LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022417\
Data File : BF093158.D
Acq On : 24 Feb 2017 21:35
Operator : SJ/MA
Sample : I1957-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SRI-SB-5(13-15)20170222

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-BF013017.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	5.002	252	255	268	rBV	1345212	2118412	43.74%	4.822%
2	5.436	290	293	295	rBV	3506031	4842910	100.00%	11.024%
3	6.476	381	384	386	rBV	4017518	4632163	95.65%	10.544%
4	6.602	392	395	397	rBV	4346524	4433216	91.54%	10.091%
5	6.830	413	415	417	rBV	1087861	902922	18.64%	2.055%
6	6.990	426	429	431	rBV	3712489	3533076	72.95%	8.042%
7	7.402	462	465	468	rBV	2638598	2857583	59.01%	6.505%
8	7.516	473	475	480	rVB	47747	68383	1.41%	0.156%
9	8.122	525	528	530	rBV	1220952	1190595	24.58%	2.710%
10	9.196	619	622	625	rBV	4306387	4580062	94.57%	10.425%
11	9.596	654	657	659	rBV	1004195	885657	18.29%	2.016%
12	9.802	673	675	679	rBV	38641	54864	1.13%	0.125%
13	9.871	679	681	684	rVB	1370963	1332979	27.52%	3.034%
14	10.305	718	719	721	rVB	111188	84281	1.74%	0.192%
15	10.522	735	738	741	rBV	35755	55561	1.15%	0.126%
16	10.671	748	751	753	rBV	2454104	2972682	61.38%	6.767%
17	10.774	759	760	767	rVB	114108	161382	3.33%	0.367%
18	11.231	798	800	801	rBV	65709	81878	1.69%	0.186%
19	11.356	809	811	814	rBV	1351423	1311728	27.09%	2.986%
20	12.957	947	951	953	rBV	3329260	4716966	97.40%	10.737%
21	13.425	986	992	995	rBV	235294	245662	5.07%	0.559%
22	13.848	1026	1029	1036	rBV	210324	401588	8.29%	0.914%
23	13.997	1040	1042	1045	rVB	1327207	1236990	25.54%	2.816%
24	14.465	1080	1083	1090	rBV4	18141	54870	1.13%	0.125%
25	14.740	1105	1107	1113	rBV2	68567	116858	2.41%	0.266%
26	14.831	1113	1115	1117	rVB	106749	100581	2.08%	0.229%
27	15.425	1165	1167	1170	rBV	739909	957832	19.78%	2.180%

Sum of corrected areas: 43931681

LSC Report - Integrated Chromatogram

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Misc :
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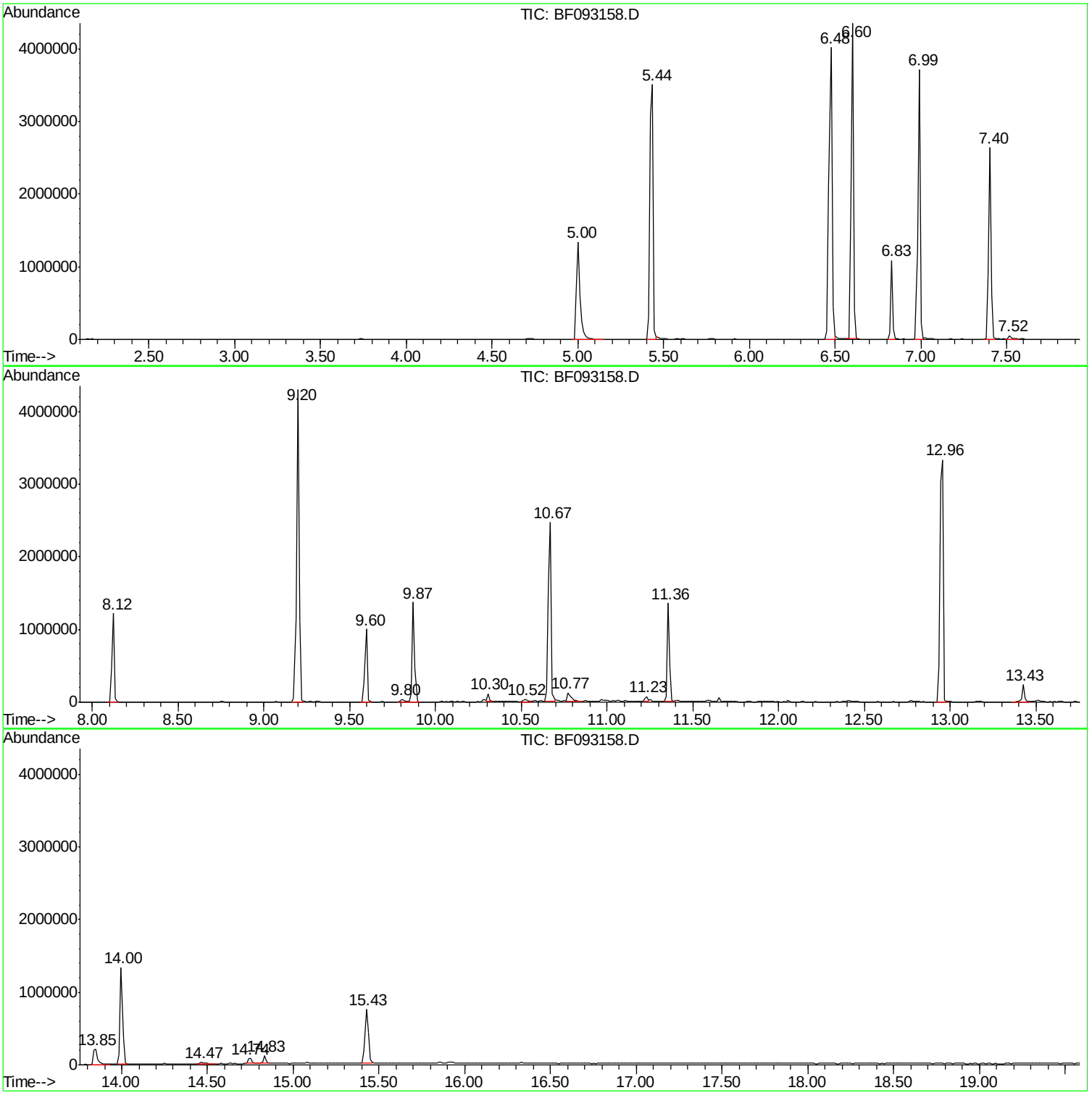
Instrument :
BNA_F
ClientSampleId :
SRI-SB-5(13-15)20170222

