

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062223\
 Data File : BF133902.D
 Acq On : 22 Jun 2023 15:32
 Operator : CG\JU
 Sample : 03321-07
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-23

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-BF060923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133902.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	6	11	rVB	377498	462427	24.03%	3.011%
2	2.240	22	26	35	rVB2	22773	42405	2.20%	0.276%
3	5.092	506	511	524	rBV	717002	839597	43.63%	5.466%
4	5.492	575	579	598	rBV	1849719	1704565	88.57%	11.098%
5	5.881	641	645	652	rBV	47608	41484	2.16%	0.270%
6	6.492	745	749	752	rBV	1834354	1668499	86.70%	10.863%
7	6.857	808	811	815	rBV	722357	579402	30.11%	3.772%
8	7.422	902	907	910	rBV	1195550	1094805	56.89%	7.128%
9	8.139	1025	1029	1032	rBV	863423	707321	36.75%	4.605%
10	9.216	1208	1212	1215	rBV	2483811	1924460	100.00%	12.529%
11	9.898	1324	1328	1333	rBV	802466	697101	36.22%	4.538%
12	10.610	1446	1449	1458	rVB	385145	326172	16.95%	2.124%
13	10.686	1458	1462	1477	rVB	1222102	1081590	56.20%	7.042%
14	10.921	1499	1502	1505	rBV	83871	65805	3.42%	0.428%
15	11.004	1512	1516	1519	rBV	101804	94855	4.93%	0.618%
16	11.298	1564	1566	1572	rVB	44183	40494	2.10%	0.264%
17	11.392	1578	1582	1585	rBV	687231	630958	32.79%	4.108%
18	11.916	1668	1671	1684	rBV2	165728	208550	10.84%	1.358%
19	12.610	1786	1789	1792	rBV	26256	25361	1.32%	0.165%
20	12.710	1803	1806	1810	rBV5	32141	36008	1.87%	0.234%
21	12.839	1825	1828	1830	rBV	24521	24255	1.26%	0.158%
22	12.986	1849	1853	1856	rBV	1953306	1660010	86.26%	10.808%
23	13.221	1888	1893	1895	rBV2	33956	43887	2.28%	0.286%
24	13.562	1948	1951	1954	rBV2	31167	26875	1.40%	0.175%
25	13.898	2005	2008	2021	rBV3	82258	189999	9.87%	1.237%
26	14.051	2030	2034	2037	rBV	661230	624649	32.46%	4.067%
27	14.521	2112	2114	2117	rBV2	30352	26256	1.36%	0.171%
28	15.556	2285	2290	2295	rBV	370834	491933	25.56%	3.203%

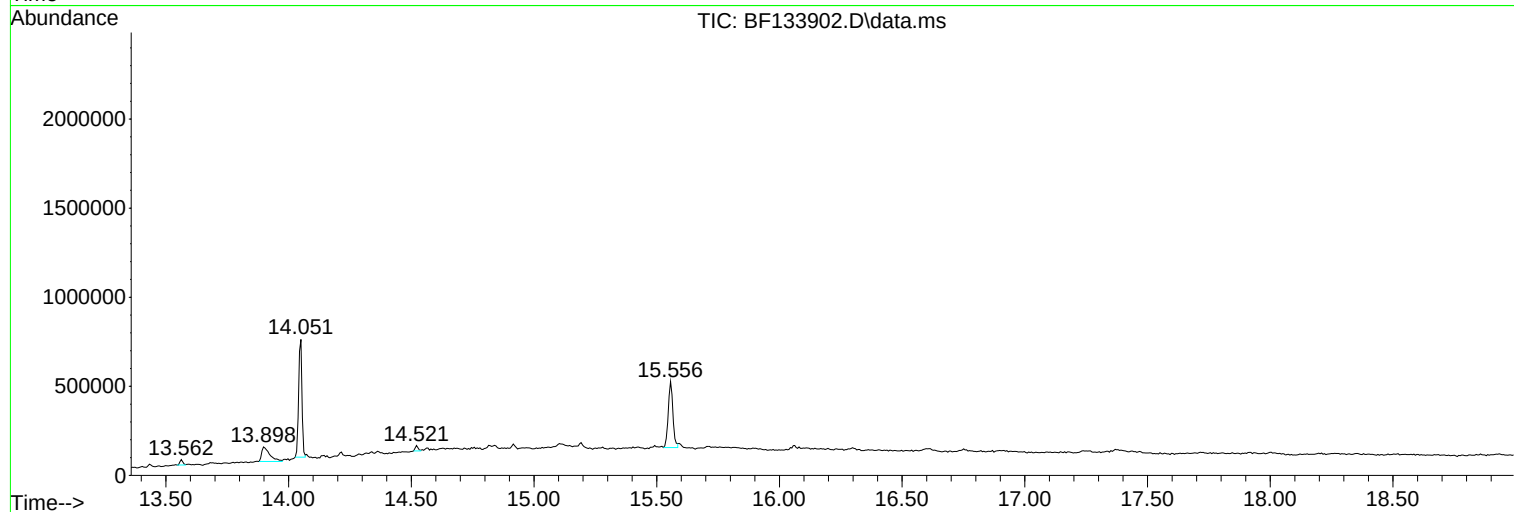
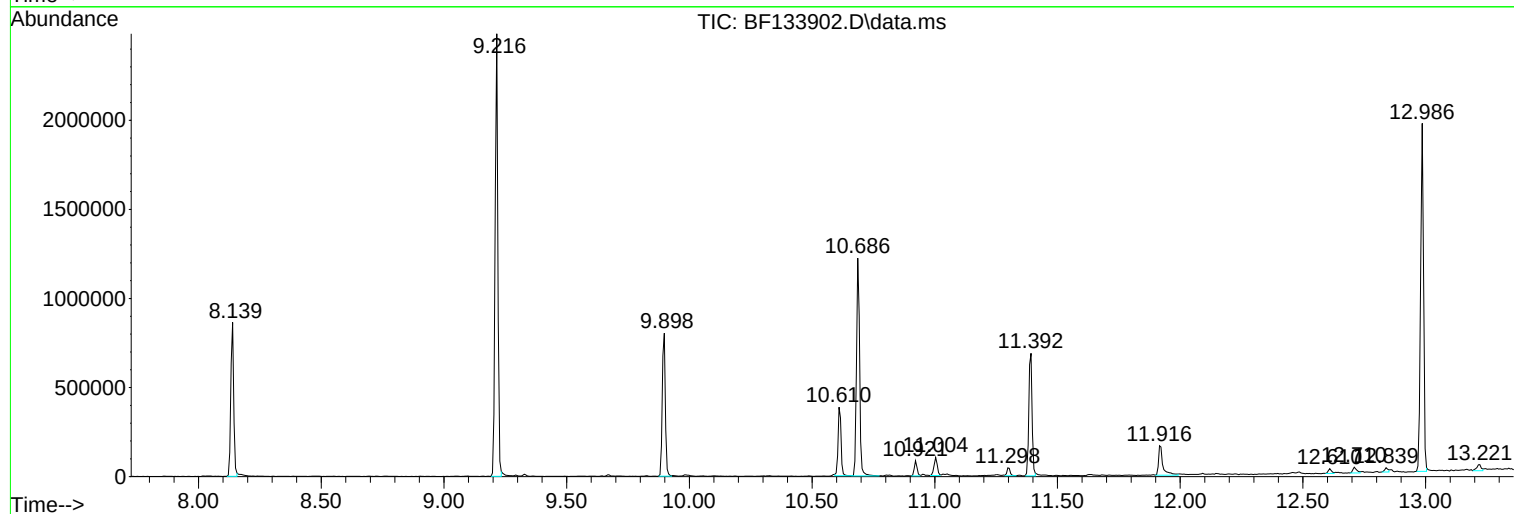
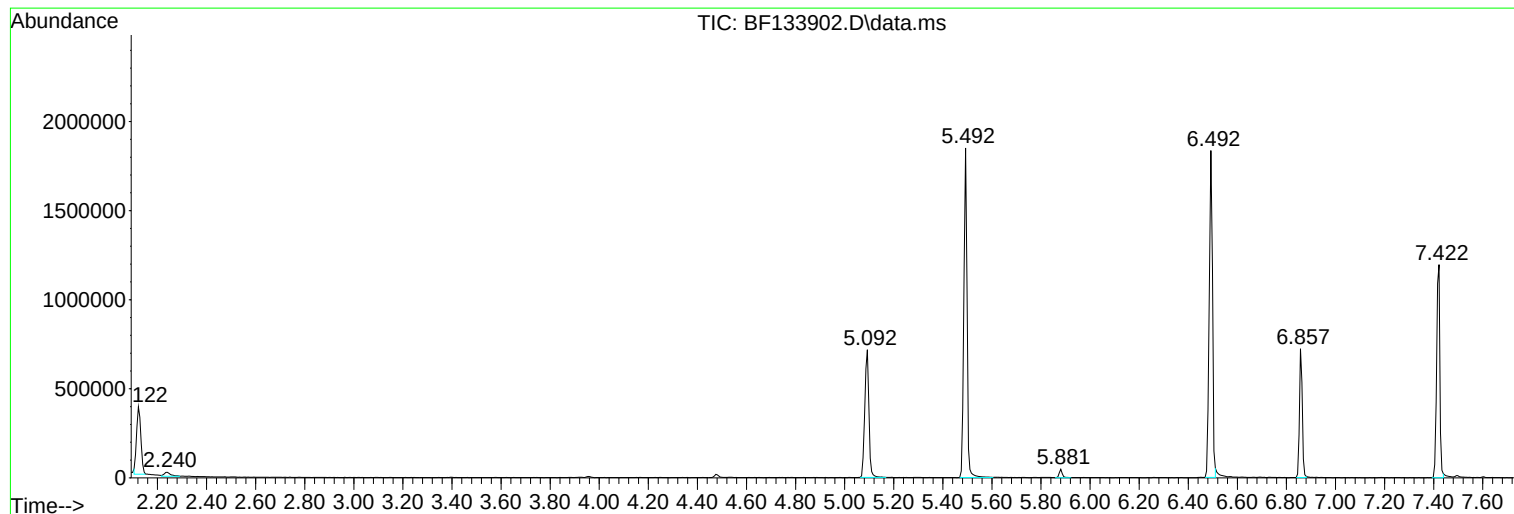
