

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112822\
 Data File : BF131448.D
 Acq On : 29 Nov 2022 01:17
 Operator : CG\JU
 Sample : N5772-04 2X
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 LOCATION-4

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-BF112122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131448.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.222	19	23	29	rVB	167094	208374	21.43%	2.340%
2	4.046	329	333	336	rVB	10566	11367	1.17%	0.128%
3	5.163	519	523	531	rBV	151950	146533	15.07%	1.646%
4	5.563	587	591	594	rBV	1074661	937933	96.45%	10.534%
5	6.569	758	762	765	rBV	1100201	972503	100.00%	10.922%
6	6.598	765	767	775	rVB	169844	141987	14.60%	1.595%
7	6.957	824	828	831	rBV	929966	742081	76.31%	8.334%
8	7.516	919	923	926	rBV	622754	478541	49.21%	5.374%
9	8.245	1043	1047	1050	rBV	686348	523682	53.85%	5.881%
10	9.322	1227	1230	1233	rBV	821367	622993	64.06%	6.997%
11	9.869	1320	1323	1327	rBV	48518	37792	3.89%	0.424%
12	10.010	1343	1347	1351	rBV	681411	542350	55.77%	6.091%
13	10.798	1478	1481	1485	rBV	518966	452873	46.57%	5.086%
14	10.922	1498	1502	1506	rBV7	15523	25773	2.65%	0.289%
15	11.022	1517	1519	1520	rBV2	13784	11129	1.14%	0.125%
