

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032117\
 Data File : BF093796.D
 Acq On : 21 Mar 2017 14:19
 Operator : SJ/MA
 Sample : I2263-14
 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-BF032017.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	2.081	14	17	22	rVB2	61947	102289	1.84%	0.215%
2	4.984	269	271	274	rBV	292079	375350	6.74%	0.789%
3	5.156	277	286	290	rVB	32070	85457	1.53%	0.180%
4	5.418	306	309	311	rBV	2243323	2052314	36.86%	4.313%
5	5.590	323	324	327	rVB	88243	119736	2.15%	0.252%
6	5.670	329	331	334	rVB	688328	650442	11.68%	1.367%
7	6.081	361	367	369	rBV	33834	69142	1.24%	0.145%
8	6.447	397	399	402	rVB2	1437562	1424323	25.58%	2.994%
9	6.596	409	412	414	rVB	3354343	4143639	74.43%	8.709%
10	6.824	430	432	434	rBV	1265382	1048045	18.82%	2.203%
11	6.893	437	438	443	rVV	83946	85009	1.53%	0.179%
12	6.984	443	446	448	rVV	4093801	3911363	70.25%	8.221%
13	7.076	450	454	456	rBV2	354324	386444	6.94%	0.812%
14	7.224	464	467	469	rBV	223140	269871	4.85%	0.567%
15	7.384	478	481	483	rBV	2713559	3086815	55.44%	6.488%
16	7.430	483	485	488	rVV	131400	165586	2.97%	0.348%
17	7.499	488	491	493	rVV2	50199	103641	1.86%	0.218%
18	7.544	493	495	499	rVB3	45730	100390	1.80%	0.211%
19	7.636	500	503	505	rBV3	33257	60884	1.09%	0.128%
20	7.887	518	525	526	rBV3	451777	1030470	18.51%	2.166%
21	7.922	526	528	529	rVV	110293	156502	2.81%	0.329%
22	7.967	529	532	535	rVB2	89420	175317	3.15%	0.368%
23	8.024	535	537	538	rBV	62544	82627	1.48%	0.174%
24	8.104	542	544	547	rVV	1132558	1405341	25.24%	2.954%
25	8.162	547	549	551	rVB	73991	71648	1.29%	0.151%
26	8.219	551	554	559	rBV3	59112	159135	2.86%	0.334%
27	8.356	562	566	567	rBV2	86037	147880	2.66%	0.311%
28	8.379	567	568	570	rVV	122080	125552	2.26%	0.264%
29	8.413	570	571	572	rVB	369660	253402	4.55%	0.533%
30	8.470	572	576	579	rBV	144391	245096	4.40%	0.515%
31	8.527	579	581	583	rBV2	107106	222538	4.00%	0.468%
32	8.653	589	592	593	rBV2	55276	98496	1.77%	0.207%
33	8.745	598	600	601	rVB	77237	63360	1.14%	0.133%
34	8.802	604	605	608	rVB	113589	100351	1.80%	0.211%

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35	8.893	611	613	616	rVB	175886	167265	3.00%	0.352%
36	9.042	622	626	629	rBV	525174	725461	13.03%	1.525%
37	9.190	636	639	641	rVB	5496360	5567498	100.00%	11.701%
38	9.316	647	650	652	rBV	63058	62681	1.13%	0.132%
39	9.373	652	655	656	rBV	117445	112056	2.01%	0.236%
40	9.476	661	664	667	rBV3	29451	60428	1.09%	0.127%
41	9.625	676	677	681	rVB	277779	315454	5.67%	0.663%
42	9.693	681	683	684	rVV	86560	104534	1.88%	0.220%
43	9.785	687	691	693	rVV	367975	526360	9.45%	1.106%
44	9.865	695	698	700	rVB	1597518	1651619	29.67%	3.471%
45	9.968	705	707	708	rVB	112636	98892	1.78%	0.208%
46	10.082	711	717	720	rBV	563012	672882	12.09%	1.414%
47	10.196	725	727	728	rVV2	84130	120904	2.17%	0.254%
48	10.230	728	730	733	rVV2	113360	164683	2.96%	0.346%
49	10.288	733	735	738	rVB2	36082	67771	1.22%	0.142%
50	10.379	740	743	746	rVB2	74569	112110	2.01%	0.236%
51	10.608	758	763	764	rBV2	145658	220051	3.95%	0.462%
52	10.642	764	766	769	rVV2	2283170	3092320	55.54%	6.499%
53	10.733	772	774	777	rVV2	180459	250539	4.50%	0.527%
54	10.779	777	778	781	rVB2	74102	88235	1.58%	0.185%
55	10.939	790	792	794	rBV2	81270	118853	2.13%	0.250%
56	11.019	796	799	800	rVV2	131773	169351	3.04%	0.356%
57	11.053	800	802	804	rVV	86997	145644	2.62%	0.306%
58	11.088	804	805	807	rVB	70106	70526	1.27%	0.148%
59	11.225	816	817	819	rVB	213463	183548	3.30%	0.386%
60	11.339	824	827	829	rVV	1779172	1608968	28.90%	3.382%
61	11.431	833	835	840	rVB4	29839	63028	1.13%	0.132%
62	11.876	872	874	876	rBV	225177	248292	4.46%	0.522%
63	11.922	876	878	884	rVB3	52107	102889	1.85%	0.216%
64	12.036	885	888	892	rVB	191227	235058	4.22%	0.494%
65	12.391	917	919	921	rBV	97366	83788	1.50%	0.176%
66	12.665	940	943	950	rVB	334016	382541	6.87%	0.804%
67	12.928	963	966	968	rBV	4595413	4801037	86.23%	10.090%
68	13.831	1042	1045	1048	rBV2	44239	64146	1.15%	0.135%
69	13.968	1054	1057	1059	rBV	1037319	1192076	21.41%	2.505%
70	14.162	1072	1074	1079	rVB	161807	178519	3.21%	0.375%
71	14.562	1107	1109	1112	rBV	144443	155663	2.80%	0.327%

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72	15.374	1177	1180	1182	rBV	620981	854942	15.36%	1.797%
73	15.728	1208	1211	1218	rBV	40207	75085	1.35%	0.158%
74	16.494	1275	1278	1283	rVB	45055	86300	1.55%	0.181%

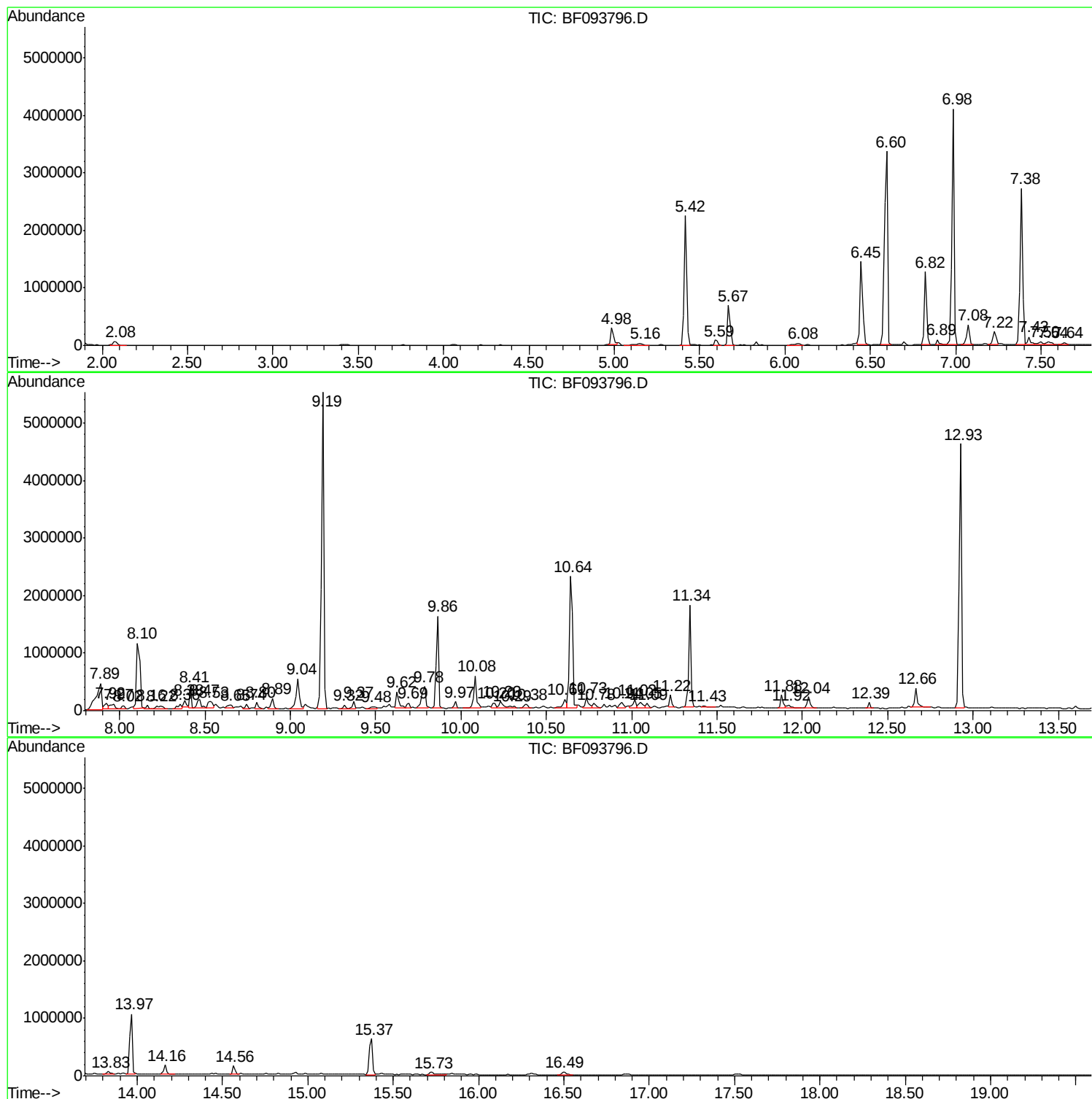
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Instrument :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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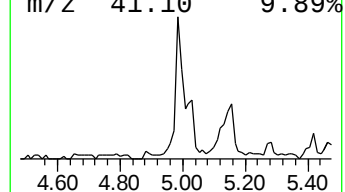
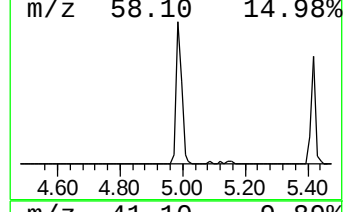
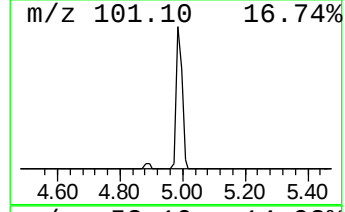
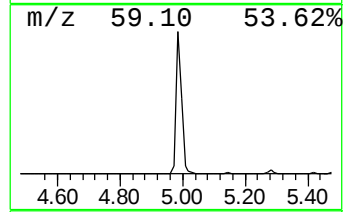
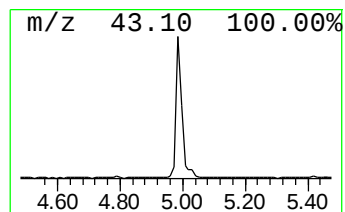
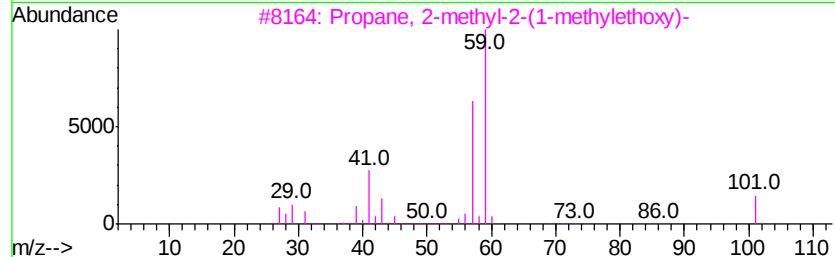
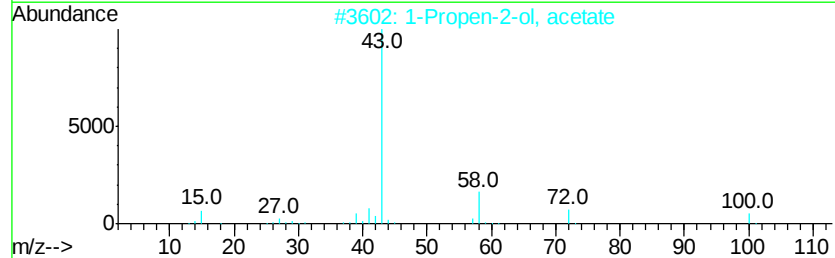
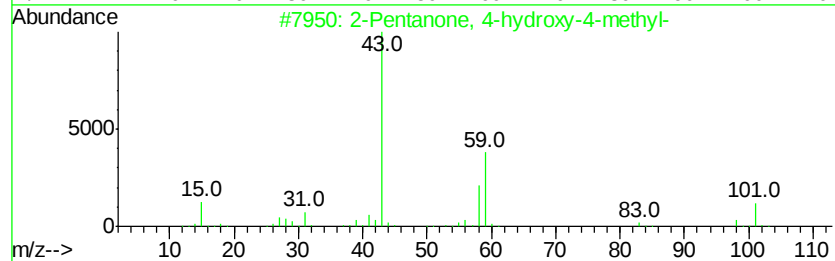
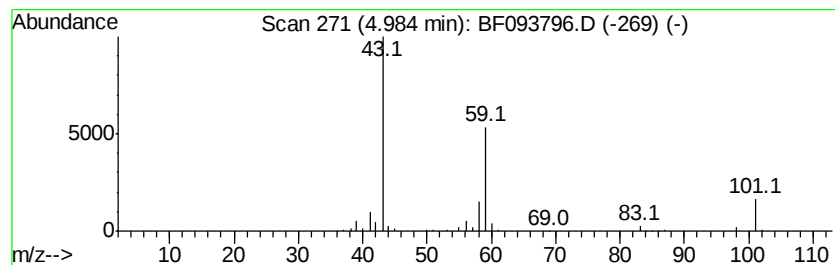
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.98	7.16 ng	375350	1,4-Dichlorobenzene-d4	6.82

