

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041723\
 Data File : BG057115.D
 Acq On : 17 Apr 2023 17:47
 Operator : CG/JU
 Sample : 02366-09
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 20230341-COMP-19

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_G\Methods\8270-BG033023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057115.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.429	316	322	329	rBB	58835	89658	7.68%	1.787%
2	5.911	397	404	414	rBB	208662	336632	28.83%	6.711%
3	7.532	672	680	691	rBB	219393	383365	32.83%	7.642%
4	8.402	822	828	834	rBB2	36357	60520	5.18%	1.206%
5	9.577	1021	1028	1036	rBB	129319	226189	19.37%	4.509%
6	11.239	1303	1311	1317	rBV	47469	81620	6.99%	1.627%
7	13.636	1712	1719	1727	rVB	535891	806144	69.04%	16.070%
8	15.010	1946	1953	1960	rBV	134291	207912	17.81%	4.145%
9	16.491	2199	2205	2215	rBV	469423	711036	60.89%	14.174%
10	17.754	2411	2420	2424	rBV	170403	256786	21.99%	5.119%
11	18.588	2557	2562	2573	rBV4	23044	35841	3.07%	0.714%
12	19.780	2760	2765	2770	rVB	15678	20819	1.78%	0.415%
13	20.139	2823	2826	2831	rVB2	13150	18666	1.60%	0.372%
14	20.321	2851	2857	2862	rBV	924233	1167675	100.00%	23.277%
15	21.625	3075	3079	3086	rBV4	33762	50866	4.36%	1.014%
16	22.066	3146	3154	3160	rBV2	152358	277294	23.75%	5.528%
17	22.113	3160	3162	3166	rVB4	9028	12957	1.11%	0.258%
18	25.596	3746	3755	3766	rVB	86564	272465	23.33%	5.431%

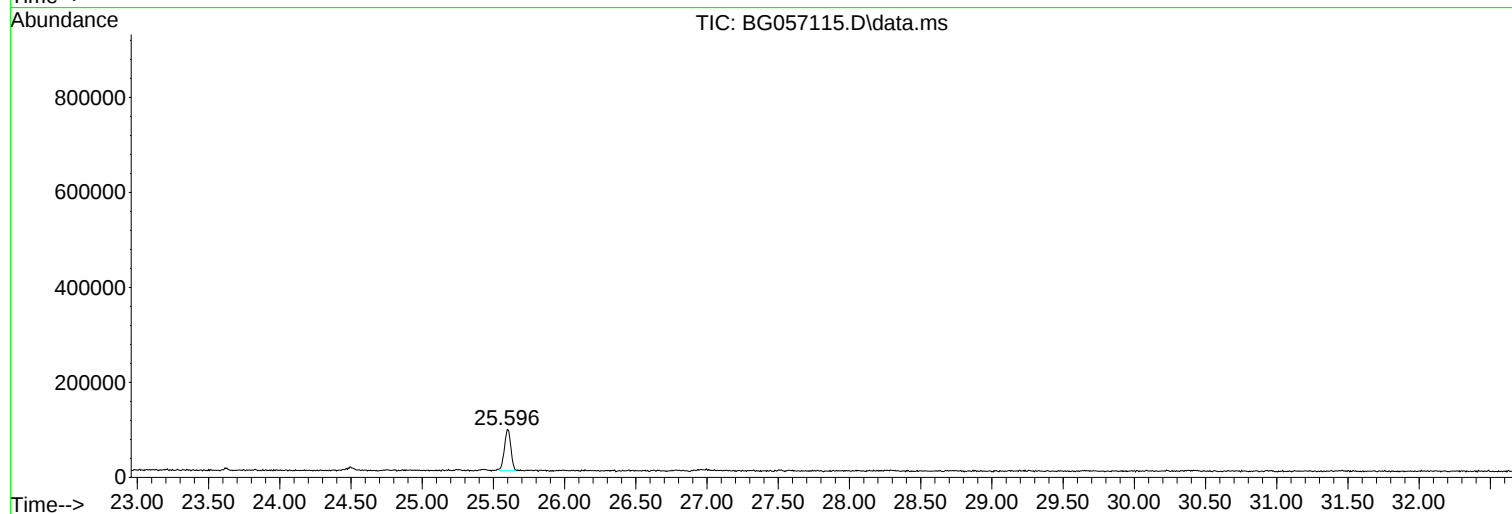
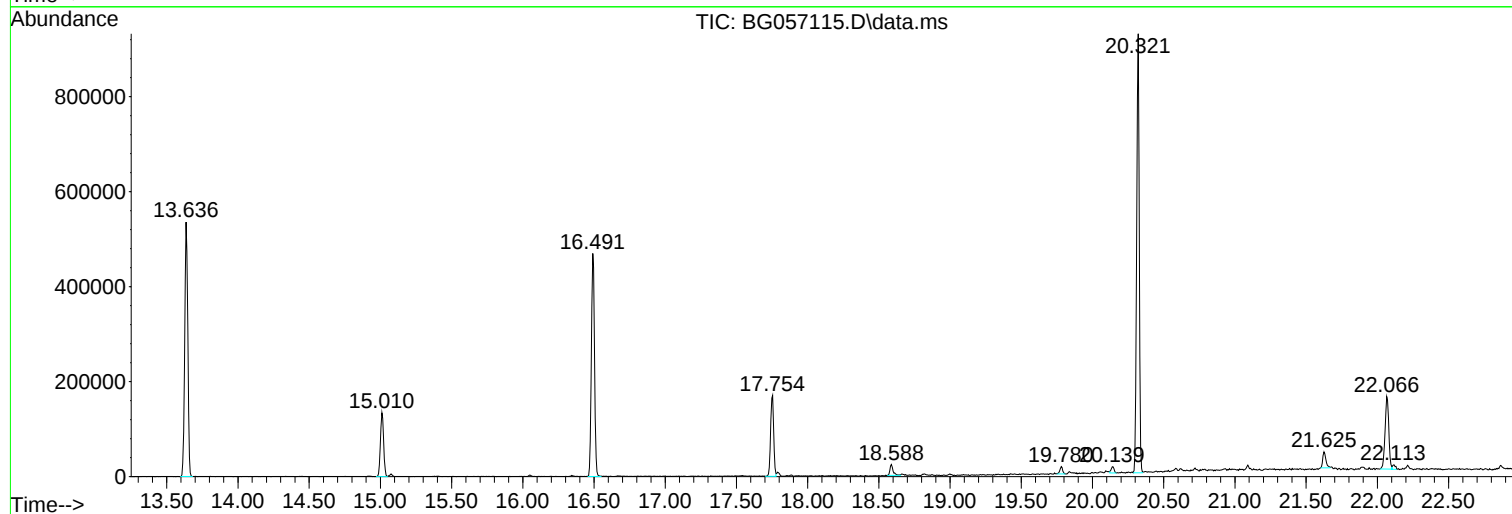
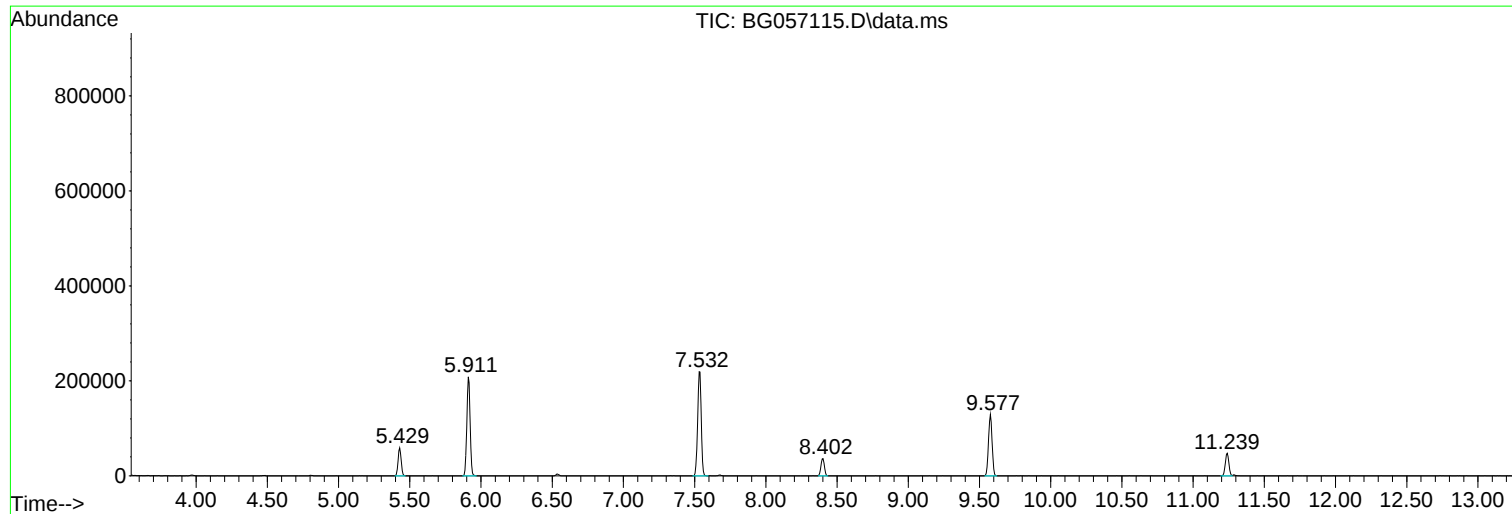
Sum of corrected areas: 5016445

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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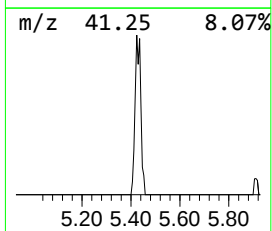
