

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092123\
 Data File : BF135382.D
 Acq On : 21 Sep 2023 16:06
 Operator : CG\JU
 Sample : 04407-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 306-TP-1-2-CS-1

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-BF091123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135382.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	4	9	19	rVB	47006	69393	2.07%	0.303%
2	4.998	491	495	503	rBV	66065	91164	2.72%	0.398%
3	5.393	558	562	579	rBV	3044291	3353157	100.00%	14.632%
4	6.404	729	734	737	rBV	3234504	3251929	96.98%	14.190%
5	6.757	790	794	805	rVB	1072444	858397	25.60%	3.746%
6	7.322	885	890	893	rBV	2298460	2142796	63.90%	9.350%
7	8.034	1007	1011	1017	rBV	1220313	1057749	31.54%	4.616%
8	9.116	1190	1195	1198	rBV	3529365	3229930	96.33%	14.094%
9	9.234	1210	1215	1219	rVB	41924	41940	1.25%	0.183%
10	9.792	1306	1310	1314	rBV	1144851	988202	29.47%	4.312%
11	10.586	1441	1445	1457	rBV	1637839	1543614	46.03%	6.736%
12	10.886	1491	1496	1500	rBV	42839	40670	1.21%	0.177%
13	11.286	1560	1564	1566	rBV	877454	831168	24.79%	3.627%
14	11.304	1566	1567	1571	rVB	83675	70259	2.10%	0.307%
15	11.580	1611	1614	1617	rBV	46719	39616	1.18%	0.173%
16	11.822	1651	1655	1666	rBV	281927	340294	10.15%	1.485%
17	12.504	1767	1771	1774	rBV	132654	122818	3.66%	0.536%
18	12.610	1786	1789	1793	rBV2	51728	55932	1.67%	0.244%
19	12.733	1805	1810	1813	rBV	109699	102427	3.05%	0.447%
20	12.880	1831	1835	1838	rBV	2593544	2414412	72.00%	10.536%
21	13.133	1873	1878	1880	rBV3	29059	45674	1.36%	0.199%
22	13.369	1913	1918	1924	rBV9	29708	66513	1.98%	0.290%
23	13.792	1987	1990	1993	rVB3	41936	46373	1.38%	0.202%
24	13.886	2000	2006	2011	rBV7	91480	275794	8.22%	1.203%
25	13.939	2011	2015	2018	rVB	774743	753392	22.47%	3.288%
26	14.139	2046	2049	2053	rBV3	44717	40038	1.19%	0.175%
27	14.792	2157	2160	2164	rVB	116742	108436	3.23%	0.473%
28	14.863	2170	2172	2176	rBV2	34680	37221	1.11%	0.162%
