

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110915\
 Data File : BF082850.D
 Acq On : 10 Nov 2015 3:17
 Operator : UM/IZ
 Sample : G4286-07
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 T-2R

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-BF110715.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	2.144	3	5	21	rVB	145355	401824	4.82%	0.524%
2	5.024	253	257	266	rVB	2566281	4012294	48.13%	5.235%
3	5.447	290	294	296	rBV	6686293	7753855	93.01%	10.117%
4	6.476	380	384	386	rBV	5210974	8336208	100.00%	10.877%
5	6.602	392	395	397	rBV	7072813	7732482	92.76%	10.089%
6	6.830	412	415	417	rBV	1738313	1685254	20.22%	2.199%
7	6.990	426	429	431	rBV	4974072	5740716	68.86%	7.490%
8	7.390	461	464	466	rBV	3989692	4390306	52.67%	5.728%
9	7.493	470	473	476	rBV	71673	99049	1.19%	0.129%
10	8.110	524	527	530	rBV	2088494	2081513	24.97%	2.716%
11	9.196	618	622	624	rVB	7036977	7702273	92.40%	10.050%
12	9.585	653	656	658	rBV	1674374	1454722	17.45%	1.898%
13	9.813	674	676	677	rBV	144671	121303	1.46%	0.158%
14	9.870	677	681	683	rBV	2177244	2437611	29.24%	3.181%
15	10.316	716	720	721	rBV	114721	165049	1.98%	0.215%
16	10.659	746	750	752	rVV	3753048	5090608	61.07%	6.642%
17	10.785	759	761	765	rVB	169333	208598	2.50%	0.272%
18	11.231	796	800	801	rBV	133839	132617	1.59%	0.173%
19	11.345	808	810	813	rVB	2547179	2293653	27.51%	2.993%
20	11.825	849	852	854	rBV	207842	197626	2.37%	0.258%
21	11.905	856	859	860	rBV3	118033	195676	2.35%	0.255%
22	12.054	870	872	874	rBV2	170917	203724	2.44%	0.266%
23	12.099	874	876	878	rVB	167771	167937	2.01%	0.219%
24	12.214	883	886	888	rVV	492758	566037	6.79%	0.739%
25	12.294	892	893	895	rVB	89940	105608	1.27%	0.138%
26	12.431	903	905	909	rVB2	213346	253417	3.04%	0.331%
27	12.602	918	920	922	rVB	103394	94926	1.14%	0.124%
28	12.659	922	925	930	rBV2	123184	206044	2.47%	0.269%
29	12.774	933	935	938	rVB	67802	92403	1.11%	0.121%
30	12.934	946	949	952	rVB	4669231	5840287	70.06%	7.620%
31	13.071	959	961	963	rBV	1125041	956250	11.47%	1.248%
32	13.185	968	971	972	rBV	41906	88002	1.06%	0.115%
33	13.208	972	973	975	rVB	105689	85783	1.03%	0.112%
34	13.859	1028	1030	1036	rBV	185604	415560	4.99%	0.542%

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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:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.985	1038	1041	1043	rBV	1895175	2321642	27.85%	3.029%
36	14.500	1081	1086	1095	rBV3	86864	292366	3.51%	0.381%
37	15.402	1162	1165	1168	rBV	1500535	1850147	22.19%	2.414%
38	17.186	1317	1321	1327	rVB	200093	440314	5.28%	0.575%
39	17.368	1333	1337	1344	rBV5	47135	175359	2.10%	0.229%
40	17.540	1349	1352	1356	rVV3	43596	97940	1.17%	0.128%
41	21.209	1666	1673	1680	rBV8	41137	153931	1.85%	0.201%

