

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041923\
 Data File : BF132917.D
 Acq On : 19 Apr 2023 18:03
 Operator : CG\JU
 Sample : 02270-26
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-16-14-16-20230413

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-BF041723.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132917.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.963	485	489	497	rVB	214456	273450	2.80%	0.455%
2	5.369	552	558	561	rBV	7034521	7045146	72.18%	11.730%
3	6.392	726	732	735	rBV	6724100	7118017	72.92%	11.851%
4	6.763	791	795	798	rBV	1884687	1428507	14.63%	2.378%
5	6.828	803	806	809	rBV	145262	109396	1.12%	0.182%
6	7.328	886	891	894	rBV	5229561	4757569	48.74%	7.921%
7	8.045	1010	1013	1016	rVB	2892386	2152718	22.05%	3.584%
8	9.127	1192	1197	1200	rBV	9874282	8240603	84.42%	13.720%
9	9.398	1240	1243	1256	rBV	751512	720761	7.38%	1.200%
10	9.798	1308	1311	1315	rVB	3041182	2559607	26.22%	4.262%
11	10.516	1425	1433	1436	rBV	686075	582019	5.96%	0.969%
12	10.586	1441	1445	1448	rBV	6011603	5720091	58.60%	9.524%
13	11.280	1559	1563	1567	rVB	3379617	2723949	27.91%	4.535%
14	11.821	1649	1655	1664	rBV2	835276	981985	10.06%	1.635%
15	12.421	1754	1757	1763	rVB	155272	133420	1.37%	0.222%
16	12.604	1782	1788	1801	rBV	239135	321468	3.29%	0.535%
17	12.874	1829	1834	1837	rBV	9810108	9761188	100.00%	16.252%
18	13.774	1981	1987	2007	rBV2	532810	1005700	10.30%	1.674%
19	13.915	2007	2011	2014	rBV	2606703	2183912	22.37%	3.636%
20	14.104	2039	2043	2045	rBV	108389	104703	1.07%	0.174%
21	14.404	2091	2094	2099	rBV	121687	129899	1.33%	0.216%
22	14.709	2142	2146	2149	rBV	104297	106096	1.09%	0.177%
23	15.033	2197	2201	2208	rVB	102552	110949	1.14%	0.185%
24	15.345	2249	2254	2260	rBV	1469950	1685021	17.26%	2.806%
25	15.868	2339	2343	2351	rBV3	42936	104862	1.07%	0.175%

