

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021417\
 Data File : BF092938.D
 Acq On : 14 Feb 2017 12:37
 Operator : SJ/MA
 Sample : I1788-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-1-021017

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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	5.047	257	259	266	rBV	560819	746630	12.76%	1.876%
2	5.481	294	297	299	rBV	2326080	2618486	44.74%	6.579%
3	6.510	384	387	390	rBV	1870927	1717910	29.35%	4.316%
4	6.647	396	399	401	rBV	4130626	4180810	71.43%	10.504%
5	6.876	417	419	421	rBV	1136923	972759	16.62%	2.444%
6	7.036	430	433	435	rBV	3665857	3899776	66.63%	9.798%
7	7.447	466	469	471	rBV	2967581	3534302	60.39%	8.880%
8	8.156	529	531	534	rBV	1116362	1239268	21.17%	3.114%
9	9.242	622	626	628	rBV	5088813	5852714	100.00%	14.705%
10	9.630	658	660	662	rVB	145786	112364	1.92%	0.282%
11	9.916	682	685	687	rVB	1267818	1487748	25.42%	3.738%
12	10.339	719	722	724	rVB	93013	106954	1.83%	0.269%
13	10.705	751	754	756	rBV	2738102	3023107	51.65%	7.595%
14	10.808	762	763	768	rVB	86147	124999	2.14%	0.314%
15	11.265	801	803	808	rVB	60908	119438	2.04%	0.300%
16	11.391	812	814	817	rBV	1341194	1408487	24.07%	3.539%
17	11.688	838	840	842	rBV	65696	62913	1.07%	0.158%
18	12.979	950	953	956	rBV	3730109	5117160	87.43%	12.856%
19	13.871	1029	1031	1036	rBV	73654	136273	2.33%	0.342%
20	14.031	1042	1045	1047	rBV	1320866	1279335	21.86%	3.214%
21	14.317	1068	1070	1075	rVB5	22537	66782	1.14%	0.168%
22	15.174	1139	1145	1156	rVB2	249749	1021949	17.46%	2.568%
23	15.460	1167	1170	1173	rBV	614707	901858	15.41%	2.266%
24	17.803	1372	1375	1379	rBV4	27771	70119	1.20%	0.176%

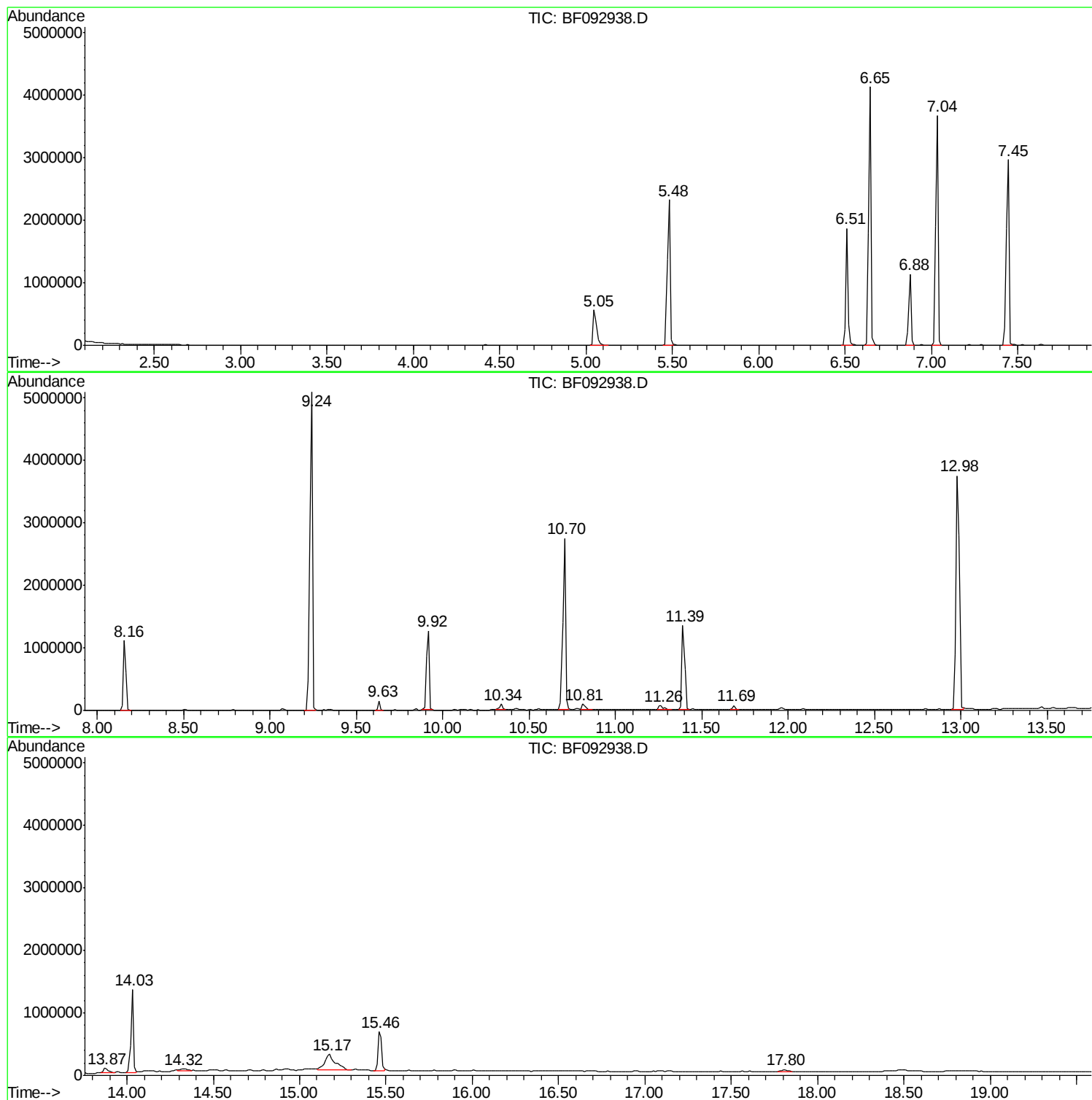
