

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081717\
 Data File : BF097804.D
 Acq On : 17 Aug 2017 23:44
 Operator : SJ/JU
 Sample : I4754-03
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 30-FINES-COMP

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-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	2.363	42	47	53	rVB2	38564	67601	1.96%	0.256%
2	4.981	487	492	500	rBV	295694	380347	11.05%	1.442%
3	5.387	556	561	565	rBV	3017427	3263516	94.77%	12.369%
4	6.410	729	735	748	rBV	3287705	3443532	100.00%	13.051%
5	6.545	753	758	761	rBV	3294971	3165105	91.91%	11.996%
6	6.775	794	797	801	rVB	1072073	866994	25.18%	3.286%
7	6.934	820	824	827	rBV	2717849	2383599	69.22%	9.034%
8	7.339	888	893	896	rBV	2176927	1966979	57.12%	7.455%
9	8.057	1011	1015	1019	rBV	1241805	1021720	29.67%	3.872%
10	9.133	1194	1198	1202	rBV	2828684	2712327	78.77%	10.280%
11	9.527	1261	1265	1269	rBV	383565	291455	8.46%	1.105%
12	9.810	1309	1313	1317	rVB	971490	858117	24.92%	3.252%
13	10.251	1385	1388	1391	rVB	63042	46757	1.36%	0.177%
14	10.598	1442	1447	1450	rBV	1480582	1251754	36.35%	4.744%
15	10.721	1465	1468	1476	rBV	59798	61814	1.80%	0.234%
16	11.292	1561	1565	1569	rBV	862331	736614	21.39%	2.792%
17	12.880	1831	1835	1839	rBV	2213093	2050793	59.55%	7.773%
18	13.780	1985	1988	1996	rBV	232628	249745	7.25%	0.947%
19	13.927	2009	2013	2017	rBV	944709	826893	24.01%	3.134%
20	15.039	2200	2202	2209	rVB4	34716	48262	1.40%	0.183%
21	15.356	2251	2256	2261	rBV	516002	597521	17.35%	2.265%
22	15.409	2262	2265	2270	rVB	32587	43538	1.26%	0.165%
23	15.827	2333	2336	2342	rBV	35104	49397	1.43%	0.187%

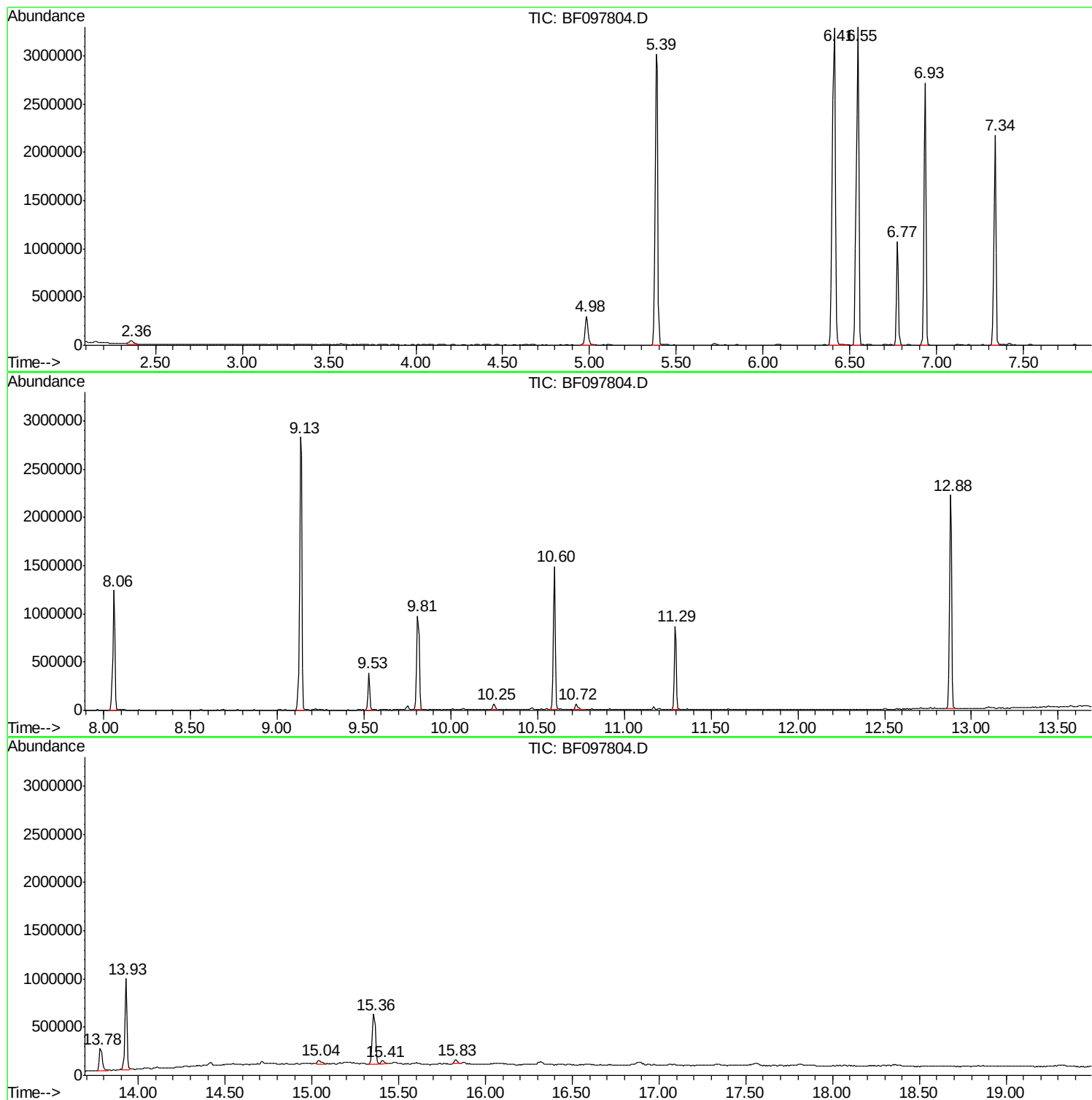
