

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040215\
 Data File : BF078227.D
 Acq On : 3 Apr 2015 6:00
 Operator : TP/IZ
 Sample : G1731-03
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-3

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	1.184	23	26	28	rBV	186070	241960	20.87%	2.327%
2	1.298	32	36	39	rBV	116184	172996	14.92%	1.664%
3	1.447	47	49	52	rVB	75099	90656	7.82%	0.872%
4	1.710	69	72	81	rVB	31252	51228	4.42%	0.493%
5	4.739	335	337	346	rBB	66367	93194	8.04%	0.896%
6	5.299	384	386	389	rBV	723569	771341	66.52%	7.419%
7	6.602	498	500	503	rBV	562838	785075	67.70%	7.551%
8	6.727	509	511	514	rBV	741161	839366	72.39%	8.073%
9	7.013	534	536	539	rBV	296832	303036	26.13%	2.915%
10	7.196	550	552	555	rBV	507933	668837	57.68%	6.433%
11	7.710	595	597	600	rBV	460150	498110	42.96%	4.791%
12	8.591	672	674	677	rBV	444968	424025	36.57%	4.078%
13	9.939	790	792	795	rBV	1080350	1013282	87.38%	9.746%
14	10.454	835	837	839	rBV	85414	73695	6.36%	0.709%
15	10.762	861	864	866	rVB	478376	490841	42.33%	4.721%
16	11.734	947	949	952	rBV	498543	548608	47.31%	5.277%
17	11.939	966	967	971	rBB	7752	12502	1.08%	0.120%
18	12.591	1022	1024	1026	rBV	532484	519617	44.81%	4.998%
19	14.088	1153	1155	1158	rBB	38740	39771	3.43%	0.383%
20	14.363	1177	1179	1182	rVB	33017	41165	3.55%	0.396%
21	14.591	1196	1199	1201	rBV	1017239	1159566	100.00%	11.153%
22	15.768	1299	1302	1308	rBV	74948	110457	9.53%	1.062%
23	15.871	1308	1311	1313	rBV	538057	619454	53.42%	5.958%
24	16.591	1372	1374	1380	rBV2	7953	15243	1.31%	0.147%
25	16.946	1402	1405	1407	rBV	57869	72691	6.27%	0.699%
26	17.163	1422	1424	1429	rBV	19637	42775	3.69%	0.411%
27	17.380	1441	1443	1447	rBV3	10888	19299	1.66%	0.186%
28	17.483	1450	1452	1456	rBV	10749	13596	1.17%	0.131%
29	17.551	1456	1458	1461	rBV	13676	19648	1.69%	0.189%
30	17.609	1461	1463	1466	rBV	439576	583021	50.28%	5.608%
