

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF070318\
 Data File : BF107089.D
 Acq On : 3 Jul 2018 18:30
 Operator : JU/SJ
 Sample : J3798-04
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DRUM-7-12

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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	5.184	480	484	496	rBV	45307	52373	3.77%	0.543%
2	5.601	551	555	569	rBV	517388	548041	39.42%	5.682%
3	6.601	722	725	739	rBV2	387172	442225	31.81%	4.585%
4	6.737	744	748	751	rVV	1038208	943732	67.88%	9.785%
5	6.784	753	756	764	rVB	10938	14700	1.06%	0.152%
6	6.954	782	785	789	rBV	388751	311590	22.41%	3.231%
7	7.007	791	794	801	rVB	17719	19591	1.41%	0.203%
8	7.113	808	812	815	rBV	1068781	904352	65.04%	9.376%
9	7.525	877	882	891	rBV	704411	680528	48.95%	7.056%
10	7.666	903	906	910	rVB	32314	27591	1.98%	0.286%
11	8.242	1000	1004	1016	rBV	366942	361000	25.96%	3.743%
12	8.525	1049	1052	1056	rBV	38480	43952	3.16%	0.456%
13	9.313	1182	1186	1194	rBV	1444800	1257033	90.41%	13.033%
14	9.419	1201	1204	1212	rVB	54627	54467	3.92%	0.565%
15	9.701	1249	1252	1259	rBV	178048	177683	12.78%	1.842%
16	10.001	1299	1303	1313	rVB	396187	358756	25.80%	3.720%
17	10.795	1434	1438	1450	rBV	734535	714300	51.37%	7.406%
18	11.495	1553	1557	1564	rBV	435949	365224	26.27%	3.787%
19	12.477	1721	1724	1728	rBV	25188	23157	1.67%	0.240%
20	13.077	1822	1826	1829	rBV	1528667	1390393	100.00%	14.416%
21	13.618	1915	1918	1921	rBV2	12591	14820	1.07%	0.154%
22	13.954	1971	1975	1983	rBV	73971	91161	6.56%	0.945%
23	14.148	2004	2008	2012	rBV	414927	377788	27.17%	3.917%
24	14.271	2026	2029	2032	rBV	15993	14806	1.06%	0.154%
25	14.577	2079	2081	2086	rBV2	22585	37701	2.71%	0.391%
26	14.895	2133	2135	2139	rVB	35601	36466	2.62%	0.378%
27	15.248	2193	2195	2199	rVB	32212	33916	2.44%	0.352%
28	15.654	2260	2264	2266	rBV	35218	43474	3.13%	0.451%
29	15.695	2266	2271	2279	rVB	190741	268271	19.29%	2.781%
30	16.112	2339	2342	2346	rVB2	27311	36017	2.59%	0.373%