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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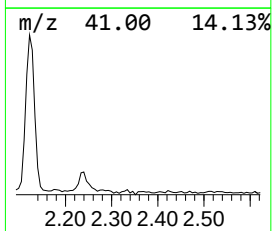
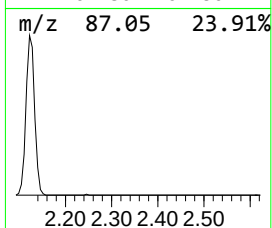
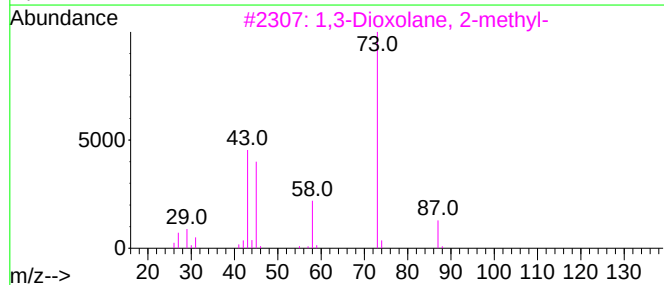
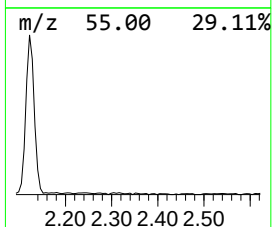
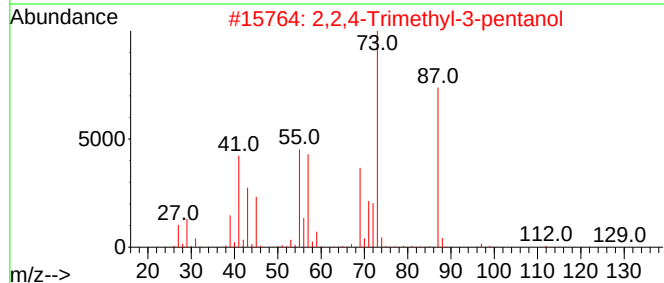
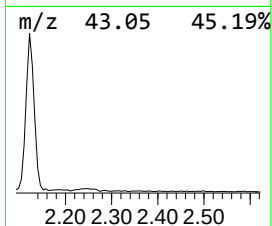
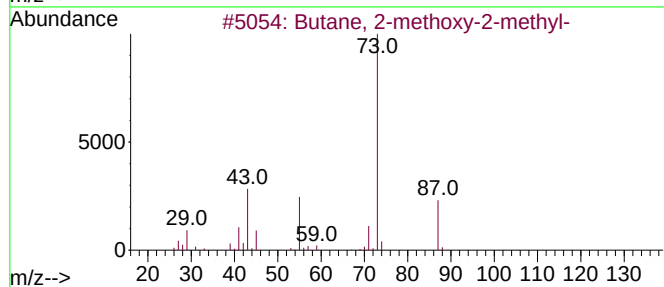
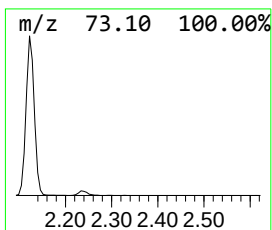
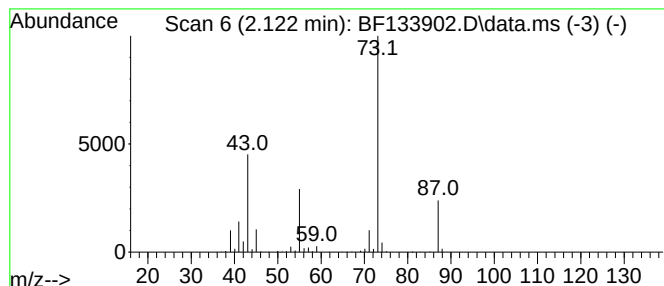
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	15.96 ng	462427	1,4-Dichlorobenzene-d4	6.857

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			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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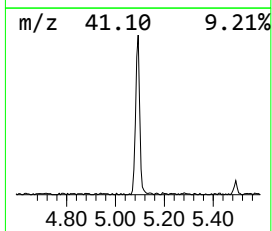
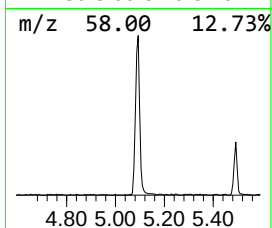
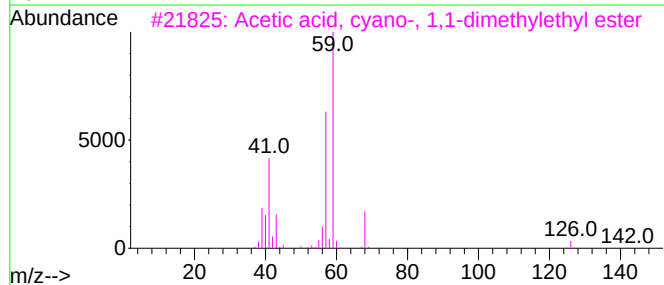
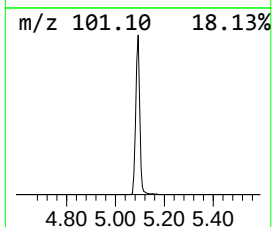
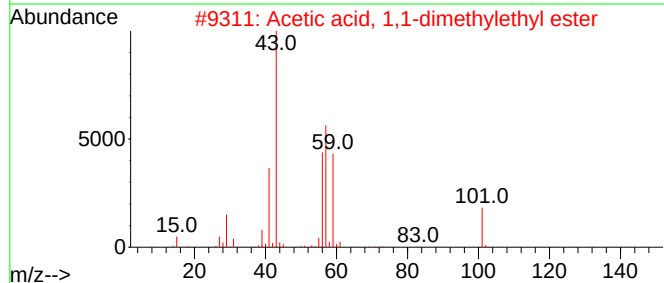
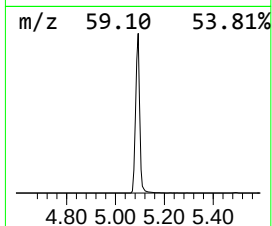
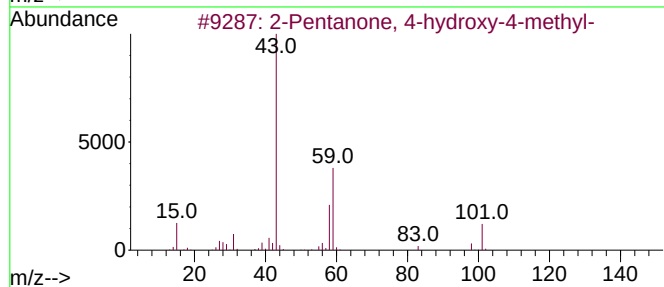
