

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM081518\
Data File : BM016405.D
Acq On : 16 Aug 2018 07:25
Operator : SJ/JU
Sample : J4462-02
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
081318-TIPC-F-D-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:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.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	5.645	396	401	413	rBV	131737	220655	12.39%	2.997%
2	7.281	675	679	698	rBB2	68143	128186	7.20%	1.741%
3	7.634	734	739	751	rBV	299453	499906	28.07%	6.789%
4	8.104	814	819	829	rBB	98305	162011	9.10%	2.200%
5	8.428	868	874	885	rBB	500521	798583	44.85%	10.845%
6	9.292	1015	1021	1033	rBV	324815	550680	30.92%	7.479%
7	10.922	1292	1298	1307	rBV	103497	176205	9.90%	2.393%
8	13.363	1707	1713	1725	rBV	839858	1159410	65.11%	15.746%
9	14.745	1941	1948	1955	rBB2	131741	203145	11.41%	2.759%
10	16.015	2160	2164	2169	rBB	35762	43034	2.42%	0.584%
11	16.233	2196	2201	2214	rBB	438449	613284	34.44%	8.329%
12	17.480	2408	2413	2426	rBB	178594	251508	14.12%	3.416%
13	18.327	2552	2557	2565	rBV2	34445	50594	2.84%	0.687%
14	19.586	2766	2771	2778	rBV2	20290	29741	1.67%	0.404%
15	20.062	2847	2852	2857	rBV	1640812	1780700	100.00%	24.183%
16	21.615	3111	3116	3122	rBV	285189	351844	19.76%	4.778%
17	23.938	3505	3511	3518	rBV	171188	343829	19.31%	4.669%

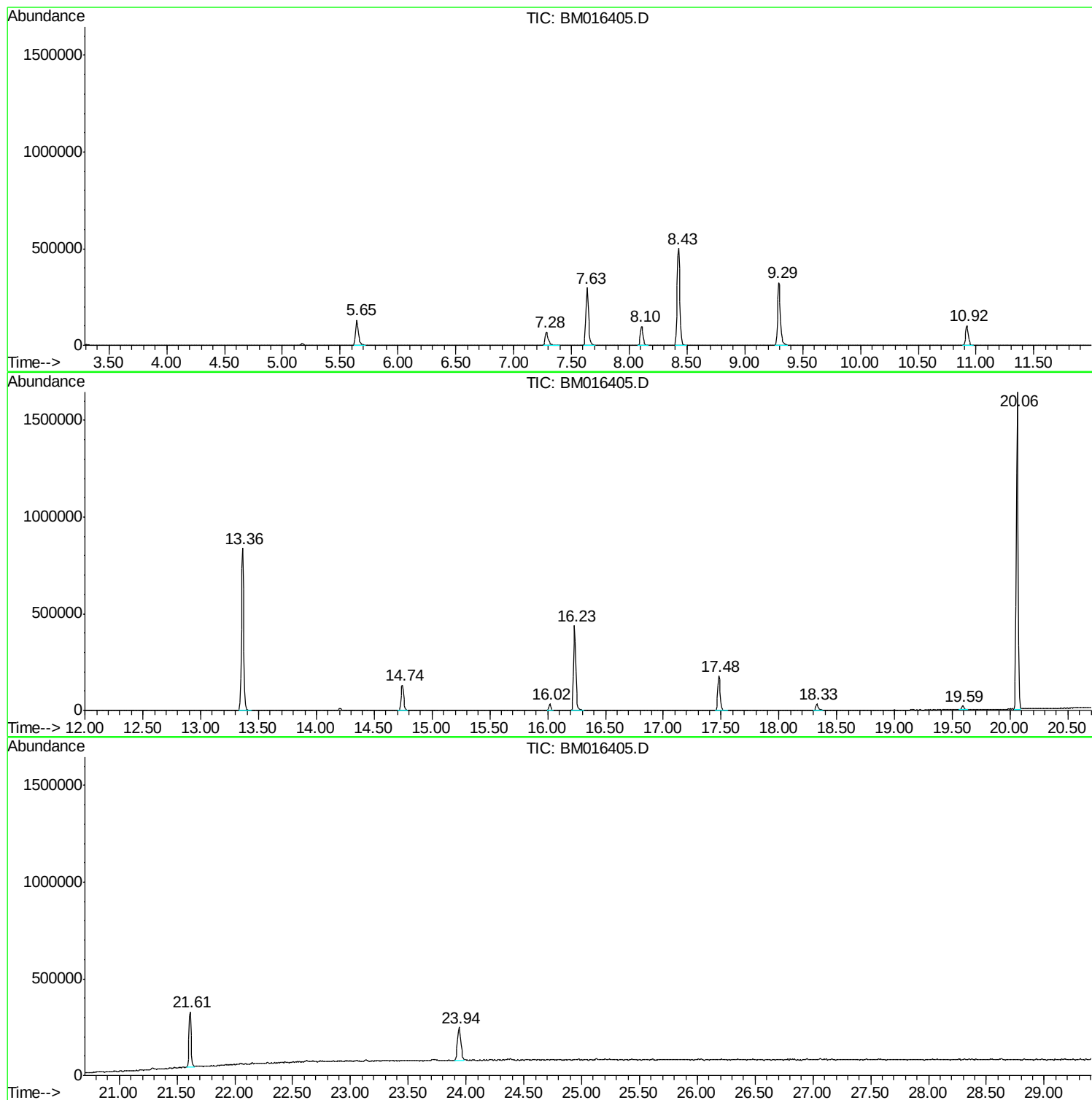
Sum of corrected areas: 7363315

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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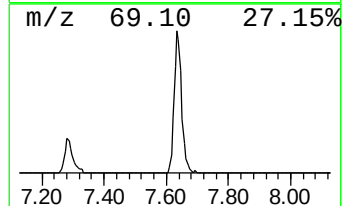
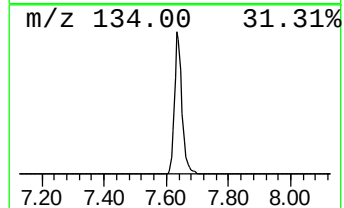
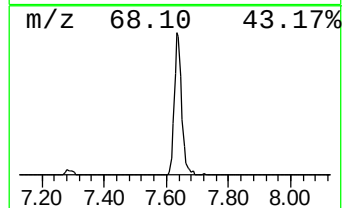
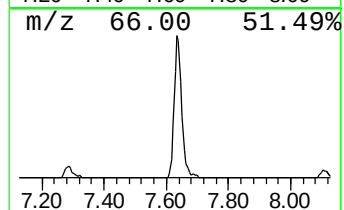
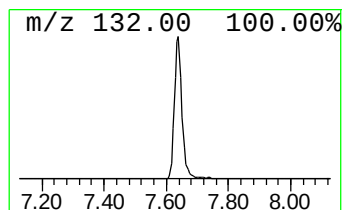
