

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022817\
 Data File : BF093250.D
 Acq On : 28 Feb 2017 16:00
 Operator : SJ/MA
 Sample : I2017-03
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :

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-BF013017.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	4.967	250	252	269	rBV	993345	1357315	40.41%	4.697%
2	5.413	288	291	293	rBV	2486634	3249251	96.74%	11.244%
3	6.453	380	382	385	rBV	2835336	3213050	95.66%	11.119%
4	6.579	390	393	395	rBV	3379879	3358711	100.00%	11.623%
5	6.807	411	413	415	rBV	764644	806275	24.01%	2.790%
6	6.956	424	426	429	rBV	2149157	2388088	71.10%	8.264%
7	7.379	460	463	465	rBV	1481478	2090399	62.24%	7.234%
8	8.088	523	525	528	rBV	1171093	1066265	31.75%	3.690%
9	9.162	617	619	622	rBV	2615156	3123124	92.99%	10.807%
10	9.562	652	654	657	rBV	275205	228020	6.79%	0.789%
11	9.779	671	673	676	rBV	24396	35556	1.06%	0.123%
12	9.848	676	679	681	rVV	854681	1102501	32.83%	3.815%
13	10.271	715	716	718	rVB	73337	56283	1.68%	0.195%
14	10.488	732	735	739	rBV	25496	38348	1.14%	0.133%
15	10.636	745	748	750	rBV	1575400	1607355	47.86%	5.562%
16	10.751	756	758	763	rVB	61988	100014	2.98%	0.346%
17	11.196	795	797	798	rBV	47271	54200	1.61%	0.188%
18	11.322	806	808	811	rBV	777031	969854	28.88%	3.356%
19	12.774	932	935	937	rBV	22410	35156	1.05%	0.122%
20	12.911	944	947	949	rBV	2359010	2117621	63.05%	7.328%
21	13.802	1023	1025	1030	rBV	60274	127773	3.80%	0.442%
22	13.962	1037	1039	1042	rBV	769535	802386	23.89%	2.777%
23	14.054	1045	1047	1053	rVB6	19779	43743	1.30%	0.151%
24	14.442	1077	1081	1083	rBV5	23111	67144	2.00%	0.232%
25	15.391	1161	1164	1170	rBV	659202	859532	25.59%	2.974%

