

Data Path : Z:\HPCHEM1\BNA F\DATA\BF043017\
 Data File : BF094728.D
 Acq On : 30 Apr 2017 21:25
 Operator : SJ/MA
 Sample : I2860-04
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HW-32

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-BF041717.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	3.366	240	243	258	rVB	481713	523876	5.50%	1.268%
2	3.919	331	337	341	rBV	1339903	1731053	18.17%	4.191%
3	4.319	402	405	419	rBV	897768	946043	9.93%	2.291%
4	4.696	465	469	474	rBV	318834	296411	3.11%	0.718%
5	5.390	583	587	602	rBV	541095	669024	7.02%	1.620%
6	5.513	605	608	613	rBV	1737292	1676919	17.61%	4.060%
7	5.760	647	650	655	rBV	710741	655044	6.88%	1.586%
8	5.943	676	681	687	rBV	2343898	2269038	23.82%	5.494%
9	6.419	756	762	765	rBV	1777800	1923581	20.20%	4.657%
10	6.866	828	838	845	rBV3	79928	136708	1.44%	0.331%
11	6.960	845	854	856	rBV6	91704	172052	1.81%	0.417%
12	7.001	857	861	865	rVV4	80504	163652	1.72%	0.396%
13	7.066	866	872	879	rVV6	85208	208870	2.19%	0.506%
14	7.148	879	886	891	rVV5	98446	249257	2.62%	0.604%
15	7.254	895	904	910	rVV	1051155	1153736	12.11%	2.793%
16	7.313	910	914	917	rVV3	88357	149983	1.57%	0.363%
17	7.372	917	924	926	rVV4	158498	333027	3.50%	0.806%
18	7.401	926	929	933	rVV	139045	182765	1.92%	0.443%
19	7.466	934	940	944	rVB3	147094	202890	2.13%	0.491%
20	7.607	959	964	966	rVB3	123337	171145	1.80%	0.414%
21	7.760	984	990	996	rBV3	284470	579999	6.09%	1.404%
22	7.825	996	1001	1008	rVB7	107346	256321	2.69%	0.621%
23	7.889	1008	1012	1015	rBV3	103805	146436	1.54%	0.355%
24	7.937	1015	1020	1025	rVB7	145366	263260	2.76%	0.637%
25	8.001	1025	1031	1034	rBV2	160743	241738	2.54%	0.585%
26	8.195	1056	1064	1066	rBV3	131112	235393	2.47%	0.570%
27	8.225	1066	1069	1072	rVV2	118739	158022	1.66%	0.383%
28	8.313	1081	1084	1087	rBV3	73428	99655	1.05%	0.241%
29	8.401	1090	1099	1102	rBV	446297	1090925	11.45%	2.641%
30	8.472	1109	1111	1116	rVB3	141109	166322	1.75%	0.403%
31	8.519	1116	1119	1124	rVB3	205932	247499	2.60%	0.599%
32	8.584	1125	1130	1133	rBV	3417624	3630344	38.12%	8.790%
33	9.084	1213	1215	1220	rVB2	221203	229540	2.41%	0.556%
34	9.389	1264	1267	1271	rBV2	942244	982332	10.31%	2.378%

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Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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35	9.513	1283	1288	1295	rVB6	301069	599515	6.29%	1.452%
36	9.878	1331	1350	1352	rBV	2720781	9524544	100.00%	23.061%
37	9.919	1355	1357	1359	rBV	197852	149647	1.57%	0.362%
38	10.054	1377	1380	1384	rBV2	162518	165855	1.74%	0.402%
39	10.195	1399	1404	1407	rBV	385777	509087	5.35%	1.233%
40	10.236	1408	1411	1414	rBV4	150996	198698	2.09%	0.481%
41	10.378	1431	1435	1438	rVB	1065930	1173653	12.32%	2.842%
42	11.142	1562	1565	1569	rVB	513637	607130	6.37%	1.470%
43	11.219	1574	1578	1582	rBV	1092873	1127128	11.83%	2.729%
44	11.977	1704	1707	1713	rVB2	335951	396013	4.16%	0.959%
45	12.936	1867	1870	1876	rVB	332478	386986	4.06%	0.937%
46	13.201	1909	1915	1918	rBV	2171322	2537765	26.64%	6.145%
47	14.471	2127	2131	2138	rVB	607240	636769	6.69%	1.542%
48	14.624	2154	2157	2164	rVB	151560	160635	1.69%	0.389%
49	16.095	2403	2407	2413	rBV	489514	592909	6.23%	1.436%
50	16.318	2441	2445	2453	rVB	185220	228004	2.39%	0.552%
51	18.636	2833	2839	2846	rVB3	65840	163829	1.72%	0.397%

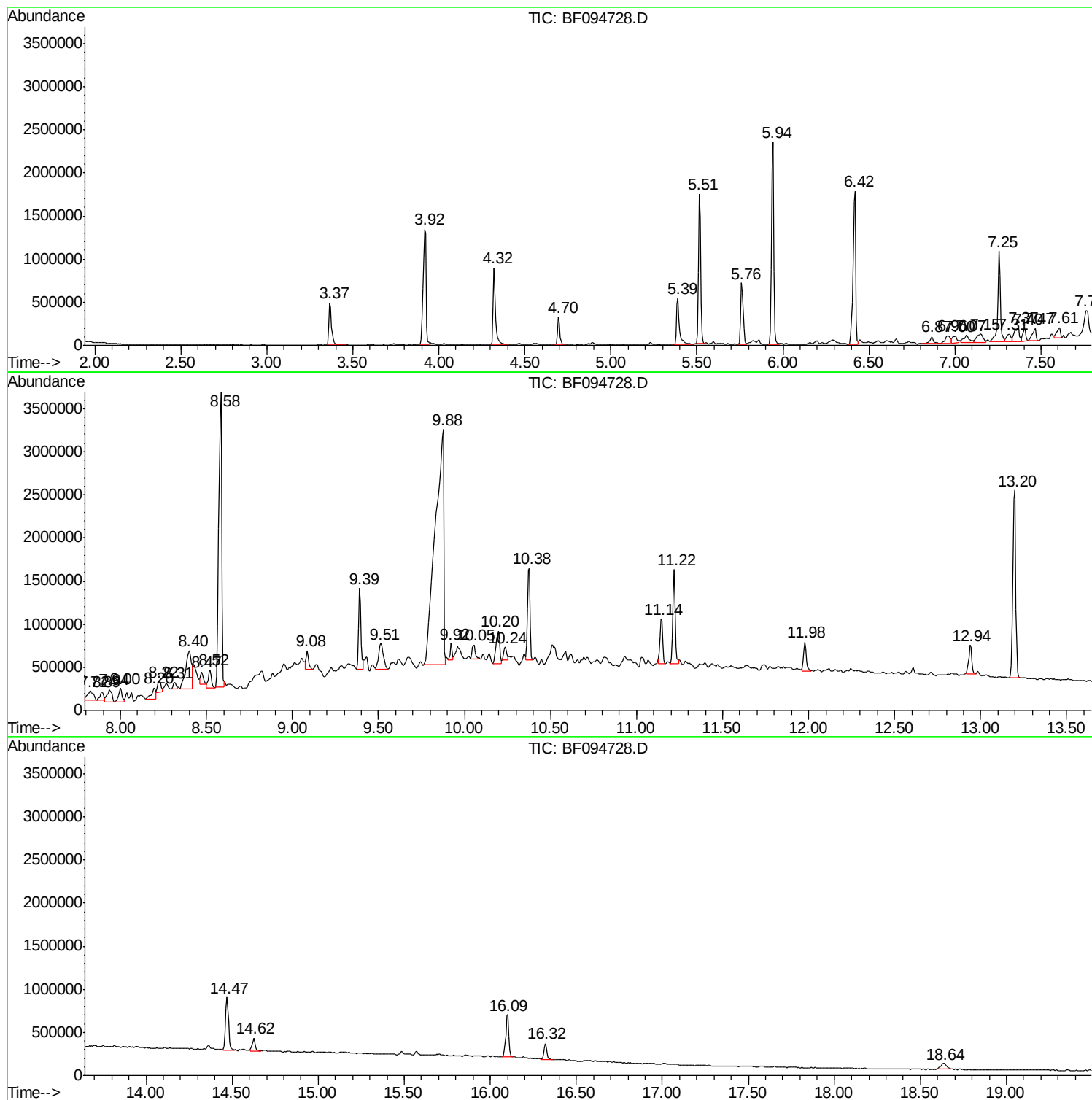
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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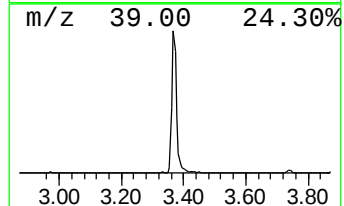
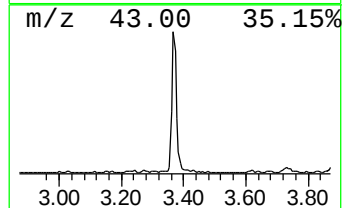
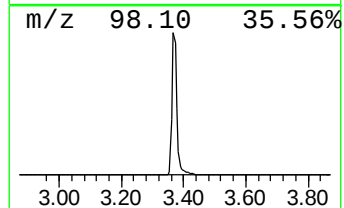
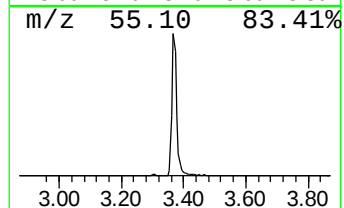
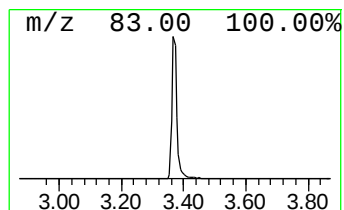
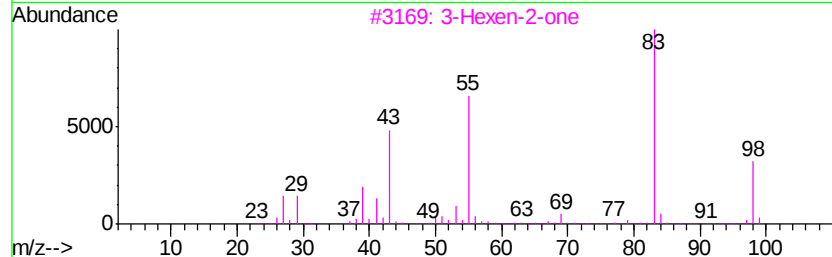
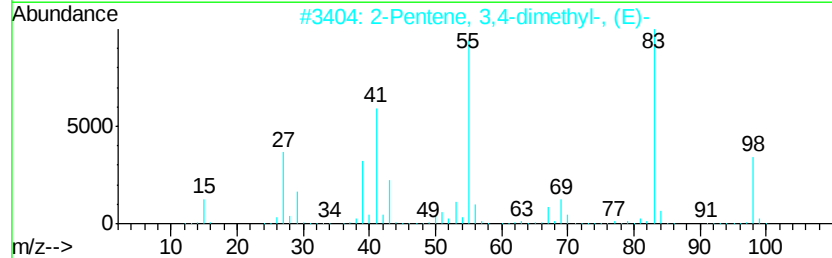
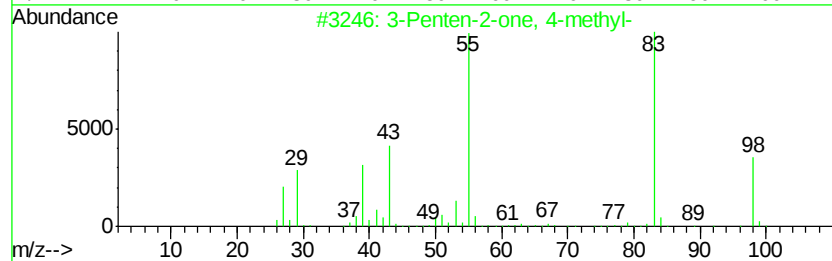
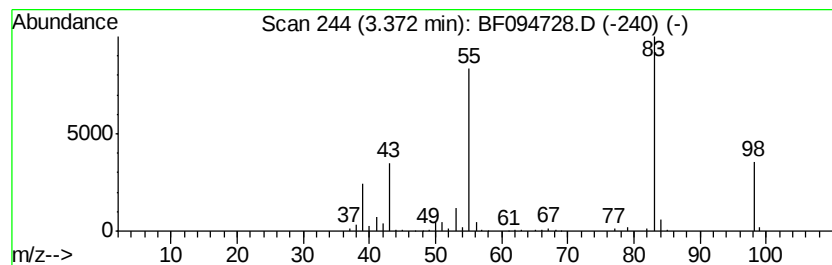
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.37	16.00 ng	523876	1,4-Dichlorobenzene-d4	5.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
3		3-Hexen-2-one	98	C6H10O	000763-93-9	90
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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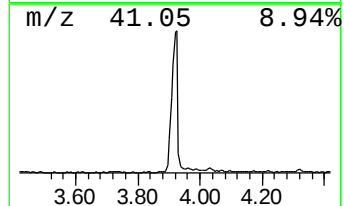
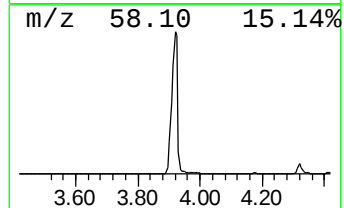
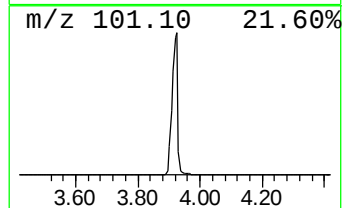
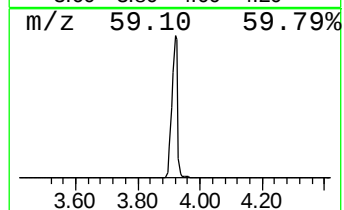
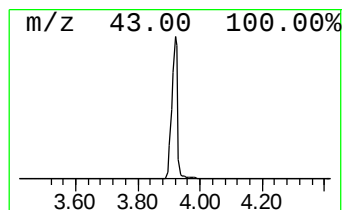
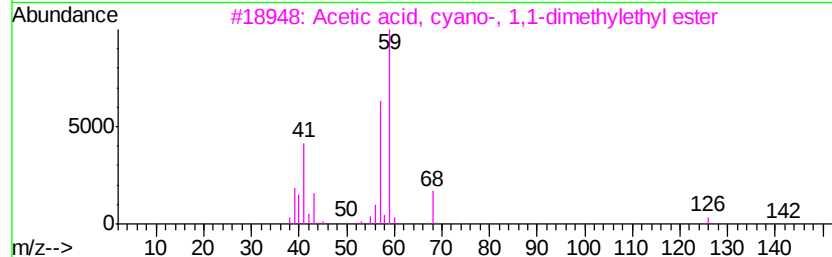
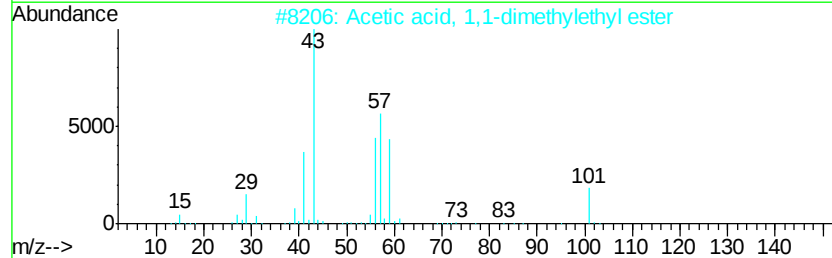
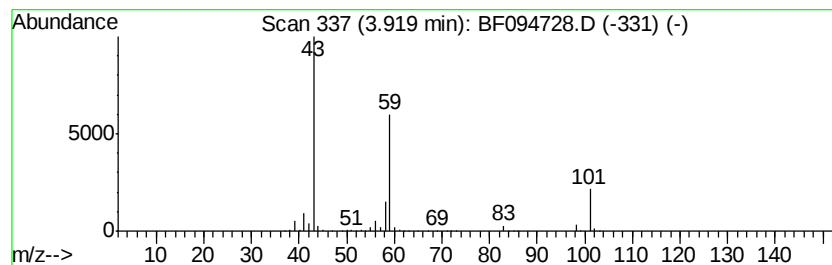
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.92	52.85 ng	1731050	1,4-Dichlorobenzene-d4	5.76

