

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
 Data File : BF135029.D
 Acq On : 31 Aug 2023 04:31
 Operator : CG\JU
 Sample : 04198-14
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OR-309-OK-370-COMP-26

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:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135029.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	7	17	rVB2	28366	42123	2.22%	0.300%
2	4.993	491	494	504	rVB	129530	140177	7.38%	0.997%
3	5.398	559	563	566	rBV	2009240	1739280	91.60%	12.377%
4	6.404	730	734	738	rBV	1791058	1740181	91.64%	12.383%
5	6.604	764	768	777	rBV	42696	49261	2.59%	0.351%
6	6.769	793	796	800	rBV	889453	759832	40.02%	5.407%
7	7.334	887	892	895	rBV	1278219	1087566	57.27%	7.739%
8	8.051	1010	1014	1017	rBV	1174025	970074	51.09%	6.903%
9	9.128	1193	1197	1200	rBV	2316551	1898854	100.00%	13.512%
10	9.251	1214	1218	1221	rVB	39302	35080	1.85%	0.250%
11	9.810	1309	1313	1316	rBV	1145386	947072	49.88%	6.739%
12	10.598	1443	1447	1451	rBV	1085719	894975	47.13%	6.369%
13	11.298	1563	1566	1570	rBV	912012	759280	39.99%	5.403%
14	11.839	1654	1658	1667	rBV2	74293	93175	4.91%	0.663%
15	12.627	1789	1792	1798	rBV3	18709	26444	1.39%	0.188%
16	12.727	1806	1809	1811	rBV	32264	26172	1.38%	0.186%
17	12.898	1834	1838	1841	rBV	1600808	1351532	71.18%	9.617%
18	13.816	1990	1994	2001	rBV	85520	128459	6.77%	0.914%
19	13.957	2014	2018	2022	rBV	743519	672379	35.41%	4.785%
20	14.445	2097	2101	2108	rBV5	20689	42640	2.25%	0.303%
21	14.821	2162	2165	2170	rVB3	26268	27671	1.46%	0.197%
22	15.427	2262	2268	2273	rBV	477467	620723	32.69%	4.417%

