

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041315\
 Data File : BF078490.D
 Acq On : 14 Apr 2015 7:30
 Operator : TP/IZ
 Sample : G1787-04
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 LS-SD02A

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-BF040115.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	1.255	4	6	9	rVB	59008	78793	4.46%	0.763%
2	1.507	26	28	35	rBV	129276	211695	11.97%	2.050%
3	1.610	35	37	62	rVB	914731	1768410	100.00%	17.127%
4	4.490	287	289	296	rBV	49242	69270	3.92%	0.671%
5	5.084	338	341	349	rBV	477875	619906	35.05%	6.004%
6	6.422	456	458	466	rBV	421396	638627	36.11%	6.185%
7	6.536	466	468	471	rBV	522379	668870	37.82%	6.478%
8	6.833	491	494	496	rBV	158689	213982	12.10%	2.072%
9	7.016	507	510	512	rBV	440328	482536	27.29%	4.673%
10	7.530	553	555	557	rBV	420420	393136	22.23%	3.807%
11	8.399	629	631	634	rBV	239456	296433	16.76%	2.871%
12	9.748	747	749	752	rVB	569655	706874	39.97%	6.846%
13	10.262	793	794	799	rBV	29336	42620	2.41%	0.413%
14	10.559	818	820	823	rBV	350956	356226	20.14%	3.450%
15	11.462	894	899	903	rBV2	42098	49901	2.82%	0.483%
16	11.531	903	905	908	rBV	446648	491677	27.80%	4.762%
17	11.771	923	926	928	rBV	16211	24358	1.38%	0.236%