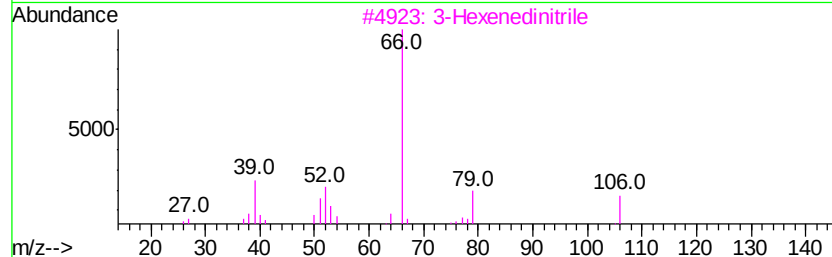
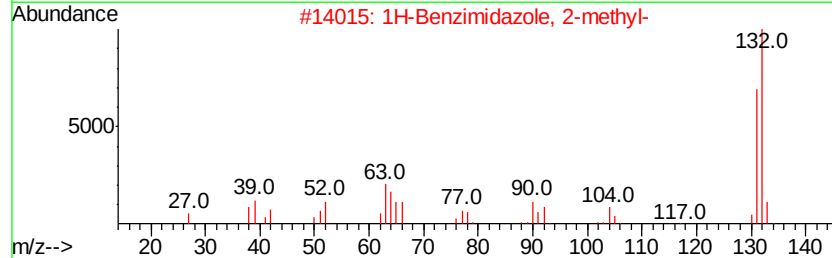
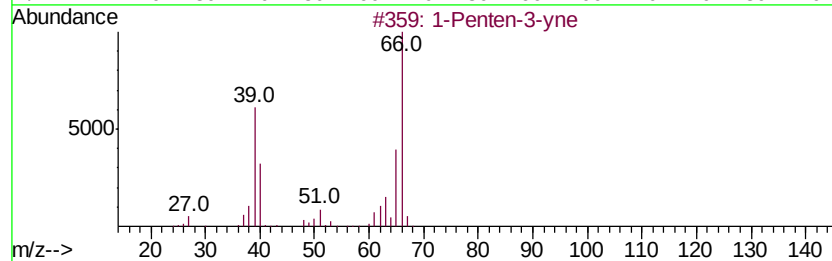
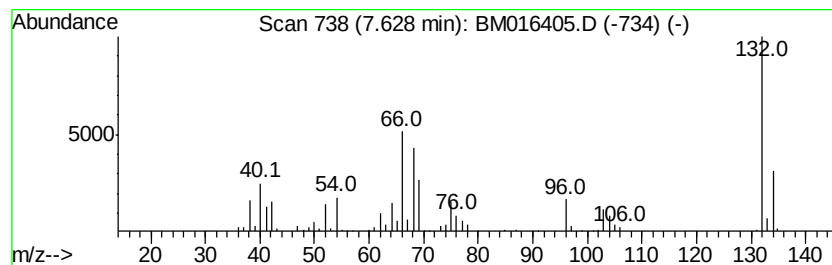
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown7.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.63	61.71 ng	499906	1,4-Dichlorobenzene-d4	8.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Penten-3-yne	66	C5H6	000646-05-9	27
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3		3-Hexenedinitrile	106	C6H6N2	001119-85-3	16
4		3-Penten-1-yne, (E)-	66	C5H6	002004-69-5	16
5		3-Penten-1-yne, (Z)-	66	C5H6	001574-40-9	16



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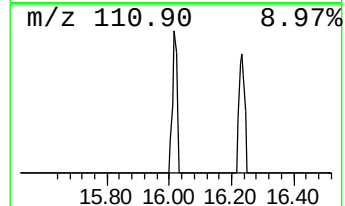
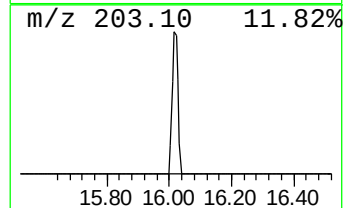
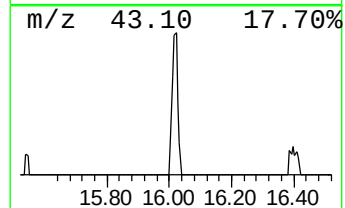
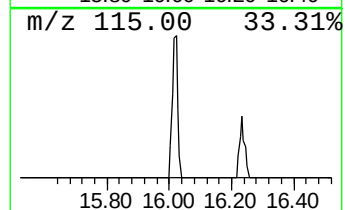