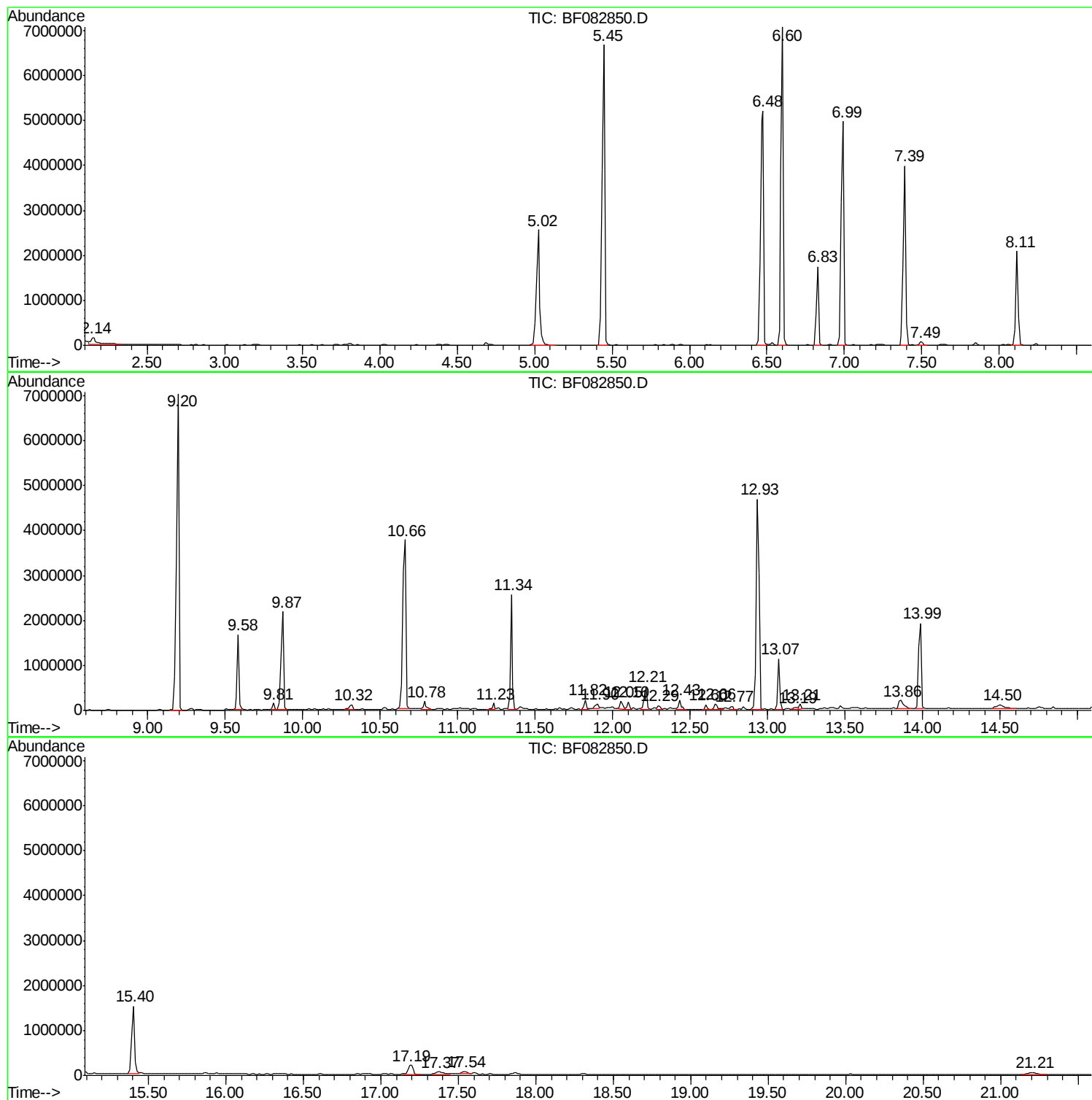
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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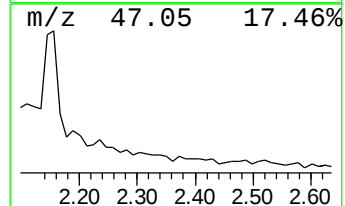
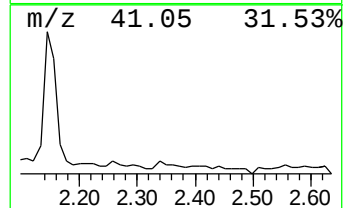
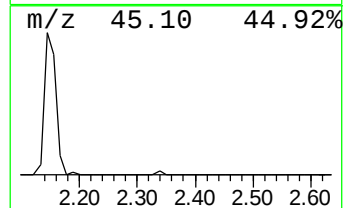
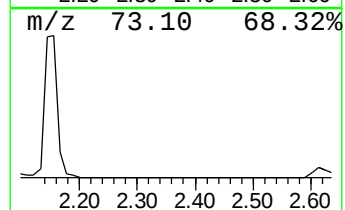
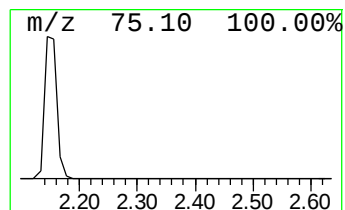
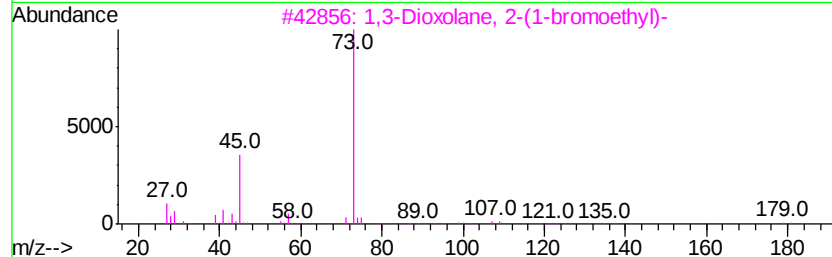
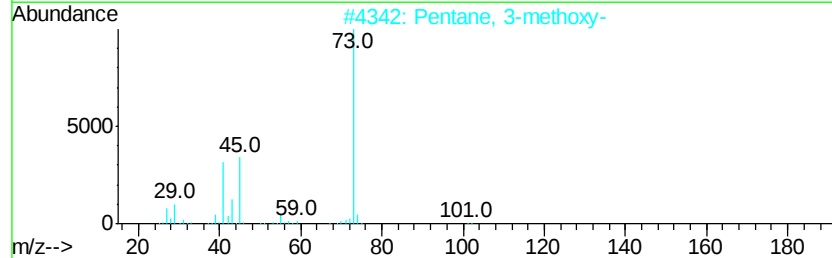
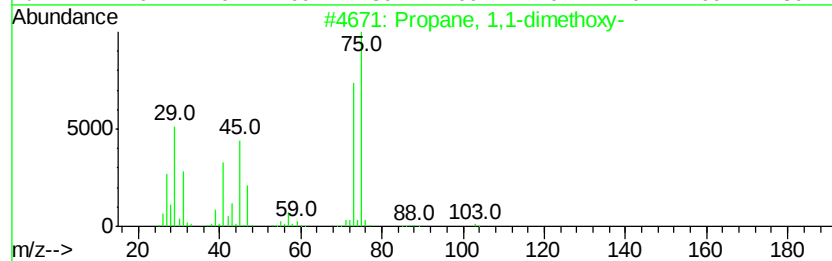
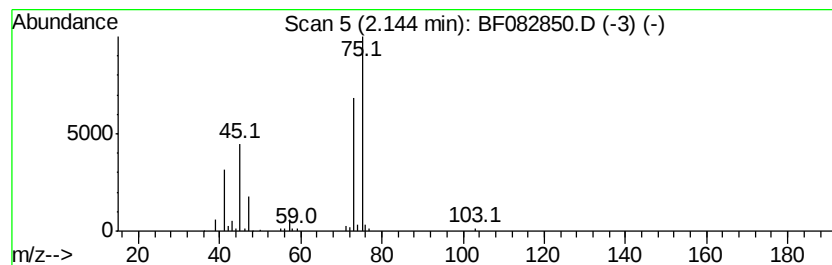
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.14	4.77 ng	401824	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	74
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	22
3		1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	12
4		Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9
5		d-(+)-Glyceric acid	106	C3H6O4	1000211-40-8	9



