

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122117\
 Data File : BF101647.D
 Acq On : 22 Dec 2017 10:43
 Operator : SJ/JU
 Sample : I7008-13
 Misc :
 ALS Vial : 49 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 121817-TIFR-E-U-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	509	rBV	72882	123495	4.15%	0.644%
2	5.422	563	567	588	rBV	631141	1060690	35.64%	5.534%
3	6.440	737	740	754	rBV2	410195	785946	26.41%	4.101%
4	6.569	758	762	769	rBV	1757633	1792052	60.22%	9.350%
5	6.798	797	801	810	rBV	734289	748581	25.16%	3.906%
6	6.951	823	827	842	rBV	2550952	2417244	81.23%	12.612%
7	7.363	894	897	914	rBV	1721480	1968508	66.15%	10.271%
8	8.081	1015	1019	1037	rBV	797600	921825	30.98%	4.810%
9	9.151	1197	1201	1211	rBV	3254447	2975707	100.00%	15.526%
10	9.833	1314	1317	1325	rVB	769995	740259	24.88%	3.862%
11	10.628	1448	1452	1465	rBV	853803	920836	30.95%	4.804%
12	11.322	1567	1570	1581	rBV	640456	676125	22.72%	3.528%
13	12.710	1802	1806	1809	rBV	90387	76811	2.58%	0.401%
14	12.904	1835	1839	1842	rBV	2568637	2309020	77.60%	12.047%
15	13.410	1922	1925	1929	rBV	65323	55850	1.88%	0.291%
16	13.792	1986	1990	1999	rBV2	45865	94683	3.18%	0.494%
17	13.969	2017	2020	2031	rBV	786360	811485	27.27%	4.234%
18	15.033	2197	2201	2206	rBV3	27166	37598	1.26%	0.196%
19	15.439	2265	2270	2282	rVB	430370	615862	20.70%	3.213%
20	15.815	2331	2334	2339	rVB2	24553	33821	1.14%	0.176%

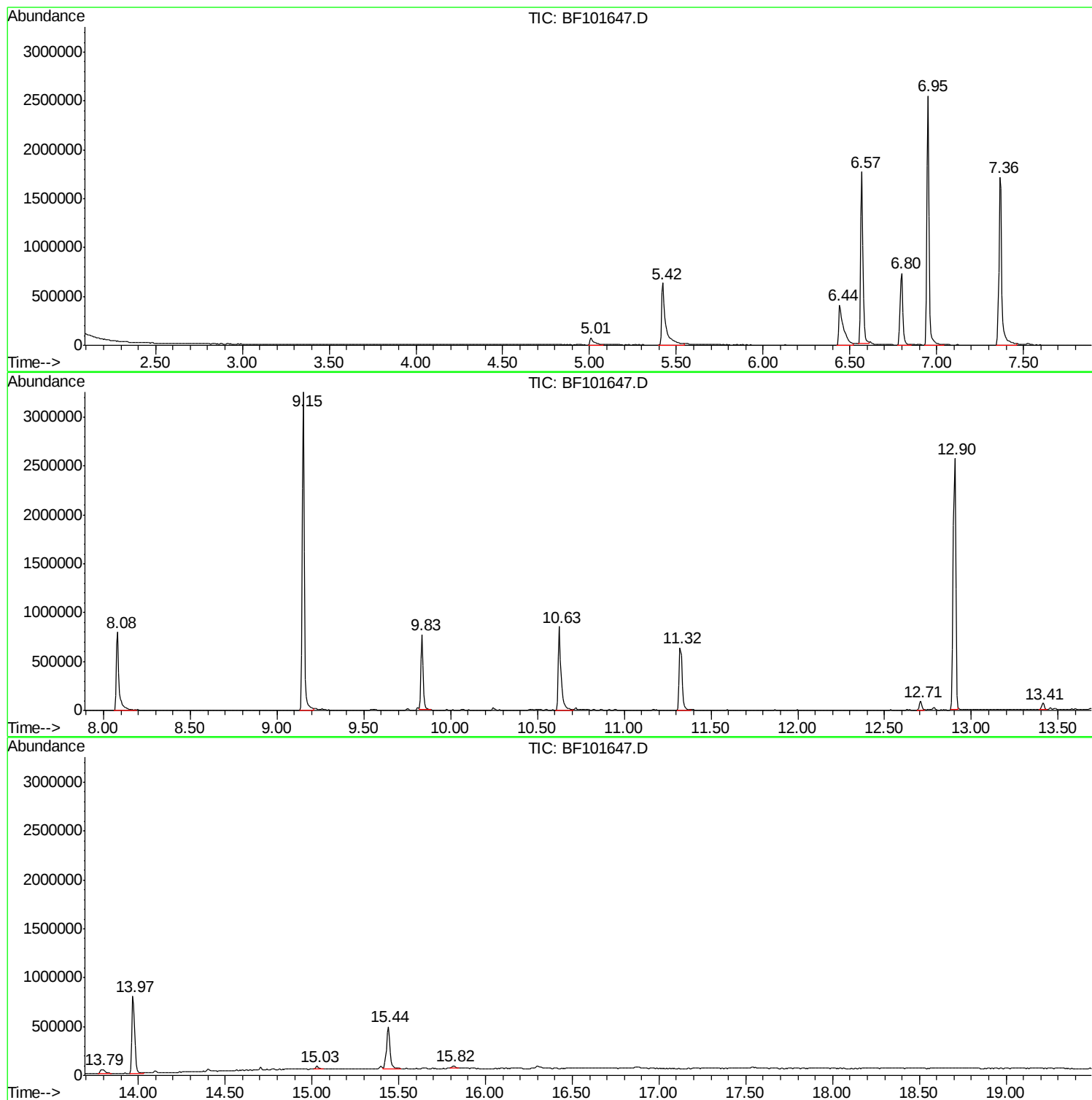
Sum of corrected areas: 19166398

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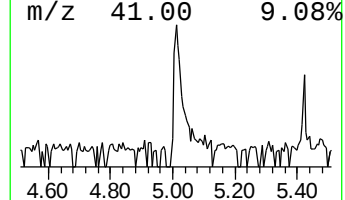
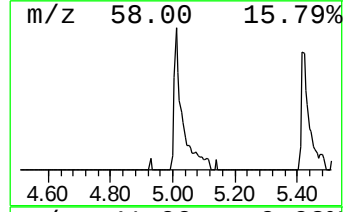
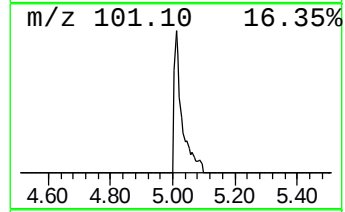
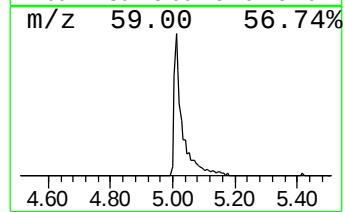
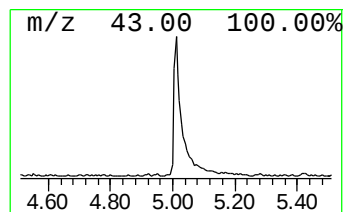
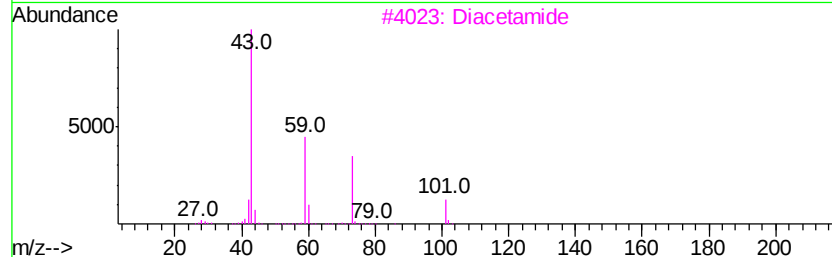
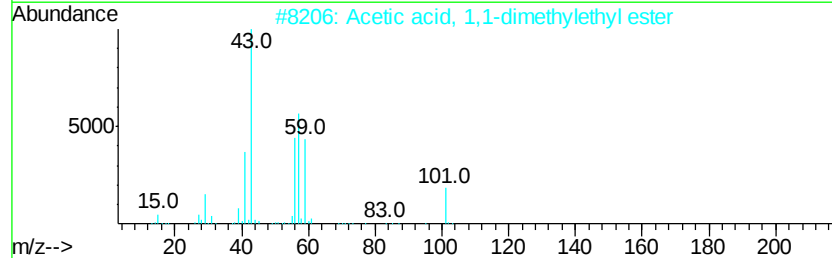
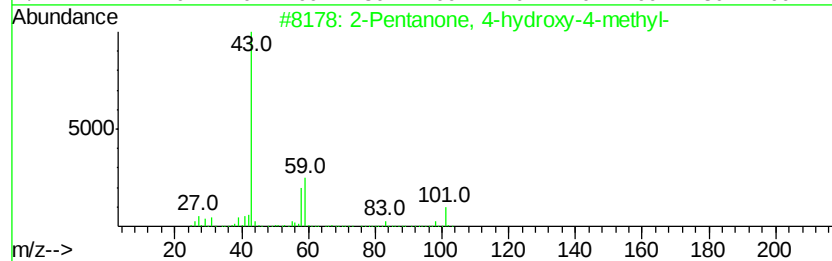
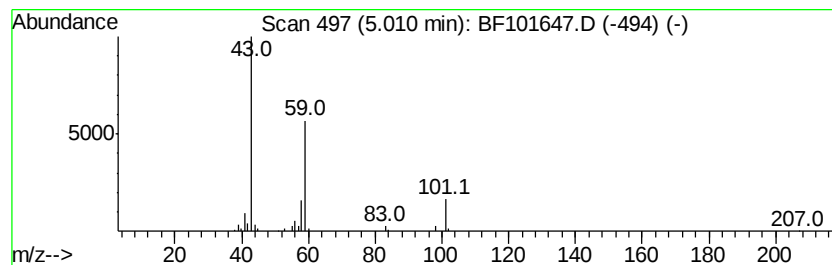