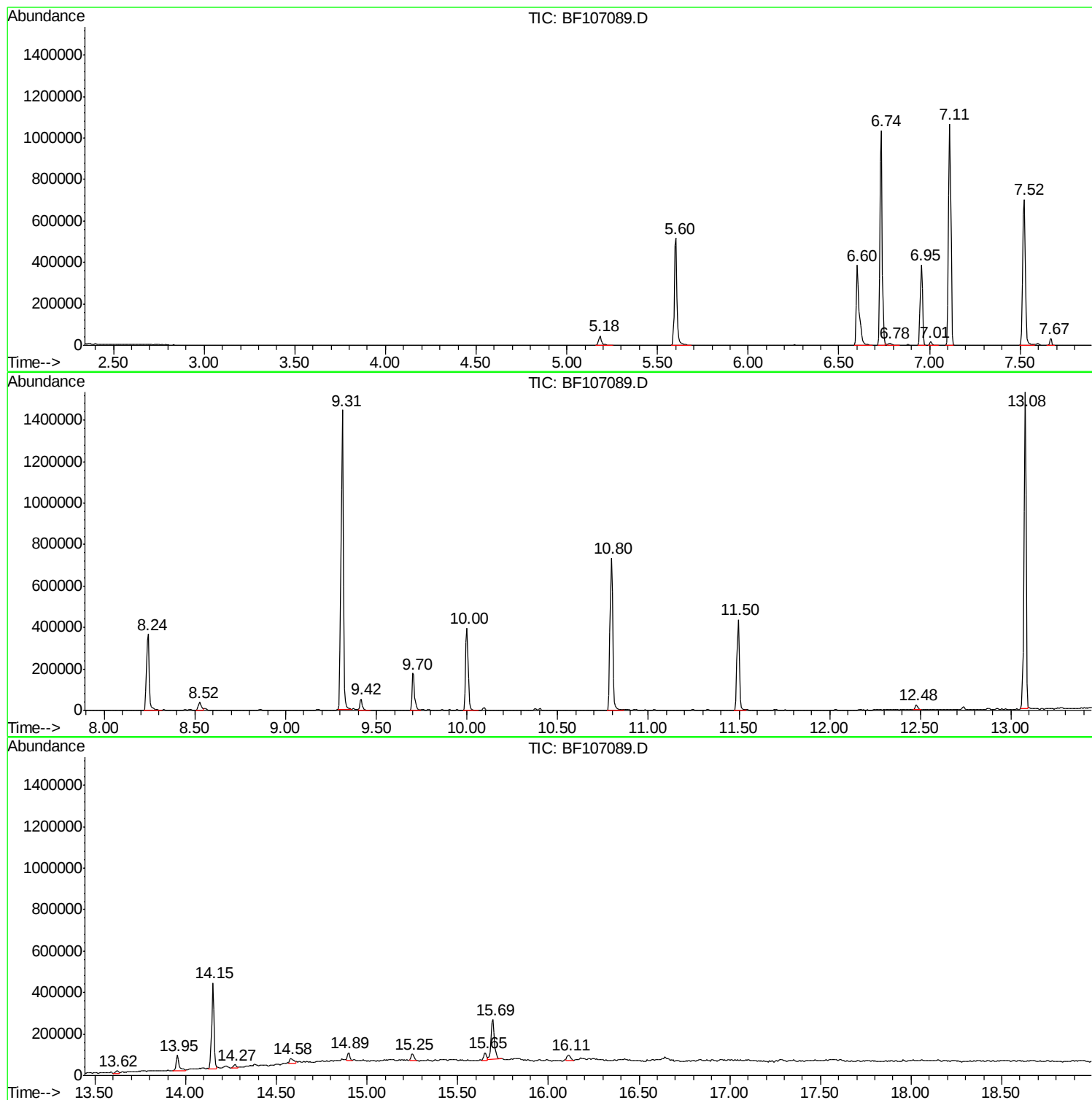
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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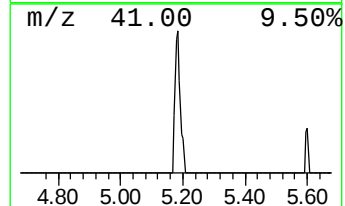
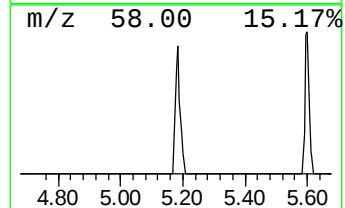
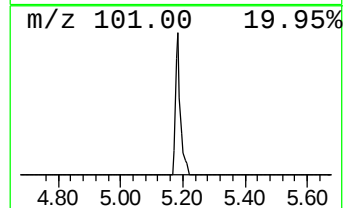
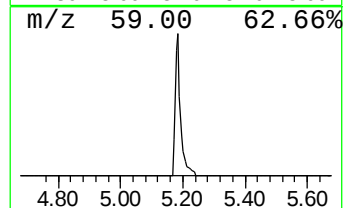
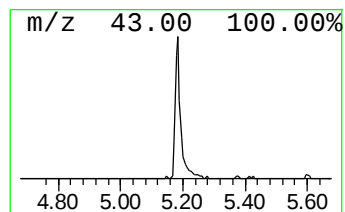
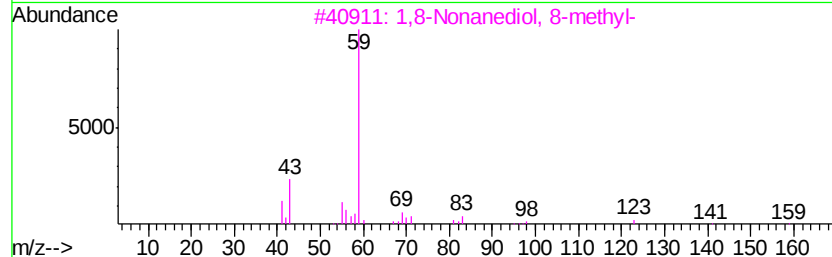
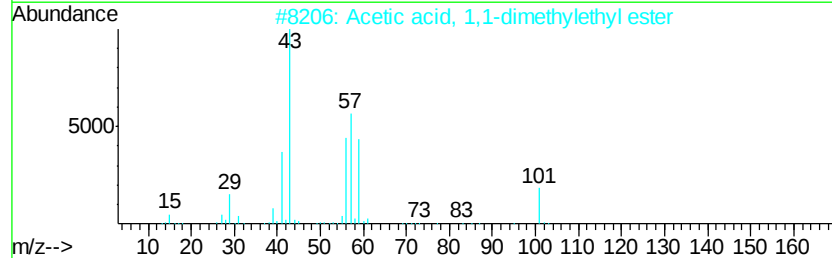
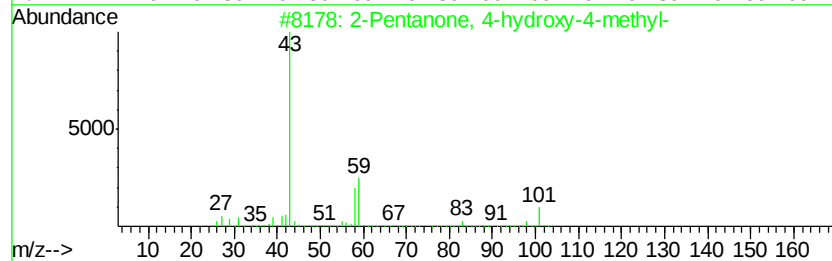
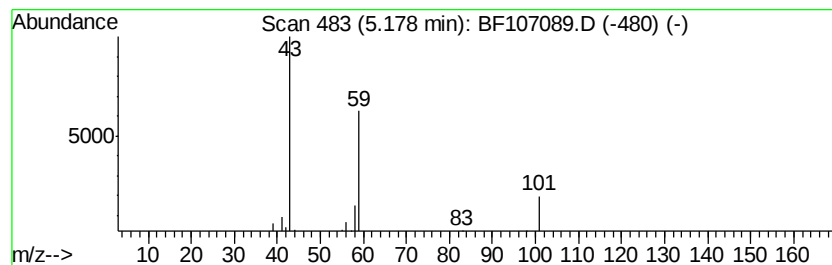
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	3.36 ng	52373	1,4-Dichlorobenzene-d4	6.95

