

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110116\
 Data File : BF090950.D
 Acq On : 1 Nov 2016 14:59
 Operator : UM/SJ
 Sample : H5445-05
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-5-4-5

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-BF102616.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	4.887	243	245	254	rBV	641146	890244	21.89%	2.553%
2	5.333	281	284	286	rBV	2775325	3264362	80.25%	9.363%
3	6.373	373	375	378	rBV	2246230	3275750	80.53%	9.396%
4	6.499	384	386	389	rBV	2921768	3261369	80.18%	9.354%
5	6.739	405	407	409	rBV	824515	896716	22.05%	2.572%
6	6.887	418	420	423	rBV	2325449	2429100	59.72%	6.967%
7	7.299	454	456	459	rBV	1749243	1912333	47.01%	5.485%
8	7.402	463	465	473	rVB	27201	67557	1.66%	0.194%
9	8.019	517	519	522	rBV	1270620	1290846	31.74%	3.702%
10	9.105	611	614	616	rBV	3890513	4067542	100.00%	11.667%
11	9.493	646	648	651	rBV	651702	742613	18.26%	2.130%
12	9.699	661	666	670	rBV2	38354	111839	2.75%	0.321%
13	9.779	670	673	675	rBV	1043691	1487889	36.58%	4.268%
14	10.213	704	711	713	rBV2	77205	126680	3.11%	0.363%
15	10.430	727	730	734	rBV	24901	47684	1.17%	0.137%
16	10.568	739	742	744	rBV2	1819687	2479276	60.95%	7.111%
17	10.693	751	753	759	rVB	67899	118876	2.92%	0.341%
18	11.139	790	792	793	rBV	49276	55581	1.37%	0.159%
19	11.253	800	802	805	rBV	1638173	1491358	36.66%	4.278%
20	11.310	805	807	814	rVB2	20861	51271	1.26%	0.147%
21	12.842	938	941	944	rBV	4021487	3885394	95.52%	11.144%
22	13.745	1017	1020	1026	rBV2	129635	207755	5.11%	0.596%
23	13.894	1030	1033	1035	rBV	954469	1337836	32.89%	3.837%
24	14.065	1046	1048	1051	rBV	52421	61213	1.50%	0.176%
25	14.374	1073	1075	1081	rVB	62666	62457	1.54%	0.179%
26	14.671	1097	1101	1104	rBV2	47852	94798	2.33%	0.272%
27	14.739	1104	1107	1109	rVV	61344	78744	1.94%	0.226%
