

Data Path : Z:\HPCHEM1\BNA G\DATA\BG062317\
 Data File : BG027649.D
 Acq On : 24 Jun 2017 3:09
 Operator : SJ/JU
 Sample : I3781-04
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-01-14.5-15.0

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-BG062117.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	5.639	291	298	310	rBV	63811	105717	4.20%	0.980%
2	6.085	367	374	387	rBV	449240	772974	30.70%	7.163%
3	7.642	631	639	652	rBV	469664	860738	34.19%	7.976%
4	8.036	697	706	716	rBV	453672	815180	32.38%	7.554%
5	8.506	778	786	792	rBV	64773	112267	4.46%	1.040%
6	8.829	834	841	851	rBB	301682	556188	22.09%	5.154%
7	9.669	976	984	992	rBV	261608	492454	19.56%	4.564%
8	11.320	1258	1265	1274	rVB	92717	173698	6.90%	1.610%
9	13.712	1664	1672	1683	rBV	812524	1265535	50.27%	11.728%
10	14.517	1803	1809	1815	rBV	120124	179220	7.12%	1.661%
11	15.087	1899	1906	1916	rBB2	162643	267773	10.64%	2.481%
12	16.573	2152	2159	2170	rBV	817955	1286658	51.11%	11.923%
13	17.836	2367	2374	2381	rBV	252689	394793	15.68%	3.658%
14	18.676	2512	2517	2529	rBV3	36203	62610	2.49%	0.580%
15	19.934	2726	2731	2737	rBV3	23330	36879	1.46%	0.342%
16	20.416	2806	2813	2822	rVB	1947384	2517623	100.00%	23.330%
17	22.208	3110	3118	3129	rVB	243304	463708	18.42%	4.297%
18	25.839	3722	3736	3748	rBV3	134810	427124	16.97%	3.958%

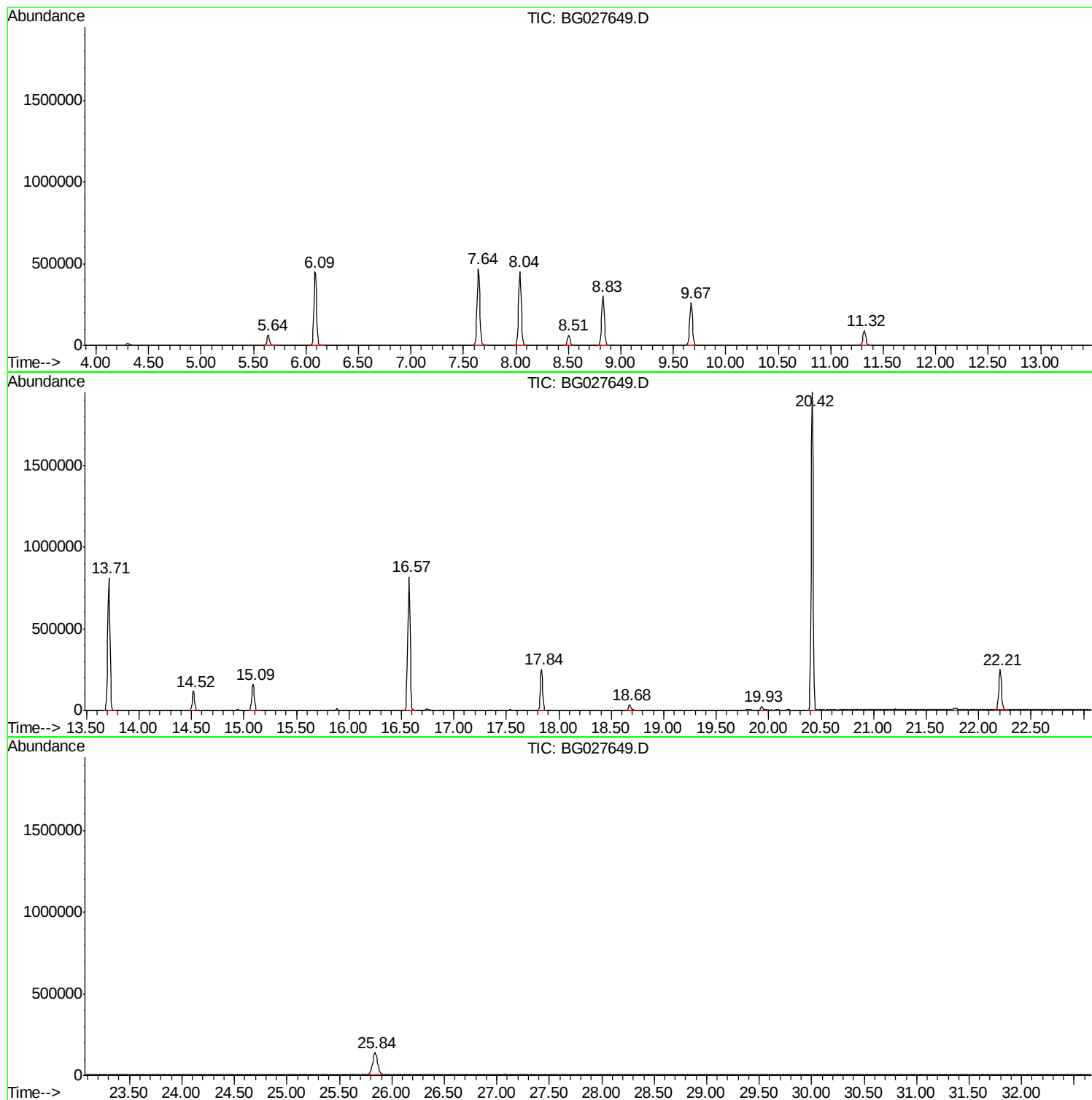
Sum of corrected areas: 10791139

