

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122817\
 Data File : BF101810.D
 Acq On : 28 Dec 2017 18:46
 Operator : SJ/JU
 Sample : I6970-11
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S5-5-10

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-BF121417.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	5.004	492	496	520	rBV	263716	499850	16.20%	1.964%
2	5.410	561	565	593	rBV	2084429	3084820	100.00%	12.122%
3	6.428	735	738	756	rBV	2208922	3062321	99.27%	12.033%
4	6.557	756	760	774	rVB	2829990	2907484	94.25%	11.425%
5	6.781	795	798	808	rBV	841074	829693	26.90%	3.260%
6	6.933	821	824	847	rVB	2115114	2280486	73.93%	8.961%
7	7.351	892	895	918	rBV	1481060	1890412	61.28%	7.428%
8	8.063	1013	1016	1032	rBV	961296	1061453	34.41%	4.171%
9	9.139	1195	1199	1208	rBV	2874079	2808940	91.06%	11.038%
10	9.539	1264	1267	1272	rVB	83058	81555	2.64%	0.320%
11	9.733	1297	1300	1304	rVB	68560	54179	1.76%	0.213%
12	9.816	1311	1314	1322	rBV	967288	962938	31.22%	3.784%
13	10.233	1382	1385	1388	rVB	72413	61892	2.01%	0.243%
14	10.616	1446	1450	1462	rBV	1222640	1310195	42.47%	5.148%
15	10.704	1462	1465	1470	rVB	73413	69887	2.27%	0.275%
16	11.310	1565	1568	1578	rBV	799067	820117	26.59%	3.223%
17	12.892	1833	1837	1840	rBV	2069010	1894304	61.41%	7.444%
18	13.774	1983	1987	1993	rBV2	64979	102714	3.33%	0.404%
19	13.962	2015	2019	2028	rBV	804973	826110	26.78%	3.246%
20	15.015	2195	2198	2205	rVB4	31486	46183	1.50%	0.181%
21	15.380	2257	2260	2264	rVB2	32734	36442	1.18%	0.143%
22	15.433	2264	2269	2279	rBV	559741	756899	24.54%	2.974%

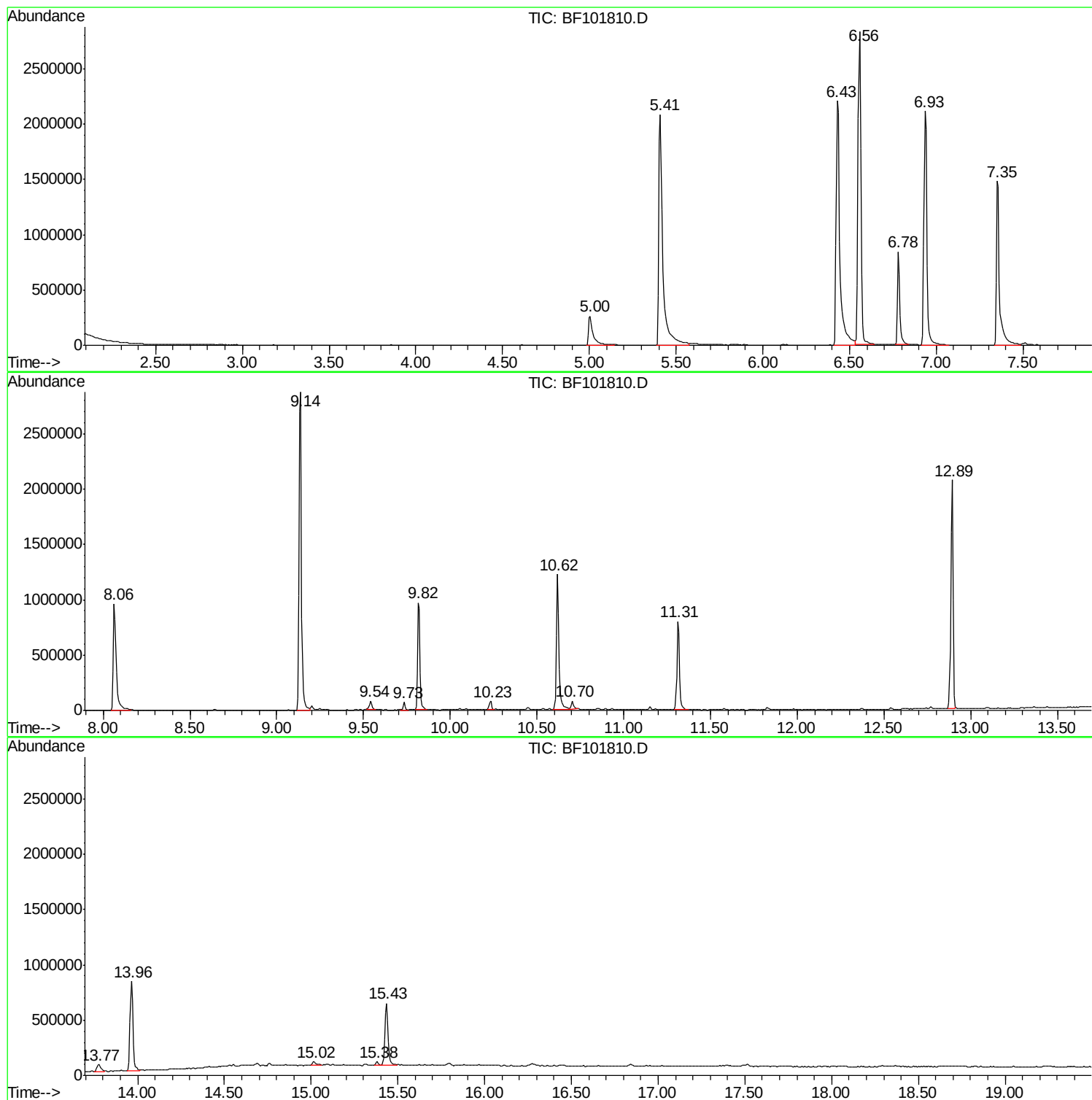
