

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022719\
 Data File : BF112736.D
 Acq On : 27 Feb 2019 23:18
 Operator : JU/SJ
 Sample : K1594-39 5X
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-9(4-5)

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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	5.334	548	552	556	rBV	706995	628125	47.59%	4.383%
2	6.357	723	726	733	rBV	744971	646578	48.99%	4.512%
3	6.504	747	751	754	rBV	804385	652048	49.41%	4.550%
4	6.740	788	791	795	rVB	1392376	1084677	82.19%	7.569%
5	6.898	814	818	821	rBV	552970	501678	38.01%	3.501%
6	7.292	881	885	892	rBV	464230	362093	27.44%	2.527%
7	8.022	1005	1009	1012	rBV	1681428	1305270	98.90%	9.108%
8	9.092	1188	1191	1195	rVB	796757	642770	48.70%	4.485%
9	9.192	1205	1208	1213	rVB2	20771	22818	1.73%	0.159%
10	9.486	1256	1258	1261	rBV	46988	32866	2.49%	0.229%
11	9.769	1302	1306	1310	rBV	1551149	1274553	96.58%	8.894%
12	10.216	1380	1382	1384	rVB	33784	23290	1.76%	0.163%
13	10.545	1435	1438	1443	rBV	398744	365197	27.67%	2.548%
14	10.686	1459	1462	1464	rBV2	44713	42630	3.23%	0.297%