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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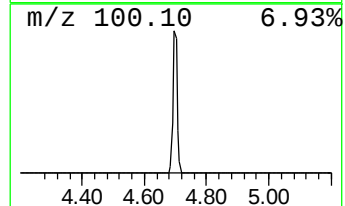
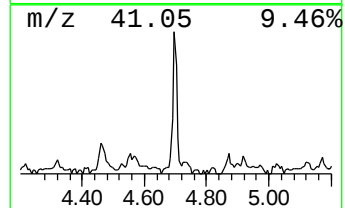
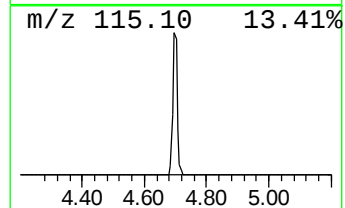
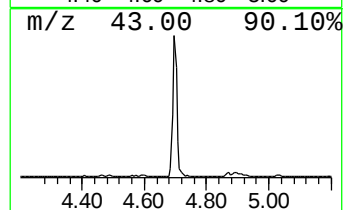
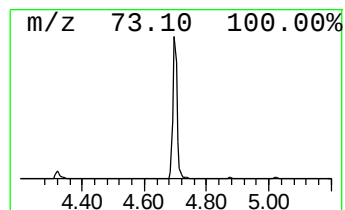
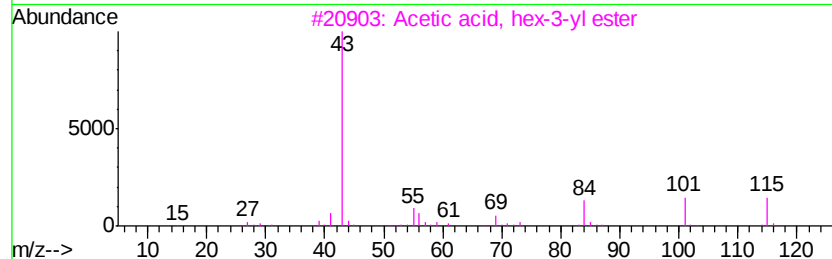
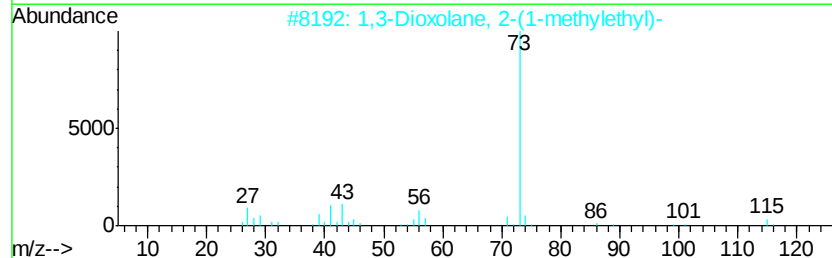
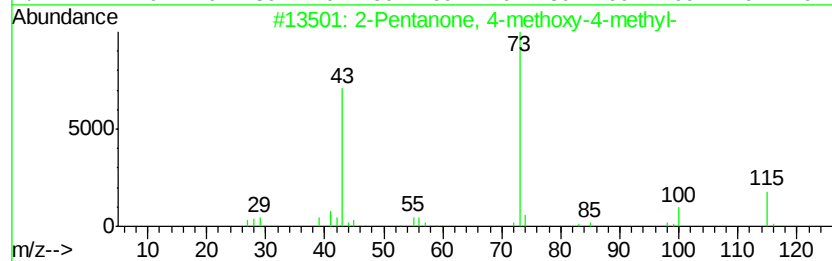
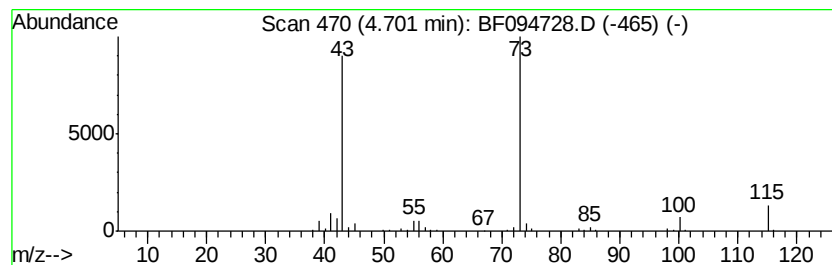
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.70	9.05 ng	296411	1,4-Dichlorobenzene-d4	5.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	32
3		Acetic acid, hex-3-yl ester	144	C8H16O2	1000367-94-5	17
4		N-Formylmorpholine	115	C5H9NO2	004394-85-8	10
5		2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10



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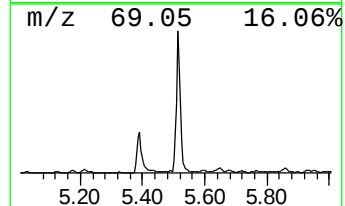
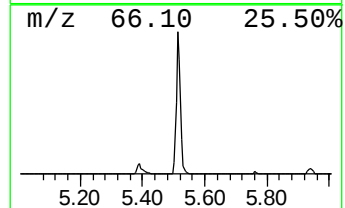
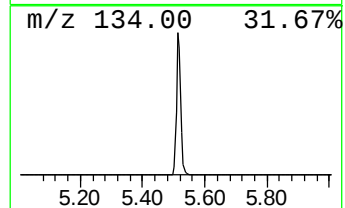
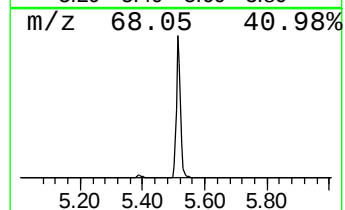
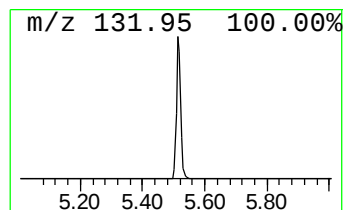
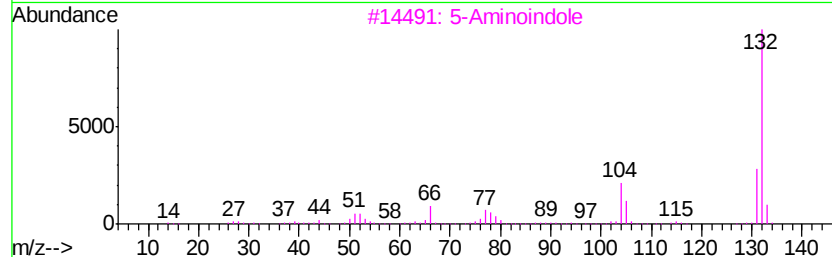
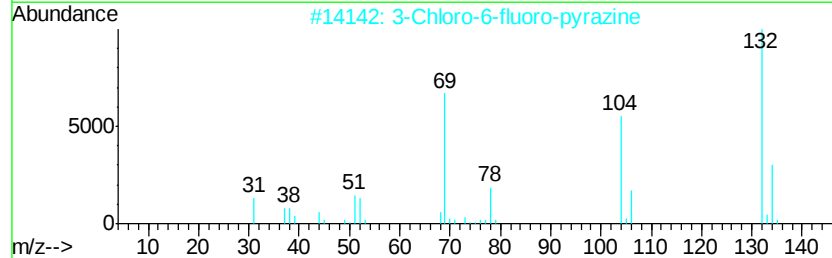
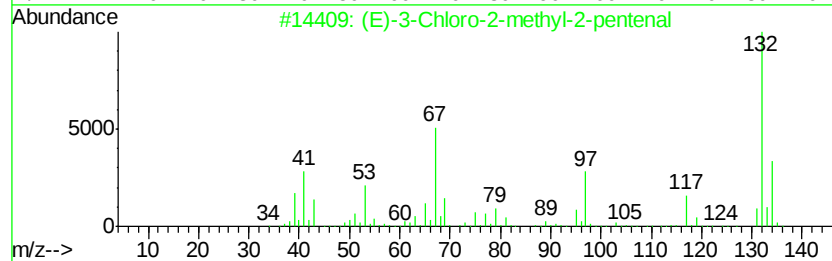
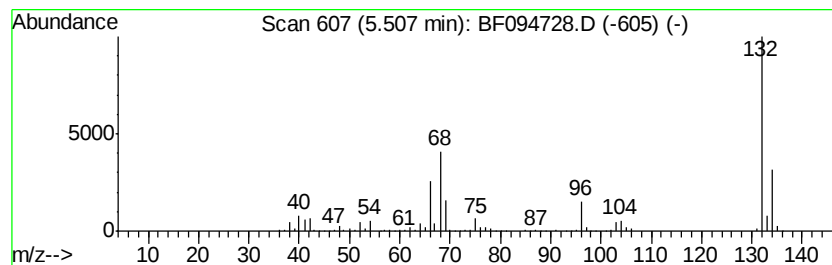
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 unknown5.51 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.51	51.20 ng	1676920	1,4-Dichlorobenzene-d4	5.76

