

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110722\
 Data File : BG055489.D
 Acq On : 7 Nov 2022 22:56
 Operator : CG/JU
 Sample : N5460-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SH-1

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_G\Methods\8270-BG110122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055489.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.480	232	237	246	rBV	16871	25537	1.42%	0.327%
2	5.115	339	345	353	rBV	118919	176551	9.84%	2.262%
3	5.608	423	429	443	rBV	320875	511035	28.49%	6.548%
4	7.242	700	707	719	rBV	336940	560144	31.22%	7.177%
5	8.082	844	850	857	rVB	74325	117526	6.55%	1.506%
6	9.257	1043	1050	1064	rBV	197382	348255	19.41%	4.462%
7	10.908	1323	1331	1341	rBV	113484	194841	10.86%	2.496%
8	13.346	1738	1746	1757	rBV	707617	1061651	59.18%	13.603%
9	14.721	1973	1980	1989	rVB	222237	331371	18.47%	4.246%
10	16.208	2226	2233	2248	rBV	585150	922632	51.43%	11.821%
11	17.459	2440	2446	2456	rBV	304213	440492	24.55%	5.644%
12	18.094	2549	2554	2559	rBV	18944	23056	1.29%	0.295%
13	18.334	2591	2595	2603	rBV2	10631	24560	1.37%	0.315%
14	20.050	2881	2887	2892	rBV	1339381	1793904	100.00%	22.985%
15	21.331	3100	3105	3121	rBV6	38254	119950	6.69%	1.537%
16	21.713	3164	3170	3177	rBV2	318801	519097	28.94%	6.651%
17	21.871	3194	3197	3201	rVB3	16505	21617	1.21%	0.277%
18	22.471	3297	3299	3306	rVB2	13920	21255	1.18%	0.272%
19	23.170	3414	3418	3423	rVB3	12534	19852	1.11%	0.254%
20	24.980	3716	3726	3738	rVB2	192778	571485	31.86%	7.322%

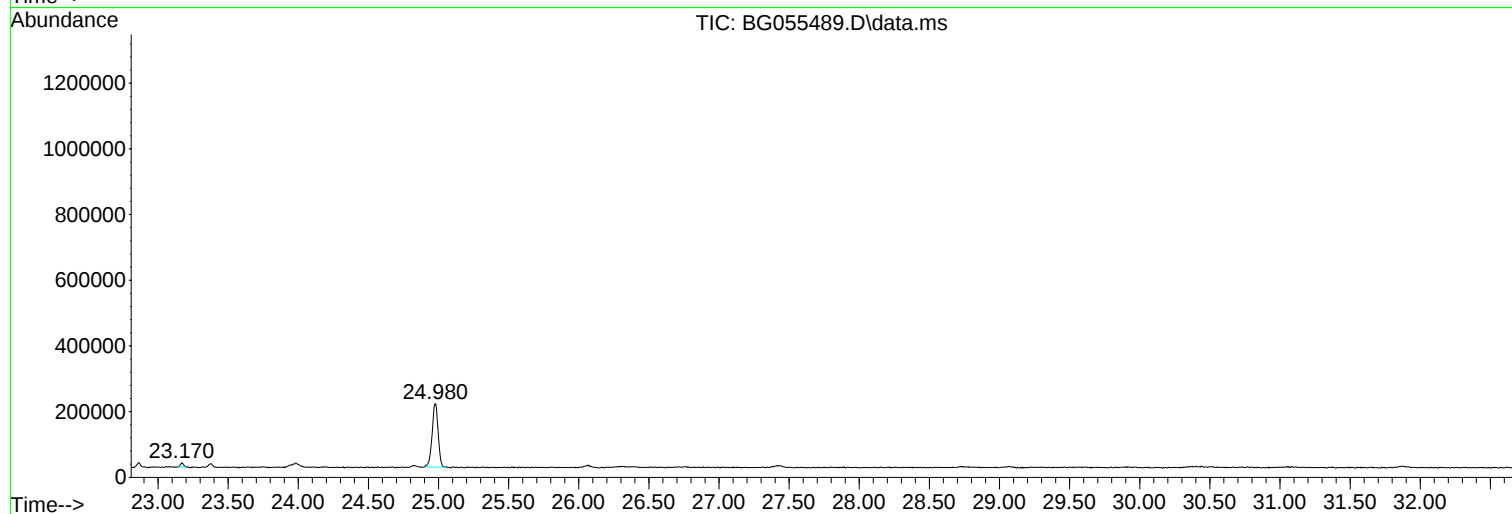
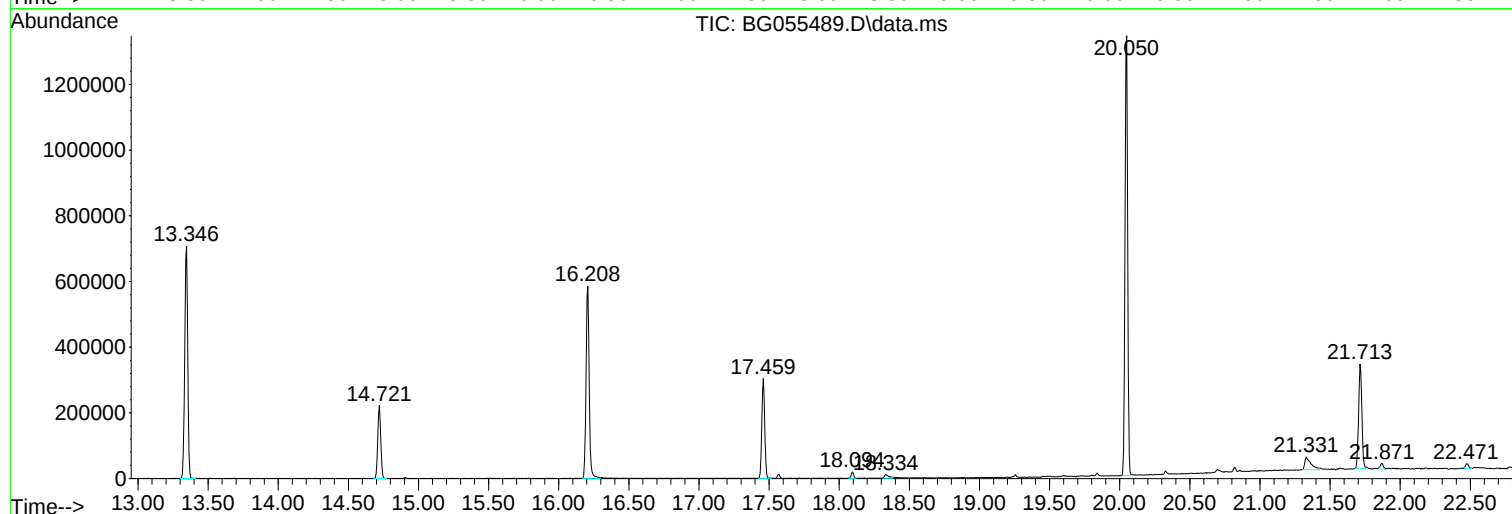
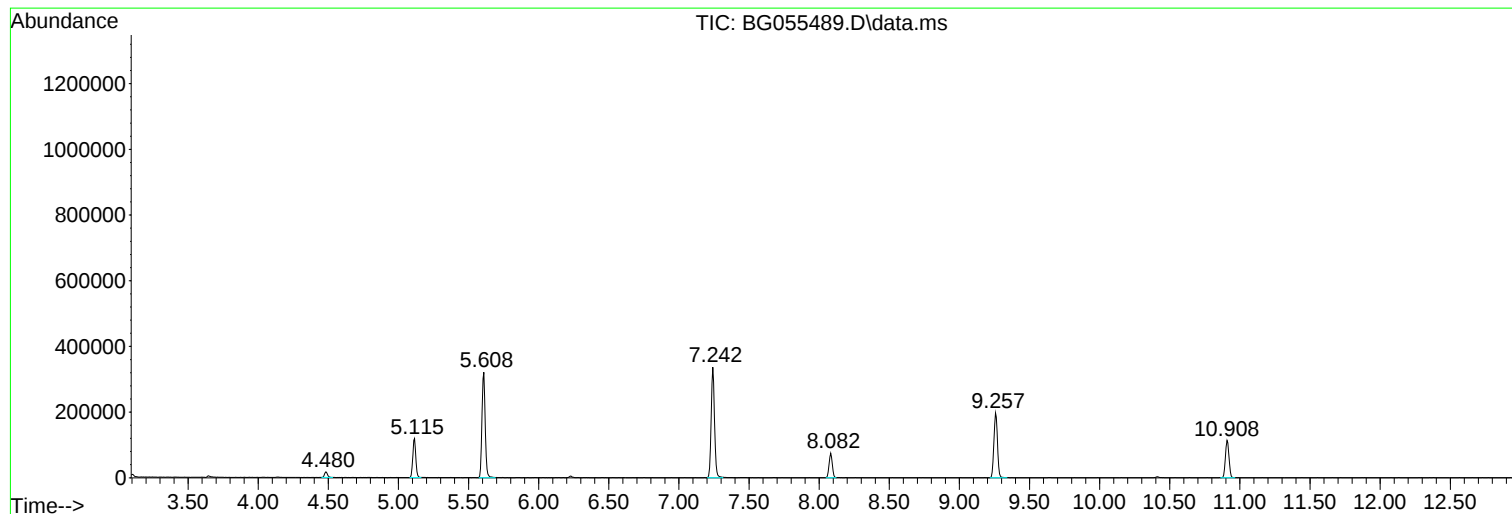
Sum of corrected areas: 7804811

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.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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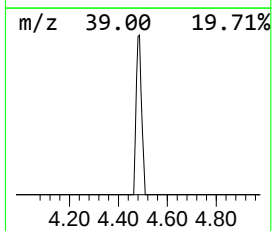
