

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120415\
 Data File : BG019908.D
 Acq On : 4 Dec 2015 17:06
 Operator : UM/NP
 Sample : G4642-01
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TW-04

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_G\METHODS\8270-BG120215.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	5.191	393	400	405	rBV	29848	44485	1.68%	0.344%
2	5.661	473	480	489	rVB	206471	338546	12.81%	2.621%
3	7.259	744	752	761	rVB	133712	236264	8.94%	1.829%
4	7.641	809	817	826	rBV	438959	763864	28.90%	5.914%
5	8.117	891	898	905	rBV	105950	175375	6.63%	1.358%
6	8.446	945	954	962	rBV	417648	733893	27.76%	5.682%
7	9.286	1088	1097	1107	rBV	387135	678164	25.66%	5.250%
8	10.937	1371	1378	1385	rBV	151582	268195	10.15%	2.076%
9	13.375	1785	1793	1802	rVB	1187982	1804475	68.27%	13.970%
10	14.744	2020	2026	2035	rVB3	264010	423244	16.01%	3.277%
11	15.585	2164	2169	2174	rVB	20856	28548	1.08%	0.221%
12	16.231	2272	2279	2289	rBV	1022197	1551501	58.70%	12.012%
13	16.442	2309	2315	2318	rBV2	23895	32901	1.24%	0.255%
14	16.883	2385	2390	2397	rVB6	12630	26776	1.01%	0.207%
15	16.948	2397	2401	2406	rBV	18093	26459	1.00%	0.205%
16	17.488	2487	2493	2499	rBV	377209	546638	20.68%	4.232%
17	18.364	2637	2642	2649	rBV2	48982	72924	2.76%	0.565%
18	19.221	2783	2788	2795	rBV2	30599	46355	1.75%	0.359%
19	19.539	2839	2842	2848	rVB2	21806	27697	1.05%	0.214%
20	19.633	2854	2858	2863	rBV3	46001	64904	2.46%	0.502%
21	19.768	2877	2881	2887	rBV	23991	31409	1.19%	0.243%
22	20.091	2930	2936	2942	rBV	2088127	2643272	100.00%	20.464%
23	20.297	2967	2971	2976	rBV	35984	47152	1.78%	0.365%
24	20.779	3049	3053	3059	rVB	64951	89132	3.37%	0.690%
25	20.855	3059	3066	3076	rBV3	54390	106354	4.02%	0.823%
26	20.996	3085	3090	3094	rBV3	43363	83836	3.17%	0.649%
27	21.043	3094	3098	3102	rVV	77951	103924	3.93%	0.805%
28	21.108	3106	3109	3115	rVB2	33347	48622	1.84%	0.376%
29	21.395	3156	3158	3165	rVB8	27667	44390	1.68%	0.344%
30	21.554	3177	3185	3189	rBV2	66969	124024	4.69%	0.960%
31	21.625	3193	3197	3201	rBV2	32213	55182	2.09%	0.427%
32	21.760	3214	3220	3228	rVB	420941	720521	27.26%	5.578%
33	22.106	3275	3279	3284	rVB2	42447	63064	2.39%	0.488%
34	22.377	3321	3325	3330	rVB4	19190	34885	1.32%	0.270%

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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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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	22.735	3381	3386	3392	rVB2	42488	74676	2.83%	0.578%
36	23.046	3434	3439	3441	rBV2	26593	47646	1.80%	0.369%
37	23.082	3443	3445	3452	rVB2	47264	75438	2.85%	0.584%
38	25.050	3770	3780	3789	rBV	228306	631855	23.90%	4.892%