15	11.133	1535	1538	1541	rVB3	42710	38757	2.94%	0.270%
16	11.169	1541	1544	1548	rVB	29446	30622	2.32%	0.214%
17	11.245	1553	1557	1560	rBV	1605878	1316307	99.74%	9.185%
18	11.463	1592	1594	1600	rBV2	17402	21945	1.66%	0.153%
19	11.557	1608	1610	1616	rBV3	40552	46886	3.55%	0.327%
20	11.780	1645	1648	1653	rBV2	89382	98569	7.47%	0.688%
21	11.857	1658	1661	1663	rBV3	29175	29181	2.21%	0.204%
22	11.963	1677	1679	1684	rVB2	41613	47377	3.59%	0.331%
23	12.298	1733	1736	1738	rBV2	47131	56818	4.31%	0.396%
24	12.351	1743	1745	1748	rVB	58965	48701	3.69%	0.340%
25	12.451	1760	1762	1764	rBV	51532	45574	3.45%	0.318%
26	12.704	1802	1805	1807	rBV	152685	151951	11.51%	1.060%
27	12.827	1822	1826	1829	rBV	789125	672150	50.93%	4.690%
28	13.416	1924	1926	1929	rBV2	103220	104199	7.90%	0.727%
29	13.868	2000	2003	2007	rVB	1399285	1319753	100.00%	9.209%
30	14.063	2034	2036	2038	rVB	167088	125999	9.55%	0.879%
31	14.663	2136	2138	2144	rBV2	232325	278862	21.13%	1.946%
32	15.280	2240	2243	2248	rVB	733307	883435	66.94%	6.164%
