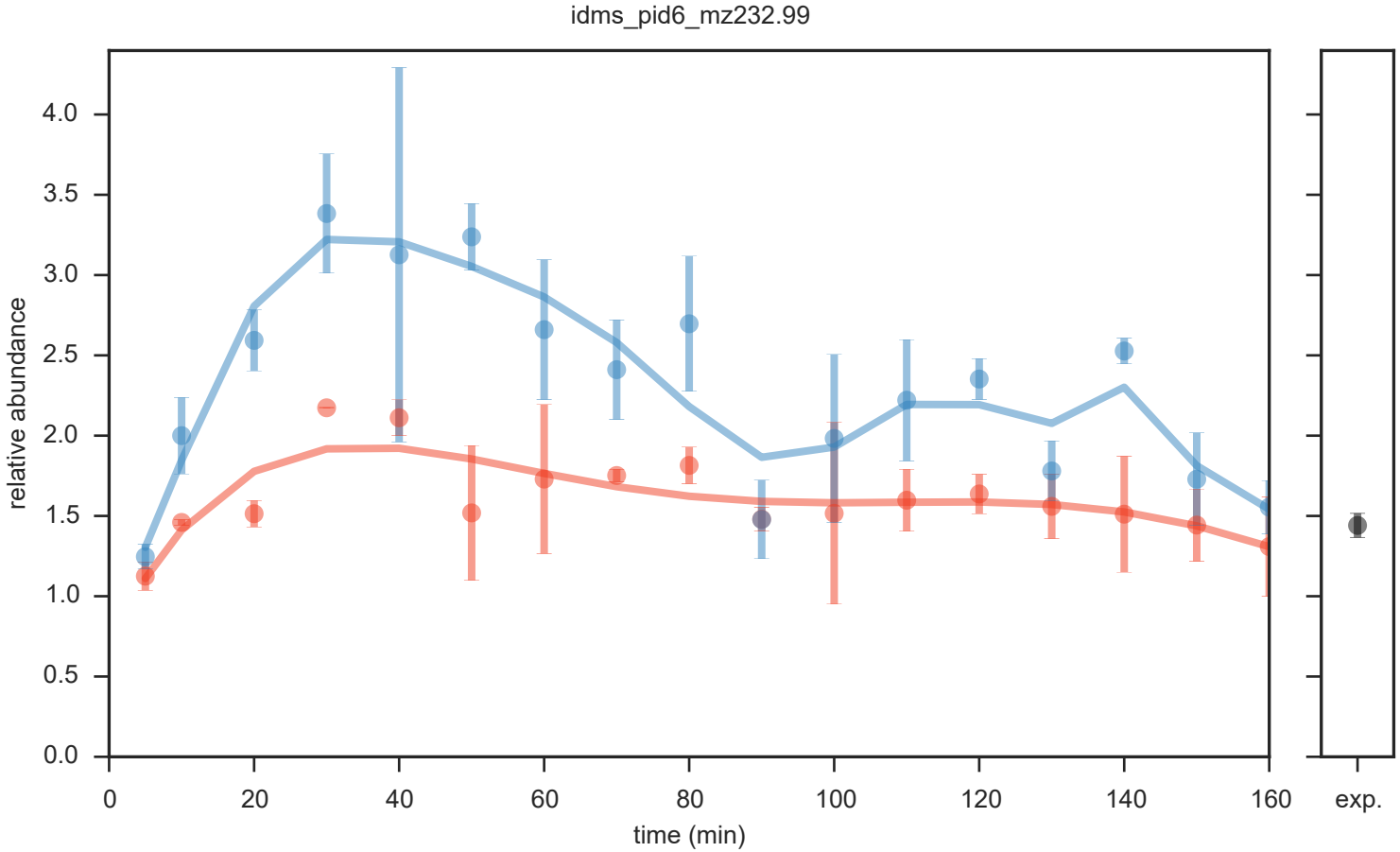
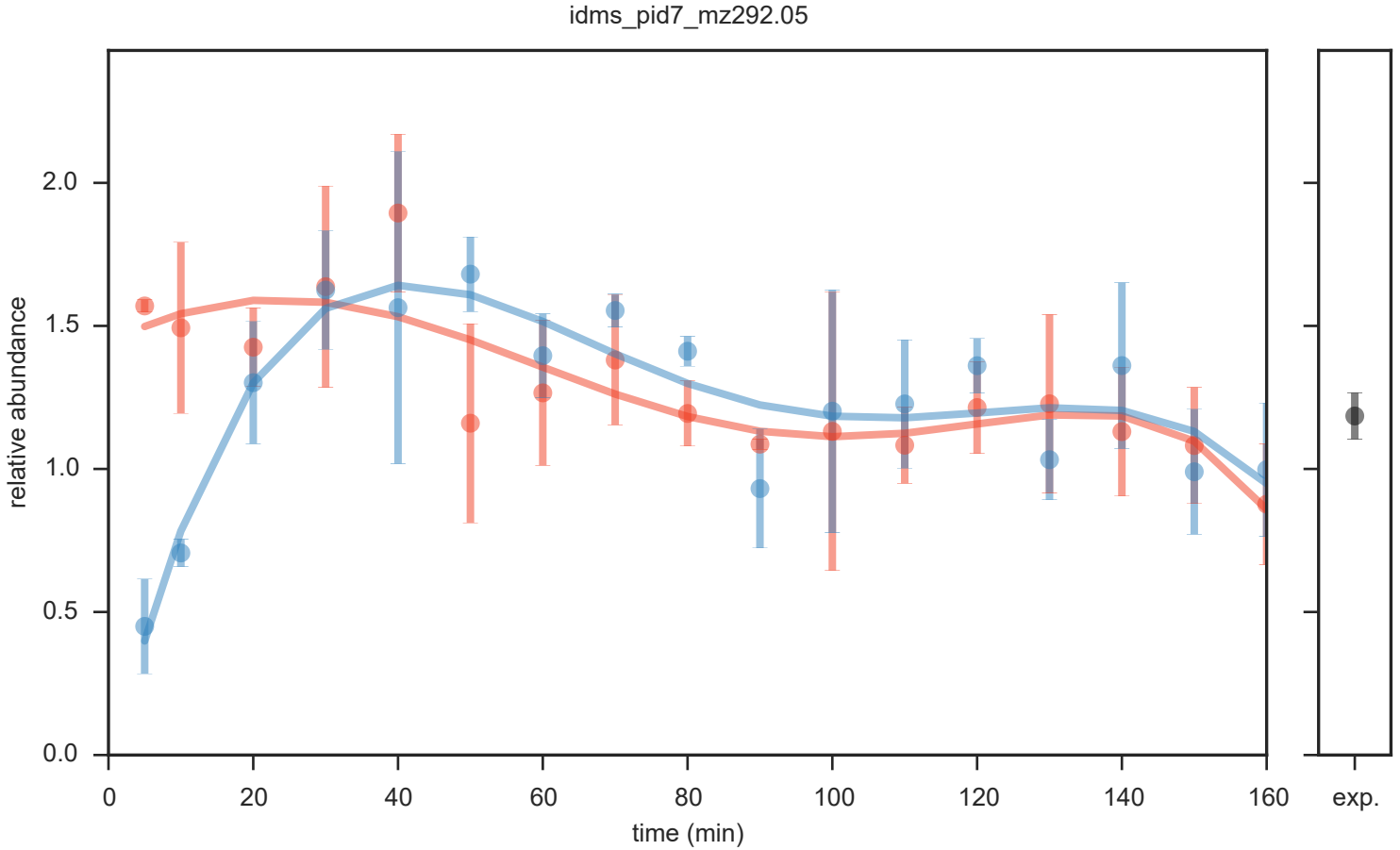
Supplemental Data 1. Metabolite abundance profiles for nLC-QEx data.

Cell-cycle dependent abundance profiles of metabolite features detected via the method nLC-QEx (negative mode); blue profiles are from synchronized, red from control cultures. Mean values +/- SD are shown (3 biological replicates per condition). The time-point (box) labeled "exp" indicates respective exponentially growing pre-cultures (n=6).


idms_pid6_mz232.99
relative abundance
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid7_mz292.05
relative abundance
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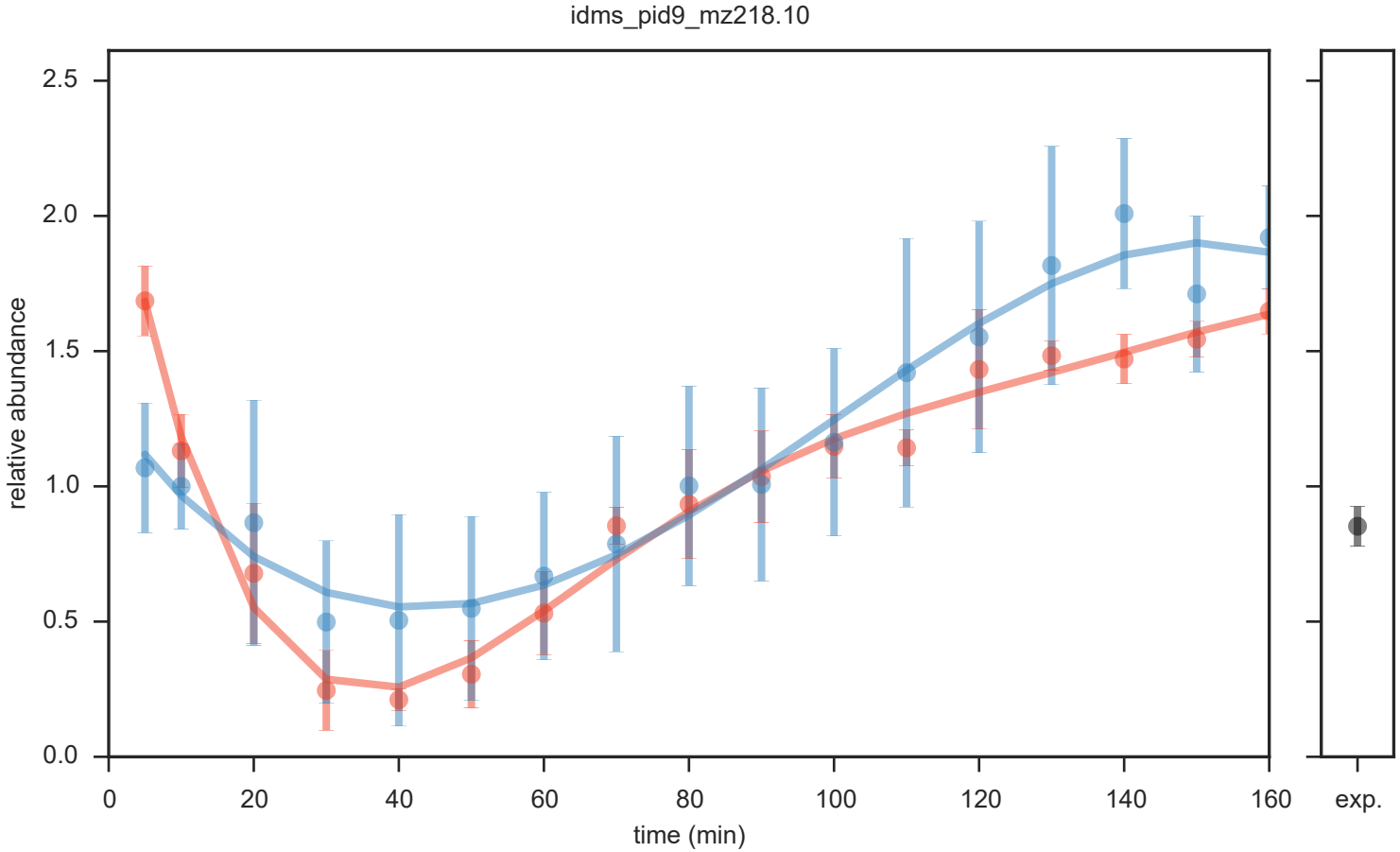
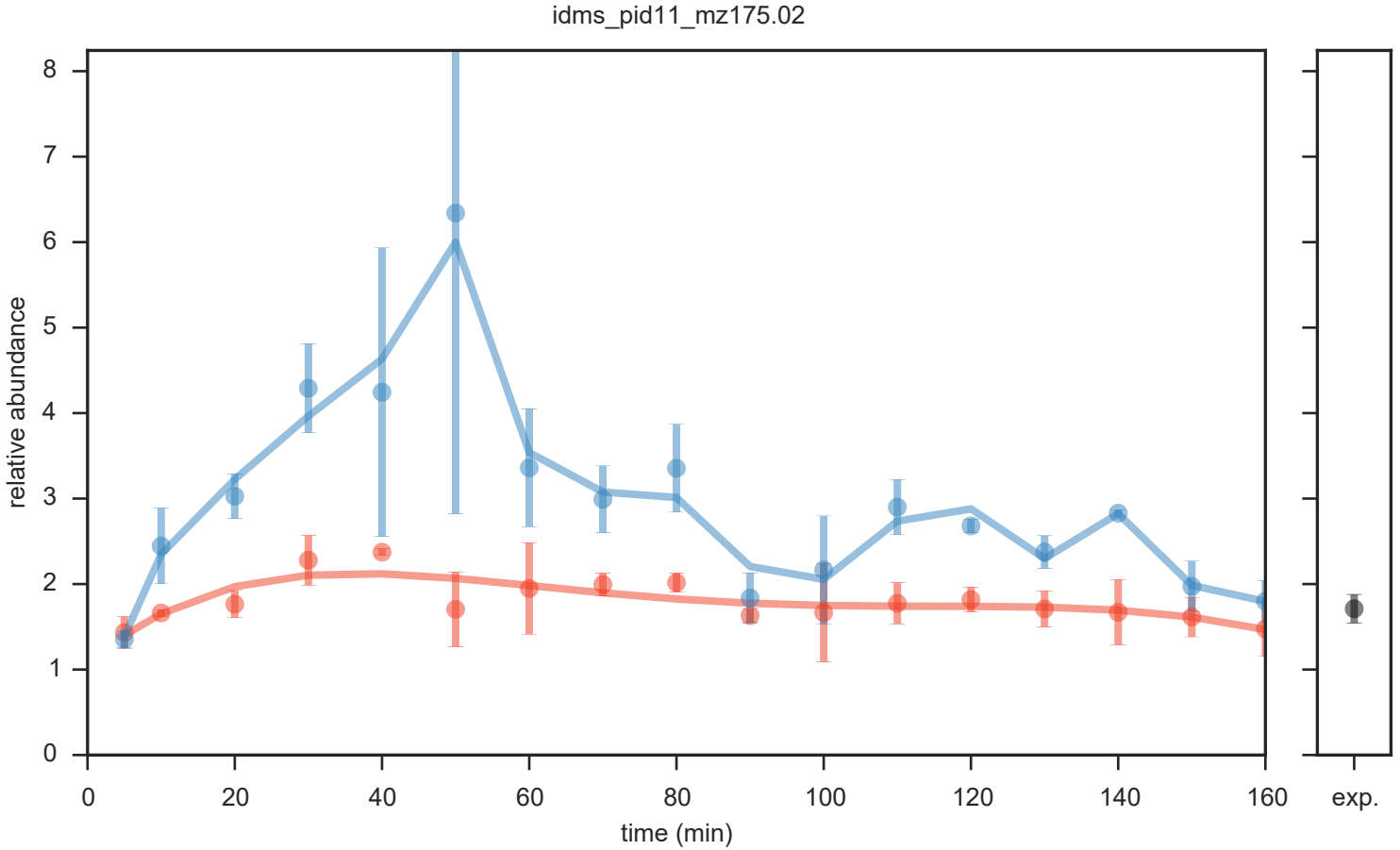
0.5
1.0
1.5
2.0
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid9_mz218.10
relative abundance
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid11_mz175.02
relative abundance
time (min)
exp.
