

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072117\
 Data File : BF096948.D
 Acq On : 21 Jul 2017 17:08
 Operator : SJ/JU
 Sample : I4290-05
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S-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:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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	4.728	462	466	481	rVB	209289	370465	9.91%	1.311%
2	5.163	535	540	543	rBV	3155792	3593491	96.12%	12.715%
3	6.216	713	719	733	rBV	3041891	3738535	100.00%	13.228%
4	6.328	733	738	741	rBV	3292677	3432404	91.81%	12.145%
5	6.551	773	776	780	rBV	847644	717163	19.18%	2.538%
6	6.710	799	803	806	rBV	2615622	2500032	66.87%	8.846%
7	7.122	867	873	876	rBV	2108347	2197565	58.78%	7.776%
8	7.834	990	994	998	rBV	1126630	979278	26.19%	3.465%
9	8.916	1172	1178	1181	rBV	3171292	3254025	87.04%	11.514%
10	9.310	1241	1245	1248	rBV	299018	234833	6.28%	0.831%
11	9.580	1287	1291	1295	rBV2	1121374	993024	26.56%	3.514%
12	10.033	1364	1368	1371	rVB	61181	49074	1.31%	0.174%
13	10.369	1421	1425	1429	rBV	1745957	1751380	46.85%	6.197%
14	10.504	1445	1448	1455	rBV	78846	80289	2.15%	0.284%
15	11.057	1538	1542	1545	rBV	956066	774720	20.72%	2.741%
16	12.645	1807	1812	1815	rBV	2200628	2213256	59.20%	7.831%
17	13.551	1962	1966	1974	rBV	167015	190410	5.09%	0.674%
18	13.680	1984	1988	1992	rBV	636529	573281	15.33%	2.028%
19	15.045	2215	2220	2226	rBV	517998	618382	16.54%	2.188%

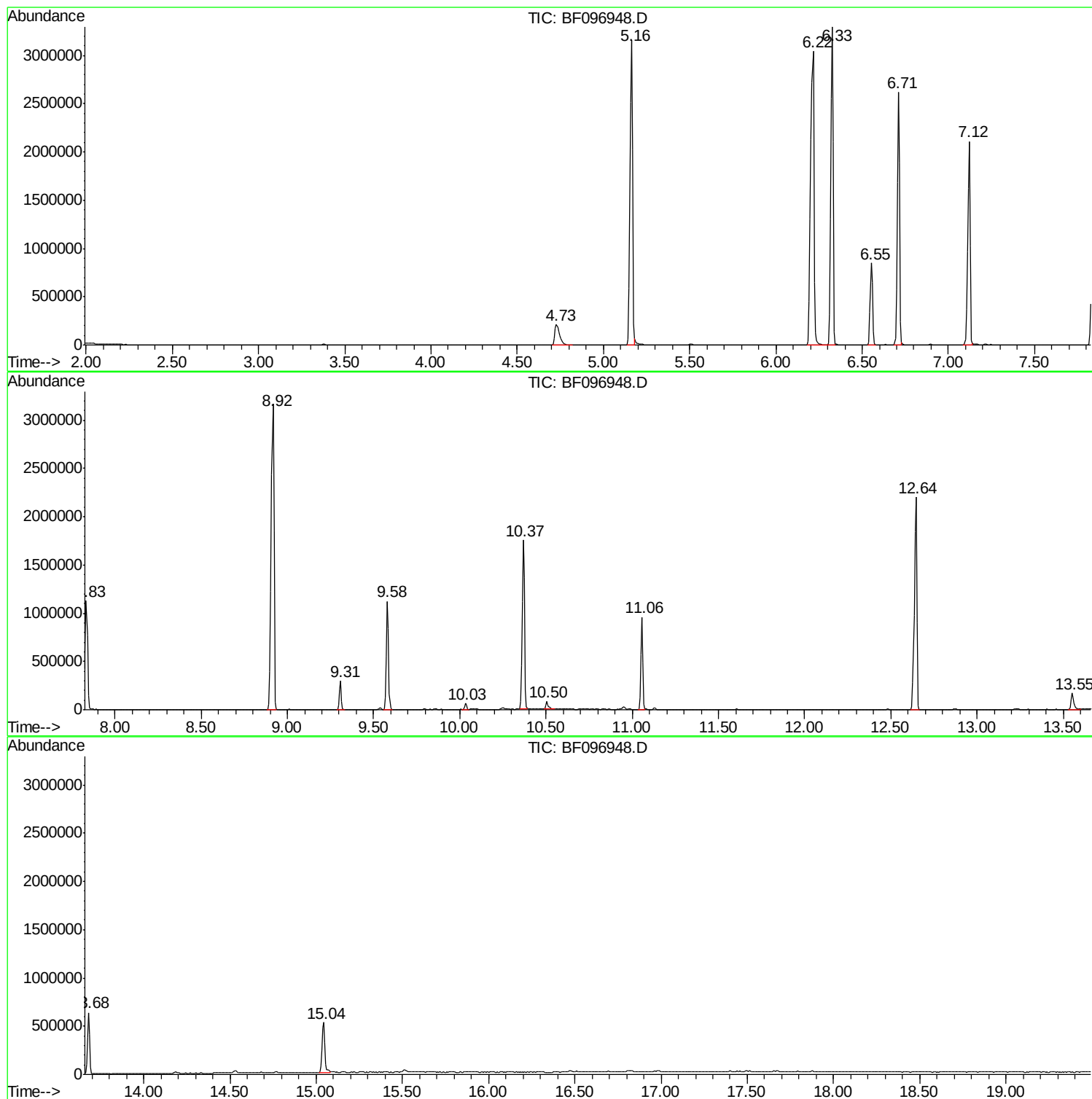
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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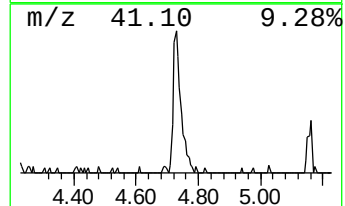
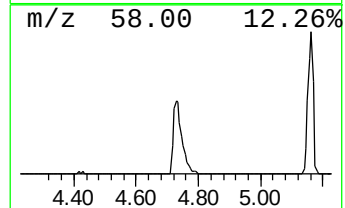
