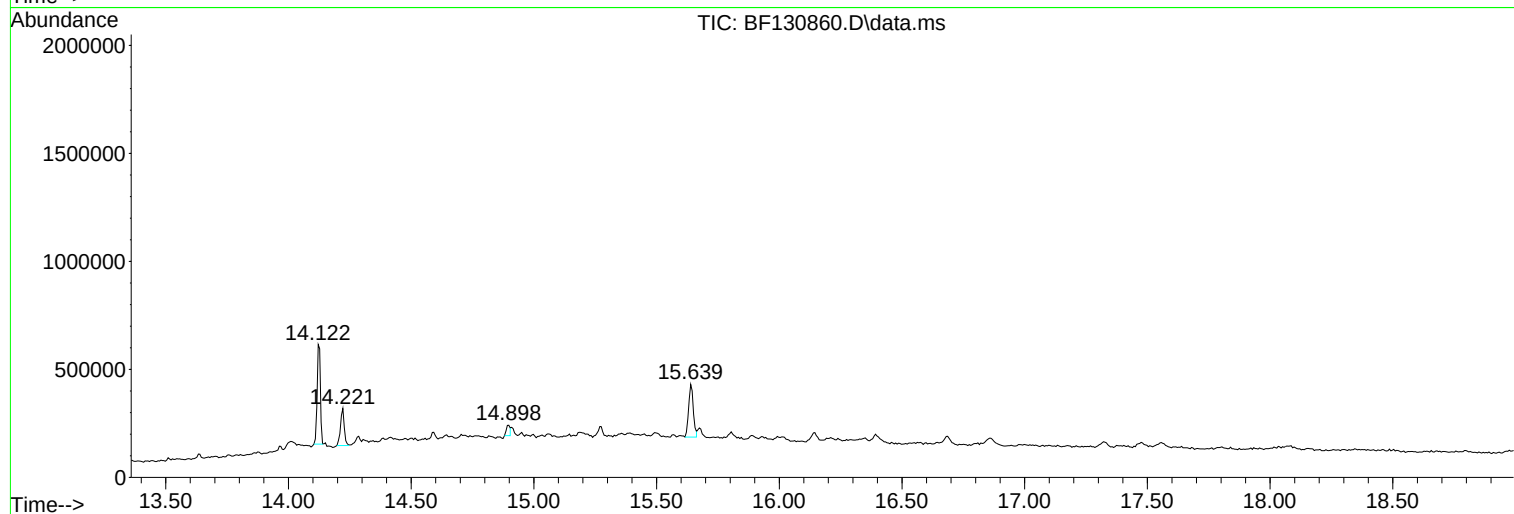
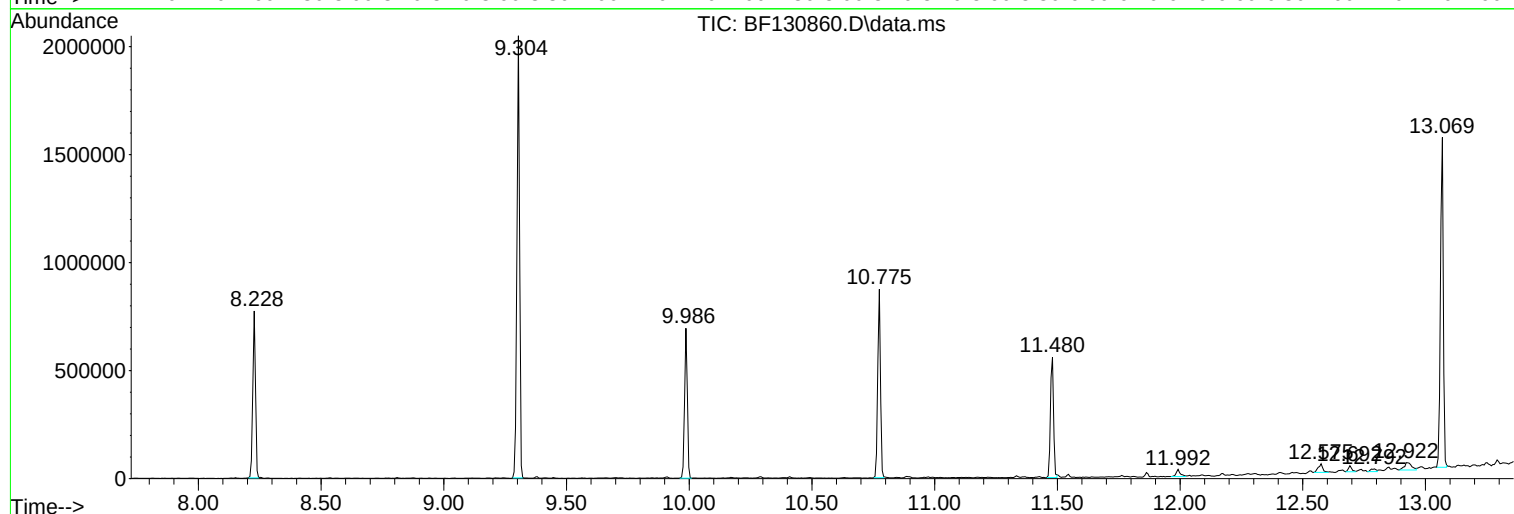
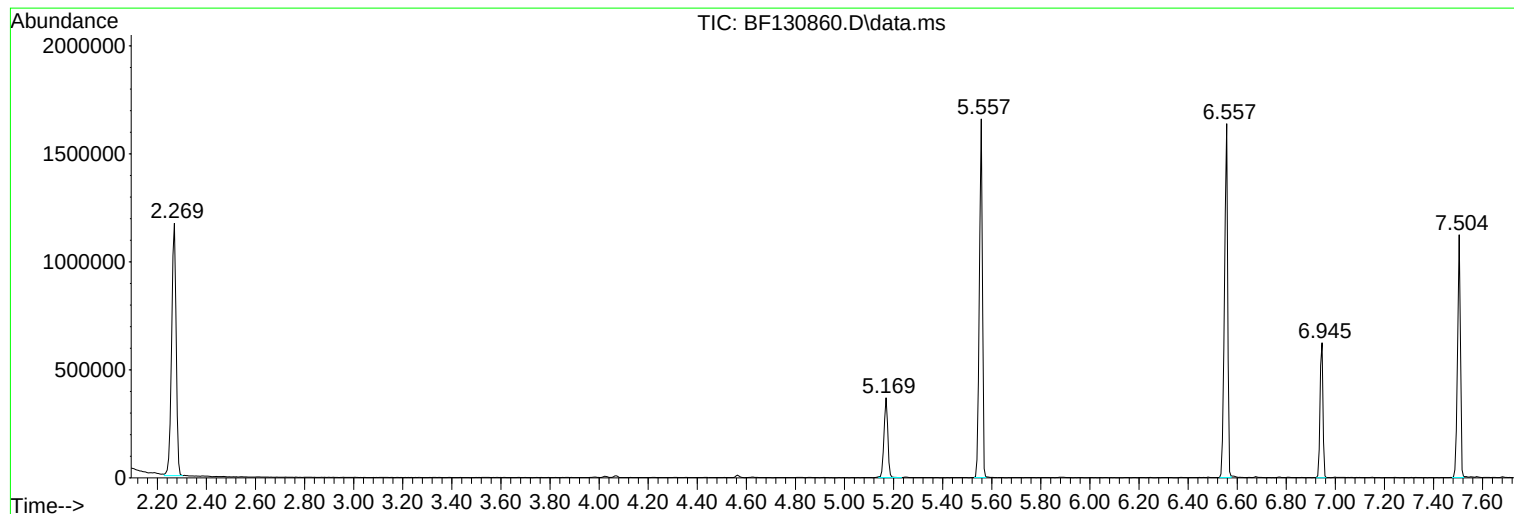
Sum of corrected areas: 12571527

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102922\
Data File : BF130860.D
Acq On : 29 Oct 2022 16:46
Operator : CG\JU
Sample : N5284-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-3-WC

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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\BF102922\
Data File : BF130860.D
Acq On : 29 Oct 2022 16:46
Operator : CG\JU
Sample : N5284-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-3-WC

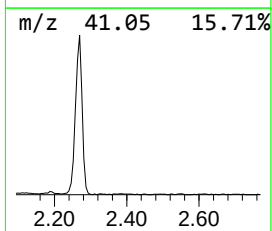
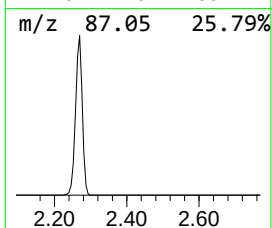
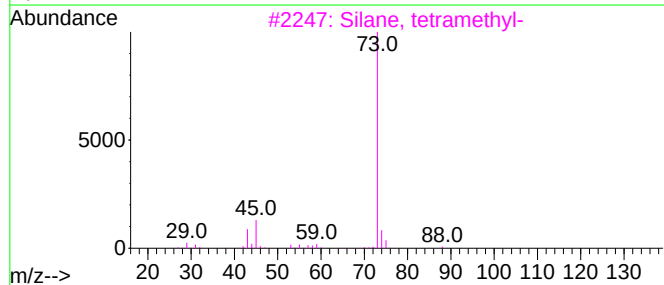
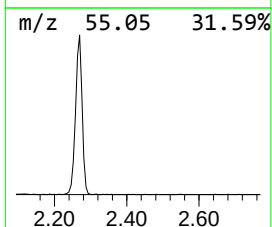
