

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011918\
 Data File : BF102245.D
 Acq On : 20 Jan 2018 4:12
 Operator : SJ/JU
 Sample : J1113-07
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-14-2.5-3.0

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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	4.934	480	484	497	rVB	221816	369327	8.23%	0.972%
2	5.339	546	553	556	rBV	3714797	4453610	99.26%	11.724%
3	6.369	721	728	731	rBV	3696798	4486711	100.00%	11.812%
4	6.492	744	749	752	rBV	4289135	4468203	99.59%	11.763%
5	6.716	784	787	791	rBV	1212004	984624	21.95%	2.592%
6	6.875	809	814	817	rBV	3599162	3467289	77.28%	9.128%
7	7.286	878	884	887	rBV	2575130	2967759	66.15%	7.813%
8	7.469	911	915	922	rVB	72001	63300	1.41%	0.167%
9	7.998	1001	1005	1009	rBV	1466106	1289931	28.75%	3.396%
10	9.080	1183	1189	1192	rBV	4617677	4363974	97.26%	11.488%
11	9.157	1198	1202	1204	rBV	82900	71379	1.59%	0.188%
12	9.469	1251	1255	1258	rBV	426264	408635	9.11%	1.076%
13	9.686	1289	1292	1296	rVB	233660	173749	3.87%	0.457%
