

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120715\
 Data File : BG019992.D
 Acq On : 7 Dec 2015 22:11
 Operator : UM/NP
 Sample : G4676-02
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-101

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	5.184	394	399	406	rVB	24825	37553	2.07%	0.441%
2	5.654	473	479	488	rVB	163654	260717	14.38%	3.061%
3	7.252	745	751	761	rBV	111230	191815	10.58%	2.252%
4	7.640	810	817	826	rBV	295763	507858	28.01%	5.963%
5	8.110	891	897	904	rBV	60818	101201	5.58%	1.188%
6	8.439	946	953	959	rBV	255419	434303	23.95%	5.099%
7	9.279	1087	1096	1107	rBV	237607	434301	23.95%	5.099%
8	10.930	1370	1377	1383	rBV	91490	161194	8.89%	1.893%
9	13.369	1782	1792	1800	rBV	718243	1102190	60.79%	12.941%
10	14.462	1973	1978	1984	rVB	15479	23201	1.28%	0.272%
11	14.744	2019	2026	2031	rBV2	151755	253640	13.99%	2.978%
12	14.802	2031	2036	2043	rVB	248708	393729	21.72%	4.623%
13	15.784	2198	2203	2209	rVB3	10367	18509	1.02%	0.217%
14	16.224	2269	2278	2288	rVB	628970	945575	52.15%	11.102%
15	16.453	2300	2317	2323	rBV3	35029	78338	4.32%	0.920%
16	16.941	2394	2400	2405	rBV3	14959	24760	1.37%	0.291%
17	17.482	2486	2492	2498	rBV2	220170	332633	18.35%	3.905%
18	18.357	2637	2641	2646	rBV2	35416	48164	2.66%	0.565%
19	18.551	2666	2674	2679	rBV2	20530	40366	2.23%	0.474%
20	19.209	2782	2786	2793	rBV4	10733	18495	1.02%	0.217%
21	19.526	2834	2840	2845	rBV2	19366	29579	1.63%	0.347%
22	19.626	2852	2857	2865	rVB2	36317	51724	2.85%	0.607%
23	19.755	2875	2879	2886	rVB4	13455	21456	1.18%	0.252%
24	19.885	2898	2901	2907	rVB	31465	48510	2.68%	0.570%
25	20.084	2929	2935	2940	rBV	1394721	1813127	100.00%	21.287%
26	20.284	2966	2969	2972	rBV	15896	19137	1.06%	0.225%
27	20.319	2972	2975	2979	rVB2	16522	19652	1.08%	0.231%
28	20.766	3047	3051	3055	rBV	31069	40459	2.23%	0.475%
29	20.831	3059	3062	3070	rVB7	15425	30620	1.69%	0.360%
30	20.978	3082	3087	3091	rBV2	23641	36108	1.99%	0.424%
31	21.025	3091	3095	3099	rVB	37731	46359	2.56%	0.544%
32	21.095	3104	3107	3113	rVB3	17915	24760	1.37%	0.291%
33	21.389	3155	3157	3164	rVB6	13656	21214	1.17%	0.249%
34	21.542	3174	3183	3187	rBV	31204	52237	2.88%	0.613%

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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 >
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35	21.612	3191	3195	3198	rBV4	13426	18770	1.04%	0.220%
36	21.753	3213	3219	3228	rVB	267789	431598	23.80%	5.067%
37	22.082	3272	3275	3281	rVB	13588	22041	1.22%	0.259%
38	25.037	3767	3778	3790	rBV2	140226	381468	21.04%	4.479%