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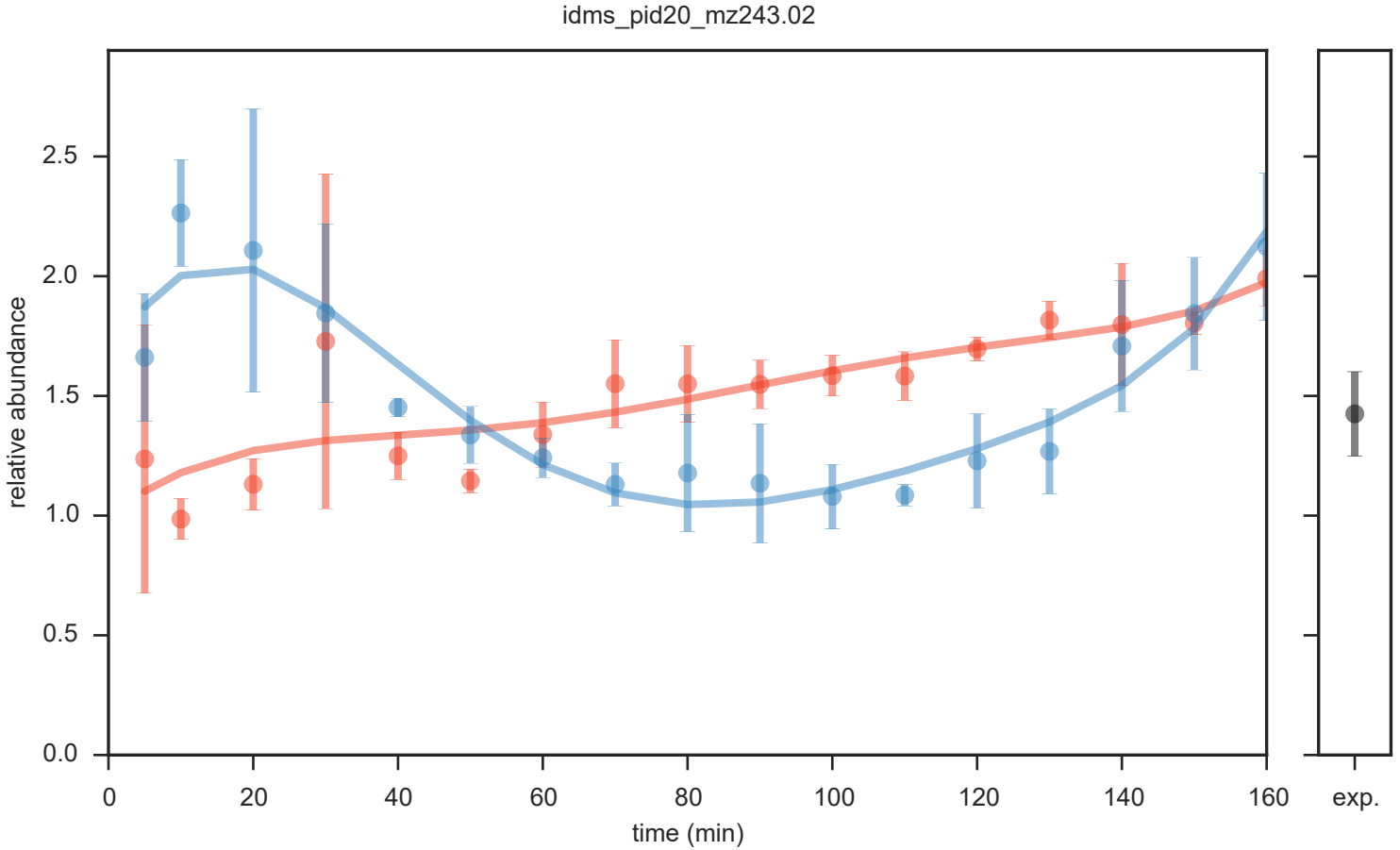
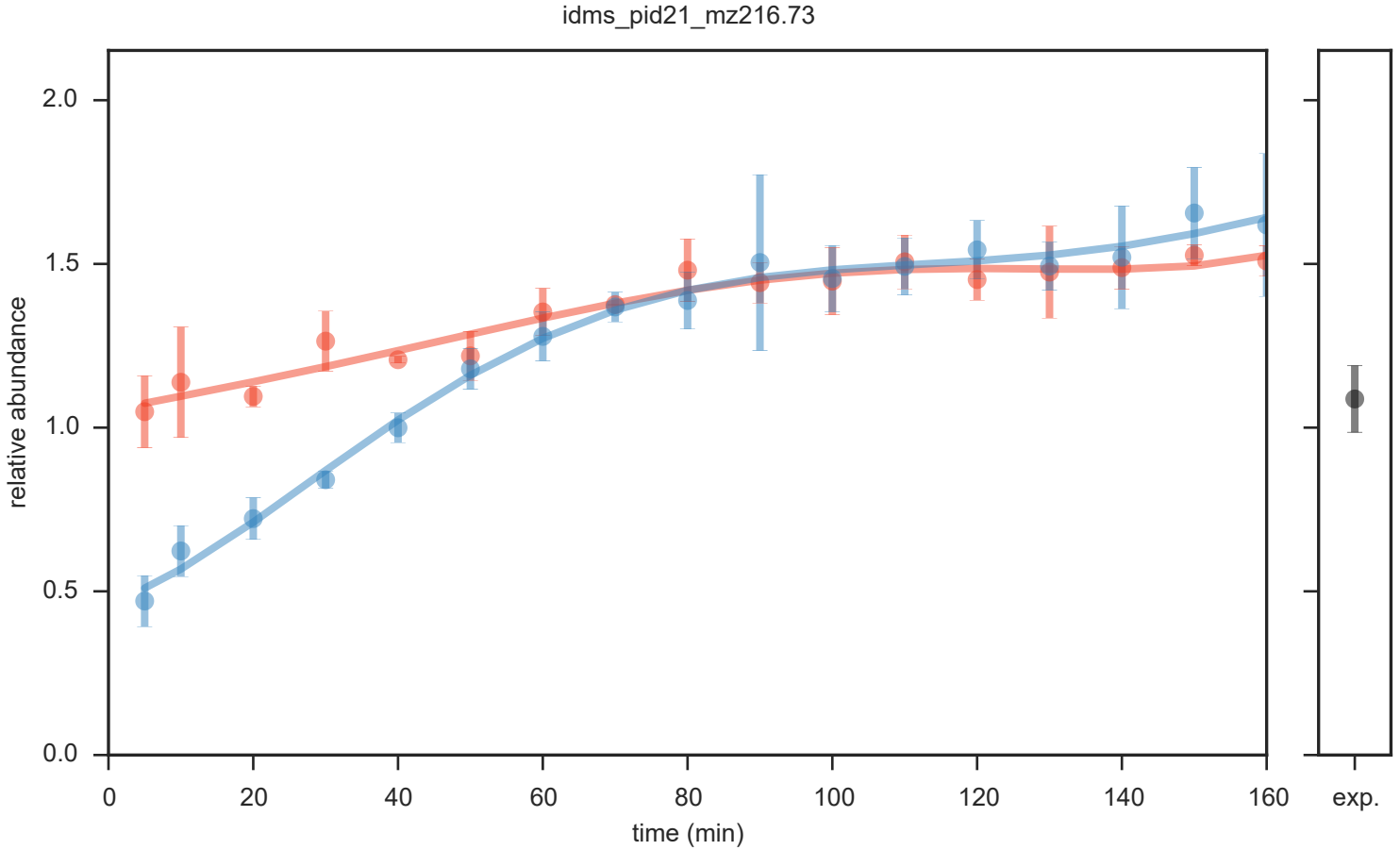
1
2
3
4
5
6
7
8
0
20
40
60
80
100
120
140
160


idms_pid20_mz243.02
relative abundance
0.0
0.5
1.0
1.5
2.0
2.5
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid21_mz216.73
relative abundance
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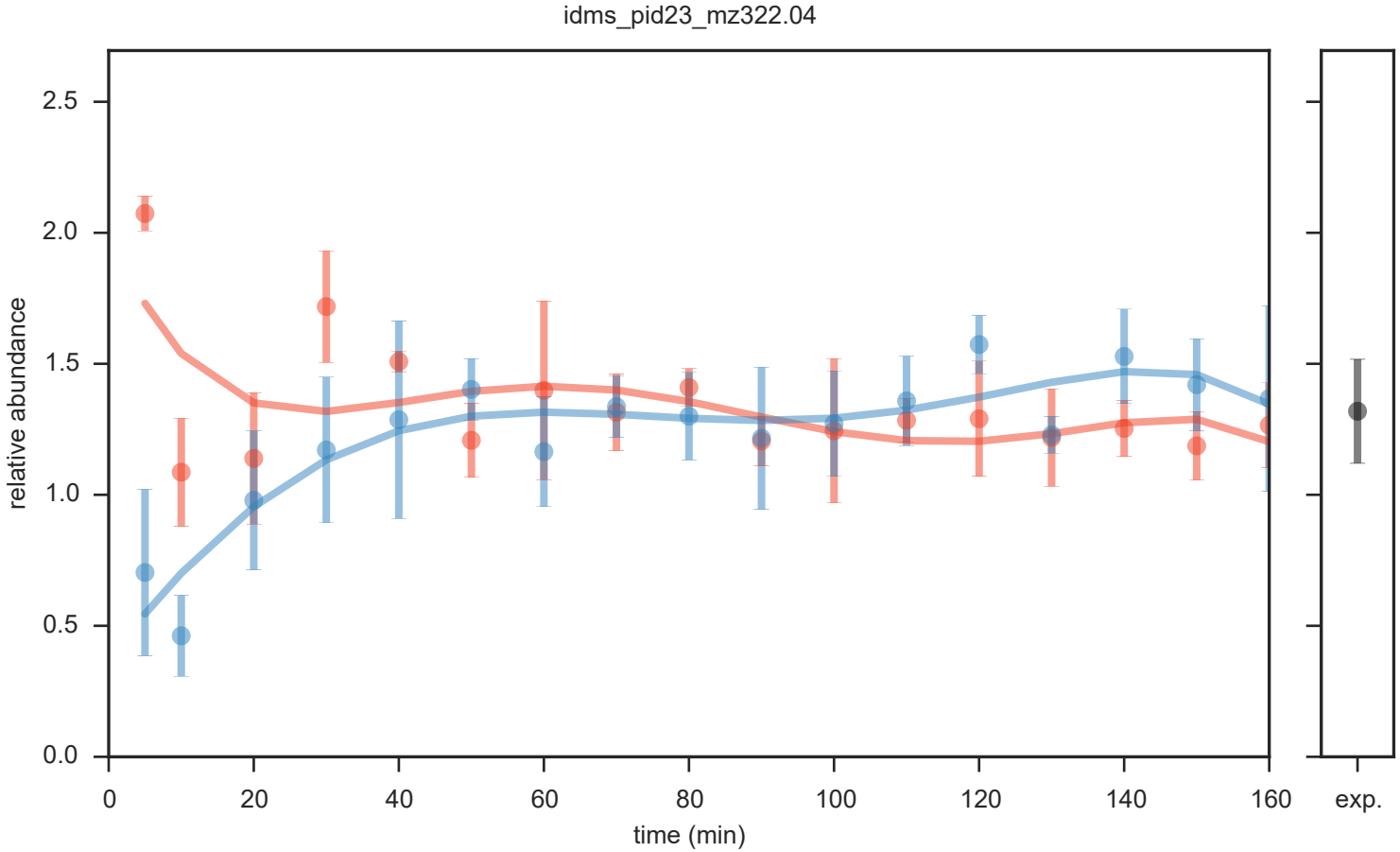
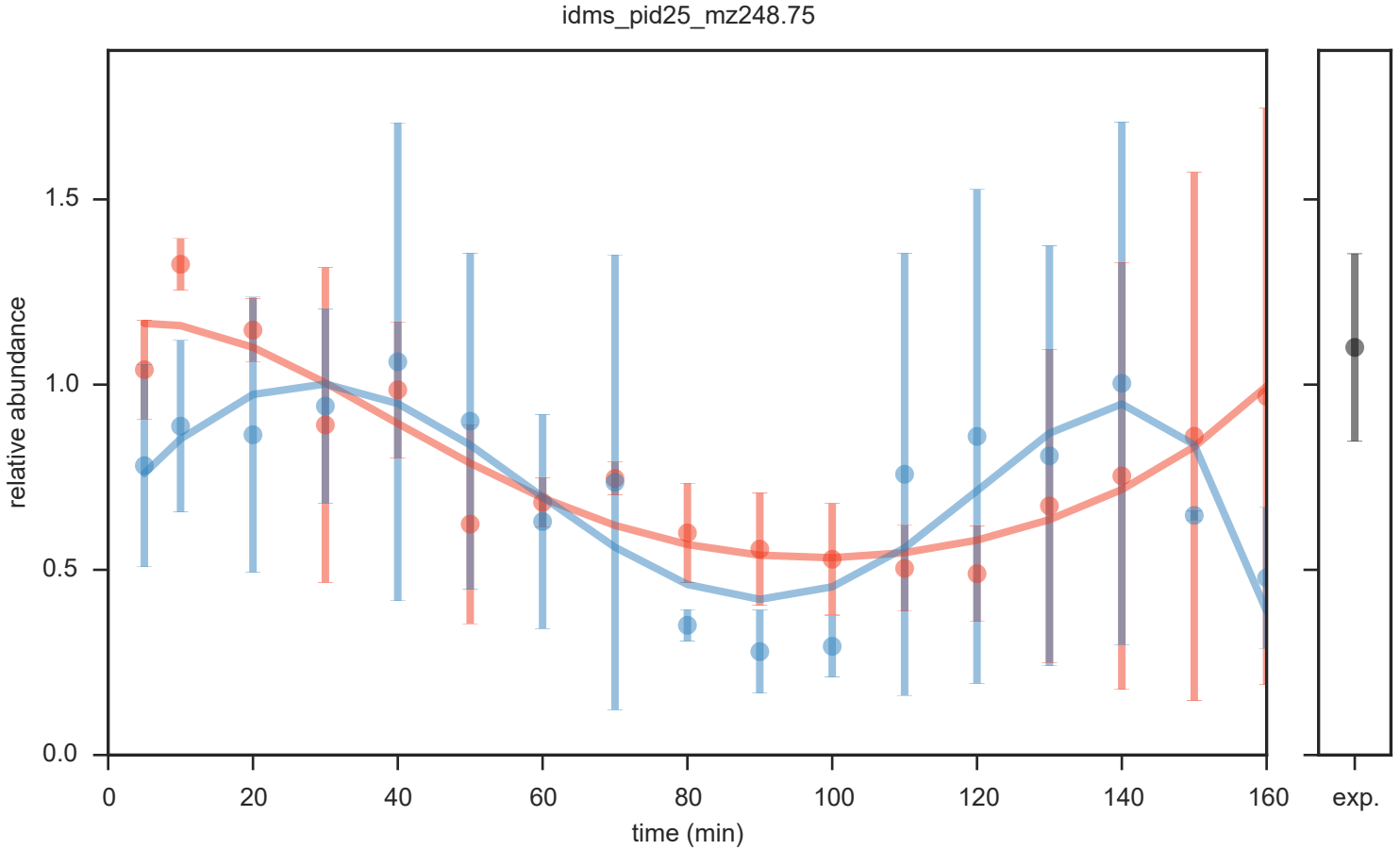
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid23_mz322.04
relative abundance
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid25_mz248.75
relative abundance
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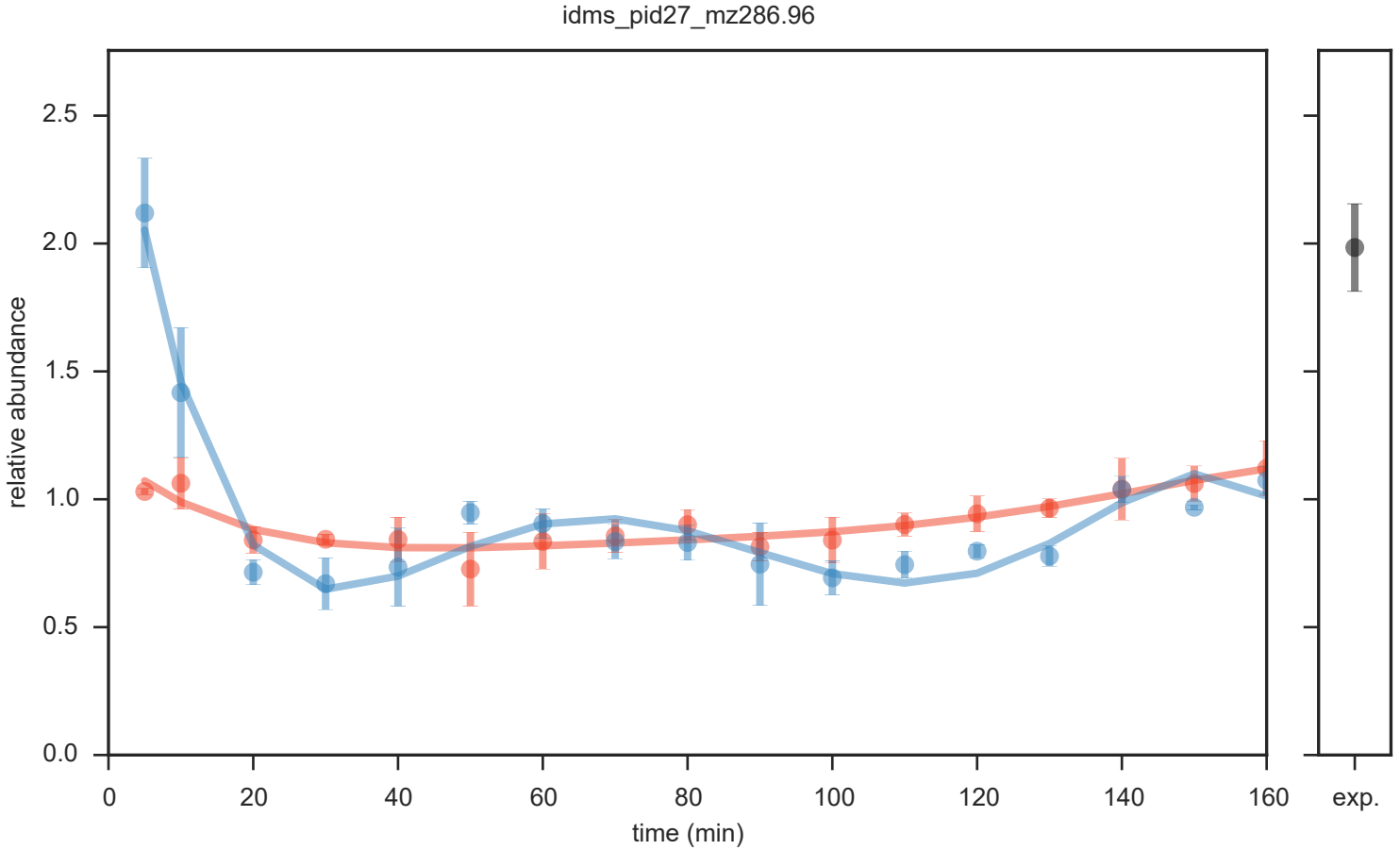