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022417\
Data File : BF093158.D
Acq On : 24 Feb 2017 21:35
Operator : SJ/MA
Sample : I1957-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SRI-SB-5(13-15)20170222

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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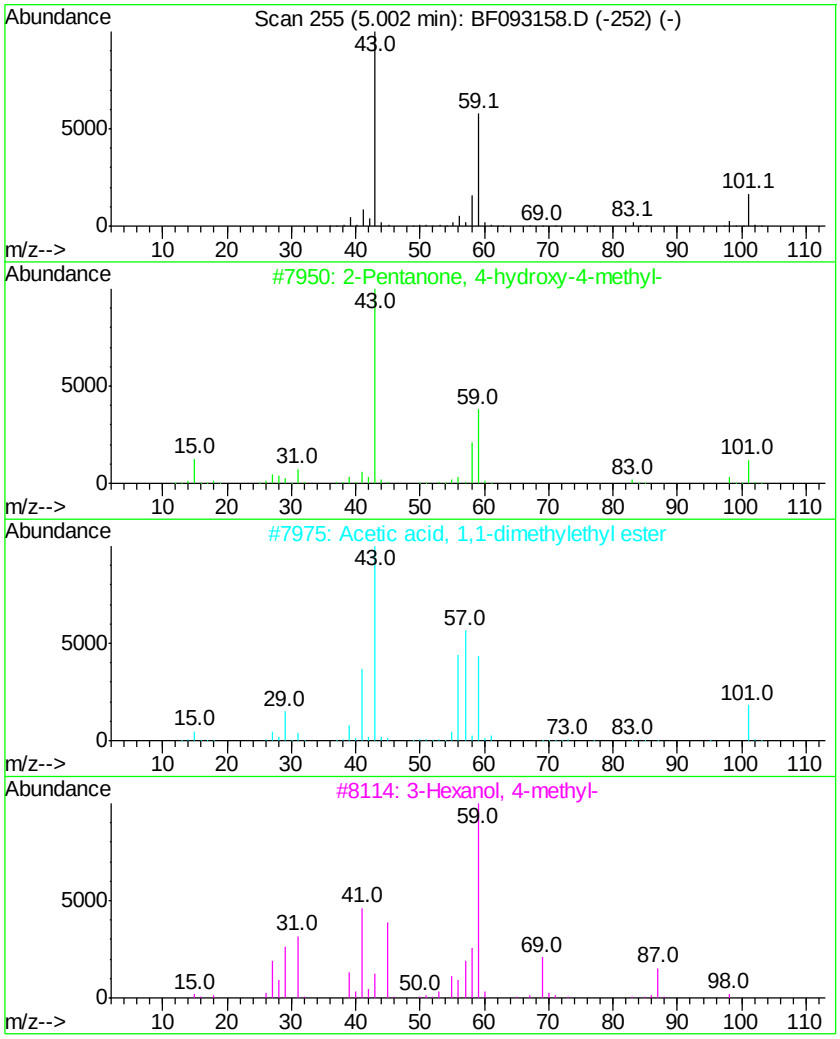
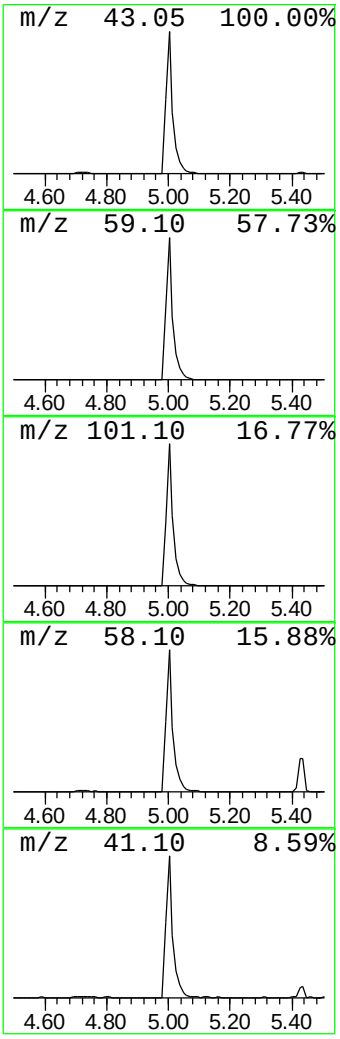
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	46.92 ng	2118410	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Instrument : BNA_F
ClientSampleId : SRI-SB-5(13-15)20170222

