

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
 Data File : BF098783.D
 Acq On : 25 Sep 2017 15:08
 Operator : SJ/JU
 Sample : I5364-03
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SASP2P-ENV-125-17(0-5)

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-BF092317.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	2.222	19	23	31	rVB	64771	88702	2.75%	0.315%
2	5.146	516	520	531	rVB	484574	582368	18.07%	2.068%
3	5.540	581	587	590	rBV	3036945	3137173	97.36%	11.139%
4	6.540	751	757	760	rBV	3031772	3189108	98.97%	11.324%
5	6.687	777	782	785	rBV	3347860	3222298	100.00%	11.441%
6	6.916	817	821	824	rVB	1128737	881926	27.37%	3.131%
7	7.075	843	848	851	rBV	2659558	2442636	75.80%	8.673%
8	7.475	911	916	919	rBV	1977544	1943182	60.30%	6.900%
9	8.198	1035	1039	1042	rBV	1361653	1122229	34.83%	3.985%
10	9.269	1216	1221	1225	rVB	3270563	3061014	94.99%	10.869%
11	9.663	1284	1288	1291	rVB	341733	297815	9.24%	1.057%
12	9.951	1333	1337	1341	rVB2	1201744	1047772	32.52%	3.720%
13	10.375	1406	1409	1412	rVB	70578	51004	1.58%	0.181%
14	10.739	1467	1471	1474	rBV	1668237	1387176	43.05%	4.925%
15	10.845	1486	1489	1499	rVB	77992	80288	2.49%	0.285%
16	11.292	1562	1565	1568	rBV	41342	37696	1.17%	0.134%
17	11.439	1586	1590	1593	rBV	1036324	837652	26.00%	2.974%
18	11.951	1672	1677	1682	rBV2	137790	145712	4.52%	0.517%
19	12.651	1792	1796	1800	rBV	115863	96240	2.99%	0.342%
20	12.833	1823	1827	1830	rBV2	45277	40793	1.27%	0.145%
21	12.880	1830	1835	1839	rBV	114865	116314	3.61%	0.413%
22	13.021	1855	1859	1862	rBV	2363298	2039444	63.29%	7.241%
23	13.904	2006	2009	2017	rVB2	176223	184478	5.73%	0.655%
24	14.051	2031	2034	2035	rBV	52350	51795	1.61%	0.184%
25	14.080	2035	2039	2041	rVV	859490	861101	26.72%	3.058%
26	14.104	2041	2043	2048	rVB	60673	54938	1.70%	0.195%
27	14.833	2164	2167	2176	rVB2	124903	163394	5.07%	0.580%
28	14.927	2180	2183	2189	rVV	233103	228658	7.10%	0.812%
29	15.127	2214	2217	2220	rBV	59792	86467	2.68%	0.307%
30	15.568	2288	2292	2303	rVB	486463	684026	21.23%	2.429%