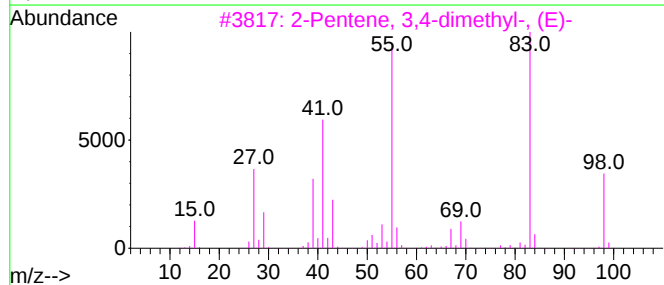
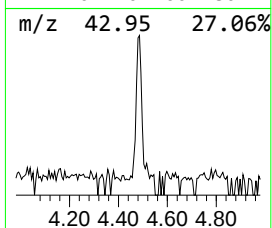
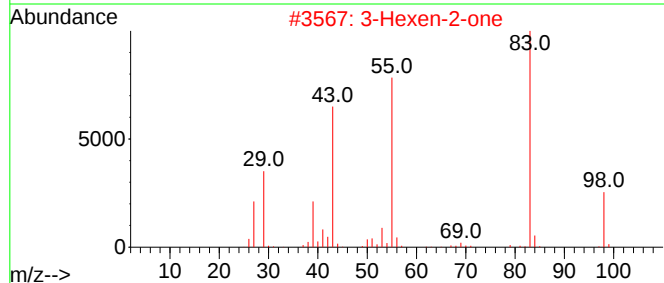
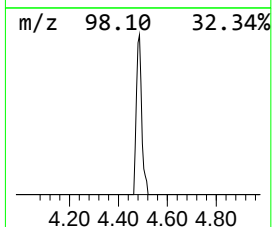
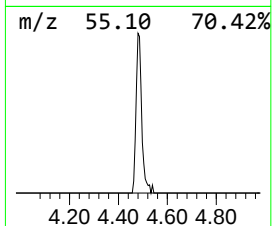
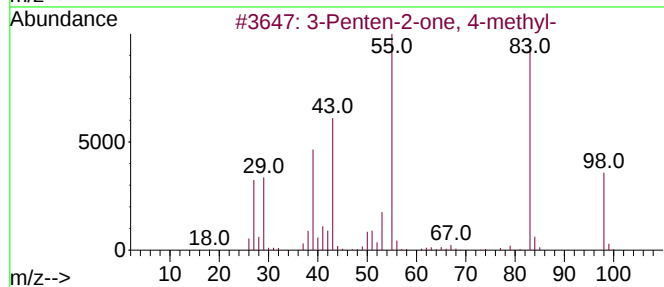
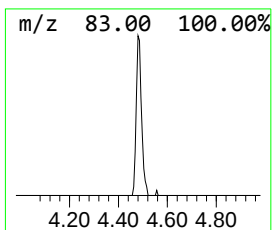
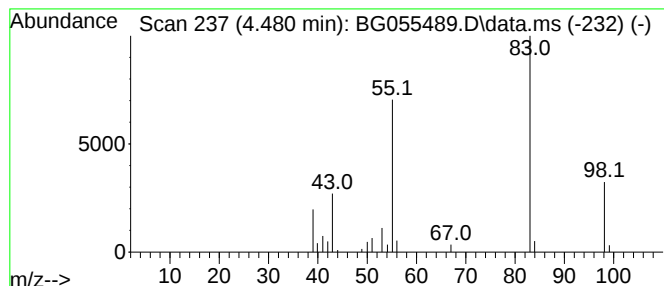
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.480	4.35 ng	25537	1,4-Dichlorobenzene-d4	8.082

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	87
2		3-Hexen-2-one	98	C6H10O	000763-93-9	86
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	80
4		2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	80
5		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78



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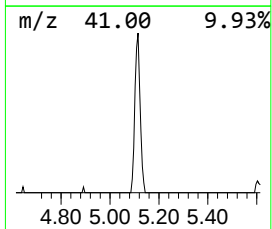