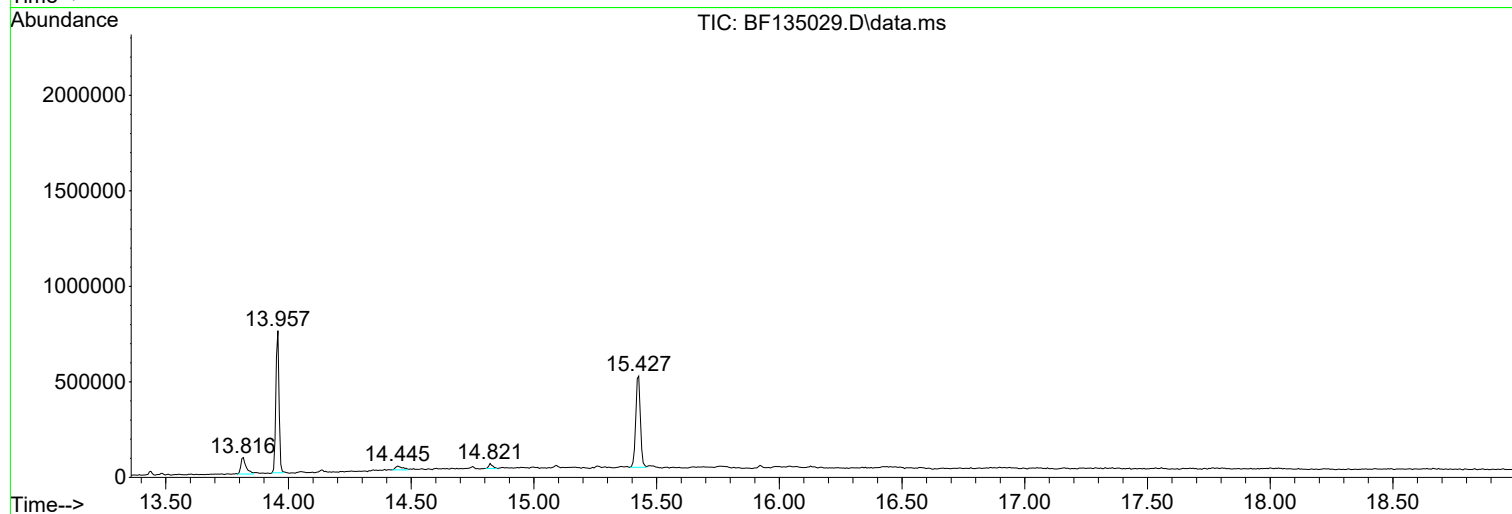
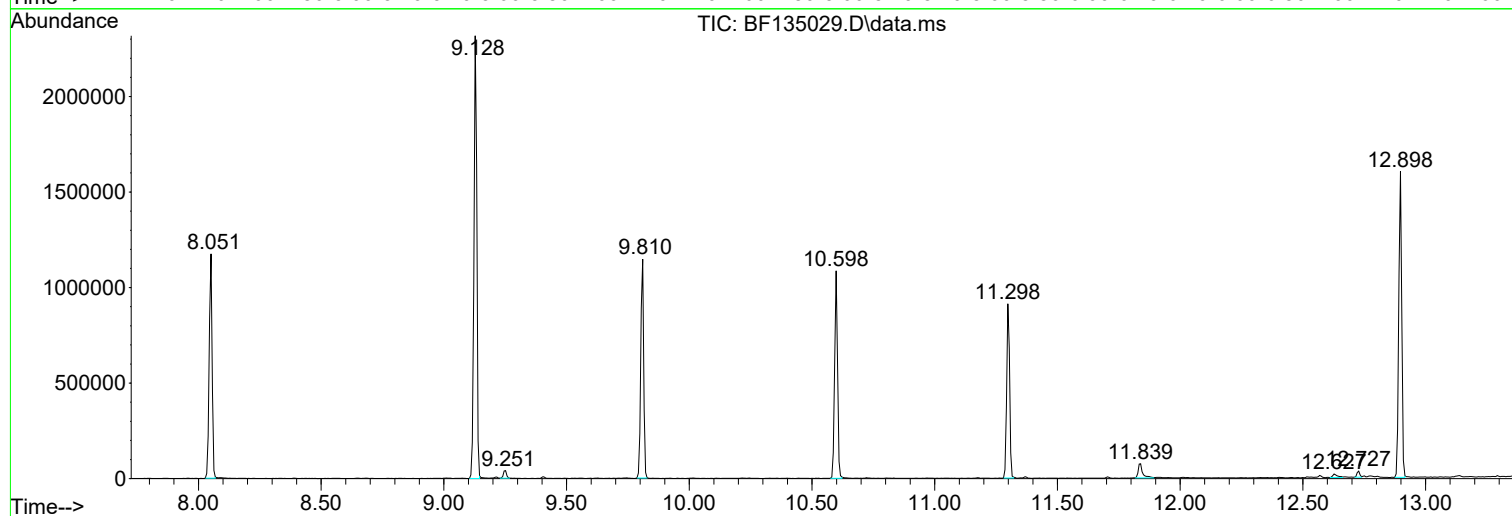
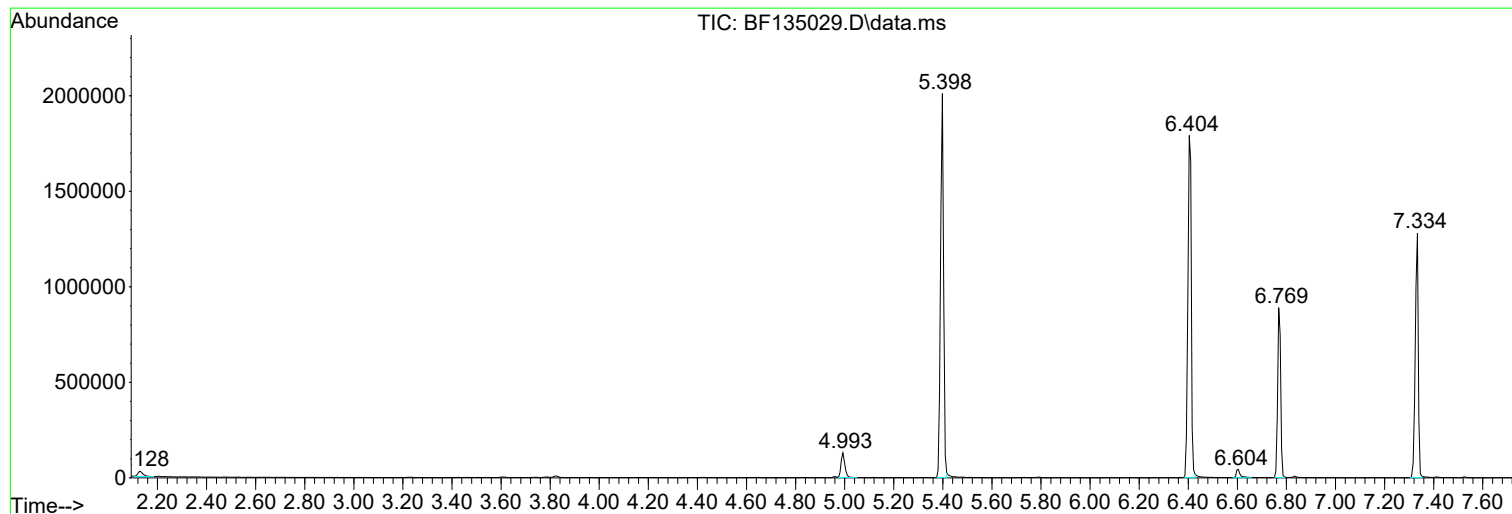
Sum of corrected areas: 14052950

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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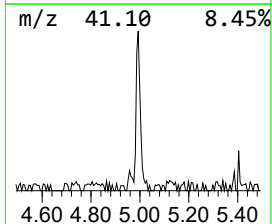
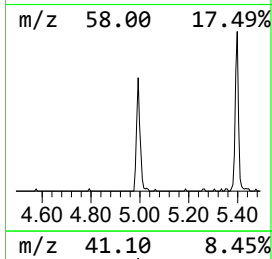
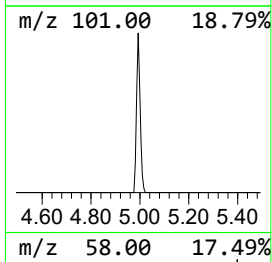
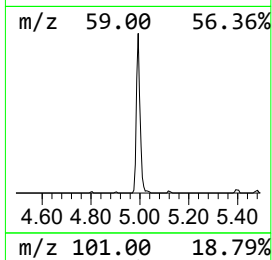
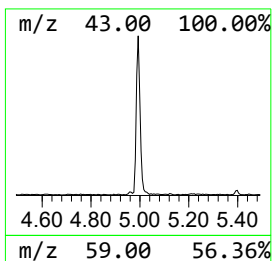
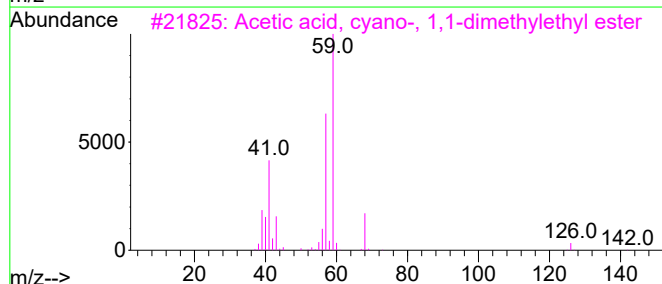
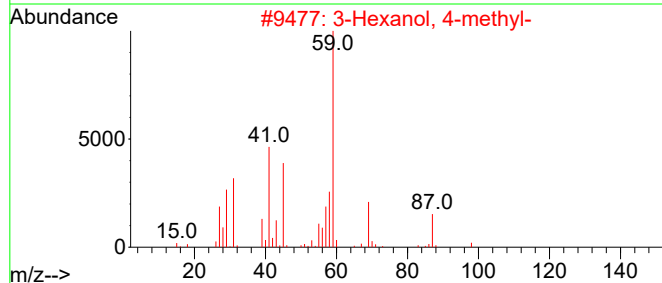
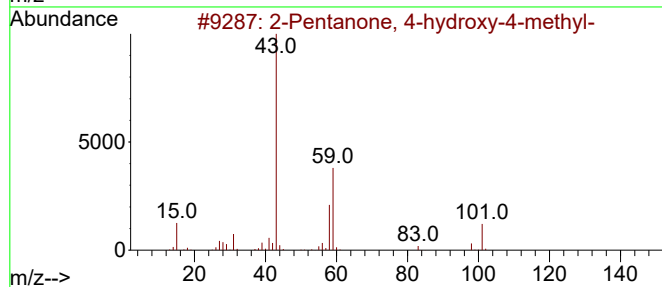
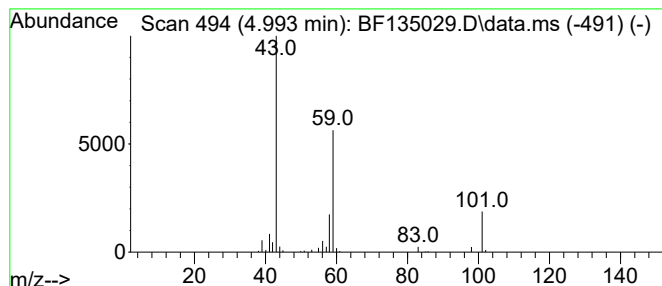
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.993	3.69 ng	140177	1,4-Dichlorobenzene-d4	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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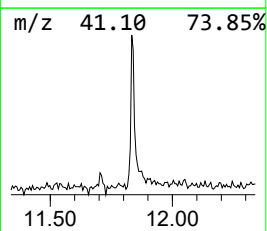