0.5
1.0
1.5
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid27_mz286.96
relative abundance
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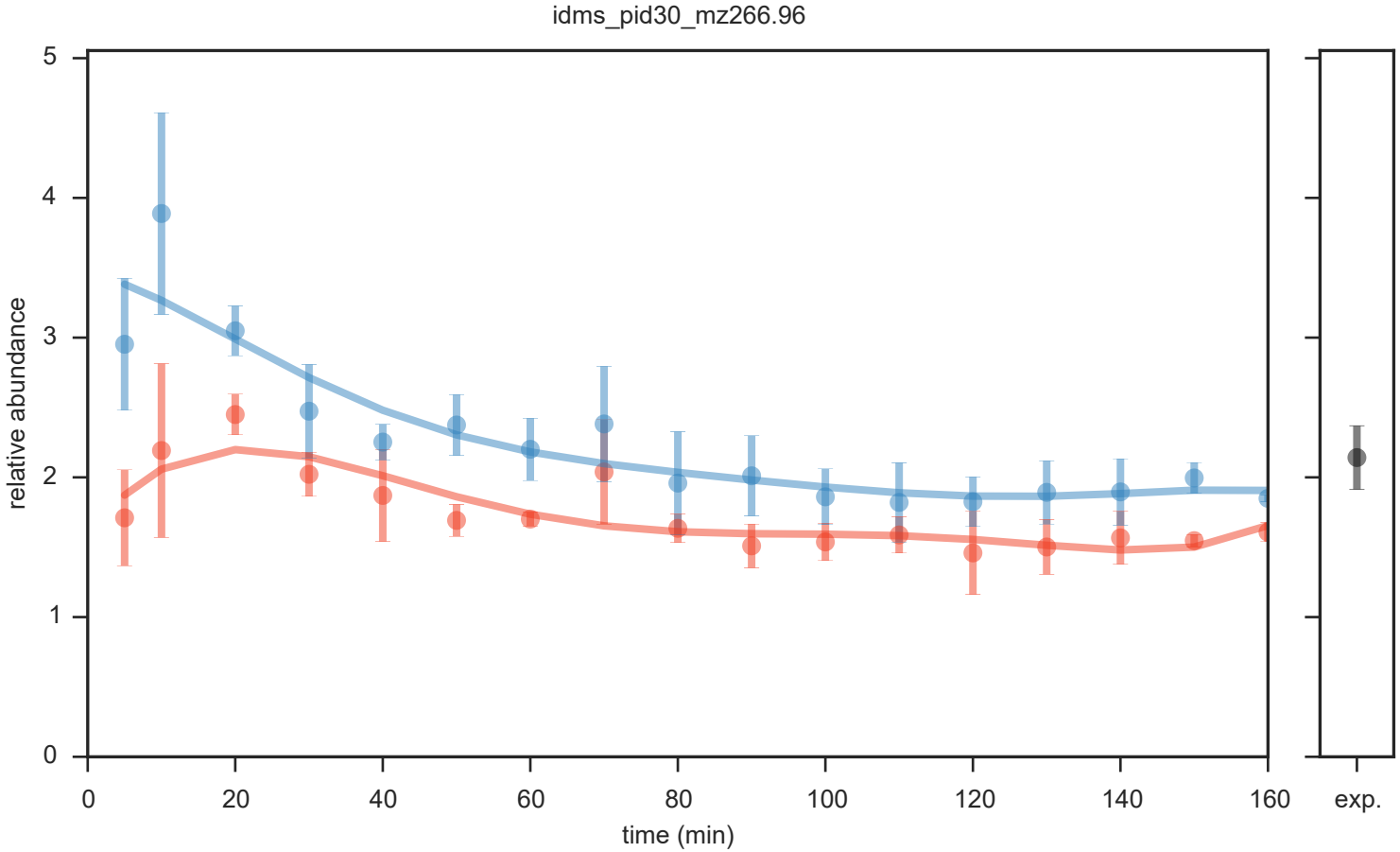
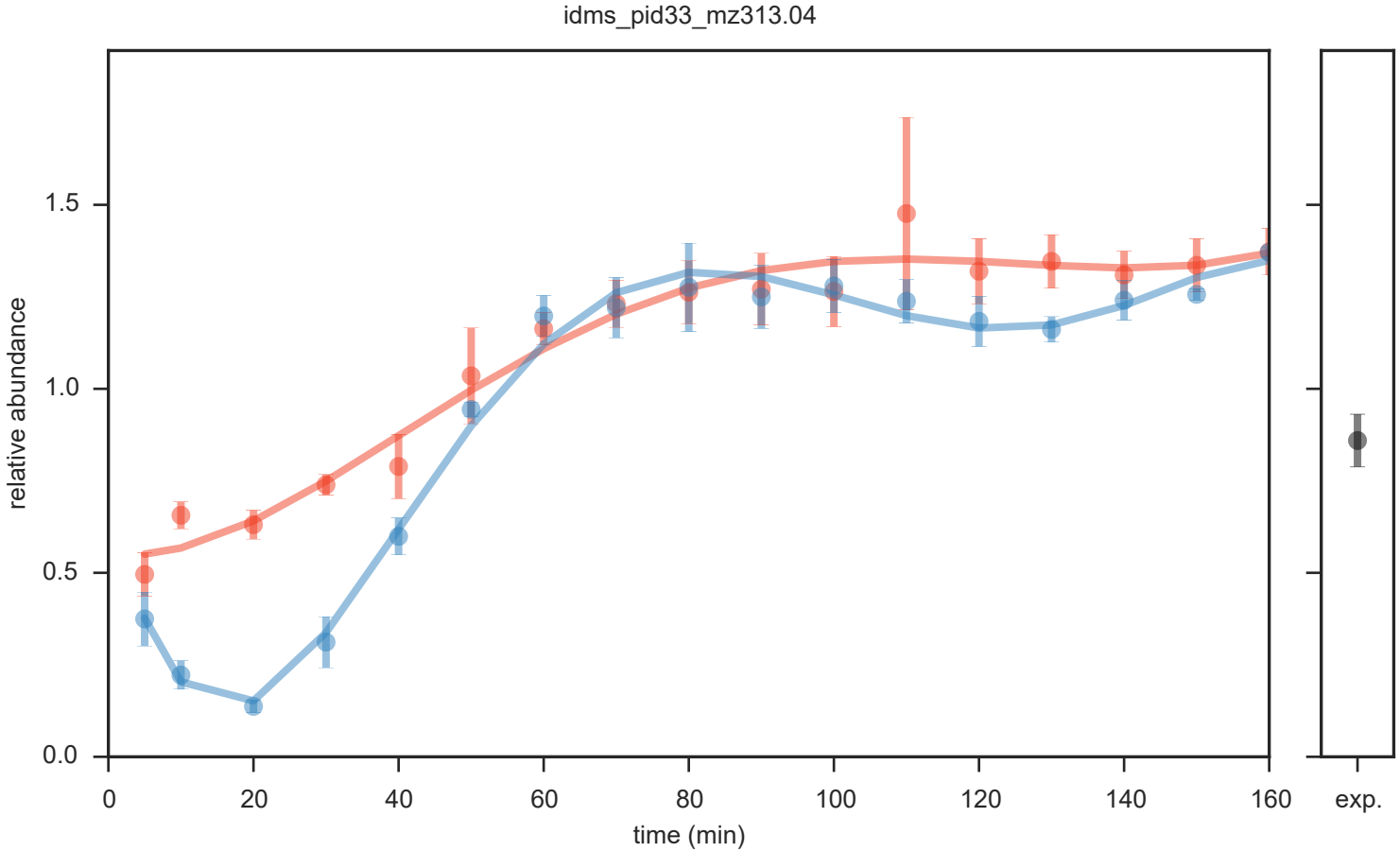
0.5
1.0
1.5
2.0
2.5
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid30_mz266.96
relative abundance
time (min)
exp.
0
1
2
3
4
5
0
20
40
60
80
100
120
140
160


idms_pid33_mz313.04
relative abundance
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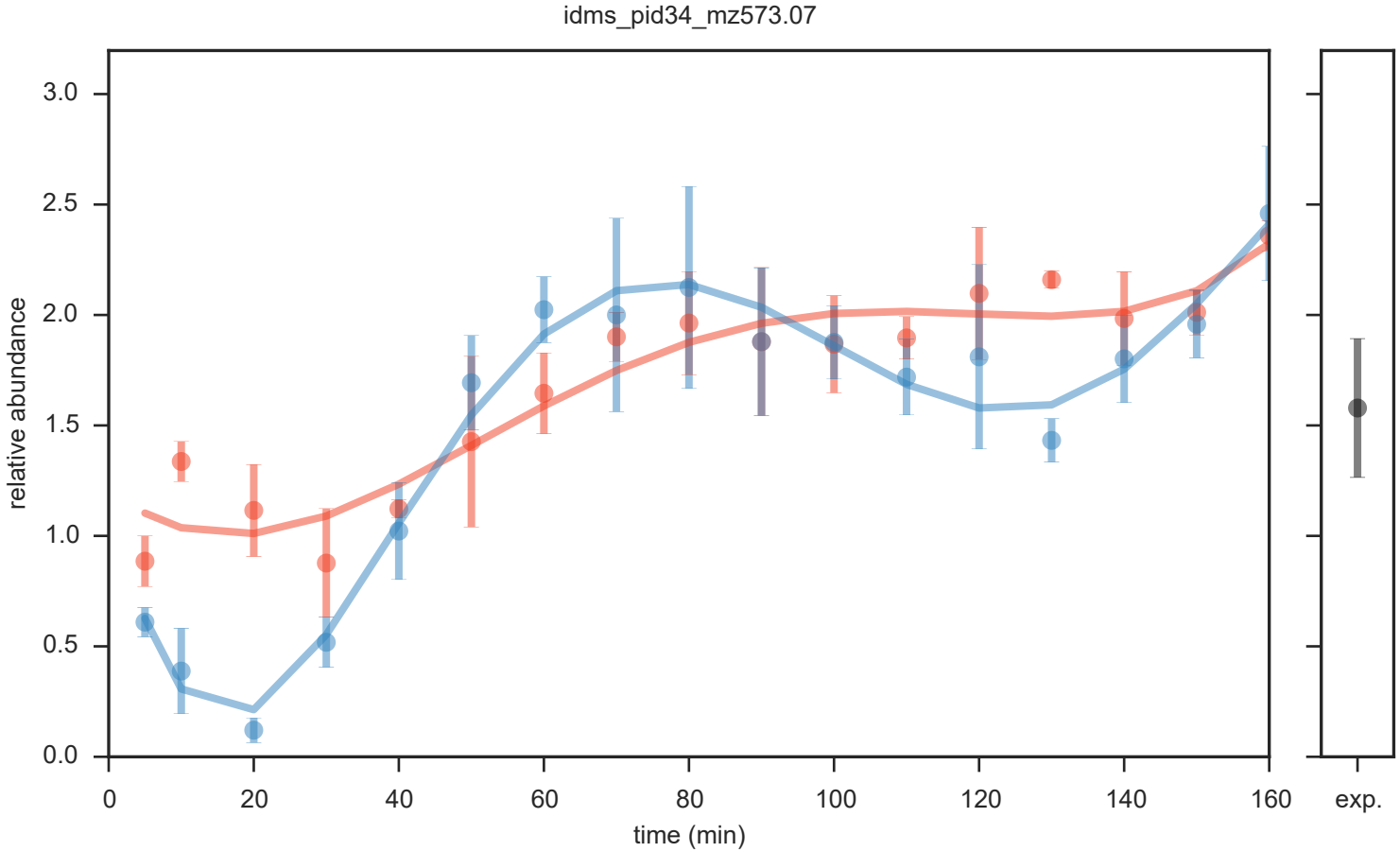
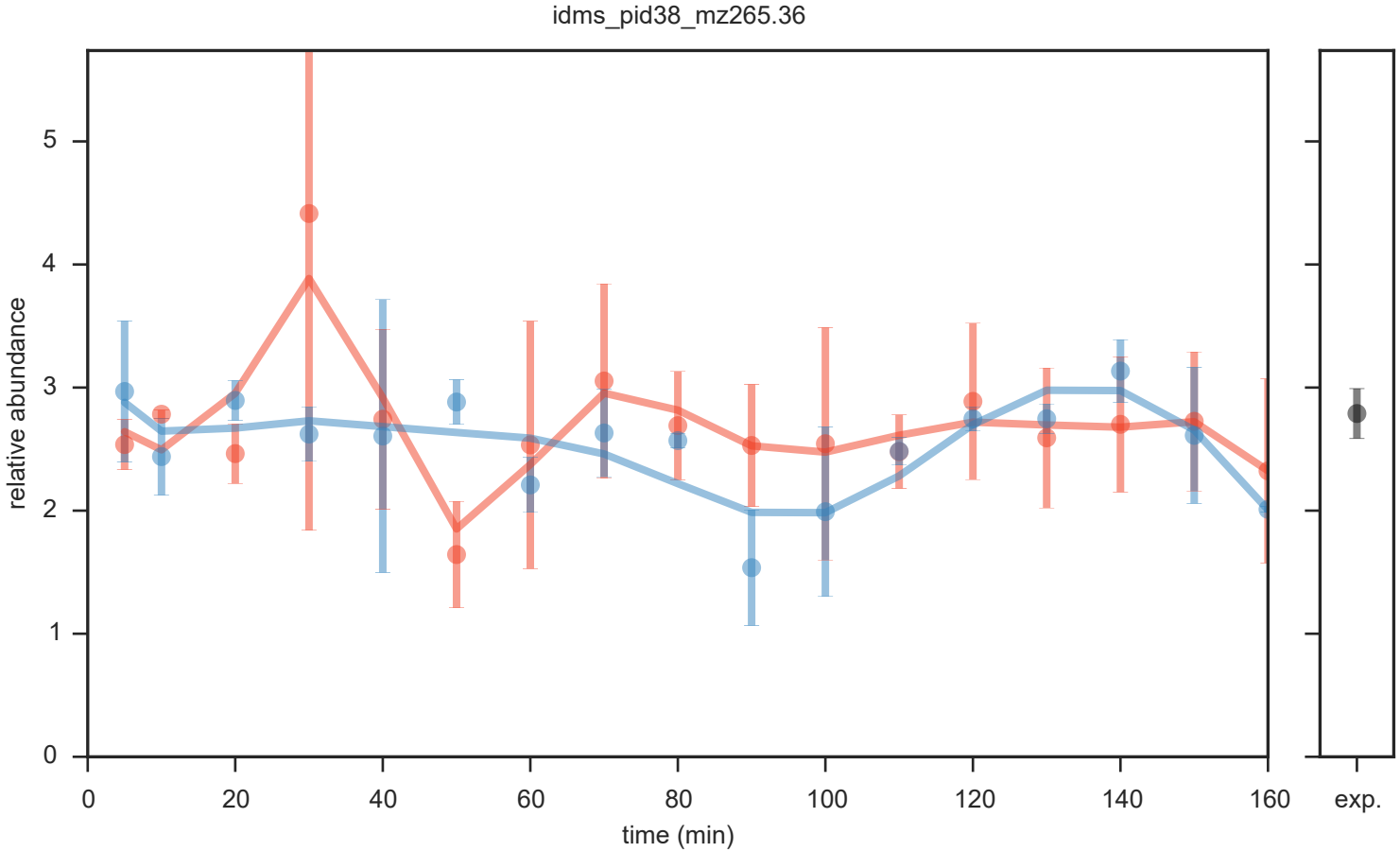
1.0
1.5
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid34_mz573.07
relative abundance
