

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062321\
 Data File : BG049062.D
 Acq On : 23 Jun 2021 15:24
 Operator : CG/JU
 Sample : M2748-12
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-10A

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-BG061121.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG049062.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.158	14	20	30	rBV	51823	102617	5.76%	1.349%
2	3.234	30	33	41	rVB3	13760	20424	1.15%	0.269%
3	5.191	360	366	373	rBV	45342	74837	4.20%	0.984%
4	5.655	439	445	457	rBV	299399	498370	27.96%	6.552%
5	7.259	710	718	728	rBV	310248	556016	31.20%	7.310%
6	8.105	856	862	868	rBV	101515	170625	9.57%	2.243%
7	9.274	1053	1061	1071	rBV	194323	368590	20.68%	4.846%
8	10.931	1333	1343	1351	rBV	127332	231805	13.01%	3.048%
9	13.370	1752	1758	1767	rVB	498140	809491	45.42%	10.643%
10	14.750	1985	1993	2000	rBV	204984	337330	18.93%	4.435%
11	15.544	2121	2128	2131	rBV	15232	22450	1.26%	0.295%
12	16.237	2239	2246	2261	rBV	447826	713620	40.04%	9.382%
13	17.500	2453	2461	2469	rBV	331805	499725	28.04%	6.570%
14	18.376	2605	2610	2619	rBV7	18935	33671	1.89%	0.443%
15	20.103	2898	2904	2911	rBV	1413332	1782132	100.00%	23.430%
16	21.419	3123	3128	3138	rBV5	42662	87233	4.89%	1.147%
17	21.783	3184	3190	3199	rVB	341147	599250	33.63%	7.878%
18	22.964	3387	3391	3393	rBV4	15035	21321	1.20%	0.280%
19	23.534	3484	3488	3496	rVB5	26167	52322	2.94%	0.688%
20	25.109	3746	3756	3773	rVB3	205168	624365	35.03%	8.209%

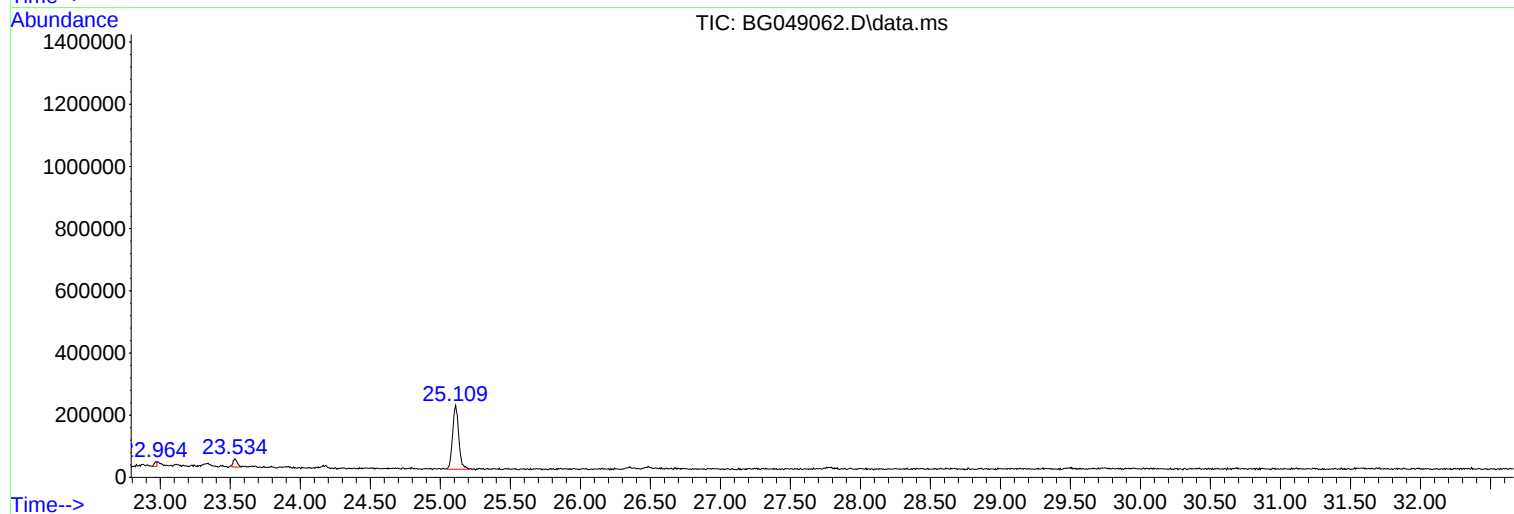
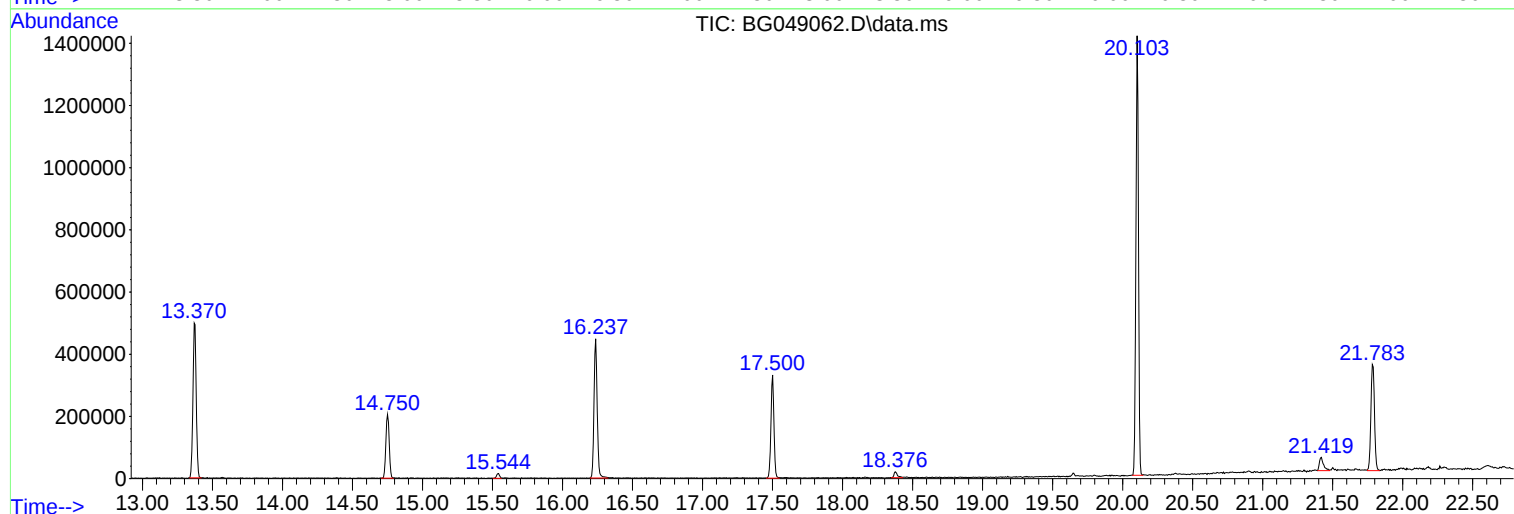
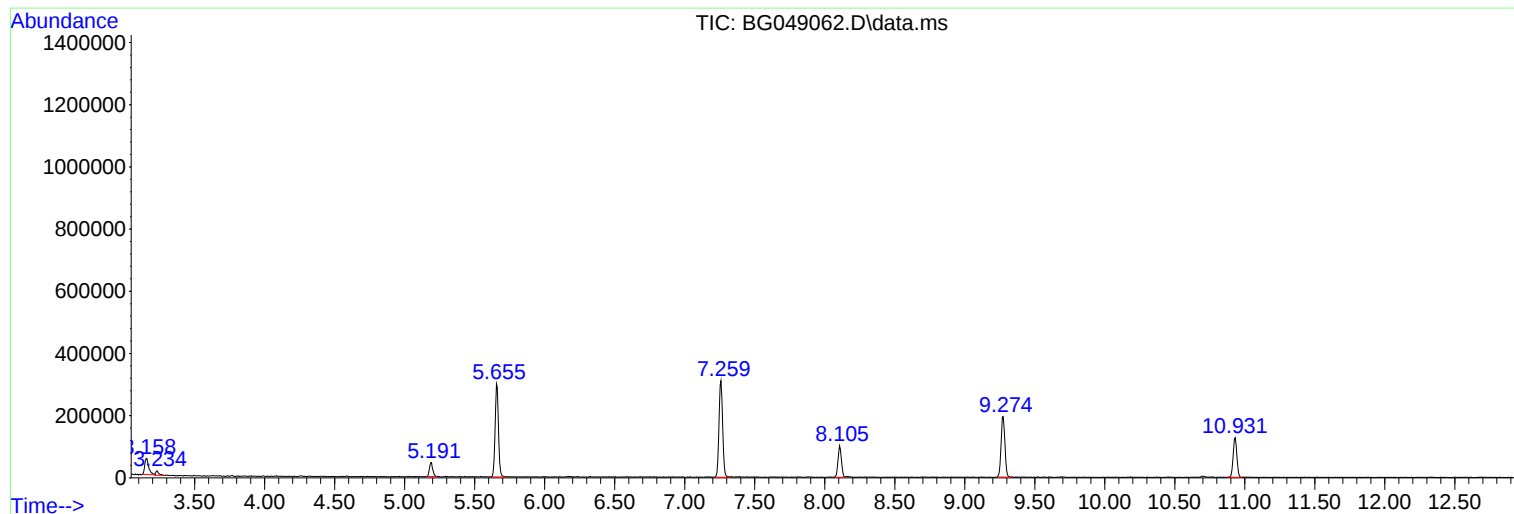
Sum of corrected areas: 7606194

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.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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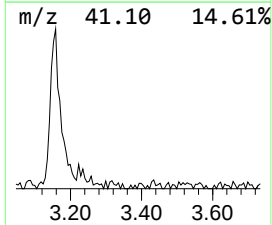