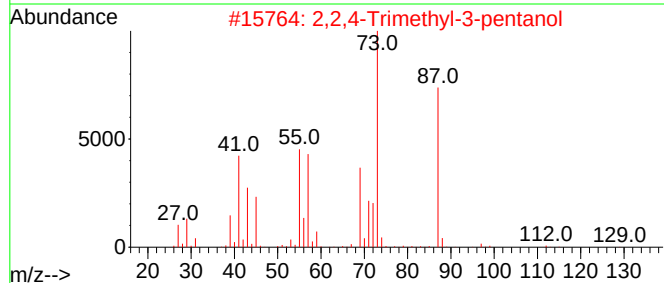
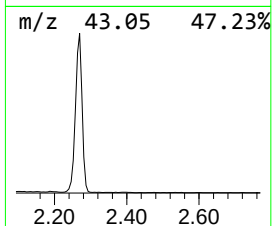
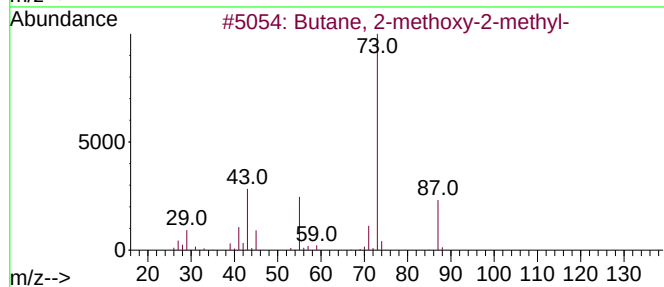
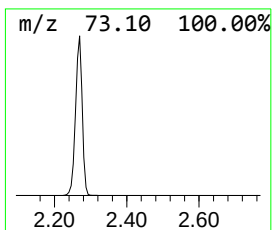
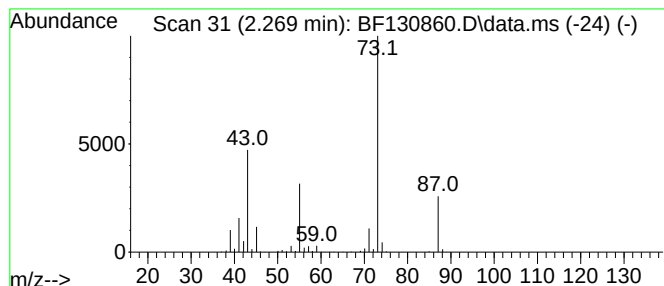
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.269	58.31 ng	1500830	1,4-Dichlorobenzene-d4	6.945

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	39
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
5			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102922\
Data File : BF130860.D
Acq On : 29 Oct 2022 16:46
Operator : CG\JU
Sample : N5284-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-3-WC

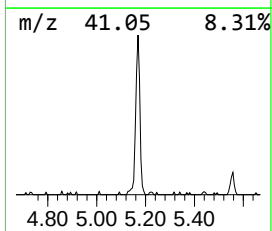
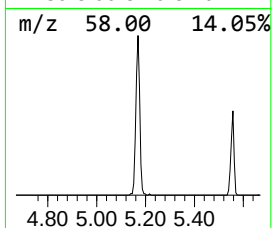
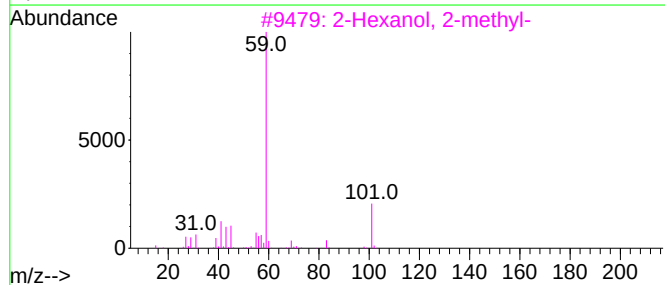