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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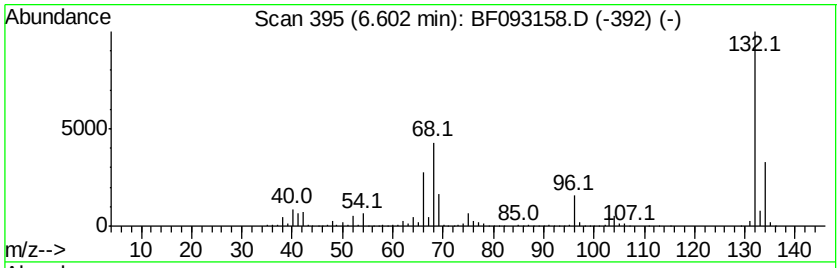
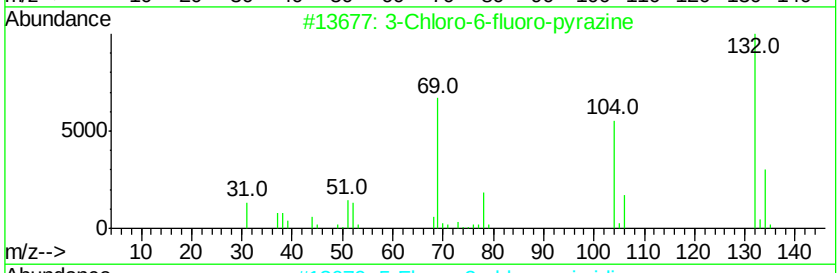
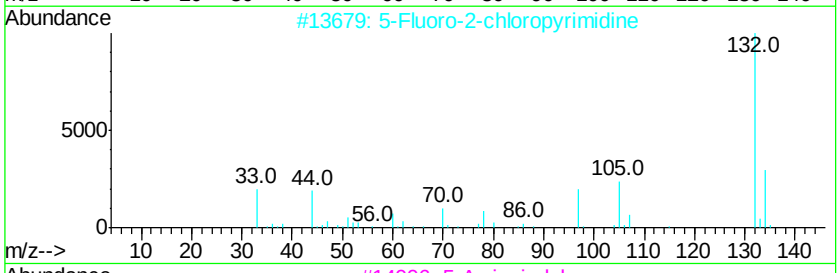
Peak Number 2 unknown6.60 Concentration Rank 1

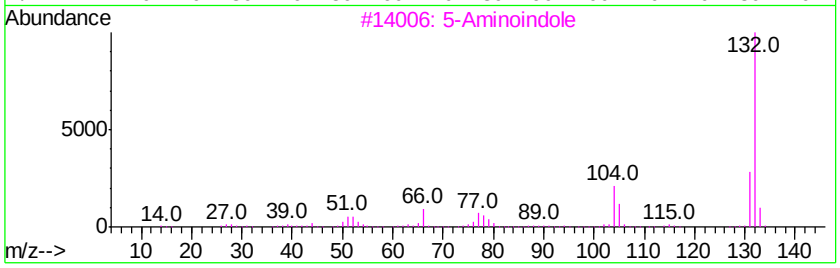
R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	98.20 ng	4433220	1,4-Dichlorobenzene-d4	6.83