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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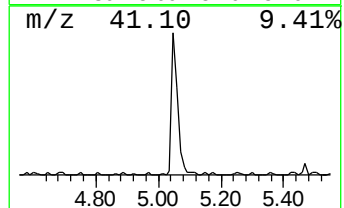
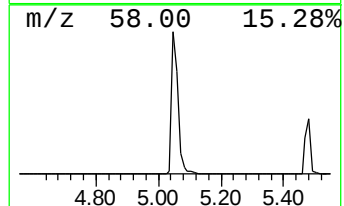
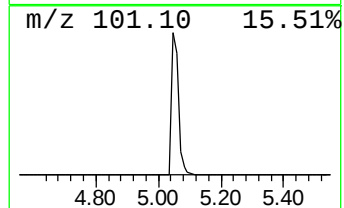
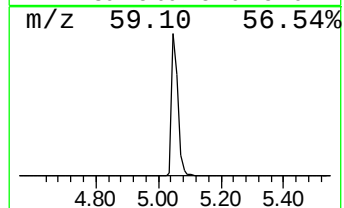
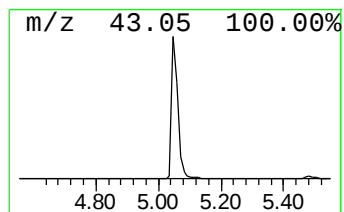
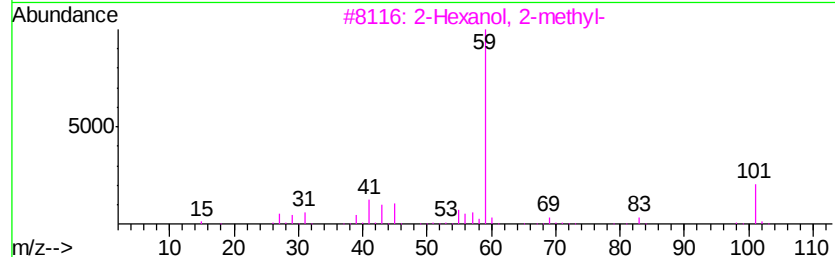
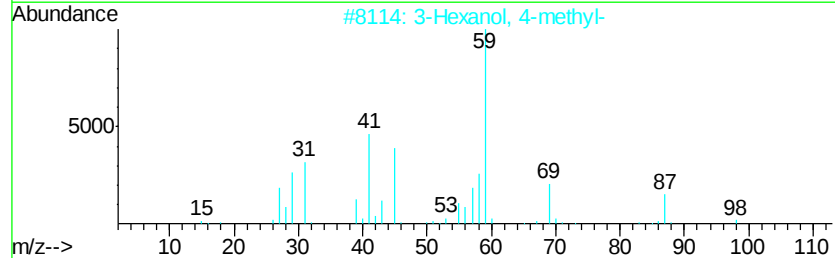
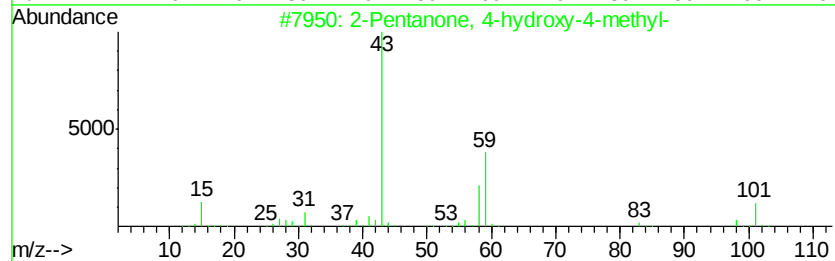
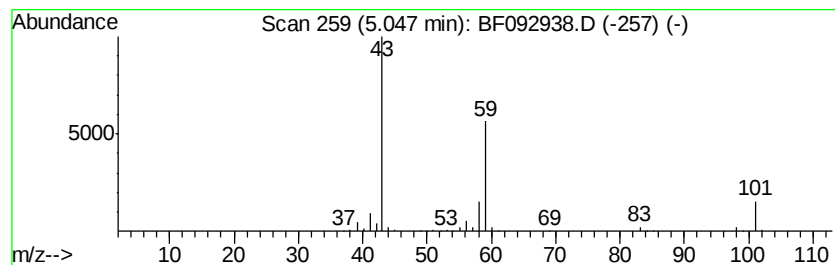
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	15.35 ng	746630	1,4-Dichlorobenzene-d4	6.88

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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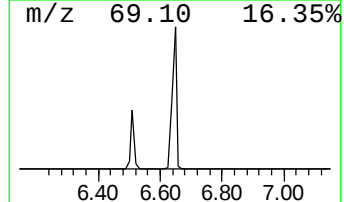
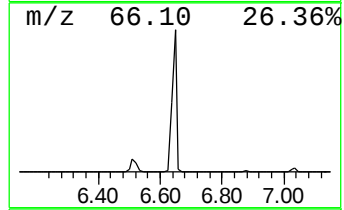
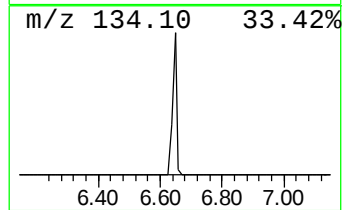
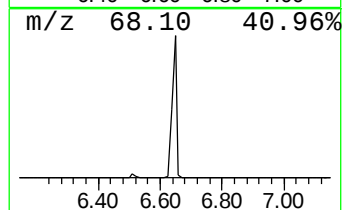
