

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111820\
 Data File : BF122367.D
 Acq On : 18 Nov 2020 14:55
 Operator : JU/CG
 Sample : L4771-05
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CD-BH-01-4-5

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-BF110920.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122367.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	4	8	33	rVB	785853	1266206	17.42%	2.631%
2	5.075	501	508	515	rBV	115051	156185	2.15%	0.325%
3	5.475	571	576	579	rBV	5194094	5049283	69.45%	10.491%
4	6.487	742	748	751	rBV	4784147	5251133	72.23%	10.910%
5	6.687	779	782	789	rBV	80501	81005	1.11%	0.168%
6	6.863	808	812	815	rBV	1827778	1378108	18.96%	2.863%
7	7.422	902	907	910	rBV	3326503	3366994	46.31%	6.996%
8	8.151	1026	1031	1034	rBV	1940800	1824190	25.09%	3.790%
9	9.228	1209	1214	1217	rBV	6386639	5882348	80.91%	12.222%
10	9.616	1276	1280	1291	rBV	1172200	958014	13.18%	1.990%
11	9.904	1325	1329	1340	rVB	2646403	2230152	30.67%	4.634%
12	10.692	1458	1463	1466	rBV	4419990	4257624	58.56%	8.846%
13	11.386	1577	1581	1585	rBV	2659998	2386479	32.83%	4.958%
14	11.916	1665	1671	1680	rBV2	260453	365983	5.03%	0.760%
15	12.369	1745	1748	1752	rBV	272152	248053	3.41%	0.515%
16	12.704	1802	1805	1811	rBV	101422	156597	2.15%	0.325%
17	12.980	1847	1852	1855	rBV	7102411	7270308	100.00%	15.105%
18	13.880	2001	2005	2021	rBV	447316	909777	12.51%	1.890%
19	14.027	2025	2030	2034	rBV	2926582	2579327	35.48%	5.359%
20	14.892	2173	2177	2181	rVB	76649	76738	1.06%	0.159%
21	15.498	2274	2280	2285	rBV	1903019	2435923	33.51%	5.061%

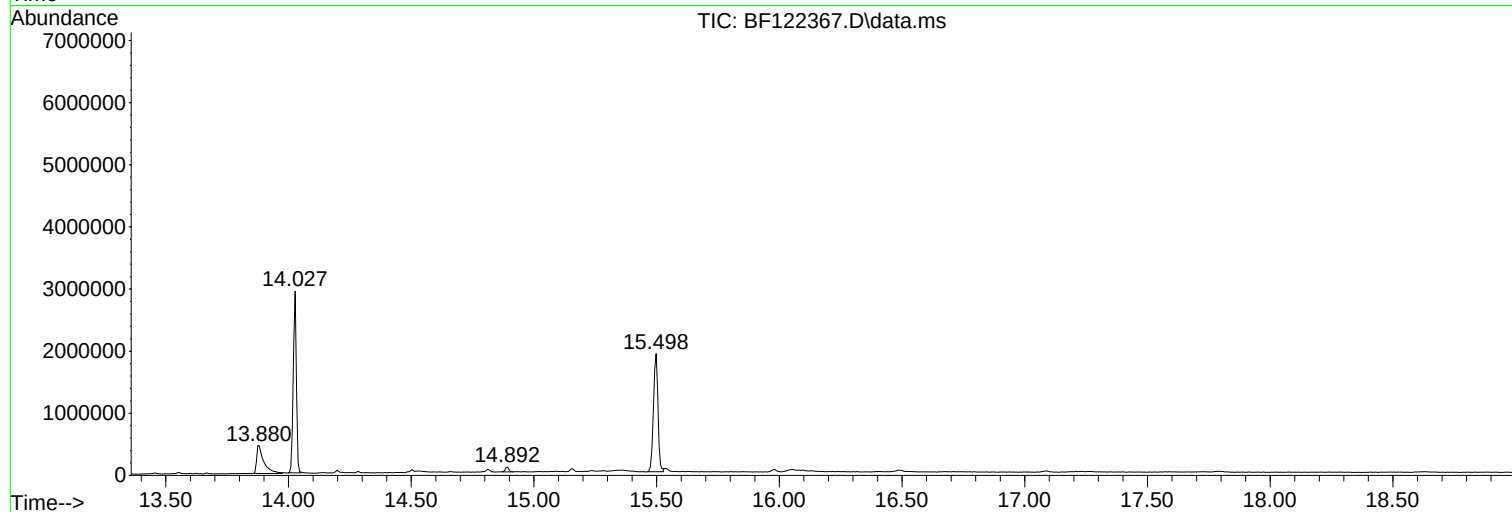
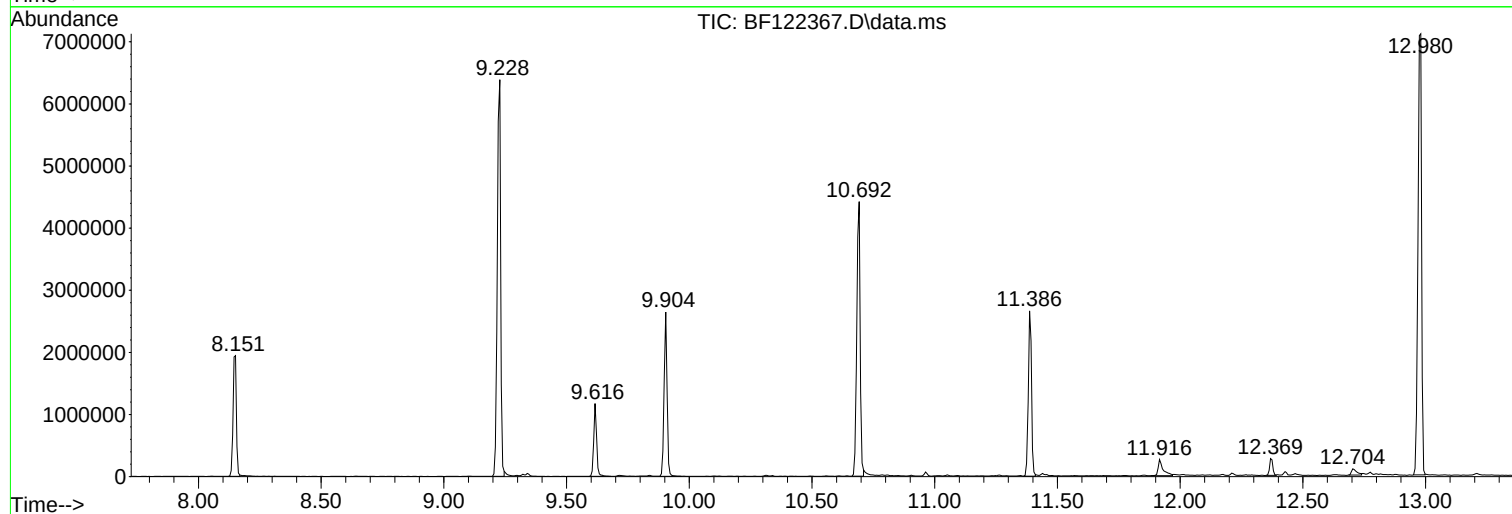
