

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042423\
 Data File : BF132995.D
 Acq On : 24 Apr 2023 15:06
 Operator : CG\JU
 Sample : 02469-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TWP-02

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-BF042123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132995.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.740	278	281	288	rVB	55223	74981	1.26%	0.219%
2	4.934	474	484	487	rBV	1194571	1328672	22.26%	3.875%
3	5.351	551	555	559	rBV	1960742	1693247	28.36%	4.938%
4	6.375	725	729	732	rBV	1322491	1019781	17.08%	2.974%
5	6.745	788	792	795	rBV	1603801	1286292	21.55%	3.751%
6	6.810	800	803	814	rBV	714686	637633	10.68%	1.860%
7	7.310	882	888	891	rBV	3937515	3725299	62.40%	10.864%
8	8.028	1006	1010	1013	rBV	2197839	1745799	29.24%	5.091%
9	9.110	1188	1194	1197	rBV	6552615	5969943	100.00%	17.410%
10	9.781	1304	1308	1311	rBV	2443236	1945943	32.60%	5.675%
11	10.198	1376	1379	1382	rBV	316750	234947	3.94%	0.685%
12	10.492	1424	1429	1432	rBV	176988	139653	2.34%	0.407%
13	10.569	1437	1442	1445	rBV	3029438	2551612	42.74%	7.441%
14	11.263	1556	1560	1563	rBV	2512911	1945114	32.58%	5.673%
15	11.798	1647	1651	1665	rBV2	380796	430341	7.21%	1.255%
16	12.586	1781	1785	1795	rBV	183045	202074	3.38%	0.589%
17	12.857	1826	1831	1834	rBV	5813681	5834967	97.74%	17.017%
18	13.786	1982	1989	1999	rBV3	117380	255350	4.28%	0.745%
19	13.898	2004	2008	2012	rBV	1686947	1441724	24.15%	4.205%
20	13.992	2020	2024	2031	rBV	99787	128217	2.15%	0.374%
21	14.757	2150	2154	2158	rVB	533039	489265	8.20%	1.427%
22	15.321	2245	2250	2256	rBV	1086182	1208946	20.25%	3.526%