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid38_mz265.36
relative abundance
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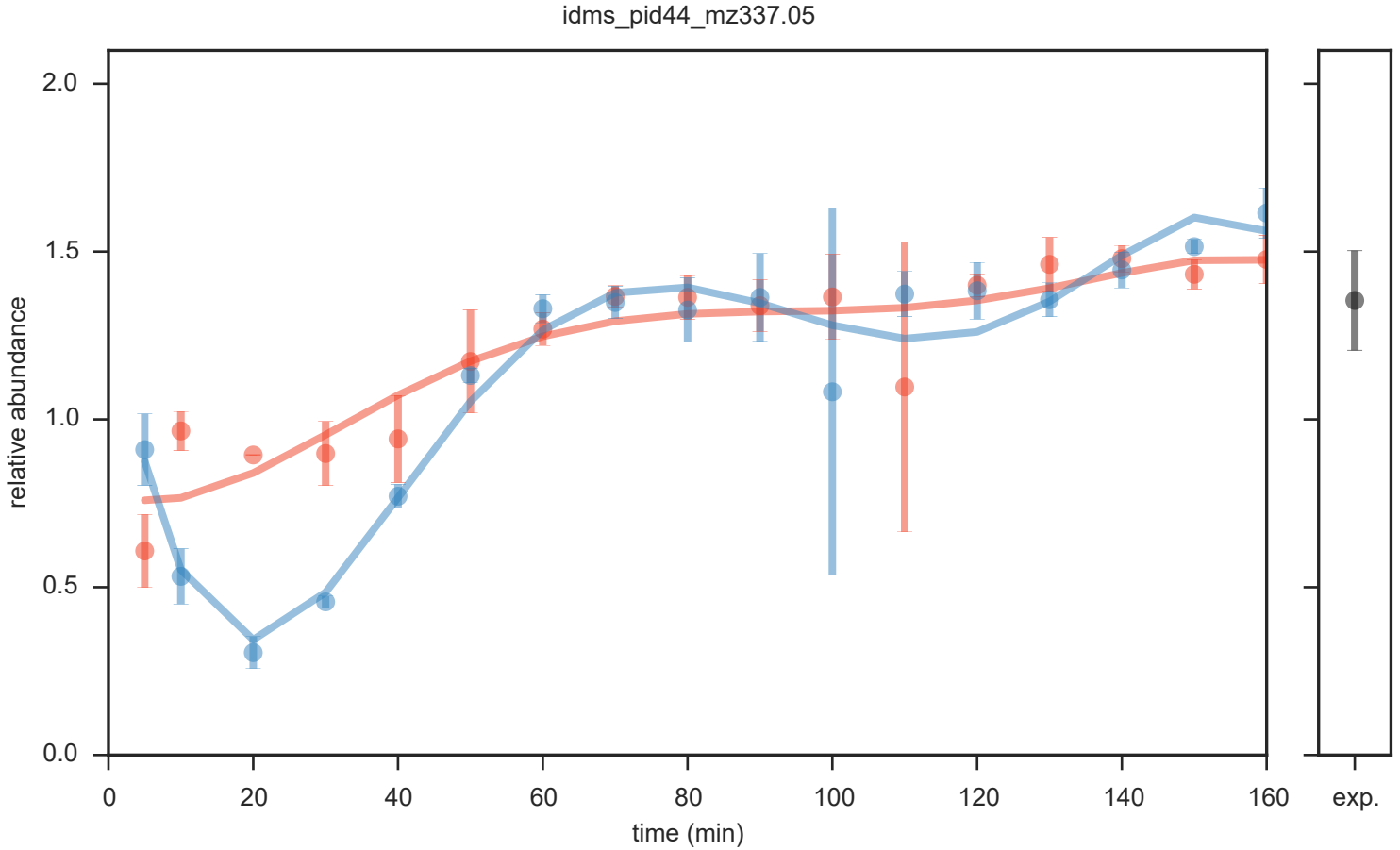
2
3
4
5
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid44_mz337.05
relative abundance
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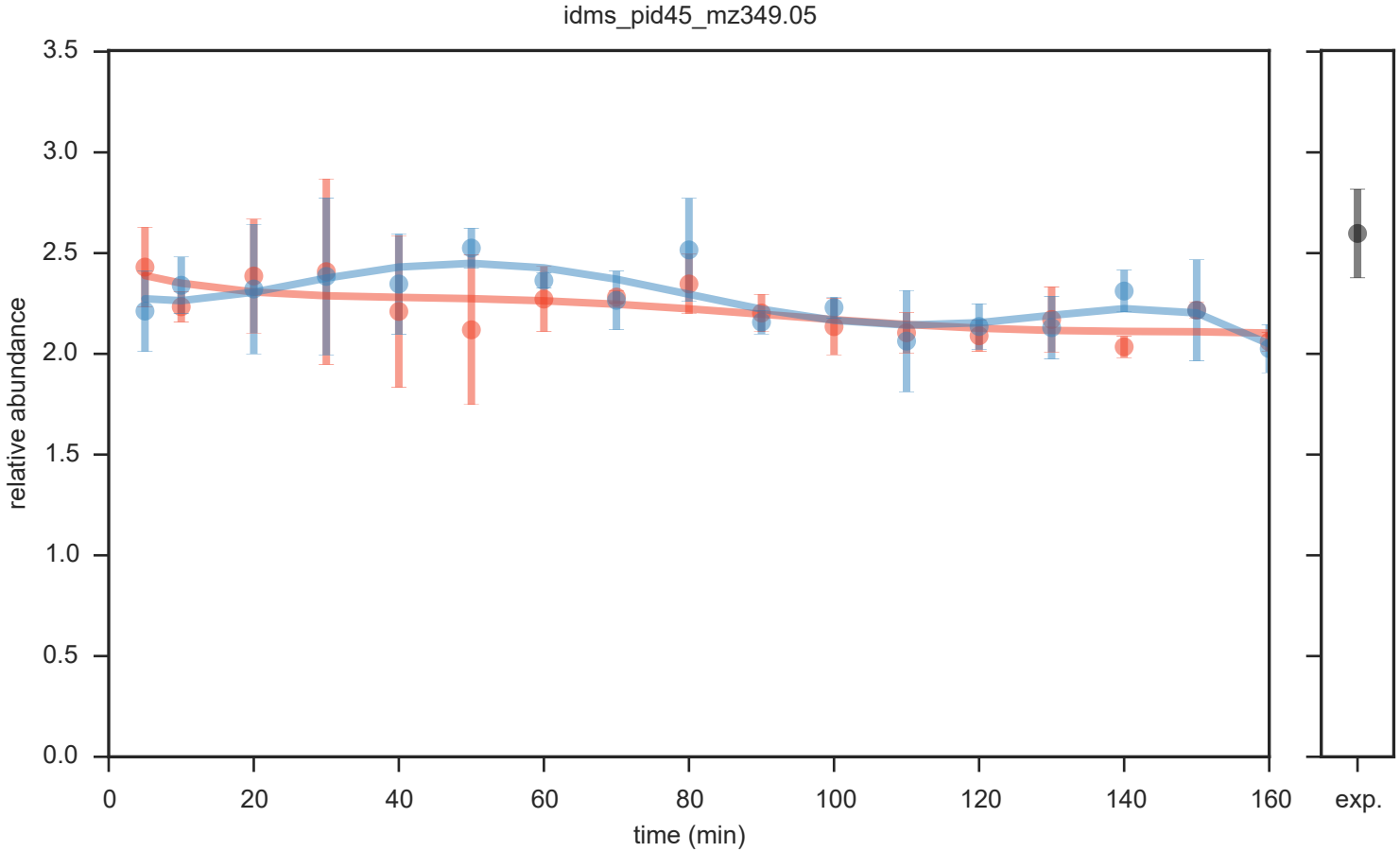
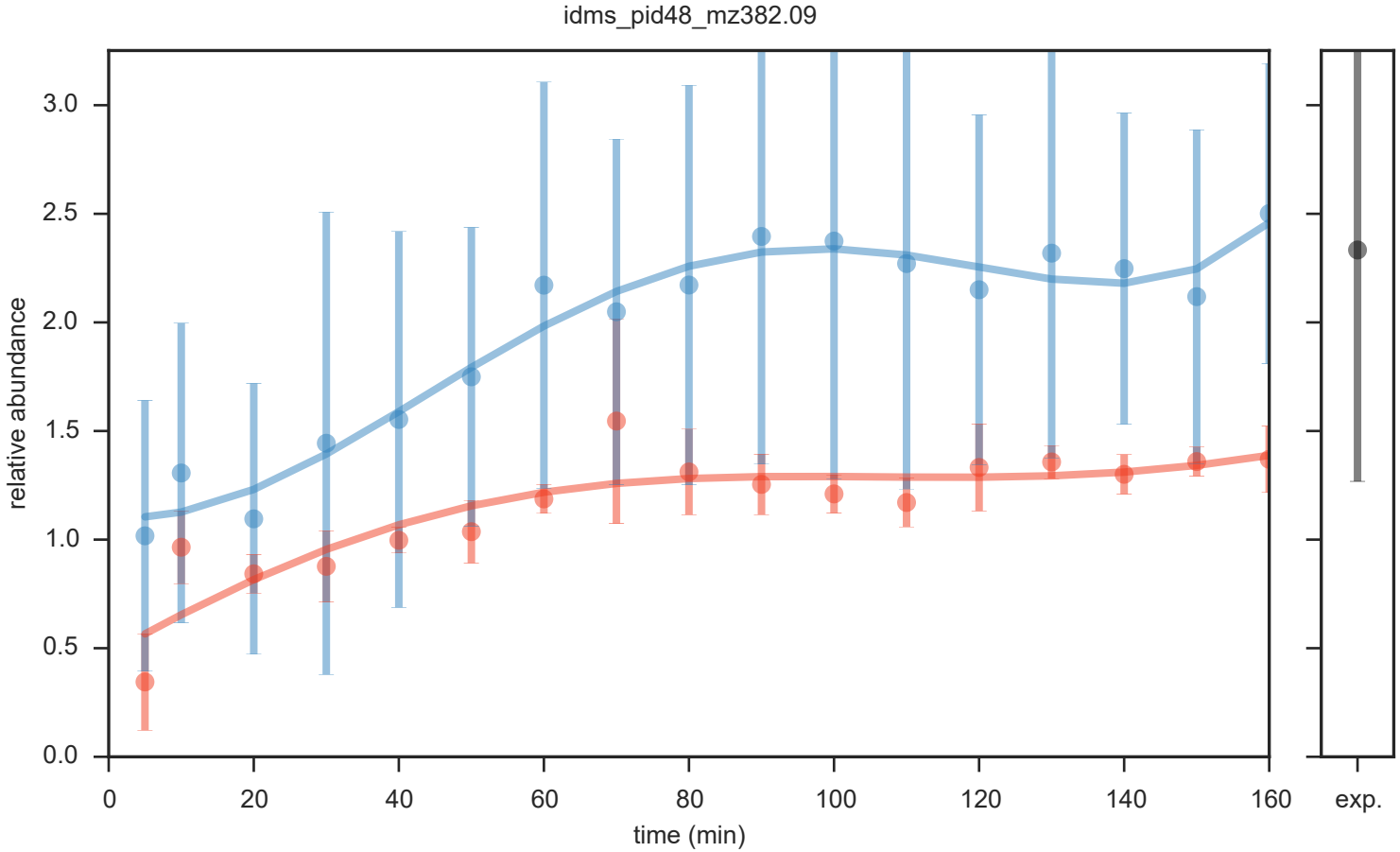
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid45_mz349.05
relative abundance
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid48_mz382.09
relative abundance
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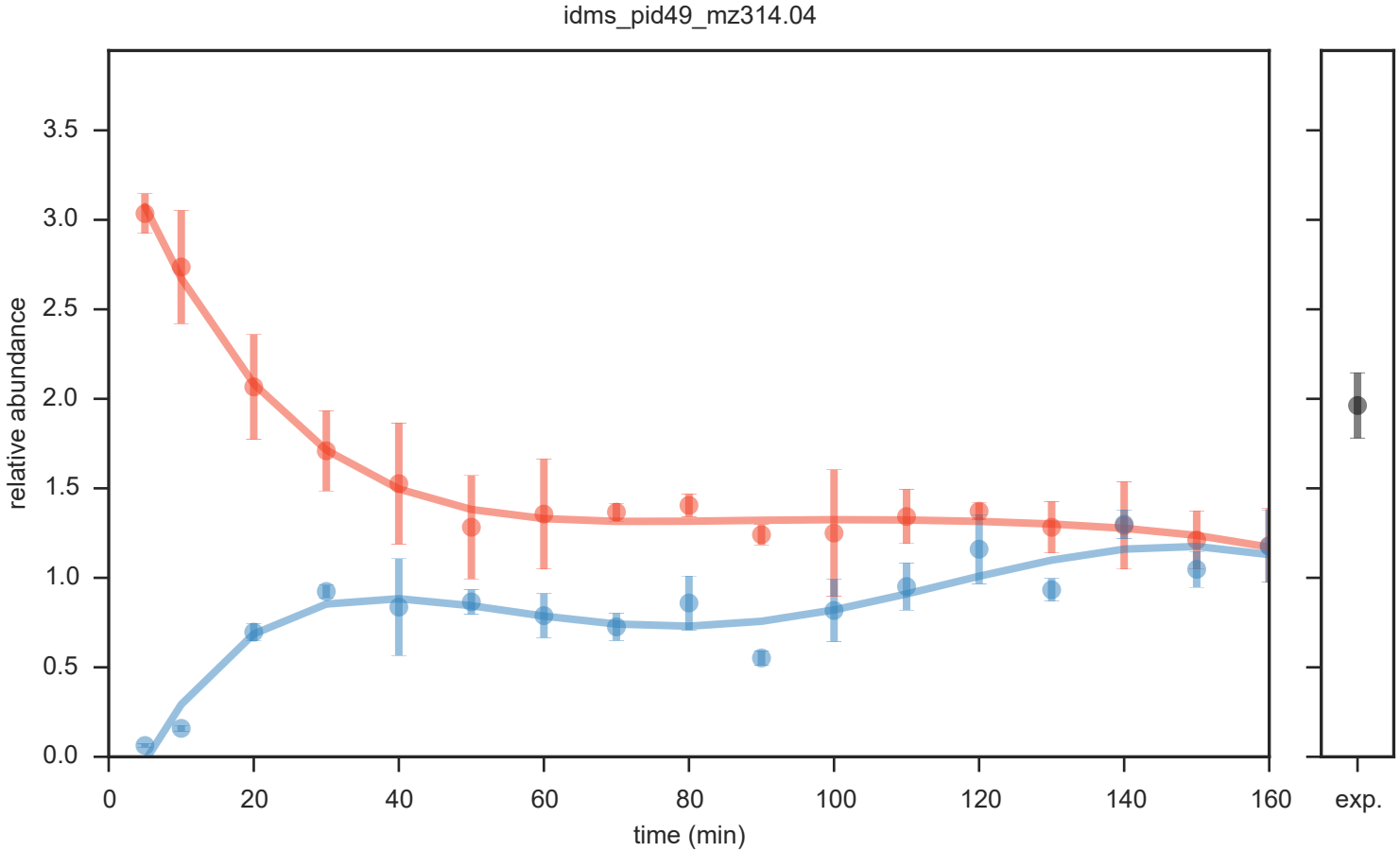
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid49_mz314.04
