

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071817\
 Data File : BF096849.D
 Acq On : 18 Jul 2017 15:49
 Operator : SJ/JU
 Sample : I4223-10
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC071417-1SE

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-BF071317.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	4.781	471	475	488	rVB	252214	405160	12.25%	1.484%
2	5.216	543	549	552	rBV	2735145	3060234	92.51%	11.208%
3	6.251	719	725	728	rBV	2678216	3308067	100.00%	12.116%
4	6.369	740	745	749	rBV	2921510	3135914	94.80%	11.485%
5	6.598	780	784	787	rBV	712763	622253	18.81%	2.279%
6	6.757	806	811	814	rBV	2260426	2278056	68.86%	8.343%
7	7.163	874	880	883	rBV	2097570	2183664	66.01%	7.998%
8	7.881	997	1002	1005	rBV	873254	836199	25.28%	3.063%
9	8.957	1179	1185	1188	rBV	2949288	3240730	97.96%	11.869%
10	9.351	1248	1252	1255	rBV	598733	463284	14.00%	1.697%
11	9.628	1294	1299	1302	rBV	959236	894748	27.05%	3.277%
12	10.416	1427	1433	1436	rBV	1810925	1850654	55.94%	6.778%
13	10.545	1452	1455	1464	rBV	51333	59375	1.79%	0.217%
14	10.992	1527	1531	1534	rBV	43745	37748	1.14%	0.138%
15	11.098	1545	1549	1553	rVB	907902	855744	25.87%	3.134%
16	12.686	1814	1819	1823	rBV	2464371	2787037	84.25%	10.207%
17	13.592	1969	1973	1981	rBV	120708	149666	4.52%	0.548%
18	13.721	1991	1995	1999	rBV	687303	644611	19.49%	2.361%
19	15.092	2223	2228	2234	rBV	431433	491032	14.84%	1.798%

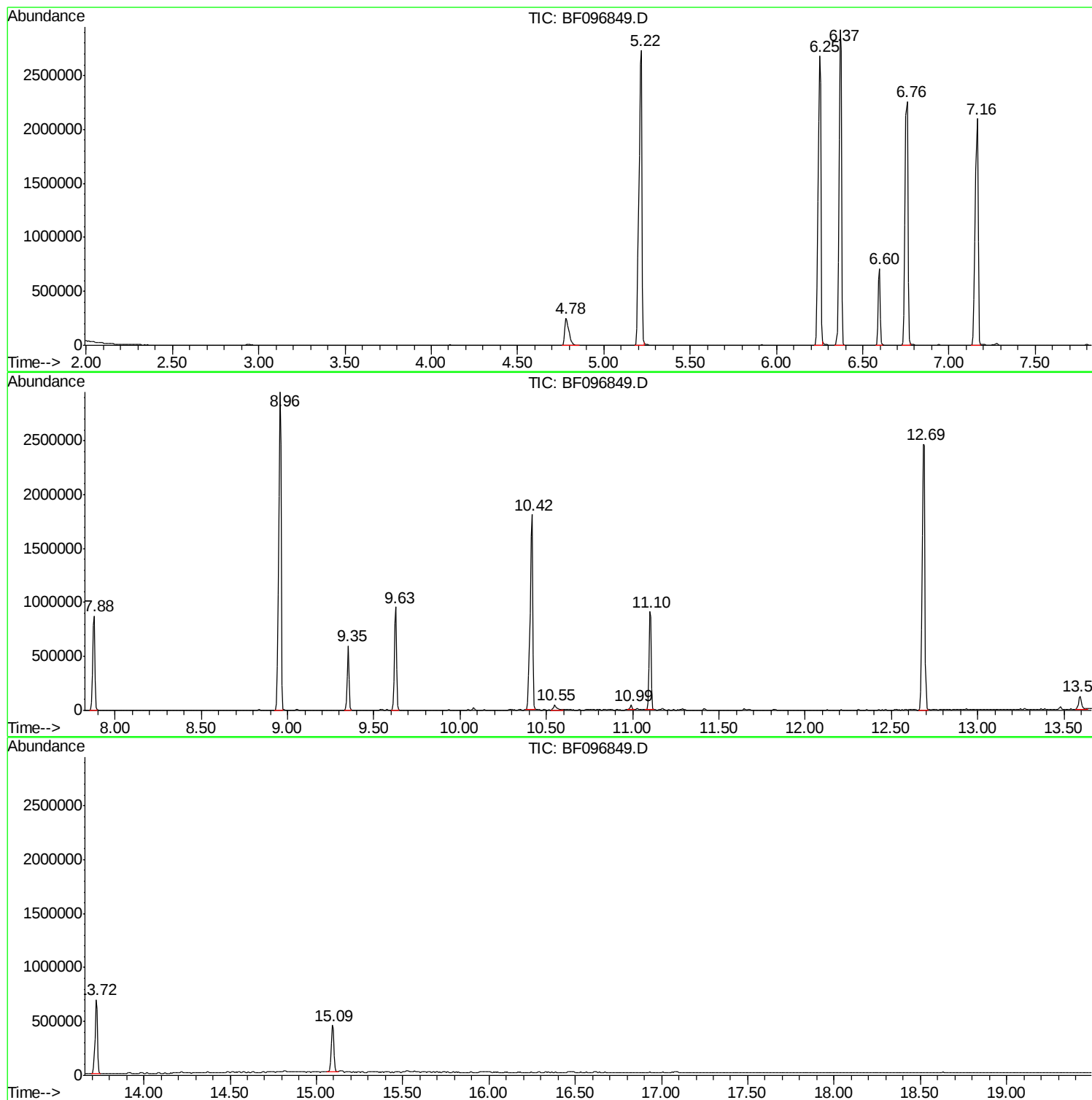
Sum of corrected areas: 27304176

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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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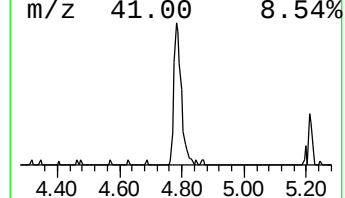