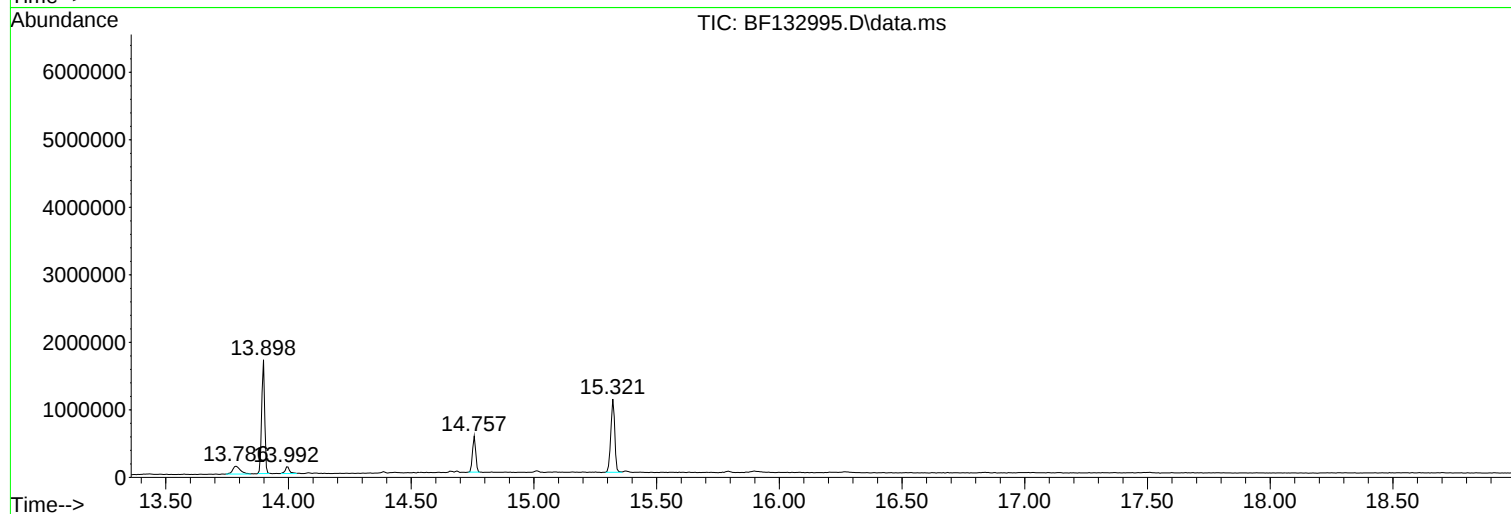
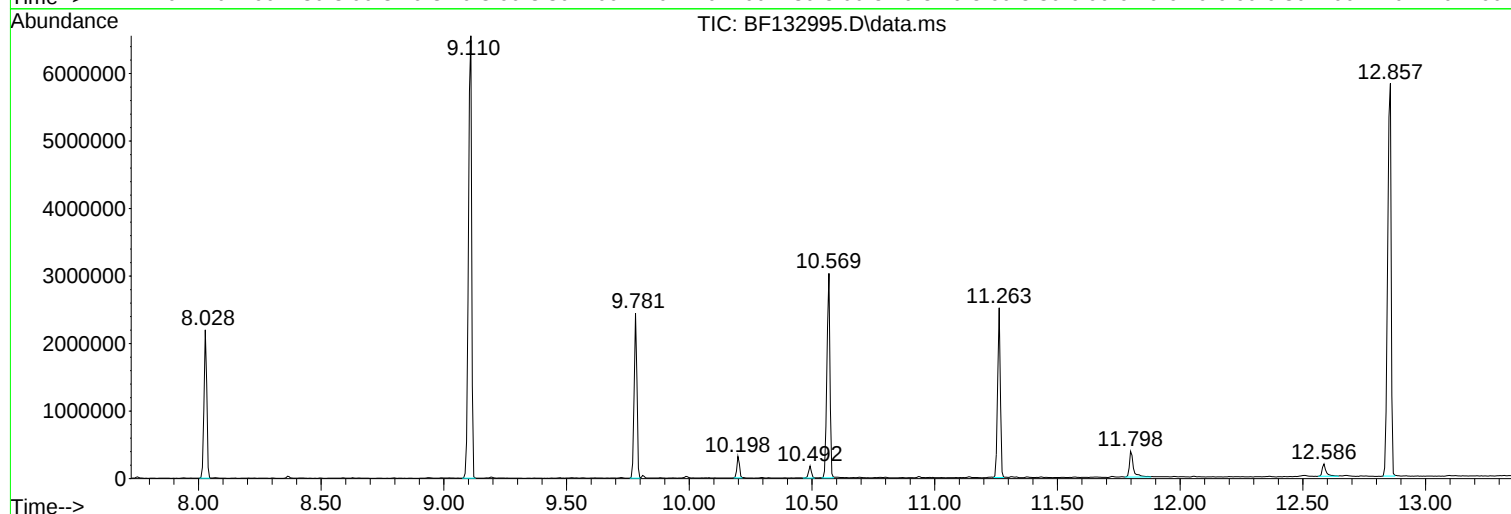
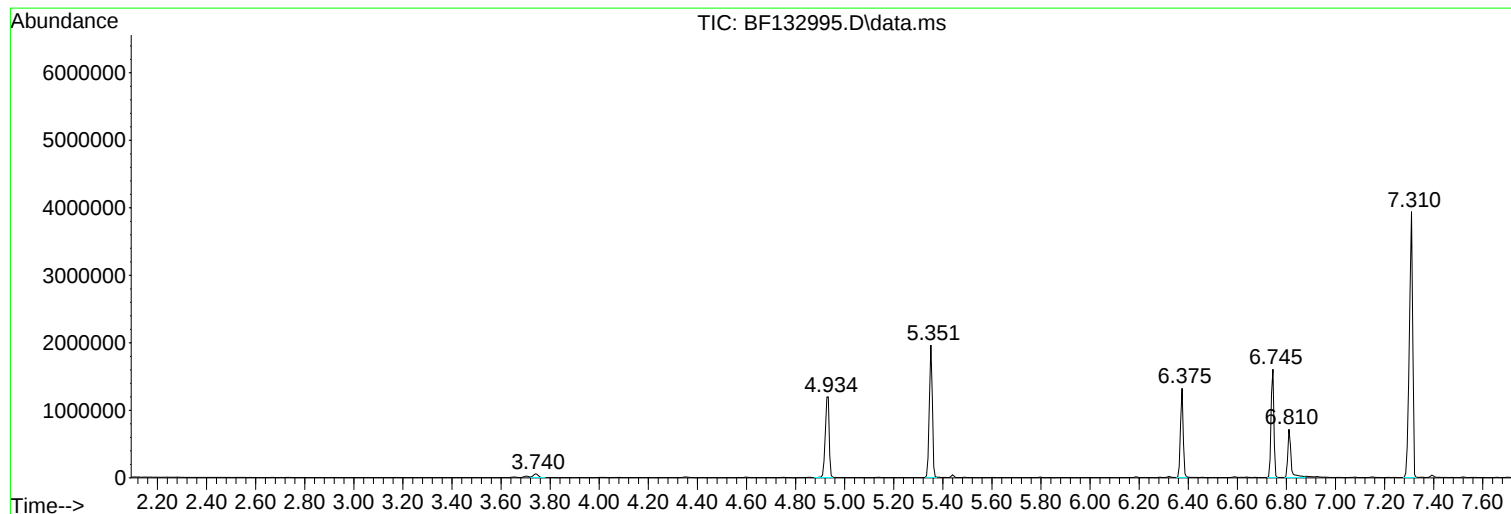
Sum of corrected areas: 34289800