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3			Propane, 2-methyl-2-(1-methylethyl)-	116	C7H16O	017348-59-3	10
4			3,3-Dimethylbutylamine	101	C6H15N	015673-00-4	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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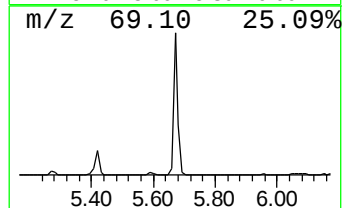
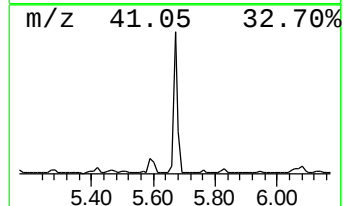
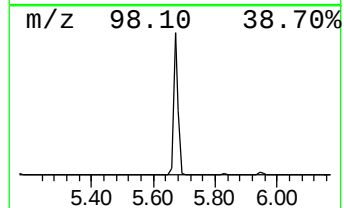
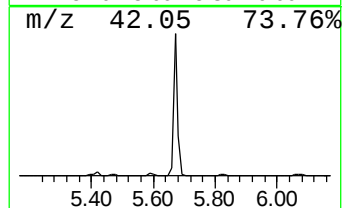
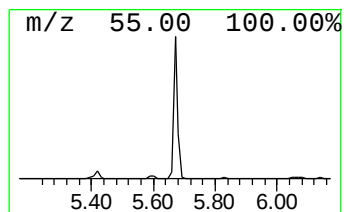
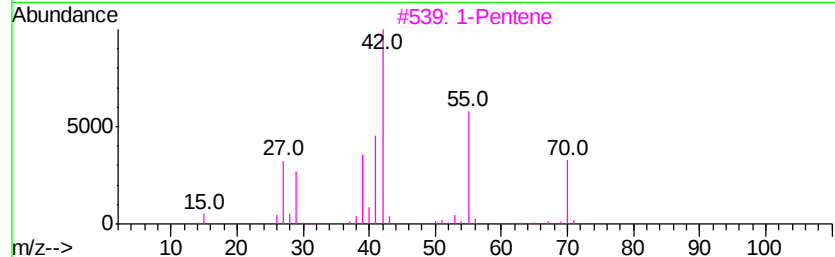
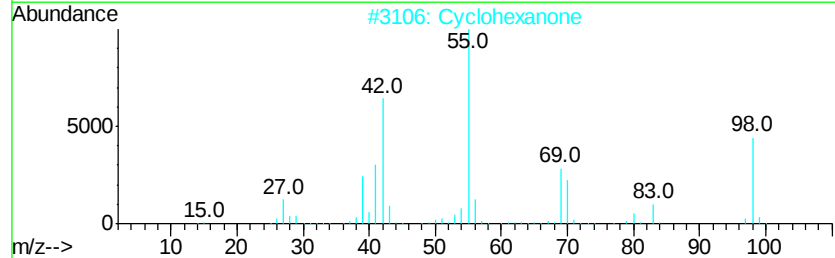
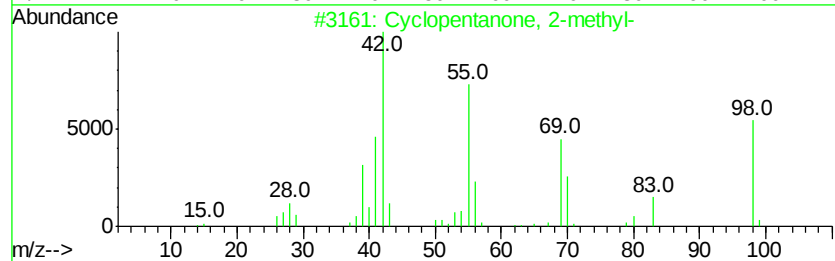
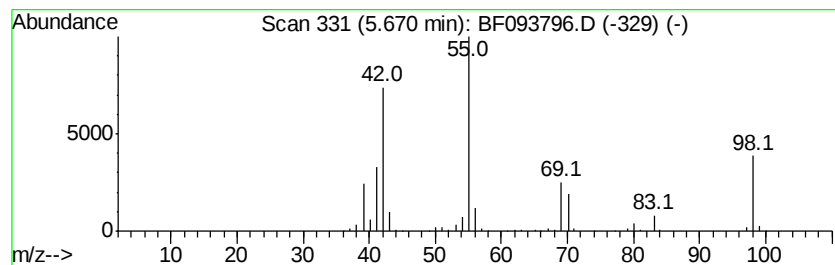
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Cyclopentanone, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.67	12.41 ng	650442	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentanone, 2-methyl-	98	C6H10O	001120-72-5	95
2		Cyclohexanone	98	C6H10O	000108-94-1	93
3		1-Pentene	70	C5H10	000109-67-1	46
4		2-Pentene, (Z)-	70	C5H10	000627-20-3	40
5		2-Pentene	70	C5H10	000109-68-2	40



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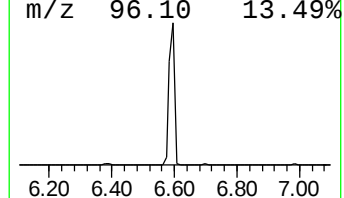
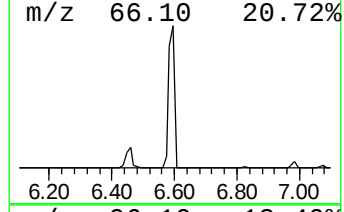
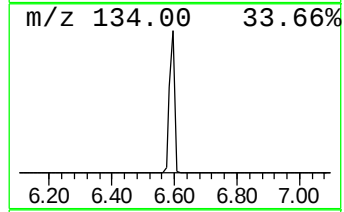
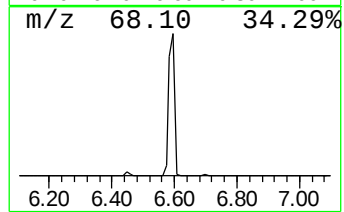
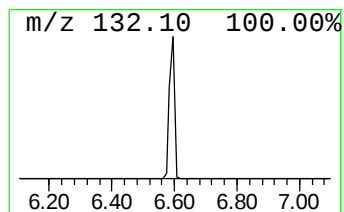
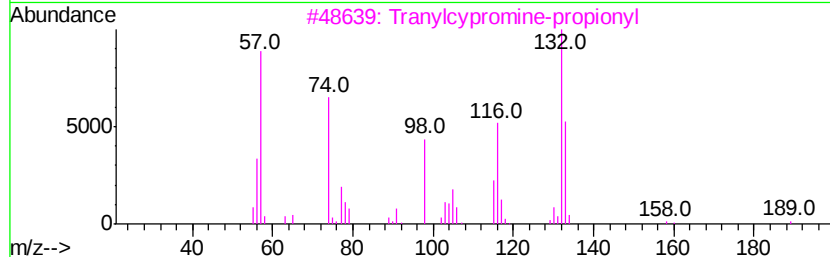
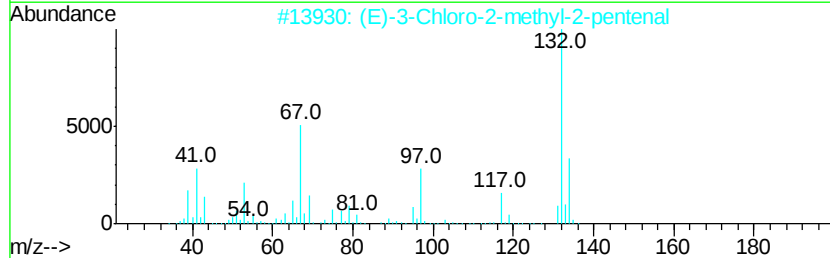
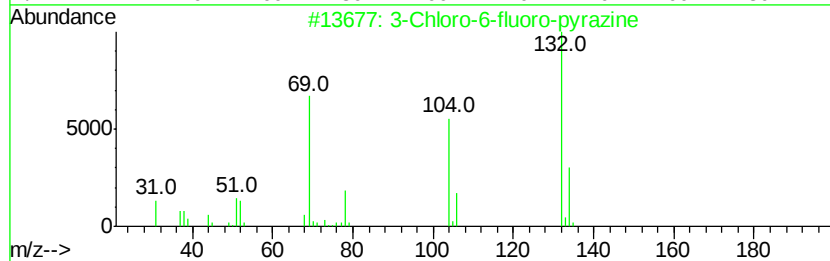
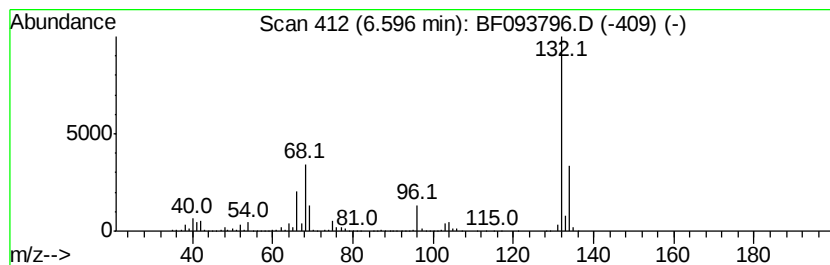
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	79.07 ng	4143640	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropane-propionyl	189	C12H15NO	1000123-86-3	16
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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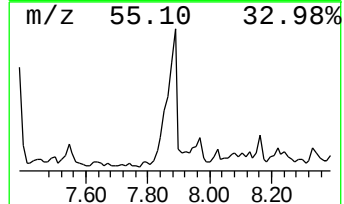
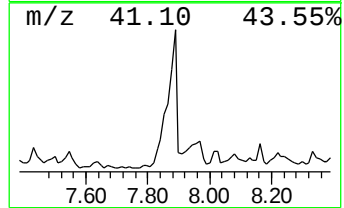
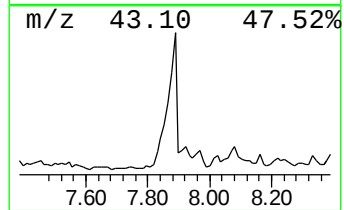
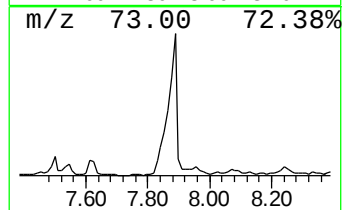
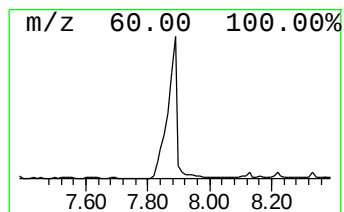
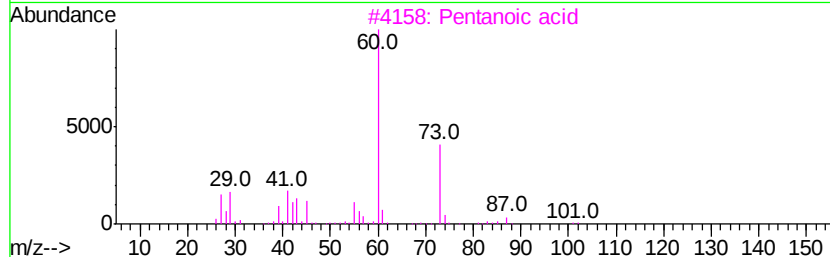
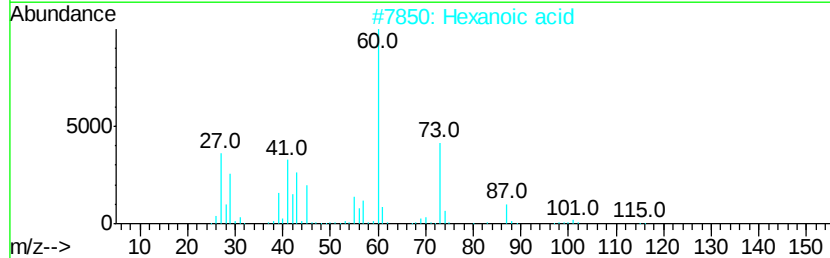
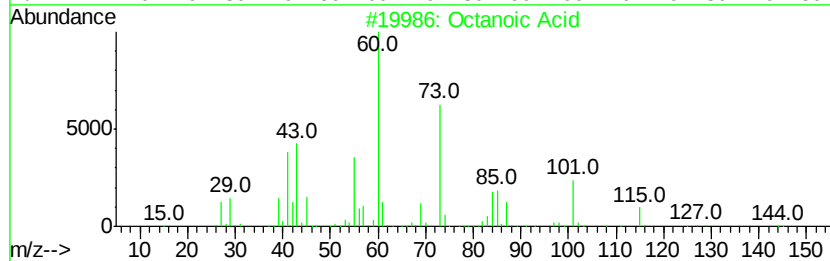
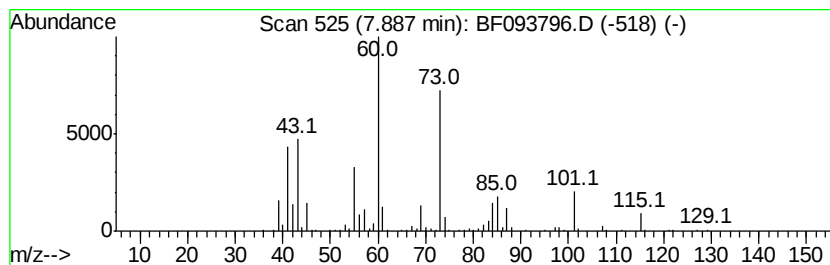
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octanoic Acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.89	14.67 ng	1030470	Napthalene-d8	8.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octanoic Acid	144	C8H16O2	000124-07-2	91
2		Hexanoic acid	116	C6H12O2	000142-62-1	53
3		Pentanoic acid	102	C5H10O2	000109-52-4	50
4		Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	50
5		Butanoic acid	88	C4H8O2	000107-92-6	47



