

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112522\
 Data File : BF131406.D
 Acq On : 25 Nov 2022 20:51
 Operator : CG\JU
 Sample : N5741-18
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-37

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: BF131406.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.252	22	28	34	rVB	1463036	1902314	67.05%	10.795%
2	3.351	208	215	220	rBV2	22657	38985	1.37%	0.221%
3	5.169	520	524	531	rVB	188632	201637	7.11%	1.144%
4	5.563	586	591	594	rBV	1382280	1246813	43.95%	7.076%
5	6.563	757	761	764	rBV	961641	818944	28.86%	4.647%
6	6.957	824	828	831	rBV	589675	531634	18.74%	3.017%
7	7.481	910	917	919	rBV	55208	65797	2.32%	0.373%
8	7.522	919	924	927	rVB	1704084	1622151	57.17%	9.206%
9	7.804	967	972	977	rVB	31507	32181	1.13%	0.183%
10	8.245	1042	1047	1050	rBV	765401	688887	24.28%	3.909%
11	9.328	1225	1231	1234	rBV	3053653	2837185	100.00%	16.101%
12	9.433	1245	1249	1252	rVB2	29704	31035	1.09%	0.176%
13	10.010	1343	1347	1350	rBV	989649	777487	27.40%	4.412%
14	10.316	1396	1399	1407	rBV	30916	45137	1.59%	0.256%
15	10.727	1465	1469	1472	rBV	167110	129394	4.56%	0.734%
16	10.804	1477	1482	1485	rBV	1981037	1845768	65.06%	10.475%
17	11.504	1597	1601	1605	rBV	935137	777098	27.39%	4.410%
18	12.027	1687	1690	1694	rBV	129016	116105	4.09%	0.659%
19	13.104	1868	1873	1876	rBV	2682518	2356729	83.07%	13.374%
20	13.998	2022	2025	2037	rBV	156393	195253	6.88%	1.108%
21	14.163	2049	2053	2057	rVB	631597	539983	19.03%	3.064%
22	14.263	2065	2070	2077	rVB	87400	95299	3.36%	0.541%
23	14.627	2130	2132	2143	rVB4	18618	30238	1.07%	0.172%
24	15.321	2246	2250	2254	rVB2	28789	31699	1.12%	0.180%
25	15.698	2309	2314	2318	rBV	360623	475376	16.76%	2.698%
26	15.733	2318	2320	2327	rVB3	39914	44810	1.58%	0.254%
27	16.209	2396	2401	2406	rVB	30571	48789	1.72%	0.277%
28	16.756	2490	2494	2501	rVB2	29549	54578	1.92%	0.310%
29	17.409	2600	2605	2612	rVB4	18818	40089	1.41%	0.228%

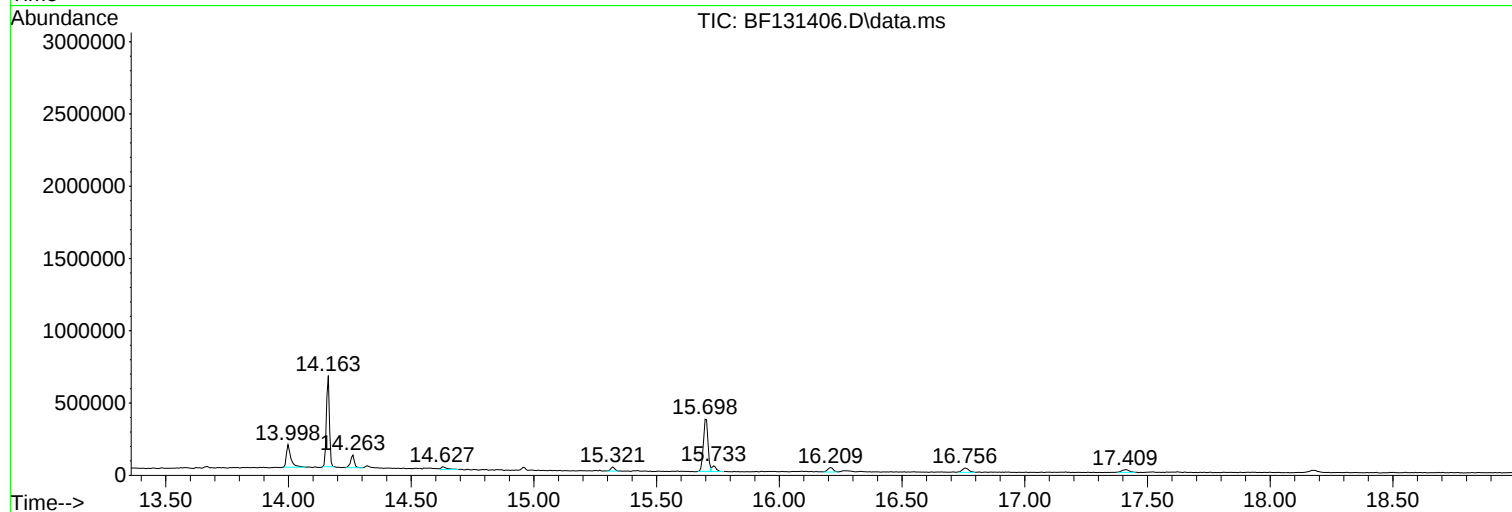
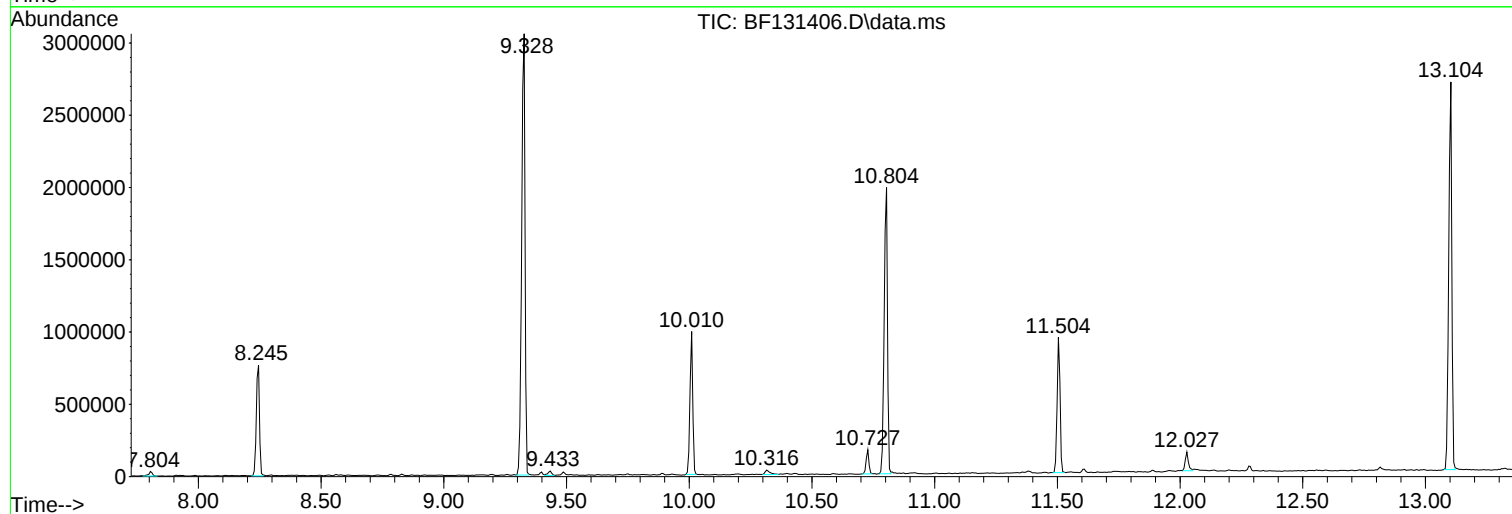
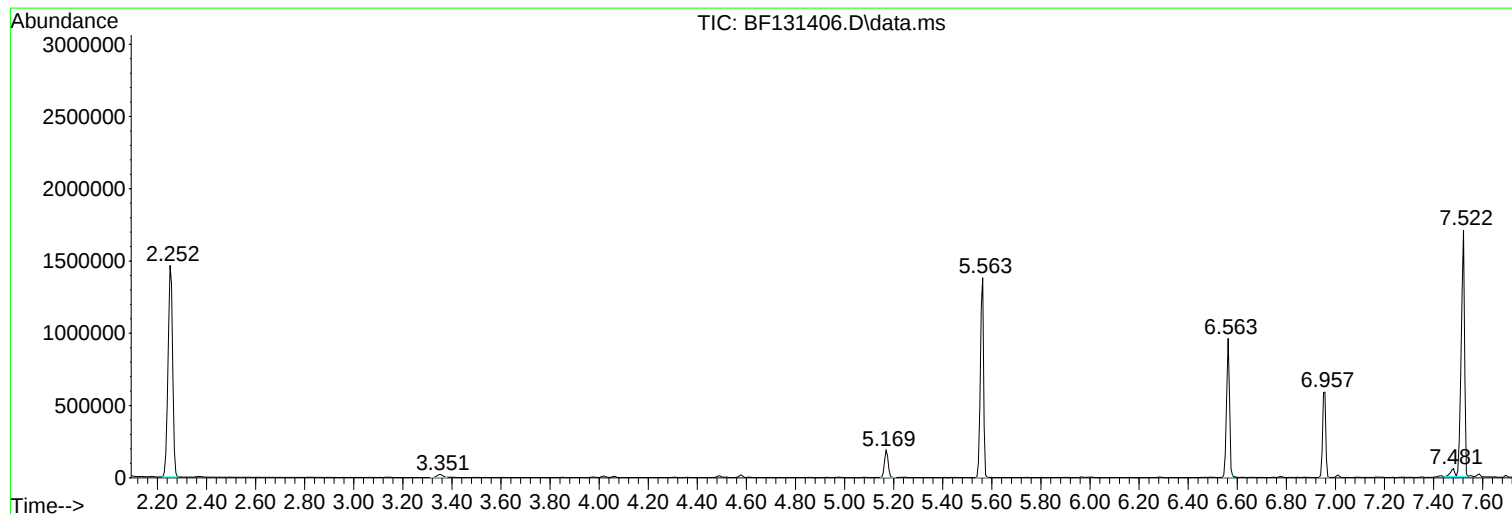