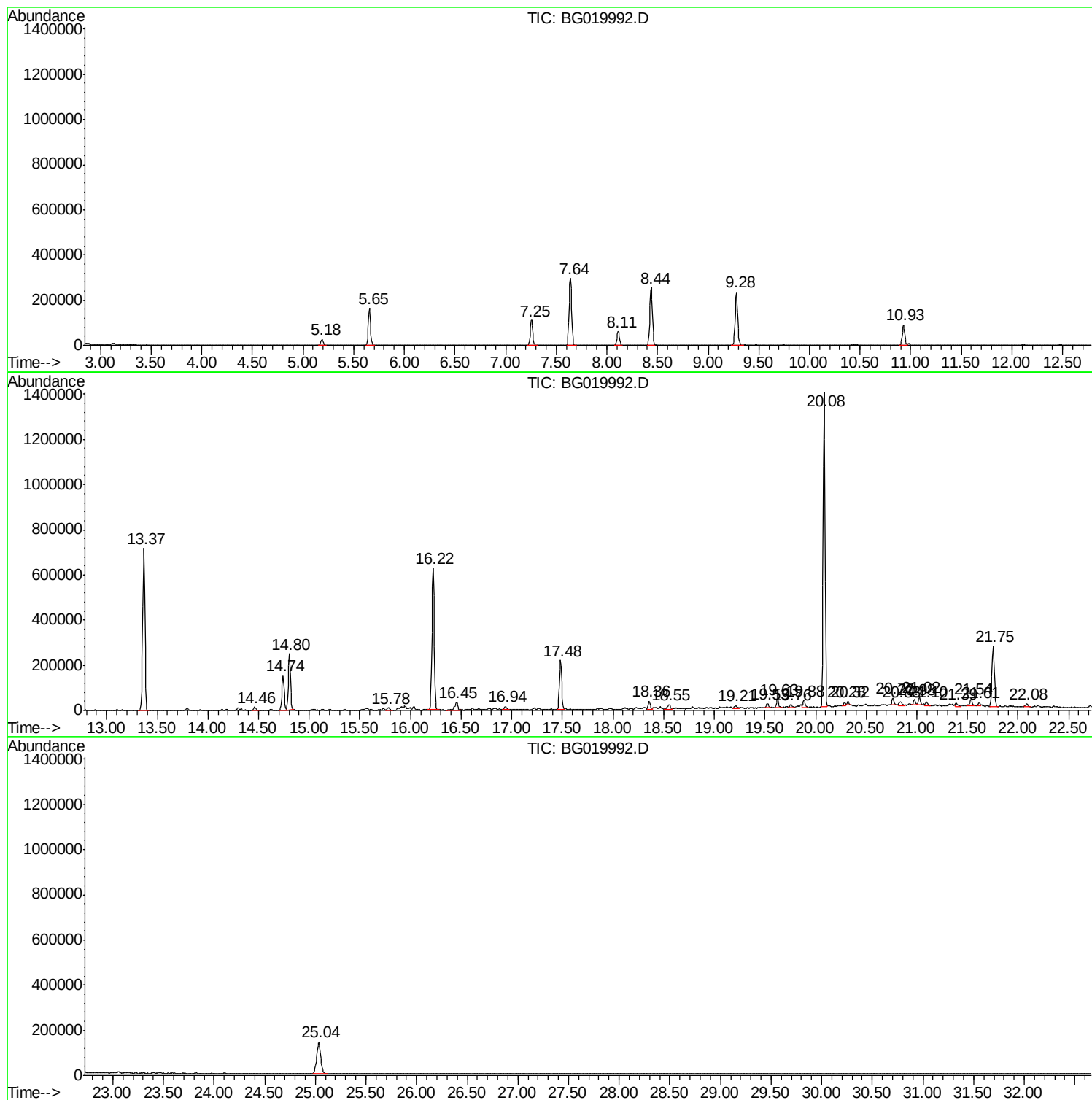
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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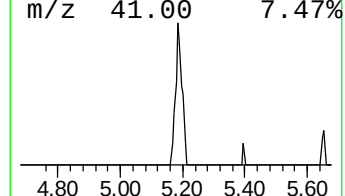
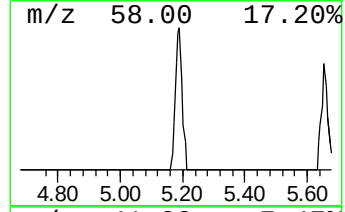
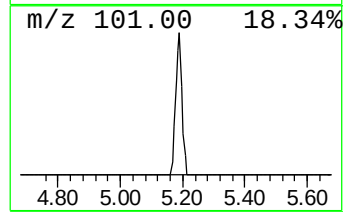
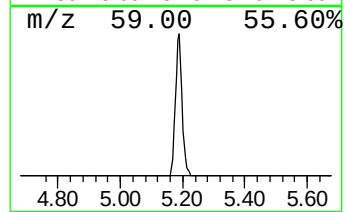
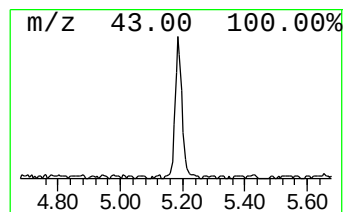
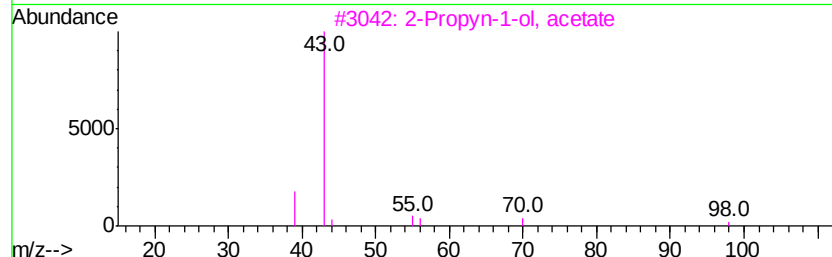
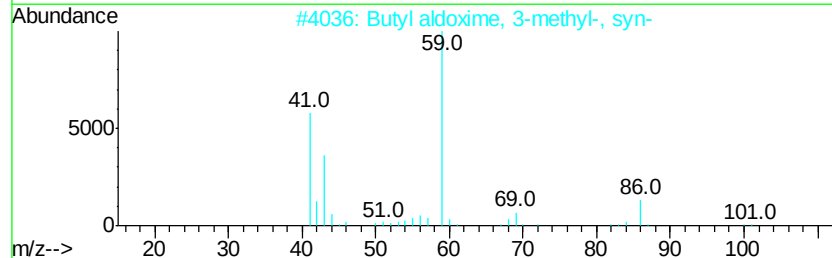
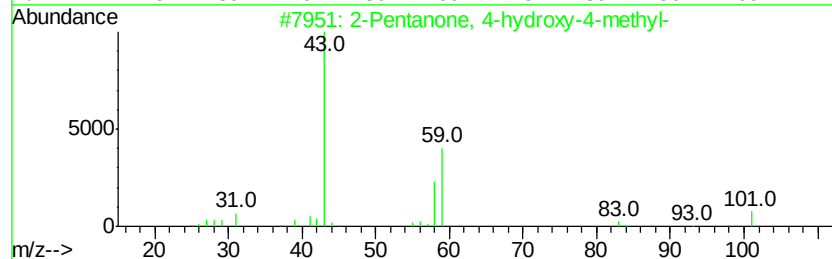
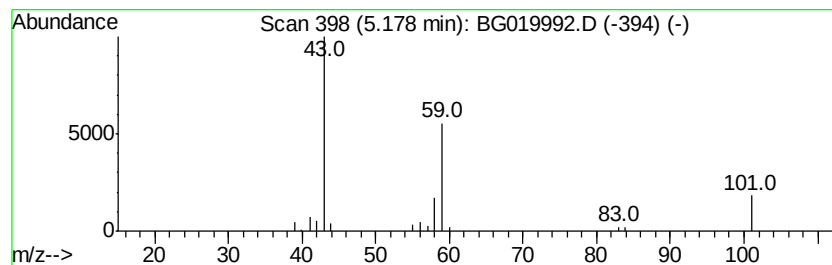
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	7.42 ng	37553	1,4-Dichlorobenzene-d4	8.11

