

Data Path : Z:\HPCHEM1\BNA G\DATA\BG113017\
 Data File : BG031296.D
 Acq On : 30 Nov 2017 20:23
 Operator : SJ/JU
 Sample : I6634-04
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 112717-JETT-E-U-S

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_G\METHODS\8270-BG111017.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	5.209	321	327	339	rVB	66528	113222	1.65%	0.464%
2	5.691	403	409	421	rBV	342743	607020	8.87%	2.487%
3	7.295	675	682	699	rBV	206493	426773	6.24%	1.748%
4	7.665	738	745	761	rBV	639493	1193487	17.44%	4.889%
5	8.129	817	824	832	rBV	231510	400319	5.85%	1.640%
6	8.452	871	879	895	rBV	972354	1779424	26.00%	7.289%
7	9.298	1015	1023	1036	rBV	704074	1365929	19.96%	5.595%
8	10.949	1296	1304	1322	rBV	263354	575490	8.41%	2.357%
9	13.376	1709	1717	1736	rBV	2370103	3902282	57.02%	15.985%
10	14.751	1942	1951	1965	rBV2	508170	902395	13.19%	3.697%
11	16.237	2198	2204	2223	rBV	1133152	1899879	27.76%	7.783%
12	17.495	2411	2418	2431	rBV	727903	1167707	17.06%	4.783%
13	18.364	2561	2566	2574	rBV3	46371	96328	1.41%	0.395%
14	19.622	2775	2780	2796	rBV2	62639	151049	2.21%	0.619%
15	20.086	2852	2859	2869	rBV	4824566	6844061	100.00%	28.036%
16	21.378	3073	3079	3091	rBV4	49226	135573	1.98%	0.555%
17	21.766	3138	3145	3162	rBV	854010	1460478	21.34%	5.983%
18	25.068	3696	3707	3723	rBV3	471200	1390075	20.31%	5.694%

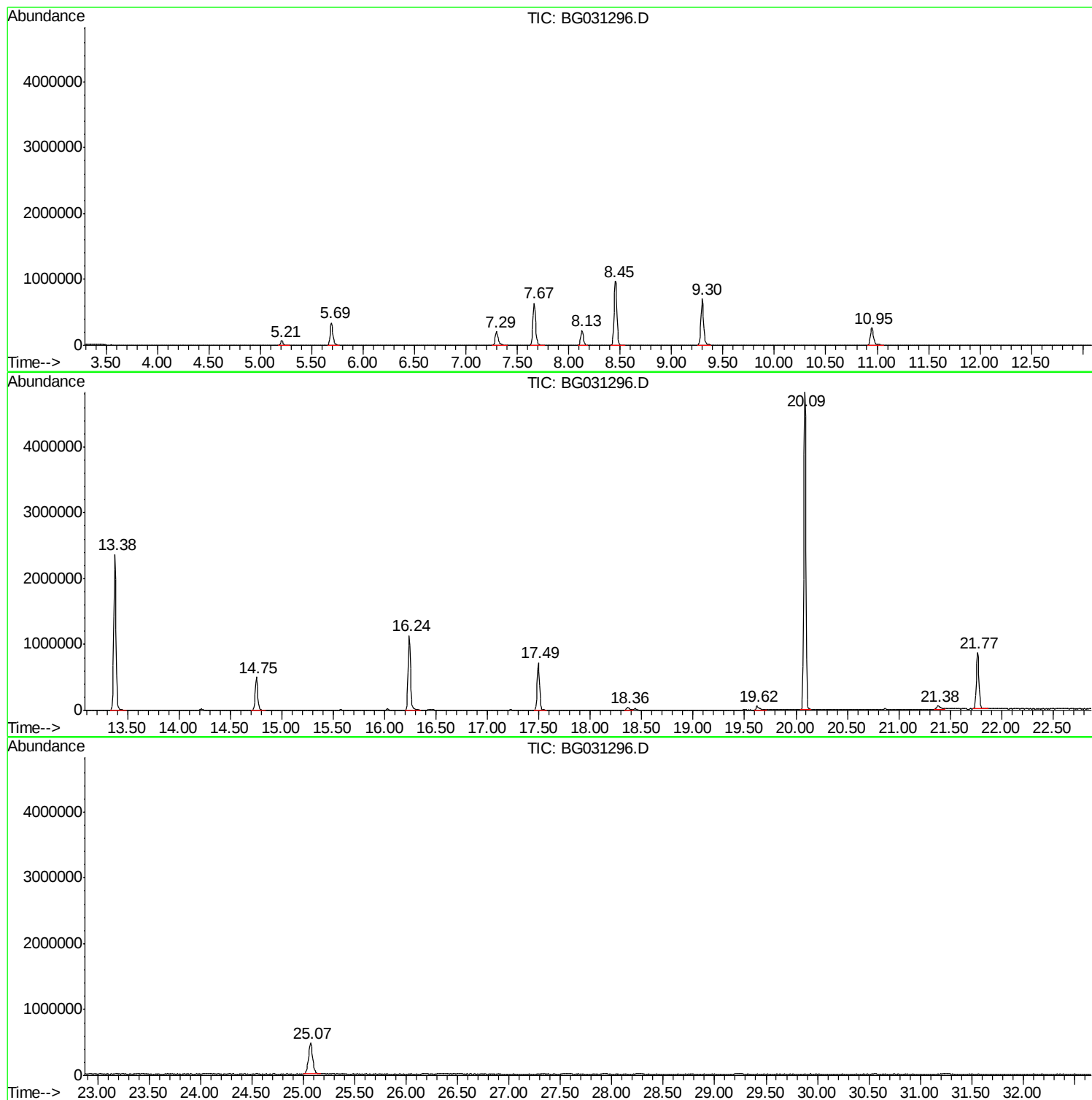
Sum of corrected areas: 24411491

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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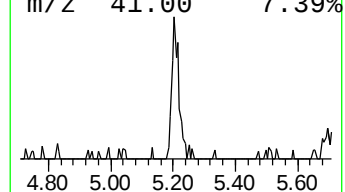
