

Data Path : Z:\HPCHEM1\BNA G\DATA\BG042018\
 Data File : BG033898.D
 Acq On : 21 Apr 2018 00:04
 Operator : SJ/JU
 Sample : J2473-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 041818-DBRI-F-D-B

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-BG041918.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	4.992	284	290	296	rBV	71783	109471	1.62%	0.436%
2	5.439	359	366	375	rBV	514627	795560	11.79%	3.171%
3	6.996	621	631	641	rBV	330035	556653	8.25%	2.219%
4	7.366	686	694	703	rBV	861323	1437965	21.31%	5.731%
5	7.830	766	773	781	rBV	249871	426659	6.32%	1.700%
6	8.147	820	827	836	rVB	1000006	1766420	26.18%	7.040%
7	8.982	959	969	977	rBV	910622	1593037	23.61%	6.349%
8	10.615	1239	1247	1259	rVB	356360	615957	9.13%	2.455%
9	13.089	1660	1668	1675	rBV	2368083	3674863	54.46%	14.646%
10	14.464	1895	1902	1910	rVB2	555566	905299	13.42%	3.608%
11	15.950	2149	2155	2165	rBV2	1349864	2080113	30.83%	8.290%
12	17.213	2362	2370	2378	rBV	776821	1173131	17.39%	4.676%
13	18.130	2520	2526	2535	rBV2	75834	128708	1.91%	0.513%
14	19.417	2740	2745	2752	rBV2	51939	87465	1.30%	0.349%
15	19.857	2813	2820	2825	rBV	4994176	6747431	100.00%	26.892%
16	21.473	3088	3095	3102	rBV	970535	1469858	21.78%	5.858%
17	24.534	3605	3616	3630	rVB2	532417	1420918	21.06%	5.663%
18	29.975	4526	4542	4543	rBV9	31293	101044	1.50%	0.403%

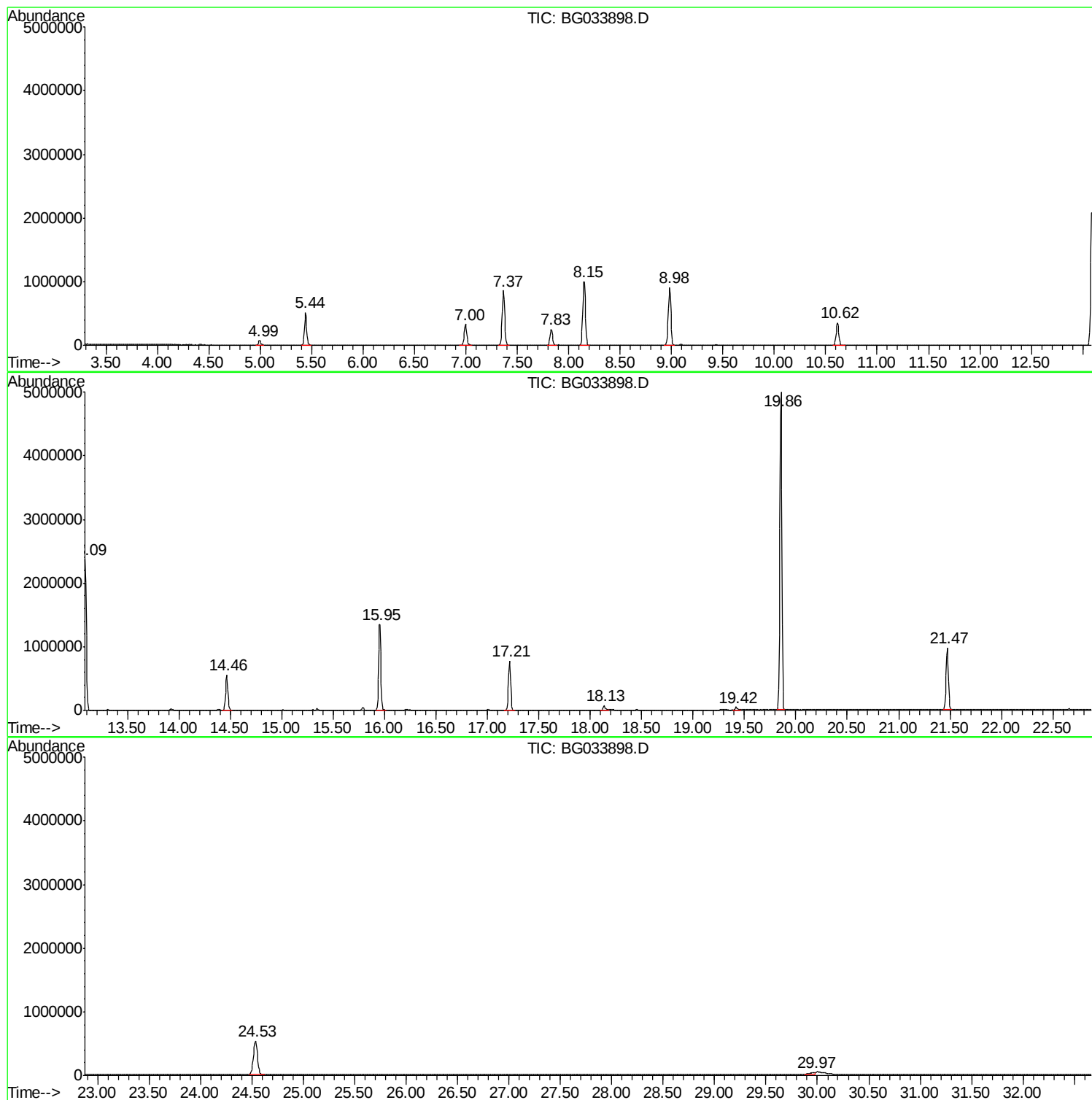
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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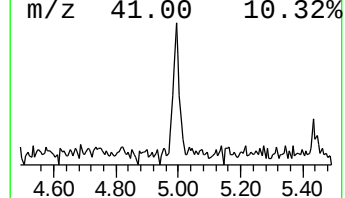