18	12.388	977	980	981	rVV	288629	377681	21.36%	3.658%
19	12.411	981	982	985	rVB	58642	47937	2.71%	0.464%
20	13.874	1107	1110	1112	rBV	79015	80332	4.54%	0.778%
21	14.148	1131	1134	1136	rBV	63703	71712	4.06%	0.695%
22	14.251	1142	1143	1146	rVB	39209	41467	2.34%	0.402%
23	14.365	1151	1153	1156	rVV	624790	824910	46.65%	7.989%
24	15.554	1253	1257	1261	rVV2	24856	64703	3.66%	0.627%
25	15.634	1261	1264	1269	rVV	436238	520558	29.44%	5.041%
26	15.714	1269	1271	1273	rVV	111318	127263	7.20%	1.233%
27	16.320	1322	1324	1325	rVV	47781	53664	3.03%	0.520%
28	16.354	1325	1327	1332	rVB	16772	25578	1.45%	0.248%
29	16.880	1371	1373	1379	rBV	26262	59153	3.34%	0.573%
30	17.108	1390	1393	1395	rBV	18861	25943	1.47%	0.251%
31	17.188	1398	1400	1402	rVV	19344	25839	1.46%	0.250%
32	17.245	1402	1405	1408	rVV2	28916	42705	2.41%	0.414%
33	17.314	1408	1411	1419	rVB	345693	470043	26.58%	4.552%
34	18.263	1492	1494	1498	rVB3	12754	26839	1.52%	0.260%

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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-BF040115.M
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35	18.526	1515	1517	1520	rVB2	10210	22400	1.27%	0.217%