29	14.980	2190	2192	2195	rBV	48013	43872	1.31%	0.191%
30	15.057	2202	2205	2209	rVB	134006	143693	4.29%	0.627%
31	15.410	2260	2265	2269	rBV	437028	585134	17.45%	2.553%
32	15.874	2340	2344	2350	rVB	90542	124809	3.72%	0.545%

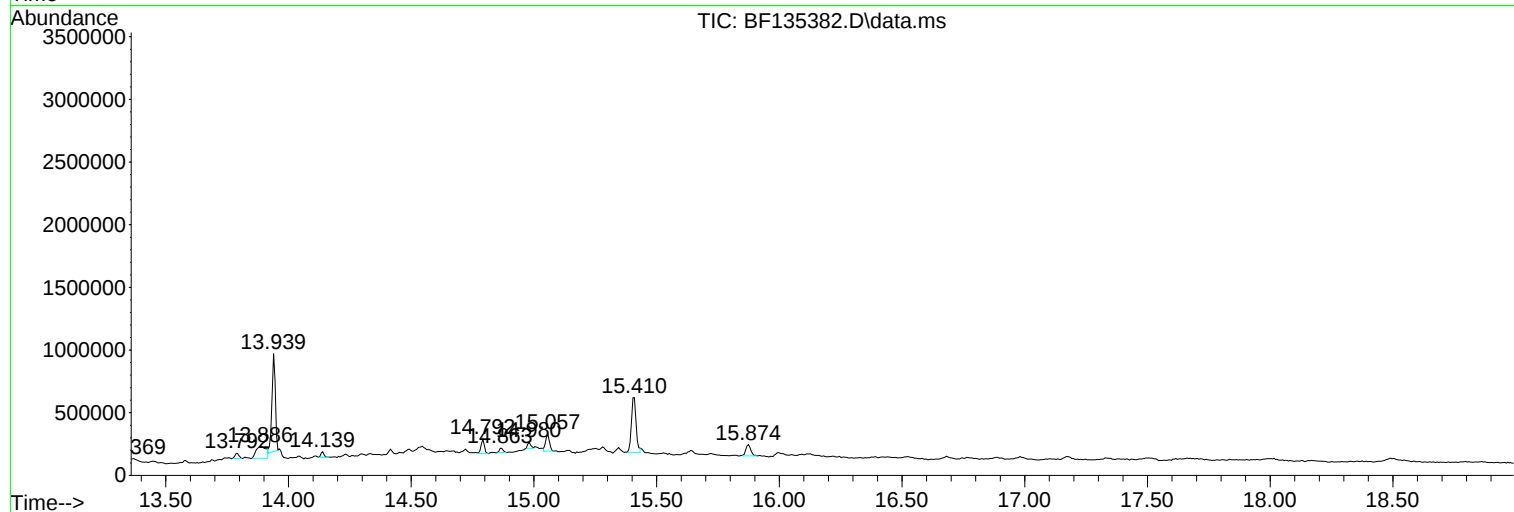
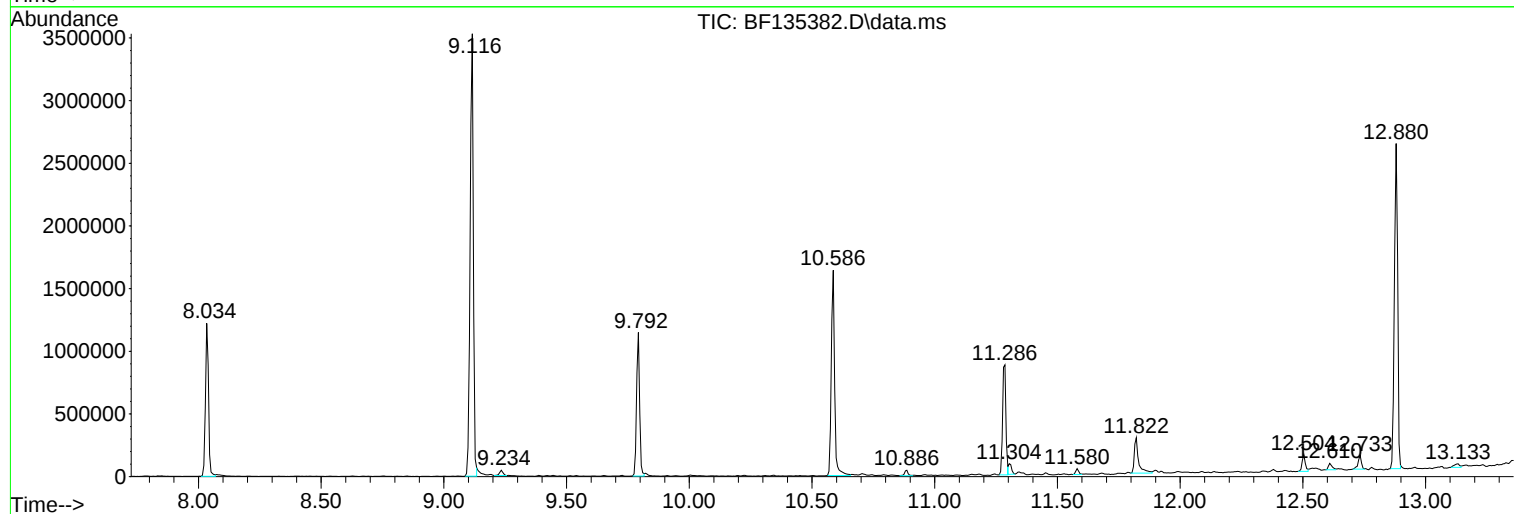
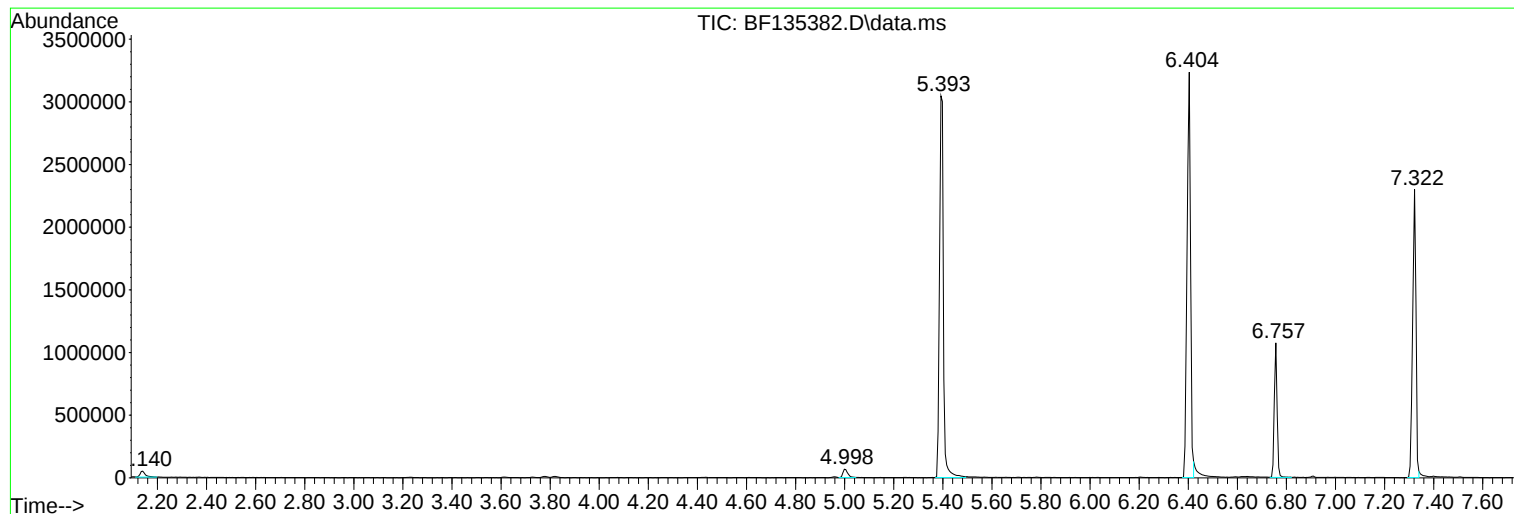
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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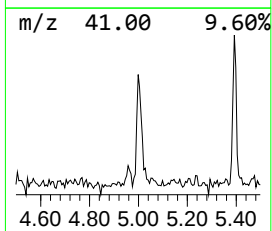
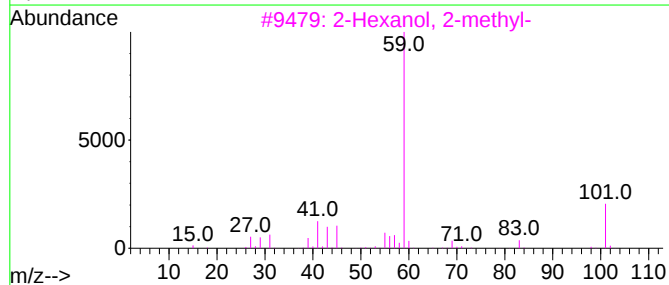
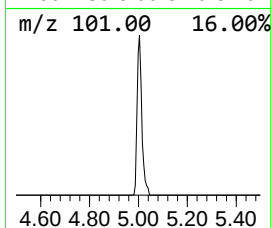
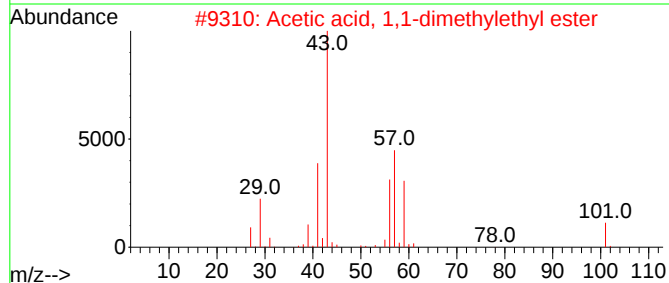
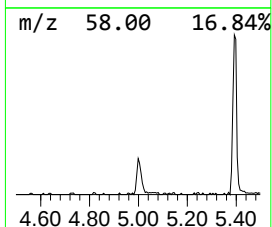
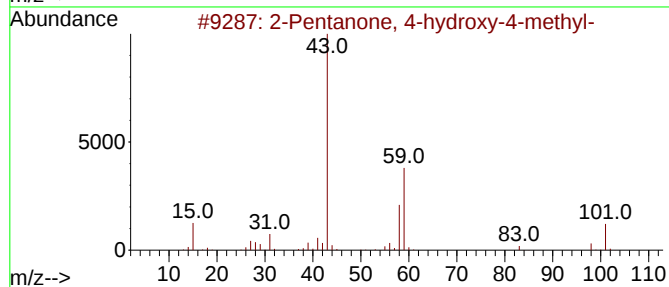
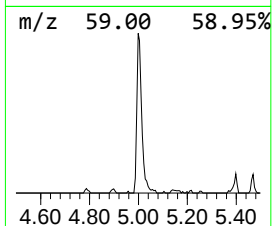
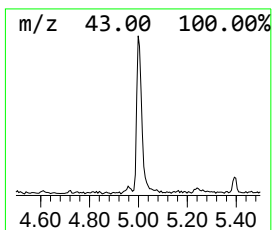
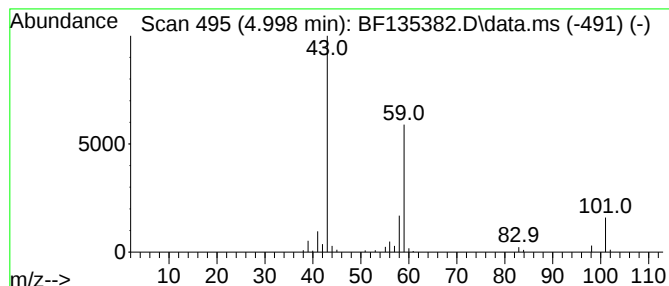
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.998	2.12 ng	91164	1,4-Dichlorobenzene-d4	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