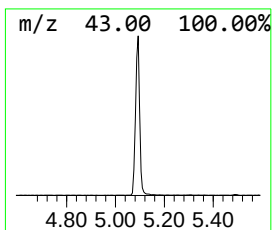
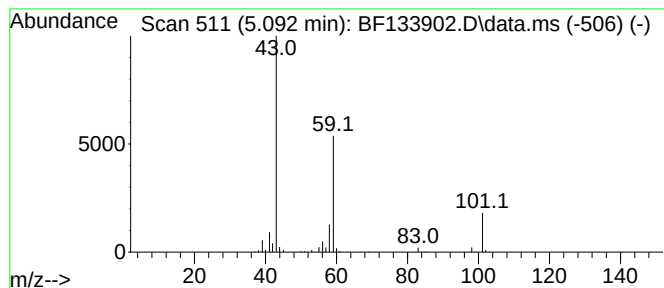
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.092	28.98 ng	839597	1,4-Dichlorobenzene-d4	6.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		



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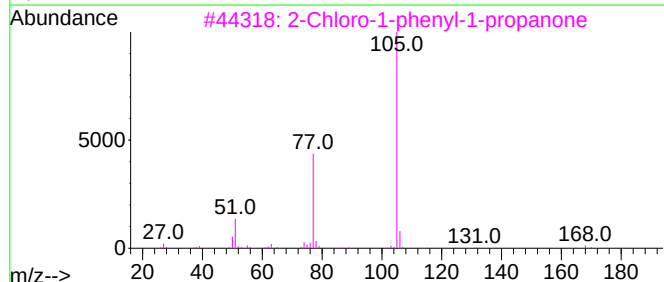
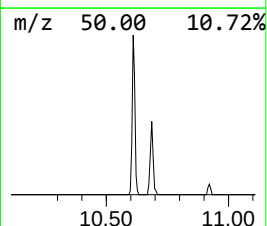
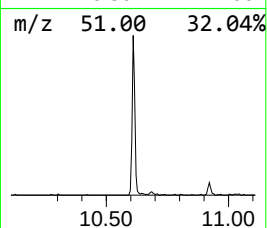
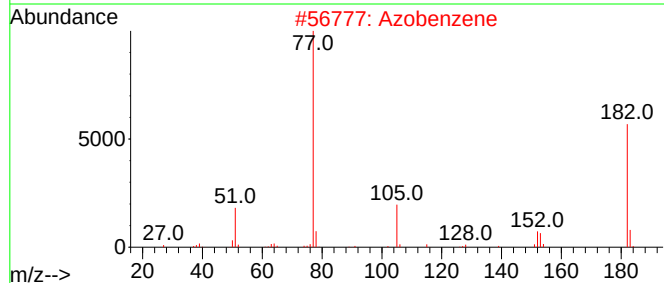
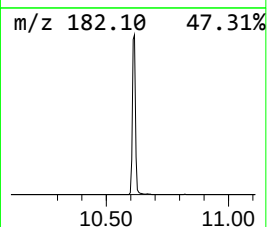
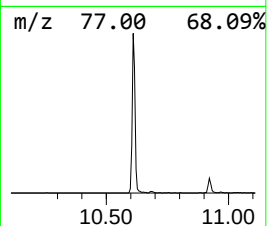
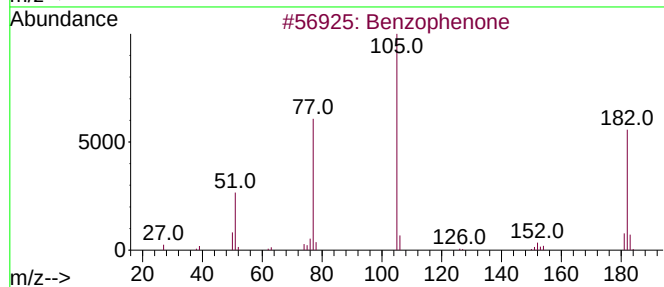
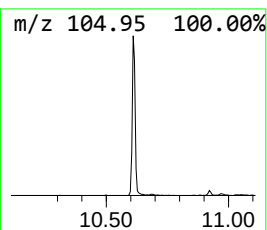
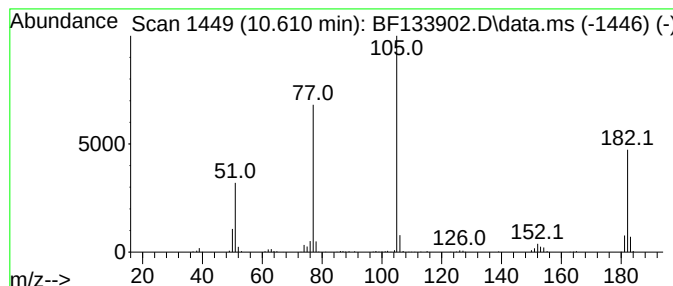
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Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.610	9.36 ng	326172	Acenaphthene-d10	9.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	53
3			2-Chloro-1-phenyl-1-propanone	168	C9H9ClO	006084-17-9	50
4			Vinyl benzoate	148	C9H8O2	000769-78-8	50