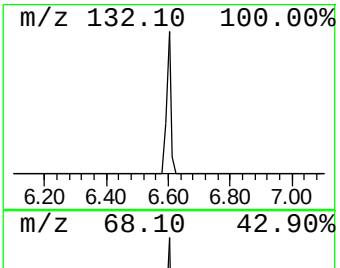
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9

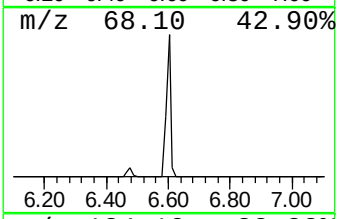


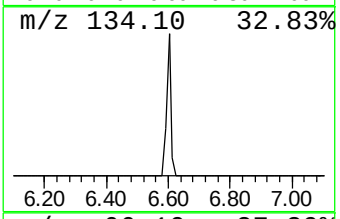


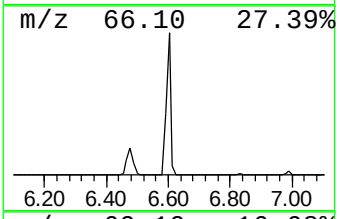


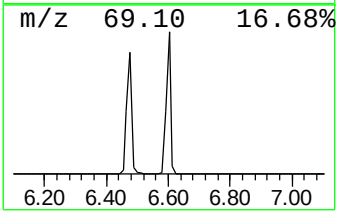












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Sample : I1957-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SRI-SB-5(13-15)20170222

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

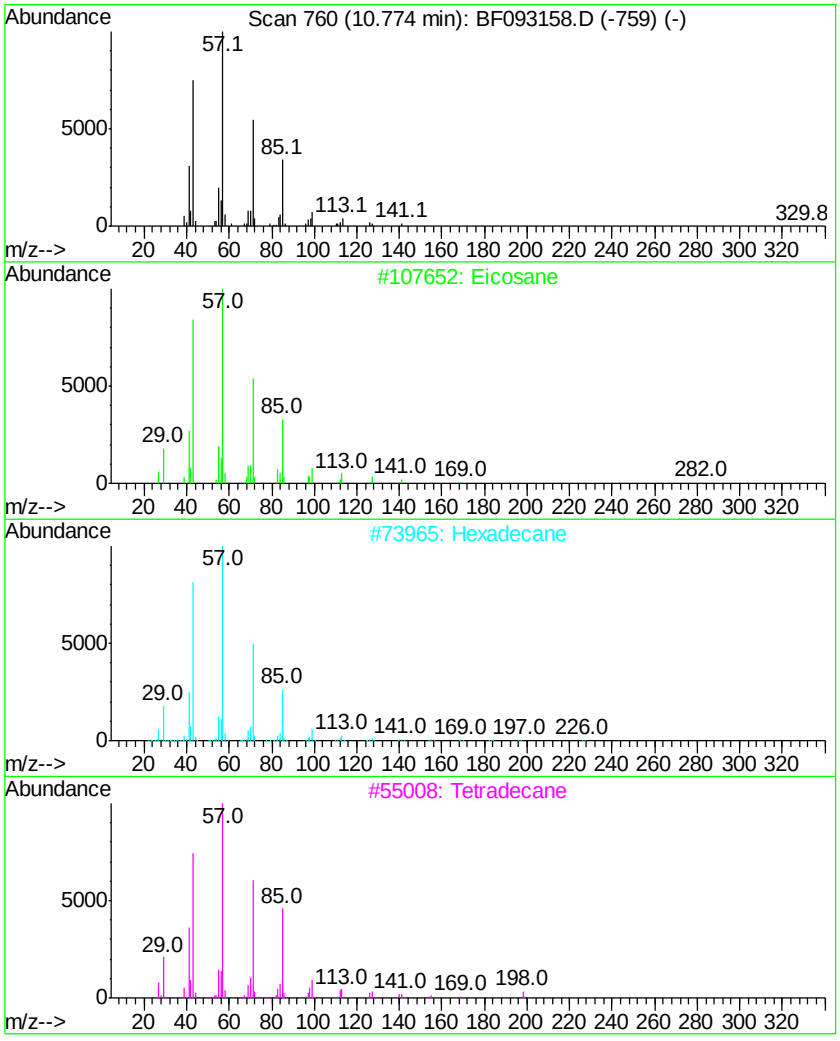
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