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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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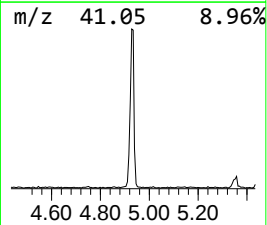
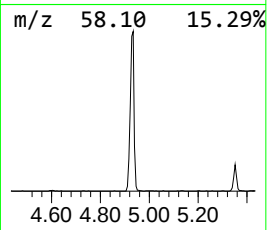
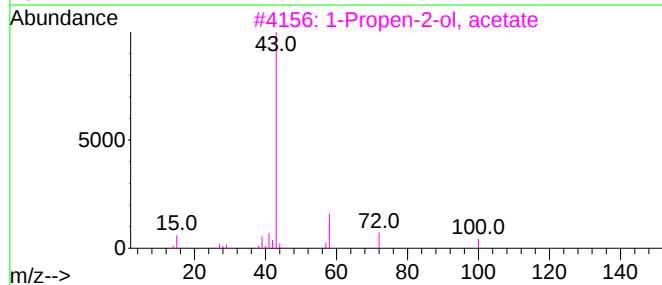
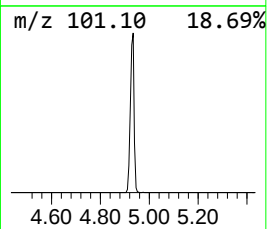
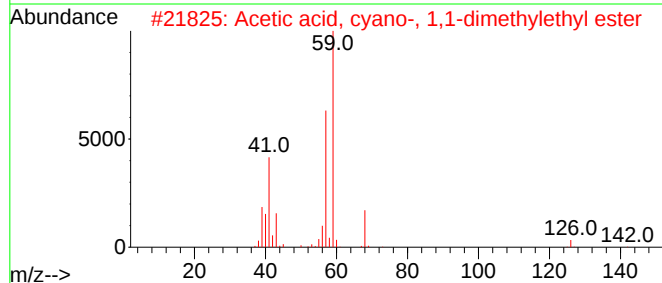
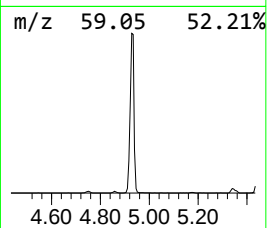
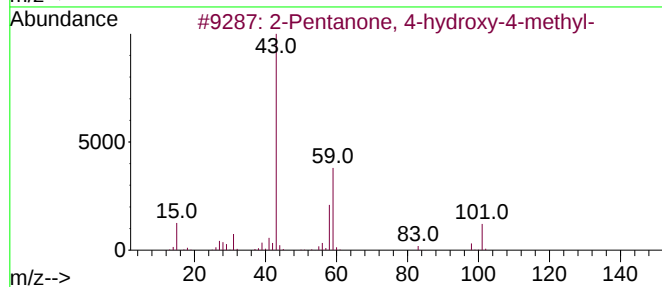
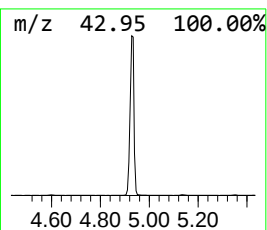
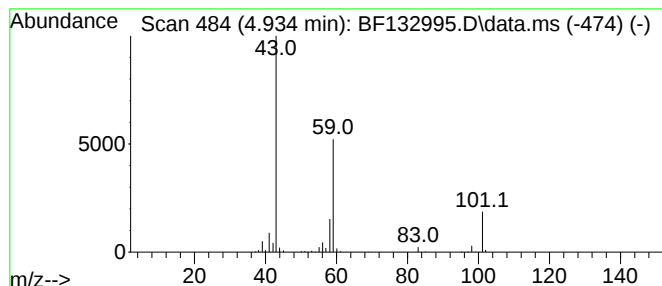
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
4.934	20.66 ng	1328670	1,4-Dichlorobenzene-d4			6.745
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, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	12
4	Morpholine, 4-methyl-		101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	9