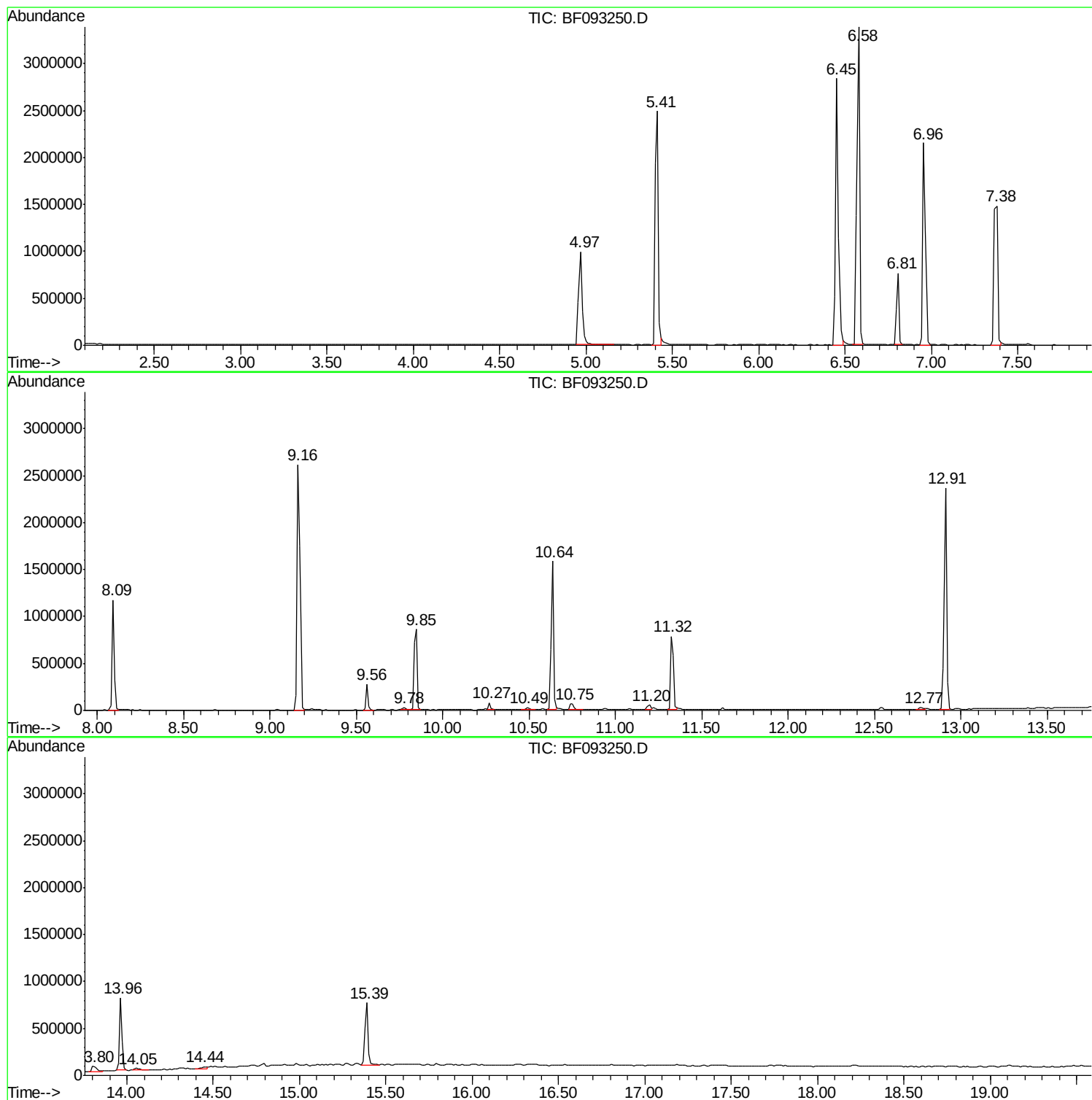
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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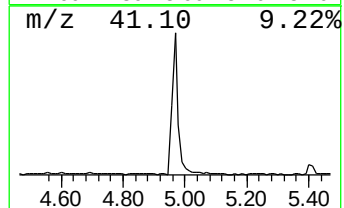
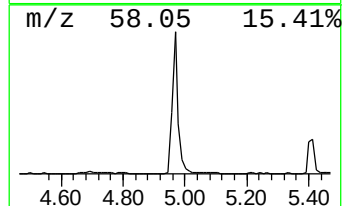
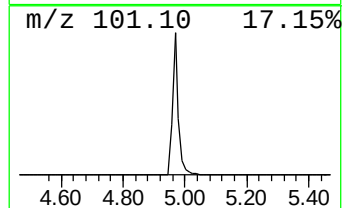
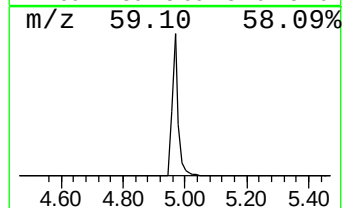
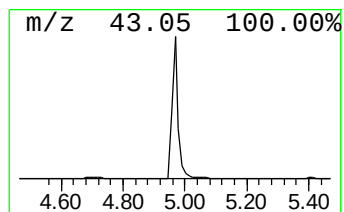
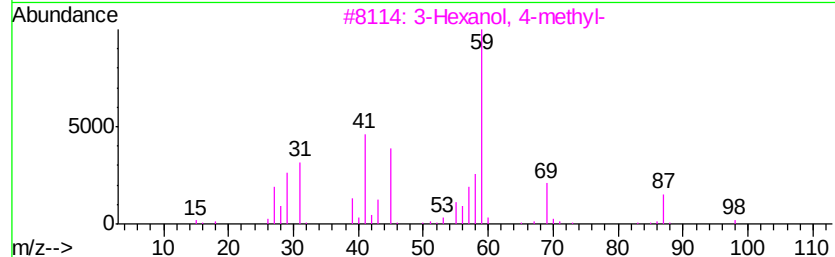
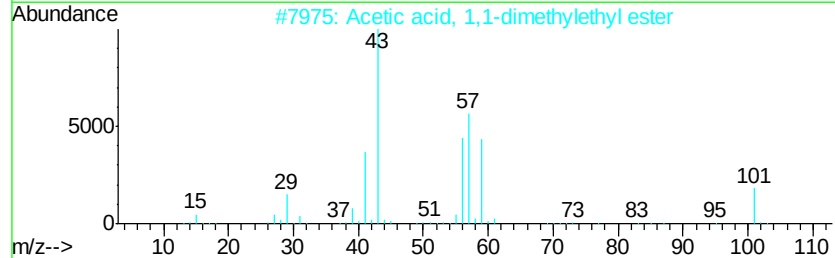
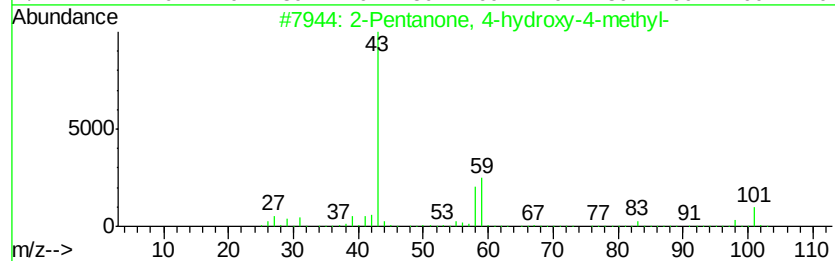
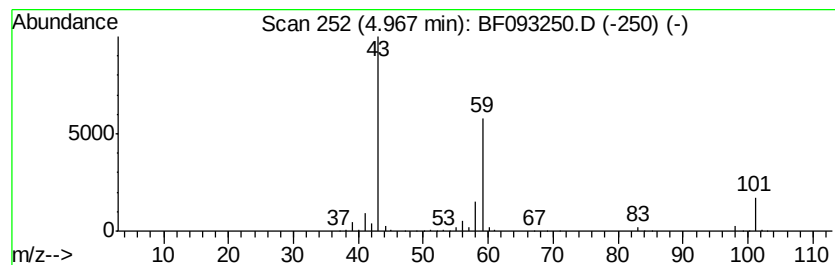
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.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.
4.97	33.67 ng	1357320	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32



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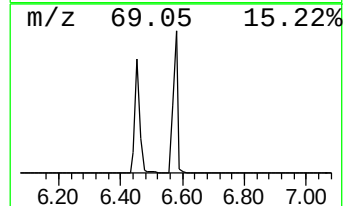
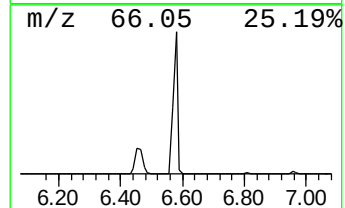
