

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072817\
 Data File : BF097173.D
 Acq On : 29 Jul 2017 00:14
 Operator : SJ/JU
 Sample : I4456-06
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DUP

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:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.693	134	137	142	rBV2	18461	41535	1.41%	0.190%
2	4.634	462	467	479	rBV	495649	737278	24.99%	3.365%
3	5.093	540	545	557	rBV	2499989	2783958	94.38%	12.704%
4	6.151	720	725	739	rBV	2670315	2949731	100.00%	13.461%
5	6.257	739	743	747	rBV	2585532	2606542	88.37%	11.895%
6	6.487	778	782	787	rBV	836756	718279	24.35%	3.278%
7	6.640	804	808	812	rBV	1876981	1868292	63.34%	8.526%
8	7.057	874	879	893	rBV	1660235	1646484	55.82%	7.514%
9	7.192	899	902	912	rVB	41861	46216	1.57%	0.211%
10	7.769	996	1000	1008	rVV	1060024	883189	29.94%	4.030%
11	8.845	1179	1183	1186	rBV	2282994	2071609	70.23%	9.454%
12	9.245	1247	1251	1254	rBV	463986	348558	11.82%	1.591%
13	9.510	1293	1296	1301	rVB	778361	736165	24.96%	3.359%
14	9.933	1362	1368	1371	rBV5	20837	32968	1.12%	0.150%
15	10.298	1426	1430	1436	rBV	1100305	994412	33.71%	4.538%
16	10.439	1451	1454	1461	rBV2	50129	79026	2.68%	0.361%
17	10.880	1526	1529	1532	rBV	42962	40605	1.38%	0.185%
18	10.986	1543	1547	1555	rVB	653858	580872	19.69%	2.651%
19	11.310	1599	1602	1606	rVB3	24407	30531	1.04%	0.139%
20	11.539	1639	1641	1644	rBV	44634	36354	1.23%	0.166%
21	12.416	1786	1790	1793	rBV	46401	43537	1.48%	0.199%
22	12.569	1812	1816	1820	rBV	1396439	1278723	43.35%	5.835%
23	13.480	1965	1971	1978	rBV3	83306	127025	4.31%	0.580%
24	13.610	1987	1993	1999	rBV	666934	603743	20.47%	2.755%
25	14.604	2160	2162	2168	rVB	28694	47580	1.61%	0.217%
26	14.957	2218	2222	2227	rBV	425584	491760	16.67%	2.244%
27	15.368	2288	2292	2295	rBV3	20996	33024	1.12%	0.151%
