

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102616\
 Data File : BF090847.D
 Acq On : 26 Oct 2016 18:34
 Operator : UM/SJ
 Sample : H5308-17
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-105D

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-BF102616.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	3.618	116	134	136	rBV2	20338	141603	2.78%	0.225%
2	4.213	176	186	196	rBV3	23478	133830	2.63%	0.212%
3	4.944	247	250	253	rBV	511157	647514	12.70%	1.028%
4	5.116	253	265	266	rBV	75715	369053	7.24%	0.586%
5	5.310	272	282	284	rVB	121588	393048	7.71%	0.624%
6	5.379	285	288	290	rBV	2635950	2701259	52.99%	4.288%
7	5.550	301	303	308	rBV2	258451	367935	7.22%	0.584%
8	5.630	308	310	313	rVB	936800	820113	16.09%	1.302%
9	6.190	346	359	361	rBV	251146	983128	19.29%	1.561%
10	6.419	377	379	388	rBV2	1588664	2280413	44.73%	3.620%
11	6.556	388	391	393	rVV	4205775	4725102	92.69%	7.500%
12	6.659	397	400	404	rVB	59817	93478	1.83%	0.148%
13	6.784	409	411	416	rBV	1345985	1282301	25.15%	2.035%
14	6.853	416	417	419	rVV	109498	173374	3.40%	0.275%
15	6.944	422	425	427	rVV	2526869	2849400	55.90%	4.523%
16	7.013	429	431	432	rVV	57043	85300	1.67%	0.135%
17	7.047	432	434	439	rVB2	866018	1158701	22.73%	1.839%
18	7.196	445	447	458	rVB	526419	1017839	19.97%	1.616%
19	7.356	458	461	463	rBV	1831395	2344889	46.00%	3.722%
20	7.402	463	465	468	rVV	174888	203134	3.98%	0.322%
21	7.573	471	480	482	rVV3	176399	567166	11.13%	0.900%
22	7.927	499	511	513	rBV	1304960	5097624	100.00%	8.092%
23	7.985	515	516	519	rVB2	81493	91353	1.79%	0.145%
24	8.076	521	524	526	rBV	1668368	1765862	34.64%	2.803%
25	8.202	533	535	537	rBV3	55757	113504	2.23%	0.180%
26	8.373	546	550	554	rBV	623174	1006080	19.74%	1.597%
27	8.453	554	557	560	rVV2	104193	287054	5.63%	0.456%
28	8.499	560	561	562	rVB	143745	102849	2.02%	0.163%
29	8.647	571	574	576	rBV3	50487	113308	2.22%	0.180%
30	8.716	579	580	583	rVB	135953	142854	2.80%	0.227%
31	8.773	583	585	589	rVB	56182	88741	1.74%	0.141%
32	8.910	589	597	600	rBV	938057	2191933	43.00%	3.479%
33	9.059	603	610	612	rVV	1701671	3755107	73.66%	5.961%
34	9.150	615	618	621	rVV	3839539	4020962	78.88%	6.383%

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35	9.299	627	631	634 rBV	92504	129700	2.54%	0.206%
36	9.390	637	639	644 rBV4	44954	96648	1.90%	0.153%
37	9.493	644	648	649 rBV3	22958	51476	1.01%	0.082%
38	9.550	650	653	655 rVV	278793	263806	5.18%	0.419%
39	9.653	660	662	664 rVB	230987	202411	3.97%	0.321%
40	9.756	668	671	675 rBV	844373	887879	17.42%	1.409%
41	9.825	675	677	680 rVB	1968346	1871976	36.72%	2.971%
42	9.939	685	687	693 rVB	127958	130950	2.57%	0.208%
43	10.065	694	698	701 rBV	617254	872452	17.11%	1.385%
44	10.225	709	712	714 rBV	116891	191700	3.76%	0.304%
45	10.270	714	716	719 rVV2	57938	85914	1.69%	0.136%
46	10.350	720	723	726 rVB3	29054	69897	1.37%	0.111%
47	10.545	738	740	741 rBV2	31256	61245	1.20%	0.097%
48	10.625	741	747	749 rVV3	2895592	4345345	85.24%	6.898%
49	10.739	755	757	761 rBV2	103535	168247	3.30%	0.267%
50	10.922	770	773	776 rBV	141482	158135	3.10%	0.251%
51	10.991	776	779	781 rVV2	141466	215463	4.23%	0.342%
52	11.048	783	784	788 rVB2	40457	55991	1.10%	0.089%
53	11.116	788	790	794 rVB2	41378	57069	1.12%	0.091%
54	11.208	794	798	801 rVB4	84339	199987	3.92%	0.317%
55	11.311	805	807	811 rBV	2012108	1917344	37.61%	3.043%
56	11.848	852	854	856 rBV	46431	80137	1.57%	0.127%
57	11.882	856	857	864 rVB3	66758	128937	2.53%	0.205%
58	12.374	898	900	902 rBV	55392	55477	1.09%	0.088%
59	12.728	929	931	934 rVB	172154	156359	3.07%	0.248%
60	12.899	943	946	949 rBV	4216536	4505280	88.38%	7.151%
61	13.437	991	993	995 rBV	131183	120652	2.37%	0.192%
62	13.802	1023	1025	1028 rBV	79004	99552	1.95%	0.158%
63	13.951	1035	1038	1040 rBV	1788229	1794996	35.21%	2.849%
64	14.134	1051	1054	1061 rVB	93862	158335	3.11%	0.251%
65	14.408	1076	1078	1087 rBV2	48929	128703	2.52%	0.204%
66	14.545	1087	1090	1092 rBV	82410	98434	1.93%	0.156%
67	15.368	1159	1162	1164 rBV	941101	1374174	26.96%	2.181%
68	15.402	1164	1165	1171 rVB	49660	69239	1.36%	0.110%
69	16.271	1238	1241	1251 rVB2	32094	78626	1.54%	0.125%

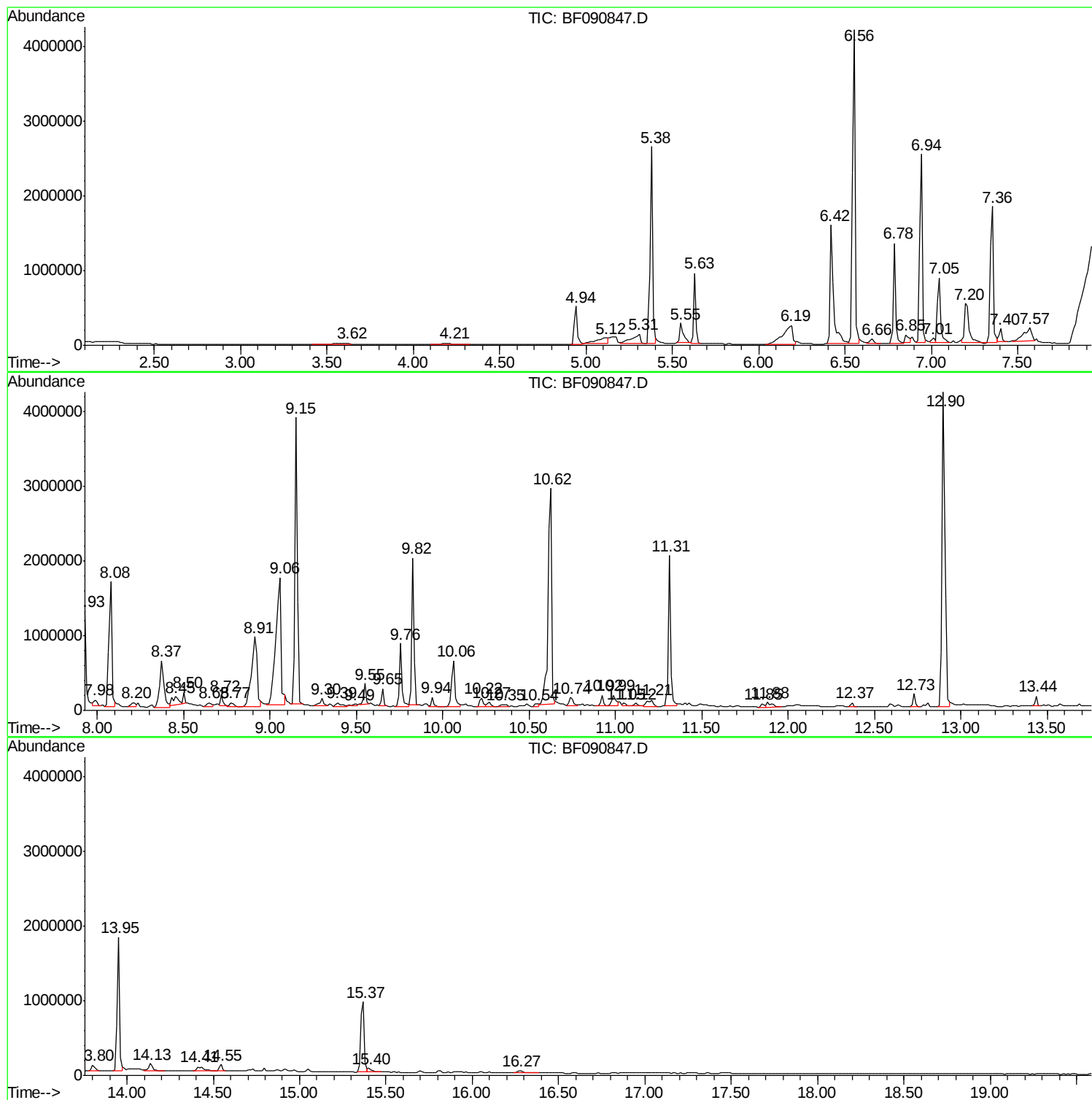
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ClientSampled :
MW-105D

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF102616.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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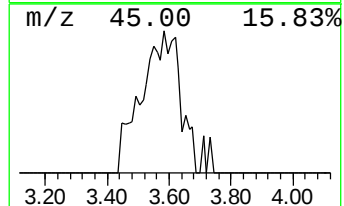
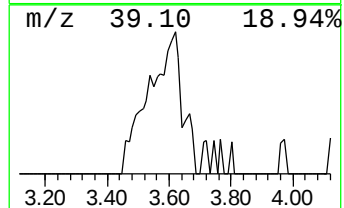
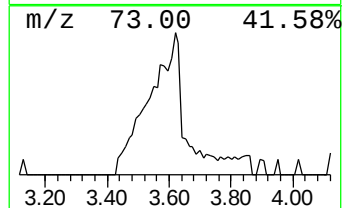
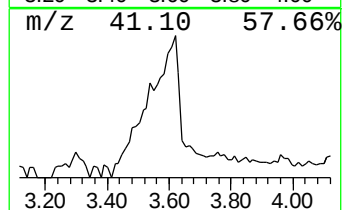
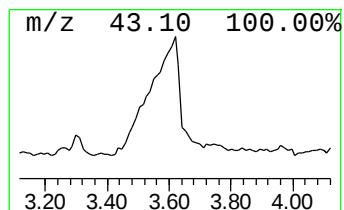
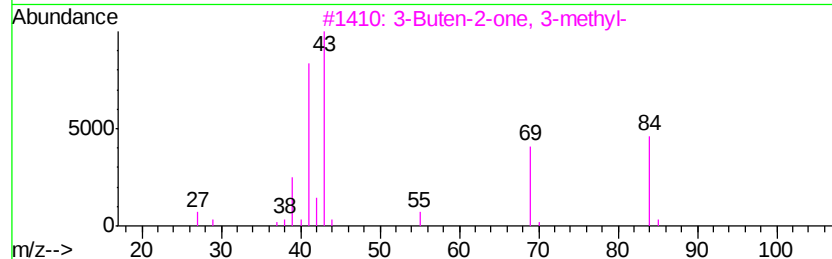
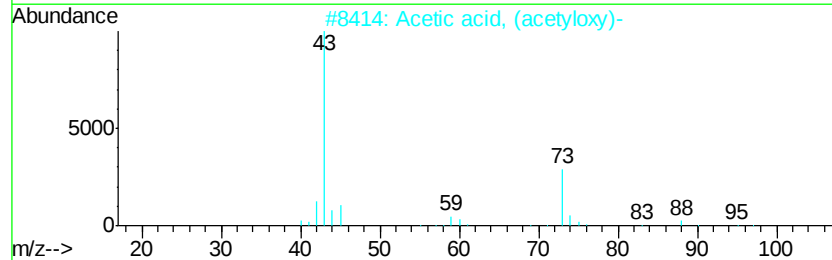
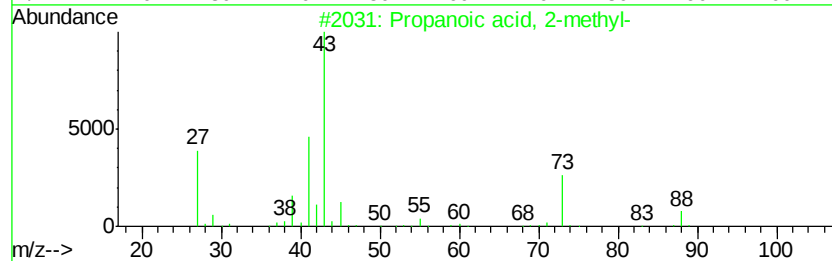
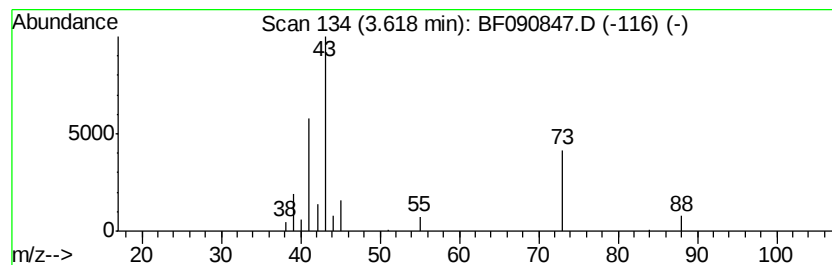
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propanoic acid, 2-methyl- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.62	2.21 ng	141603	1,4-Dichlorobenzene-d4	6.78

