

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020316\
 Data File : BF084825.D
 Acq On : 4 Feb 2016 10:12
 Operator : SJ/IZ
 Sample : H1322-09
 Misc :
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S4-B020(20-22)

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-BF020116.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	4.133	178	179	184	rBV	40218	67462	1.35%	0.156%
2	4.841	238	241	253	rVB	1159097	1824535	36.45%	4.211%
3	5.276	277	279	282	rBV	3180705	4316671	86.24%	9.964%
4	5.687	313	315	318	rVB	54866	54175	1.08%	0.125%
5	6.339	369	372	374	rBV	4245170	4626821	92.43%	10.680%
6	6.453	379	382	385	rBV	4466499	4209722	84.10%	9.717%
7	6.681	400	402	404	rBV	1276724	1098520	21.95%	2.536%
8	6.841	413	416	418	rBV	4009609	3548078	70.88%	8.190%
9	7.253	449	452	455	rBV	2499104	2702502	53.99%	6.238%
10	7.379	459	463	467	rBV	38560	72434	1.45%	0.167%
11	7.722	491	493	501	rBV	38132	57460	1.15%	0.133%
12	7.973	512	515	517	rBV	1710954	1505390	30.07%	3.475%
13	9.059	607	610	612	rBV	4202985	5005538	100.00%	11.554%
14	9.447	642	644	647	rBV	848034	849356	16.97%	1.960%
15	9.665	661	663	666	rBV	71020	80596	1.61%	0.186%
16	9.722	666	668	671	rVB	1711030	1493266	29.83%	3.447%
17	10.168	706	707	709	rVB	147802	105571	2.11%	0.244%
18	10.385	723	726	729	rBV	46972	69294	1.38%	0.160%
19	10.510	734	737	739	rBV	2919373	2679177	53.52%	6.184%
20	10.636	746	748	755	rVB	148850	176836	3.53%	0.408%
21	11.082	786	787	789	rBV	90164	88762	1.77%	0.205%
22	11.196	795	797	800	rBV	1186644	1288310	25.74%	2.974%
23	11.276	800	804	807	rVB5	27620	52881	1.06%	0.122%
24	11.448	815	819	822	rBV4	30173	71241	1.42%	0.164%
25	11.516	822	825	826	rVV2	35011	68119	1.36%	0.157%
26	11.539	826	827	830	rVB	163047	136787	2.73%	0.316%
27	11.916	856	860	862	rBV	38617	62411	1.25%	0.144%
28	11.996	865	867	872	rVB2	56060	65728	1.31%	0.152%
29	12.339	892	897	899	rVB	235441	390532	7.80%	0.901%
30	12.408	901	903	905	rVB	73577	70649	1.41%	0.163%
31	12.625	920	922	925	rBV2	94043	122969	2.46%	0.284%
32	12.705	925	929	930	rVB2	32573	59950	1.20%	0.138%
33	12.785	934	936	939	rVV	3015454	3540580	70.73%	8.172%
34	13.322	981	983	985	rBV2	33152	53483	1.07%	0.123%

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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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Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
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35	13.699	1014	1016	1024	rVB	169569	324414	6.48%	0.749%
36	13.825	1025	1027	1030	rBV	880998	1014364	20.26%	2.341%
37	14.831	1112	1115	1118	rVB	35202	69651	1.39%	0.161%
38	15.208	1145	1148	1150	rBV	701784	901806	18.02%	2.082%
39	15.631	1183	1185	1188	rBV3	29903	61120	1.22%	0.141%
40	15.814	1199	1201	1207	rVB5	41514	95493	1.91%	0.220%
41	16.191	1232	1234	1241	rVB6	35229	74613	1.49%	0.172%
42	16.408	1250	1253	1258	rBV	48825	111754	2.23%	0.258%
43	16.694	1275	1278	1281	rBV4	23456	54430	1.09%	0.126%