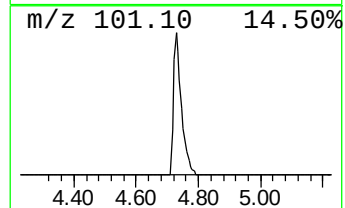
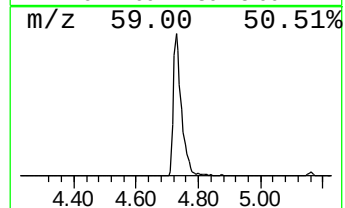
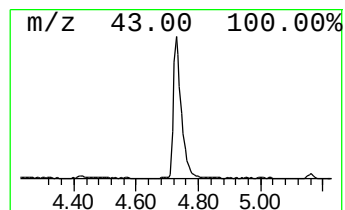
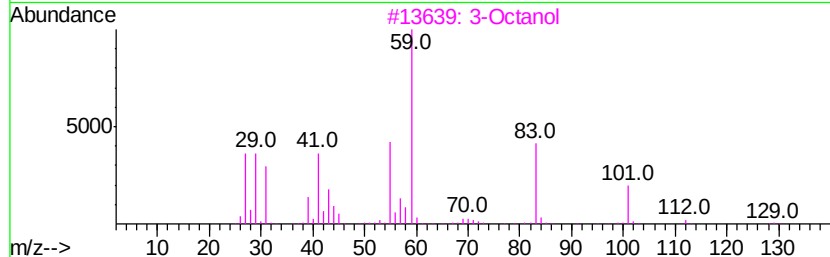
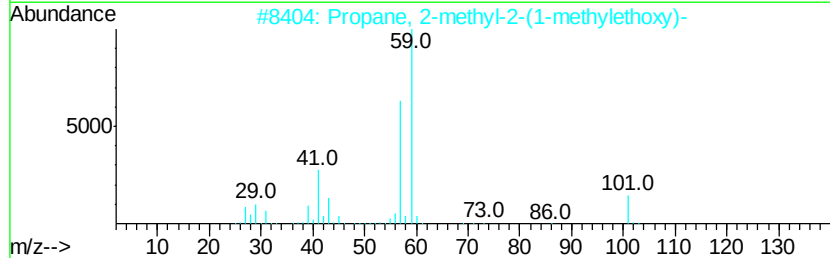
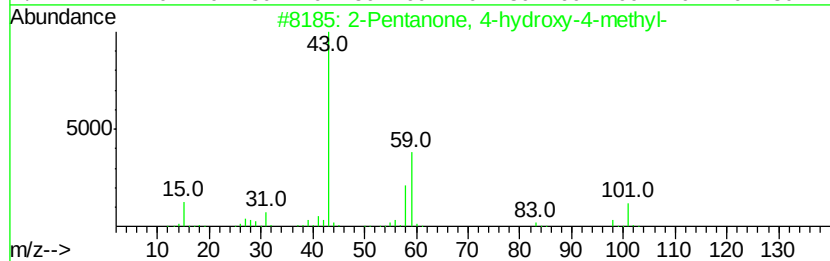
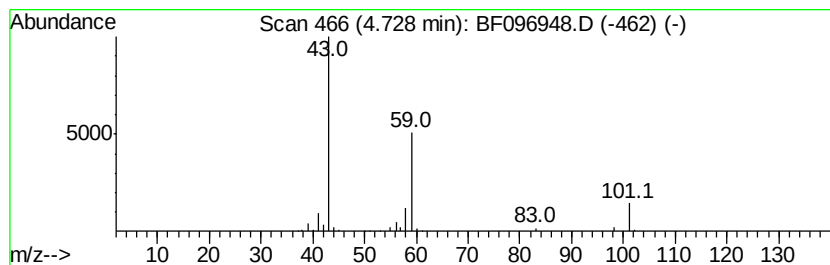
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.73	10.33 ng	370465	1,4-Dichlorobenzene-d4	6.55	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Octanol	130	C8H18O	000589-98-0	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28



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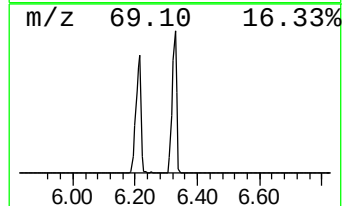
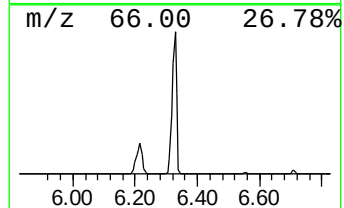
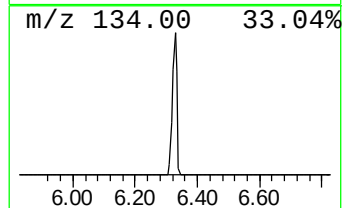
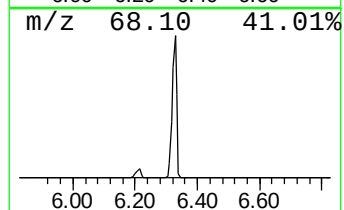
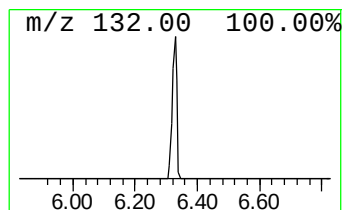