relative abundance
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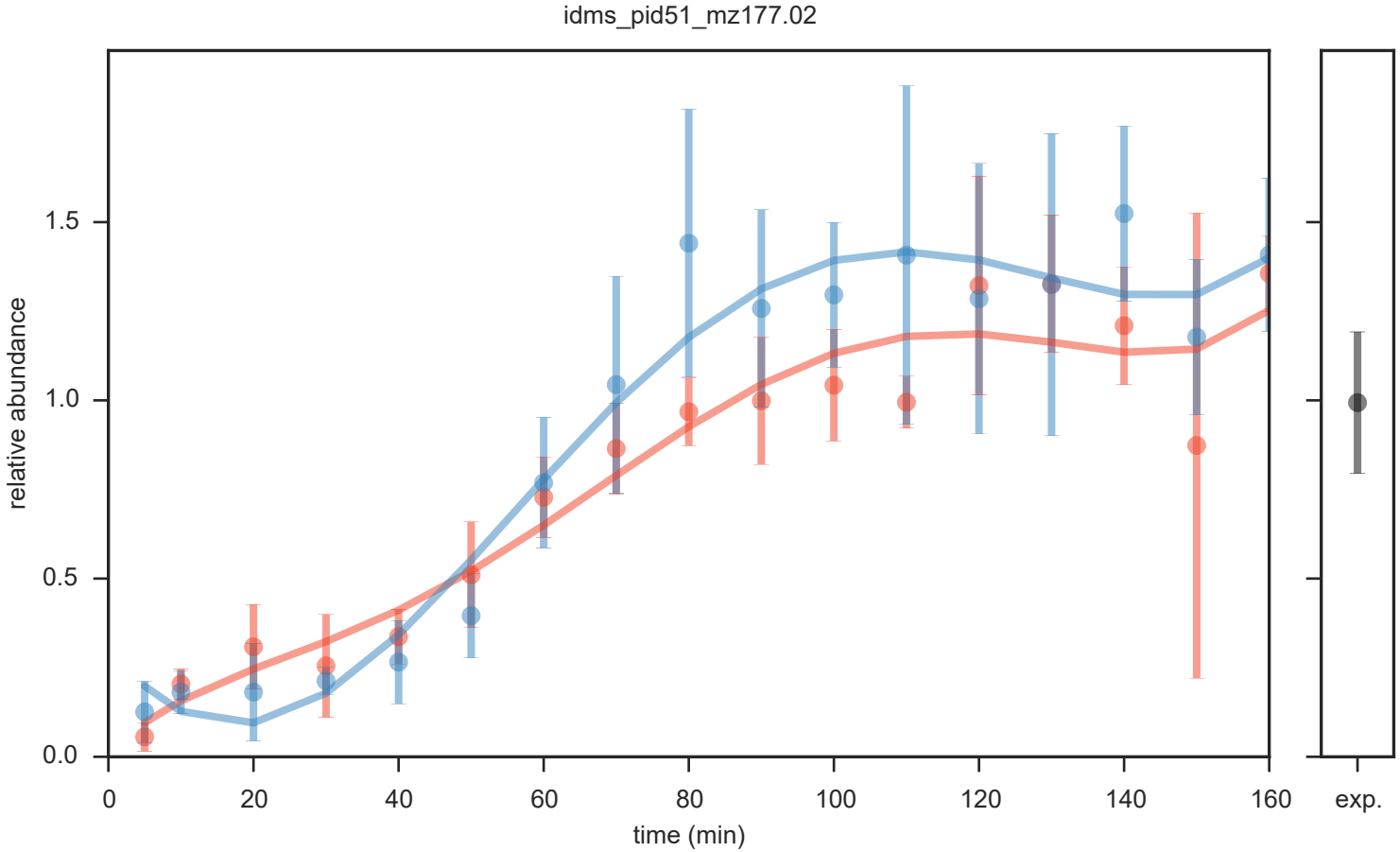
0.5
1.0
1.5
2.0
2.5
3.0
3.5
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid51_mz177.02
relative abundance
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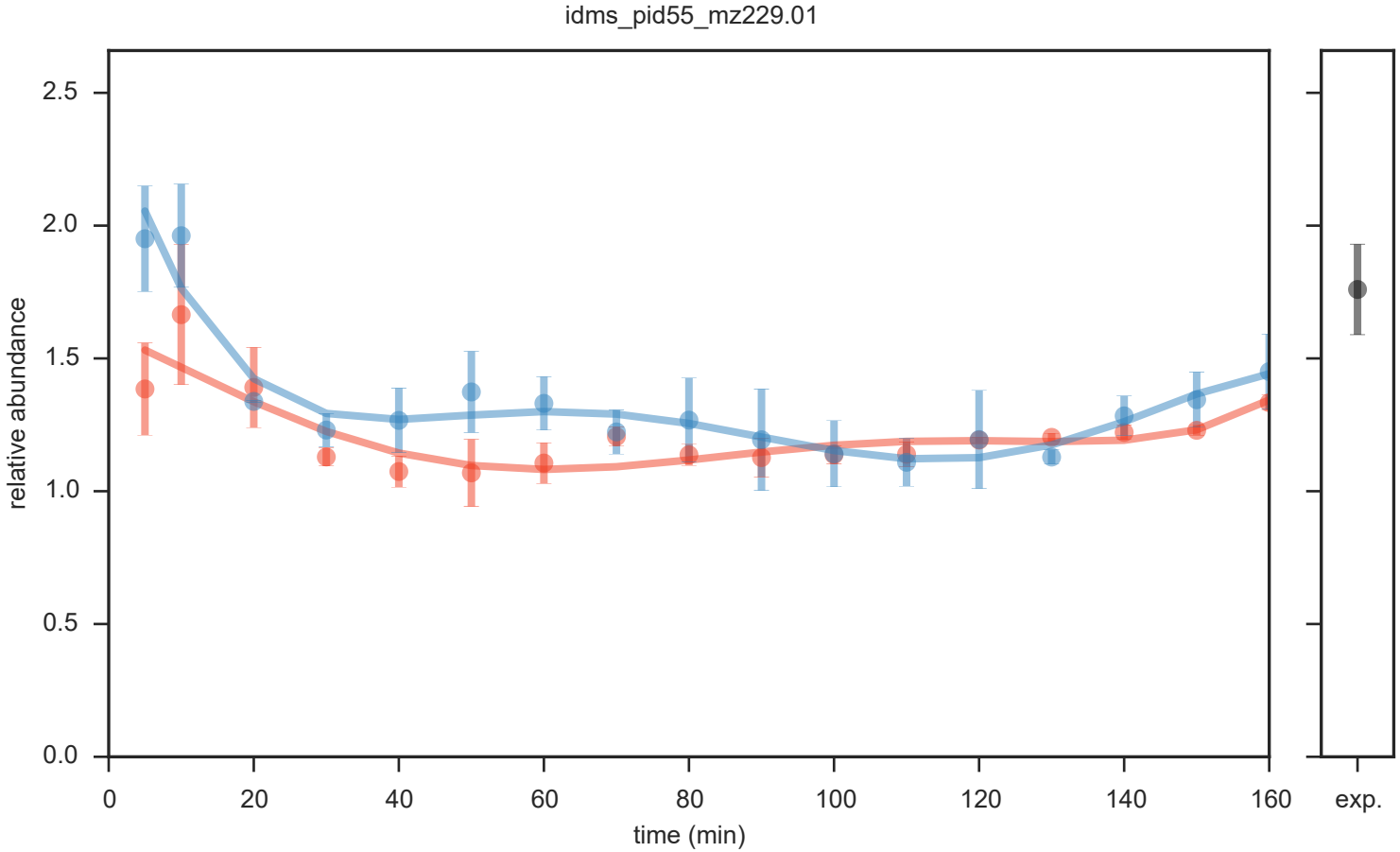
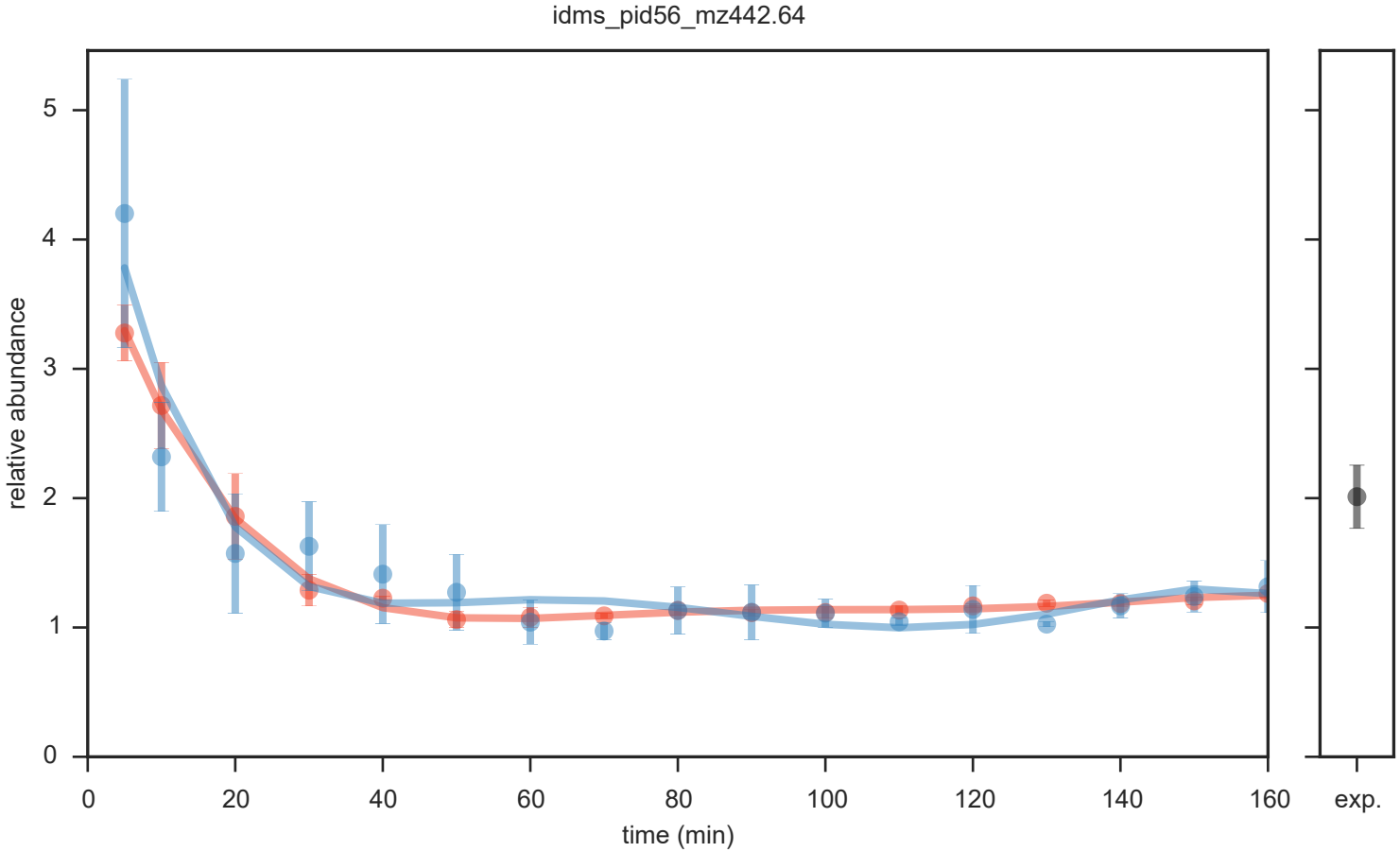
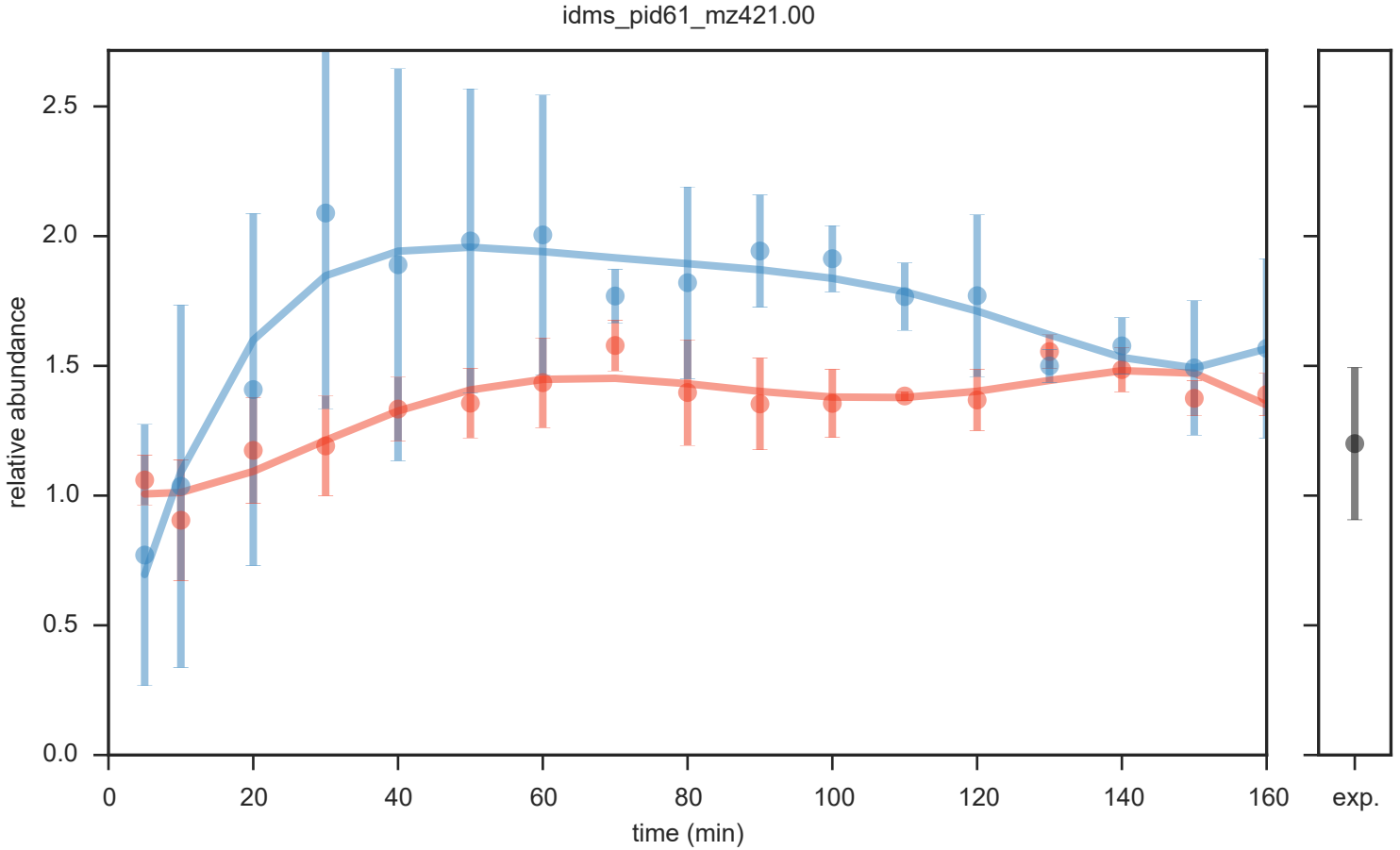
1.0
1.5
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid55_mz229.01
relative abundance
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid56_mz442.64
relative abundance
0
1
2
3
4
5
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid61_mz421.00
relative abundance
0.0
