

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010821\
 Data File : BG047900.D
 Acq On : 9 Jan 2021 00:05
 Operator : CG/JU
 Sample : M1044-17
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-10

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: BG047900.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.512	24	29	36	rVB2	84170	105553	3.15%	0.646%
2	4.704	226	232	239	rBV	130062	190823	5.70%	1.167%
3	5.174	306	312	316	rBV	82259	123731	3.70%	0.757%
4	5.215	316	319	326	rVB	42103	61483	1.84%	0.376%
5	5.750	401	410	421	rBV	879848	1576009	47.10%	9.642%
6	7.395	682	690	708	rBV	711528	1658288	49.56%	10.145%
7	8.165	814	821	830	rBV	173019	311422	9.31%	1.905%
8	9.334	1012	1020	1028	rBV	636222	1139939	34.07%	6.974%
9	10.991	1294	1302	1308	rBV	216744	387923	11.59%	2.373%
10	13.418	1705	1715	1724	rBV	1616692	2470360	73.83%	15.113%
11	14.228	1848	1853	1860	rBV	34028	50484	1.51%	0.309%
12	14.792	1942	1949	1956	rVB2	353218	559087	16.71%	3.420%
13	16.285	2196	2203	2215	rBV	1550231	2314098	69.16%	14.157%
14	17.530	2409	2415	2421	rBV	489530	745506	22.28%	4.561%
15	20.127	2850	2857	2862	rBV	2493598	3346229	100.00%	20.472%
16	21.426	3073	3078	3083	rBV8	28646	59319	1.77%	0.363%
17	21.808	3136	3143	3151	rBV	369919	621613	18.58%	3.803%
18	25.133	3698	3709	3719	rBV2	205300	623543	18.63%	3.815%

