

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090123\
 Data File : BF135075.D
 Acq On : 01 Sep 2023 14:33
 Operator : CG\JU
 Sample : 04203-05
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-6(12-12.5)

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-BF083023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135075.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	5	9	14	rVB	27264	33899	1.42%	0.218%
2	5.004	493	496	506	rVB	59593	74133	3.11%	0.477%
3	5.404	559	564	567	rBV	2438420	2237105	93.97%	14.401%
4	6.410	730	735	738	rBV	2356405	2164709	90.93%	13.935%
5	6.604	765	768	778	rBV	36727	46501	1.95%	0.299%
6	6.769	793	796	800	rBV	700003	560910	23.56%	3.611%
7	7.334	887	892	895	rBV	1611717	1410645	59.25%	9.081%
8	8.051	1010	1014	1017	rBV	794356	715305	30.05%	4.605%
9	9.128	1193	1197	1200	rBV	2732347	2380730	100.00%	15.325%
10	9.804	1308	1312	1316	rBV	860377	710169	29.83%	4.572%
11	10.598	1443	1447	1450	rBV	1435368	1186829	49.85%	7.640%
12	11.298	1562	1566	1570	rBV	725964	584878	24.57%	3.765%
13	11.833	1654	1657	1668	rBV2	106934	122634	5.15%	0.789%
14	12.627	1789	1792	1797	rBV2	28068	32135	1.35%	0.207%
15	12.898	1834	1838	1841	rBV	2171828	1874370	78.73%	12.066%
16	13.827	1990	1996	2012	rBV2	60147	156716	6.58%	1.009%
17	13.951	2013	2017	2024	rVV	640806	588105	24.70%	3.786%
18	14.815	2161	2164	2169	rBV	24299	26761	1.12%	0.172%
19	15.421	2261	2267	2272	rBV	511452	628129	26.38%	4.043%

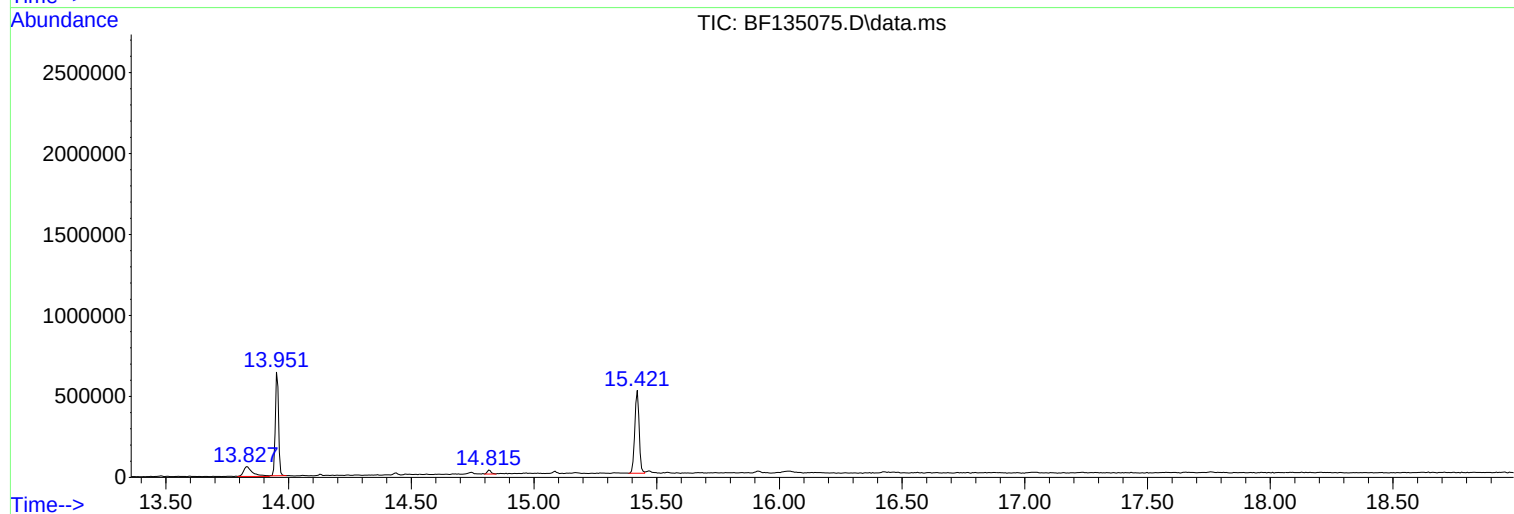
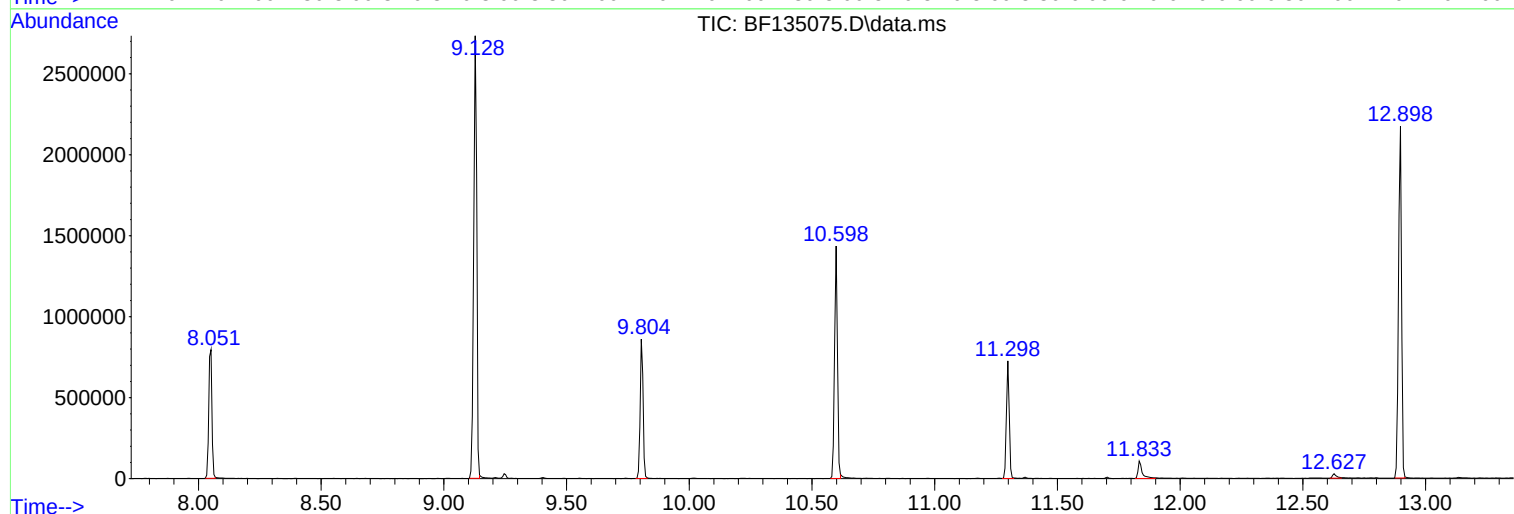
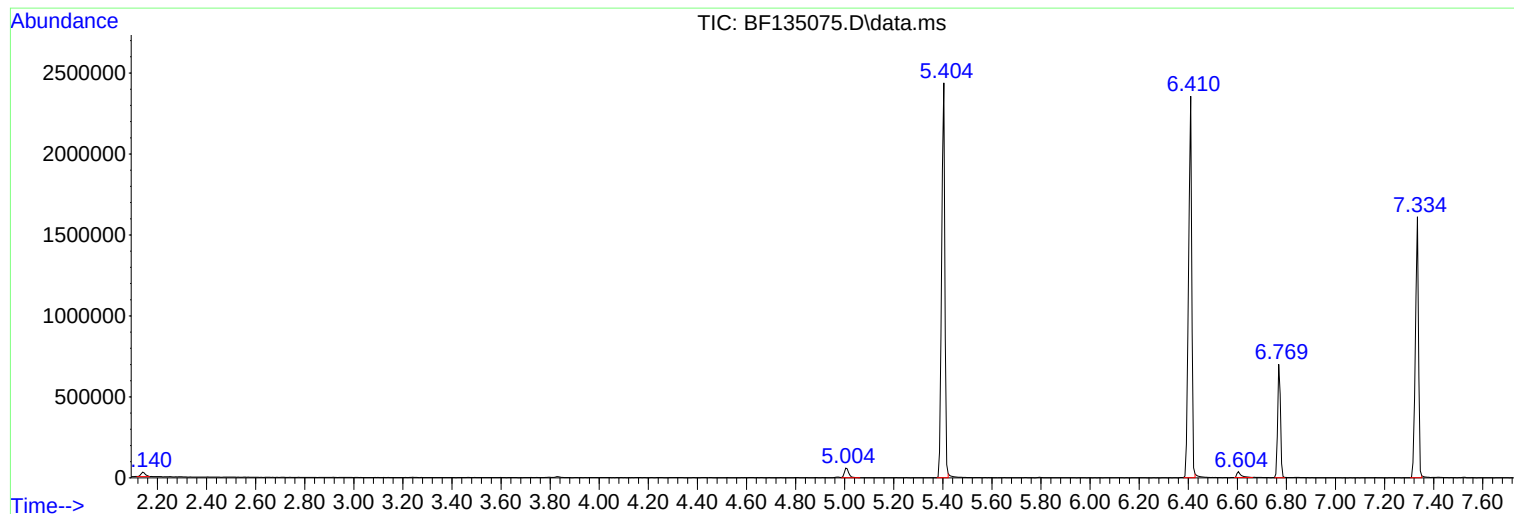
Sum of corrected areas: 15534663