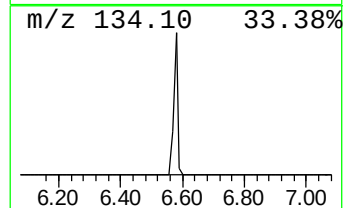
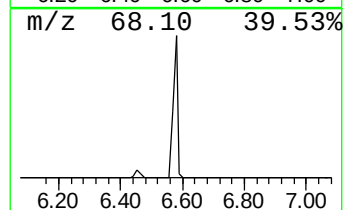
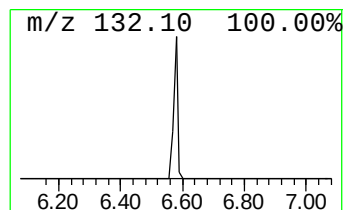
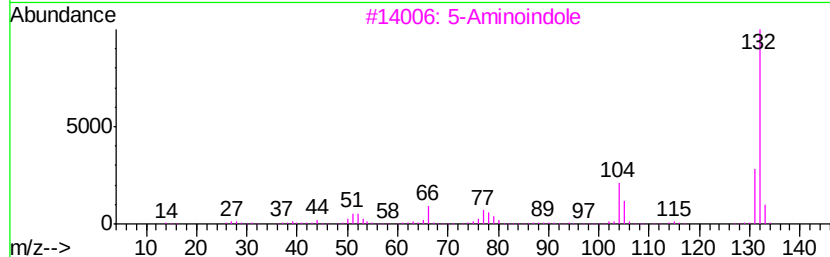
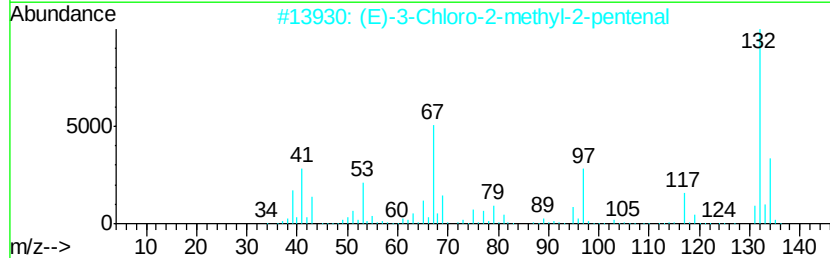
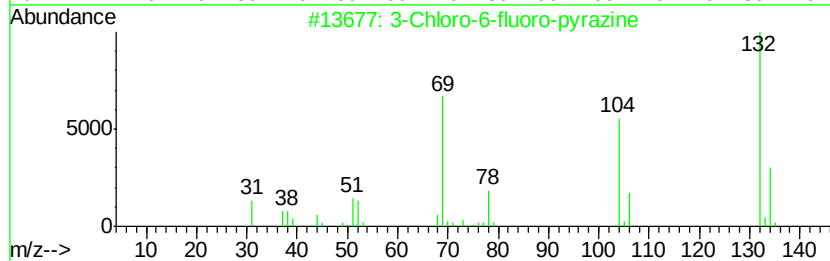
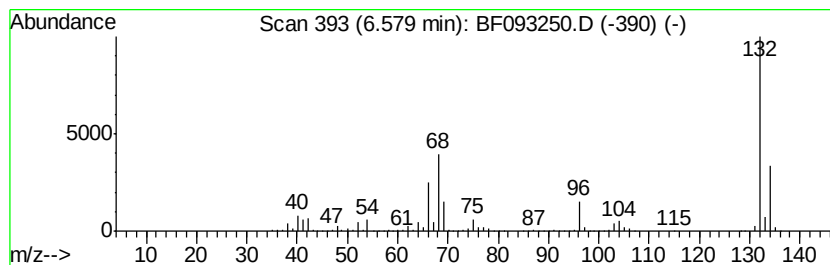
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Peak Number 2 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	83.31 ng	3358710	1,4-Dichlorobenzene-d4	6.81

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		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



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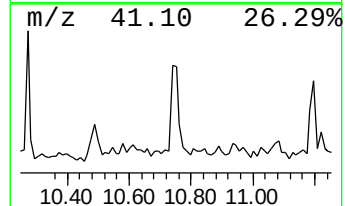
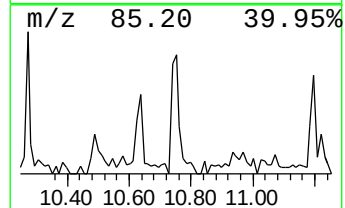
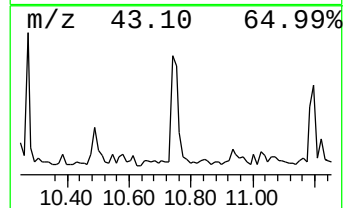
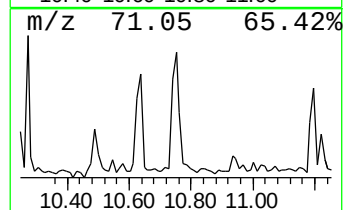
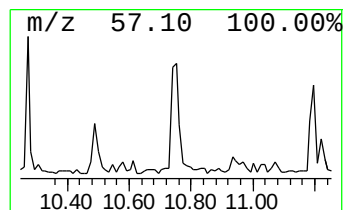
