

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090123\
 Data File : BF135073.D
 Acq On : 01 Sep 2023 13:30
 Operator : CG\JU
 Sample : 04203-03
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-3(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: BF135073.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.110	3	4	9	rVB	23585	23715	1.38%	0.186%
2	4.992	491	494	503	rVB	54745	65673	3.82%	0.516%
3	5.398	559	563	566	rBV	1981957	1698618	98.86%	13.351%
4	6.410	730	735	738	rBV	1811238	1680080	97.79%	13.205%
5	6.604	765	768	777	rBV	64732	73513	4.28%	0.578%
6	6.769	793	796	800	rBV	643734	528573	30.76%	4.154%
7	7.333	887	892	895	rBV	1231188	1036035	60.30%	8.143%
8	8.051	1010	1014	1017	rBV	772877	678102	39.47%	5.330%
9	9.127	1193	1197	1200	rBV	2189506	1718125	100.00%	13.504%
10	9.245	1214	1217	1225	rVB	46514	43317	2.52%	0.340%
11	9.804	1309	1312	1316	rBV	840722	675661	39.33%	5.311%
12	10.598	1443	1447	1461	rBV	1168739	981505	57.13%	7.714%
13	11.298	1562	1566	1570	rBV	722749	577010	33.58%	4.535%
14	11.833	1654	1657	1668	rBV	139297	159729	9.30%	1.255%
15	12.627	1789	1792	1801	rBV	35363	46813	2.72%	0.368%
16	12.898	1833	1838	1841	rBV	1617903	1398664	81.41%	10.993%
17	13.827	1991	1996	2006	rBV3	53710	127004	7.39%	0.998%
18	13.951	2013	2017	2021	rBV	558687	550968	32.07%	4.330%
19	14.815	2161	2164	2168	rVB	72209	75721	4.41%	0.595%
20	15.421	2262	2267	2273	rBV	465979	563364	32.79%	4.428%
21	15.915	2347	2351	2354	rVB4	14200	20821	1.21%	0.164%

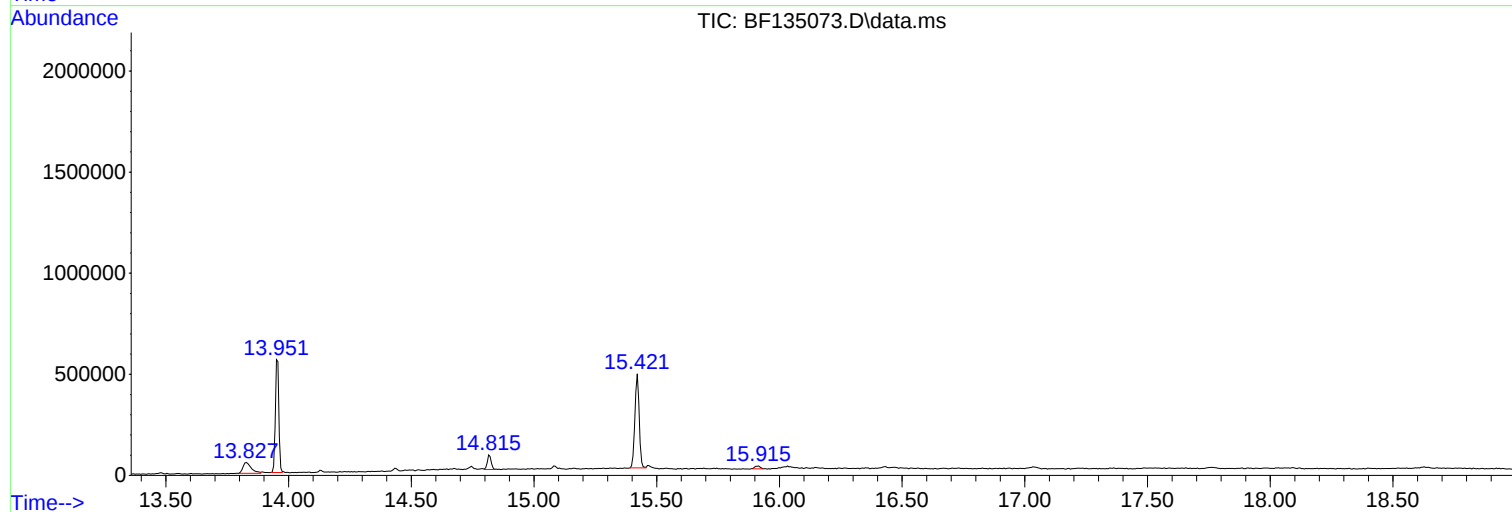
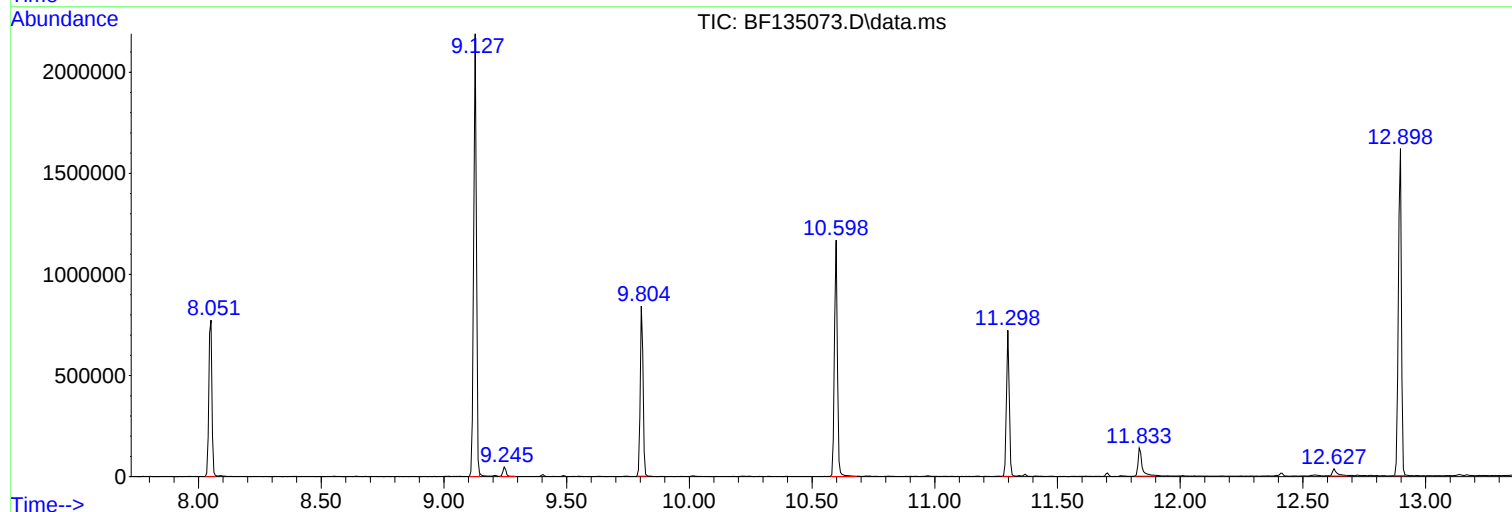
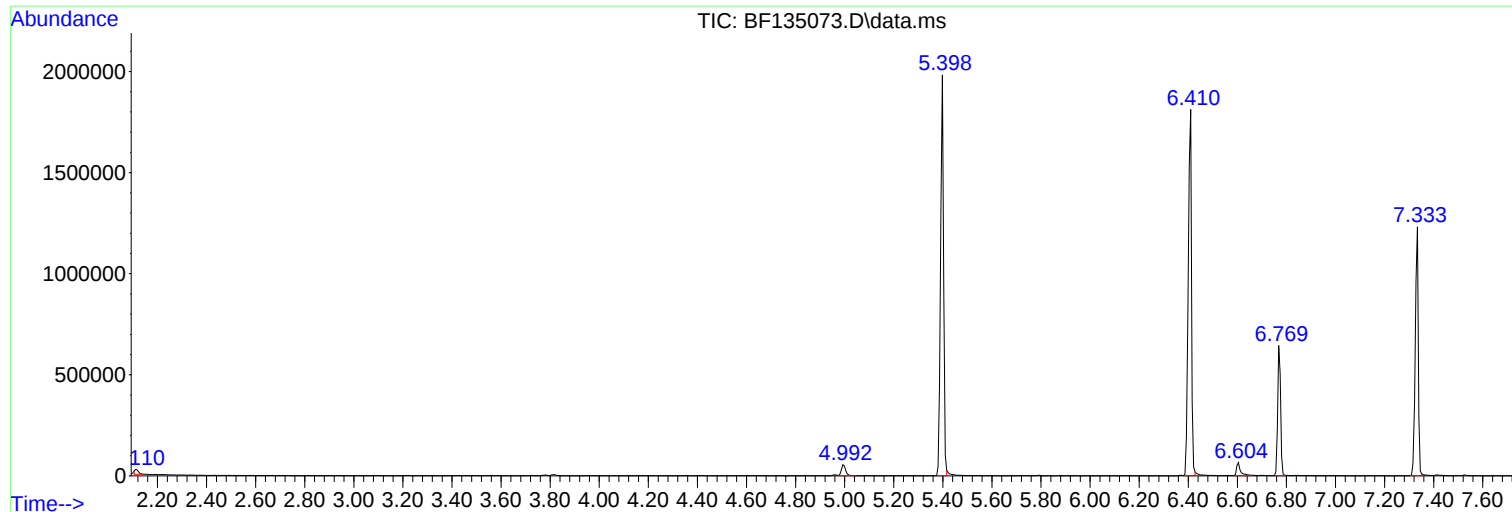