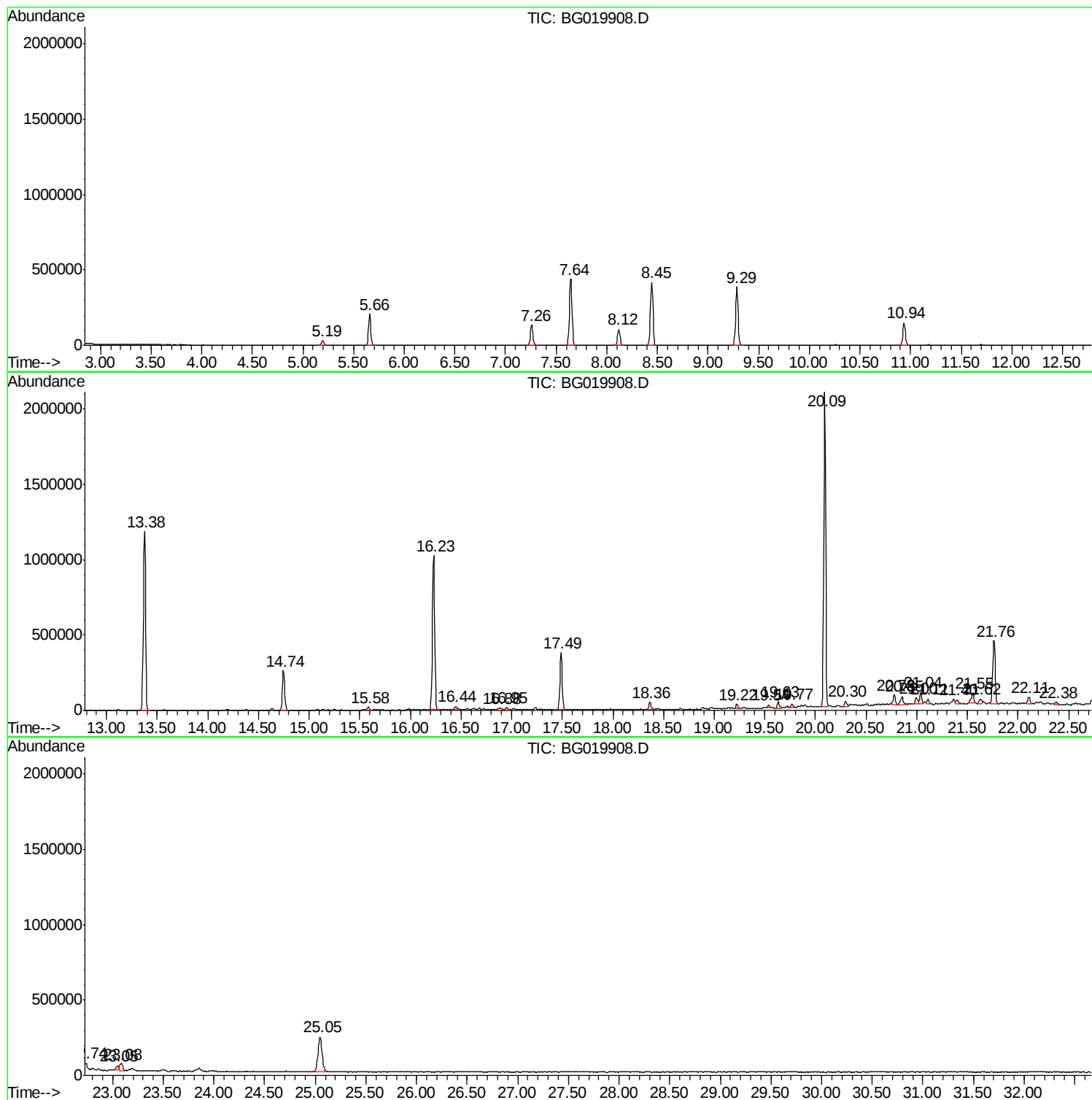
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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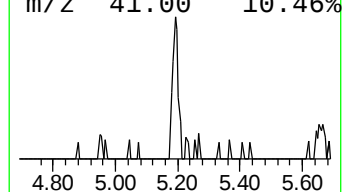
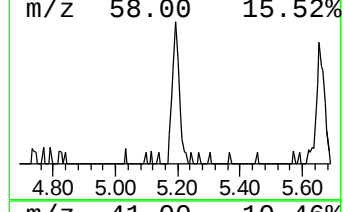
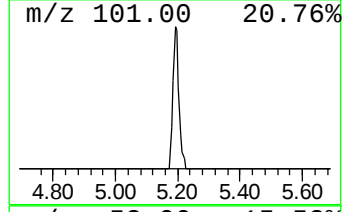
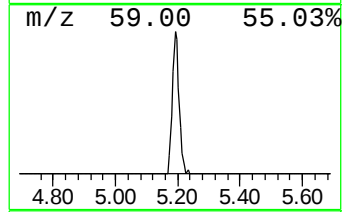
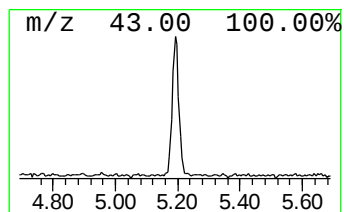
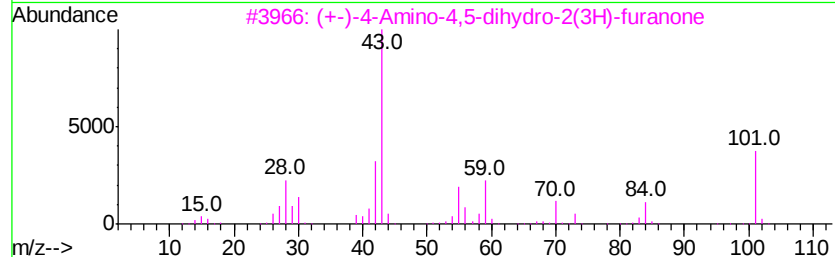
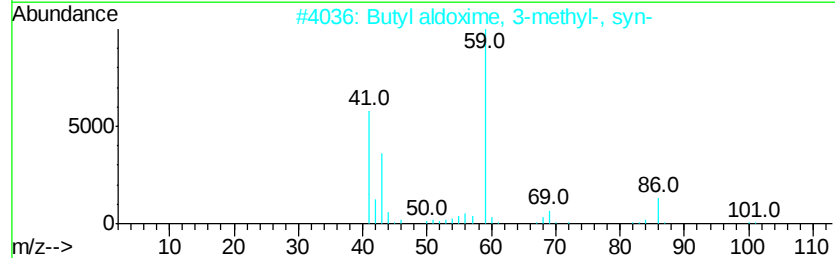
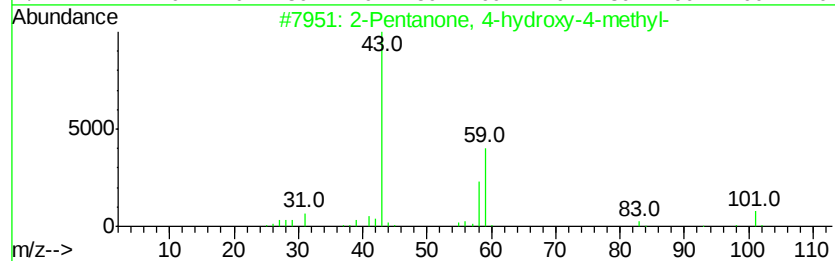
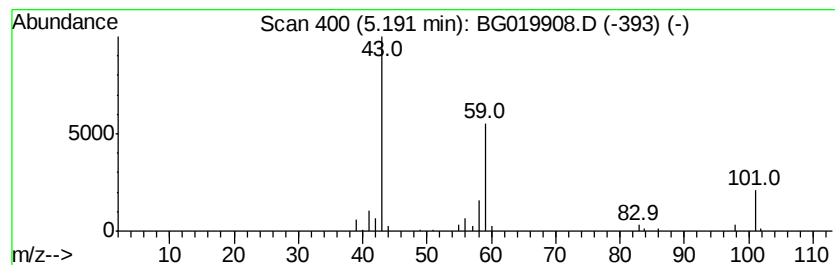
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.19	5.07 ng	44485	1,4-Dichlorobenzene-d4	8.12