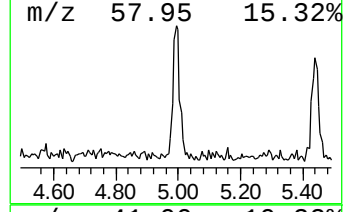
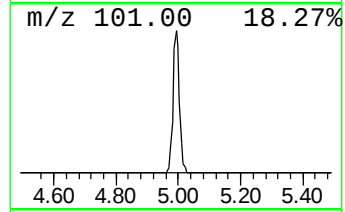
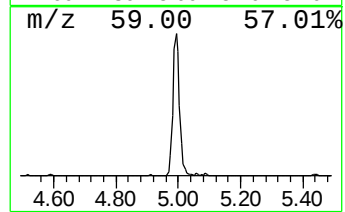
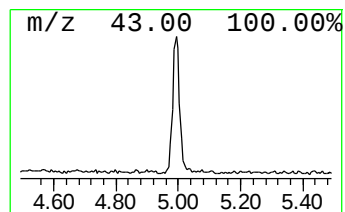
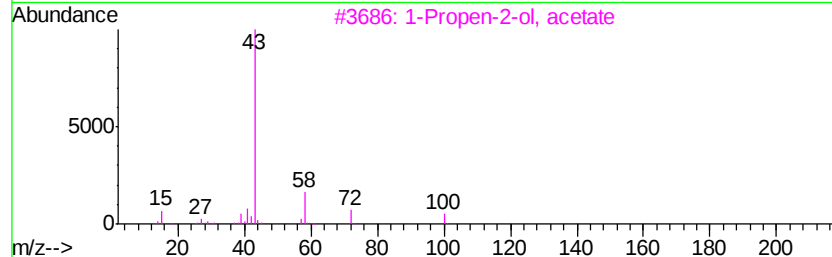
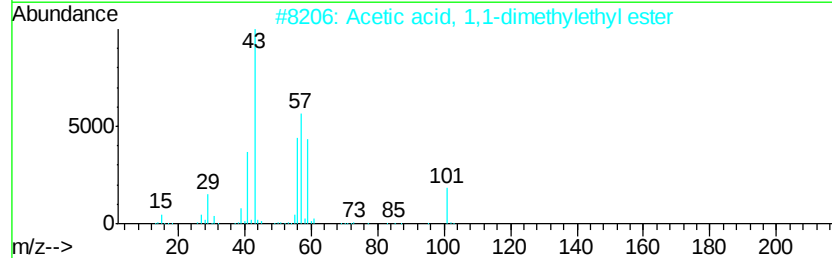
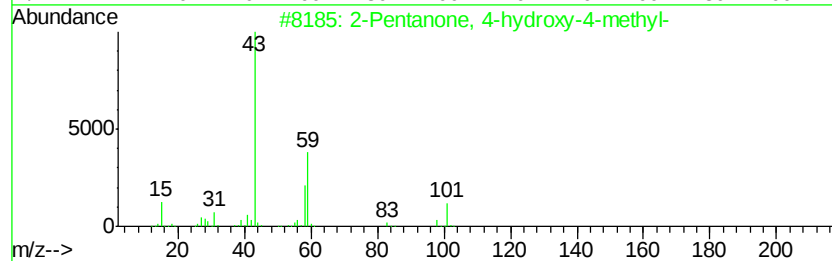
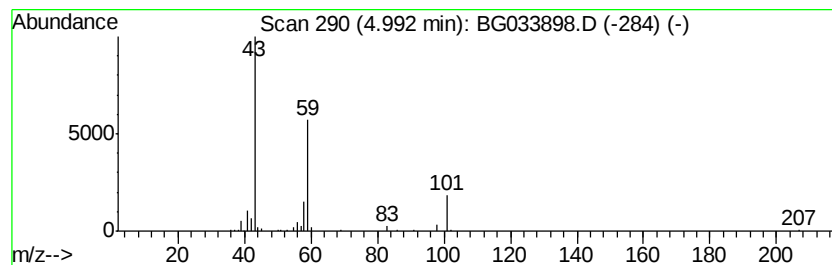
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.99	5.13 ng	109471	1,4-Dichlorobenzene-d4	7.83	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	2-Pentanone	86	C5H10O	000107-87-9	10
5	Glycine, N-(2-methoxyethoxycarbo...	235	C9H17NO6	1000328-06-4	9



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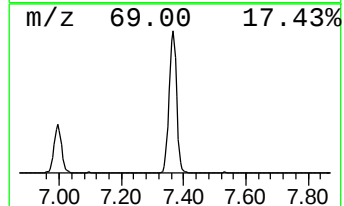
