

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111315\
 Data File : BF082933.D
 Acq On : 14 Nov 2015 9:37
 Operator : UM/IZ
 Sample : G4331-03
 Misc :
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 LIBERTY-SF-002-02

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-BF110715.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	4.967	249	252	255	rVB	855319	908162	14.04%	2.051%
2	5.413	289	291	294	rVB	2167132	2152658	33.27%	4.863%
3	6.453	380	382	384	rBV	1748117	1449815	22.41%	3.275%
4	6.579	390	393	395	rBV	4769373	4658013	71.99%	10.522%
5	6.796	410	412	414	rBV	1026915	1170603	18.09%	2.644%
6	6.876	416	419	424	rBV2	66722	78282	1.21%	0.177%
7	6.956	424	426	429	rBV	3601990	4294532	66.37%	9.701%
8	7.367	459	462	464	rBV	3295656	3538908	54.70%	7.994%
9	7.482	468	472	475	rBV	84941	121727	1.88%	0.275%
10	7.836	500	503	505	rBV2	138206	184938	2.86%	0.418%
11	8.007	515	518	519	rBV	48334	66428	1.03%	0.150%
12	8.087	523	525	529	rBV	1820877	1659009	25.64%	3.748%
13	8.556	561	566	568	rBV2	39644	66592	1.03%	0.150%
14	8.590	568	569	572	rVB	51552	72031	1.11%	0.163%
15	8.808	585	588	589	rVB2	51115	69521	1.07%	0.157%
16	8.899	593	596	599	rBV2	105733	138076	2.13%	0.312%
17	9.048	607	609	615	rVB	168386	195153	3.02%	0.441%
18	9.173	617	620	622	rVV	6891732	6470184	100.00%	14.616%
19	9.425	640	642	645	rBV2	71930	113842	1.76%	0.257%
20	9.505	645	649	650	rBV	167425	181879	2.81%	0.411%
21	9.562	653	654	657	rVB	437276	343558	5.31%	0.776%
22	9.619	657	659	662	rBV2	62355	103314	1.60%	0.233%
23	9.848	676	679	681	rBV	1817785	1778577	27.49%	4.018%
24	10.053	694	697	699	rBV2	43227	80247	1.24%	0.181%
25	10.259	713	715	719	rVB3	120444	189654	2.93%	0.428%
26	10.339	719	722	723	rBV	102986	100011	1.55%	0.226%
27	10.636	745	748	750	rBV	3674892	3529581	54.55%	7.973%
28	10.762	757	759	765	rVB	76925	110155	1.70%	0.249%
29	10.853	765	767	771	rBV2	52089	84911	1.31%	0.192%
30	11.105	787	789	792	rVB	213305	187894	2.90%	0.424%
31	11.208	796	798	799	rBV	115550	94300	1.46%	0.213%
32	11.322	806	808	811	rBV2	1247000	1476812	22.82%	3.336%
33	11.562	826	829	833	rVV2	57145	104581	1.62%	0.236%
34	11.631	833	835	839	rVV	65506	79561	1.23%	0.180%

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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

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Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
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35	11.722	842	843	846	rVB	151607	129289	2.00%	0.292%
36	11.894	857	858	860	rVB	253928	268714	4.15%	0.607%
37	12.168	880	882	884	rVB	140514	111458	1.72%	0.252%
38	12.922	945	948	950	rBV	4511991	5288341	81.73%	11.946%
39	13.825	1024	1027	1032	rBV2	69922	96776	1.50%	0.219%
40	13.962	1037	1039	1041	rBV	1290905	1155369	17.86%	2.610%
41	14.820	1112	1114	1116	rBV	85904	96534	1.49%	0.218%
42	15.380	1160	1163	1166	rBV	768141	1117768	17.28%	2.525%
43	15.848	1201	1204	1207	rBV	39171	72030	1.11%	0.163%
44	16.317	1243	1245	1251	rVB3	40458	79155	1.22%	0.179%