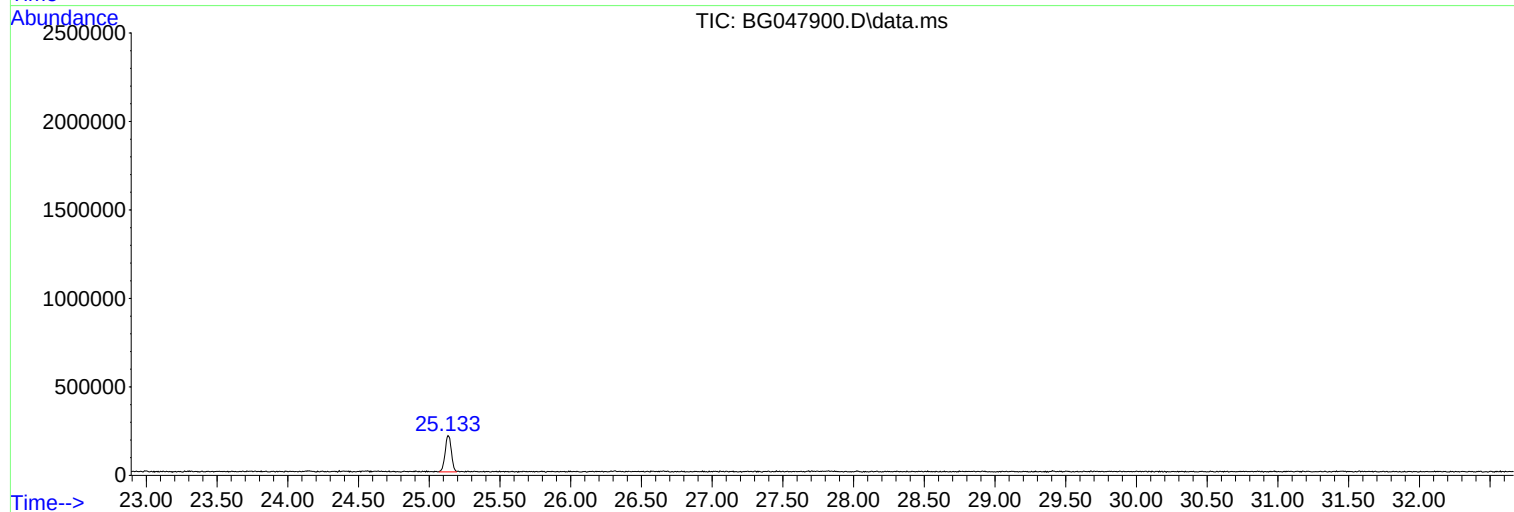
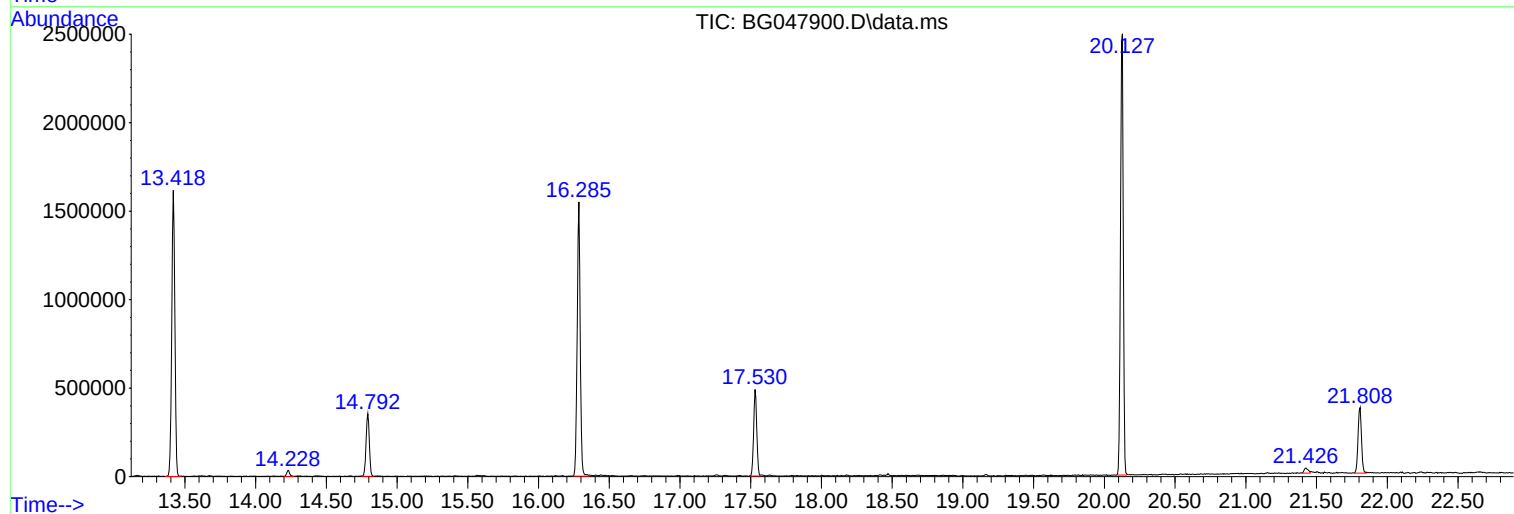
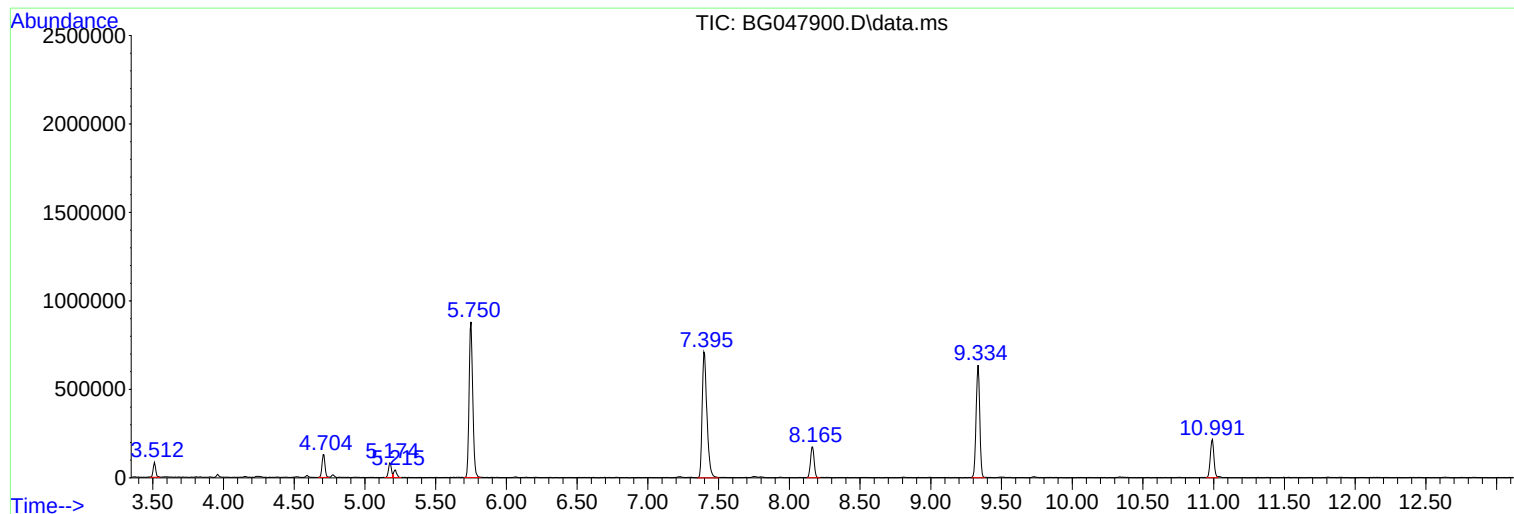
Sum of corrected areas: 16345410

