

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010821\
 Data File : BG047898.D
 Acq On : 8 Jan 2021 22:45
 Operator : CG/JU
 Sample : M1044-15
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-6

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-BG121720.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG047898.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.508	18	29	34	rBV	72828	101173	2.36%	0.663%
2	4.707	228	233	241	rBV	106917	147970	3.46%	0.969%
3	5.177	308	313	316	rBV2	60279	90012	2.10%	0.589%
4	5.212	316	319	325	rVB	49059	67854	1.58%	0.444%
5	5.747	403	410	424	rVB	815889	1417237	33.10%	9.281%
6	7.398	683	691	707	rBV	635161	1481820	34.61%	9.704%
7	8.162	814	821	830	rVB2	164986	287227	6.71%	1.881%
8	9.337	1013	1021	1029	rBV	389377	694069	16.21%	4.545%
9	10.988	1295	1302	1309	rVB	132100	233641	5.46%	1.530%
10	13.420	1709	1716	1724	rVB	1279867	1960821	45.80%	12.841%
11	14.231	1849	1854	1861	rVB	47267	67194	1.57%	0.440%
12	14.789	1941	1949	1958	rVB	278432	448847	10.48%	2.939%
13	16.282	2197	2203	2216	rBV	1279806	1977140	46.18%	12.948%
14	17.533	2410	2416	2422	rBV	412897	610270	14.25%	3.996%
15	20.124	2850	2857	2863	rBV	3354019	4281134	100.00%	28.036%
16	21.810	3137	3144	3150	rBV	478806	798175	18.64%	5.227%
17	25.136	3699	3710	3721	rBV2	207859	605747	14.15%	3.967%

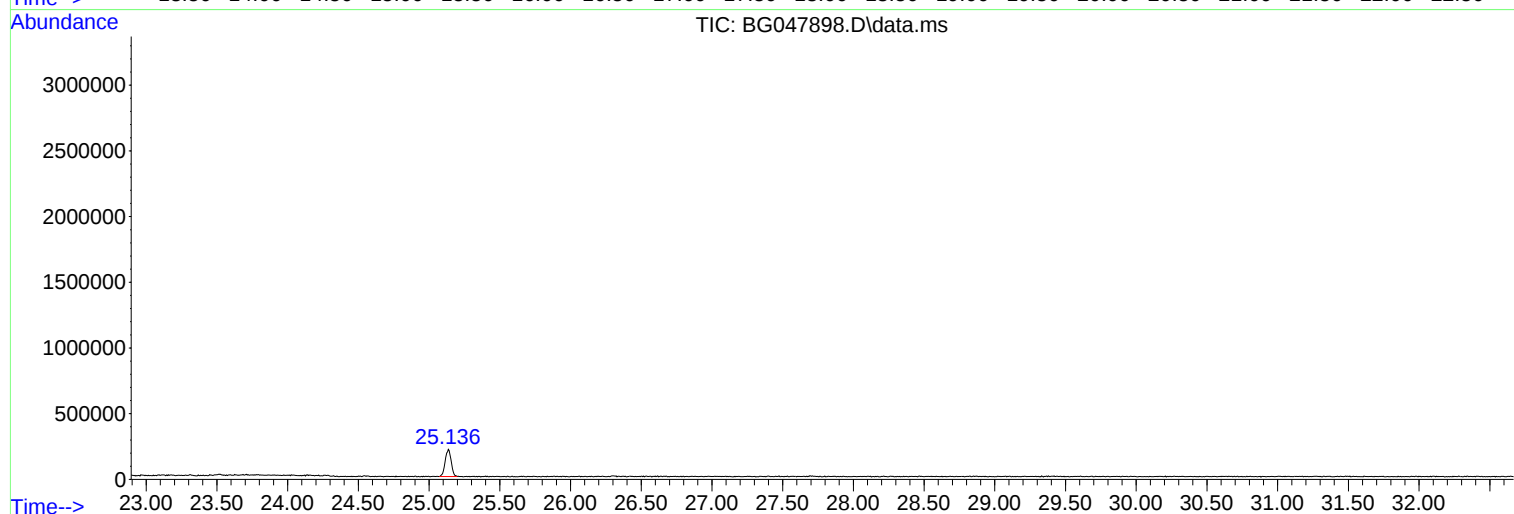
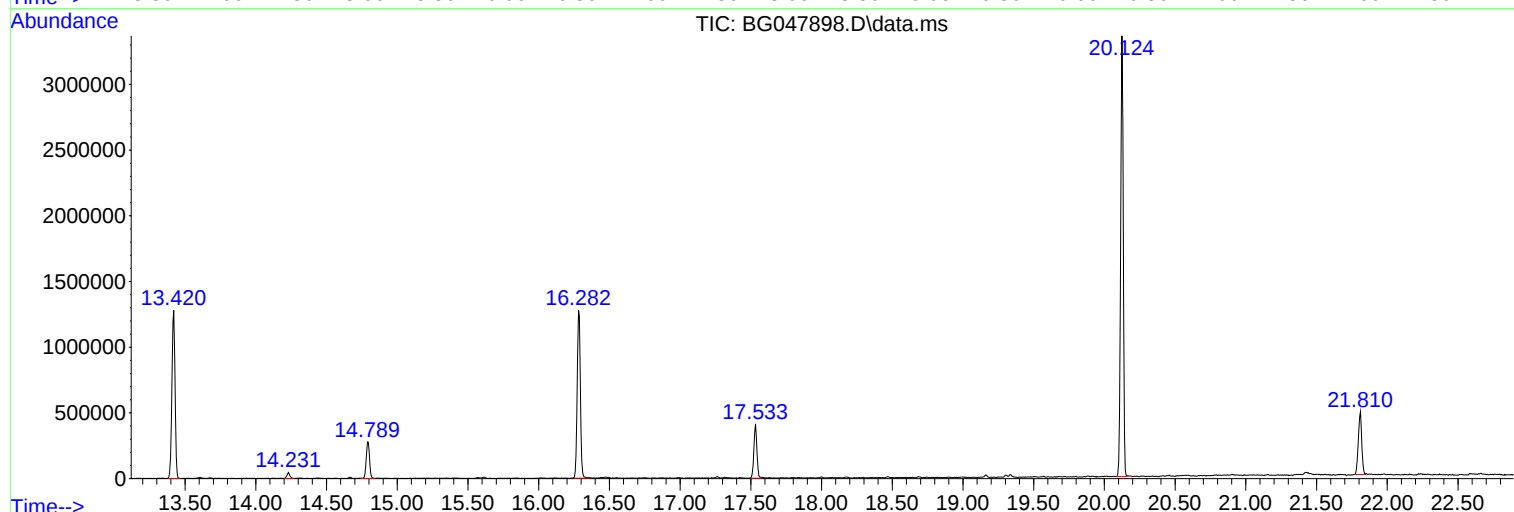
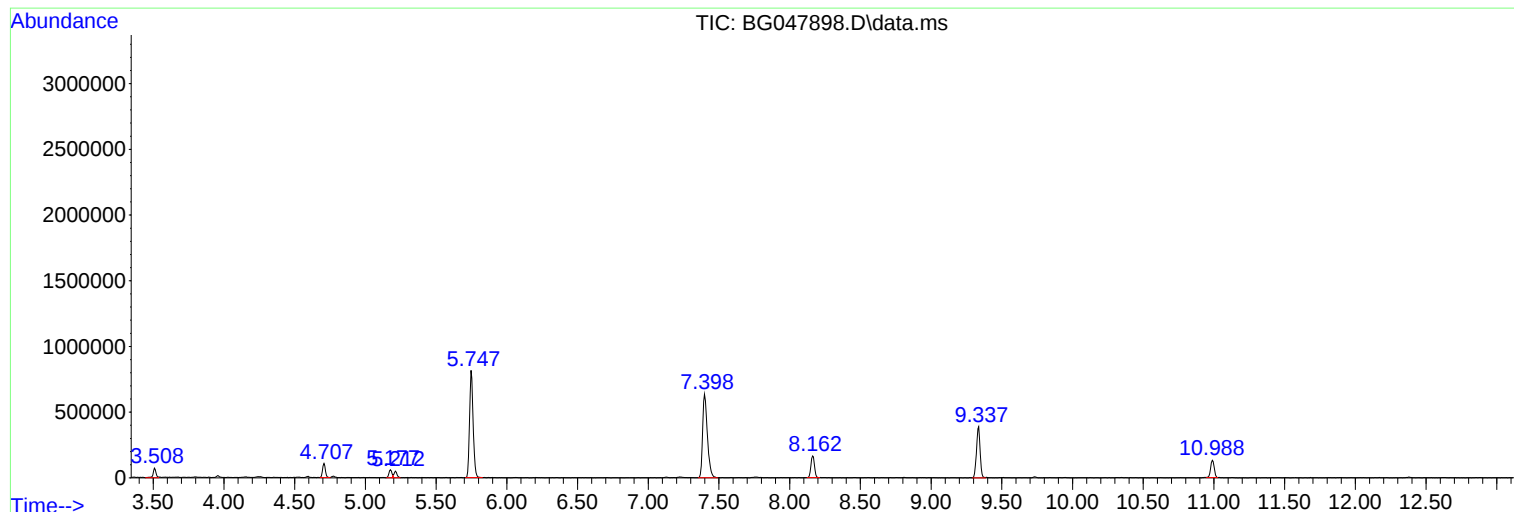
Sum of corrected areas: 15270331

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010821\
Data File : BG047898.D
Acq On : 8 Jan 2021 22:45
Operator : CG/JU
Sample : M1044-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121720.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\BG010821\
