

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050615\
 Data File : BF078953.D
 Acq On : 6 May 2015 11:48
 Operator : TP/IZ
 Sample : G2114-16
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GRID-6(0-6)

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-BF043015.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	1.495	24	27	29	rVB	2845820	3588231	71.14%	12.614%
2	1.633	37	39	49	rVB	162409	329502	6.53%	1.158%
3	1.770	49	51	53	rVV	150141	237923	4.72%	0.836%
4	1.815	53	55	60	rVV	133041	217539	4.31%	0.765%
5	1.895	60	62	103	rVB	2709739	5044044	100.00%	17.732%
6	5.153	345	347	353	rVB	62821	92311	1.83%	0.325%
7	5.644	387	390	392	rBV	690474	926265	18.36%	3.256%
8	6.890	497	499	502	rBV	1062522	995759	19.74%	3.500%
9	7.050	511	513	516	rBV	956219	995884	19.74%	3.501%
10	7.347	536	539	541	rBV	439640	394415	7.82%	1.387%
11	7.530	553	555	558	rVB	802147	732463	14.52%	2.575%
12	8.033	597	599	602	rBV	699992	599528	11.89%	2.108%
13	8.925	674	677	679	rBV	579367	563414	11.17%	1.981%
14	10.273	792	795	797	rBV	835906	1158712	22.97%	4.073%
15	10.776	837	839	841	rBV	45594	56626	1.12%	0.199%
16	11.096	865	867	869	rBV2	590154	620955	12.31%	2.183%
17	11.999	943	946	949	rVB	146085	130565	2.59%	0.459%
18	12.079	950	953	955	rBV	801401	805541	15.97%	2.832%
19	12.948	1026	1029	1030	rBV	636304	677172	13.43%	2.380%
20	12.971	1030	1031	1033	rVV	272857	259443	5.14%	0.912%
21	13.039	1033	1037	1039	rVV	80421	80157	1.59%	0.282%
22	13.611	1085	1087	1089	rVB	55163	54244	1.08%	0.191%
23	13.657	1089	1091	1093	rBV2	35904	59448	1.18%	0.209%
24	13.702	1093	1095	1097	rBV2	47063	72186	1.43%	0.254%
25	13.954	1115	1117	1122	rVB	27469	54232	1.08%	0.191%
26	14.457	1158	1161	1163	rBV	499663	565374	11.21%	1.987%
27	14.731	1182	1185	1188	rVV	515192	626658	12.42%	2.203%
28	14.800	1189	1191	1197	rVV	312406	478305	9.48%	1.681%
29	14.937	1201	1203	1206	rVV	1244514	1449489	28.74%	5.095%
30	15.017	1206	1210	1212	rVB2	31002	56021	1.11%	0.197%
31	15.154	1215	1222	1224	rBV2	55942	134738	2.67%	0.474%
32	15.280	1231	1233	1235	rVV	74059	75932	1.51%	0.267%
33	15.782	1274	1277	1281	rVB	52776	79013	1.57%	0.278%
34	15.920	1286	1289	1292	rBV3	47010	108113	2.14%	0.380%

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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

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35	15.965	1292	1293	1296	rVV2	48337	97689	1.94%	0.343%
36	16.045	1299	1300	1304	rVV	35735	55033	1.09%	0.193%
37	16.125	1304	1307	1313	rVV4	135227	259700	5.15%	0.913%
38	16.251	1313	1318	1320	rVV2	850849	1389272	27.54%	4.884%
39	16.285	1320	1321	1323	rVV	277225	243552	4.83%	0.856%
40	16.377	1326	1329	1331	rBV2	47414	80202	1.59%	0.282%
41	16.434	1331	1334	1338	rVV4	31438	76720	1.52%	0.270%
42	16.548	1342	1344	1346	rVB	45257	54944	1.09%	0.193%
43	16.754	1360	1362	1365	rVV	56758	95834	1.90%	0.337%
44	16.960	1378	1380	1384	rVB5	61203	120271	2.38%	0.423%
45	17.360	1413	1415	1417	rBV	54643	76279	1.51%	0.268%
46	17.577	1431	1434	1441	rBV	297532	713975	14.15%	2.510%
47	17.703	1442	1445	1447	rVB	55000	80808	1.60%	0.284%
48	17.908	1460	1463	1466	rVB	201678	263365	5.22%	0.926%
49	17.966	1466	1468	1471	rBV	313032	397294	7.88%	1.397%
50	18.034	1471	1474	1476	rBV	606926	881872	17.48%	3.100%
51	18.171	1483	1486	1488	rBV3	22187	51504	1.02%	0.181%
52	18.628	1522	1526	1529	rBV2	31628	74563	1.48%	0.262%
53	18.983	1555	1557	1561	rVB5	28843	70237	1.39%	0.247%
54	19.371	1588	1591	1598	rVB2	40299	106079	2.10%	0.373%
55	19.531	1602	1605	1611	rVB2	133296	301644	5.98%	1.060%
56	19.634	1612	1614	1617	rVB2	32326	62472	1.24%	0.220%
57	19.726	1619	1622	1624	rBV	25709	57773	1.15%	0.203%
58	19.977	1640	1644	1654	rVB	129838	334371	6.63%	1.175%
59	20.194	1659	1663	1669	rVB2	54461	181070	3.59%	0.637%