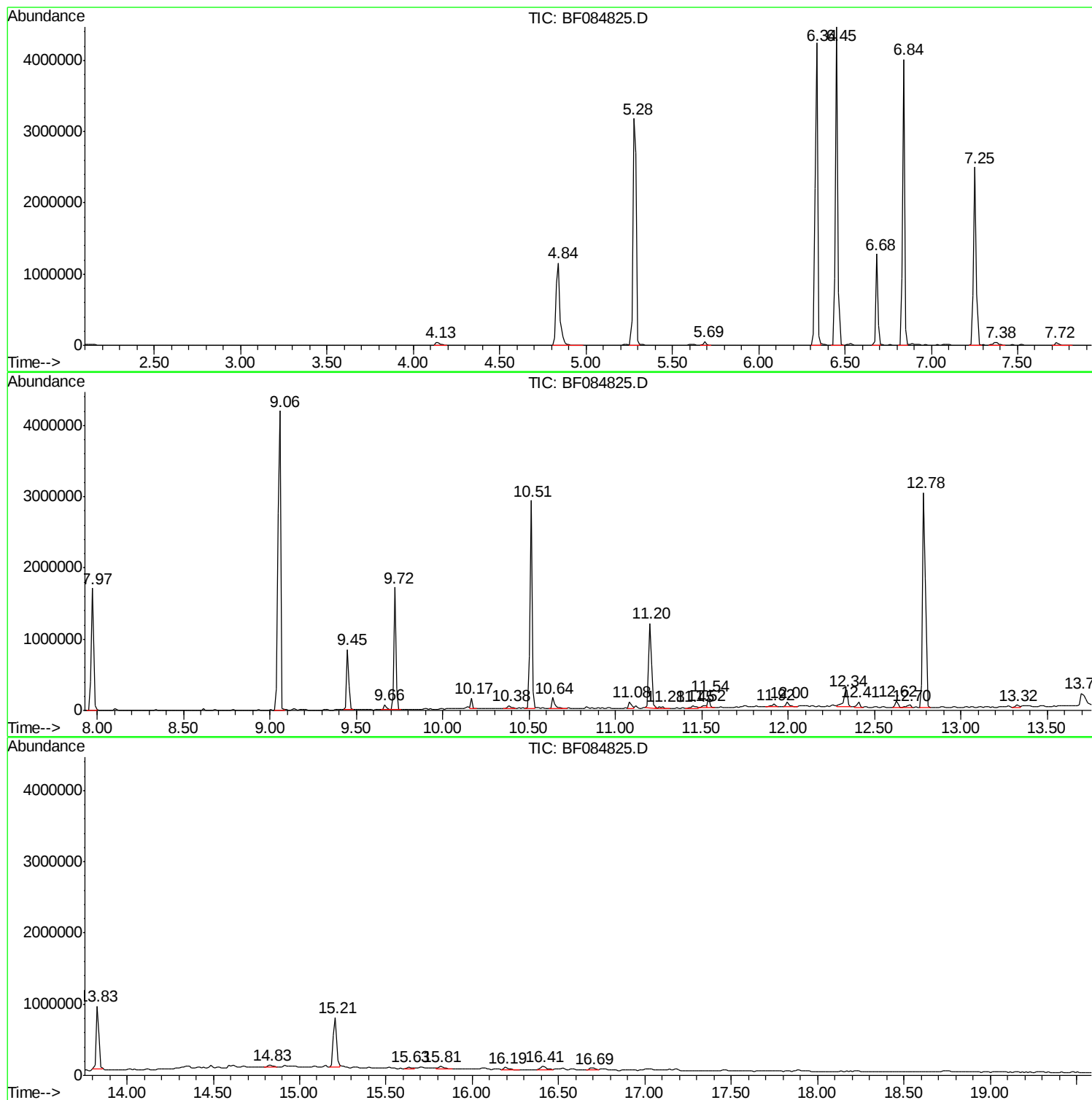
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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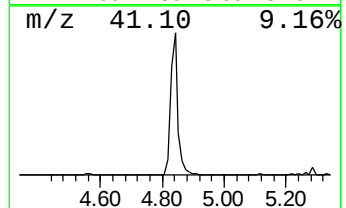
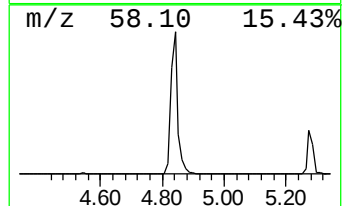
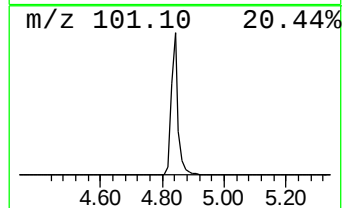
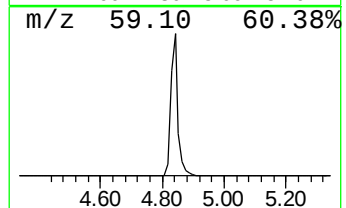
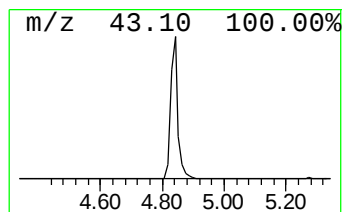
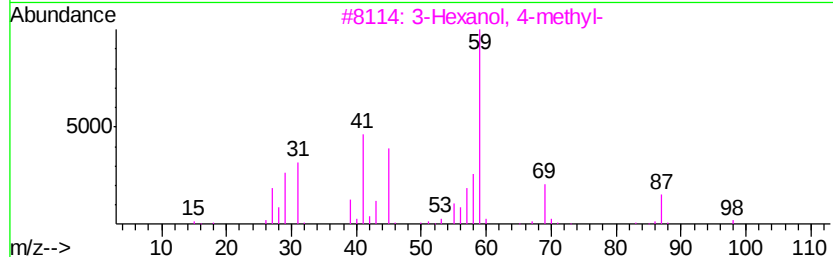
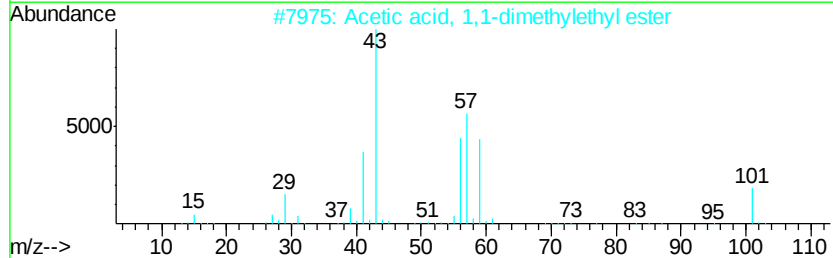
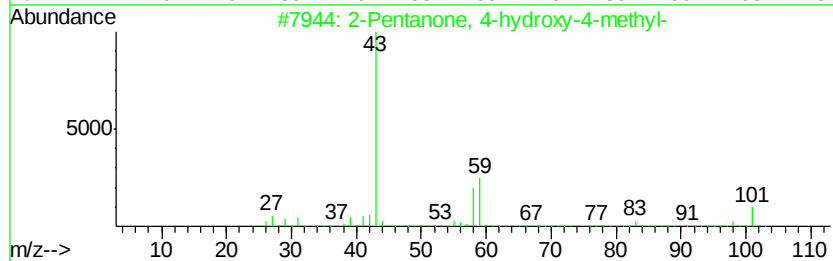
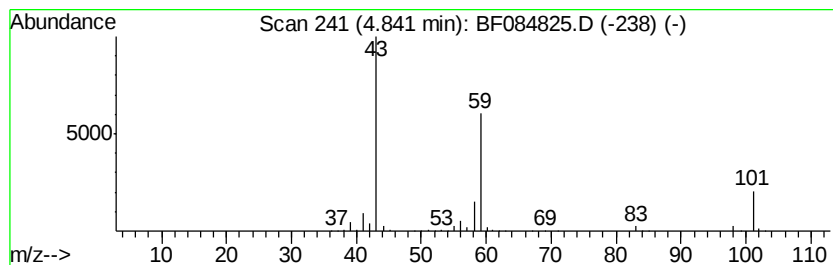
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.84	33.22 ng	1824540	1,4-Dichlorobenzene-d4	6.68