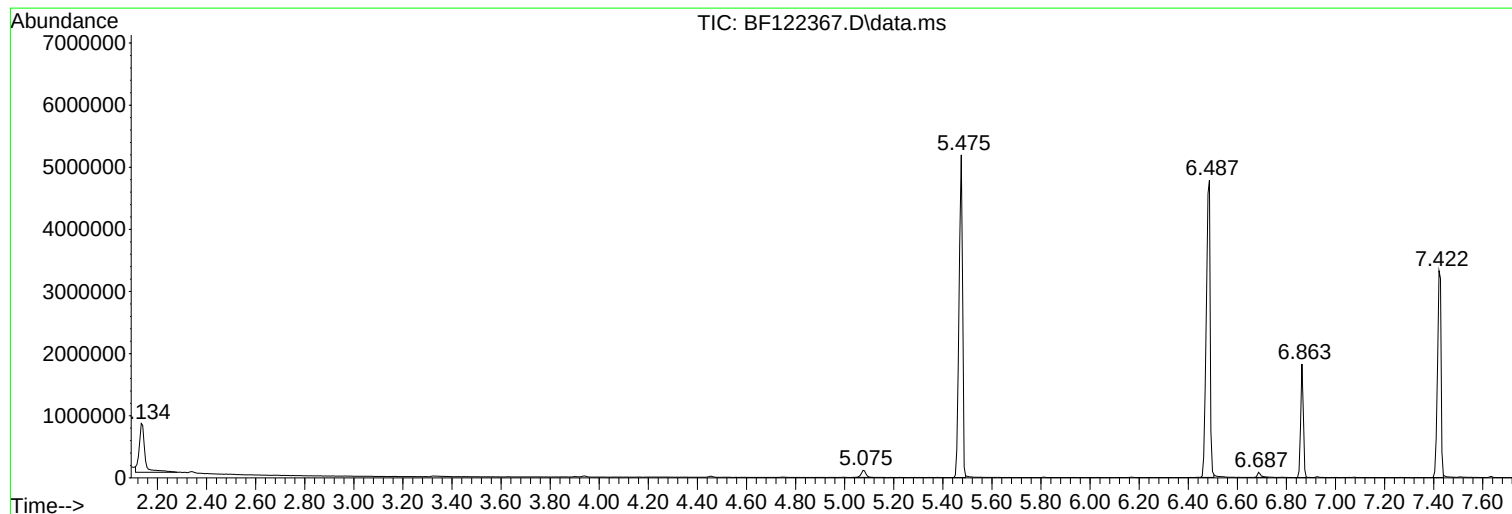
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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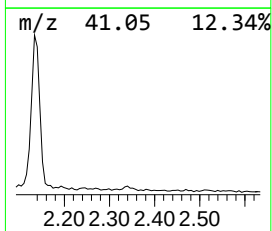
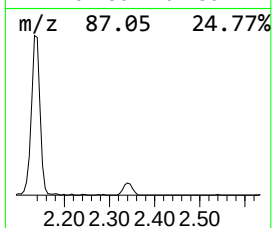
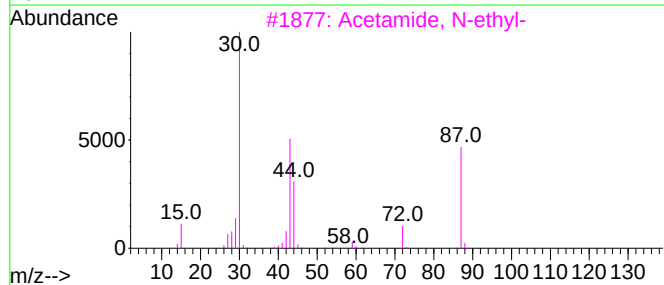
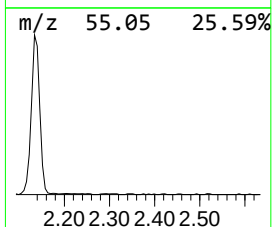
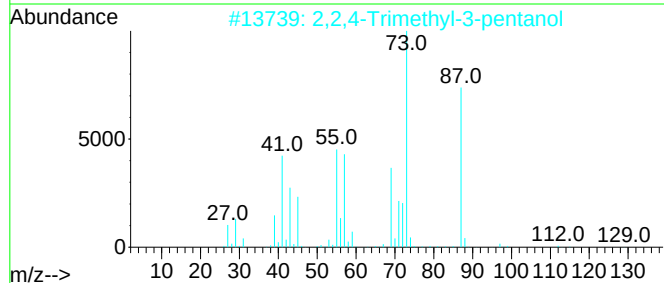
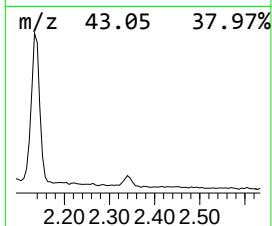
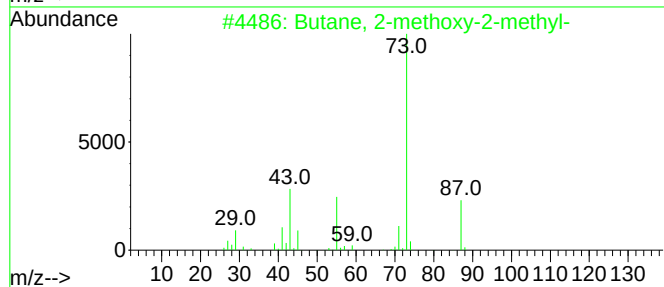
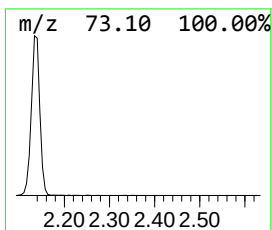
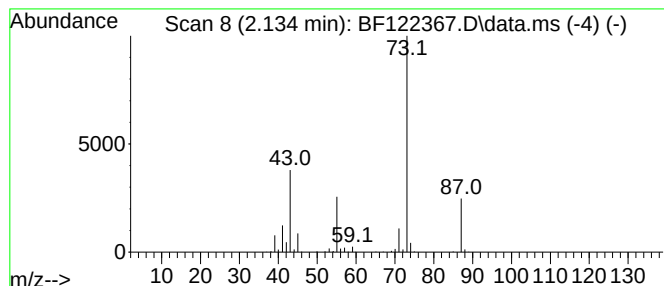
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	18.38 ng	1266210	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	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12



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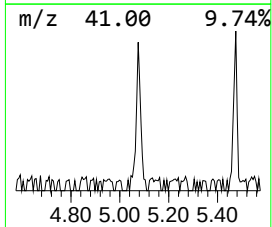