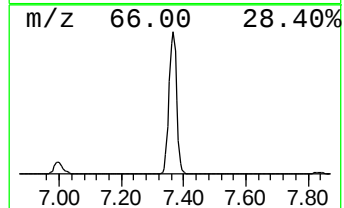
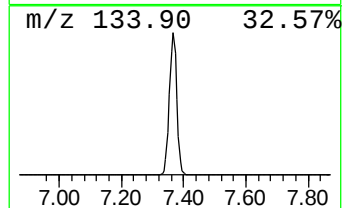
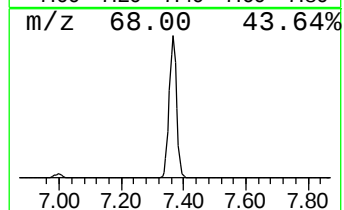
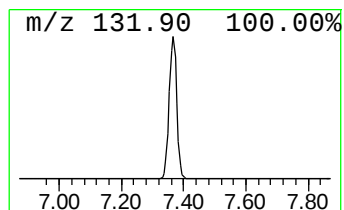
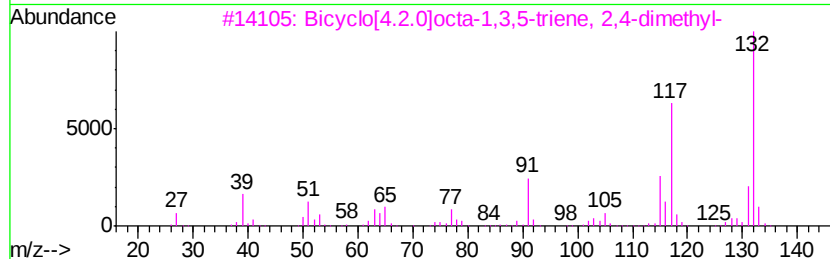
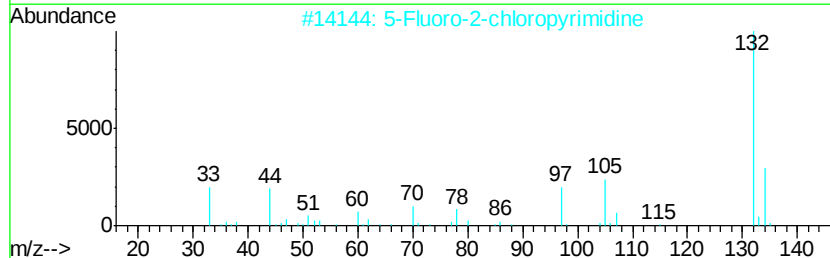
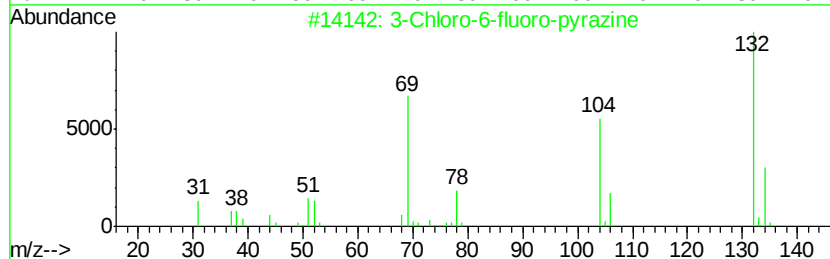
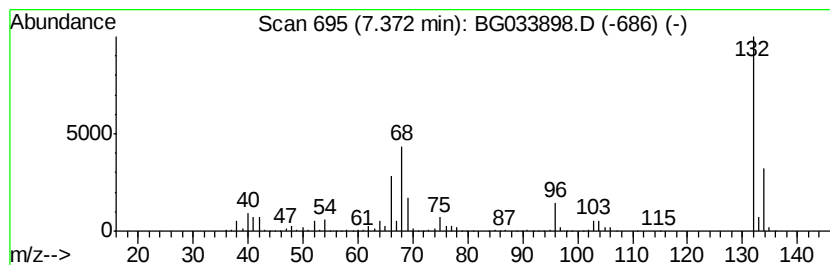
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Peak Number 2 unknown7.37 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.37	67.41 ng	1437970	1,4-Dichlorobenzene-d4	7.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



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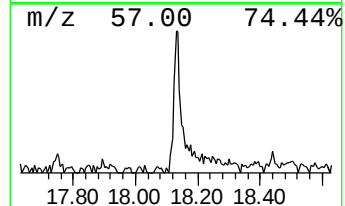
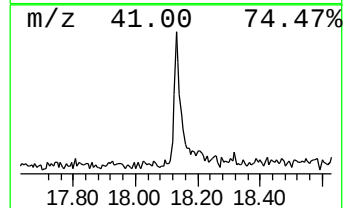