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
3			(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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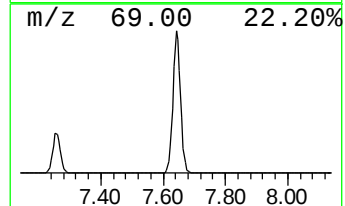
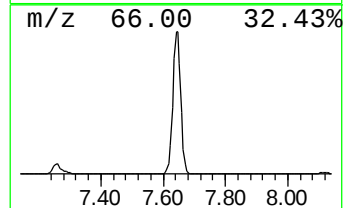
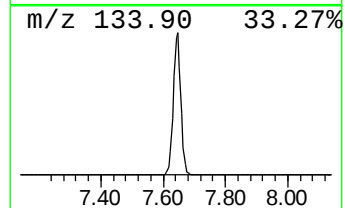
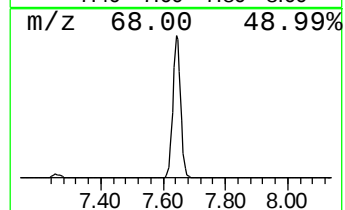
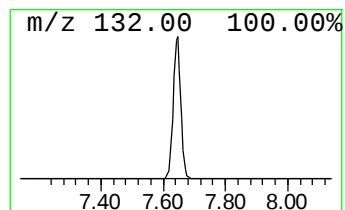
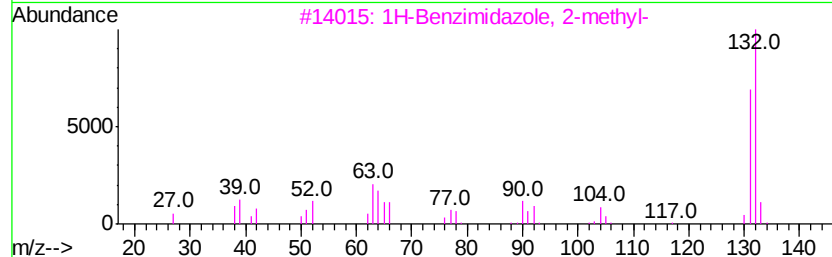
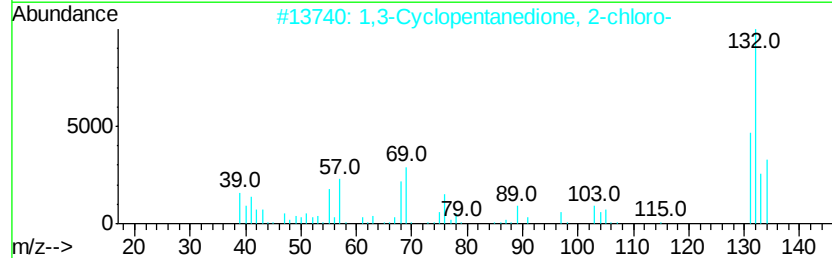
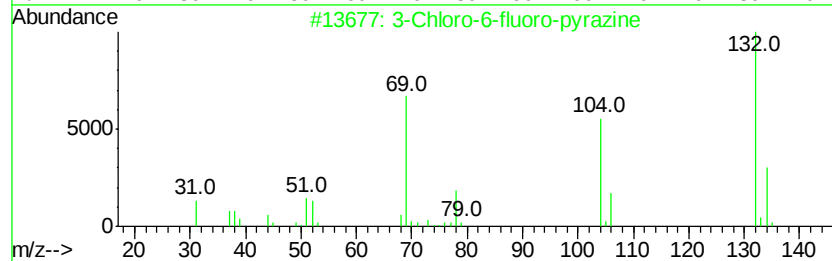
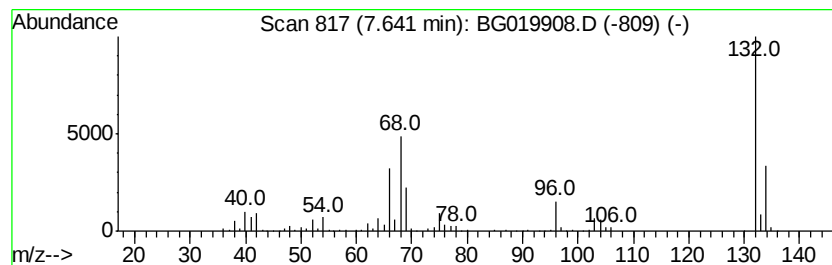
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown7.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.64	87.11 ng	763864	1,4-Dichlorobenzene-d4	8.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12
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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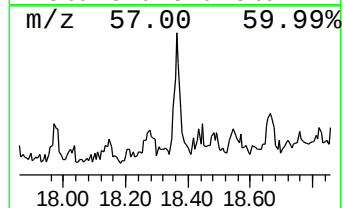
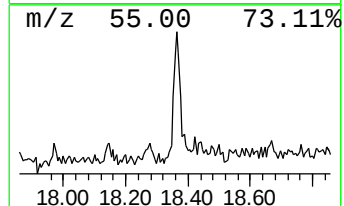
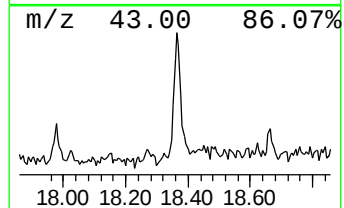
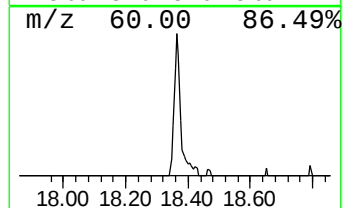
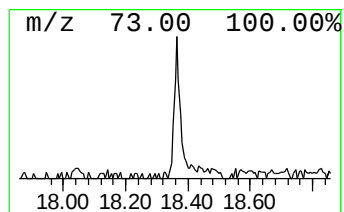
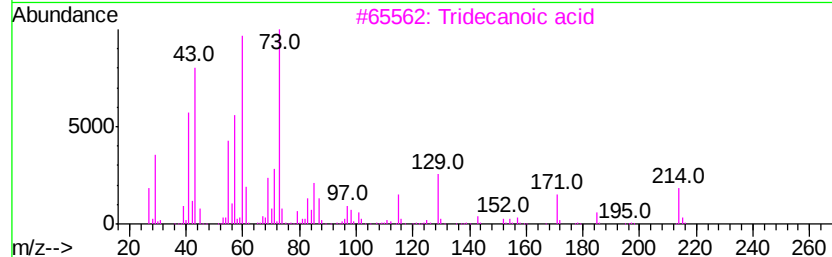
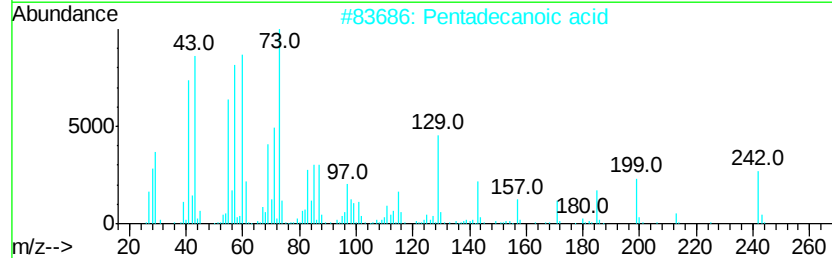
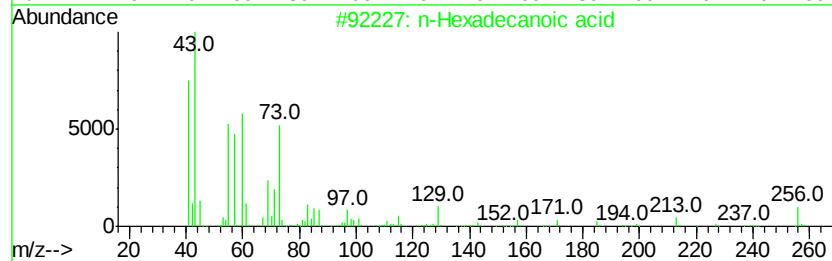
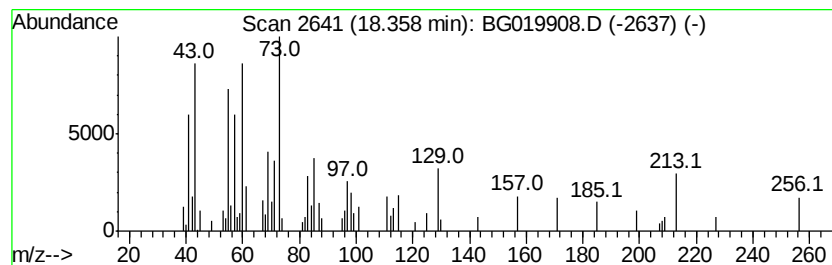
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.36	2.67 ng	72924	Phenanthrene-d10	17.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3		Tridecanoic acid	214	C13H26O2	000638-53-9	76
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5		n-Decanoic acid	172	C10H20O2	000334-48-5	47



