

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081717\
 Data File : BF097806.D
 Acq On : 18 Aug 2017 00:41
 Operator : SJ/JU
 Sample : I4761-01
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RUSB-01

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-BF081517.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	4.963	485	489	497	rBV	578237	575538	45.54%	4.390%
2	5.375	555	559	563	rBV	1049177	943367	74.65%	7.196%
3	6.398	729	733	743	rBV	1498425	1263783	100.00%	9.640%
4	6.539	753	757	760	rBV	1326833	1089054	86.17%	8.307%
5	6.775	793	797	800	rBV	1077675	810574	64.14%	6.183%
6	6.928	820	823	827	rBV	1131636	985462	77.98%	7.517%
7	7.334	888	892	895	rBV	903164	742216	58.73%	5.662%
8	8.057	1011	1015	1019	rBV	1180514	979425	77.50%	7.471%
9	9.133	1194	1198	1201	rBV	1540841	1245709	98.57%	9.502%
10	9.527	1261	1265	1270	rBV	140034	103261	8.17%	0.788%
11	9.722	1290	1298	1300	rBV5	7680	15135	1.20%	0.115%
12	9.751	1300	1303	1305	rVB	19428	14987	1.19%	0.114%
13	9.810	1309	1313	1317	rBV	976851	855057	67.66%	6.522%
14	10.251	1385	1388	1391	rVB	27051	20968	1.66%	0.160%
15	10.592	1443	1446	1451	rBV	304133	244772	19.37%	1.867%
16	10.722	1465	1468	1475	rBV	28162	28939	2.29%	0.221%
17	11.292	1561	1565	1569	rBV	892487	759130	60.07%	5.791%
18	12.710	1803	1806	1811	rBV	32866	24088	1.91%	0.184%
19	12.880	1831	1835	1838	rBV	1137739	951829	75.32%	7.260%
20	13.415	1923	1926	1929	rBV	24410	19279	1.53%	0.147%
21	13.780	1985	1988	1994	rBV	69930	81535	6.45%	0.622%
22	13.927	2009	2013	2016	rBV	904215	763011	60.38%	5.820%
23	14.415	2093	2096	2099	rBV4	21575	22637	1.79%	0.173%
24	15.357	2251	2256	2262	rBV	468885	570042	45.11%	4.348%

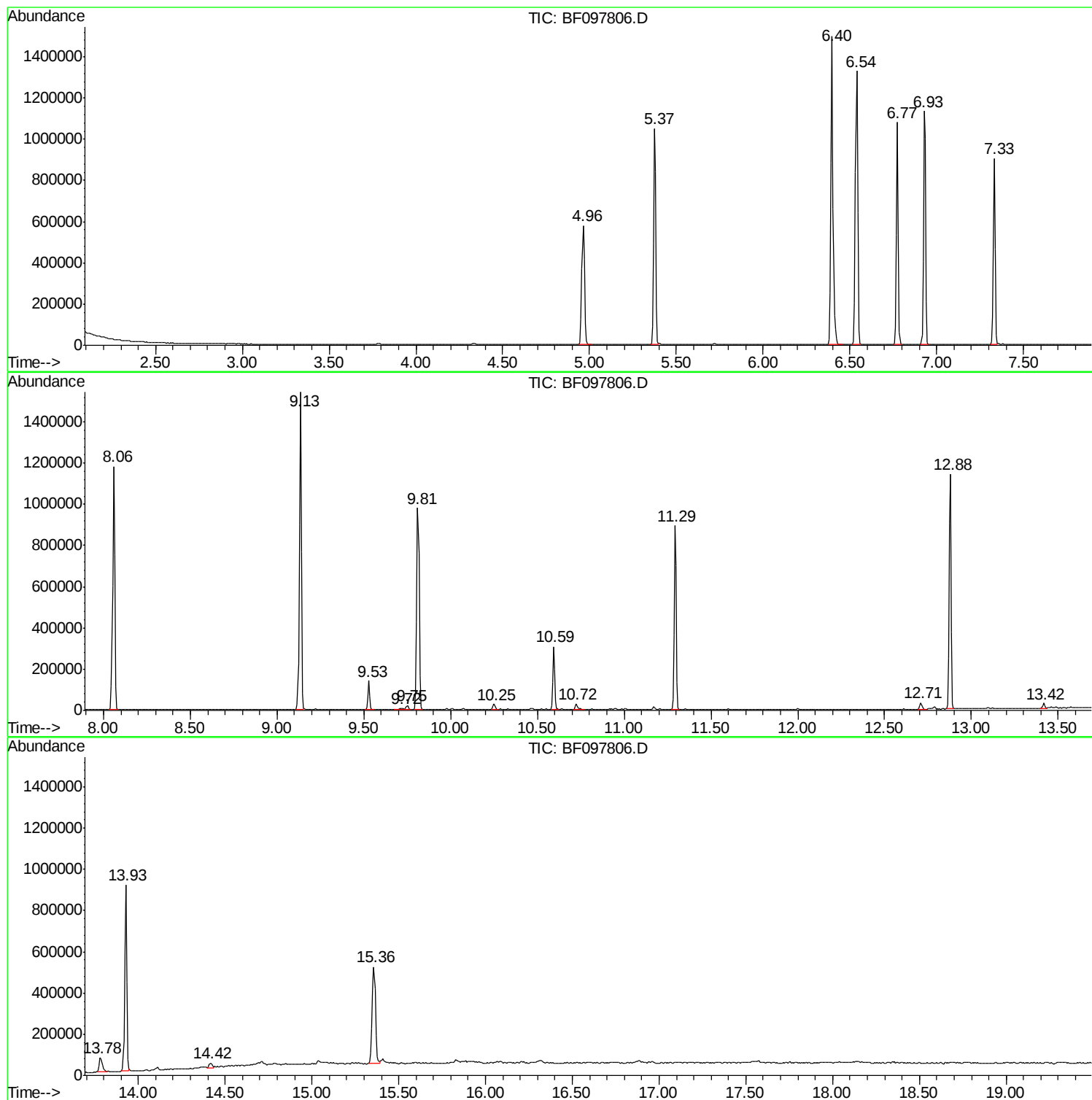
Sum of corrected areas: 13109798