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	25
3			2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			3-Heptanol	116	C7H16O	000589-82-2	9



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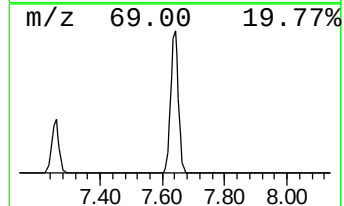
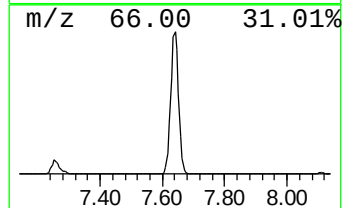
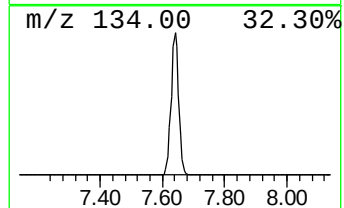
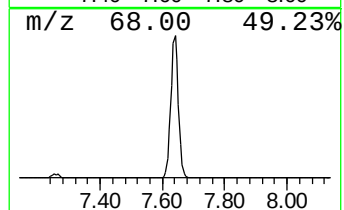
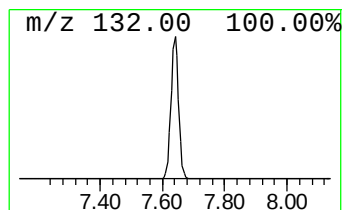
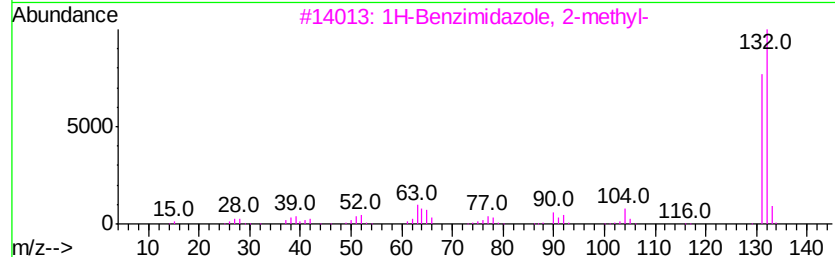
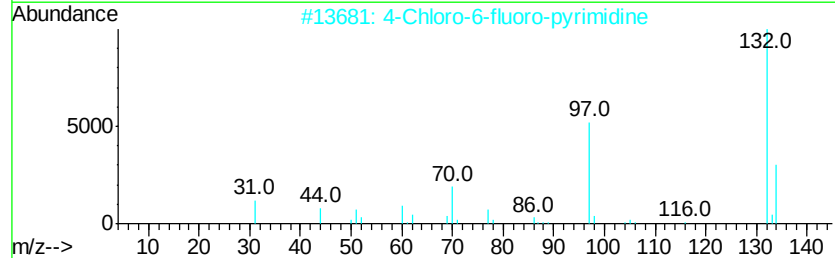
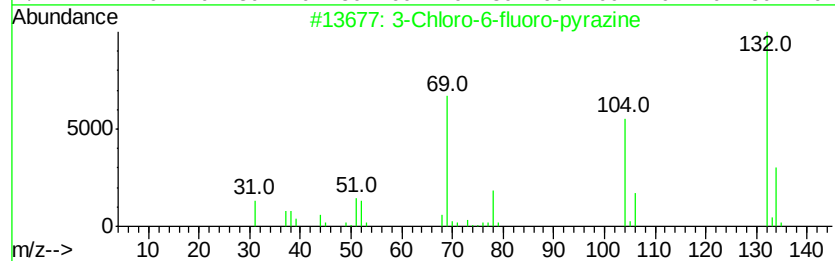
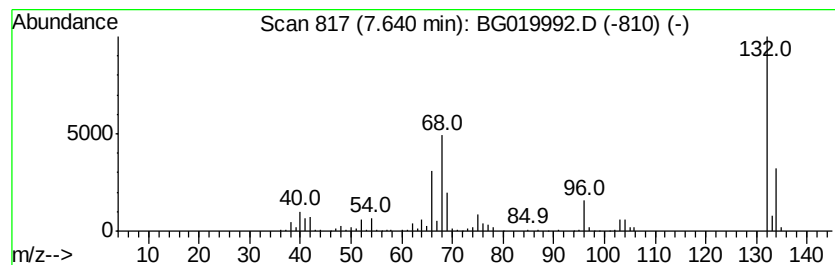
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.64	100.37 ng	507858	1,4-Dichlorobenzene-d4	8.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
5		5-Aminoindole	132	C8H8N2	005192-03-0	10



