

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032423\
 Data File : BM039140.D
 Acq On : 24 Mar 2023 14:00
 Operator : CG/JU
 Sample : PB151460BL
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PB151460BL

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-BM030823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039140.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.428	189	194	205	rVB	234320	327121	1.71%	0.370%
2	5.040	292	298	306	rBV	2368462	3204242	16.72%	3.621%
3	5.510	371	378	393	rBV	5743420	8141254	42.48%	9.201%
4	7.122	644	652	666	rBV	5501313	8577508	44.75%	9.694%
5	7.951	786	793	802	rVB	942366	1467774	7.66%	1.659%
6	9.122	983	992	1004	rBV	3325886	5399837	28.17%	6.103%
7	10.763	1261	1271	1280	rBV	1293436	2168909	11.32%	2.451%
8	13.221	1682	1689	1703	rBV	8817326	12795161	66.76%	14.461%
9	14.598	1915	1923	1936	rBV	2039219	3056949	15.95%	3.455%
10	16.086	2168	2176	2199	rBV	7287843	10489186	54.73%	11.855%
11	17.339	2383	2389	2400	rBV	2754477	3805774	19.86%	4.301%
12	18.233	2536	2541	2551	rBV	230446	438162	2.29%	0.495%
13	19.509	2754	2758	2769	rBV2	144133	289647	1.51%	0.327%
14	19.656	2779	2783	2788	rBV	214916	240696	1.26%	0.272%
15	19.962	2829	2835	2840	rBV	14995905	19166844	100.00%	21.662%
16	20.697	2957	2960	2966	rBV	312265	353472	1.84%	0.399%
17	21.521	3095	3100	3106	rBV	3286262	4228093	22.06%	4.779%
18	23.950	3506	3513	3524	rVB2	2102377	4329418	22.59%	4.893%

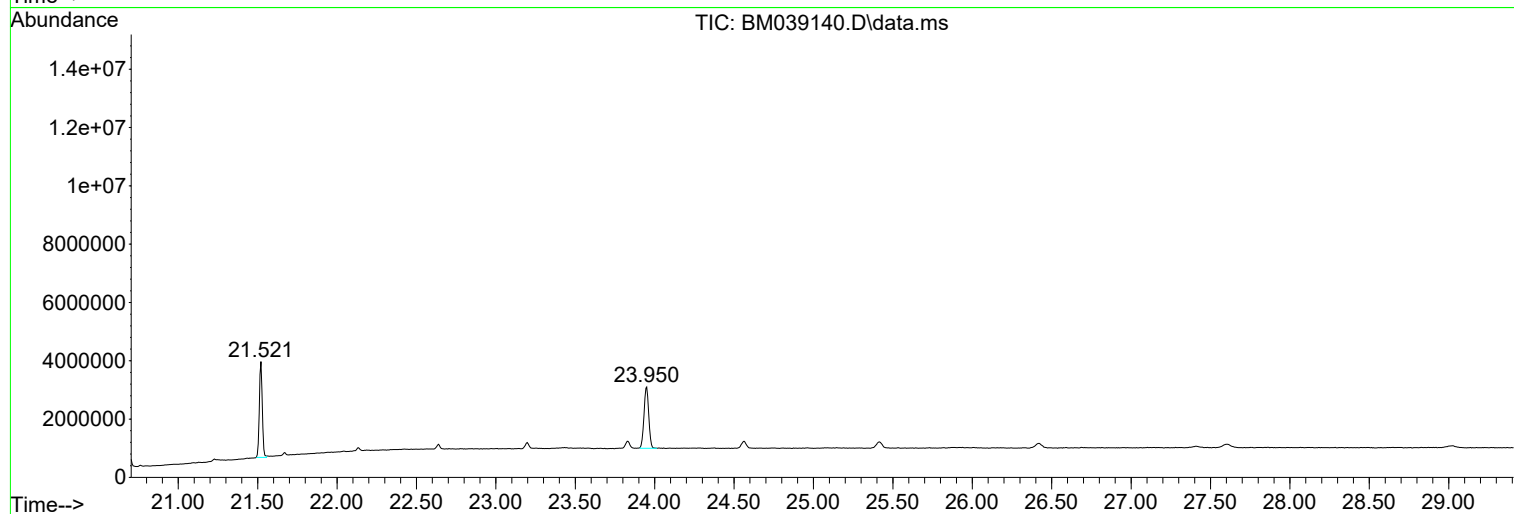