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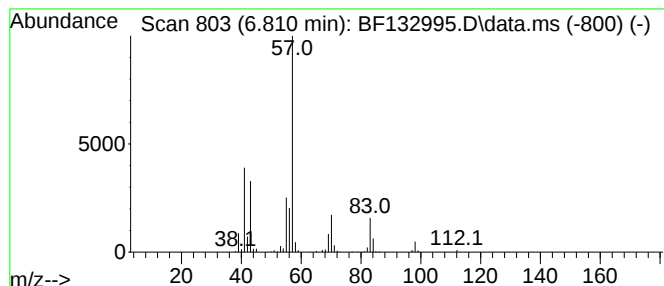
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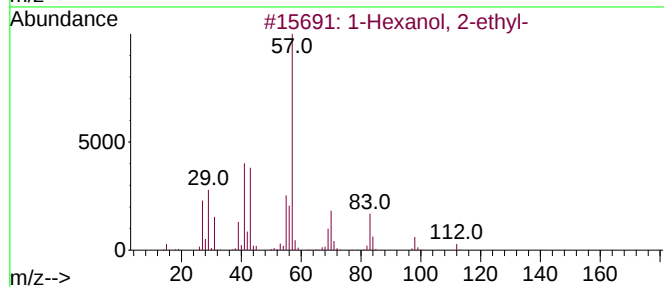
Peak Number 2 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
0.000	0.00 ng	637633	1,4-Dichlorobenzene-d4	6.745

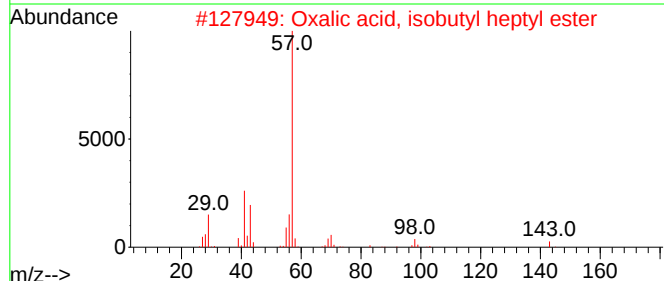
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2			Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	59
3			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	56
4			1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	50
5			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	50



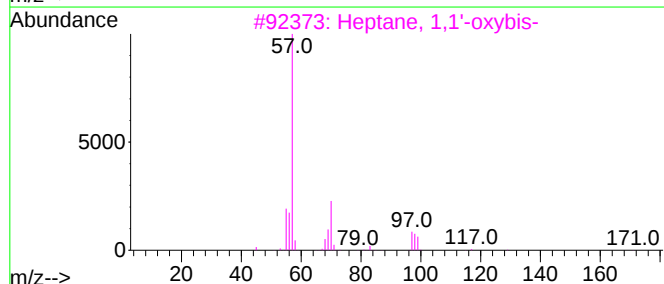
m/z	57.05	100.00%
	2.20 2.40 2.60 2.80 3.00	
m/z	41.05	39.04%



