

Data Path : Z:\HPCHEM1\BNA G\DATA\BG121015\
 Data File : BG020060.D
 Acq On : 10 Dec 2015 1:46
 Operator : UM/SJ
 Sample : G4659-04
 Misc :
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 A8-4C

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	2.991	20	26	43	rVB	966121	1389048	88.58%	14.646%
2	5.183	394	399	408	rVB	62006	93135	5.94%	0.982%
3	5.659	472	480	492	rBV	334520	523451	33.38%	5.519%
4	7.263	745	753	763	rBV	356327	606937	38.71%	6.399%
5	7.639	810	817	827	rBV	344557	579510	36.96%	6.110%
6	8.109	890	897	904	rVB	61871	99820	6.37%	1.052%
7	8.438	945	953	959	rBV	237906	414961	26.46%	4.375%
8	9.278	1086	1096	1104	rBV	209664	371426	23.69%	3.916%
9	10.929	1368	1377	1385	rBV	88423	156597	9.99%	1.651%
10	13.362	1784	1791	1800	rBV	621153	962543	61.38%	10.149%
11	14.184	1925	1931	1937	rVB	58155	82553	5.26%	0.870%
12	14.736	2019	2025	2034	rVB2	152037	248103	15.82%	2.616%
13	16.223	2271	2278	2286	rBV	537639	801027	51.08%	8.446%
14	16.429	2308	2313	2321	rBV2	9889	17499	1.12%	0.185%
15	17.480	2486	2492	2498	rBV2	204195	304640	19.43%	3.212%
16	18.350	2632	2640	2648	rBV	47366	63183	4.03%	0.666%
17	19.619	2852	2856	2860	rBV2	24138	32652	2.08%	0.344%
18	19.666	2860	2864	2870	rVB2	58599	68116	4.34%	0.718%
19	19.830	2888	2892	2894	rBV2	52866	71689	4.57%	0.756%
20	19.854	2894	2896	2900	rVB2	42044	44810	2.86%	0.472%
21	20.083	2929	2935	2941	rBV	1220868	1568108	100.00%	16.534%
22	21.376	3150	3155	3166	rBV2	61970	111452	7.11%	1.175%
23	21.752	3213	3219	3226	rVB	240574	403140	25.71%	4.251%
24	23.462	3505	3510	3518	rVB7	7597	16245	1.04%	0.171%
25	24.078	3611	3615	3621	rVB5	12238	23539	1.50%	0.248%
26	25.024	3767	3776	3789	rVB2	132494	374196	23.86%	3.945%
27	26.211	3969	3978	3989	rVB3	18288	55756	3.56%	0.588%