28	14.979	1125	1128	1130	rBV	42981	49295	1.21%	0.141%
29	15.288	1152	1155	1157	rBV	828351	1018602	25.04%	2.922%

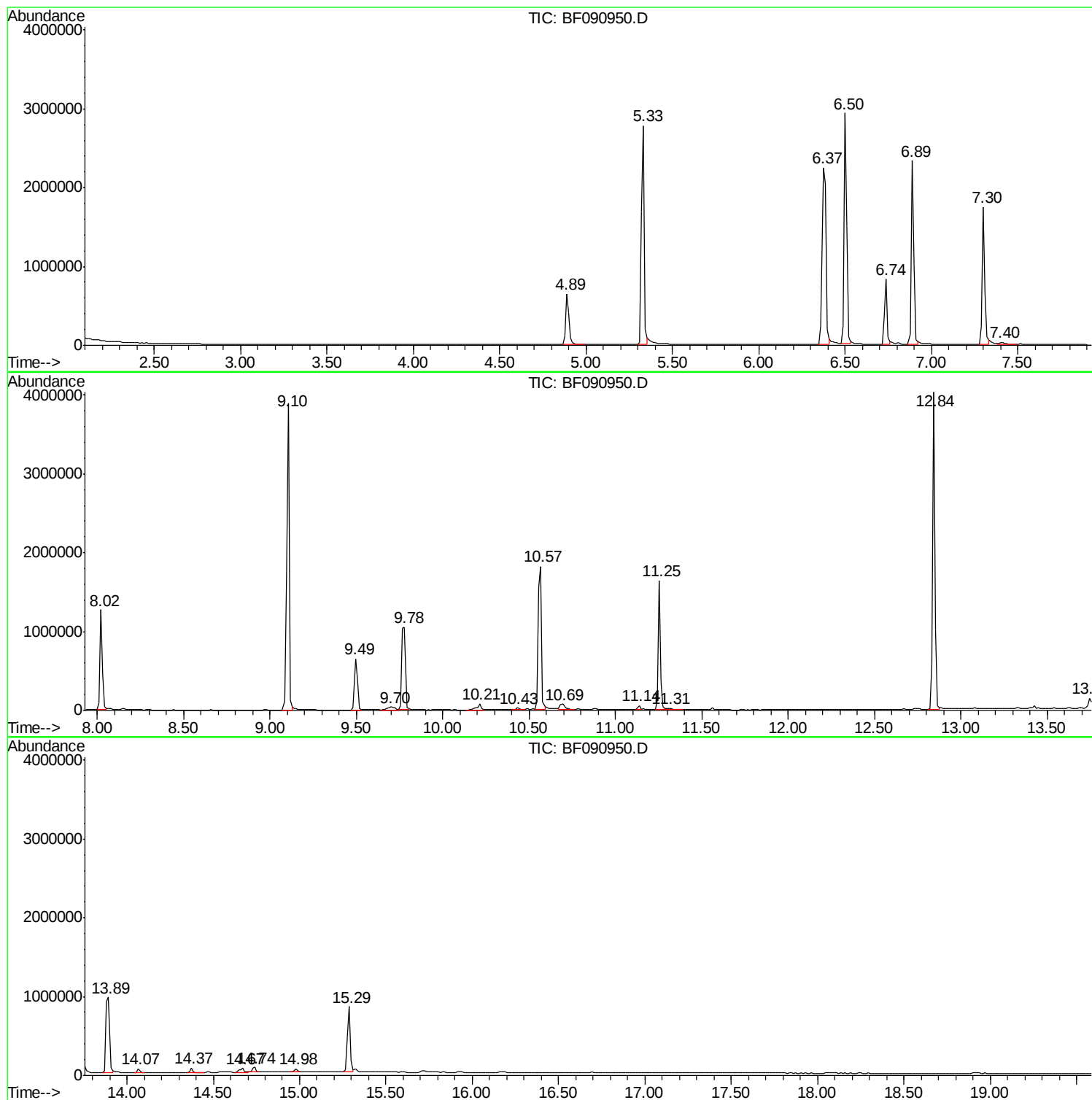
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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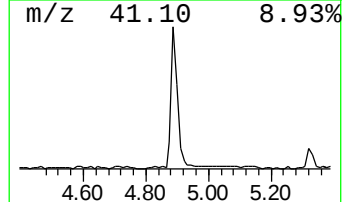
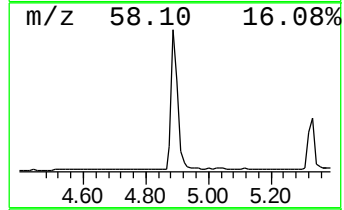
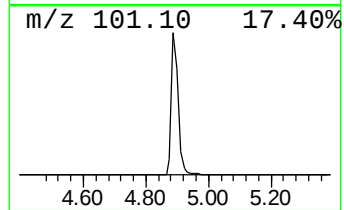
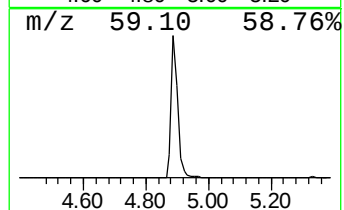
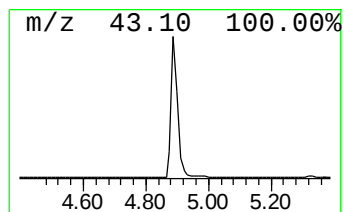
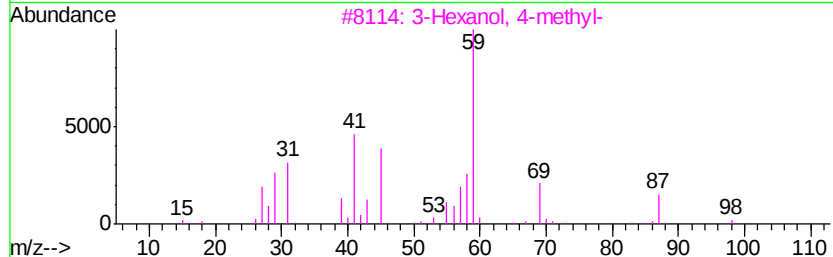
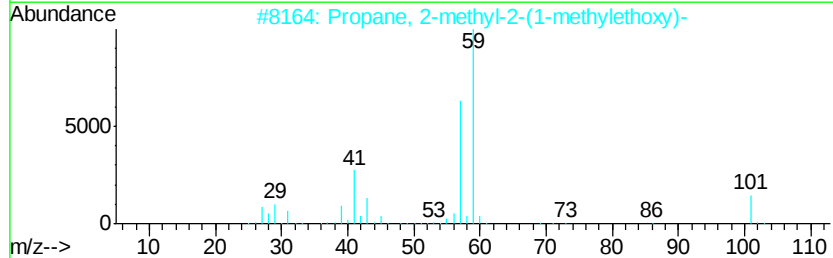
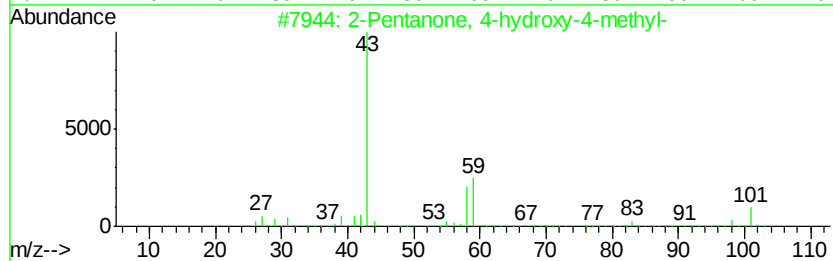
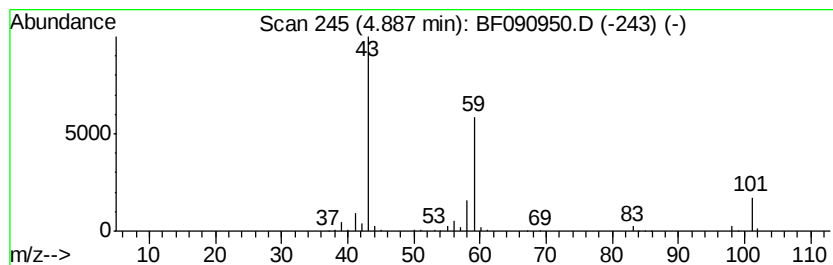
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.89	19.86 ng	890244	1,4-Dichlorobenzene-d4	6.74

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
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			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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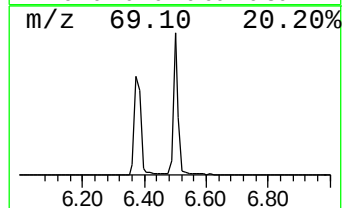