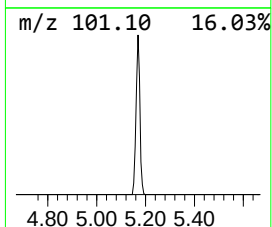
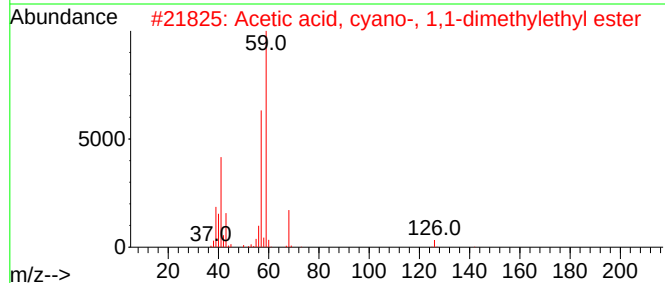
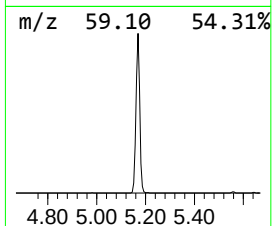
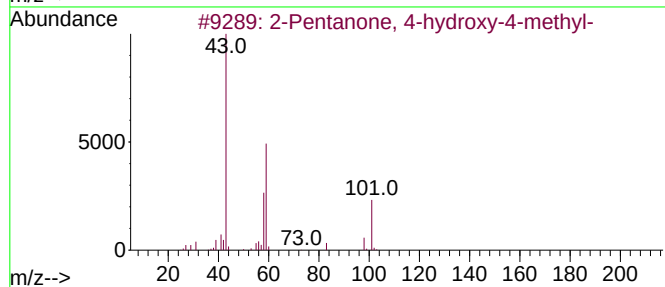
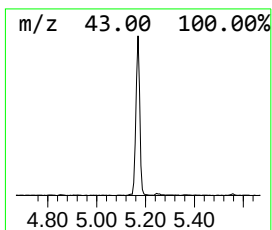
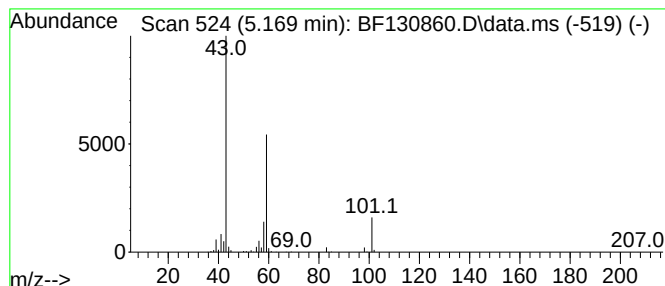
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.169	15.48 ng	398440	1,4-Dichlorobenzene-d4	6.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102922\
Data File : BF130860.D
Acq On : 29 Oct 2022 16:46
Operator : CG\JU
Sample : N5284-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-3-WC

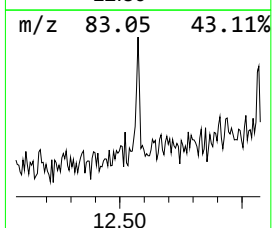
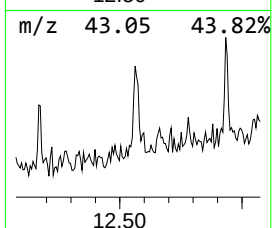
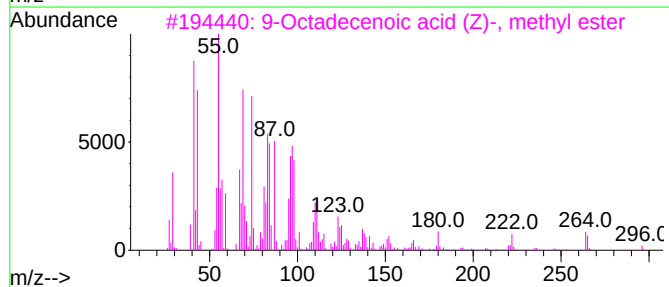
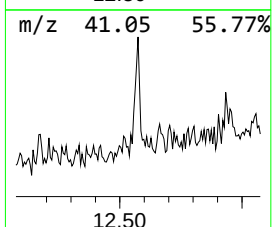
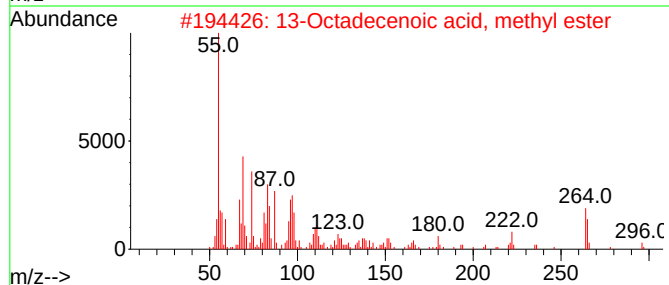
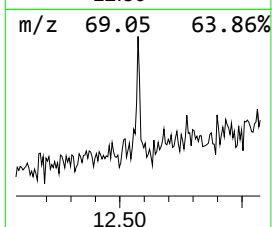