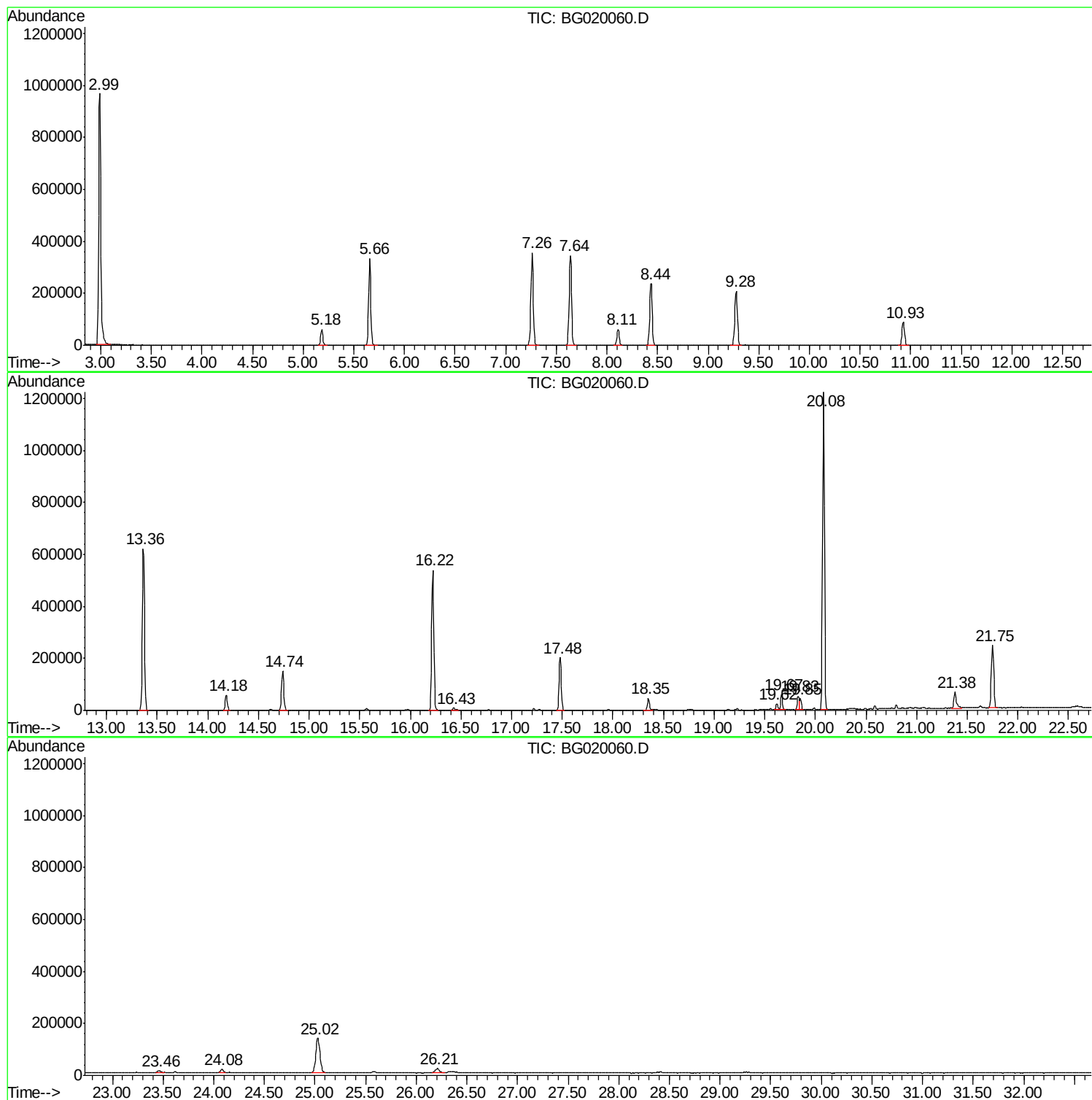
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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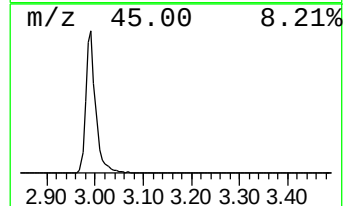
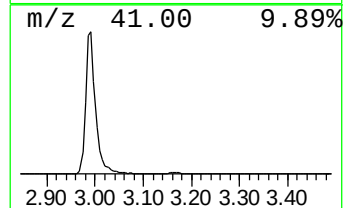
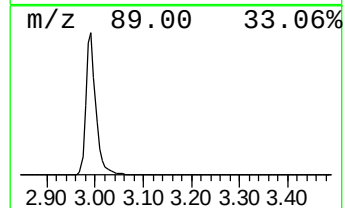
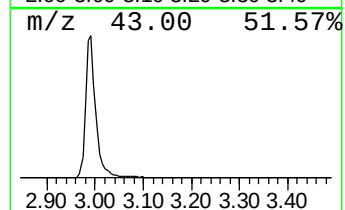
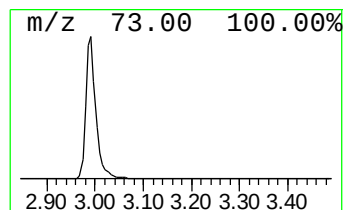
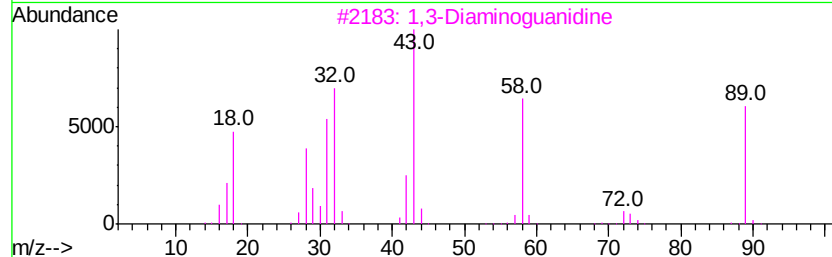
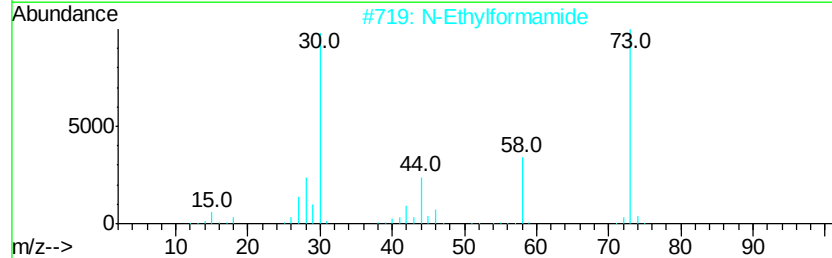
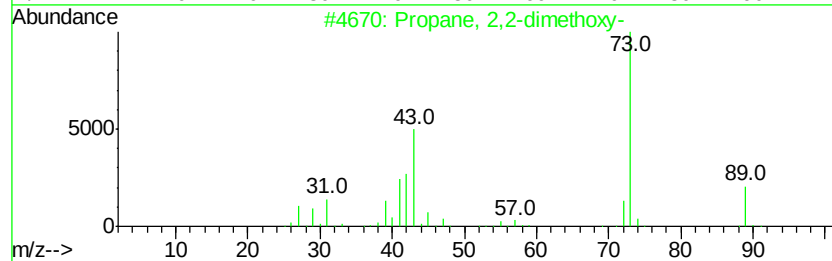
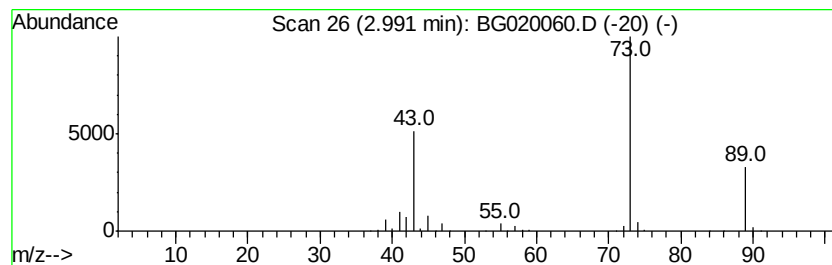
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown2.99 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.99	278.31 ng	1389050	1,4-Dichlorobenzene-d4	8.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2		N-Ethylformamide	73	C3H7NO	000627-45-2	9
3		1,3-Diaminoquanidine	89	CH7N5	004364-78-7	9
4		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5		1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9



