LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050617\
Data File : BF094965.D
Acq On : 8 May 2017 3:03
Operator : SJ/MA
Sample : I2947-15
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-05-4.0-4.5

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_F\METHODS\8270-BF050217.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	5.042	524	528	546	rBV	145928	308767	9.94%	1.220%
2	5.666	629	634	660	rBV	1768691	2698175	86.84%	10.661%
3	7.260	900	905	921	rBV	1772796	2670556	85.95%	10.552%
4	7.383	921	926	935	rVB	2129250	2825799	90.94%	11.165%
5	7.719	979	983	994	rVB	418039	497365	16.01%	1.965%
6	7.960	1019	1024	1037	rBV	1766604	2107180	67.82%	8.326%
7	8.619	1131	1136	1157	rBV	1155632	1599619	51.48%	6.320%
8	9.742	1322	1327	1348	rBV	502876	710898	22.88%	2.809%
9	11.513	1623	1628	1649	rBV	2327764	3107200	100.00%	12.277%
10	12.207	1741	1746	1757	rBV	313845	409796	13.19%	1.619%
11	12.571	1803	1808	1828	rBV2	587147	831989	26.78%	3.287%
12	13.413	1947	1951	1956	rBV	37124	39706	1.28%	0.157%
13	13.865	2023	2028	2042	rBV	1231475	1843945	59.34%	7.286%
14	14.183	2078	2082	2086	rBV	30232	38030	1.22%	0.150%
15	14.971	2211	2216	2232	rBV2	535556	765096	24.62%	3.023%
16	15.936	2375	2380	2391	rBV	80177	119093	3.83%	0.471%
17	16.765	2518	2521	2532	rBB	26841	33784	1.09%	0.133%
18	17.065	2569	2572	2579	rVV	30381	44578	1.43%	0.176%
19	17.142	2581	2585	2589	rVB	55731	52615	1.69%	0.208%
20	17.301	2606	2612	2615	rBV	2385092	2859238	92.02%	11.297%
21	18.065	2738	2742	2746	rBV	35776	35177	1.13%	0.139%
22	18.595	2820	2832	2835	rBV6	35530	105956	3.41%	0.419%
23	18.636	2835	2839	2856	rVB	633923	870518	28.02%	3.440%
24	19.912	3053	3056	3068	rVB	23713	51711	1.66%	0.204%
25	20.300	3118	3122	3135	rBV	429217	611454	19.68%	2.416%
26	20.771	3196	3202	3210	rBV2	21530	36568	1.18%	0.144%
27	21.200	3269	3275	3284	rBV7	16674	33903	1.09%	0.134%