Sum of corrected areas: 26384380

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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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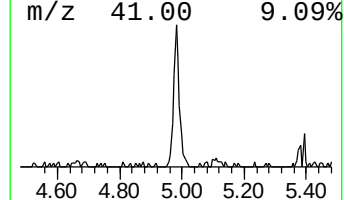
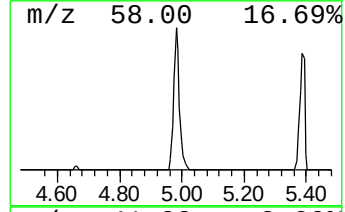
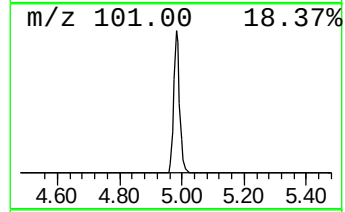
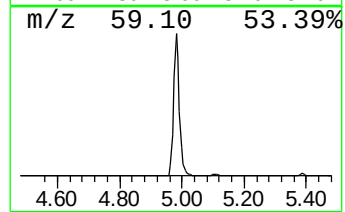
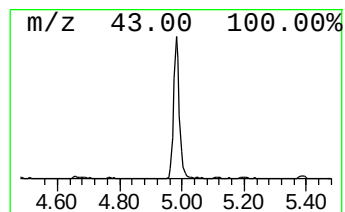
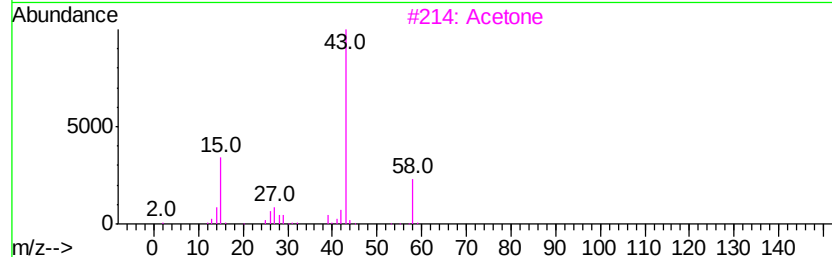
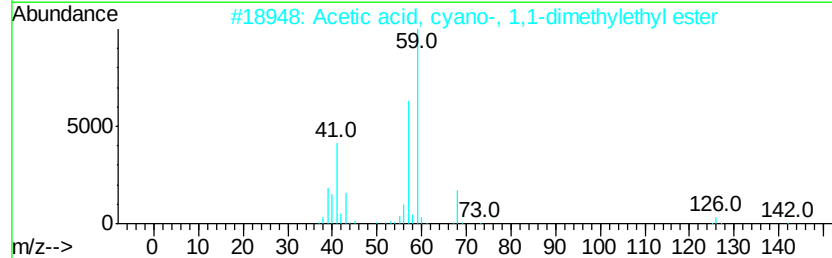
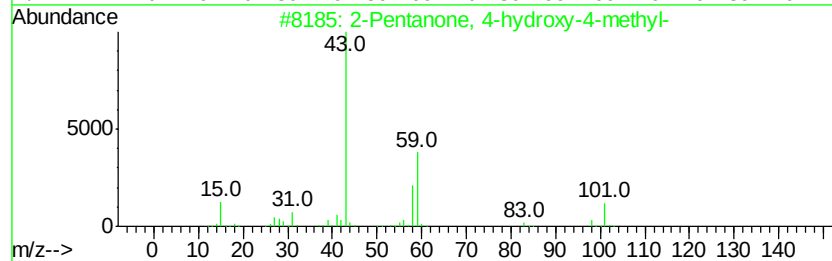
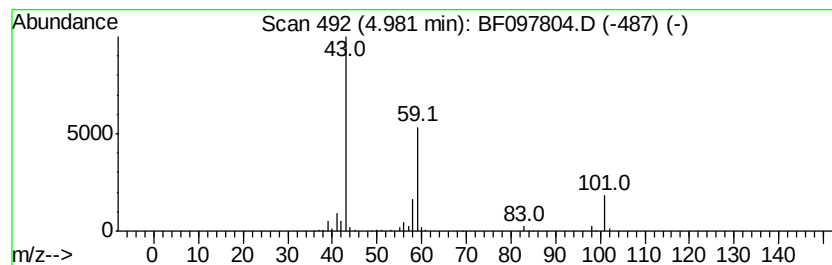
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.98	8.77 ng	380347	1,4-Dichlorobenzene-d4	6.77

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, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		Acetone	58	C3H6O	000067-64-1	12