36	18.594	1520	1523	1529	rVV2	87103	163988	9.27%	1.588%
37	18.731	1532	1535	1543	rVV8	12659	44999	2.54%	0.436%
38	18.868	1544	1547	1551	rVB	13840	32222	1.82%	0.312%
39	19.680	1615	1618	1626	rVB4	24657	62262	3.52%	0.603%

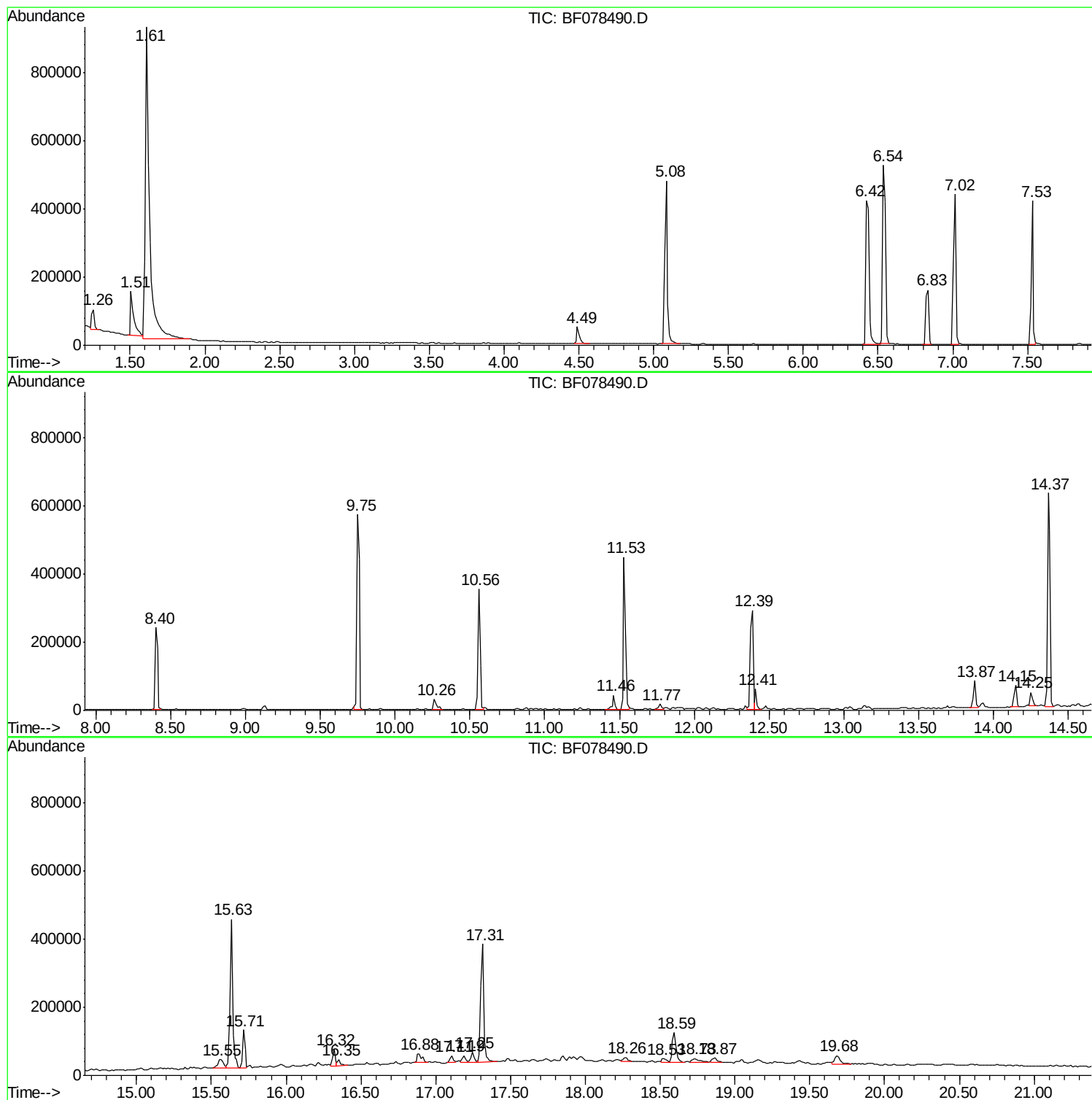
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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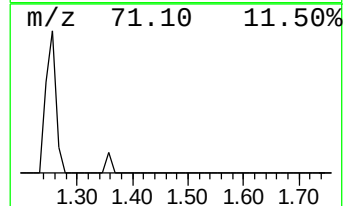
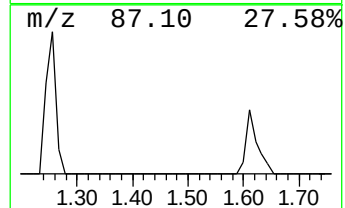
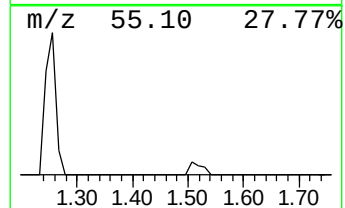
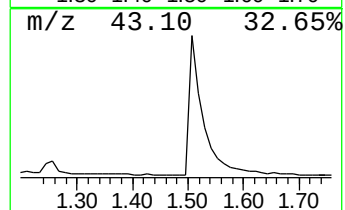
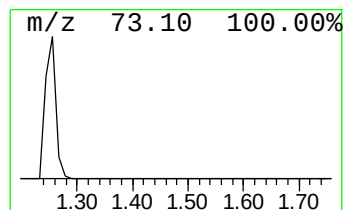
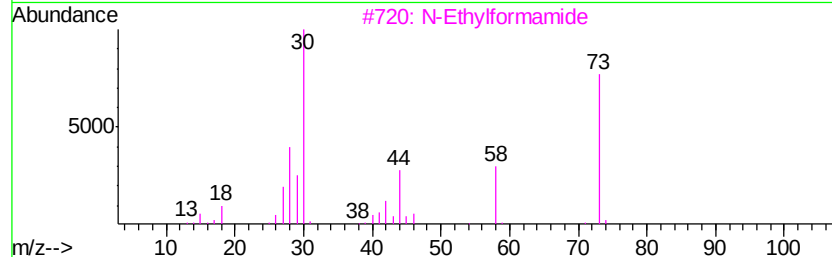
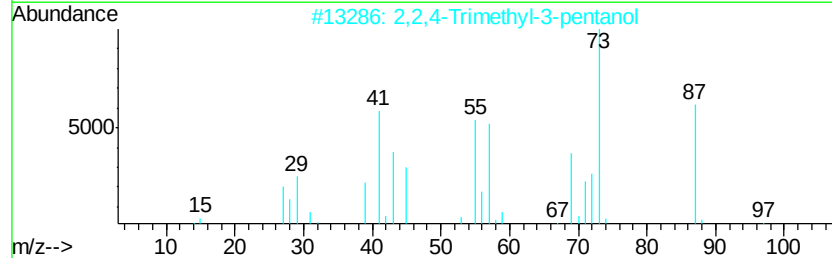
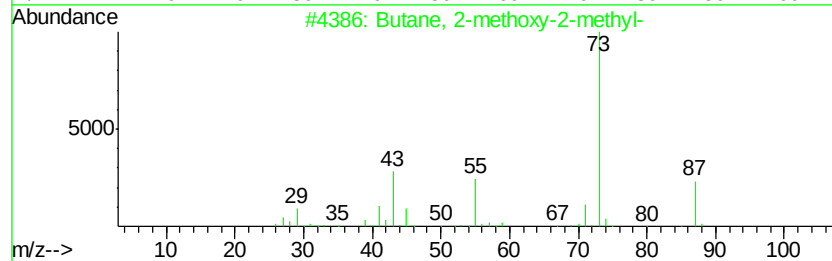
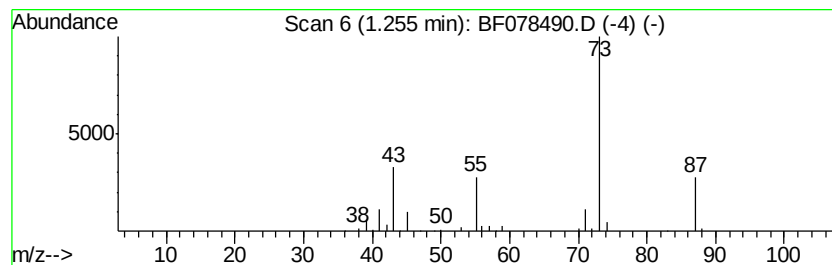
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.26	7.36 ng	78793	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	90
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	43
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	9
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9



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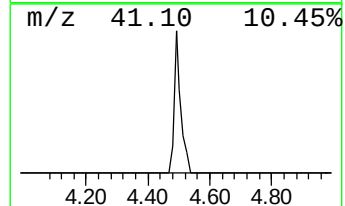
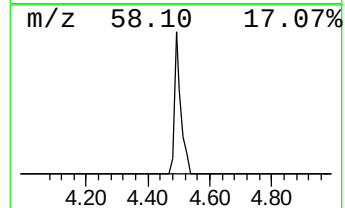
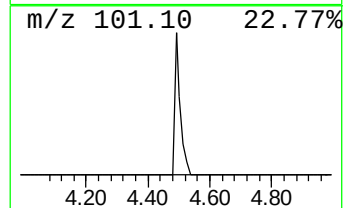
