LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
Data File : BF088649.D
Acq On : 3 Jul 2016 15:04
Operator : UM/SJ
Sample : H3837-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C1.2-6

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-BF063016.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	1.850	21	23	35	rVB	67525	97485	3.16%	0.346%
2	2.021	35	38	43	rBV2	33445	47906	1.55%	0.170%
3	4.958	292	295	301	rBB	184239	297475	9.63%	1.057%
4	5.381	329	332	334	rBV	2483728	2568322	83.19%	9.123%
5	6.421	420	423	425	rVB	2486804	2790914	90.40%	9.913%
6	6.547	431	434	437	rBV	2272254	2501401	81.02%	8.885%
7	6.787	452	455	456	rBV	571081	679617	22.01%	2.414%
8	6.936	466	468	471	rBV	1749046	2048036	66.33%	7.275%
9	7.347	501	504	506	rBV	1755220	1775470	57.51%	6.306%
10	7.439	510	512	516	rBV	25013	31871	1.03%	0.113%
11	8.067	565	567	569	rBV	1136192	981768	31.80%	3.487%
12	9.142	658	661	663	rBV	2414447	3087452	100.00%	10.967%
13	9.542	693	696	698	rVB	1694105	1498395	48.53%	5.322%
14	9.816	717	720	722	rBB	1156340	1039612	33.67%	3.693%
15	10.239	755	757	758	rBV	128861	108443	3.51%	0.385%
16	10.605	786	789	791	rBV	1913138	2009770	65.09%	7.139%
17	10.730	798	800	805	rVB	43420	51466	1.67%	0.183%
18	11.176	837	839	841	rBV	44632	41275	1.34%	0.147%
19	11.291	847	849	852	rVB	1079714	1077547	34.90%	3.827%
20	11.599	874	876	883	rBV2	21426	43825	1.42%	0.156%
21	11.839	894	897	898	rBV	48371	48944	1.59%	0.174%
22	12.879	985	988	991	rBV	2710037	3051477	98.83%	10.839%
23	13.839	1069	1072	1077	rBV	82823	235342	7.62%	0.836%
24	13.919	1077	1079	1081	rVB	1287995	1145611	37.11%	4.069%
25	14.674	1143	1145	1150	rBV3	21003	39695	1.29%	0.141%
26	15.314	1198	1201	1204	rBV	742712	854274	27.67%	3.034%