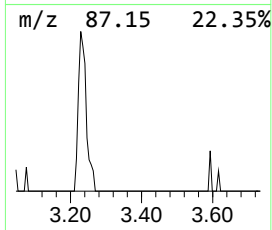
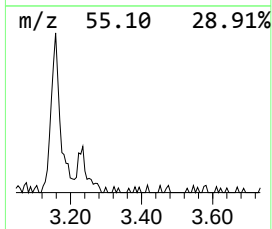
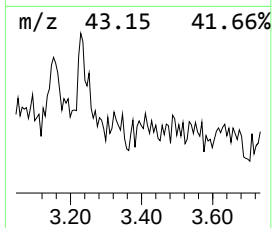
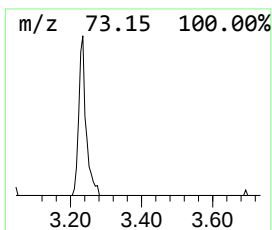
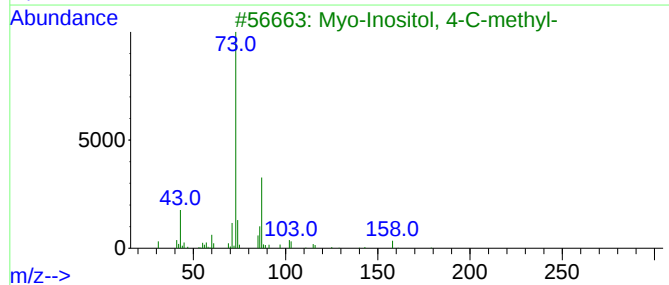
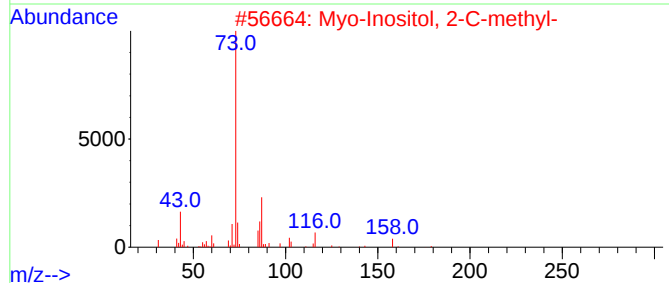
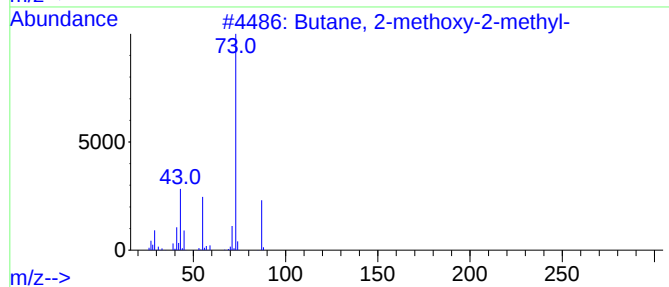
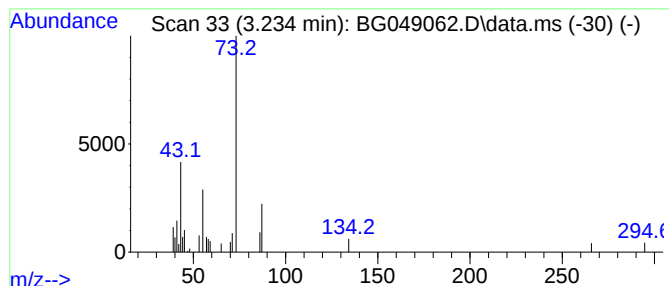
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown3.234 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.234	2.39 ng	20424	1,4-Dichlorobenzene-d4	8.111

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	40
2		Myo-Inositol, 2-C-methyl-	194	C7H14O6	000472-96-8	28
3		Myo-Inositol, 4-C-methyl-	194	C7H14O6	000472-95-7	28
4		Isobutylamine	73	C4H11N	000078-81-9	9
5		N-(2-Thioethyl) N'-methyl urea	134	C4H10N2OS	072545-68-7	9



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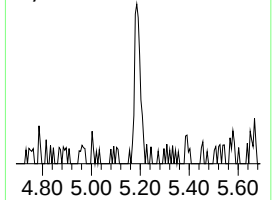
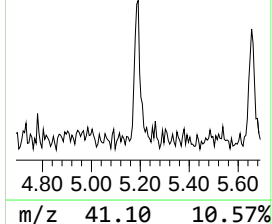
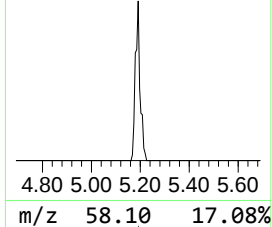
