

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
Data File : BG022992.D
Acq On : 10 Jul 2016 9:29
Operator : UM/SJ
Sample : H3921-13
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
N8-B4(6-12)C

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_G\METHODS\8270-BG070816.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	3.039	29	34	55	rBV	3831144	5555143	69.55%	9.752%
2	5.219	401	405	411	rBV	124455	198360	2.48%	0.348%
3	5.695	479	486	497	rBV	2176429	3520248	44.07%	6.180%
4	7.305	752	760	771	rBV	2513131	4346772	54.42%	7.631%
5	7.681	817	824	833	rBV	2321566	3980551	49.83%	6.988%
6	8.151	898	904	912	rVB	432676	716871	8.97%	1.258%
7	8.474	951	959	968	rBV	1504317	2731446	34.20%	4.795%
8	9.326	1095	1104	1113	rBV	1508547	2791983	34.95%	4.901%
9	10.977	1377	1385	1395	rVB	636594	1189625	14.89%	2.088%
10	13.415	1791	1800	1811	rBV	3727866	5887396	73.71%	10.335%
11	14.238	1931	1940	1946	rBV	523269	787606	9.86%	1.383%
12	14.796	2026	2035	2043	rBV2	1181014	1864650	23.34%	3.273%
13	15.613	2171	2174	2178	rVB	71225	90800	1.14%	0.159%
14	16.288	2282	2289	2303	rBV	3854871	5896281	73.82%	10.351%
15	16.482	2317	2322	2324	rBV2	79993	106610	1.33%	0.187%
16	17.276	2453	2457	2462	rVB3	68061	81278	1.02%	0.143%
17	17.552	2496	2504	2510	rBV	1455698	2241121	28.06%	3.934%
18	18.415	2647	2651	2659	rBV3	269990	417865	5.23%	0.734%
19	19.602	2849	2853	2860	rVB	131814	198200	2.48%	0.348%
20	19.684	2863	2867	2873	rVB4	78094	104398	1.31%	0.183%
21	19.961	2910	2914	2919	rVB	120005	180547	2.26%	0.317%
22	20.154	2941	2947	2953	rBV	5754422	7987649	100.00%	14.022%
23	21.453	3163	3168	3181	rVB3	282473	616165	7.71%	1.082%
24	21.847	3227	3235	3241	rBV2	1544626	2741183	34.32%	4.812%
25	22.693	3374	3379	3387	rVB6	105351	245388	3.07%	0.431%
26	25.201	3796	3806	3818	rBV2	864420	2487068	31.14%	4.366%