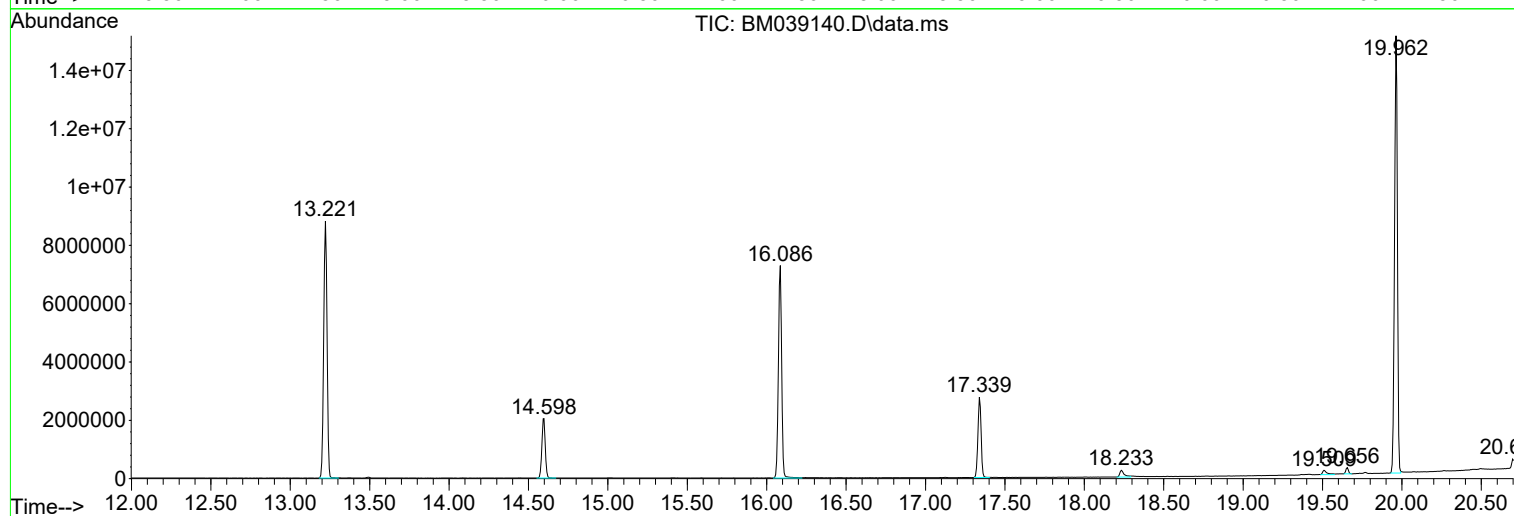
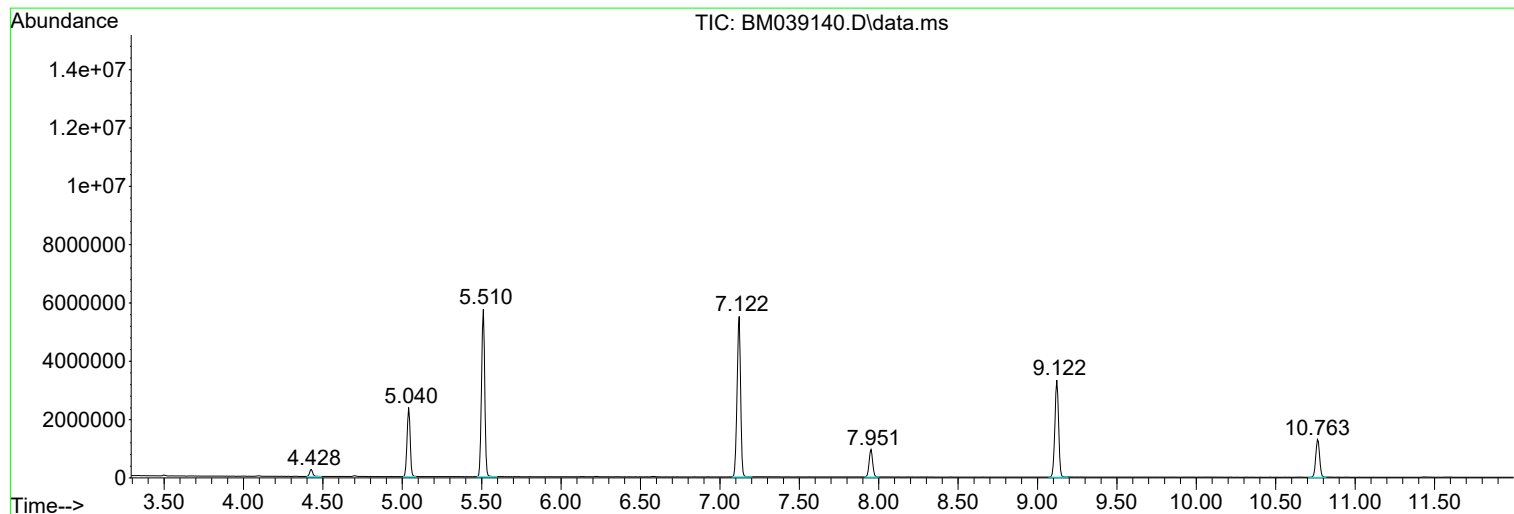
Sum of corrected areas: 88480047

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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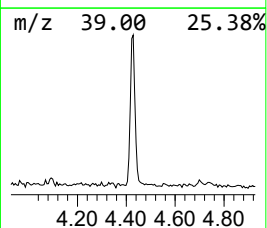
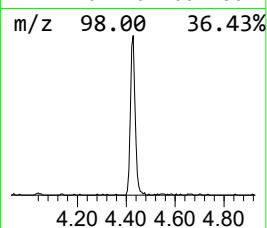
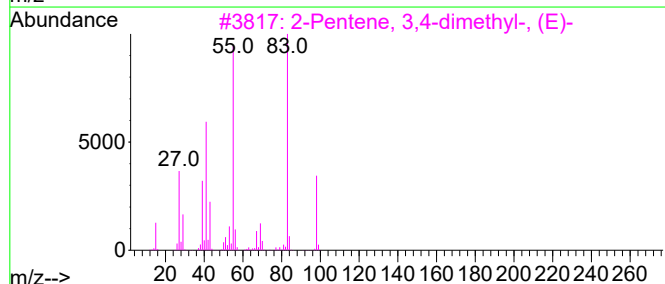
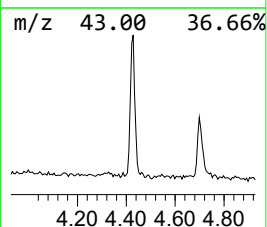
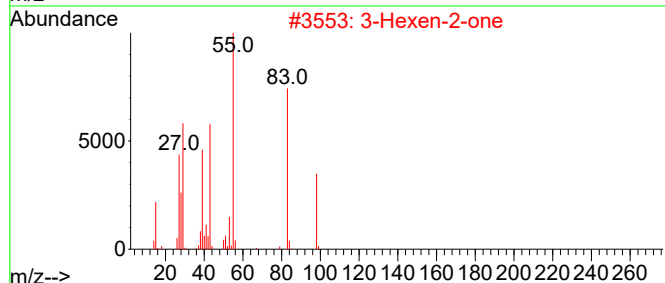
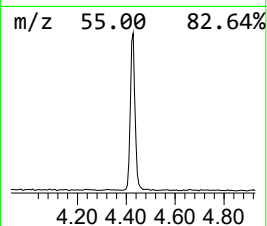
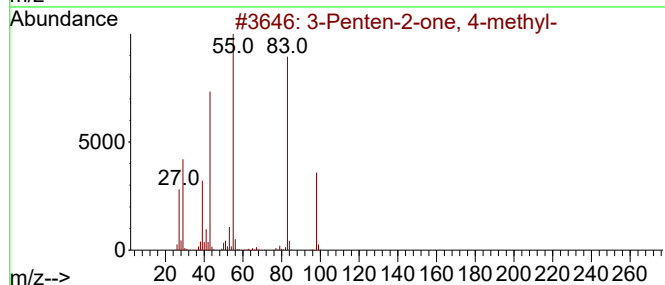
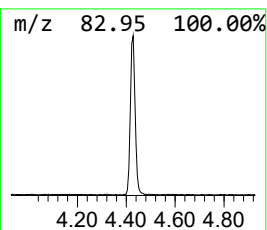
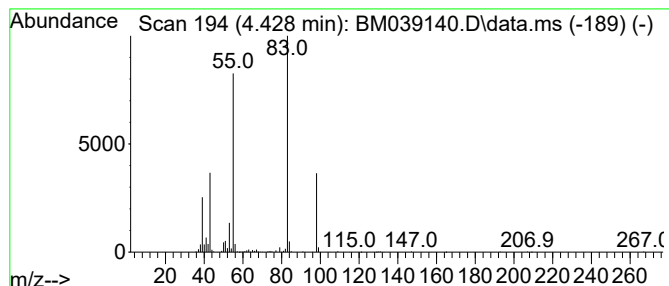
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.428	4.46 ng	327121	1,4-Dichlorobenzene-d4	7.951

