

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
 Data File : BF084095.D
 Acq On : 24 Dec 2015 22:52
 Operator : UM/SJ
 Sample : G4644-02
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S8-0528

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-BF122415.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	4.967	250	252	259	rBV	75053	91553	4.47%	0.655%
2	5.413	289	291	303	rBB	708127	668865	32.64%	4.788%
3	6.442	380	381	384	rBV	300538	397269	19.38%	2.844%
4	6.567	390	392	395	rBV	1256531	1262360	61.59%	9.036%
5	6.796	410	412	415	rBV	412438	349165	17.04%	2.499%
6	6.956	423	426	428	rBV	1557739	1428769	69.71%	10.227%
7	7.036	431	433	436	rBV	18344	34247	1.67%	0.245%
8	7.367	459	462	464	rBV	1069074	1113083	54.31%	7.967%
9	7.413	464	466	468	rVB	17553	24027	1.17%	0.172%
10	7.653	482	487	490	rBV3	33982	68644	3.35%	0.491%
11	8.019	516	519	523	rVB2	15315	22993	1.12%	0.165%
12	8.087	523	525	527	rBV	360608	458332	22.36%	3.281%
13	8.213	532	536	539	rBV3	14640	44711	2.18%	0.320%
14	8.327	542	546	547	rBV4	13392	24596	1.20%	0.176%
15	8.510	560	562	565	rVB3	11779	21691	1.06%	0.155%
16	8.830	584	590	592	rBV4	17457	51699	2.52%	0.370%
17	8.910	594	597	599	rBV3	17294	26812	1.31%	0.192%
18	8.956	599	601	604	rVB4	12294	25088	1.22%	0.180%
