

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041117\
 Data File : BF094368.D
 Acq On : 11 Apr 2017 23:32
 Operator : SJ/MA
 Sample : I2611-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VIRGINROCK-1

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-BF032217.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	3.416	256	260	266	rBV	820314	818285	33.19%	4.023%
2	3.957	348	352	358	rBV	384178	379652	15.40%	1.867%
3	4.381	420	424	438	rBV	1223839	1229733	49.88%	6.046%
4	5.457	603	607	615	rVB	1784503	1842508	74.73%	9.059%
5	5.581	624	628	639	rVB	1741087	1648134	66.85%	8.104%
6	5.828	666	670	674	rBV	897013	782003	31.72%	3.845%
7	6.004	696	700	704	rBV	1840590	1750327	70.99%	8.606%
8	6.475	774	780	783	rBV	1335449	1320130	53.54%	6.491%
9	7.333	920	926	929	rBV	1011468	1022432	41.47%	5.027%
10	8.657	1143	1151	1154	rVB	2338956	2465568	100.00%	12.123%
11	9.151	1231	1235	1239	rBV	75029	72314	2.93%	0.356%
12	9.469	1281	1289	1294	rBV2	944345	1017571	41.27%	5.003%
13	10.063	1386	1390	1393	rVB	70923	65377	2.65%	0.321%