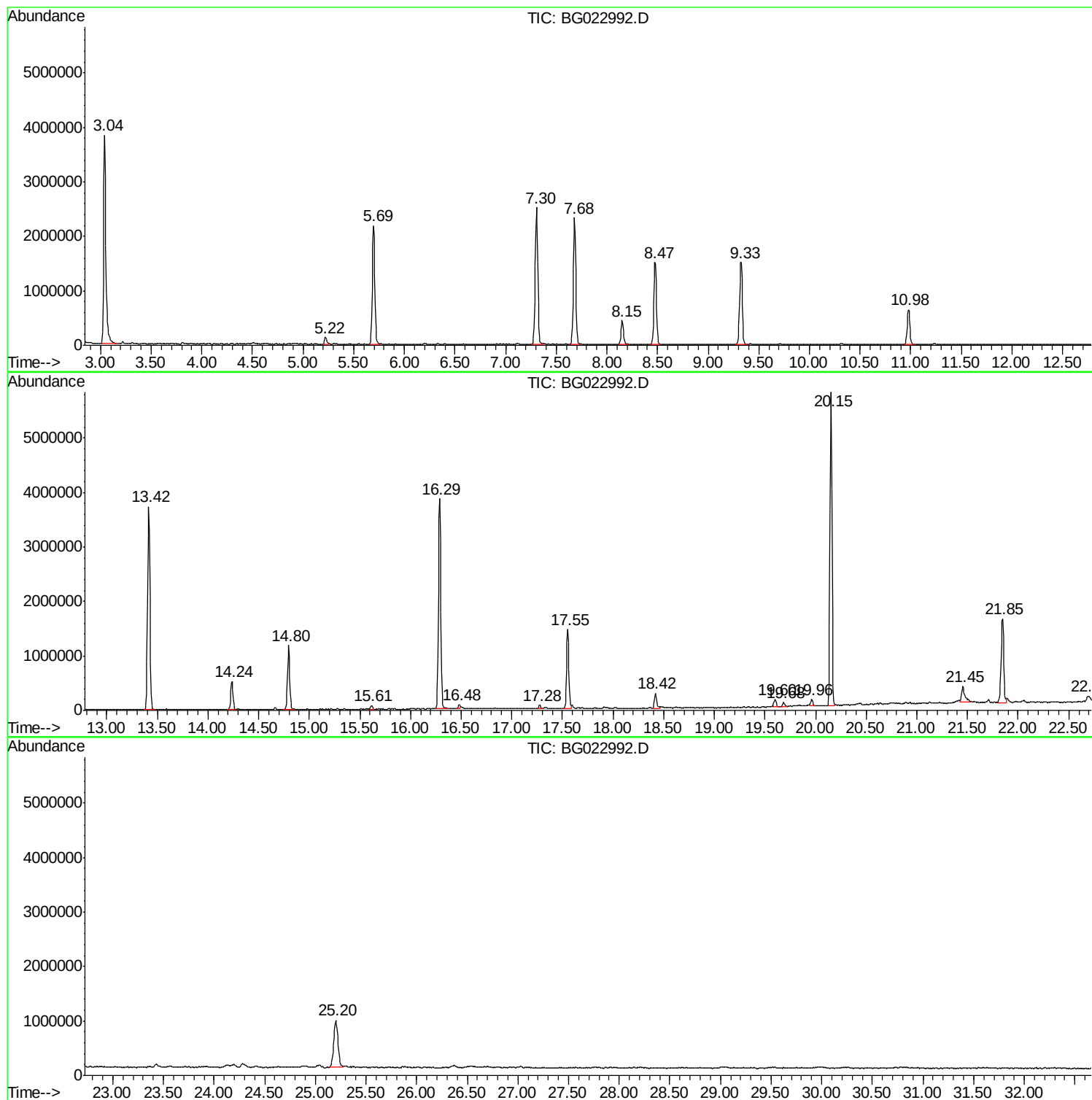
Sum of corrected areas: 56965204

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
Data File : BG022992.D
Acq On : 10 Jul 2016 9:29
Operator : UM/SJ
Sample : H3921-13
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
N8-B4(6-12)C

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
Data File : BG022992.D
Acq On : 10 Jul 2016 9:29
Operator : UM/SJ
Sample : H3921-13
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
N8-B4(6-12)C