19	9.048	604	609	611	rBV2	23255	51239	2.50%	0.367%
20	9.116	613	615	616	rBV	23140	28782	1.40%	0.206%
21	9.162	616	619	621	rBV	2166043	2049484	100.00%	14.670%
22	9.322	631	633	634	rBV2	16662	24430	1.19%	0.175%
23	9.345	634	635	637	rVB	42770	34426	1.68%	0.246%
24	9.448	643	644	647	rBV3	18999	36577	1.78%	0.262%
25	9.493	647	648	650	rVV2	29052	39423	1.92%	0.282%
26	9.539	650	652	656	rVV4	16715	44967	2.19%	0.322%
27	9.653	659	662	664	rVV2	51220	85805	4.19%	0.614%
28	9.768	668	672	675	rBV5	11594	33724	1.65%	0.241%
29	9.836	675	678	680	rBV	599862	553789	27.02%	3.964%
30	10.099	699	701	703	rBV	33180	40779	1.99%	0.292%
31	10.133	703	704	706	rVV2	40328	63547	3.10%	0.455%
32	10.168	706	707	713	rVB5	57897	93713	4.57%	0.671%
33	10.271	713	716	722	rBV5	22541	45645	2.23%	0.327%
34	10.625	744	747	750	rBV	1171982	1237488	60.38%	8.858%

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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

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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122415.M
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35	11.185	794	796	798	rVB	38634	42117	2.06%	0.301%
36	11.322	805	808	810	rBV	510795	509933	24.88%	3.650%
37	11.551	826	828	832	rBV4	14509	37313	1.82%	0.267%