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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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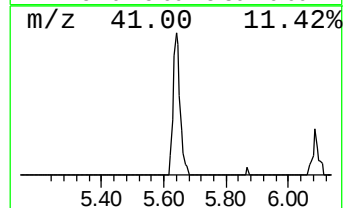
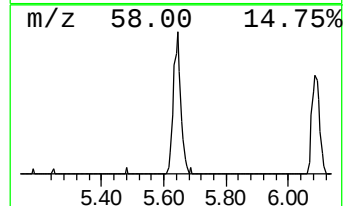
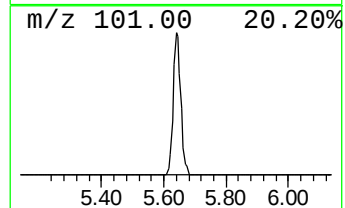
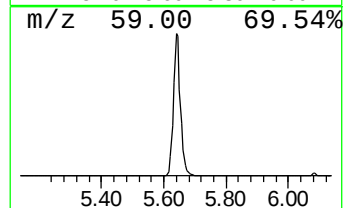
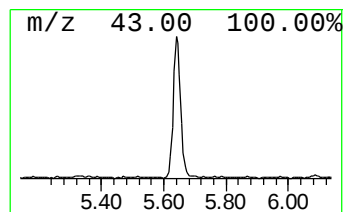
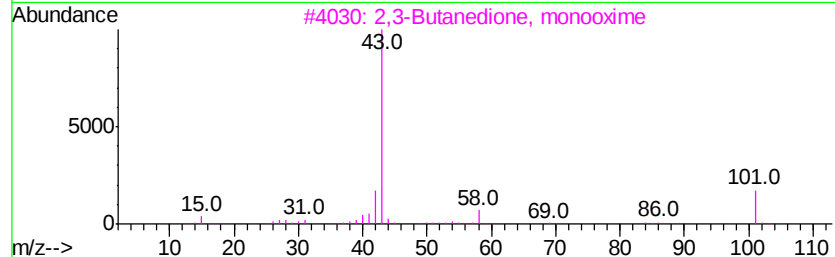
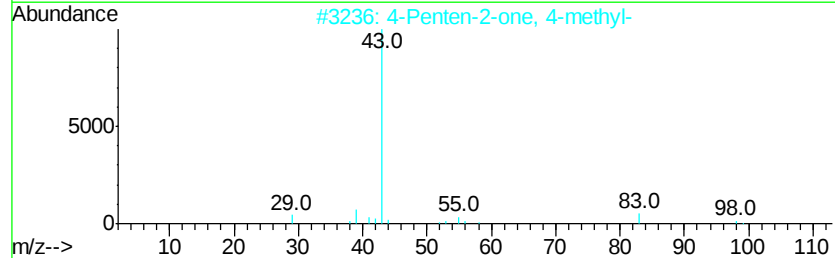
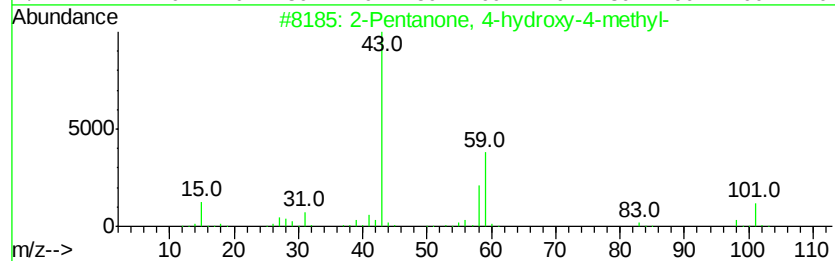
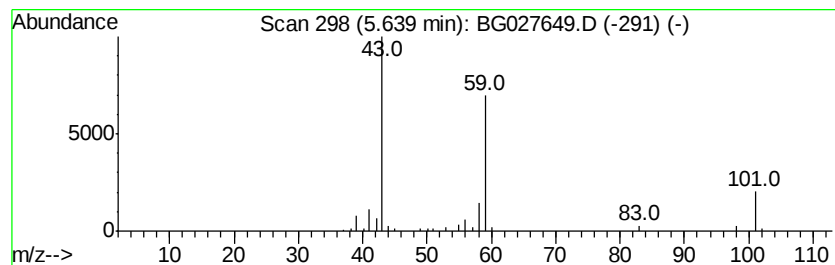
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.64	18.83 ng	105717	1,4-Dichlorobenzene-d4	8.51

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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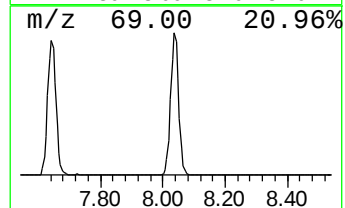
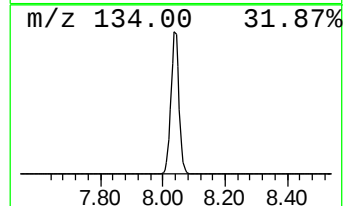