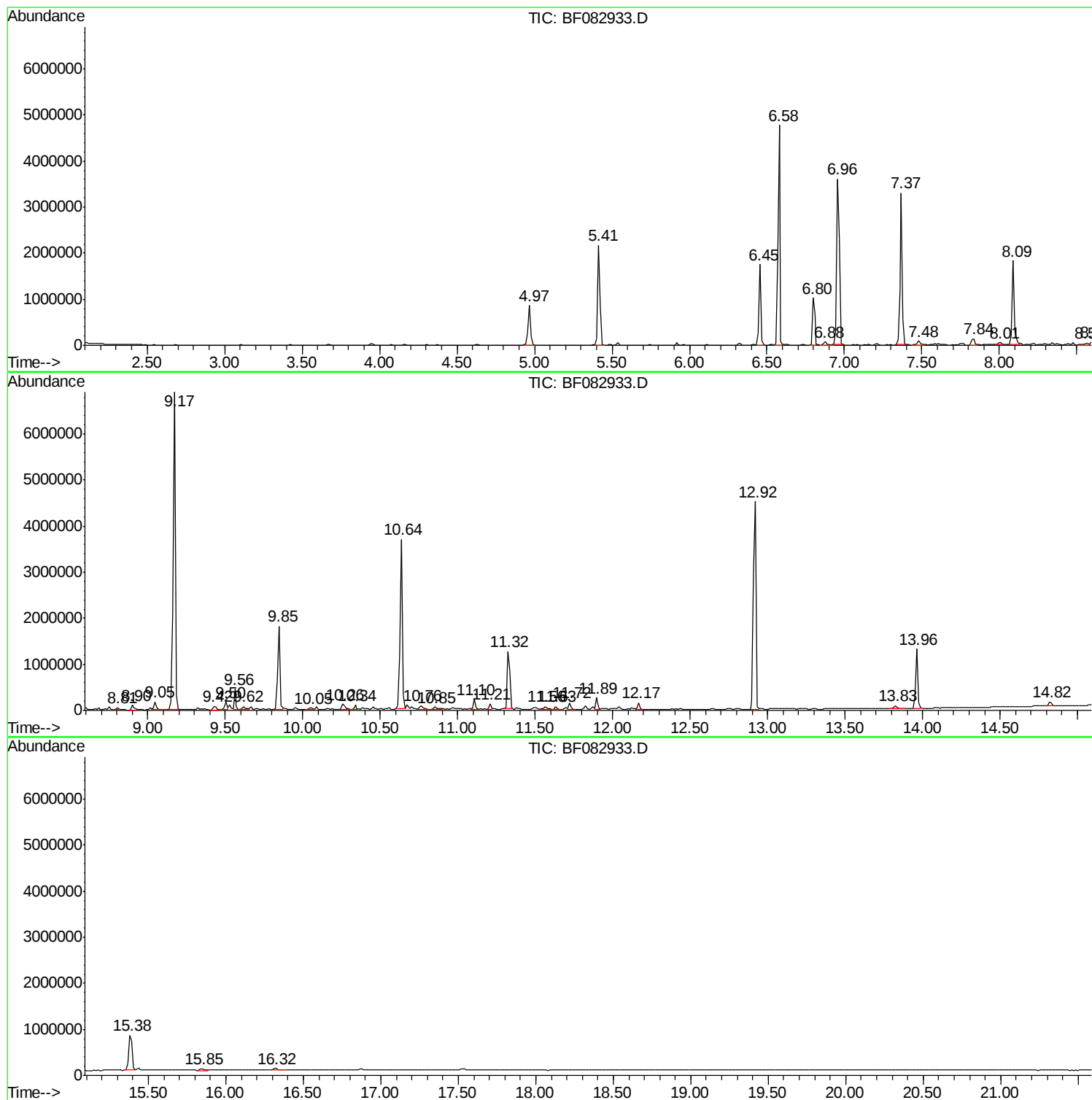
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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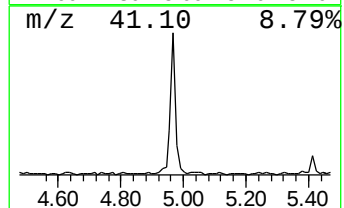
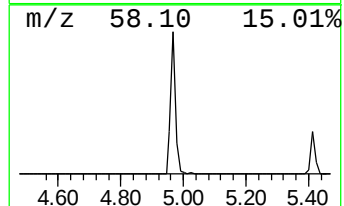
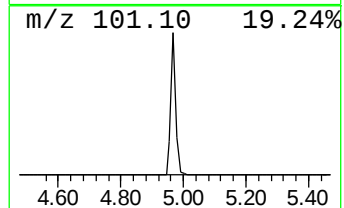
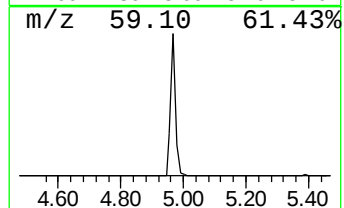
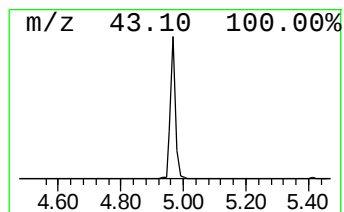
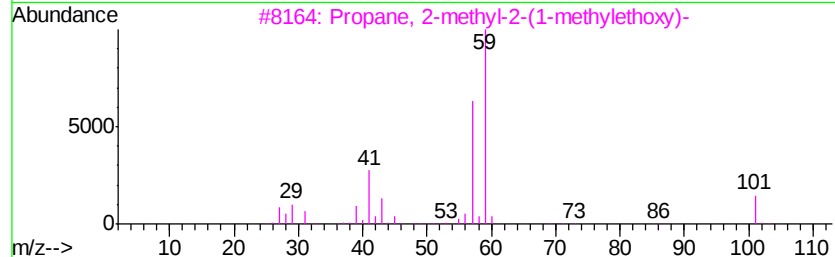
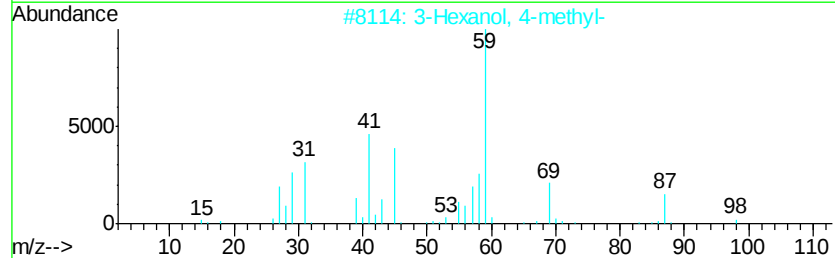
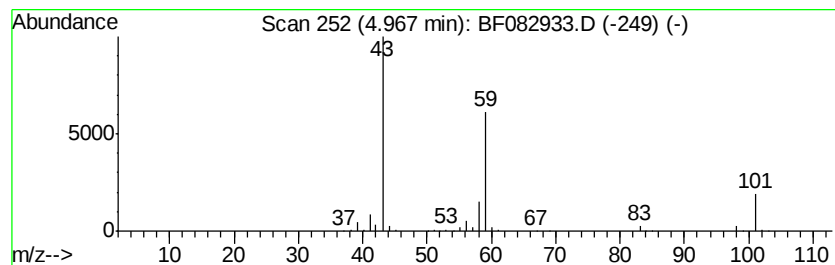
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	15.52 ng	908162	1,4-Dichlorobenzene-d4	6.80