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		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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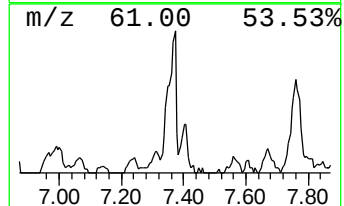
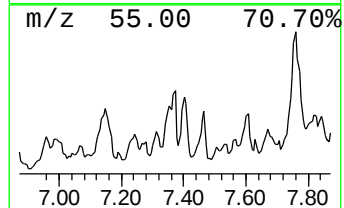
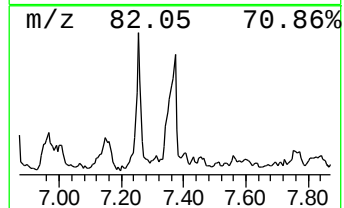
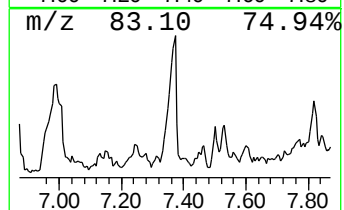
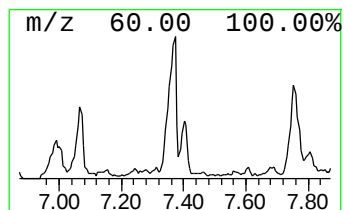
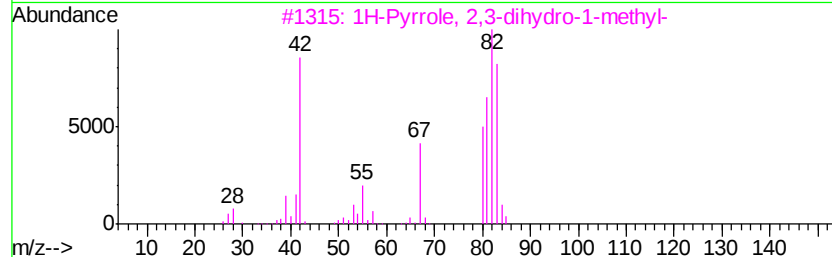
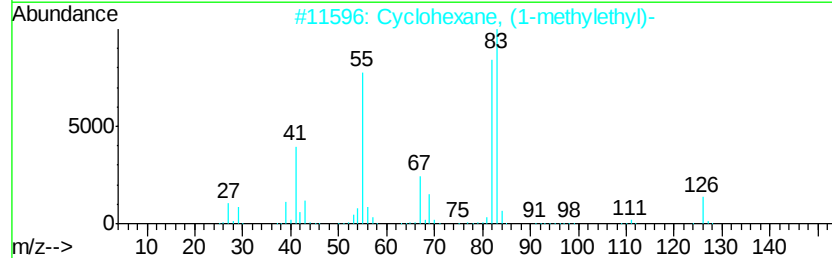
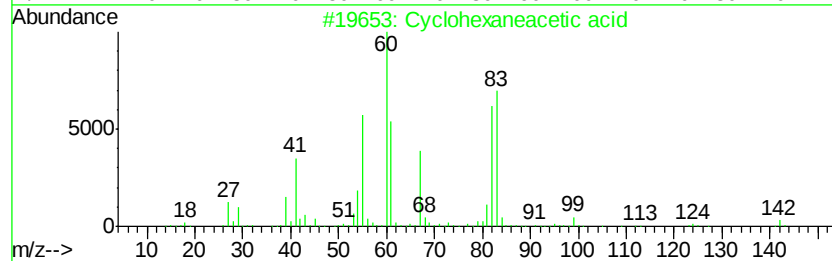
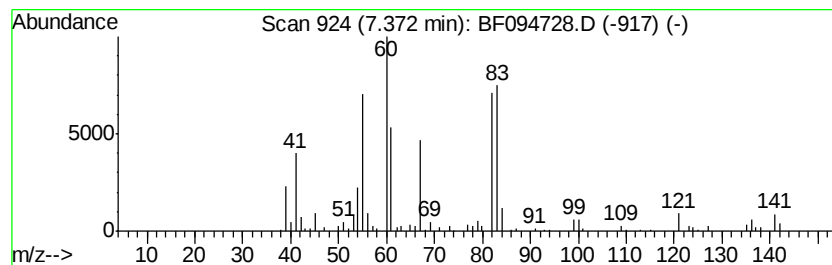
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Cyclohexaneacetic acid Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.37	5.77 ng	333027	Naphthalene-d8	7.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexaneacetic acid	142	C8H14O2	005292-21-7	94
2		Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	35
3		1H-Pyrrole, 2,3-dihydro-1-methyl-	83	C5H9N	033838-11-8	35
4		Cyclohexane, octyl-	196	C14H28	001795-15-9	25
5		Tricyclo[4.2.1.0(3,7)]nonane-3,8...	154	C9H14O2	106435-09-0	22



Data Path : Z:\HPCHEM1\BNA F\DATA\BF043017\
Data File : BF094728.D
Acq On : 30 Apr 2017 21:25
Operator : SJ/MA
Sample : I2860-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

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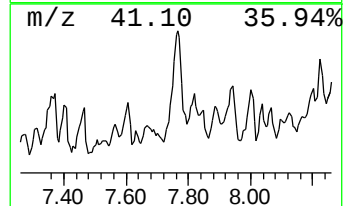
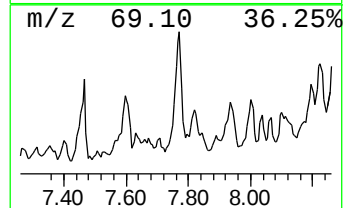
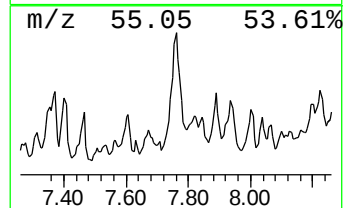
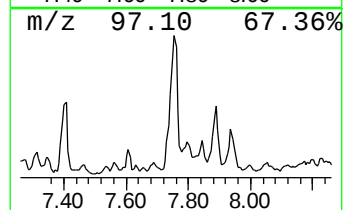
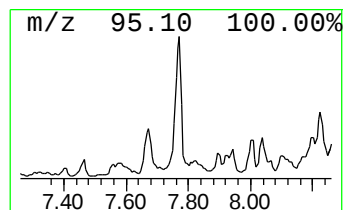
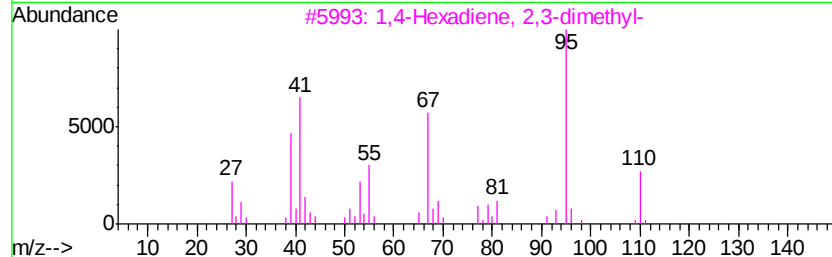
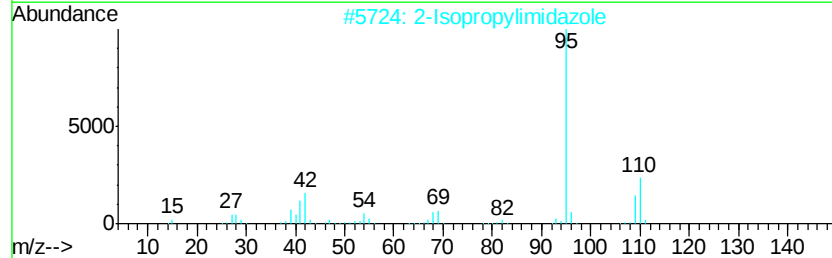
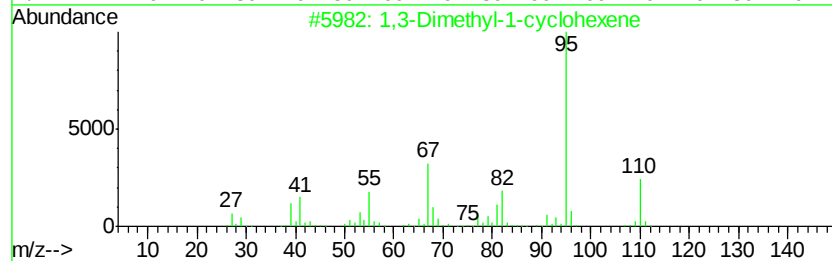
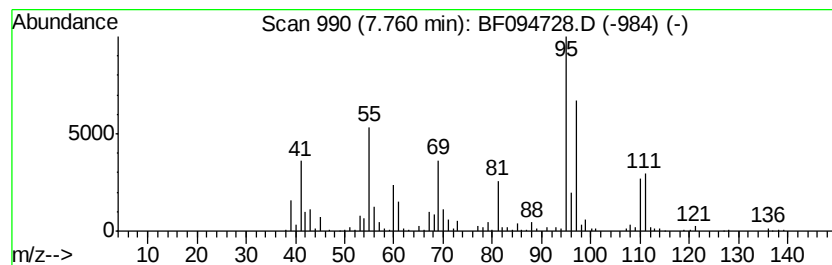
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown7.76 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.76	10.05 ng	579999	Napthalene-d8	7.25

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	35
2			2-Isopropylimidazole	110	C6H10N2	036947-68-9	25
3			1,4-Hexadiene, 2,3-dimethyl-	110	C8H14	018669-52-8	25
4			5,6-Dibromo-5-methyl-hex-1-ene	254	C7H12Br2	1000192-24-6	12
5			5-Amino-3-methylpyrazole	97	C4H7N3	031230-17-8	11



Data Path : Z:\HPCHEM1\BNA F\DATA\BF043017\
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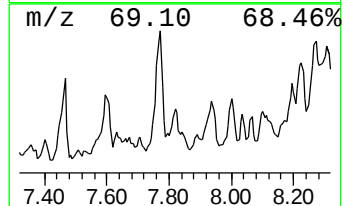
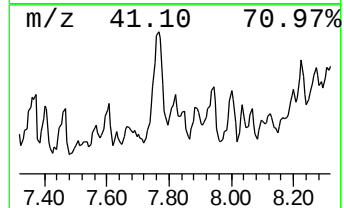
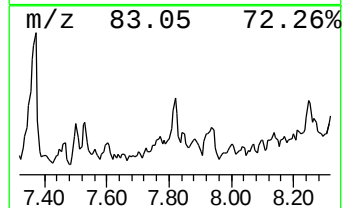
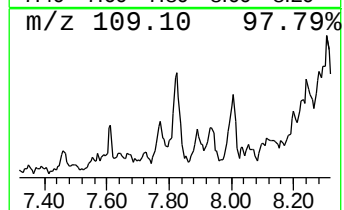
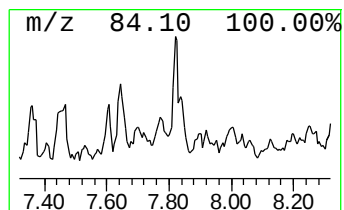
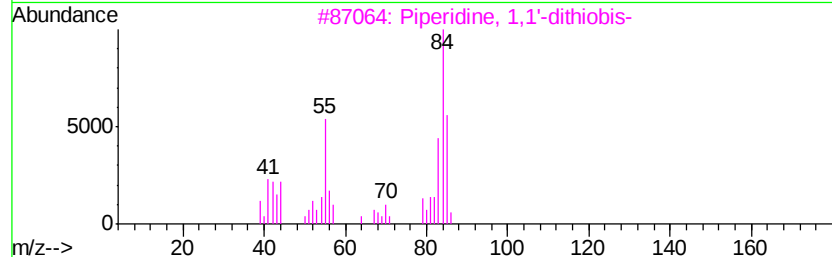
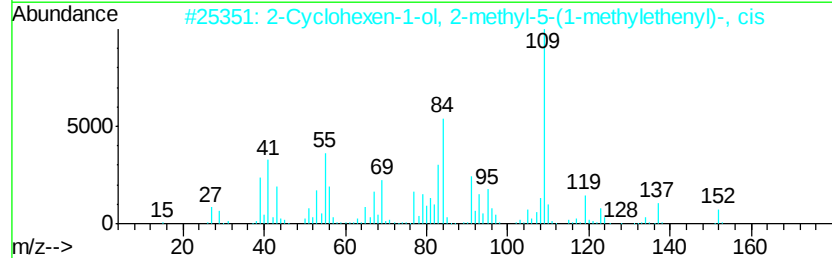
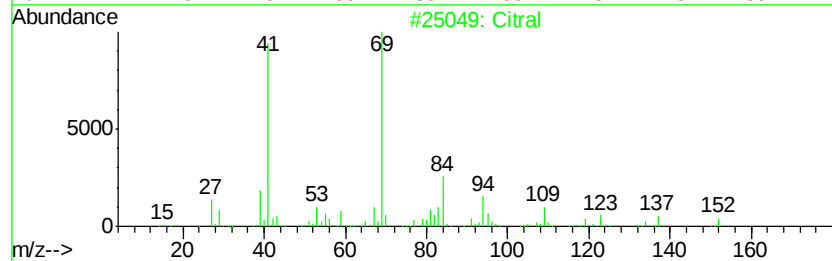
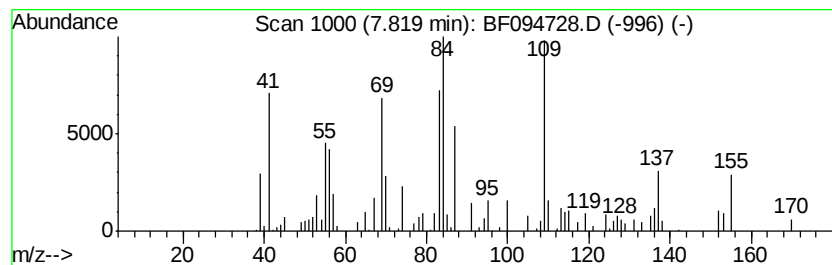
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown7.82 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.82	4.44 ng	256321	Naphthalene-d8	7.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Citral	152	C10H16O	005392-40-5	27
2		2-Cyclohexen-1-ol, 2-methyl-5-(1-methylethenyl)-, cis	152	C10H16O	001197-06-4	25
3		Piperidine, 1,1'-dithiobis-	232	C10H20N2S2	010220-20-9	22
4		2-Butenal, 3-methyl-	84	C5H8O	000107-86-8	22
5		Benzenamine, 3-ethoxy-	137	C8H11NO	000621-33-0	18