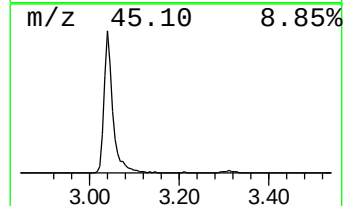
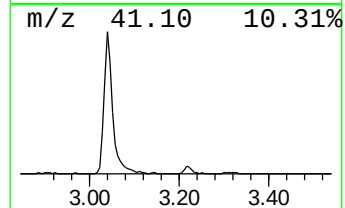
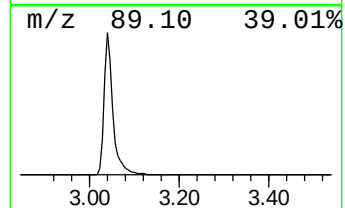
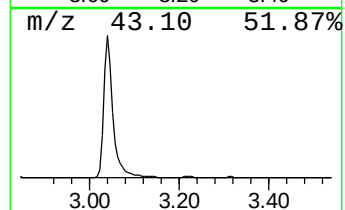
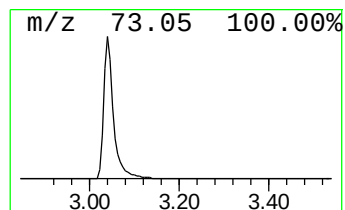
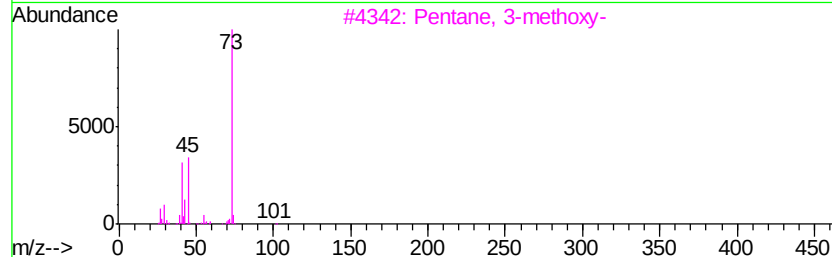
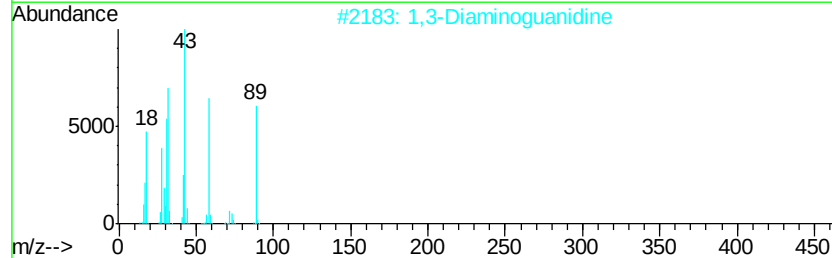
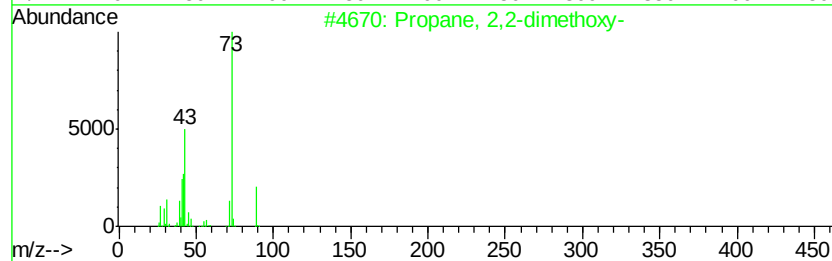
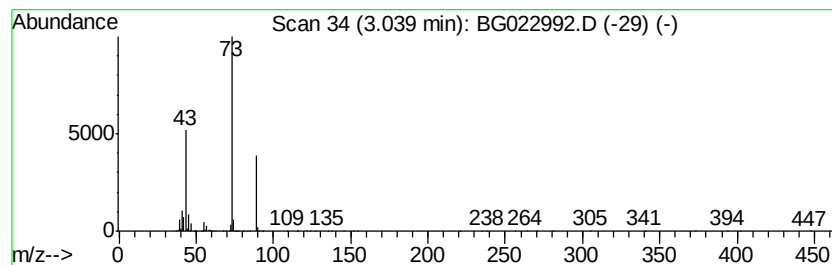
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.04	154.98 ng	5555140	1,4-Dichlorobenzene-d4	8.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56	
2	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	25	
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10	
4	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9	
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9	



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
Data File : BG022992.D
Acq On : 10 Jul 2016 9:29
Operator : UM/SJ
Sample : H3921-13
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
N8-B4(6-12)C

