

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112120\
 Data File : BF122430.D
 Acq On : 21 Nov 2020 20:12
 Operator : JU/CG
 Sample : L4839-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B3-9-10

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-BF110920.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122430.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	6	11	22	rVB	321427	437946	6.97%	1.089%
2	2.257	26	29	40	rVB	63137	97901	1.56%	0.243%
3	5.075	502	508	518	rBV	965729	1230740	19.59%	3.060%
4	5.487	573	578	581	rBV	4309521	4407830	70.15%	10.958%
5	5.875	641	644	651	rVB	138019	110046	1.75%	0.274%
6	6.498	744	750	754	rBV	4199382	4752335	75.64%	11.814%
7	6.687	779	782	790	rBV	79806	79311	1.26%	0.197%
8	6.863	808	812	815	rBV	1525701	1186976	18.89%	2.951%
9	7.428	902	908	911	rBV	2736896	2948244	46.92%	7.329%
10	8.151	1026	1031	1034	rBV	1624369	1525028	24.27%	3.791%
11	9.228	1209	1214	1217	rBV	5990355	5346858	85.10%	13.292%
12	9.622	1277	1281	1285	rBV	257811	250236	3.98%	0.622%
13	9.839	1310	1318	1325	rBV6	28891	66879	1.06%	0.166%
14	9.904	1325	1329	1333	rBV	1961621	1801863	28.68%	4.479%
15	10.698	1459	1464	1478	rBV	3261454	3347717	53.28%	8.322%
16	11.392	1578	1582	1589	rBV	2091980	1910791	30.41%	4.750%
17	11.922	1666	1672	1680	rBV2	70733	122155	1.94%	0.304%
18	12.716	1802	1807	1819	rBV	159311	278184	4.43%	0.692%
19	12.986	1848	1853	1856	rBV	6303964	6283028	100.00%	15.619%
20	13.886	2002	2006	2021	rBV	264320	420329	6.69%	1.045%
21	14.039	2028	2032	2043	rVB	2213586	1930724	30.73%	4.800%
22	14.515	2108	2113	2121	rBV4	40138	67871	1.08%	0.169%