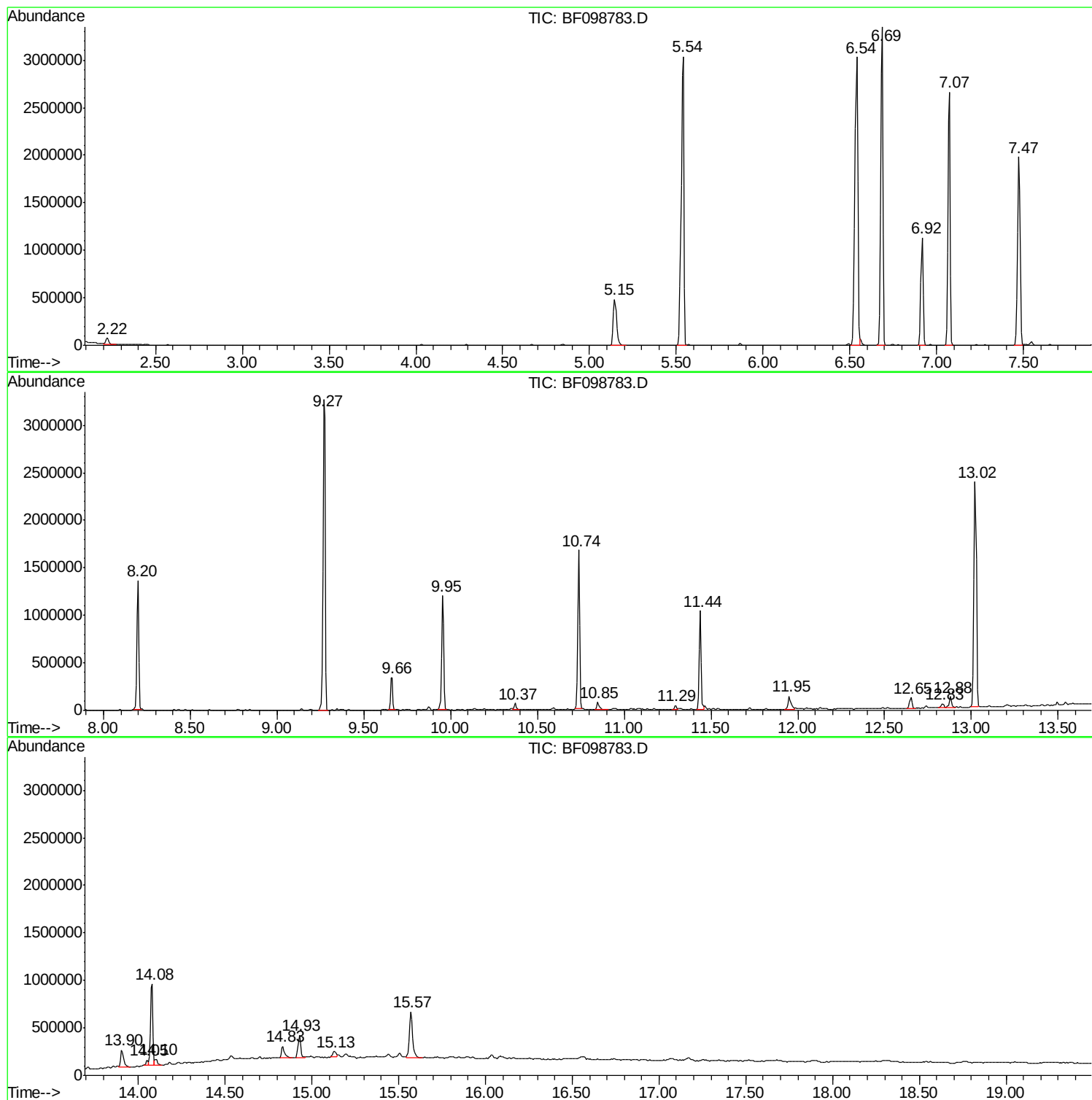
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-ENV-125-17(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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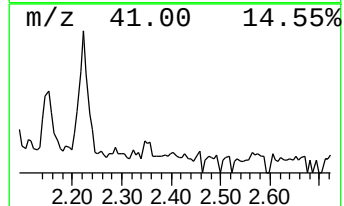
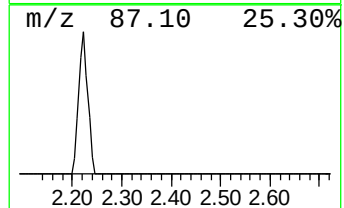
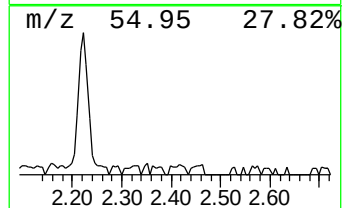
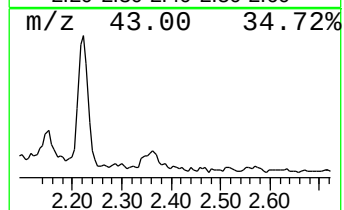
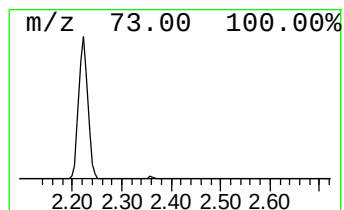
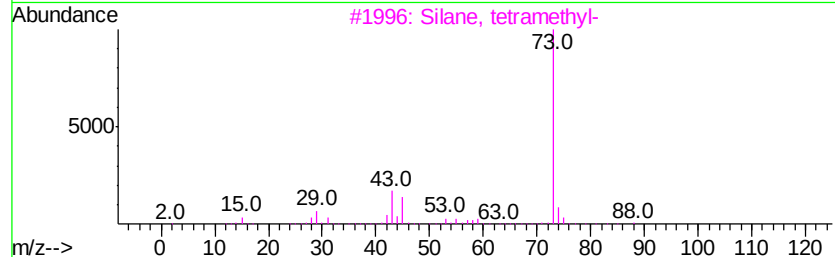
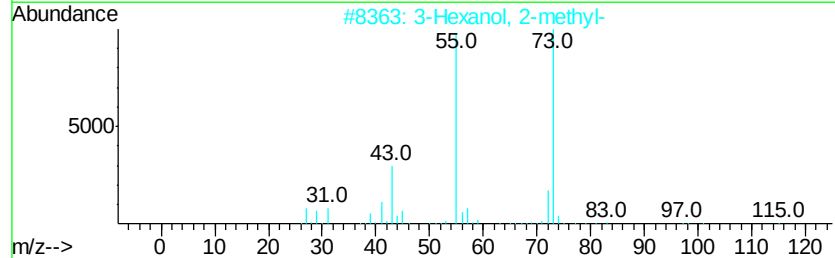
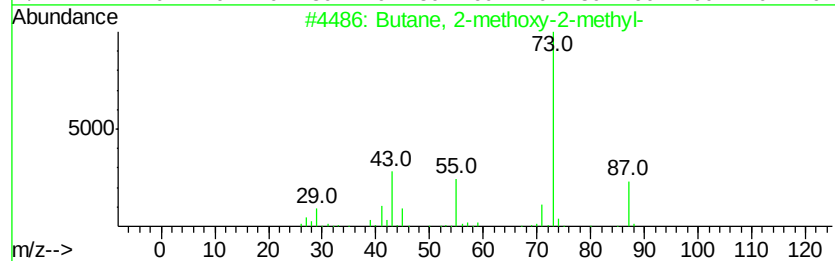
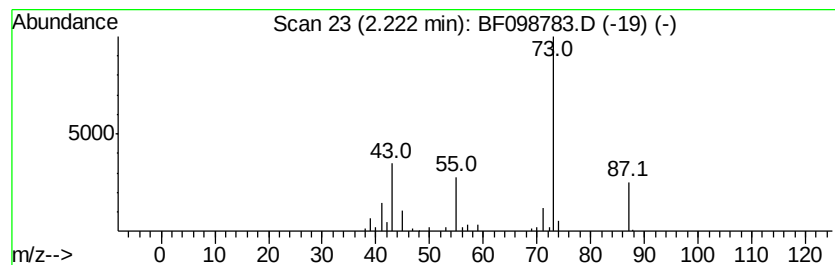
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	2.01 ng	88702	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	23
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
4		Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	10
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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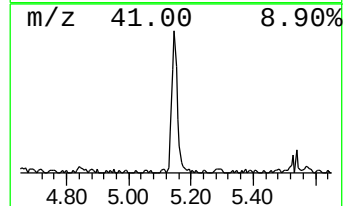
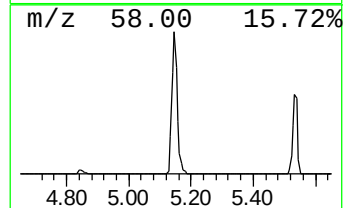
