

Data Path : Z:\HPCHEM1\BNA_F\Data\BF071217\
 Data File : BF096703.D
 Acq On : 12 Jul 2017 20:35
 Operator : SJ/JU
 Sample : I4140-02
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EP-05

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-BF070117.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	4.851	466	470	481	rVB	268561	382588	14.41%	1.825%
2	5.281	538	543	546	rBV	2401364	2441265	91.95%	11.644%
3	6.310	713	718	721	rBV	2300195	2511124	94.59%	11.977%
4	6.440	735	740	743	rBV	2554191	2428229	91.46%	11.582%
5	6.663	775	778	782	rBV	671009	605149	22.79%	2.886%
6	6.822	801	805	809	rBV	2005928	1820634	68.58%	8.684%
7	7.228	869	874	877	rBV	1597147	1546317	58.24%	7.375%
8	7.945	992	996	1000	rBV	921555	819322	30.86%	3.908%
9	9.028	1174	1180	1183	rBV	2886527	2654871	100.00%	12.663%
10	9.416	1243	1246	1250	rBV	310378	261148	9.84%	1.246%
11	9.698	1290	1294	1298	rBV	979545	794593	29.93%	3.790%
12	10.145	1367	1370	1373	rVB	46173	34667	1.31%	0.165%
13	10.486	1423	1428	1431	rBV	1222216	1217357	45.85%	5.806%
14	10.616	1447	1450	1457	rBV	72110	75092	2.83%	0.358%
15	11.063	1523	1526	1529	rBV2	35984	28666	1.08%	0.137%
16	11.175	1542	1545	1549	rVB	721831	613691	23.12%	2.927%
17	12.763	1810	1815	1818	rBV	1575189	1467523	55.28%	6.999%
18	13.663	1965	1968	1978	rBV	209603	247758	9.33%	1.182%
19	13.804	1988	1992	1997	rVB	557463	489583	18.44%	2.335%
20	15.198	2224	2229	2235	rVB	426310	489974	18.46%	2.337%
21	15.680	2309	2311	2317	rBV6	22921	36687	1.38%	0.175%

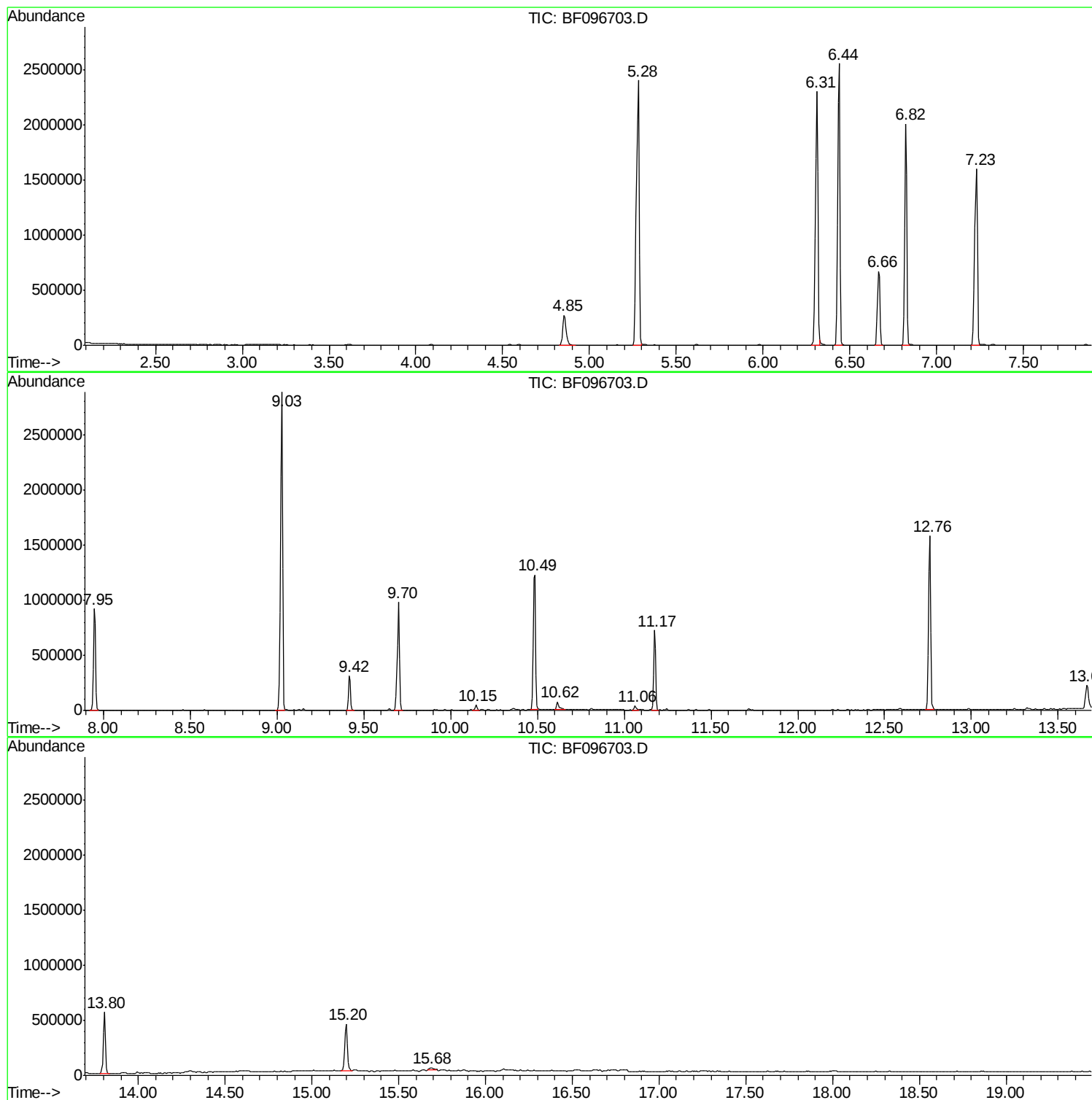
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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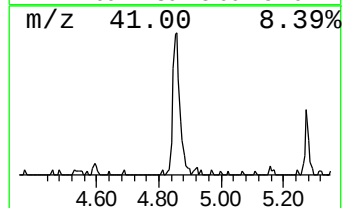
