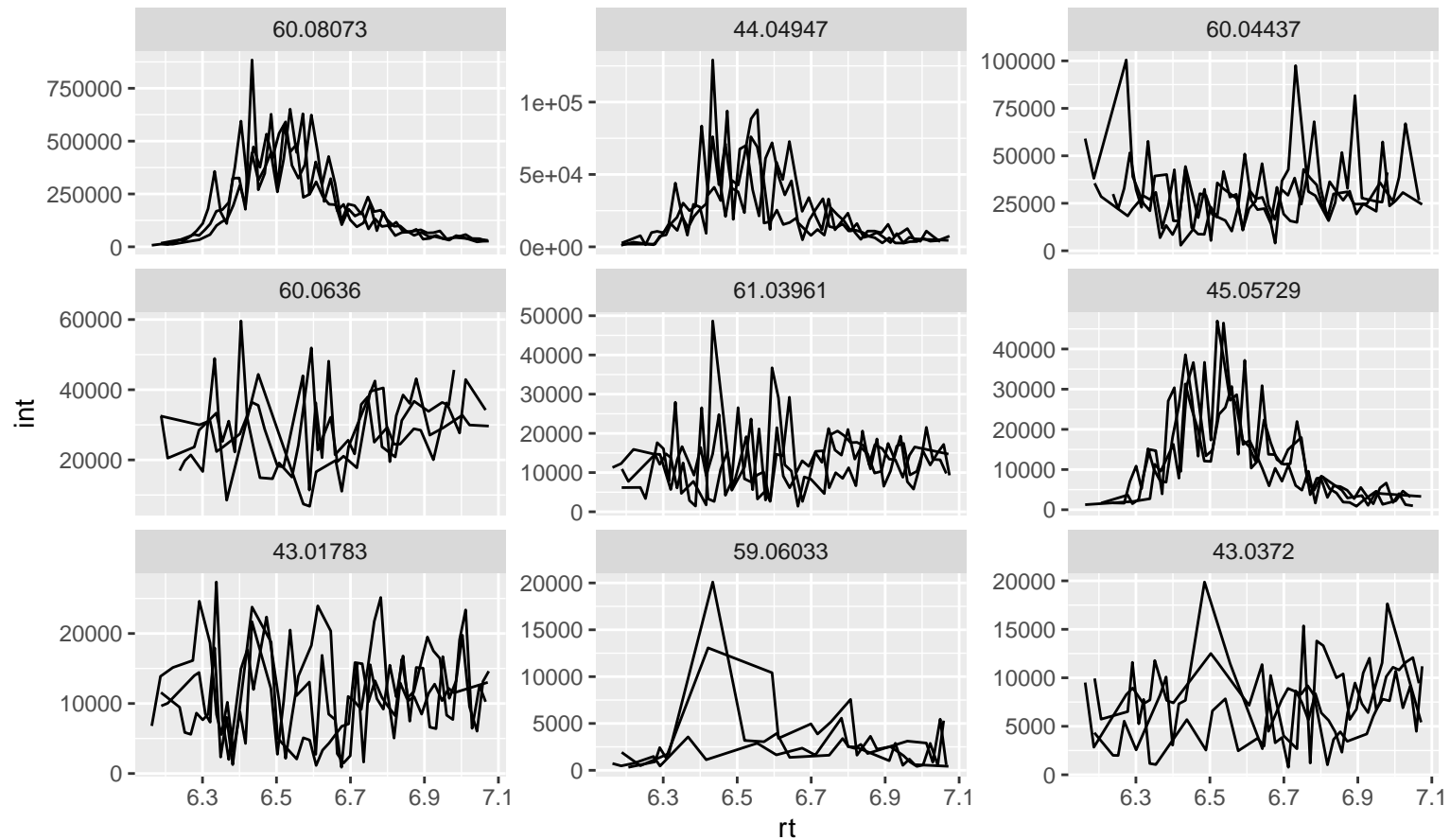
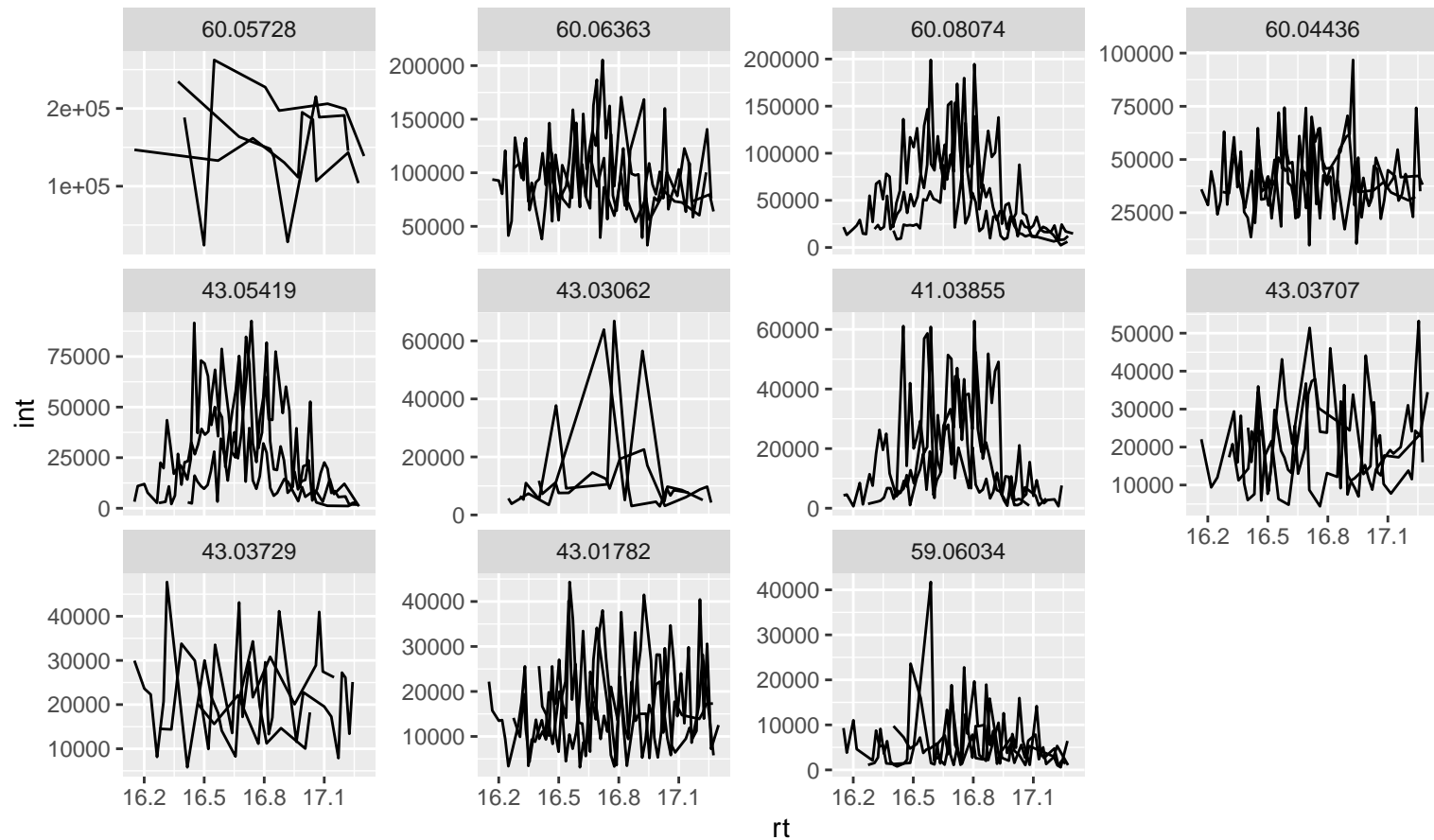


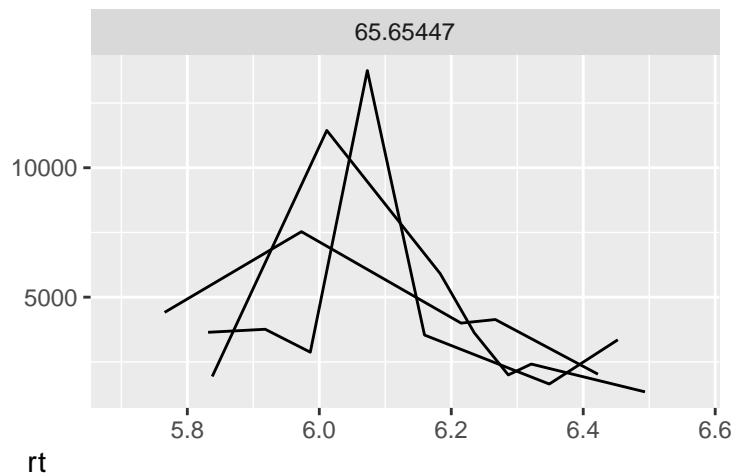
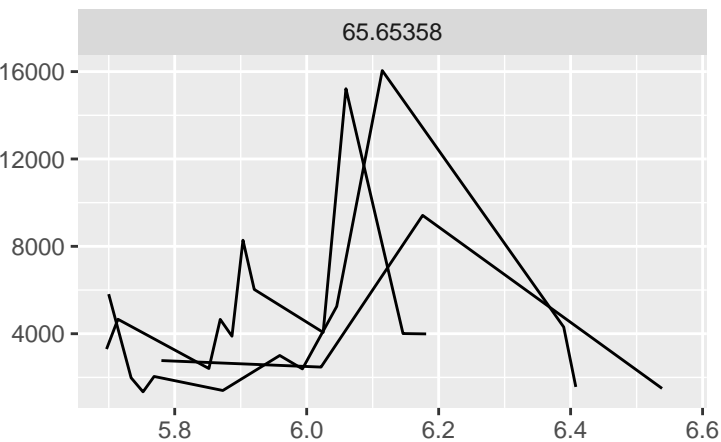
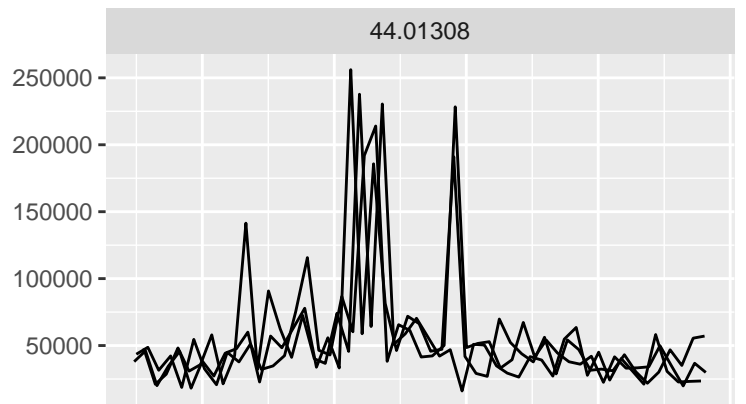
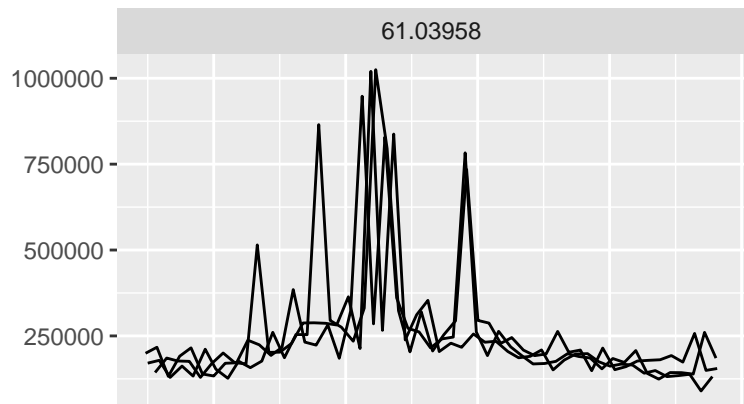
Trimethylamine (pos) 60.080775



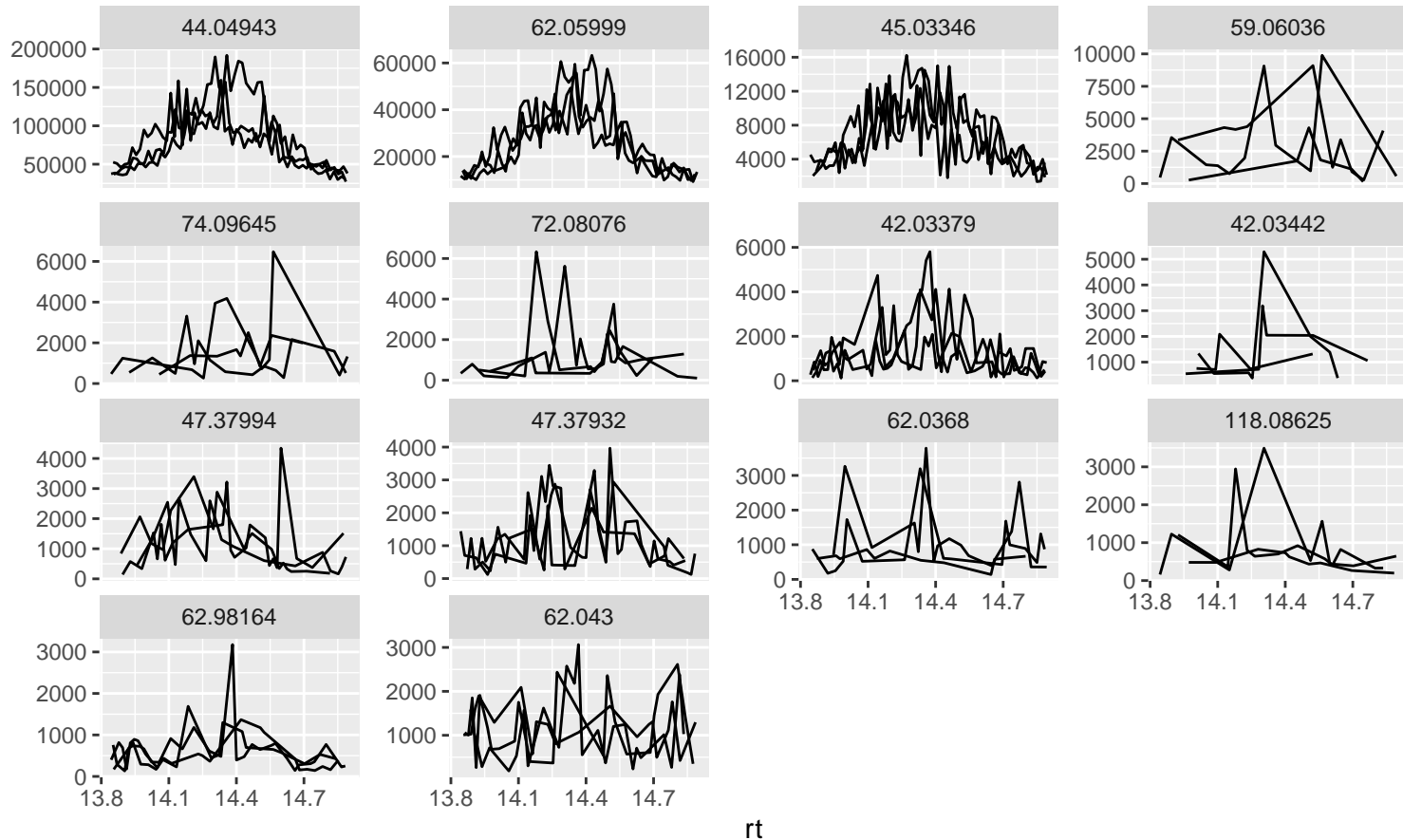
Propylamine (pos) 60.080775



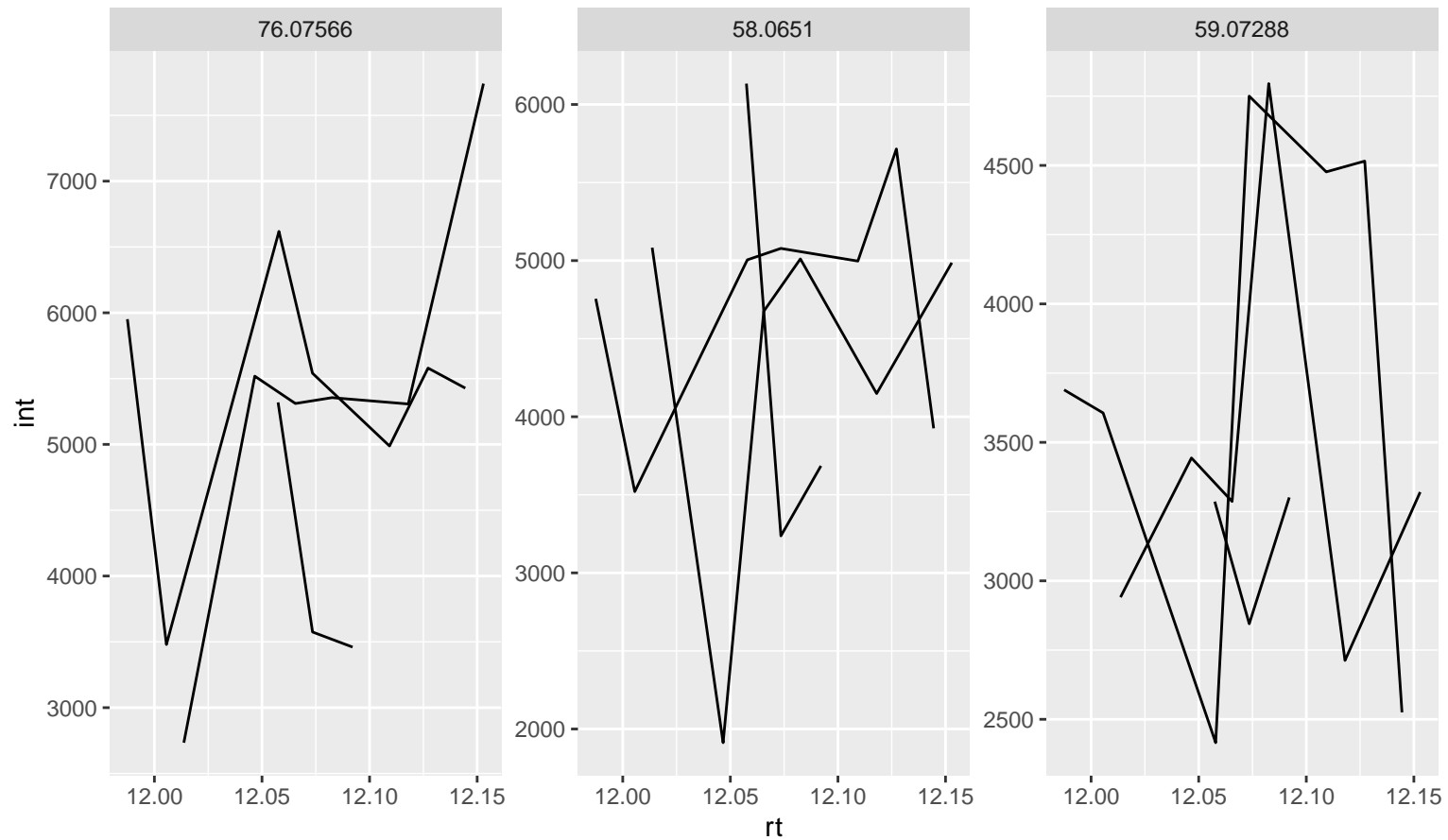
Urea (pos) 61.039639



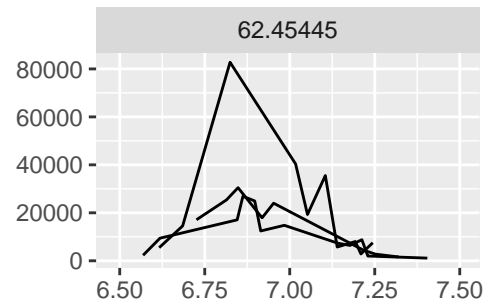
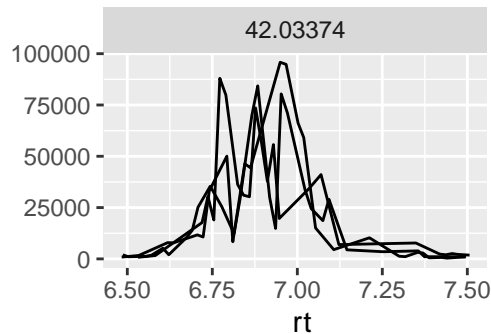
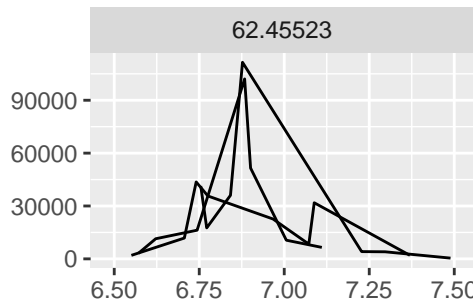
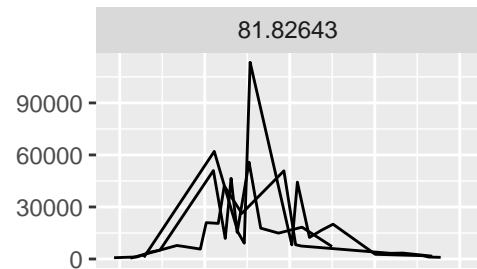
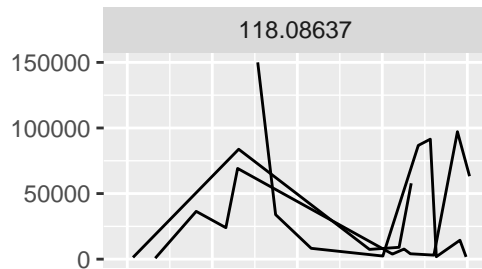
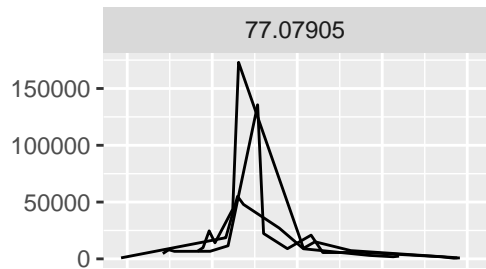
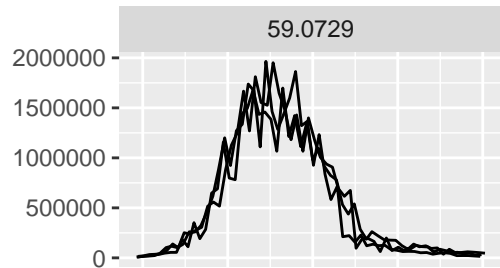
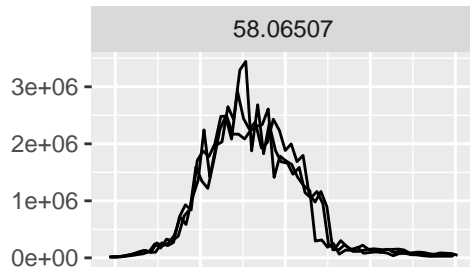
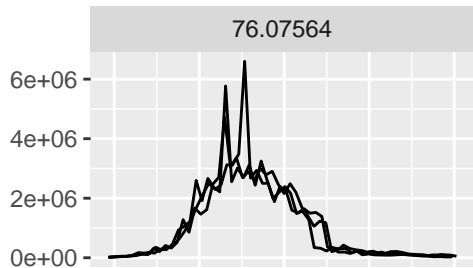
Ethanolamine (pos) 62.06004



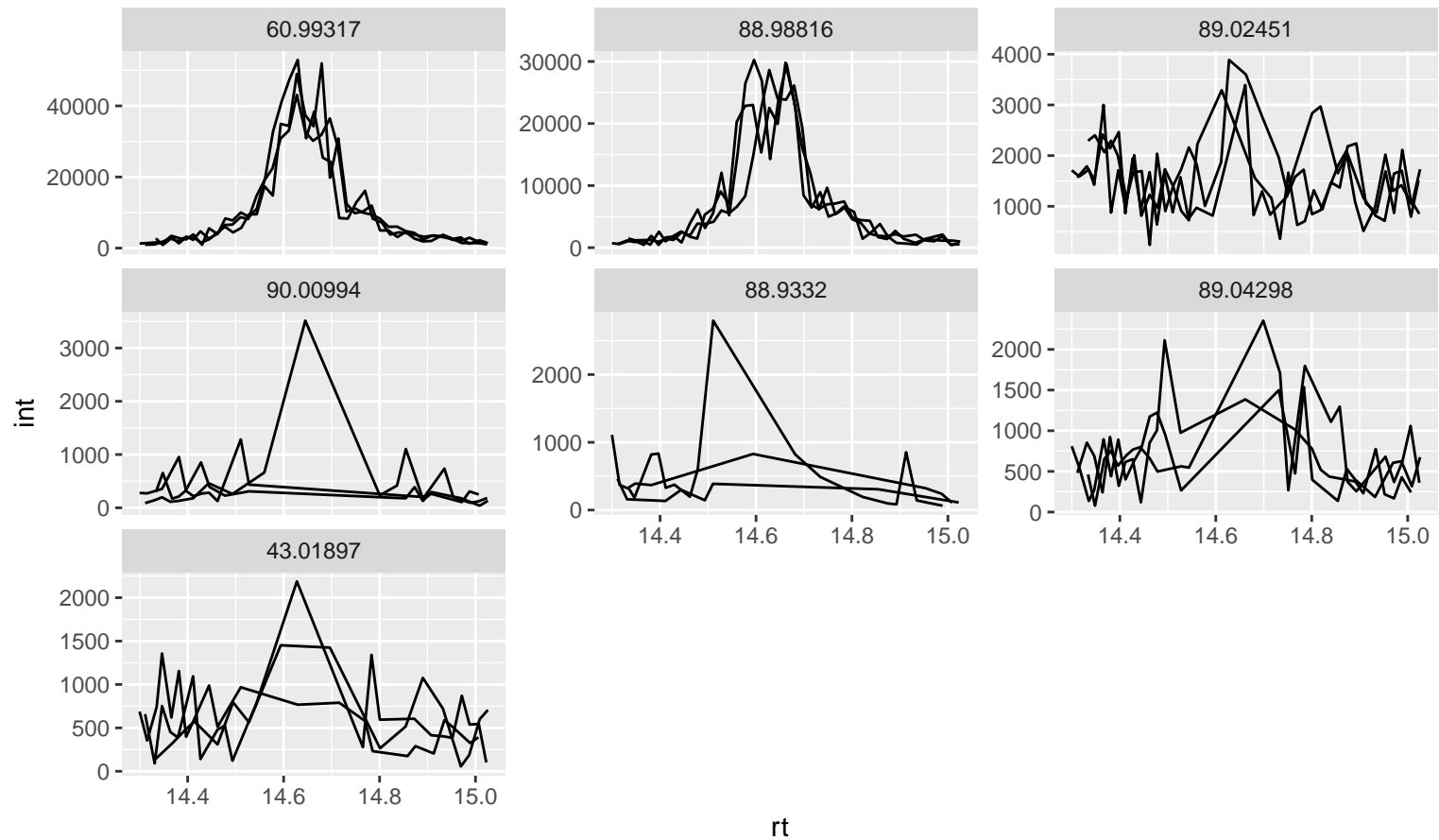
Glycine (pos) 76.039305



Trimethylamine N-oxide (pos) 76.07569

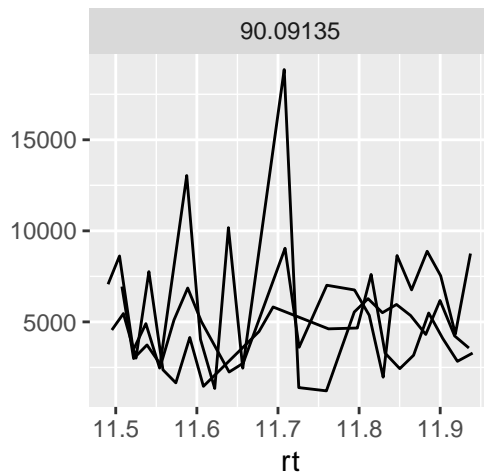
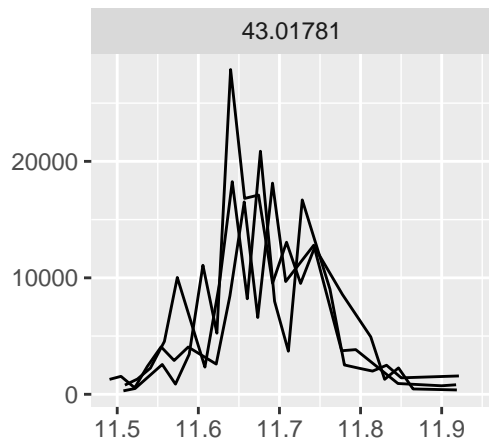
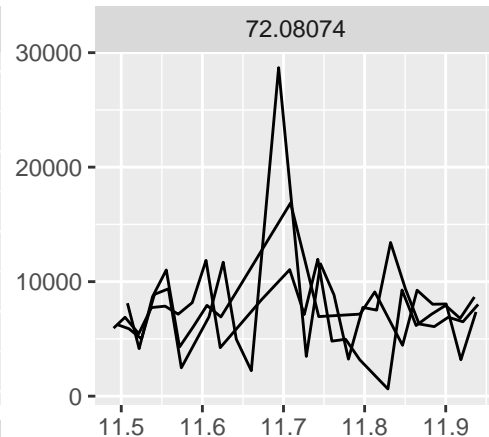
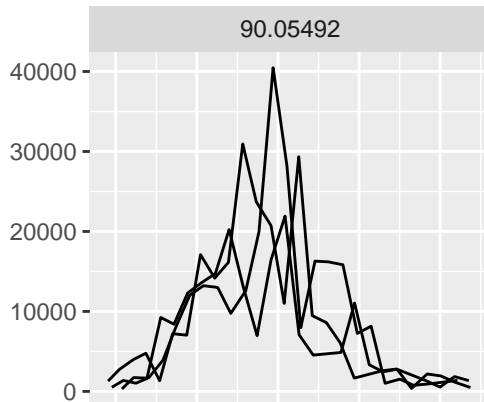
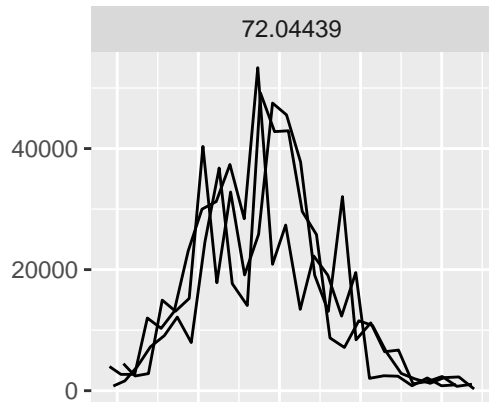


Oxalic acid (neg) 88.988034



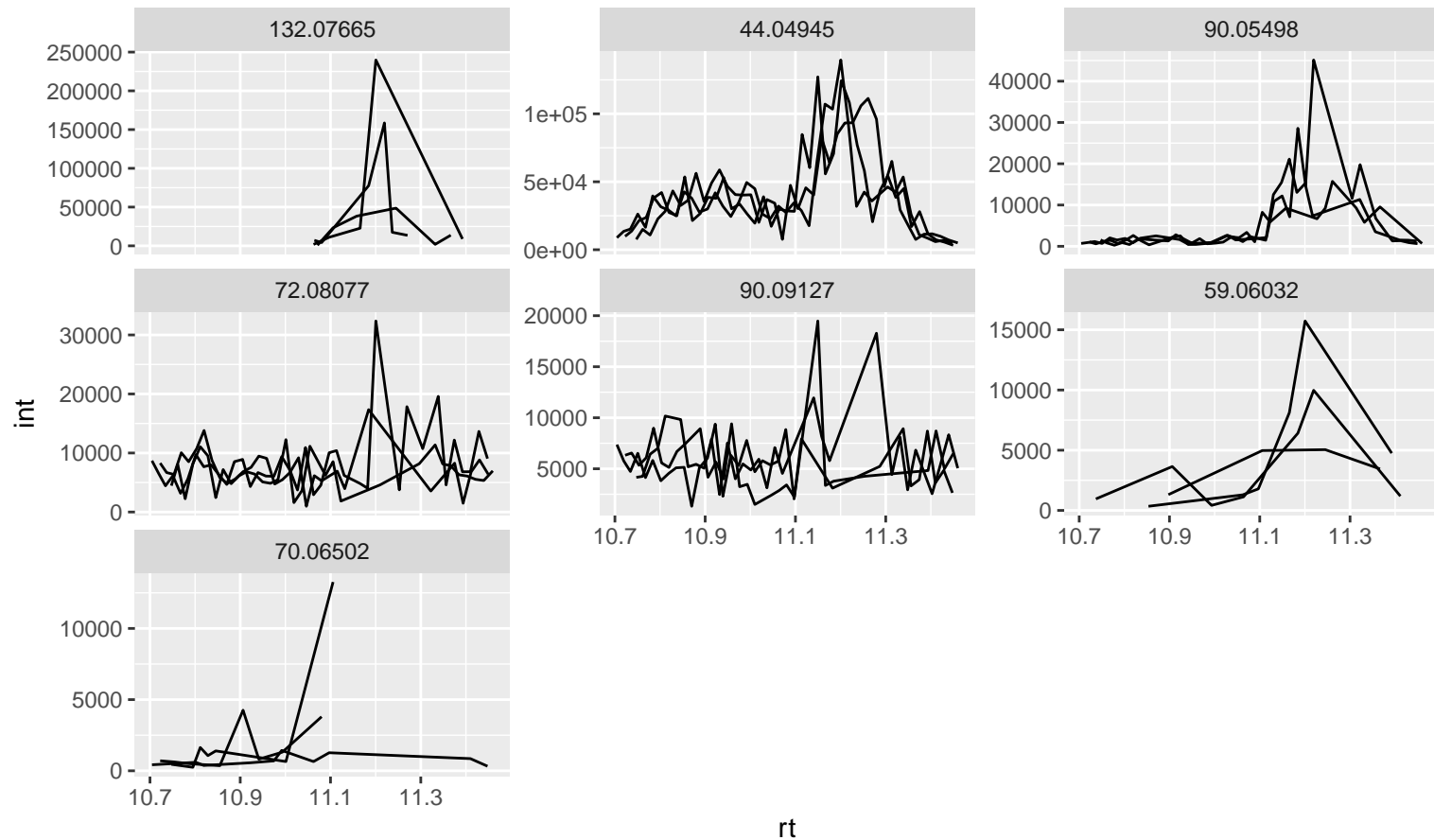
beta-Alanine (pos) 90.054955

int

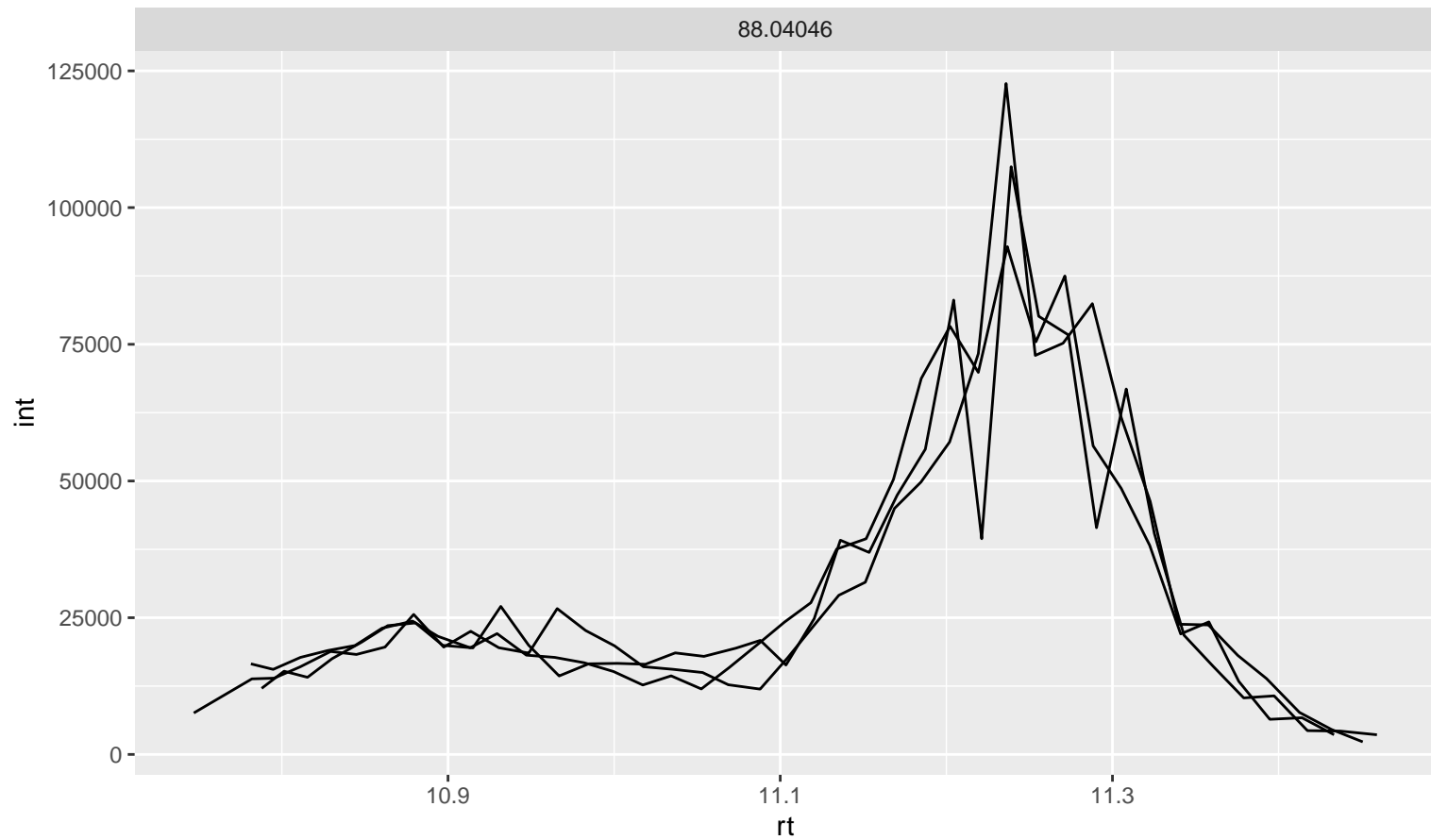


rt

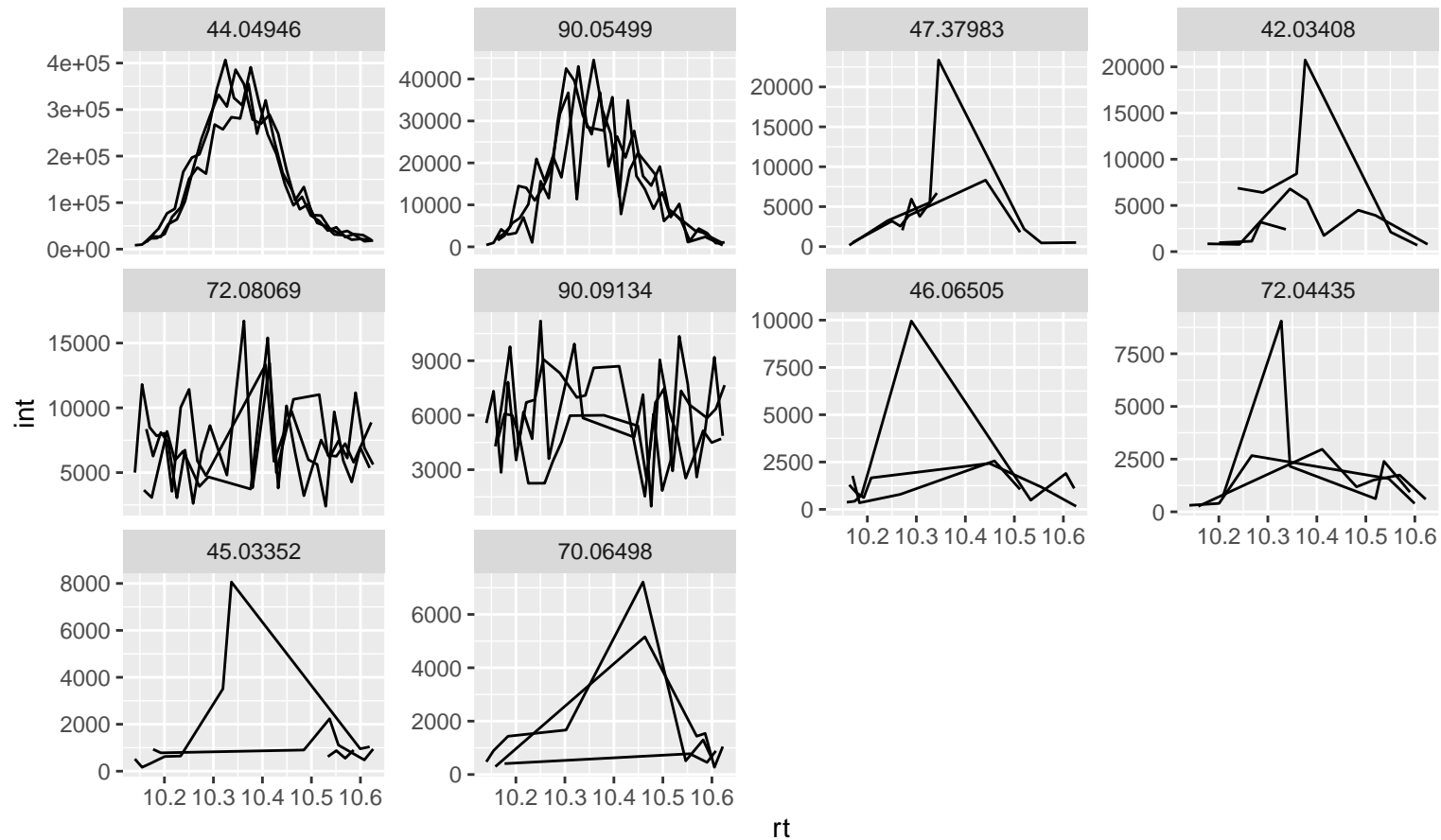
L-Alanine (pos) 90.054955



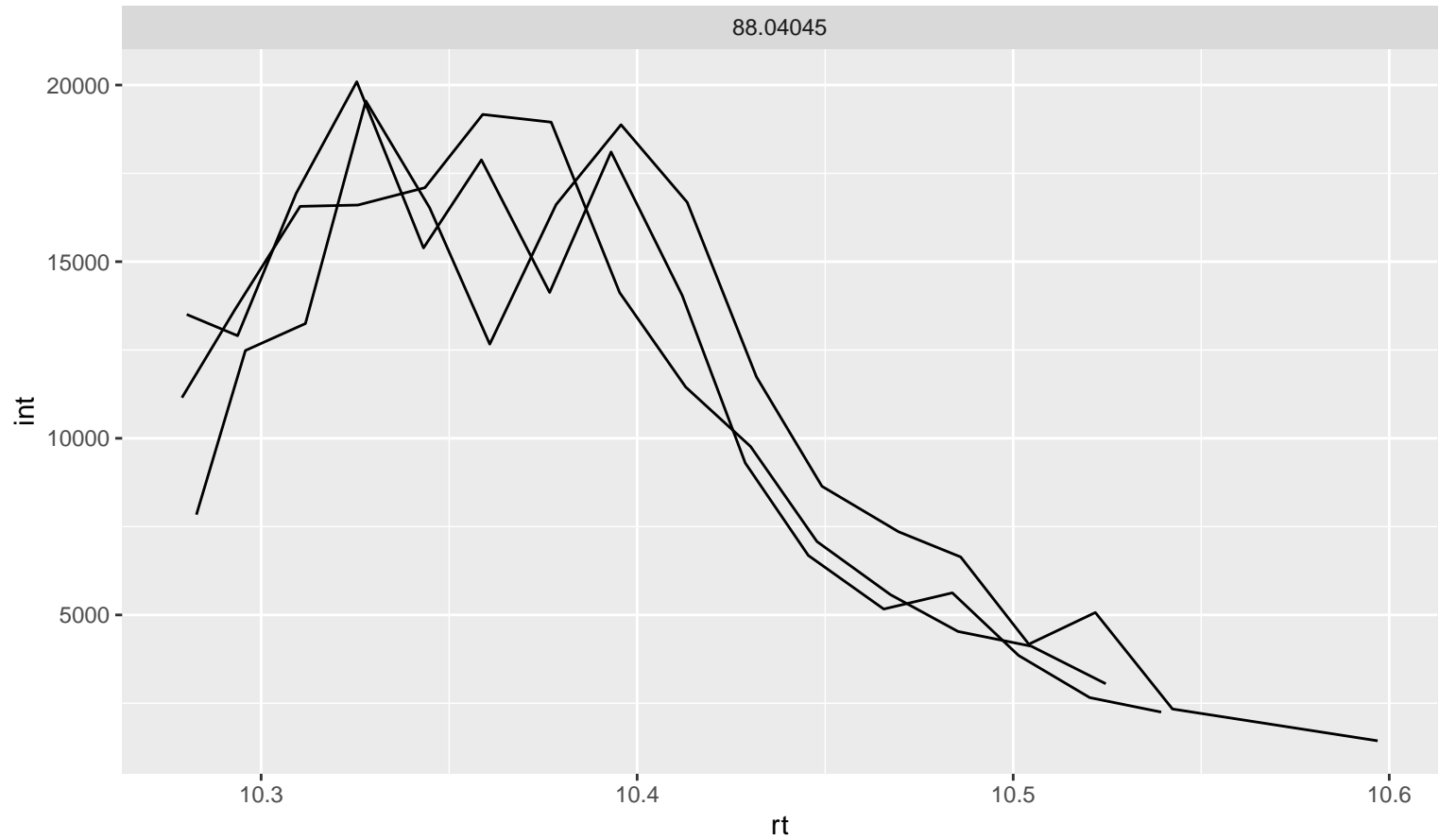
L-Alanine (neg) 88.040403



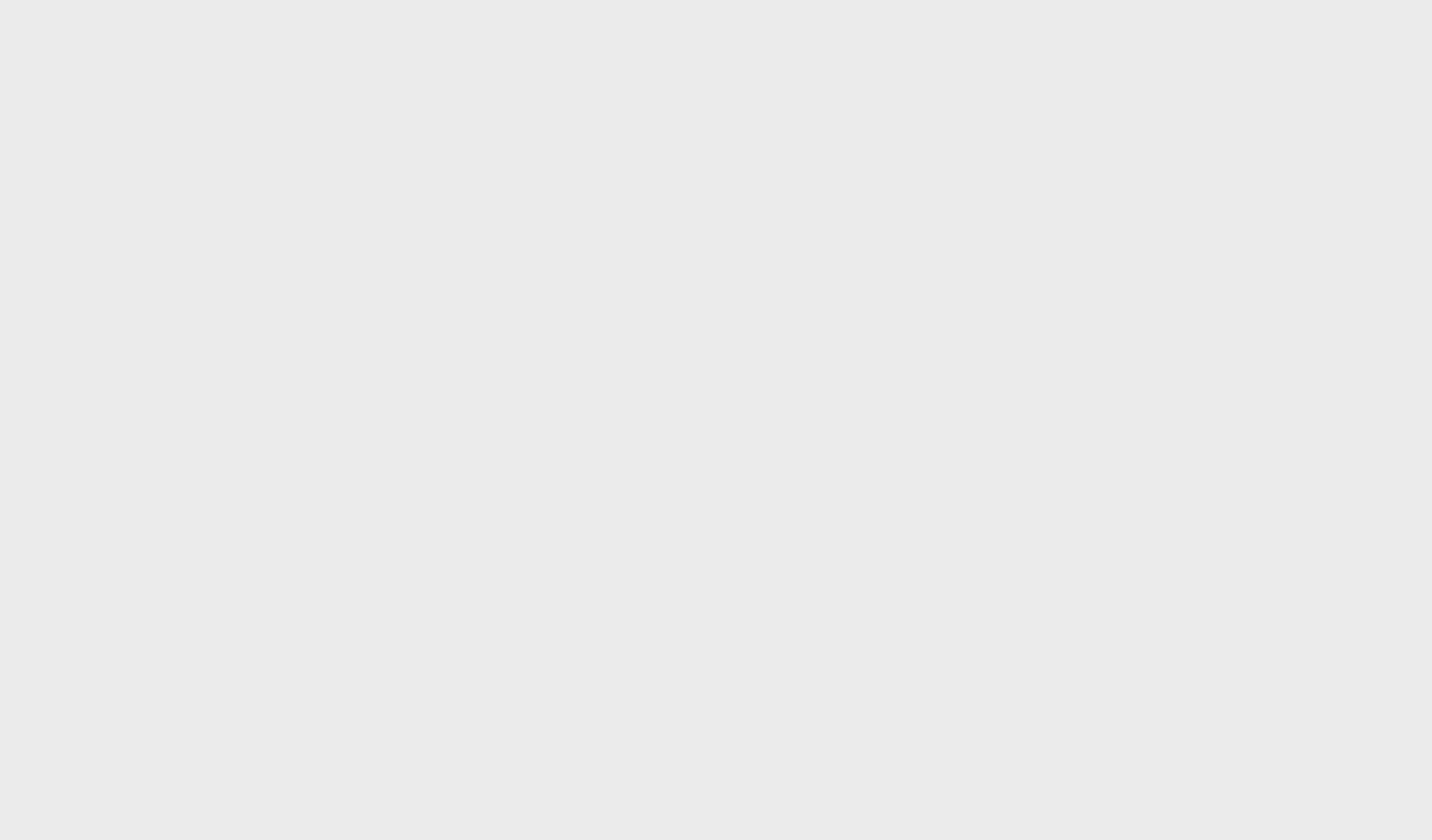
Sarcosine (pos) 90.054955



Sarcosine (neg) 88.040403

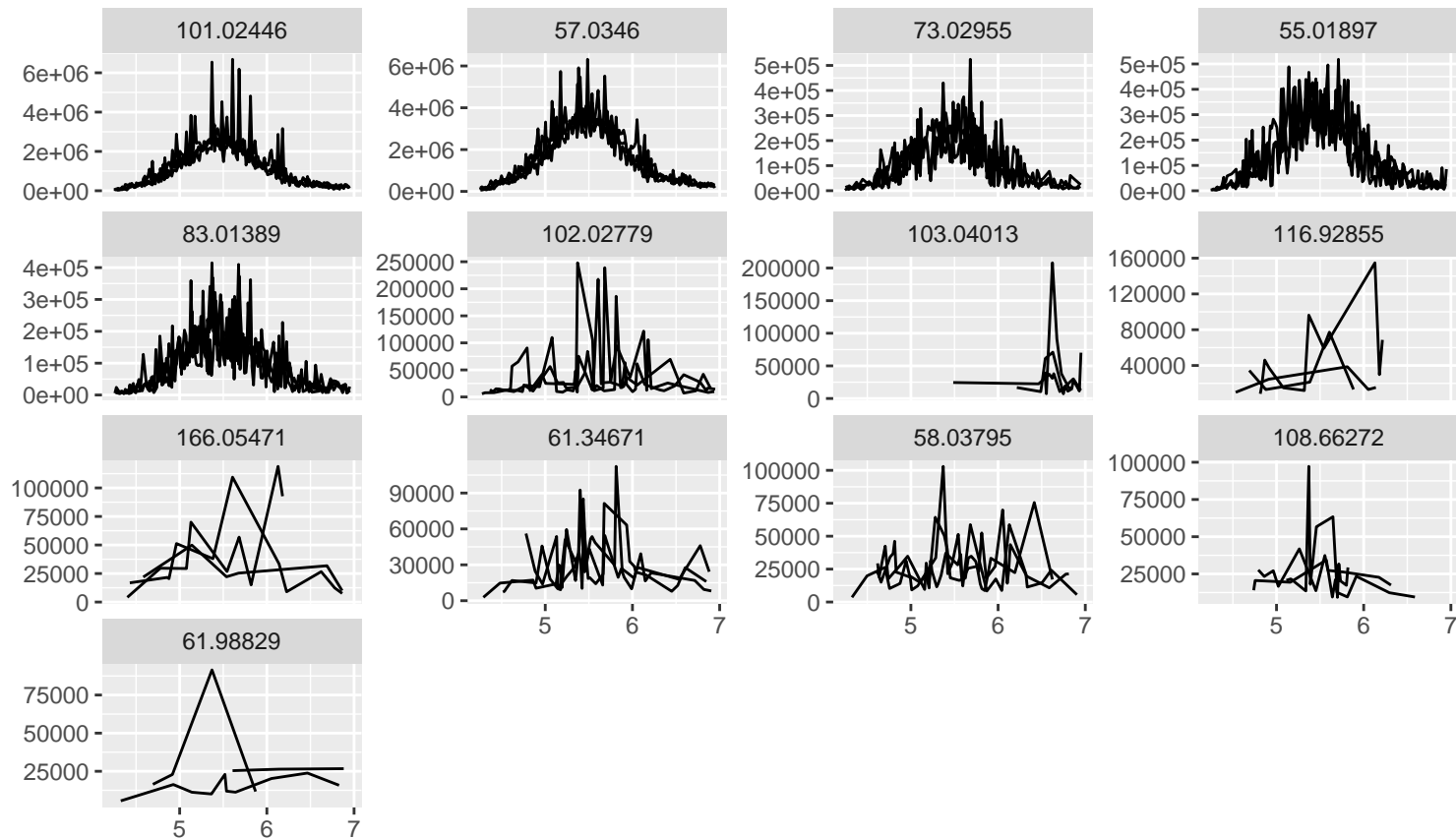


Methylphosphonic acid (pos) 97.004909



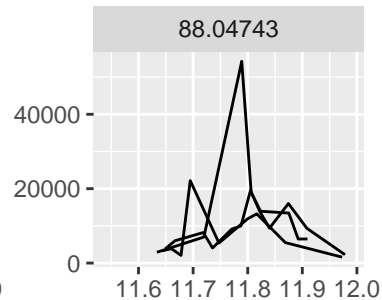
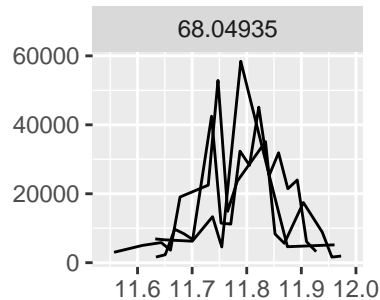
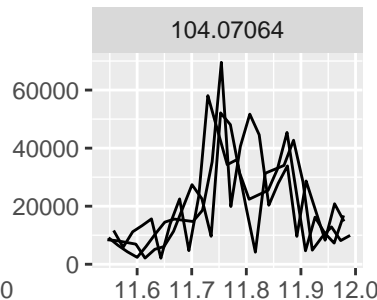
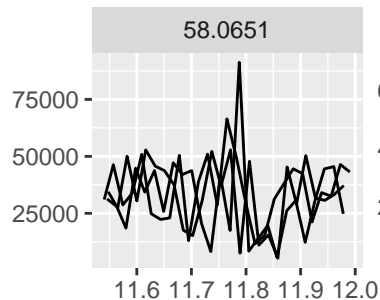
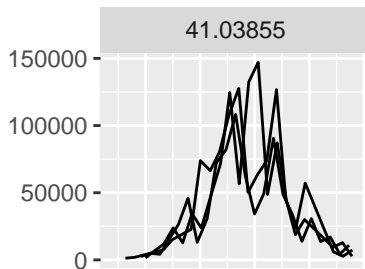
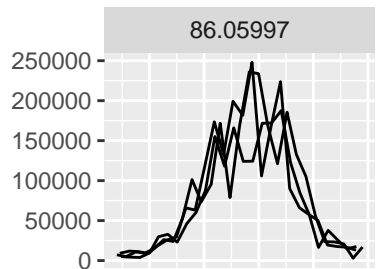
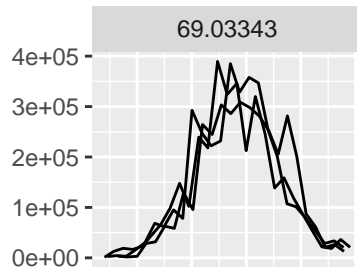
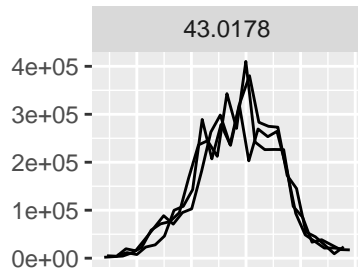
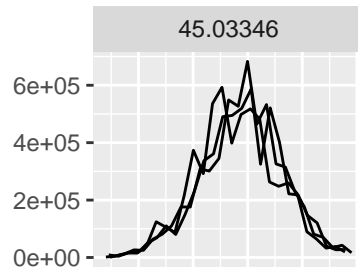
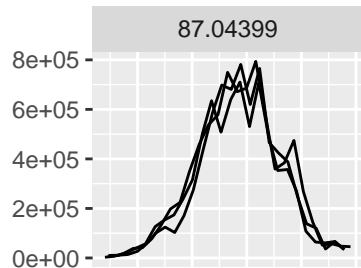
Succinic semialdehyde (neg) 101.024419

int



rt

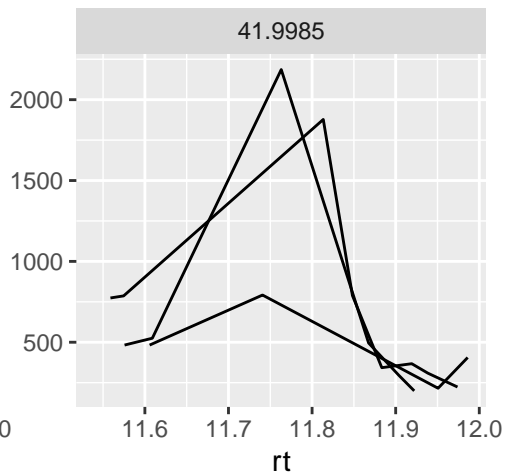
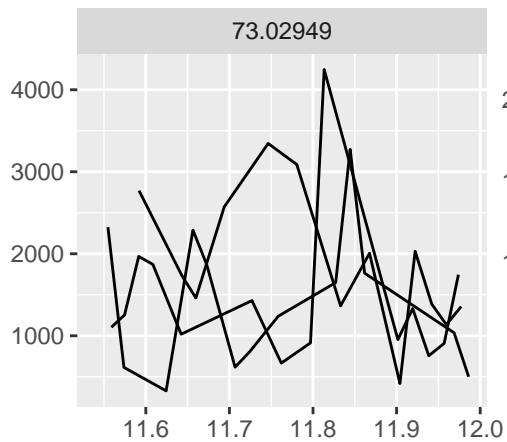
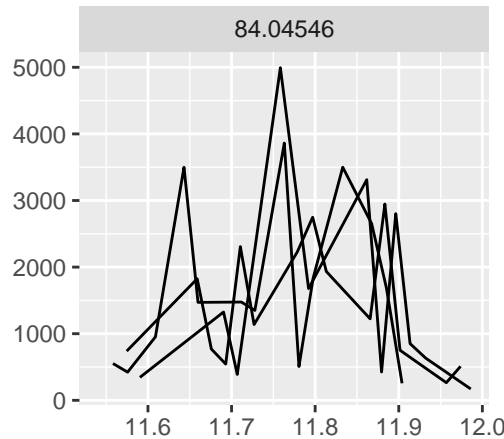
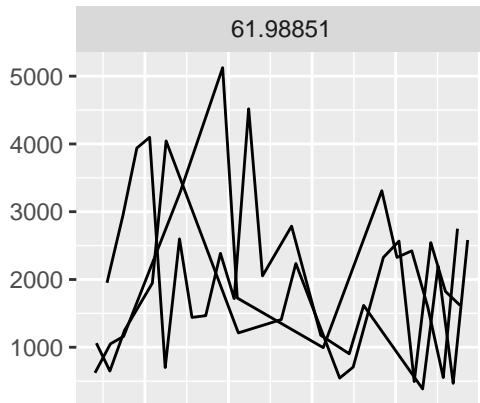
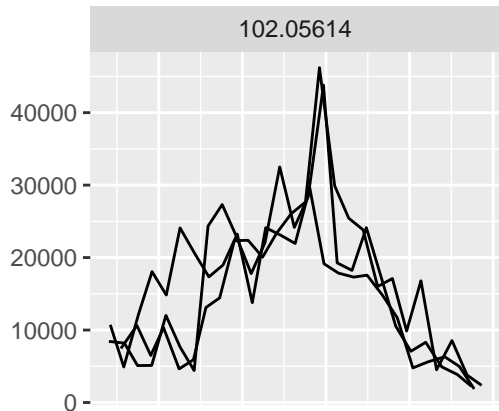
4-Aminobutyric acid (pos) 104.070605



rt

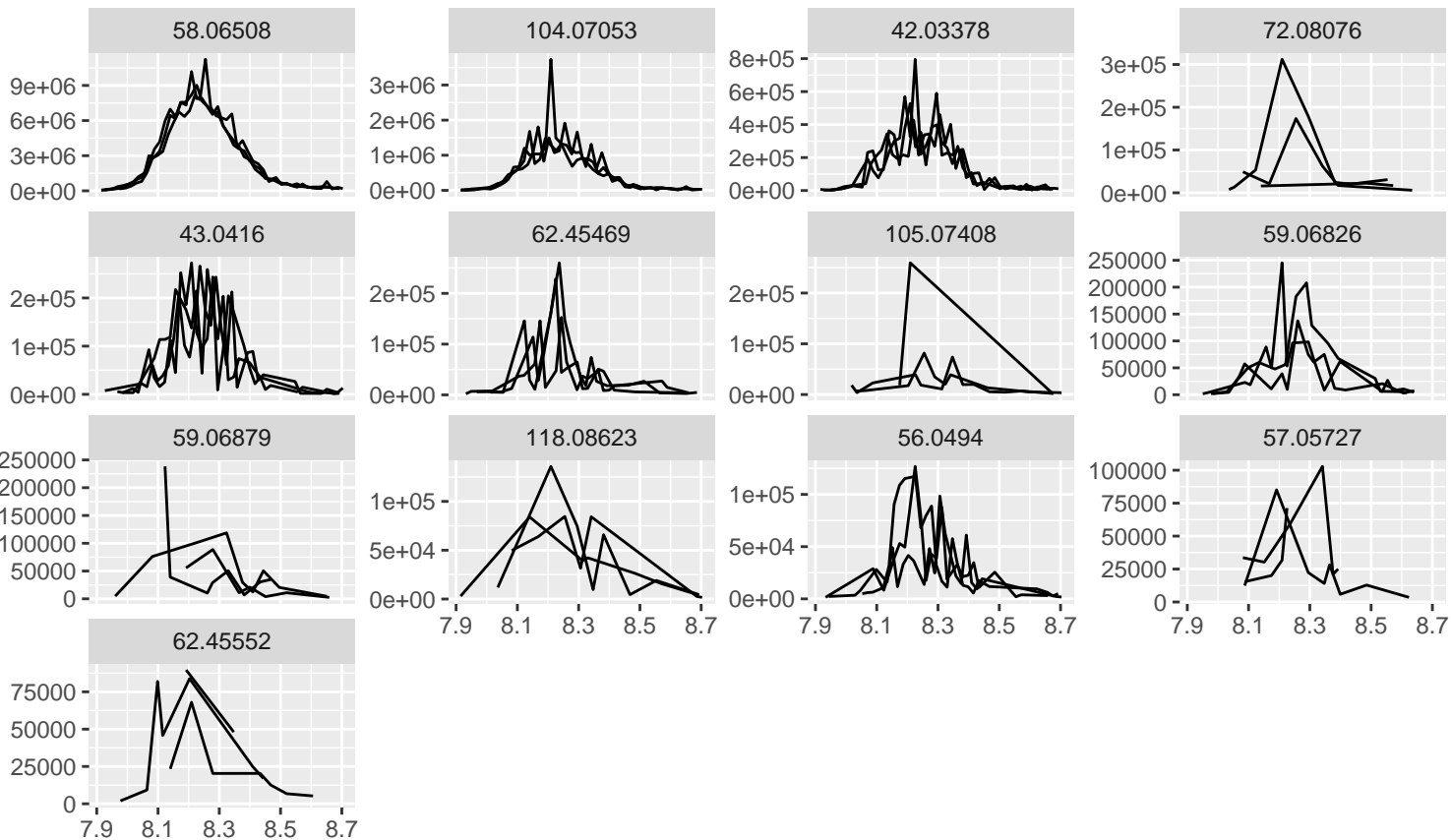
4-Aminobutyric acid (neg) 102.056053

int



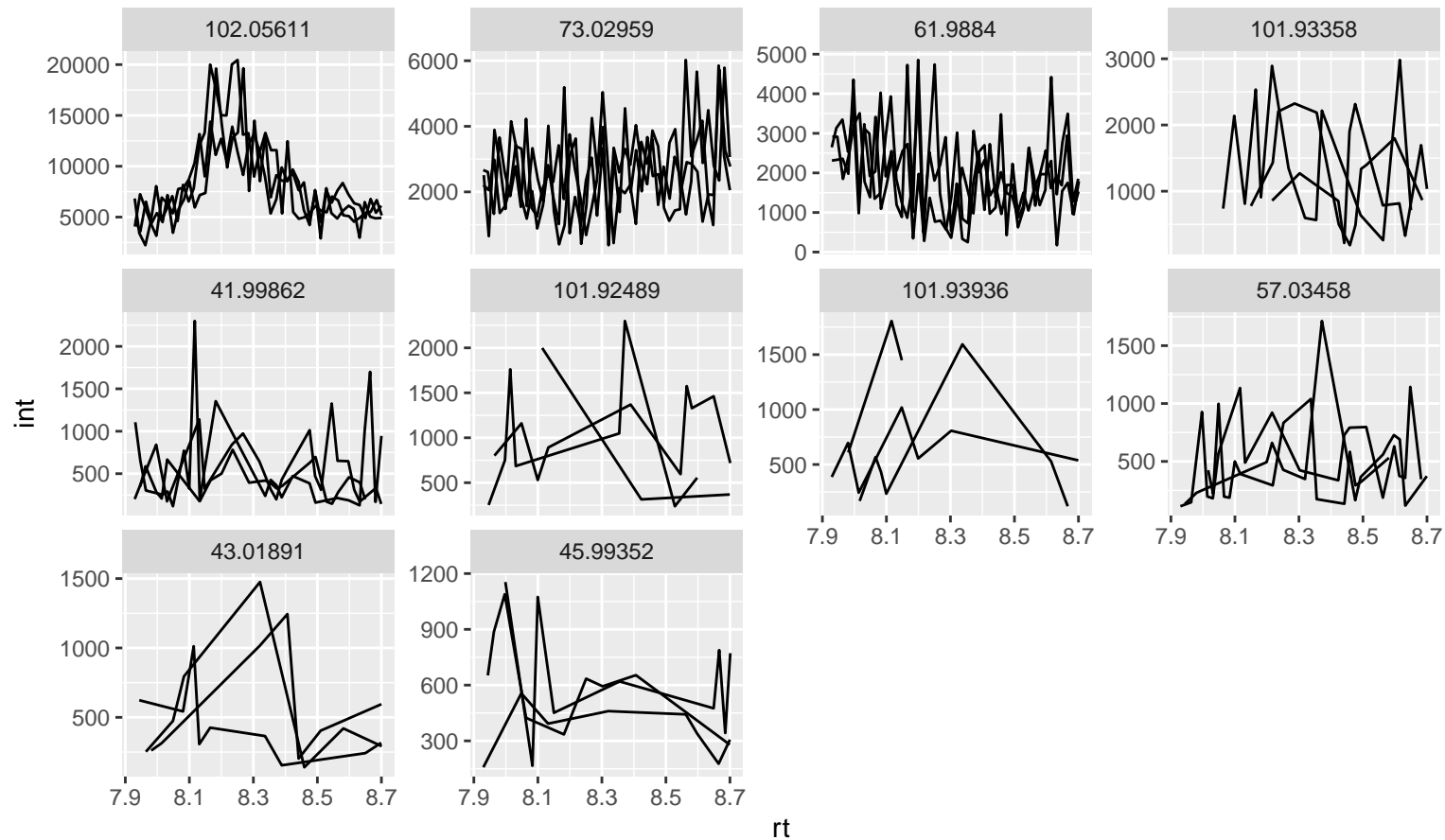
Dimethylglycine (pos) 104.070605

int



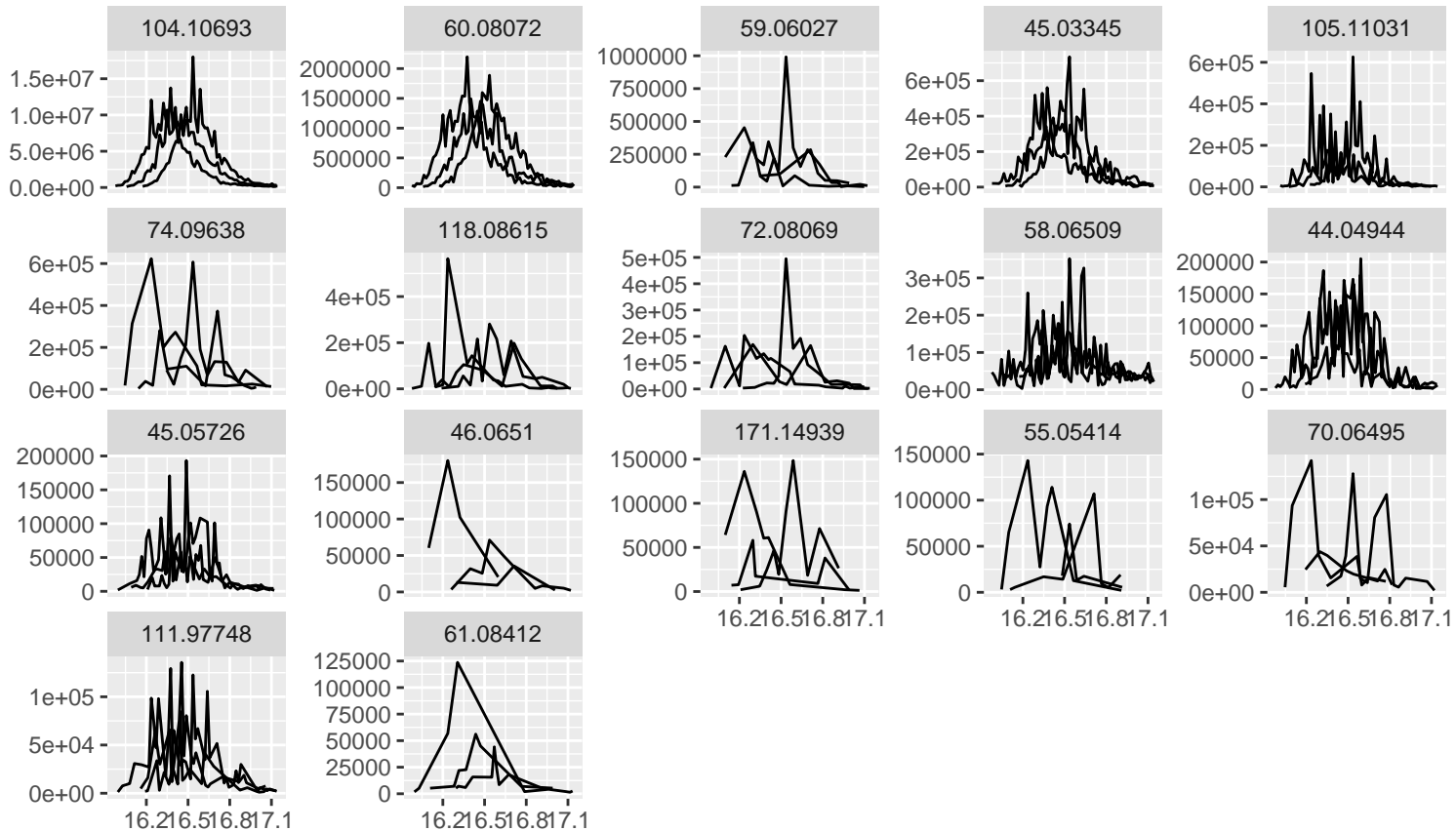
rt

Dimethylglycine (neg) 102.056053



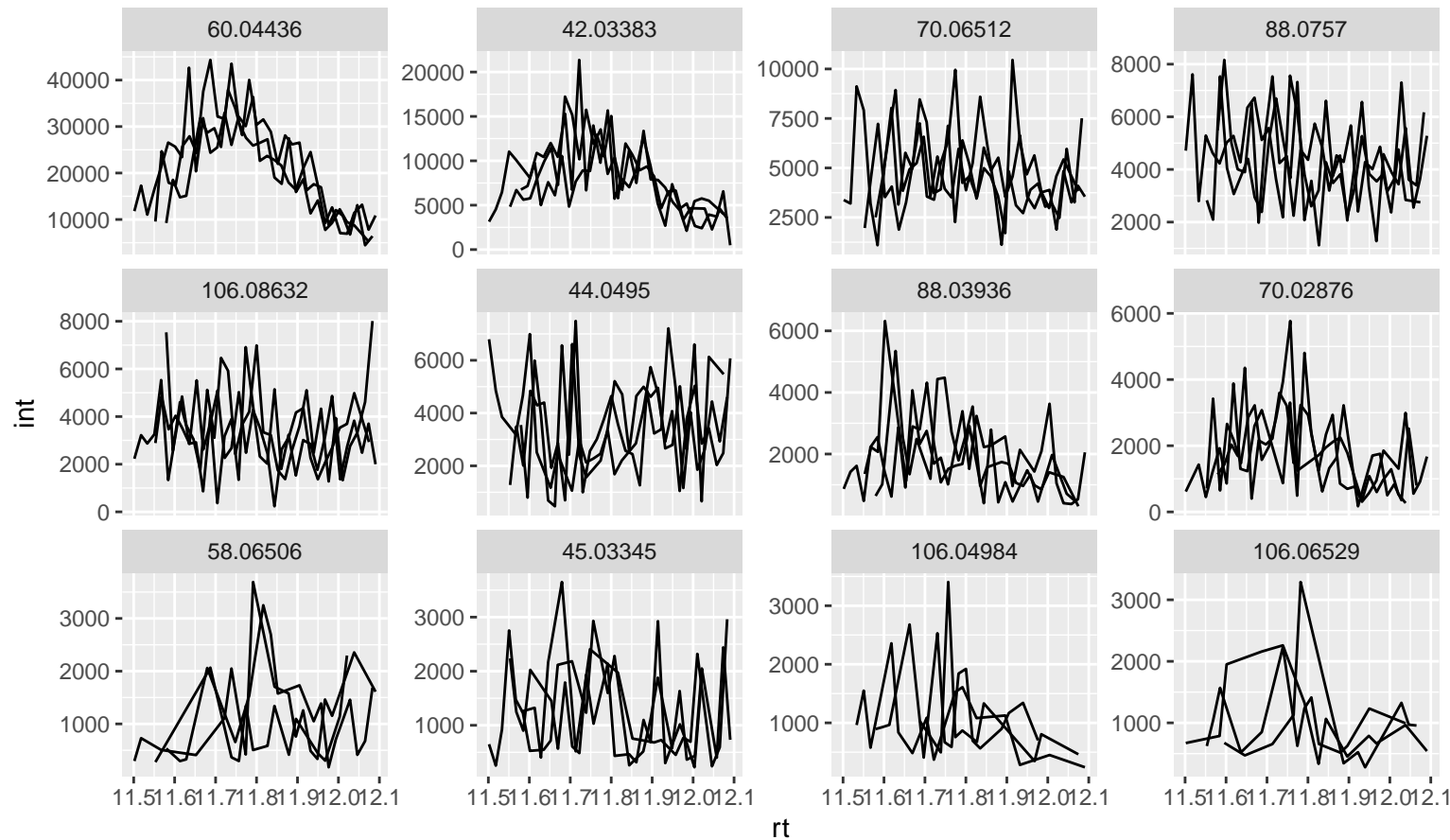
Choline (pos) 104.1069042

int

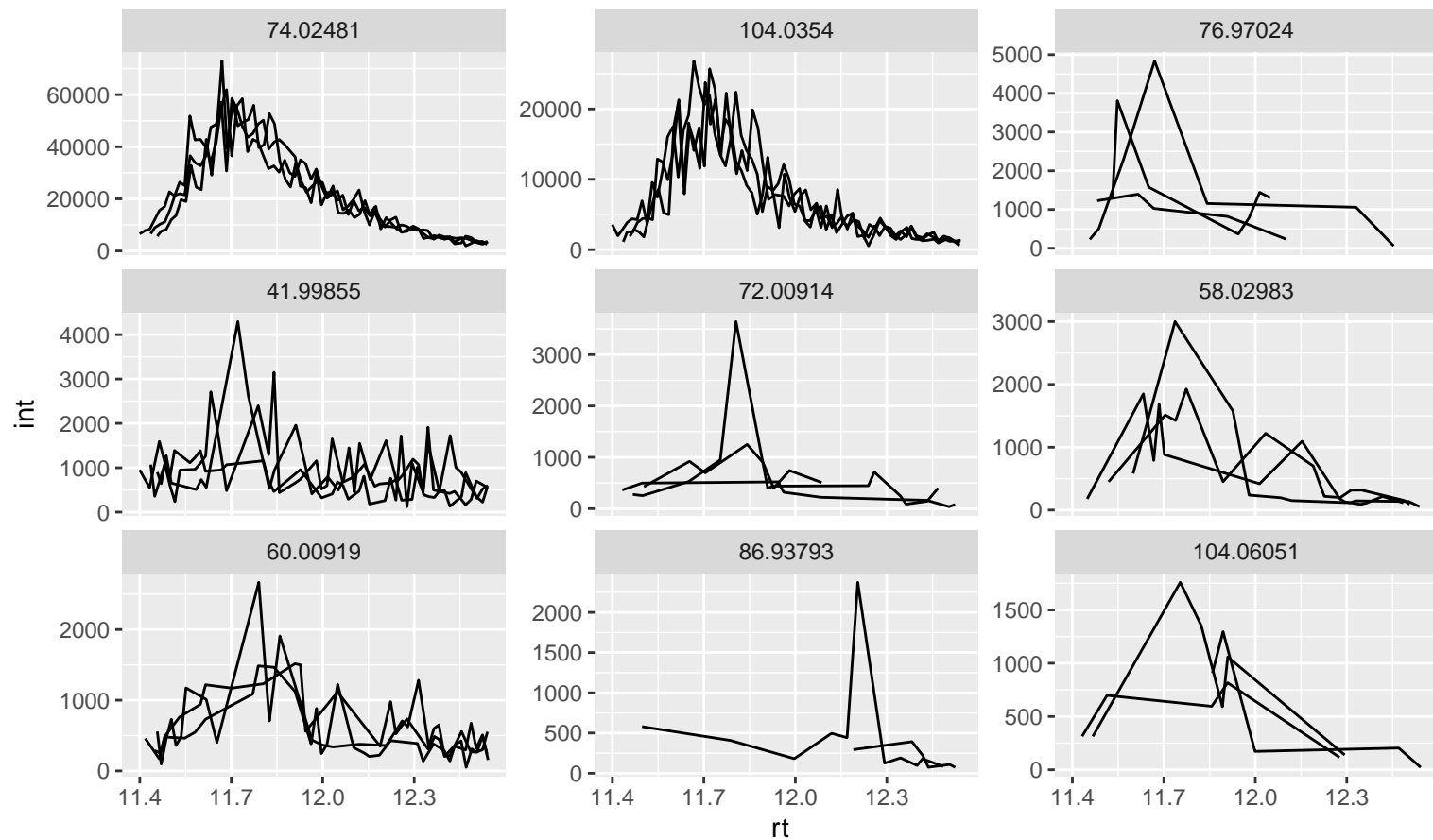


rt

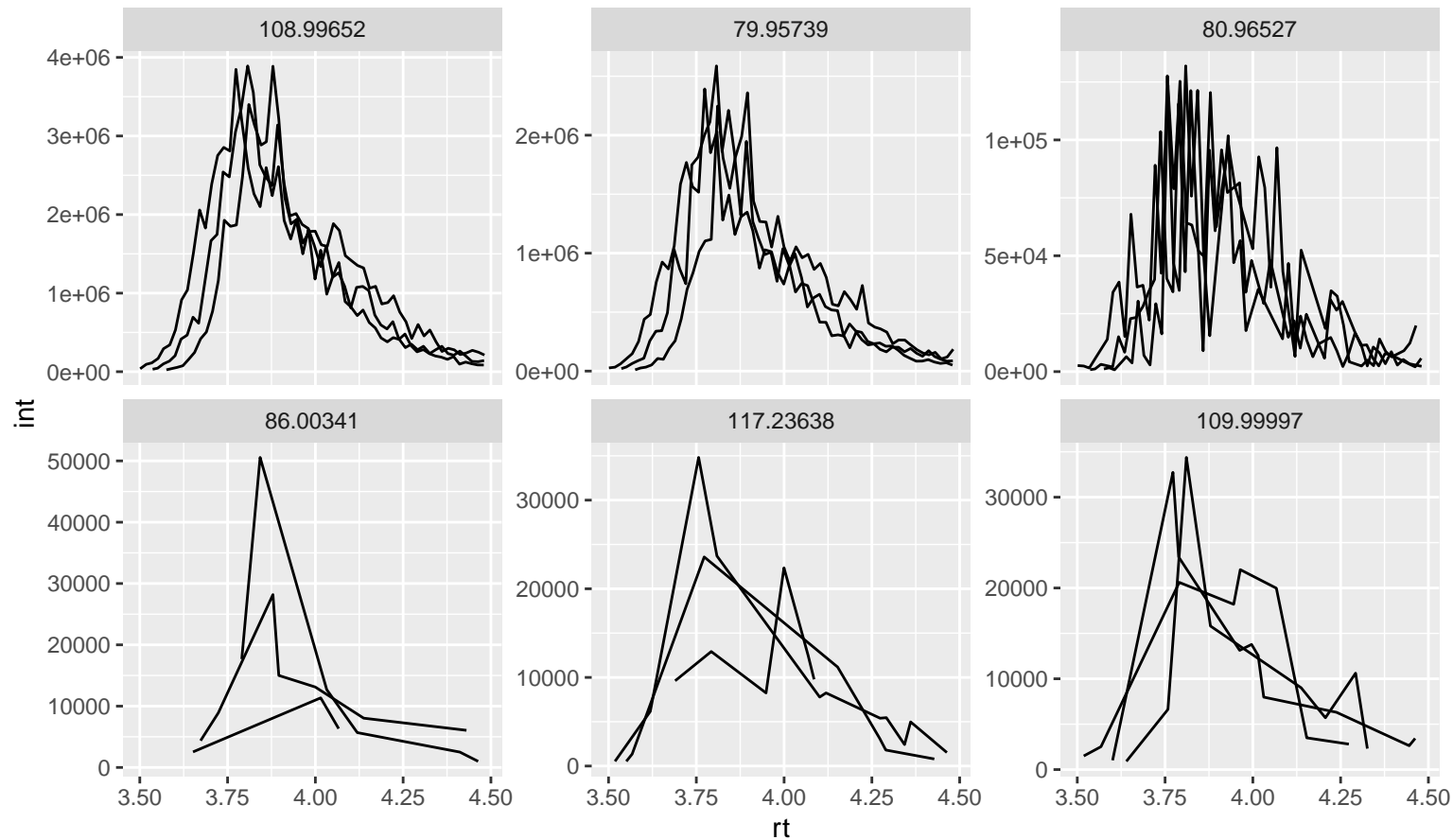
L-Serine (pos) 106.04987



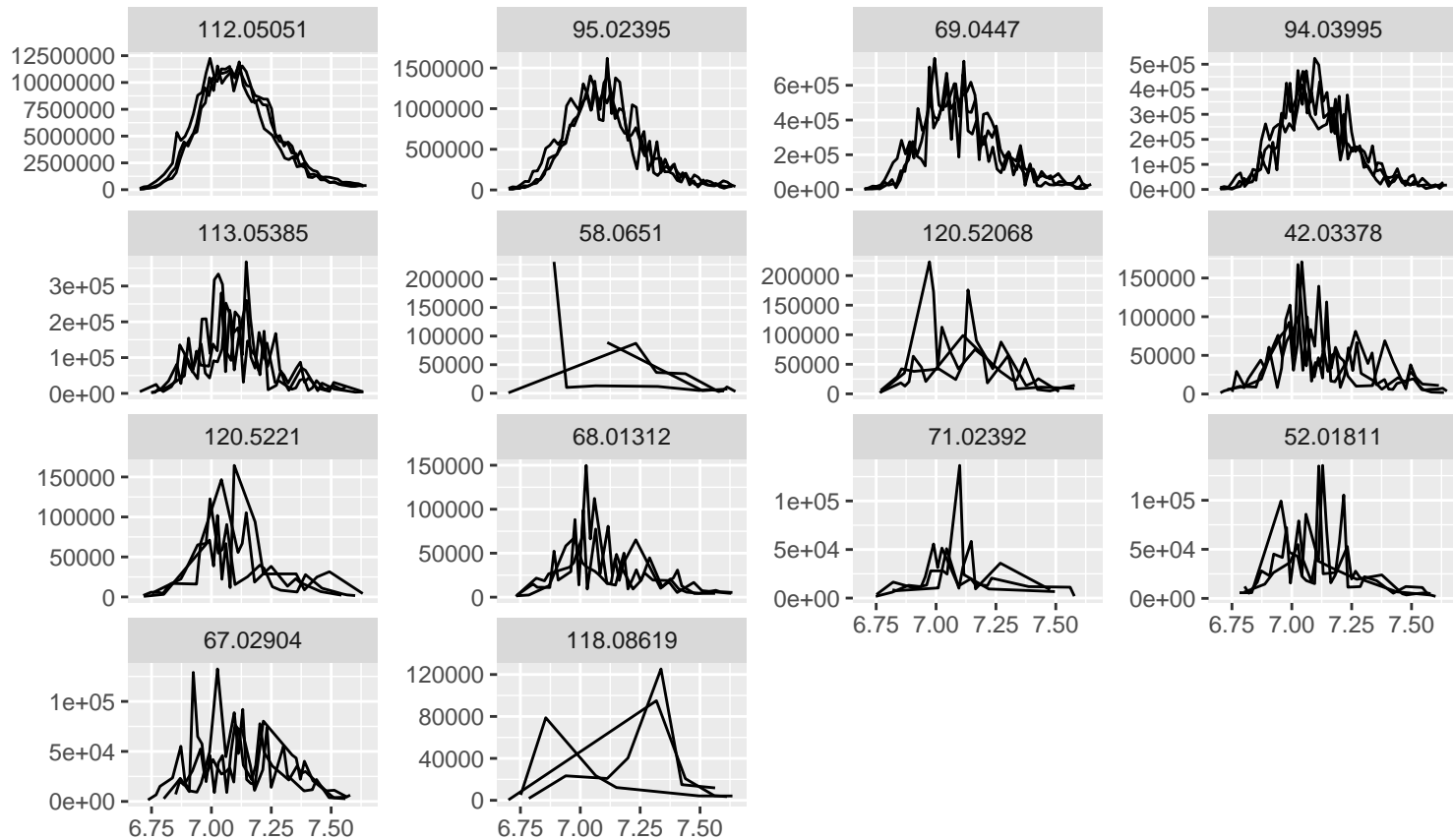
L-Serine (neg) 104.035318



Ethanesulfonic acid (neg) 108.996491

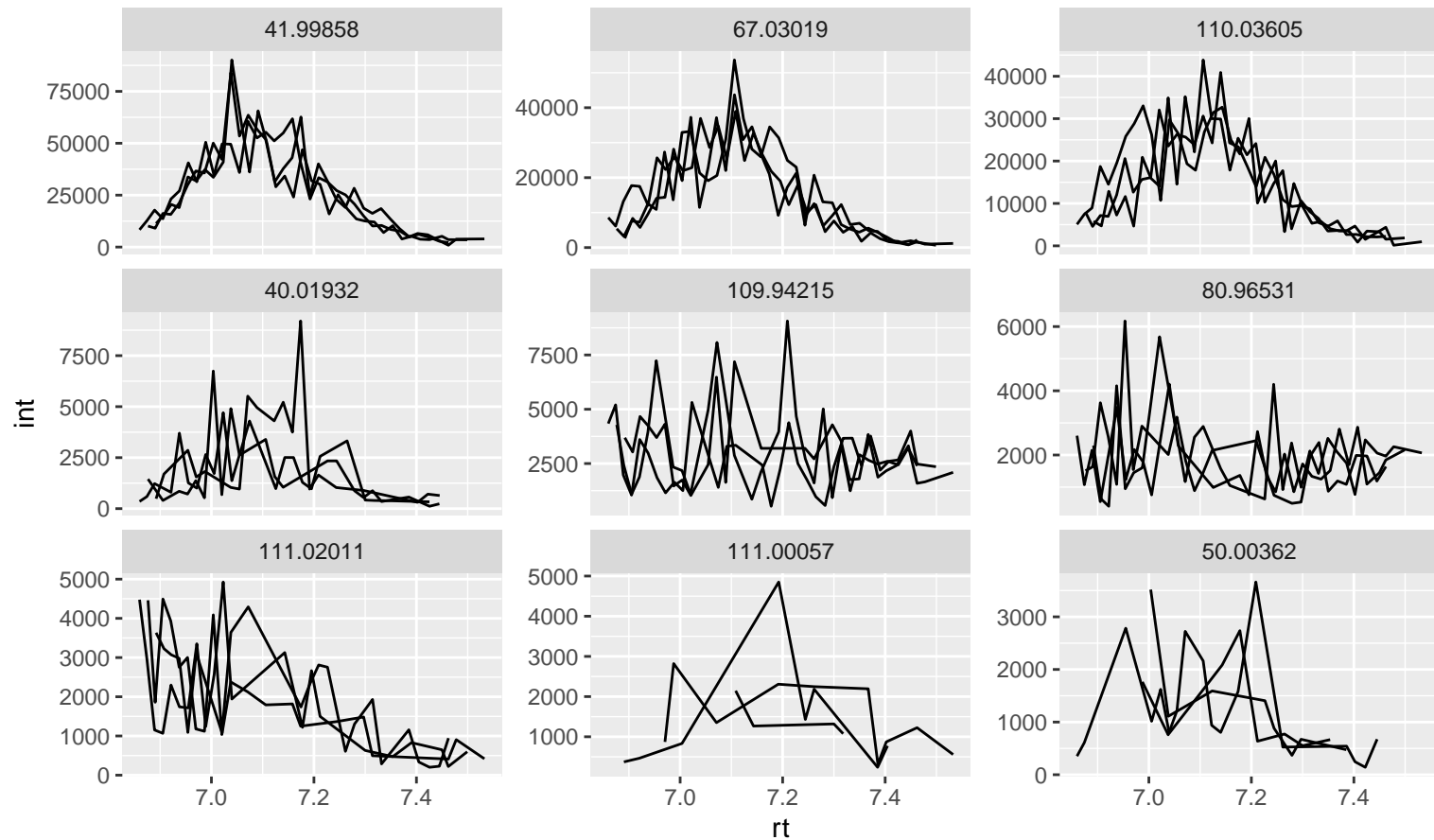


Cytosine (pos) 112.050538



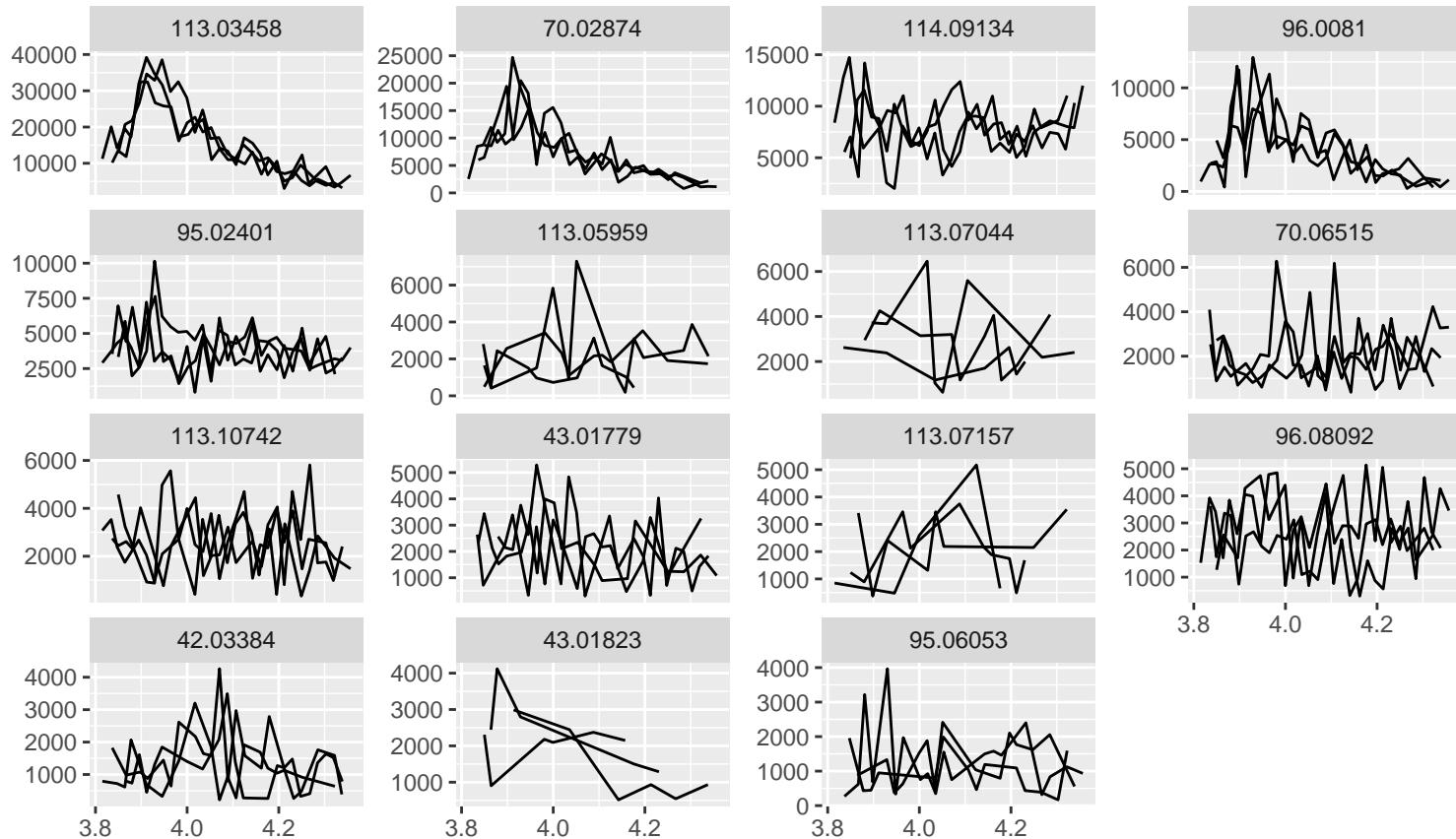
rt

Cytosine (neg) 110.035986



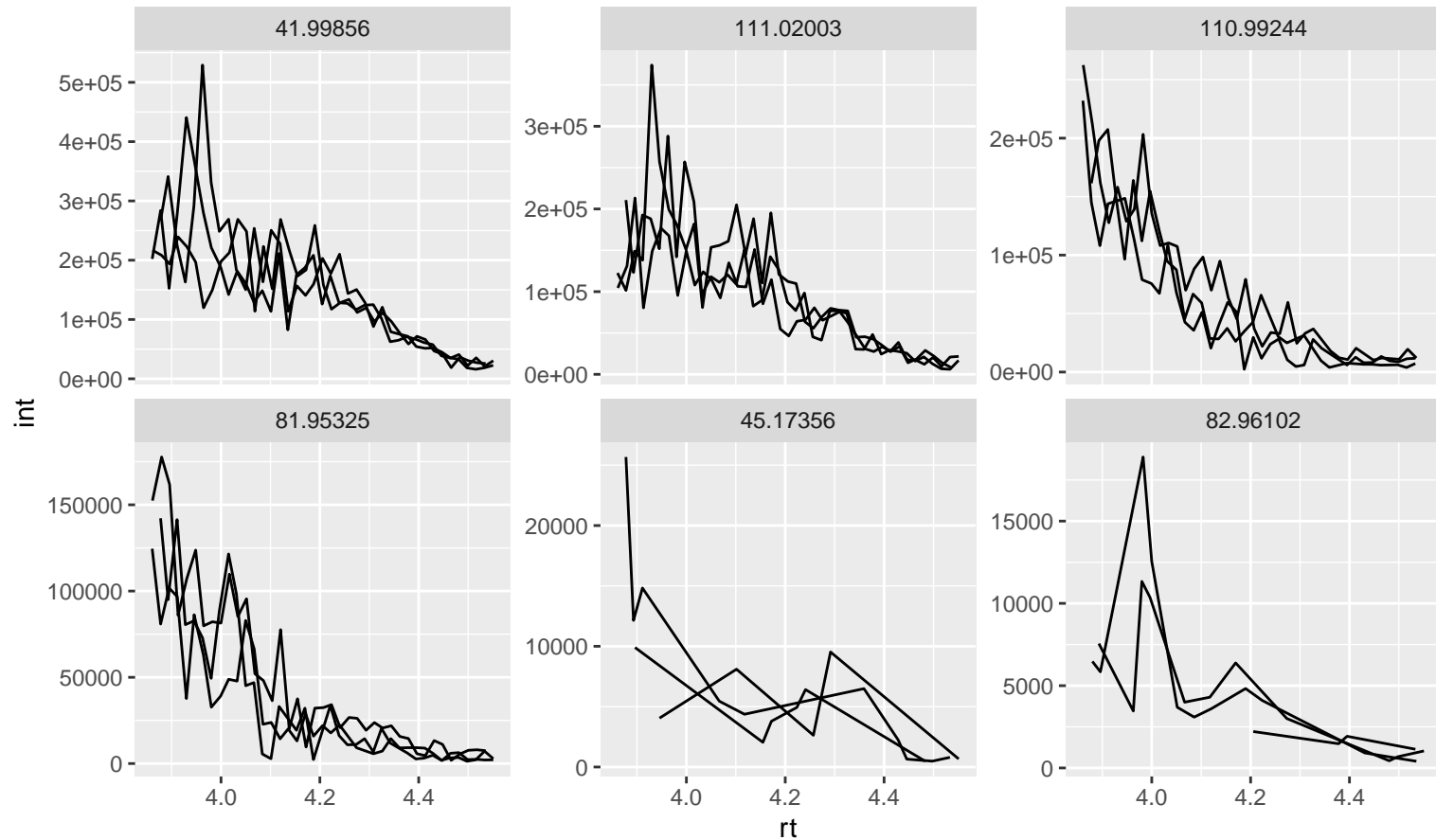
Uracil (pos) 113.034554

int

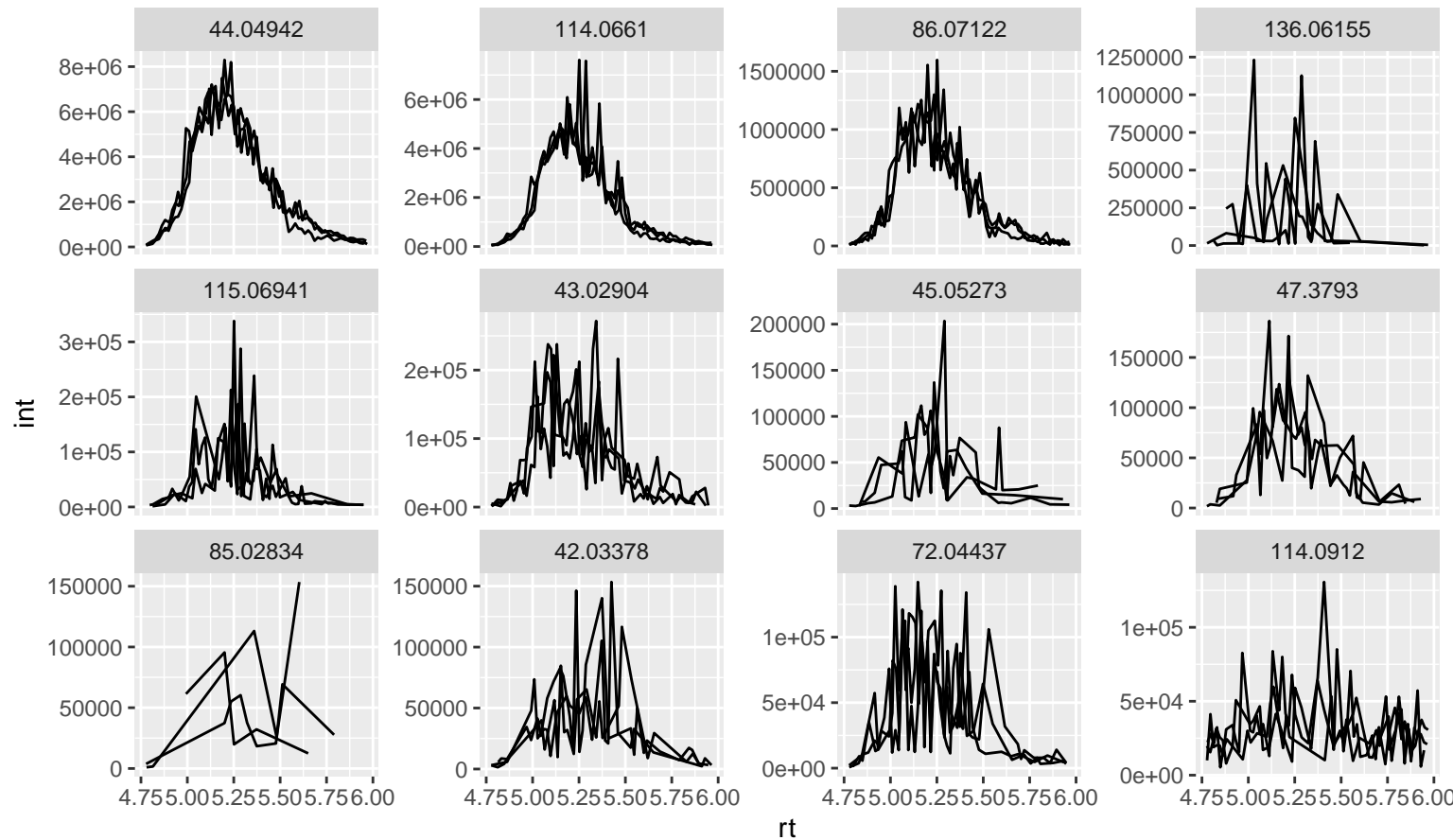


rt

Uracil (neg) 111.020002

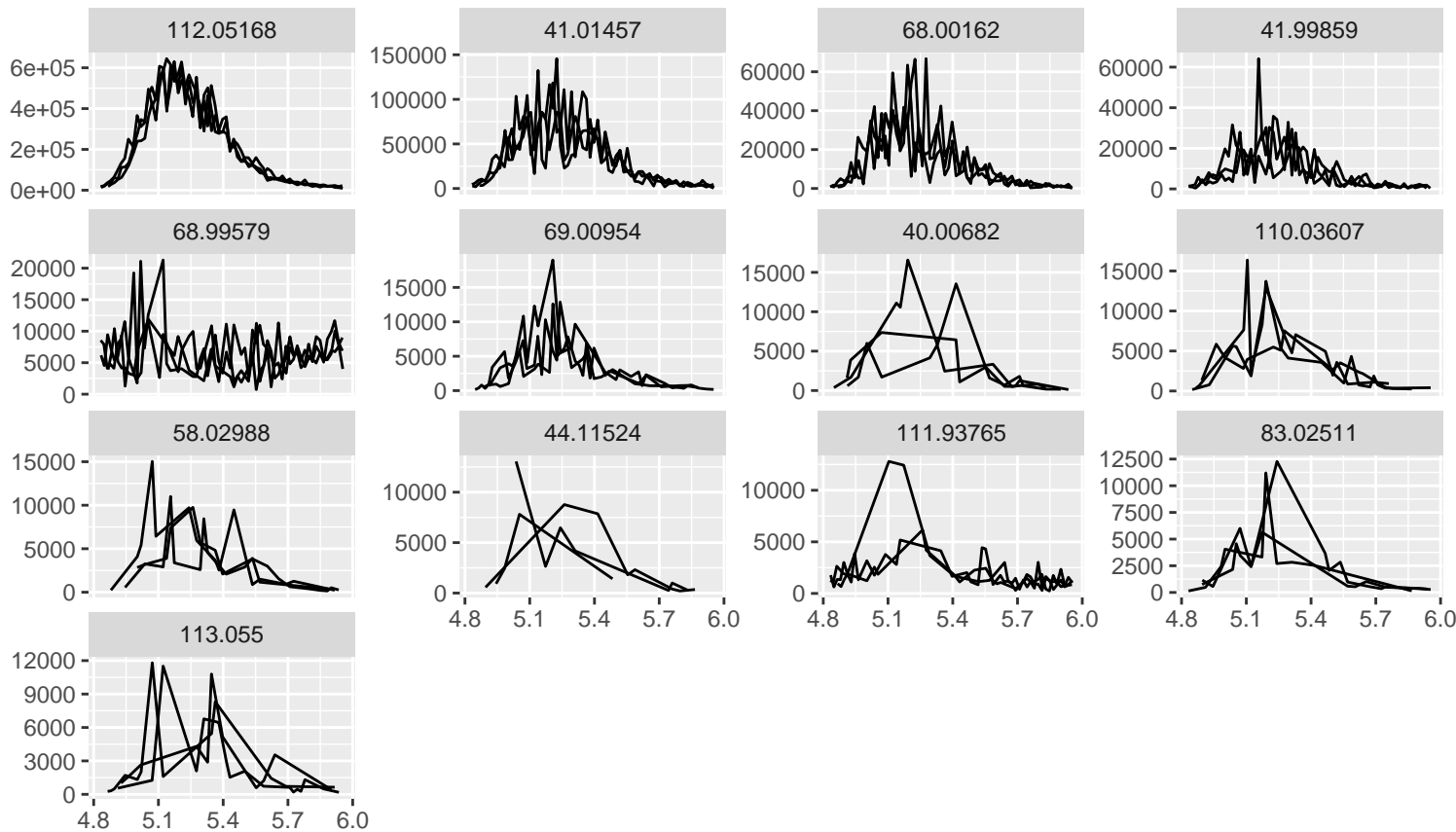


Creatinine (pos) 114.066188



Creatinine (neg) 112.051636

int



rt

Fumaric acid (neg) 115.003684

114.93422

40000

30000

20000

10000

int

115.07648

20000

15000

10000

5000

0

13.2

13.4

13.6

13.8

71.01387

25000

20000

15000

10000

5000

0

13.2

13.4

13.6

13.8

rt

97.93143

15000

10000

5000

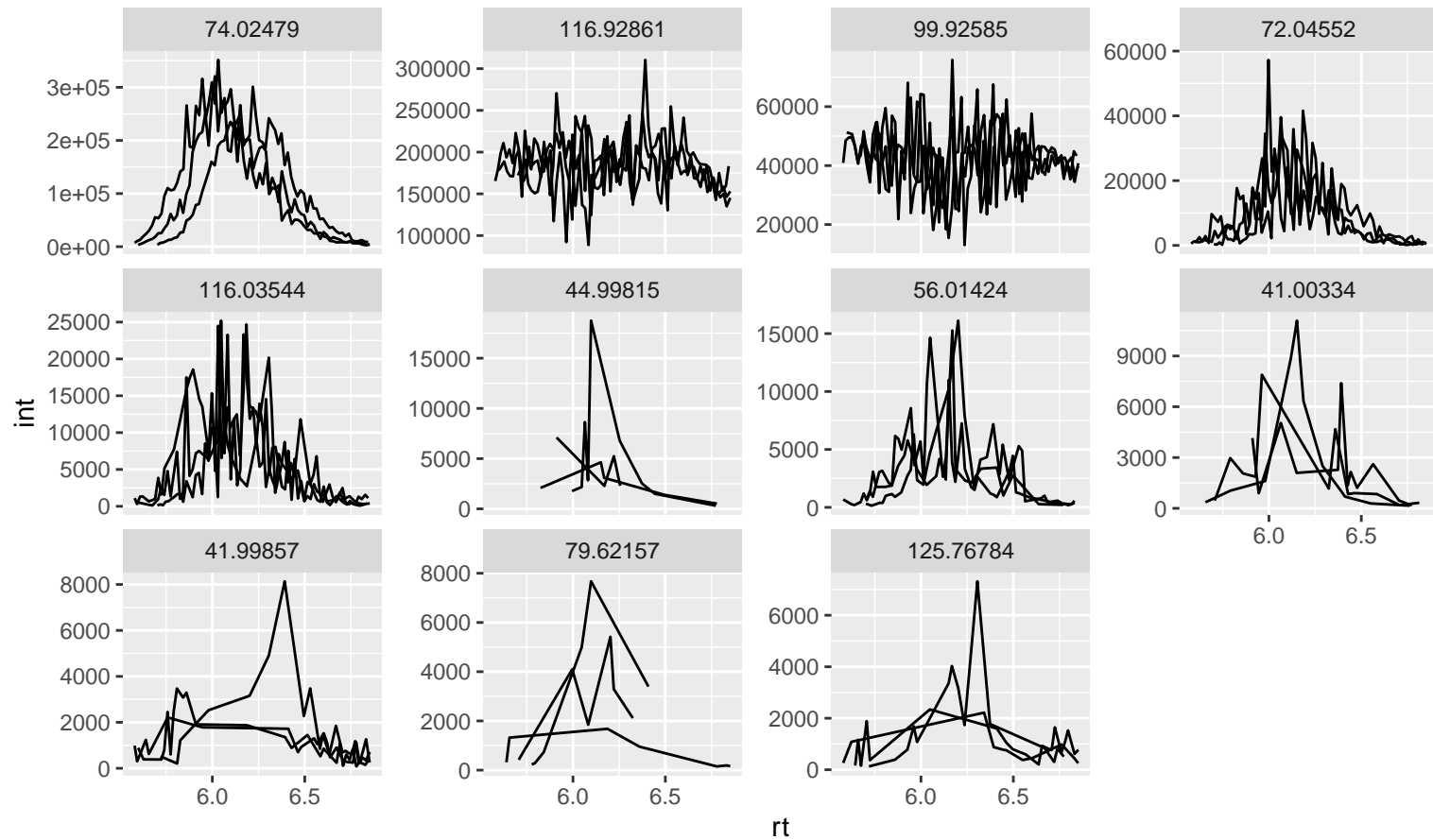
13.2

13.4

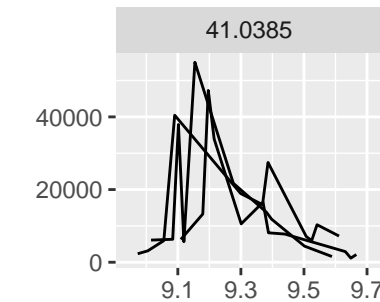
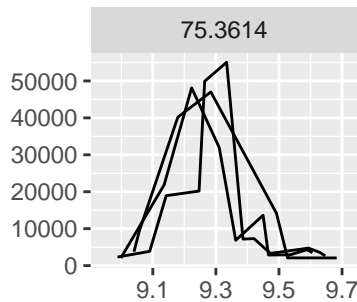
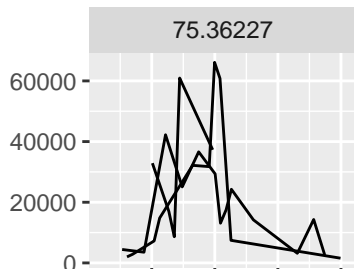
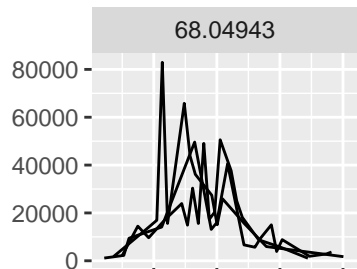
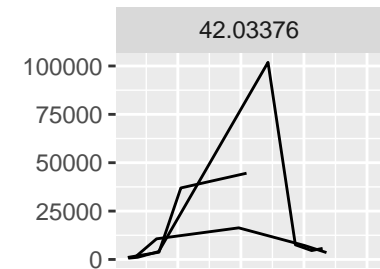
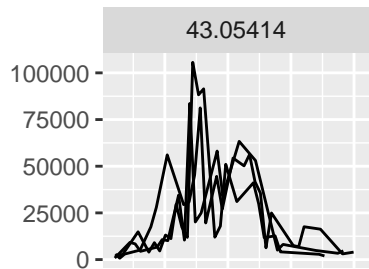
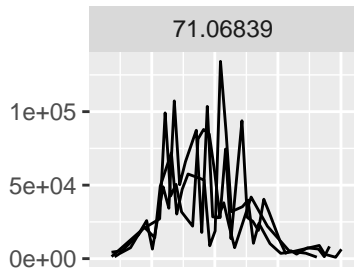
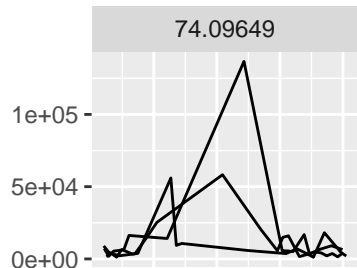
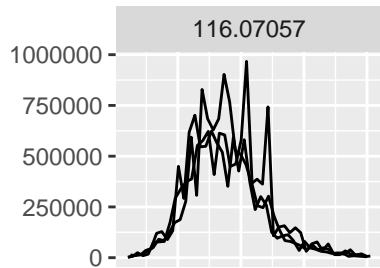
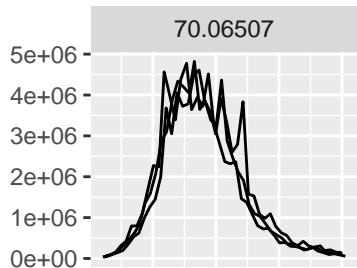
13.6

13.8

Acetylglycine (neg) 116.035318

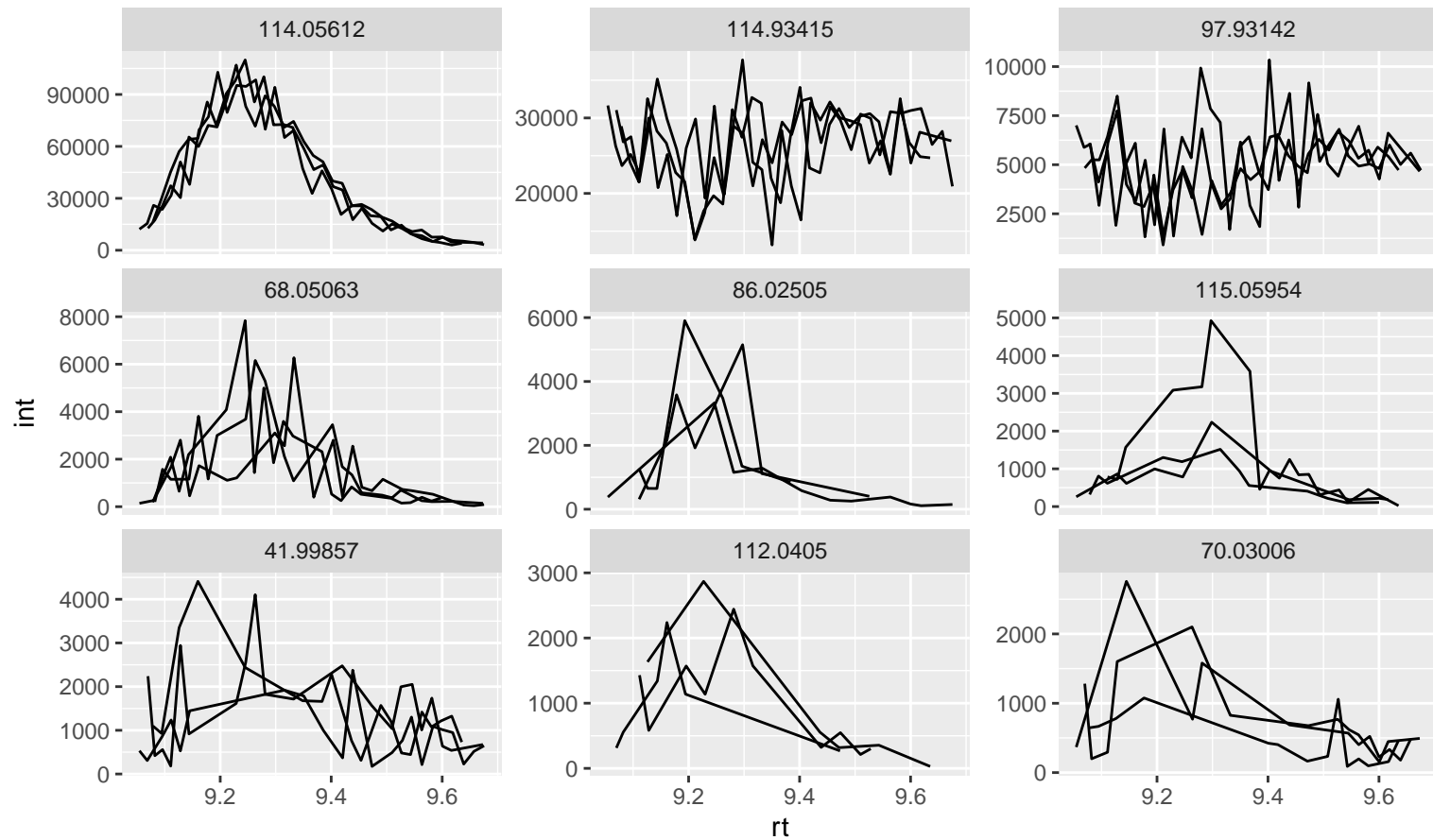


L-Proline (pos) 116.070605

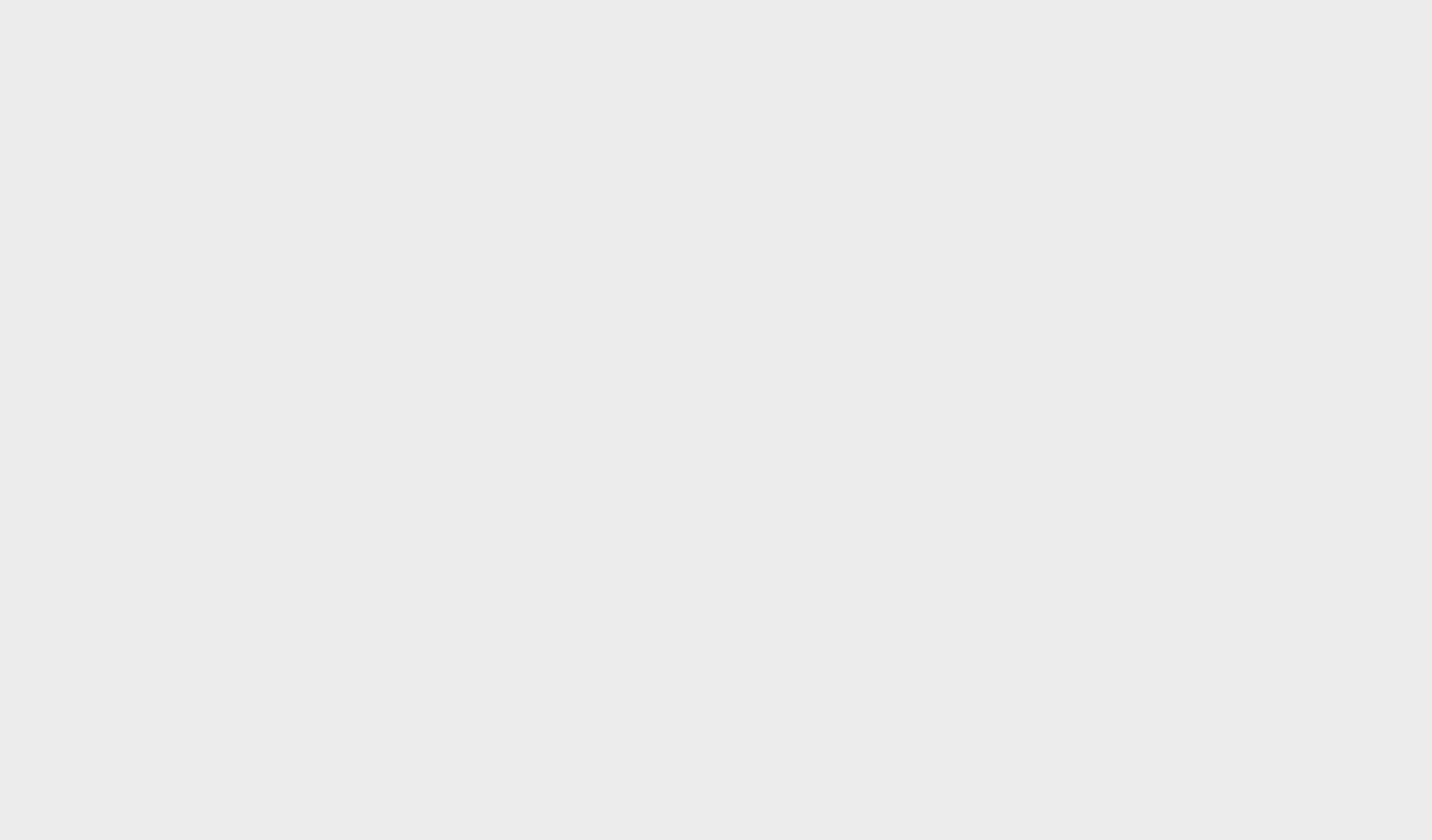


rt

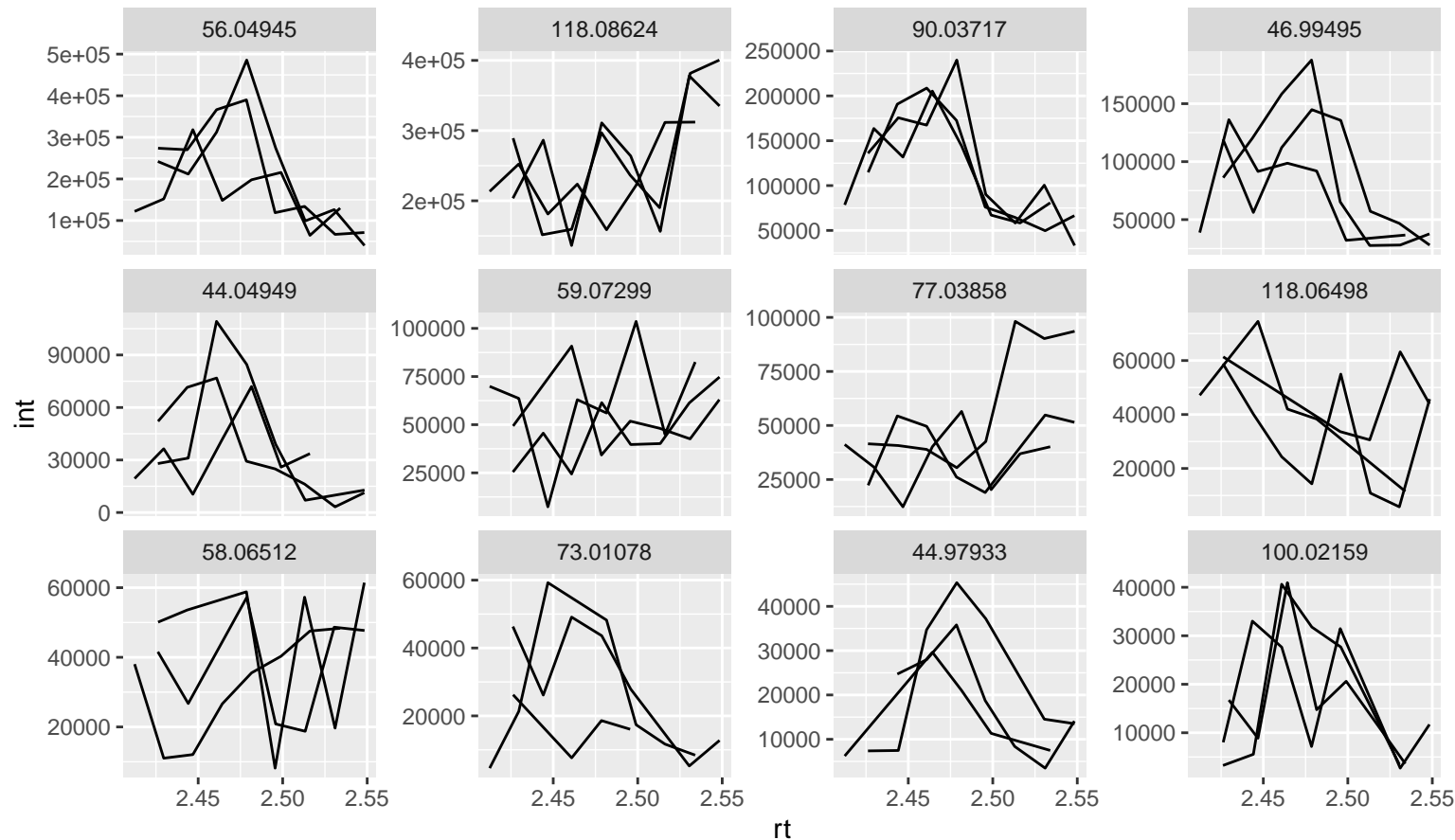
L-Proline (neg) 114.056053



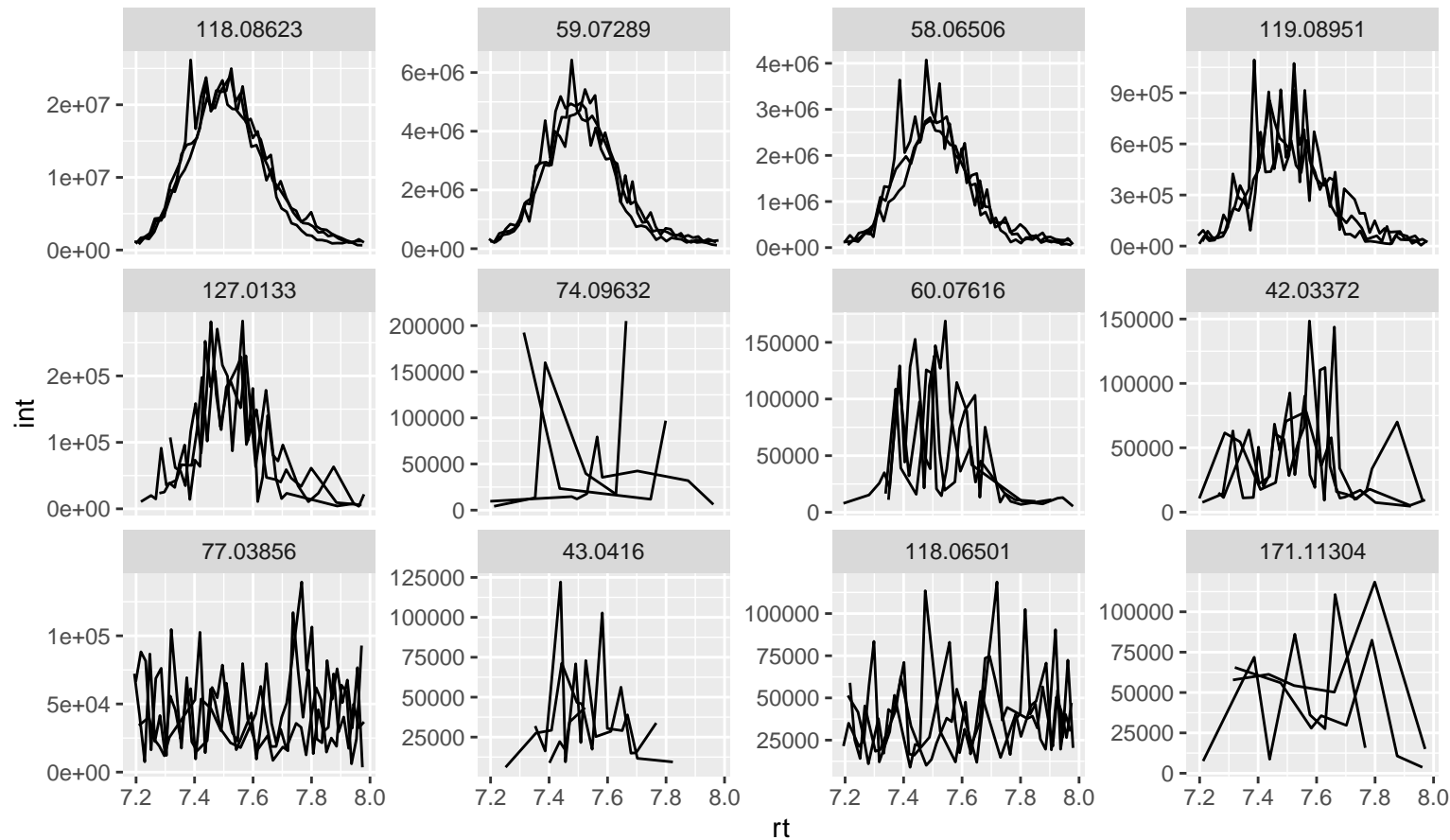
Succinic acid (neg) 117.019334



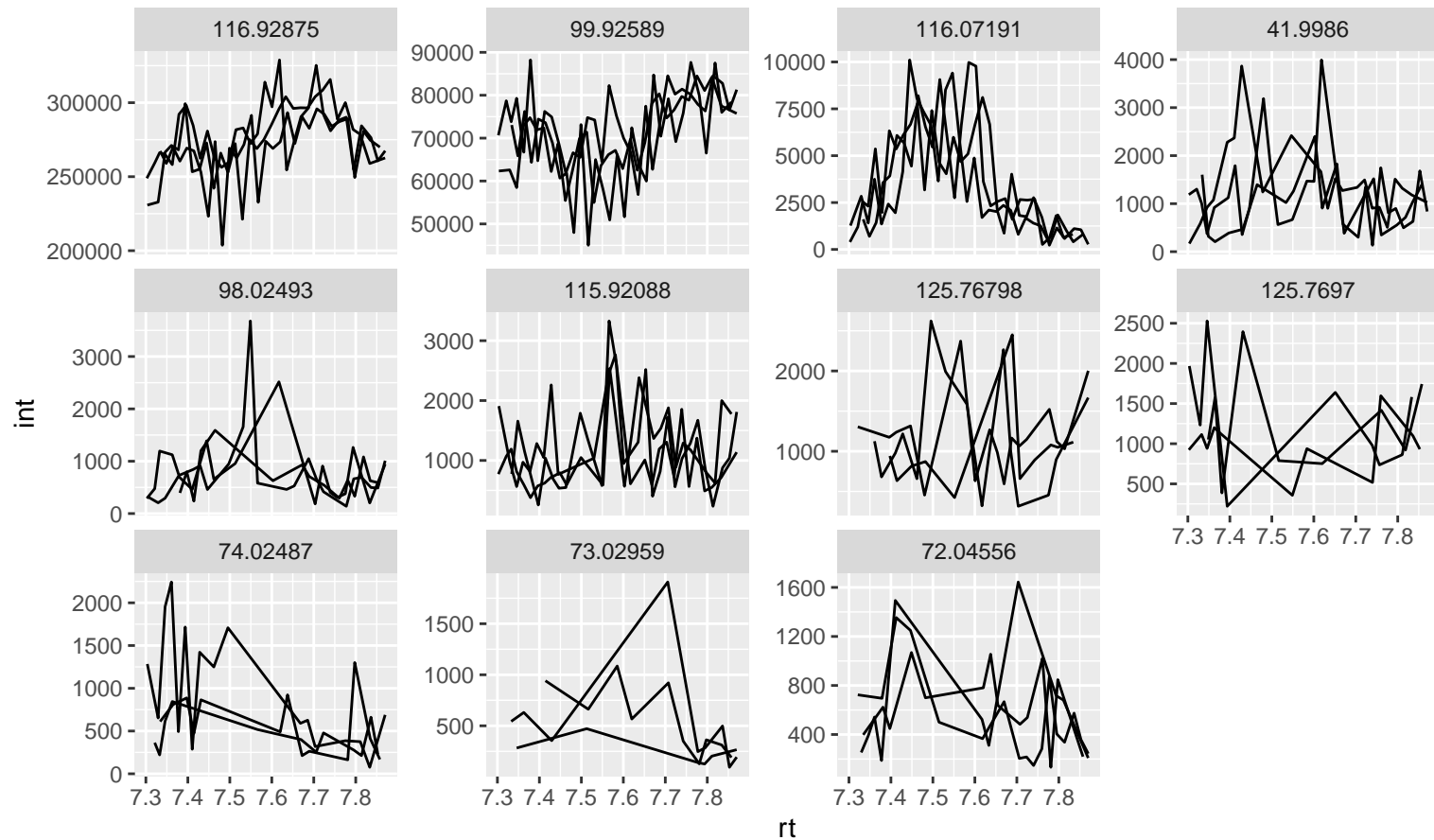
Homocysteine thiolactone (pos) 118.032112



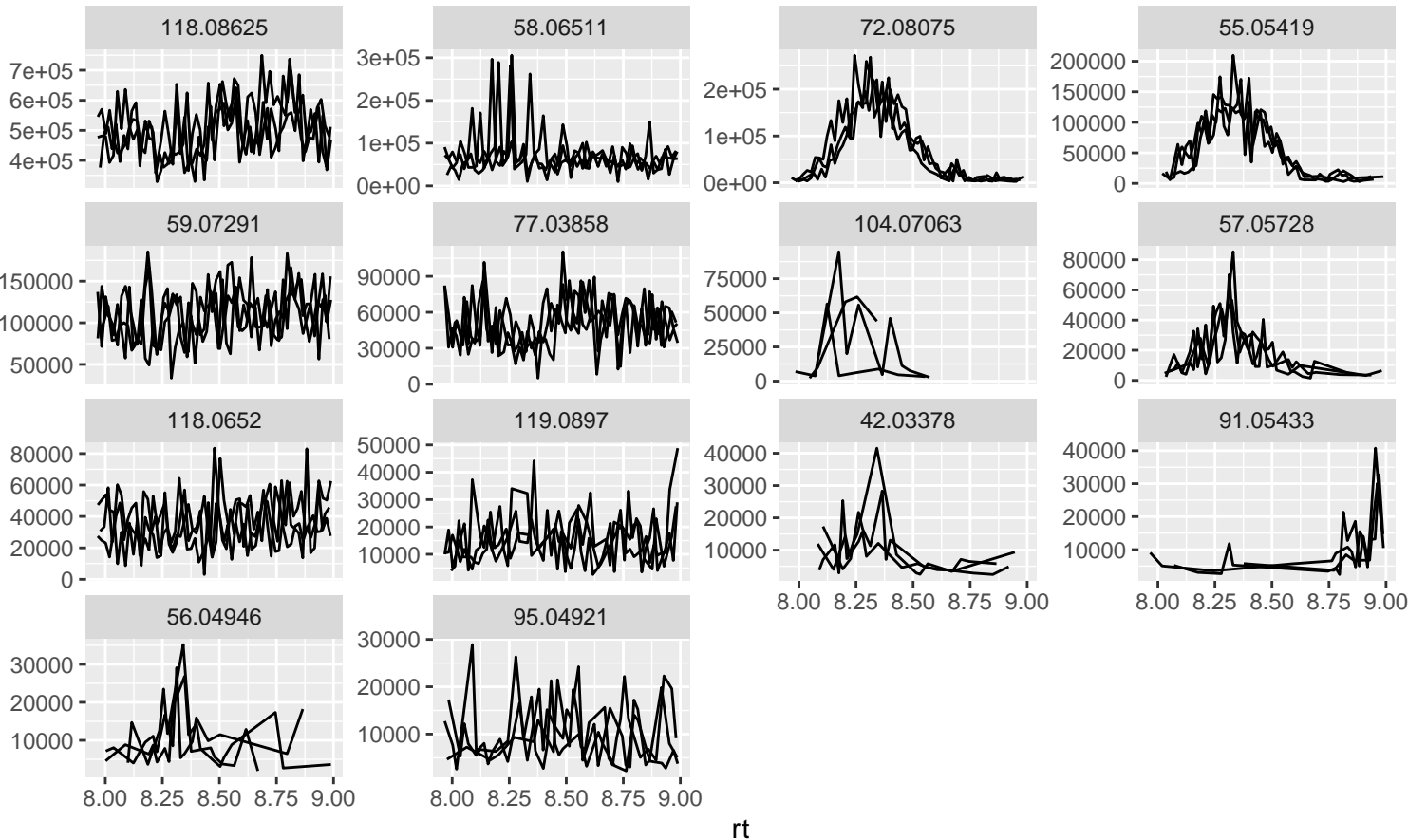
Glycine betaine (pos) 118.086255



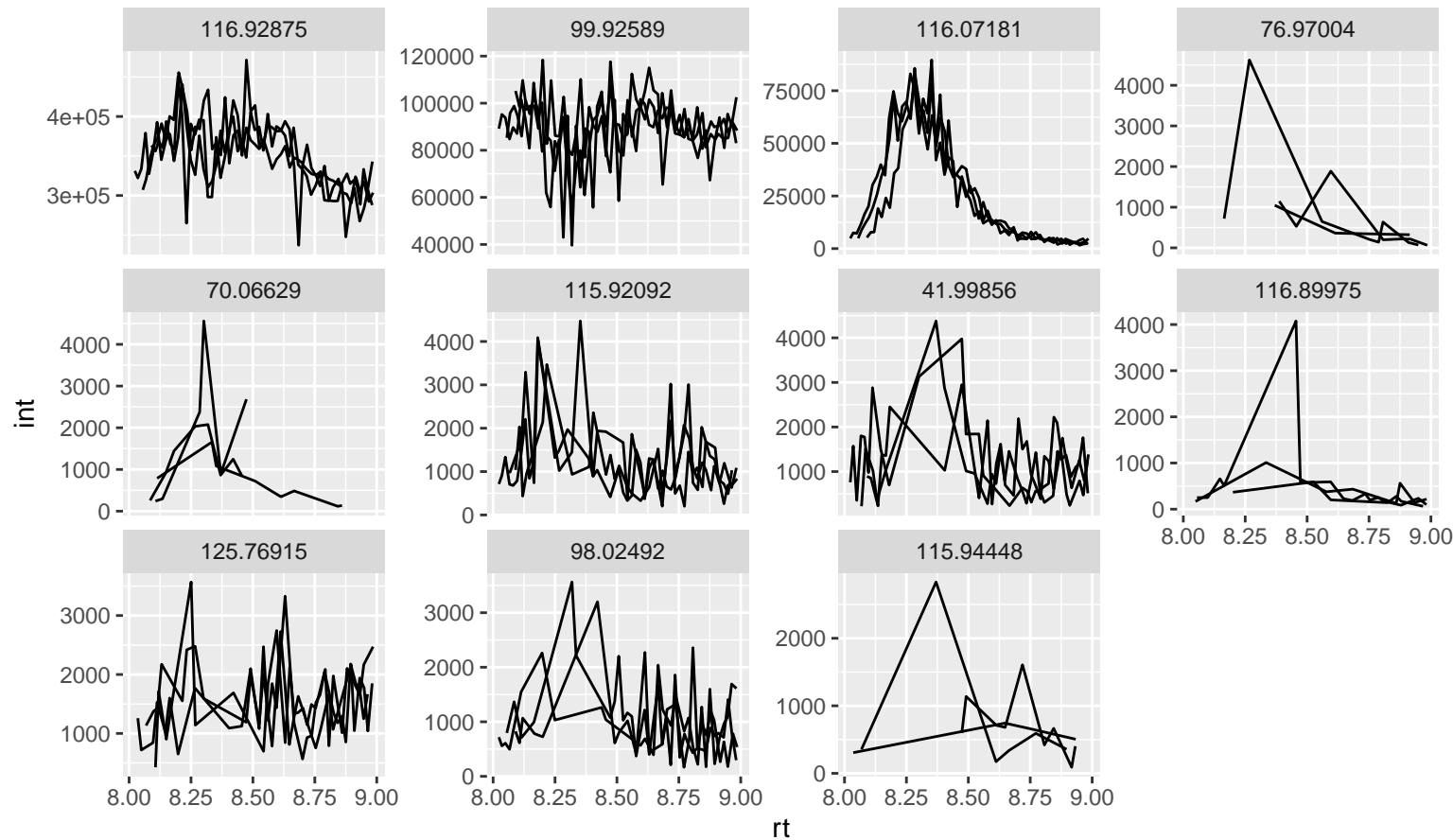
Glycine betaine (neg) 116.071703



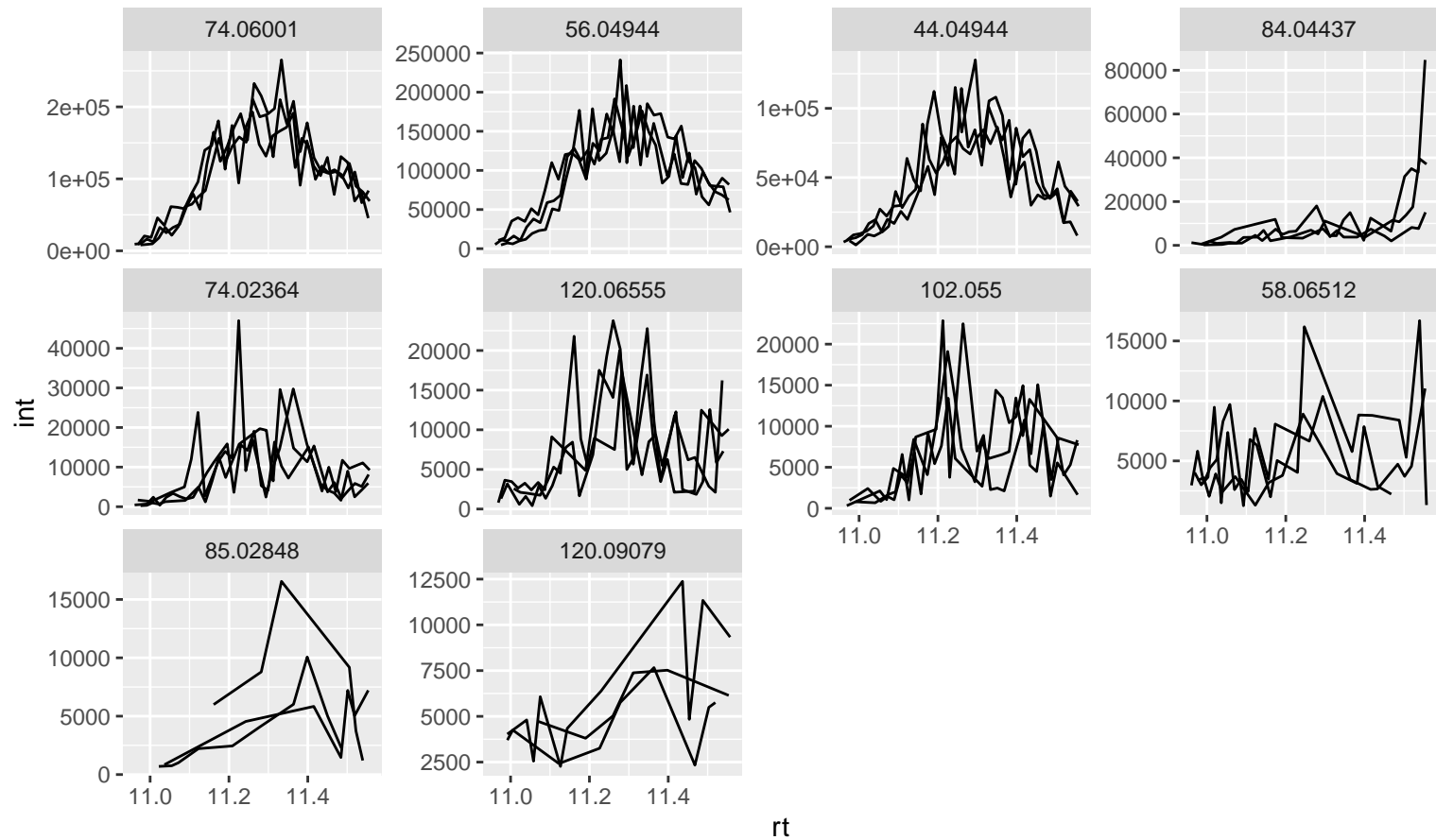
L-Valine (pos) 118.08625



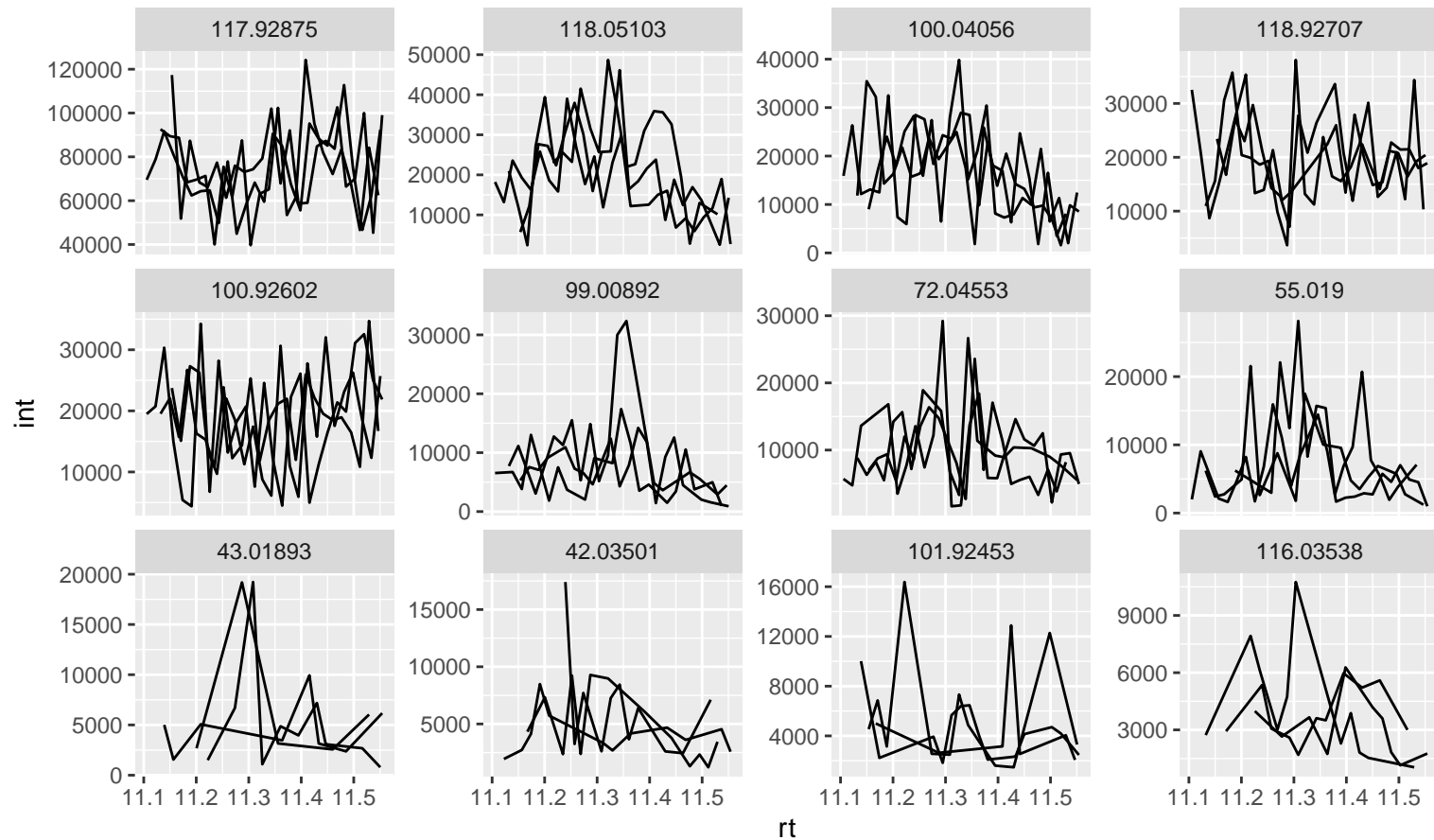
L-Valine (neg) 116.071703



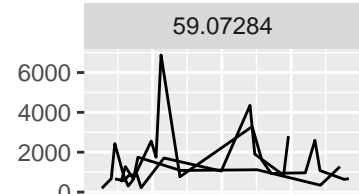
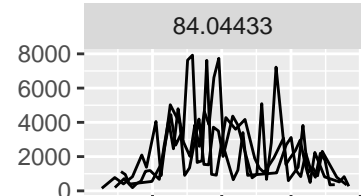
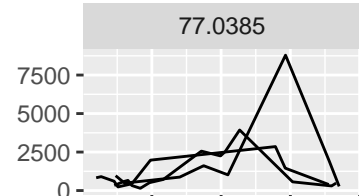
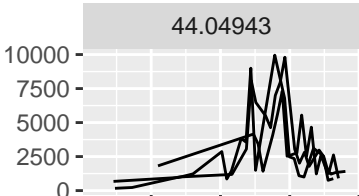
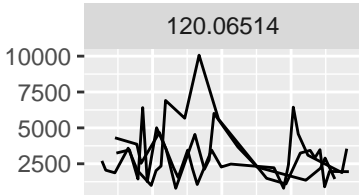
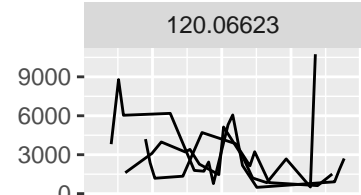
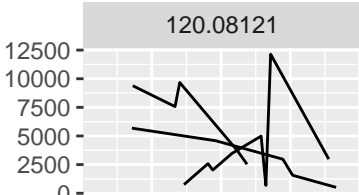
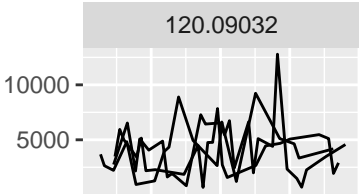
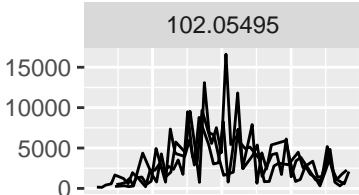
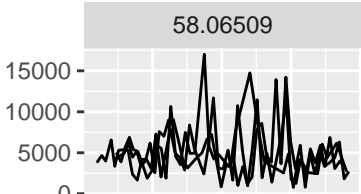
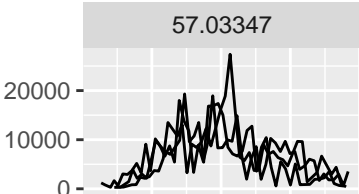
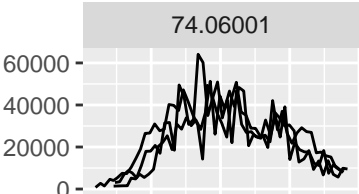
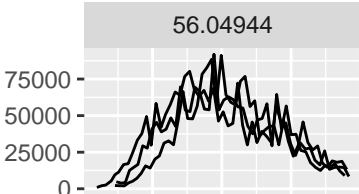
L-Homoserine (pos) 120.06552



L-Homoserine (neg) 118.050968

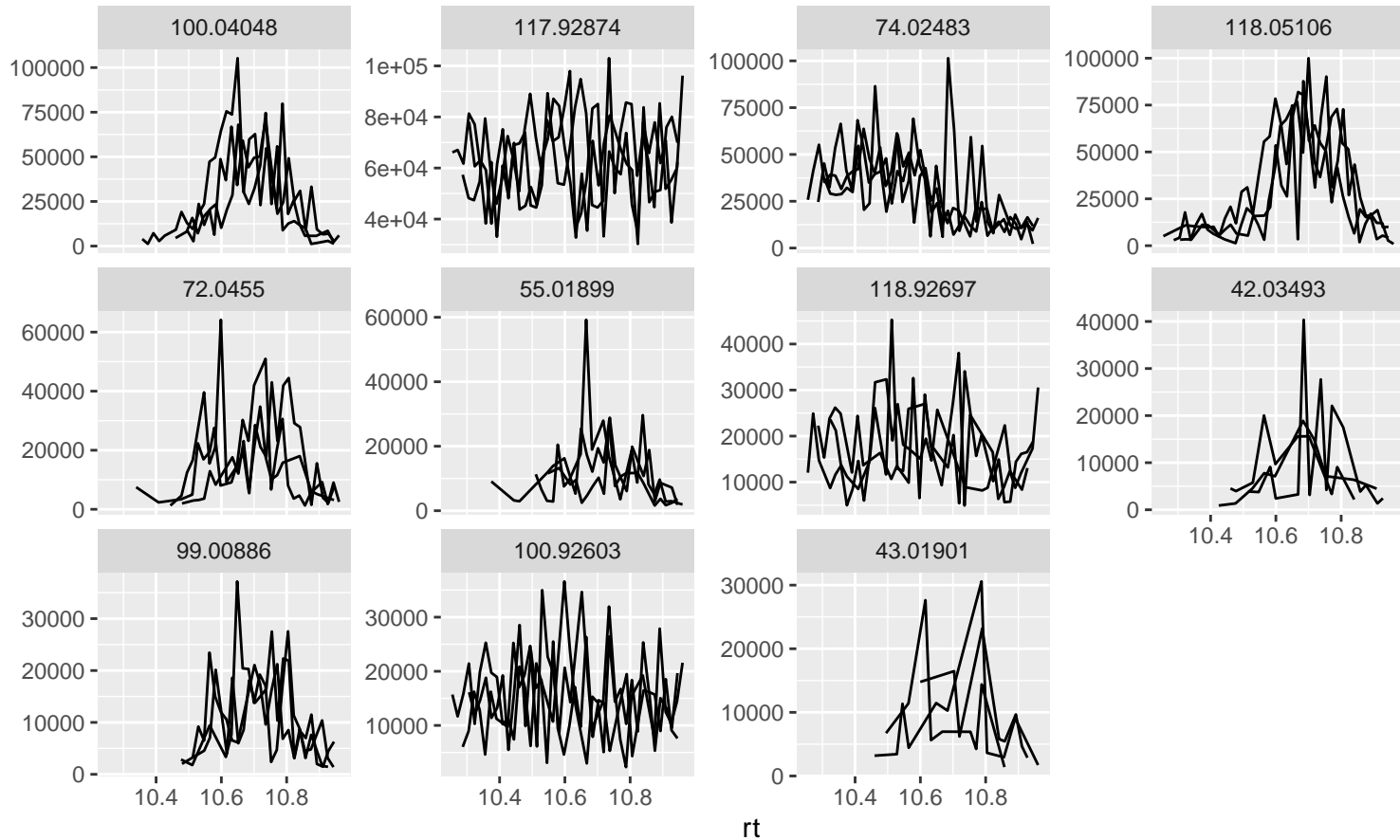


L-Threonine (pos) 120.06552



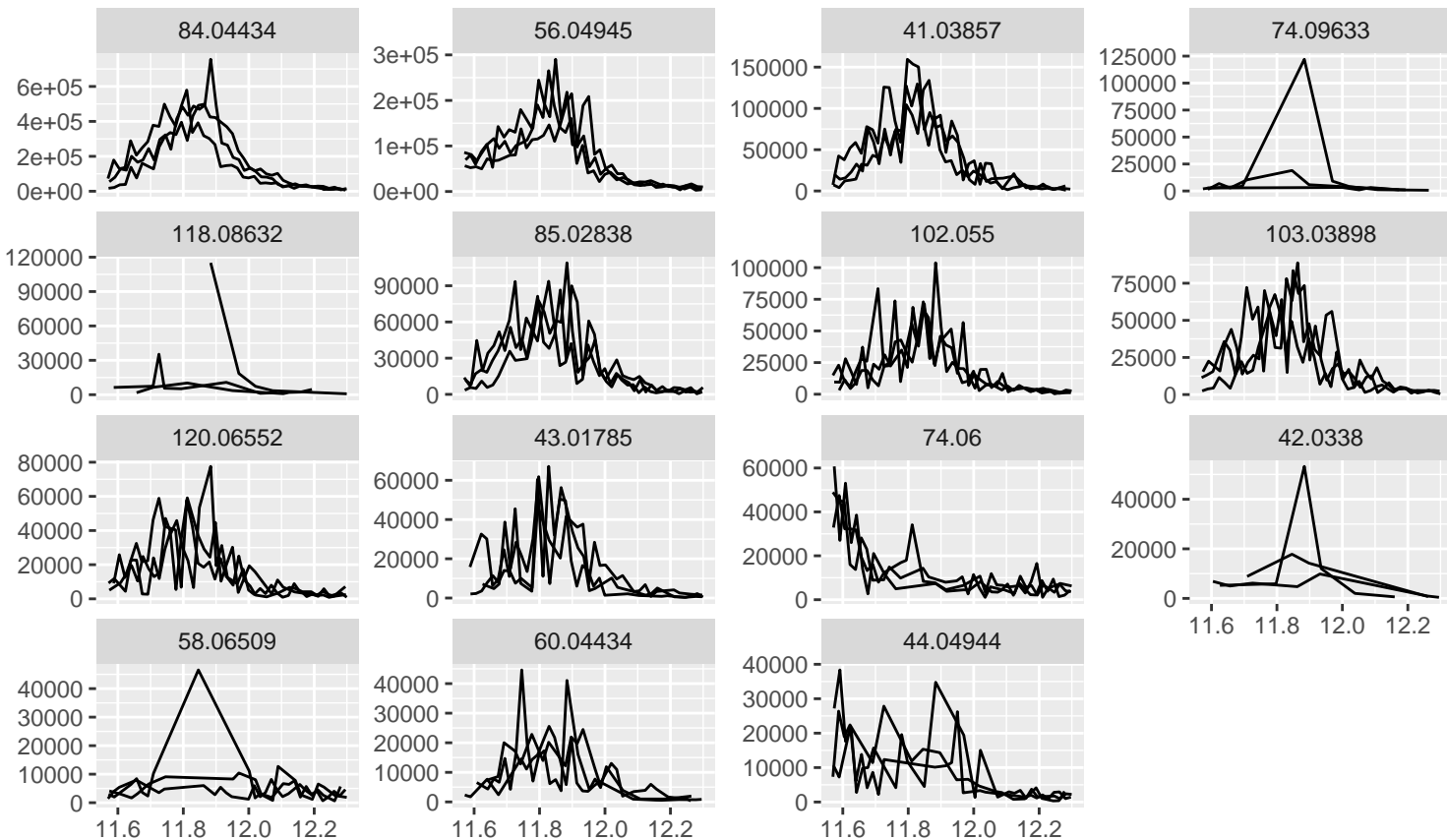
rt

L-Threonine (neg) 118.050968



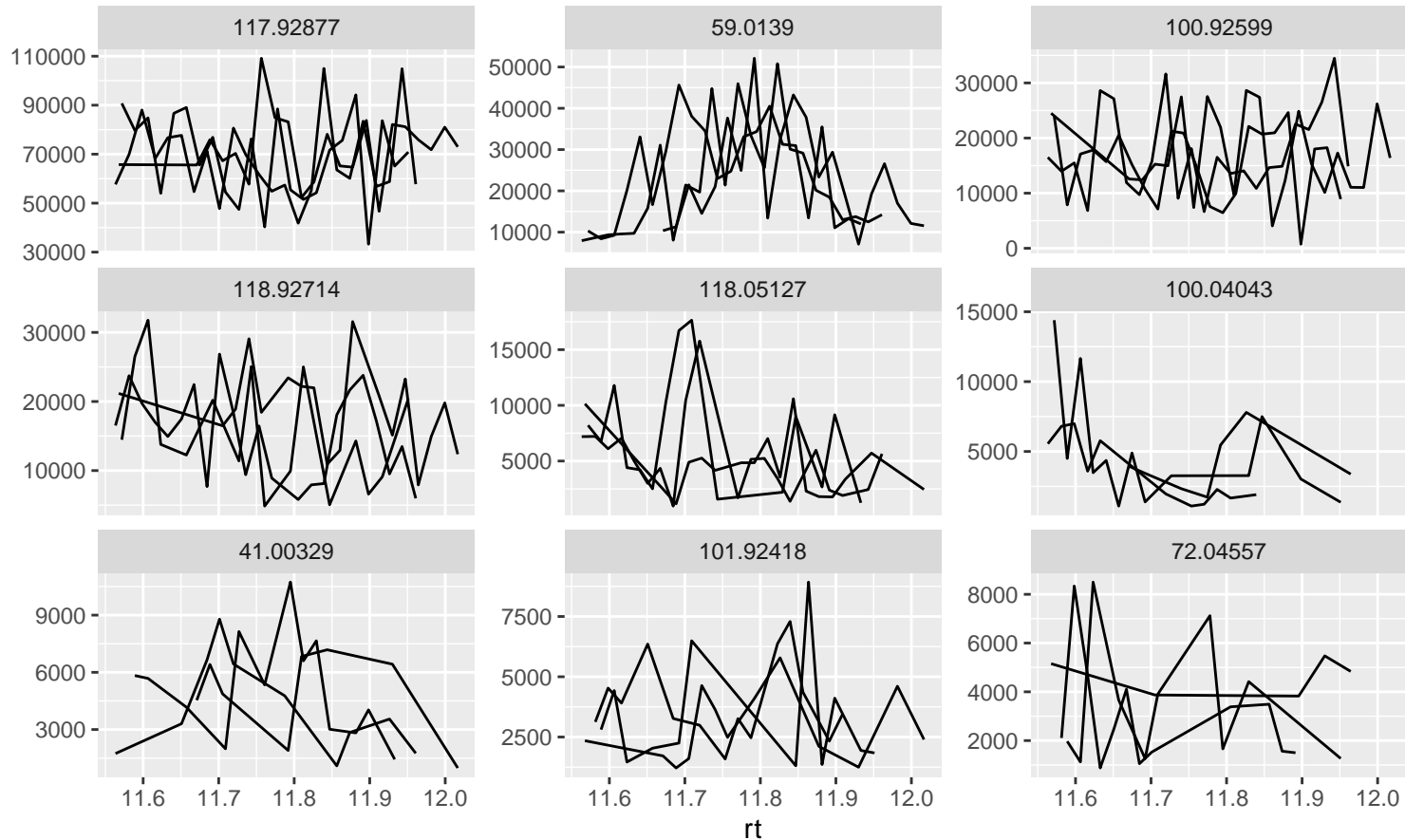
gamma-Amino-beta-hydroxybutyric acid (pos) 120.0652

int

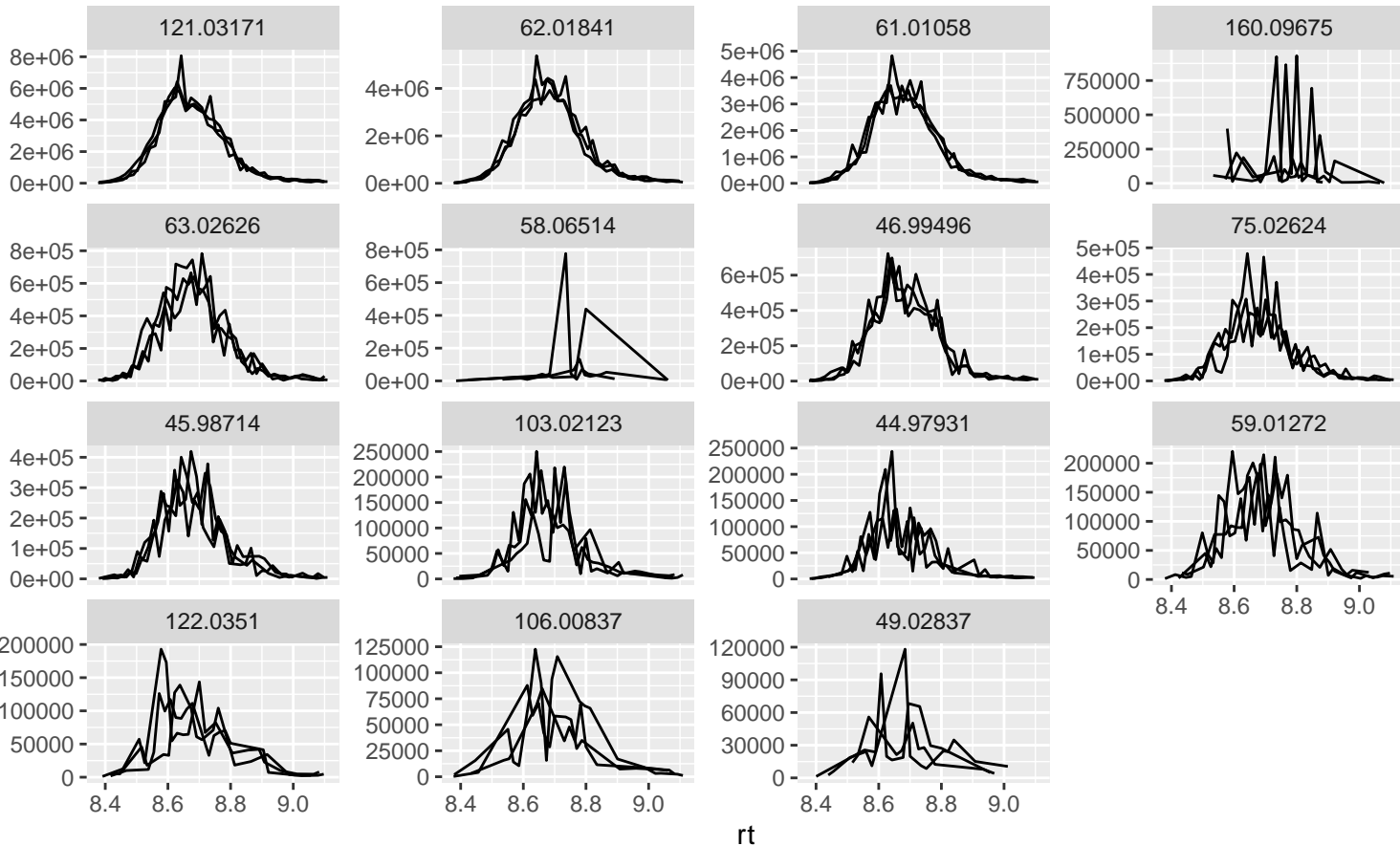


rt

gamma-Amino-beta-hydroxybutyric acid (neg) 118.050968

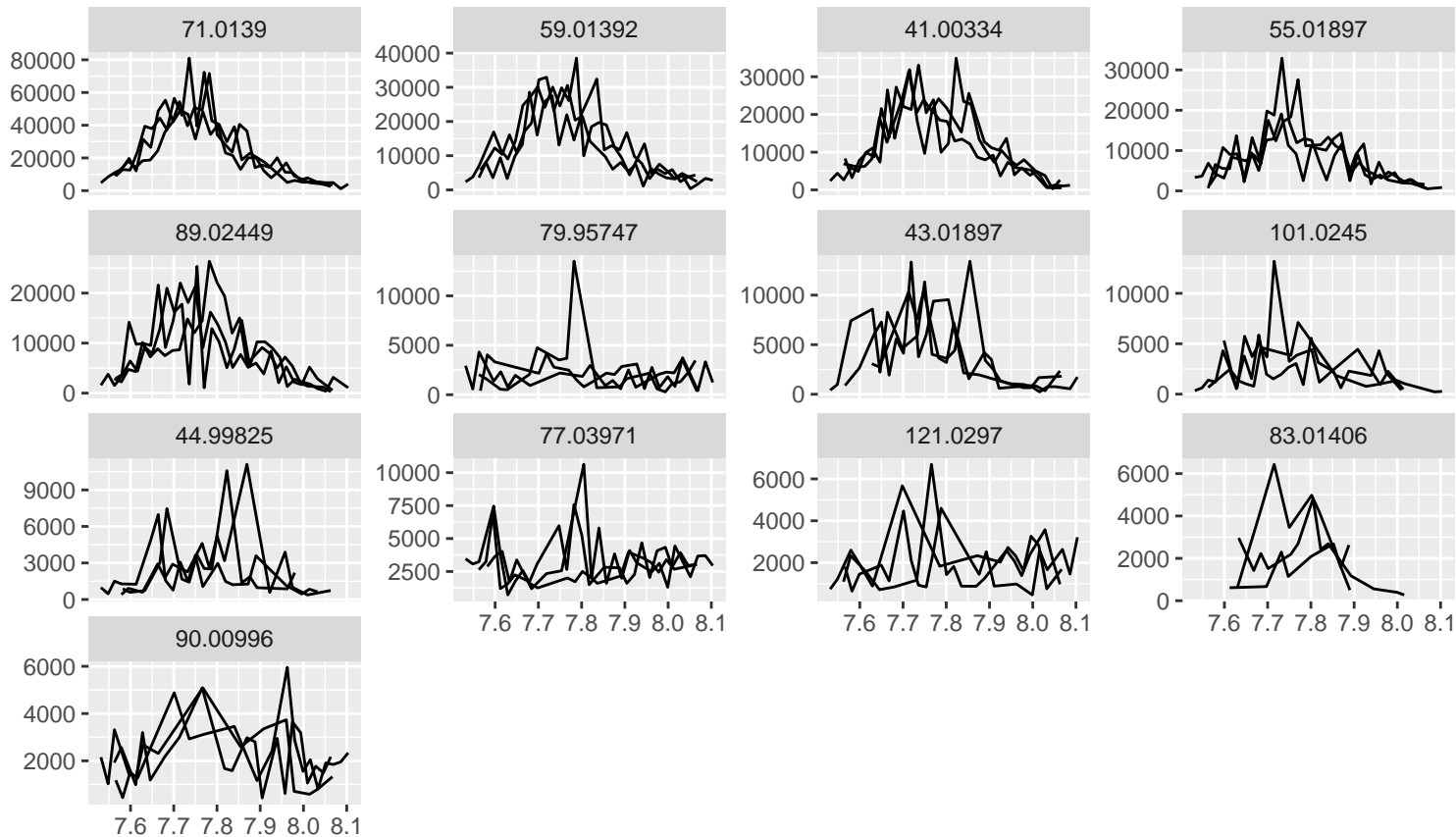


Dimethylsulfonioacetate (pos) 121.031778



Erythritol (neg) 121.050634

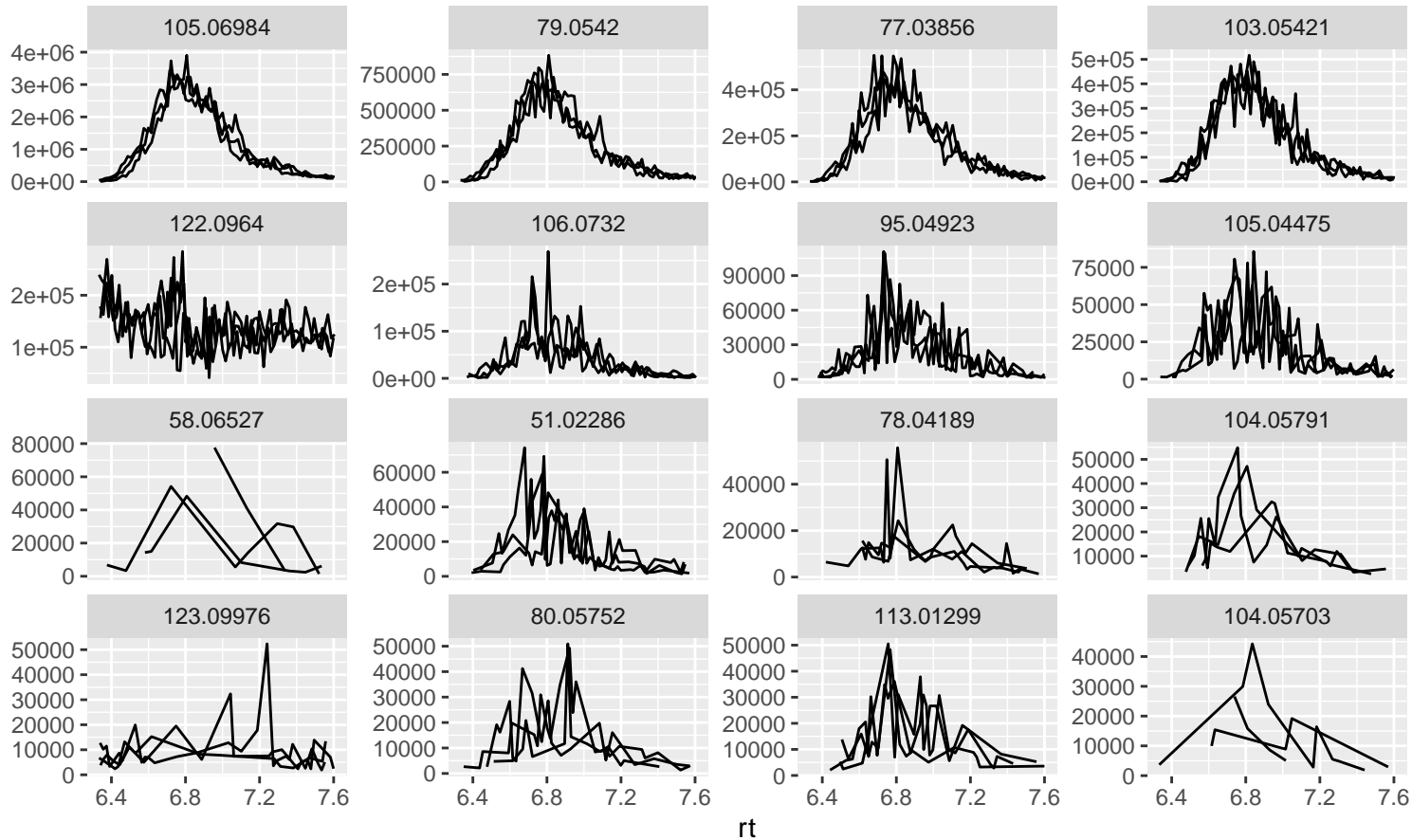
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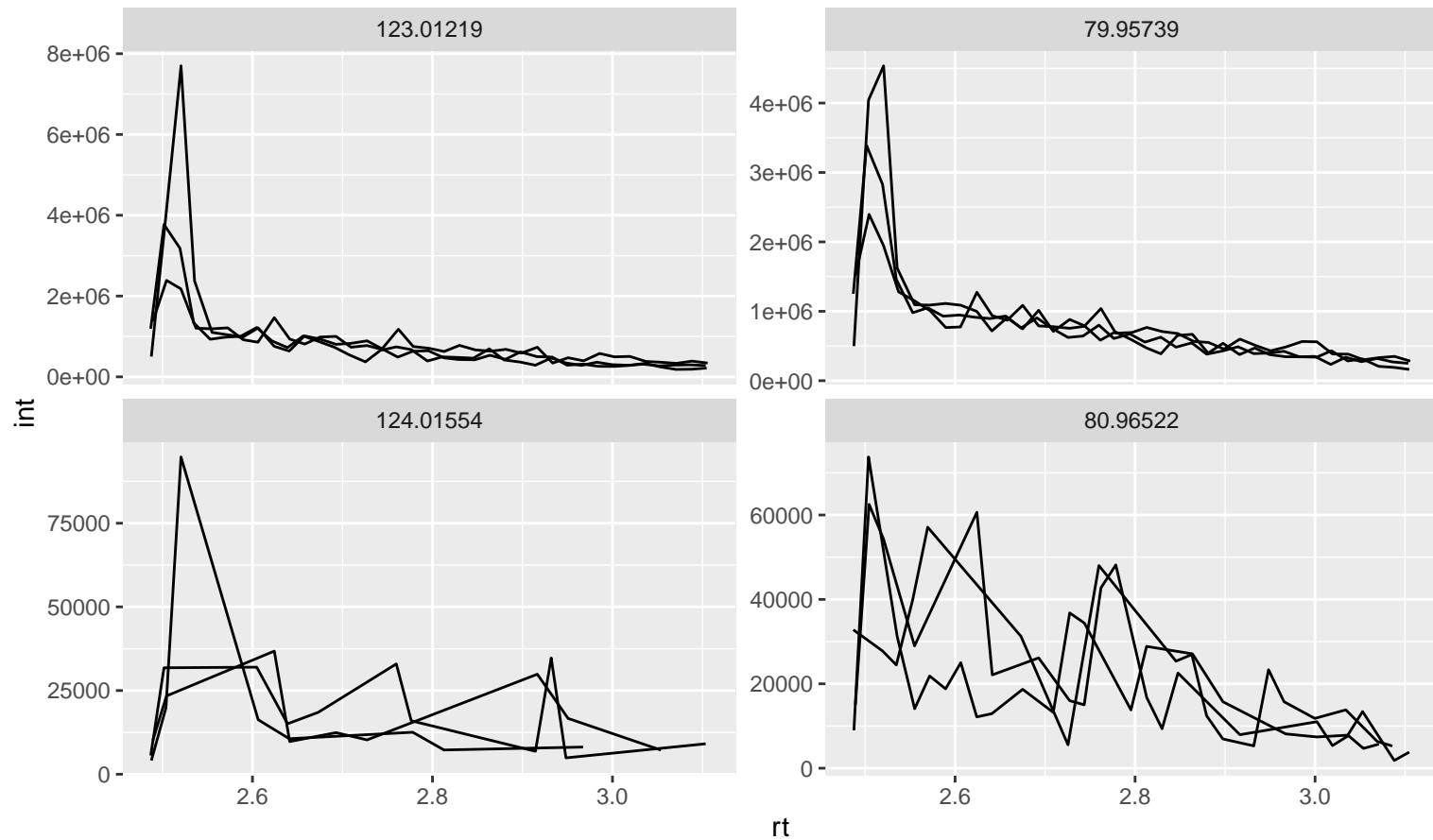
rt