4	Acetone	58	C3H6O	000067-64-1	9		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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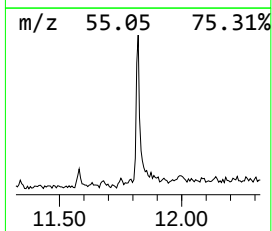
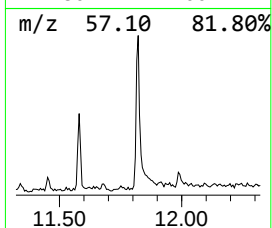
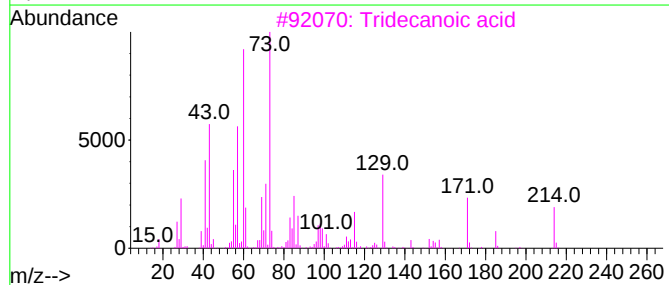
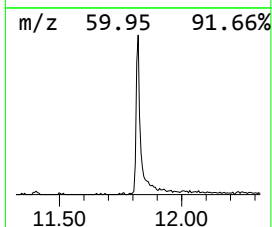
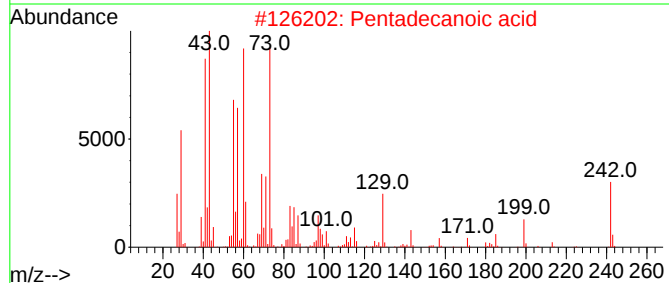
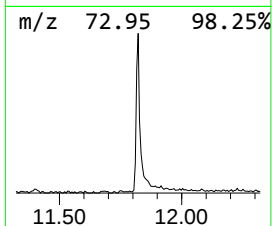
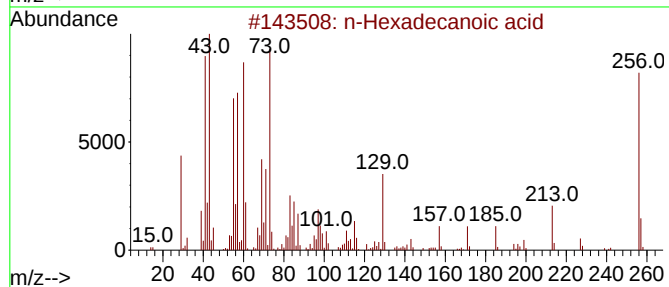
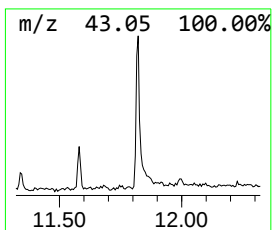
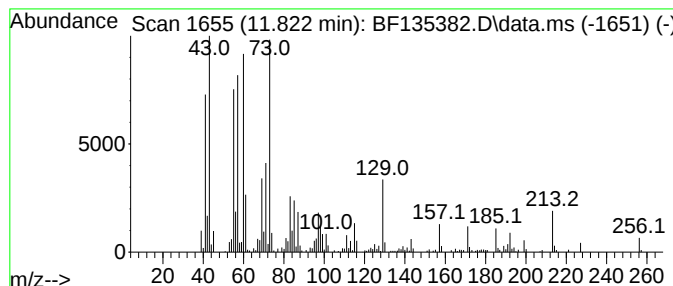
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.822	8.19 ng	340294	Phenanthrene-d10	11.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3			Tridecanoic acid	214	C13H26O2	000638-53-9	76
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			Octanoic acid	144	C8H16O2	000124-07-2	49



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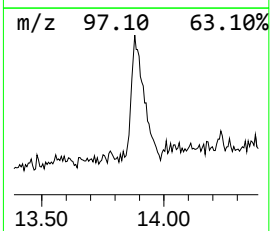
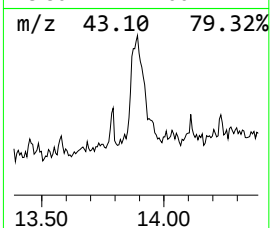
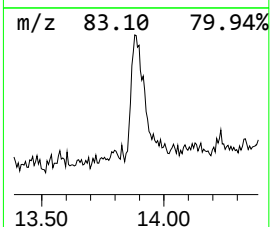
