

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103019\
 Data File : BG043417.D
 Acq On : 31 Oct 2019 1:43
 Operator : JU
 Sample : K5599-09
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 Z3-22A

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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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	3.187	13	17	28	rVB	120013	192781	6.81%	1.376%
2	5.126	342	347	355	rBV	95882	154421	5.46%	1.102%
3	5.608	422	429	444	rBV	452985	805254	28.46%	5.747%
4	7.206	693	701	724	rBV	485645	953254	33.69%	6.803%
5	7.564	754	762	772	rBV	499306	915109	32.34%	6.531%
6	8.023	832	840	850	rBV	133659	234330	8.28%	1.672%
7	8.346	887	895	909	rBV	395274	710367	25.11%	5.070%
8	9.186	1028	1038	1054	rBV	244579	538458	19.03%	3.843%
9	10.831	1310	1318	1327	rBV	143068	300649	10.63%	2.146%
10	13.269	1725	1733	1750	rBV	832305	1485653	52.51%	10.603%
11	14.104	1867	1875	1888	rBV	45141	99335	3.51%	0.709%
12	14.650	1961	1968	1980	rBV	308875	527742	18.65%	3.766%
13	16.137	2214	2221	2234	rBV	748804	1315966	46.51%	9.392%
14	17.394	2429	2435	2450	rBV2	372568	677915	23.96%	4.838%
15	17.517	2451	2456	2464	rVB4	20222	36532	1.29%	0.261%
16	18.287	2582	2587	2597	rBV4	28880	60878	2.15%	0.434%
17	20.003	2873	2879	2895	rBV	2017636	2829296	100.00%	20.192%
18	21.301	3095	3100	3110	rBV3	73896	159149	5.63%	1.136%
19	21.389	3111	3115	3121	rVB	19280	35027	1.24%	0.250%
20	21.659	3150	3161	3173	rBV	465958	888480	31.40%	6.341%
21	23.134	3406	3412	3420	rVB7	24044	42064	1.49%	0.300%
22	23.927	3541	3547	3553	rVB6	26390	56056	1.98%	0.400%
23	24.856	3694	3705	3718	rBV	307846	942873	33.33%	6.729%
24	25.984	3889	3897	3908	rVB6	18117	50588	1.79%	0.361%

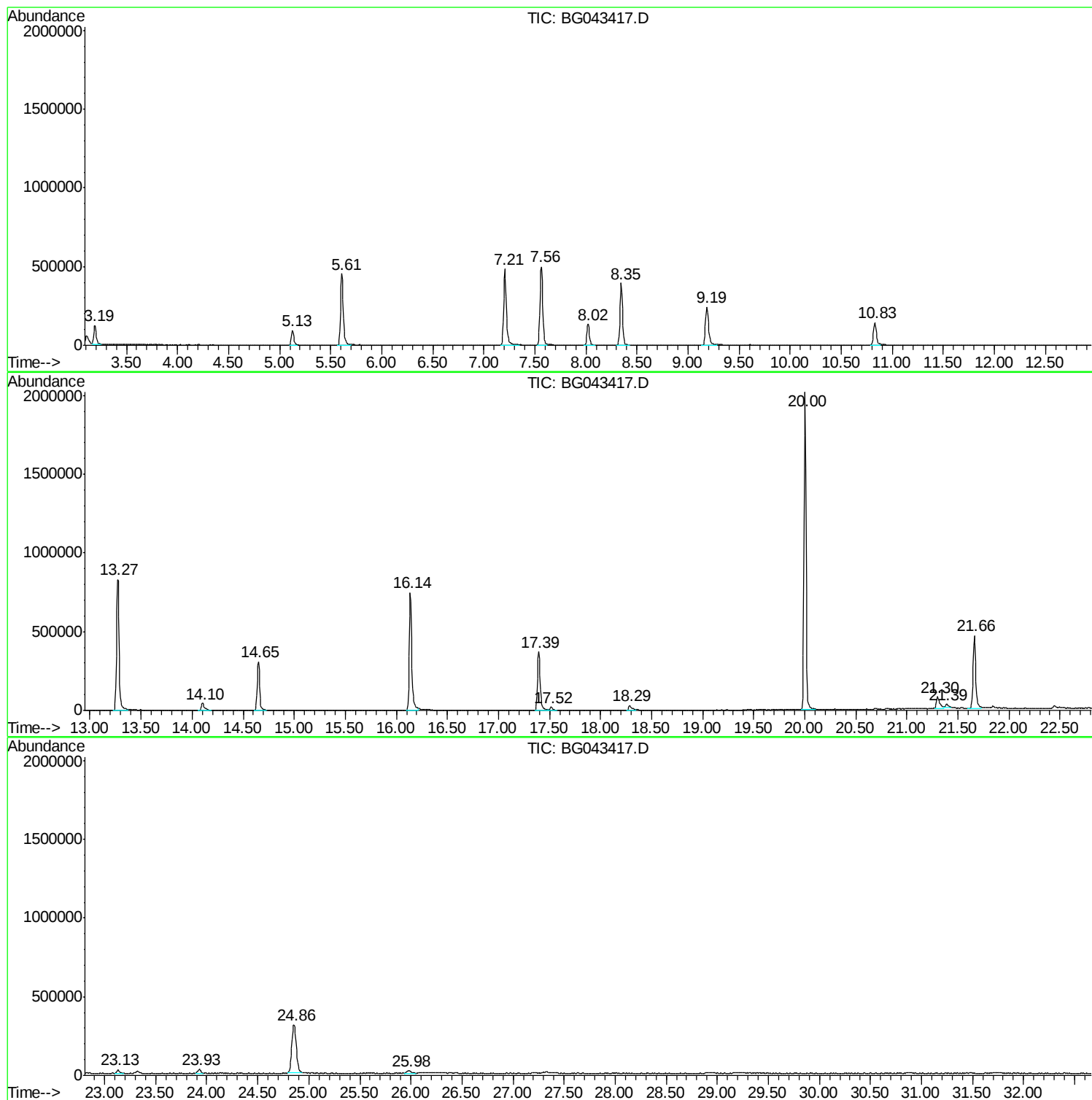
Sum of corrected areas: 14012177

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103019\
Data File : BG043417.D
Acq On : 31 Oct 2019 1:43
Operator : JU
Sample : K5599-09
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
Z3-22A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103019\