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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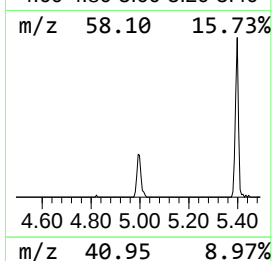
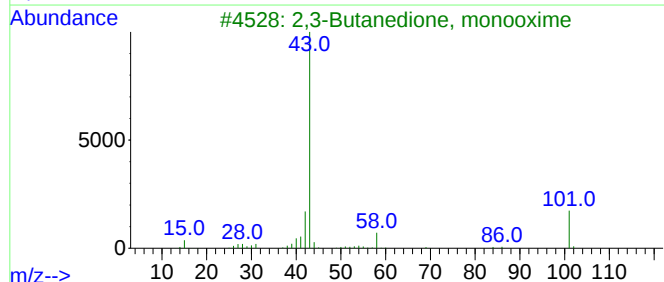
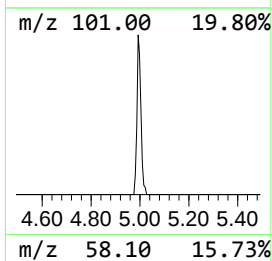
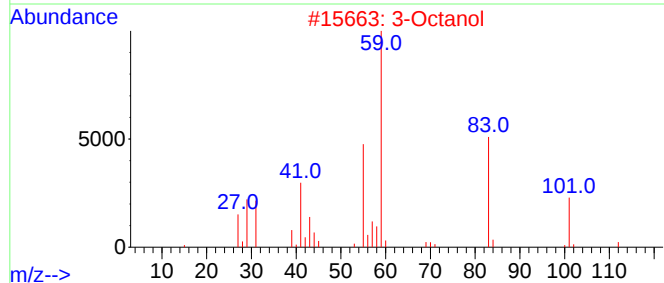
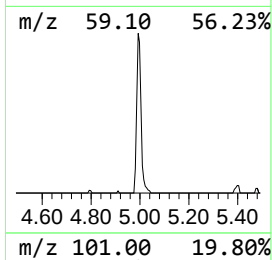
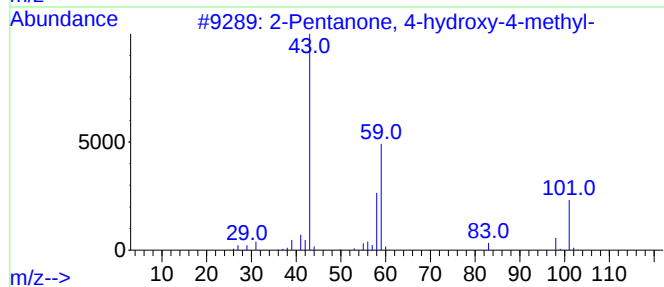
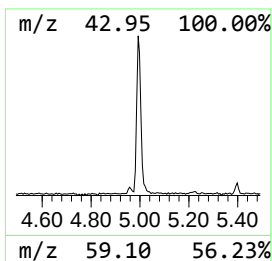
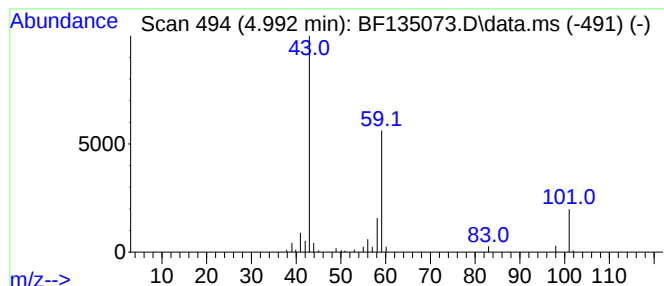
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.992	2.48 ng	65673	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	56		
2	3-Octanol	130	C8H18O	000589-98-0	33		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
5	Acetone	58	C3H6O	000067-64-1	9		



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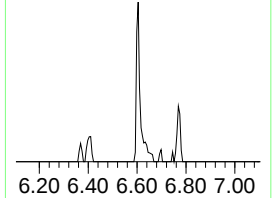
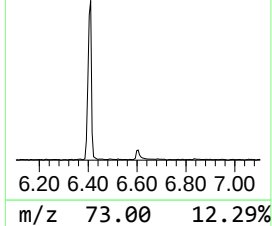
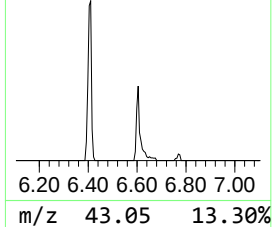