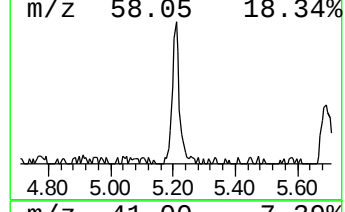
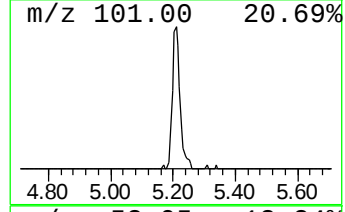
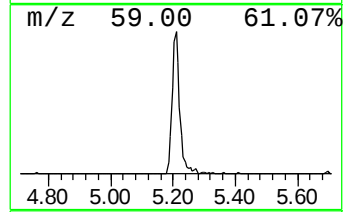
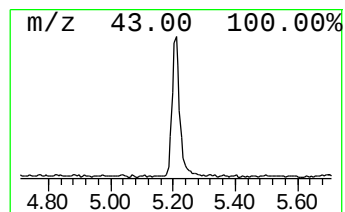
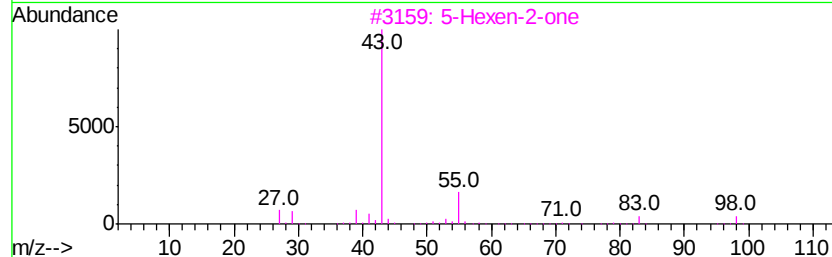
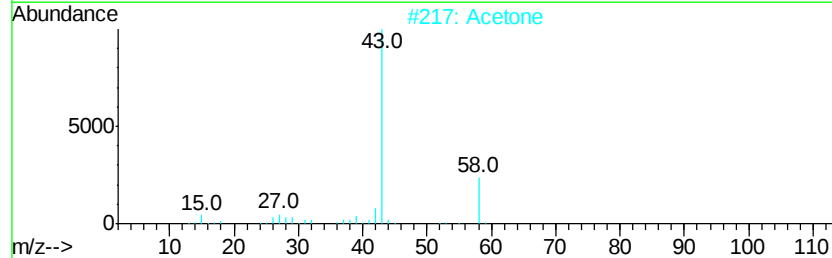
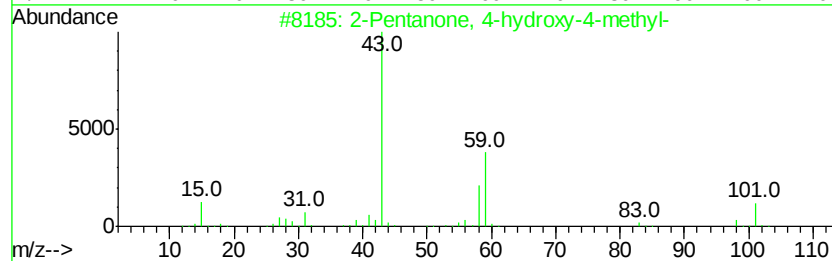
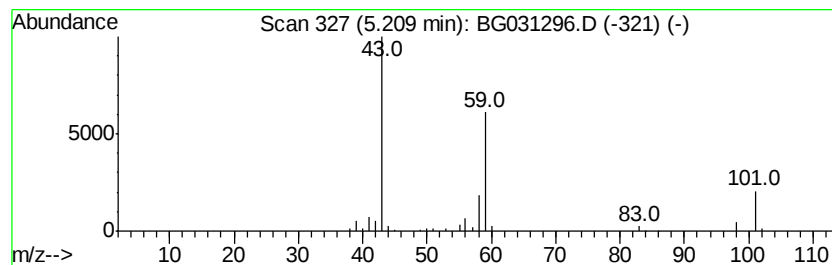
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	5.66 ng	113222	1,4-Dichlorobenzene-d4	8.13

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2		000123-42-2	40
2	Acetone	58	C3H6O		000067-64-1	14
3	5-Hexen-2-one	98	C6H10O		000109-49-9	9
4	Guanidine	59	CH5N3		000113-00-8	9
5	Butane, 1-ethoxy-	102	C6H14O		000628-81-9	9



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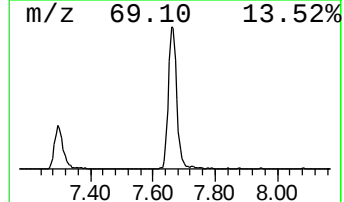
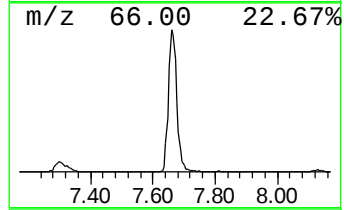