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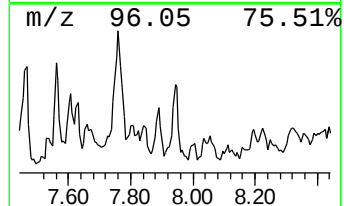
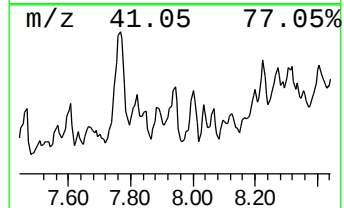
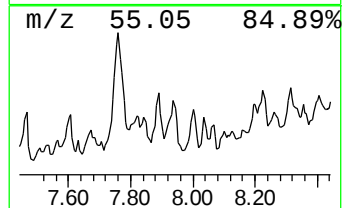
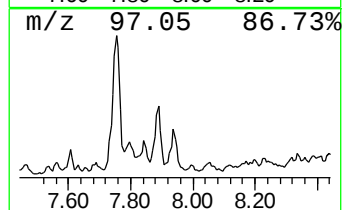
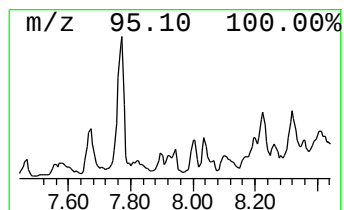
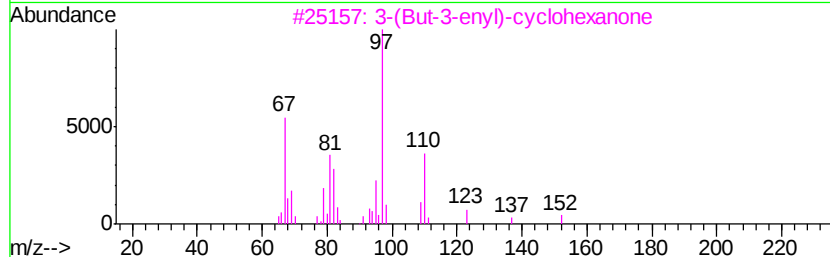
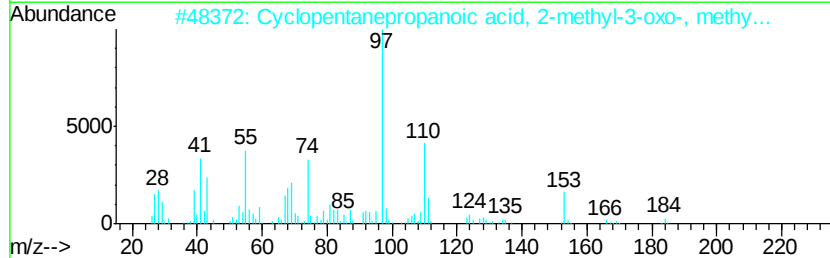
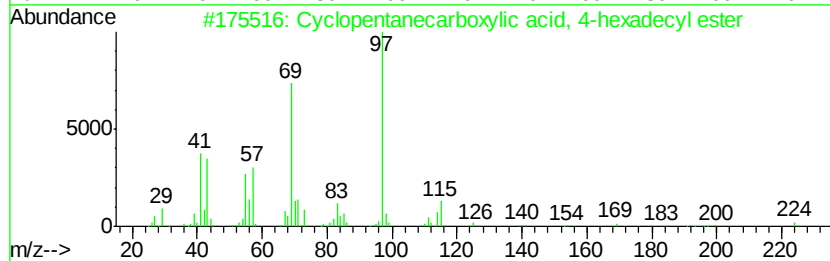
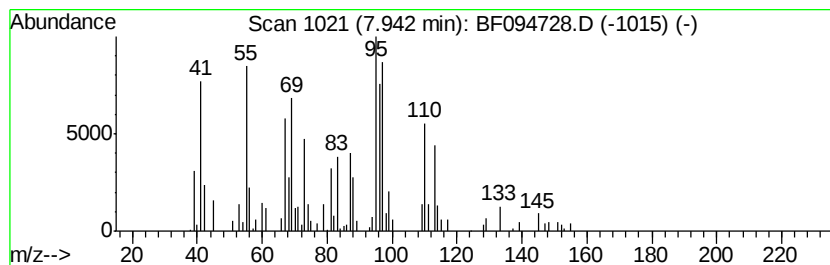
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown7.94 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.94	4.56 ng	263260	Naphthalene-d8	7.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentanecarboxylic acid, 4-h...	338	C22H42O2	1000282-77-5	35
2		Cyclopentanepropanoic acid, 2-me...	184	C10H16O3	092486-10-7	27
3		3-(But-3-enyl)-cyclohexanone	152	C10H16O	003636-03-1	25
4		2-Propen-1-one, 1-cyclopropyl-	96	C6H8O	059819-62-4	25
5		(5-Ethylcyclopent-1-enyl)methanol	126	C8H14O	036431-59-1	22