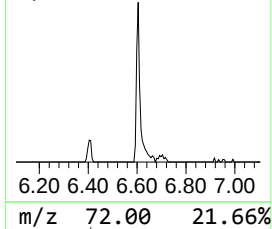
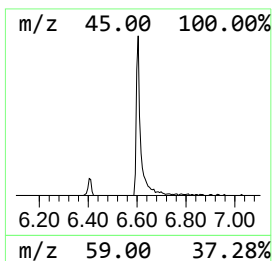
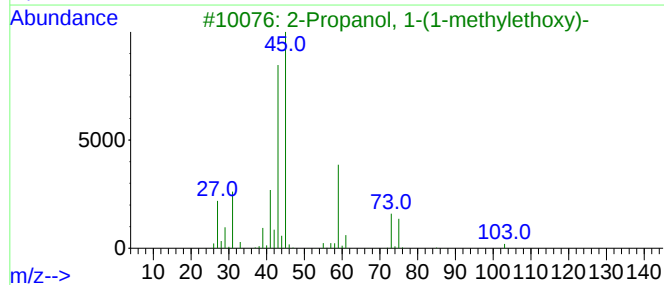
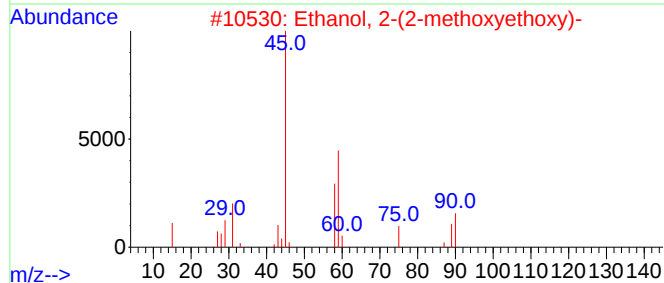
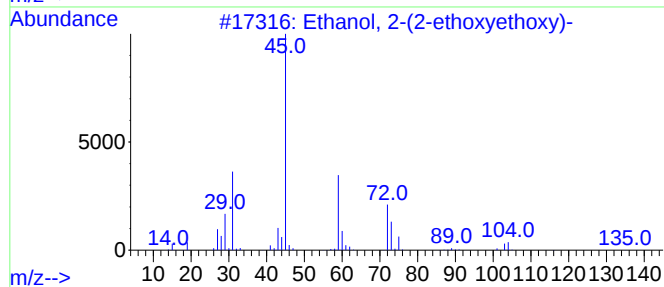
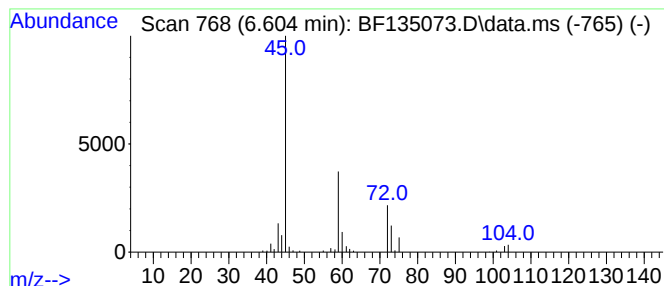
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.604	2.78 ng	73513	1,4-Dichlorobenzene-d4	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2			Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	45
3			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	38
4			Carbonic acid, dimethyl ester	90	C3H6O3	000616-38-6	36
5			.beta.-Methoxyethoxymethyl chloride	124	C4H9ClO2	003970-21-6	36



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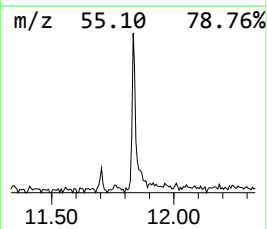
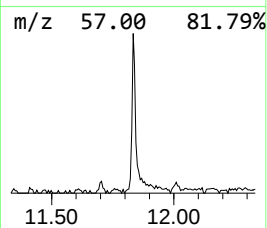
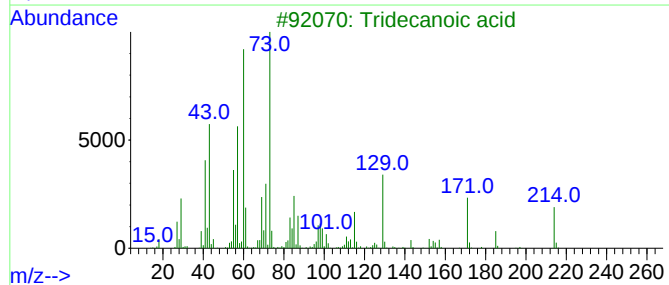