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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



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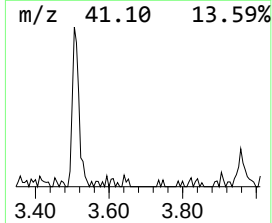
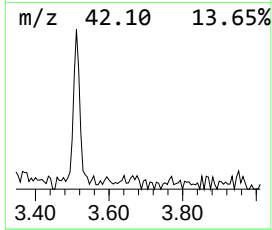
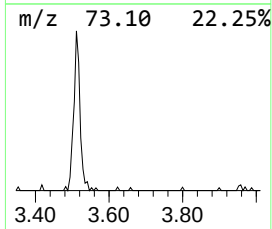
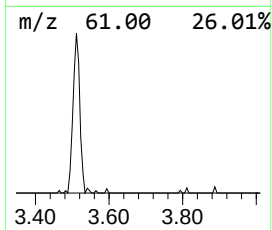
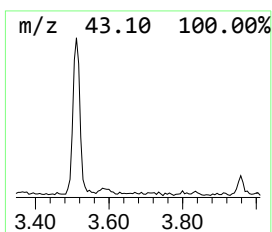
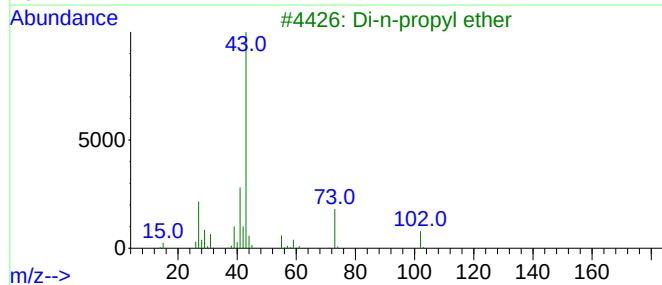
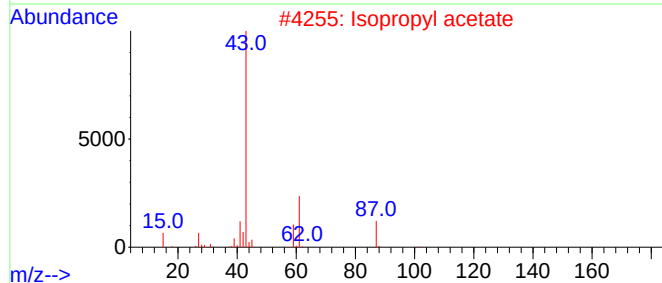
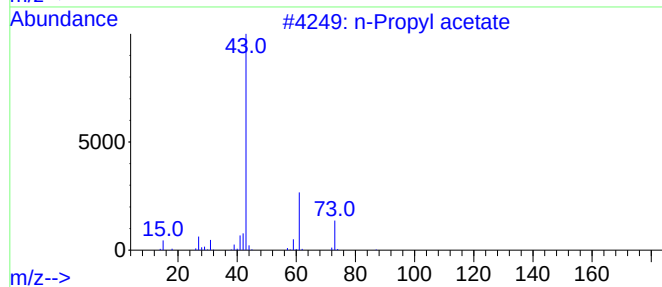
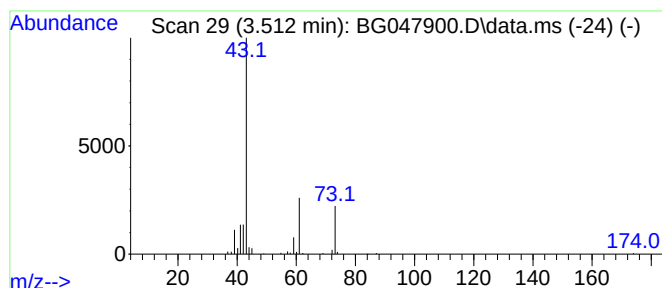
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.512 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.512	6.78 ng	105553	1,4-Dichlorobenzene-d4	8.159