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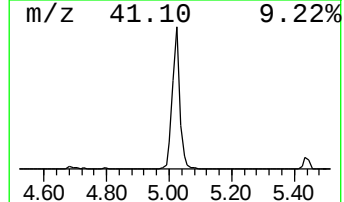
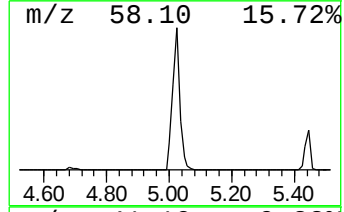
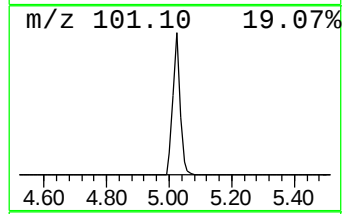
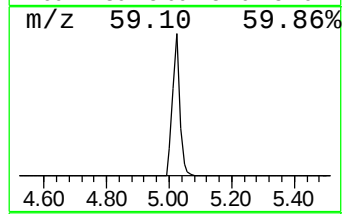
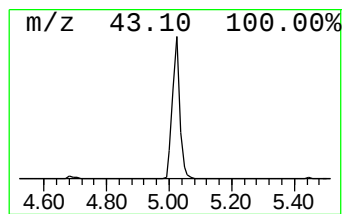
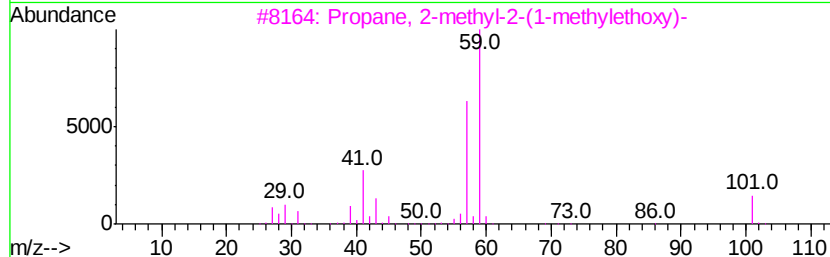
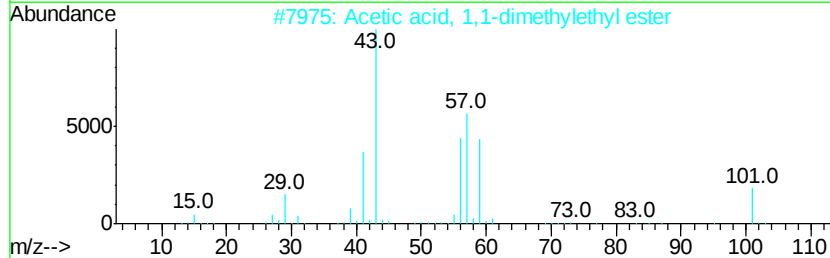
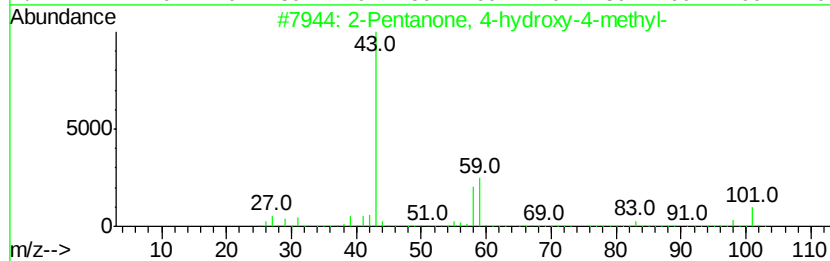
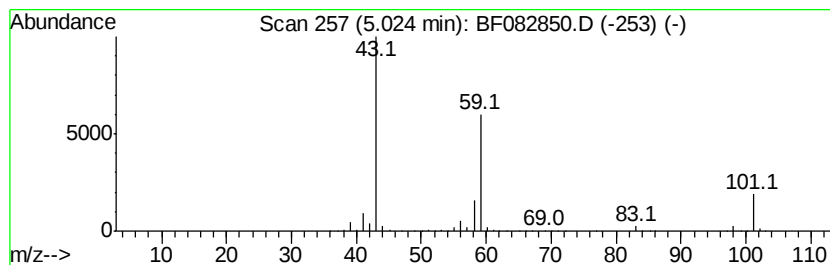
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	47.62 ng	4012290	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
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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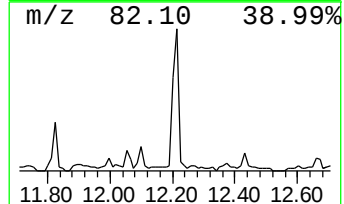
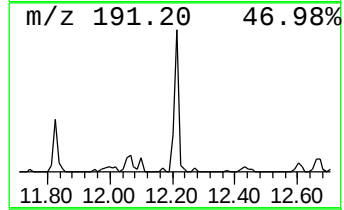
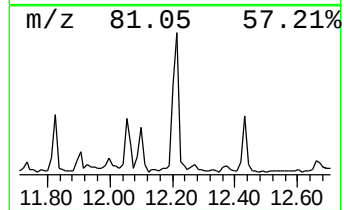
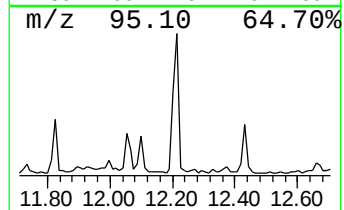
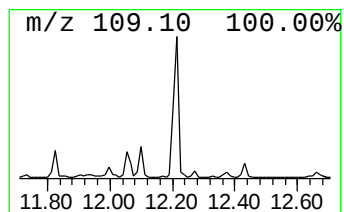
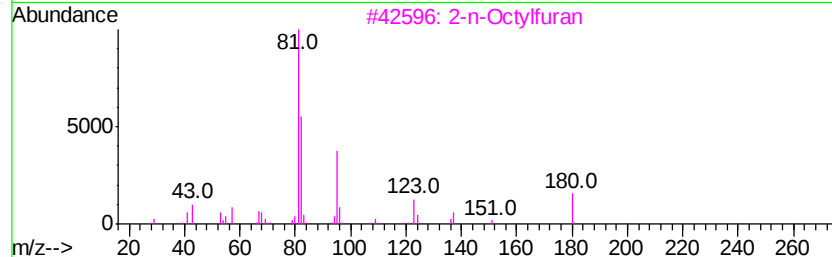
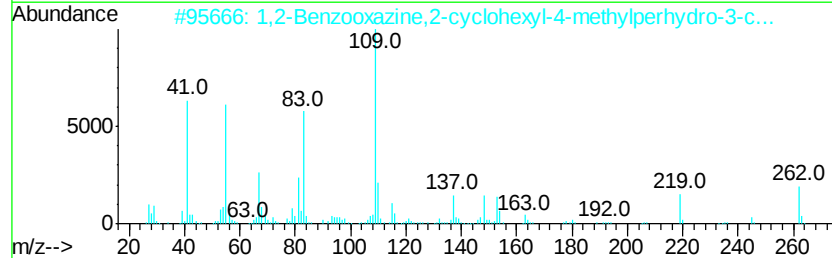
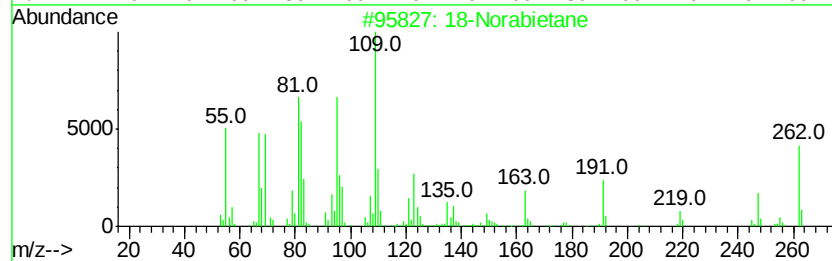
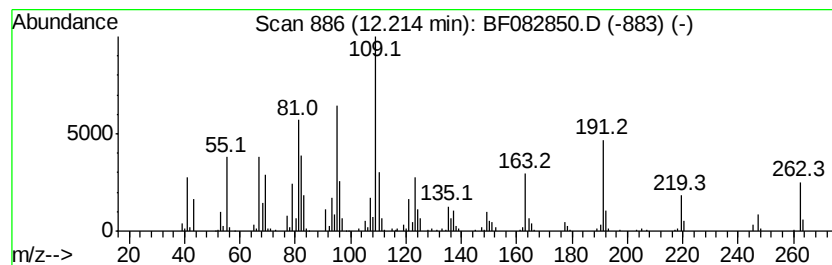
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 18-Norabietane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.21	4.94 ng	566037	Phenanthrene-d10	11.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	18-Norabietane	262	C19H34	1000293-16-6	58
2		1,2-Benzooxazine,2-cyclohexyl-4-...	262	C16H26N2O	037898-39-8	38
3		2-n-Octylfuran	180	C12H20O	004179-38-8	22
4		1-Methyl-2-methylenecyclohexane	110	C8H14	002808-75-5	22
5		1,1-Dimethyl-4-methylenecyclohexane	124	C9H16	006007-96-1	16