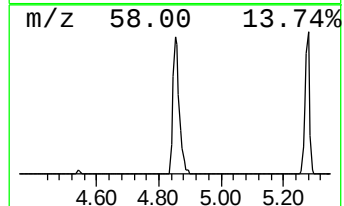
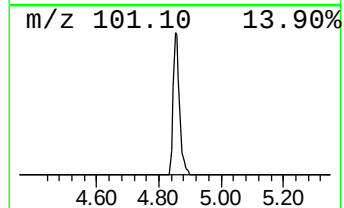
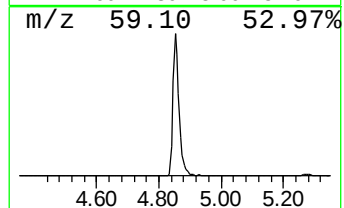
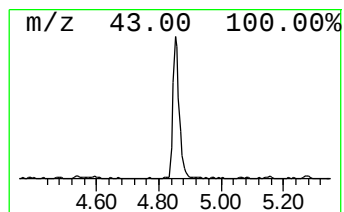
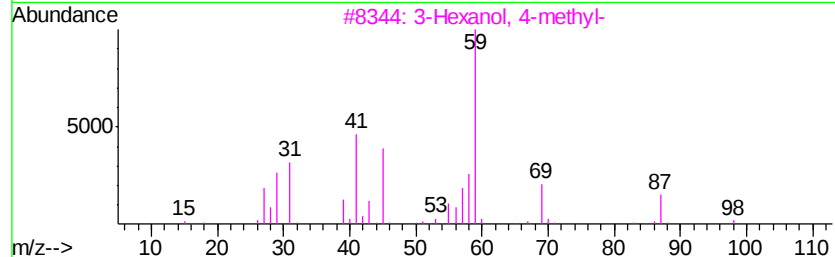
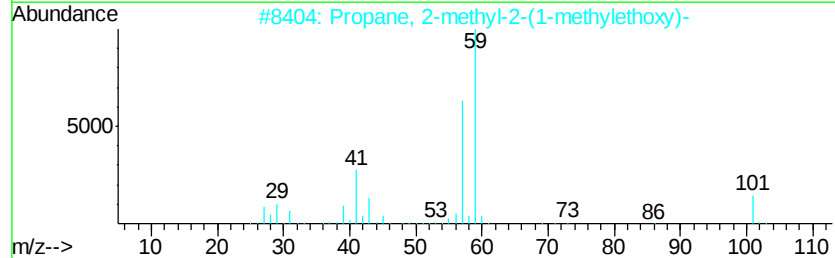
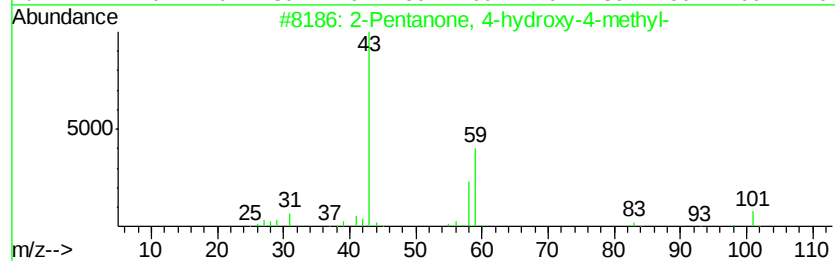
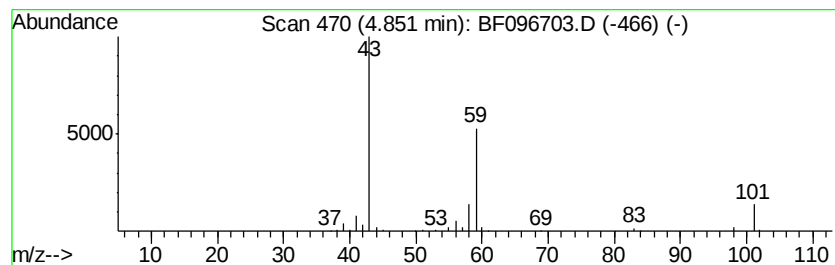
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.85	12.64 ng	382588	1,4-Dichlorobenzene-d4	6.66

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			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28



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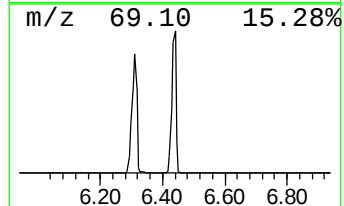
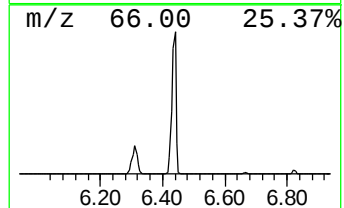
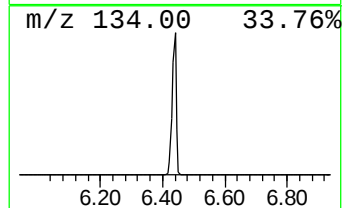
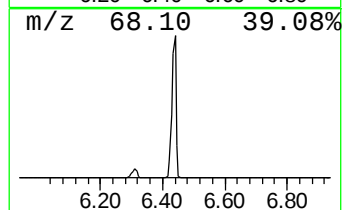