	2.20 2.40 2.60 2.80 3.00	
m/z	43.05	32.84%



	2.20 2.40 2.60 2.80 3.00	
m/z	55.05	25.26%



	2.20 2.40 2.60 2.80 3.00	
m/z	56.05	20.40%
	2.20 2.40 2.60 2.80 3.00	

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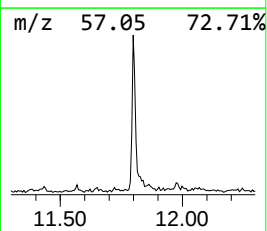
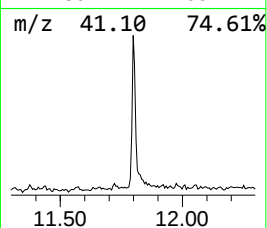
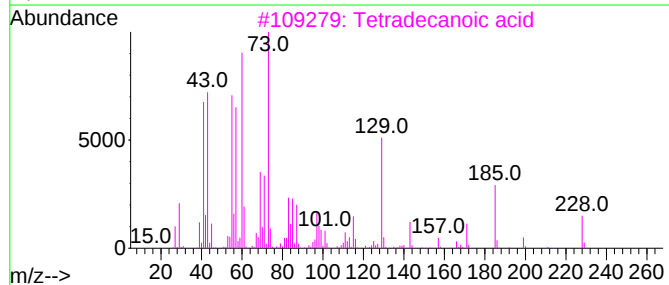
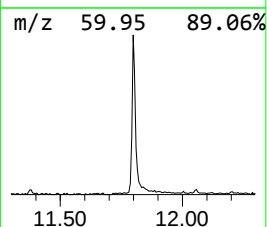
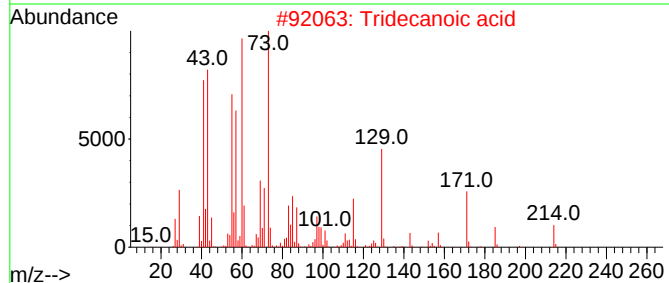
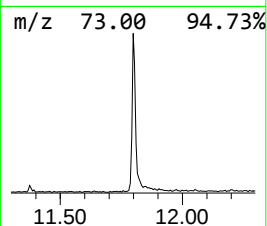
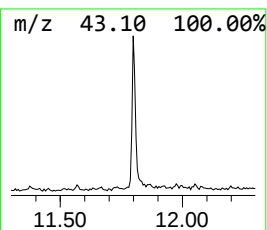
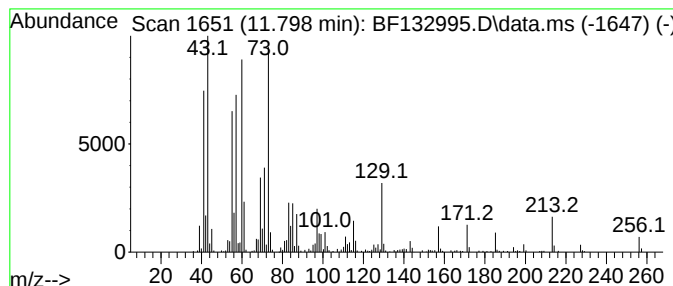
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.798	4.42 ng	430341	Phenanthrene-d10	11.263

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			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	35