Data File : BG043417.D
Acq On : 31 Oct 2019 1:43
Operator : JU
Sample : K5599-09
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
Z3-22A

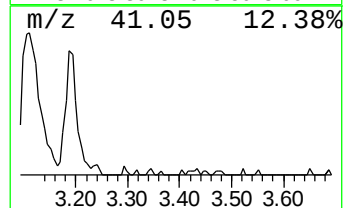
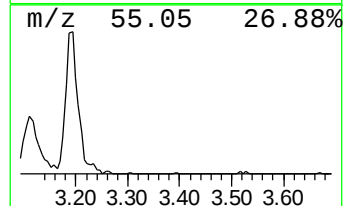
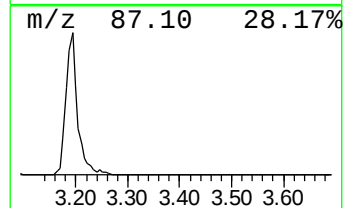
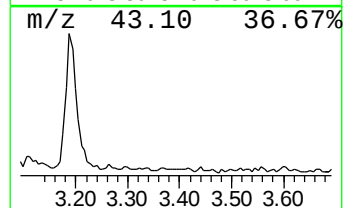
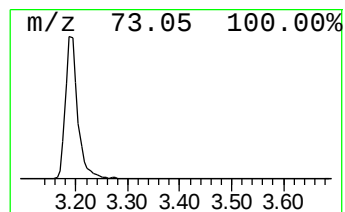
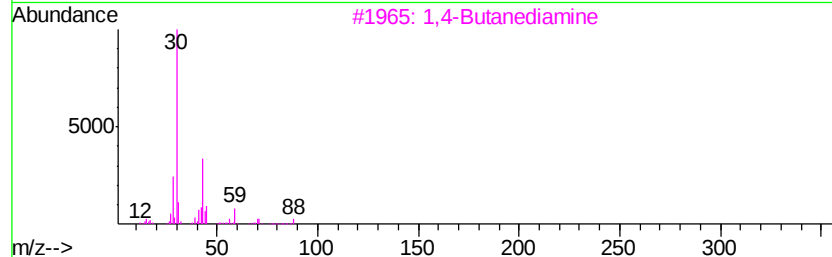
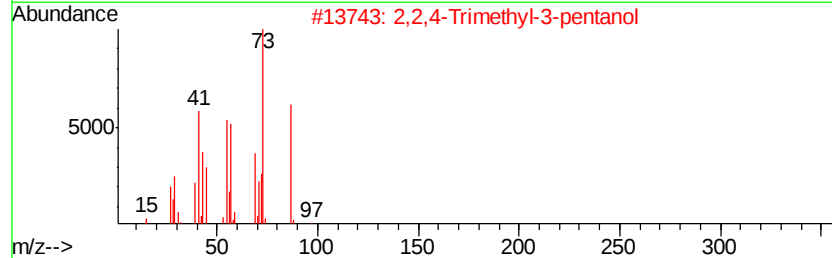
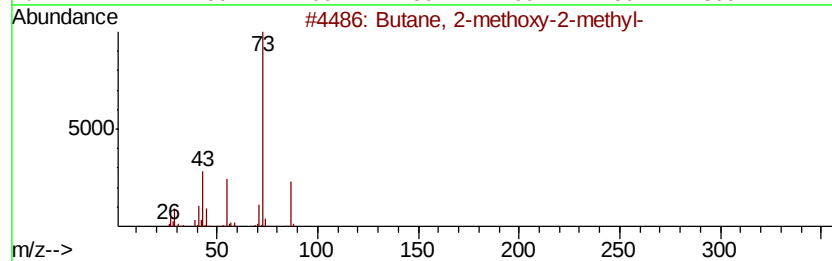
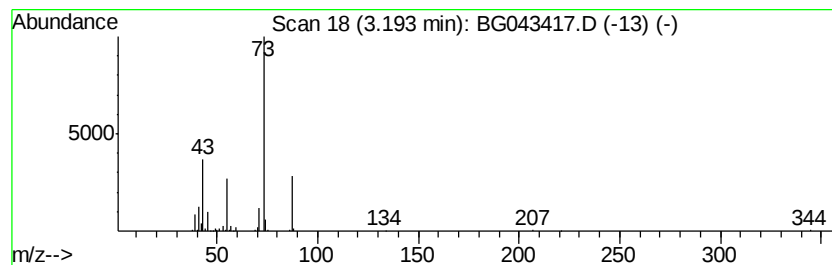
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.19	16.45 ng	192781	1,4-Dichlorobenzene-d4	8.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	43
3		1,4-Butanediamine	88	C4H12N2	000110-60-1	9
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5		Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103019\
Data File : BG043417.D
Acq On : 31 Oct 2019 1:43
Operator : JU
Sample : K5599-09
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
Z3-22A