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3		Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	28
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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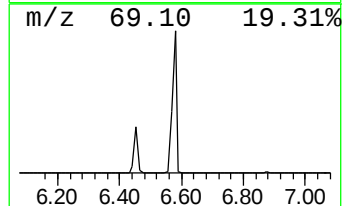
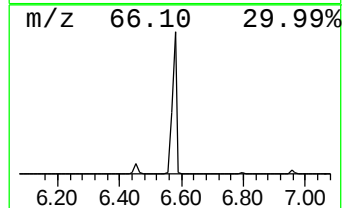
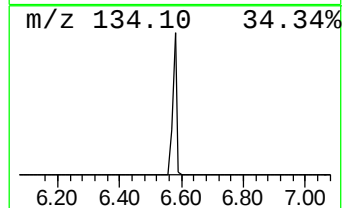
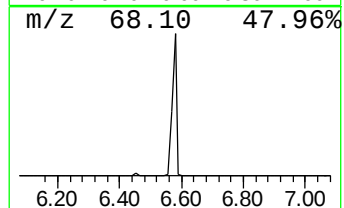
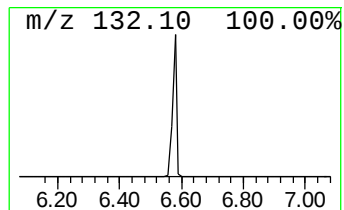
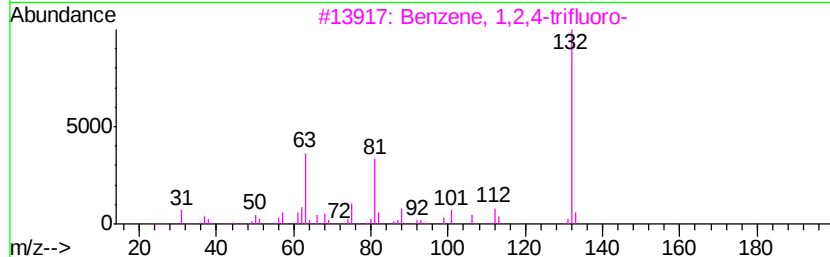
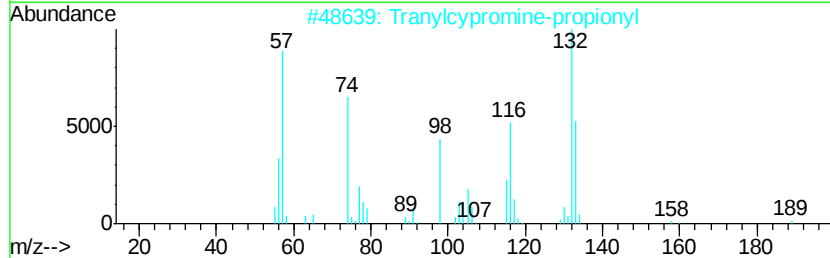
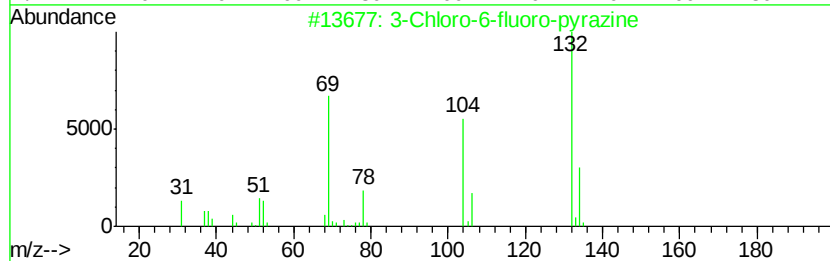
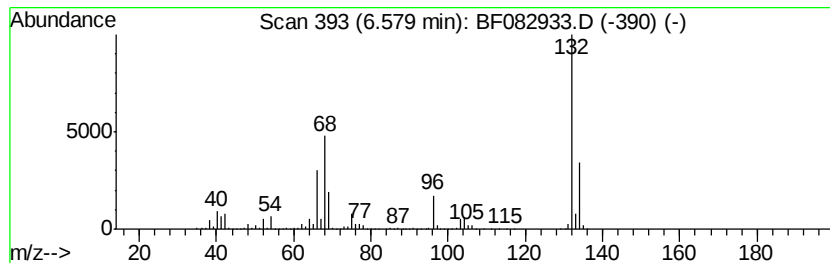
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	79.58 ng	4658010	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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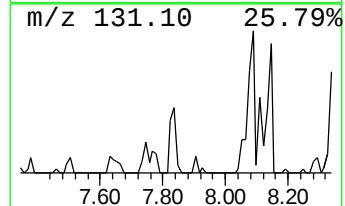