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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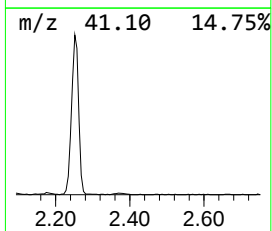
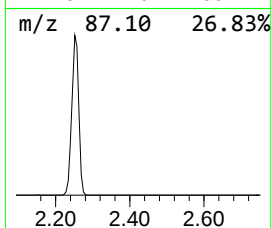
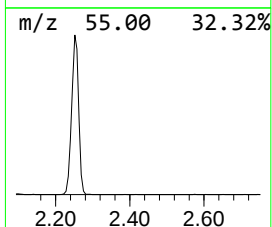
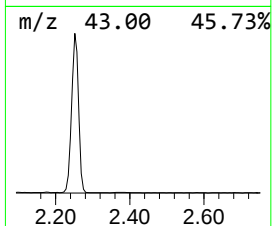
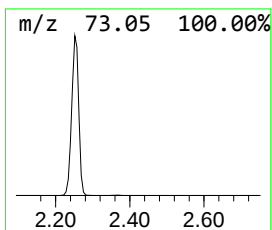
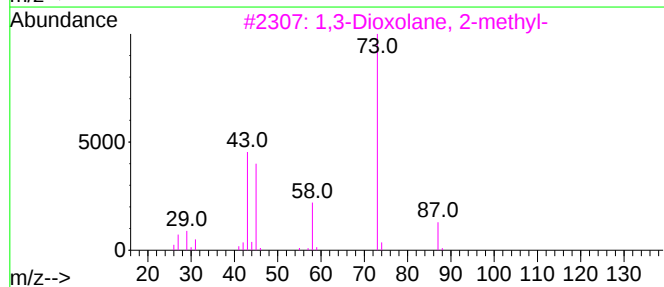
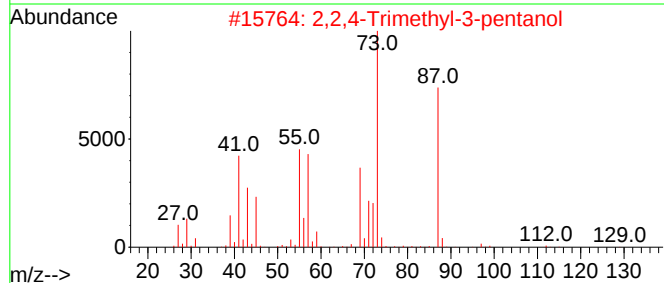
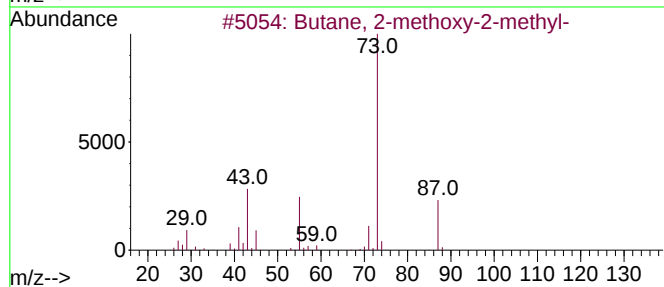
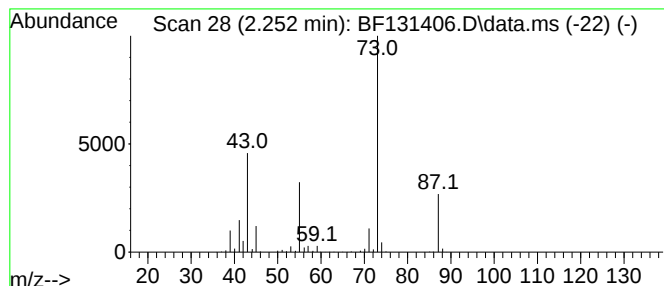
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.252	71.56 ng	1902310	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	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12



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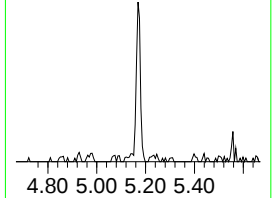
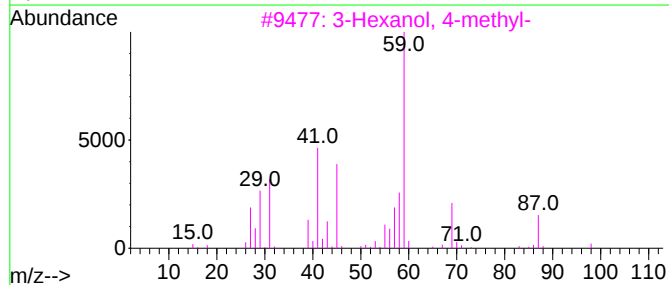
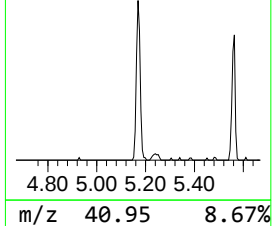
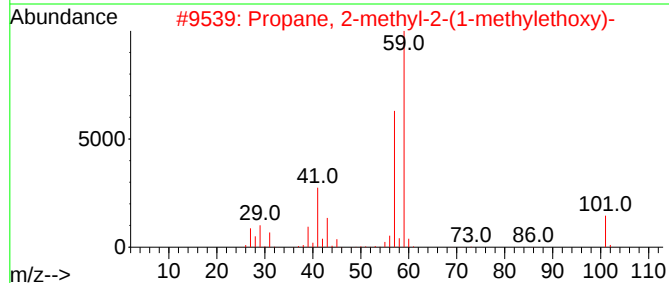
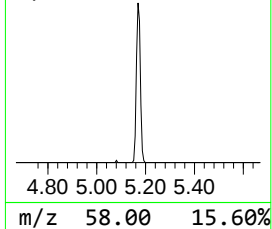
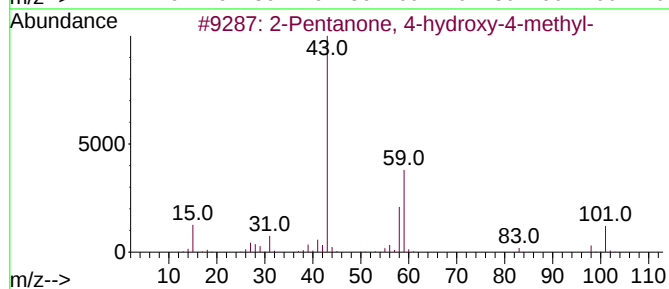
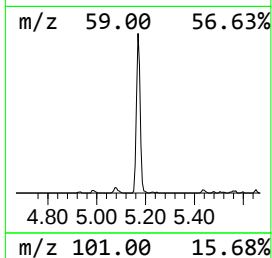