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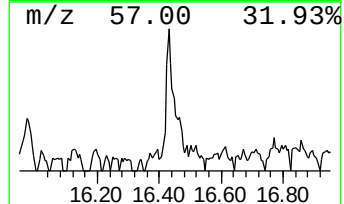
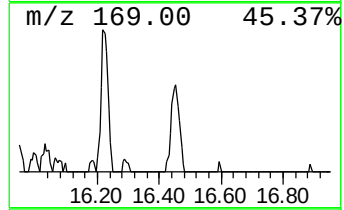
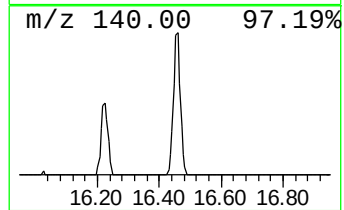
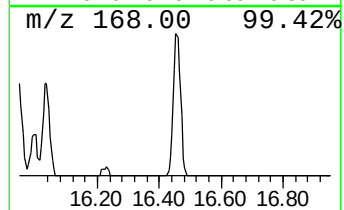
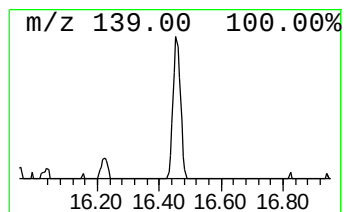
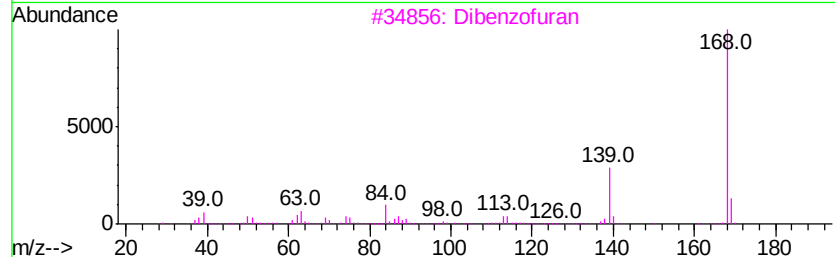
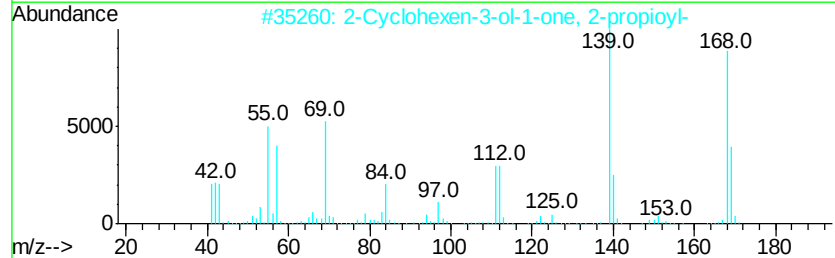
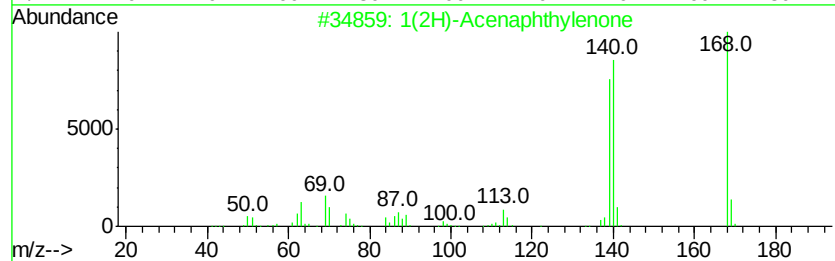
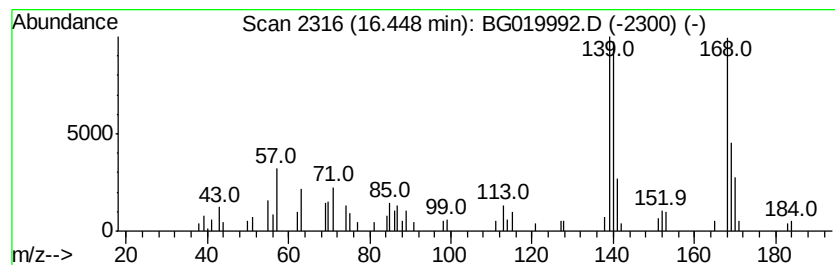
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1(2H)-Acenaphthylenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.45	4.71 ng	78338	Phenanthrene-d10	17.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1(2H)-Acenaphthylenone	168	C12H8O	002235-15-6	95
2		2-Cyclohexen-3-ol-1-one, 2-propyl...	168	C9H12O3	062847-90-9	50
3		Dibenzofuran	168	C12H8O	000132-64-9	47
4		Cyclobuta[de]naphthalene	140	C11H8	024973-91-9	46
5		Benzaldehyde, 2-fluoro-4-hydroxy-	140	C7H5FO2	000348-27-6	38