14	9.751	1296	1303	1307	rBV	1359901	1357658	30.26%	3.574%
15	10.004	1344	1346	1350	rBV3	50321	55962	1.25%	0.147%
16	10.186	1374	1377	1379	rVB	269360	187797	4.19%	0.494%
17	10.545	1433	1438	1441	rBV	2296640	2182235	48.64%	5.745%
18	10.657	1454	1457	1464	rBV	227043	241176	5.38%	0.635%
19	11.104	1531	1533	1536	rBV2	71360	65444	1.46%	0.172%
20	11.239	1552	1556	1558	rBV	1120453	994191	22.16%	2.617%
21	11.257	1558	1559	1564	rVB	209990	180600	4.03%	0.475%
22	12.445	1759	1761	1765	rVB	132738	119019	2.65%	0.313%
23	12.645	1793	1795	1798	rVB	232976	174236	3.88%	0.459%
24	12.674	1798	1800	1803	rVB	183258	139591	3.11%	0.367%
25	12.827	1821	1826	1829	rBV	2729969	2566984	57.21%	6.758%
26	13.351	1913	1915	1919	rVB	164383	137637	3.07%	0.362%
27	13.721	1975	1978	1982	rBV	510358	499227	11.13%	1.314%
28	13.874	2001	2004	2007	rVB	843881	739608	16.48%	1.947%
29	15.304	2243	2247	2260	rVB	524386	776036	17.30%	2.043%

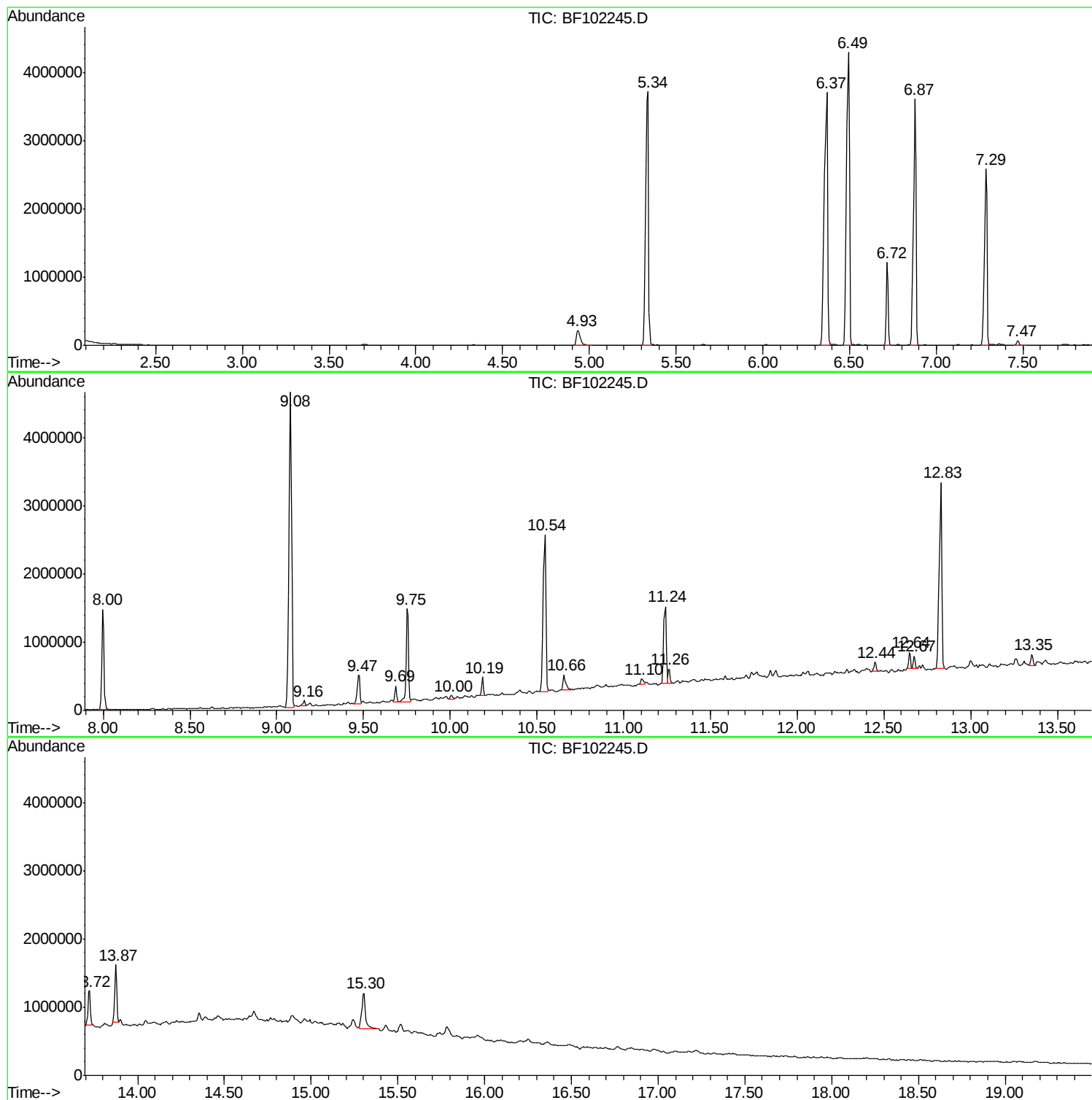
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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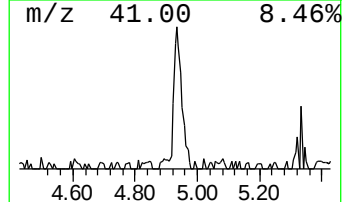