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	90
2			Acetic acid, (acetyloxy)-	118	C4H6O4	013831-30-6	39
3			3-Buten-2-one, 3-methyl-	84	C5H8O	000814-78-8	28
4			Propane, 2-nitro-	89	C3H7NO2	000079-46-9	9
5			sec-Butyl nitrite	103	C4H9NO2	000924-43-6	9



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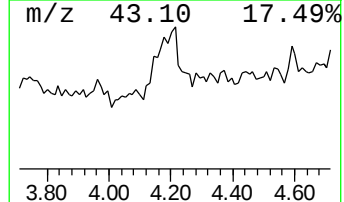
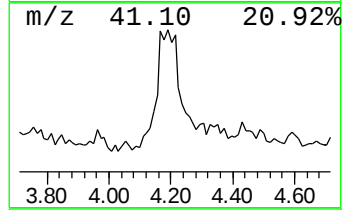
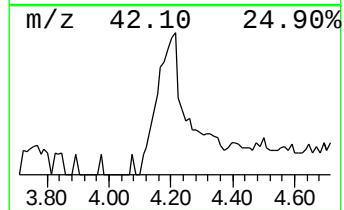
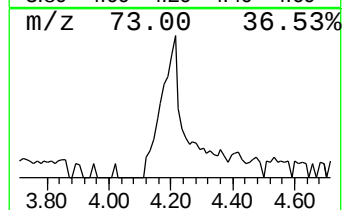
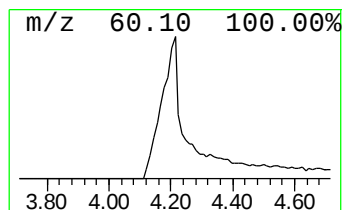
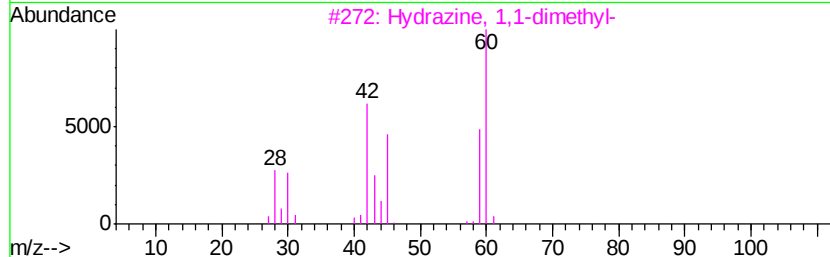
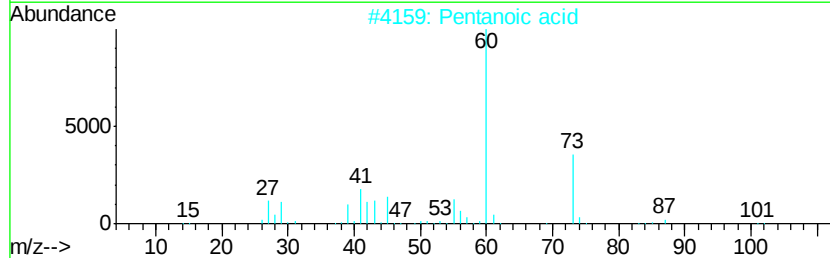
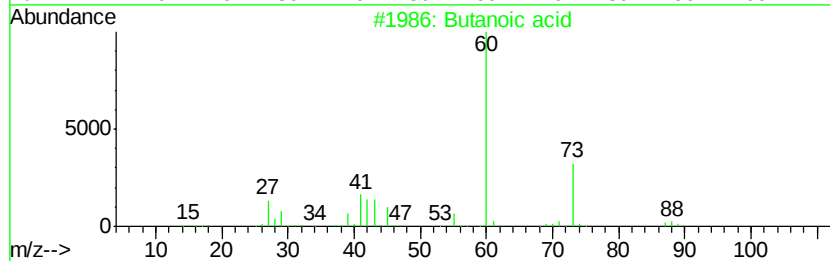
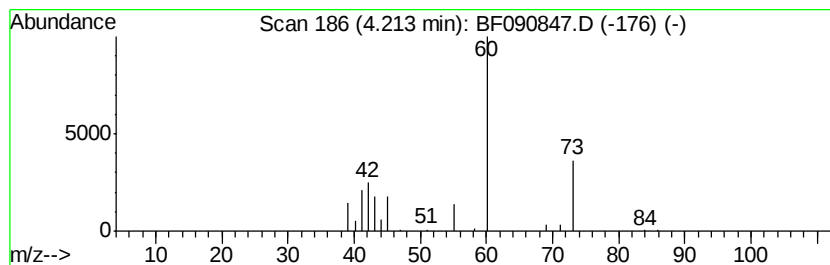
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown4.21 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.21	2.09 ng	133830	1,4-Dichlorobenzene-d4	6.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid	88	C4H8O2	000107-92-6	9
2		Pentanoic acid	102	C5H10O2	000109-52-4	9
3		Hvdrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	5
4		1-Propanol	60	C3H8O	000071-23-8	5
5		Formic acid hydrazide	60	CH4N2O	000624-84-0	4



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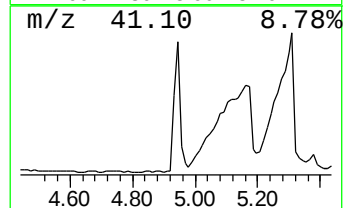
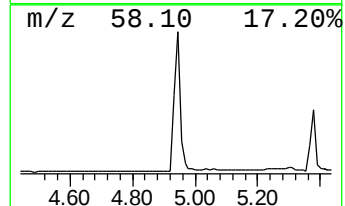
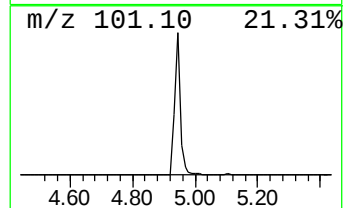
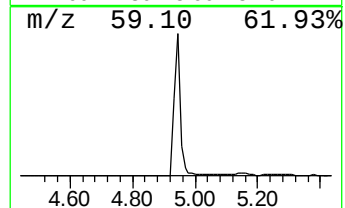
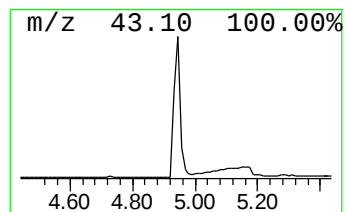
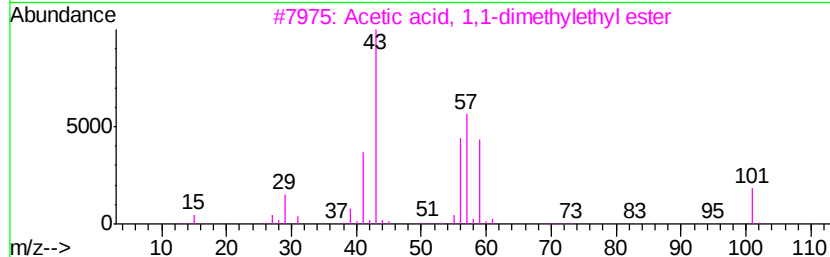
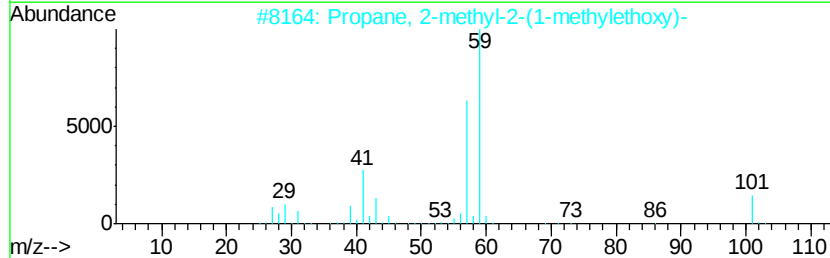
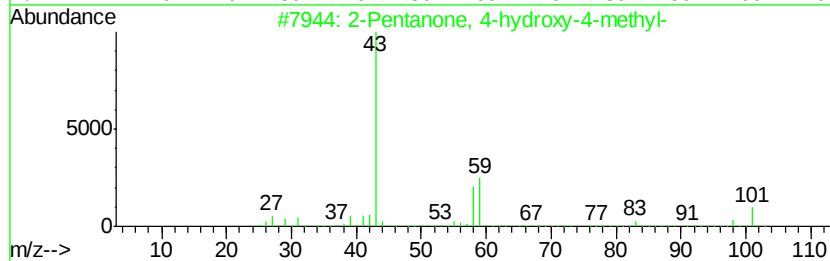
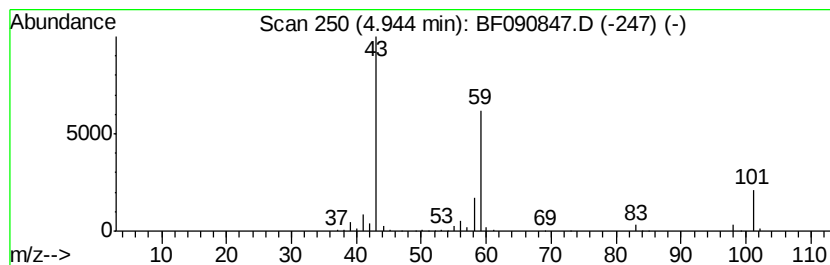
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	10.10 ng	647514	1,4-Dichlorobenzene-d4	6.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Propane, 2-methyl-2-(1-methylethyl)-	116	C7H16O	017348-59-3	53
3		Acetic acid, 1,1-dimethylethyl ester	116	C6H12O2	000540-88-5	39
4		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	23
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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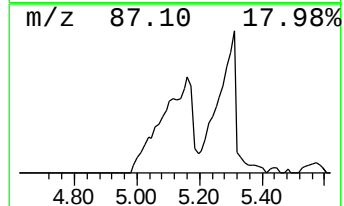
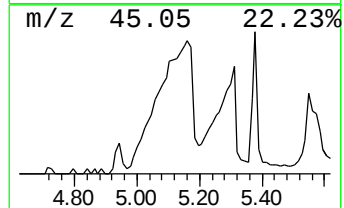
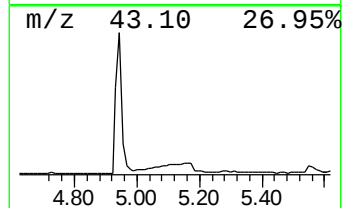
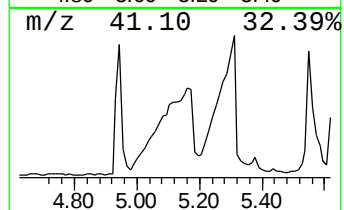
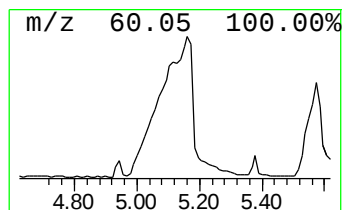
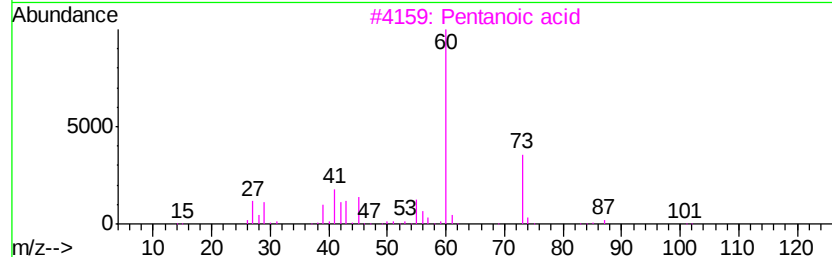
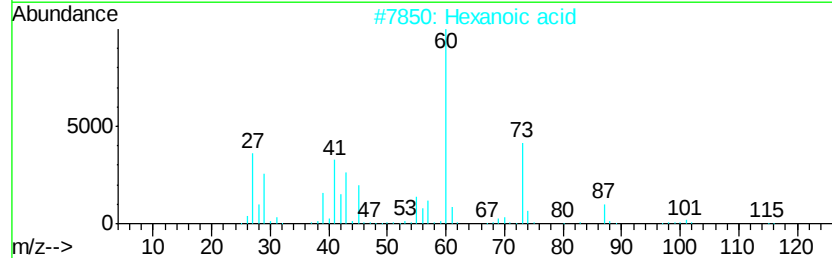
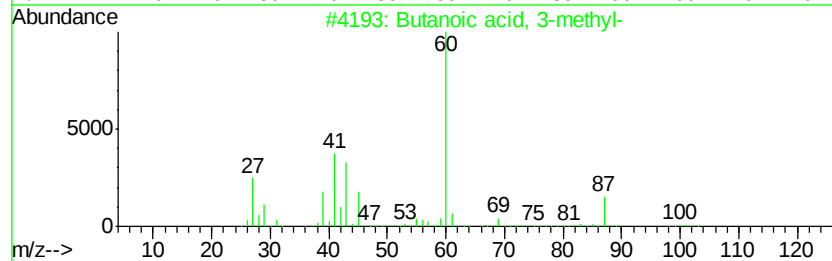
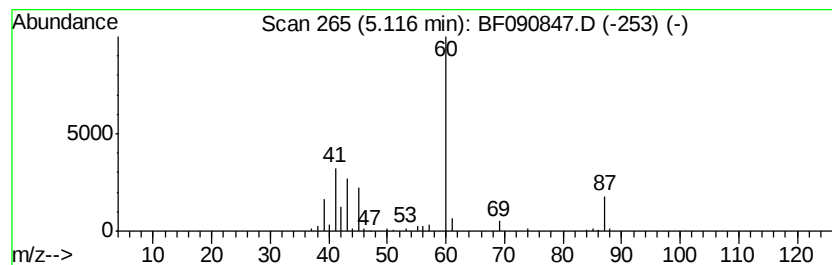
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 Butanoic acid, 3-methyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	5.76 ng	369053	1,4-Dichlorobenzene-d4	6.78