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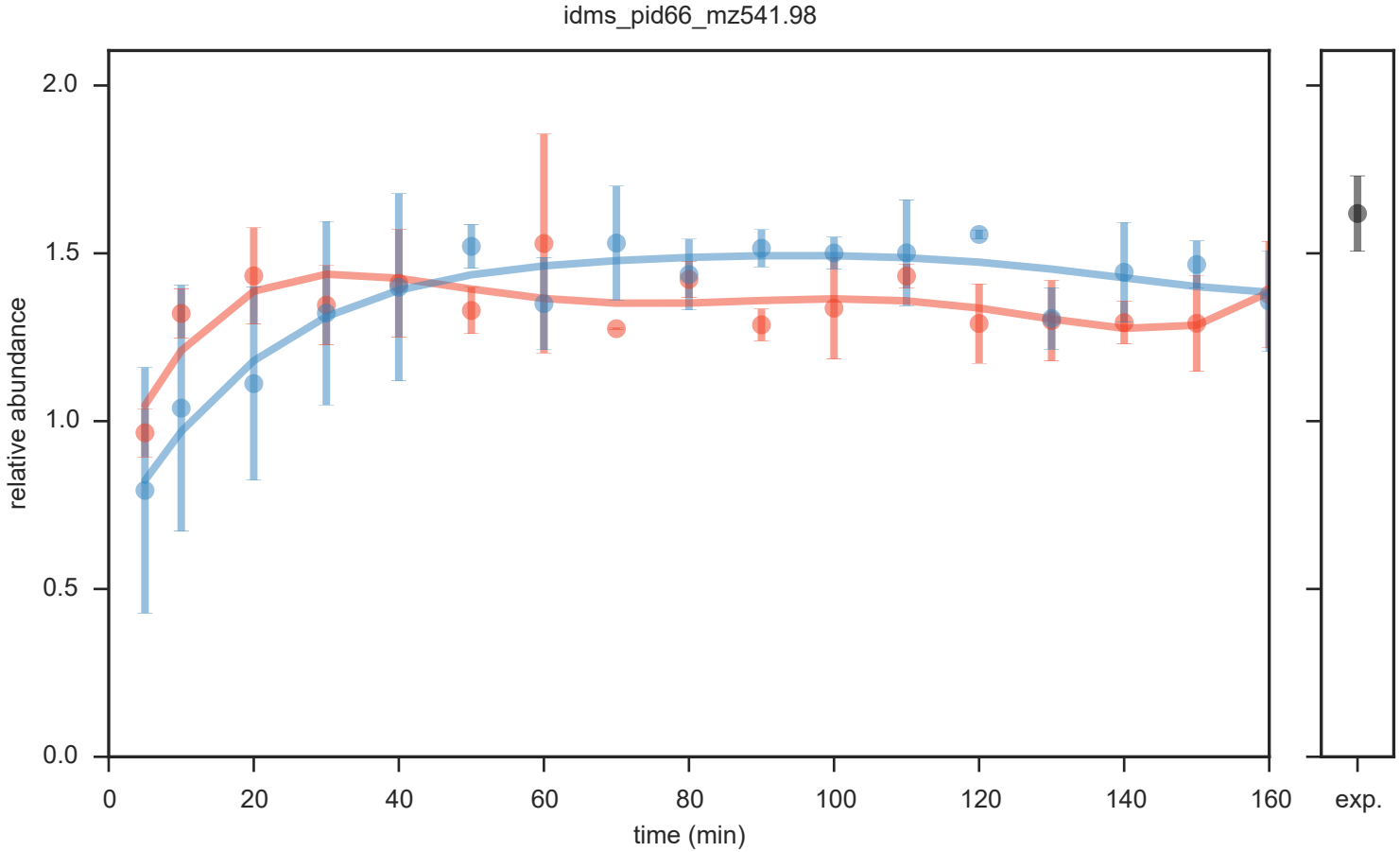
1.0
1.5
2.0
2.5
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid66_mz541.98
relative abundance
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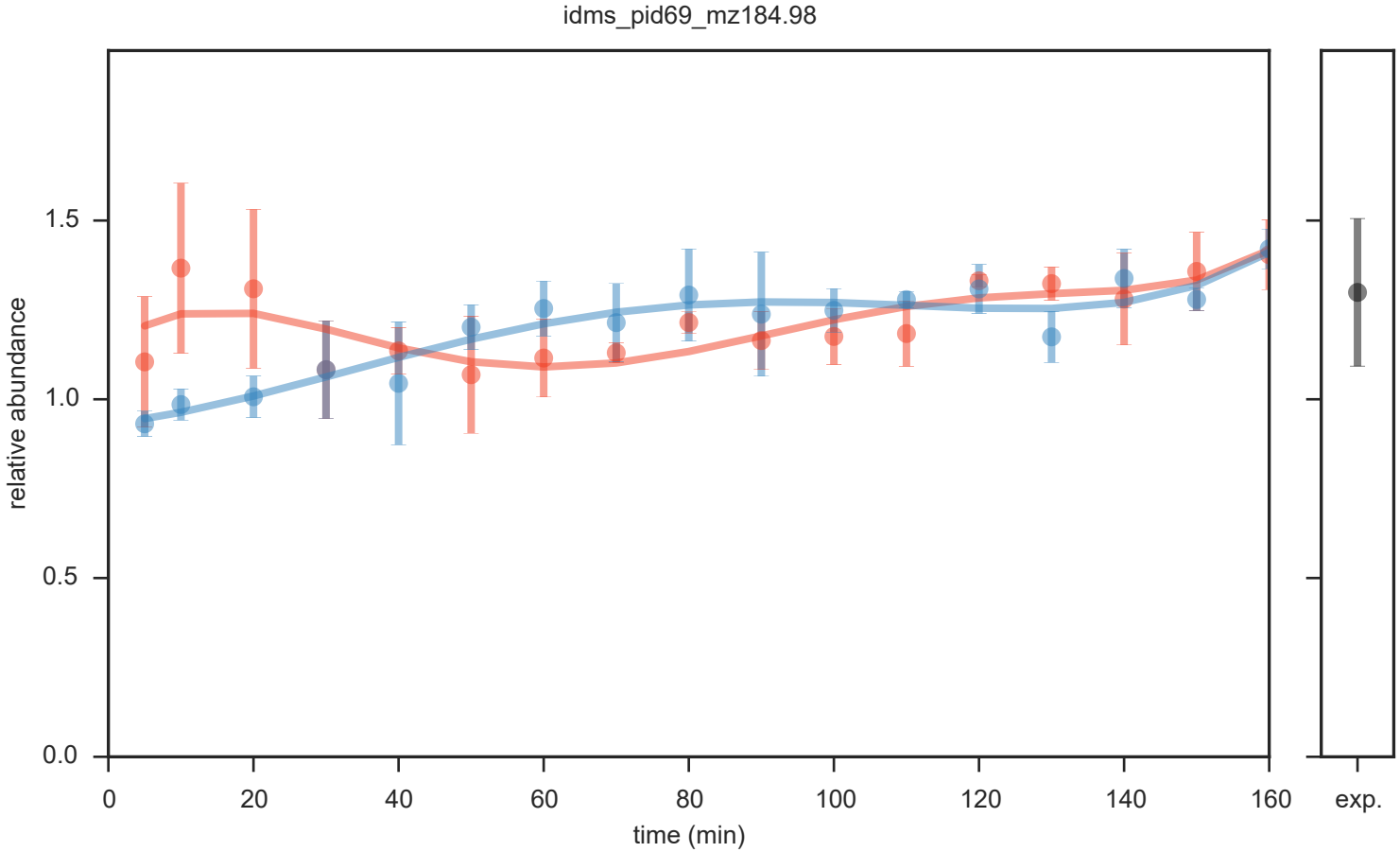
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid69_mz184.98
relative abundance
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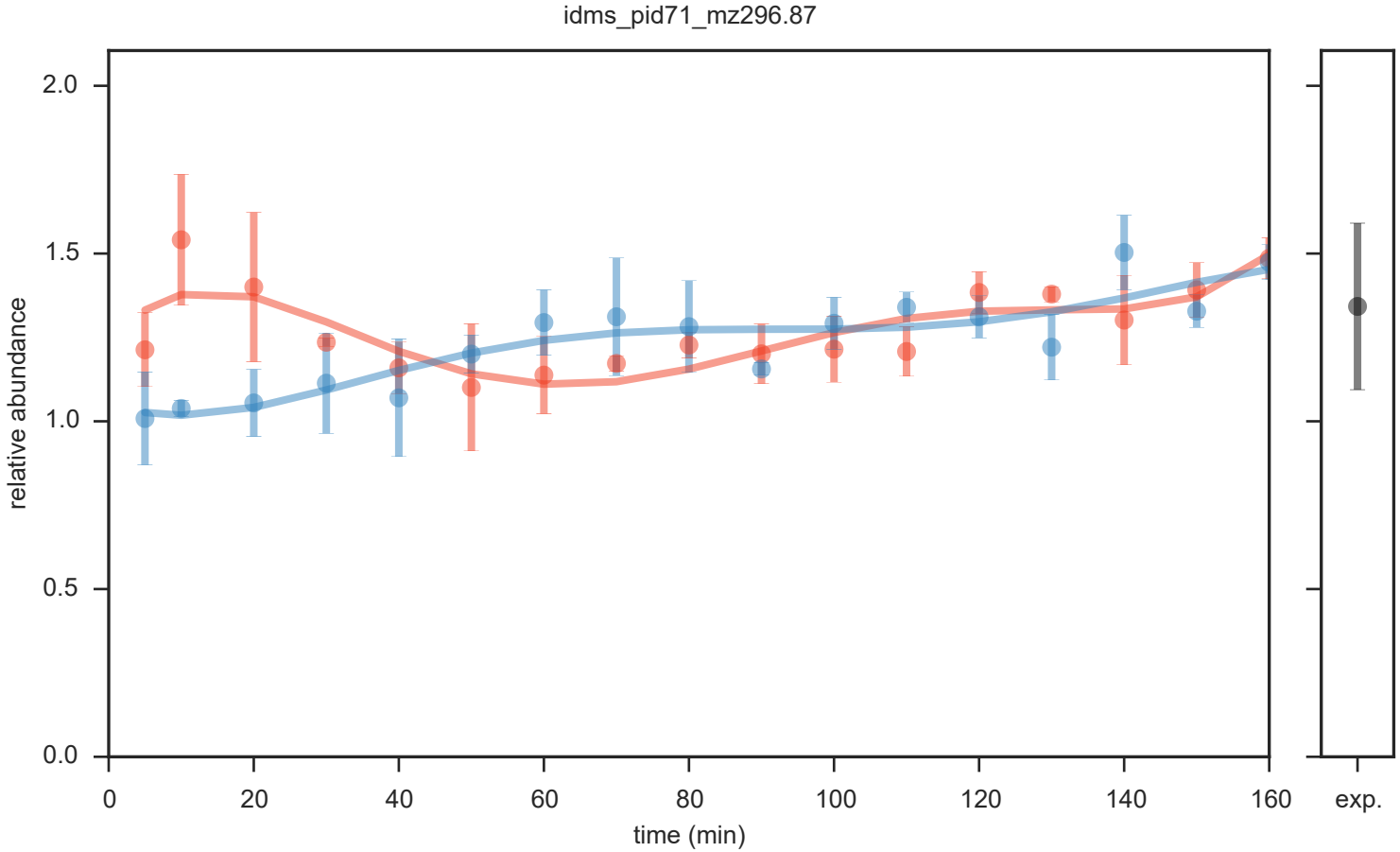
1.0
1.5
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid71_mz296.87
relative abundance
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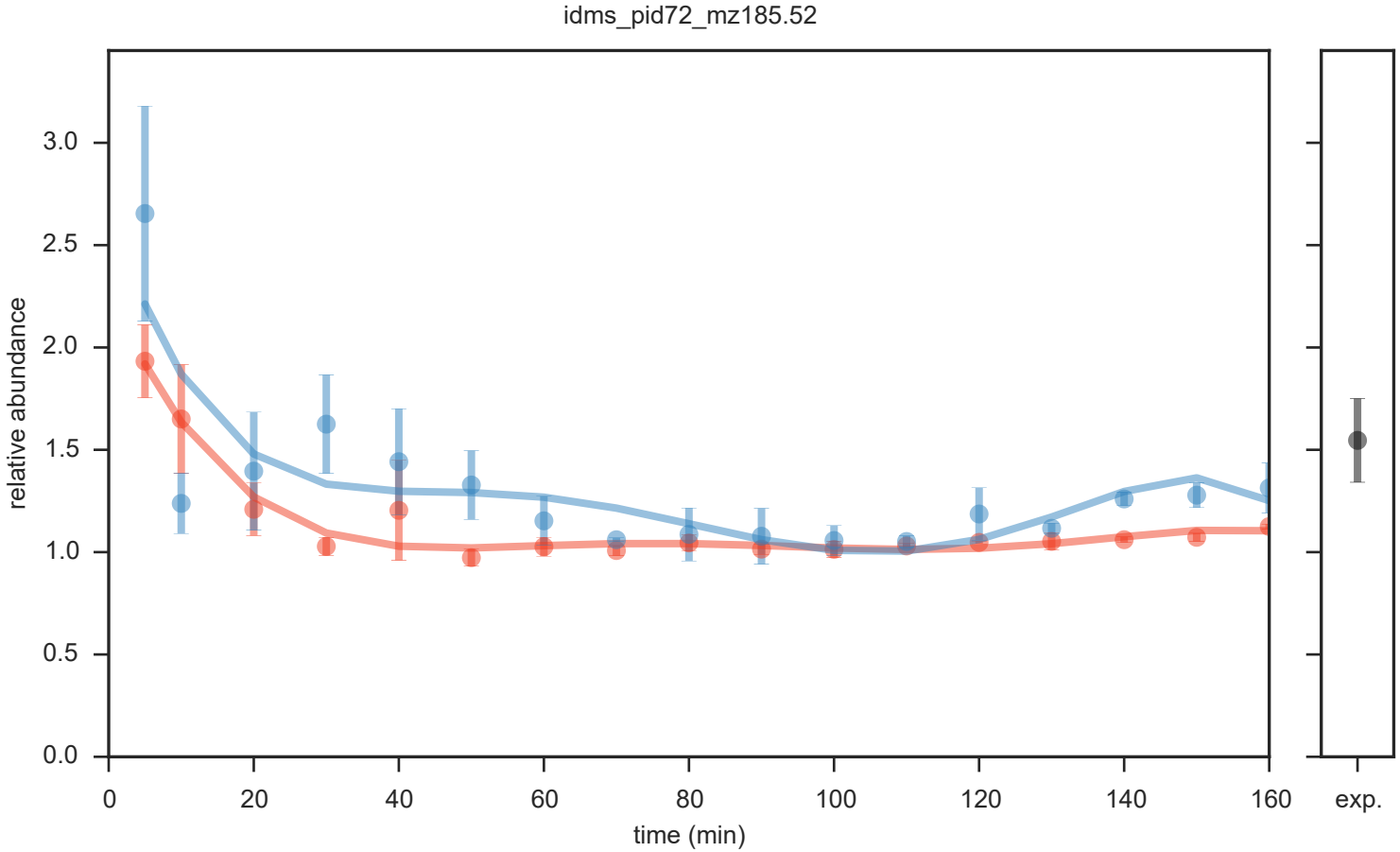
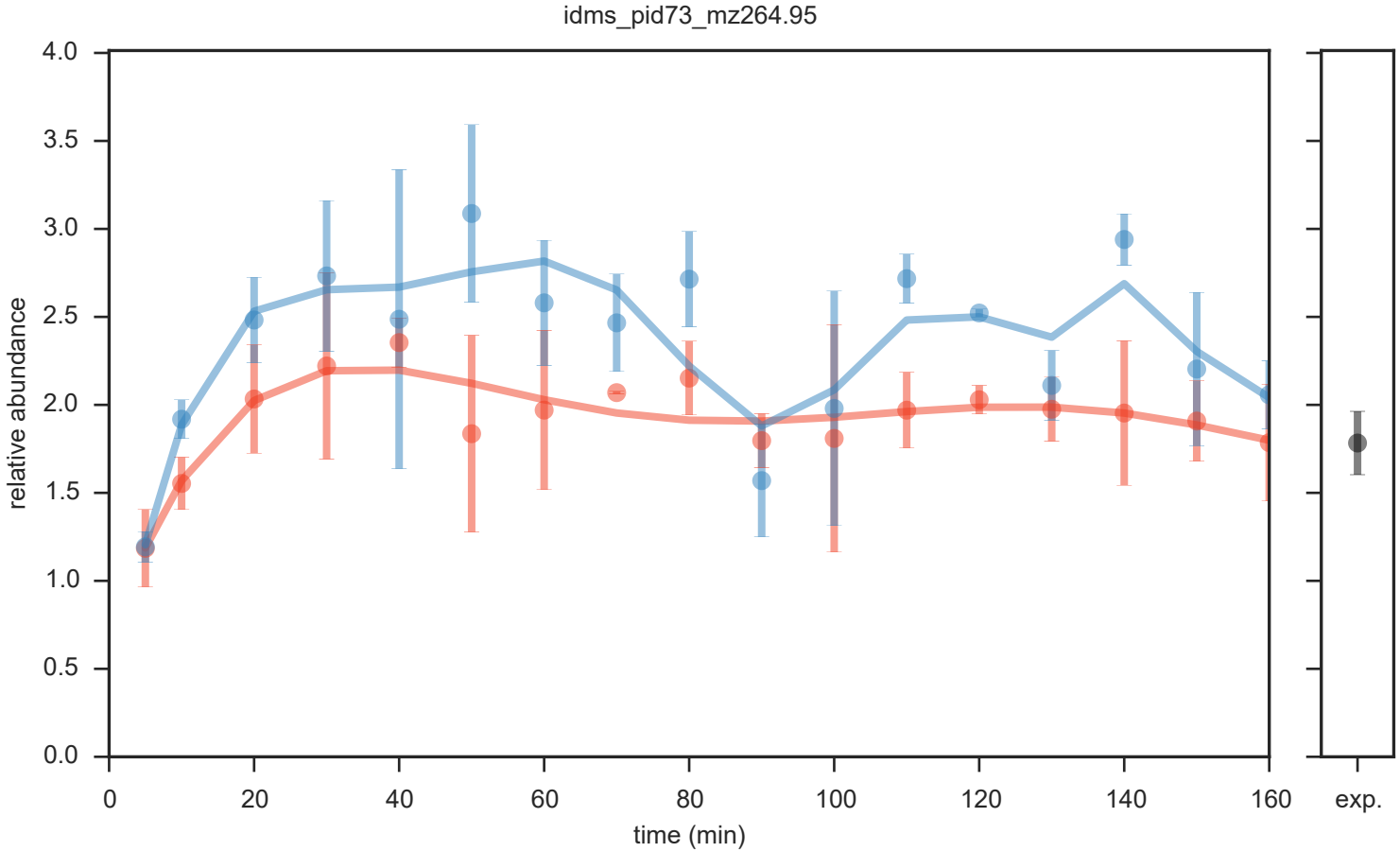
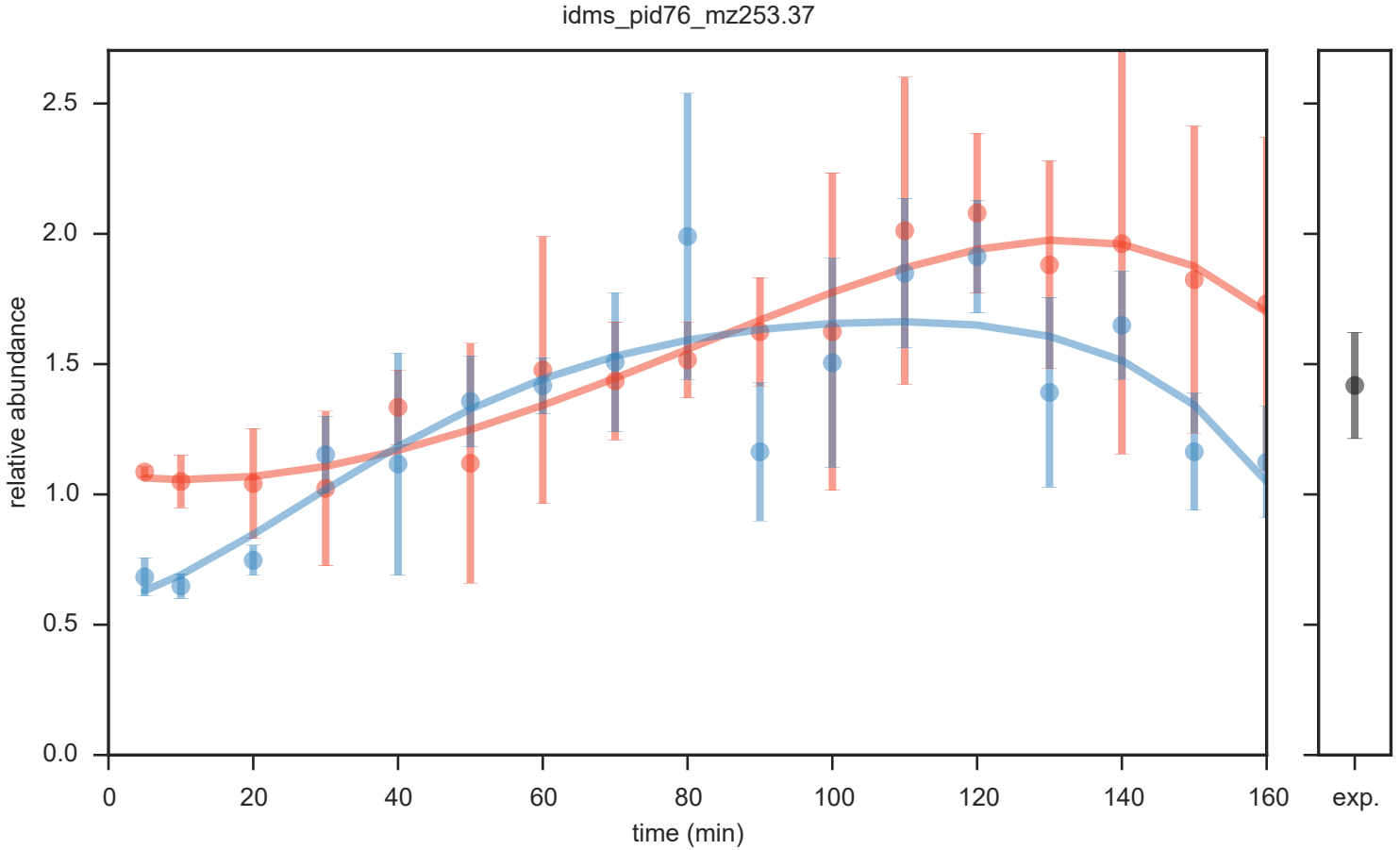