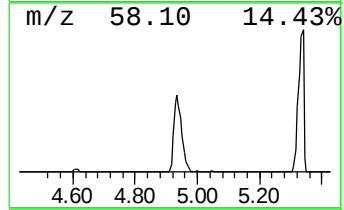
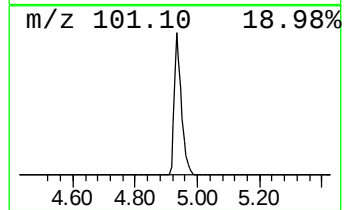
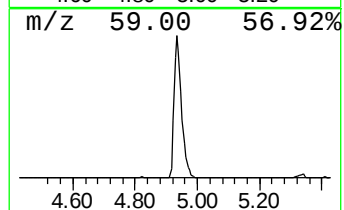
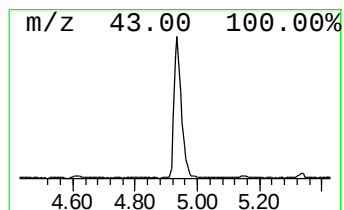
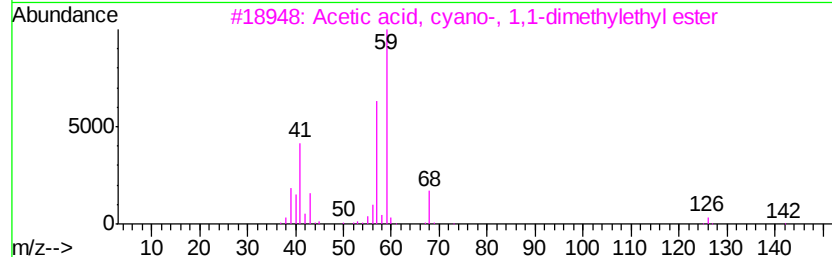
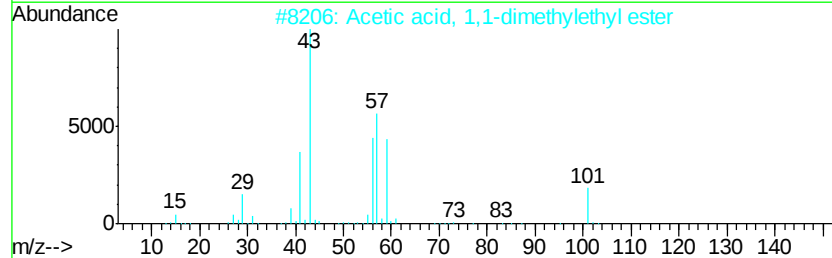
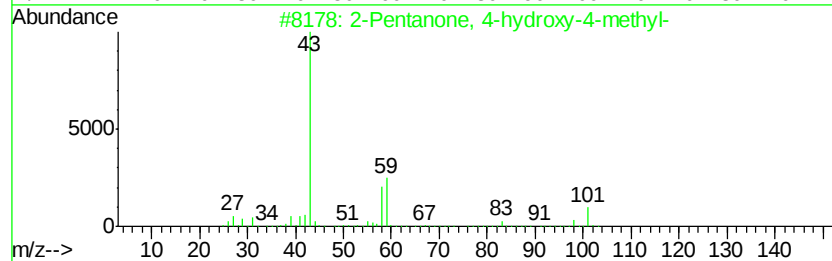
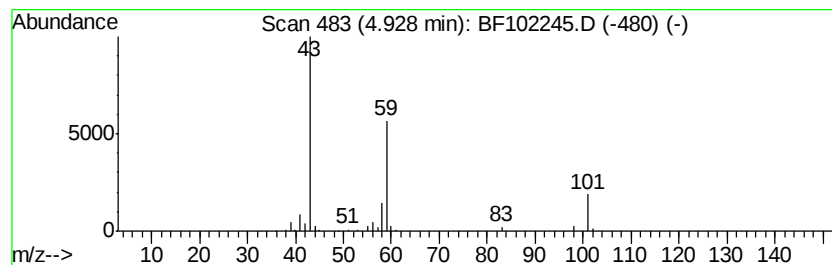
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	7.50 ng	369327	1,4-Dichlorobenzene-d4	6.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	32
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5			Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17



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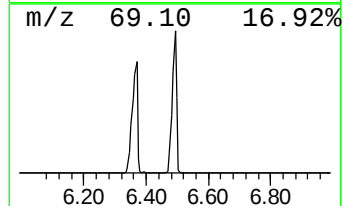
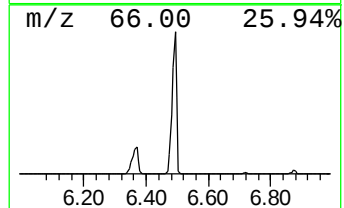
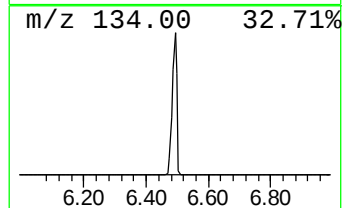
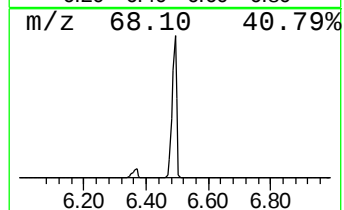
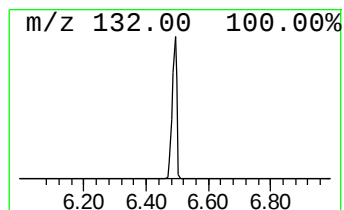
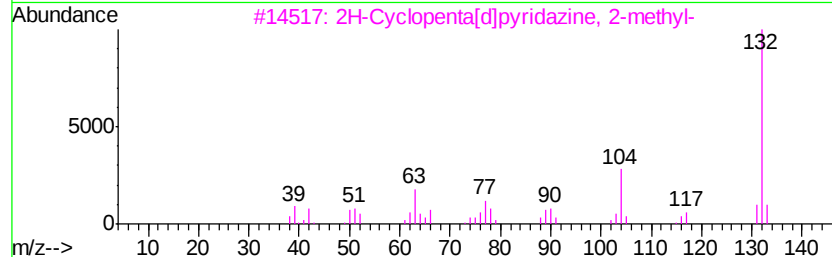
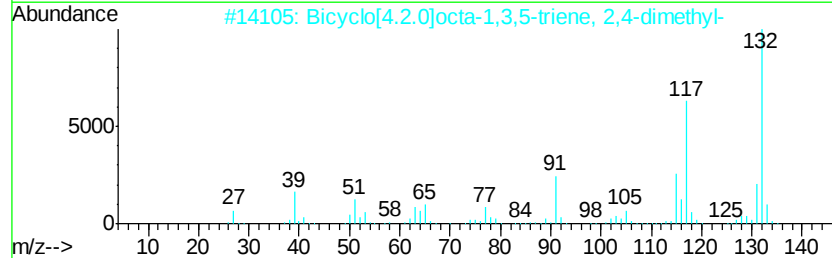
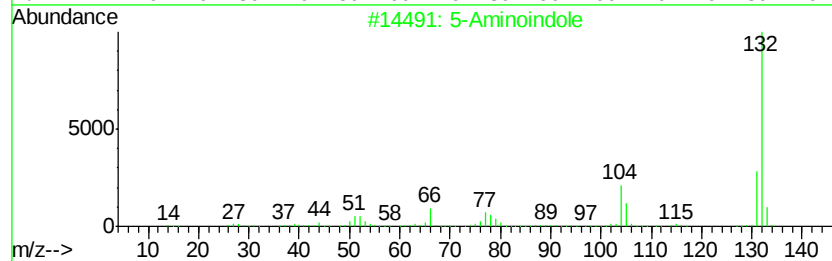
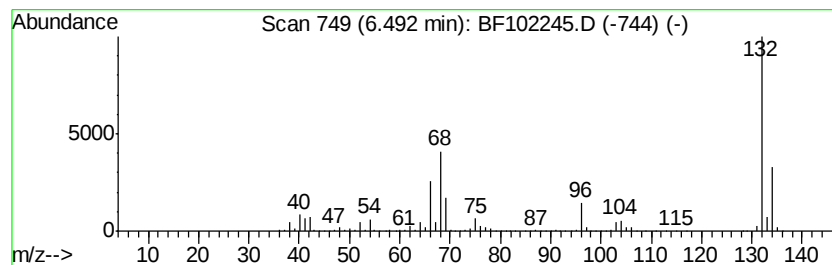