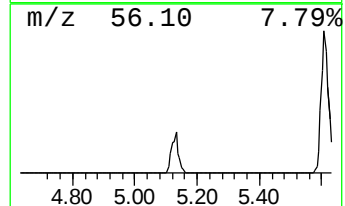
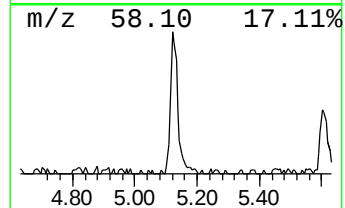
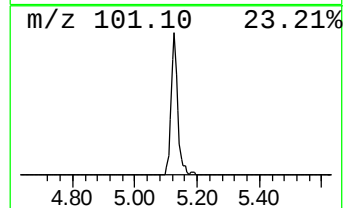
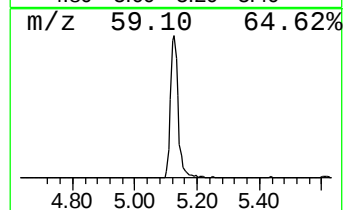
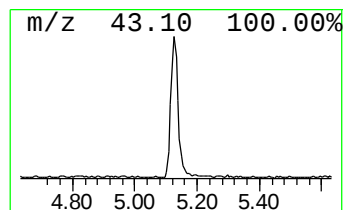
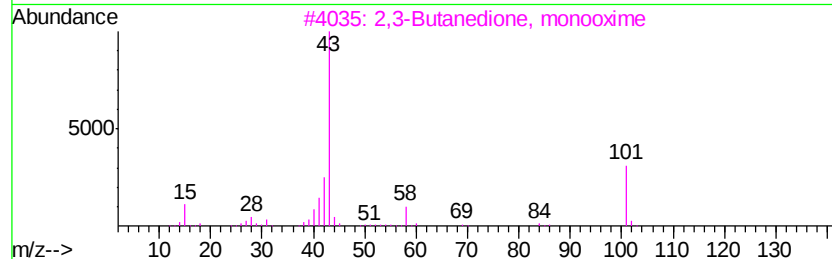
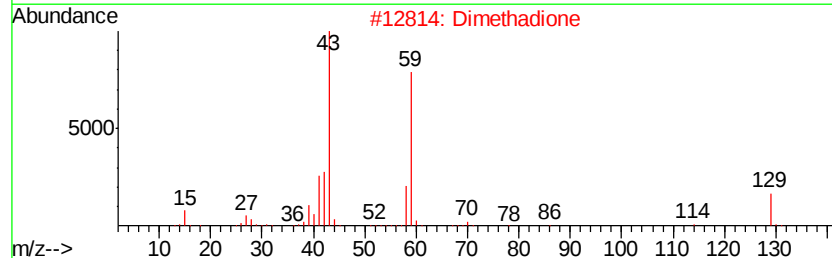
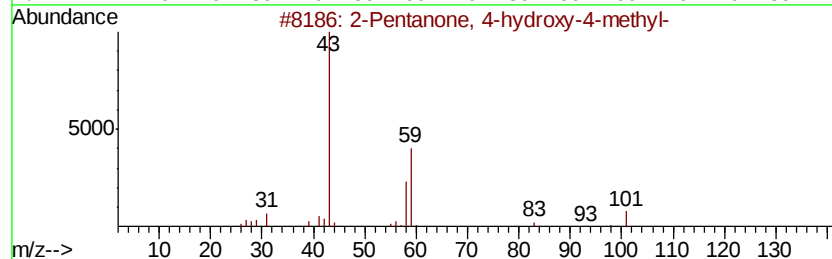
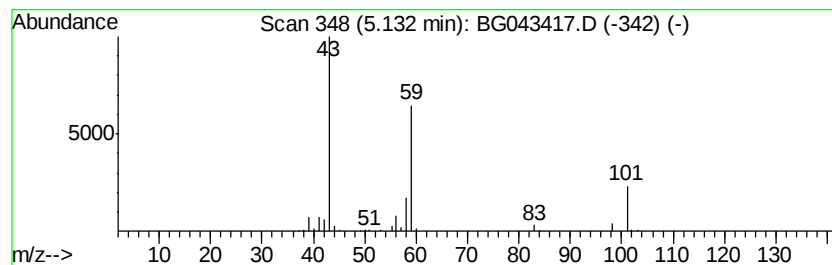
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.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.
5.13	13.18 ng	154421	1,4-Dichlorobenzene-d4	8.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Dimethadione	129	C5H7NO3	000695-53-4	33
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
5		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103019\
Data File : BG043417.D
Acq On : 31 Oct 2019 1:43
Operator : JU
Sample : K5599-09
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
Z3-22A

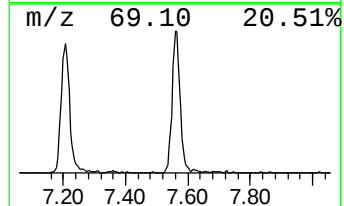
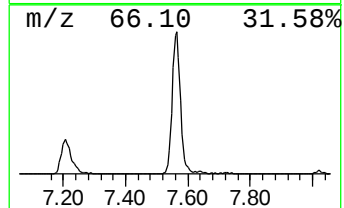
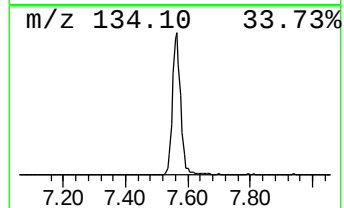