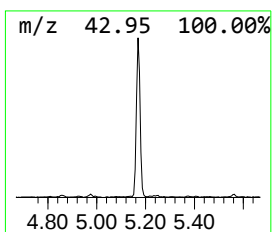
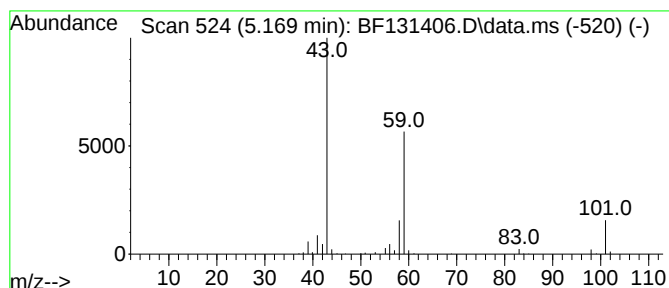
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.169	7.59 ng	201637	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			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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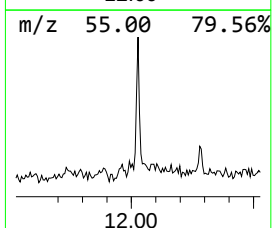
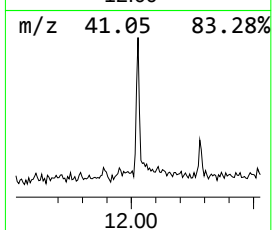
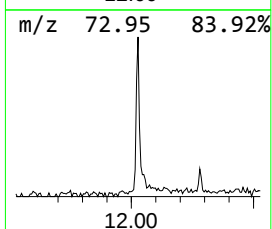
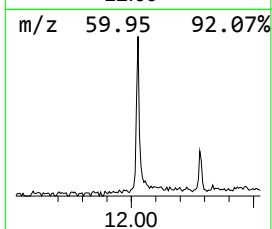
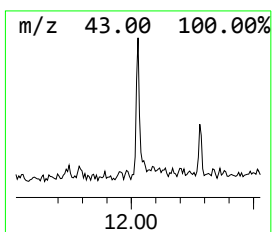
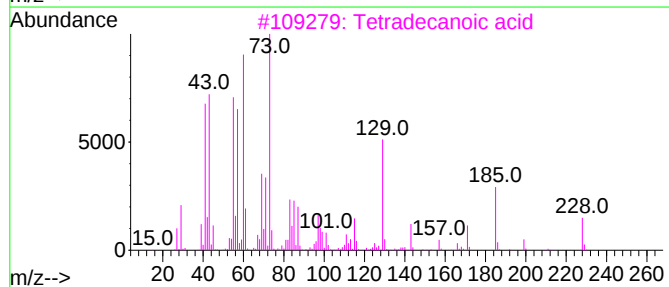
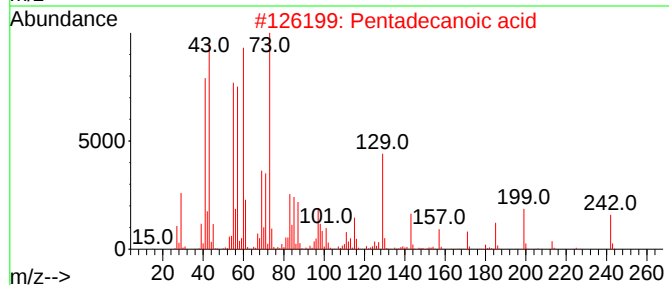
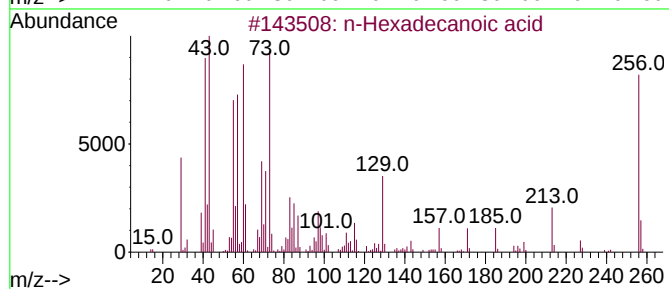
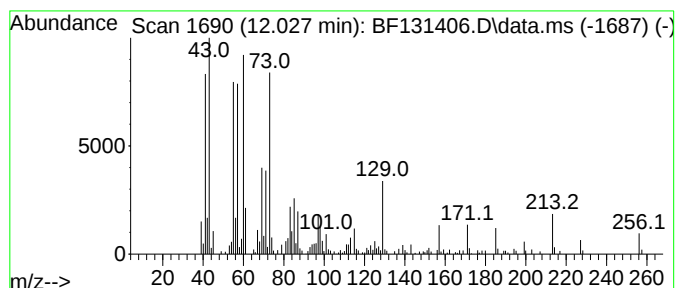
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.027	2.99 ng	116105	Phenanthrene-d10	11.504	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Tridecanoic acid	214	C13H26O2	000638-53-9	52
5	.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	18



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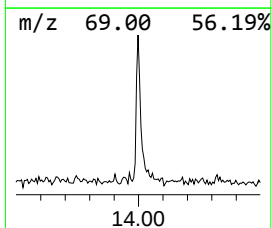