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	38
3			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			2-Butanol, 1-chloro-	108	C4H9ClO	001873-25-2	9



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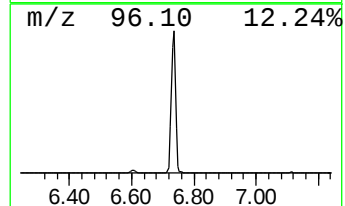
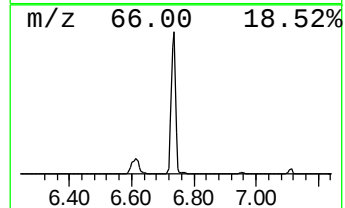
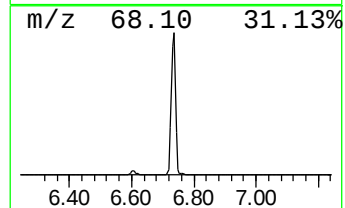
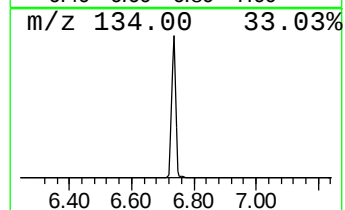
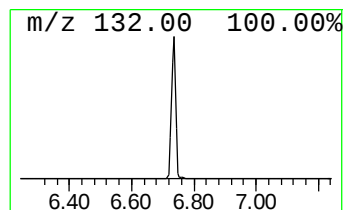
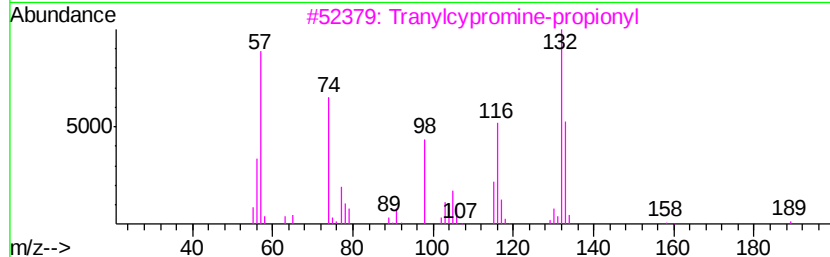
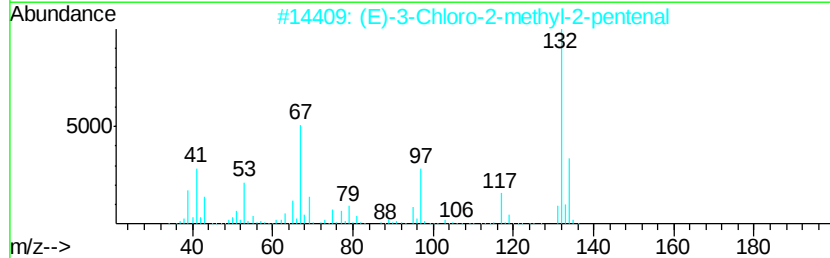
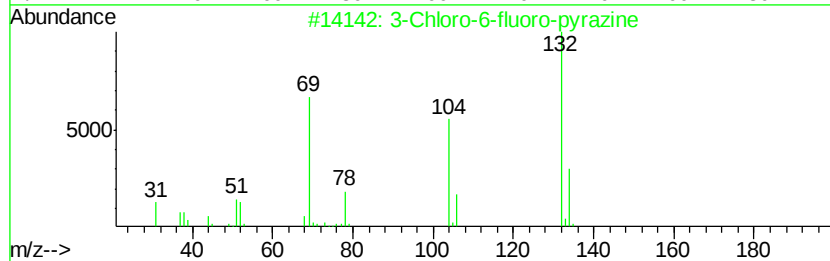
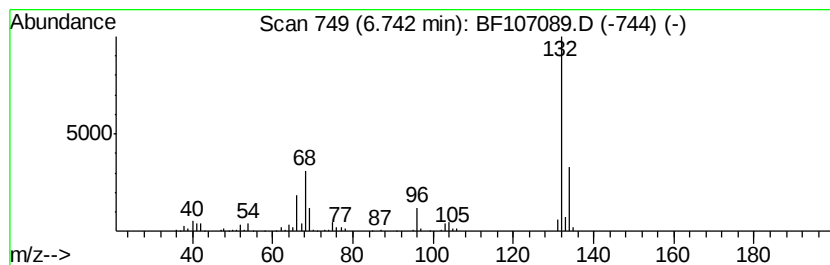
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Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	60.58 ng	943732	1,4-Dichlorobenzene-d4	6.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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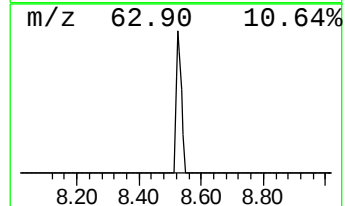