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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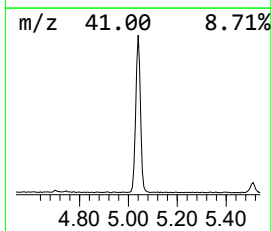
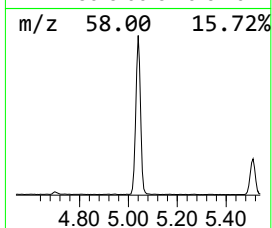
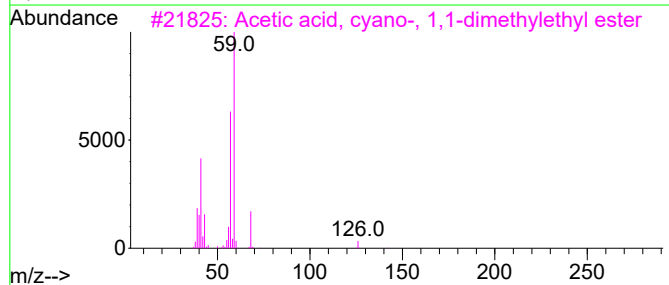
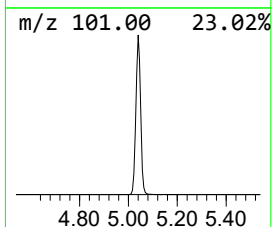
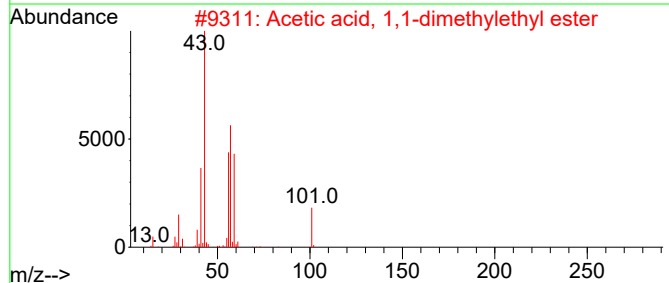
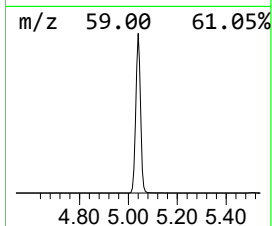
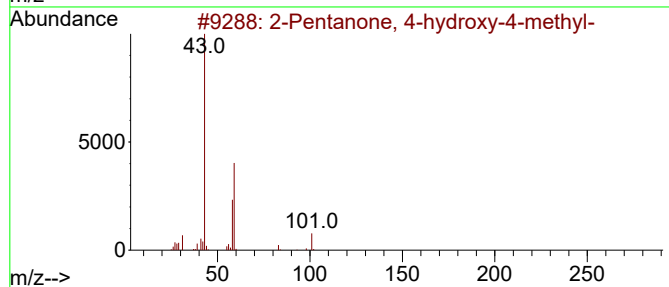
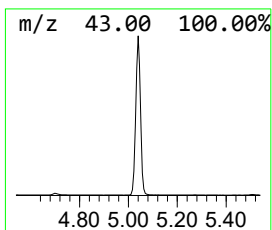
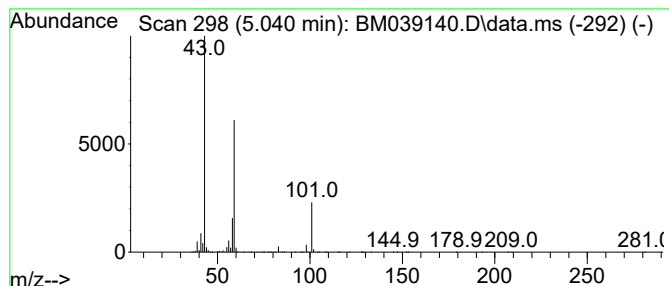
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.040	43.66 ng	3204240	1,4-Dichlorobenzene-d4	7.951	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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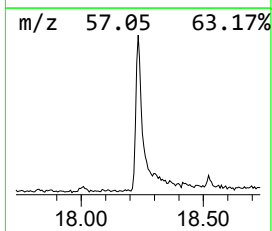
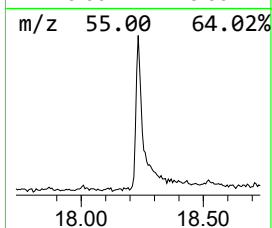
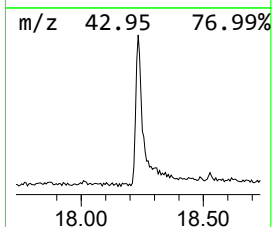