14	10.333	1432	1436	1440	rVB	28306	37987	1.54%	0.187%
15	10.445	1451	1455	1459	rBV	367337	362787	14.71%	1.784%
16	10.592	1477	1480	1485	rVB	35462	38610	1.57%	0.190%
17	10.645	1486	1489	1491	rBV	81360	79711	3.23%	0.392%
18	11.204	1580	1584	1587	rBV	79821	80765	3.28%	0.397%
19	11.239	1587	1590	1595	rVB3	36746	46938	1.90%	0.231%
20	11.292	1595	1599	1603	rBV	811471	843699	34.22%	4.148%
21	11.733	1670	1674	1677	rBV	49102	54382	2.21%	0.267%
22	12.039	1721	1726	1732	rVB8	41686	74379	3.02%	0.366%
23	12.233	1757	1759	1764	rVB	41989	38289	1.55%	0.188%
24	12.633	1824	1827	1831	rVB5	50929	63935	2.59%	0.314%
25	12.715	1838	1841	1844	rBV2	54639	75417	3.06%	0.371%
26	12.751	1844	1847	1851	rVV5	80222	128784	5.22%	0.633%
27	12.786	1851	1853	1857	rVB	39618	38458	1.56%	0.189%
28	13.062	1897	1900	1904	rBV	37279	45967	1.86%	0.226%
29	13.180	1917	1920	1923	rBV2	32502	46395	1.88%	0.228%
30	13.274	1931	1936	1940	rBV	1750983	1845744	74.86%	9.075%
31	13.315	1941	1943	1952	rVB5	93407	139392	5.65%	0.685%
32	13.904	2039	2043	2049	rVB	118239	195971	7.95%	0.964%