23	15.515	2277	2283	2288	rBV	1256136	1623576	25.84%	4.036%

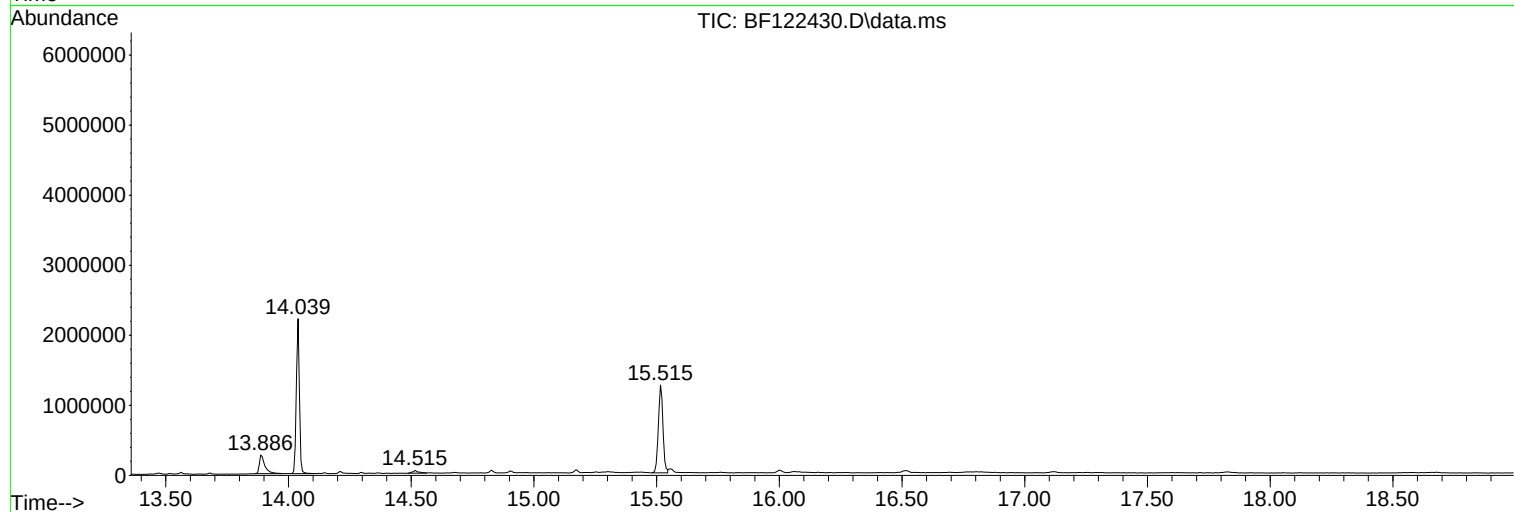
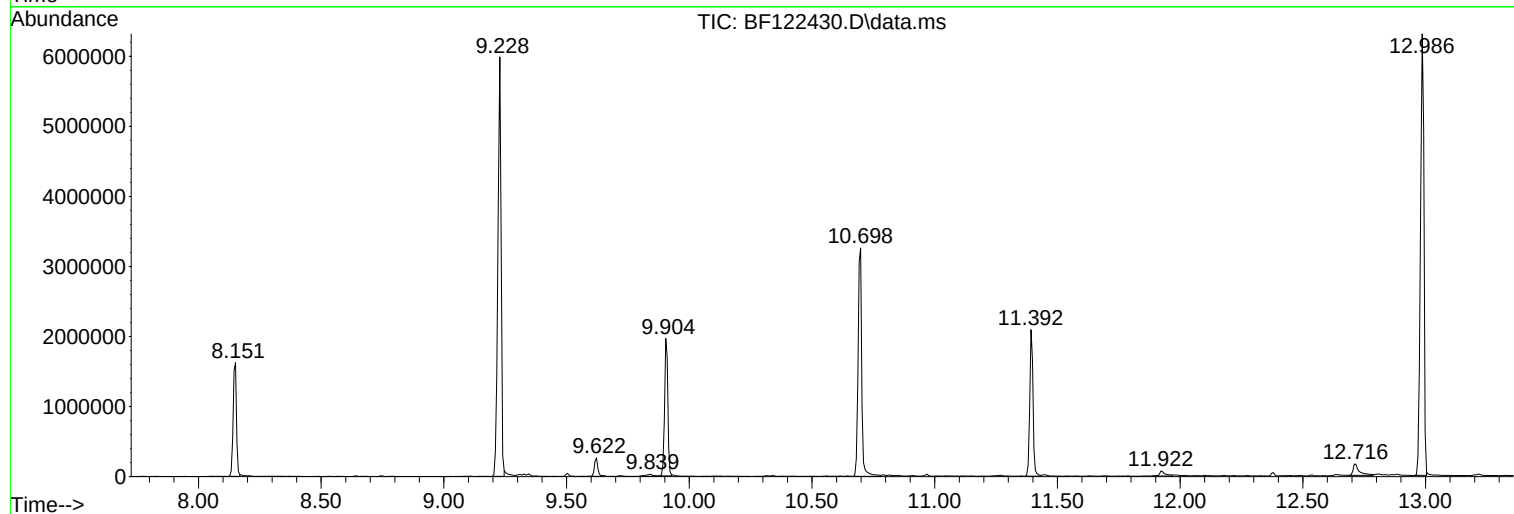
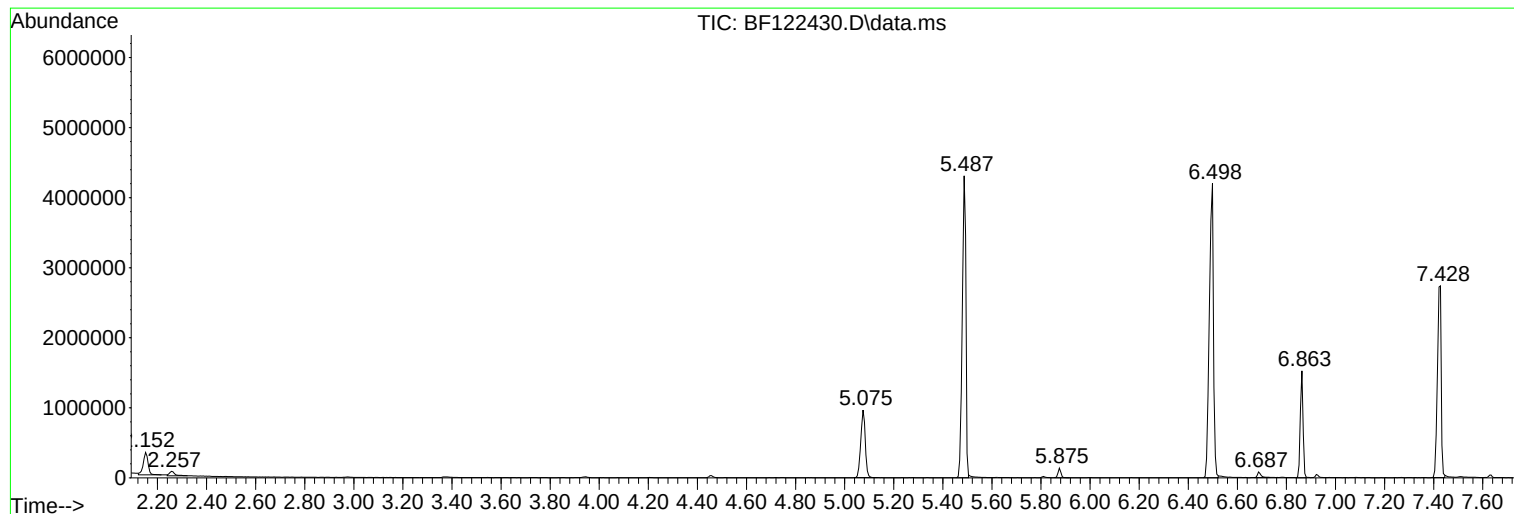
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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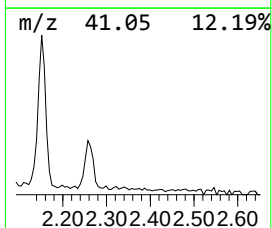
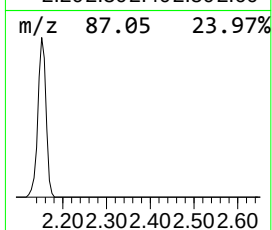
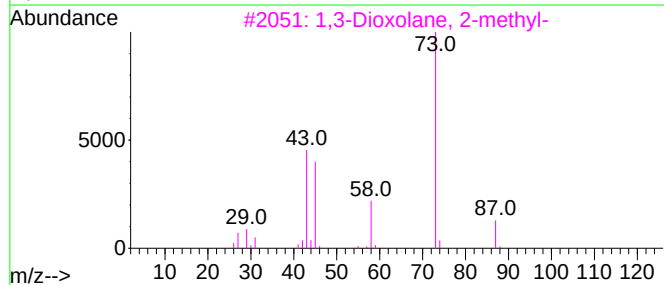
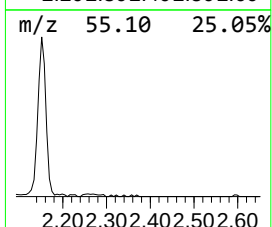
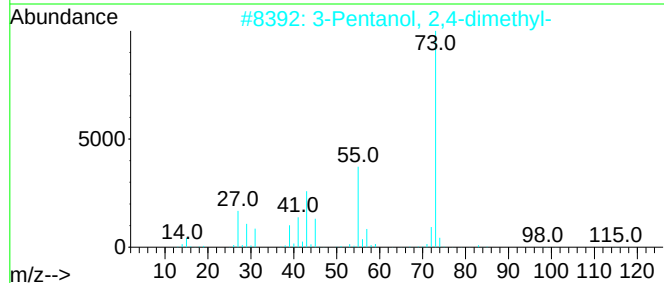
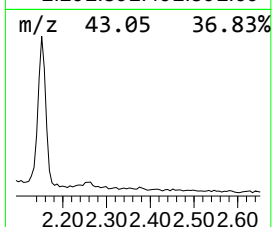
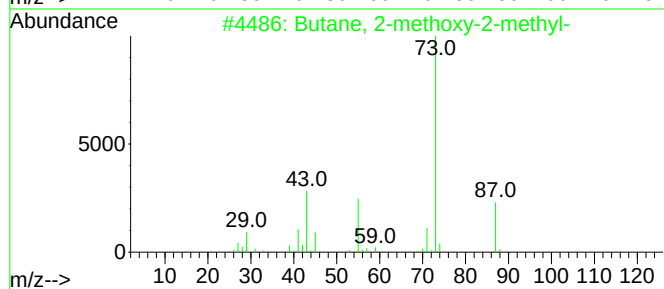
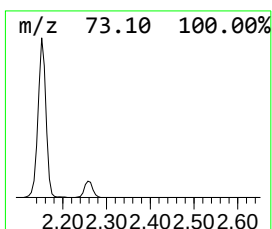
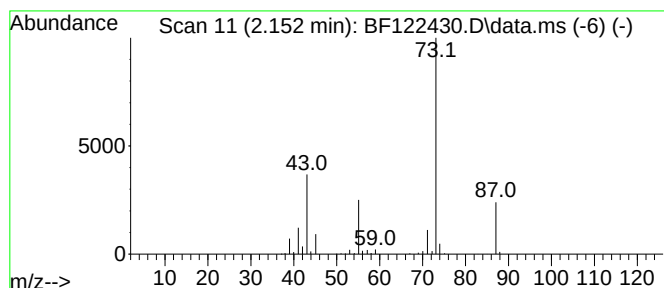
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.152	7.38 ng	437946	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12