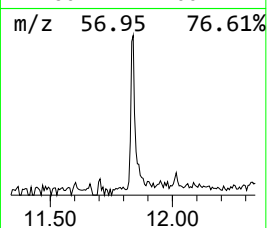
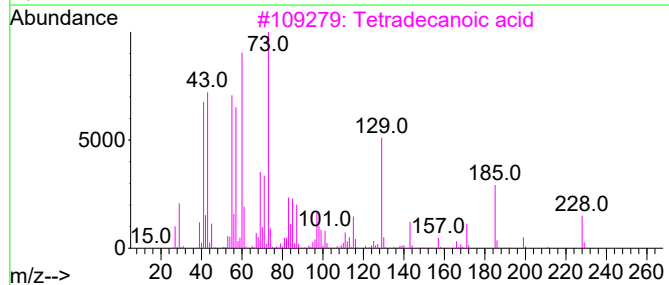
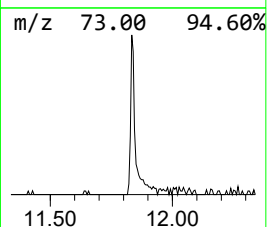
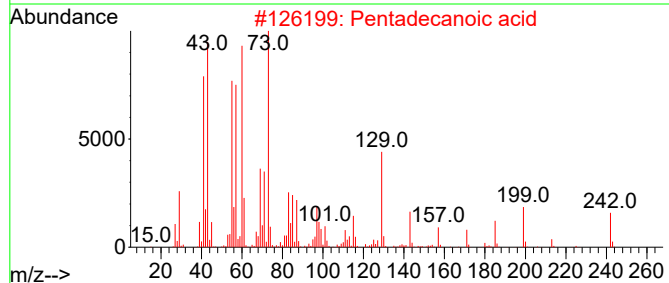
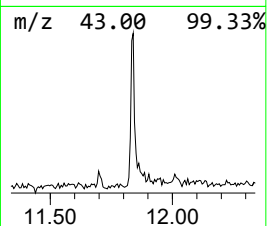
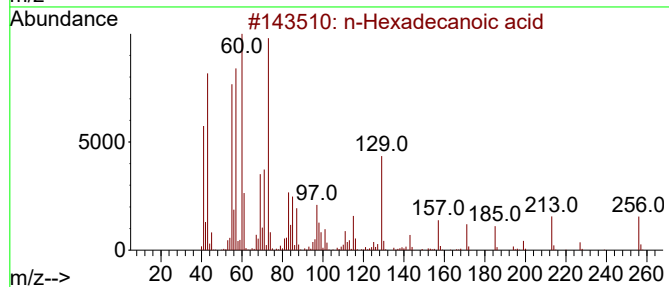
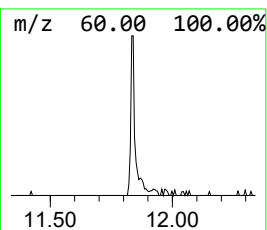
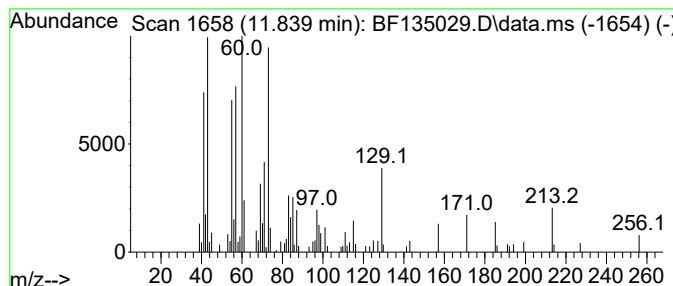
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	2.45 ng	93175	Phenanthrene-d10	11.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4			Tridecanoic acid	214	C13H26O2	000638-53-9	80
5			Undecanoic acid	186	C11H22O2	000112-37-8	68



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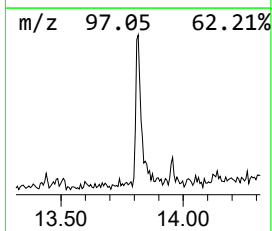
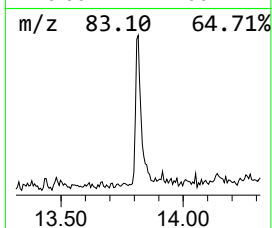
