

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031616\
 Data File : BF085469.D
 Acq On : 16 Mar 2016 18:40
 Operator : UM/SJ
 Sample : H1769-01
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DRUM-325-359-COMPOSITE

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-BF031516.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	5.098	244	246	253	rVB	183410	241880	5.80%	0.720%
2	5.510	279	282	284	rBV	3105740	3461616	82.98%	10.302%
3	6.539	369	372	374	rBV	2792757	3678292	88.18%	10.947%
4	6.676	381	384	386	rBV	2524273	3577107	85.75%	10.646%
5	6.904	401	404	406	rBV	759325	735703	17.64%	2.189%
6	7.053	415	417	420	rBV	2032526	2789327	66.87%	8.301%
7	7.464	450	453	455	rBV	2168466	2187882	52.45%	6.511%
8	7.910	488	492	496	rBV4	23122	47522	1.14%	0.141%
9	8.184	514	516	519	rBV	1146930	997026	23.90%	2.967%
10	9.270	608	611	613	rBV	3361437	4171566	100.00%	12.415%
11	9.659	643	645	647	rBV	703644	595311	14.27%	1.772%
12	9.945	667	670	672	rVB	1187592	1082347	25.95%	3.221%
13	10.367	704	707	709	rVB2	40800	63306	1.52%	0.188%
14	10.733	736	739	741	rBV	2437801	2377505	56.99%	7.076%