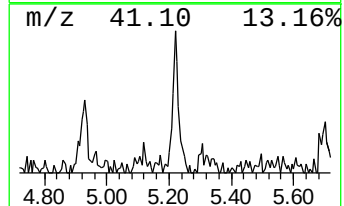
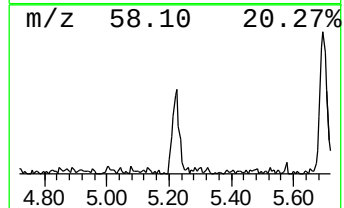
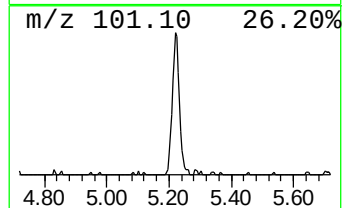
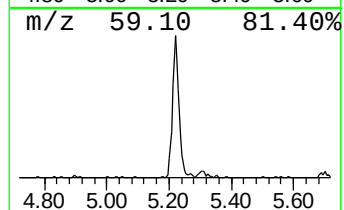
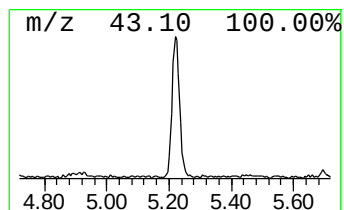
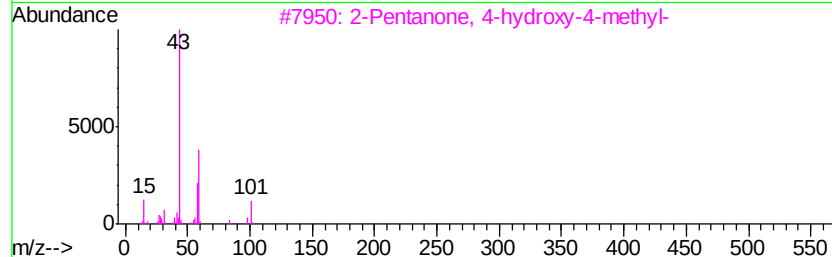
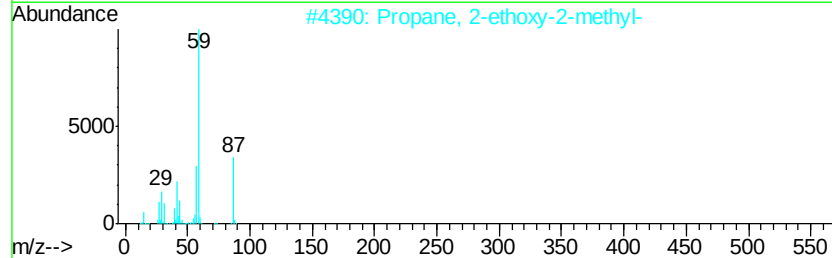
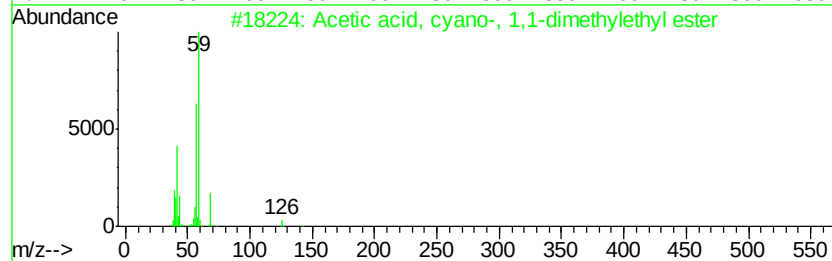
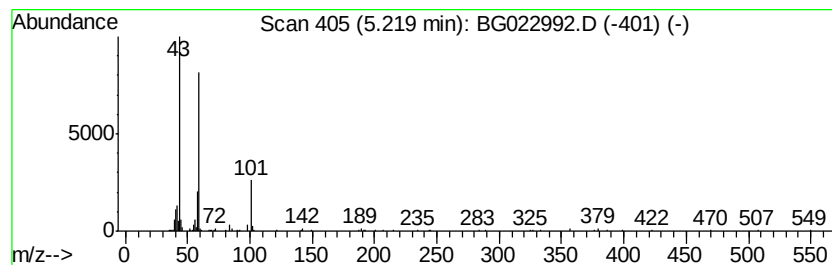
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown5.22 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	5.53 ng	198360	1,4-Dichlorobenzene-d4	8.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	28
2		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	25
3		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	12
4		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5		Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
Data File : BG022992.D
Acq On : 10 Jul 2016 9:29
Operator : UM/SJ
Sample : H3921-13
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
N8-B4(6-12)C