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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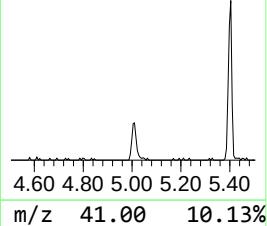
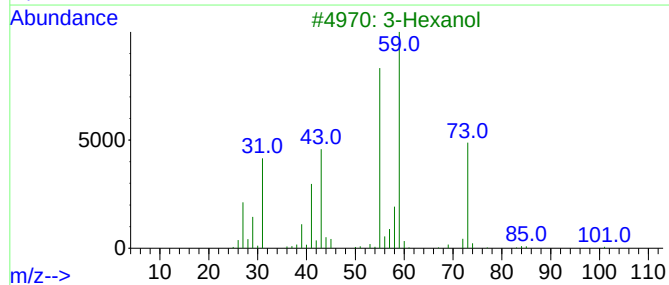
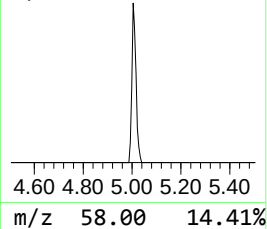
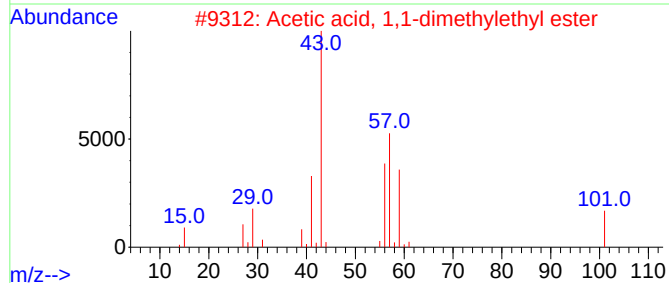
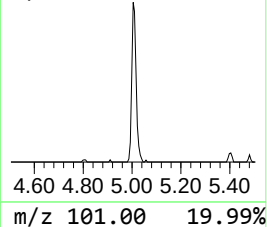
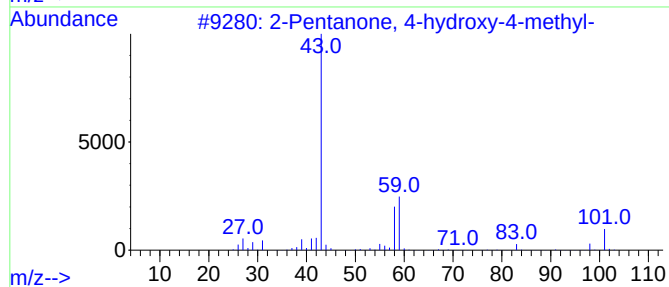
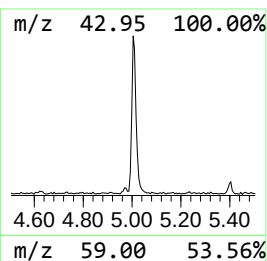
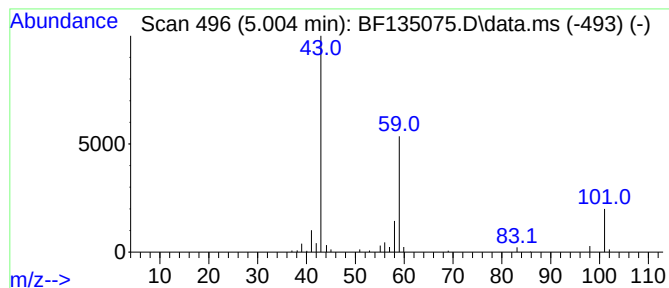
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.004	2.64 ng	74133	1,4-Dichlorobenzene-d4	6.769

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64	
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	50	
3	3-Hexanol	102	C6H14O	000623-37-0	28	
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25	
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17	