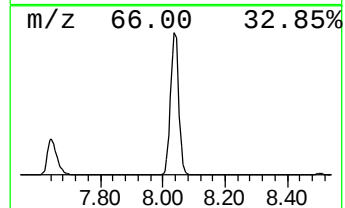
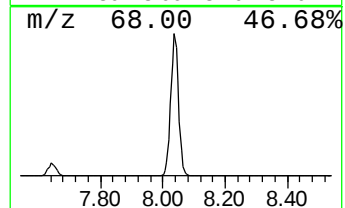
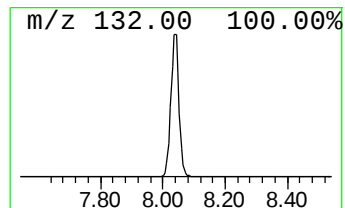
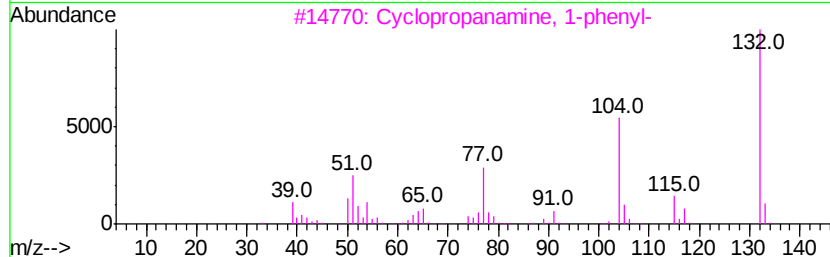
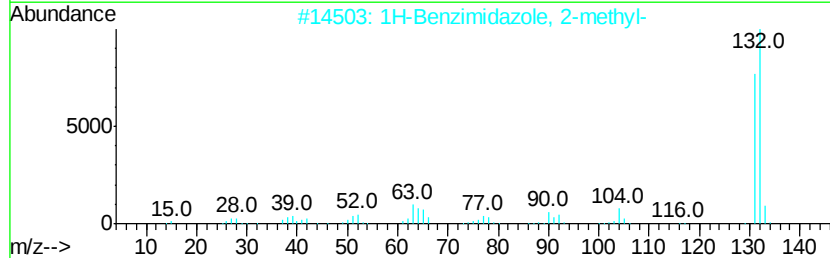
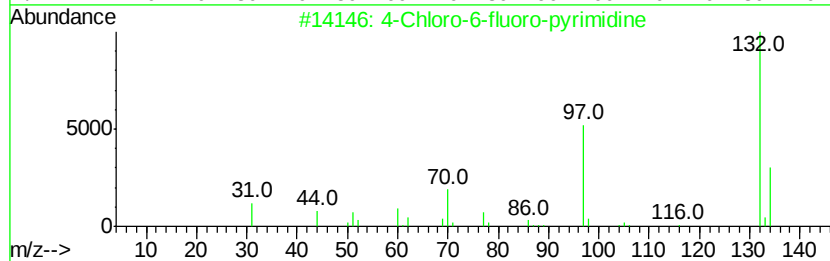
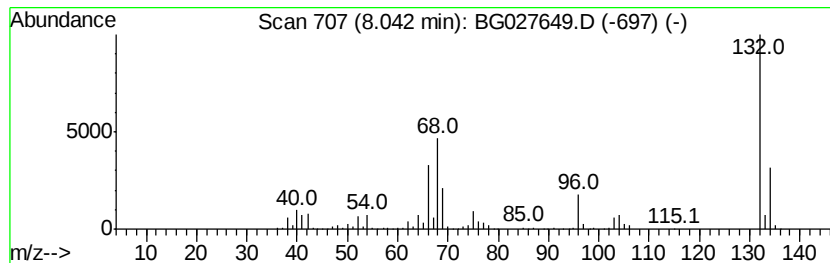
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Peak Number 2 unknown8.04 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.04	145.22 ng	815180	1,4-Dichlorobenzene-d4	8.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	22
4		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	22
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	16



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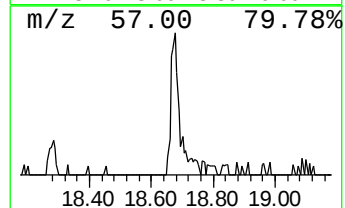