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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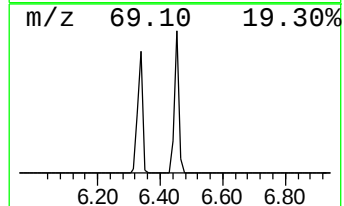
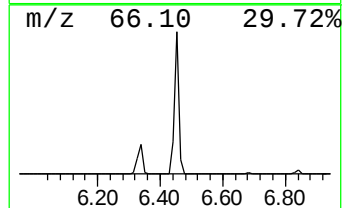
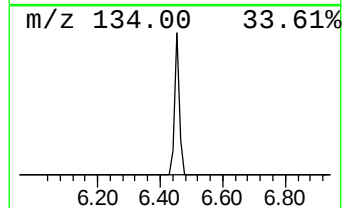
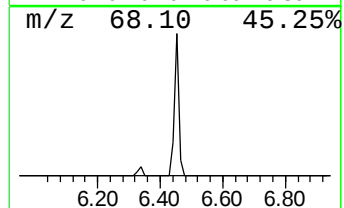
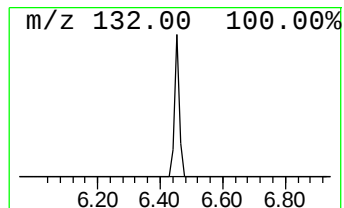
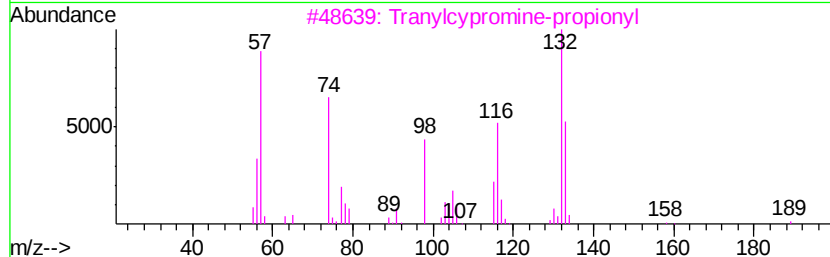
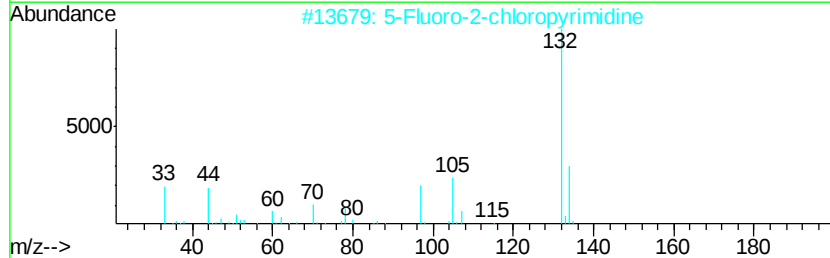
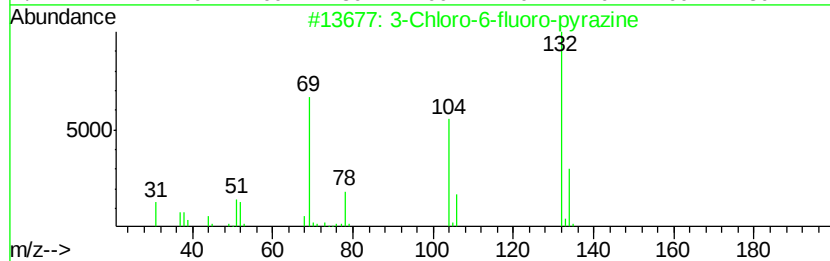
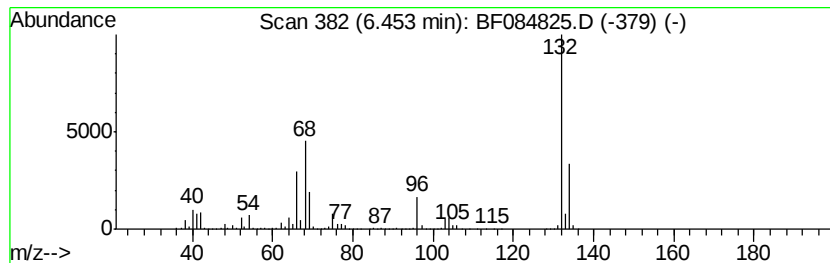
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Peak Number 2 unknown6.45 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.45	76.64 ng	4209720	1,4-Dichlorobenzene-d4	6.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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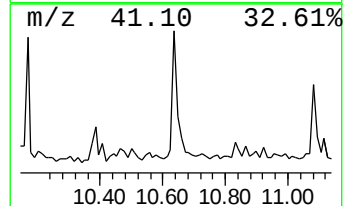
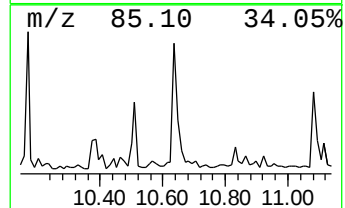
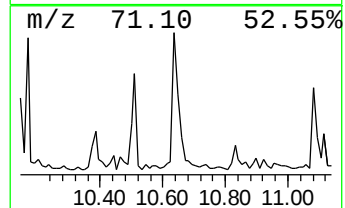
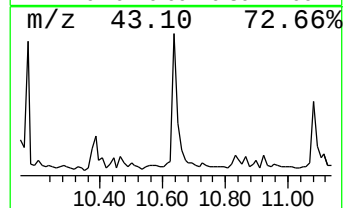
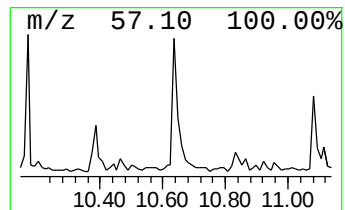
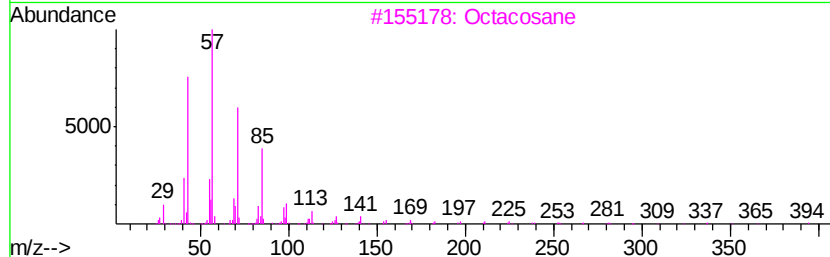
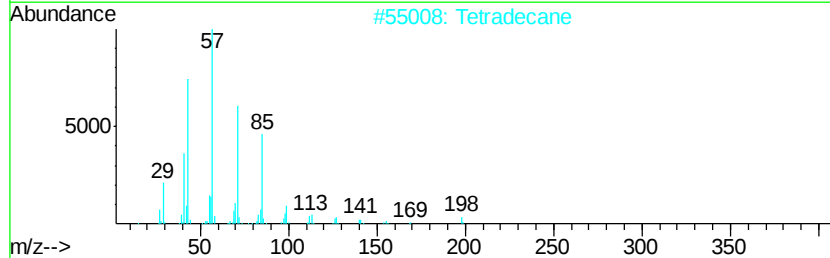
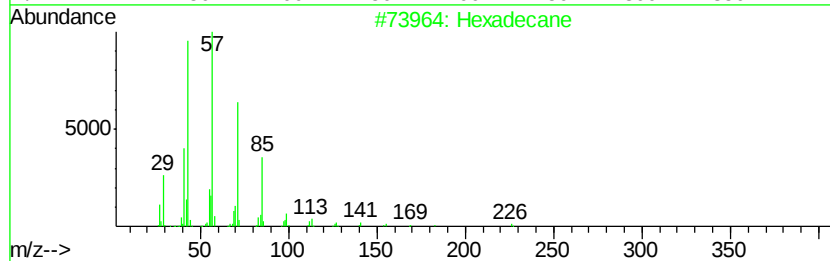
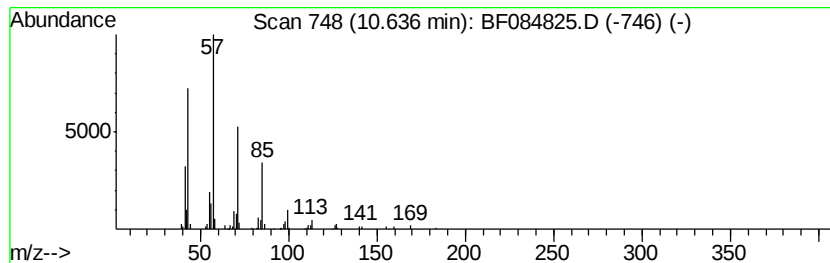
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.64	2.75 ng	176836	Phenanthrene-d10	11.20	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Tetradecane	198	C14H30	000629-59-4	90
3	Octacosane	394	C28H58	000630-02-4	86
4	Pentadecane	212	C15H32	000629-62-9	86
5	Octadecane	254	C18H38	000593-45-3	86



