

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032217\
 Data File : BF093869.D
 Acq On : 23 Mar 2017 8:35
 Operator : SJ/MA
 Sample : I2350-06
 Misc :
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VNJ-238-210-221-COMP

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-BF032217.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	2.104	34	37	46	rVB	132132	172655	3.04%	0.352%
2	4.140	378	383	394	rVB	687533	1018523	17.96%	2.075%
3	4.516	441	447	450	rBV	4267524	5294424	93.37%	10.784%
4	4.910	511	514	520	rVB	65298	61750	1.09%	0.126%
5	5.204	561	564	574	rVB	62217	64075	1.13%	0.131%
6	5.575	619	627	631	rVB	4036679	5670205	100.00%	11.550%
7	5.728	647	653	657	rBV	4324622	5491966	96.86%	11.187%
8	5.986	693	697	701	rVB	1252870	1131816	19.96%	2.305%
9	6.169	722	728	731	rVB	3980169	4176729	73.66%	8.508%
10	6.633	800	807	810	rBV	2797686	3636860	64.14%	7.408%
11	7.486	947	952	956	rBV	1437033	1524229	26.88%	3.105%
12	8.816	1171	1178	1182	rBV	4658303	5604443	98.84%	11.416%
13	9.304	1256	1261	1265	rBV	593900	514817	9.08%	1.049%
14	9.633	1308	1317	1321	rBV2	1620750	1625749	28.67%	3.312%
15	10.180	1407	1410	1413	rVB	107260	95541	1.68%	0.195%
16	10.222	1413	1417	1421	rBV	108944	100106	1.77%	0.204%
17	10.498	1457	1464	1467	rBV	38951	57825	1.02%	0.118%
18	10.604	1476	1482	1486	rBV	2576045	3115804	54.95%	6.347%
19	10.810	1513	1517	1519	rBV	132443	146189	2.58%	0.298%
20	11.363	1607	1611	1614	rBV	120799	108691	1.92%	0.221%
21	11.457	1622	1627	1630	rBV	1531723	1440139	25.40%	2.933%
22	11.892	1695	1701	1705	rVB2	80292	89967	1.59%	0.183%
23	12.174	1745	1749	1752	rBV	119911	125947	2.22%	0.257%
24	12.945	1872	1880	1883	rBV	114252	115560	2.04%	0.235%
25	13.221	1923	1927	1931	rBV	88210	91864	1.62%	0.187%
26	13.268	1931	1935	1938	rVB	127792	114615	2.02%	0.233%
27	13.439	1958	1964	1967	rBV	3540844	3927374	69.26%	8.000%
28	14.145	2080	2084	2089	rBV	82665	87846	1.55%	0.179%
29	14.592	2157	2160	2170	rBV2	201418	306916	5.41%	0.625%
30	14.704	2174	2179	2183	rVV	988487	1064242	18.77%	2.168%
31	15.380	2291	2294	2300	rBV	64037	79463	1.40%	0.162%
32	16.098	2412	2416	2427	rBV3	127504	268518	4.74%	0.547%
33	16.345	2453	2458	2471	rBV	774369	966282	17.04%	1.968%
34	16.892	2547	2551	2555	rBV	55483	82658	1.46%	0.168%

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Integration Parameters: rteint.p
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Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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35	16.939	2555	2559	2566	rVB4	32856	57098	1.01%	0.116%
36	17.933	2720	2728	2736	rBV7	49505	133748	2.36%	0.272%
37	18.339	2791	2797	2808	rBV8	85455	212521	3.75%	0.433%
38	18.850	2878	2884	2894	rVB7	53927	137507	2.43%	0.280%
39	19.080	2917	2923	2937	rBV9	41679	120756	2.13%	0.246%
40	19.291	2953	2959	2966	rBV7	24557	58136	1.03%	0.118%