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	3.30 ng	123495	1,4-Dichlorobenzene-d4	6.80

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38		
3	Diacetamide	101	C4H7NO2	000625-77-4	36		
4	3-Hexanol	102	C6H14O	000623-37-0	33		
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		



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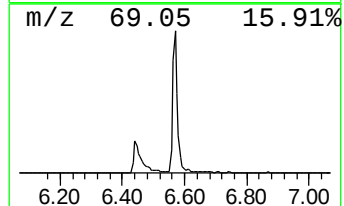
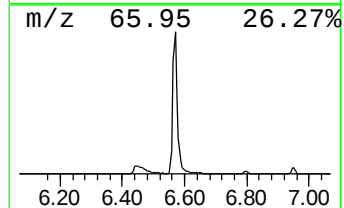
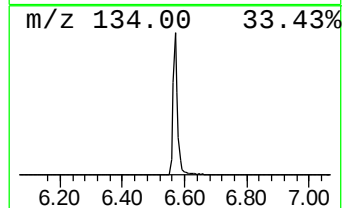
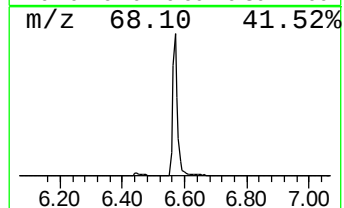
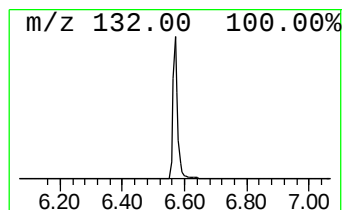
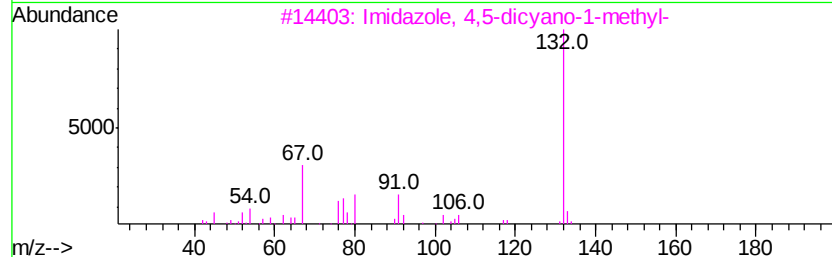
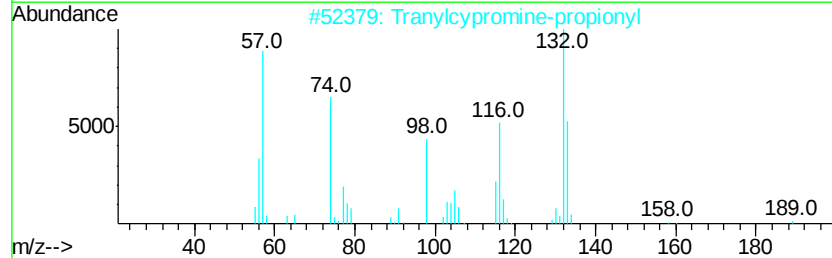
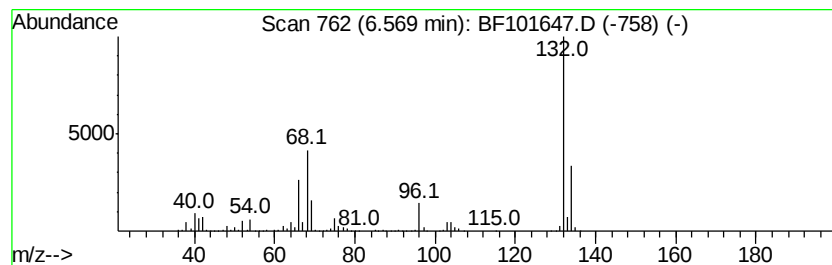
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Peak Number 2 unknown6.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	47.88 ng	1792050	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		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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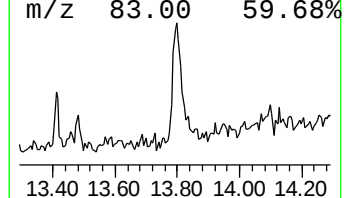