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Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	90.76 ng	4468200	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Aminoindole	132	C8H8N2	005192-03-0	12
2		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



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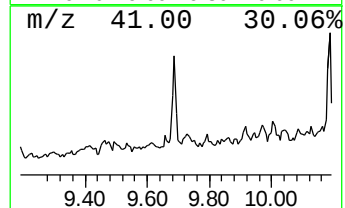
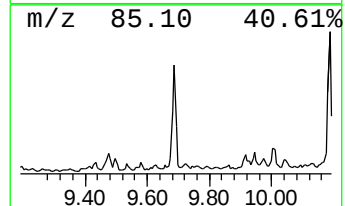
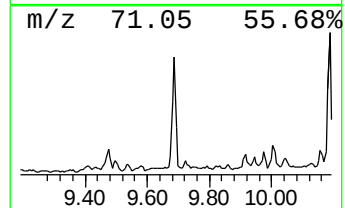
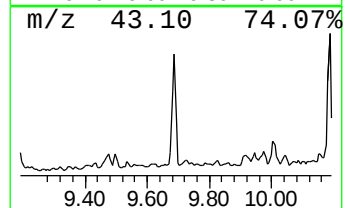
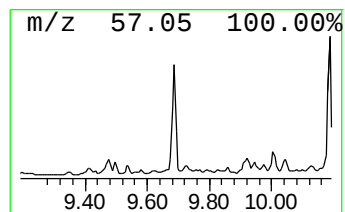
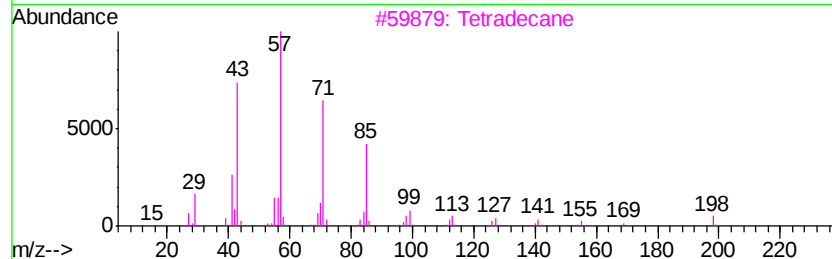
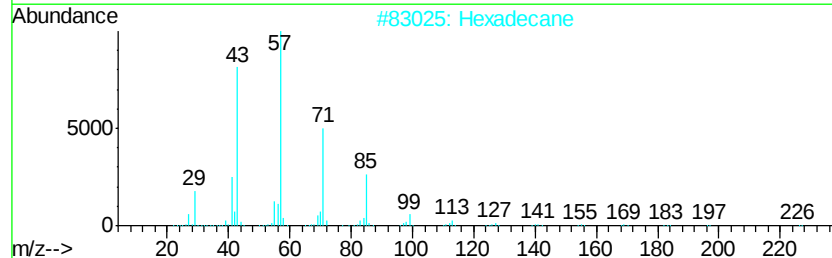
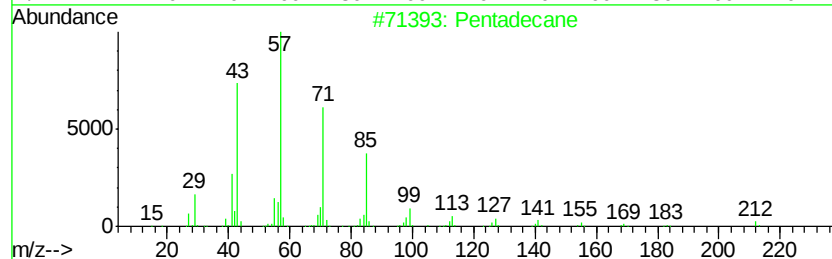
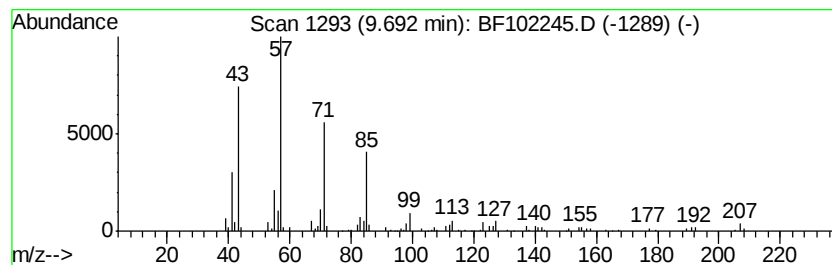
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Pentadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.69	2.56 ng	173749	Acenaphthene-d10	9.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane		212	C15H32	000629-62-9	94
2	Hexadecane		226	C16H34	000544-76-3	90
3	Tetradecane		198	C14H30	000629-59-4	90
4	Tridecane		184	C13H28	000629-50-5	83