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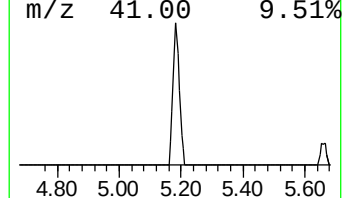
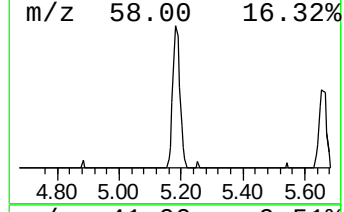
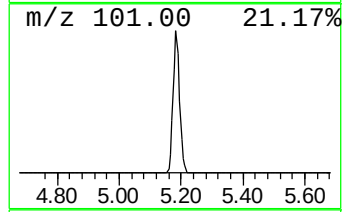
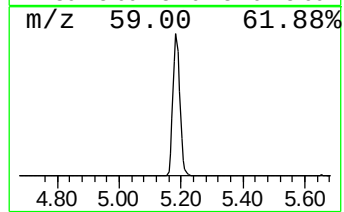
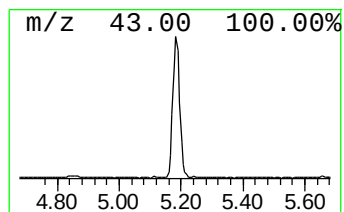
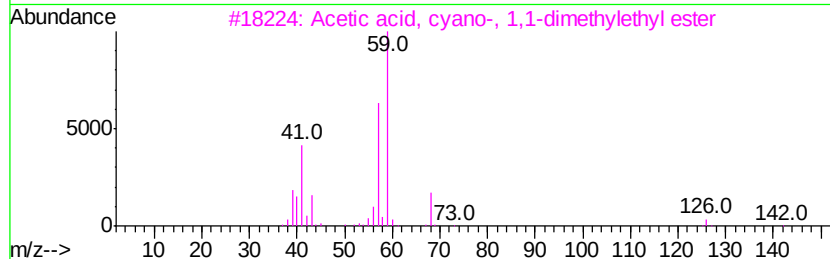
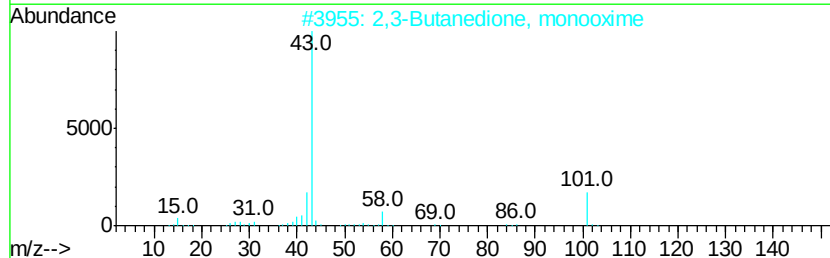
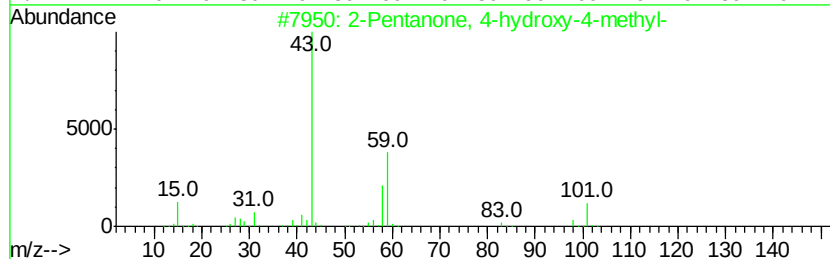
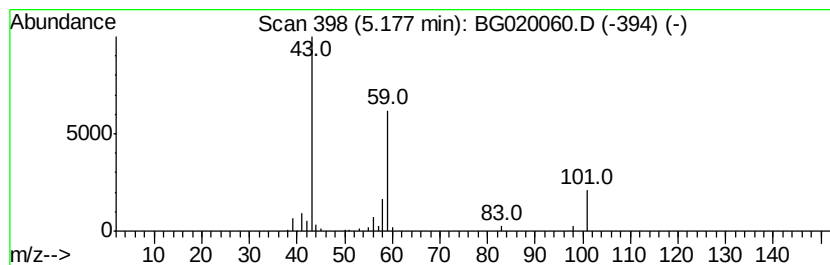
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	18.66 ng	93135	1,4-Dichlorobenzene-d4	8.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
5		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9