38	12.899	943	946	949	rBV	1547311	2024107	98.76%	14.488%
39	13.814	1023	1026	1030	rVB2	16783	29619	1.45%	0.212%
40	13.951	1036	1038	1041	rBV2	379587	430098	20.99%	3.079%
41	15.380	1161	1163	1167	rVB	220800	319843	15.61%	2.289%

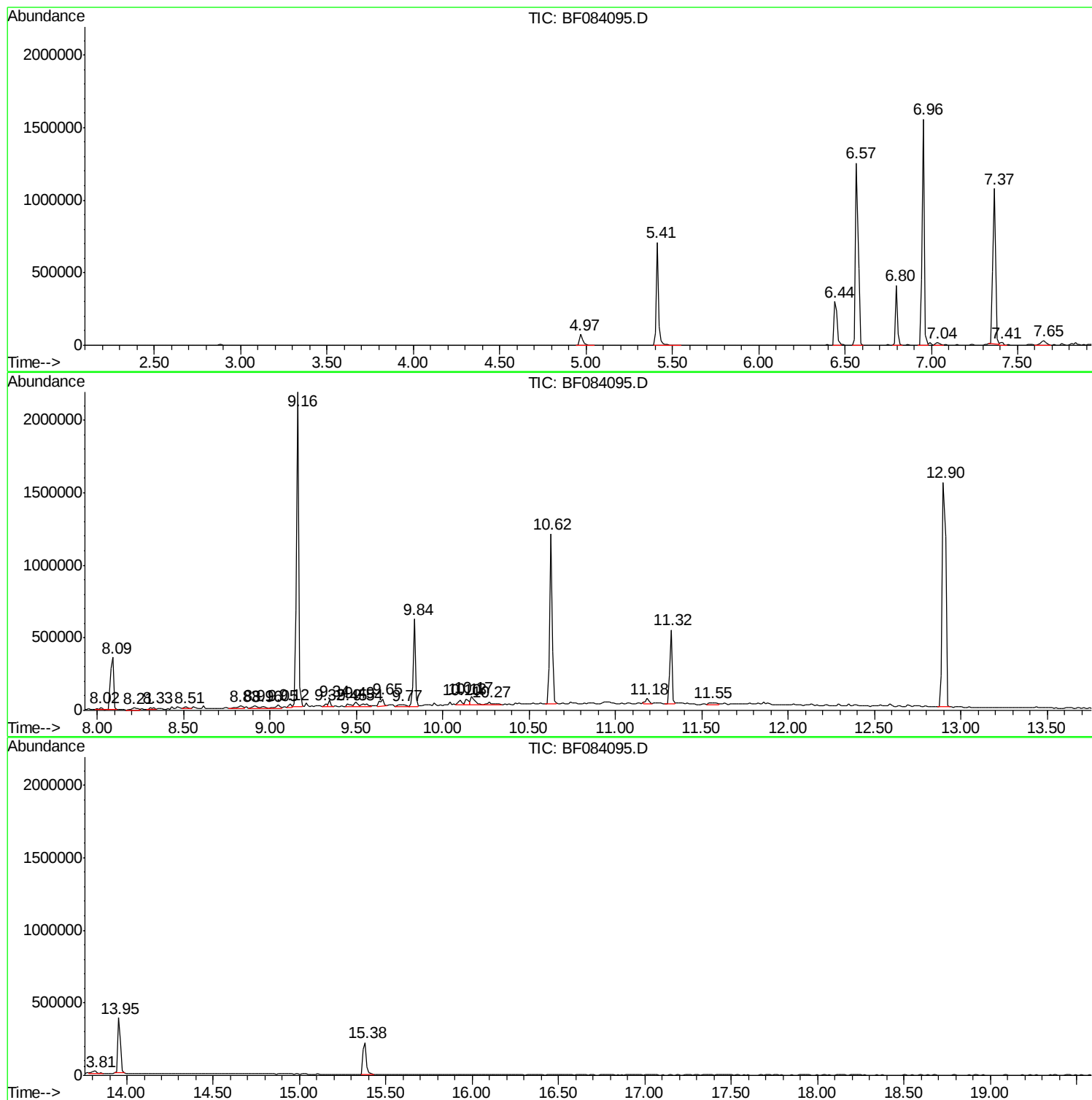
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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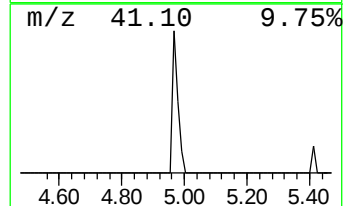
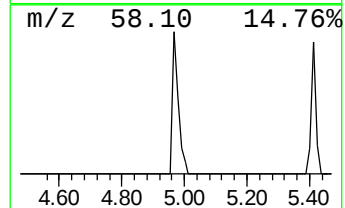
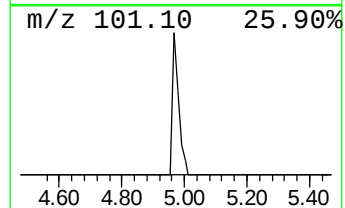
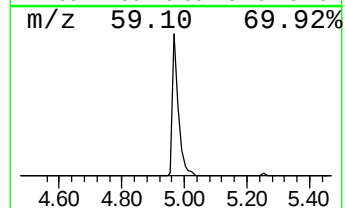
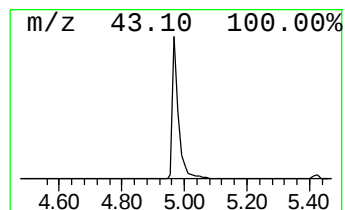
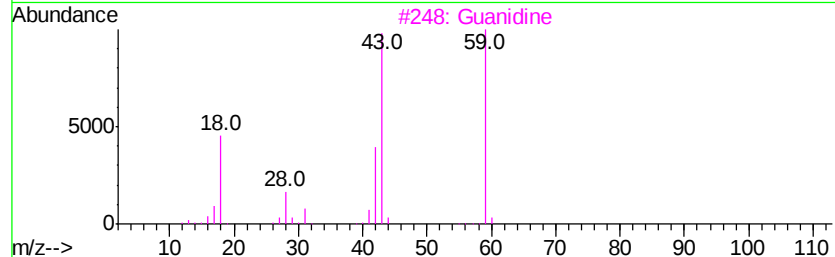
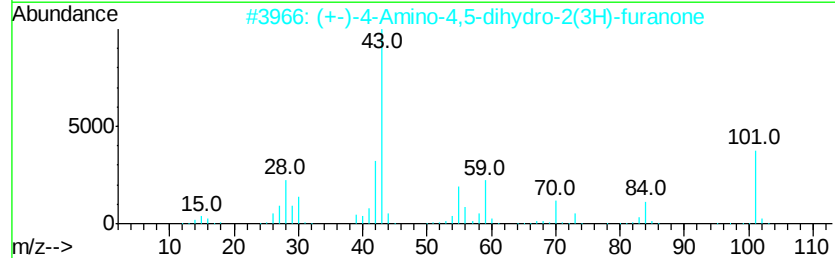
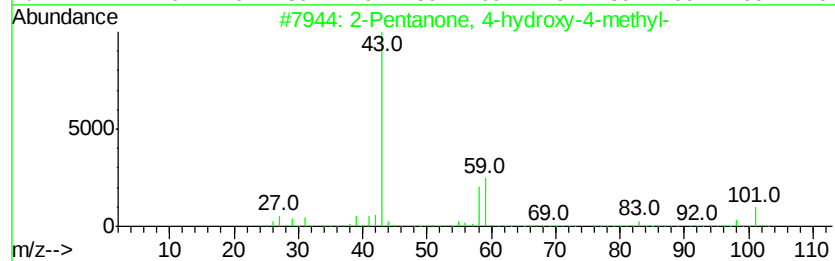
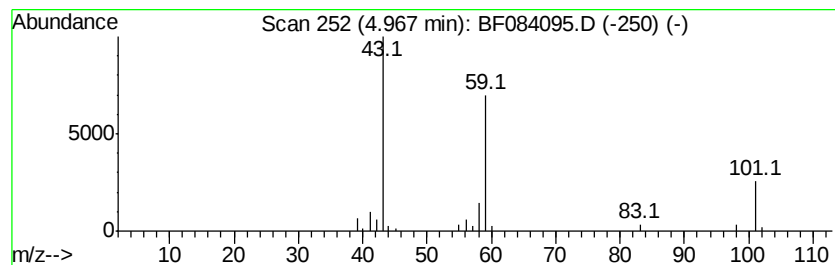
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122415.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	5.24 ng	91553	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	47
3		Guanidine	59	CH5N3	000113-00-8	43
4		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	17
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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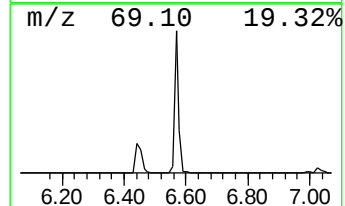
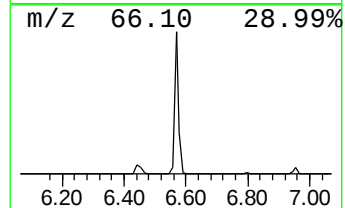