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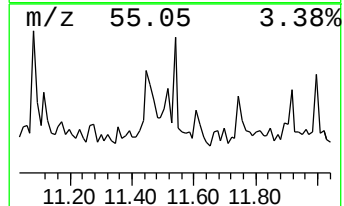
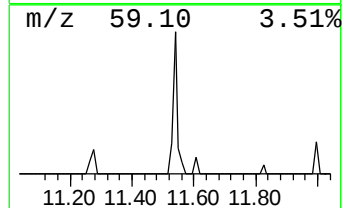
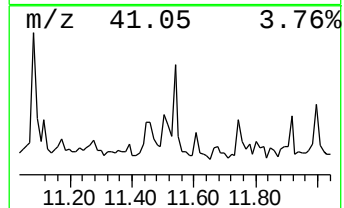
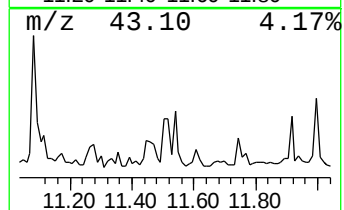
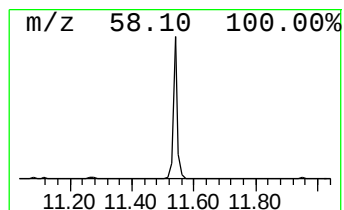
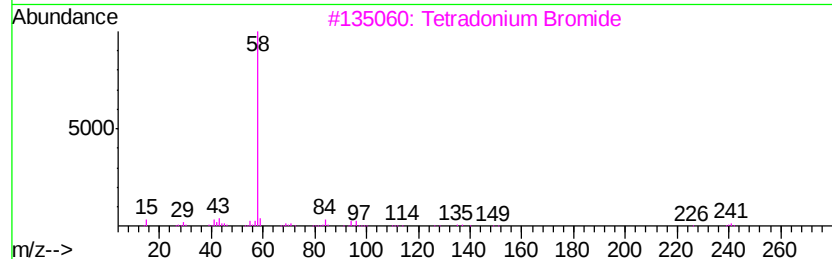
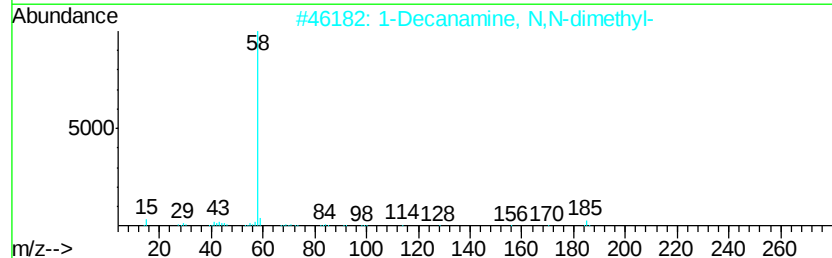
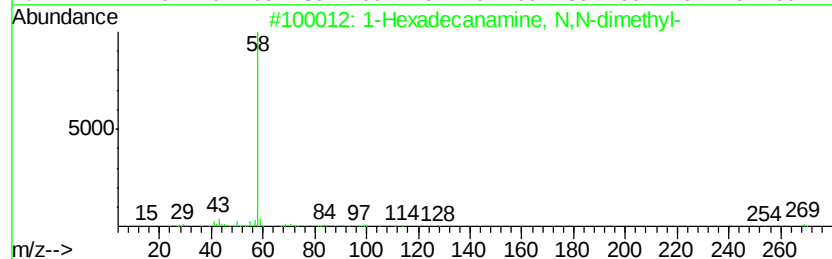
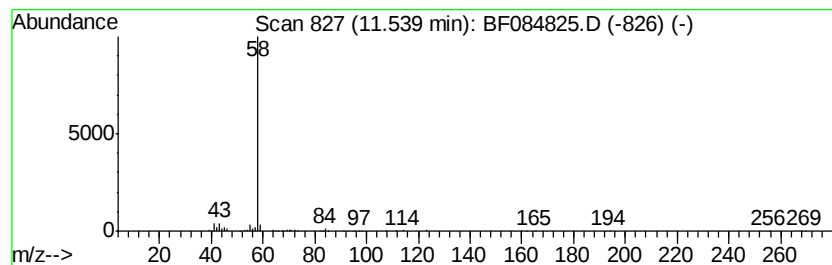
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Hexadecanamine, N,N-dimet... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.54	2.12 ng	136787	Phenanthrene-d10	11.20