33	14.139	2078	2083	2088	rBV3	125053	188486	7.64%	0.927%
34	14.551	2148	2153	2158	rBV	702254	825334	33.47%	4.058%

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

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

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35	16.180	2426	2430	2436	rVB	574747	672555	27.28%	3.307%
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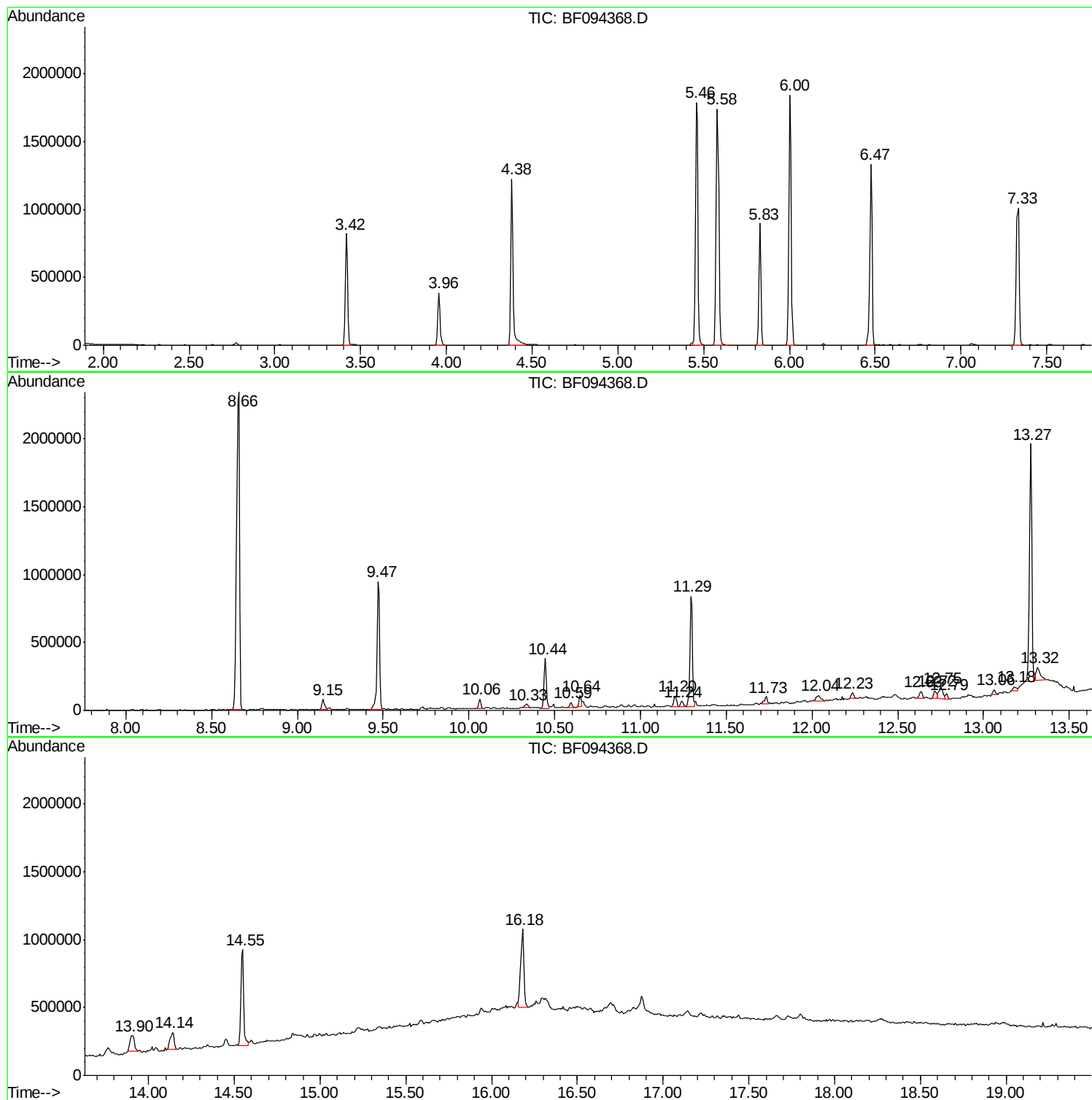
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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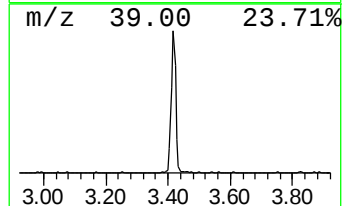
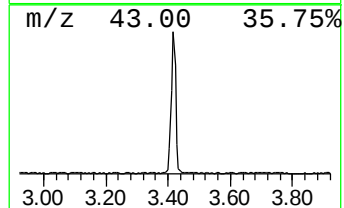
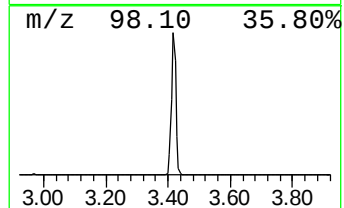
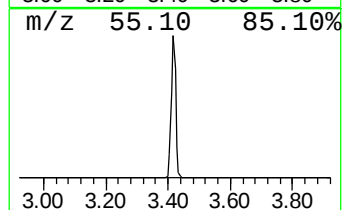
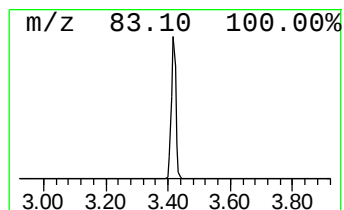
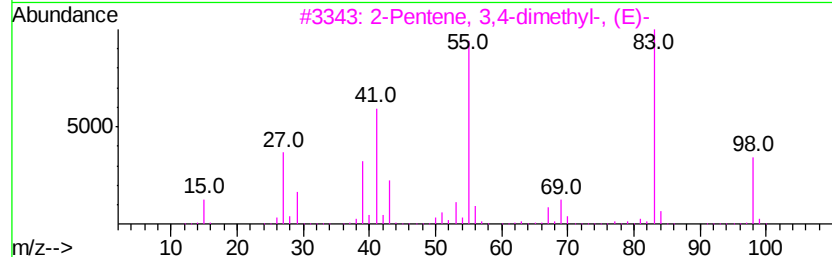
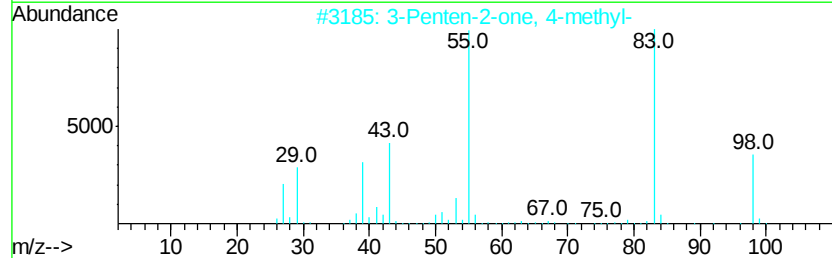
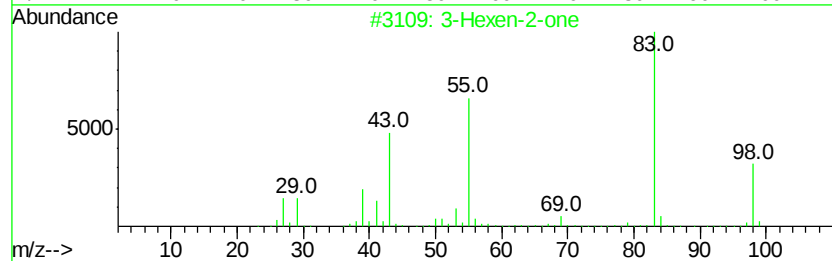
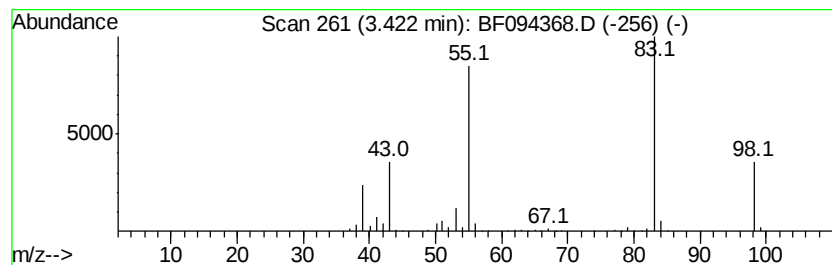
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Hexen-2-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.42	20.93 ng	818285	1,4-Dichlorobenzene-d4	5.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Hexen-2-one	98	C6H10O	000763-93-9	91