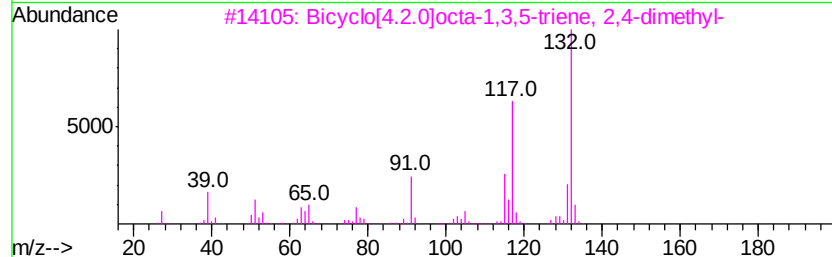
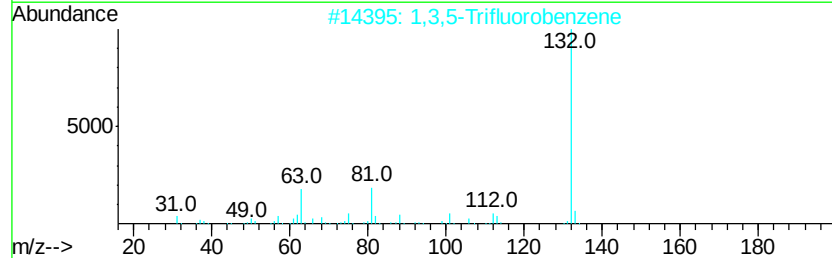
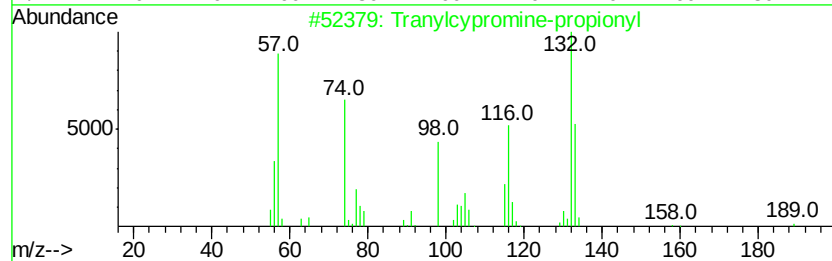
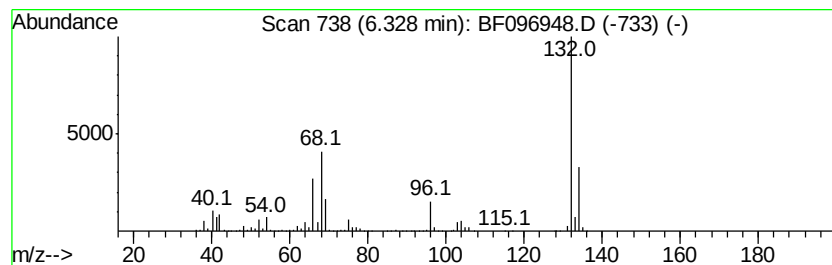
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Peak Number 2 unknown6.33 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.33	95.72 ng	3432400	1,4-Dichlorobenzene-d4	6.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
2		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
3		Bicyclo[4.2.0]octa-1,3,5-triene...	132	C10H12	028749-81-7	9
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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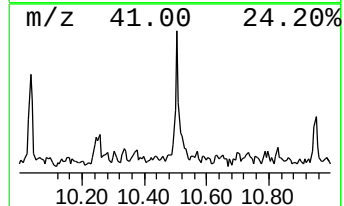
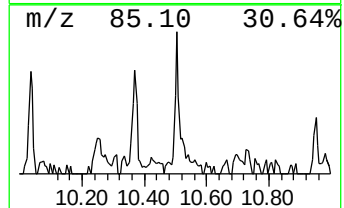
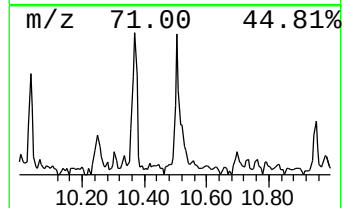
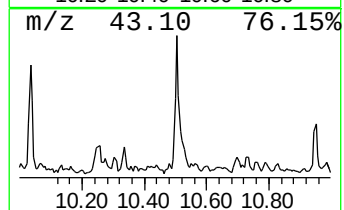
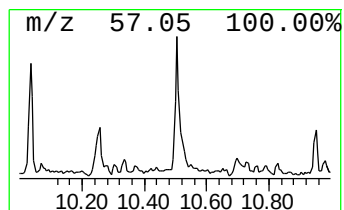