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Data File : BF093796.D
Acq On : 21 Mar 2017 14:19
Operator : SJ/MA
Sample : I2263-14
Misc :
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Instrument :
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ClientSampleId :
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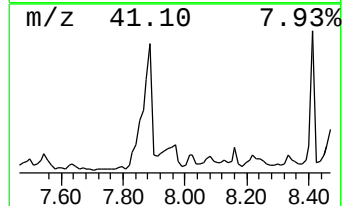
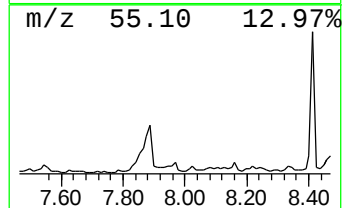
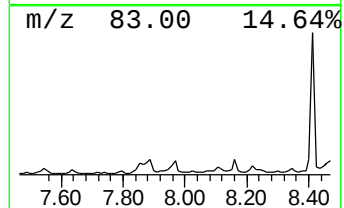
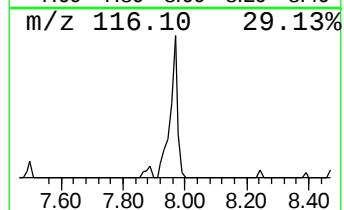
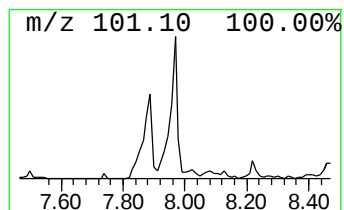
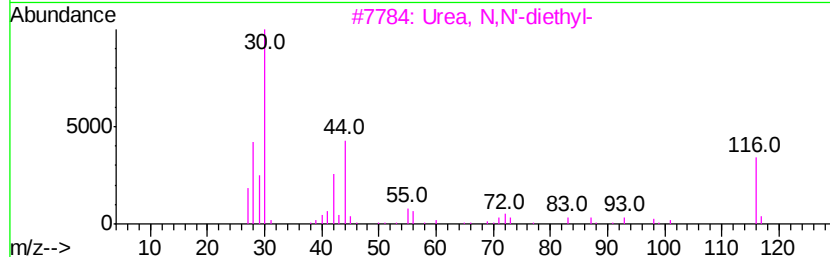
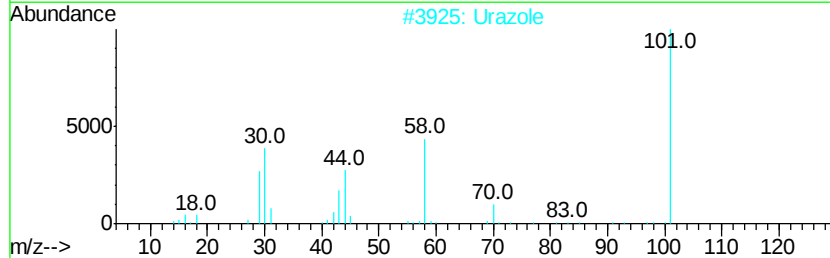
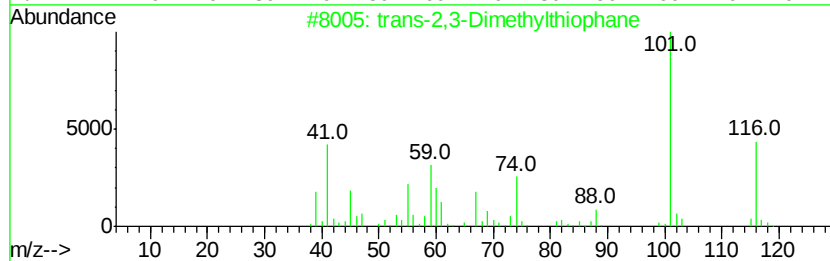
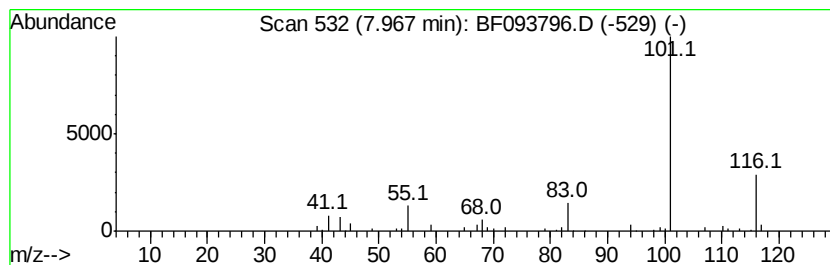
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown7.97 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.97	2.50 ng	175317	Naphthalene-d8	8.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	trans-2,3-Dimethylthiophane	116	C6H12S	005161-78-4	9
2		Urazole	101	C2H3N3O2	003232-84-6	7
3		Urea, N,N'-diethyl-	116	C5H12N2O	000623-76-7	5
4		Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-14-8	5
5		Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-13-7	5



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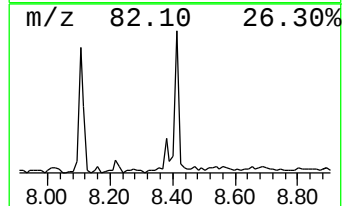
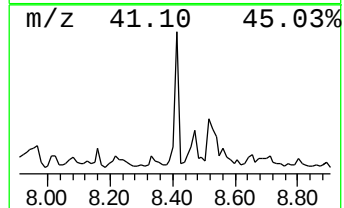
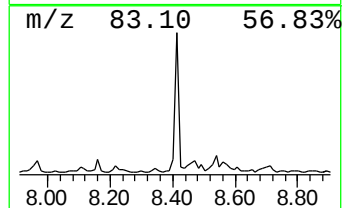
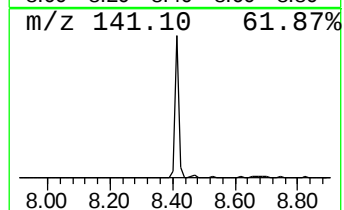
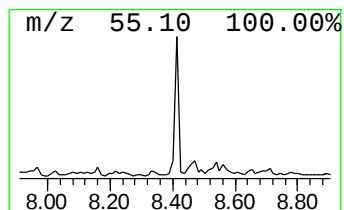
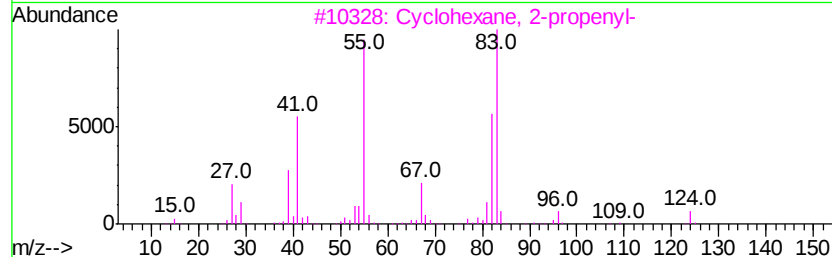
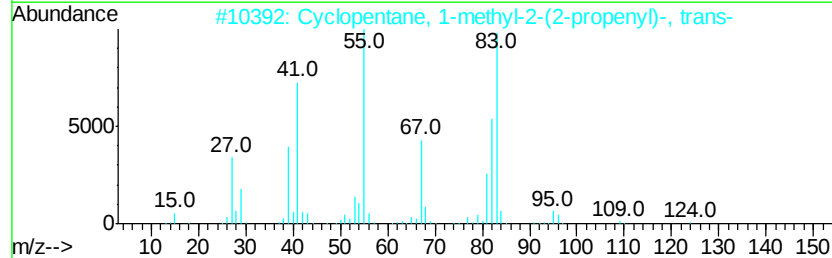
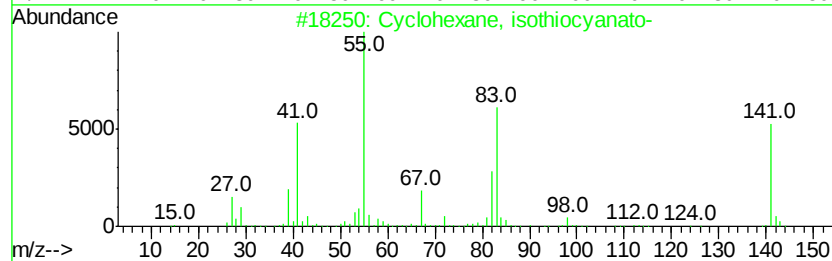
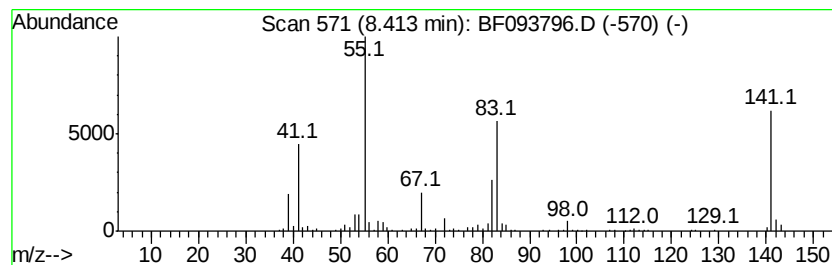
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Cyclohexane, isothiocyanato- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.41	3.61 ng	253402	Naphthalene-d8	8.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, isothiocyanato-	141	C7H11NS	001122-82-3	97
2		Cyclopentane, 1-methyl-2-(2-propenyl)-, trans-	124	C9H16	050746-53-7	46
3		Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	38
4		1-Hexene, 6-bromo-	162	C6H11Br	002695-47-8	38
5		Cyclohexane, bromo-	162	C6H11Br	000108-85-0	35