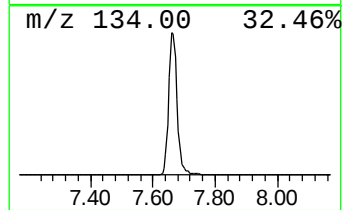
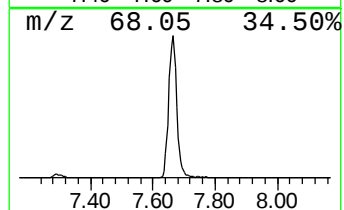
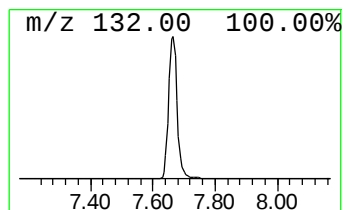
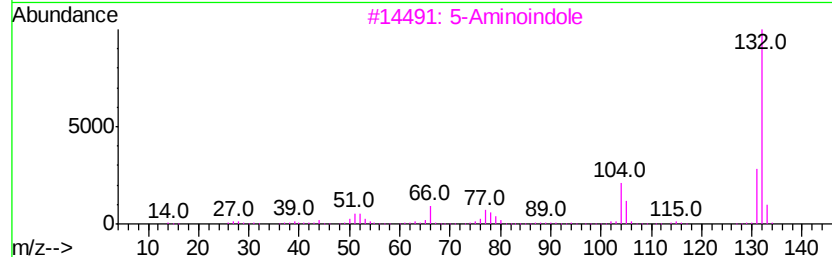
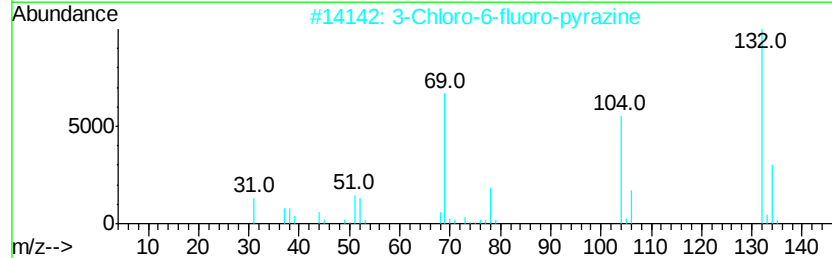
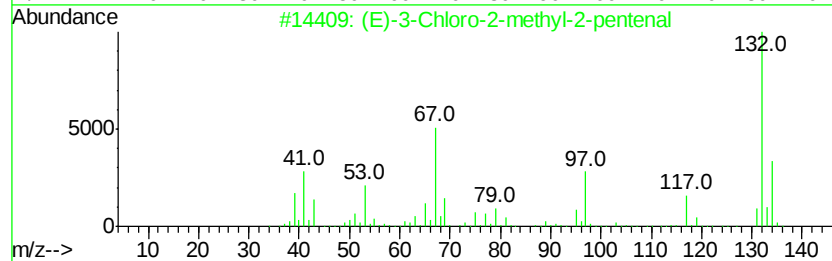
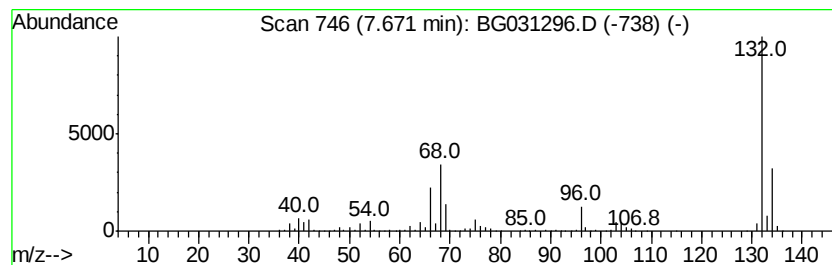
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Peak Number 2 unknown7.67 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.67	59.63 ng	1193490	1,4-Dichlorobenzene-d4	8.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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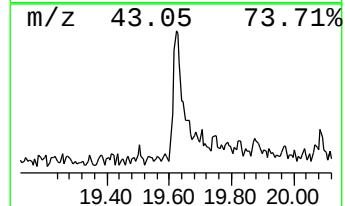
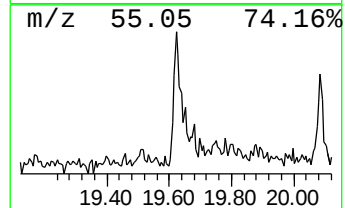
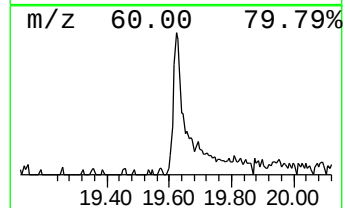
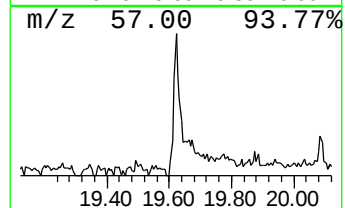
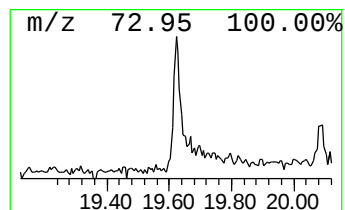