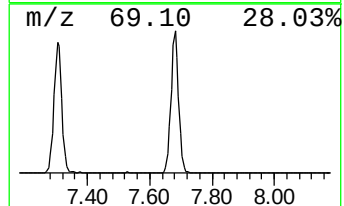
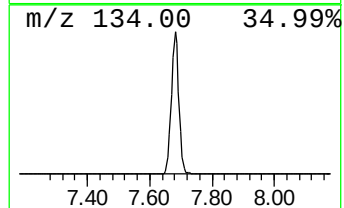
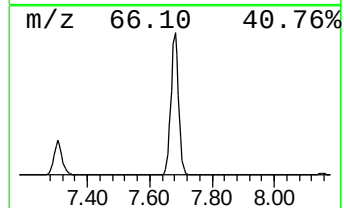
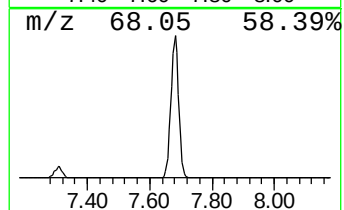
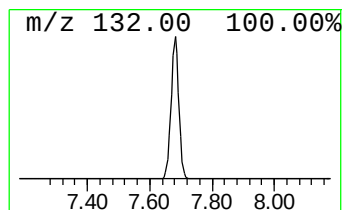
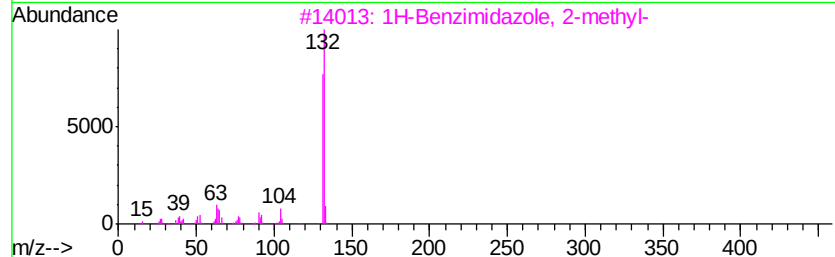
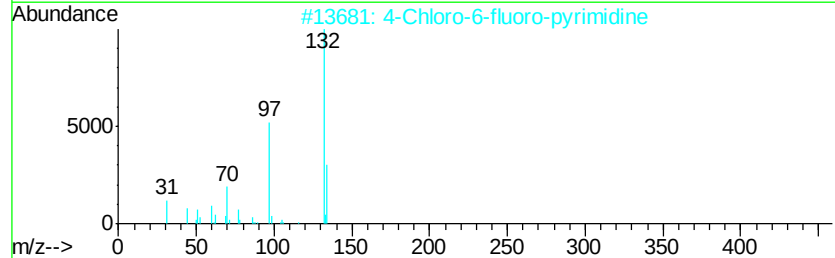
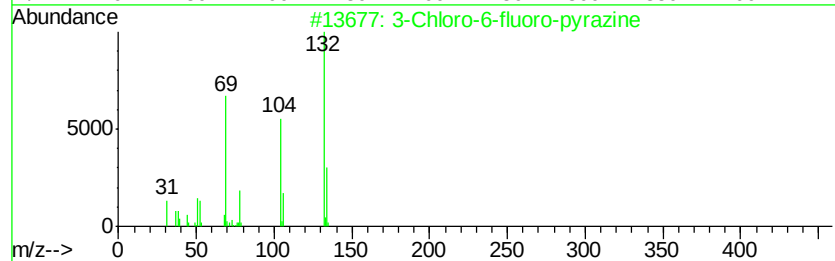
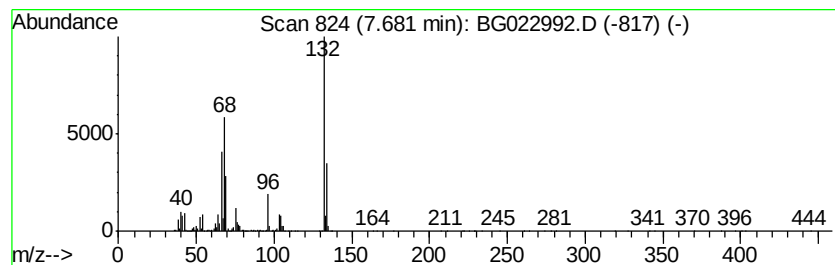
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown7.68 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	111.05 ng	3980550	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4	Xenon	132	Xe	007440-63-3	9
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
Data File : BG022992.D
Acq On : 10 Jul 2016 9:29
Operator : UM/SJ
Sample : H3921-13
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
N8-B4(6-12)C