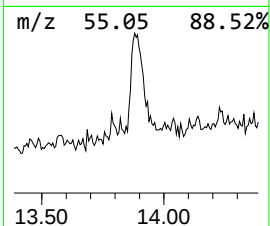
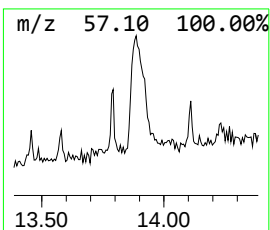
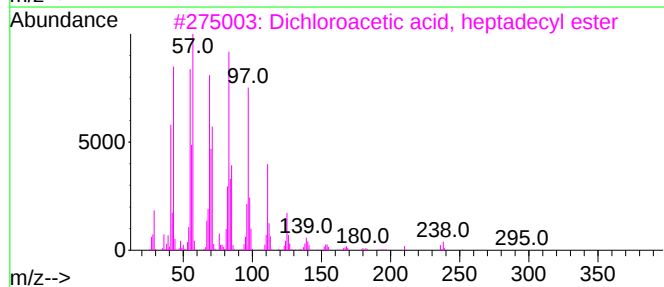
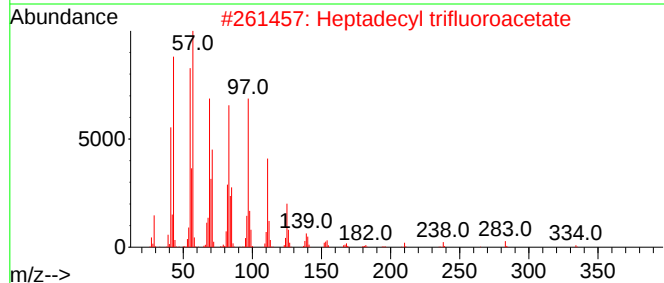
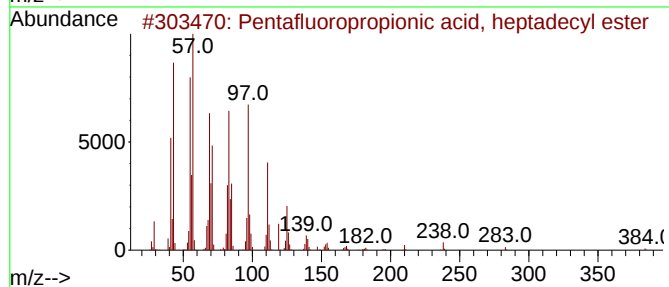
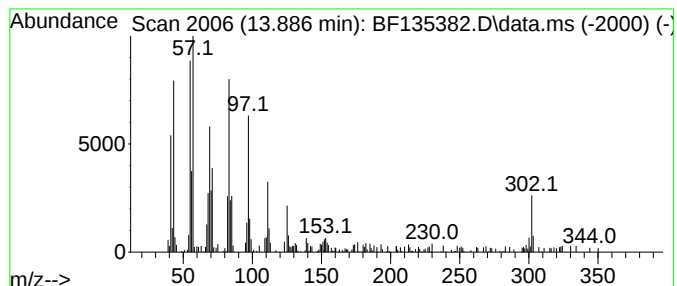
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Peak Number 4 Pentafluoropropionic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	7.32 ng	275794	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	93
2			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	93
3			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
4			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93
5			1-Hexacosene	364	C26H52	018835-33-1	93



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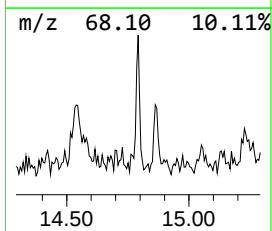
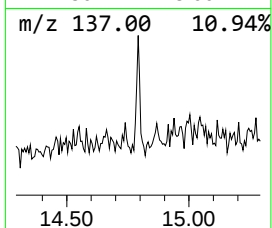
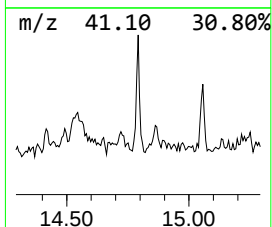
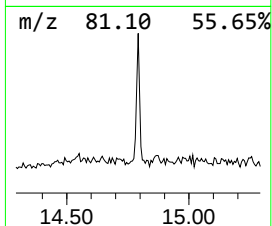
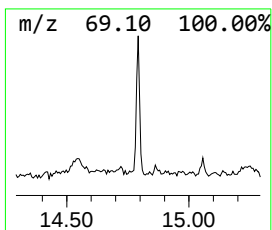