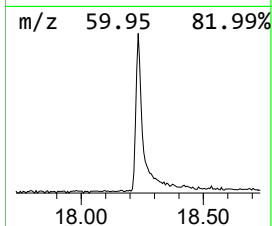
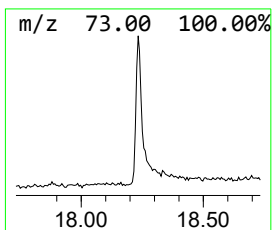
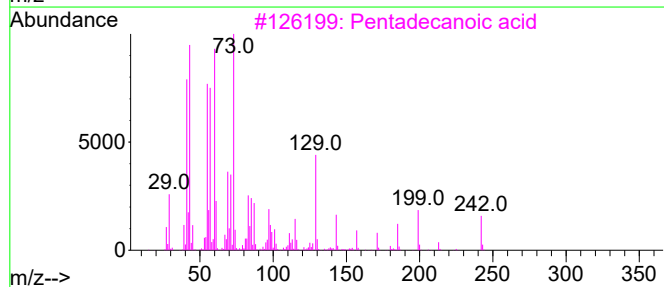
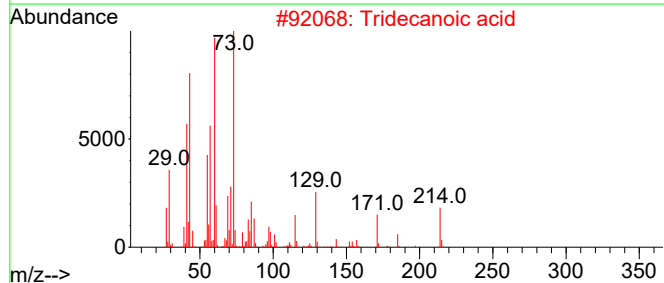
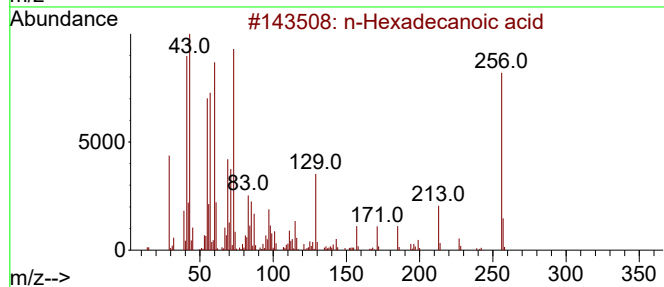
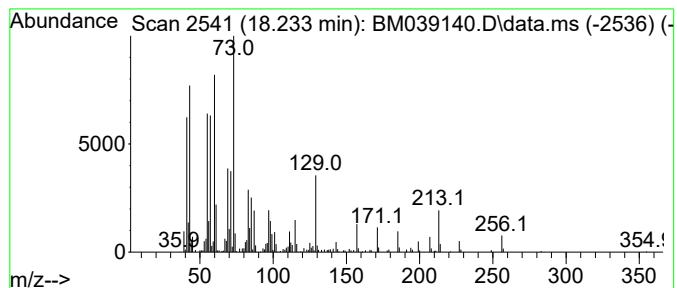
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.233	2.30 ng	438162	Phenanthrene-d10	17.339

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	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Octadecanoic acid	284	C18H36O2	000057-11-4	87
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one,...	4.428	4.5	ng	327121	1	7.951	1467770	20.0
2-Pentanone, 4-...	5.040	43.7	ng	3204240	1	7.951	1467770	20.0
n-Hexadecanoic ...	18.233	2.3	ng	438162	4	17.339	3805770	20.0