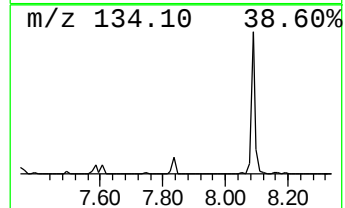
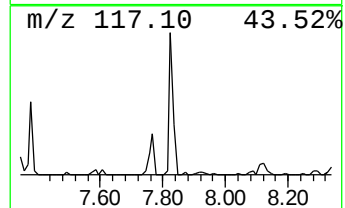
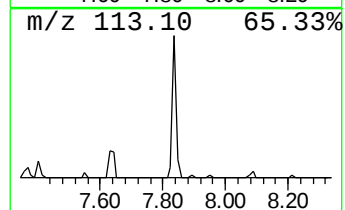
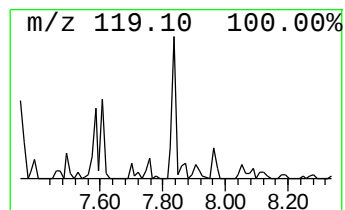
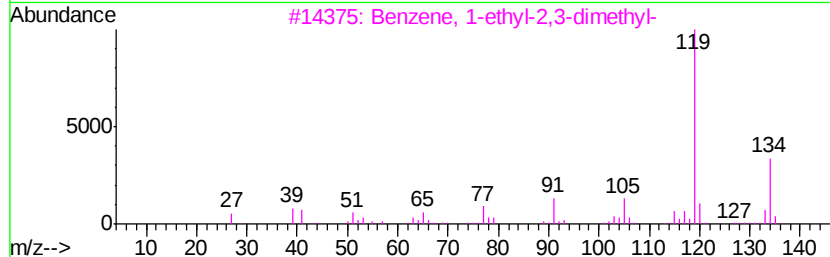
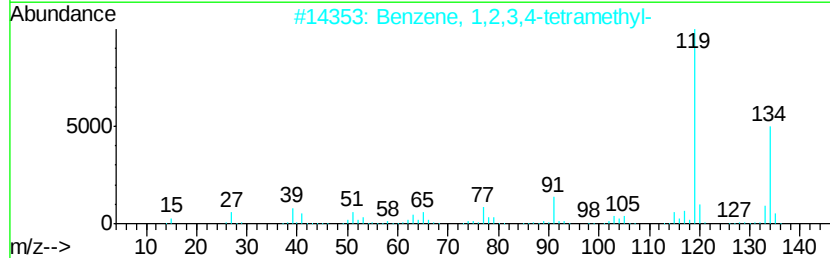
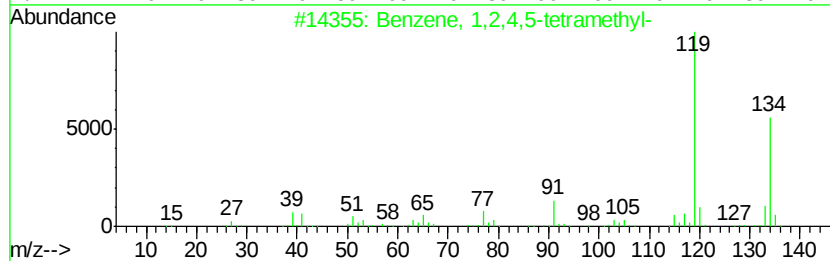
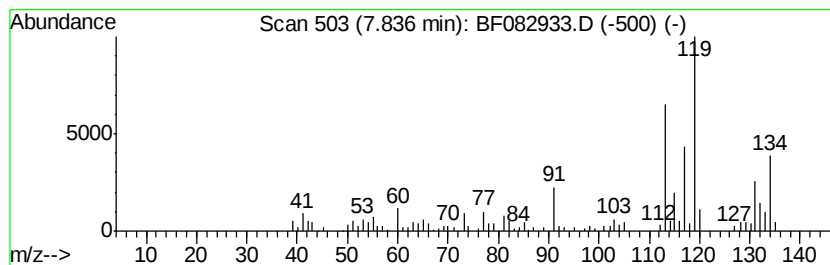
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.84	2.23 ng	184938	Naphthalene-d8	8.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	55
2		Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	55
3		Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	55
4		Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	55
5		Benzene, 1-methyl-2-(1-methyleth...	134	C10H14	000527-84-4	50