Data Path : Z:\HPCHEM1\BNA F\DATA\BF043017\
Data File : BF094728.D
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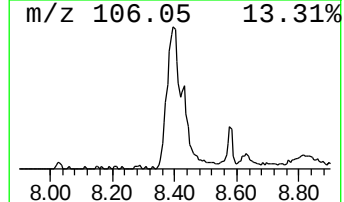
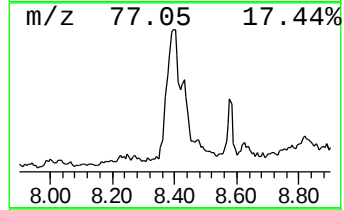
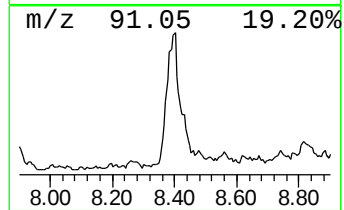
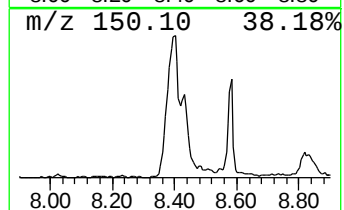
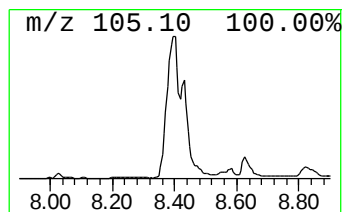
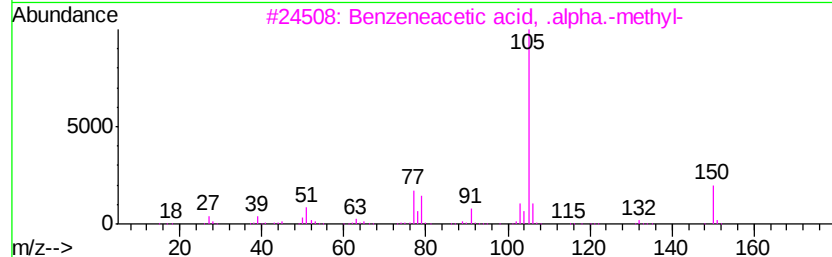
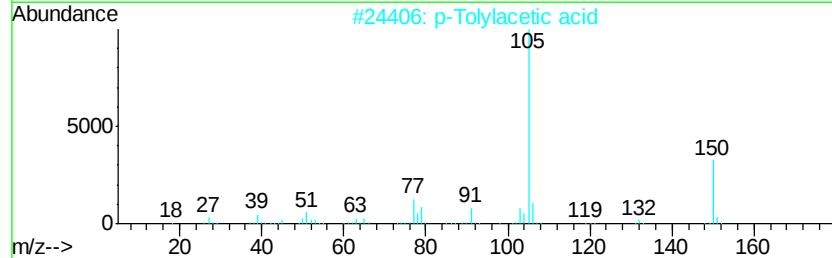
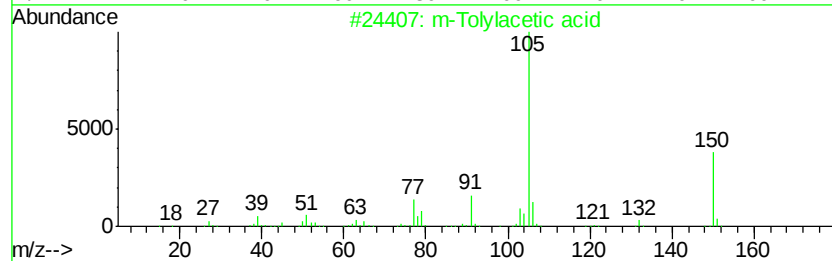
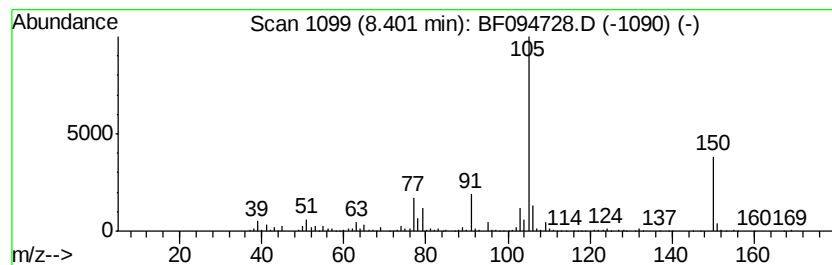
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 m-Tolylacetic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.40	22.21 ng	1090930	Acenaphthene-d10	9.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	m-Tolylacetic acid	150	C9H10O2	000621-36-3	94
2		p-Tolylacetic acid	150	C9H10O2	000622-47-9	90
3		Benzeneacetic acid, .alpha.-methvl-	150	C9H10O2	000492-37-5	90
4		o-Tolylacetic acid	150	C9H10O2	000644-36-0	87
5		Benzeneacetic acid, .alpha.-meth...	150	C9H10O2	007782-26-5	74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF043017\
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Acq On : 30 Apr 2017 21:25
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Misc :
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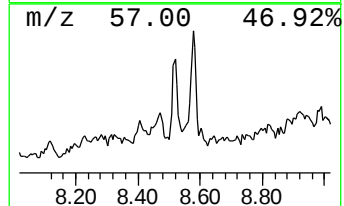
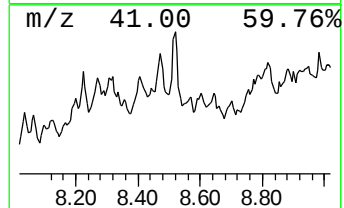
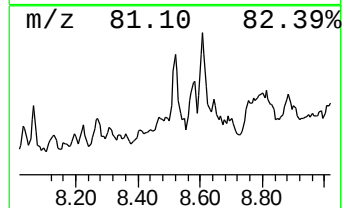
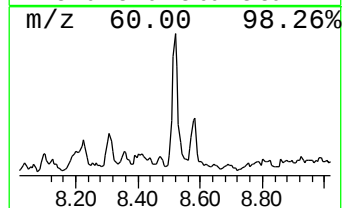
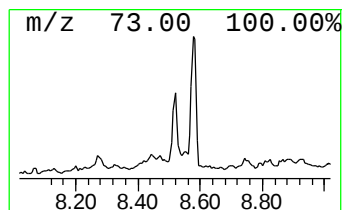
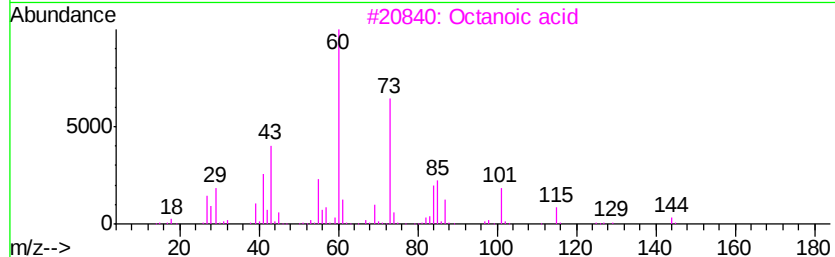
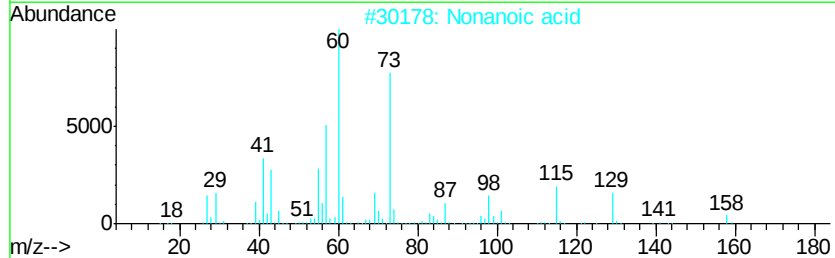
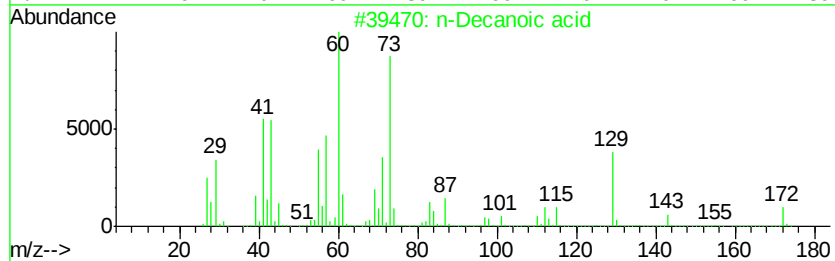
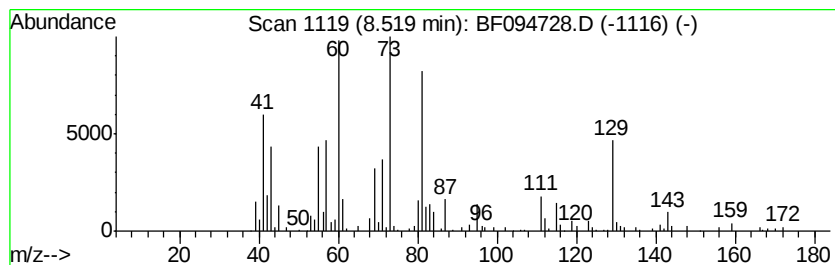
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 unknown8.52 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.52	5.04 ng	247499	Acenaphthene-d10	9.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Decanoic acid	172	C10H20O2	000334-48-5	49
2		Nonanoic acid	158	C9H18O2	000112-05-0	32
3		Octanoic acid	144	C8H16O2	000124-07-2	22
4		2,4-Undecadienal, (E,E)-	166	C11H18O	030361-29-6	14
5		2,4-Decadienal, (E,E)-	152	C10H16O	025152-84-5	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF043017\
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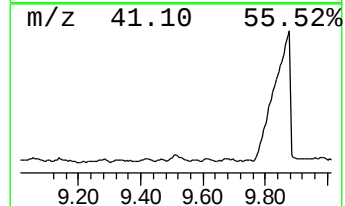
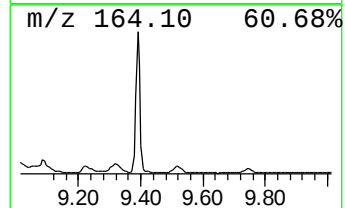
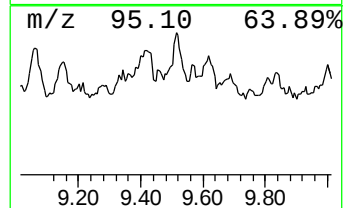
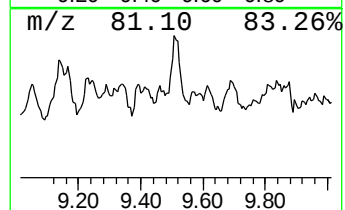
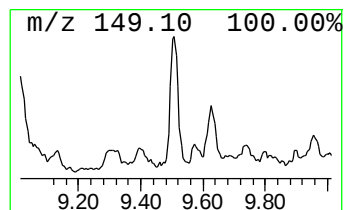
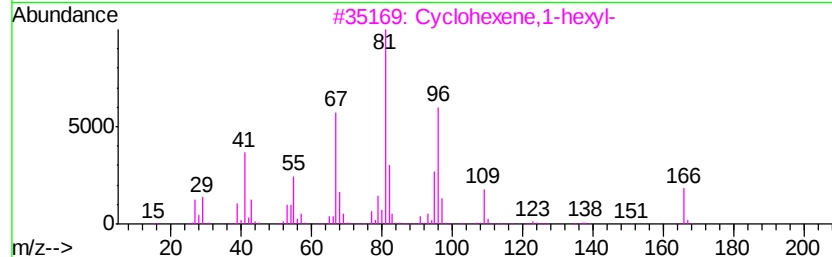
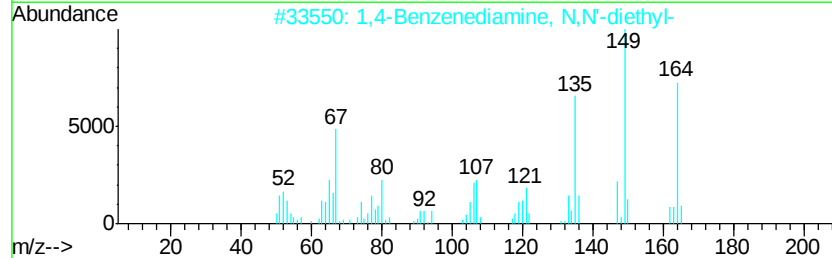
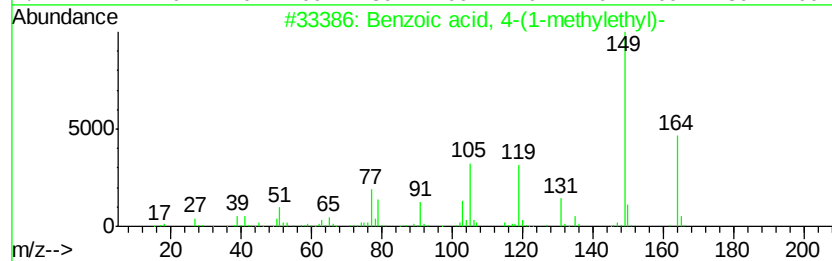
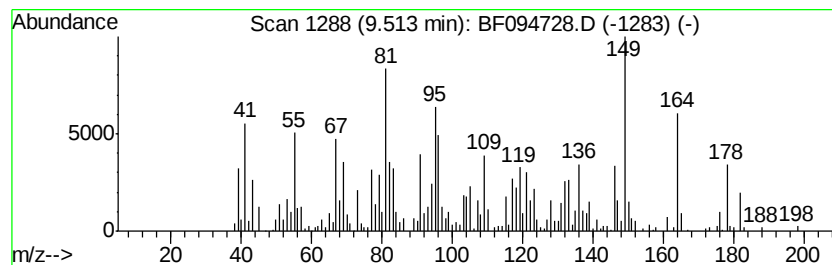
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 unknown9.51 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.51	12.21 ng	599515	Acenaphthene-d10	9.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzoic acid, 4-(1-methylethyl)-	164	C10H12O2	000536-66-3	35
2		1,4-Benzenediamine, N,N'-diethyl-	164	C10H16N2	003010-30-8	35
3		Cyclohexene, 1-hexyl-	166	C12H22	003964-66-7	25
4		tert-Butyl-p-benzoquinone	164	C10H12O2	003602-55-9	22
5		o-Isopropylphenetole	164	C11H16O	056631-59-5	20



Data Path : Z:\HPCHEM1\BNA F\DATA\BF043017\
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Misc :
ALS Vial : 23 Sample Multiplier: 1

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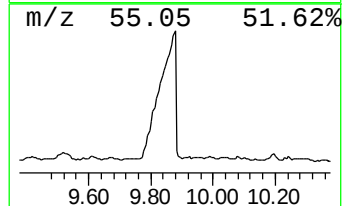
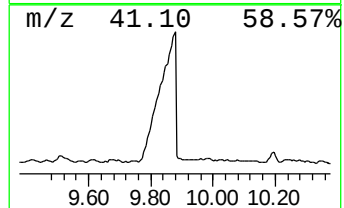
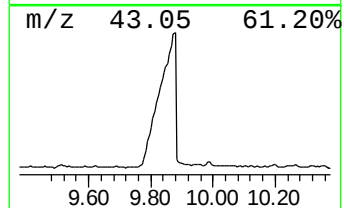
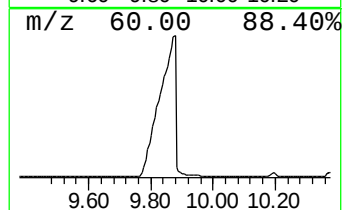
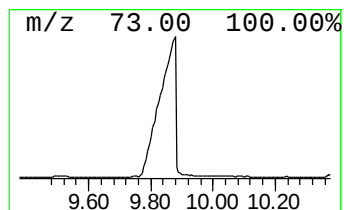
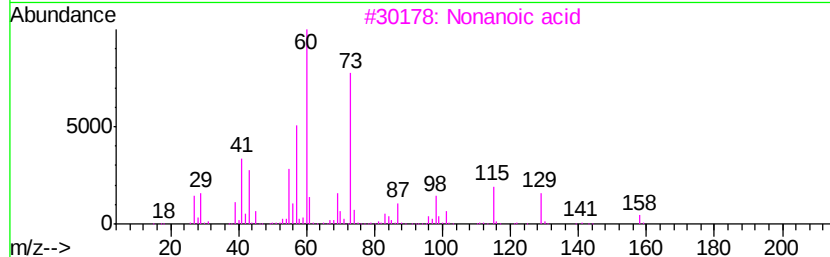
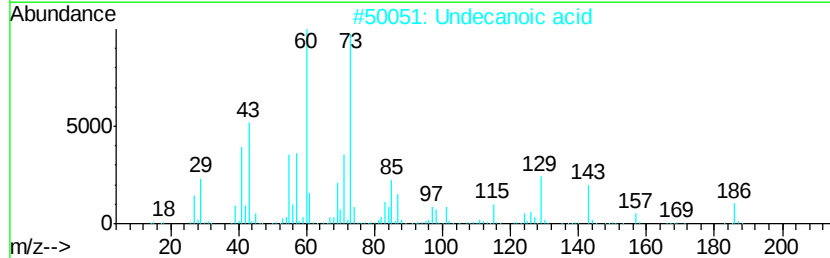
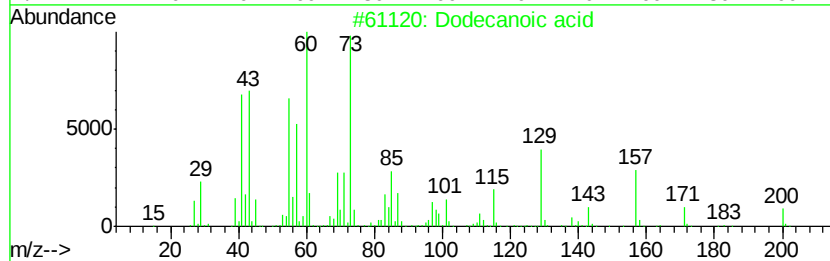
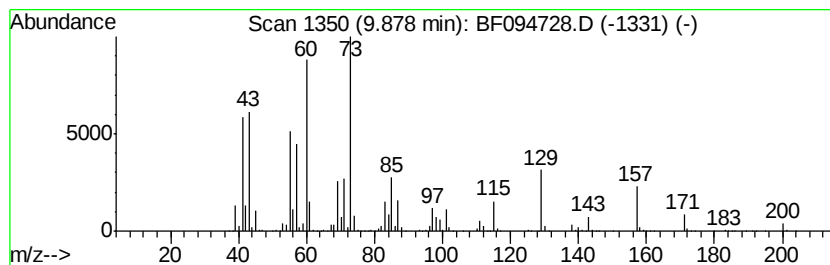
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Dodecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.88	193.92 ng	9524540	Acenaphthene-d10	9.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecanoic acid	200	C12H24O2	000143-07-7	97
2		Undecanoic acid	186	C11H22O2	000112-37-8	72
3		Nonanoic acid	158	C9H18O2	000112-05-0	60
4		n-Decanoic acid	172	C10H20O2	000334-48-5	59
5		Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	46