16	11.192	1547	1548	1552	rBV4	13161	16308	1.68%	0.183%
17	11.251	1557	1558	1560	rBV2	13694	11016	1.13%	0.124%
18	11.310	1565	1568	1569	rBV2	12393	13946	1.43%	0.157%
19	11.328	1569	1571	1573	rVV3	15381	12933	1.33%	0.145%
20	11.404	1583	1584	1589	rVB5	22687	22762	2.34%	0.256%
21	11.510	1598	1602	1604	rBV	696677	580136	59.65%	6.515%
22	11.533	1604	1606	1610	rVV	73435	61017	6.27%	0.685%
23	11.581	1612	1614	1617	rVB	22203	19411	2.00%	0.218%
24	12.010	1685	1687	1690	rBV2	17422	18434	1.90%	0.207%
25	12.039	1690	1692	1695	rVB	29992	24437	2.51%	0.274%
26	12.122	1704	1706	1709	rBV3	31042	34602	3.56%	0.389%
27	12.563	1779	1781	1784	rVB	28793	22483	2.31%	0.252%
28	12.727	1806	1809	1813	rBV	188658	161922	16.65%	1.818%
29	12.963	1846	1849	1855	rVB	183443	176406	18.14%	1.981%
30	13.104	1869	1873	1877	rVB	570653	503998	51.82%	5.660%
31	14.169	2050	2054	2057	rBV2	543939	538375	55.36%	6.046%
32	15.710	2313	2316	2321	rBV	218245	279683	28.76%	3.141%
33	17.480	2615	2617	2621	rVB3	90054	81178	8.35%	0.912%
34	17.851	2678	2680	2683	rBV3	88540	79205	8.14%	0.890%
35	18.515	2791	2793	2797	rBV4	104357	131060	13.48%	1.472%
36	18.633	2811	2813	2818	rBV5	98481	83162	8.55%	0.934%

