

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122117\
 Data File : BF101644.D
 Acq On : 22 Dec 2017 9:22
 Operator : SJ/JU
 Sample : I7008-10
 Misc :
 ALS Vial : 46 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 121817-TIFR-E-D-M

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	5.010	494	497	508	rBV	56753	93309	2.78%	0.445%
2	5.422	563	567	595	rBV	661021	1137636	33.87%	5.429%
3	6.445	737	741	758	rBV2	401265	822648	24.49%	3.926%
4	6.569	758	762	777	rVB	1959508	2016786	60.05%	9.625%
5	6.798	797	801	809	rBV	842503	837636	24.94%	3.998%
6	6.951	823	827	846	rBV	2823362	2661853	79.25%	12.704%
7	7.369	894	898	917	rBV	1926982	2188539	65.16%	10.445%
8	8.081	1015	1019	1036	rBV	968217	1034027	30.79%	4.935%
9	9.151	1197	1201	1211	rBV	3547276	3358615	100.00%	16.029%
10	9.786	1306	1309	1311	rBV	58476	62706	1.87%	0.299%
11	9.833	1314	1317	1329	rVB2	963145	919413	27.37%	4.388%
12	10.628	1448	1452	1465	rBV	916864	992086	29.54%	4.735%
13	11.322	1567	1570	1579	rBV	731598	744594	22.17%	3.554%
14	12.710	1802	1806	1810	rVB	61227	51447	1.53%	0.246%
15	12.904	1835	1839	1842	rBV	2556078	2367135	70.48%	11.297%
16	13.410	1923	1925	1928	rVB2	40205	35753	1.06%	0.171%
17	13.792	1986	1990	2002	rBV2	79247	132404	3.94%	0.632%
18	13.974	2017	2021	2030	rBV	840922	872798	25.99%	4.165%
19	15.439	2265	2270	2282	rVB	450147	623705	18.57%	2.977%

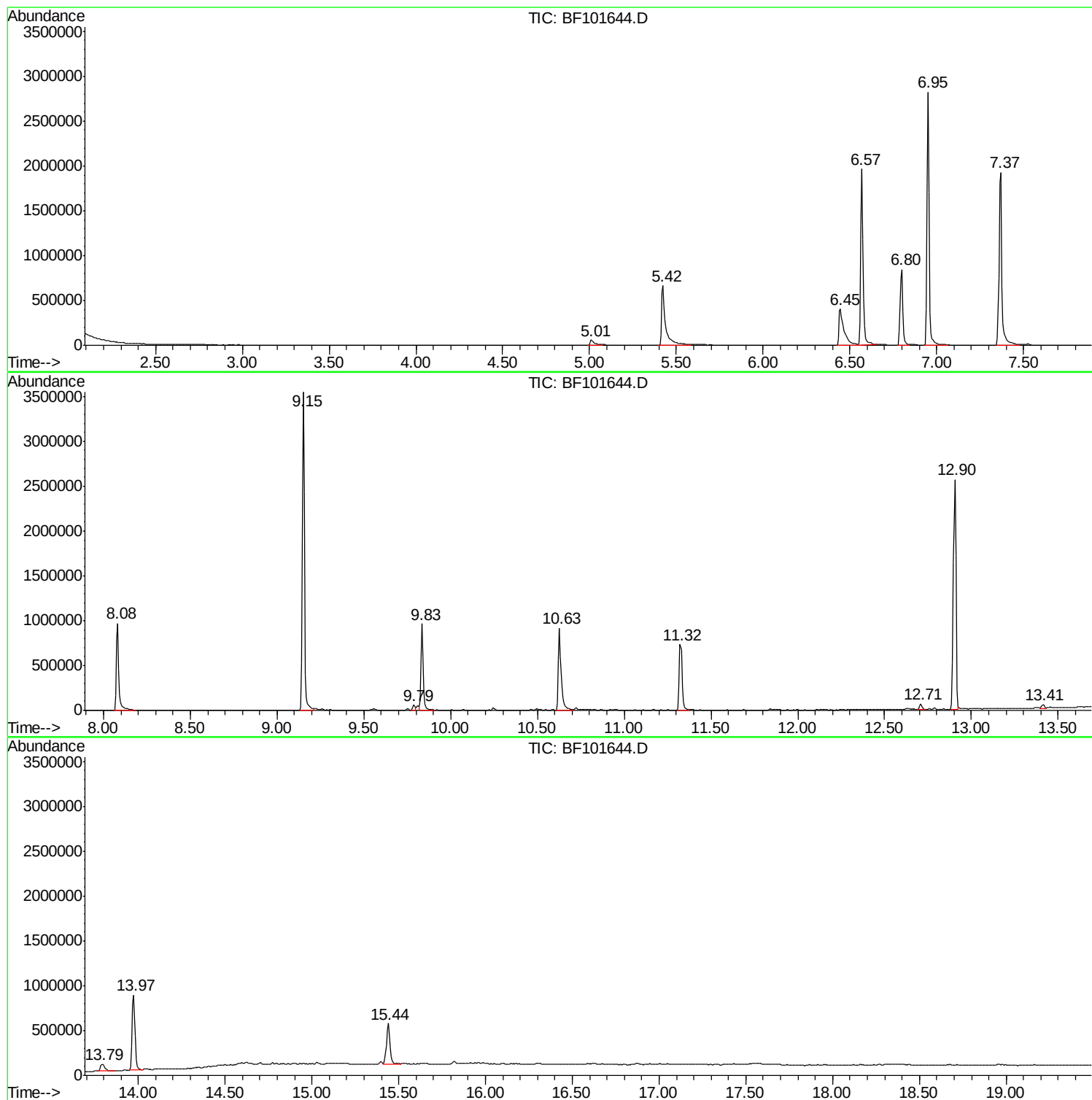
Sum of corrected areas: 20953090

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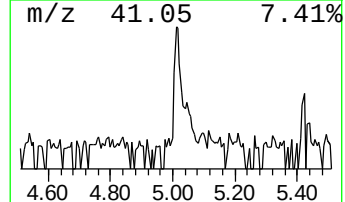