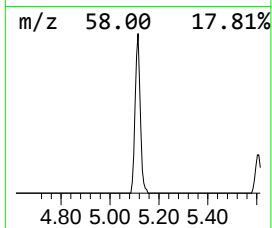
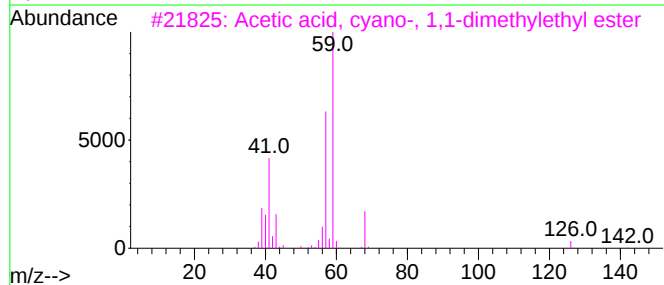
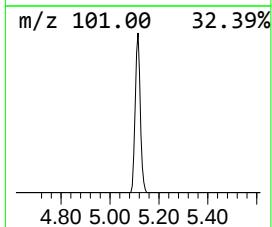
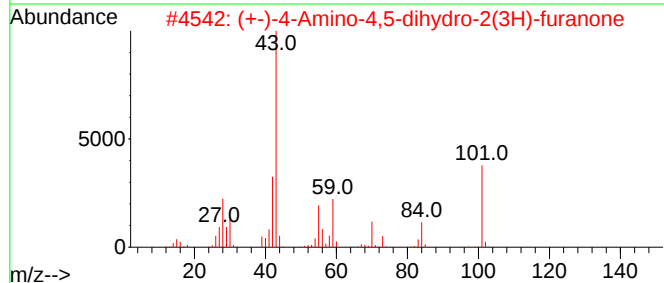
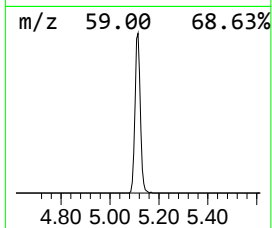
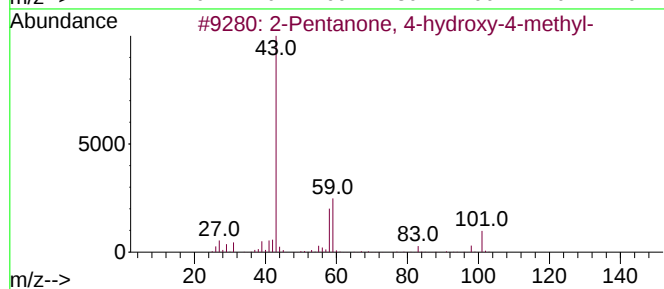
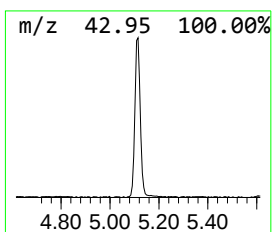
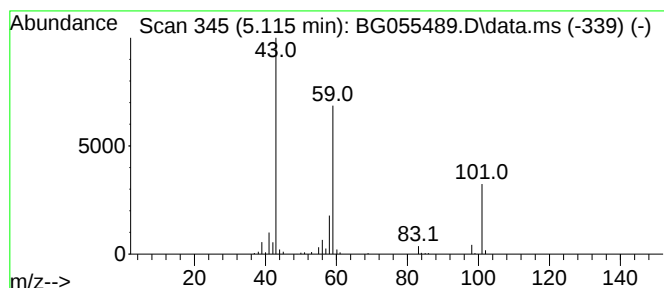
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.115	30.04 ng	176551	1,4-Dichlorobenzene-d4	8.082

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	47
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4		Acetone	58	C3H6O	000067-64-1	10
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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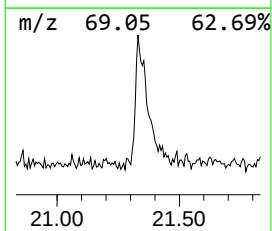
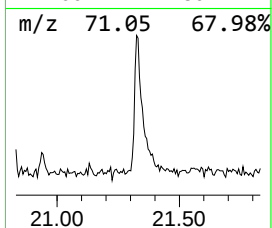
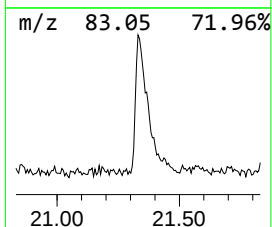
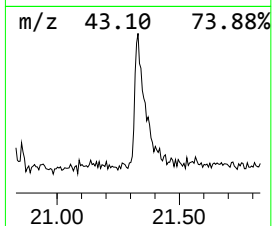
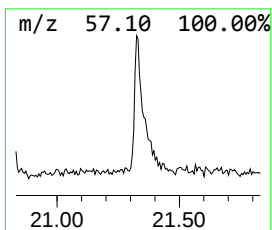