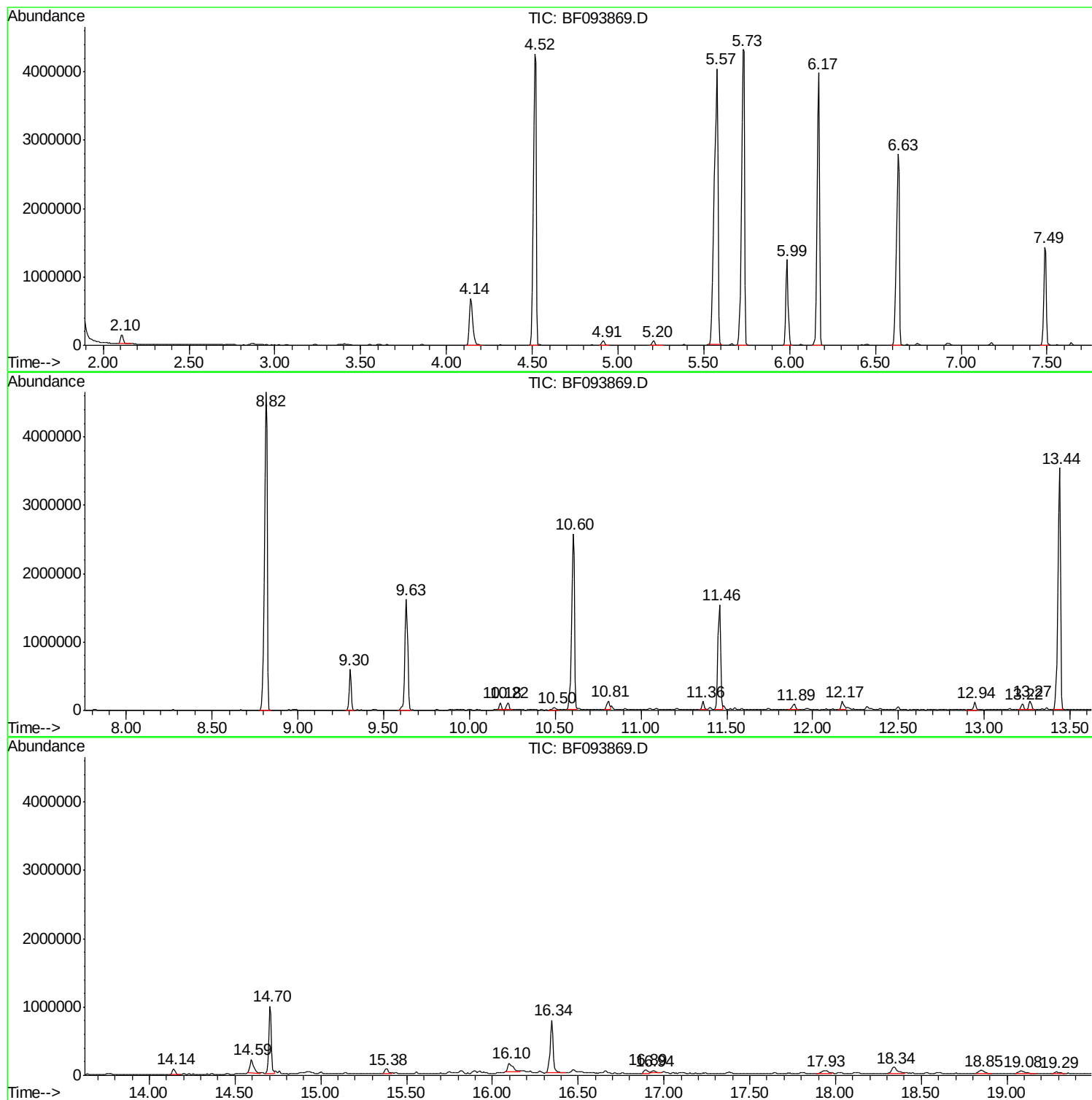
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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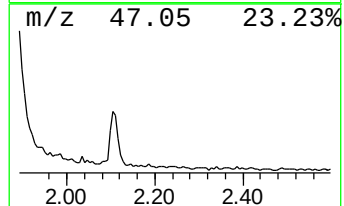
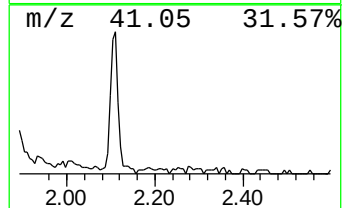
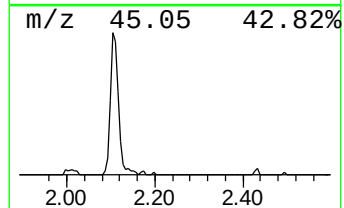
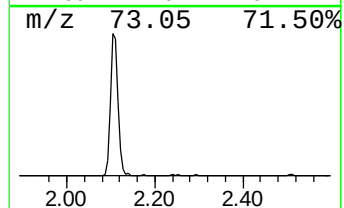
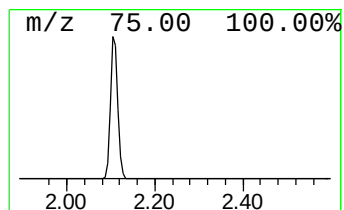
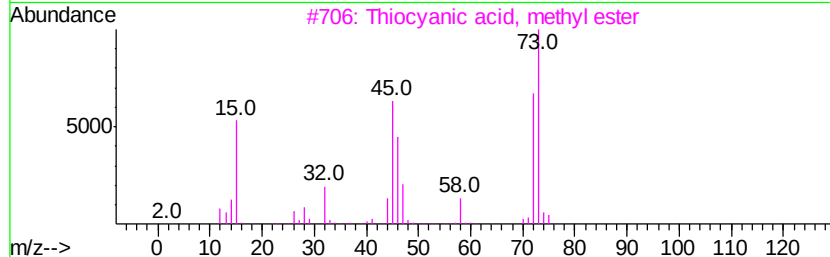
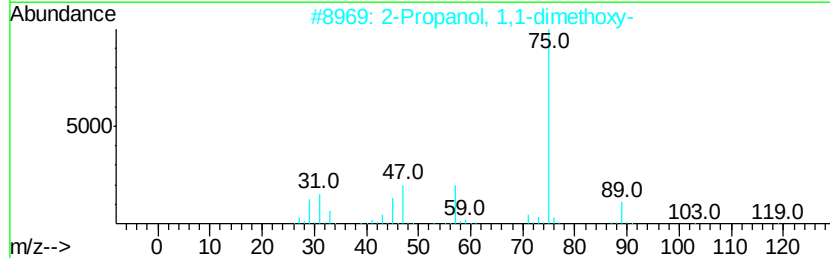
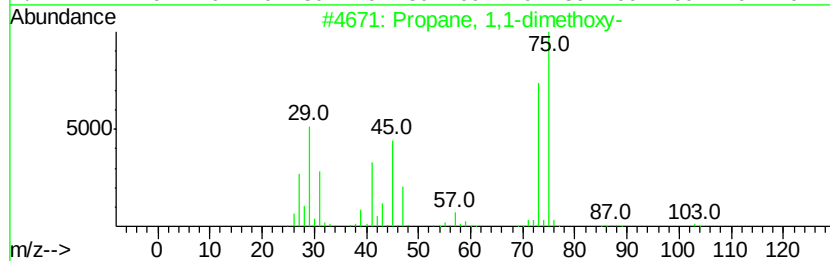
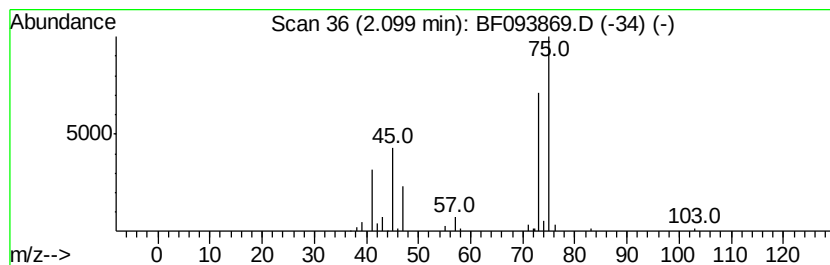
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.10	3.05 ng	172655	1,4-Dichlorobenzene-d4	5.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2		2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	42
3		Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	27
4		2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	10
5		Chloromethyl cyanide	75	C2H2ClN	000107-14-2	9



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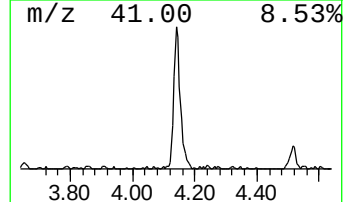
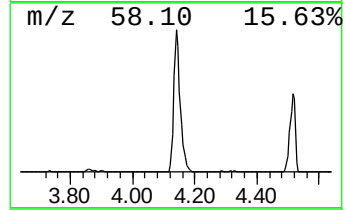
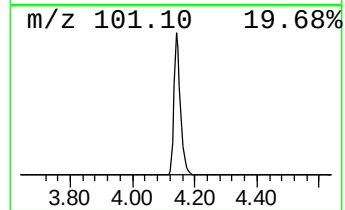
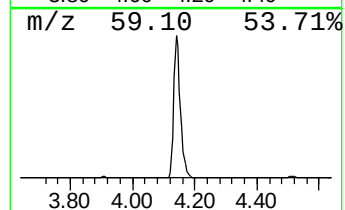
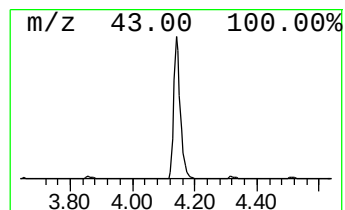
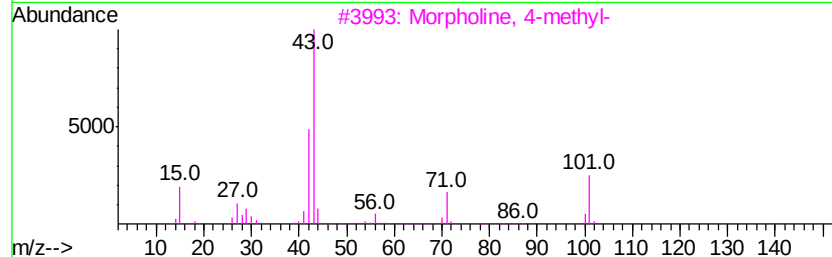
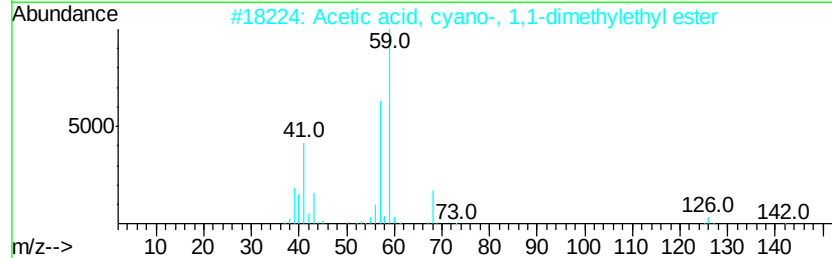
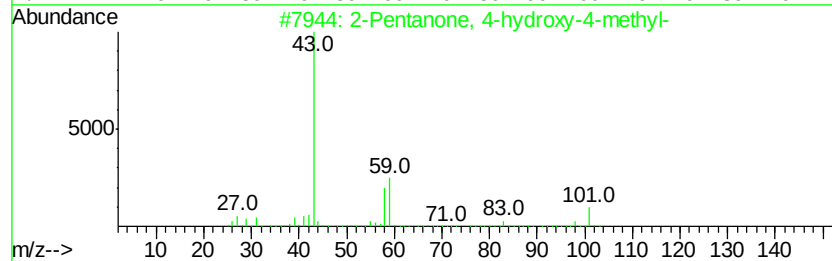
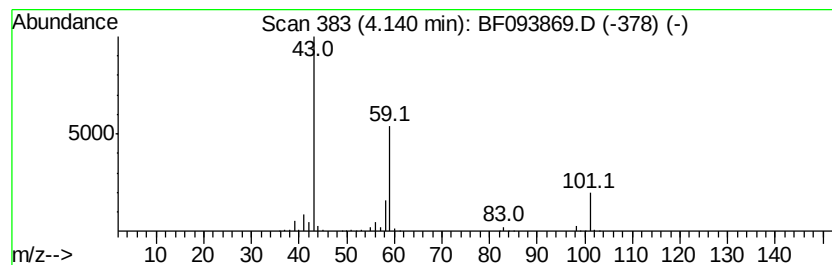
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.14	18.00 ng	1018520	1,4-Dichlorobenzene-d4	5.99