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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-BF112122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	18.751	2829	2833	2834	rBV3	108122	175860	18.08%	1.975%
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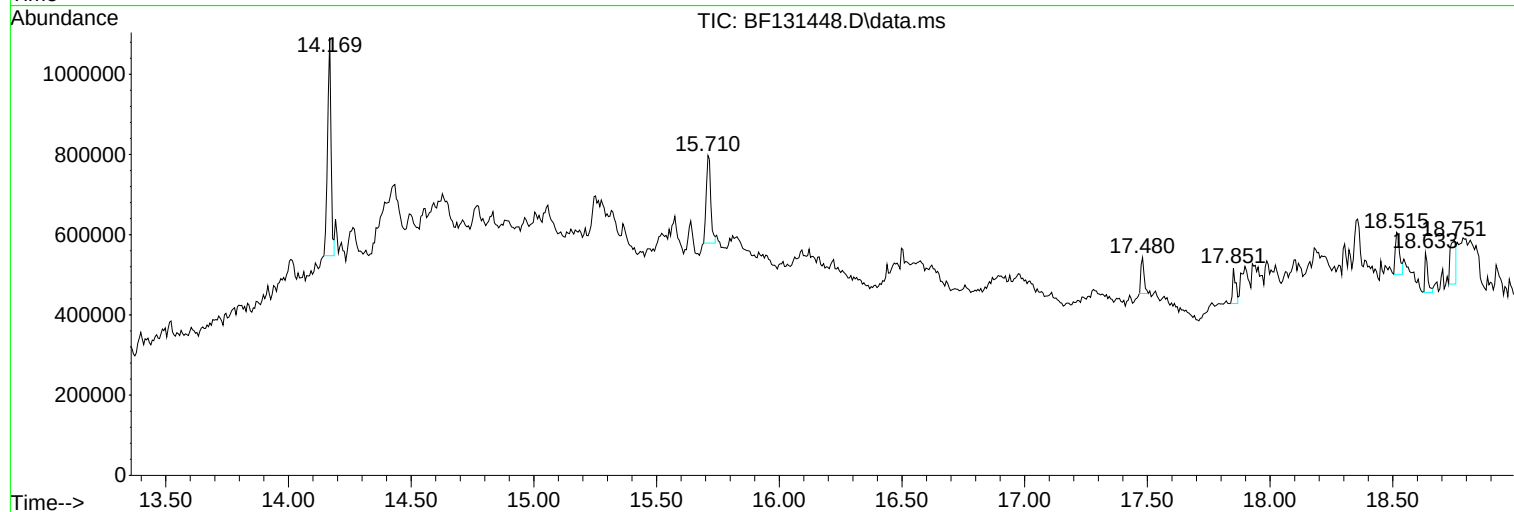
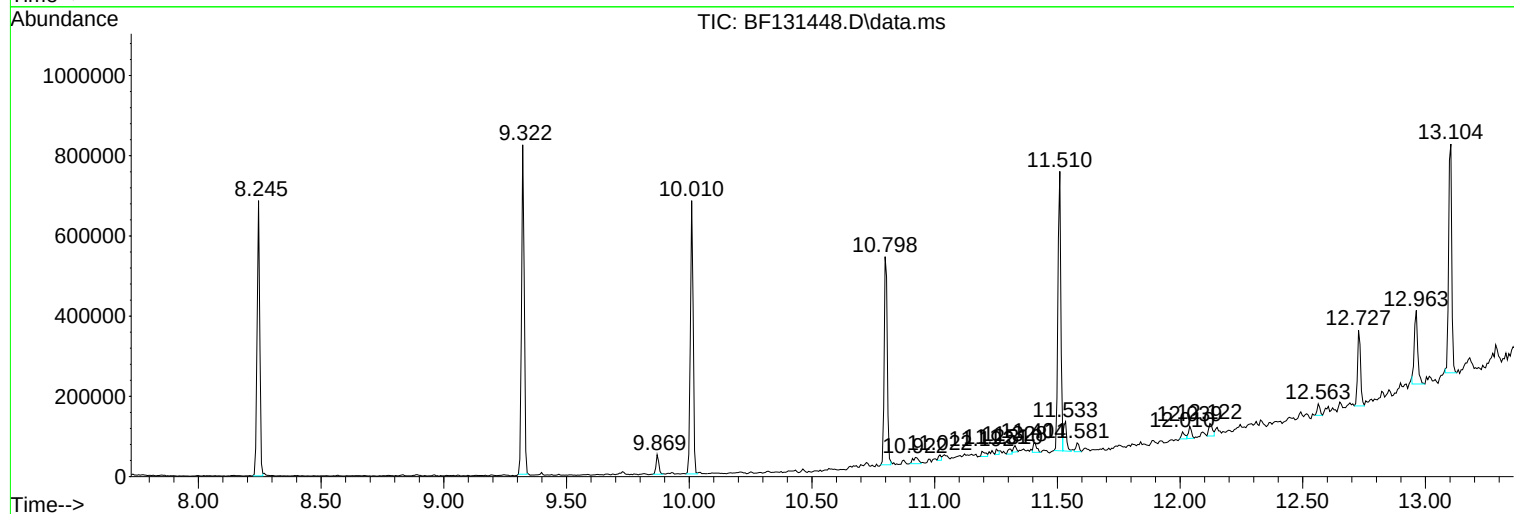
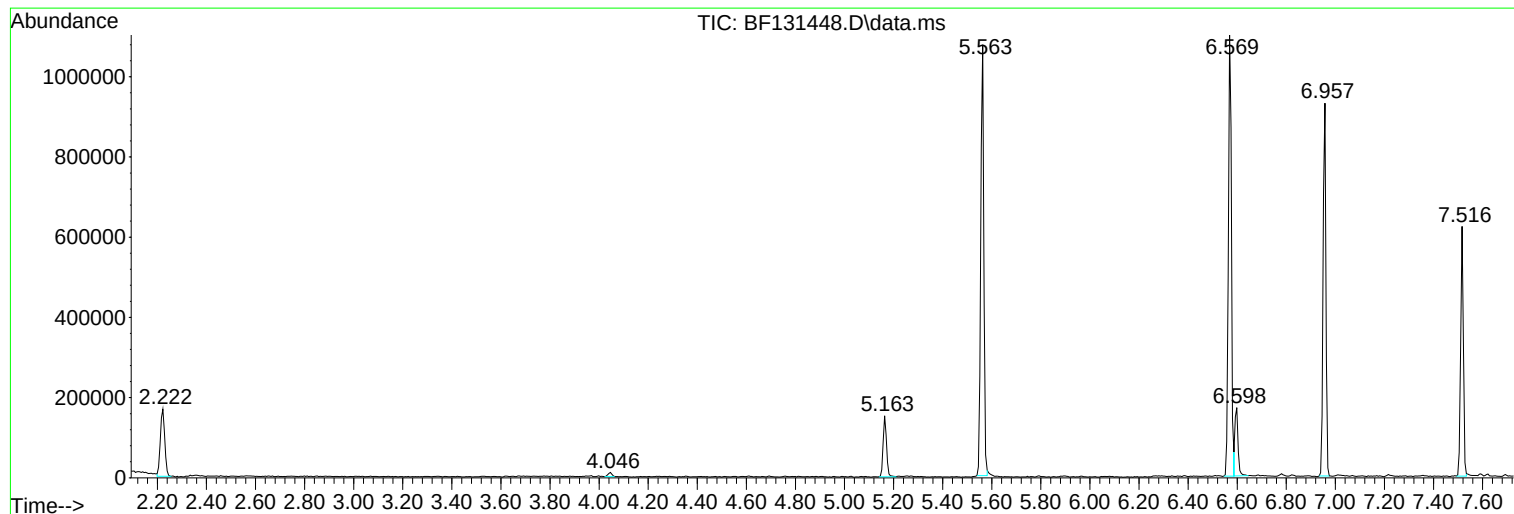
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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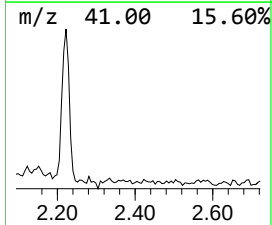
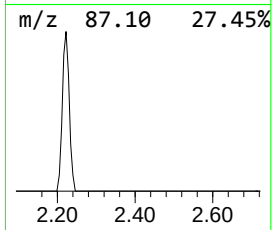
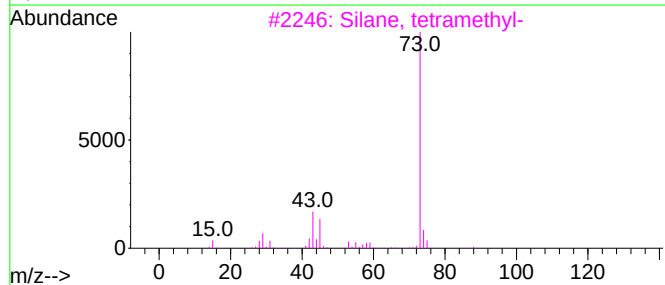
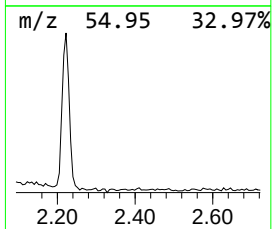
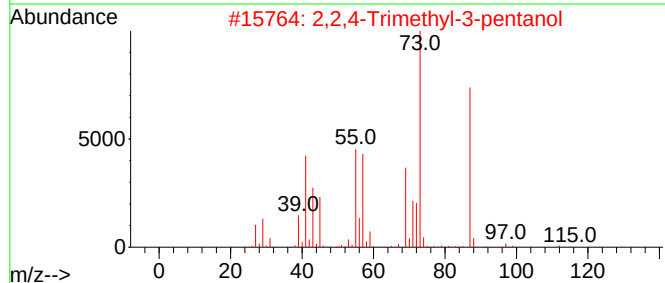
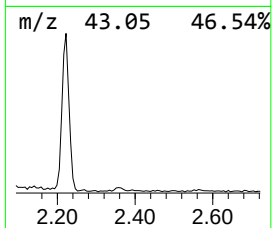
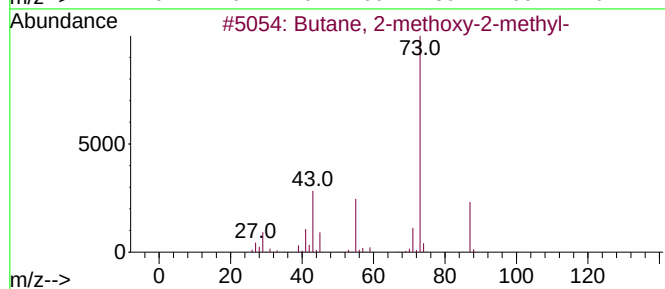
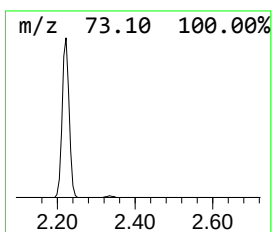
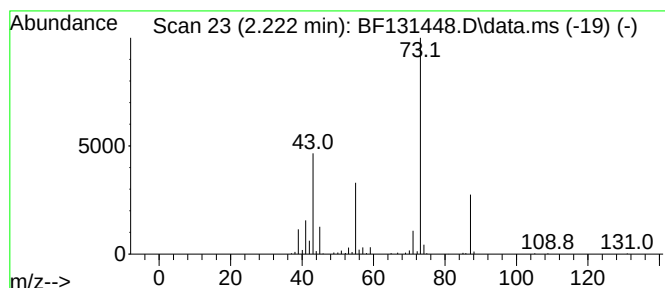
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.222	5.62 ng	208374	1,4-Dichlorobenzene-d4	6.957

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			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	38
5			Butanoic acid, 2-hydroxy-2-methy...	132	C6H12O3	032793-34-3	32



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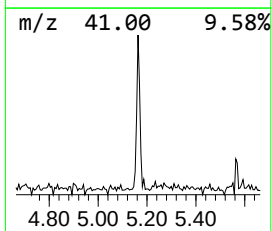