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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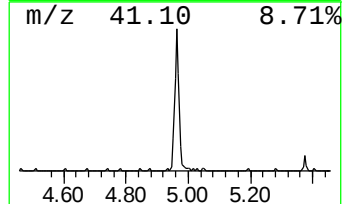
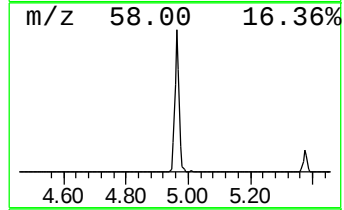
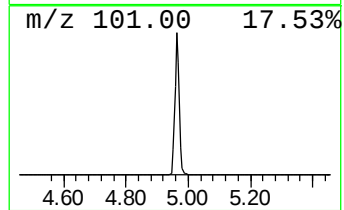
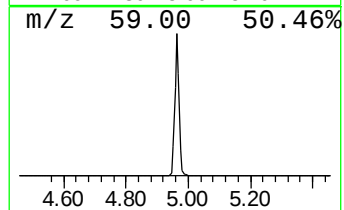
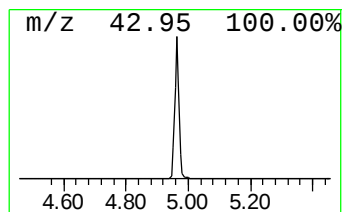
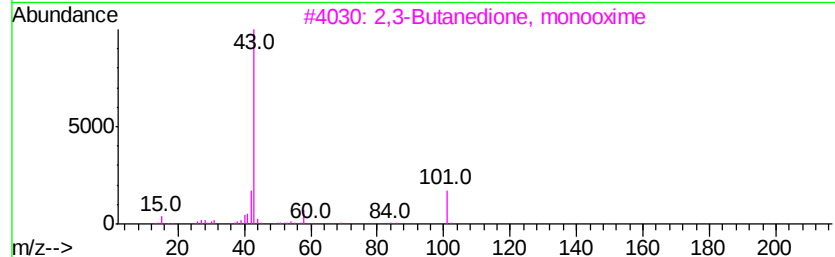
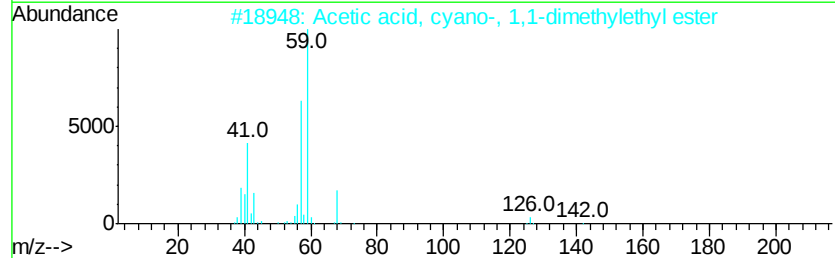
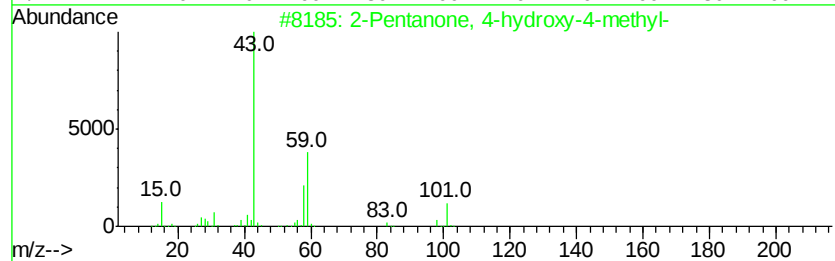
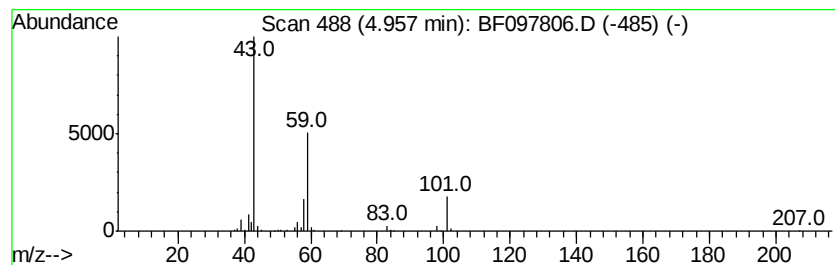
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.96	14.20 ng	575538	1,4-Dichlorobenzene-d4	6.77

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59	
2	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25	
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16	
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10	
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9	