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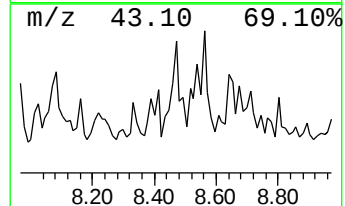
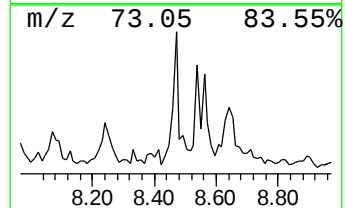
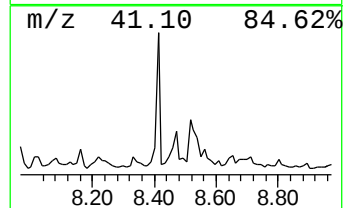
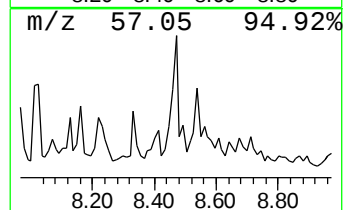
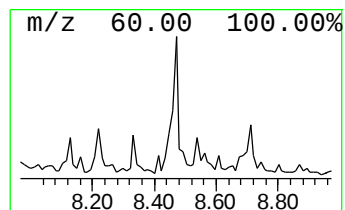
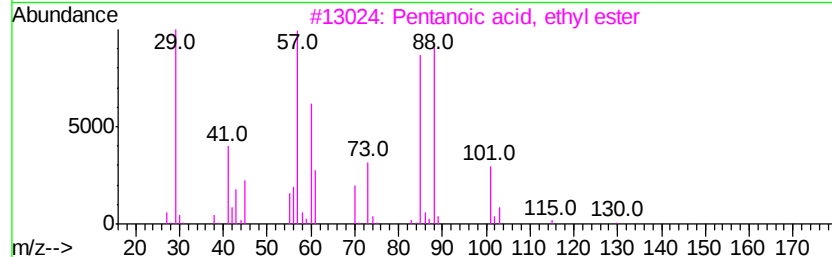
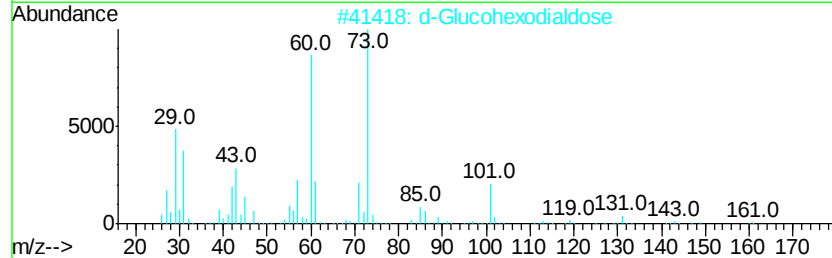
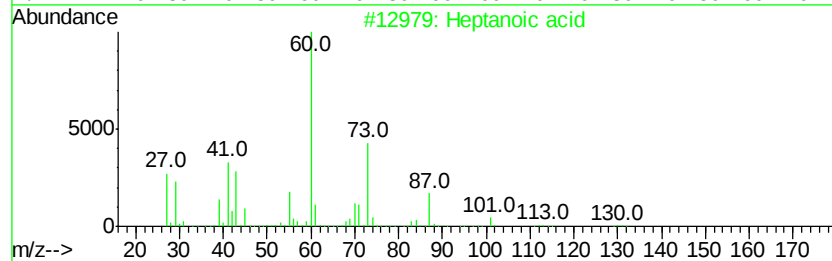
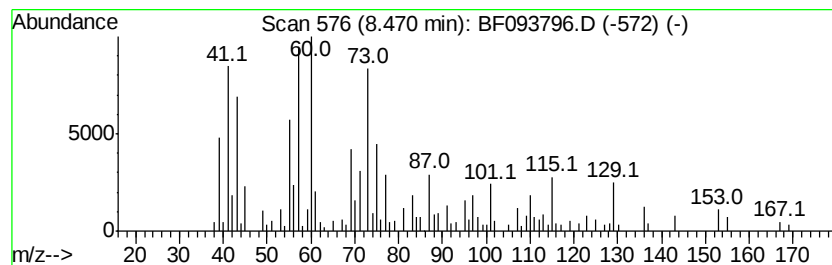
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown8.47 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.47	3.49 ng	245096	Napthalene-d8	8.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptanoic acid	130	C7H14O2	000111-14-8	38
2		d-Glucohexodialdose	178	C6H10O6	1000149-19-1	37
3		Pentanoic acid, ethyl ester	130	C7H14O2	000539-82-2	27
4		1-(p-Toluidino)-1-deoxy-.beta.-d...	269	C13H19NO5	1000226-06-4	25
5		l-Tyrosinol	167	C9H13NO2	1000131-27-0	22



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032117\
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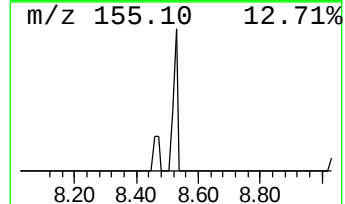
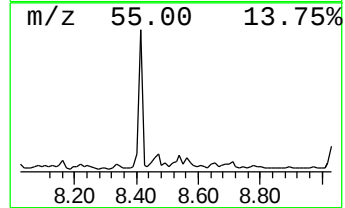
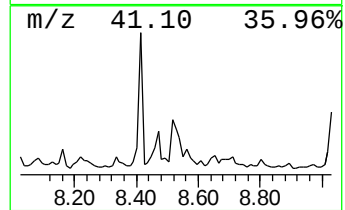
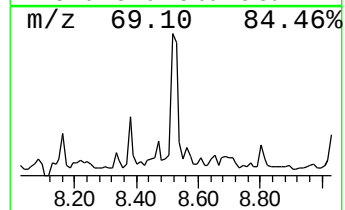
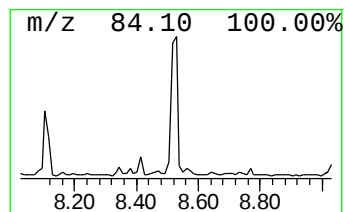
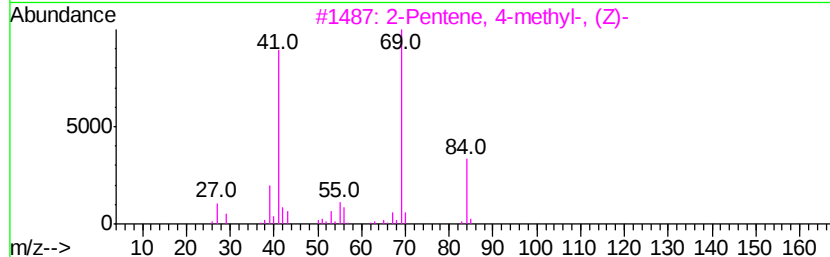
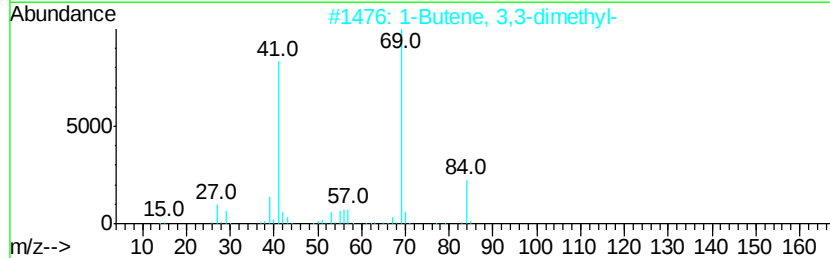
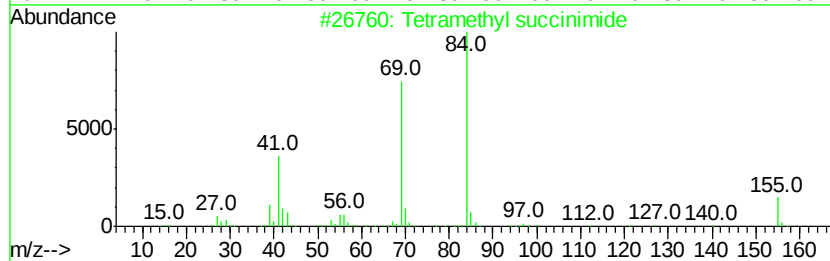
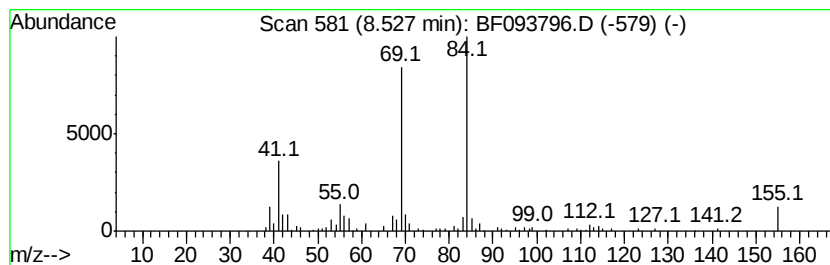
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetramethyl succinimide Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.53	3.17 ng	222538	Naphthalene-d8	8.10

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetramethyl succinimide	155	C8H13NO2	003566-61-8	80
2			1-Butene, 3,3-dimethyl-	84	C6H12	000558-37-2	72
3			2-Pentene, 4-methyl-, (Z)-	84	C6H12	000691-38-3	64
4			Pyrrolidin-2-one, 5-pentyl-	155	C9H17NO	003817-18-3	38
5			2-Azetidinone, 3,3,4,4-tetramethyl-	127	C7H13NO	013423-22-8	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032117\
Data File : BF093796.D
Acq On : 21 Mar 2017 14:19
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Misc :
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ClientSampleId :
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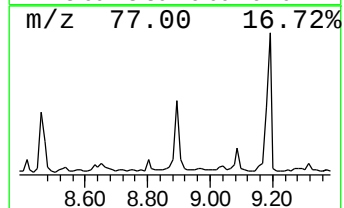
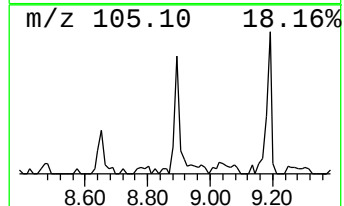
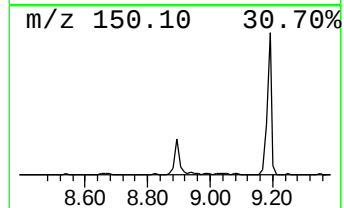
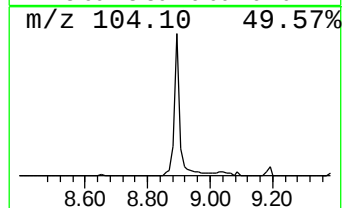
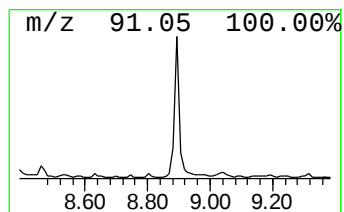
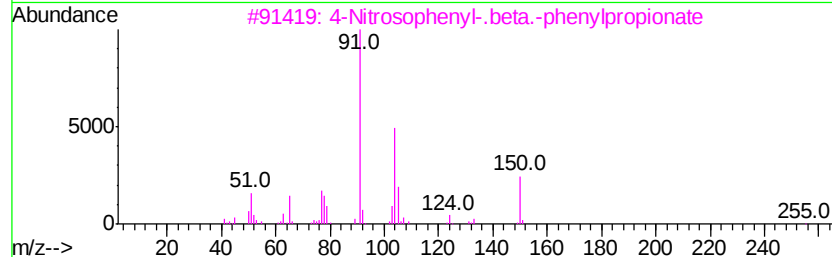
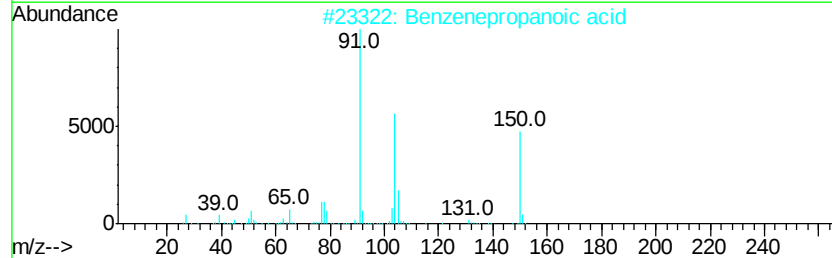
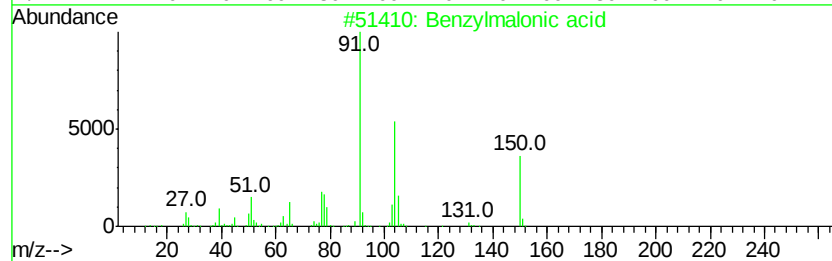
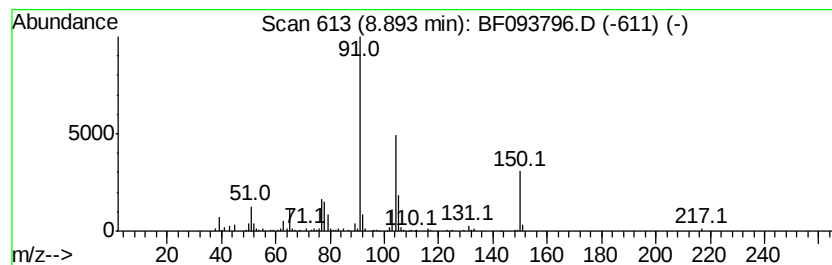
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Benzylmalonic acid Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.89	2.38 ng	167265	Naphthalene-d8	8.10