Data Path : Z:\HPCHEM1\BNA F\DATA\BF043017\
Data File : BF094728.D
Acq On : 30 Apr 2017 21:25
Operator : SJ/MA
Sample : I2860-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HW-32

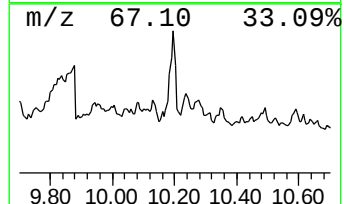
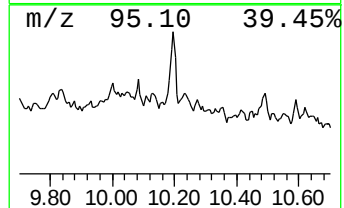
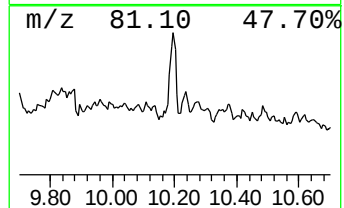
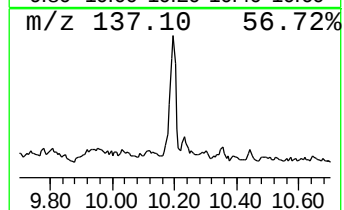
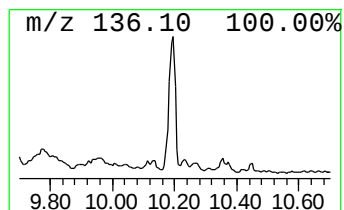
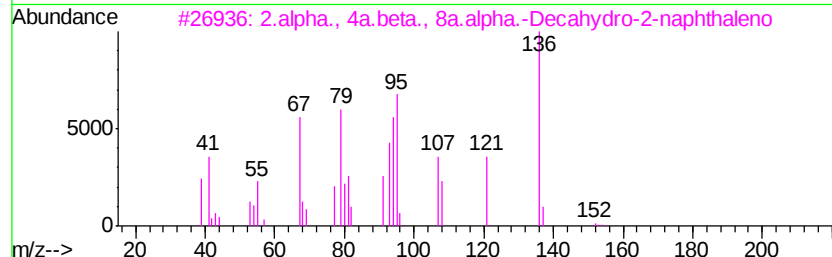
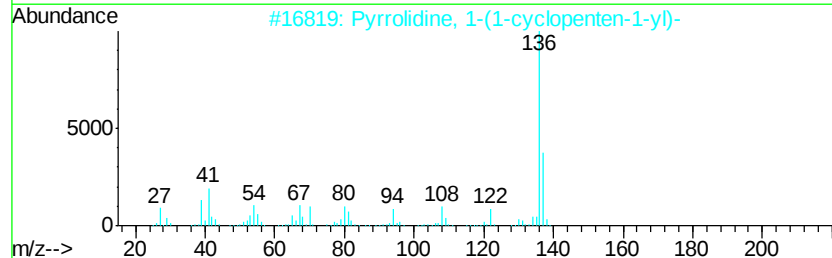
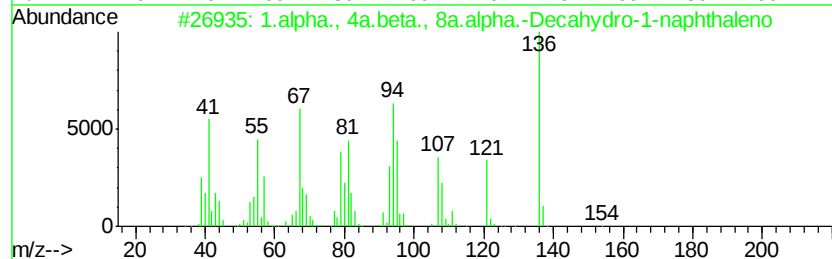
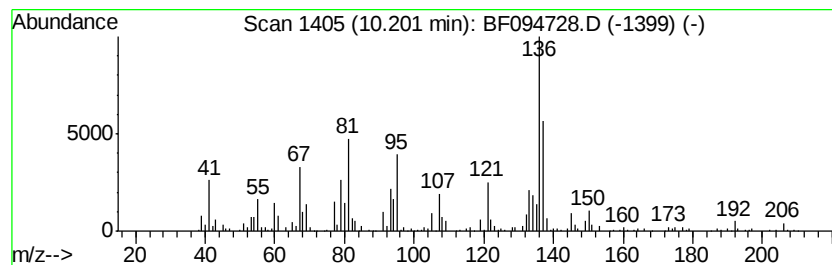
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 1.alpha., 4a.beta., 8a.alpha... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.20	10.36 ng	509087	Acenaphthene-d10	9.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1.alpha., 4a.beta., 8a.alpha.-De...	154	C10H18O	036159-47-4	58
2		Pyrrolidine, 1-(1-cyclopenten-1-...	137	C9H15N	007148-07-4	47
3		2.alpha., 4a.beta., 8a.alpha.-De...	154	C10H18O	005779-35-1	46
4		3,5,7-Trimethyl-1,2(4H)-diazepine	136	C8H12N2	088829-73-6	43
5		2,5-Methano-1H-indene, octahydro-	136	C10H16	019026-94-9	43



Data Path : Z:\HPCHEM1\BNA F\DATA\BF043017\
Data File : BF094728.D
Acq On : 30 Apr 2017 21:25
Operator : SJ/MA
Sample : I2860-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
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ClientSampleId :
HW-32

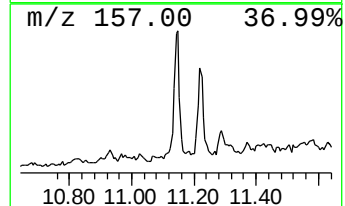
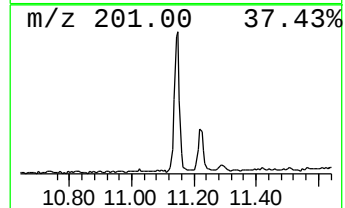
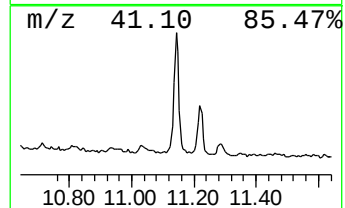
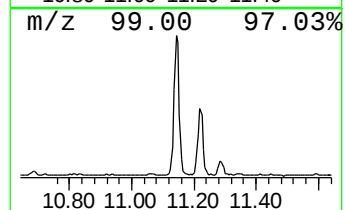
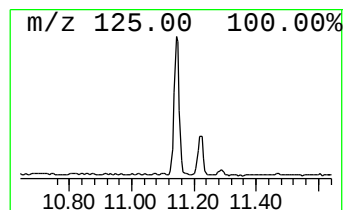
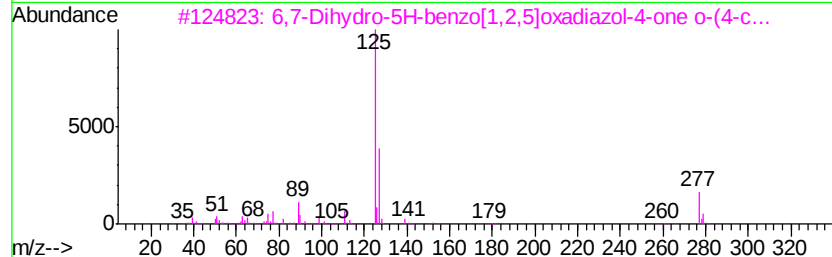
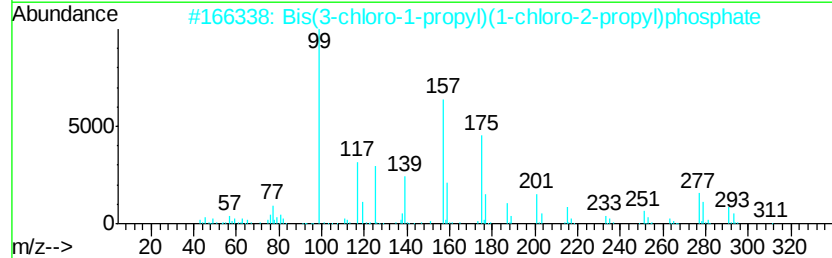
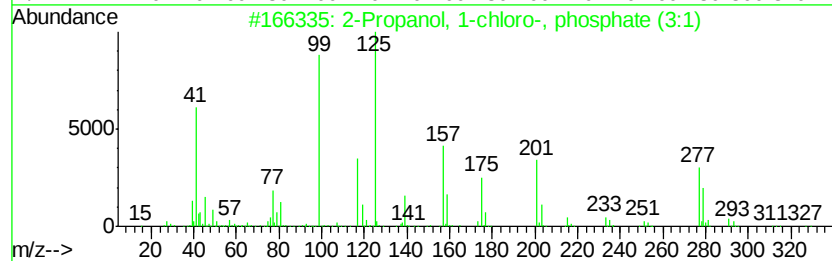
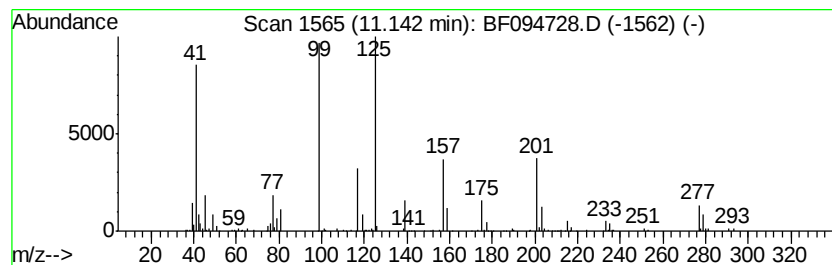
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 2-Propanol, 1-chloro-, phos... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.14	10.77 ng	607130	Phenanthrene-d10	11.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Propanol, 1-chloro-, phosphate...	326	C9H18Cl3O4P	013674-84-5	91
2		Bis(3-chloro-1-propyl)(1-chloro-...	326	C9H18Cl3O4P	137888-35-8	16
3		6,7-Dihydro-5H-benzo[1,2,5]oxadi...	277	C13H12ClN3O2	1000301-42-2	10
4		4-Chloro-2-nitrobenzoic acid	201	C7H4ClN04	006280-88-2	10
5		Benzoic acid, 4-[[2-(1-piperazin...	277	C14H19N3O3	1000350-32-6	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF043017\
Data File : BF094728.D
Acq On : 30 Apr 2017 21:25
Operator : SJ/MA
Sample : I2860-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HW-32