5			2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	50



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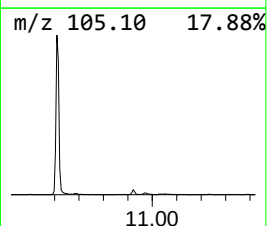
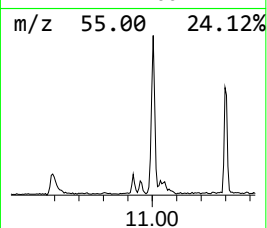
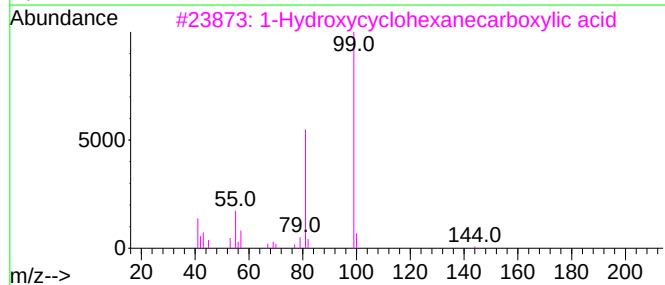
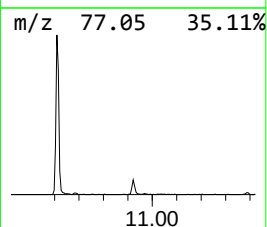
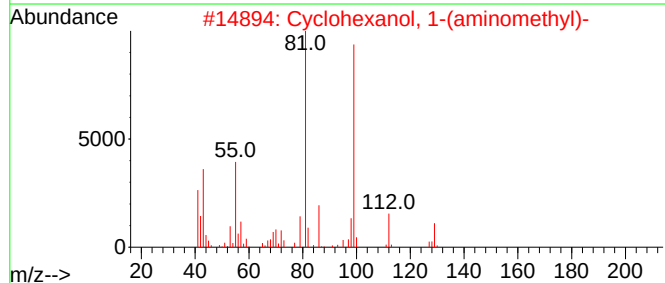
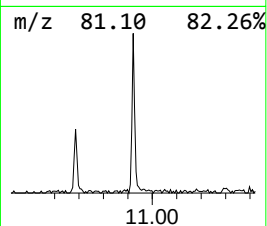
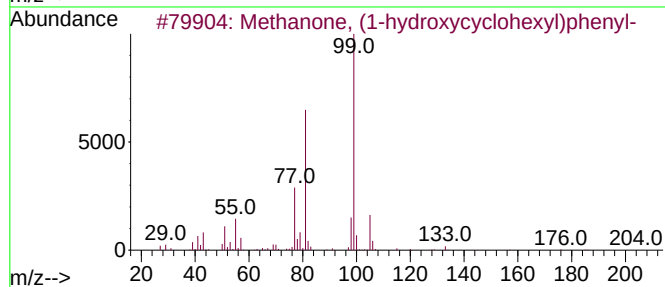
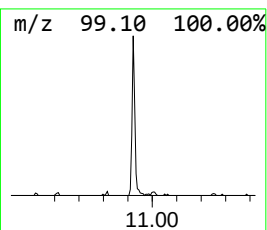
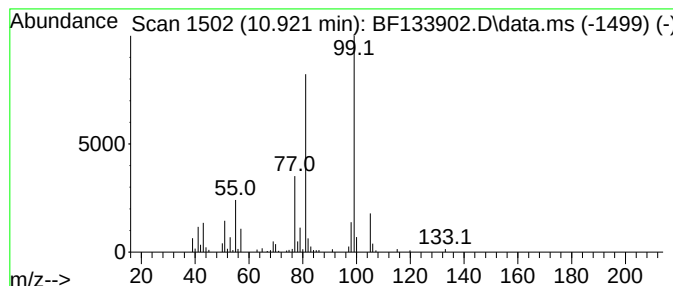
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Peak Number 4 Methanone, (1-hydroxycyclohexyl) Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.922	2.09 ng	65805	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	90
2			Cyclohexanol, 1-(aminomethyl)-	129	C7H15NO	004000-72-0	64
3			1-Hydroxycyclohexanecarboxylic acid	144	C7H12O3	001123-28-0	45
4			2-Methylcyclosarin	194	C8H16F02P	085473-32-1	42
5			3-Methylcyclohexyl methylphospho...	194	C8H16F02P	113548-86-0	42



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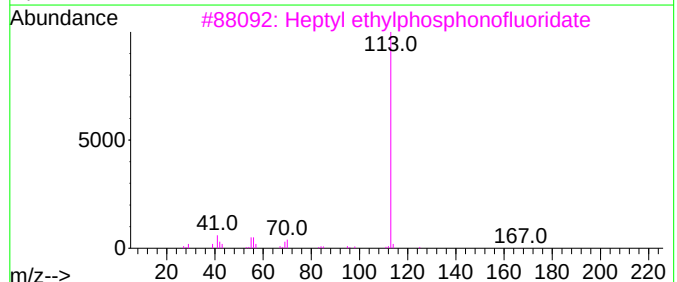