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	64
2			Hexanoic acid	116	C6H12O2	000142-62-1	40
3			Pentanoic acid	102	C5H10O2	000109-52-4	38
4			Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	28
5			Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	9



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MW-105D

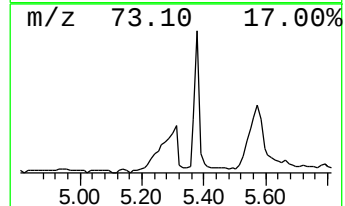
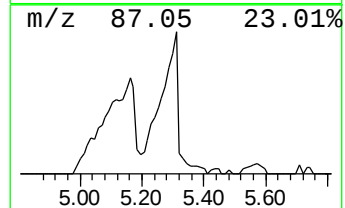
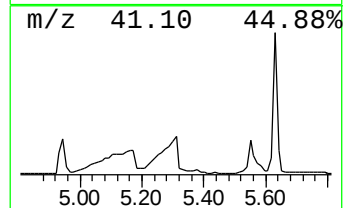
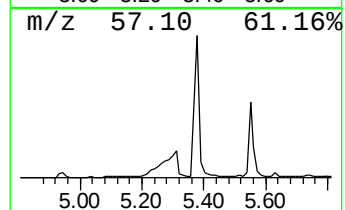
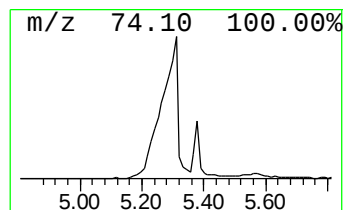
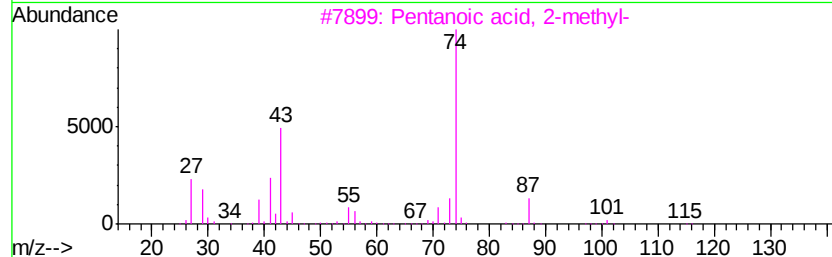
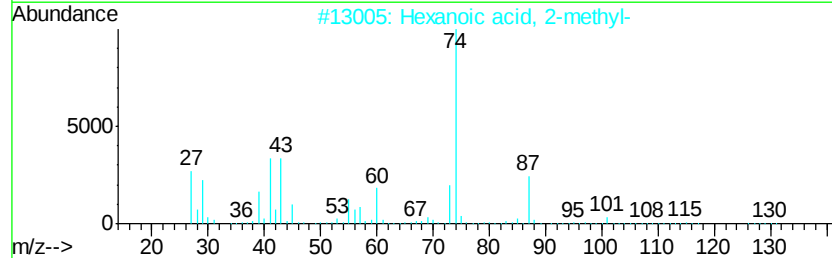
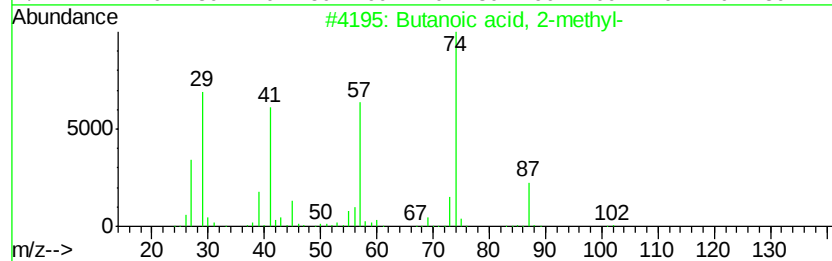
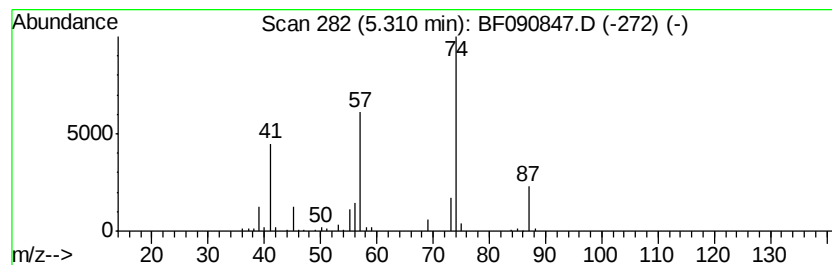
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Butanoic acid, 2-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.31	6.13 ng	393048	1,4-Dichlorobenzene-d4	6.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	83
2		Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	72
3		Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	50
4		Oxirane, (butoxymethyl)-	130	C7H14O2	002426-08-6	9
5		5-Hydroxy-2,2-dimethylhexan-3-one	144	C8H16O2	173343-33-4	8



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102616\
Data File : BF090847.D
Acq On : 26 Oct 2016 18:34
Operator : UM/SJ
Sample : H5308-17
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-105D