15	10.848	746	749	752	rBV	64157	83999	2.01%	0.250%
16	11.430	797	800	802	rBV	1003086	1101714	26.41%	3.279%
17	11.499	802	806	808	rVB	43741	68229	1.64%	0.203%
18	11.945	843	845	847	rBV2	87934	119676	2.87%	0.356%
19	11.979	847	848	851	rVB	33353	43561	1.04%	0.130%
20	12.733	911	914	921	rBV	119489	169216	4.06%	0.504%
21	13.019	936	939	941	rBV	2852300	3984877	95.52%	11.859%
22	13.899	1014	1016	1024	rBV2	89106	136379	3.27%	0.406%
23	14.059	1026	1030	1033	rBV	910569	894121	21.43%	2.661%
24	14.814	1093	1096	1100	rBV4	23566	45406	1.09%	0.135%
25	15.511	1154	1157	1165	rVB	418417	568231	13.62%	1.691%
26	16.025	1198	1202	1209	rBV4	18742	58659	1.41%	0.175%
27	16.322	1223	1228	1237	rBV2	70293	321118	7.70%	0.956%

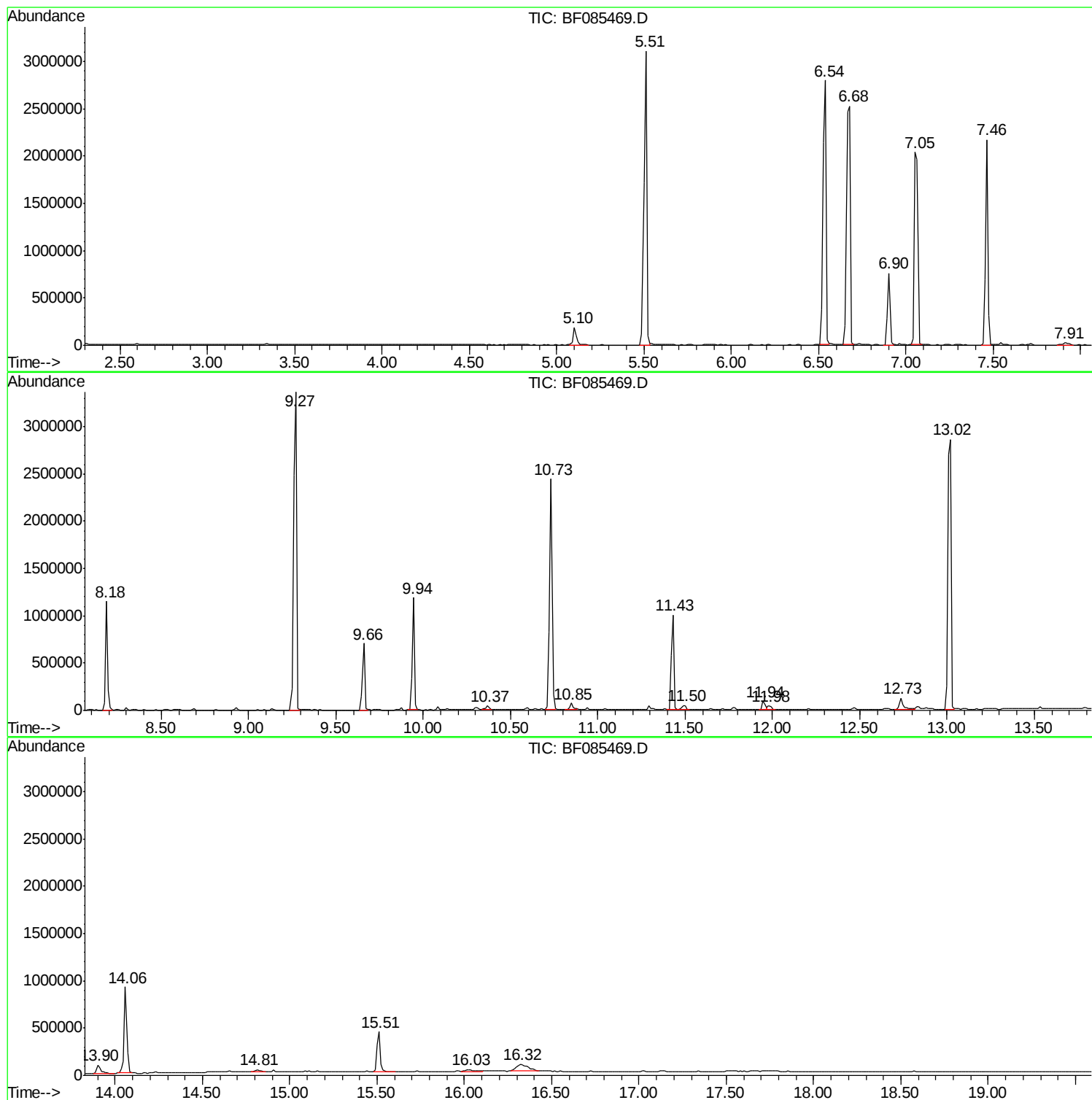
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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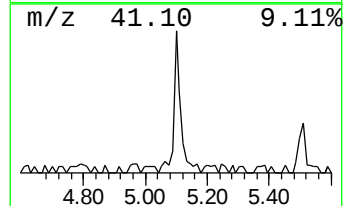
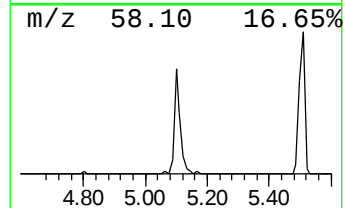
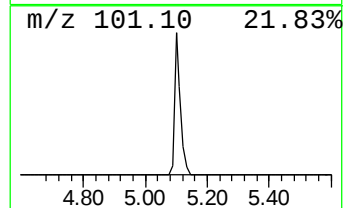
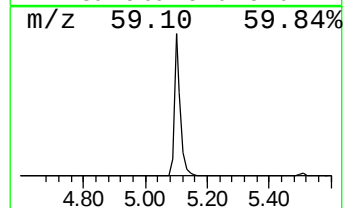
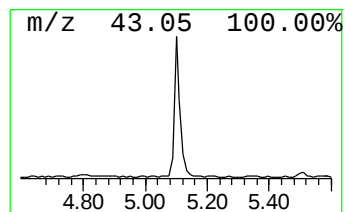