28	15.527	2316	2319	2329	rBV3	24905	55440	1.88%	0.253%

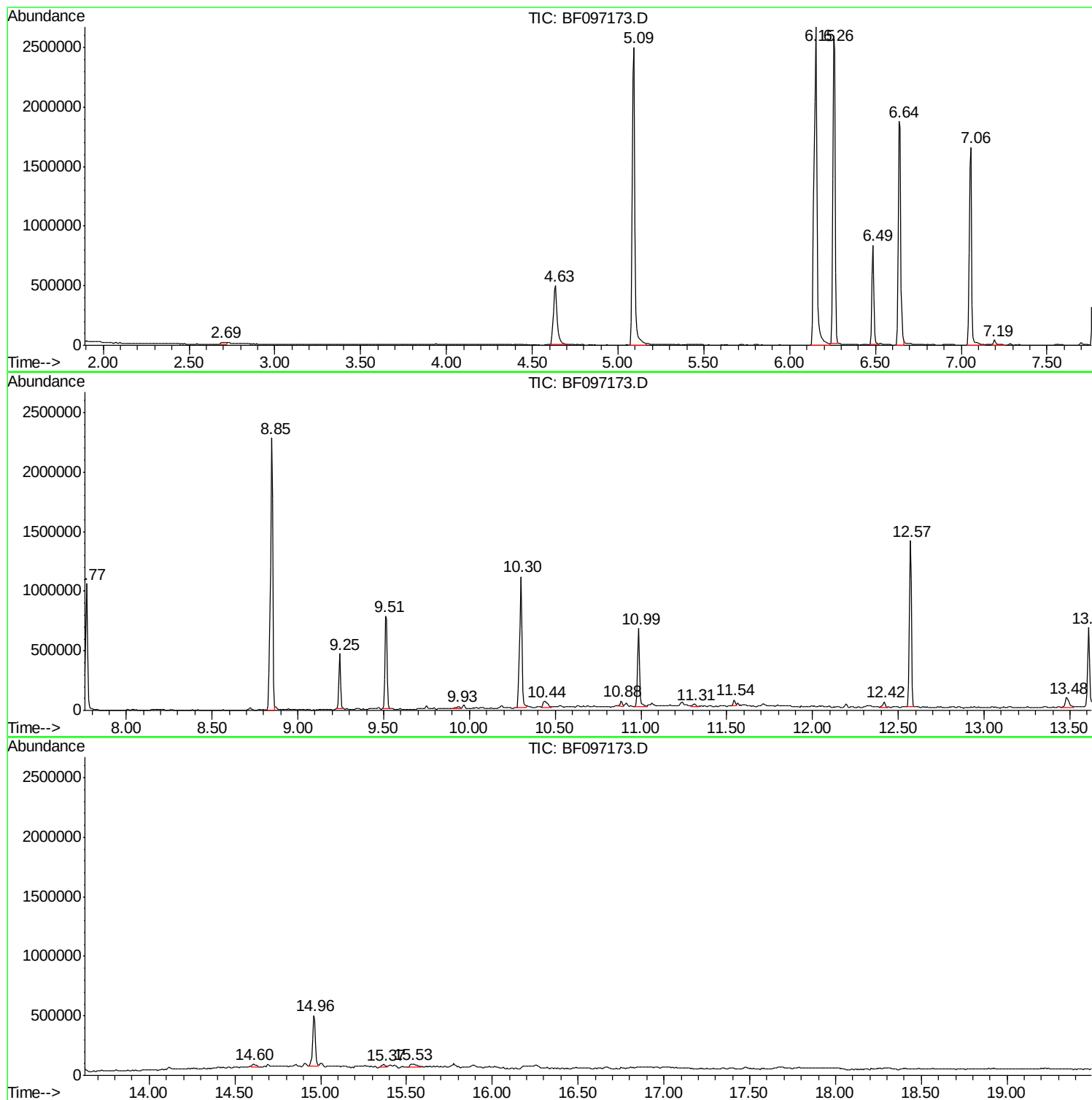
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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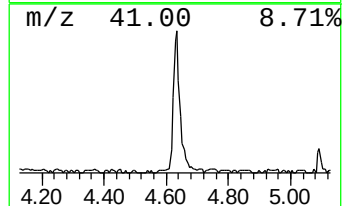
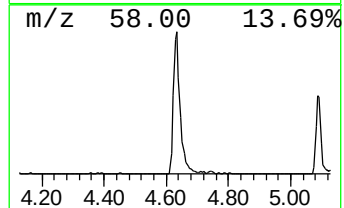
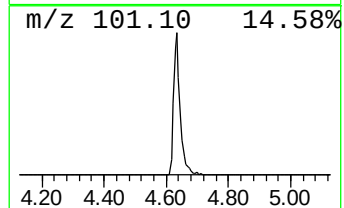
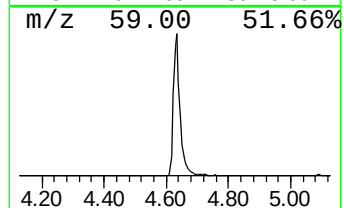
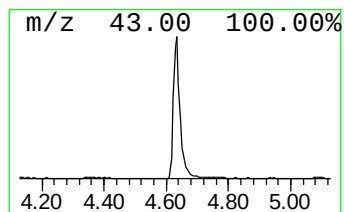
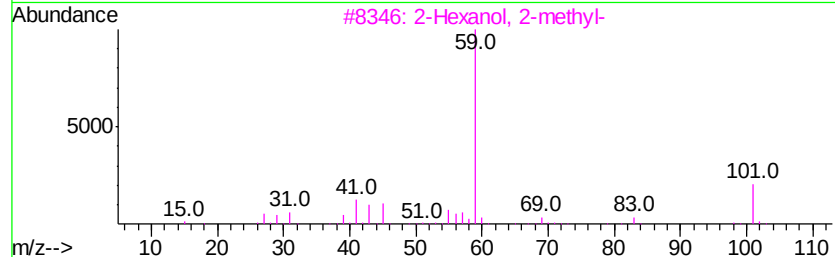
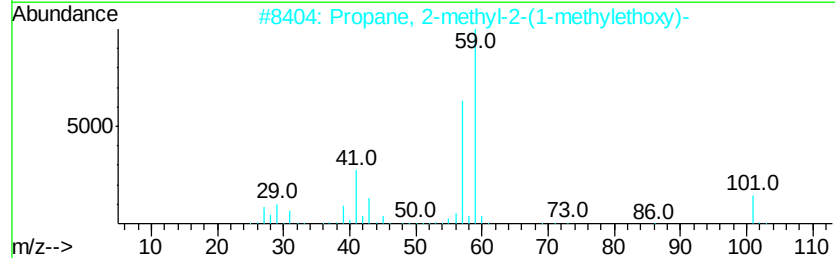
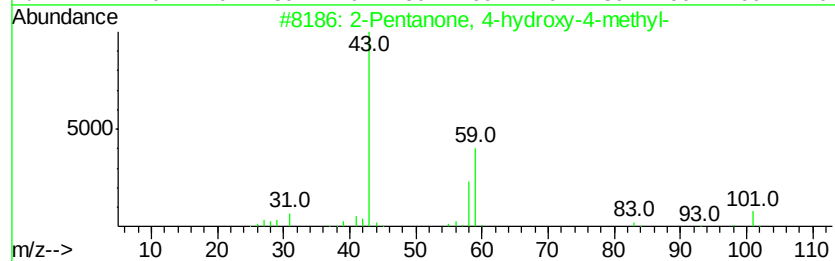
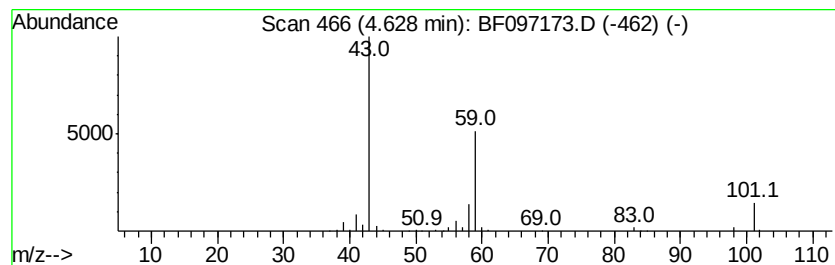
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.		
4.63	20.53 ng	737278	1,4-Dichlorobenzene-d4	6.49		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36	
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33	
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33	
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25	