31	18.226	1515	1517	1520	rBV3	6848	12508	1.08%	0.120%
32	18.660	1553	1555	1559	rVB3	8040	16390	1.41%	0.158%
33	18.934	1577	1579	1582	rBV2	8741	16059	1.38%	0.154%
34	19.312	1610	1612	1616	rVB	8109	16655	1.44%	0.160%

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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
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

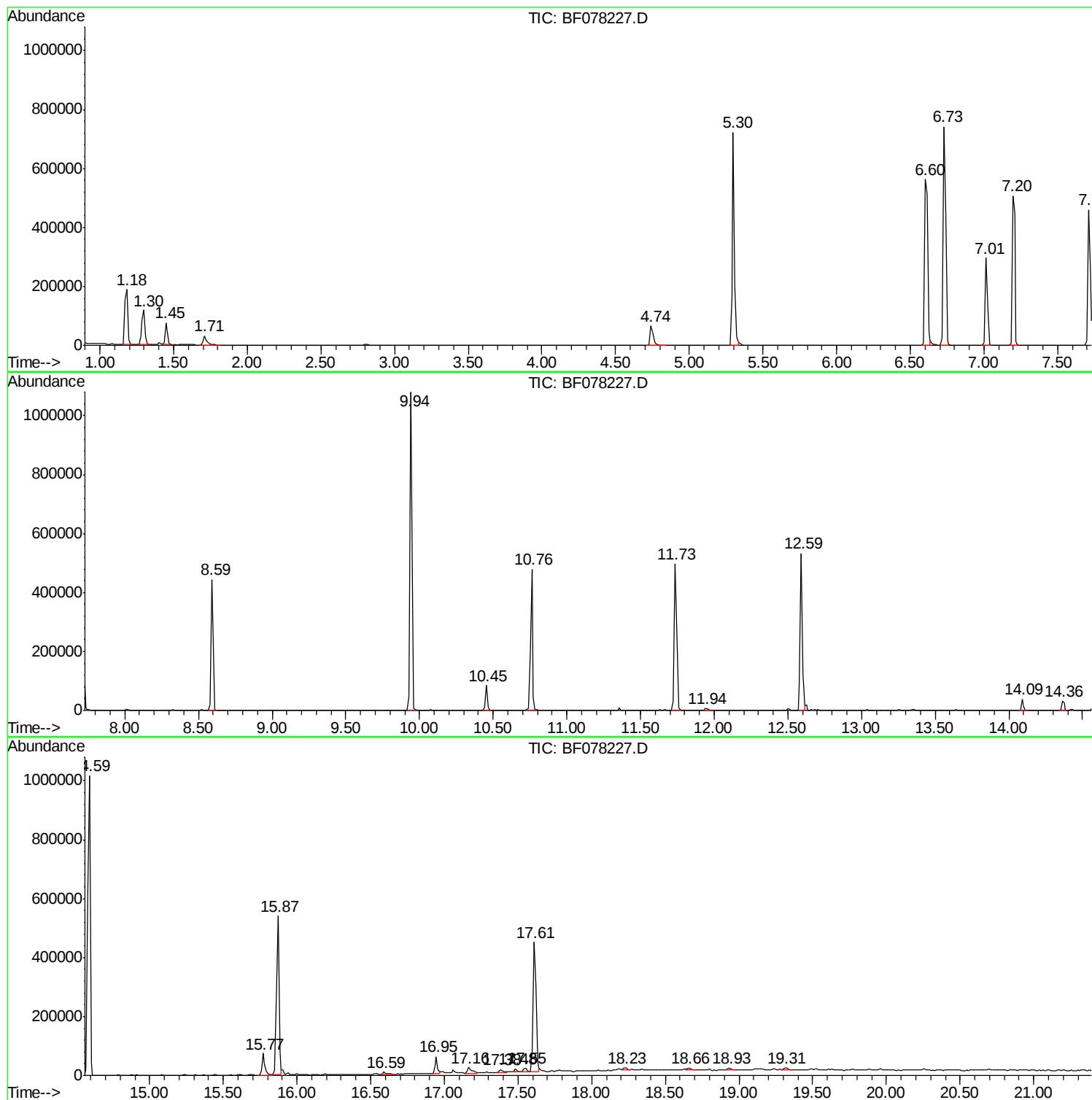
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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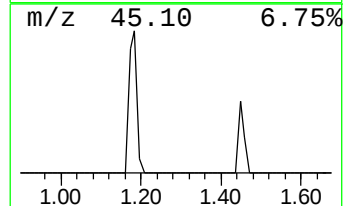
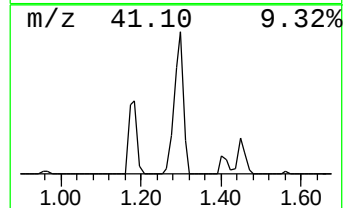
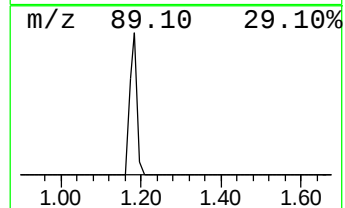
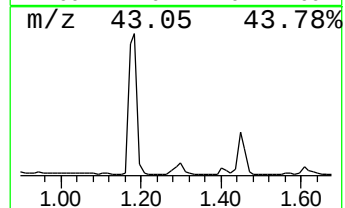
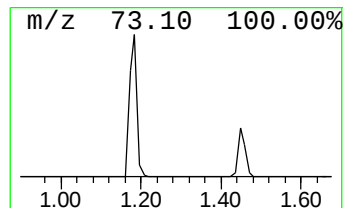
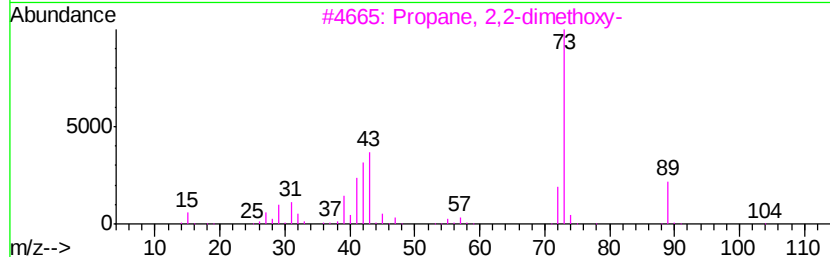
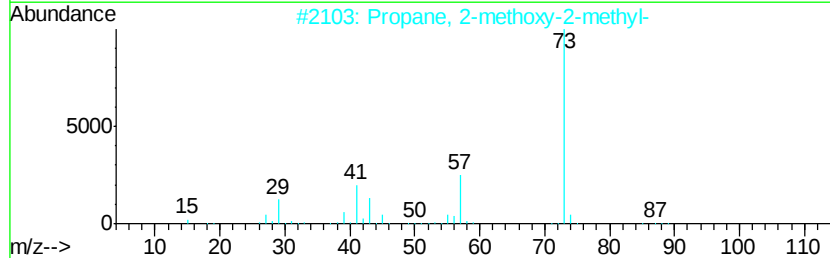
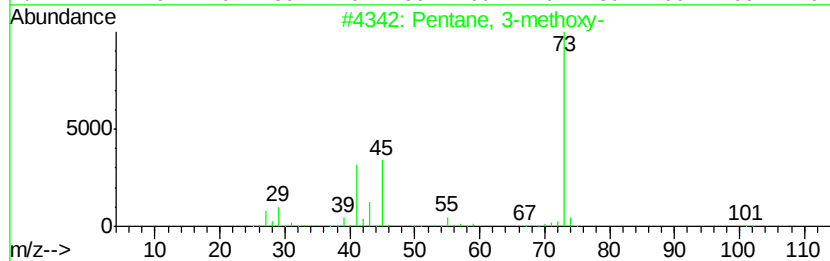
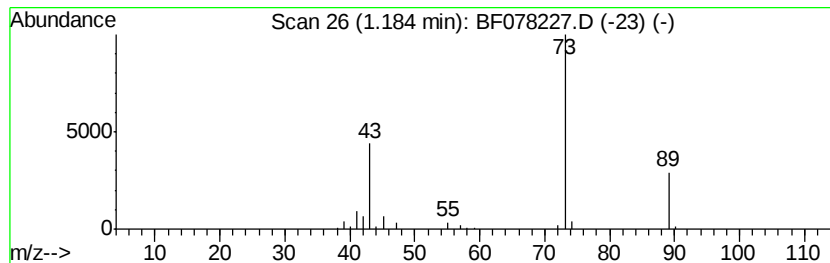