Sum of corrected areas: 28153393

LSC Report - Integrated Chromatogram

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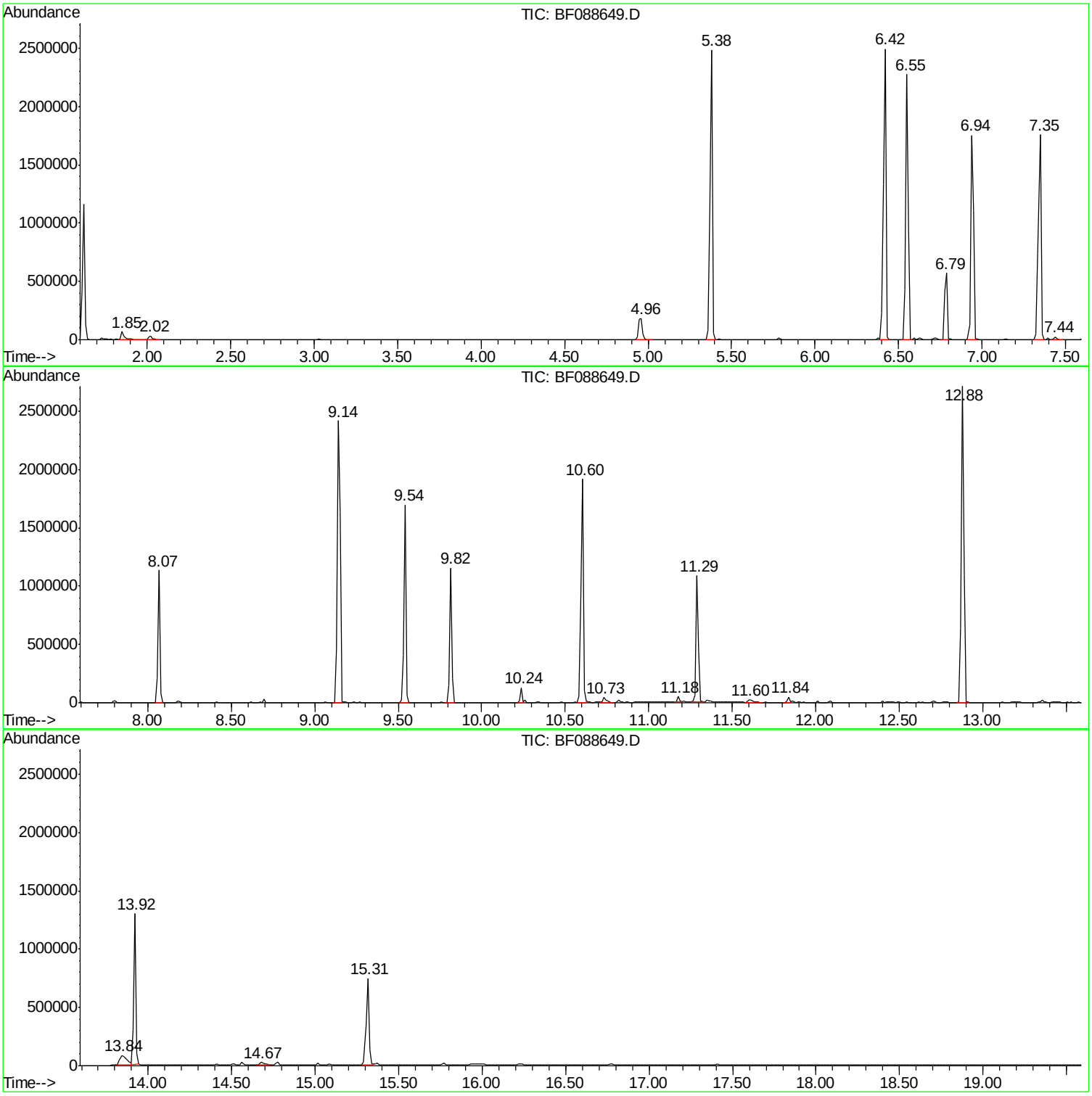
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