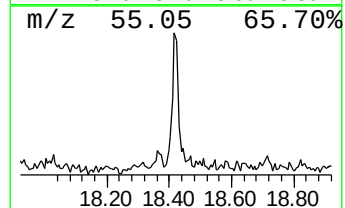
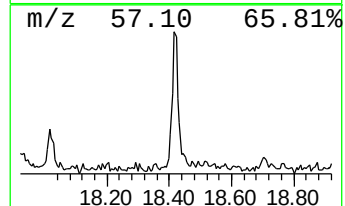
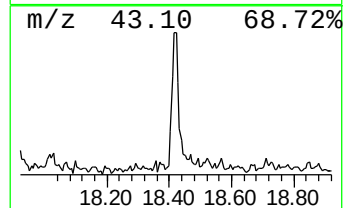
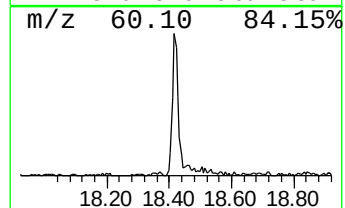
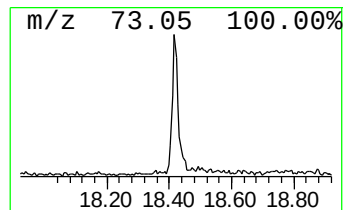
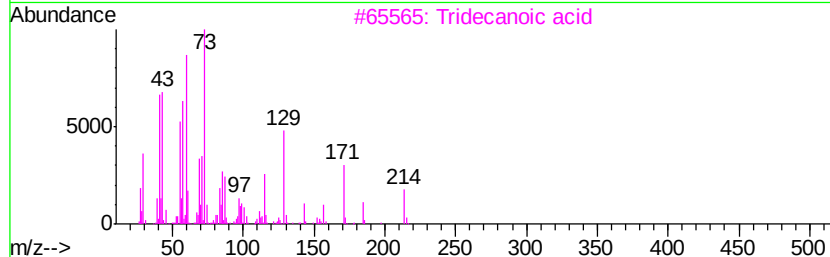
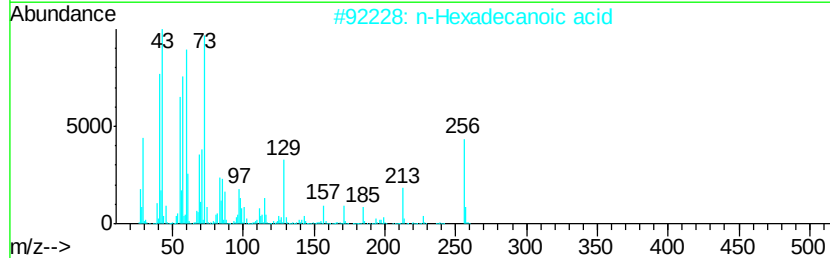
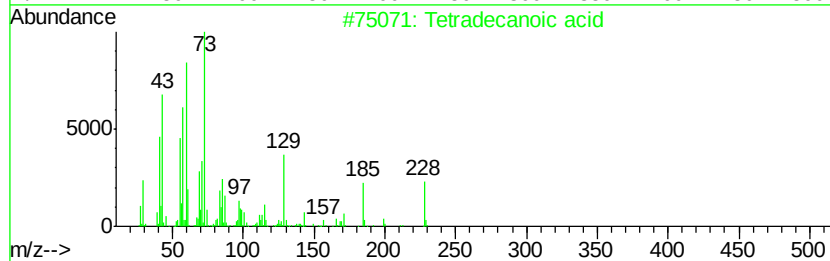
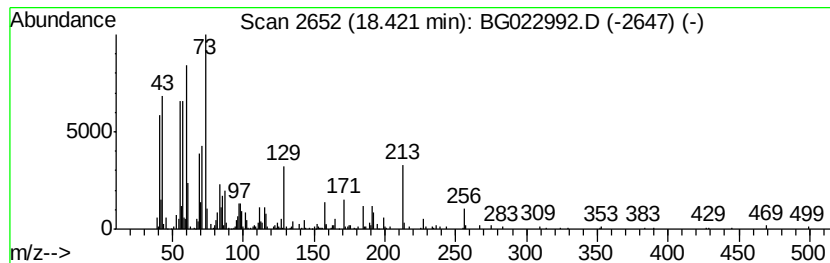
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Tetradecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.42	3.73 ng	417865	Phenanthrene-d10	17.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	95
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	70
4	Undecanoic acid	186	C11H22O2	000112-37-8	59
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	46