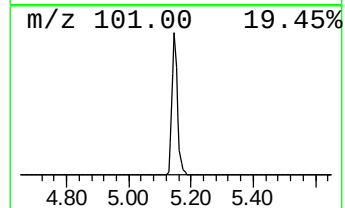
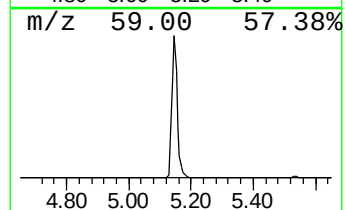
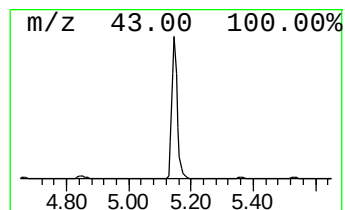
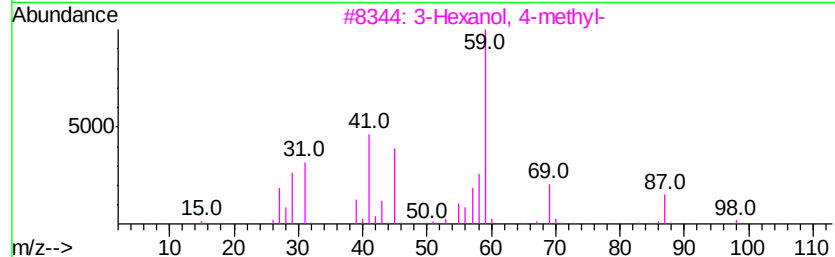
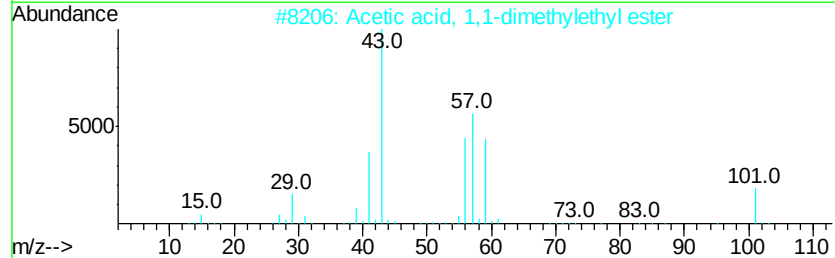
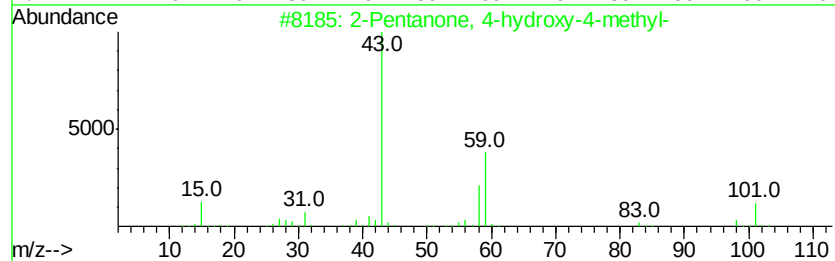
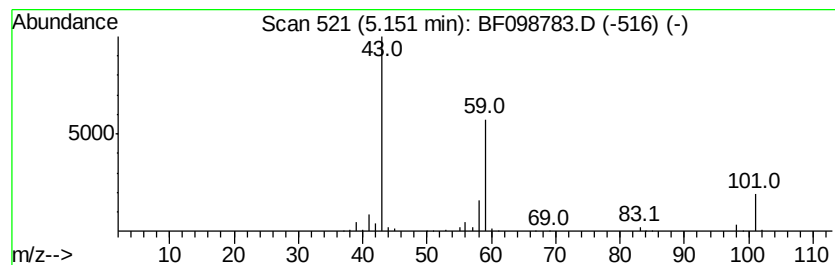
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	13.21 ng	582368	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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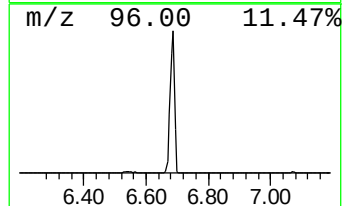
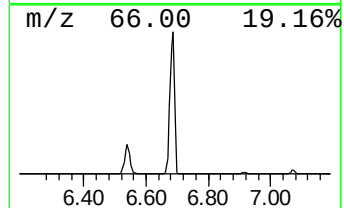
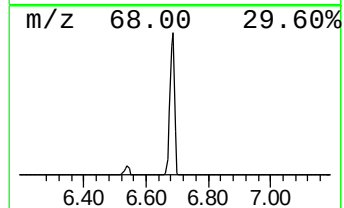
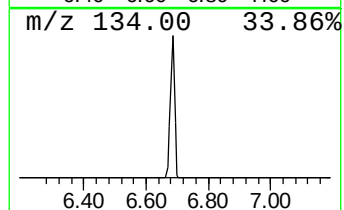
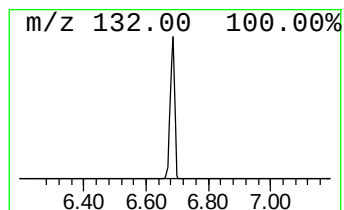
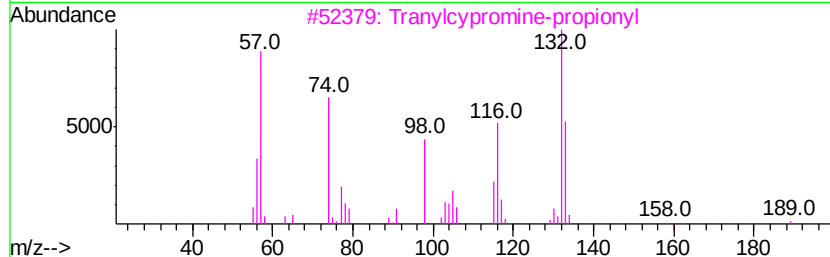
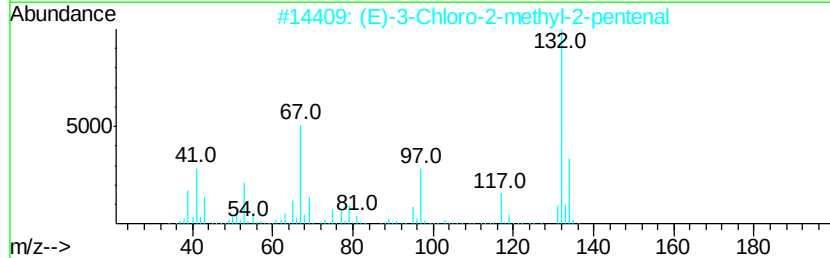
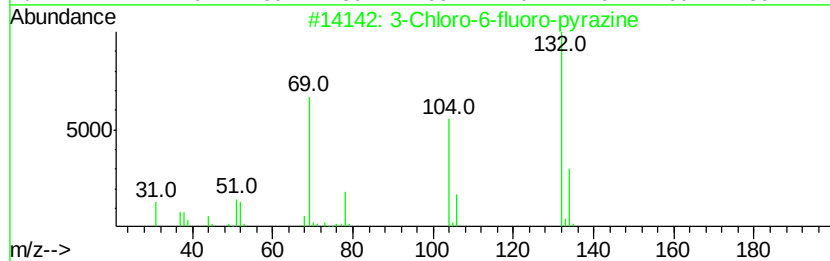
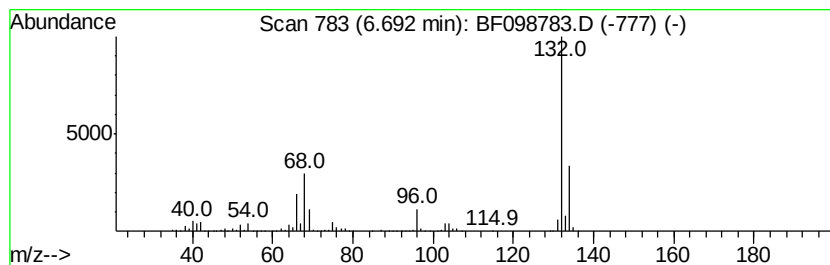
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Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	73.07 ng	3222300	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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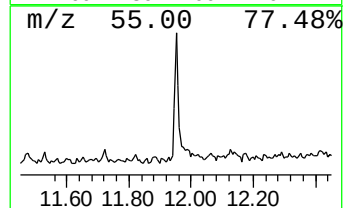