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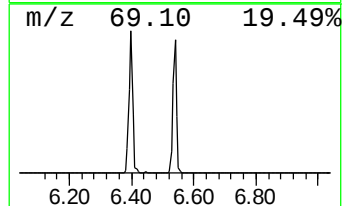
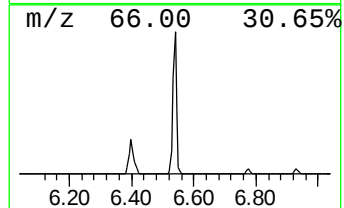
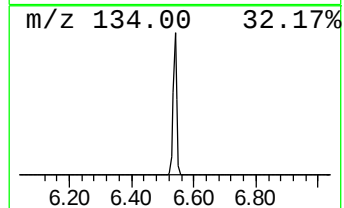
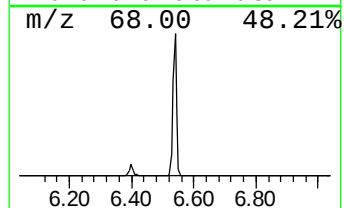
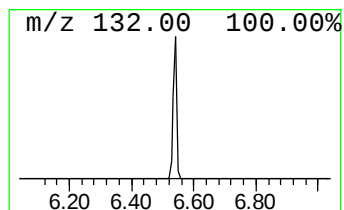
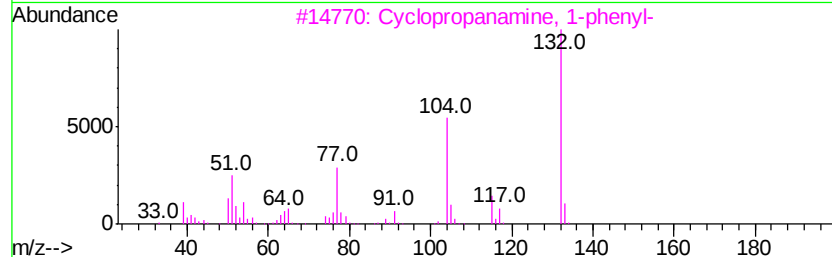
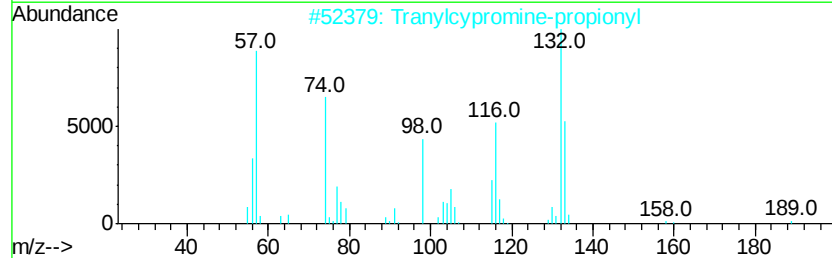
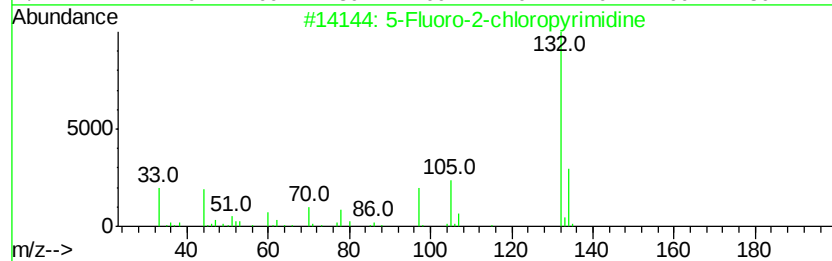
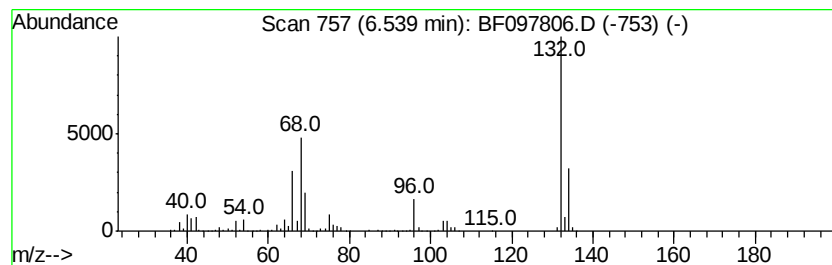
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Peak Number 2 unknown6.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	26.87 ng	1089050	1,4-Dichlorobenzene-d4	6.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
4		5-Aminoindole	132	C8H8N2	005192-03-0	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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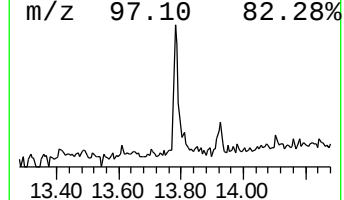
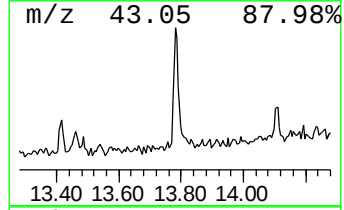