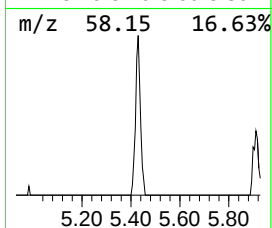
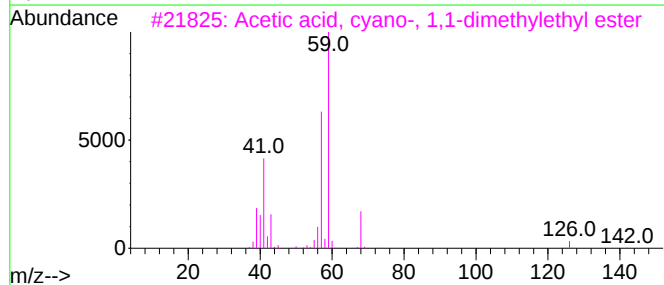
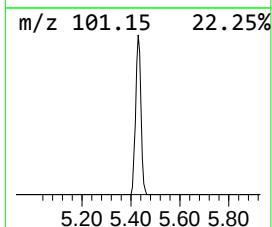
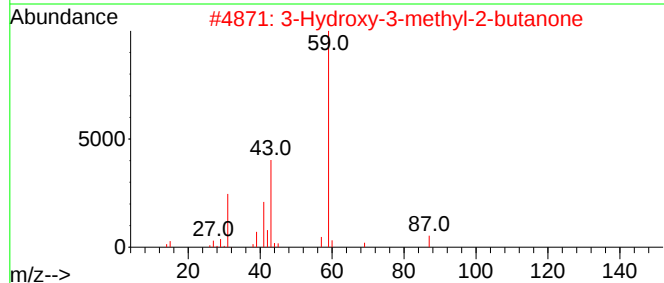
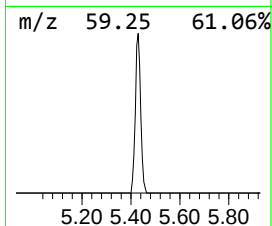
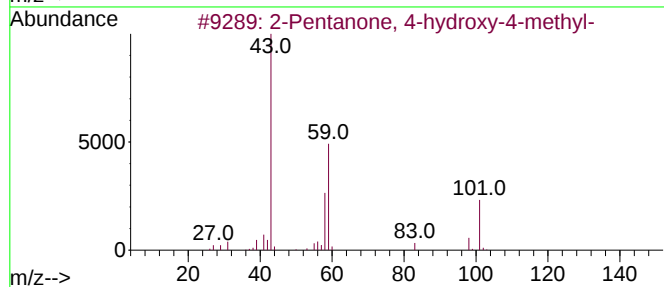
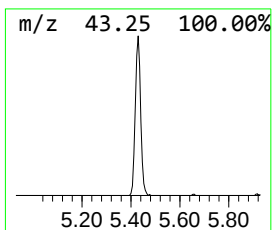
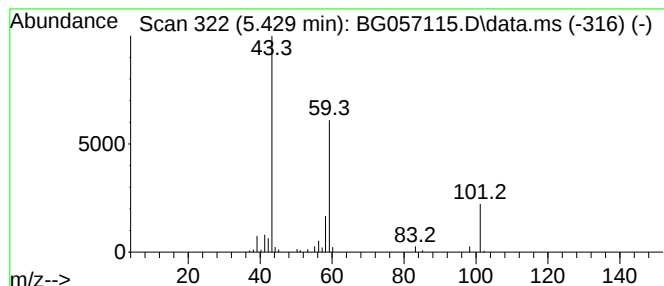
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.429	29.63 ng	89658	1,4-Dichlorobenzene-d4	8.396

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	Acetone	58	C3H6O	000067-64-1	9		



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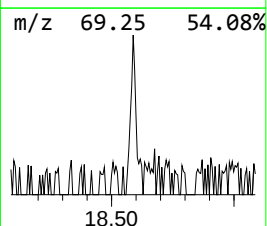
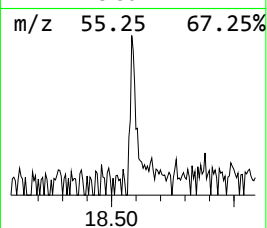
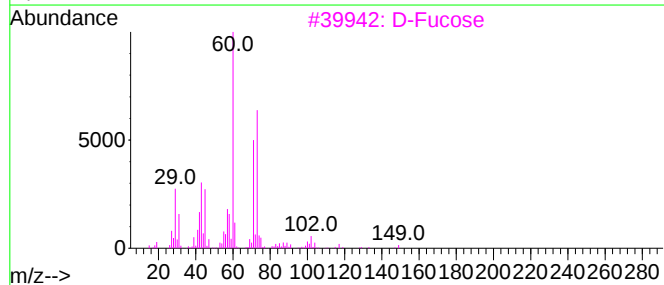
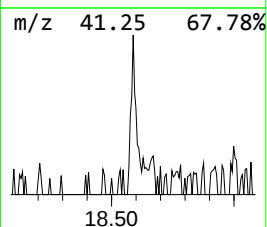
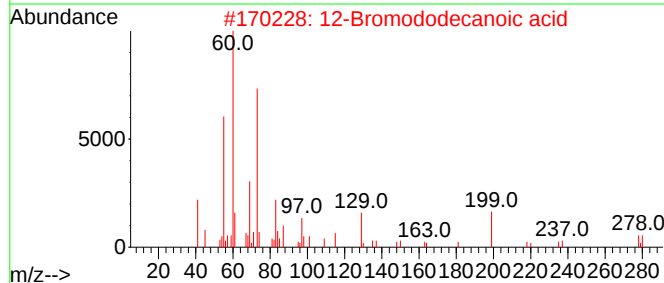
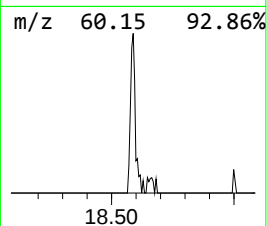