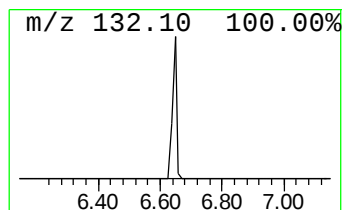
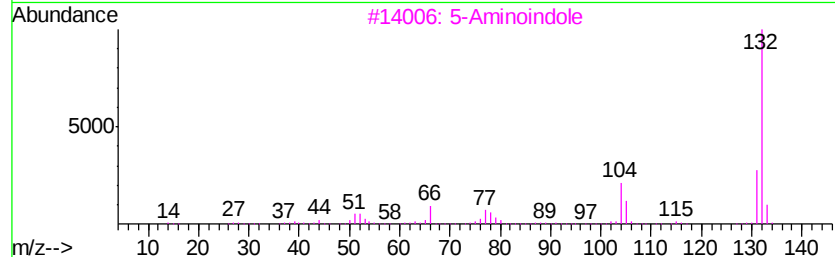
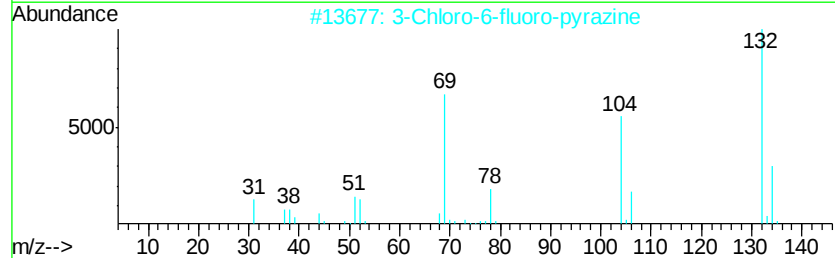
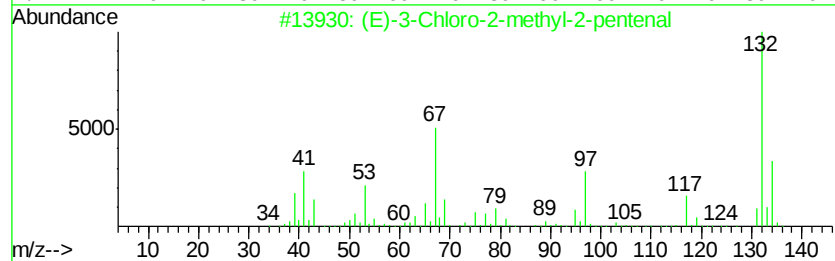
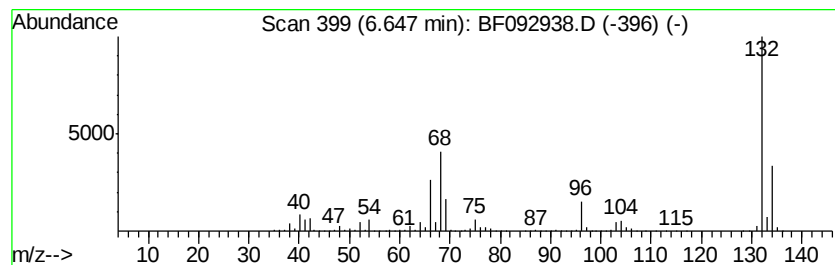
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Peak Number 2 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	85.96 ng	4180810	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
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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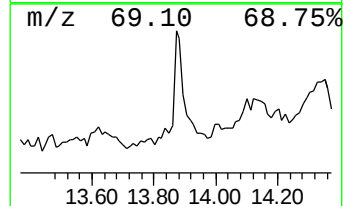
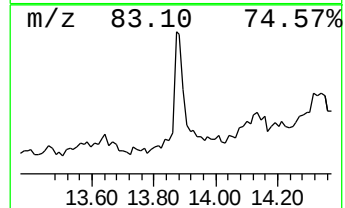
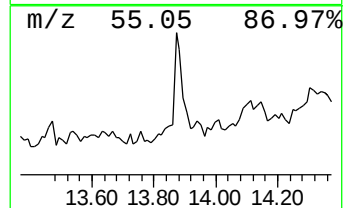
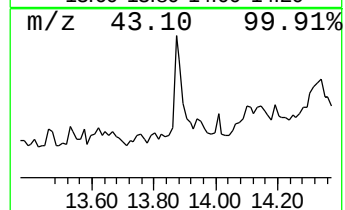
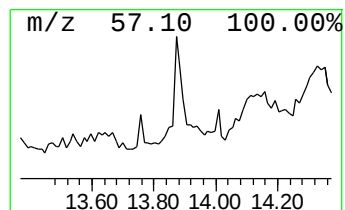
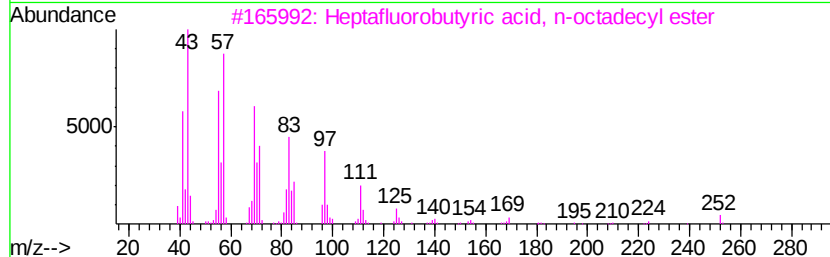
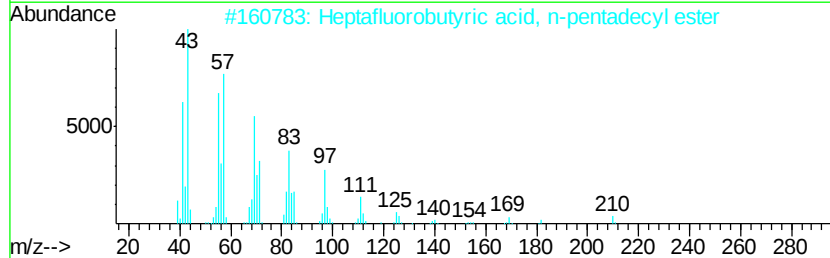
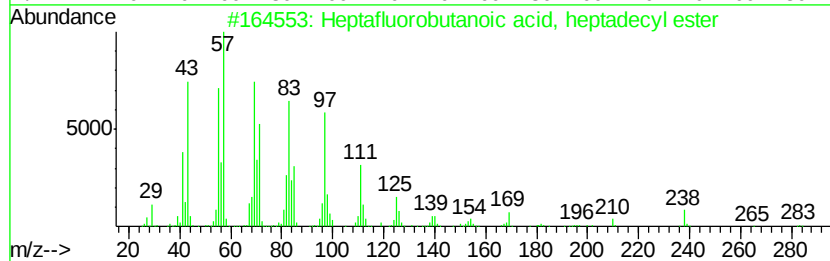