33	15.962	2356	2359	2366	rVB	455973	747985	56.68%	5.219%
34	16.368	2425	2428	2438	rVB	366394	681536	51.64%	4.756%

LSC Area Percent Report

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

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

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
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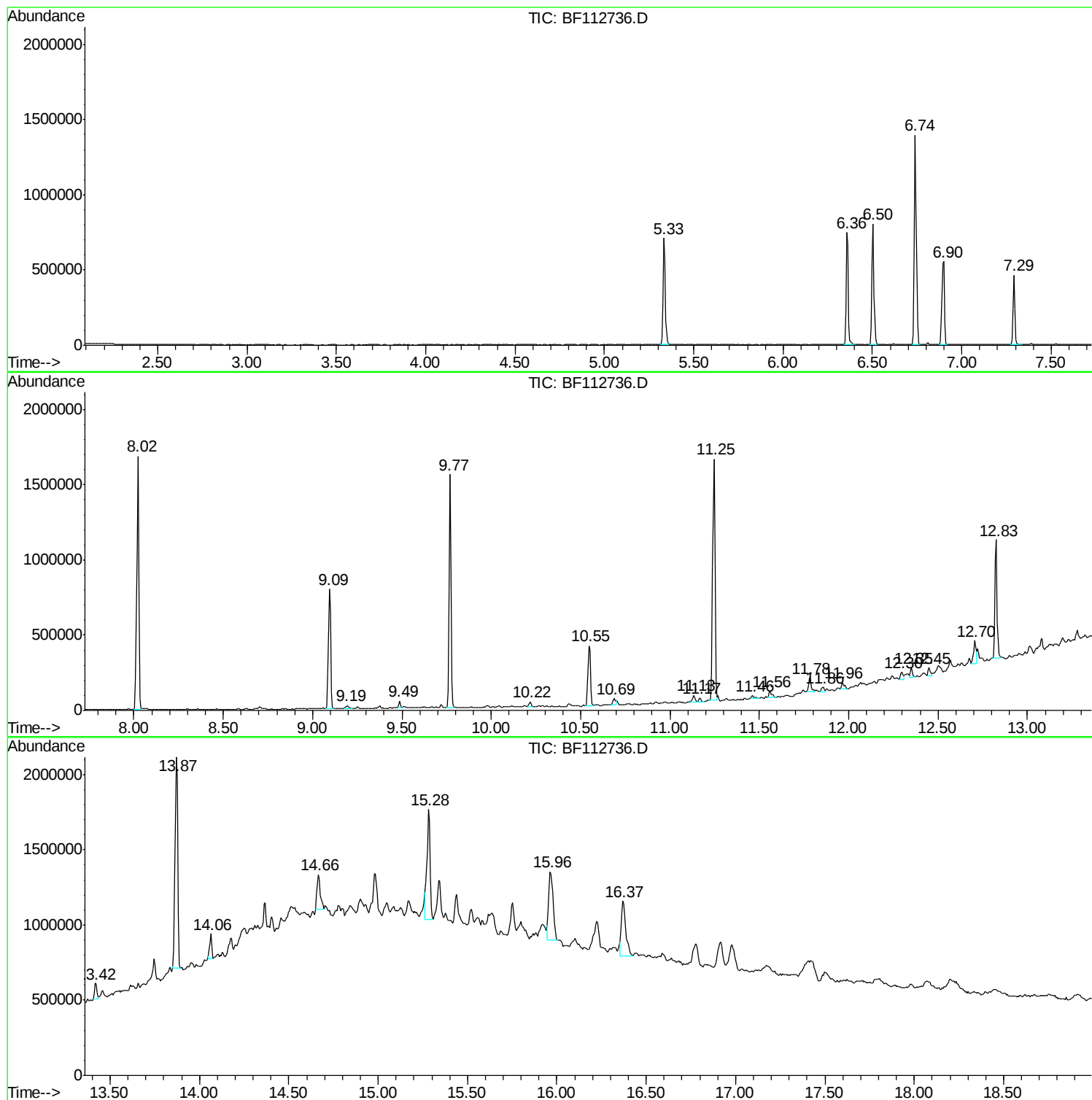
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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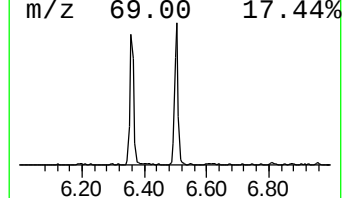
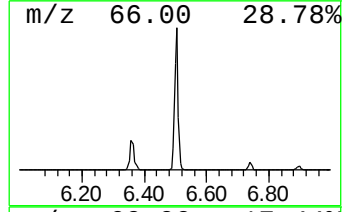
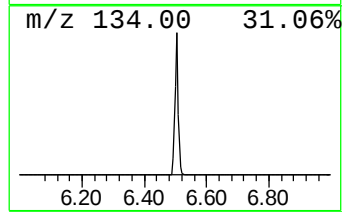
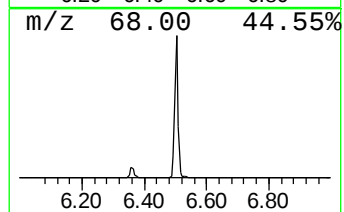
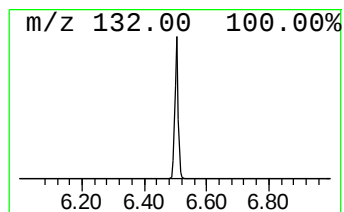
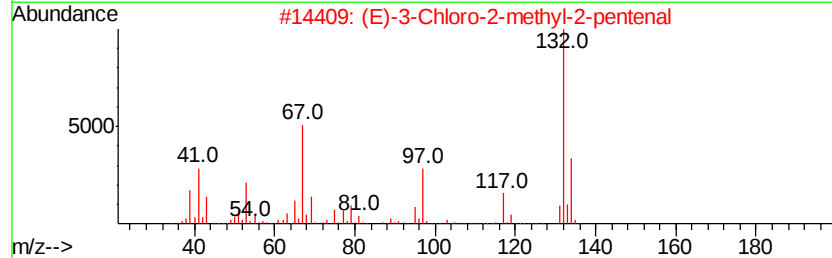
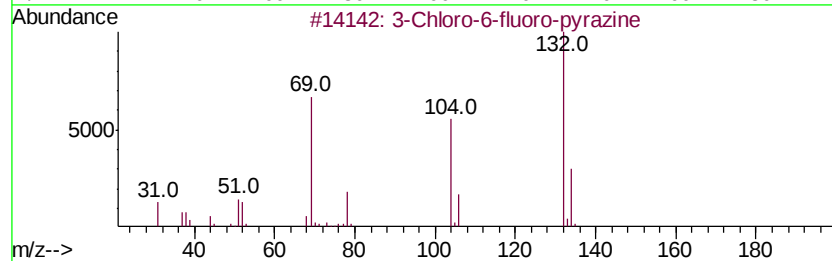
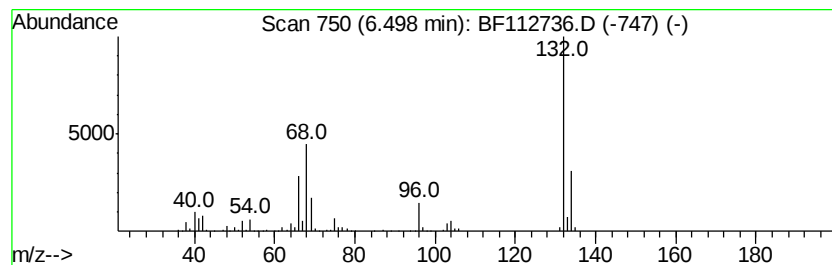
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.50 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	12.02 ng	652048	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	12