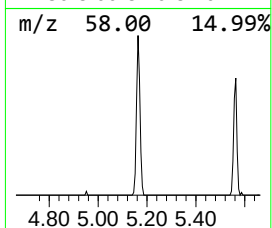
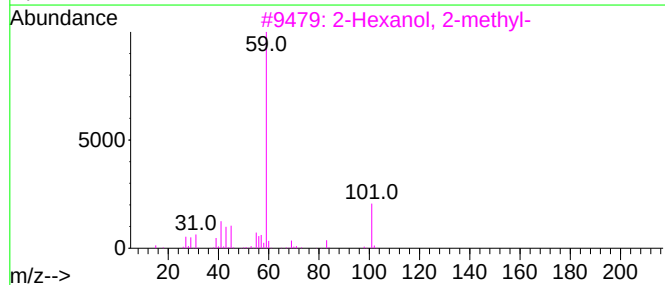
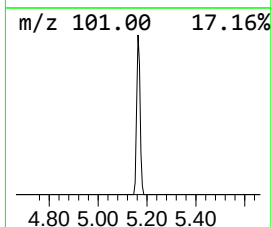
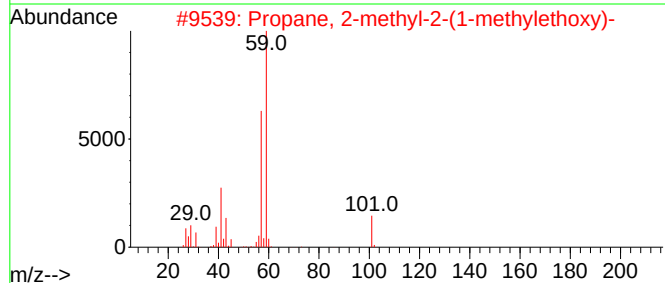
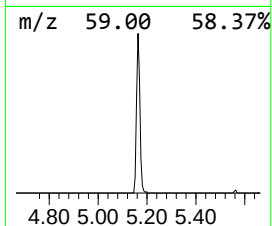
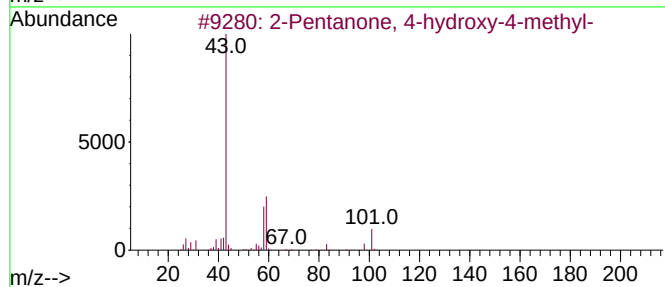
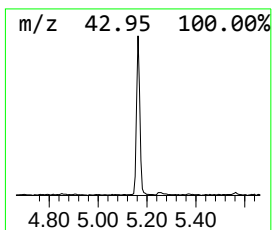
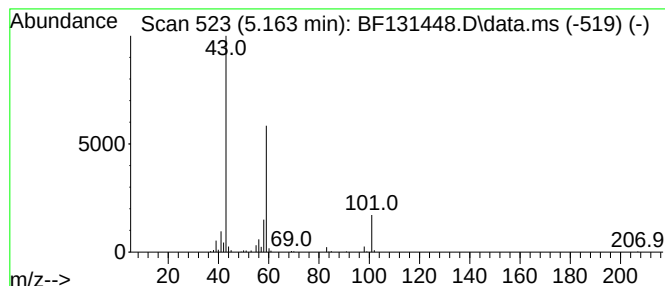
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.163	3.95 ng	146533	1,4-Dichlorobenzene-d4	6.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12



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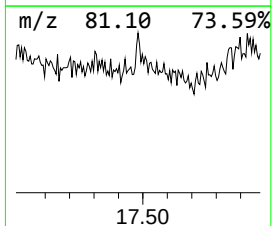
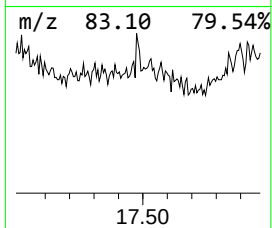
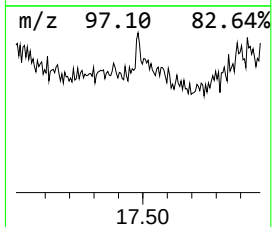
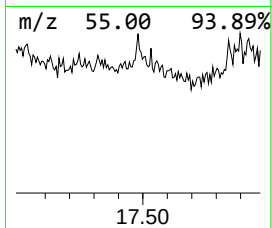
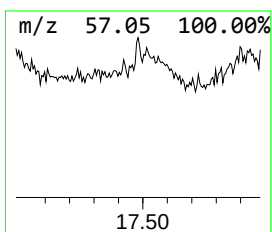
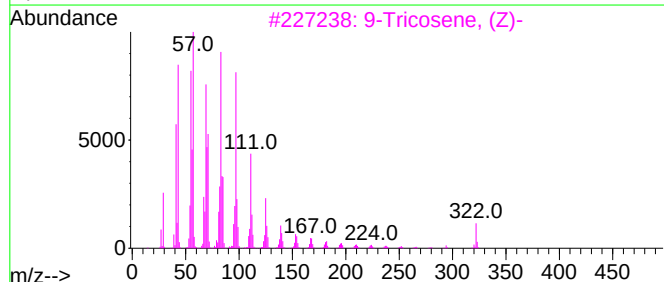
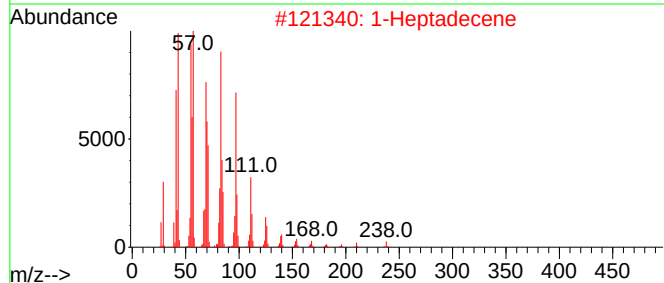
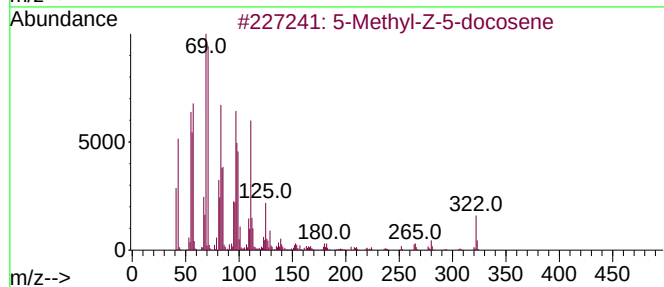
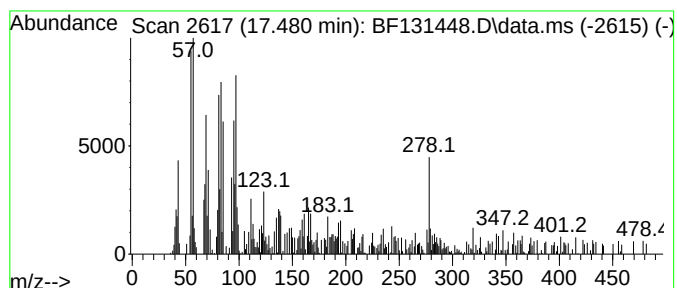
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown17.480 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.480	5.80 ng	81178	Perylene-d12	15.710

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Methyl-Z-5-docosene	322	C23H46	1000131-17-1	46
2			1-Heptadecene	238	C17H34	006765-39-5	46