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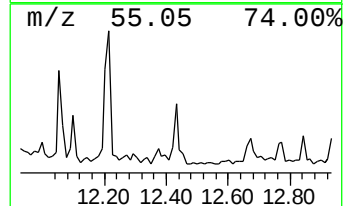
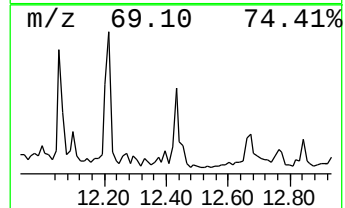
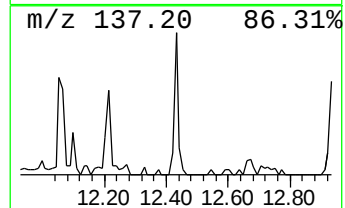
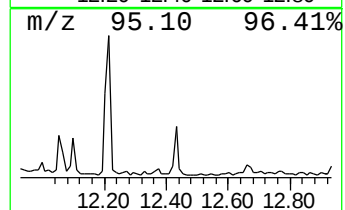
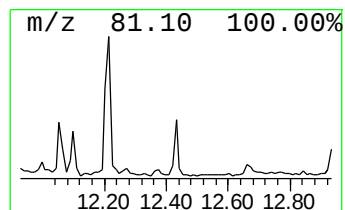
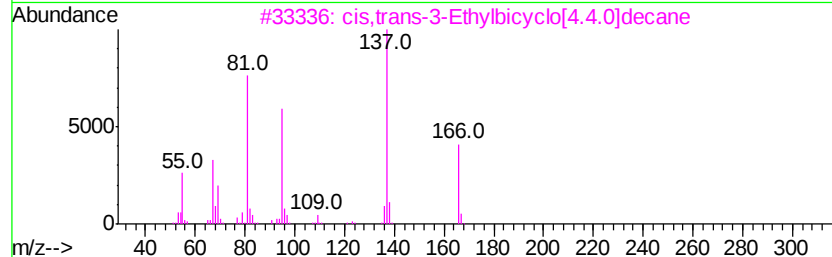
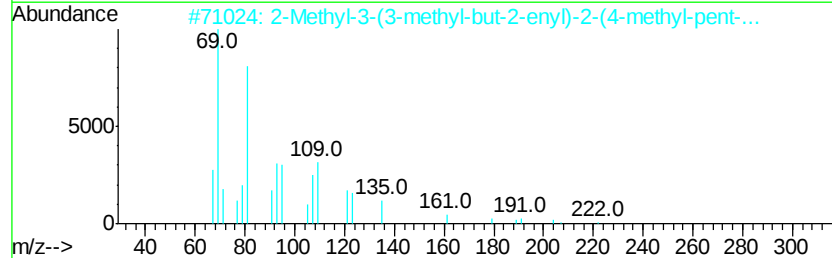
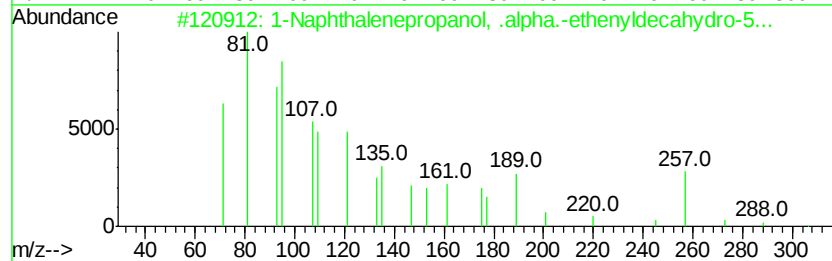
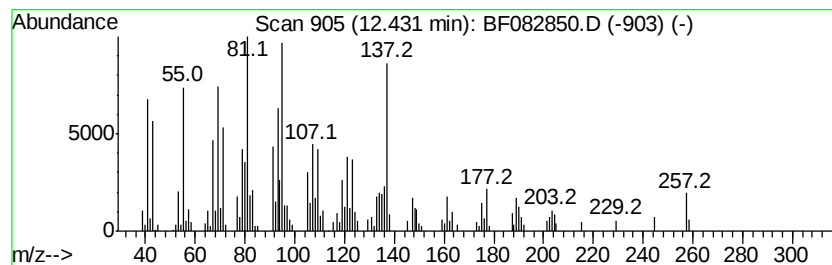
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown12.43 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.43	2.21 ng	253417	Phenanthrene-d10	11.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Naphthalenepropanol, .alpha.-e...	306	C20H34O2	003650-30-4	46
2		2-Methyl-3-(3-methyl-but-2-enyl)...	222	C15H26O	1000144-10-2	43
3		cis,trans-3-Ethylbicyclo[4.4.0]d...	166	C12H22	066660-41-1	38
4		2(1H)-Pyridone, 1-ethyl-4-methyl-	137	C8H11NO	019006-62-3	35
5		2,2-Dimethyl-3-(3,7,16,20-tetram...	412	C29H48O	1000194-78-6	27