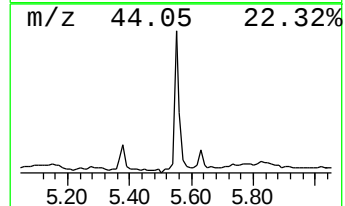
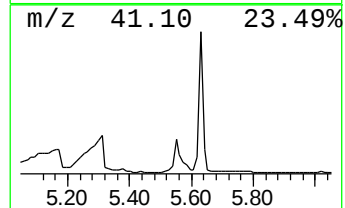
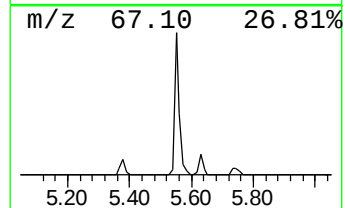
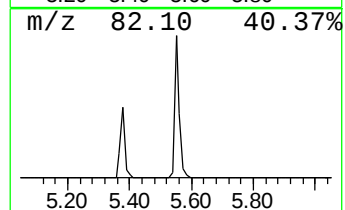
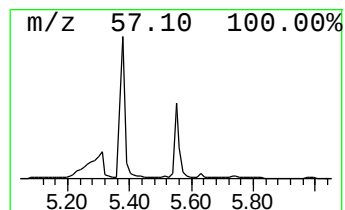
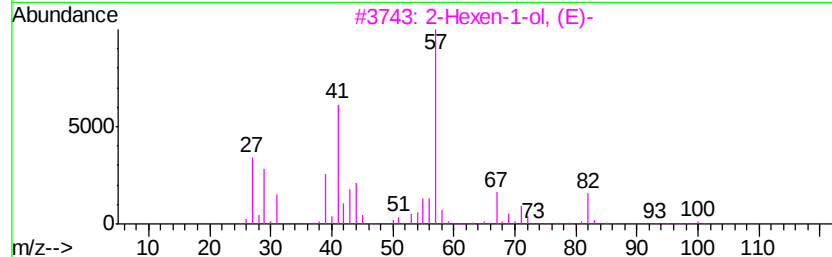
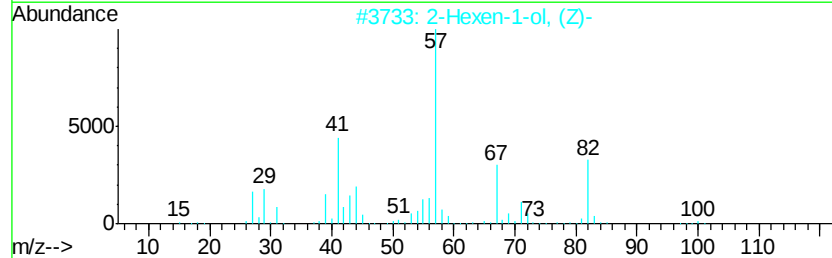
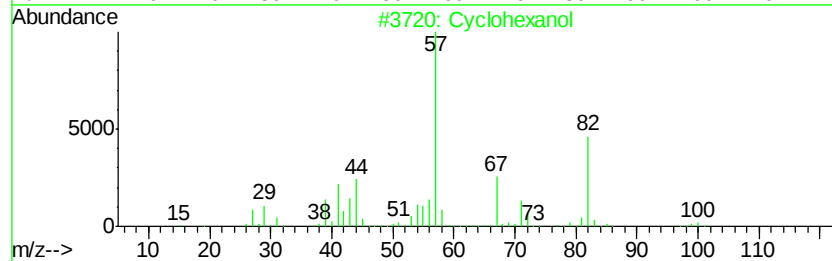
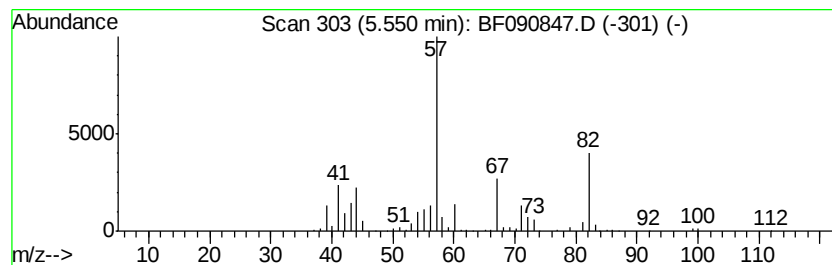
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclohexanol Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.55	5.74 ng	367935	1,4-Dichlorobenzene-d4	6.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexanol	100	C6H12O	000108-93-0	93
2		2-Hexen-1-ol, (Z)-	100	C6H12O	000928-94-9	74
3		2-Hexen-1-ol, (E)-	100	C6H12O	000928-95-0	53
4		Cyclopentanol, 2-methyl-	100	C6H12O	024070-77-7	38
5		Nitrous acid, cyclohexyl ester	129	C6H11NO2	005156-40-1	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102616\
Data File : BF090847.D
Acq On : 26 Oct 2016 18:34
Operator : UM/SJ
Sample : H5308-17
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampled :
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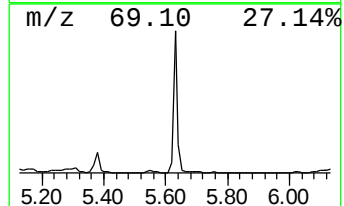
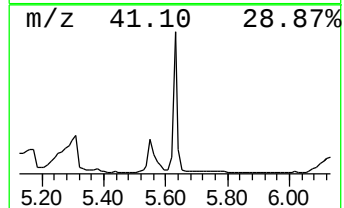
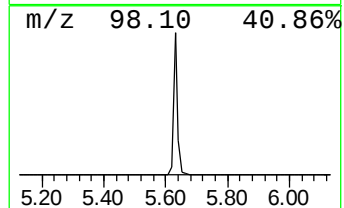
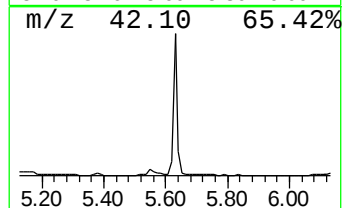
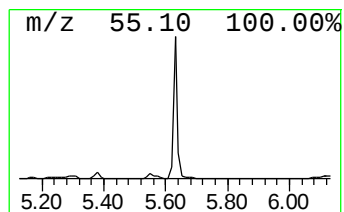
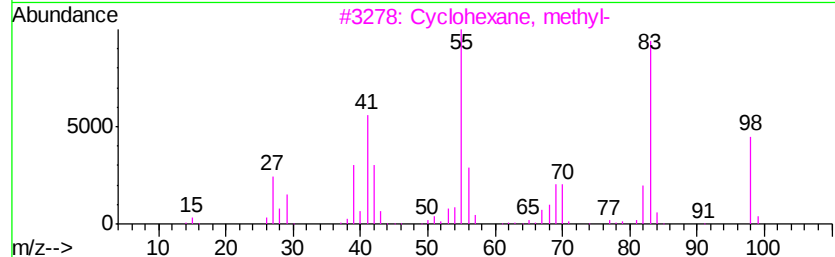
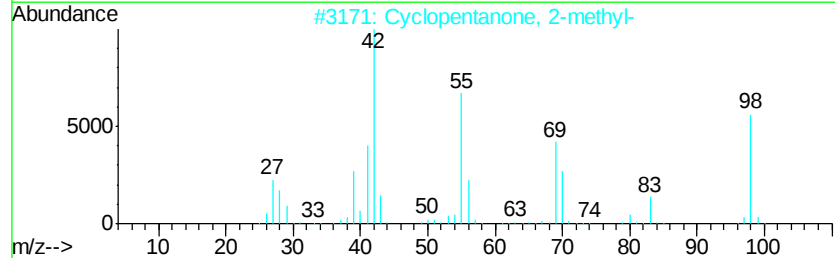
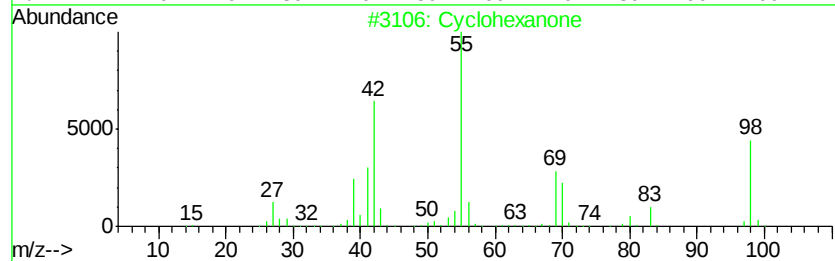
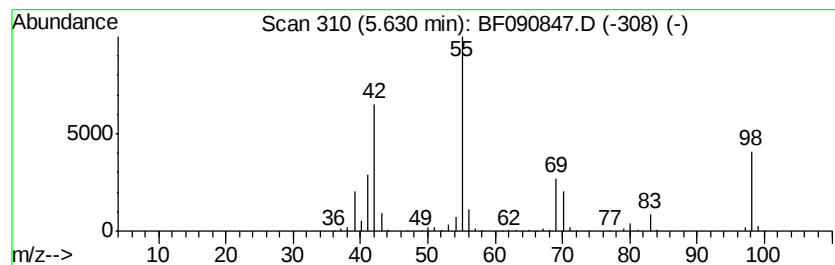
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclohexanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.63	12.79 ng	820113	1,4-Dichlorobenzene-d4	6.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexanone	98	C6H10O	000108-94-1	94
2		Cyclopentanone, 2-methyl-	98	C6H10O	001120-72-5	74
3		Cyclohexane, methyl-	98	C7H14	000108-87-2	45
4		6-Oxa-bicyclo[3.1.0]hexan-3-one	98	C5H6O2	074017-10-0	38
5		1-Pentene	70	C5H10	000109-67-1	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102616\
Data File : BF090847.D
Acq On : 26 Oct 2016 18:34
Operator : UM/SJ
Sample : H5308-17
Misc :
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Instrument :
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ClientSampleId :
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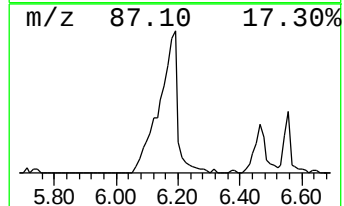
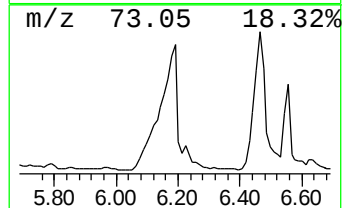
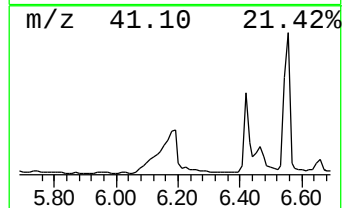
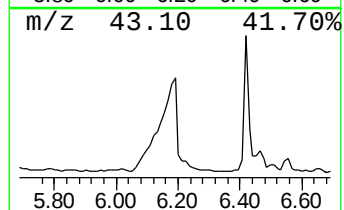
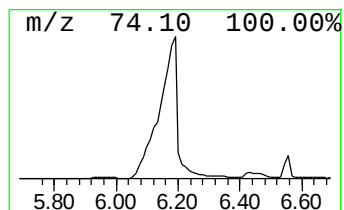
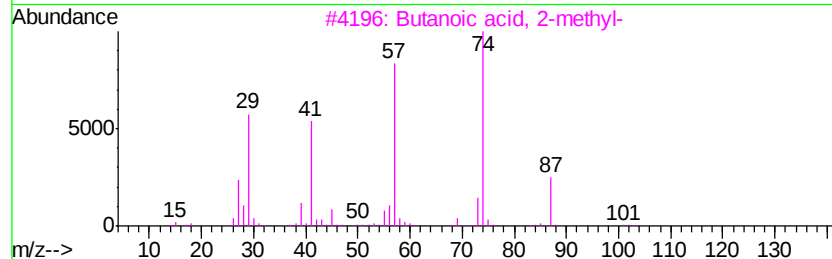
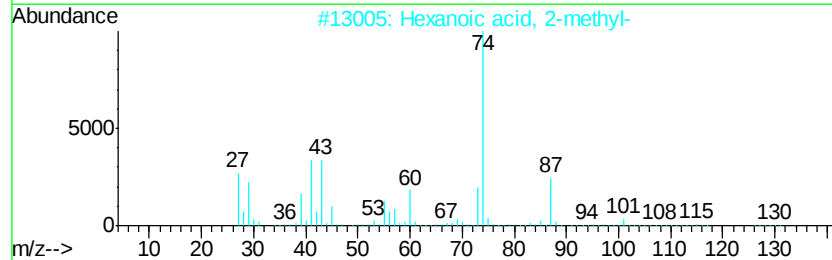
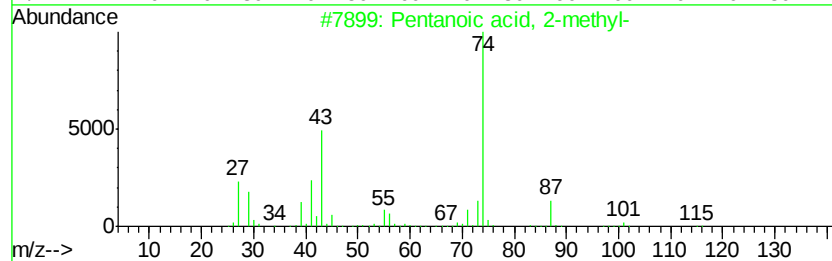
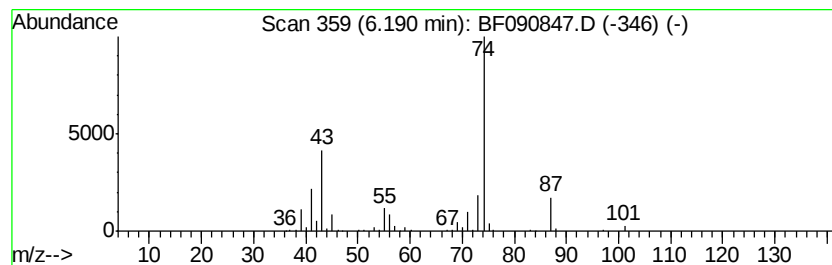
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentanoic acid, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.19	15.33 ng	983128	1,4-Dichlorobenzene-d4	6.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	83
2		Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	72
3		Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	38
4		Hexanoic acid, methyl ester	130	C7H14O2	000106-70-7	23
5		Propanoic acid	74	C3H6O2	000079-09-4	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102616\
Data File : BF090847.D
Acq On : 26 Oct 2016 18:34
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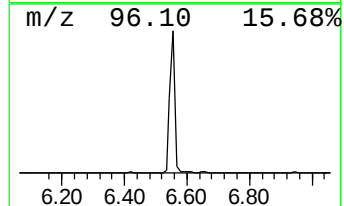
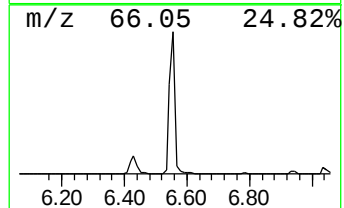
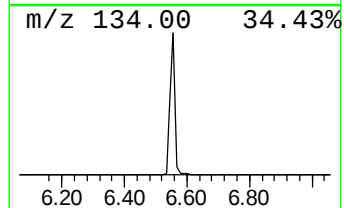
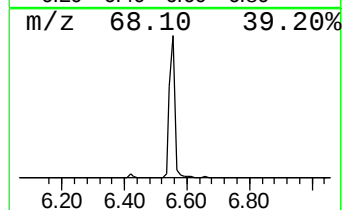
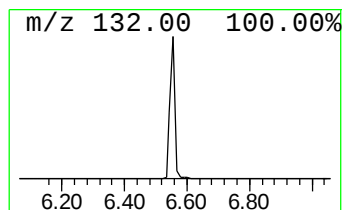
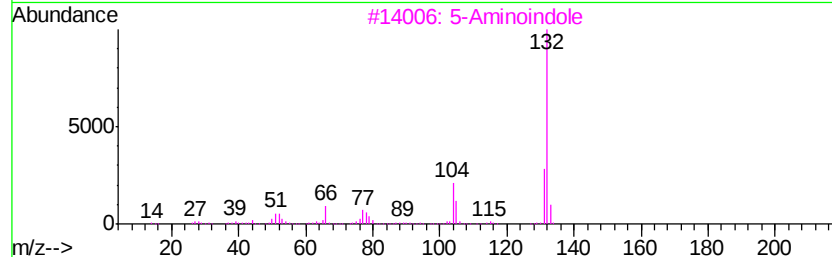
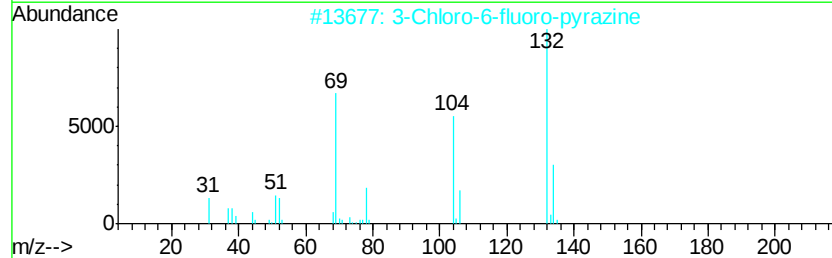
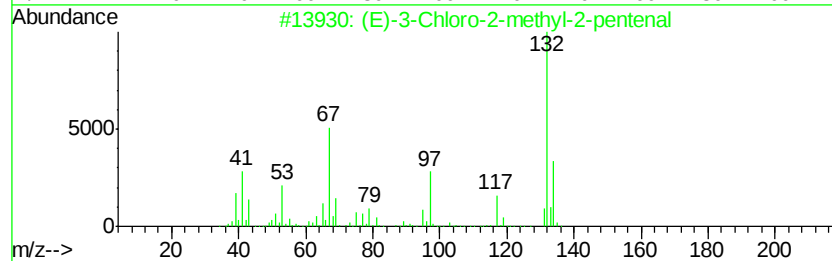
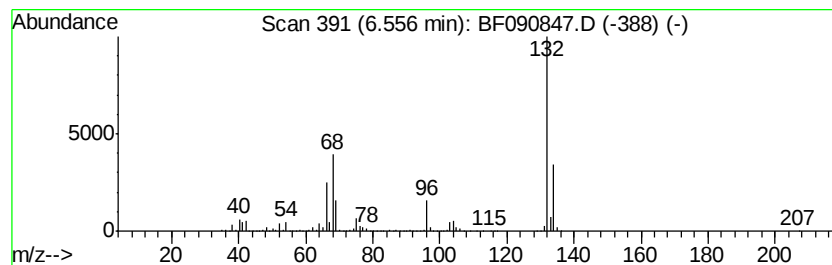
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	73.70 ng	4725100	1,4-Dichlorobenzene-d4	6.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102616\
Data File : BF090847.D
Acq On : 26 Oct 2016 18:34
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Misc :
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ClientSampleId :
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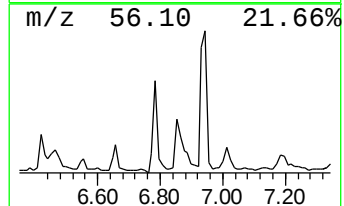
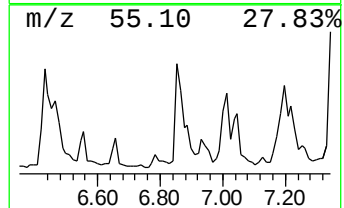
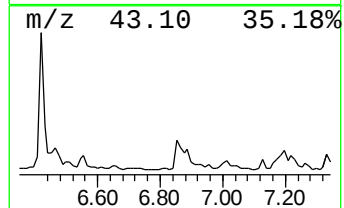
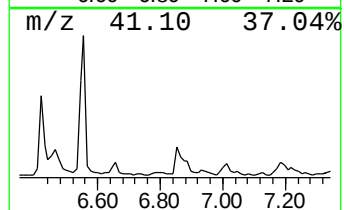
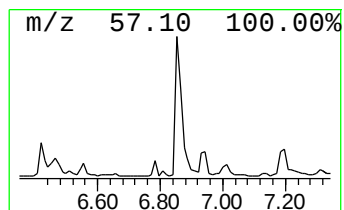
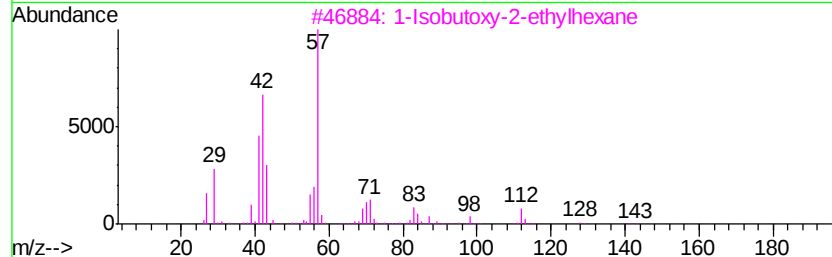
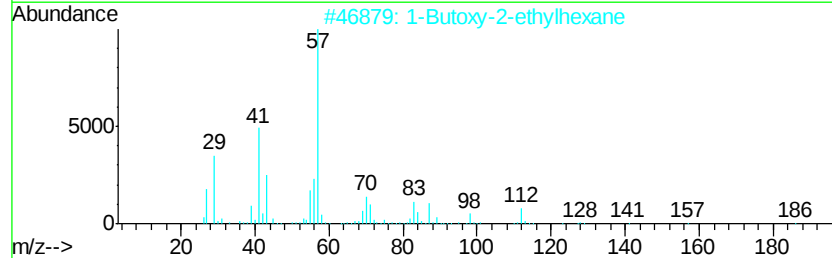
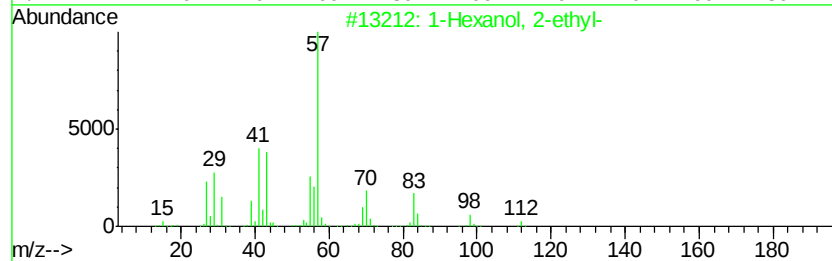
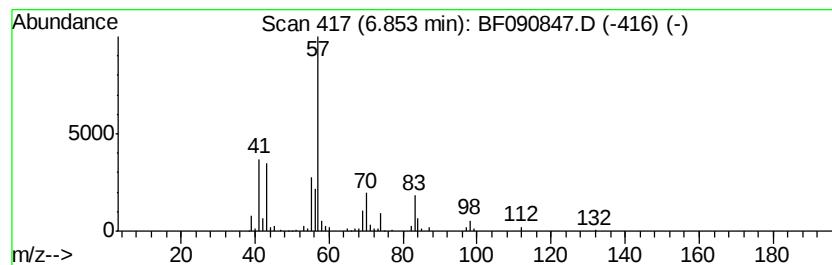
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Hexanol, 2-ethyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.85	2.70 ng	173374	1,4-Dichlorobenzene-d4	6.78