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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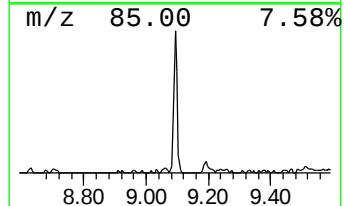
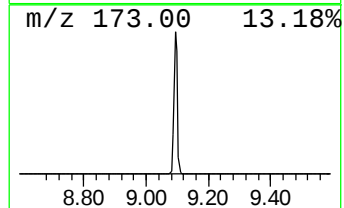
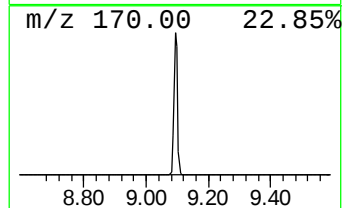
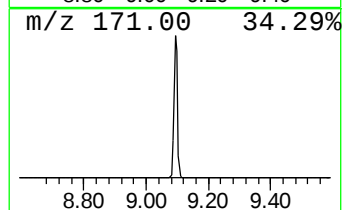
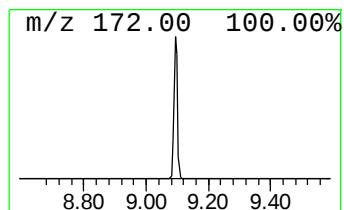
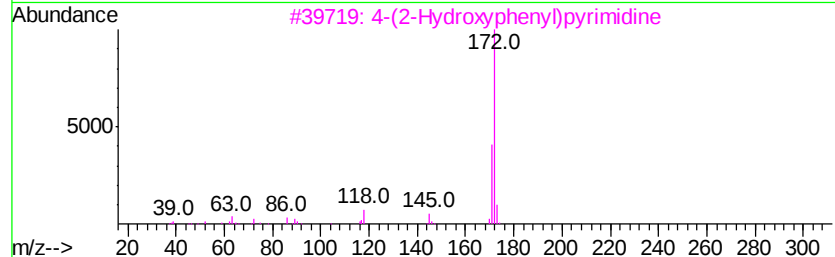
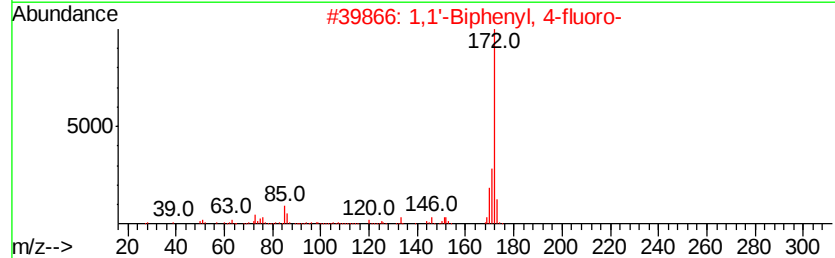
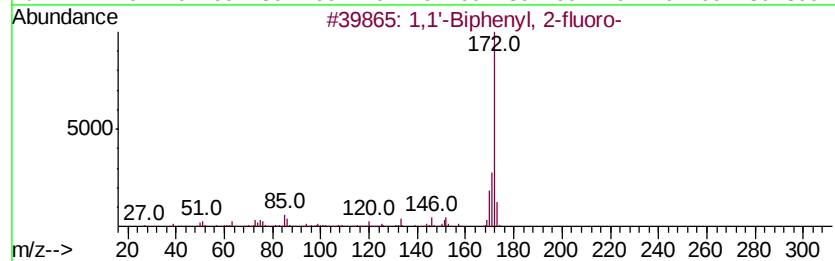
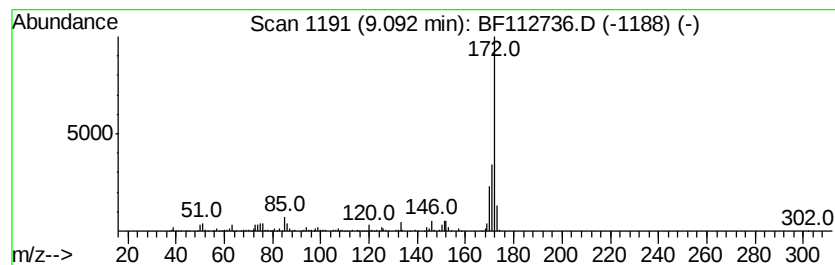
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1,1'-Biphenyl, 2-fluoro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.09	10.09 ng	642770	Acenaphthene-d10	9.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,1'-Biphenyl, 2-fluoro-	172	C12H9F	000321-60-8	96
2		1,1'-Biphenyl, 4-fluoro-	172	C12H9F	000324-74-3	94
3		4-(2-Hydroxyphenyl)pyrimidine	172	C10H8N2O	068535-55-7	59
4		4-Pyrimidinol, 5-phenyl-	172	C10H8N2O	022433-69-8	42
5		2-Naphthalenecarboxylic acid	172	C11H8O2	000093-09-4	38



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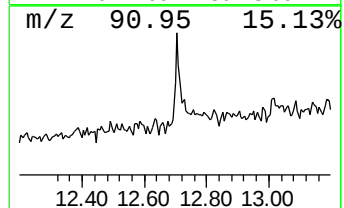
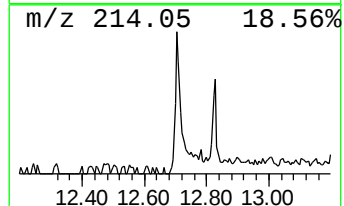