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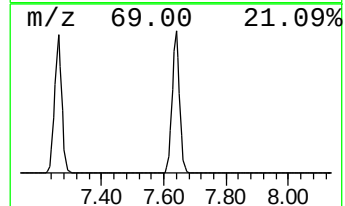
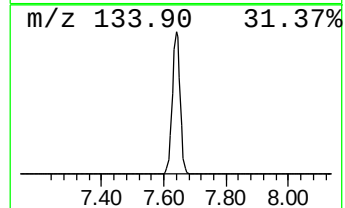
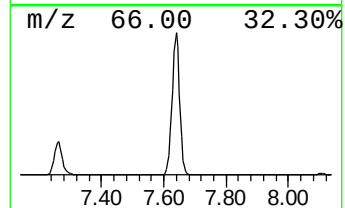
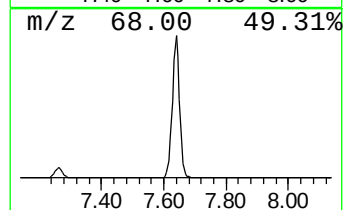
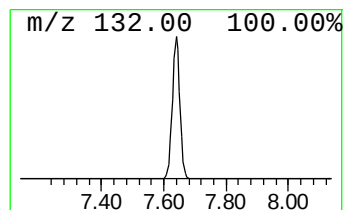
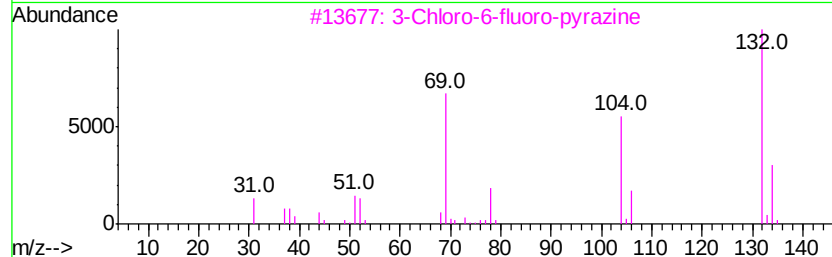
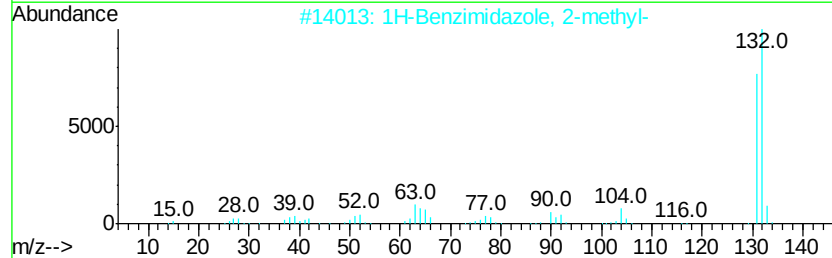
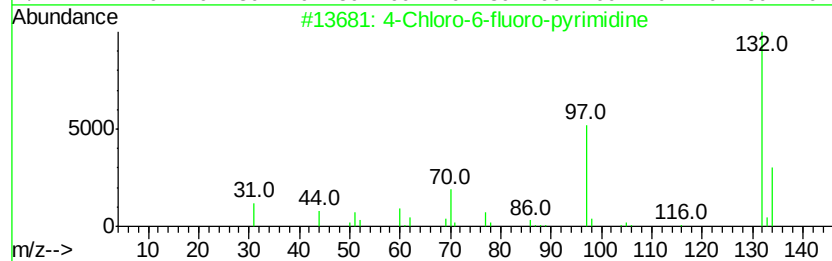
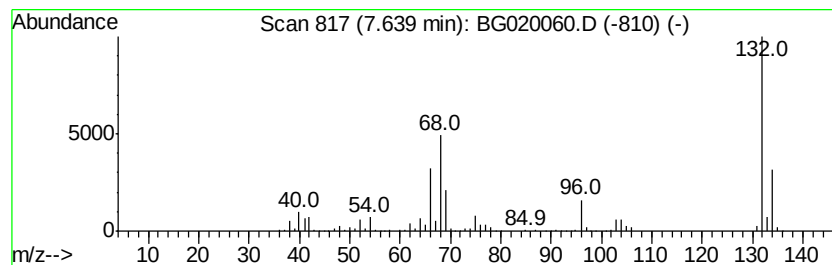
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Peak Number 3 unknown7.64 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.64	116.11 ng	579510	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	1,2,3-Trifluorobenzene	132	C6H3F3	001489-53-8	9



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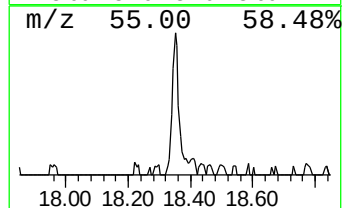
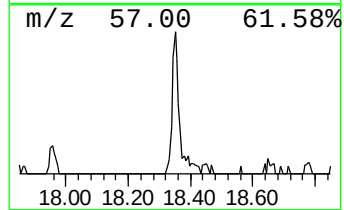
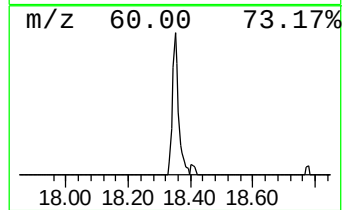
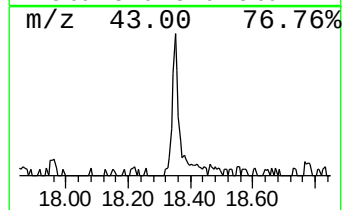
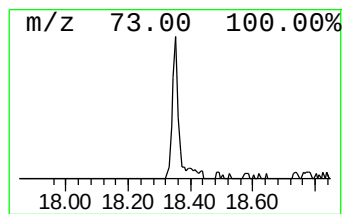
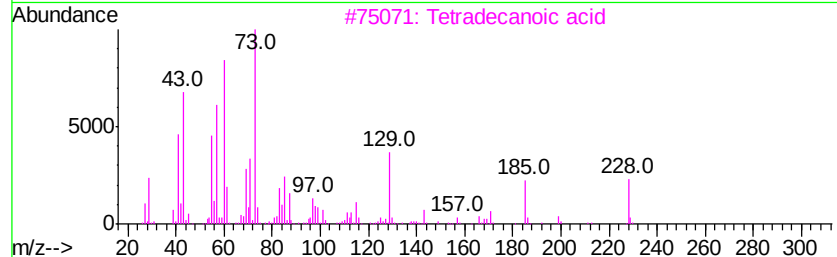
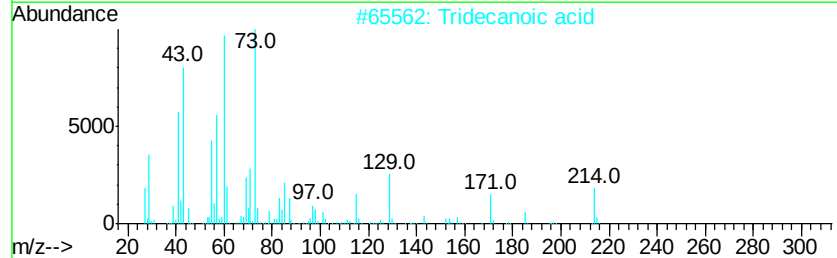
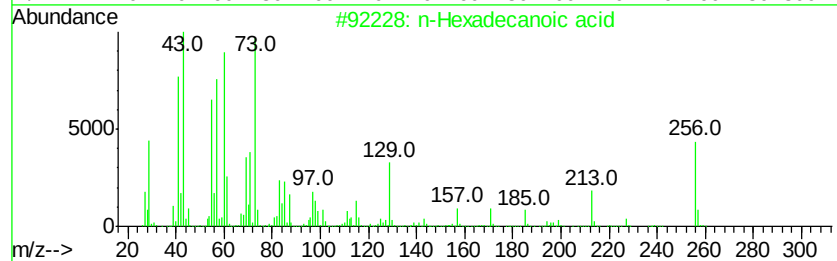
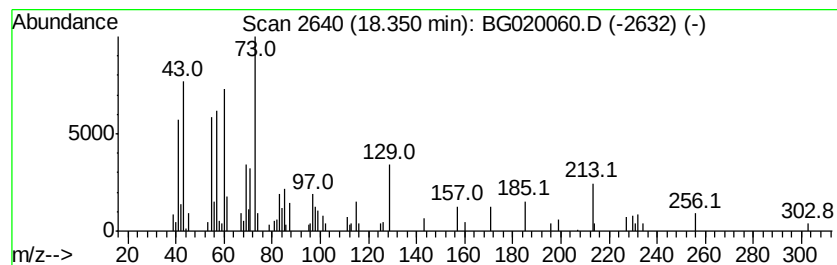
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.35	4.15 ng	63183	Phenanthrene-d10	17.48