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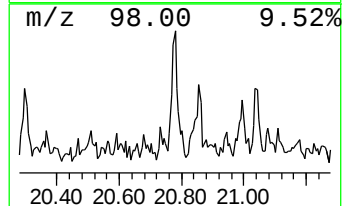
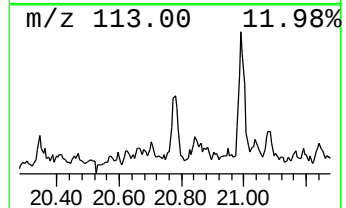
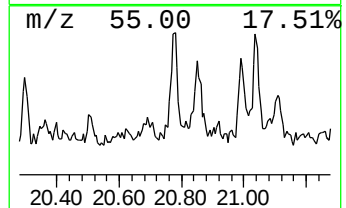
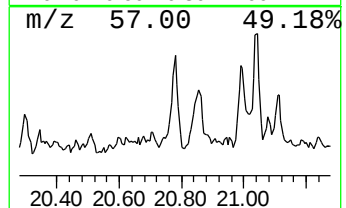
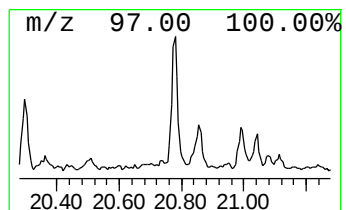
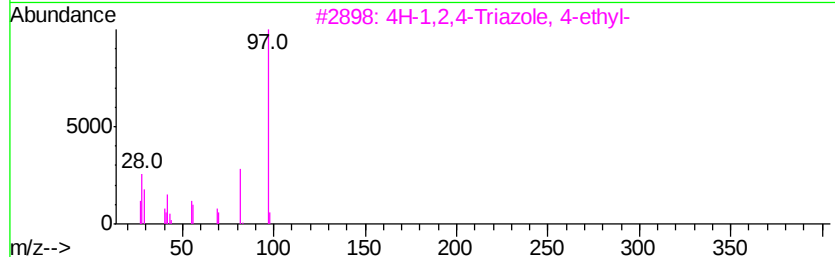
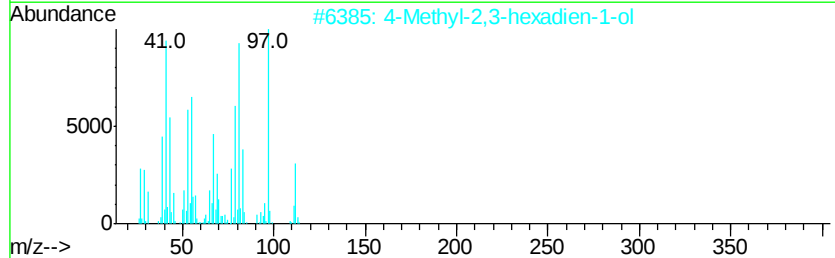
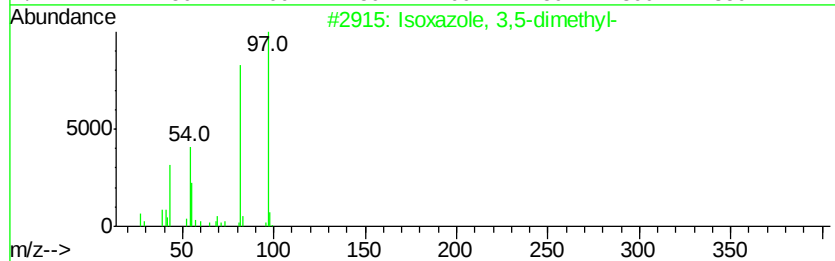
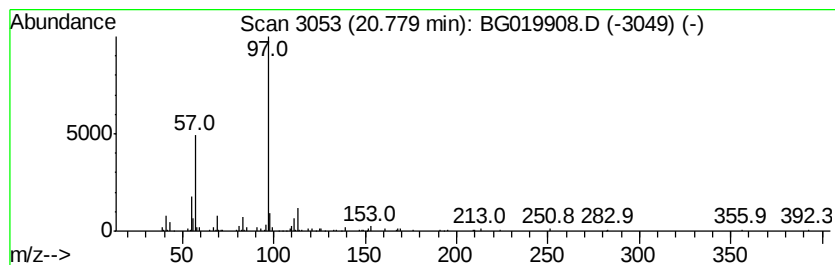
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Isoxazole, 3,5-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.78	2.47 ng	89132	Chrysene-d12	21.76

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isoxazole, 3,5-dimethyl-	97	C5H7NO	000300-87-8	53
2		4-Methyl-2,3-hexadien-1-ol	112	C7H12O	1000196-09-6	50
3		4H-1,2,4-Triazole, 4-ethyl-	97	C4H7N3	043183-55-7	40
4		Thiophene, 2-ethyl-	112	C6H8S	000872-55-9	38
5		2H-Pyran-2-one, 5,6-dihydro-6-pe...	168	C10H16O2	054814-64-1	38



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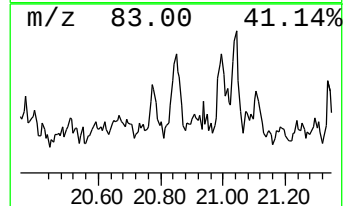
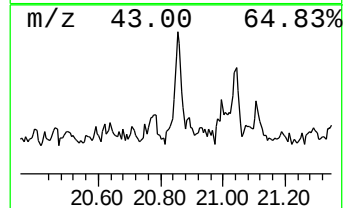
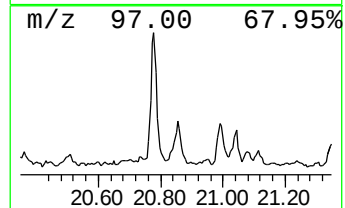
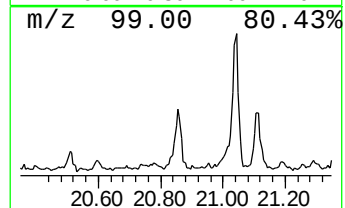
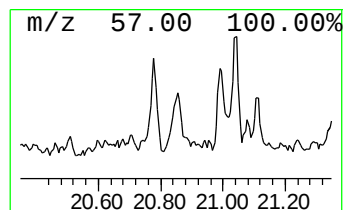
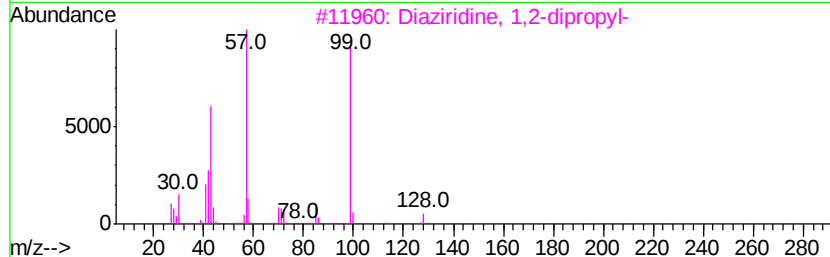
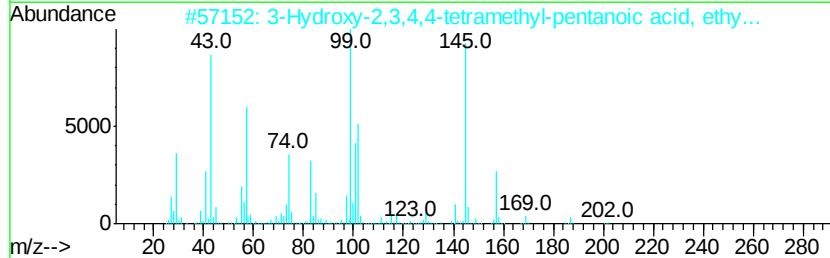
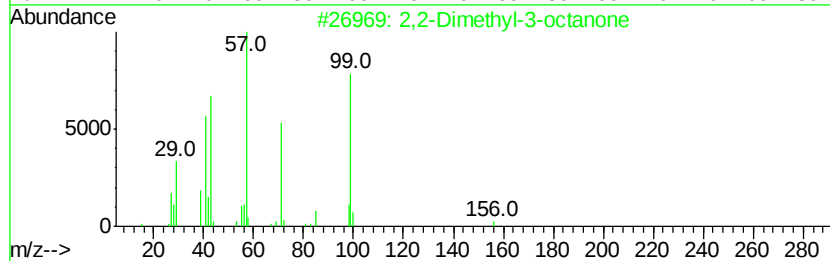
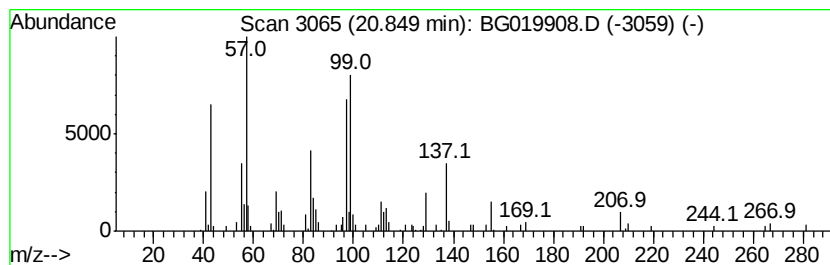
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown20.85 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.85	2.95 ng	106354	Chrysene-d12	21.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,2-Dimethyl-3-octanone	156	C10H20O	005340-64-7	35
2		3-Hydroxy-2,3,4,4-tetramethyl-pe...	202	C11H22O3	1000194-64-5	35
3		Diaziridine, 1,2-dipropyl-	128	C7H16N2	006794-92-9	27
4		Cyclohexanol, 1-(aminomethyl)-	129	C7H15NO	004000-72-0	27
5		Hexanoic acid, 2-tetradecyl ester	312	C20H40O2	055193-21-0	25