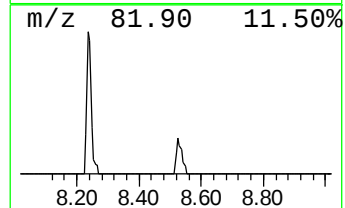
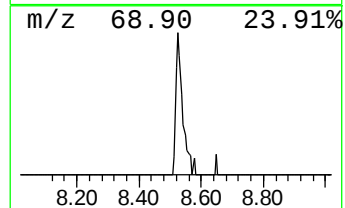
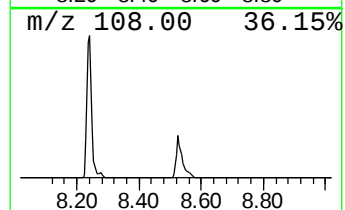
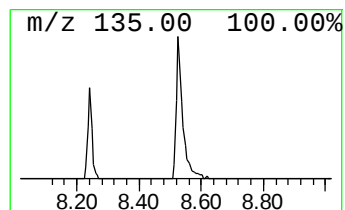
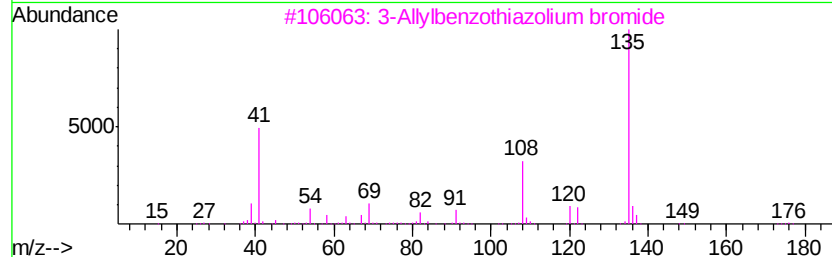
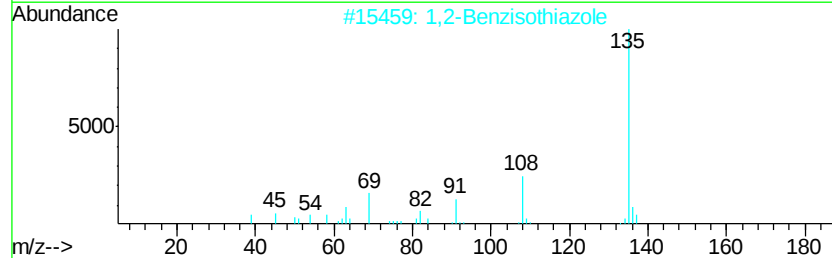
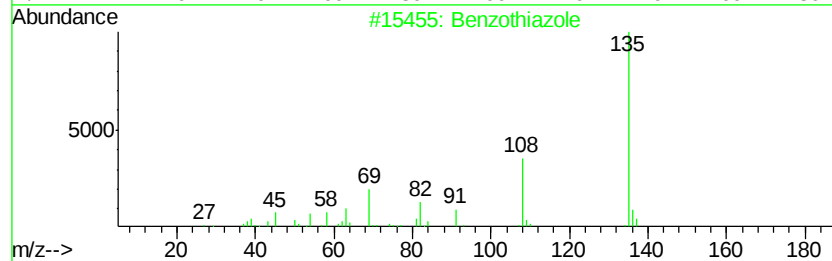
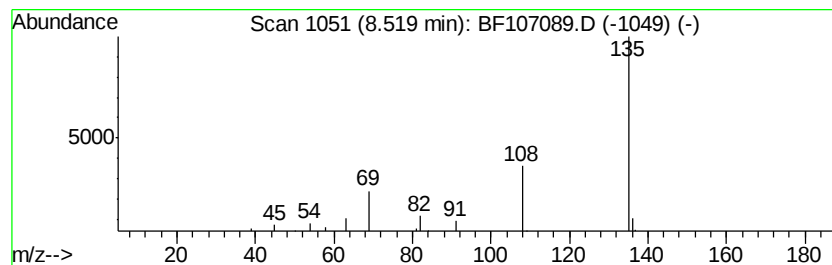
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Peak Number 4 Benzothiazole Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.52	2.44 ng	43952	Naphthalene-d8	8.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzothiazole	135	C7H5NS	000095-16-9	95
2		1,2-Benzisothiazole	135	C7H5NS	000272-16-2	91
3		3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	74
4		2-Fluoro-4-cyanotoluene	135	C8H6FN	170572-49-3	64
5		1H-Indole, 5-fluoro-	135	C8H6FN	000399-52-0	64