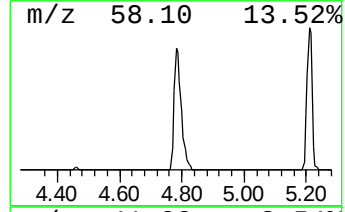
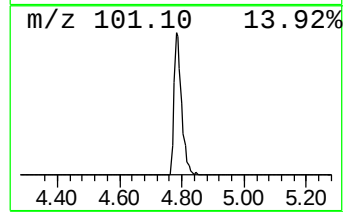
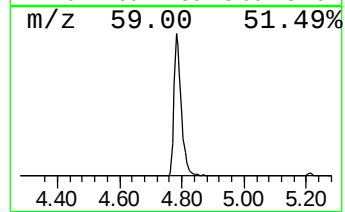
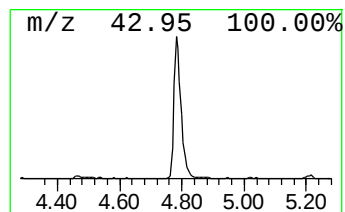
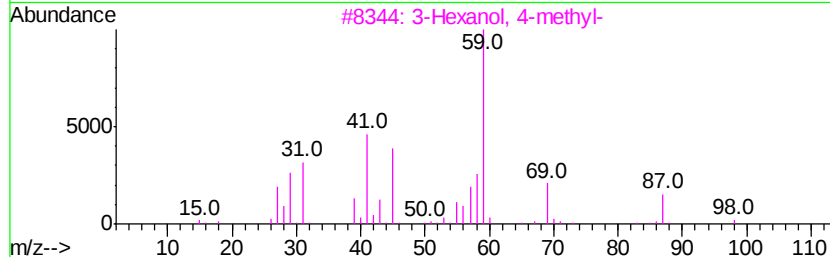
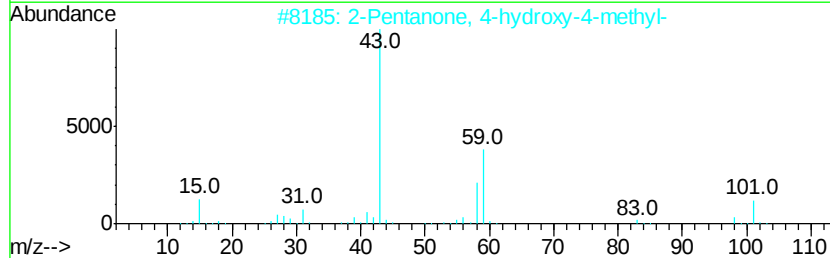
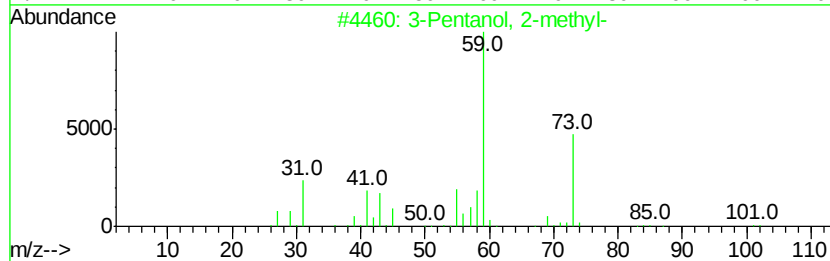
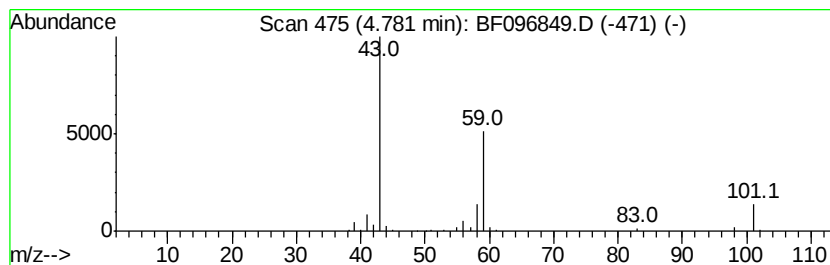
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Pentanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.78	13.02 ng	405160	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	50
2		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		3-Hexanol	102	C6H14O	000623-37-0	33
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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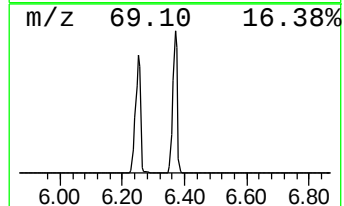
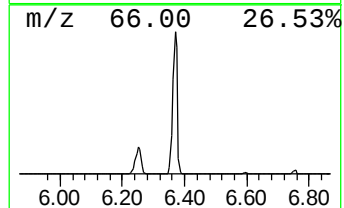
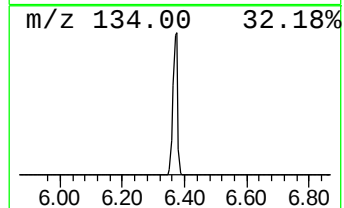