Sum of corrected areas: 25308716

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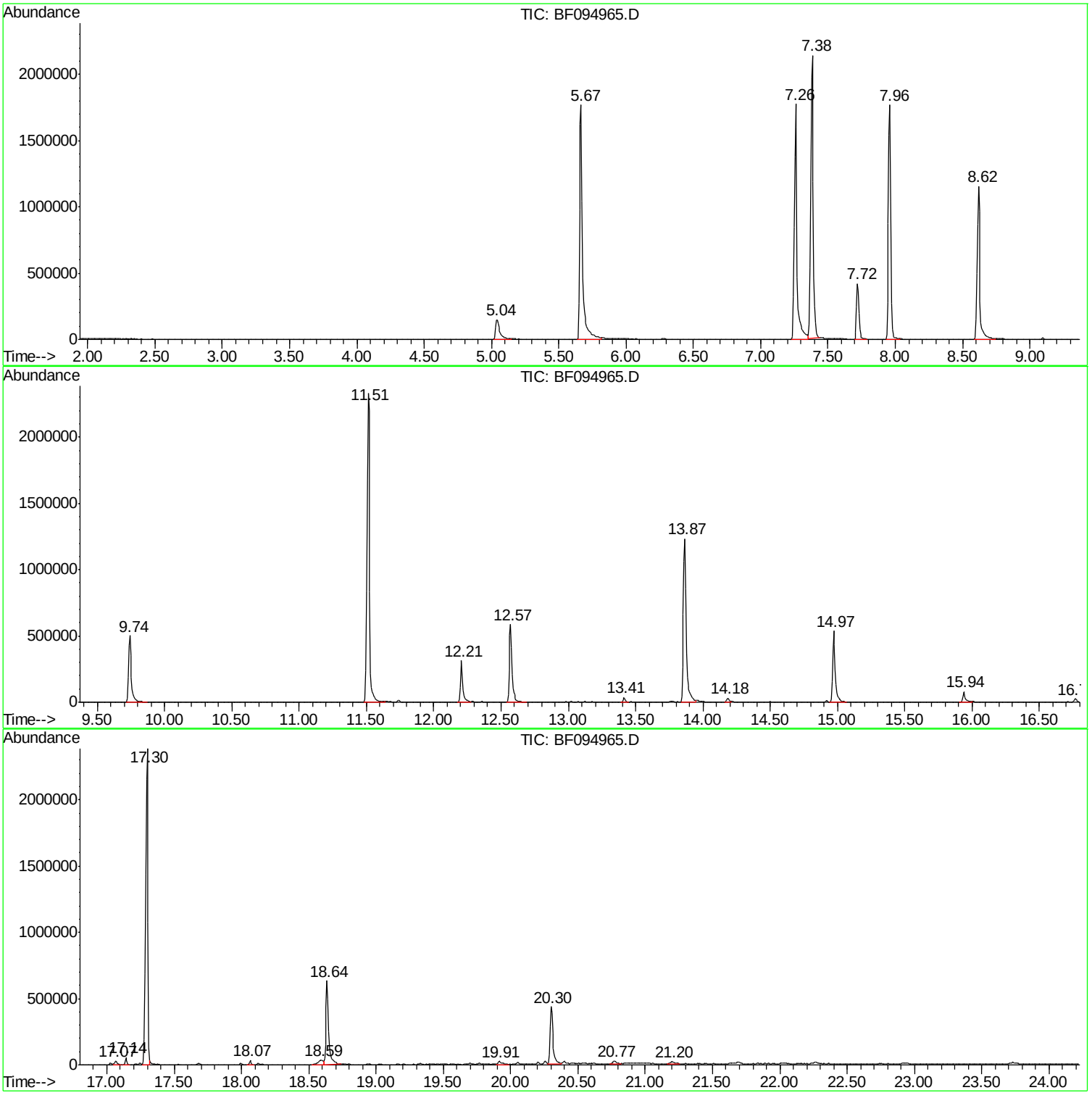
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050617\
Data File : BF094965.D
Acq On : 8 May 2017 3:03
Operator : SJ/MA
Sample : I2947-15
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-05-4.0-4.