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Propyl acetate	102	C5H10O2	000109-60-4	45
2			Isopropyl acetate	102	C5H10O2	000108-21-4	38
3			Di-n-propyl ether	102	C6H14O	000111-43-3	28
4			Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	28
5			Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	9



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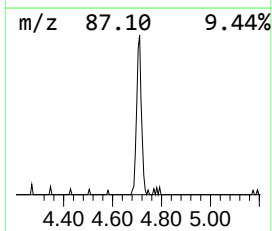
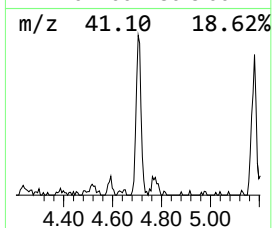
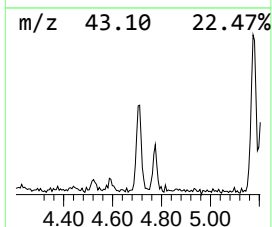
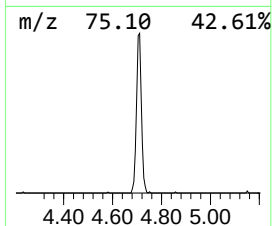
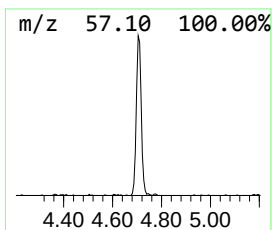
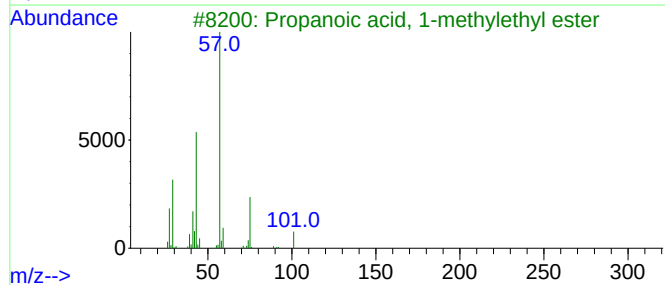
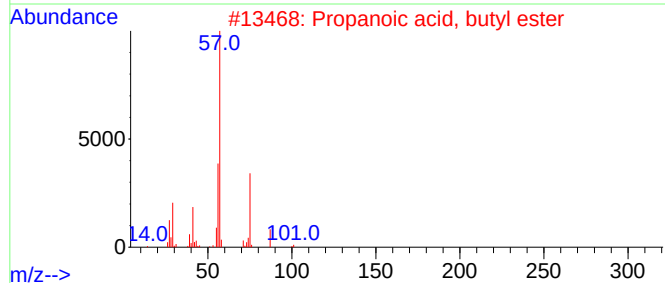
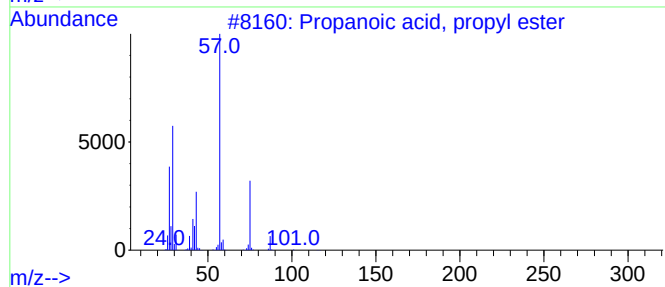
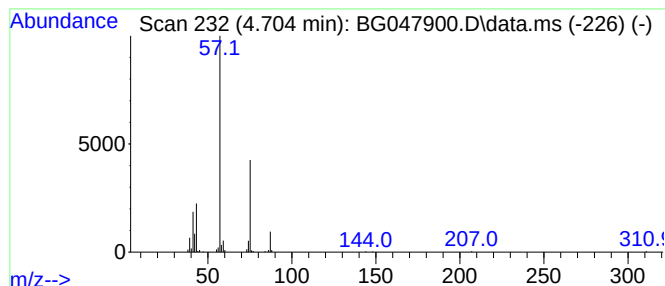
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.704	12.25 ng	190823	1,4-Dichlorobenzene-d4	8.159