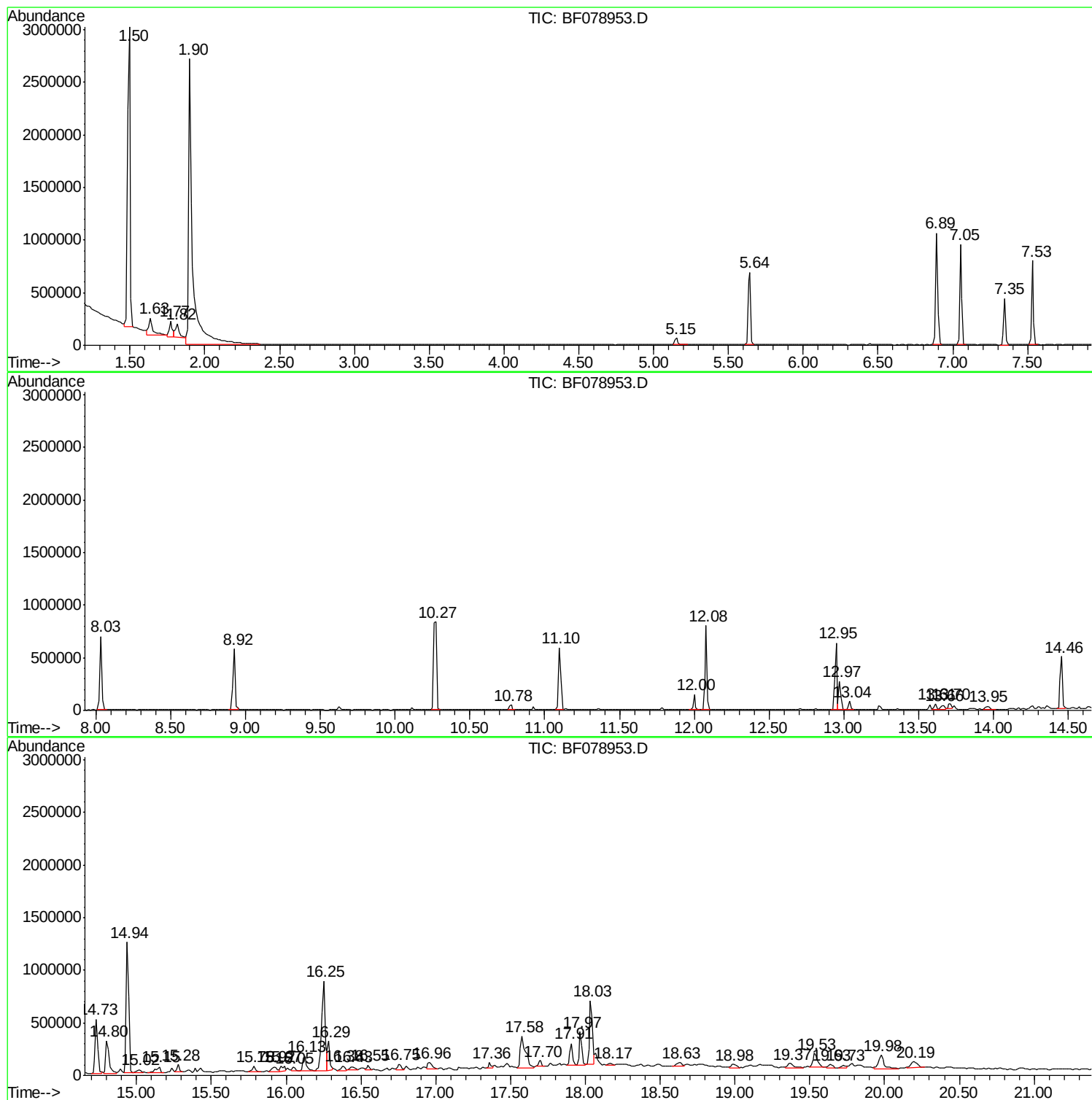
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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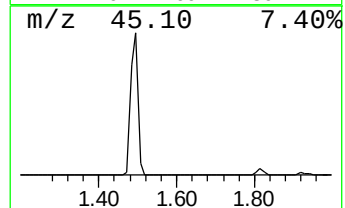
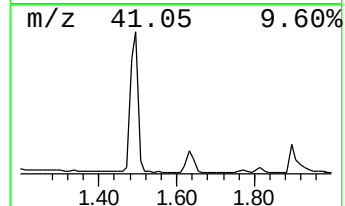
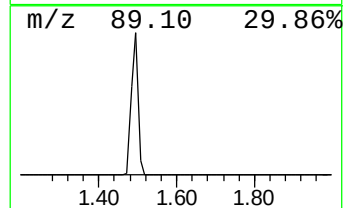
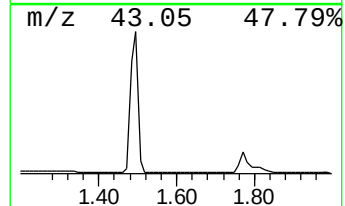
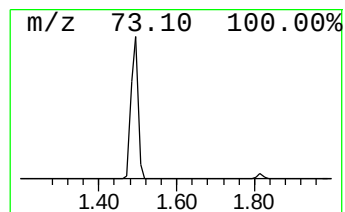
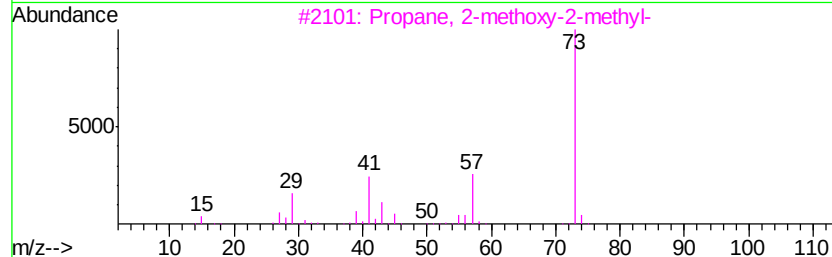
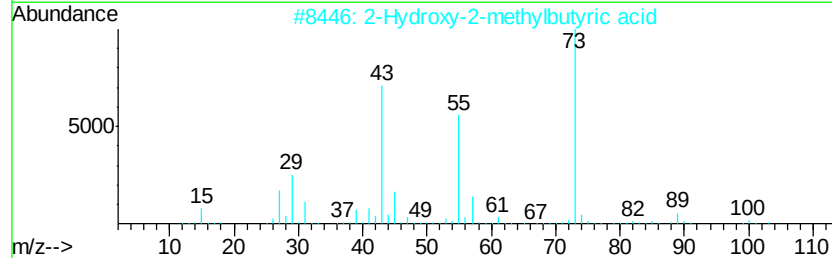
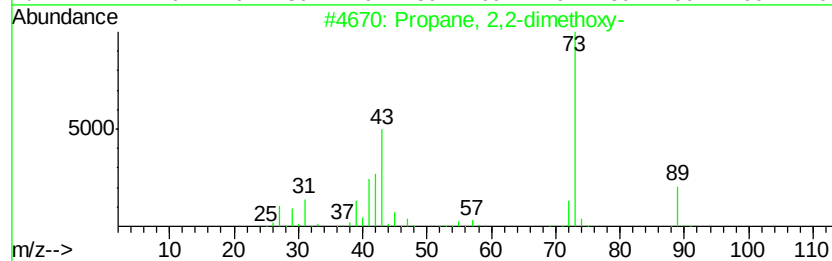
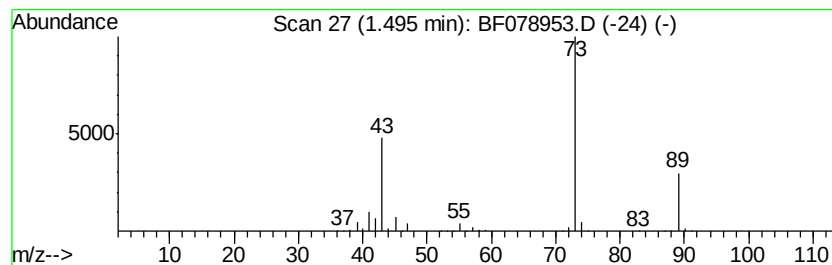
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown1.50 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.50	181.95 ng	3588230	1,4-Dichlorobenzene-d4	7.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
3		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5		N-Ethylformamide	73	C3H7NO	000627-45-2	5