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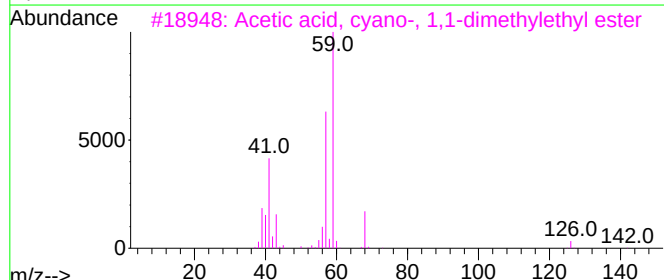
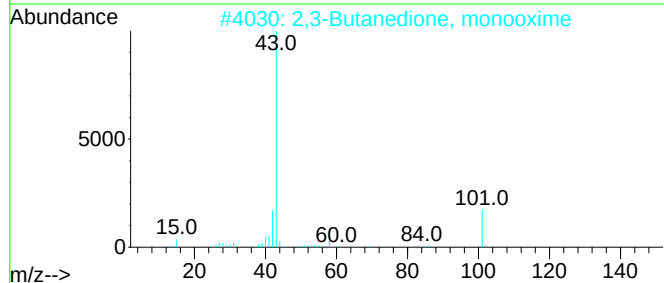
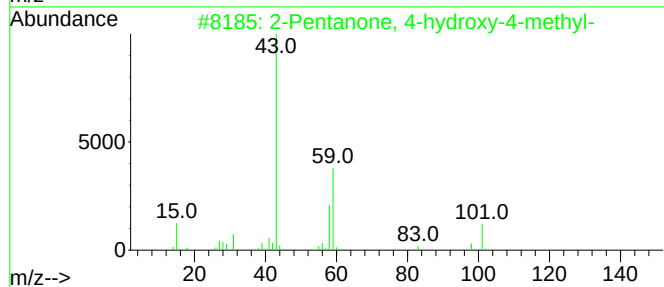
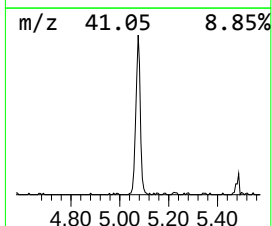
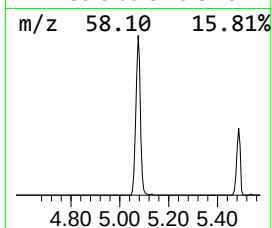
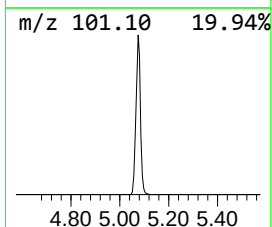
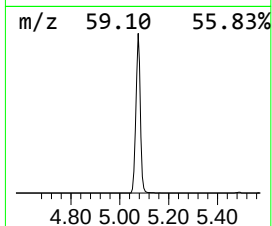
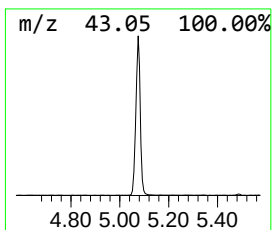
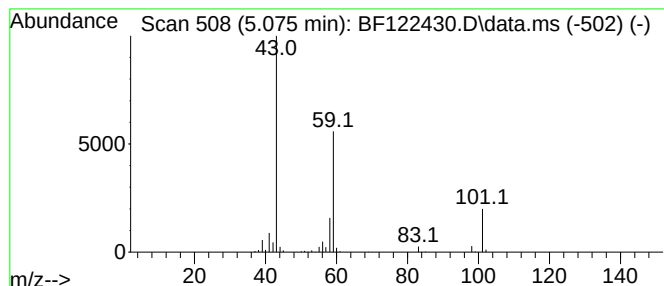
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	20.74 ng	1230740	1,4-Dichlorobenzene-d4	6.863

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25	
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17	
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9	
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9	