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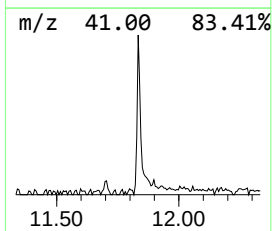
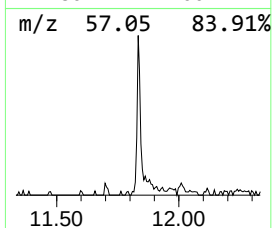
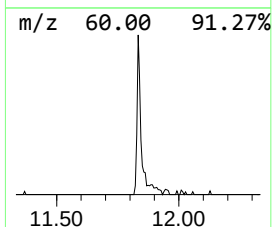
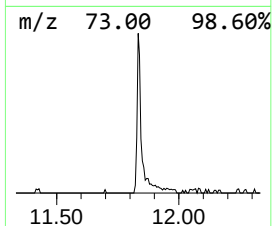
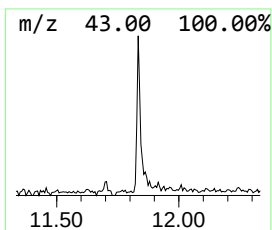
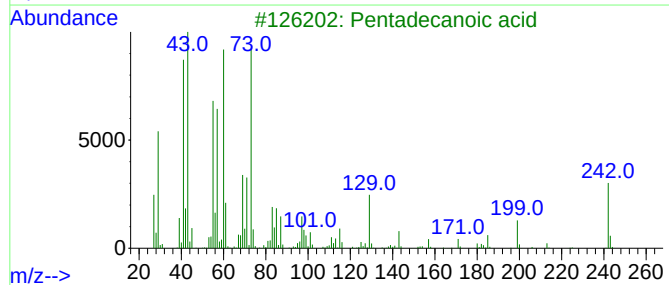
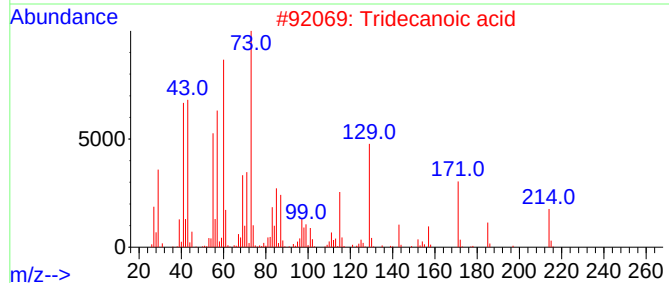
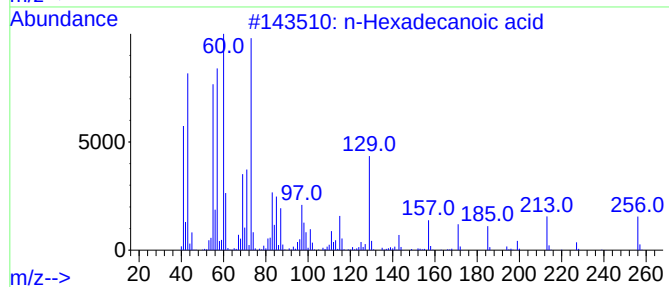
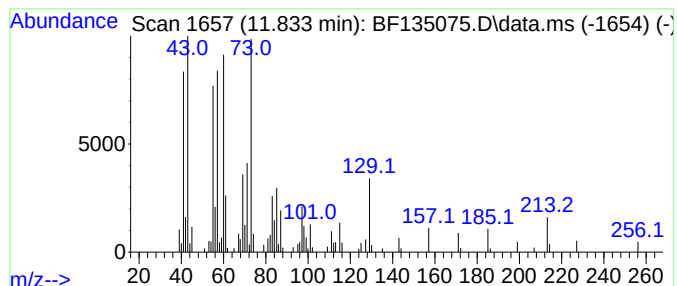
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.833	4.19 ng	122634	Phenanthrene-d10	11.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Tridecanoic acid	214	C13H26O2	000638-53-9	87
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	78



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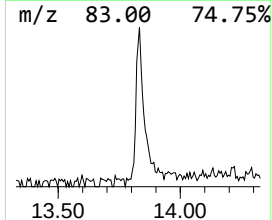
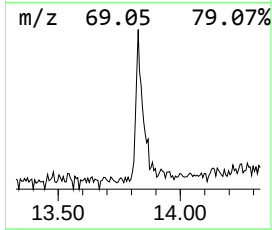
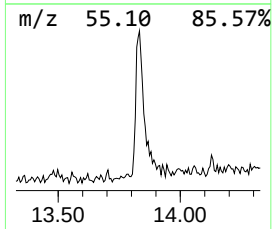