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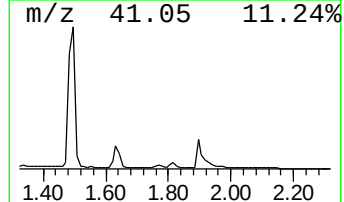
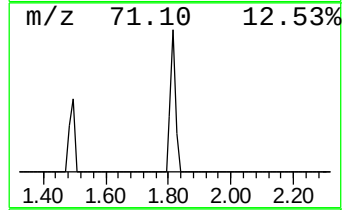
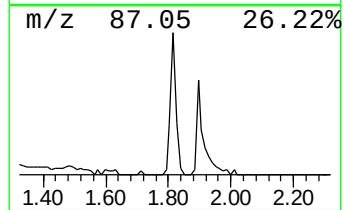
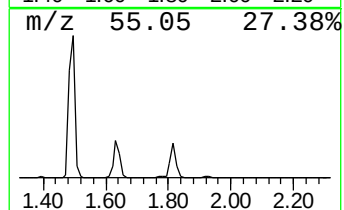
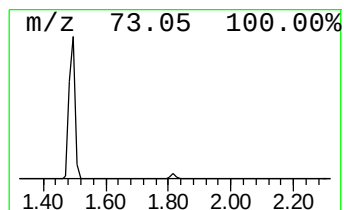
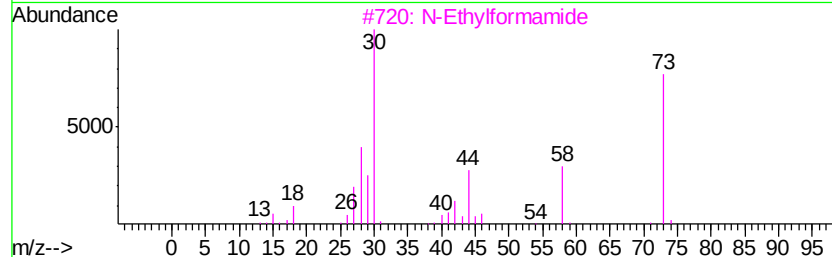
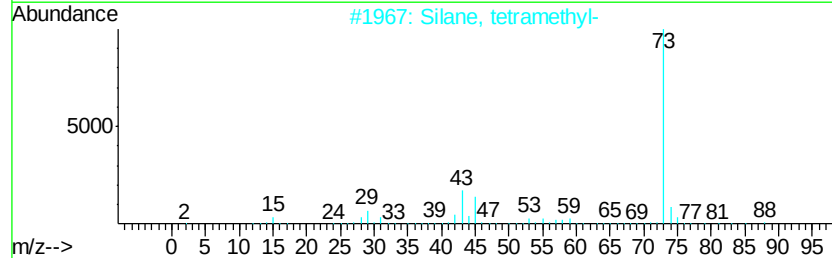
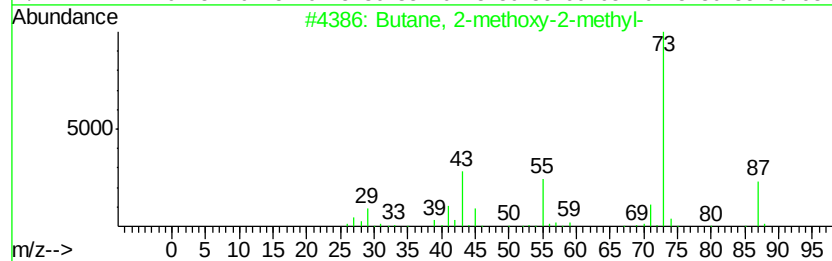
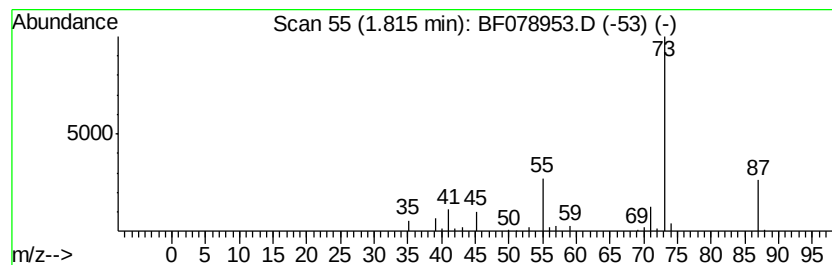
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF043015.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.82	11.03 ng	217539	1,4-Dichlorobenzene-d4	7.35

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	9
5		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	9



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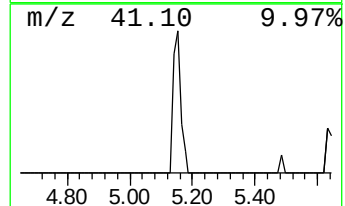
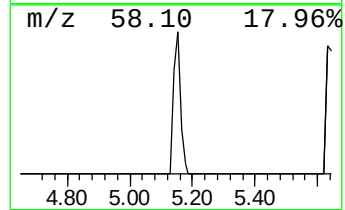
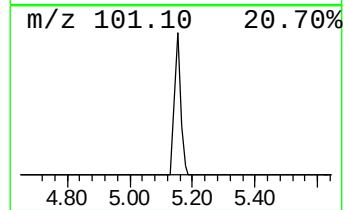
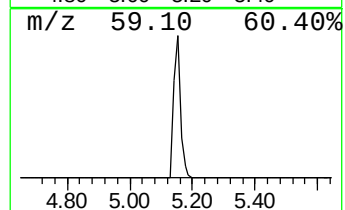
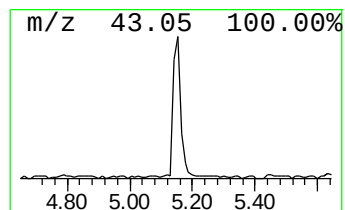
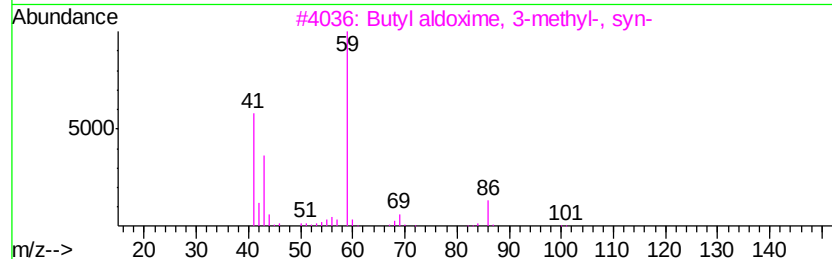
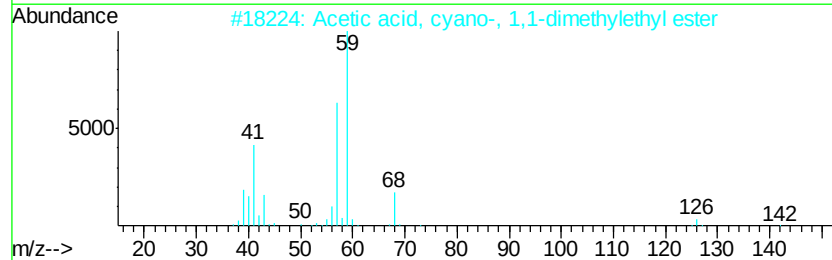
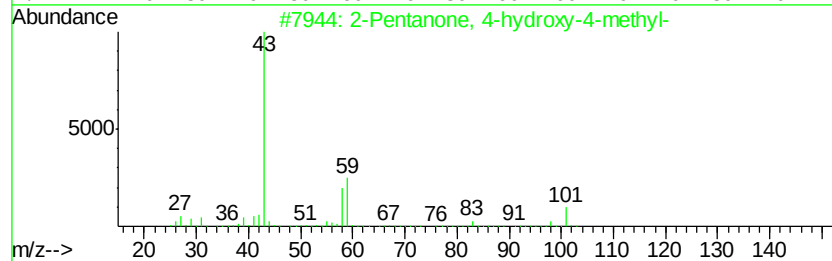
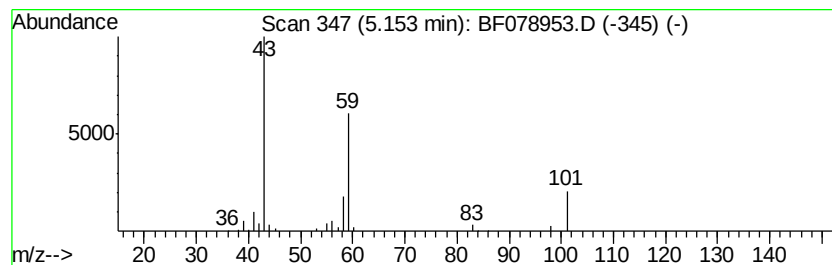
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	4.68 ng	92311	1,4-Dichlorobenzene-d4	7.35