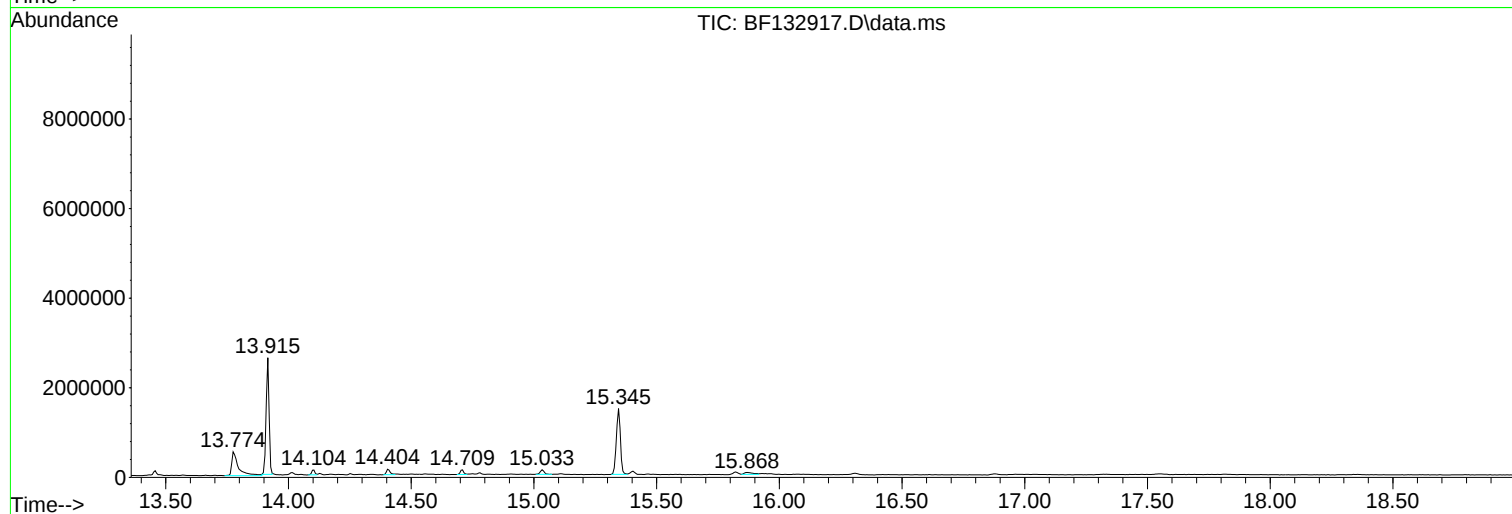
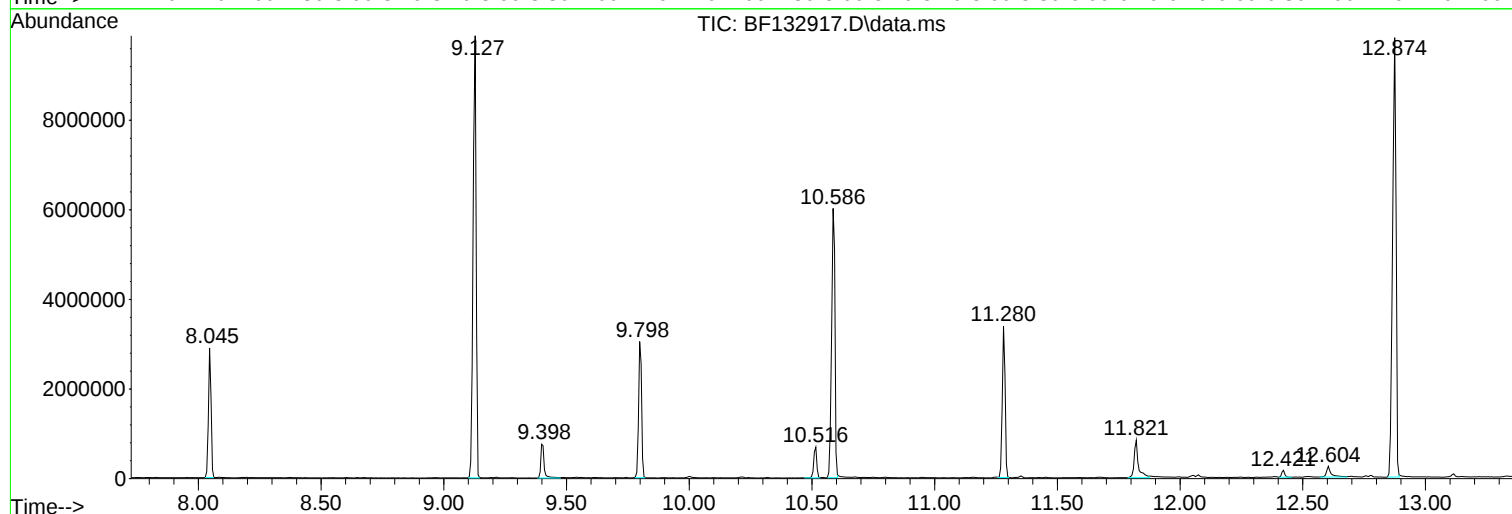
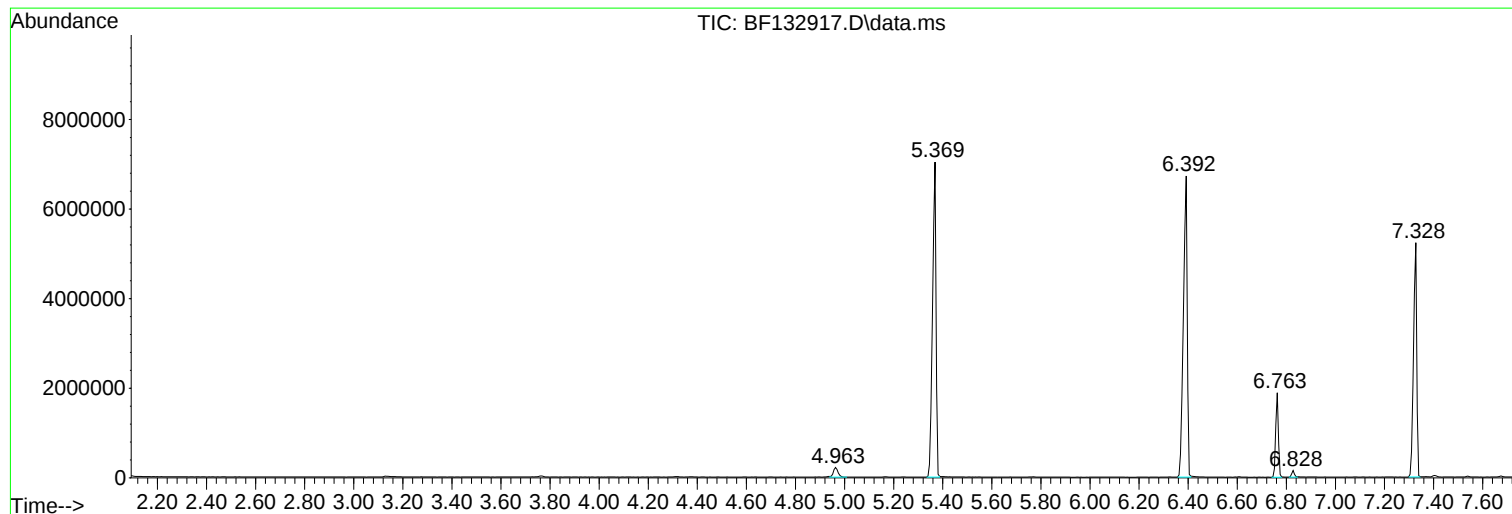
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF041723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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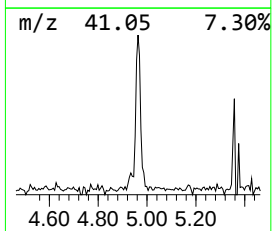
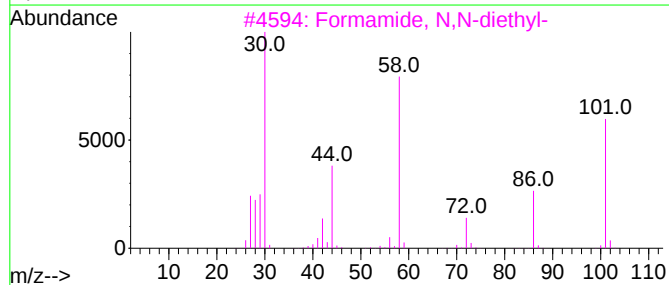
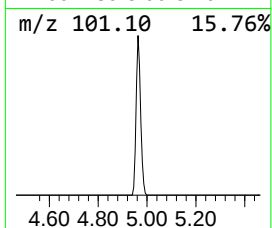
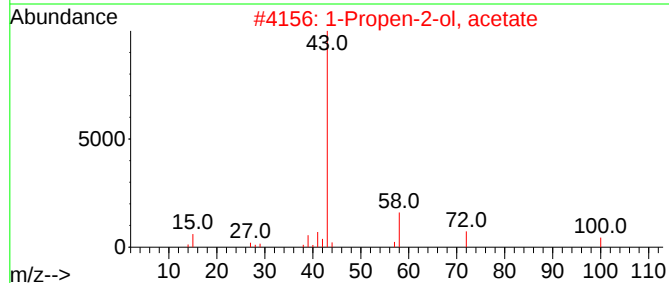
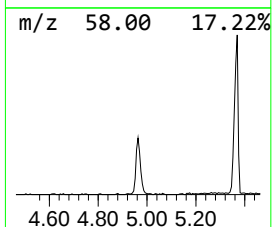
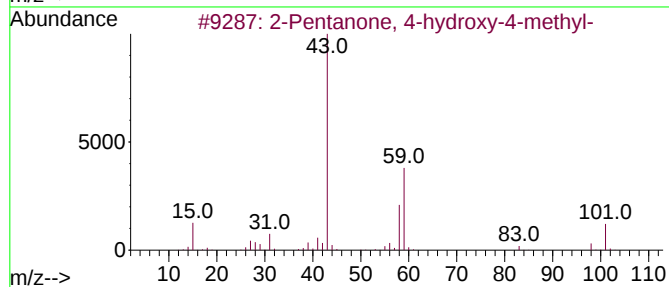
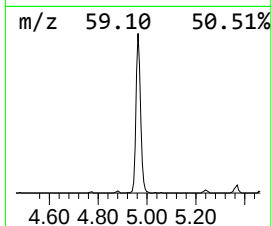
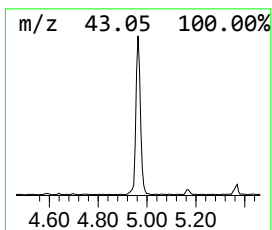
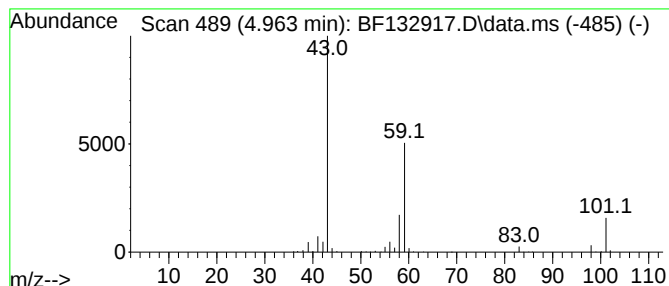
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.963	3.83 ng	273450	1,4-Dichlorobenzene-d4	6.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3		Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9
4		Acetone	58	C3H6O	000067-64-1	9