Data File : BG047898.D
Acq On : 8 Jan 2021 22:45
Operator : CG/JU
Sample : M1044-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-6

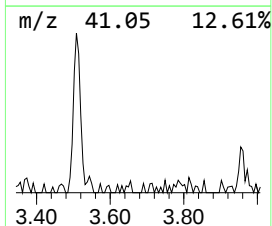
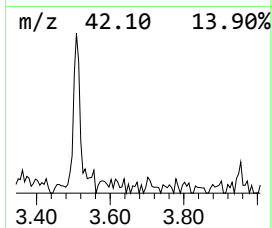
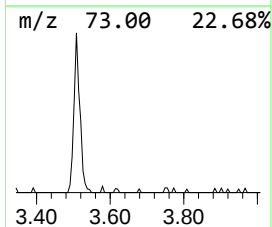
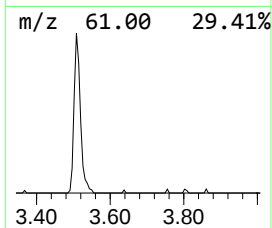
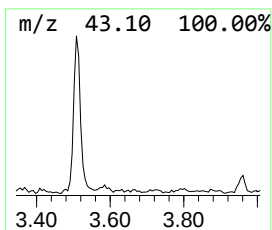
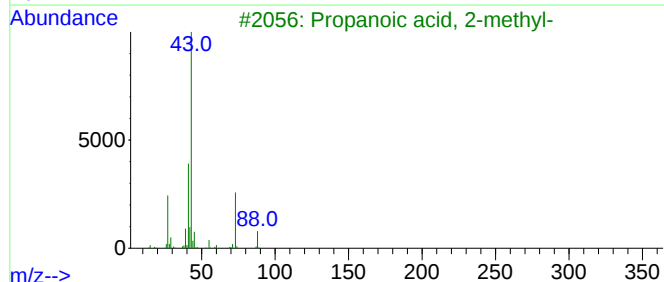
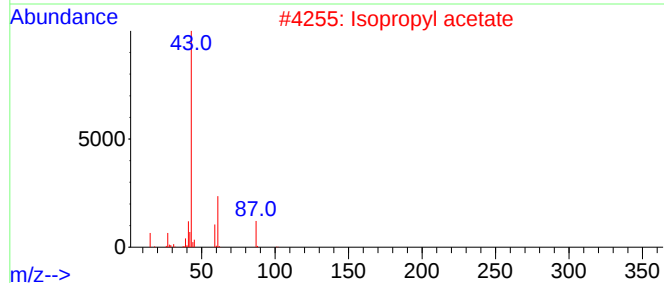
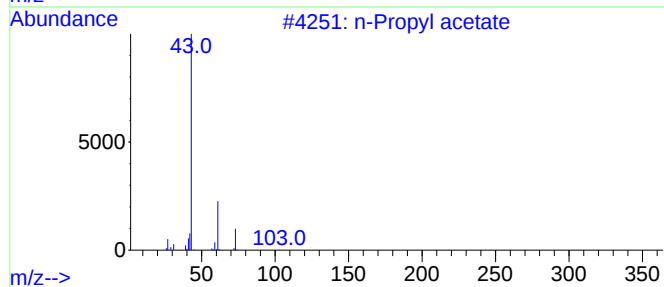
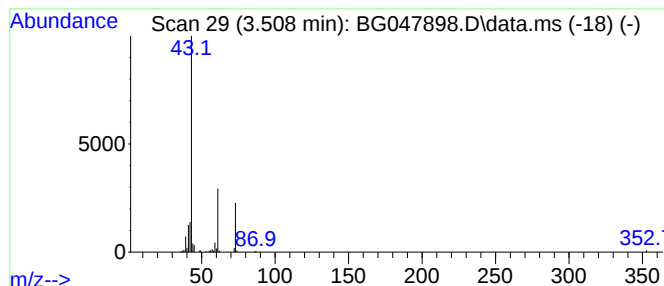
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.508	7.04 ng	101173	1,4-Dichlorobenzene-d4	8.162

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Propyl acetate	102	C5H10O2	000109-60-4	72
2		Isopropyl acetate	102	C5H10O2	000108-21-4	28
3		Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	28