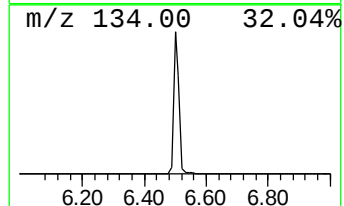
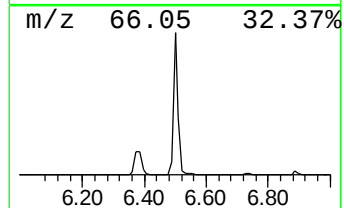
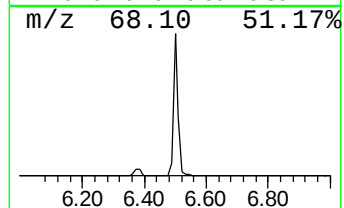
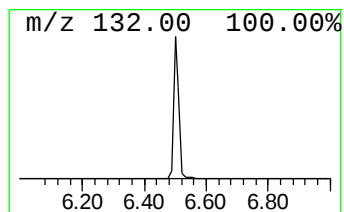
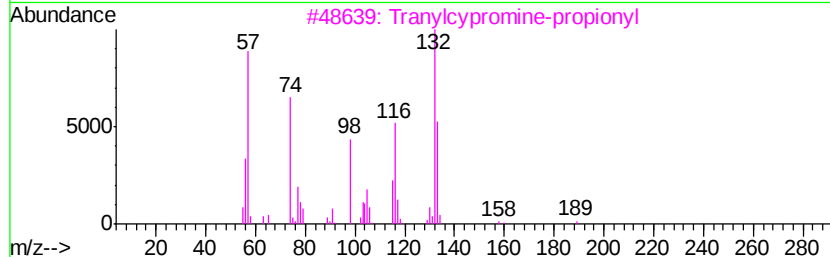
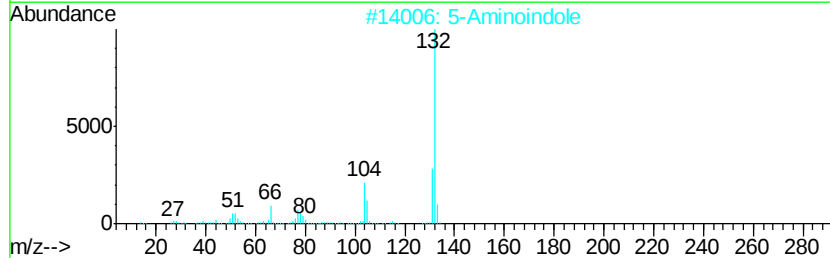
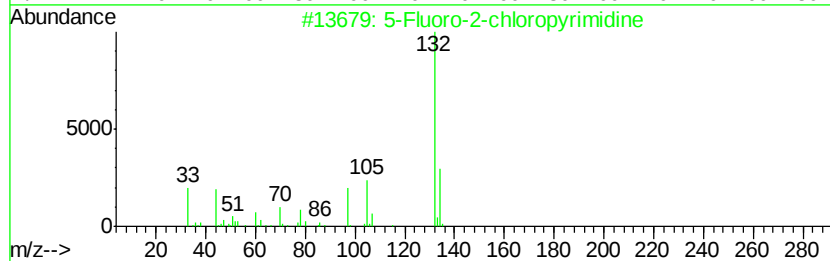
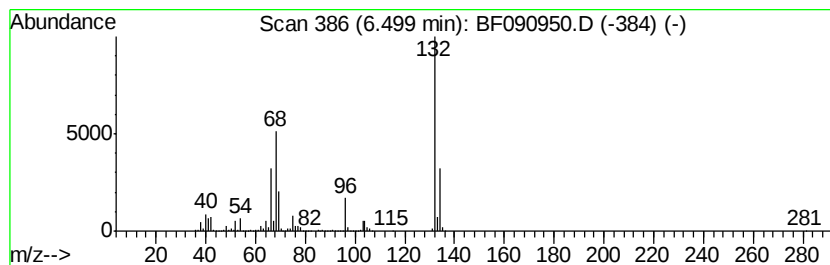
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Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	72.74 ng	3261370	1,4-Dichlorobenzene-d4	6.74

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4			2-Cyclohexen-1-one	96	C6H8O	000930-68-7	9
5			Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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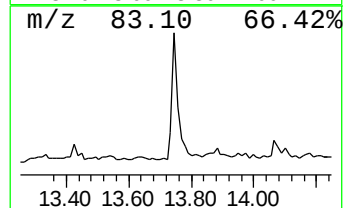
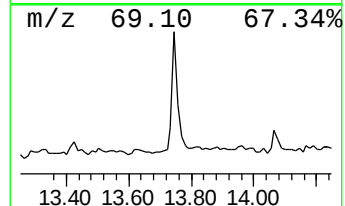
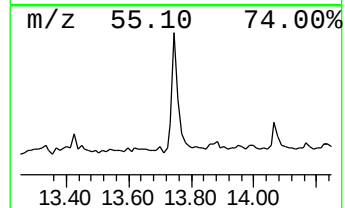
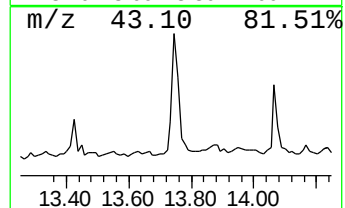