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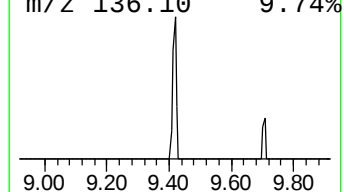
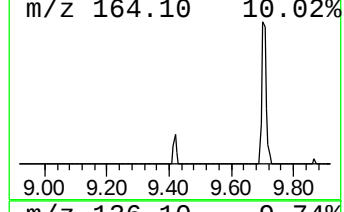
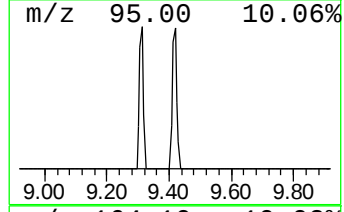
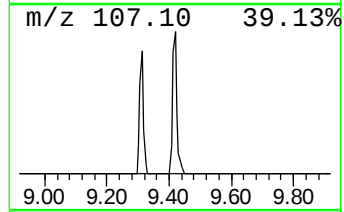
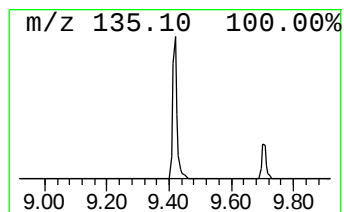
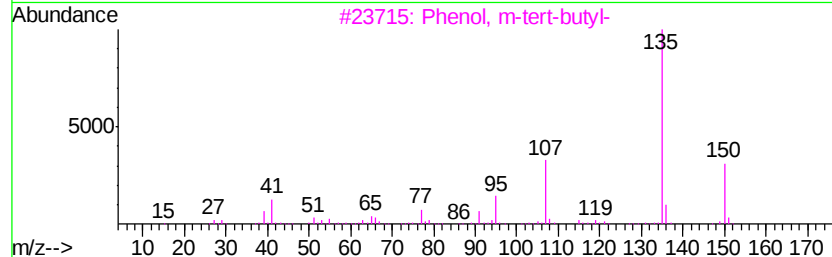
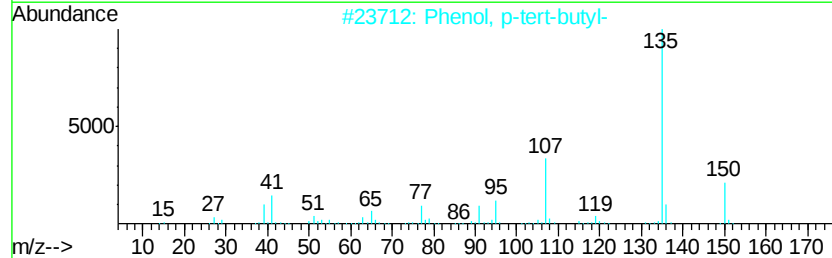
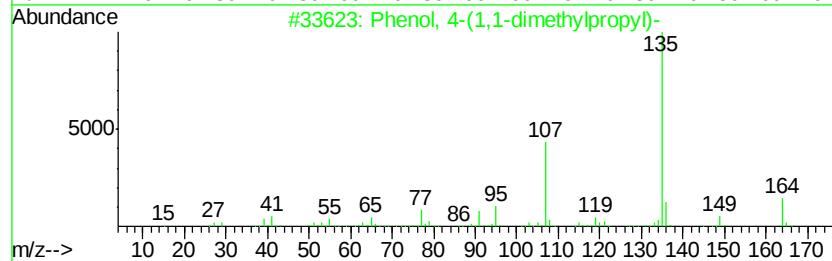
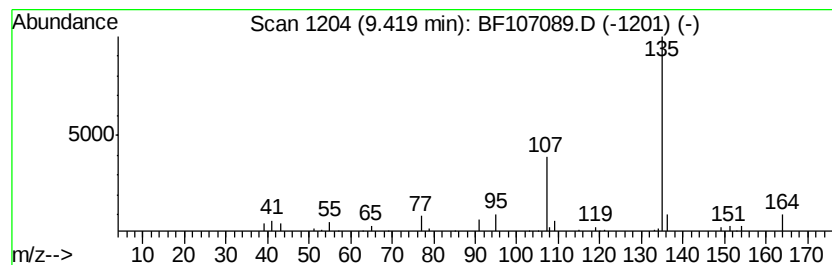
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Peak Number 5 Phenol, 4-(1,1-dimethylprop... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.42	3.04 ng	54467	Acenaphthene-d10	10.00

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	94	
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	72	
3	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	64	
4	Hexestrol, 0-trifluoroacetyl-	366	C20H21F3O3	1000365-31-7	59	
5	Hexestrol	270	C18H22O2	005635-50-7	59	