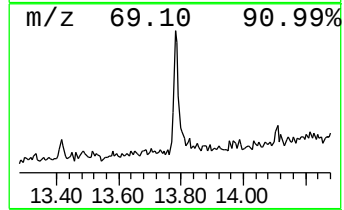
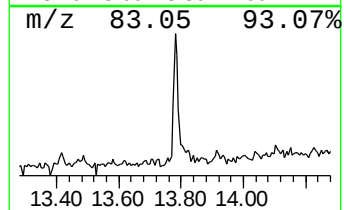
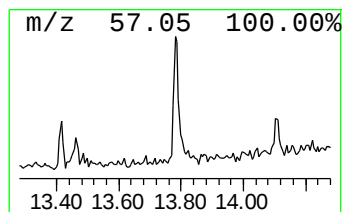
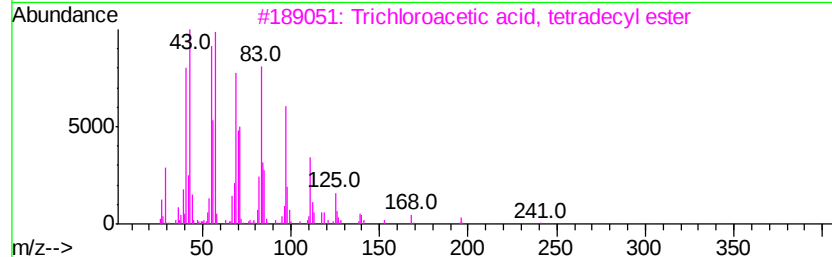
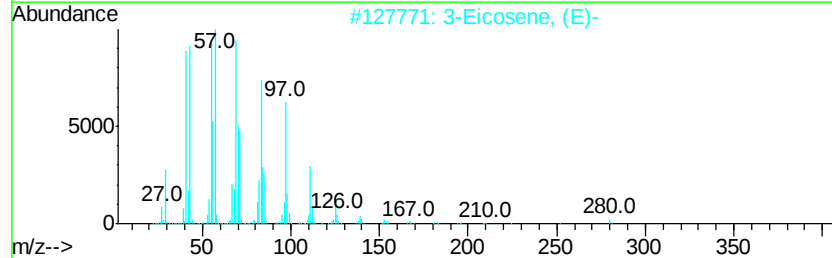
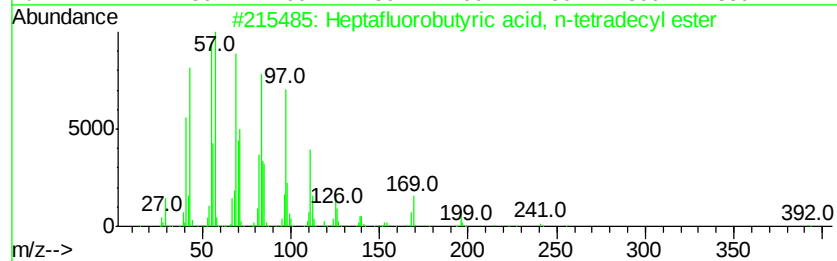
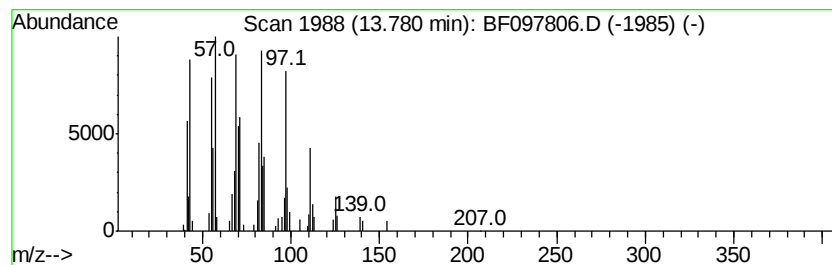
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Peak Number 4 Heptafluorobutyric acid, n-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.78	2.14 ng	81535	Chrysene-d12	13.93	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	95
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
5	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	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...	4.96	14.2	ng	575538	1	6.77	810574	20.0
unknown6.54	6.54	26.9	ng	1089050	1	6.77	810574	20.0
Heptafluorobutyri...	13.78	2.1	ng	81535	5	13.93	763011	20.0