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexadecanamine, N,N-dimethyl-	269	C18H39N	000112-69-6	86
2		1-Decanamine, N,N-dimethyl-	185	C12H27N	001120-24-7	72
3		Tetradonium Bromide	335	C17H38BrN	001119-97-7	72
4		1-Undecanamine, N,N-dimethyl-	199	C13H29N	017373-28-3	72
5		1-Pentadecanamine, N,N-dimethyl-	255	C17H37N	017678-60-3	64



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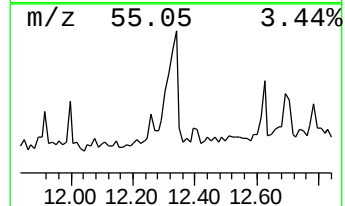
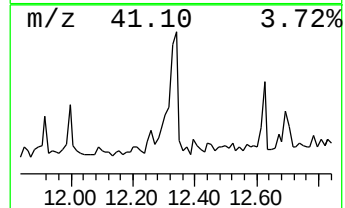
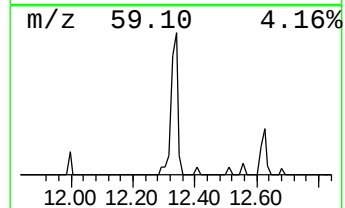
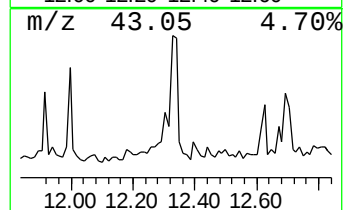
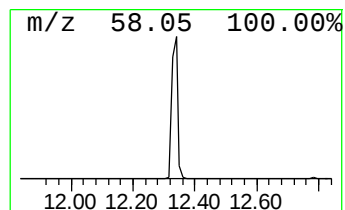
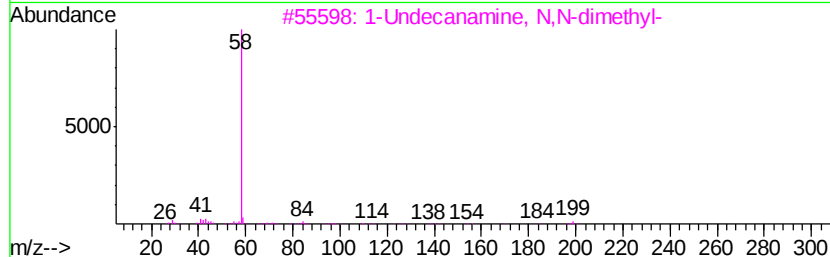
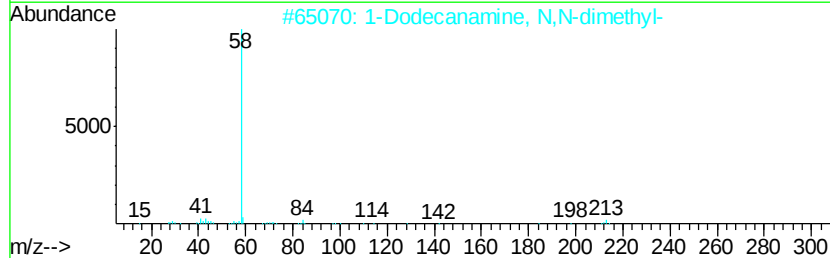
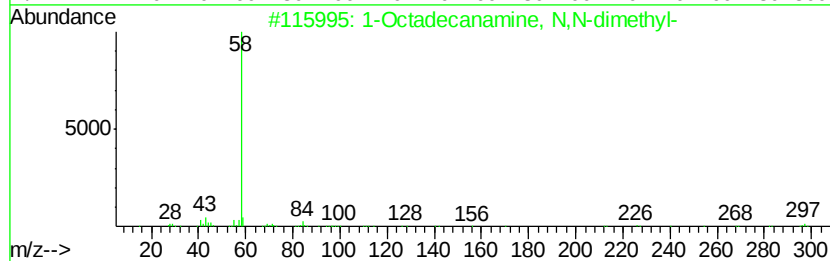
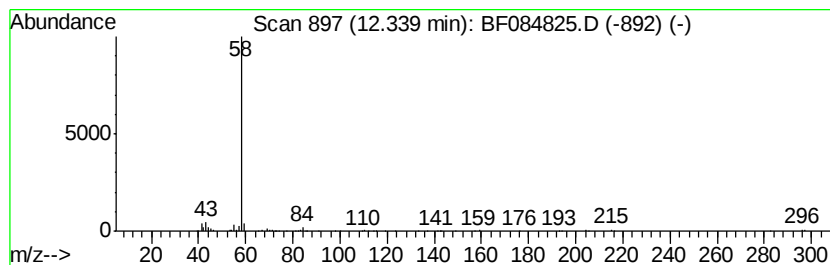
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Octadecanamine, N,N-dimet... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.34	6.06 ng	390532	Phenanthrene-d10	11.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Octadecanamine, N,N-dimethyl-	297	C20H43N	000124-28-7	91
2		1-Dodecanamine, N,N-dimethyl-	213	C14H31N	000112-18-5	78
3		1-Undecanamine, N,N-dimethyl-	199	C13H29N	017373-28-3	72
4		Tetradonium Bromide	335	C17H38BrN	001119-97-7	72
5		1-Nonadecanamine, N,N-dimethyl-	311	C21H45N	049859-87-2	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020316\
Data File : BF084825.D
Acq On : 4 Feb 2016 10:12
Operator : SJ/IZ
Sample : H1322-09
Misc :
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Instrument :
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ClientSampleId :
S4-B020(20-22)