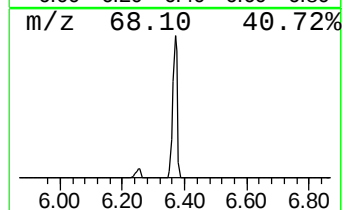
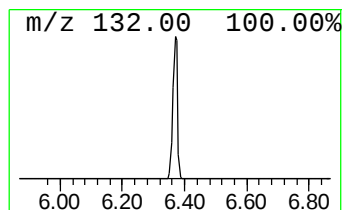
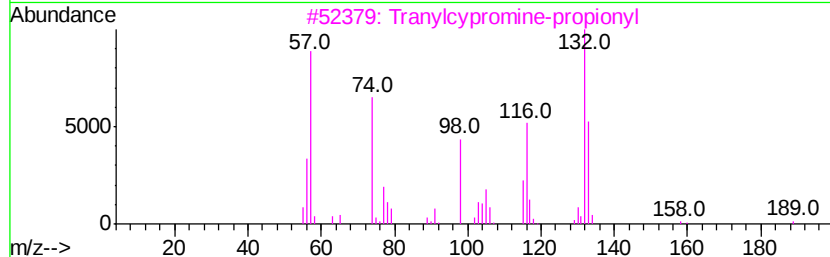
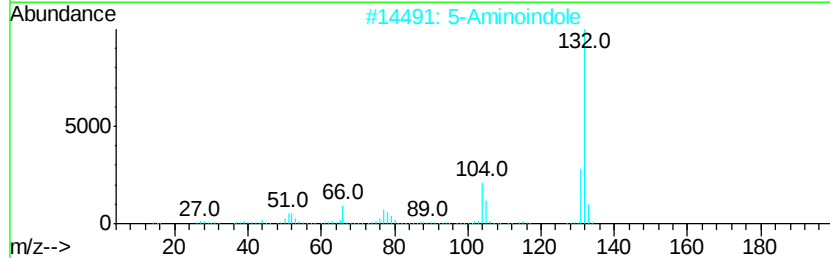
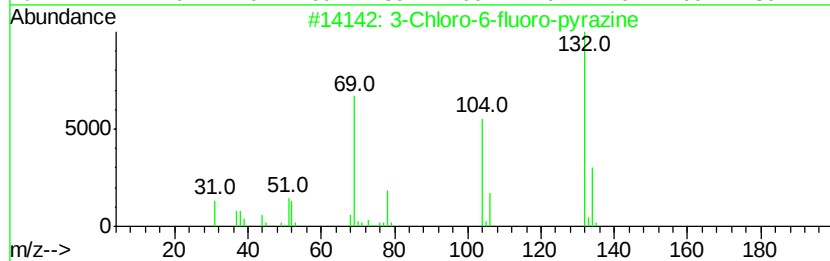
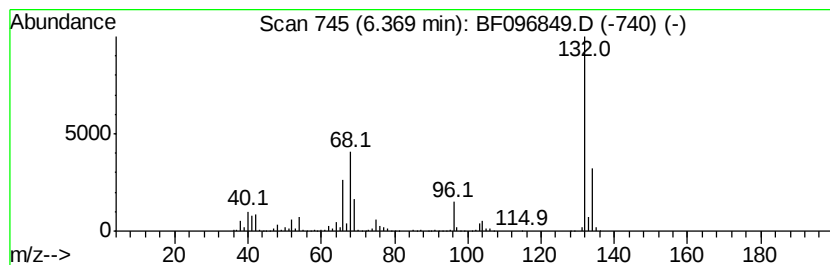
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Peak Number 2 unknown6.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.37	100.79 ng	3135910	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	5-Aminoindole	132	C8H8N2	005192-03-0	12	
3	Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10	
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9	
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9	



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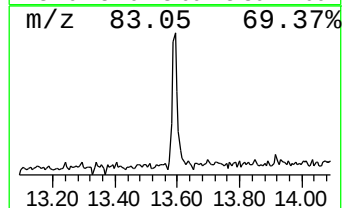
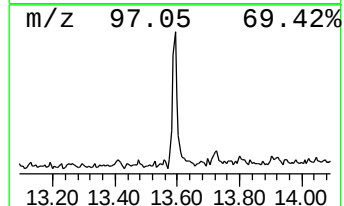