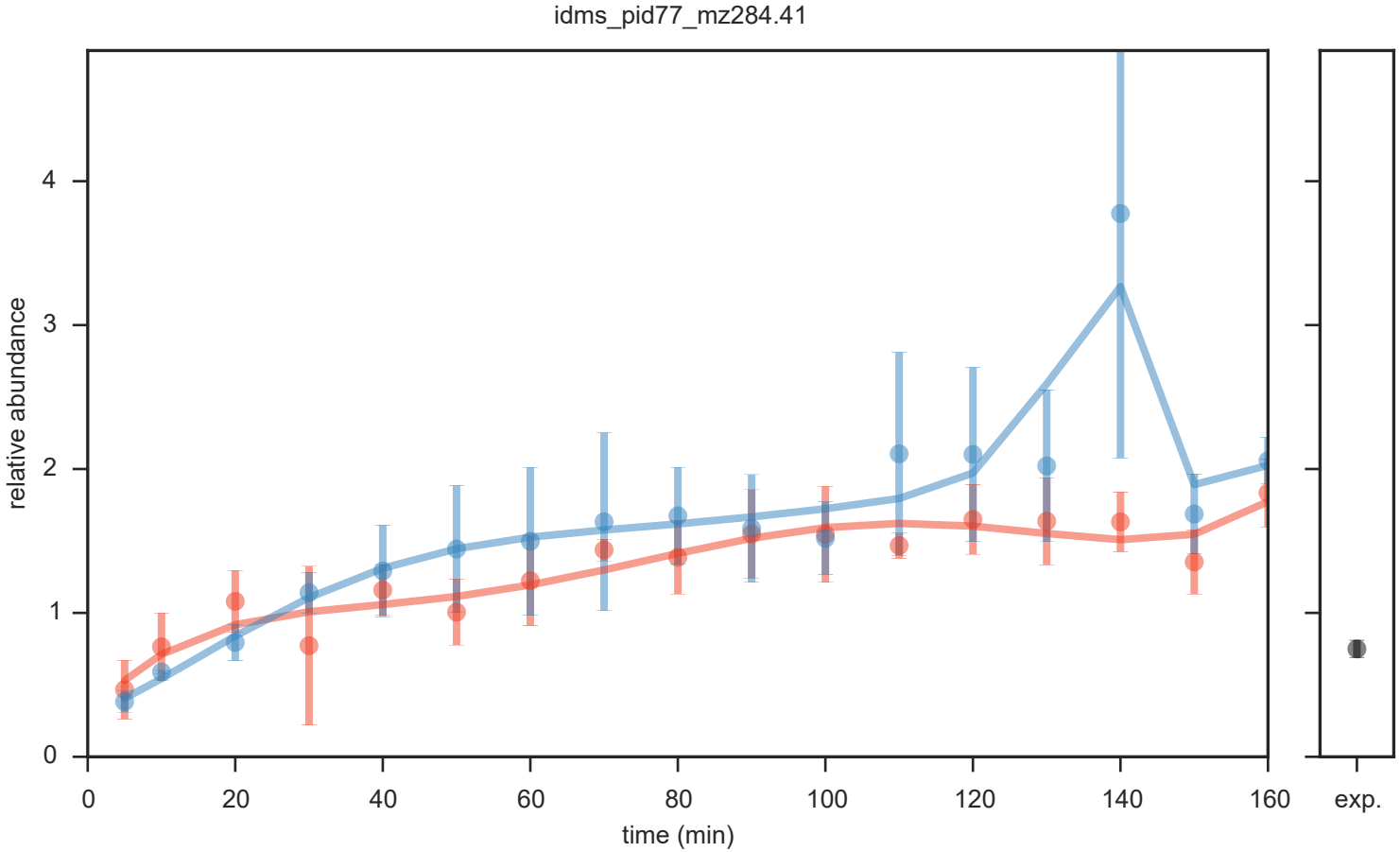
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid72_mz185.52
relative abundance
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid73_mz264.95
relative abundance
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid76_mz253.37
relative abundance
0.0
0.5
1.0
1.5
2.0
2.5
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid77_mz284.41
relative abundance
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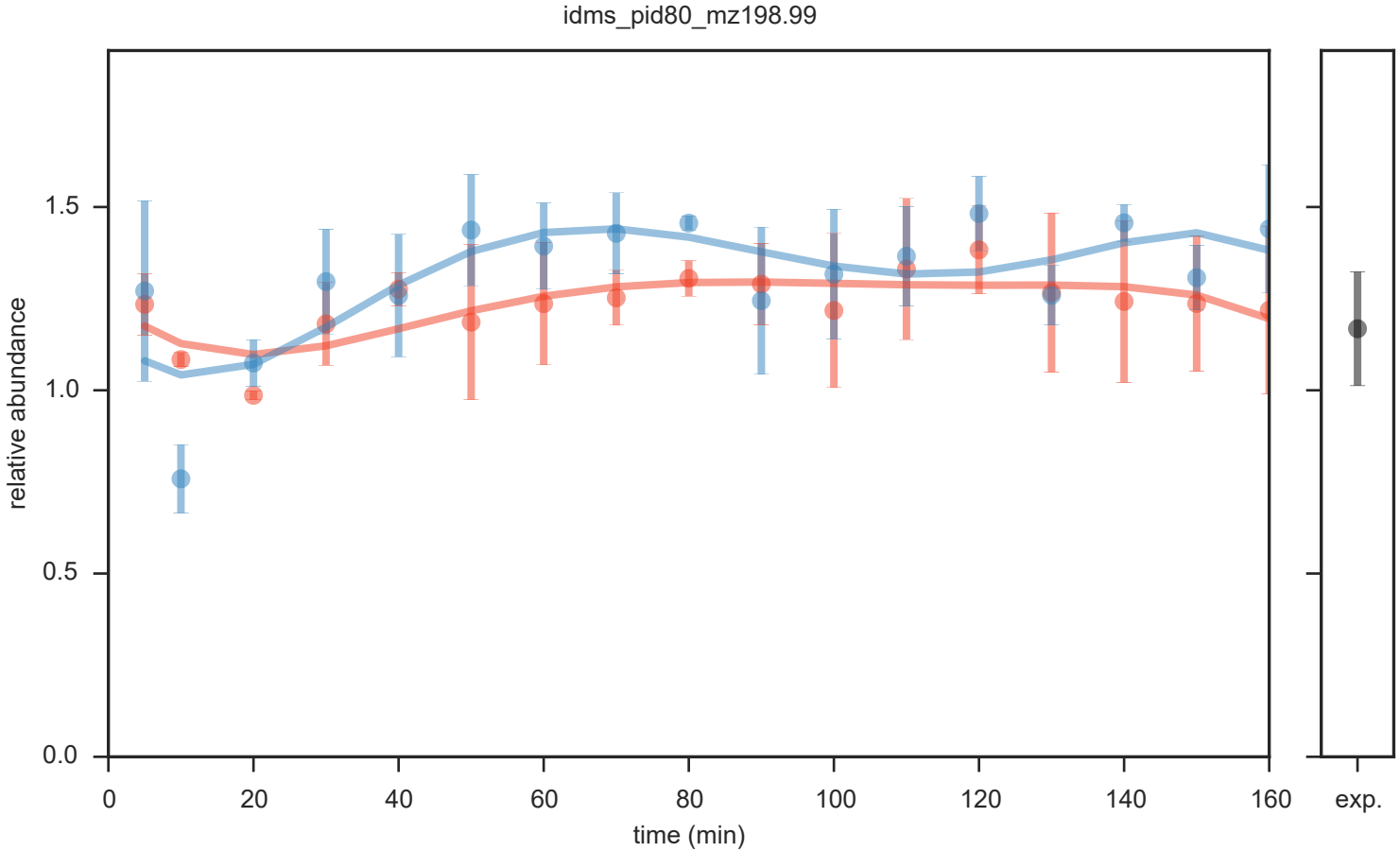
1
2
3
4
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid80_mz198.99
relative abundance
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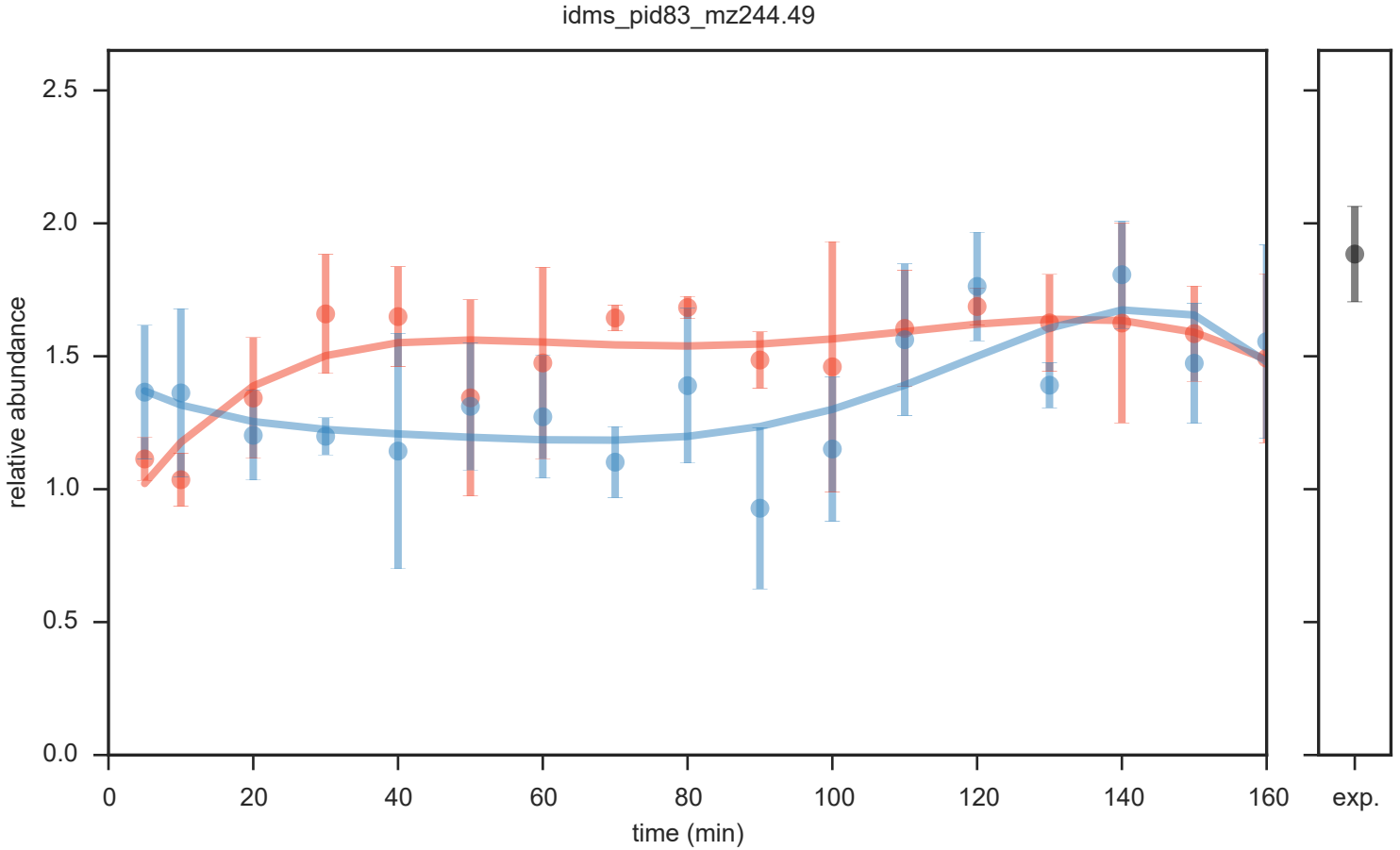
1.0
1.5