Phenylethylamine (pos) 122.096425

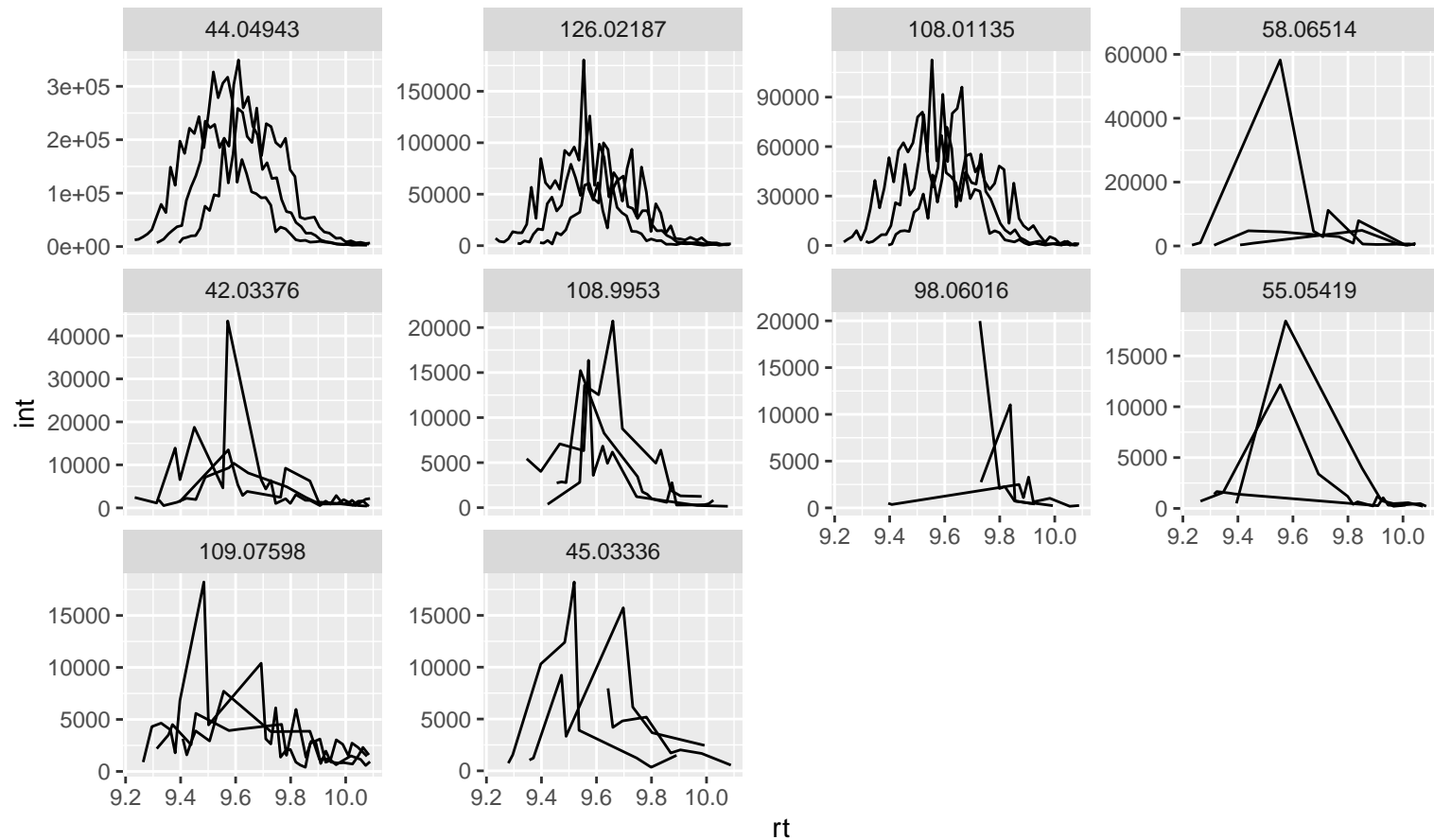
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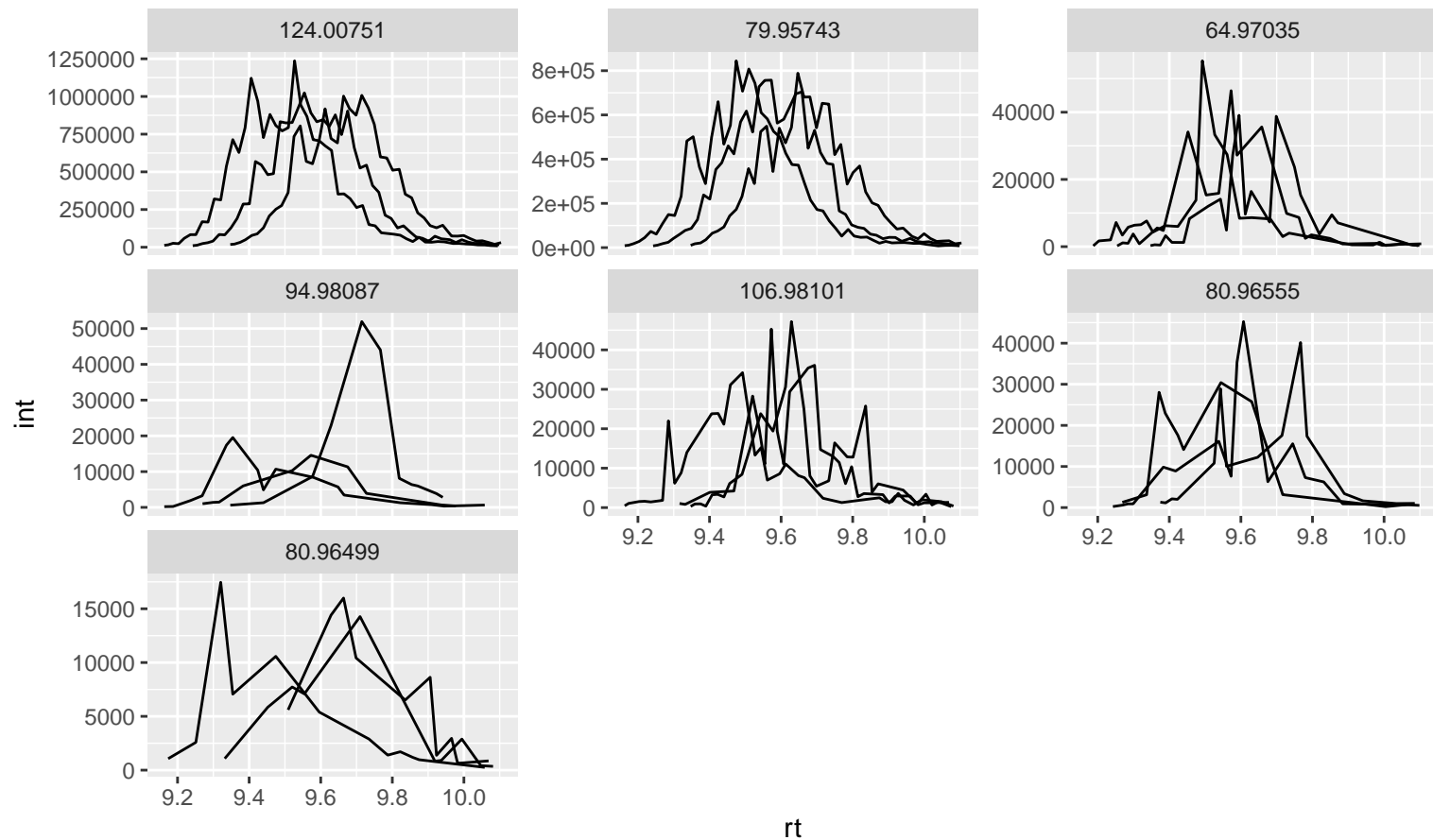
1-Propanesulfonate (neg) 123.01214058



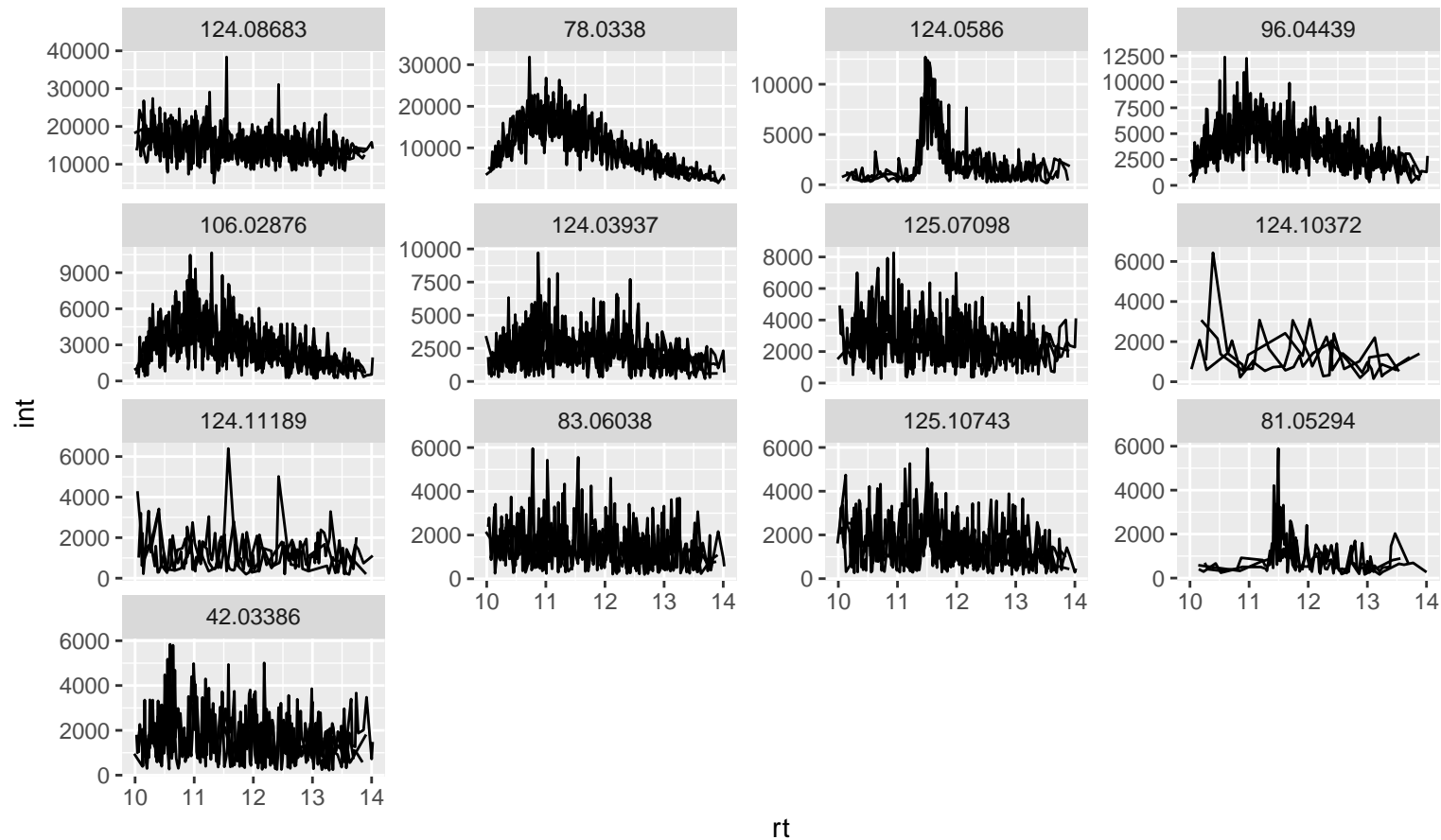
Taurine (pos) 126.021942



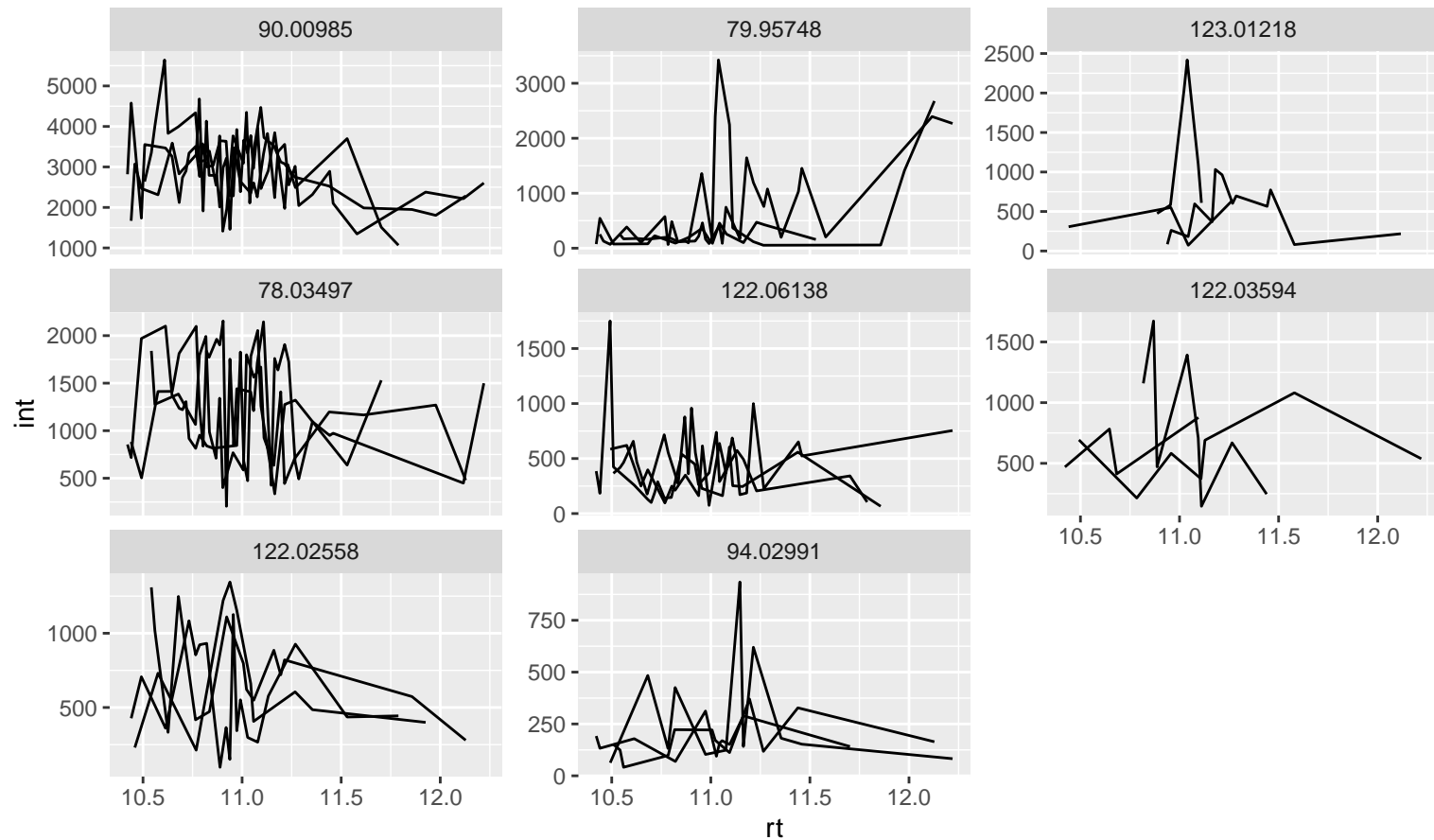
Taurine (neg) 124.00739



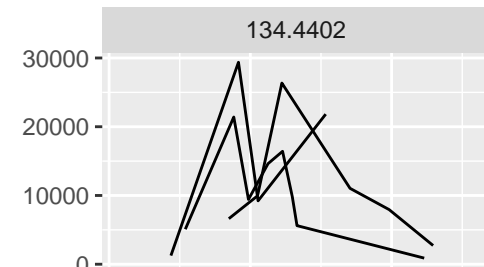
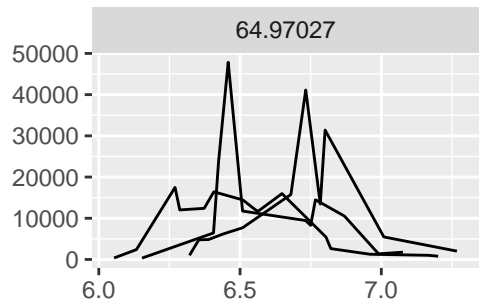
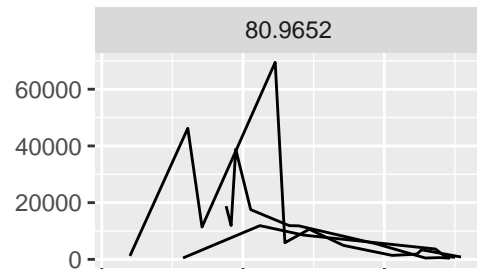
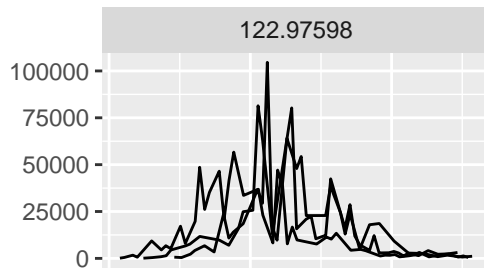
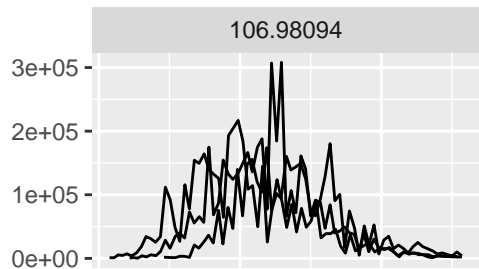
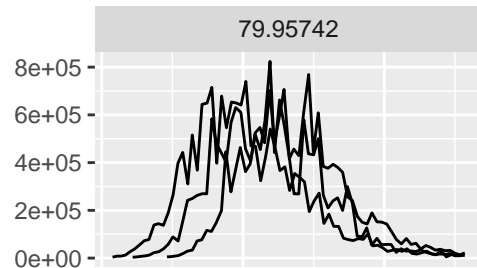
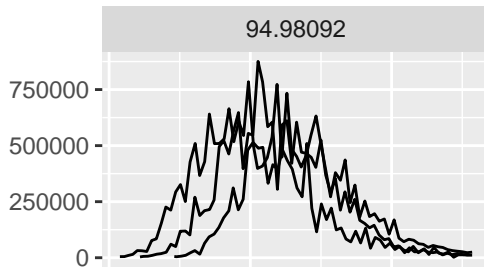
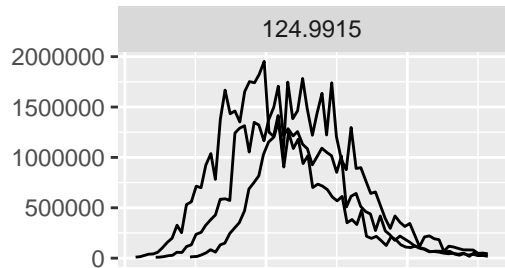
Picolinic acid (pos) 124.039305



Picolinic acid (neg) 122.024753



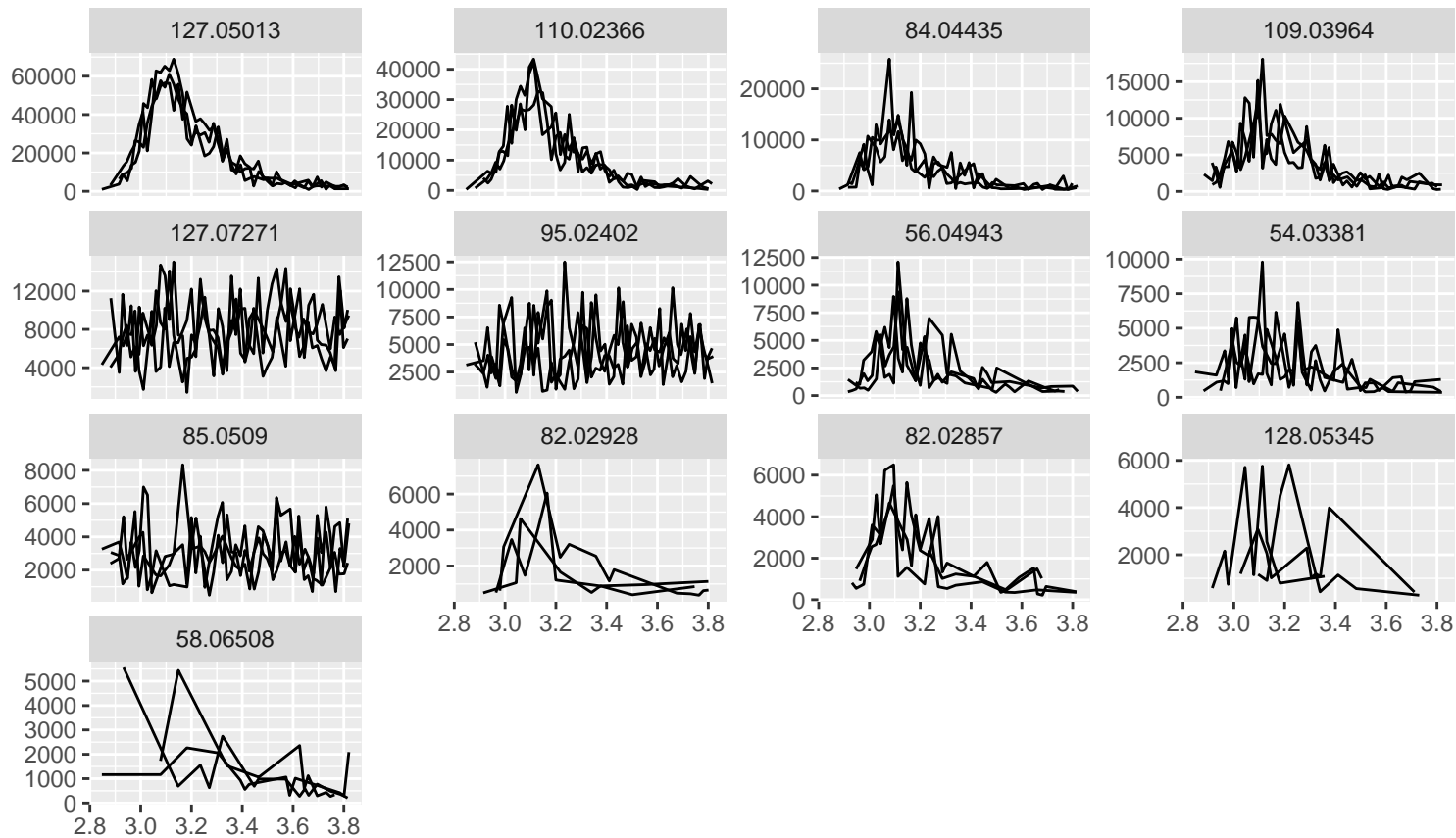
Isethionic acid (neg) 124.991406



rt

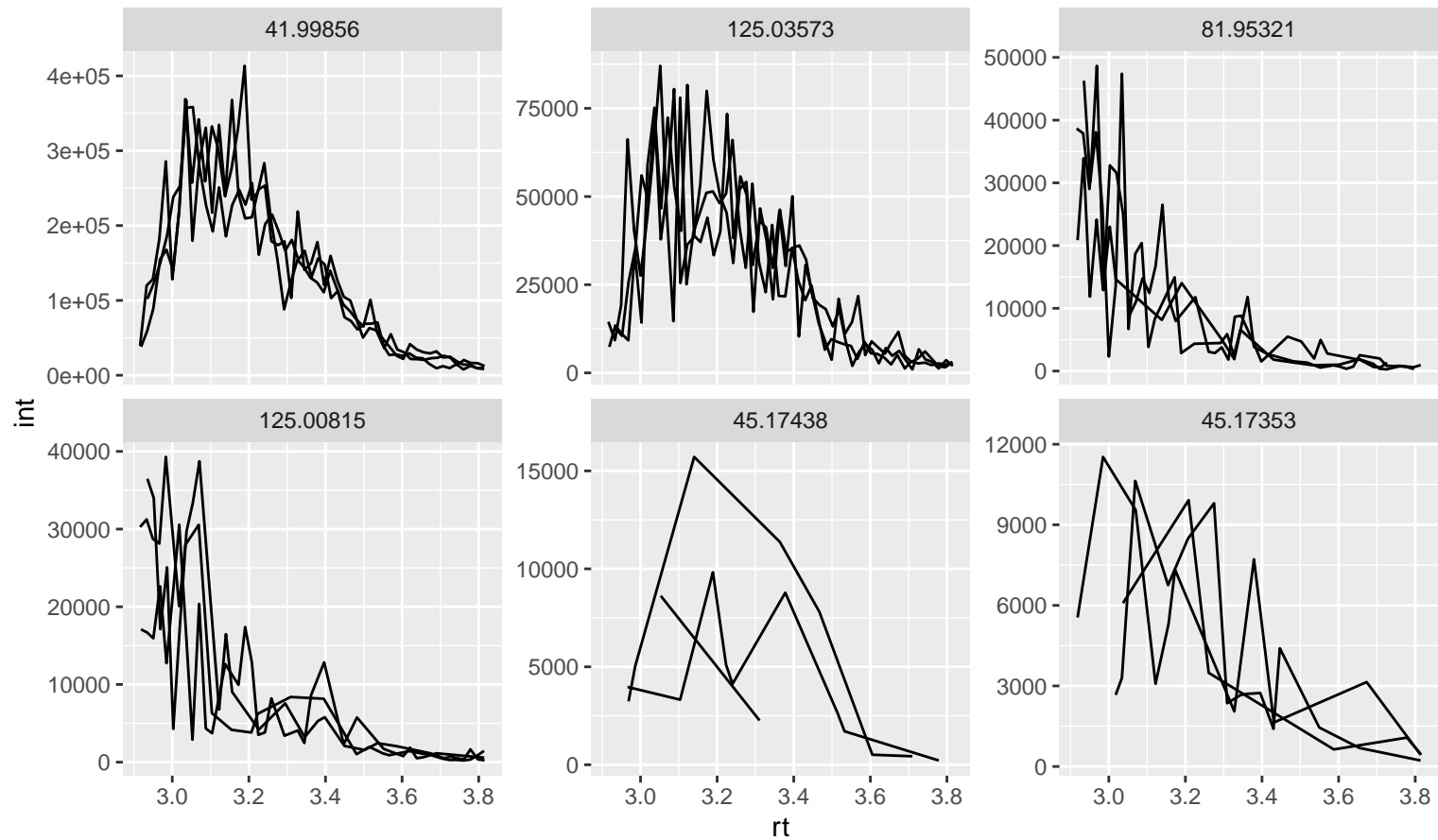
Thymine (pos) 127.050204

int



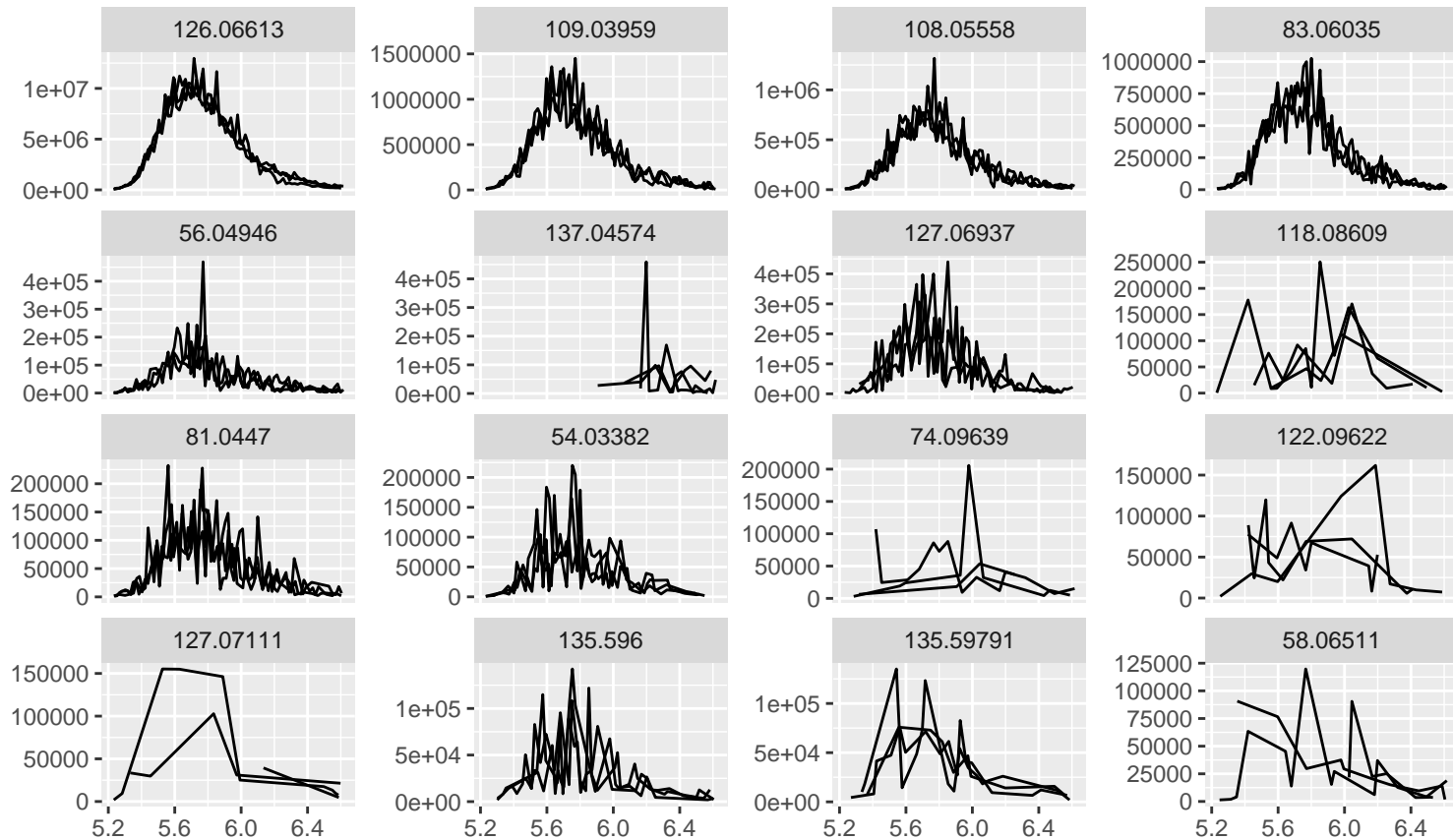
rt

Thymine (neg) 125.035652



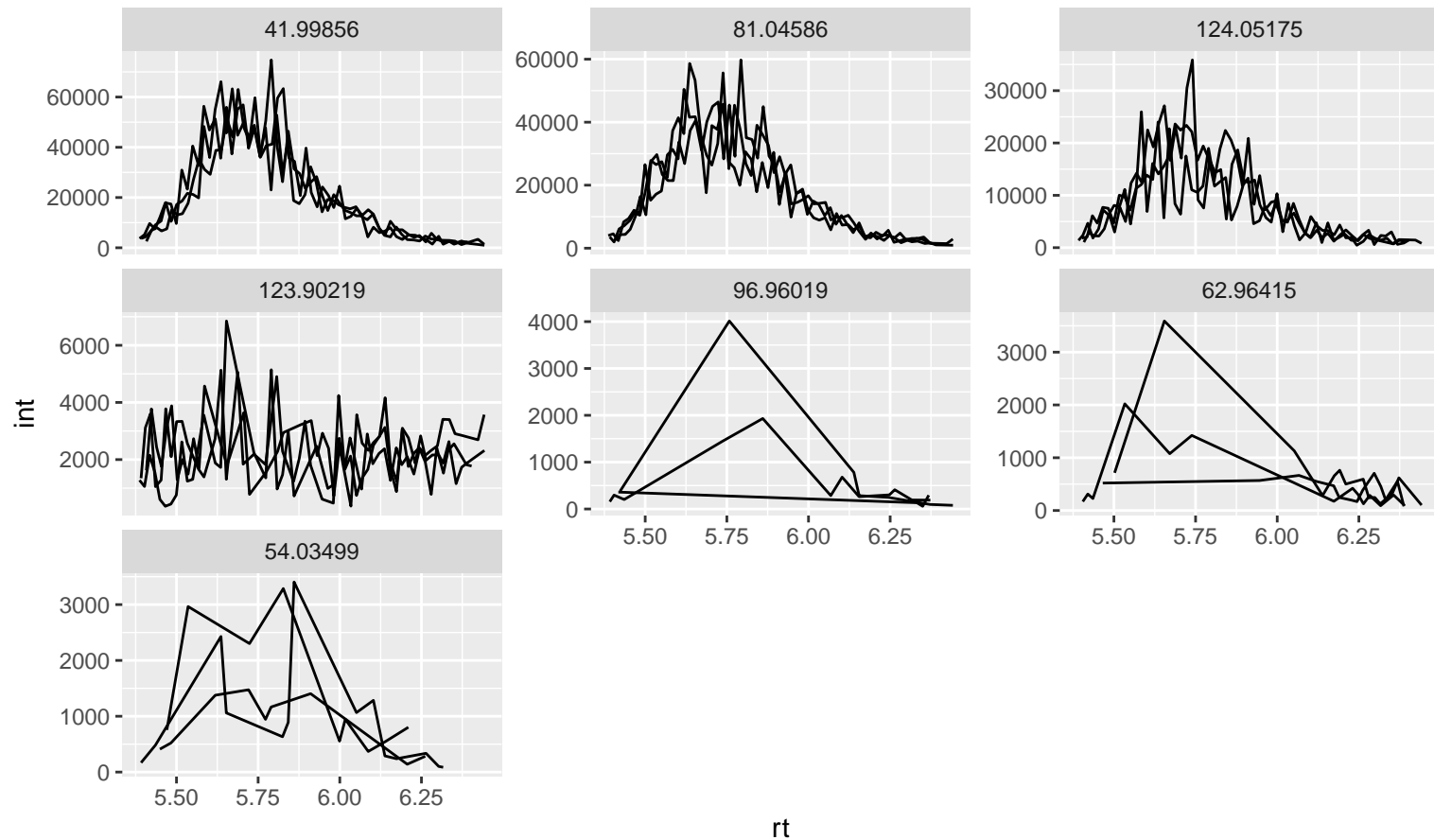
5-Methylcytosine (pos) 126.066188

int

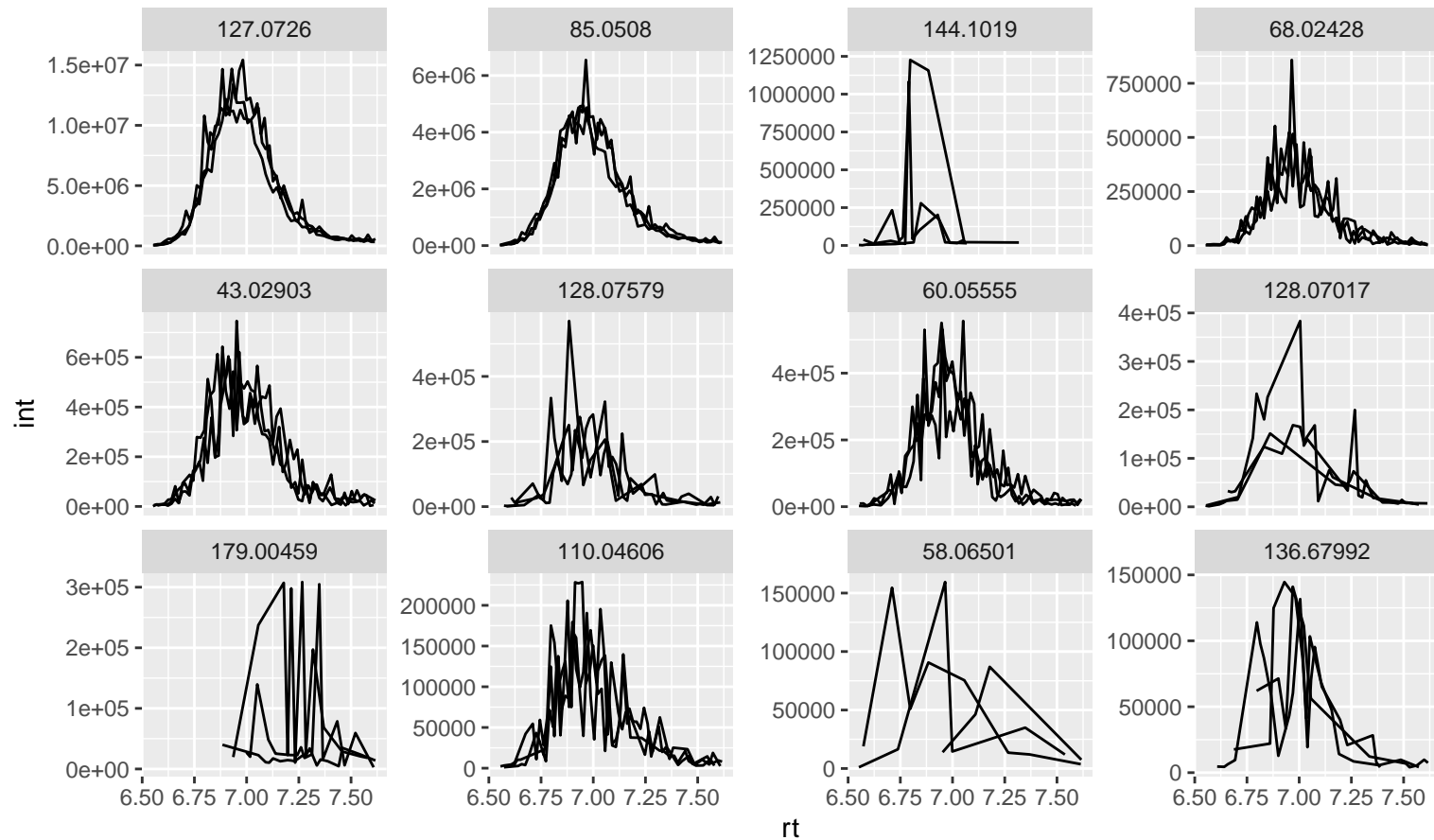


rt

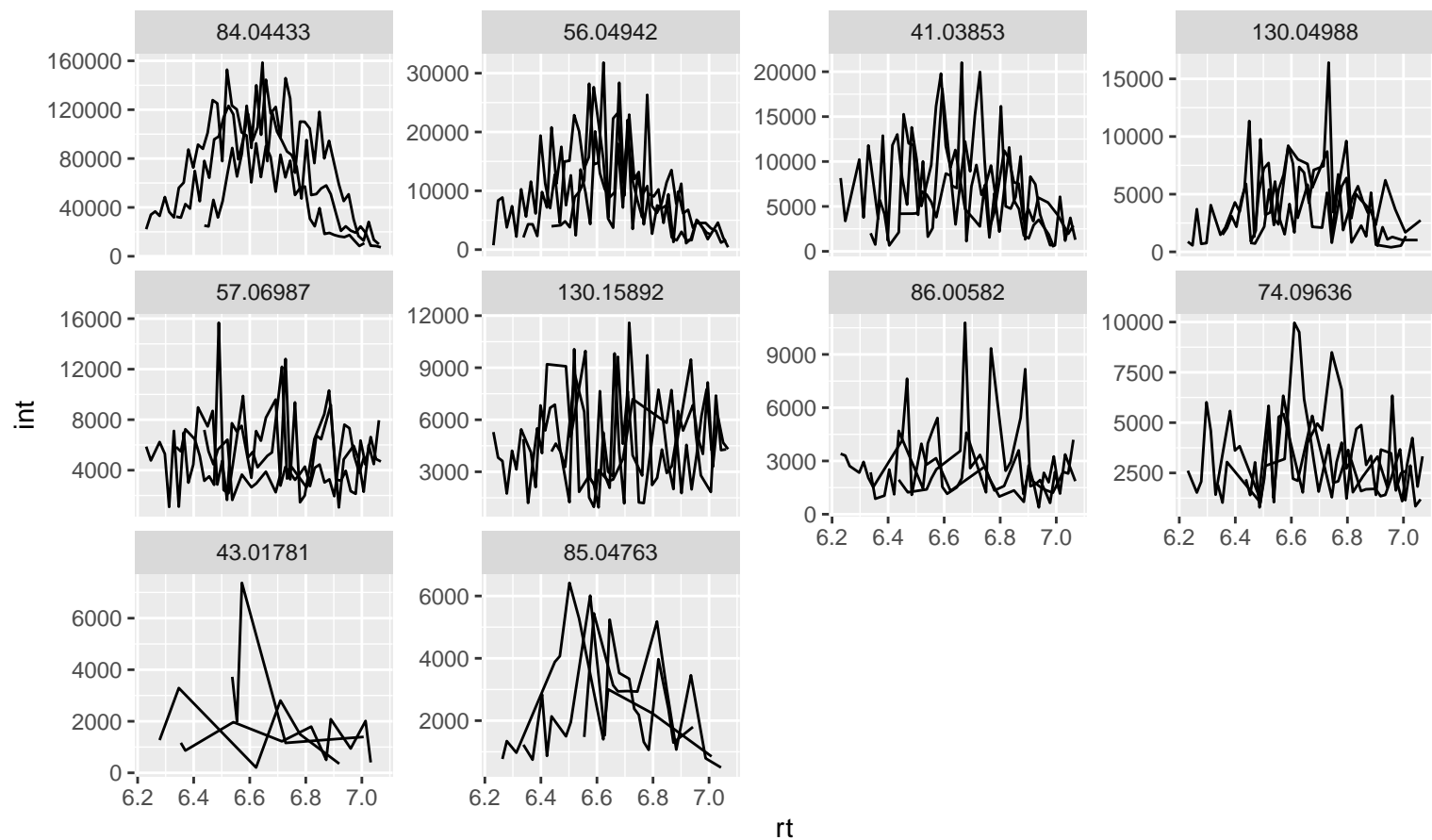
5-Methylcytosine (neg) 124.051636



Melamine (pos) 127.07267

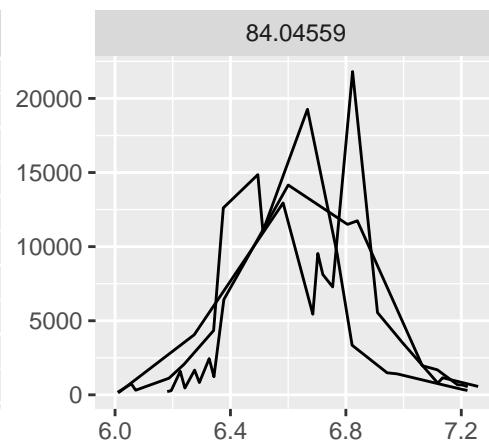
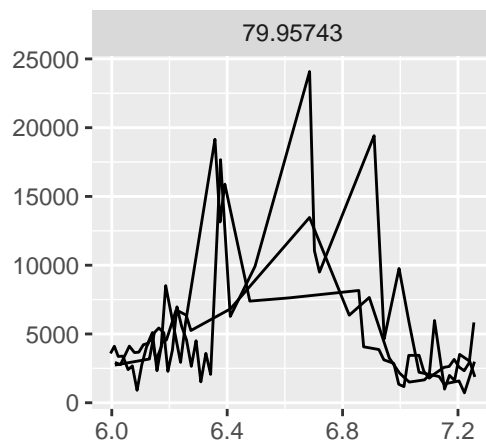
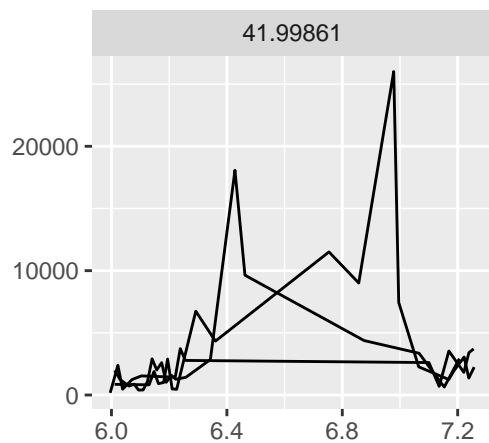
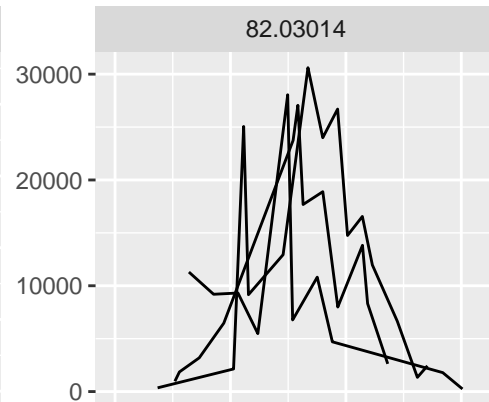
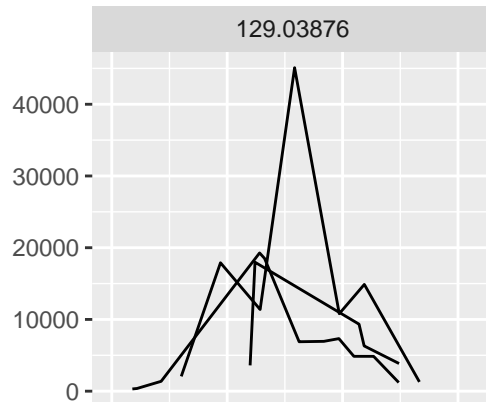
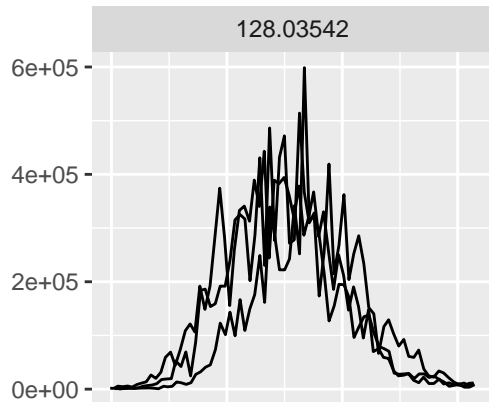


5-Oxoproline (pos) 130.04987



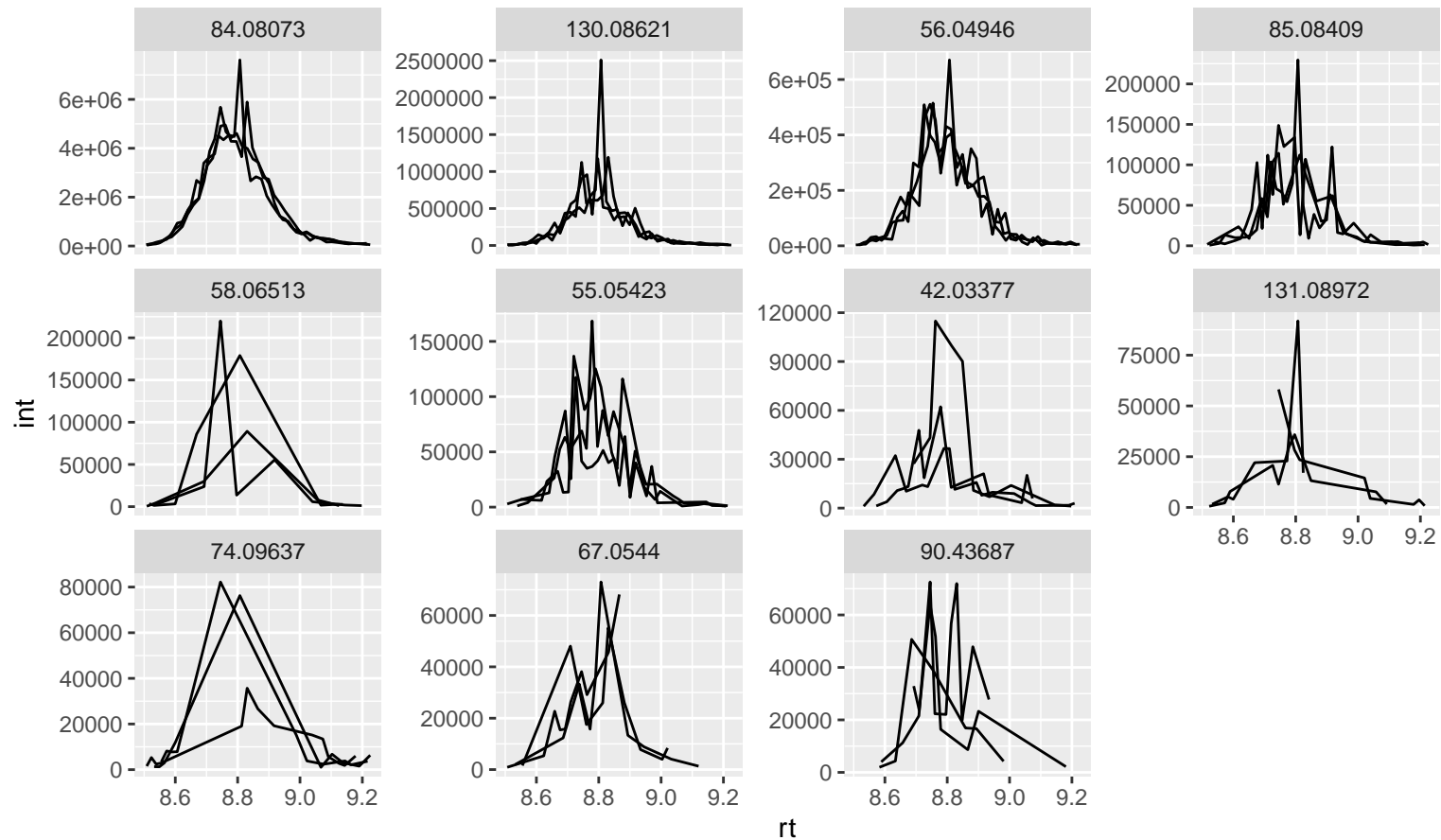
5-Oxoprolone (neg) 128.035318

int

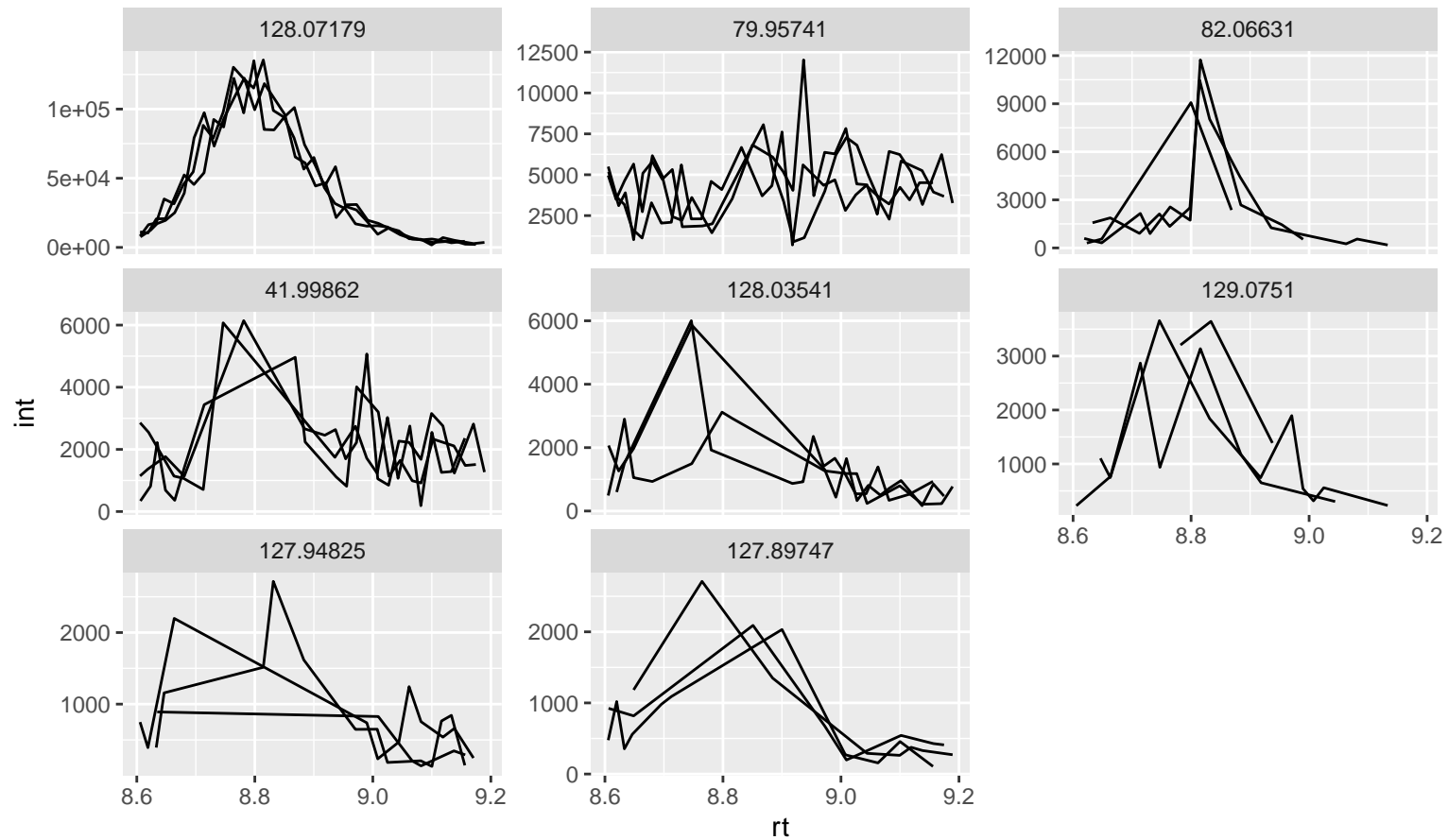


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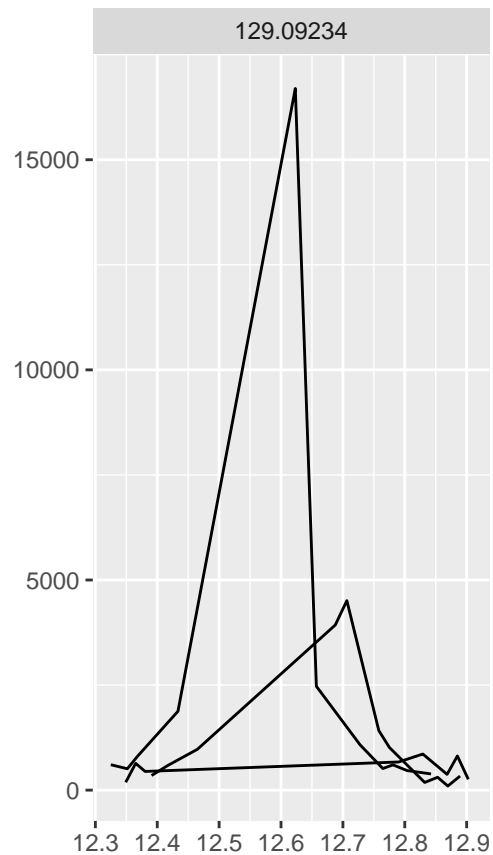
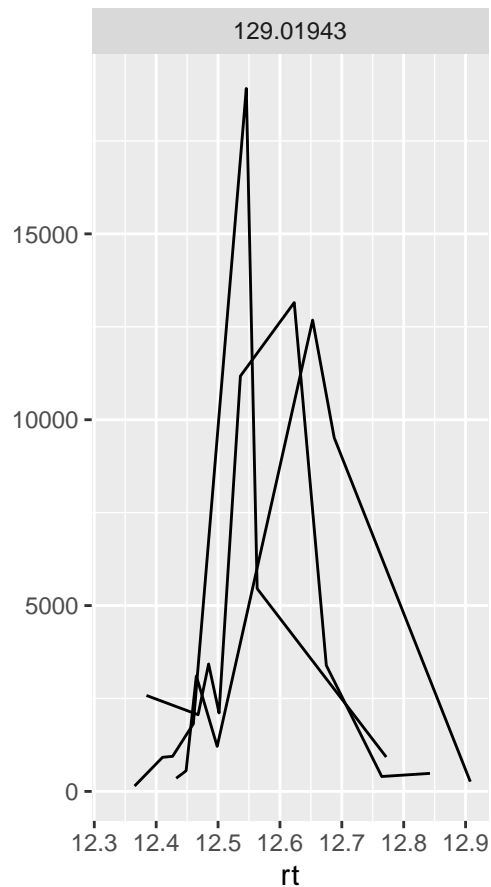
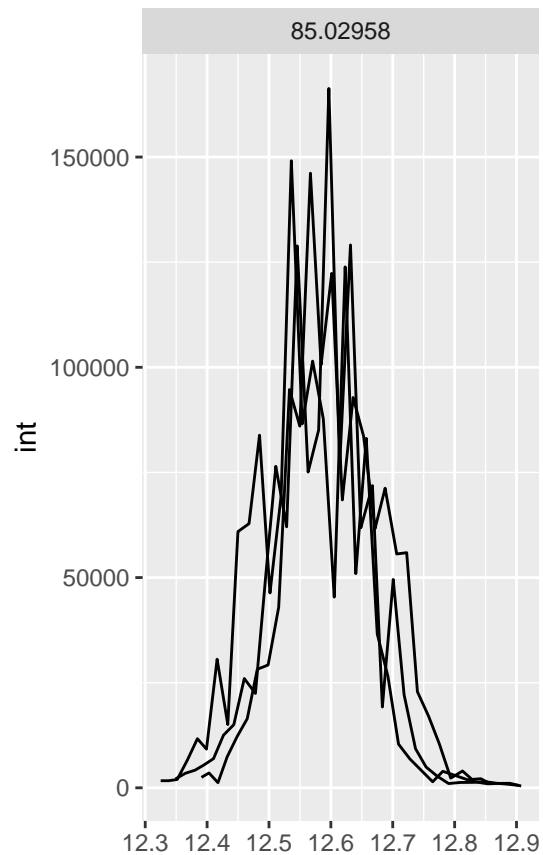
Pipecolic acid (pos) 130.086255



Pipecolic acid (neg) 128.071703

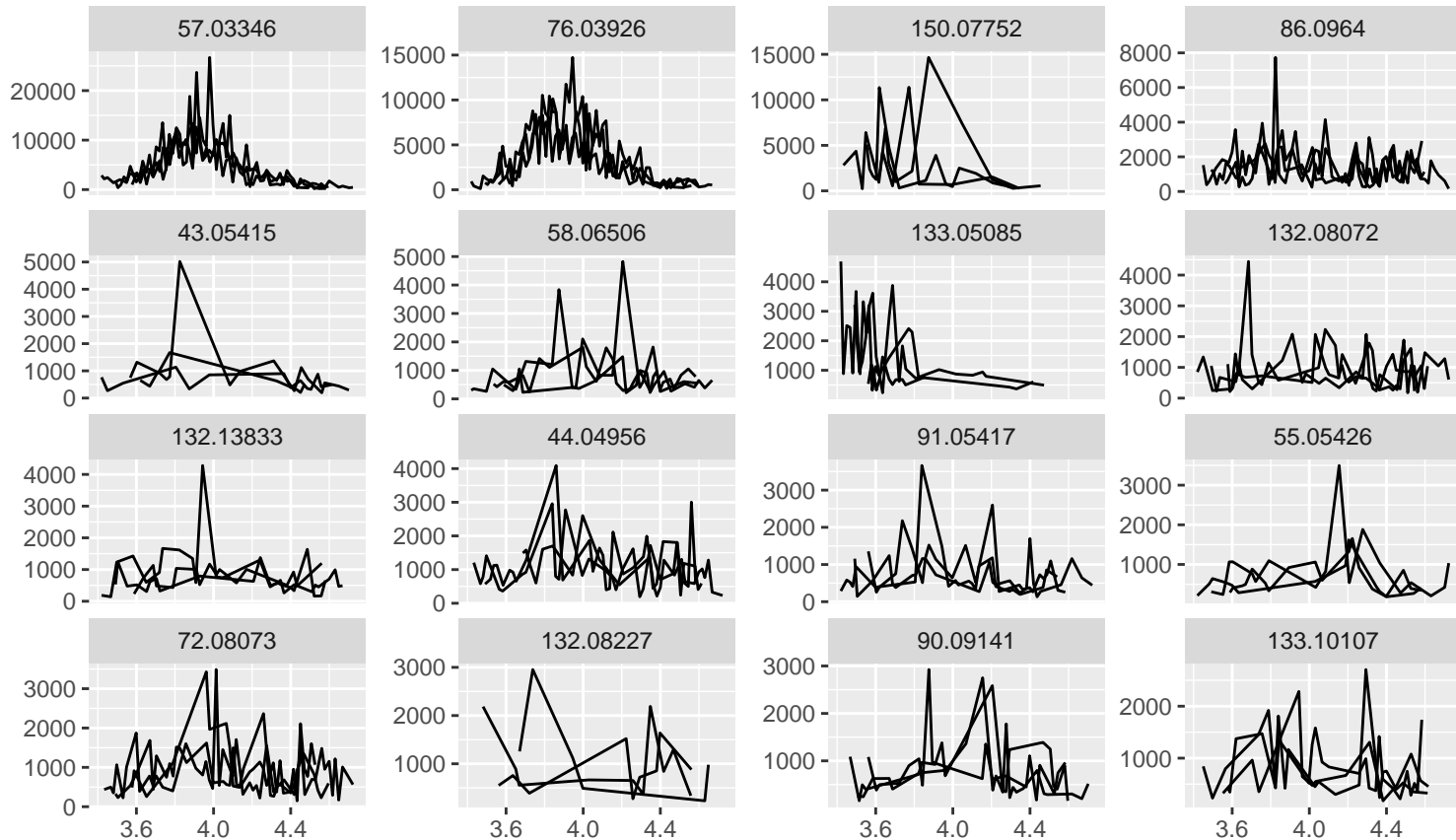


Itaconic acid (neg) 129.019334



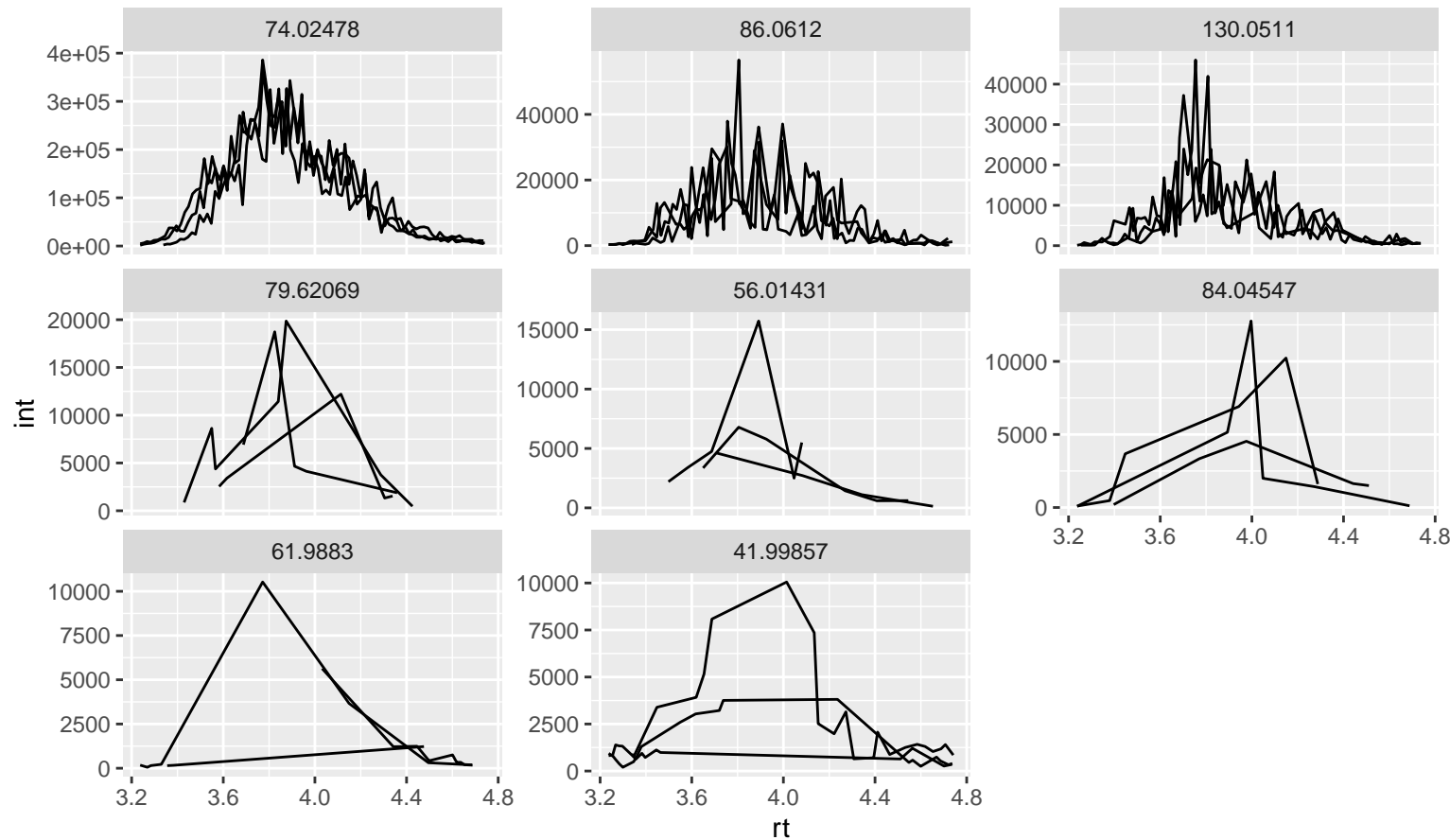
Propionylglycine (pos) 132.06552

int

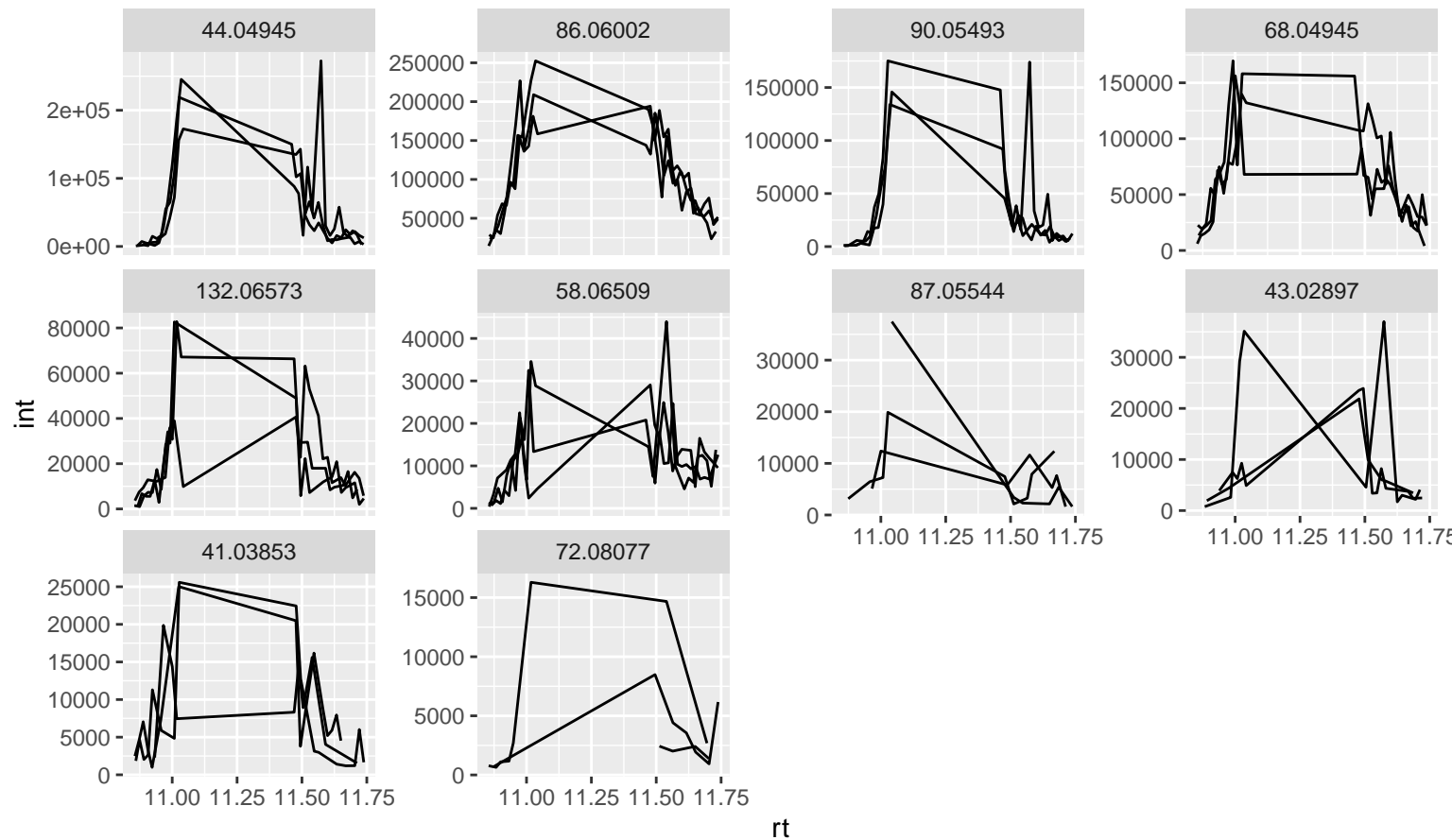


rt

Propionylglycine (neg) 130.050968

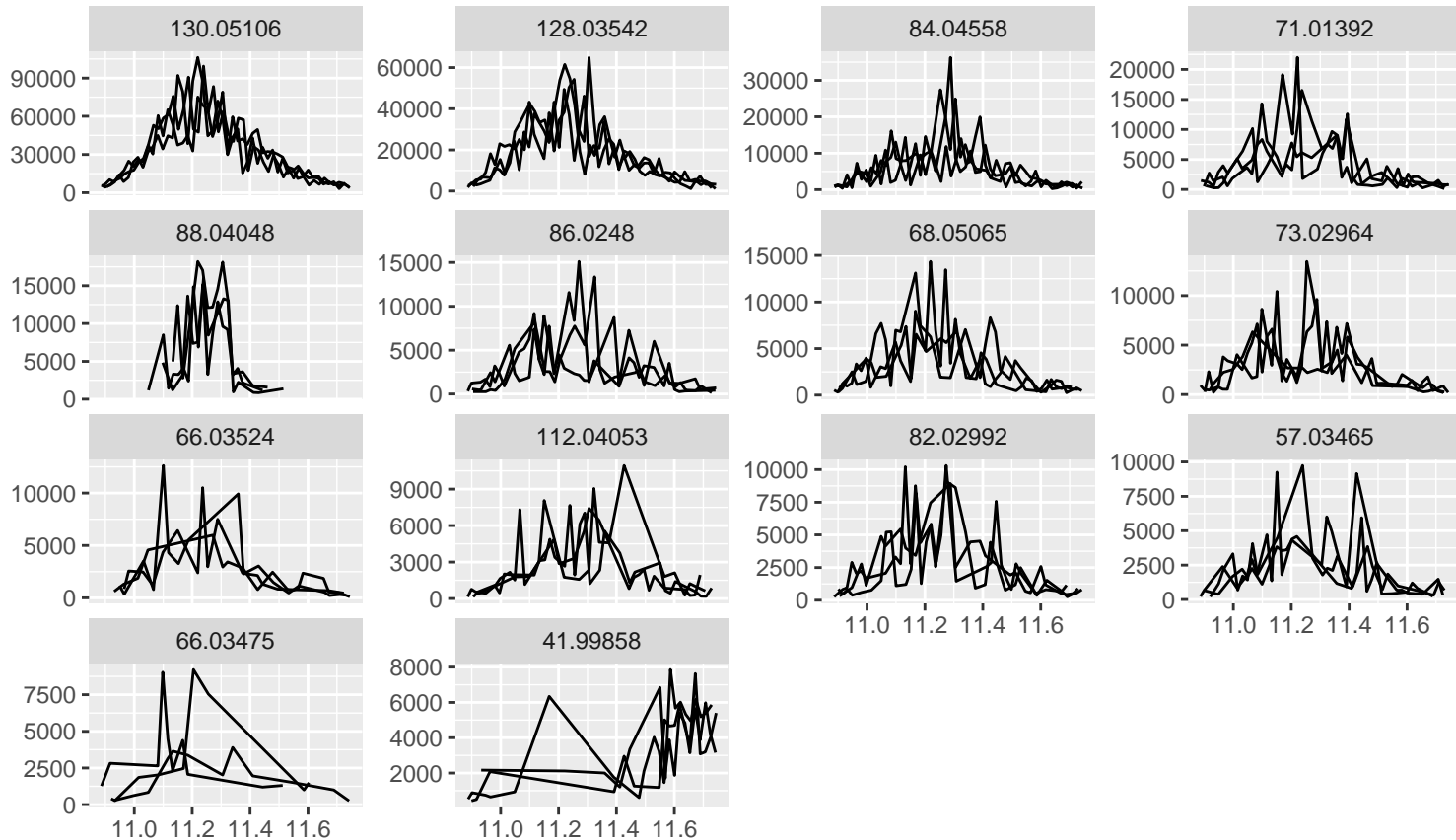


Hydroxyproline (pos) 132.06552



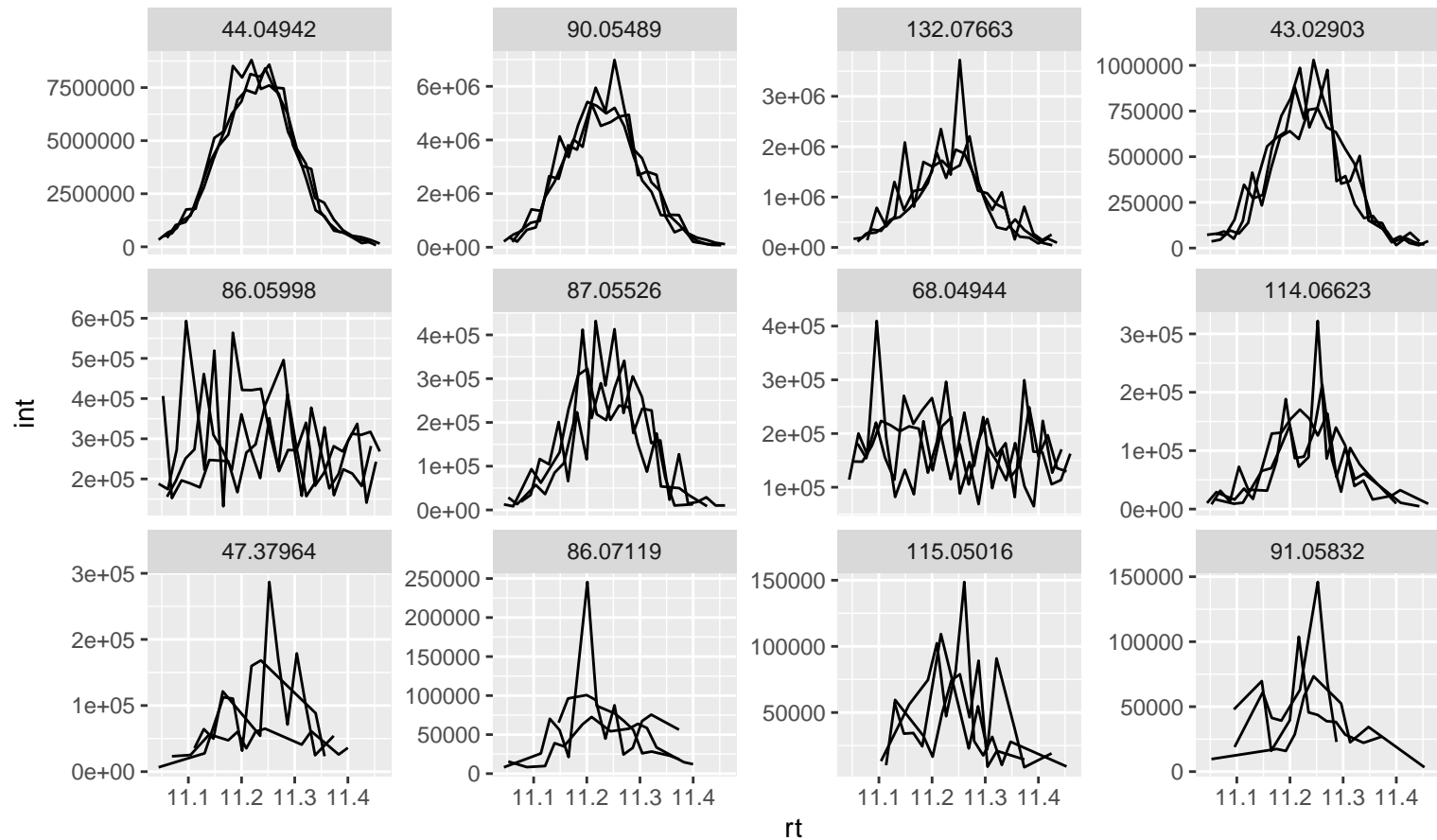
Hydroxyproline (neg) 130.050968

int

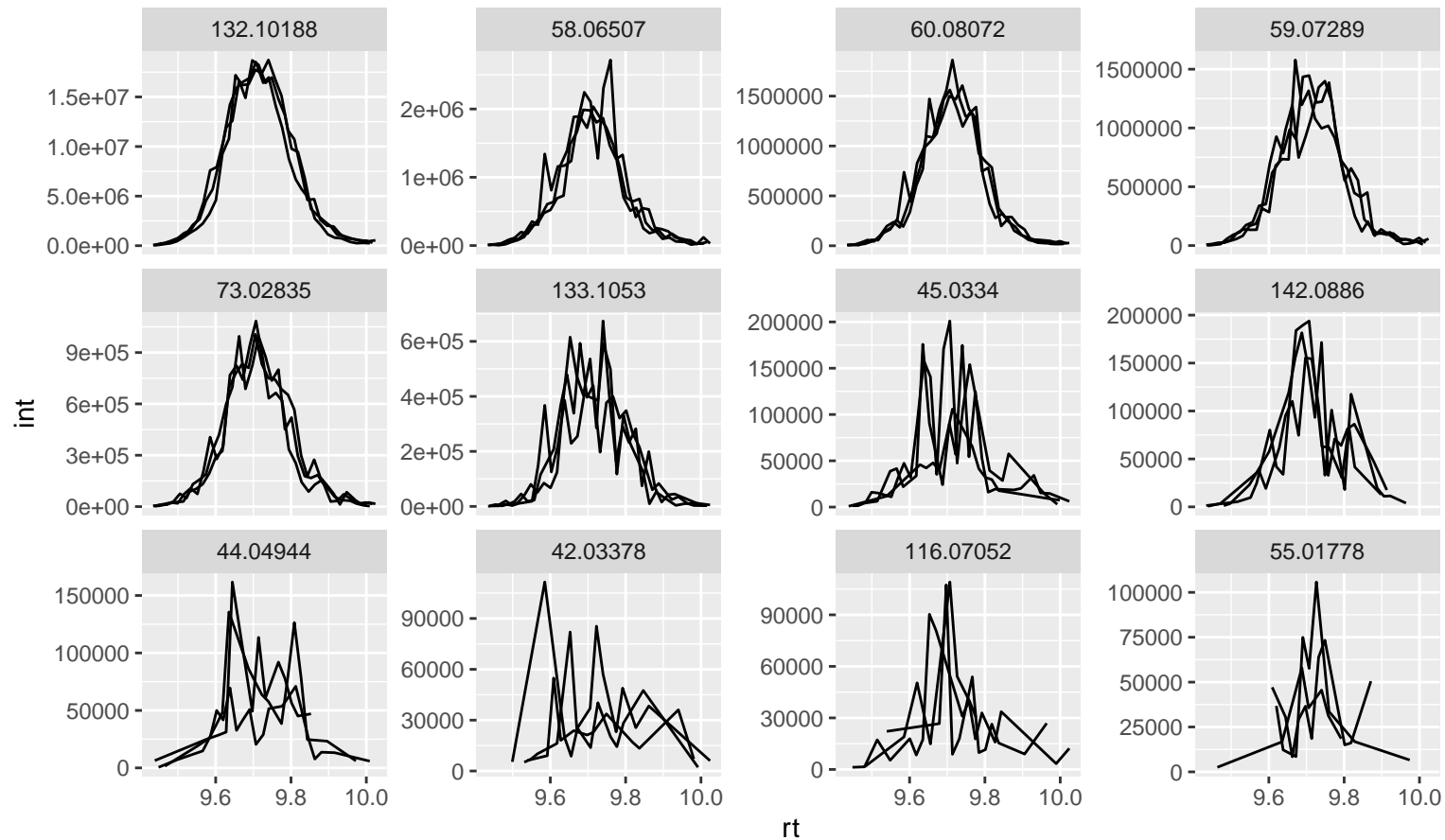


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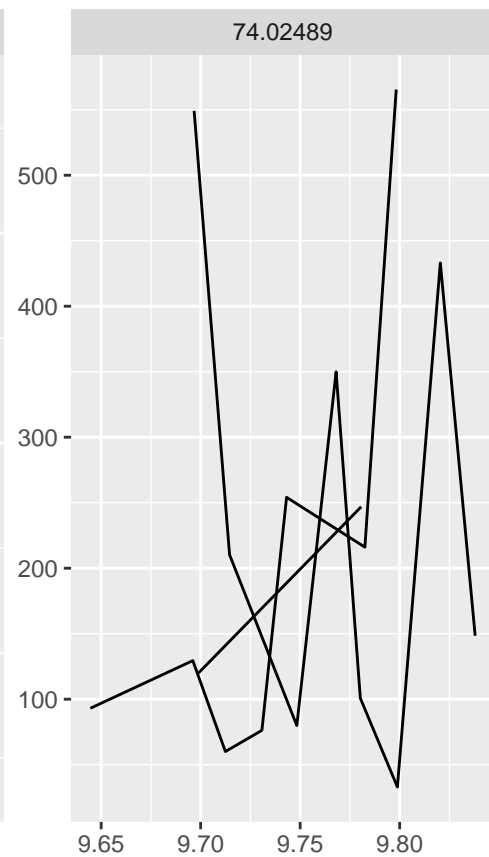
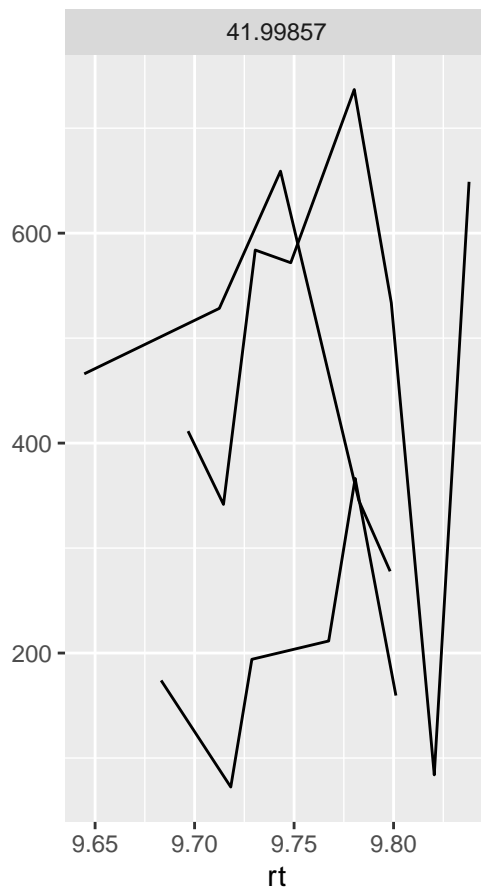
Creatine (pos) 132.076753



beta-Alaninebetaine (pos) 132.101905

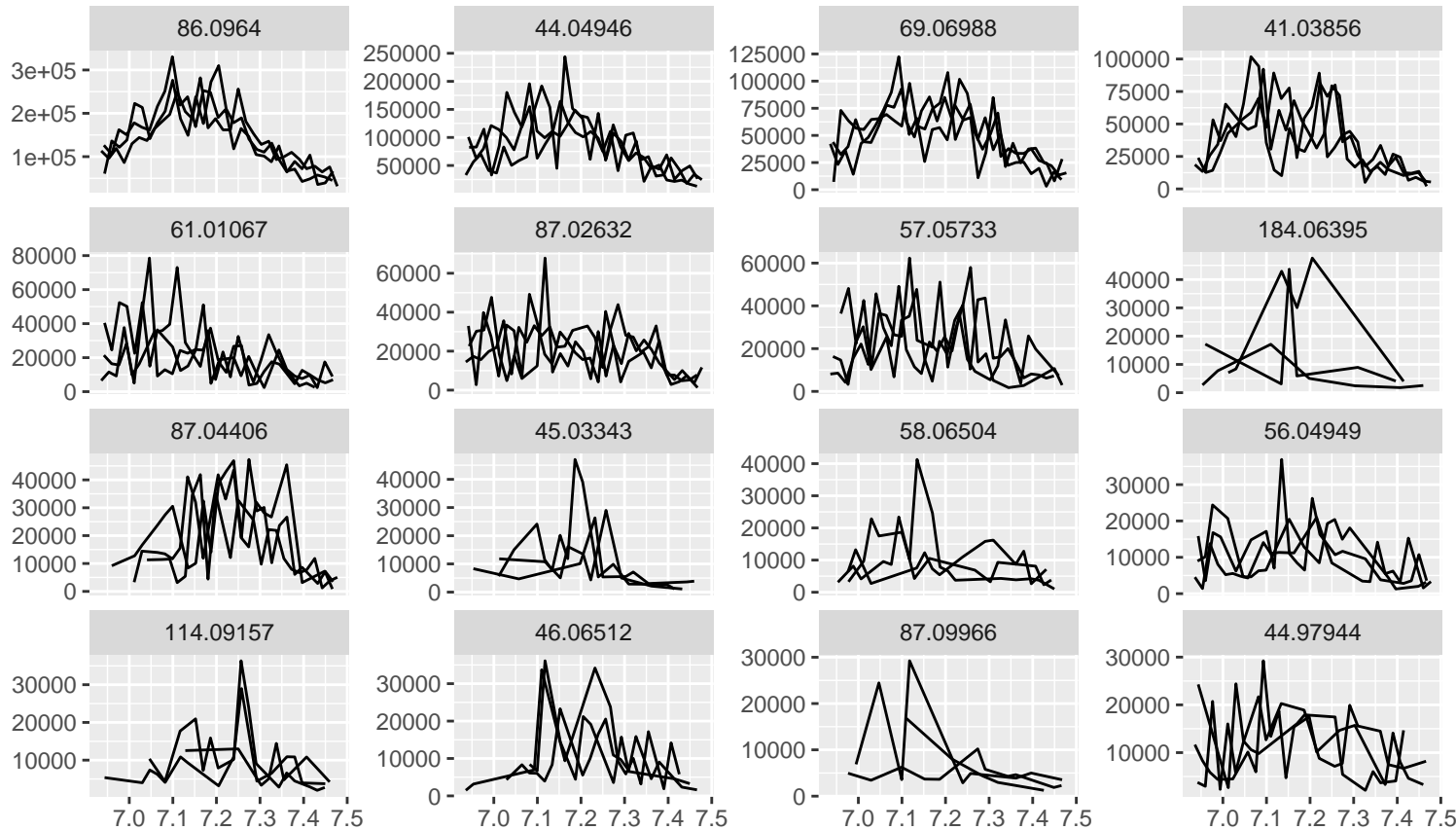


beta-Alaninebetaine (neg) 130.087353



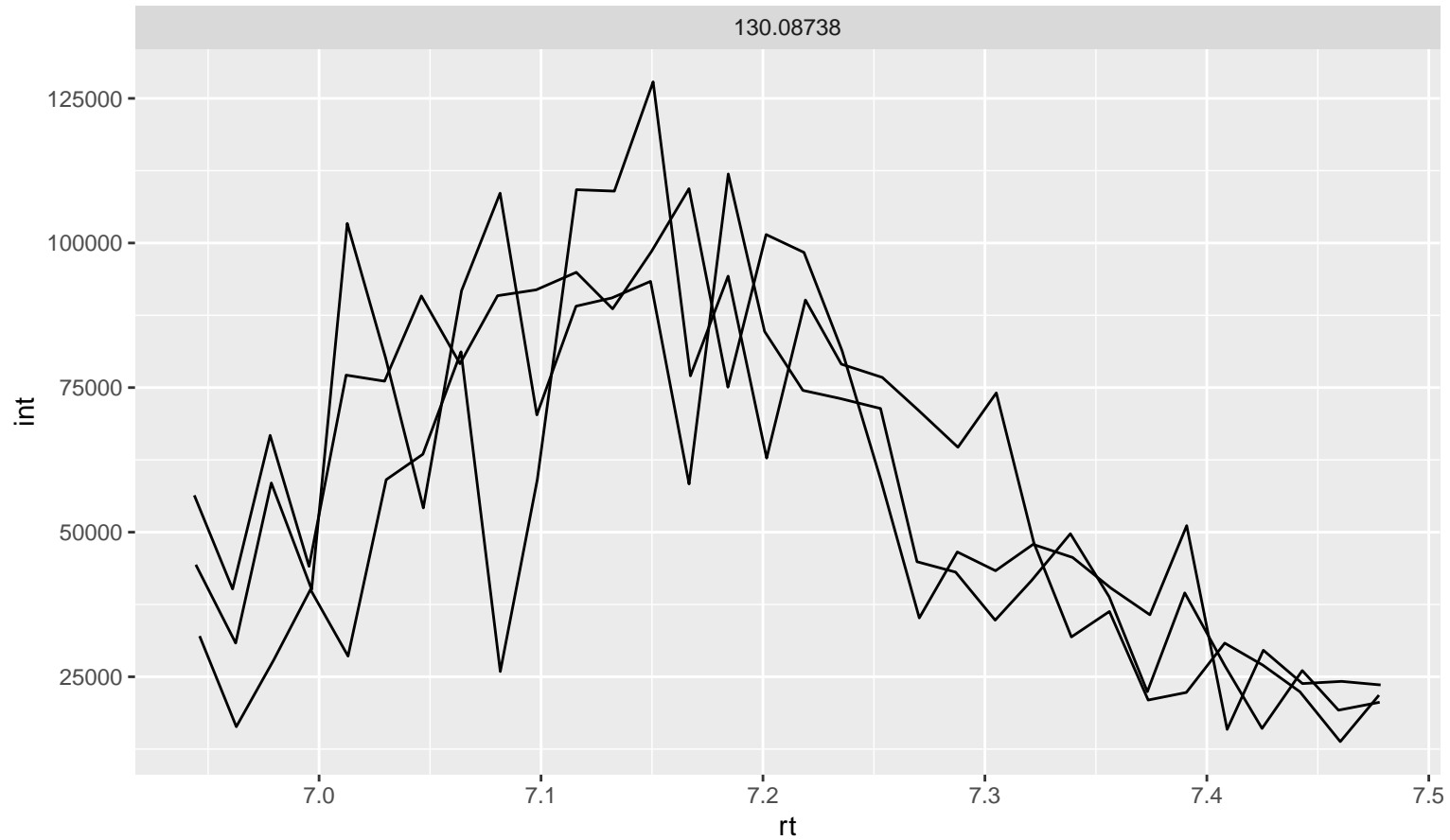
L-Isoleucine (pos) 132.101905

int

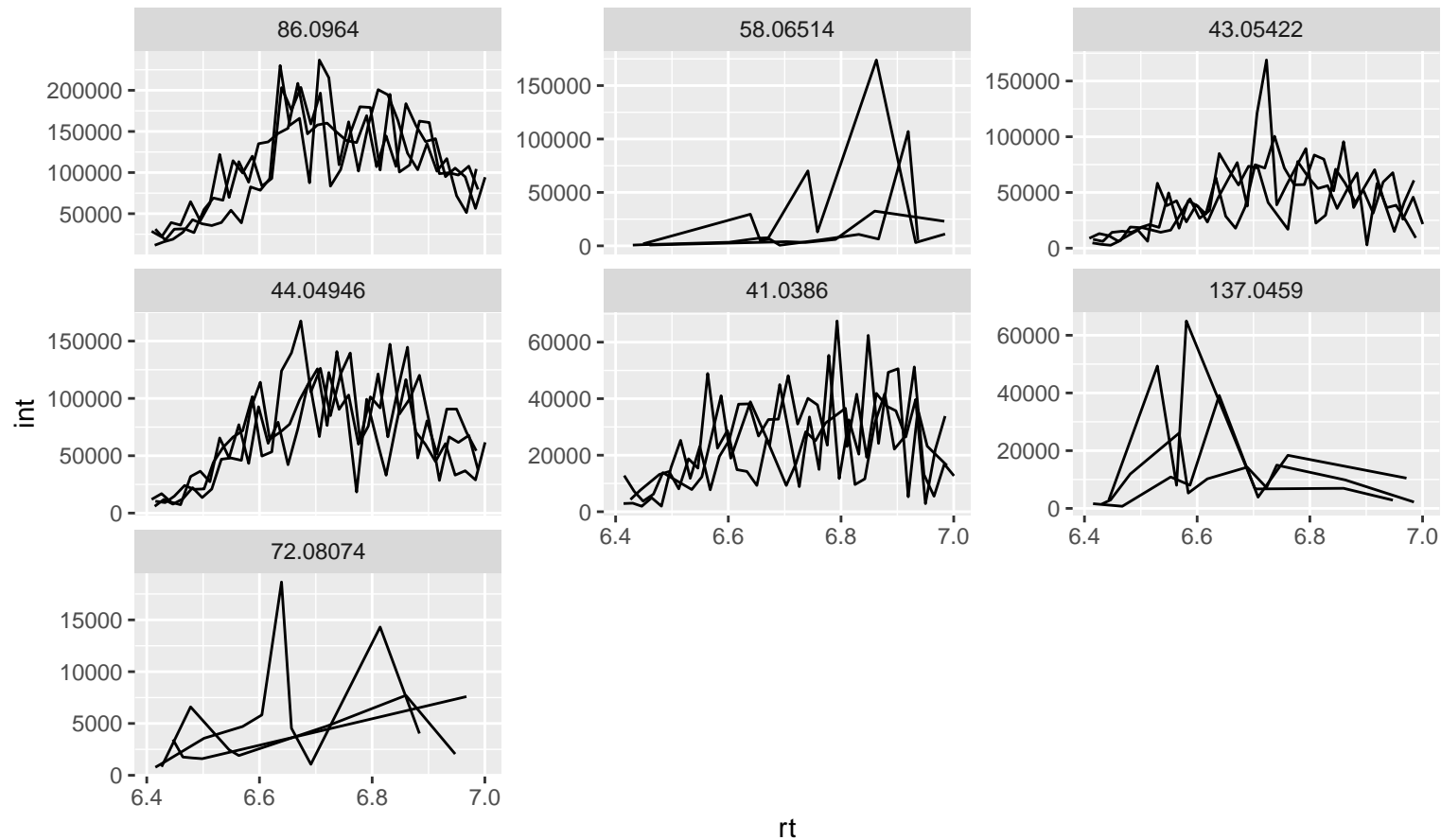


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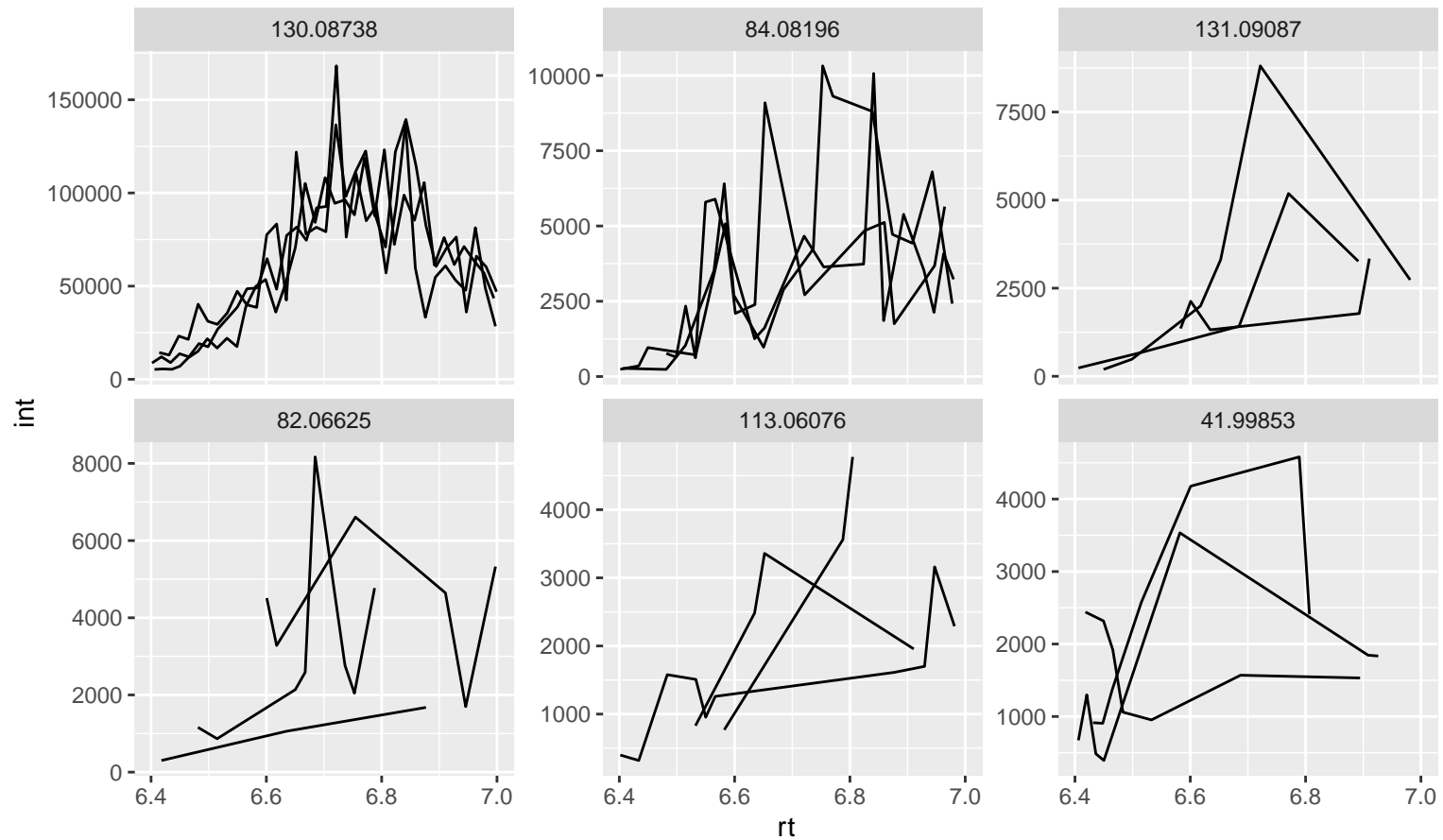
L-Isoleucine (neg) 130.087353



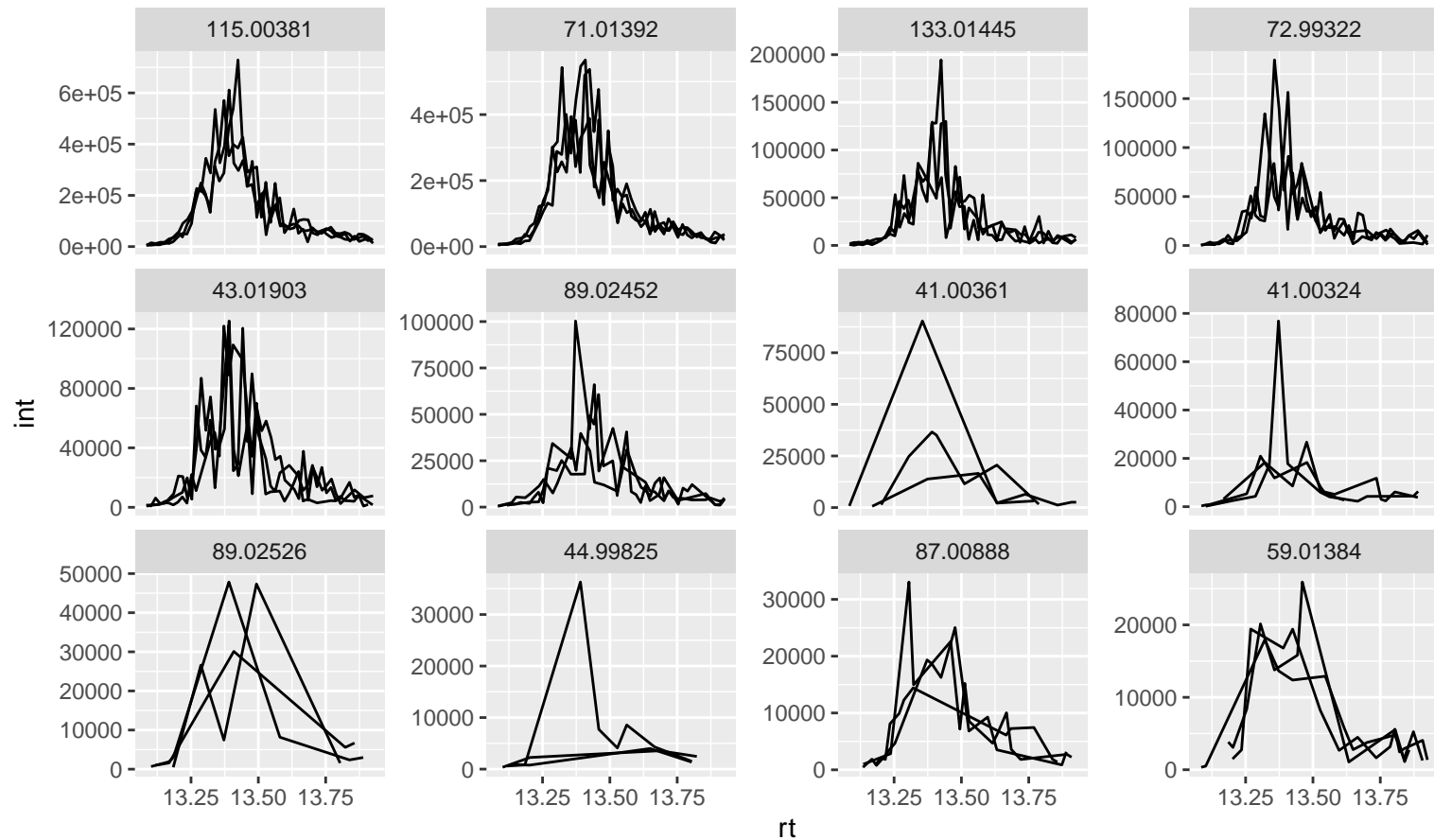
L-Leucine (pos) 132.101905



L-Leucine (neg) 130.087353

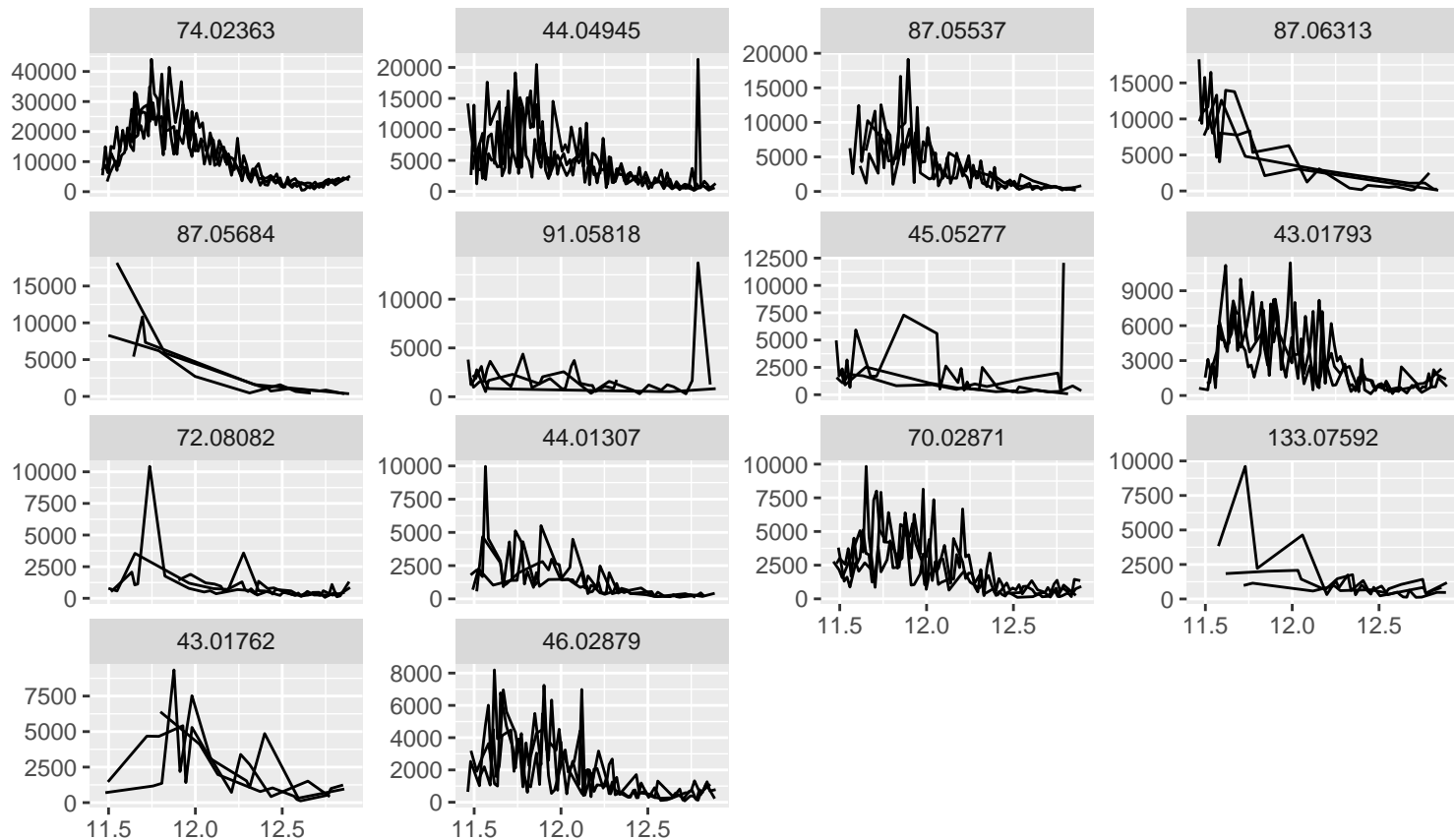


Malic acid (neg) 133.014249



L-Asparagine (pos) 133.060769

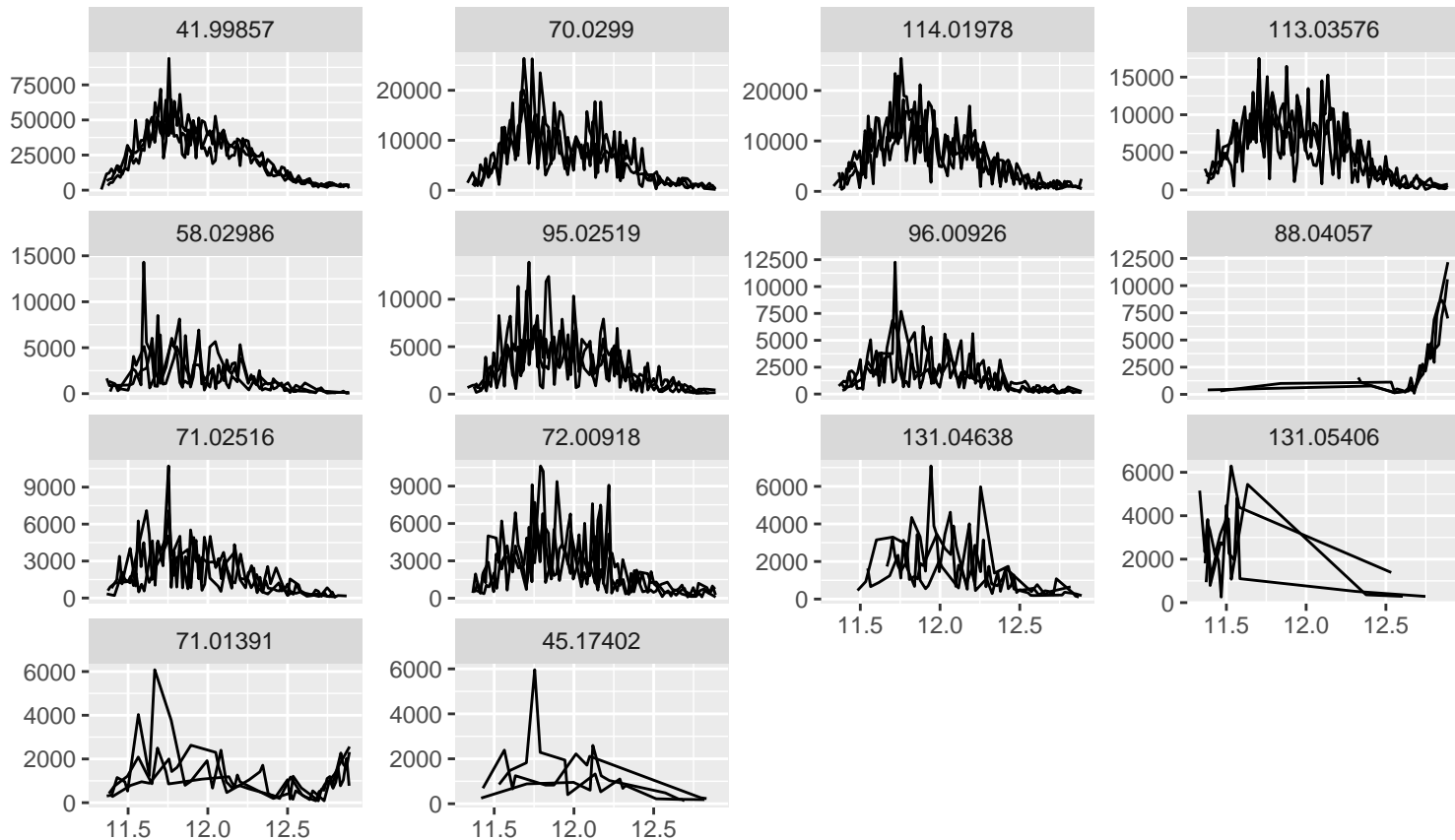
int



rt

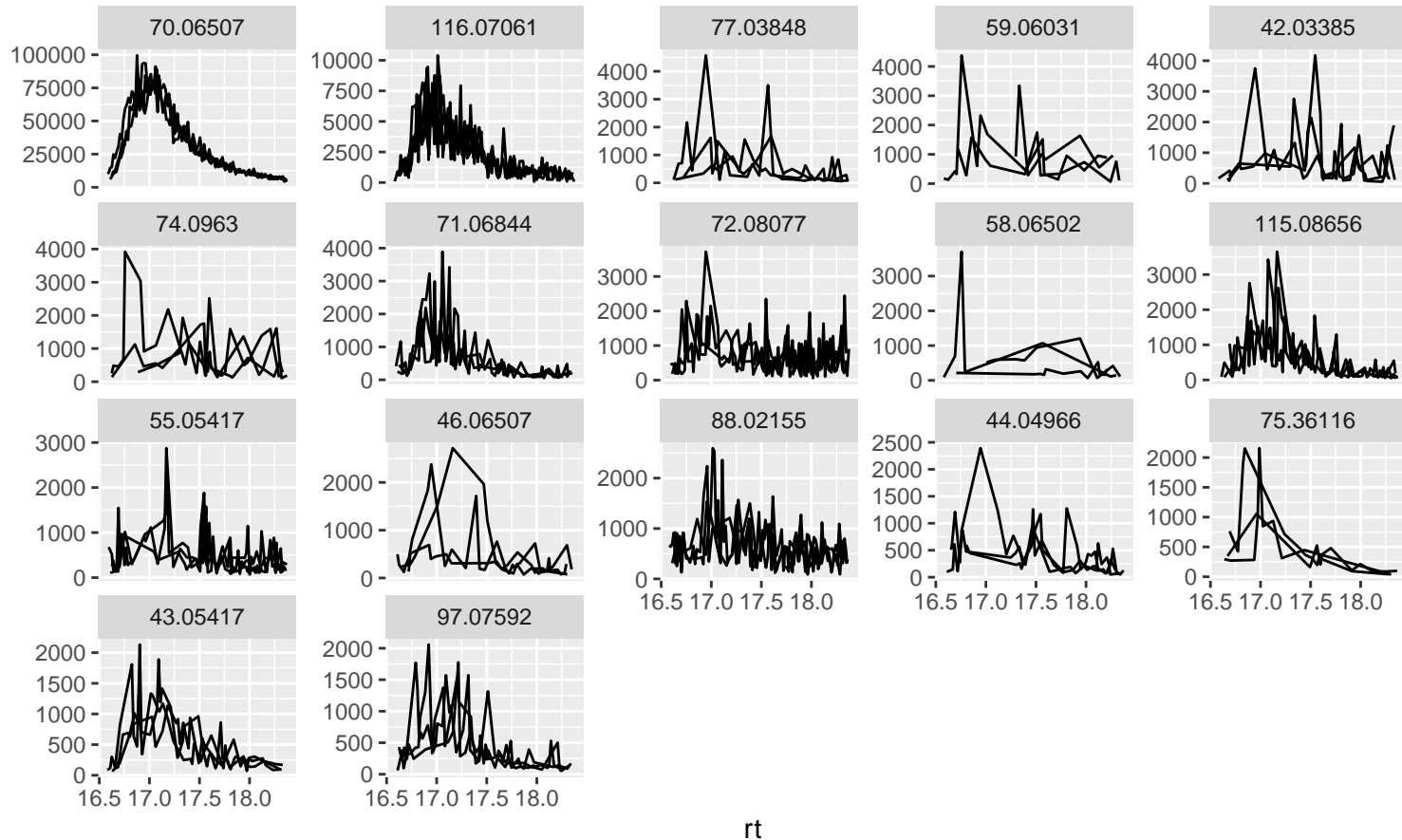
L-Asparagine (neg) 131.046217

int

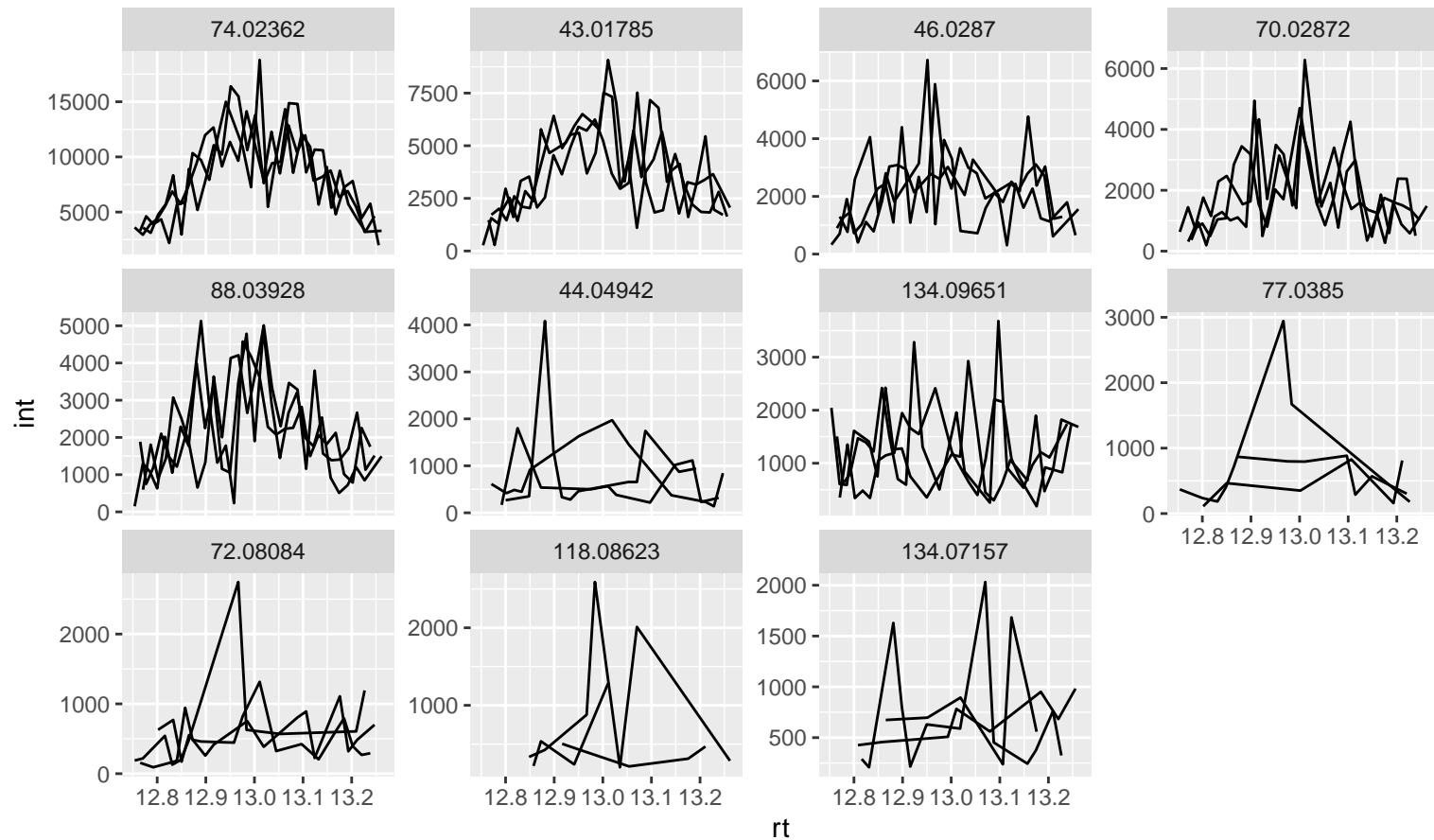


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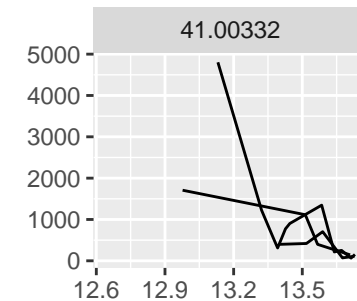
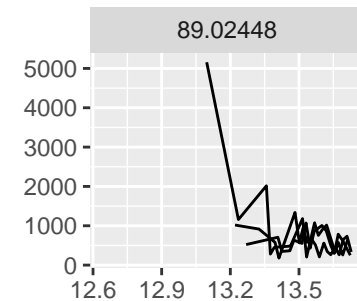
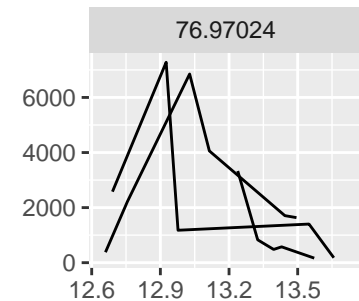
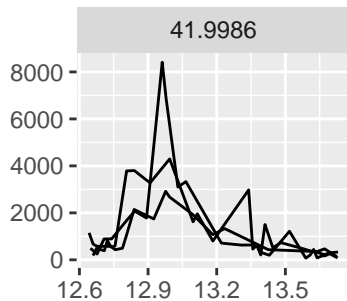
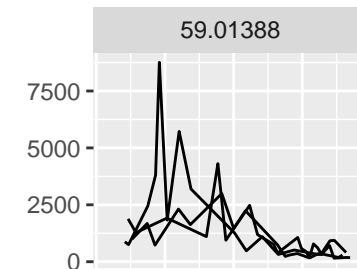
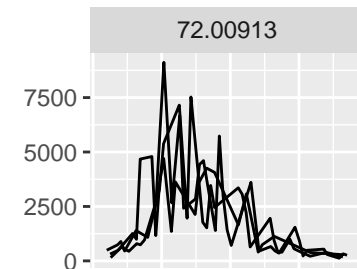
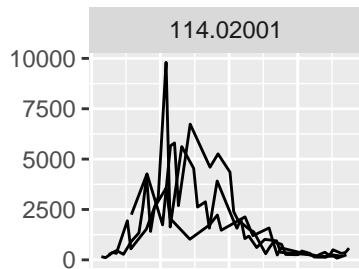
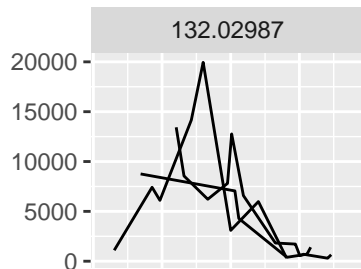
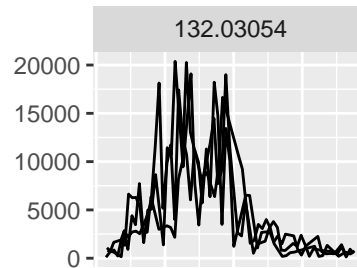
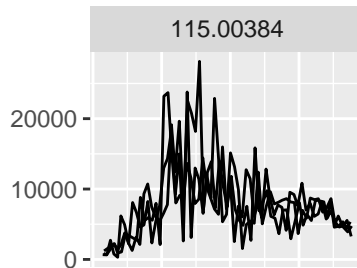
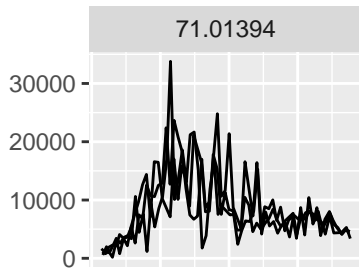
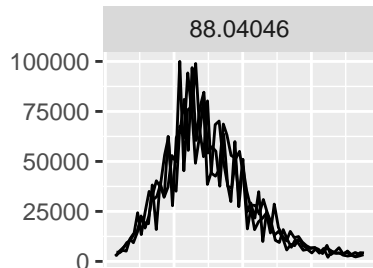
L-Ornithine (pos) 133.097154



L-Aspartic acid (pos) 134.044785

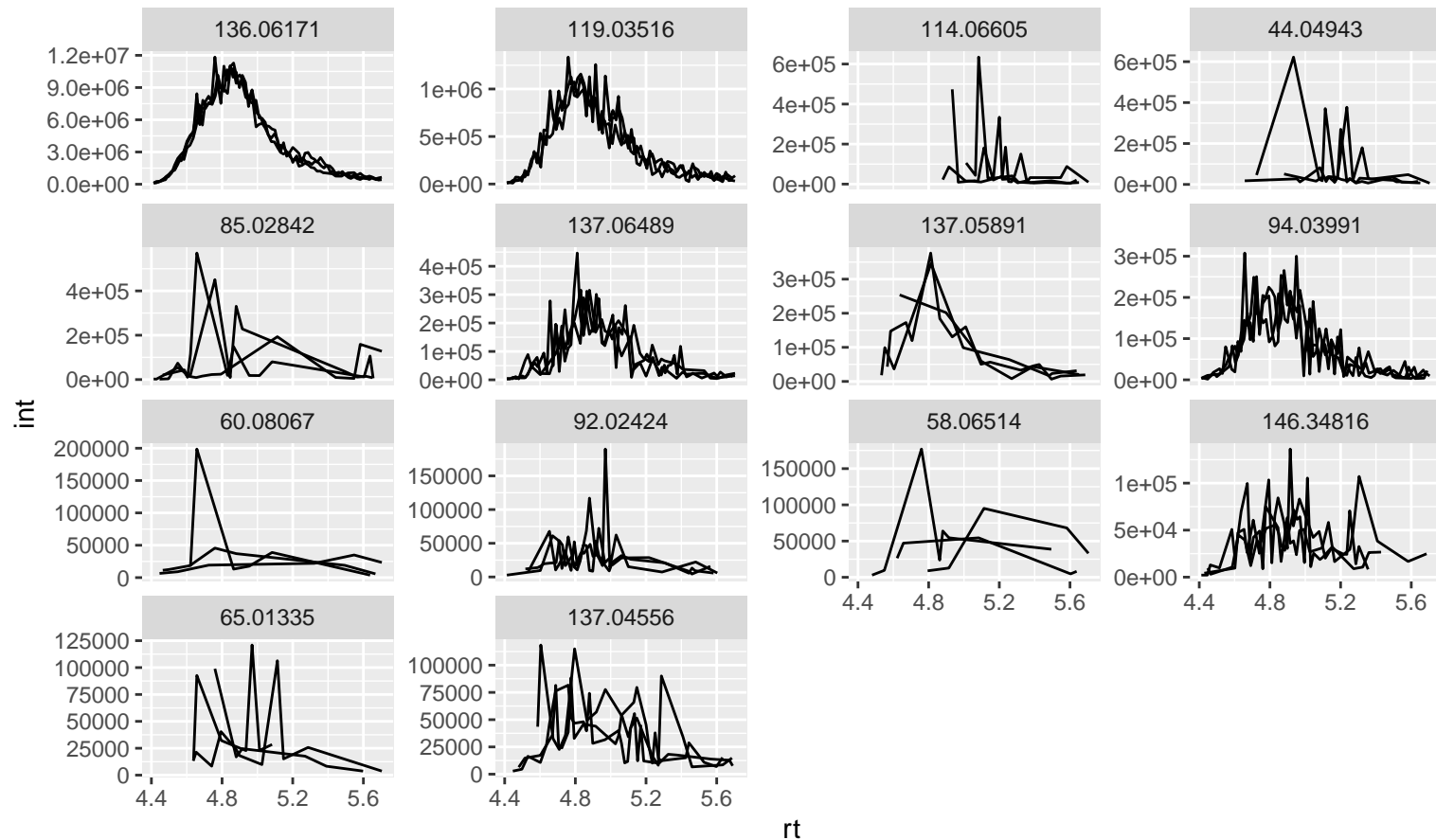


L-Aspartic acid (neg) 132.030233

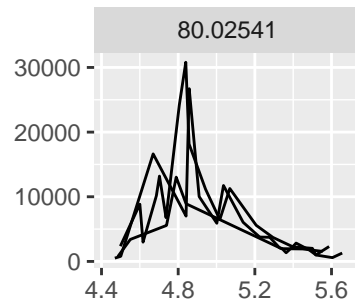
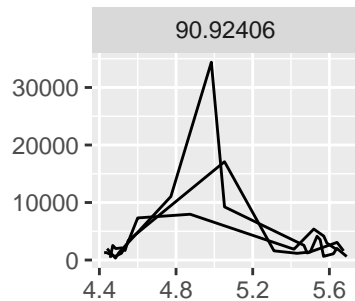
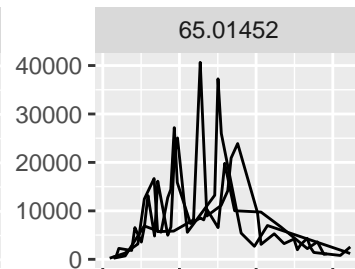
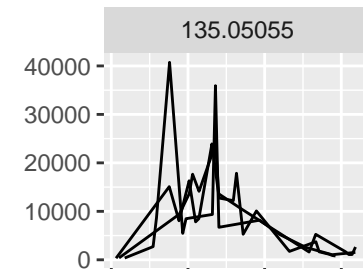
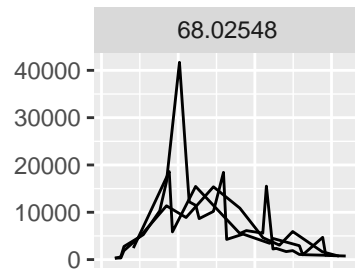
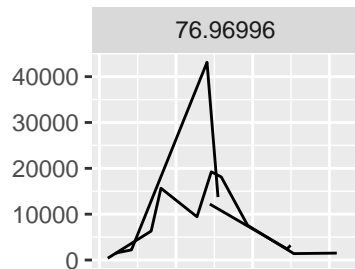
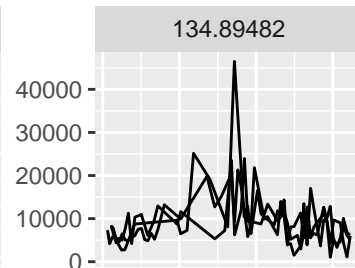
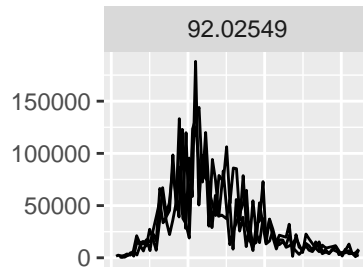
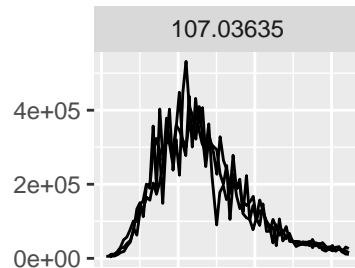
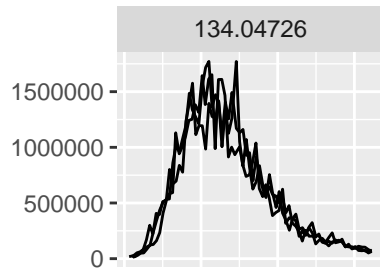


rt

Adenine (pos) 136.061771

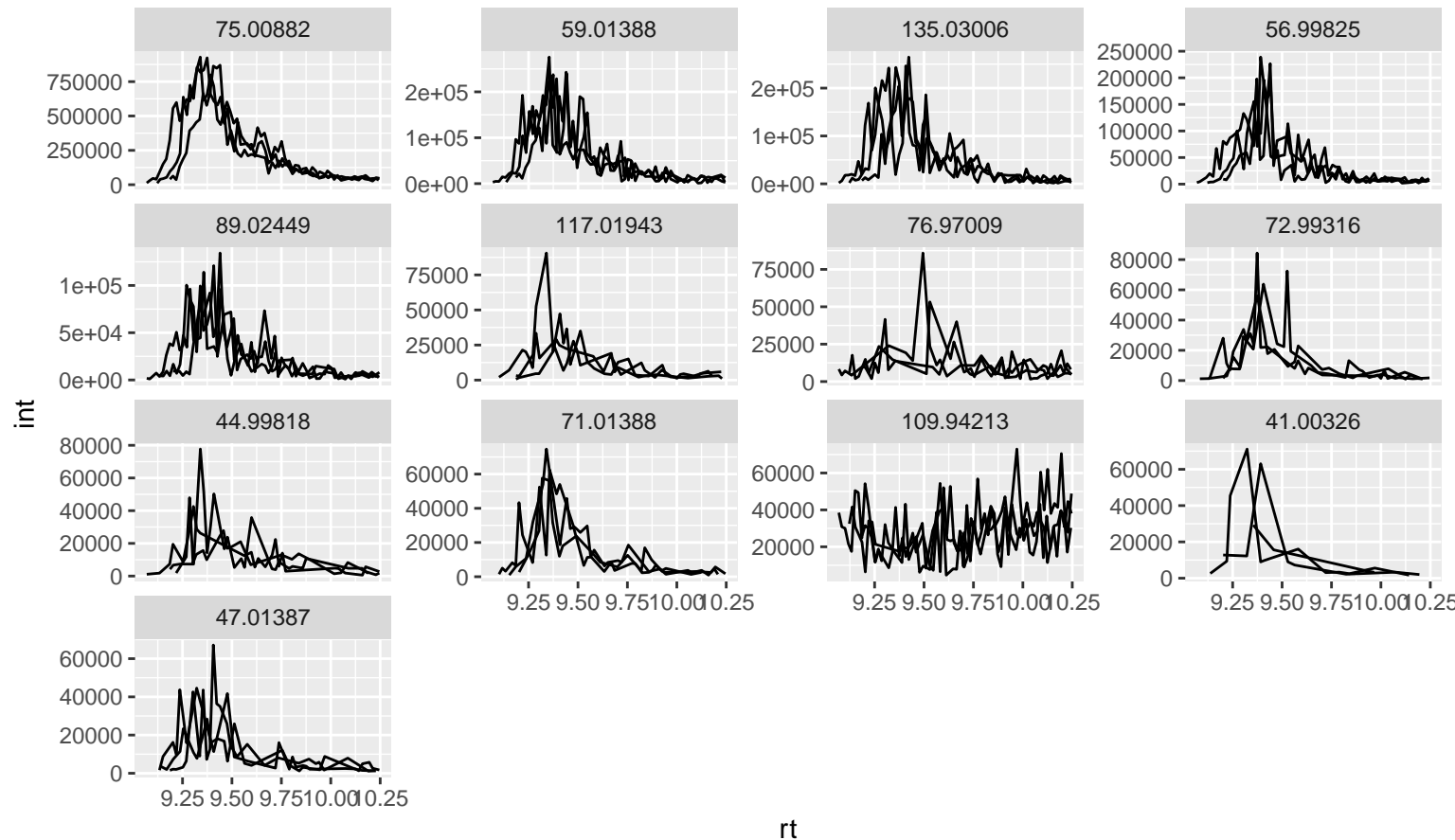


Adenine (neg) 134.047219

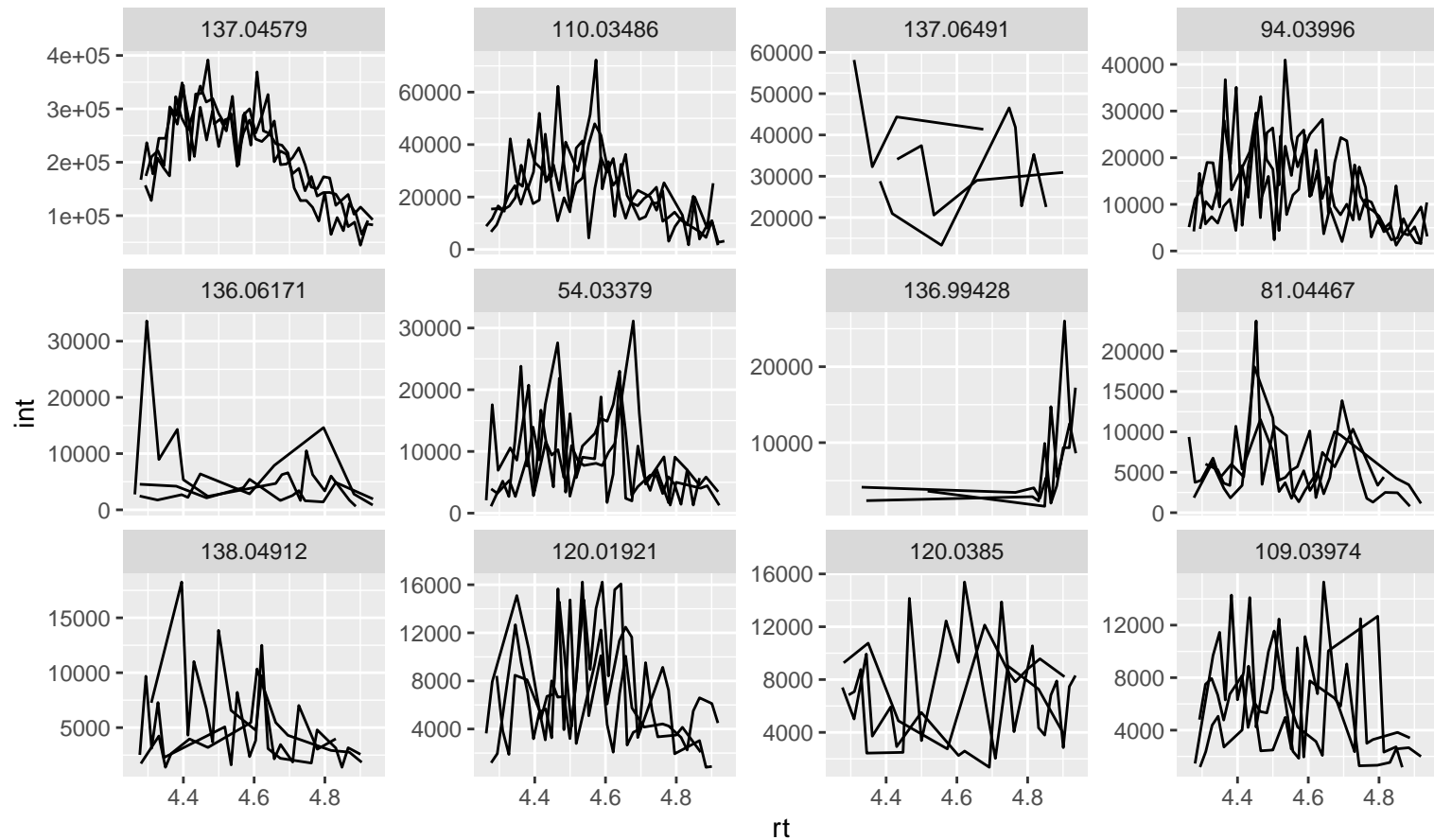


rt

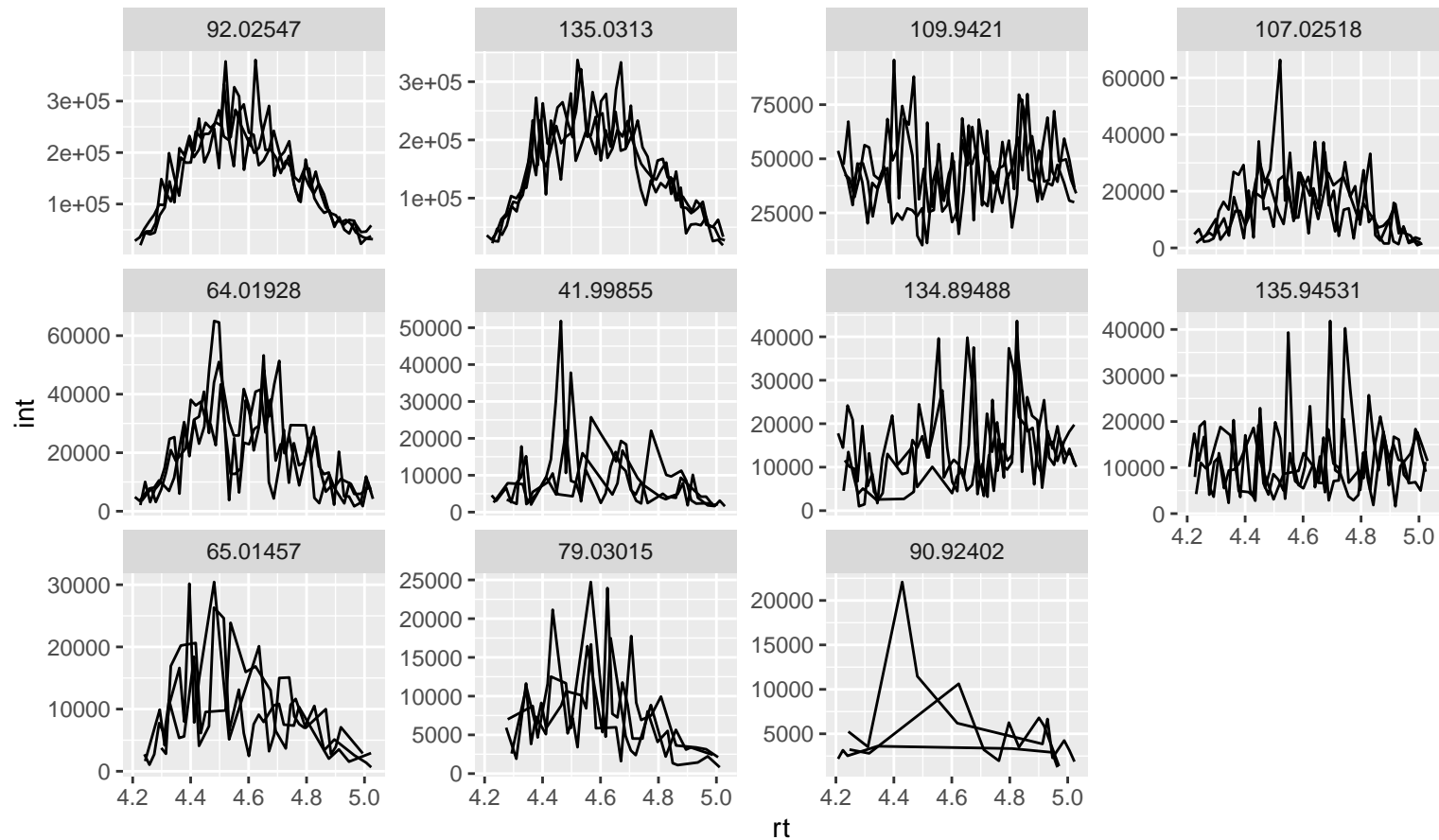
Threonic acid (neg) 135.029899



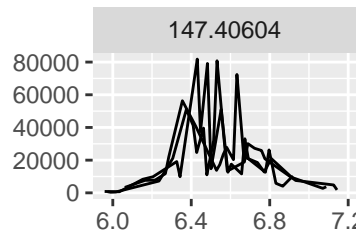
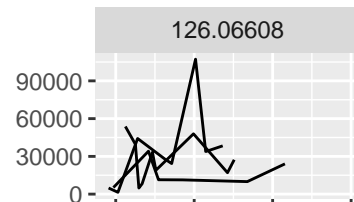
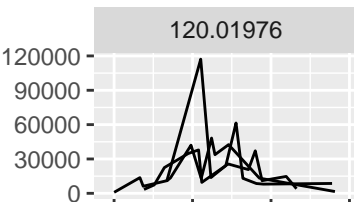
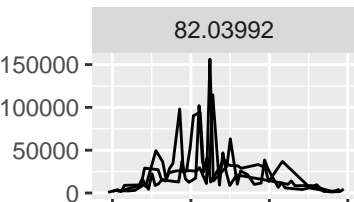
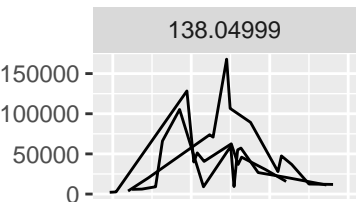
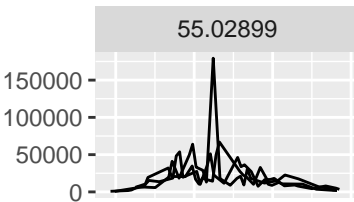
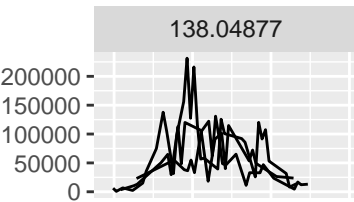
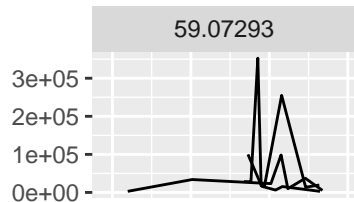
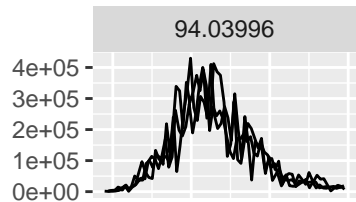
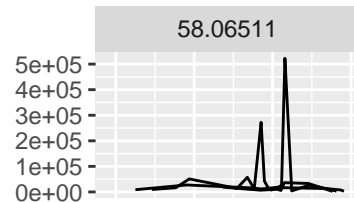
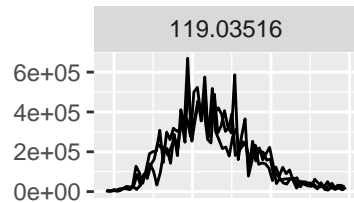
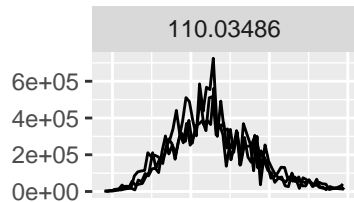
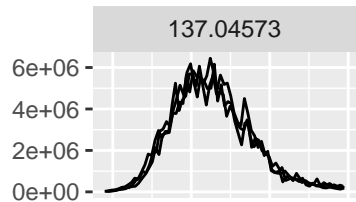
Allopurinol (pos) 137.045787



Allopurinol (neg) 135.031235



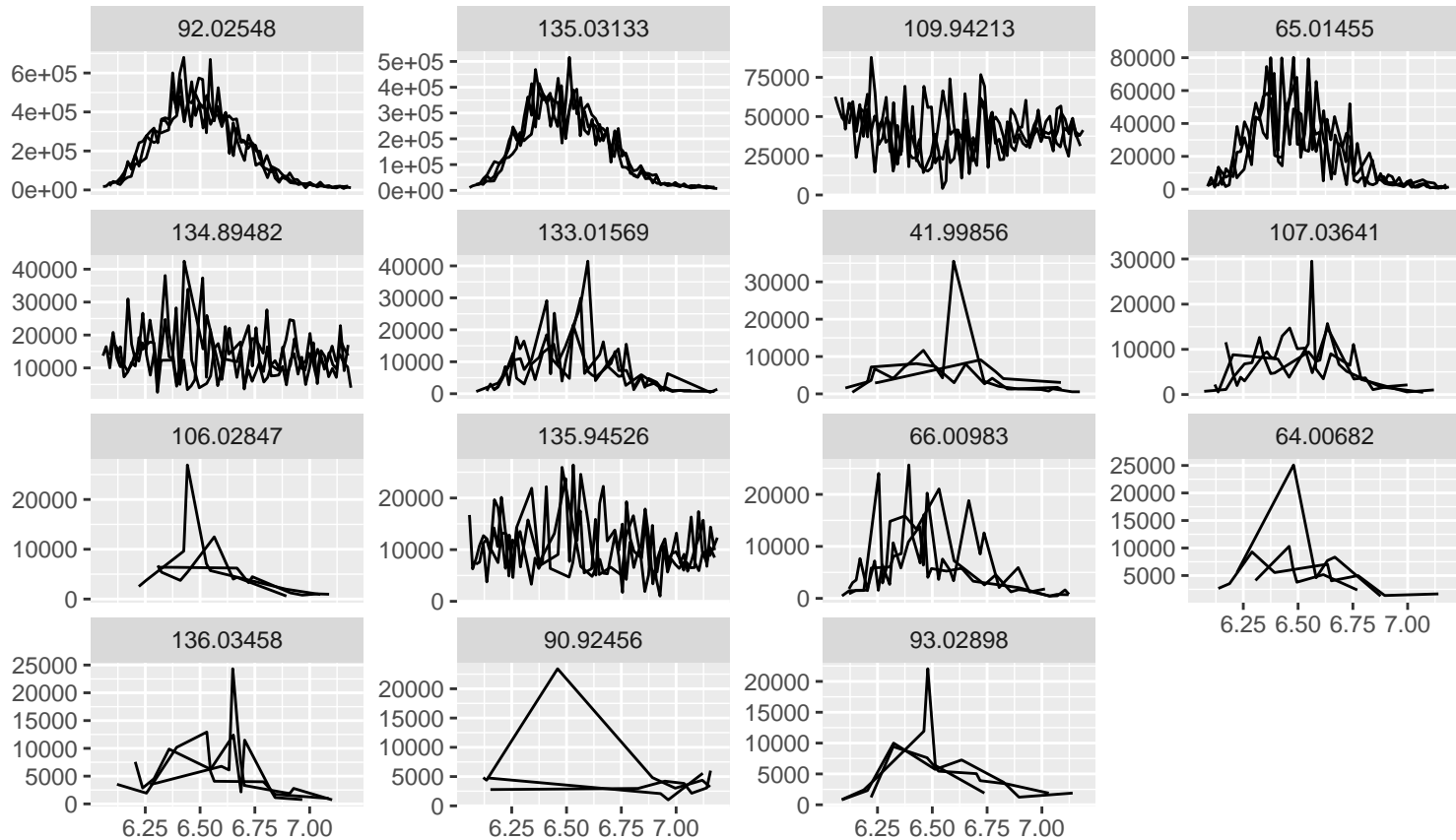
Hypoxanthine (pos) 137.045787



rt

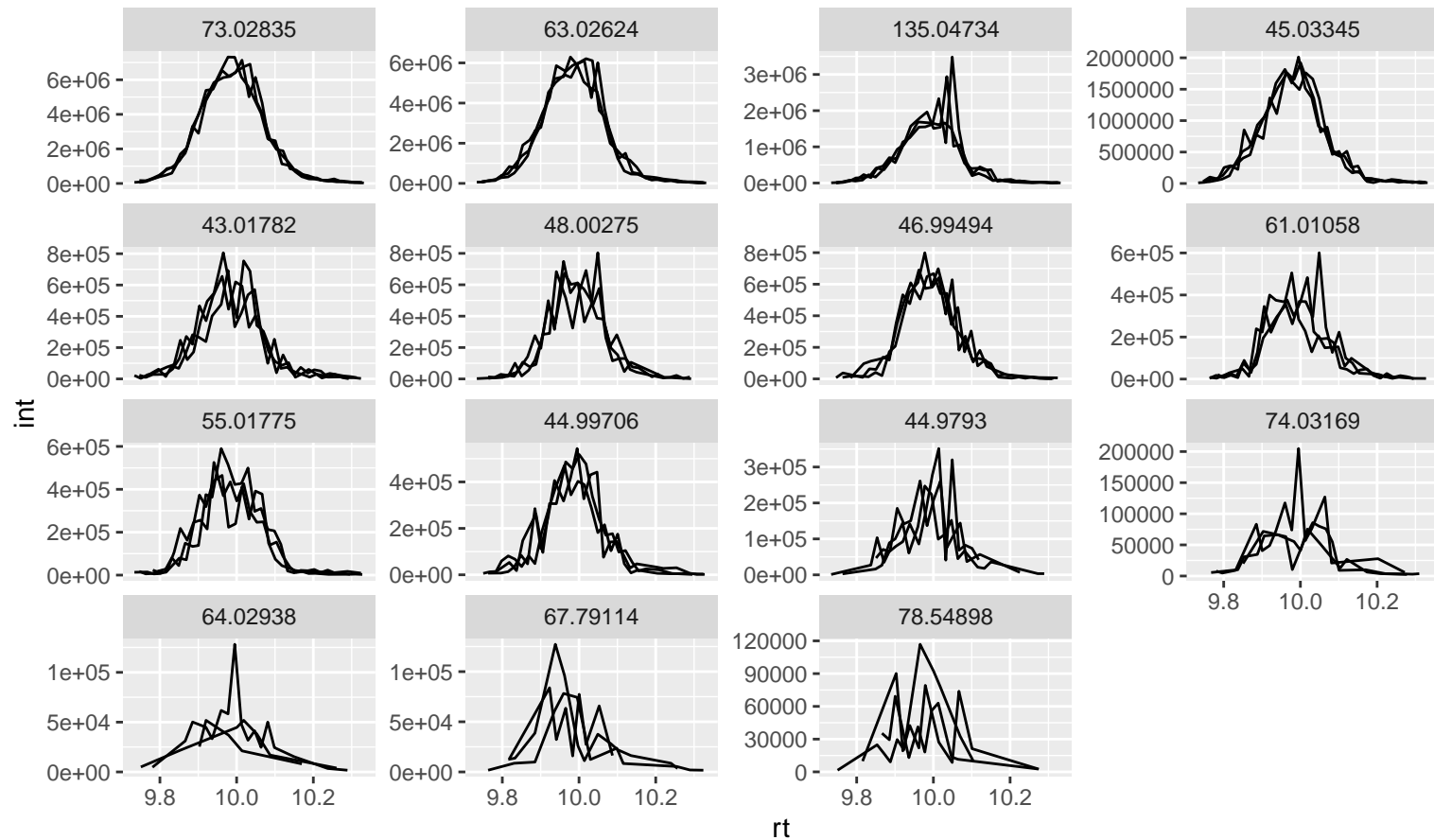
Hypoxanthine (neg) 135.031235

int

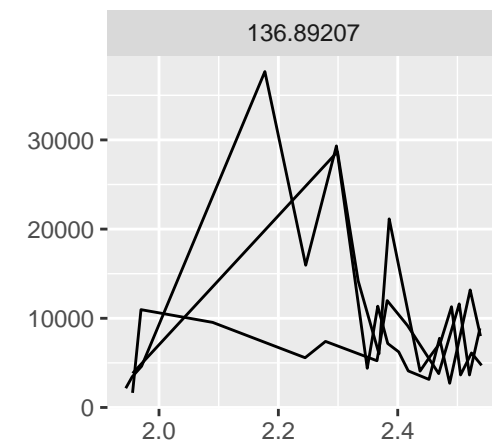
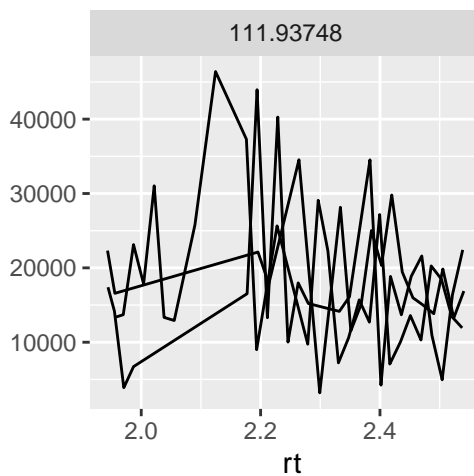
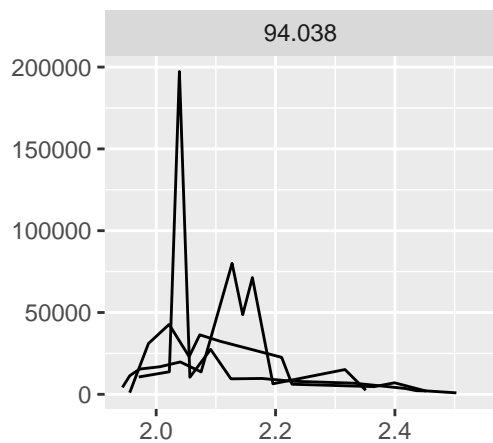
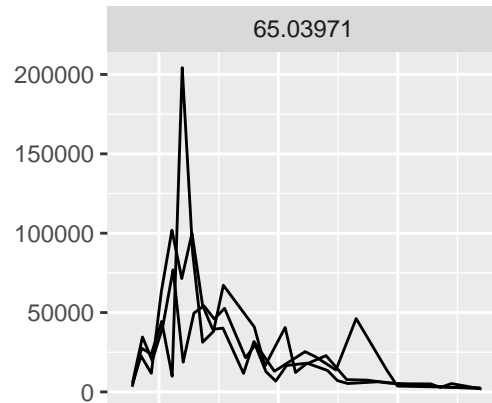
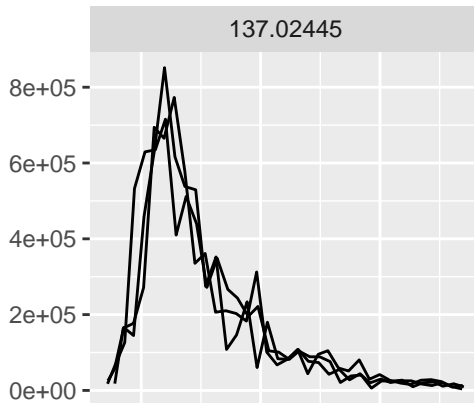
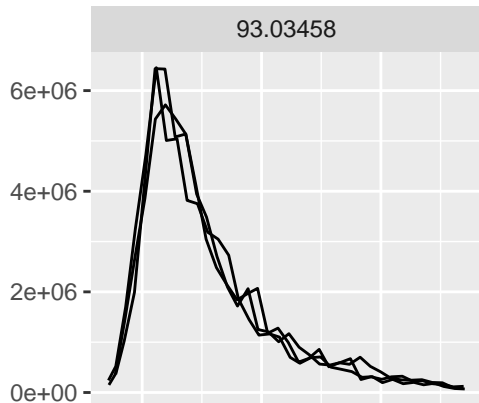