Sum of corrected areas: 25448874

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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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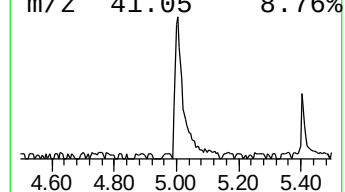
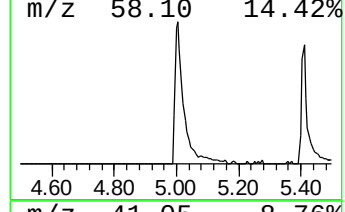
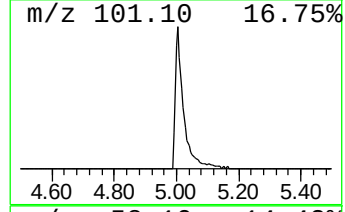
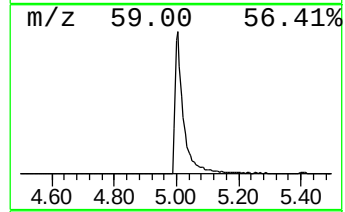
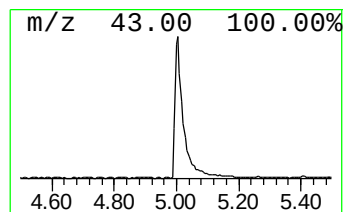
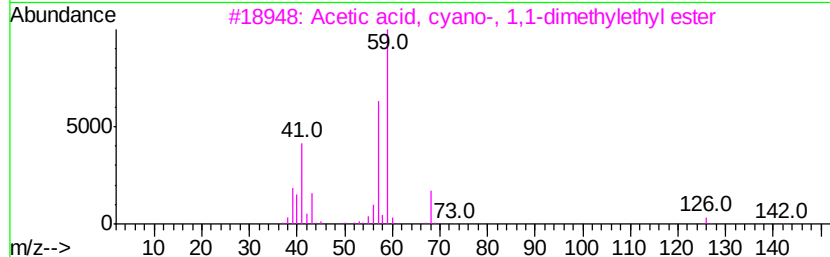
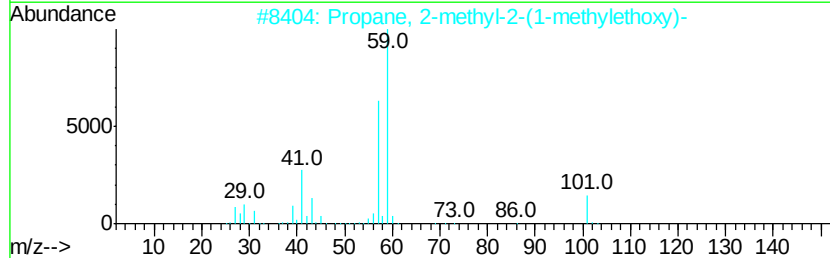
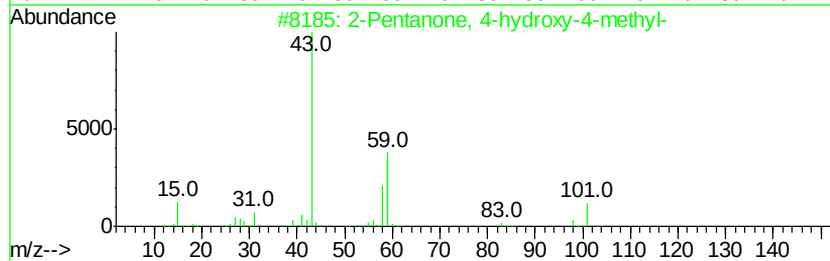
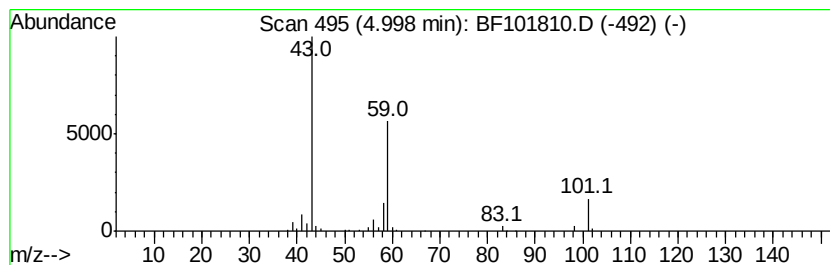
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	12.05 ng	499850	1,4-Dichlorobenzene-d4	6.78

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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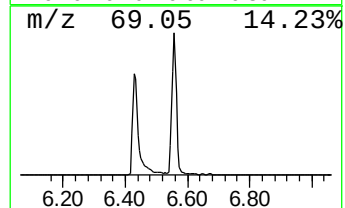