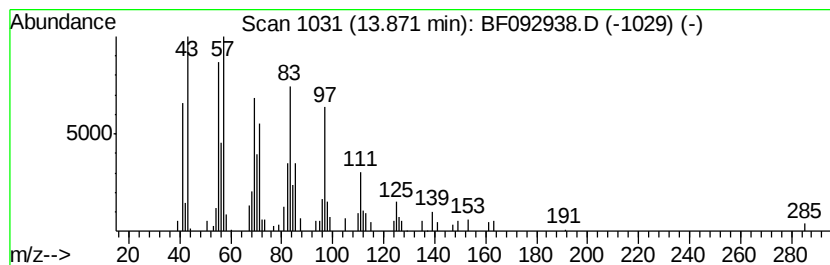
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Peak Number 4 Heptafluorobutanoic acid, h... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	2.13 ng	136273	Chrysene-d12	14.03

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	95
2		Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	91
3		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
4		Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	91
5		17-Pentatriacontene	491	C35H70	006971-40-0	91



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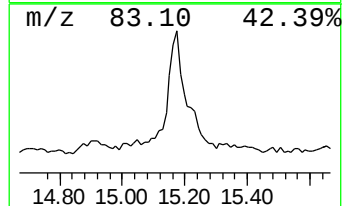
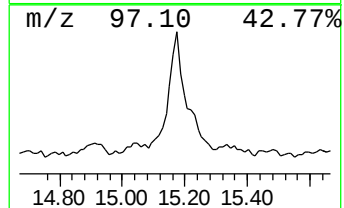
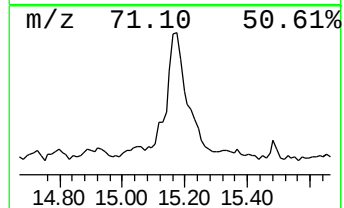
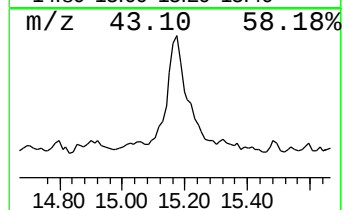
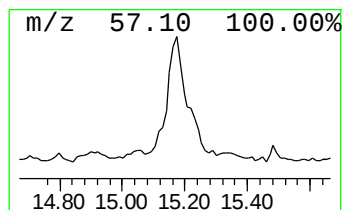
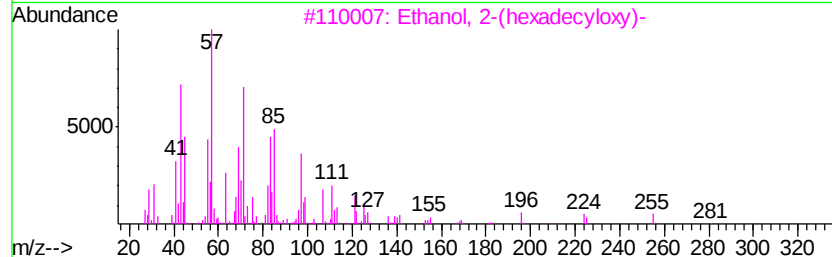
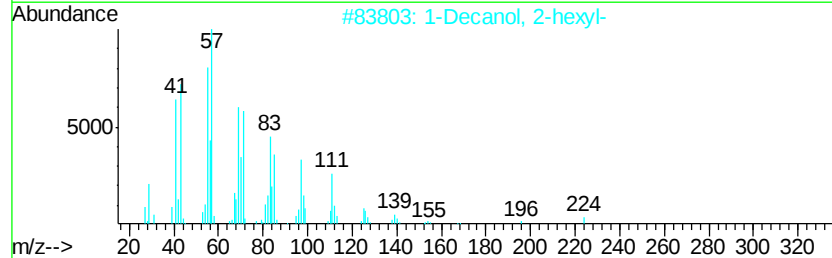