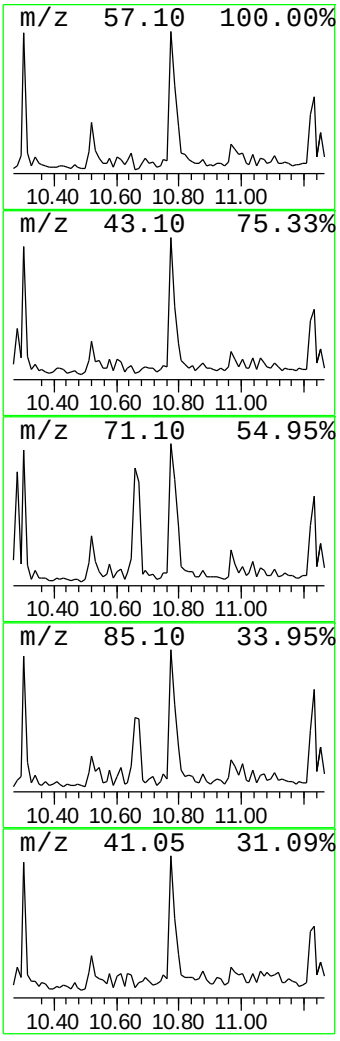
****

Peak Number 4 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.77	2.46 ng	161382	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Hexadecane	226	C16H34	000544-76-3	91
3	Tetradecane	198	C14H30	000629-59-4	90
4	Octacosane	394	C28H58	000630-02-4	83
5	Tridecane	184	C13H28	000629-50-5	83





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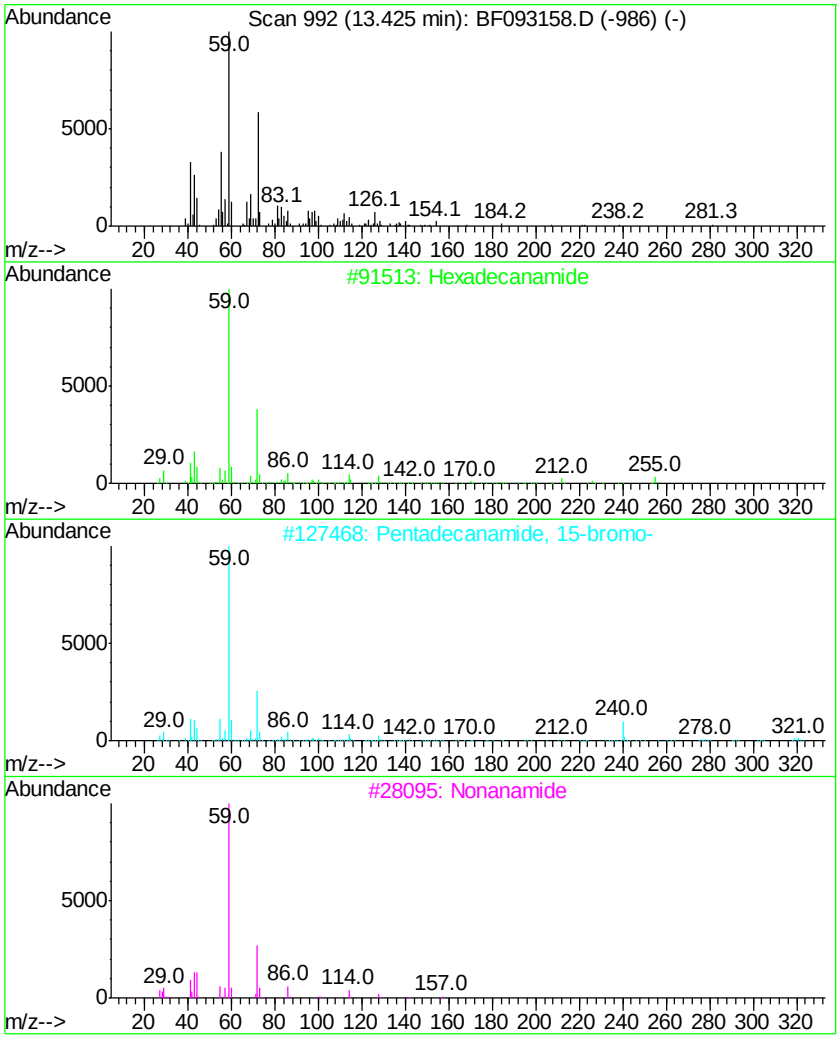
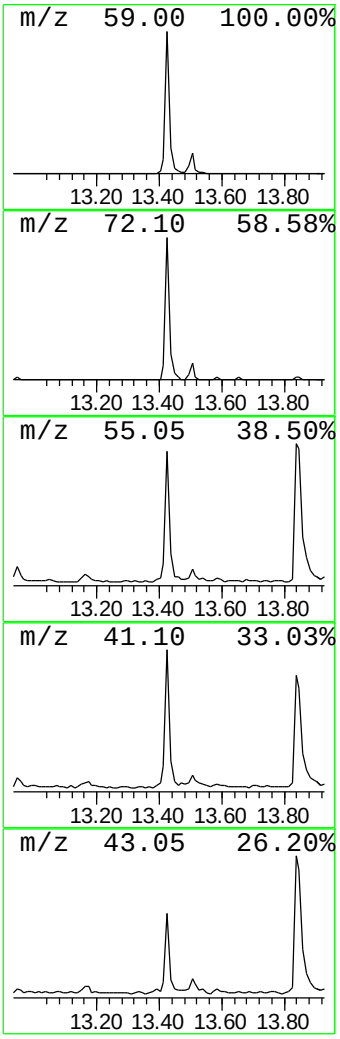
****