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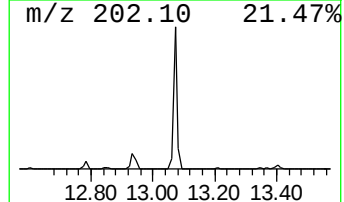
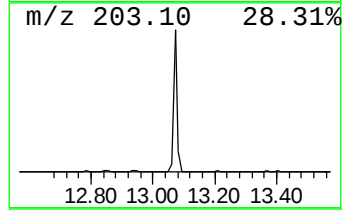
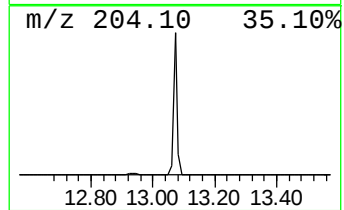
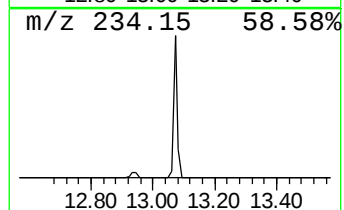
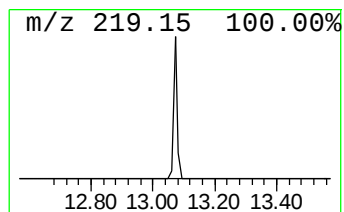
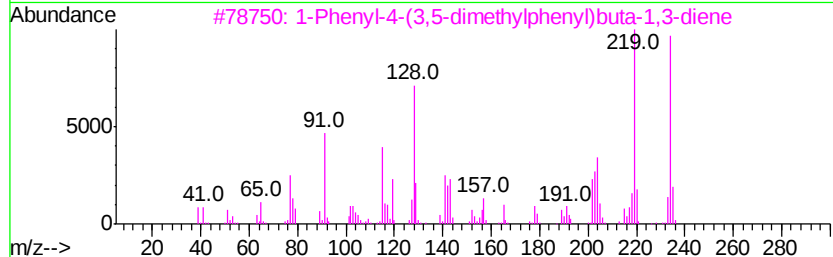
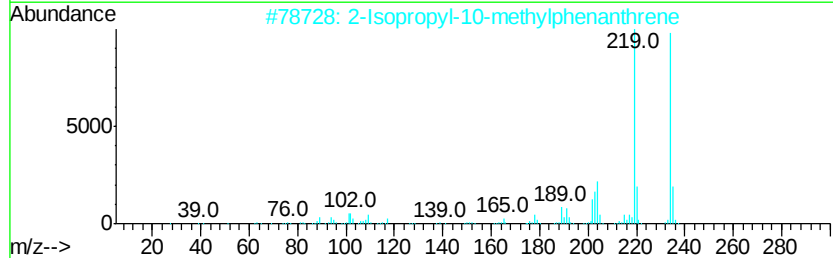
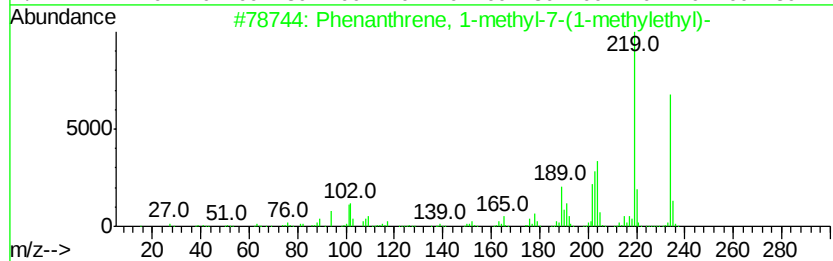
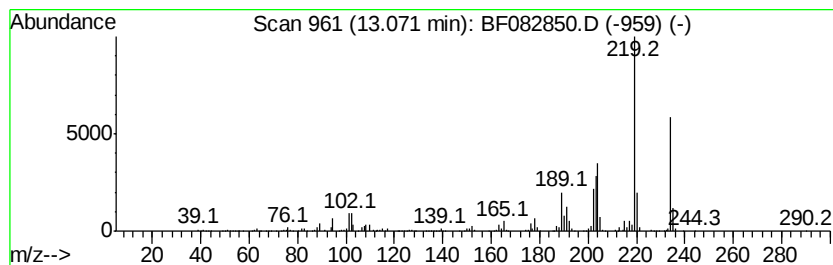
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TIC Integration Parameters: LSCINT.P