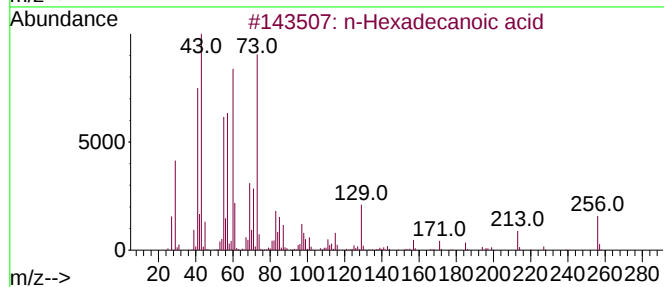
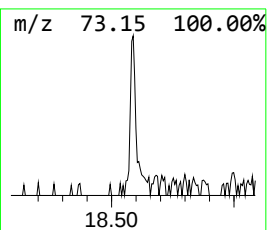
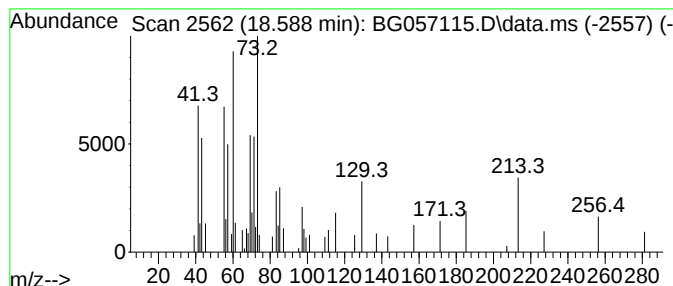
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.588	2.79 ng	35841	Phenanthrene-d10		17.754	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	55
2	12-Bromododecanoic acid		278	C12H23BrO2	073367-80-3	43
3	D-Fucose		164	C6H12O5	003615-37-0	38
4	11-Bromoundecanoic acid		264	C11H21BrO2	002834-05-1	38
5	.alpha.-D-Glucopyranose, 4-O-.be...		342	C12H22O11	014641-93-1	27



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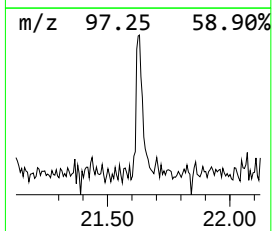
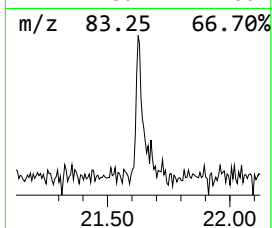
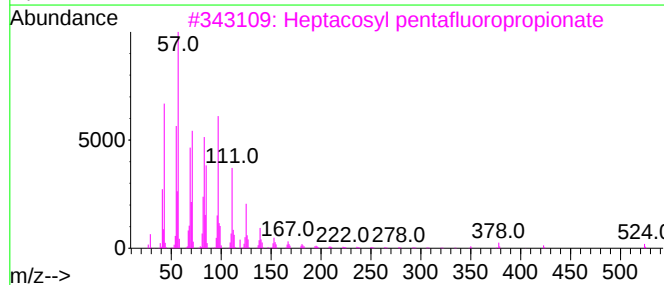
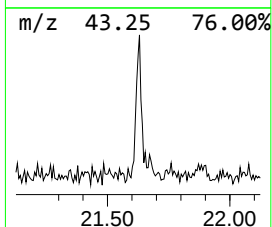
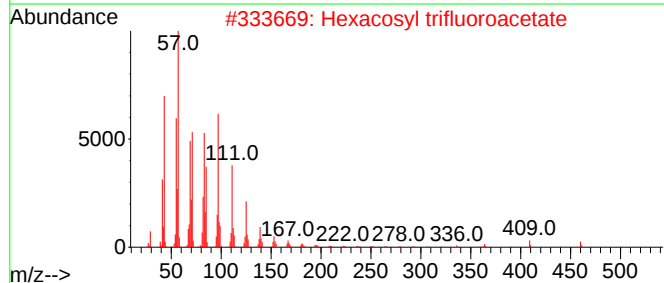
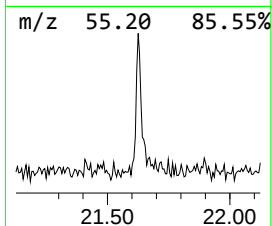
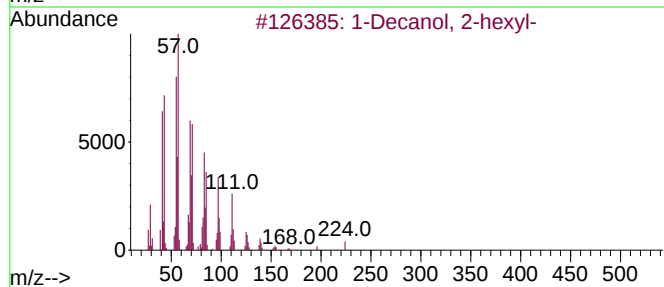