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2			1-Butoxy-2-ethylhexane	186	C12H26O	062625-25-6	72
3			1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	56
4			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	50
5			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102616\
Data File : BF090847.D
Acq On : 26 Oct 2016 18:34
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Misc :
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ClientSampleId :
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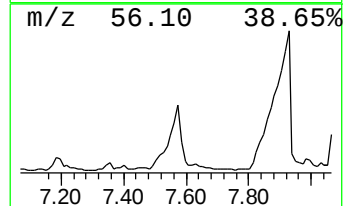
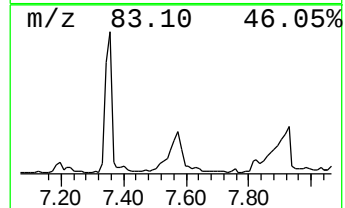
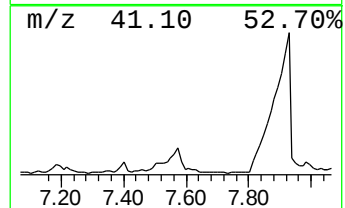
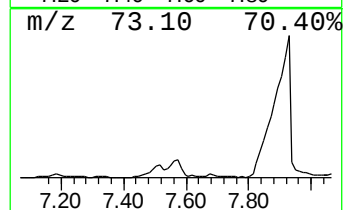
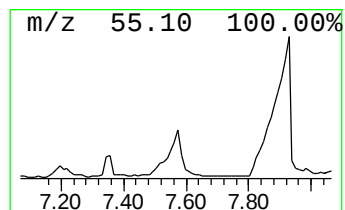
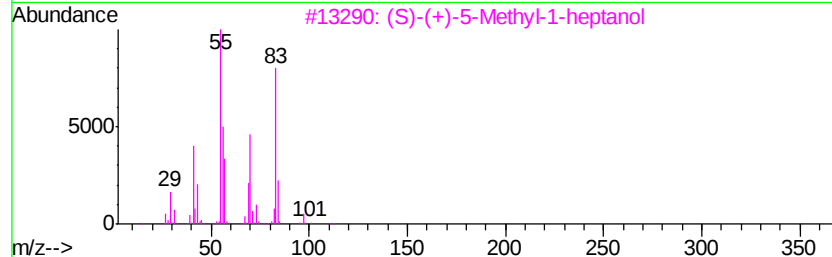
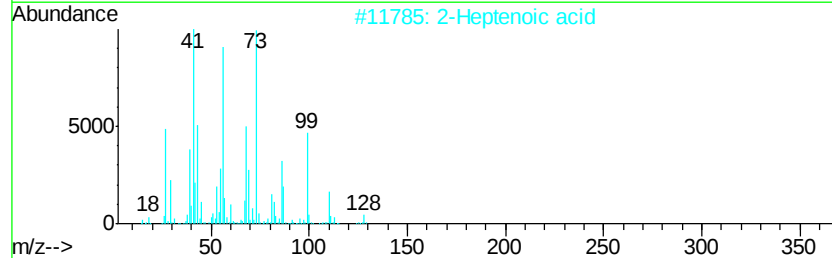
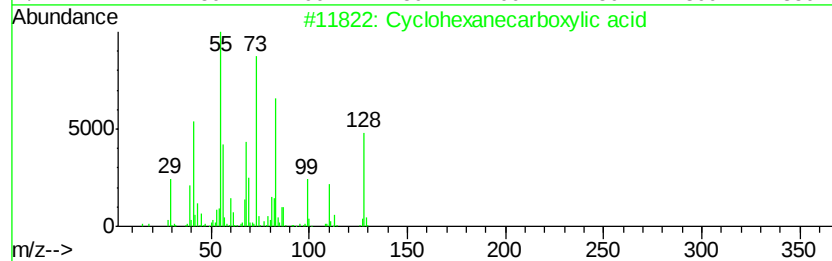
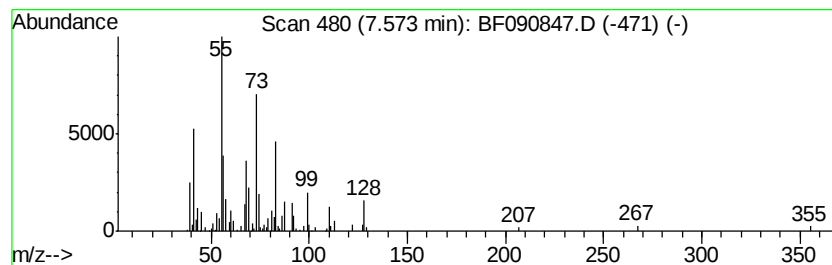
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Cyclohexanecarboxylic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.57	6.42 ng	567166	Napthalene-d8	8.08

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanecarboxylic acid	128	C7H12O2	000098-89-5	81
2			2-Heptenoic acid	128	C7H12O2	018999-28-5	38
3			(S)-(+)-5-Methyl-1-heptanol	130	C8H18O	057803-73-3	25
4			Cyclopentane, 1-ethyl-3-methyl-	112	C8H16	003726-47-4	16
5			3-Penten-1-ol	86	C5H10O	039161-19-8	14