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, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9



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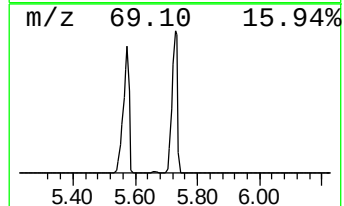
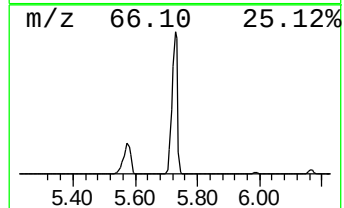
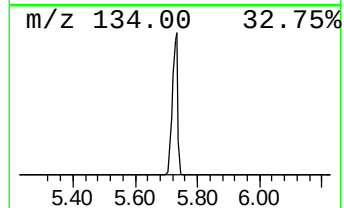
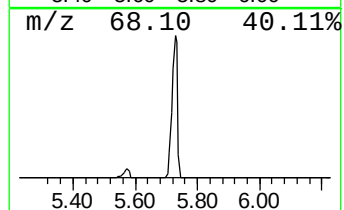
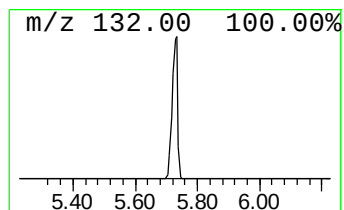
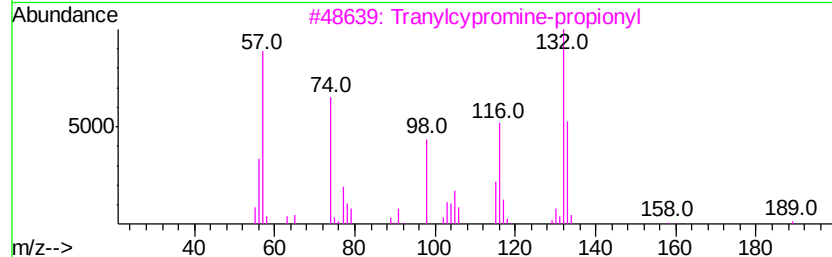
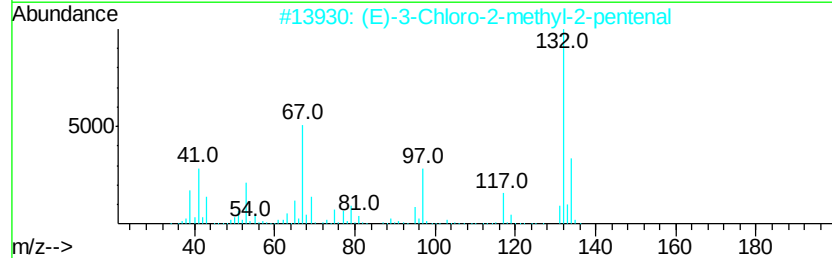
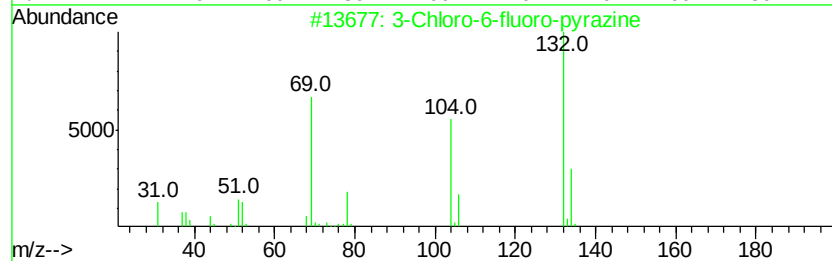
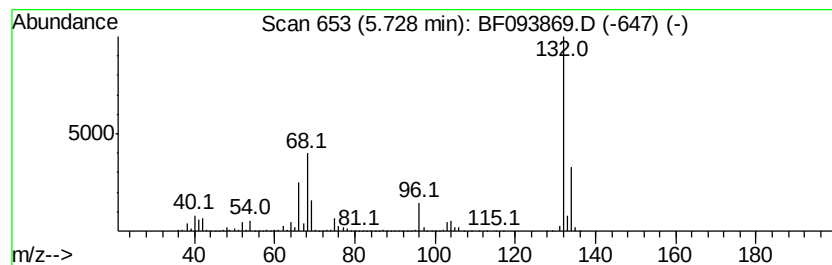
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Peak Number 3 unknown5.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.73	97.05 ng	5491970	1,4-Dichlorobenzene-d4	5.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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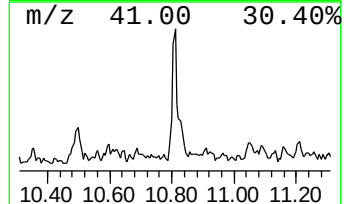
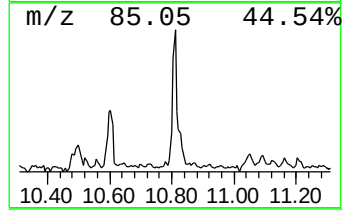
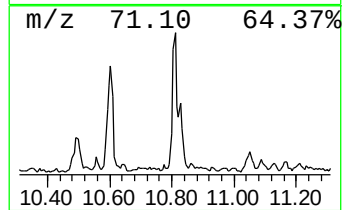
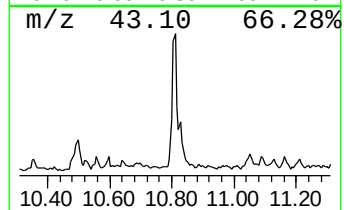
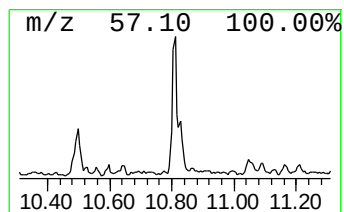
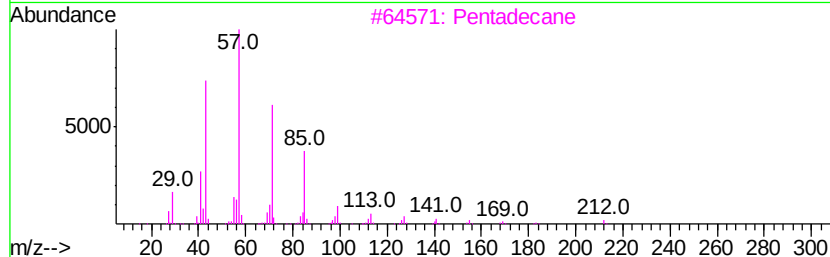
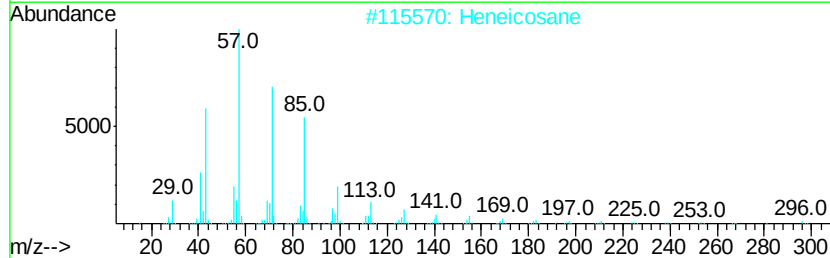
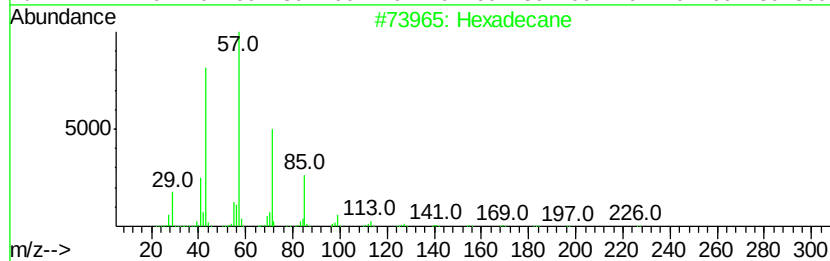
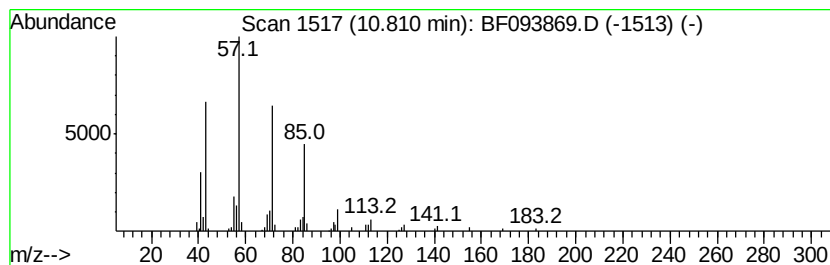
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.81	2.03 ng	146189	Phenanthrene-d10	11.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	90
2		Heneicosane	296	C21H44	000629-94-7	90
3		Pentadecane	212	C15H32	000629-62-9	87
4		Tetradecane	198	C14H30	000629-59-4	86
5		Nonacosane	408	C29H60	000630-03-5	86