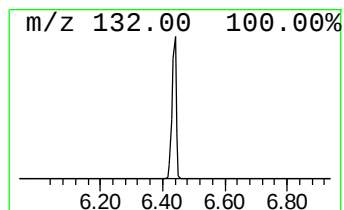
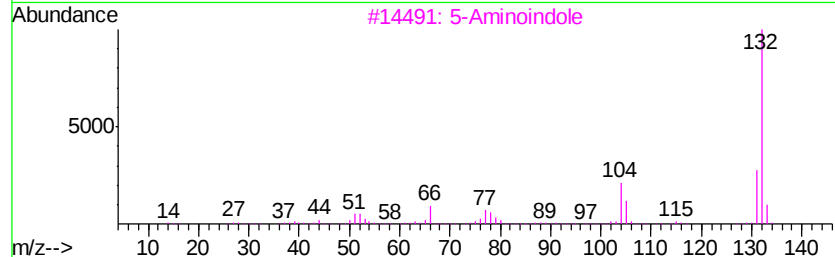
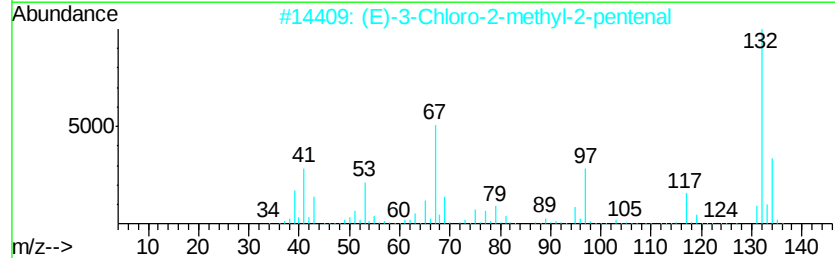
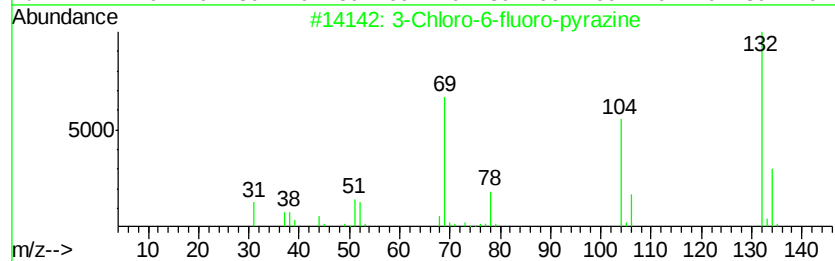
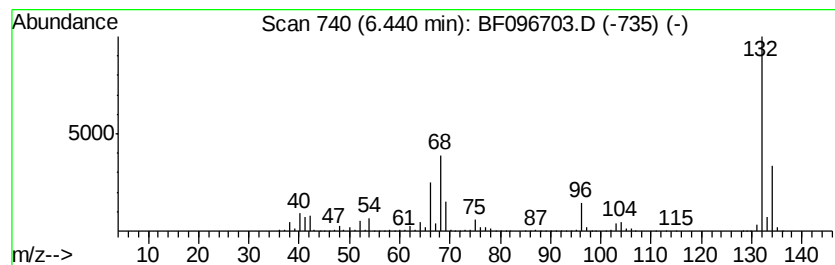
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Peak Number 2 unknown6.44 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.44	80.25 ng	2428230	1,4-Dichlorobenzene-d4	6.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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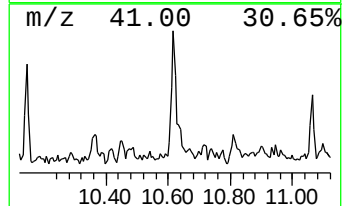
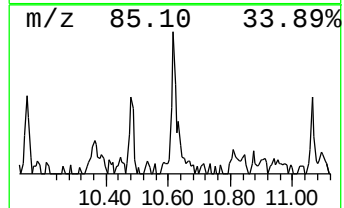
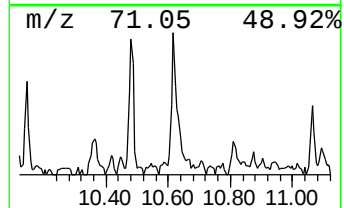
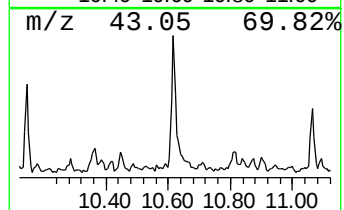
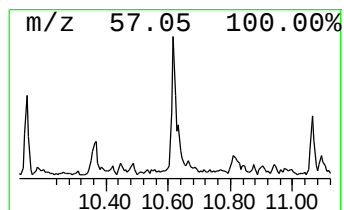
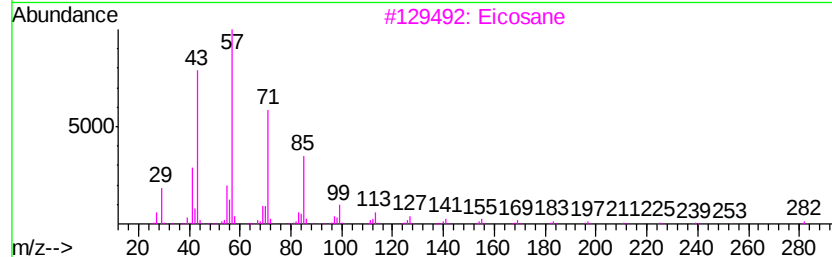
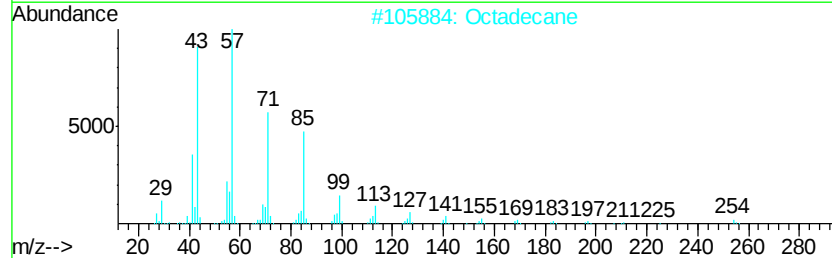