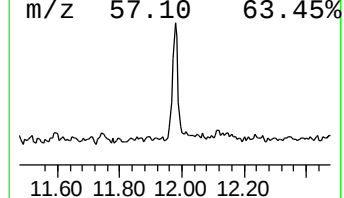
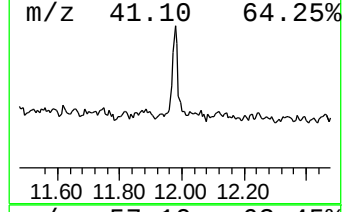
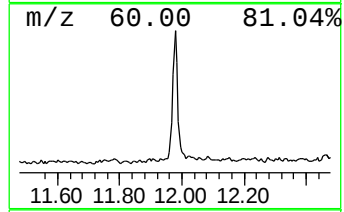
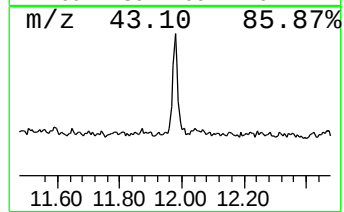
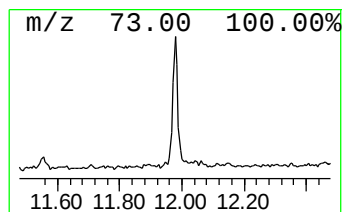
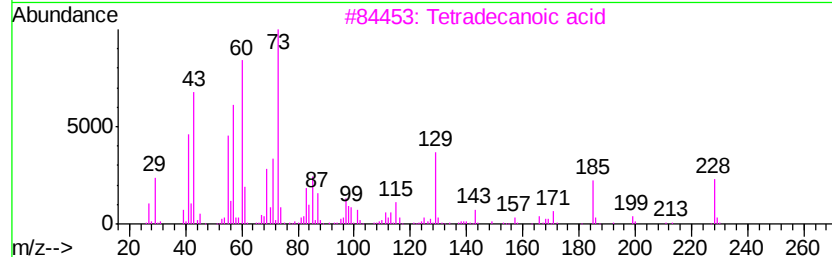
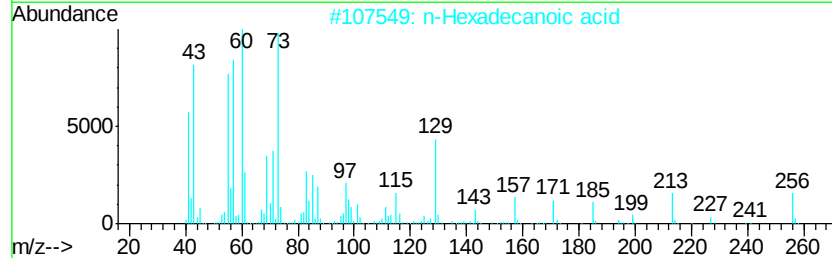
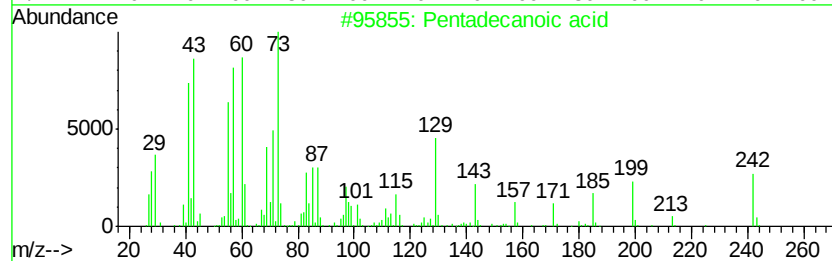
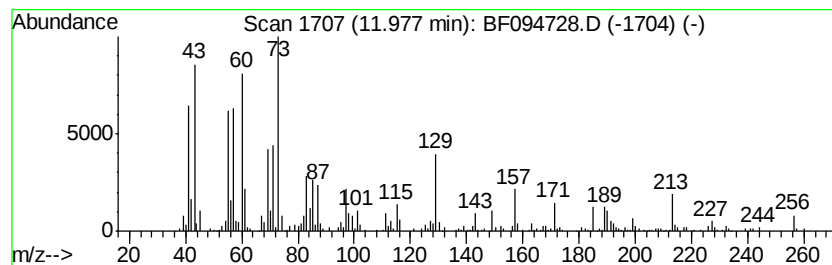
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 Pentadecanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.98	7.03 ng	396013	Phenanthrene-d10	11.22

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	94
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	81
4			Tridecanoic acid	214	C13H26O2	000638-53-9	80
5			n-Decanoic acid	172	C10H20O2	000334-48-5	76



Data Path : Z:\HPCHEM1\BNA F\DATA\BF043017\
Data File : BF094728.D
Acq On : 30 Apr 2017 21:25
Operator : SJ/MA
Sample : I2860-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

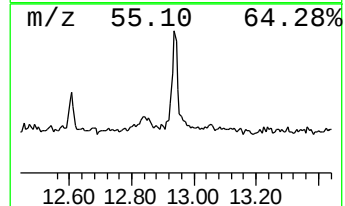
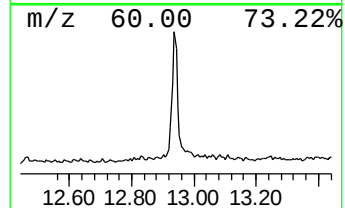
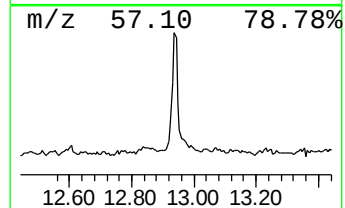
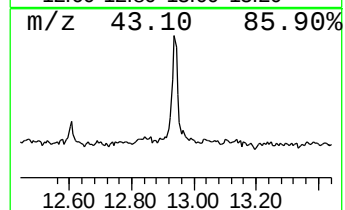
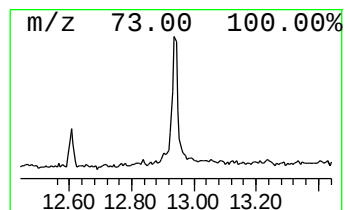
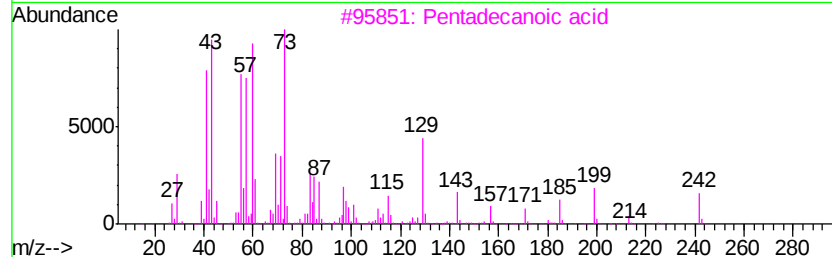
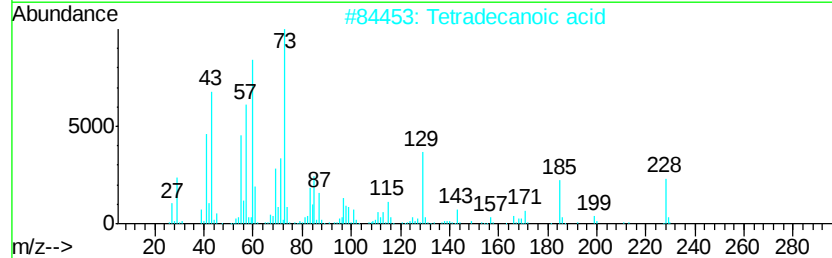
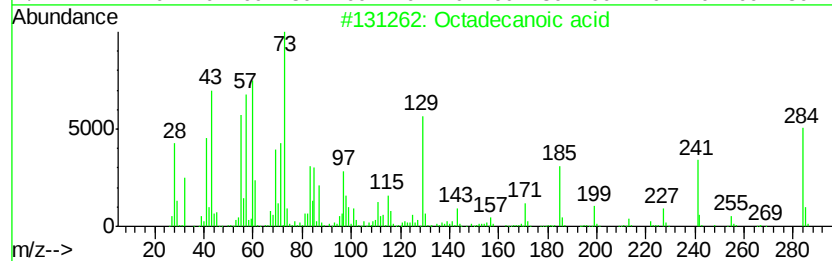
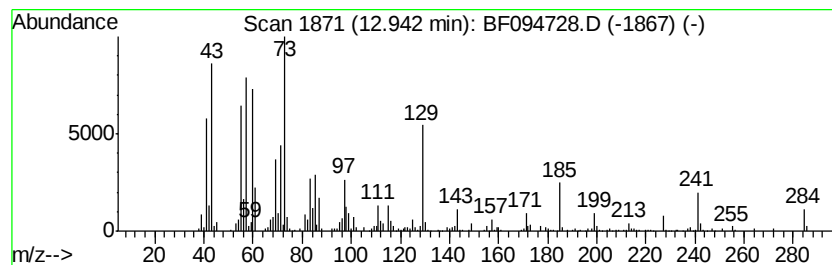
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.		
12.94	12.15 ng	386986	Chrysene-d12		14.47		
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	83
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			n-Decanoic acid	172	C10H20O2	000334-48-5	78
5			Tridecanoic acid	214	C13H26O2	000638-53-9	70



Data Path : Z:\HPCHEM1\BNA F\DATA\BF043017\
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Acq On : 30 Apr 2017 21:25
Operator : SJ/MA
Sample : I2860-04
Misc :
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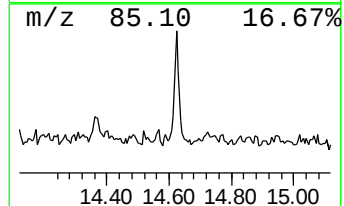
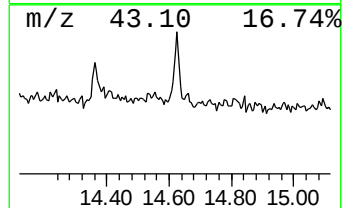
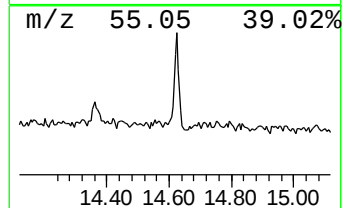
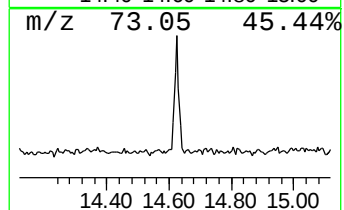
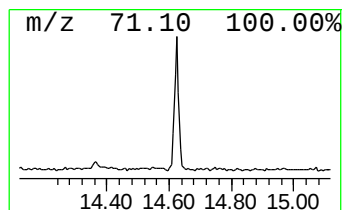
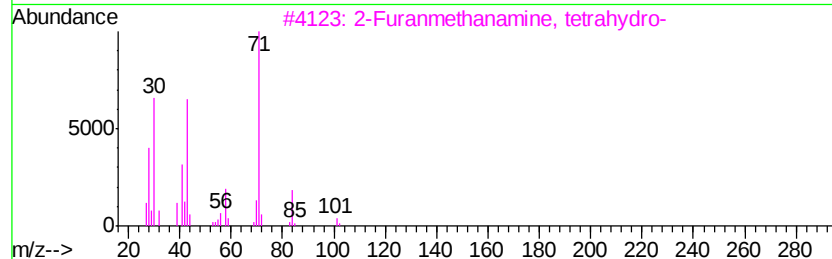
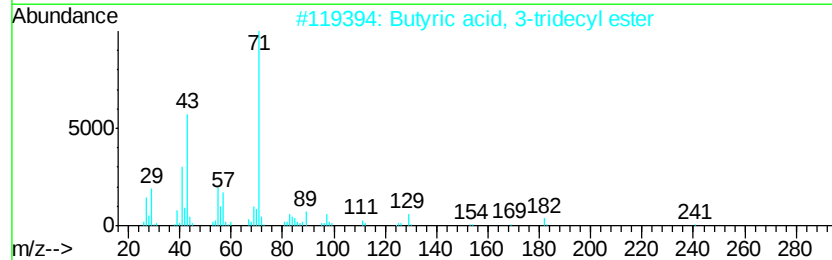
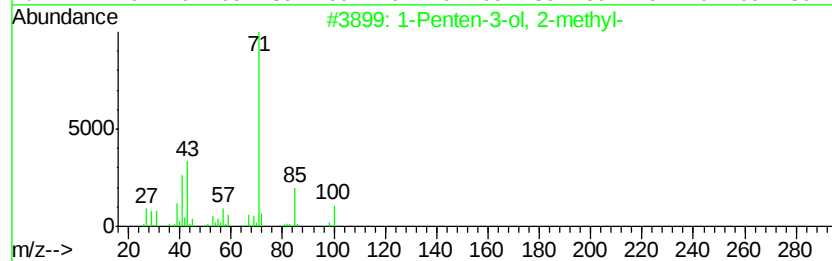
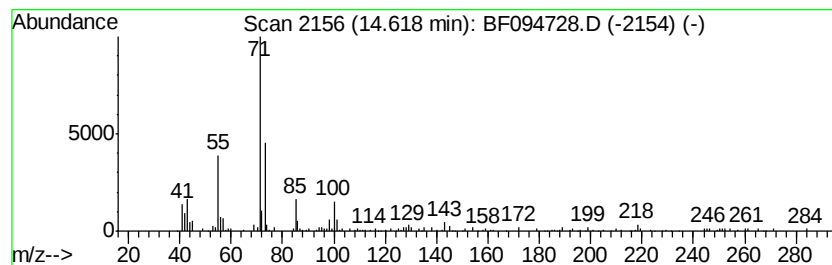
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 1-Penten-3-ol, 2-methyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.62	5.05 ng	160635	Chrysene-d12	14.47	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Penten-3-ol, 2-methyl-	100	C6H12O	002088-07-5	64
2	Butyric acid, 3-tridecyl ester	270	C17H34O2	1000280-56-8	53
3	2-Furanmethanamine, tetrahydro-	101	C5H11NO	004795-29-3	50
4	Furan, 2-butyltetrahydro-	128	C8H16O	001004-29-1	50
5	1-Methylcycloheptanol	128	C8H16O	003761-94-2	45