5	Octacosane		394	C28H58	000630-02-4	83



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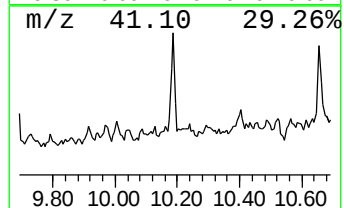
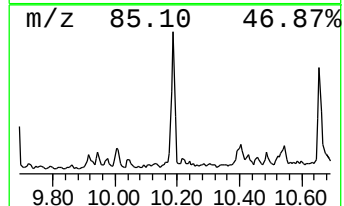
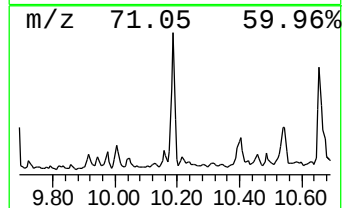
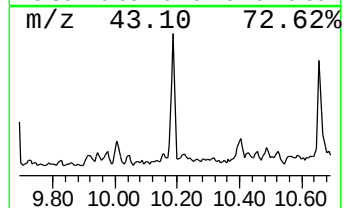
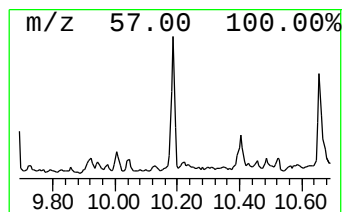
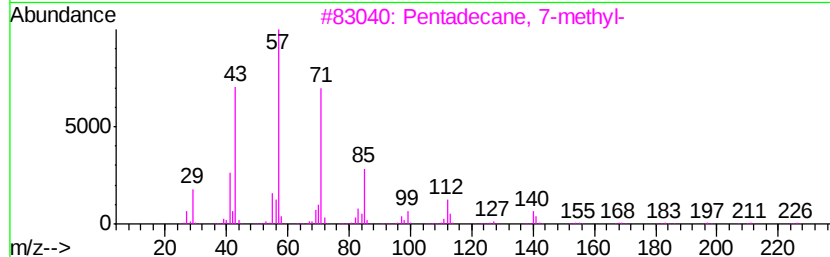
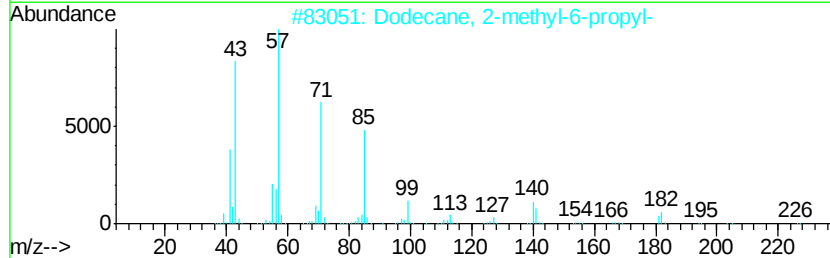
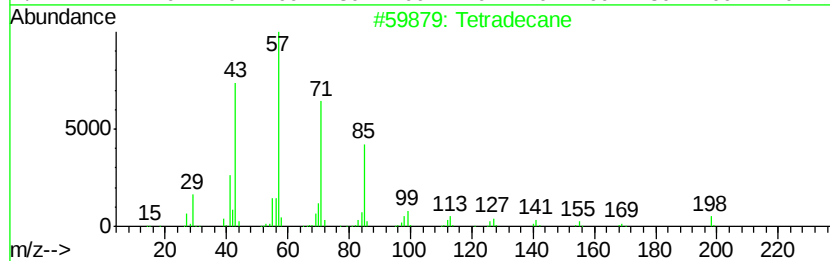
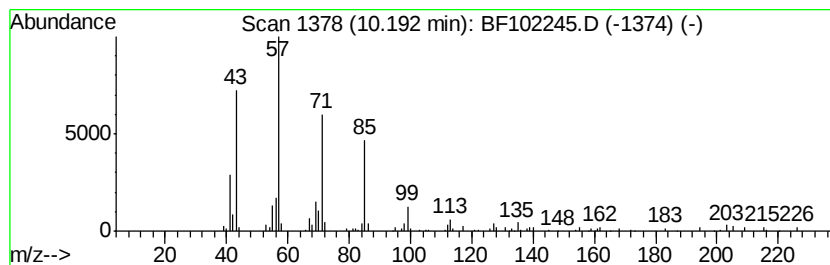
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Peak Number 5 Tetradecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.19	2.77 ng	187797	Acenaphthene-d10	9.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecane	198	C14H30	000629-59-4	86
2		Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	80
3		Pentadecane, 7-methyl-	226	C16H34	006165-40-8	72
4		Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	72
5		Sulfurous acid, 2-propyl tetradec...	320	C17H36O3S	1000309-12-5	64



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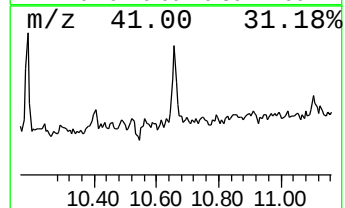