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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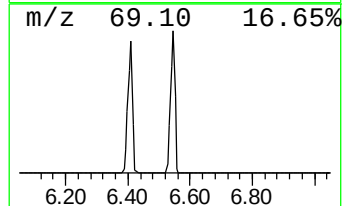
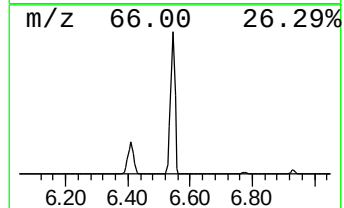
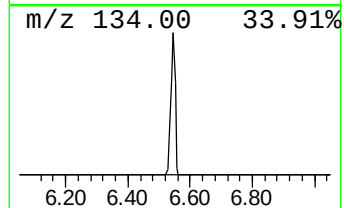
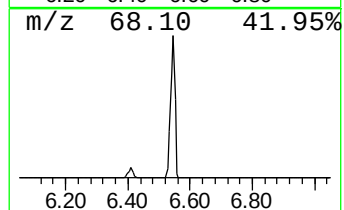
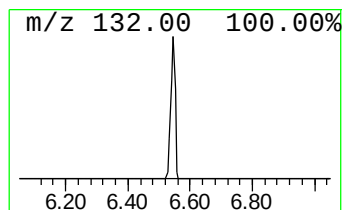
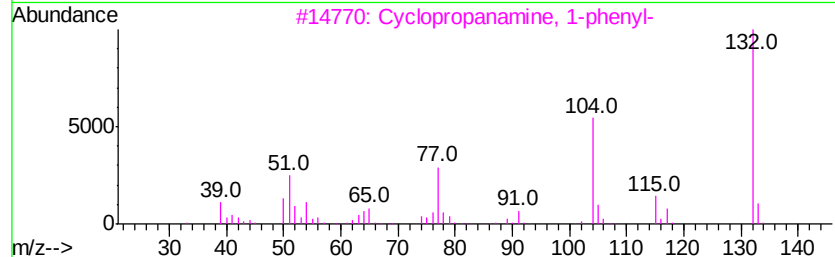
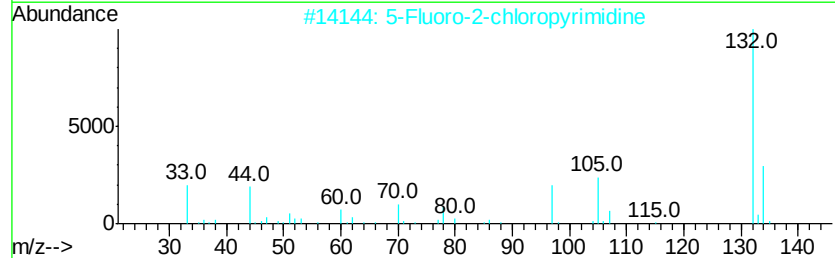
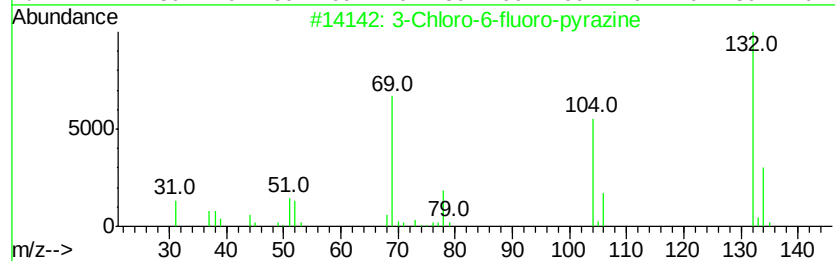
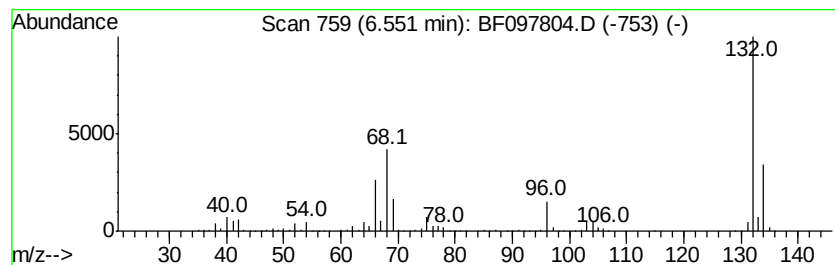
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Peak Number 2 unknown6.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	73.01 ng	3165110	1,4-Dichlorobenzene-d4	6.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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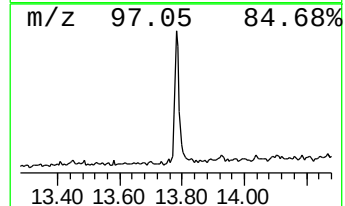
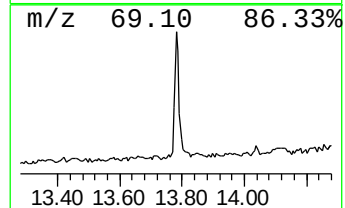