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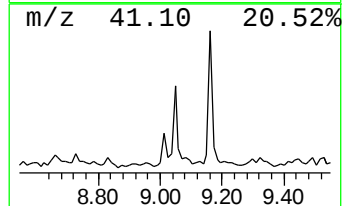
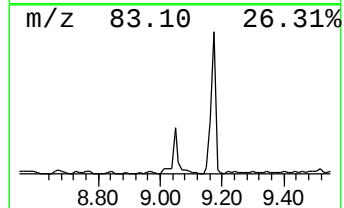
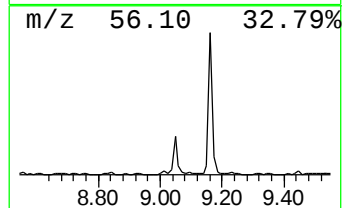
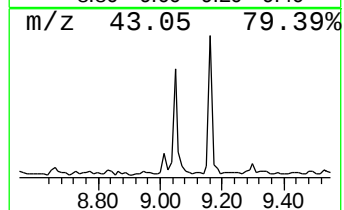
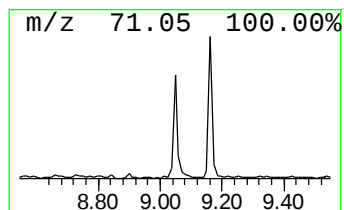
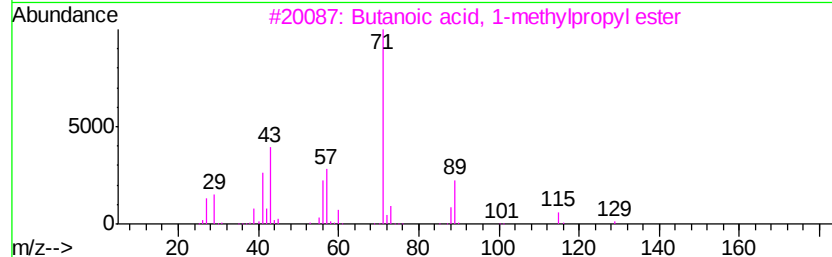
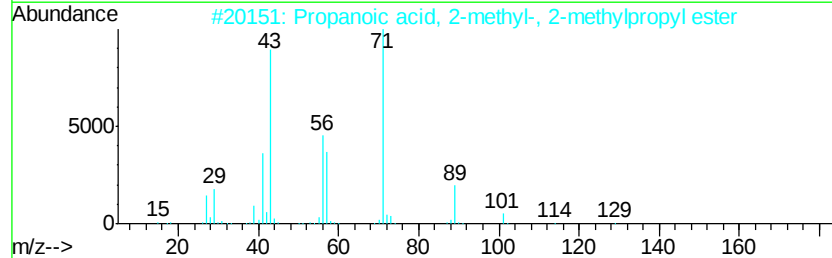
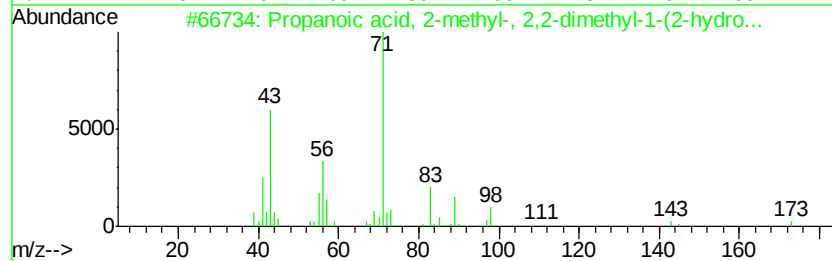
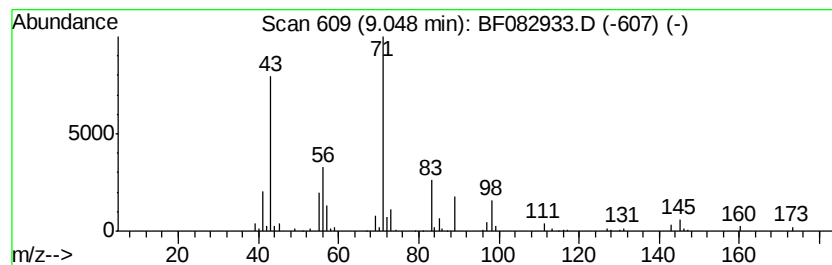
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.05	2.19 ng	195153	Acenaphthene-d10	9.85