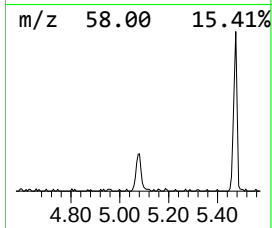
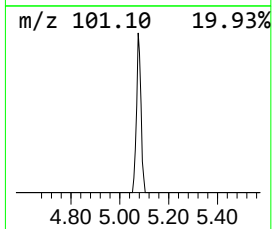
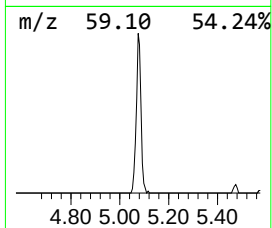
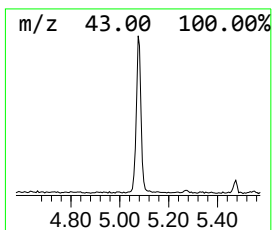
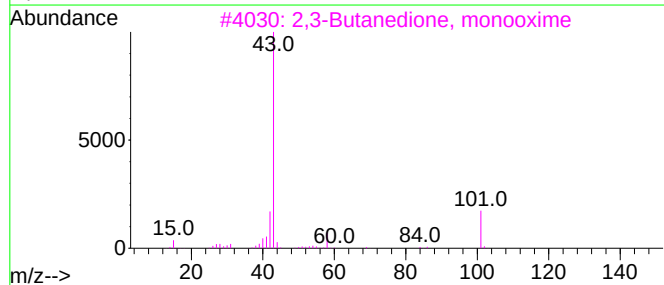
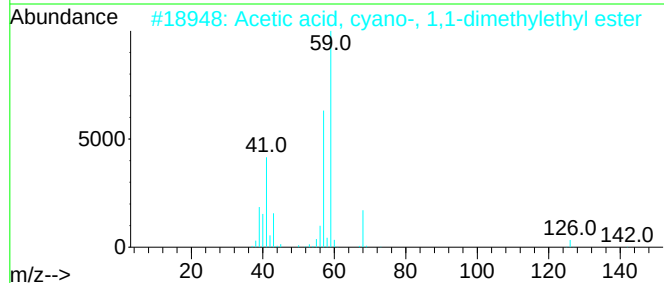
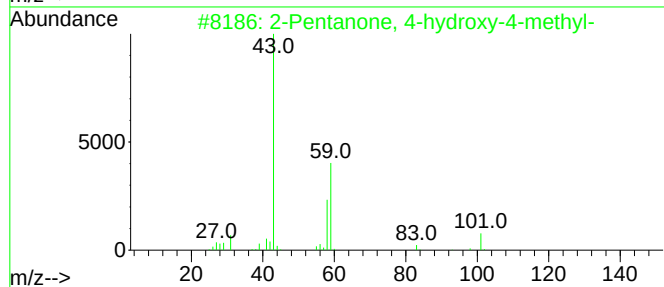
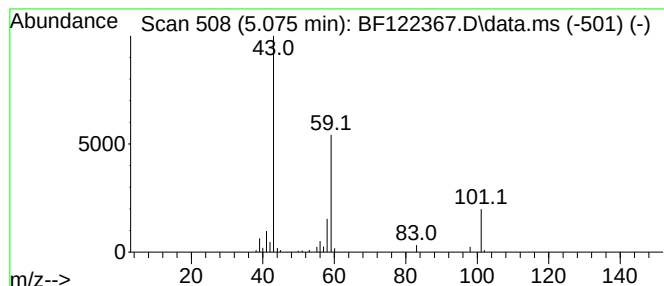
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	2.27 ng	156185	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	56
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9
5			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9



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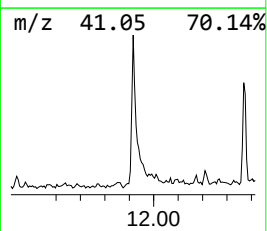
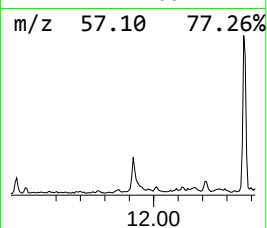
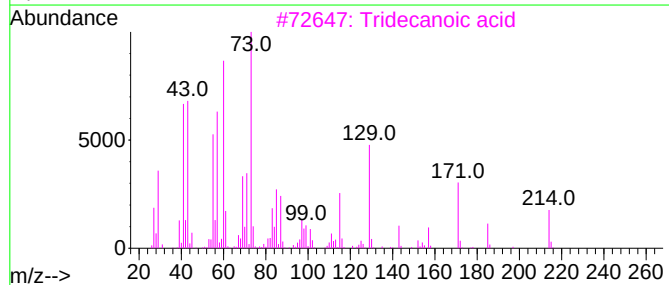
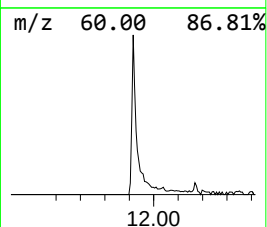
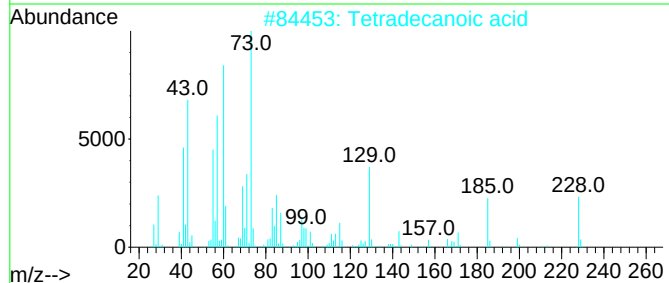