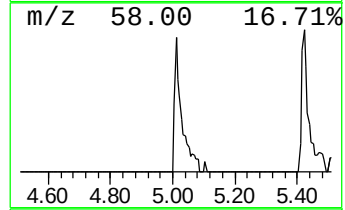
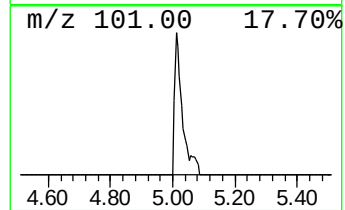
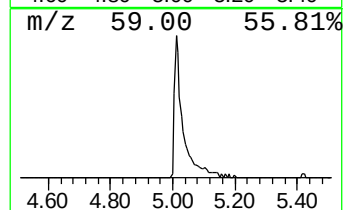
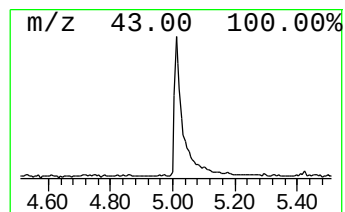
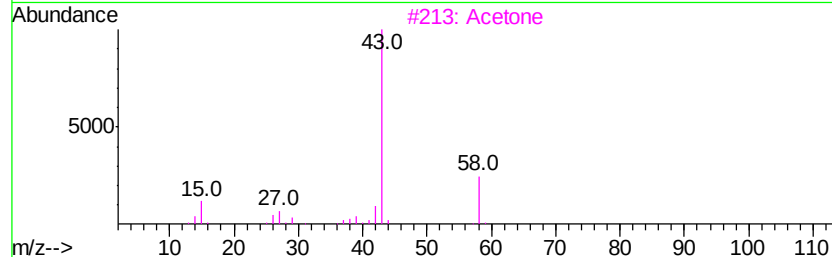
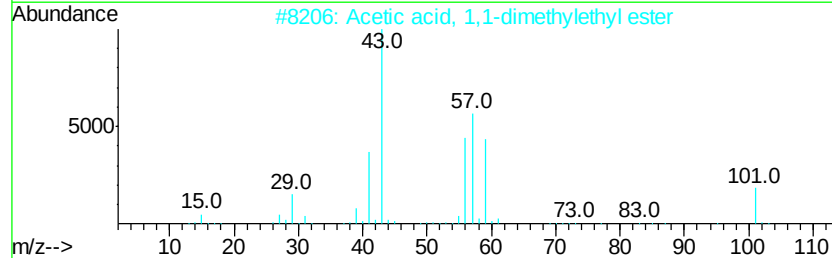
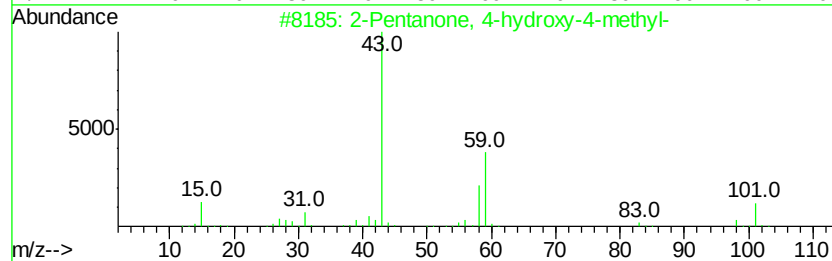
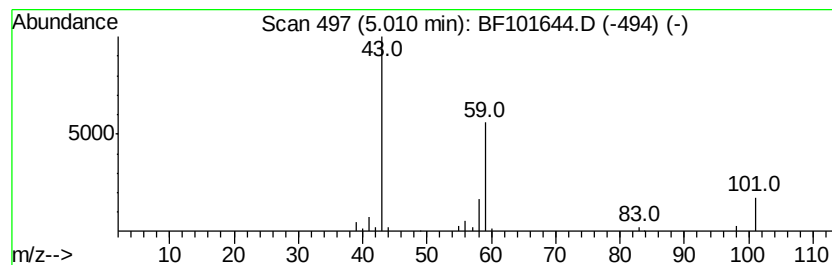
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	2.23 ng	93309	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3		Acetone	58	C3H6O	000067-64-1	9
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9
5		Silane, trimethyl-	74	C3H10Si	000993-07-7	9



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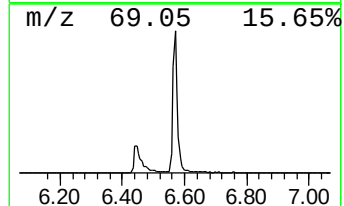
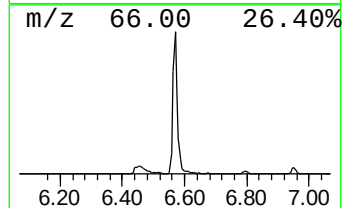
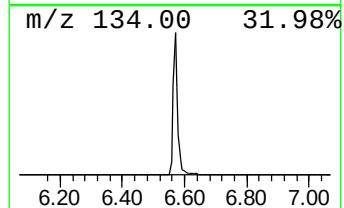