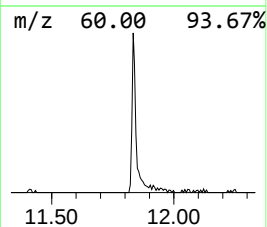
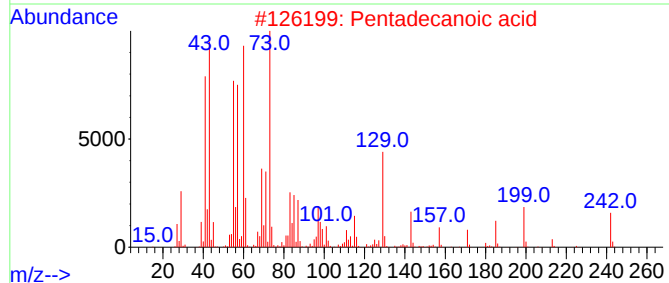
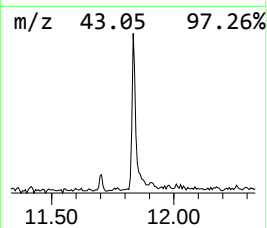
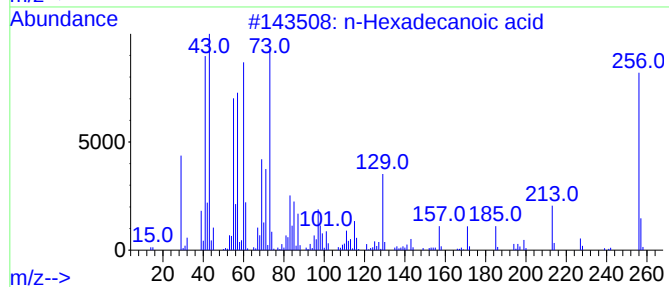
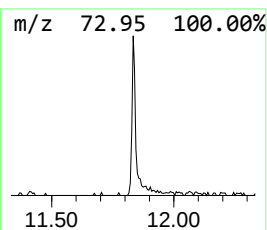
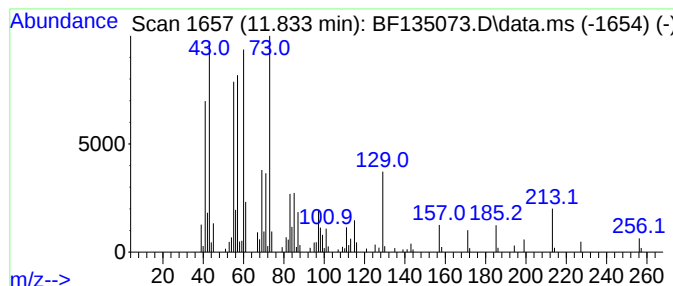
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.833	5.54 ng	159729	Phenanthrene-d10	11.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Tridecanoic acid	214	C13H26O2	000638-53-9	89
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			n-Decanoic acid	172	C10H20O2	000334-48-5	55



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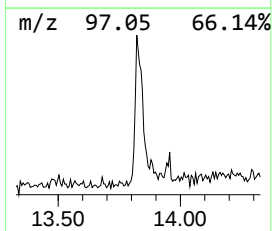
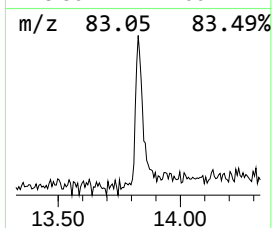
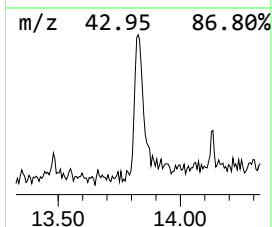
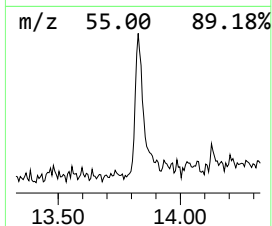
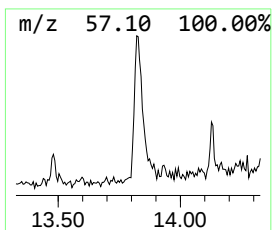
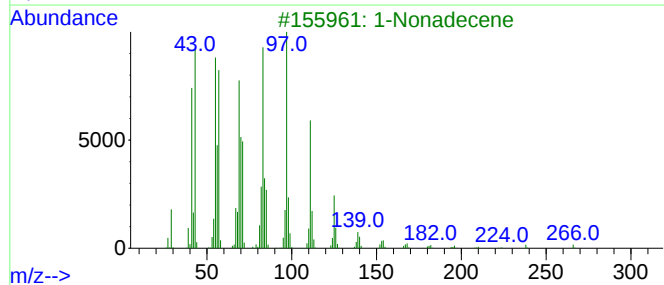
