

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032715\
 Data File : BF078075.D
 Acq On : 28 Mar 2015 11:43
 Operator : TP/IZ
 Sample : G1667-12
 Misc :
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 REC-7-1-1(1.5-2.0)

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-BF031115.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	1.230	27	30	32	rBV	449771	534456	55.40%	5.351%
2	1.344	37	40	43	rVB	47986	86298	8.94%	0.864%
3	1.504	52	54	57	rVB	45153	50102	5.19%	0.502%
4	1.744	72	75	88	rVB	31004	69526	7.21%	0.696%
5	4.807	341	343	350	rVB	53793	73220	7.59%	0.733%
6	5.367	389	392	401	rBV	501765	612986	63.54%	6.137%
7	6.659	503	505	508	rBV	631114	618484	64.11%	6.192%
8	6.784	514	516	519	rBV	615406	660127	68.42%	6.609%
9	7.070	539	541	544	rBB	227865	217124	22.50%	2.174%
10	7.253	555	557	560	rBV	441935	514209	53.30%	5.148%
11	7.767	600	602	605	rBV	462932	397757	41.23%	3.982%
12	8.647	677	679	682	rBV	341519	302888	31.39%	3.032%
13	9.996	795	797	799	rBV	912957	806728	83.62%	8.077%
14	10.511	840	842	844	rBB	11827	14572	1.51%	0.146%
15	10.819	867	869	871	rVB	312930	346678	35.93%	3.471%
16	11.791	952	954	957	rBV	453954	462709	47.96%	4.632%
17	11.996	970	972	975	rBB	10115	11419	1.18%	0.114%
18	12.648	1027	1029	1031	rBV	397957	405358	42.02%	4.058%
19	12.682	1031	1032	1034	rVV	65315	47809	4.96%	0.479%
20	12.739	1035	1037	1040	rVB	13523	14553	1.51%	0.146%
21	13.276	1082	1084	1086	rBV	10198	10484	1.09%	0.105%
22	13.311	1086	1087	1090	rVB	14223	11614	1.20%	0.116%
23	13.402	1094	1095	1097	rBV	11183	16819	1.74%	0.168%
24	14.145	1158	1160	1163	rBV	171343	185682	19.25%	1.859%
25	14.419	1182	1184	1187	rBV	150143	198239	20.55%	1.985%
26	14.637	1201	1203	1206	rVV	746278	964787	100.00%	9.659%
27	14.717	1206	1210	1212	rVB	7701	14680	1.52%	0.147%
28	14.842	1217	1221	1223	rVB	15818	28184	2.92%	0.282%
29	14.968	1230	1232	1234	rBV	16987	19006	1.97%	0.190%
30	15.471	1272	1276	1279	rBV2	11493	14979	1.55%	0.150%
31	15.608	1286	1288	1290	rBV	13295	13835	1.43%	0.139%