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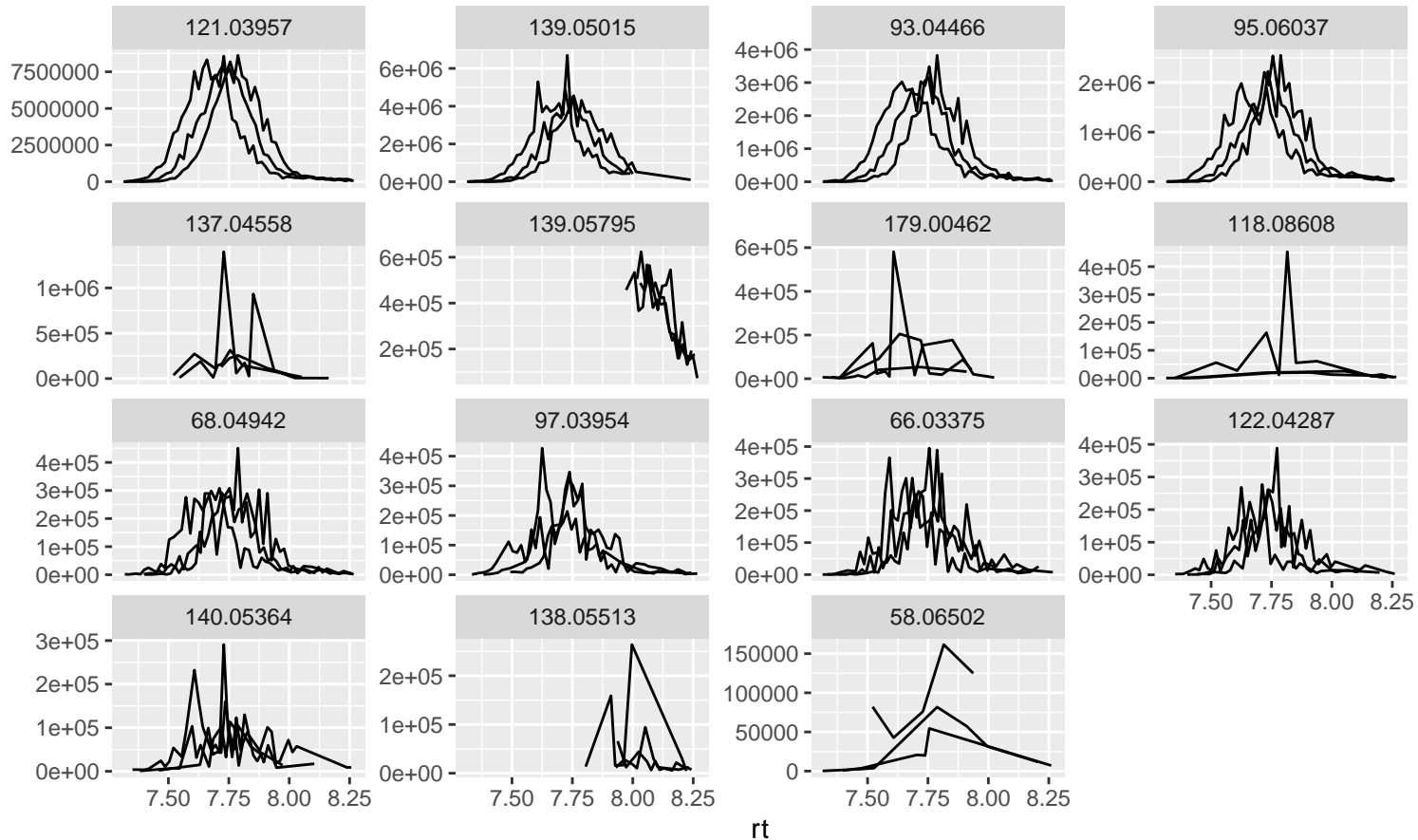
Dimethylsulfonylpropionate (pos) 135.047428



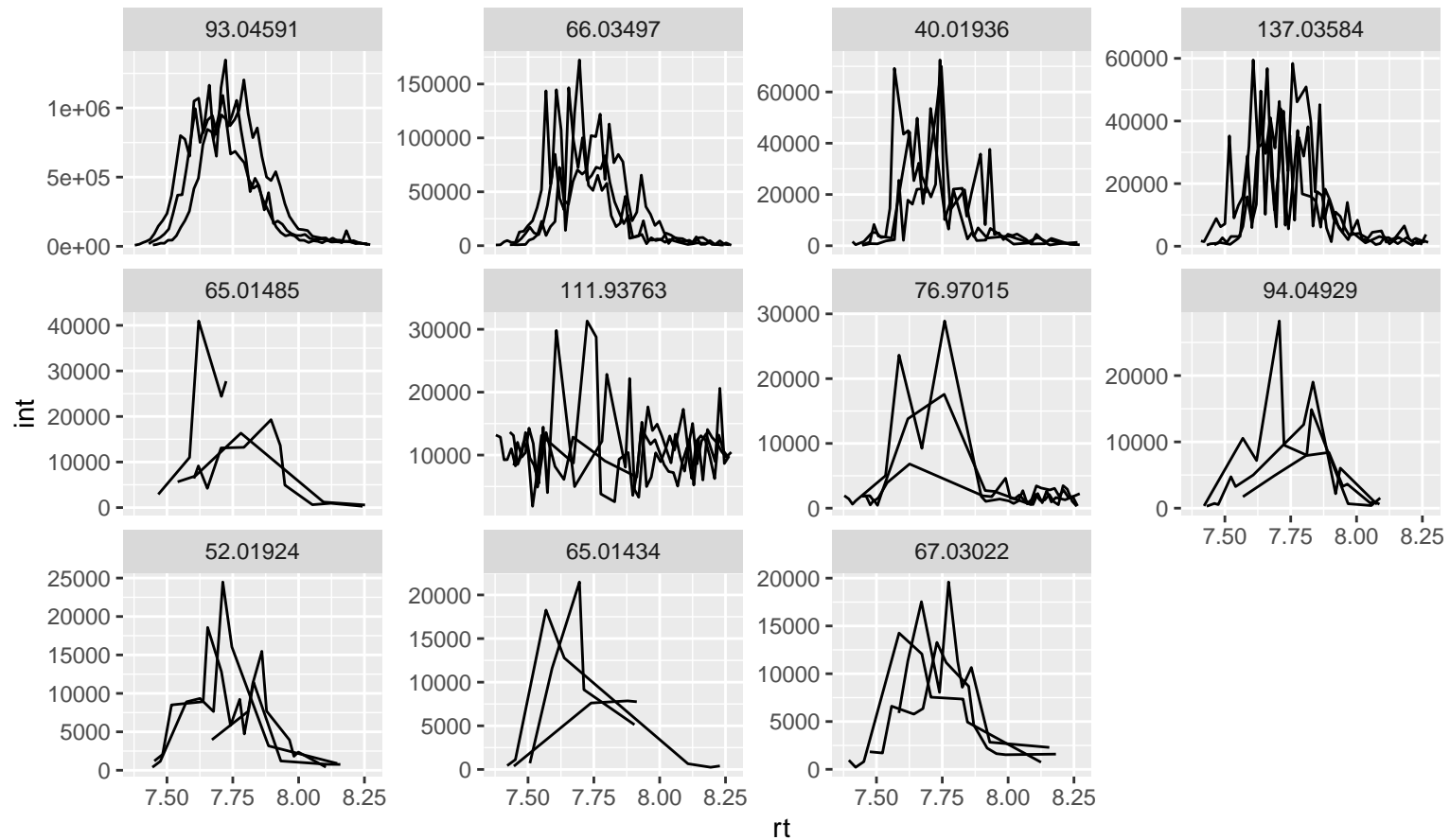
Salicylic acid (neg) 137.024419



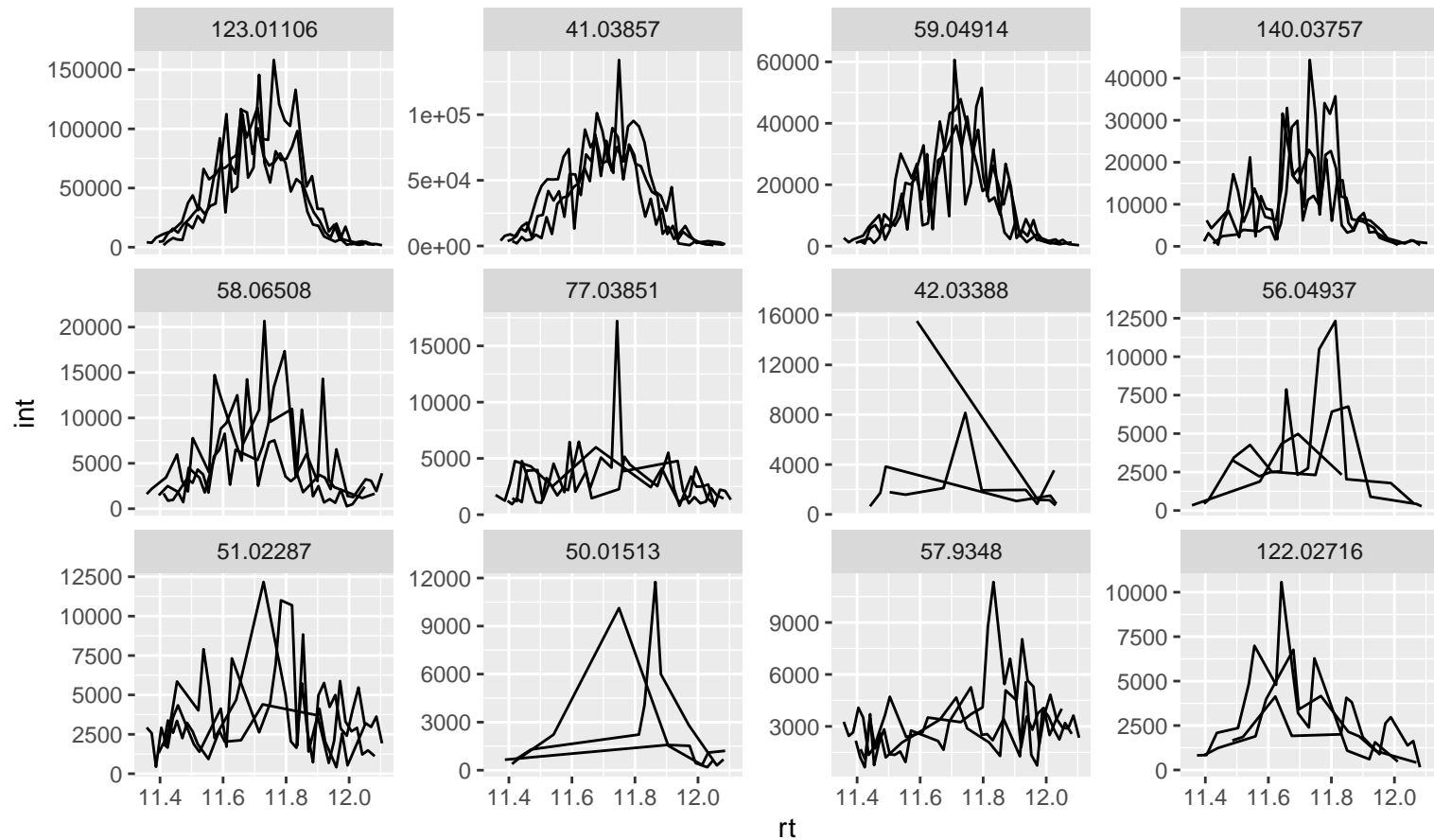
Urocanic acid (pos) 139.050204



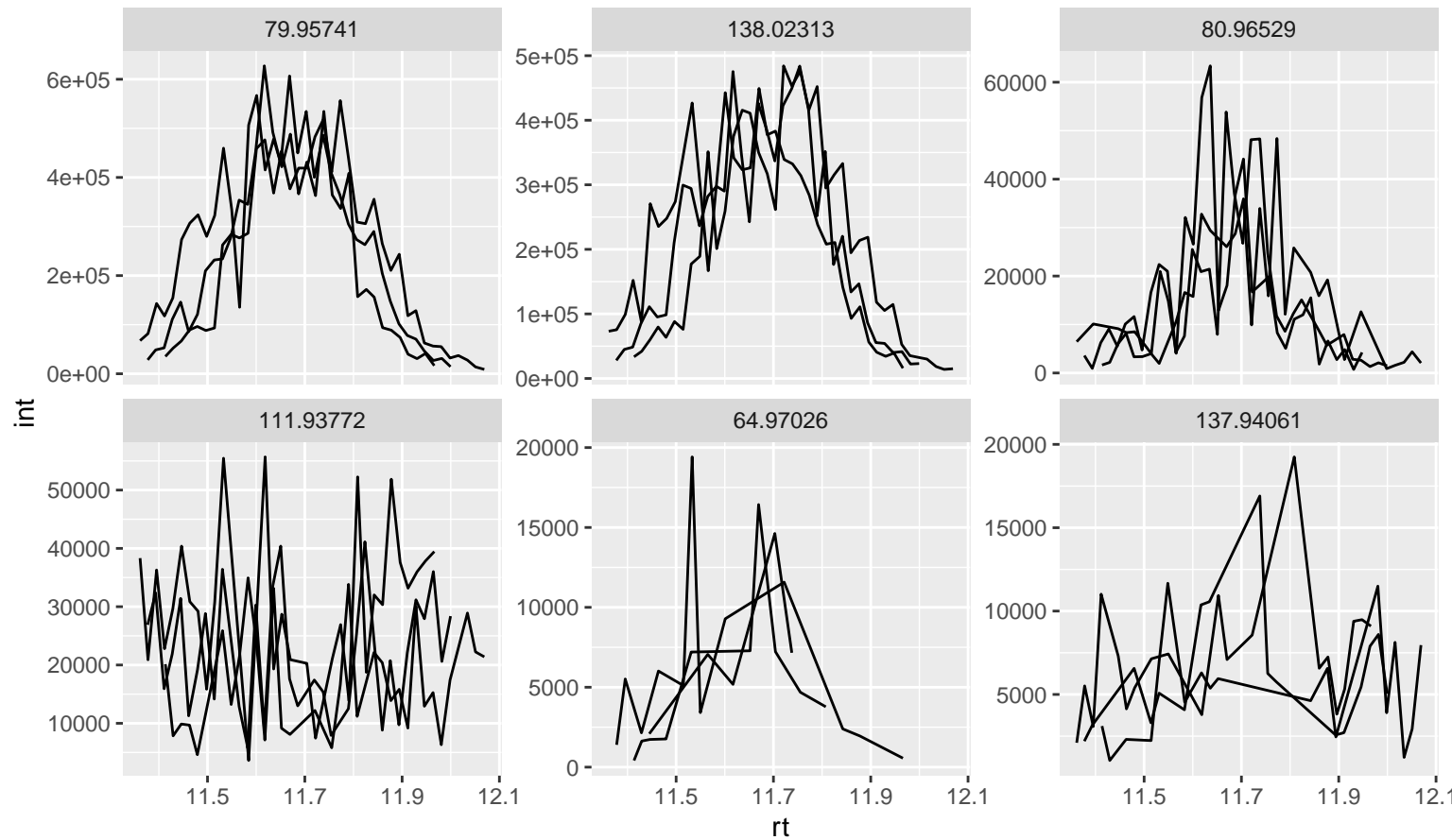
Urocanic acid (neg) 137.035652



3-Aminopropanesulfonate (pos) 140.037592

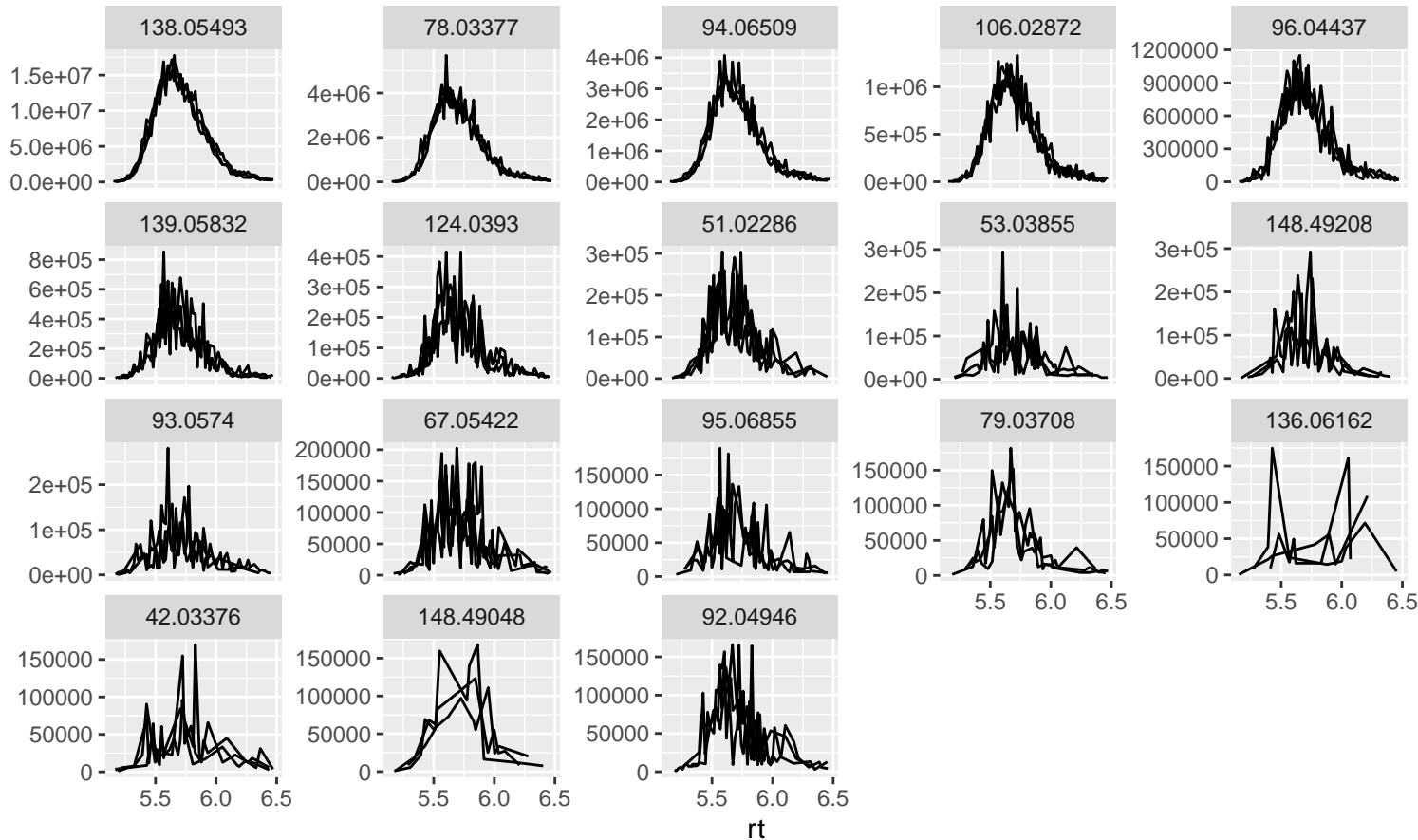


3-Aminopropanesulfonate (neg) 138.02304



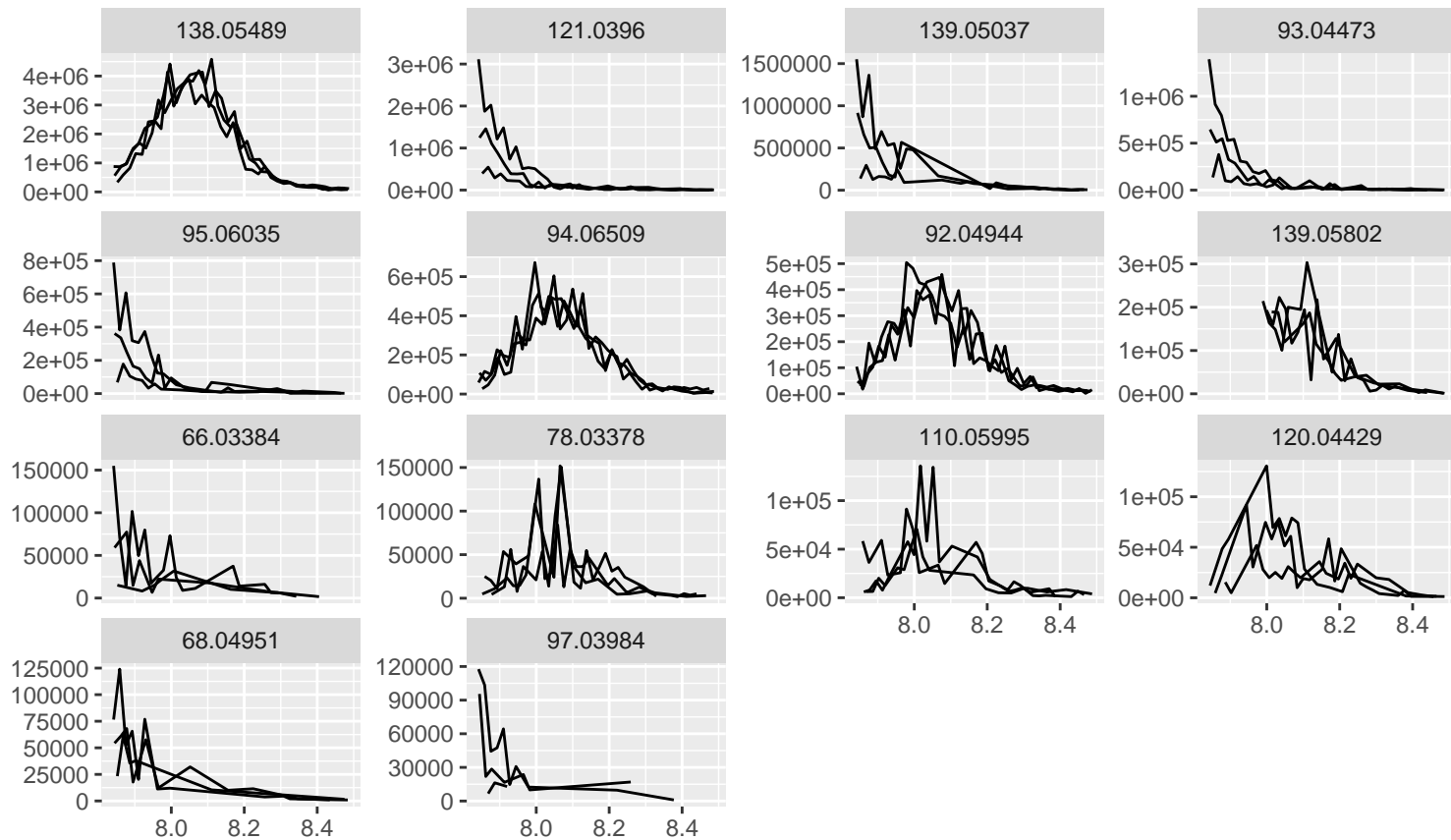
Homarine (pos) 138.054955

int



Trigonelline (pos) 138.054955

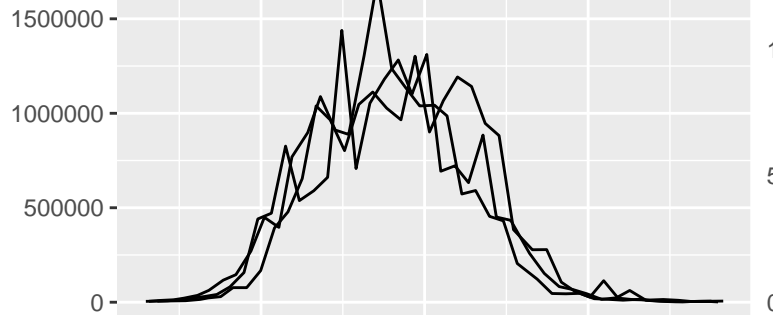
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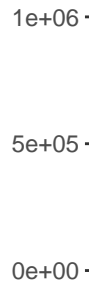
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Sulfoacetic acid (neg) 138.970671

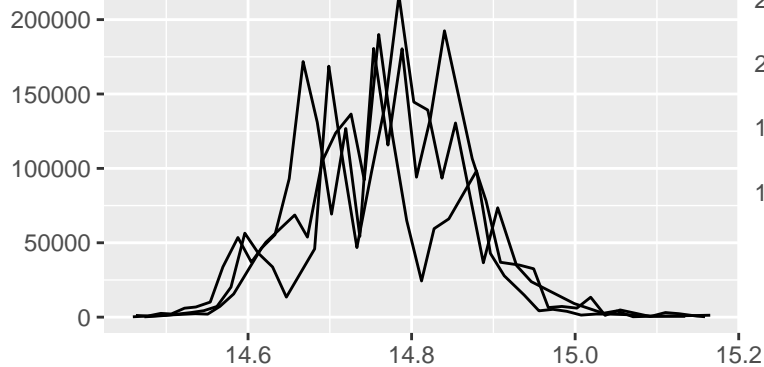
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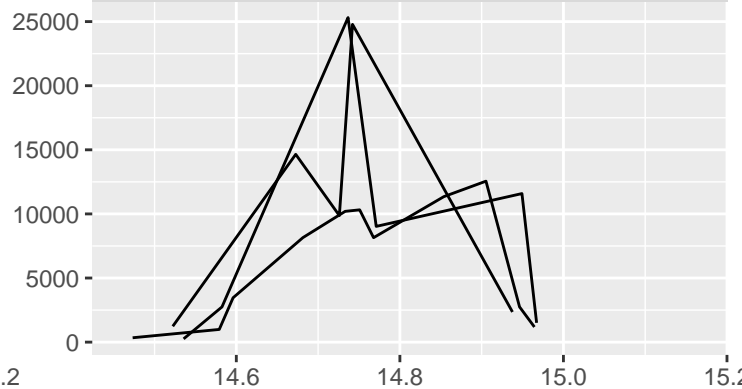
79.95743



138.97088



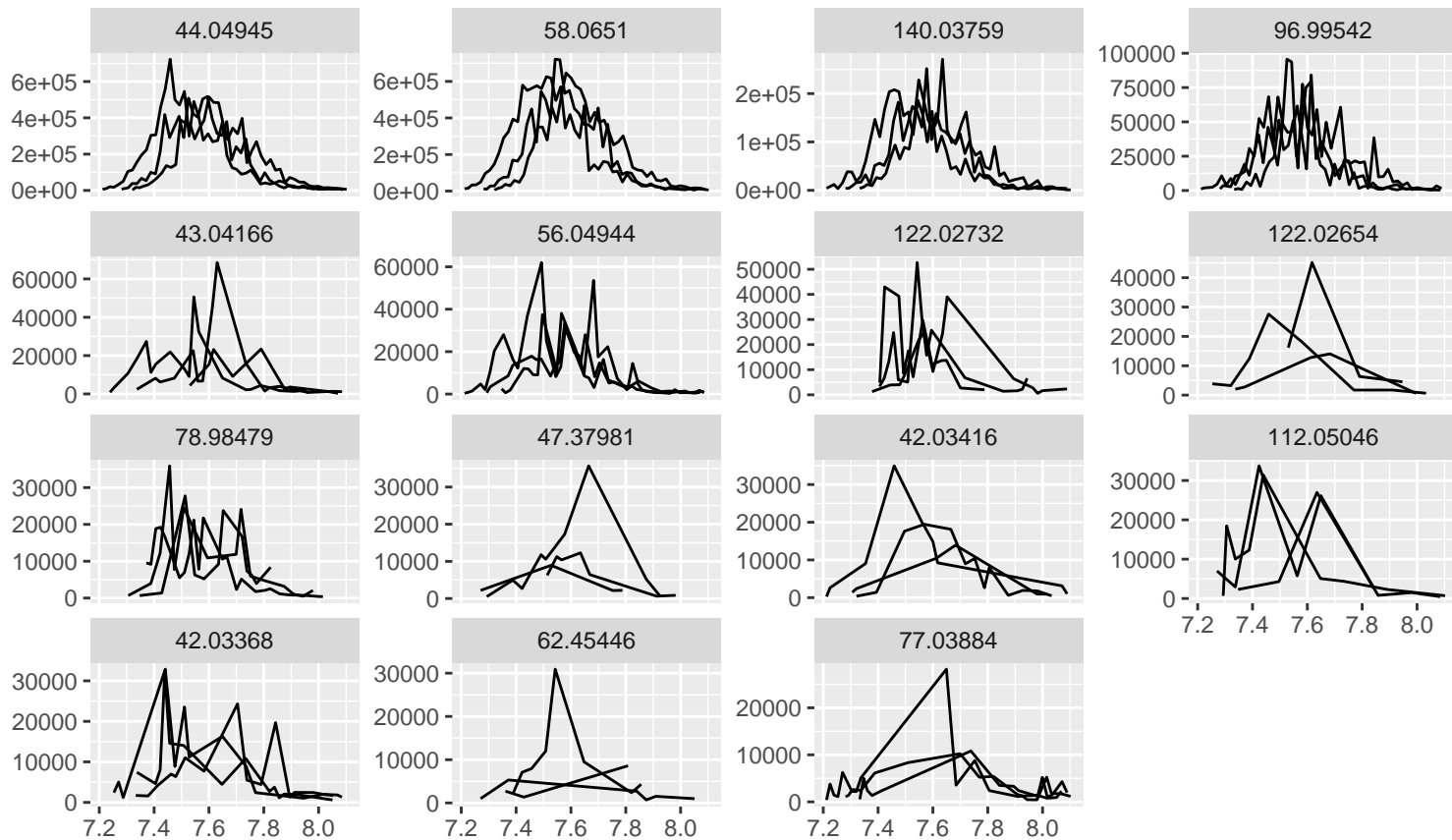
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rt

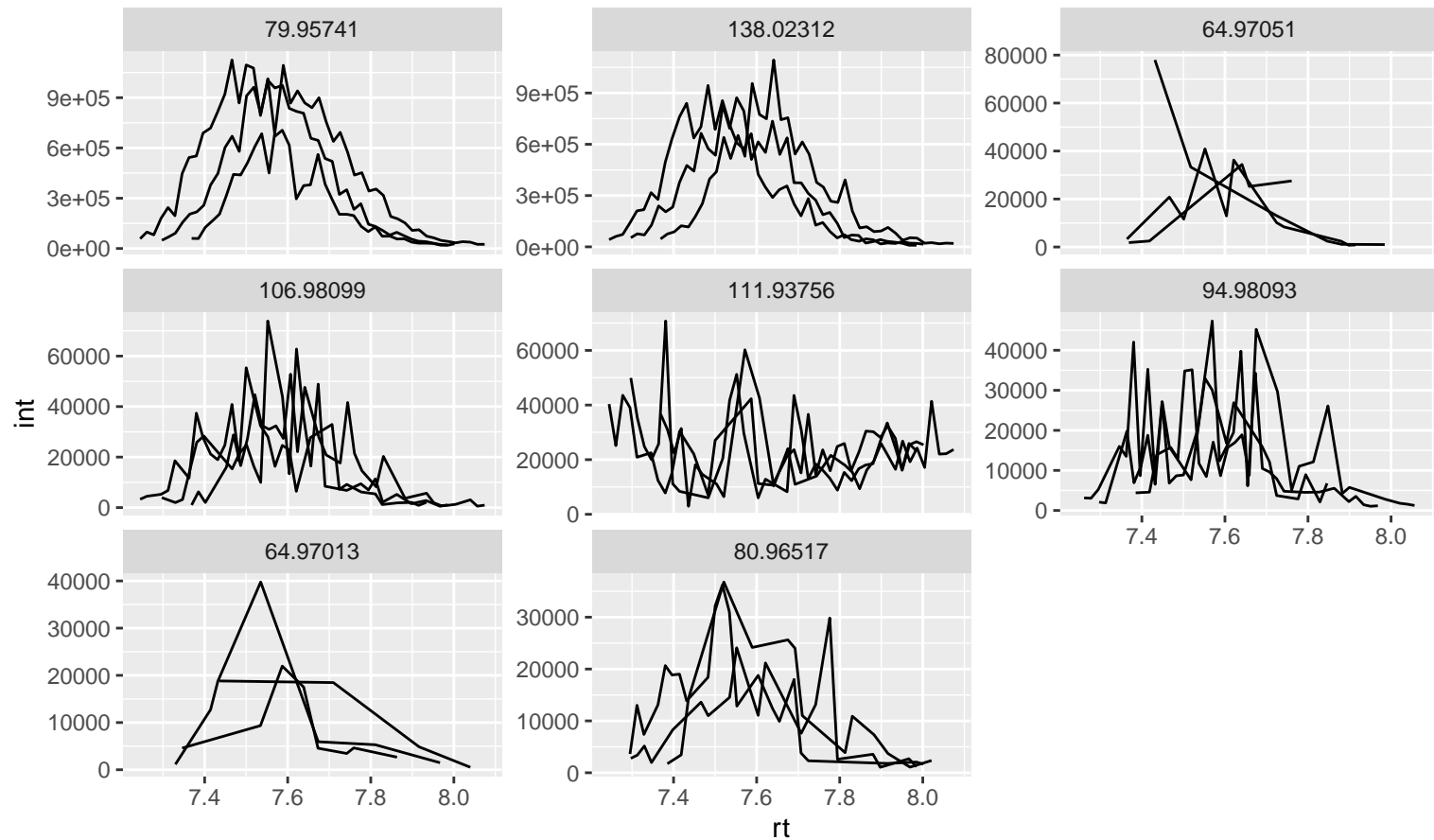
N-Methyltaurine (pos) 140.037592

int



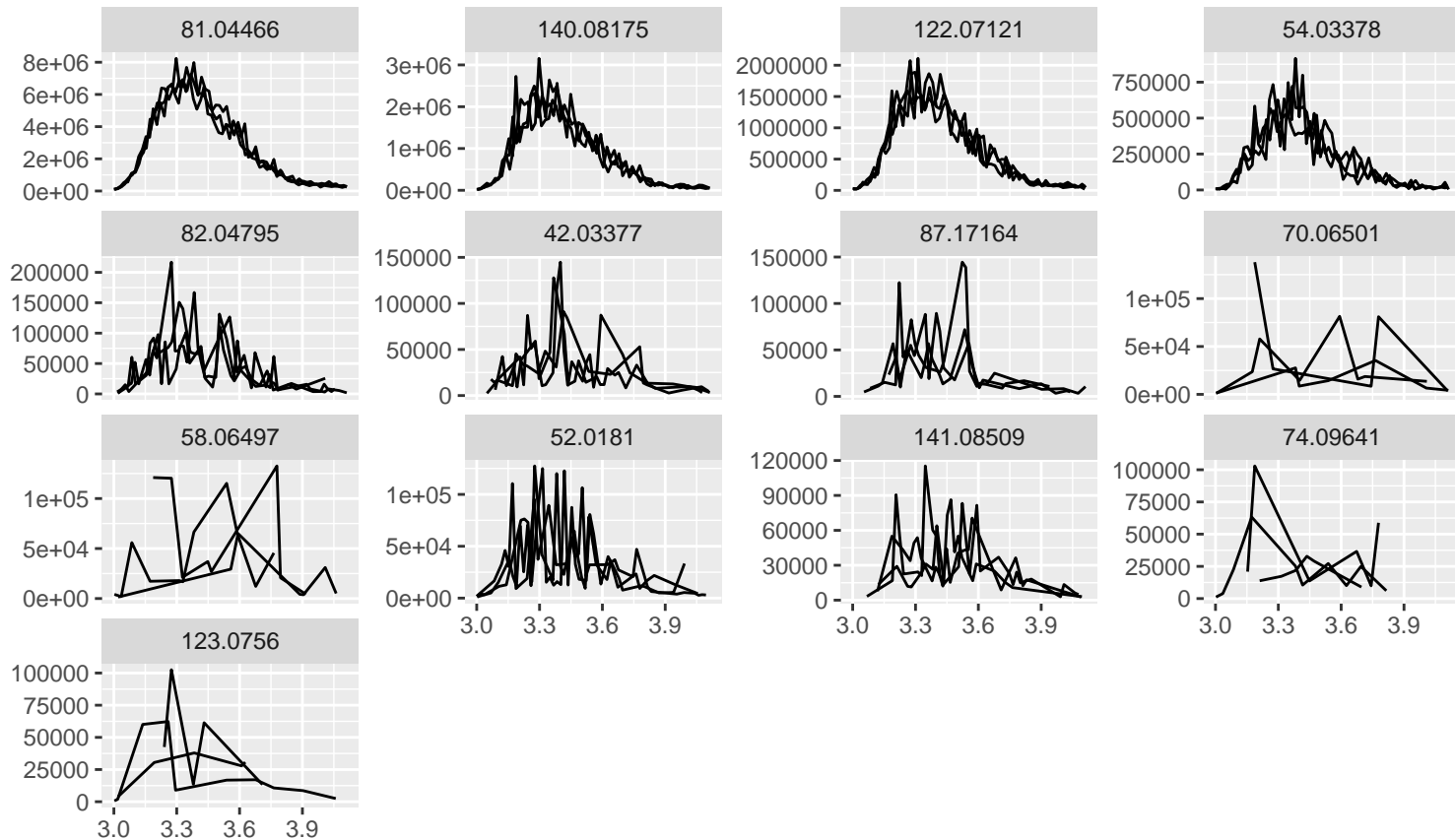
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N-Methyltaurine (neg) 138.02304



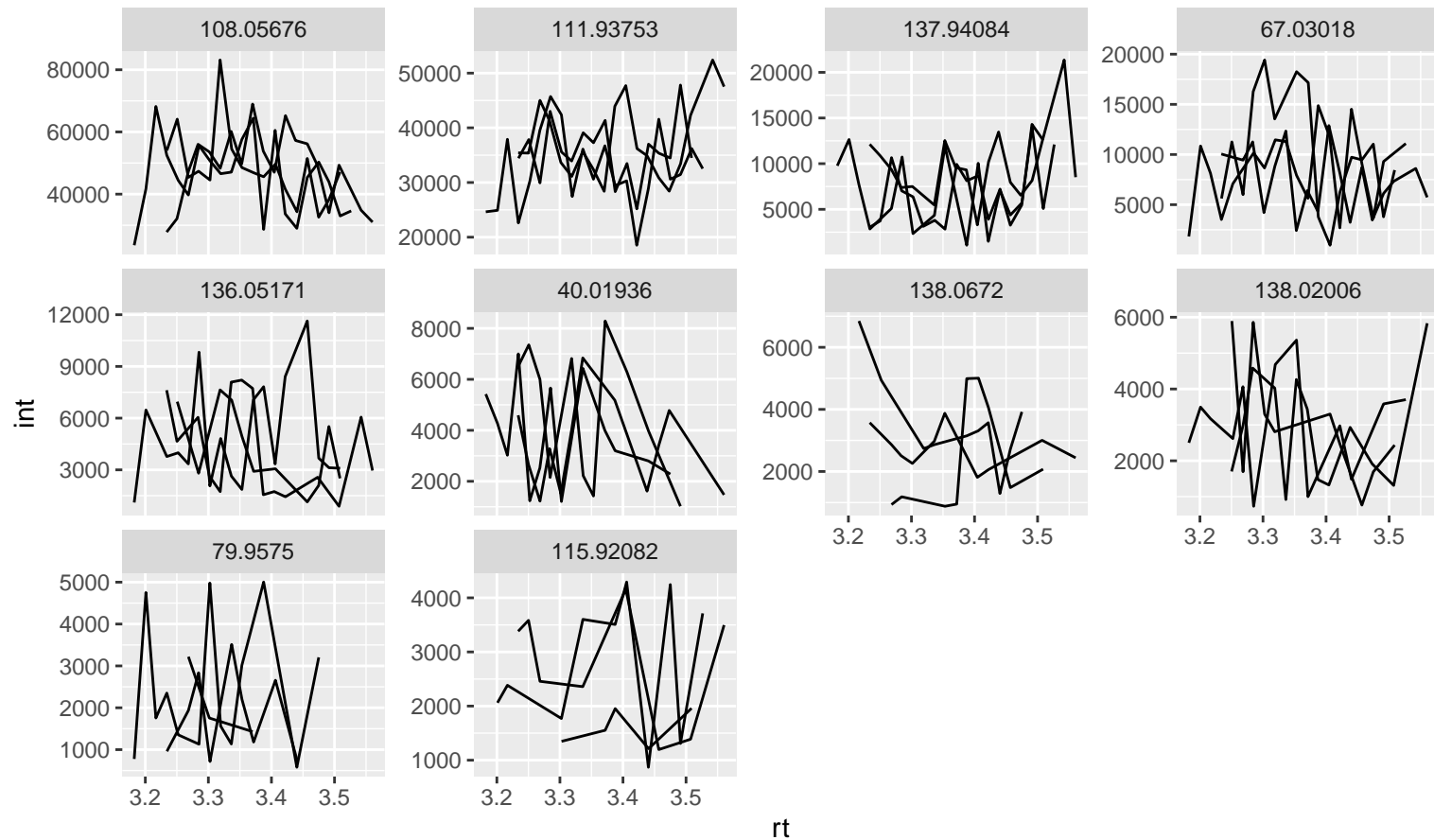
Toxopyrimidine (pos) 140.081838

int



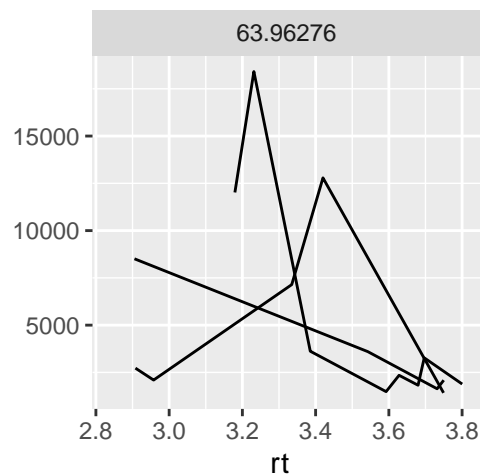
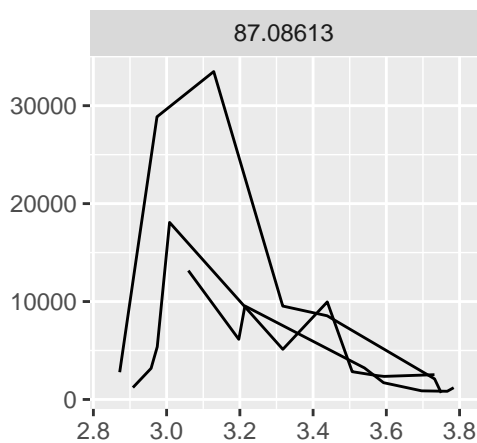
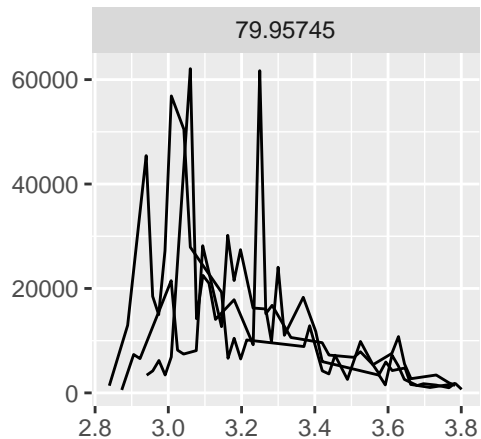
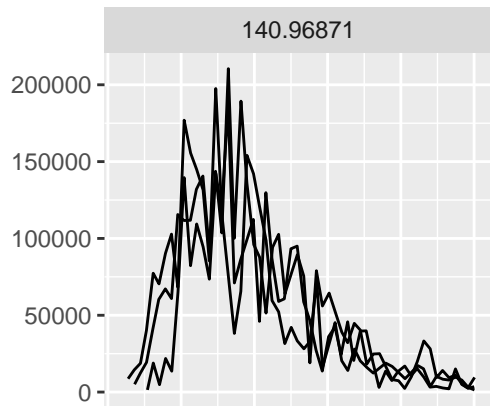
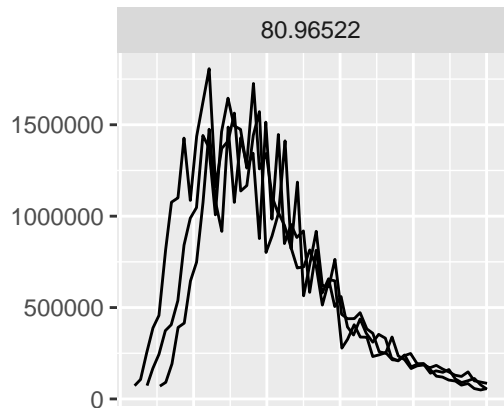
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Toxopyrimidine (neg) 138.067286



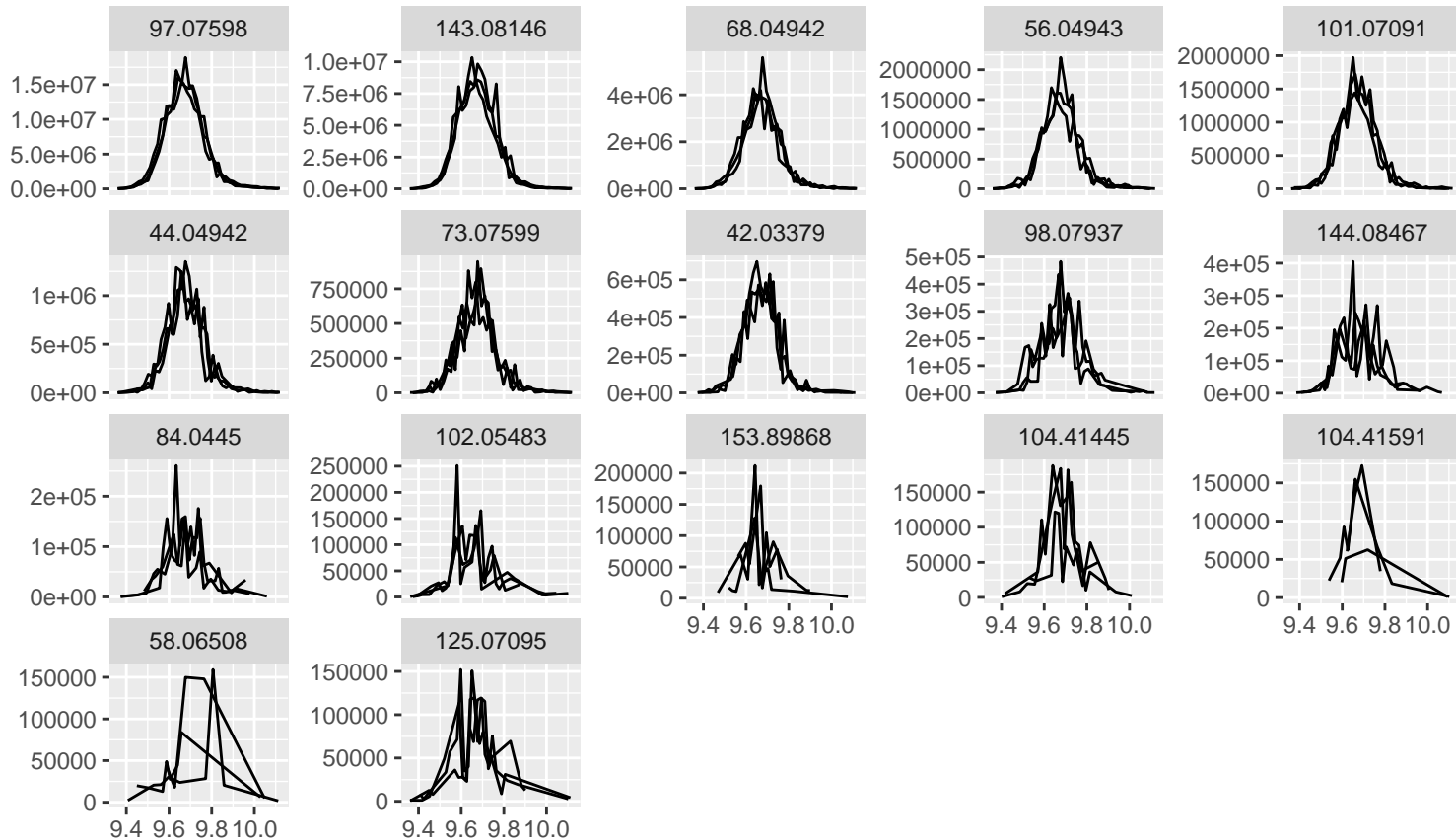
2-mercaptoethanesulfonic acid (neg) 140.968563

int



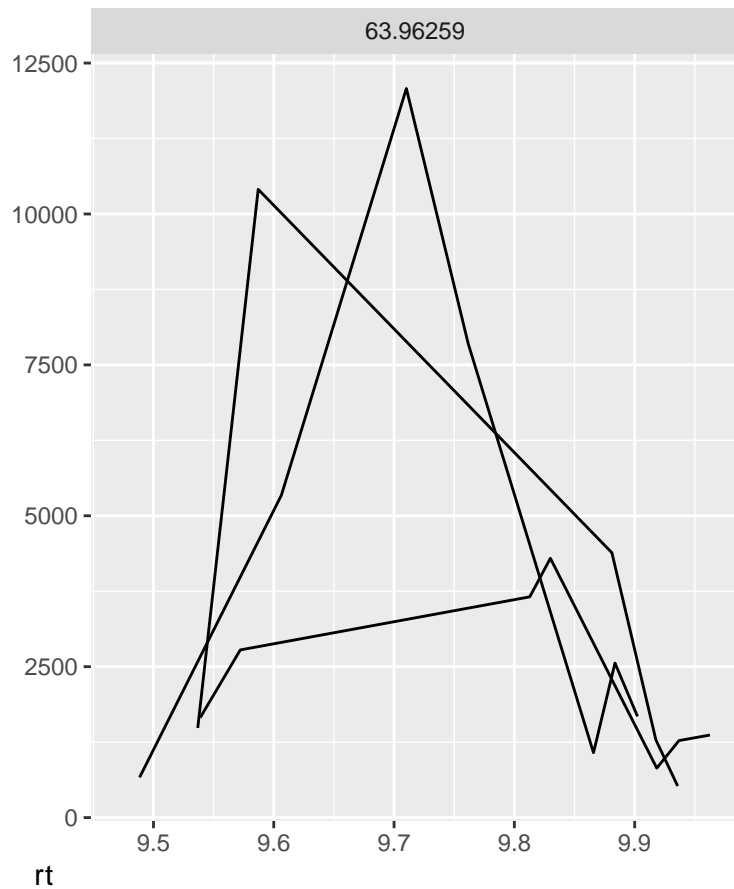
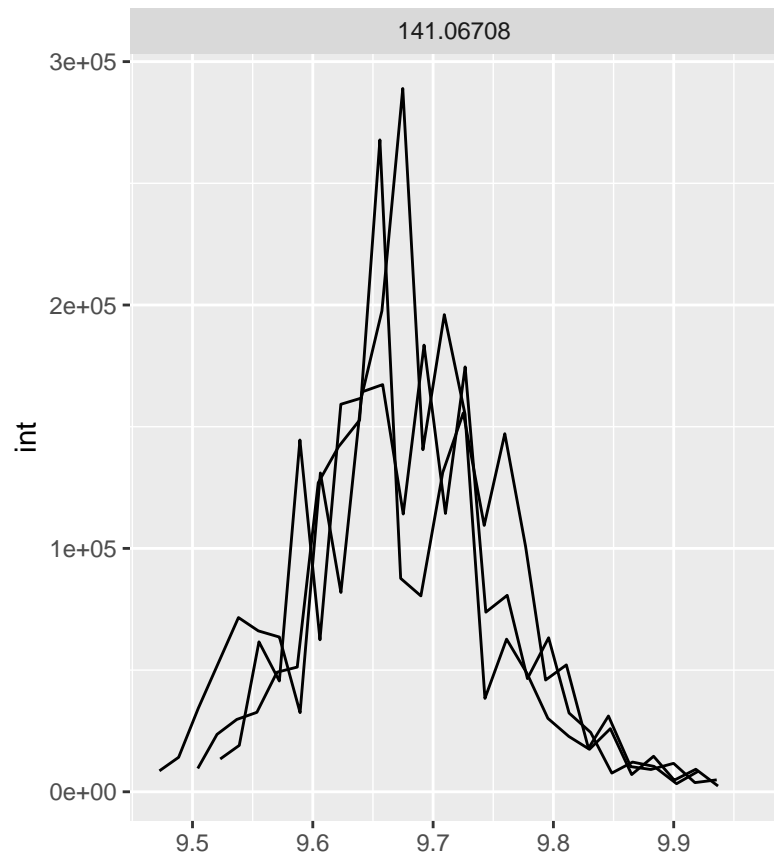
Ectoine (pos) 143.081504

int

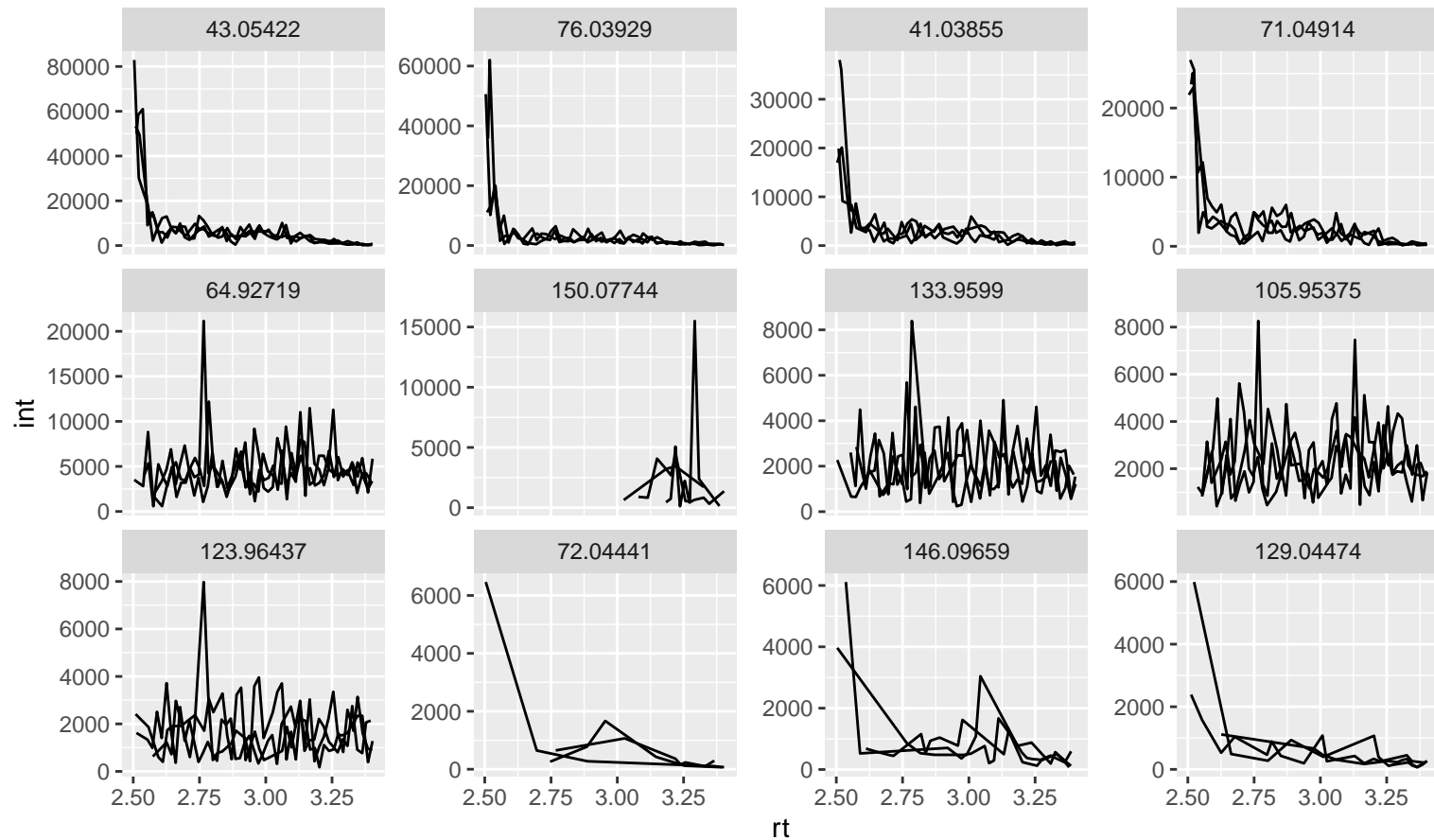


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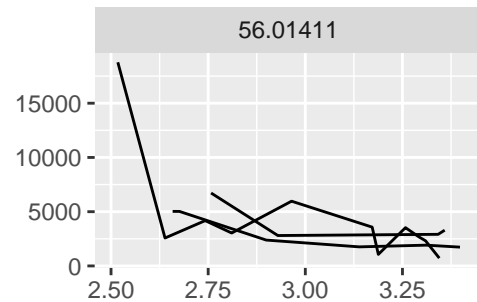
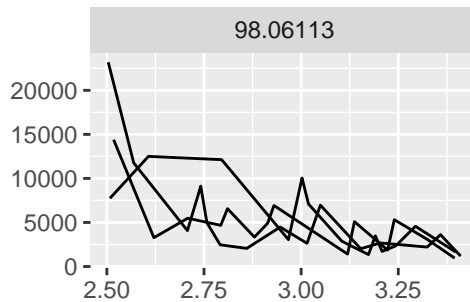
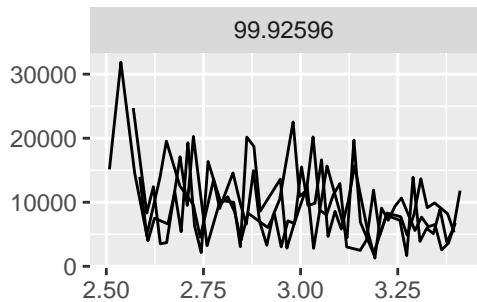
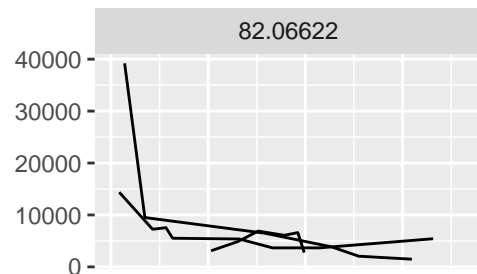
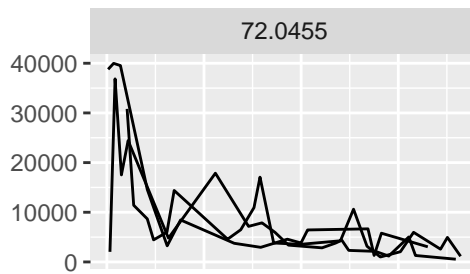
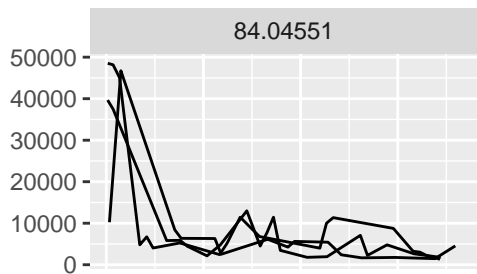
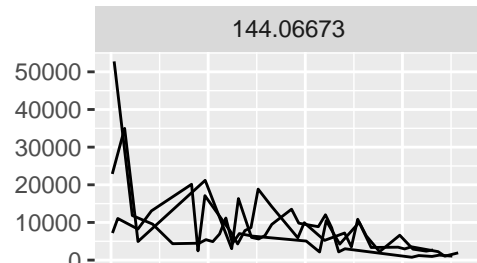
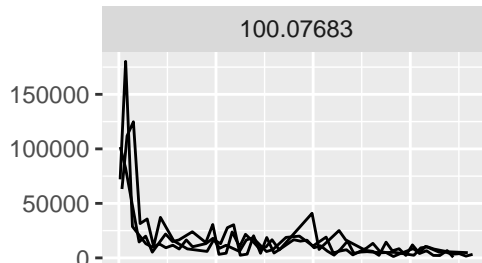
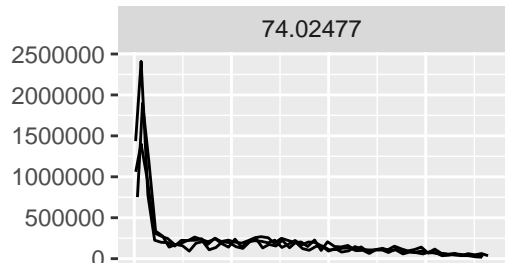
Ectoine (neg) 141.066952



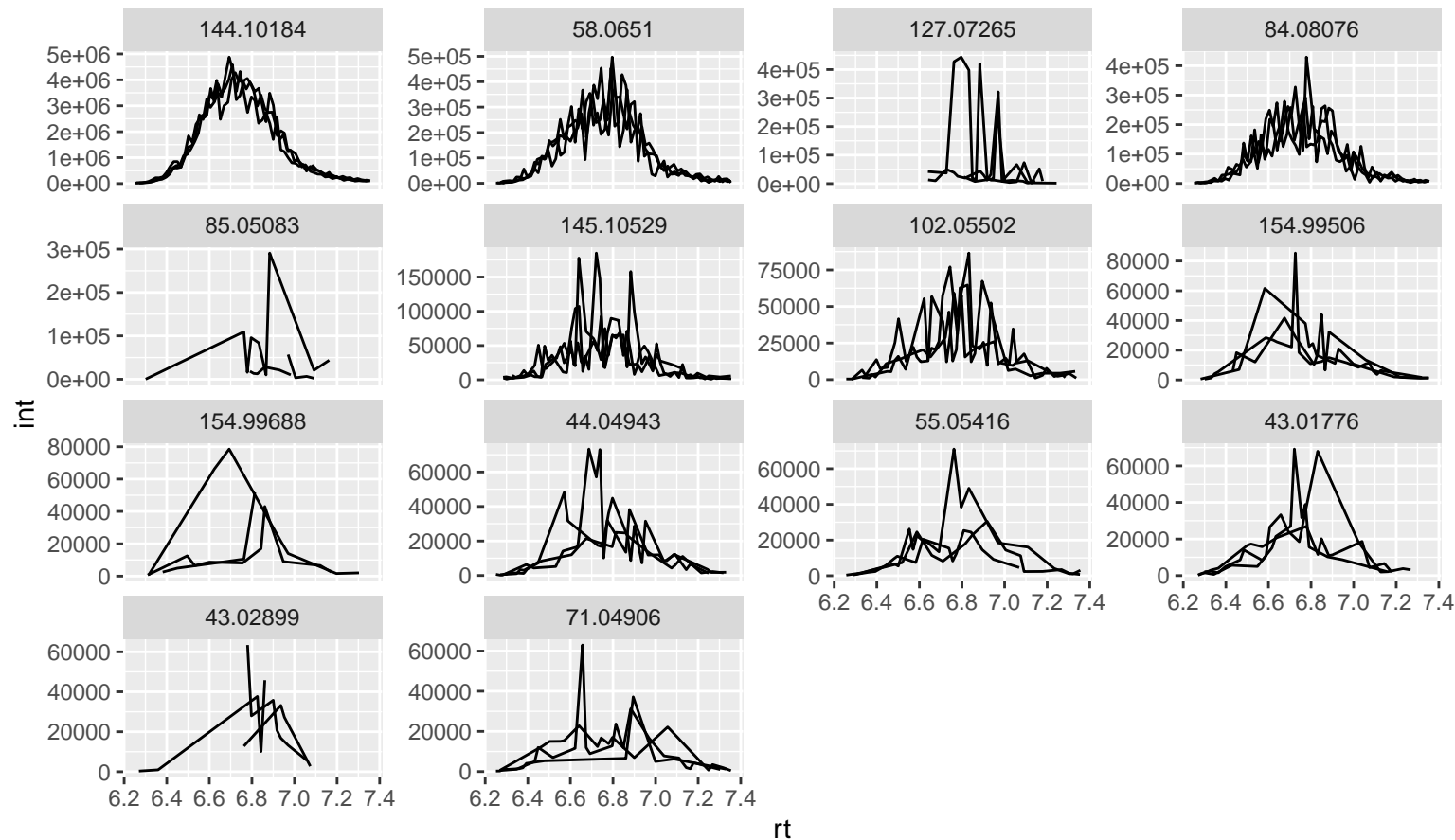
Butyrylglycine (pos) 146.08117



Butyrylglycine (neg) 144.066618

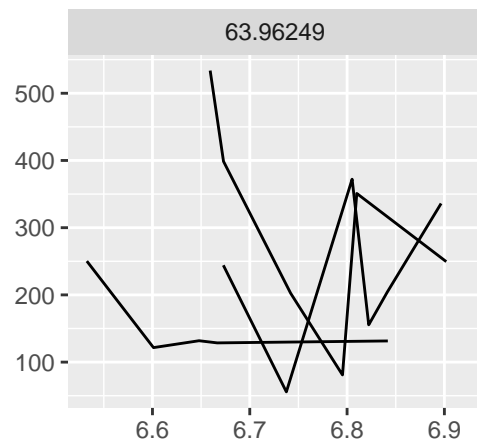
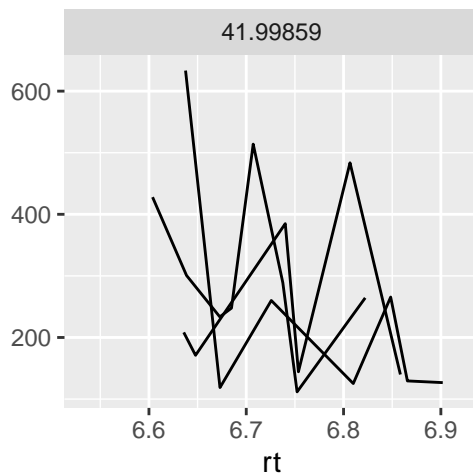
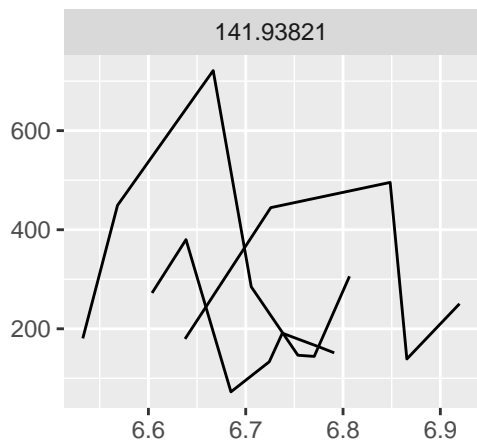
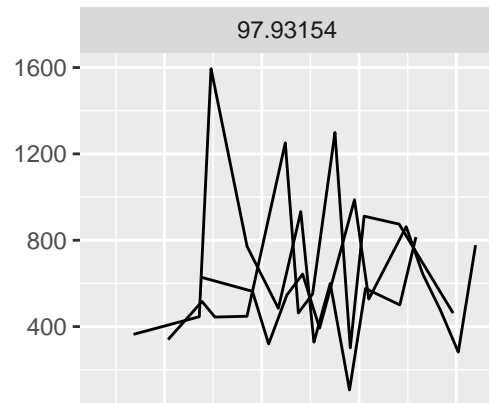
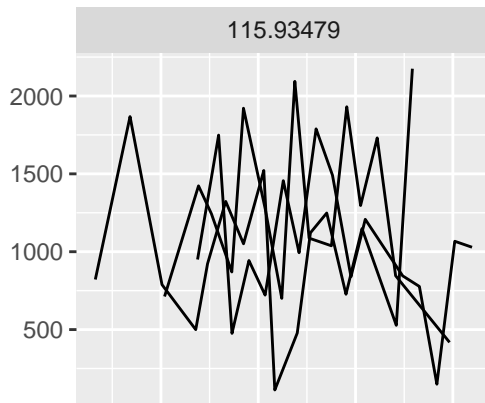
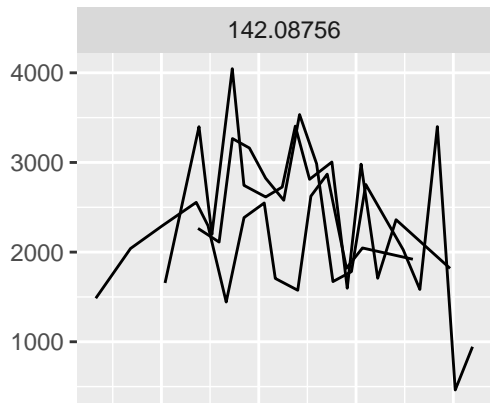


Proline betaine (pos) 144.101905

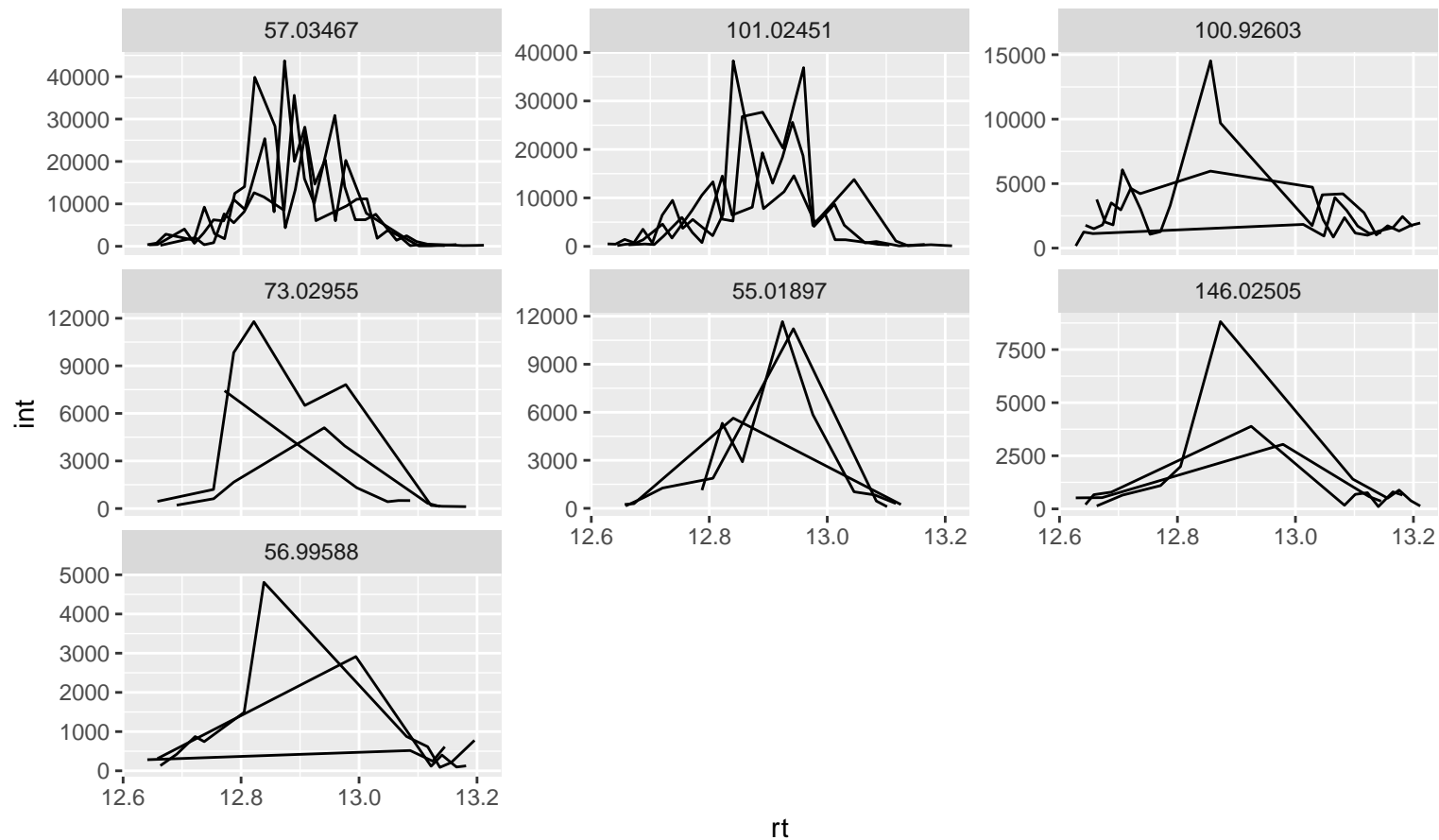


Proline betaine (neg) 142.087353

int

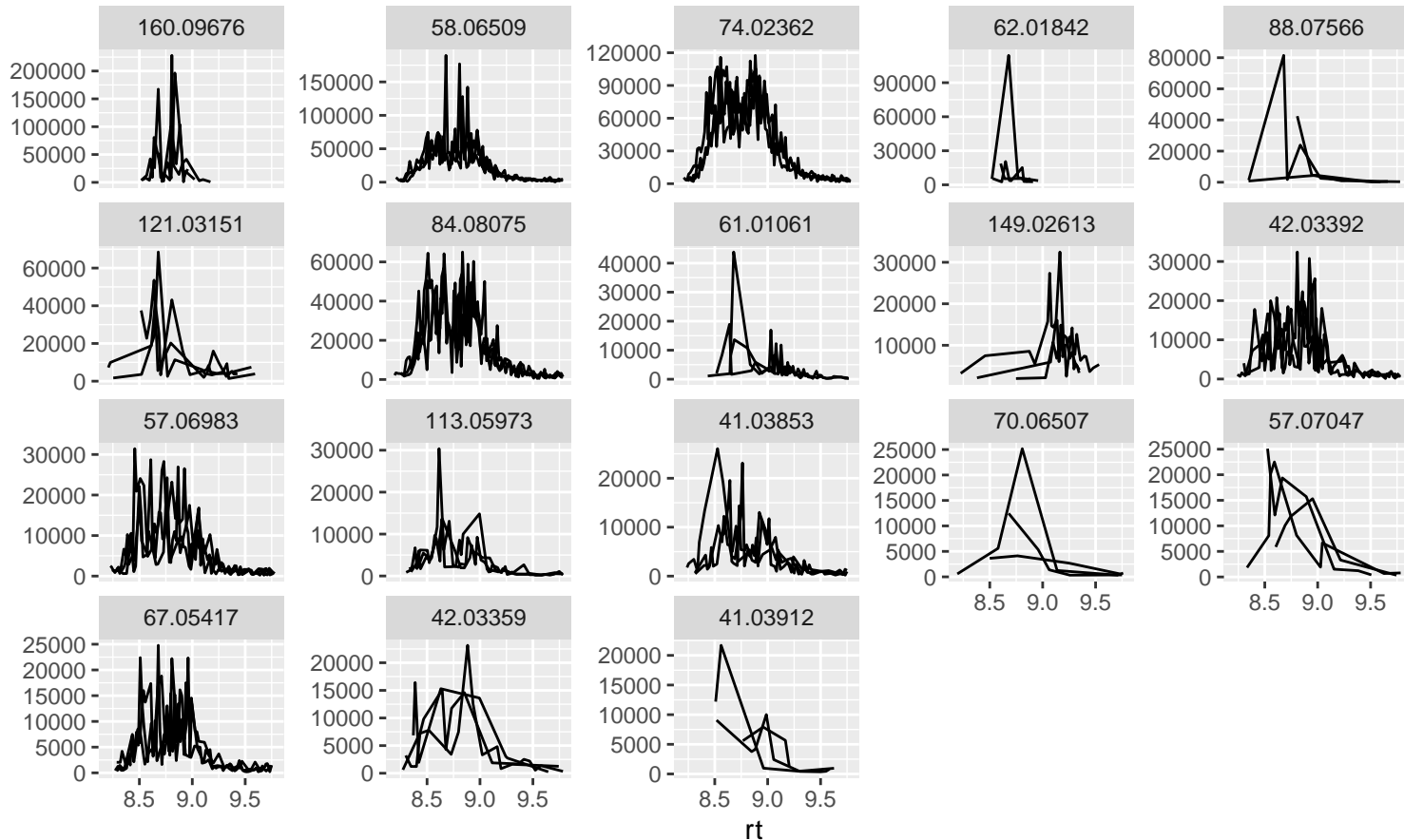


2-Ketoglutaric acid (neg) 145.014249



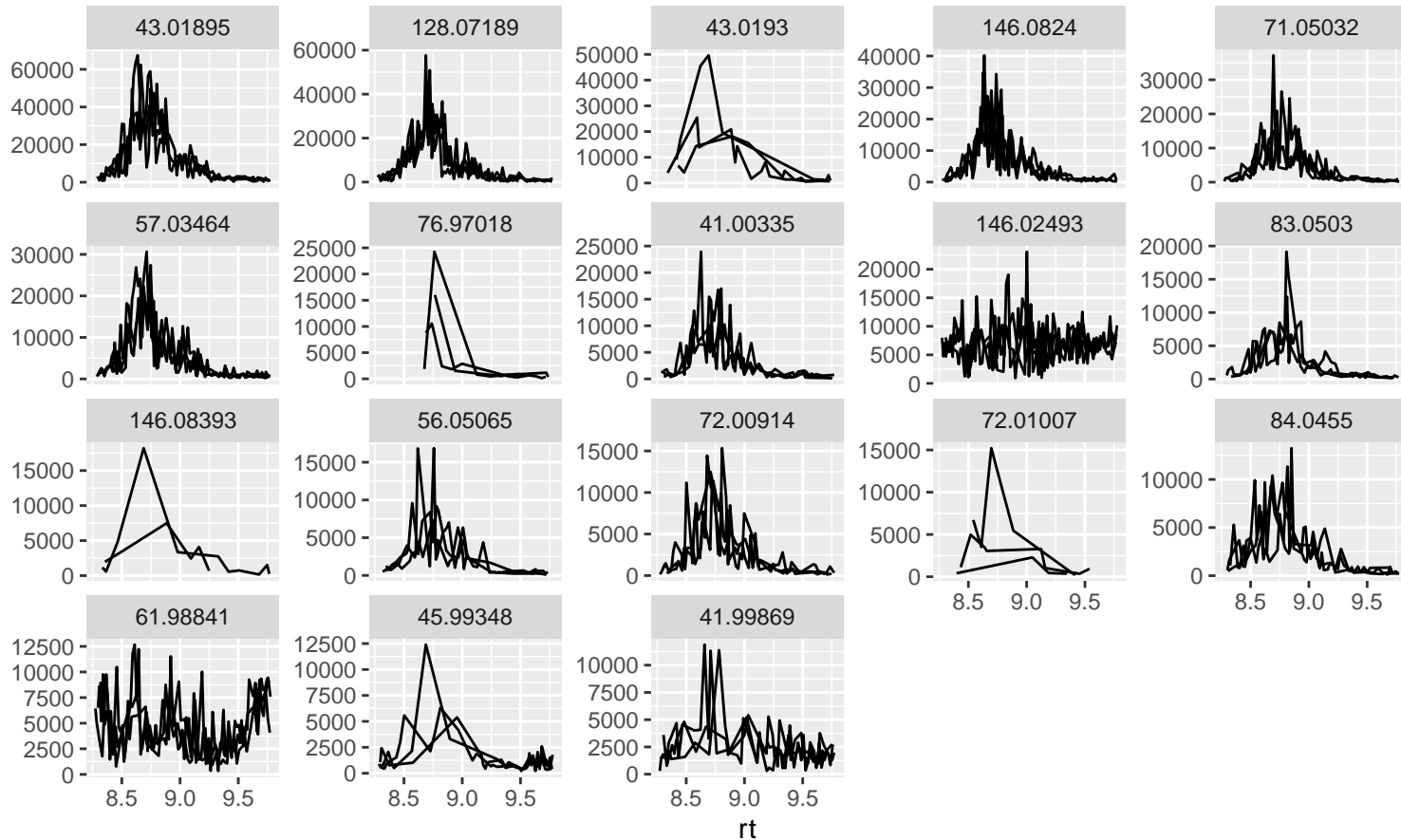
Hydroxyisoleucine (pos) 148.09682

int



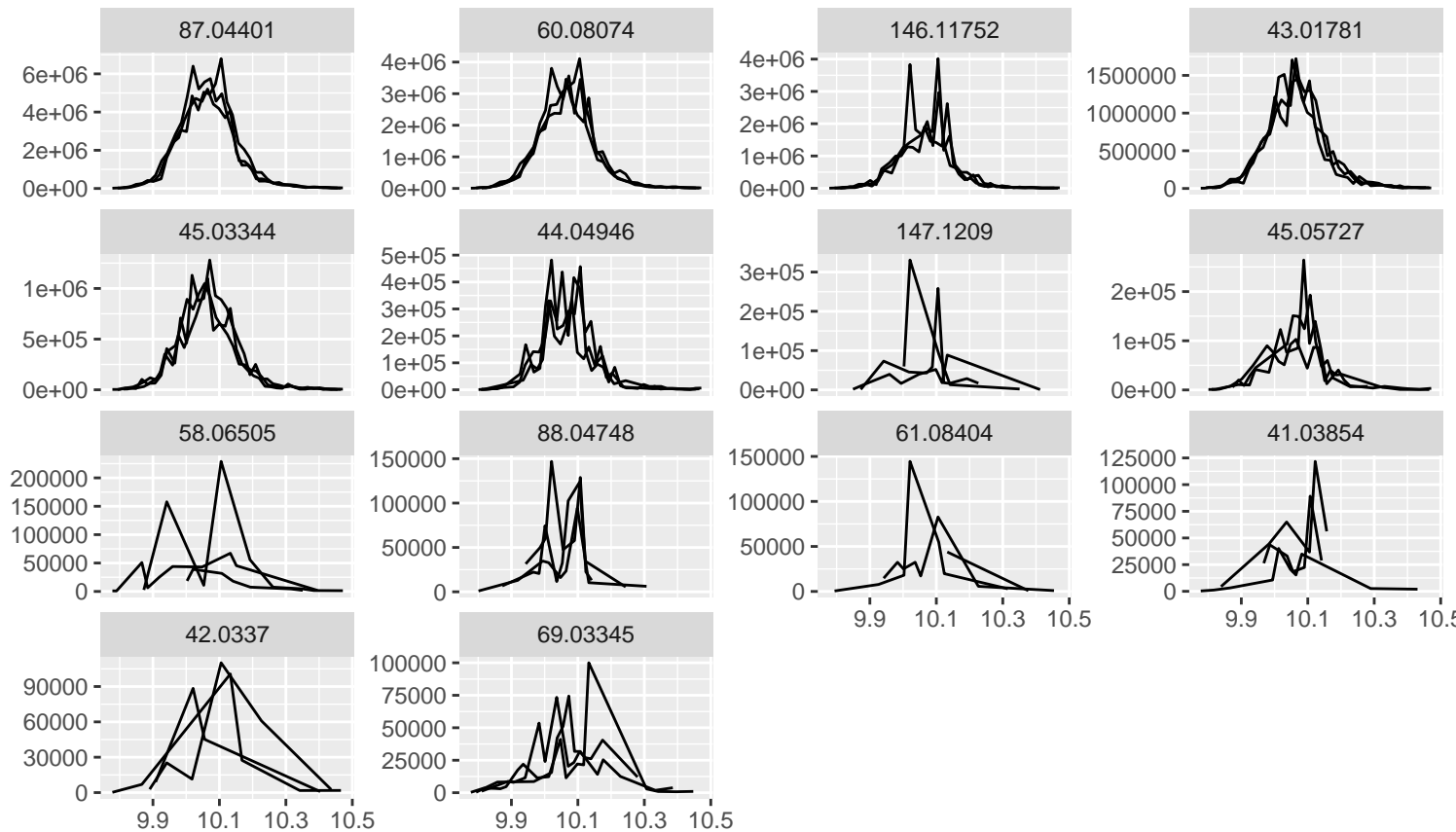
Hydroxyisoleucine (neg) 146.082268

int



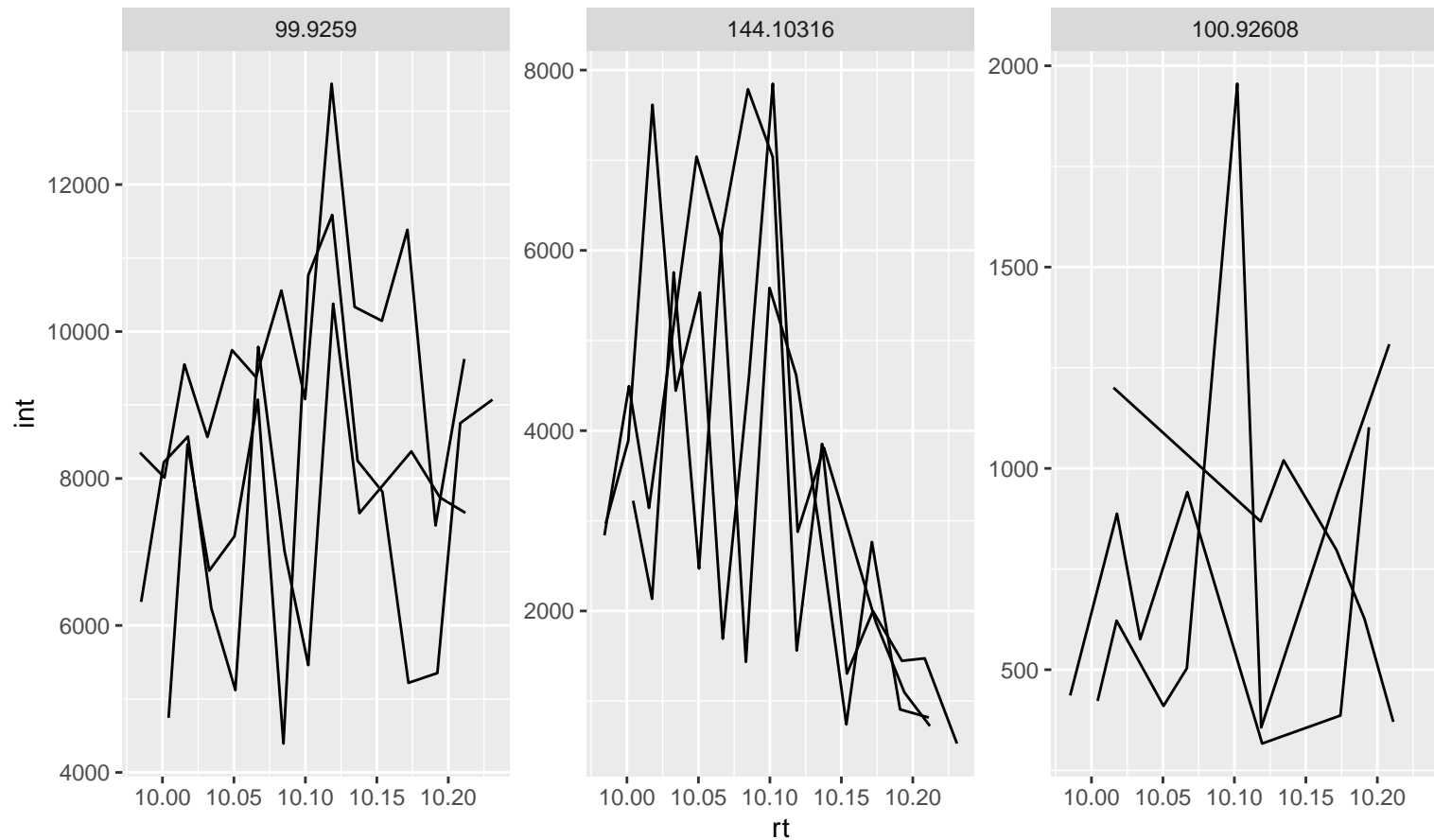
(3-Carboxypentyl)trimethylammonium (pos) 146.117555

int

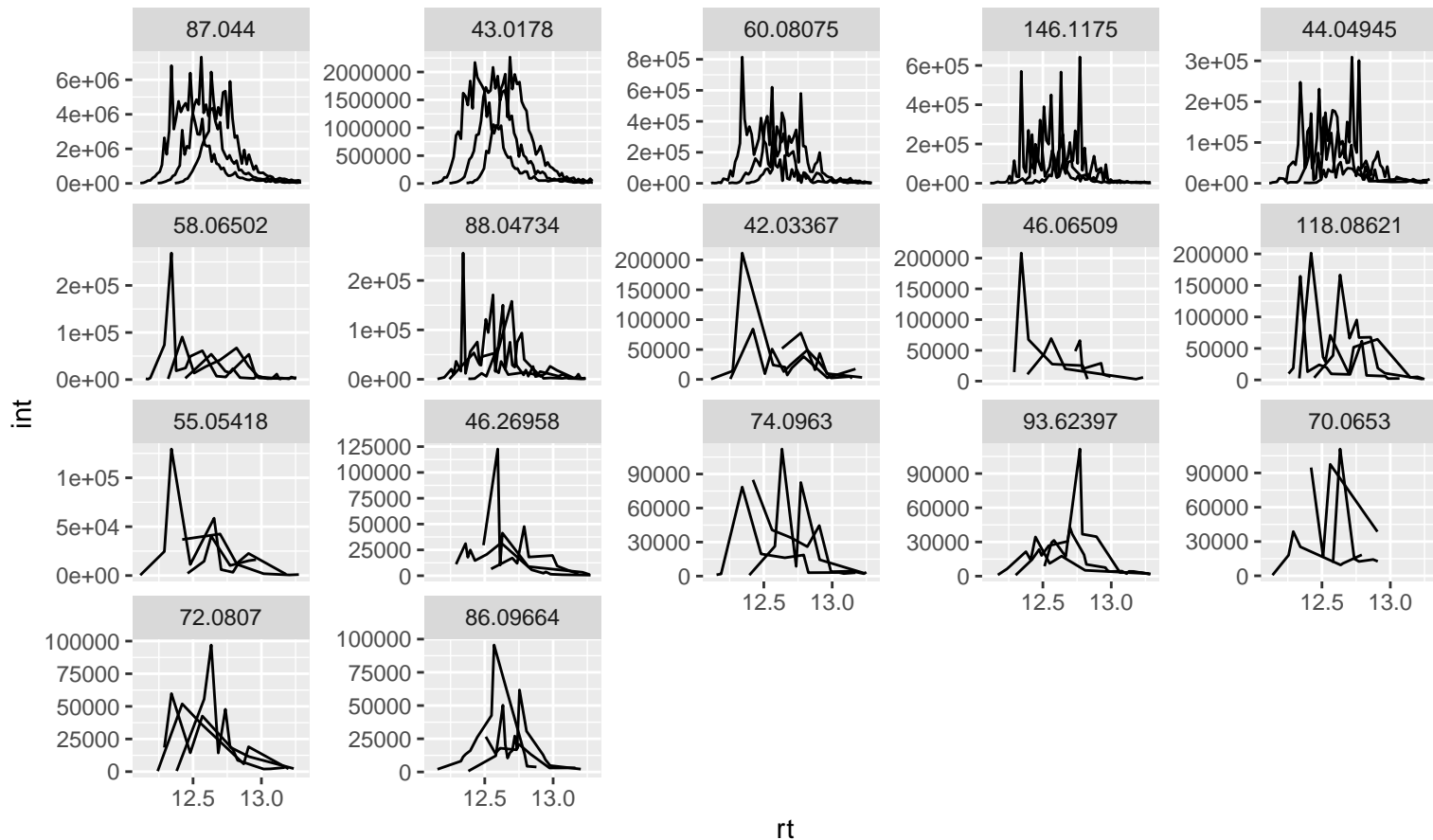


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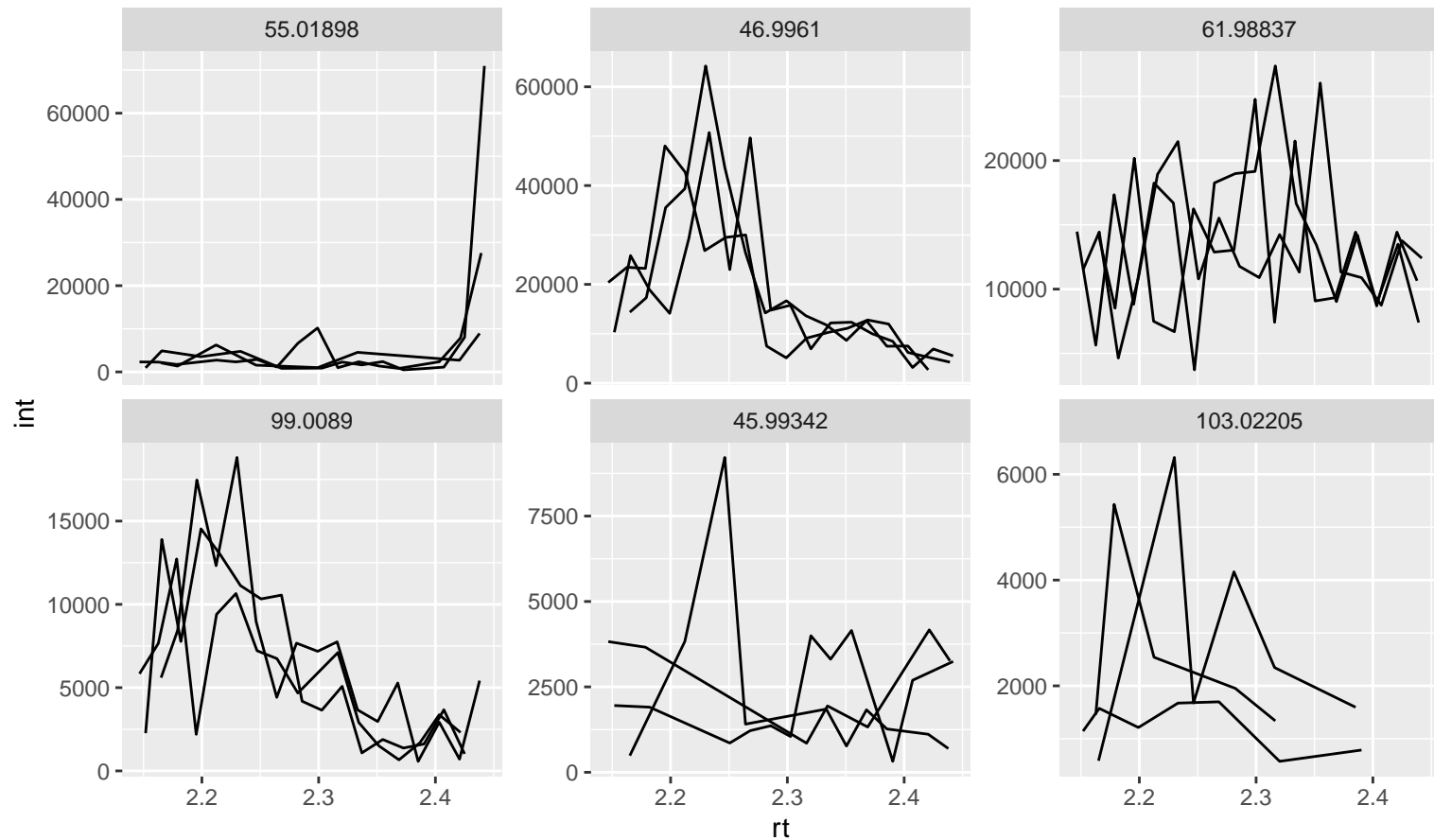
(3-Carboxypropyl)trimethylammonium (neg) 144.103003



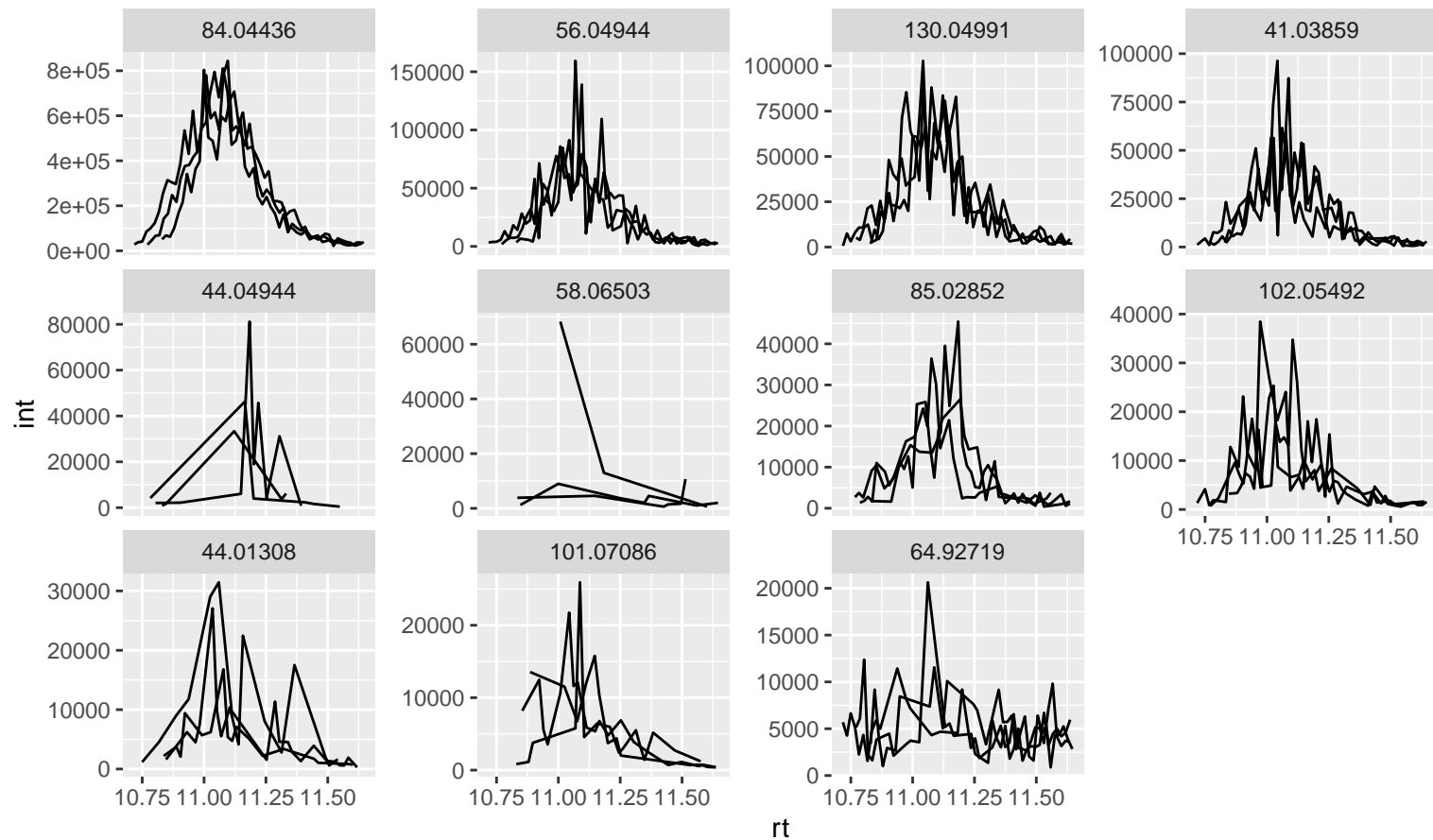
Acetylcholine (pos) 146.1175542



2-keto-4-methylthiobutyric acid (neg) 147.012141

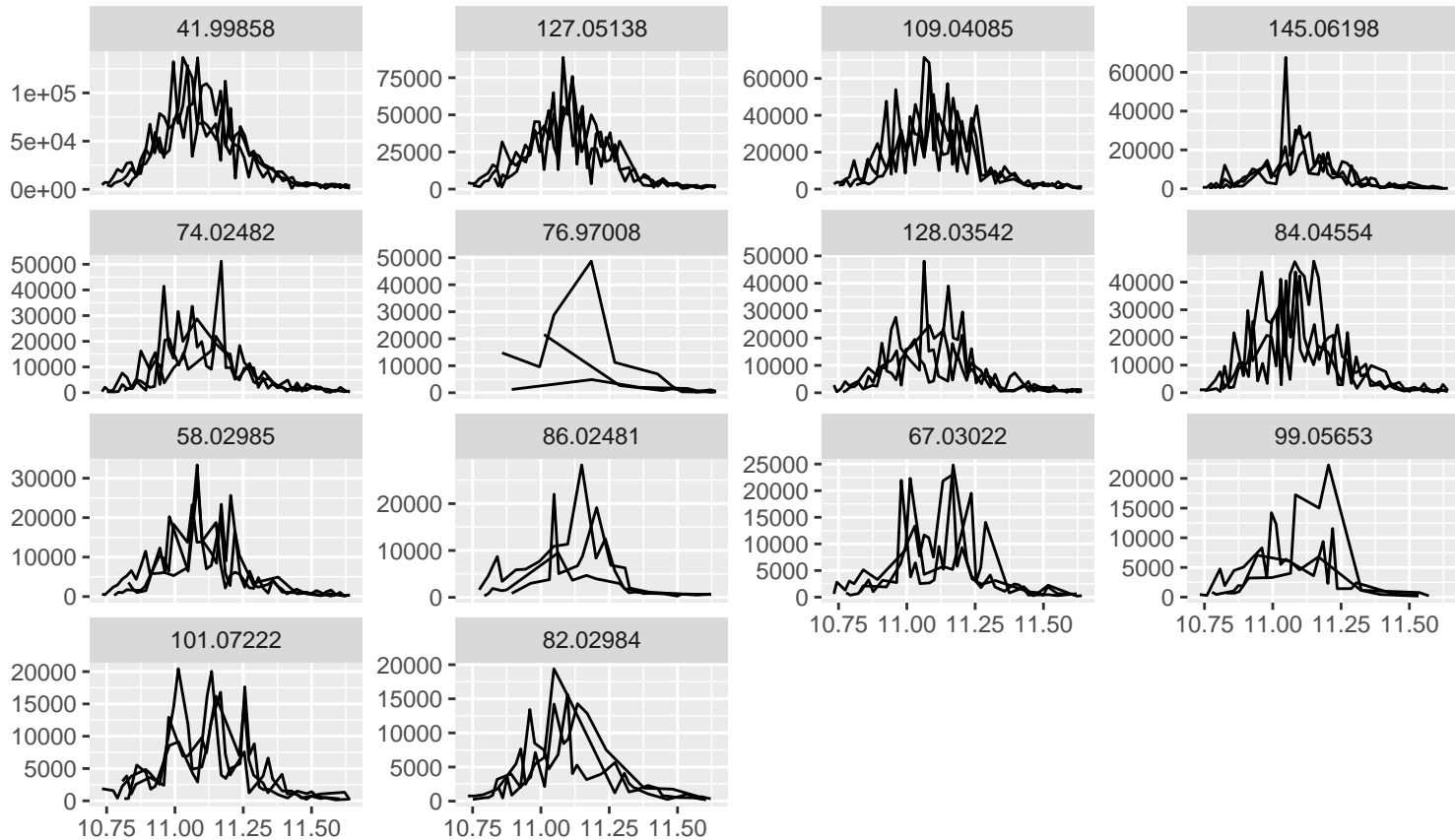


L-Glutamine (pos) 147.076419



L-Glutamine (neg) 145.061867

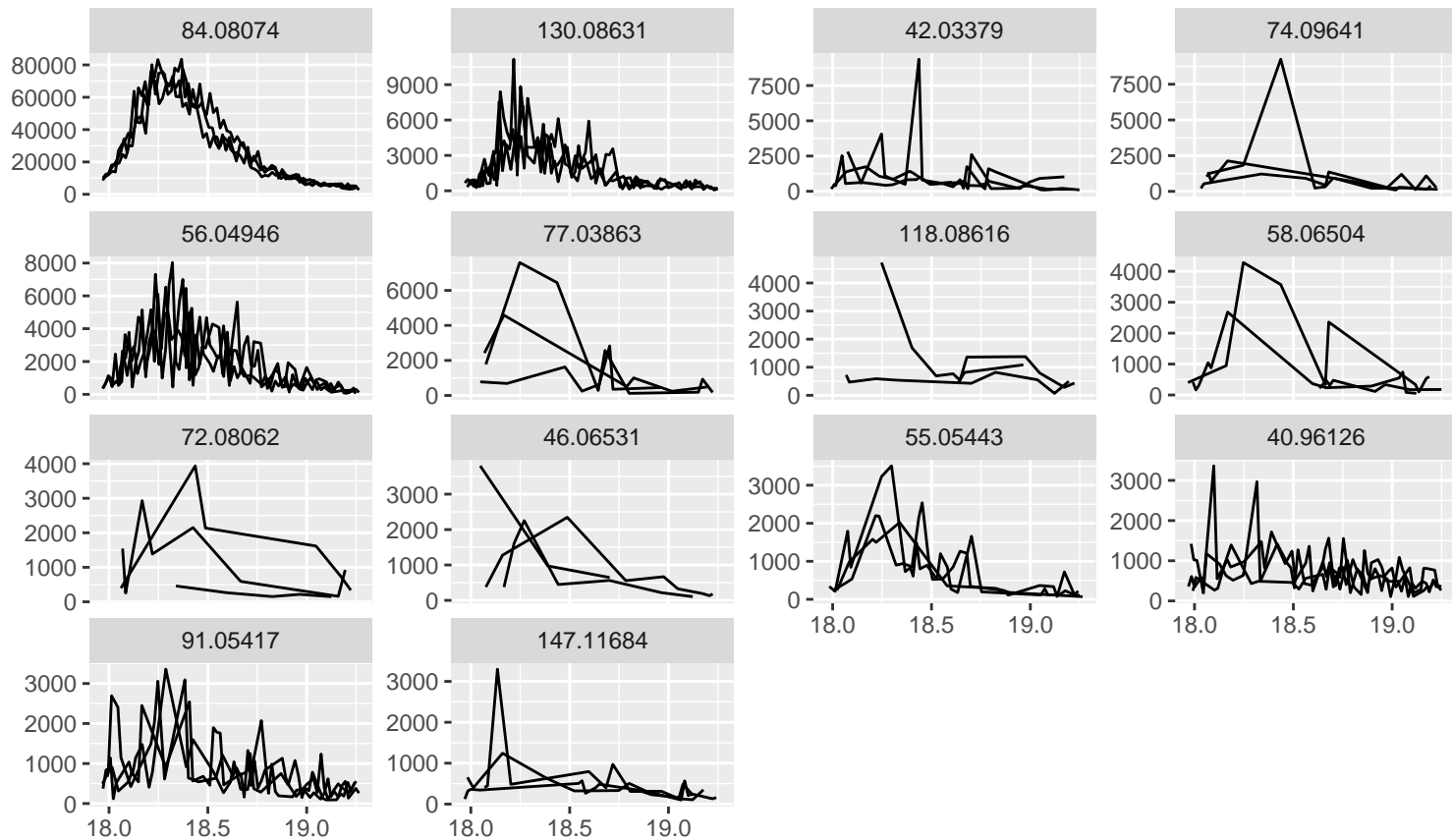
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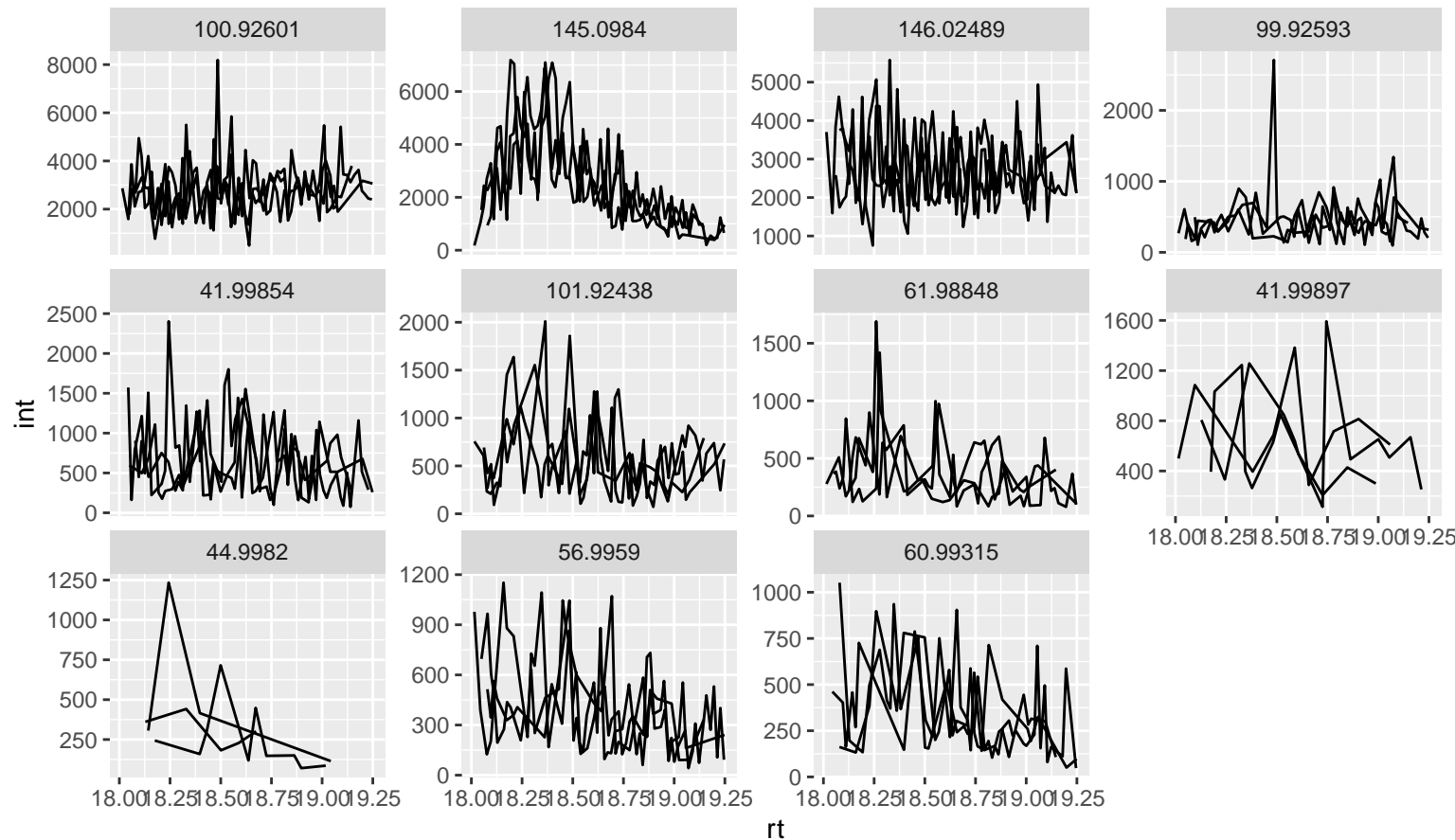
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L-Lysine (pos) 147.112804

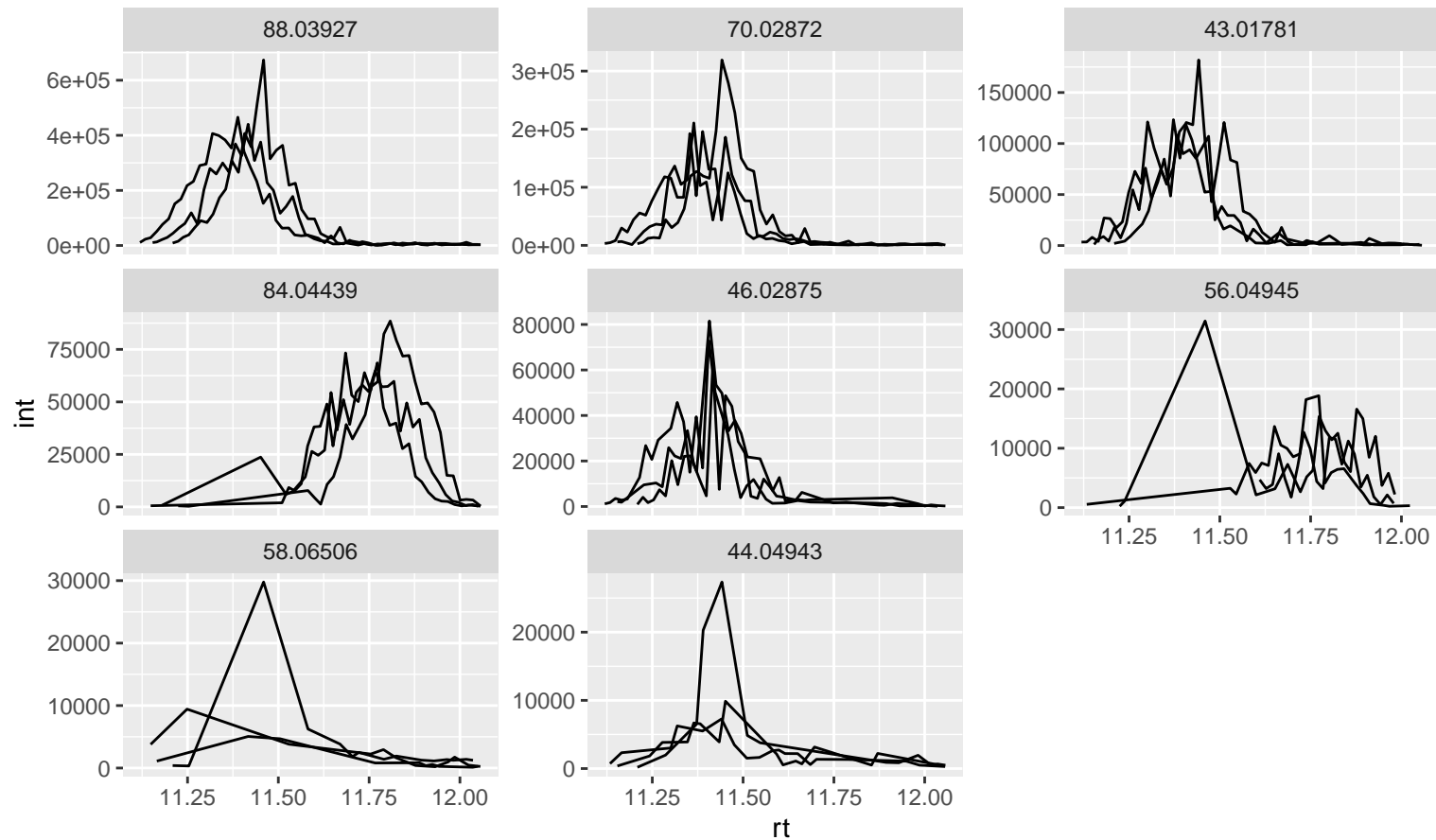
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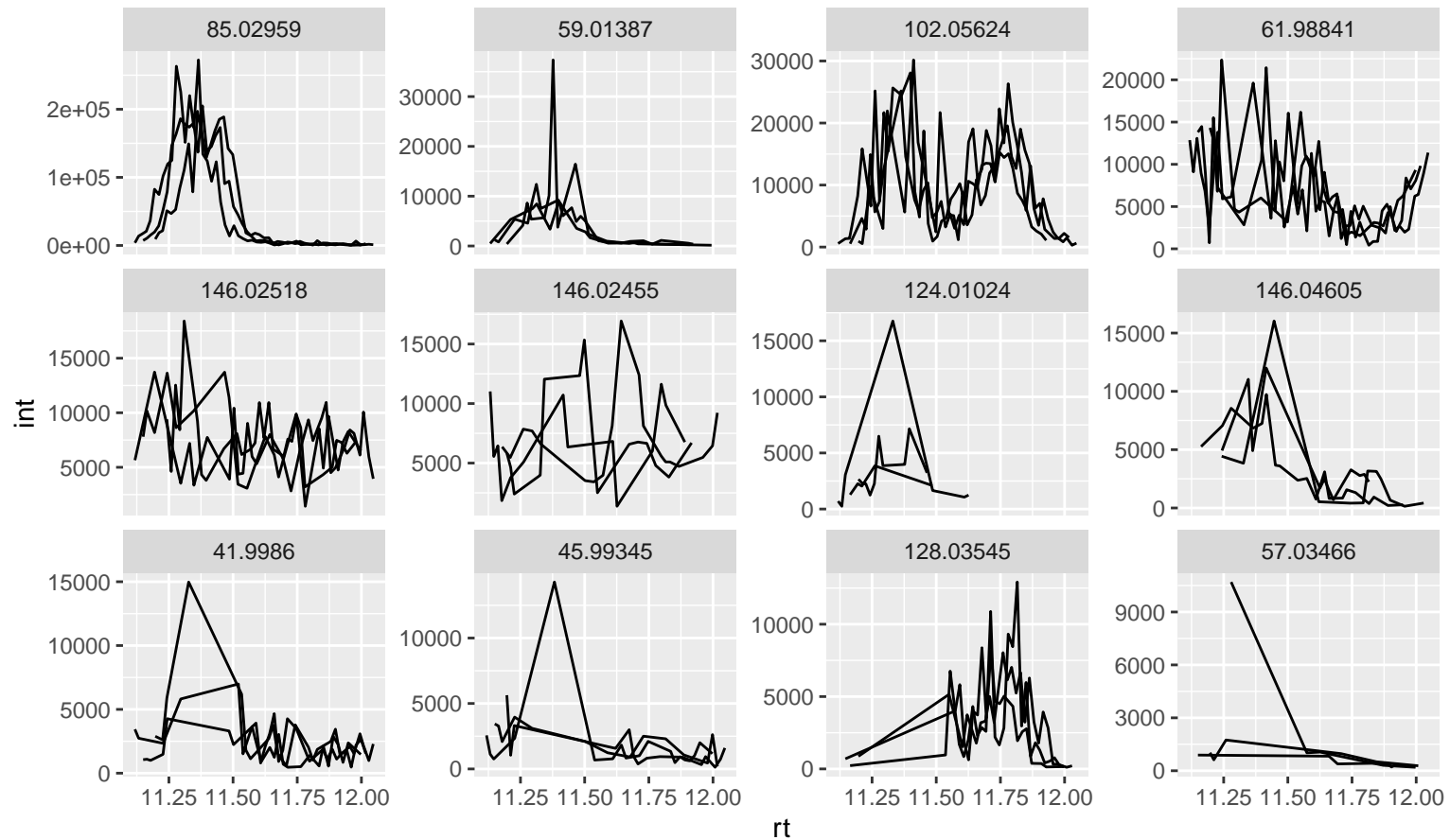
L-Lysine (neg) 145.098252



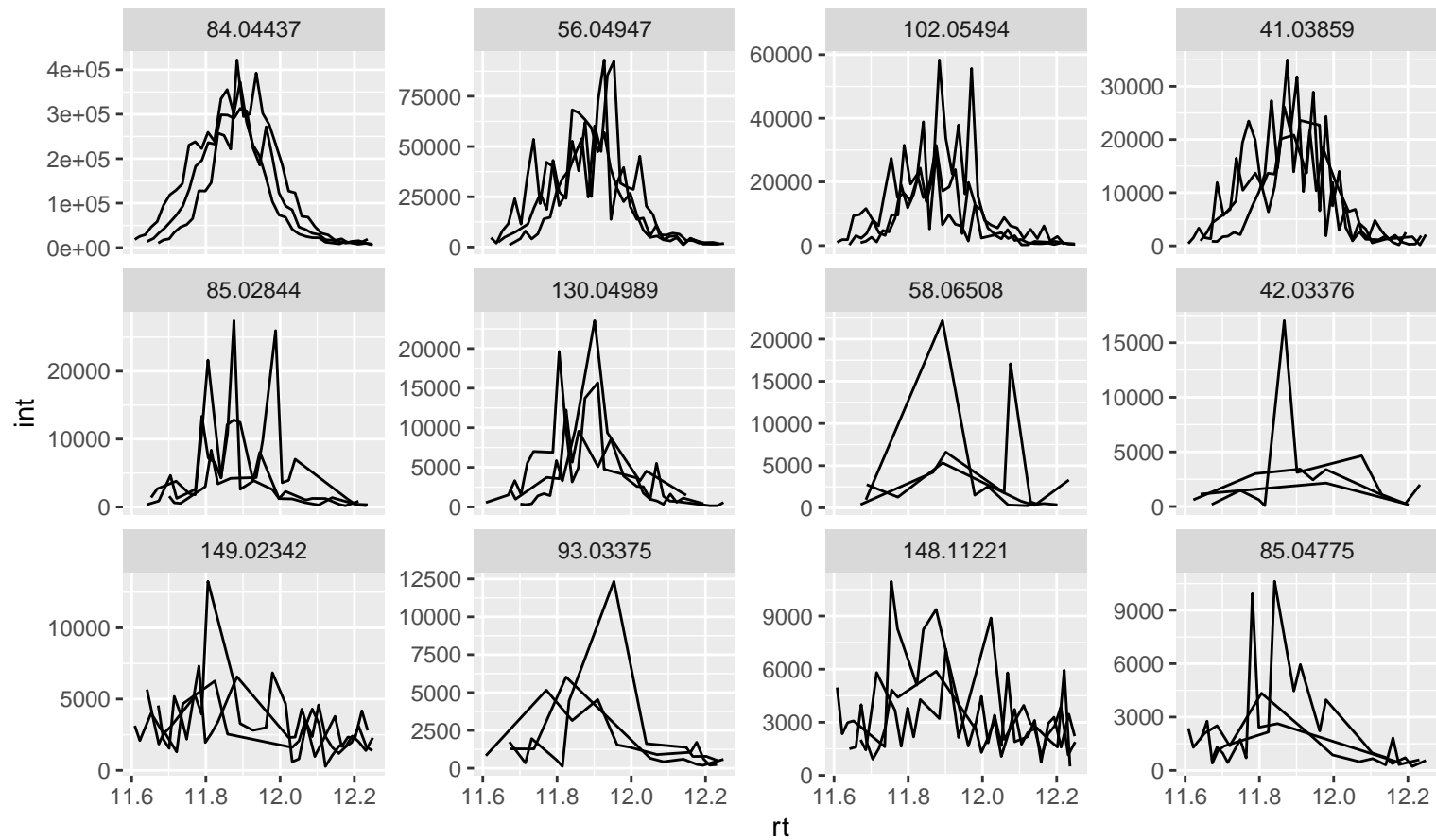
beta-Glutamic acid (pos) 148.060435



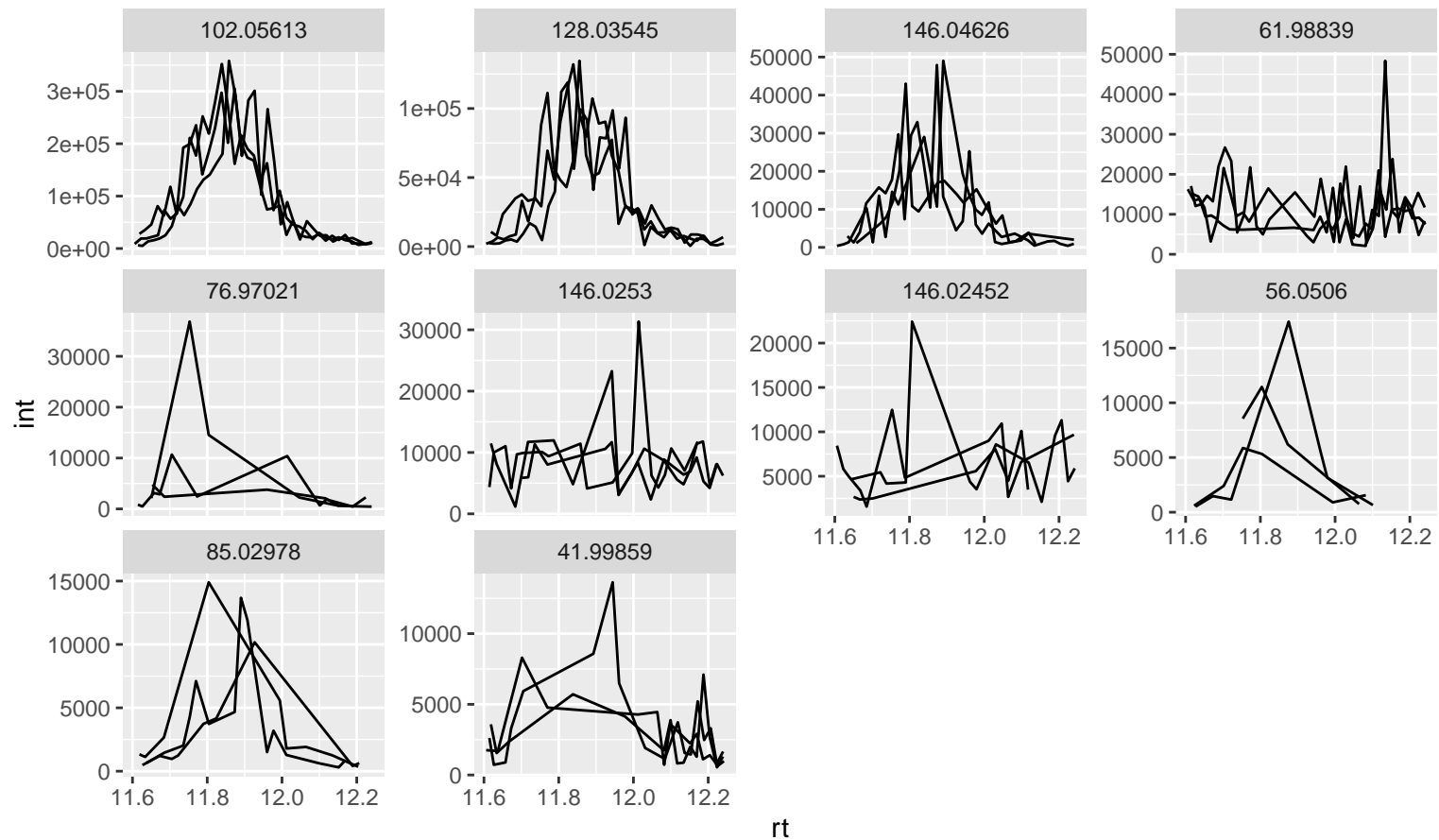
beta-Glutamic acid (neg) 146.045883



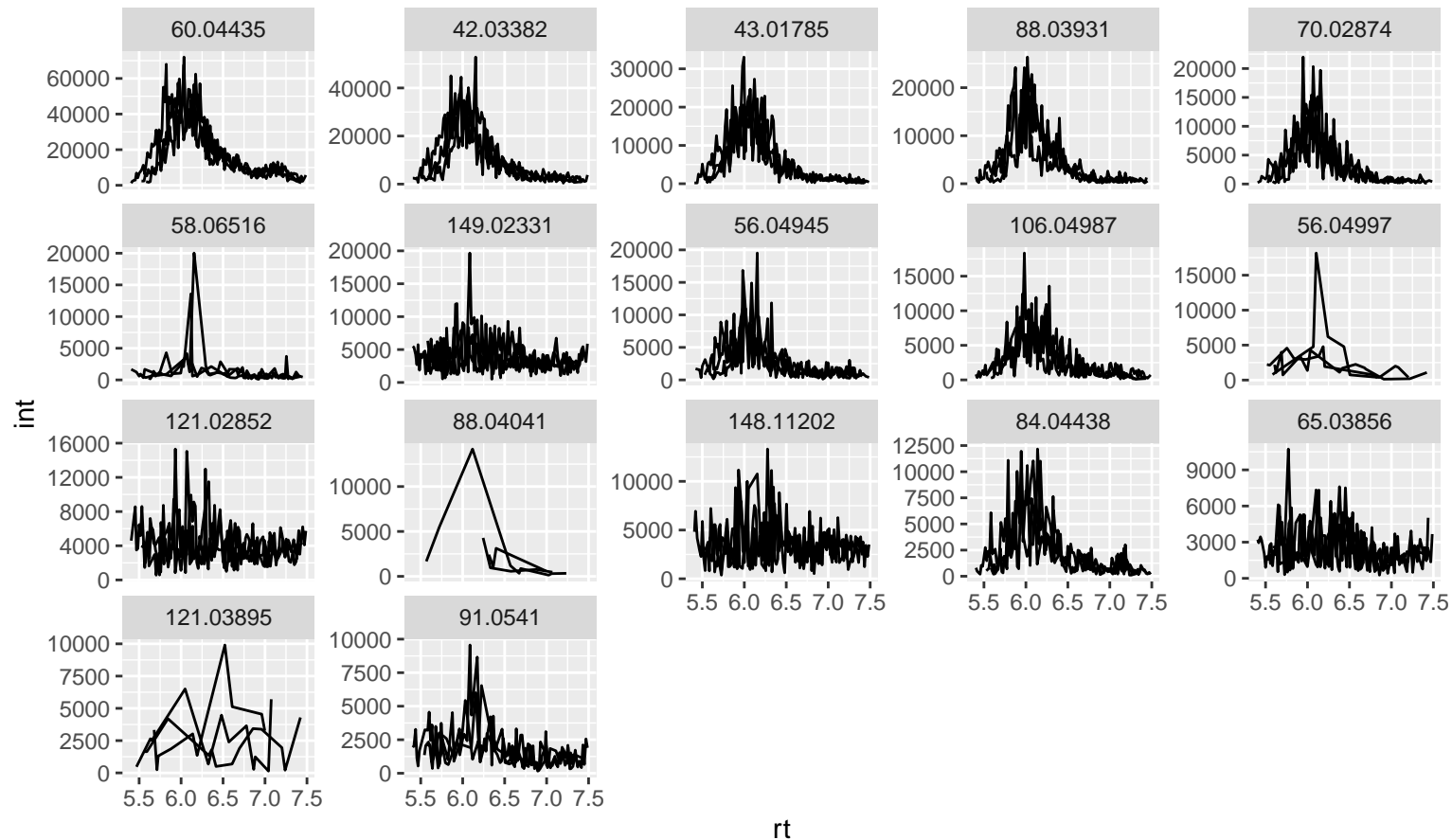
L-Glutamic acid (pos) 148.060435



L-Glutamic acid (neg) 146.045883

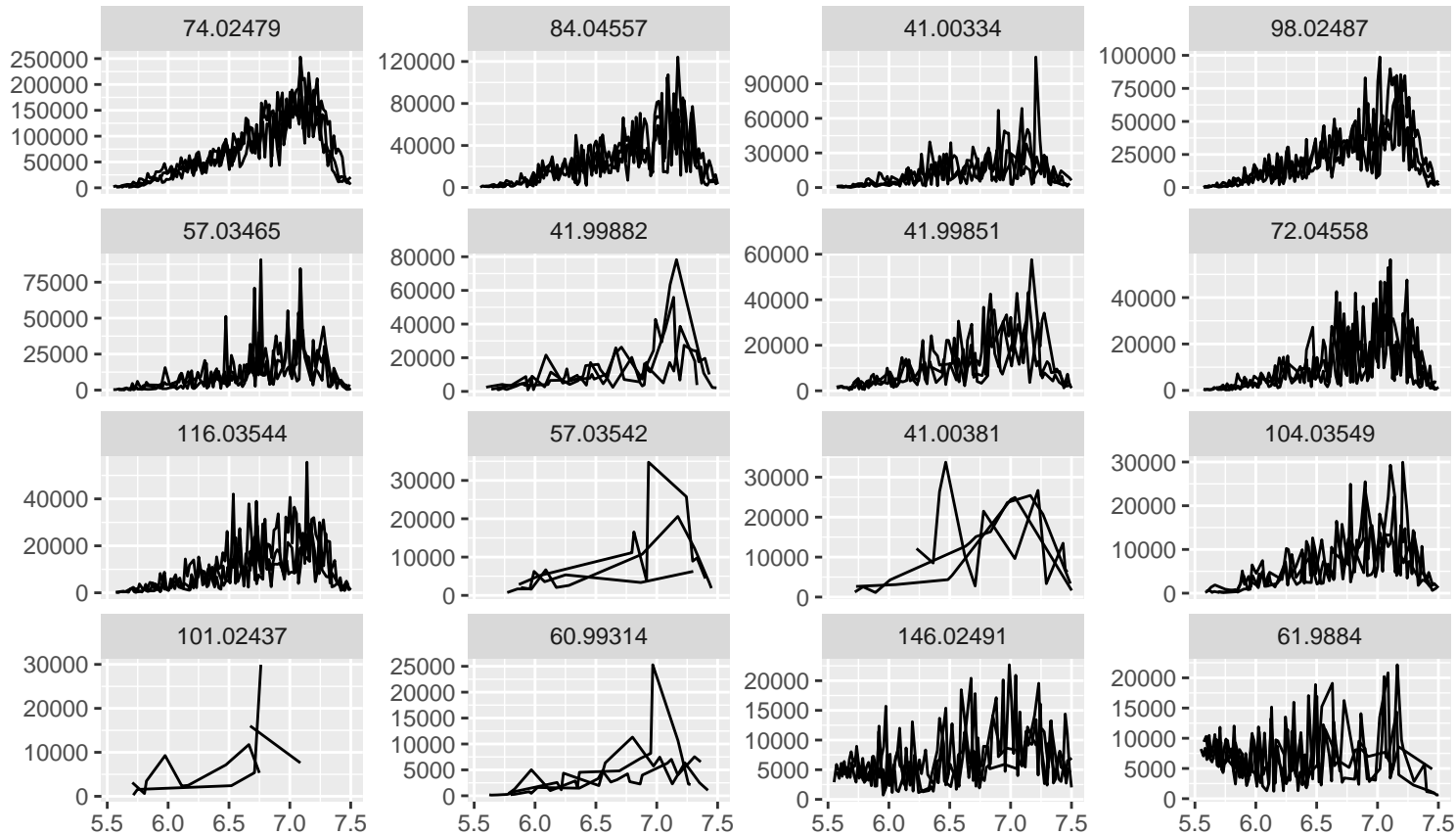


O-Acetyl-L-serine (pos) 148.060435



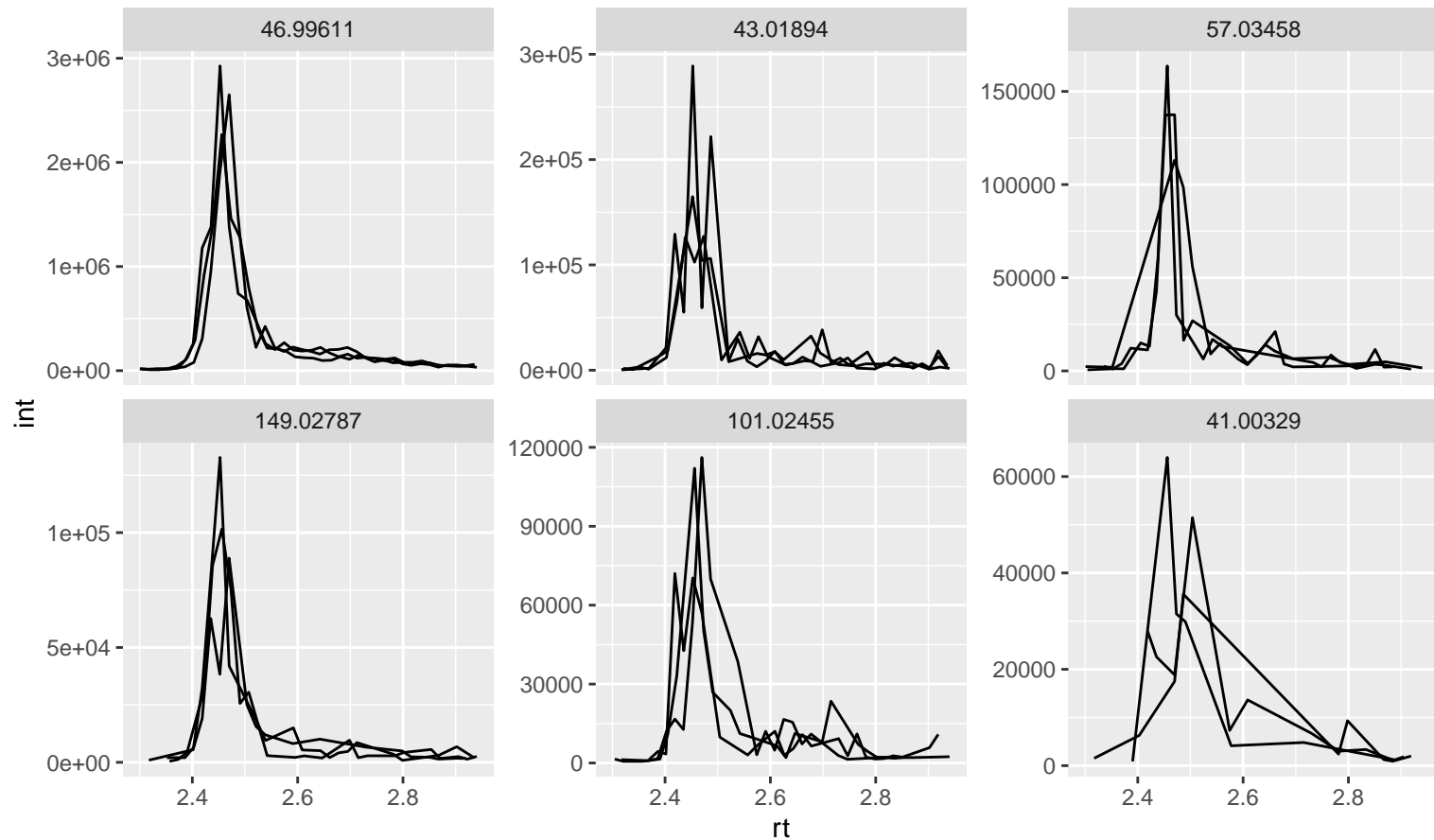
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int

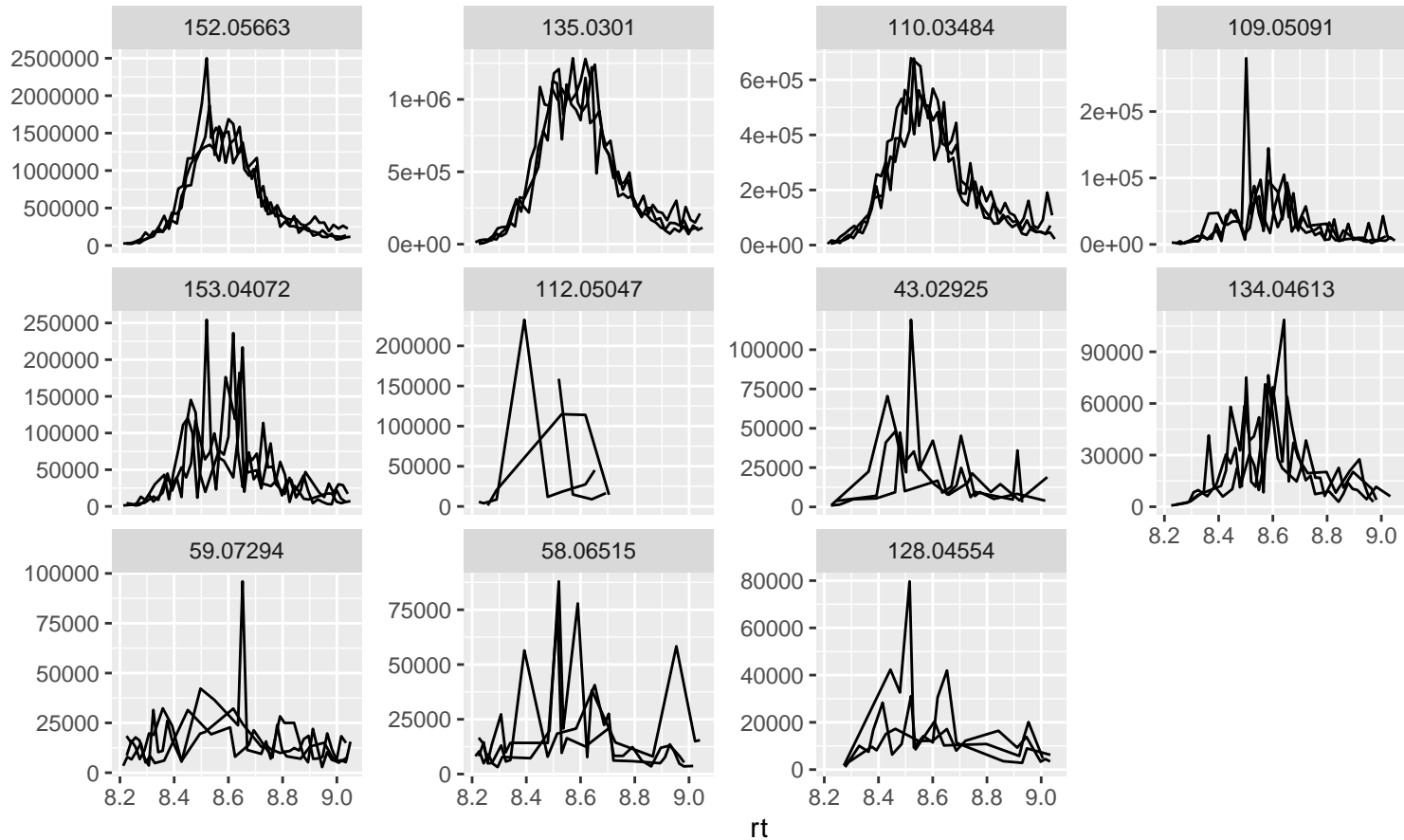


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2-Hydroxy-4-(methylthio)butyric acid (neg) 149.027791

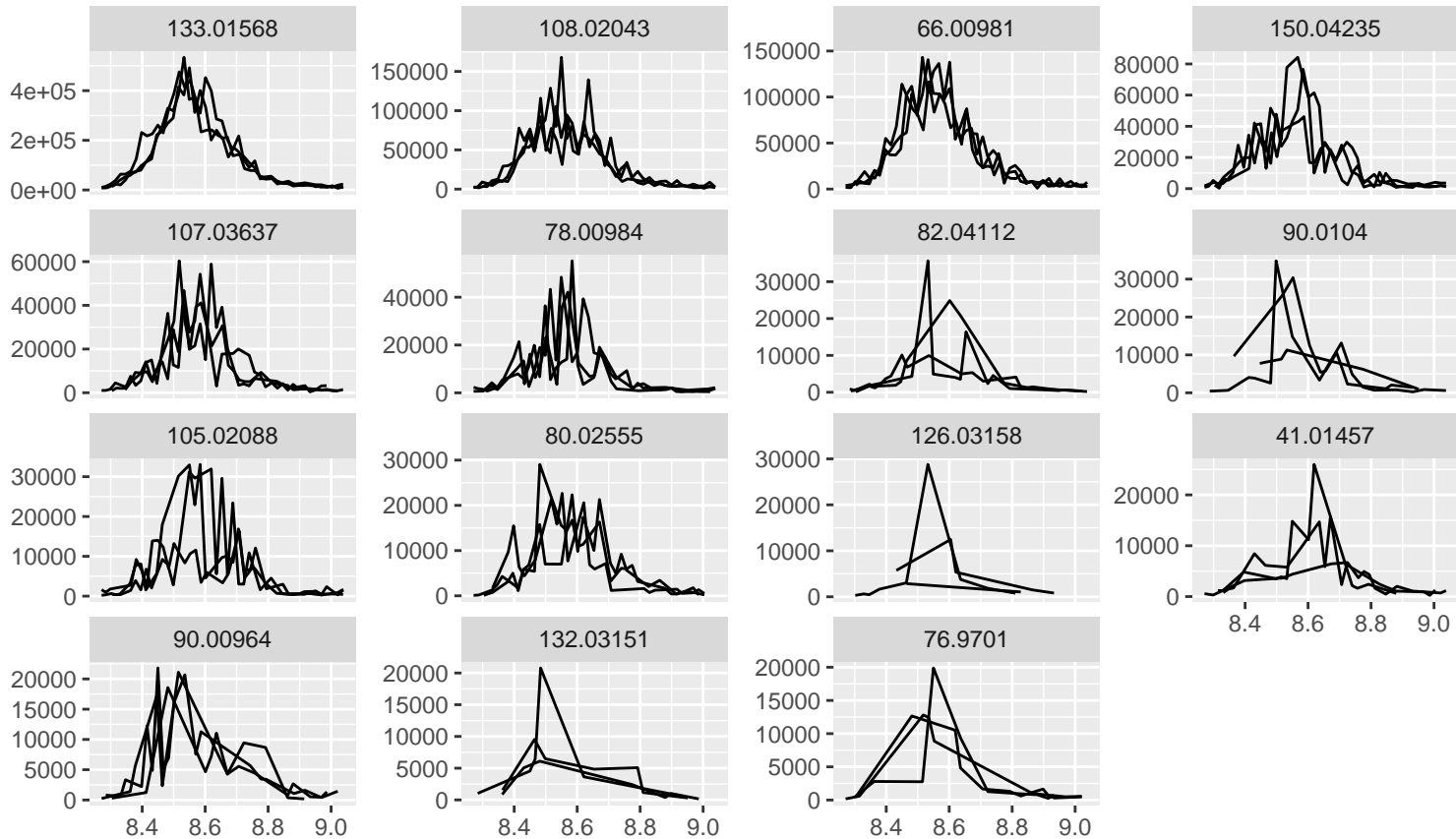


Guanine (pos) 152.05686



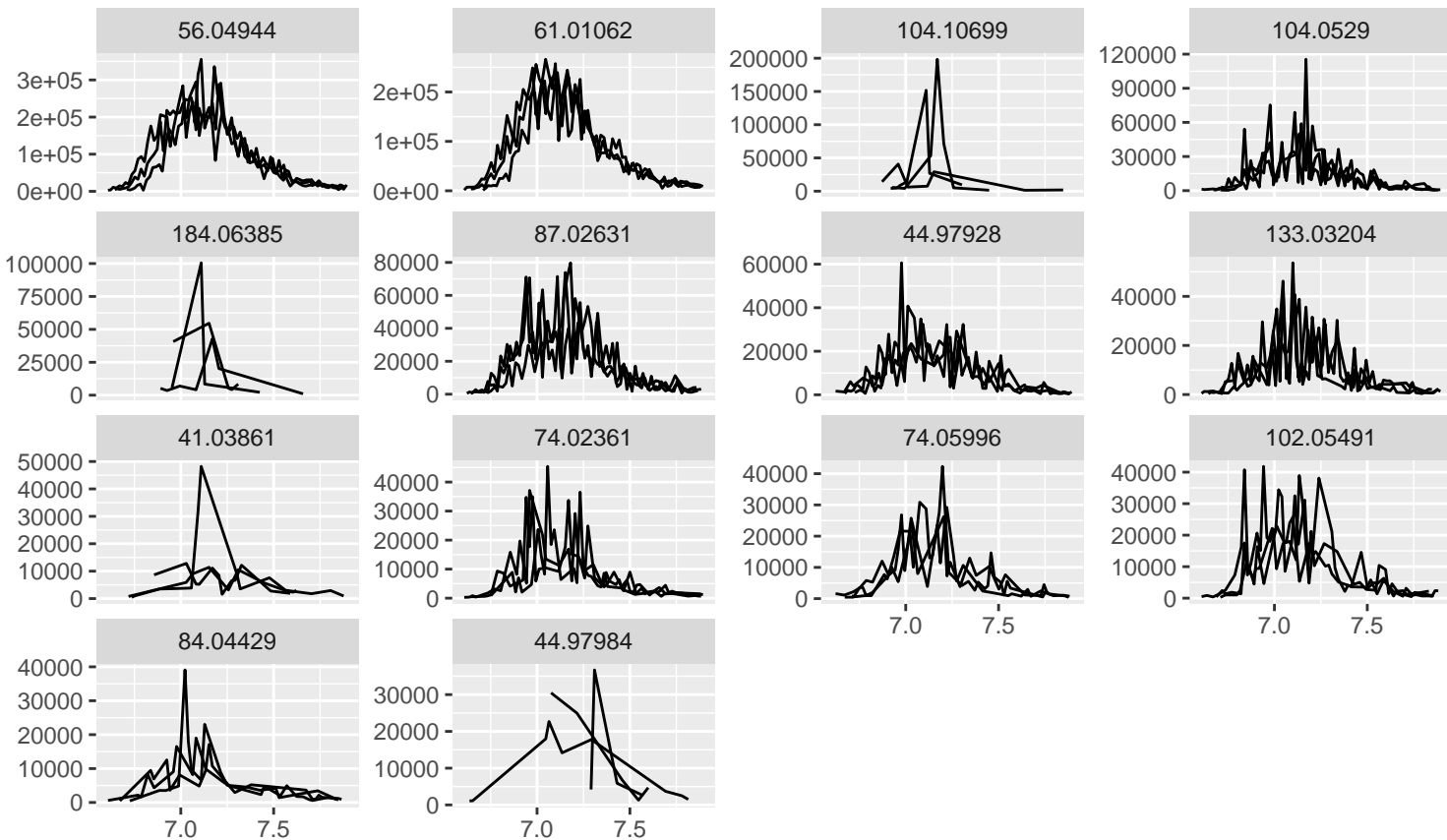
Guanine (neg) 150.042134

int

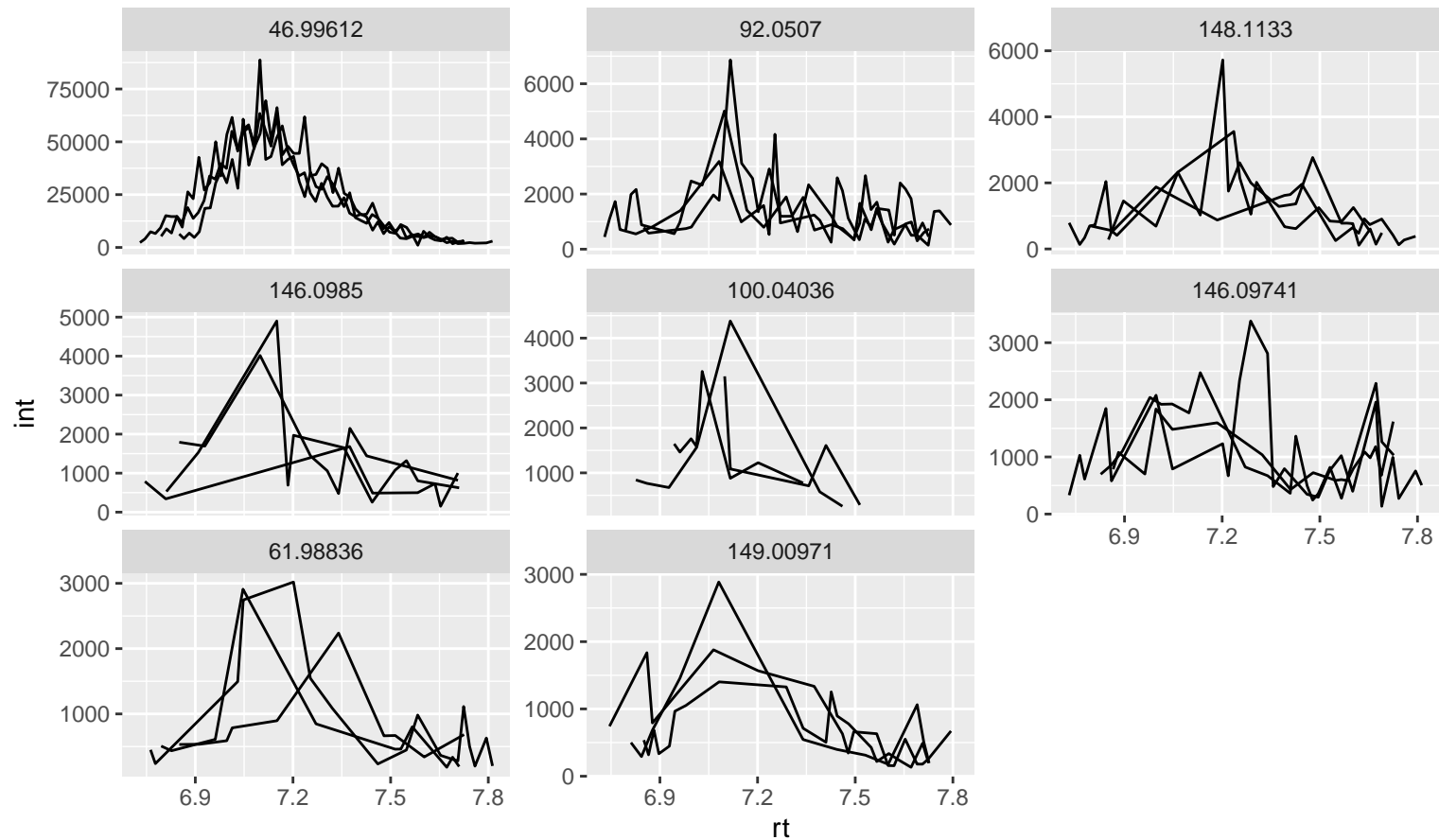


L-Methionine (pos) 150.058327

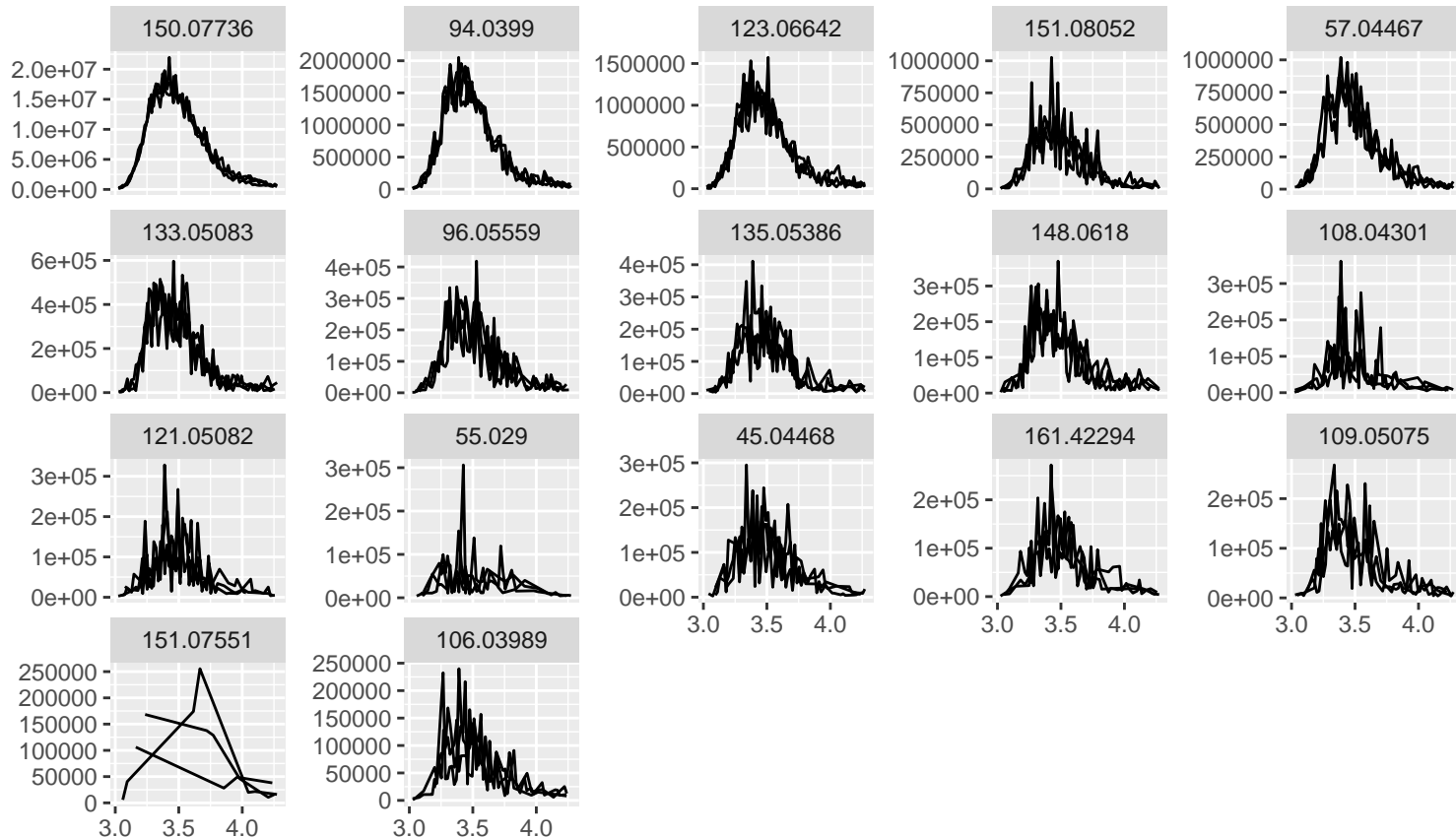
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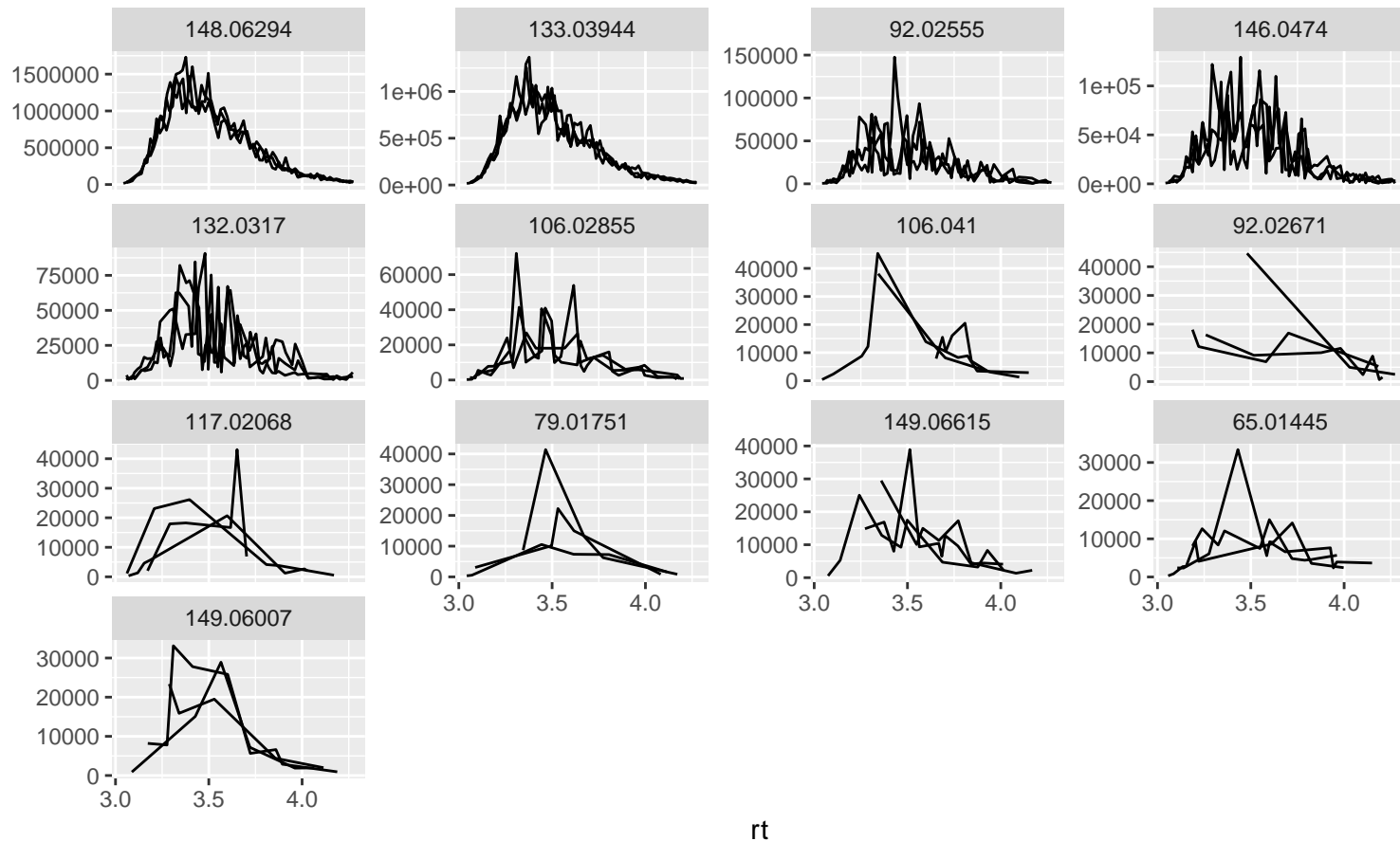
L-Methionine (neg) 148.043775