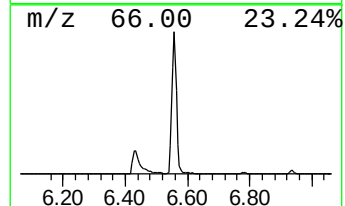
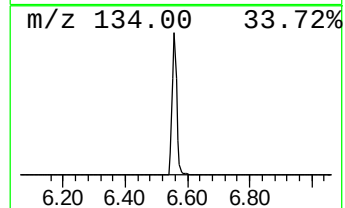
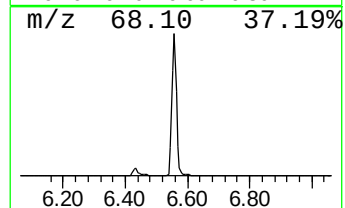
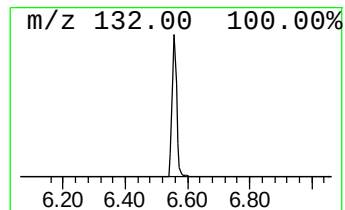
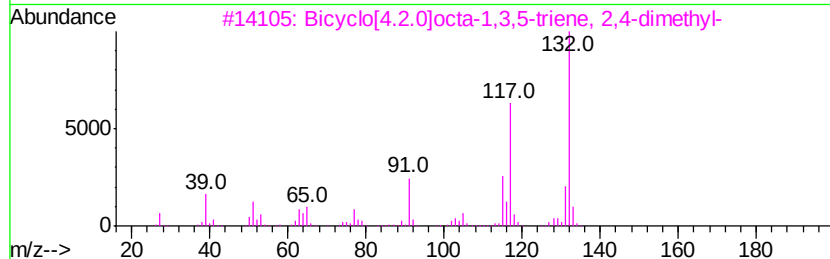
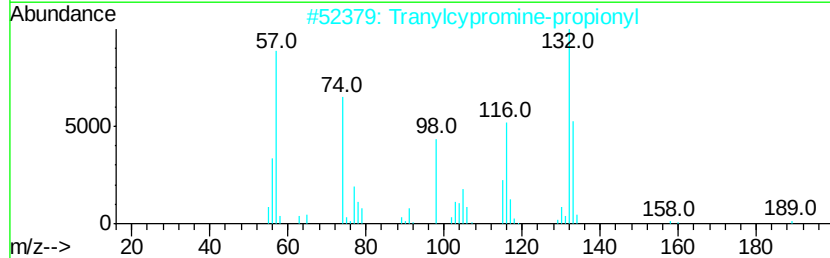
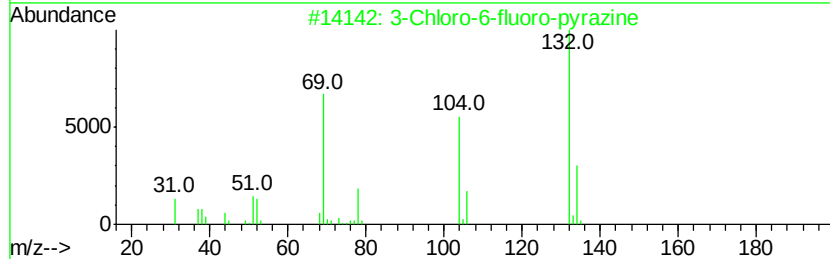
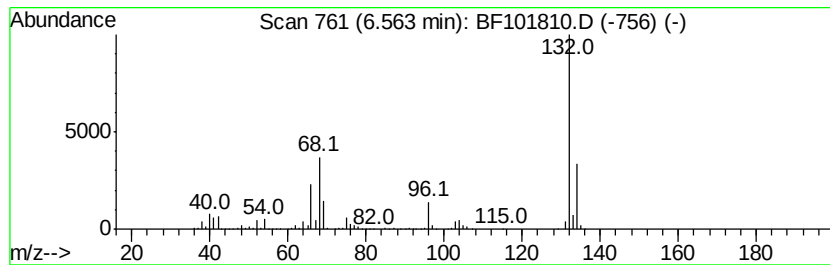
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Peak Number 2 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	70.09 ng	2907480	1,4-Dichlorobenzene-d4	6.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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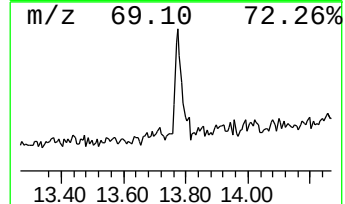
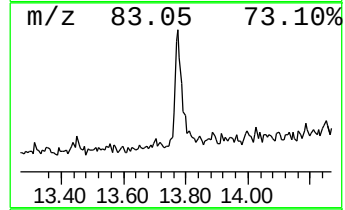
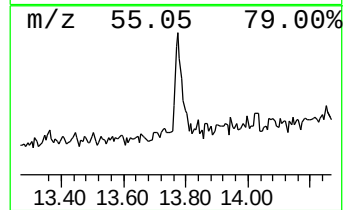
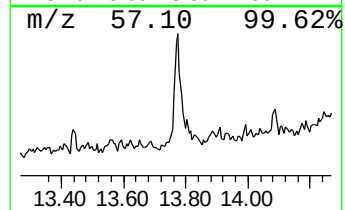