2		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78



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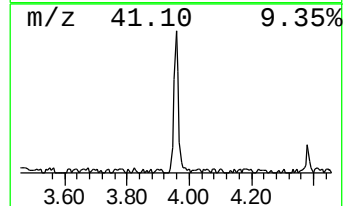
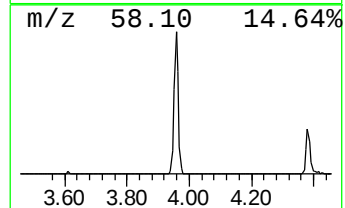
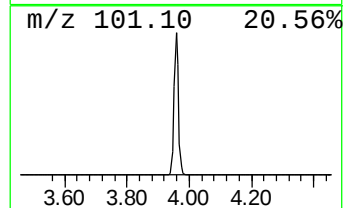
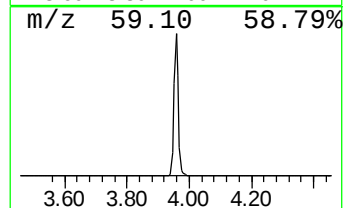
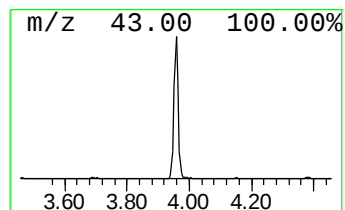
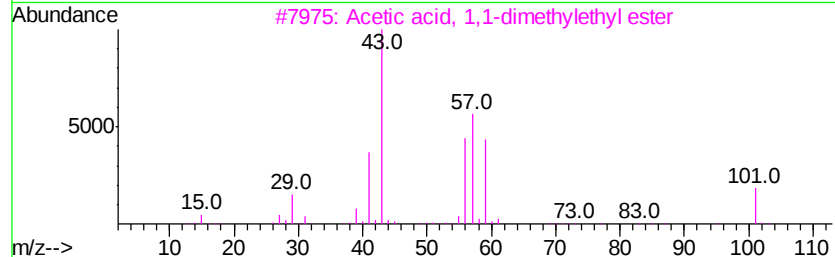
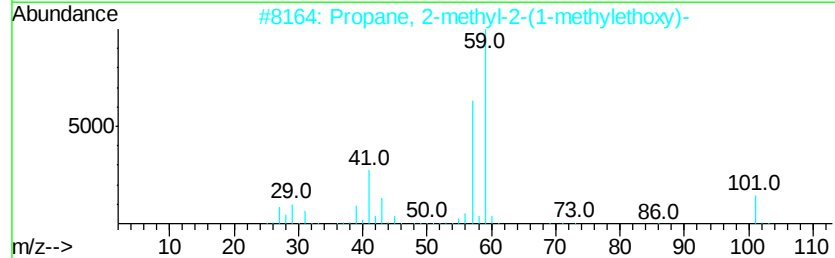
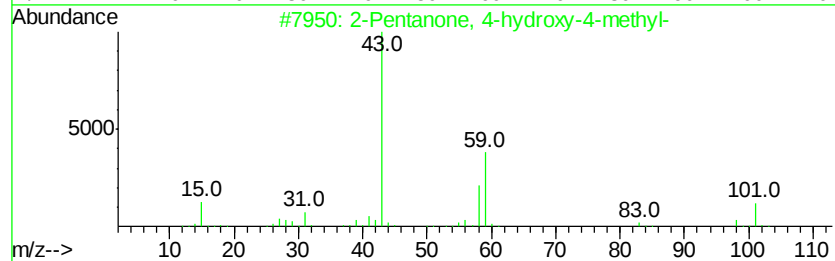
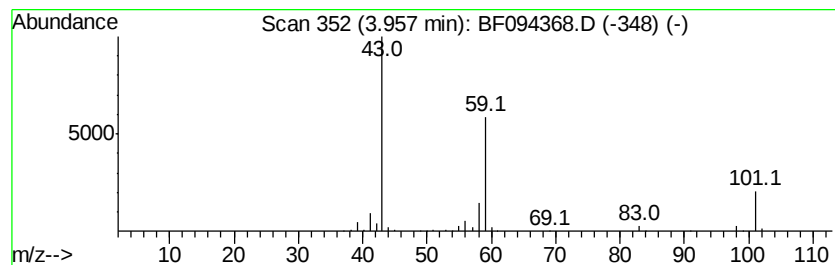
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.96	9.71 ng	379652	1,4-Dichlorobenzene-d4	5.83

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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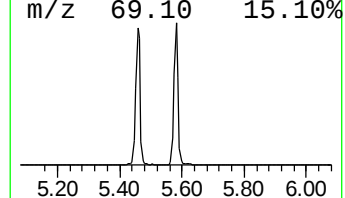
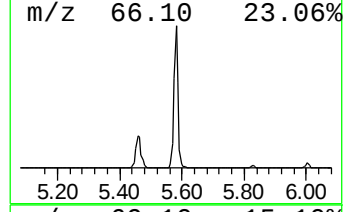
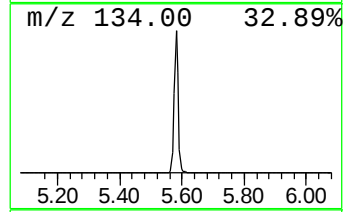
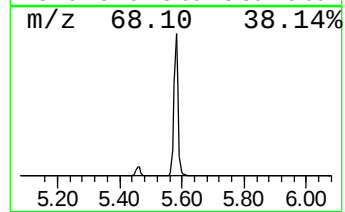
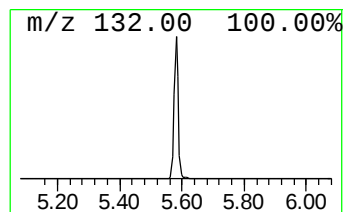
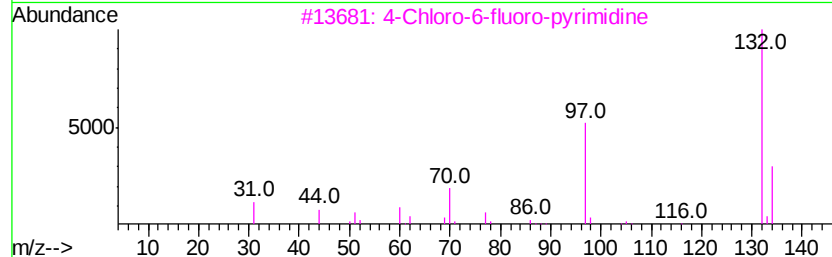
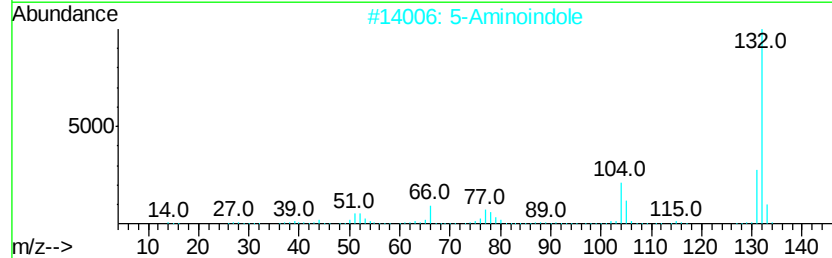