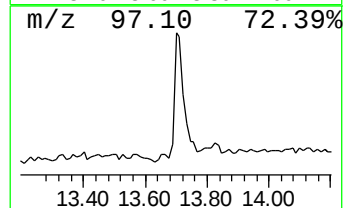
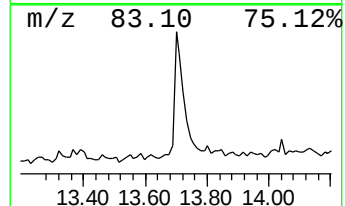
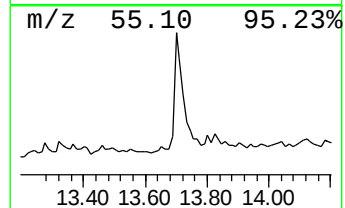
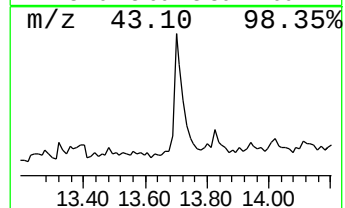
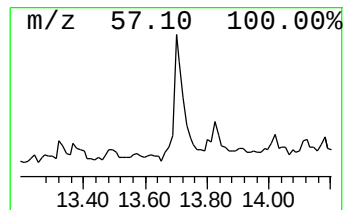
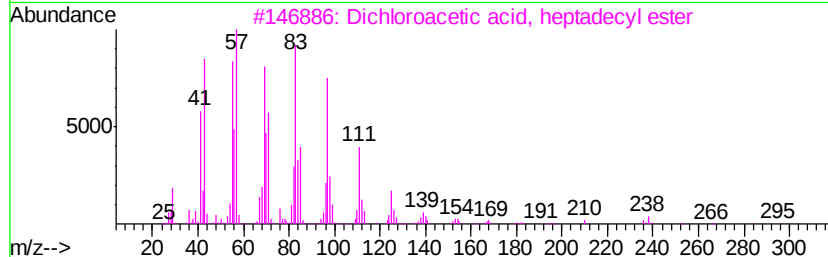
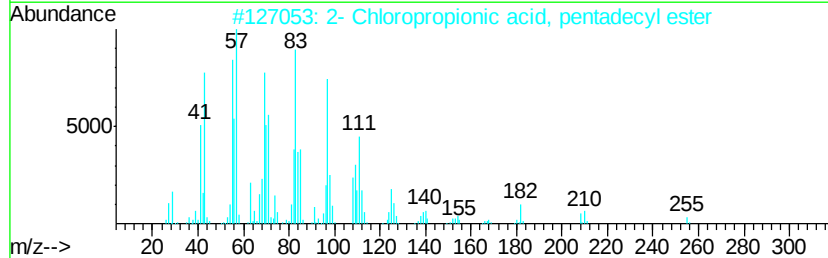
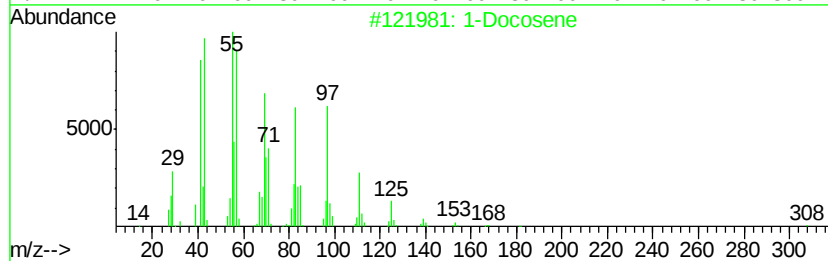
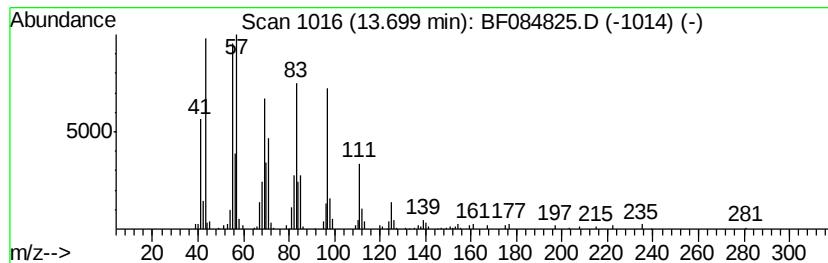
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	6.40 ng	324414	Chrysene-d12	13.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	94
2		2- Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	91
3		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
4		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
5		1-Nonadecene	266	C19H38	018435-45-5	91