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzylmalonic acid	194	C10H10O4	000616-75-1	91
2			Benzenepropanoic acid	150	C9H10O2	000501-52-0	90
3			4-Nitrosophenyl-.beta.-phenylpro...	255	C15H13NO3	1000129-40-0	86
4			3-Phenyl-propionic acid, isoprop...	192	C12H16O2	022767-95-9	64
5			Benzeneacetic acid, methyl ester	150	C9H10O2	000101-41-7	38



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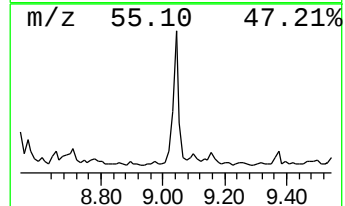
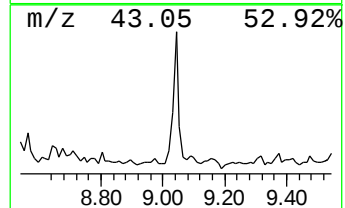
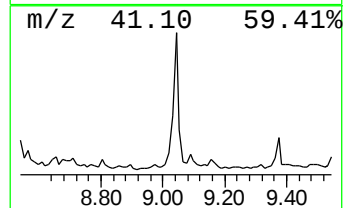
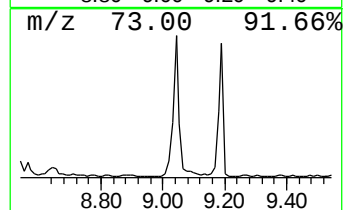
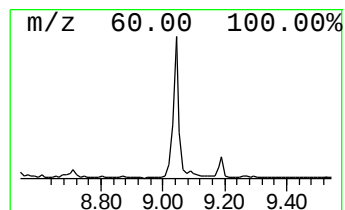
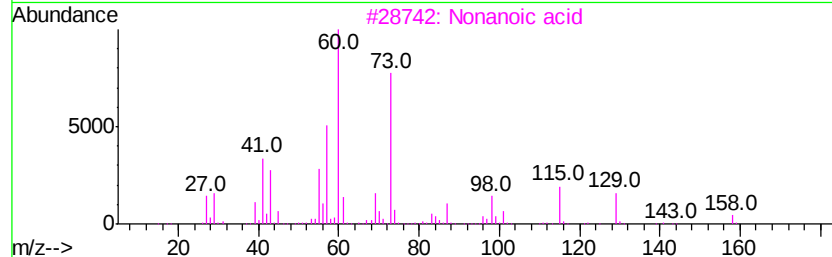
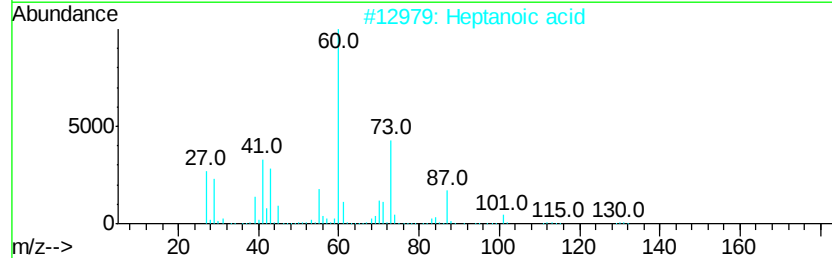
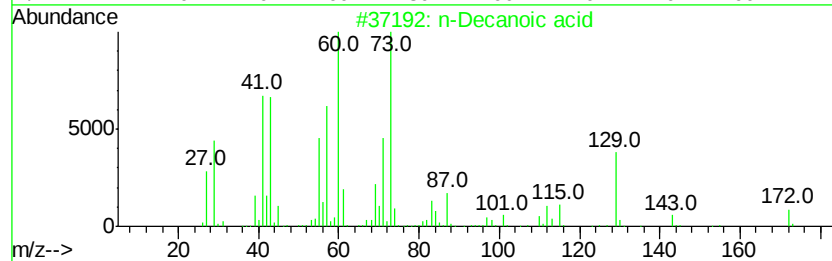
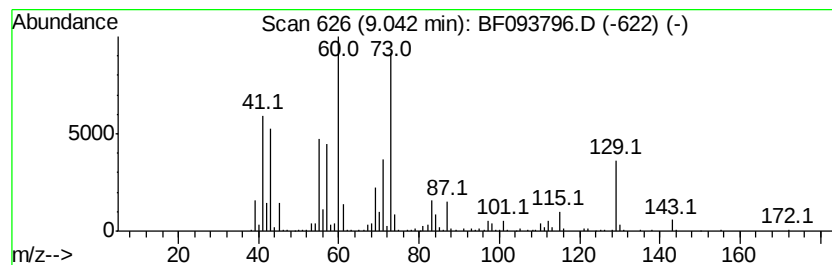
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 n-Decanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.04	8.78 ng	725461	Acenaphthene-d10	9.86

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	53
3		Nonanoic acid	158	C9H18O2	000112-05-0	53
4		Octanoic Acid	144	C8H16O2	000124-07-2	50
5		Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	50



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ClientSampleId :
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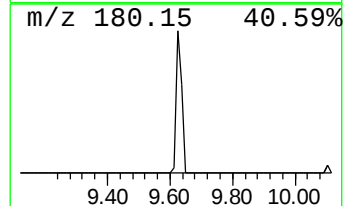
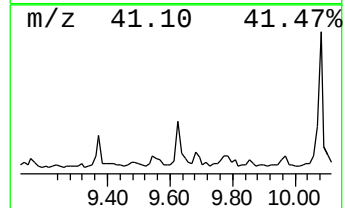
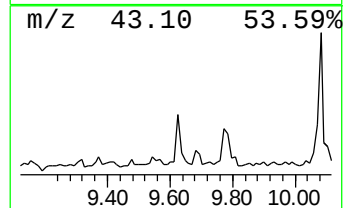
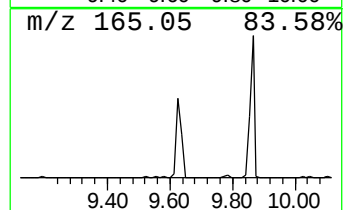
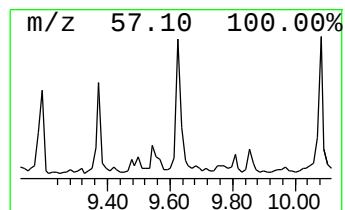
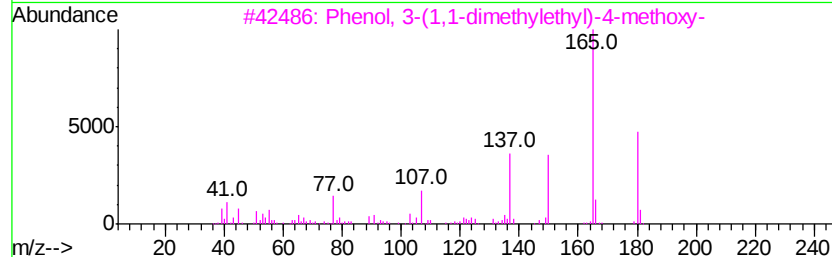
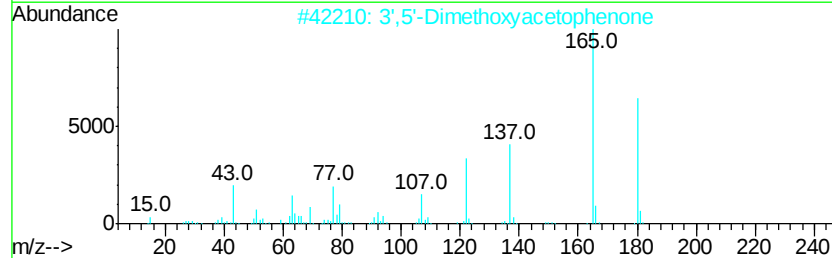
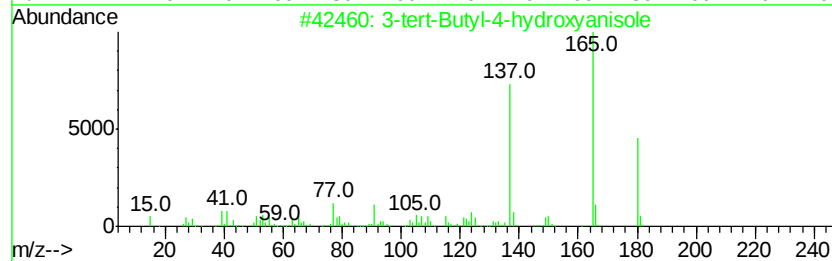
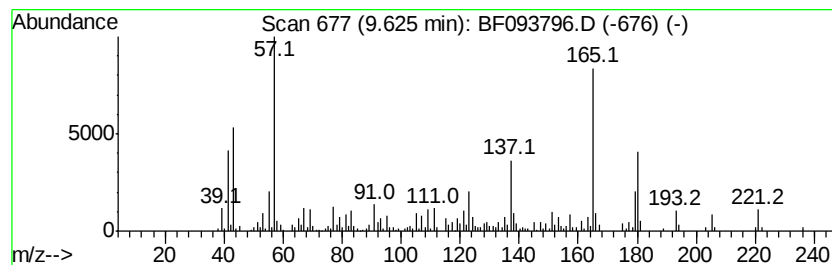
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 3-tert-Butyl-4-hydroxyanisole Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.62	3.82 ng	315454	Acenaphthene-d10	9.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-tert-Butyl-4-hydroxyanisole	180	C11H16O2	000121-00-6	64
2			3',5'-Dimethoxyacetophenone	180	C10H12O3	039151-19-4	58
3			Phenol, 3-(1,1-dimethylethyl)-4-...	180	C11H16O2	000088-32-4	58
4			Benzenamine, N-ethyl-N-methyl-4-...	180	C9H12N2O2	056269-48-8	55
5			Ethanone, 1-(2,5-dimethoxyphenyl)-	180	C10H12O3	001201-38-3	55



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032117\
Data File : BF093796.D
Acq On : 21 Mar 2017 14:19
Operator : SJ/MA
Sample : I2263-14
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-105D