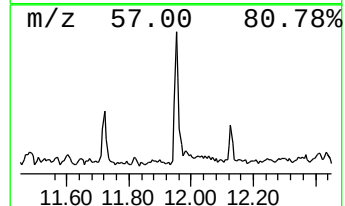
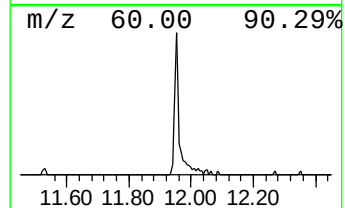
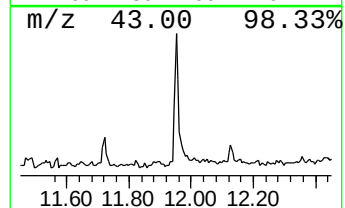
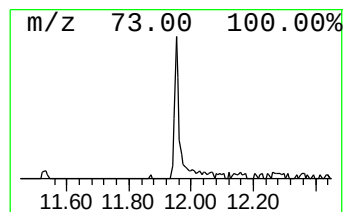
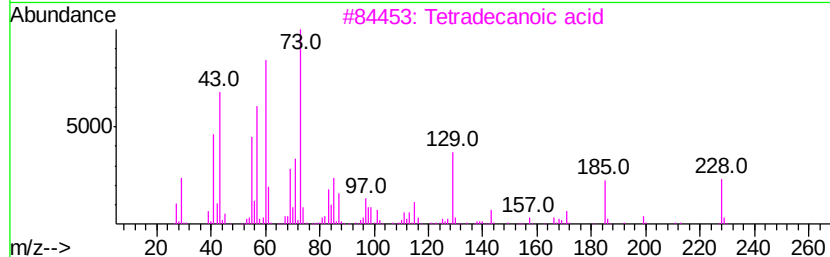
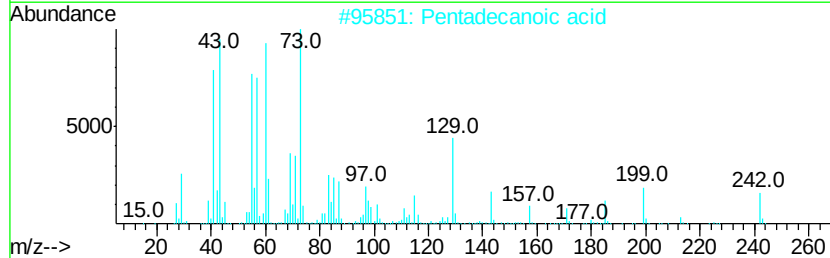
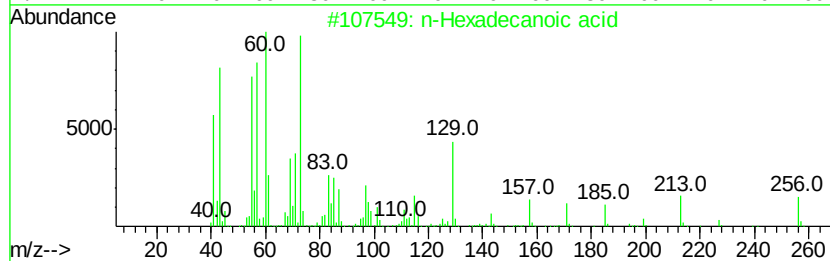
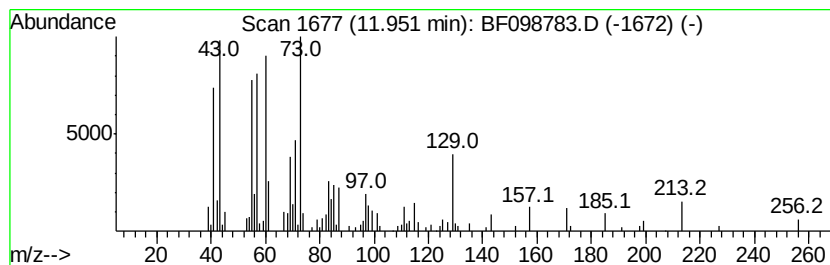
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	3.48 ng	145712	Phenanthrene-d10	11.44

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4		n-Decanoic acid	172	C10H20O2	000334-48-5	76
5		Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	18



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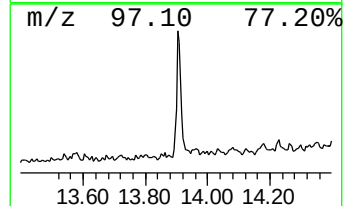
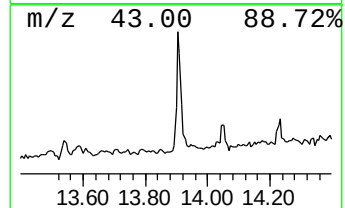
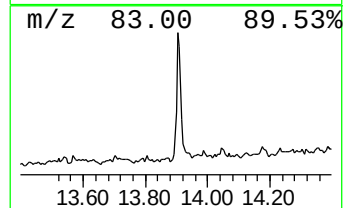
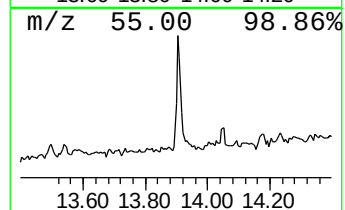
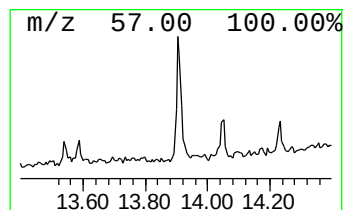
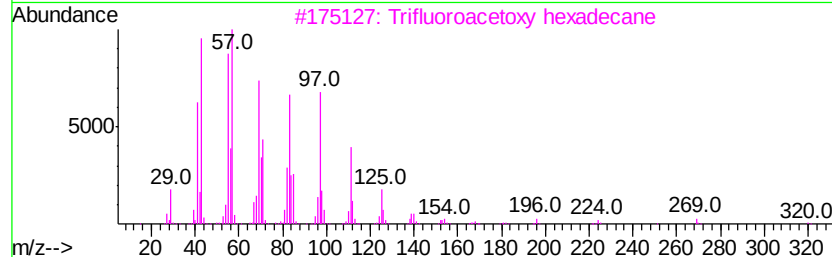