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
4			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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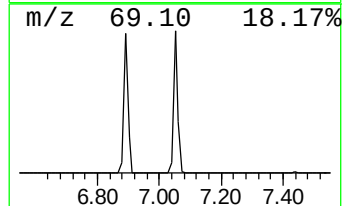
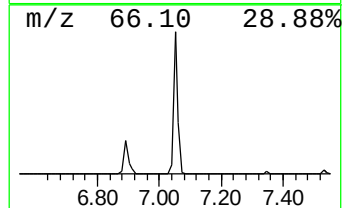
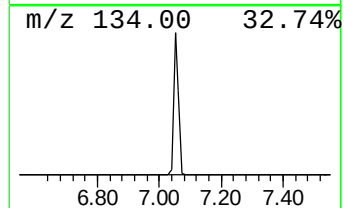
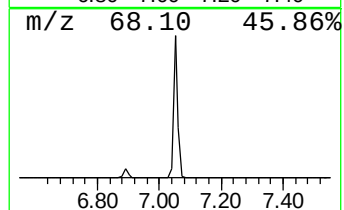
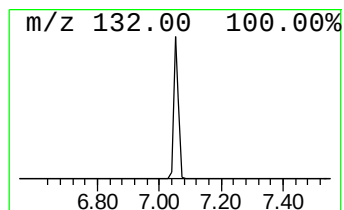
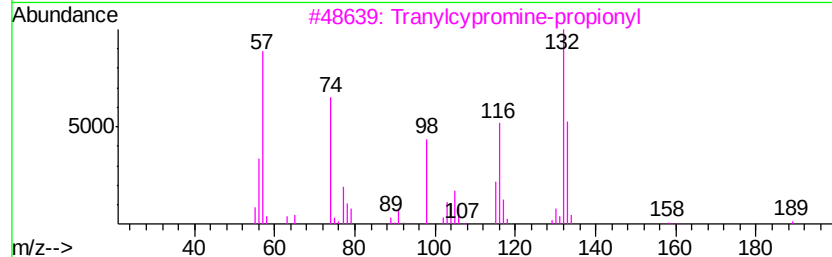
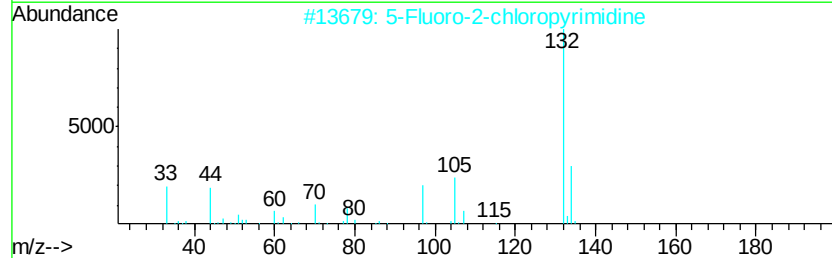
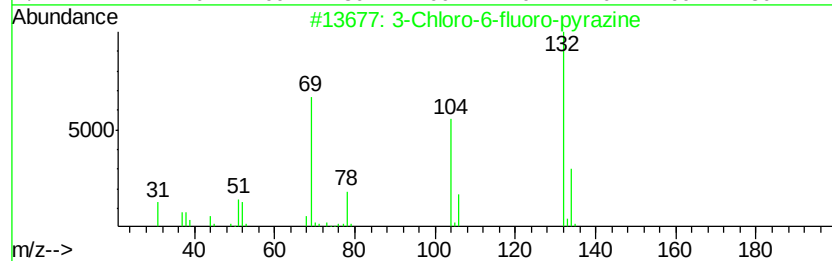
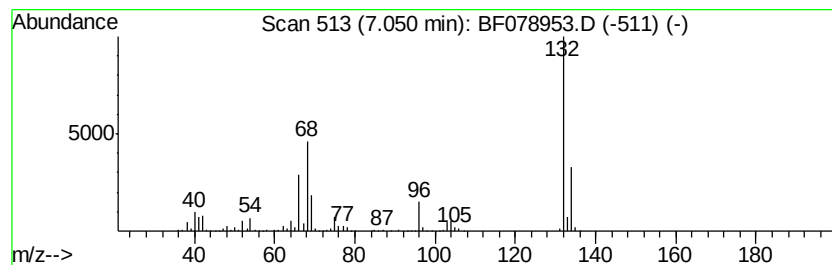
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown7.05 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.05	50.50 ng	995884	1,4-Dichlorobenzene-d4	7.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		5-Aminoindole	132	C8H8N2	005192-03-0	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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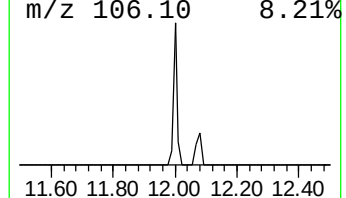
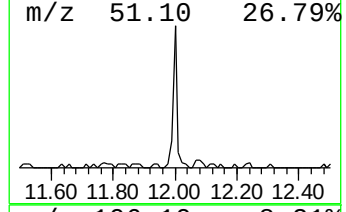
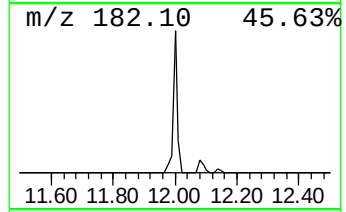
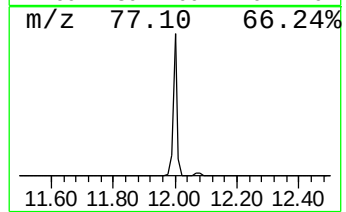
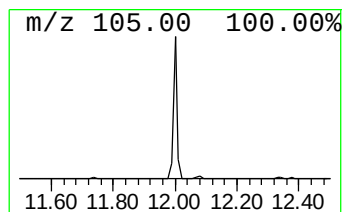
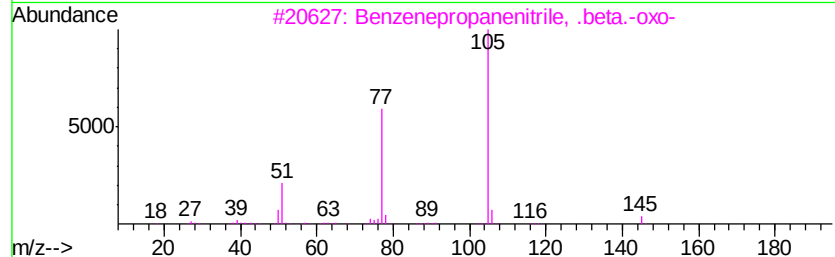
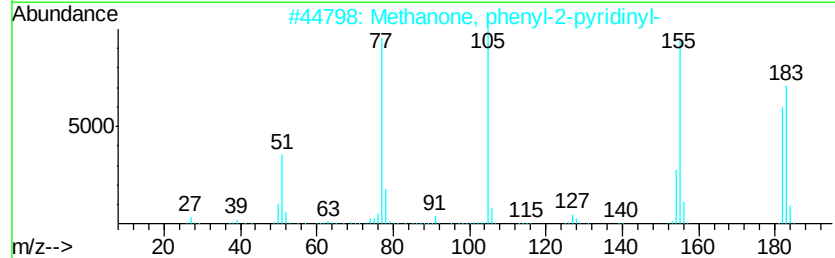
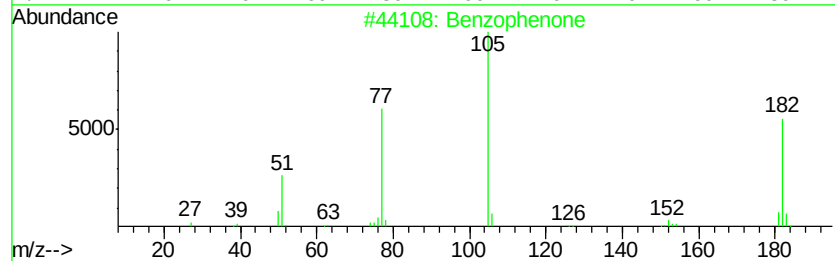
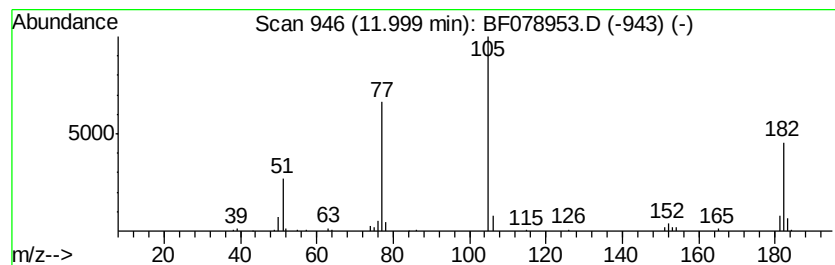
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzophenone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.00	4.21 ng	130565	Acenaphthene-d10	11.10
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzophenone	182 C13H10O	000119-61-9 96
2		Methanone, phenyl-2-pyridinyl-	183 C12H9NO	000091-02-1 72
3		Benzenepropanenitrile, .beta.-oxo-	145 C9H7NO	000614-16-4 47
4		Acetophenone, 2-chloro-	154 C8H7ClO	000532-27-4 47
5		Ethanone, 2-bromo-1-phenyl-	198 C8H7BrO	000070-11-1 47