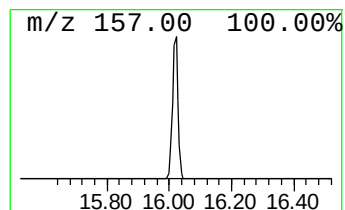
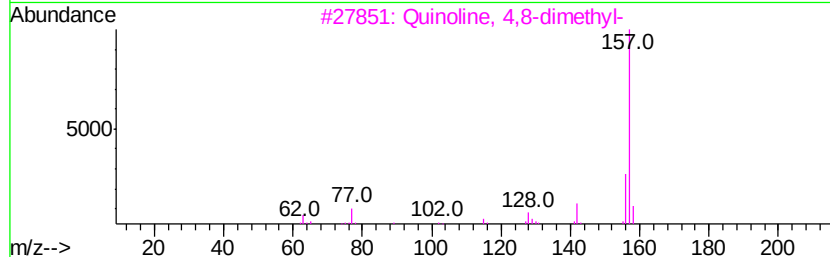
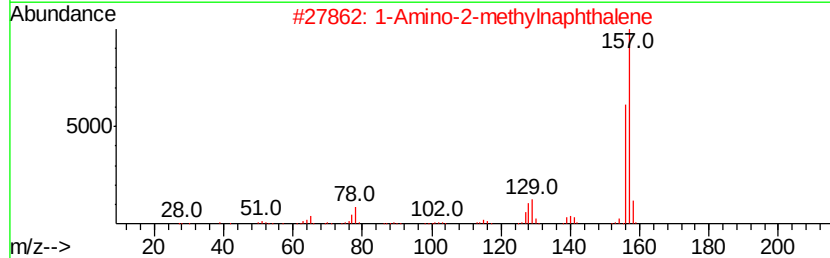
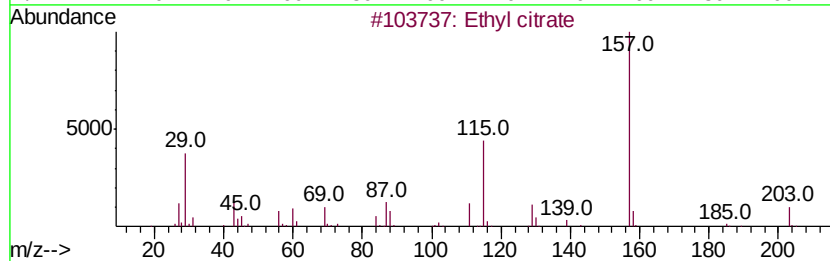
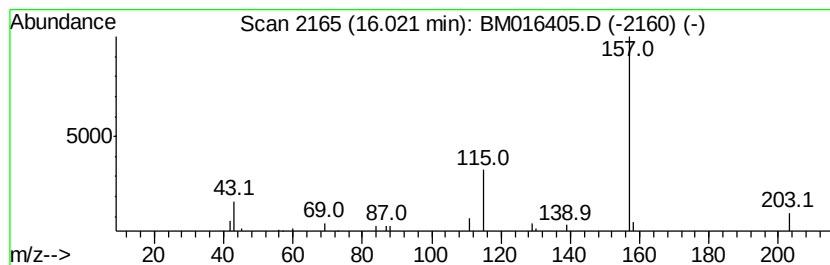
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Peak Number 3 Ethyl citrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.02	4.24 ng	43034	Acenaphthene-d10	14.74
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Ethyl citrate	276 C12H20O7	000077-93-0 83
2		1-Amino-2-methylnaphthalene	157 C11H11N	002246-44-8 50
3		Quinoline, 4,8-dimethyl-	157 C11H11N	013362-80-6 40
4		Pyrimidine, 2-methylthio-4-hydro...	157 C5H7N3OS	001074-41-5 38
5		1,4-Dioxaspiro[4.4]nonane, 7,8-b...	188 C9H16O4	1000155-54-9 33



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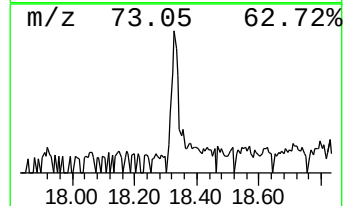
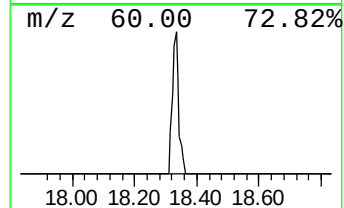