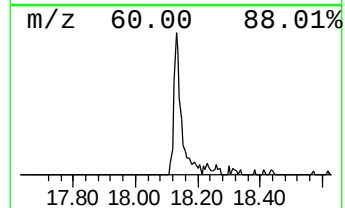
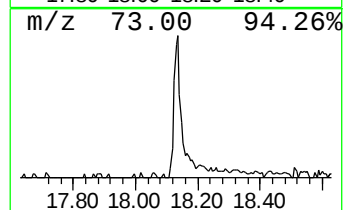
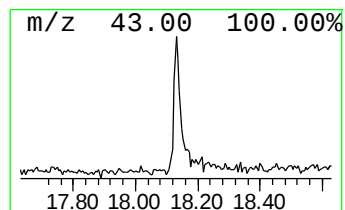
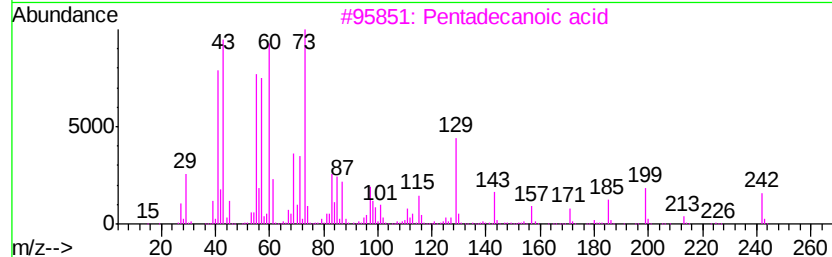
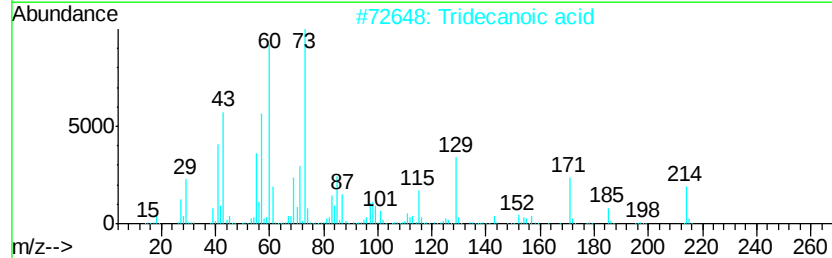
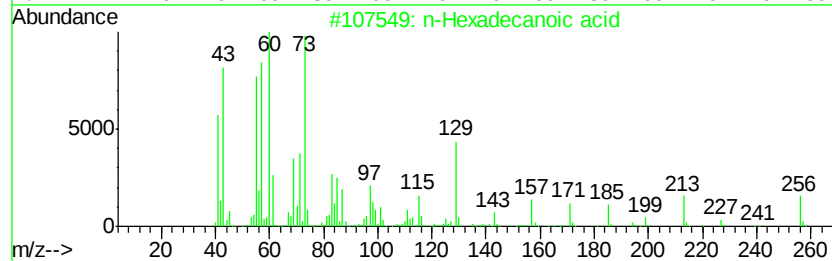
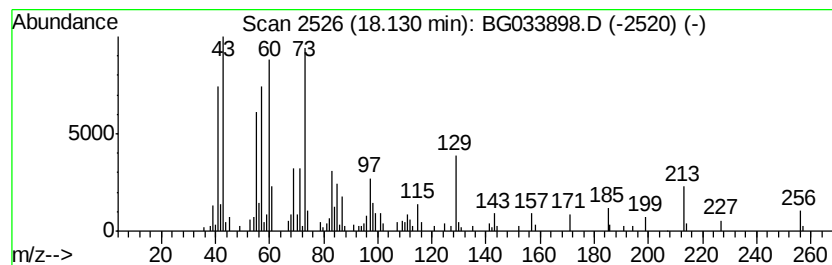
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.13	2.19 ng	128708	Phenanthrene-d10	17.21

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	81
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5		Undecanoic acid	186	C11H22O2	000112-37-8	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.99	5.1	ng	109471	1	7.83	426659	20.0
unknown7.37	7.37	67.4	ng	1437970	1	7.83	426659	20.0
n-Hexadecanoic acid	18.13	2.2	ng	128708	4	17.21	1173130	20.0