Data Path : Z:\HPCHEM1\BNA G\DATA\BG120415\
Data File : BG019908.D
Acq On : 4 Dec 2015 17:06
Operator : UM/NP
Sample : G4642-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TW-04

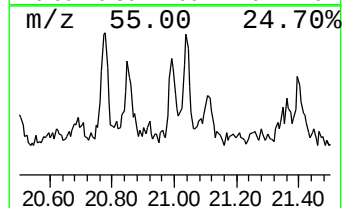
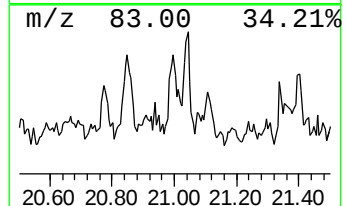
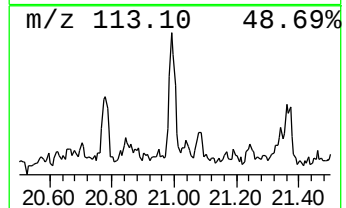
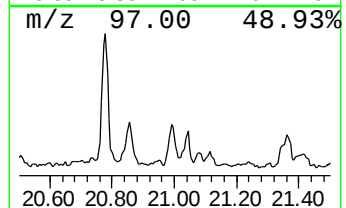
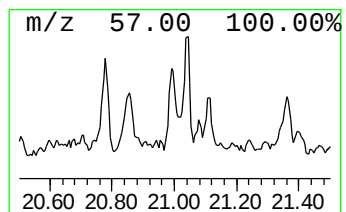
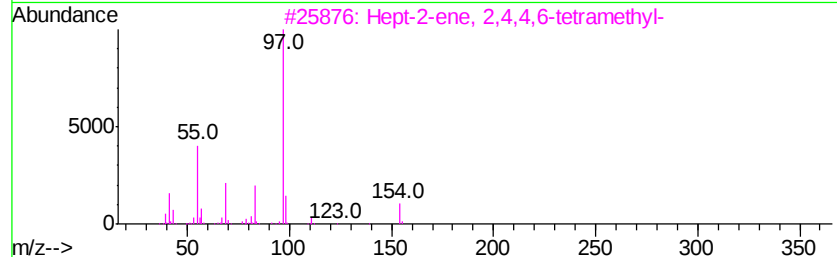
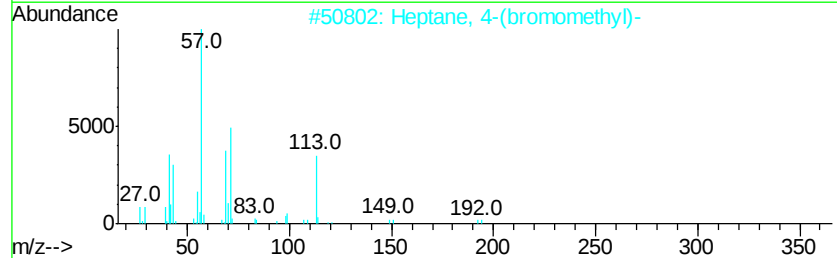
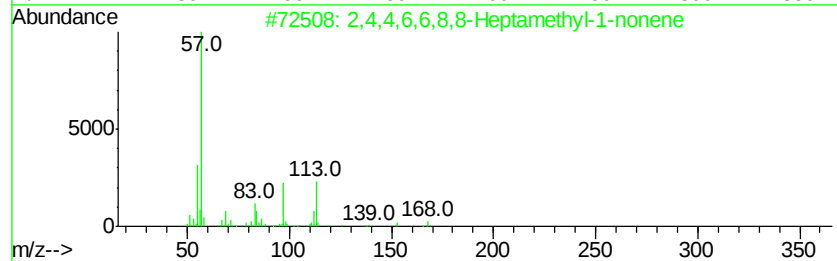
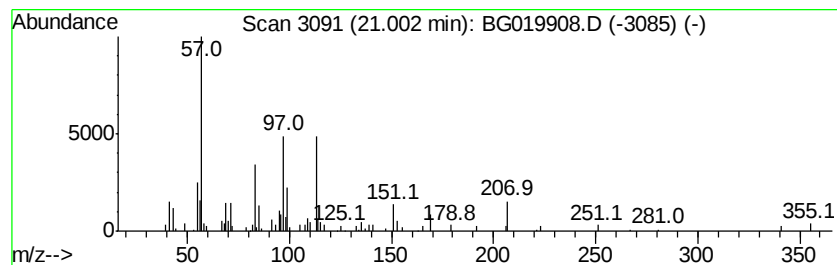
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.00	2.33 ng	83836	Chrysene-d12	21.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	50
2		Heptane, 4-(bromomethyl)-	192	C8H17Br	101654-29-9	25
3		Hept-2-ene, 2,4,4,6-tetramethyl-	154	C11H22	103982-58-7	22
4		Disulfide, di-tert-dodecyl	402	C24H50S2	027458-90-8	17
5		Octane, 2-bromo-	192	C8H17Br	000557-35-7	12



Data Path : Z:\HPCHEM1\BNA G\DATA\BG120415\
Data File : BG019908.D
Acq On : 4 Dec 2015 17:06
Operator : UM/NP
Sample : G4642-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TW-04