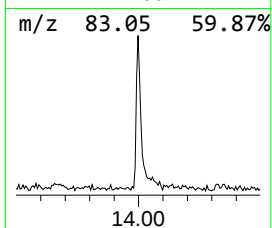
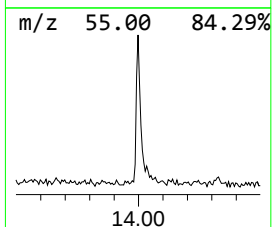
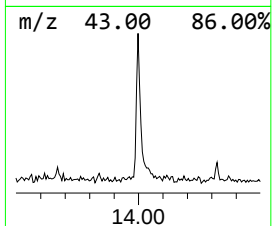
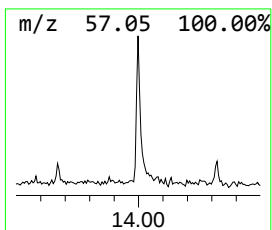
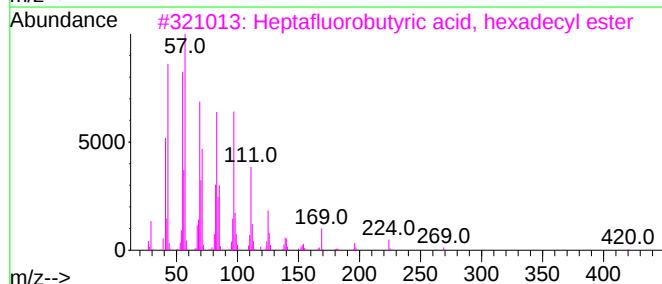
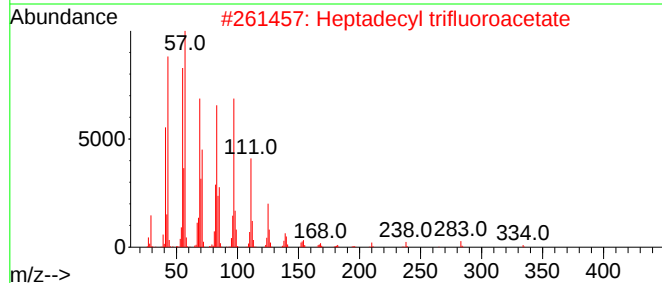
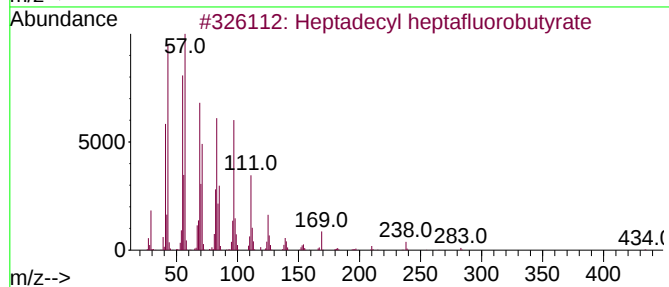
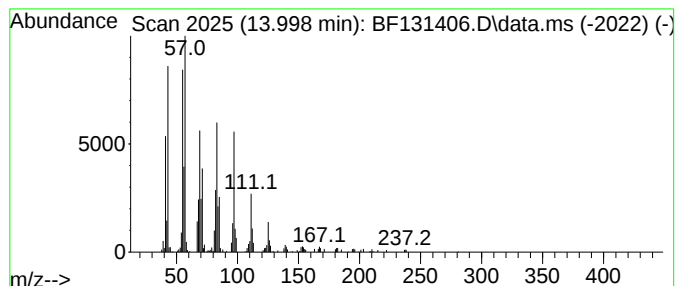
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Peak Number 4 Heptadecyl heptafluorobutyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.998	7.23 ng	195253	Chrysene-d12	14.163	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
3	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
4	Octacosanol	410	C28H58O	000557-61-9	91
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	91



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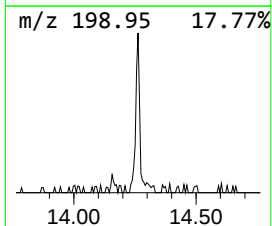
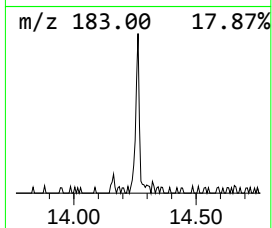
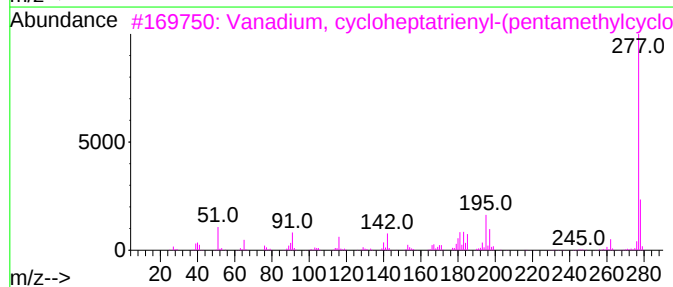
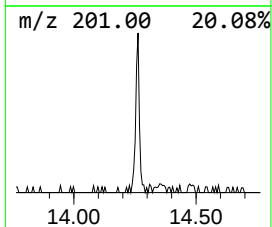
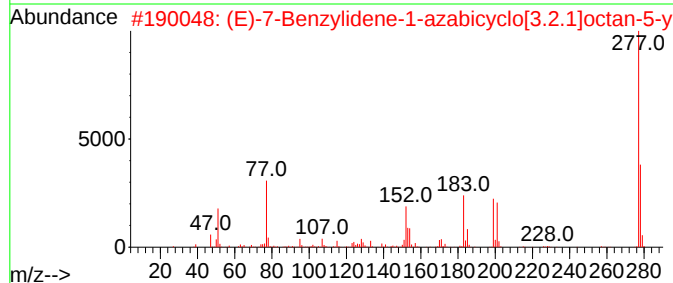
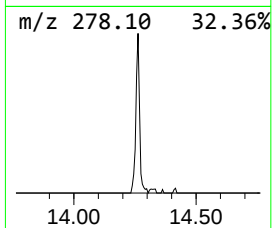