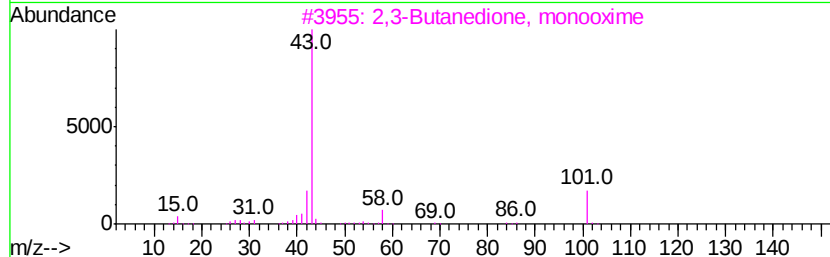
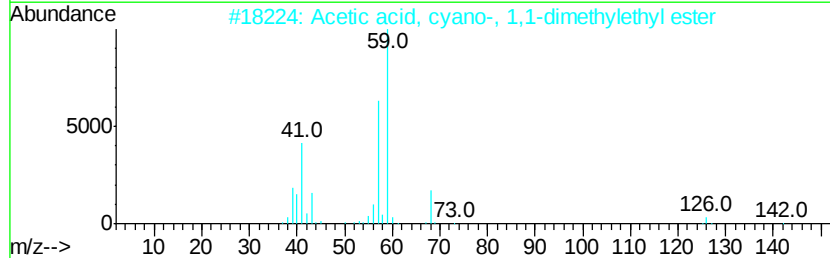
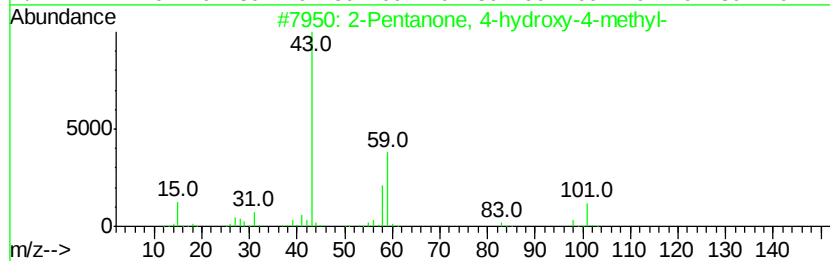
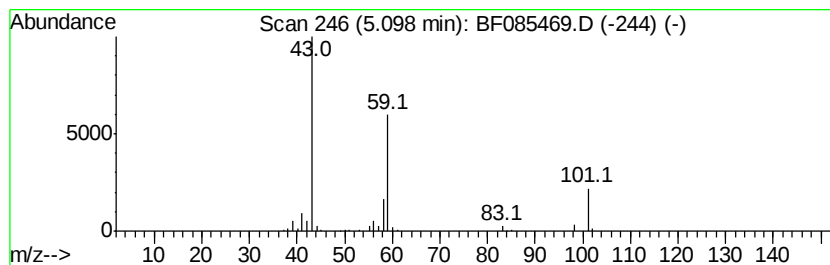
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	6.58 ng	241880	1,4-Dichlorobenzene-d4	6.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	32
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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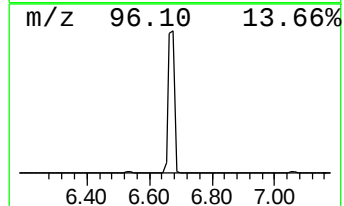
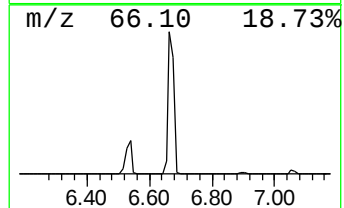
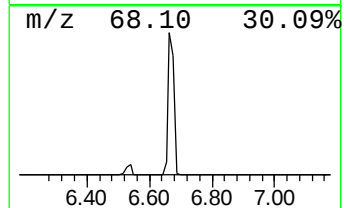
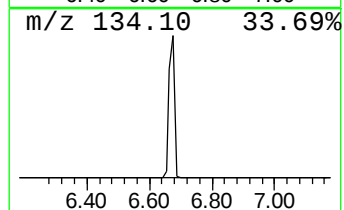
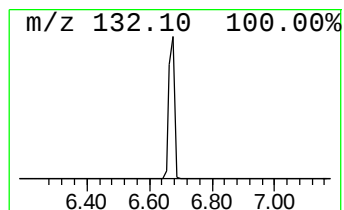
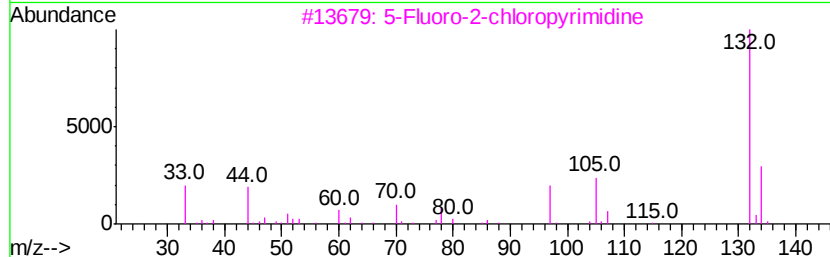
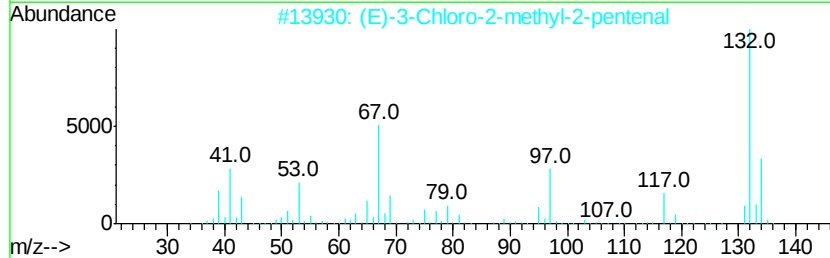
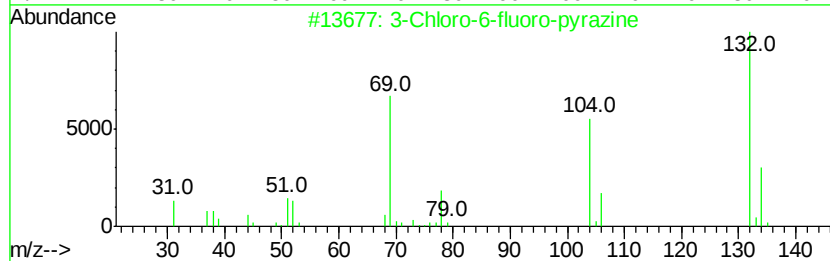
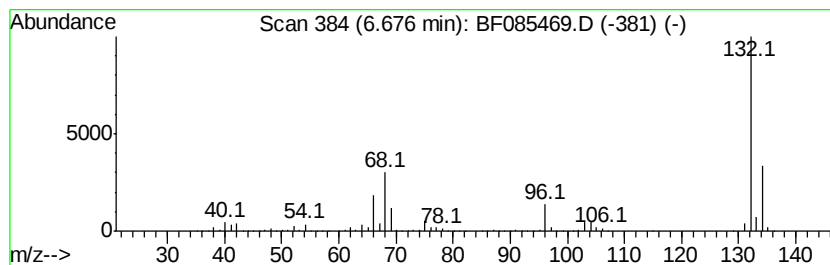
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 3-Chloro-6-fluoro-pyrazine Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	97.24 ng	3577110	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	52
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	33