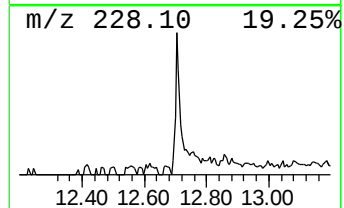
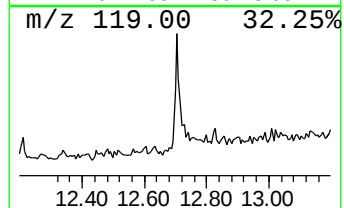
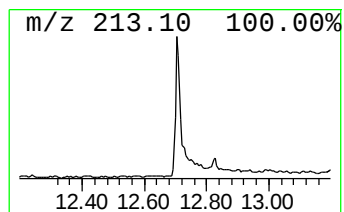
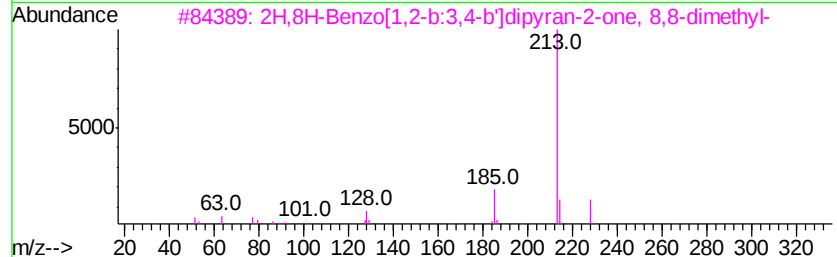
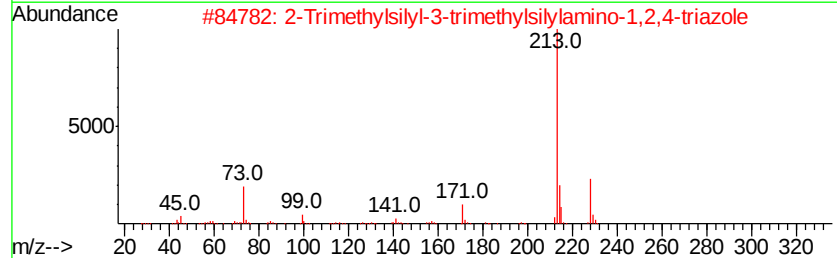
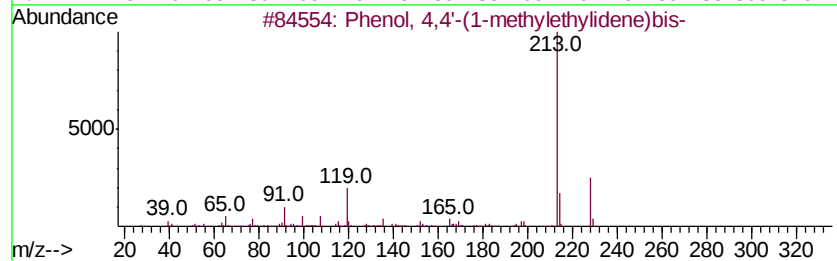
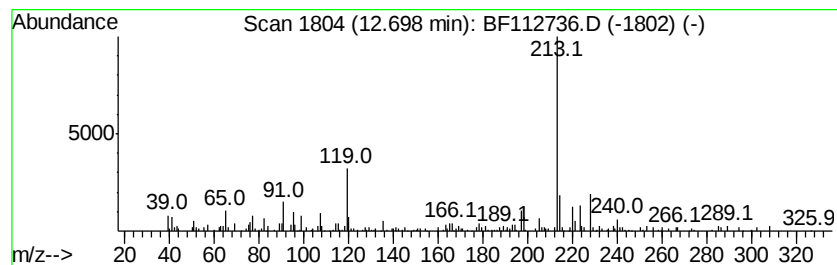
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Phenol, 4,4'-(1-methylethyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.70	2.30 ng	151951	Chrysene-d12	13.87	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene)bis-	228	C15H16O2	000080-05-7	94
2	2-Trimethylsilyl-3-trimethylsilyl-4,4'-biphenyl	228	C8H20N4Si2	1000373-05-5	53
3	2H,8H-Benzo[1,2-b:3,4-b']dipyrroline	228	C14H12O3	000523-59-1	53
4	Carbamic acid, [1,1'-biphenyl]-3-yl	213	C13H11NO2	055030-29-0	47
5	Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	47



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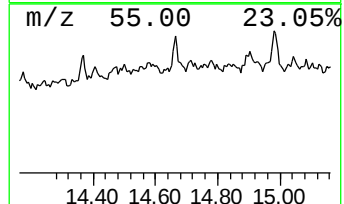
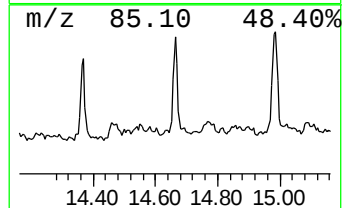
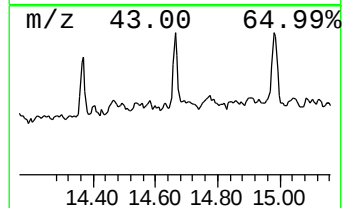
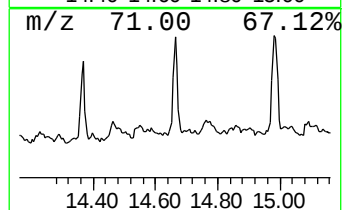