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	93
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	62
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	53
5		Isopropyl Palmitate	298	C19H38O2	000142-91-6	50



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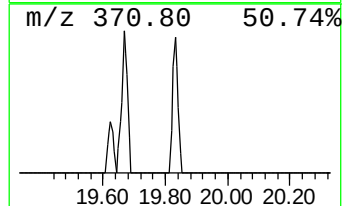
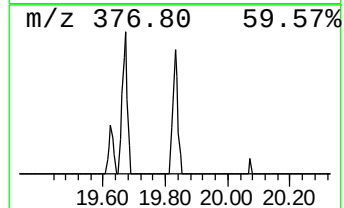
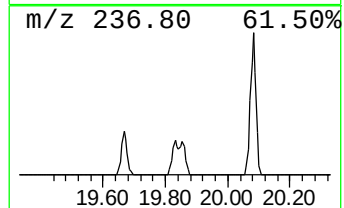
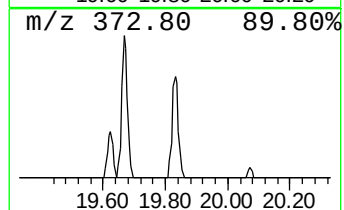
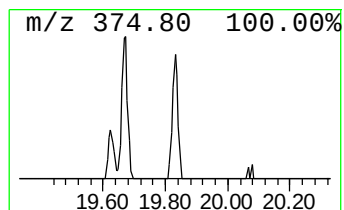
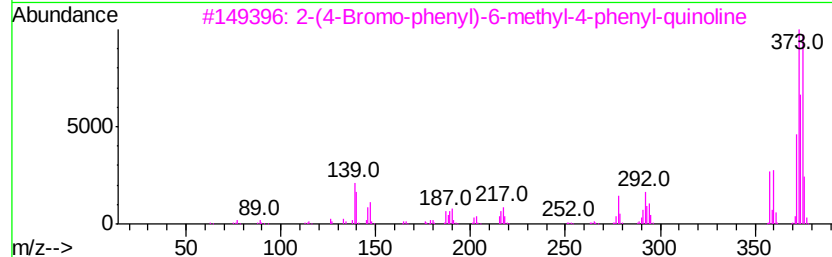
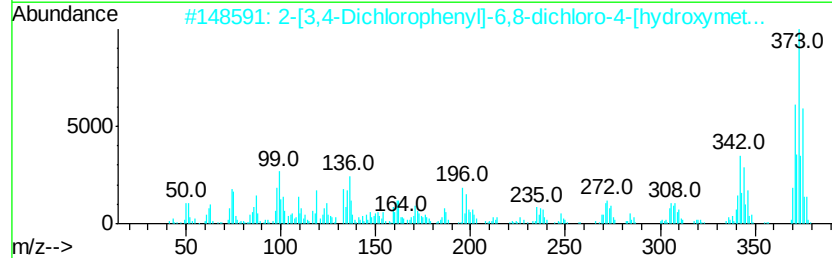
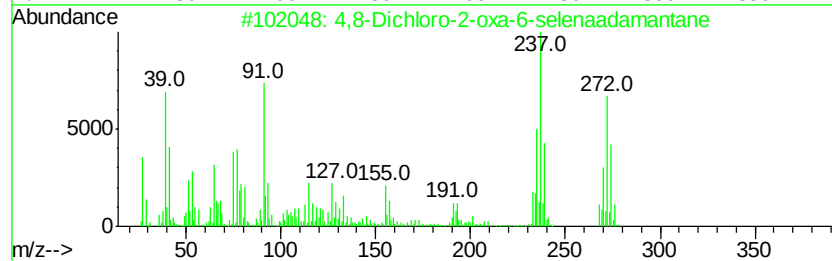
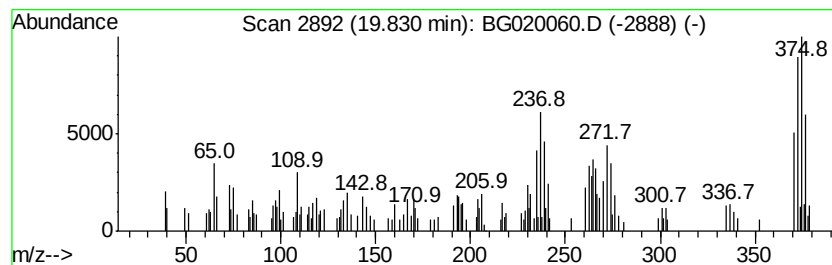
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 7 unknown19.83 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.83	3.56 ng	71689	Chrysene-d12	21.75