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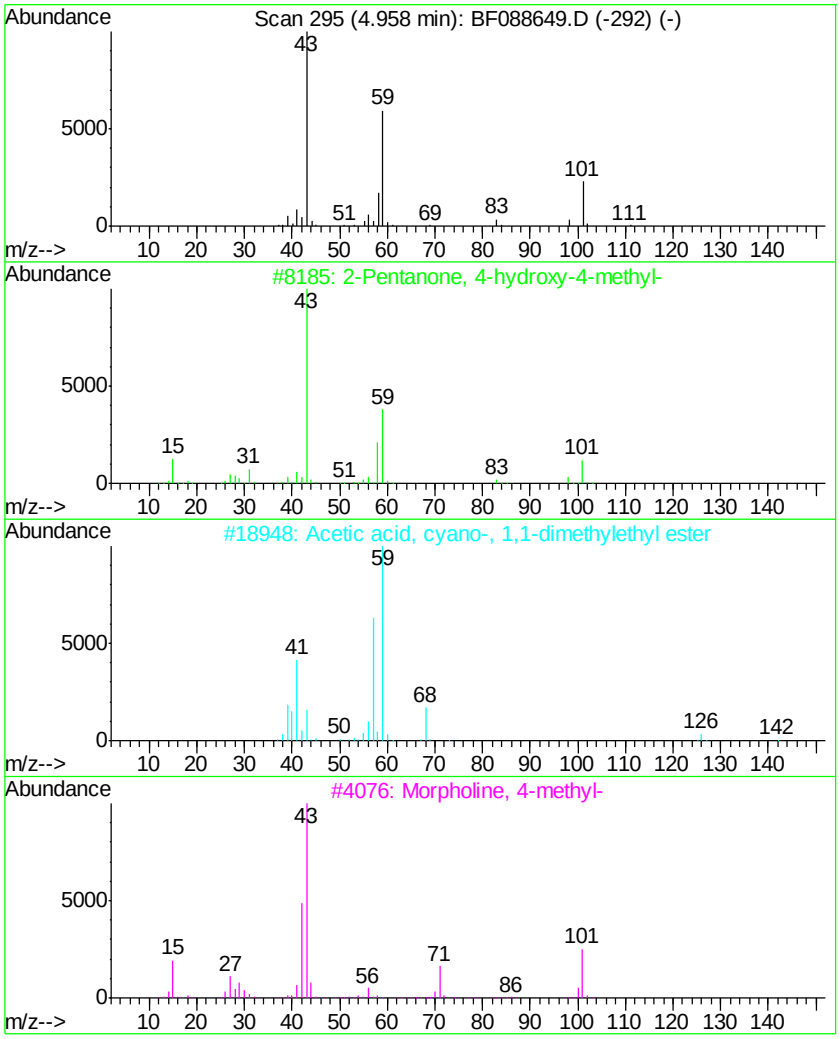
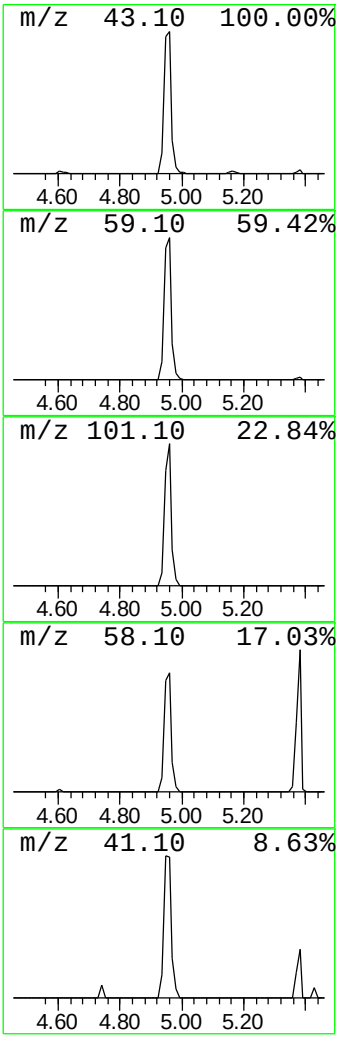
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	8.75 ng	297475	1,4-Dichlorobenzene-d4	6.79