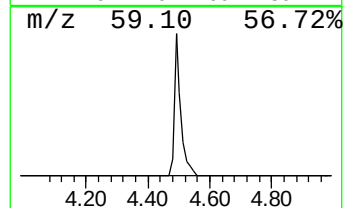
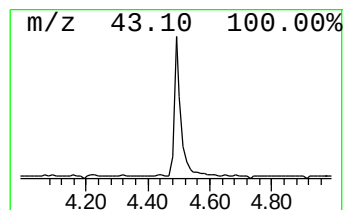
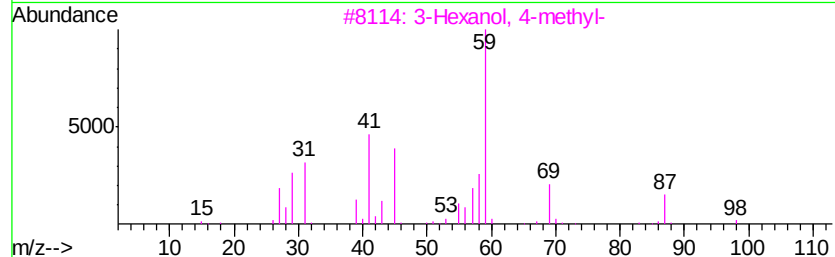
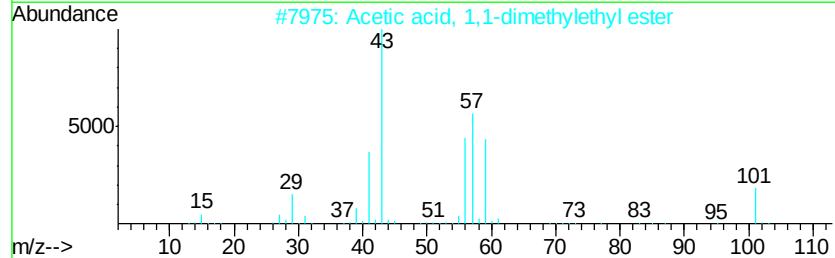
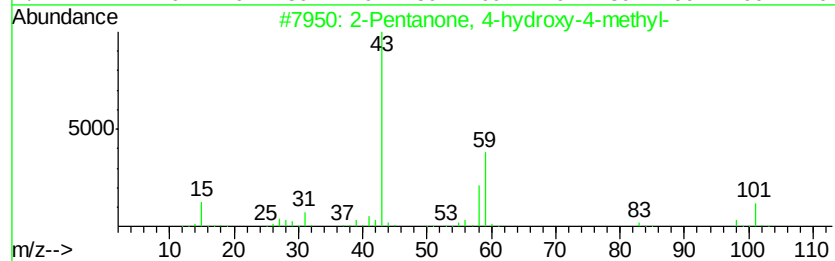
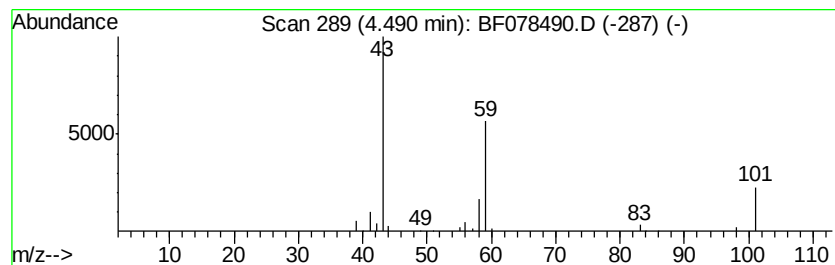
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.49	6.47 ng	69270	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	9



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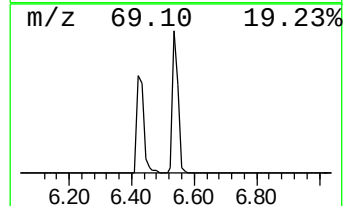
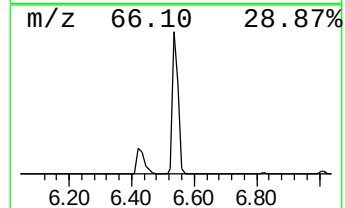
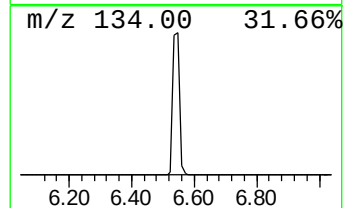
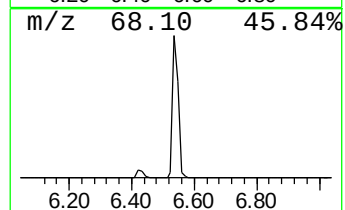
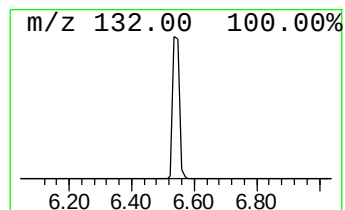
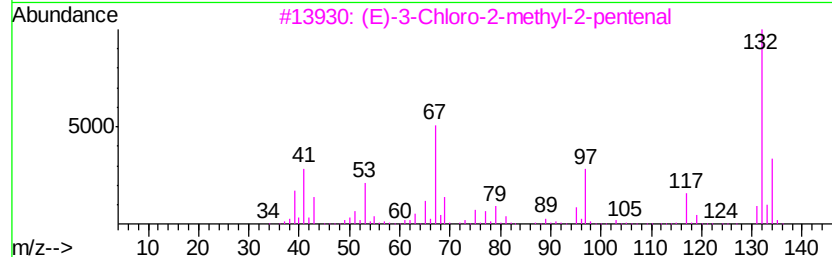
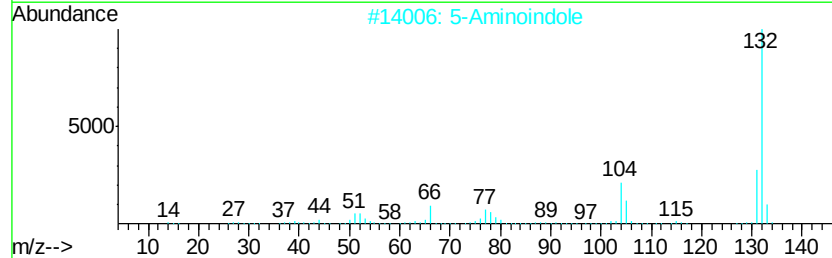
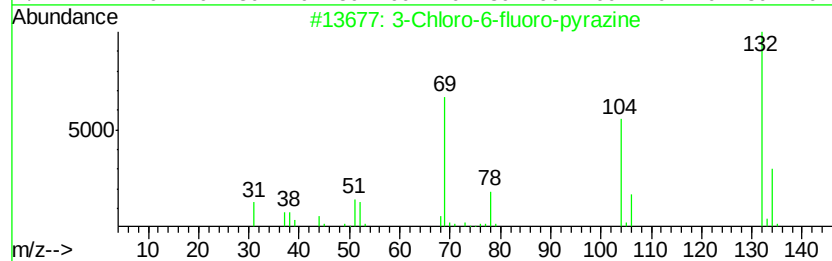
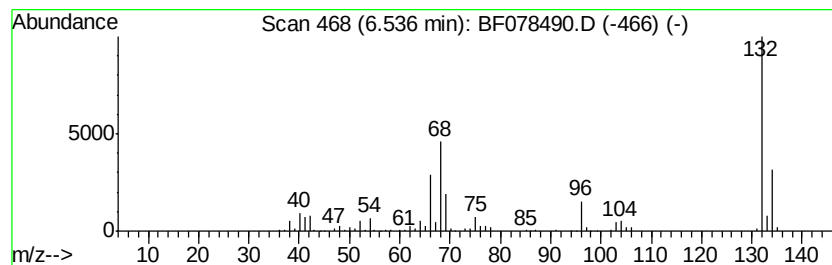
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown6.54 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	62.52 ng	668870	1,4-Dichlorobenzene-d4	6.83

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16		
2	5-Aminoindole	132	C8H8N2	005192-03-0	10		
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9		
4	Bicyclo[4.2.0]octa-1,3,5-triene, ...	132	C10H12	028749-81-7	9		