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown1.18 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.18	15.97 ng	241960	1,4-Dichlorobenzene-d4	7.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
2		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
3		Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	9
4		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
5		N-Ethylformamide	73	C3H7NO	000627-45-2	5



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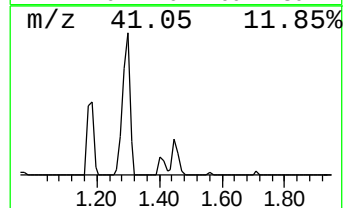
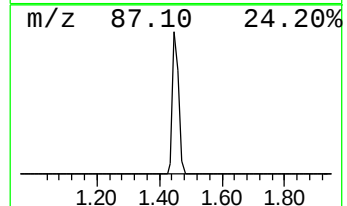
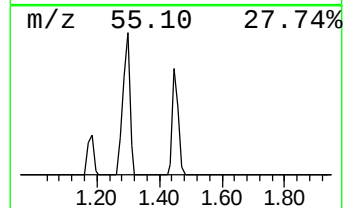
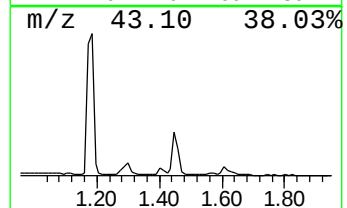
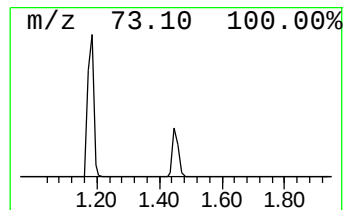
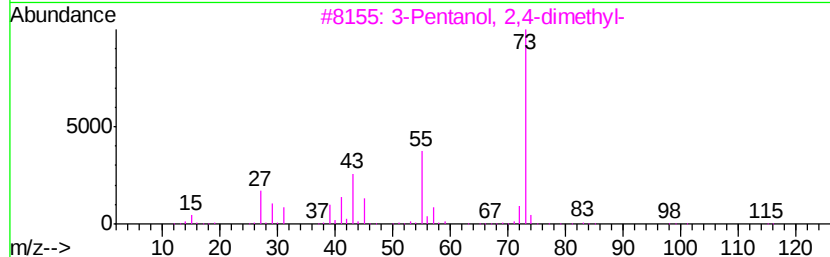
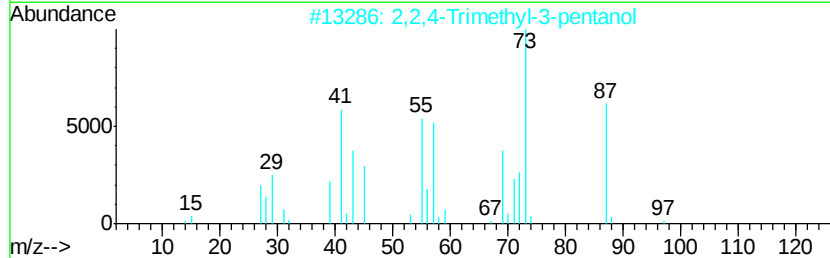
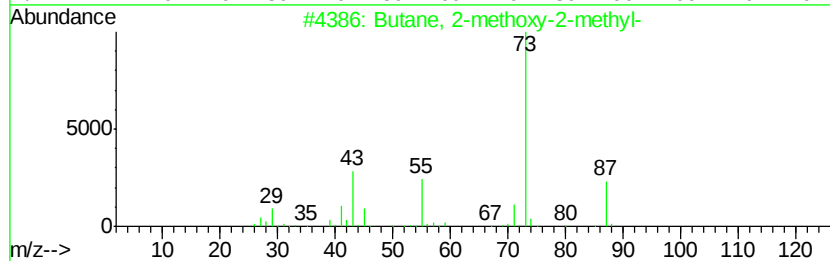
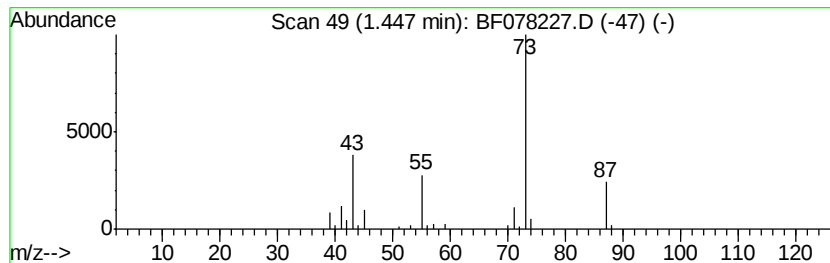
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.45	5.98 ng	90656	1,4-Dichlorobenzene-d4	7.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10