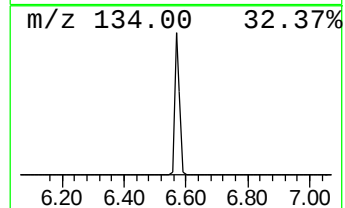
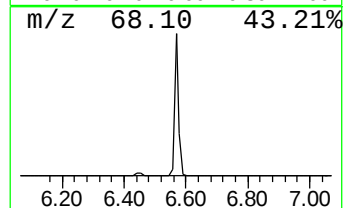
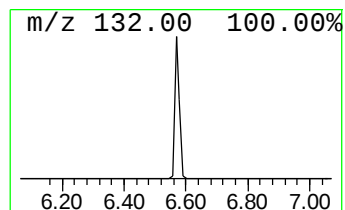
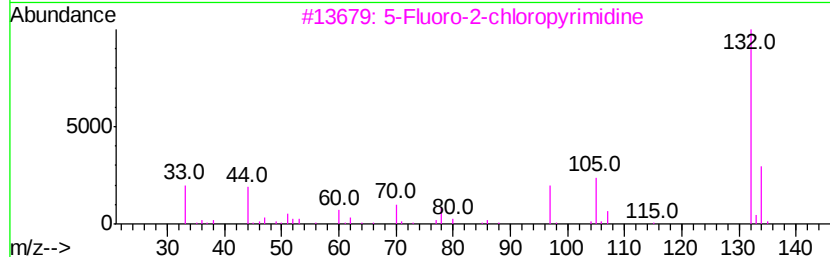
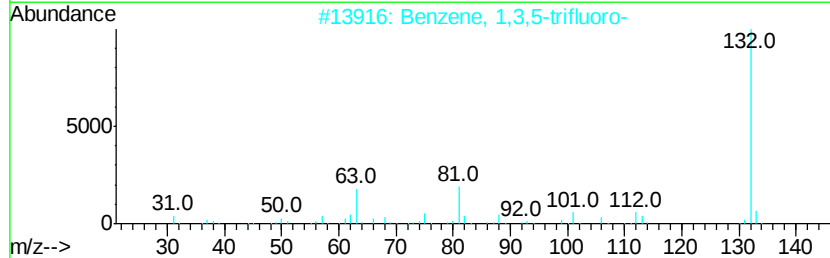
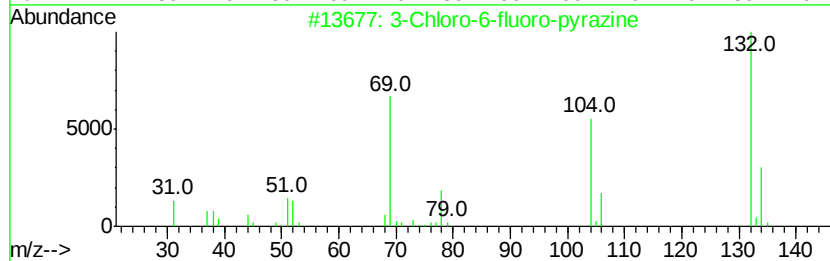
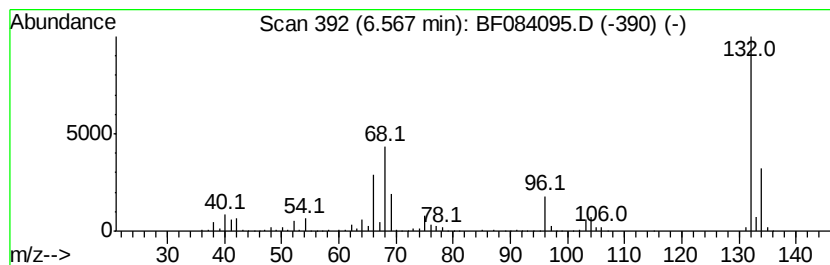
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	72.31 ng	1262360	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	14
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,2,3-Trifluorobenzene	132	C6H3F3	001489-53-8	9



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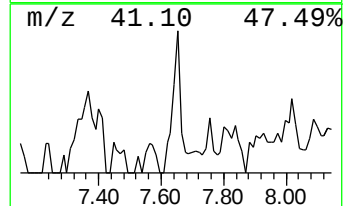
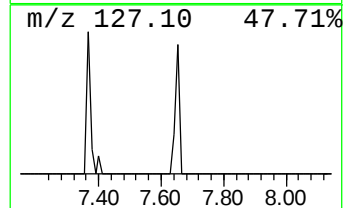
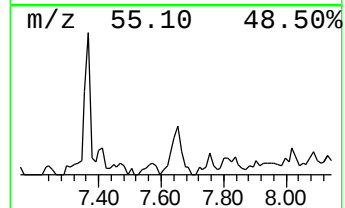
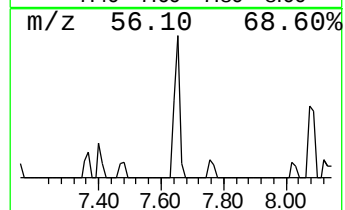
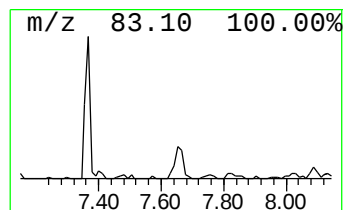
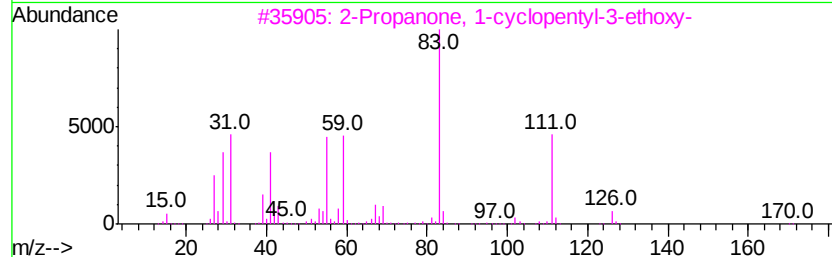
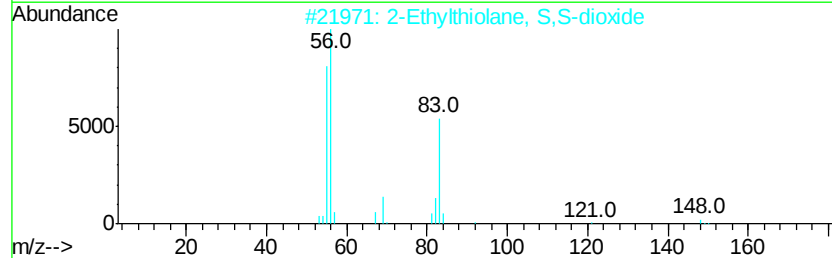
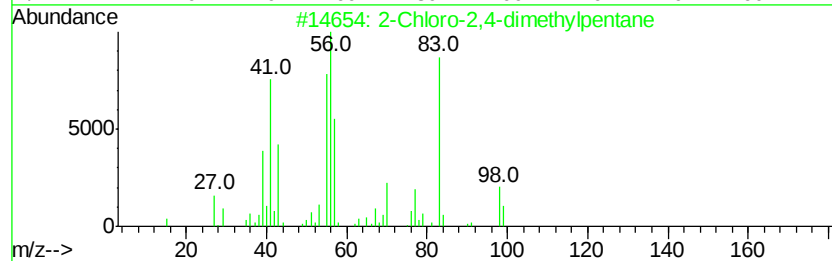
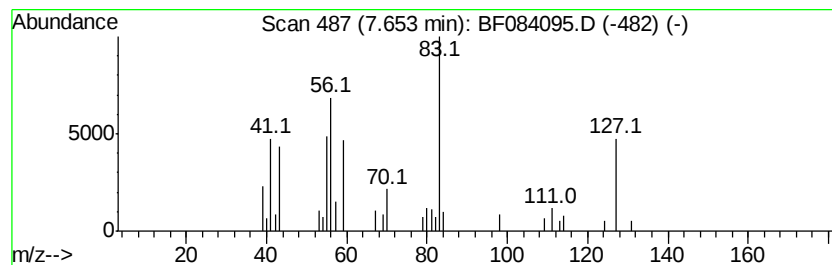
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 unknown7.65 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.65	3.00 ng	68644	Naphthalene-d8	8.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Chloro-2,4-dimethylpentane	134	C7H15Cl	035951-33-8	37
2		2-Ethylthiolane, S,S-dioxide	148	C6H12O2S	010178-59-3	32