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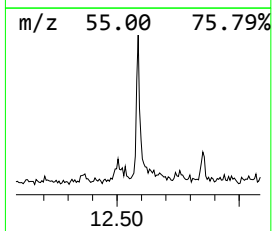
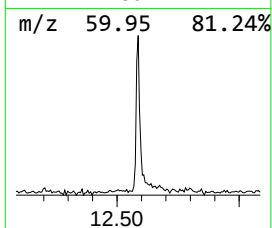
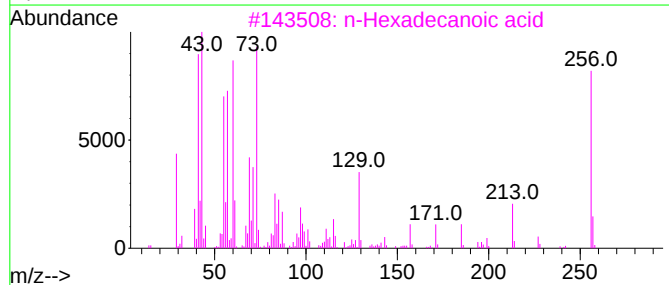
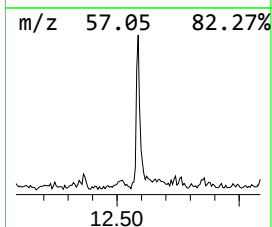
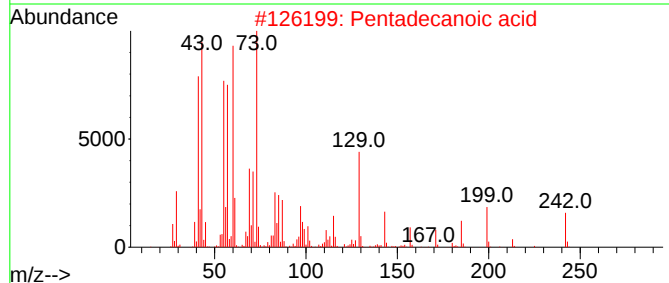
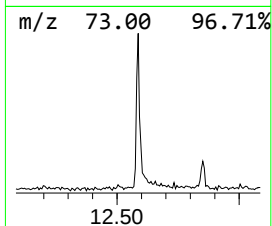
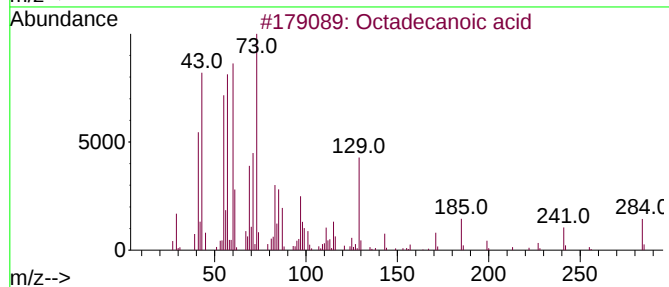
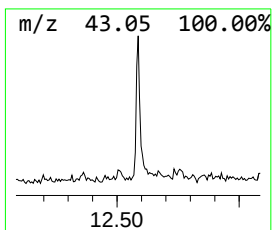
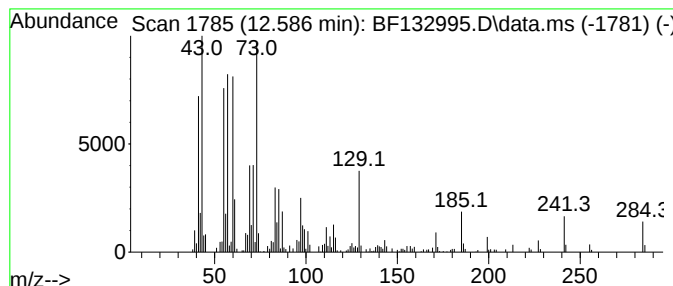
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Peak Number 4 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.586	2.80 ng	202074	Chrysene-d12	13.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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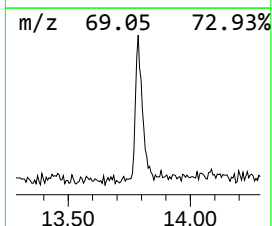
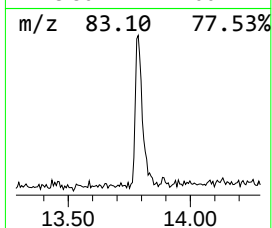