32	15.665	1290	1293	1294	rBV2	11755	24146	2.50%	0.242%
33	15.734	1298	1299	1302	rVB	9453	9932	1.03%	0.099%
34	15.825	1304	1307	1311	rBV	30268	59779	6.20%	0.598%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.917	1312	1315	1317	rBV2	422517	612667	63.50%	6.134%
36	16.042	1324	1326	1328	rBV	9101	12154	1.26%	0.122%
37	16.408	1356	1358	1360	rBV	17186	25462	2.64%	0.255%
38	16.454	1360	1362	1365	rVB	9341	11685	1.21%	0.117%
39	16.534	1365	1369	1370	rBV3	7250	16531	1.71%	0.165%
40	16.568	1370	1372	1375	rVB3	7259	14042	1.46%	0.141%
41	17.014	1407	1411	1413	rBV2	5896	11997	1.24%	0.120%
42	17.185	1423	1426	1431	rBV	127506	276856	28.70%	2.772%
43	17.300	1432	1436	1438	rVB2	19033	26342	2.73%	0.264%
44	17.414	1441	1446	1448	rBV3	6468	18178	1.88%	0.182%
45	17.494	1450	1453	1456	rBV	70341	106295	11.02%	1.064%
46	17.551	1456	1458	1461	rVB	126724	143397	14.86%	1.436%
47	17.608	1461	1463	1466	rBV	333610	477162	49.46%	4.777%
48	17.814	1479	1481	1486	rVB4	6583	17009	1.76%	0.170%