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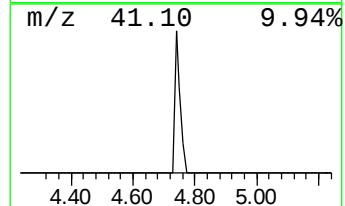
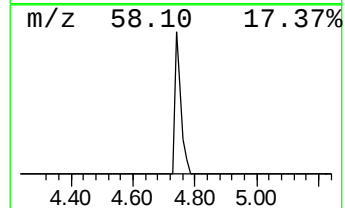
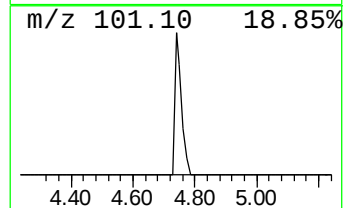
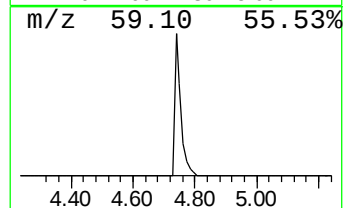
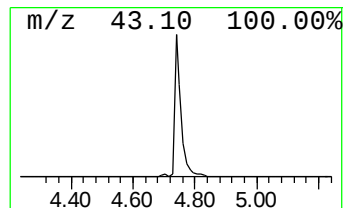
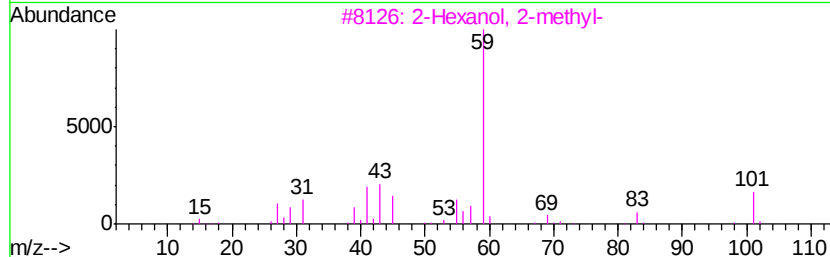
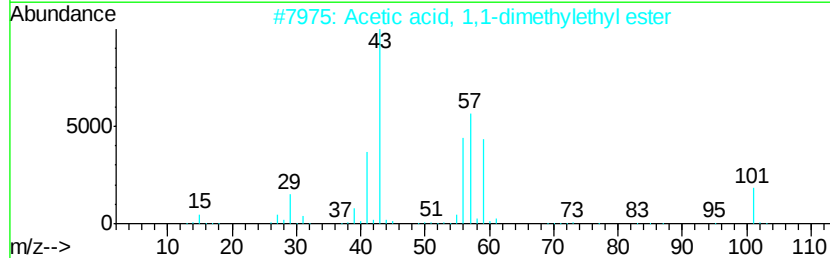
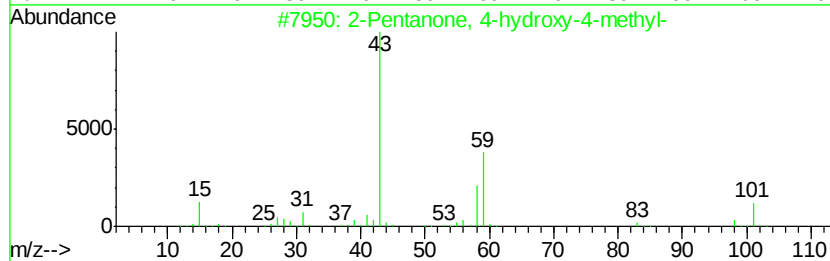
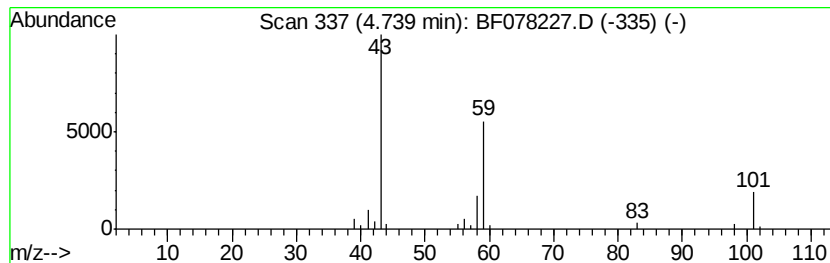
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.74	6.15 ng	93194	1,4-Dichlorobenzene-d4	7.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		Acetone	58	C3H6O	000067-64-1	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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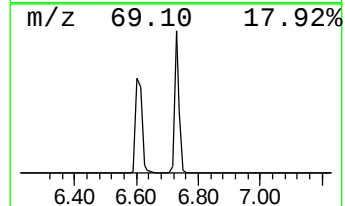
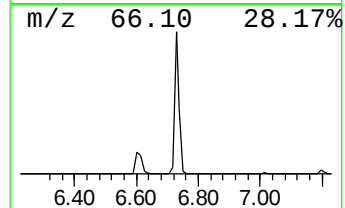
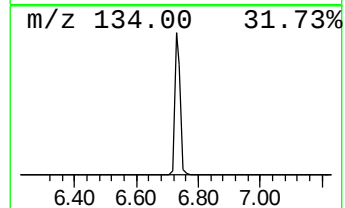
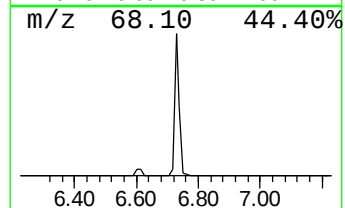