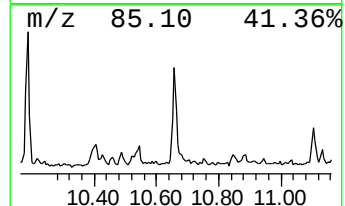
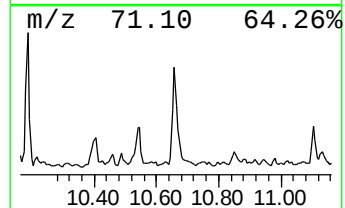
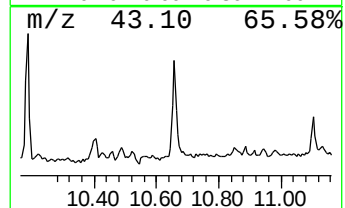
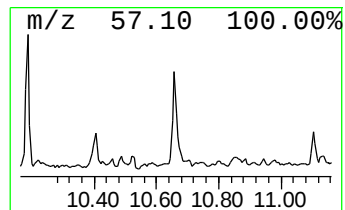
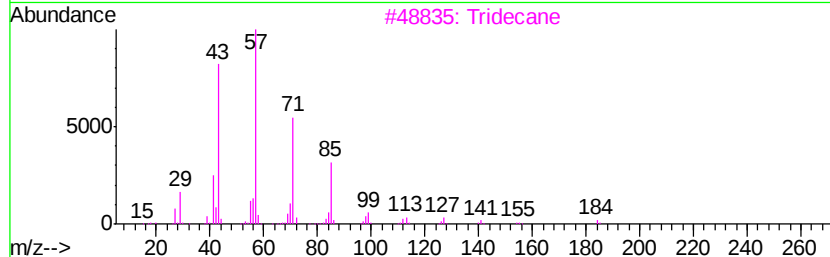
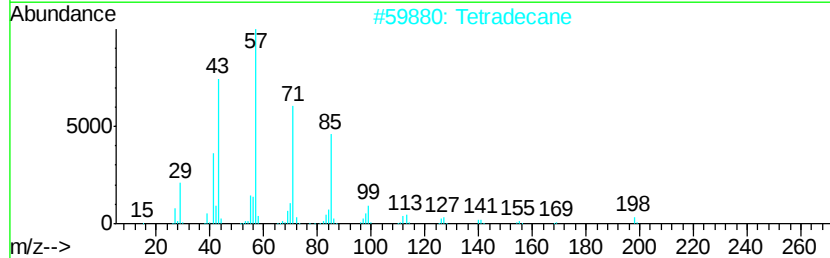
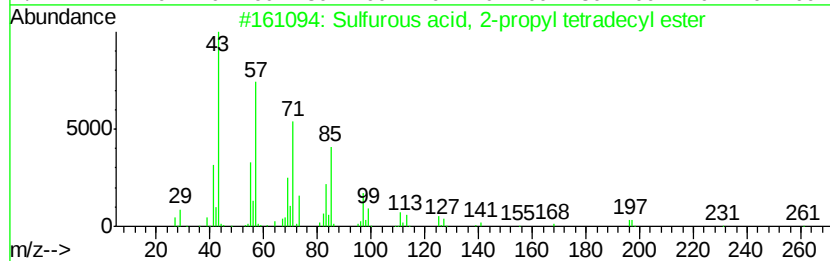
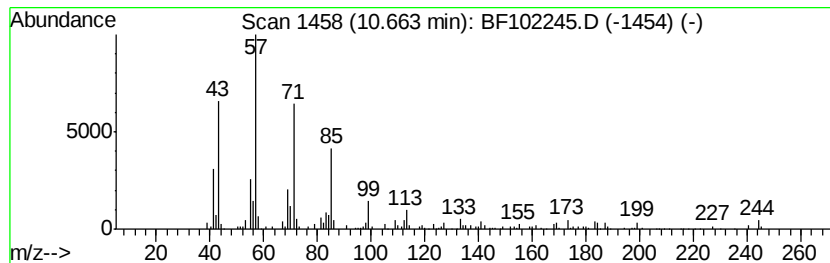
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Peak Number 6 Sulfurous acid, 2-propyl te... Concentration Rank 5

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10.66	4.85 ng	241176	Phenanthrene-d10	11.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, 2-propyl tetradec...	320	C17H36O3S	1000309-12-5	90
2		Tetradecane	198	C14H30	000629-59-4	90
3		Tridecane	184	C13H28	000629-50-5	86
4		Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	86
5		Tridecane, 7-propyl-	226	C16H34	055045-09-5	64



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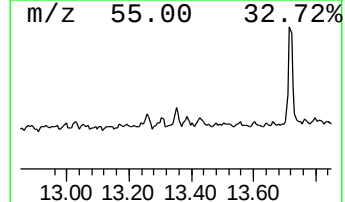
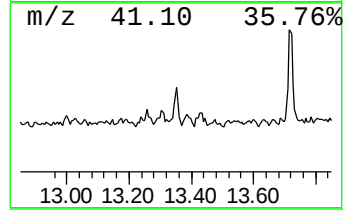
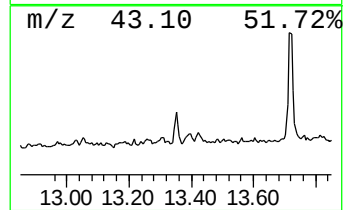
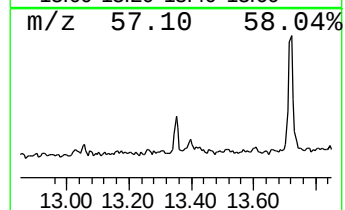