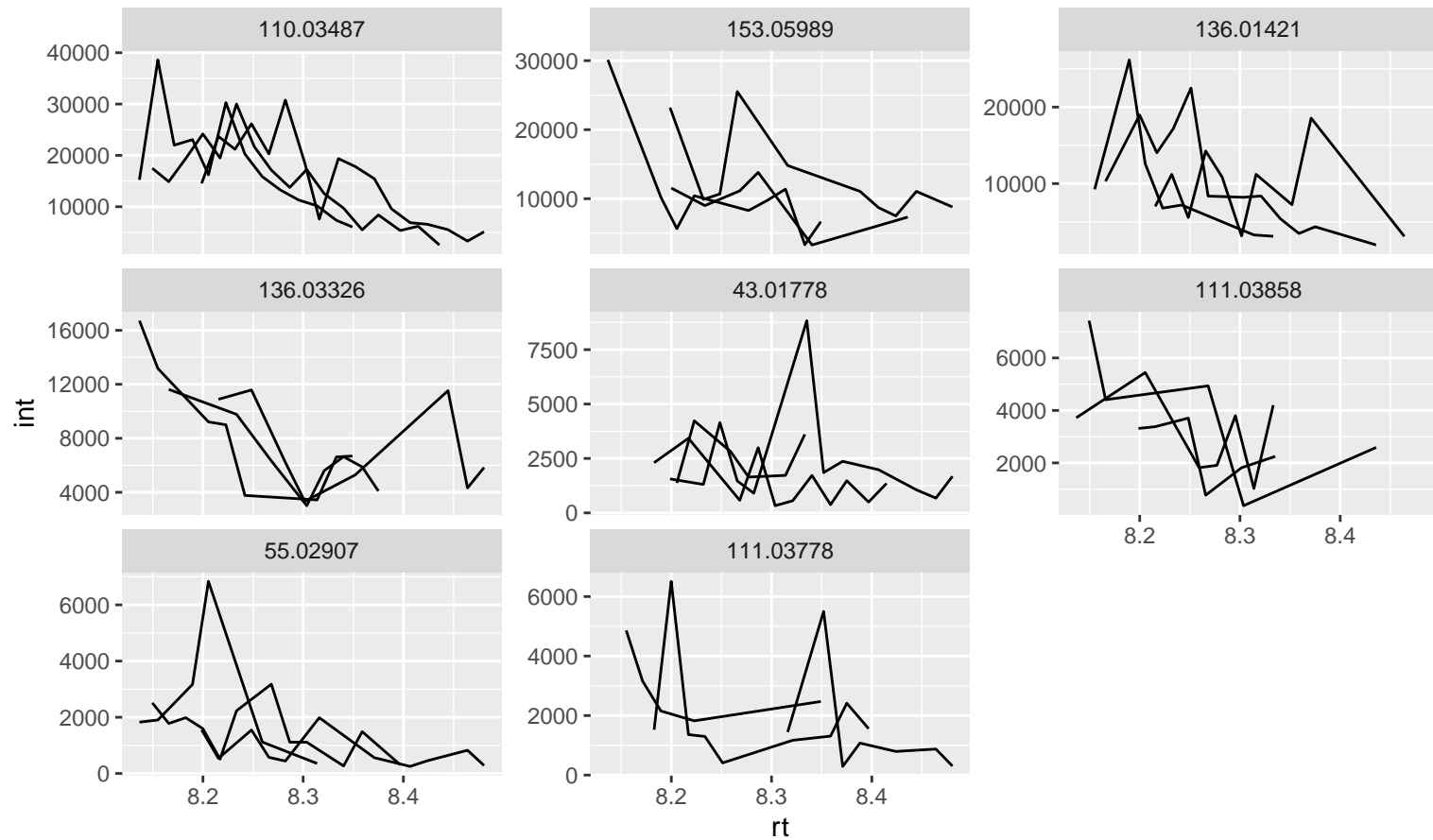
N6-Methyladenine (pos) 150.077421



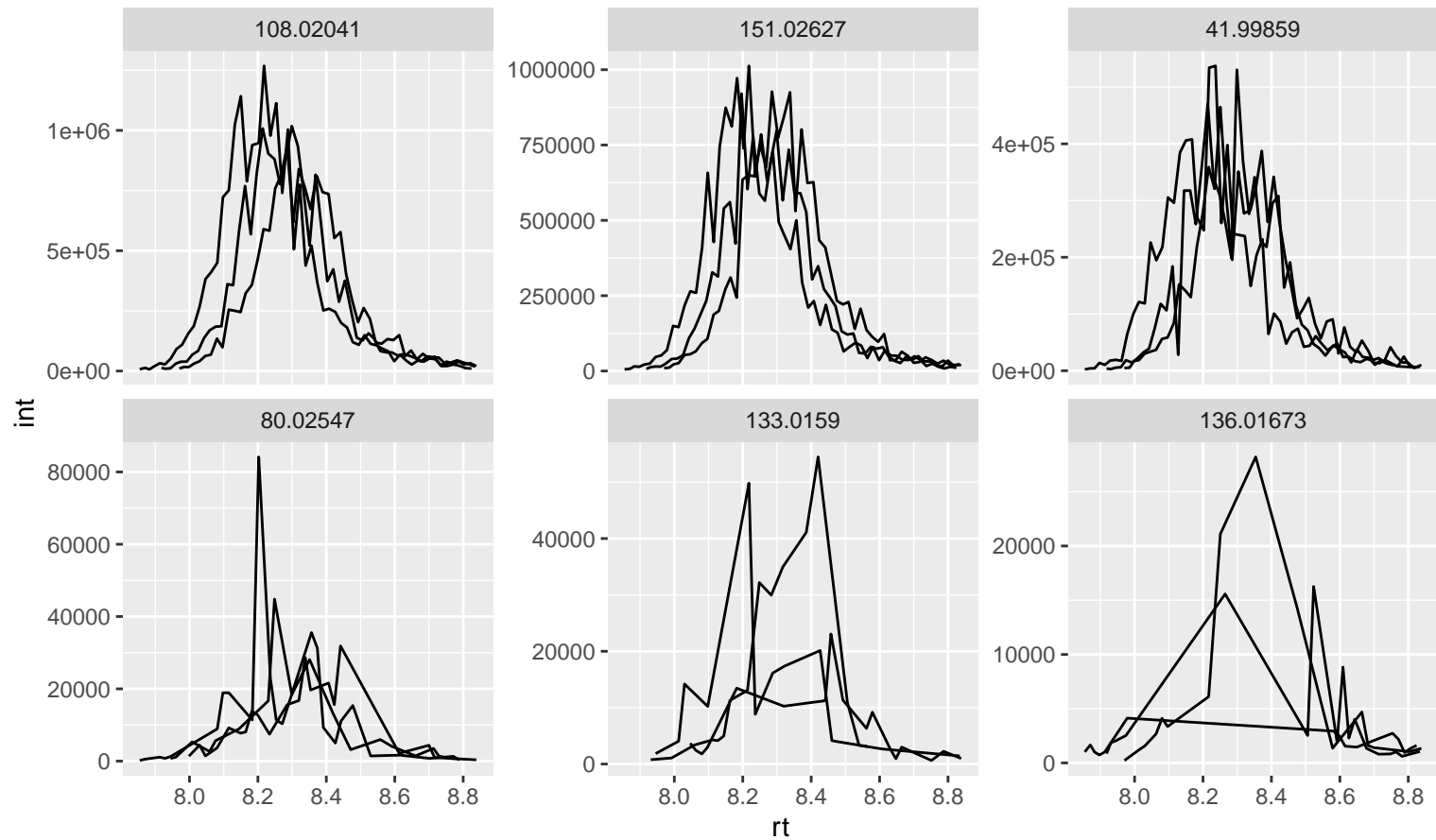
N6-Methyladenine (neg) 148.062869



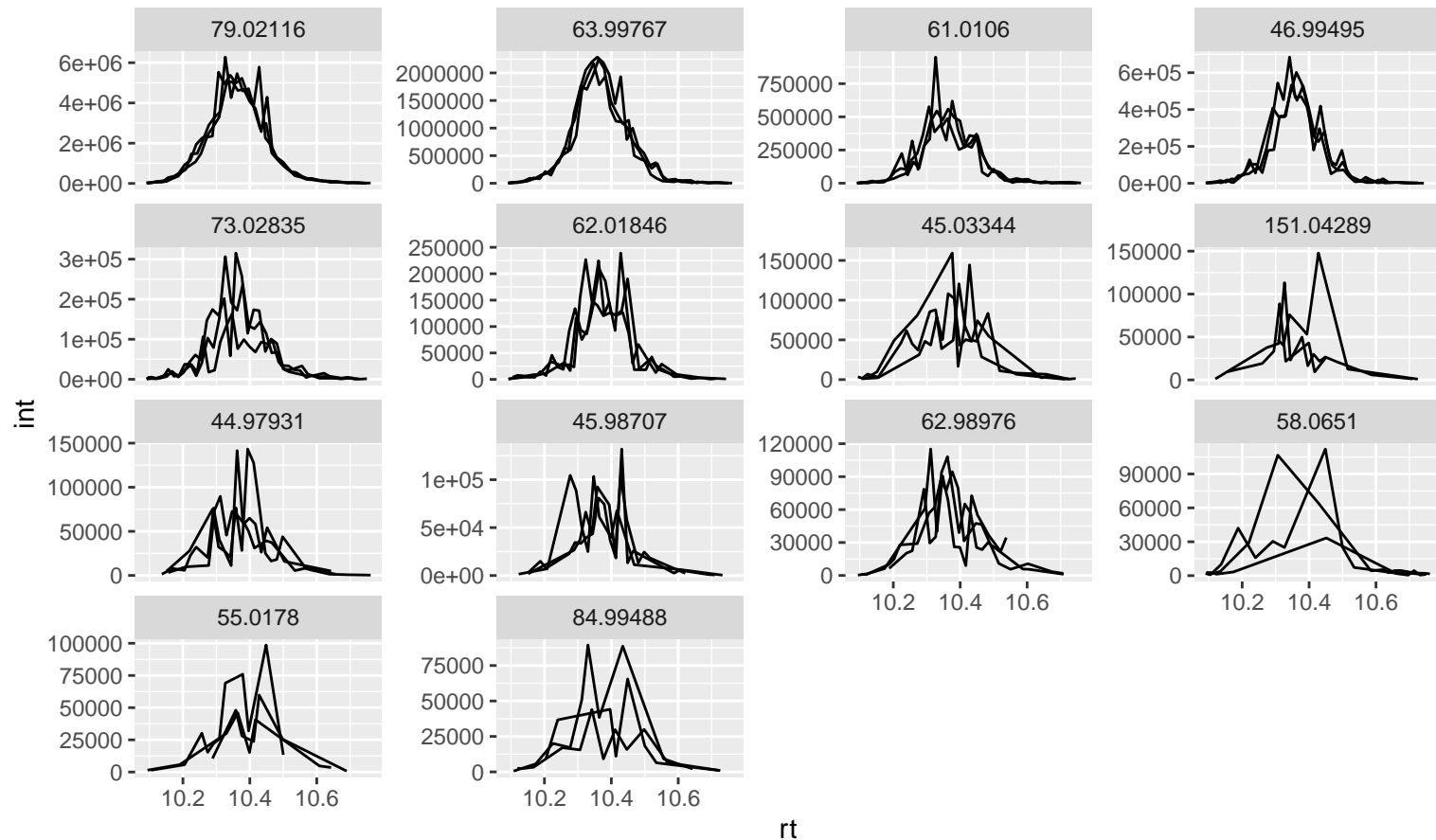
Xanthine (pos) 153.040702



Xanthine (neg) 151.02615

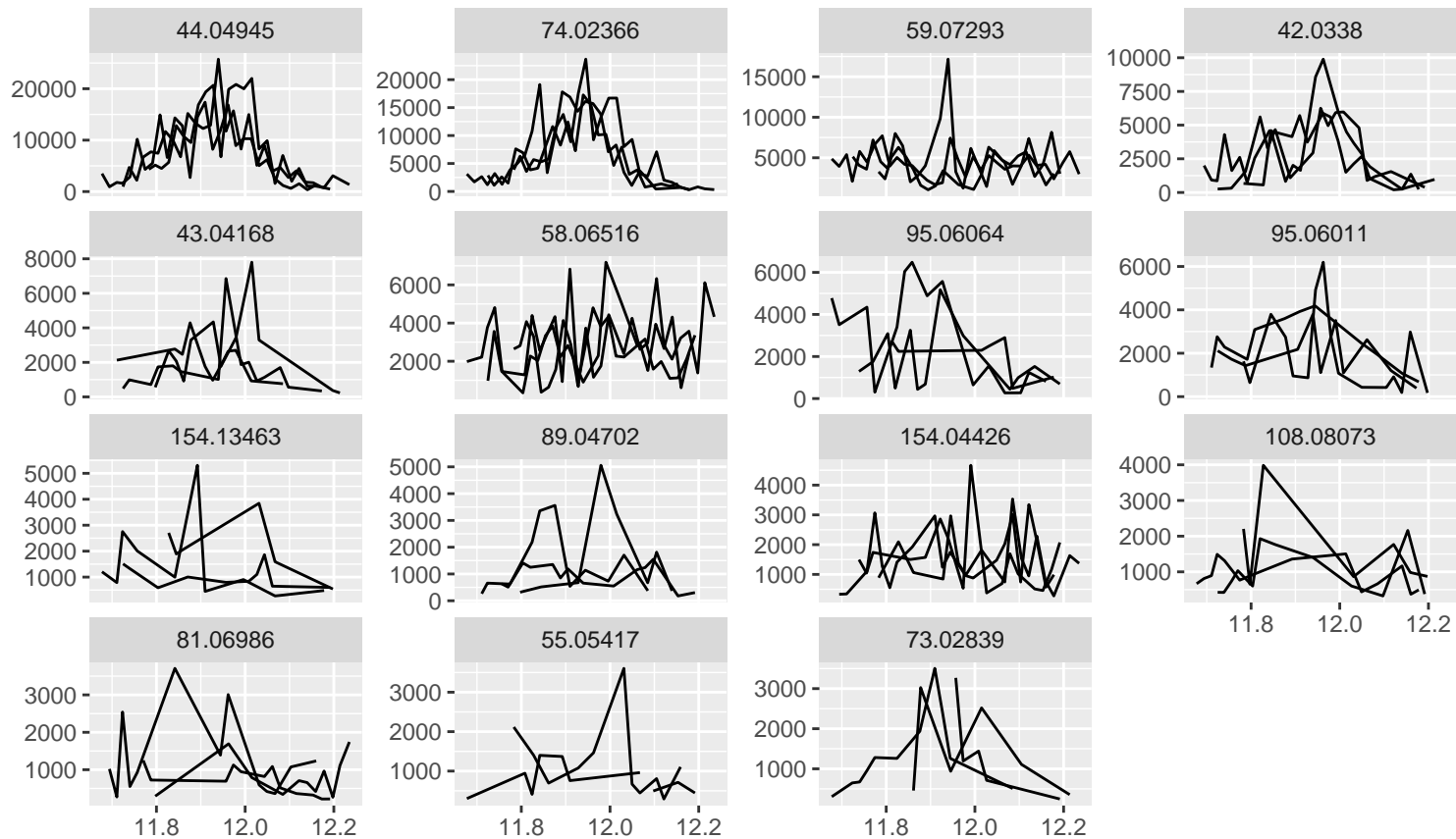


Dimethylsulfoxonium propionate (pos) 151.042343



L-Cysteinesulfinic acid (pos) 154.016857

int



rt

L-Cysteinesulfinic acid (neg) 152.002305

88.04045

int

150000

100000

50000

0

11.6 11.8 12.0 12.2

71.01387

7500

5000

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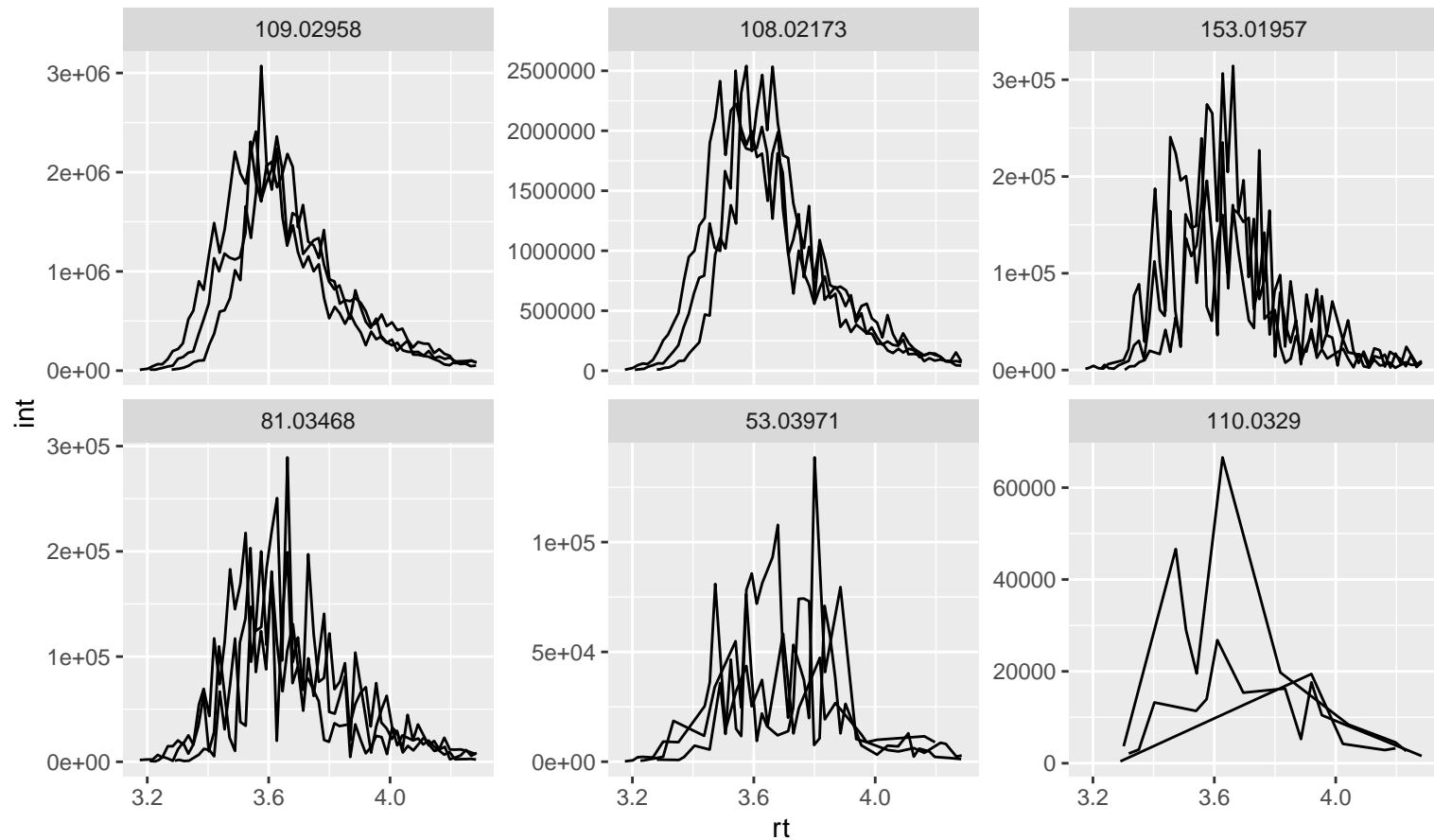
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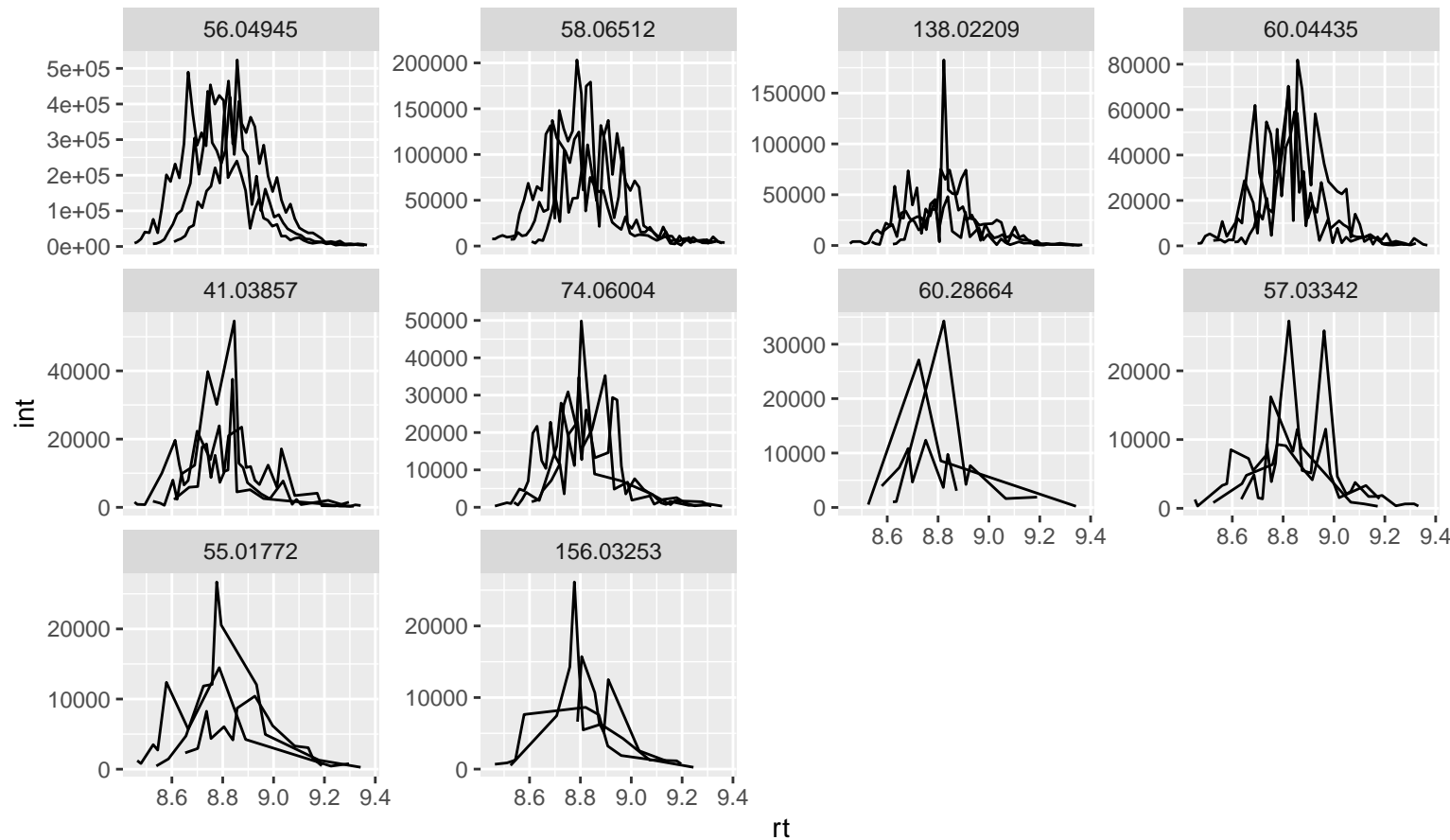
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rt

2,5-Dihydroxybenzoic acid (neg) 153.019334

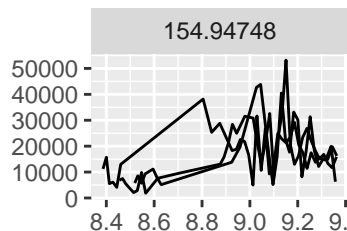
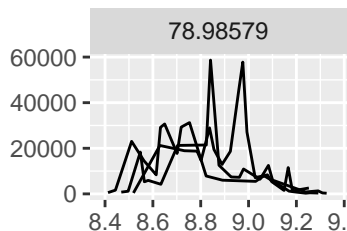
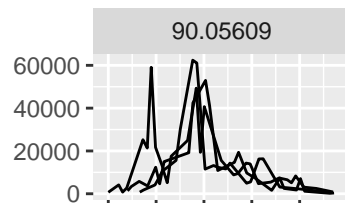
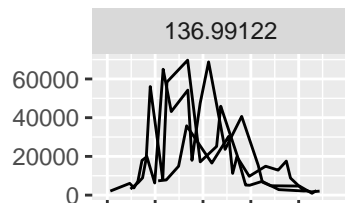
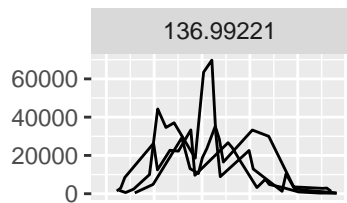
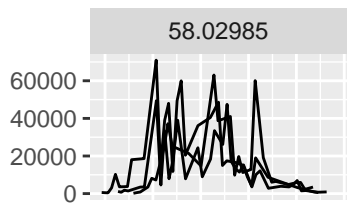
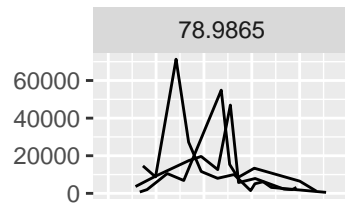
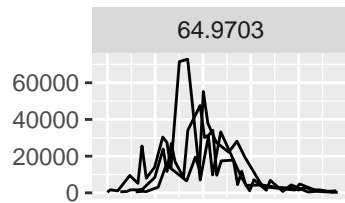
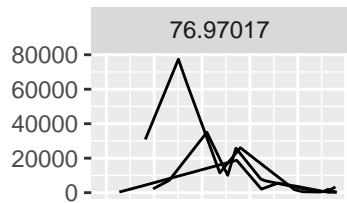
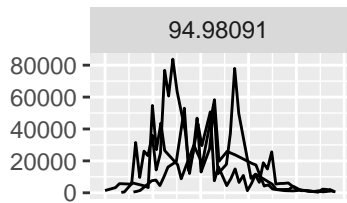
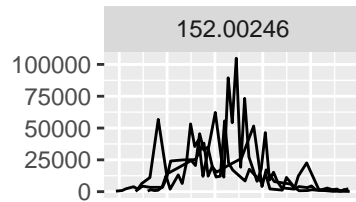
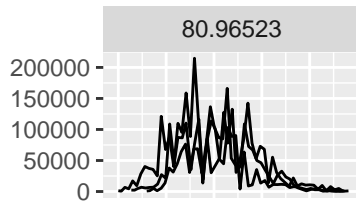
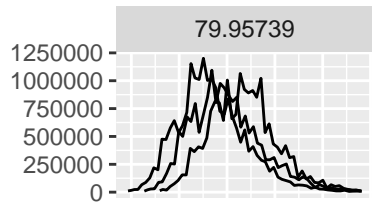
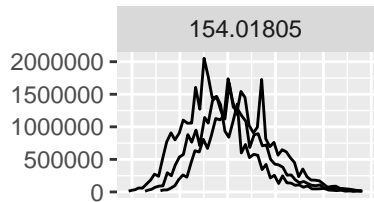


Cysteinolic acid (pos) 156.032507



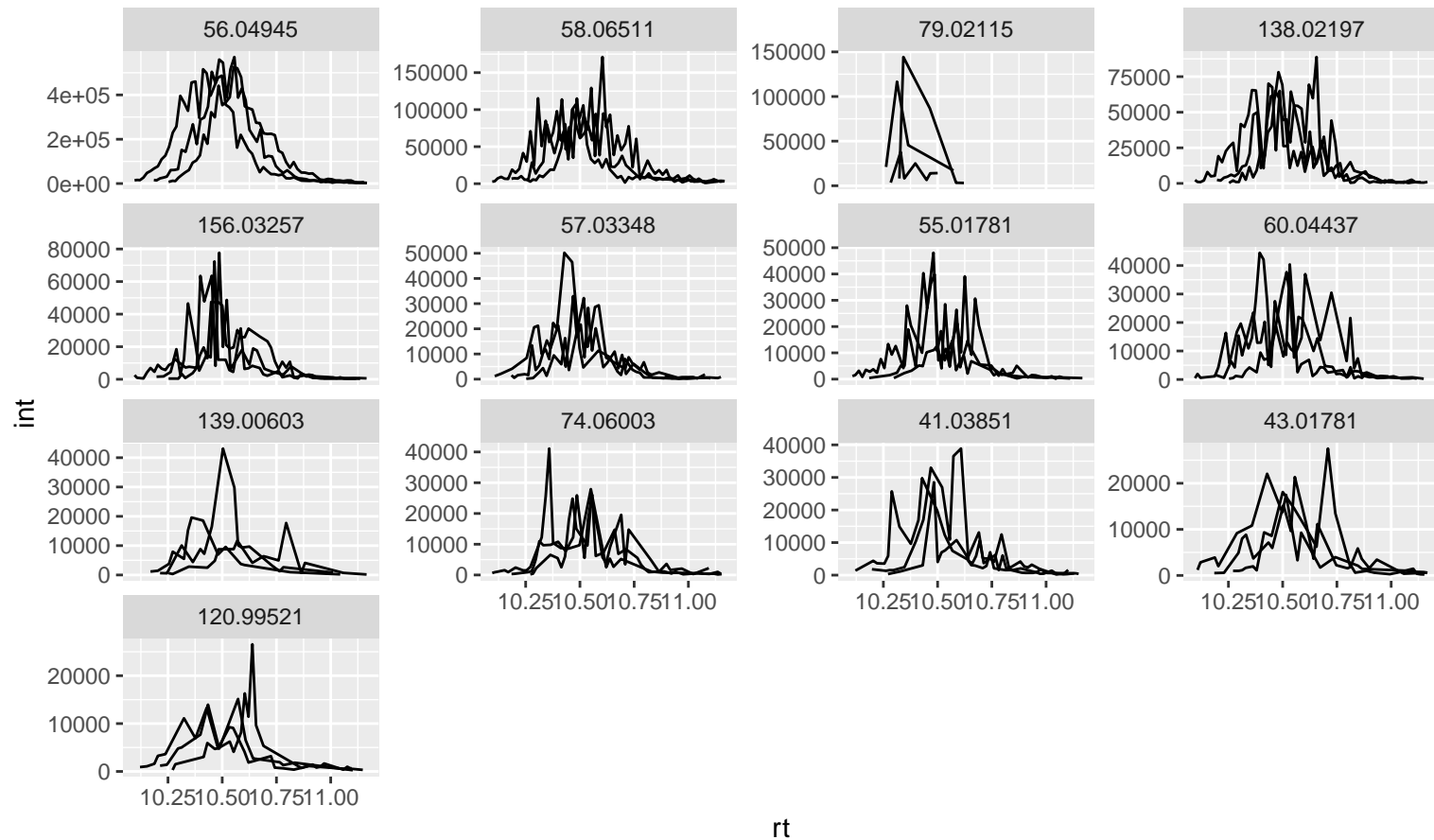
Cysteinolic acid (neg) 154.017955

int

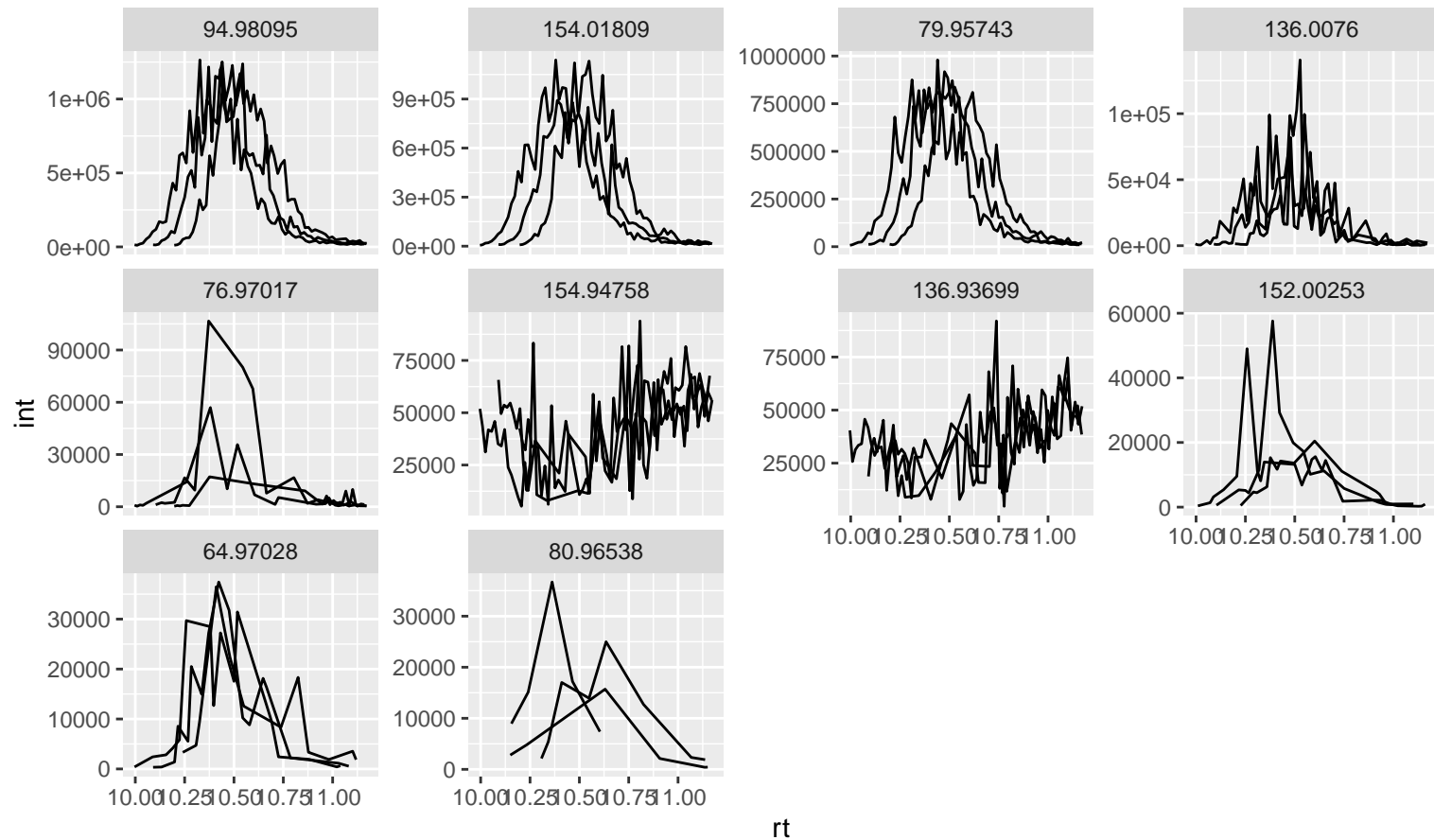


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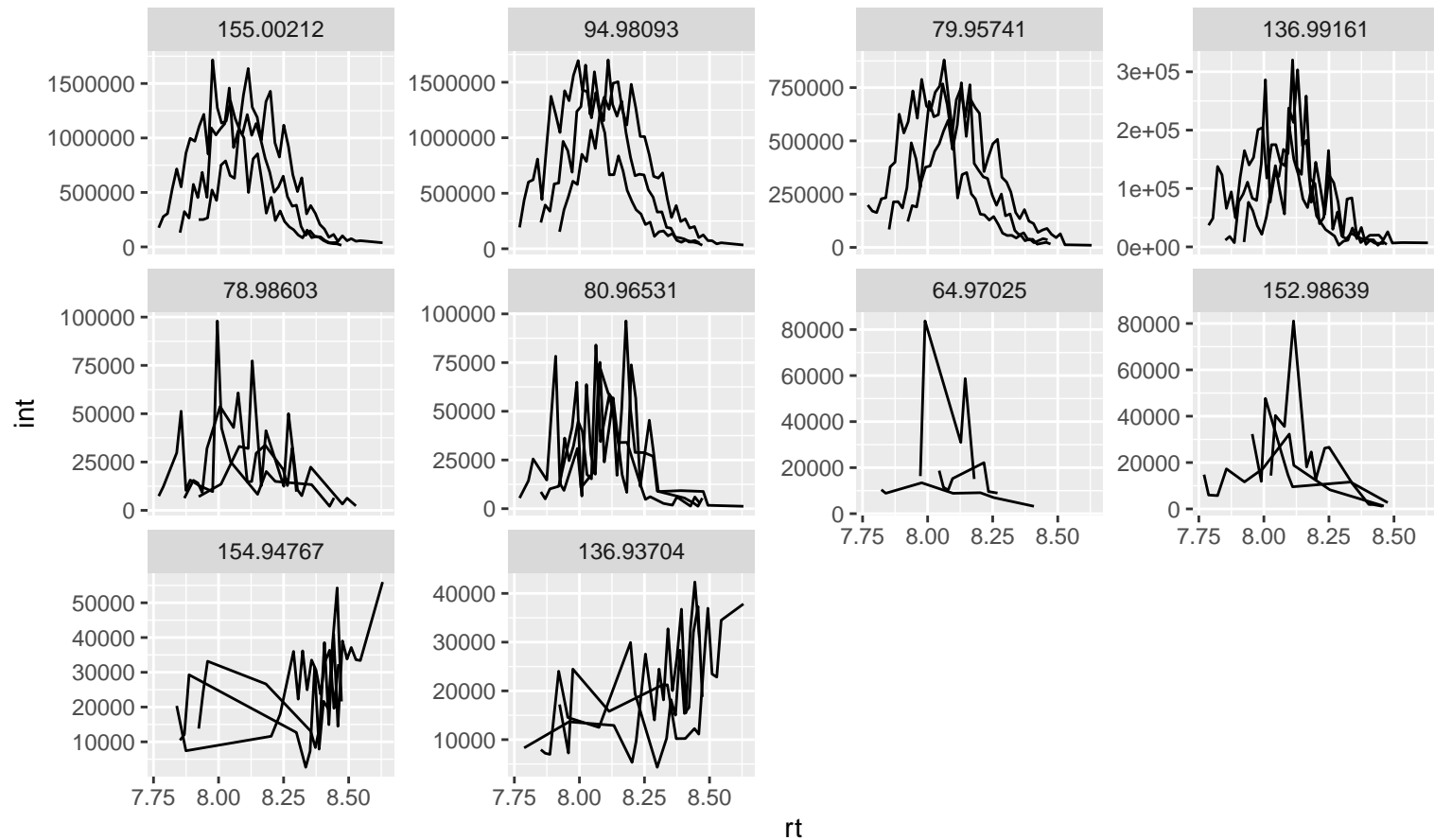
Amino hydroxypropanesulfonate (pos) 156.032507



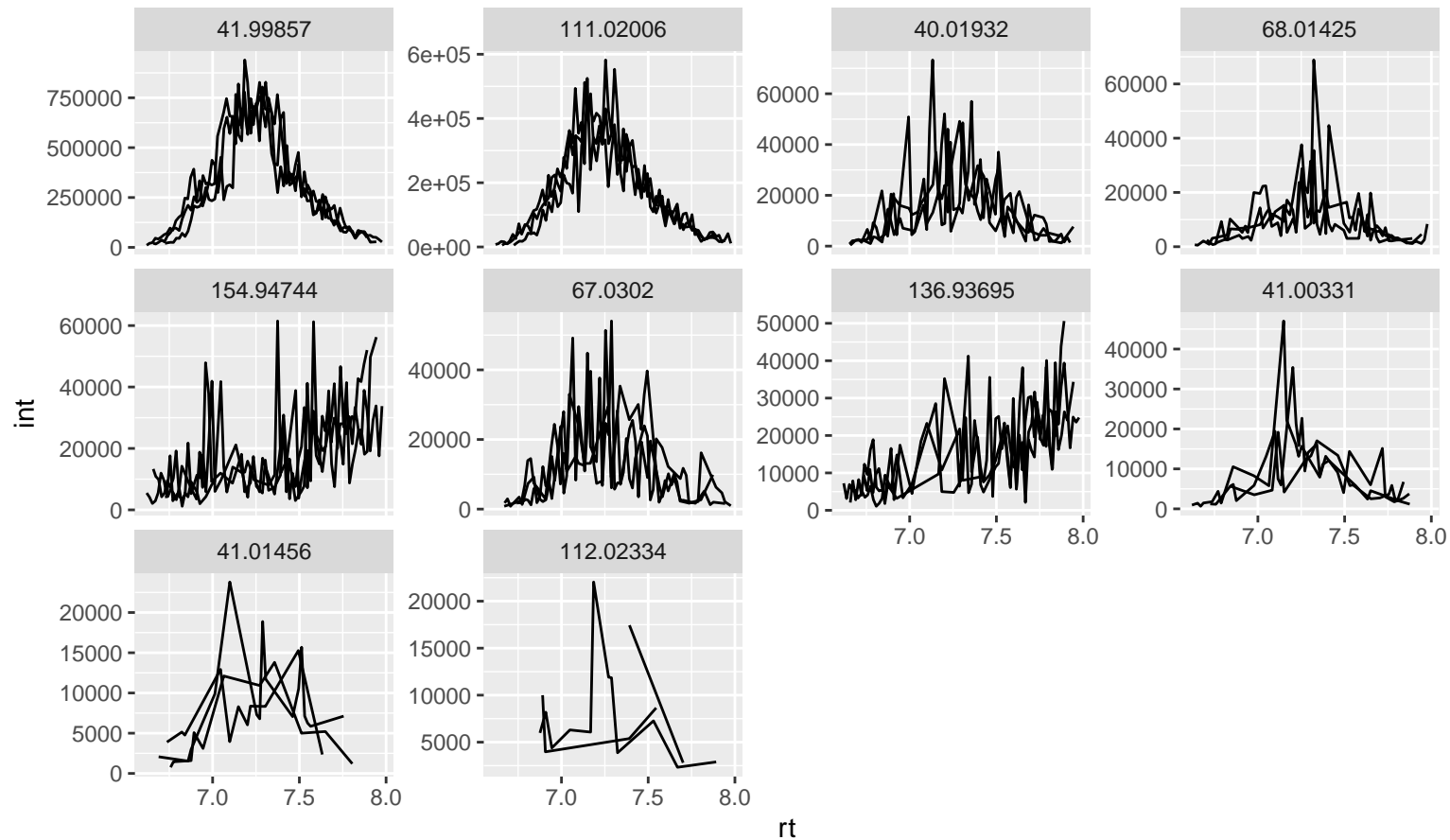
Amino hydroxypropanesulfonate (neg) 154.017955



(R)-2,3-Dihydroxypropane-1-sulfonate (neg) 155.001971

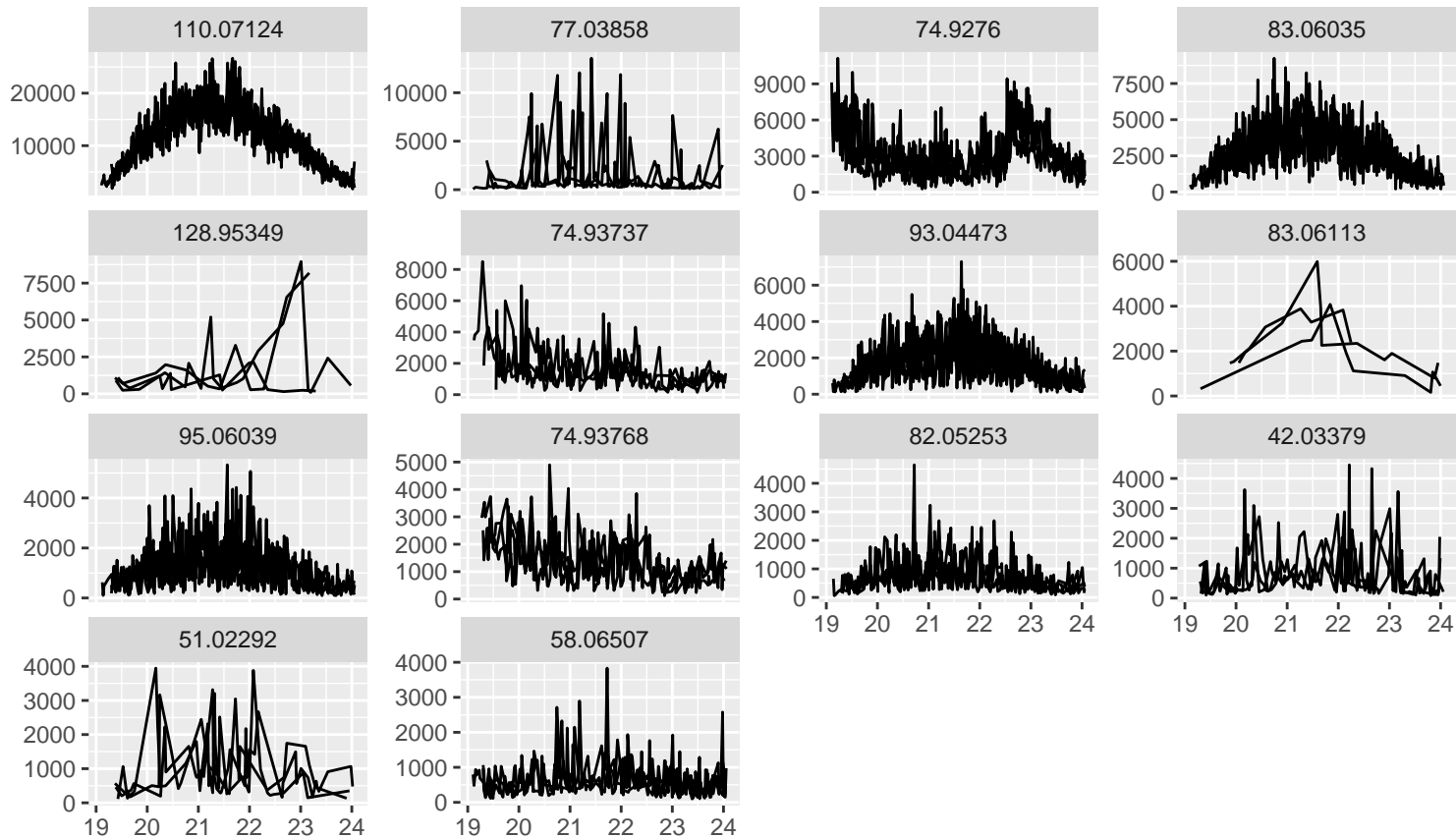


Orotic acid (neg) 155.009832



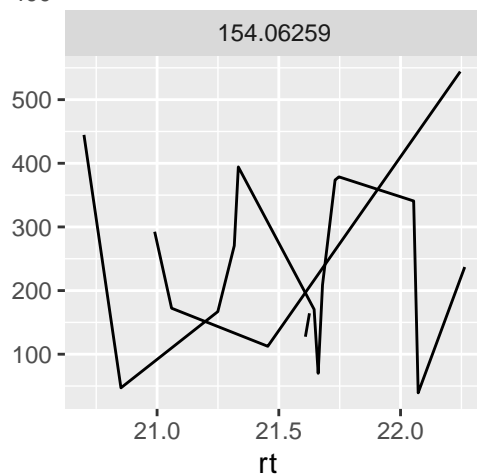
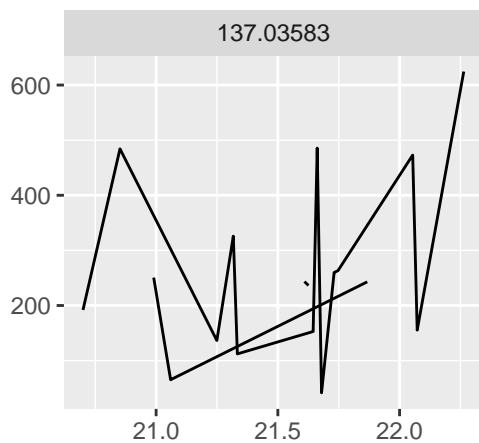
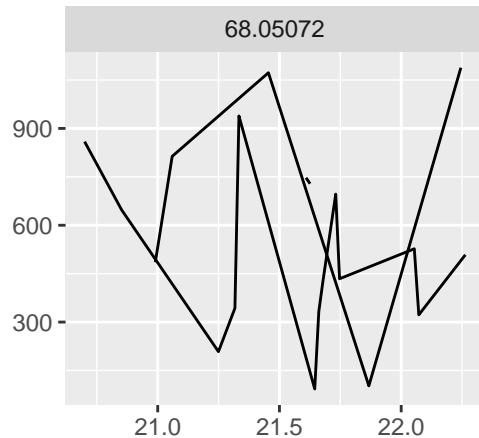
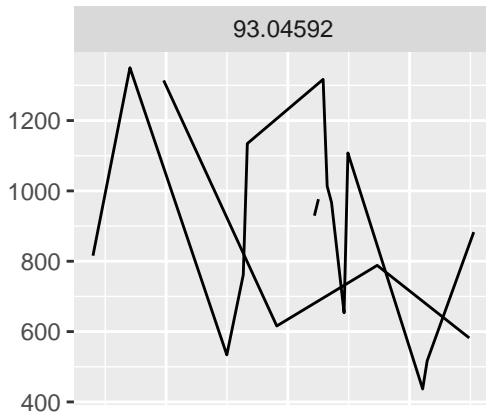
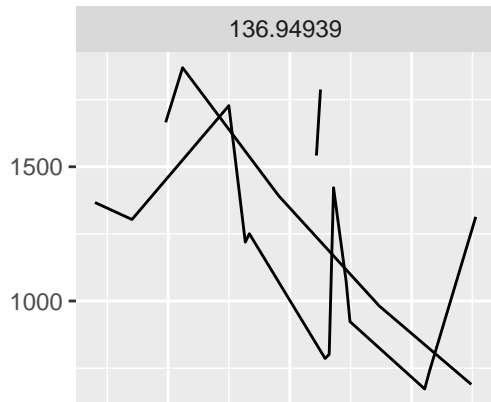
L-Histidine (pos) 156.076753

int

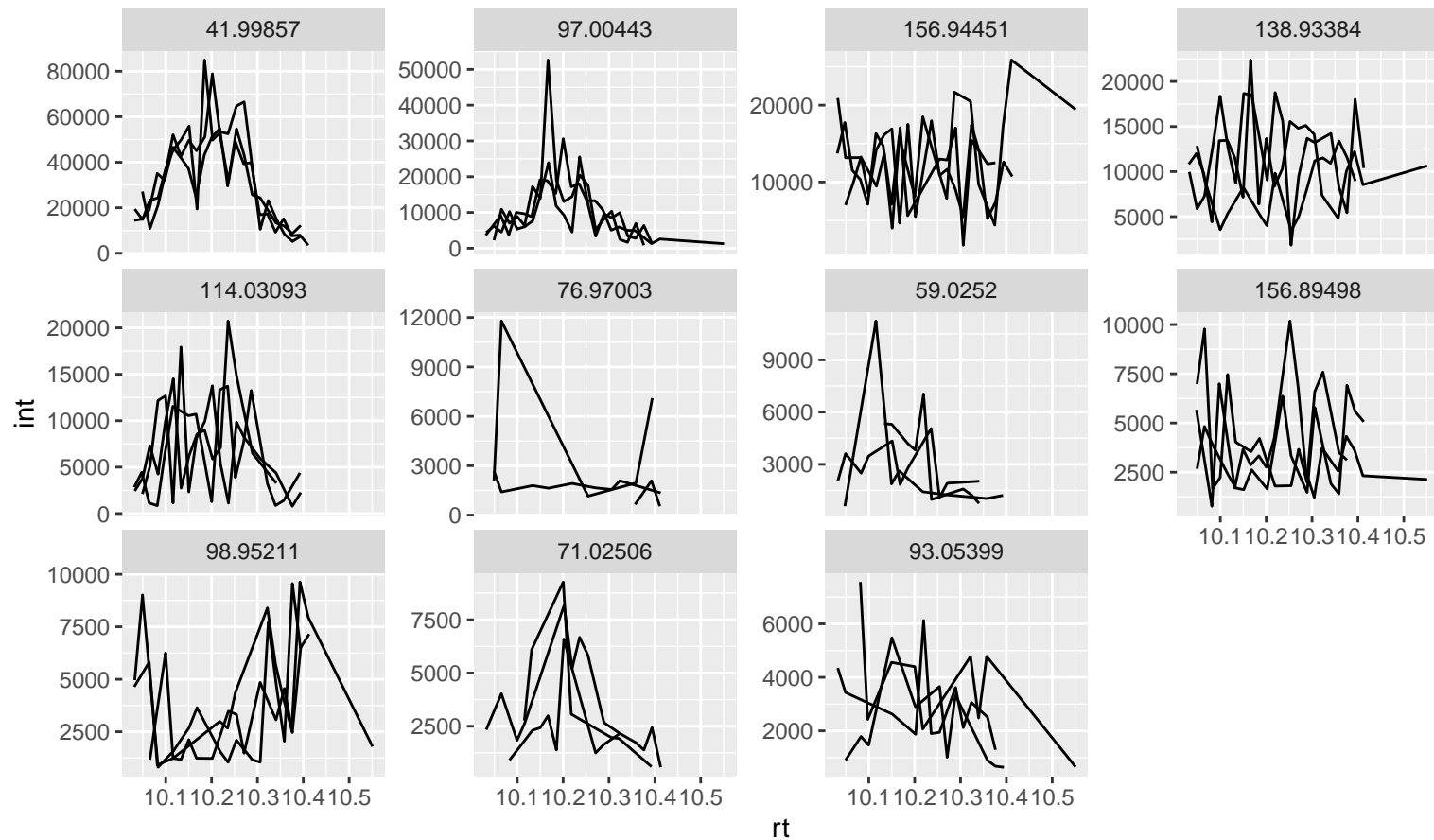


L-Histidine (neg) 154.062201

int

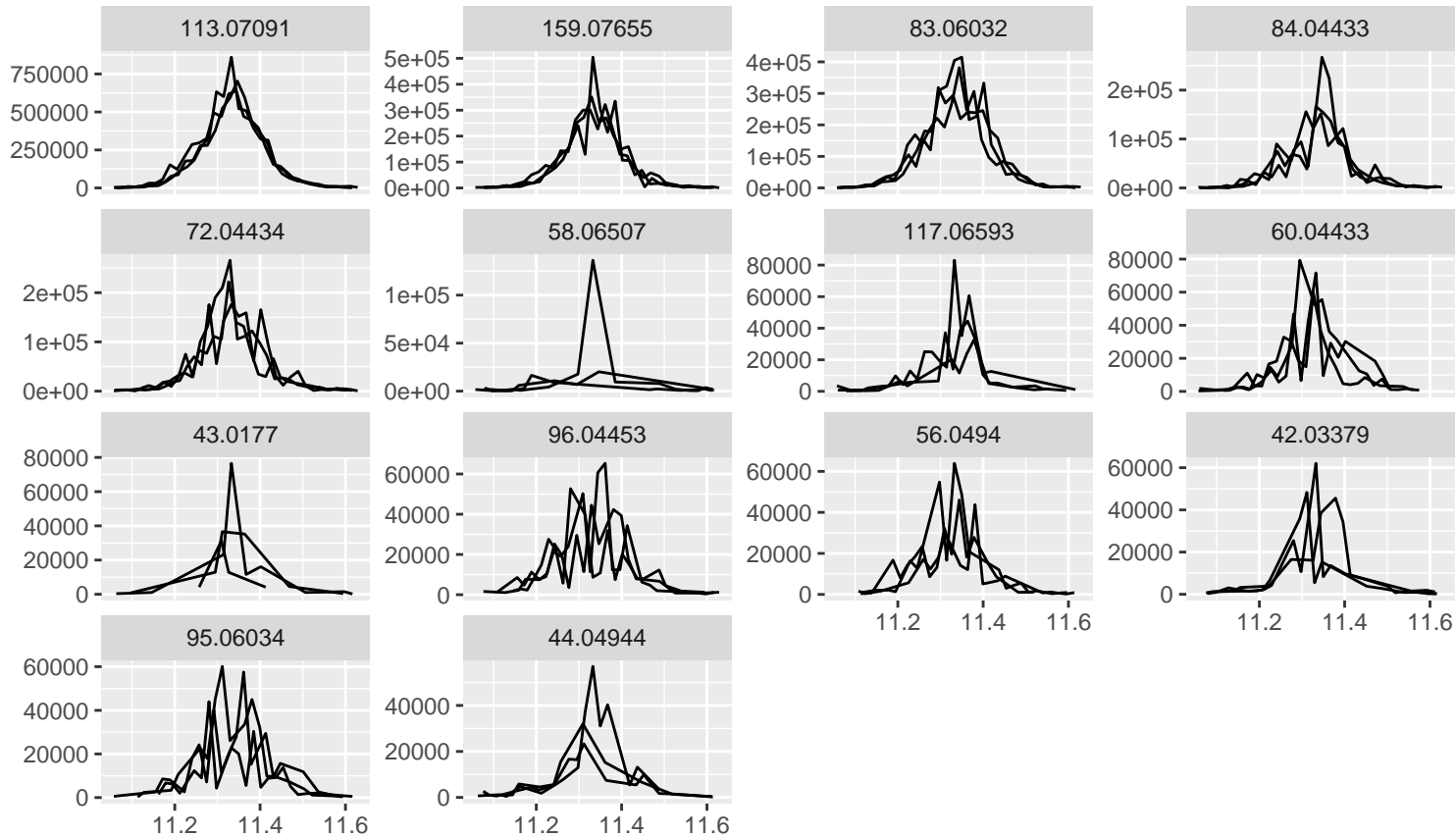


Allantoin (neg) 157.036715



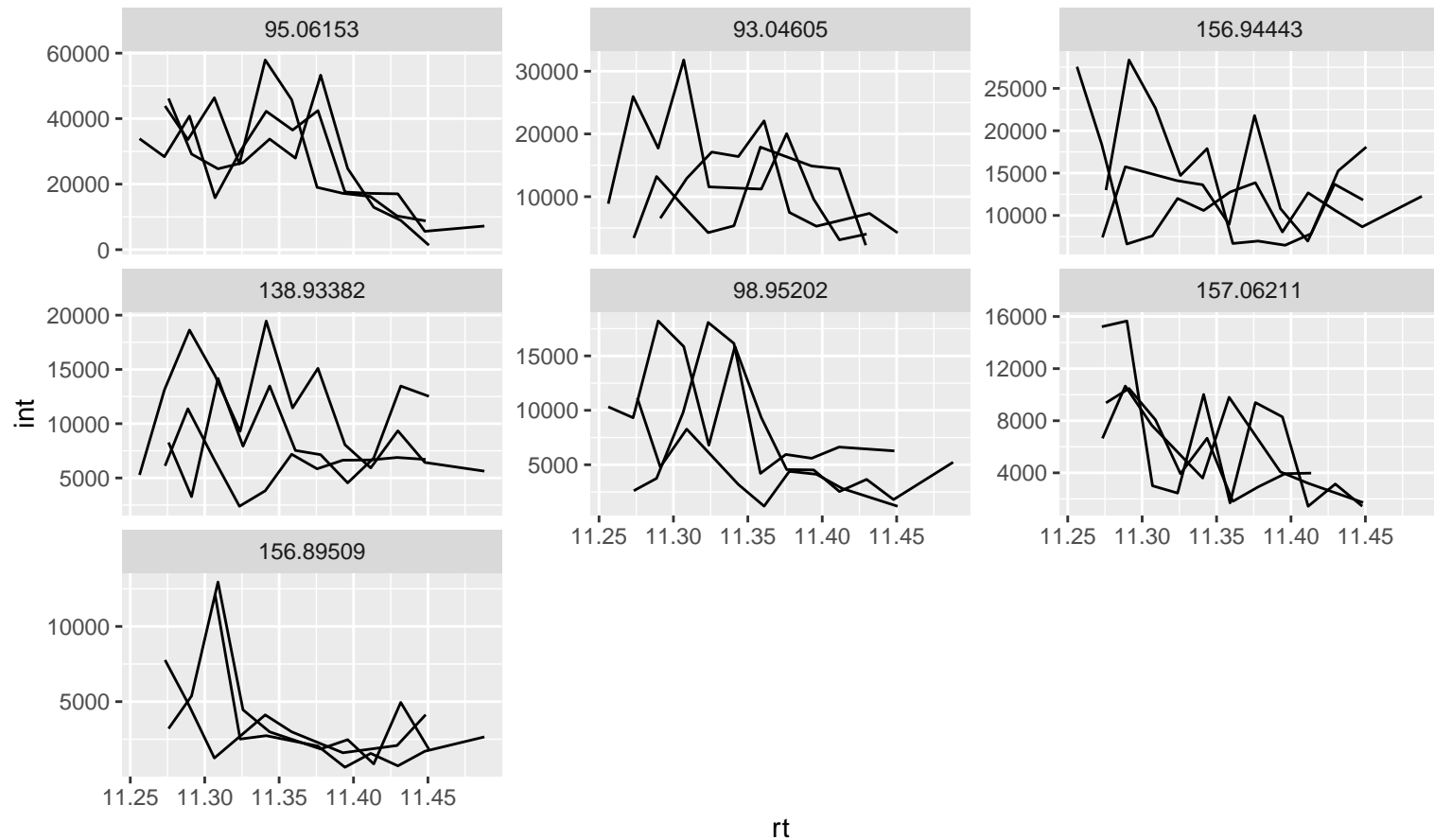
5-Hydroxyectoine (pos) 159.076419

int

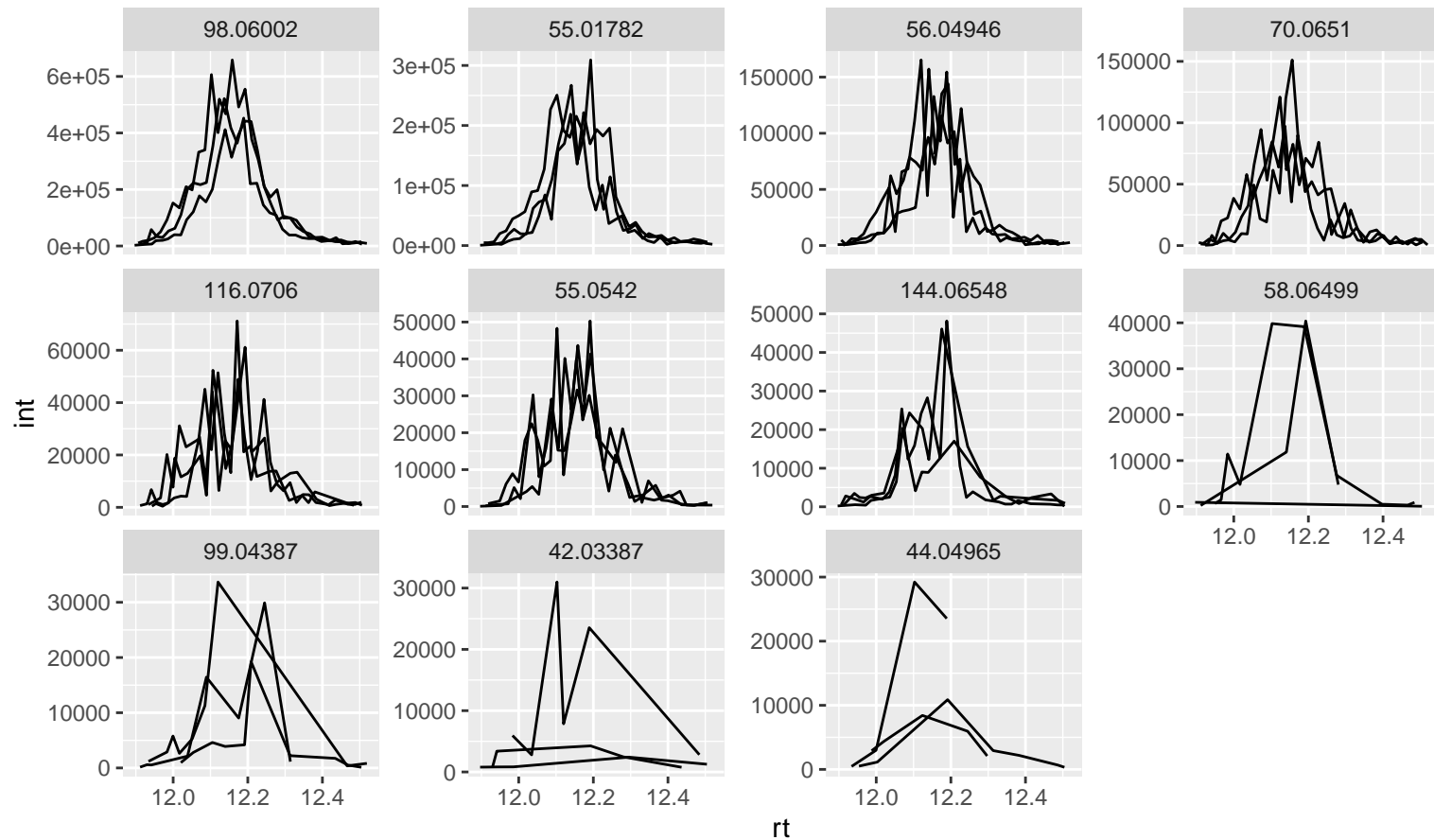


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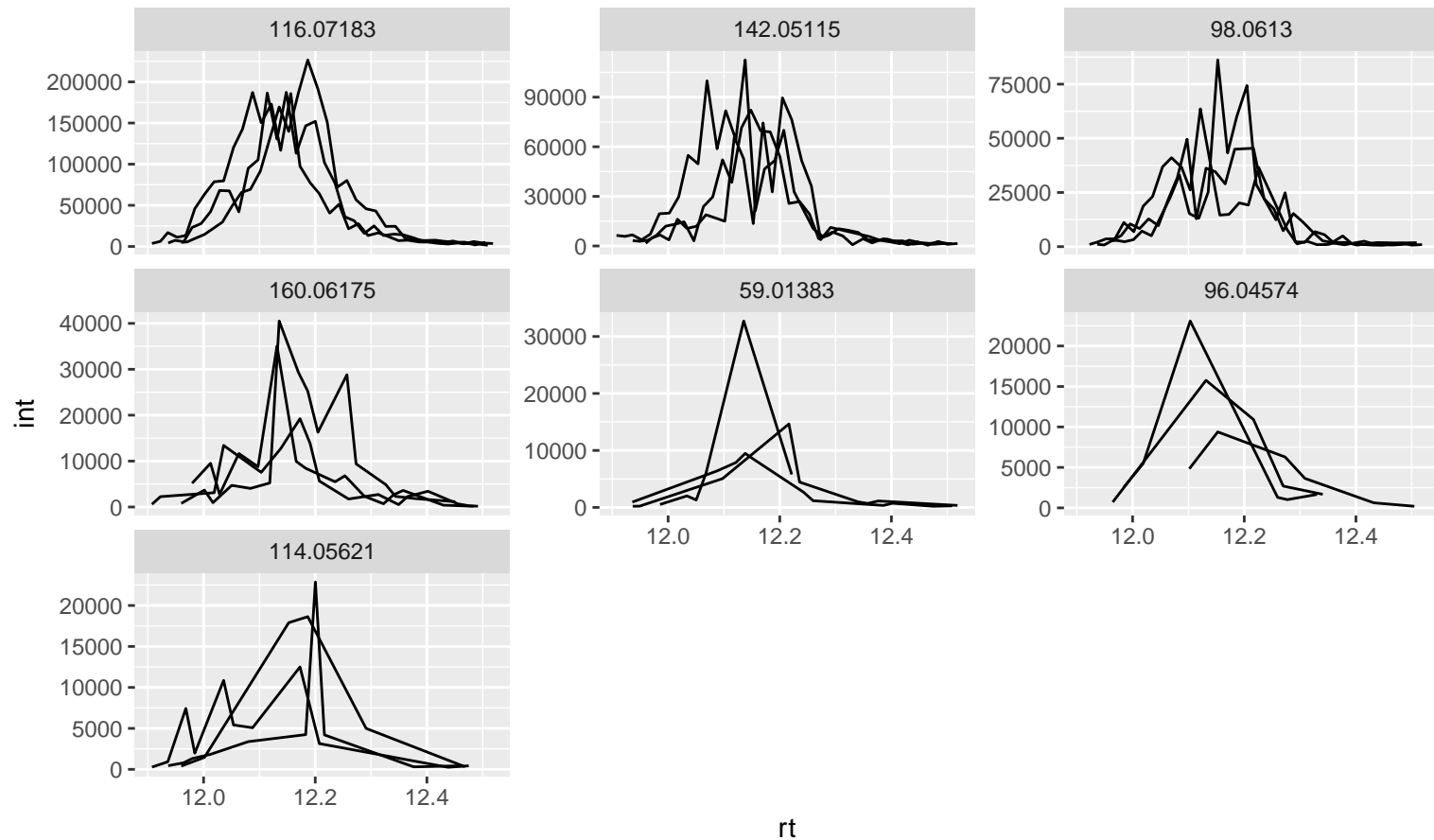
5-Hydroxyectoine (neg) 157.061867



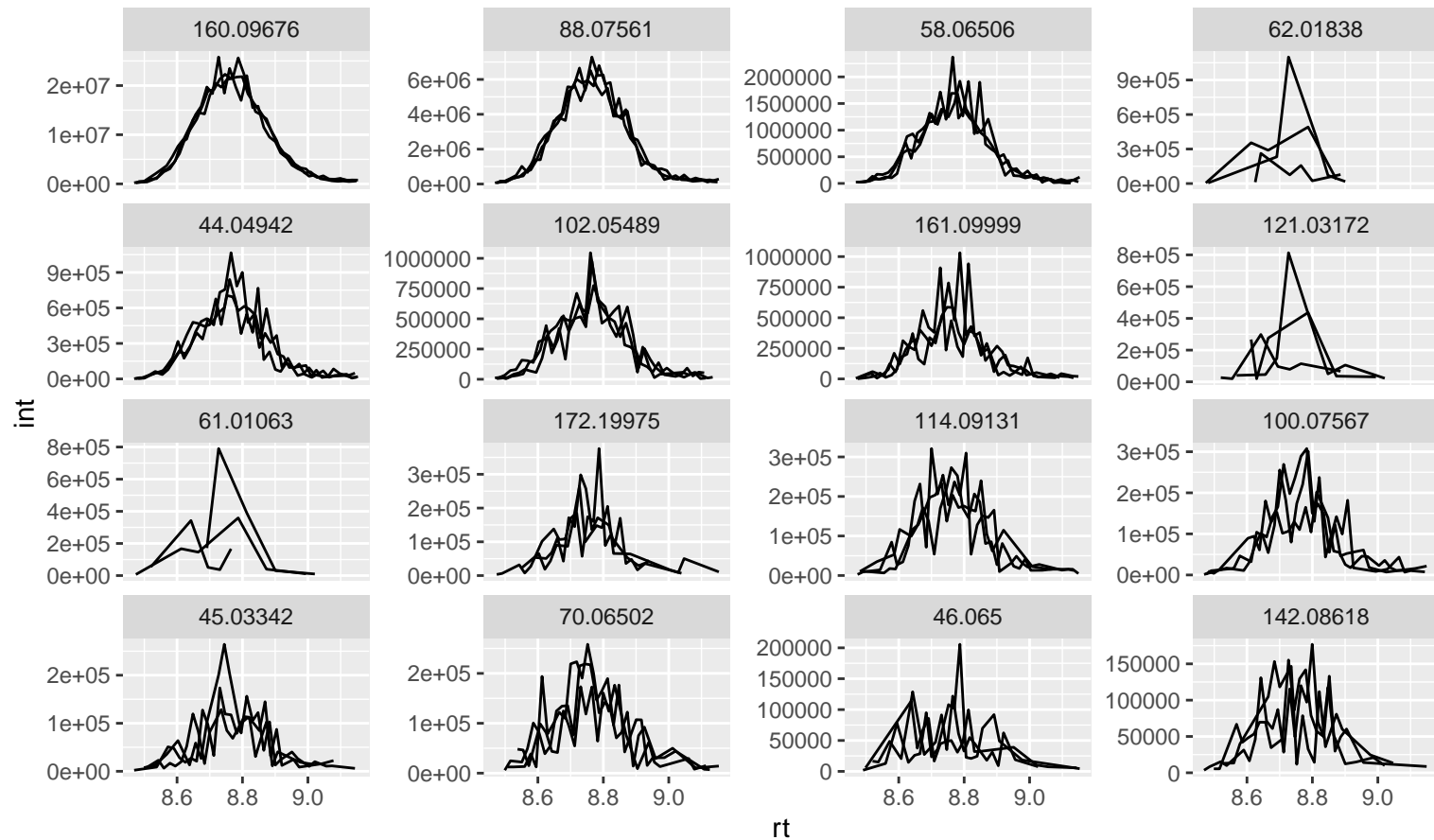
L-2-Aminoadipic acid (pos) 162.076085



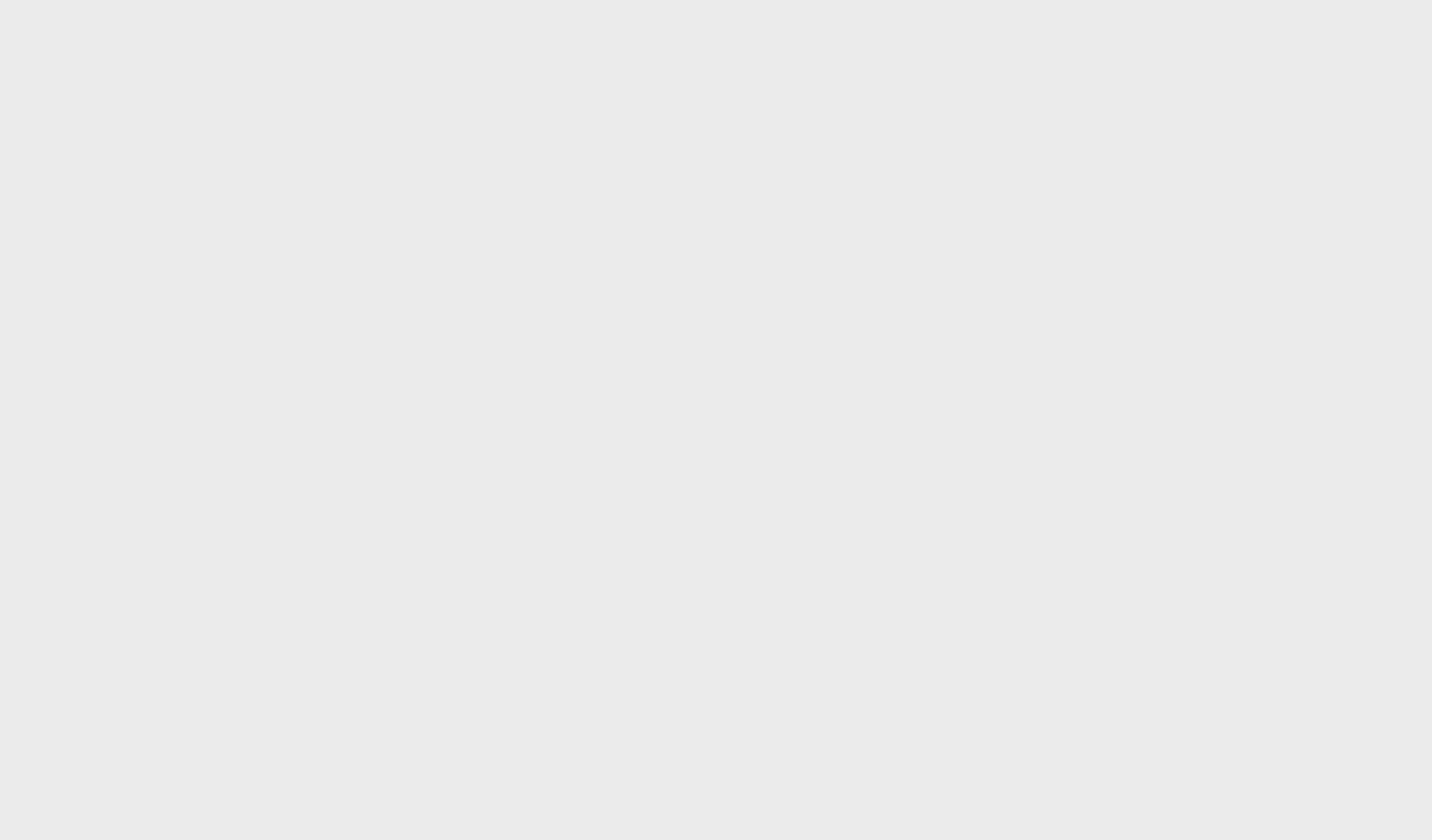
L-2-Aminoadipic acid (neg) 160.061533



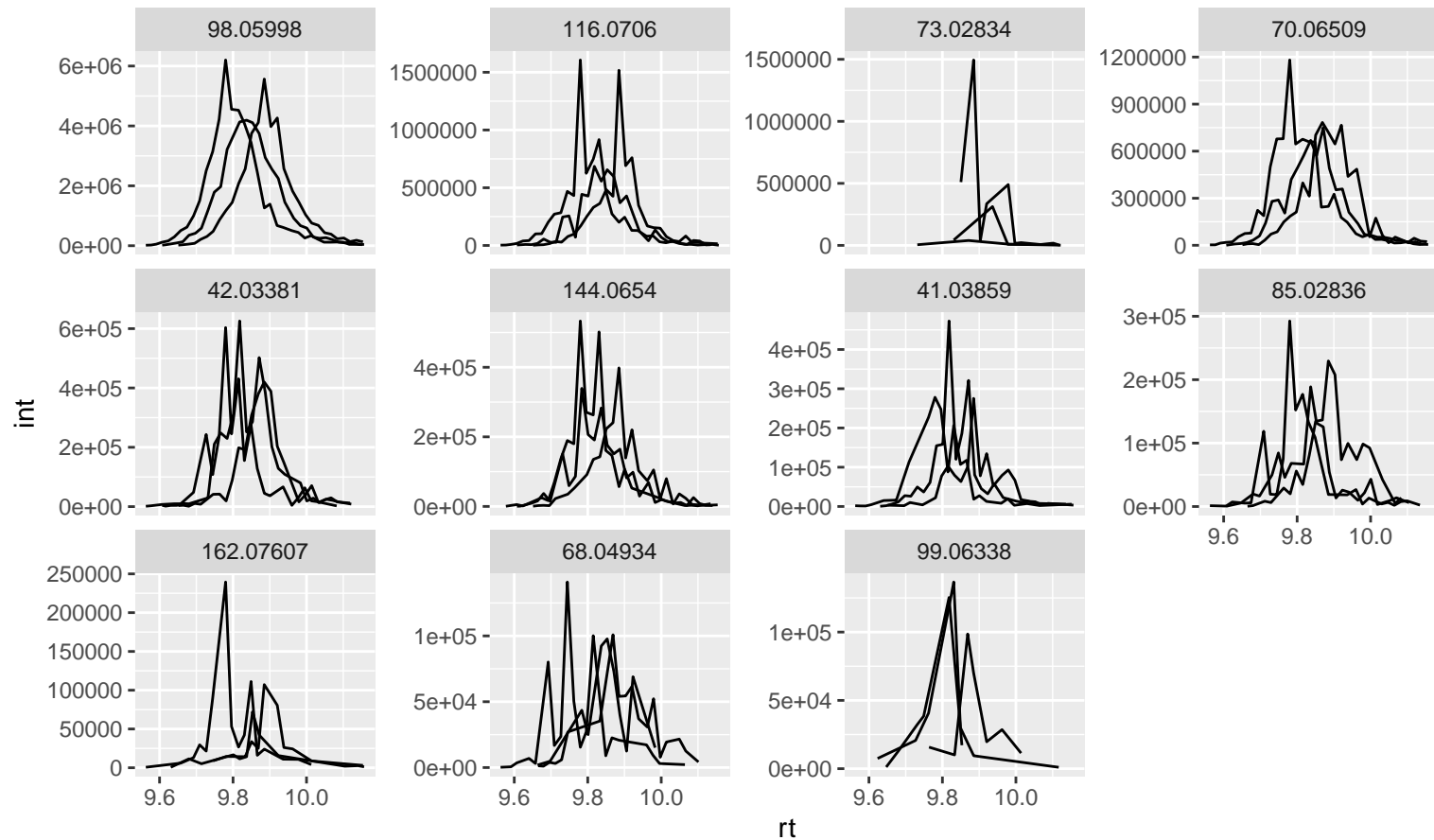
Betonicine (pos) 160.09682



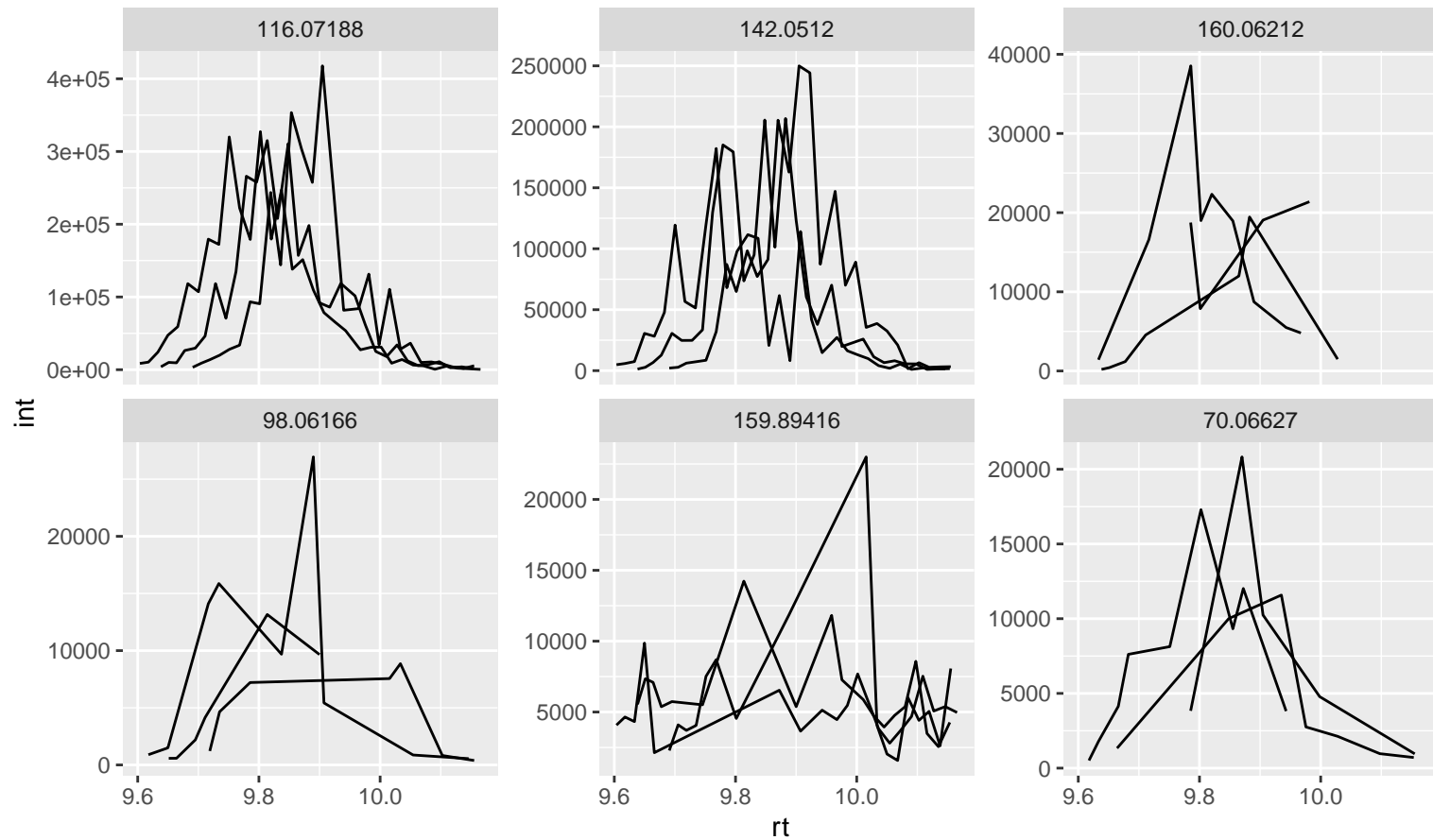
Betonicine (neg) 158.082268



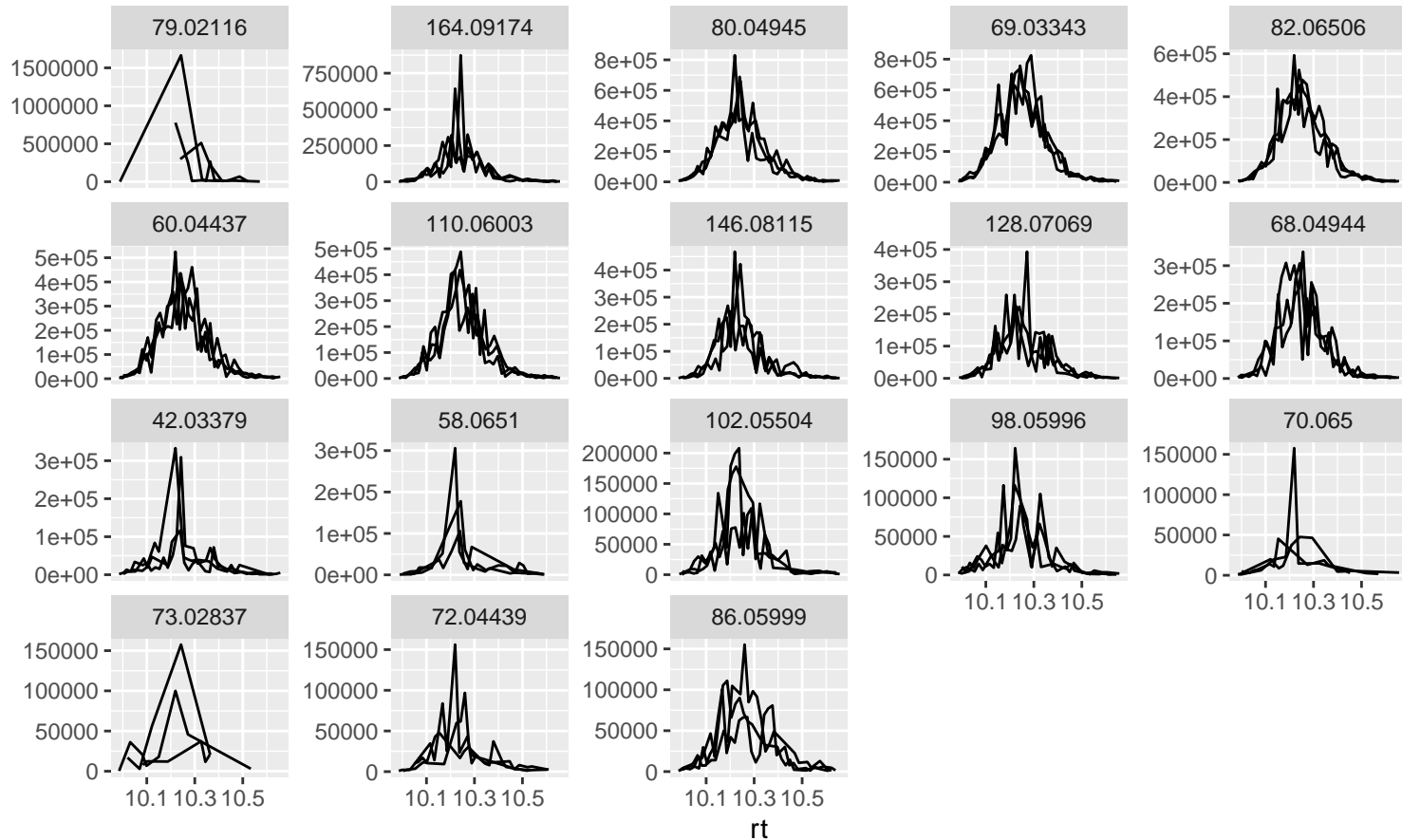
N-Methyl-L-glutamic acid (pos) 162.076085



N-Methyl-L-glutamic acid (neg) 160.061533

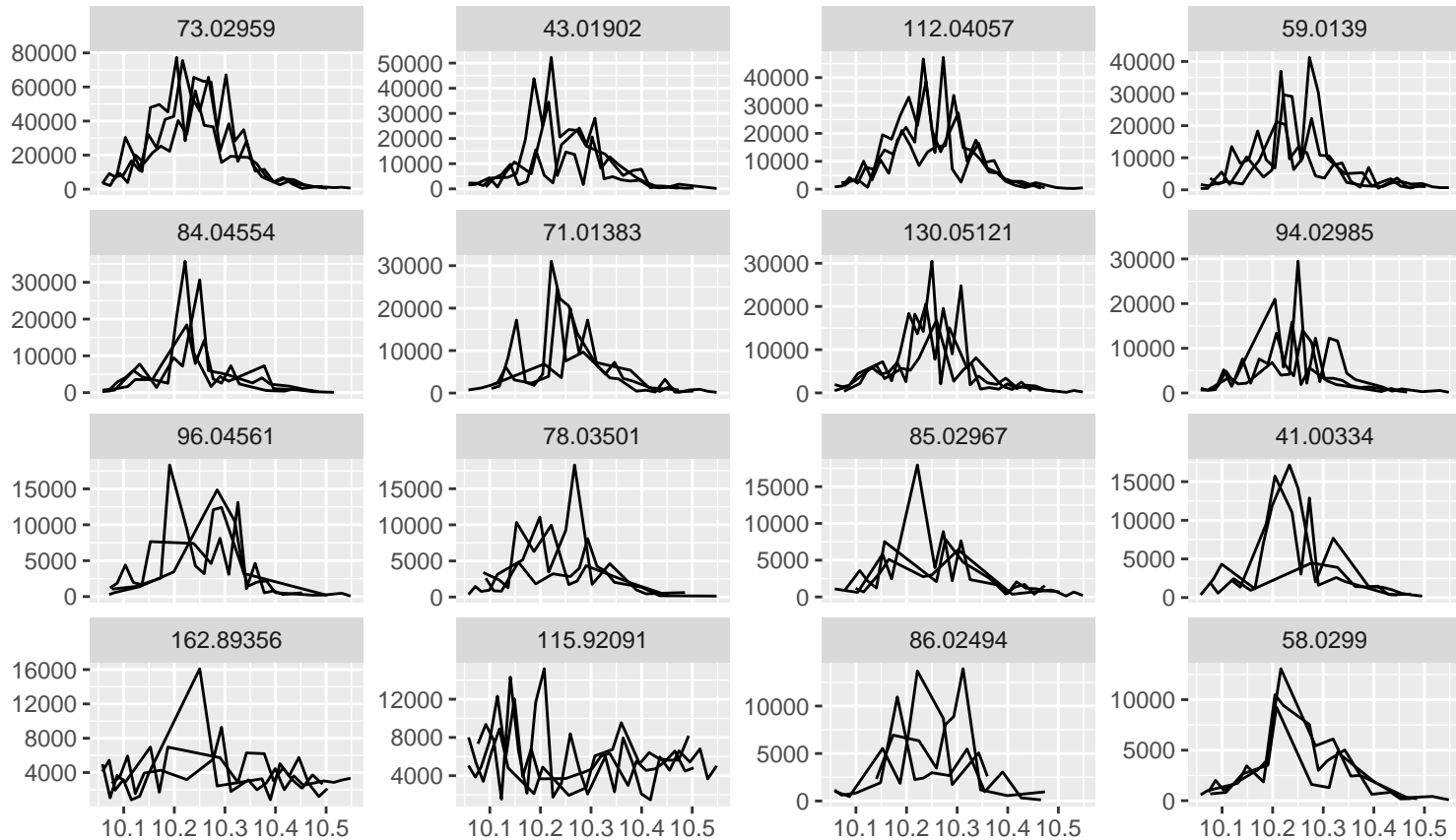


Deoxynojirimycin (pos) 164.091735



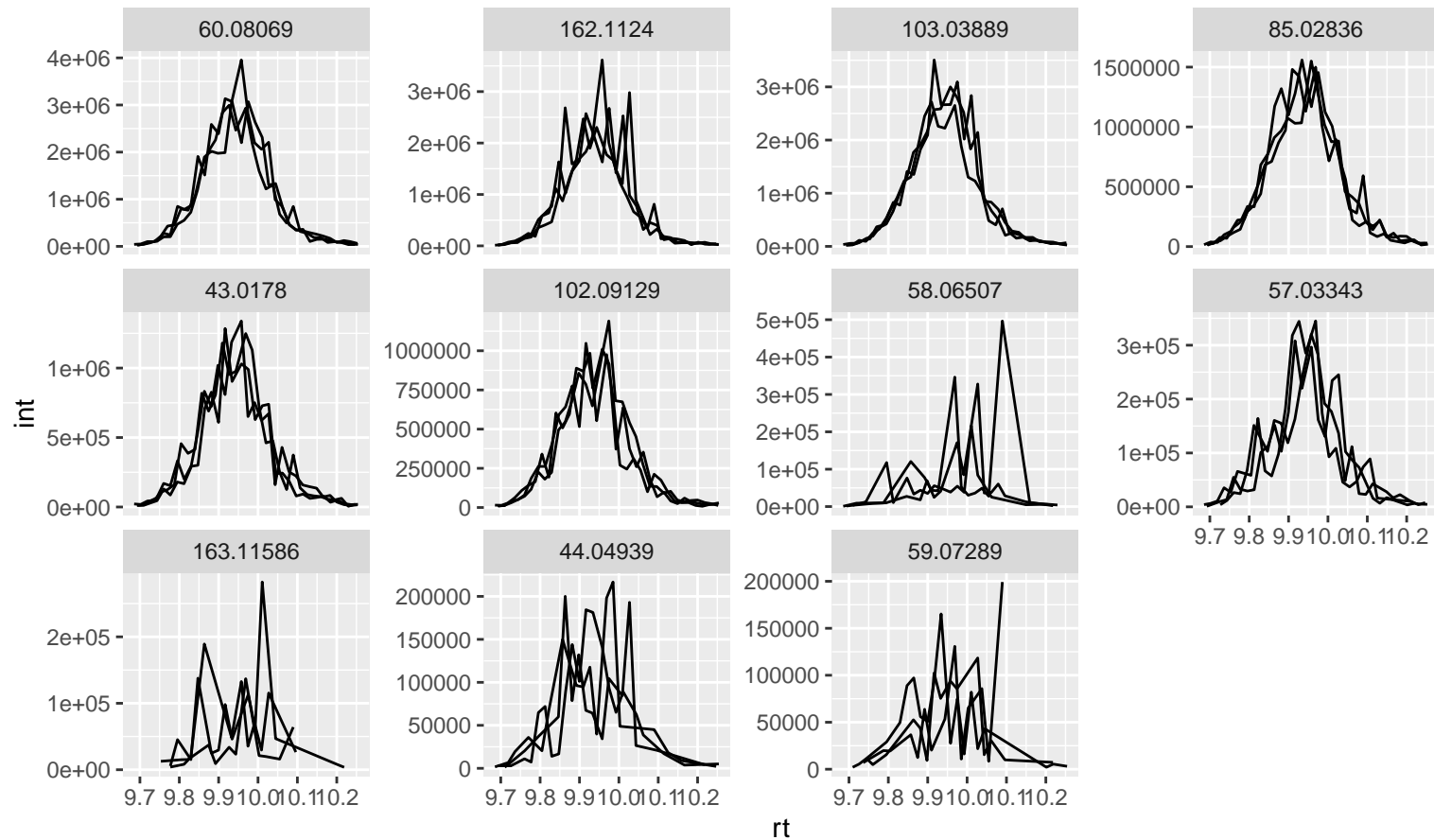
Deoxynojirimycin (neg) 162.077183

int

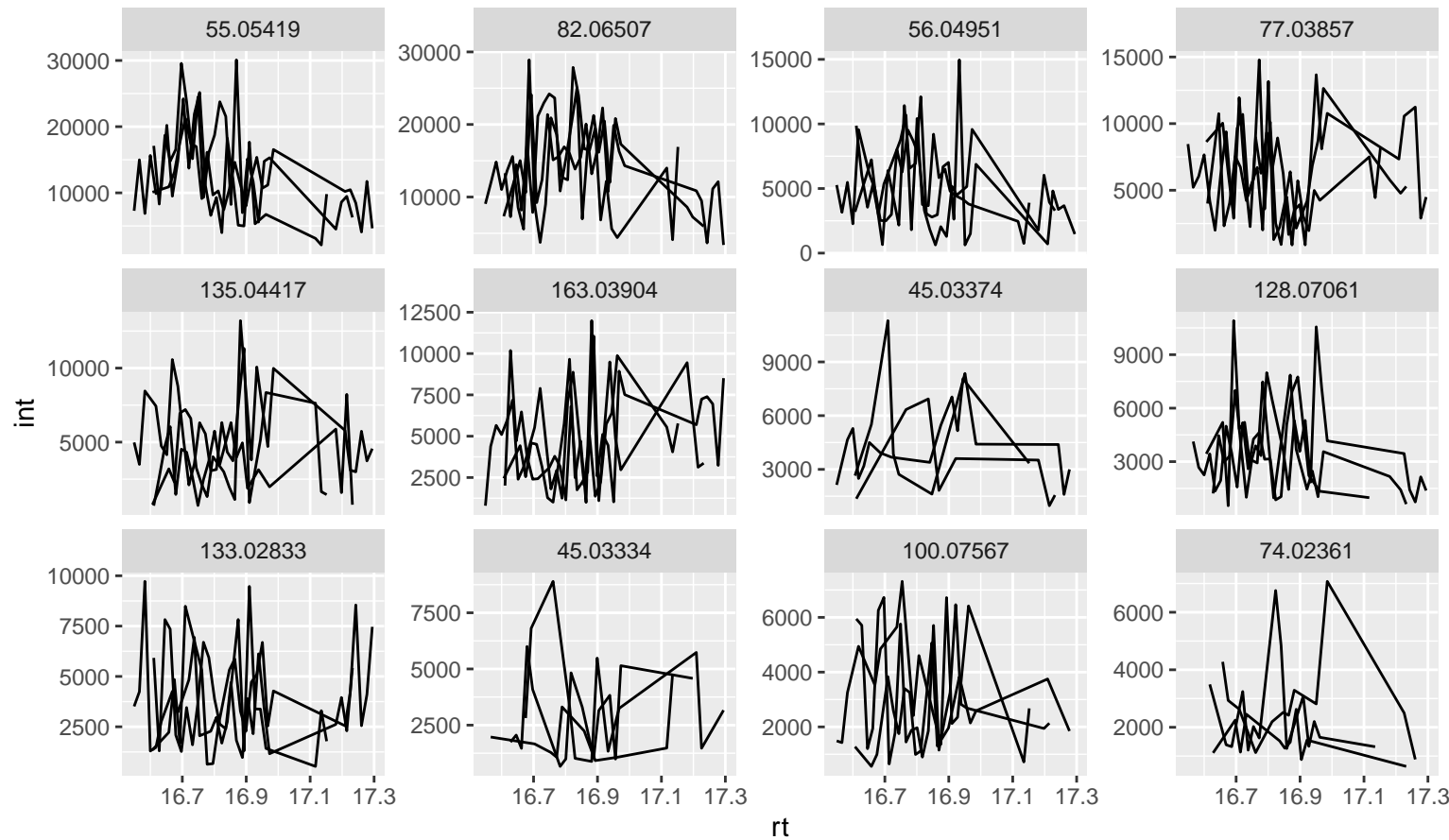


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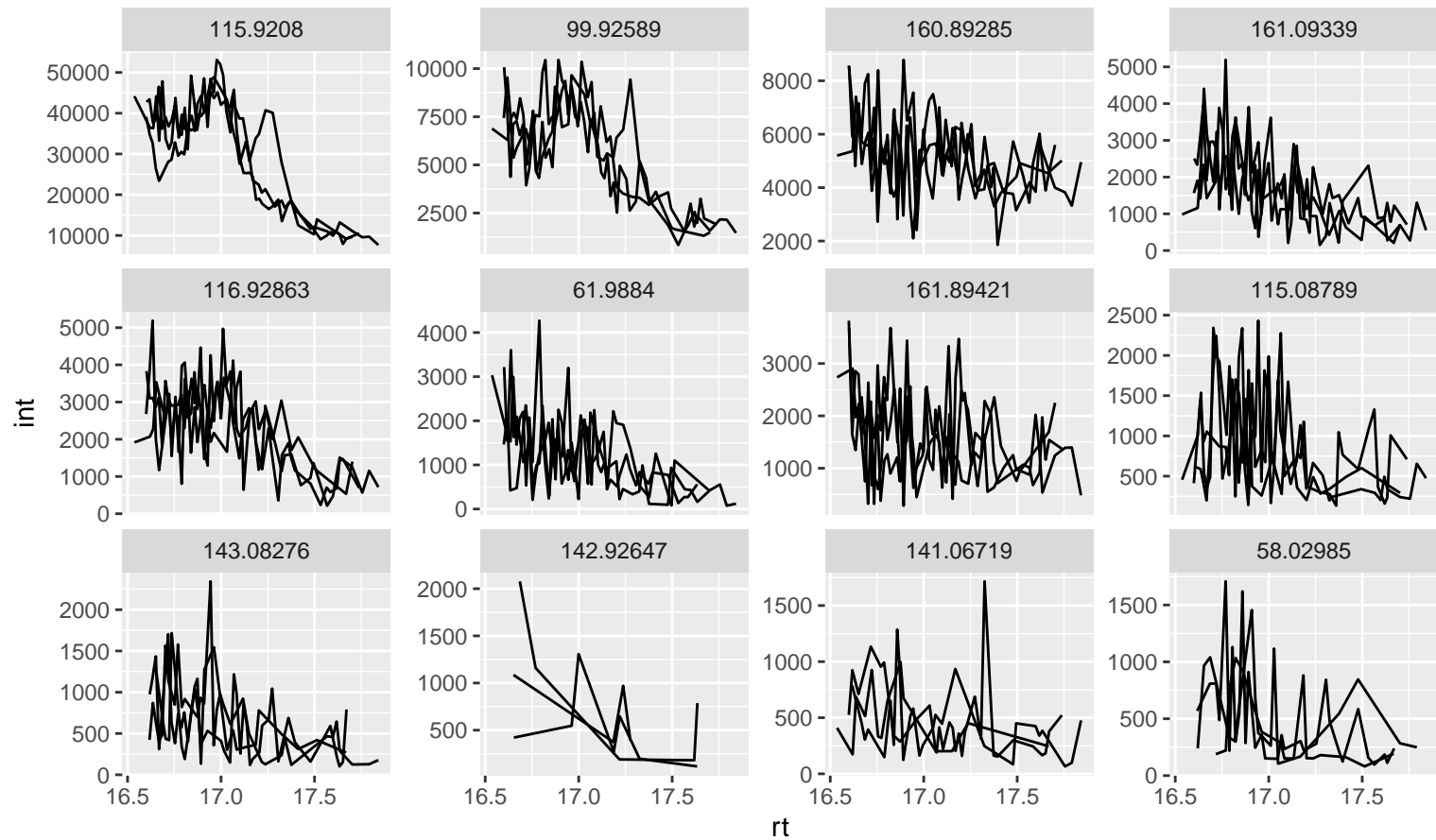
Carnitine (pos) 162.11247



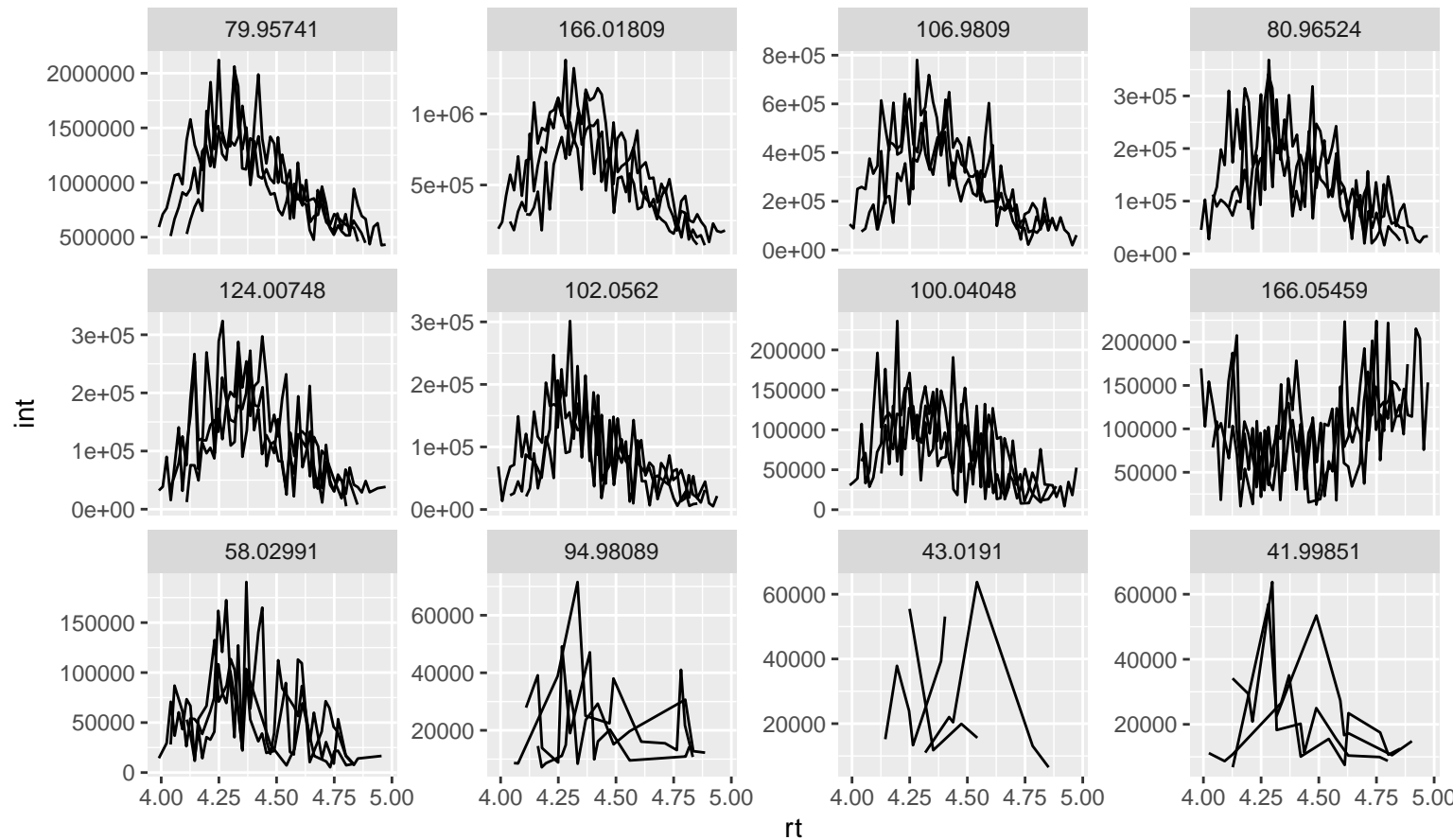
L-Hydroxylysine (pos) 163.107719



L-Hydroxylysine (neg) 161.093167

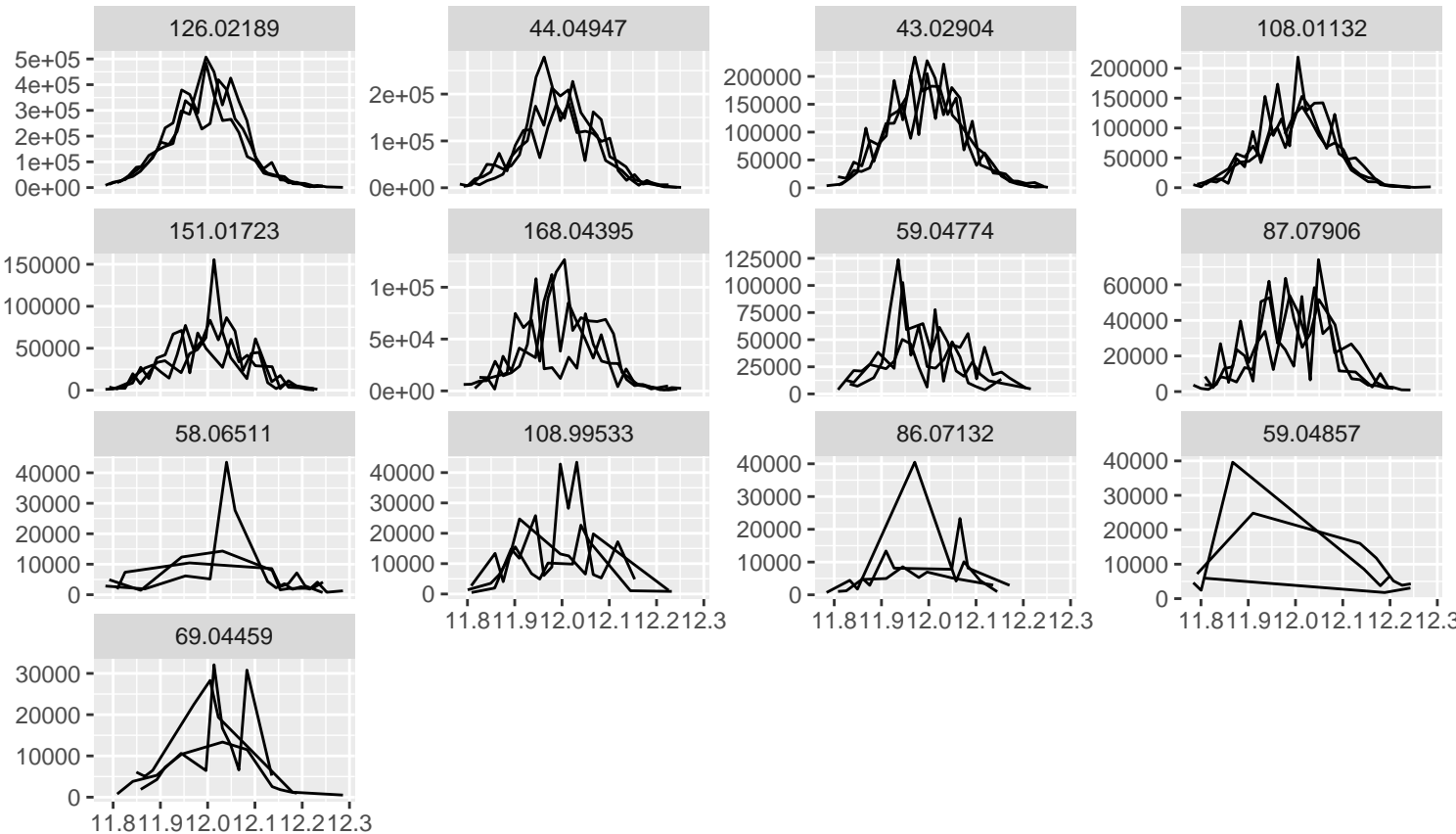


N-Acetyltaurine (neg) 166.017955



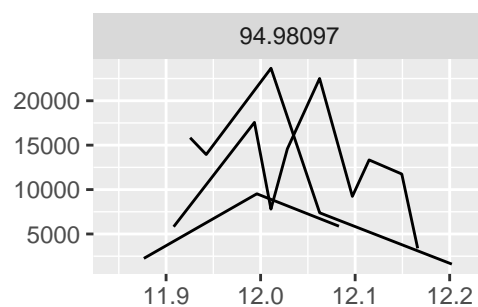
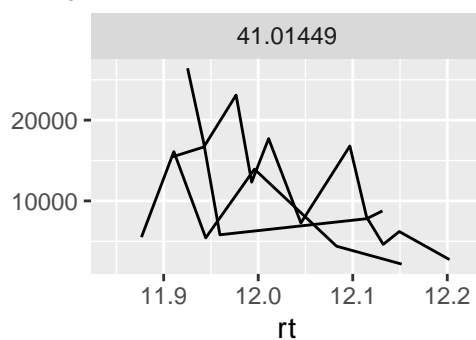
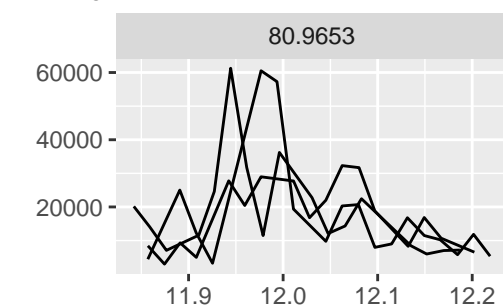
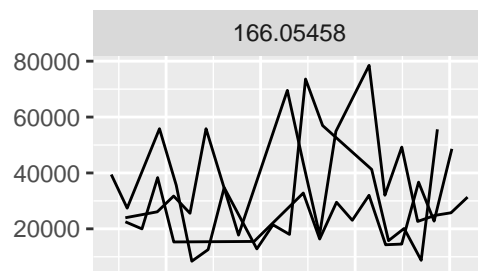
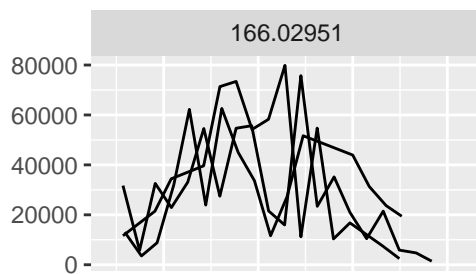
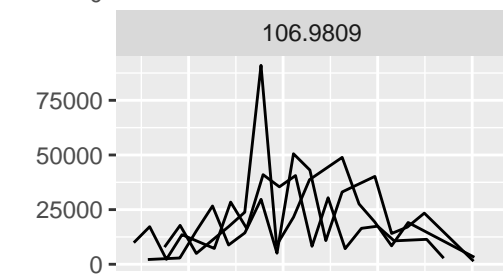
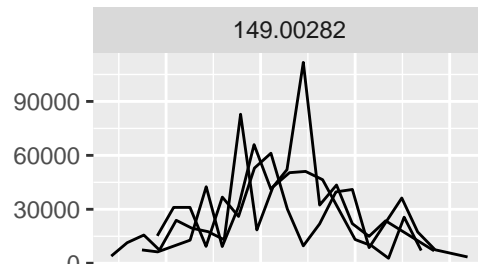
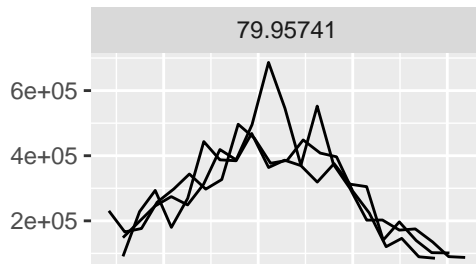
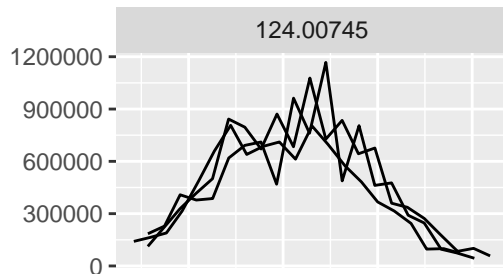
Taurocyamine (pos) 168.04374

int



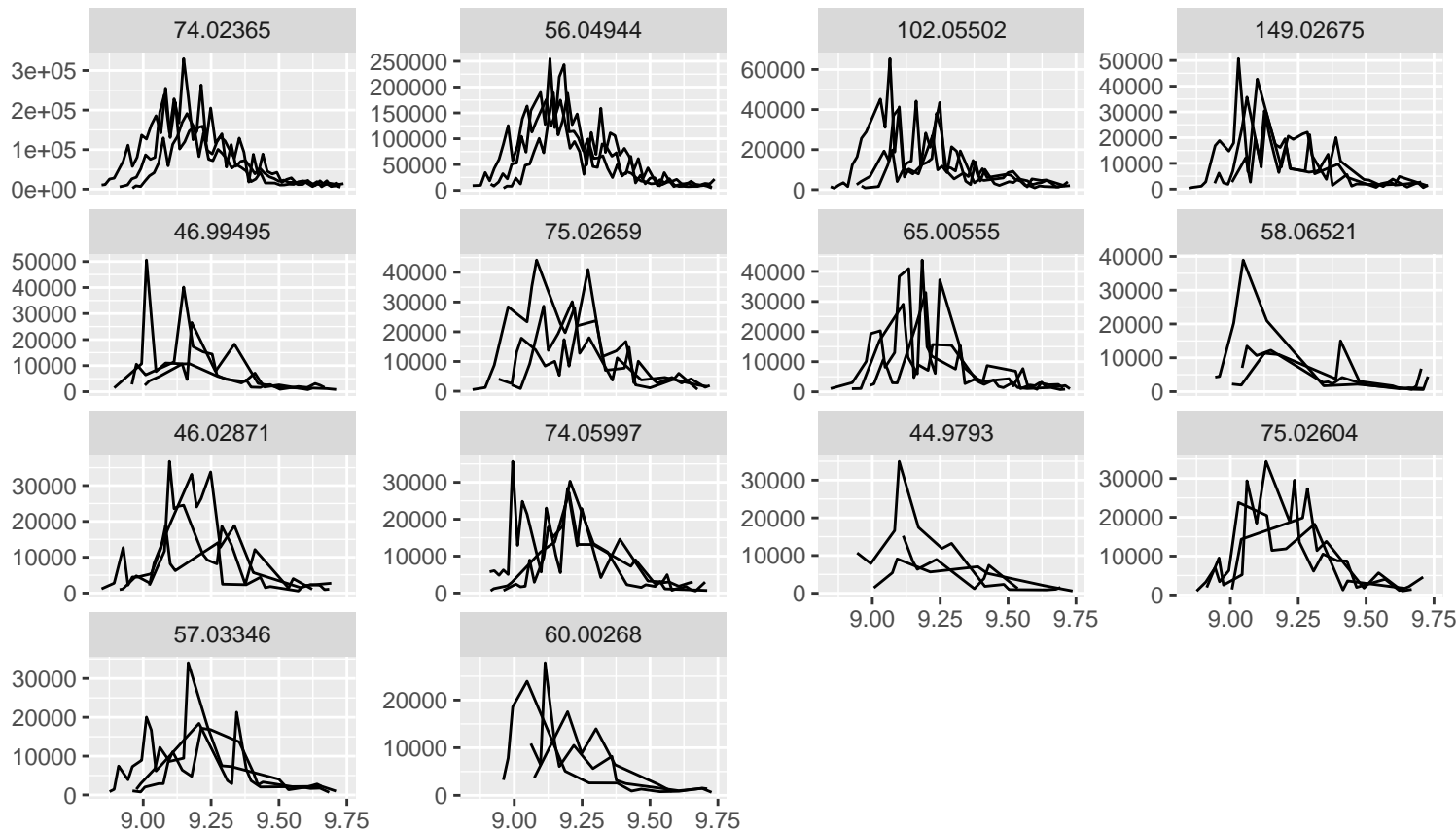
rt

Taurocyamine (neg) 166.029188



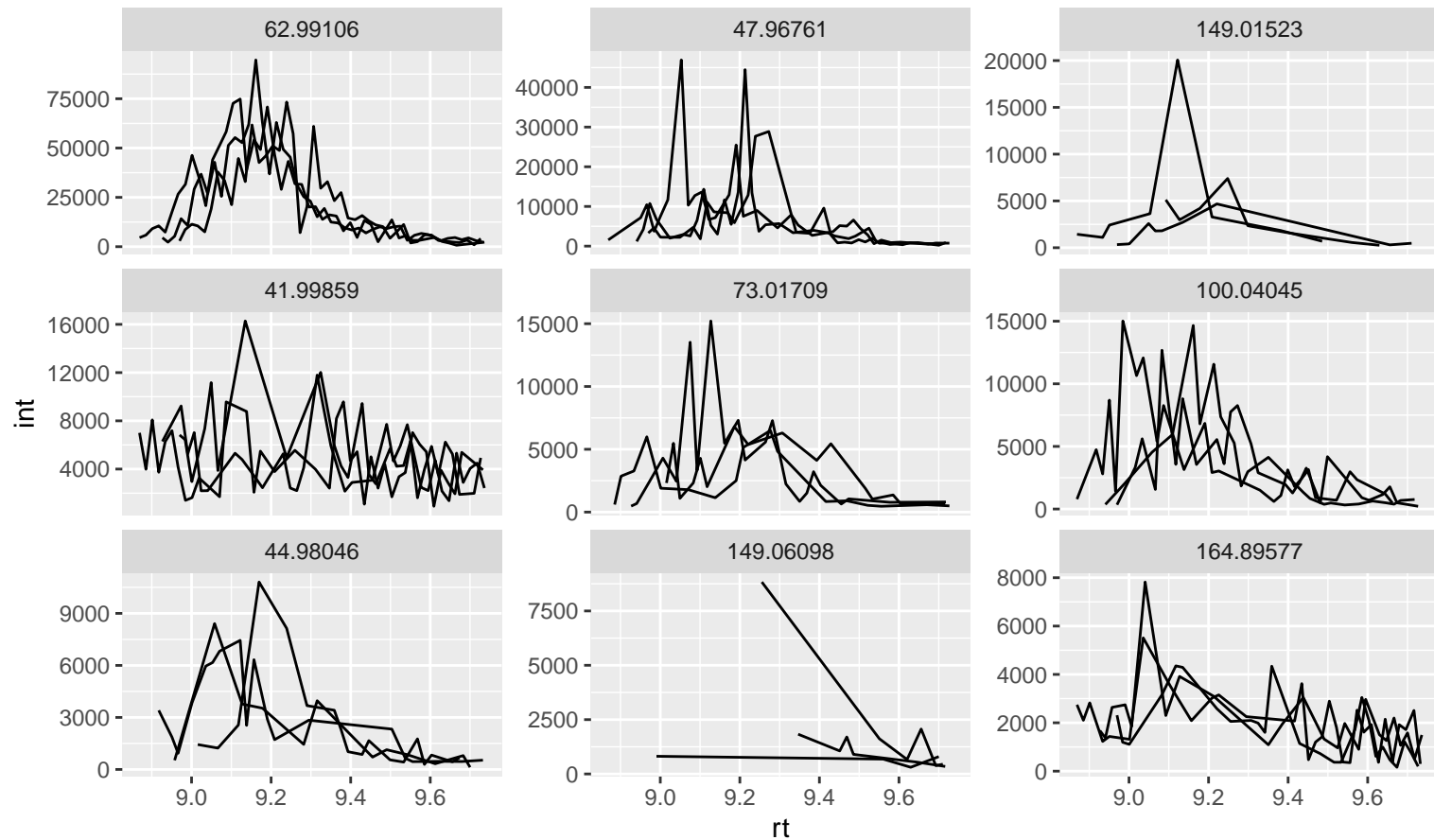
L-Methionine S-oxide (pos) 166.053242

int



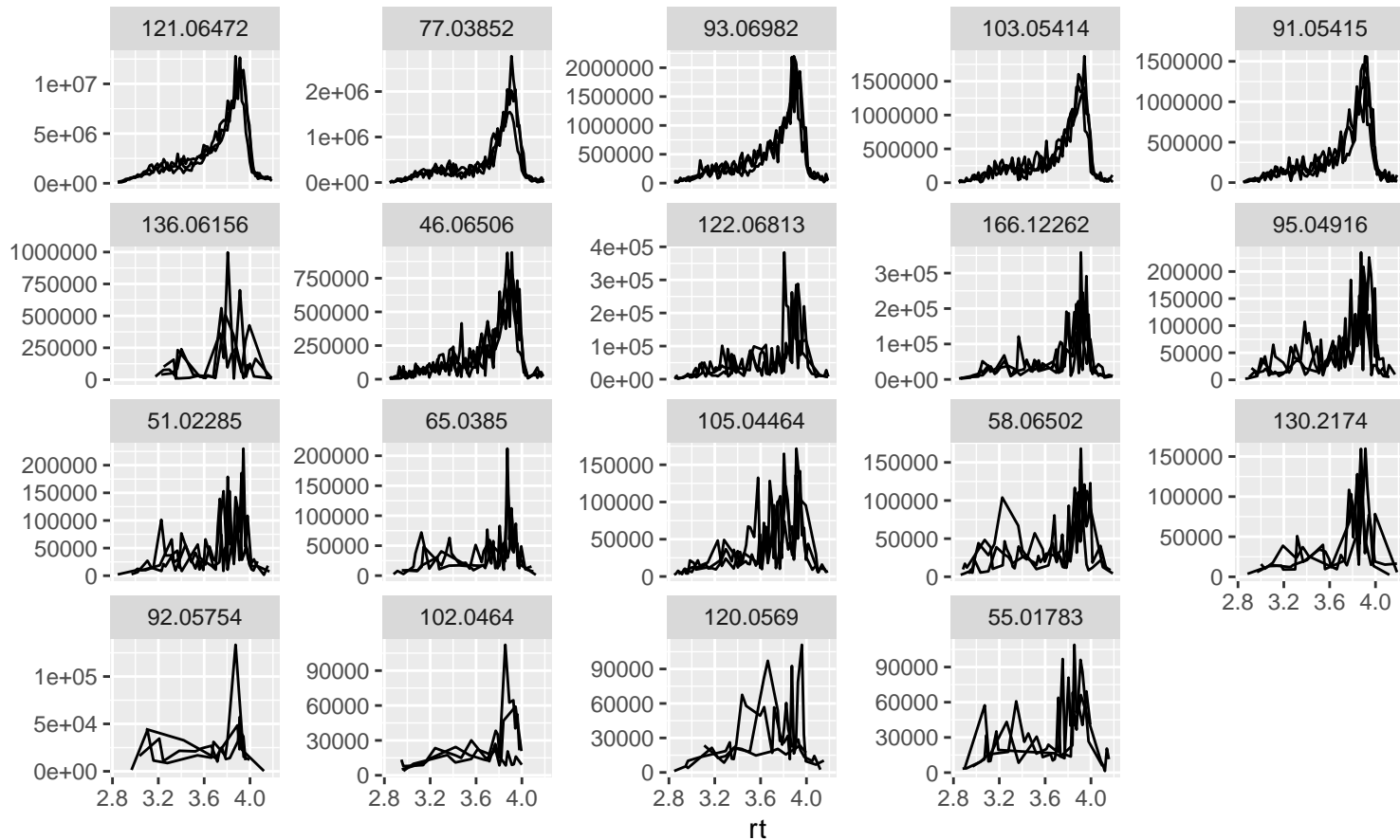
rt

L-Methionine S-oxide (neg) 164.03869

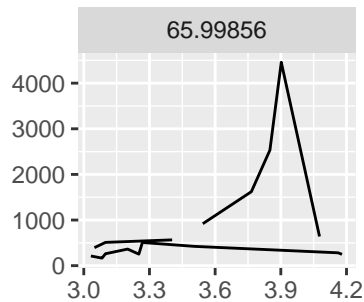
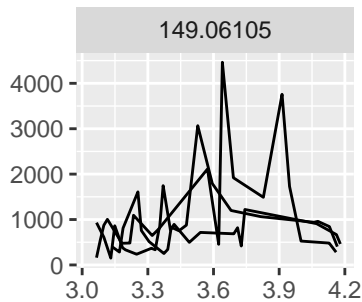
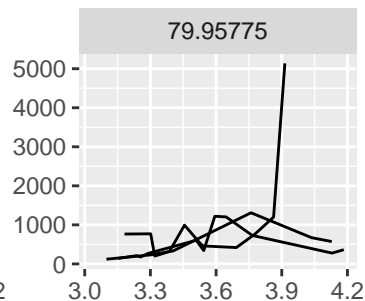
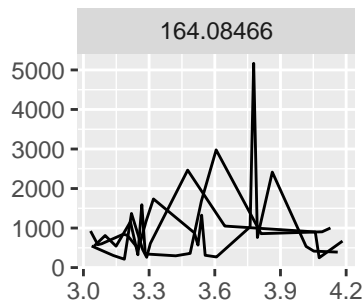
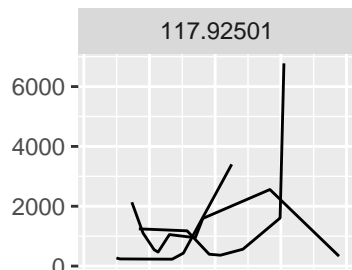
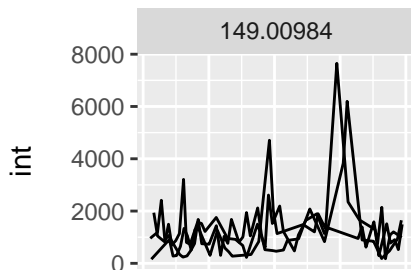
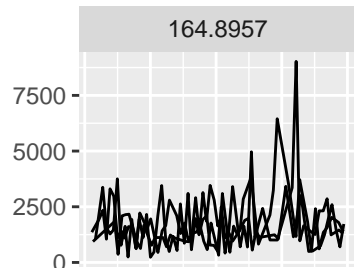
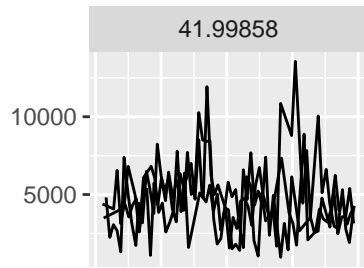
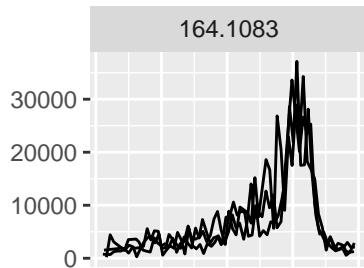
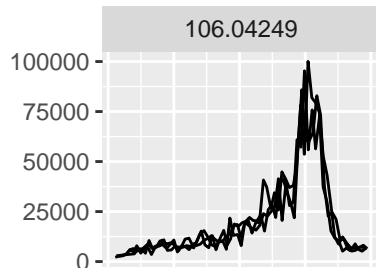


Hordenine (pos) 166.12264

int

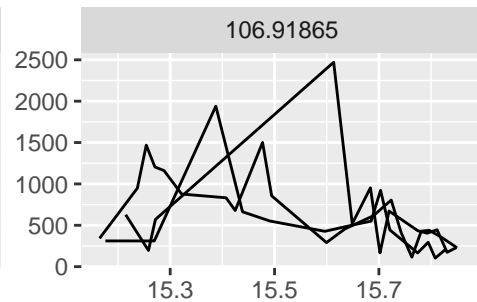
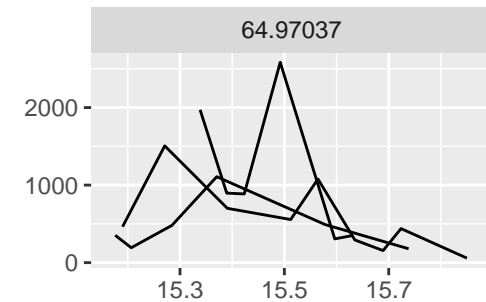
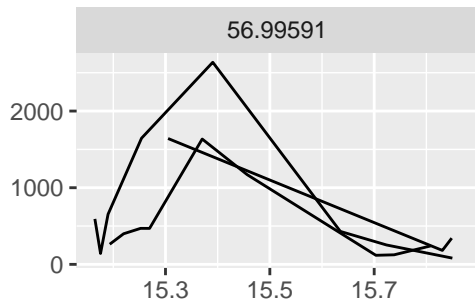
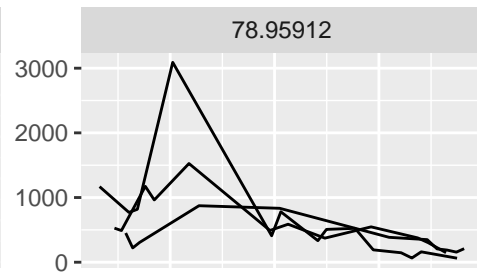
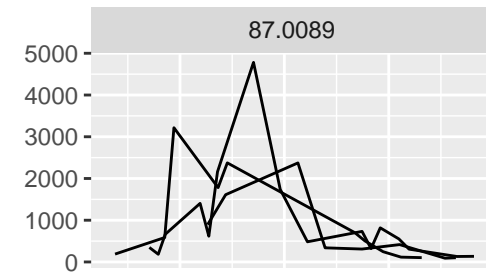
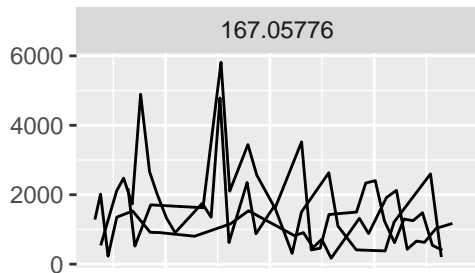
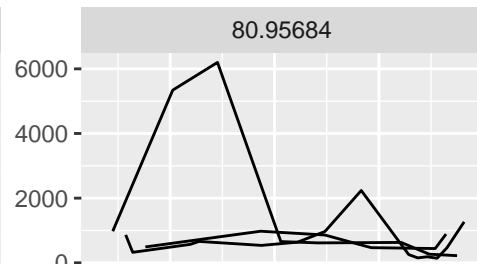
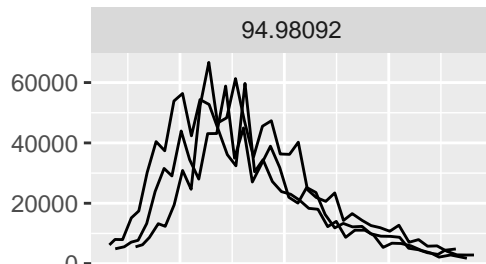
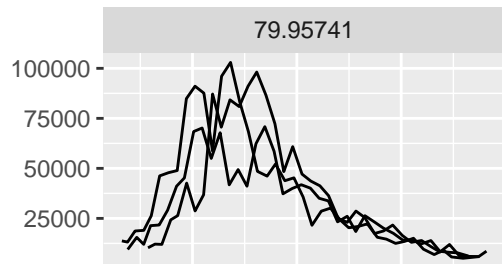


Hordenine (neg) 164.108088

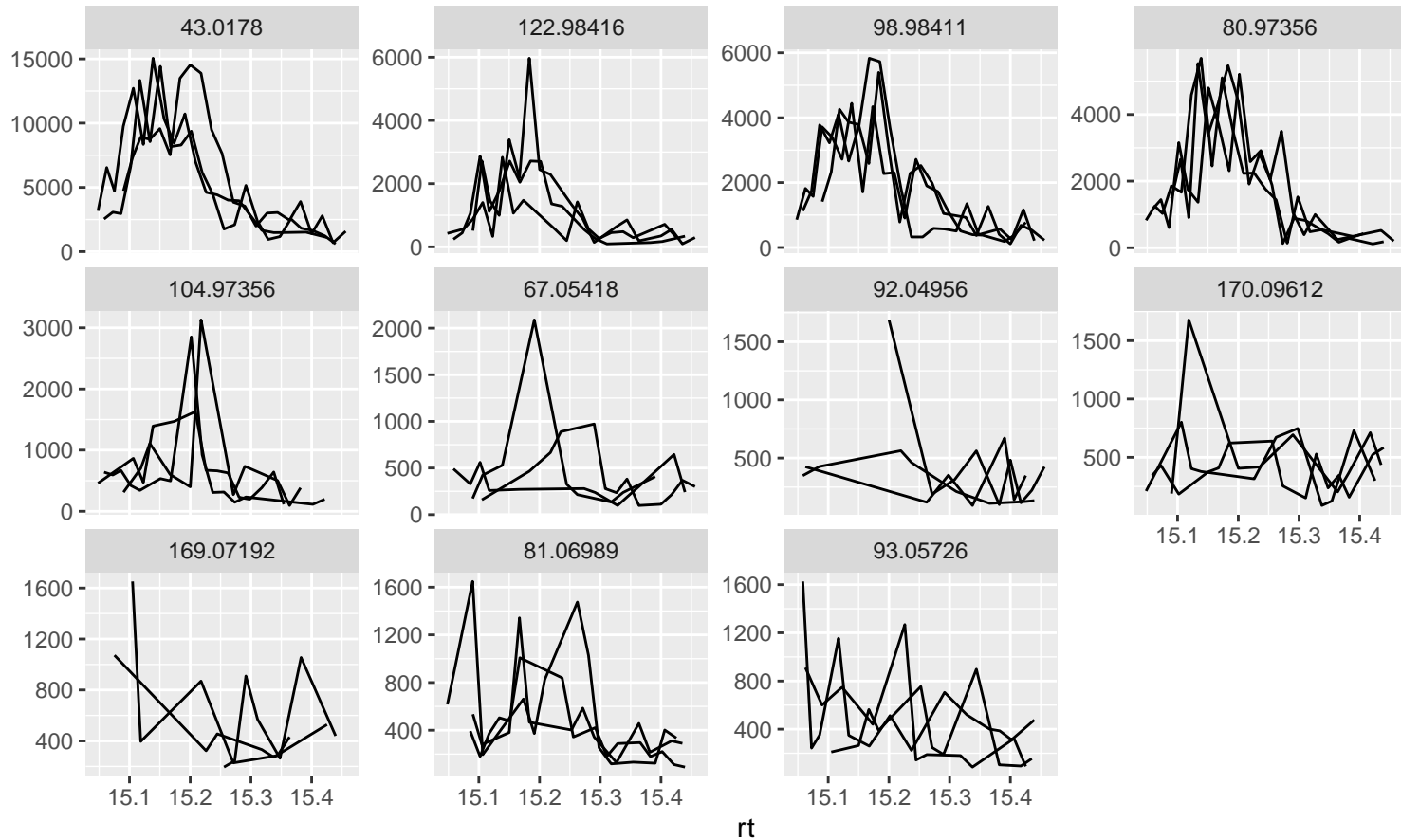


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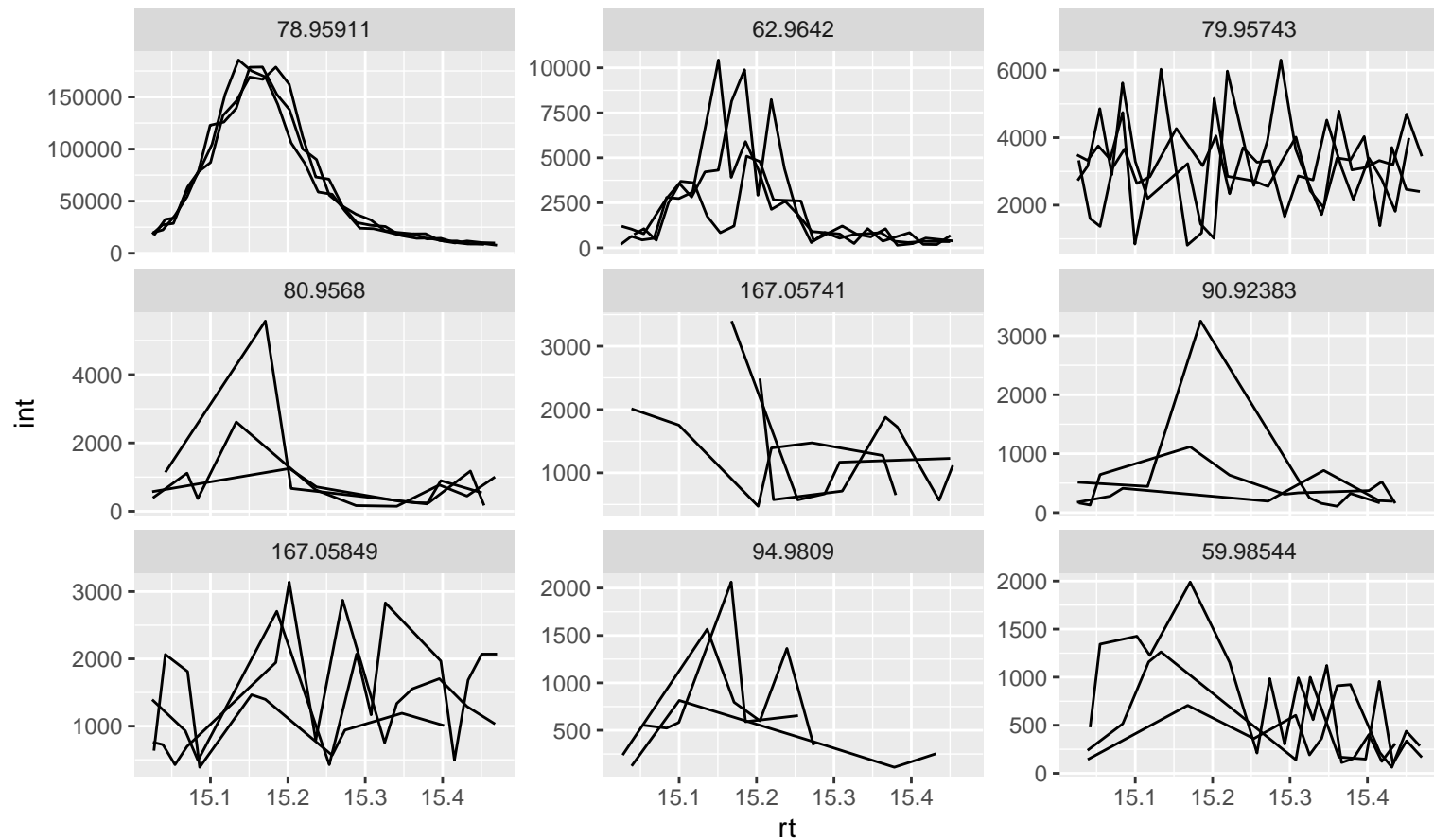
3-Sulfolpyruvic acid (neg) 166.965586



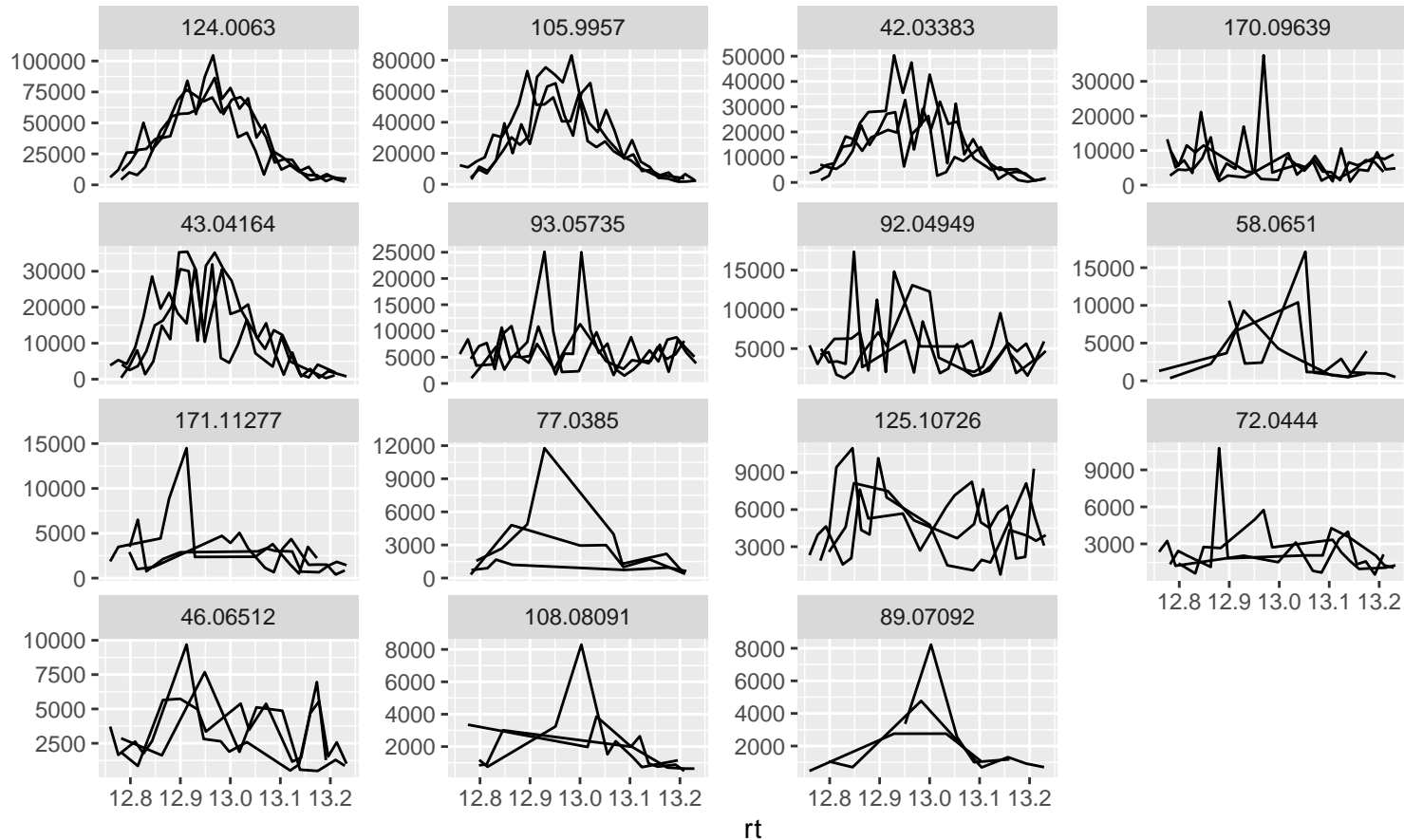
Phosphoenolpyruvic acid (pos) 168.989654



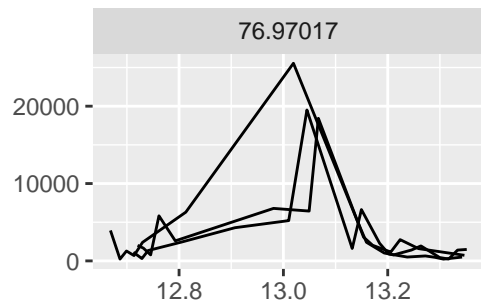
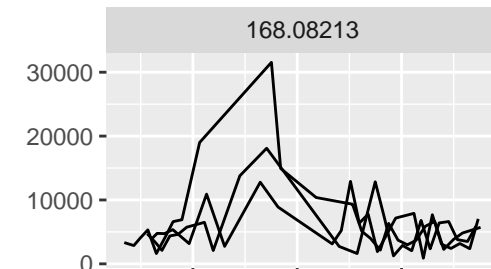
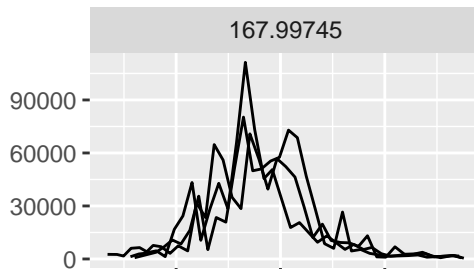
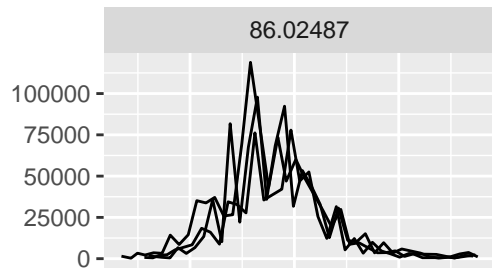
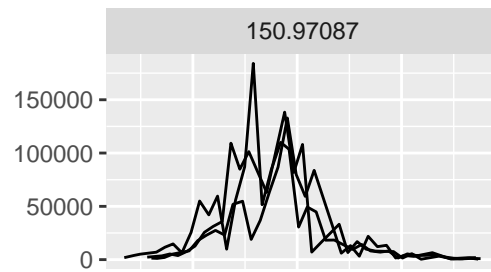
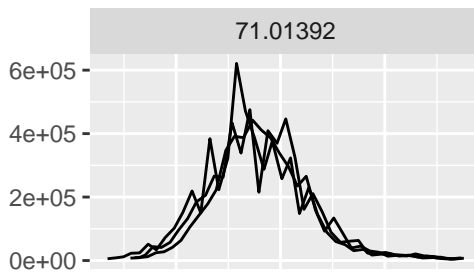
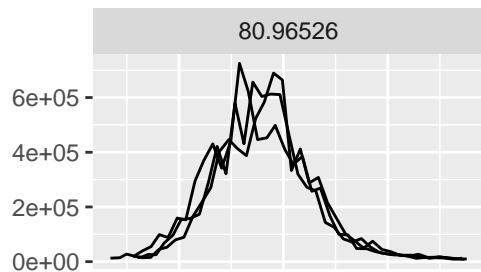
Phosphoenolpyruvic acid (neg) 166.975102



L-Cysteic acid (pos) 170.011772

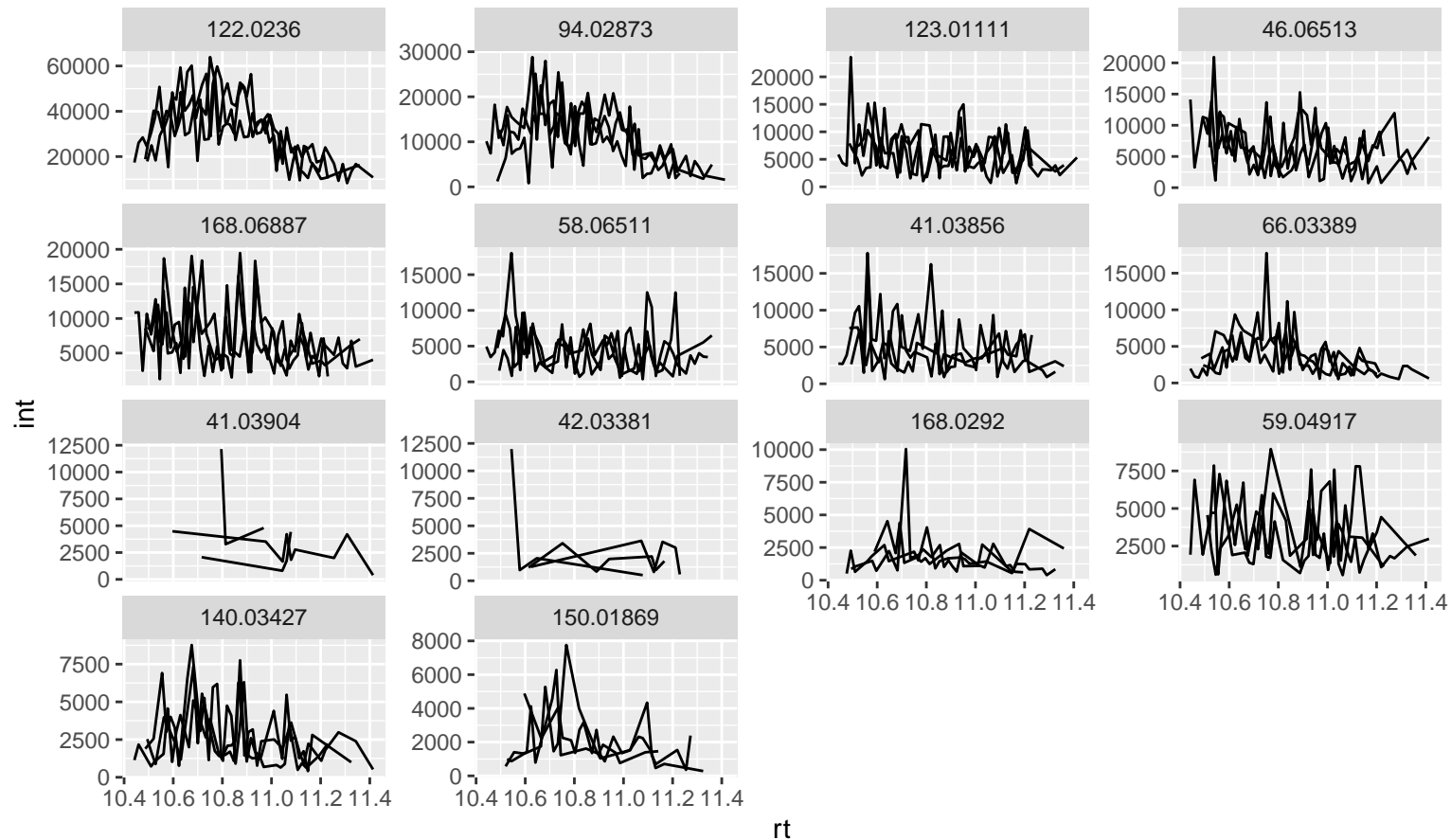


L-Cysteic acid (neg) 167.99722

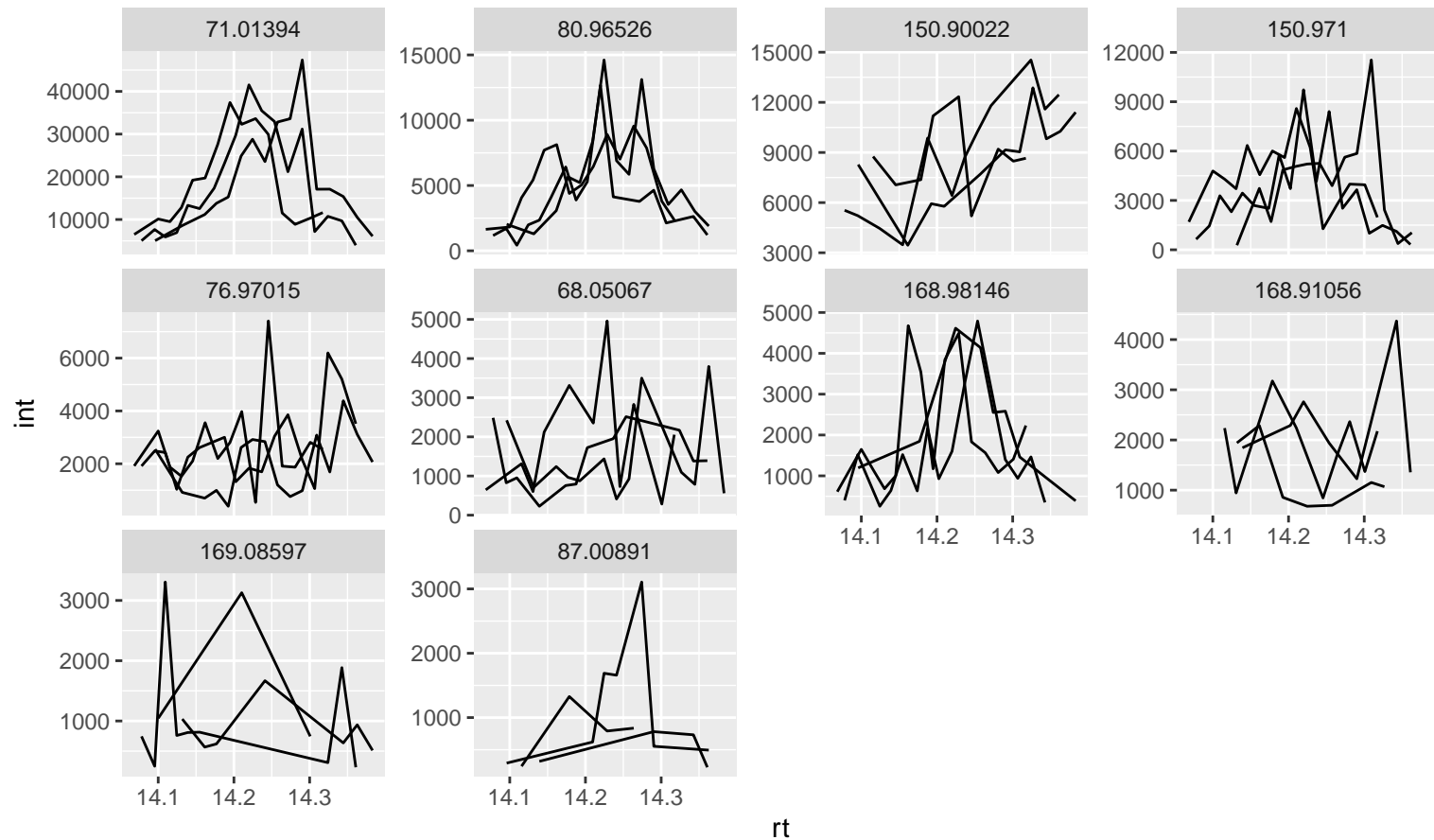


rt

2,3-Pyridinedicarboxylic acid (pos) 168.029135

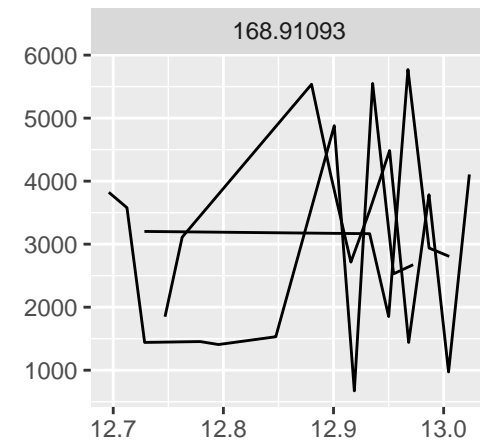
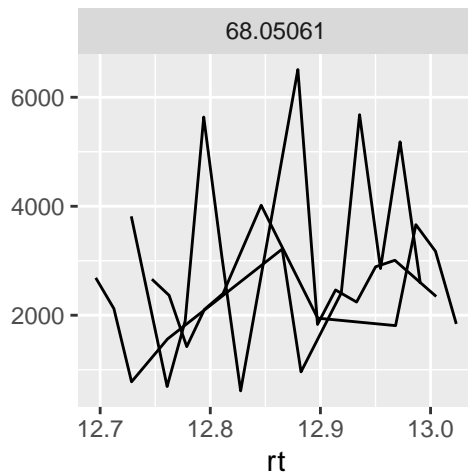
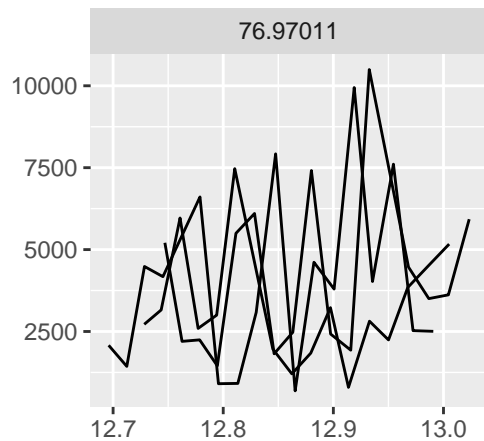
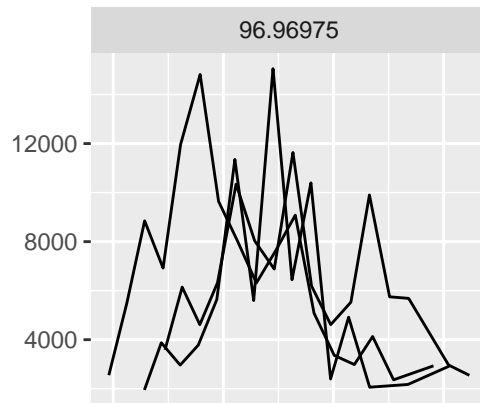
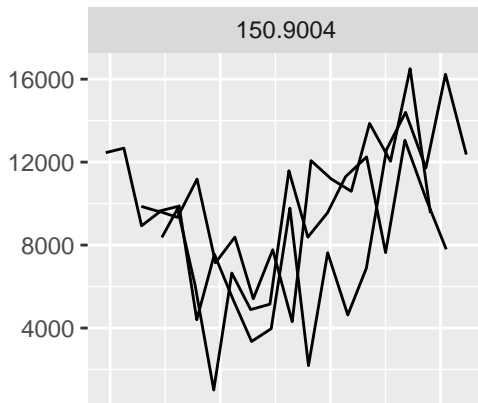
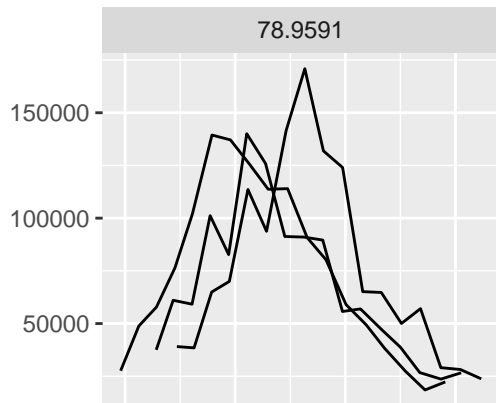


3-Sulfolactate (neg) 168.98123558



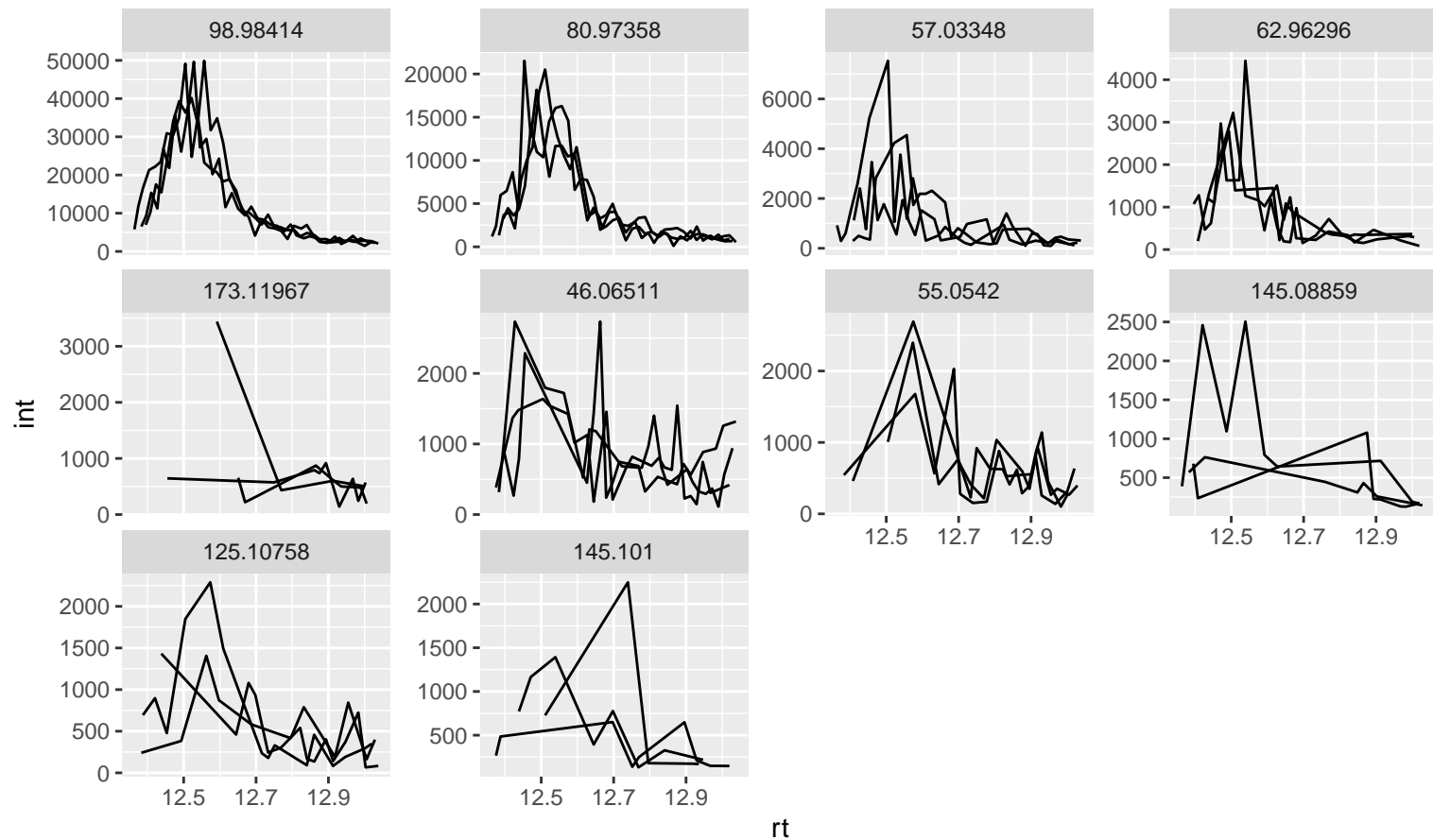
Dihydroxyacetone phosphate (neg) 168.990752

int

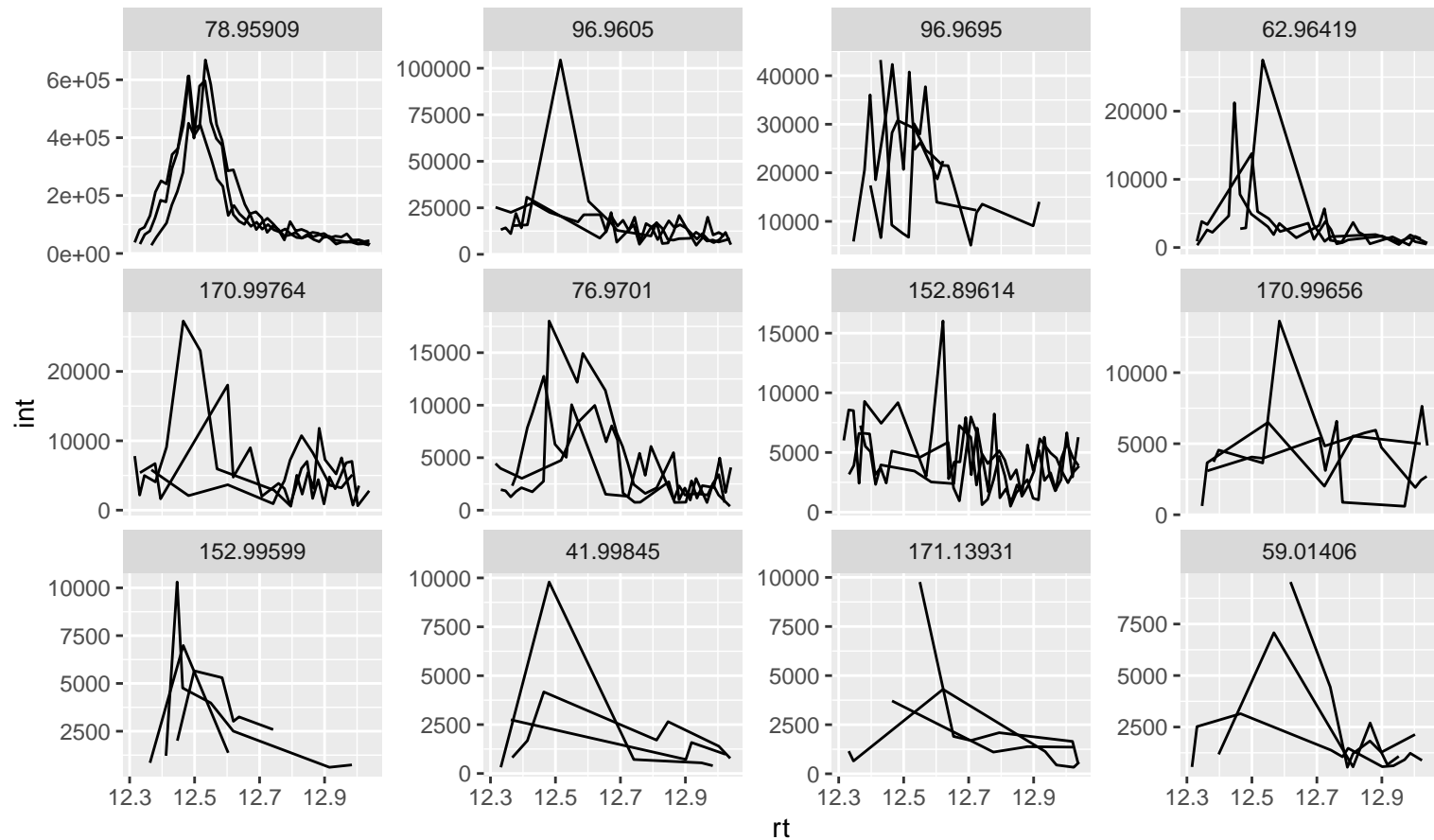


rt

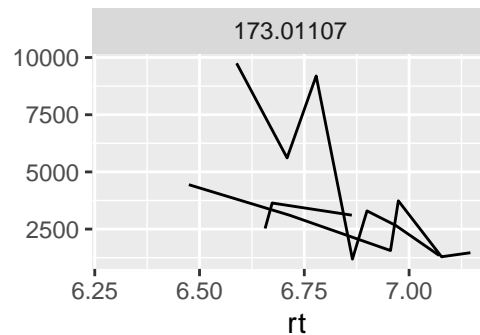
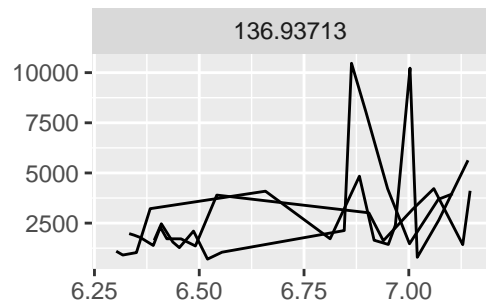
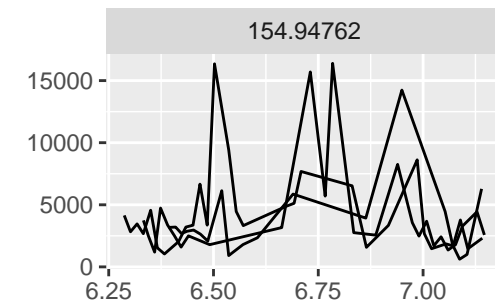
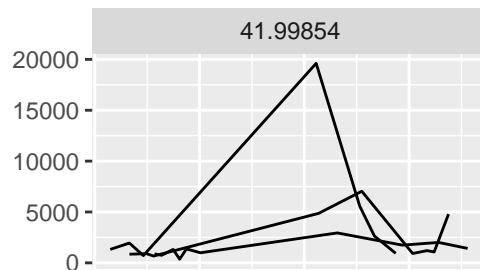
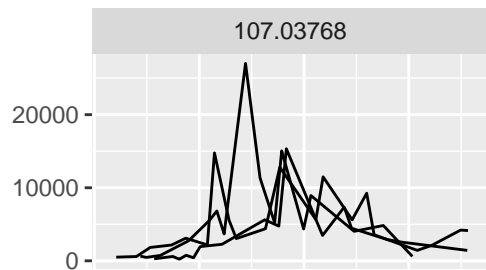
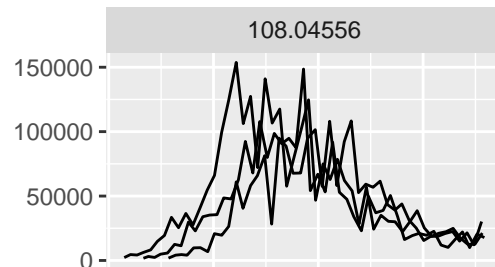
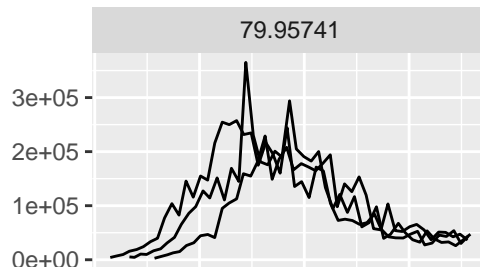
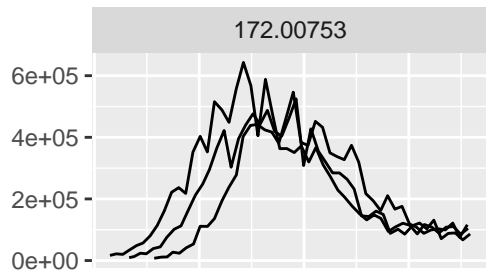
Glycerophosphoric acid (pos) 173.020954