Data Path : Z:\HPCHEM1\BNA F\DATA\BF050615\
Data File : BF078953.D
Acq On : 6 May 2015 11:48
Operator : TP/IZ
Sample : G2114-16
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GRID-6(0-6)

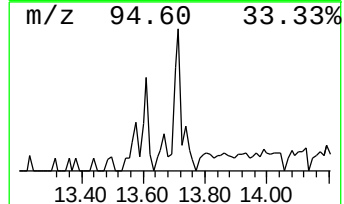
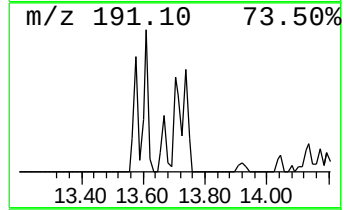
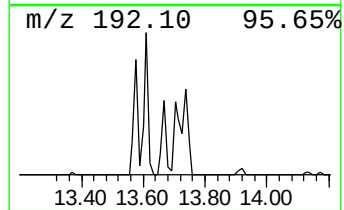
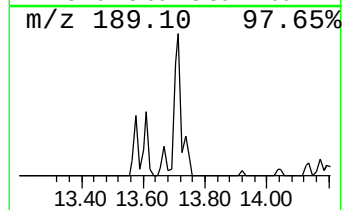
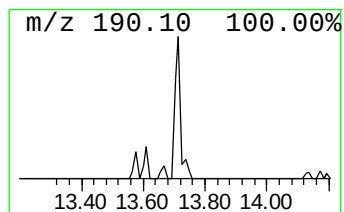
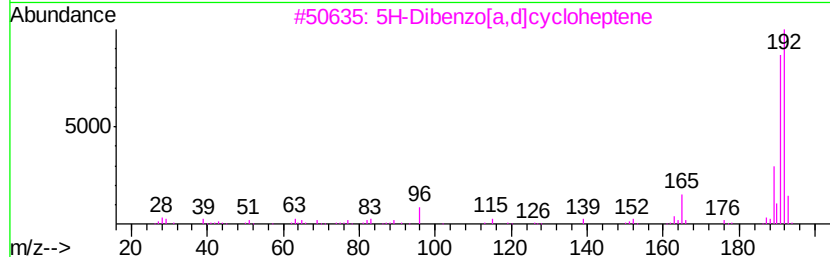
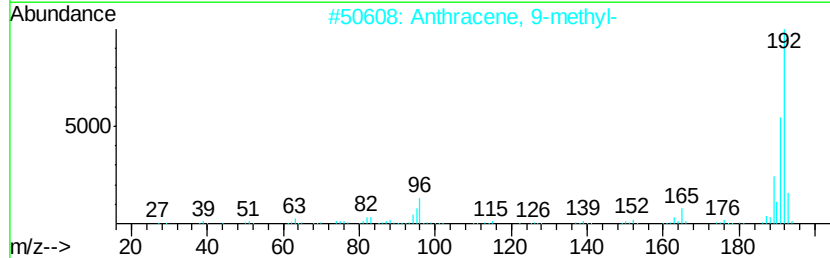
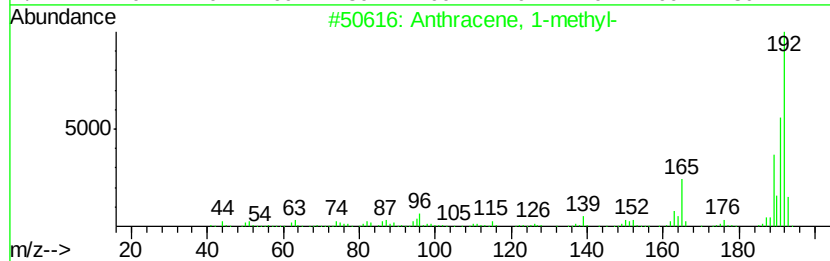
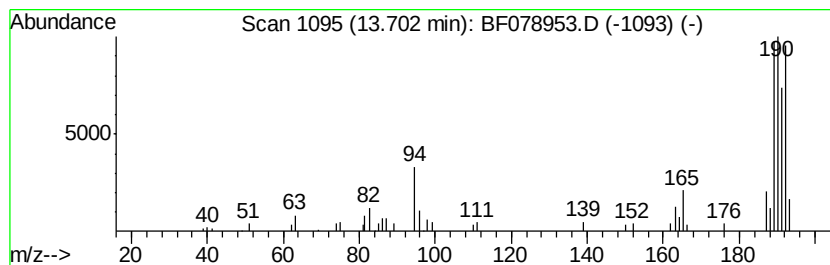
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Anthracene, 1-methyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	2.13 ng	72186	Phenanthrene-d10	12.95

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene, 1-methyl-	192	C15H12	000610-48-0	86
2			Anthracene, 9-methyl-	192	C15H12	000779-02-2	55
3			5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	50
4			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	50
5			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	46