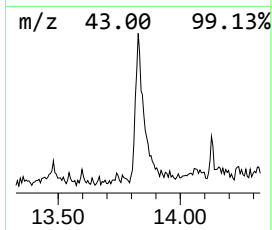
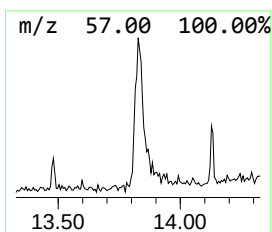
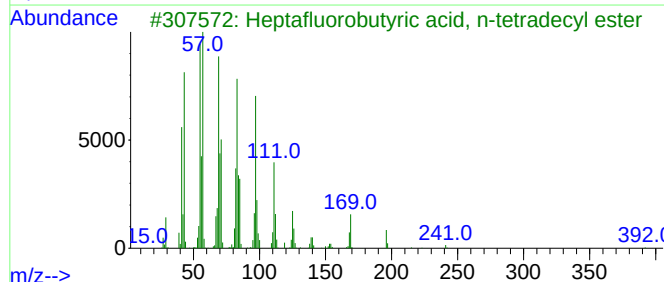
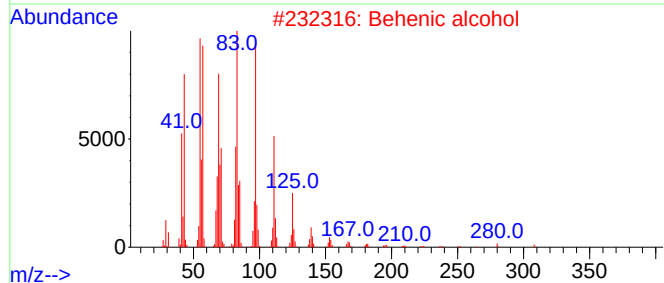
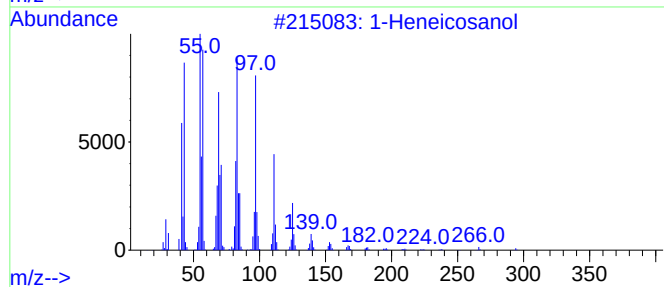
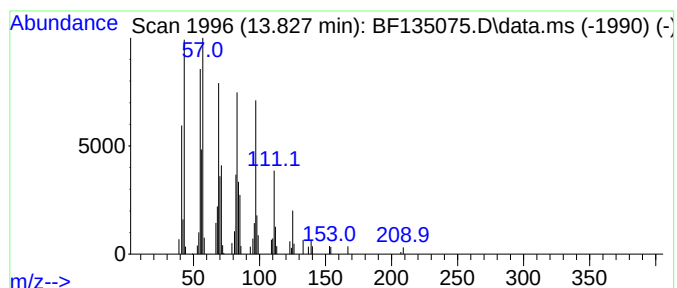
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Peak Number 3 1-Heneicosanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	5.33 ng	156716	Chrysene-d12	13.951

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			Behenic alcohol	326	C22H46O	000661-19-8	94
3			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5			11-Tricosene	322	C23H46	052078-56-5	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.004	2.6	ng	74133	1	6.769	560910	20.0
n-Hexadecanoic ...	11.833	4.2	ng	122634	4	11.298	584878	20.0
1-Heneicosanol	13.827	5.3	ng	156716	5	13.951	588105	20.0