Peak Number 5 Hexadecanamide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.43	3.97 ng	245662	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanamide	255	C16H33NO	000629-54-9	72
2	Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	56
3	Nonanamide	157	C9H19NO	001120-07-6	50
4	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	47
5	Methyl 17-methoxy-10-methoxycarb...	386	C22H42O5	1000110-20-7	47





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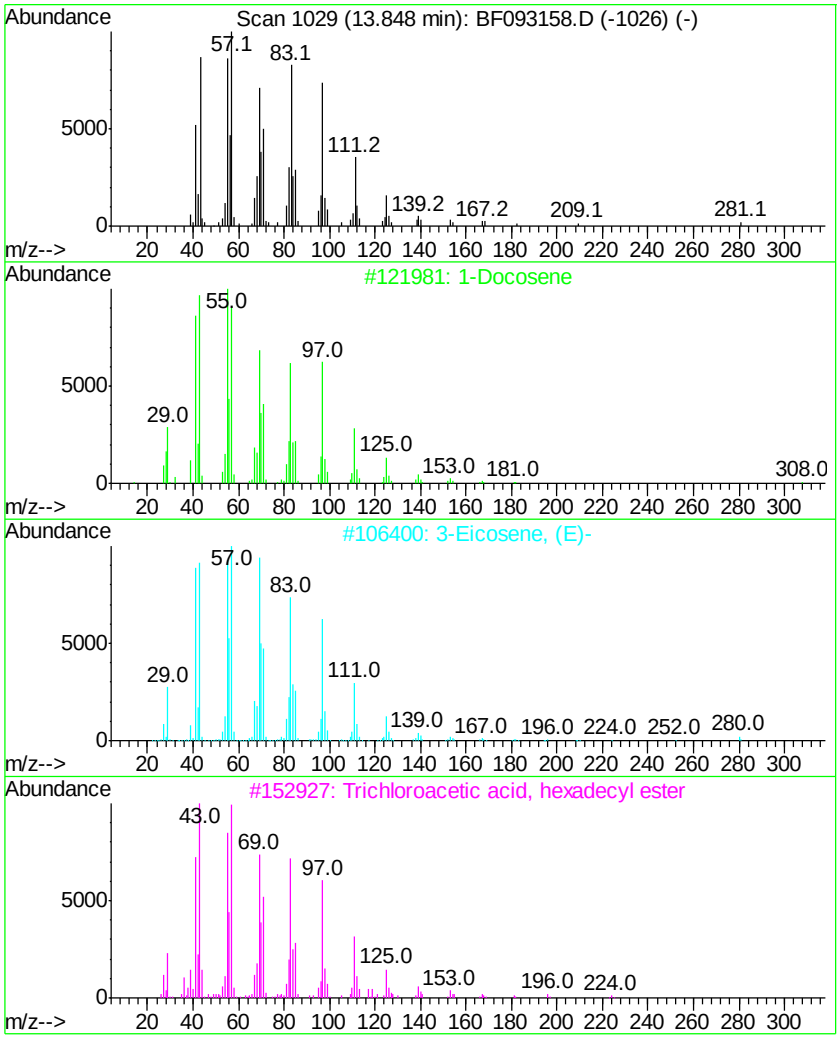
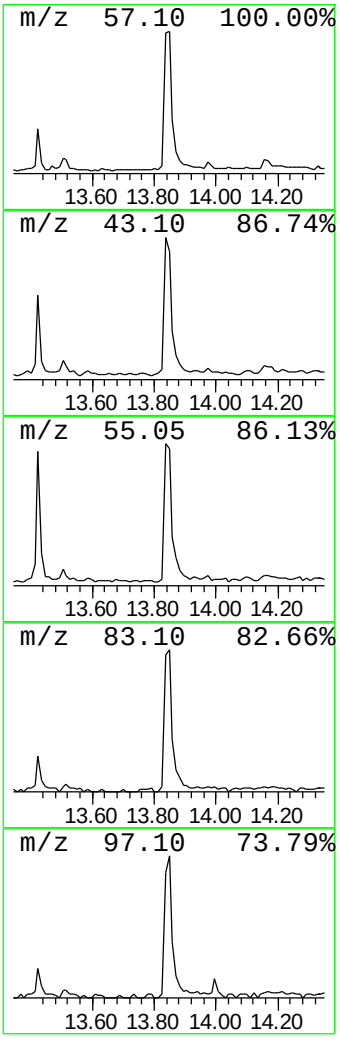
Peak Number 6 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	6.49 ng	401588	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	94
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4	2- Bromopropionic acid, pentadec...	362	C18H35BrO2	1000292-44-2	91
5	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91