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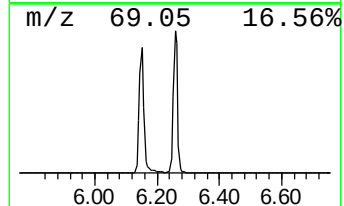
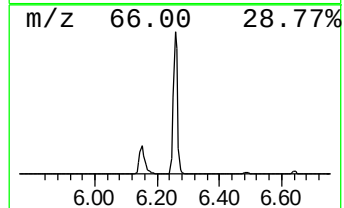
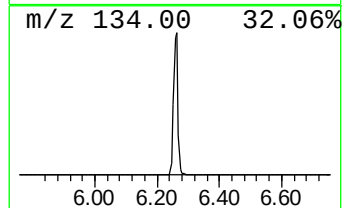
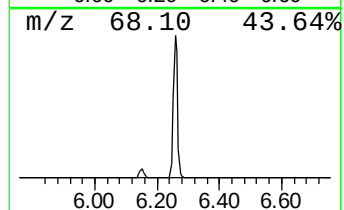
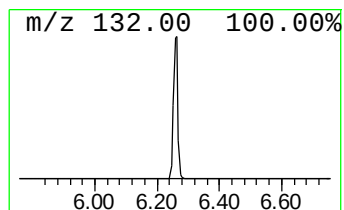
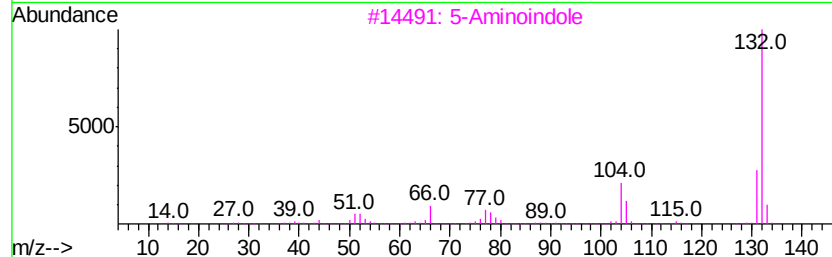
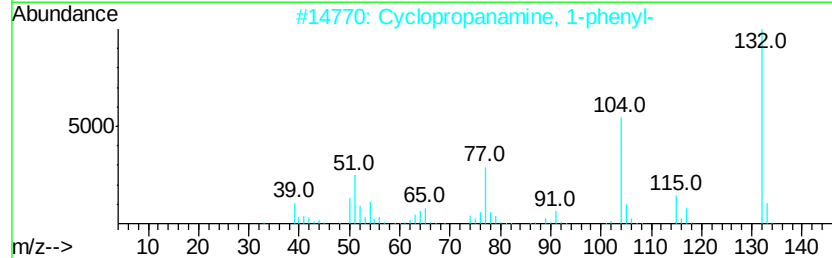
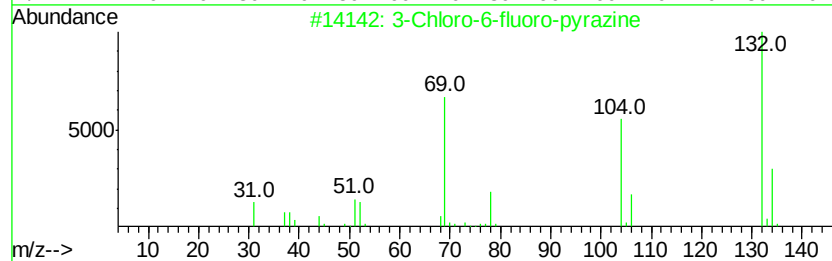
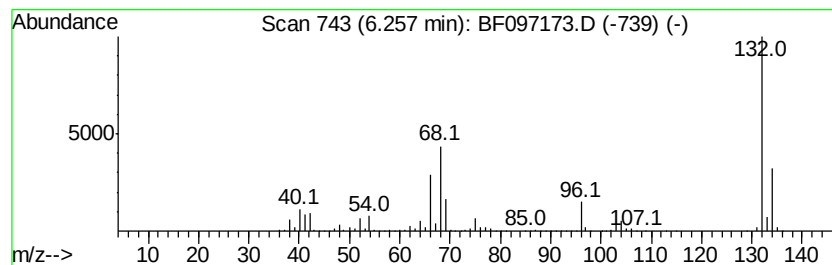
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Peak Number 2 unknown6.26 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.26	72.58 ng	2606540	1,4-Dichlorobenzene-d4	6.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	14
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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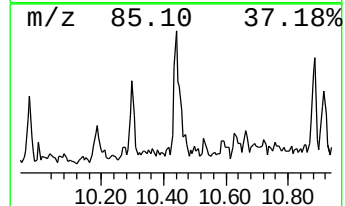
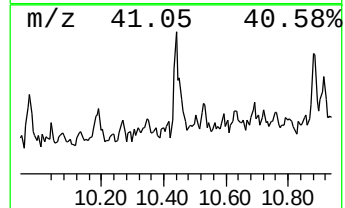
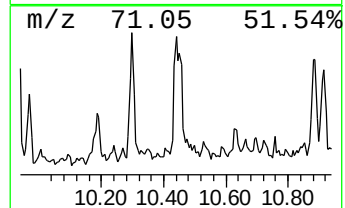