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4		Xenon	132	Xe	007440-63-3	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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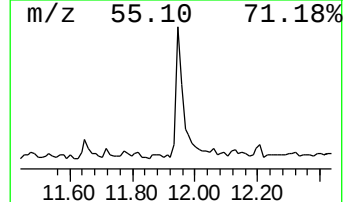
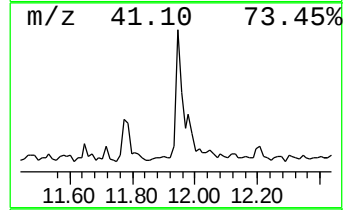
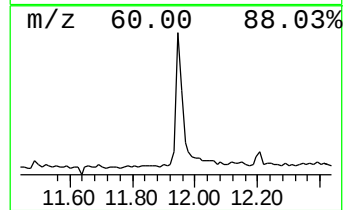
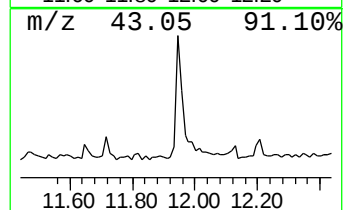
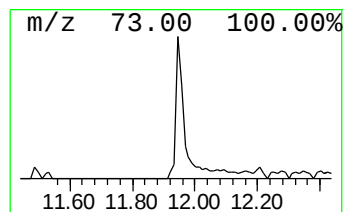
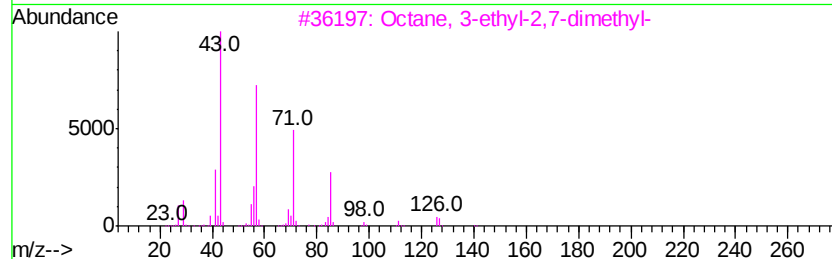
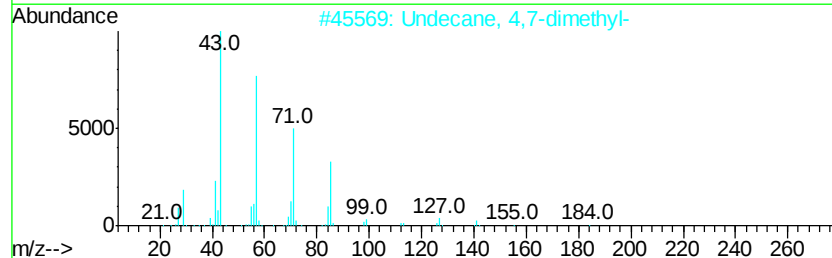
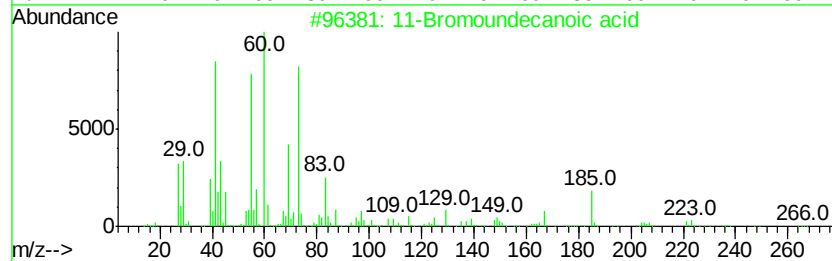
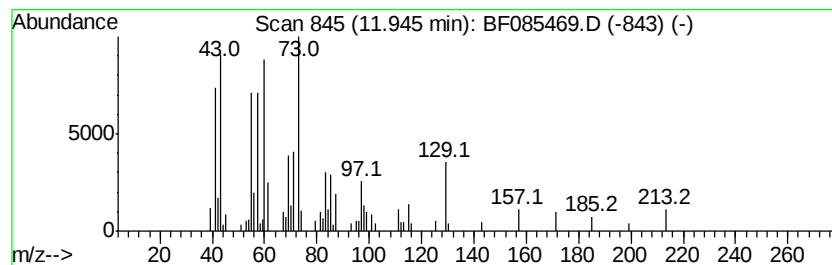
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Peak Number 4 unknown11.94 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	2.17 ng	119676	Phenanthrene-d10	11.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	35
2		Undecane, 4,7-dimethyl-	184	C13H28	017301-32-5	10
3		Octane, 3-ethyl-2,7-dimethyl-	170	C12H26	062183-55-5	10
4		Tridecane	184	C13H28	000629-50-5	10
5		Pentadecane	212	C15H32	000629-62-9	10



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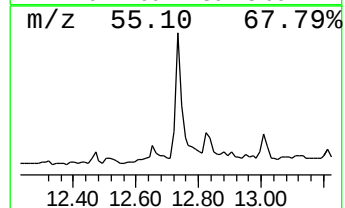
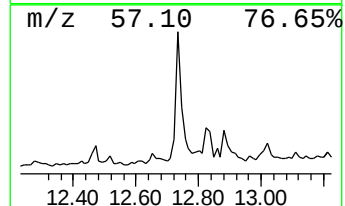