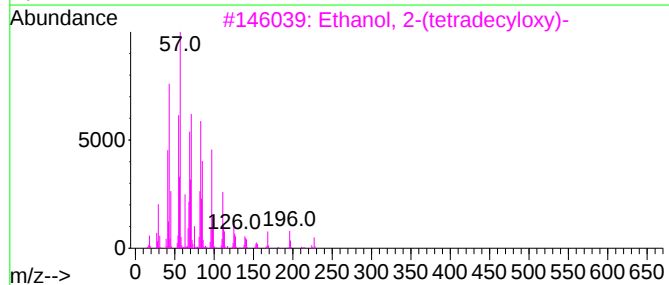
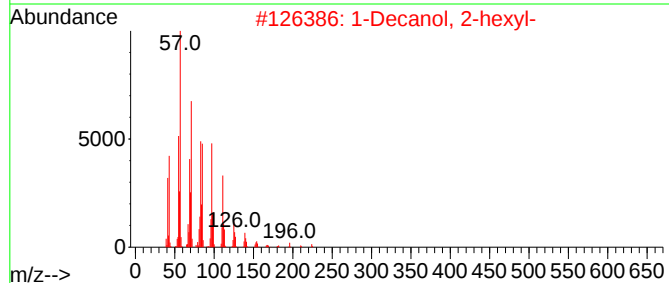
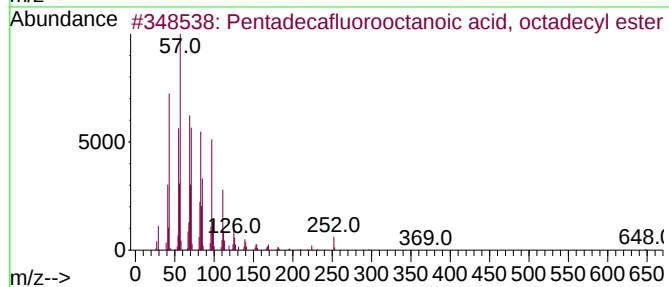
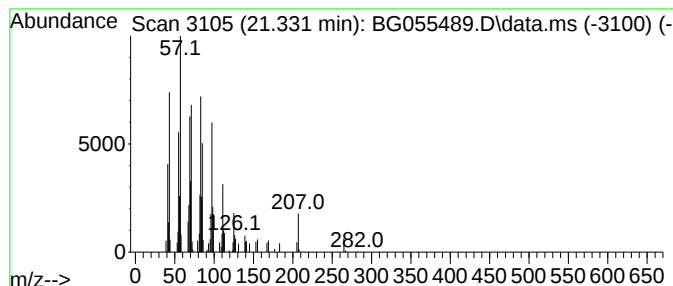
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Peak Number 3 Pentadecafluorooctanoic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.331	4.62 ng	119950	Chrysene-d12	21.713

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	90
2			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	90
3			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90
4			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	87
5			Octacosyl heptafluorobutyrate	606	C32H57F7O2	1010351-83-6	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one,...	4.480	4.3	ng	25537	1	8.082	117526	20.0
2-Pentanone, 4-...	5.115	30.0	ng	176551	1	8.082	117526	20.0
Pentadecafluoro...	21.331	4.6	ng	119950	5	21.713	519097	20.0