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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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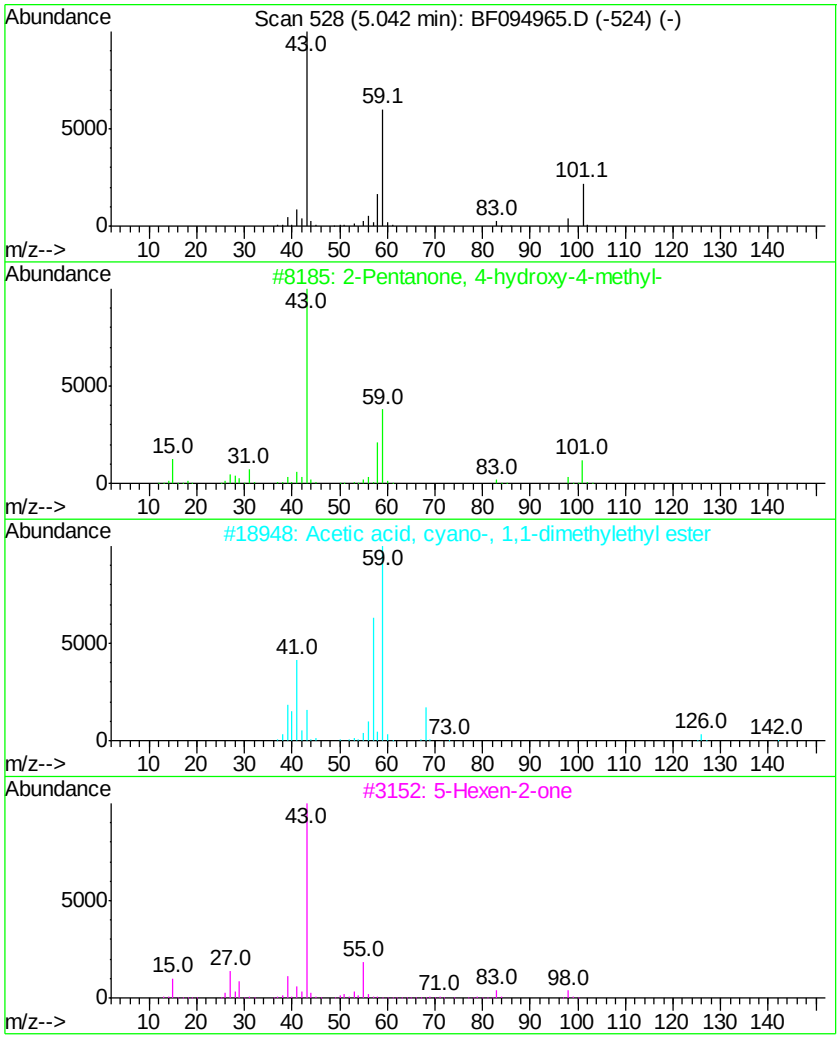
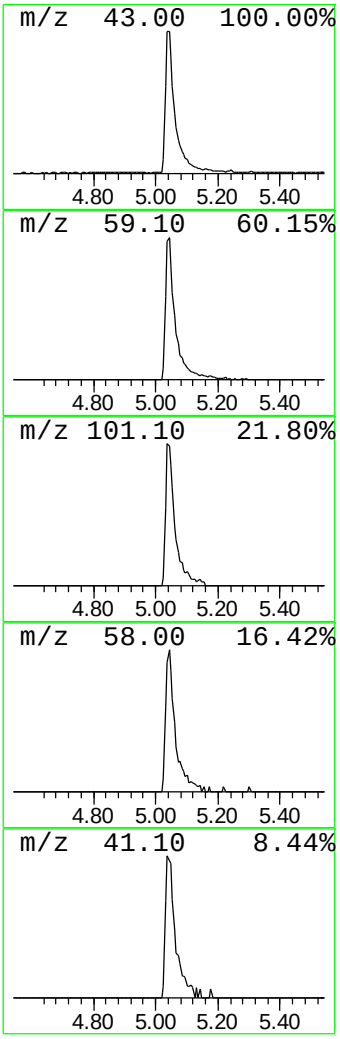
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	12.42 ng	308767	1,4-Dichlorobenzene-d4	7.72