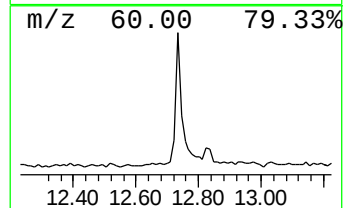
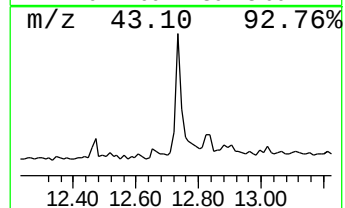
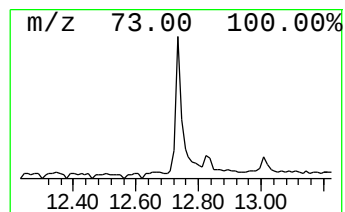
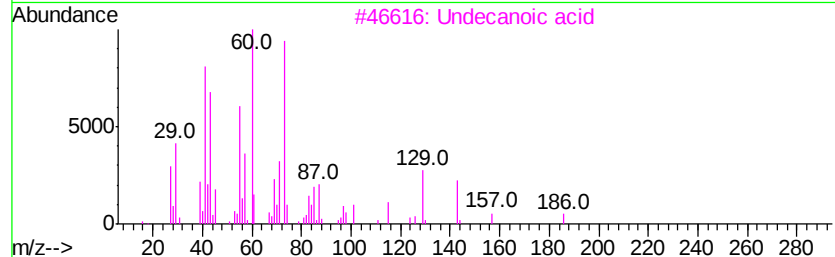
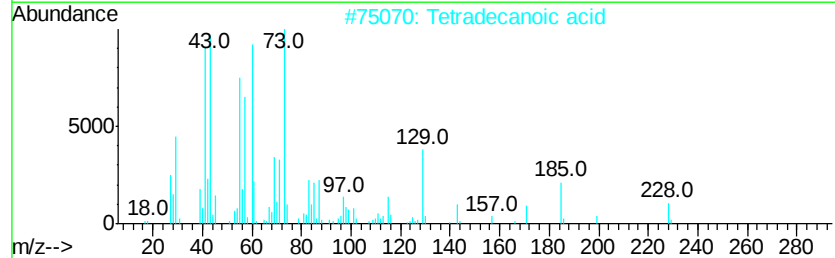
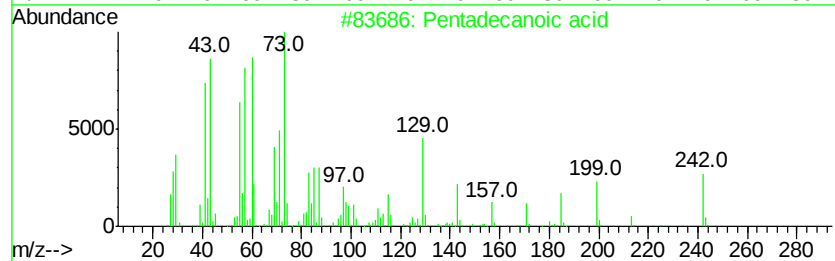
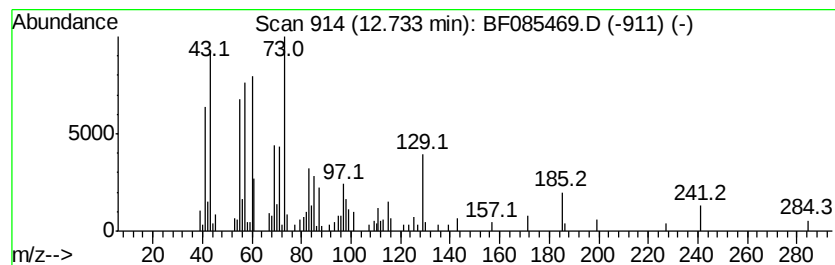
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Peak Number 5 Pentadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.73	3.07 ng	169216	Phenanthrene-d10	11.43	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3	Undecanoic acid	186	C11H22O2	000112-37-8	58
4	Tridecane	184	C13H28	000629-50-5	11
5	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	11



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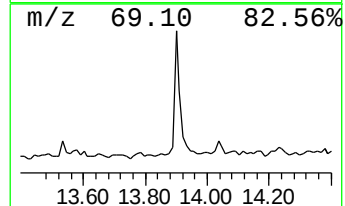
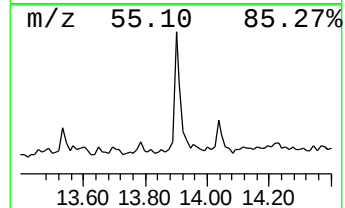
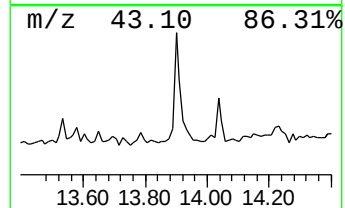
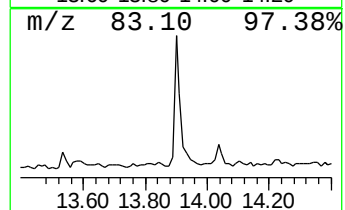
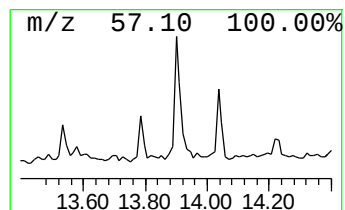
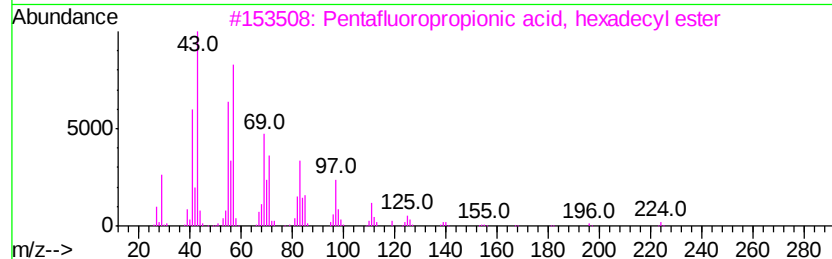
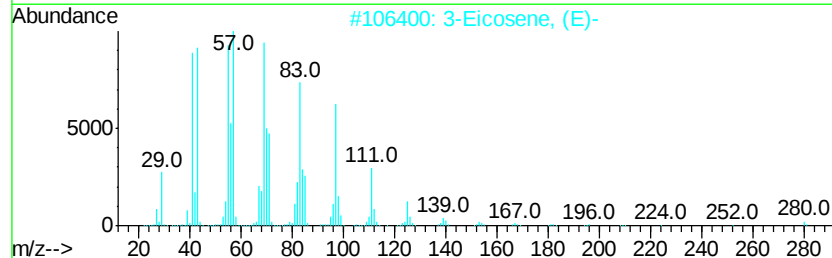
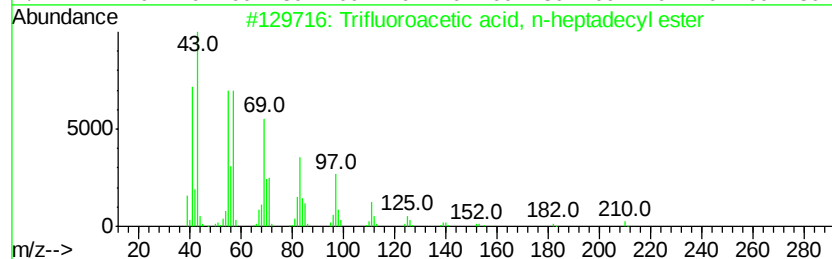
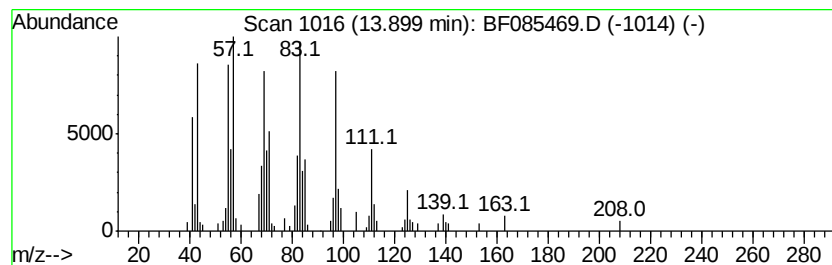