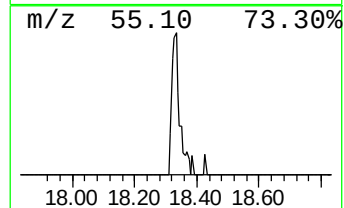
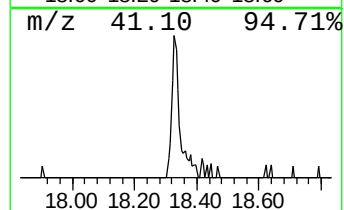
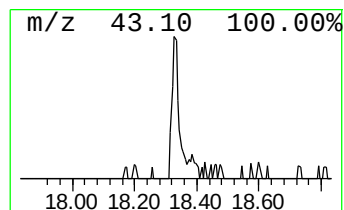
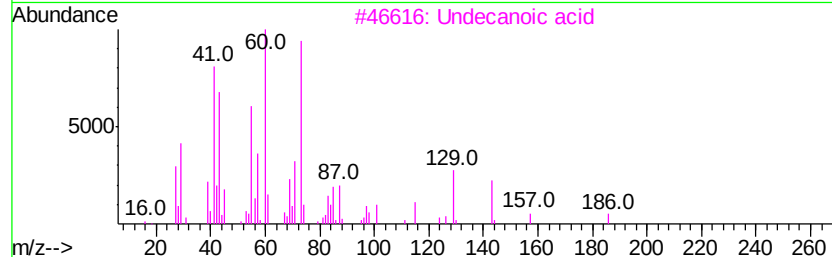
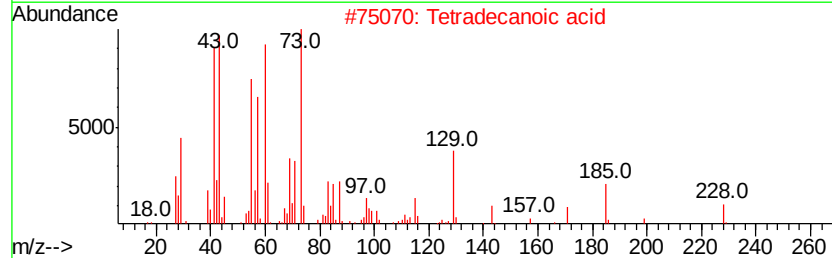
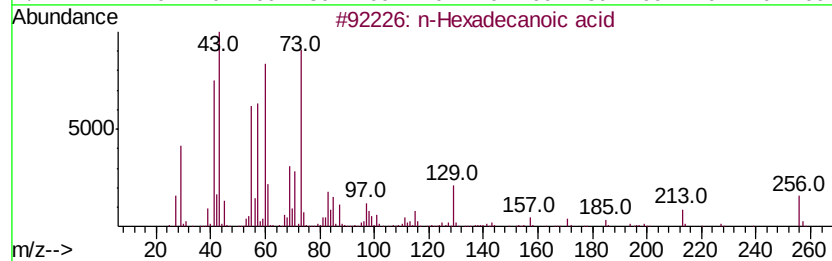
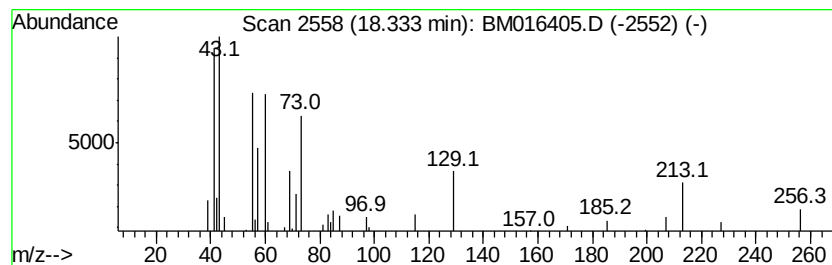
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.33	4.02 ng	50594	Phenanthrene-d10	17.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	50
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	49
3	Undecanoic acid	186	C11H22O2	000112-37-8	35
4	n-Decanoic acid	172	C10H20O2	000334-48-5	27
5	Dodecanoic acid	200	C12H24O2	000143-07-7	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown7.63	7.63	61.7	ng	499906	1	8.10	162011	20.0
Ethyl citrate	16.02	4.2	ng	43034	3	14.74	203145	20.0
n-Hexadecanoic acid	18.33	4.0	ng	50594	4	17.48	251508	20.0