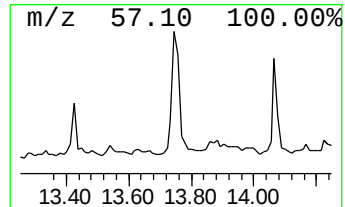
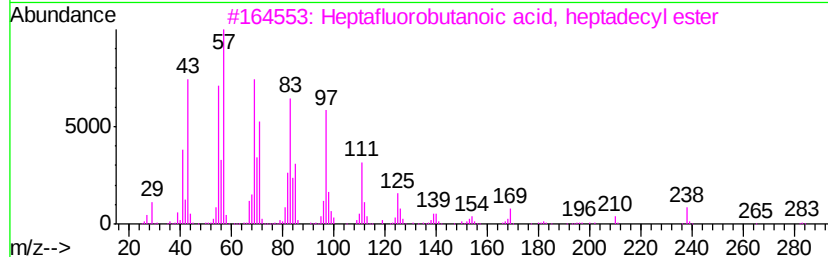
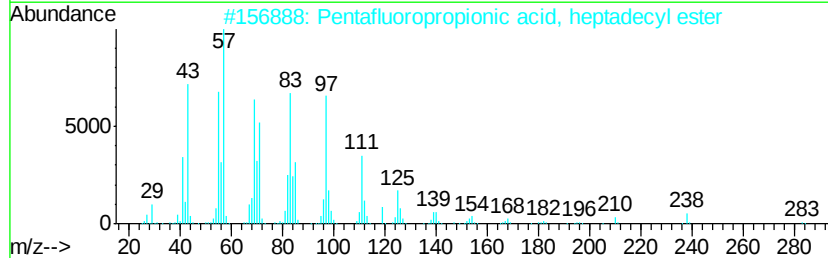
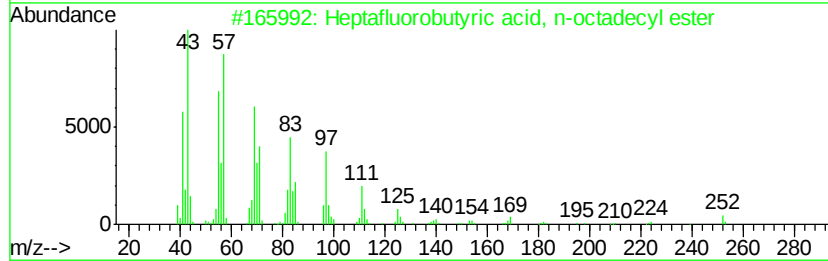
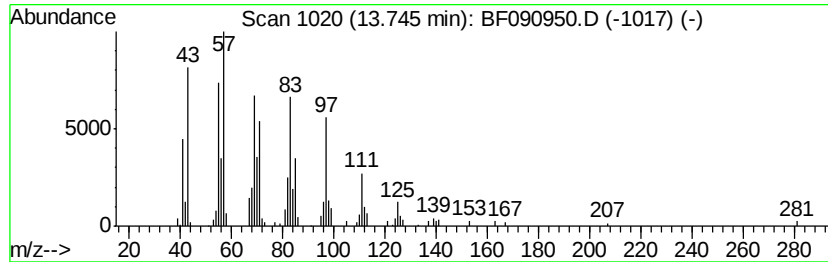
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Peak Number 4 Heptafluorobutyric acid, n-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.		
13.75	3.11 ng	207755	Chrysene-d12		13.89		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	91
2			Pentafluoropropionic acid, heptadecyl ester	402	C20H35F5O2	1000283-04-2	91
3			Heptafluorobutanoic acid, heptadecyl ester	452	C21H35F7O2	1000282-97-3	91
4			Trifluoroacetic acid, n-octadecyl ester	366	C20H37F3O2	079392-43-1	91
5			1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.89	19.9	ng	890244	1	6.74	896716	20.0
unknown6.50	6.50	72.7	ng	3261370	1	6.74	896716	20.0
Heptafluorobutyri...	13.75	3.1	ng	207755	5	13.89	1337840	20.0