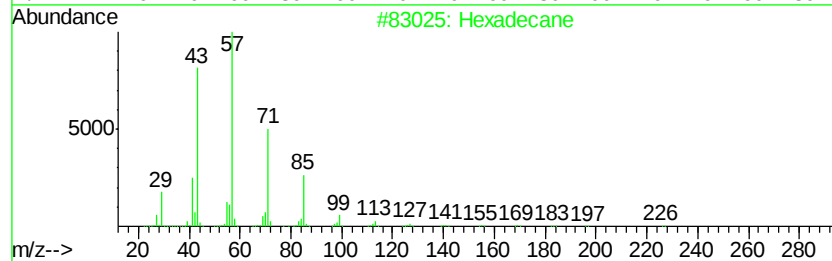
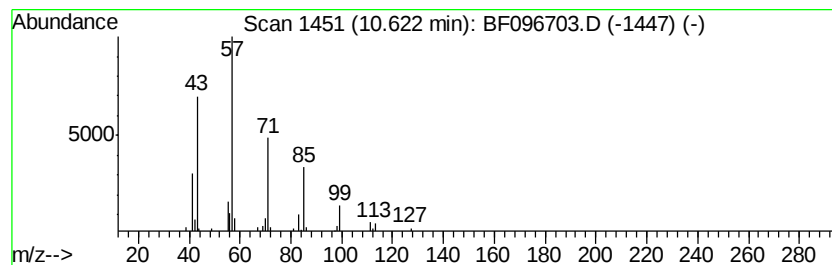
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Peak Number 4 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.62	2.45 ng	75092	Phenanthrene-d10	11.17

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	87
2	Octadecane		254	C18H38	000593-45-3	86
3	Eicosane		282	C20H42	000112-95-8	78
4	Pentadecane		212	C15H32	000629-62-9	72
5	Heneicosane		296	C21H44	000629-94-7	72



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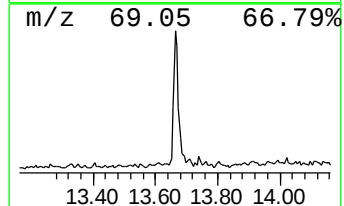
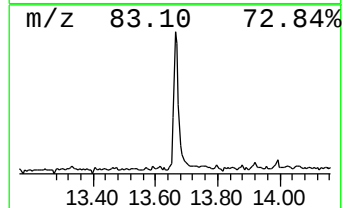
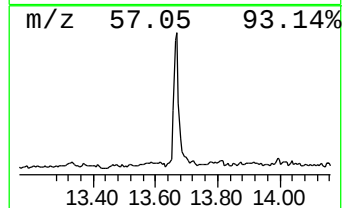
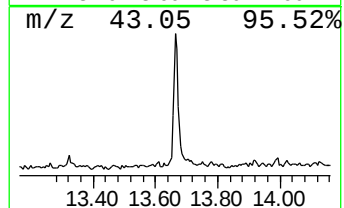
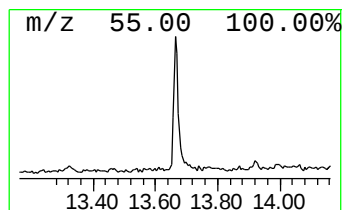
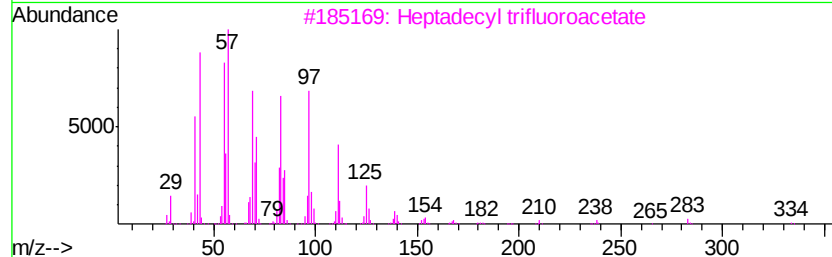
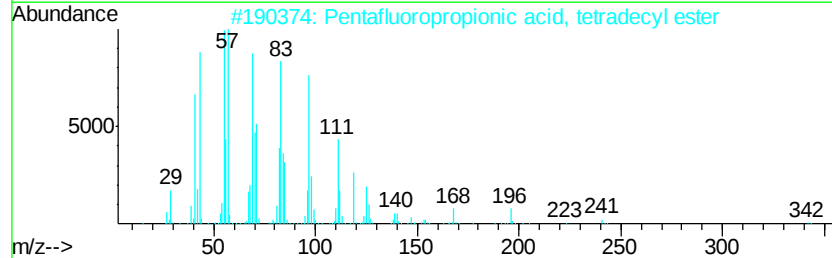