3		2-Propanone, 1-cyclopentyl-3-eth...	170	C10H18O2	051149-71-4	32
4		Cyclohexanecarbonyl chloride	146	C7H11ClO	002719-27-9	27
5		7-Oxabicyclo[4.1.0]heptane	98	C6H10O	000286-20-4	25



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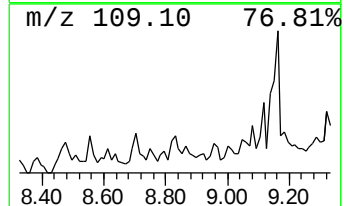
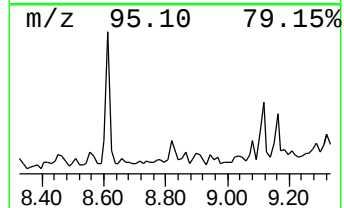
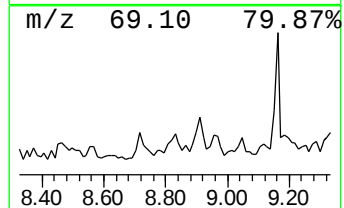
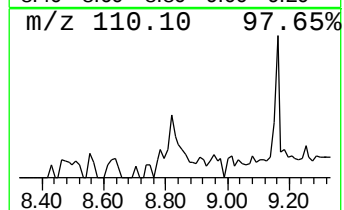
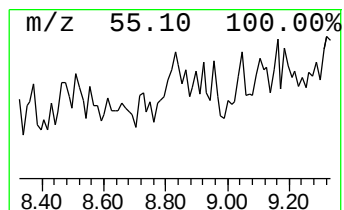
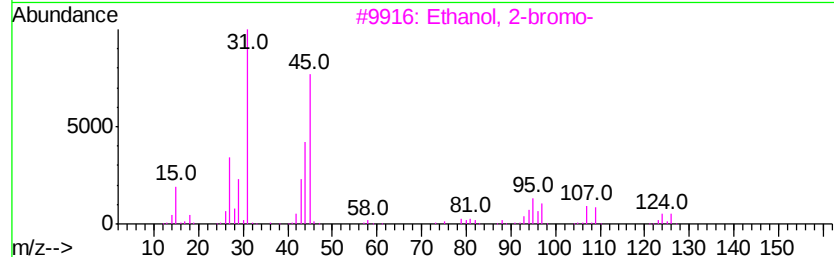
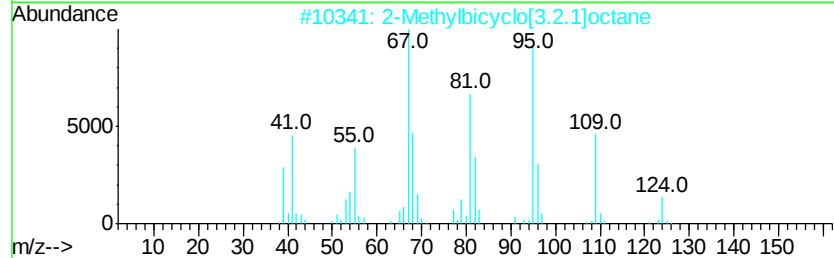
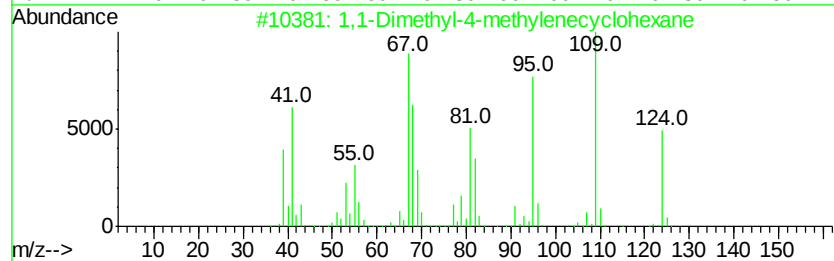
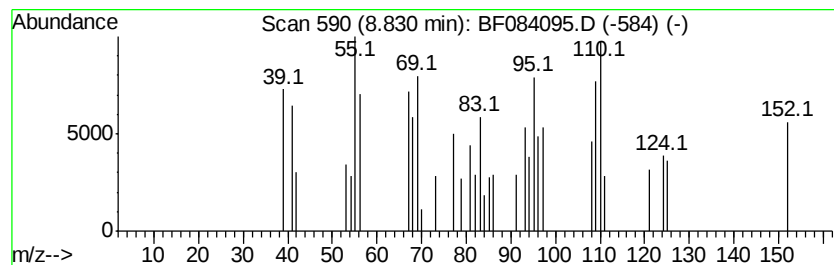
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 unknown8.83 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.83	2.26 ng	51699	Napthalene-d8	8.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,1-Dimethyl-4-methylenecyclohexane	124	C9H16	006007-96-1	42
2		2-Methylbicyclo[3.2.1]octane	124	C9H16	1000215-28-0	35
3		Ethanol, 2-bromo-	124	C2H5BrO	000540-51-2	35
4		1-Methoxy-1,3-cyclohexadiene	110	C7H10O	002161-90-2	35
5		1-Methoxy-1,4-cyclohexadiene	110	C7H10O	002886-59-1	25



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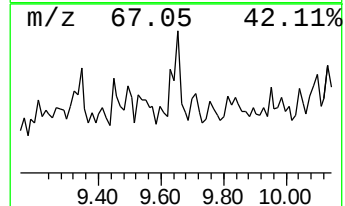
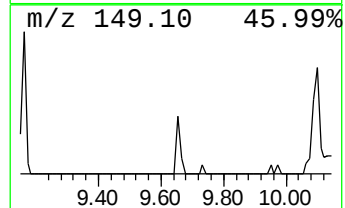