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propanoic acid, 2-methyl-, 2,2-d...	216	C12H24O3	074367-33-2	86
2		Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	50
3		Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	42
4		Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	40
5		Propanoic acid, 2-methyl-, 3-hyd...	216	C12H24O3	074367-34-3	38



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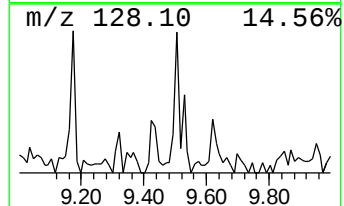
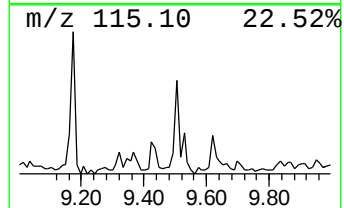
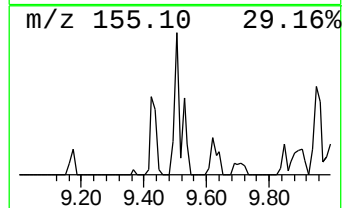
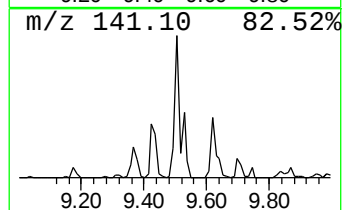
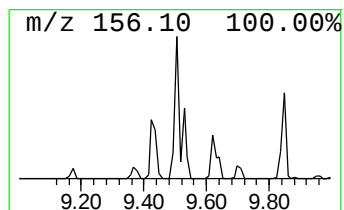
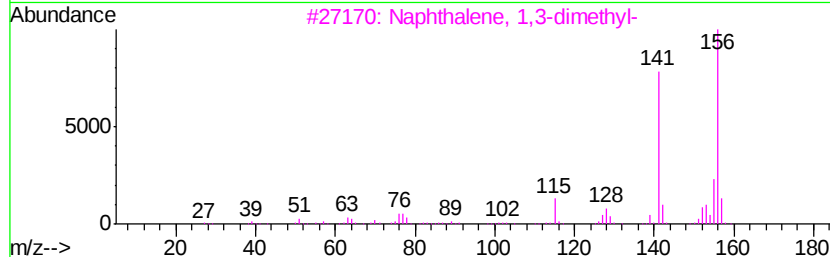
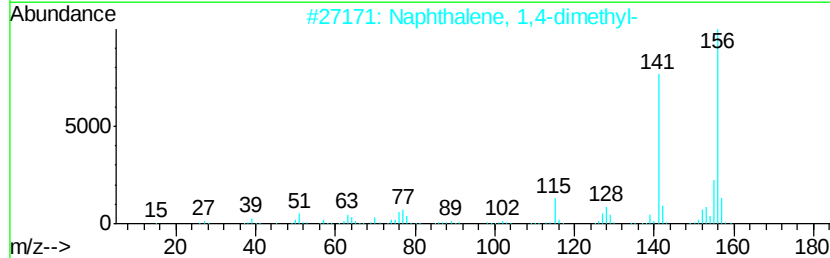
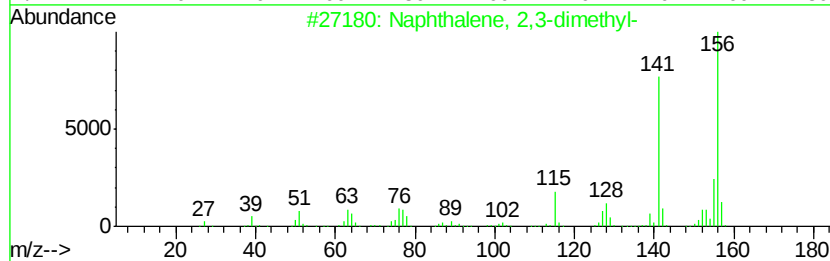
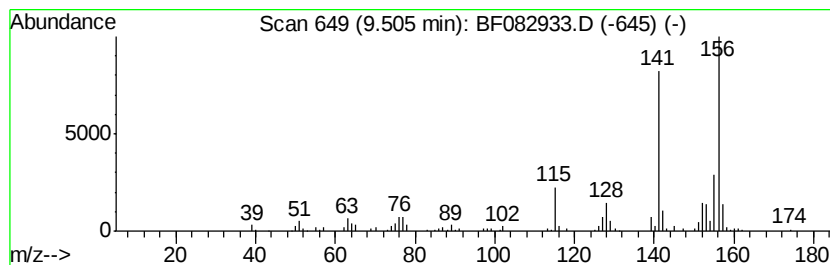
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TIC Integration Parameters: LSCINT.P

Peak Number 6 Naphthalene, 2,3-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.50	2.05 ng	181879	Acenaphthene-d10	9.85

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
2			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	96
3			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96
4			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	95
5			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	95



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111315\
Data File : BF082933.D
Acq On : 14 Nov 2015 9:37
Operator : UM/IZ
Sample : G4331-03
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LIBERTY-SF-002-02