5		Guanidine	59	CH5N3	000113-00-8	9



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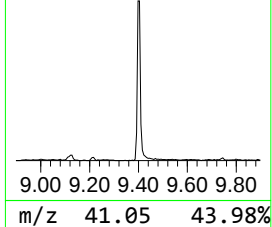
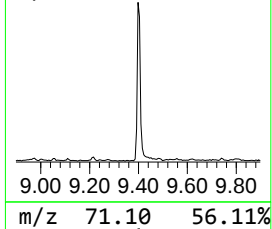
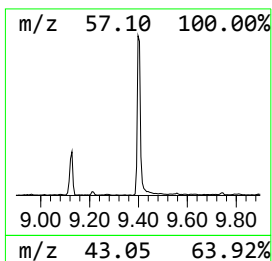
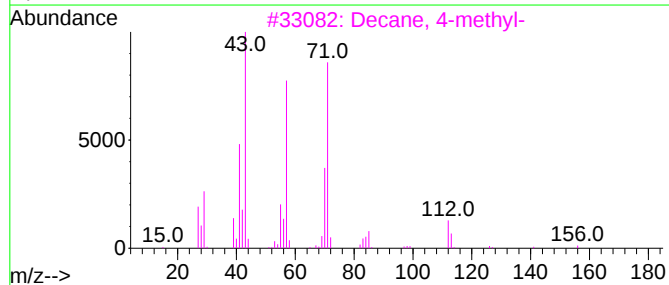
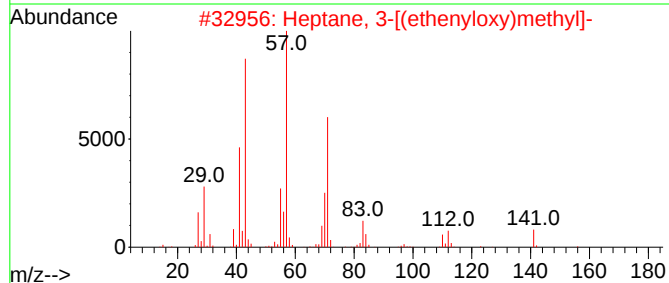
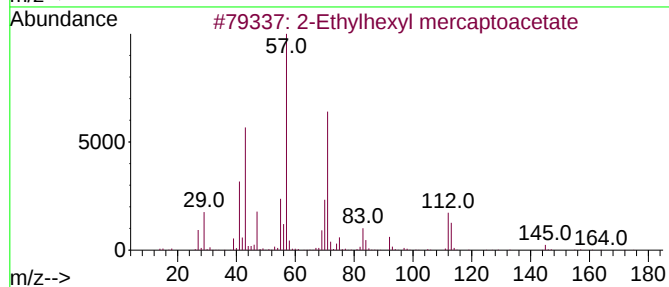
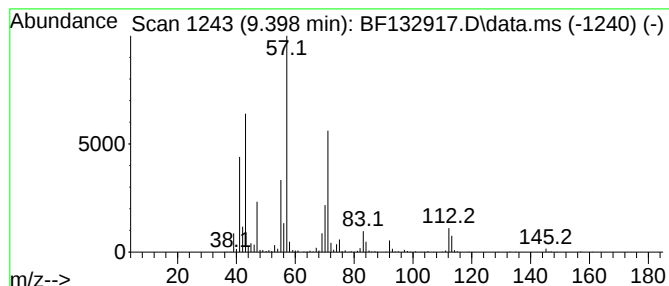
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF041723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Ethylhexyl mercaptoacetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.398	5.63 ng	720761	Acenaphthene-d10	9.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Ethylhexyl mercaptoacetate	204	C10H20O2S	007659-86-1	83
2			Heptane, 3-[(ethenyloxy)methyl]-	156	C10H20O	000103-44-6	59
3			Decane, 4-methyl-	156	C11H24	002847-72-5	50
4			Carbonic acid, neopentyl 2-ethyl...	244	C14H28O3	1000357-85-7	50