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9		



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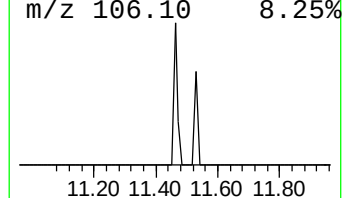
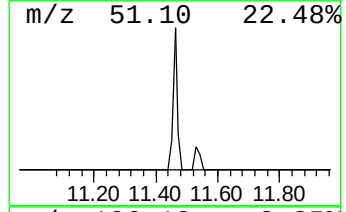
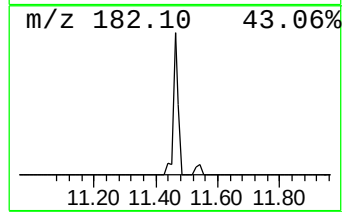
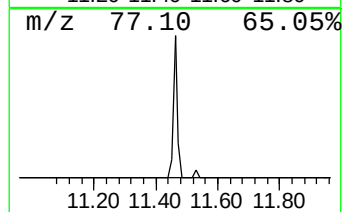
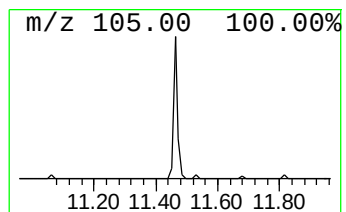
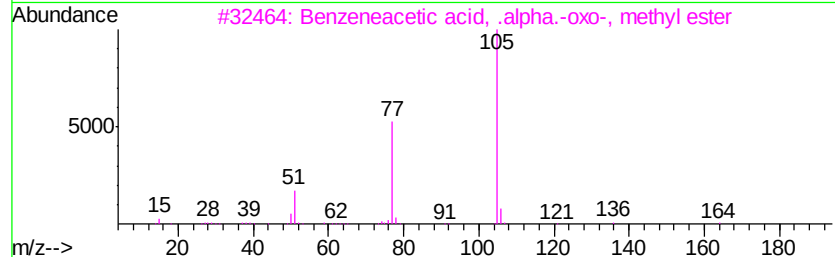
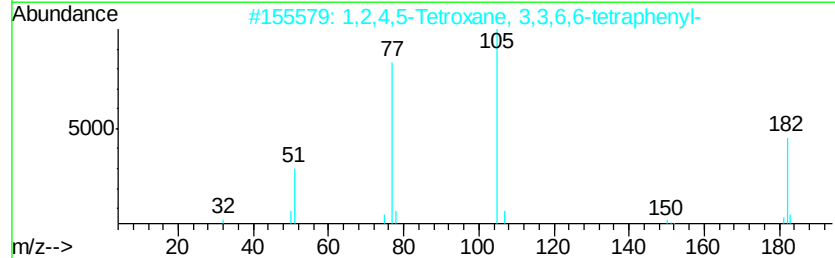
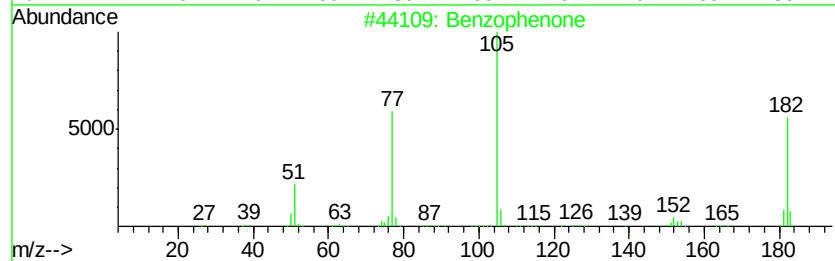
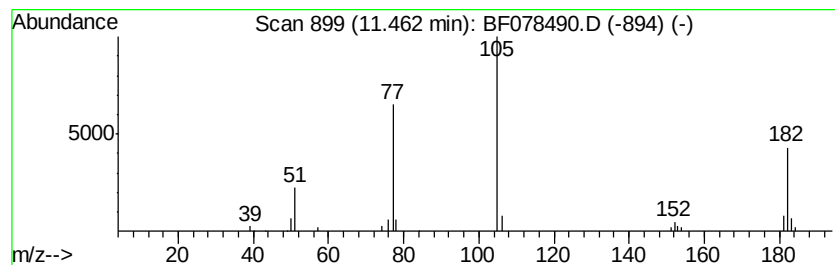
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Benzophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.46	2.80 ng	49901	Acenaphthene-d10	10.56
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzophenone	182 C13H10O	000119-61-9 97
2		1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396 C26H20O4	016204-36-7 78
3		Benzeneacetic acid, .alpha.-oxo-...	164 C9H8O3	015206-55-0 47
4		N-(1-Cyanovinyl)benzamide	172 C10H8N2O	1000186-19-1 47
5		2-(2-Oxo-2-phenyl-ethyl)-malonon...	184 C11H8N2O	1000296-76-9 47



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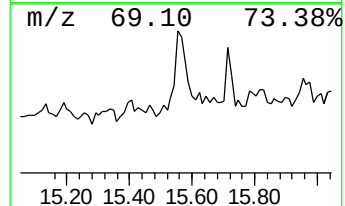
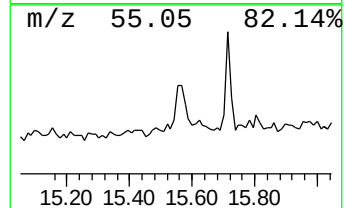
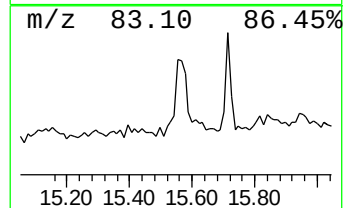