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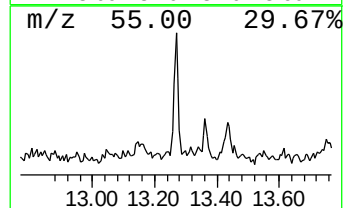
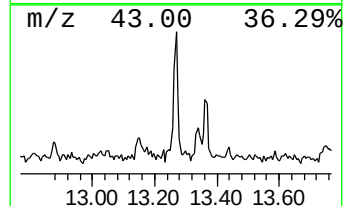
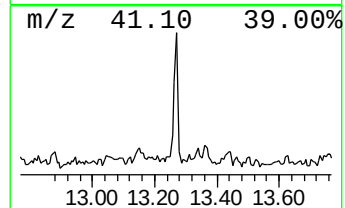
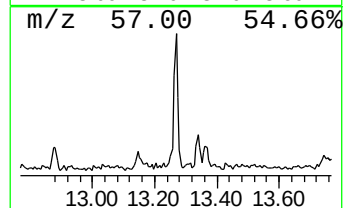
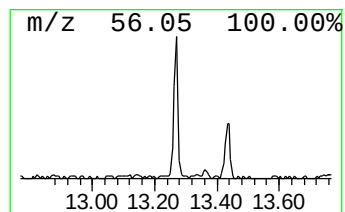
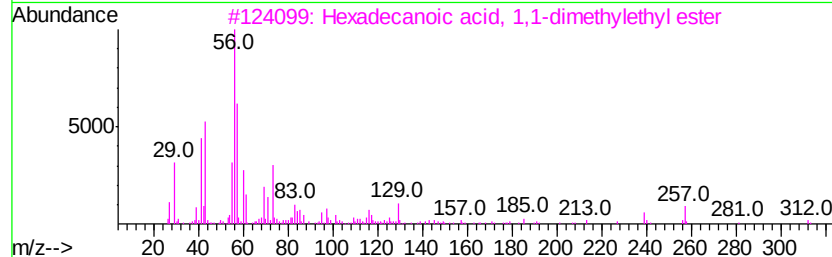
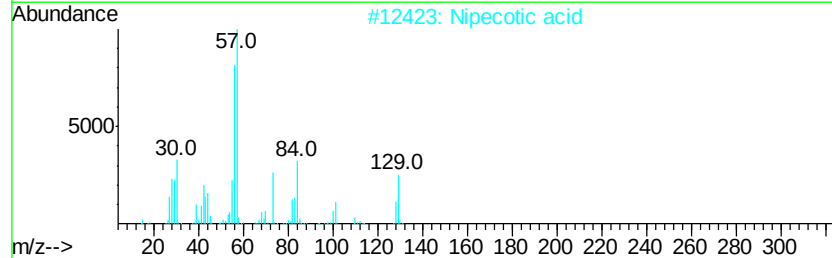
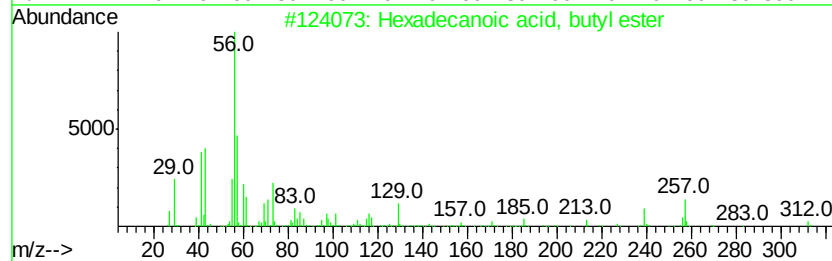
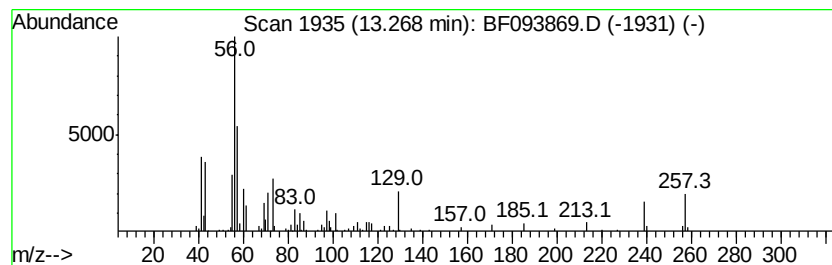
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.27	2.15 ng	114615	Chrysene-d12	14.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	83
2		Nipecotic acid	129	C6H11NO2	000498-95-3	47
3		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	43
4		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	38
5		Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	27