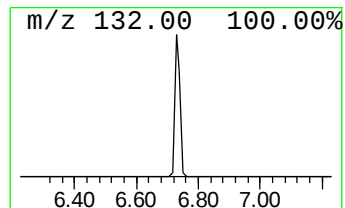
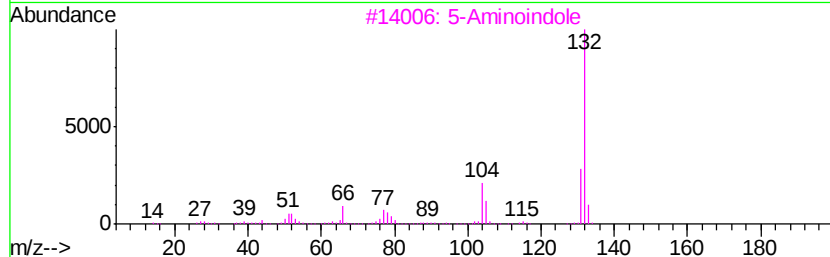
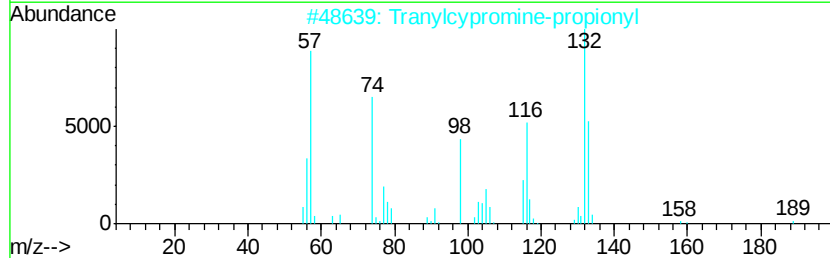
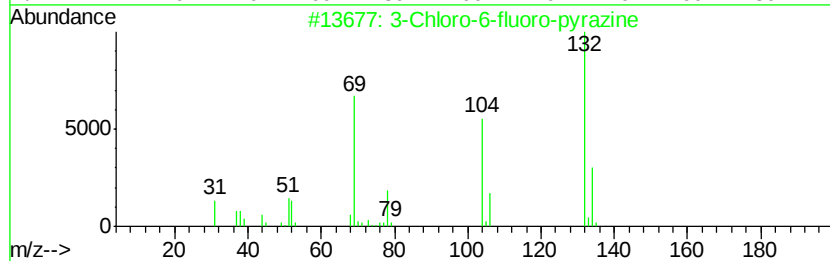
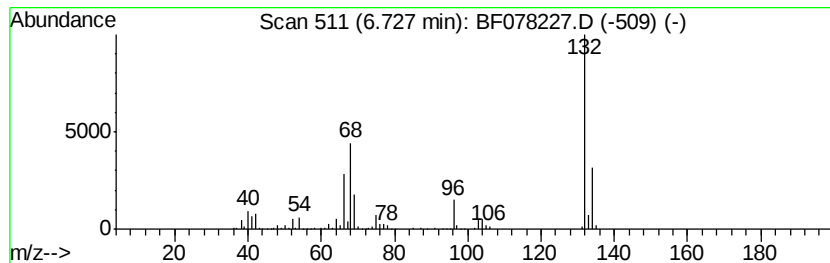
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	55.40 ng	839366	1,4-Dichlorobenzene-d4	7.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		5-Aminoindole	132	C8H8N2	005192-03-0	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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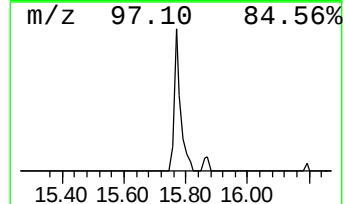
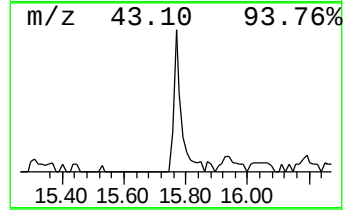
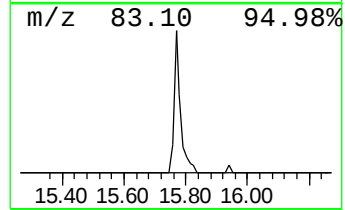
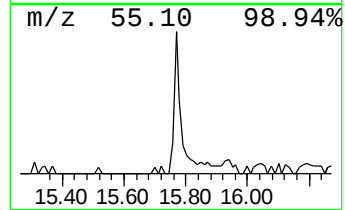
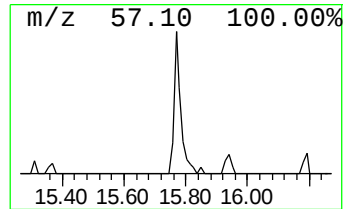
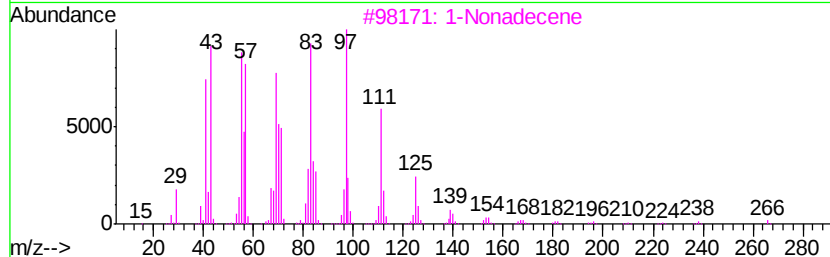
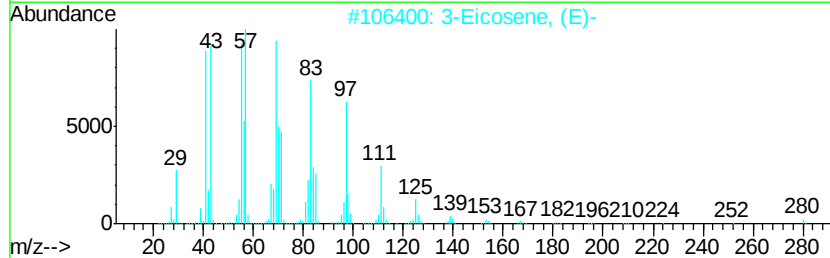
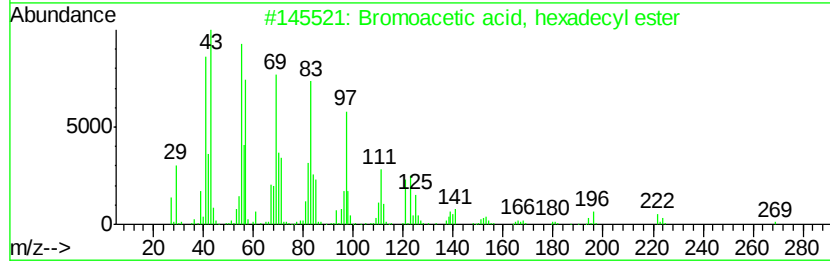
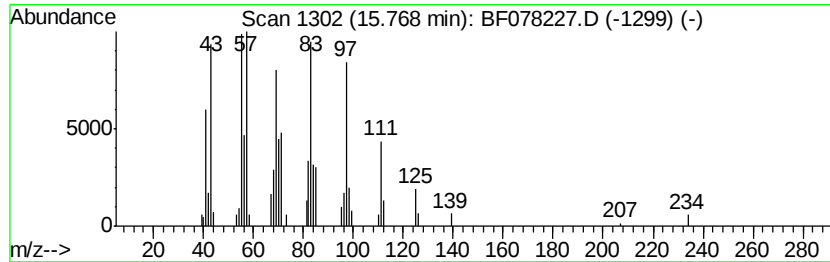