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78
2			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	39
3			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	23
4			3-Pentanol, 3-(1,1-dimethylethyl...	200	C13H28O	041902-42-5	16
5			Isobutyl ether	130	C8H18O	000628-55-7	12



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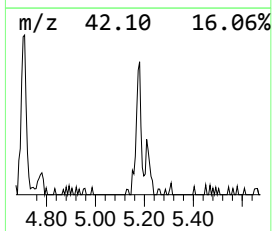
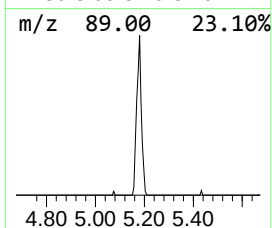
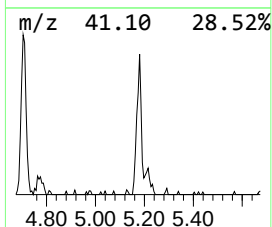
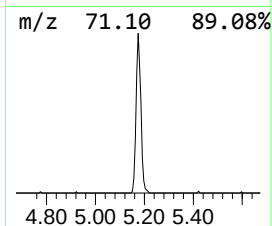
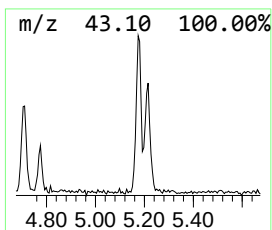
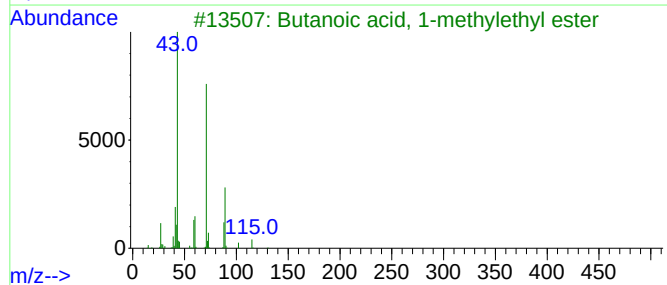
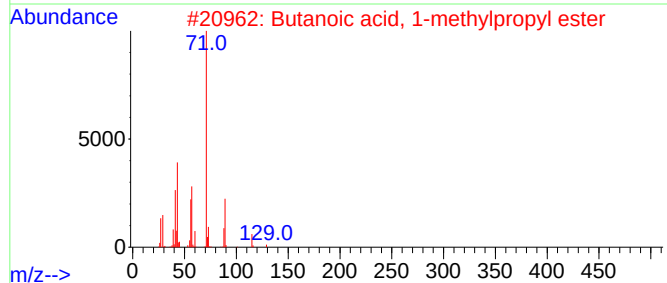
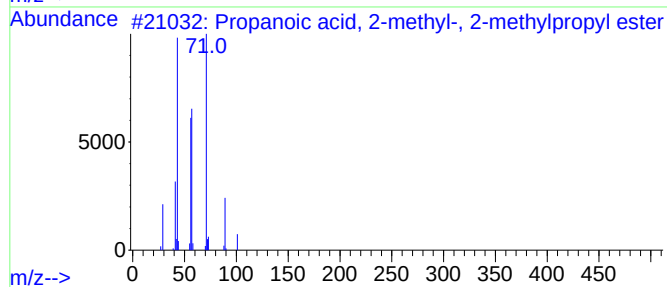
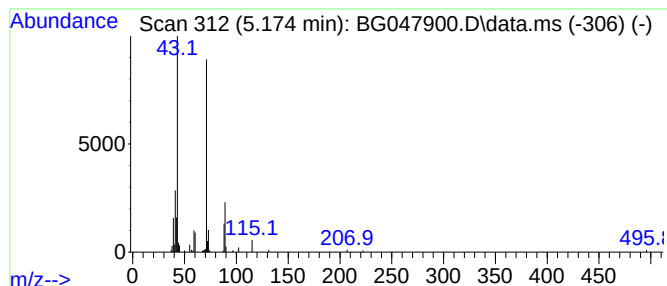
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Peak Number 3 Propanoic acid, 2-methyl-, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.174	7.95 ng	123731	1,4-Dichlorobenzene-d4	8.159

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	64
2			Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	56
3			Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	56
4			Butanoic acid, anhydride	158	C8H14O3	000106-31-0	53
5			Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	50