49	17.917	1486	1490	1492	rBV4	5253	13642	1.41%	0.137%
50	18.568	1544	1547	1550	rBV5	4028	10429	1.08%	0.104%
51	18.797	1563	1567	1571	rBV2	13897	32963	3.42%	0.330%
52	18.946	1577	1580	1585	rVB2	52666	114932	11.91%	1.151%
53	19.026	1585	1587	1591	rVB	6427	11602	1.20%	0.116%
54	19.117	1591	1595	1596	rBV	11992	23703	2.46%	0.237%
55	19.163	1596	1599	1606	rVB5	14344	38278	3.97%	0.383%
56	19.334	1610	1614	1619	rBV	50359	103290	10.71%	1.034%
57	19.540	1629	1632	1635	rVB	10663	20354	2.11%	0.204%
58	21.323	1783	1788	1790	rBV3	10313	30411	3.15%	0.304%

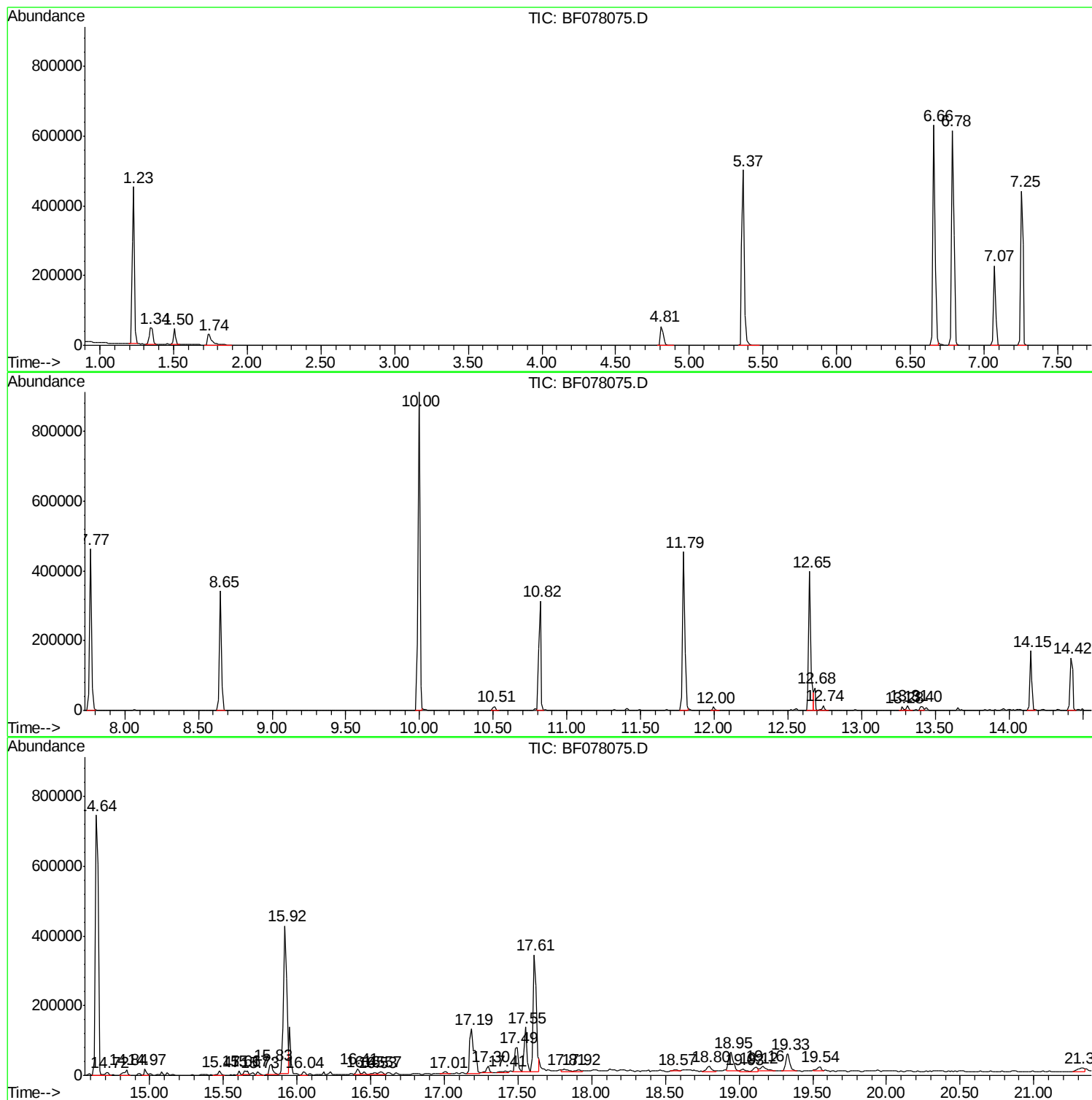
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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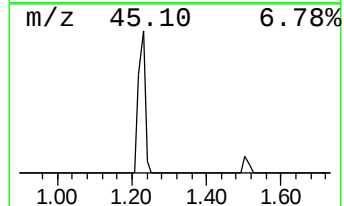
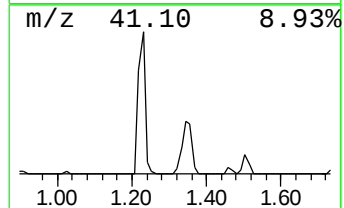
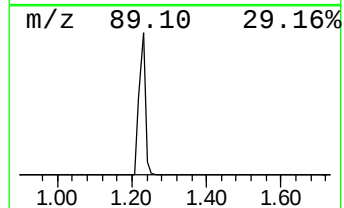
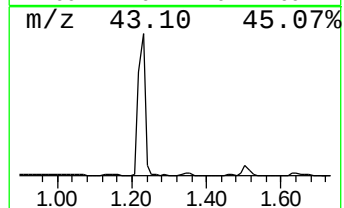
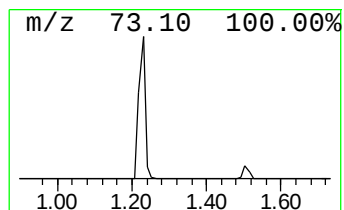
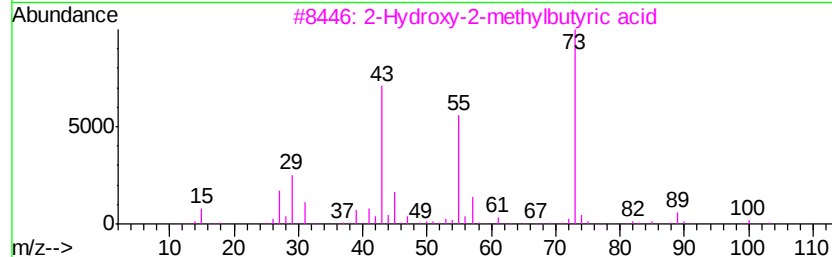
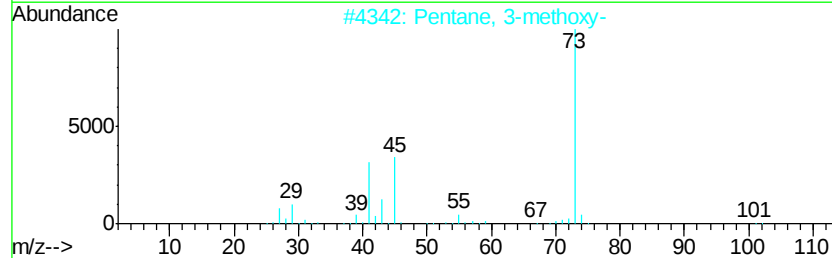