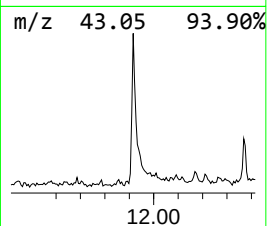
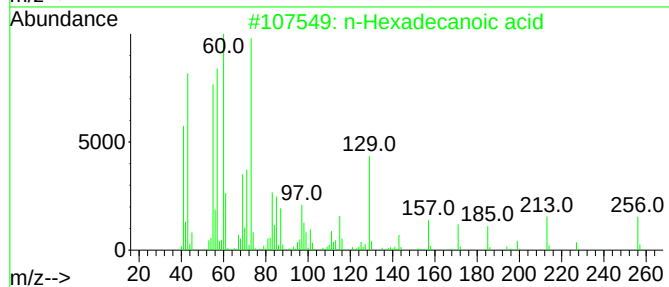
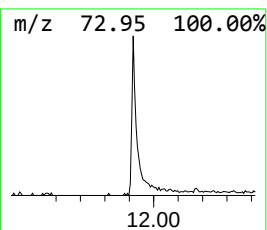
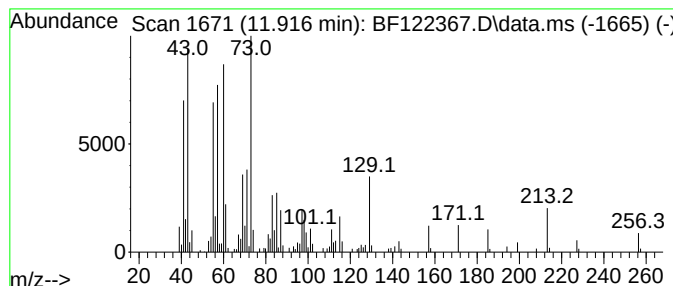
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	3.07 ng	365983	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			Tridecanoic acid	214	C13H26O2	000638-53-9	92
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5			Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	20



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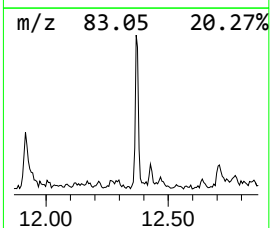
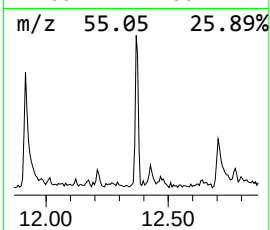
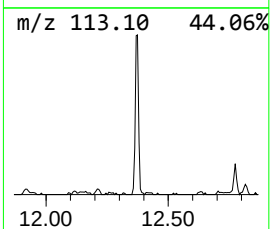
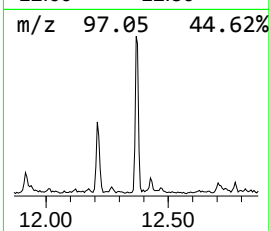
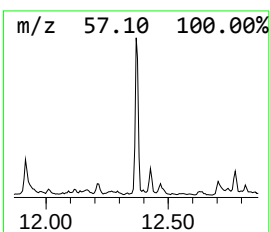
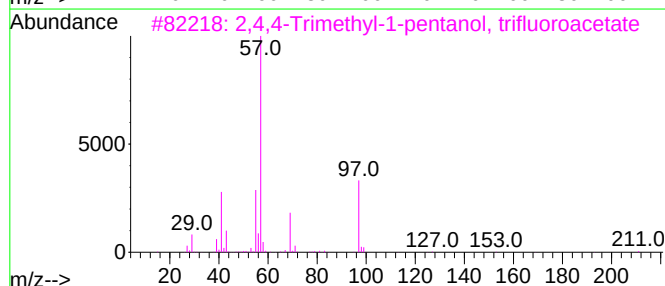
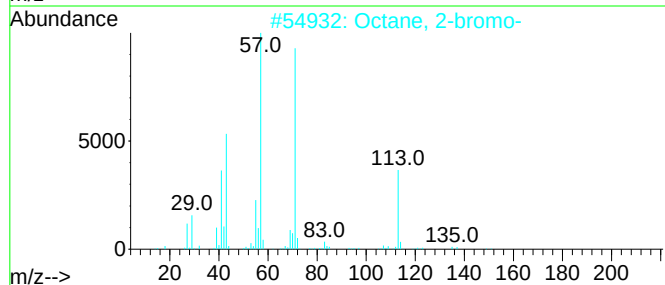
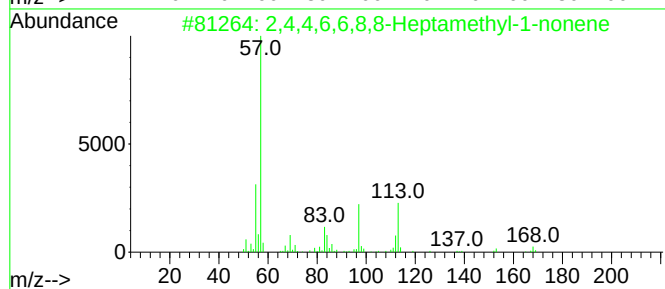