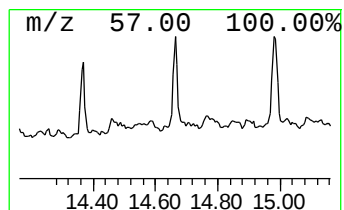
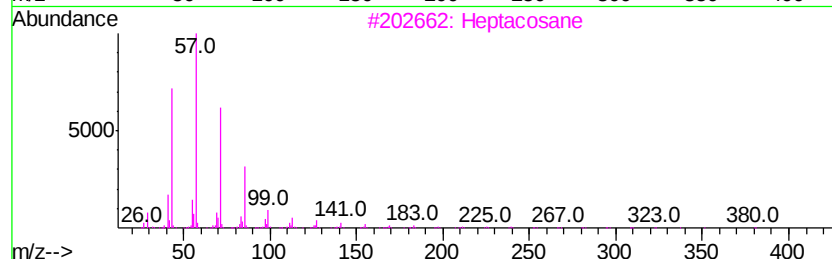
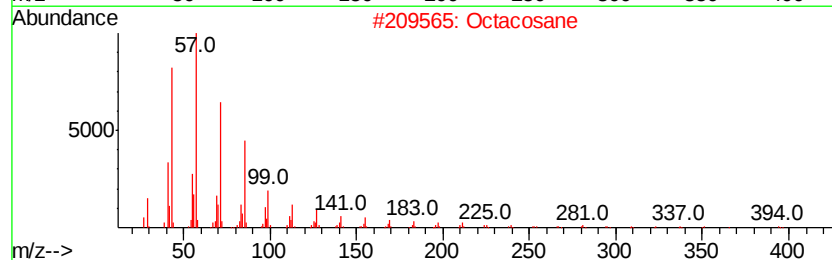
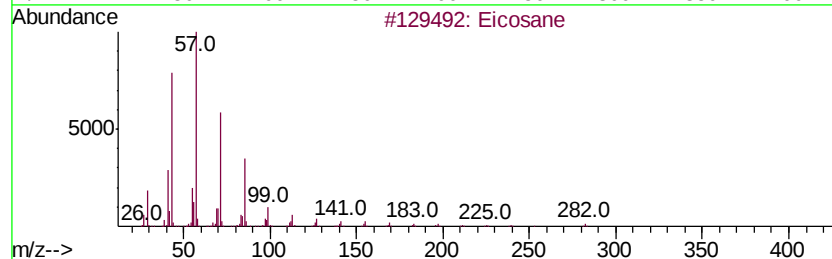
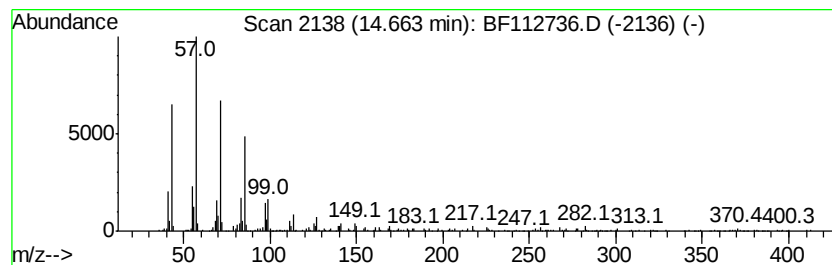
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	6.31 ng	278862	Perylene-d12	15.28

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	96
2	Octacosane		394	C28H58	000630-02-4	93
3	Heptacosane		380	C27H56	000593-49-7	83
4	Heneicosane		296	C21H44	000629-94-7	74
5	Hexadecane		226	C16H34	000544-76-3	74



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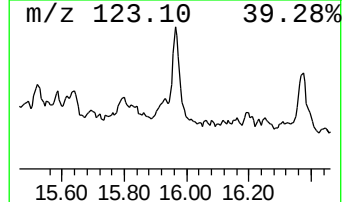
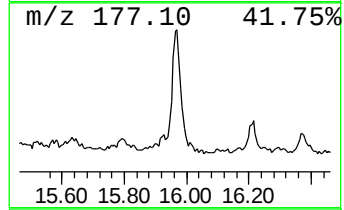
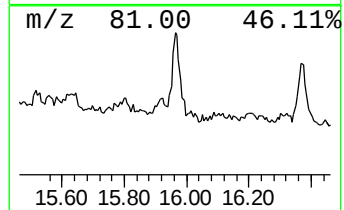
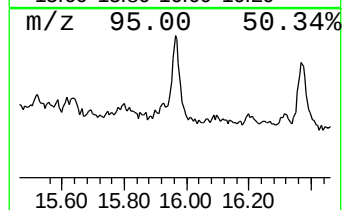
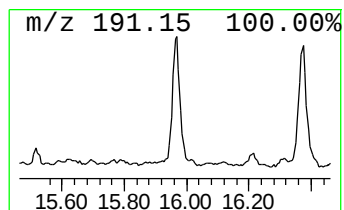
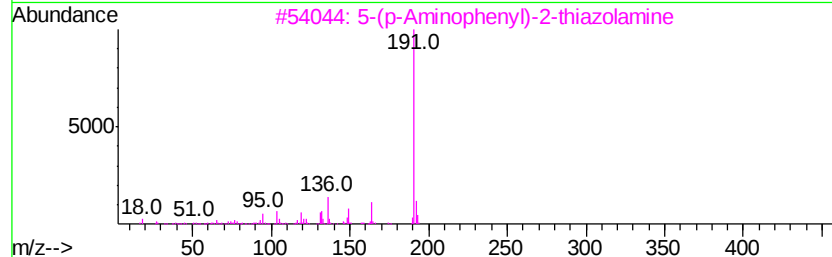
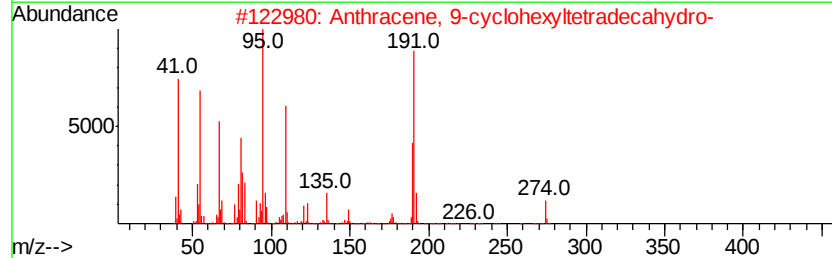
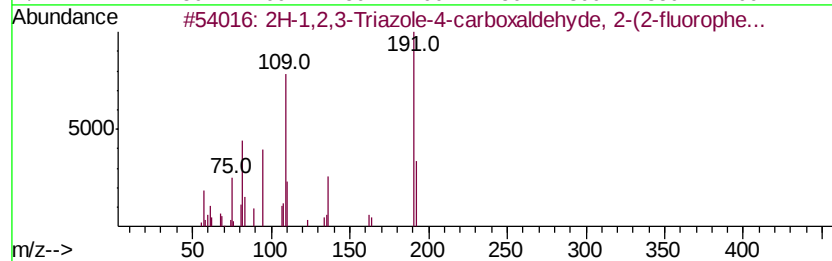
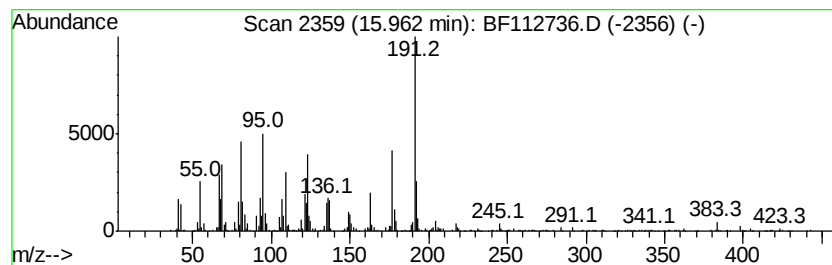
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown15.96 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.96	16.93 ng	747985	Perylene-d12	15.28		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-1,2,3-Triazole-4-carboxaldehv...	191	C9H6FN3O	051306-43-5	38	