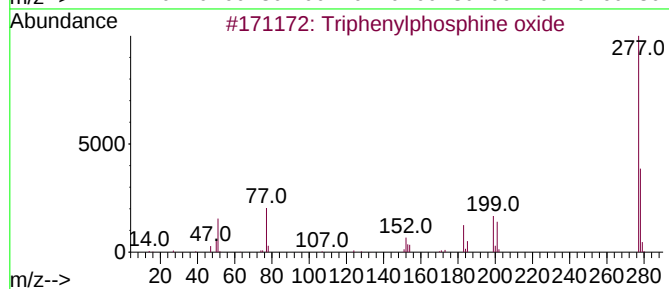
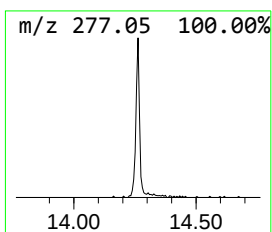
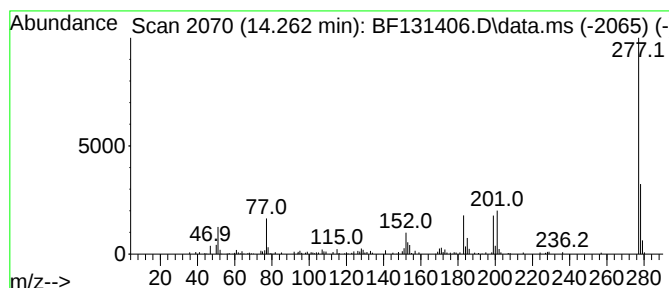
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.262	3.53 ng	95299	Chrysene-d12	14.163

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	86
3			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	53
4			Cobalt, (.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	47
5			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45



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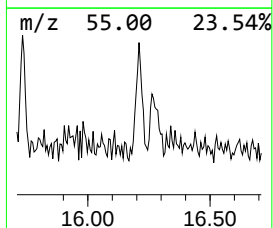
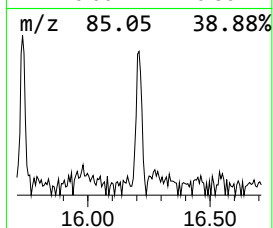
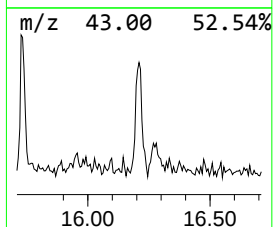
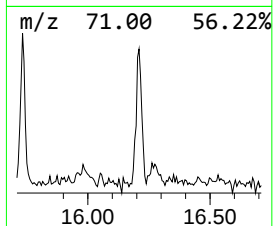
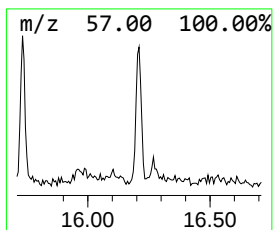
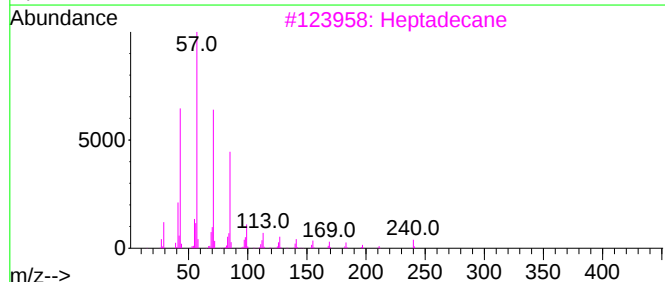
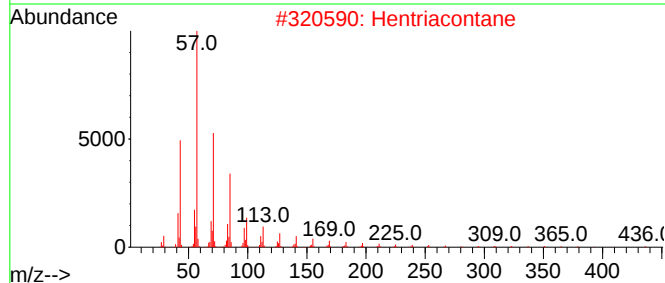
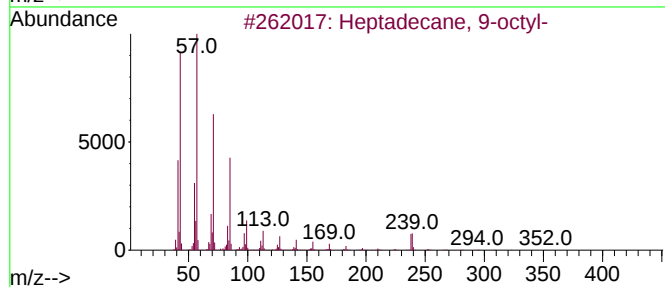
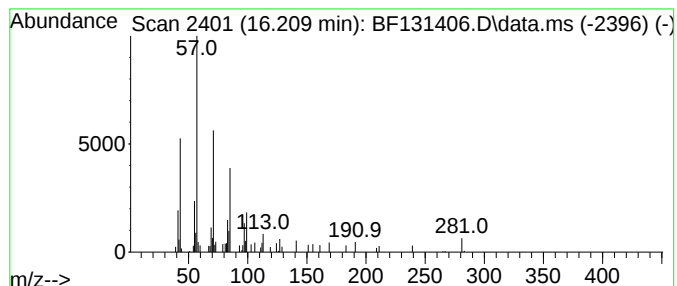
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptadecane, 9-octyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.209	2.05 ng	48789	Perylene-d12	15.704