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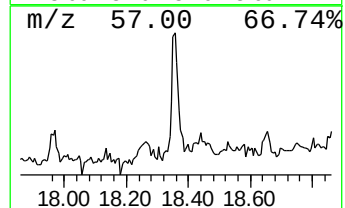
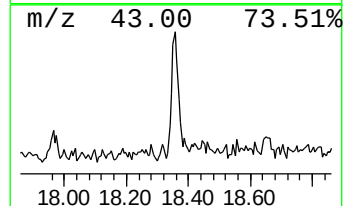
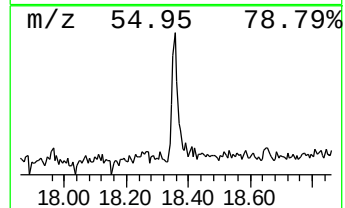
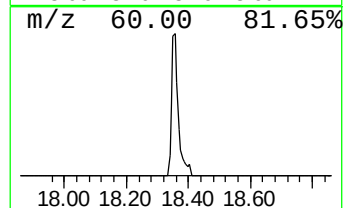
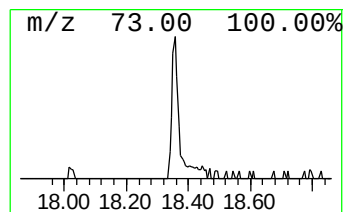
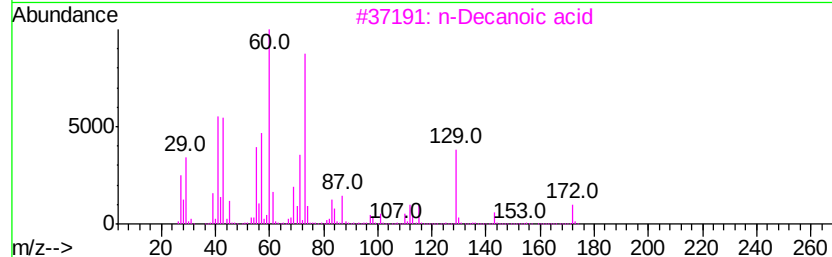
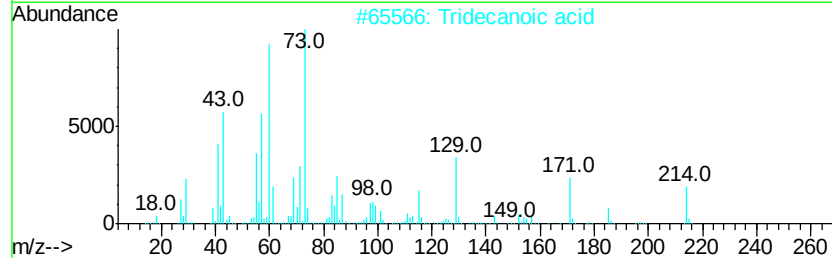
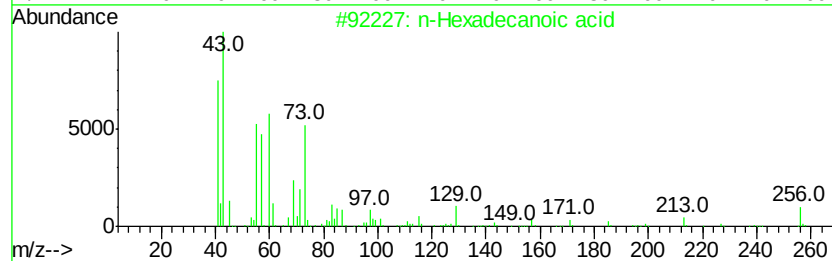
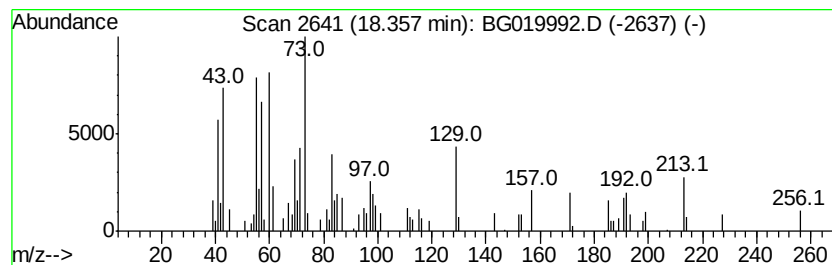
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.36	2.90 ng	48164	Phenanthrene-d10	17.48

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
2		Tridecanoic acid	214	C13H26O2	000638-53-9	60
3		n-Decanoic acid	172	C10H20O2	000334-48-5	50
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	47
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	43



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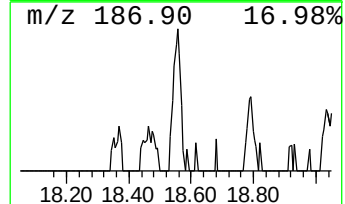
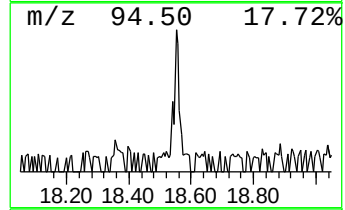
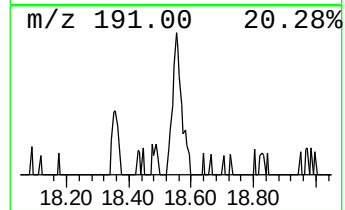
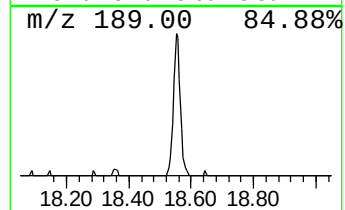
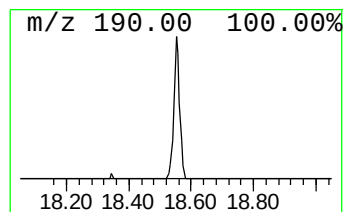
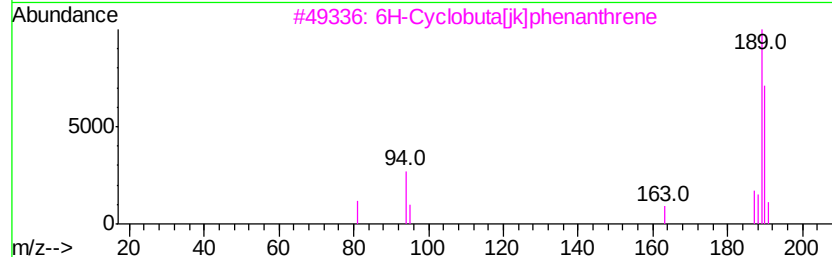
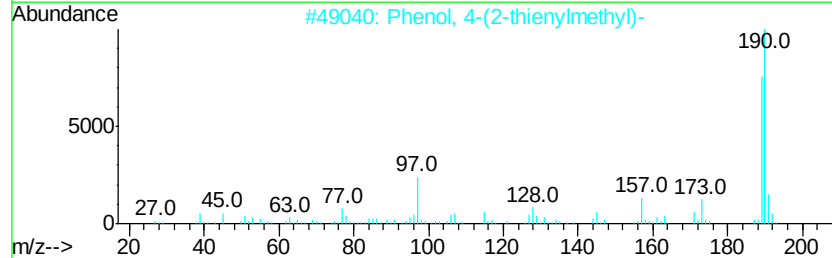
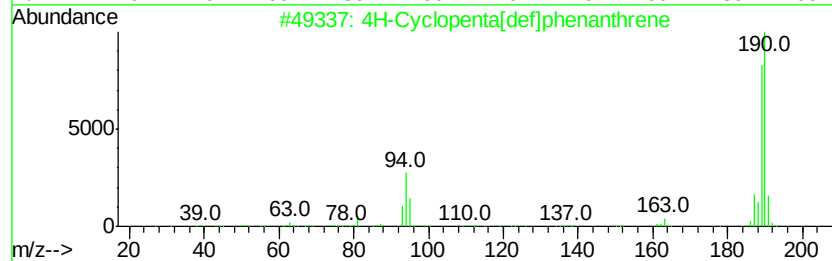
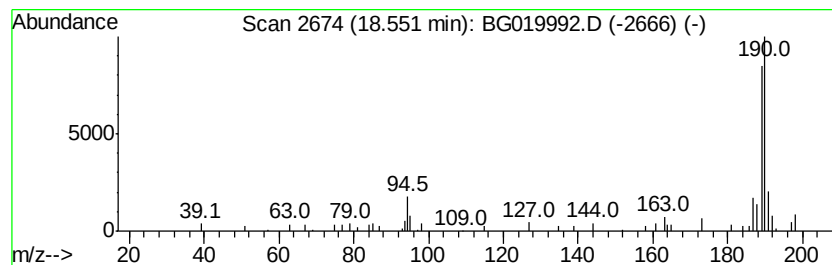
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TIC Integration Parameters: LSCINT.P