Data Path : Z:\HPCHEM1\BNA F\DATA\BF050615\
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Sample : G2114-16
Misc :
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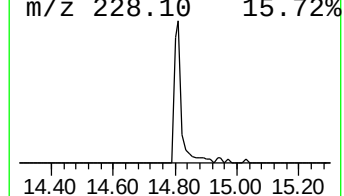
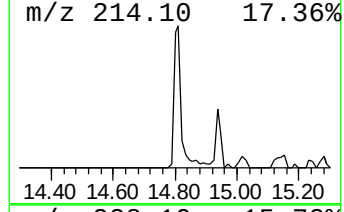
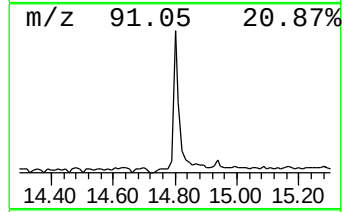
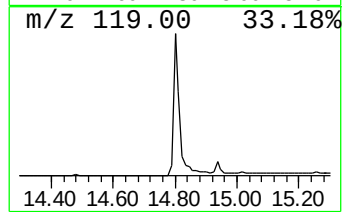
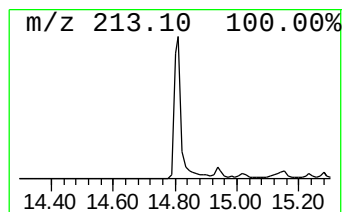
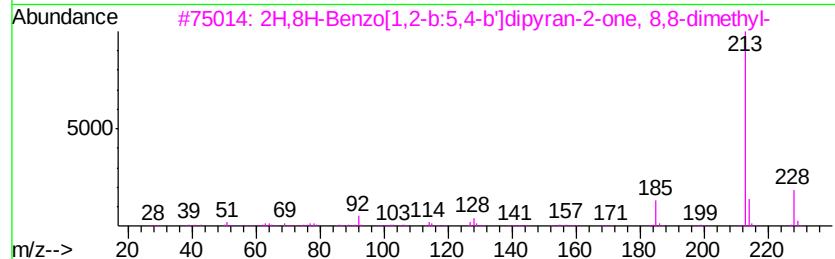
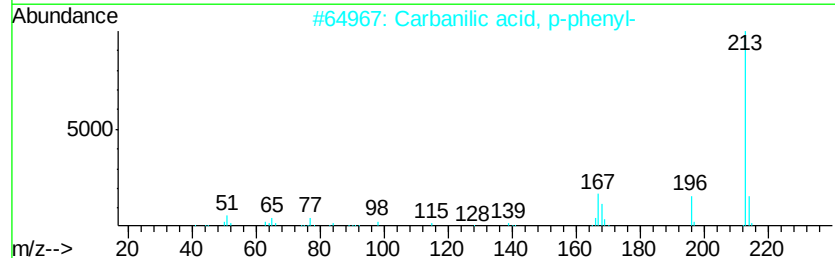
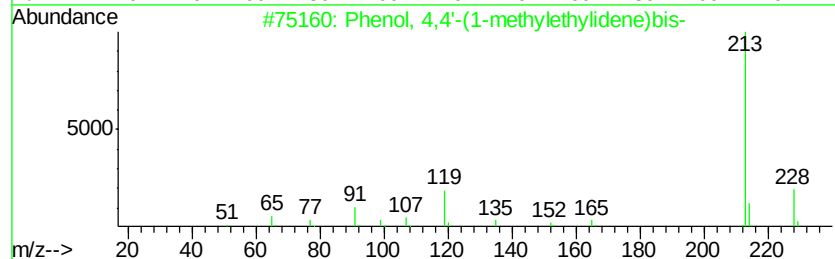
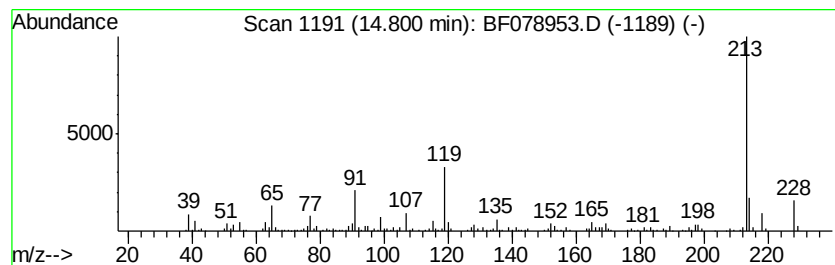
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Phenol, 4,4'-(1-methylethyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.80	6.89 ng	478305	Chrysene-d12	16.25	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	96
2	Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	53
3	2H,8H-Benzo[1,2-b:5,4-b']ldipyr...	228	C14H12O3	000553-19-5	52
4	2H,8H-Benzo[1,2-b:3,4-b']ldipyr...	228	C14H12O3	000523-59-1	52
5	Carbamic acid, [1,1'-biphenyl]-3...	213	C13H11NO2	055030-29-0	49



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050615\
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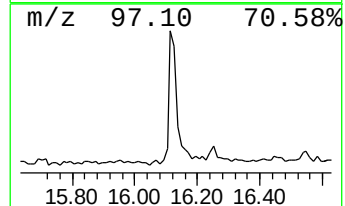
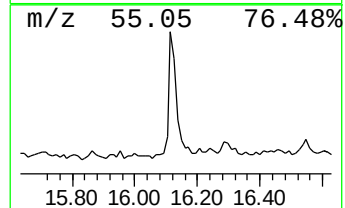
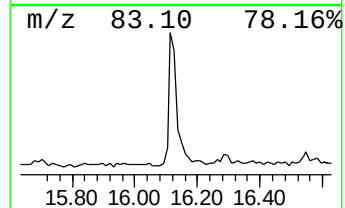
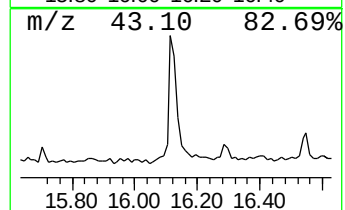
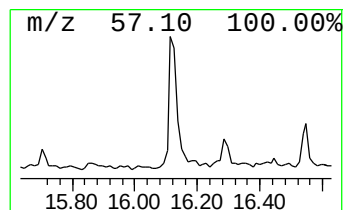
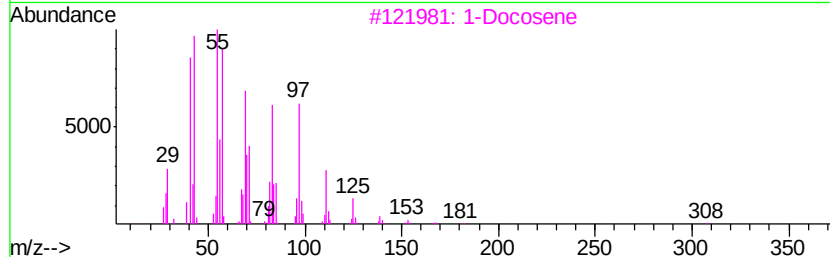
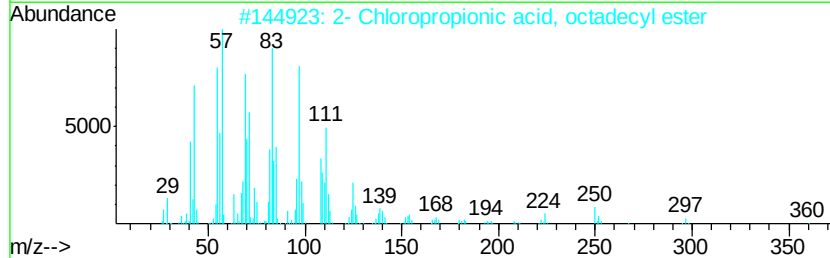
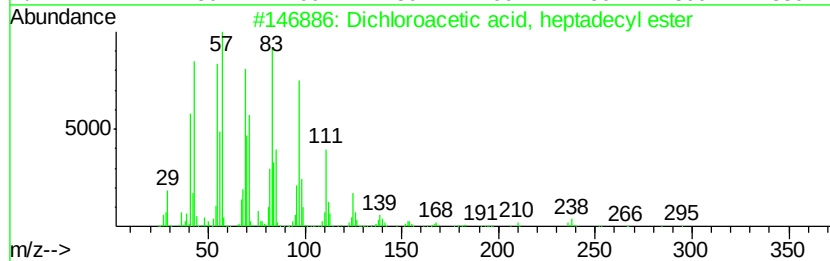
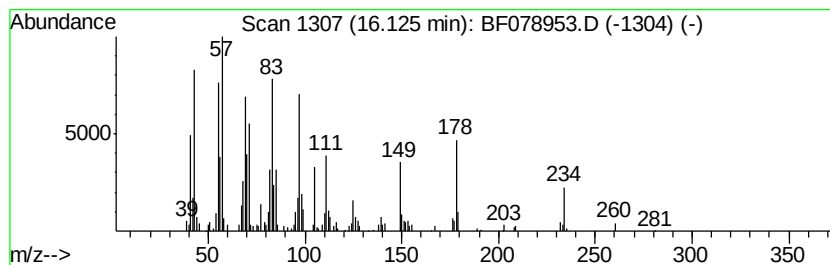
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Dichloroacetic acid, heptad... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	3.74 ng	259700	Chrysene-d12	16.25

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
2			2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	89
3			1-Docosene	308	C22H44	001599-67-3	76
4			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	76
5			Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	76