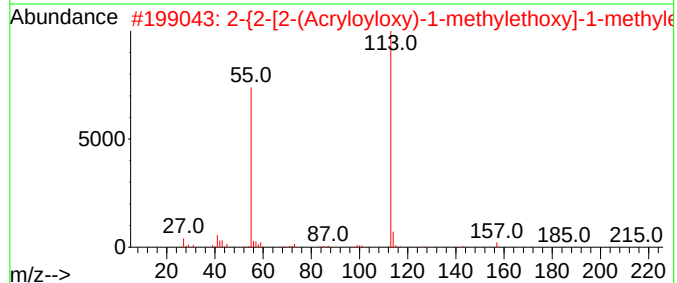
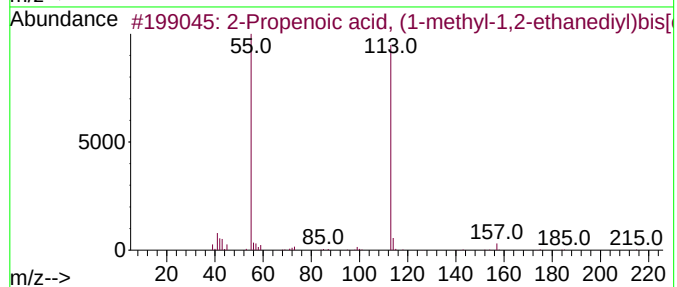
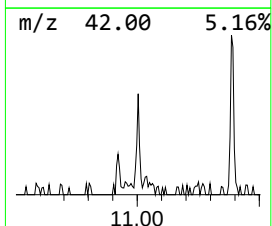
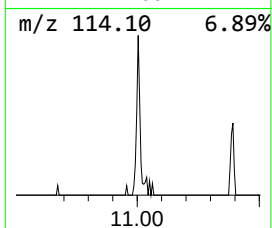
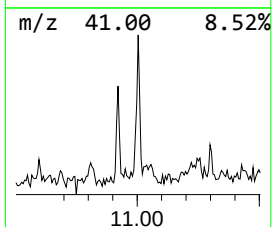
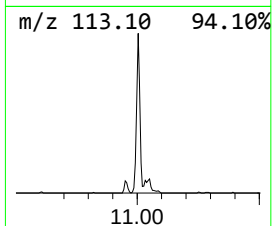
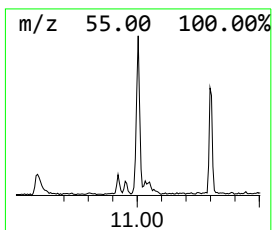
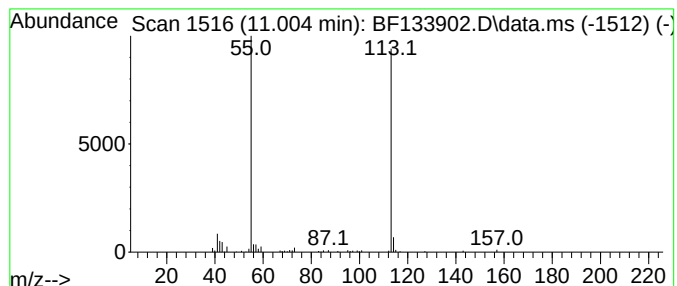
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Peak Number 5 2-Propenoic acid, (1-methyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.004	3.01 ng	94855	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenoic acid, (1-methyl-1,2-...	300	C15H24O6	042978-66-5	83		
2	2-{2-[2-(Acryloyloxy)-1-methylet...	300	C15H24O6	094120-00-0	83		
3	Heptyl ethylphosphonofluoridate	210	C9H20FO2P	162085-85-0	36		
4	2-Fluoro-5-hydroxypyridine	113	C5H4FN0	055758-32-2	9		
5	Vardenafil	488	C23H32N6O4S	224785-90-4	9		



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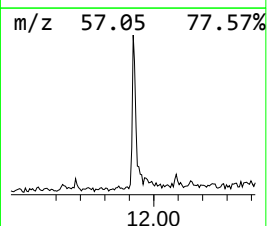
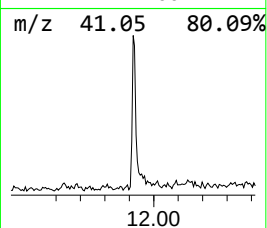