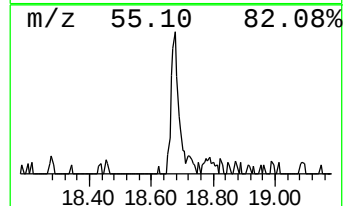
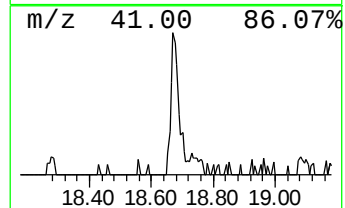
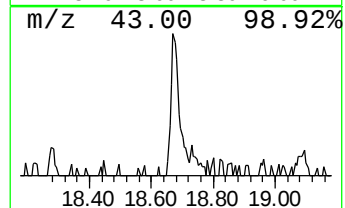
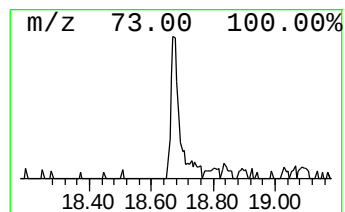
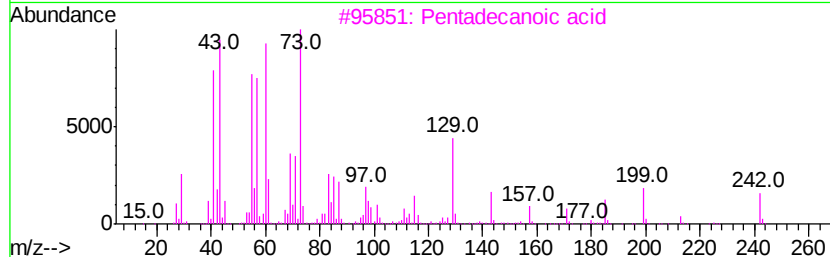
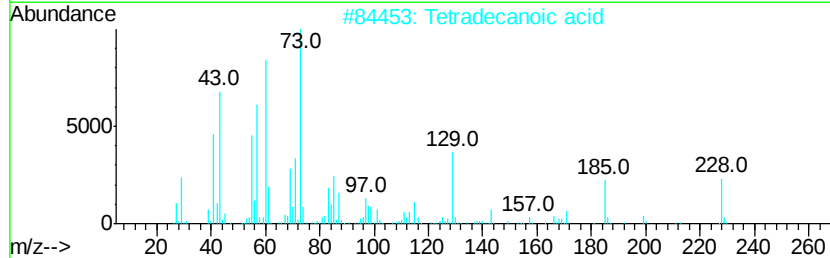
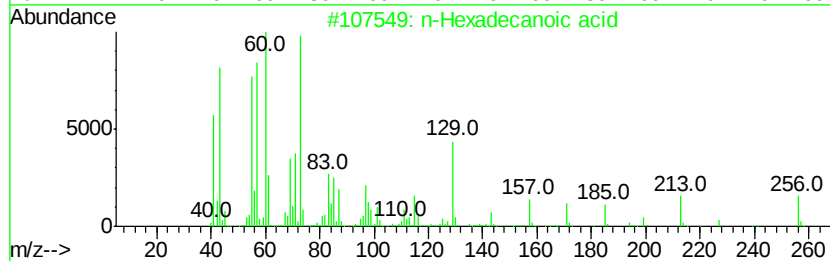
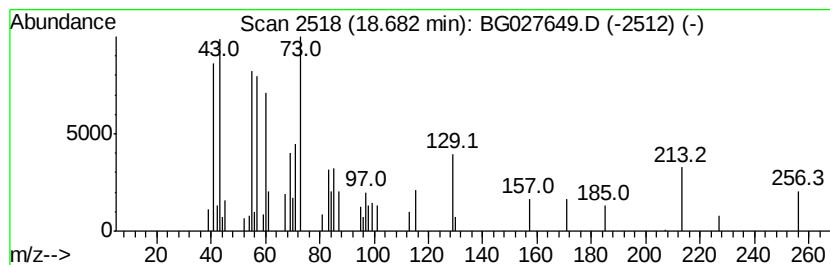
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.68	3.17 ng	62610	Phenanthrene-d10	17.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	64
5	Tridecanoic acid	214	C13H26O2	000638-53-9	62



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.64	18.8	ng	105717	1	8.51	112267	20.0
unknown8.04	8.04	145.2	ng	815180	1	8.51	112267	20.0
n-Hexadecanoic acid	18.68	3.2	ng	62610	4	17.84	394793	20.0