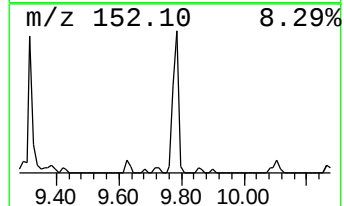
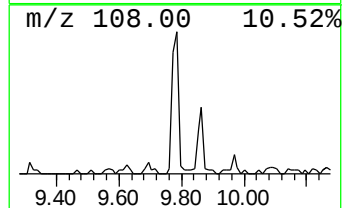
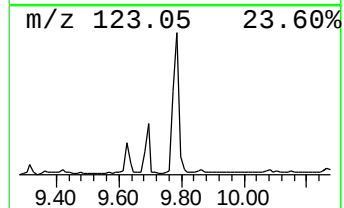
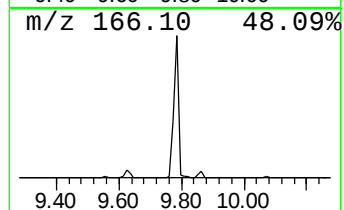
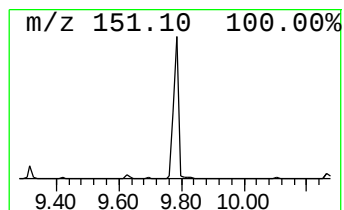
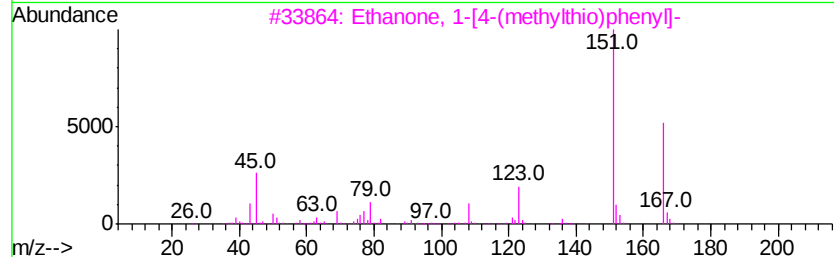
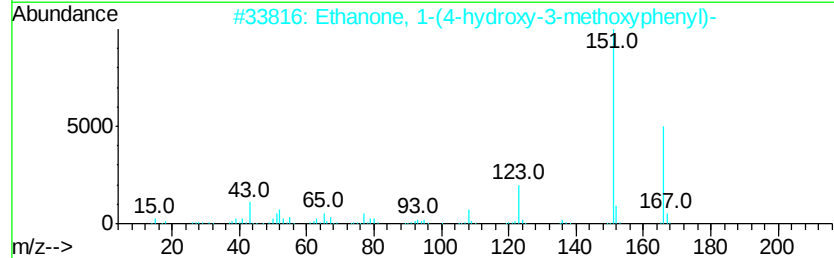
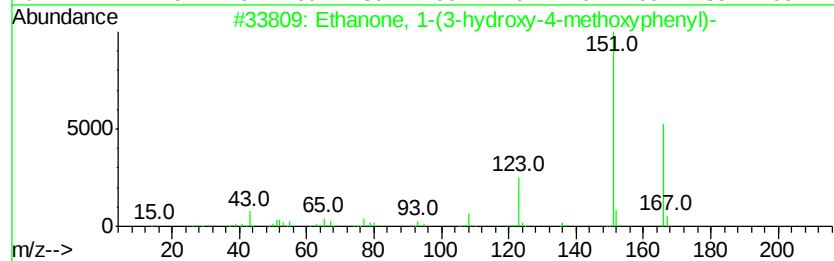
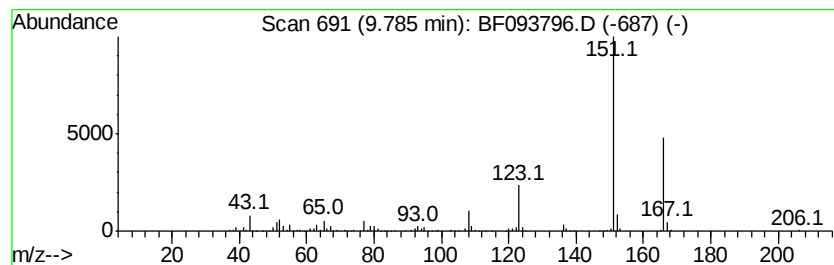
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Ethanone, 1-(3-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.78	6.37 ng	526360	Acenaphthene-d10	9.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanone, 1-(3-hydroxy-4-methoxy...	166	C9H10O3	006100-74-9	97
2		Ethanone, 1-(4-hydroxy-3-methoxy...	166	C9H10O3	000498-02-2	97
3		Ethanone, 1-[4-(methylthio)phenyl]-	166	C9H10OS	001778-09-2	90
4		Ethanone, 1-(2-hydroxy-6-methoxy...	166	C9H10O3	000703-23-1	80
5		Stibine, trimethyl-	166	C3H9Sb	000594-10-5	78



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032117\
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Acq On : 21 Mar 2017 14:19
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Sample : I2263-14
Misc :
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ClientSampleId :
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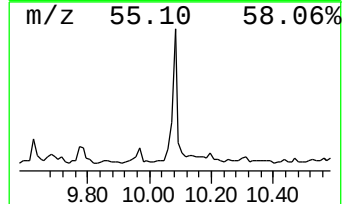
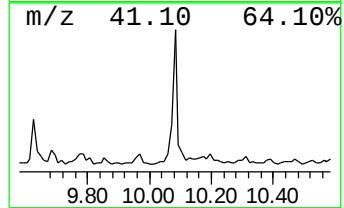
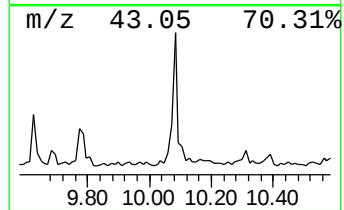
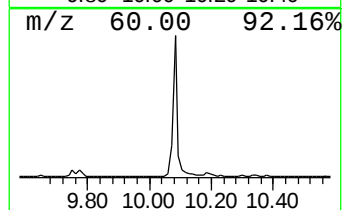
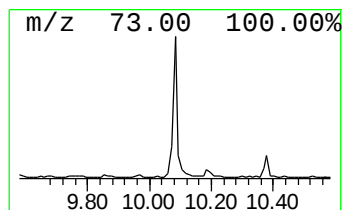
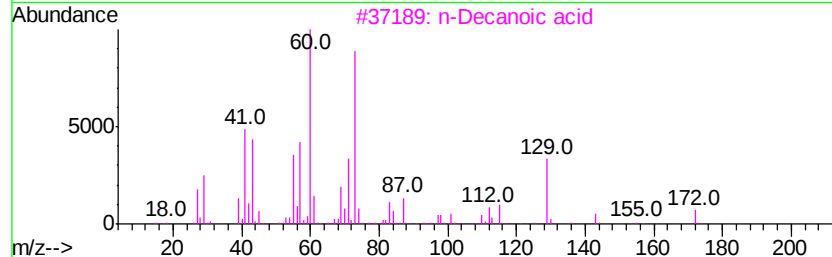
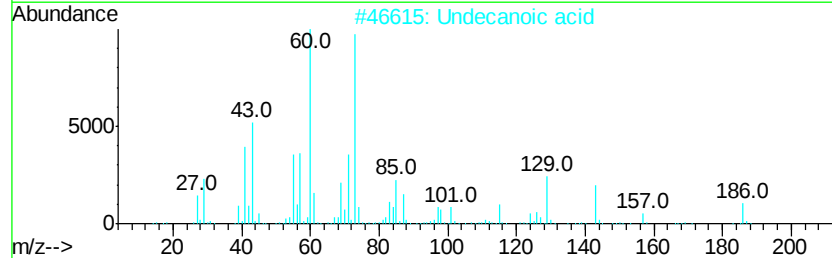
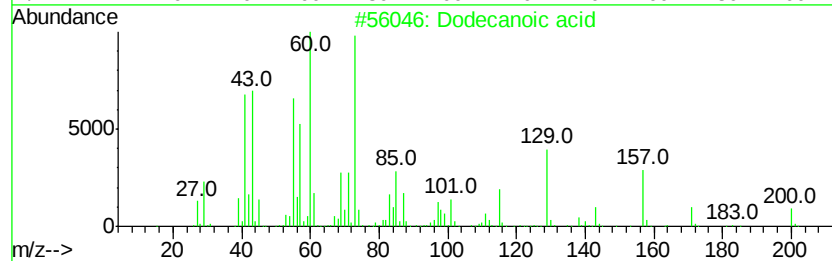
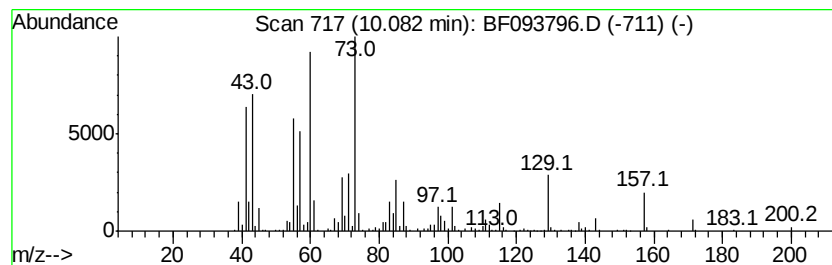
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Dodecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.08	8.15 ng	672882	Acenaphthene-d10	9.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecanoic acid	200	C12H24O2	000143-07-7	95
2		Undecanoic acid	186	C11H22O2	000112-37-8	86
3		n-Decanoic acid	172	C10H20O2	000334-48-5	59
4		Hexanoic acid	116	C6H12O2	000142-62-1	38
5		Butanoic acid	88	C4H8O2	000107-92-6	35



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Acq On : 21 Mar 2017 14:19
Operator : SJ/MA
Sample : I2263-14
Misc :
ALS Vial : 6 Sample Multiplier: 1

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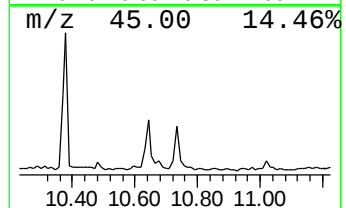
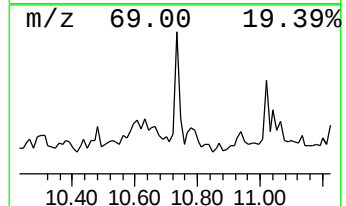
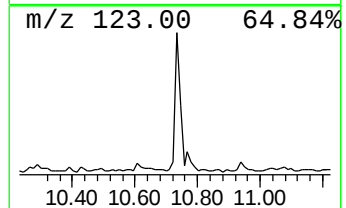
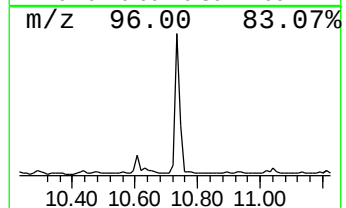
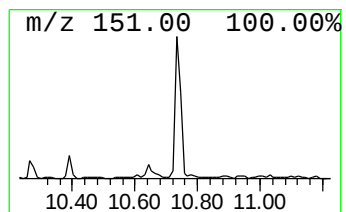
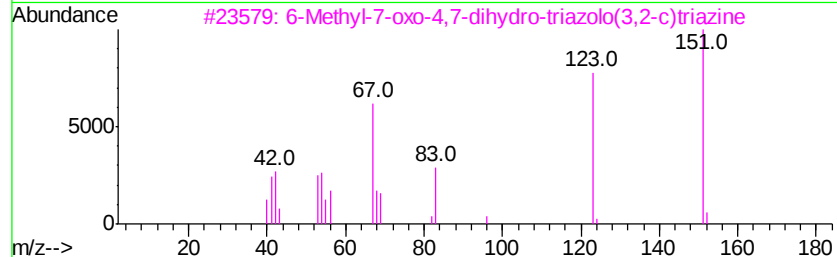
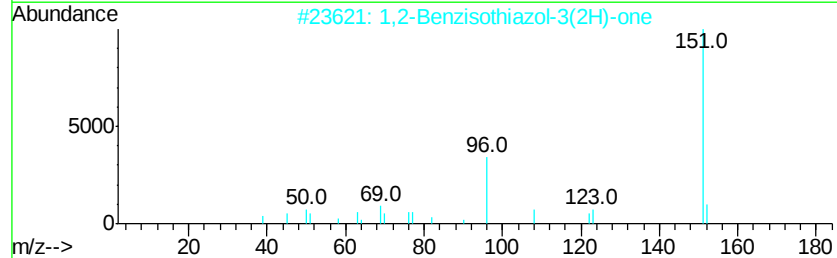
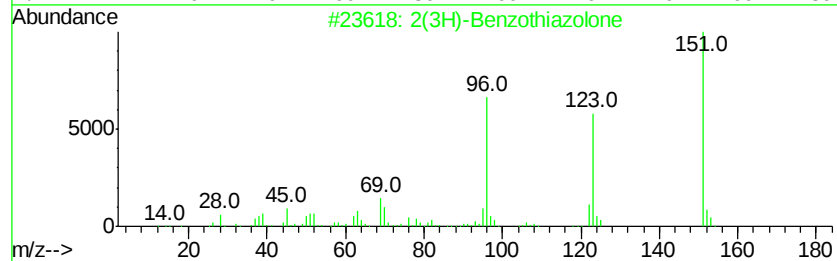
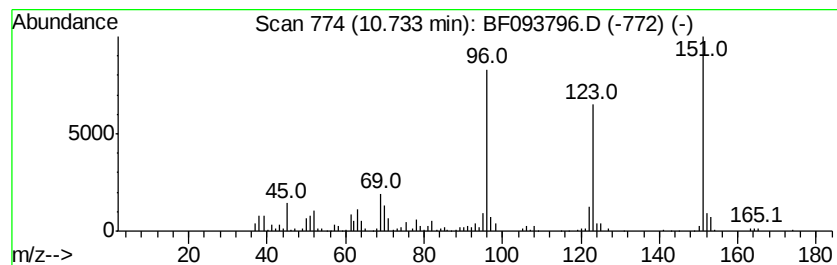
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 2(3H)-Benzothiazolone Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.73	3.11 ng	250539	Phenanthrene-d10	11.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	97
2		1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	59
3		6-Methyl-7-oxo-4,7-dihydro-triazol...	151	C5H5N5O	057250-39-2	43
4		1,4-Benzenediol, 2-(1,1-dimethyl...	166	C10H14O2	001948-33-0	43
5		4-Methoxyformanilide	151	C8H9NO2	023896-88-0	35



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032117\
Data File : BF093796.D
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Sample : I2263-14
Misc :
ALS Vial : 6 Sample Multiplier: 1