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Peak Number 6 Trifluoroacetic acid, n-hep... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	3.05 ng	136379	Chrysene-d12	14.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	91
2		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3		Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	90
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
5		1-Nonadecene	266	C19H38	018435-45-5	90



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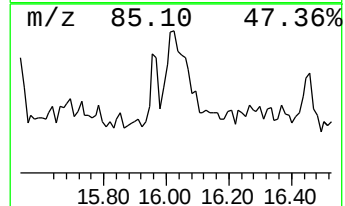
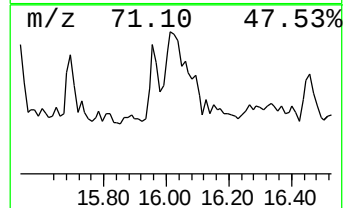
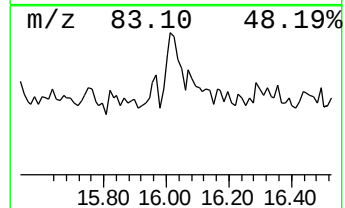
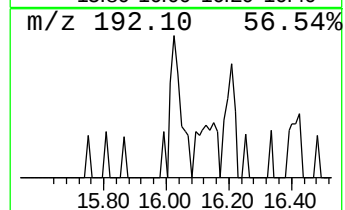
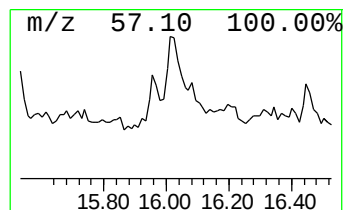
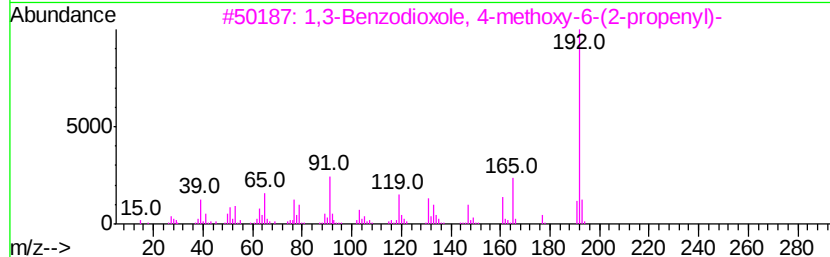
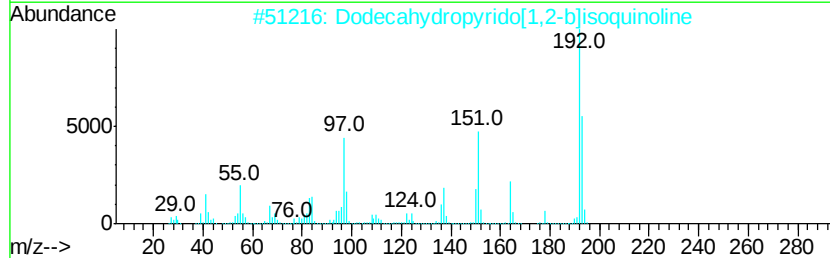
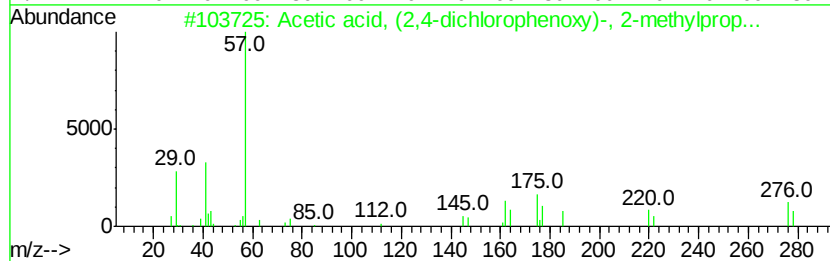
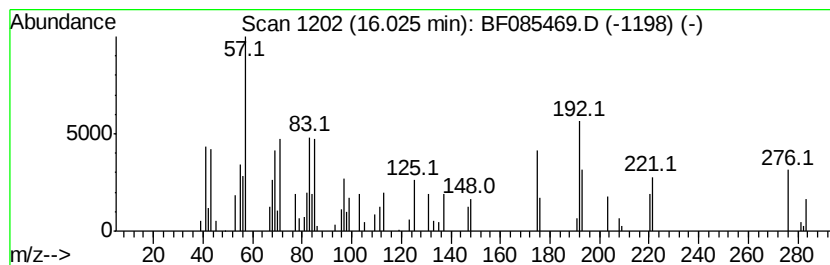
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown16.03 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.03	2.06 ng	58659	Perylene-d12	15.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetic acid, (2,4-dichlorophenox...	276	C12H14Cl2O3	001713-15-1	14