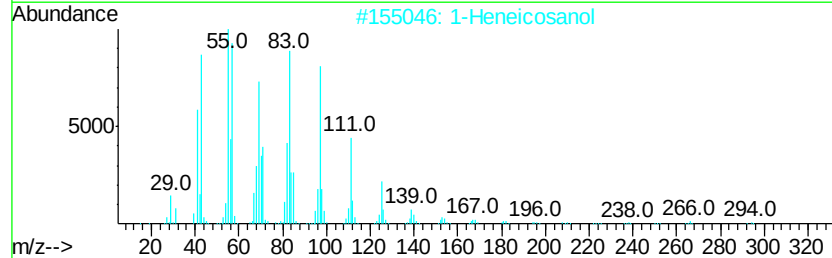
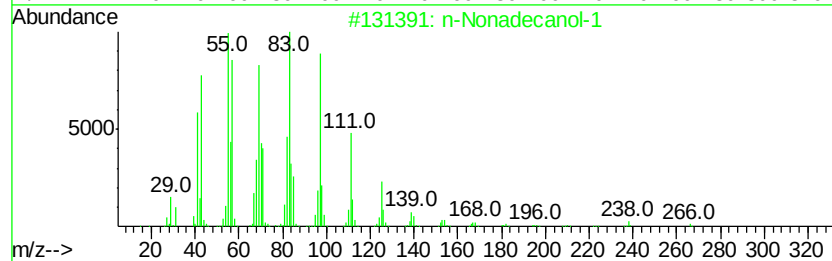
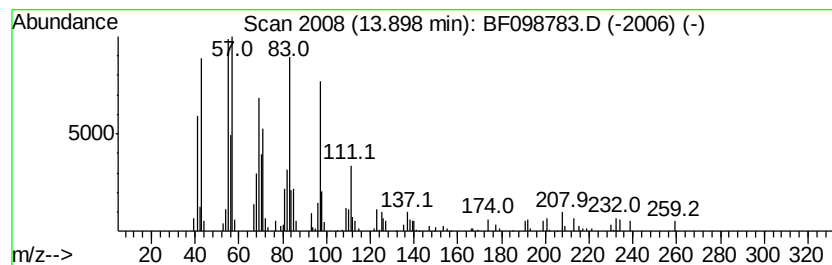
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Peak Number 7 n-Nonadecanol-1 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.90	4.28 ng	184478	Chrysene-d12	14.08	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
2	1-Heneicosanol	312	C21H44O	015594-90-8	94
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4	Behenic alcohol	326	C22H46O	000661-19-8	94
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94



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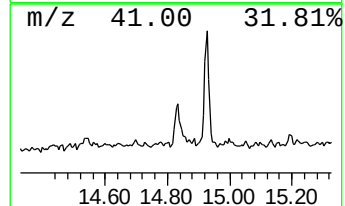
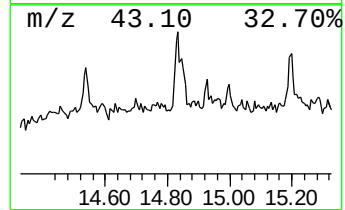
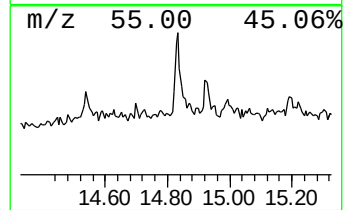
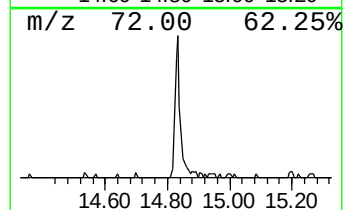
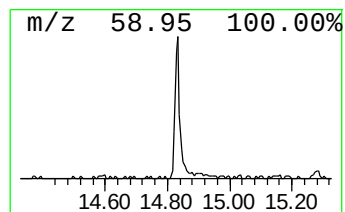
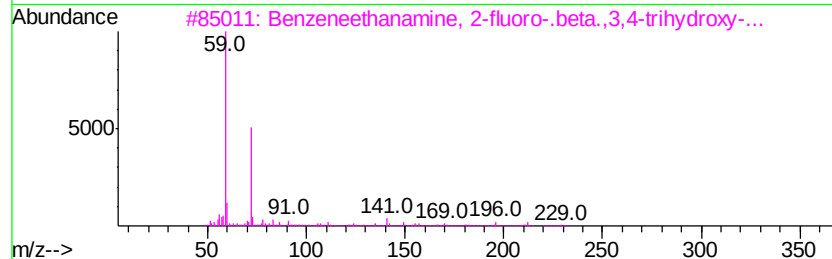
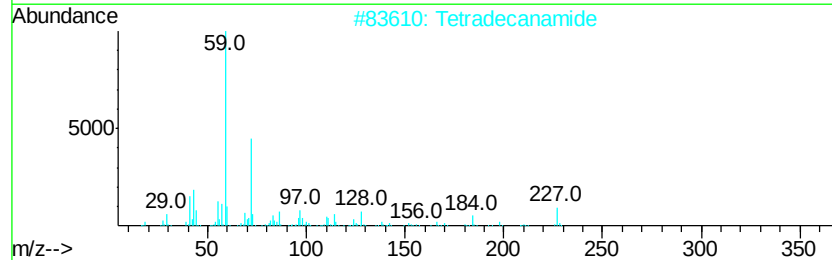
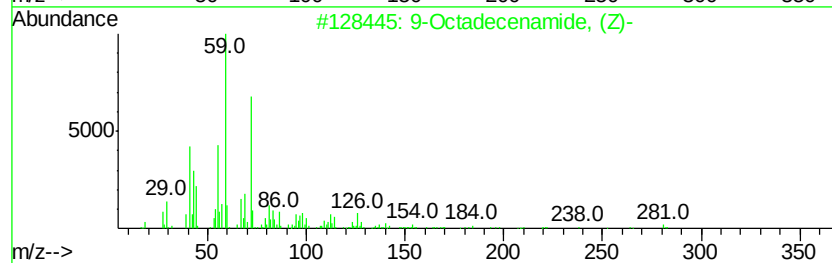
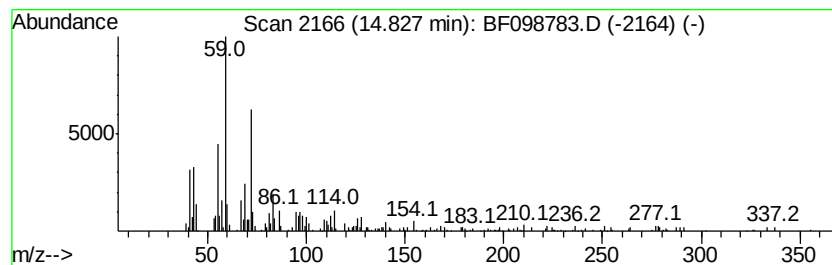