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ClientSampleId :
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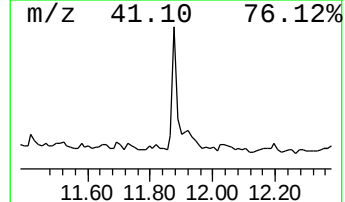
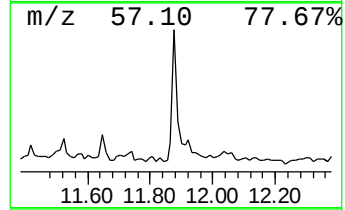
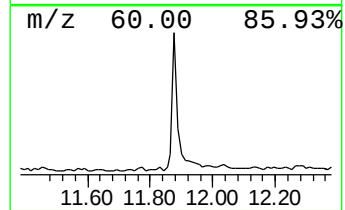
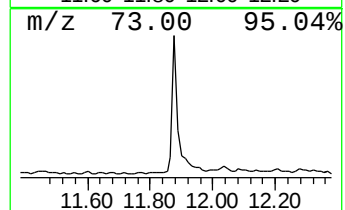
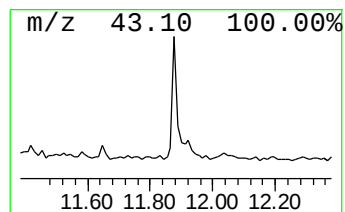
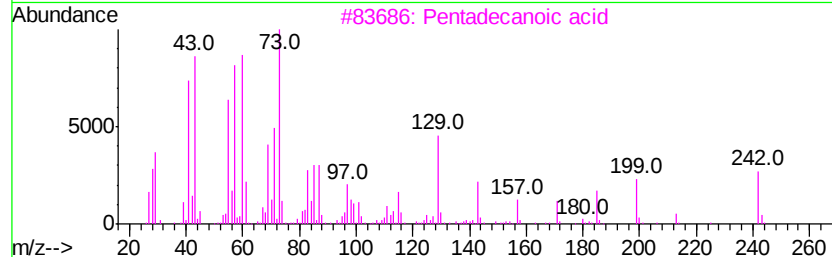
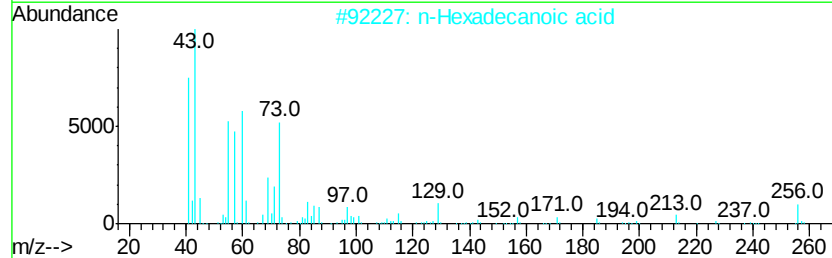
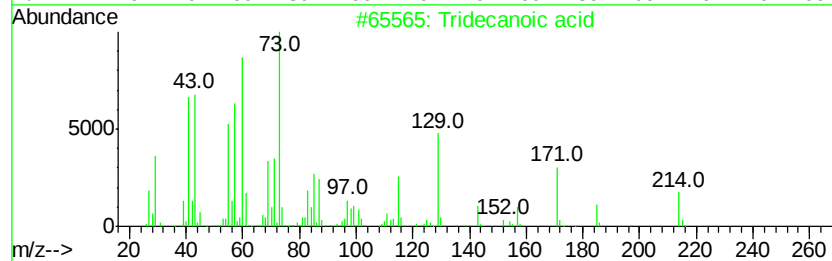
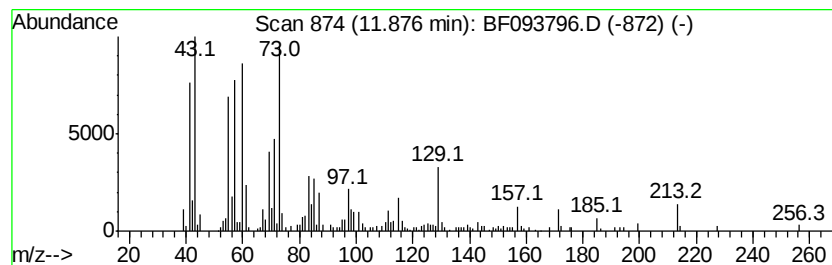
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Tridecanoic acid Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	3.09 ng	248292	Phenanthrene-d10	11.34

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	95
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			n-Decanoic acid	172	C10H20O2	000334-48-5	59
5			Undecane	156	C11H24	001120-21-4	11



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032117\
Data File : BF093796.D
Acq On : 21 Mar 2017 14:19
Operator : SJ/MA
Sample : I2263-14
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-105D

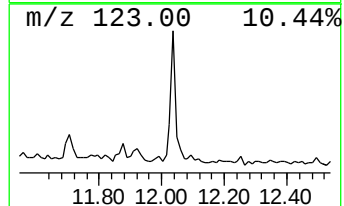
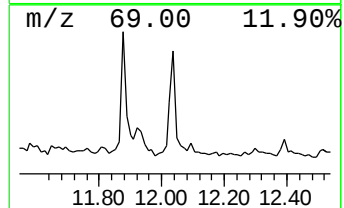
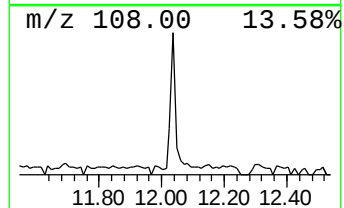
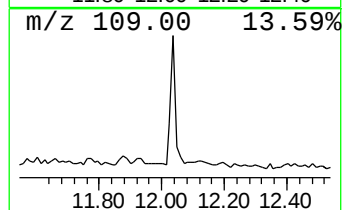
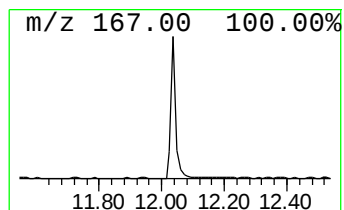
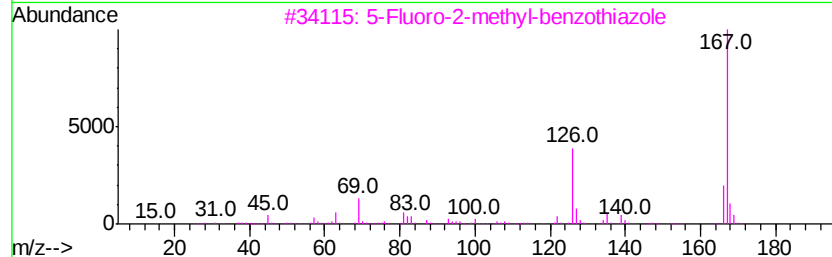
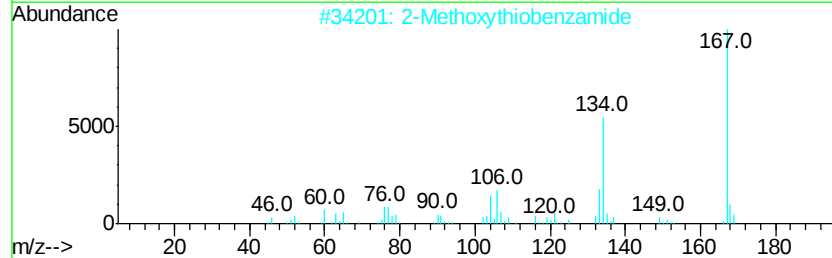
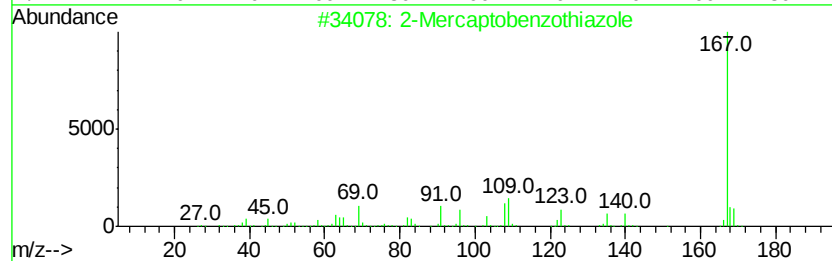
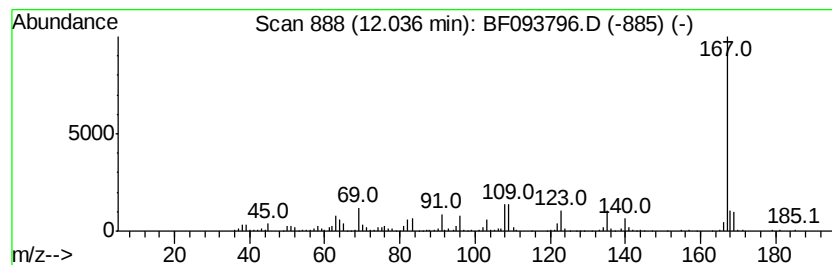
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 2-Mercaptobenzothiazole Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.04	2.92 ng	235058	Phenanthrene-d10	11.34

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Mercaptobenzothiazole	167	C7H5NS2	000149-30-4	96
2			2-Methoxythiobenzamide	167	C8H9NOS	042590-97-6	53
3			5-Fluoro-2-methyl-benzothiazole	167	C8H6FNS	000399-75-7	52
4			2',4'-Dihydroxyacetophenone oxime	167	C8H9NO3	1000212-89-5	46
5			3-Methoxythiobenzamide	167	C8H9NOS	064559-06-4	45



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032117\
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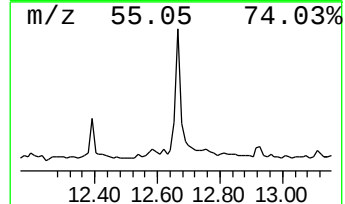
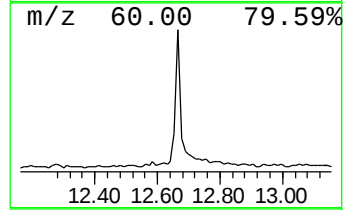
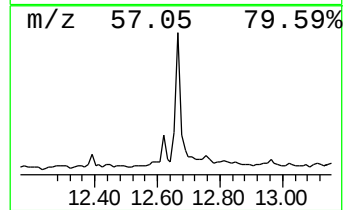
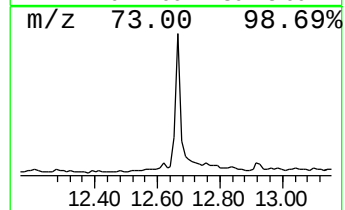
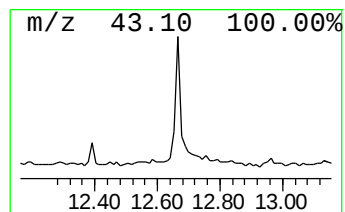
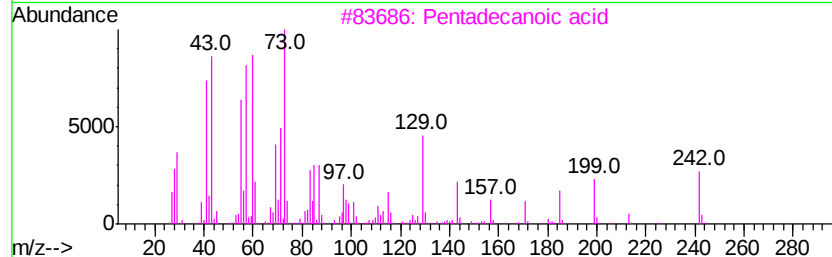
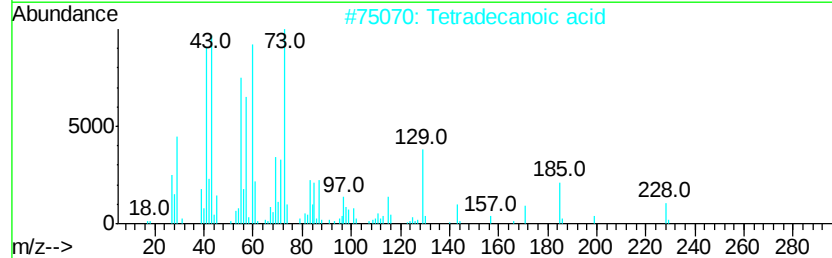
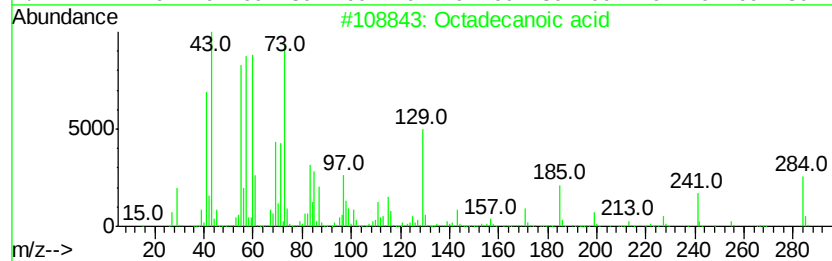
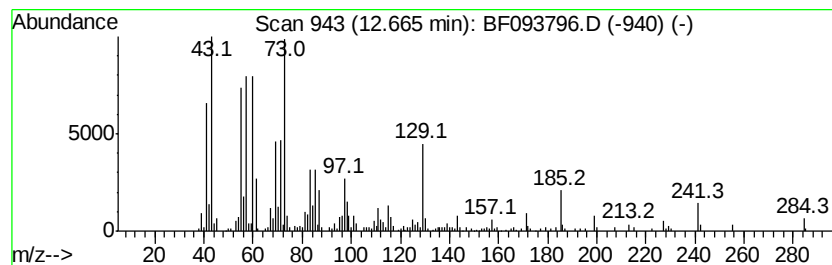
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.66	6.42 ng	382541	Chrysene-d12		13.97
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	n-Decanoic acid	172	C10H20O2	000334-48-5	68
5	Undecanoic acid	186	C11H22O2	000112-37-8	46