Data Path : Z:\HPCHEM1\BNA F\DATA\BF050615\
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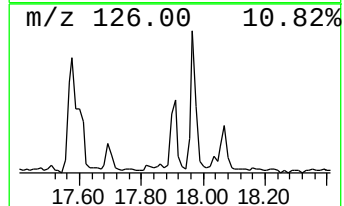
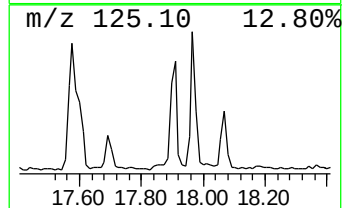
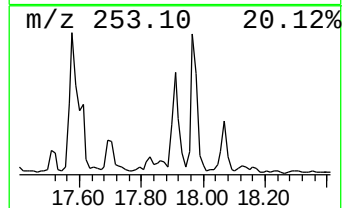
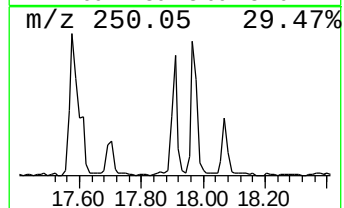
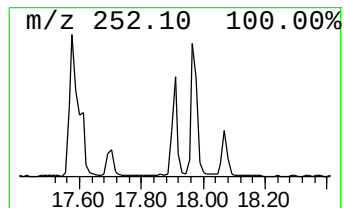
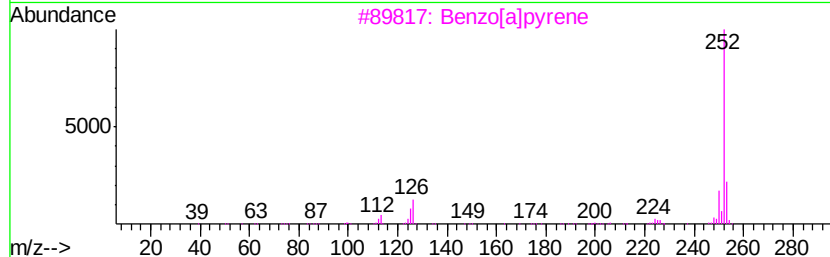
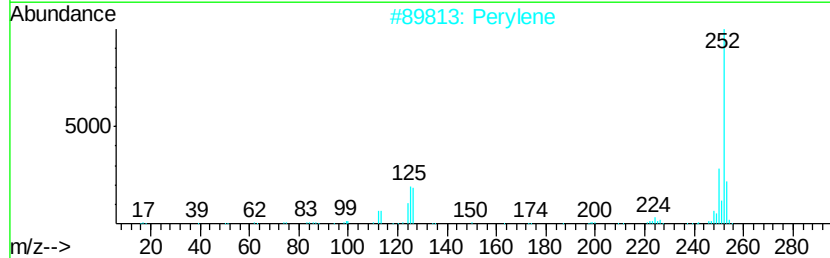
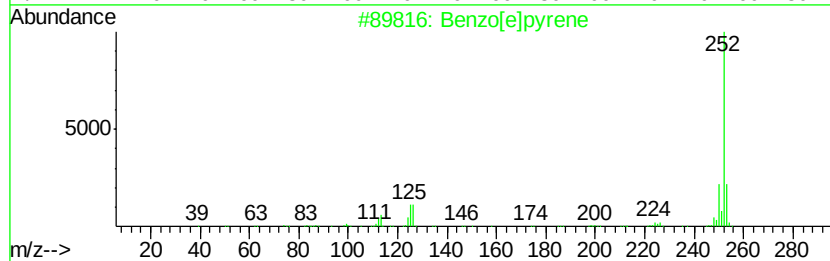
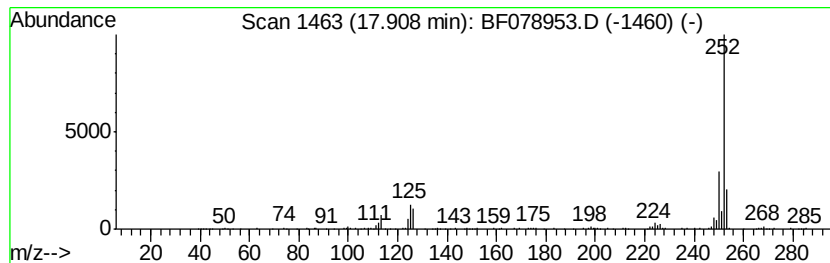
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Benzo[e]pyrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.91	5.97 ng	263365	Perylene-d12	18.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[e]pyrene	252	C20H12	000192-97-2	94
2		Perylene	252	C20H12	000198-55-0	93
3		Benzo[a]pyrene	252	C20H12	000050-32-8	93
4		Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	91
5		Benzo[k]fluoranthene	252	C20H12	000207-08-9	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050615\
Data File : BF078953.D
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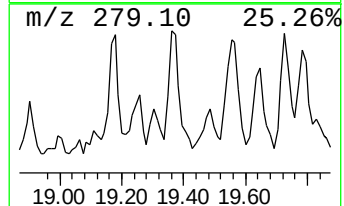
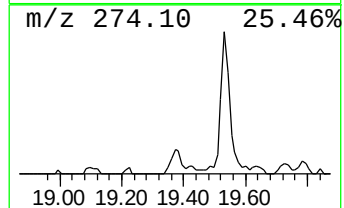
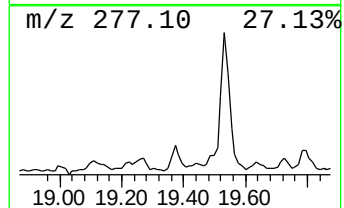
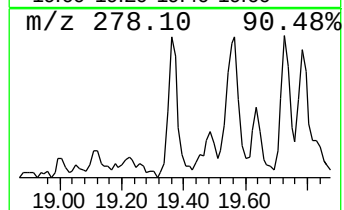
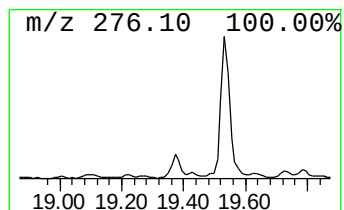
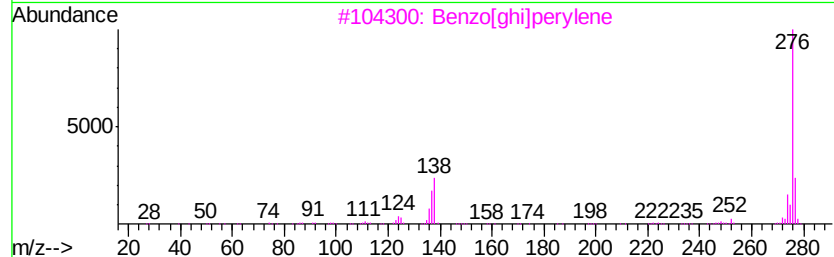
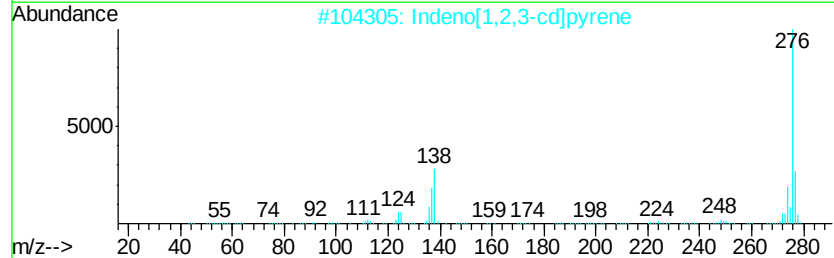
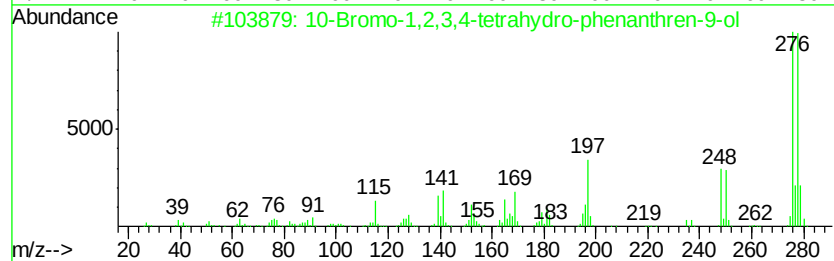
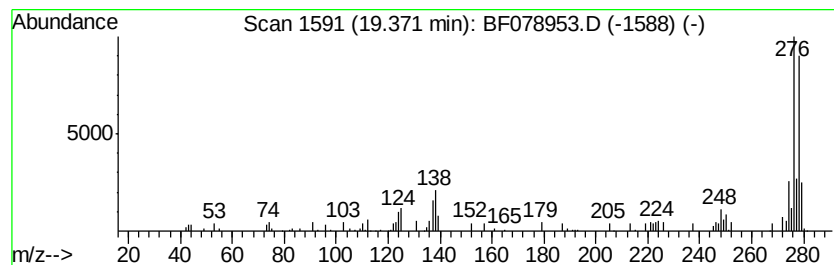
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 10-Bromo-1,2,3,4-tetrahydro... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.37	2.41 ng	106079	Perylene-d12	18.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	10-Bromo-1,2,3,4-tetrahydro-phen...	276	C14H13BrO	1000190-54-9	64
2		Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	50
3		Benzo[ghi]perylene	276	C22H12	000191-24-2	50
4		Indeno[1,2,3-cd]fluoranthene	276	C22H12	000193-43-1	50
5		Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050615\
Data File : BF078953.D
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ALS Vial : 3 Sample Multiplier: 1