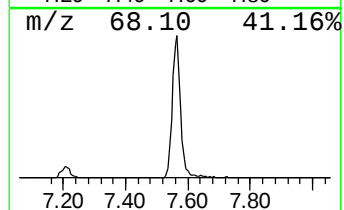
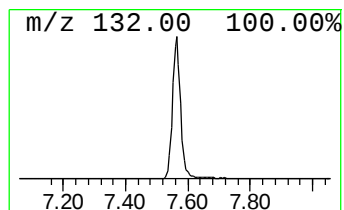
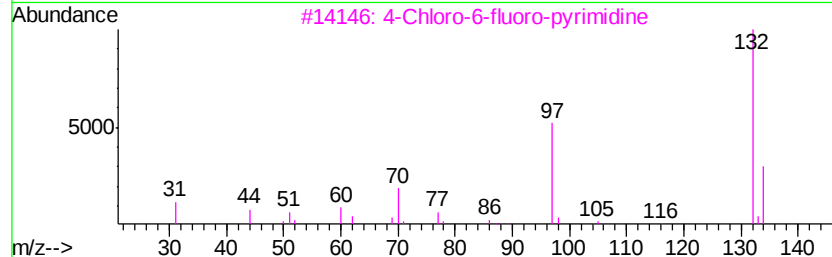
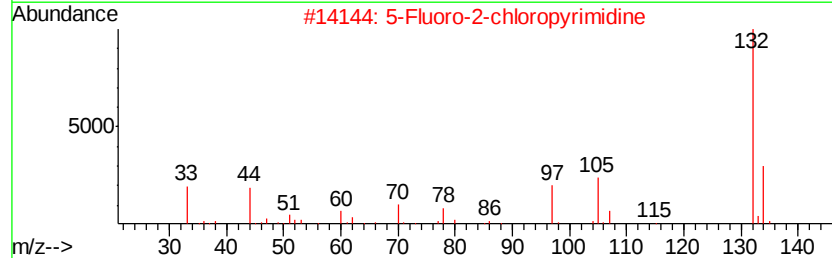
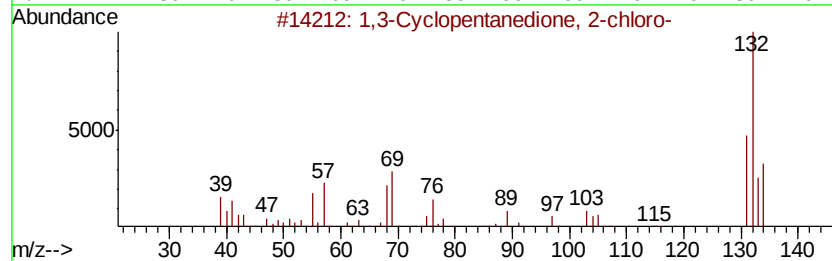
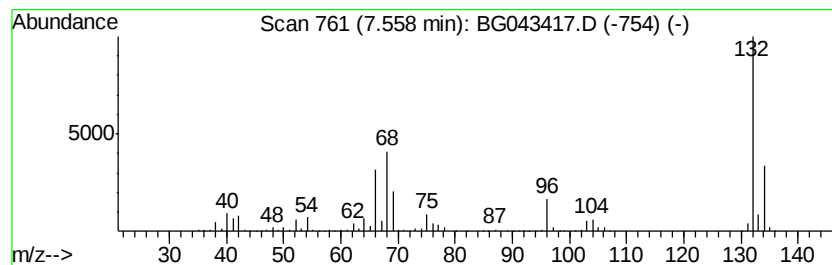
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown7.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.56	78.10 ng	915109	1,4-Dichlorobenzene-d4	8.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	38
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
3		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	12



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG103019\
Data File : BG043417.D
Acq On : 31 Oct 2019 1:43
Operator : JU
Sample : K5599-09
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
Z3-22A

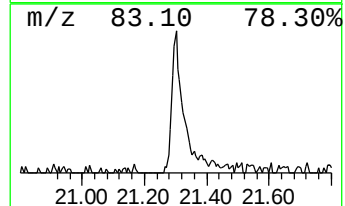
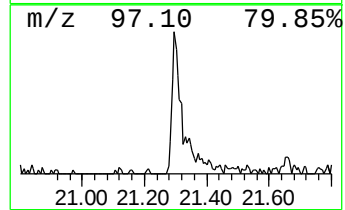
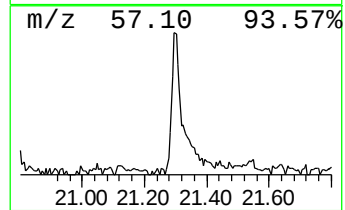
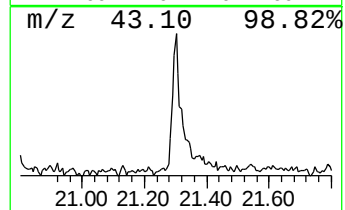
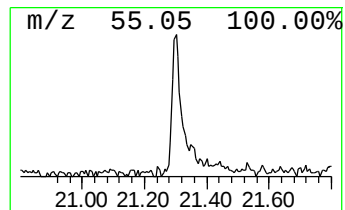
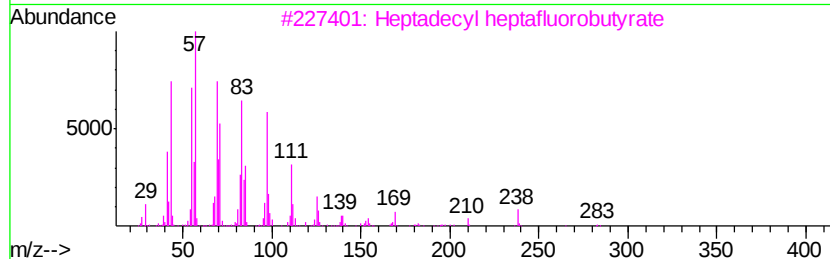