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Sample : H1322-09
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
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ClientSampleId :
S4-B020(20-22)

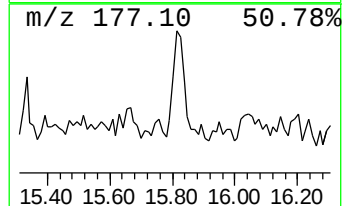
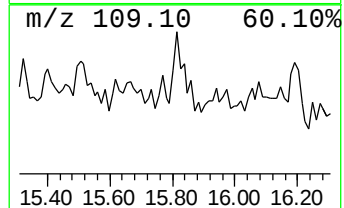
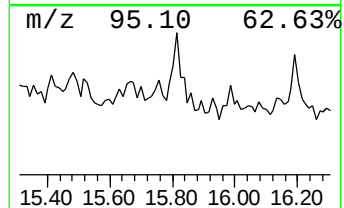
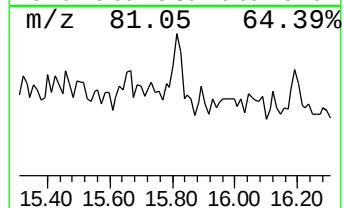
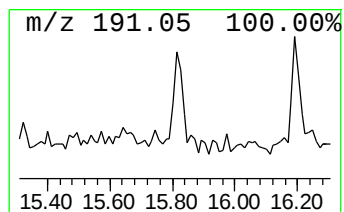
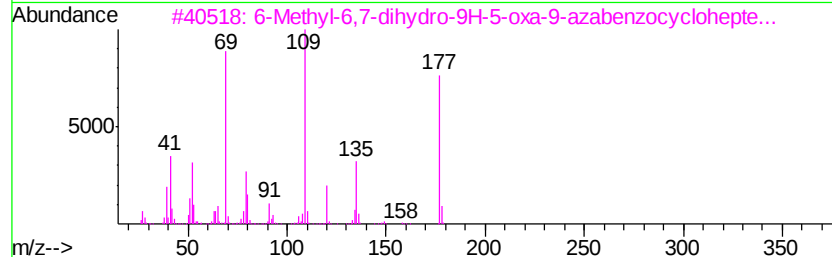
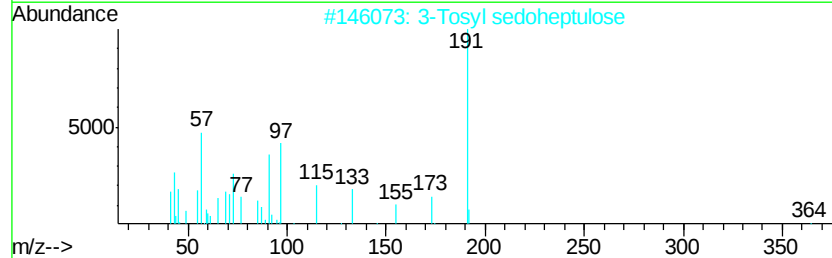
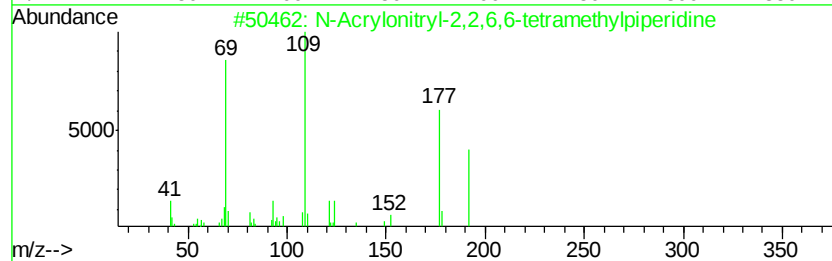
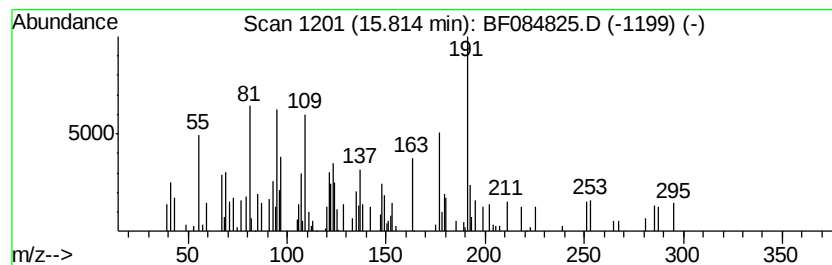
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 9 unknown15.81 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.81	2.12 ng	95493	Perylene-d12	15.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	N-Acrylonitril-2,2,6,6-tetrameth...	192	C12H20N2	077376-88-6	18
2		3-Tosyl sedoheptulose	364	C14H20O9S	1000126-65-3	16
3		6-Methyl-6,7-dihydro-9H-5-oxa-9-...	177	C10H11N02	1000210-20-2	15
4		Tricyclohexylborane	260	C18H33B	001088-01-3	14
5		Amiphenazole	191	C9H9N3S	000490-55-1	14



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ALS Vial : 38 Sample Multiplier: 1