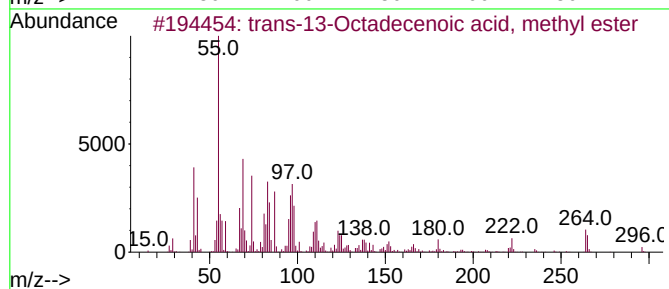
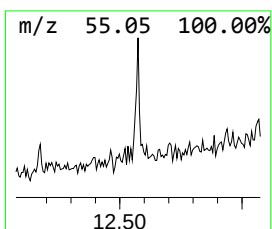
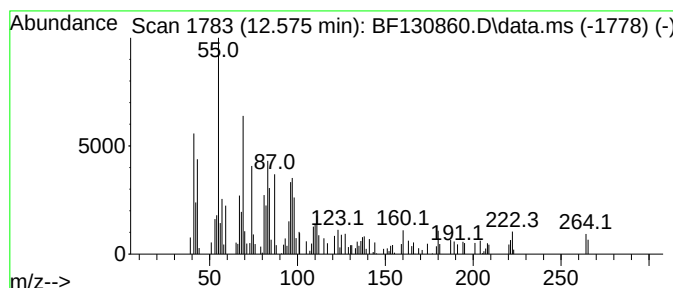
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 trans-13-Octadecenoic acid,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.575	2.11 ng	50579	Phenanthrene-d10	11.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	87
2			13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	87
3			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	87
4			9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	60
5			9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102922\
Data File : BF130860.D
Acq On : 29 Oct 2022 16:46
Operator : CG\JU
Sample : N5284-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-3-WC