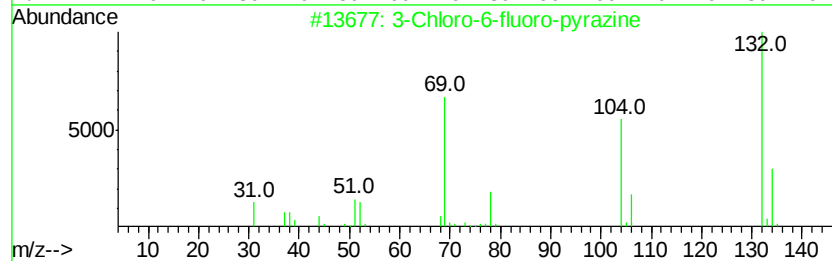
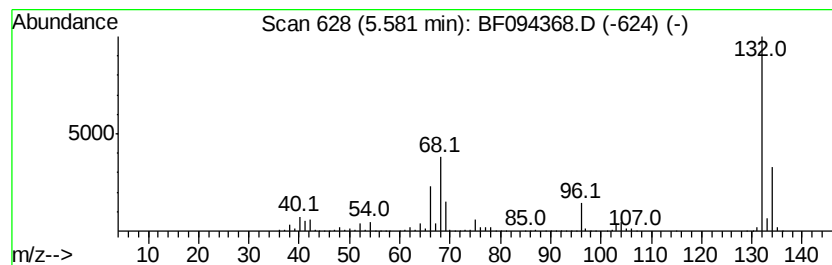
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown5.58 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.58	42.15 ng	1648130	1,4-Dichlorobenzene-d4	5.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3	Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	5	Aminoindole	132	C8H8N2	005192-03-0	12
3	4	Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
4	5	Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	1H	Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9



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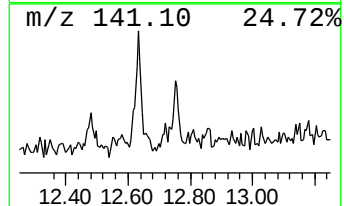
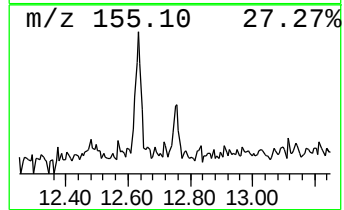
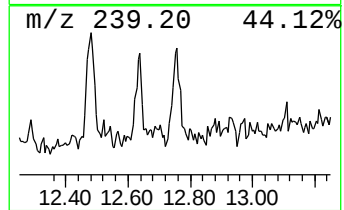
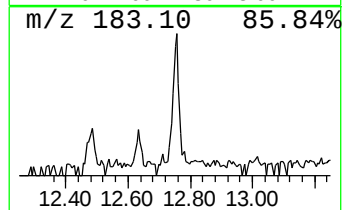
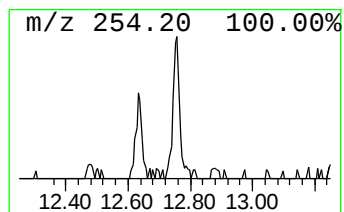
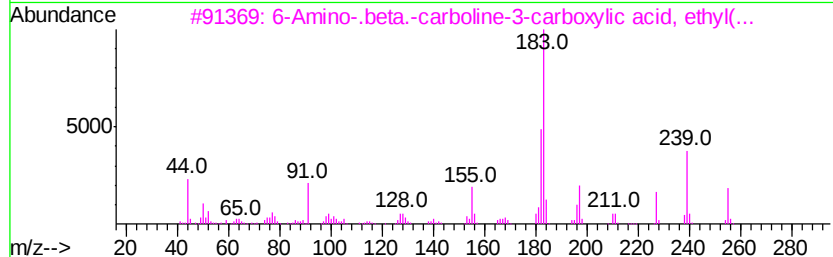
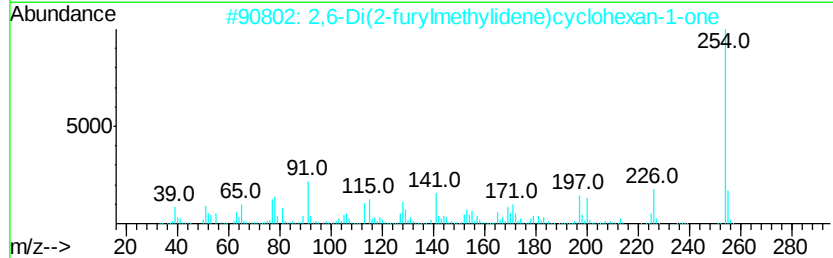
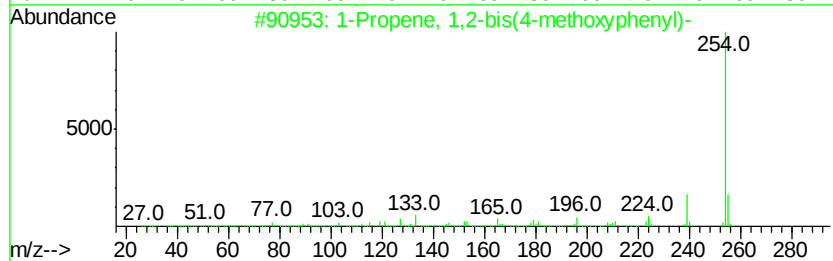
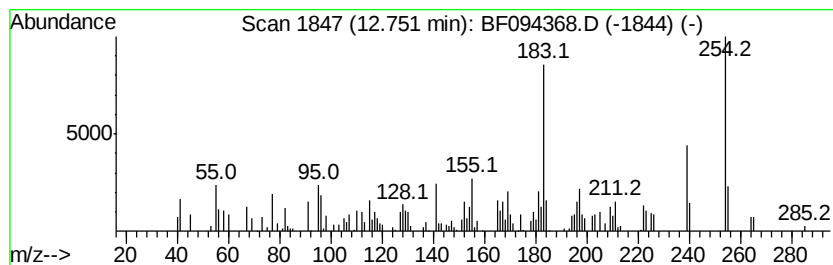