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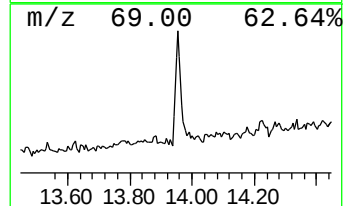
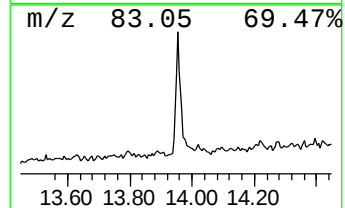
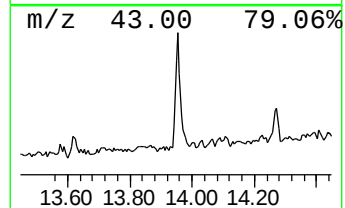
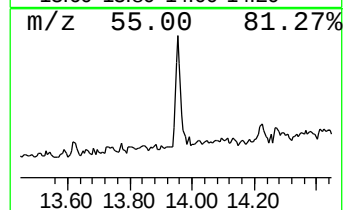
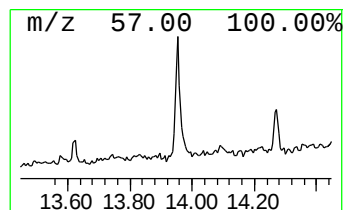
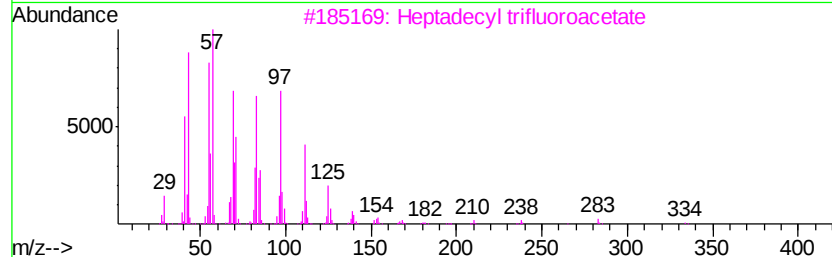
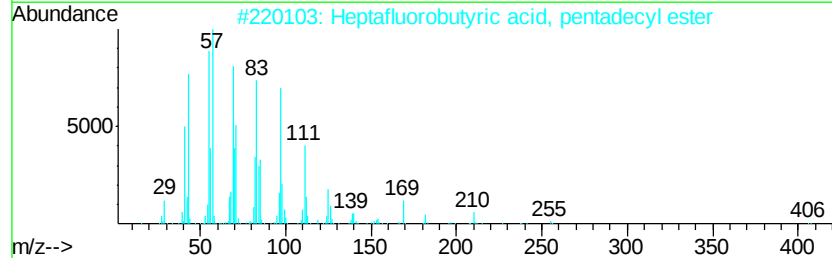
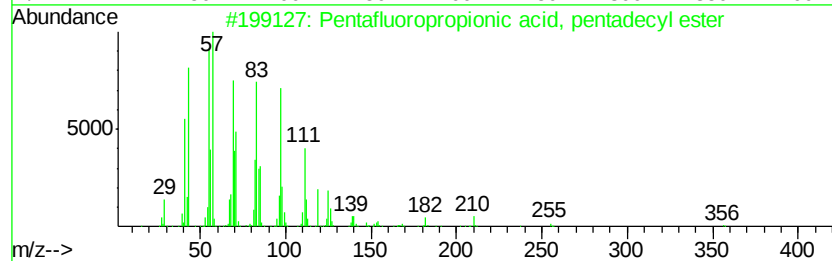
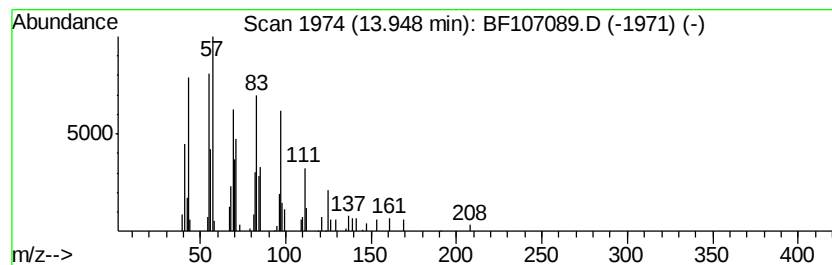
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	4.83 ng	91161	Chrysene-d12	14.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
2		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	95
3		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	95
4		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	95
5		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	95