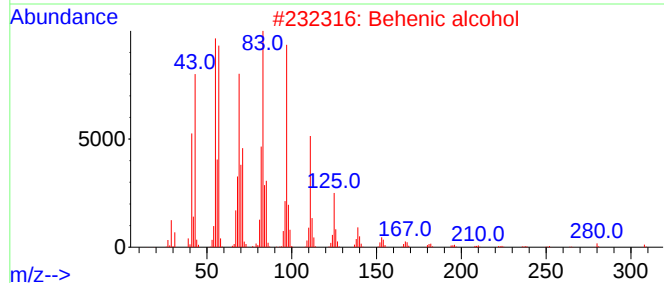
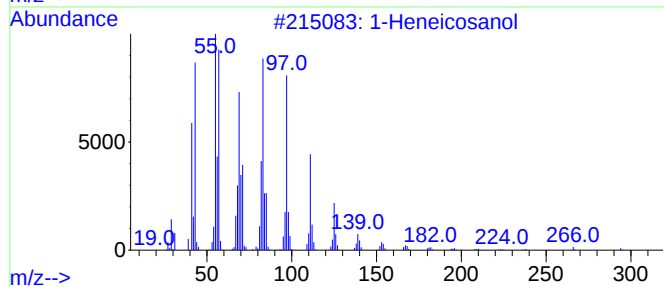
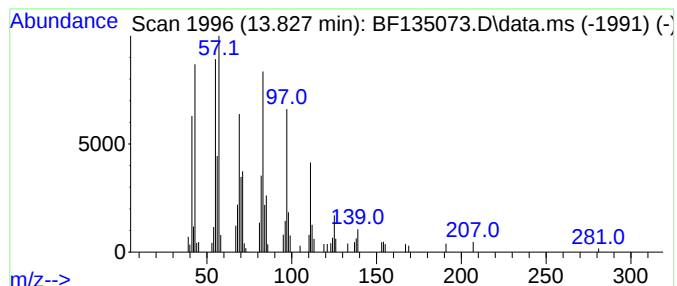
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Heneicosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	4.61 ng	127004	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	93
3			1-Nonadecene	266	C19H38	018435-45-5	91
4			3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	90
5			n-Heptadecanol-1	256	C17H36O	001454-85-9	90



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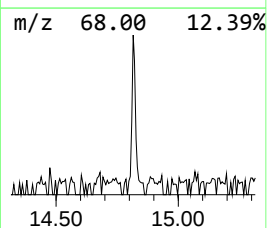
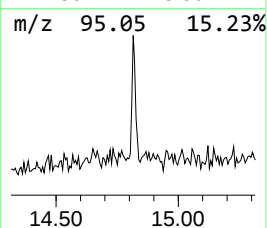
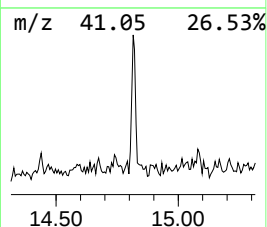
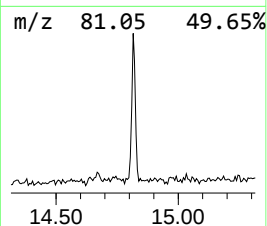
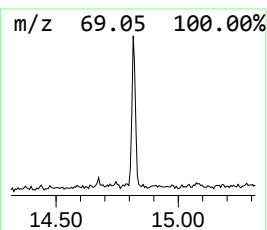
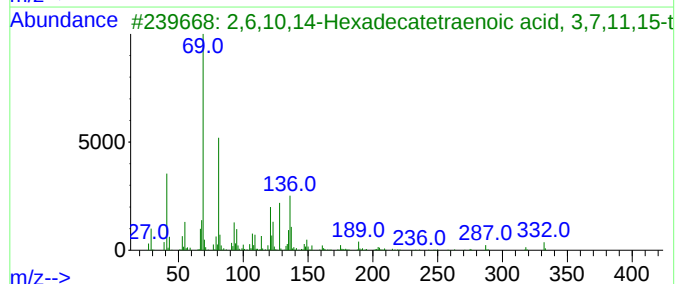
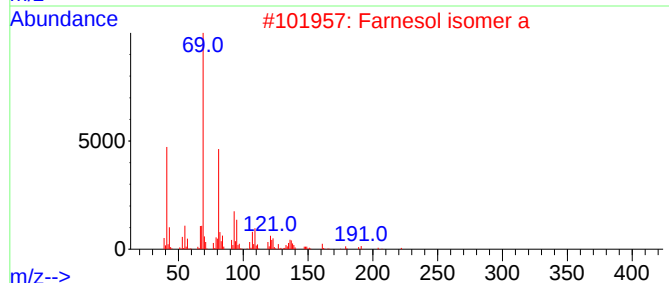