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032117\
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ALS Vial : 6 Sample Multiplier: 1

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ClientSampleId :
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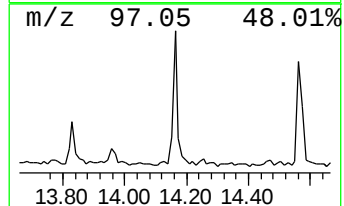
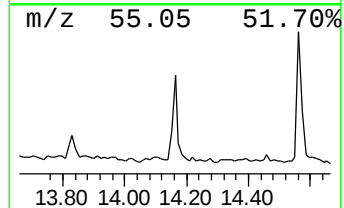
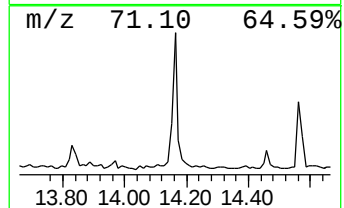
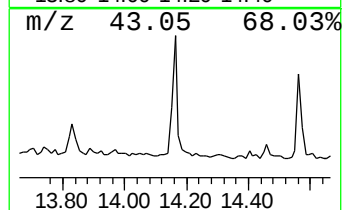
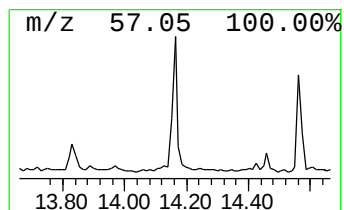
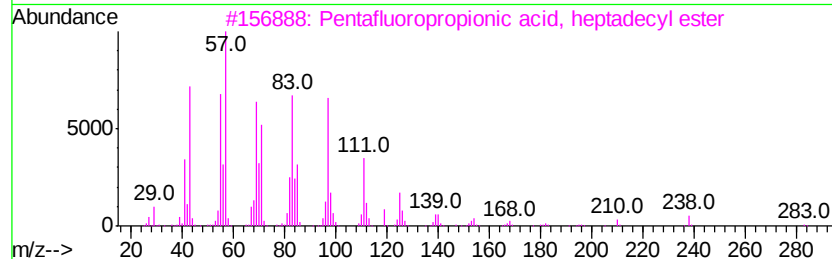
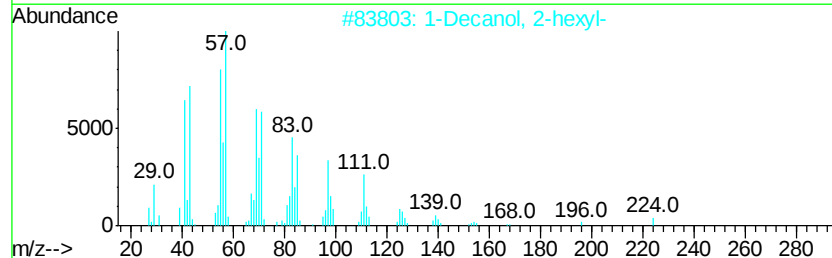
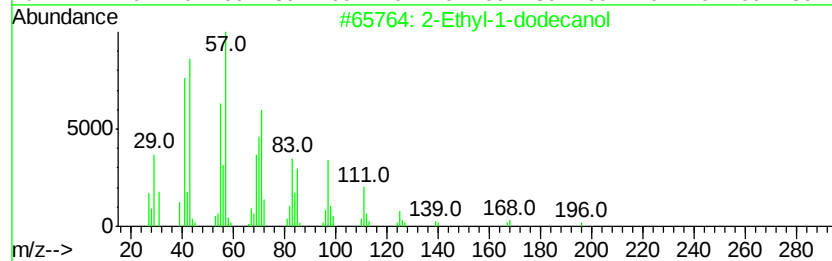
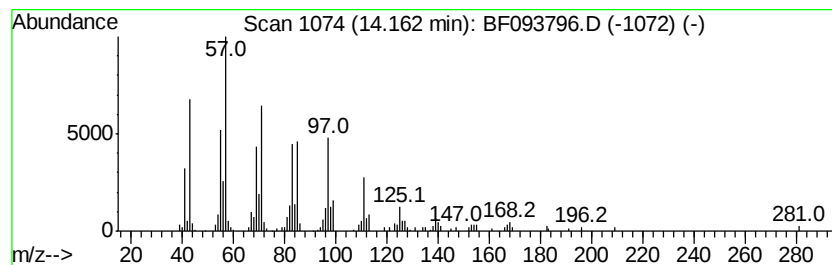
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 2-Ethyl-1-dodecanol Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.16	3.00 ng	178519	Chrysene-d12	13.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Ethyl-1-dodecanol	214	C14H30O	019780-33-7	80
2			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	72
3			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	70
4			2-Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	68
5			Eicosane, 9-cyclohexyl-	364	C26H52	004443-61-2	64



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032117\
Data File : BF093796.D
Acq On : 21 Mar 2017 14:19
Operator : SJ/MA
Sample : I2263-14
Misc :
ALS Vial : 6 Sample Multiplier: 1

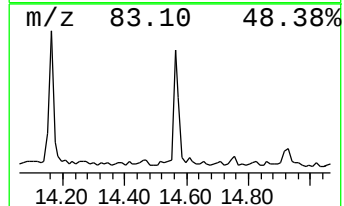
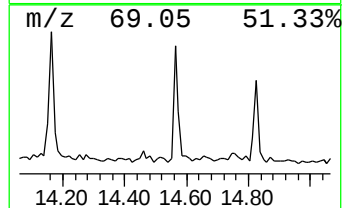
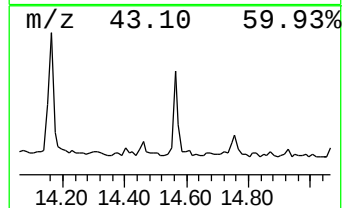
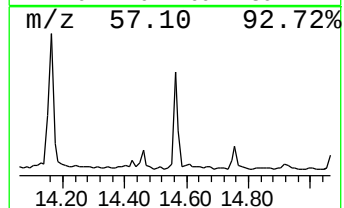
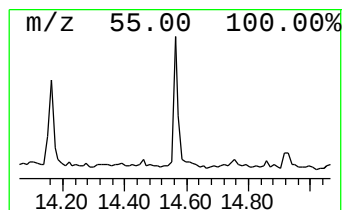
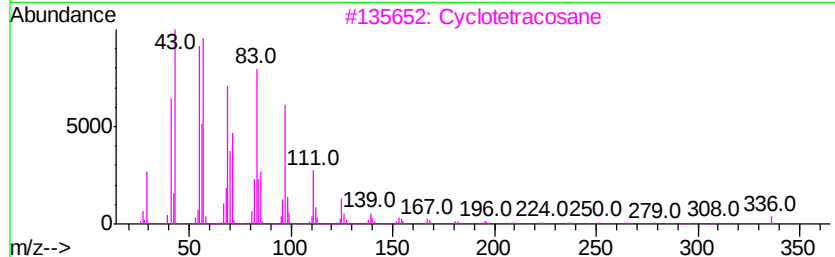
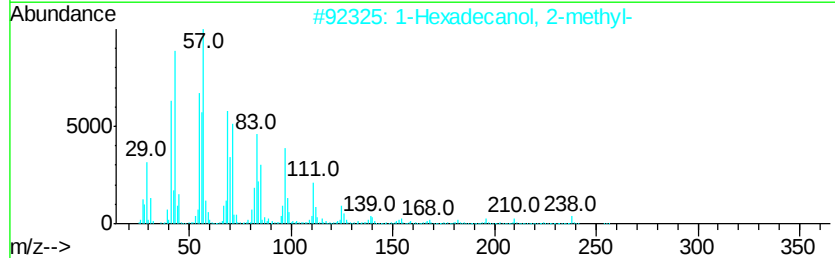
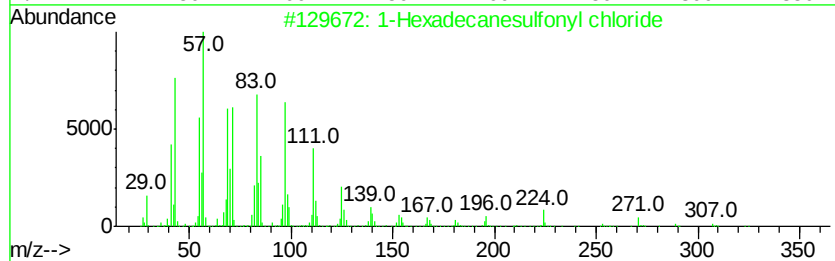
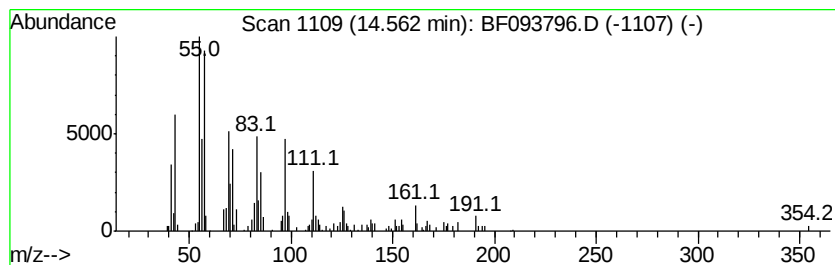
Instrument :
BNA_F
ClientSampleId :
MW-105D

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 1-Hexadecanesulfonyl chloride Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.56	2.61 ng	155663	Chrysene-d12	13.97		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	81
2		1-Hexadecanol, 2-methyl-	256	C17H36O	002490-48-4	72
3		Cyclotetracosane	336	C24H48	000297-03-0	68
4		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	68
5		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	62



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032117\
 Data File : BF093796.D
 Acq On : 21 Mar 2017 14:19
 Operator : SJ/MA
 Sample : I2263-14
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-105D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.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
2-Pentanone, 4-hy...	4.98	7.2 ng		375350	1	6.82	1048050	20.0
Cyclopentanone, 2...	5.67	12.4 ng		650442	1	6.82	1048050	20.0
unknown6.60	6.60	79.1 ng		4143640	1	6.82	1048050	20.0
Octanoic Acid	7.89	14.7 ng		1030470	2	8.10	1405340	20.0
unknown7.97	7.97	2.5 ng		175317	2	8.10	1405340	20.0
Cyclohexane, isot...	8.41	3.6 ng		253402	2	8.10	1405340	20.0
unknown8.47	8.47	3.5 ng		245096	2	8.10	1405340	20.0
Tetramethyl succi...	8.53	3.2 ng		222538	2	8.10	1405340	20.0
Benzylmalonic acid	8.89	2.4 ng		167265	2	8.10	1405340	20.0
n-Decanoic acid	9.04	8.8 ng		725461	3	9.86	1651620	20.0
3-tert-Butyl-4-hy...	9.62	3.8 ng		315454	3	9.86	1651620	20.0
Ethanone, 1-(3-hy...	9.78	6.4 ng		526360	3	9.86	1651620	20.0
Dodecanoic acid	10.08	8.2 ng		672882	3	9.86	1651620	20.0
2(3H)-Benzothiazo...	10.73	3.1 ng		250539	4	11.34	1608970	20.0
Tridecanoic acid	11.88	3.1 ng		248292	4	11.34	1608970	20.0
2-Mercaptobenzoth...	12.04	2.9 ng		235058	4	11.34	1608970	20.0
Octadecanoic acid	12.66	6.4 ng		382541	5	13.97	1192080	20.0
2-Ethyl-1-dodecanol	14.16	3.0 ng		178519	5	13.97	1192080	20.0
1-Hexadecanesulfo...	14.56	2.6 ng		155663	5	13.97	1192080	20.0