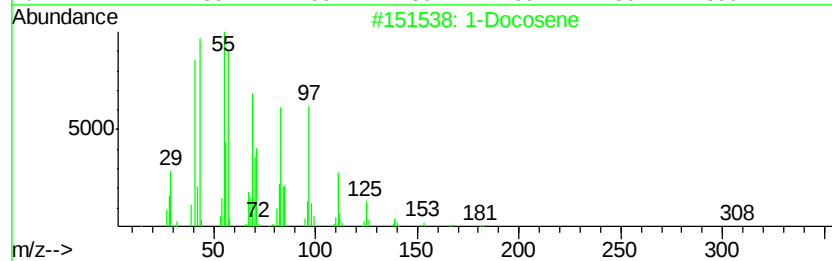
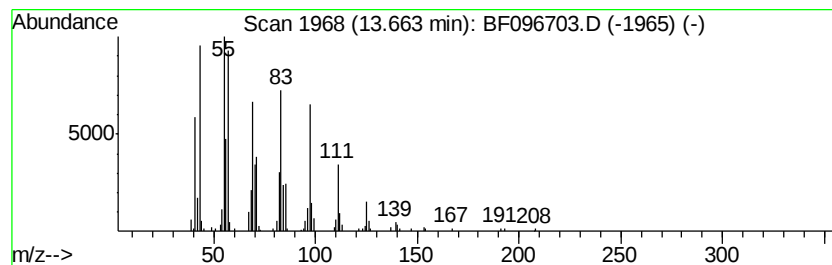
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Peak Number 5 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.66	10.12 ng	247758	Chrysene-d12	13.80

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene		308	C22H44	001599-67-3	95
2	Pentafluoropropionic acid, tetra...		360	C17H29F5O2	006222-06-6	94
3	Heptadecyl trifluoroacetate		352	C19H35F3O2	1000351-87-0	94
4	Trifluoroacetoxy hexadecane		338	C18H33F3O2	006222-03-3	94
5	1-Heneicosanol		312	C21H44O	015594-90-8	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.85	12.6	ng	382588	1	6.66	605149	20.0
unknown6.44	6.44	80.3	ng	2428230	1	6.66	605149	20.0
Hexadecane	10.62	2.5	ng	75092	4	11.17	613691	20.0
1-Docosene	13.66	10.1	ng	247758	5	13.80	489583	20.0