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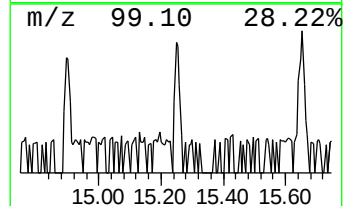
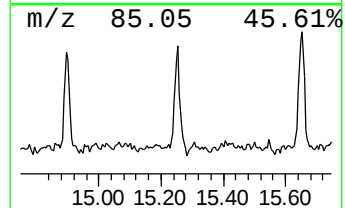
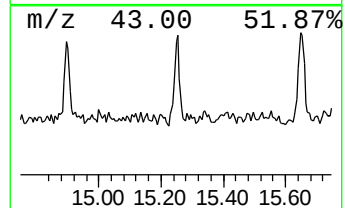
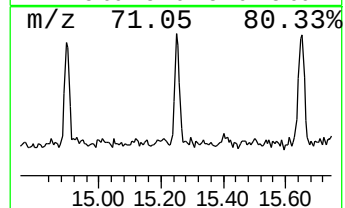
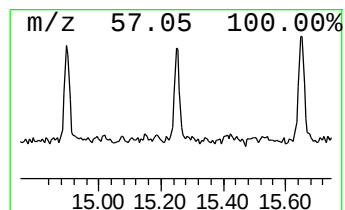
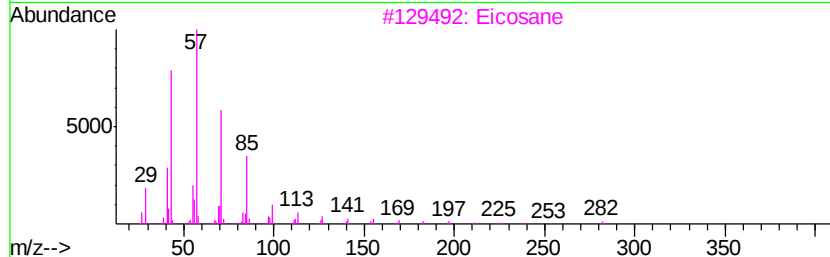
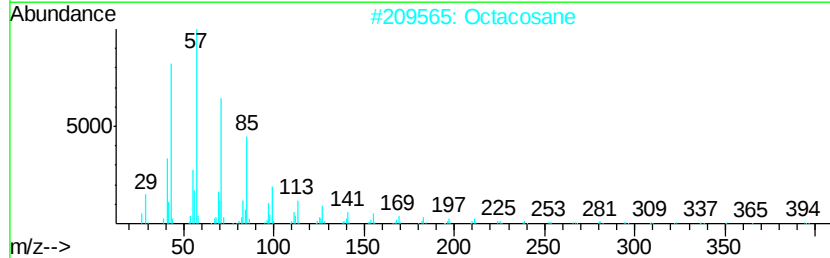
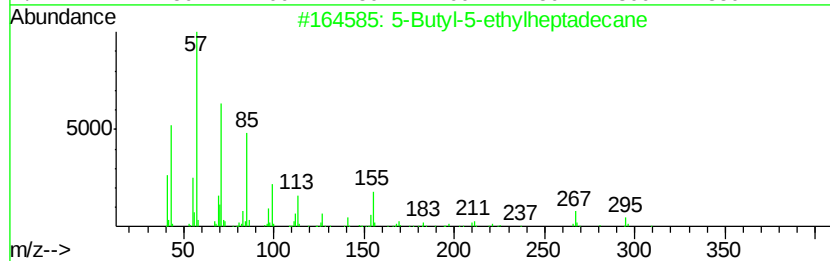
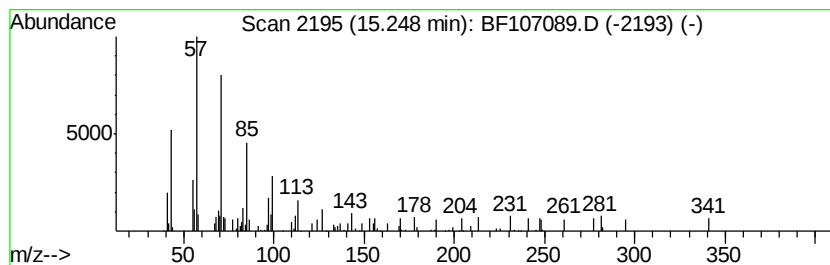
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 5-Butyl-5-ethylheptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.25	2.53 ng	33916	Perylene-d12	15.69

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Butyl-5-ethylheptadecane			324	C23H48	1000360-43-0	72
2	Octacosane			394	C28H58	000630-02-4	64
3	Eicosane			282	C20H42	000112-95-8	64
4	Tridecane, 3-methyl-			198	C14H30	006418-41-3	64
5	Undecane, 3-ethyl-			184	C13H28	017312-58-2	59



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF070318\
Data File : BF107089.D
Acq On : 3 Jul 2018 18:30
Operator : JU/SJ
Sample : J3798-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DRUM-7-12