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032217\
Data File : BF093869.D
Acq On : 23 Mar 2017 8:35
Operator : SJ/MA
Sample : I2350-06
Misc :
ALS Vial : 38 Sample Multiplier: 1

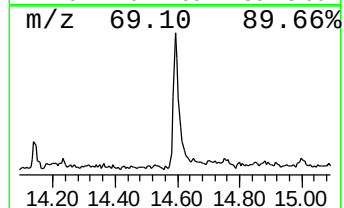
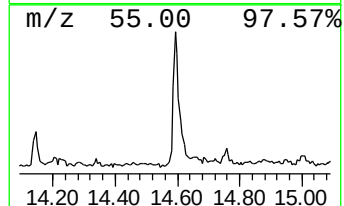
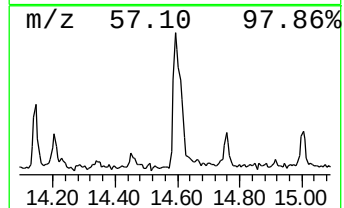
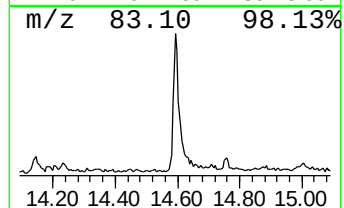
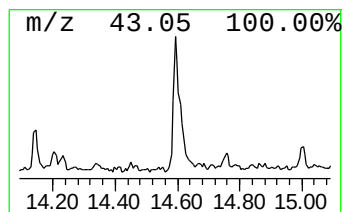
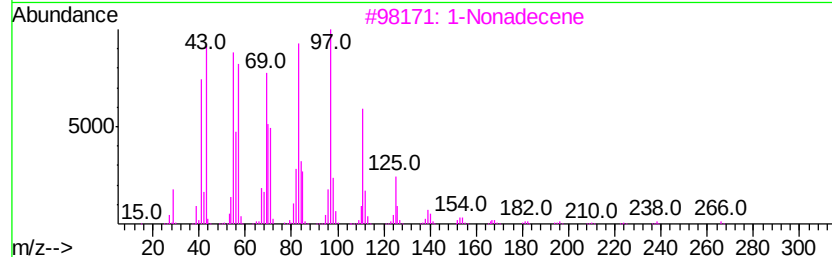
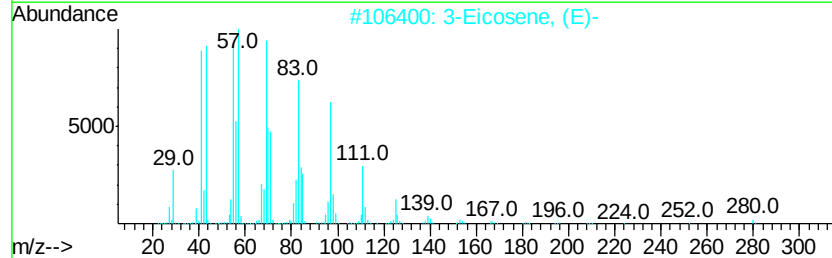
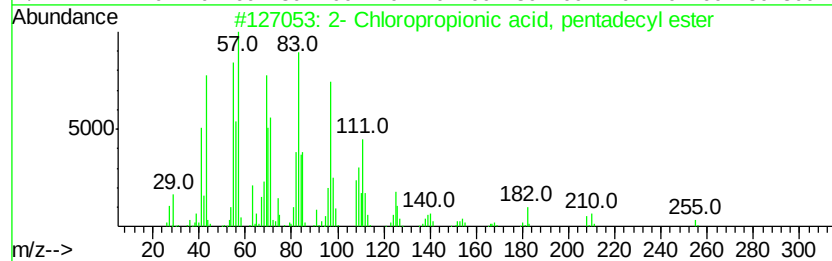
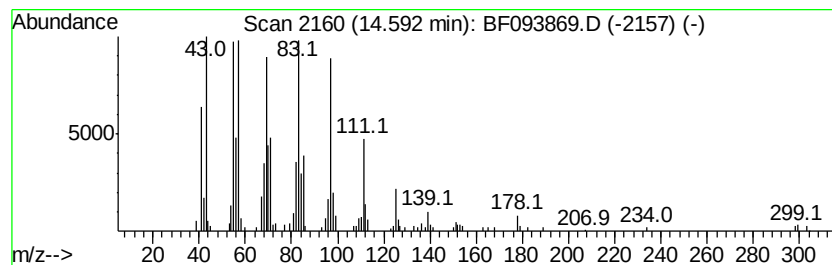
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2- Chloropropionic acid, pe... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.59	5.77 ng	306916	Chrysene-d12	14.70	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	91
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3	1-Nonadecene	266	C19H38	018435-45-5	91
4	1-Octadecanol	270	C18H38O	000112-92-5	91
5	Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032217\
Data File : BF093869.D
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Operator : SJ/MA
Sample : I2350-06
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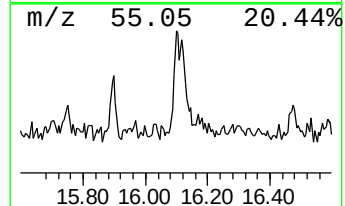
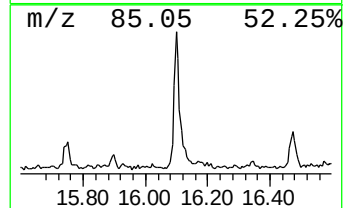
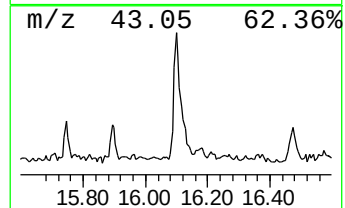
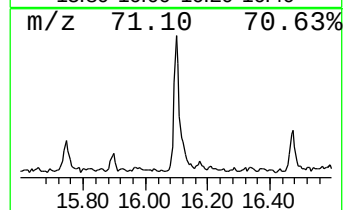
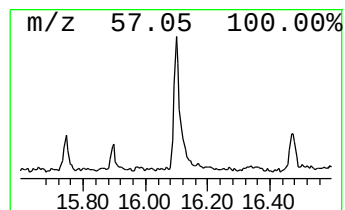
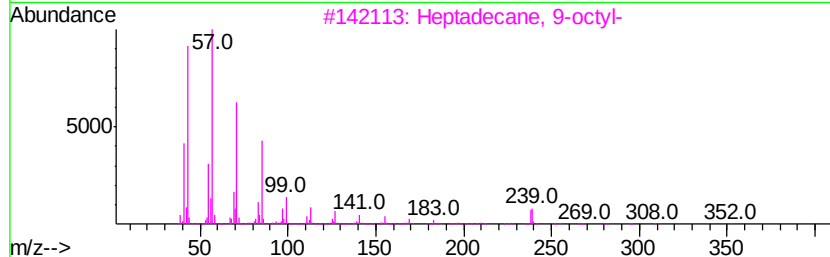
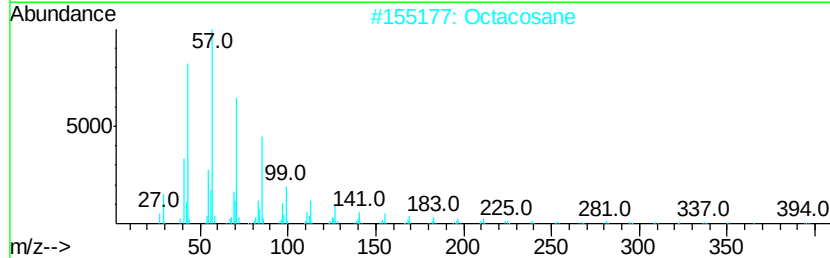
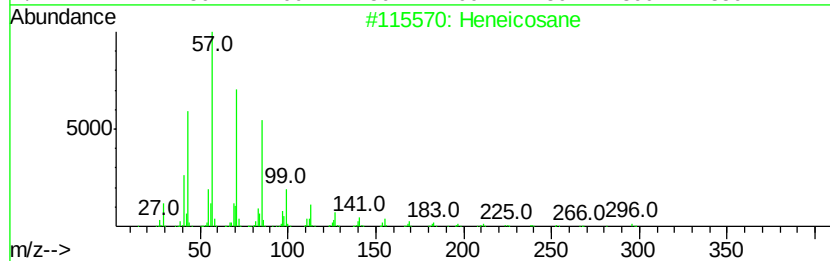
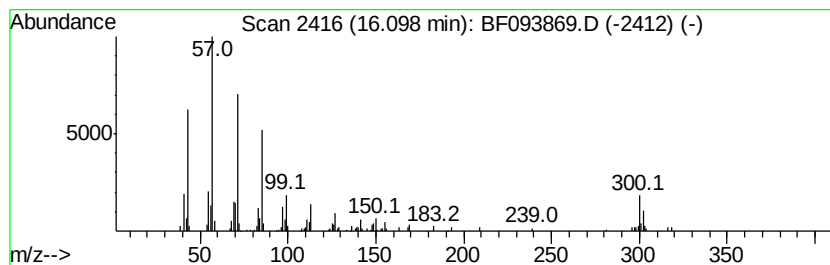
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.10	5.56 ng	268518	Perylene-d12	16.34	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	99
2	Octacosane	394	C28H58	000630-02-4	87
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	83
5	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032217\
Data File : BF093869.D
Acq On : 23 Mar 2017 8:35
Operator : SJ/MA
Sample : I2350-06
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Instrument :
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ClientSampleId :
VNJ-238-210-221-COMP