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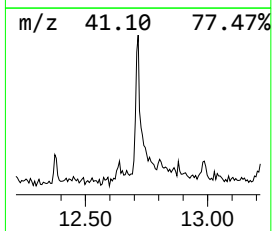
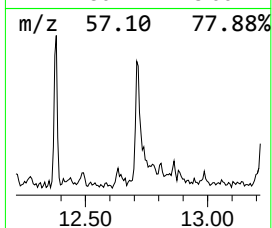
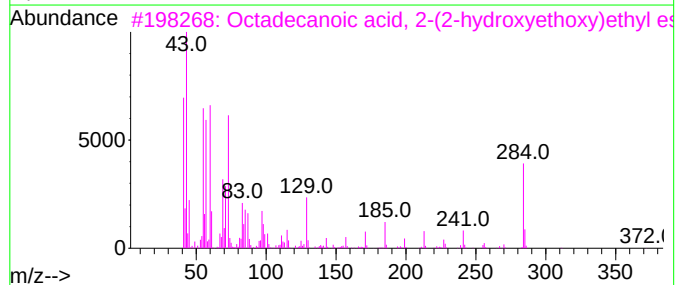
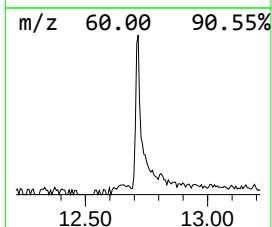
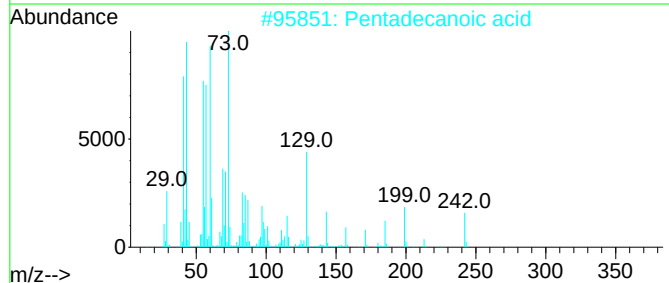
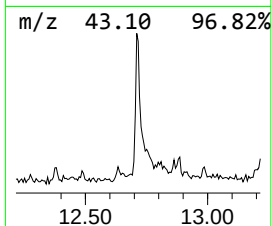
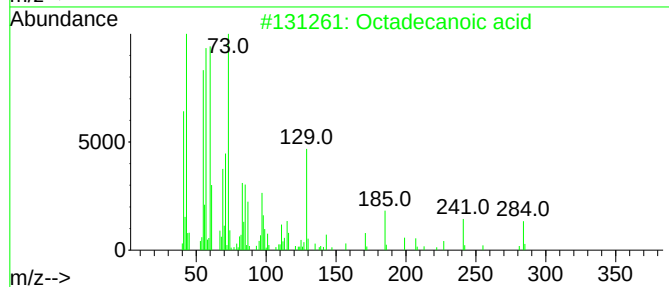
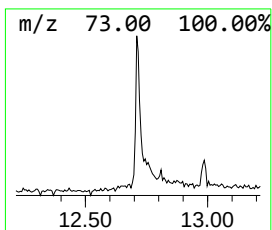
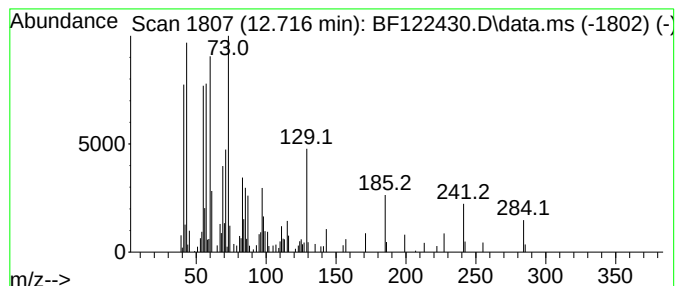
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Peak Number 3 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.716	2.91 ng	278184	Phenanthrene-d10	11.392

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	91
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
5			Undecanoic acid	186	C11H22O2	000112-37-8	81



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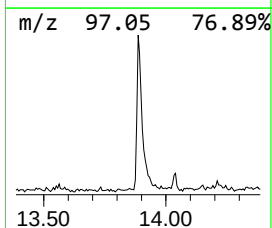