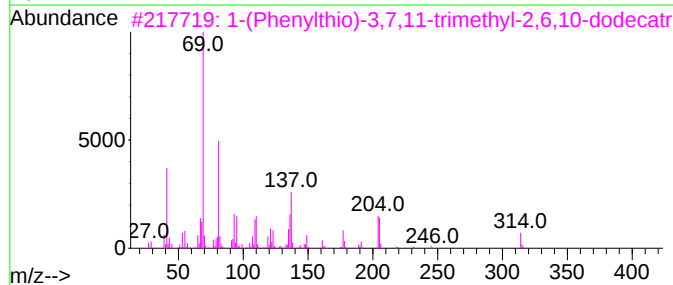
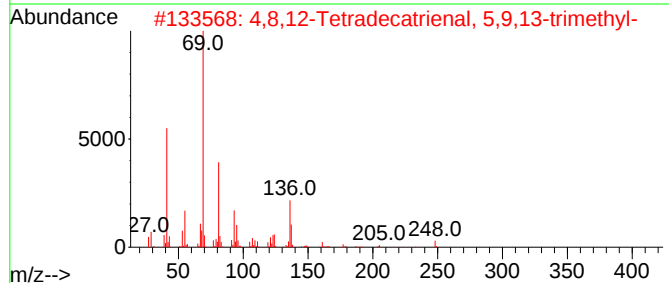
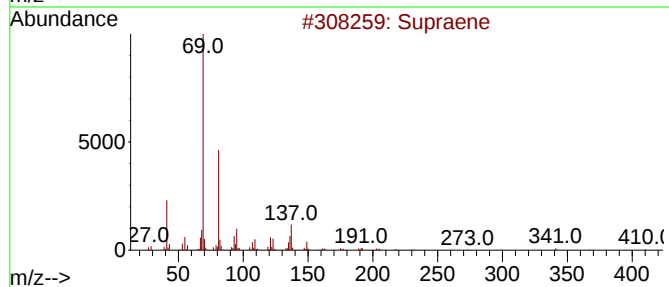
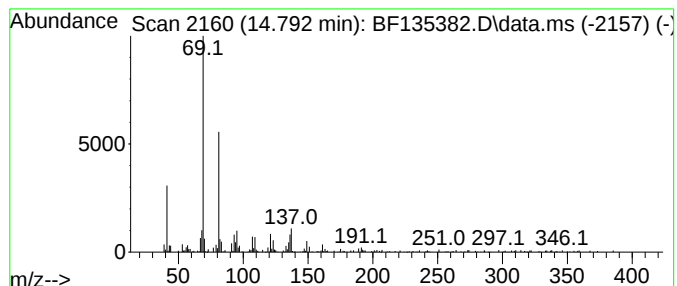
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Peak Number 5 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.792	3.71 ng	108436	Perylene-d12	15.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	90
2			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
3			1-(Phenylthio)-3,7,11-trimethyl-...	314	C21H30S	028413-57-2	72
4			Furan, 3-(4,8-dimethyl-3,7-nonad...	218	C15H22O	023262-34-2	64
5			1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	59



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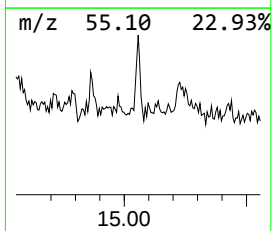
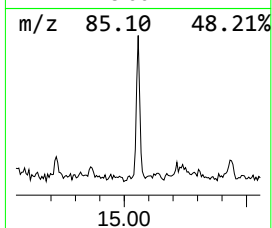
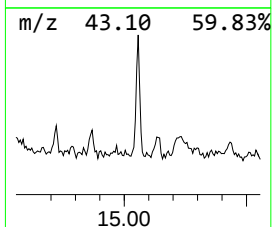
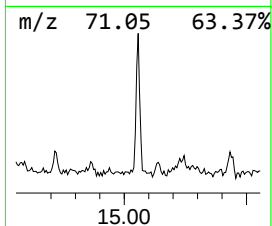
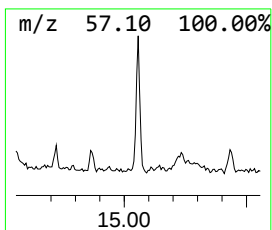
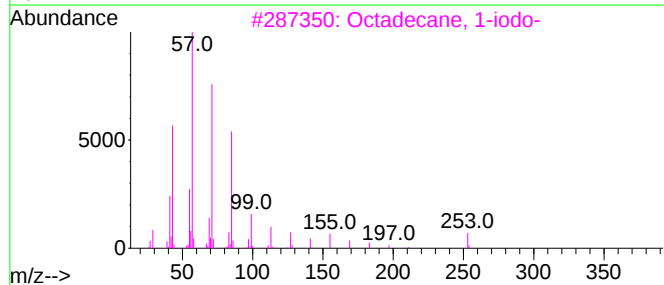
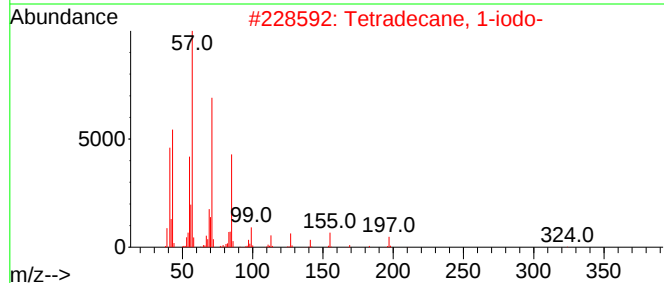