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	9
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9





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ClientSampleId : SB-05-4.0-4.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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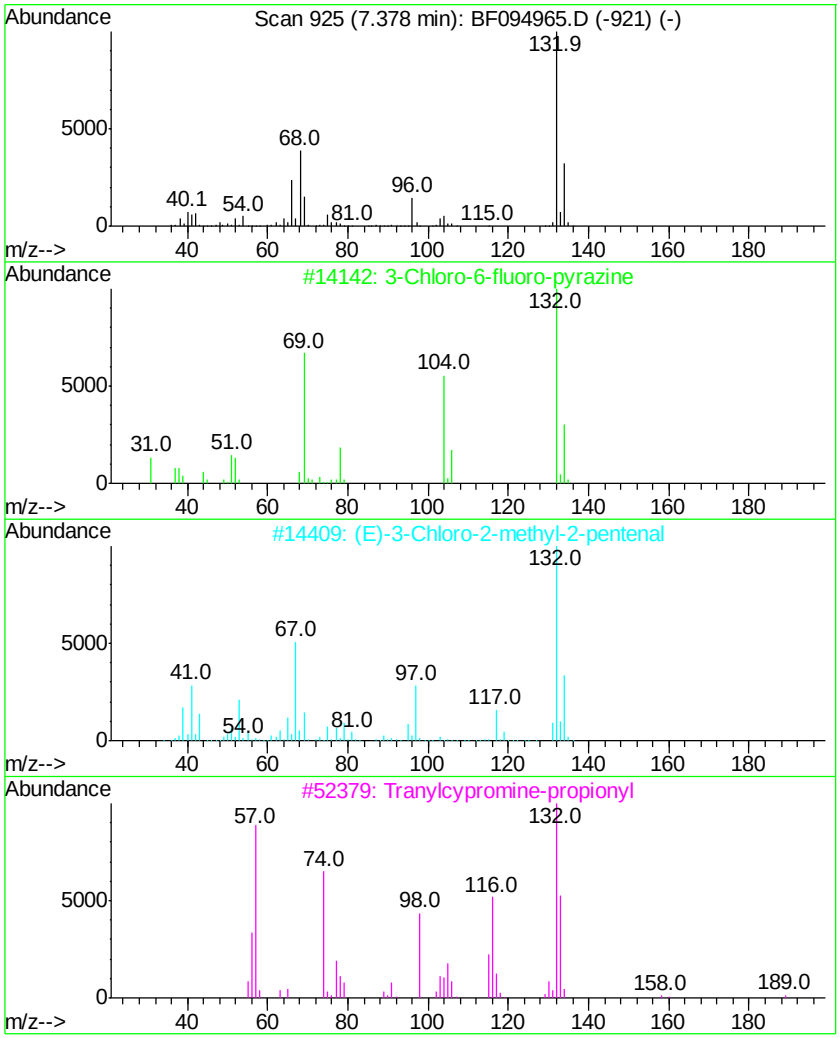
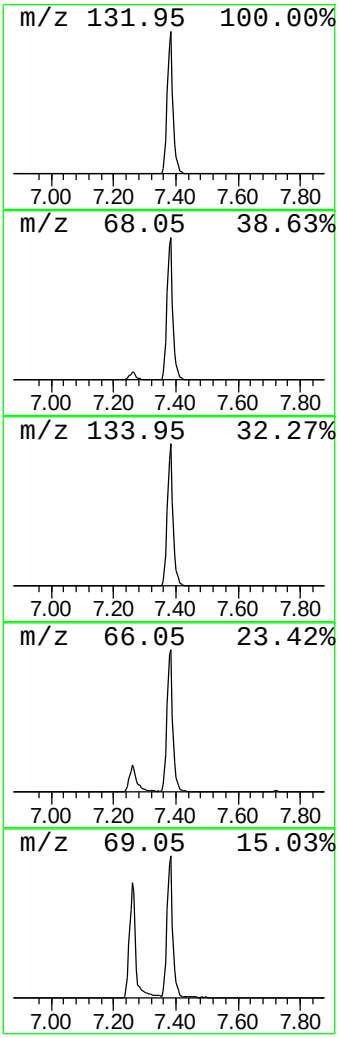
Peak Number 2 unknown7.38 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.38	113.63 ng	2825800	1,4-Dichlorobenzene-d4	7.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10