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Bromoacetic acid, hexadecyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.77	3.57 ng	110457	Chrysene-d12	15.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
2			3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3			1-Nonadecene	266	C19H38	018435-45-5	91
4			Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	91
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90



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COMP-3

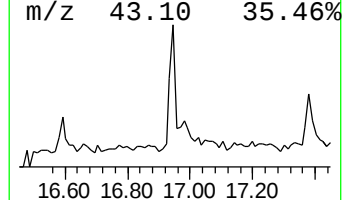
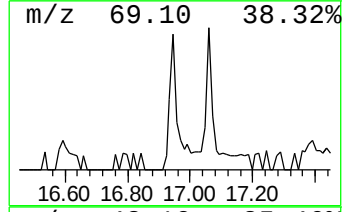
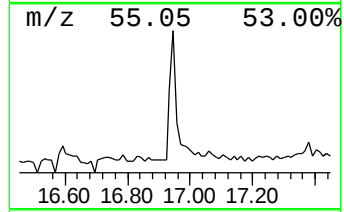
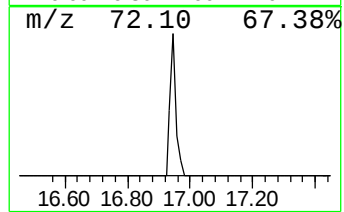
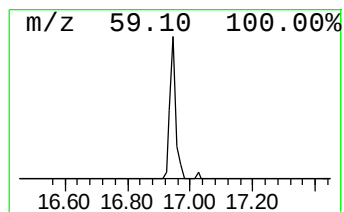
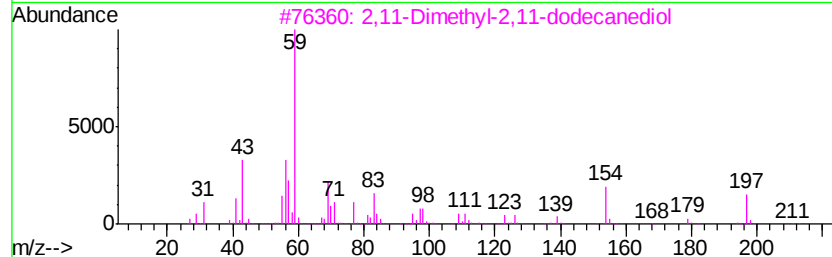
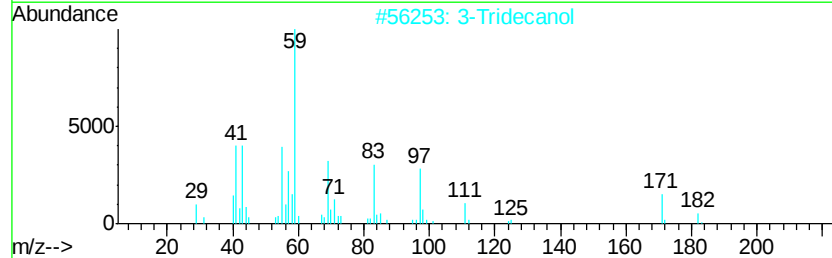
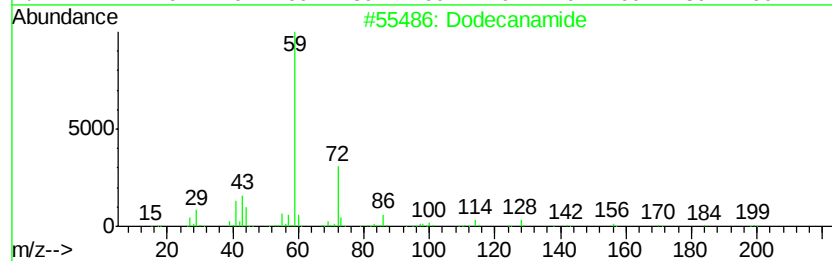
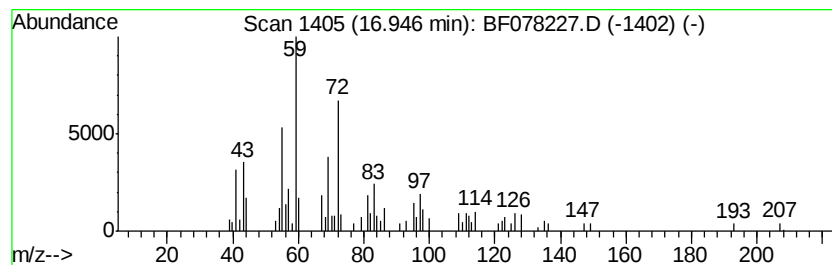
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Dodecanamide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.95	2.49 ng	72691	Perylene-d12	17.61

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanamide		199	C12H25NO	001120-16-7	50
2	3-Tridecanol		200	C13H28O	010289-68-6	43
3	2,11-Dimethyl-2,11-dodecanediol		230	C14H30O2	022092-59-7	40
4	2-Methyl-tridecane-2,12-diol		230	C14H30O2	1000187-03-5	38
5	2-Octanol, 2-methyl-6-methylene-		156	C10H20O	018479-59-9	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040215\
Data File : BF078227.D
Acq On : 3 Apr 2015 6:00
Operator : TP/IZ
Sample : G1731-03
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-3

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
unknown1.18	1.18	16.0	ng	241960	1	7.01	303036	20.0
Butane, 2-methoxy...	1.45	6.0	ng	90656	1	7.01	303036	20.0
2-Pentanone, 4-hy...	4.74	6.2	ng	93194	1	7.01	303036	20.0
unknown6.73	6.73	55.4	ng	839366	1	7.01	303036	20.0
Bromoacetic acid,...	15.77	3.6	ng	110457	5	15.87	619454	20.0
Dodecanamide	16.95	2.5	ng	72691	6	17.61	583021	20.0