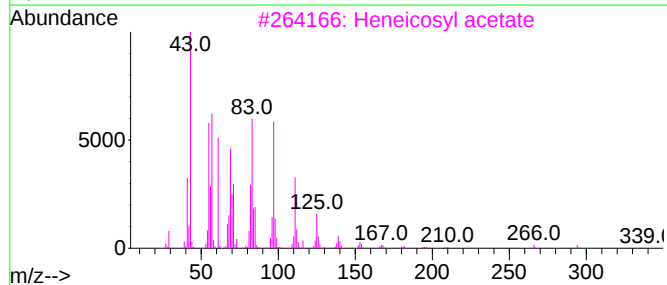
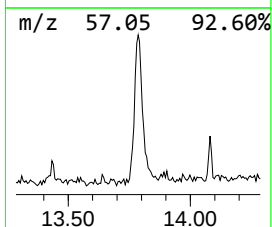
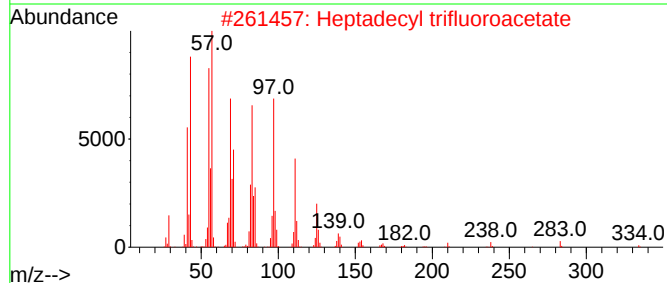
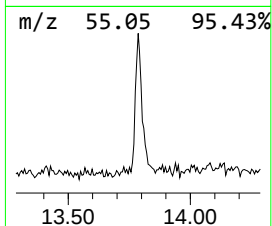
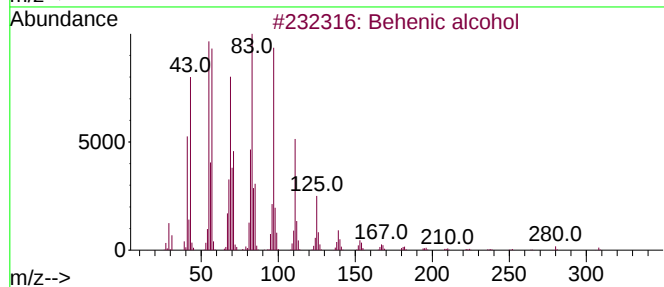
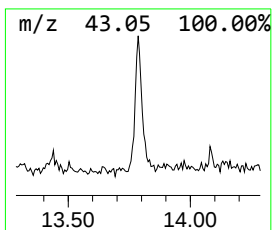
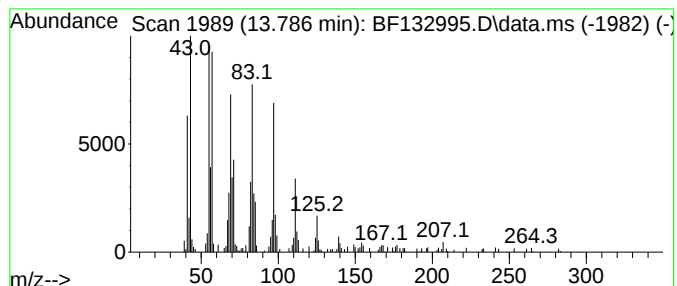
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Peak Number 5 Behenic alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.786	3.54 ng	255350	Chrysene-d12	13.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	95
2			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
3			Heneicosyl acetate	354	C23H46O2	1000351-77-3	94
4			Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	94
5			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94