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown12.75 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.75	3.05 ng	128784	Phenanthrene-d10	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 1,2-bis(4-methoxyphen...	254	C17H18O2	020802-02-2	38
2	2,6-Di(2-furylmethylidene)cyclohex...	254	C16H14O3	000893-00-5	30
3	6-Amino-.beta.-carboline-3-carbo...	255	C14H13N3O2	078539-57-8	30
4	.beta.-Carboline, 3-ethoxycarbon...	254	C15H14N2O2	124487-93-0	30
5	Benzoic acid, 4-[2-(3-methoxyphe...	254	C16H14O3	1000197-90-6	30



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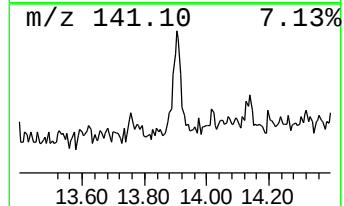
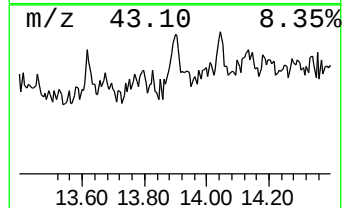
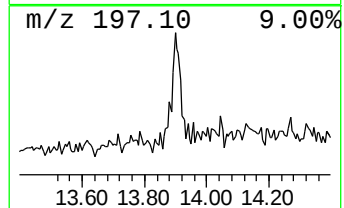
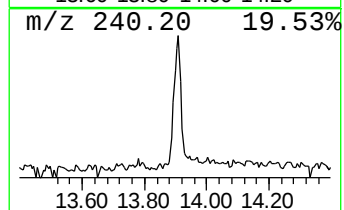
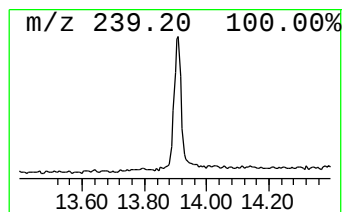
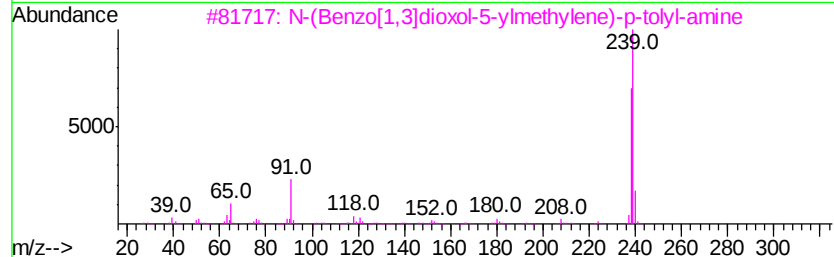
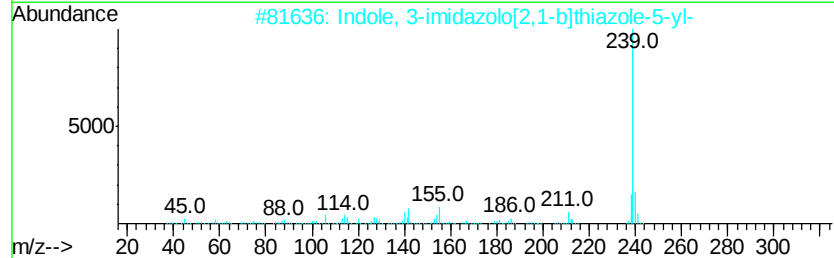
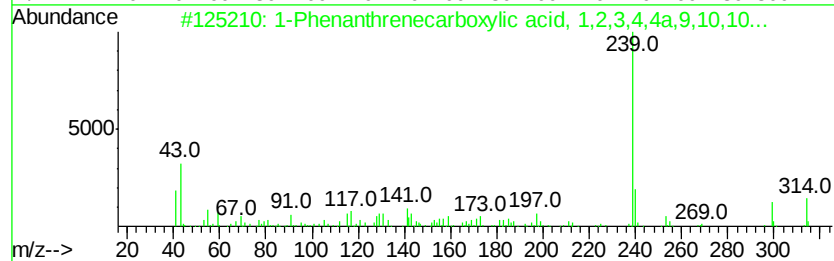
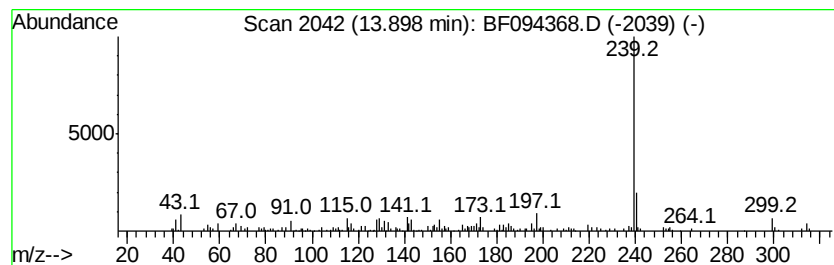
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Phenanthrenecarboxylic ac... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	4.75 ng	195971	Chrysene-d12	14.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Phenanthrenecarboxylic acid, 1...	314	C21H30O2	001235-74-1	95