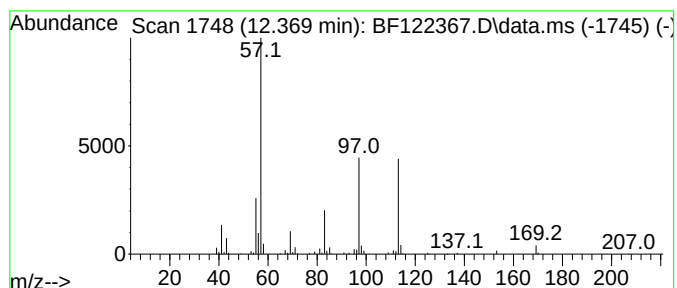
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 unknown12.36 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.369	2.08 ng	248053	Phenanthrene-d10	11.386

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	43
2		Octane, 2-bromo-	192	C8H17Br	000557-35-7	37
3		2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	35
4		2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	32
5		1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	28



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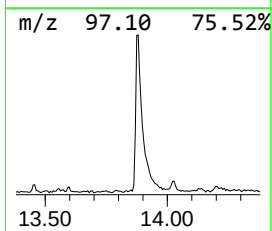
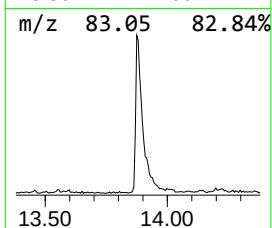
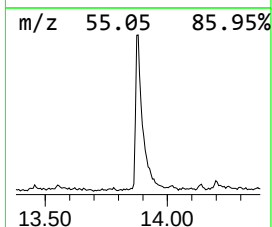
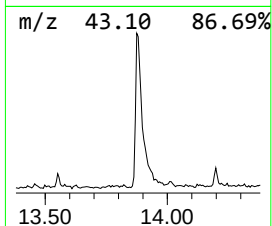
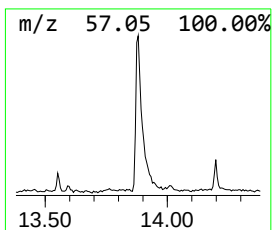
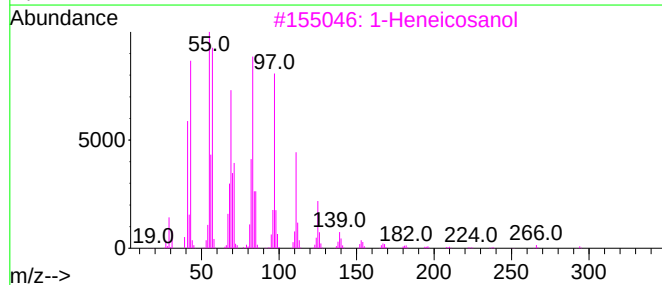
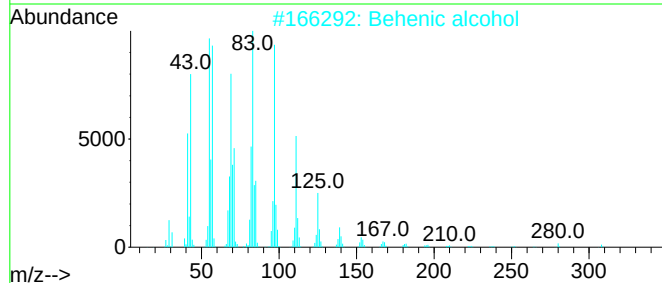