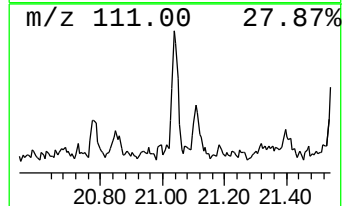
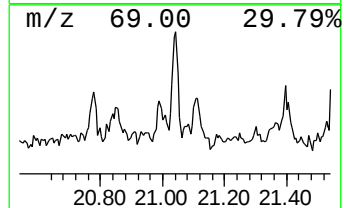
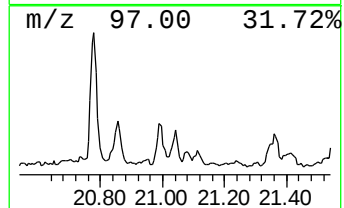
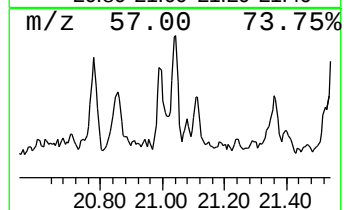
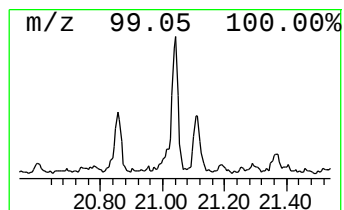
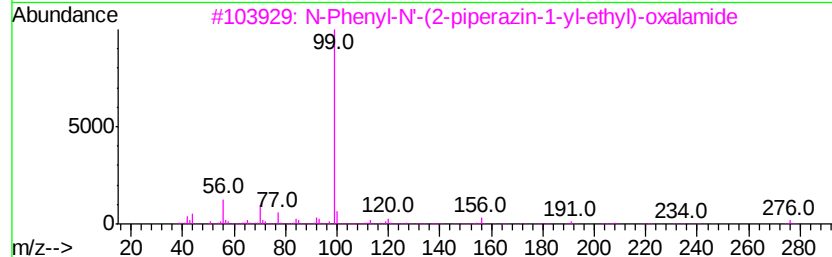
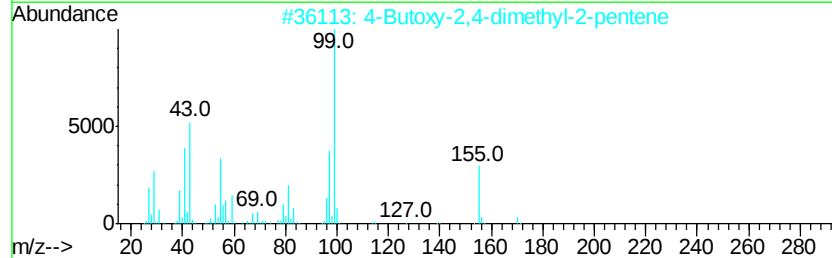
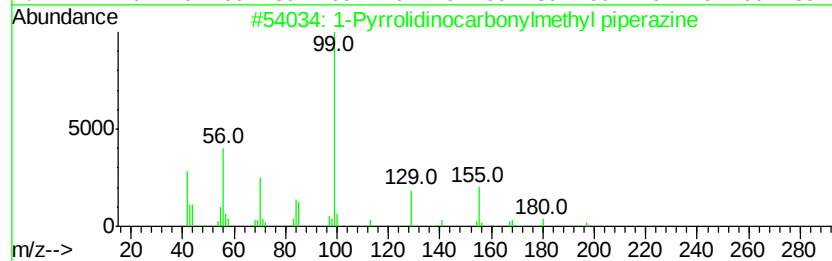
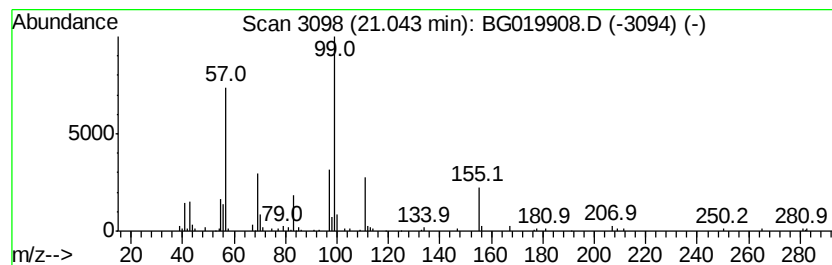
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown21.04 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.04	2.88 ng	103924	Chrysene-d12	21.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Pyrrolidinocarbonylmethyl pipe...	197	C10H19N3O	039890-45-4	47
2		4-Butoxy-2,4-dimethyl-2-pentene	170	C11H22O	1000159-08-7	45
3		N-Phenyl-N'-(2-piperazin-1-yl-ethyl-...	276	C14H20N4O2	332404-00-9	38
4		2-Propylthiazole	127	C6H9NS	017626-75-4	35
5		N-(4-Bromo-3-methyl-phenyl)-N'-(...	368	C15H21BrN4O2	1000294-59-4	35