2		Indole, 3-imidazo[2,1-b]thiazolo...	239	C13H9N3S	292855-05-1	59
3		N-(Benzo[1,3]dioxol-5-yl)methyl-...	239	C15H13NO2	007402-58-6	59
4		2-(p-Acetylanilino)tropone	239	C15H13NO2	1000241-52-9	50
5		4-Amino-2-(5-methyl-2-benzimidaz...	239	C14H13N3O	1000258-88-5	45



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041117\
Data File : BF094368.D
Acq On : 11 Apr 2017 23:32
Operator : SJ/MA
Sample : I2611-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VIRGINROCK-1

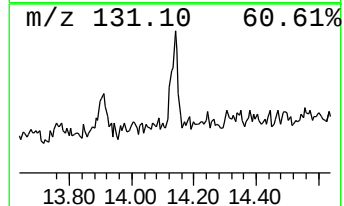
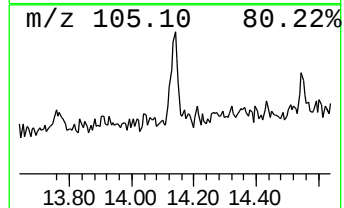
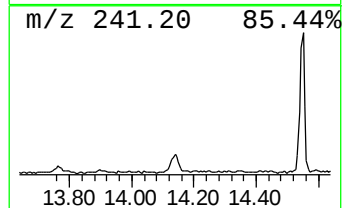
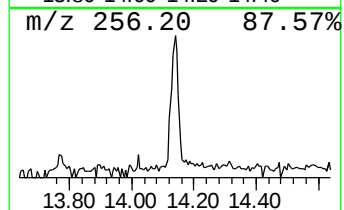
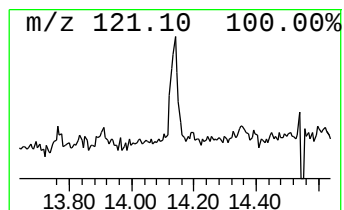
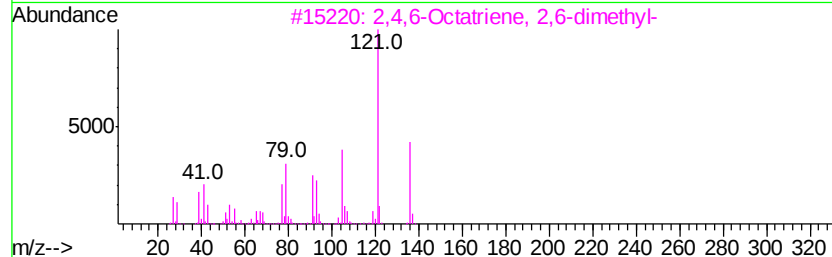
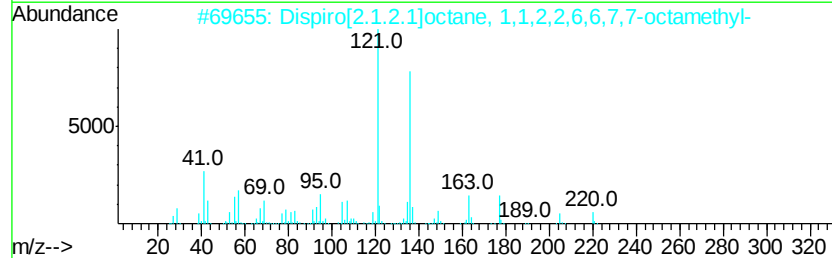
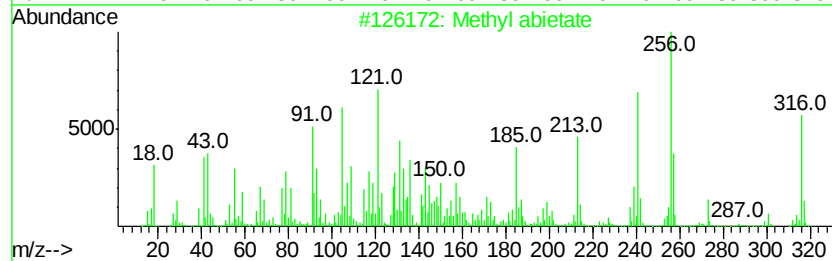
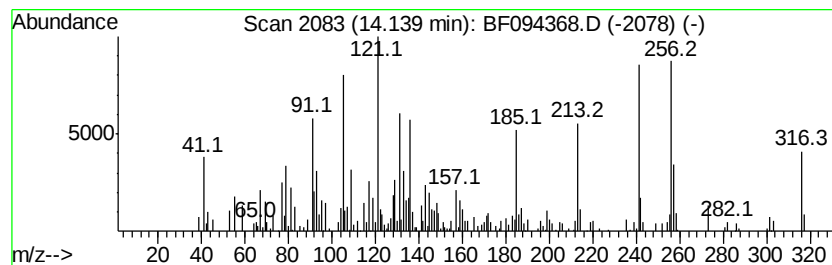
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Methyl abietate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.14	4.57 ng	188486	Chrysene-d12	14.55

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Methyl abietate	316	C21H32O2	000127-25-3	89
2		Dispiro[2.1.2.1]octane, 1,1,2,2,...	220	C16H28	1000159-45-5	53
3		2,4,6-Octatriene, 2,6-dimethyl-	136	C10H16	000673-84-7	45
4		2,4,6-Octatriene, 2,6-dimethyl-,...	136	C10H16	007216-56-0	45
5		Phenol, 2-[5-(2-furyl)pyrazol-3-...	256	C14H12N2O3	309923-40-8	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041117\
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Sample : I2611-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VIRGINROCK-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.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
3-Hexen-2-one	3.42	20.9	ng	818285	1	5.83	782003	20.0
2-Pentanone, 4-hy...	3.96	9.7	ng	379652	1	5.83	782003	20.0
unknown5.58	5.58	42.1	ng	1648130	1	5.83	782003	20.0
unknown12.75	12.75	3.0	ng	128784	4	11.29	843699	20.0
1-Phenanthrenecar...	13.90	4.8	ng	195971	5	14.55	825334	20.0
Methyl abietate	14.14	4.6	ng	188486	5	14.55	825334	20.0