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4,8-Dichloro-2-oxa-6-selenaadama...	272	C8H10Cl2OSe	1000189-96-4	49
2			2-[3,4-Dichlorophenyl]-6,8-dichl...	371	C16H9Cl4NO	038599-01-8	25
3			2-(4-Bromo-phenyl)-6-methyl-4-ph...	373	C22H16BrN	071858-09-8	10
4			7-Fluoro-3,4-dihydro-3-[4-(trifl...	375	C20H13F4NO2	144155-10-2	10
5			1,3-Cyclopentadiene, 1,2,3,4,5,5...	270	C5Cl6	000077-47-4	10



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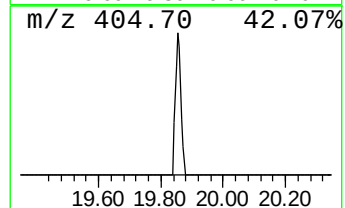
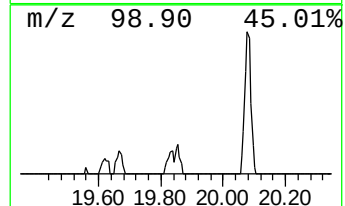
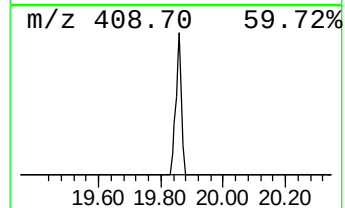
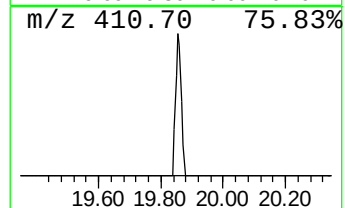
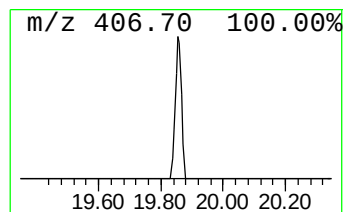
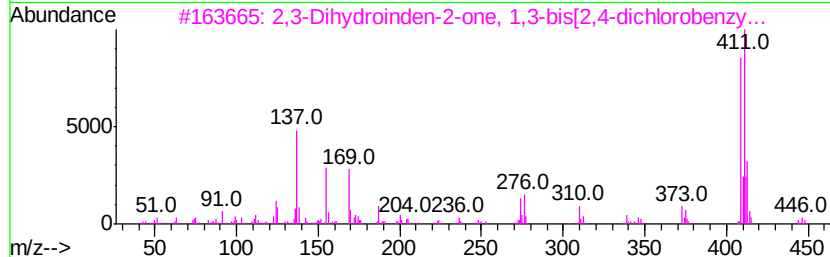
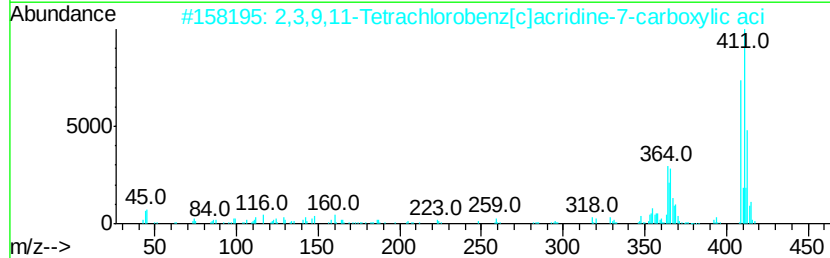
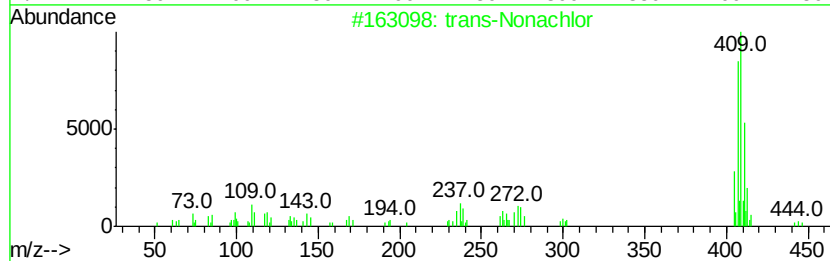
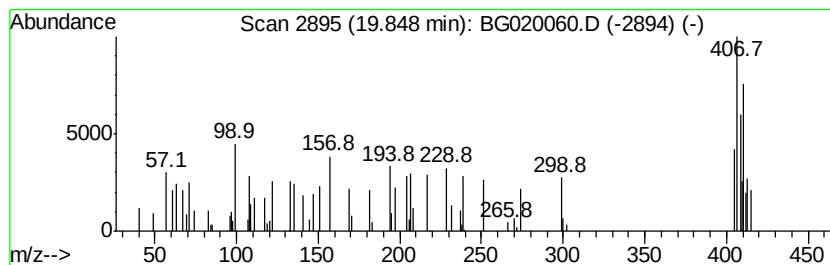
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown19.85 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.85	2.22 ng	44810	Chrysene-d12	21.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	trans-Nonachlor	440	C10H5Cl9	039765-80-5	42
2		2,3,9,11-Tetrachlorobenz[c]acrid...	409	C18H7Cl4N02	034623-48-8	35
3		2,3-Dihydroinden-2-one, 1,3-bis[...	444	C23H12Cl4O	1000252-11-0	23
4		Benzothiazole, 2-[5-(4-bromo-5-m...	407	C15H10BrN3O2S2	1000270-84-4	17
5		2,3-Distyryl-5,8-dimethoxy-6-am...	409	C26H23N3O2	056393-61-4	11