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9





Library Search Compound Report

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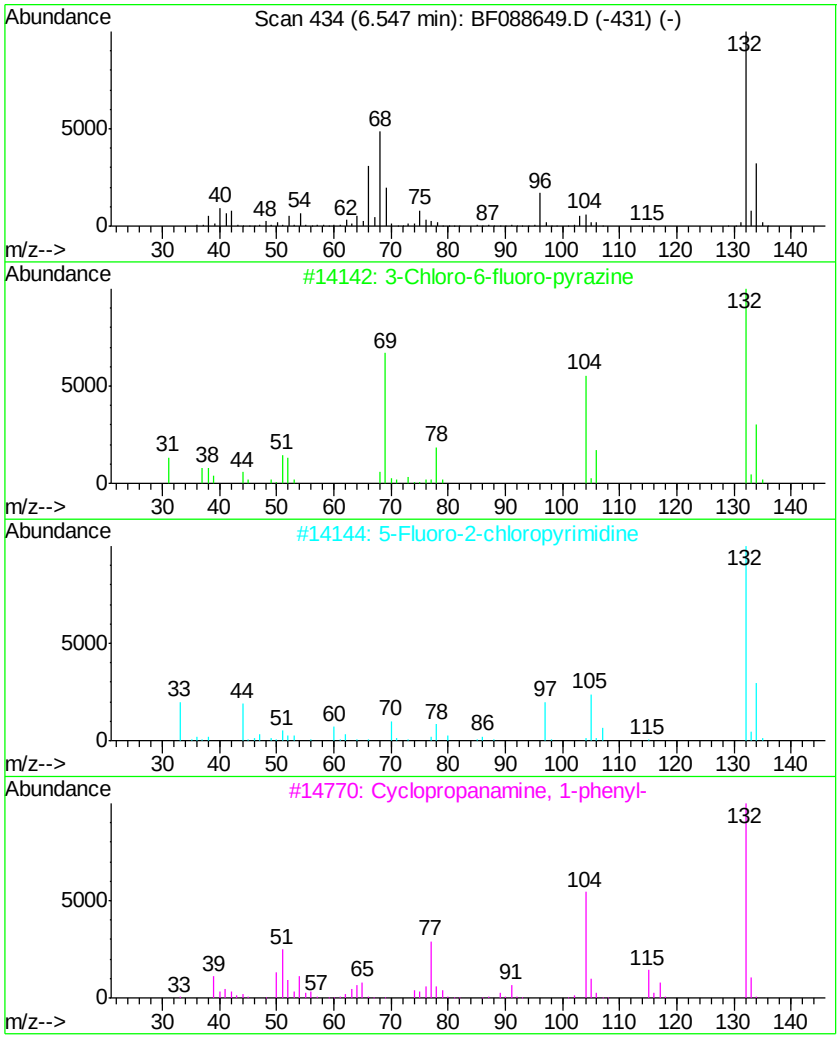
TIC Integration Parameters: LSCINT.P

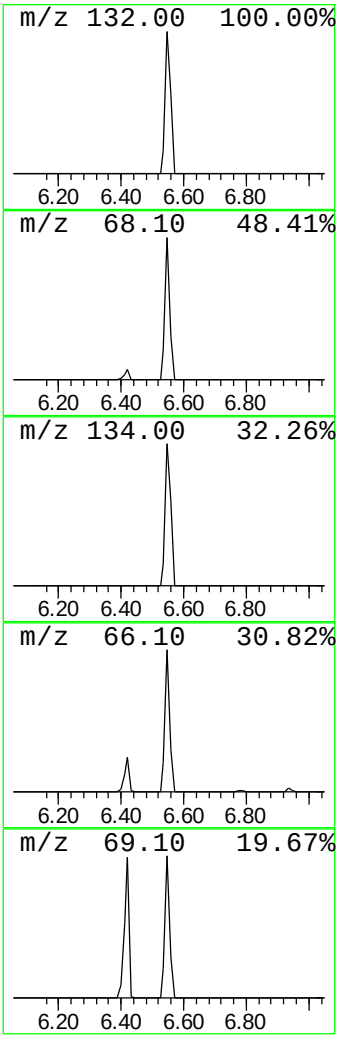
****

Peak Number 3 unknown6.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	73.61 ng	2501400	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