Data Path : Z:\HPCHEM1\BNA F\DATA\BF043017\
Data File : BF094728.D
Acq On : 30 Apr 2017 21:25
Operator : SJ/MA
Sample : I2860-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HW-32

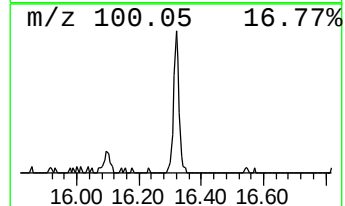
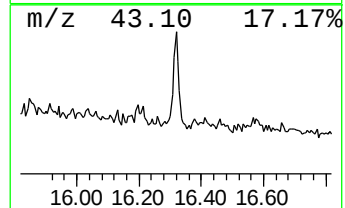
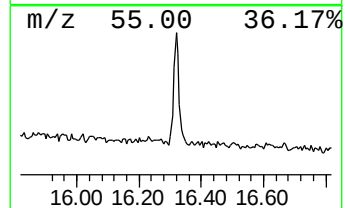
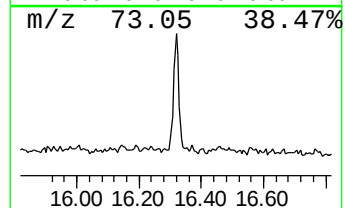
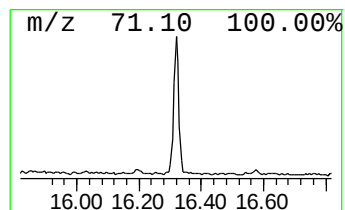
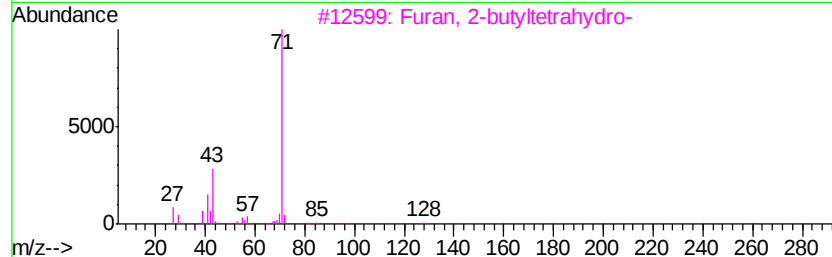
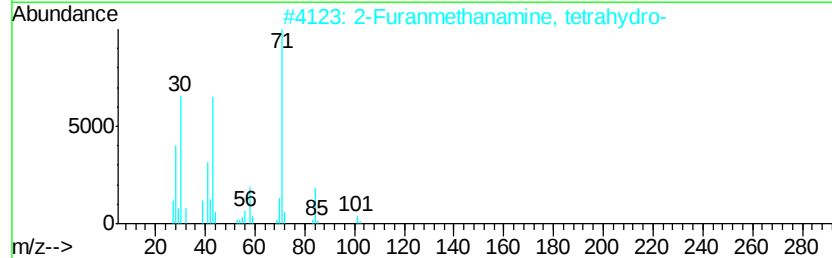
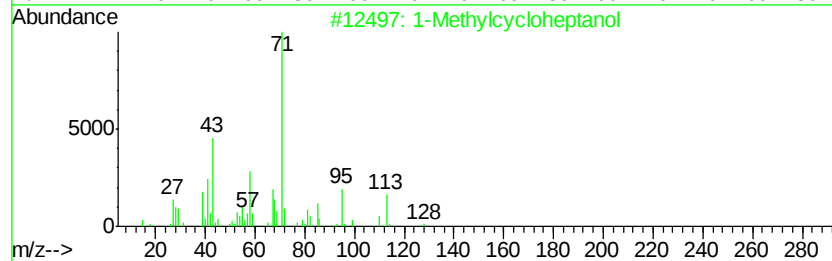
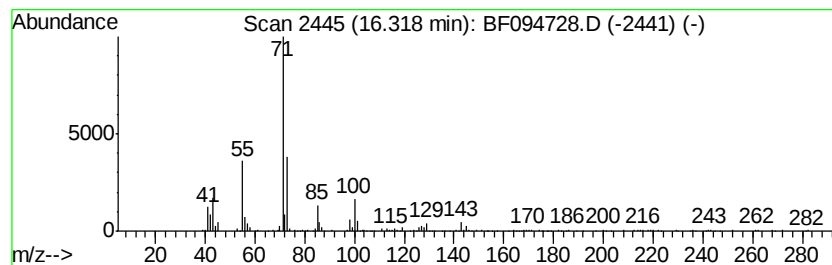
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 19 1-Methylcycloheptanol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.32	7.69 ng	228004	Perylene-d12	16.10

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Methylcycloheptanol	128	C8H16O	003761-94-2	53
2			2-Furanmethanamine, tetrahydro-	101	C5H11NO	004795-29-3	52
3			Furan, 2-butyltetrahydro-	128	C8H16O	001004-29-1	47
4			Diethylmalonic acid, monochlorid...	262	C12H19ClO4	1000370-65-0	42
5			Butanoic acid, 2-butoxy-1-methyl...	216	C11H20O4	007492-70-8	40



Data Path : Z:\HPCHEM1\BNA F\DATA\BF043017\
Data File : BF094728.D
Acq On : 30 Apr 2017 21:25
Operator : SJ/MA
Sample : I2860-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HW-32

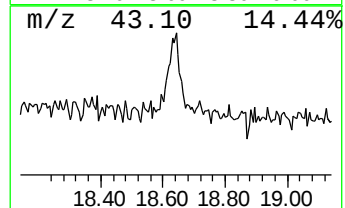
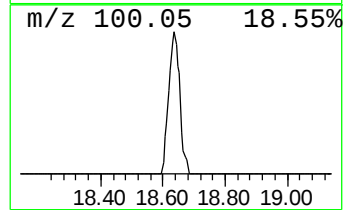
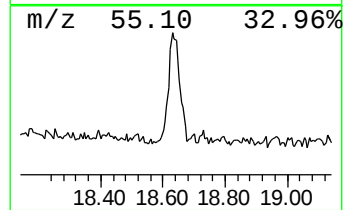
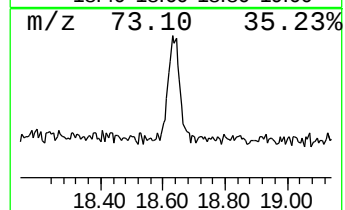
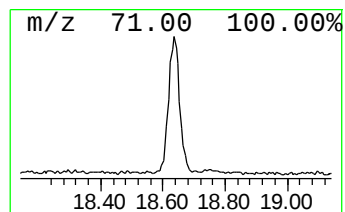
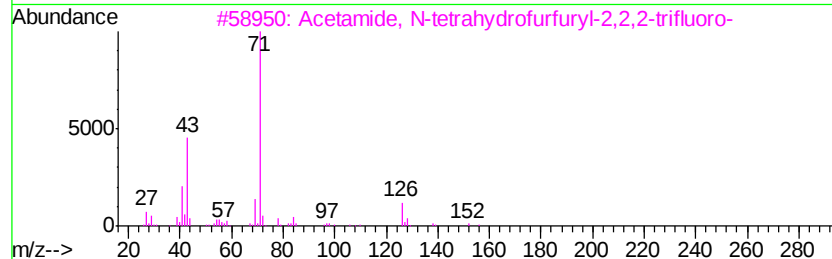
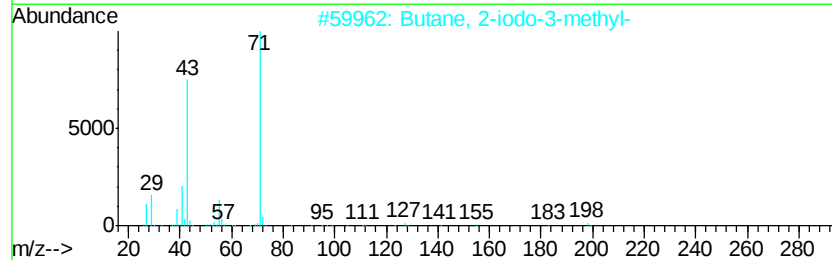
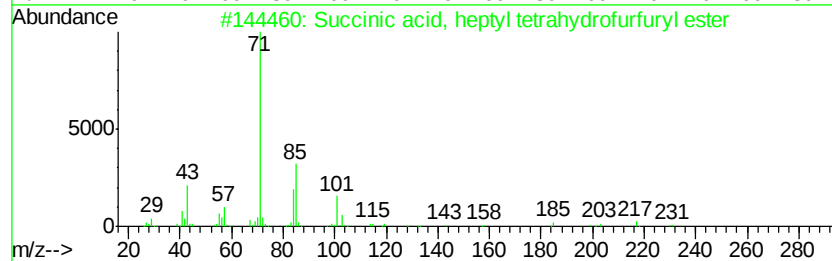
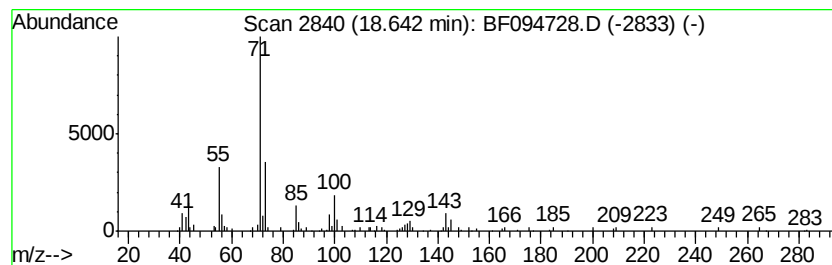
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 20 unknown18.64 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.64	5.53 ng	163829	Perylene-d12	16.10

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Succinic acid, heptyl tetrahydro...	300	C16H28O5	1000329-86-5	37
2			Butane, 2-iodo-3-methyl-	198	C5H11I	018295-27-7	37
3			Acetamide, N-tetrahydrofurfuryl-	197	C7H10F3NO2	1000307-30-7	37
4			Isobutyramide, N-methyl-	141	C8H15NO	1000339-96-0	37
5			2,2-Dimethylperhydro-1,3-oxazine	115	C6H13NO	073155-29-0	36



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF043017\
 Data File : BF094728.D
 Acq On : 30 Apr 2017 21:25
 Operator : SJ/MA
 Sample : I2860-04
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HW-32

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	3.37	16.0	ng	523876	1	5.76	655044	20.0
2-Pentanone, 4-hy...	3.92	52.9	ng	1731050	1	5.76	655044	20.0
2-Pentanone, 4-me...	4.70	9.1	ng	296411	1	5.76	655044	20.0
unknown5.51	5.51	51.2	ng	1676920	1	5.76	655044	20.0
Cyclohexaneacetic...	7.37	5.8	ng	333027	2	7.25	1153740	20.0
unknown7.76	7.76	10.1	ng	579999	2	7.25	1153740	20.0
unknown7.82	7.82	4.4	ng	256321	2	7.25	1153740	20.0
unknown7.94	7.94	4.6	ng	263260	2	7.25	1153740	20.0
m-Tolylacetic acid	8.40	22.2	ng	1090930	3	9.39	982332	20.0
unknown8.52	8.52	5.0	ng	247499	3	9.39	982332	20.0
unknown9.51	9.51	12.2	ng	599515	3	9.39	982332	20.0
Dodecanoic acid	9.88	193.9	ng	9524540	3	9.39	982332	20.0
1.alpha., 4a.beta...	10.20	10.4	ng	509087	3	9.39	982332	20.0
2-Propanol, 1-chl...	11.14	10.8	ng	607130	4	11.22	1127130	20.0
Pentadecanoic acid	11.98	7.0	ng	396013	4	11.22	1127130	20.0
Octadecanoic acid	12.94	12.2	ng	386986	5	14.47	636769	20.0
1-Penten-3-ol, 2-...	14.62	5.0	ng	160635	5	14.47	636769	20.0
1-Methylcyclohept...	16.32	7.7	ng	228004	6	16.10	592909	20.0
unknown18.64	18.64	5.5	ng	163829	6	16.10	592909	20.0