Data Path : Z:\HPCHEM1\BNA G\DATA\BG121015\
Data File : BG020060.D
Acq On : 10 Dec 2015 1:46
Operator : UM/SJ
Sample : G4659-04
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A8-4C

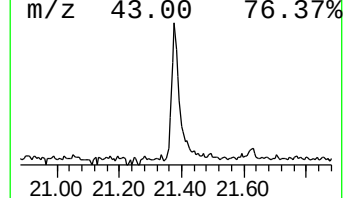
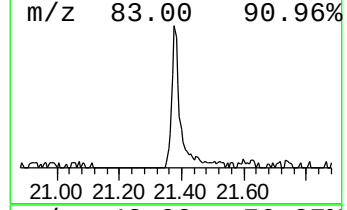
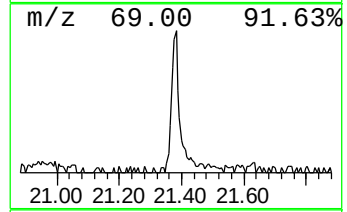
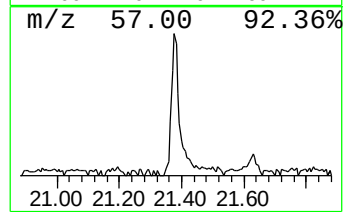
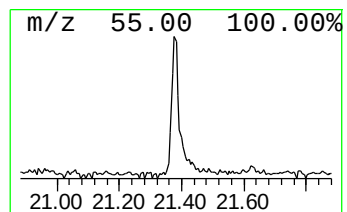
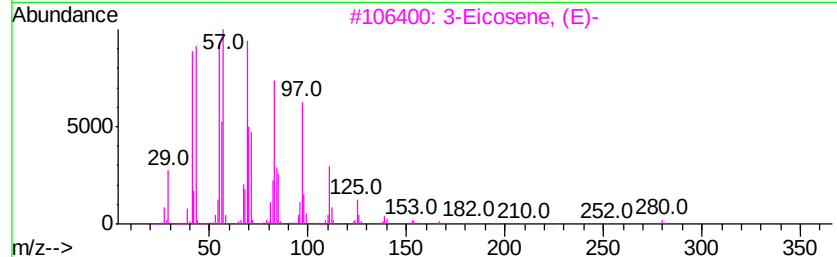
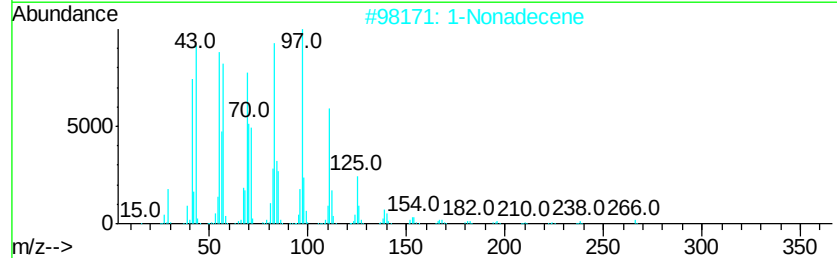
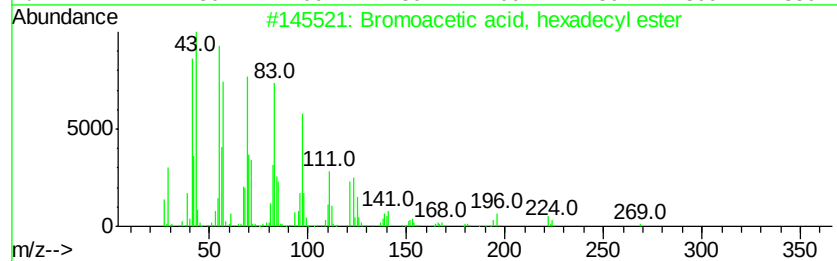
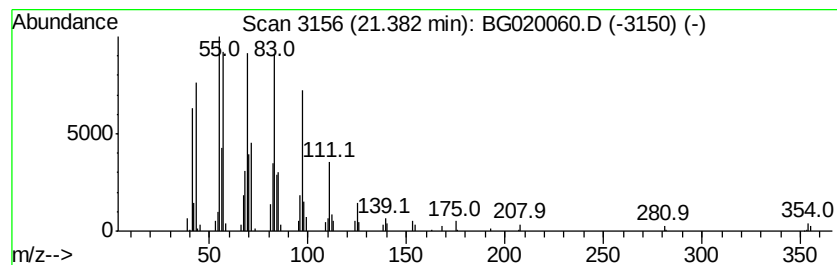
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Bromoacetic acid, hexadecyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.38	5.53 ng	111452	Chrysene-d12	21.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	94
2		1-Nonadecene	266	C19H38	018435-45-5	91
3		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4		2-Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	91
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91



Data Path : Z:\HPCHEM1\BNA G\DATA\BG121015\
Data File : BG020060.D
Acq On : 10 Dec 2015 1:46
Operator : UM/SJ
Sample : G4659-04
Misc :
ALS Vial : 30 Sample Multiplier: 1