Data Path : Z:\HPCHEM1\BNA G\DATA\BG120415\
Data File : BG019908.D
Acq On : 4 Dec 2015 17:06
Operator : UM/NP
Sample : G4642-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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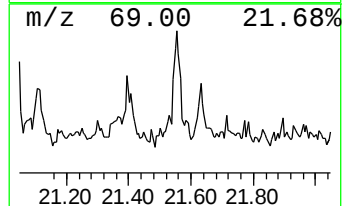
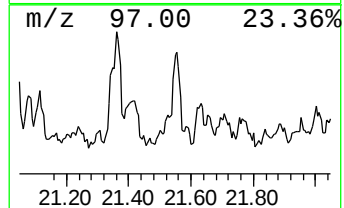
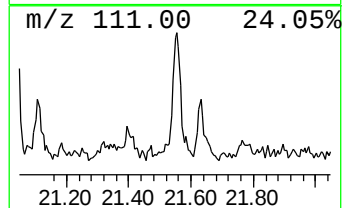
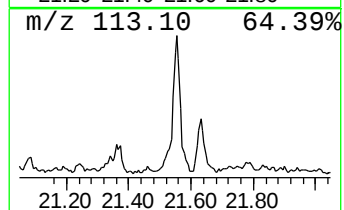
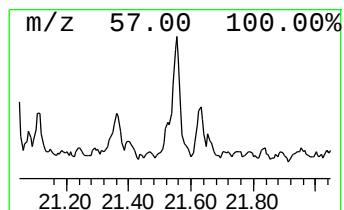
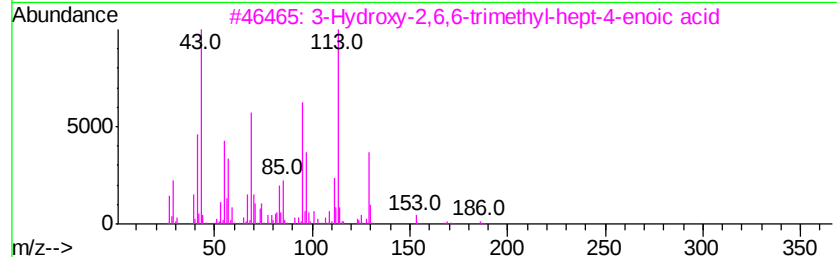
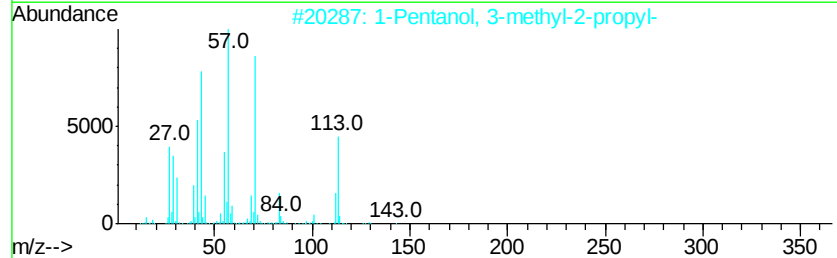
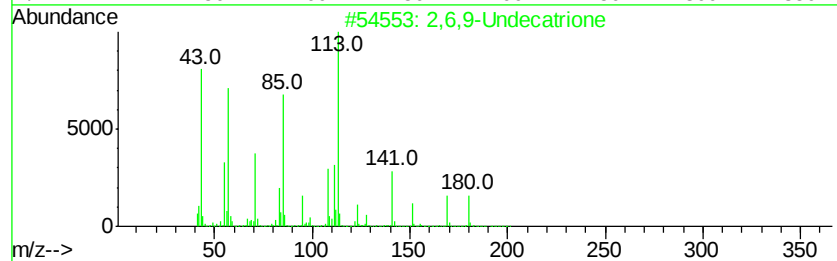
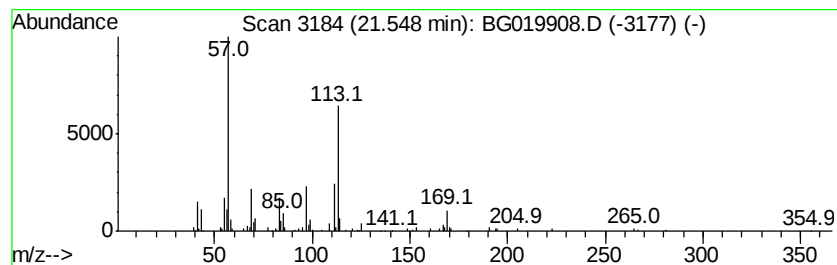
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown21.55 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.55	3.44 ng	124024	Chrysene-d12	21.76

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,9-Undecatriene			198	C11H18O3	078975-91-4	38
2	1-Pentanol, 3-methyl-2-propyl-			144	C9H20O	054004-40-9	37
3	3-Hydroxy-2,6,6-trimethyl-hept-4...			186	C10H18O3	1000185-34-0	37
4	1-Ethyl-2,2-dimethylpropyl ethyl...			210	C9H20F02P	1000298-32-8	32
5	5-Nonanone, 2,2,8,8-tetramethyl-			198	C13H26O	005709-95-5	25



Data Path : Z:\HPCHEM1\BNA G\DATA\BG120415\
Data File : BG019908.D
Acq On : 4 Dec 2015 17:06
Operator : UM/NP
Sample : G4642-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TW-04

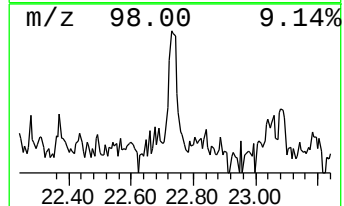
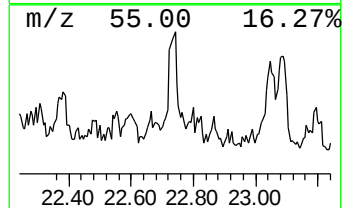
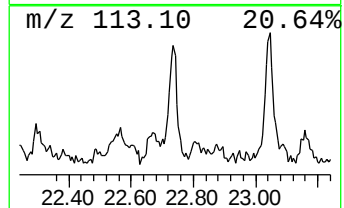
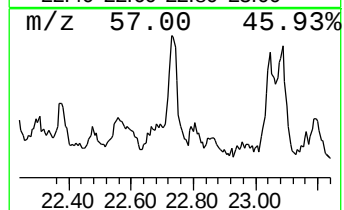
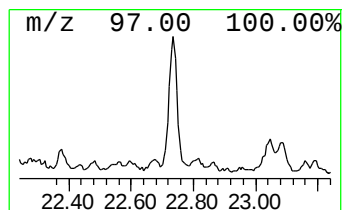
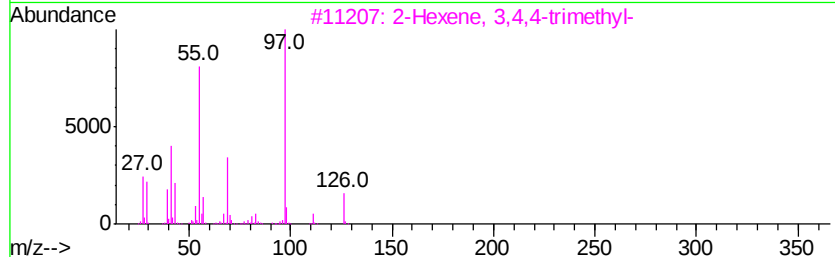
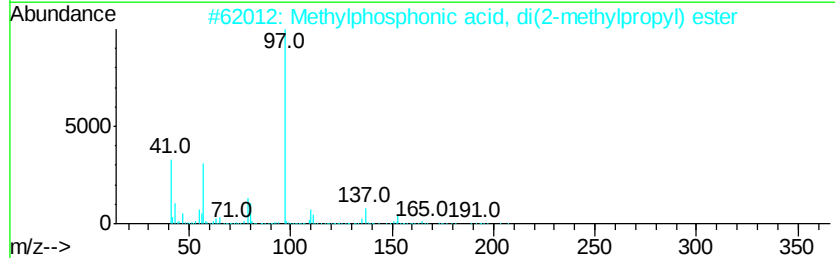
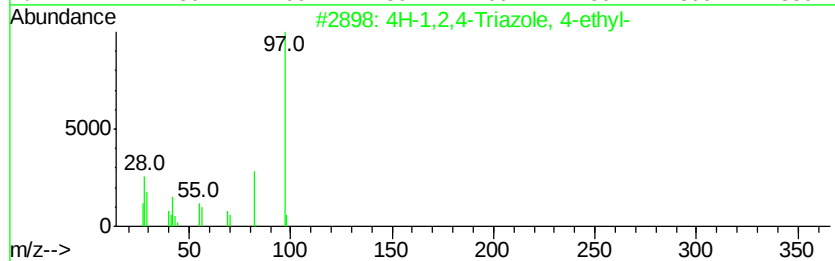
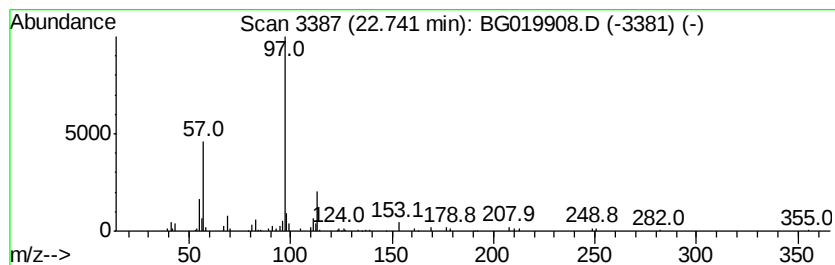
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown22.74 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.74	2.07 ng	74676	Chrysene-d12	21.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4H-1,2,4-Triazole, 4-ethyl-	97	C4H7N3	043183-55-7	47
2		Methylphosphonic acid, di(2-meth...	208	C9H21O3P	105263-11-4	45
3		2-Hexene, 3,4,4-trimethyl-	126	C9H18	053941-19-8	42
4		2H-Pyran-2-one, 5,6-dihydro-6-pe...	168	C10H16O2	054814-64-1	40
5		2-Thiopheneacetic acid, 3-methyl...	212	C11H16O2S	1000278-95-5	40