3			9-Tricosene, (Z)-	322	C23H46	027519-02-4	45
4			Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	43
5			Hexadecanoic acid, 2-hydroxy-, m...	286	C17H34O3	016742-51-1	38



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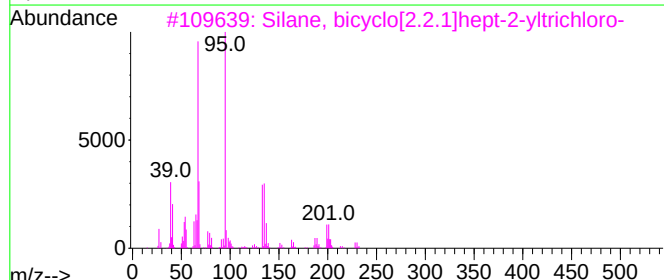
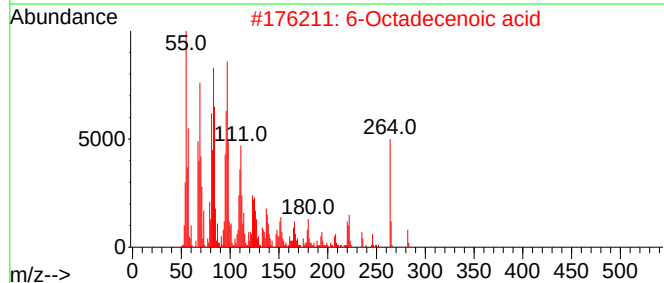
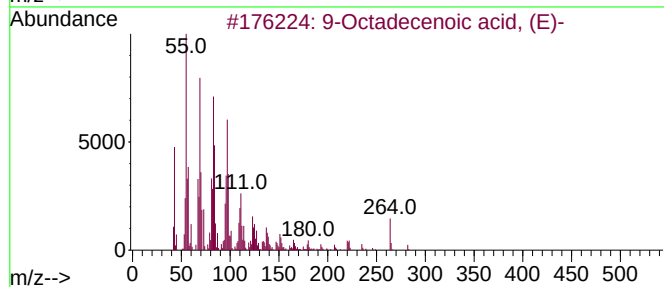
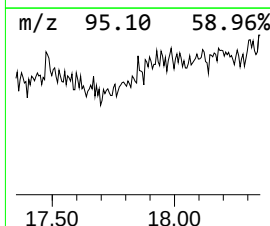
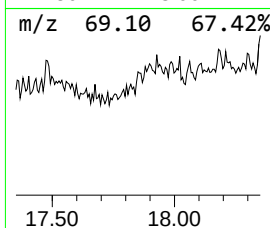
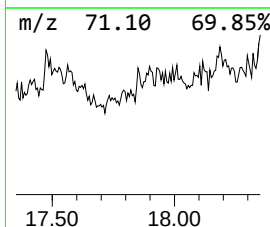
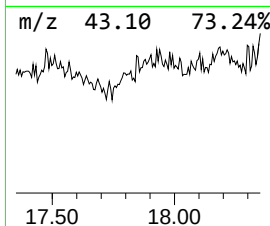
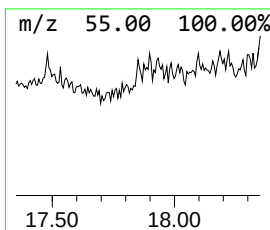
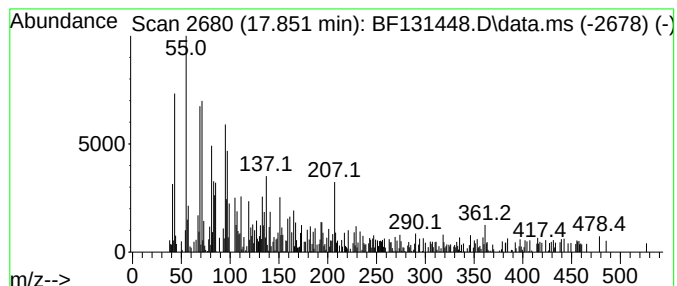
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown17.851 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.851	5.66 ng	79205	Perylene-d12	15.710

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	38
2			6-Octadecenoic acid	282	C18H34O2	1000336-66-8	38
3			Silane, bicyclo[2.2.1]hept-2-ylt...	228	C7H11Cl3Si	018245-29-9	35
4			Spiro[4.5]decan-7-one, 1,8-dimet...	236	C15H24O2	061050-91-7	35
5			Cyclohexane, 1-(cyclohexylmethyl...	194	C14H26	054823-98-2	30



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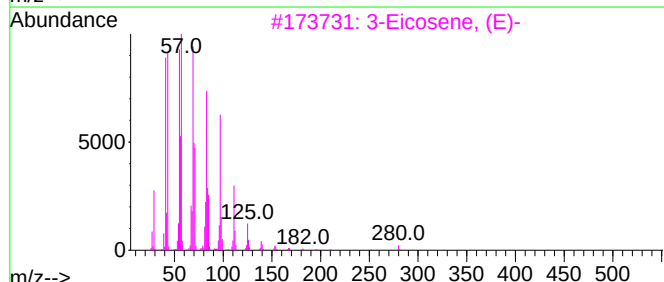
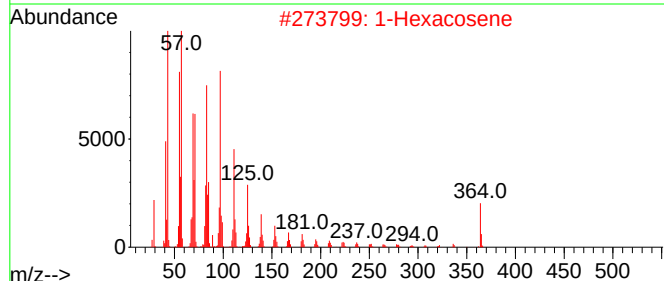