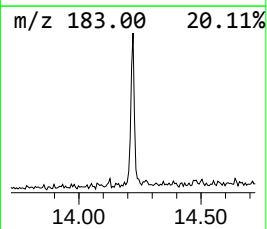
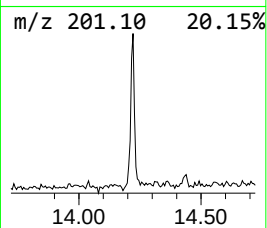
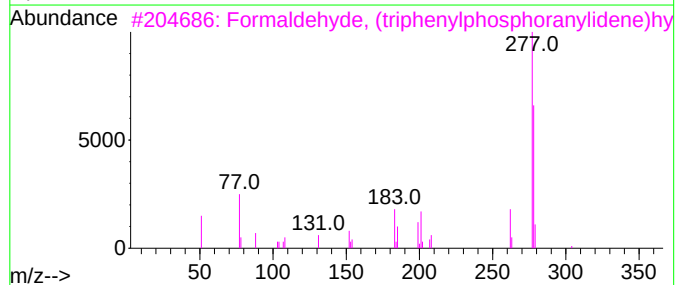
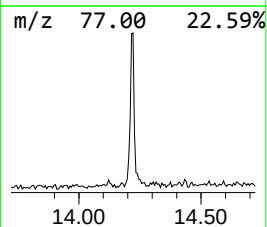
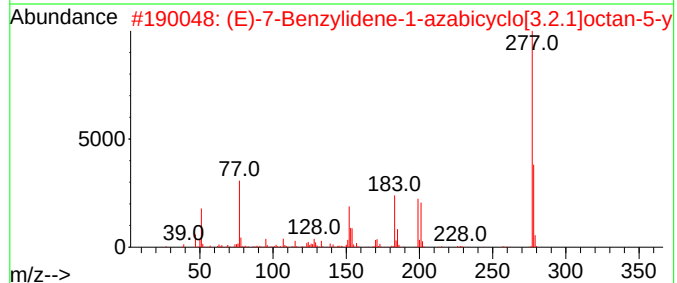
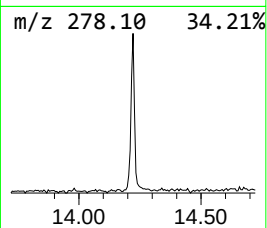
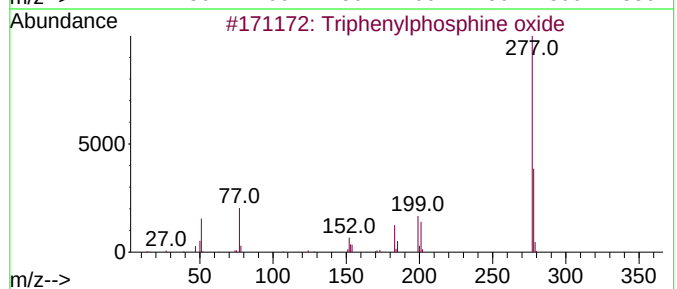
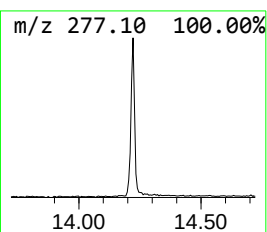
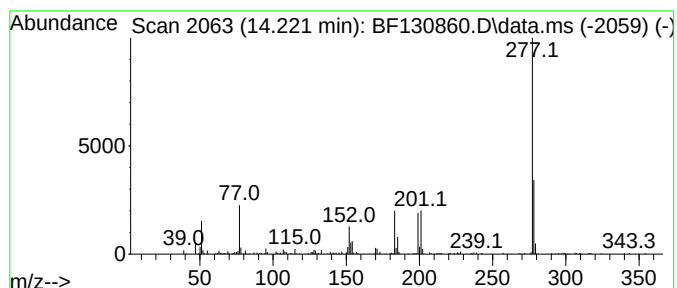
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.222	8.49 ng	179565	Chrysene-d12	14.127

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	94
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	90
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	45
4			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	38
5			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	23



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102922\