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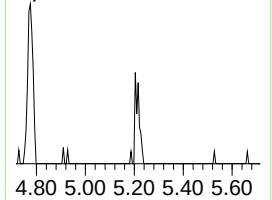
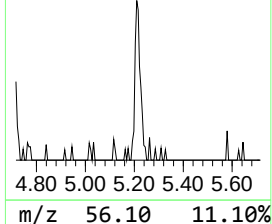
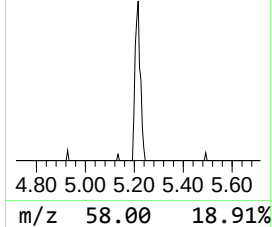
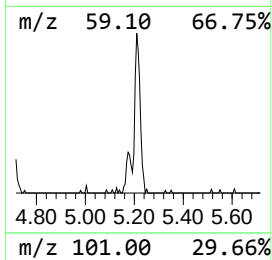
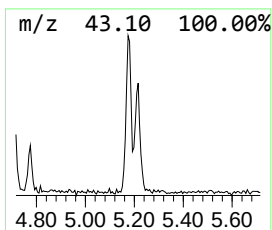
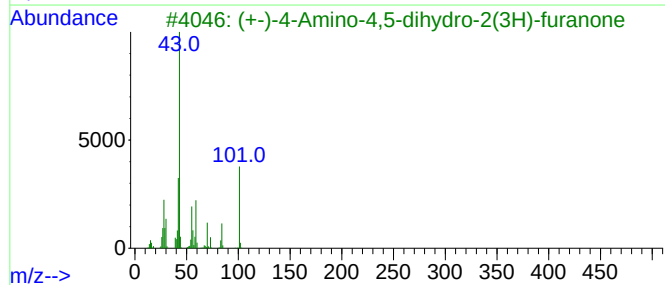
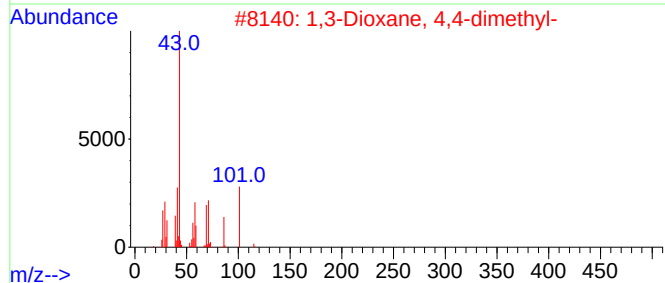
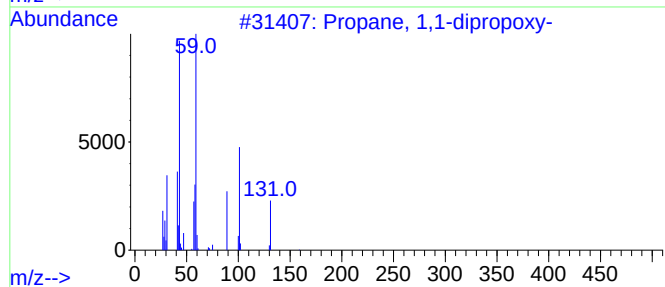
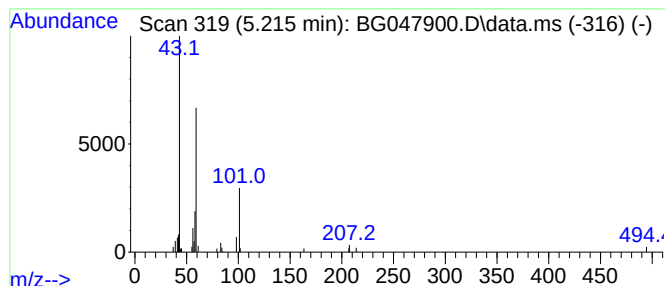
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Peak Number 4 unknown5.215 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.215	3.95 ng	61483	1,4-Dichlorobenzene-d4	8.159

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	33
2			1,3-Dioxane, 4,4-dimethyl-	116	C6H12O2	000766-15-4	28
3			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	25
4			1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	23
5			Guanidine	59	CH5N3	000113-00-8	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Propanoic acid,...	4.704	12.3	ng	190823	1	8.159	311422	20.0
Propanoic acid,...	5.174	8.0	ng	123731	1	8.159	311422	20.0
unknown5.215	5.215	4.0	ng	61483	1	8.159	311422	20.0