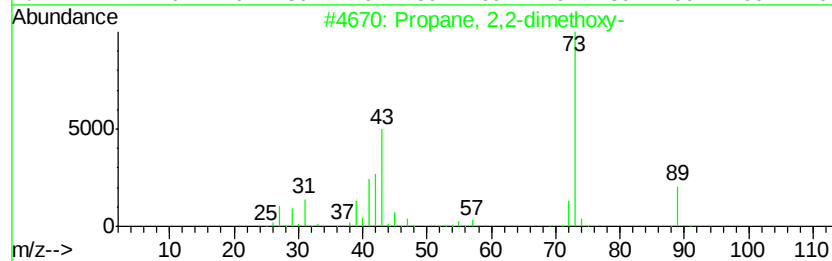
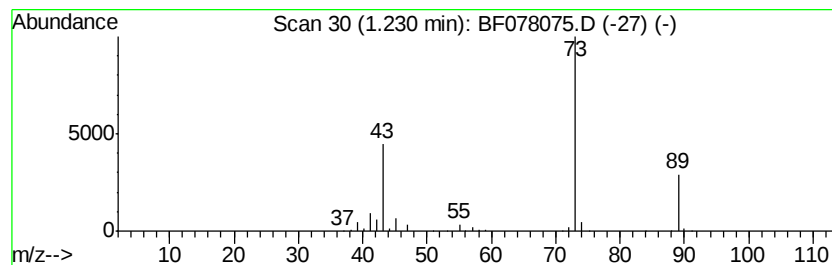
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.23	49.23 ng	534456	1,4-Dichlorobenzene-d4	7.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	50
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
3		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
4		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5		Methane, isothiocyanato-	73	C2H3NS	000556-61-6	7



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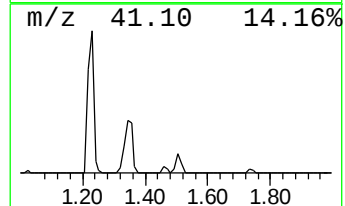
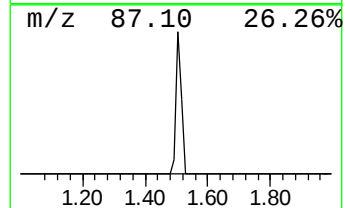
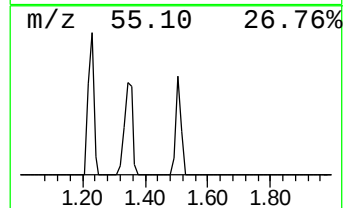
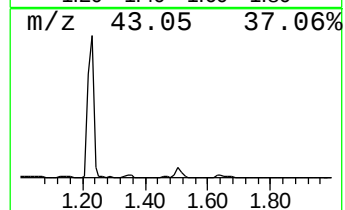
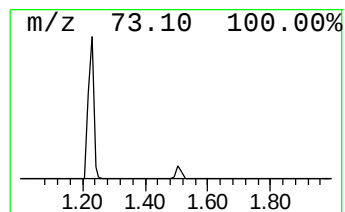
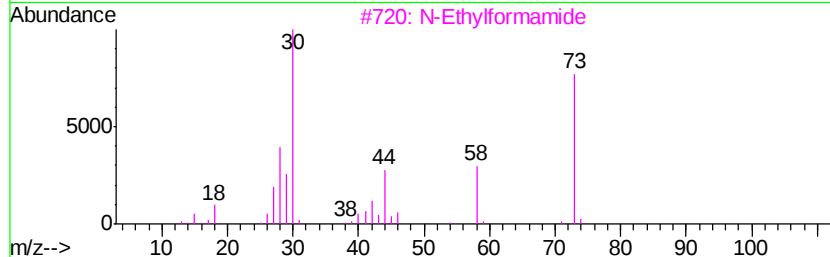
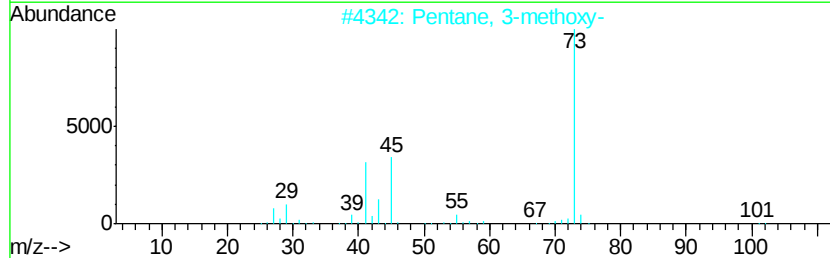
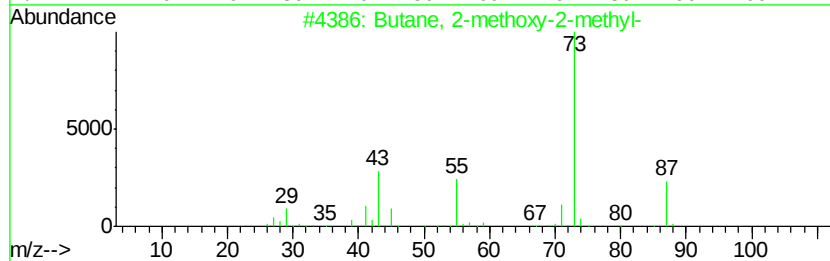
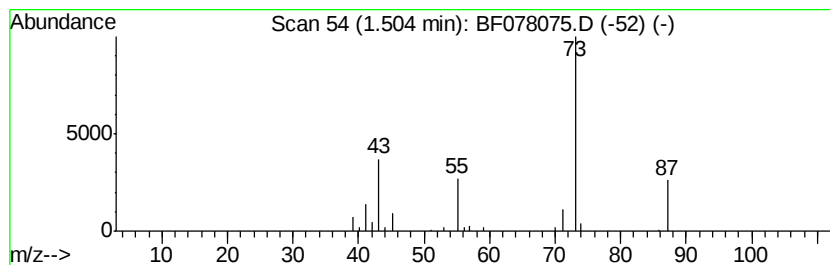
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.50	4.62 ng	50102	1,4-Dichlorobenzene-d4	7.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5		1,4-Butanediamine	88	C4H12N2	000110-60-1	9