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Operator : UM/SJ
Sample : H5308-17
Misc :
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Instrument :
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ClientSampleId :
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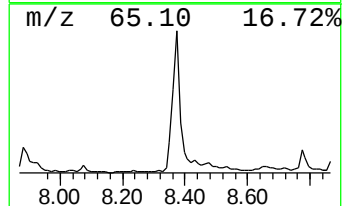
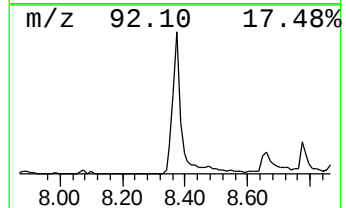
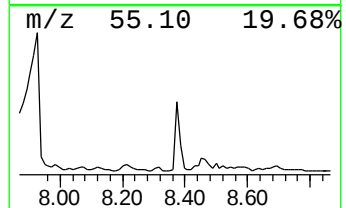
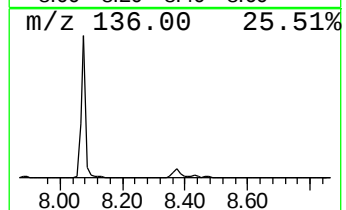
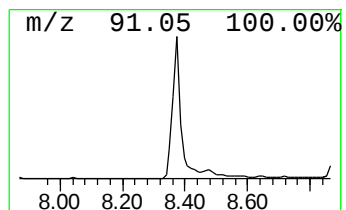
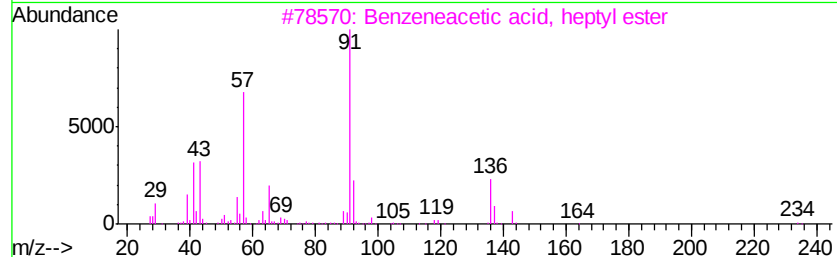
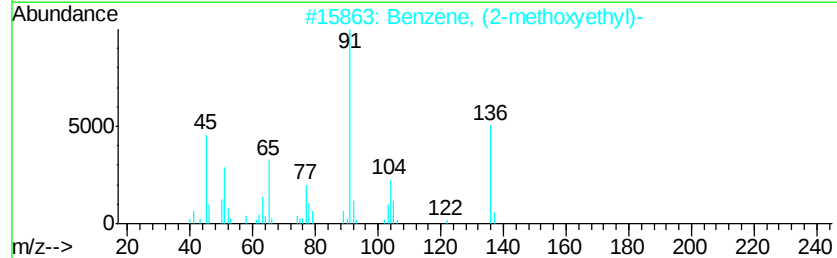
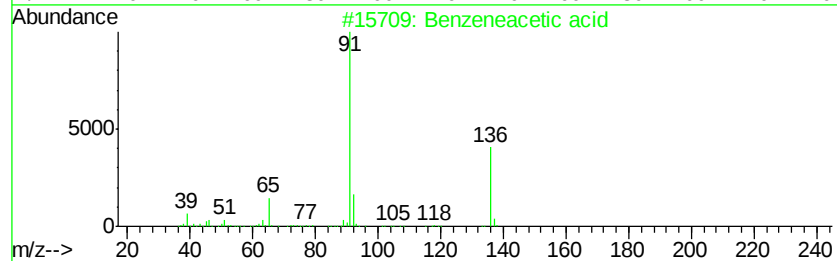
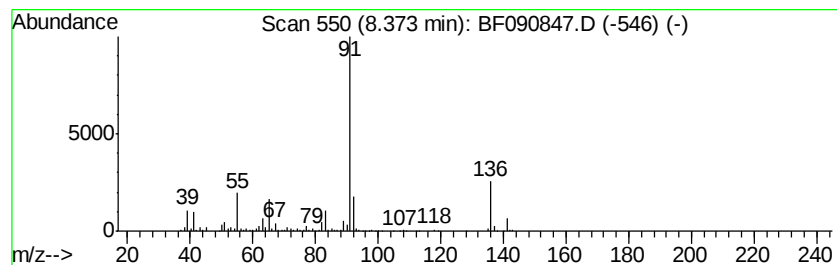
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Benzeneacetic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.37	11.39 ng	1006080	Naphthalene-d8	8.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzeneacetic acid	136	C8H8O2	000103-82-2	81
2		Benzene, (2-methoxyethyl)-	136	C9H12O	003558-60-9	59
3		Benzeneacetic acid, heptyl ester	234	C15H22O2	039736-25-9	59
4		Propanedioic acid, phenyl-	180	C9H8O4	002613-89-0	59
5		Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	49



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Data File : BF090847.D
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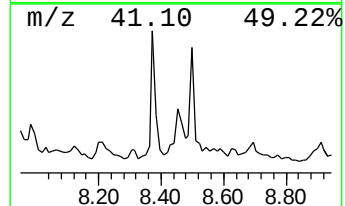
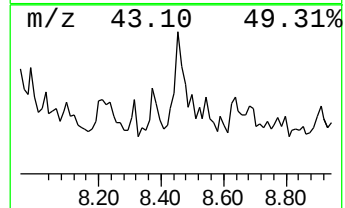
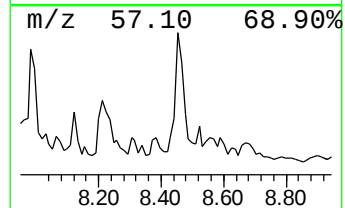
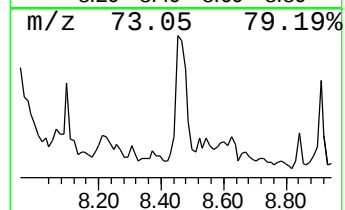
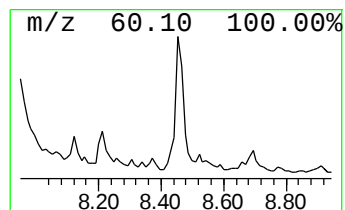
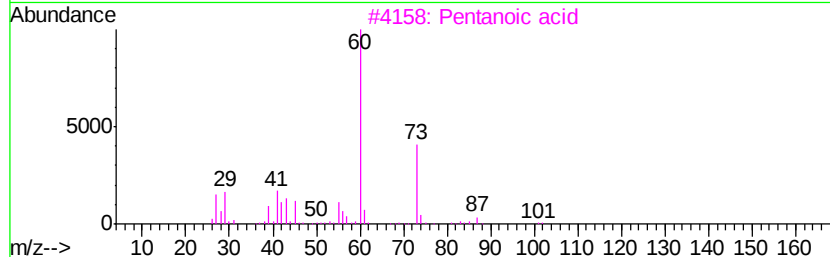
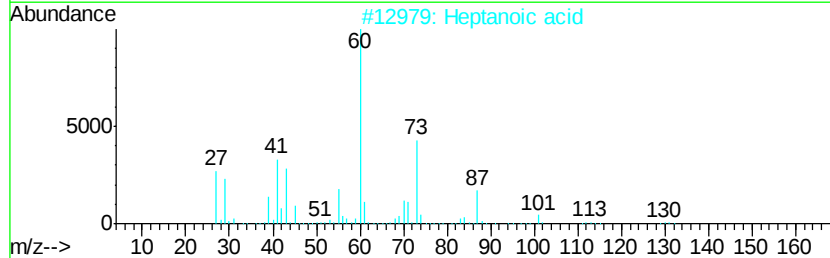
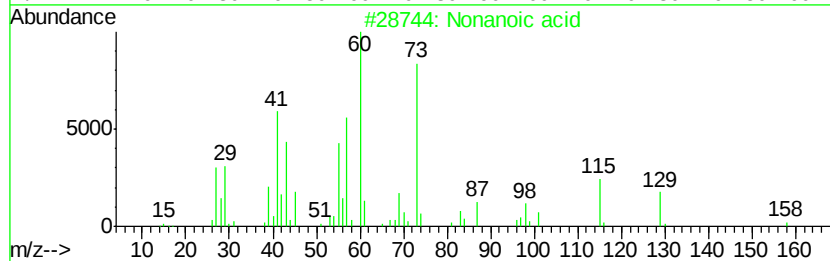
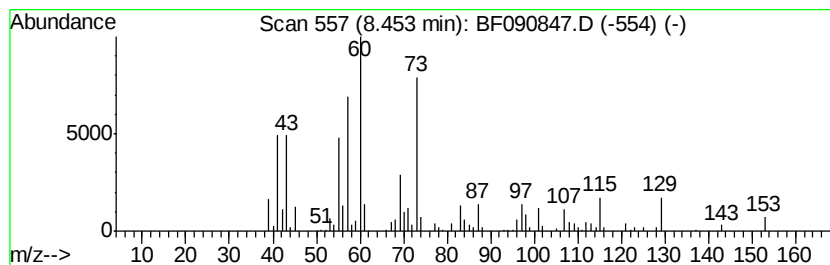
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Nonanoic acid Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.45	3.25 ng	287054	Naphthalene-d8	8.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonanoic acid	158	C9H18O2	000112-05-0	64
2		Heptanoic acid	130	C7H14O2	000111-14-8	53
3		Pentanoic acid	102	C5H10O2	000109-52-4	53
4		Hexanoic acid	116	C6H12O2	000142-62-1	50
5		Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	47



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Sample : H5308-17
Misc :
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ClientSampleId :
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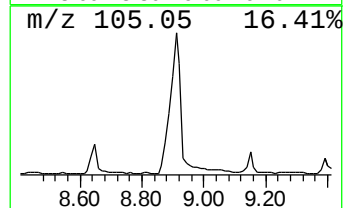
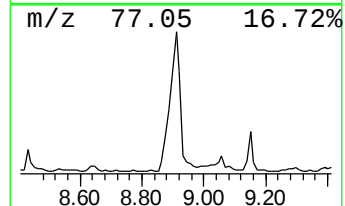
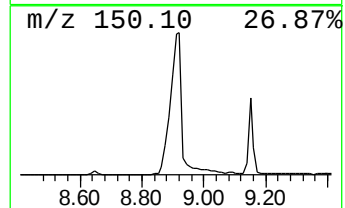
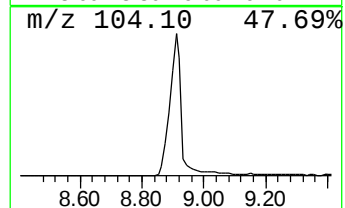
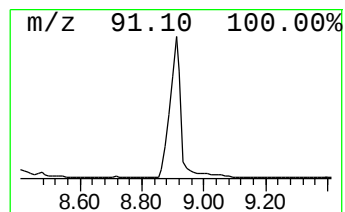
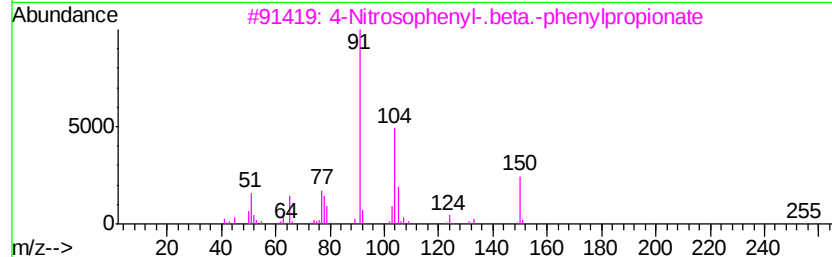
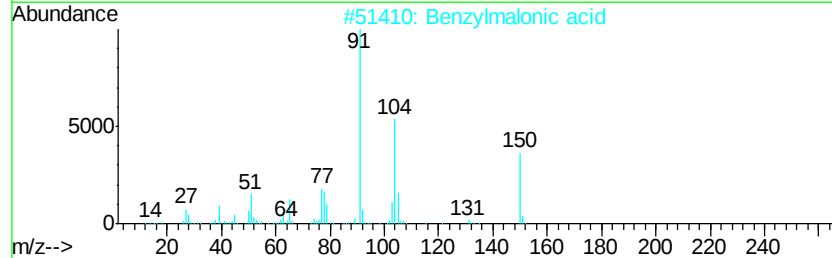
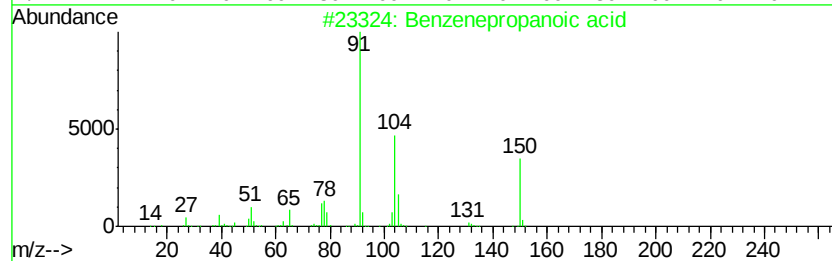
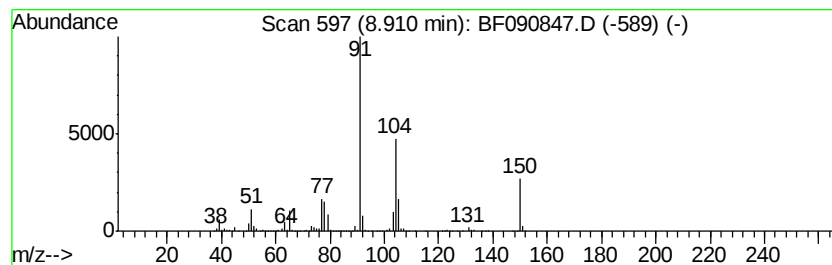
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Benzenepropanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.91	24.83 ng	2191930	Napthalene-d8	8.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzenepropanoic acid	150	C9H10O2	000501-52-0	94
2		Benzylmalonic acid	194	C10H10O4	000616-75-1	91
3		4-Nitrosophenyl-.beta.-phenylpro...	255	C15H13NO3	1000129-40-0	86
4		3-Phenyl-propionic acid, isoprop...	192	C12H16O2	022767-95-9	56
5		Benzeneacetic acid, methyl ester	150	C9H10O2	000101-41-7	27