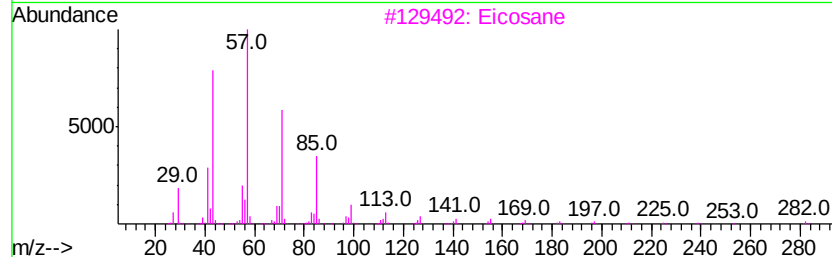
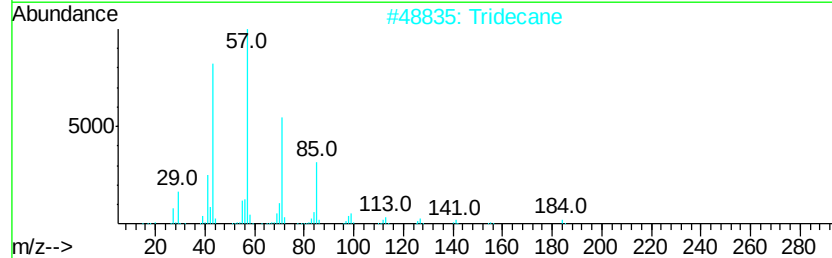
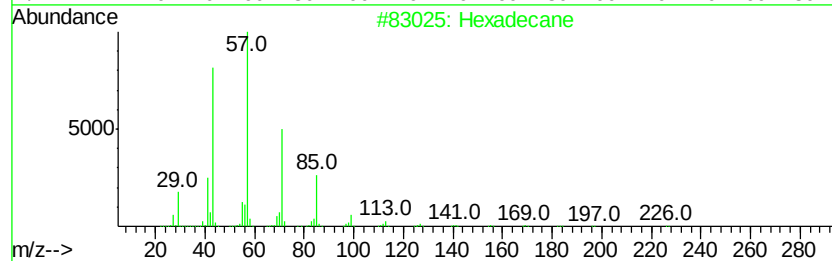
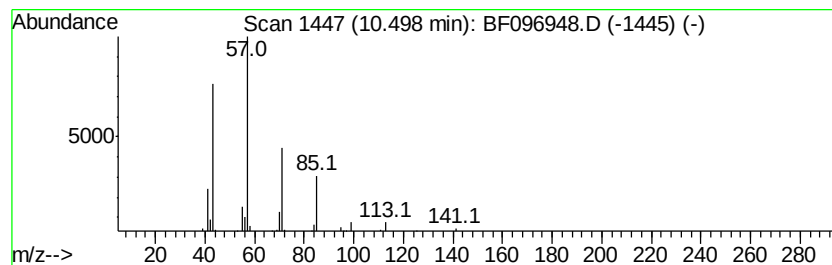
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Peak Number 4 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.50	2.07 ng	80289	Phenanthrene-d10	11.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Tridecane	184	C13H28	000629-50-5	90
3	Eicosane	282	C20H42	000112-95-8	90
4	Heptacosane	380	C27H56	000593-49-7	86
5	Nonadecane	268	C19H40	000629-92-5	86



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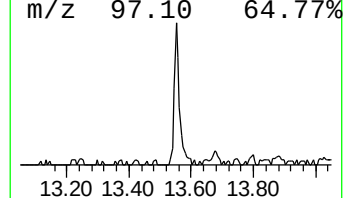
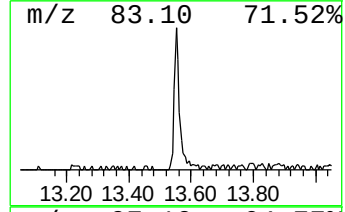
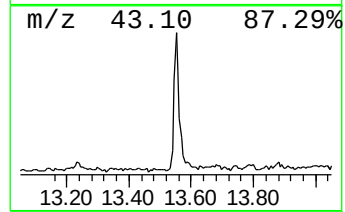
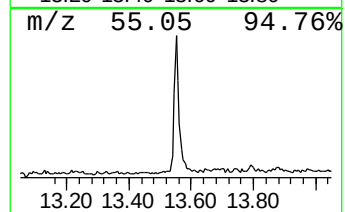
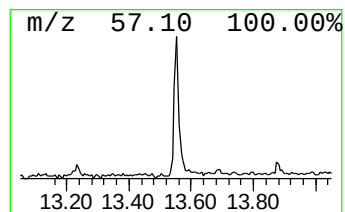
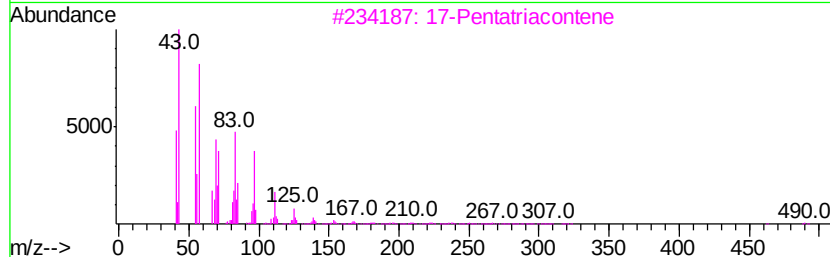