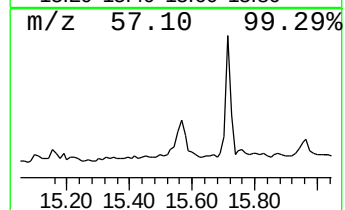
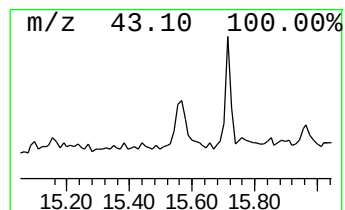
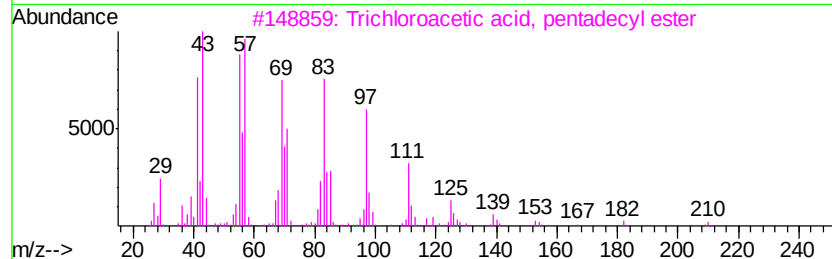
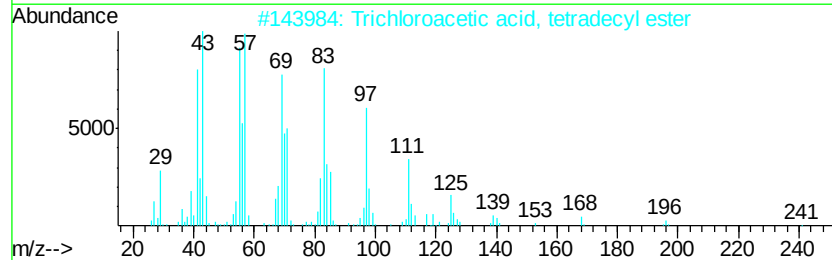
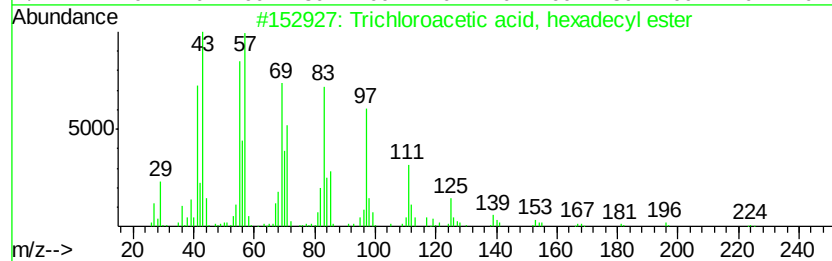
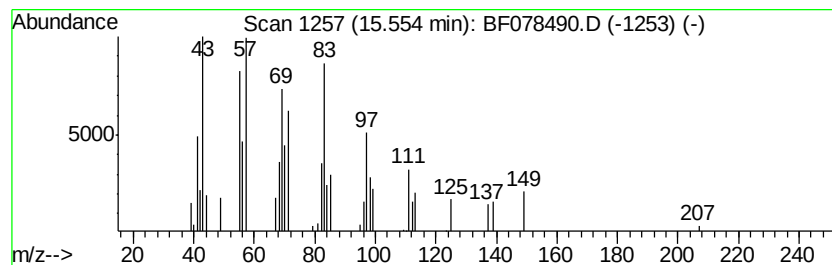
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Trichloroacetic acid, hexad... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.55	2.49 ng	64703	Chrysene-d12	15.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	81
2		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	81
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	81
4		1-Tetracosanol	354	C24H50O	000506-51-4	81
5		1-Hexadecanol	242	C16H34O	036653-82-4	76



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041315\
Data File : BF078490.D
Acq On : 14 Apr 2015 7:30
Operator : TP/IZ
Sample : G1787-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LS-SD02A

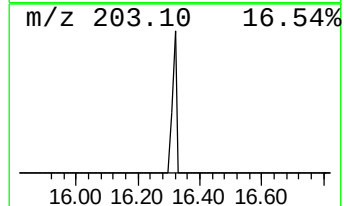
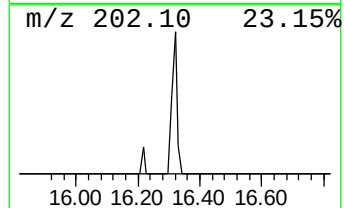
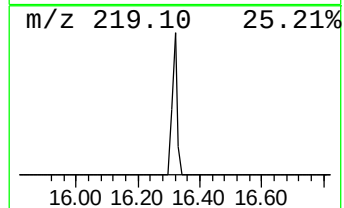
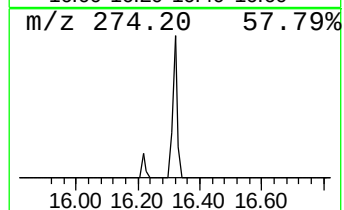
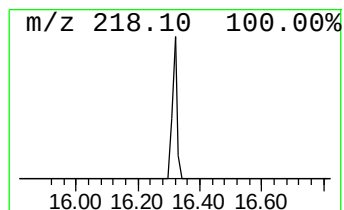
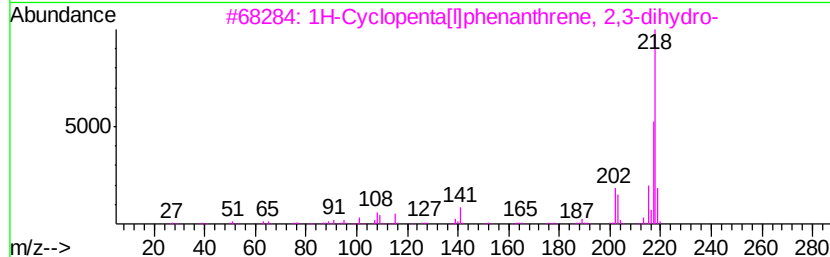
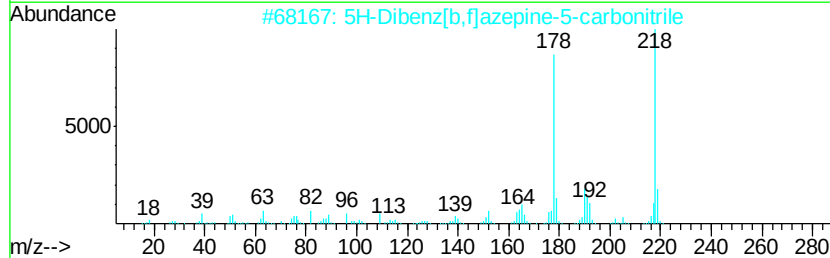
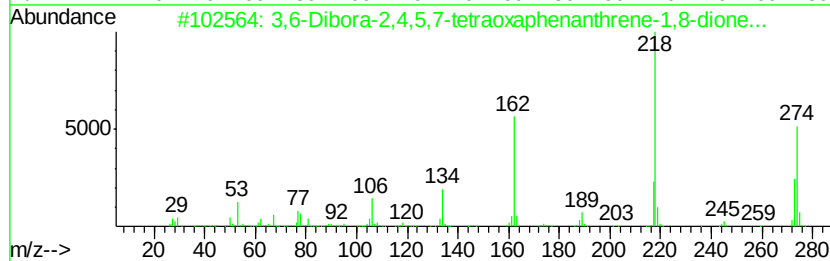