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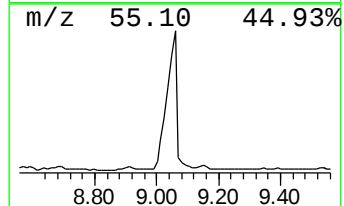
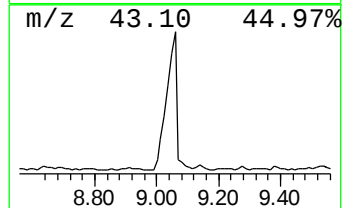
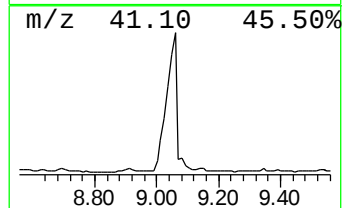
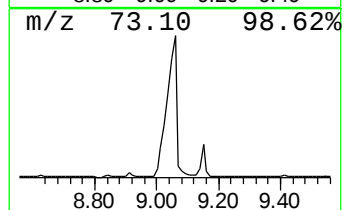
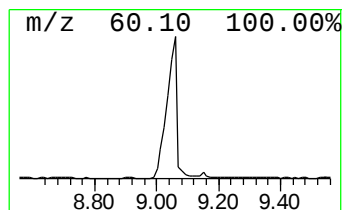
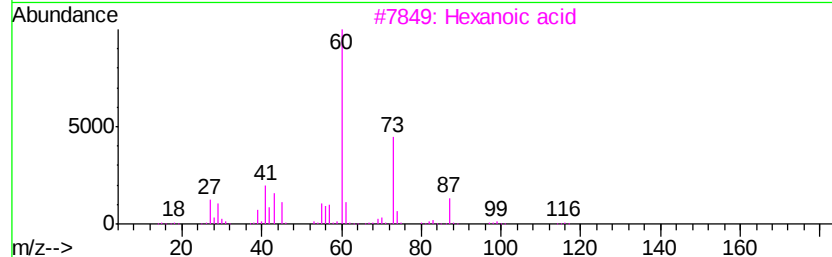
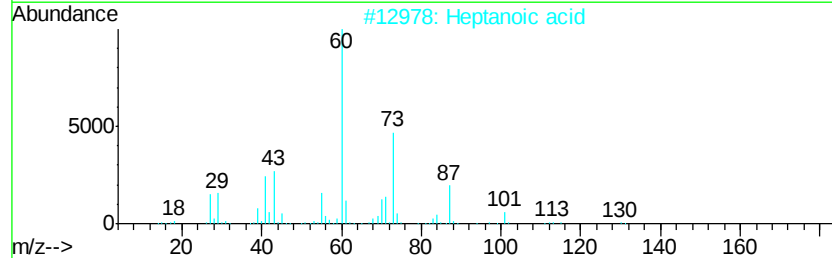
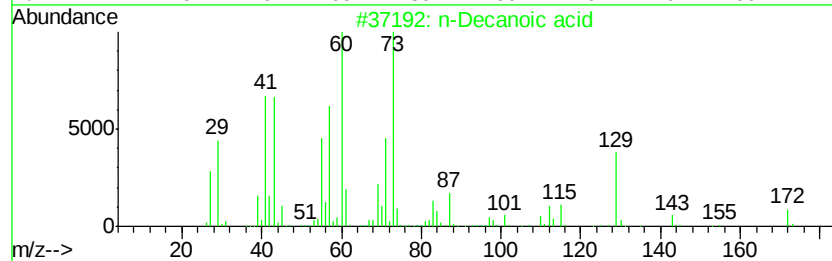
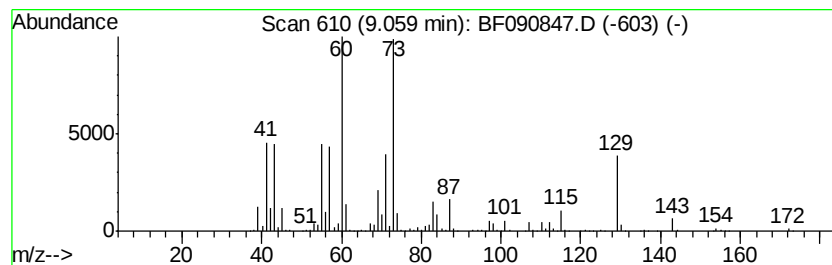
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 n-Decanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.06	40.12 ng	3755110	Acenaphthene-d10	9.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Decanoic acid	172	C10H20O2	000334-48-5	91
2		Heptanoic acid	130	C7H14O2	000111-14-8	43
3		Hexanoic acid	116	C6H12O2	000142-62-1	43
4		Alpha-l-rhamnopyranose	164	C6H12O5	035810-56-1	40
5		Pentanoic acid	102	C5H10O2	000109-52-4	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102616\
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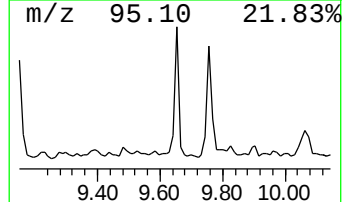
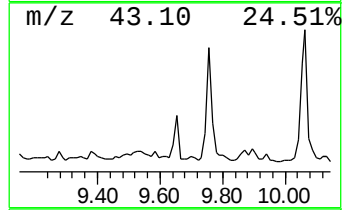
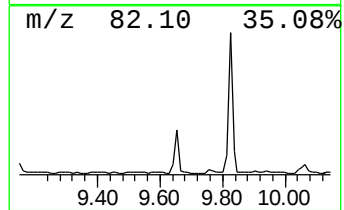
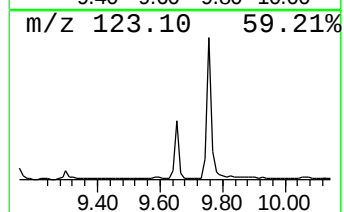
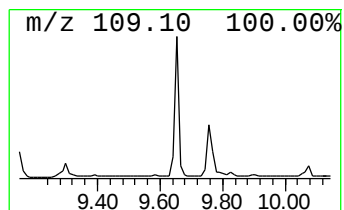
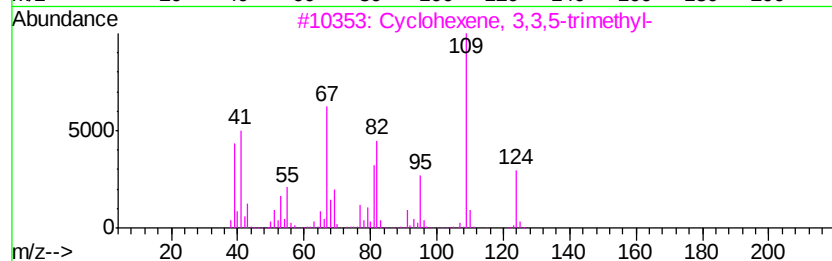
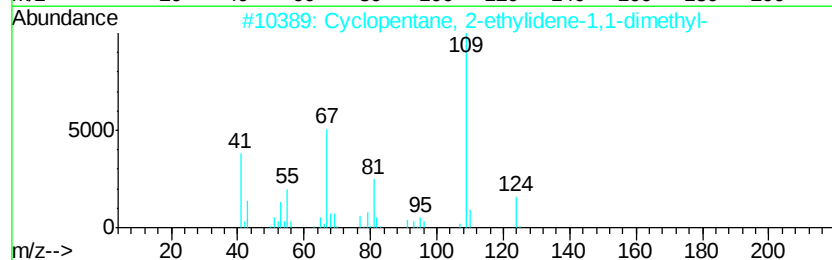
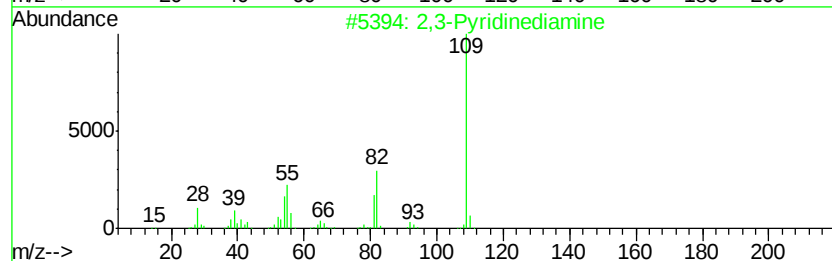
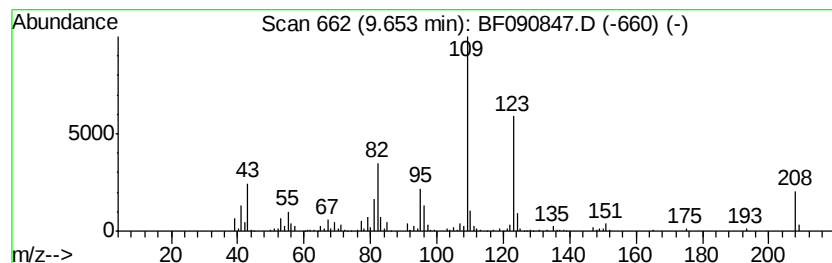
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 unknown9.65 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.65	2.16 ng	202411	Acenaphthene-d10	9.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,3-Pyridinediamine	109	C5H7N3	000452-58-4	38
2		Cyclopentane, 2-ethylidene-1,1-d...	124	C9H16	056324-66-4	38
3		Cyclohexene, 3,3,5-trimethyl-	124	C9H16	000503-45-7	38
4		6,6-Dimethylhepta-2,4-diene	124	C9H16	1000195-03-3	38
5		Diaminopyridine	109	C5H7N3	004318-76-7	35



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102616\
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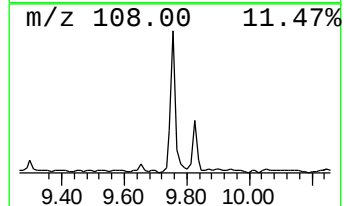
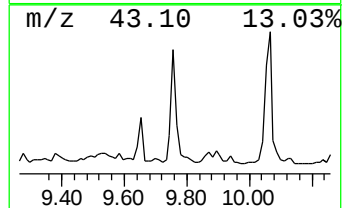
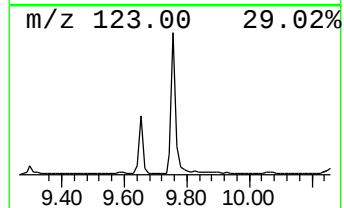
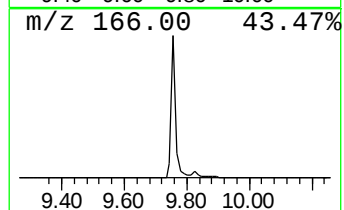
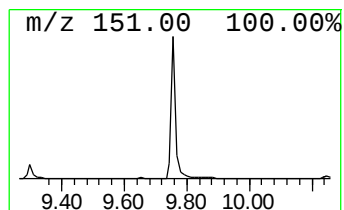
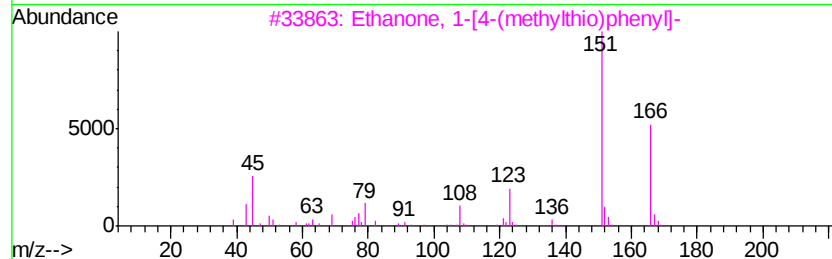
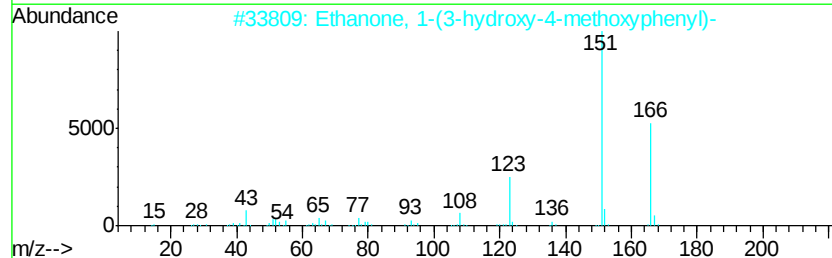
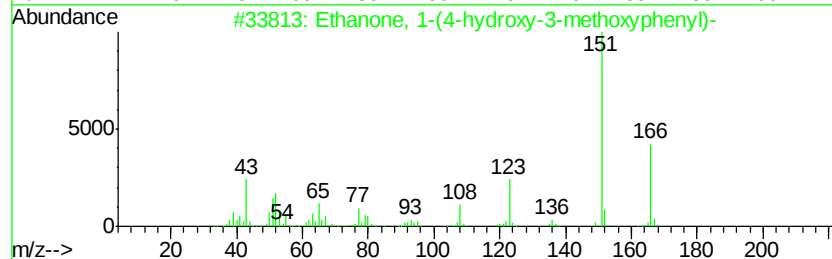
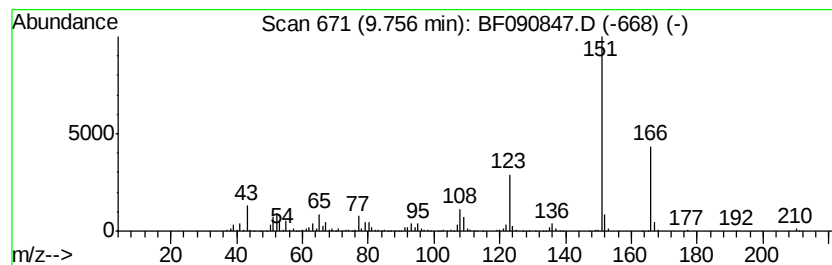
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Ethanone, 1-(4-hydroxy-3-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.76	9.49 ng	887879	Acenaphthene-d10	9.82