Data File : BF130860.D
Acq On : 29 Oct 2022 16:46
Operator : CG\JU
Sample : N5284-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-3-WC

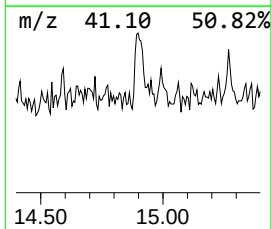
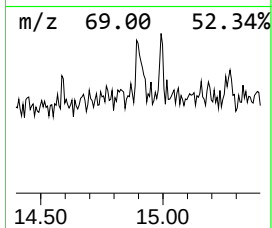
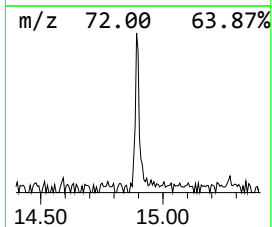
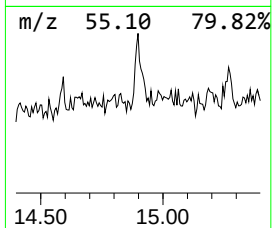
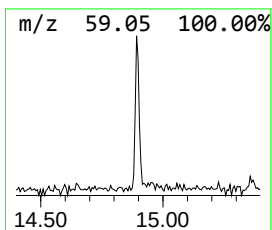
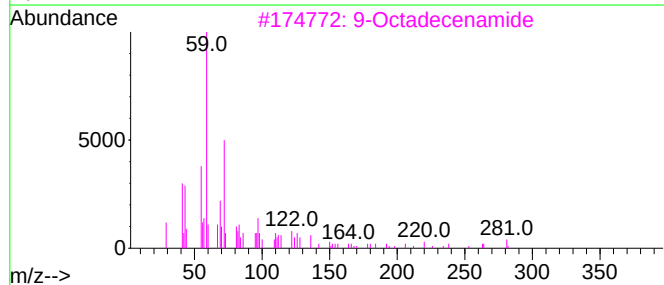
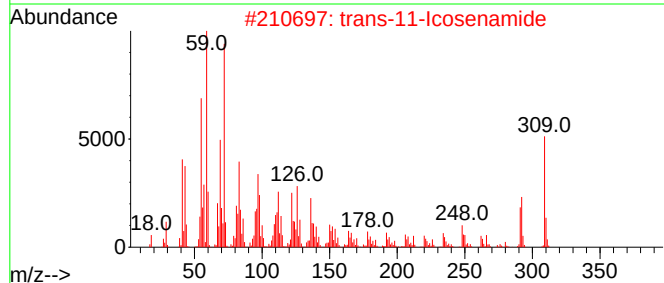
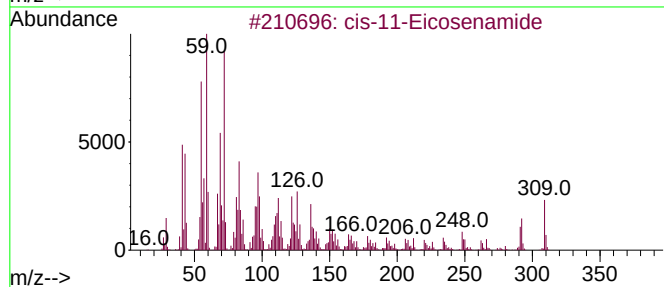
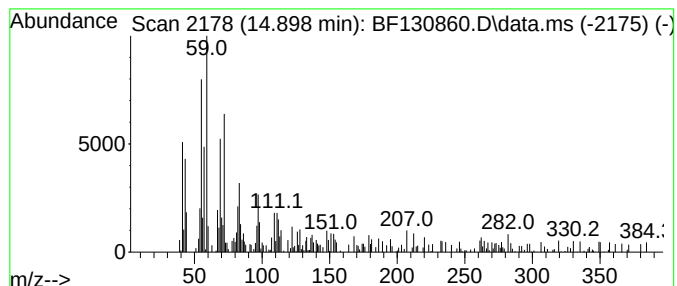
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 cis-11-Eicosenamide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.898	3.30 ng	53617	Perylene-d12	15.639

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-11-Eicosenamide	309	C20H39NO	010436-08-5	81
2			trans-11-Icosenamide	309	C20H39NO	010586-57-9	72
3			9-Octadecenamide	281	C18H35NO	003322-62-1	59
4			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	59
5			Decanamide-	171	C10H21NO	002319-29-1	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102922\
Data File : BF130860.D
Acq On : 29 Oct 2022 16:46
Operator : CG\JU
Sample : N5284-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-3-WC

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.269	58.3	ng	1500830	1	6.945	514789	20.0
2-Pentanone, 4-...	5.169	15.5	ng	398440	1	6.945	514789	20.0
trans-13-Octade...	12.575	2.1	ng	50579	4	11.480	478862	20.0
Triphenylphosph...	14.222	8.5	ng	179565	5	14.127	422982	20.0
cis-11-Eicosena...	14.898	3.3	ng	53617	6	15.639	324501	20.0