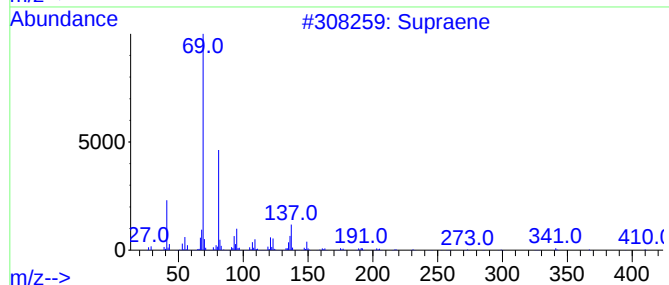
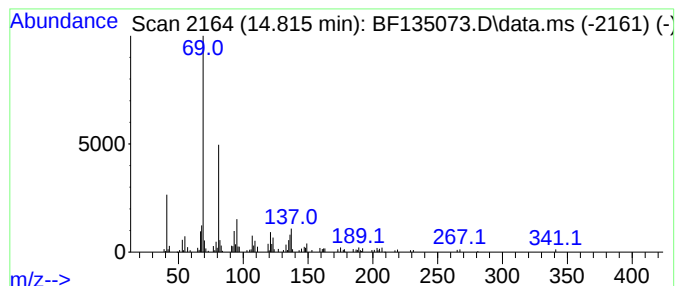
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.815	2.69 ng	75721	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	86
2			Farnesol isomer a	222	C15H26O	1000108-92-4	72
3			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64
4			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
5			5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	001117-52-8	59



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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-...	4.992	2.5	ng	65673	1	6.769	528573	20.0
Ethanol, 2-(2-e...	6.604	2.8	ng	73513	1	6.769	528573	20.0
n-Hexadecanoic ...	11.833	5.5	ng	159729	4	11.298	577010	20.0
1-Heneicosanol	13.827	4.6	ng	127004	5	13.951	550968	20.0
Supraene	14.815	2.7	ng	75721	6	15.421	563364	20.0