5			Undecane, 2,5-dimethyl-	184	C13H28	017301-22-3	50



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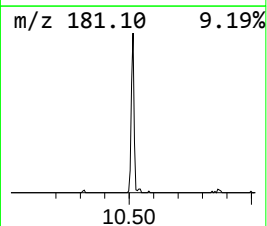
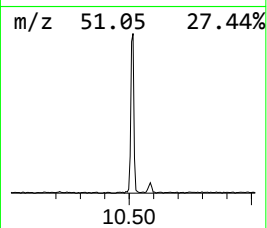
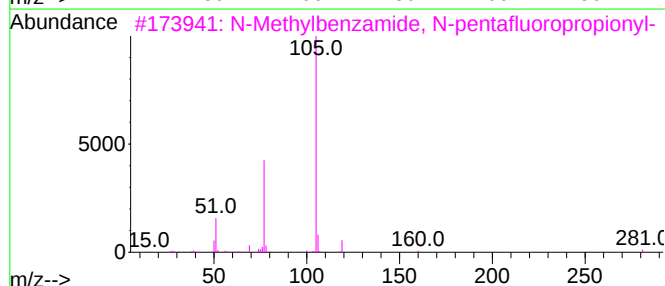
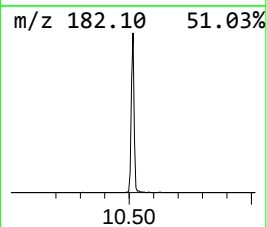
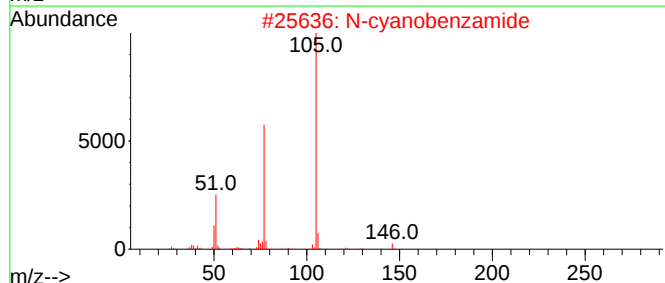
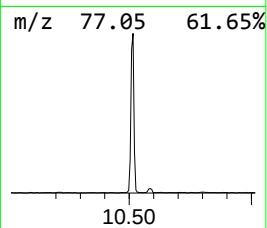
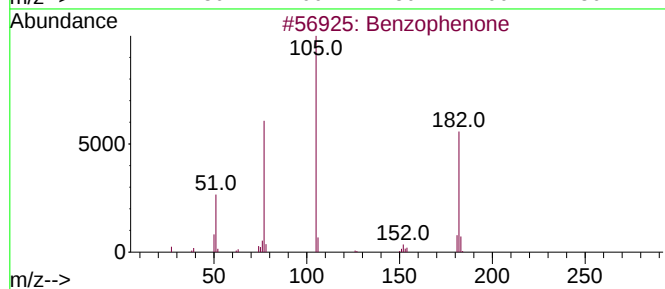
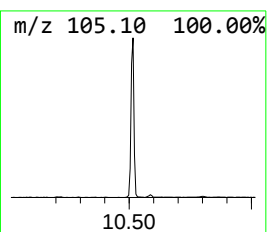
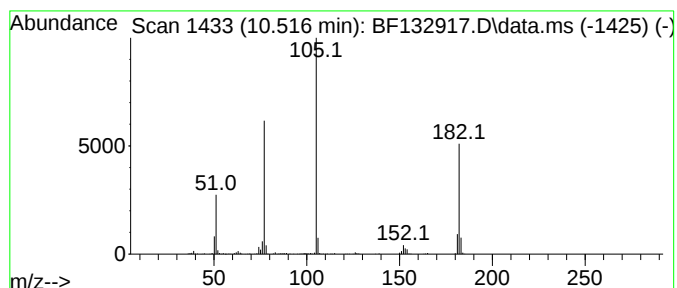
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.516	4.55 ng	582019	Acenaphthene-d10	9.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			N-cyanobenzamide	146	C8H6N2O	015150-25-1	47
3			N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	47
4			2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47
5			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47