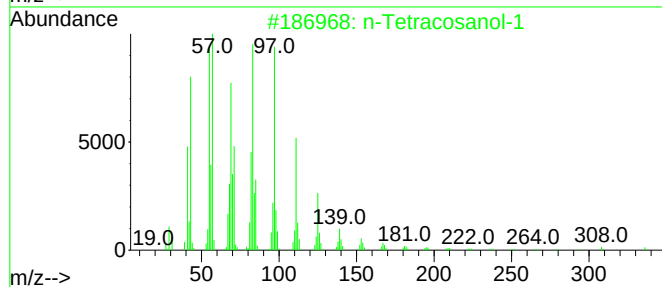
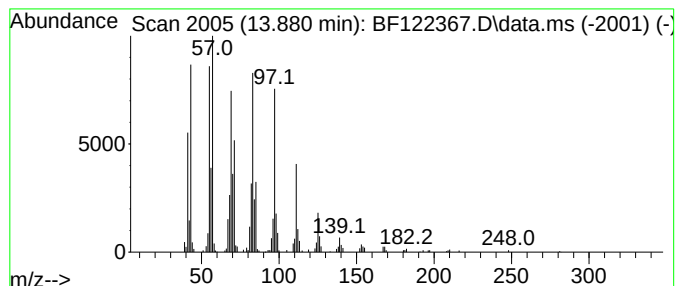
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 n-Tetracosanol-1 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	7.05 ng	909777	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Tetracosanol-1	354	C24H50O	000506-51-4	95
2			Behenic alcohol	326	C22H46O	000661-19-8	95
3			1-Heneicosanol	312	C21H44O	015594-90-8	95
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	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...	2.134	18.4	ng	1266210	1	6.863	1378110	20.0
2-Pentanone, 4-...	5.075	2.3	ng	156185	1	6.863	1378110	20.0
n-Hexadecanoic ...	11.916	3.1	ng	365983	4	11.386	2386480	20.0
unknown12.36	12.369	2.1	ng	248053	4	11.386	2386480	20.0
n-Tetracosanol-1	13.880	7.0	ng	909777	5	14.027	2579330	20.0