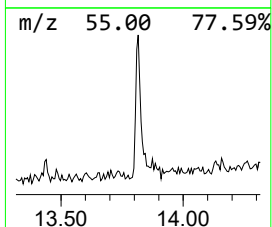
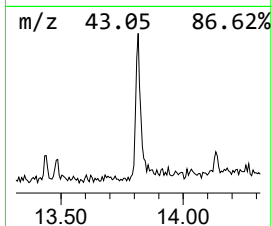
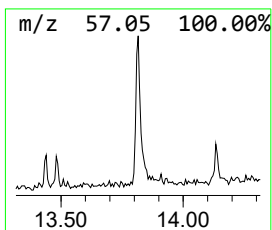
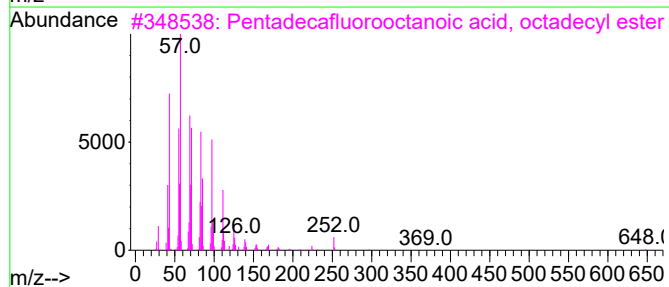
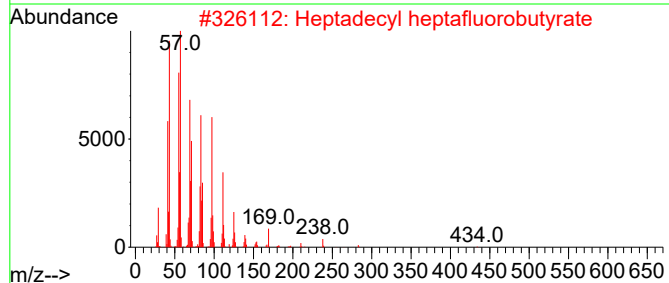
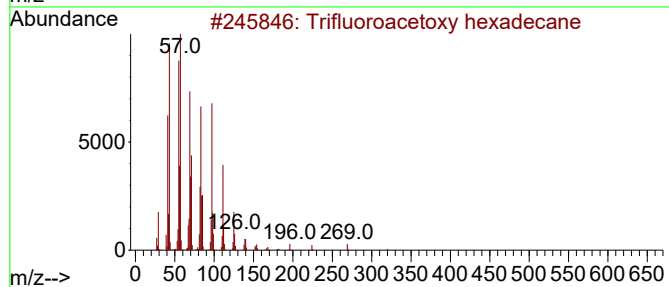
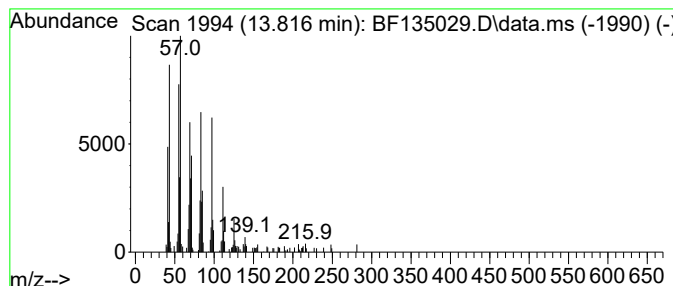
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Peak Number 3 Trifluoroacetoxy hexadecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.816	3.82 ng	128459	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
4			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	93
5			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.993	3.7	ng	140177	1	6.769	759832	20.0
n-Hexadecanoic ...	11.839	2.5	ng	93175	4	11.298	759280	20.0
Trifluoroacetox...	13.816	3.8	ng	128459	5	13.957	672379	20.0