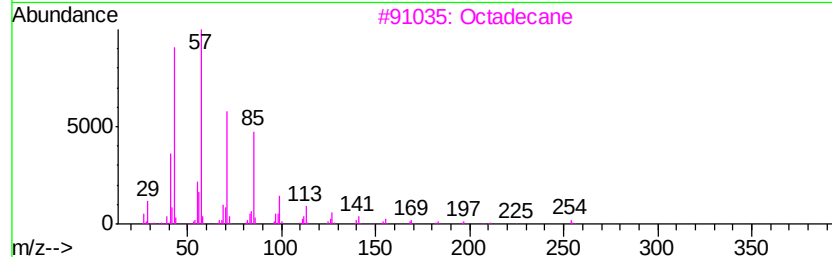
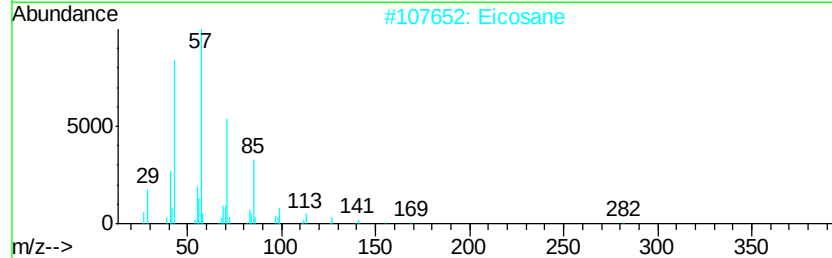
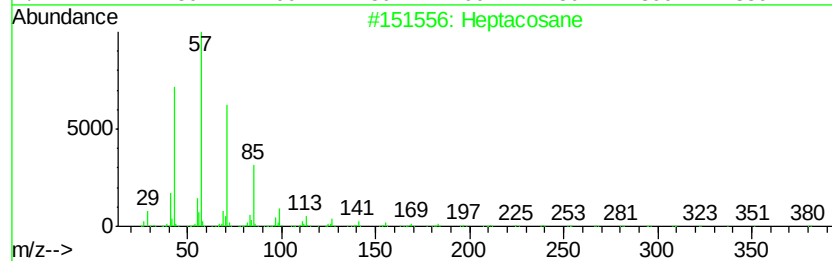
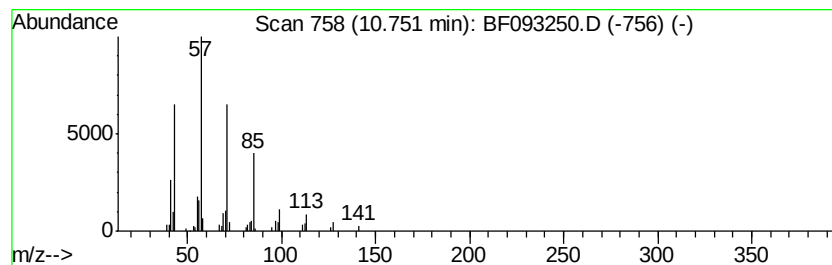
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Peak Number 4 Heptacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.75	2.06 ng	100014	Phenanthrene-d10	11.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	91
2	Eicosane		282	C20H42	000112-95-8	91
3	Octadecane		254	C18H38	000593-45-3	90
4	Heptadecane		240	C17H36	000629-78-7	90
5	Tetracosane		338	C24H50	000646-31-1	90



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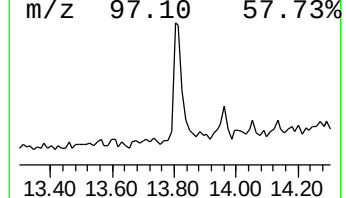
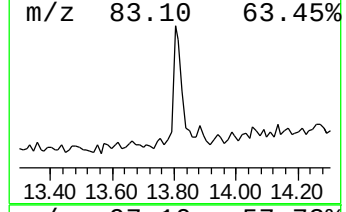
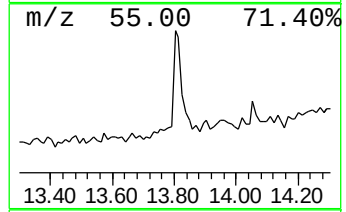
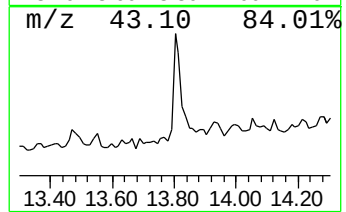
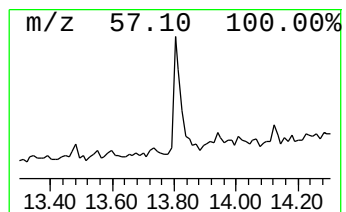
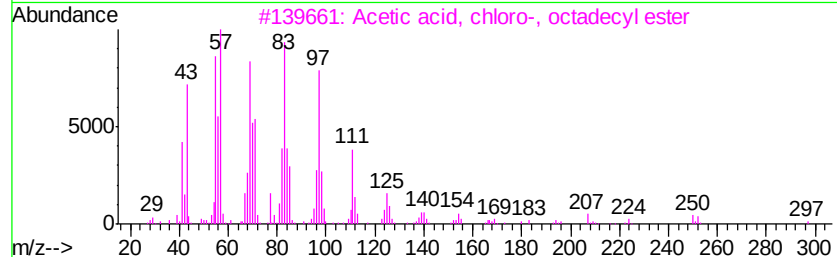