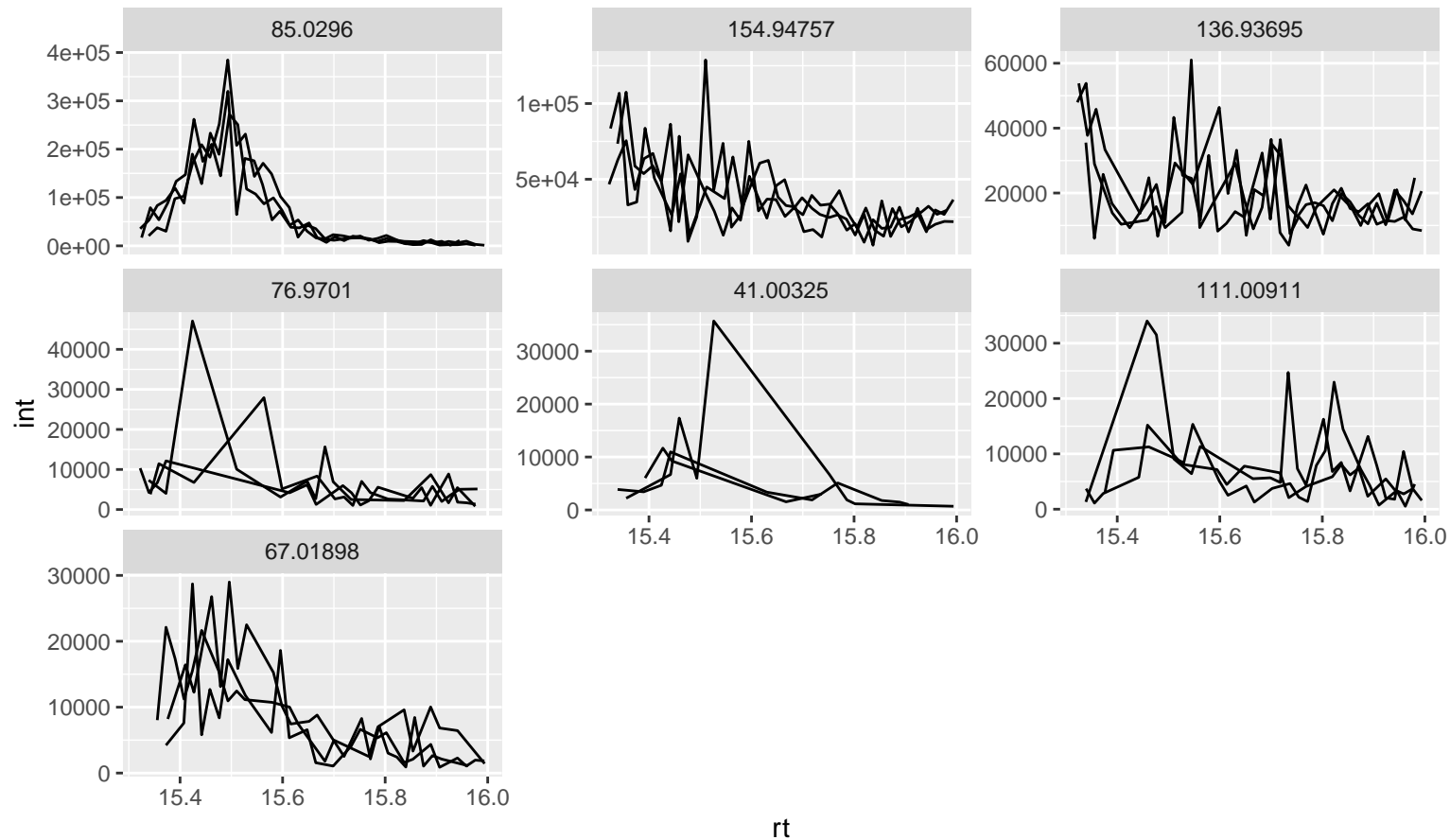
Glycerophosphoric acid (neg) 171.006402



Sulfanilic acid (neg) 172.00739

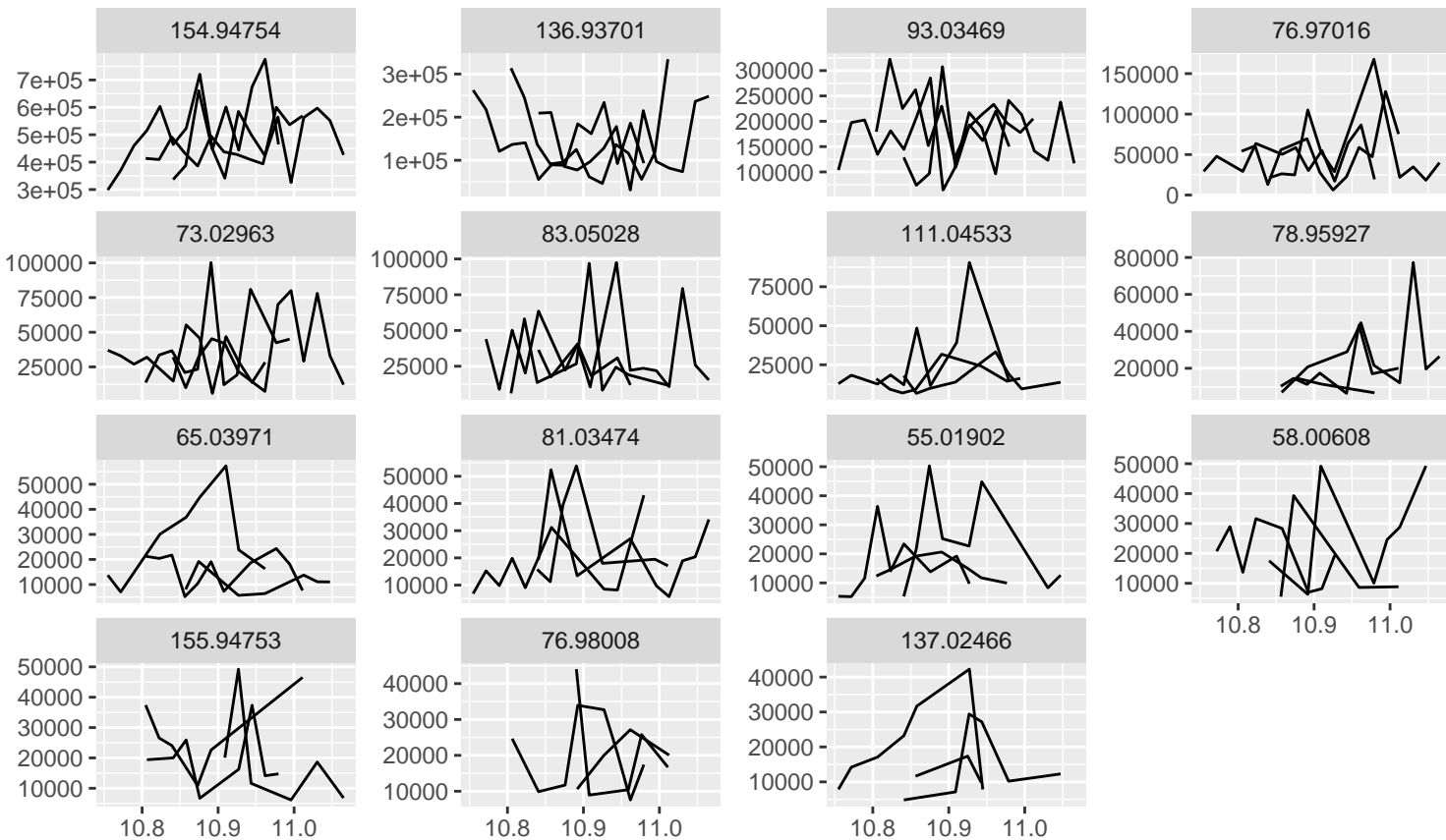


cis-Aconitic acid (neg) 173.009164



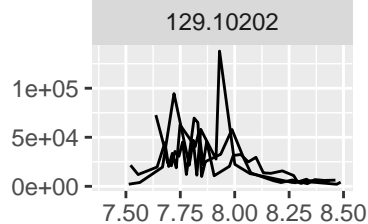
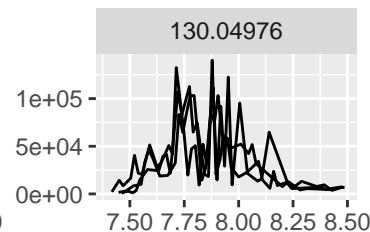
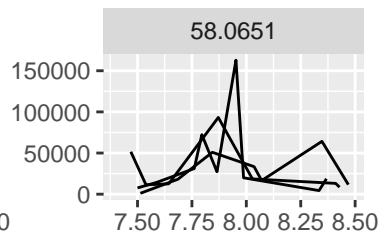
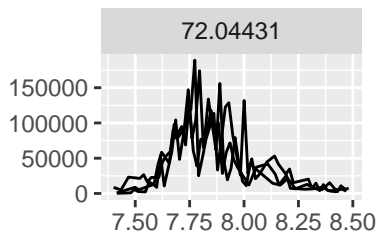
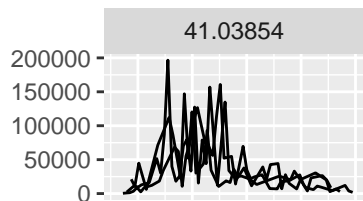
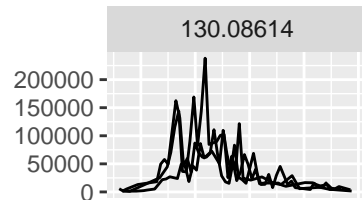
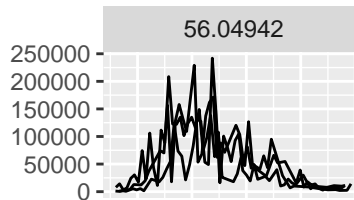
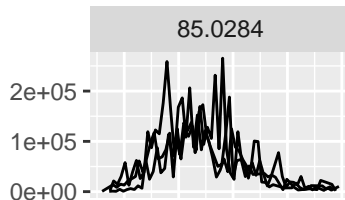
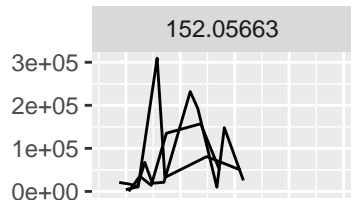
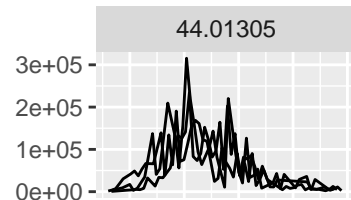
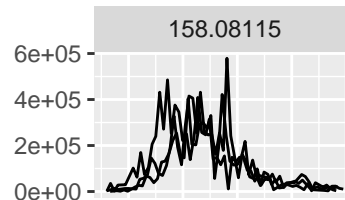
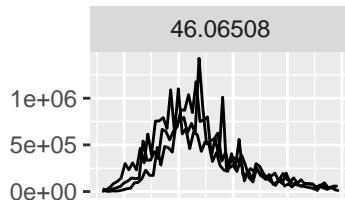
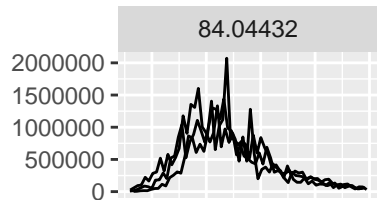
Shikimic acid (neg) 173.045549

int



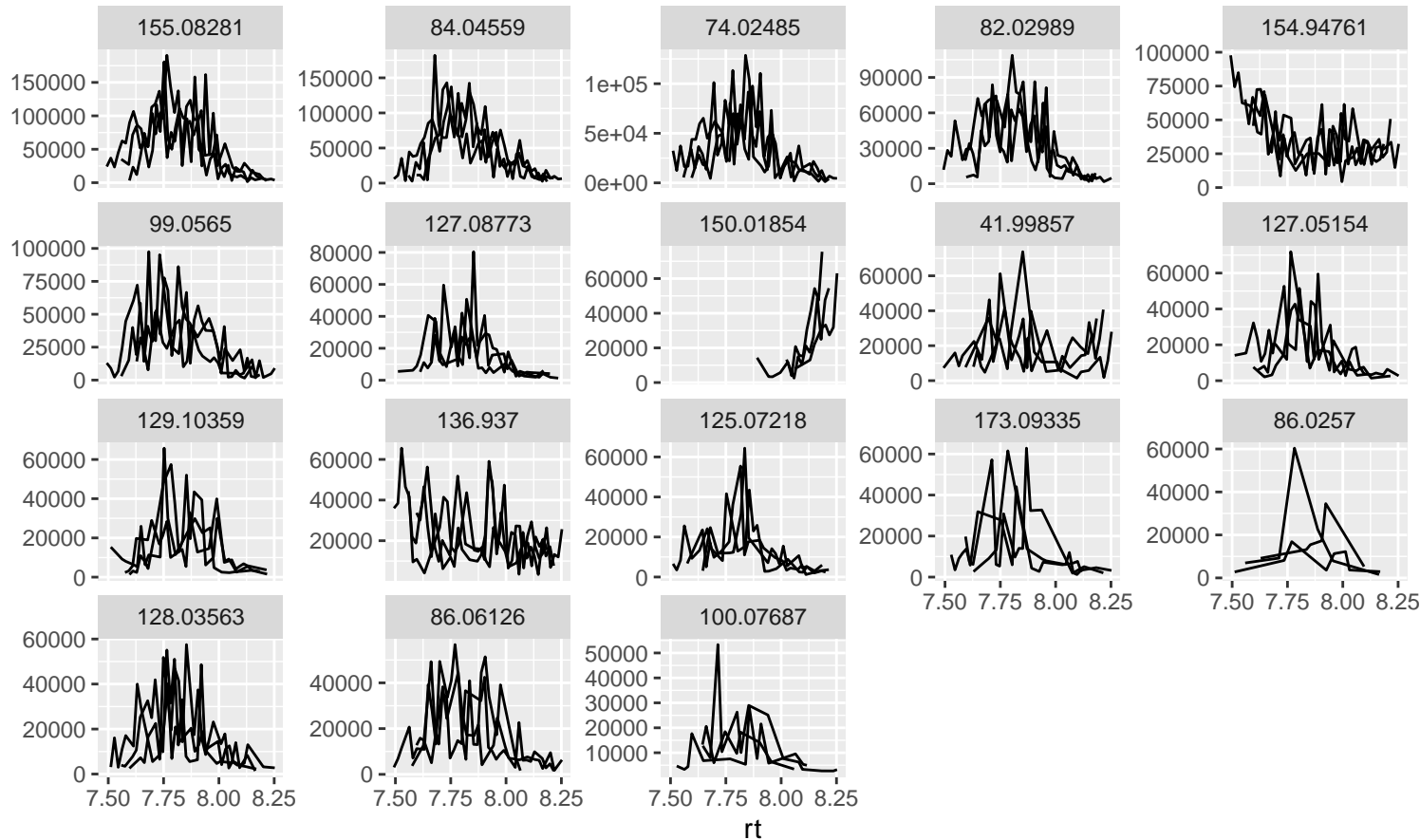
rt

L-Theanine (pos) 175.107719



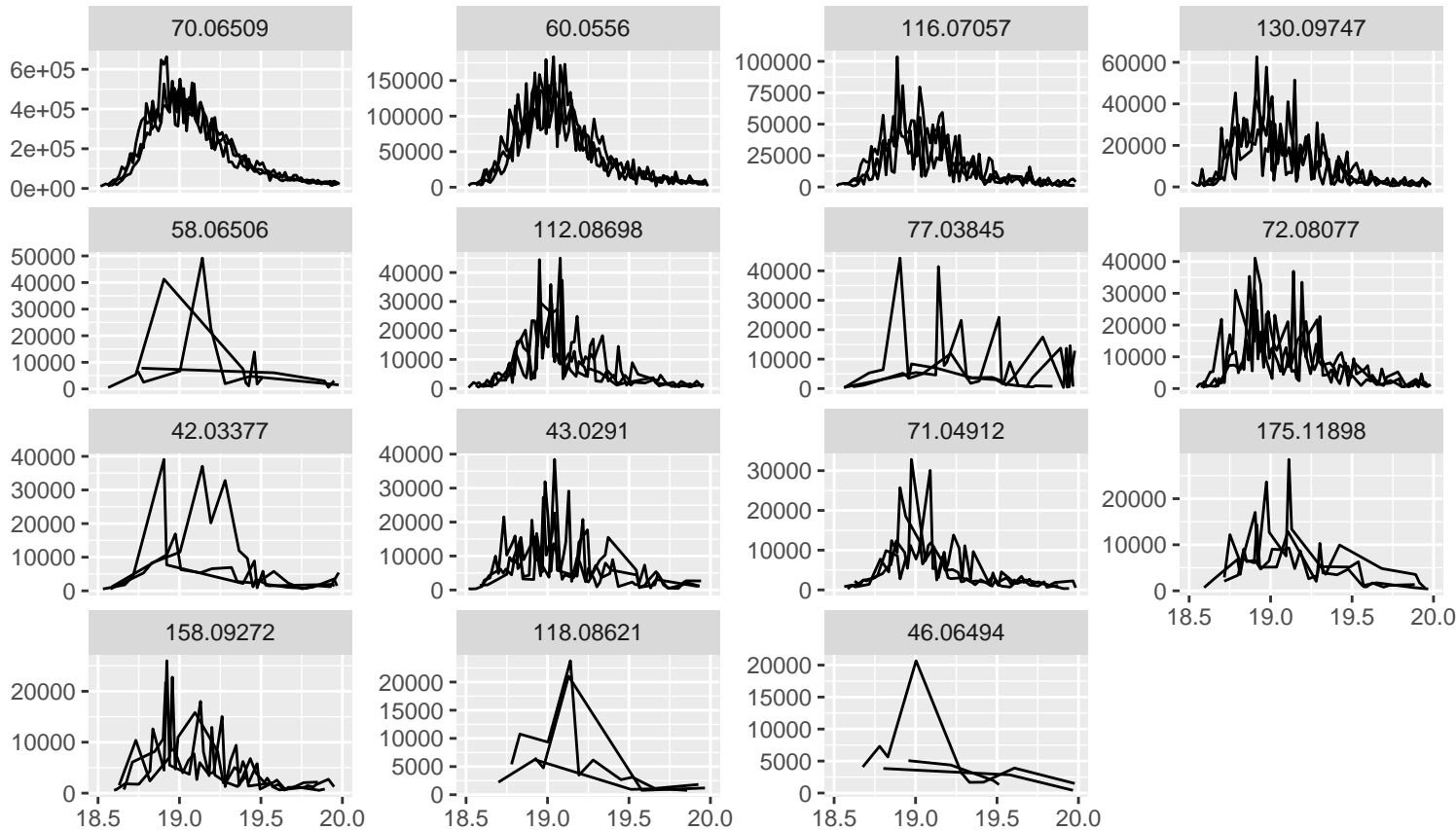
rt

L-Theanine (neg) 173.093167



L-Arginine (pos) 175.118952

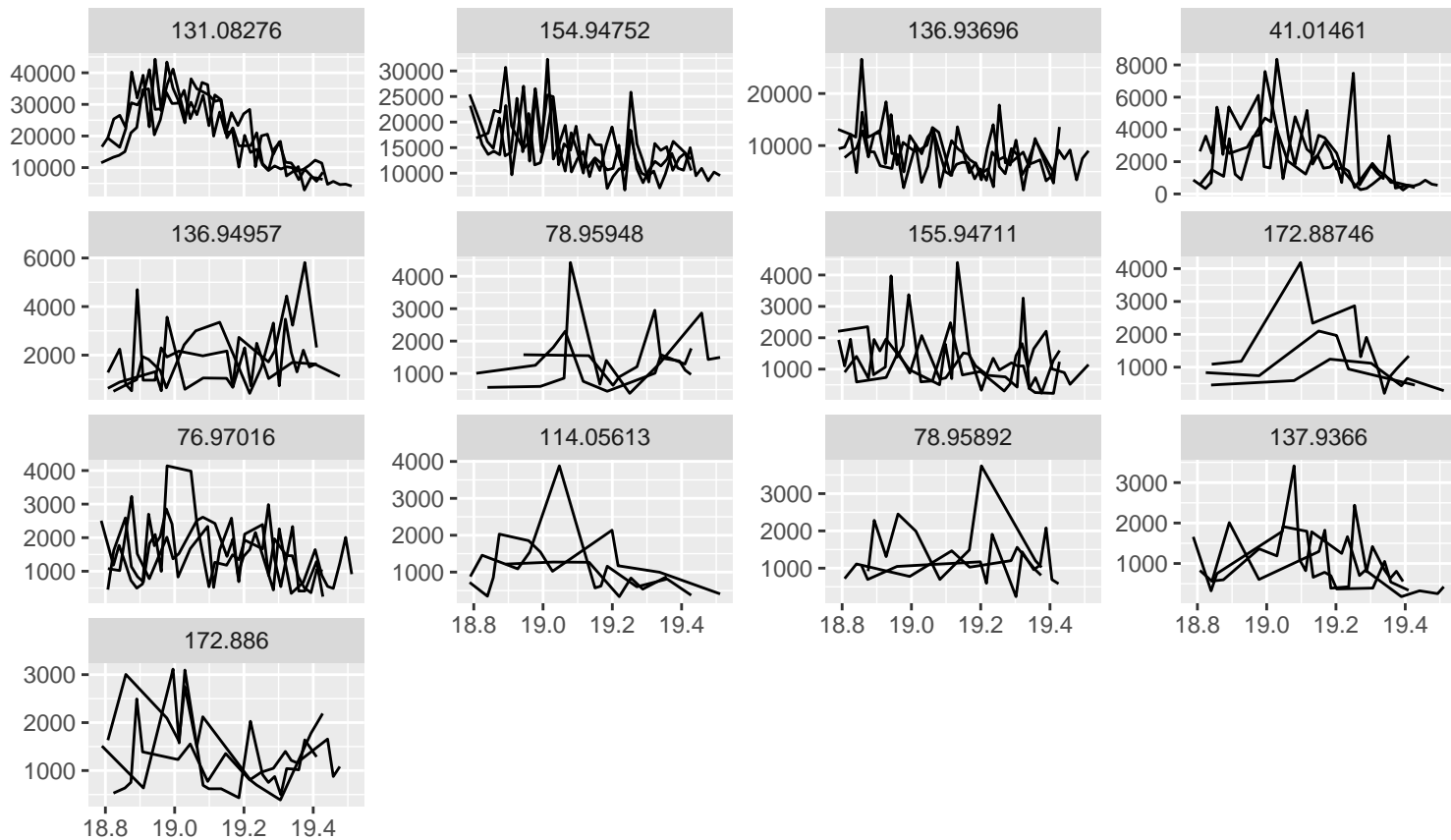
int



rt

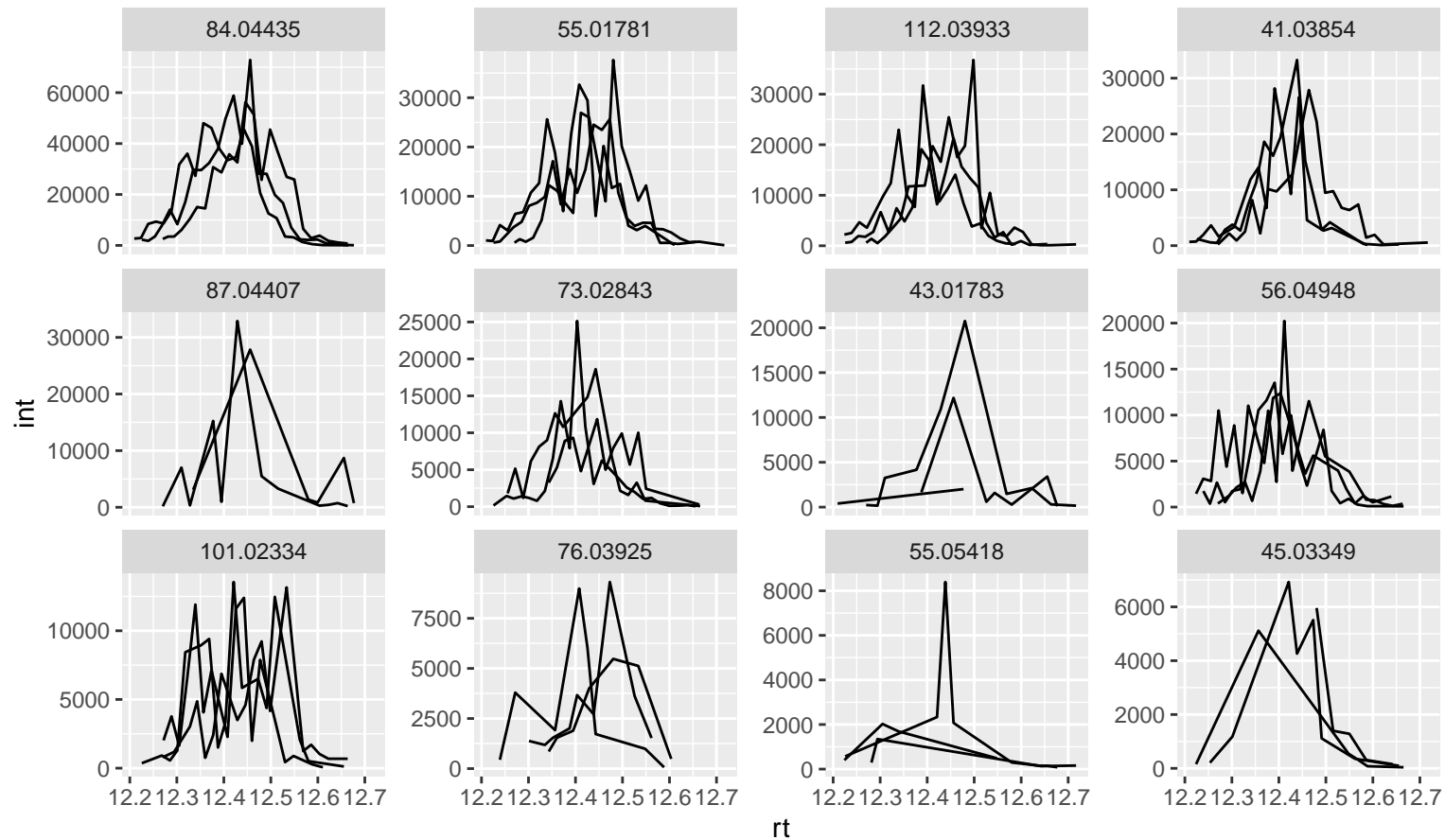
L-Arginine (neg) 173.1044

int

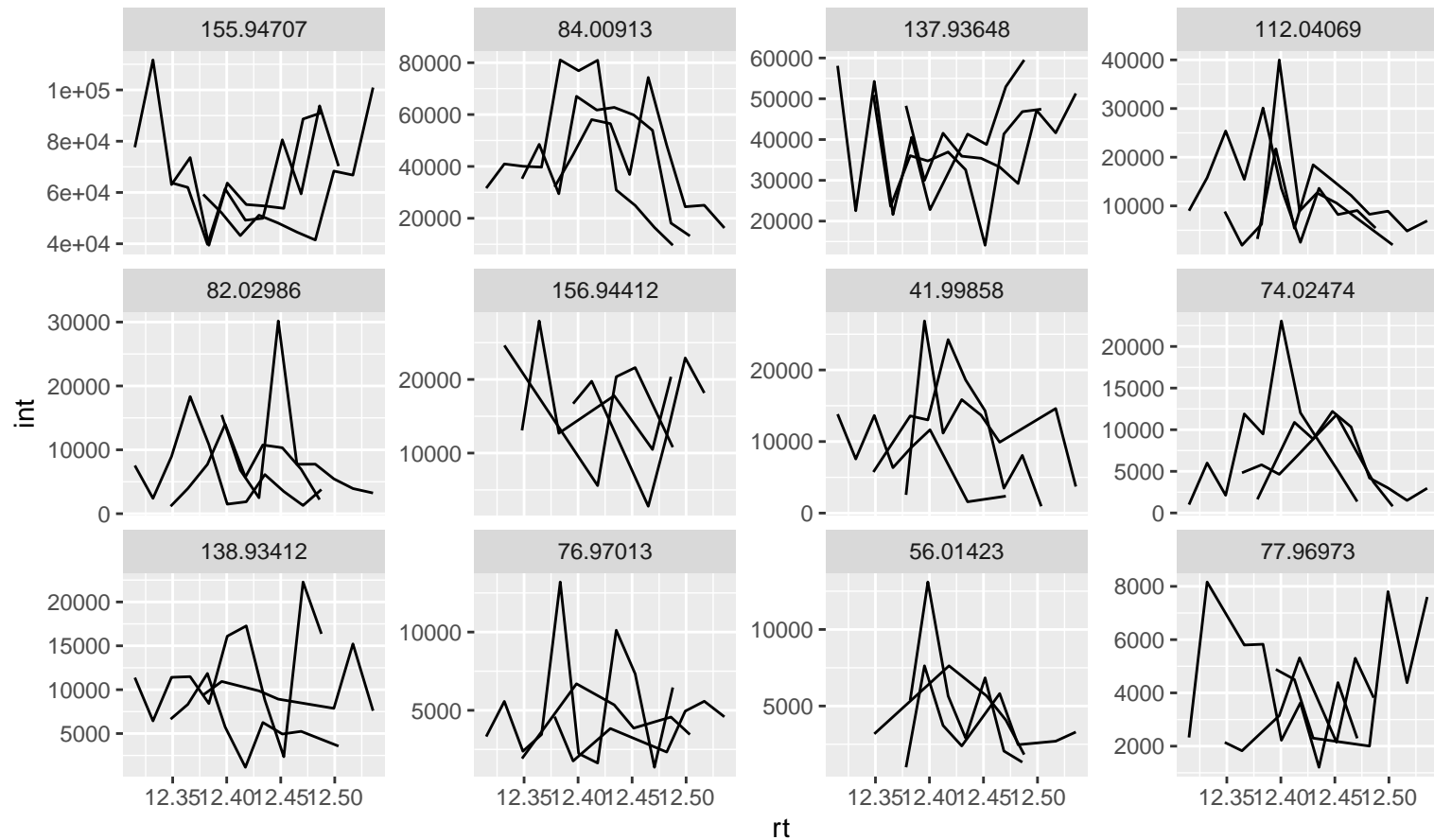


rt

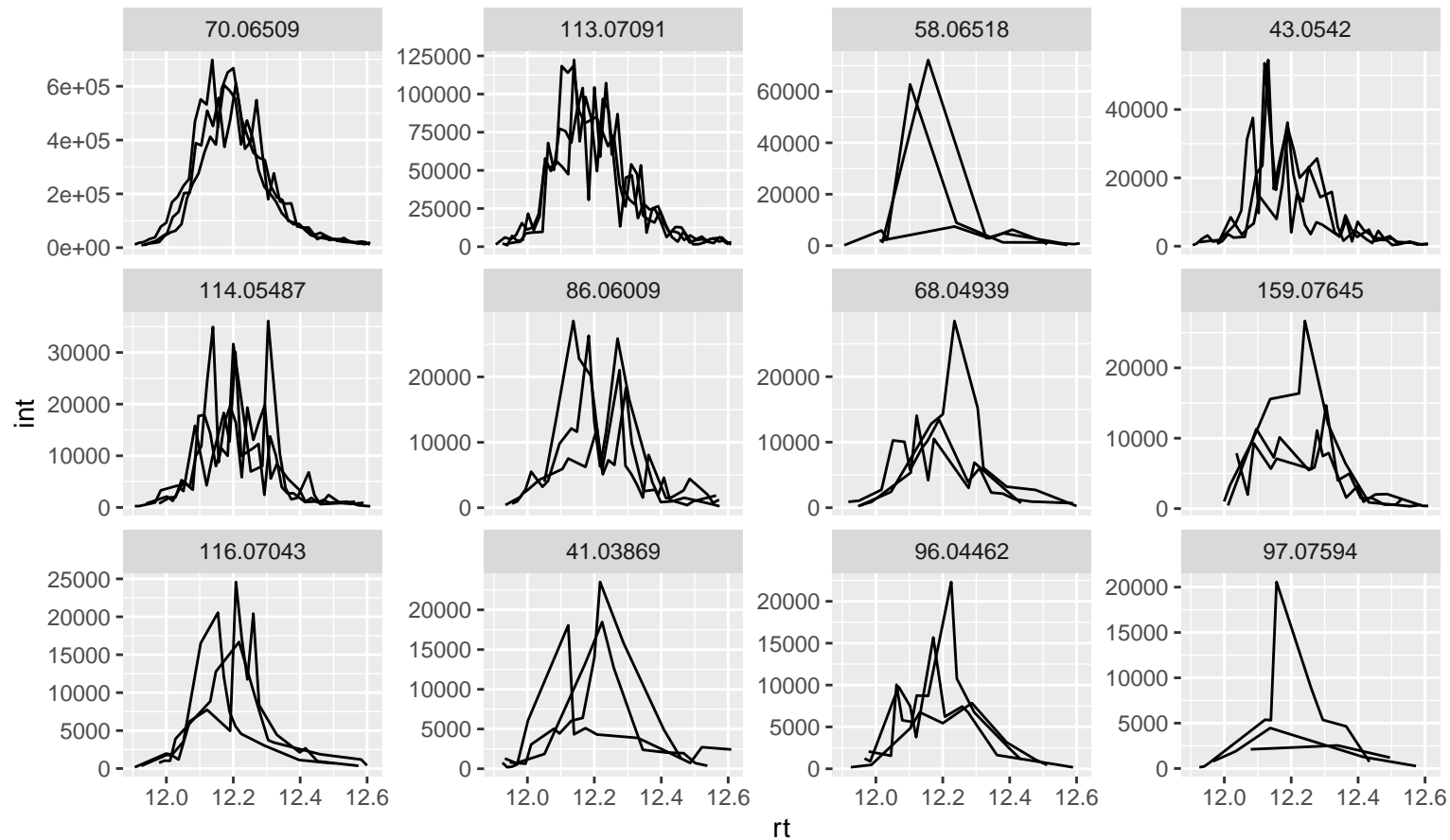
Succinylglycine (pos) 176.05535



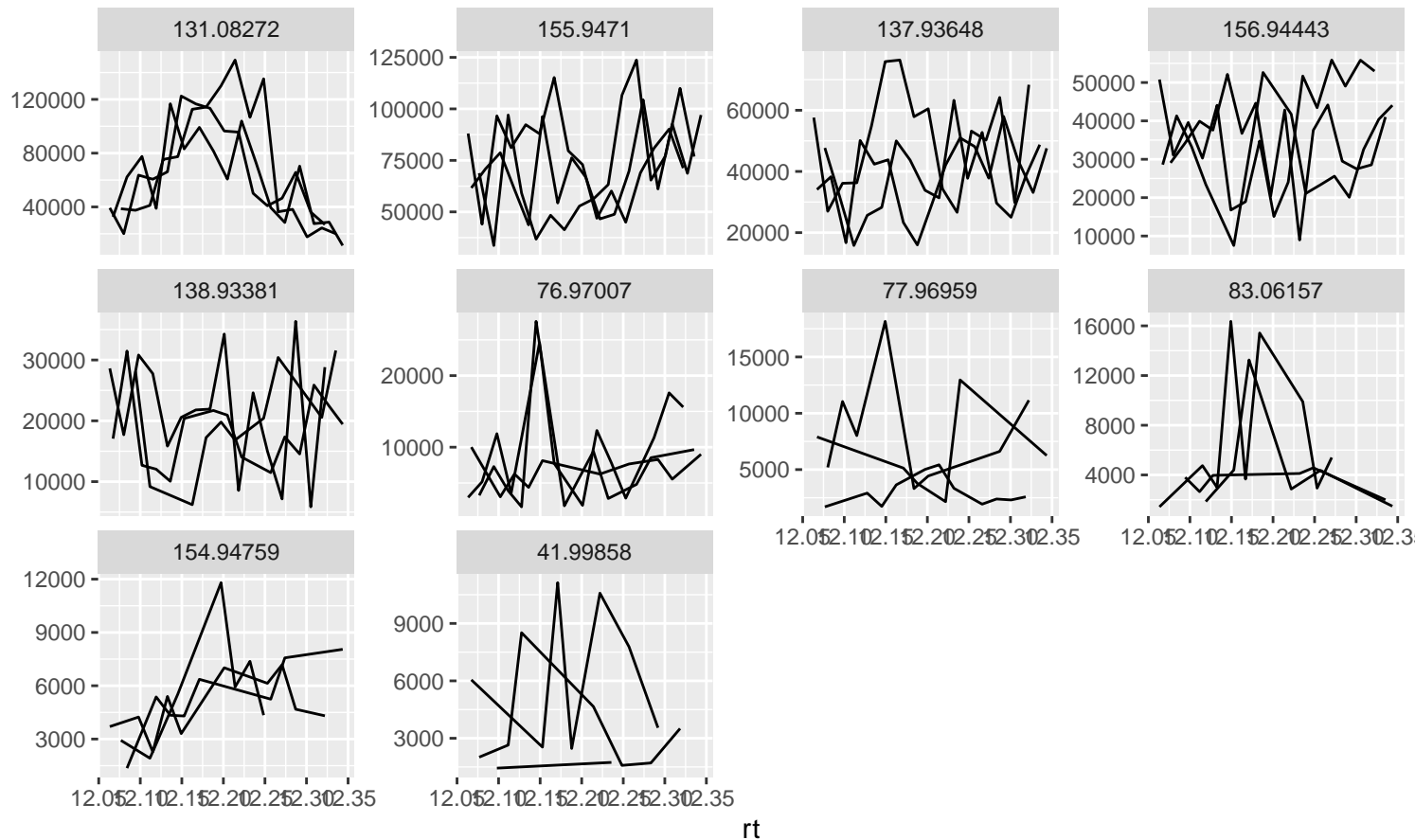
Succinylglycine (neg) 174.040798



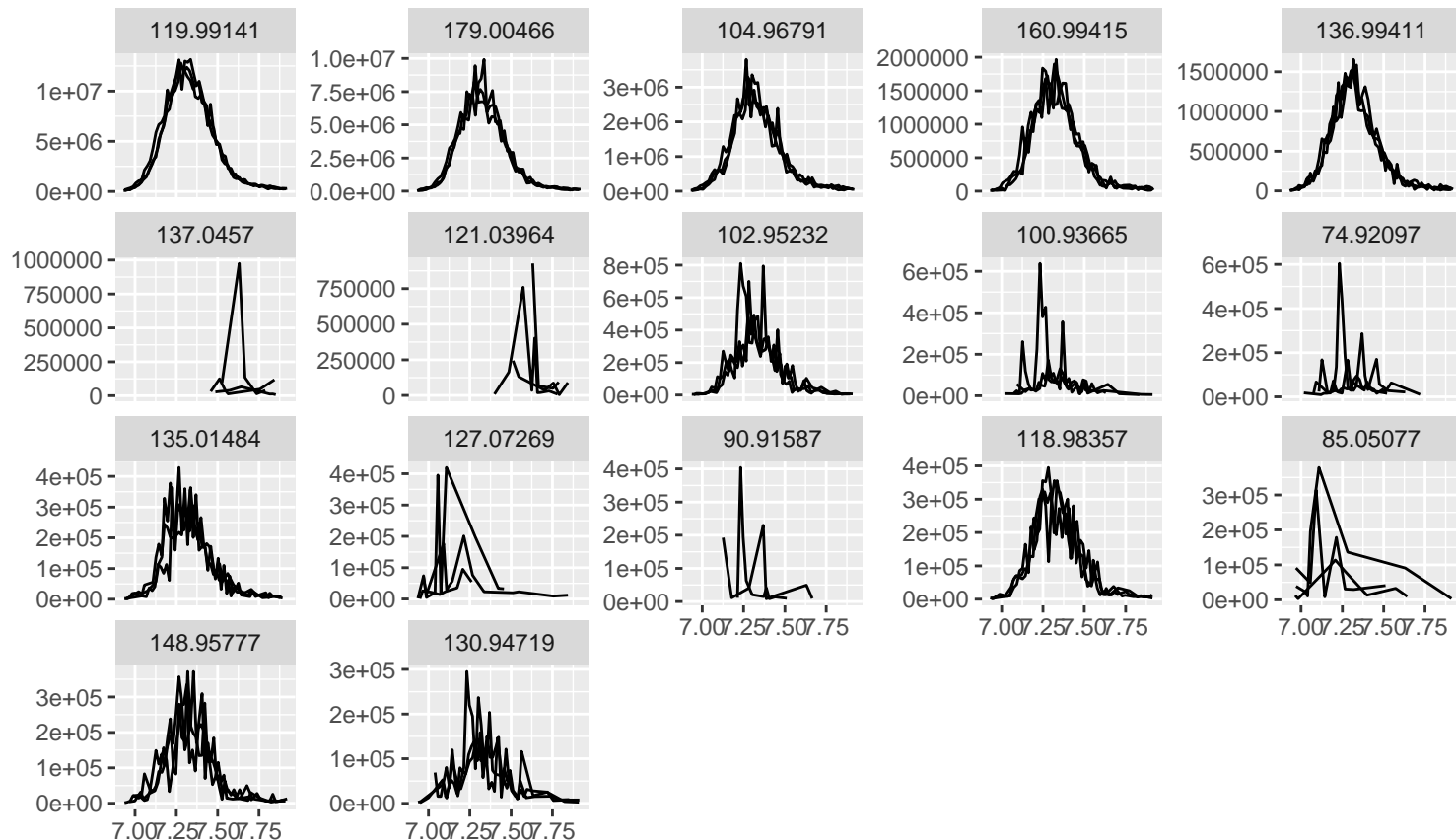
Citrulline (pos) 176.102968



Citrulline (neg) 174.088416



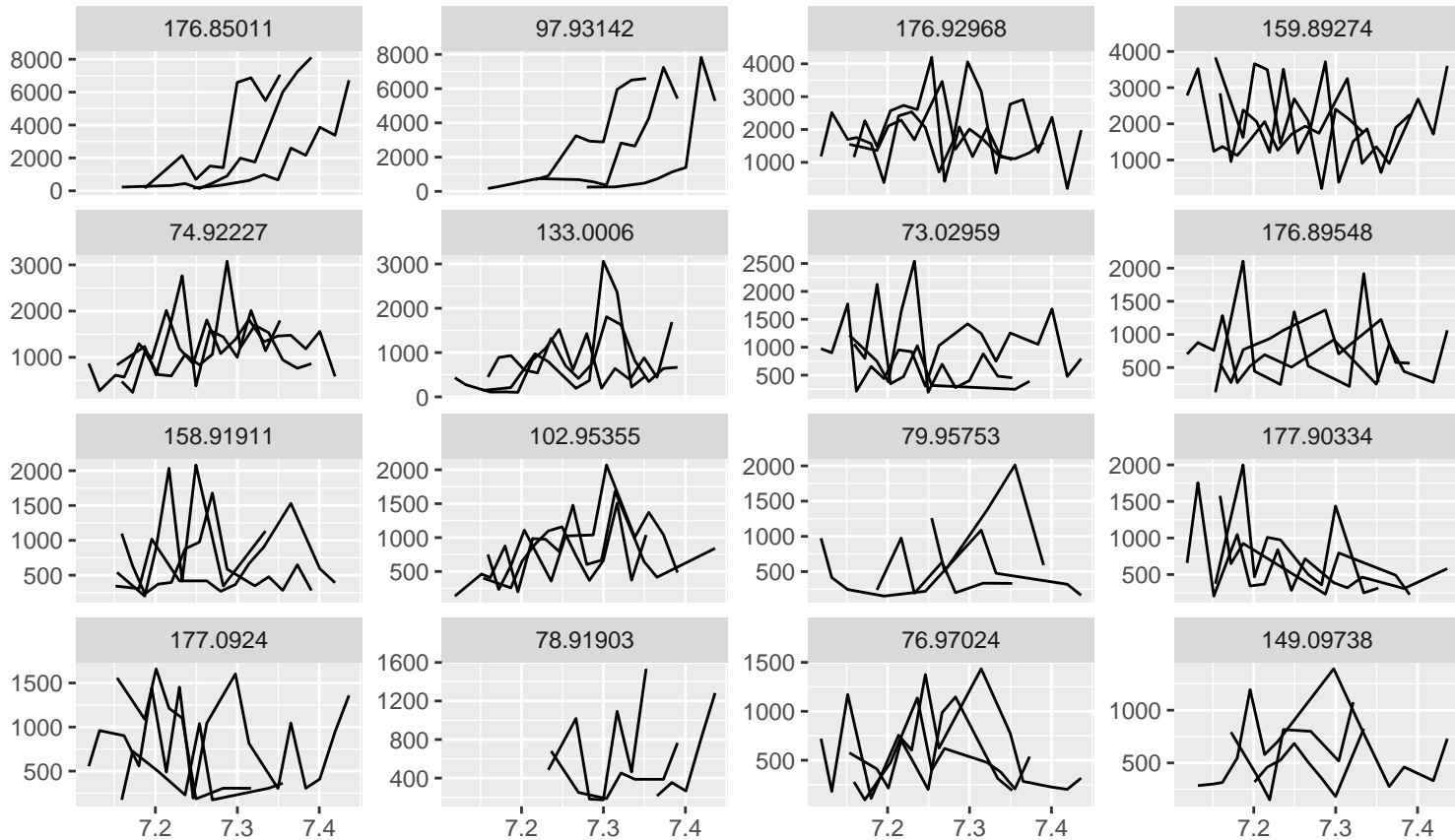
Arsenobetaine (pos) 179.004777



rt

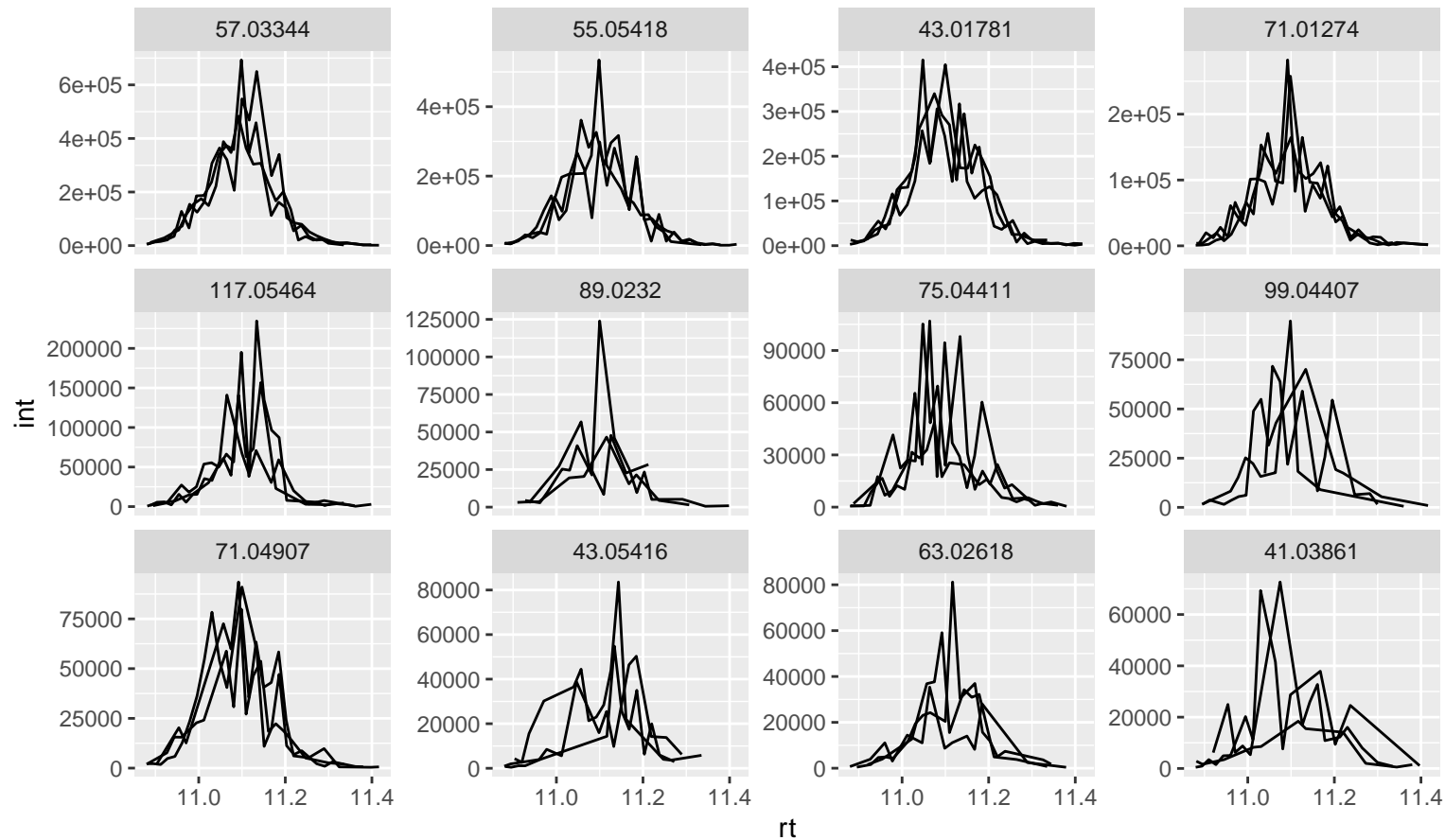
Arsenobetaine (neg) 176.990225

int



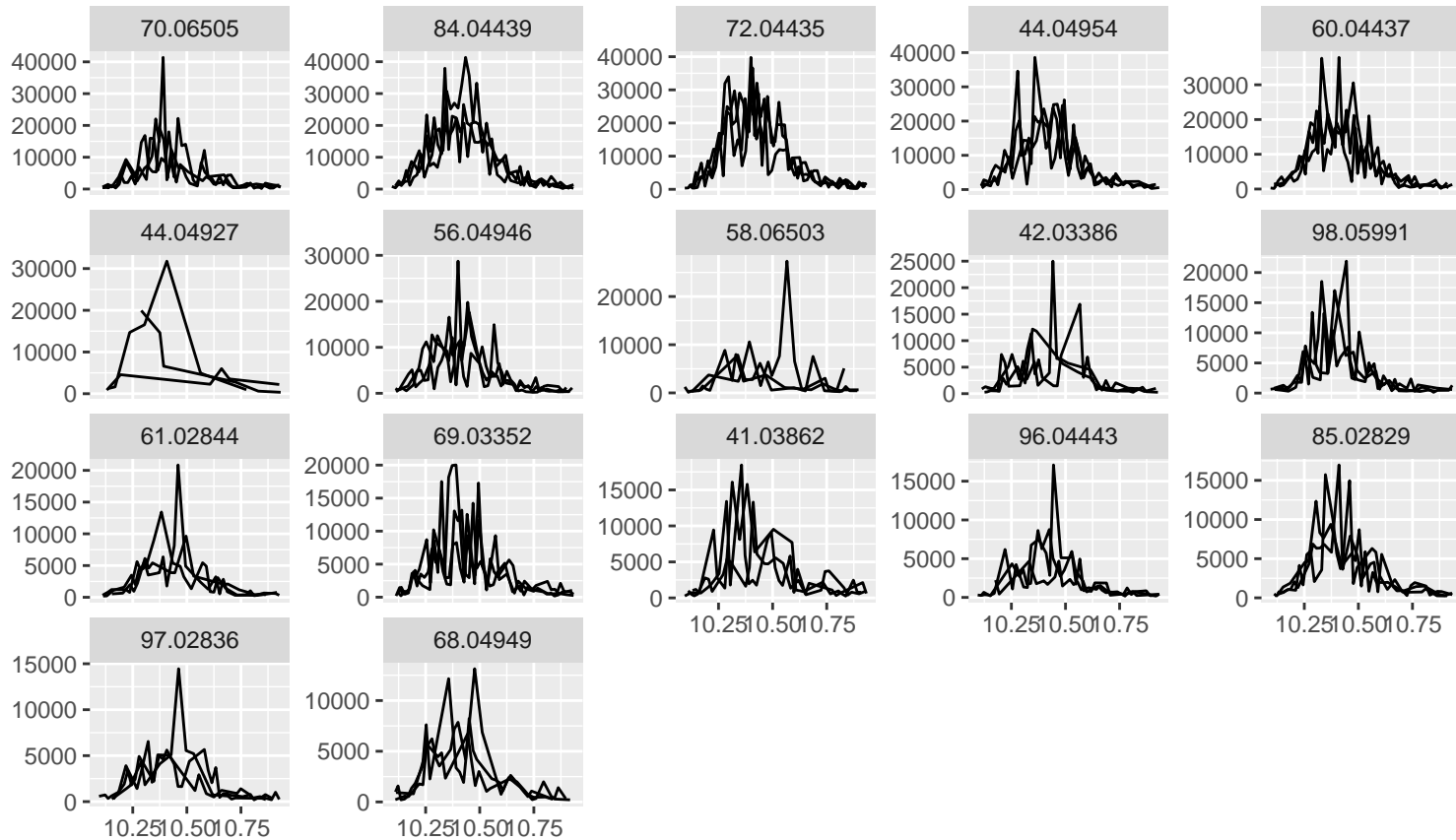
rt

Gonyol (pos) 179.073643



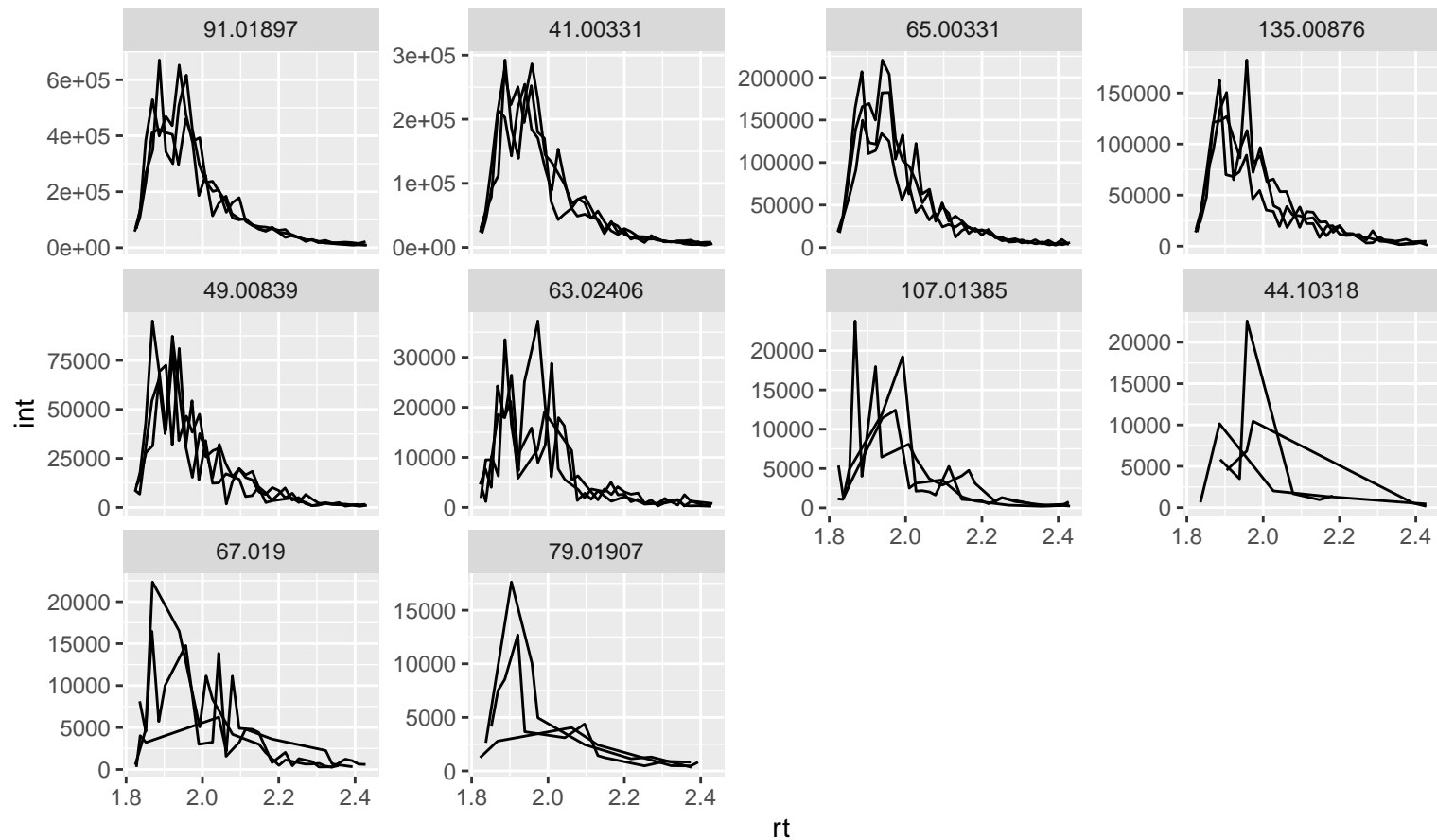
Glucosamine (pos) 180.08665

int



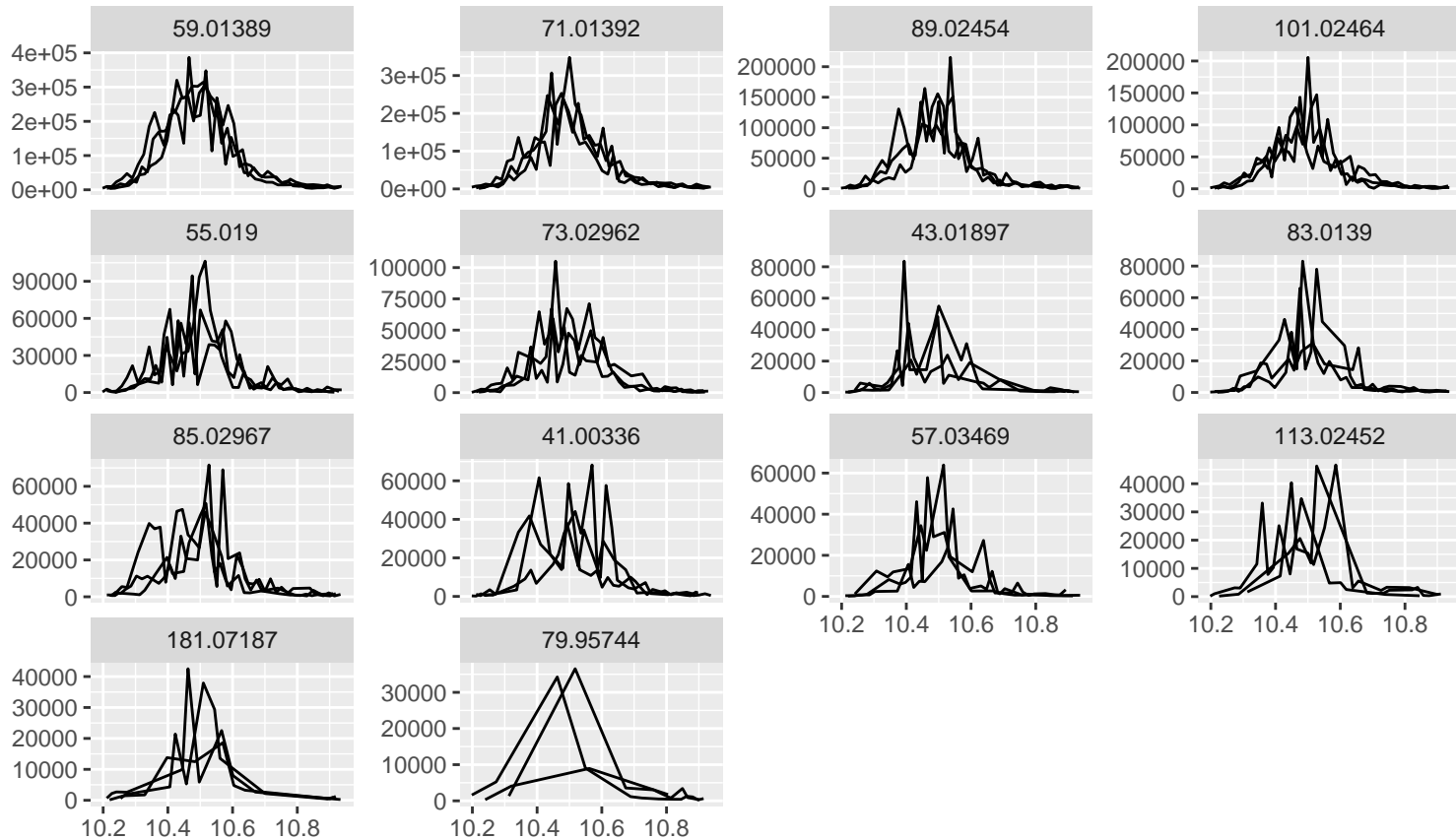
rt

Ethyl dihydroxybenzoate (neg) 181.050634



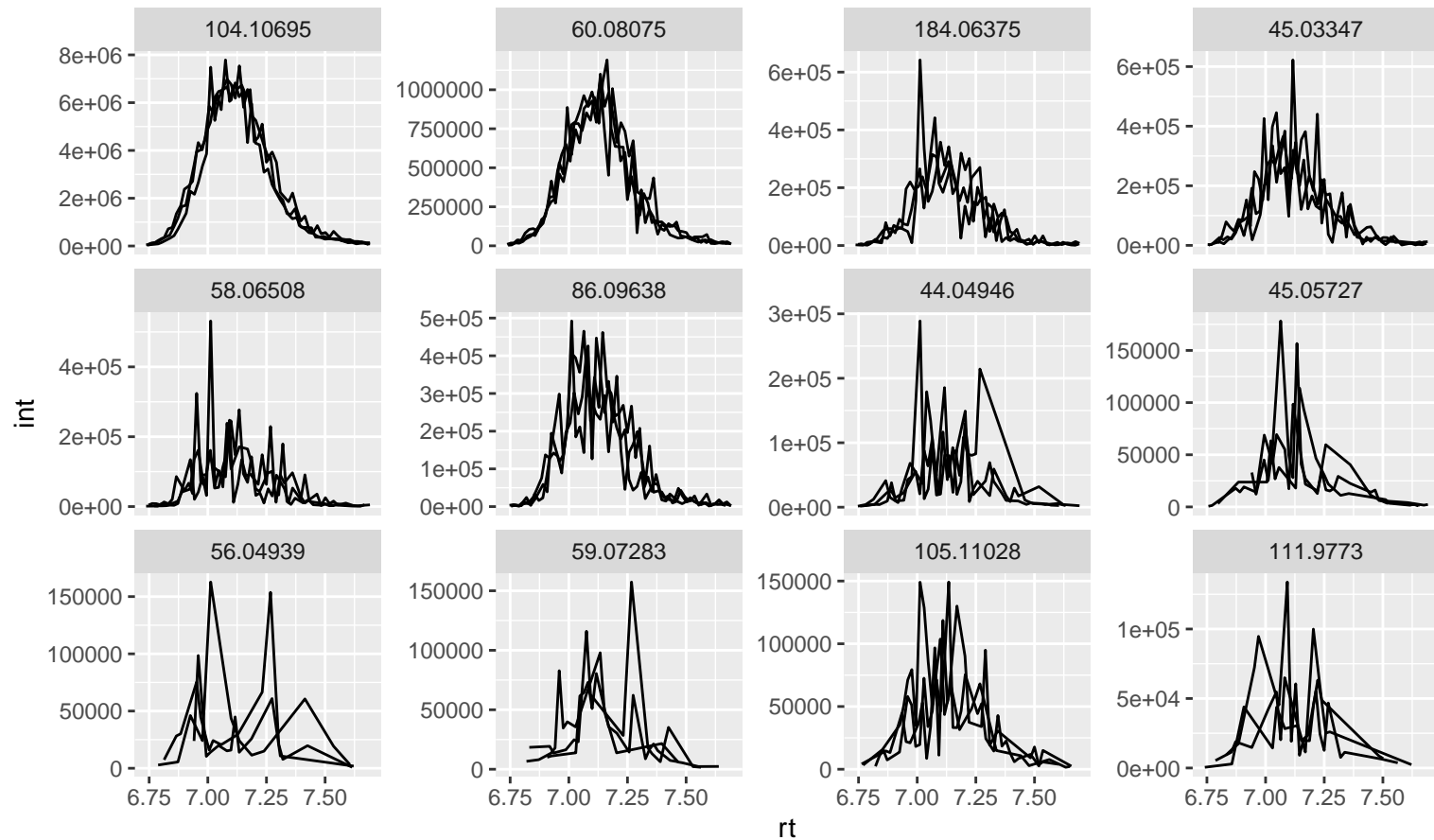
Mannitol (neg) 181.071764

int

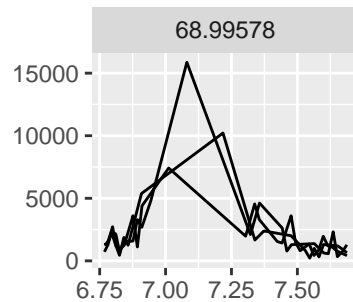
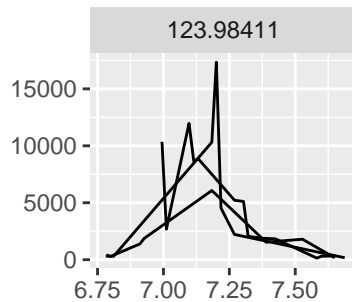
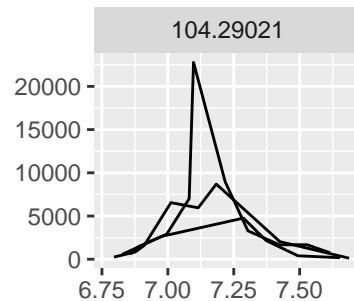
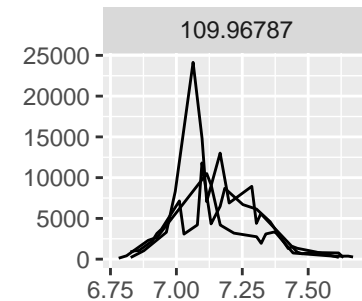
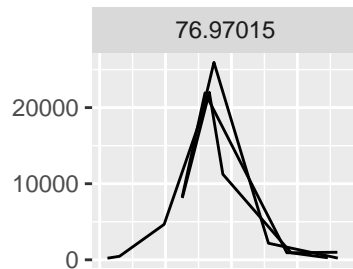
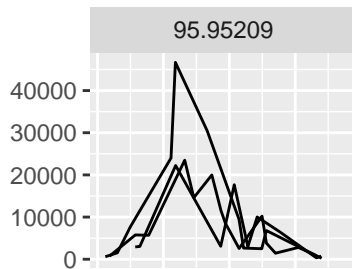
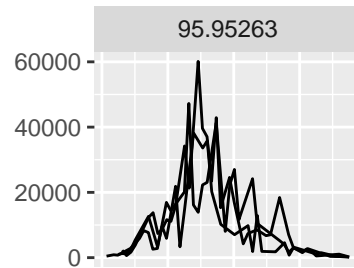
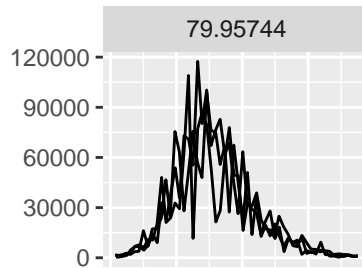
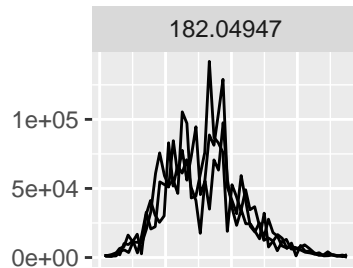
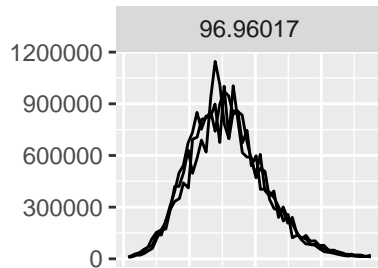


rt

Choline sulfate (pos) 184.063807



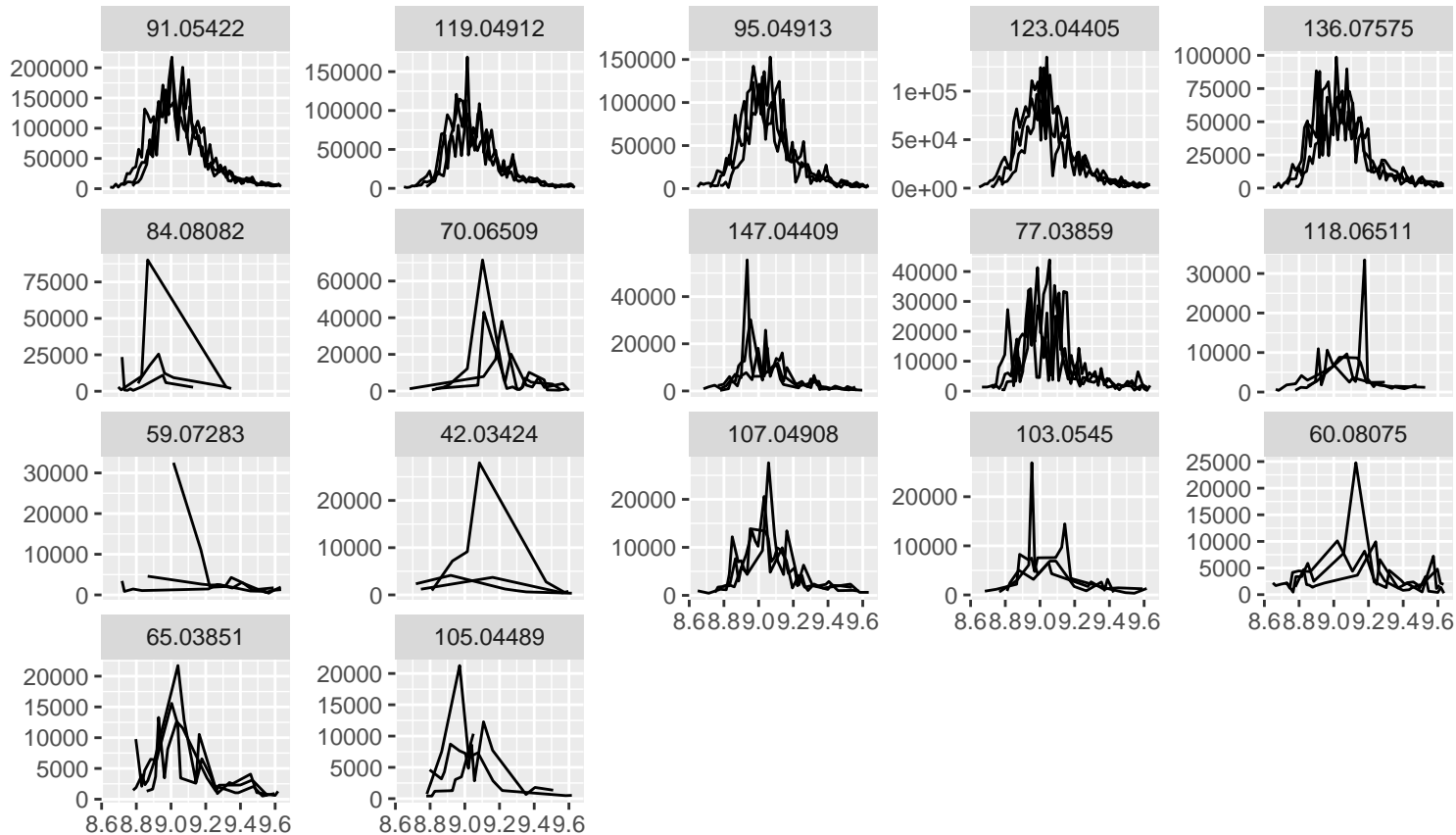
Choline sulfate (neg) 182.049255



rt

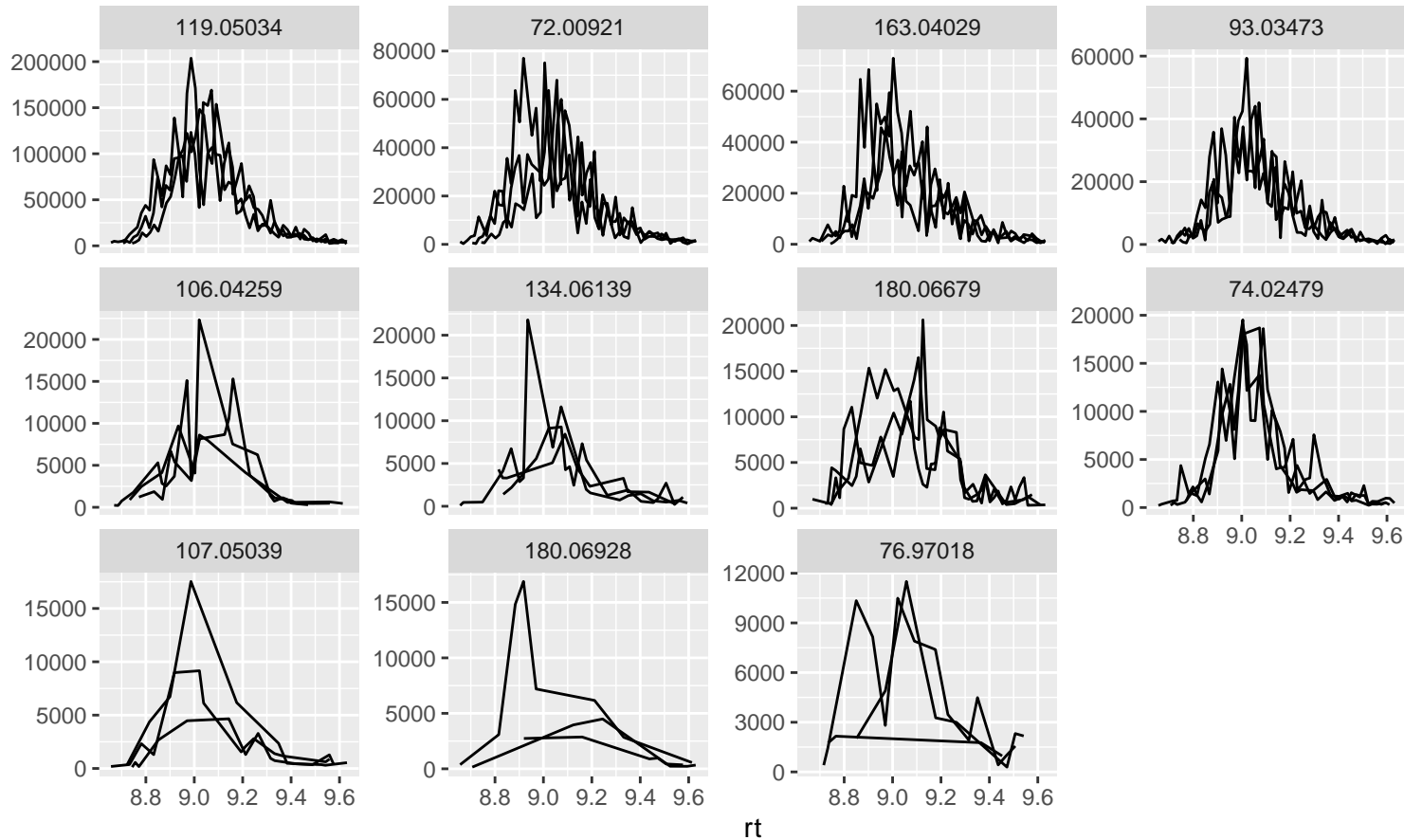
L-Tyrosine (pos) 182.08117

int



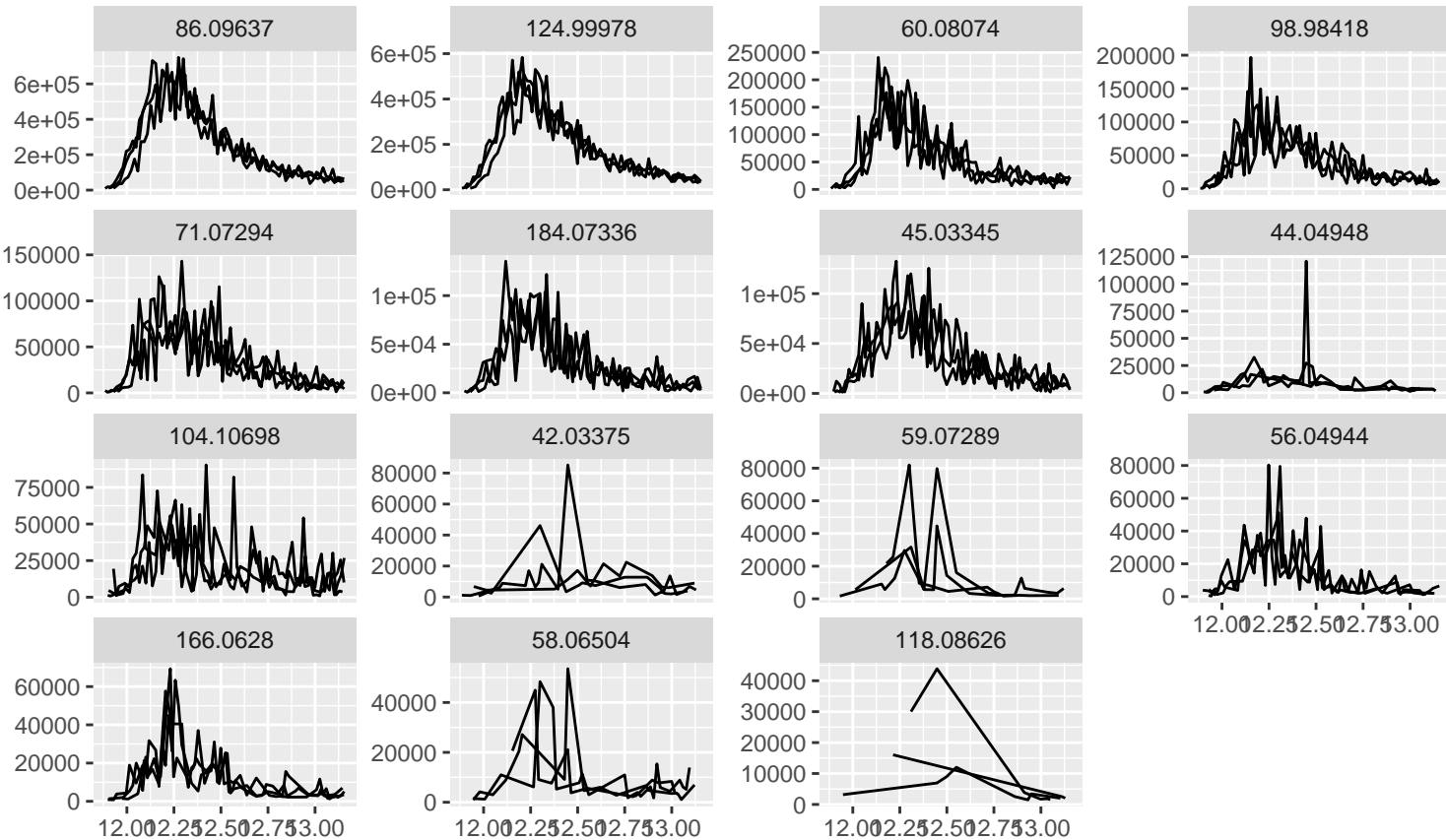
rt

L-Tyrosine (neg) 180.06618



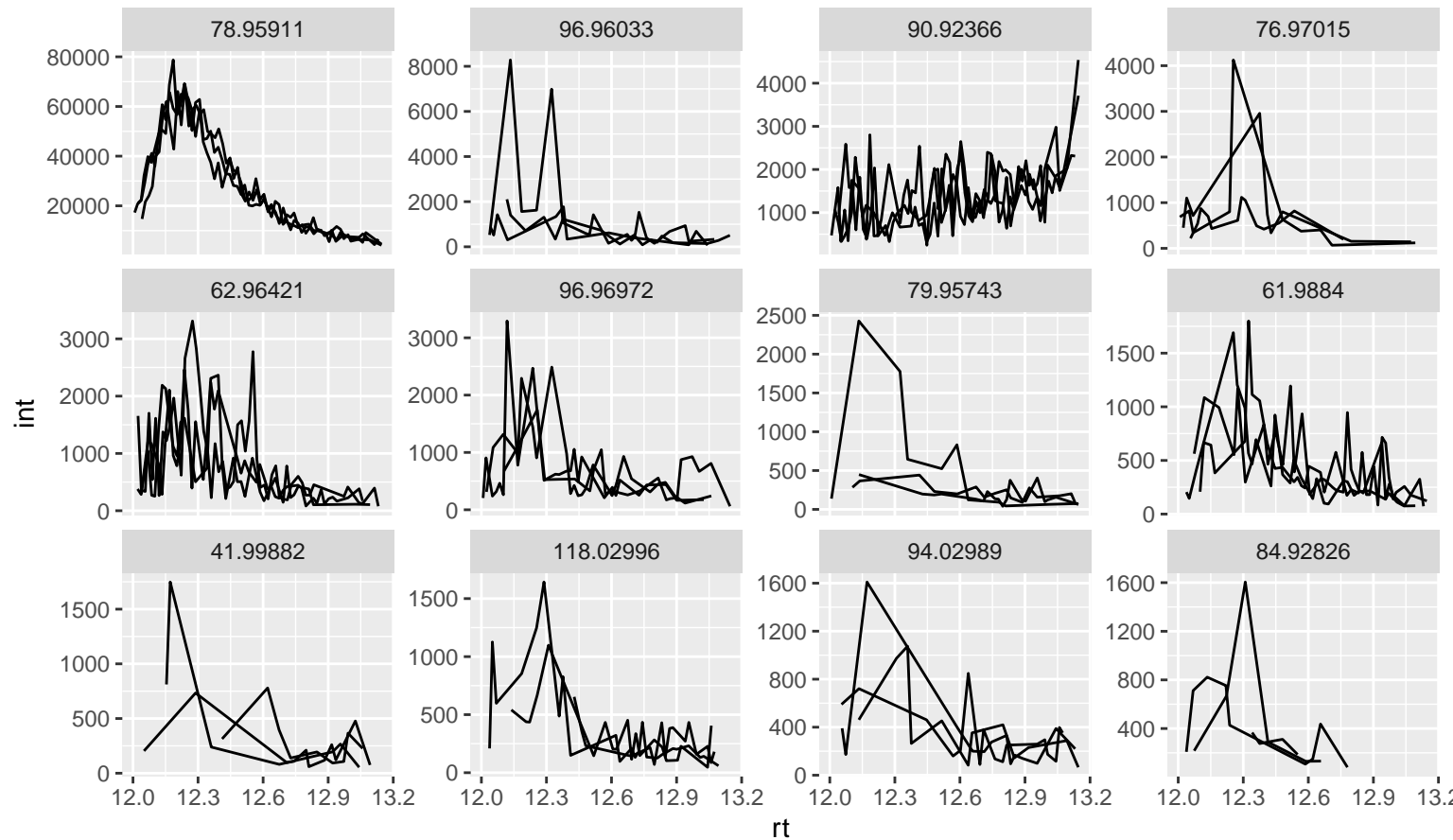
Phosphocholine (pos) 184.07323

int

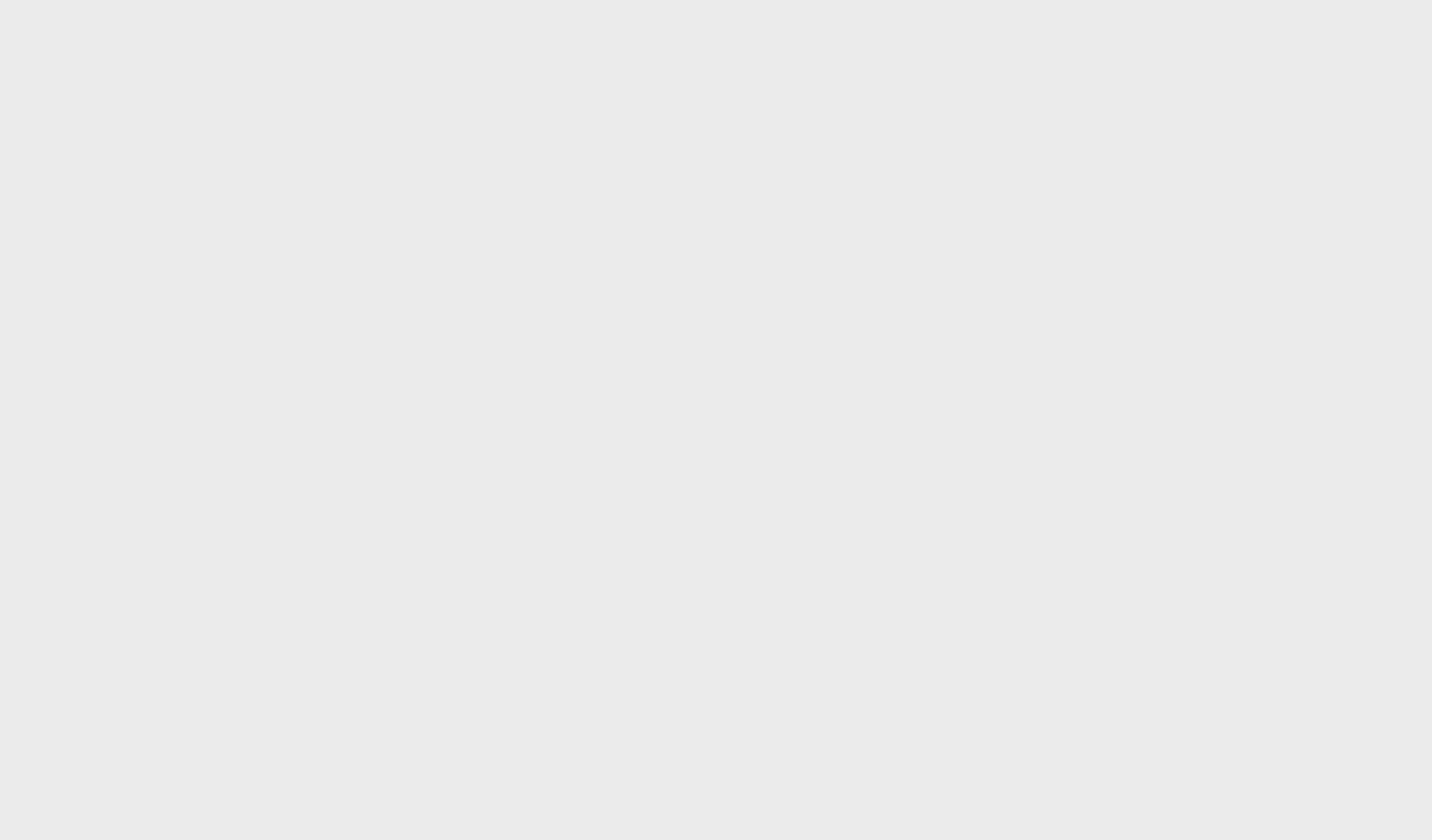


rt

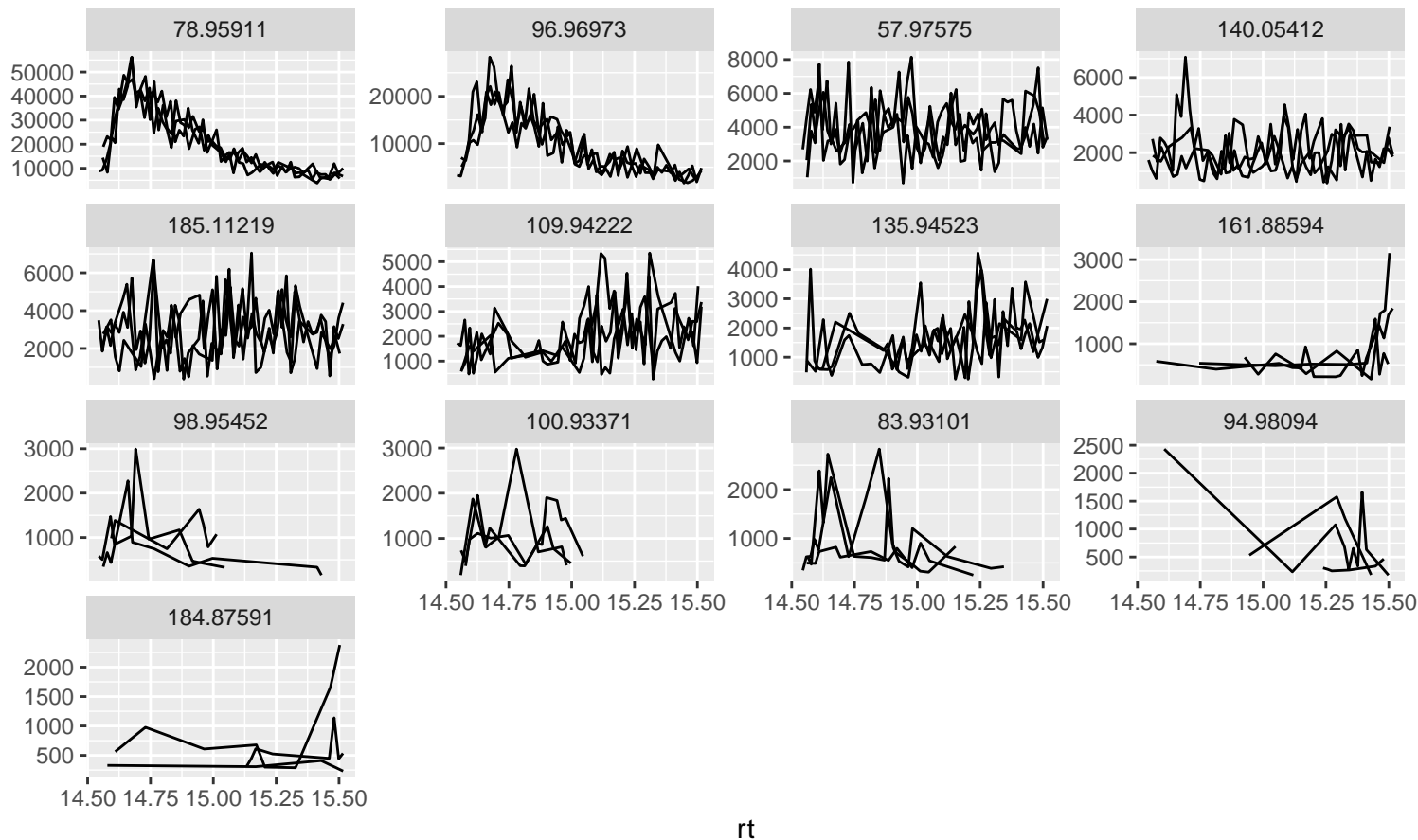
Phosphocholine (neg) 182.058771



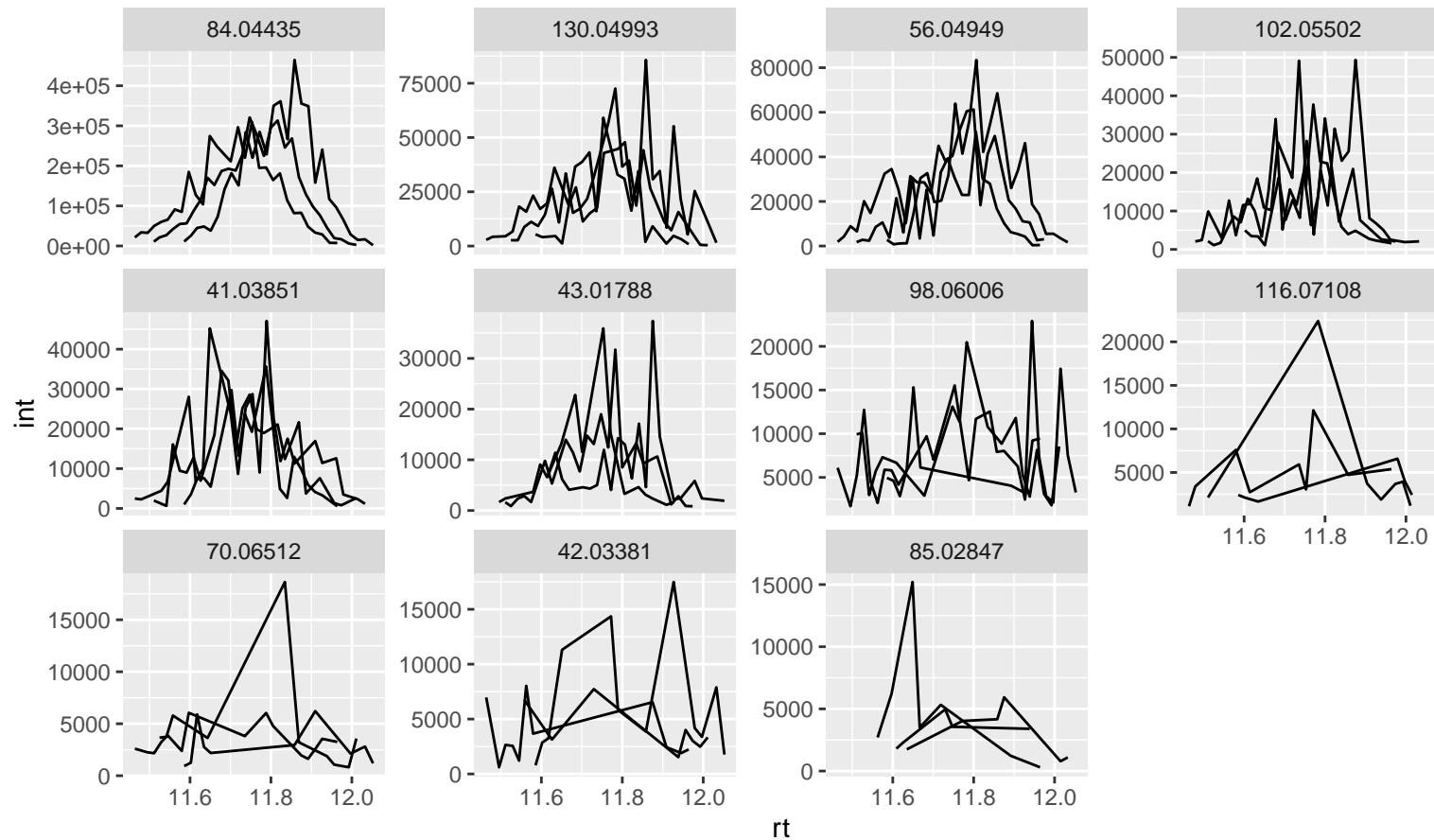
3-Phosphoglycerate (pos) 187.000219



3-Phosphoglycerate (neg) 184.985667

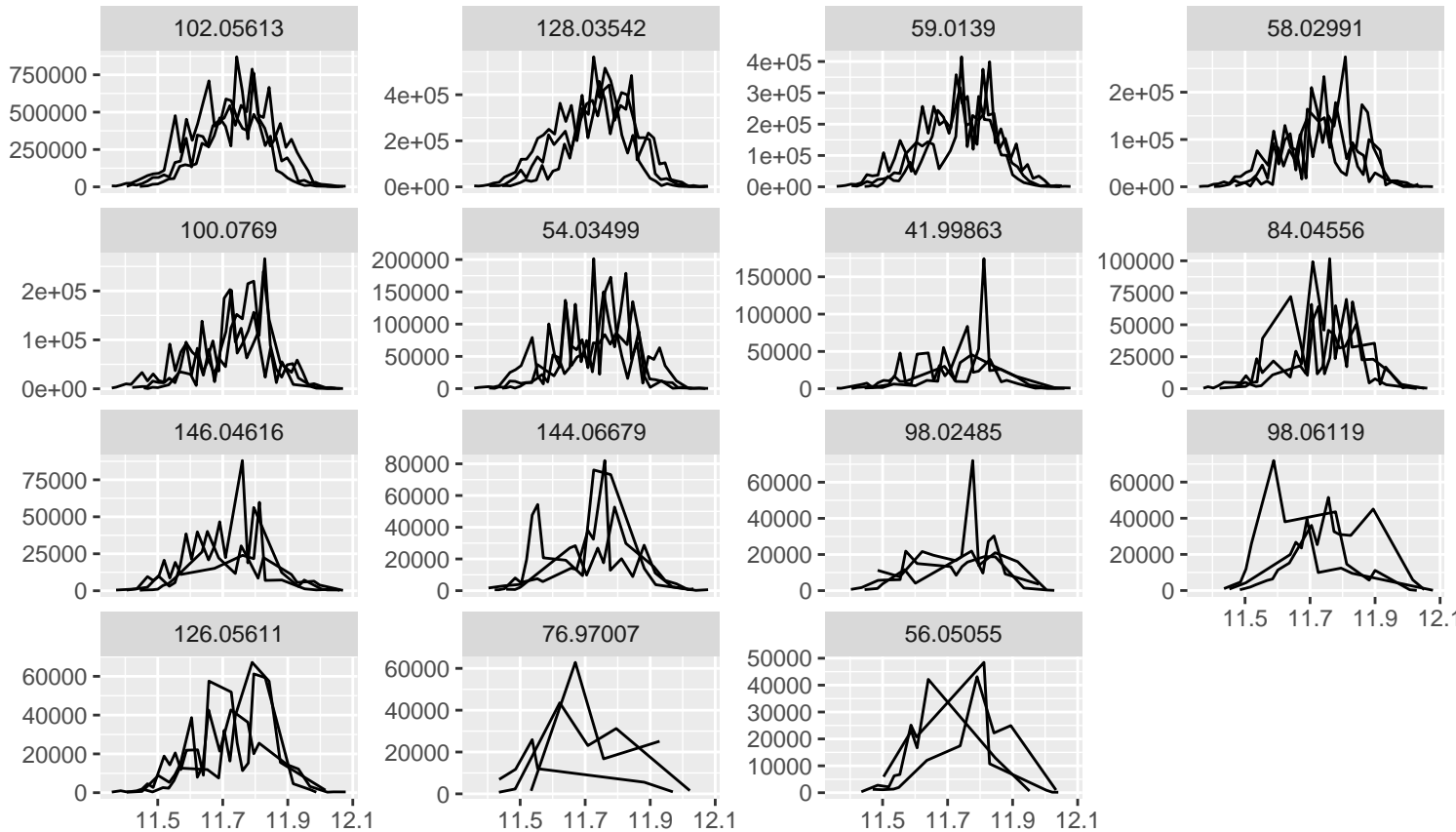


N-Acetyl-L-glutamic acid (pos) 190.071



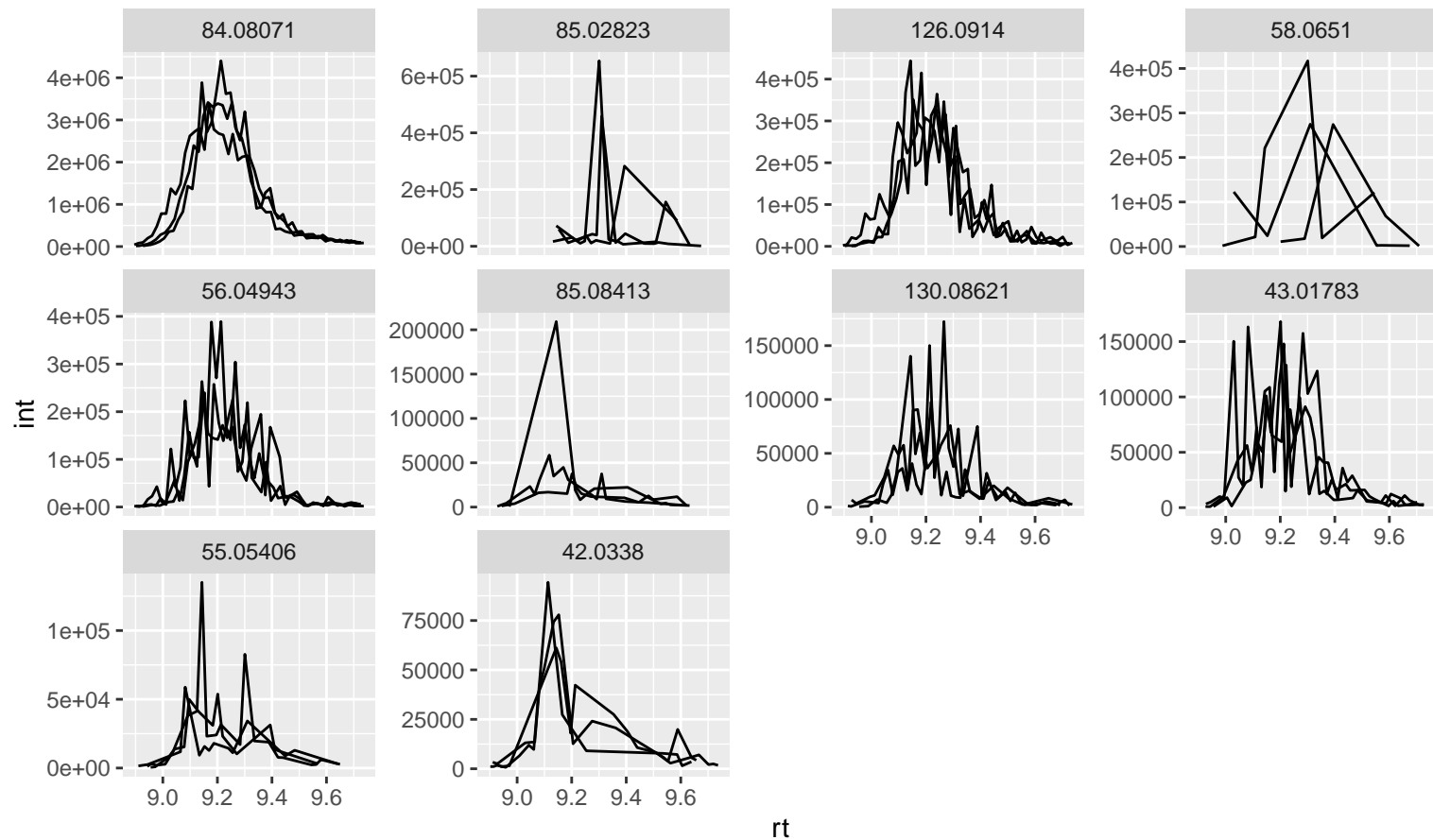
N-Acetyl-L-glutamic acid (neg) 188.056448

int

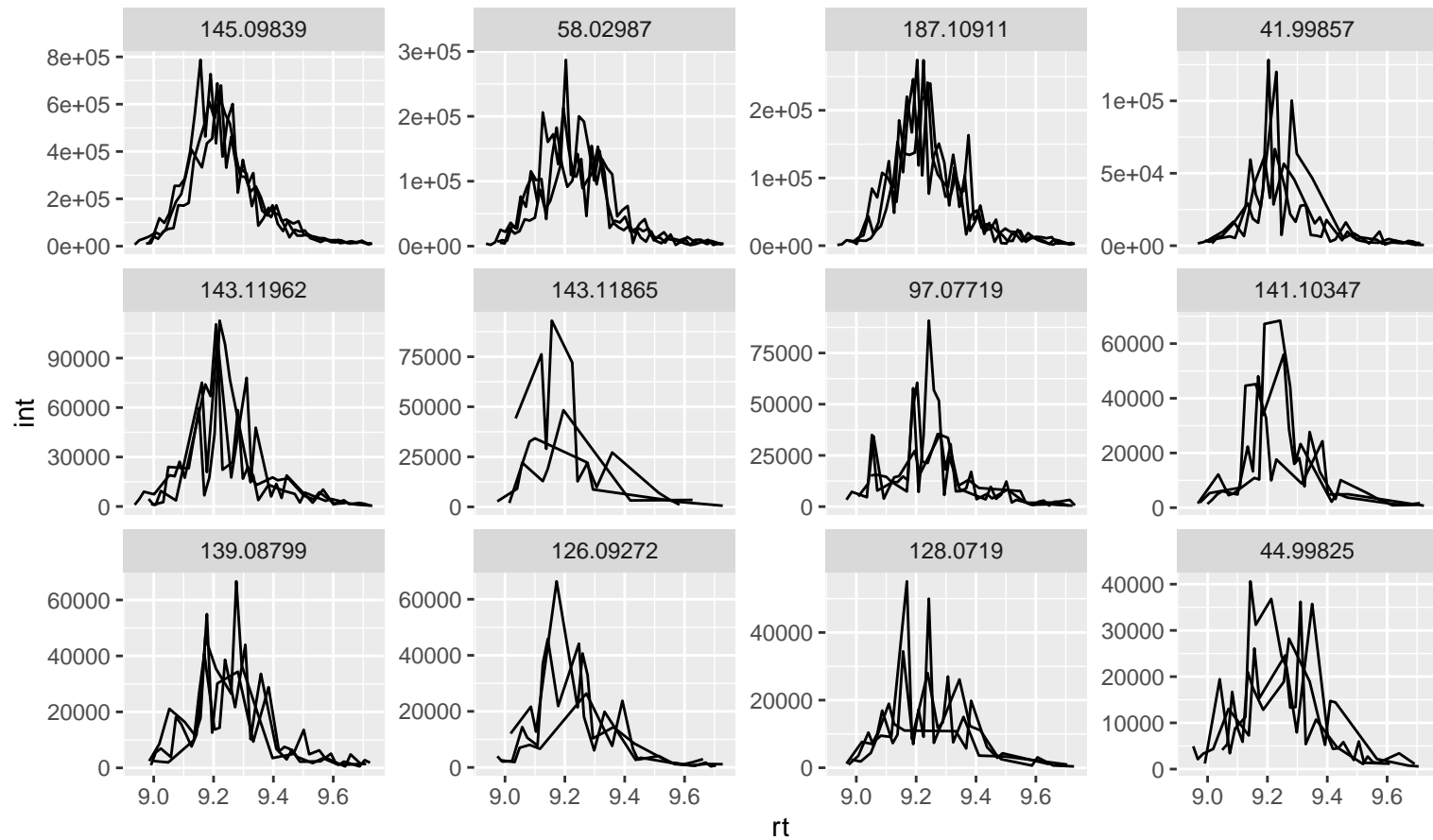


rt

N6-Acetyl-L-lysine (pos) 189.123369

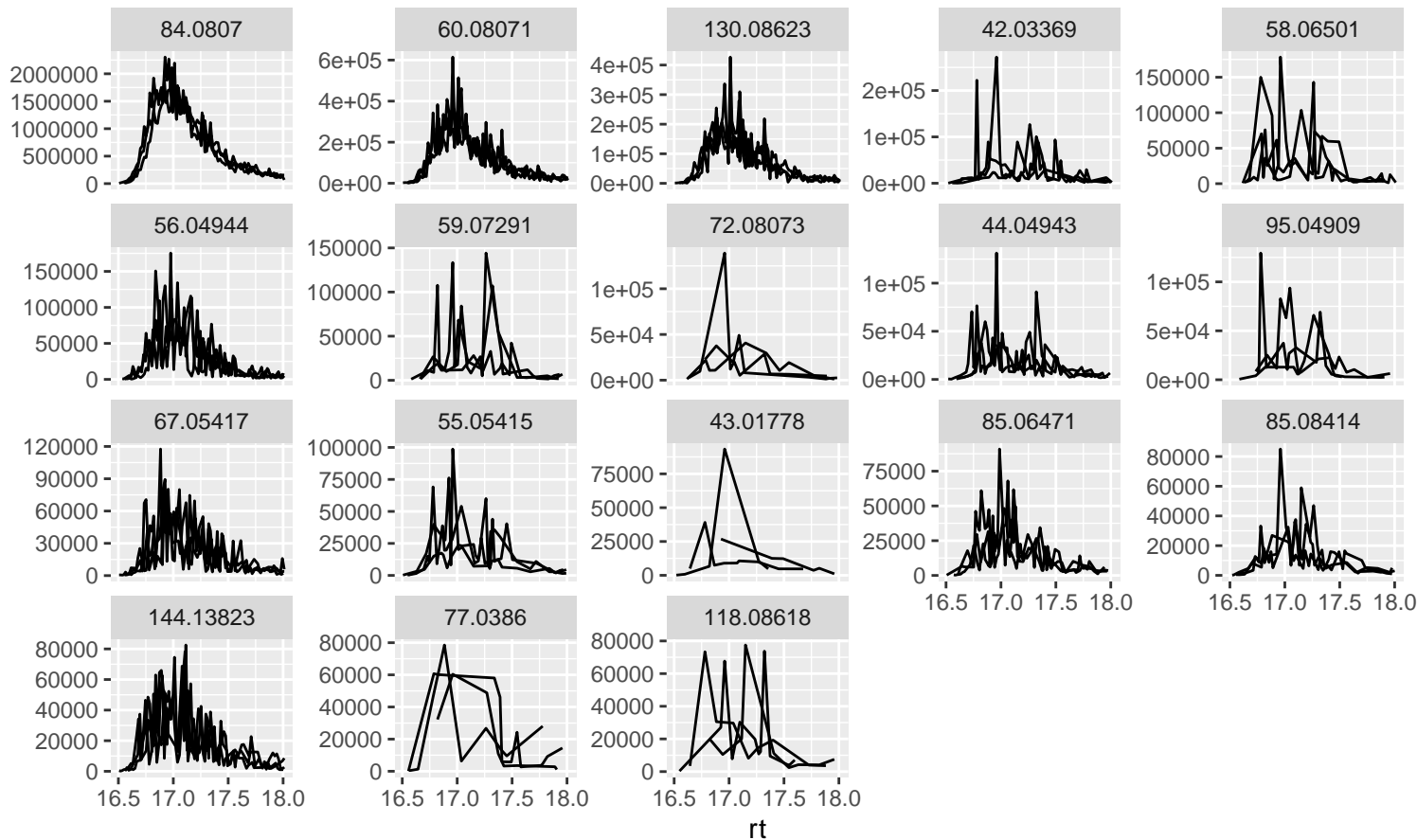


N6-Acetyl-L-lysine (neg) 187.108817

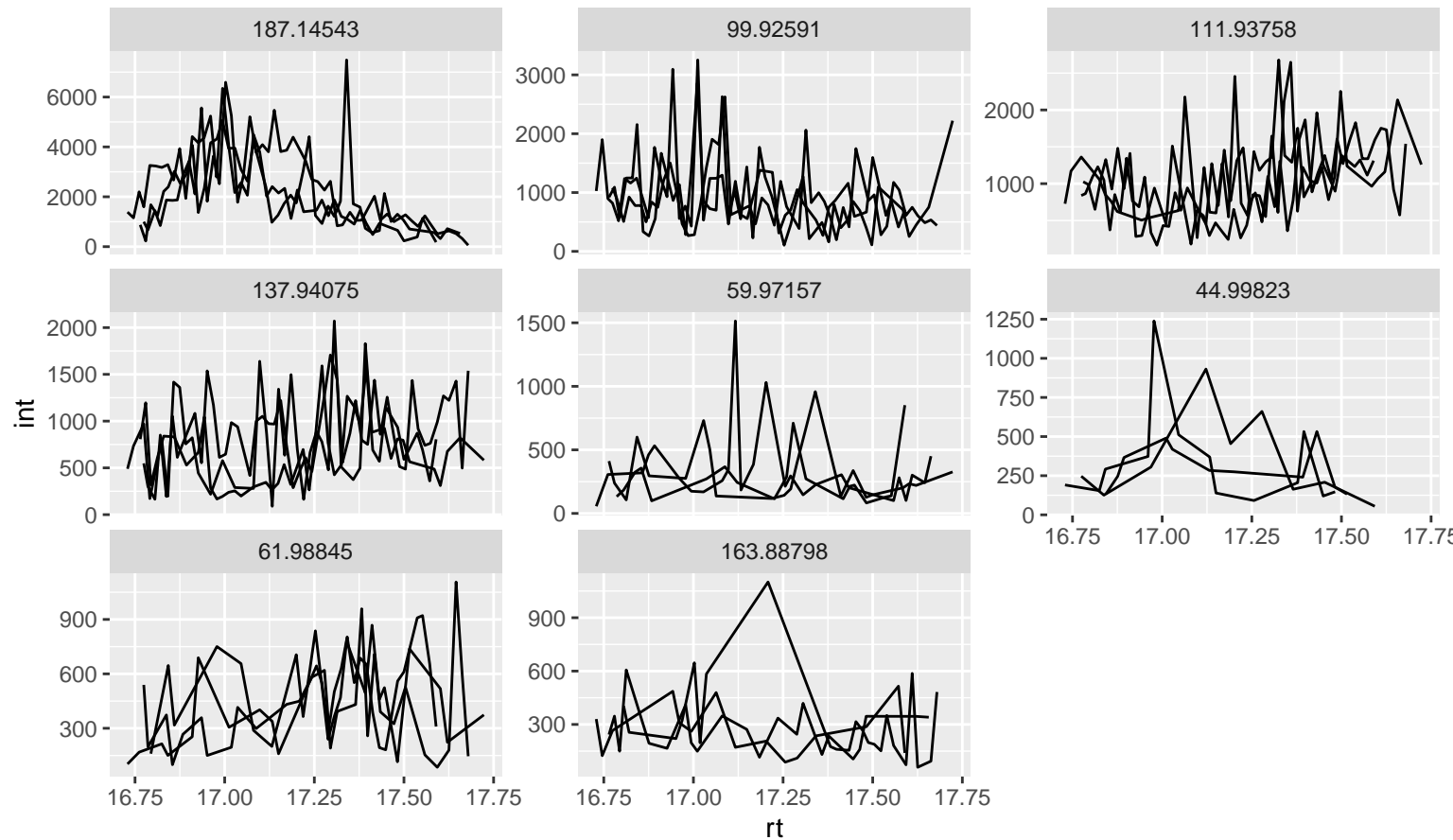


N6,N6,N6-Trimethyl-L-lysine (pos) 189.159754

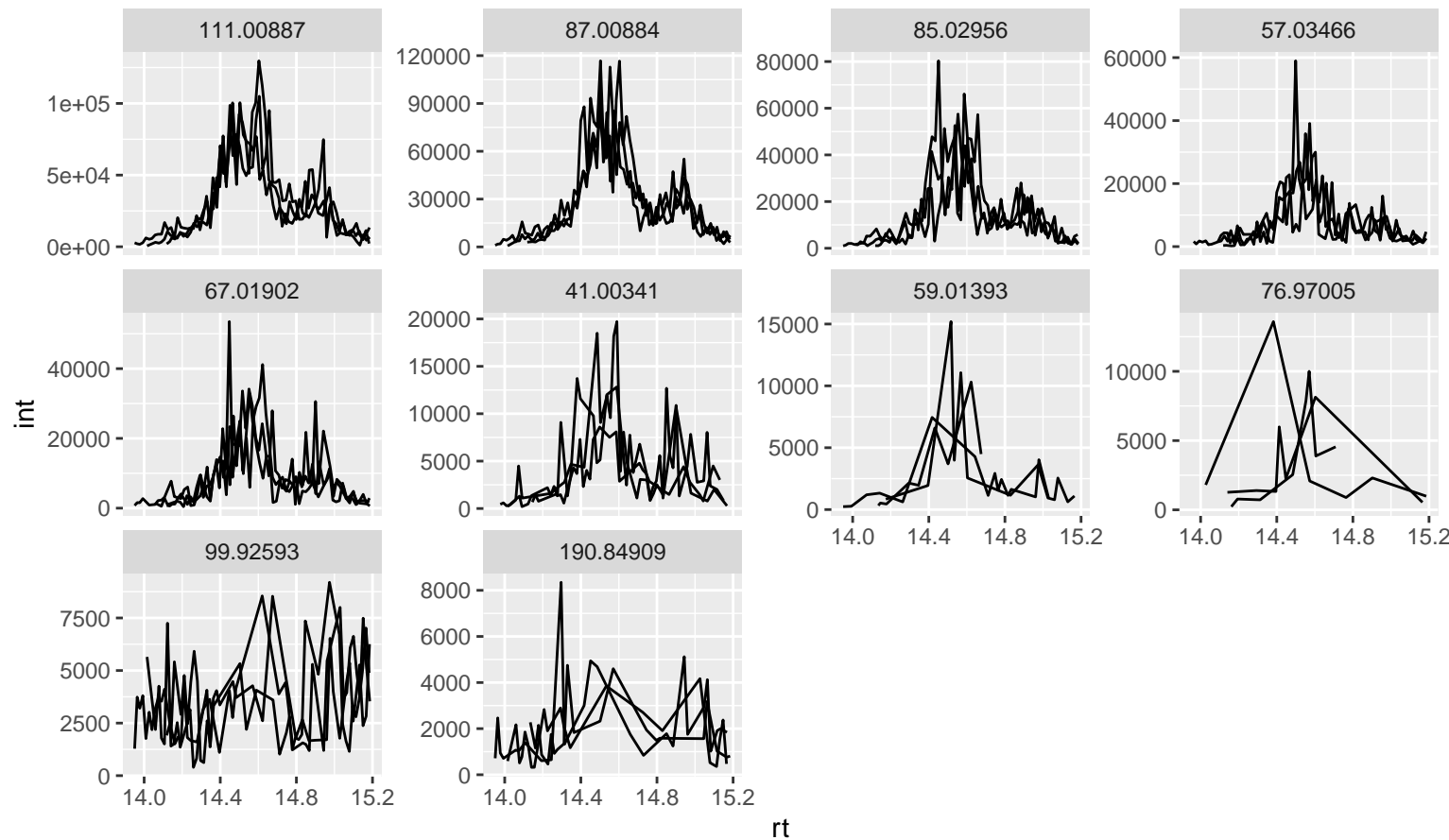
int



N6,N6,N6-Trimethyl-L-lysine (neg) 187.145202

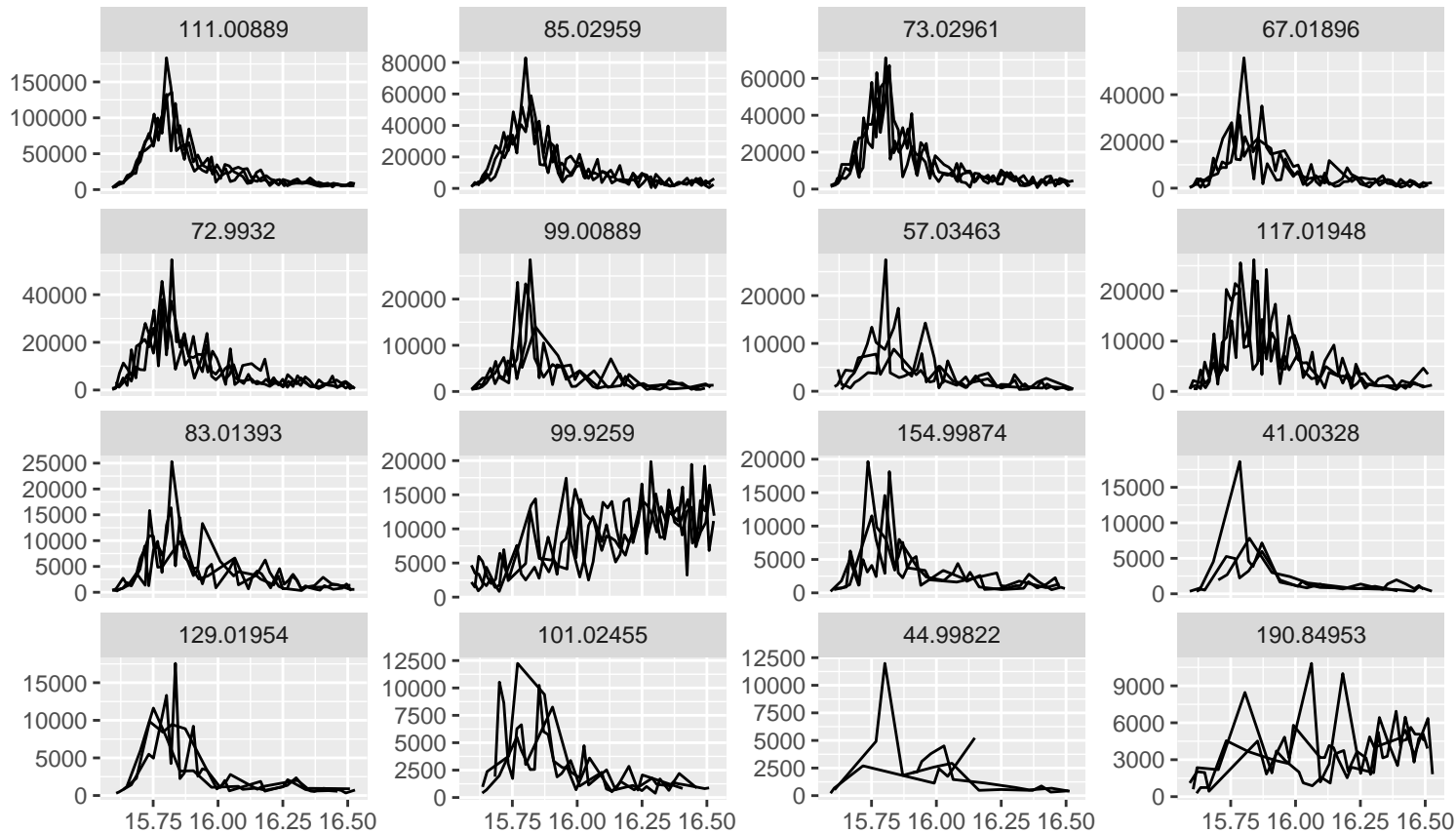


Citric acid (neg) 191.019729



Isocitric acid (neg) 191.019729

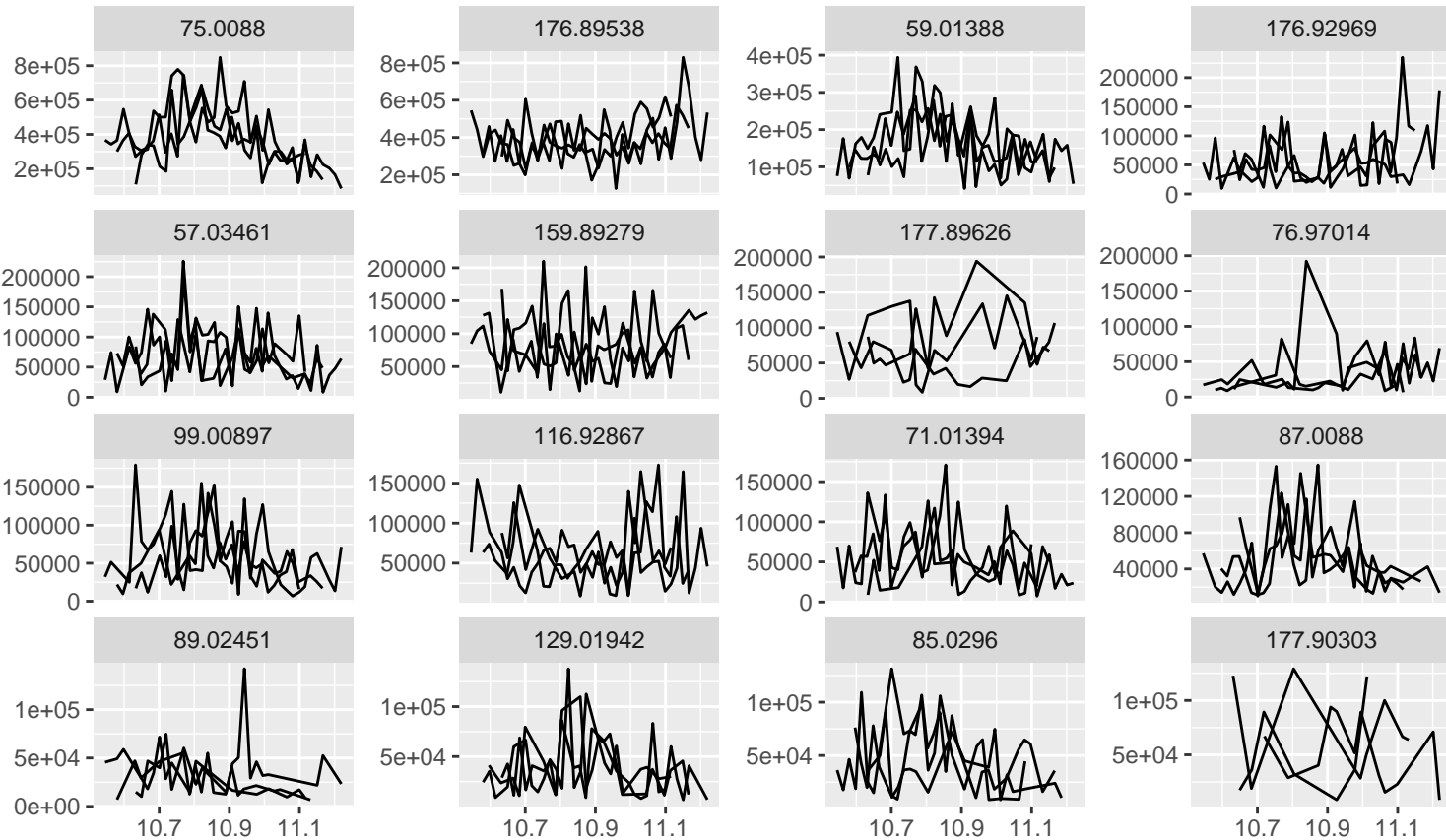
int



rt

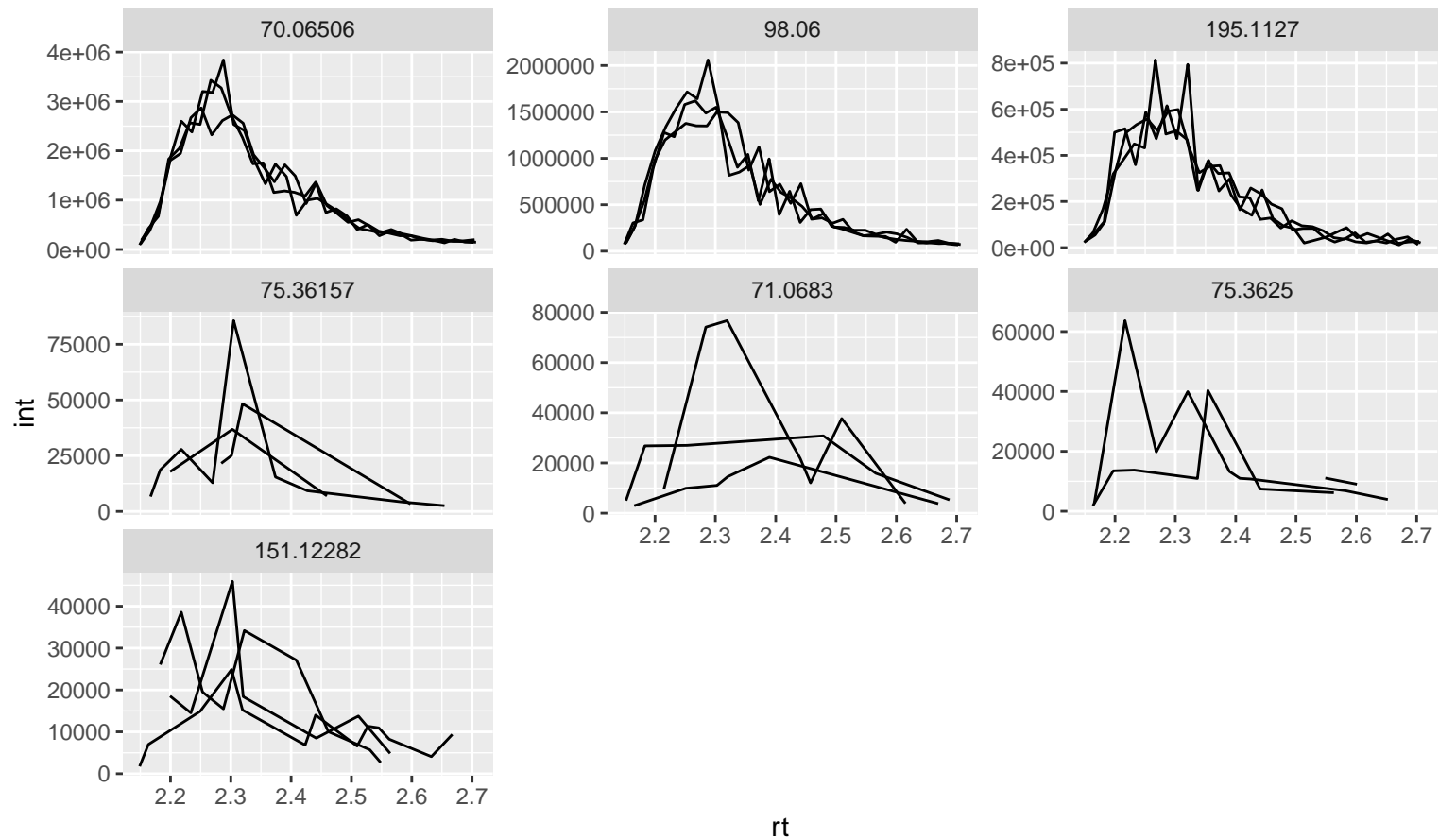
D-Gluconic acid (neg) 195.051029

int



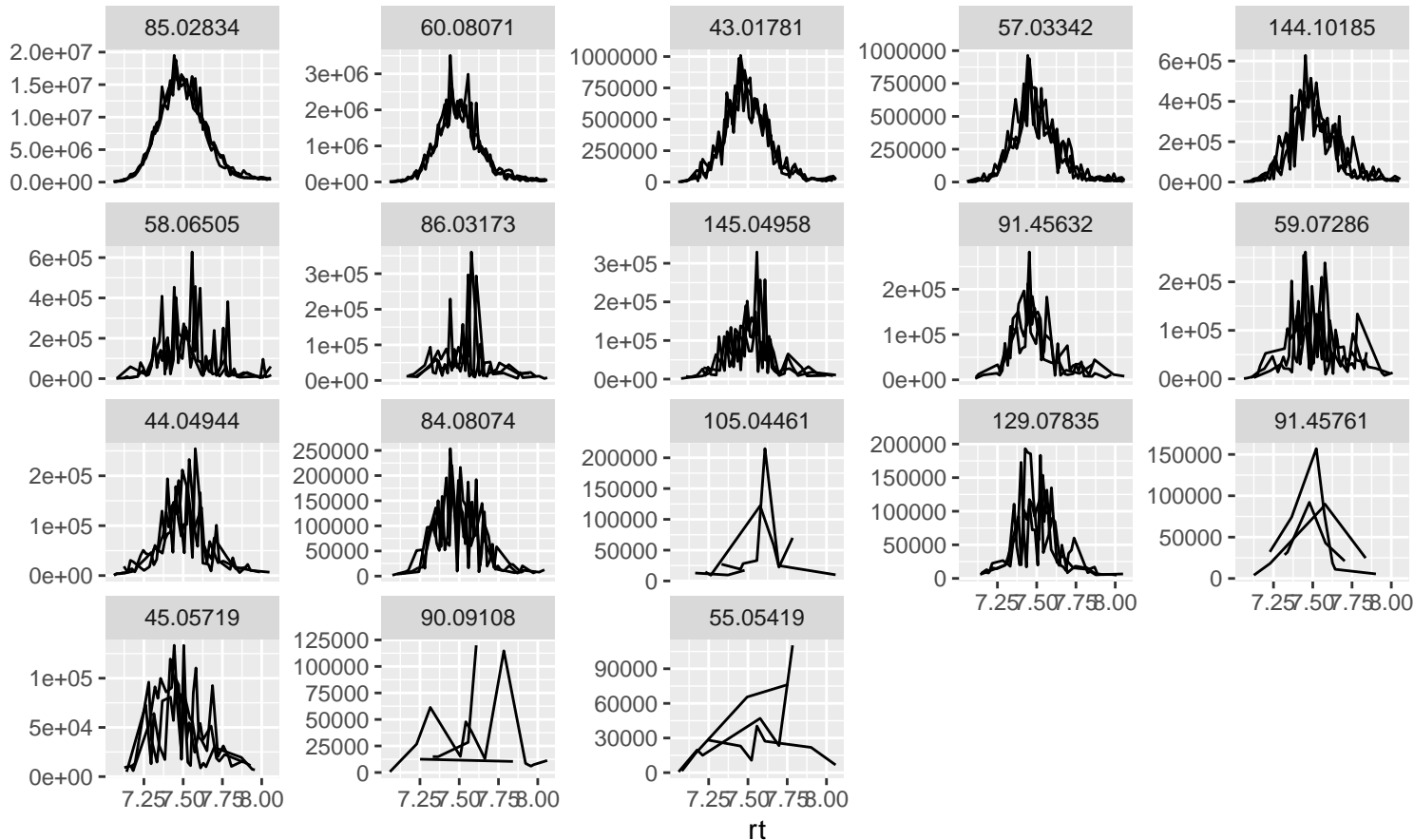
rt

Cyclo(Pro-Pro) (pos) 195.112804

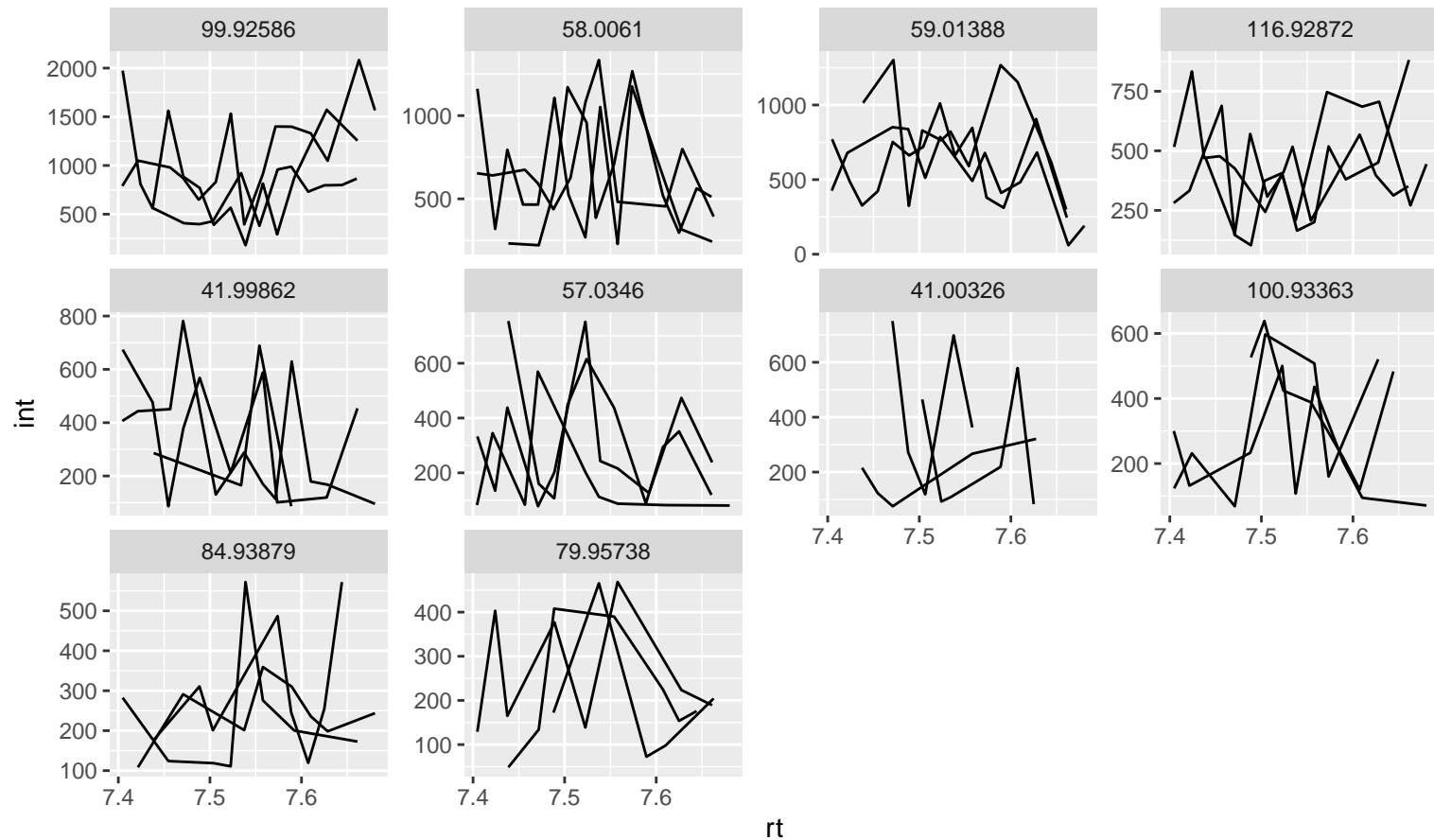


O-Acetylcarnitine (pos) 204.123035

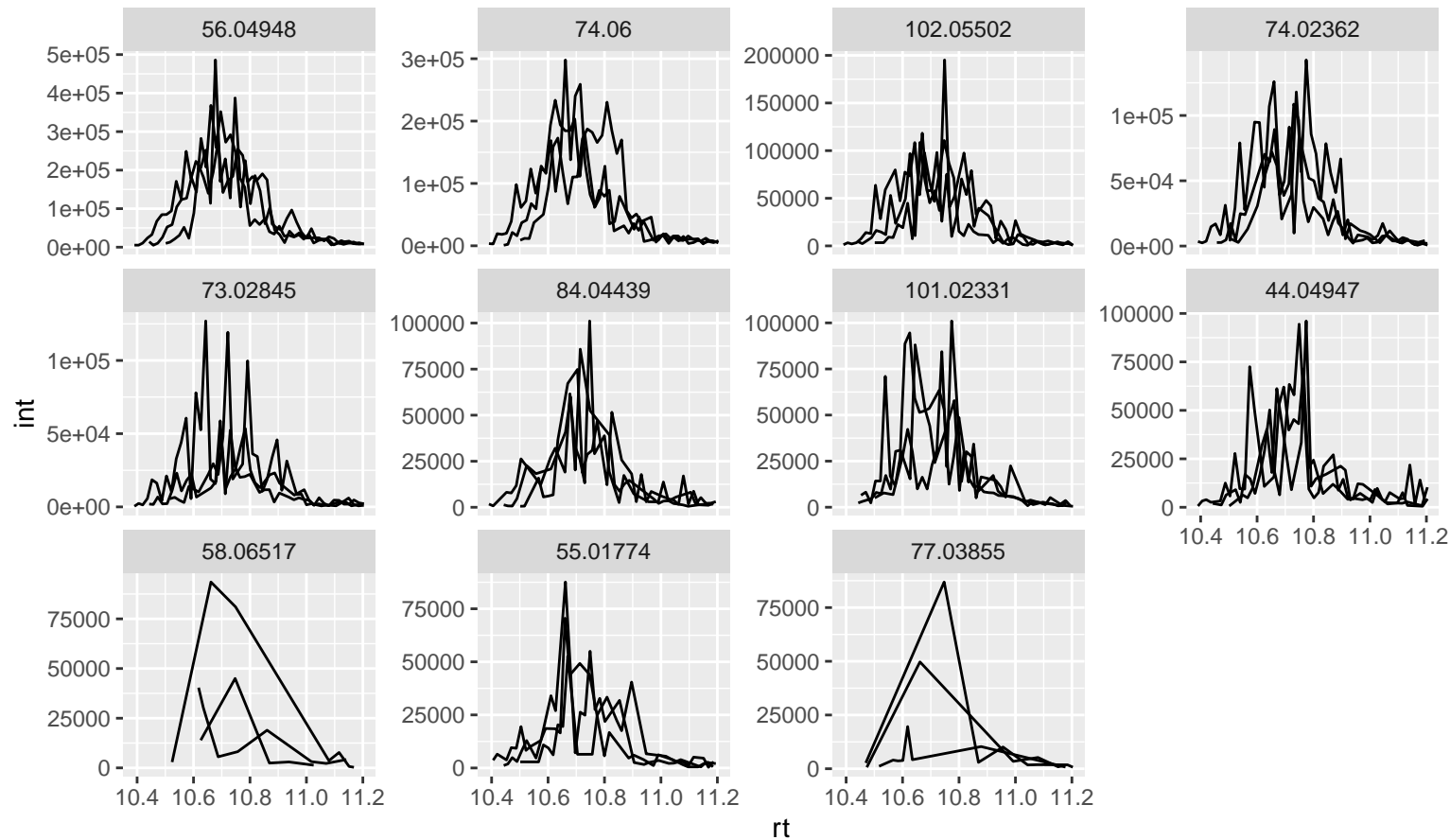
int



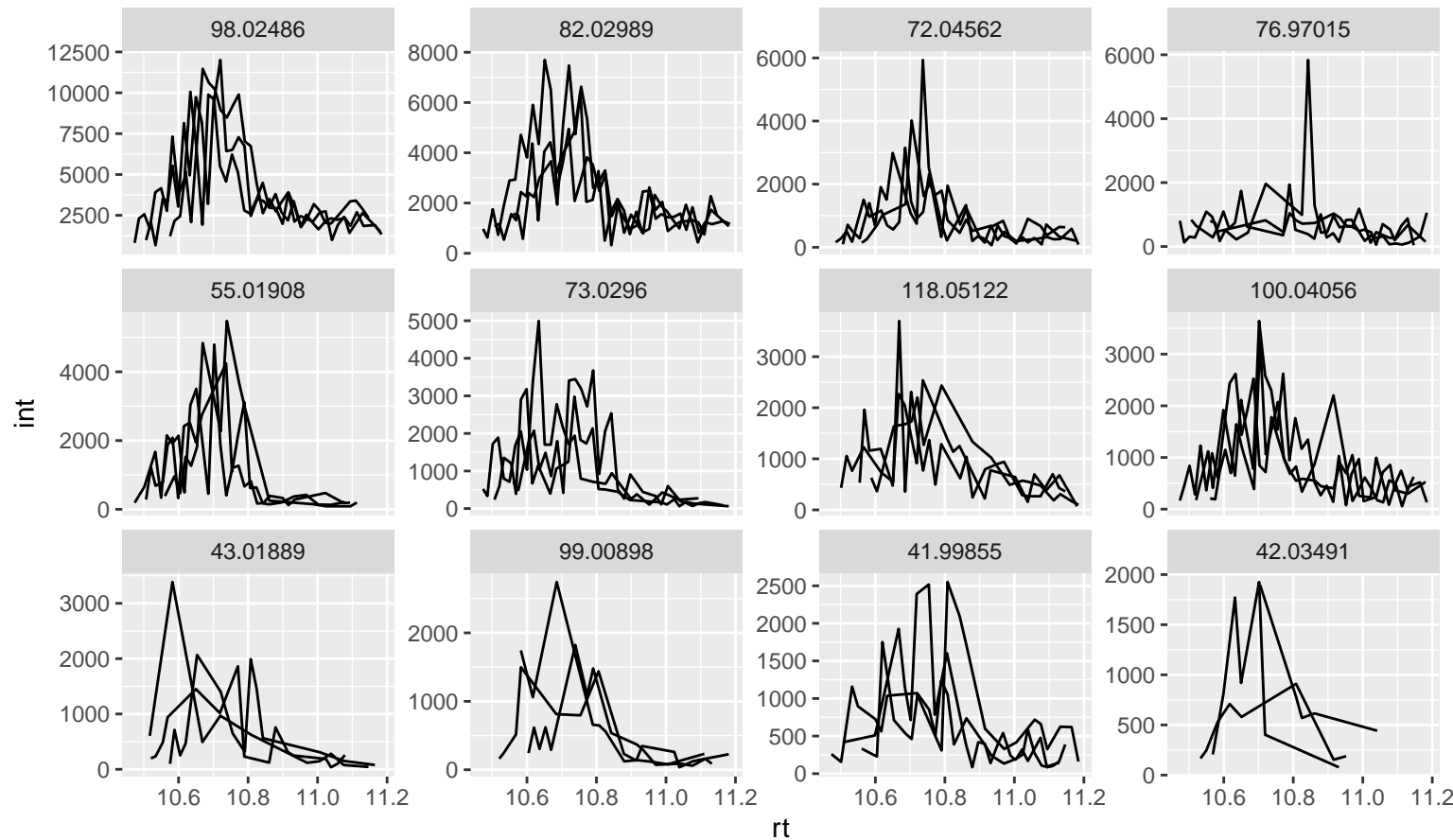
O-Acetylcarnitine (neg) 202.108483



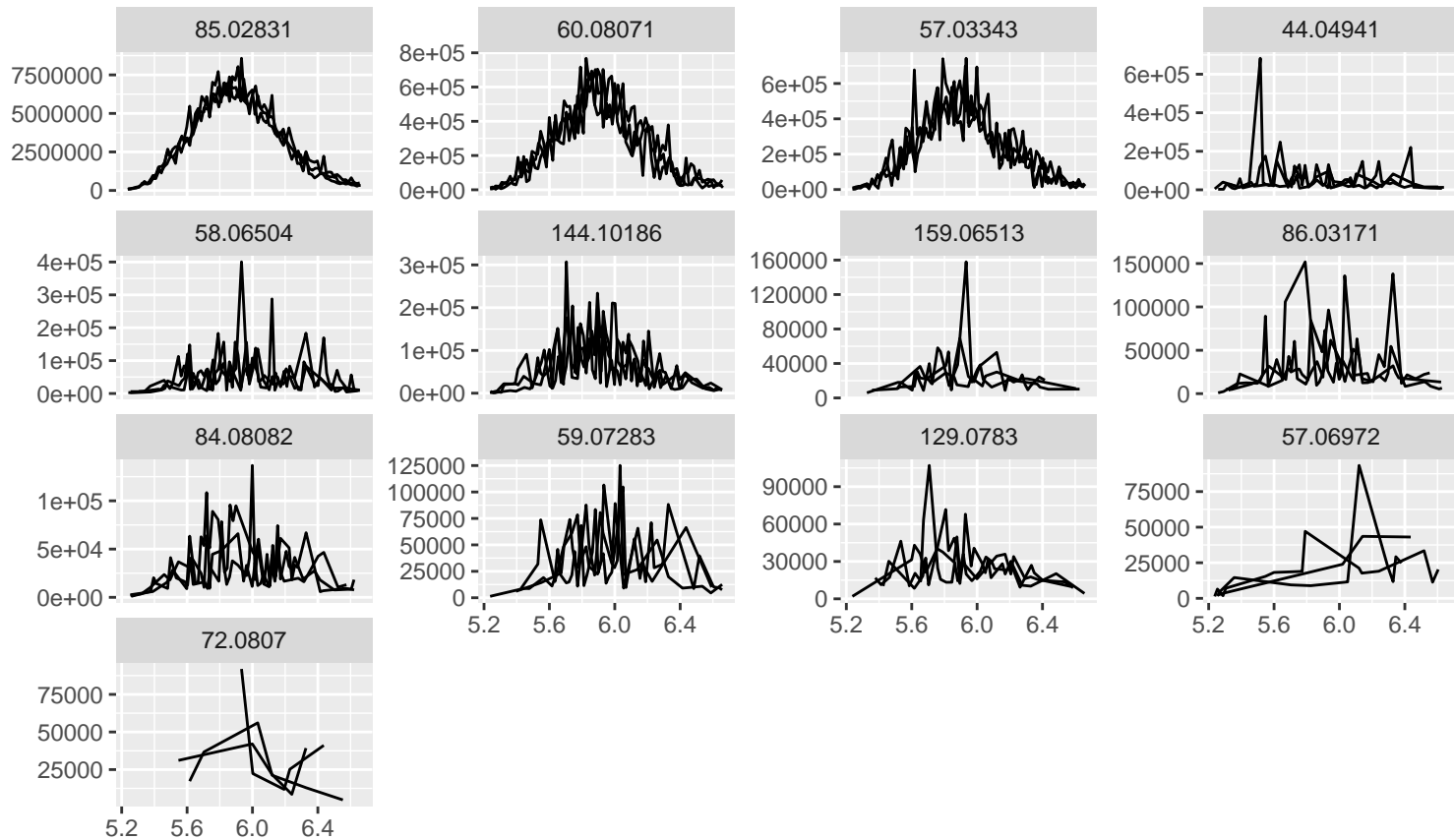
O-Succinylhomoserine (pos) 220.081565



O-Succinylhomoserine (neg) 218.067013



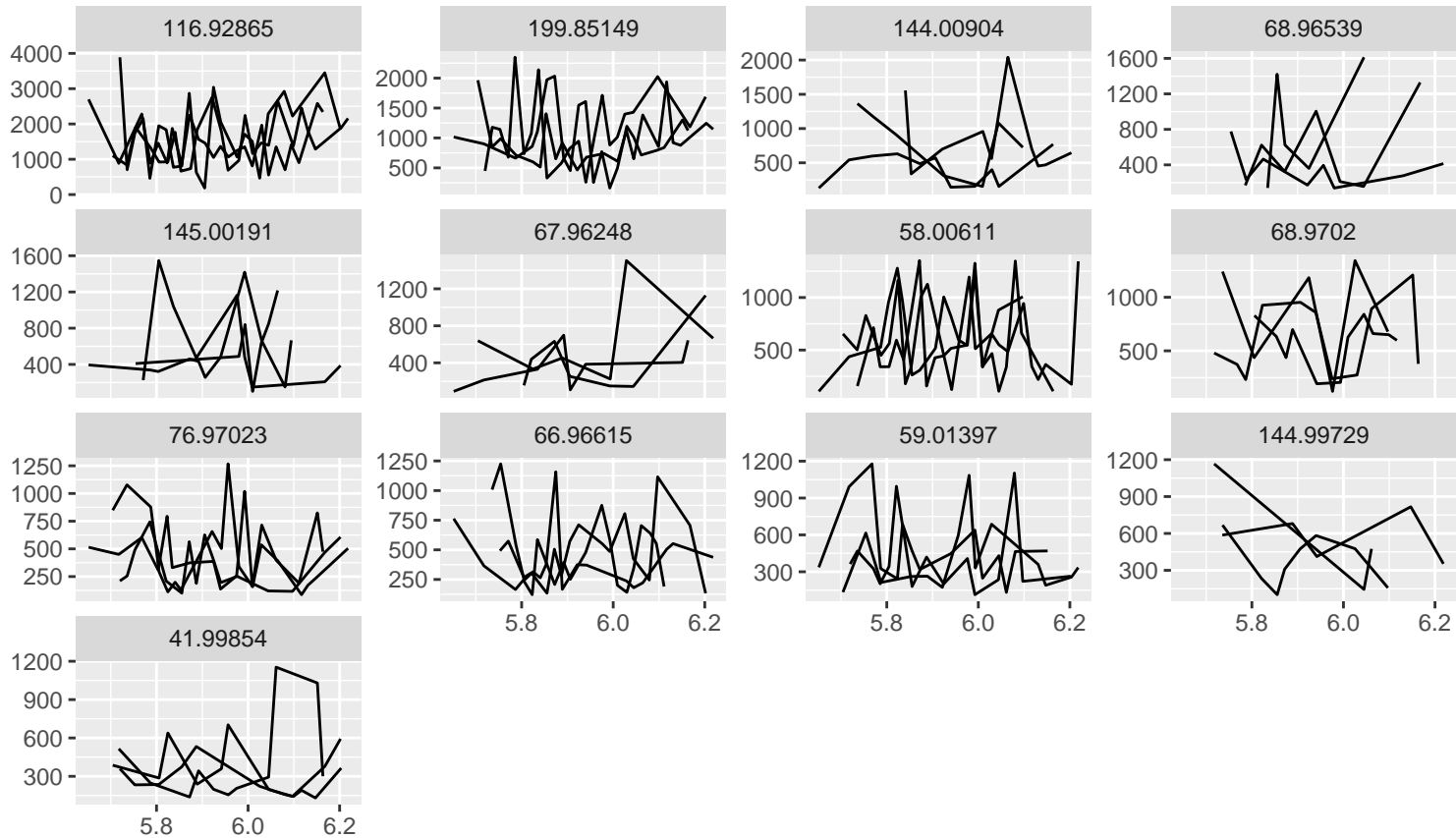
O-Propionylcarnitine (pos) 218.138685



rt

O-Propionylcarnitine (neg) 216.124133

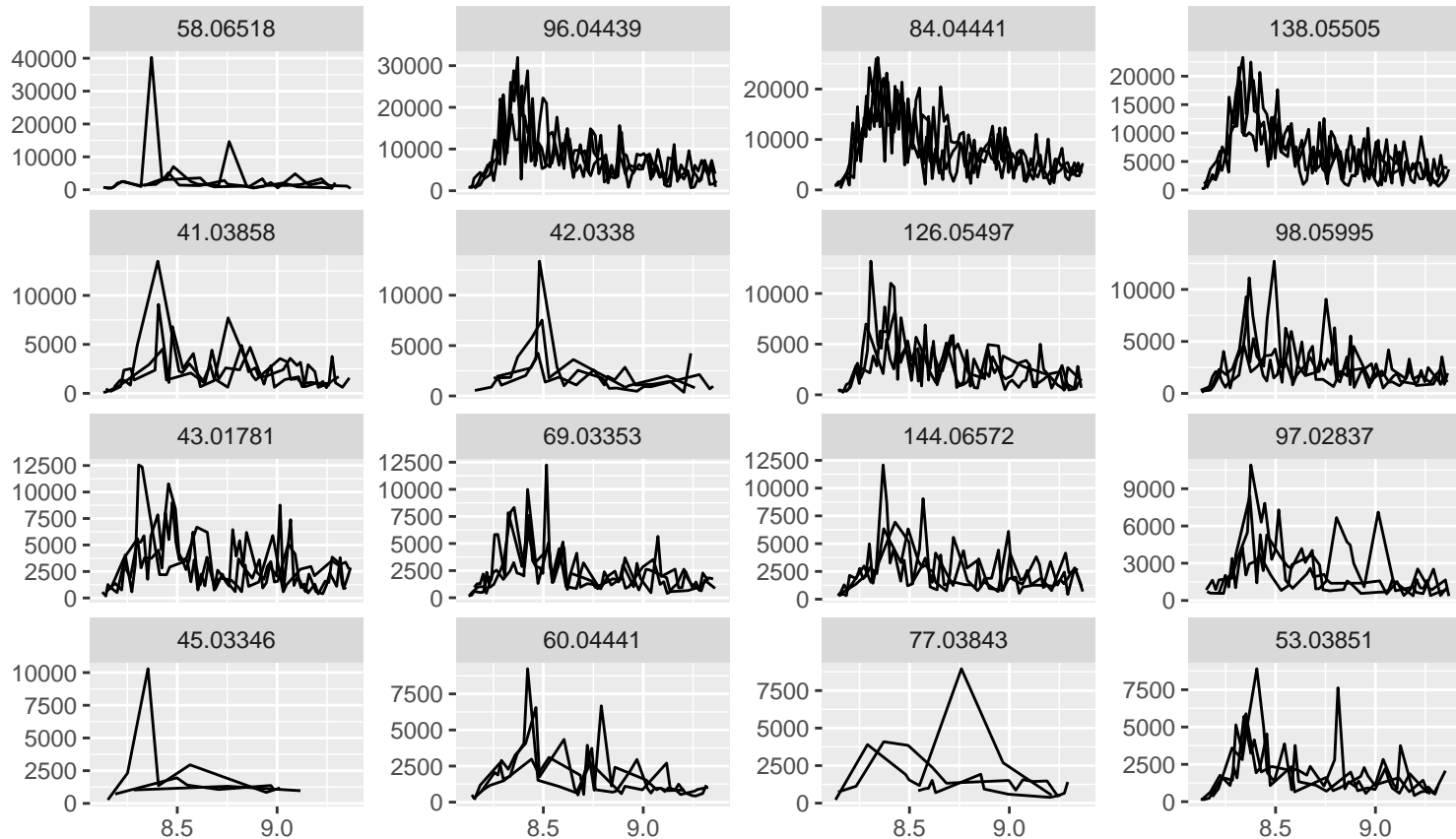
int



rt

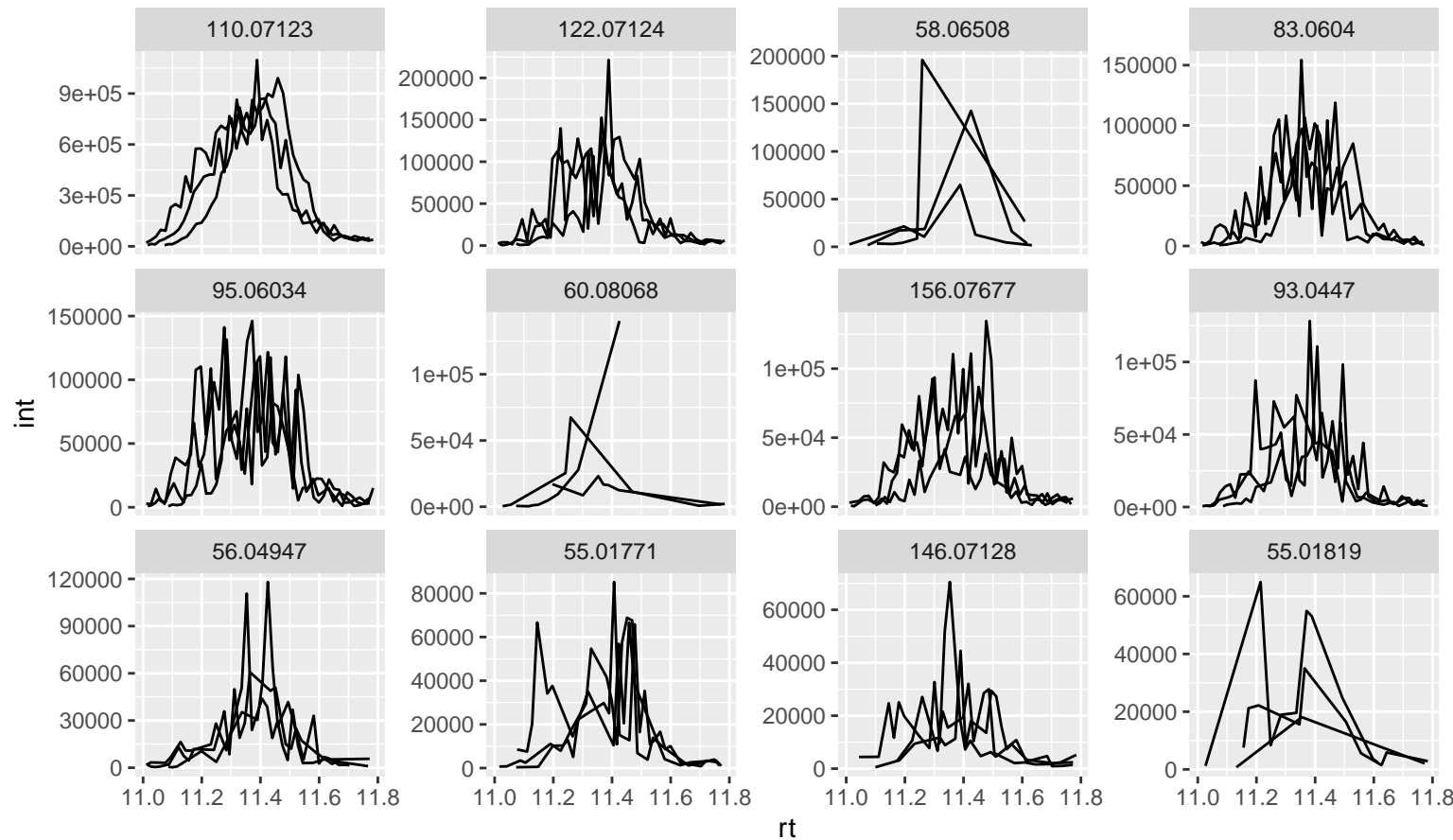
N-Acetyl-D-glucosamine (pos) 222.097215

int



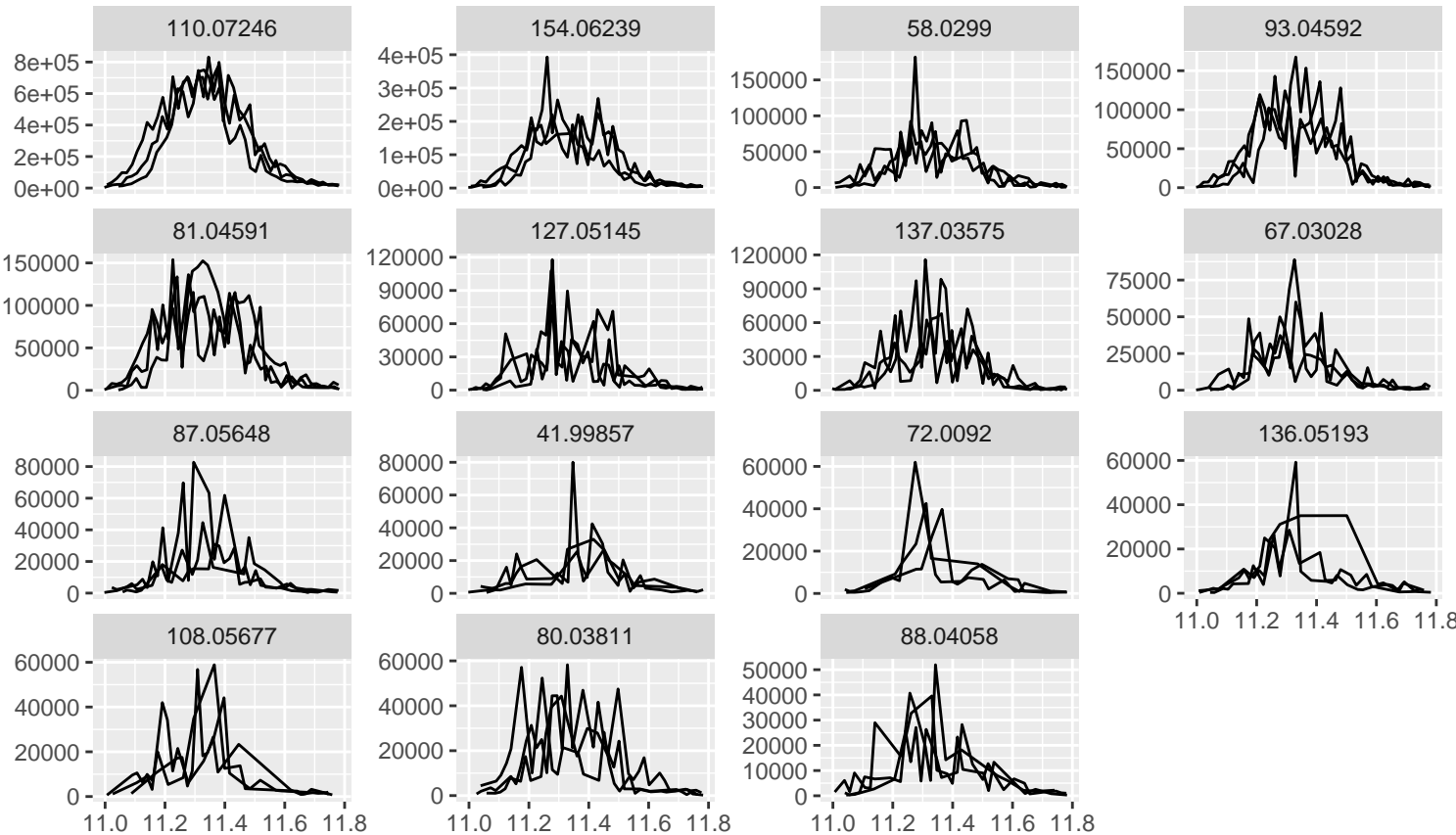
rt

Carnosine (pos) 227.113867



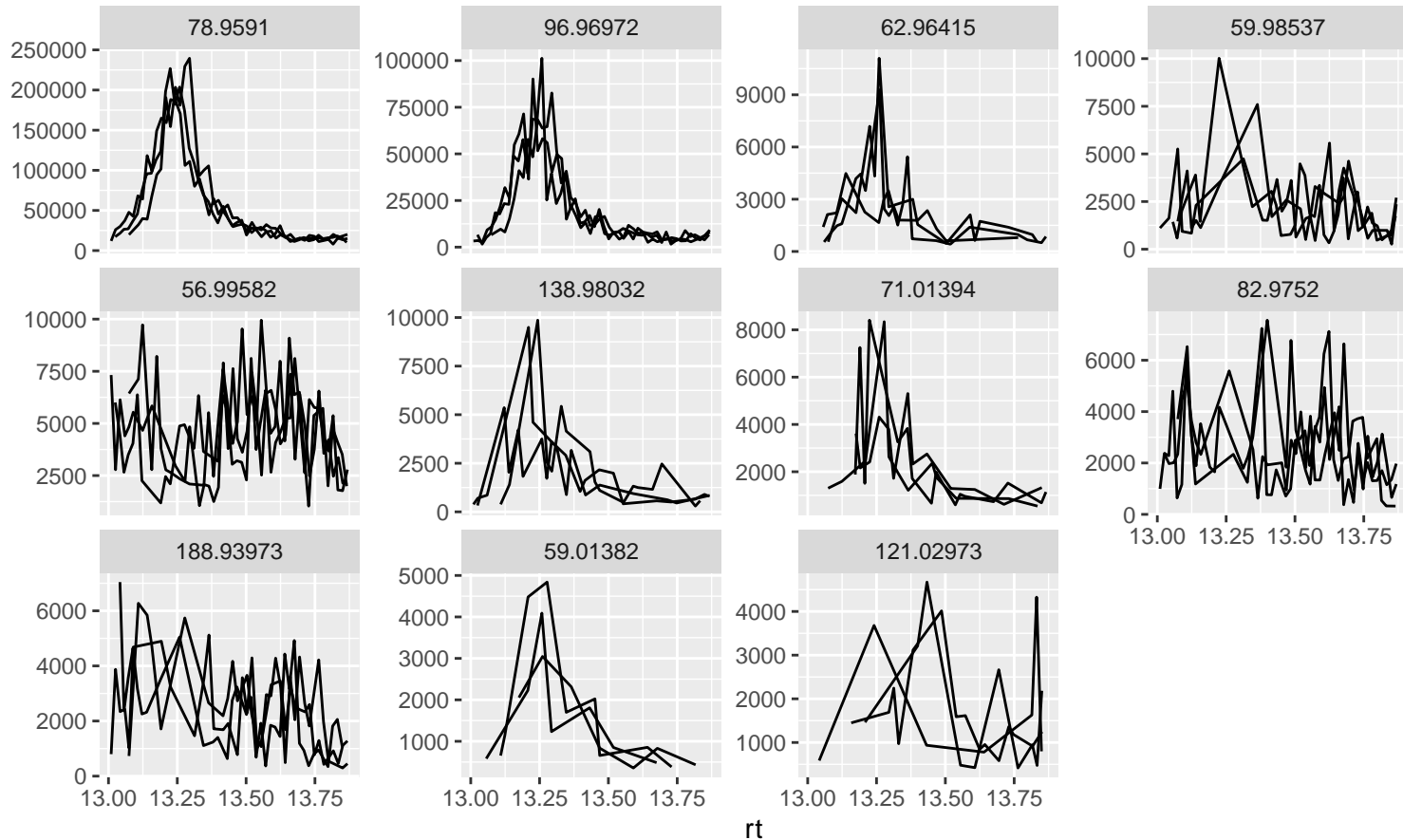
Carnosine (neg) 225.099315

int



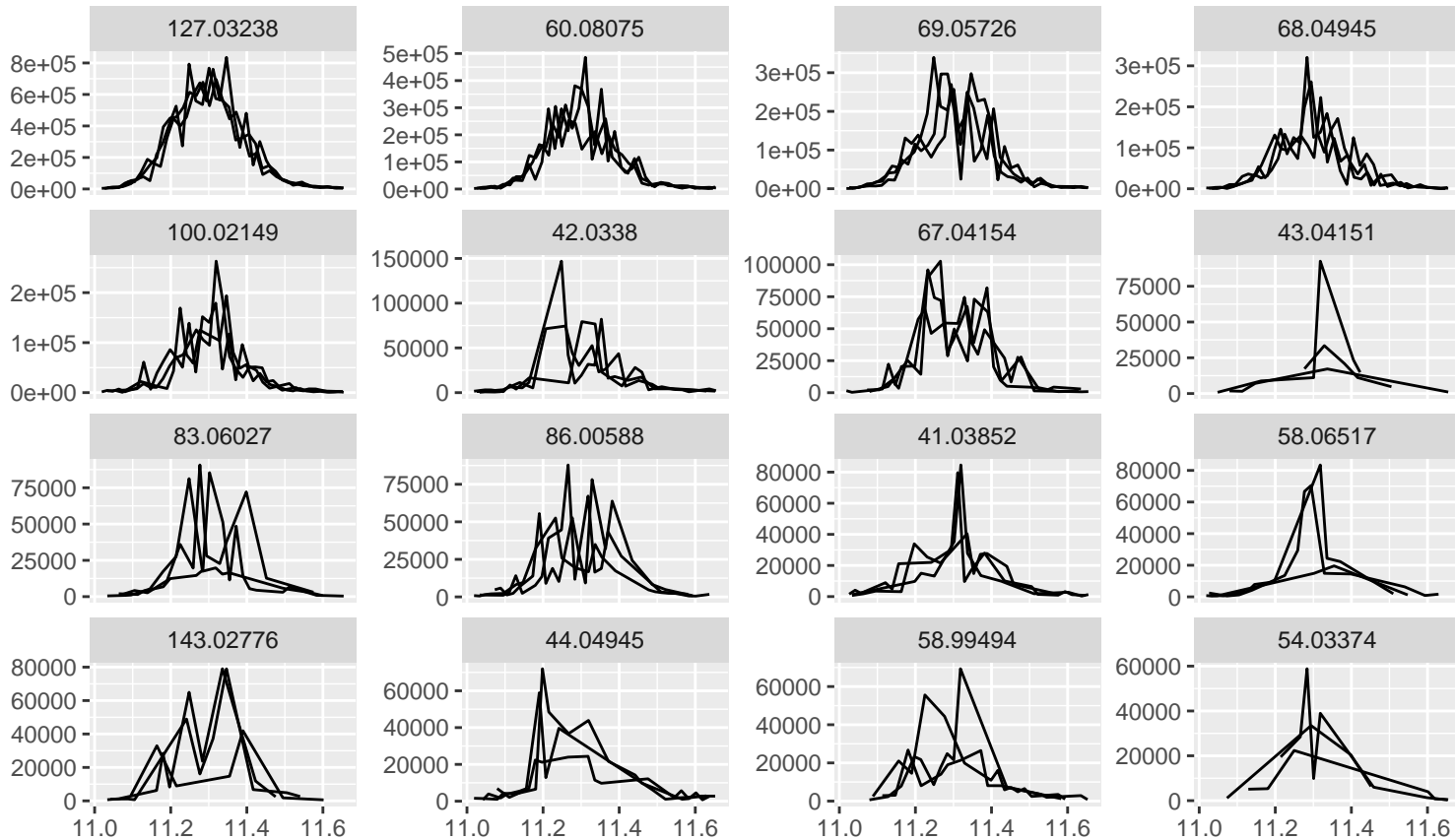
rt

D-Ribose 5-phosphate (neg) 229.011882



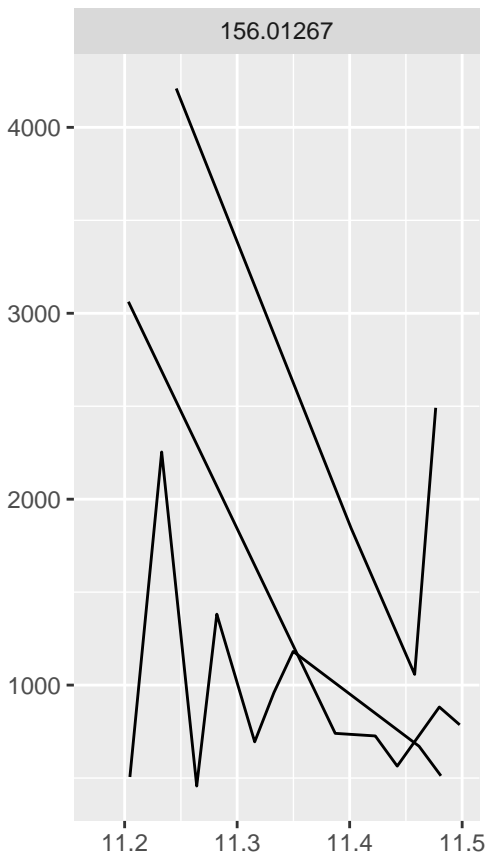
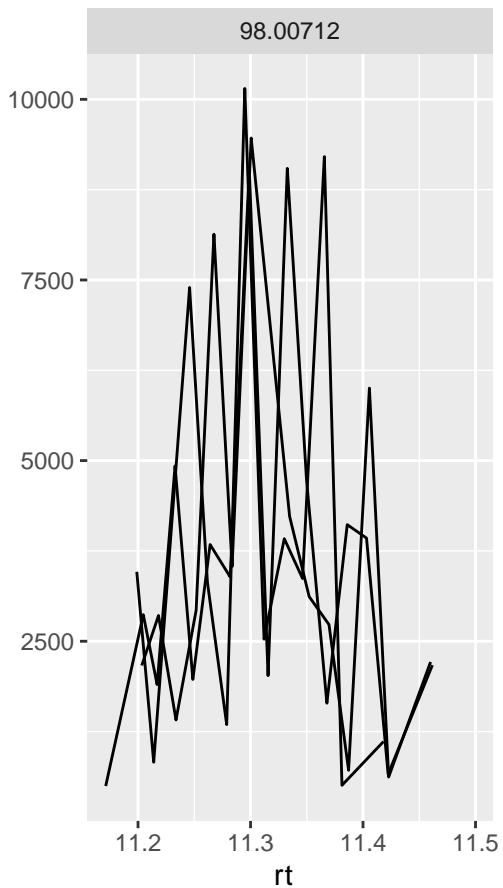
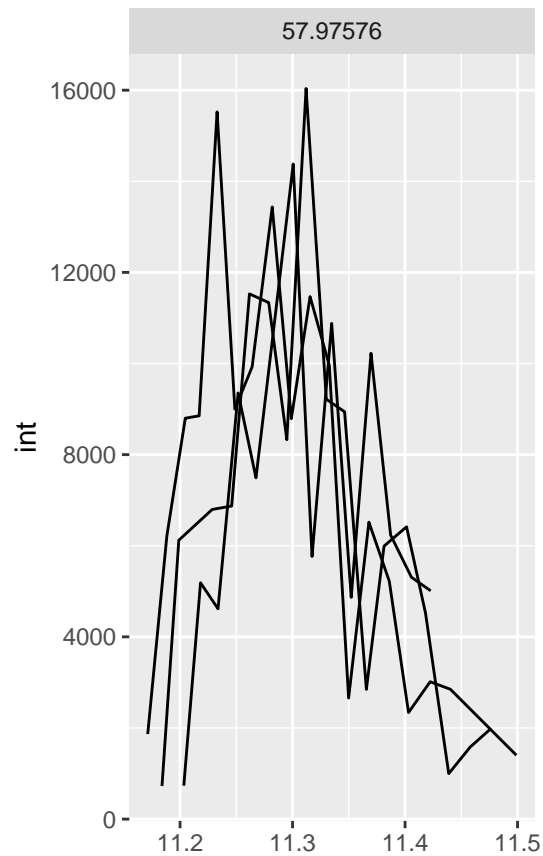
Ergothioneine (pos) 230.095775