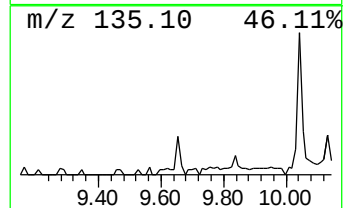
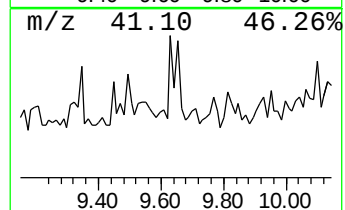
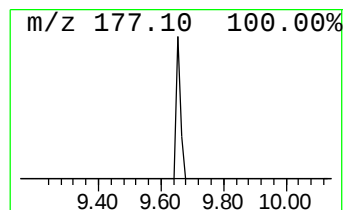
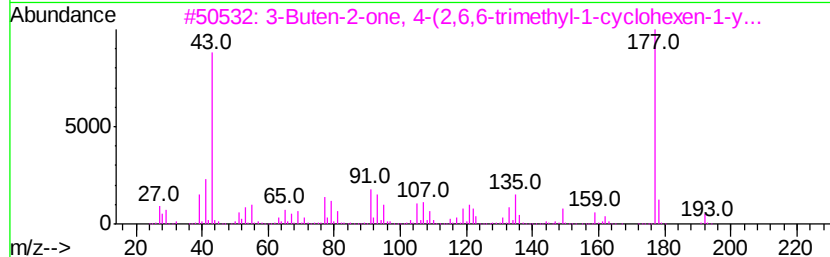
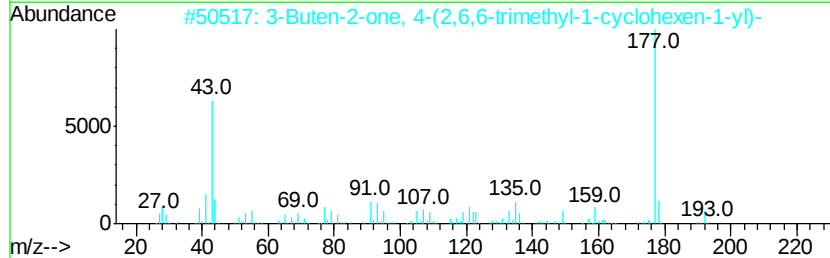
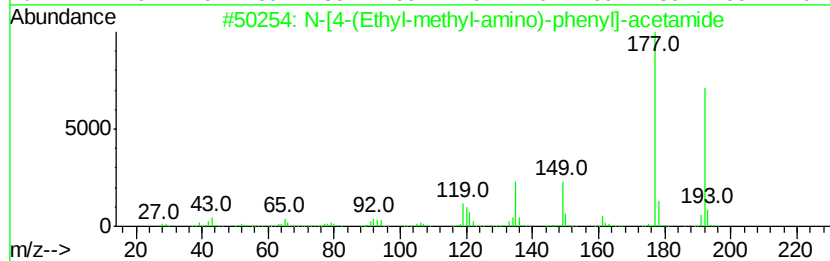
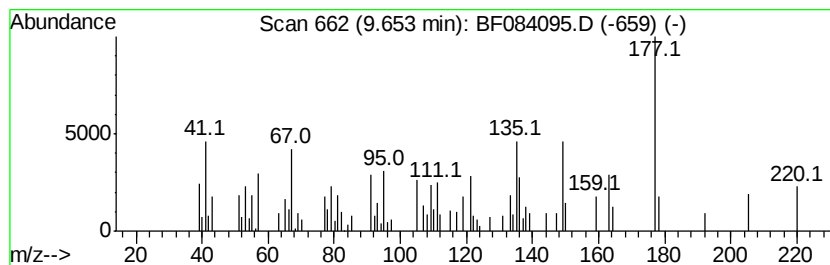
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown9.65 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.65	3.10 ng	85805	Acenaphthene-d10	9.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	N-[4-(Ethyl-methyl-amino)-phenyl]...	192	C11H16N2O	099981-45-0	49
2		3-Buten-2-one, 4-(2,6,6-trimethy...	192	C13H20O	014901-07-6	30
3		3-Buten-2-one, 4-(2,6,6-trimethy...	192	C13H20O	000079-77-6	30
4		5-Ethyl-3,4-dimethyl-1H-pyrano[2...	192	C10H12N2O2	1000296-60-7	25
5		2H-1-Benzopyran, 3,5,6,8a-tetra...	192	C13H20O	041678-29-9	25



Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
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Acq On : 24 Dec 2015 22:52
Operator : UM/SJ
Sample : G4644-02
Misc :
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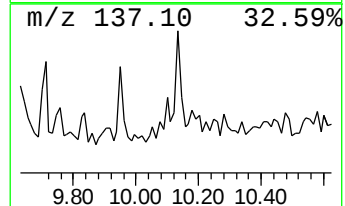
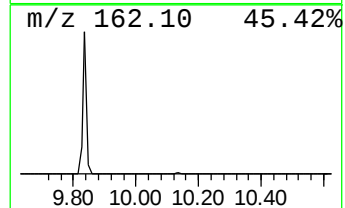
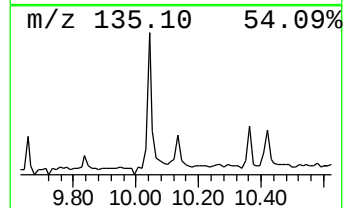
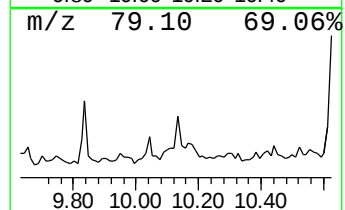
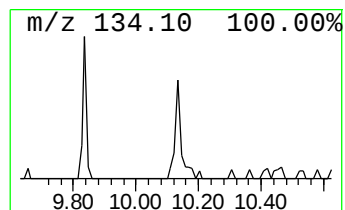