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
2			Hentriacontane	437	C31H64	000630-04-6	86
3			Heptadecane	240	C17H36	000629-78-7	80
4			Triacontane	422	C30H62	000638-68-6	80
5			Methoxyacetic acid, 2-tetradecyl...	286	C17H34O3	1000282-04-8	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112522\
Data File : BF131406.D
Acq On : 25 Nov 2022 20:51
Operator : CG\JU
Sample : N5741-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-37

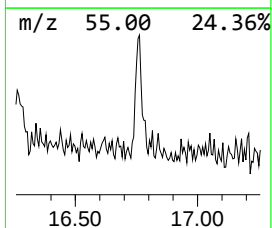
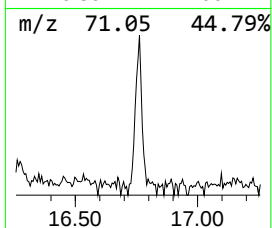
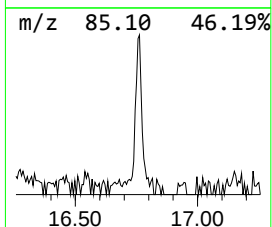
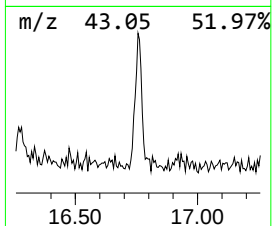
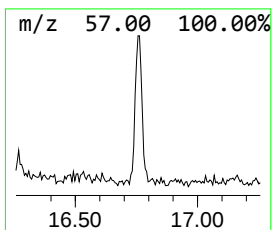
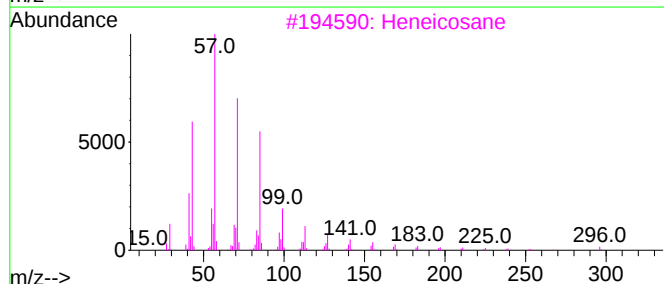
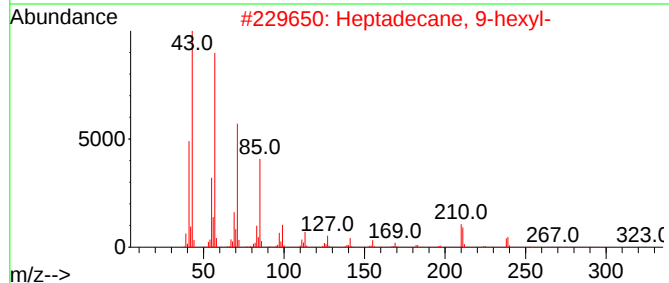
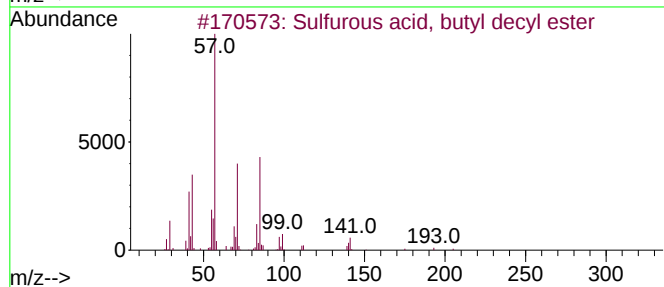
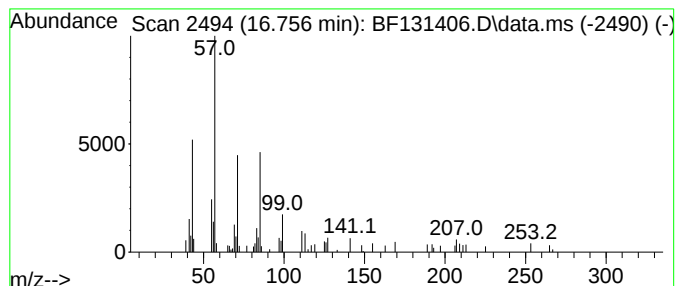
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Sulfurous acid, butyl decyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.756	2.30 ng	54578	Perylene-d12	15.704

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Sulfurous acid, butyl decyl ester	278	C14H30O3S	1000309-17-7	64
2		Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	64
3		Heneicosane	296	C21H44	000629-94-7	62
4		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	58
5		Heptadecane, 2-methyl-	254	C18H38	001560-89-0	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112522\
Data File : BF131406.D
Acq On : 25 Nov 2022 20:51
Operator : CG\JU
Sample : N5741-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-37

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...	2.252	71.6	ng	1902310	1	6.957	531634	20.0
2-Pentanone, 4-...	5.169	7.6	ng	201637	1	6.957	531634	20.0
n-Hexadecanoic ...	12.027	3.0	ng	116105	4	11.504	777098	20.0
Heptadecyl hept...	13.998	7.2	ng	195253	5	14.163	539983	20.0
Triphenylphosph...	14.262	3.5	ng	95299	5	14.163	539983	20.0
Heptadecane, 9-...	16.209	2.0	ng	48789	6	15.704	475376	20.0
Sulfurous acid,...	16.756	2.3	ng	54578	6	15.704	475376	20.0