4		Di-n-propyl ether	102	C6H14O	000111-43-3	9
5		Cyclobutylamine	71	C4H9N	002516-34-9	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010821\
Data File : BG047898.D
Acq On : 8 Jan 2021 22:45
Operator : CG/JU
Sample : M1044-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-6

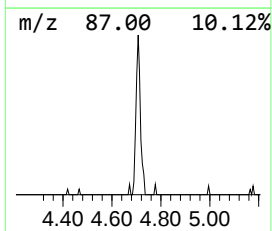
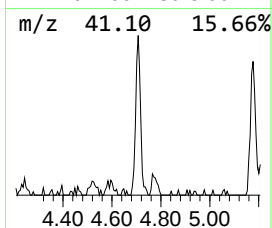
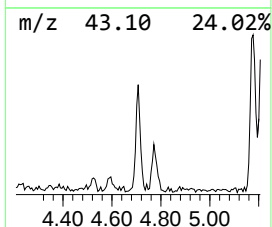
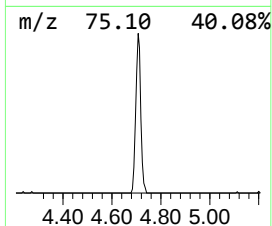
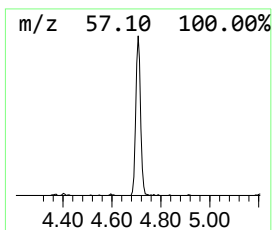
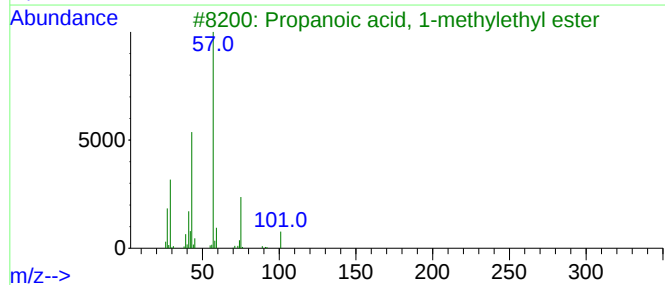
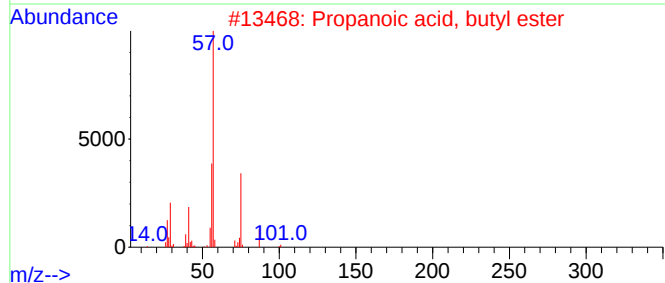
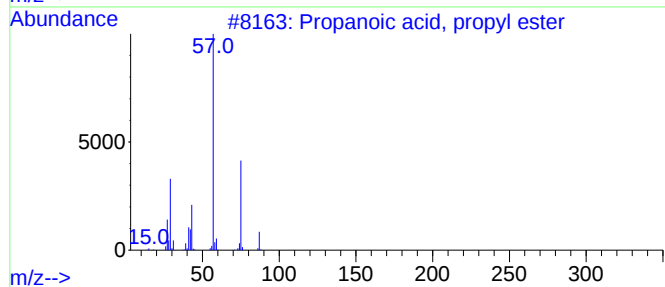
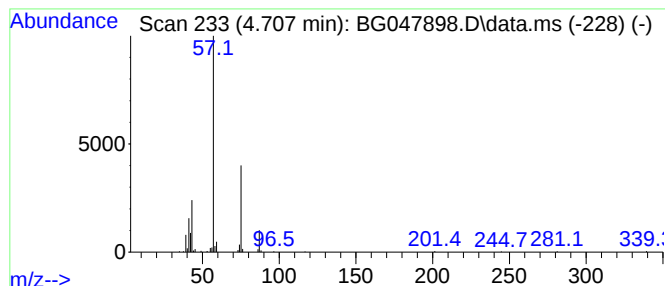
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.707	10.30 ng	147970	1,4-Dichlorobenzene-d4	8.162

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	72
2			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	50