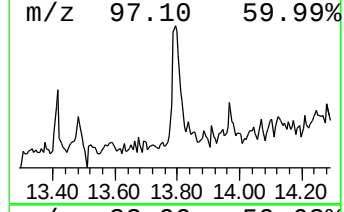
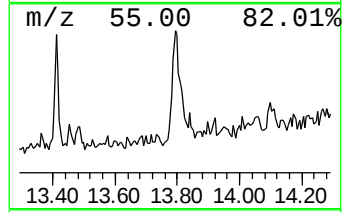
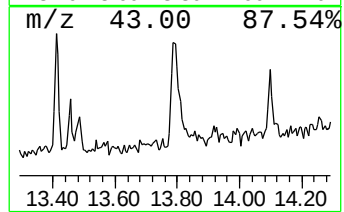
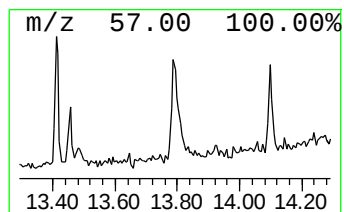
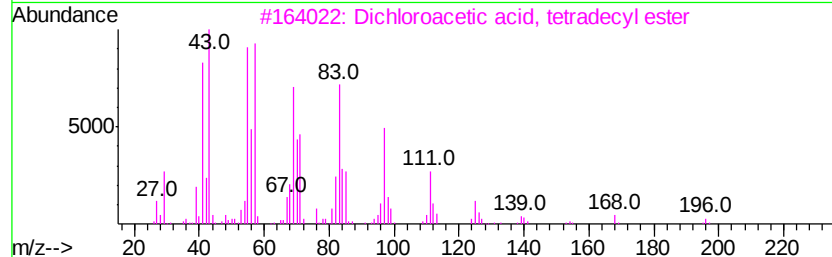
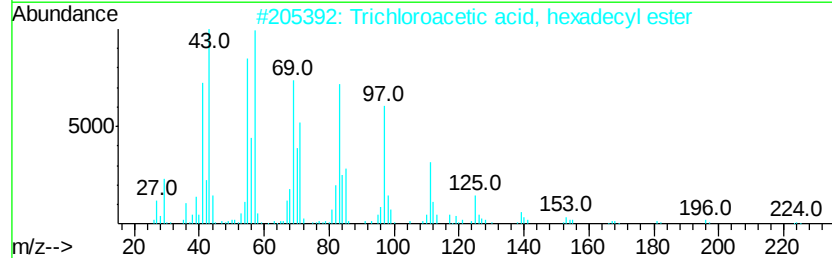
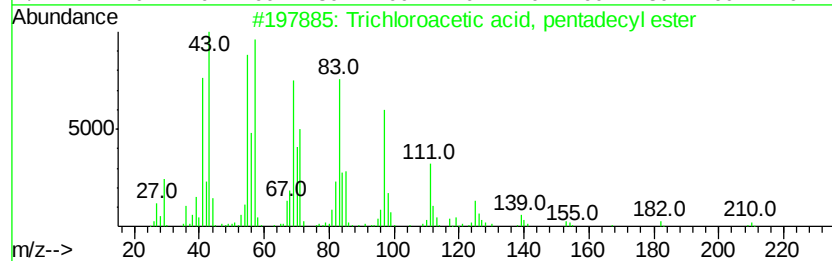
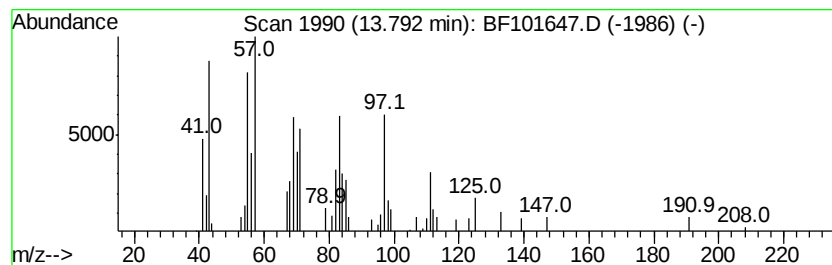
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Peak Number 4 Trichloroacetic acid, penta... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	2.33 ng	94683	Chrysene-d12	13.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3			Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	91
4			Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
5			Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.01	3.3	ng	123495	1	6.80	748581	20.0
unknown6.57	6.57	47.9	ng	1792050	1	6.80	748581	20.0
Trichloroacetic a...	13.79	2.3	ng	94683	5	13.97	811485	20.0