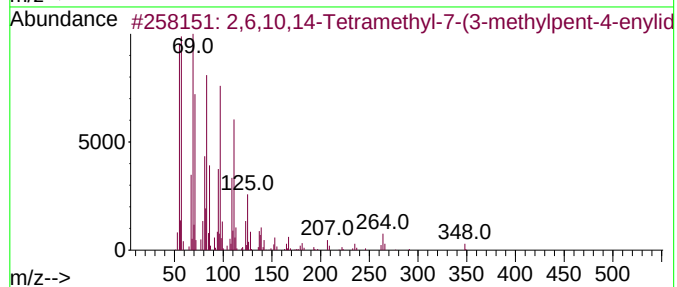
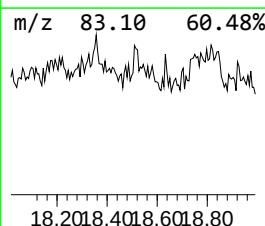
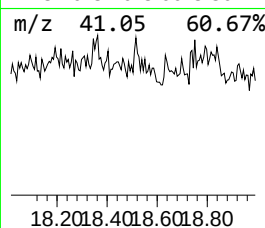
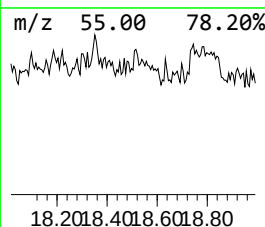
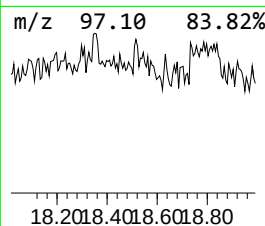
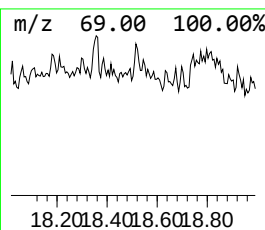
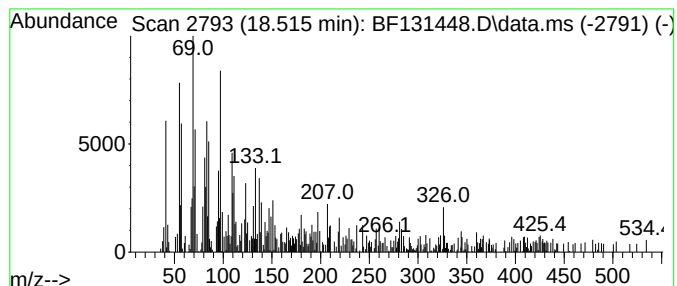
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2,6,10,14-Tetramethyl-7-(3-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.515	9.37 ng	131060	Perylene-d12	15.710

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14-Tetramethyl-7-(3-methy...	348	C25H48	1000370-41-6	53		
2	1-Hexacosene	364	C26H52	018835-33-1	49		
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	49		
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	46		
5	9-Octadecene, (E)-	252	C18H36	007206-25-9	46		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112822\
Data File : BF131448.D
Acq On : 29 Nov 2022 01:17
Operator : CG\JU
Sample : N5772-04 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LOCATION-4

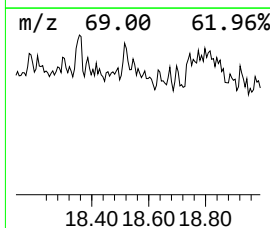
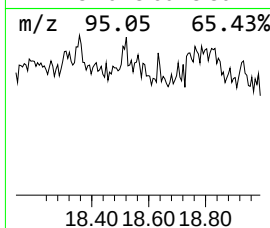
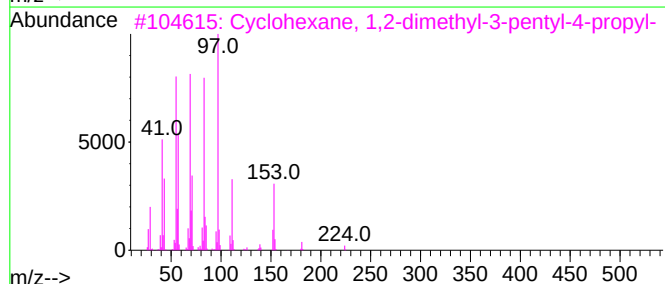
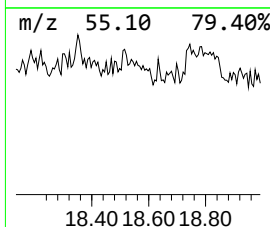
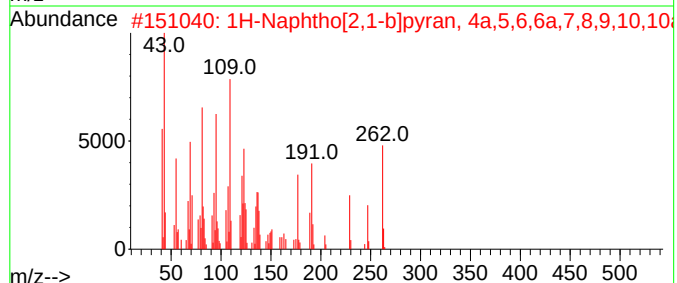