int



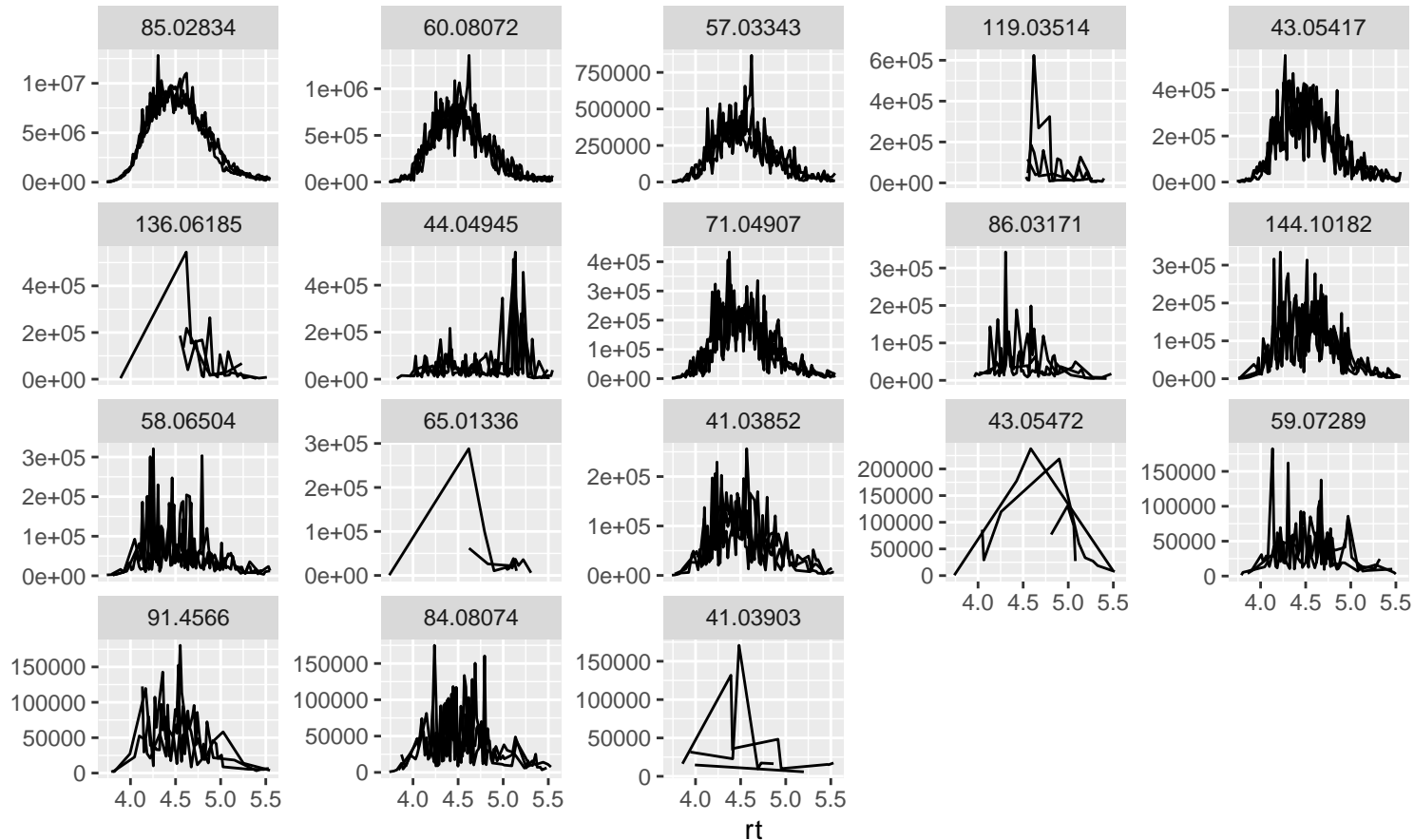
rt

Ergothioneine (neg) 228.081223

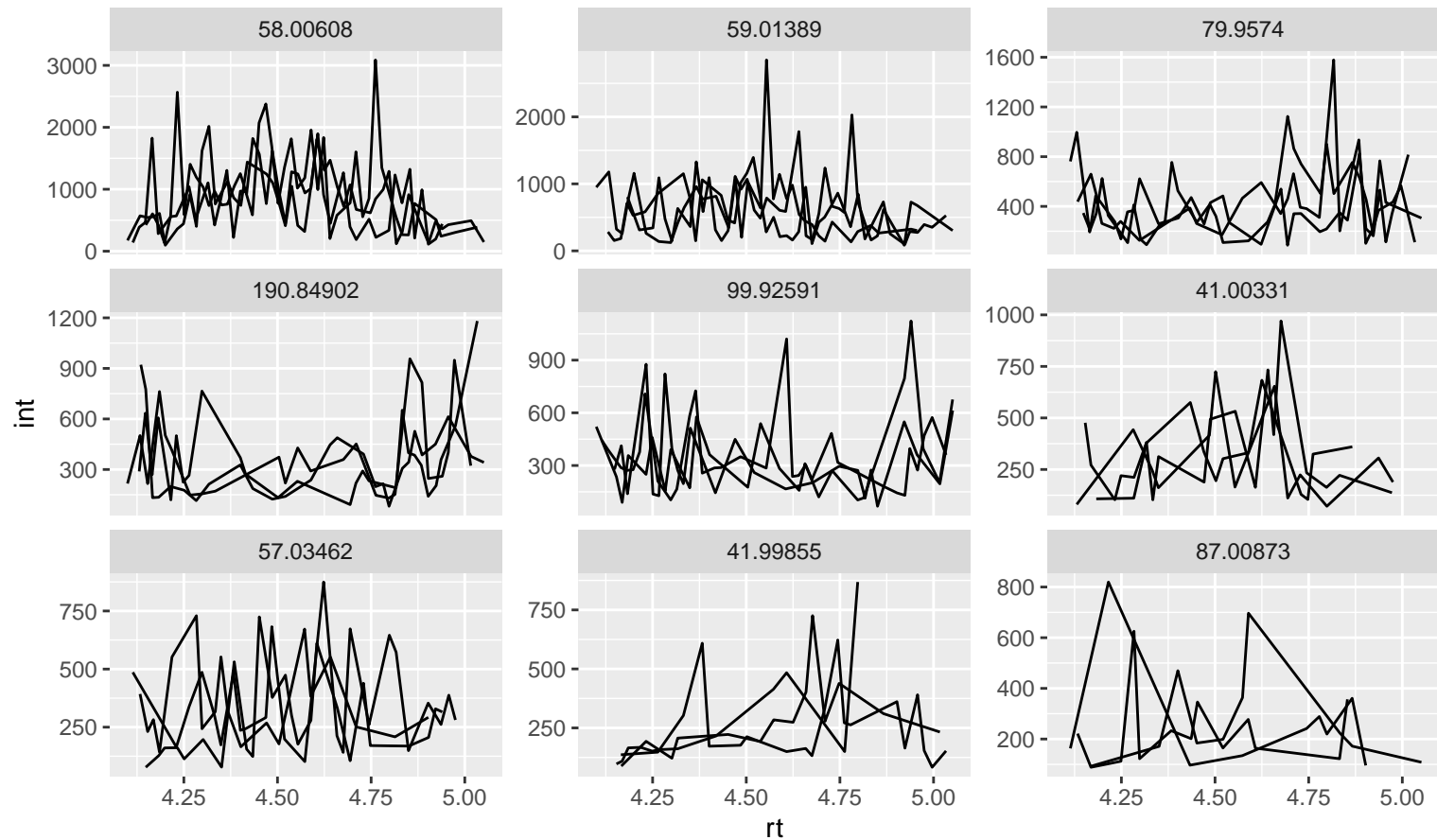


Butyrylcarnitine (pos) 232.154335

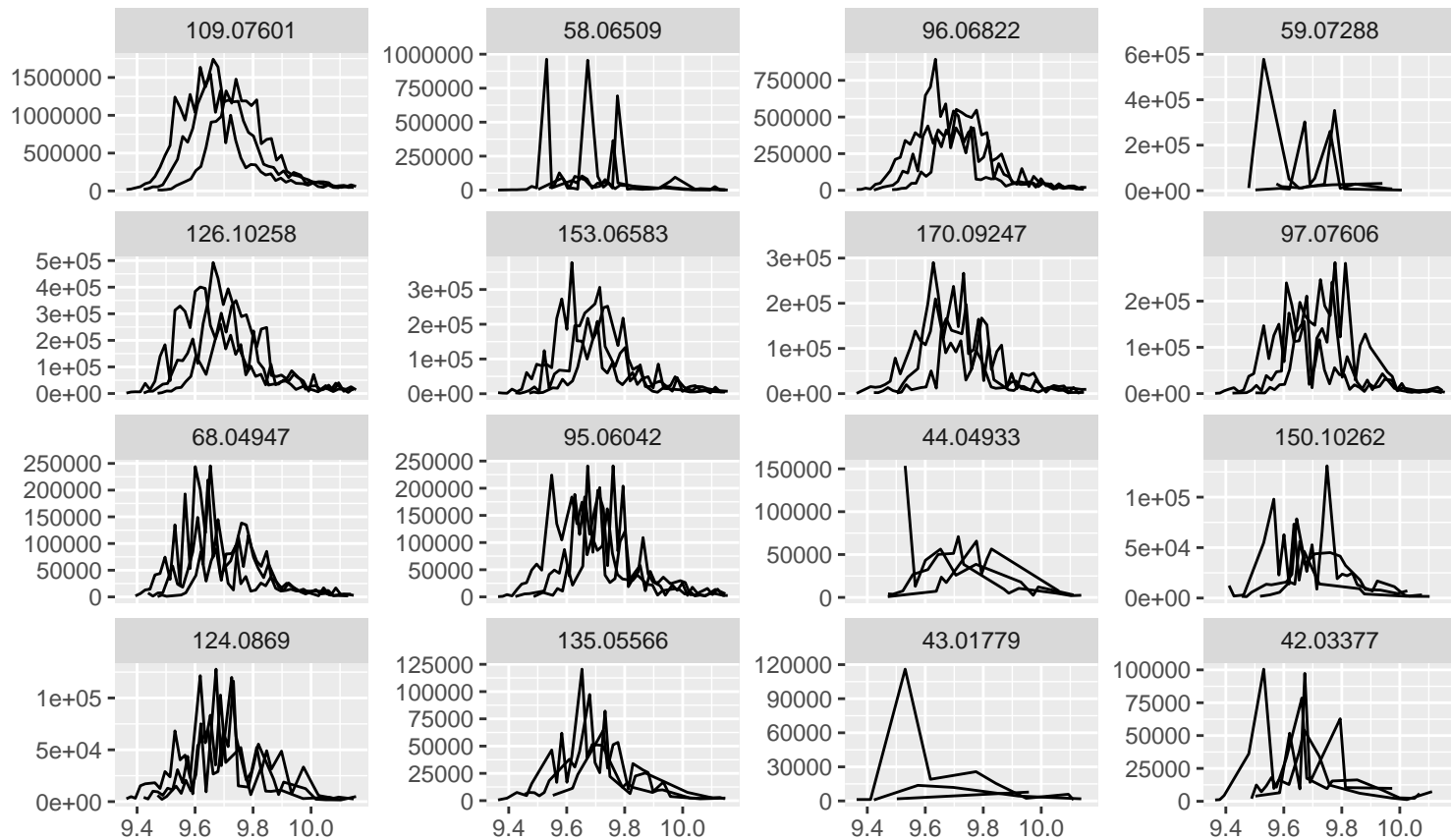
int



Butyrylcarnitine (neg) 230.139783

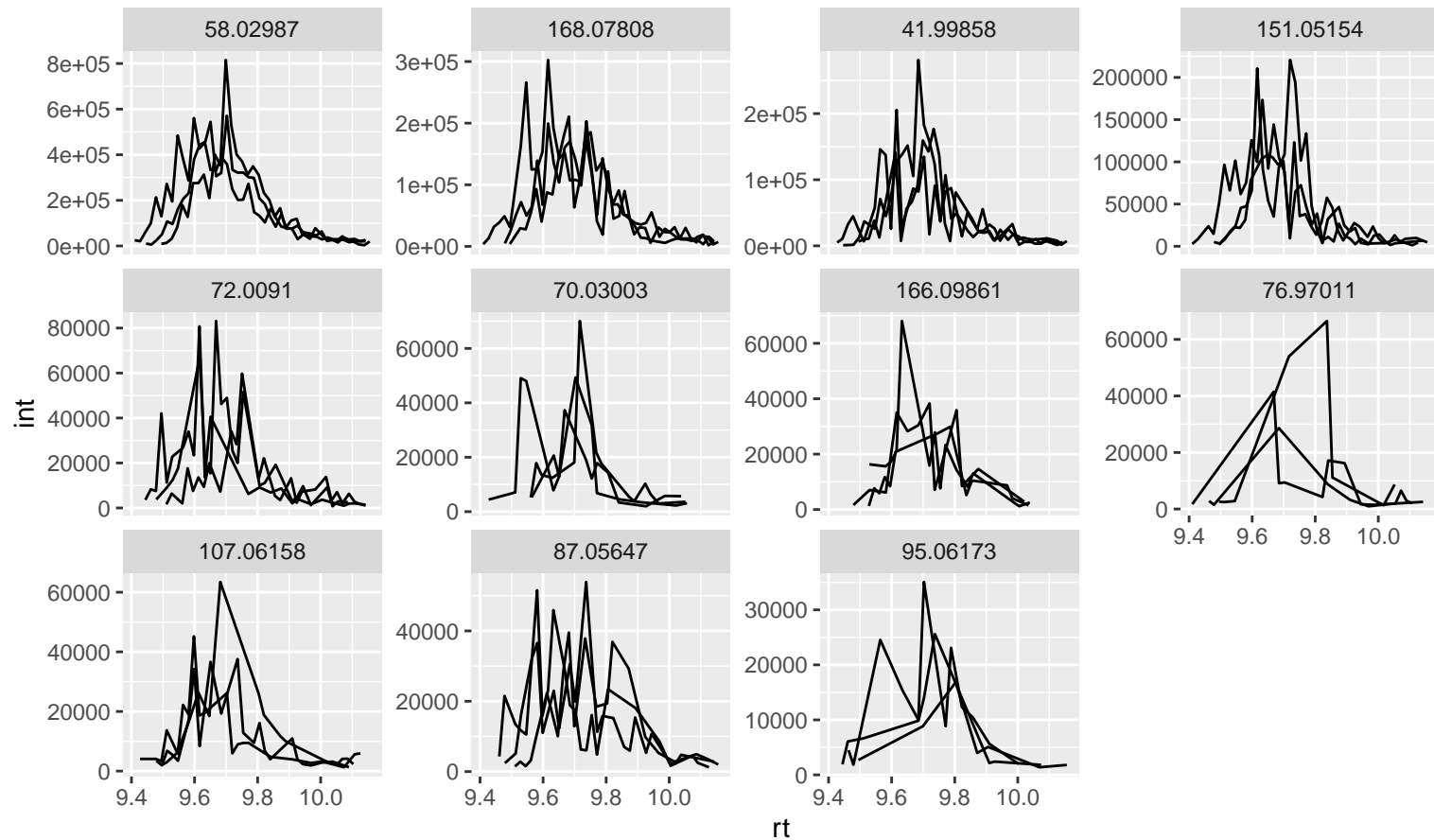


Anserine (pos) 241.129517



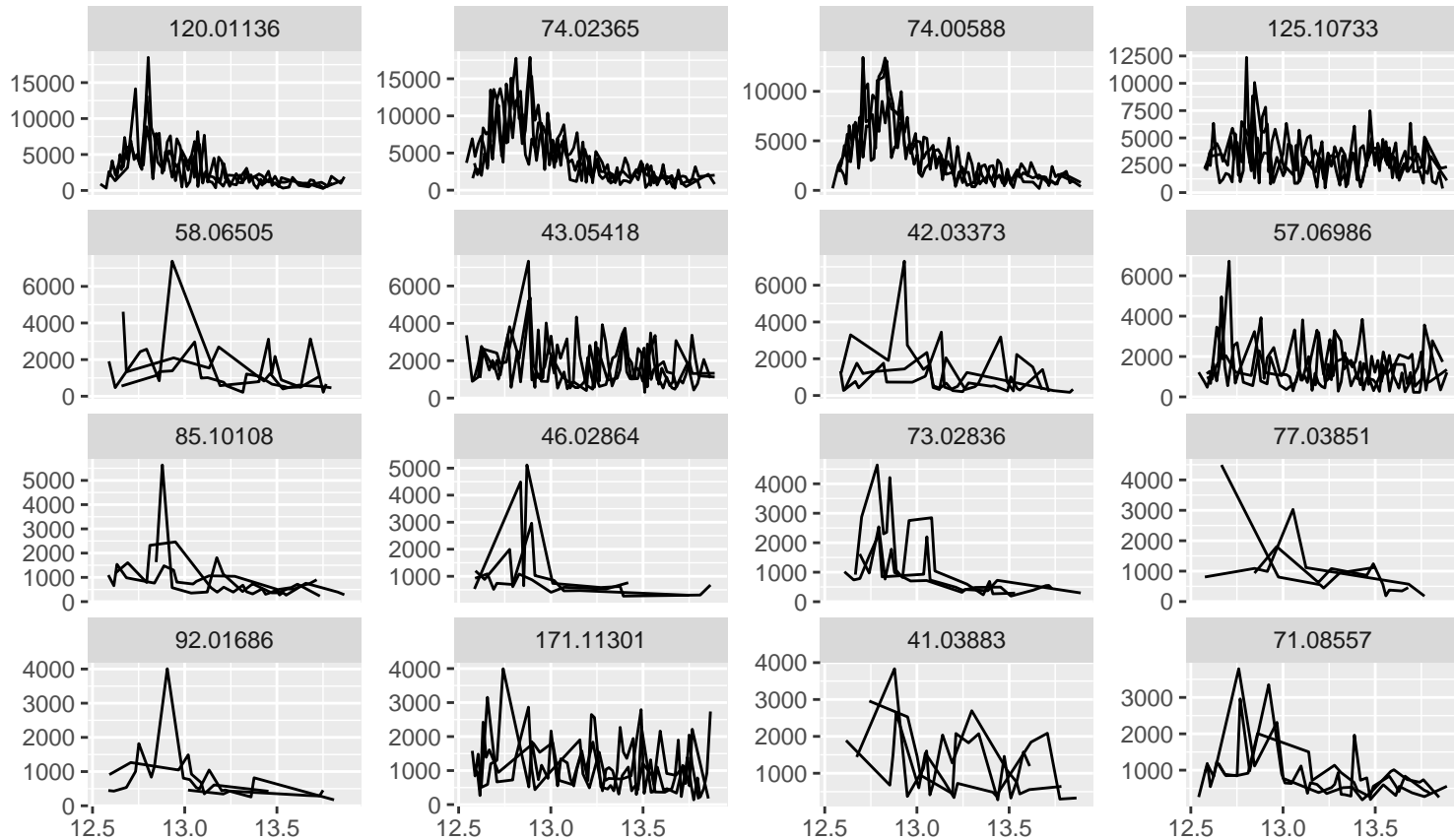
rt

Anserine (neg) 239.114965



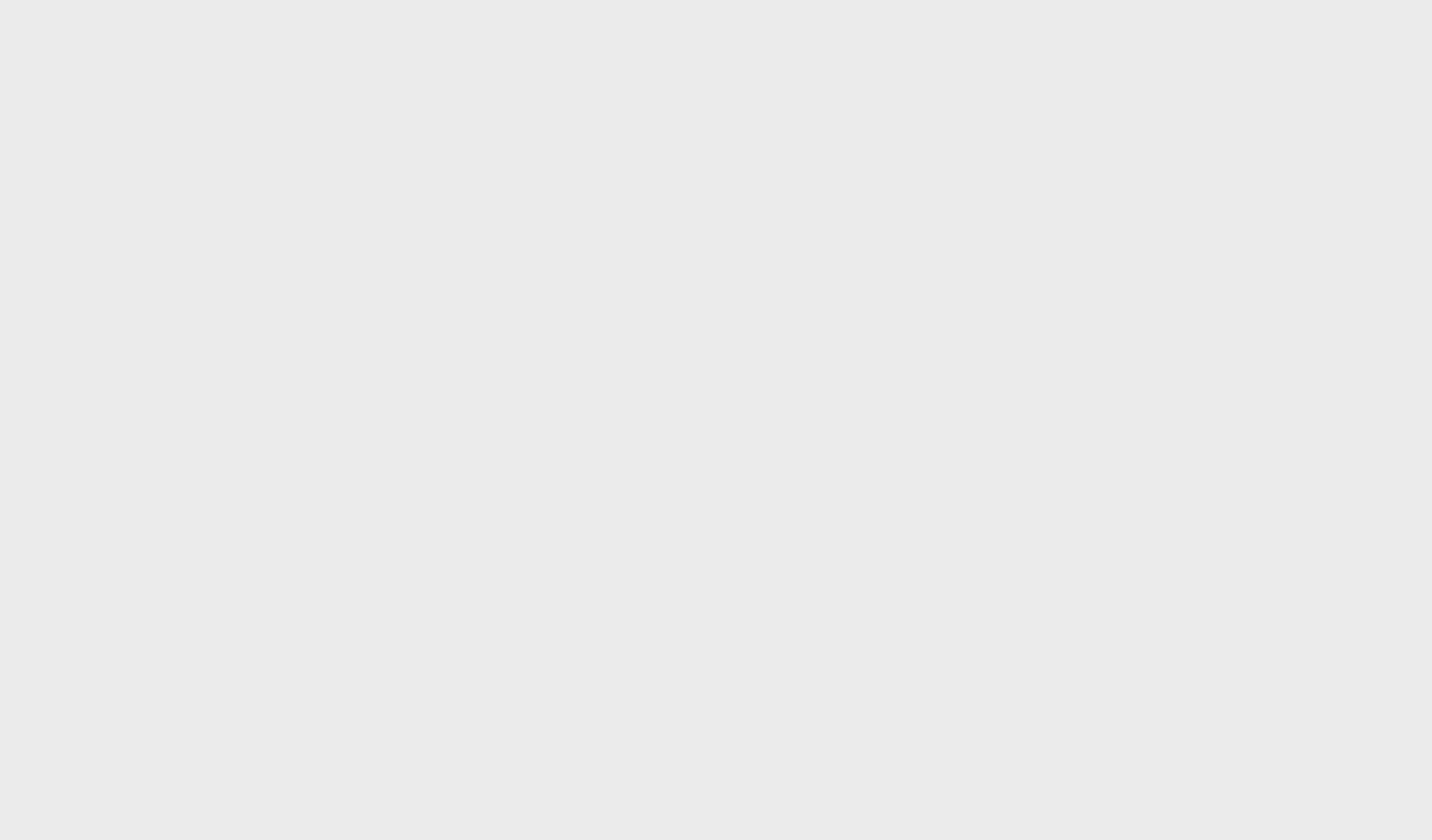
L-Cystine (pos) 241.031128

int



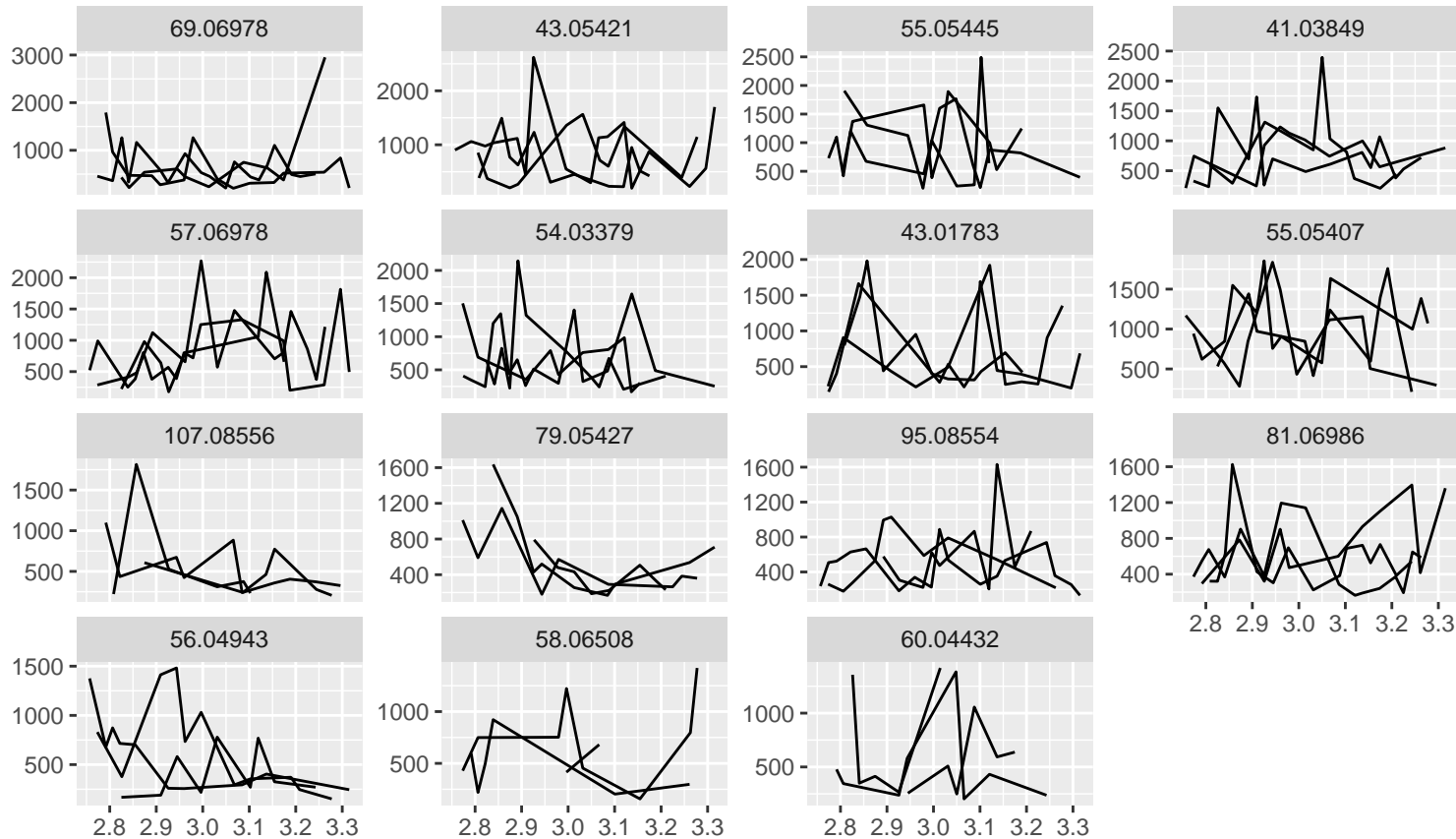
rt

L-Cystine (neg) 239.016576



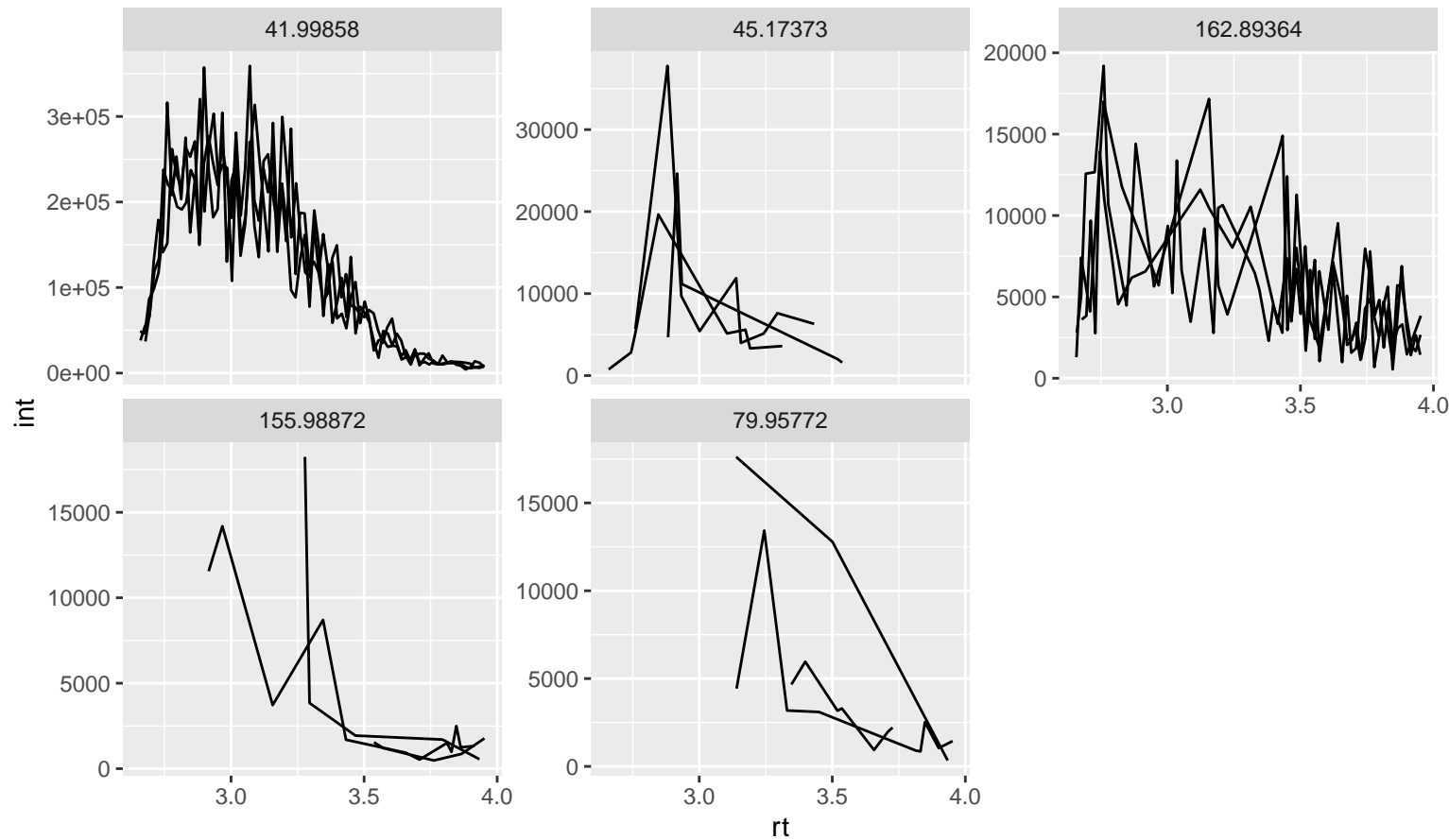
Thymidine (pos) 243.097549

int

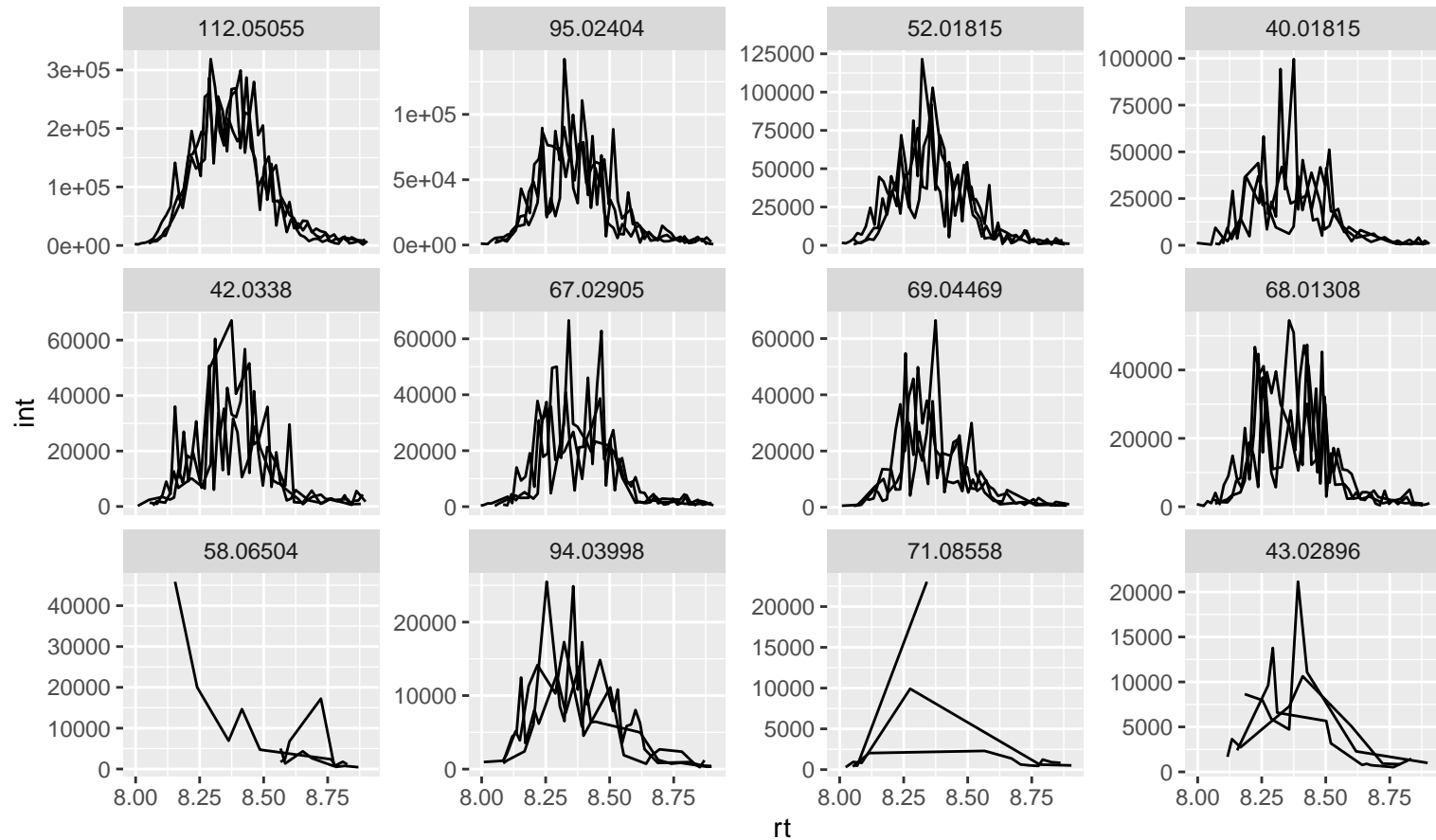


rt

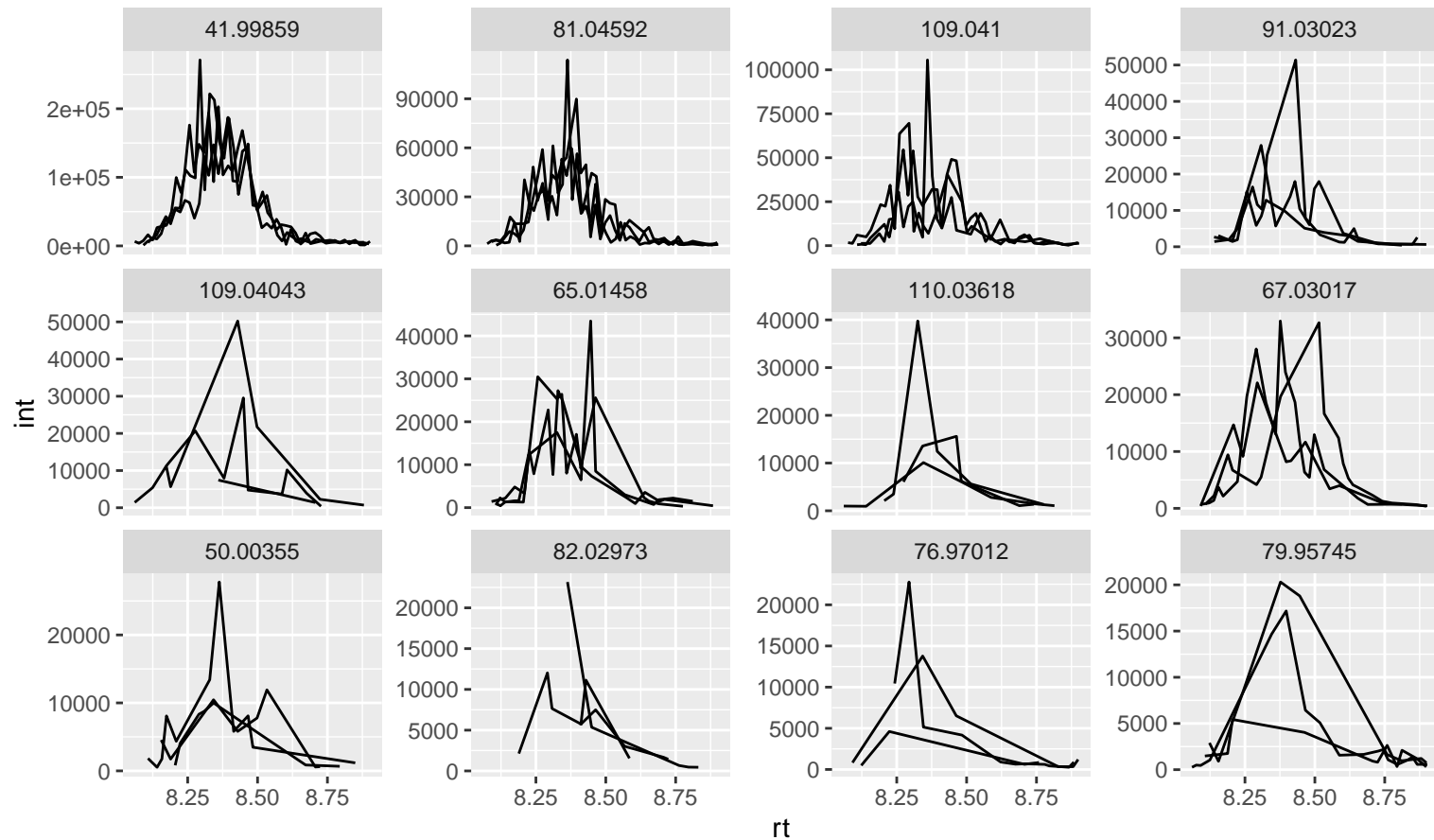
Thymidine (neg) 241.082997



Cytidine (pos) 244.092798

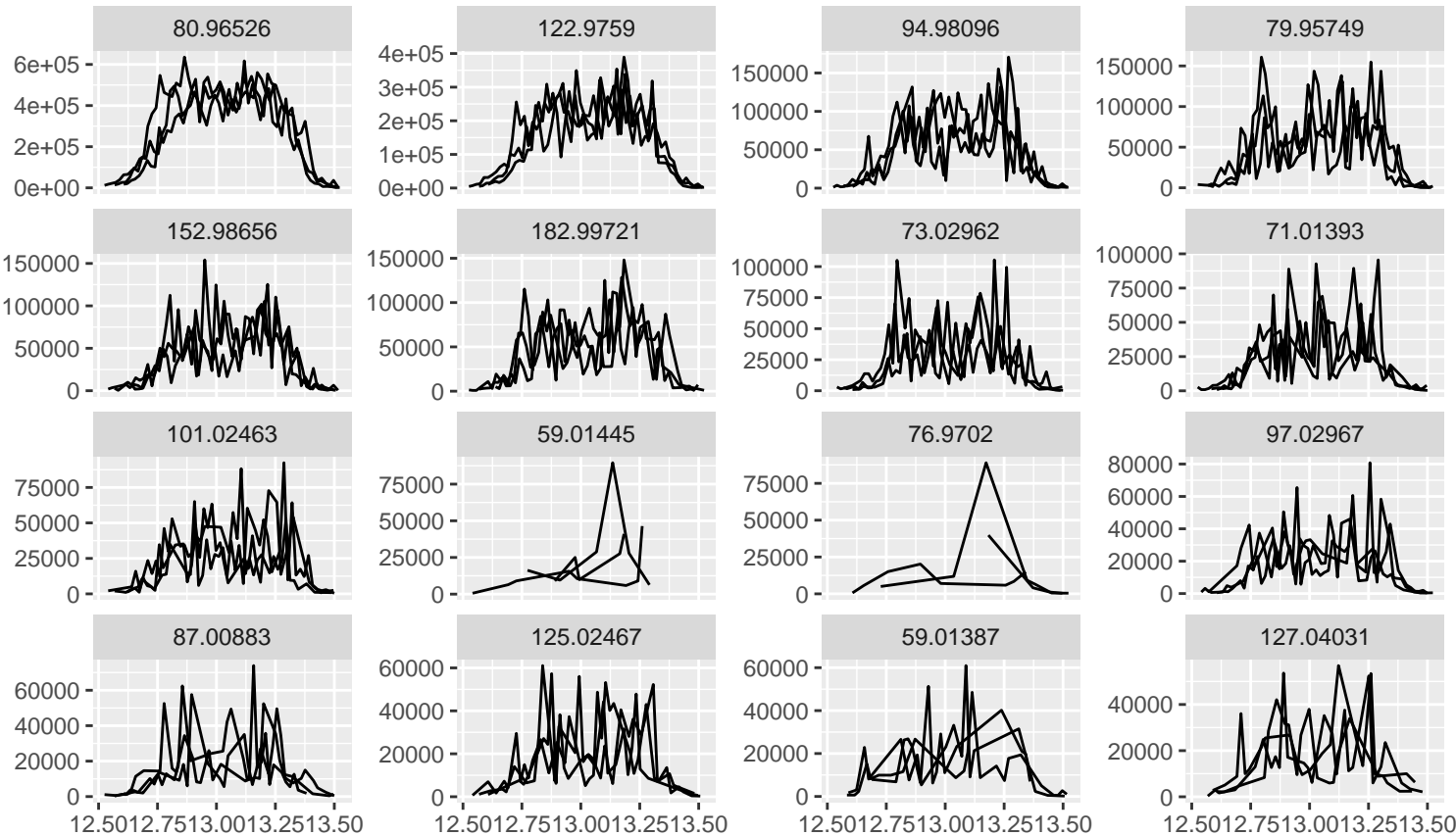


Cytidine (neg) 242.078246



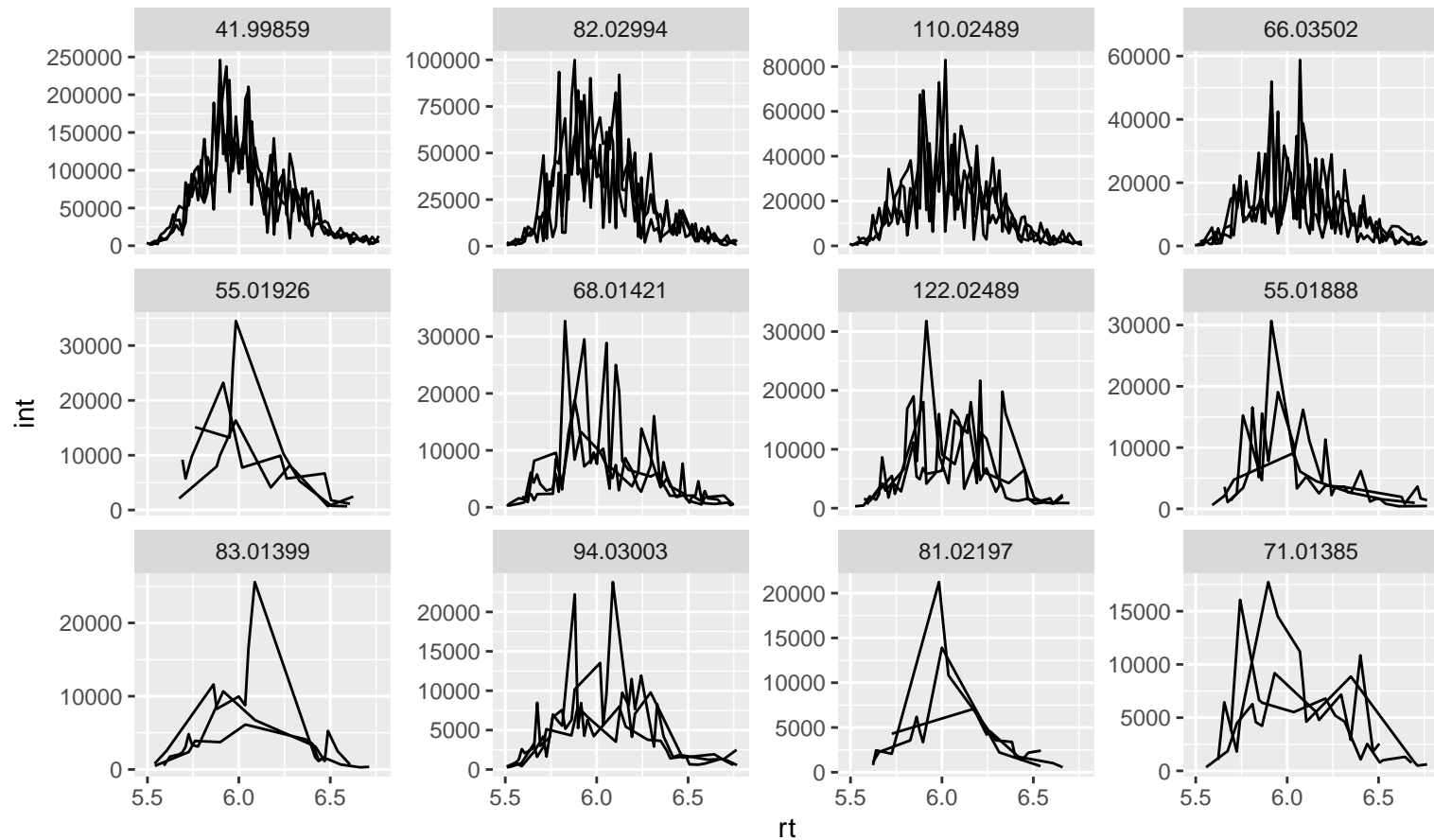
Sulfoquinovose (neg) 243.018016

int

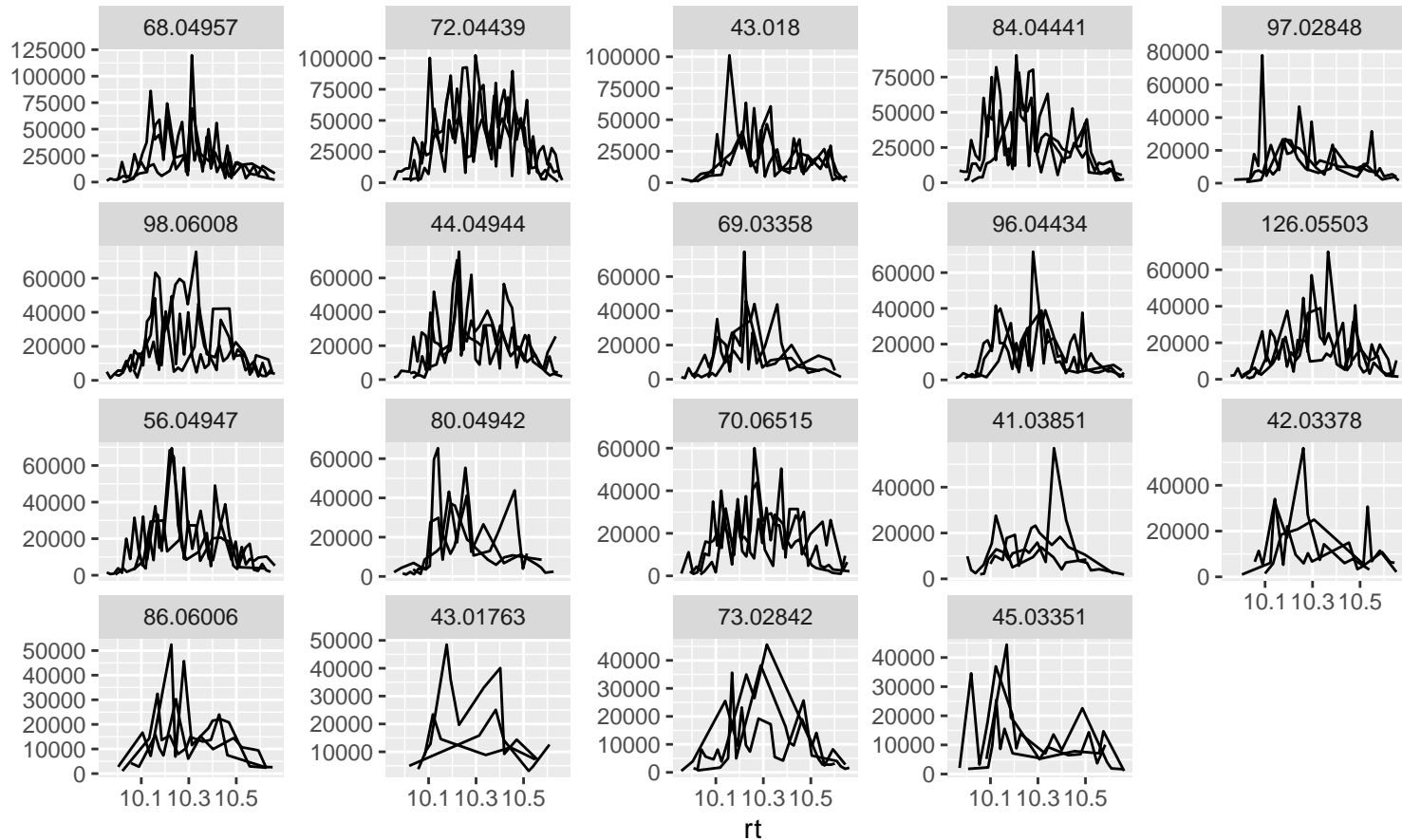


rt

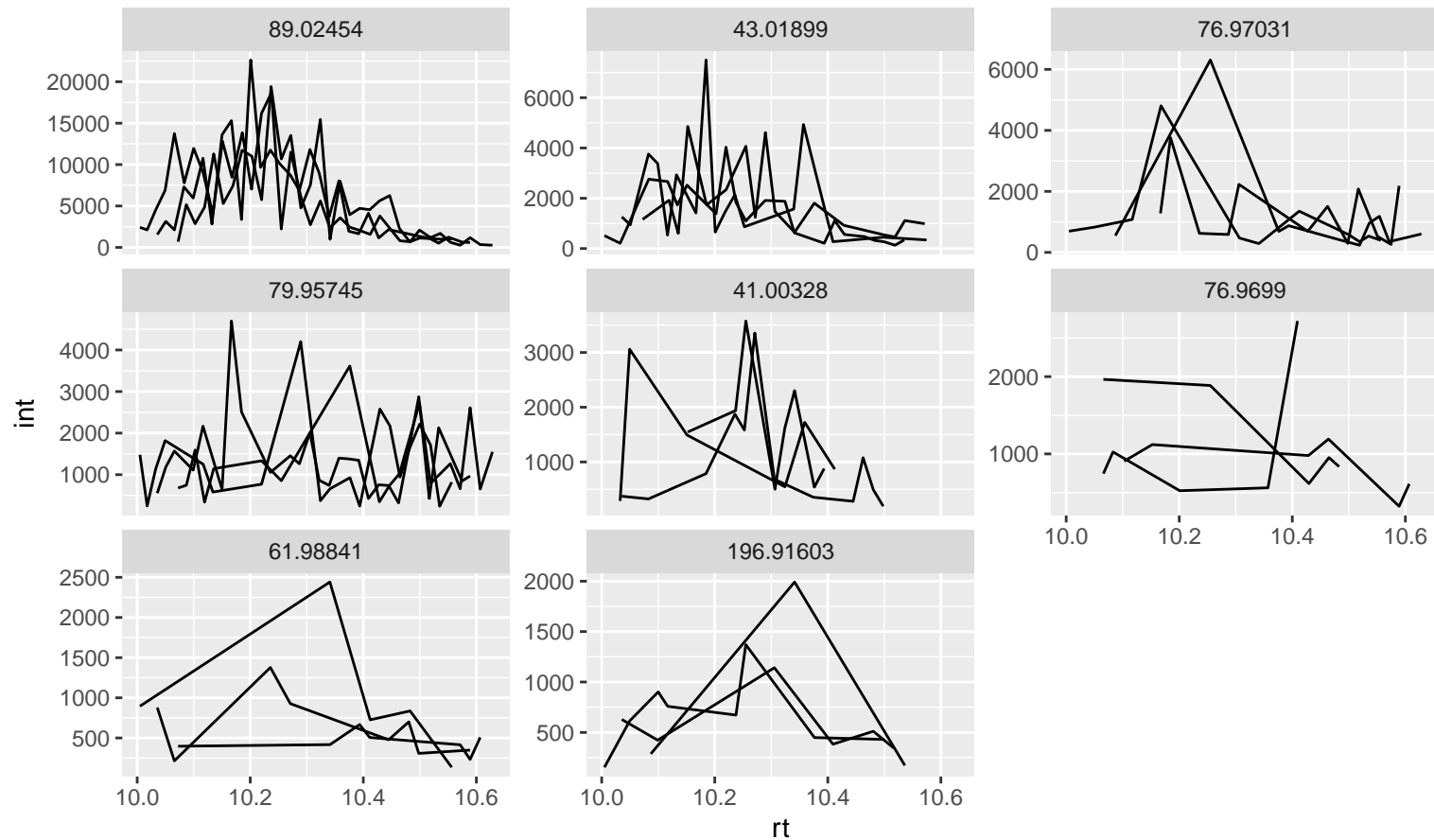
Uridine (neg) 243.062262



Muramic acid (pos) 252.10778

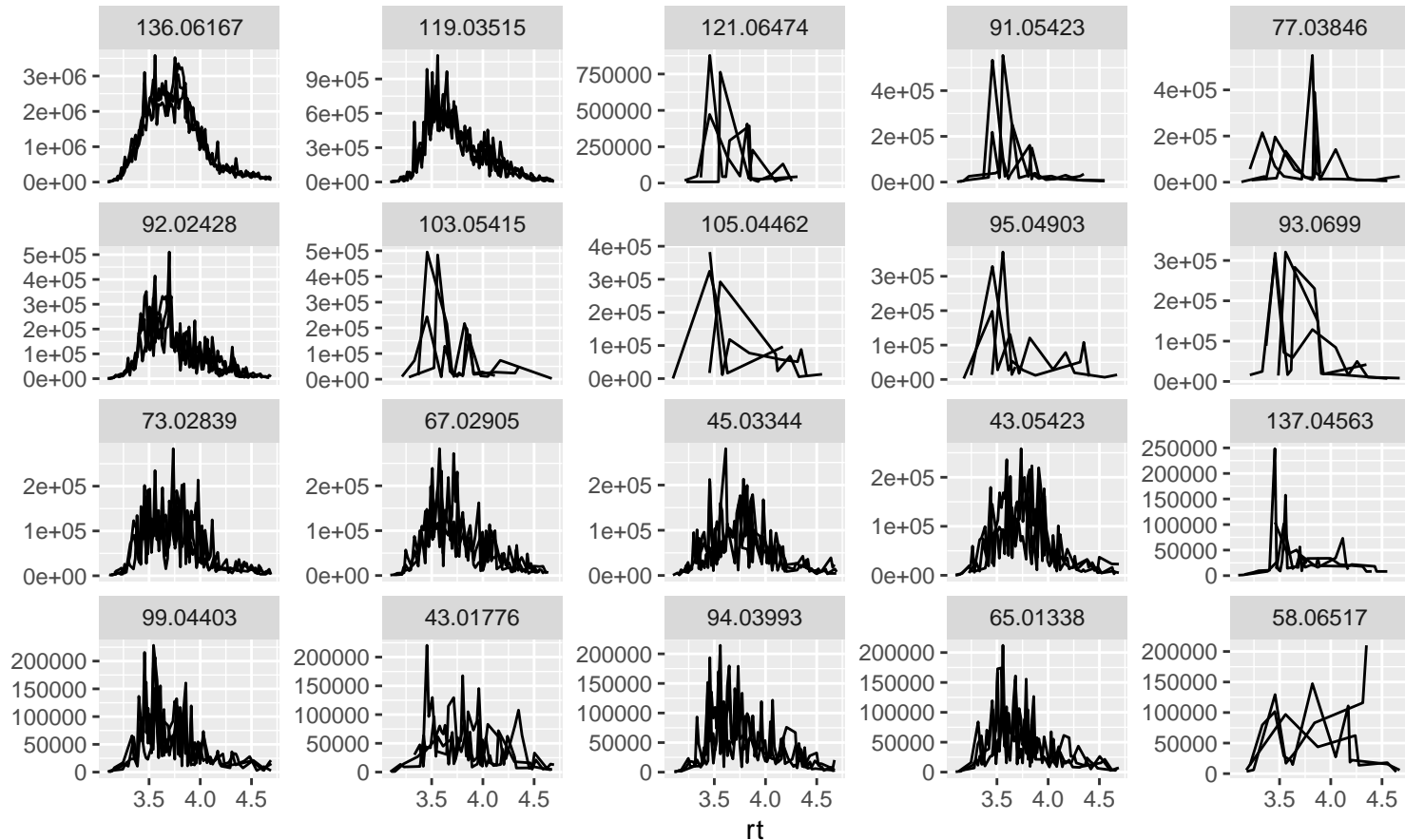


Muramic acid (neg) 250.093228



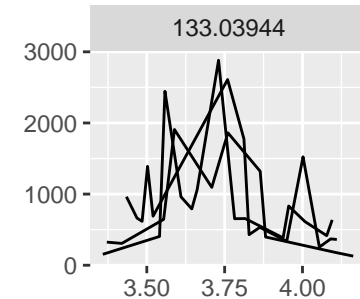
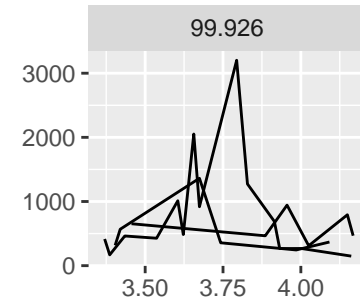
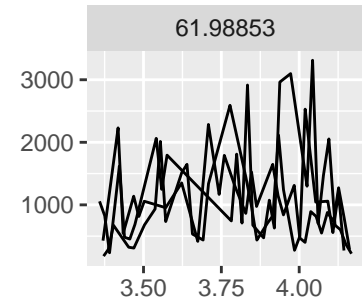
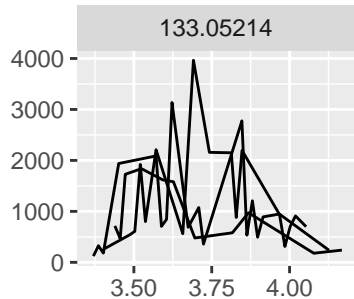
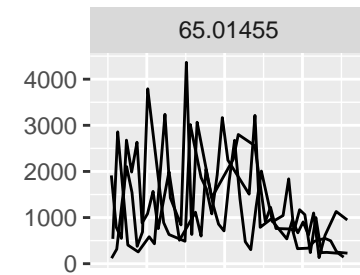
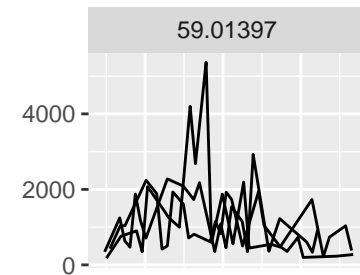
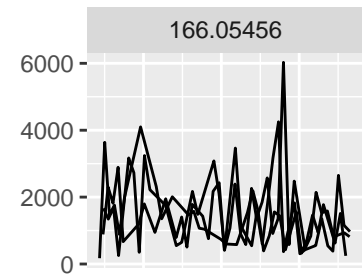
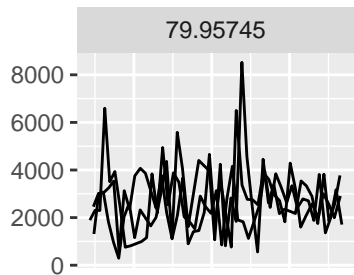
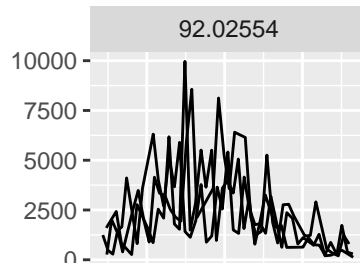
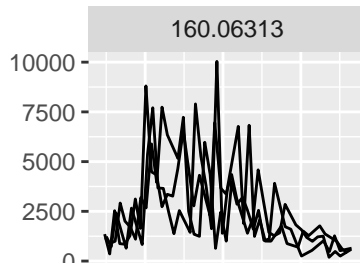
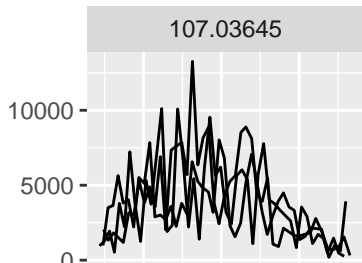
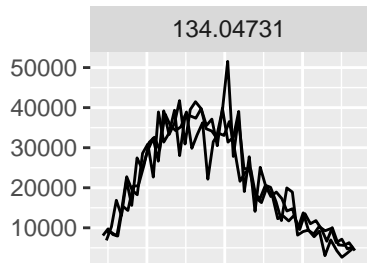
Deoxyadenosine (pos) 252.109116

int



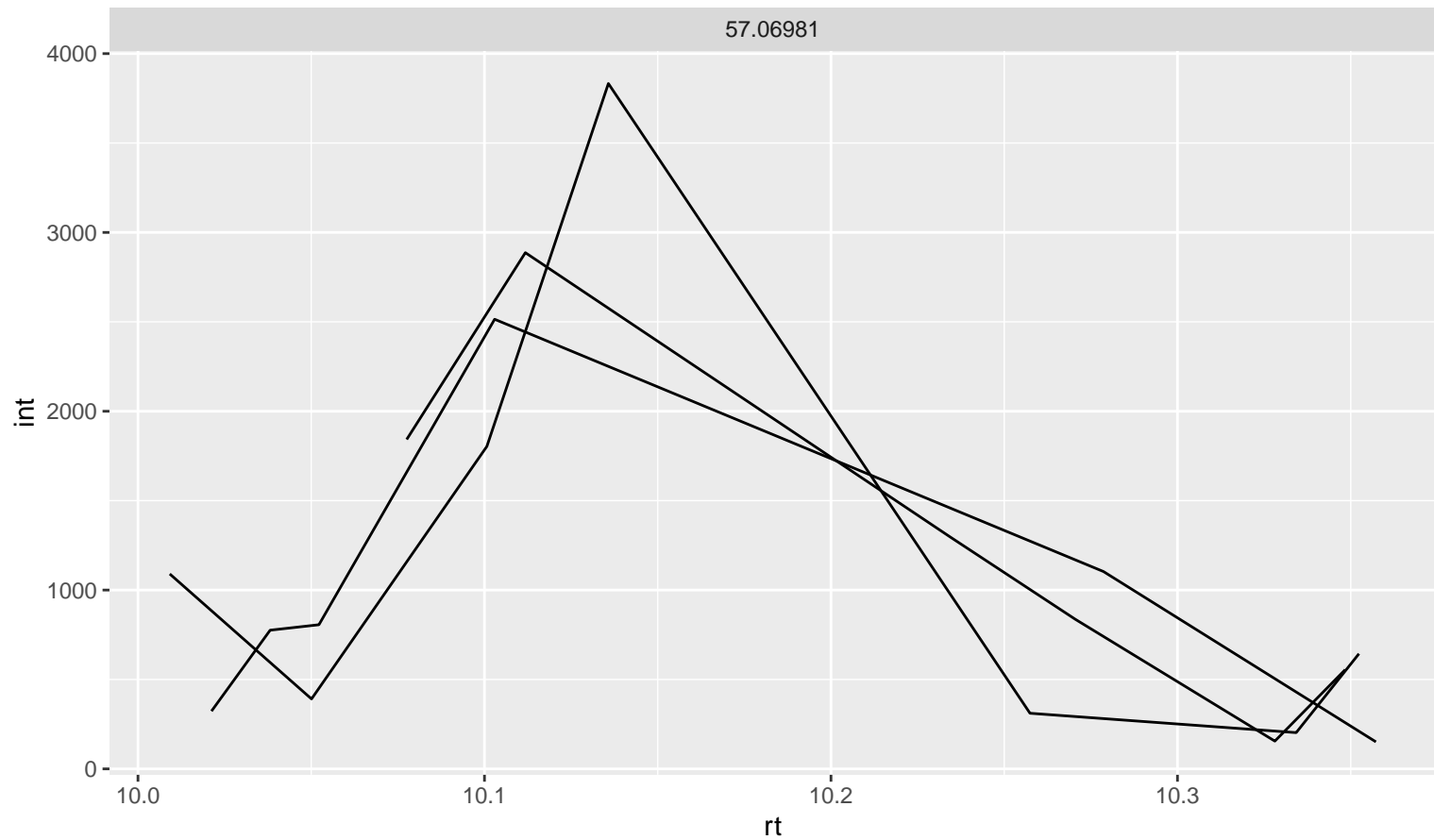
Deoxyadenosine (neg) 250.094564

int

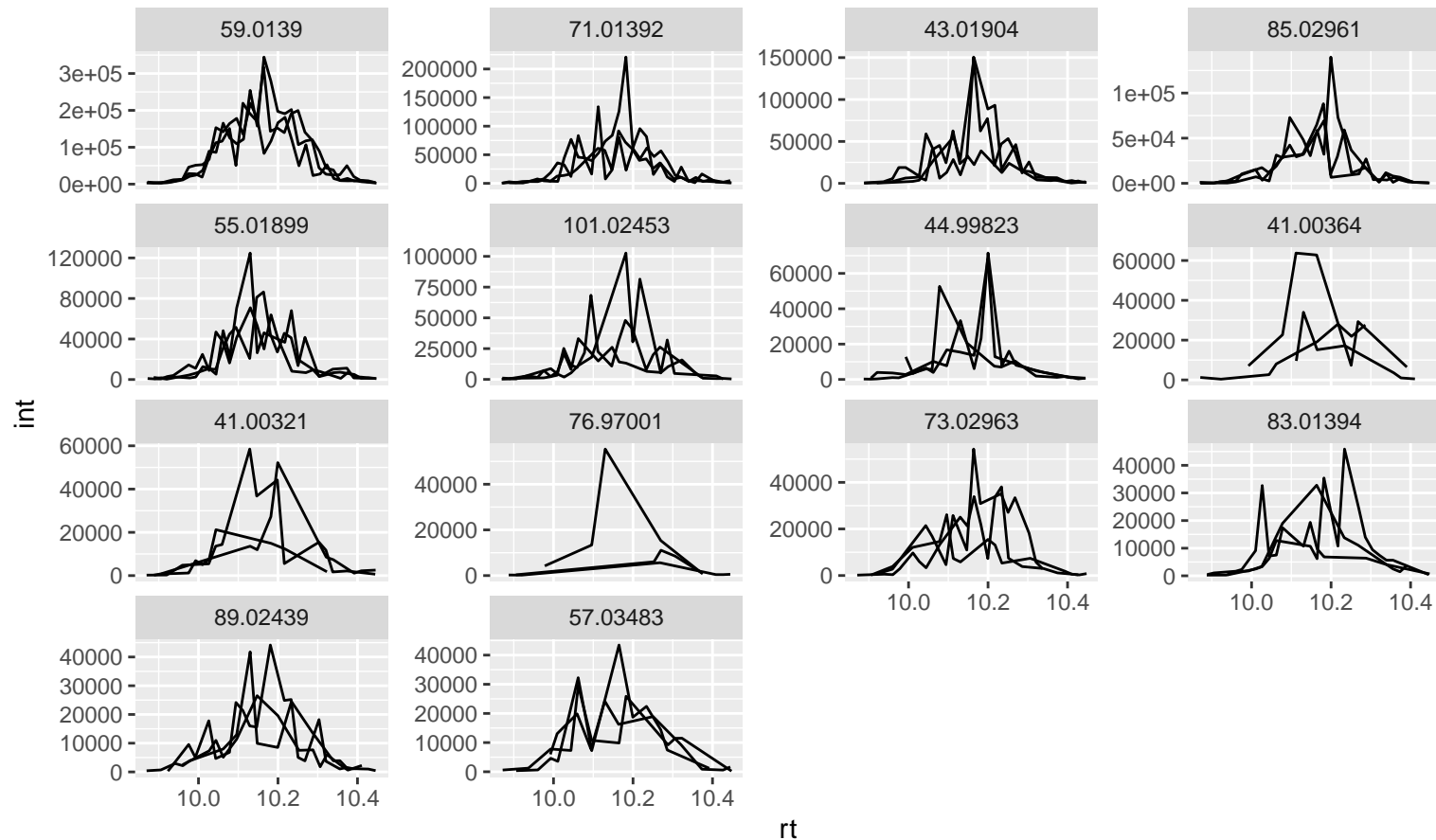


rt

2-O-alpha-D-Glucosylglycerol (pos) 255.107446

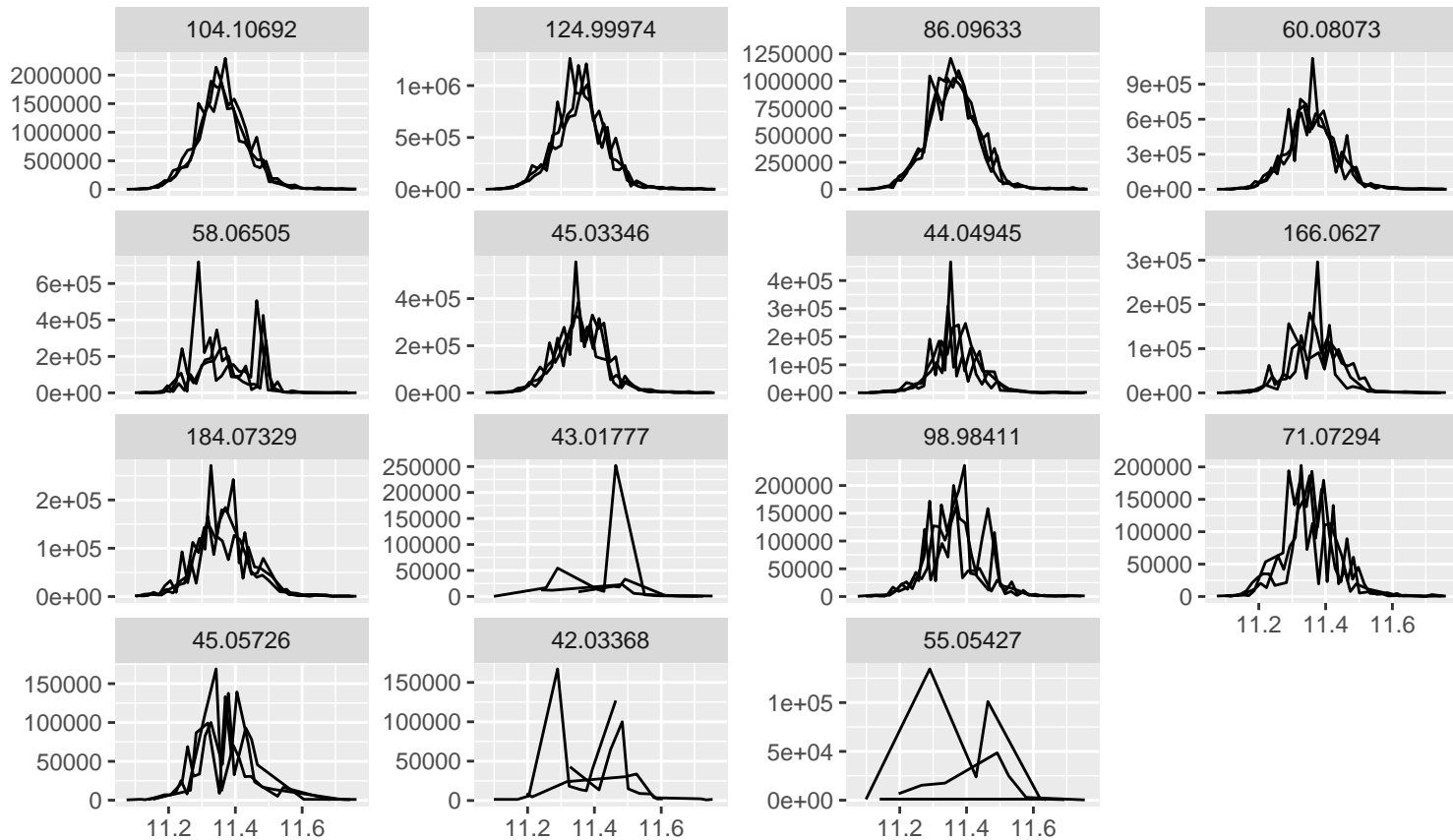


2-O-alpha-D-Glucosylglycerol (neg) 253.092894



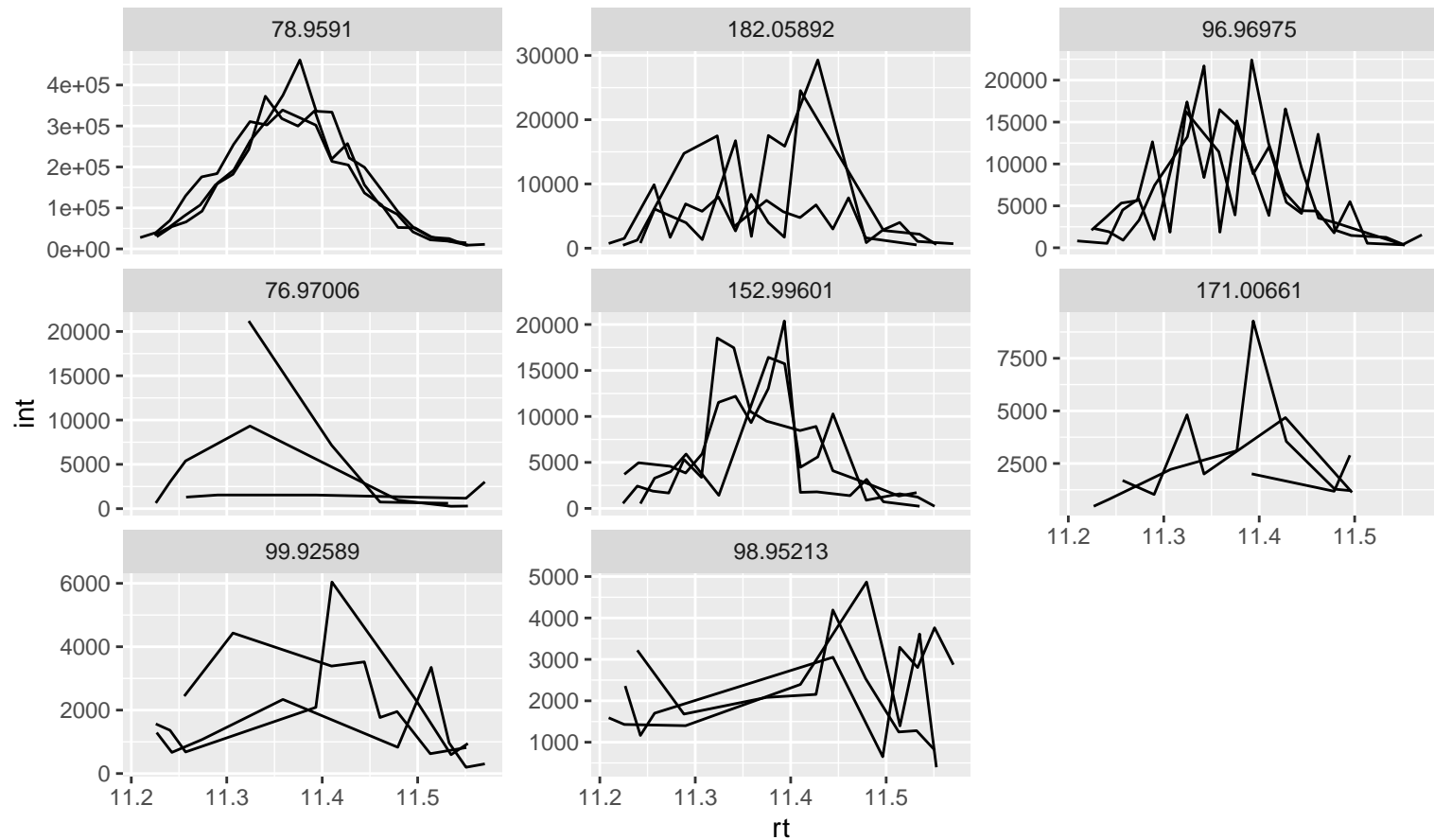
Glycerophosphocholine (pos) 258.110103

int

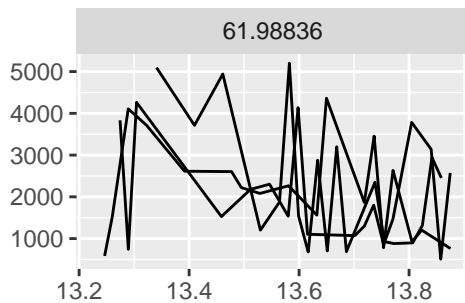
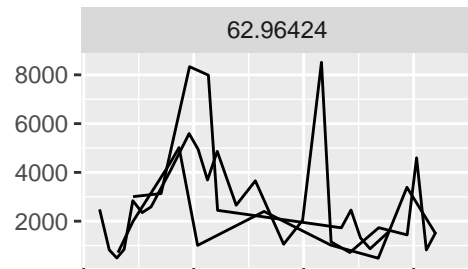
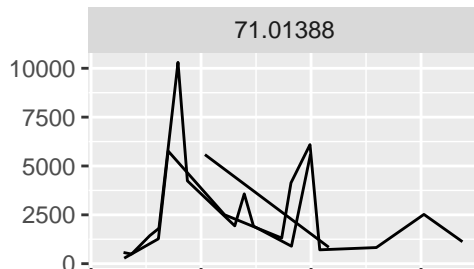
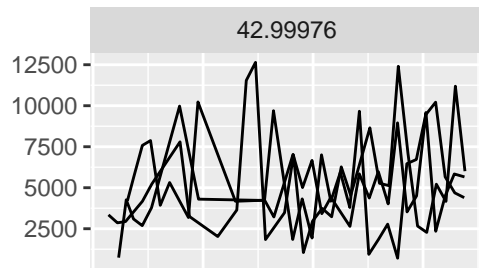
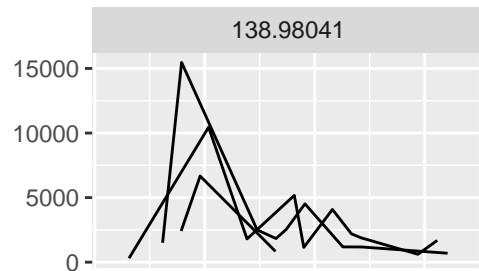
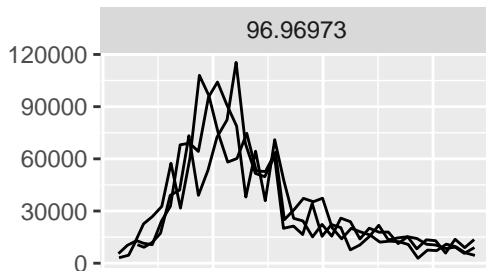
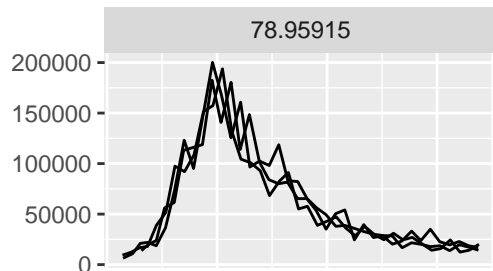


rt

Glycerophosphocholine (neg) 256.095551

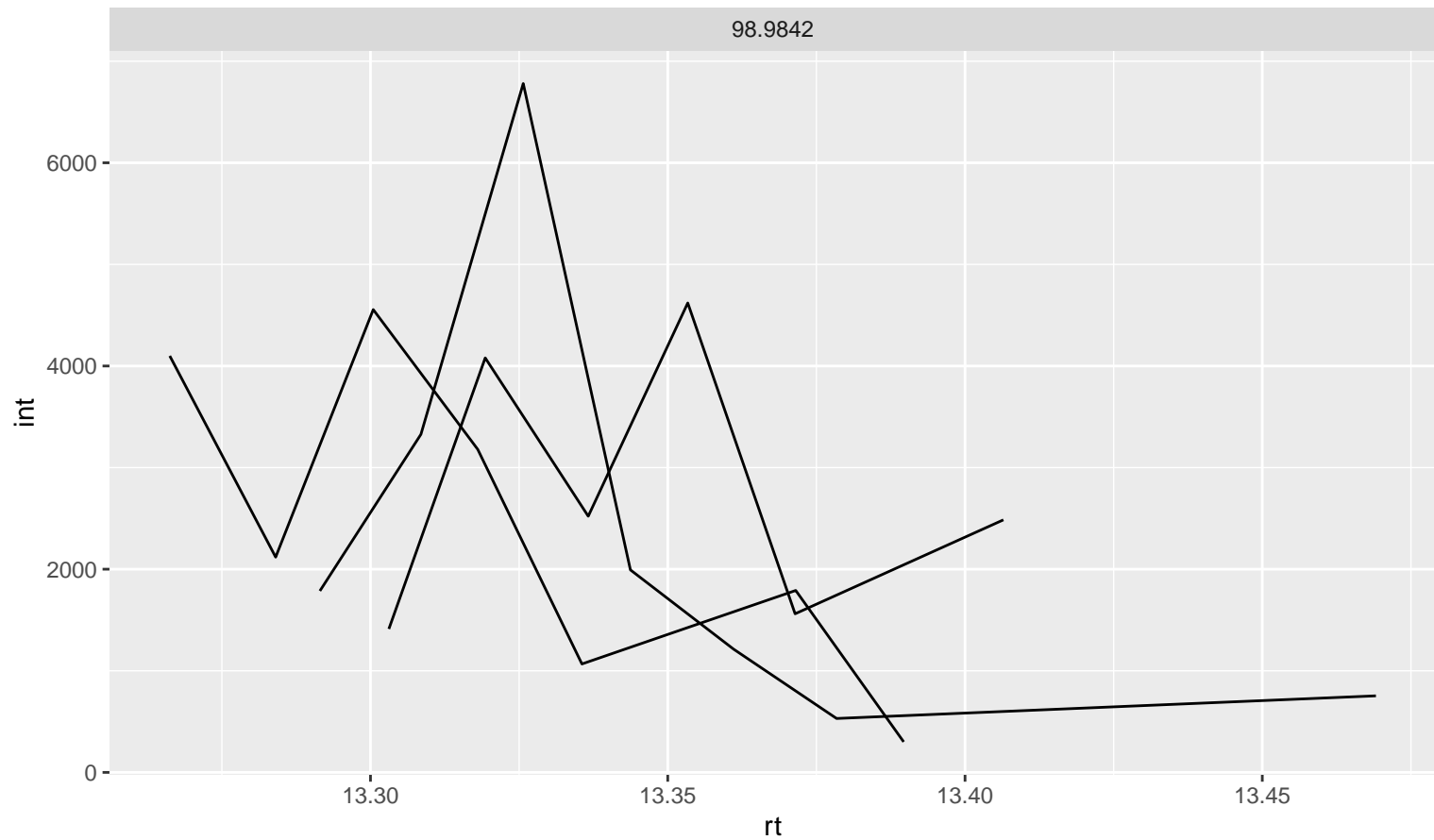


D-Fructose 6-phosphate (neg) 259.022447

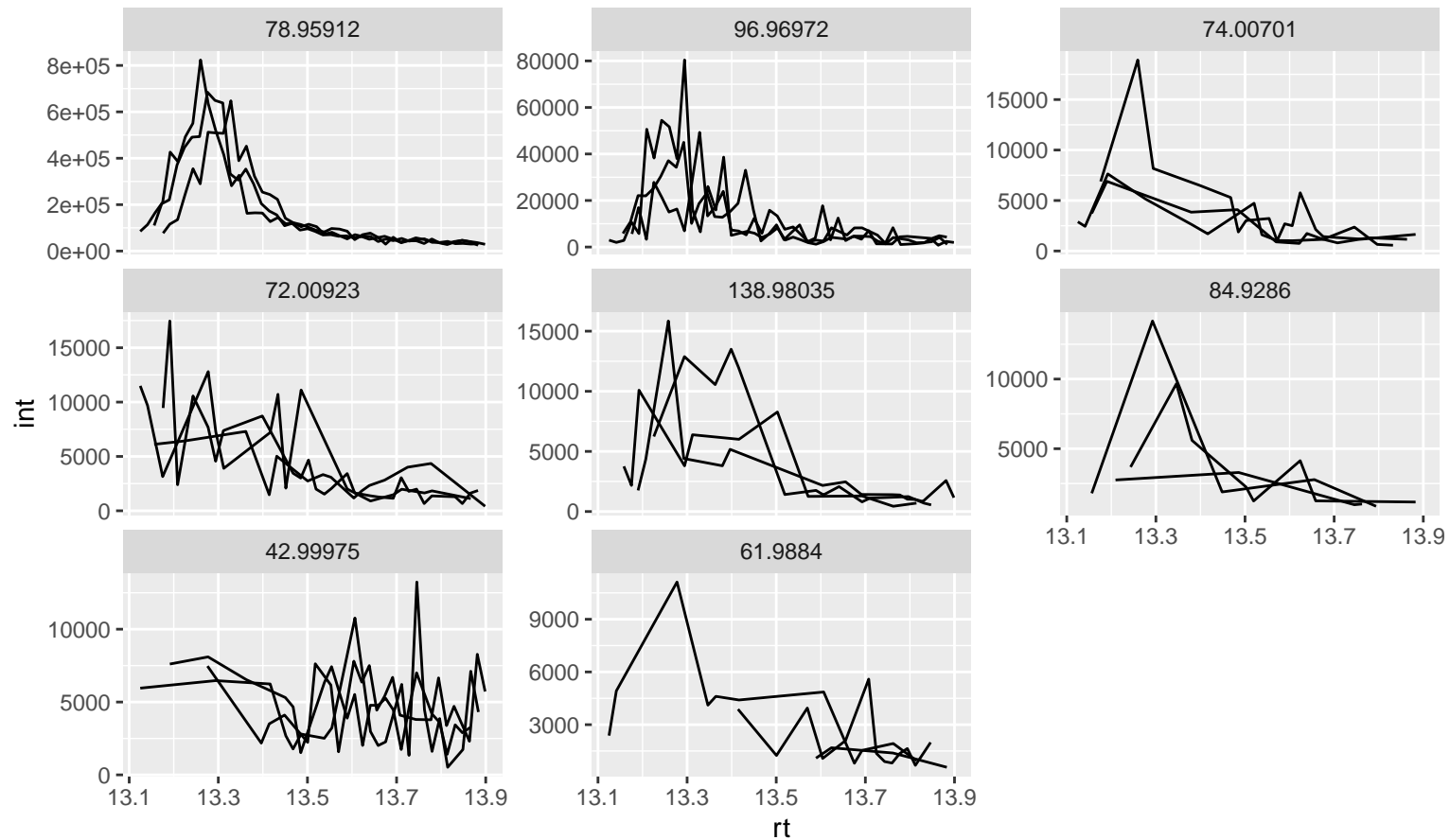


rt

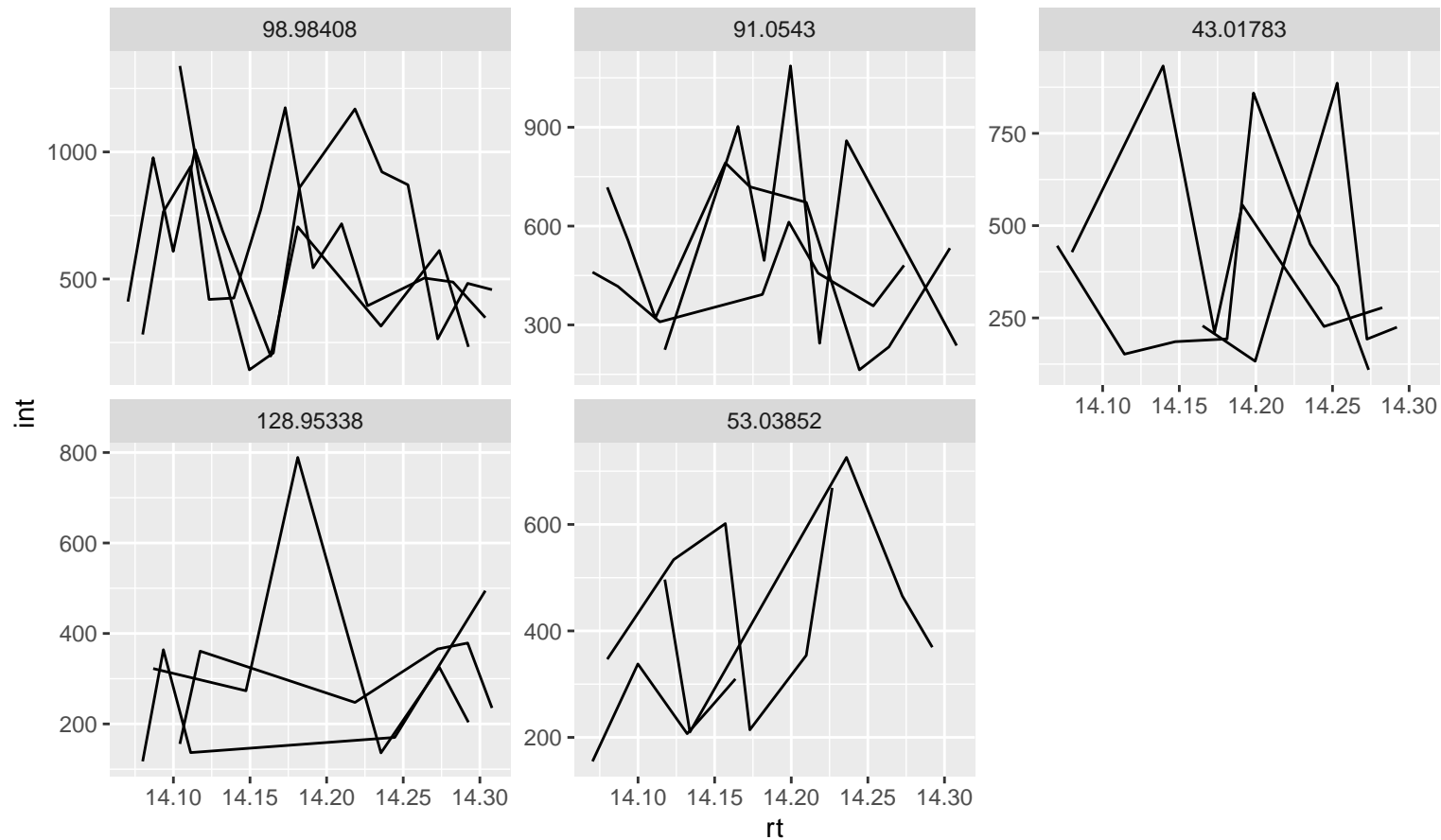
D-Glucose 1-phosphate (pos) 261.036999



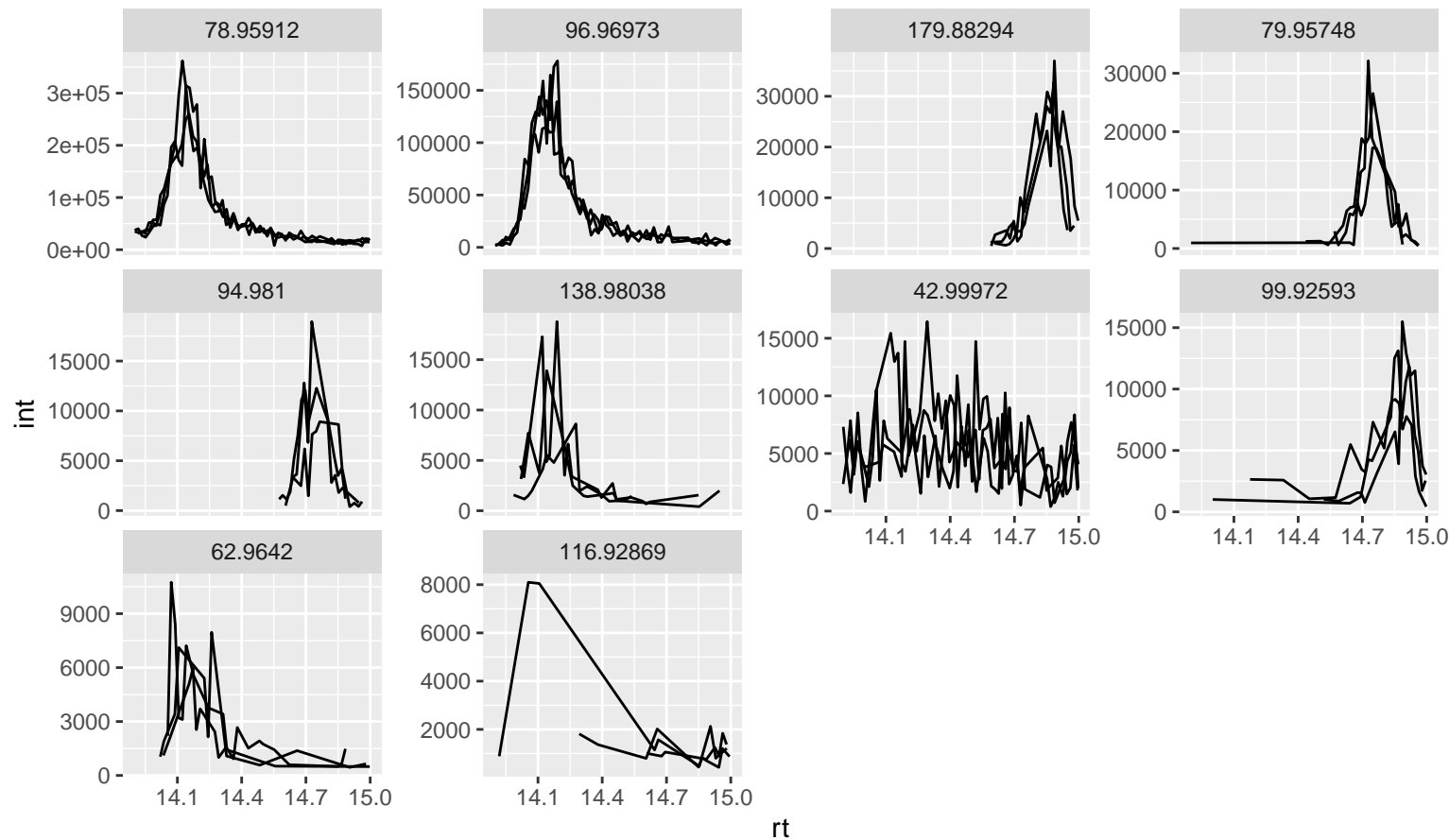
D-Glucose 1-phosphate (neg) 259.022447



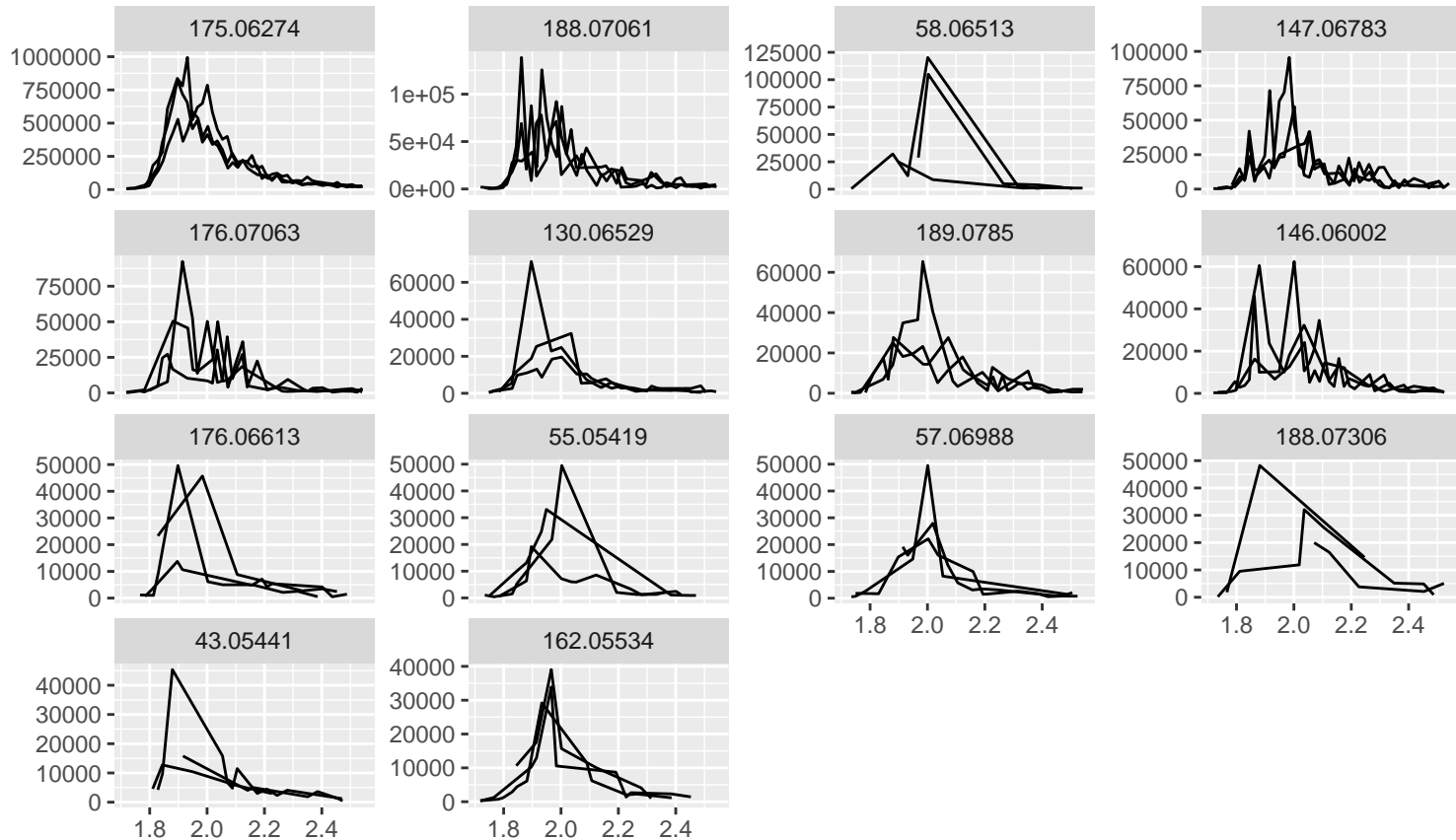
D-Glucose 6-phosphate (pos) 261.036999



D-Glucose 6-phosphate (neg) 259.022447



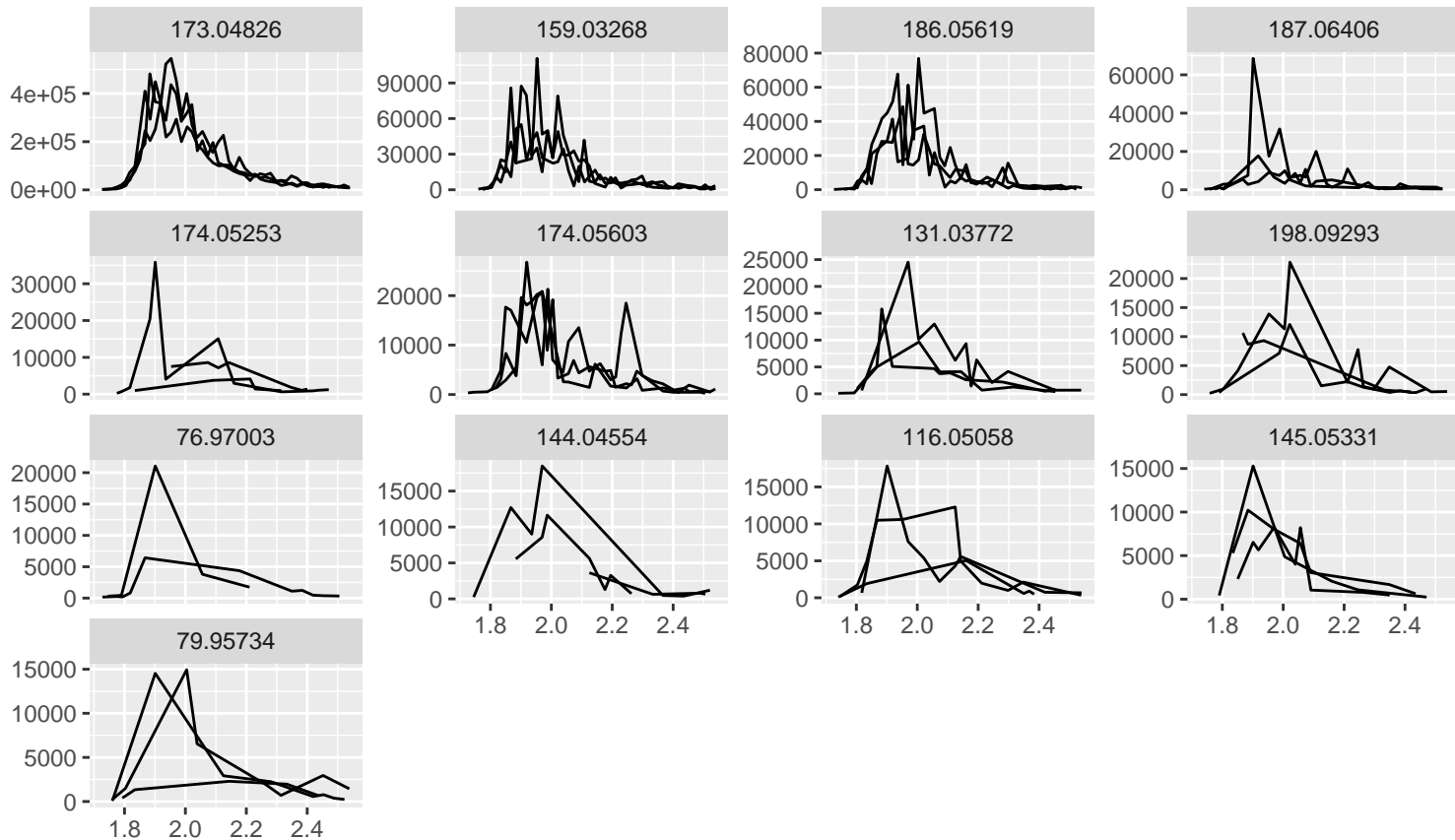
2-Heptyl-3-hydroxy-quinolone (pos) 260.164505



rt

2-Heptyl-3-hydroxy-quinolone (neg) 258.149953

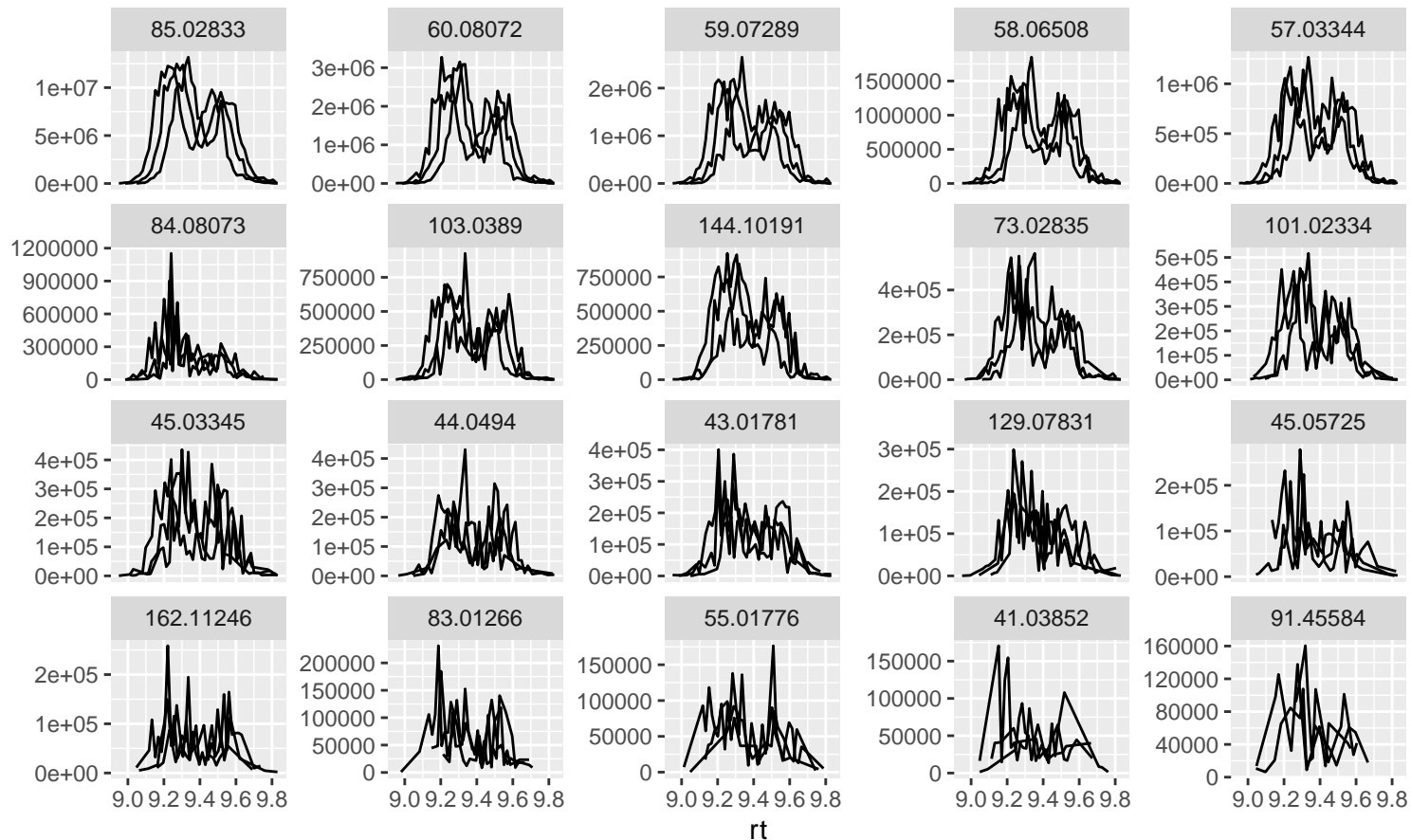
int



rt

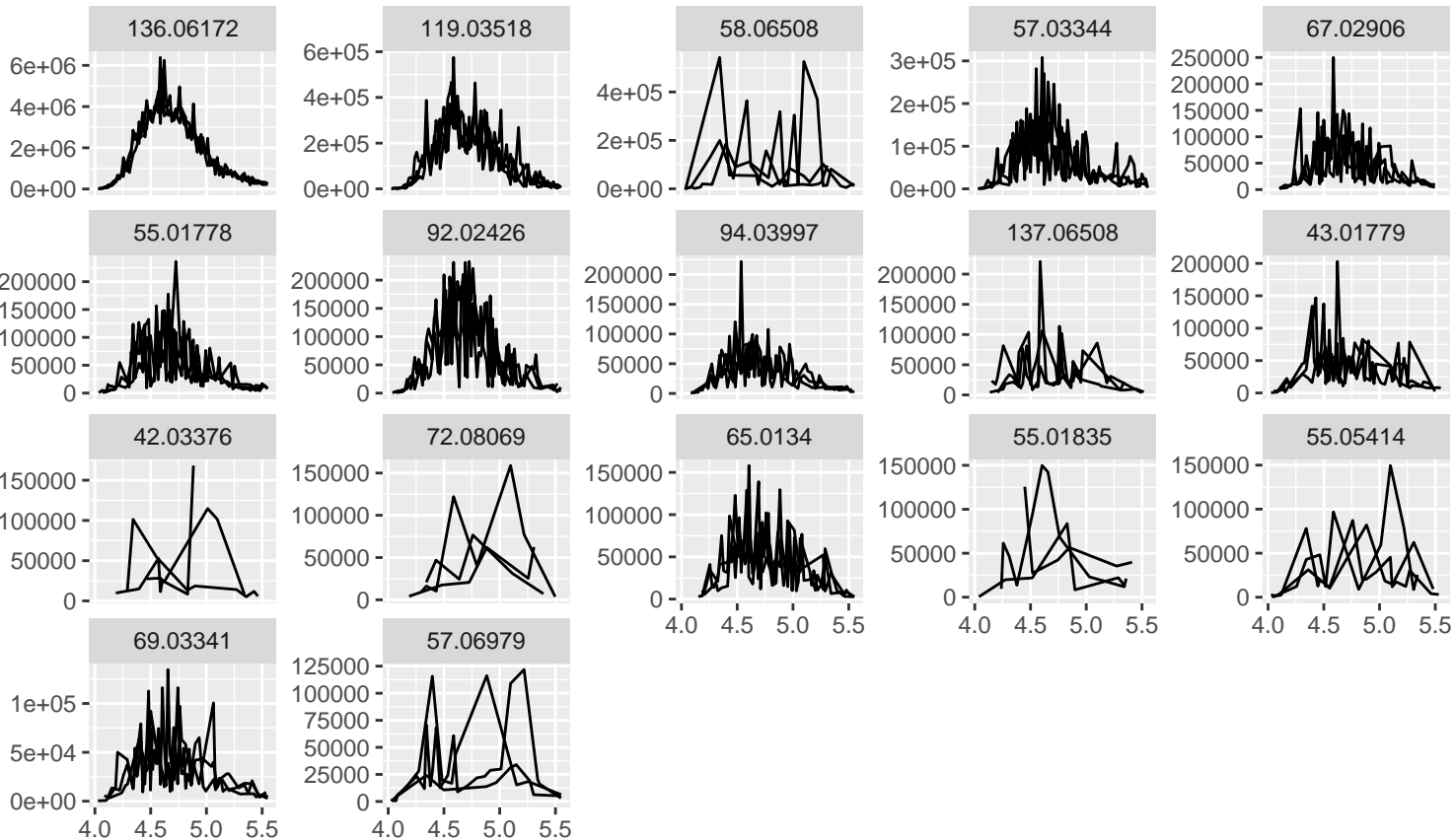
O-Methylmalonyl-L-carnitine (pos) 262.128515

int



Adenosine (pos) 268.104031

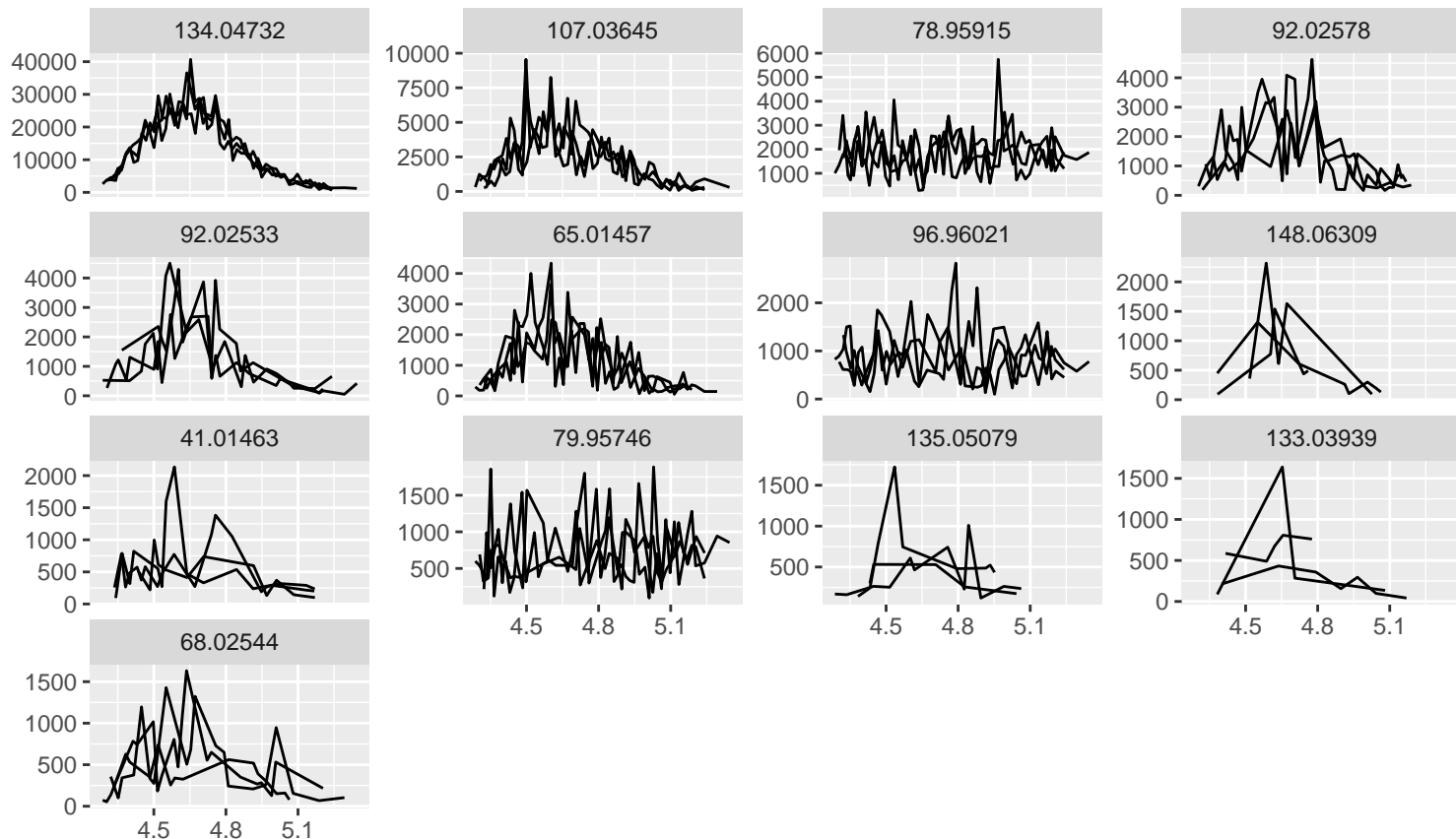
int



rt

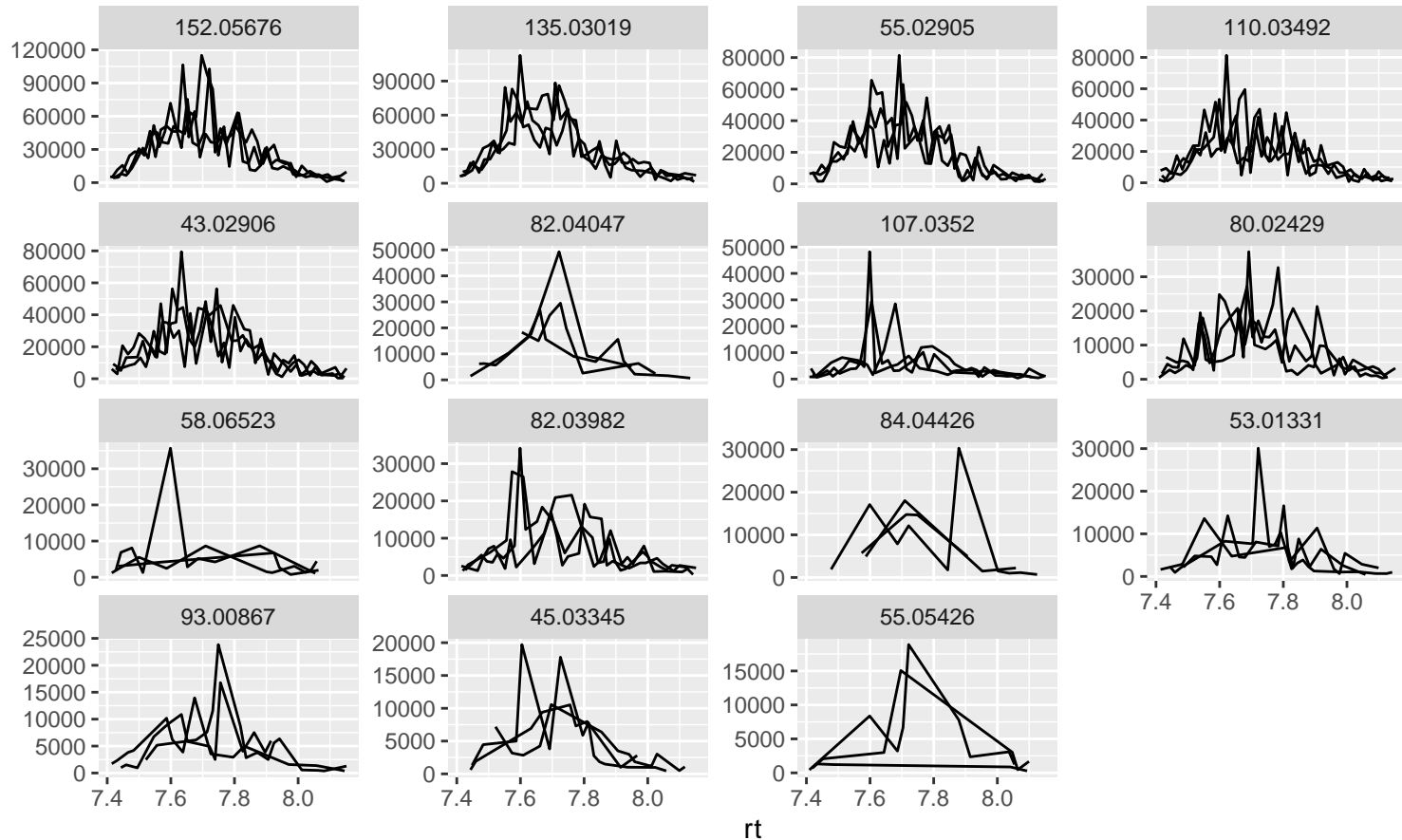
Adenosine (neg) 266.089479

int



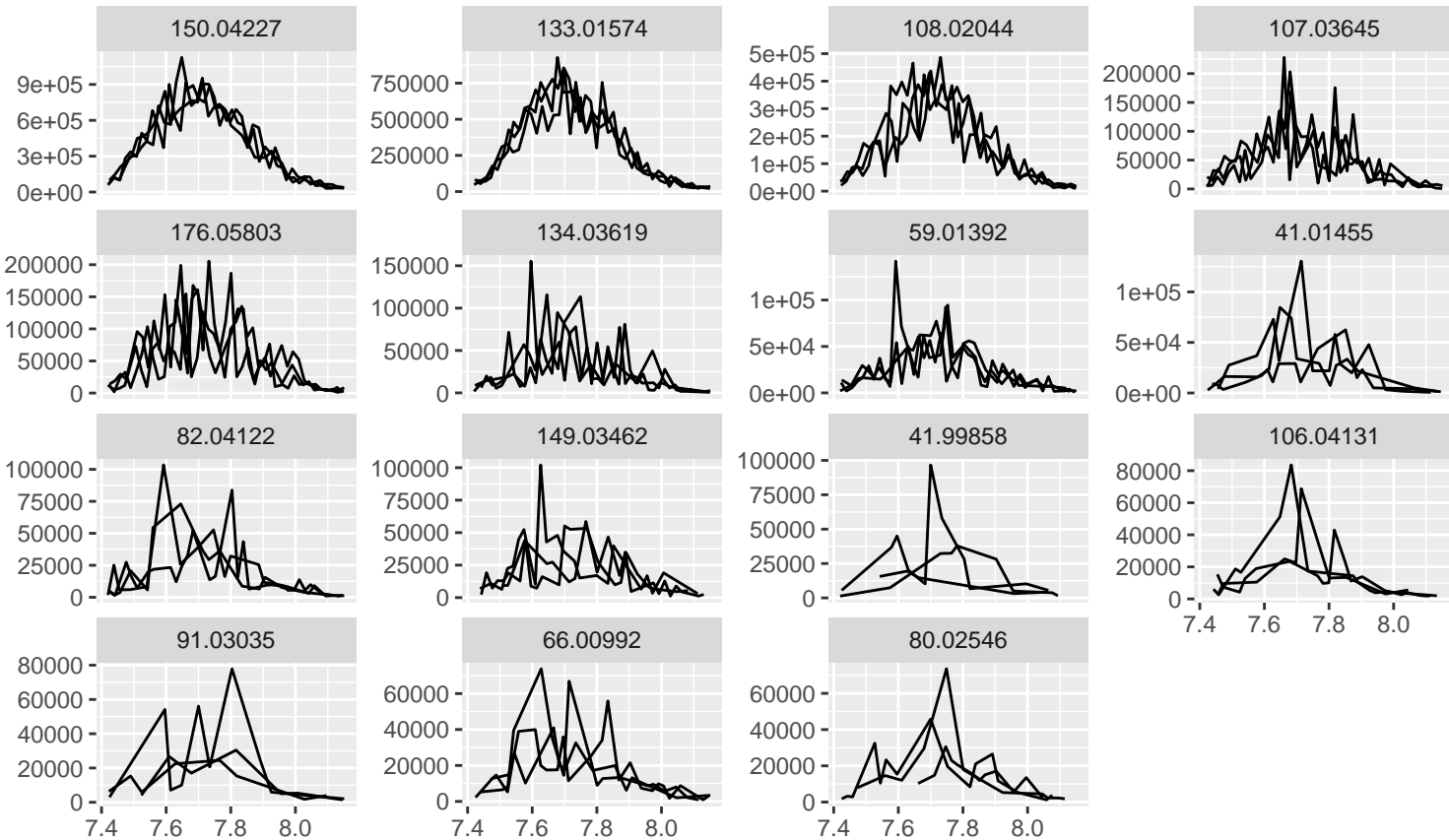
rt

Deoxyguanosine (pos) 268.104031

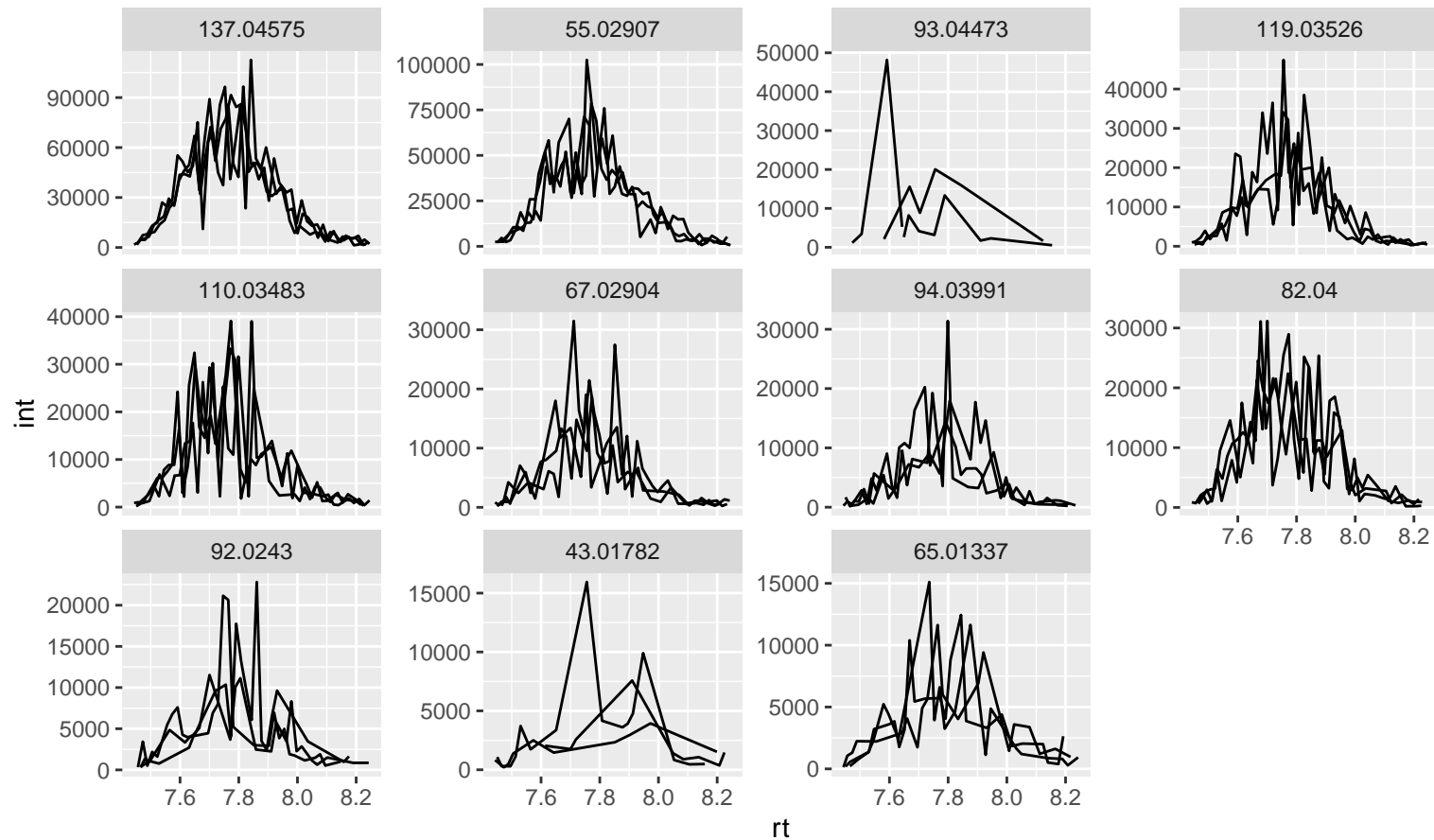


Deoxyguanosine (neg) 266.089479

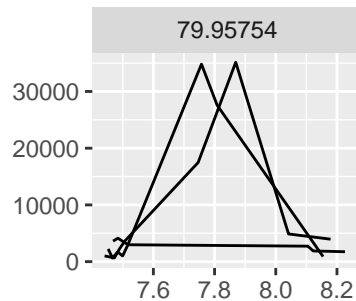
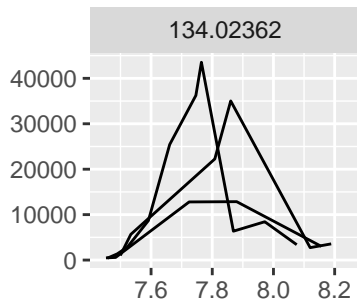
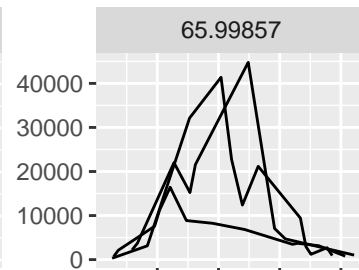
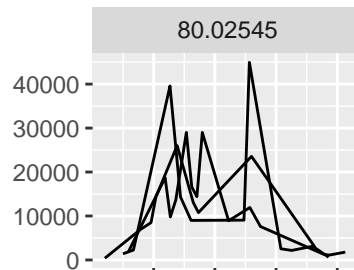
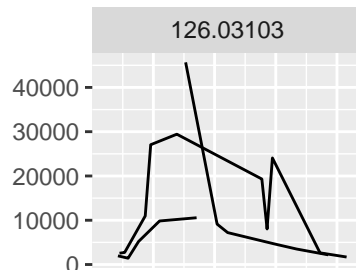
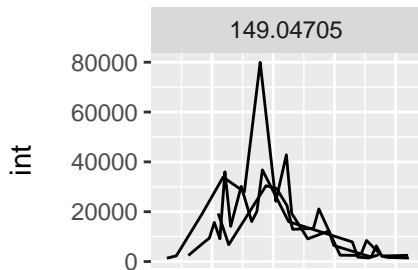
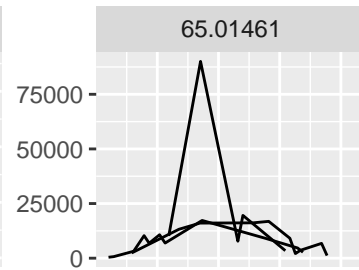
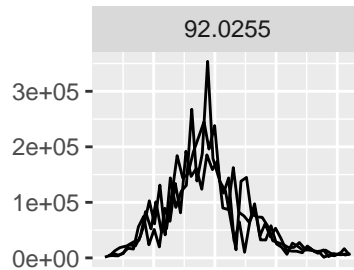
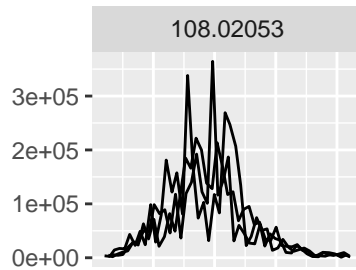
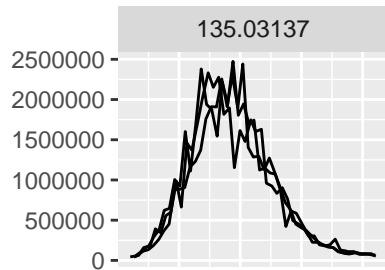
int