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

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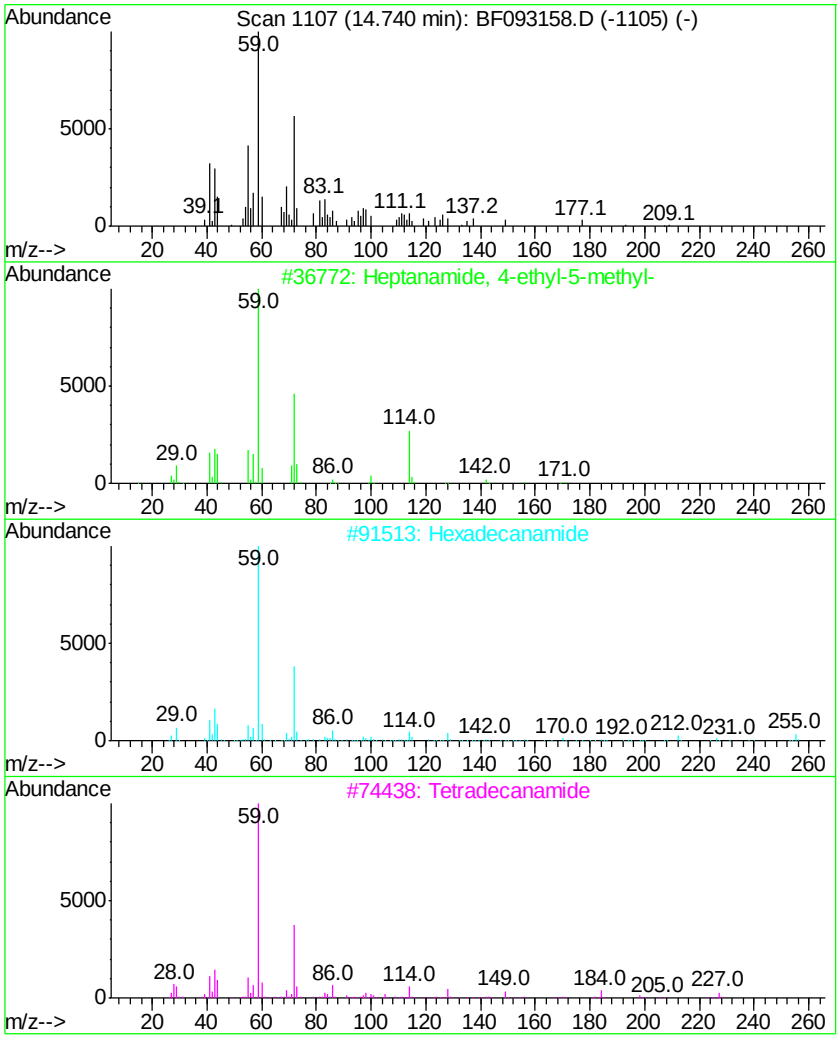
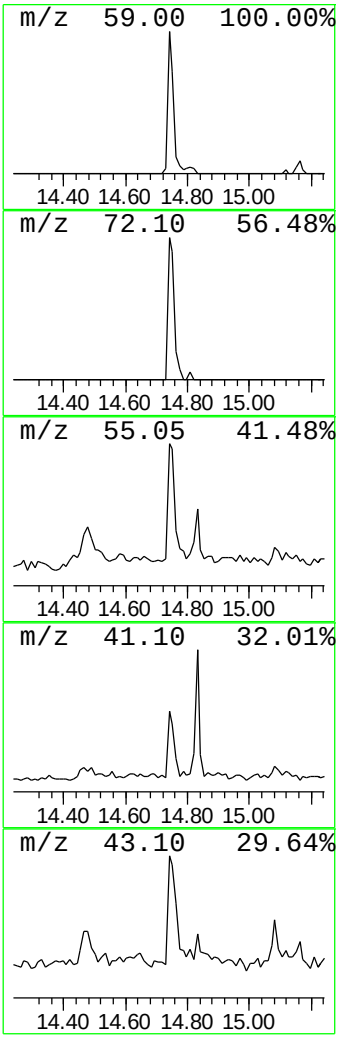
Peak Number 7 Heptanamide, 4-ethyl-5-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.74	2.44 ng	116858	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	59
2	Hexadecanamide	255	C16H33NO	000629-54-9	56
3	Tetradecanamide	227	C14H29NO	000638-58-4	53
4	Nonanamide	157	C9H19NO	001120-07-6	53
5	Octanamide	143	C8H17NO	000629-01-6	50