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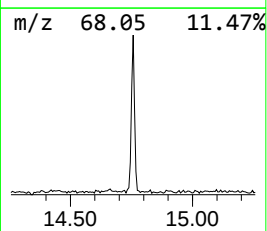
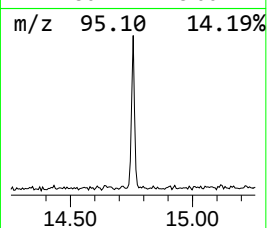
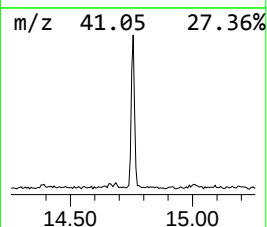
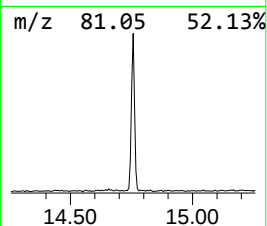
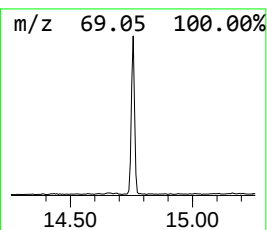
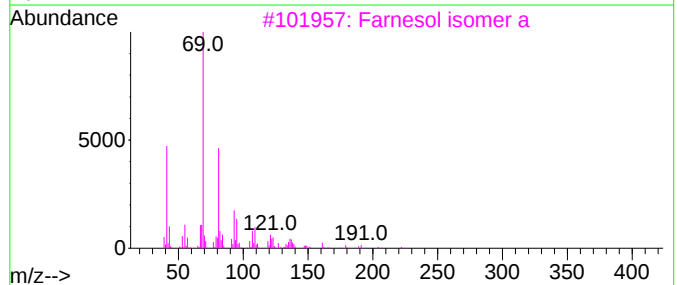
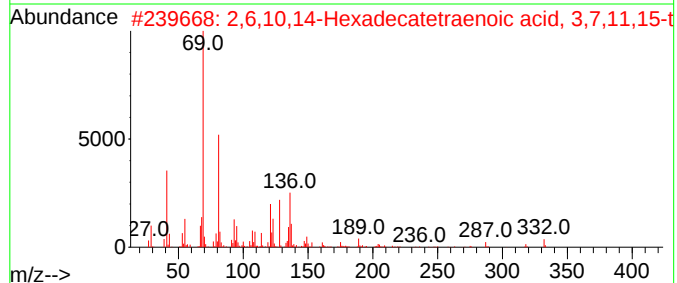
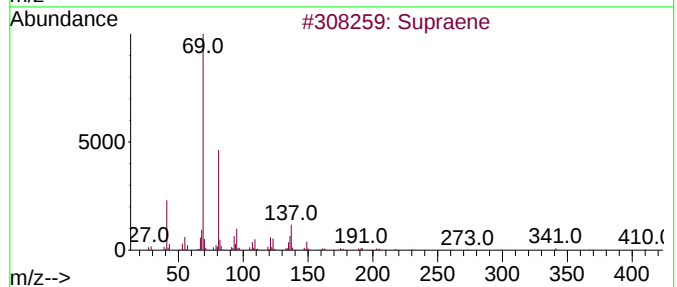
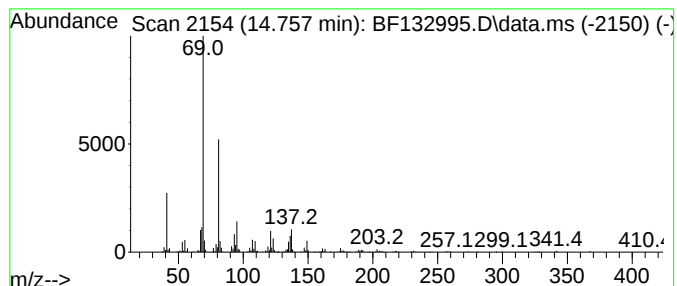
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.757	8.09 ng	489265	Perylene-d12	15.321

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
3			Farnesol isomer a	222	C15H26O	1000108-92-4	64
4			1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	52
5			2,6-Octadiene, 4-methyl-	124	C9H16	074498-94-5	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042423\
Data File : BF132995.D
Acq On : 24 Apr 2023 15:06
Operator : CG\JU
Sample : 02469-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TWP-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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
2-Pentanone, 4-...	4.934	20.7	ng	1328670	1	6.745	1286290	20.0
1-Hexanol, 2-et...	0.000	0.0	ng	637633	1	6.745	1286290	20.0
n-Hexadecanoic ...	11.798	4.4	ng	430341	4	11.263	1945110	20.0
Octadecanoic acid	12.586	2.8	ng	202074	5	13.898	1441720	20.0
Behenic alcohol	13.786	3.5	ng	255350	5	13.898	1441720	20.0
Supraene	14.757	8.1	ng	489265	6	15.321	1208950	20.0