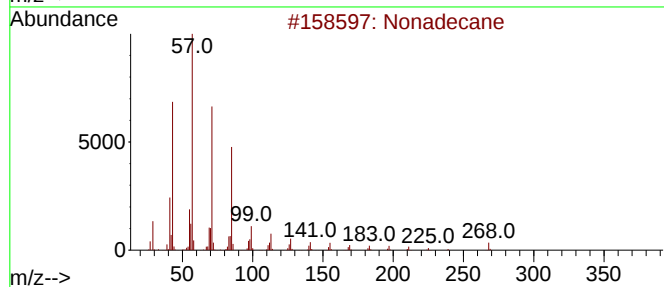
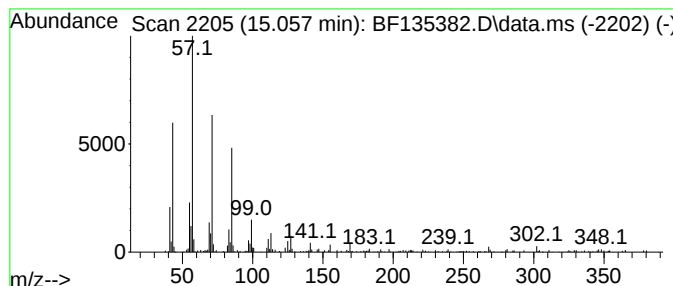
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Peak Number 6 Nonadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.057	4.91 ng	143693	Perylene-d12	15.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	93
2			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	83
3			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	83
4			Borane, diethyl(decyloxy)-	226	C14H31BO	1000152-34-3	83
5			Docosane, 1-iodo-	436	C22H45I	1000406-31-9	83



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306-TP-1-2-CS-1

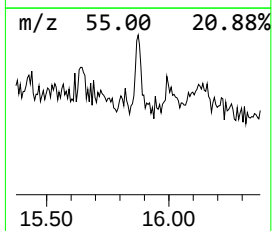
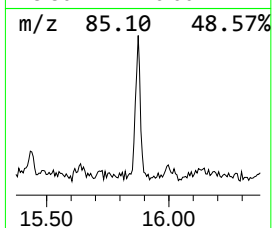
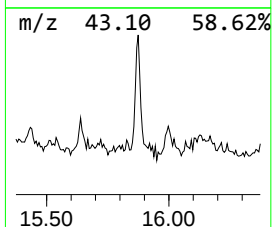
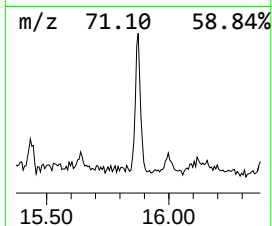
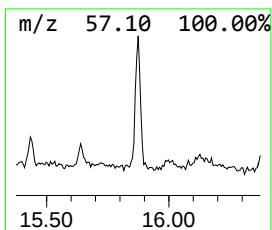
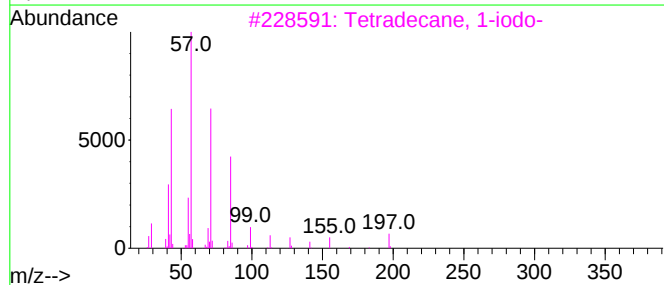
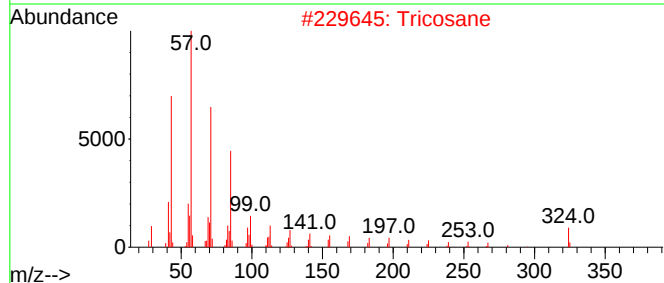
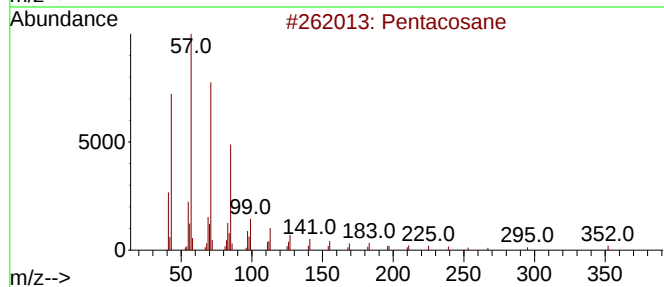
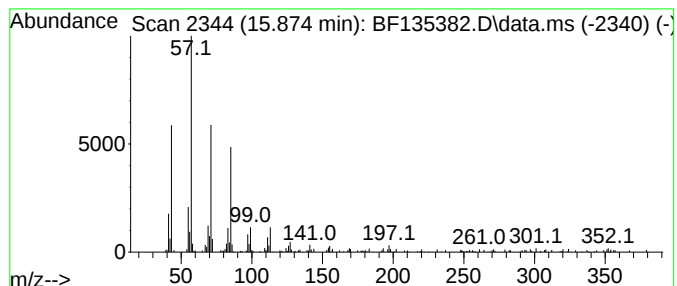
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.874	4.27 ng	124809	Perylene-d12	15.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	98
2			Tricosane	324	C23H48	000638-67-5	89
3			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	87
4			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	87
5			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092123\
Data File : BF135382.D
Acq On : 21 Sep 2023 16:06
Operator : CG\JU
Sample : 04407-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
306-TP-1-2-CS-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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-...	4.998	2.1	ng	91164	1	6.757	858397	20.0
n-Hexadecanoic ...	11.822	8.2	ng	340294	4	11.286	831168	20.0
Pentafluoroprop...	13.886	7.3	ng	275794	5	13.939	753392	20.0
Supraene	14.792	3.7	ng	108436	6	15.410	585134	20.0
Nonadecane	15.057	4.9	ng	143693	6	15.410	585134	20.0
Pentacosane	15.874	4.3	ng	124809	6	15.410	585134	20.0