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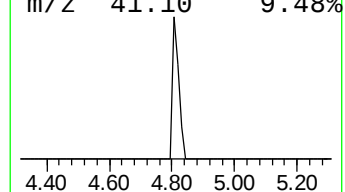
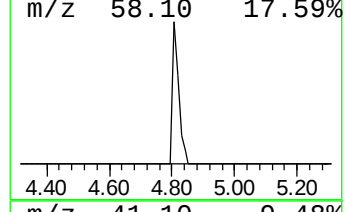
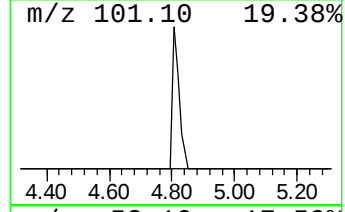
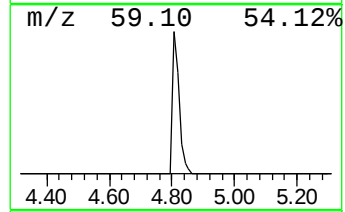
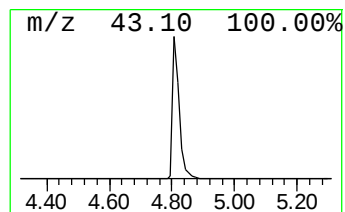
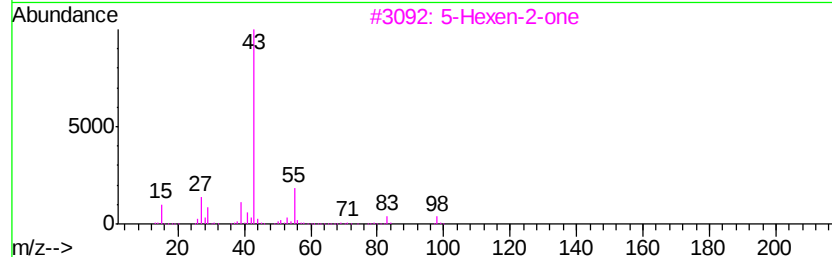
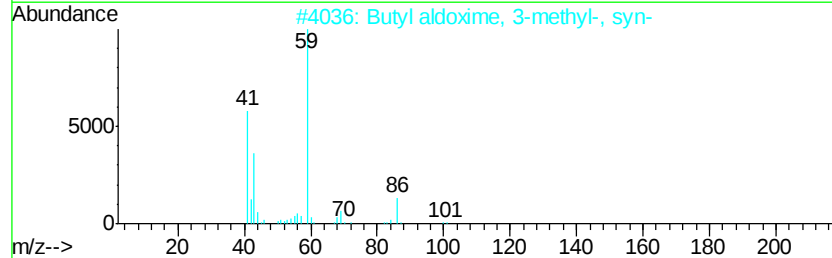
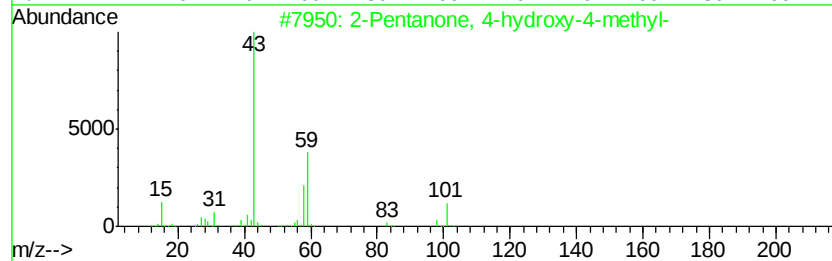
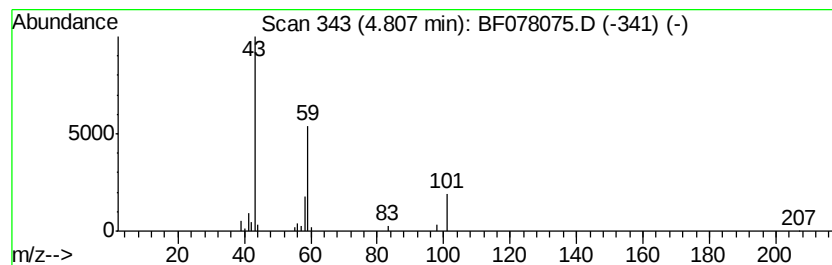
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.81	6.74 ng	73220	1,4-Dichlorobenzene-d4	7.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5		4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	9



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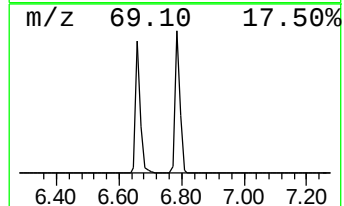
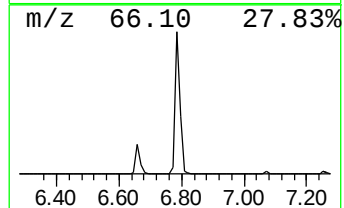
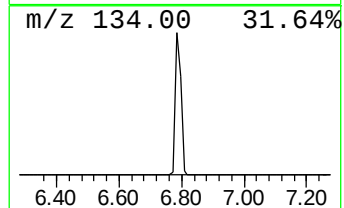
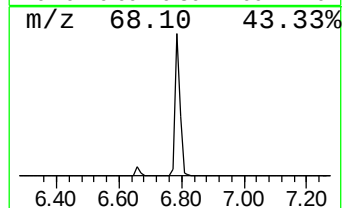
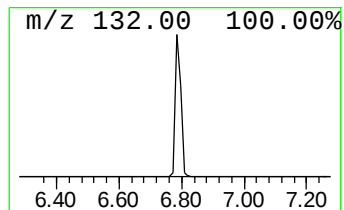