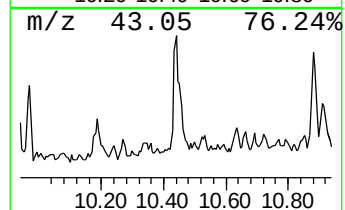
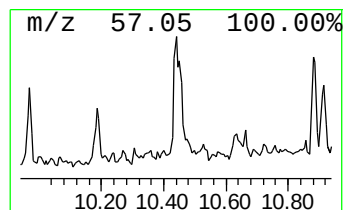
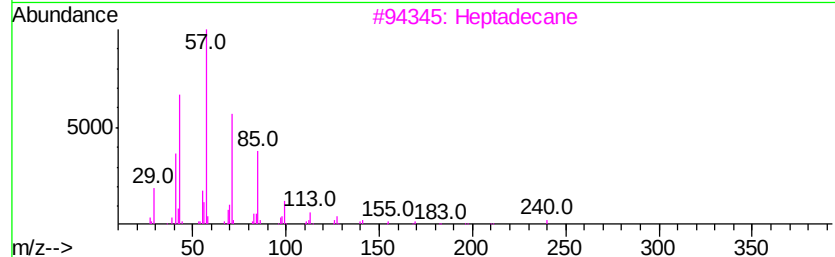
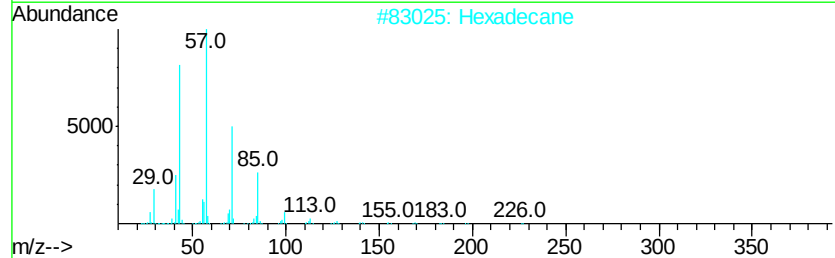
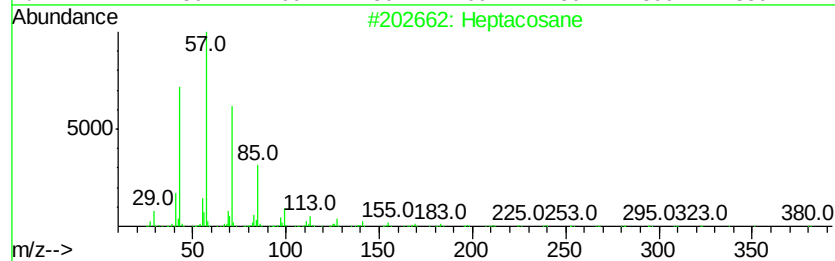
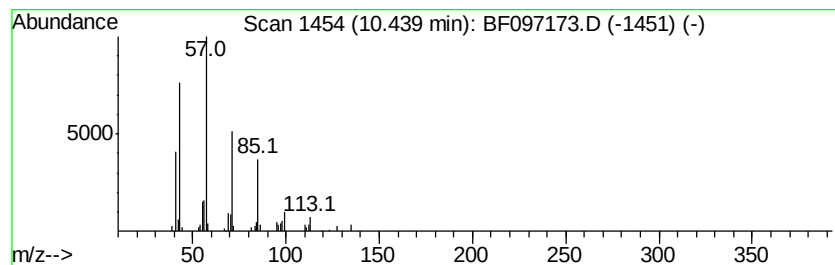
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Heptacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.44	2.72 ng	79026	Phenanthrene-d10		10.99
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	80
2	Hexadecane	226	C16H34	000544-76-3	78
3	Heptadecane	240	C17H36	000629-78-7	72
4	Pentadecane	212	C15H32	000629-62-9	72
5	Eicosane	282	C20H42	000112-95-8	64



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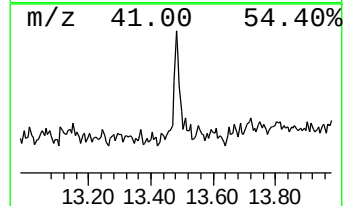
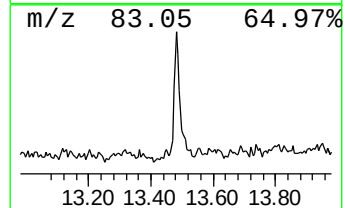
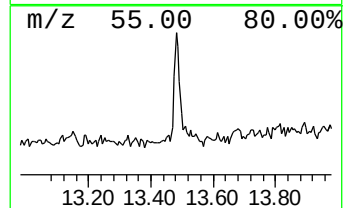
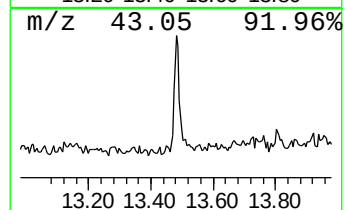
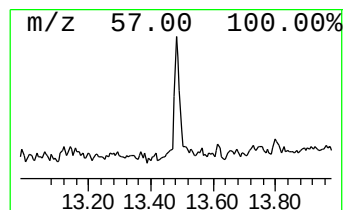
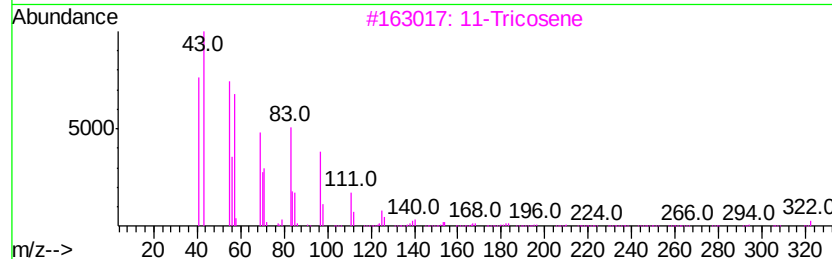