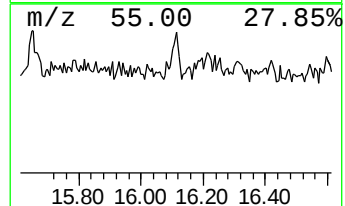
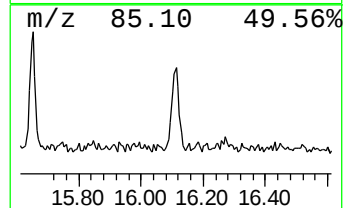
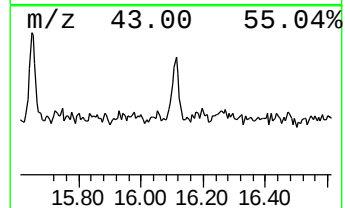
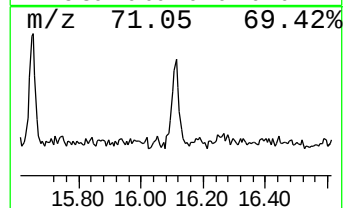
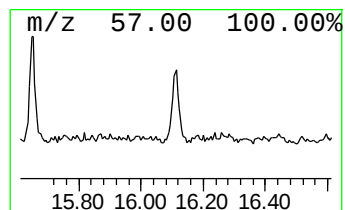
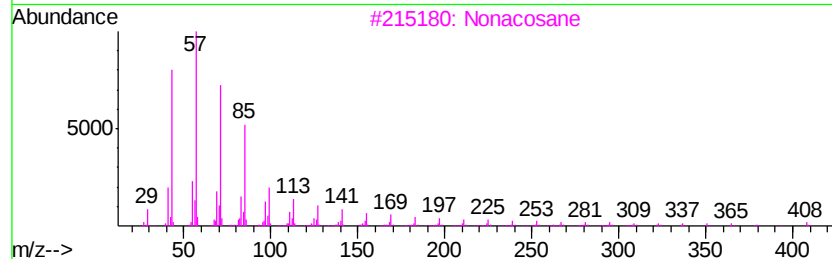
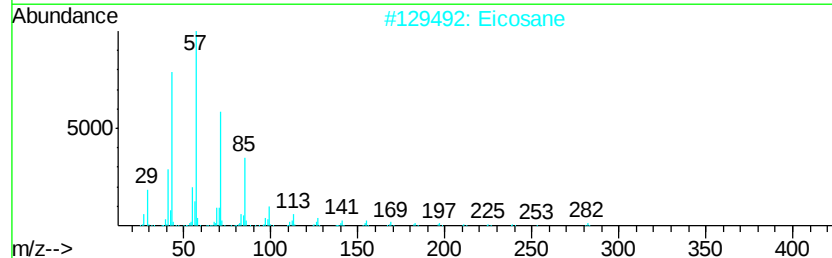
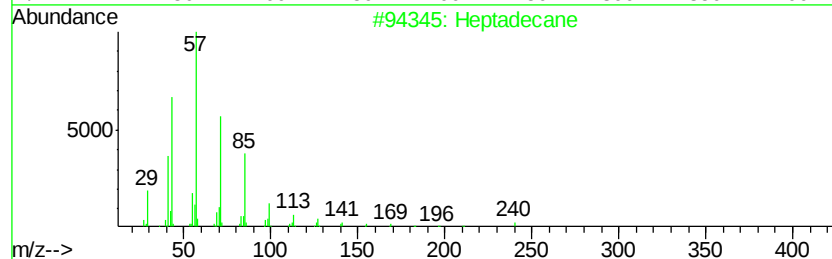
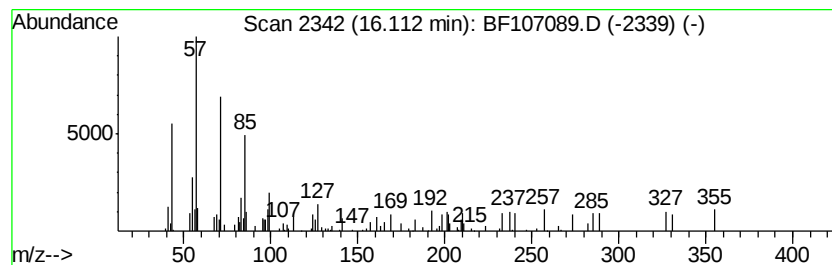
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.11	2.69 ng	36017	Perylene-d12	15.69

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	64
2	Eicosane		282	C20H42	000112-95-8	55
3	Nonacosane		408	C29H60	000630-03-5	47
4	Tetradecane		198	C14H30	000629-59-4	43
5	3,5-Dimethyldodecane		198	C14H30	107770-99-0	43



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF070318\
Data File : BF107089.D
Acq On : 3 Jul 2018 18:30
Operator : JU/SJ
Sample : J3798-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DRUM-7-12

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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...	5.18	3.4	ng	52373	1	6.95	311590	20.0
unknown6.74	6.74	60.6	ng	943732	1	6.95	311590	20.0
Benzothiazole	8.52	2.4	ng	43952	2	8.24	361000	20.0
Phenol, 4-(1,1-di...	9.42	3.0	ng	54467	3	10.00	358756	20.0
Pentafluoropropio...	13.95	4.8	ng	91161	5	14.15	377788	20.0
5-Butyl-5-ethylhe...	15.25	2.5	ng	33916	6	15.69	268271	20.0
Heptadecane	16.11	2.7	ng	36017	6	15.69	268271	20.0