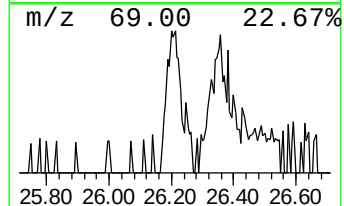
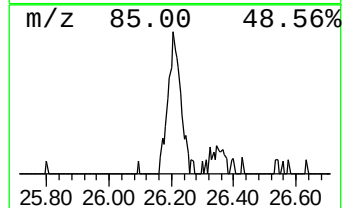
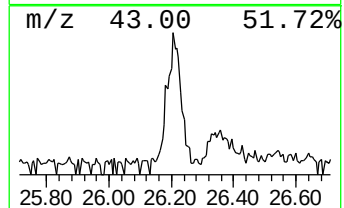
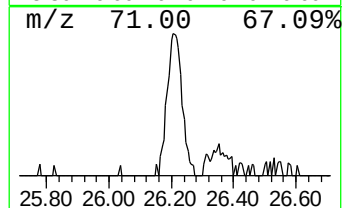
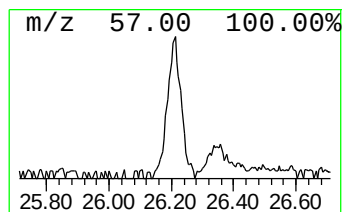
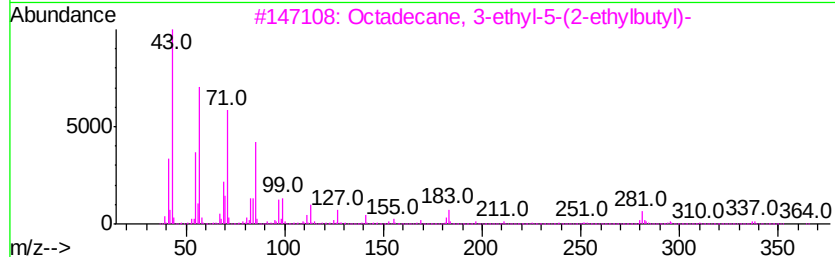
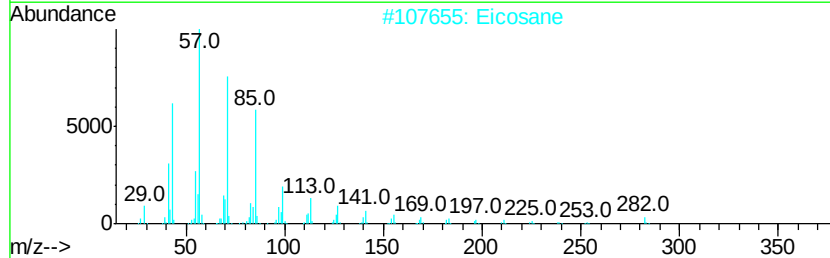
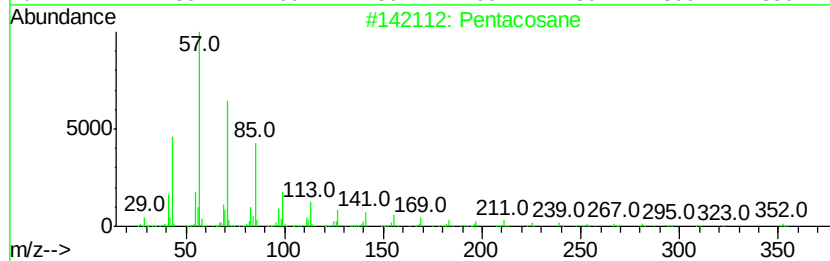
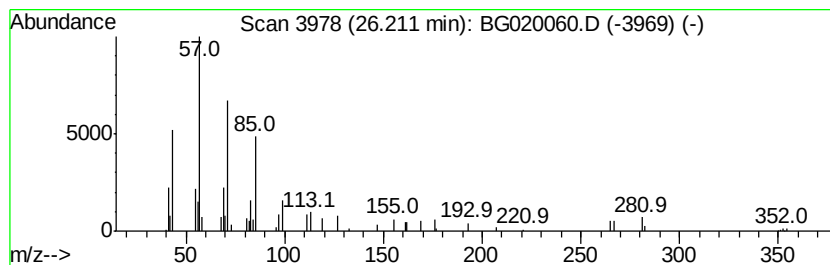
Instrument :
BNA_G
ClientSampleId :
A8-4C

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 Pentacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.21	2.98 ng	55756	Perylene-d12	25.02
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Pentacosane	352	C25H52	000629-99-2 95
2	Eicosane	282	C20H42	000112-95-8 90
3	Octadecane, 3-ethyl-5-(2-ethylbu...	366	C26H54	055282-12-7 86
4	Tetracosane	338	C24H50	000646-31-1 86
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1 83



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG121015\
Data File : BG020060.D
Acq On : 10 Dec 2015 1:46
Operator : UM/SJ
Sample : G4659-04
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A8-4C

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
unknown2.99	2.99	278.3	ng	1389050	1	8.11	99820	20.0
2-Pentanone, 4-hy...	5.18	18.7	ng	93135	1	8.11	99820	20.0
unknown7.64	7.64	116.1	ng	579510	1	8.11	99820	20.0
n-Hexadecanoic acid	18.35	4.2	ng	63183	4	17.48	304640	20.0
unknown19.83	19.83	3.6	ng	71689	5	21.75	403140	20.0
unknown19.85	19.85	2.2	ng	44810	5	21.75	403140	20.0
Bromoacetic acid,...	21.38	5.5	ng	111452	5	21.75	403140	20.0
Pentacosane	26.21	3.0	ng	55756	6	25.02	374196	20.0