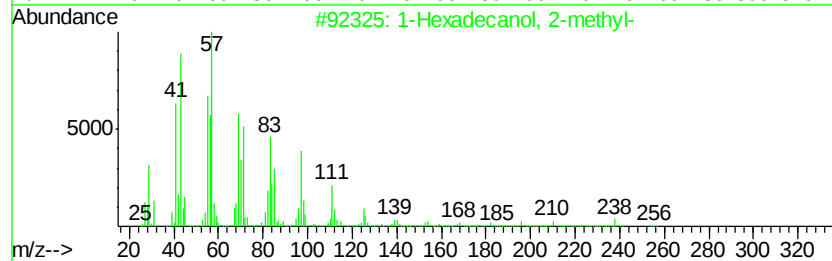
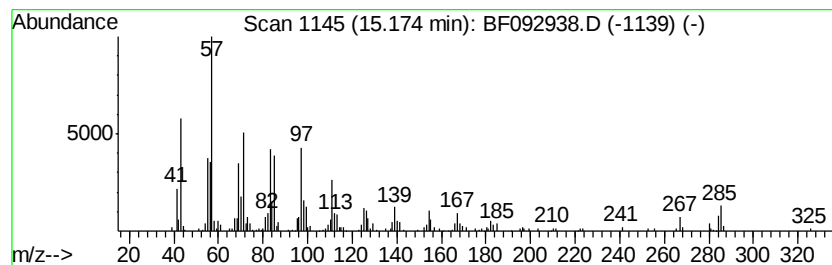
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Peak Number 5 1-Hexadecanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	22.66 ng	1021950	Perylene-d12	15.46

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexadecanol, 2-methyl-	256	C17H36O	002490-48-4	72
2		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	62
3		Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	52
4		Cycloundecane, (1-methylethyl)-	196	C14H28	062338-56-1	44
5		Nonadecane	268	C19H40	000629-92-5	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.05	15.4	ng	746630	1	6.88	972759	20.0
unknown6.65	6.65	86.0	ng	4180810	1	6.88	972759	20.0
Heptafluorobutano...	13.87	2.1	ng	136273	5	14.03	1279340	20.0
1-Hexadecanol, 2-...	15.17	22.7	ng	1021950	6	15.46	901858	20.0