2	Anthracene, 9-cyclohexyltetradec...	274	C20H34	055255-70-4	35	
3	5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	25	
4	2-Amino-4-methyl-6-(2-thienyl)pv...	191	C9H9N3S	026963-43-9	22	
5	3-Fluoro-4-trifluoromethylbenzoi...	352	C14H6Cl2F4O2	1000357-94-6	22	



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022719\
Data File : BF112736.D
Acq On : 27 Feb 2019 23:18
Operator : JU/SJ
Sample : K1594-39 5X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
B-9(4-5)

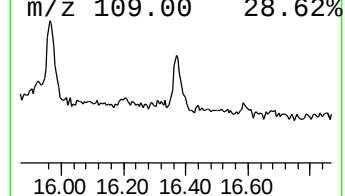
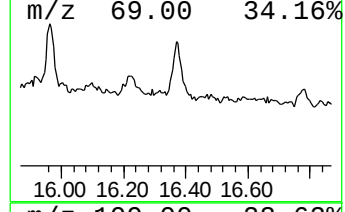
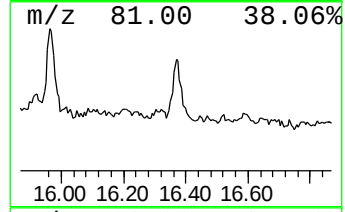
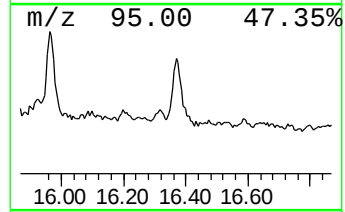
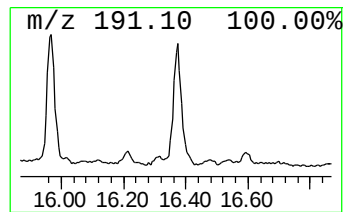
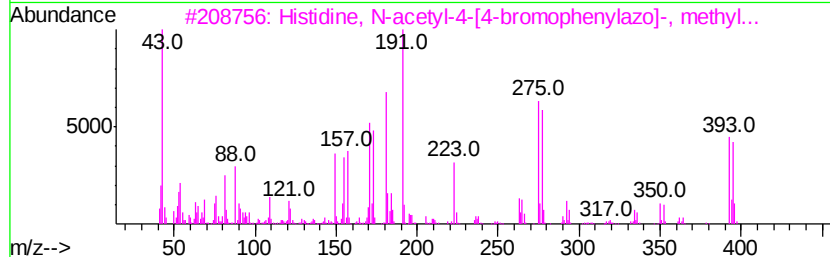
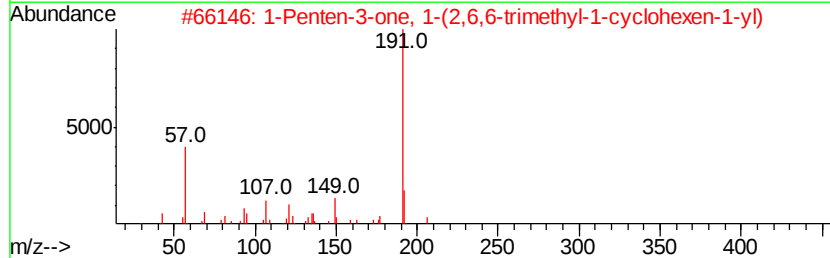
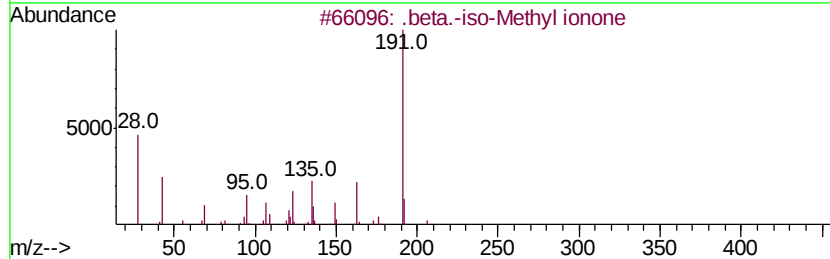
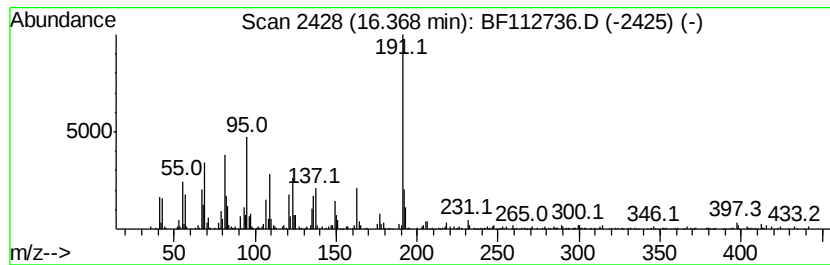
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 .beta.-iso-Methyl ionone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.37	15.43 ng	681536	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	74
2		1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	45
3		Histidine, N-acetyl-4-[4-bromoph...	393	C15H16BrN5O3	039037-16-6	42
4		Anthracene, 9-butyltetradecahydro-	248	C18H32	055133-89-6	40
5		2-Fluoro-5-(trifluoromethyl) ben...	226	C8H3ClF4O	1000342-45-1	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF022719\
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Operator : JU/SJ
Sample : K1594-39 5X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-9(4-5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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
unknown6.50	6.50	12.0	ng	652048	1	6.74	1084680	20.0
1,1'-Biphenyl, 2-...	9.09	10.1	ng	642770	3	9.77	1274550	20.0
Phenol, 4,4'-(1-m...	12.70	2.3	ng	151951	5	13.87	1319750	20.0
Eicosane	14.66	6.3	ng	278862	6	15.28	883435	20.0
unknown15.96	15.96	16.9	ng	747985	6	15.28	883435	20.0
.beta.-iso-Methyl...	16.37	15.4	ng	681536	6	15.28	883435	20.0