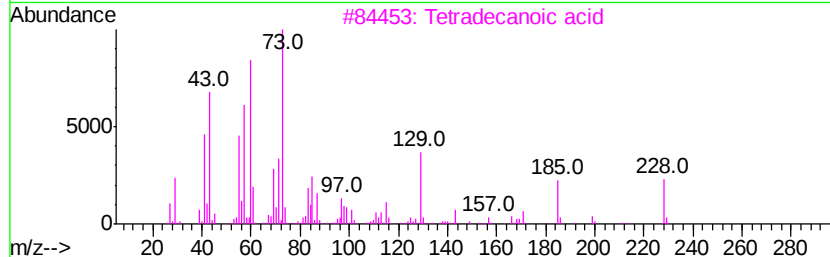
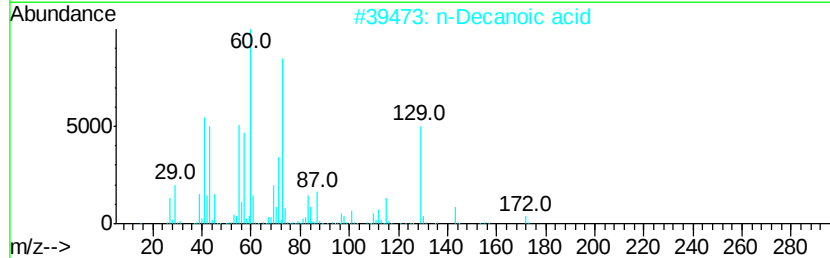
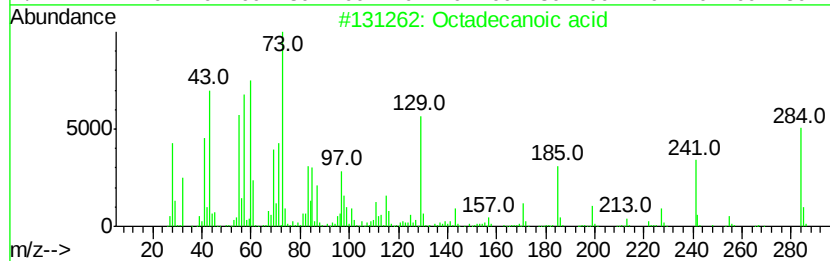
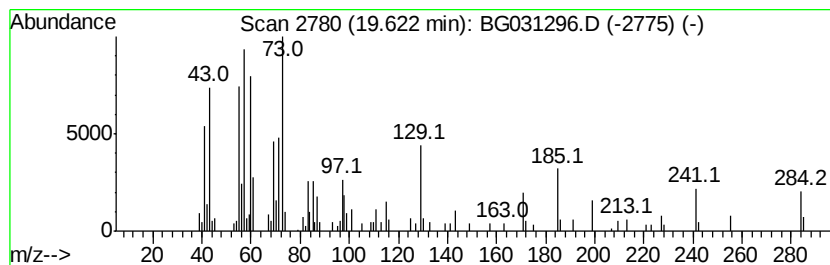
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Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.62	2.59 ng	151049	Phenanthrene-d10	17.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		n-Decanoic acid	172	C10H20O2	000334-48-5	87
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4		Tridecanoic acid	214	C13H26O2	000638-53-9	53
5		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	52



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.21	5.7	ng	113222	1	8.13	400319	20.0
unknown7.67	7.67	59.6	ng	1193490	1	8.13	400319	20.0
Octadecanoic acid	19.62	2.6	ng	151049	4	17.49	1167710	20.0