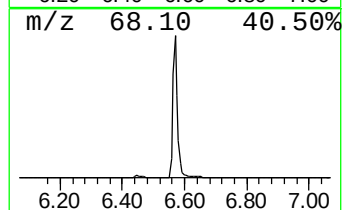
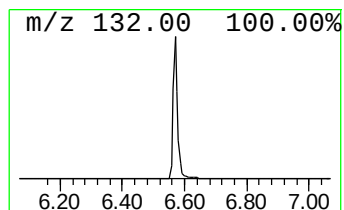
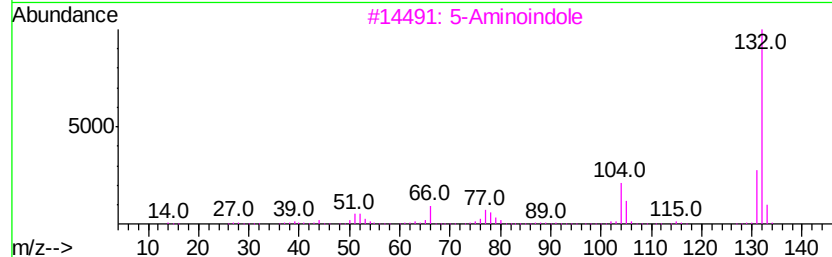
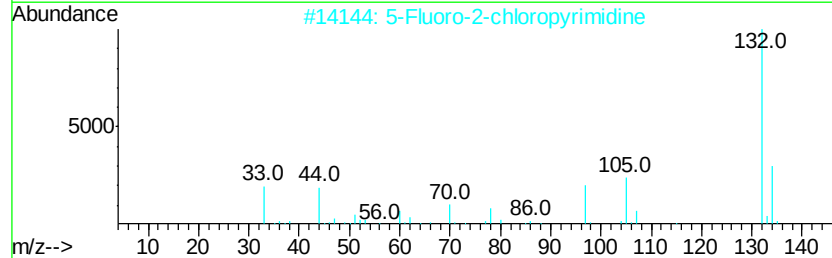
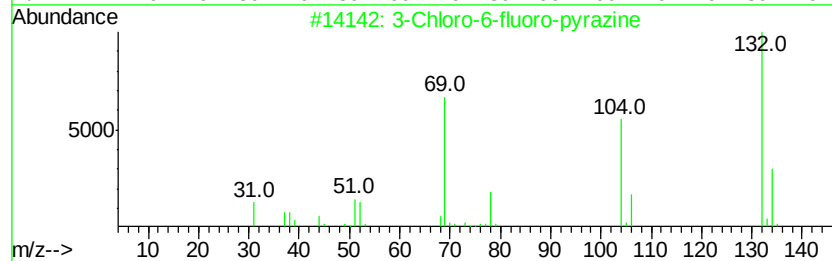
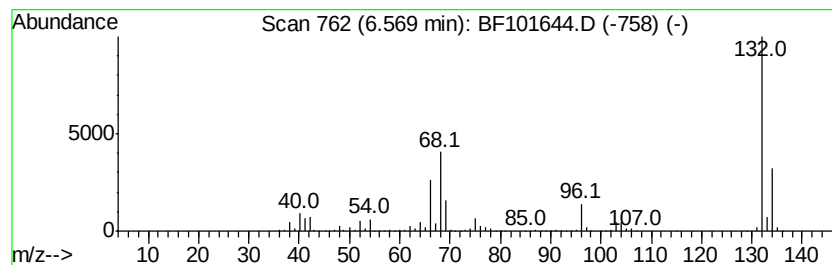
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Peak Number 2 unknown6.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	48.15 ng	2016790	1,4-Dichlorobenzene-d4	6.80

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	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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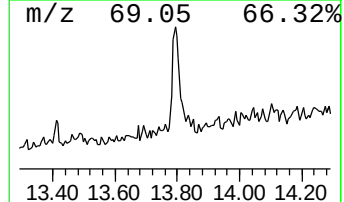
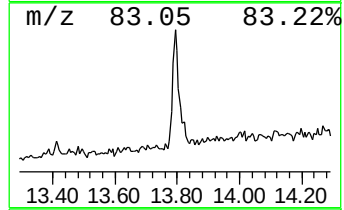
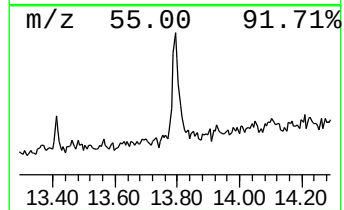
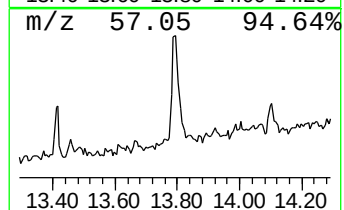
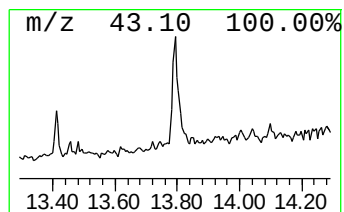