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.55	2.43 ng	40366	Phenanthrene-d10	17.48	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	91
2	Phenol, 4-(2-thienylmethyl)-	190	C11H10OS	091680-55-6	64
3	6H-Cyclobuta[ikl]phenanthrene	190	C15H10	083469-43-6	50
4	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	45
5	1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	43



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Misc :
ALS Vial : 15 Sample Multiplier: 1

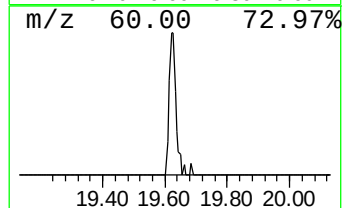
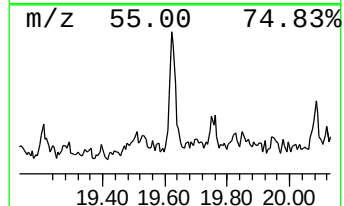
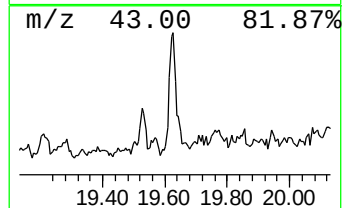
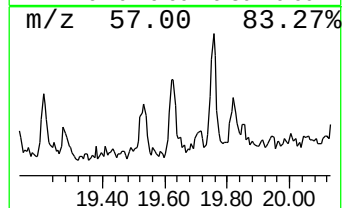
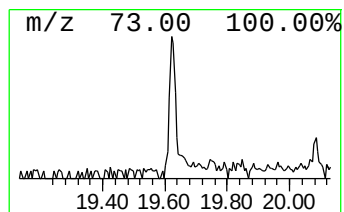
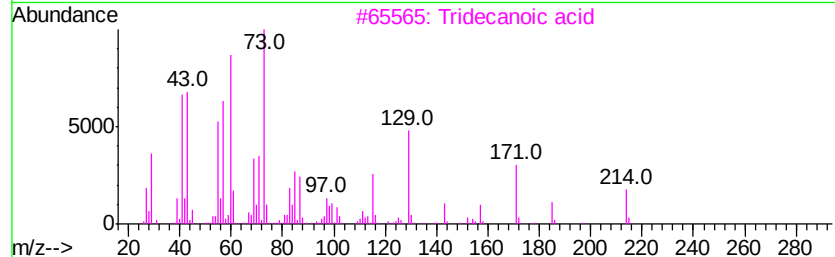
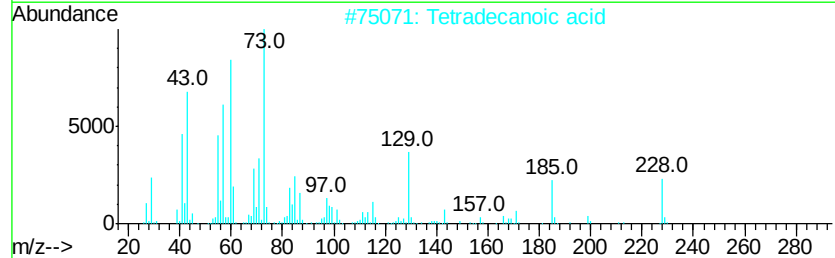
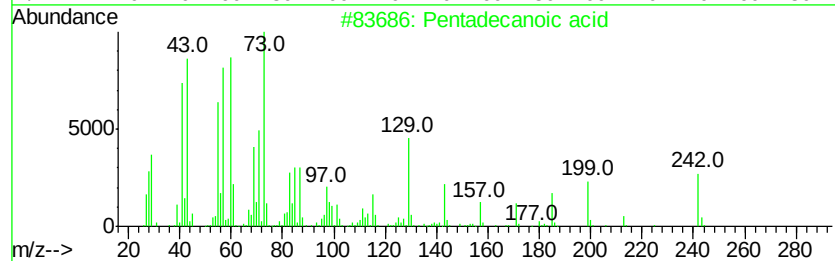
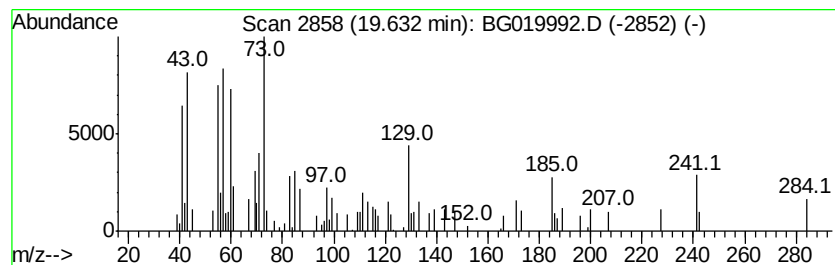
Instrument :
BNA_G
ClientSampleId :
MW-101