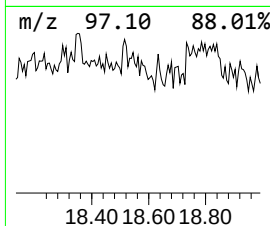
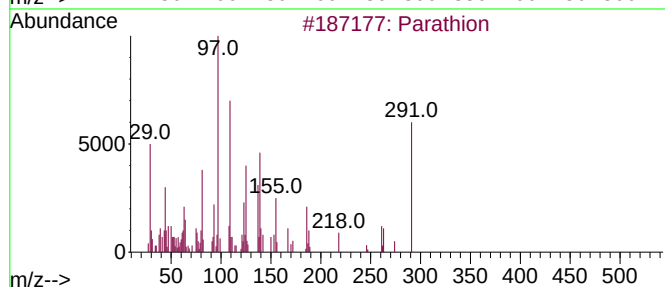
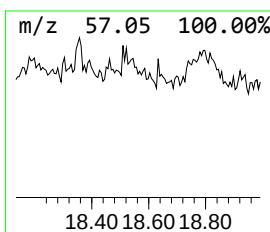
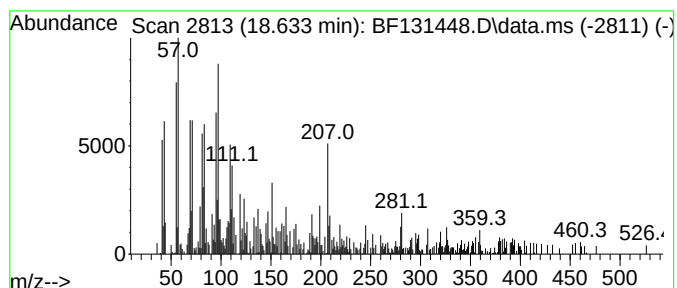
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown18.633 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.633	5.95 ng	83162	Perylene-d12	15.710

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Parathion	291	C10H14NO5PS	000056-38-2	46
2			1H-Naphtho[2,1-b]pyran, 4a,5,6,6...	262	C18H30O	005153-92-4	44
3			Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	42
4			9-Tricosene, (Z)-	322	C23H46	027519-02-4	41
5			W-18	421	C19H20C1N3O4S	093101-02-1	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112822\
Data File : BF131448.D
Acq On : 29 Nov 2022 01:17
Operator : CG\JU
Sample : N5772-04 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

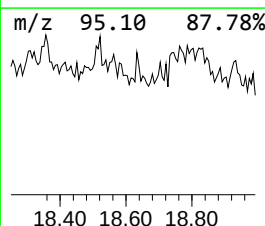
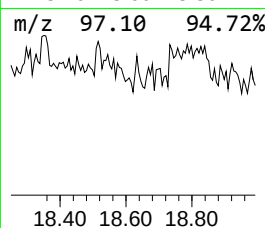
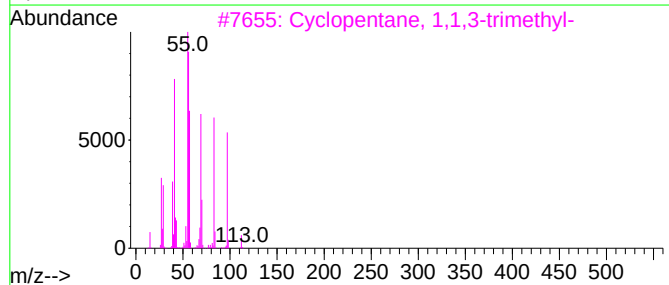
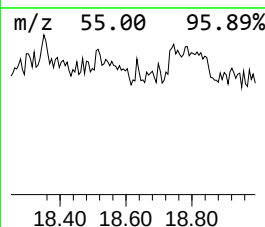
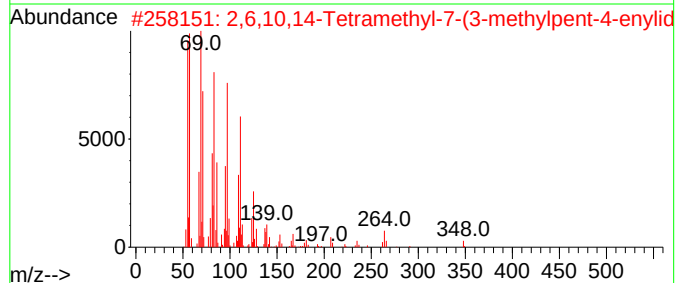
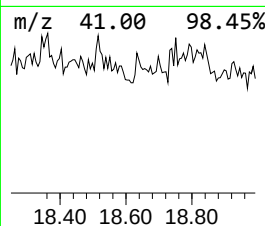
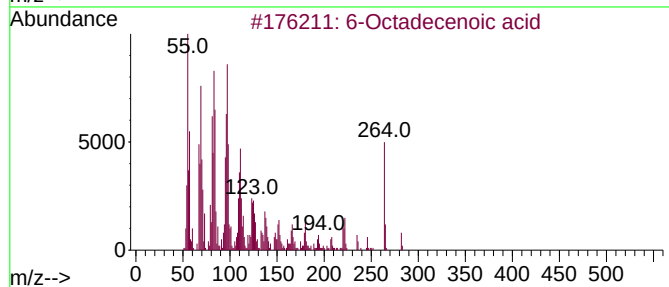
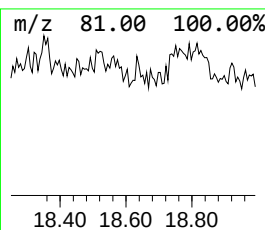
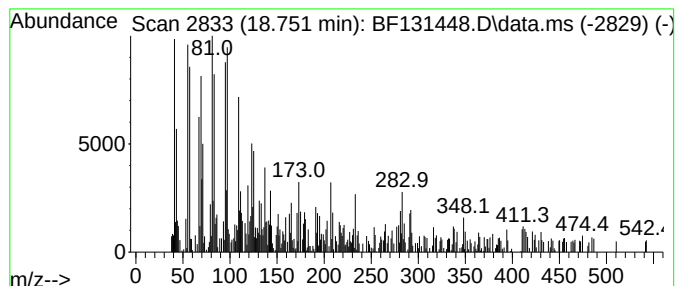
Instrument :
BNA_F
ClientSampleId :
LOCATION-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 6-Octadecenoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.751	12.58 ng	175860	Perylene-d12	15.710	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Octadecenoic acid	282	C18H34O2	1000336-66-8	50
2	2,6,10,14-Tetramethyl-7-(3-methy...	348	C25H48	1000370-41-6	45
3	Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	38
4	Z-12-Pentacosene	350	C25H50	1000131-09-4	38
5	1H-Indene, 5-butyl-6-hexyloctahy...	264	C19H36	055044-36-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112822\
Data File : BF131448.D
Acq On : 29 Nov 2022 01:17
Operator : CG\JU
Sample : N5772-04 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LOCATION-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.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...	2.222	5.6	ng	208374	1	6.957	742081	20.0
2-Pentanone, 4-...	5.163	4.0	ng	146533	1	6.957	742081	20.0
unknown17.480	17.480	5.8	ng	81178	6	15.710	279683	20.0
unknown17.851	17.851	5.7	ng	79205	6	15.710	279683	20.0
2,6,10,14-Tetra...	18.515	9.4	ng	131060	6	15.710	279683	20.0
unknown18.633	18.633	6.0	ng	83162	6	15.710	279683	20.0
6-Octadecenoic ...	18.751	12.6	ng	175860	6	15.710	279683	20.0