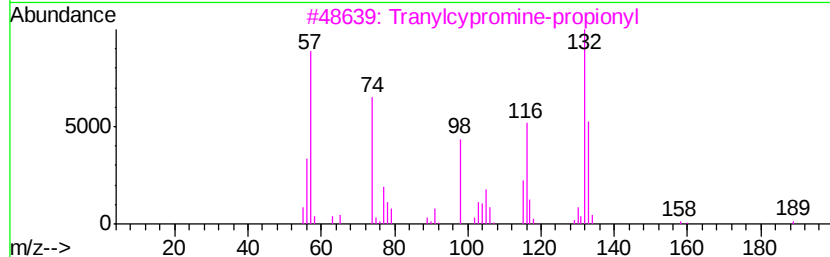
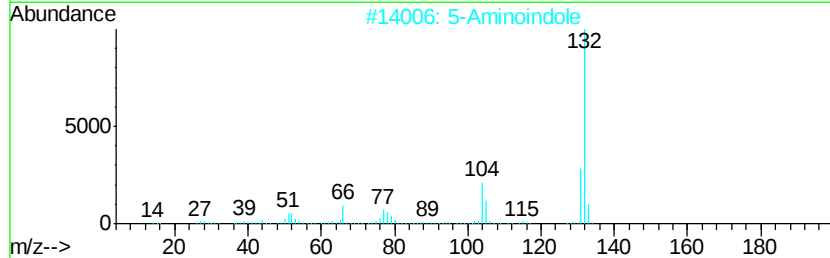
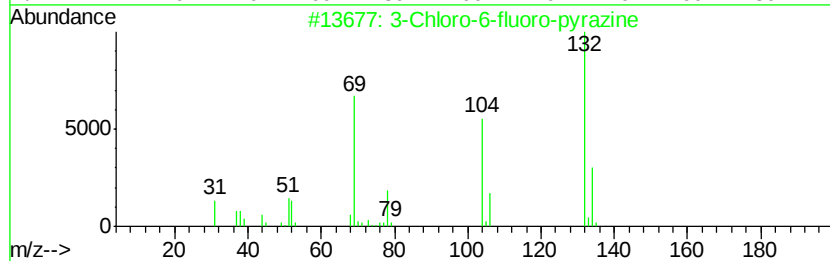
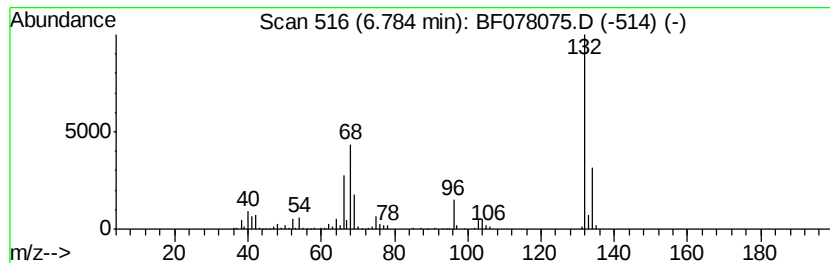
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown6.78 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.78	60.81 ng	660127	1,4-Dichlorobenzene-d4	7.07

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	12
3			Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
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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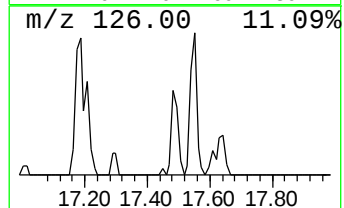
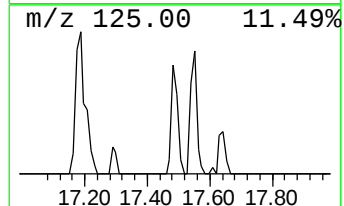
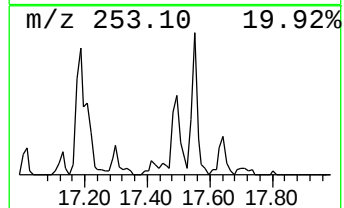
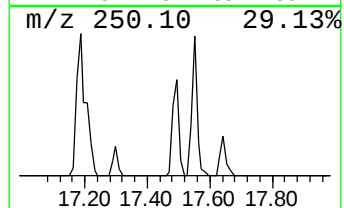
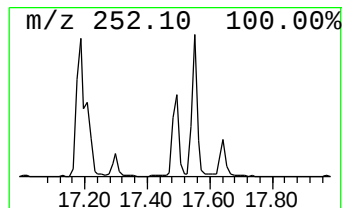
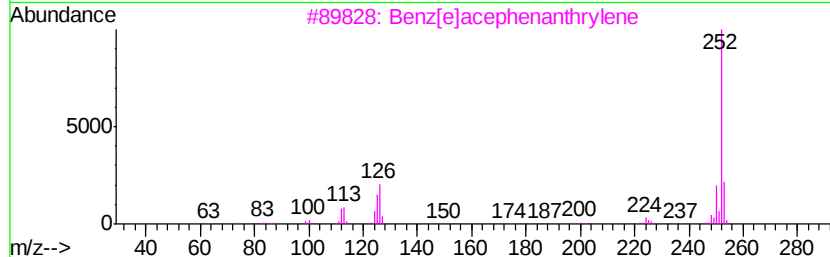
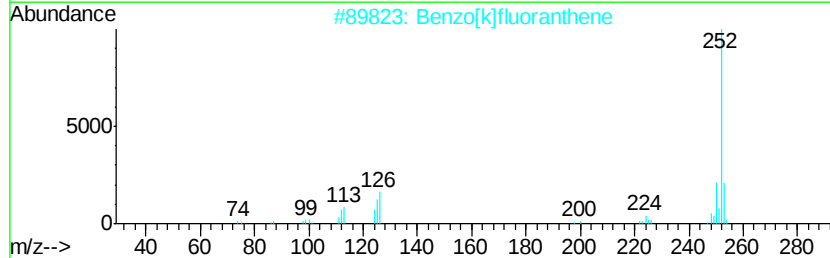
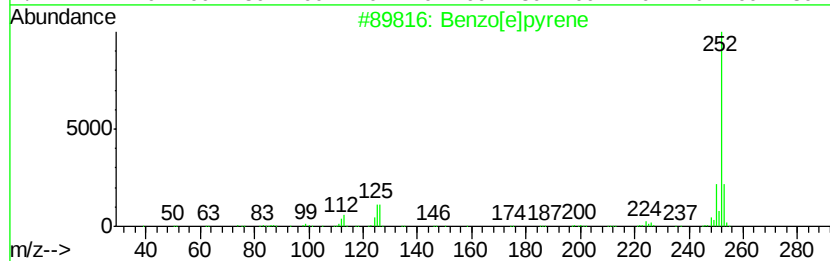
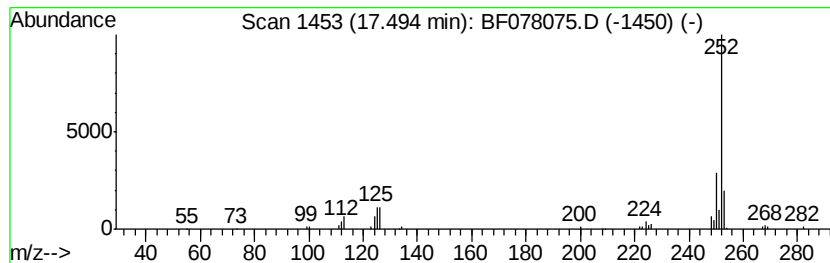
Instrument :
BNA_F
ClientSampleId :
REC-7-1-1(1.5-2.0)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzo[e]pyrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.49	4.46 ng	106295	Perylene-d12	17.61	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	93
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
3	Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	91
4	Benzo[a]pyrene	252	C20H12	000050-32-8	91
5	Perylene	252	C20H12	000198-55-0	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032715\
Data File : BF078075.D
Acq On : 28 Mar 2015 11:43
Operator : TP/IZ
Sample : G1667-12
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
REC-7-1-1(1.5-2.0)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.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
Propane, 2,2-dime...	1.23	49.2	ng	534456	1	7.07	217124	20.0
Butane, 2-methoxy...	1.50	4.6	ng	50102	1	7.07	217124	20.0
2-Pentanone, 4-hy...	4.81	6.7	ng	73220	1	7.07	217124	20.0
unknown6.78	6.78	60.8	ng	660127	1	7.07	217124	20.0
Benzo[e]pyrene	17.49	4.5	ng	106295	6	17.61	477162	20.0