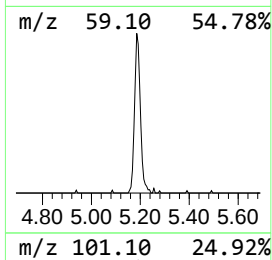
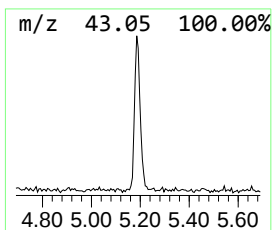
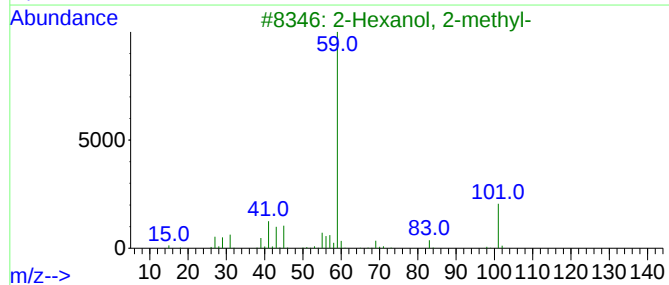
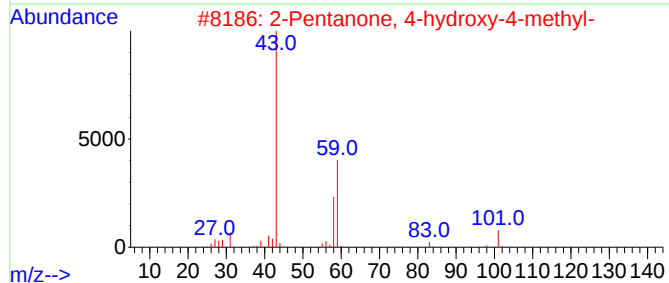
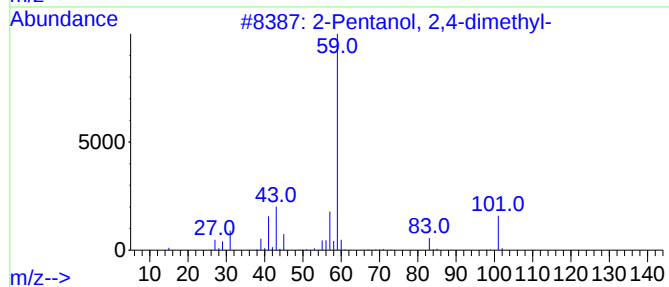
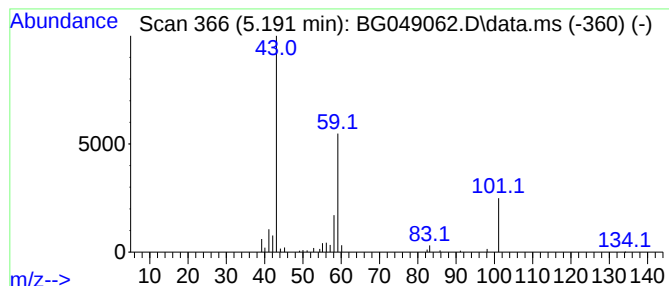
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TIC Library : C:\Database\NIST11.L
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Peak Number 3 unknown5.191 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.191	8.77 ng	74837	1,4-Dichlorobenzene-d4	8.111

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	42
2		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		3-Pentanol	88	C5H12O	000584-02-1	23
5		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23



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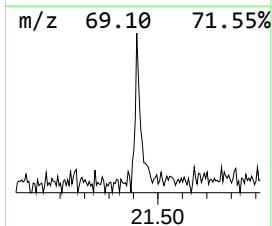
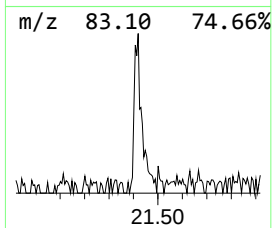
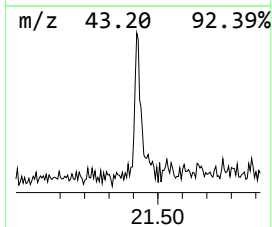