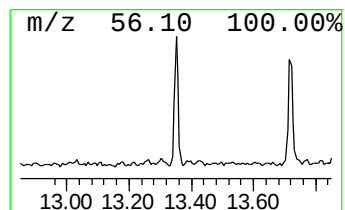
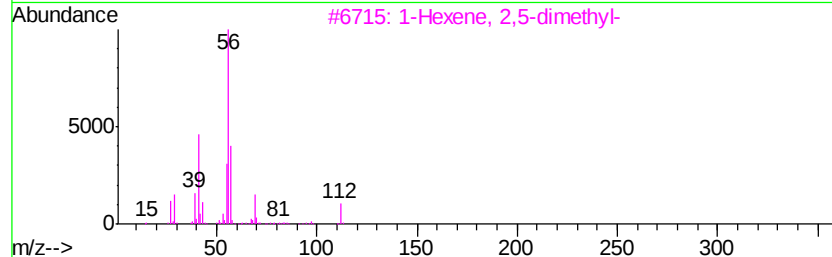
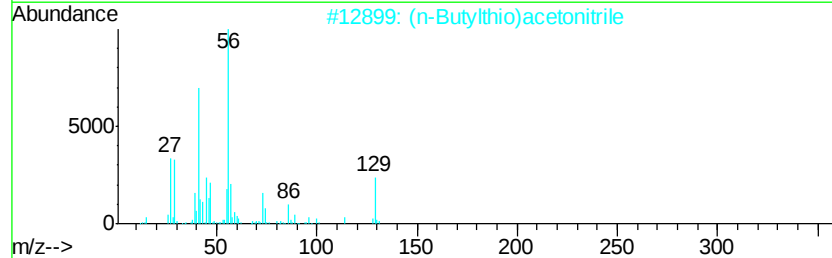
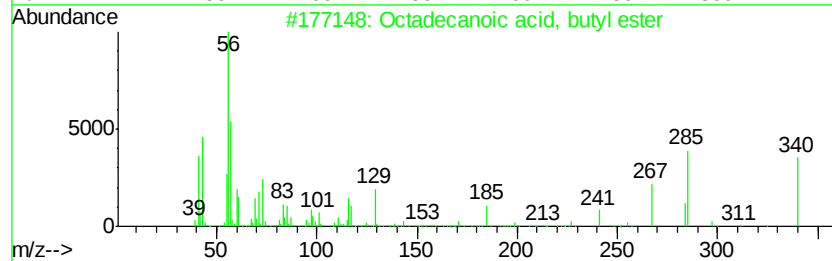
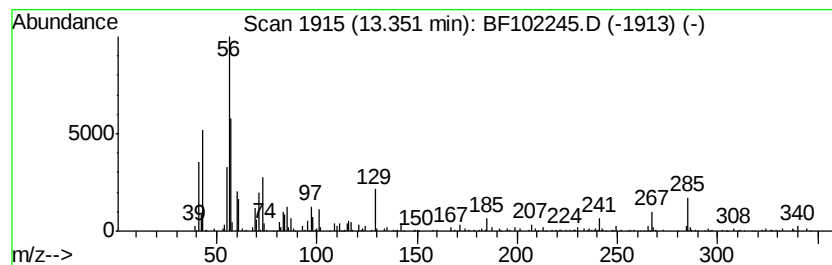
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.35	3.72 ng	137637	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	78
2		(n-Butylthio)acetonitrile	129	C6H11NS	071037-08-6	47
3		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27
4		Docosanoic acid	340	C22H44O2	000112-85-6	25
5		1-Undecene, 10-methyl-	168	C12H24	022370-55-4	25



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
Data File : BF102245.D
Acq On : 20 Jan 2018 4:12
Operator : SJ/JU
Sample : J1113-07
Misc :
ALS Vial : 21 Sample Multiplier: 1

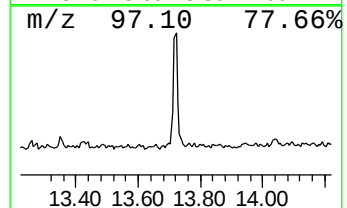
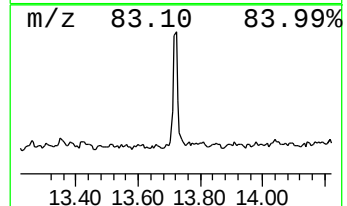
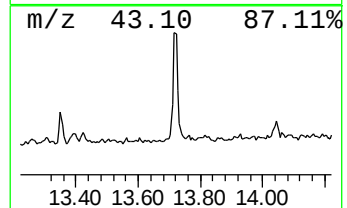
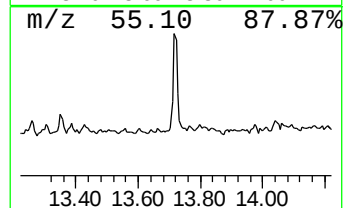
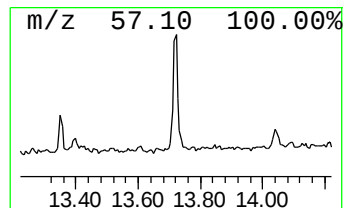
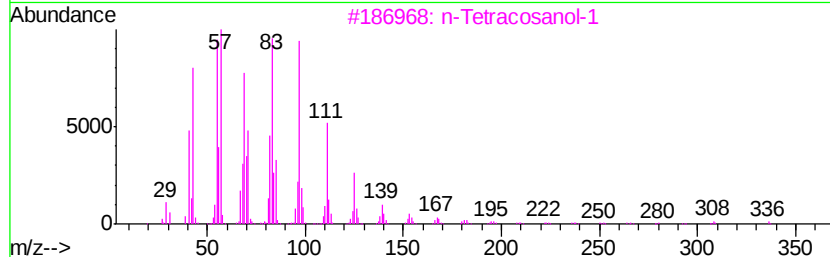
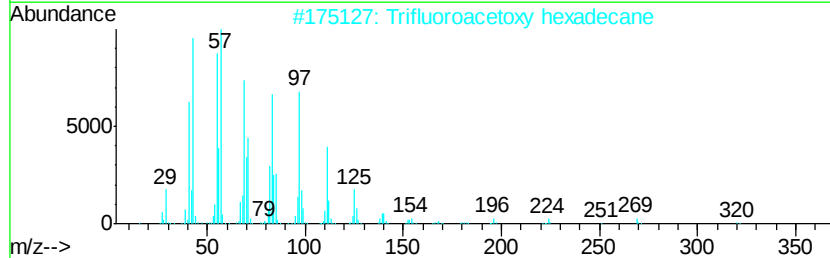