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Instrument : BNA_F
ClientSampleId : SB-05-4.0-4.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
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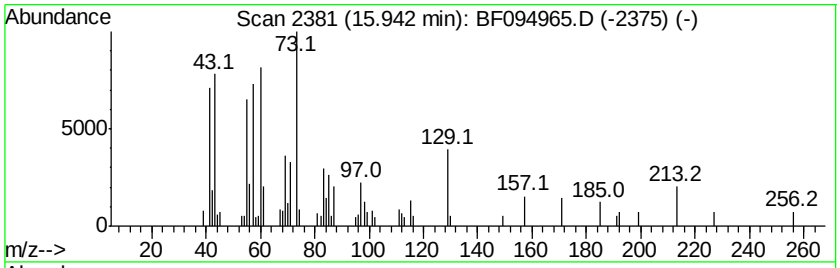
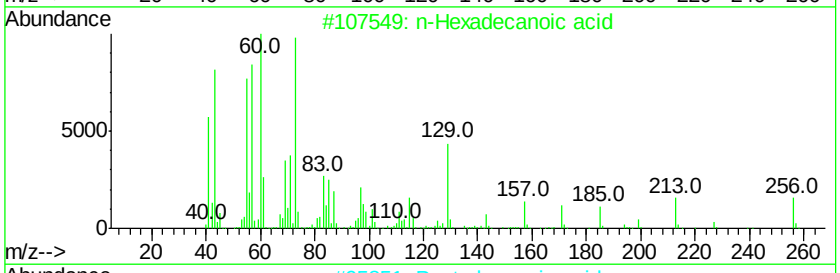
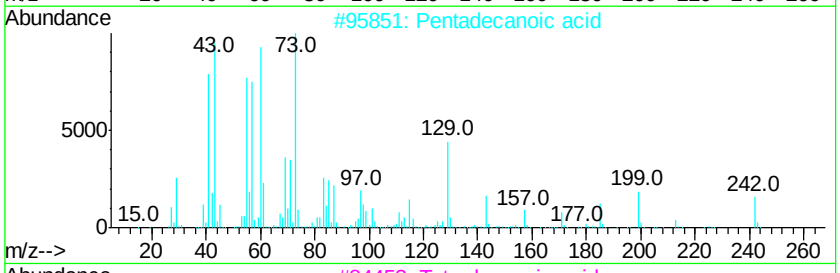
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

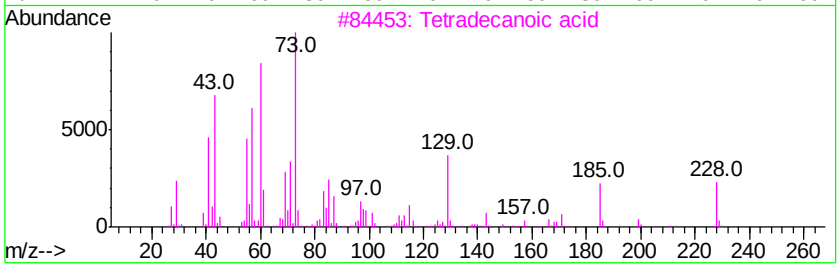
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	3.11 ng	119093	Phenanthrene-d10	14.97

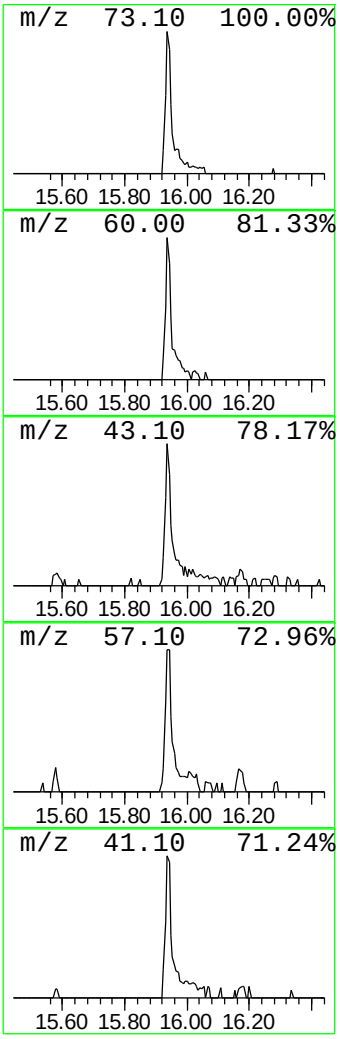
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	80
5	Dodecanoic acid	200	C12H24O2	000143-07-7	72











Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.04	12.4	ng	308767	1	7.72	497365	20.0
unknown7.38	7.38	113.6	ng	2825800	1	7.72	497365	20.0
n-Hexadecanoic acid	15.94	3.1	ng	119093	4	14.97	765096	20.0