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanone, 1-(4-hydroxy-3-methoxy...	166	C9H10O3	000498-02-2	93
2			Ethanone, 1-(3-hydroxy-4-methoxy...	166	C9H10O3	006100-74-9	90
3			Ethanone, 1-[4-(methylthio)phenyl]-	166	C9H10OS	001778-09-2	80
4			4-Acetoxy-3-methoxyacetophenone	208	C11H12O4	054771-60-7	72
5			Ethanone, 1-(2-hydroxy-6-methoxy...	166	C9H10O3	000703-23-1	72



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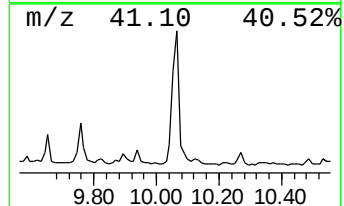
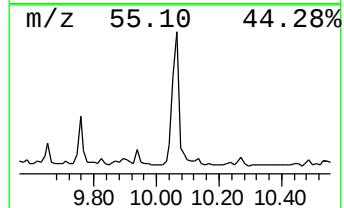
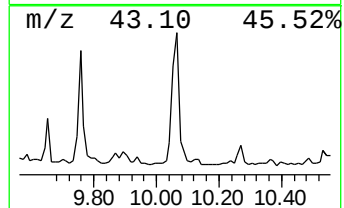
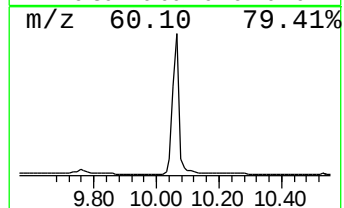
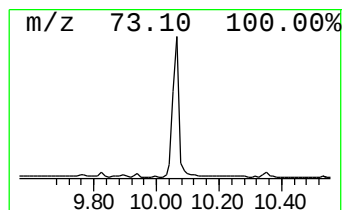
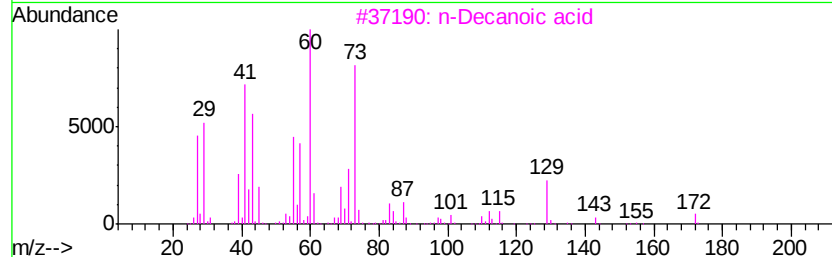
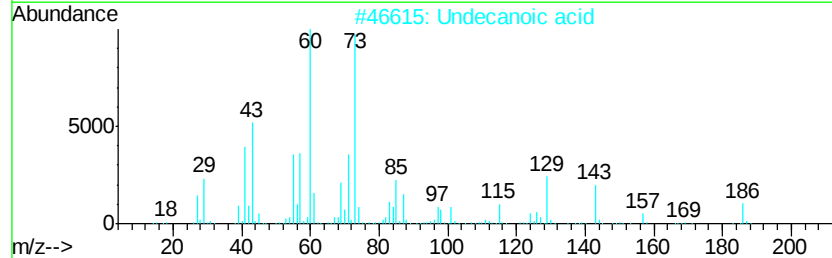
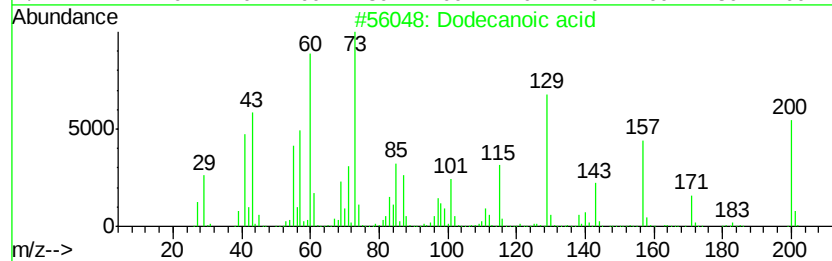
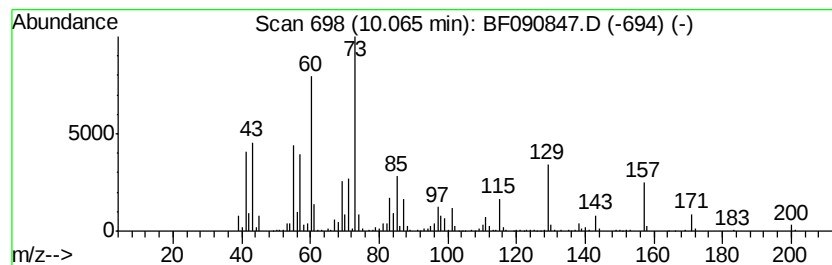
Instrument :
 BNA_F
 ClientSampleId :
 MW-105D

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF102616.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 19 Dodecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.06	9.32 ng	872452	Acenaphthene-d10		9.82
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	95
2	Undecanoic acid	186	C11H22O2	000112-37-8	72
3	n-Decanoic acid	172	C10H20O2	000334-48-5	64
4	Nonanoic acid	158	C9H18O2	000112-05-0	58
5	Methyl-.alpha.-d-ribofuranoside	164	C6H12O5	1000129-83-1	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102616\
Data File : BF090847.D
Acq On : 26 Oct 2016 18:34
Operator : UM/SJ
Sample : H5308-17
Misc :
ALS Vial : 6 Sample Multiplier: 1

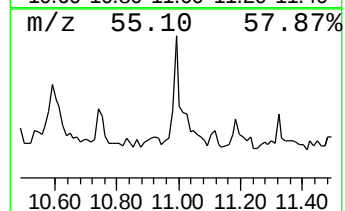
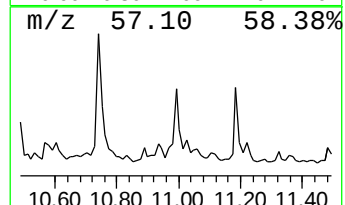
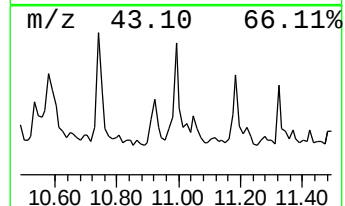
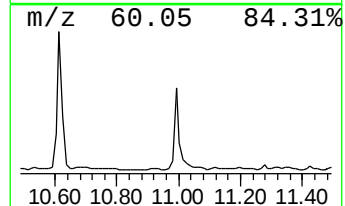
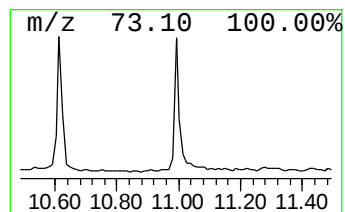
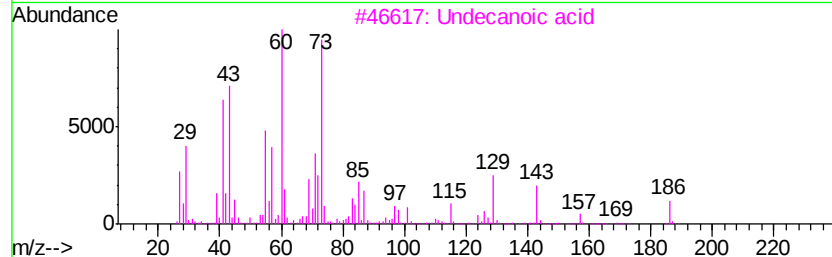
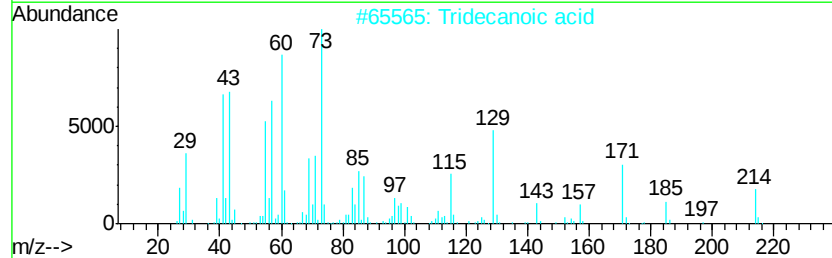
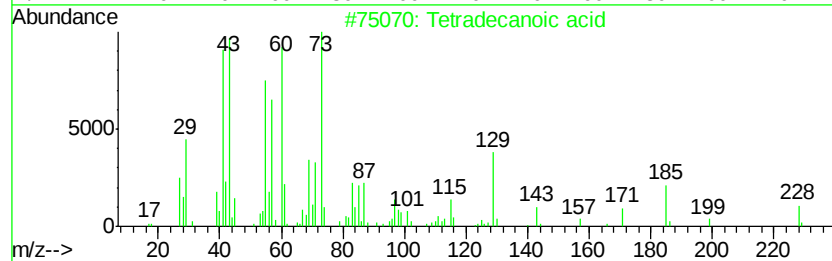
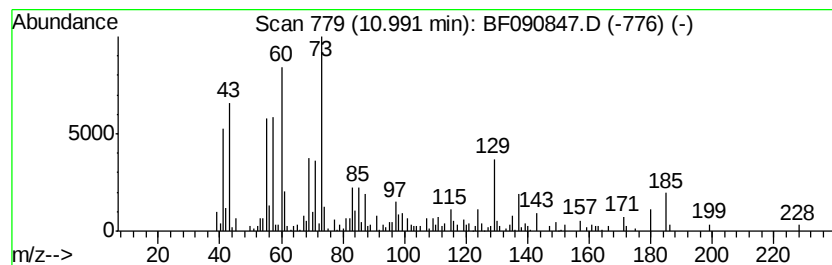
Instrument :
BNA_F
ClientSampleId :
MW-105D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Tetradecanoic acid Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.99	2.25 ng	215463	Phenanthrene-d10	11.31
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Tetradecanoic acid	228 C14H28O2	000544-63-8 87
2		Tridecanoic acid	214 C13H26O2	000638-53-9 72
3		Undecanoic acid	186 C11H22O2	000112-37-8 59
4		.alpha.-d-6,3-Furanose, methyl-....	192 C7H12O6	1000149-62-6 50
5		n-Decanoic acid	172 C10H20O2	000334-48-5 49



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102616\
 Data File : BF090847.D
 Acq On : 26 Oct 2016 18:34
 Operator : UM/SJ
 Sample : H5308-17
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-105D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.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
Propanoic acid, 2...	3.62	2.2	ng	141603	1	6.78	1282300	20.0
unknown4.21	4.21	2.1	ng	133830	1	6.78	1282300	20.0
2-Pentanone, 4-hy...	4.94	10.1	ng	647514	1	6.78	1282300	20.0
Butanoic acid, 3-...	5.12	5.8	ng	369053	1	6.78	1282300	20.0
Butanoic acid, 2-...	5.31	6.1	ng	393048	1	6.78	1282300	20.0
Cyclohexanol	5.55	5.7	ng	367935	1	6.78	1282300	20.0
Cyclohexanone	5.63	12.8	ng	820113	1	6.78	1282300	20.0
Pentanoic acid, 2...	6.19	15.3	ng	983128	1	6.78	1282300	20.0
unknown6.56	6.56	73.7	ng	4725100	1	6.78	1282300	20.0
1-Hexanol, 2-ethyl-	6.85	2.7	ng	173374	1	6.78	1282300	20.0
Cyclohexanecarbox...	7.57	6.4	ng	567166	2	8.08	1765860	20.0
Benzeneacetic acid	8.37	11.4	ng	1006080	2	8.08	1765860	20.0
Nonanoic acid	8.45	3.3	ng	287054	2	8.08	1765860	20.0
Benzenepropanoic ...	8.91	24.8	ng	2191930	2	8.08	1765860	20.0
n-Decanoic acid	9.06	40.1	ng	3755110	3	9.82	1871980	20.0
unknown9.65	9.65	2.2	ng	202411	3	9.82	1871980	20.0
Ethanone, 1-(4-hy...	9.76	9.5	ng	887879	3	9.82	1871980	20.0
Dodecanoic acid	10.06	9.3	ng	872452	3	9.82	1871980	20.0
Tetradecanoic acid	10.99	2.3	ng	215463	4	11.31	1917340	20.0