Inosine (pos) 269.088047



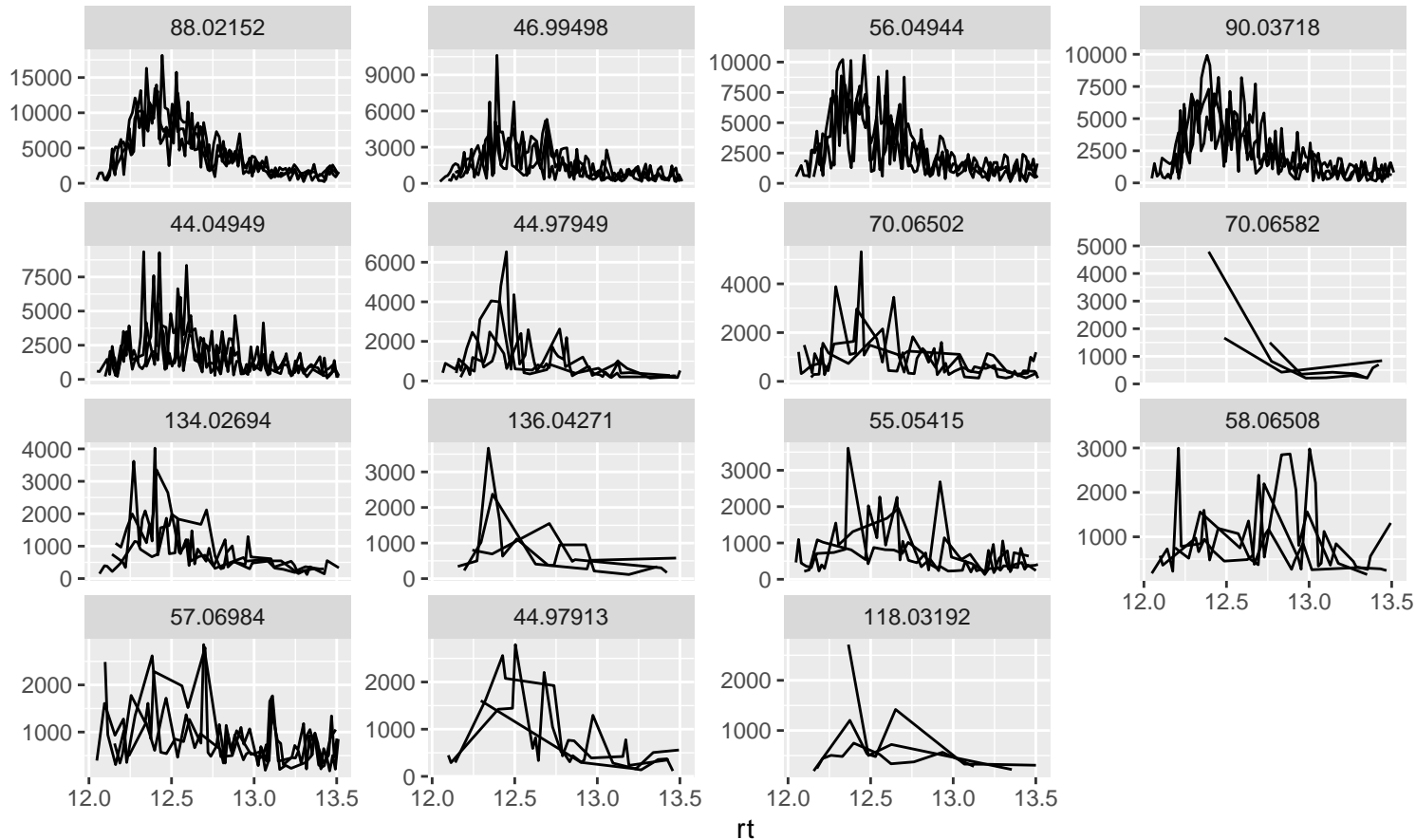
Inosine (neg) 267.073495



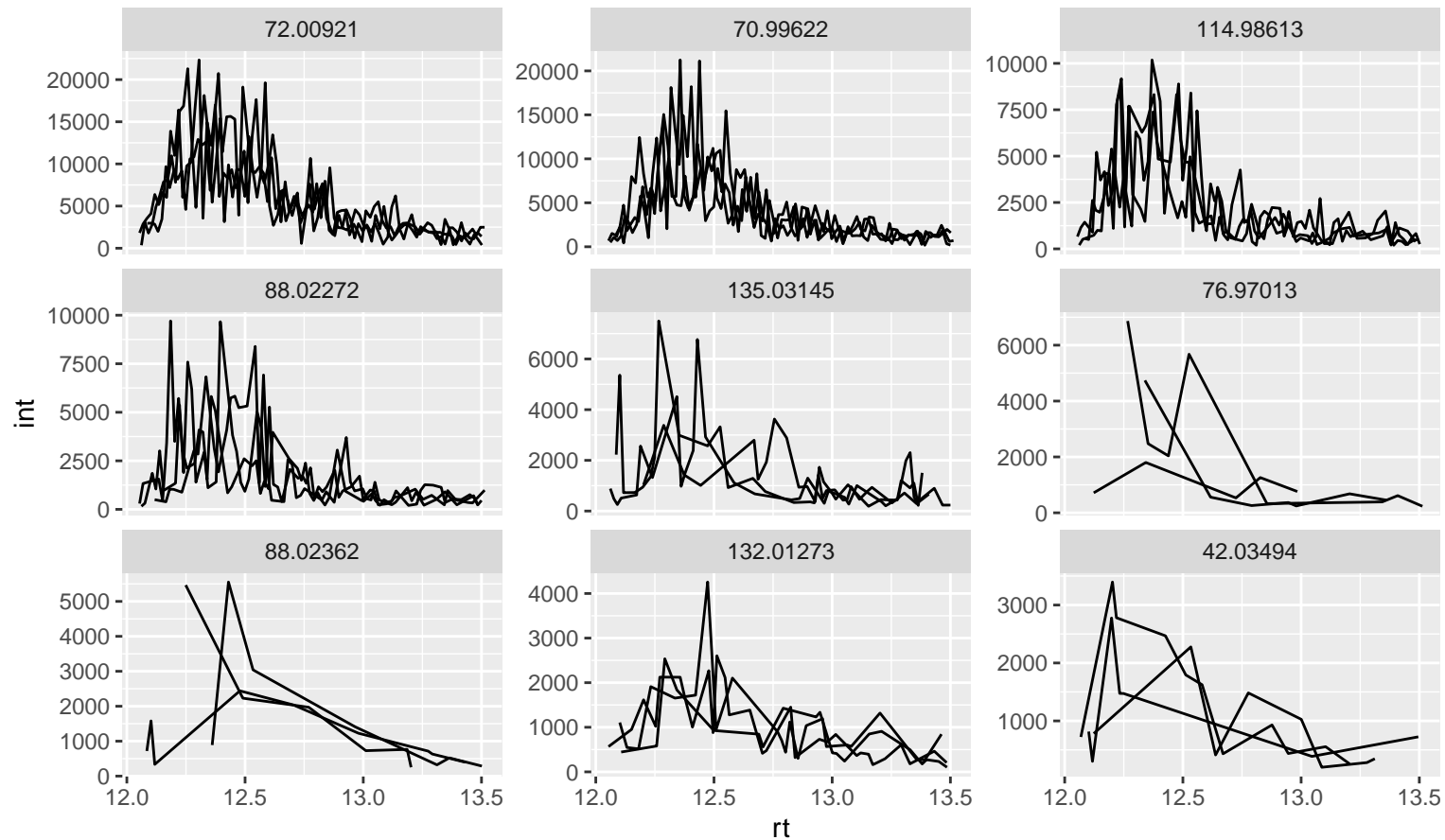
rt

L-Homocystine (pos) 269.062428

int

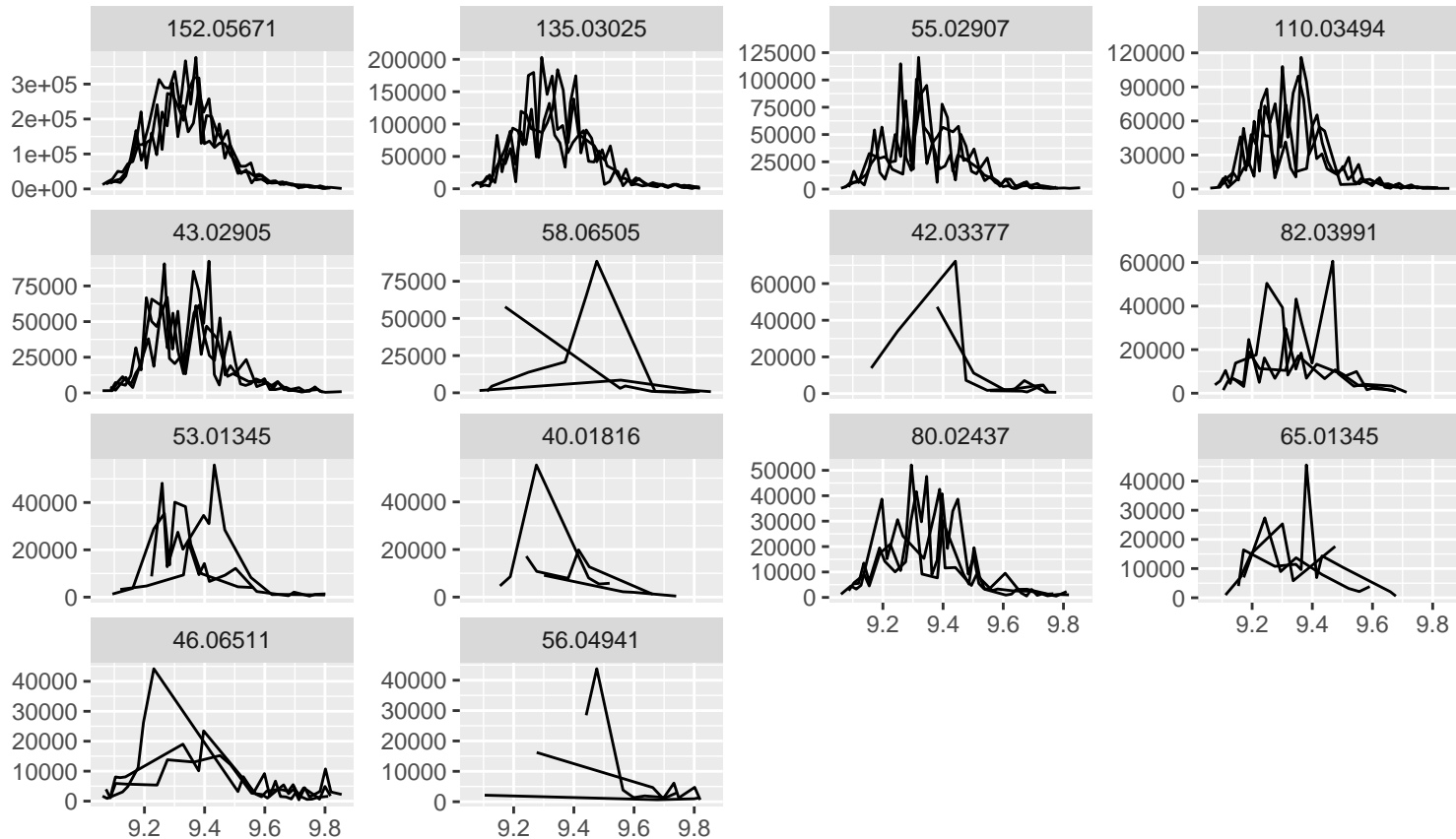


L-Homocystine (neg) 267.047876



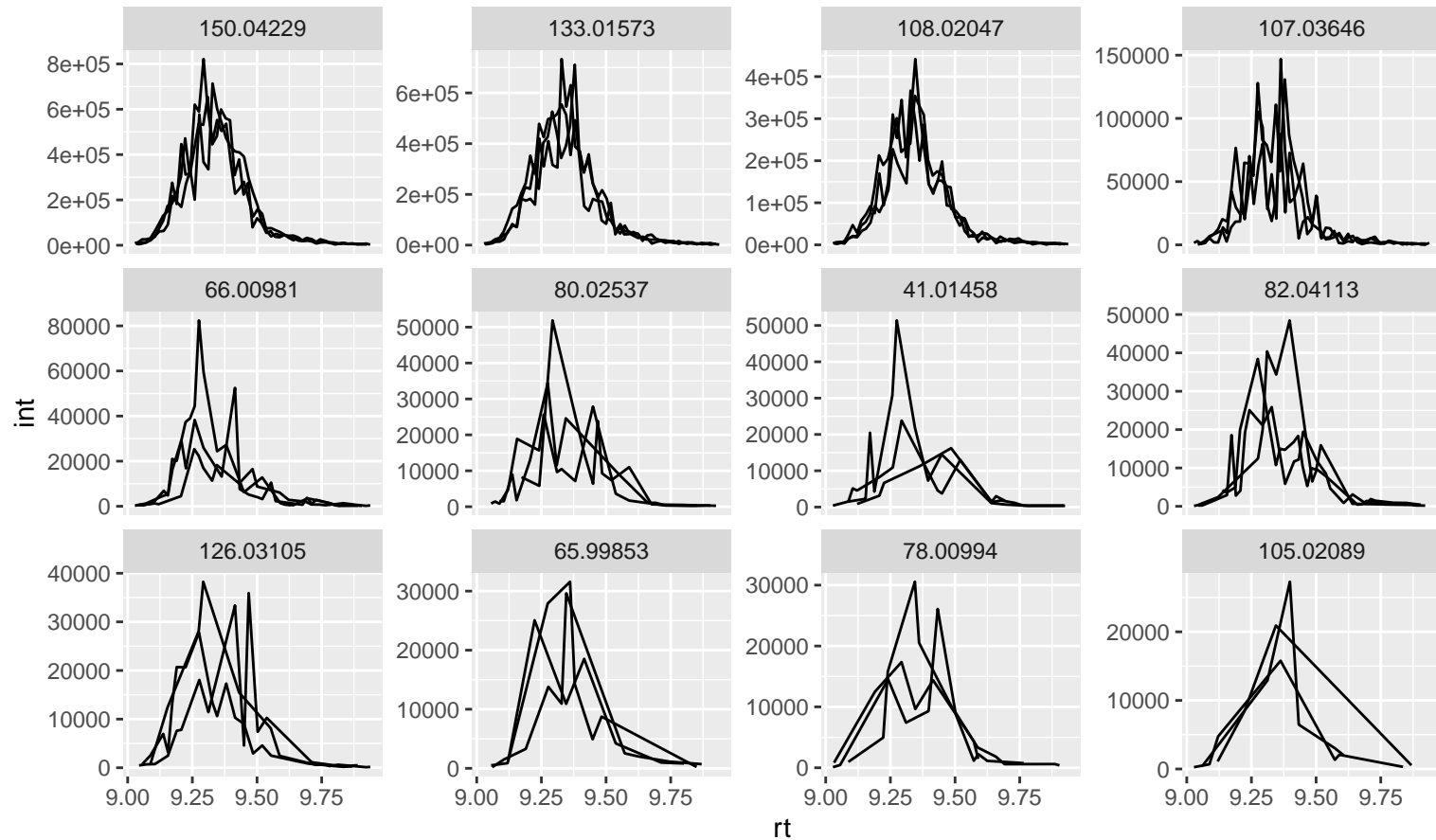
Guanosine (pos) 284.098946

int

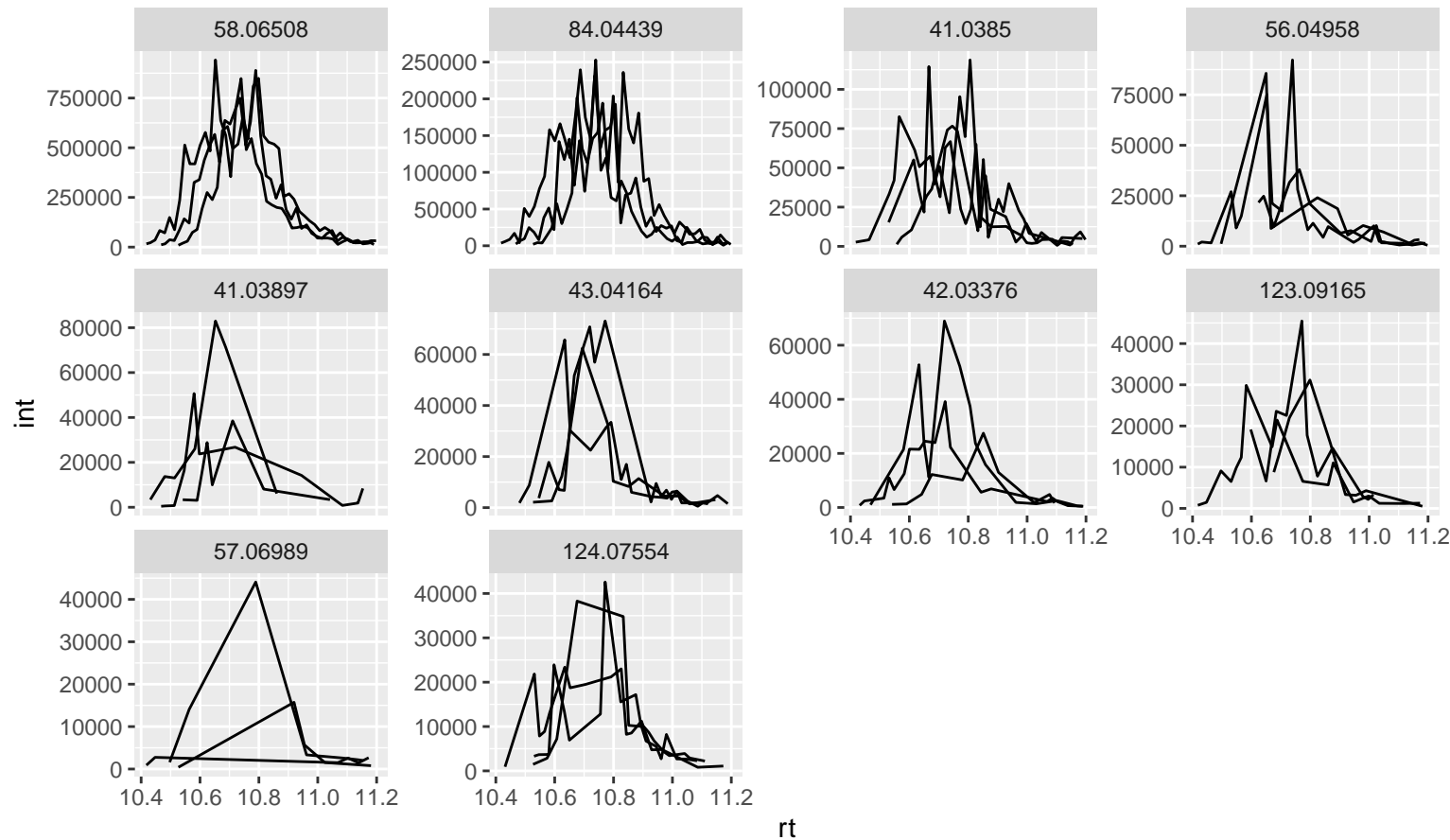


rt

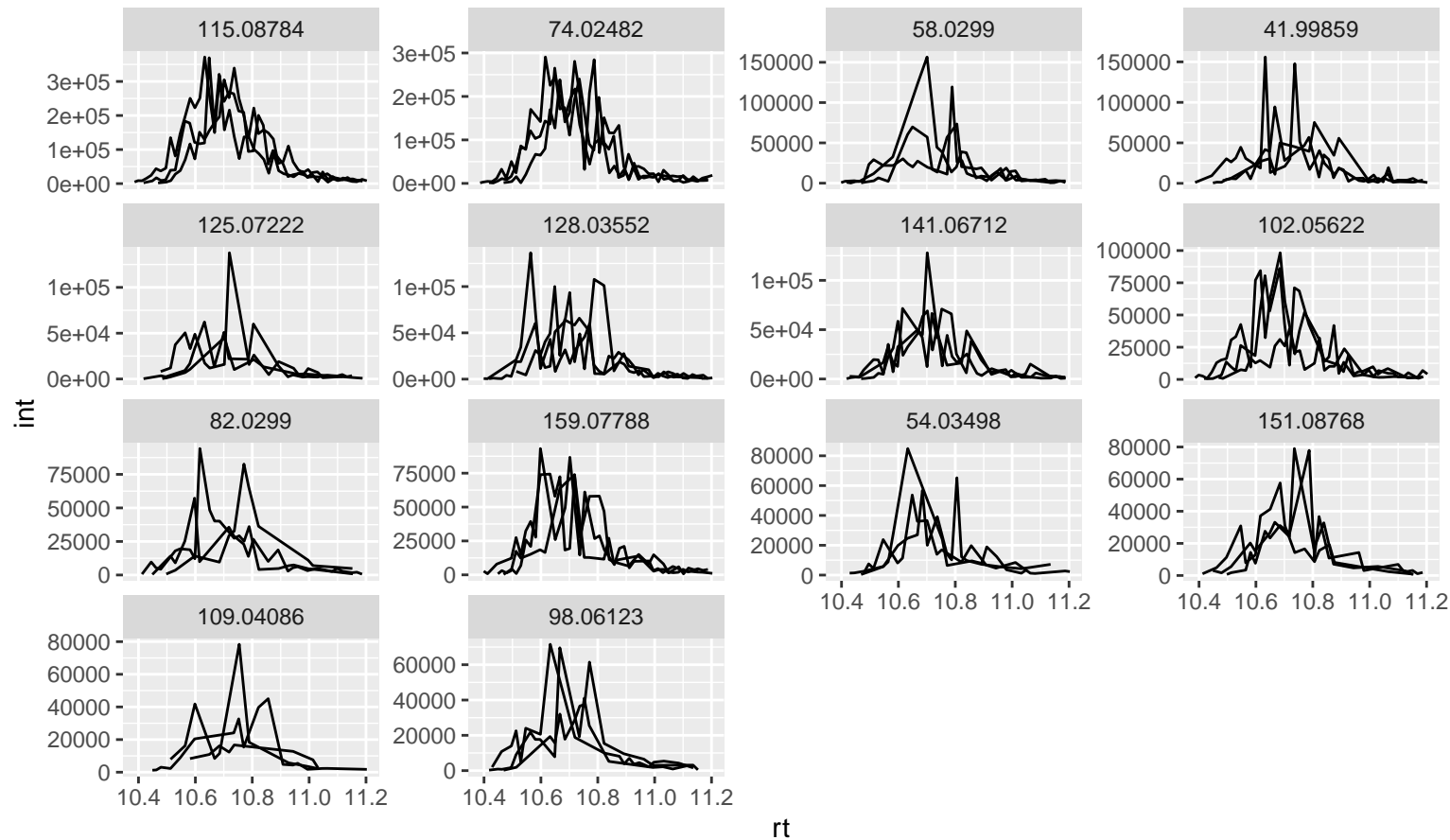
Guanosine (neg) 282.084394



Ophthalmic acid (pos) 290.134663

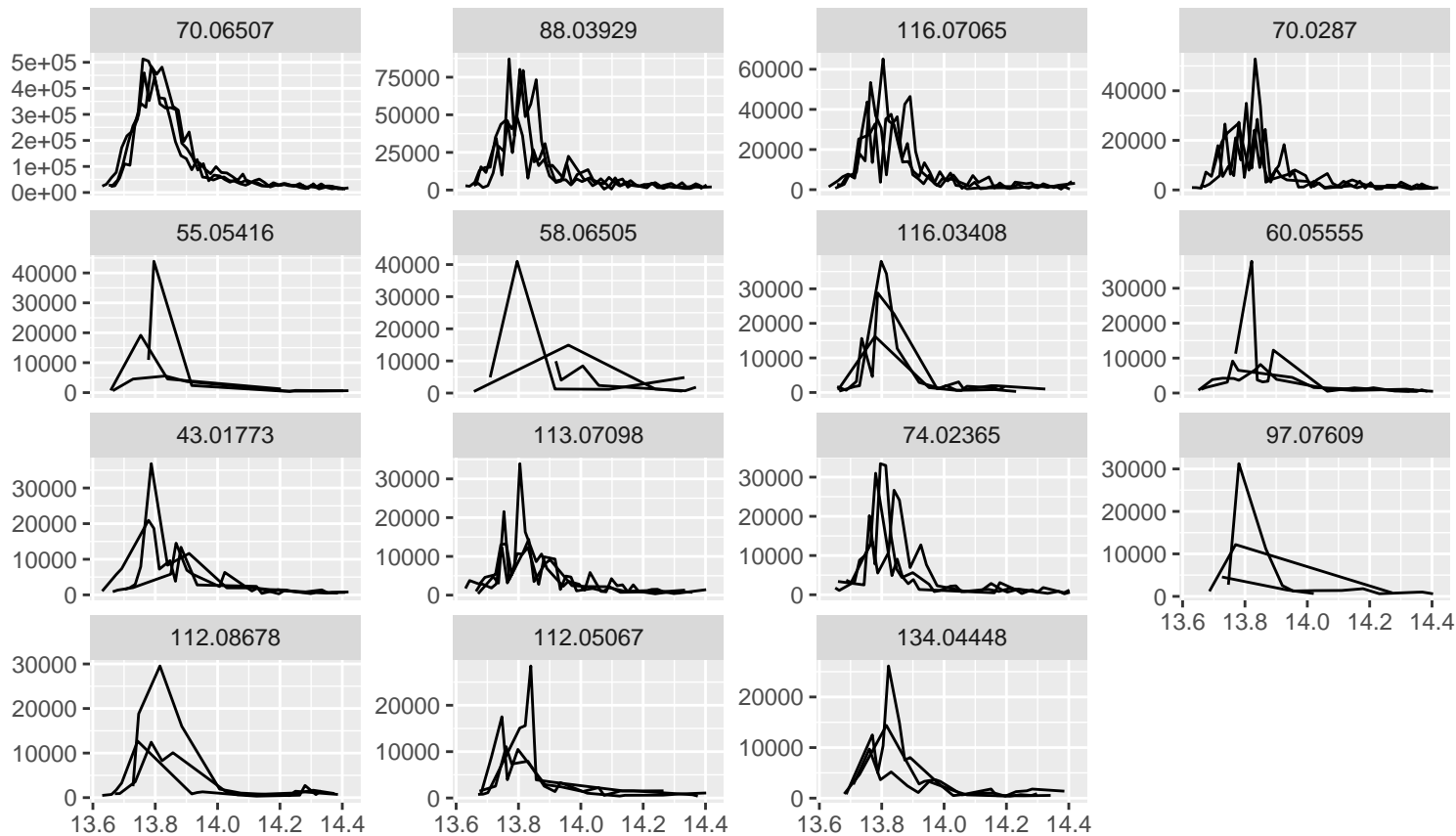


Ophthalmic acid (neg) 288.120111



L-Argininosuccinic acid (pos) 291.129912

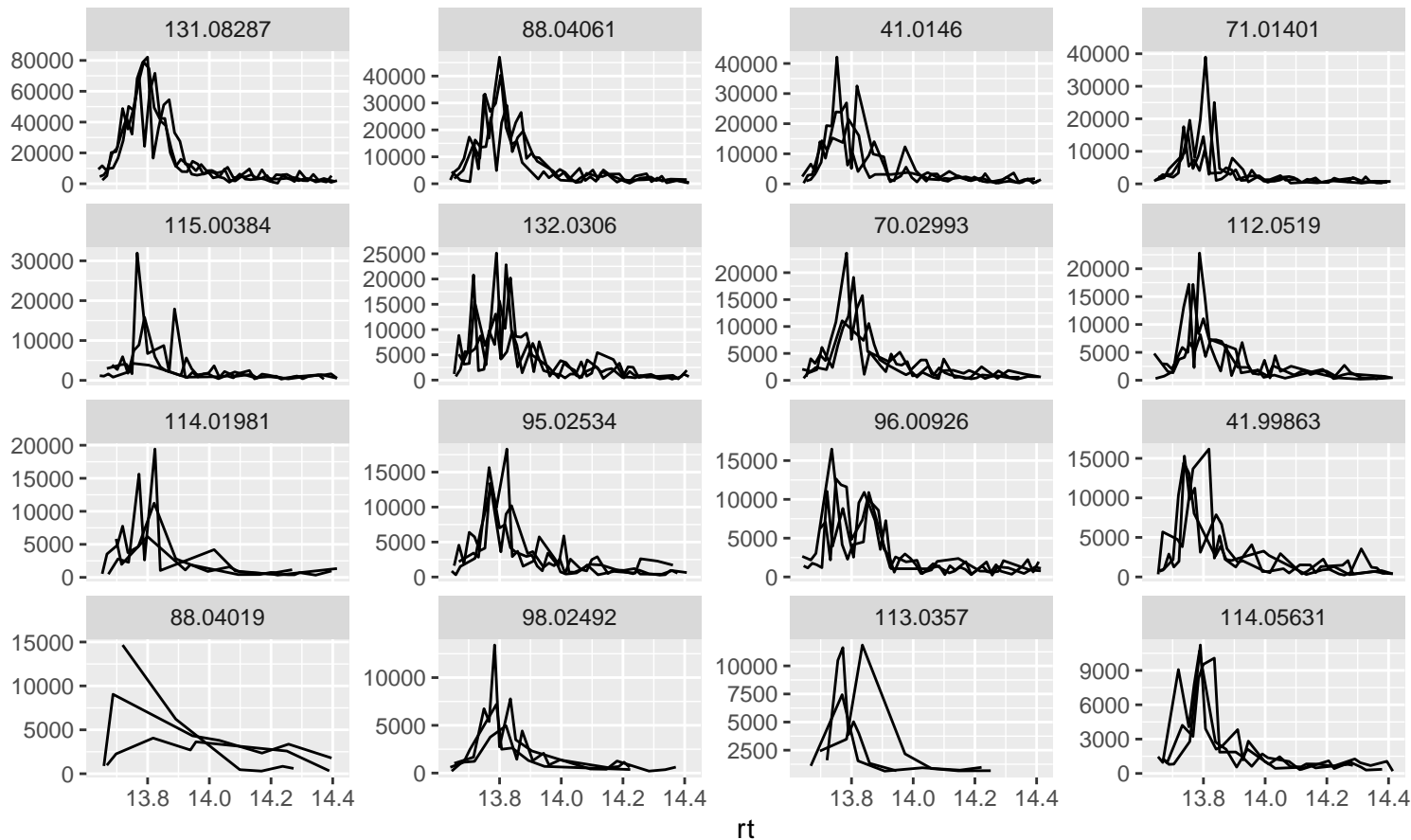
int



rt

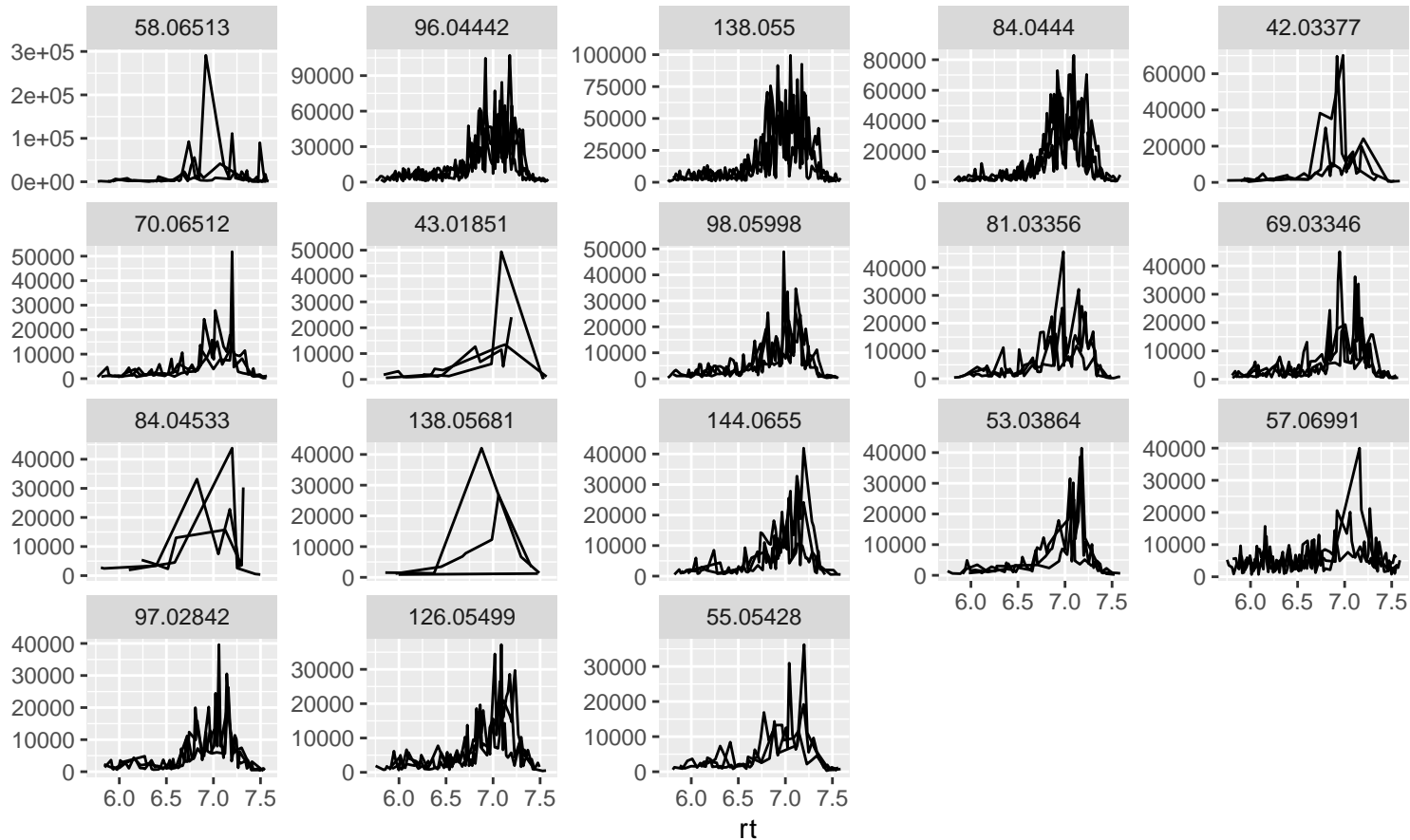
L-Arginosuccinic acid (neg) 289.11536

int

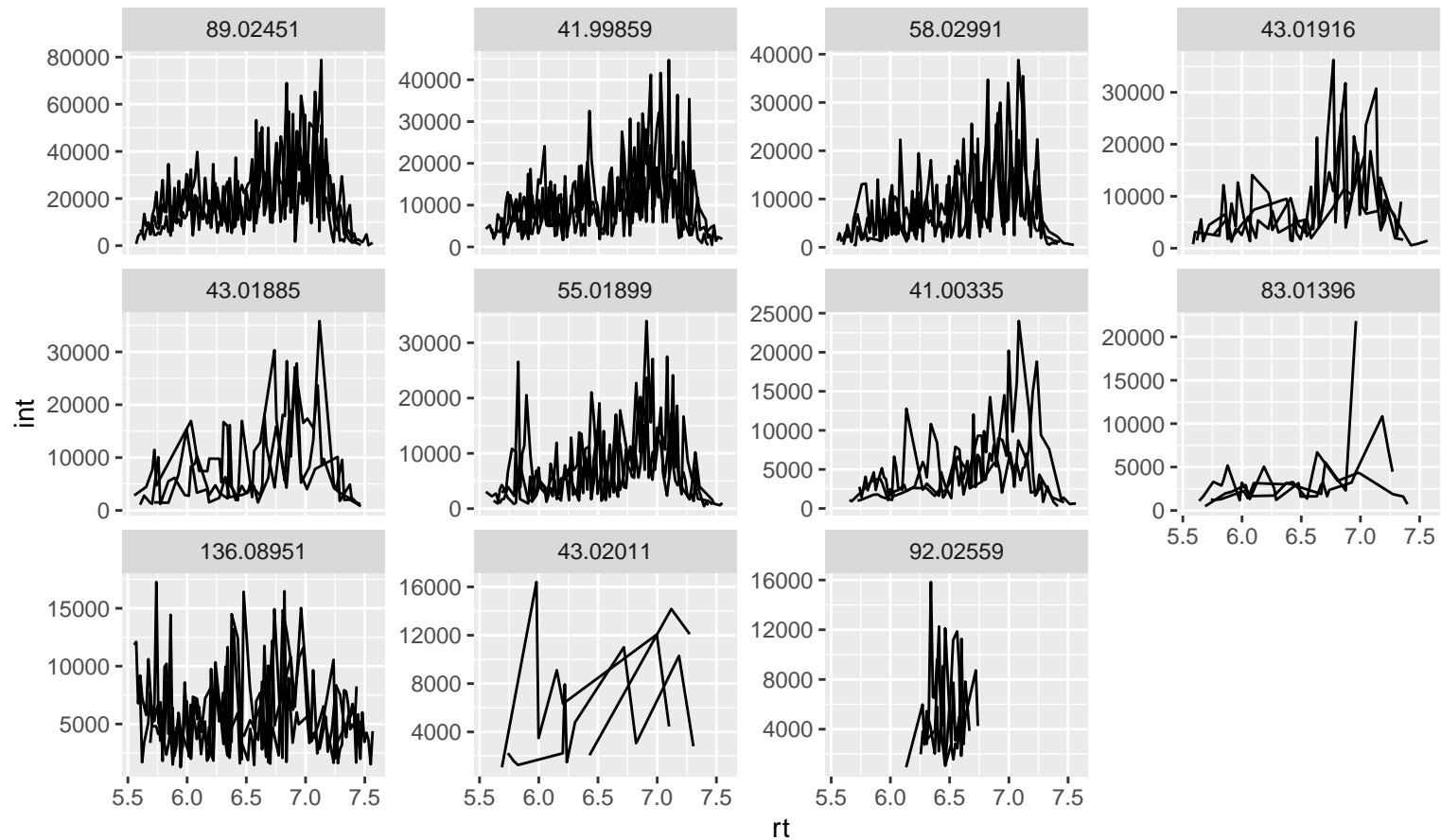


N-Acetylmuramic acid (pos) 294.118345

int

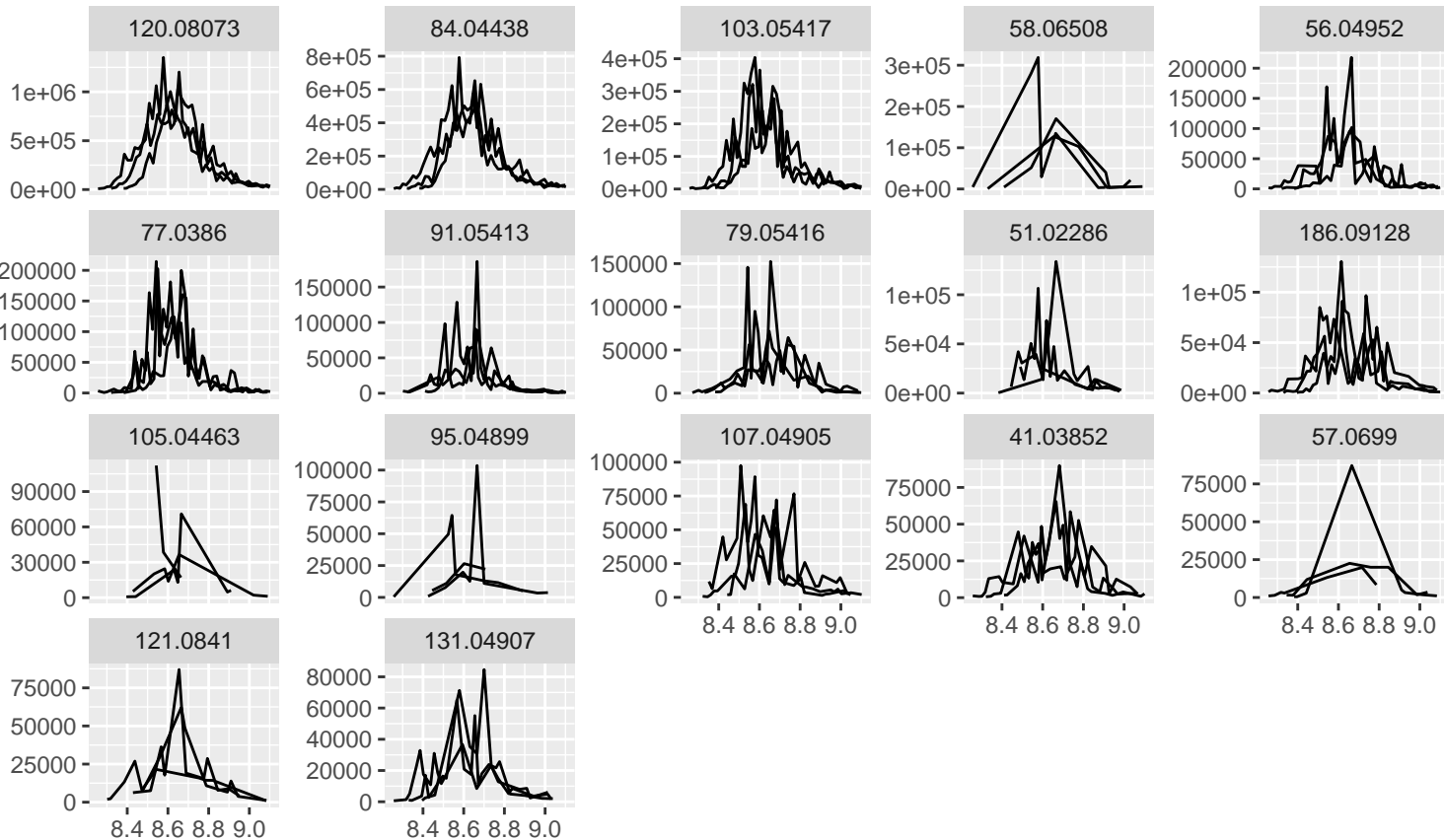


N-Acetylmuramic acid (neg) 292.103793



Glutamylphenylalanine (pos) 295.128849

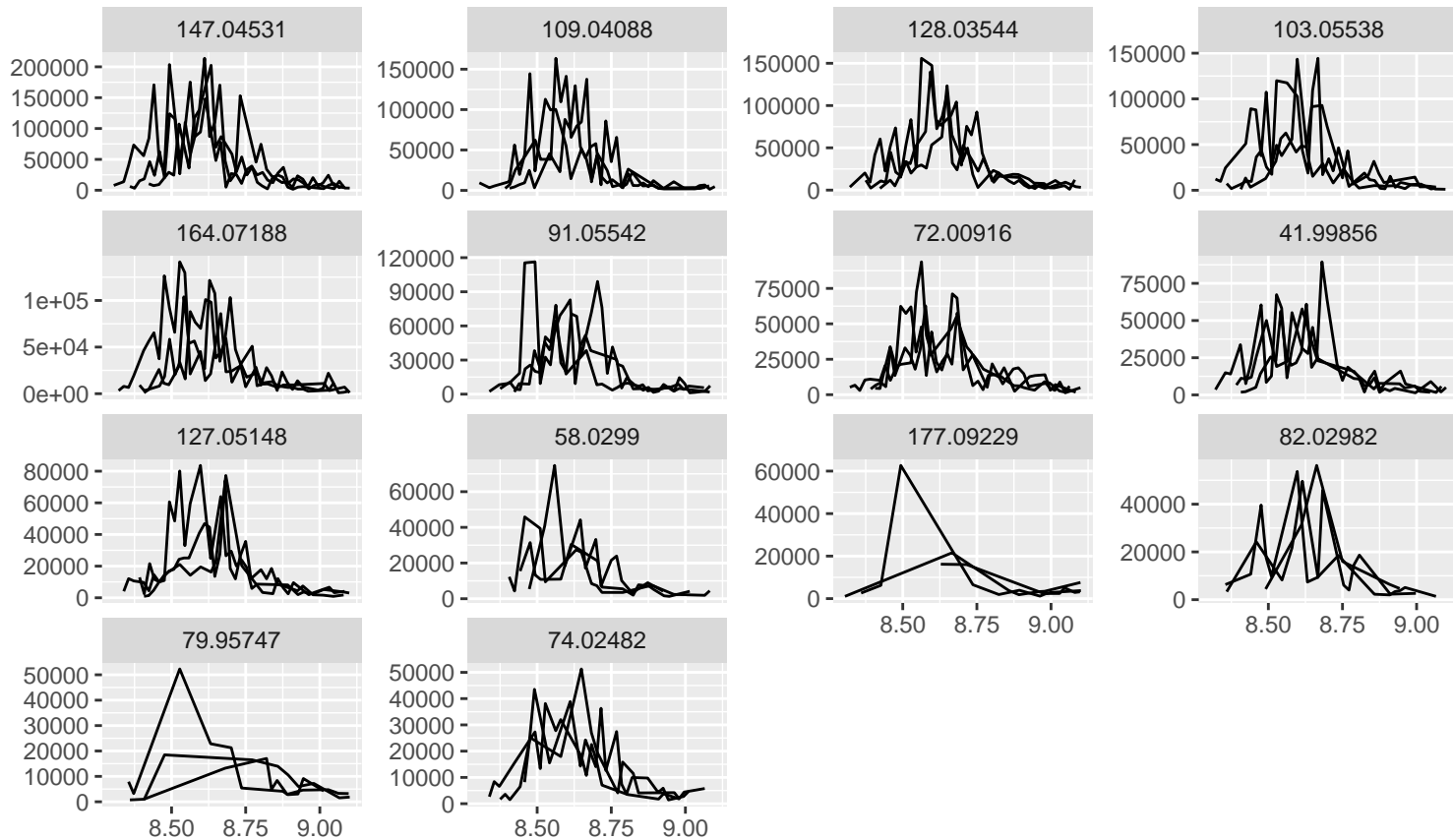
int



rt

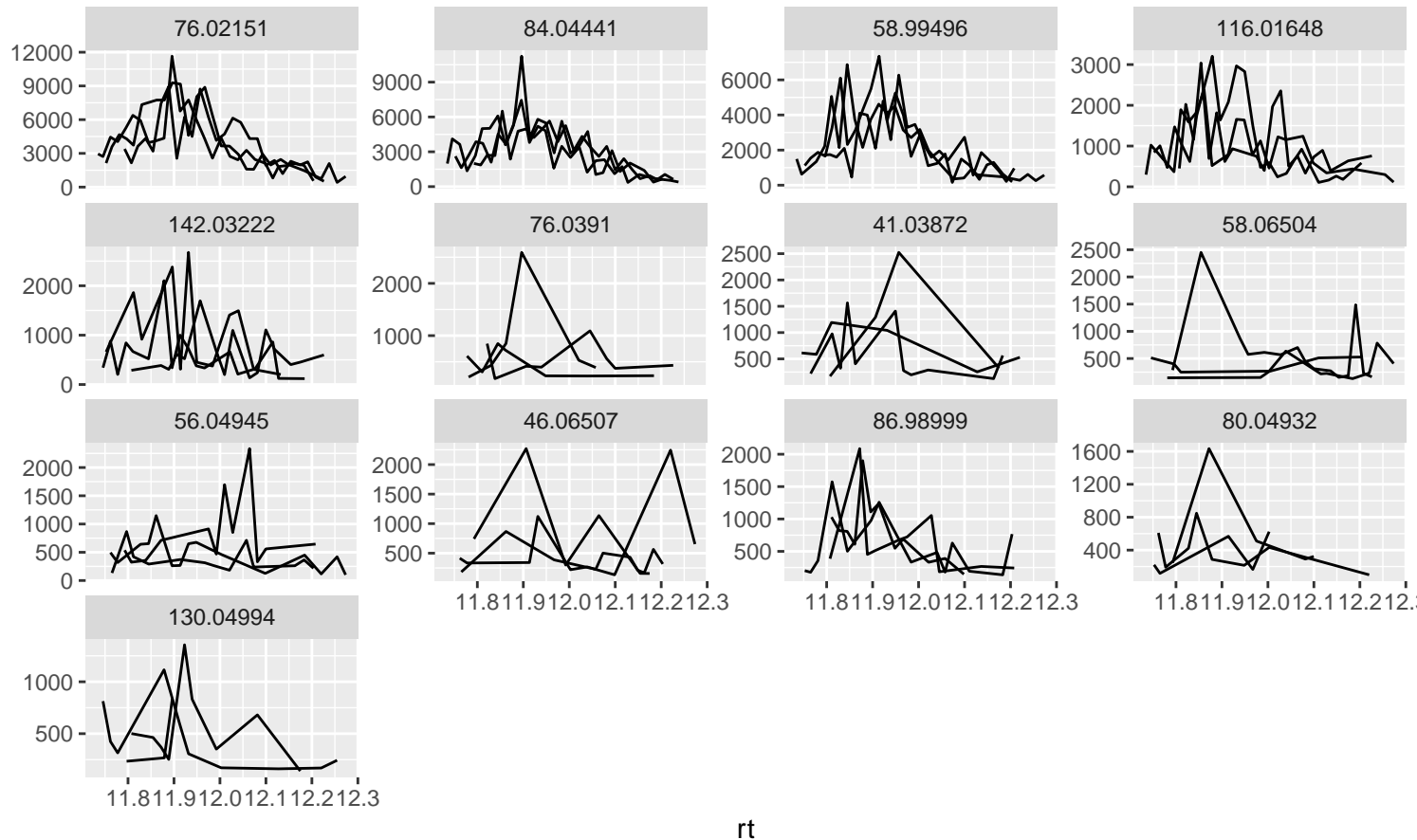
Glutamylphenylalanine (neg) 293.114297

int

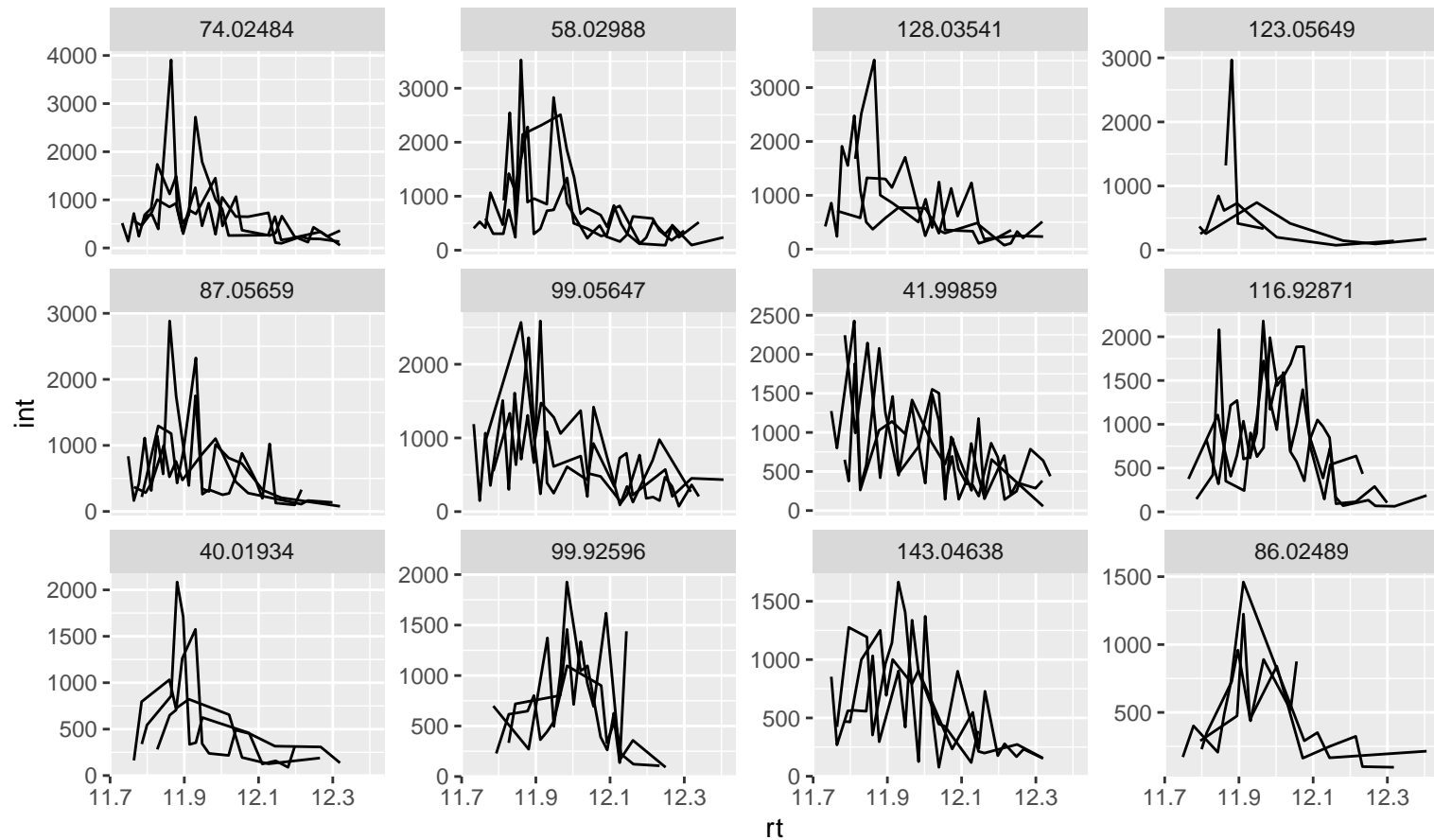


rt

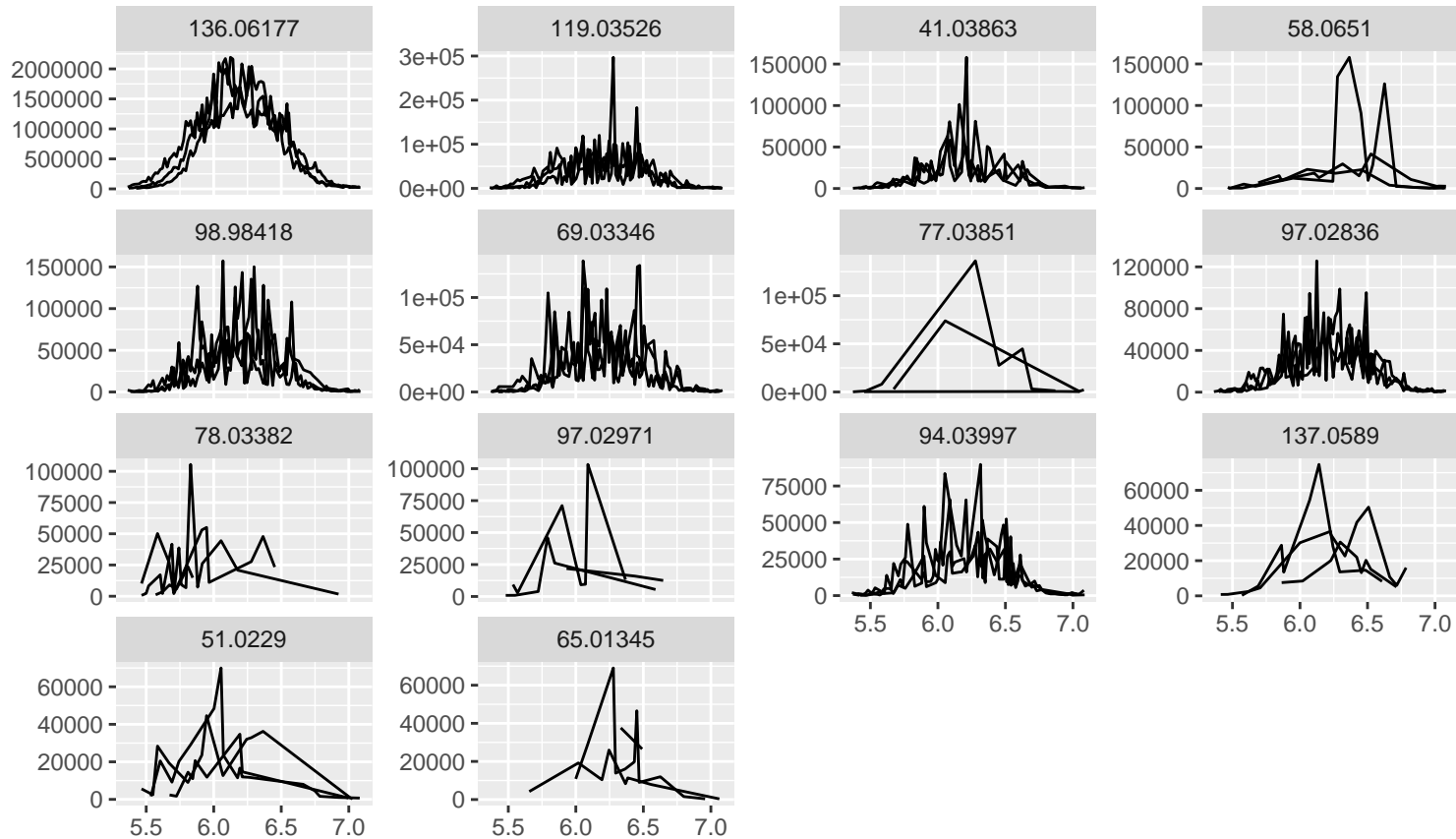
Glutathione (pos) 308.091085



Glutathione (neg) 306.076533



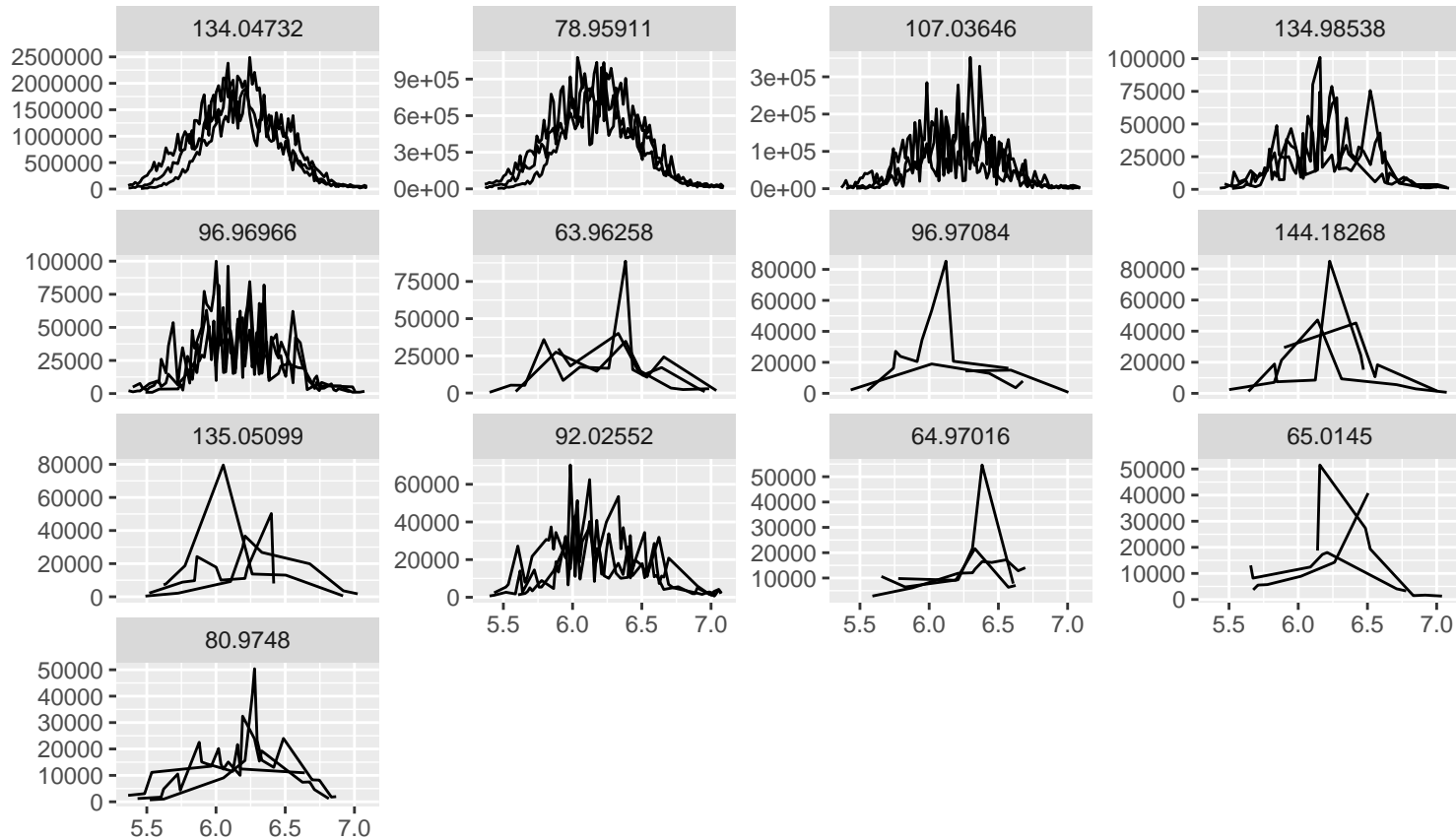
3',5'-Cyclic AMP (pos) 330.059799



rt

3',5'-Cyclic AMP (neg) 328.045247

int



rt

Sucrose (pos) 343.123491

57.0698

2000

1000

int

1500

1000

500

11.9

12.0

55.05419

1500

1000

500

11.9

12.0

43.05411

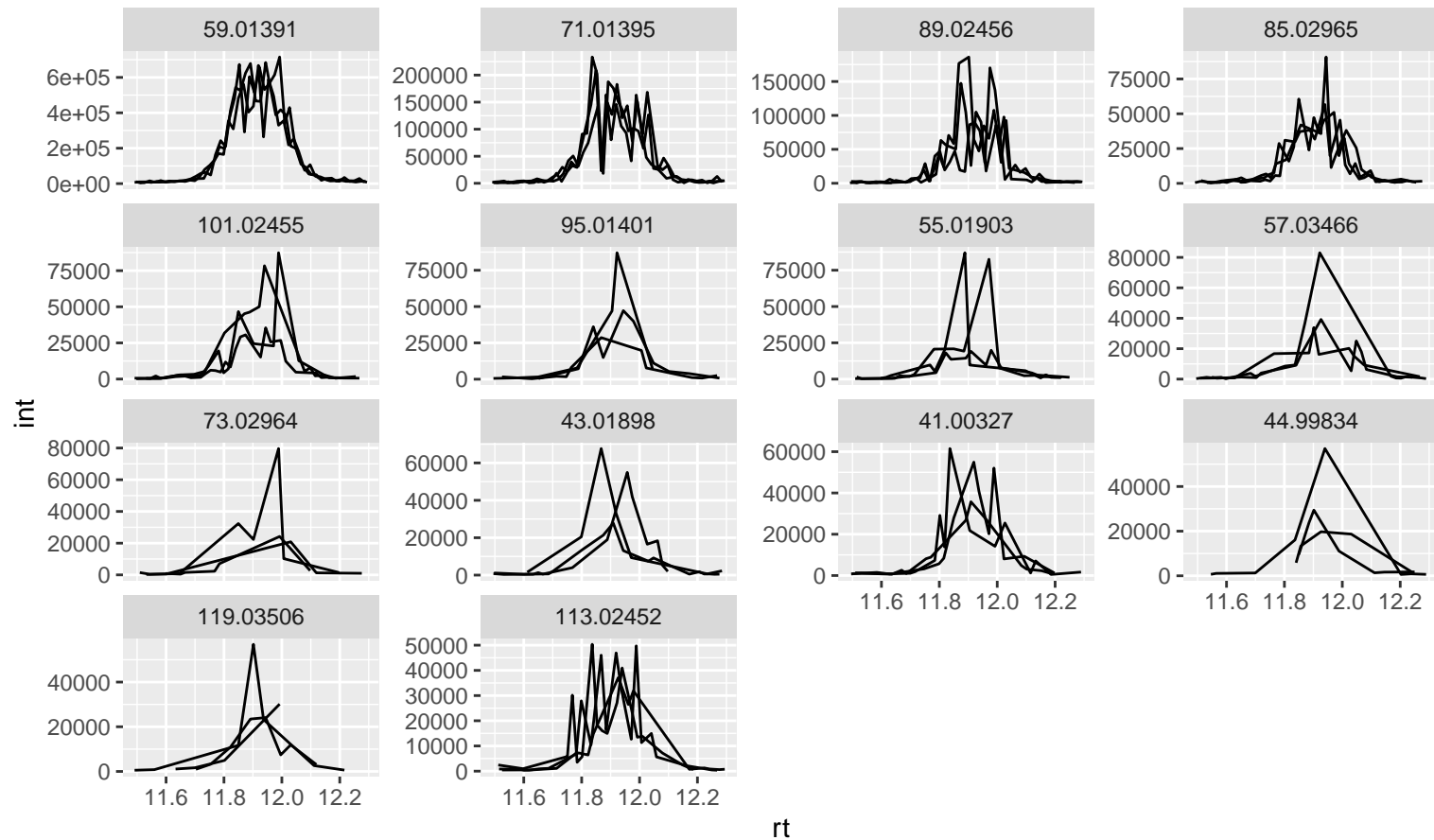
1500

1000

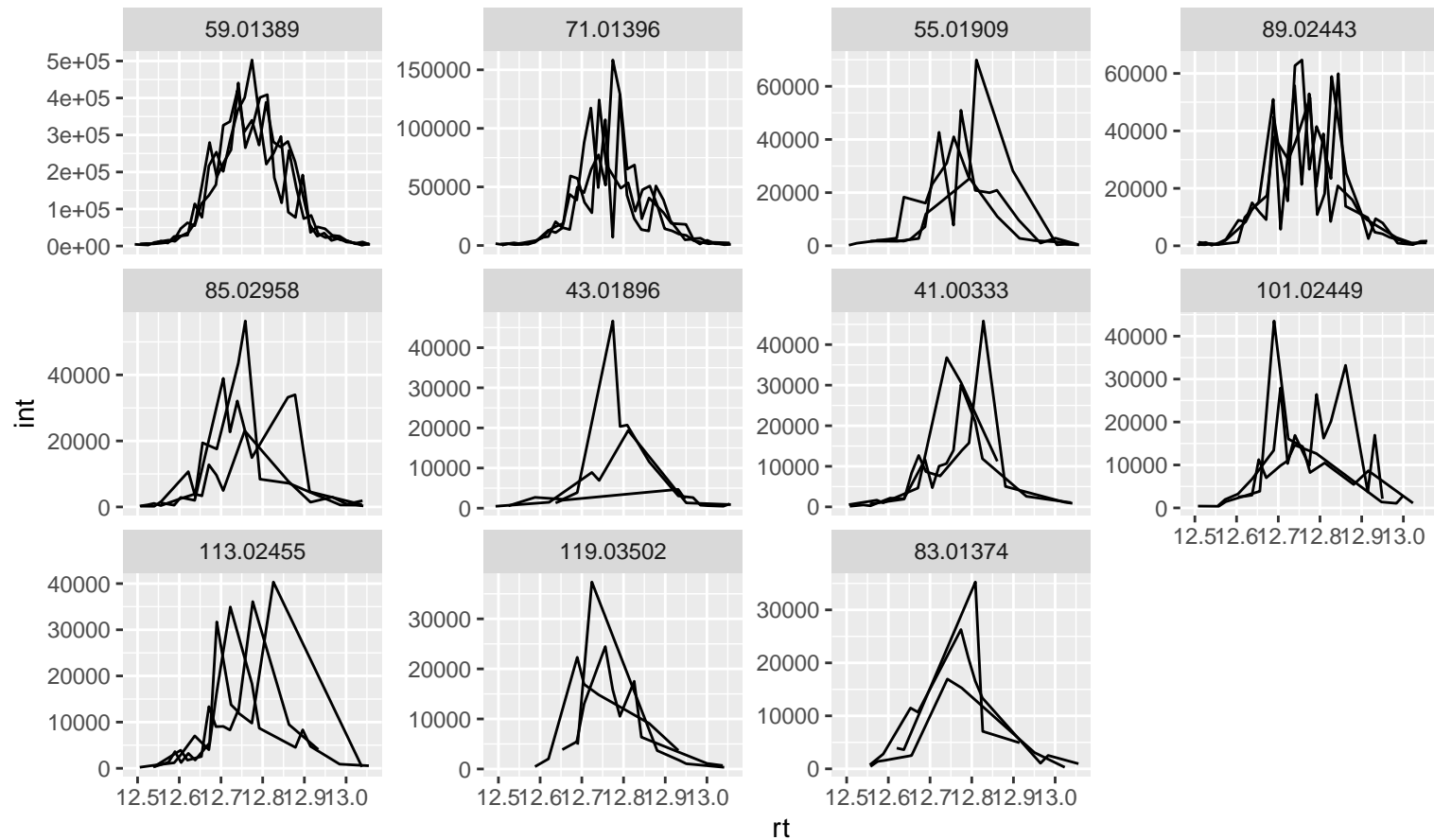
500

rt

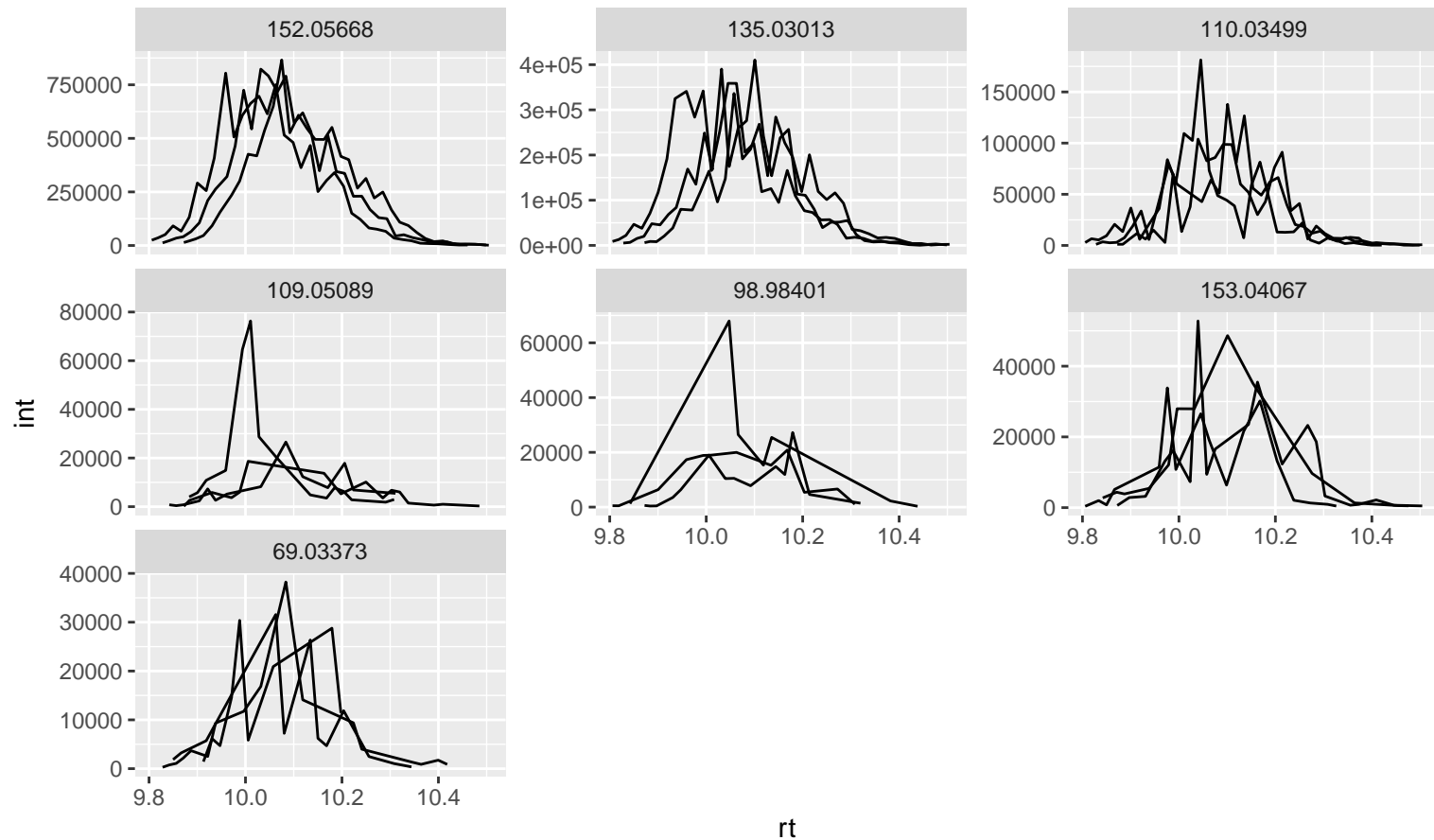
Sucrose (neg) 341.108939



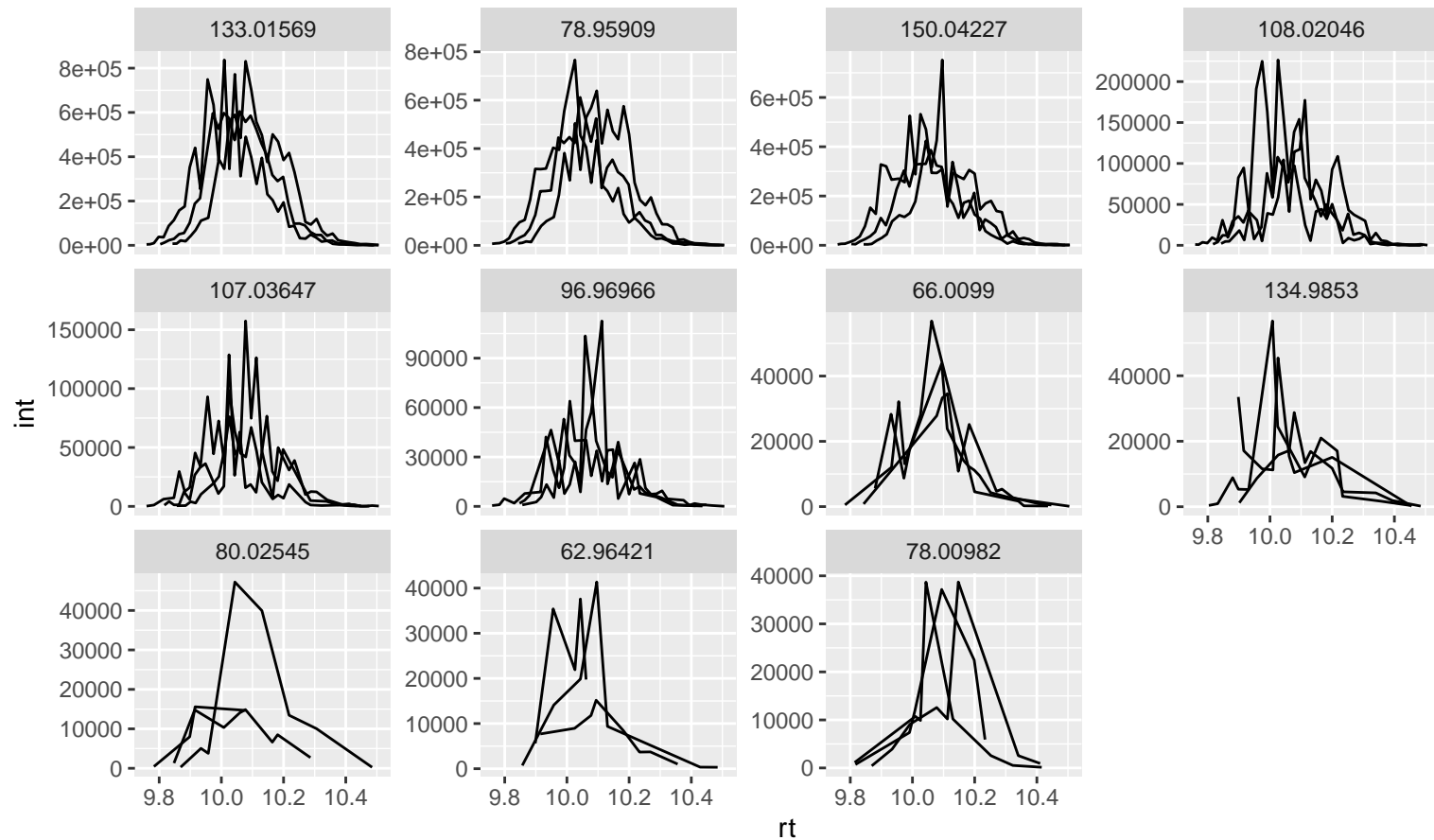
Trehalose (neg) 341.108939



3',5'-Cyclic GMP (pos) 346.054714

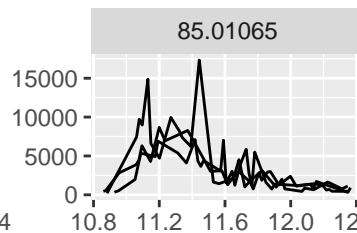
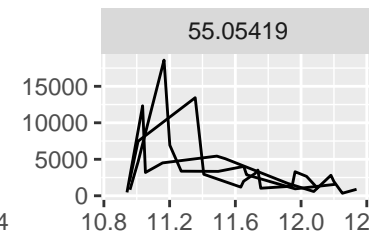
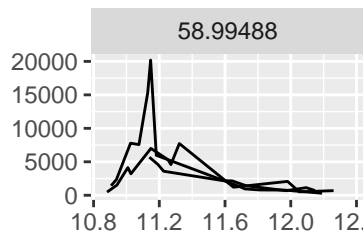
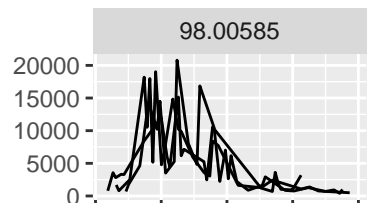
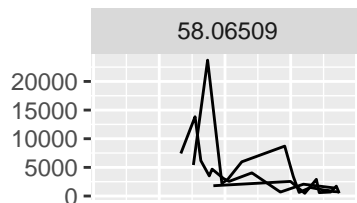
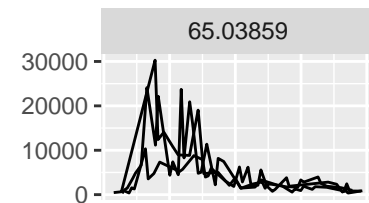
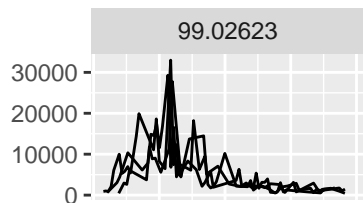
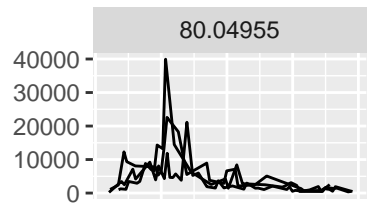
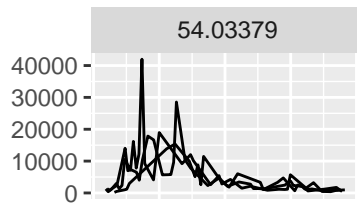
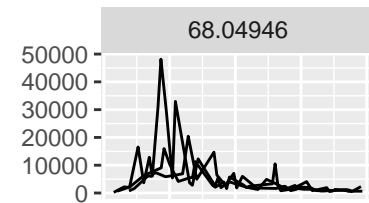
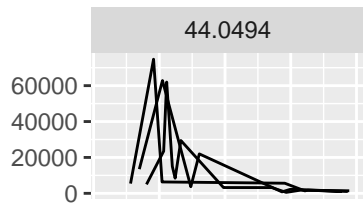
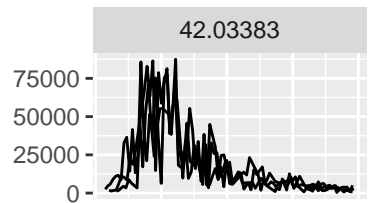
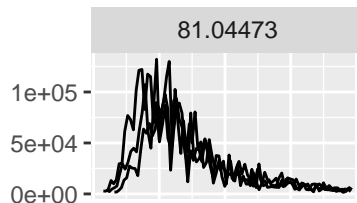
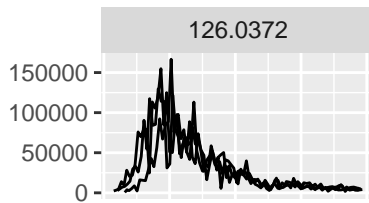
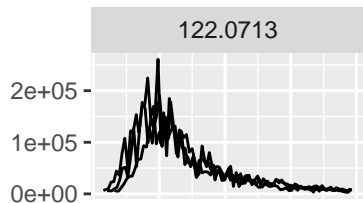


3',5'-Cyclic GMP (neg) 344.040162



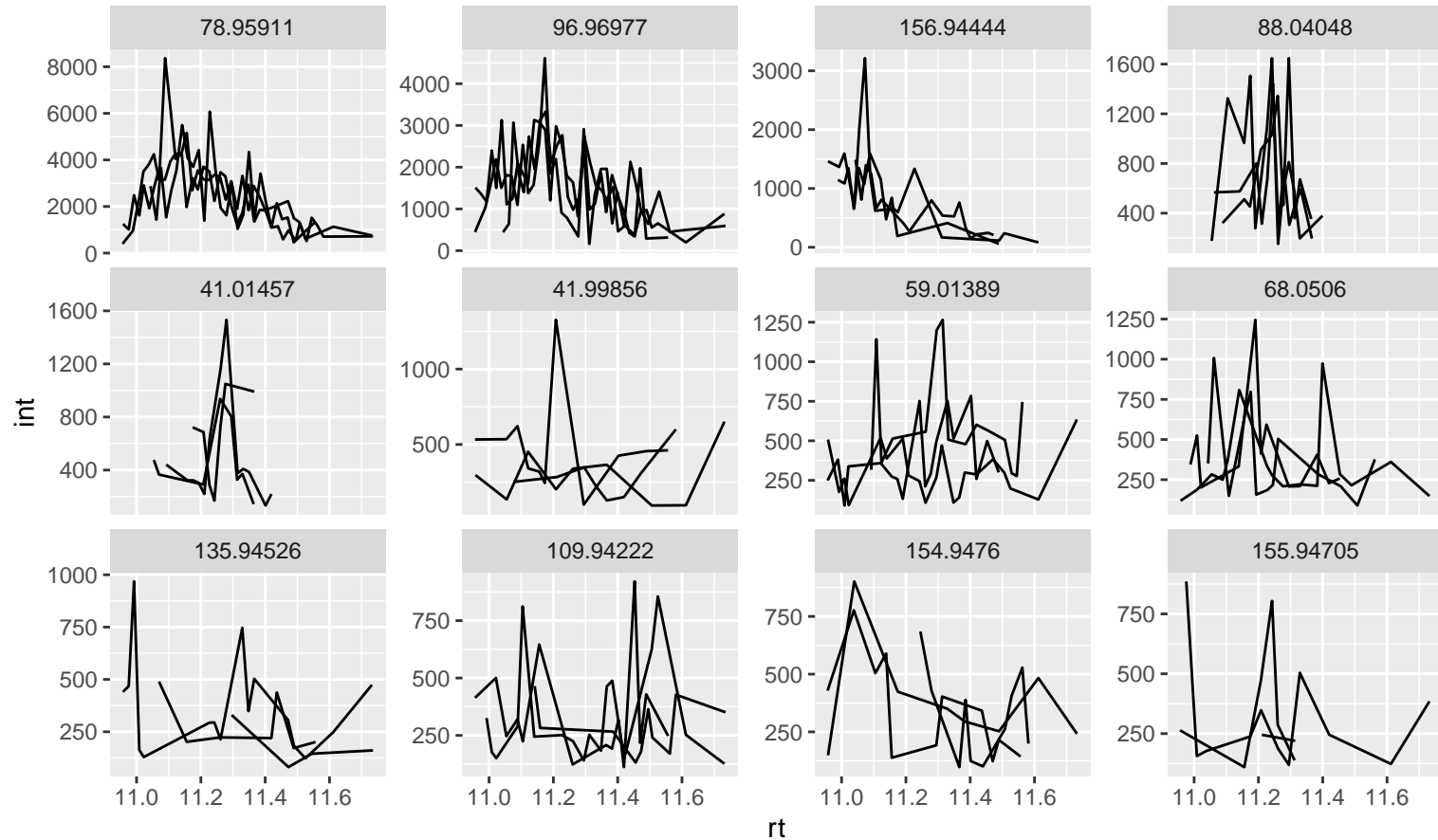
Thiamine monophosphate (pos) 345.078092

int

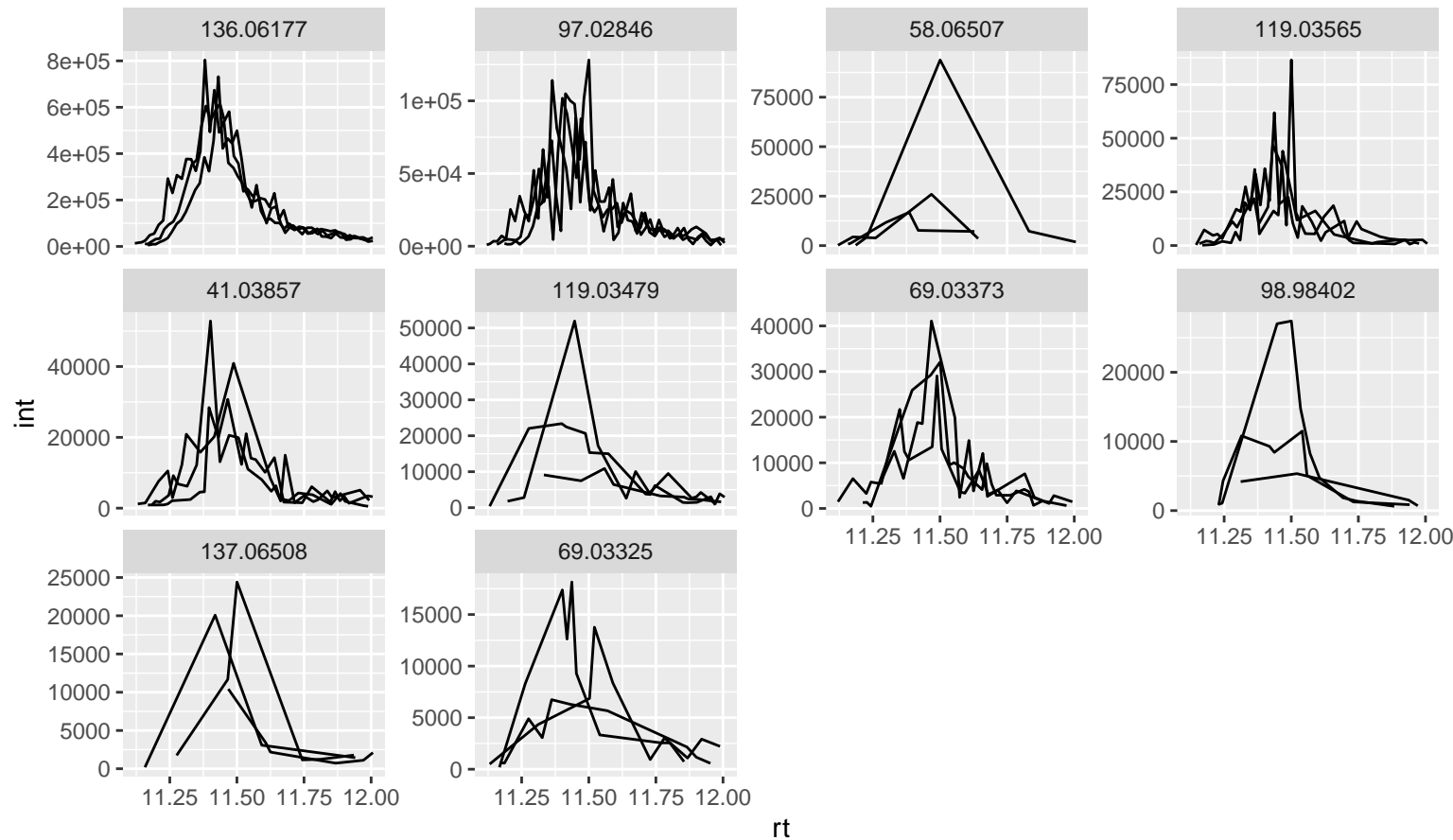


rt

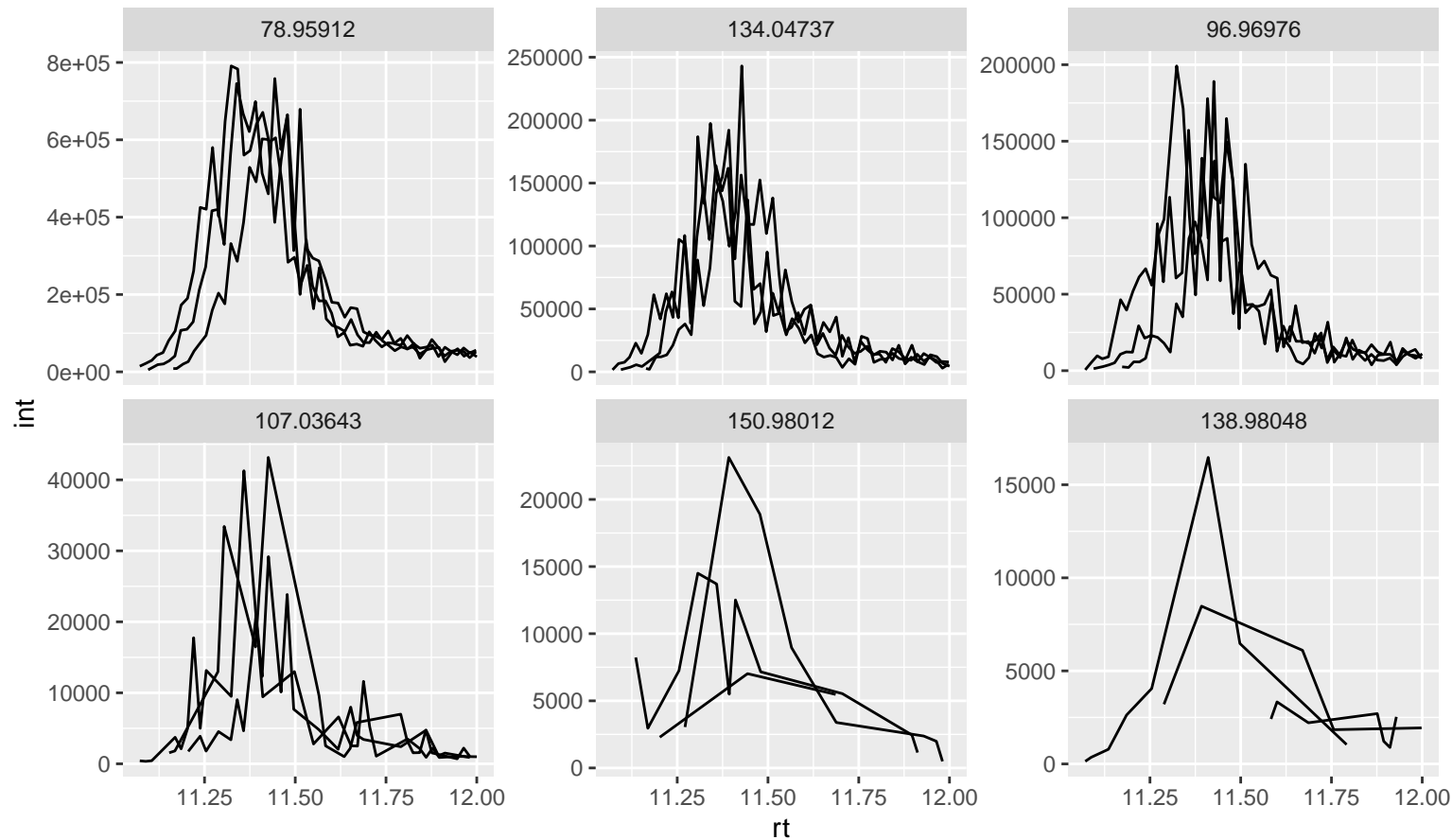
Thiamine monophosphate (neg) 343.06354



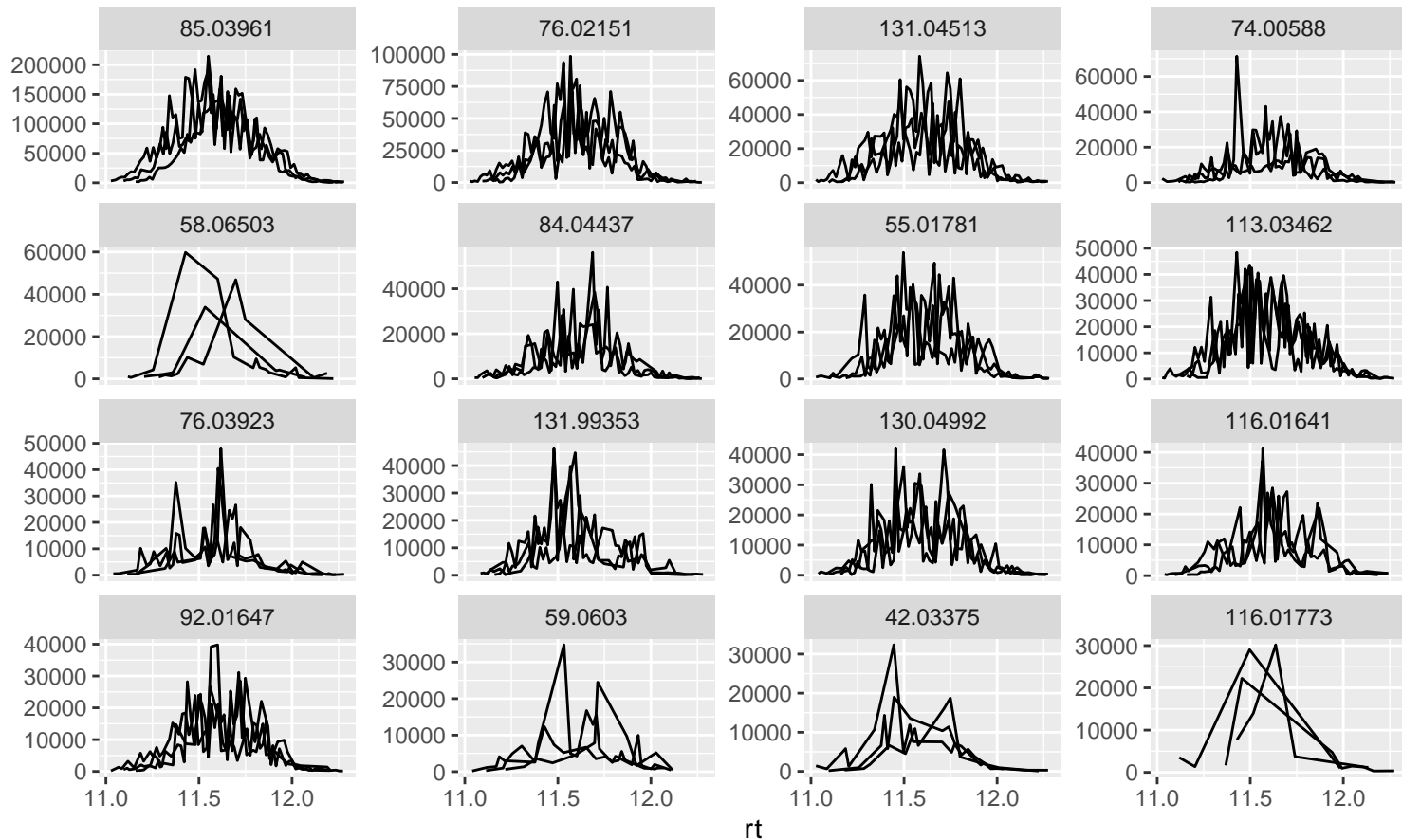
Adenosine monophosphate (pos) 348.070364



Adenosine monophosphate (neg) 346.055812

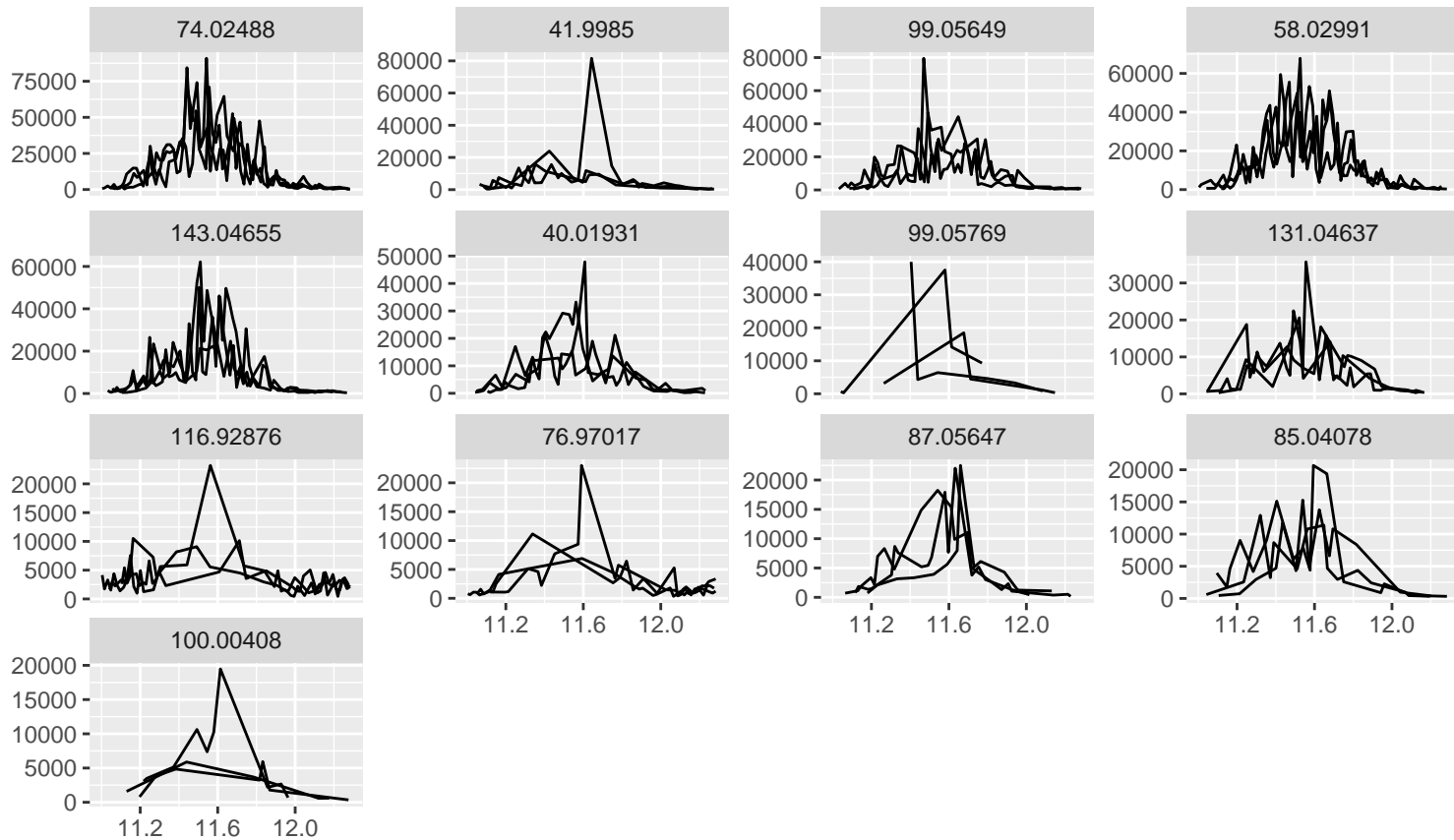


Cys–Gly, oxidized (pos) 355.074056



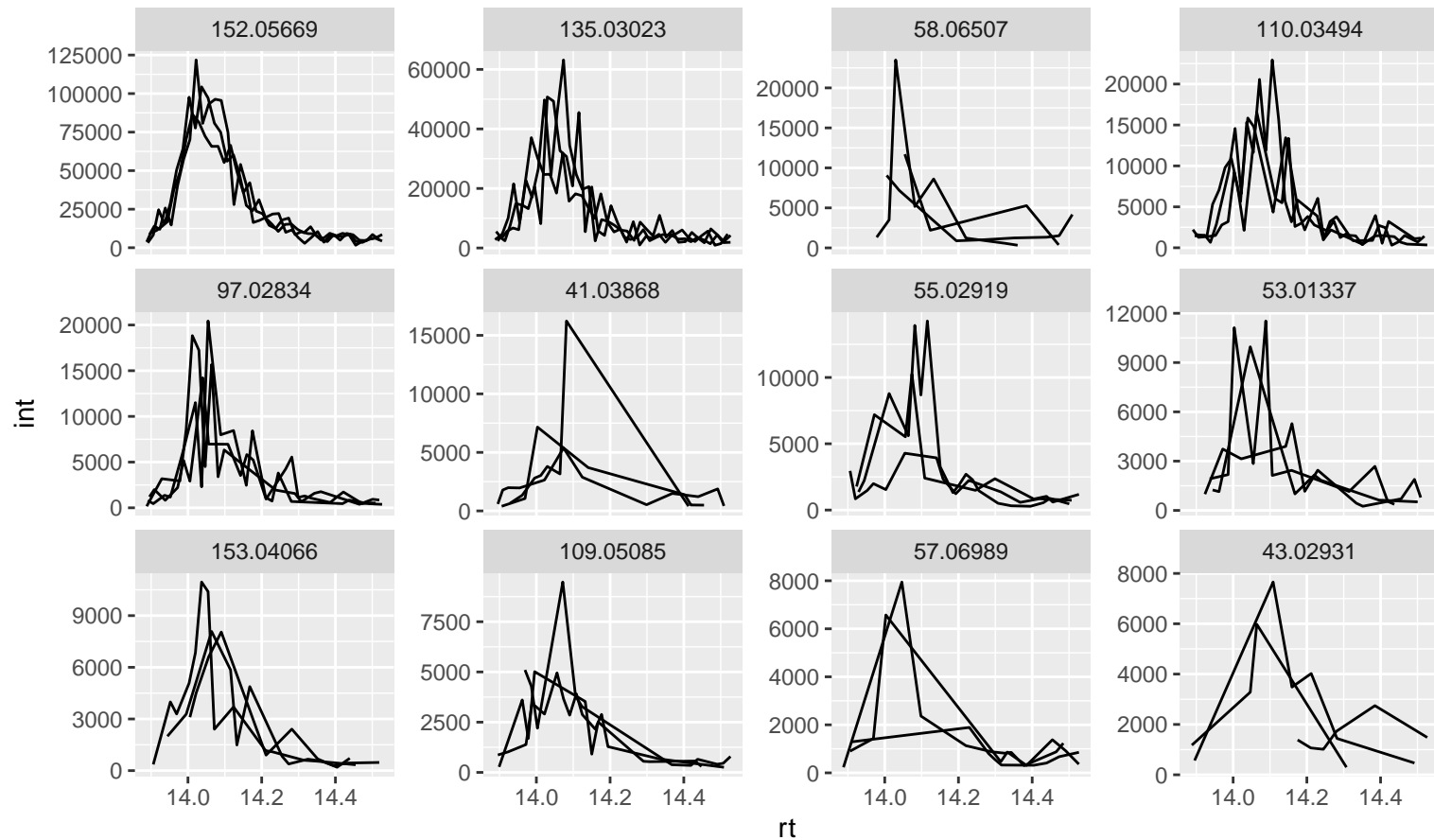
Cys–Gly, oxidized (neg) 353.059504

int

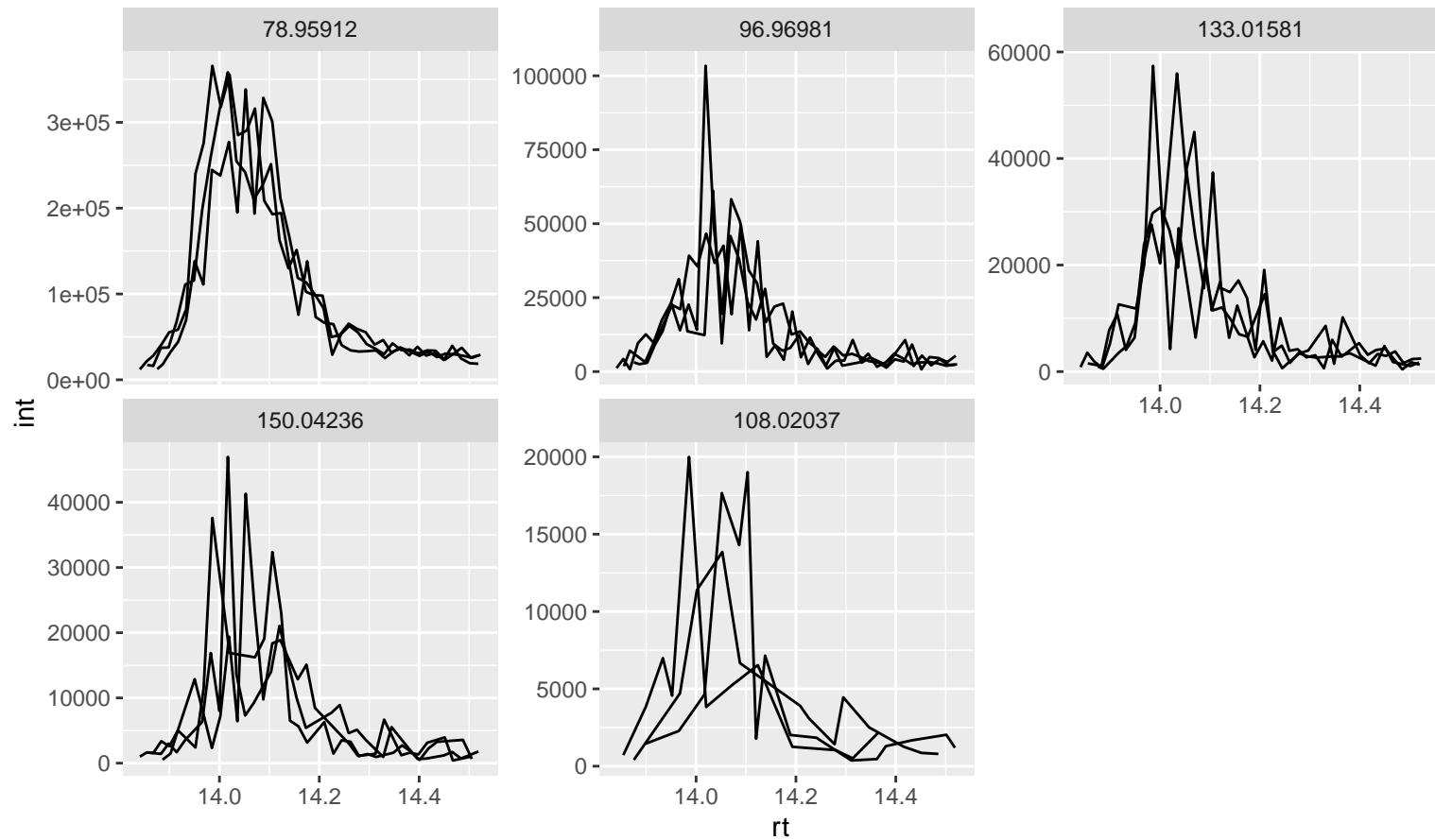


rt

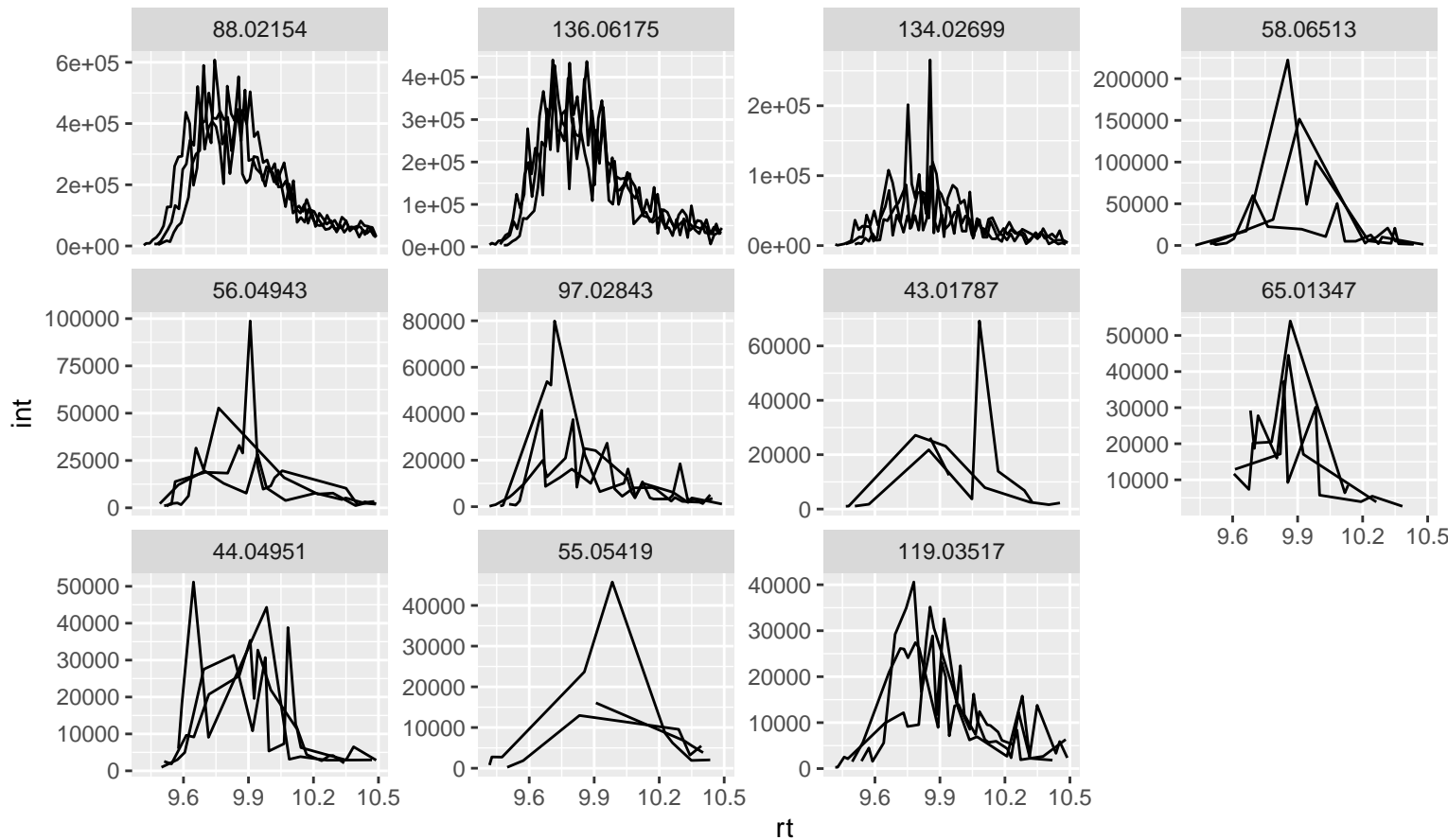
Guanosine monophosphate (pos) 364.065279



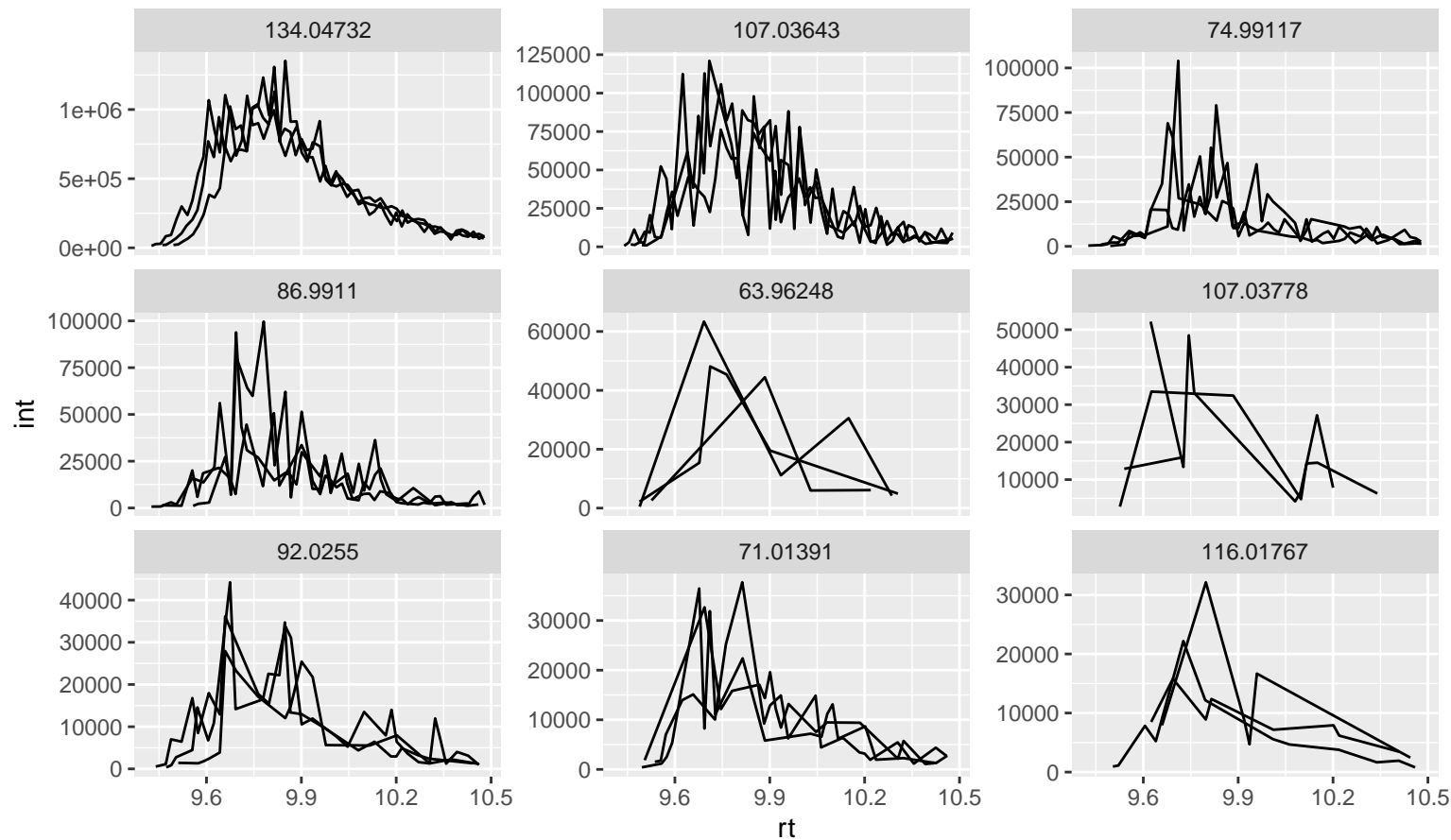
Guanosine monophosphate (neg) 362.050727



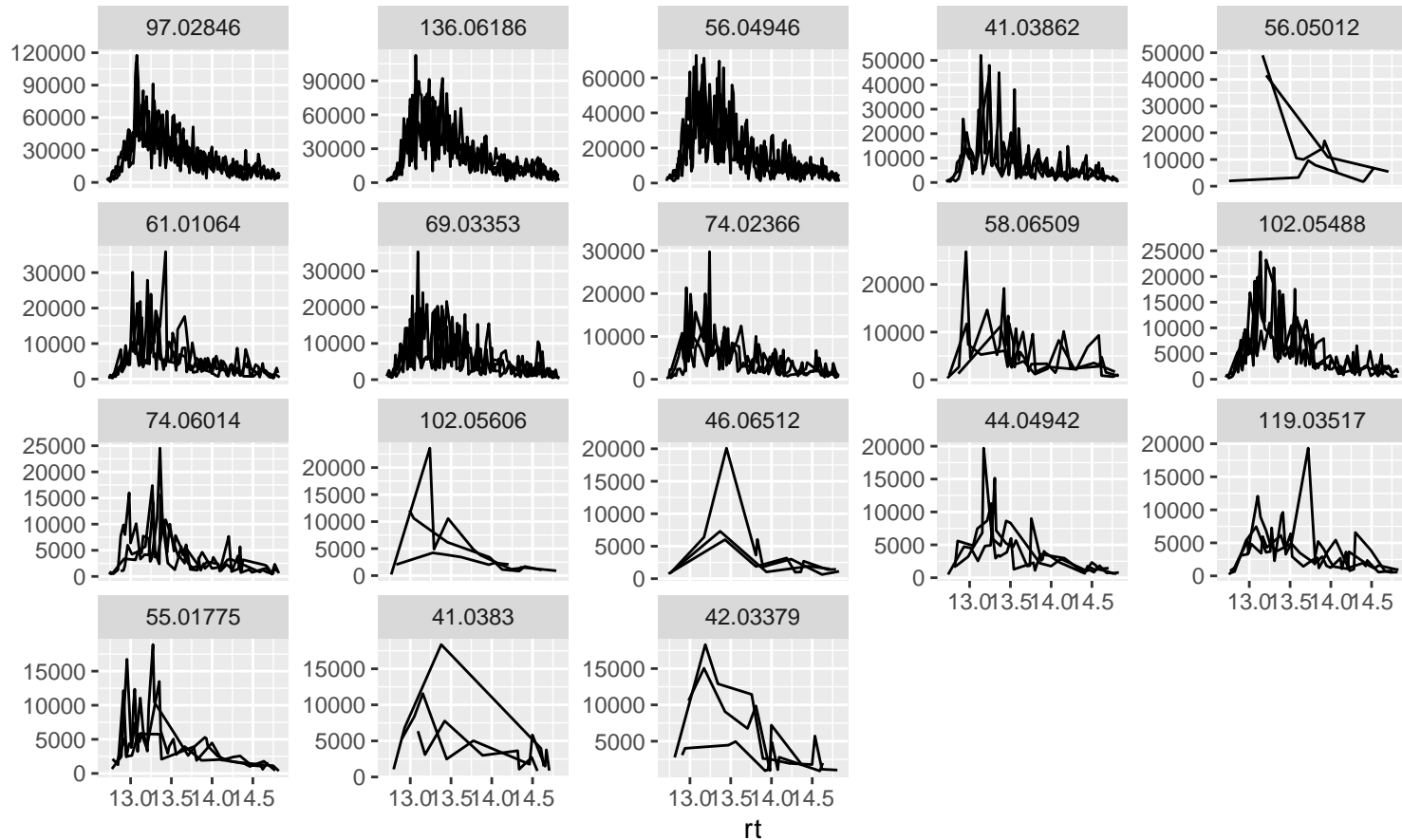
S-Adenosylhomocysteine (pos) 385.128867



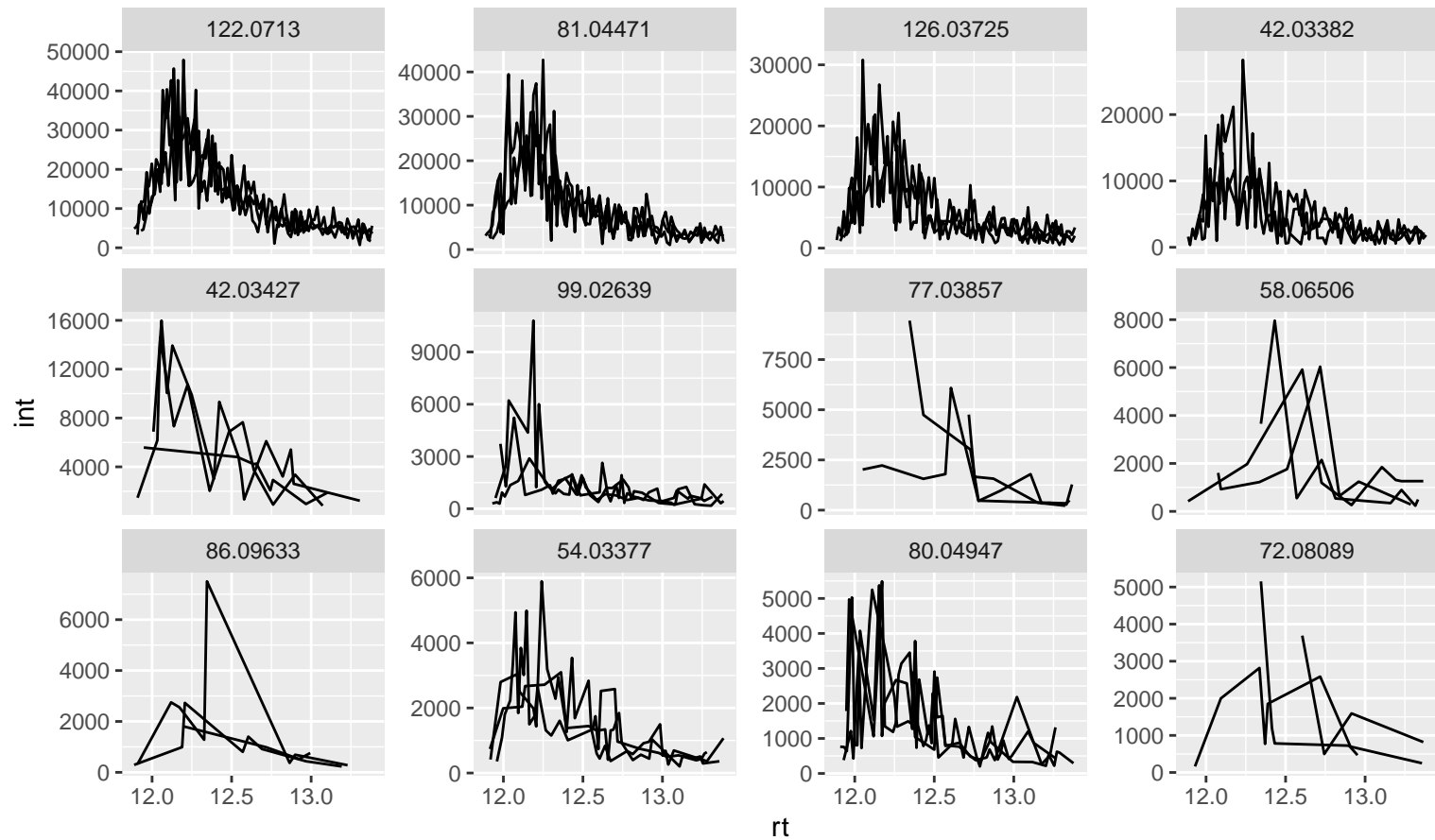
S-Adenosylhomocysteine (neg) 383.114315



S-Adenosylmethionine (pos) 399.144517

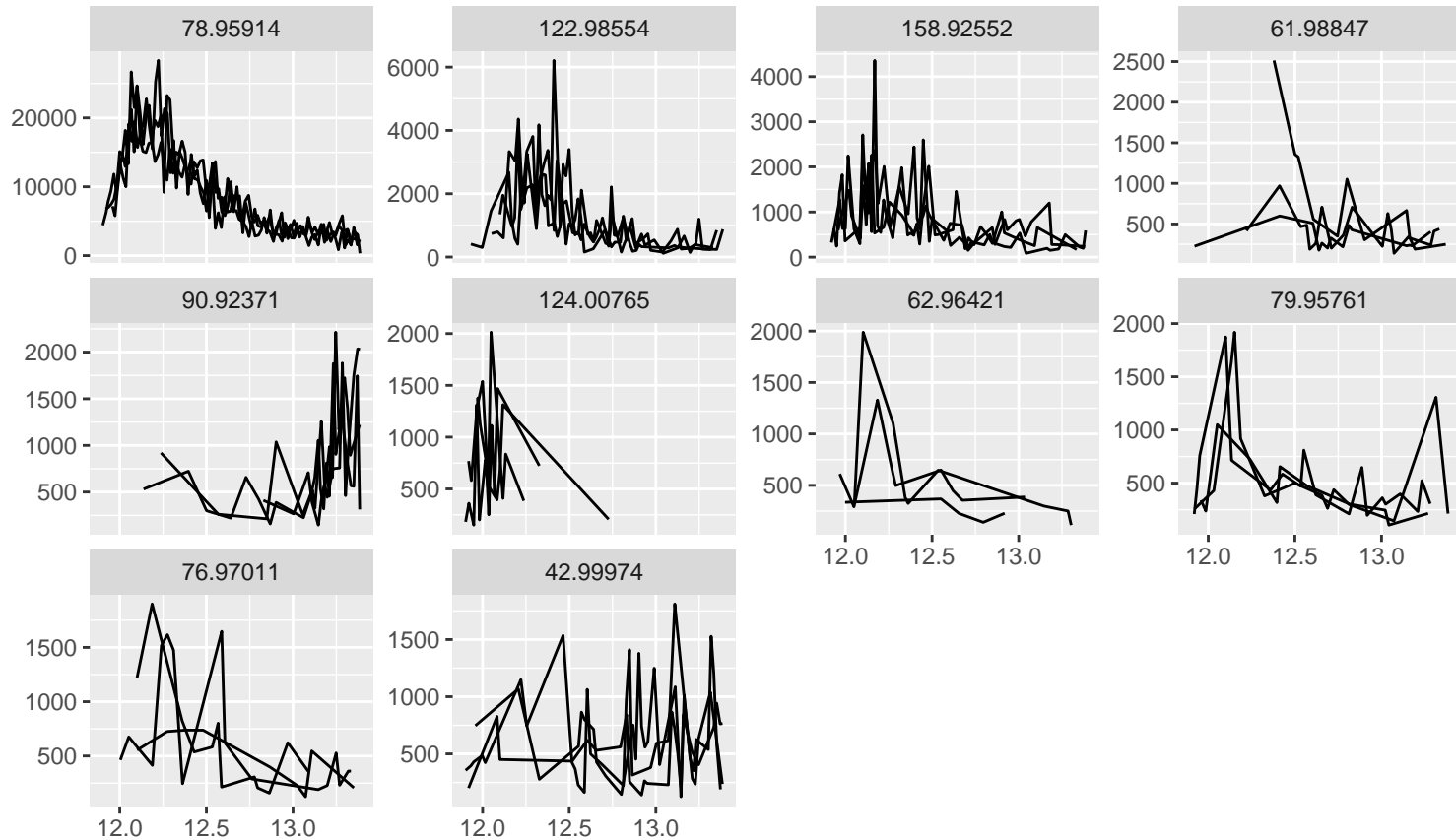


Thiamine diphosphate (pos) 425.044425



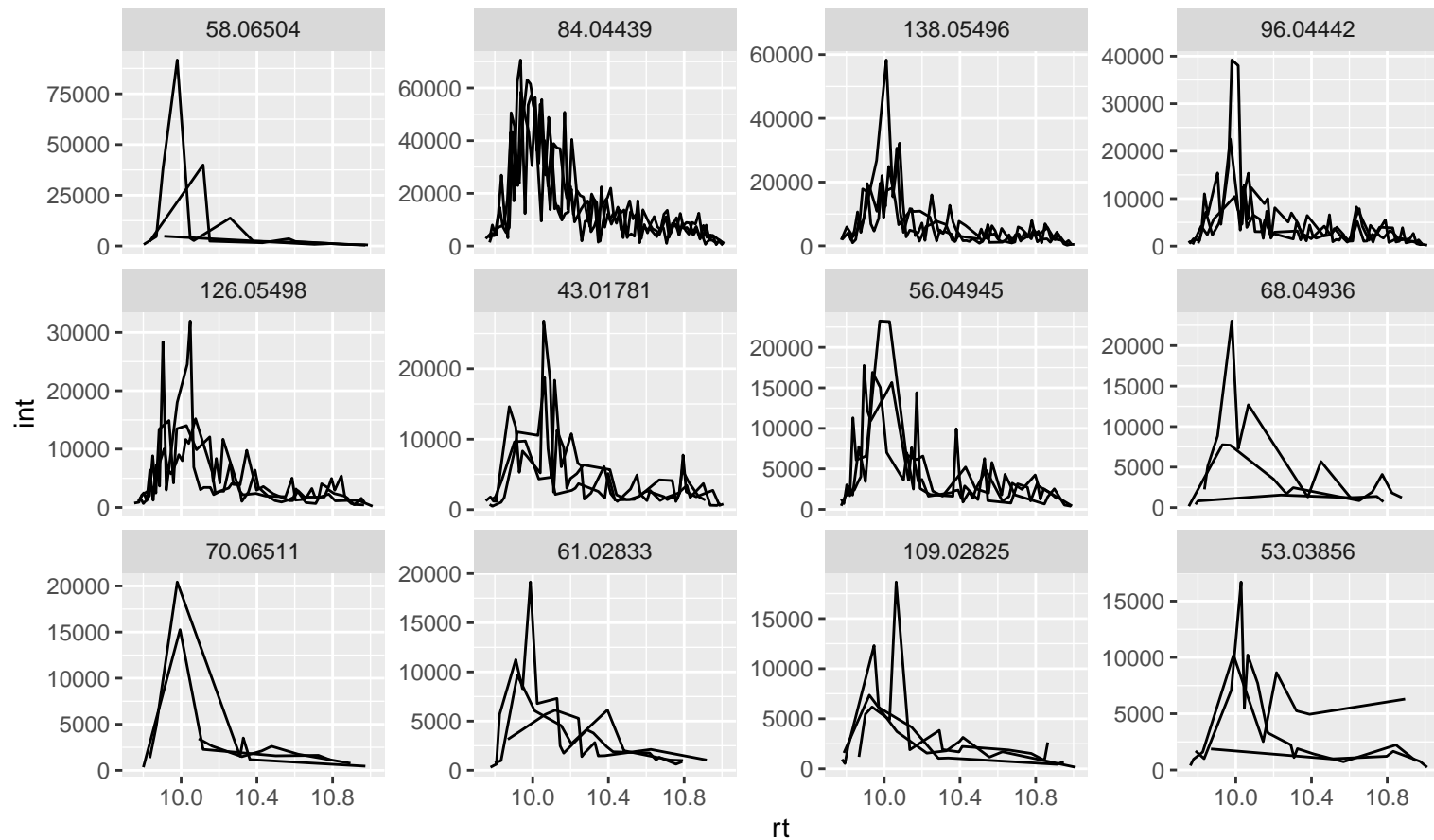
Thiamine diphosphate (neg) 423.029873

int

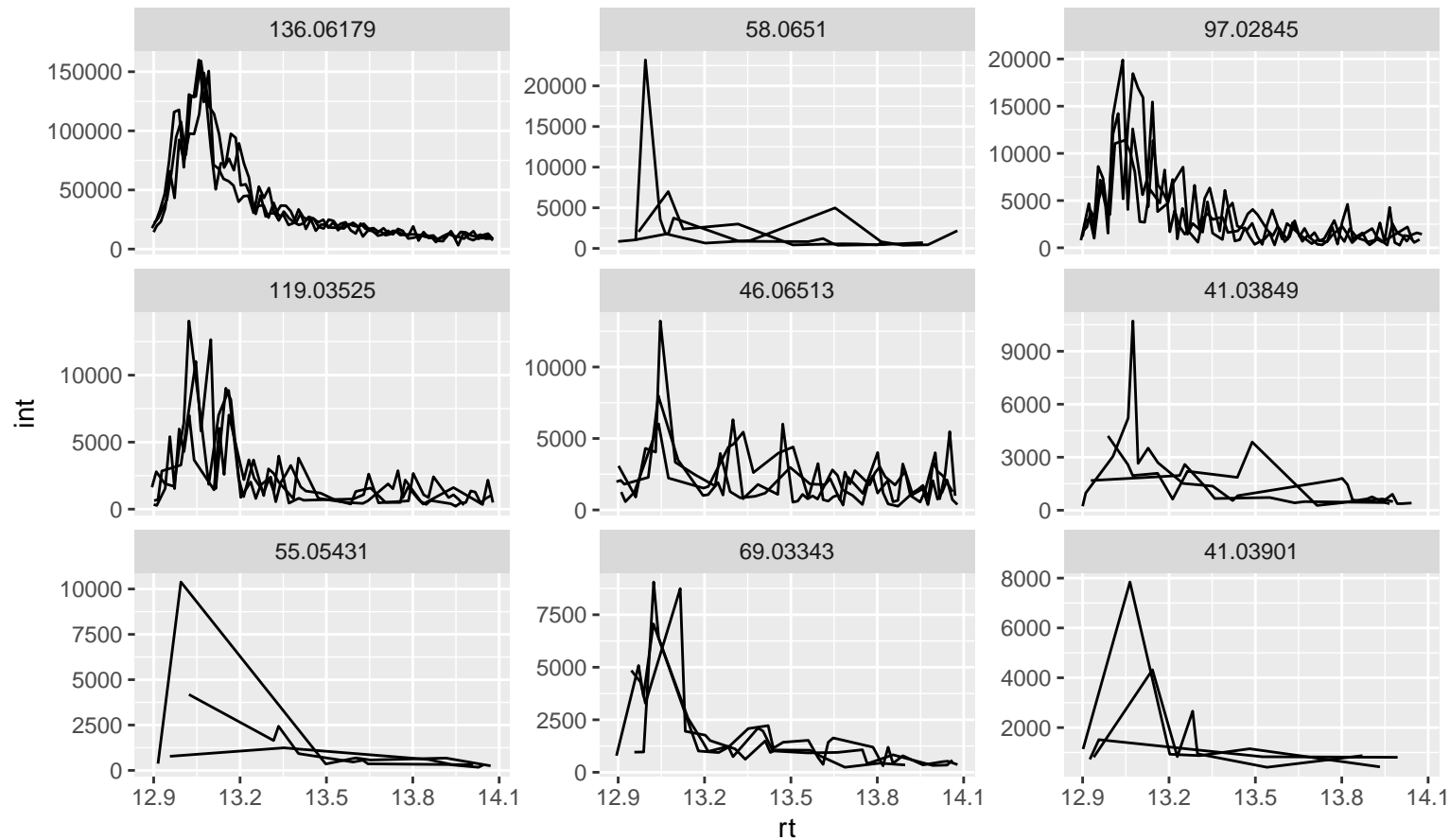


rt

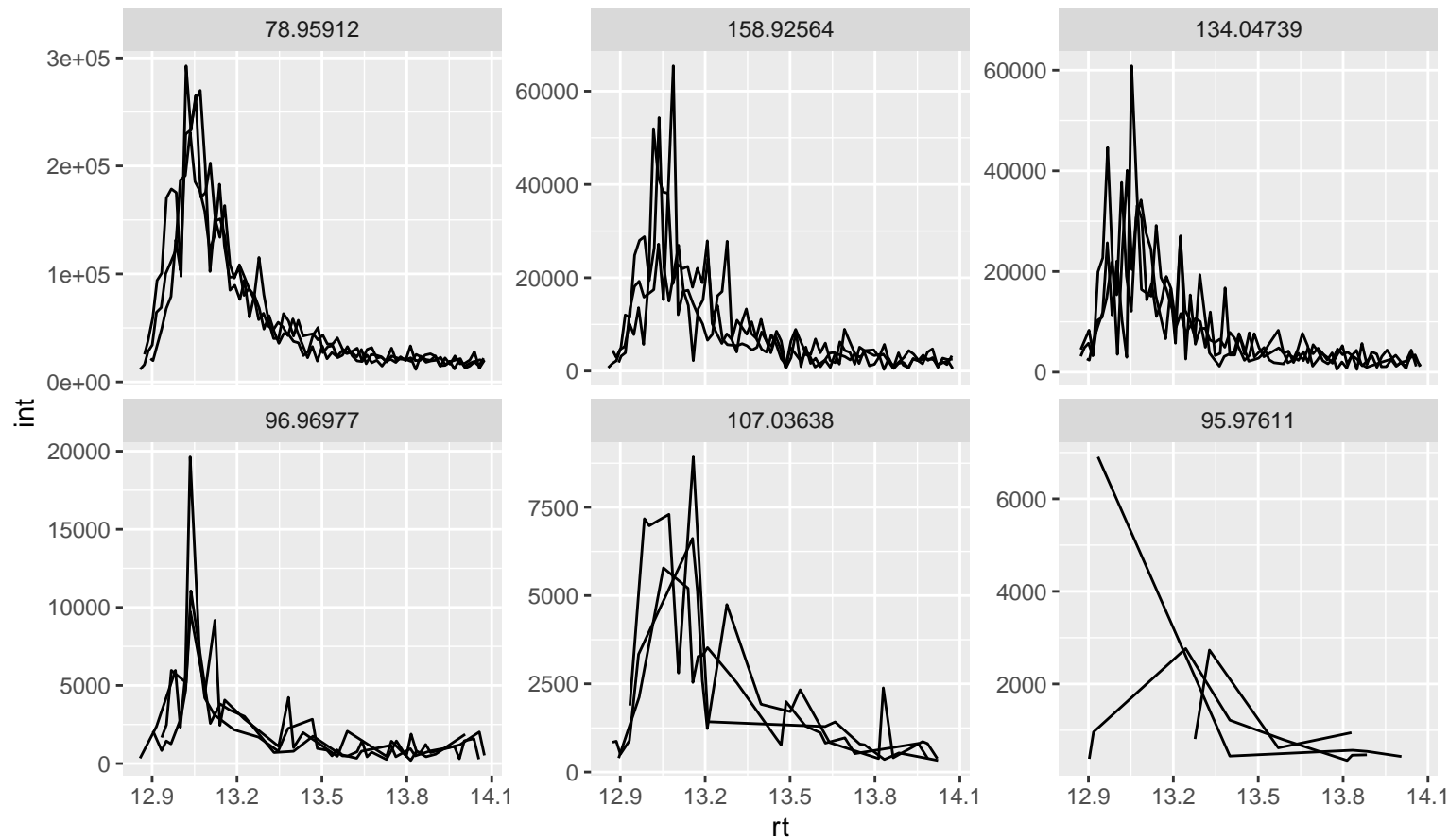
Chitobiose (pos) 425.176589



Adenosine diphosphate (pos) 428.036697

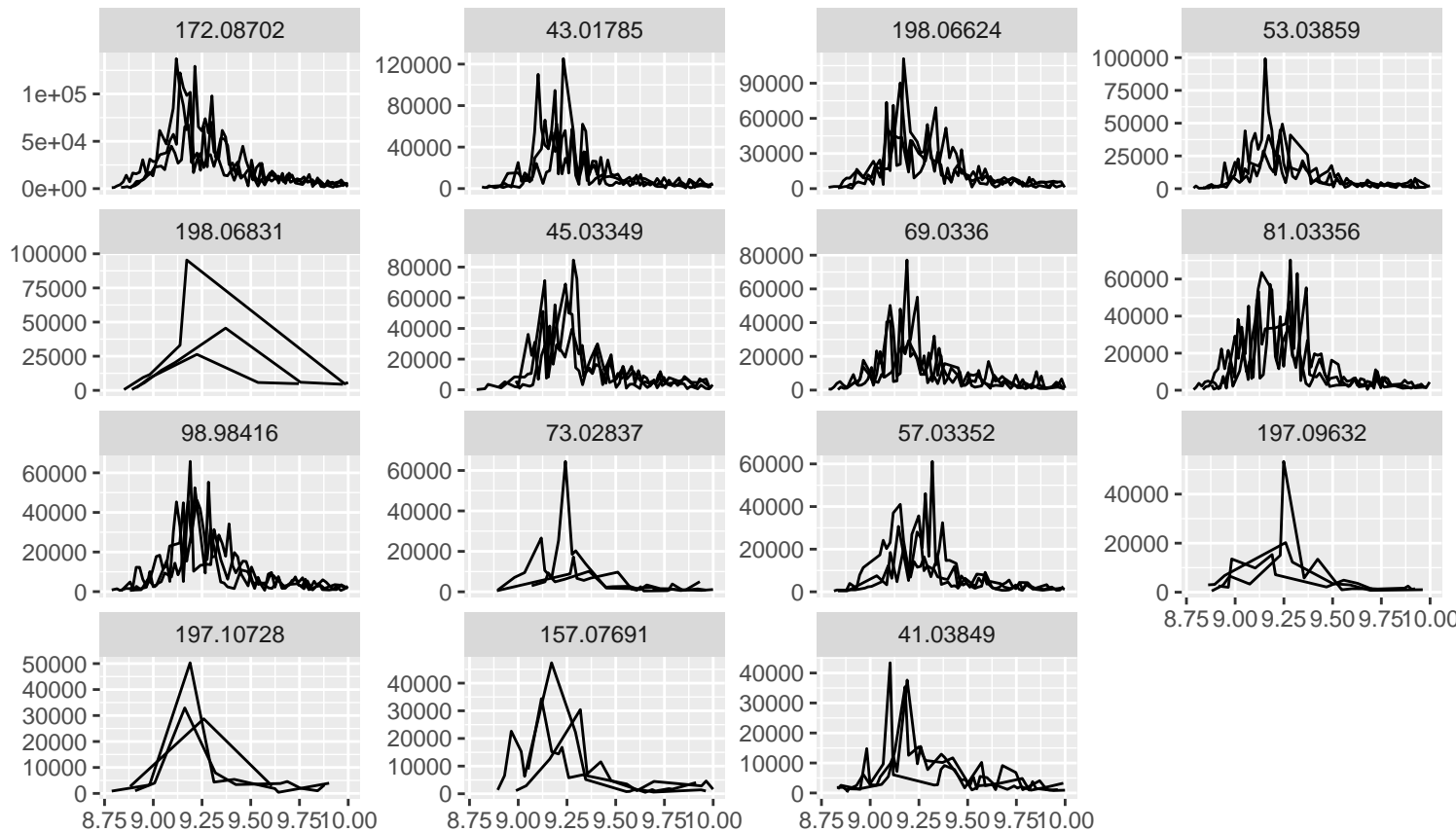


Adenosine diphosphate (neg) 426.022145



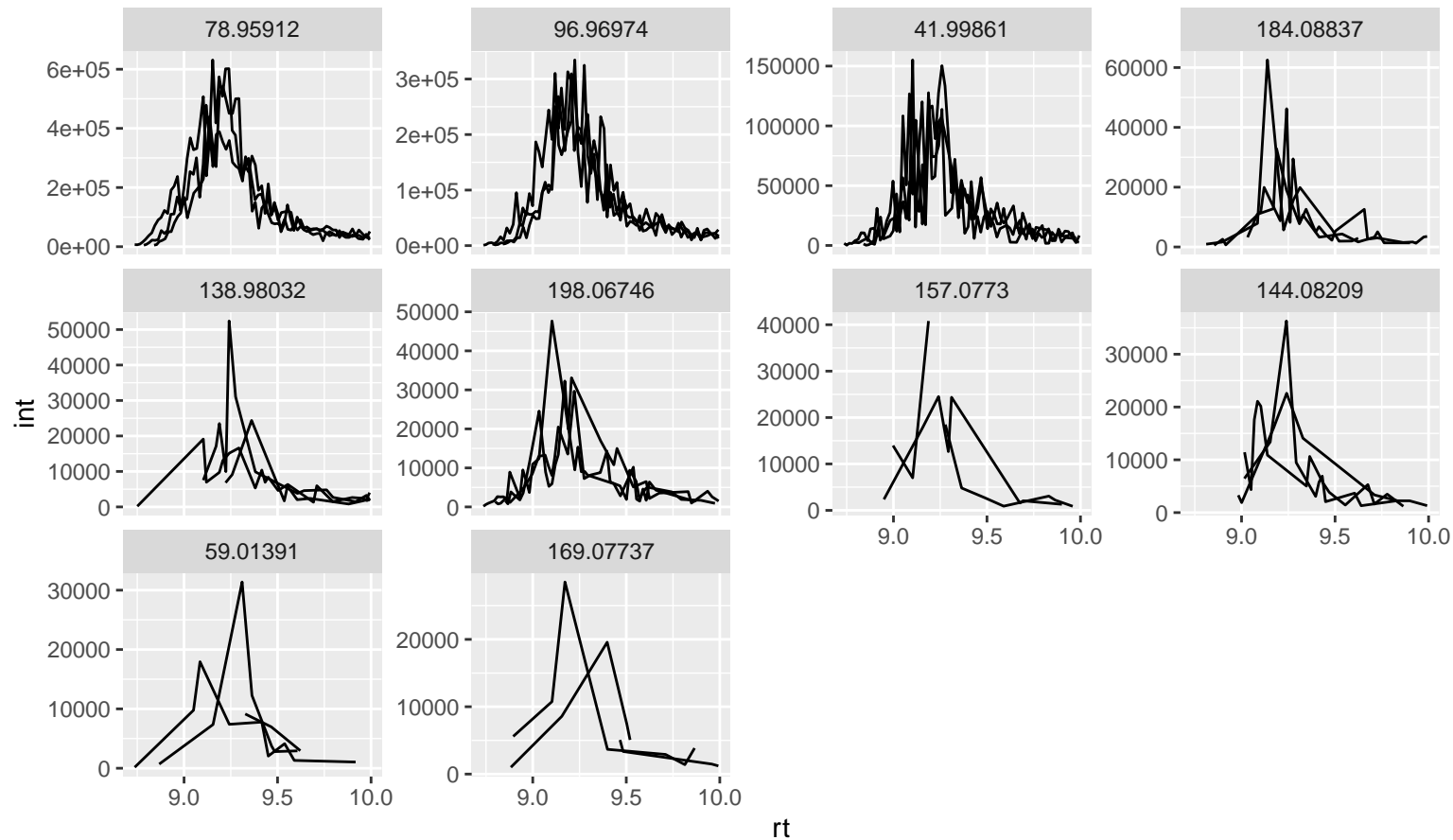
Riboflavin-5-phosphate (pos) 457.111895

int



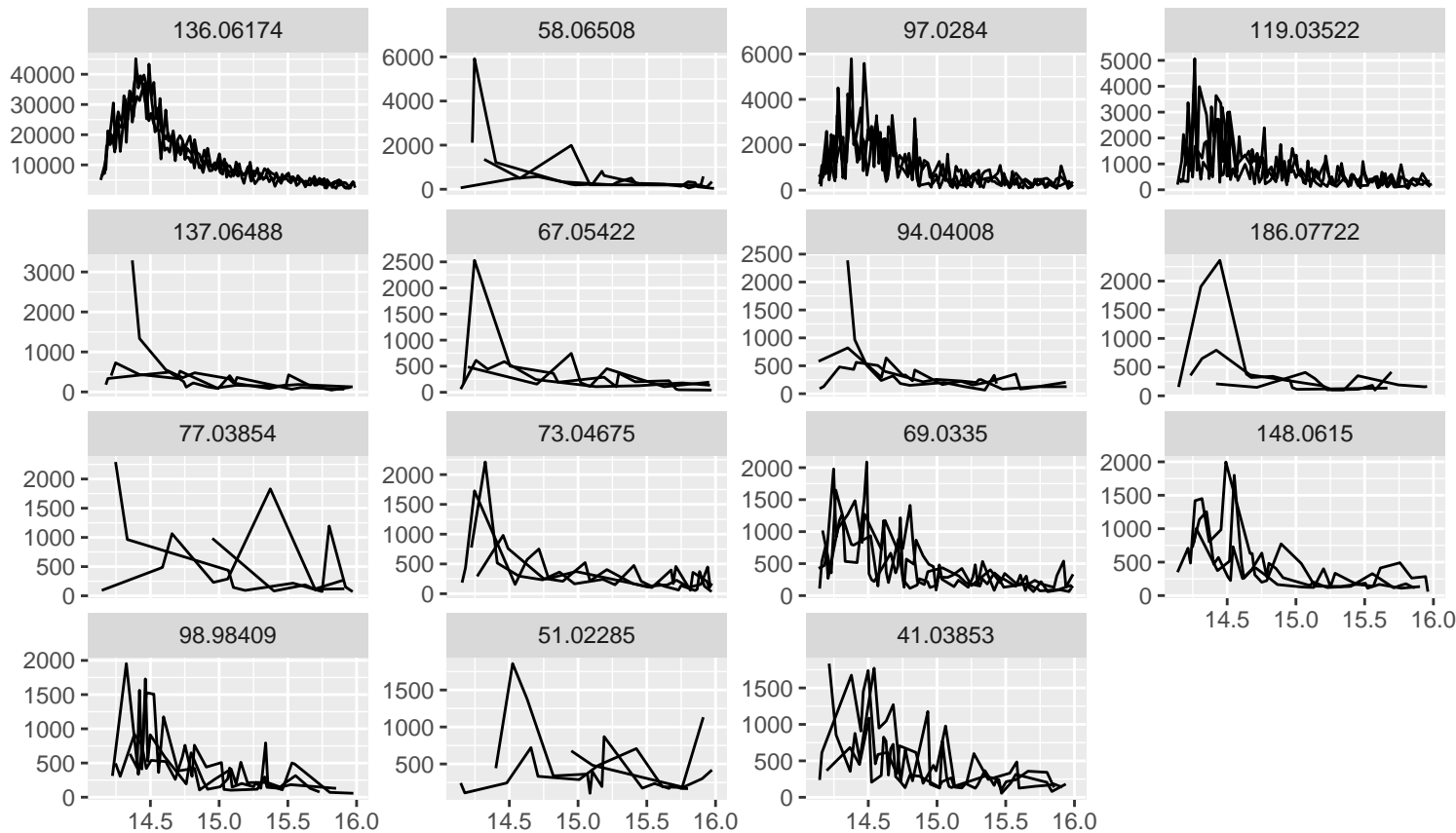
rt

Riboflavin-5-phosphate (neg) 455.097343



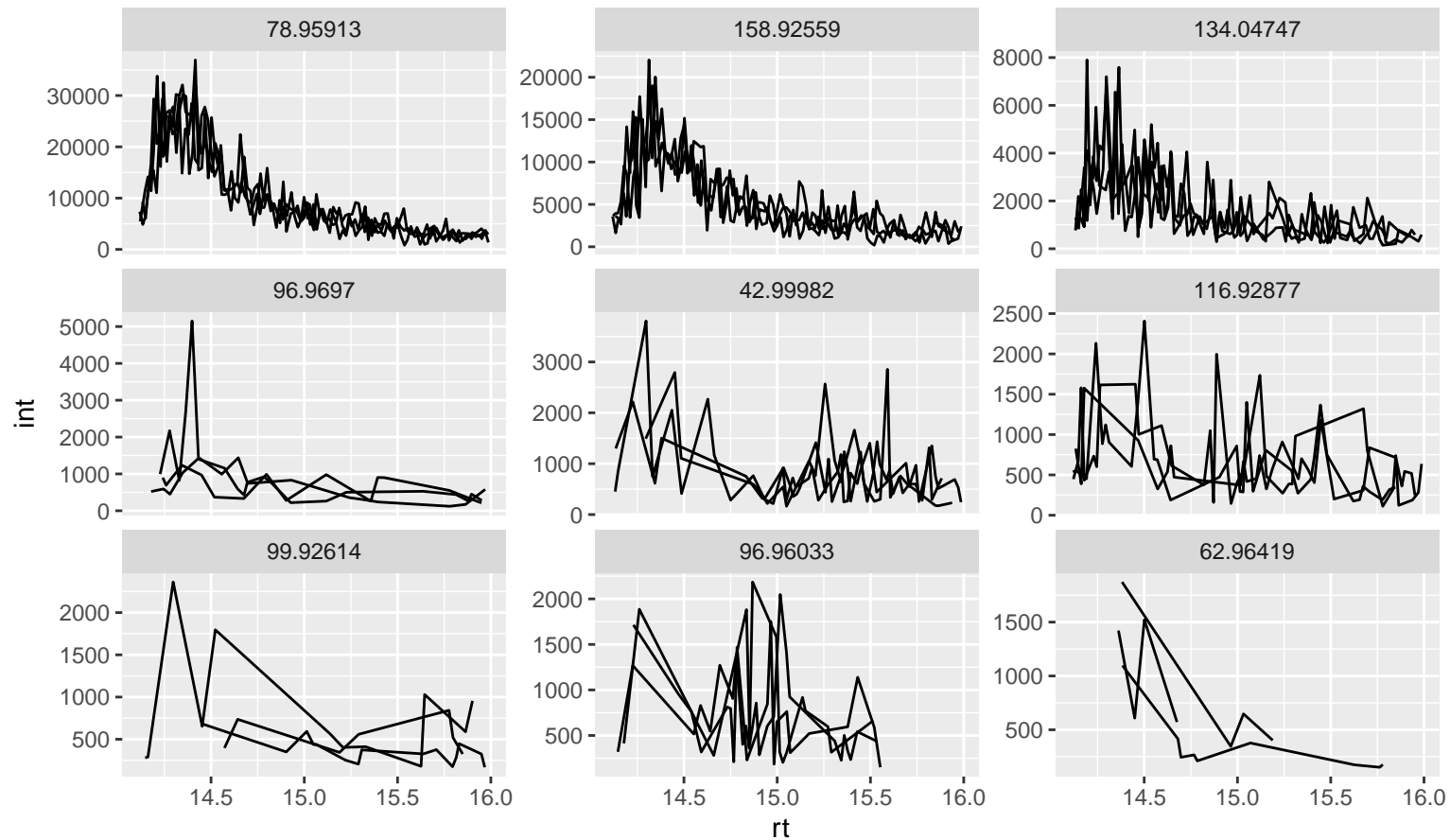
Adenosine triphosphate (pos) 508.00303

int

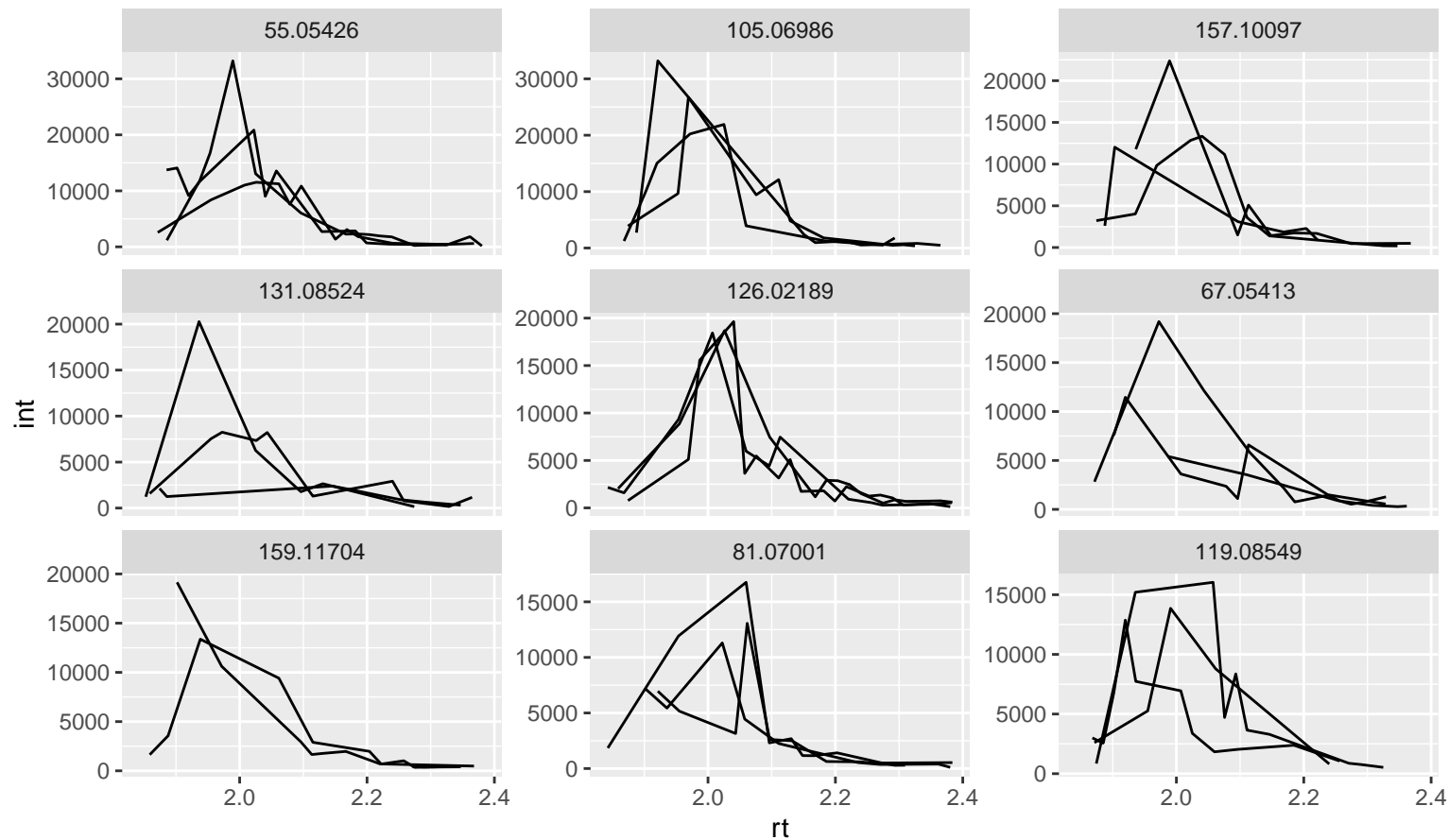


rt

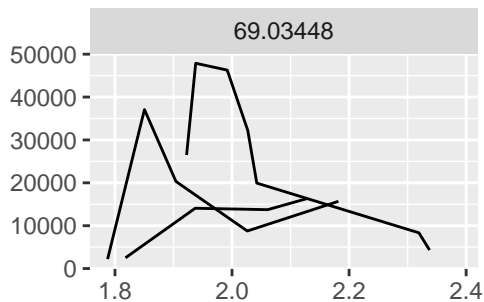
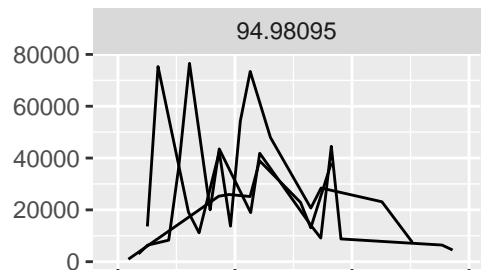
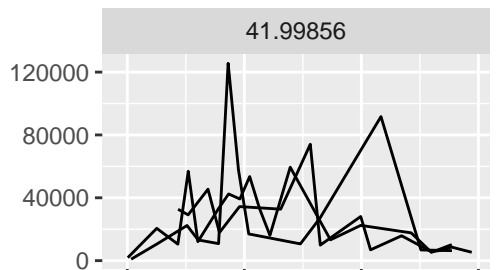
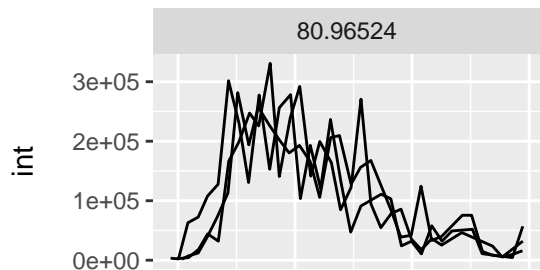
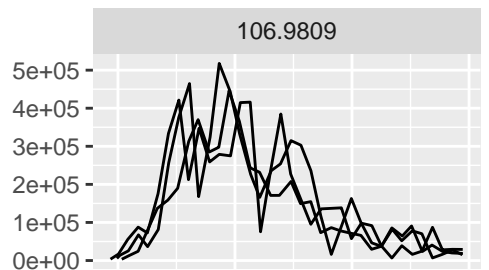
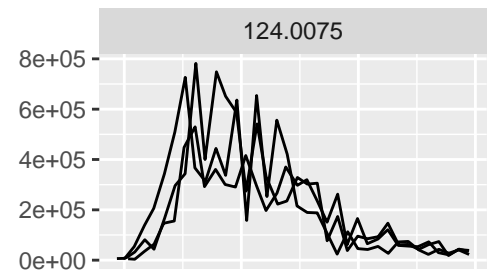
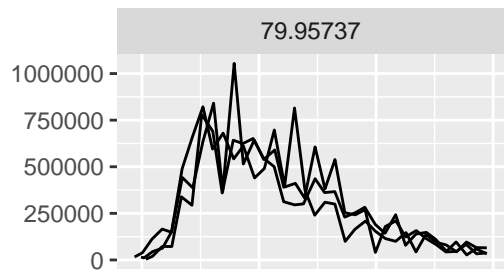
Adenosine triphosphate (neg) 505.988478



Taurocholic acid (pos) 516.298952

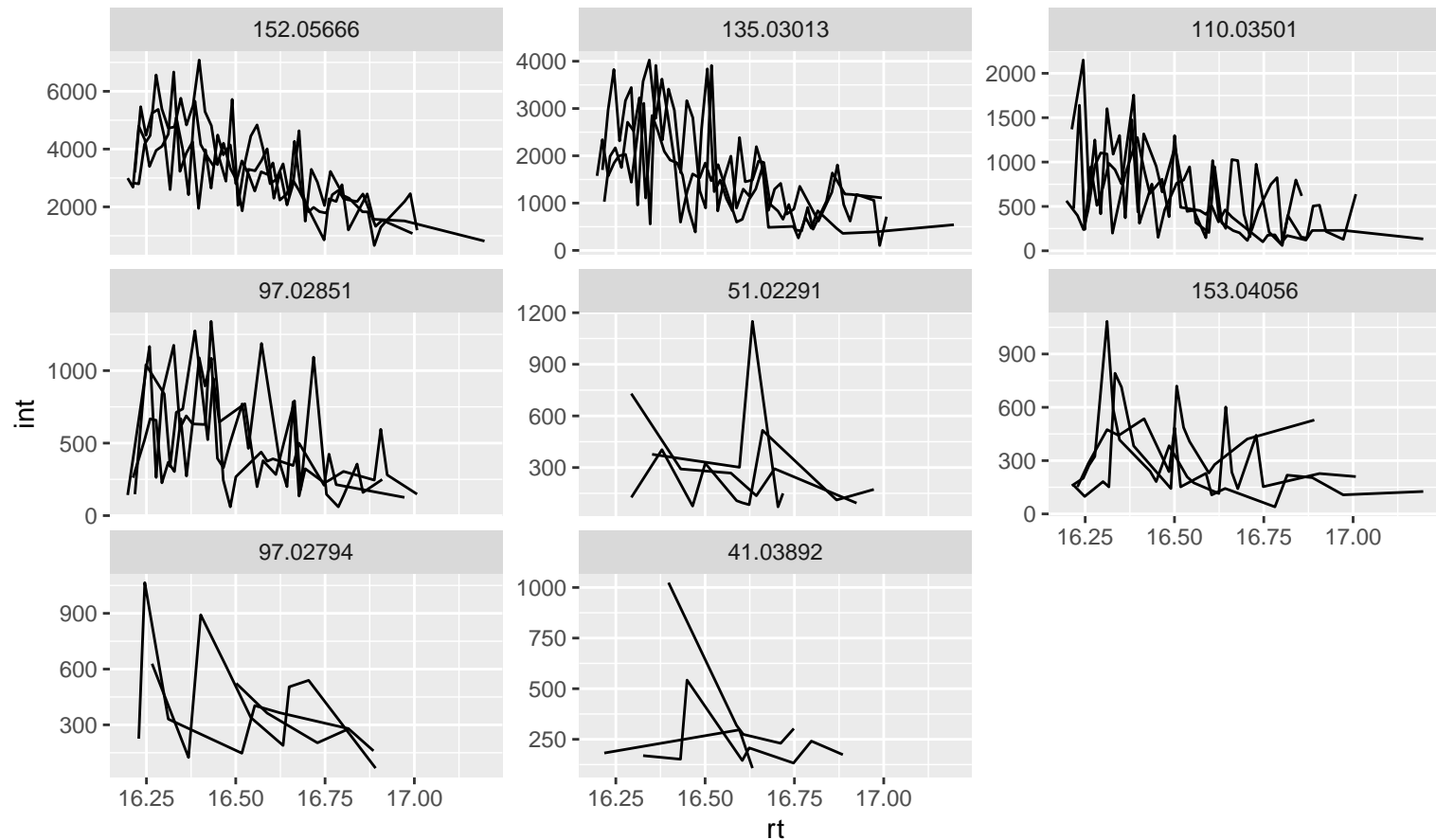


Taurocholic acid (neg) 514.2844

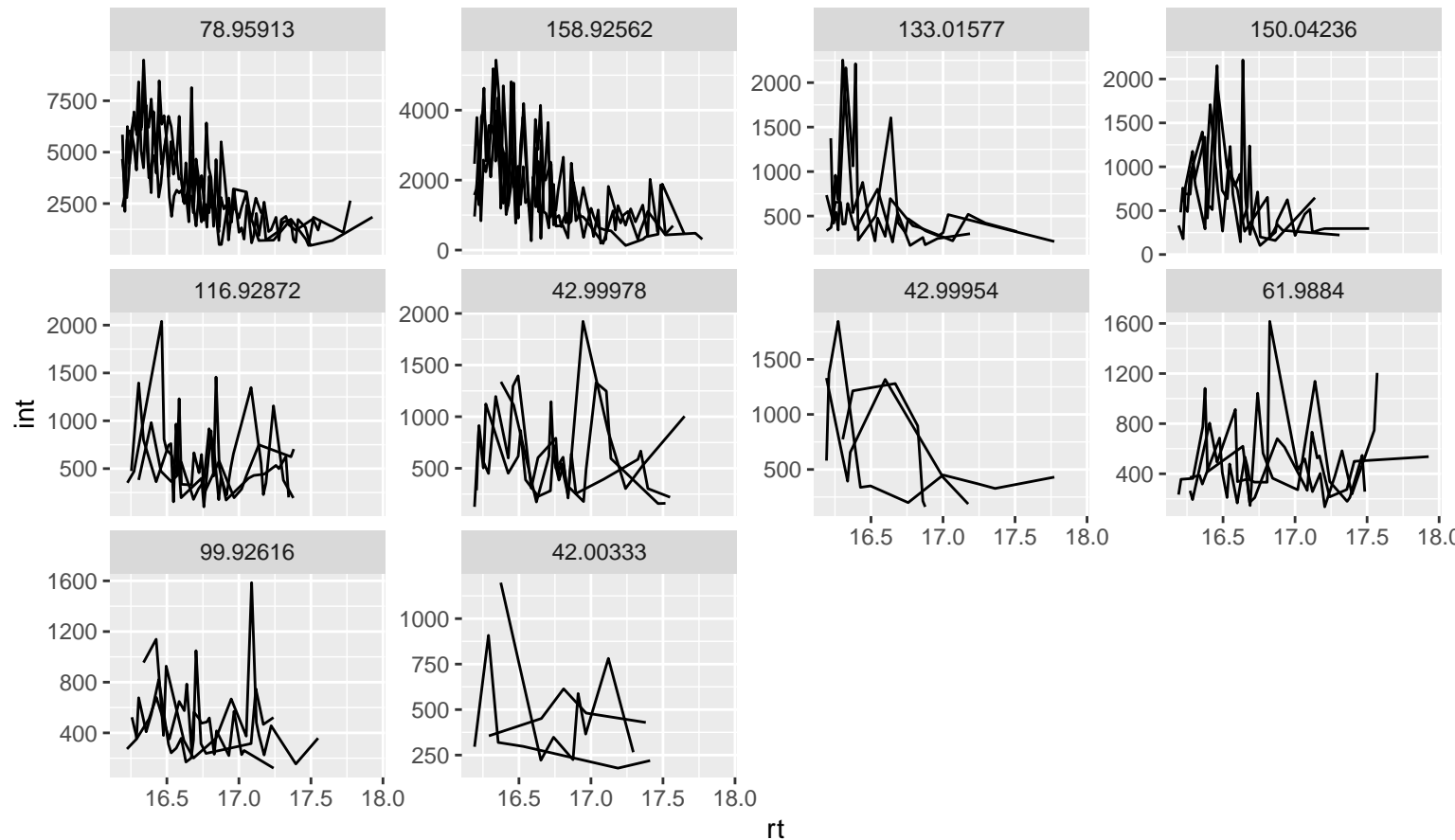


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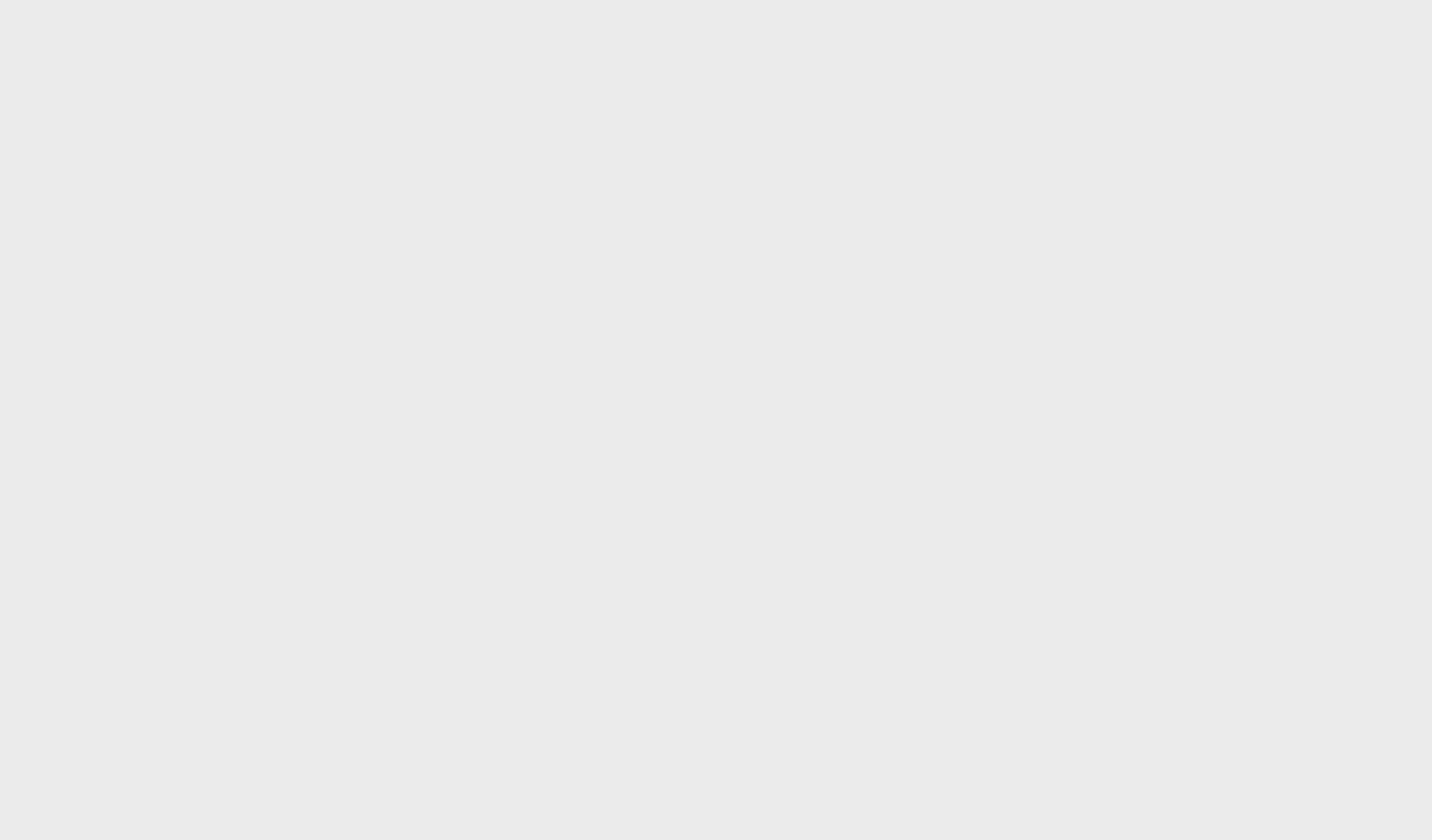
Guanosine triphosphate (pos) 523.997945



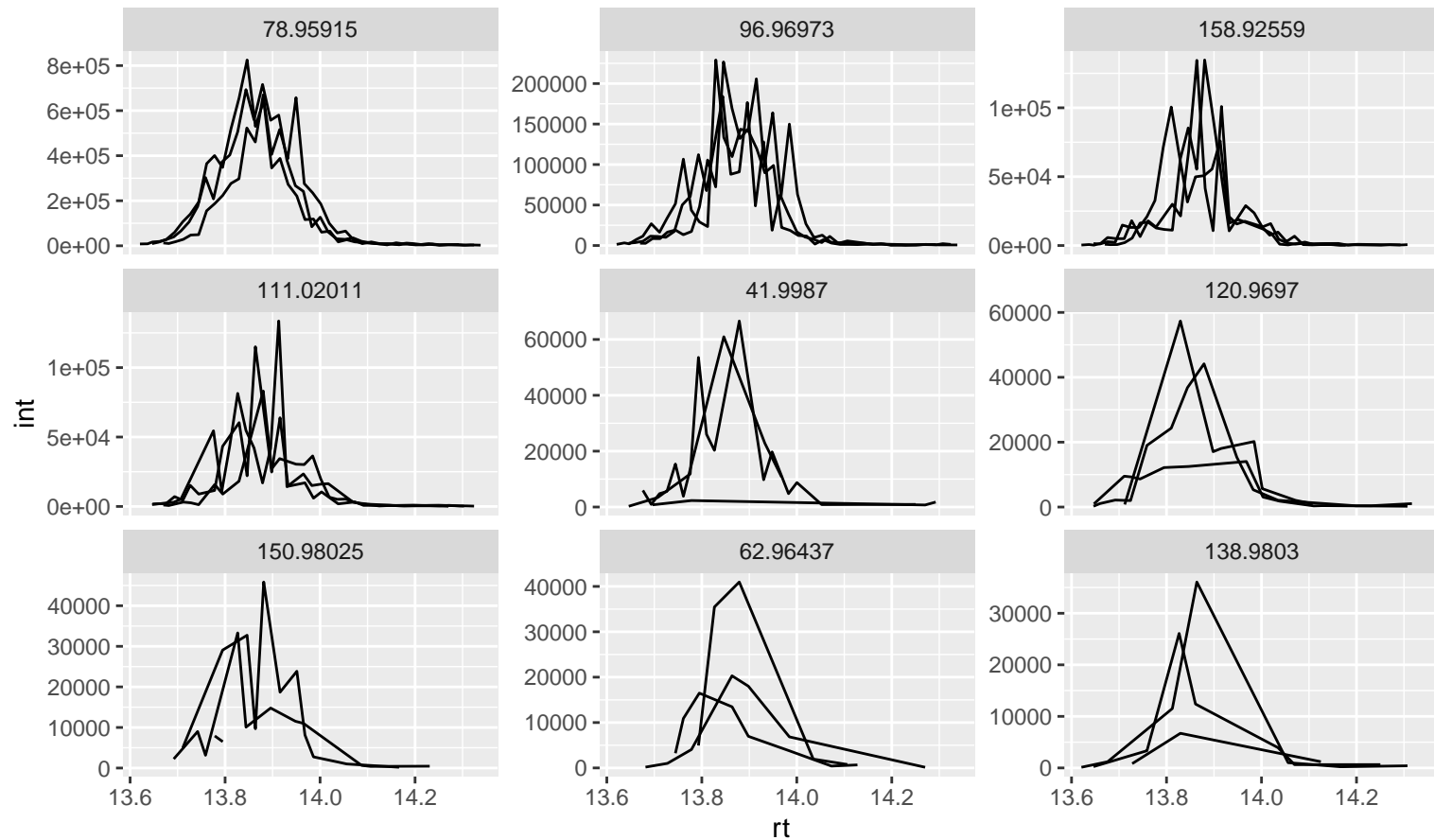
Guanosine triphosphate (neg) 521.983393



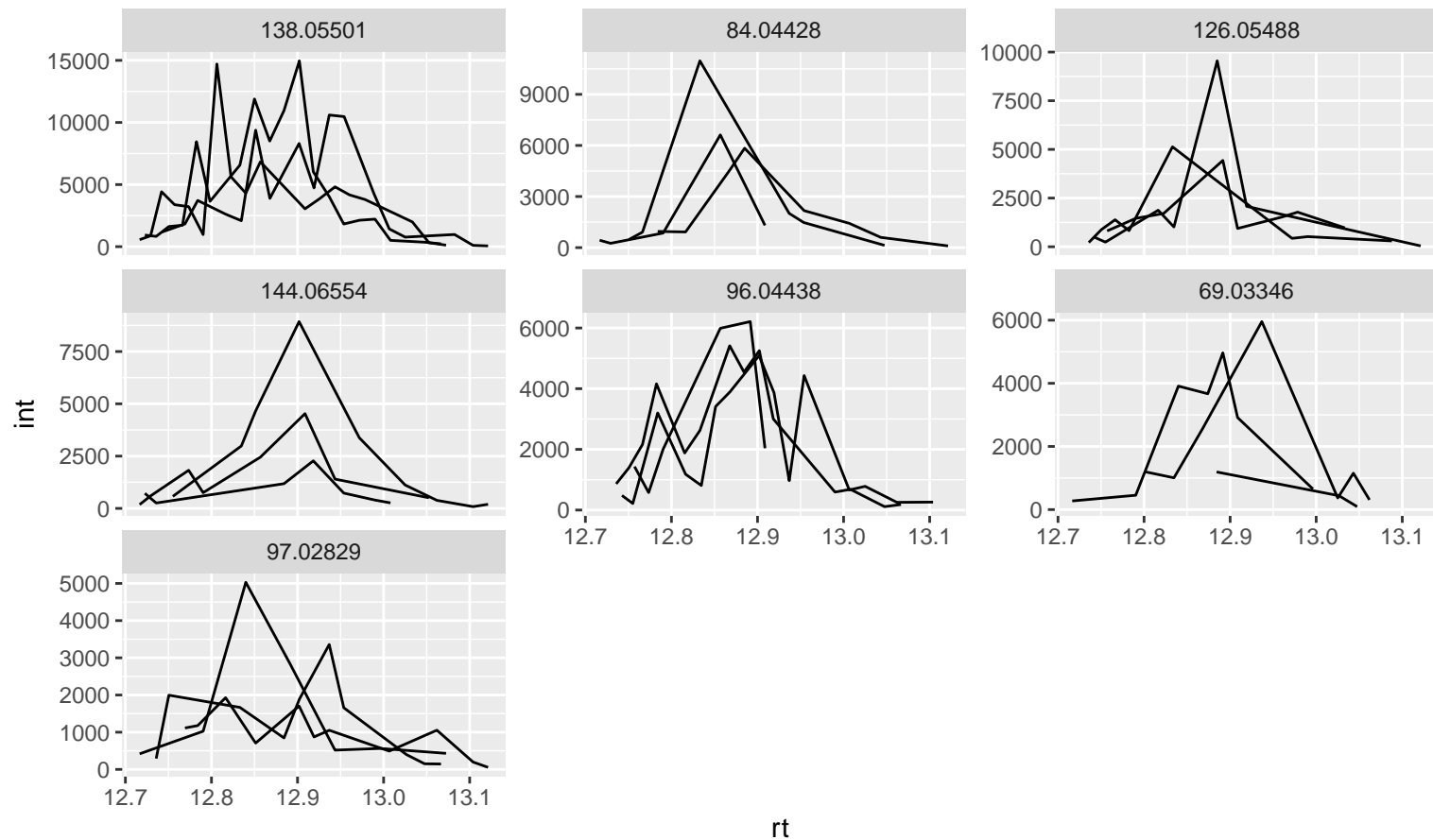
UDP-glucose (pos) 567.062305



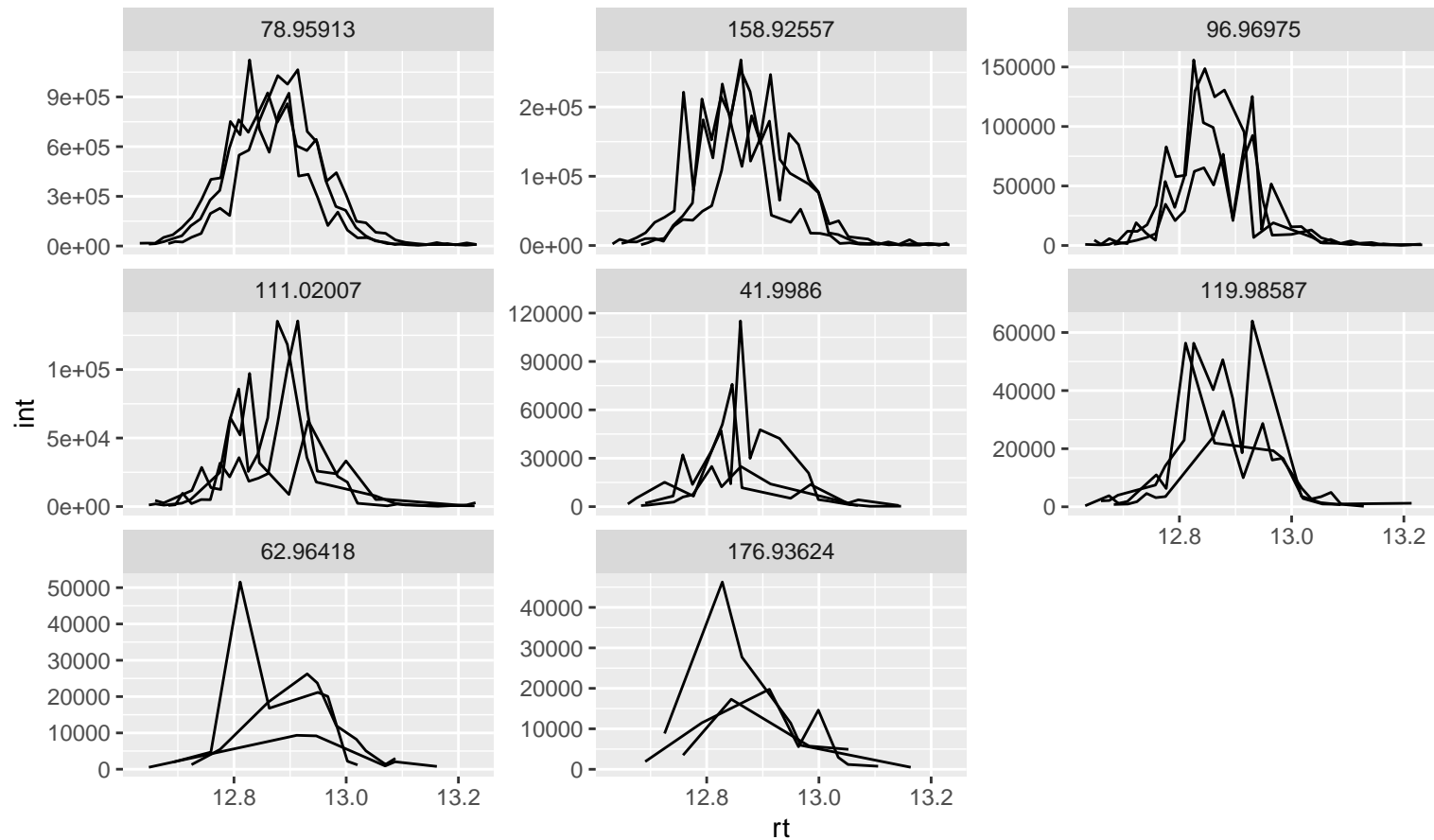
UDP-glucose (neg) 565.047753



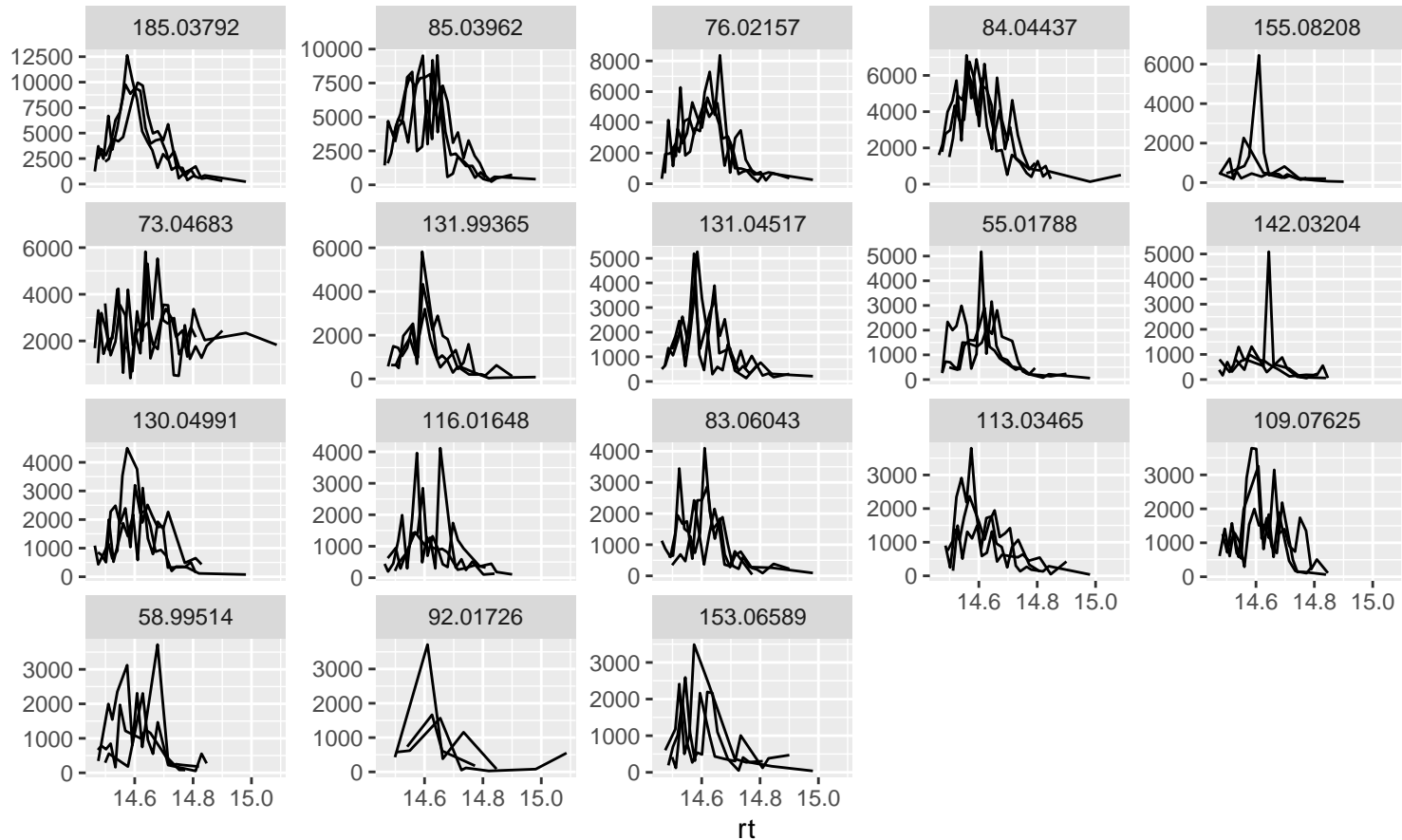
UDP-N-acetylglucosamine (pos) 608.08854



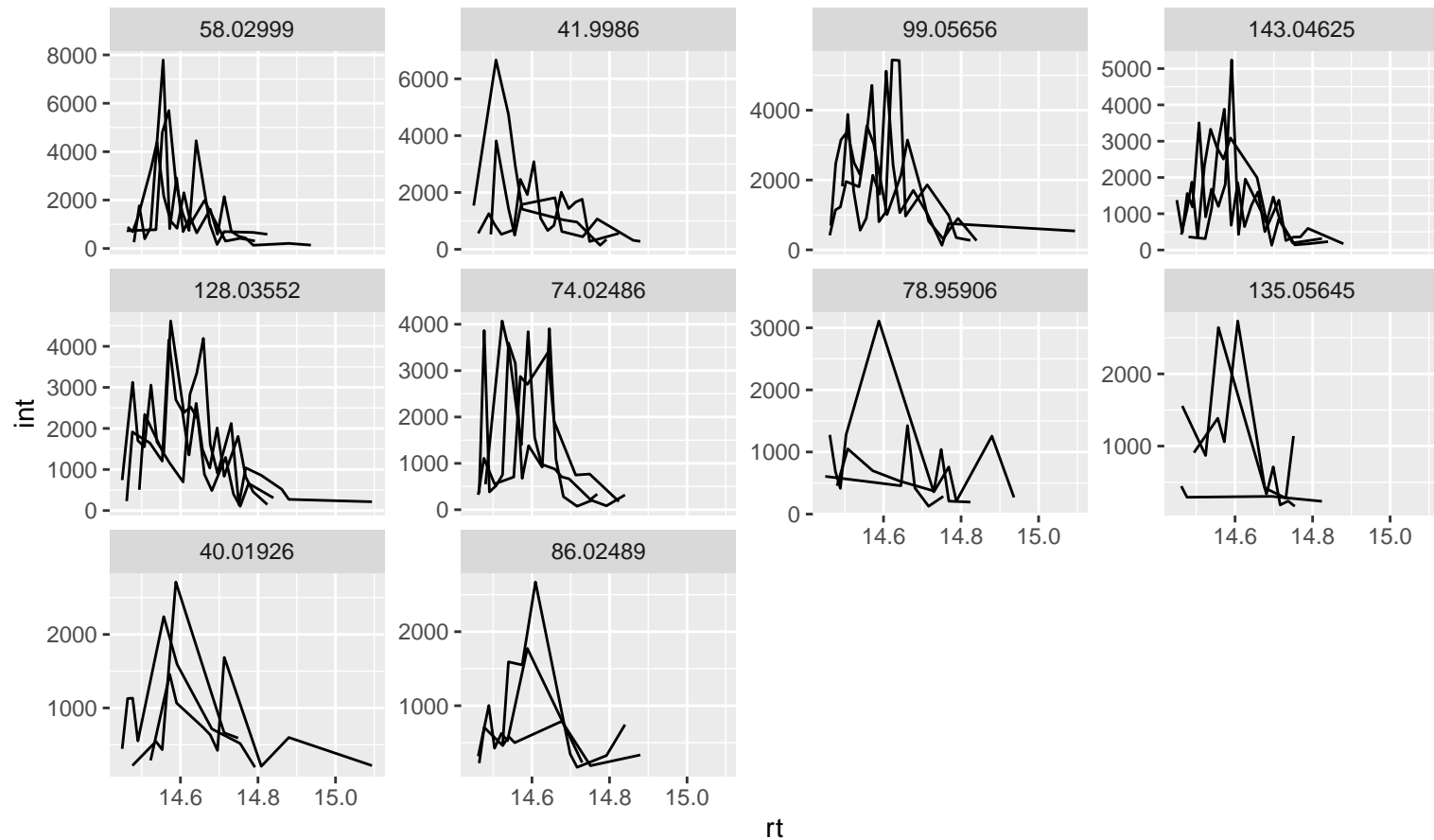
UDP-N-acetylglucosamine (neg) 606.074302



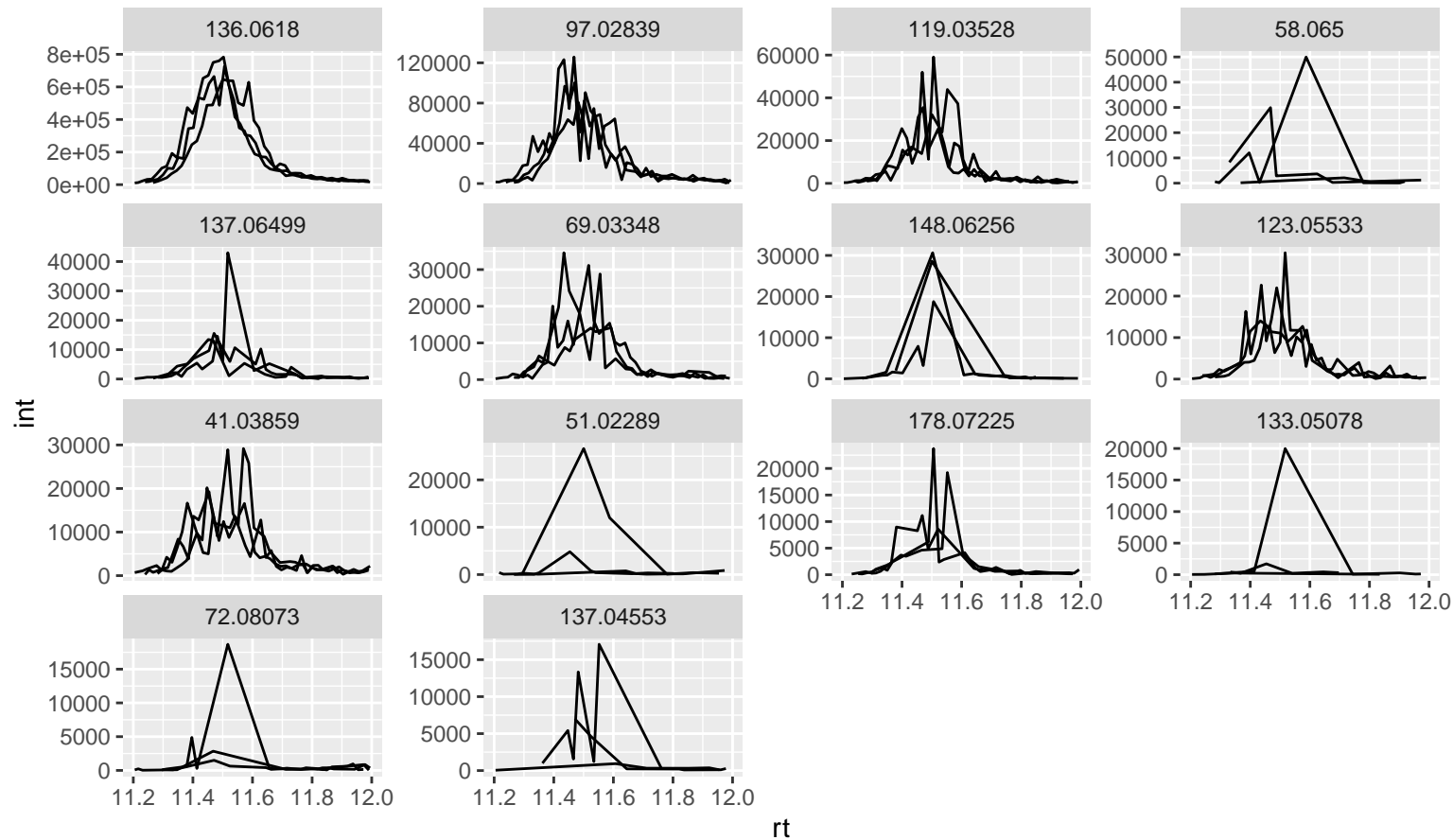
Glutathione disulfide (pos) 613.159244



Glutathione disulfide (neg) 611.144692

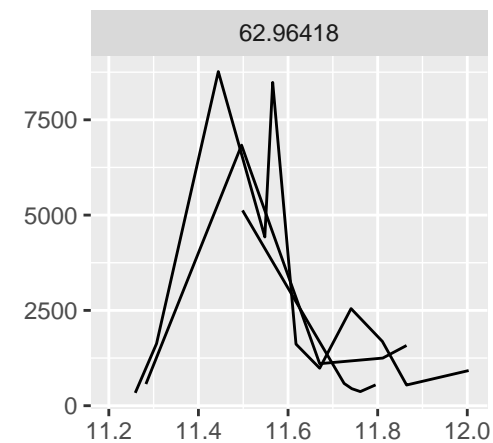
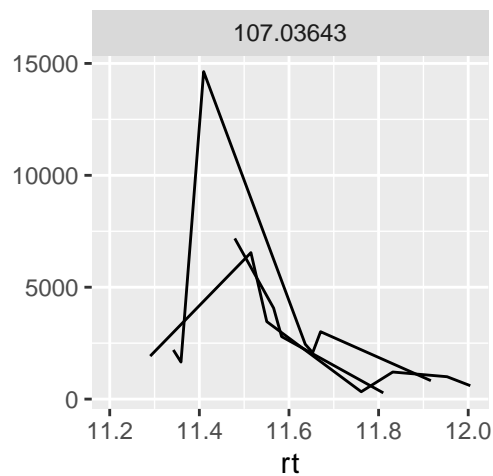
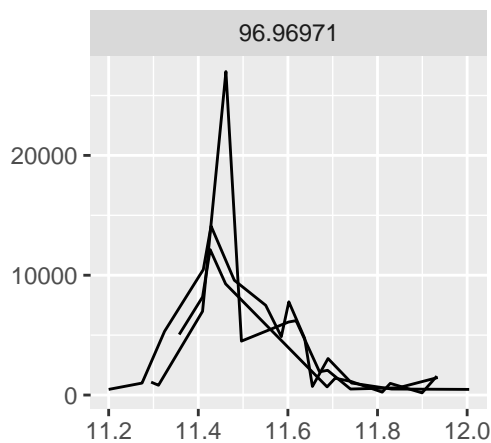
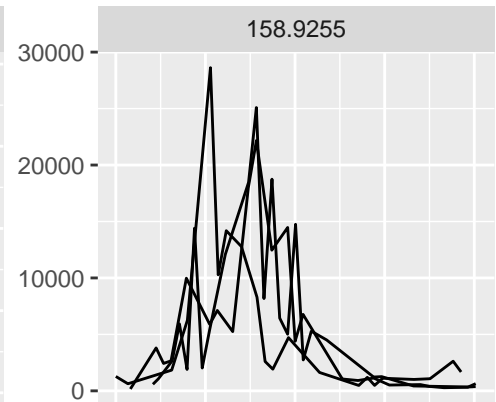
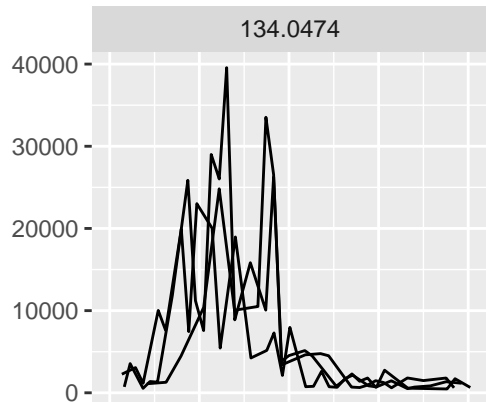
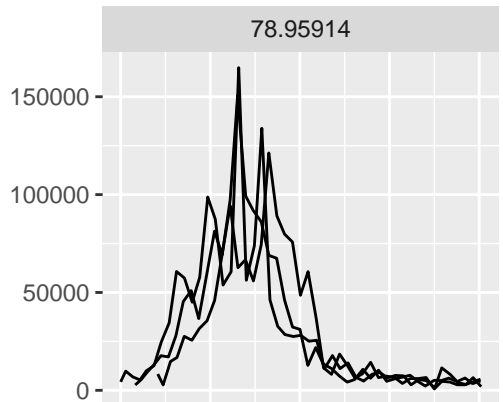