2		Dodecahydropyrido[1,2-b]isoquino...	193	C13H23N	113039-29-5	10
3		1,3-Benzodioxole, 4-methoxy-6-(2...	192	C11H12O3	000607-91-0	9
4		3-(2-Methoxy-5-methylphenyl)acry...	192	C11H12O3	103986-76-1	9
5		Pyridazin-3(2H)-one, 4,5-dihydro...	192	C10H9FN2O	039499-62-2	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031616\
Data File : BF085469.D
Acq On : 16 Mar 2016 18:40
Operator : UM/SJ
Sample : H1769-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DRUM-325-359-COMPOSITE

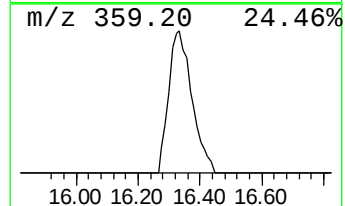
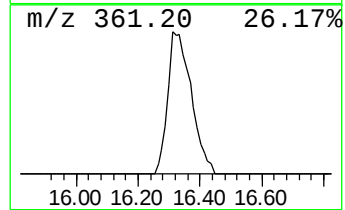
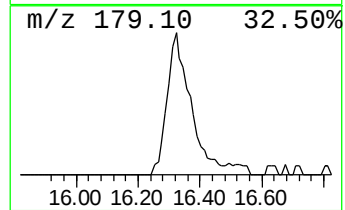
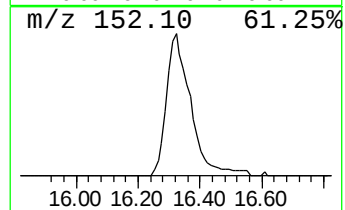
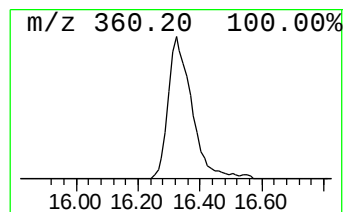
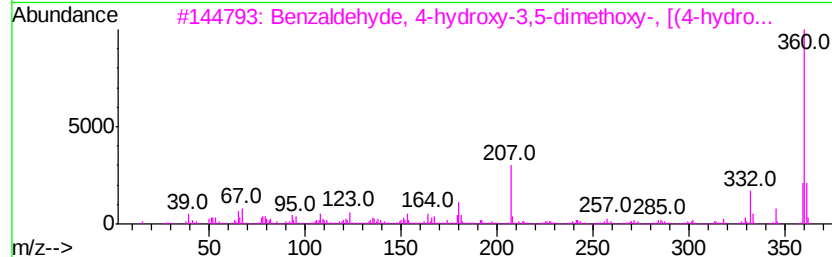
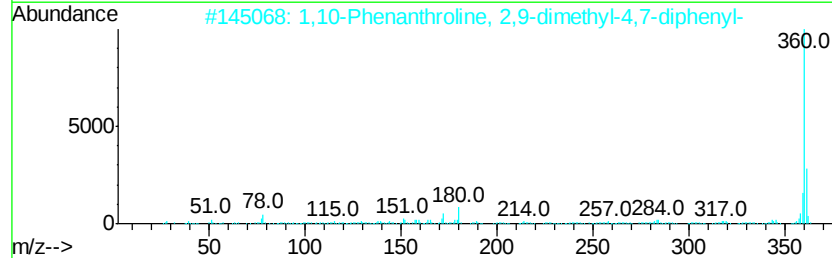
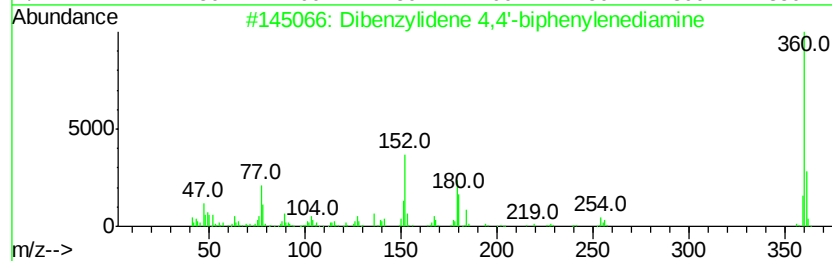
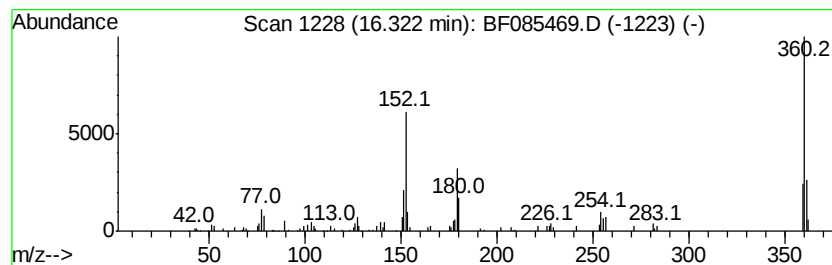
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Dibenzylidene 4,4'-biphenyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.32	11.30 ng	321118	Perylene-d12	15.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dibenzylidene 4,4'-biphenylenedi...	360	C26H20N2	006311-48-4	93
2		1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	46
3		Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	43
4		1,3,2-Dioxaborolane, bis(spiro[4...	360	C20H13B06	1000150-23-7	43
5		N,N'-di-2-Naphthyl-p-phenylenedi...	360	C26H20N2	000093-46-9	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031616\
Data File : BF085469.D
Acq On : 16 Mar 2016 18:40
Operator : UM/SJ
Sample : H1769-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DRUM-325-359-COMPOSITE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.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
2-Pentanone, 4-hy...	5.10	6.6	ng	241880	1	6.90	735703	20.0
3-Chloro-6-fluoro...	6.68	97.2	ng	3577110	1	6.90	735703	20.0
unknown11.94	11.94	2.2	ng	119676	4	11.43	1101710	20.0
Pentadecanoic acid	12.73	3.1	ng	169216	4	11.43	1101710	20.0
Trifluoroacetic a...	13.90	3.0	ng	136379	5	14.06	894121	20.0
unknown16.03	16.03	2.1	ng	58659	6	15.51	568231	20.0
Dibenzylidene 4,4...	16.32	11.3	ng	321118	6	15.51	568231	20.0