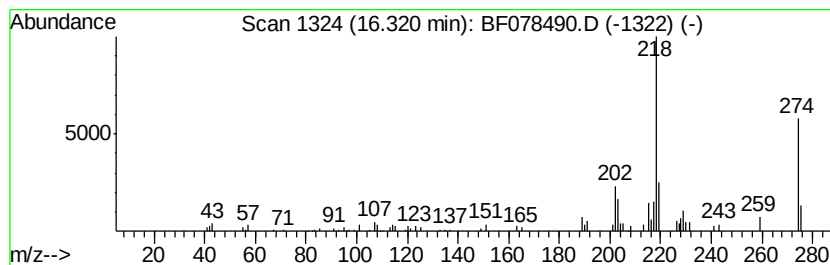
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 3,6-Dibora-2,4,5,7-tetraoxa... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.32	2.06 ng	53664	Chrysene-d12	15.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3,6-Dibora-2,4,5,7-tetraoxaphena...	274	C12H12B2O6	1000159-66-2	53
2		5H-Dibenz[b,f]azepine-5-carbonit...	218	C15H10N2	042787-75-7	46
3		1H-Cyclopenta[l]phenanthrene, 2,...	218	C17H14	000723-98-8	43
4		Naphthalene, 2-(phenylmethyl)-	218	C17H14	000613-59-2	43
5		Naphthalene, 1-(phenylmethyl)-	218	C17H14	000611-45-0	37



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041315\
Data File : BF078490.D
Acq On : 14 Apr 2015 7:30
Operator : TP/IZ
Sample : G1787-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LS-SD02A

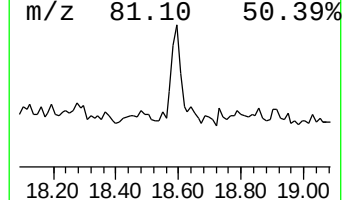
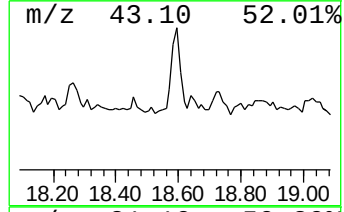
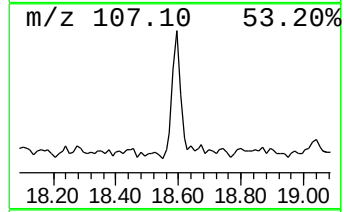
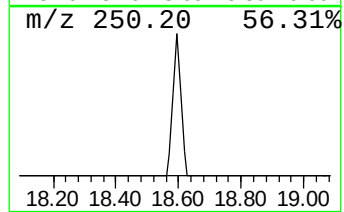
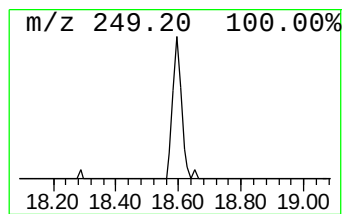
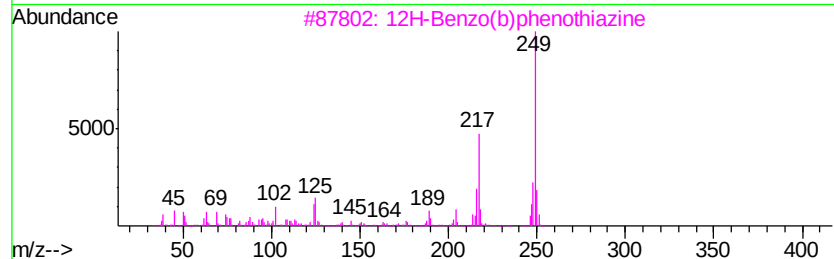
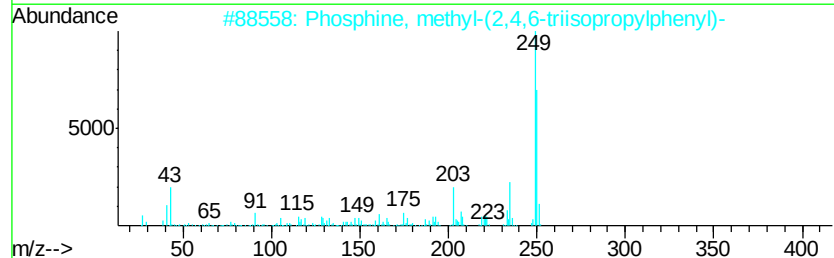
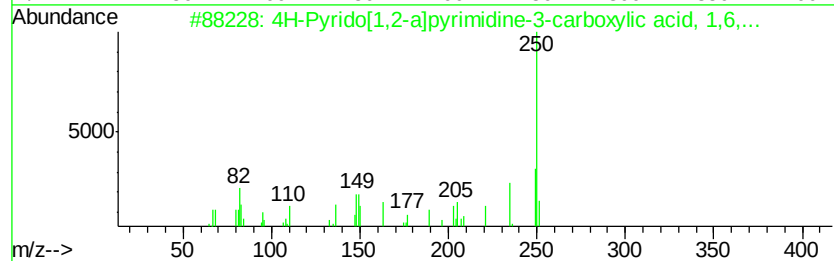
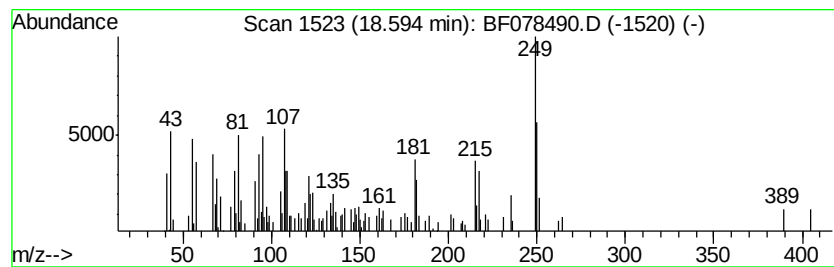