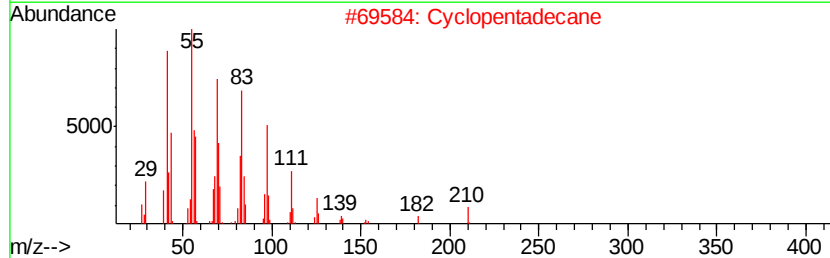
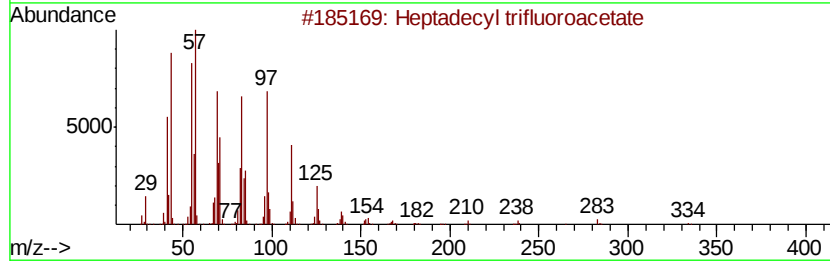
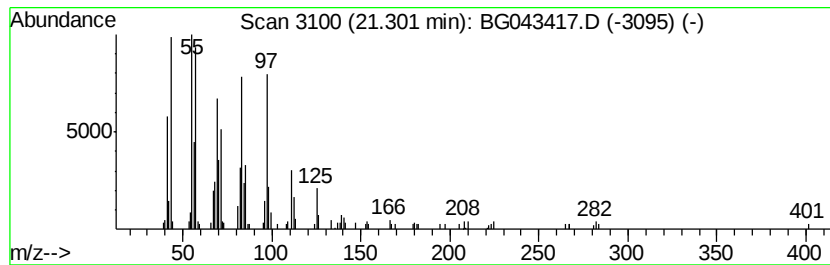
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptadecyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.30	3.58 ng	159149	Chrysene-d12	21.66

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
2		Cyclopentadecane	210	C15H30	000295-48-7	92
3		Heptadecyl heptafluorobutyrte	452	C21H35F7O2	959085-66-6	91
4		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
5		1-Tricosanol	340	C23H48O	003133-01-5	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG103019\
Data File : BG043417.D
Acq On : 31 Oct 2019 1:43
Operator : JU
Sample : K5599-09
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
Z3-22A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.19	16.4	ng	192781	1	8.02	234330	20.0
2-Pentanone, 4-hy...	5.13	13.2	ng	154421	1	8.02	234330	20.0
unknown7.56	7.56	78.1	ng	915109	1	8.02	234330	20.0
Heptadecyl triflu...	21.30	3.6	ng	159149	5	21.66	888480	20.0