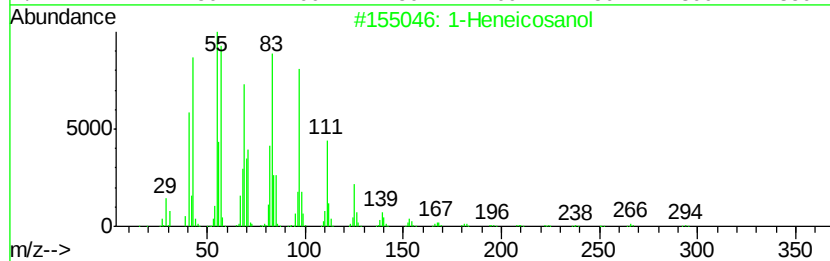
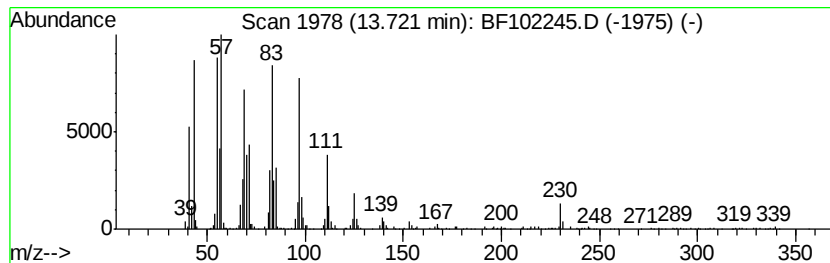
Instrument :
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ClientSampleId :
SB-14-2.5-3.0

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.72	13.50 ng	499227	Chrysene-d12	13.87		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	95
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	93
4		1-Docosene	308	C22H44	001599-67-3	91
5		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011918\
Data File : BF102245.D
Acq On : 20 Jan 2018 4:12
Operator : SJ/JU
Sample : J1113-07
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-14-2.5-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.93	7.5	ng	369327	1	6.72	984624	20.0
unknown6.49	6.49	90.8	ng	4468200	1	6.72	984624	20.0
Pentadecane	9.69	2.6	ng	173749	3	9.75	1357660	20.0
Tetradecane	10.19	2.8	ng	187797	3	9.75	1357660	20.0
Sulfurous acid, 2...	10.66	4.8	ng	241176	4	11.24	994191	20.0
Octadecanoic acid...	13.35	3.7	ng	137637	5	13.87	739608	20.0
1-Heneicosanol	13.72	13.5	ng	499227	5	13.87	739608	20.0