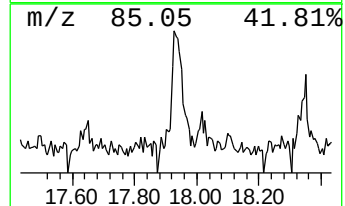
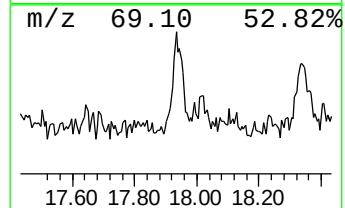
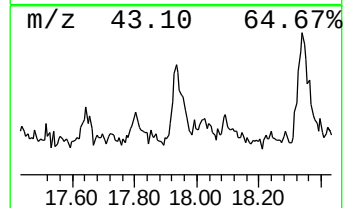
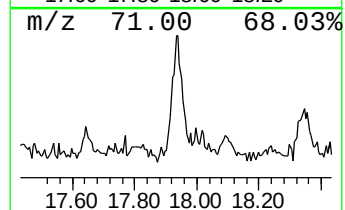
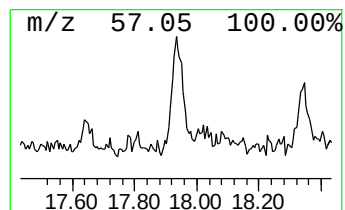
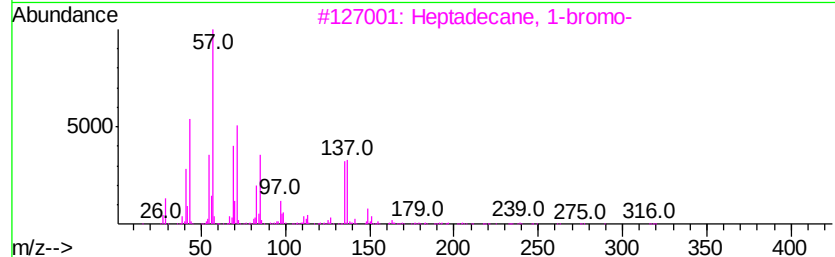
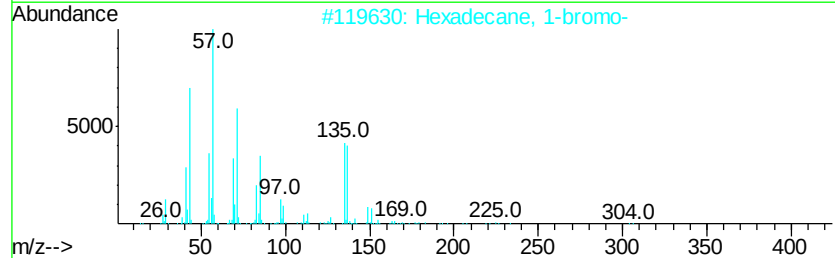
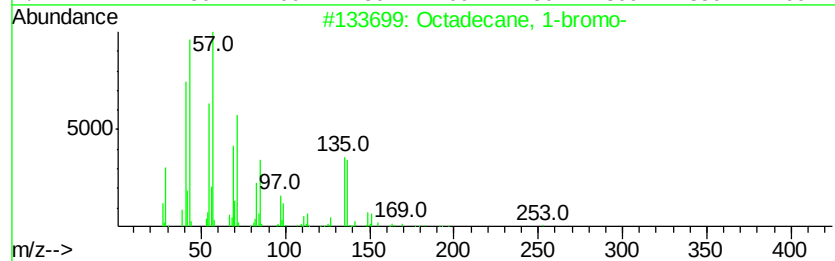
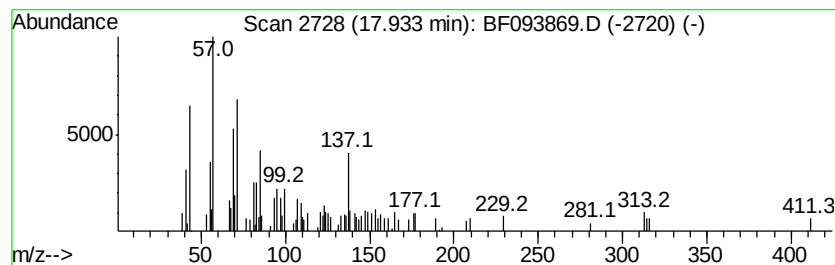
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecane, 1-bromo- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.93	2.77 ng	133748	Perylene-d12	16.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane, 1-bromo-	332	C18H37Br	000112-89-0	58
2		Hexadecane, 1-bromo-	304	C16H33Br	000112-82-3	52
3		Heptadecane, 1-bromo-	318	C17H35Br	003508-00-7	52
4		1-Bromoeicosane	360	C20H41Br	004276-49-7	52
5		1-Chloroeicosane	316	C20H41Cl	042217-02-7	45



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032217\
Data File : BF093869.D
Acq On : 23 Mar 2017 8:35
Operator : SJ/MA
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ALS Vial : 38 Sample Multiplier: 1