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
Data File : BG022992.D
Acq On : 10 Jul 2016 9:29
Operator : UM/SJ
Sample : H3921-13
Misc :
ALS Vial : 25 Sample Multiplier: 1

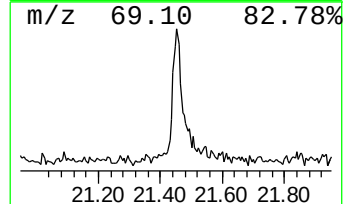
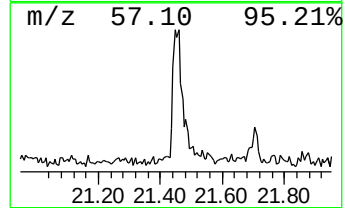
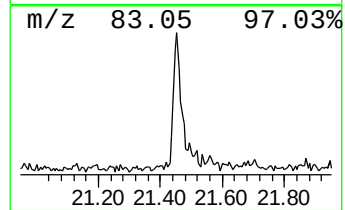
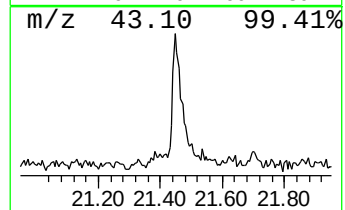
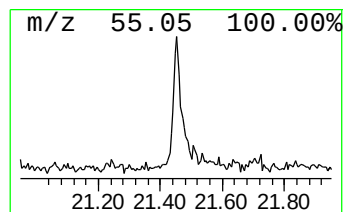
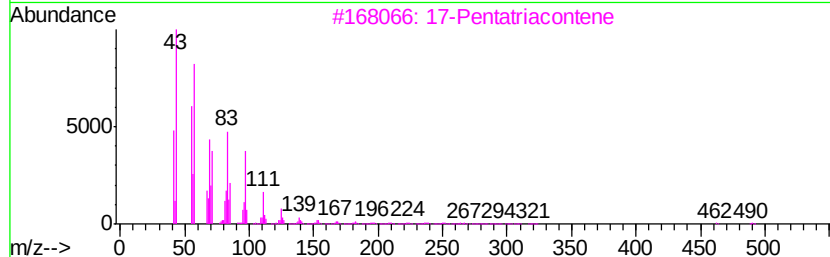
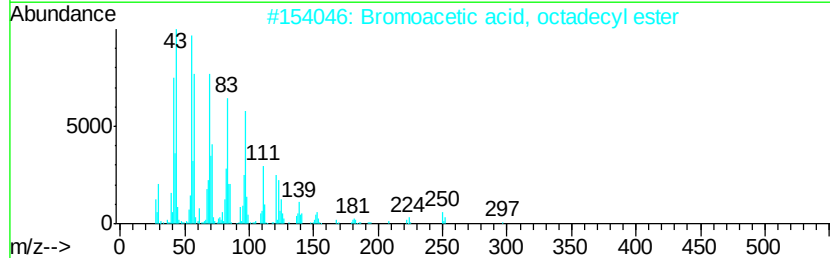
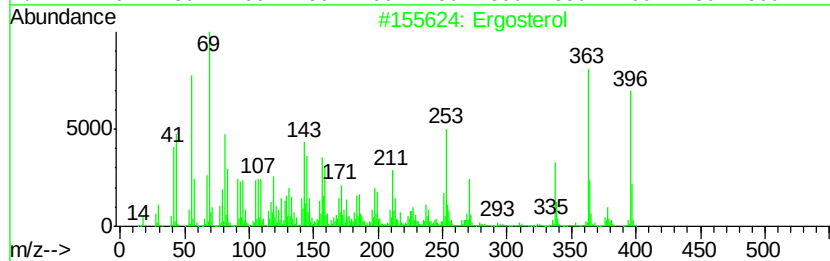
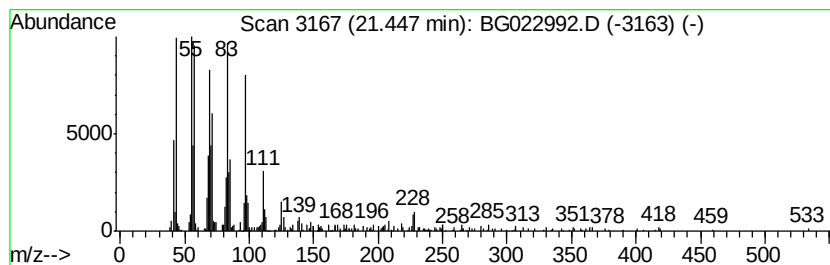
Instrument :
BNA_G
ClientSampleId :
N8-B4(6-12)C

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Ergosterol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.45	4.50 ng	616165	Chrysene-d12	21.85	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ergosterol	396	C28H44O	000057-87-4	90
2	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	90
3	17-Pentatriacontene	491	C35H70	006971-40-0	90
4	1-Docosene	308	C22H44	001599-67-3	83
5	1-Tetracosanol	354	C24H50O	000506-51-4	83



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
Data File : BG022992.D
Acq On : 10 Jul 2016 9:29
Operator : UM/SJ
Sample : H3921-13
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
N8-B4(6-12)C

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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, 2,2-dime...	3.04	155.0	ng	5555140	1	8.15	716871	20.0
unknown5.22	5.22	5.5	ng	198360	1	8.15	716871	20.0
unknown7.68	7.68	111.1	ng	3980550	1	8.15	716871	20.0
Tetradecanoic acid	18.42	3.7	ng	417865	4	17.55	2241120	20.0
Ergosterol	21.45	4.5	ng	616165	5	21.85	2741180	20.0