Instrument :
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ClientSampleId :
S4-B020(20-22)

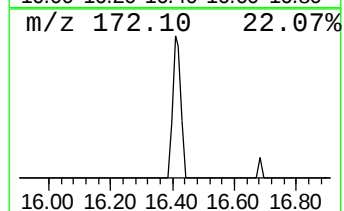
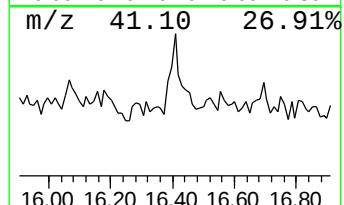
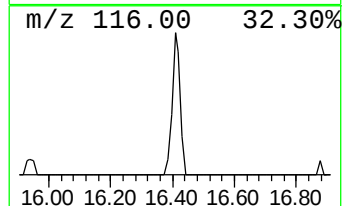
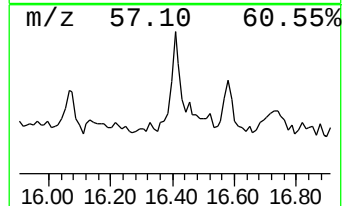
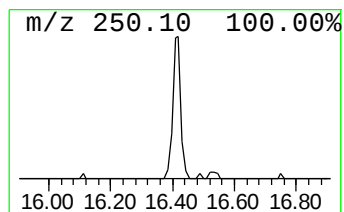
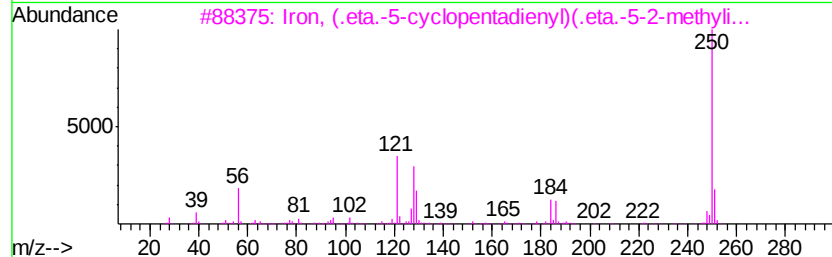
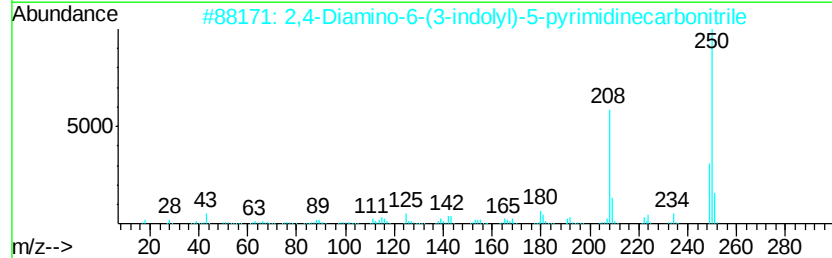
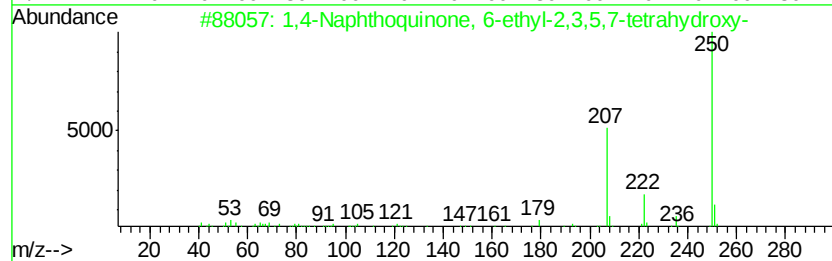
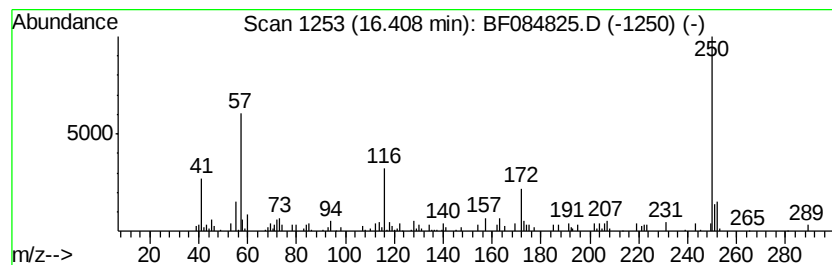
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown16.41 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.41	2.48 ng	111754	Perylene-d12	15.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,4-Naphthoquinone, 6-ethyl-2,3,...	250	C12H10O6	013378-99-9	49
2		2,4-Diamino-6-(3-indolyl)-5-pyri...	250	C13H10N6	018234-36-1	47
3		Iron, (.eta.-5-cyclopentadienyl)...	250	C15H14Fe	1000155-35-1	47
4		4-Phenyl-2-(3-fluorophenyl)pyrim...	250	C16H11FN2	076128-69-3	43
5		3-Heptyne, 7-iodo-2,2-dimethyl-	250	C9H15I	055402-07-8	43



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Instrument :
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ClientSampleId :
S4-B020(20-22)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.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...	4.84	33.2	ng	1824540	1	6.68	1098520	20.0
unknown6.45	6.45	76.6	ng	4209720	1	6.68	1098520	20.0
Hexadecane	10.64	2.8	ng	176836	4	11.20	1288310	20.0
1-Hexadecanamine,...	11.54	2.1	ng	136787	4	11.20	1288310	20.0
1-Octadecanamine,...	12.34	6.1	ng	390532	4	11.20	1288310	20.0
1-Docosene	13.70	6.4	ng	324414	5	13.82	1014360	20.0
unknown15.81	15.81	2.1	ng	95493	6	15.21	901806	20.0
unknown16.41	16.41	2.5	ng	111754	6	15.21	901806	20.0