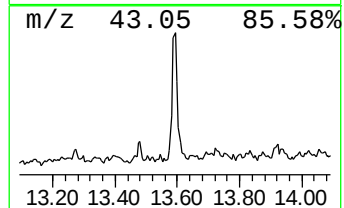
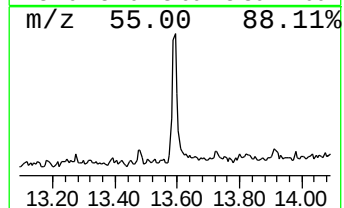
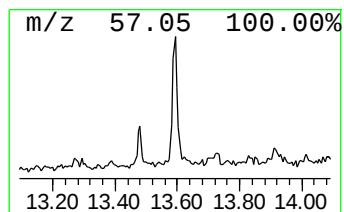
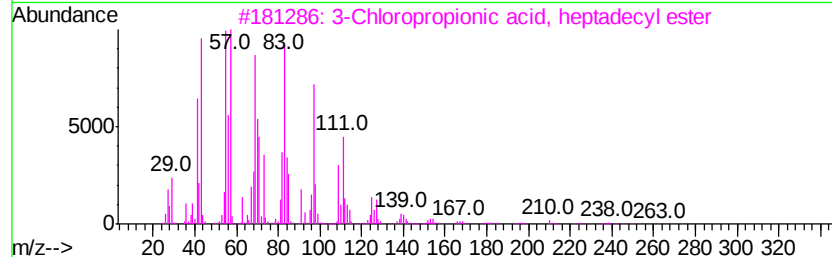
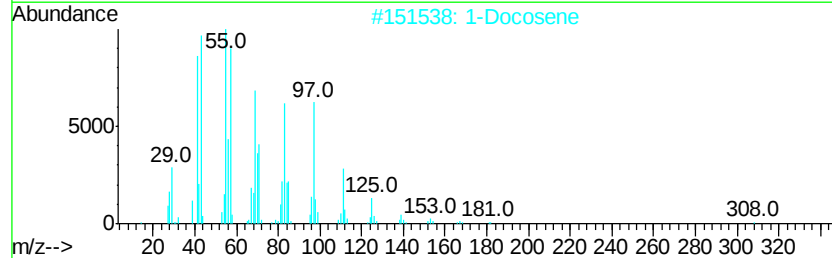
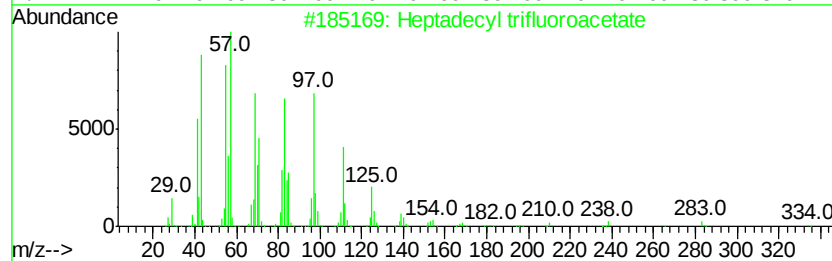
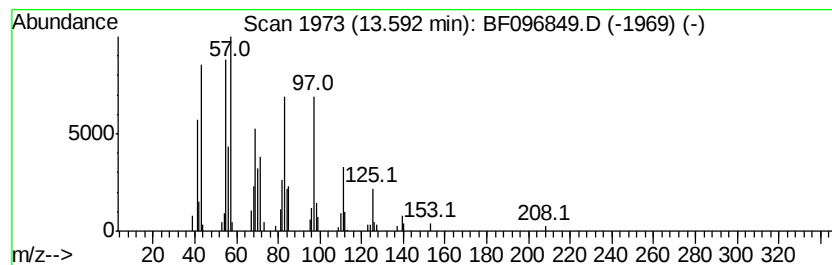
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Peak Number 4 Heptadecyl trifluoroacetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.59	4.64 ng	149666	Chrysene-d12	13.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
2		1-Docosene	308	C22H44	001599-67-3	91
3		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
5		Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Pentanol, 2-met...	4.78	13.0	ng	405160	1	6.60	622253	20.0
unknown6.37	6.37	100.8	ng	3135910	1	6.60	622253	20.0
Heptadecyl triflu...	13.59	4.6	ng	149666	5	13.72	644611	20.0