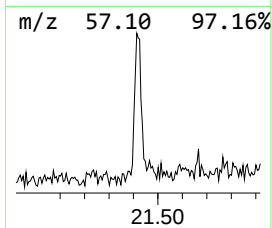
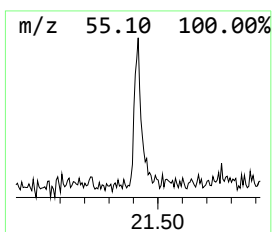
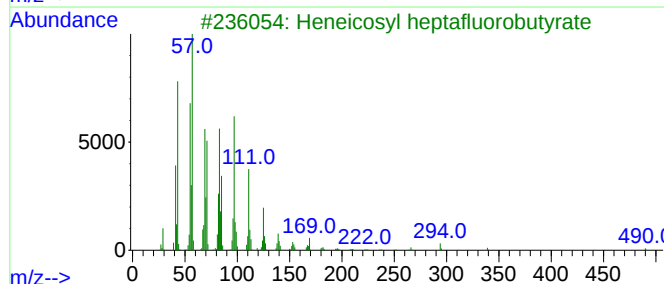
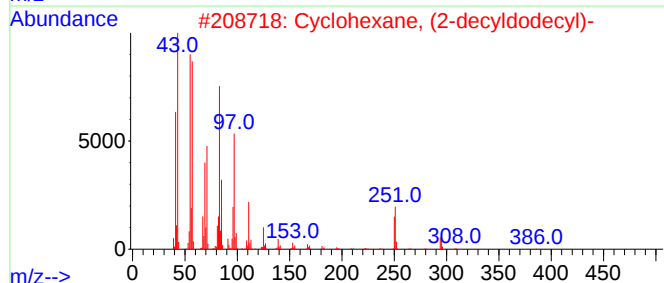
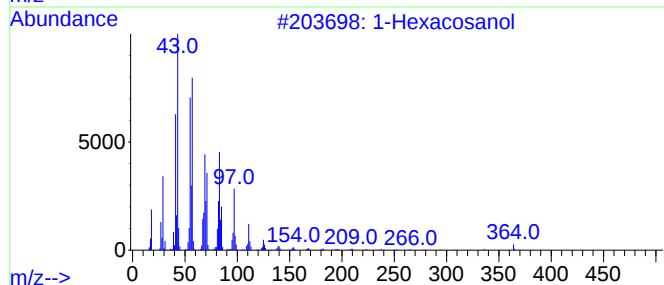
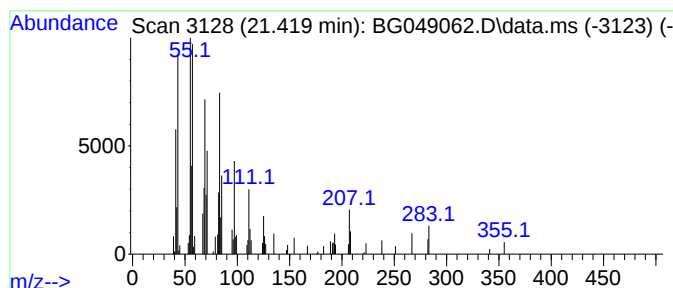
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Peak Number 4 1-Hexacosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.419	2.91 ng	87233	Chrysene-d12	21.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosanol			382	C26H54O	000506-52-5	72
2	Cyclohexane, (2-decyldodecyl)-			392	C28H56	006704-00-3	58
3	Heneicosyl heptafluorobutyrate			508	C25H43F7O2	1000351-83-8	58
4	Cyclopentane, (4-octyldodecyl)-			350	C25H50	005638-09-5	58
5	2-Methyl-E-7-hexadecene			238	C17H34	064183-52-4	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.234	3.234	2.4	ng	20424	1	8.111	170625	20.0
unknown5.191	5.191	8.8	ng	74837	1	8.111	170625	20.0
1-Hexacosanol	21.419	2.9	ng	87233	5	21.783	599250	20.0