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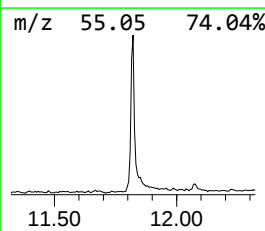
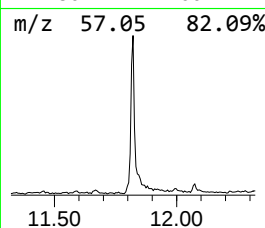
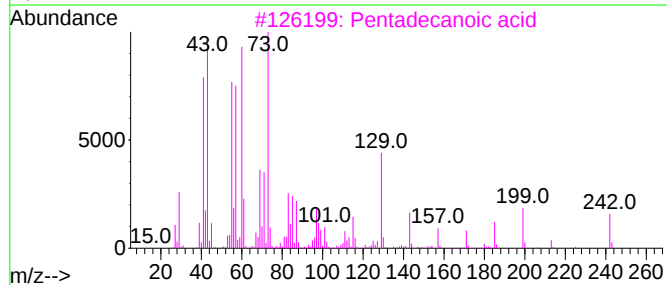
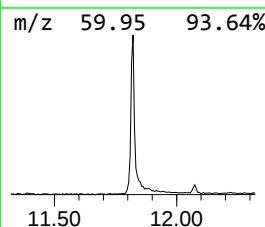
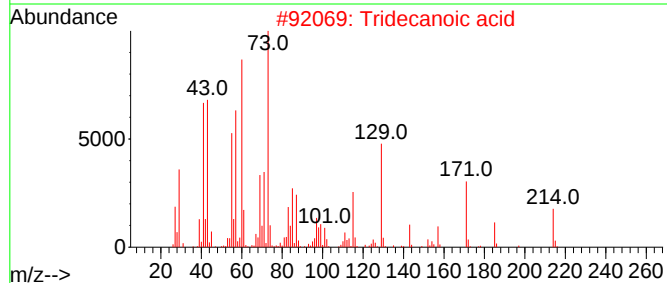
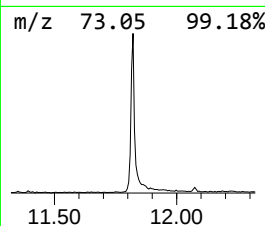
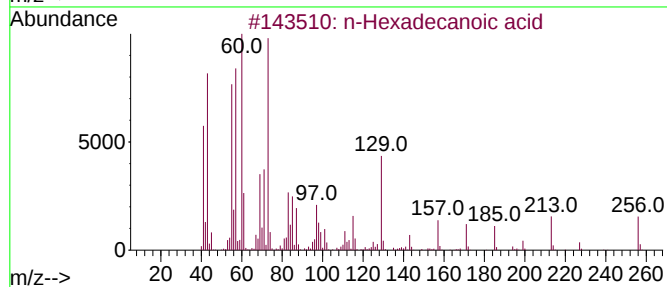
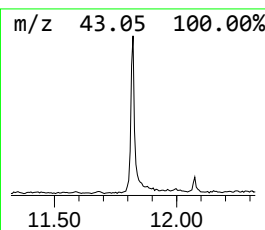
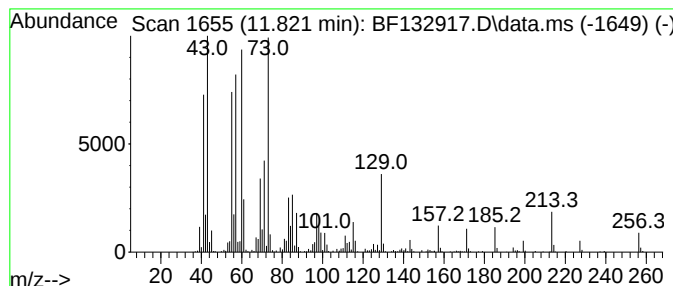
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.821	7.21 ng	981985	Phenanthrene-d10	11.280

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	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	49



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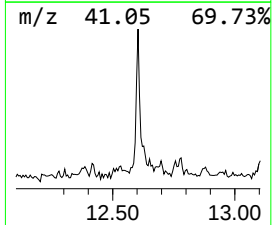
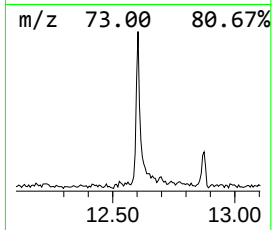
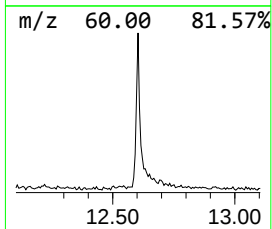
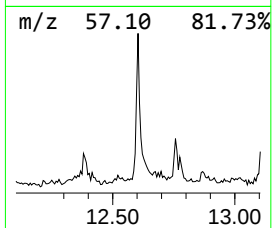
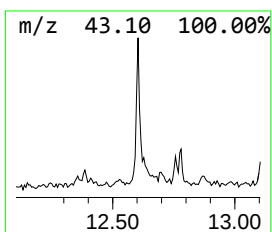
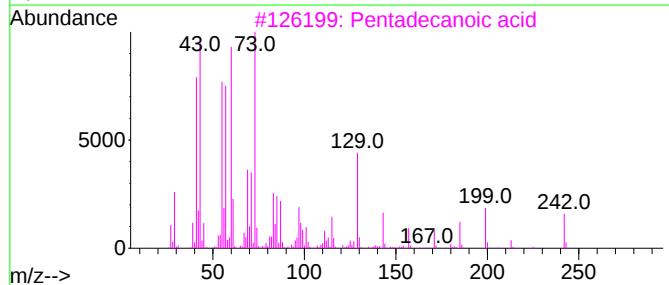