Data Path : Z:\HPCHEM1\BNA G\DATA\BG120415\
Data File : BG019908.D
Acq On : 4 Dec 2015 17:06
Operator : UM/NP
Sample : G4642-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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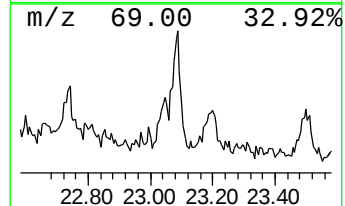
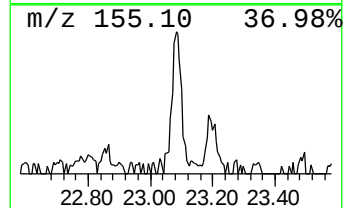
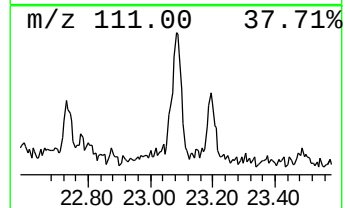
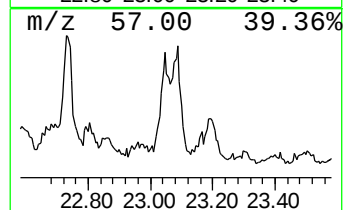
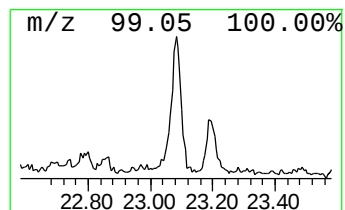
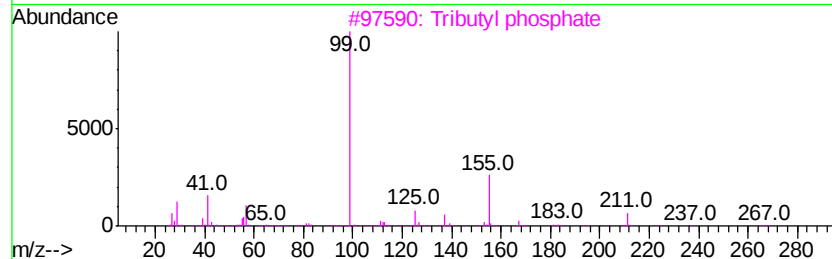
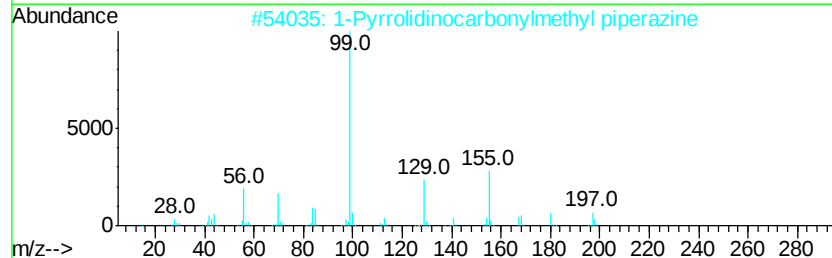
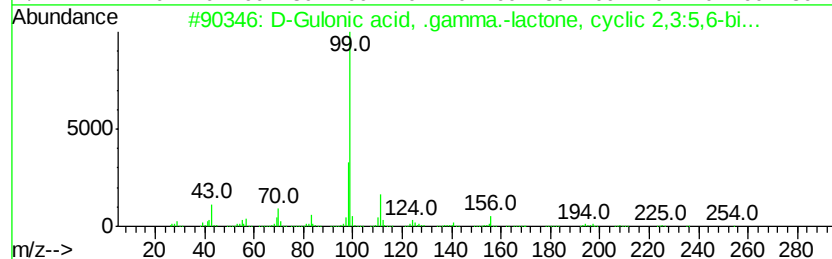
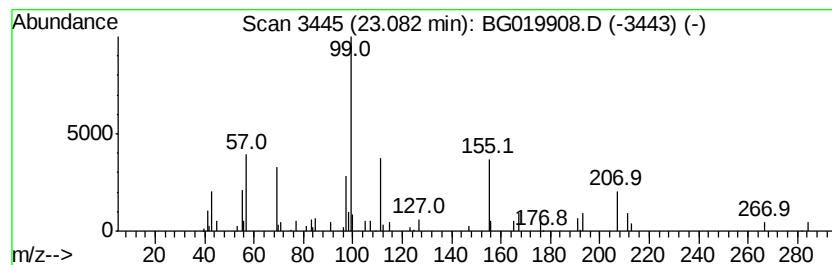
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown23.08 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.08	2.09 ng	75438	Chrysene-d12	21.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	D-Gulonic acid, .gamma.-lactone,...	254	C10H16B206	074128-60-2	32
2		1-Pyrrolidinocarbonylmethyl pipe...	197	C10H19N30	039890-45-4	28
3		Tributyl phosphate	266	C12H27O4P	000126-73-8	25
4		1,4-Dioxaspiro[4.14]nonadecane	268	C17H32O2	000184-41-8	25
5		3'-O-Acetylthymidine	284	C12H16N2O6	021090-30-2	17



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG120415\
Data File : BG019908.D
Acq On : 4 Dec 2015 17:06
Operator : UM/NP
Sample : G4642-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.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...	5.19	5.1 ng		44485	1	8.12	175375	20.0
unknown7.64	7.64	87.1 ng		763864	1	8.12	175375	20.0
n-Hexadecanoic acid	18.36	2.7 ng		72924	4	17.49	546638	20.0
Isoxazole, 3,5-di...	20.78	2.5 ng		89132	5	21.76	720521	20.0
unknown20.85	20.85	3.0 ng		106354	5	21.76	720521	20.0
2,4,4,6,6,8,8-Hep...	21.00	2.3 ng		83836	5	21.76	720521	20.0
unknown21.04	21.04	2.9 ng		103924	5	21.76	720521	20.0
unknown21.55	21.55	3.4 ng		124024	5	21.76	720521	20.0
unknown22.74	22.74	2.1 ng		74676	5	21.76	720521	20.0
unknown23.08	23.08	2.1 ng		75438	5	21.76	720521	20.0