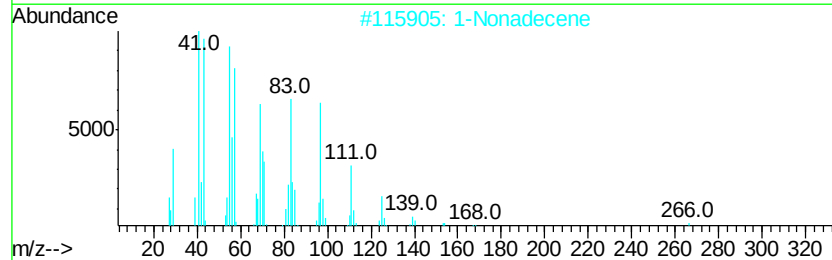
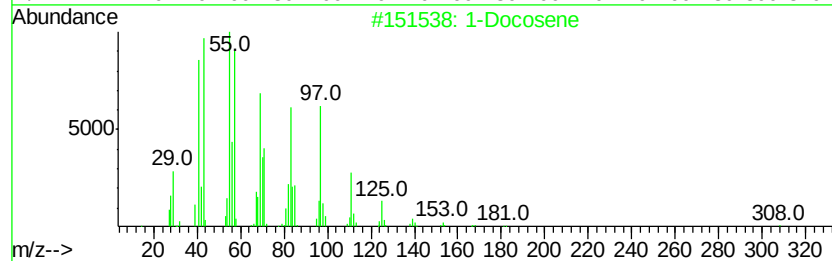
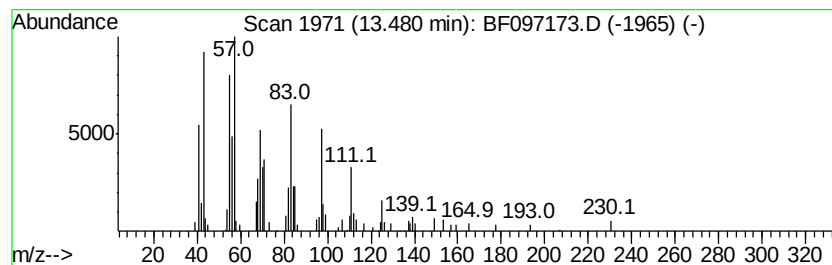
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.48	4.21 ng	127025	Chrysene-d12	13.61
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Docosene		308 C22H44	001599-67-3 94
2	1-Nonadecene		266 C19H38	018435-45-5 91
3	11-Tricosene		322 C23H46	052078-56-5 87
4	Octadecyl trifluoroacetate		366 C20H37F3O2	079392-43-1 87
5	Trichloroacetic acid, pentadecyl...		372 C17H31Cl3O2	074339-53-0 87



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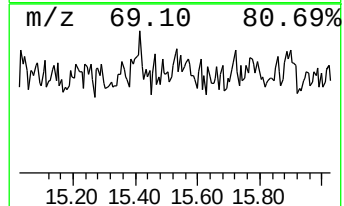
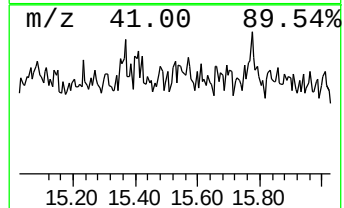
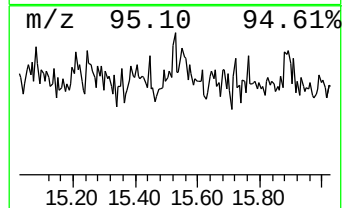
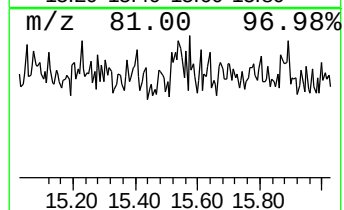
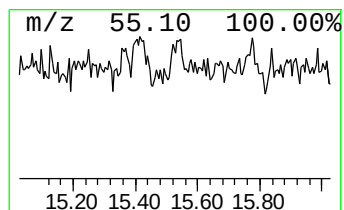
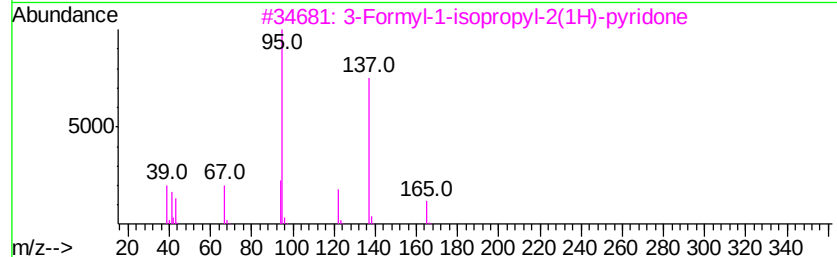
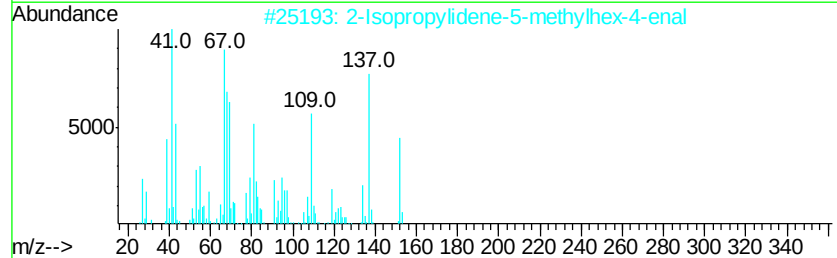