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 4H-Pyrido[1,2-a]pyrimidine-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.59	6.98 ng	163988	Perylene-d12	17.31

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4H-Pyrido[1,2-a]pyrimidine-3-car...	250	C13H18N2O3	035569-43-8	62
2		Phosphine, methyl-(2,4,6-triisop...	250	C16H27P	158748-69-7	43
3		12H-Benzo(b)phenothiazine	249	C16H11NS	000258-08-2	38
4		12H-Benzo[a]phenothiazine	249	C16H11NS	000225-83-2	35
5		7H-Benzo(c)phenothiazine	249	C16H11NS	000226-06-2	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041315\
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Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LS-SD02A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.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
Butane, 2-methoxy...	1.26	7.4	ng	78793	1	6.83	213982	20.0
2-Pentanone, 4-hy...	4.49	6.5	ng	69270	1	6.83	213982	20.0
unknown6.54	6.54	62.5	ng	668870	1	6.83	213982	20.0
Benzophenone	11.46	2.8	ng	49901	3	10.56	356226	20.0
Trichloroacetic a...	15.55	2.5	ng	64703	5	15.63	520558	20.0
3,6-Dibora-2,4,5,...	16.32	2.1	ng	53664	5	15.63	520558	20.0
4H-Pyrido[1,2-a]p...	18.59	7.0	ng	163988	6	17.31	470043	20.0