3			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	17
4			Isobutyl ether	130	C8H18O	000628-55-7	10
5			Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010821\
Data File : BG047898.D
Acq On : 8 Jan 2021 22:45
Operator : CG/JU
Sample : M1044-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-6

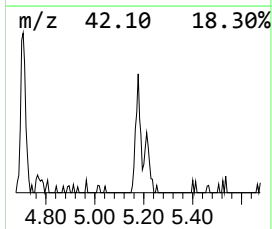
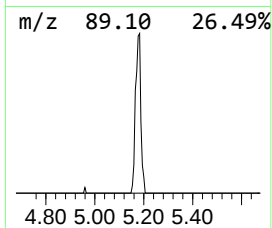
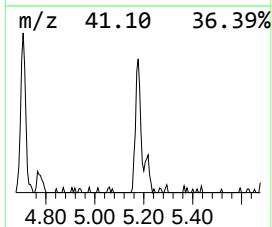
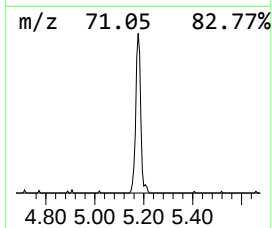
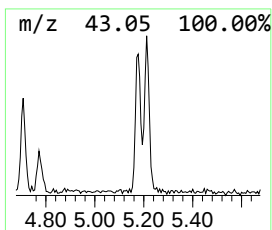
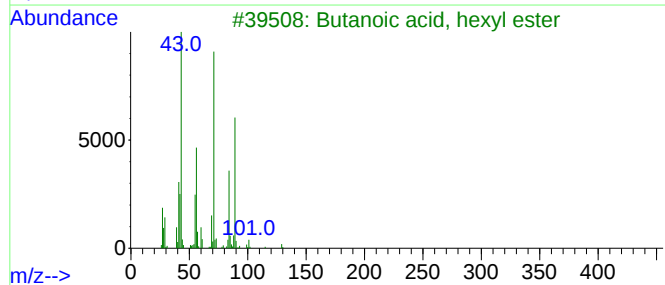
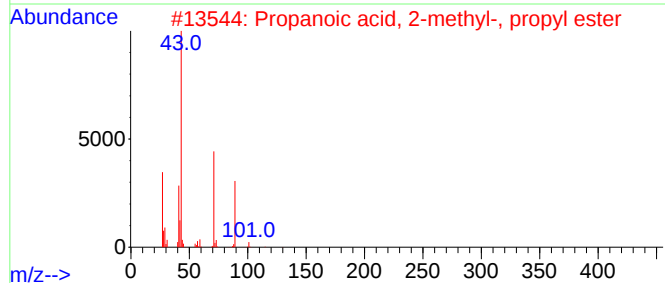
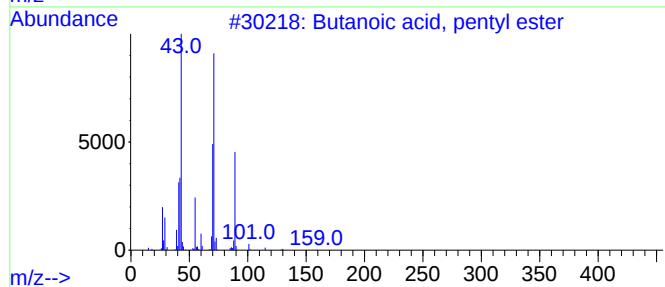
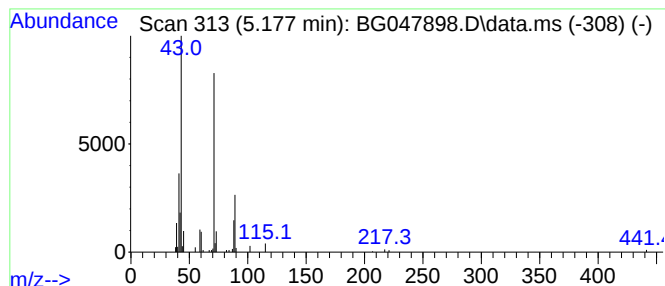
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Butanoic acid, pentyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.177	6.27 ng	90012	1,4-Dichlorobenzene-d4	8.162