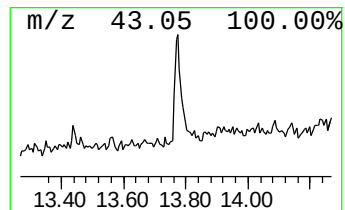
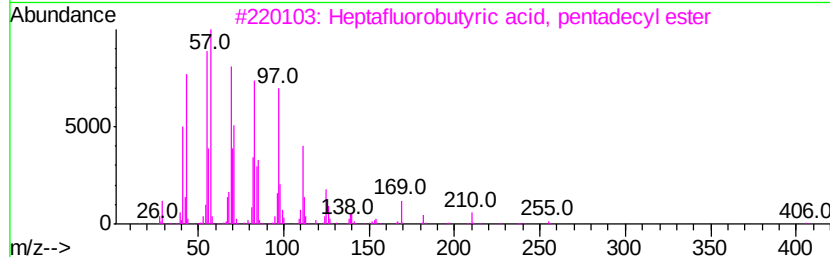
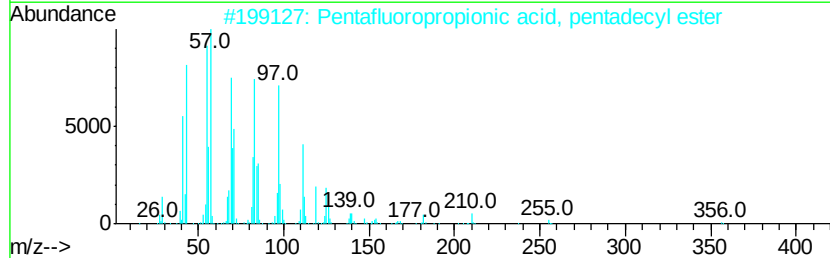
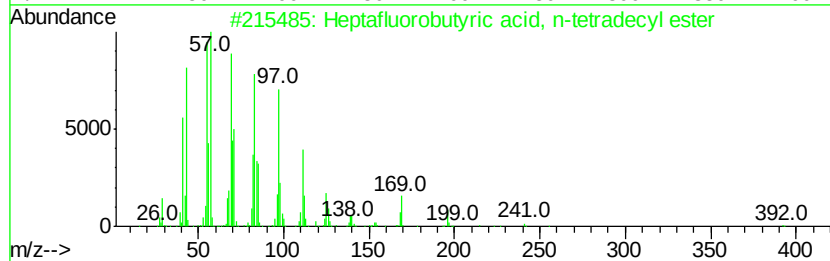
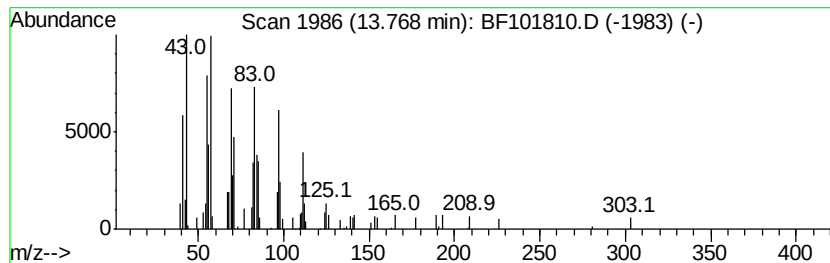
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Peak Number 4 Heptafluorobutyric acid, n-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	2.49 ng	102714	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	95
2		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
3		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	95
4		Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	94
5		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.00	12.1	ng	499850	1	6.78	829693	20.0
unknown6.56	6.56	70.1	ng	2907480	1	6.78	829693	20.0
Heptafluorobutyri...	13.77	2.5	ng	102714	5	13.96	826110	20.0