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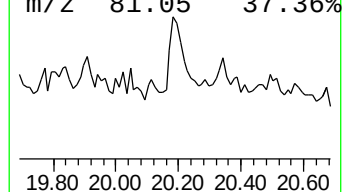
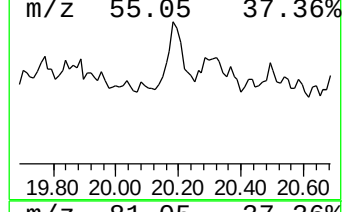
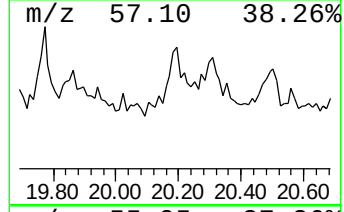
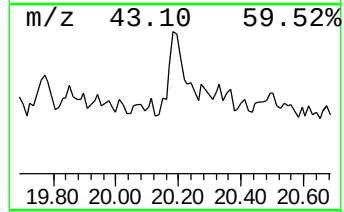
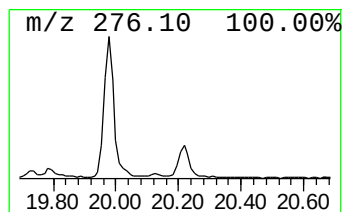
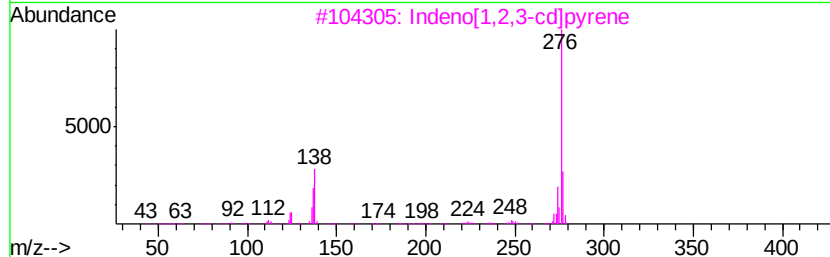
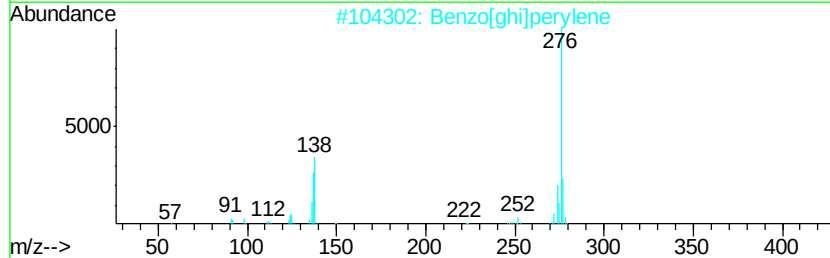
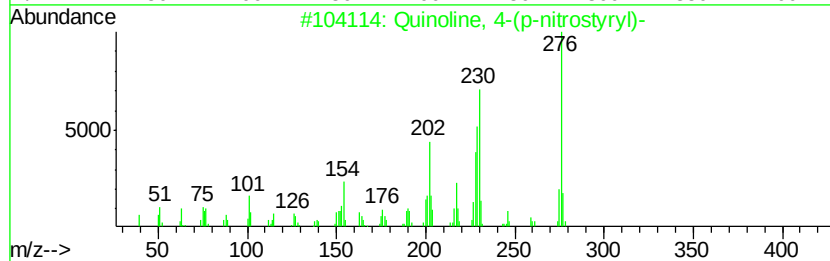
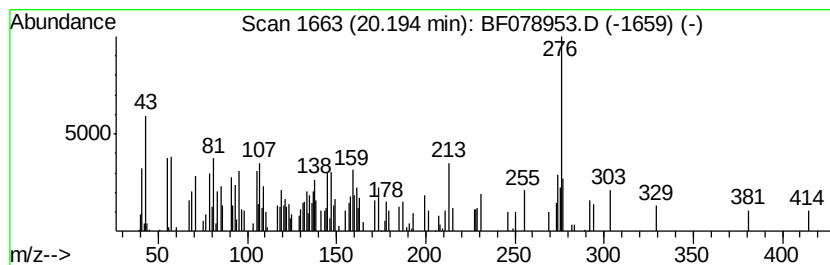
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown20.19 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.19	4.11 ng	181070	Perylene-d12	18.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Quinoline, 4-(p-nitrostyryl)-	276	C17H12N2O2	004594-97-2	47
2		Benzo[ghi]perylene	276	C22H12	000191-24-2	45
3		Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	45
4		Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	43
5		Diphenyl(4-tolyl)phosphine	276	C19H17P	001031-93-2	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050615\
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown1.50	1.50	181.9	ng	3588230	1	7.35	394415	20.0
Butane, 2-methoxy...	1.82	11.0	ng	217539	1	7.35	394415	20.0
2-Pentanone, 4-hy...	5.15	4.7	ng	92311	1	7.35	394415	20.0
unknown7.05	7.05	50.5	ng	995884	1	7.35	394415	20.0
Benzophenone	12.00	4.2	ng	130565	3	11.10	620955	20.0
Anthracene, 1-met...	13.70	2.1	ng	72186	4	12.95	677172	20.0
Phenol, 4,4'-(1-m...	14.80	6.9	ng	478305	5	16.25	1389270	20.0
Dichloroacetic ac...	16.13	3.7	ng	259700	5	16.25	1389270	20.0
Benzo[e]pyrene	17.91	6.0	ng	263365	6	18.03	881872	20.0
10-Bromo-1,2,3,4-...	19.37	2.4	ng	106079	6	18.03	881872	20.0
unknown20.19	20.19	4.1	ng	181070	6	18.03	881872	20.0