Peak Number 7 Phenanthrene, 1-methyl-7-(1... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.07	8.24 ng	956250	Chrysene-d12	13.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenanthrene, 1-methyl-7-(1-meth...	234	C18H18	000483-65-8	99
2		2-Isopropyl-10-methylphenanthrene	234	C18H18	066552-97-4	95
3		1-Phenyl-4-(3,5-dimethylphenyl)b...	234	C18H18	1000202-15-0	83
4		2,5-Diphenyl-2,4-hexadiene	234	C18H18	016819-47-9	64
5		3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	50



Data Path : Z:\HPCHEM1\BNA F\DATA\BF110915\
Data File : BF082850.D
Acq On : 10 Nov 2015 3:17
Operator : UM/IZ
Sample : G4286-07
Misc :
ALS Vial : 21 Sample Multiplier: 1

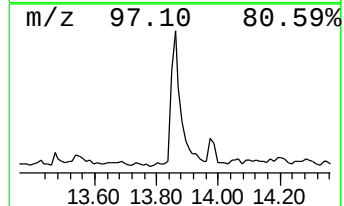
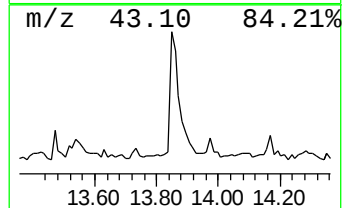
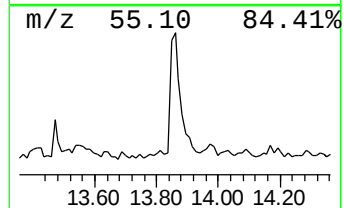
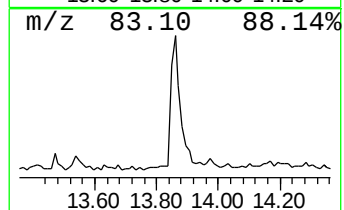
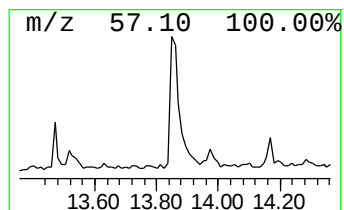
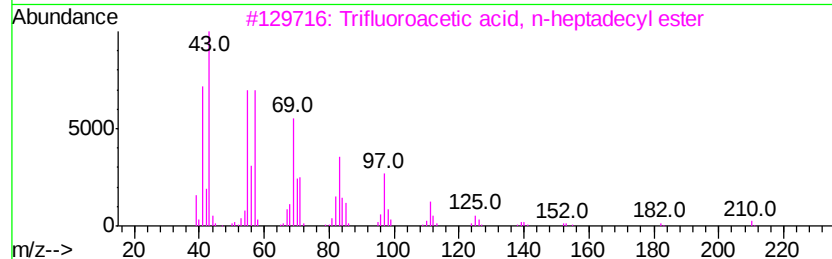
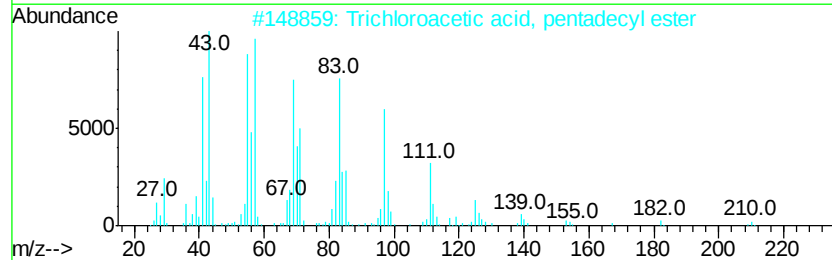
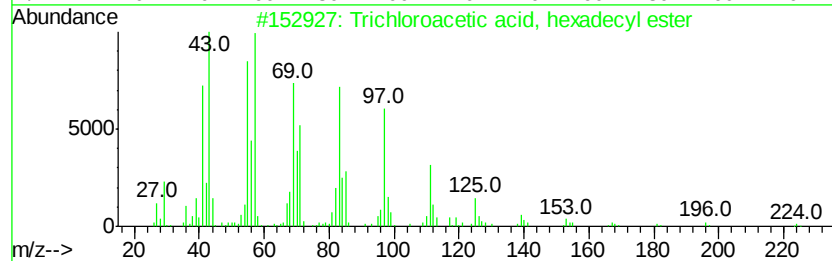
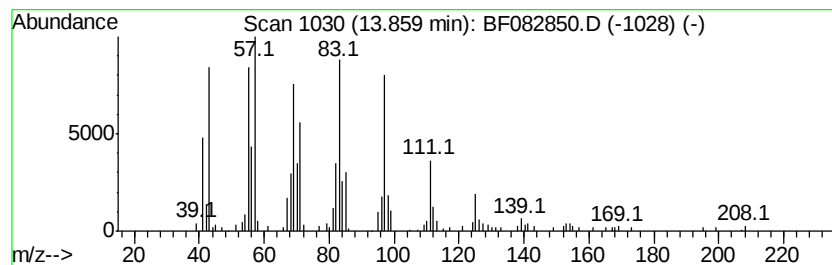
Instrument :
BNA_F
ClientSampleId :
T-2R