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 7 Pentadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.63	2.40 ng	51724	Chrysene-d12	21.75
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Pentadecanoic acid	242 C15H30O2	001002-84-2 90
2		Tetradecanoic acid	228 C14H28O2	000544-63-8 72
3		Tridecanoic acid	214 C13H26O2	000638-53-9 59
4		Undecanoic acid	186 C11H22O2	000112-37-8 43
5		d-Glucohexodialdose	178 C6H10O6	1000149-19-1 27



Data Path : Z:\HPCHEM1\BNA G\DATA\BG120715\
Data File : BG019992.D
Acq On : 7 Dec 2015 22:11
Operator : UM/NP
Sample : G4676-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-101

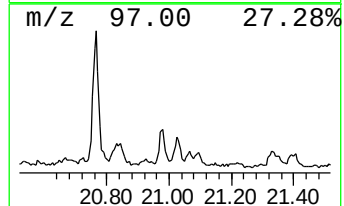
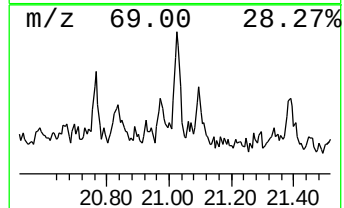
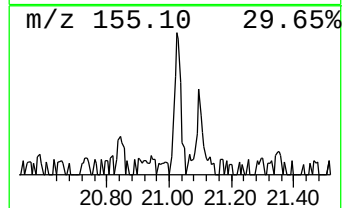
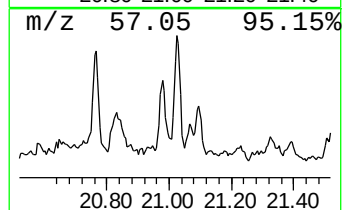
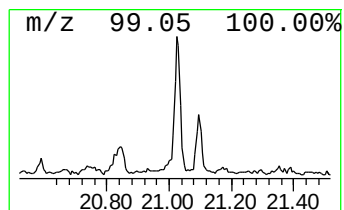
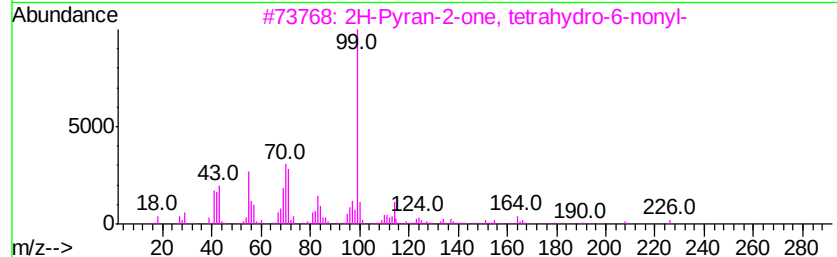
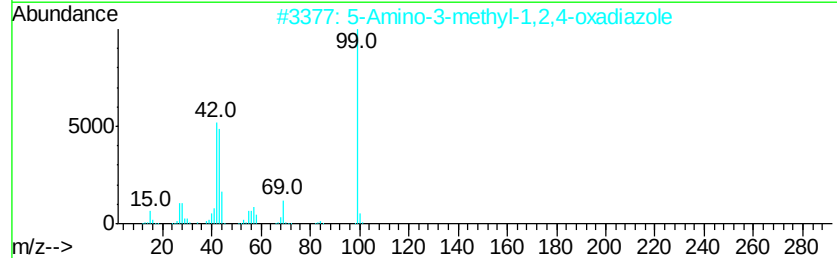
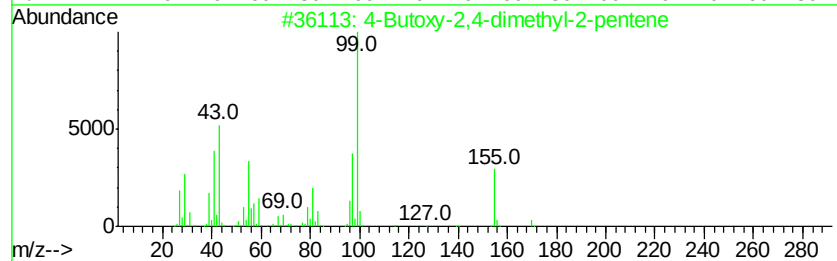
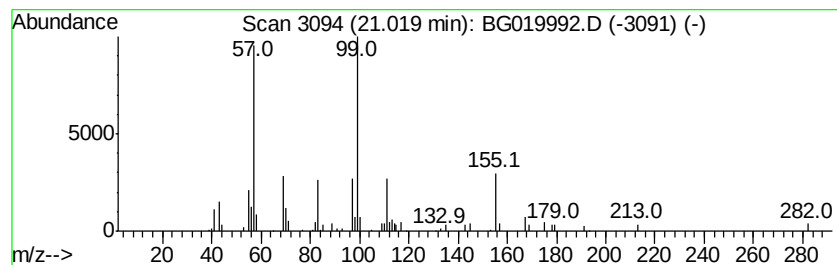
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown21.02 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.02	2.15 ng	46359	Chrysene-d12	21.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Butoxy-2,4-dimethyl-2-pentene	170	C11H22O	1000159-08-7	40
2		5-Amino-3-methyl-1,2,4-oxadiazole	99	C3H5N3O	003663-39-6	38
3		2H-Pyran-2-one, tetrahydro-6-nonyl-	226	C14H26O2	002721-22-4	38
4		Heptane, 2-iodo-	226	C7H15I	018589-29-2	38
5		Hexanoic acid, 6-tridecyl ester	298	C19H38O2	1000279-29-5	35



Data Path : Z:\HPCHEM1\BNA G\DATA\BG120715\
Data File : BG019992.D
Acq On : 7 Dec 2015 22:11
Operator : UM/NP
Sample : G4676-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-101