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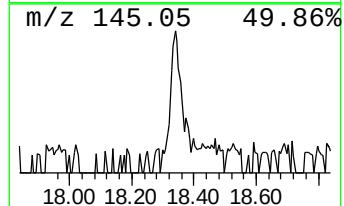
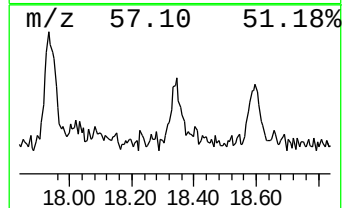
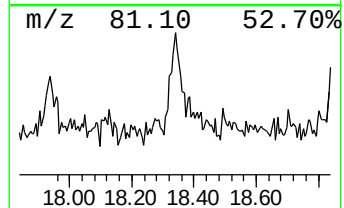
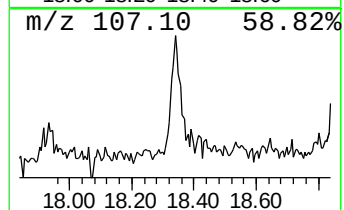
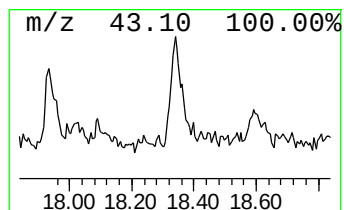
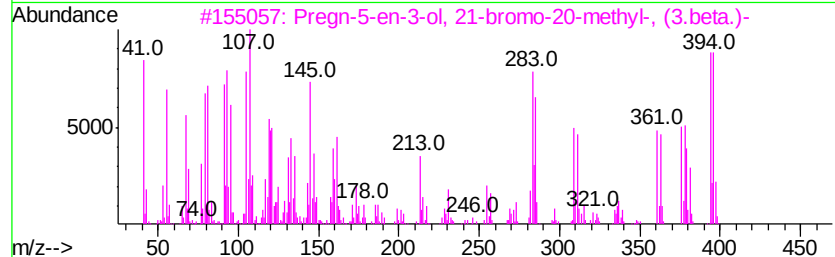
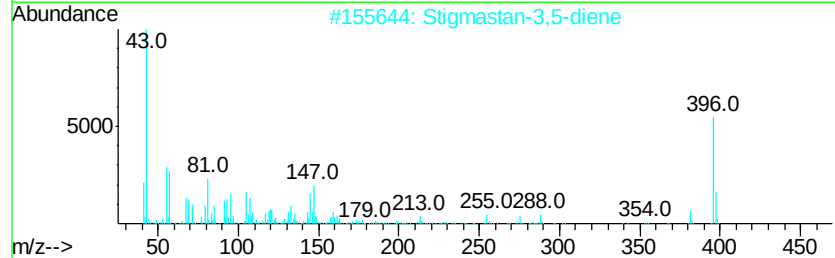
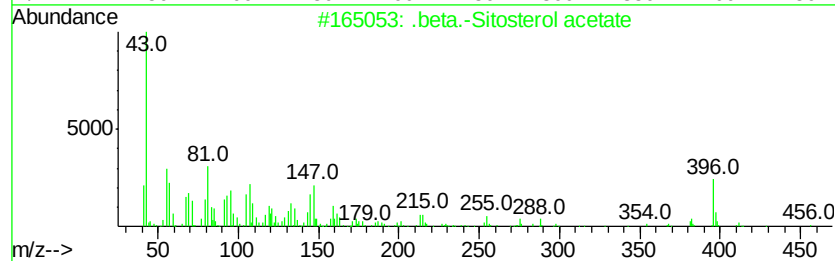
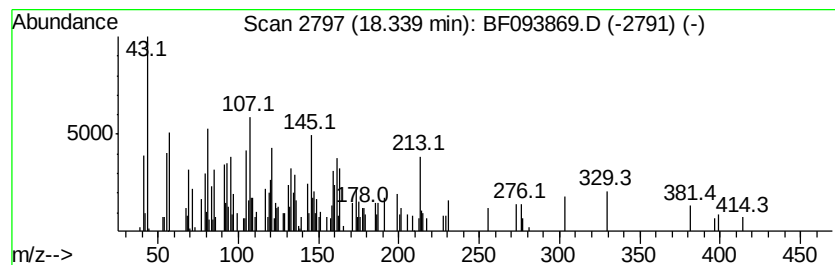
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown18.34 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.34	4.40 ng	212521	Perylene-d12	16.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	37
2		Stigmastan-3,5-diene	396	C29H48	1000214-16-4	32
3		Pregn-5-en-3-ol, 21-bromo-20-met...	394	C22H35BrO	055103-80-5	30
4		Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	17
5		Clionasterol acetate	456	C31H52O2	004651-54-1	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032217\
Data File : BF093869.D
Acq On : 23 Mar 2017 8:35
Operator : SJ/MA
Sample : I2350-06
Misc :
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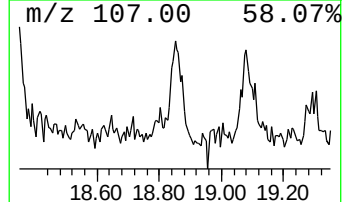
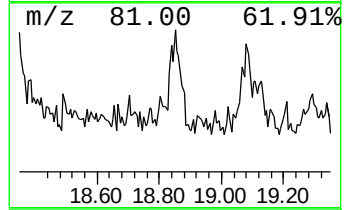
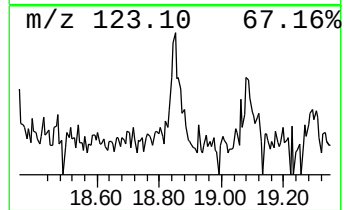
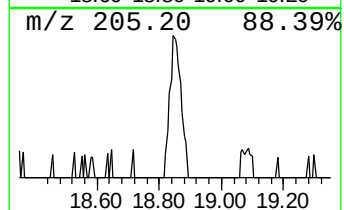
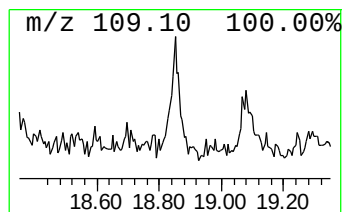
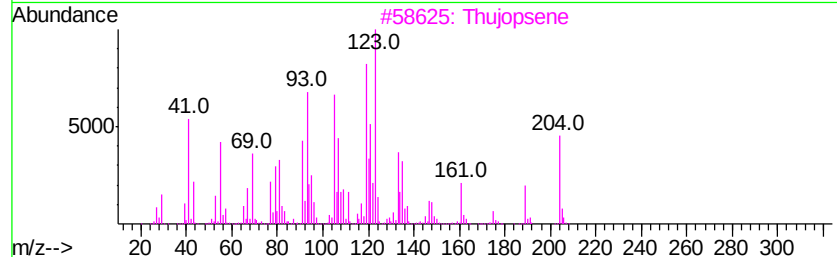
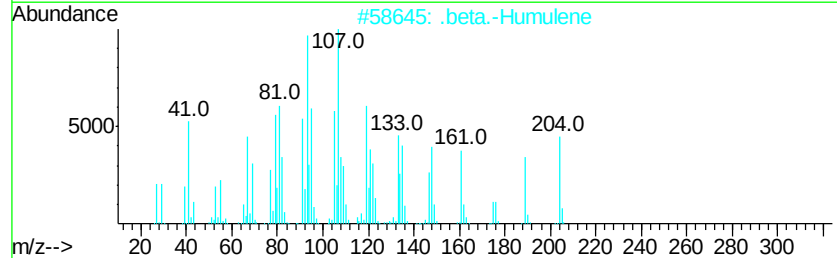
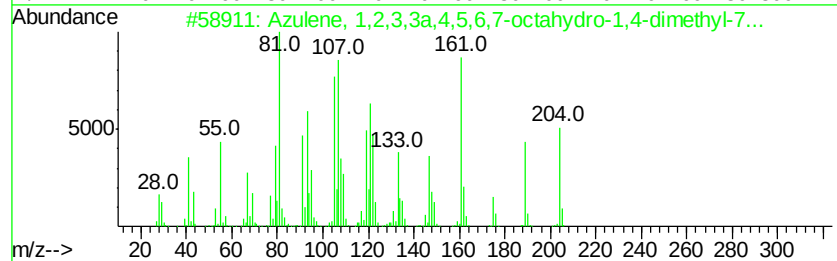
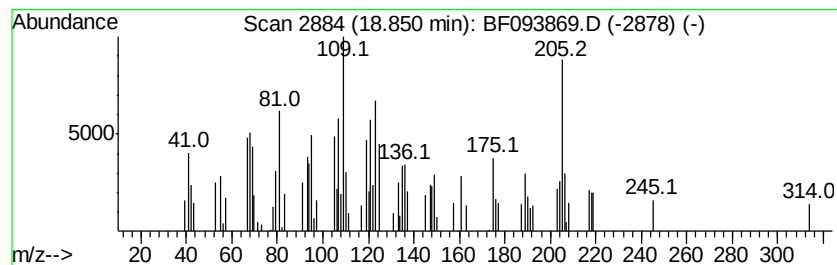
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Azulene, 1,2,3,3a,4,5,6,7-o... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.85	2.85 ng	137507	Perylene-d12	16.34	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Azulene, 1,2,3,3a,4,5,6,7-octahy...	204	C15H24	022567-17-5	53
2	.beta.-Humulene	204	C15H24	000116-04-1	47
3	Thuiopsene	204	C15H24	000470-40-6	25
4	1R,4S,7S,11R-2,2,4,8-Tetramethyl...	204	C15H24	1000140-07-6	25
5	1-Chloro-1-ethyl-3-methyl-1-germ...	206	C7H13ClGe	026311-76-2	25