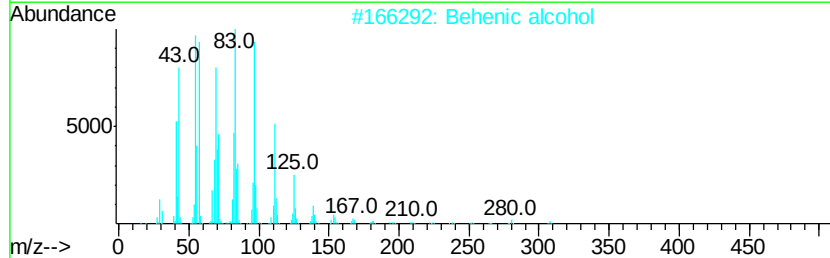
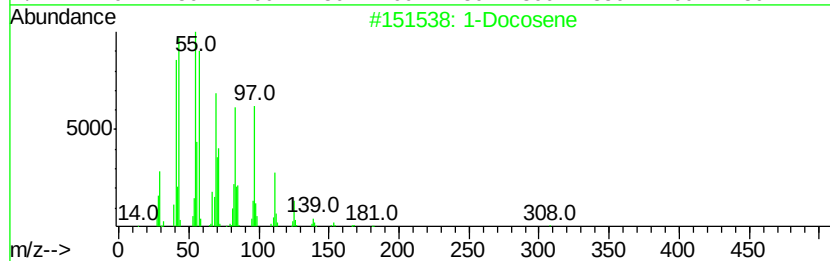
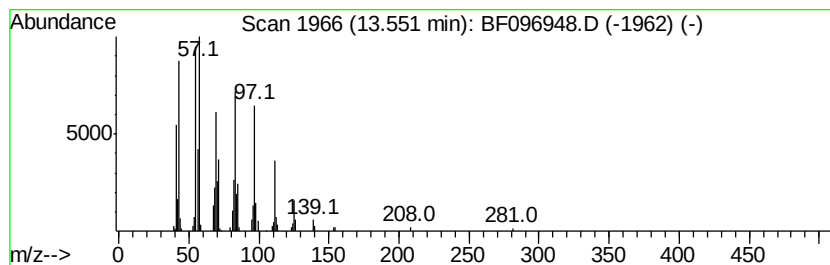
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Peak Number 5 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	6.64 ng	190410	Chrysene-d12	13.68

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene		308	C22H44	001599-67-3	94
2	Behenic alcohol		326	C22H46O	000661-19-8	93
3	17-Pentatriacontene		491	C35H70	006971-40-0	91
4	Heptadecyl heptafluorobutyrte		452	C21H35F7O2	959085-66-6	90
5	Heptadecyl trifluoroacetate		352	C19H35F3O2	1000351-87-0	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.73	10.3	ng	370465	1	6.55	717163	20.0
unknown6.33	6.33	95.7	ng	3432400	1	6.55	717163	20.0
Hexadecane	10.50	2.1	ng	80289	4	11.06	774720	20.0
1-Docosene	13.55	6.6	ng	190410	5	13.68	573281	20.0