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Trichloroacetic acid, hexad... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.86	3.58 ng	415560	Chrysene-d12	13.99	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87
3	Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	83
4	1-Heptadecanol	256	C17H36O	001454-85-9	81
5	1-Docosene	308	C22H44	001599-67-3	81



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110915\
Data File : BF082850.D
Acq On : 10 Nov 2015 3:17
Operator : UM/IZ
Sample : G4286-07
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T-2R

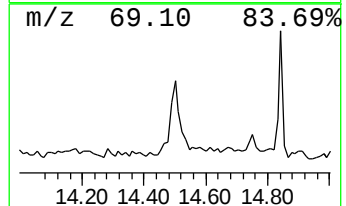
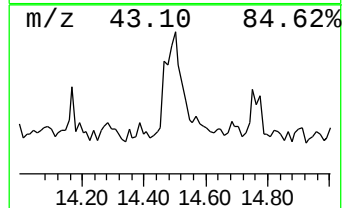
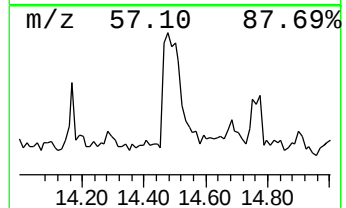
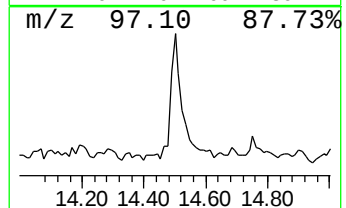
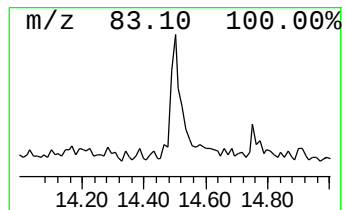
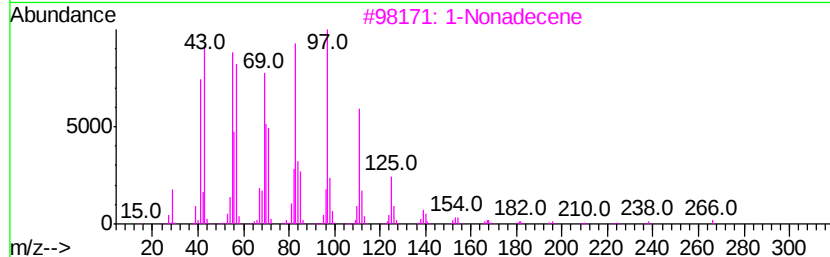
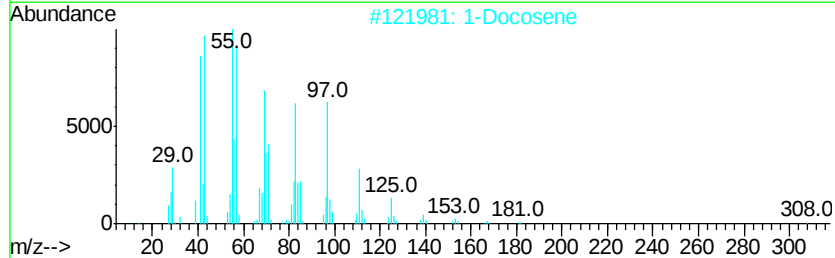
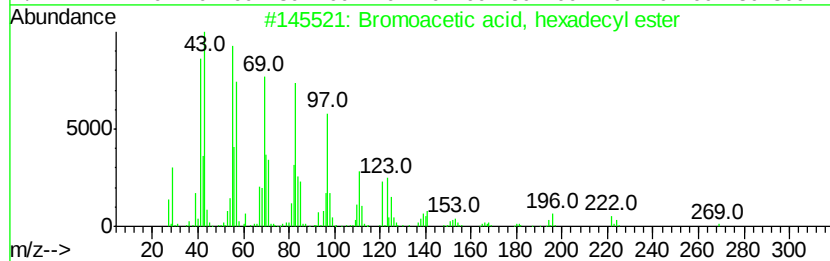
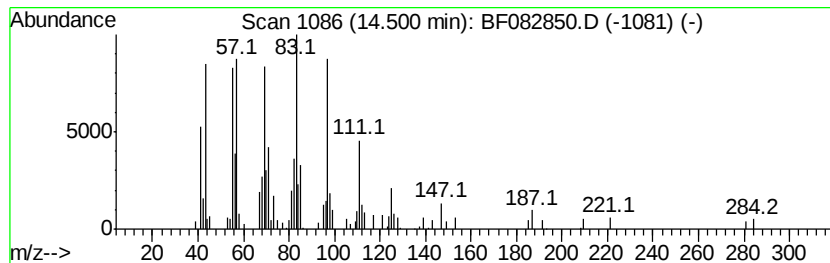
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Bromoacetic acid, hexadecyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.50	2.52 ng	292366	Chrysene-d12	13.99

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	70
2		1-Docosene	308	C22H44	001599-67-3	62
3		1-Nonadecene	266	C19H38	018435-45-5	62
4		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	58
5		1-Tetracosanol	354	C24H50O	000506-51-4	58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110915\
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Sample : G4286-07
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T-2R