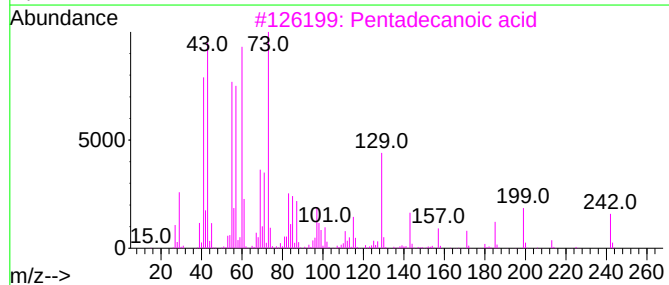
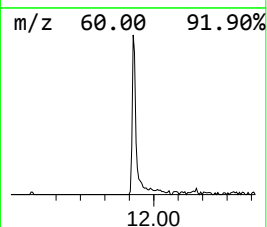
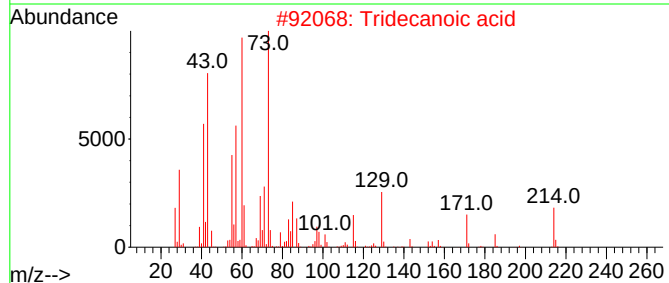
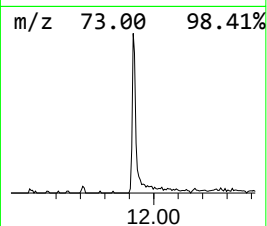
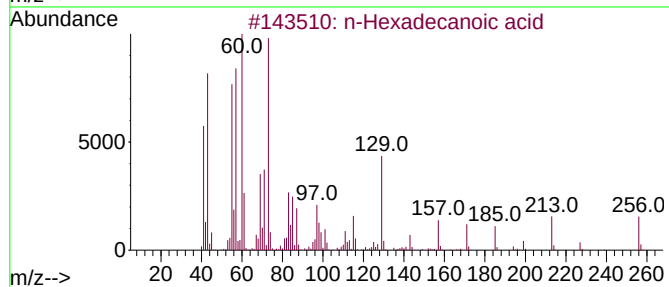
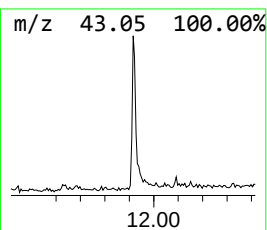
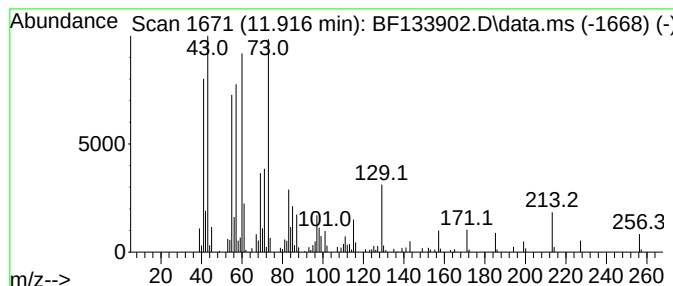
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	6.61 ng	208550	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Undecanoic acid	186	C11H22O2	000112-37-8	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062223\
Data File : BF133902.D
Acq On : 22 Jun 2023 15:32
Operator : CG\JU
Sample : 03321-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-23

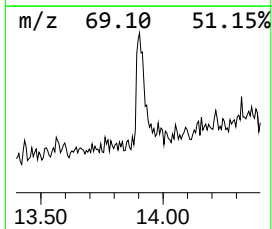
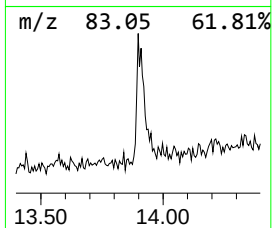
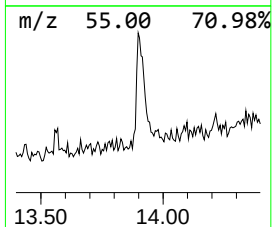
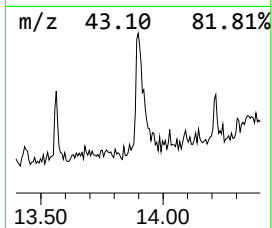
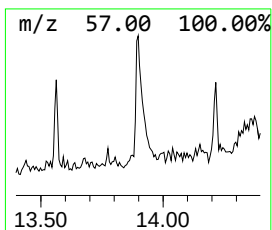
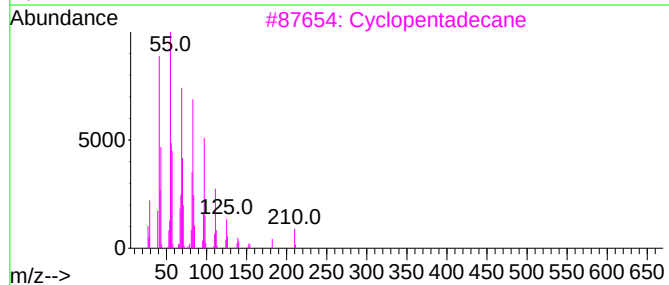
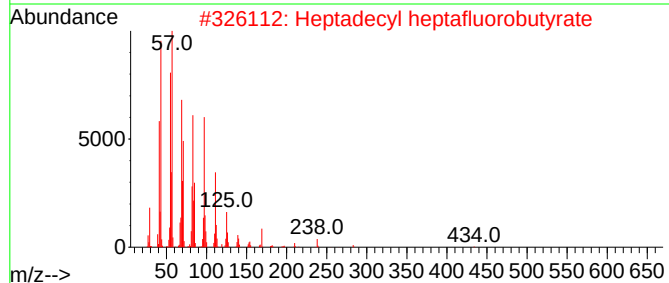
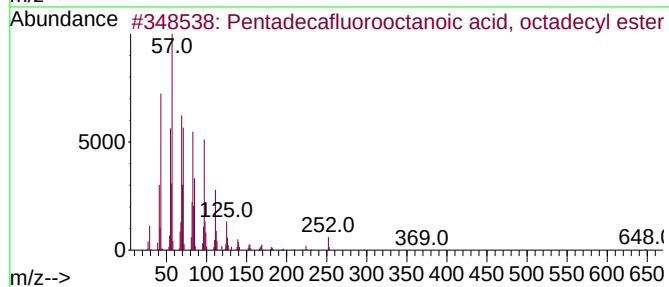
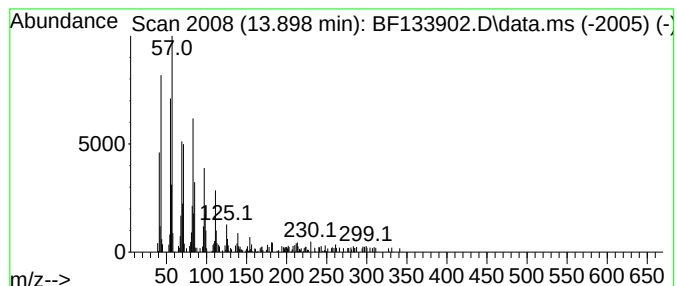
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentadecafluorooctanoic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	6.08 ng	189999	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
3			Cyclopentadecane	210	C15H30	000295-48-7	87
4			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
5			Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062223\
Data File : BF133902.D
Acq On : 22 Jun 2023 15:32
Operator : CG\JU
Sample : 03321-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-23

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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...	2.122	16.0	ng	462427	1	6.857	579402	20.0
2-Pentanone, 4-...	5.092	29.0	ng	839597	1	6.857	579402	20.0
Benzophenone	10.610	9.4	ng	326172	3	9.898	697101	20.0
Methanone, (1-h...	10.922	2.1	ng	65805	4	11.392	630958	20.0
2-Propenoic aci...	11.004	3.0	ng	94855	4	11.392	630958	20.0
n-Hexadecanoic ...	11.916	6.6	ng	208550	4	11.392	630958	20.0
Pentadecafluoro...	13.898	6.1	ng	189999	5	14.051	624649	20.0