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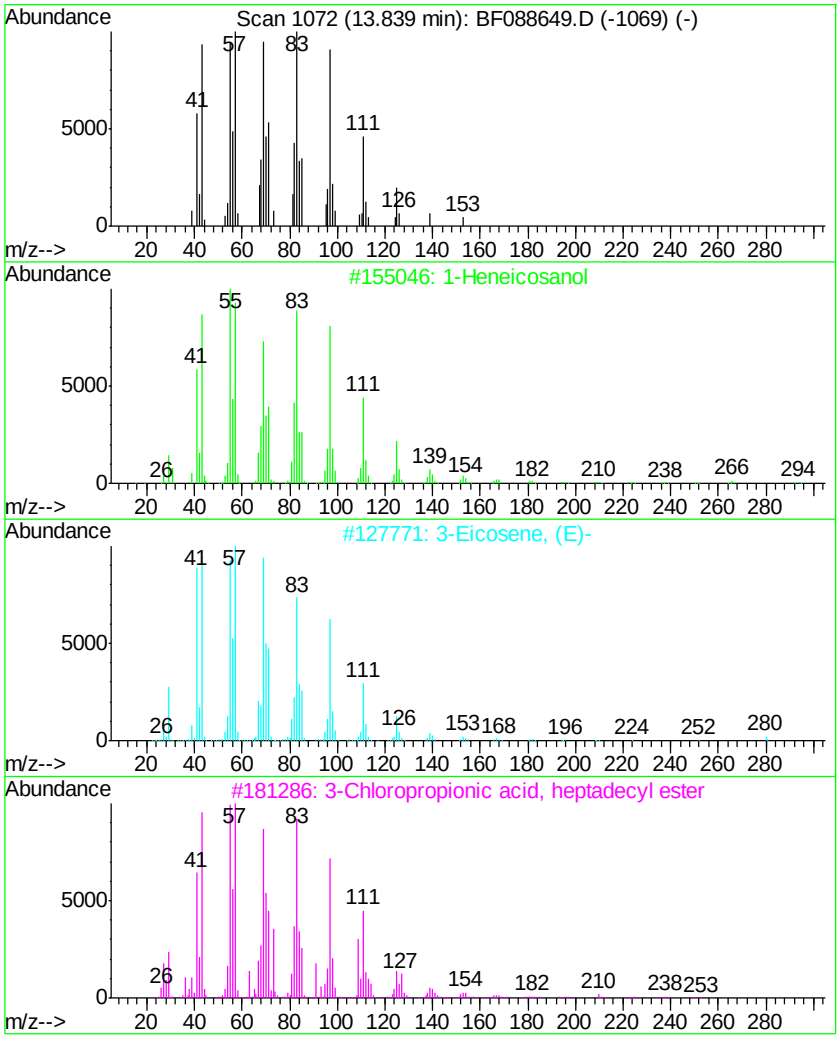
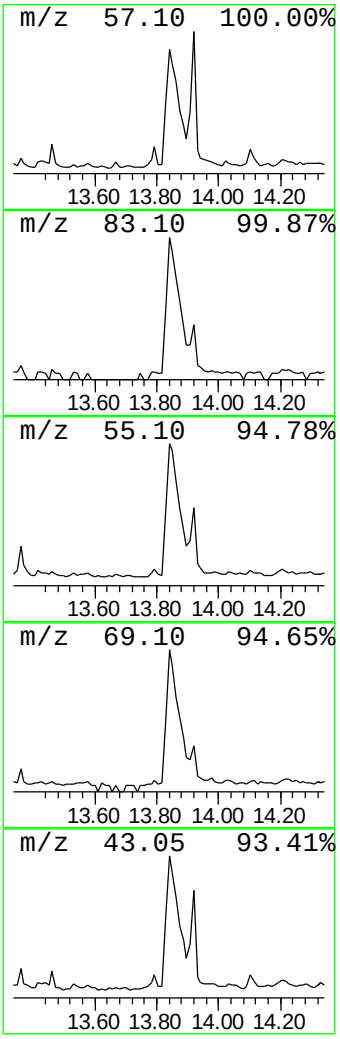
Peak Number 5 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	4.11 ng	235342	Chrysene-d12	13.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
4	1-Hexadecanol	242	C16H34O	036653-82-4	91
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91





Tentatively Identified Compound (LSC) summary

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TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
2-Pentanone, 4-hy...	4.96	8.8	ng	297475	1	6.79	679617	20.0
unknown6.55	6.55	73.6	ng	2501400	1	6.79	679617	20.0
1-Heneicosanol	13.84	4.1	ng	235342	5	13.92	1145610	20.0