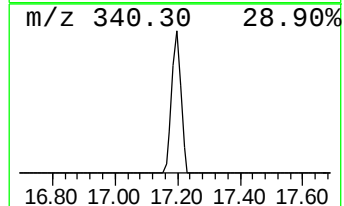
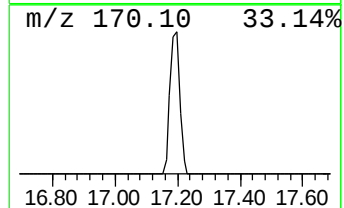
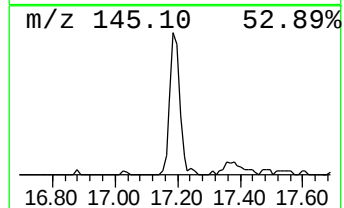
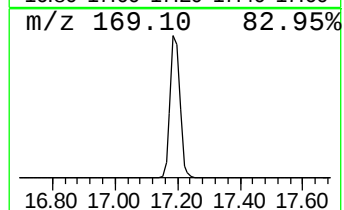
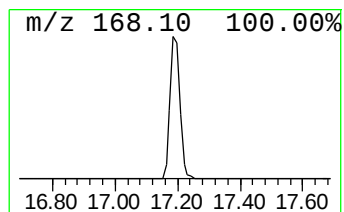
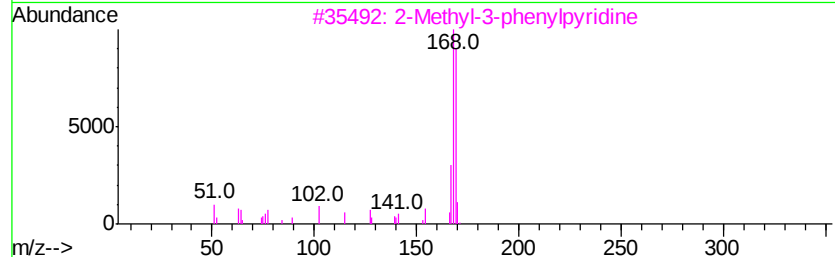
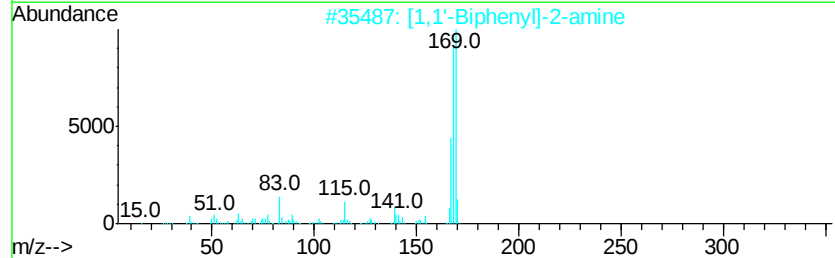
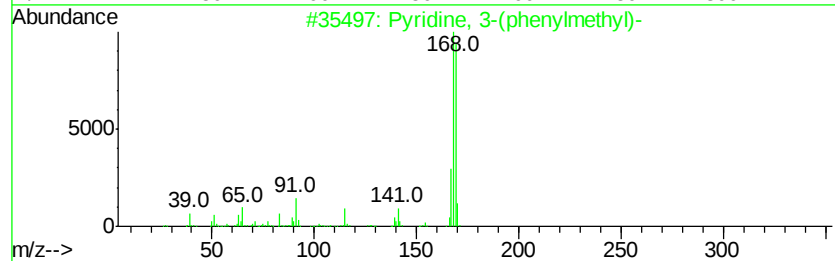
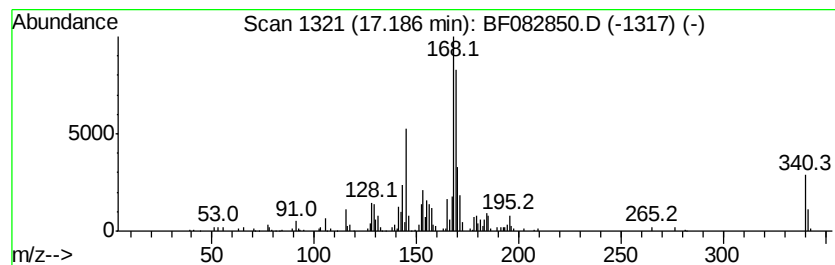
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown17.19 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.19	4.76 ng	440314	Perylene-d12	15.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyridine, 3-(phenylmethyl)-	169	C12H11N	000620-95-1	43
2		[1,1'-Biphenyl]-2-amine	169	C12H11N	000090-41-5	43
3		2-Methyl-3-phenylpyridine	169	C12H11N	003256-89-1	43
4		Benzeneacetamide, N,N-diphenyl-	287	C20H17NO	033675-70-6	43
5		1,2-Dihydro-5-acenaphthylenamine	169	C12H11N	004657-93-6	37



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110915\
Data File : BF082850.D
Acq On : 10 Nov 2015 3:17
Operator : UM/IZ
Sample : G4286-07
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T-2R

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.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
Propane, 1,1-dime...	2.14	4.8	ng	401824	1	6.83	1685250	20.0
2-Pentanone, 4-hy...	5.02	47.6	ng	4012290	1	6.83	1685250	20.0
18-Norabietane	12.21	4.9	ng	566037	4	11.34	2293650	20.0
unknown12.43	12.43	2.2	ng	253417	4	11.34	2293650	20.0
Phenanthrene, 1-m...	13.07	8.2	ng	956250	5	13.99	2321640	20.0
Trichloroacetic a...	13.86	3.6	ng	415560	5	13.99	2321640	20.0
Bromoacetic acid,...	14.50	2.5	ng	292366	5	13.99	2321640	20.0
unknown17.19	17.19	4.8	ng	440314	6	15.40	1850150	20.0