NAD (pos) 664.116405



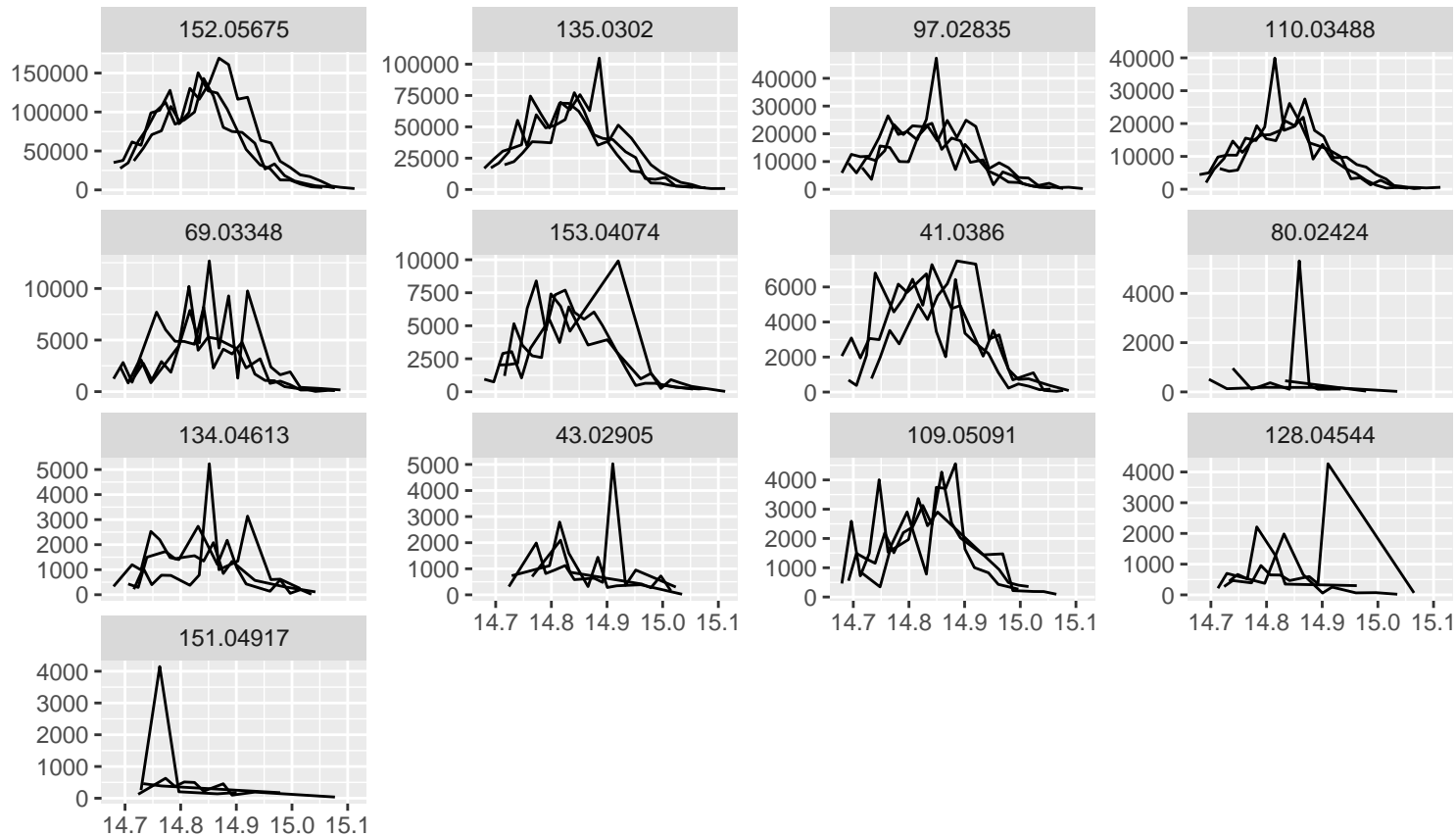
NAD (neg) 662.101853

int



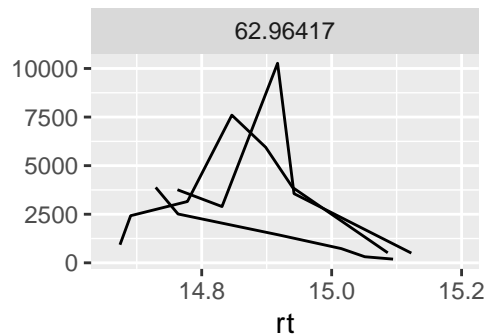
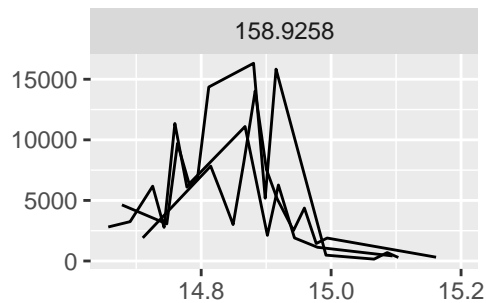
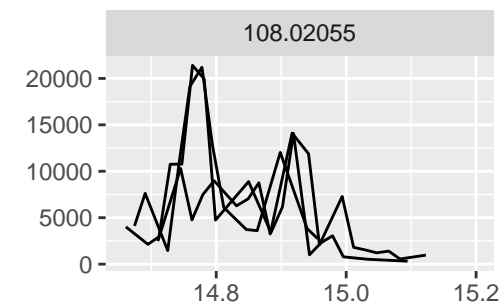
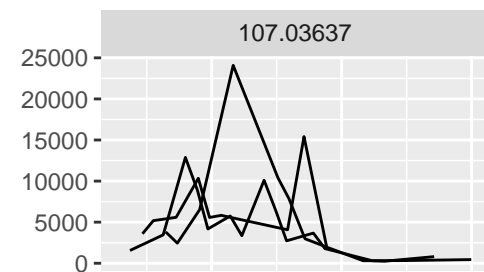
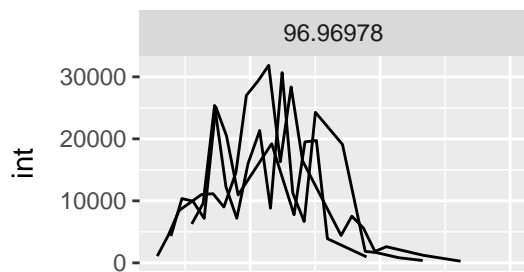
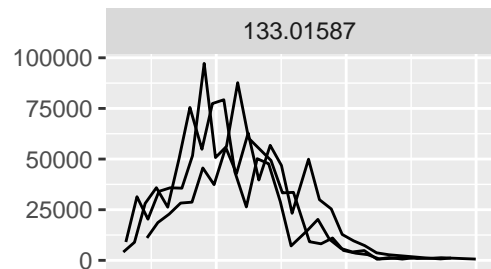
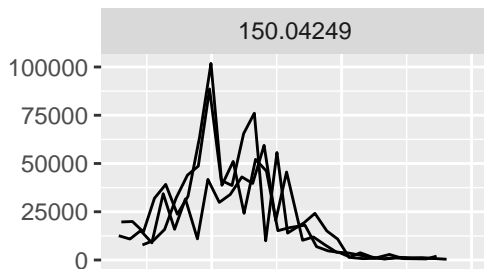
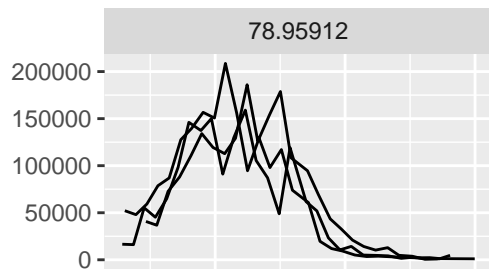
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3',5'-Cyclic diGMP (pos) 691.102152

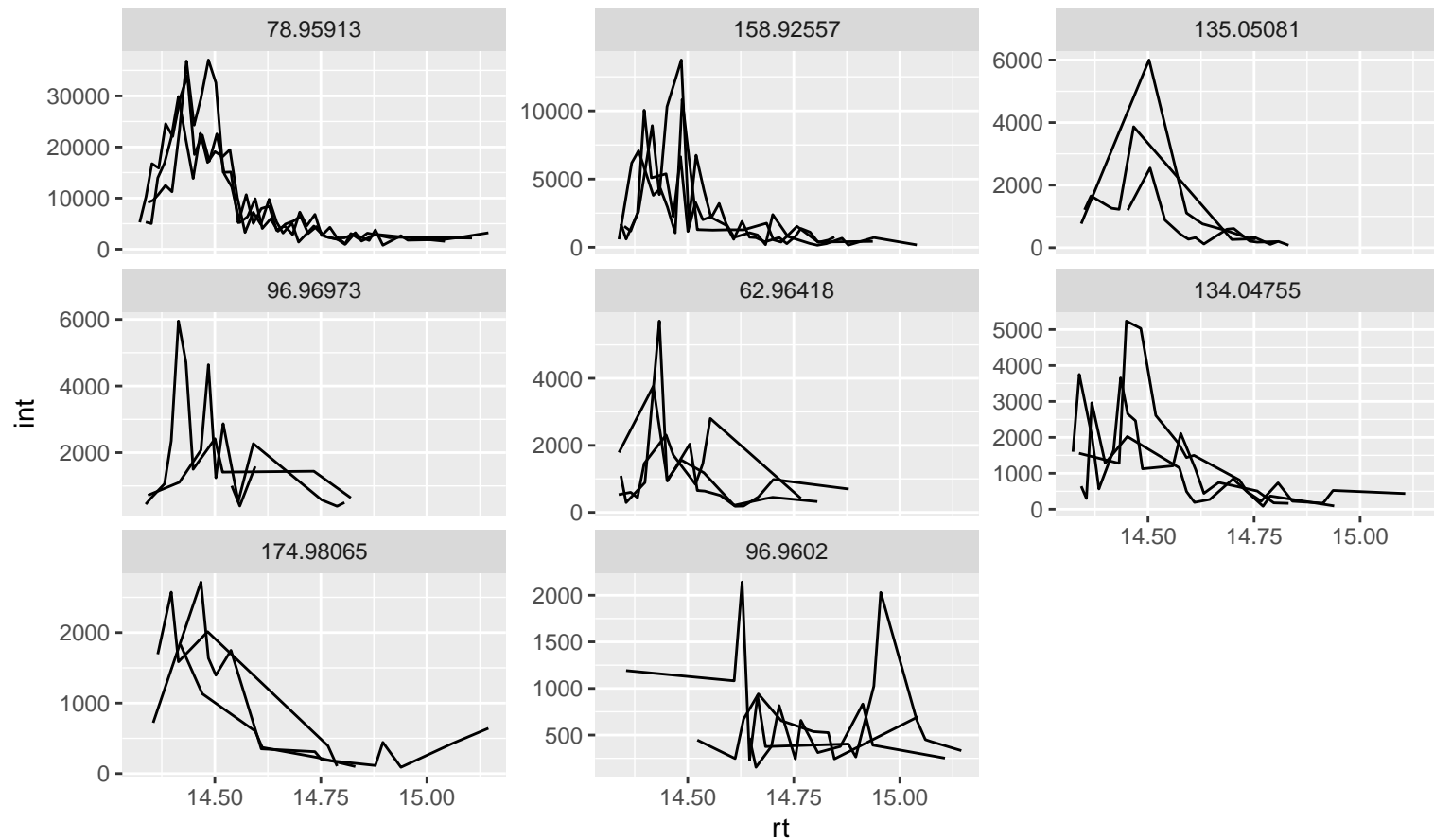


rt

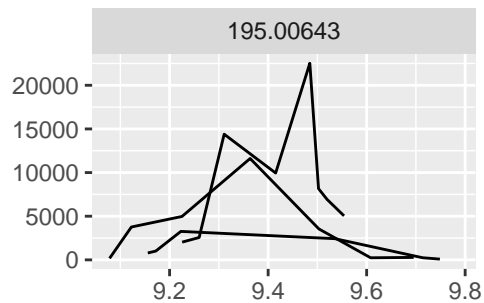
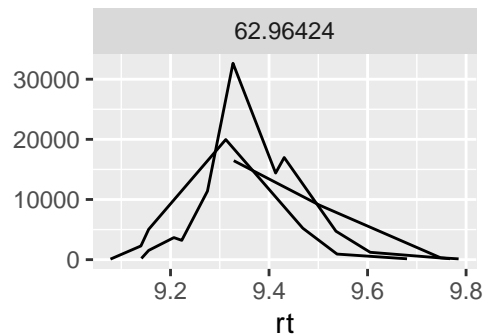
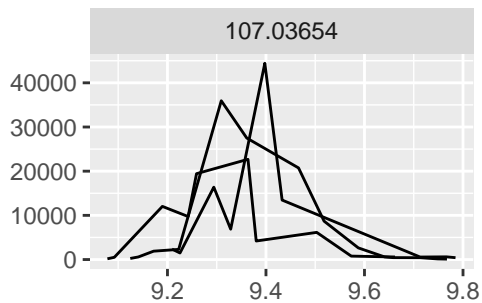
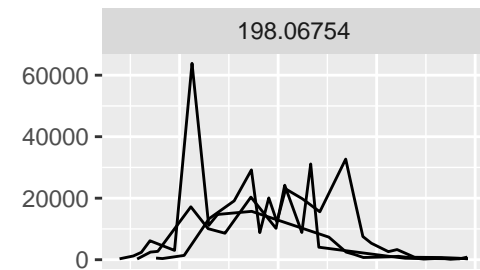
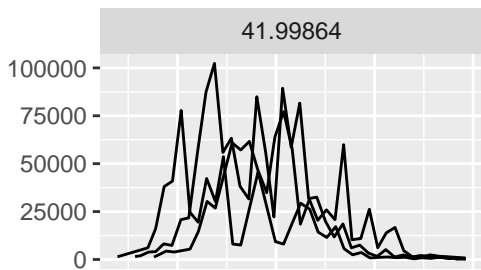
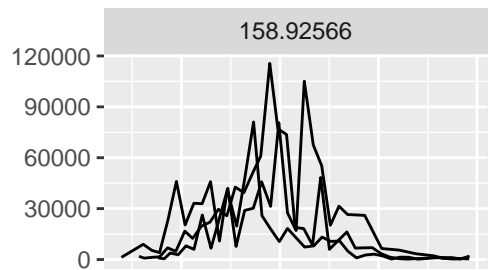
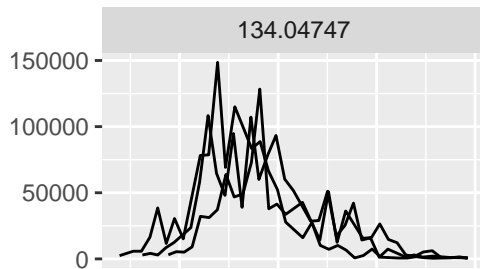
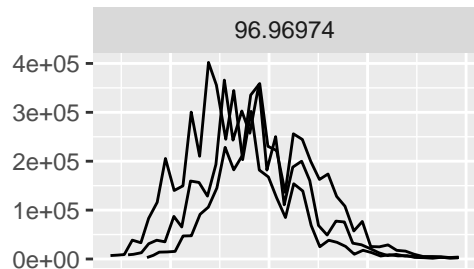
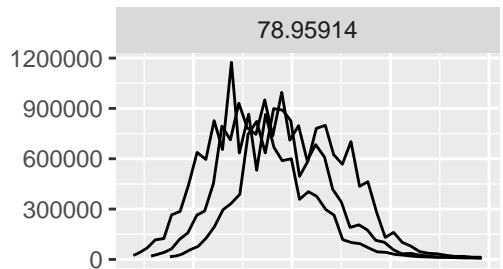
3',5'-Cyclic diGMP (neg) 689.0876



NADP (neg) 743.076011

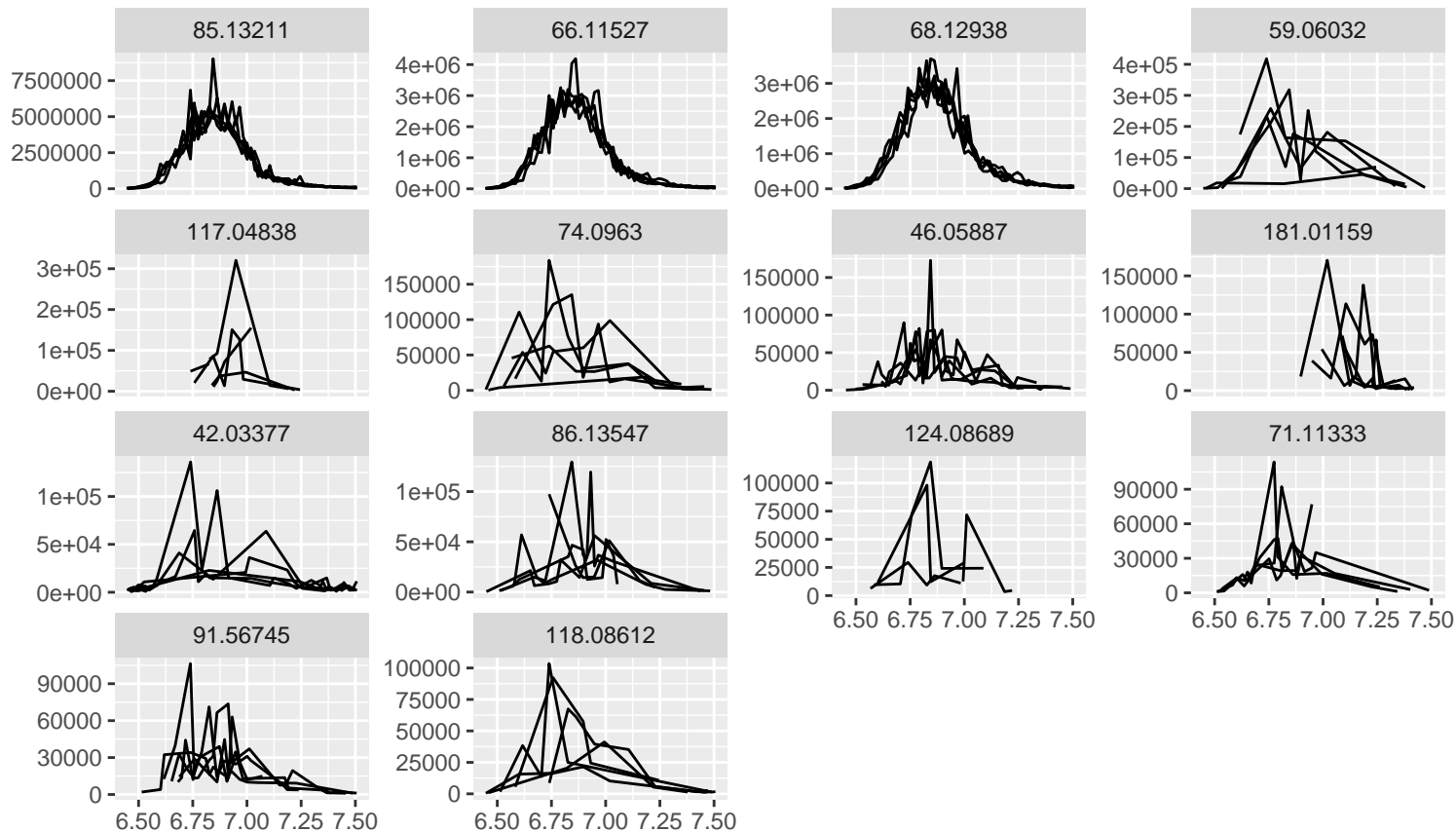


Flavin adenine dinucleotide (neg) 784.149866



Trimethylamine N-oxide, 2H9 (pos) 85.132183

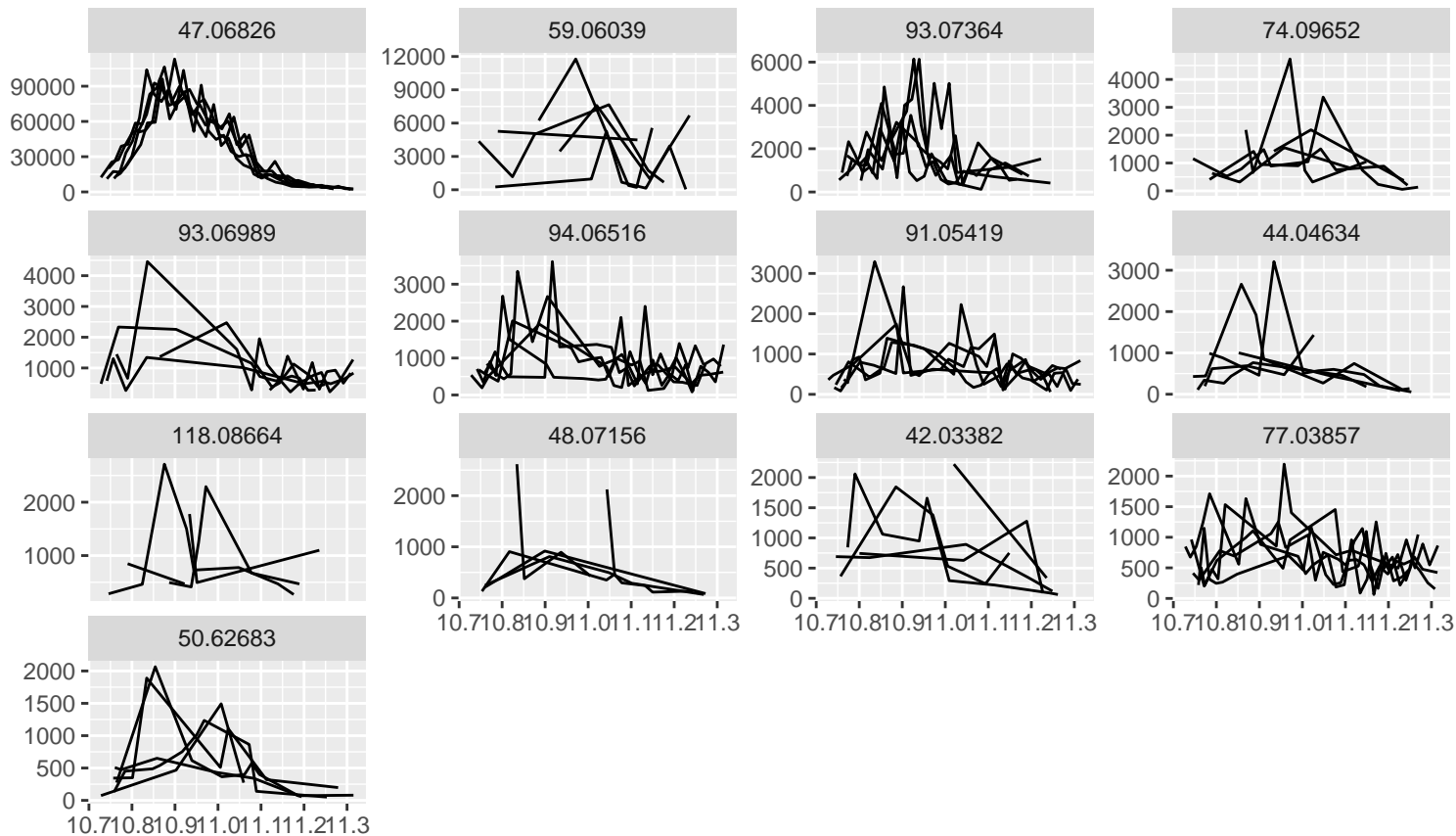
int



rt

L-Alanine, 2H3 (pos) 93.073786

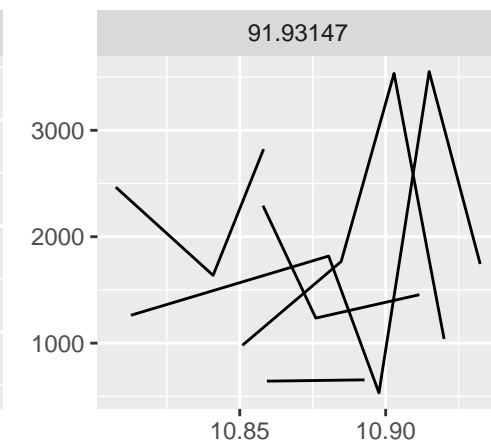
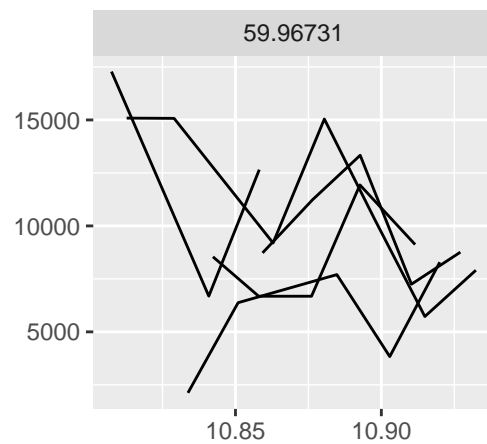
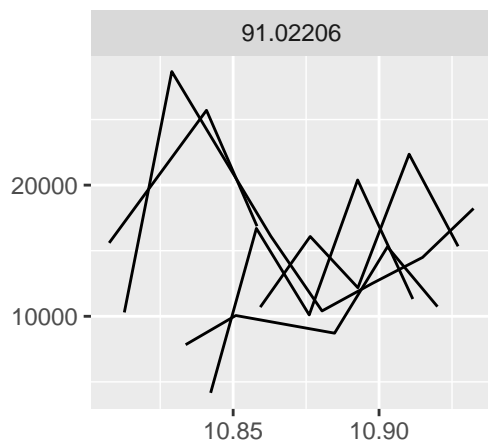
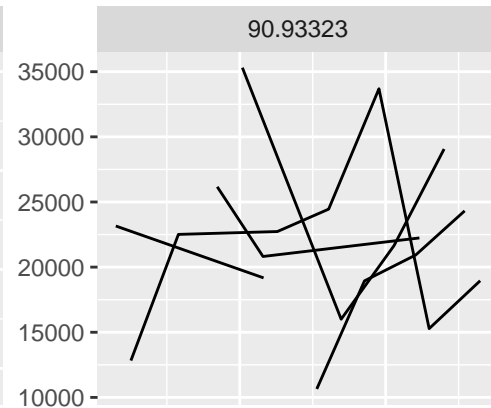
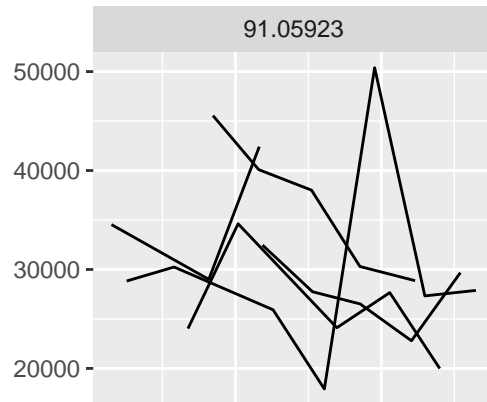
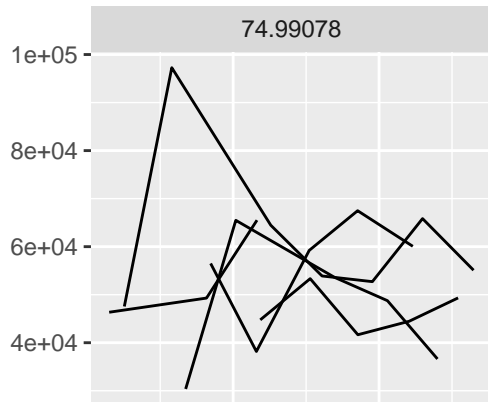
int



rt

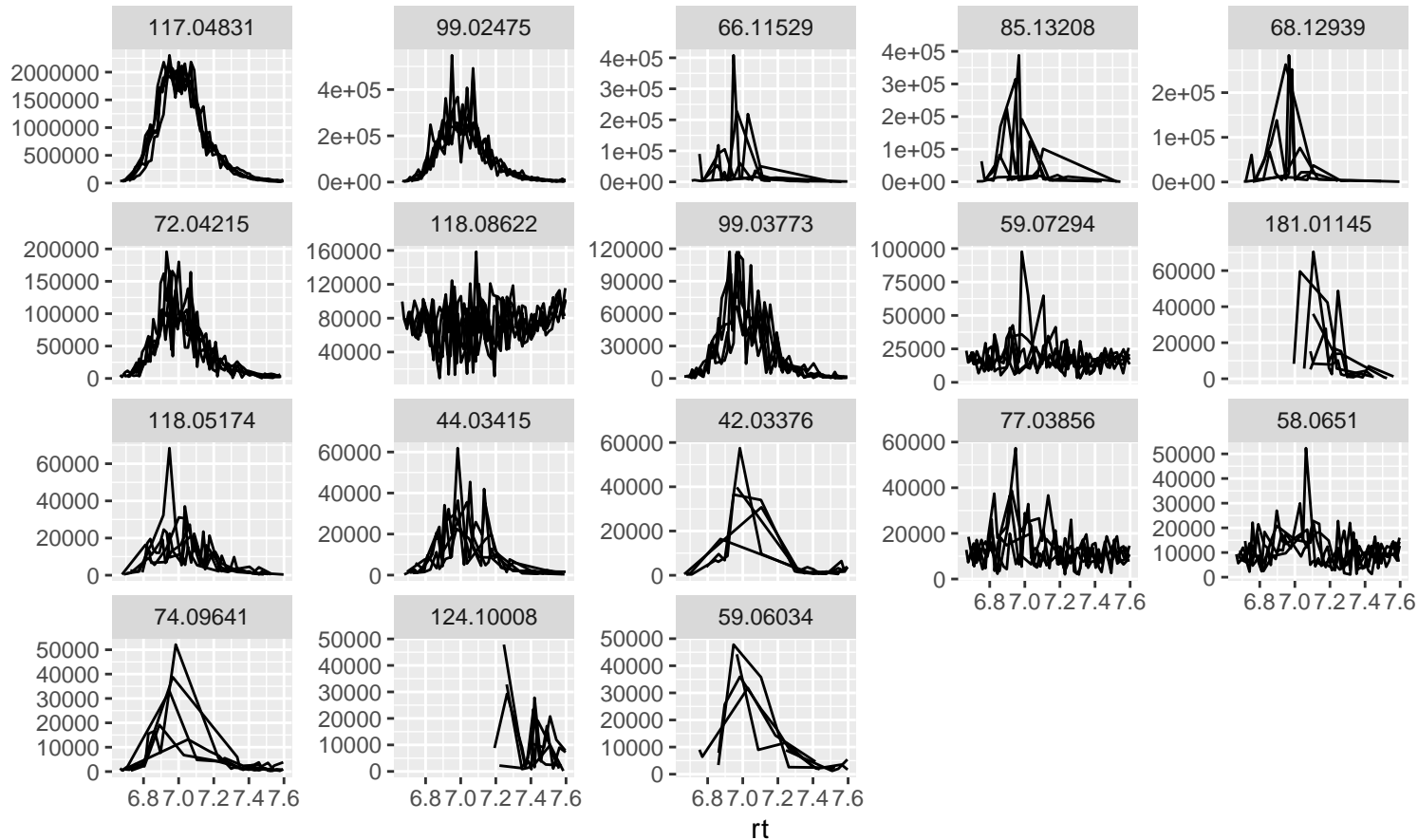
L-Alanine, 2H3 (neg) 91.059234

int

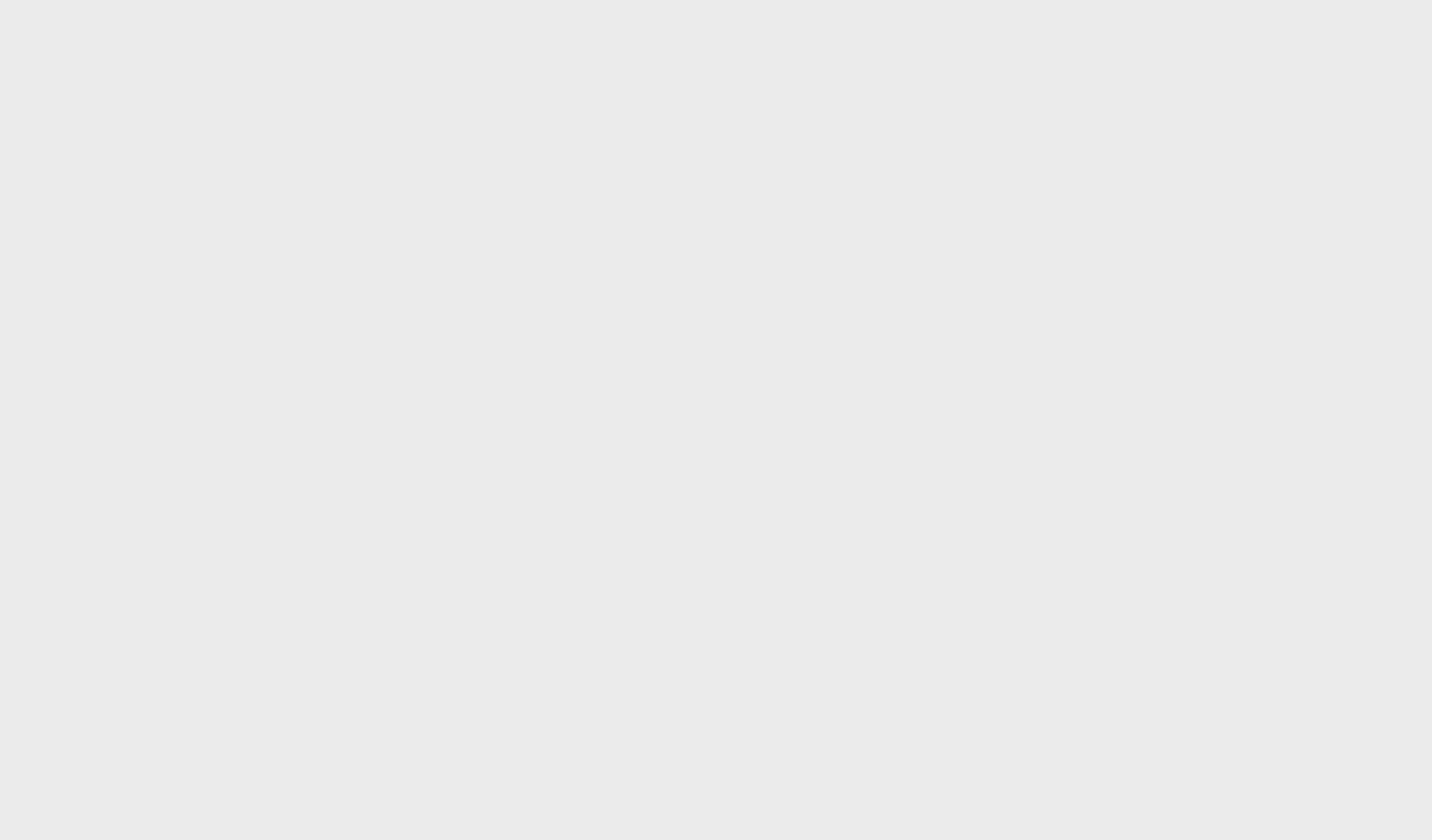


rt

Cytosine, 13C2, 15N3 (pos) 117.048353

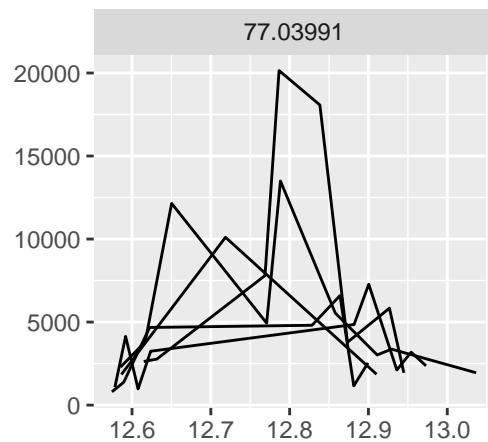
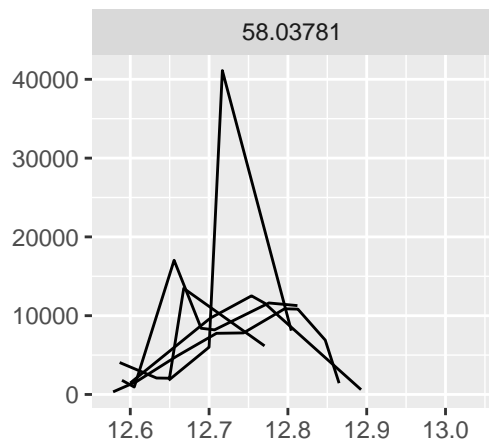
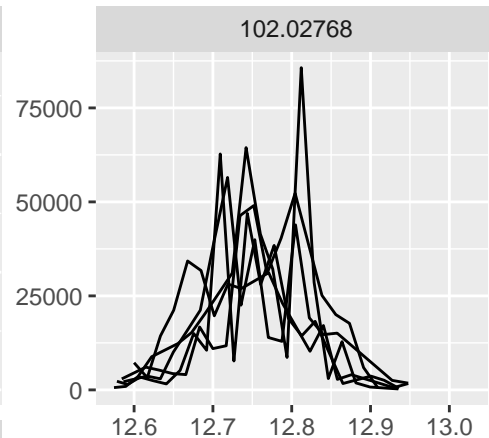
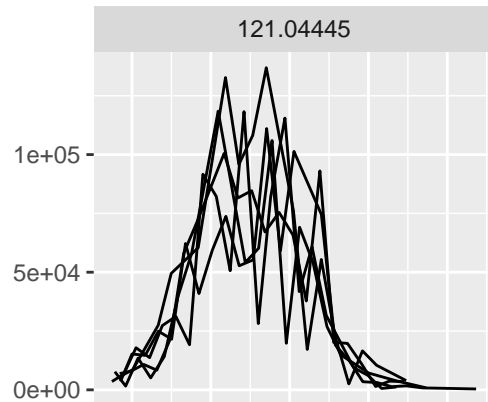
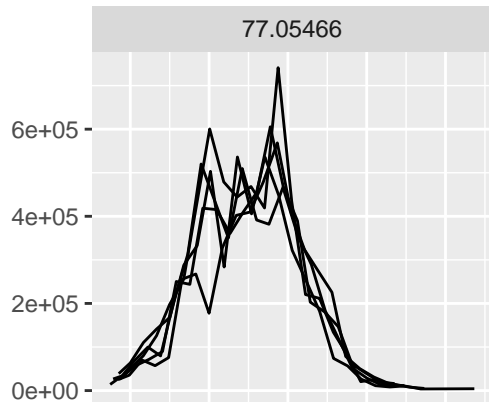


Cytosine, ¹³C₂, ¹⁵N₃ (neg) 115.033801



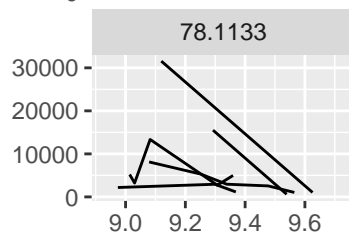
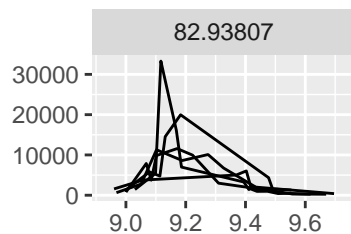
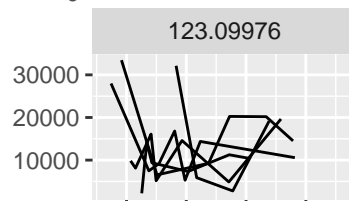
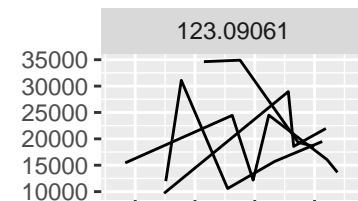
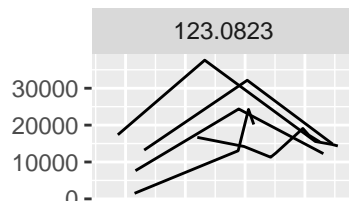
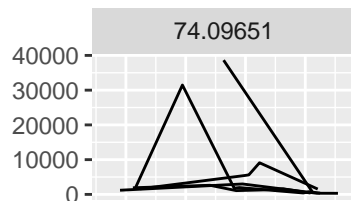
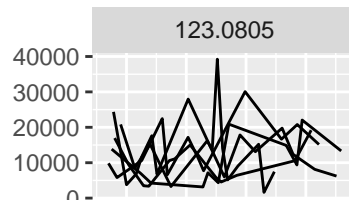
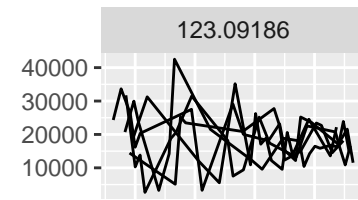
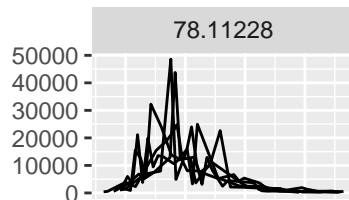
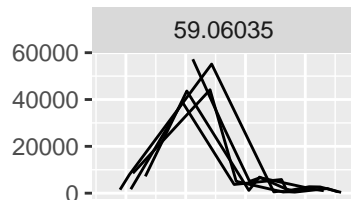
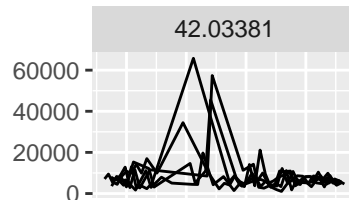
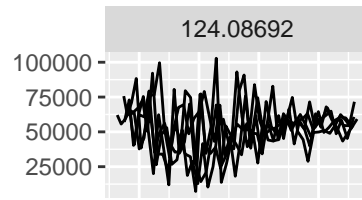
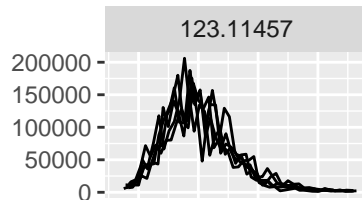
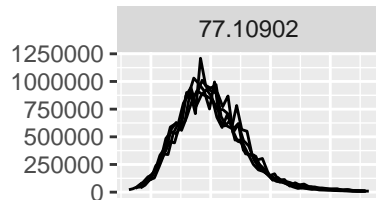
Succinic acid, 2H4 (neg) 121.04442

int



rt

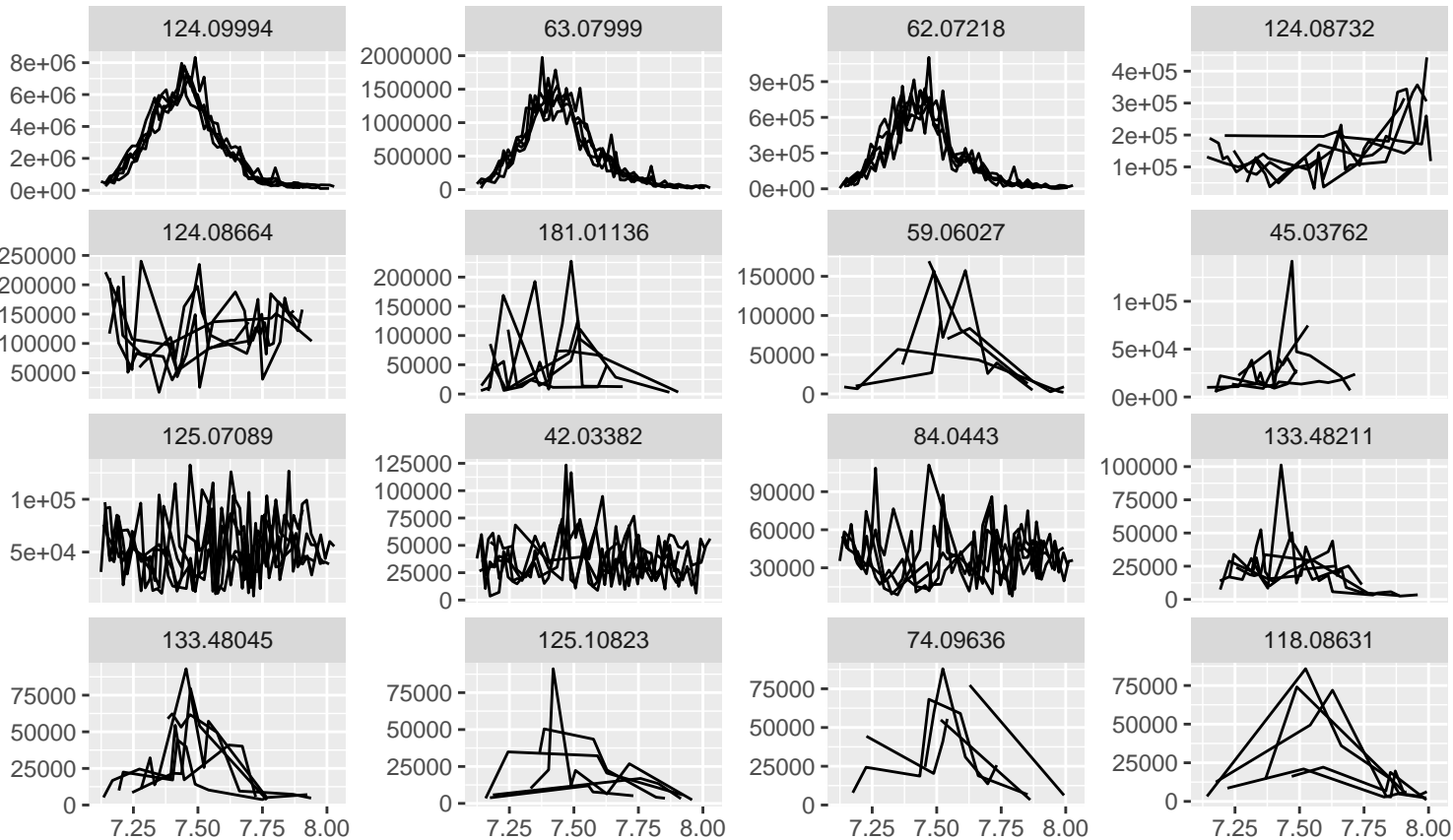
L-Proline, 2H7 (pos) 123.114544



rt

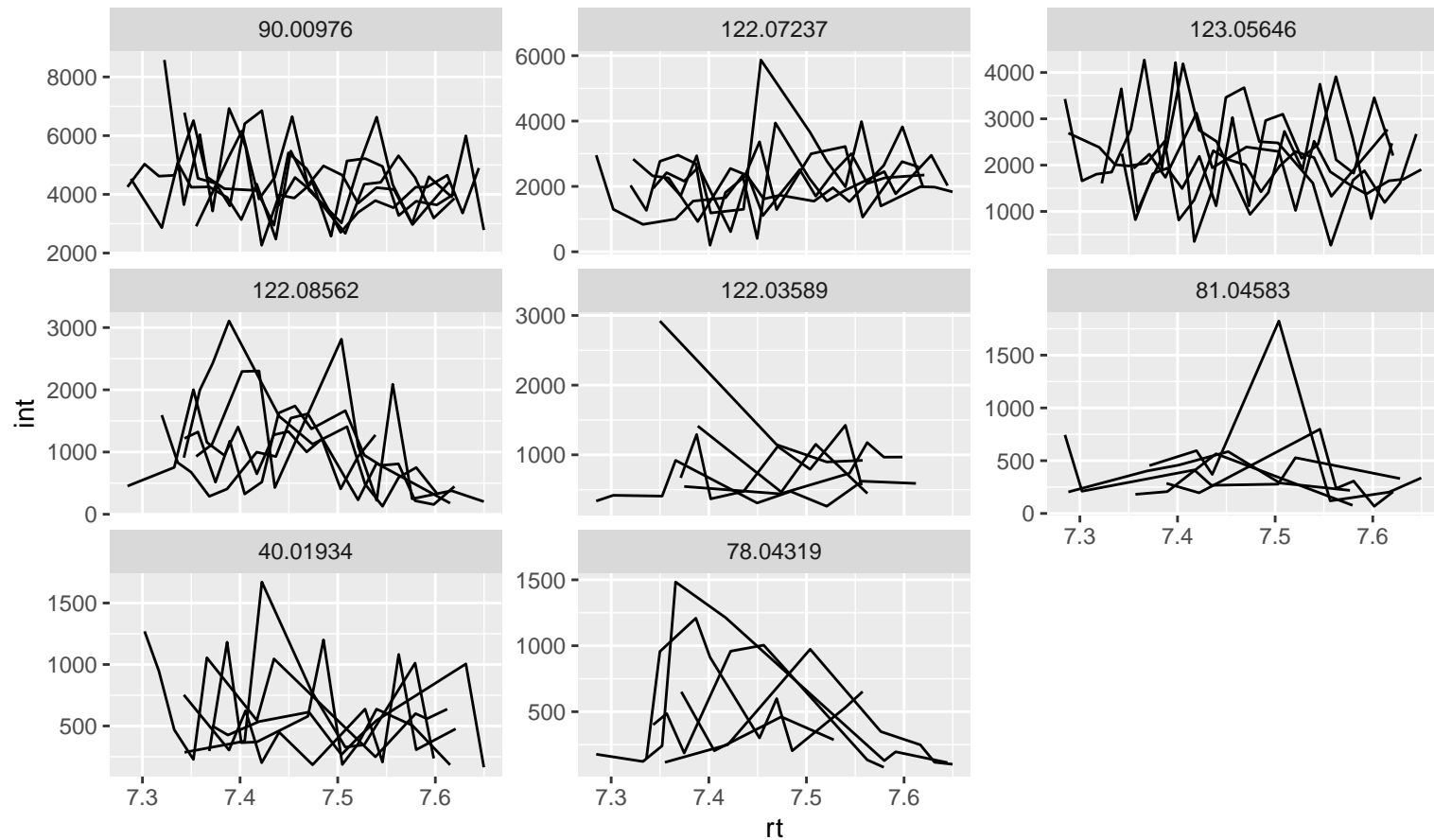
Glycine betaine, $^{13}\text{C}5$, ^{15}N (pos) 124.100065

int

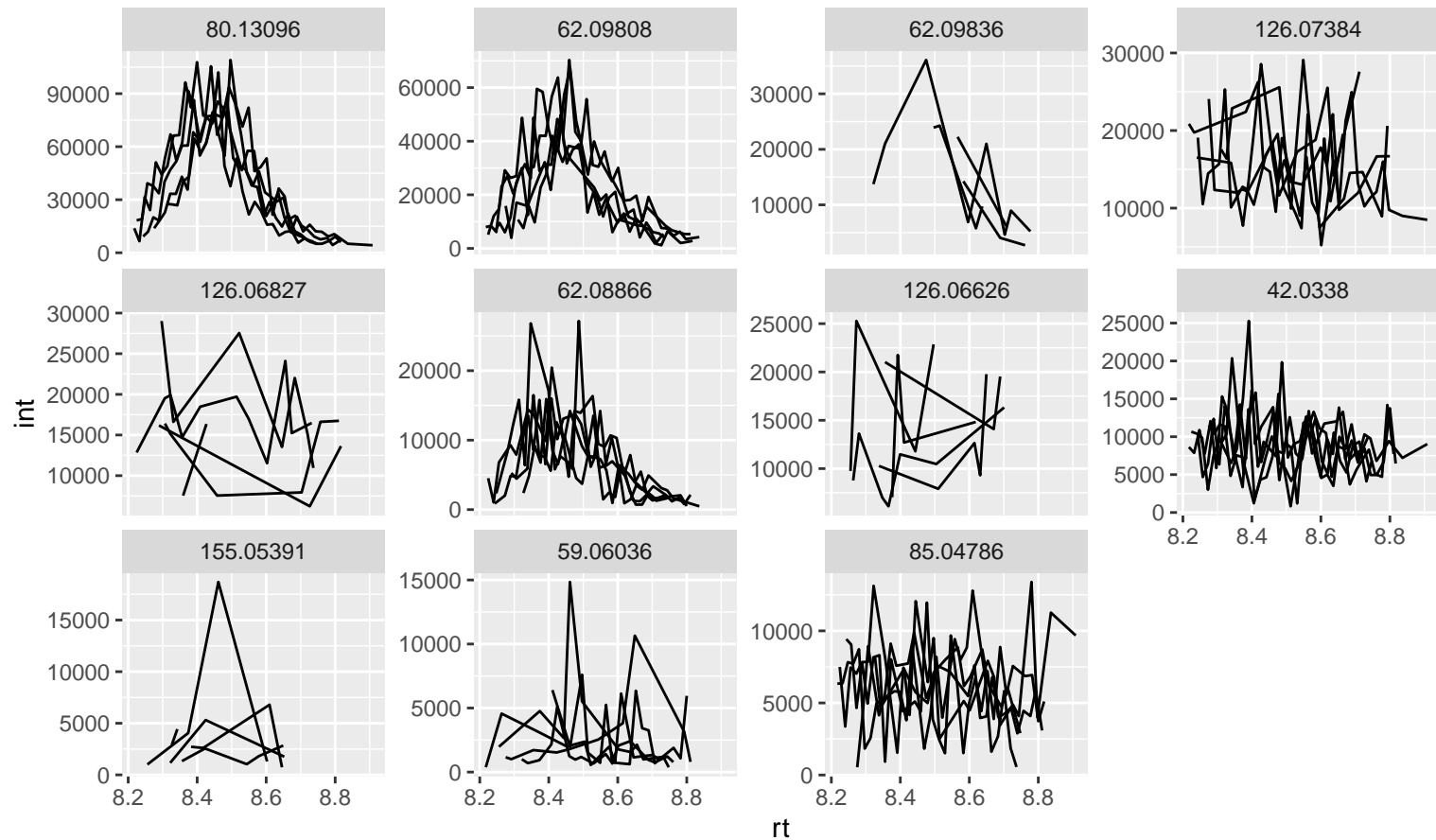


rt

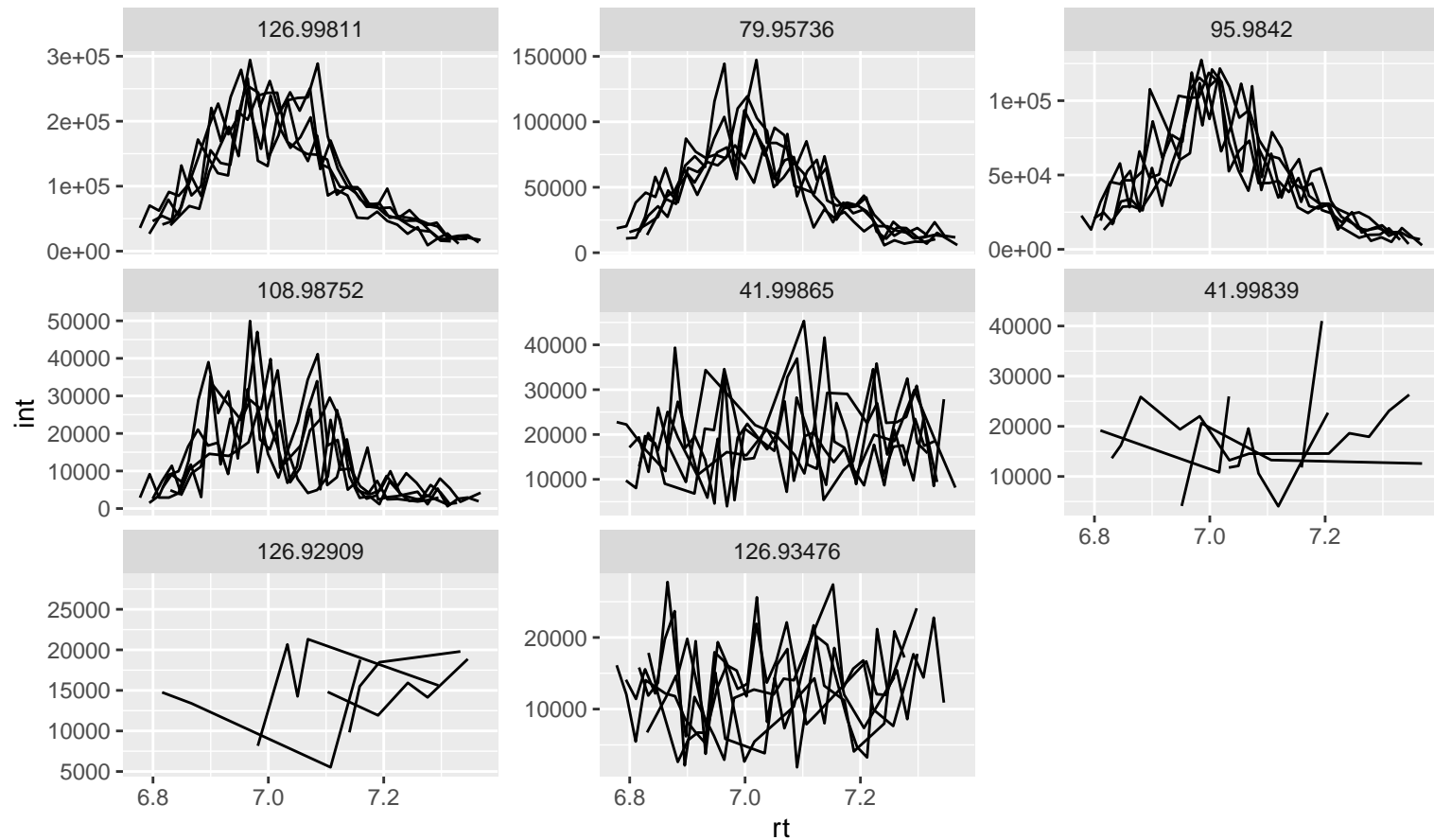
Glycine betaine, $^{13}\text{C}5$, ^{15}N (neg) 122.085513



L-Valine, 2H8 (pos) 126.136471

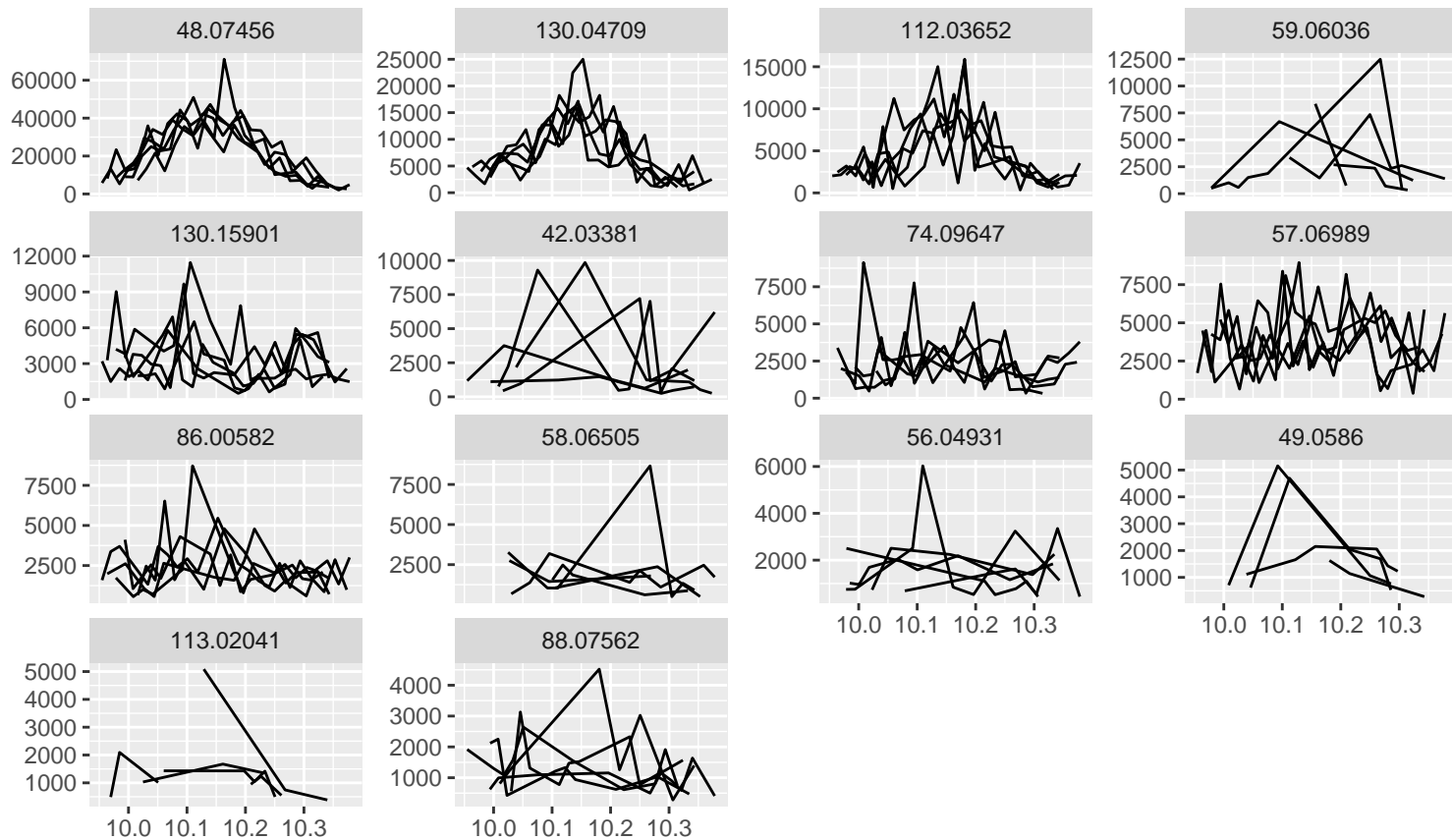


Isethionic acid, 13C2 (neg) 126.998116



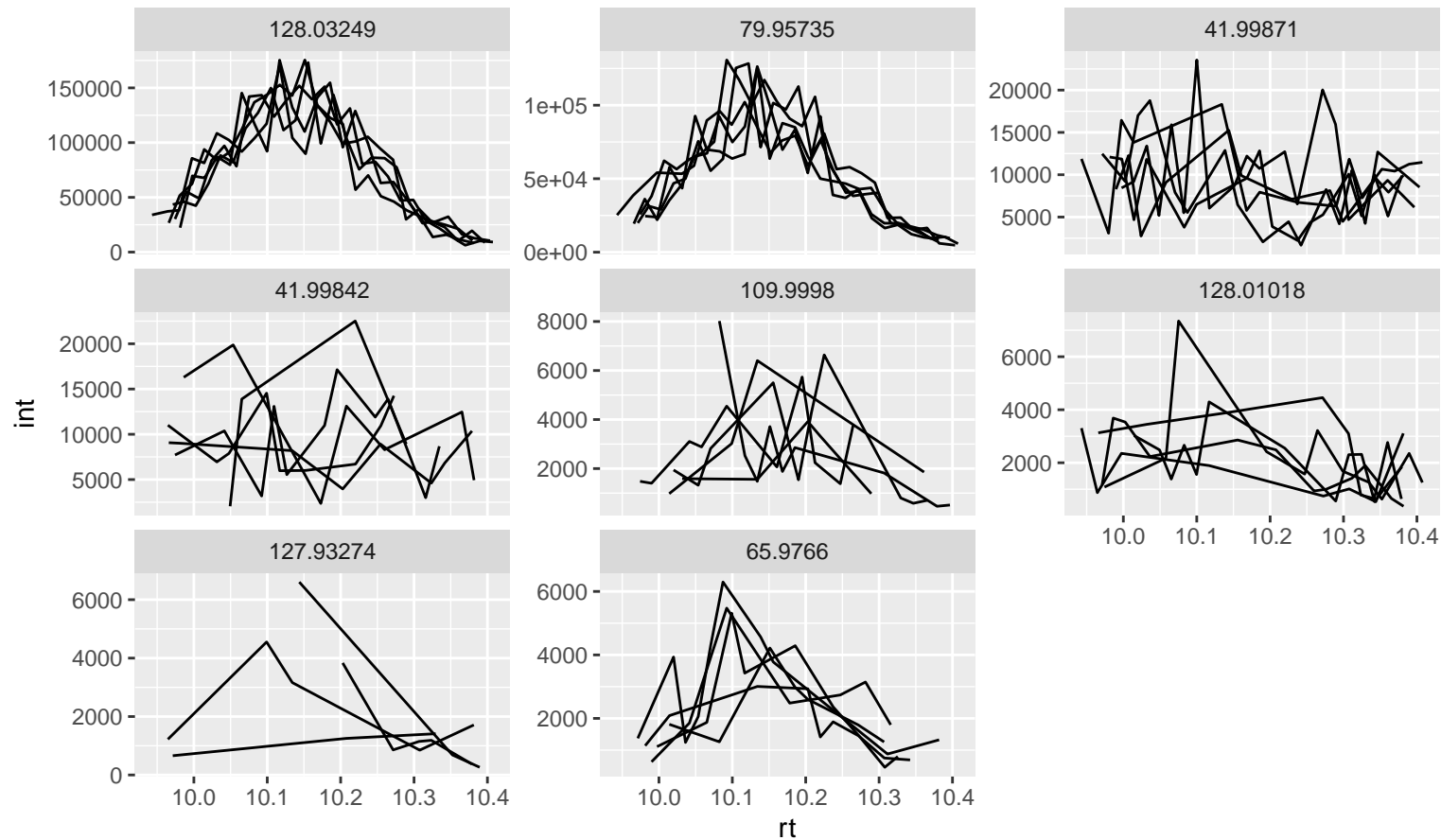
Taurine, 2H4 (pos) 130.04705

int



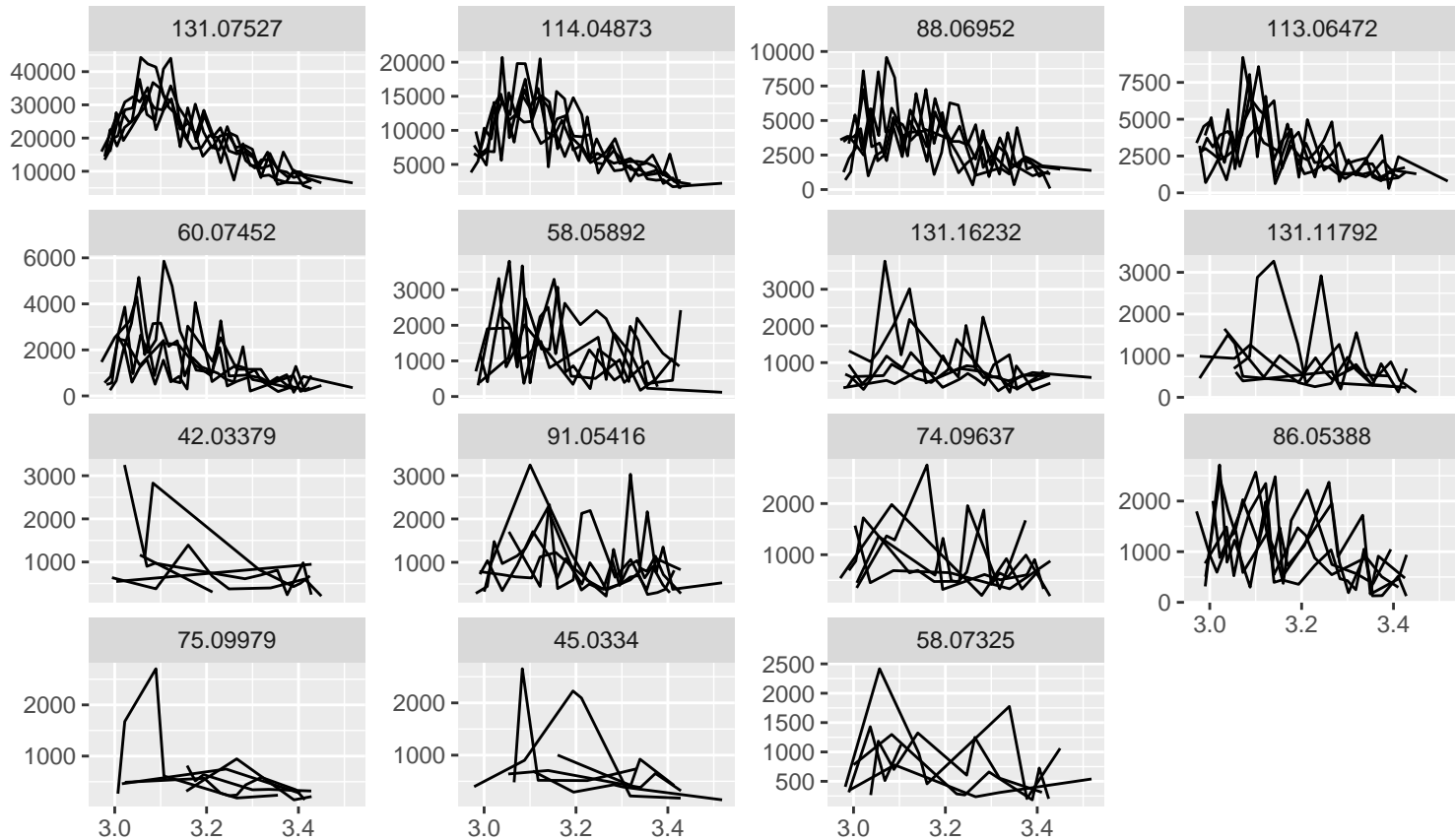
rt

Taurine, 2H4 (neg) 128.032498



Thymine, 2H4 (pos) 131.075312

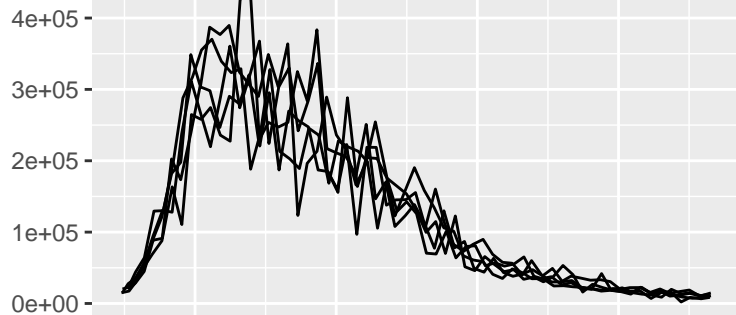
int



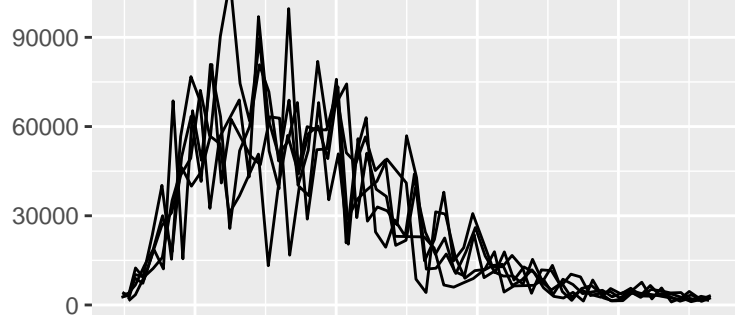
rt

Thymine, 2H4 (neg) 129.06076

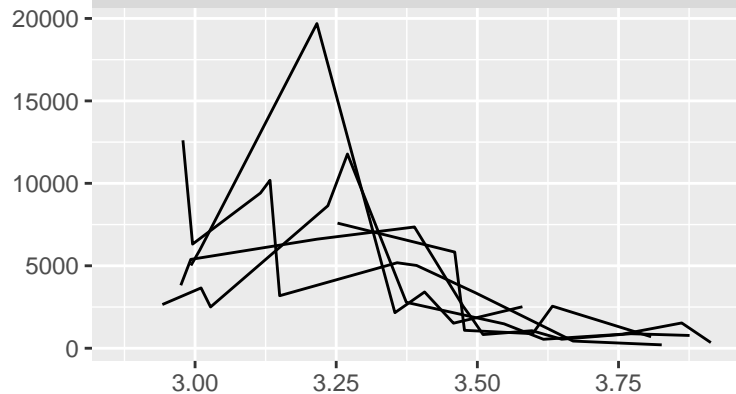
41.99858



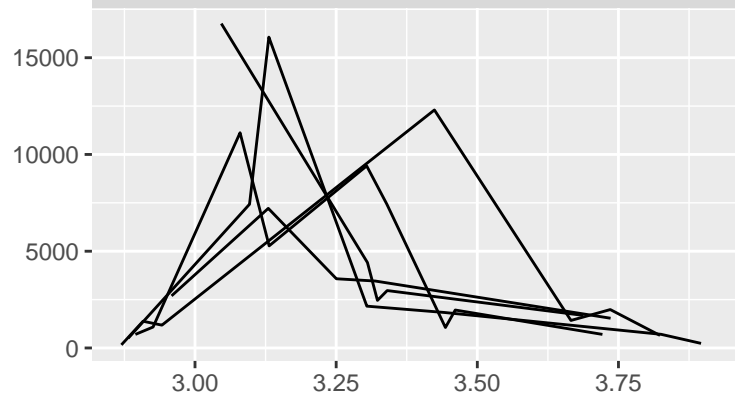
129.06084



45.17346

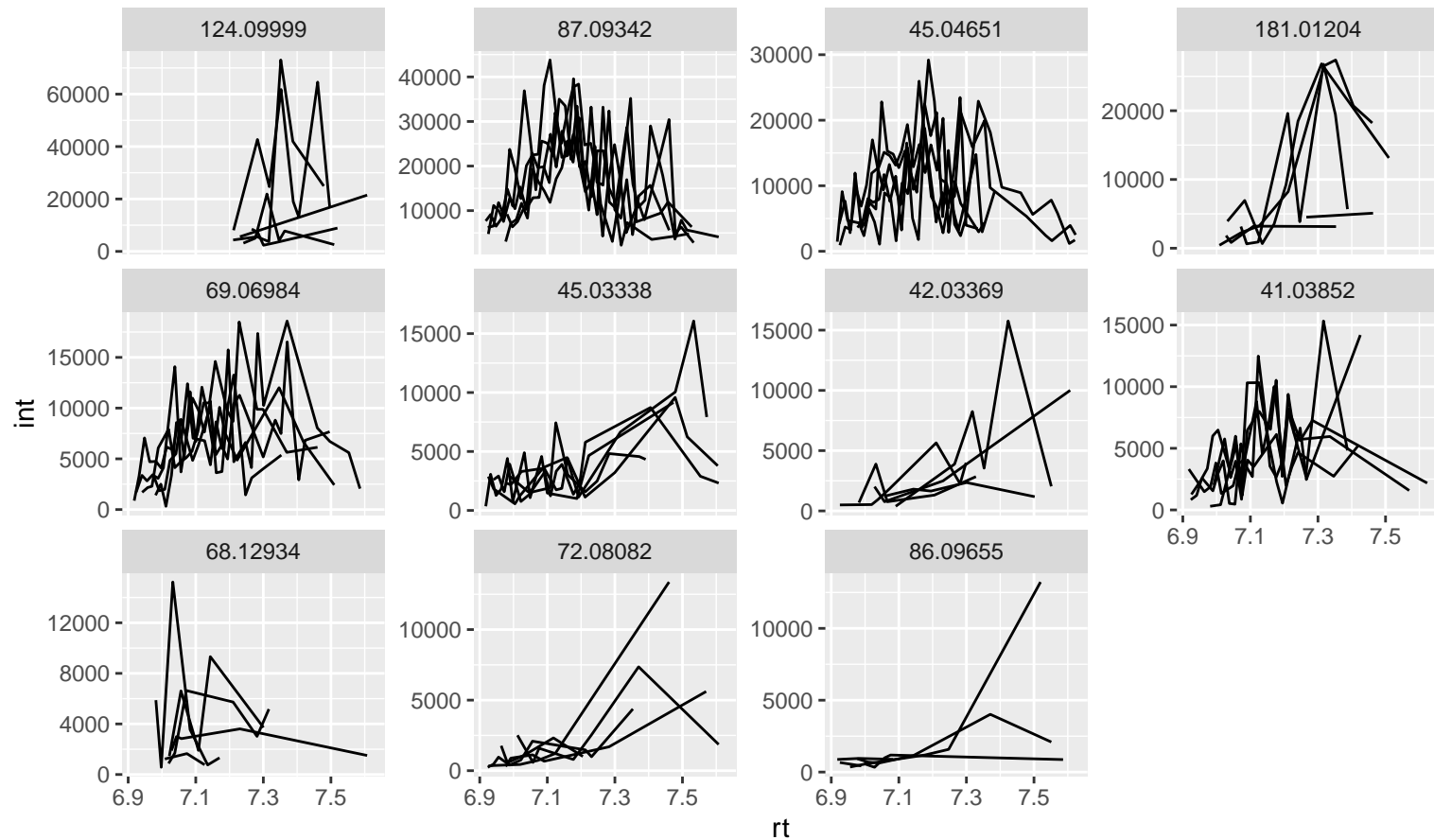


45.17397

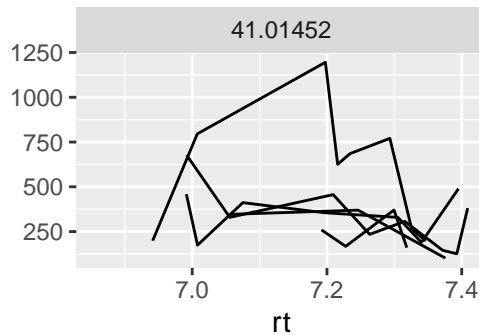
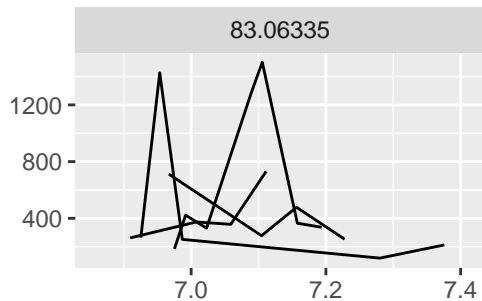
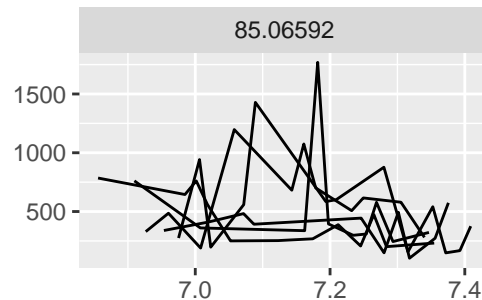
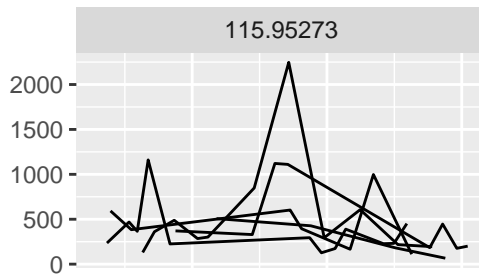
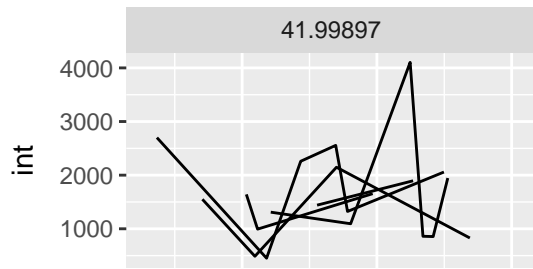
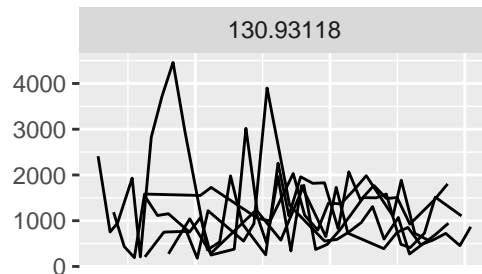
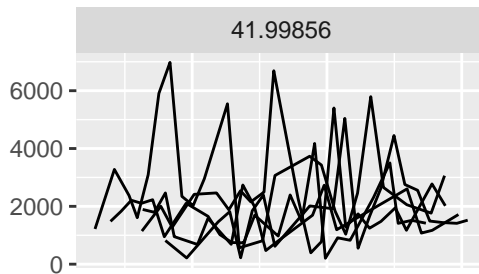
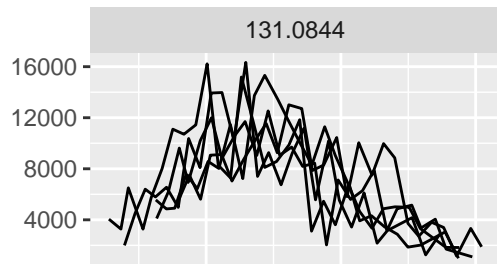


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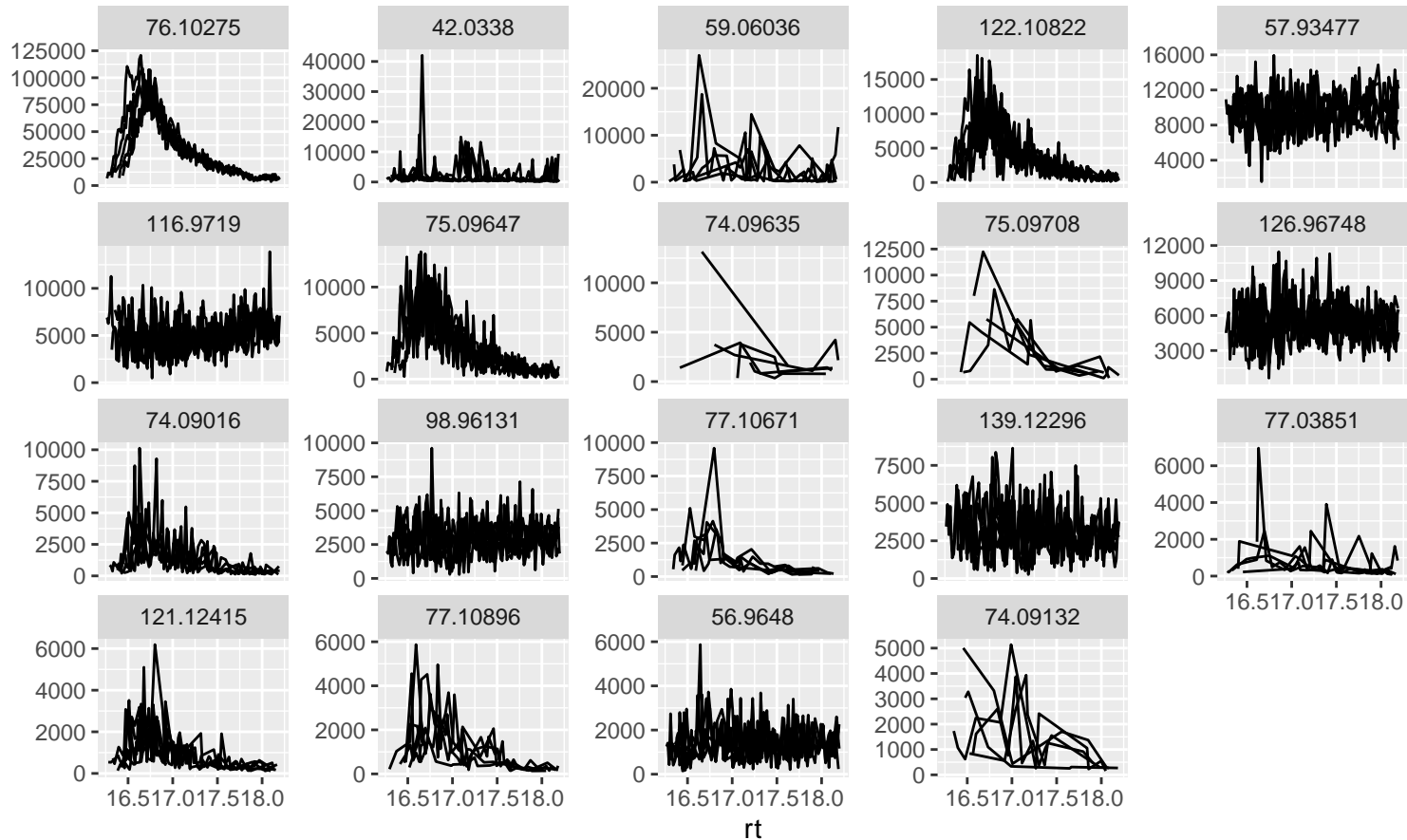
L-Isoleucine, 15N (pos) 133.09894



L-Isoleucine, 15N (neg) 131.084388

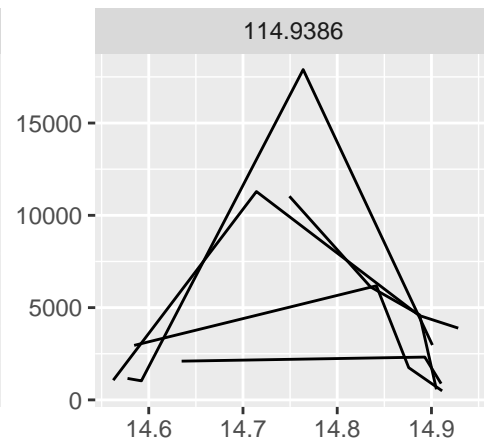
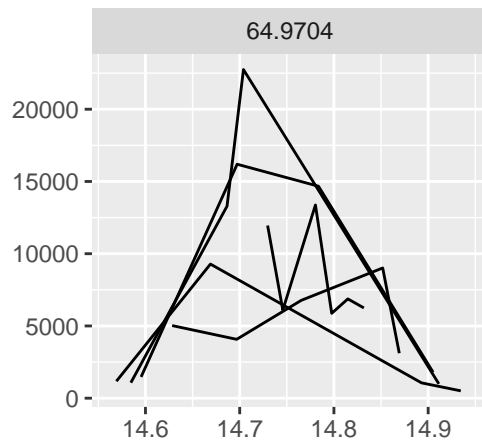
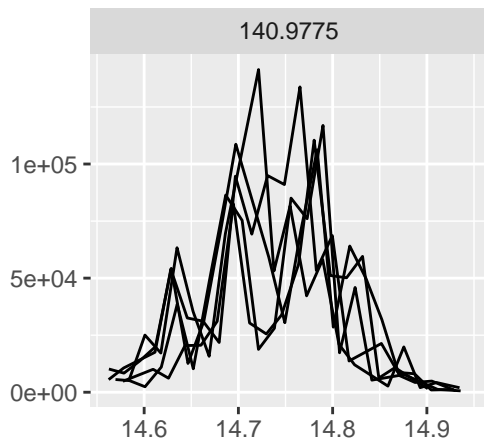
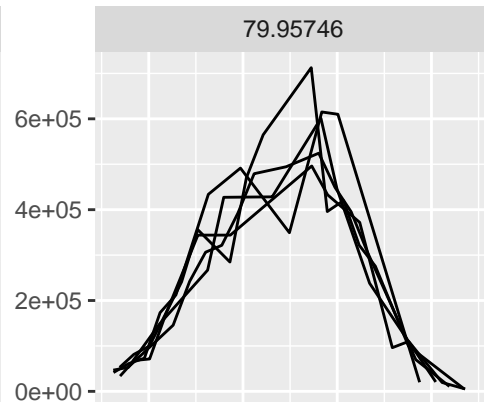
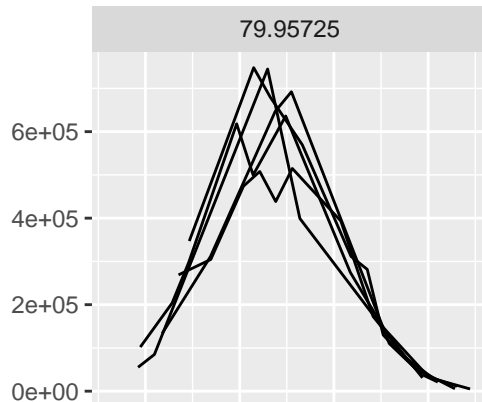
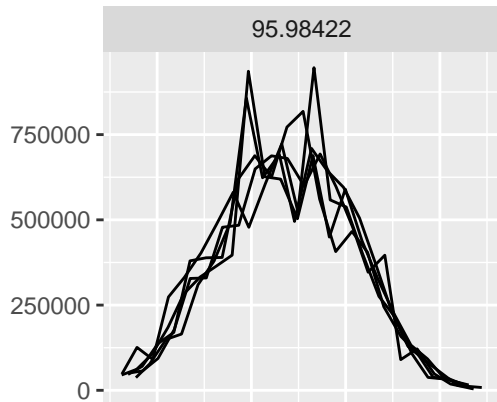


Ornithine, 2H6 (pos) 139.134816



Sulfoacetic acid, $^{13}\text{C}2$ (neg) 140.977381

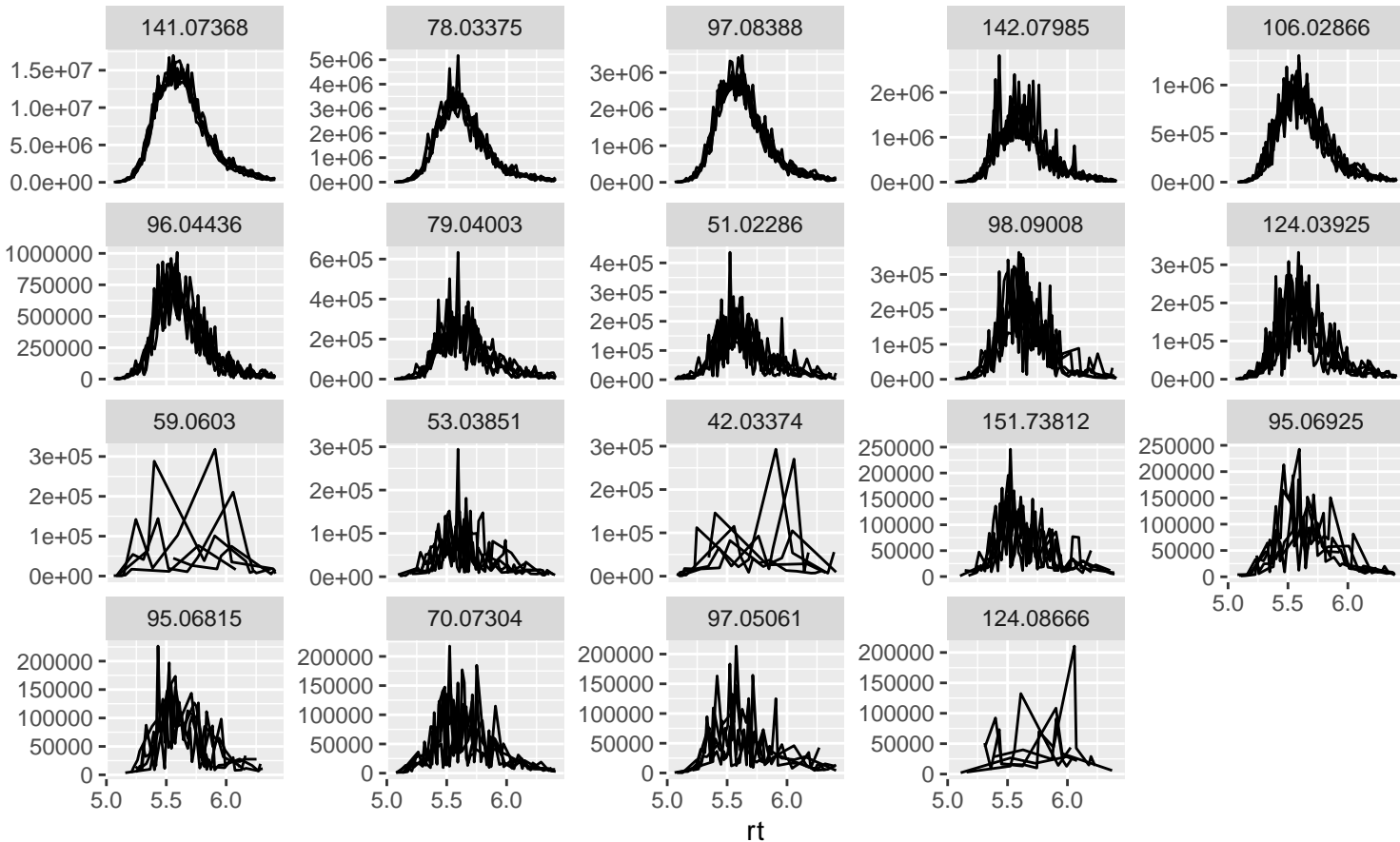
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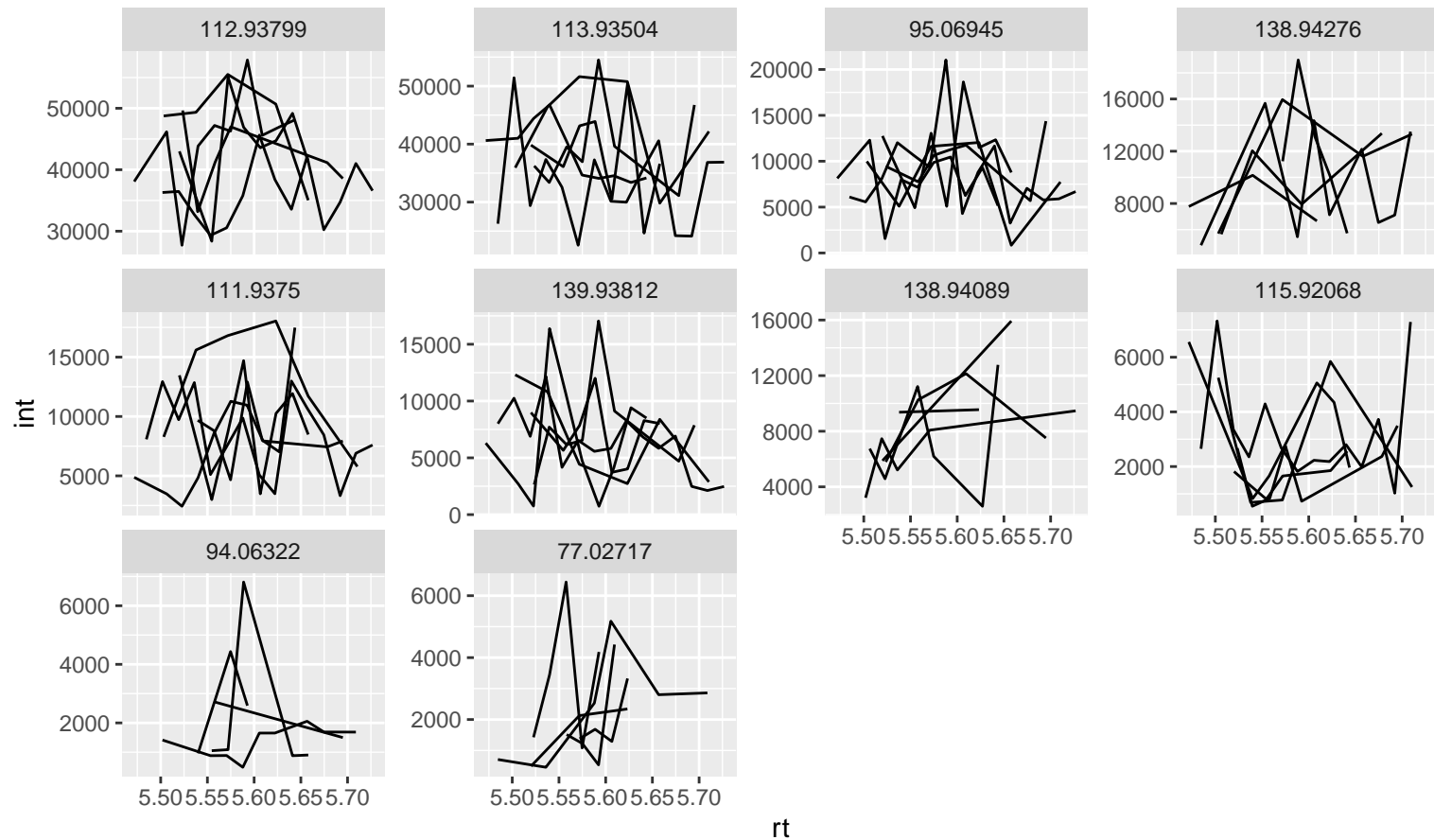
rt

Homarine, 2H3 (pos) 141.073786

int

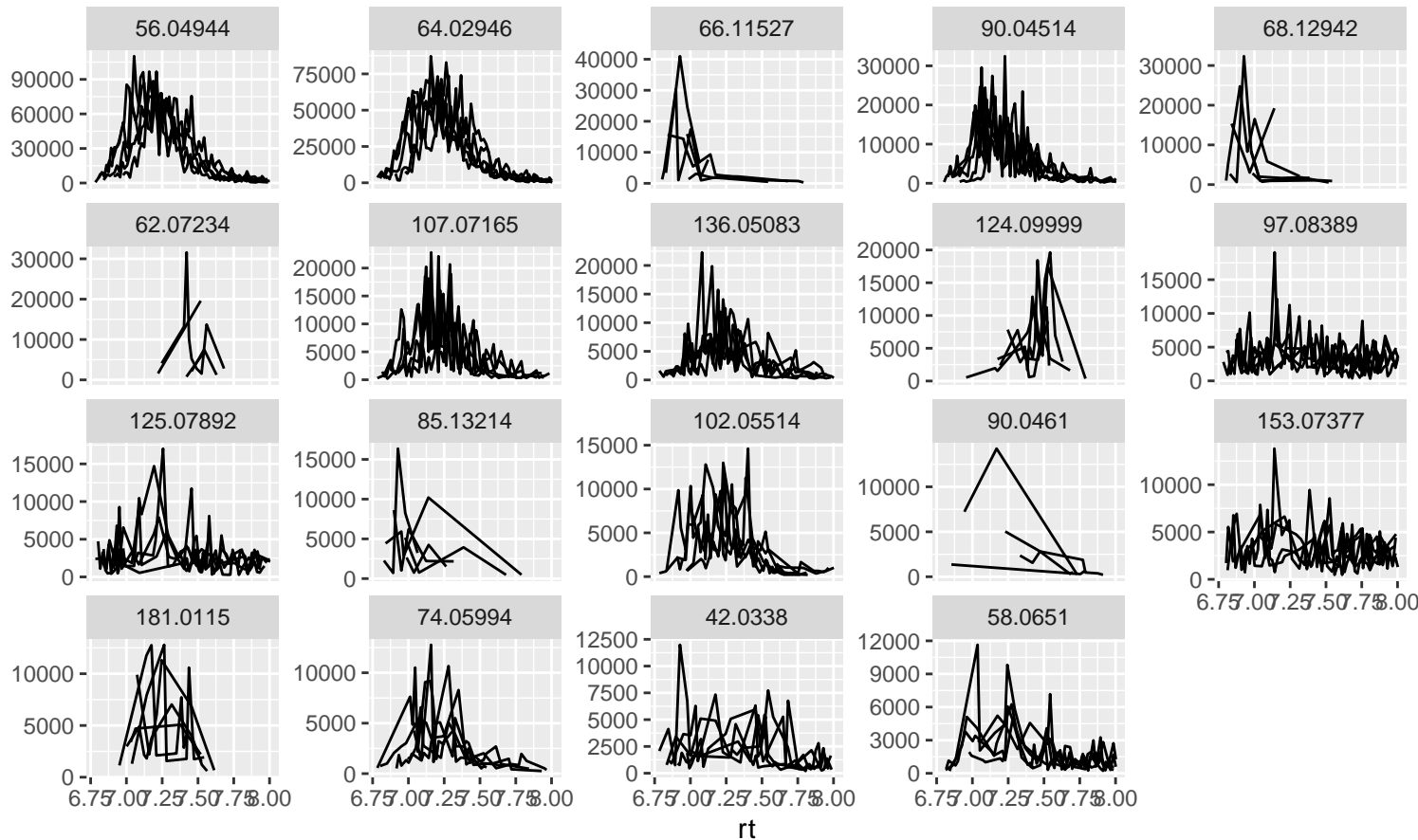


Homarine, 2H3 (neg) 139.059234

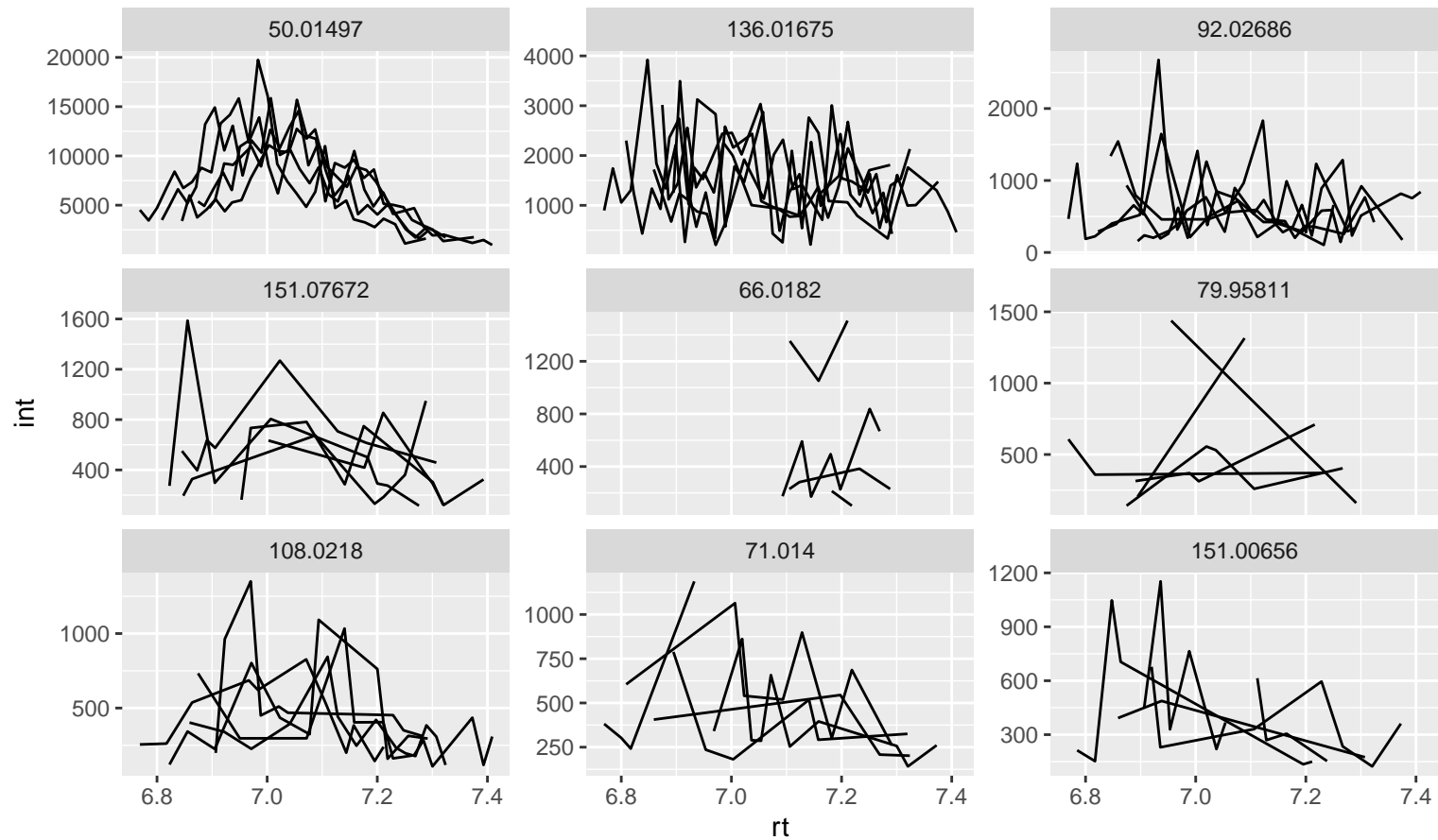


L-Methionine, 2H3 (pos) 153.077158

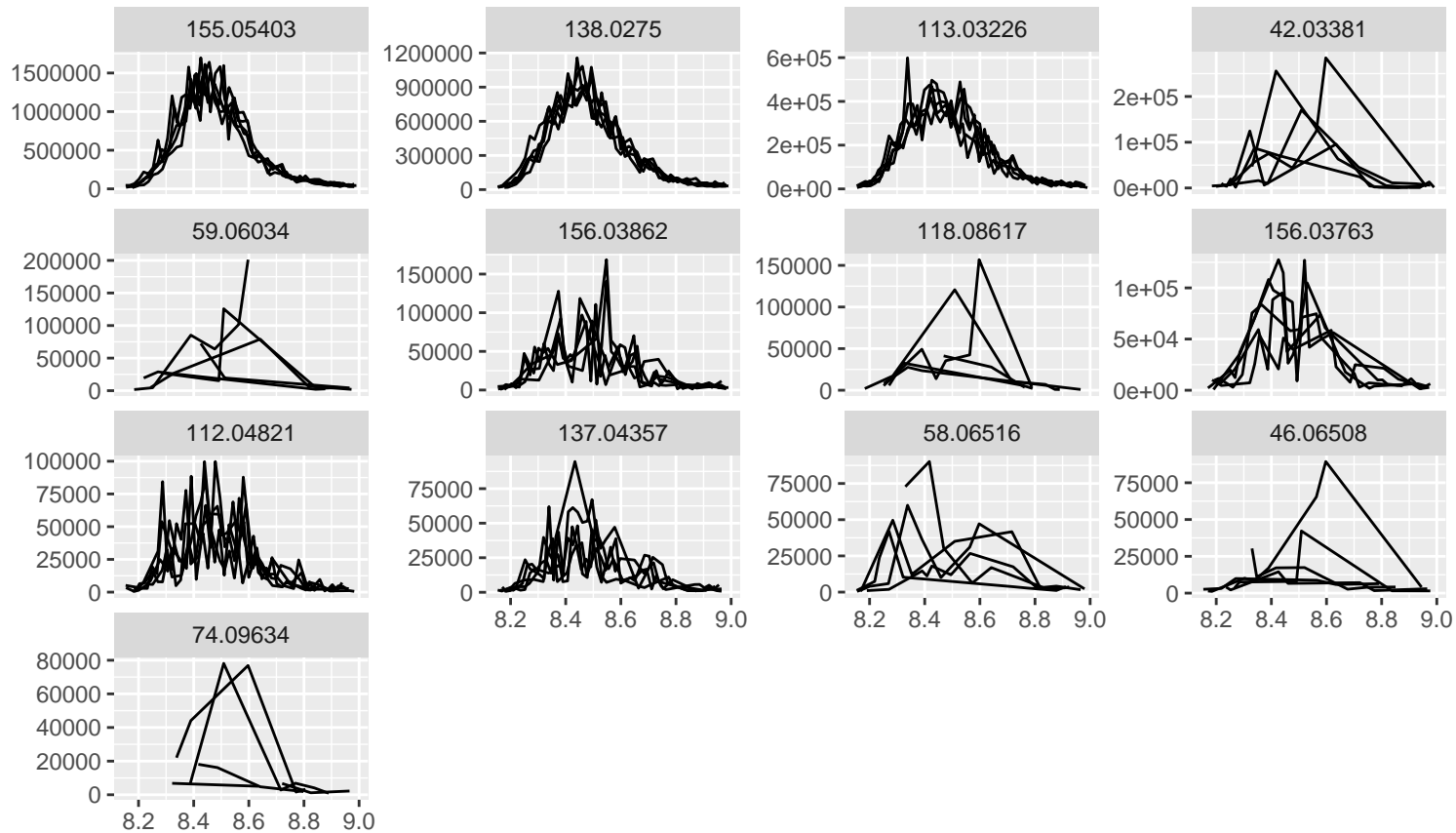
int



L-Methionine, 2H3 (neg) 151.062606

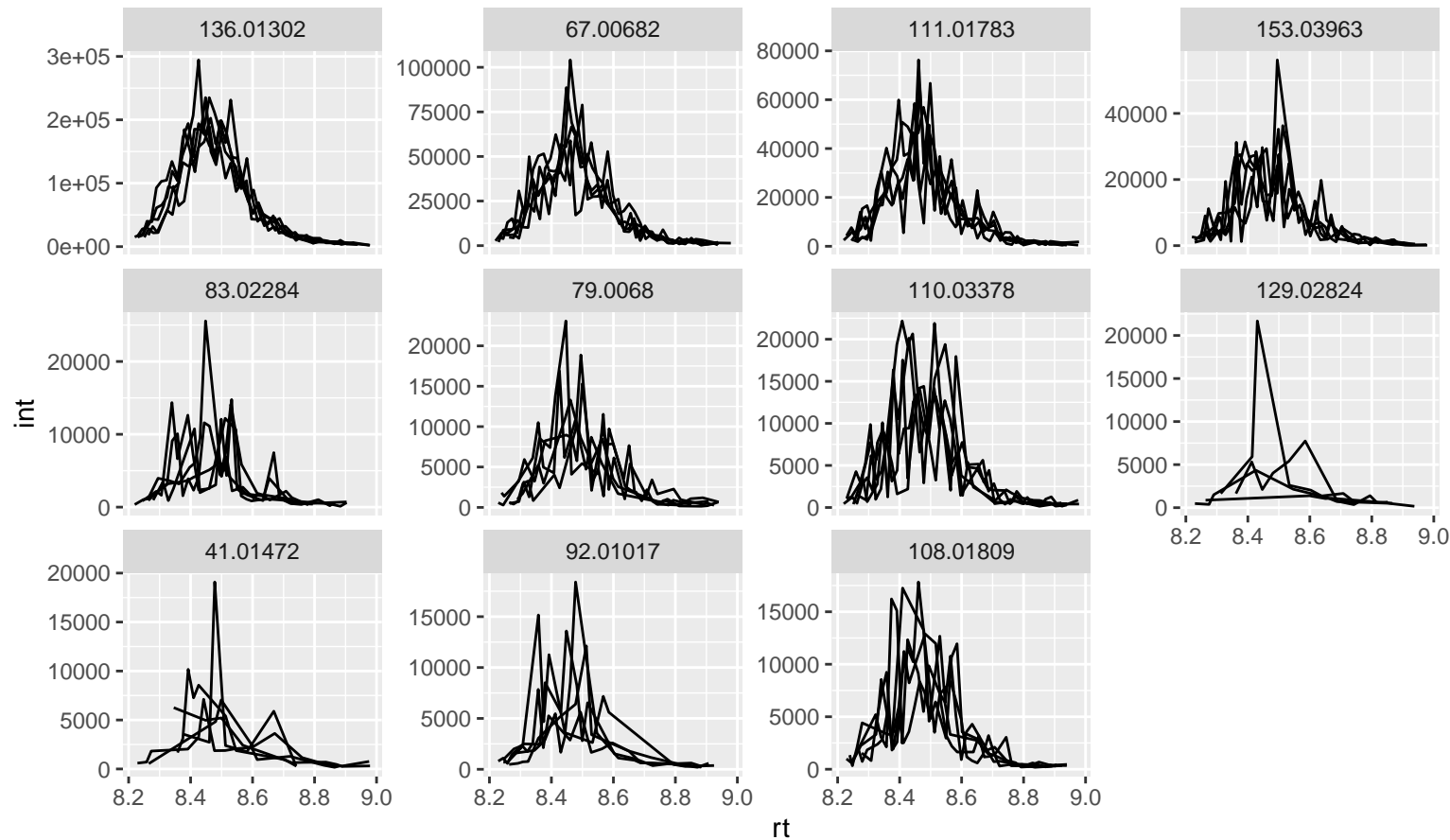


Guanine, 13C, 15N2 (pos) 155.054111



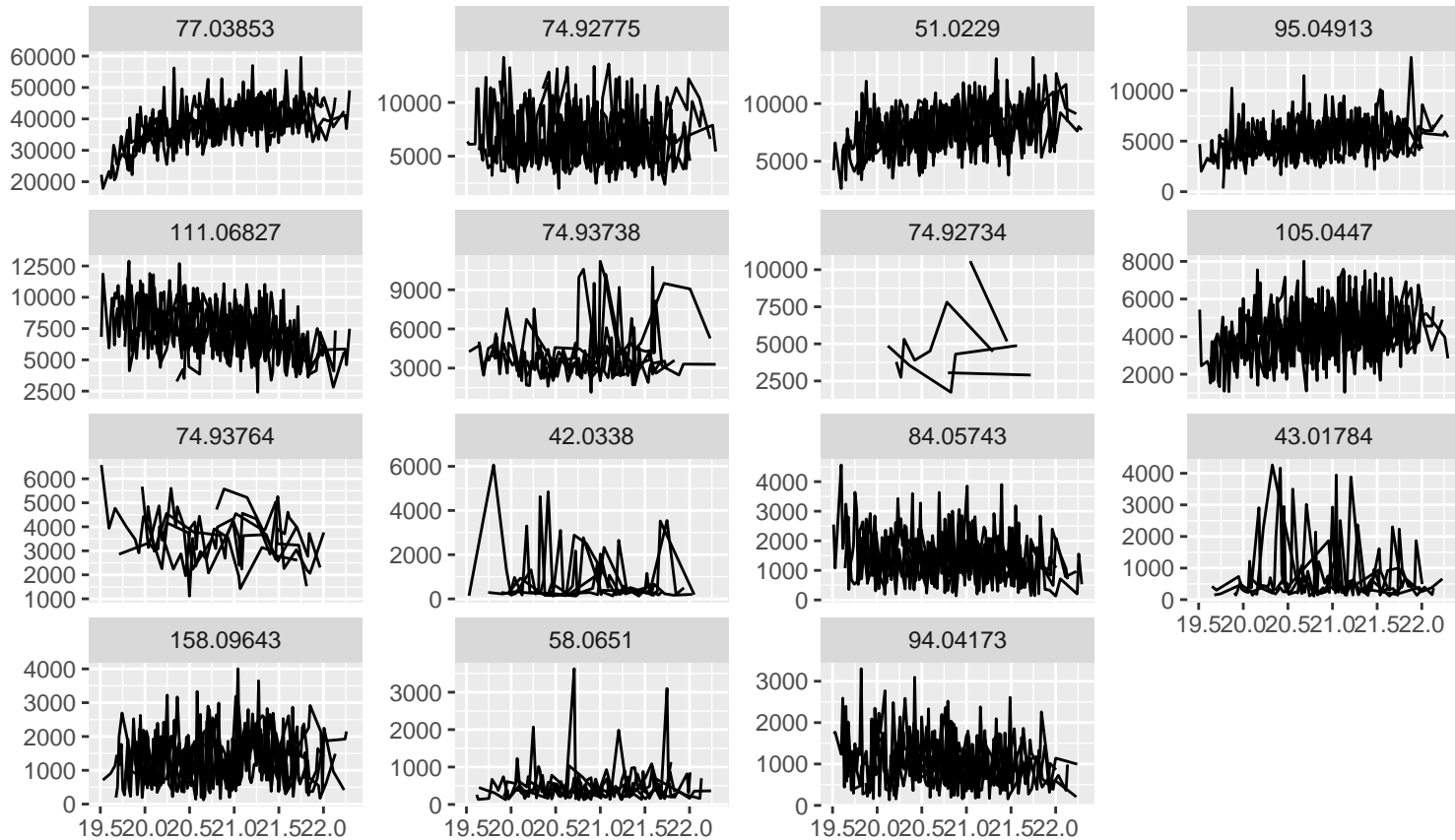
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Guanine, 13C, 15N2 (neg) 153.039559



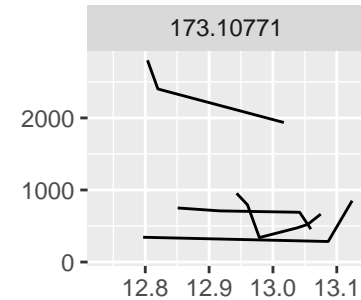
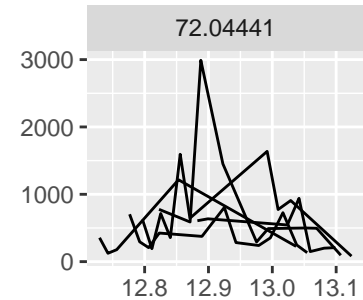
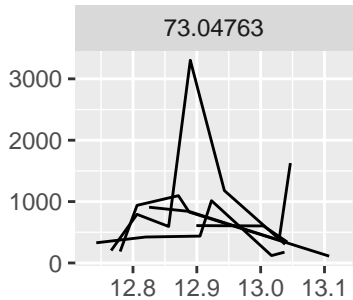
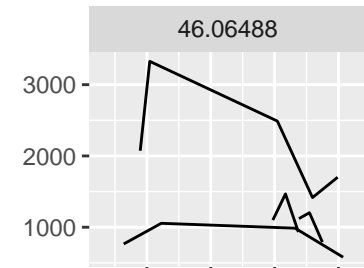
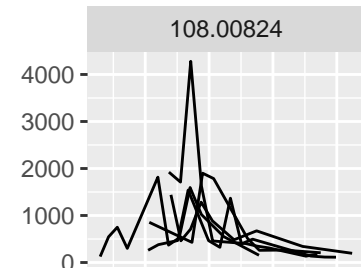
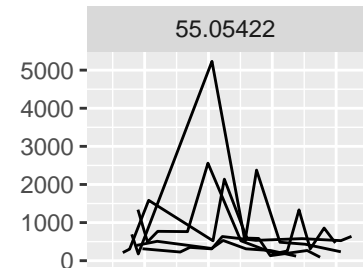
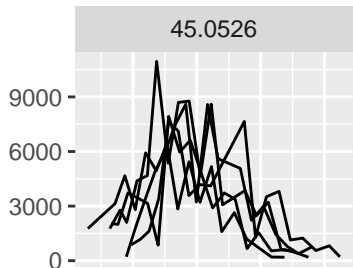
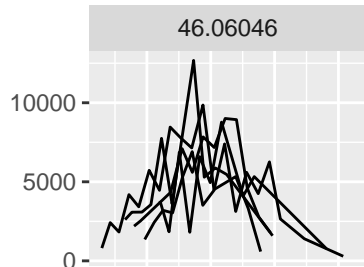
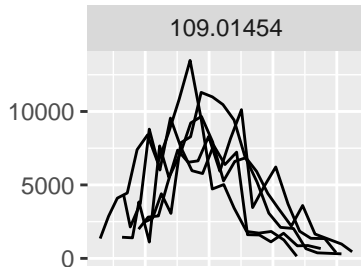
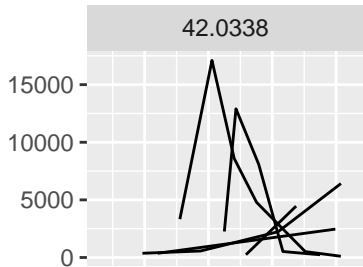
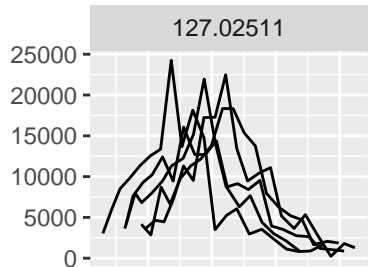
L-Histidine, 15N (pos) 157.073788

int



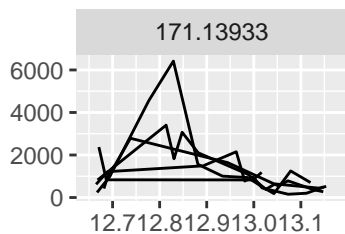
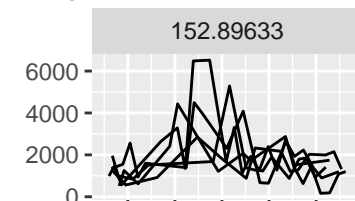
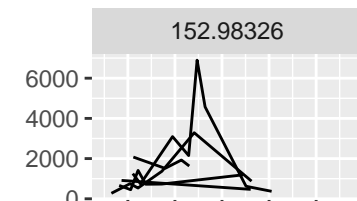
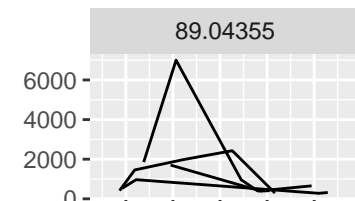
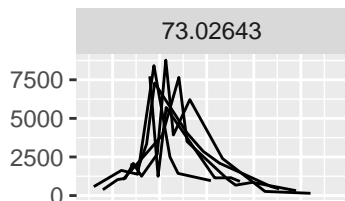
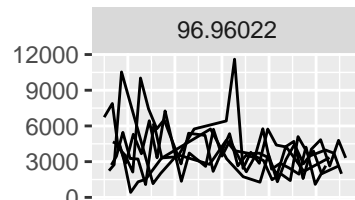
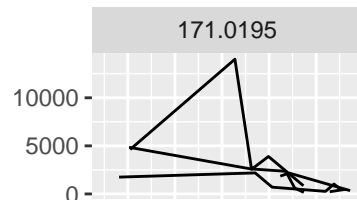
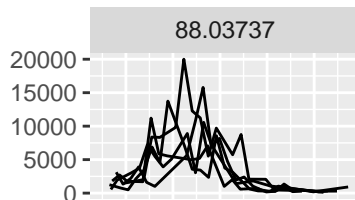
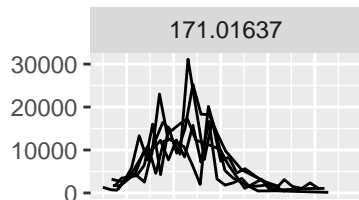
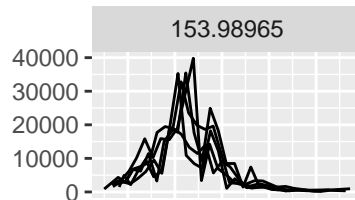
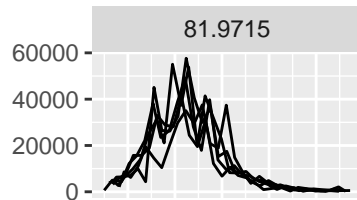
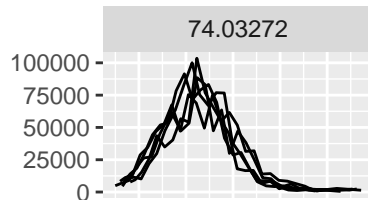
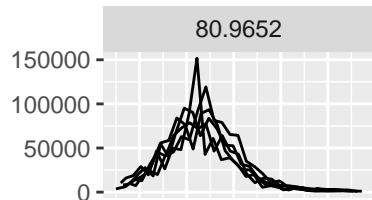
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L-Cysteic acid, 2H3 (pos) 173.030603



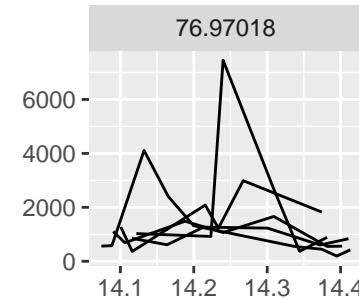
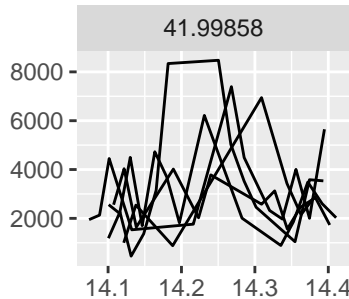
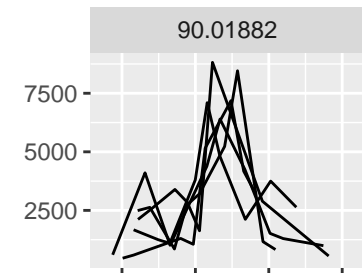
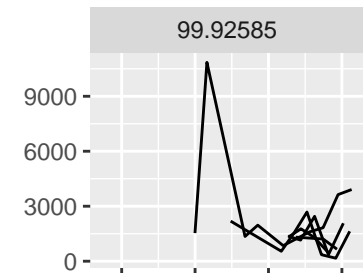
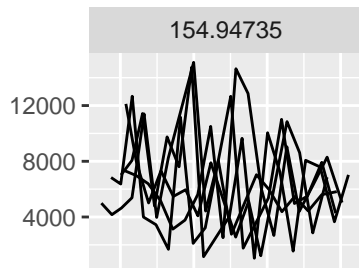
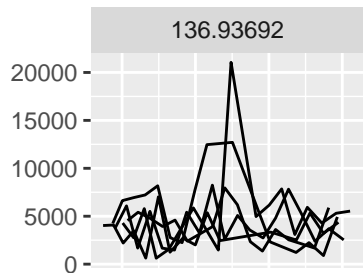
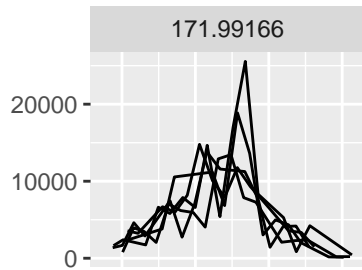
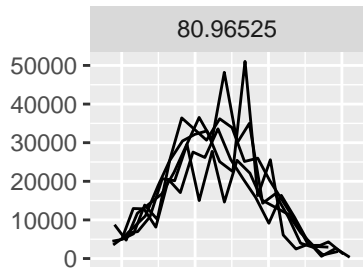
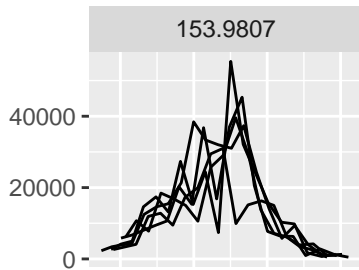
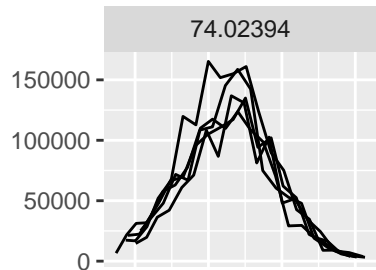
rt

L-Cysteic acid, 2H3 (neg) 171.016051



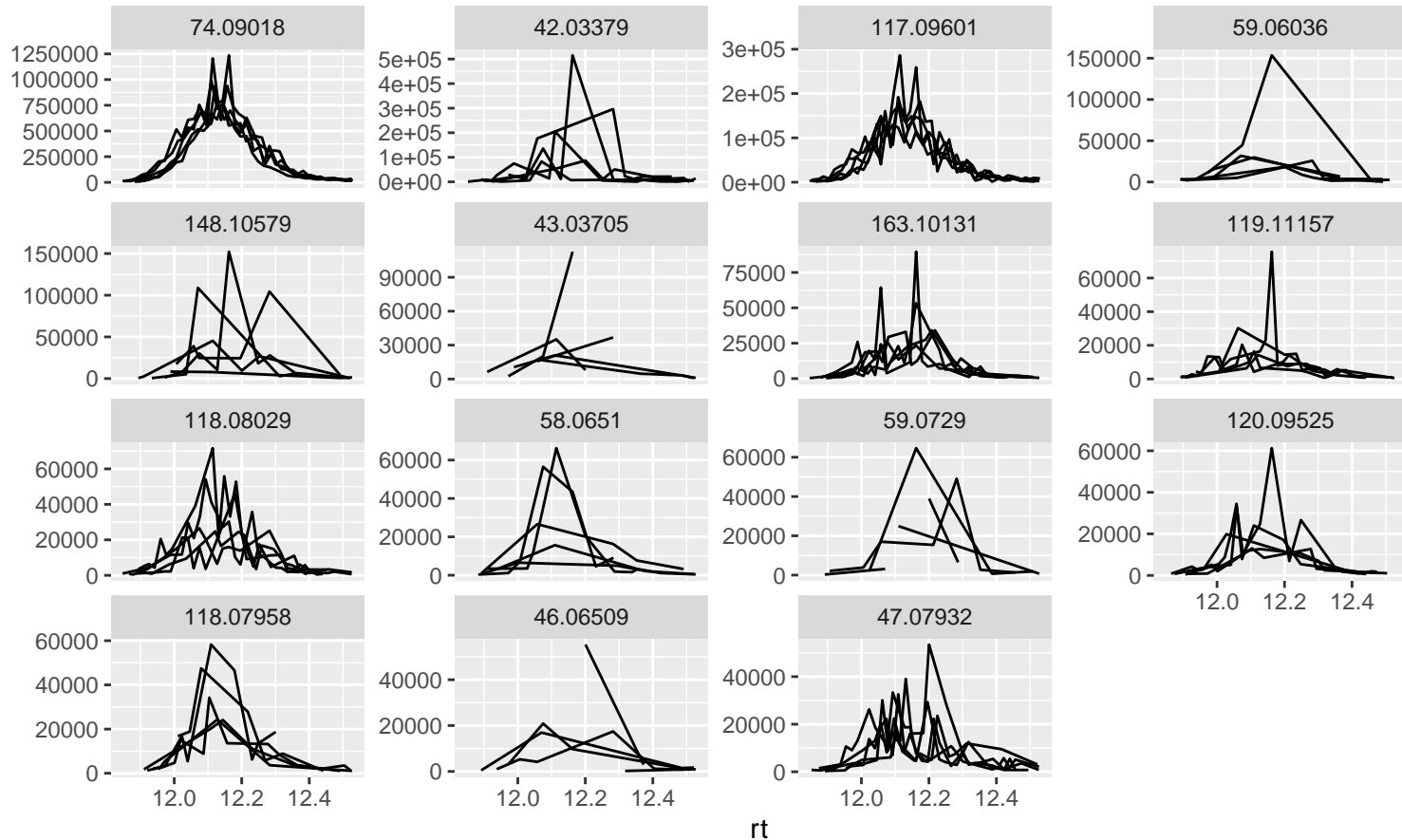
rt

3-Sulfolactate, $^{13}\text{C}3$ (neg) 171.99130058

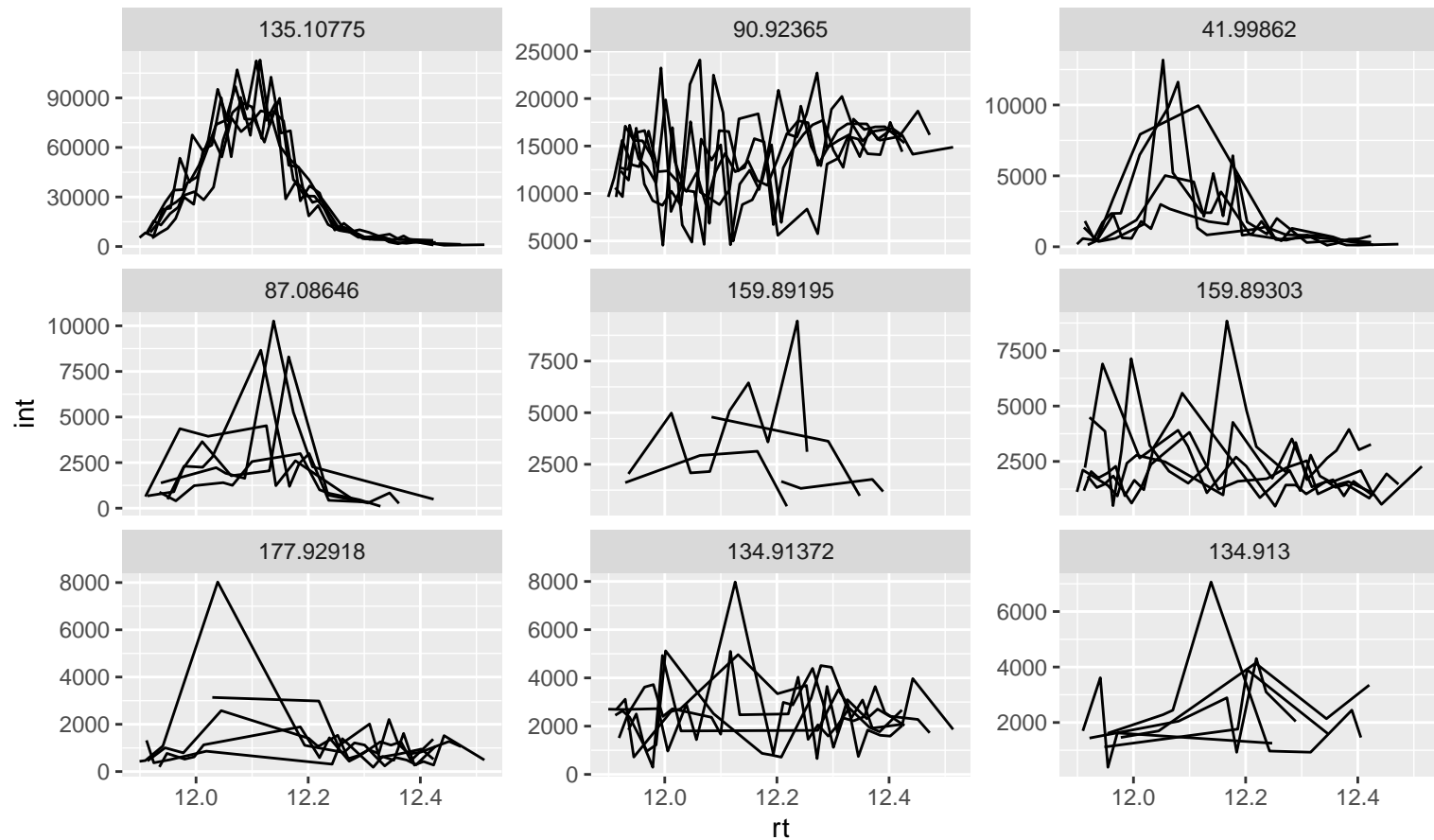


rt

Citrulline, 2H4 (pos) 180.128076

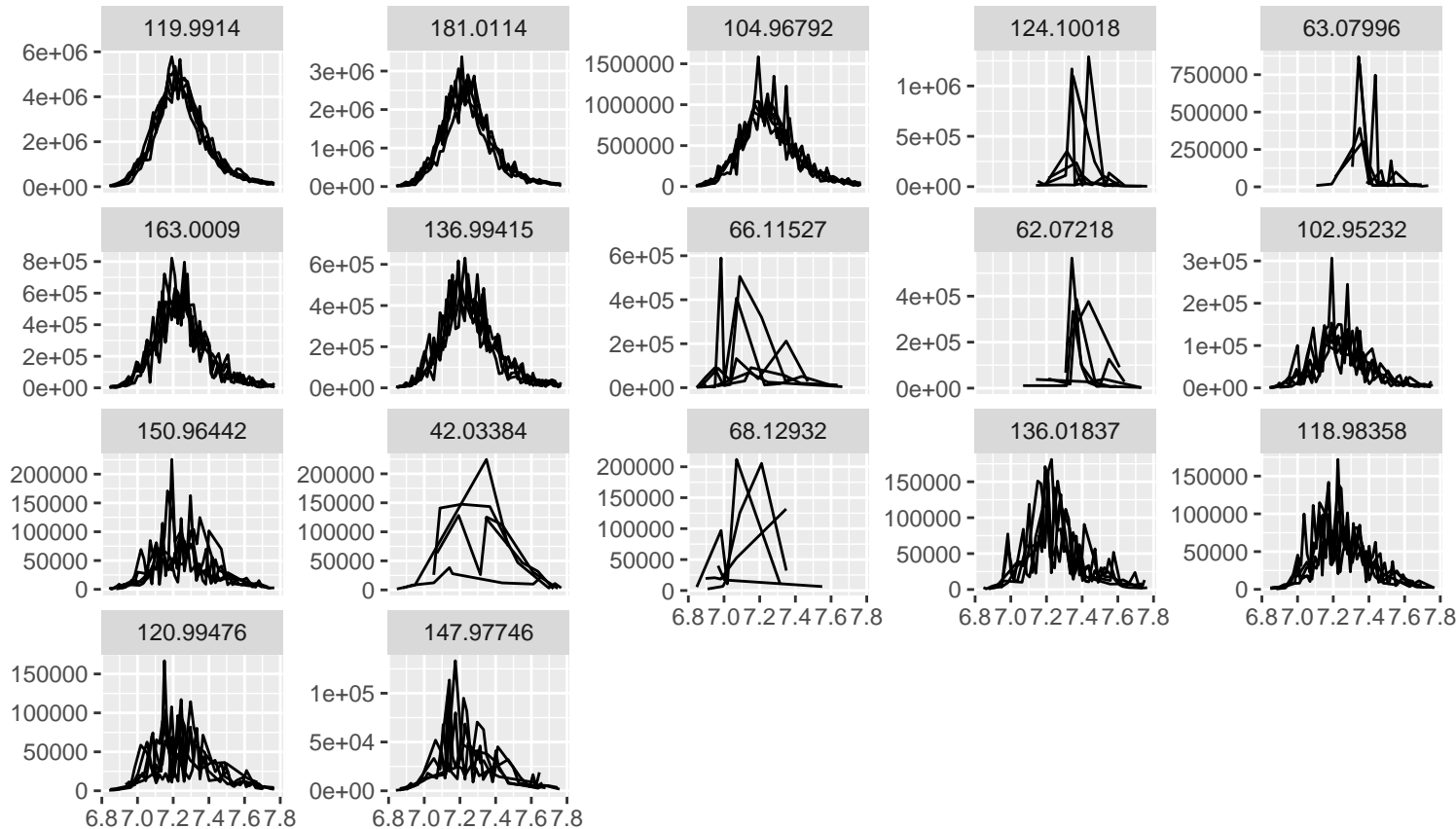


Citrulline, 2H4 (neg) 178.113524



Arsenobetaine, 13C2 (pos) 181.011487

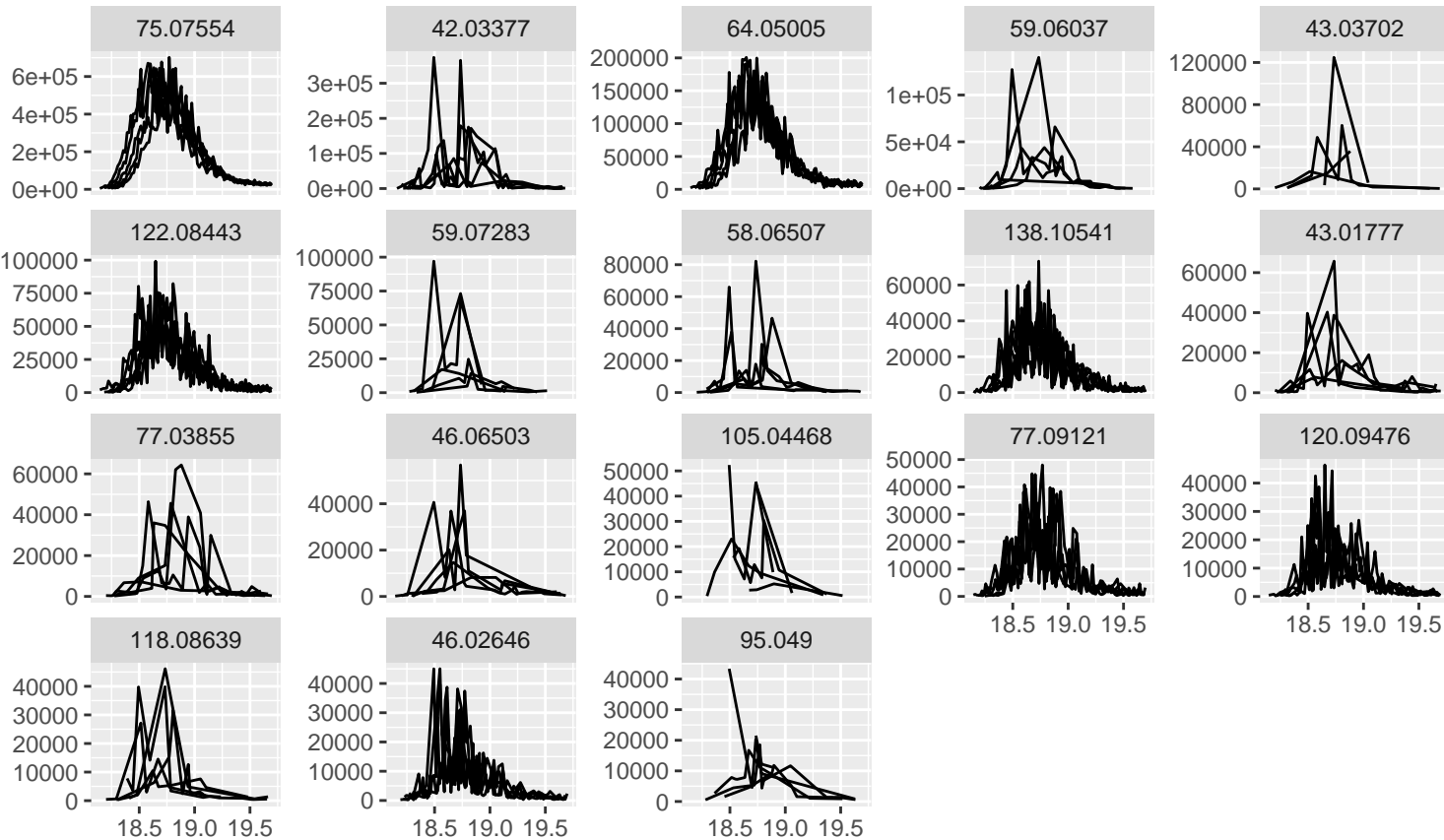
int



rt

L-Arginine, 13C6, 15N4 (pos) 185.127222

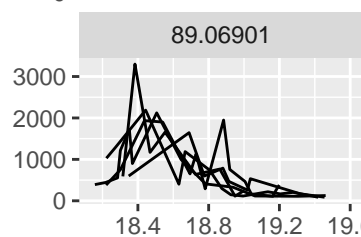
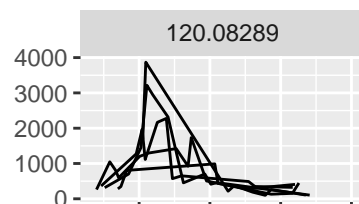
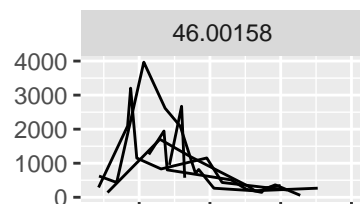
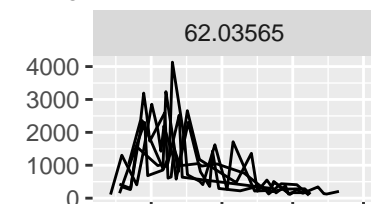
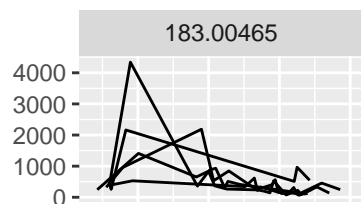
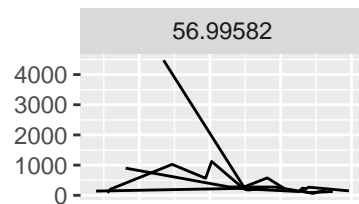
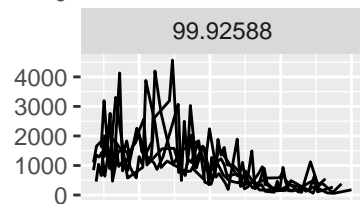
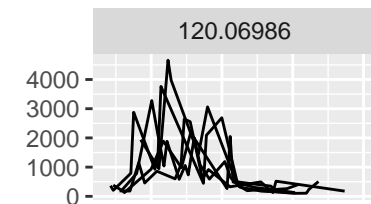
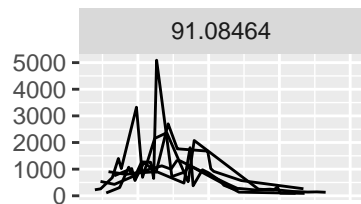
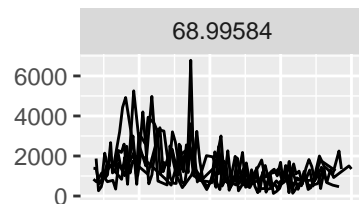
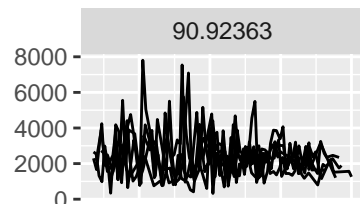
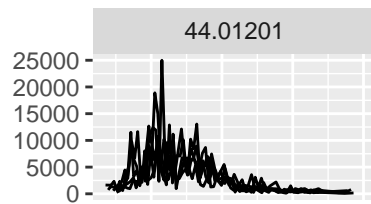
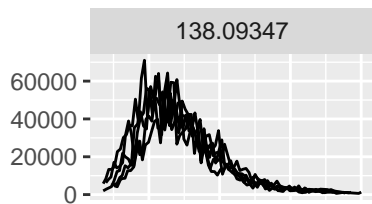
int



rt

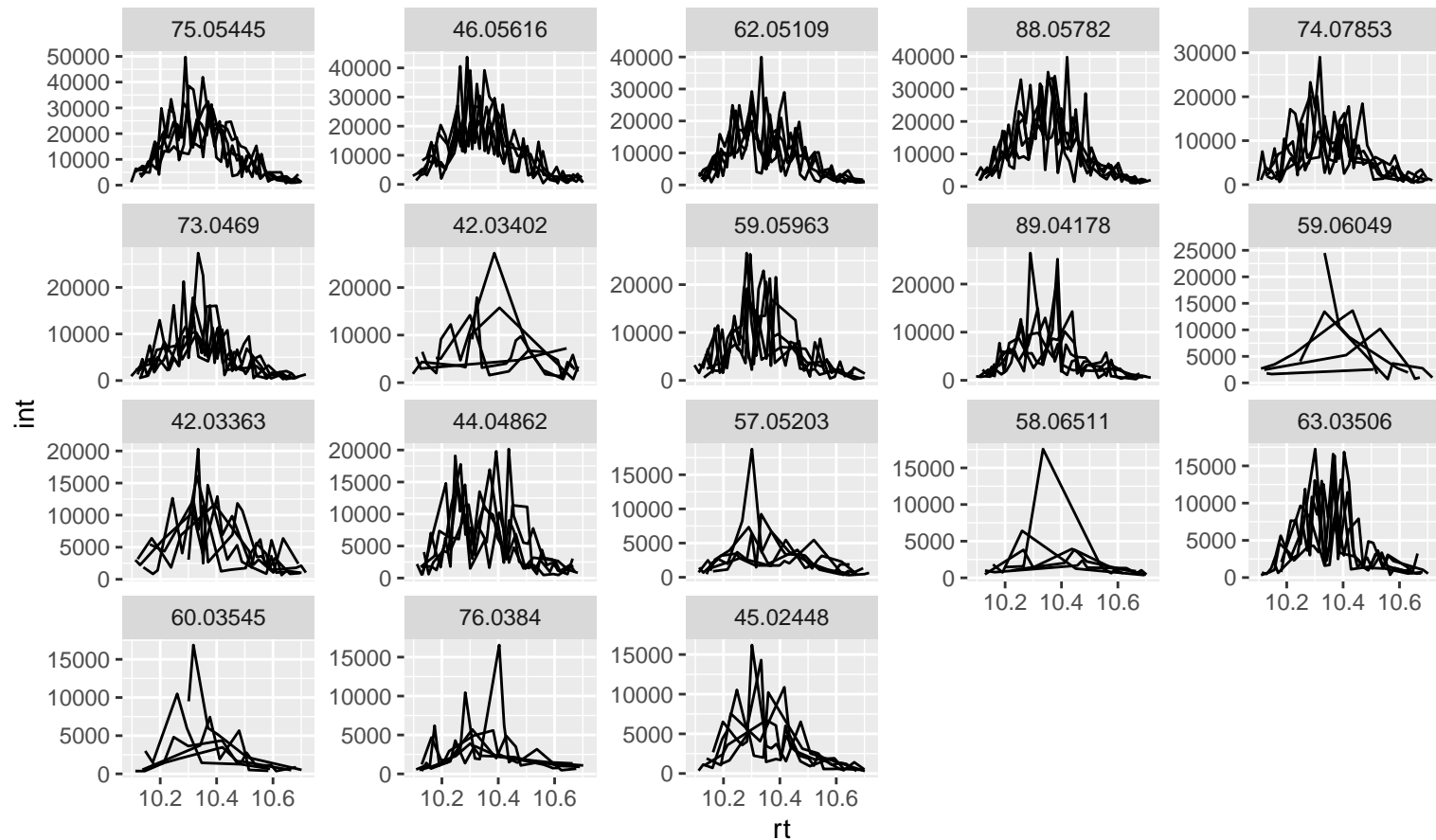
L-Arginine, $^{13}\text{C}_6$, $^{15}\text{N}_4$ (neg) 183.11267

int

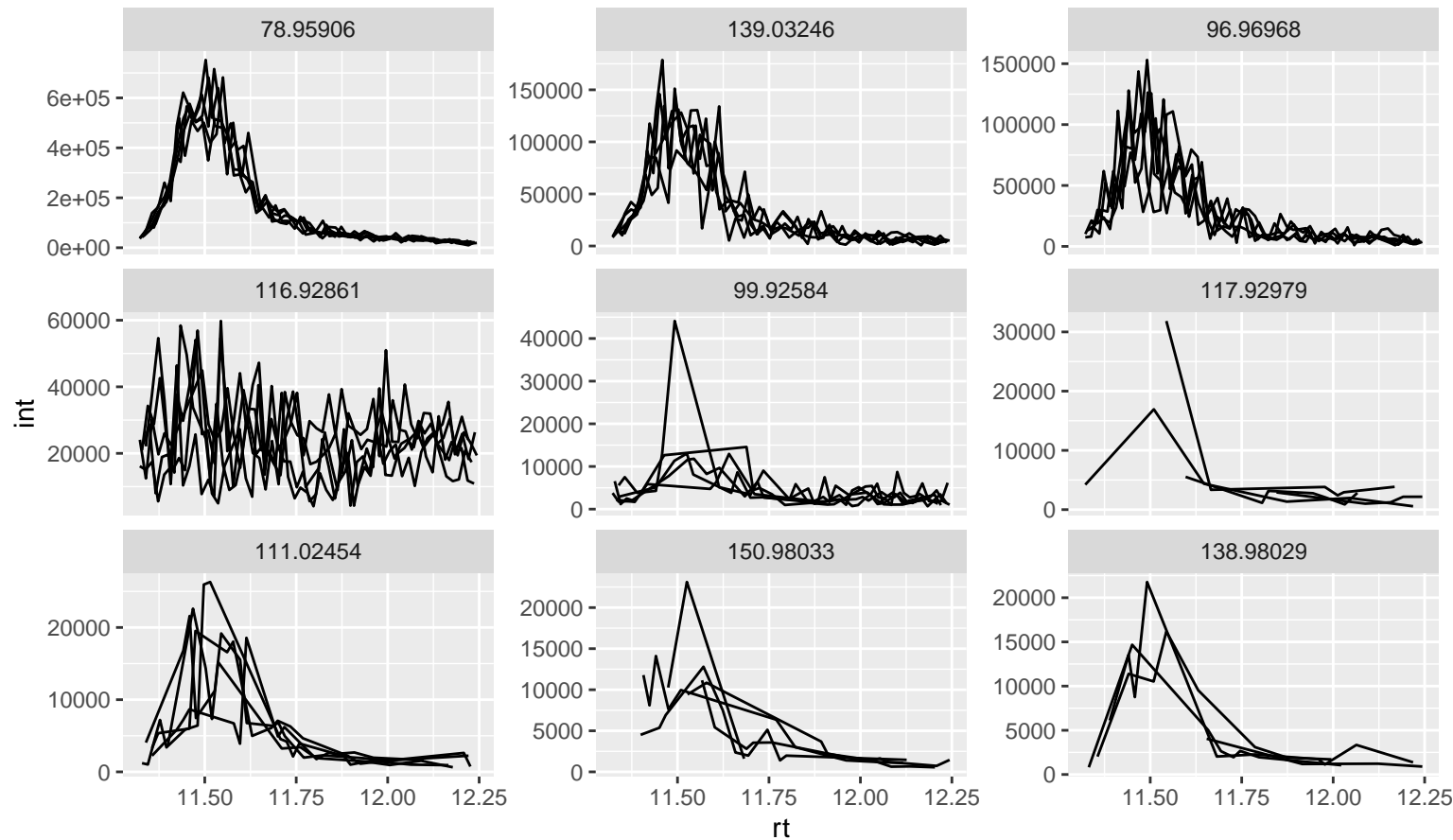


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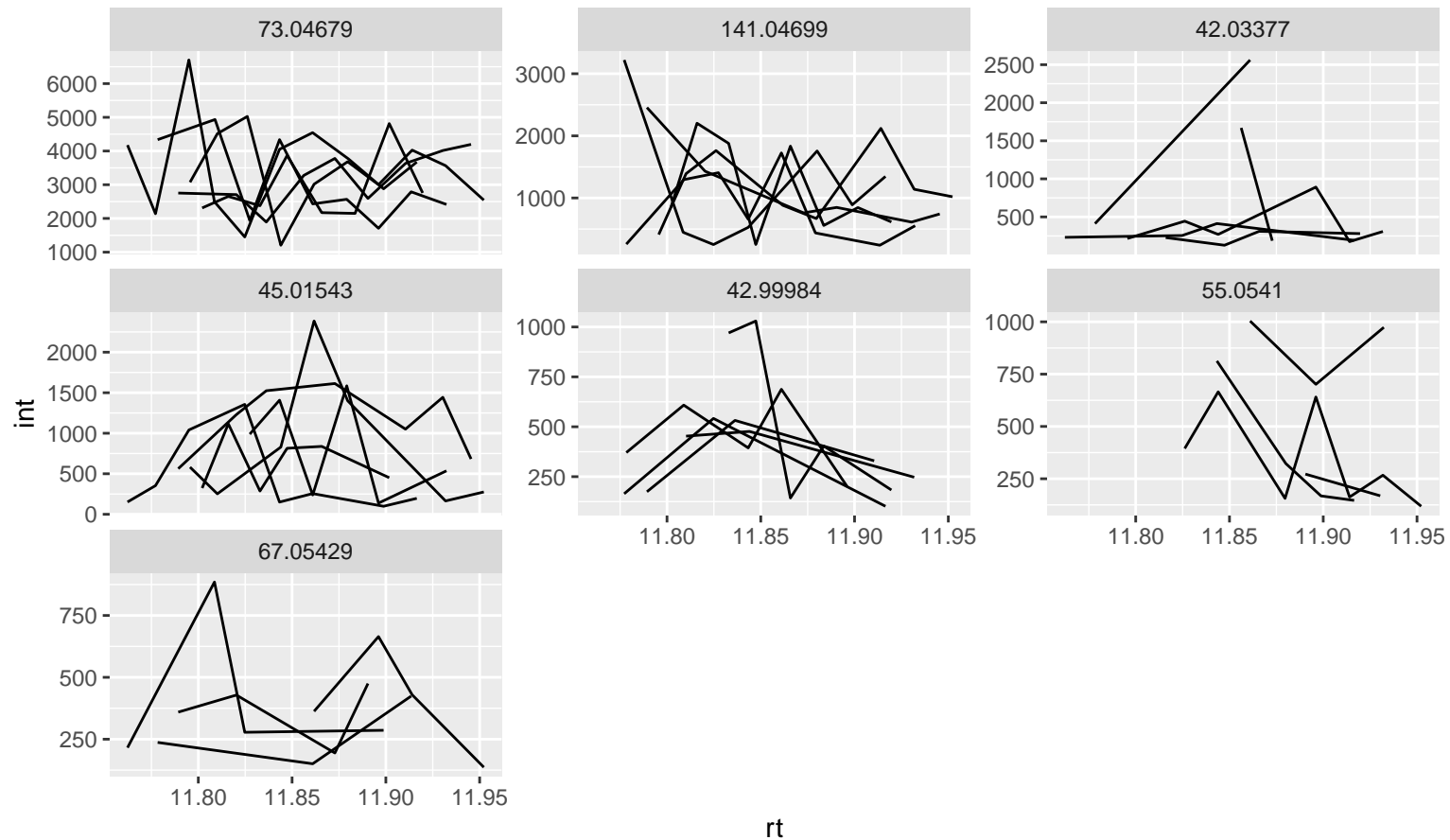
Glucosamine, 13C6 (pos) 186.10678



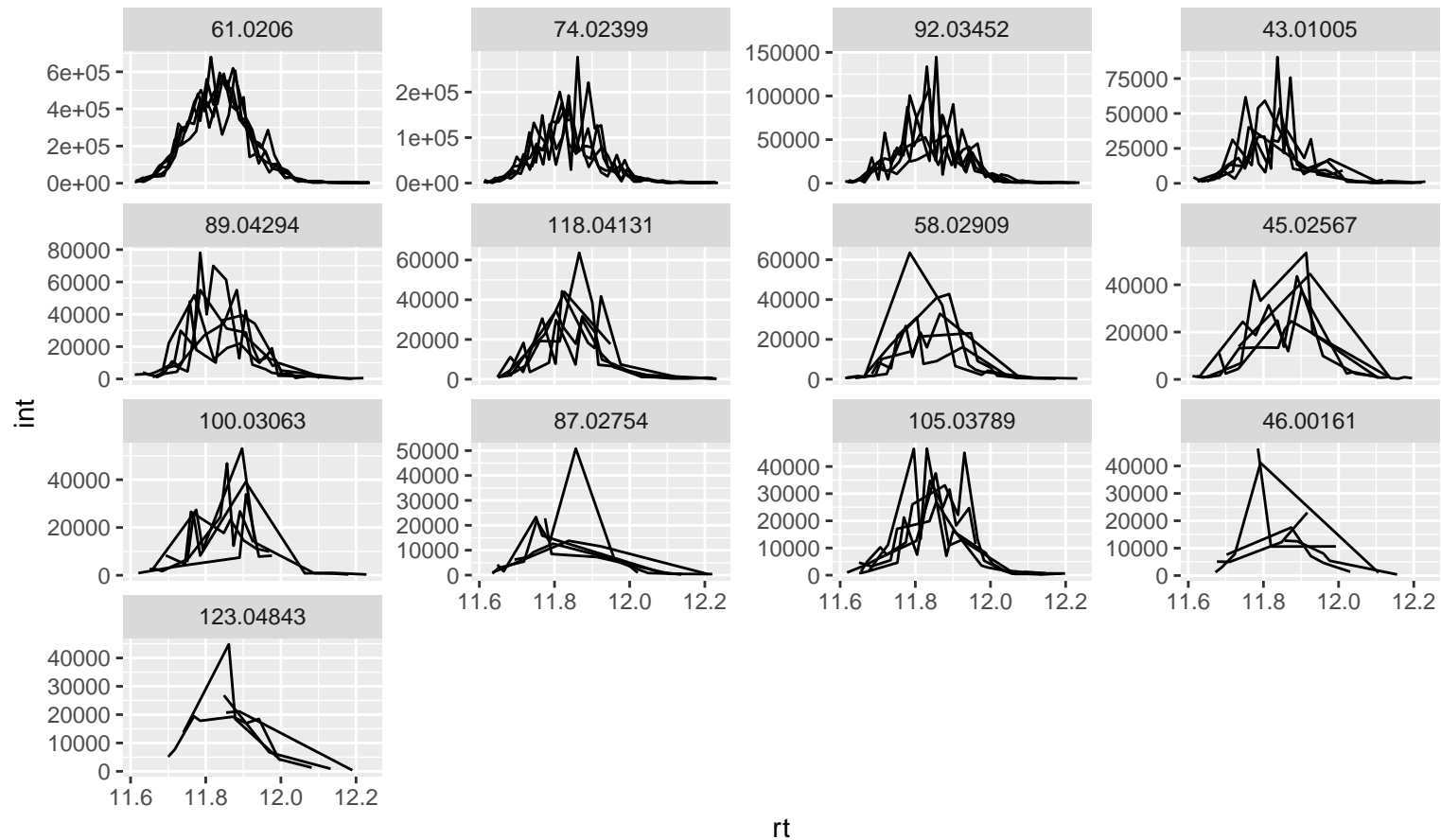
Adenosine monophosphate, 15N5 (neg) 351.040987



Sucrose, 13C12 (pos) 355.163751

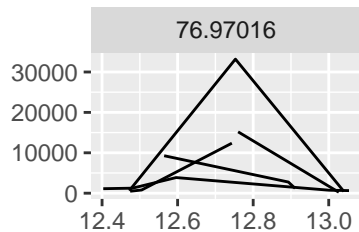
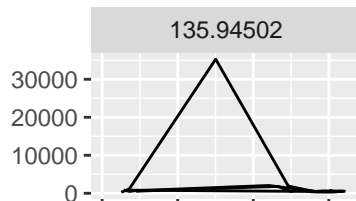
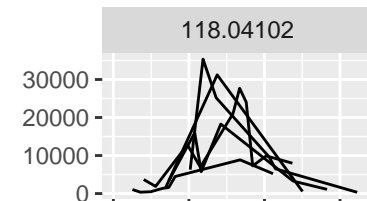
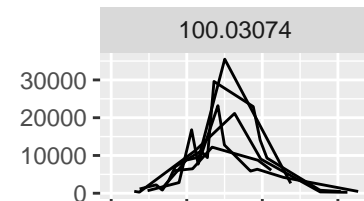
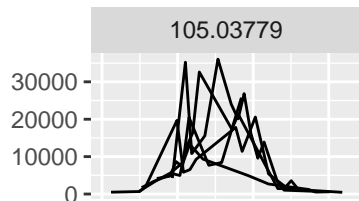
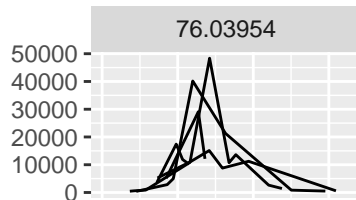
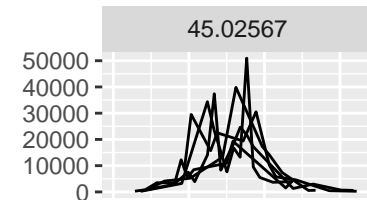
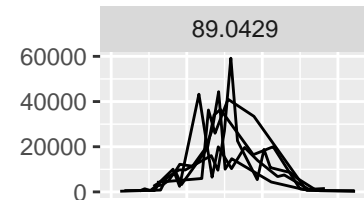
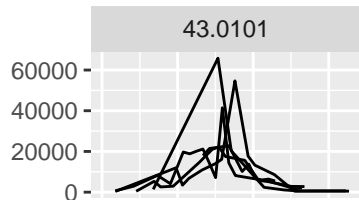
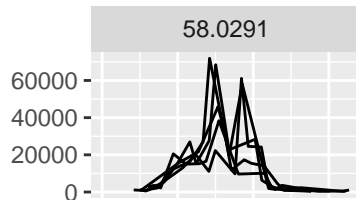
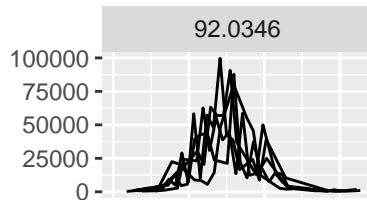
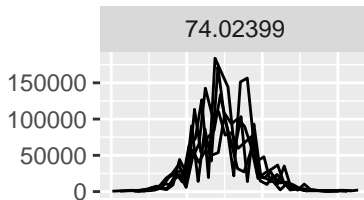
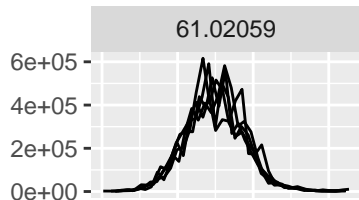


Sucrose, 13C12 (neg) 353.149199



Trehalose, $^{13}\text{C}_{12}$ (neg) 353.149199

int



rt

Guanosine monophosphate, 15N5 (neg) 367.035902