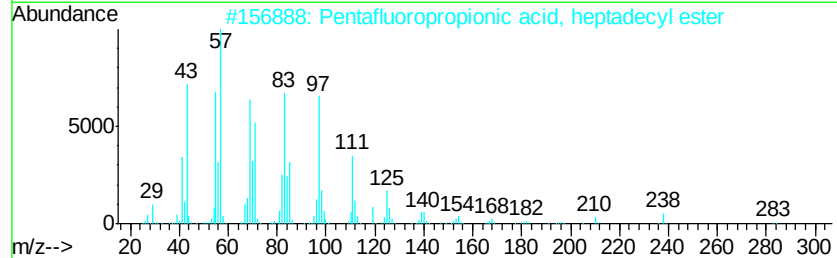
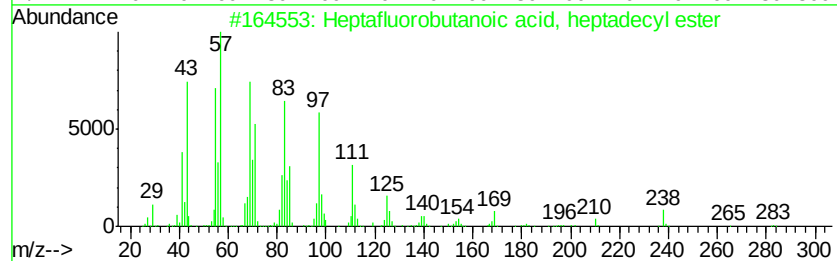
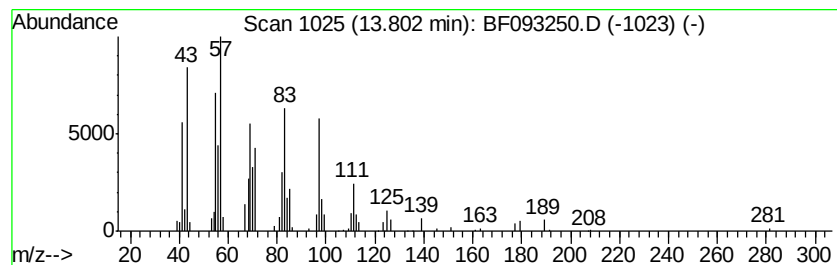
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Peak Number 5 Heptafluorobutanoic acid, h... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	3.18 ng	127773	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	90
2		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	87
3		Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	87
4		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87
5		1-Nonadecene	266	C19H38	018435-45-5	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.97	33.7	ng	1357320	1	6.81	806275	20.0
unknown6.58	6.58	83.3	ng	3358710	1	6.81	806275	20.0
Heptacosane	10.75	2.1	ng	100014	4	11.32	969854	20.0
Heptafluorobutano...	13.80	3.2	ng	127773	5	13.96	802386	20.0