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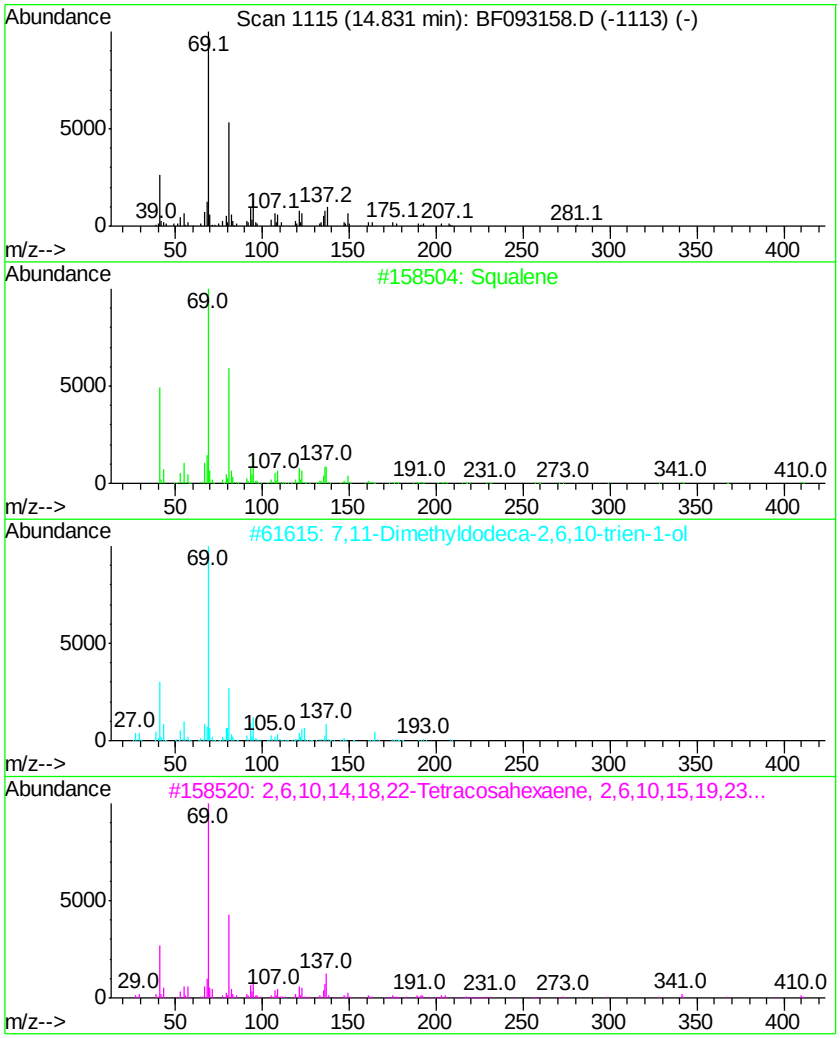
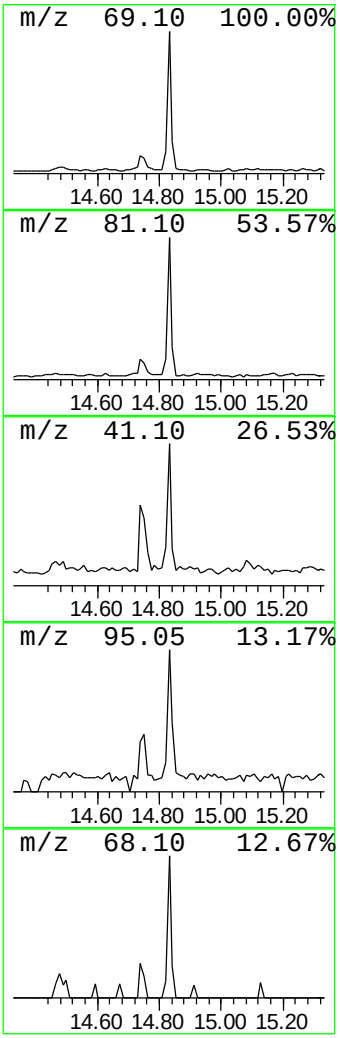
Peak Number 8 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	2.10 ng	100581	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	91
2	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	87
3	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	86
4	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	74
5	3,7,11-Tridecatrienenitrile, 4,8...	231	C16H25N	006006-01-5	72





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.00	46.9	ng	2118410	1	6.83	902922	20.0
unknown6.60	6.60	98.2	ng	4433220	1	6.83	902922	20.0
Eicosane	10.77	2.5	ng	161382	4	11.36	1311730	20.0
Hexadecanamide	13.43	4.0	ng	245662	5	14.00	1236990	20.0
1-Docosene	13.85	6.5	ng	401588	5	14.00	1236990	20.0
Heptanamide, 4-et...	14.74	2.4	ng	116858	6	15.43	957832	20.0
Squalene	14.83	2.1	ng	100581	6	15.43	957832	20.0