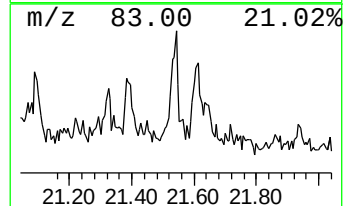
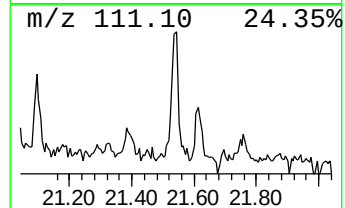
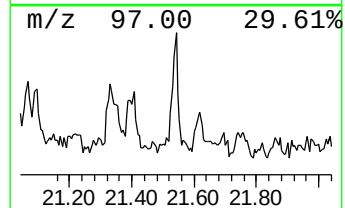
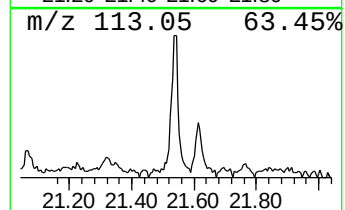
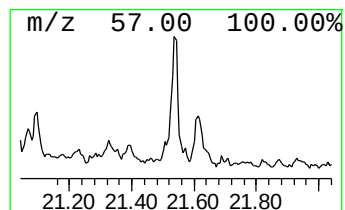
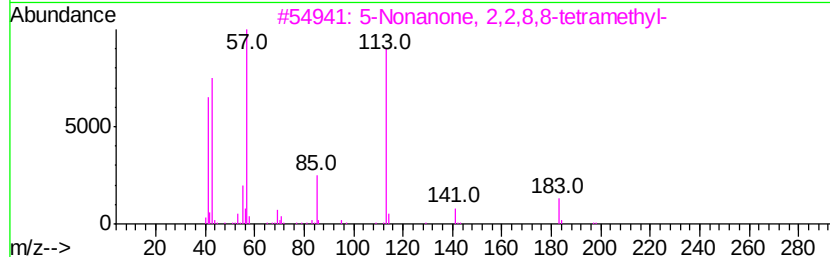
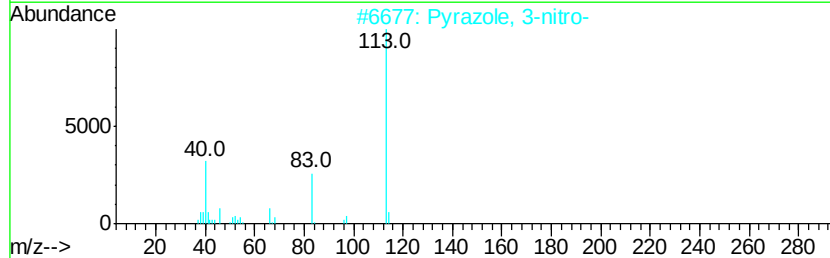
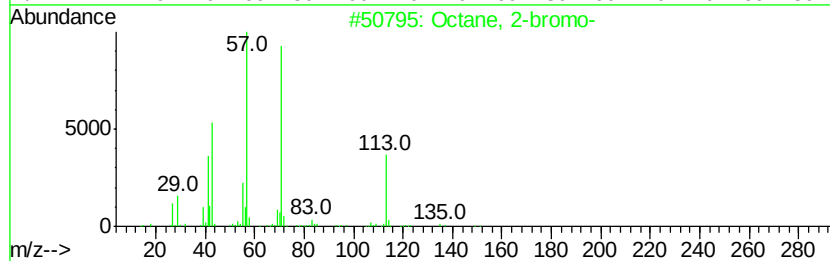
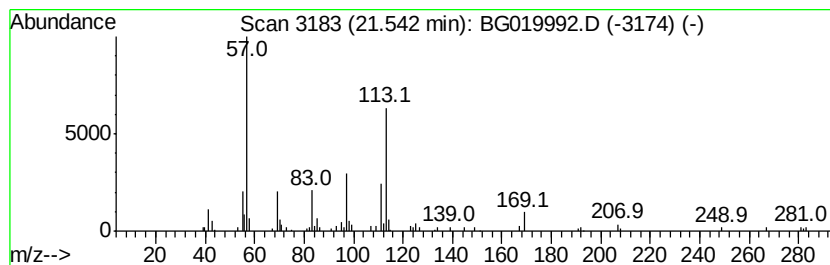
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown21.54 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.54	2.42 ng	52237	Chrysene-d12	21.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octane, 2-bromo-	192	C8H17Br	000557-35-7	35
2		Pyrazole, 3-nitro-	113	C3H3N3O2	026621-44-3	25
3		5-Nonanone, 2,2,8,8-tetramethyl-	198	C13H26O	005709-95-5	25
4		6-Undecen-3-one, 5-butyl-2,2-dim...	252	C17H32O	055976-05-1	23
5		Heptane, 4-(bromomethyl)-	192	C8H17Br	101654-29-9	14



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG120715\
Data File : BG019992.D
Acq On : 7 Dec 2015 22:11
Operator : UM/NP
Sample : G4676-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-101

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...	5.18	7.4	ng	37553	1	8.11	101201	20.0
unknown7.64	7.64	100.4	ng	507858	1	8.11	101201	20.0
1(2H)-Acenaphthyl...	16.45	4.7	ng	78338	4	17.48	332633	20.0
n-Hexadecanoic acid	18.36	2.9	ng	48164	4	17.48	332633	20.0
4H-Cyclopenta[def...	18.55	2.4	ng	40366	4	17.48	332633	20.0
Pentadecanoic acid	19.63	2.4	ng	51724	5	21.75	431598	20.0
unknown21.02	21.02	2.1	ng	46359	5	21.75	431598	20.0
unknown21.54	21.54	2.4	ng	52237	5	21.75	431598	20.0