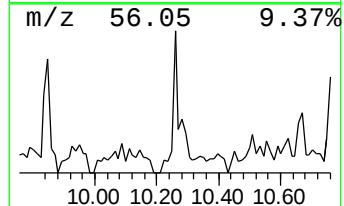
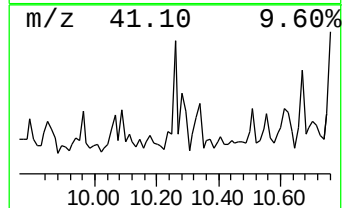
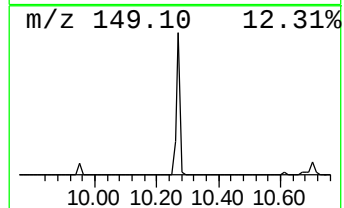
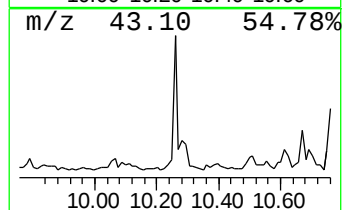
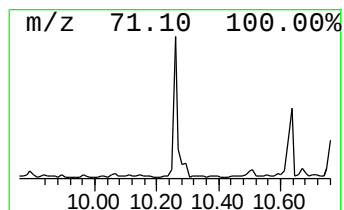
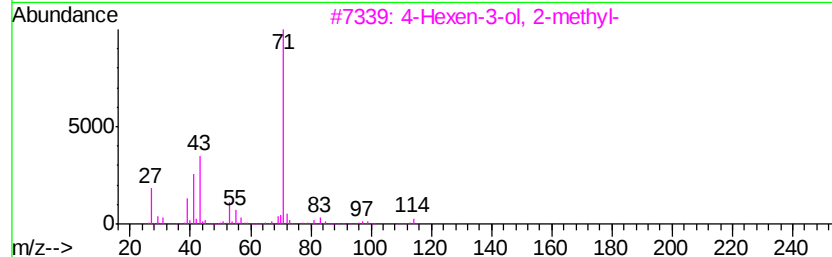
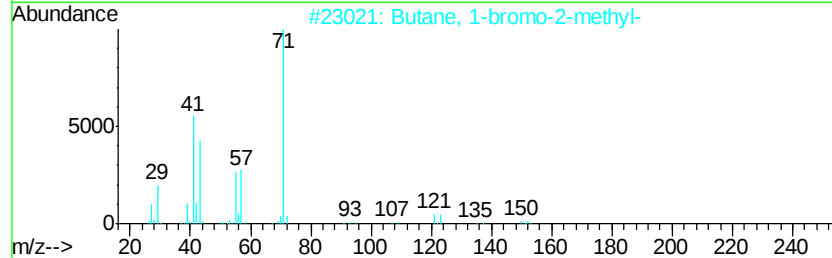
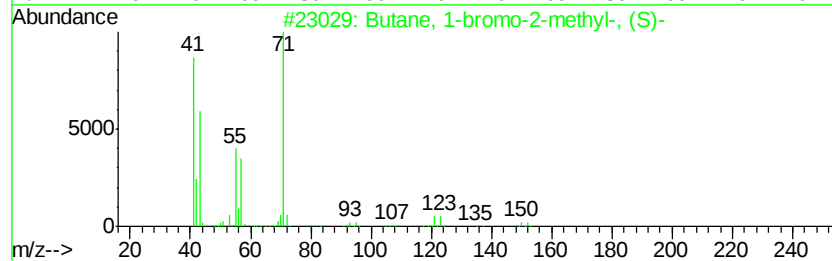
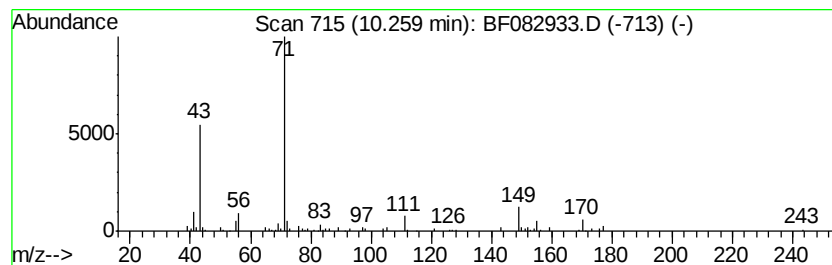
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Butane, 1-bromo-2-methyl-, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.26	2.13 ng	189654	Acenaphthene-d10	9.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 1-bromo-2-methyl-, (S)-	150	C5H11Br	000534-00-9	59
2		Butane, 1-bromo-2-methyl-	150	C5H11Br	010422-35-2	59
3		4-Hexen-3-ol, 2-methyl-	114	C7H14O	004798-60-1	50
4		Butyric acid, m-nitrophenyl ester	209	C10H11NO4	014617-97-1	50
5		2-Furanmethanol, tetrahydro-, ac...	144	C7H12O3	000637-64-9	40



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111315\
Data File : BF082933.D
Acq On : 14 Nov 2015 9:37
Operator : UM/IZ
Sample : G4331-03
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LIBERTY-SF-002-02