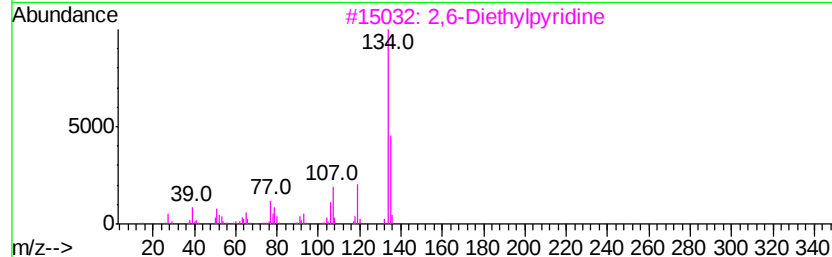
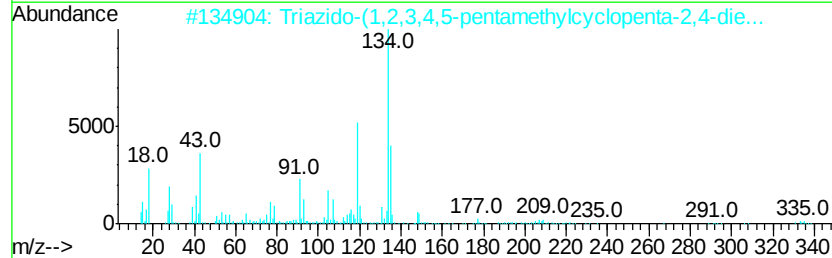
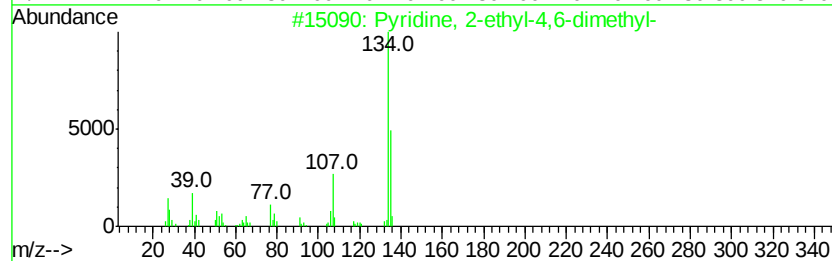
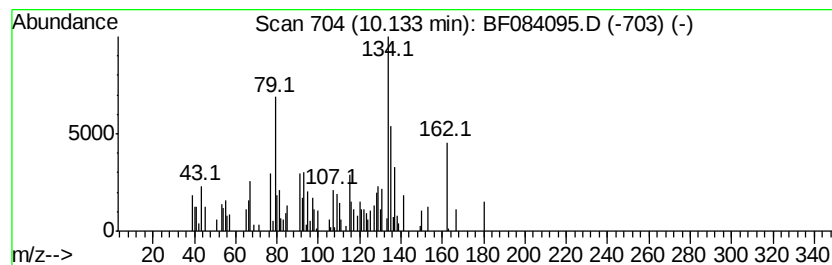
Instrument :
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ClientSampleId :
S8-0528

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown10.13 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.13	2.29 ng	63547	Acenaphthene-d10	9.84	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine, 2-ethyl-4,6-dimethyl-	135	C9H13N	001124-35-2	35
2	Triazido-(1,2,3,4,5-pentamethylc...	335	C10H15GeN9	1000288-06-4	35
3	2,6-Diethylpyridine	135	C9H13N	000935-28-4	35
4	Benzenamine, N,N,3-trimethyl-	135	C9H13N	000121-72-2	27
5	Benzimidazole, 2-ethoxy-	162	C9H10N2O	022219-23-4	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122415\
Data File : BF084095.D
Acq On : 24 Dec 2015 22:52
Operator : UM/SJ
Sample : G4644-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

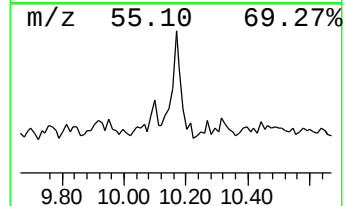
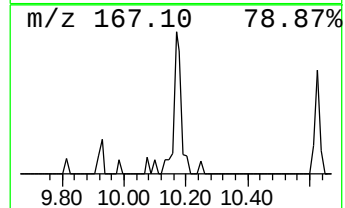
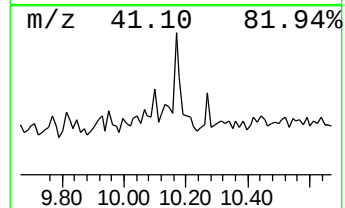
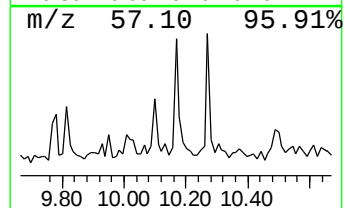
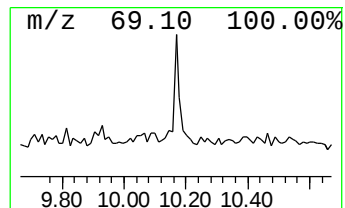
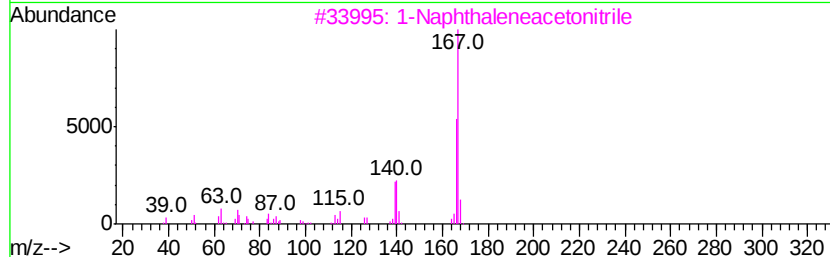
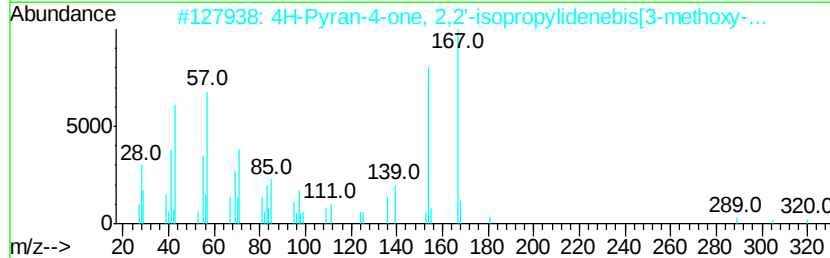