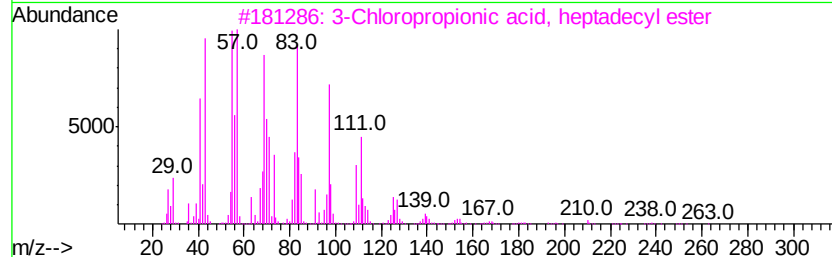
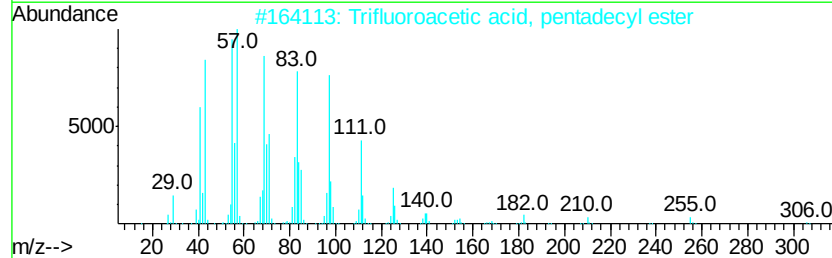
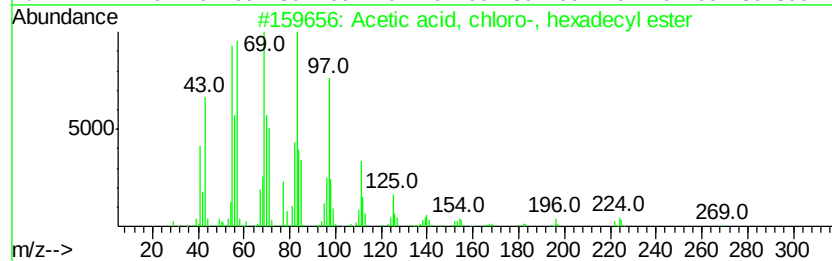
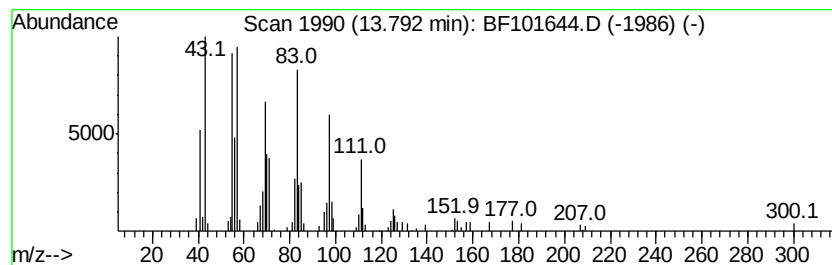
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Peak Number 4 Acetic acid, chloro-, hexad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	3.03 ng	132404	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	95
2		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
3		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	94
4		Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91
5		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.01	2.2	ng	93309	1	6.80	837636	20.0
unknown6.57	6.57	48.1	ng	2016790	1	6.80	837636	20.0
Acetic acid, chlo...	13.79	3.0	ng	132404	5	13.97	872798	20.0