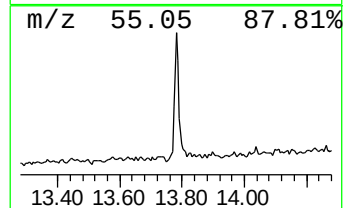
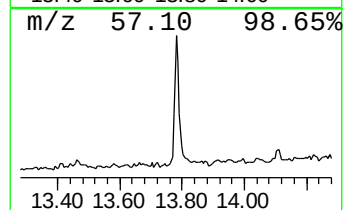
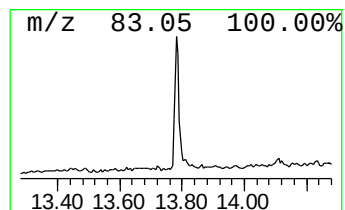
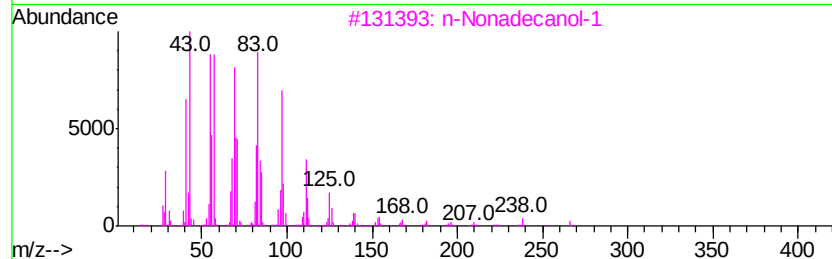
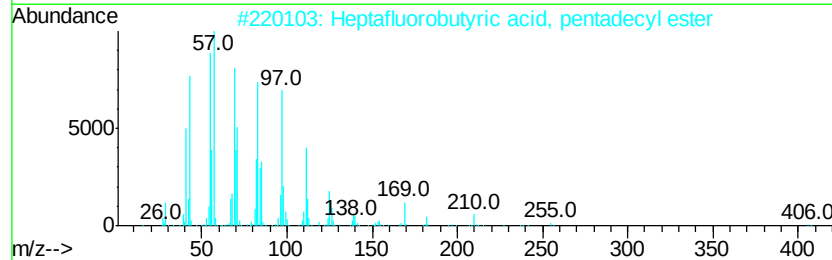
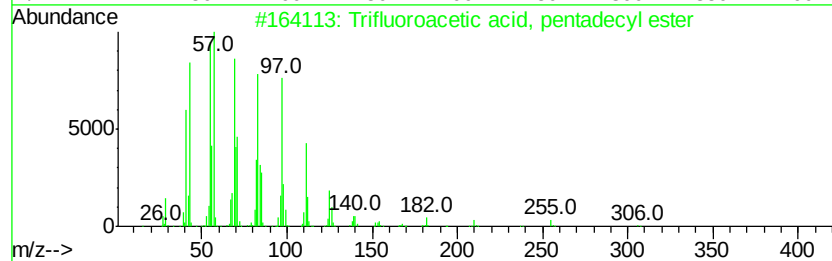
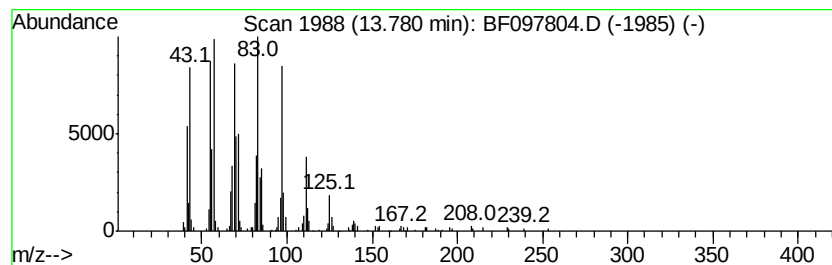
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Peak Number 4 Trifluoroacetic acid, penta... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.78	6.04 ng	249745	Chrysene-d12	13.93	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
4	1-Heptacosanol	396	C27H56O	002004-39-9	93
5	Behenic alcohol	326	C22H46O	000661-19-8	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.98	8.8	ng	380347	1	6.77	866994	20.0
unknown6.55	6.55	73.0	ng	3165110	1	6.77	866994	20.0
Trifluoroacetic a...	13.78	6.0	ng	249745	5	13.93	826893	20.0