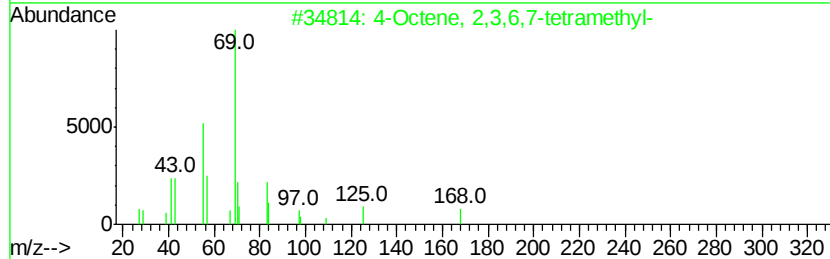
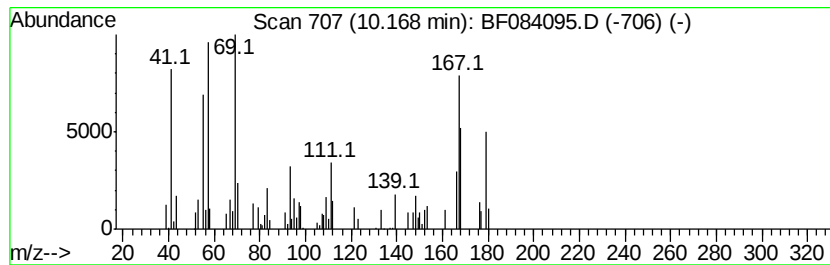
Instrument :
BNA_F
ClientSampleId :
S8-0528

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown10.17 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.17	3.38 ng	93713	Acenaphthene-d10	9.84	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Octene, 2,3,6,7-tetramethyl-	168	C12H24	063830-66-0	22
2	4H-Pyran-4-one, 2,2'-isopropylid...	320	C17H20O6	033771-01-6	14
3	1-Naphthaleneacetonitrile	167	C12H9N	000132-75-2	14
4	Heptane, 4-methylene-	112	C8H16	015918-08-8	11
5	2,5-Dimethyl-3-hexene	112	C8H16	1000118-16-2	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122415\
Data File : BF084095.D
Acq On : 24 Dec 2015 22:52
Operator : UM/SJ
Sample : G4644-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S8-0528

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122415.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...	4.97	5.2	ng	91553	1	6.80	349165	20.0
unknown6.57	6.57	72.3	ng	1262360	1	6.80	349165	20.0
unknown7.65	7.65	3.0	ng	68644	2	8.09	458332	20.0
unknown8.83	8.83	2.3	ng	51699	2	8.09	458332	20.0
unknown9.65	9.65	3.1	ng	85805	3	9.84	553789	20.0
unknown10.13	10.13	2.3	ng	63547	3	9.84	553789	20.0
unknown10.17	10.17	3.4	ng	93713	3	9.84	553789	20.0