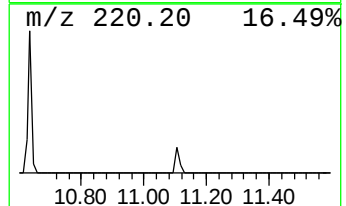
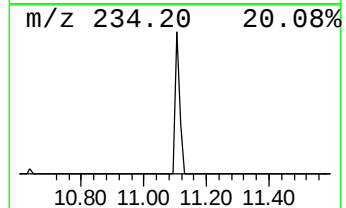
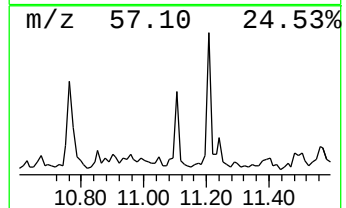
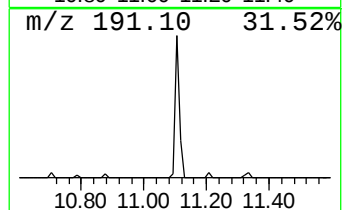
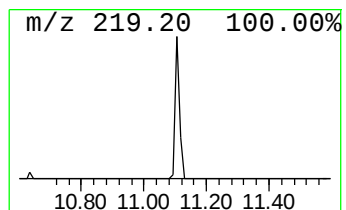
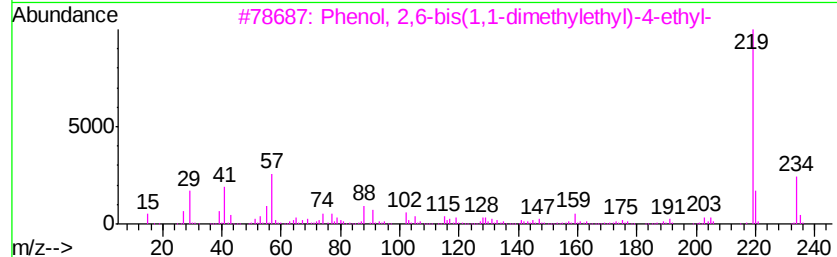
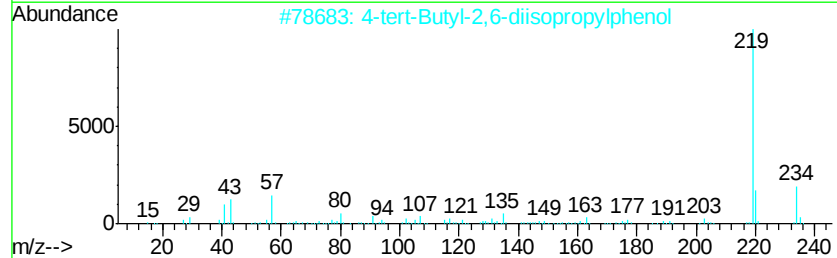
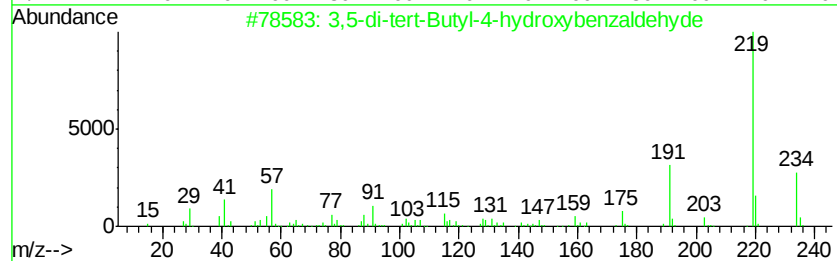
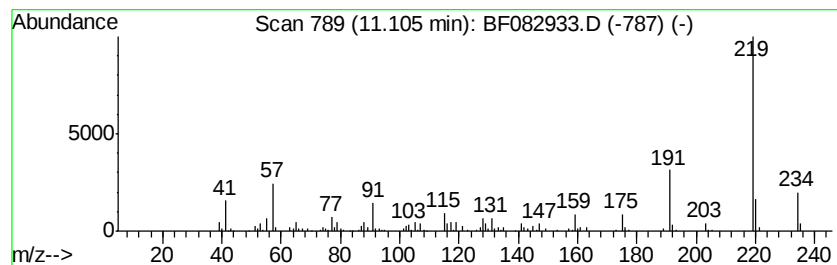
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 3,5-di-tert-Butyl-4-hydroxy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.10	2.54 ng	187894	Phenanthrene-d10	11.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	96
2		4-tert-Butyl-2,6-diisopropylphenol	234	C16H26O	057354-65-1	81
3		Phenol, 2,6-bis(1,1-dimethylethyl)...	234	C16H26O	004130-42-1	74
4		6-Tert-butyl-2,3-dicyanonaphthalen	234	C16H14N2	032703-82-5	72
5		3,5-Di-tert-butylbenzoic acid	234	C15H22O2	016225-26-6	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111315\
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Acq On : 14 Nov 2015 9:37
Operator : UM/IZ
Sample : G4331-03
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LIBERTY-SF-002-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.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...	4.97	15.5	ng	908162	1	6.80	1170600	20.0
unknown6.58	6.58	79.6	ng	4658010	1	6.80	1170600	20.0
Benzene, 1,2,4,5-...	7.84	2.2	ng	184938	2	8.09	1659010	20.0
Propanoic acid, 2...	9.05	2.2	ng	195153	3	9.85	1778580	20.0
Naphthalene, 2,3-...	9.50	2.0	ng	181879	3	9.85	1778580	20.0
Butane, 1-bromo-2...	10.26	2.1	ng	189654	3	9.85	1778580	20.0
3,5-di-tert-Butyl...	11.10	2.5	ng	187894	4	11.32	1476810	20.0