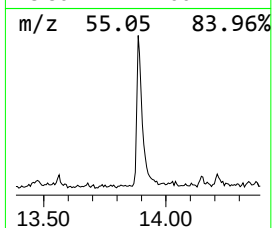
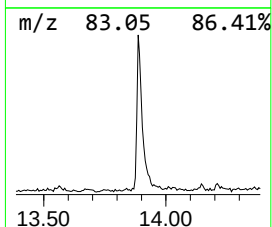
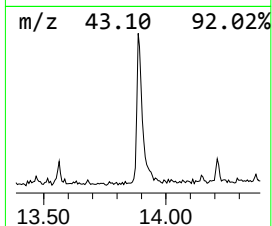
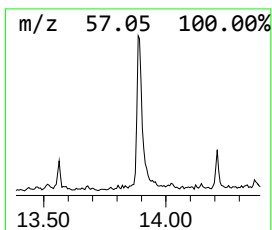
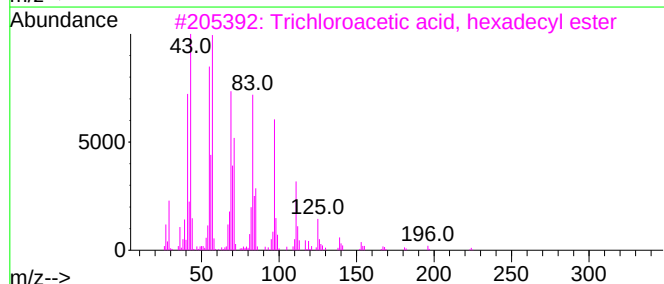
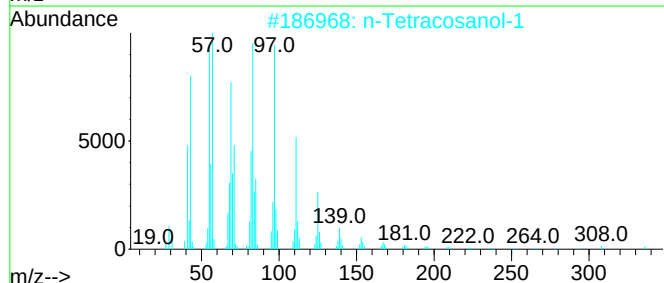
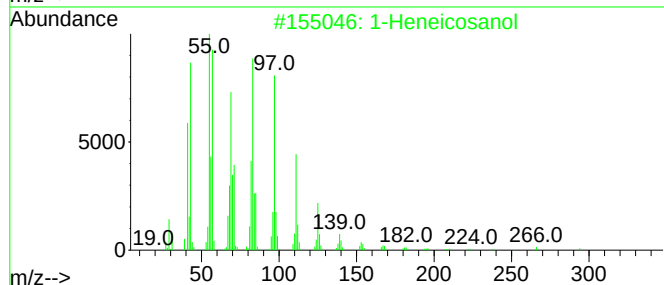
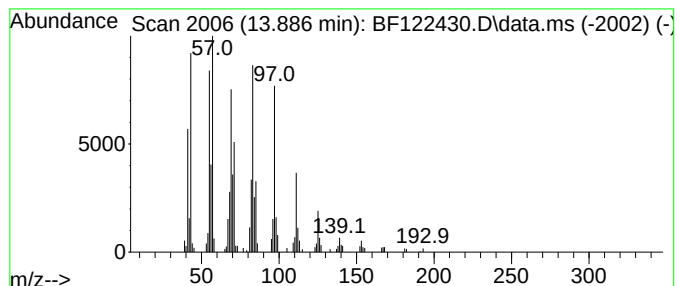
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	4.35 ng	420329	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4			Behenic alcohol	326	C22H46O	000661-19-8	94
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.152	7.4	ng	437946	1	6.863	1186980	20.0
2-Pentanone, 4-...	5.075	20.7	ng	1230740	1	6.863	1186980	20.0
Octadecanoic acid	12.716	2.9	ng	278184	4	11.392	1910790	20.0
1-Heneicosanol	13.886	4.3	ng	420329	5	14.039	1930720	20.0