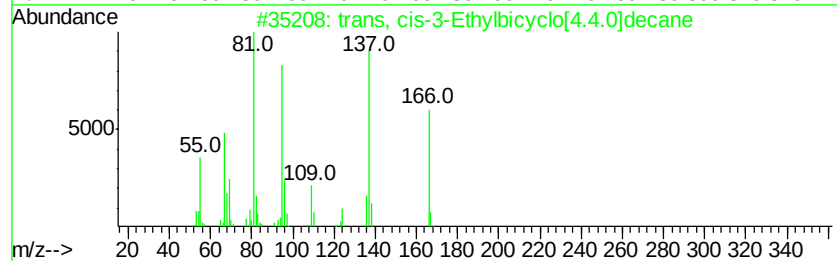
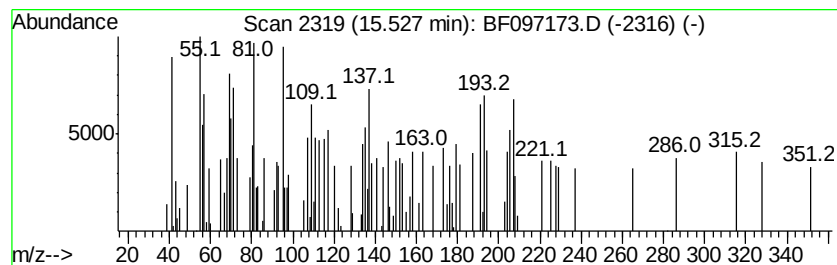
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown15.53 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.53	2.25 ng	55440	Perylene-d12	14.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	trans, cis-3-Ethylbicyclo[4.4.0]...	166	C12H22	066660-43-3	35
2		2-Isopropylidene-5-methylhex-4-enal	152	C10H16O	003304-28-7	25
3		3-Formyl-1-isopropyl-2(1H)-pyridone	165	C9H11NO2	1000306-46-8	22
4		2,5-Cyclohexadiene-1,4-dione, 2,...	236	C8H6Cl2O4	007210-71-1	22
5		5-(1-Bromo-1-methyl-ethyl)-2-met...	234	C10H19BrO	1000188-65-7	22



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.63	20.5	ng	737278	1	6.49	718279	20.0
unknown6.26	6.26	72.6	ng	2606540	1	6.49	718279	20.0
Heptacosane	10.44	2.7	ng	79026	4	10.99	580872	20.0
1-Docosene	13.48	4.2	ng	127025	5	13.61	603743	20.0
unknown15.53	15.53	2.3	ng	55440	6	14.96	491760	20.0