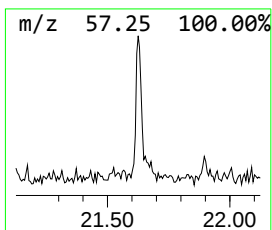
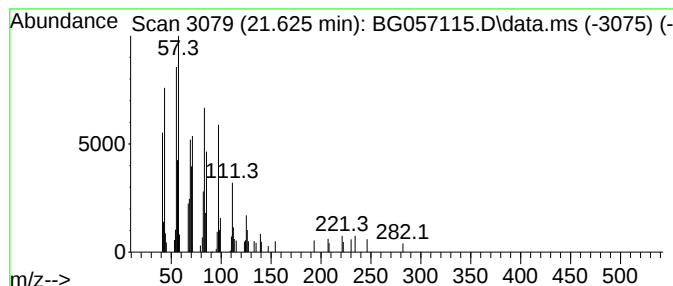
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Peak Number 3 1-Decanol, 2-hexyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.625	3.67 ng	50866	Chrysene-d12		22.066	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-Decanol, 2-hexyl-		242	C16H34O	002425-77-6	83
2	Hexacosyl trifluoroacetate		478	C28H53F3O2	1000351-75-0	81
3	Heptacosyl pentafluoropropionate		542	C30H55F5O2	1000351-81-6	81
4	Hexacosyl pentafluoropropionate		528	C29H53F5O2	1000351-81-2	81
5	Heptadecyl heptafluorobutyrate		452	C21H35F7O2	959085-66-6	81



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.429	29.6	ng	89658	1	8.396	60520	20.0
n-Hexadecanoic ...	18.588	2.8	ng	35841	4	17.754	256786	20.0
1-Decanol, 2-he...	21.625	3.7	ng	50866	5	22.066	277294	20.0