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032217\
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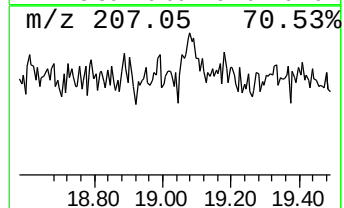
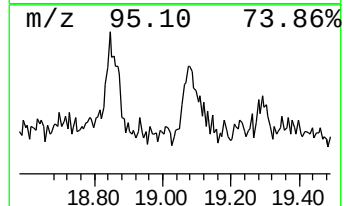
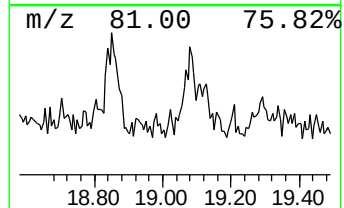
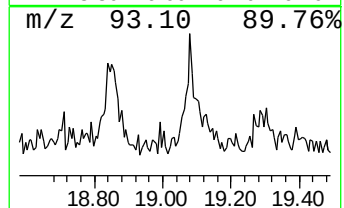
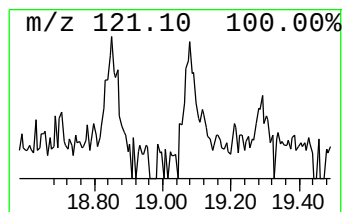
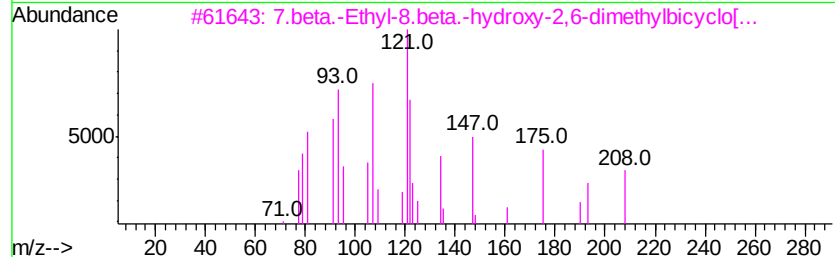
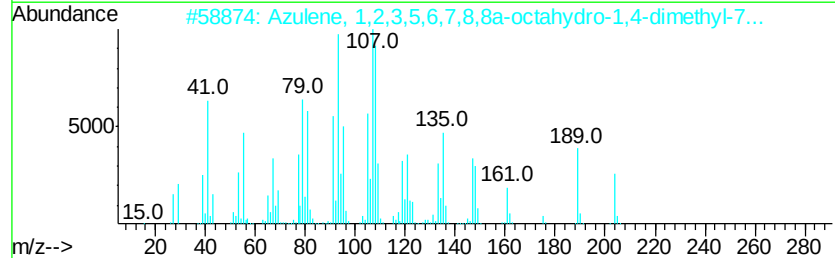
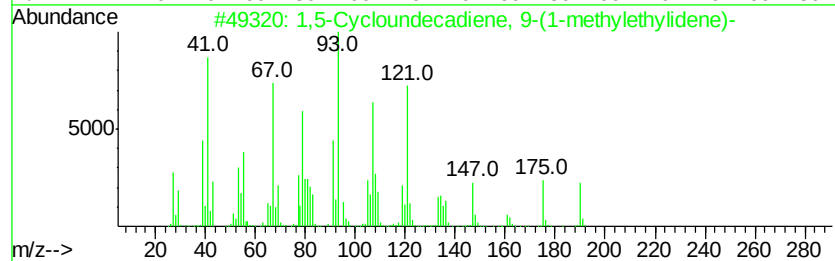
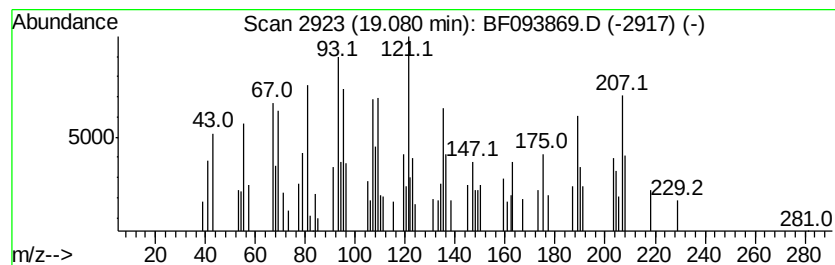
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown19.08 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.08	2.50 ng	120756	Perylene-d12	16.34

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,5-Cycloundecadiene, 9-(1-methy...	190	C14H22	062338-55-0	43
2			Azulene, 1,2,3,5,6,7,8,8a-octahy...	204	C15H24	003691-11-0	38
3			7.beta.-Ethyl-8.beta.-hydroxy-2,...	208	C14H24O	1000077-92-5	38
4			2,6a-Methano-6aH-indeno[4,5-b]ox...	150	C10H14O	016489-32-0	38
5			4,8-Methanoazulen-9-ol, decahydr...	222	C15H26O	004586-22-5	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032217\
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Operator : SJ/MA
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Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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2-Pentanone, 4-hy...	4.14	18.0	ng	1018520	1	5.99	1131820	20.0
unknown5.73	5.73	97.0	ng	5491970	1	5.99	1131820	20.0
Hexadecane	10.81	2.0	ng	146189	4	11.46	1440140	20.0
Hexadecanoic acid...	13.27	2.1	ng	114615	5	14.70	1064240	20.0
2-Chloropropioni...	14.59	5.8	ng	306916	5	14.70	1064240	20.0
Heneicosane	16.10	5.6	ng	268518	6	16.34	966282	20.0
Octadecane, 1-bromo-	17.93	2.8	ng	133748	6	16.34	966282	20.0
unknown18.34	18.34	4.4	ng	212521	6	16.34	966282	20.0
Azulene, 1,2,3,3a...	18.85	2.9	ng	137507	6	16.34	966282	20.0
unknown19.08	19.08	2.5	ng	120756	6	16.34	966282	20.0