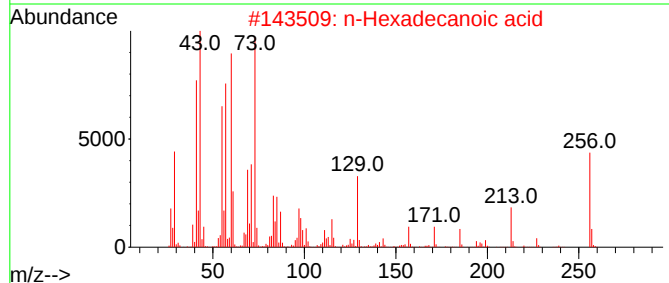
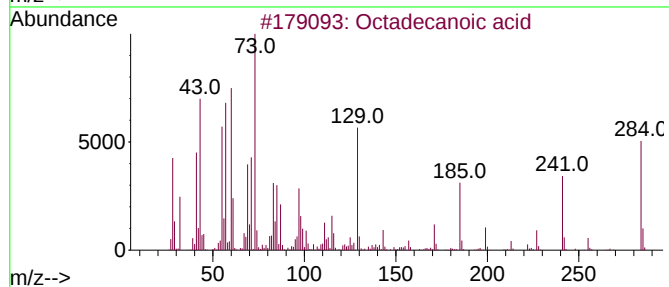
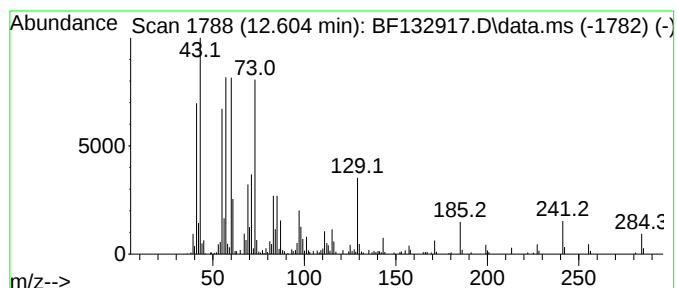
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.604	2.94 ng	321468	Chrysene-d12	13.915

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
5			Undecanoic acid	186	C11H22O2	000112-37-8	70



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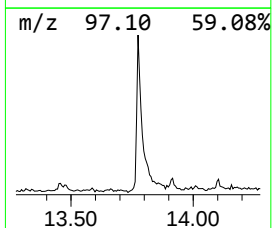
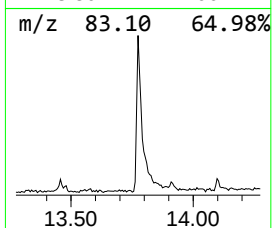
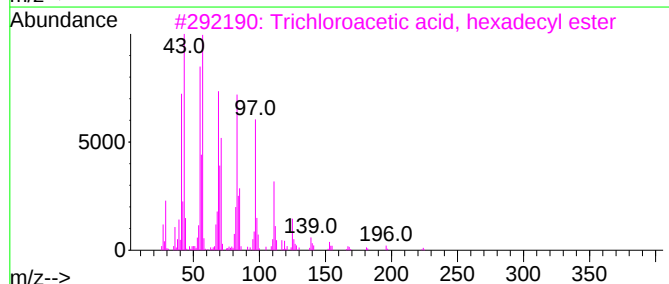
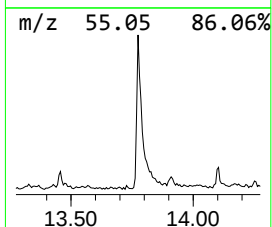
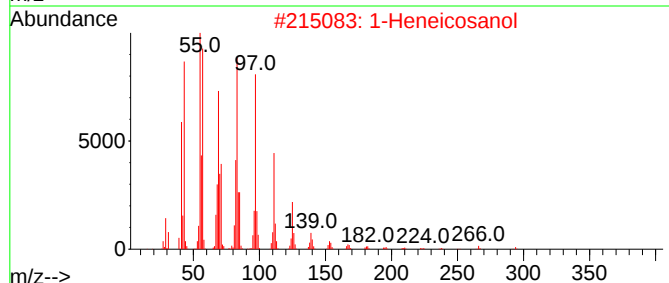
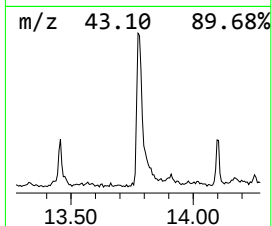
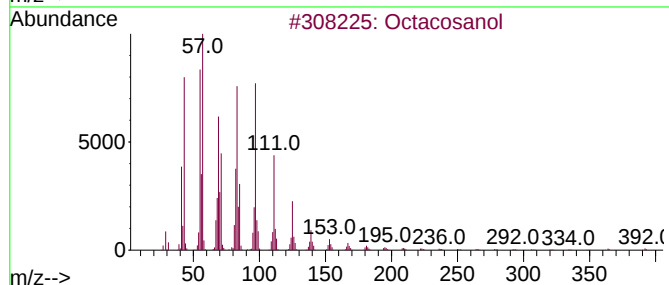
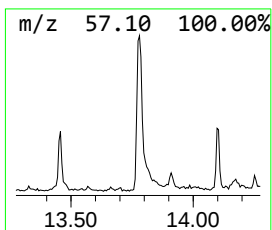
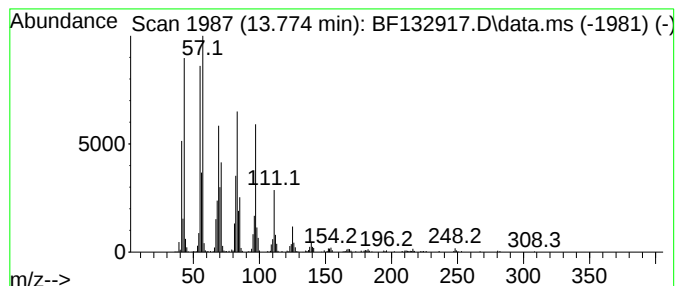
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octacosanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	9.21 ng	1005700	Chrysene-d12	13.915

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosanol	410	C28H58O	000557-61-9	94
2			1-Heneicosanol	312	C21H44O	015594-90-8	94
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5			1-Hexacosanol	382	C26H54O	000506-52-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041923\
Data File : BF132917.D
Acq On : 19 Apr 2023 18:03
Operator : CG\JU
Sample : 02270-26
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-16-14-16-20230413

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF041723.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-...	4.963	3.8	ng	273450	1	6.763	1428510	20.0
2-Ethylhexyl me...	9.398	5.6	ng	720761	3	9.798	2559610	20.0
Benzophenone	10.516	4.5	ng	582019	3	9.798	2559610	20.0
n-Hexadecanoic ...	11.821	7.2	ng	981985	4	11.280	2723950	20.0
Octadecanoic acid	12.604	2.9	ng	321468	5	13.915	2183910	20.0
Octacosanol	13.774	9.2	ng	1005700	5	13.915	2183910	20.0