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64
2			Propanoic acid, 2-methyl-, propyl...	130	C7H14O2	000644-49-5	64
3			Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	59
4			Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	56
5			Butanoic acid, 1-methylbutyl ester	158	C9H18O2	060415-61-4	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010821\
Data File : BG047898.D
Acq On : 8 Jan 2021 22:45
Operator : CG/JU
Sample : M1044-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-6

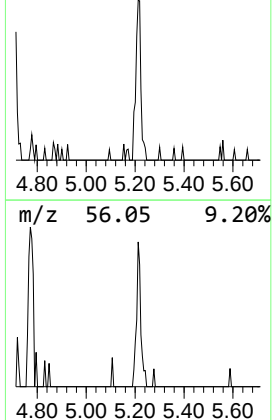
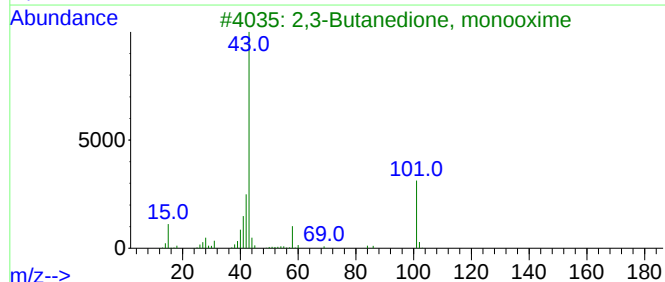
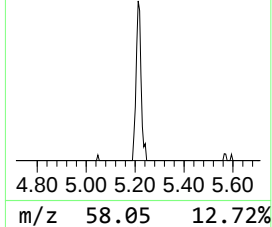
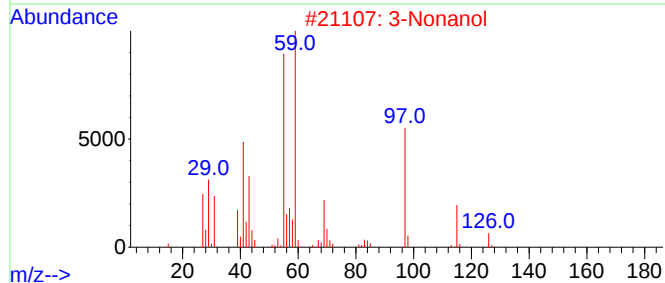
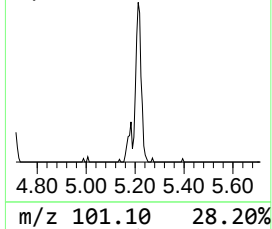
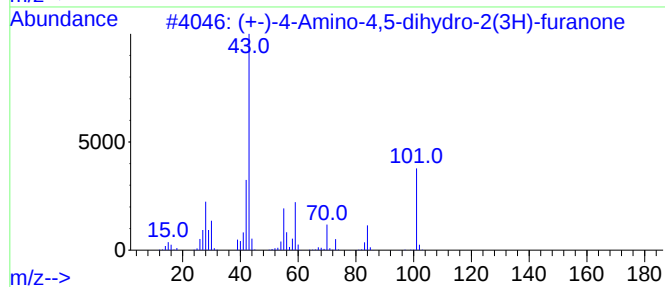
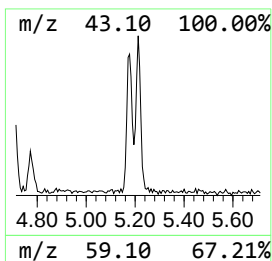
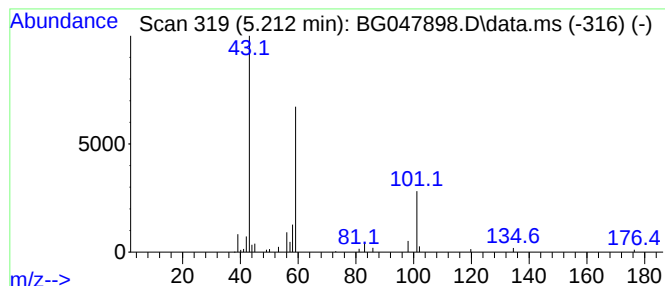
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown5.212 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.212	4.72 ng	67854	1,4-Dichlorobenzene-d4	8.162

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7N02	016504-58-8	45		
2	3-Nonanol	144	C9H20O	000624-51-1	25		
3	2,3-Butanedione, monooxime	101	C4H7N02	000057-71-6	16		
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9		
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010821\
Data File : BG047898.D
Acq On : 8 Jan 2021 22:45
Operator : CG/JU
Sample : M1044-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121720.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
n-Propyl acetate	3.508	7.0	ng	101173	1	8.162	287227	20.0
Propanoic acid,...	4.707	10.3	ng	147970	1	8.162	287227	20.0
Butanoic acid, ...	5.177	6.3	ng	90012	1	8.162	287227	20.0
unknown5.212	5.212	4.7	ng	67854	1	8.162	287227	20.0