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	4.78 ng	163394	Perylene-d12	15.57

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2		Tetradecanamide	227	C14H29NO	000638-58-4	78
3		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	64
4		3-Hydroxy-3-methyl-butvric acid,...	132	C5H12N2O2	1000193-80-2	53
5		Dodecanamide	199	C12H25NO	001120-16-7	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092517\
Data File : BF098783.D
Acq On : 25 Sep 2017 15:08
Operator : SJ/JU
Sample : I5364-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-ENV-125-17(0-5)

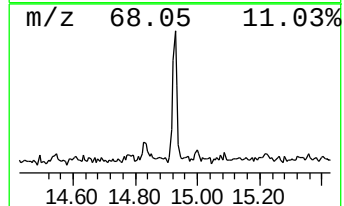
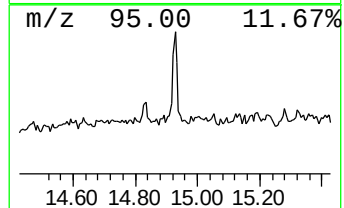
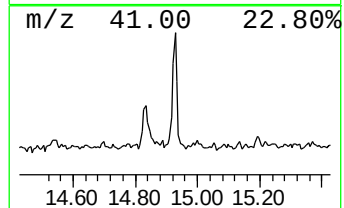
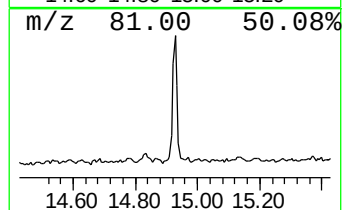
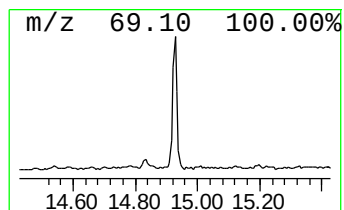
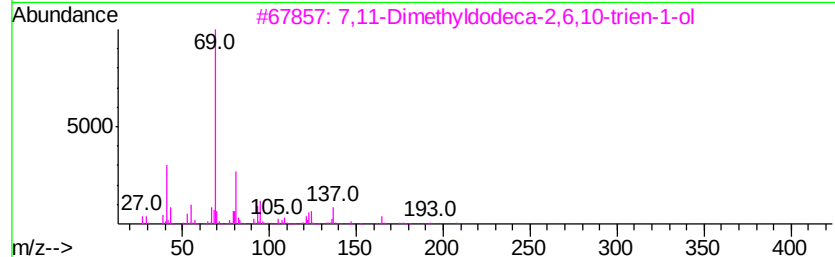
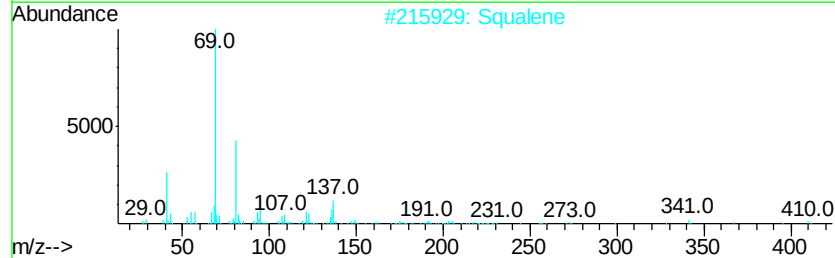
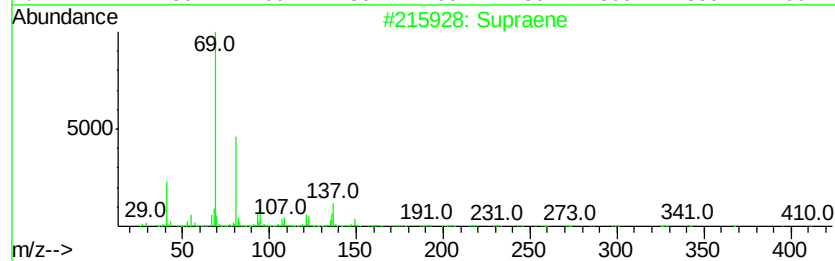
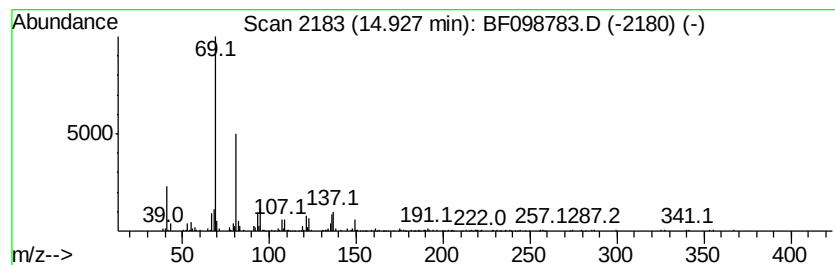
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.93	6.69 ng	228658	Perylene-d12	15.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	91
2		Squalene	410	C30H50	000111-02-4	86
3		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4		2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	53
5		Methanone, dicyclopropyl-	110	C7H10O	001121-37-5	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092517\
Data File : BF098783.D
Acq On : 25 Sep 2017 15:08
Operator : SJ/JU
Sample : I5364-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-ENV-125-17(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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
Butane, 2-methoxy...	2.22	2.0	ng	88702	1	6.92	881926	20.0
2-Pentanone, 4-hy...	5.15	13.2	ng	582368	1	6.92	881926	20.0
unknown6.69	6.69	73.1	ng	3222300	1	6.92	881926	20.0
n-Hexadecanoic acid	11.95	3.5	ng	145712	4	11.44	837652	20.0
n-Nonadecanol-1	13.90	4.3	ng	184478	5	14.08	861101	20.0
9-Octadecenamide, ...	14.83	4.8	ng	163394	6	15.57	684026	20.0
Supraene	14.93	6.7	ng	228658	6	15.57	684026	20.0