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid83_mz244.49
relative abundance
2.5
2.0
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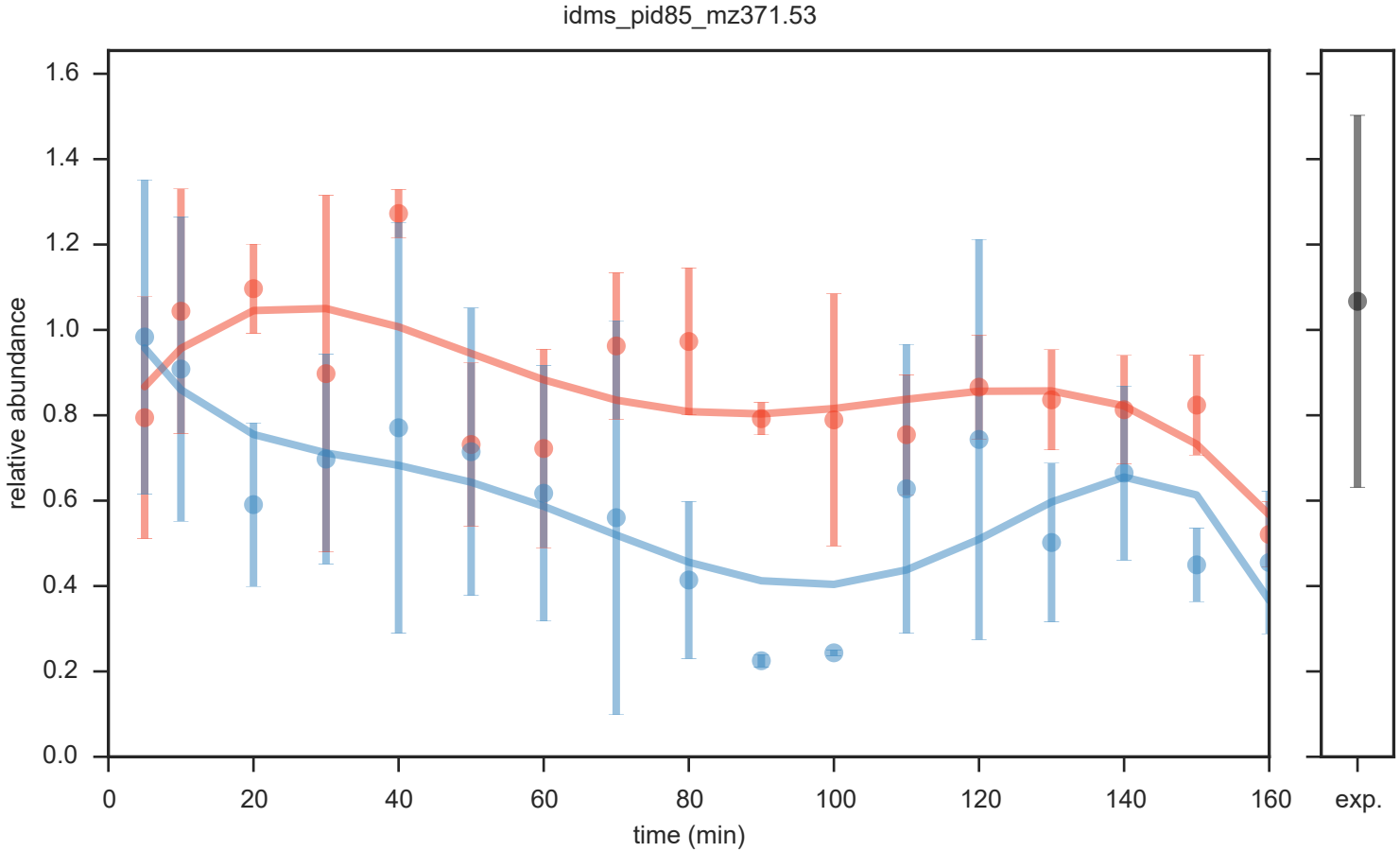
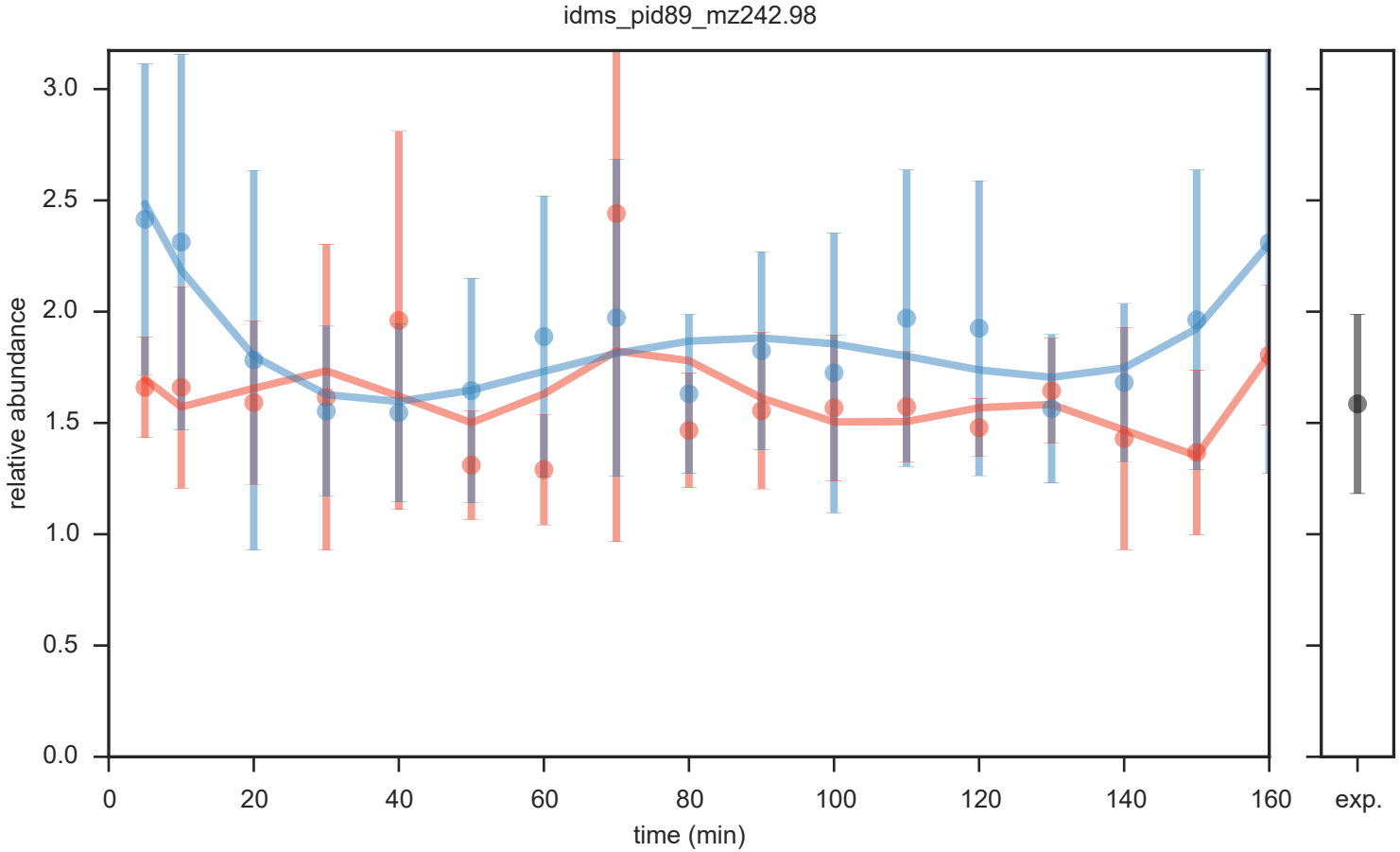
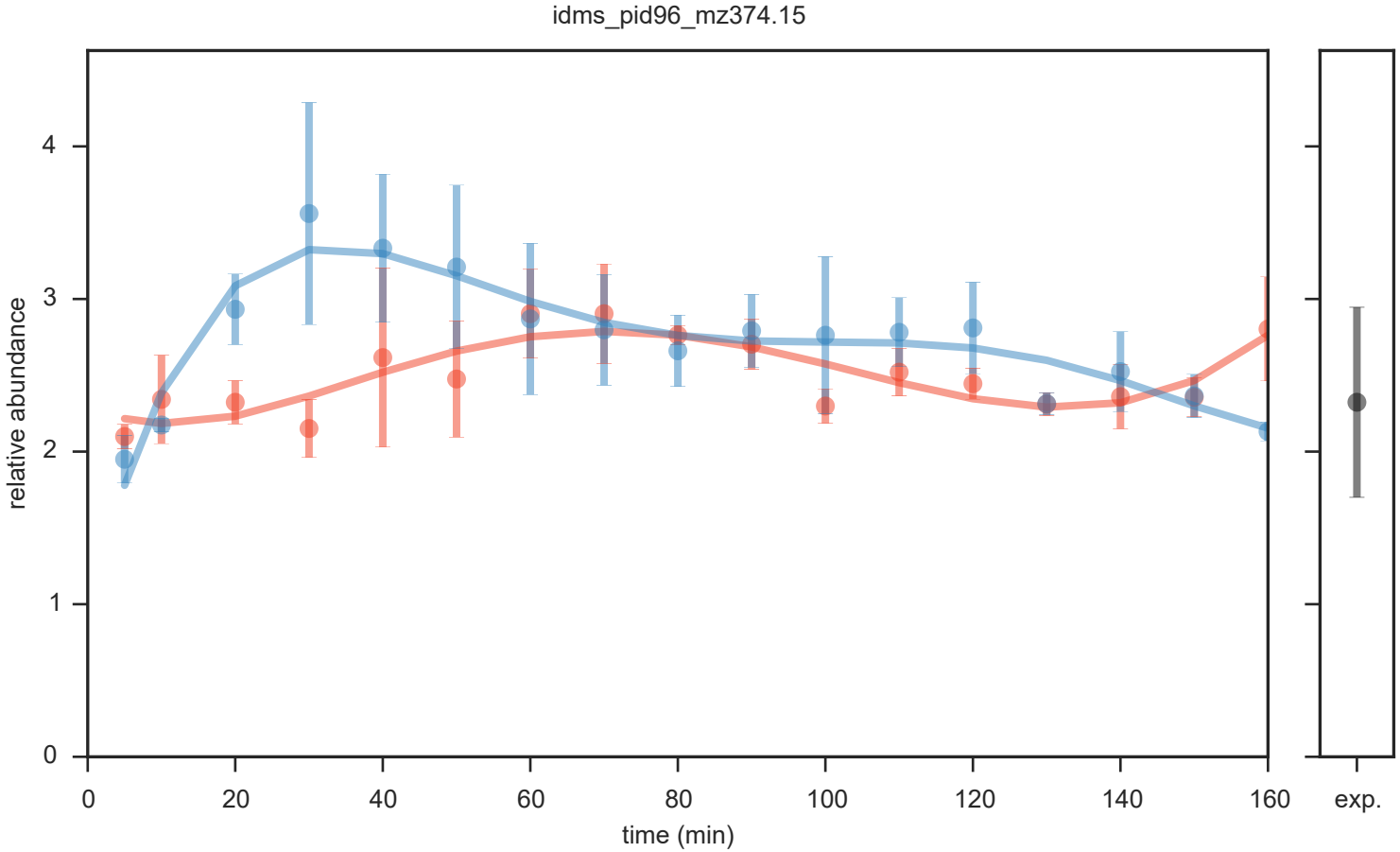
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid85_mz371.53
relative abundance
time (min)
exp.
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
0
20
40
60
80
100
120
140
160


idms_pid89_mz242.98
relative abundance
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid96_mz374.15
relative abundance
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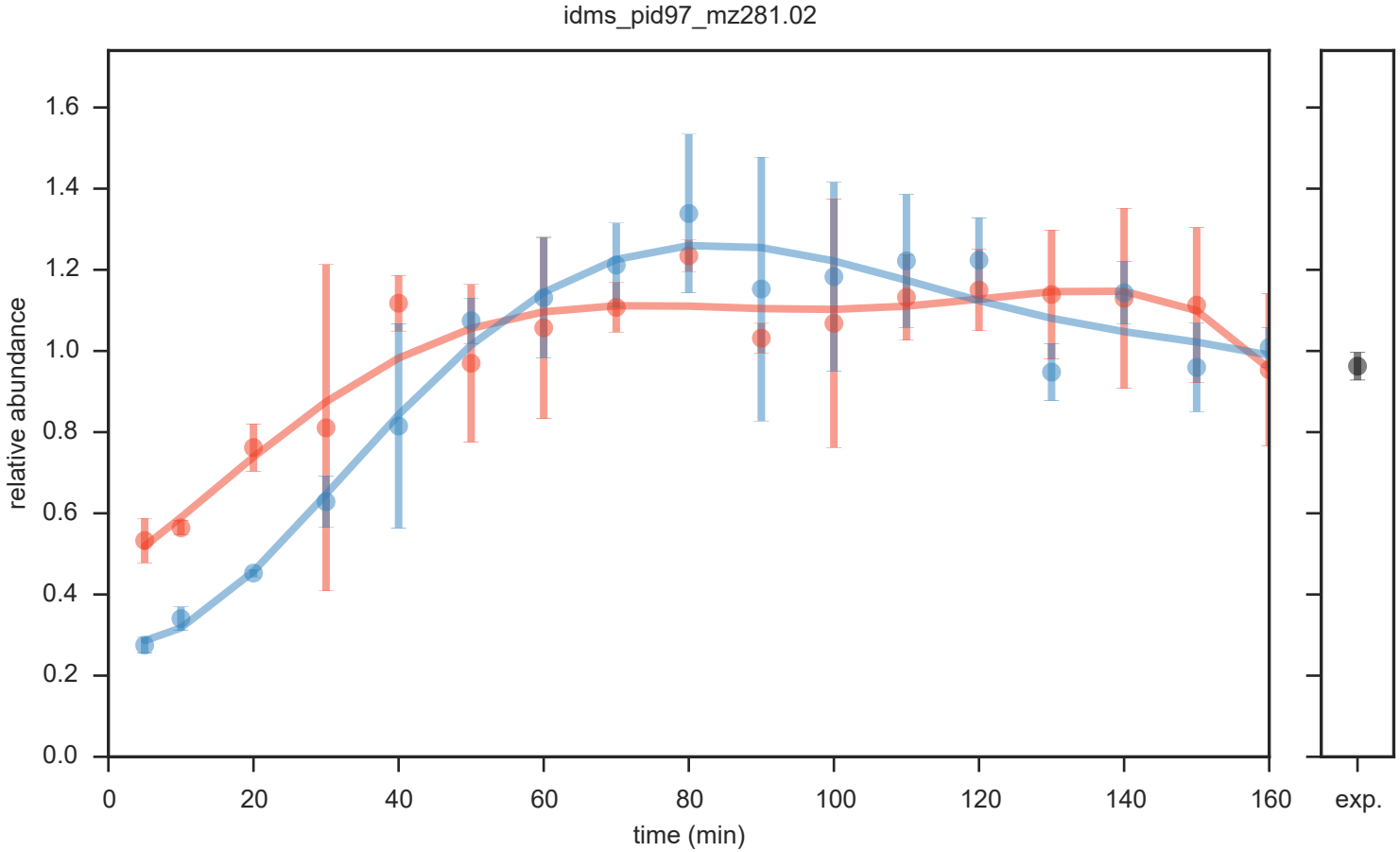
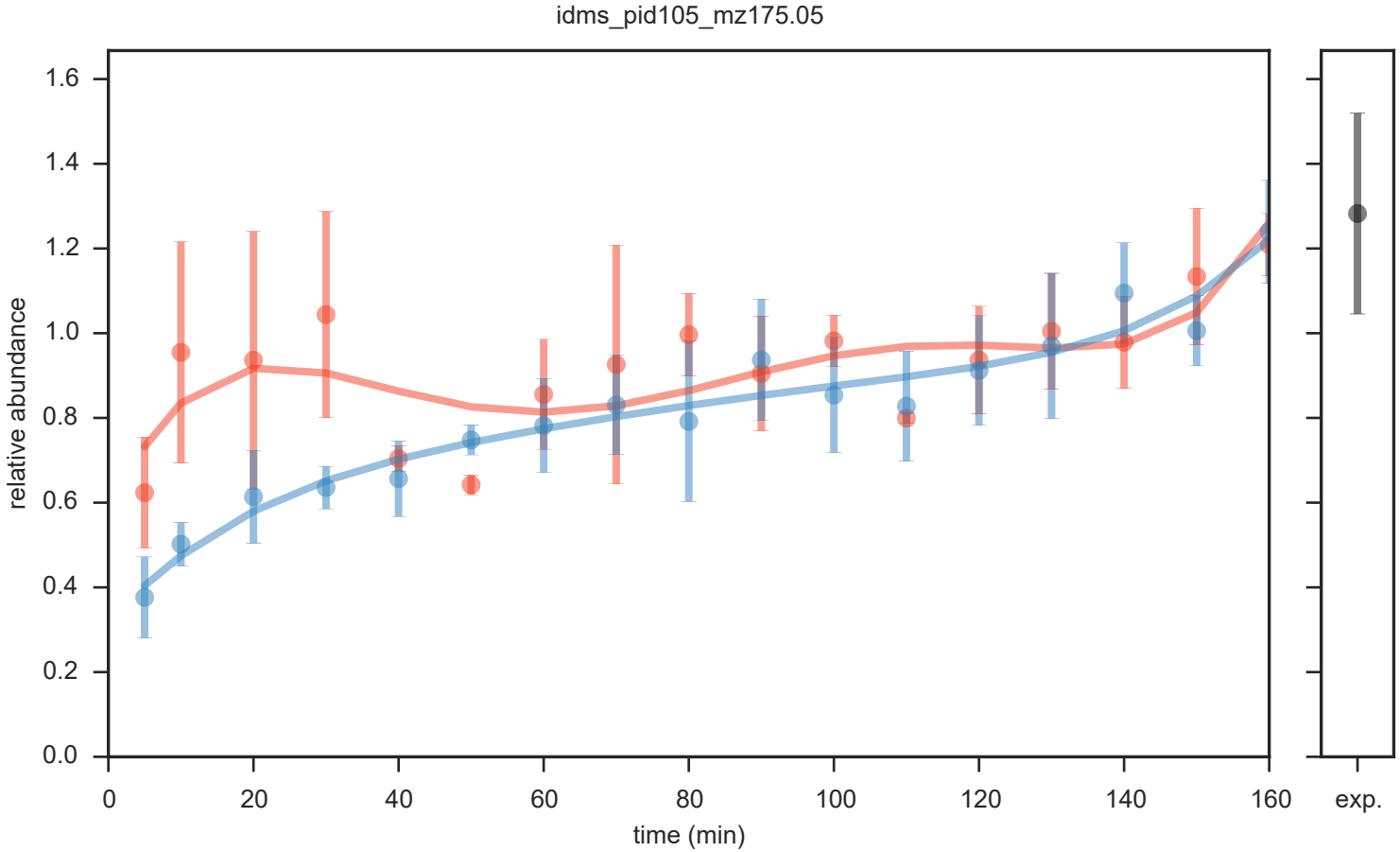
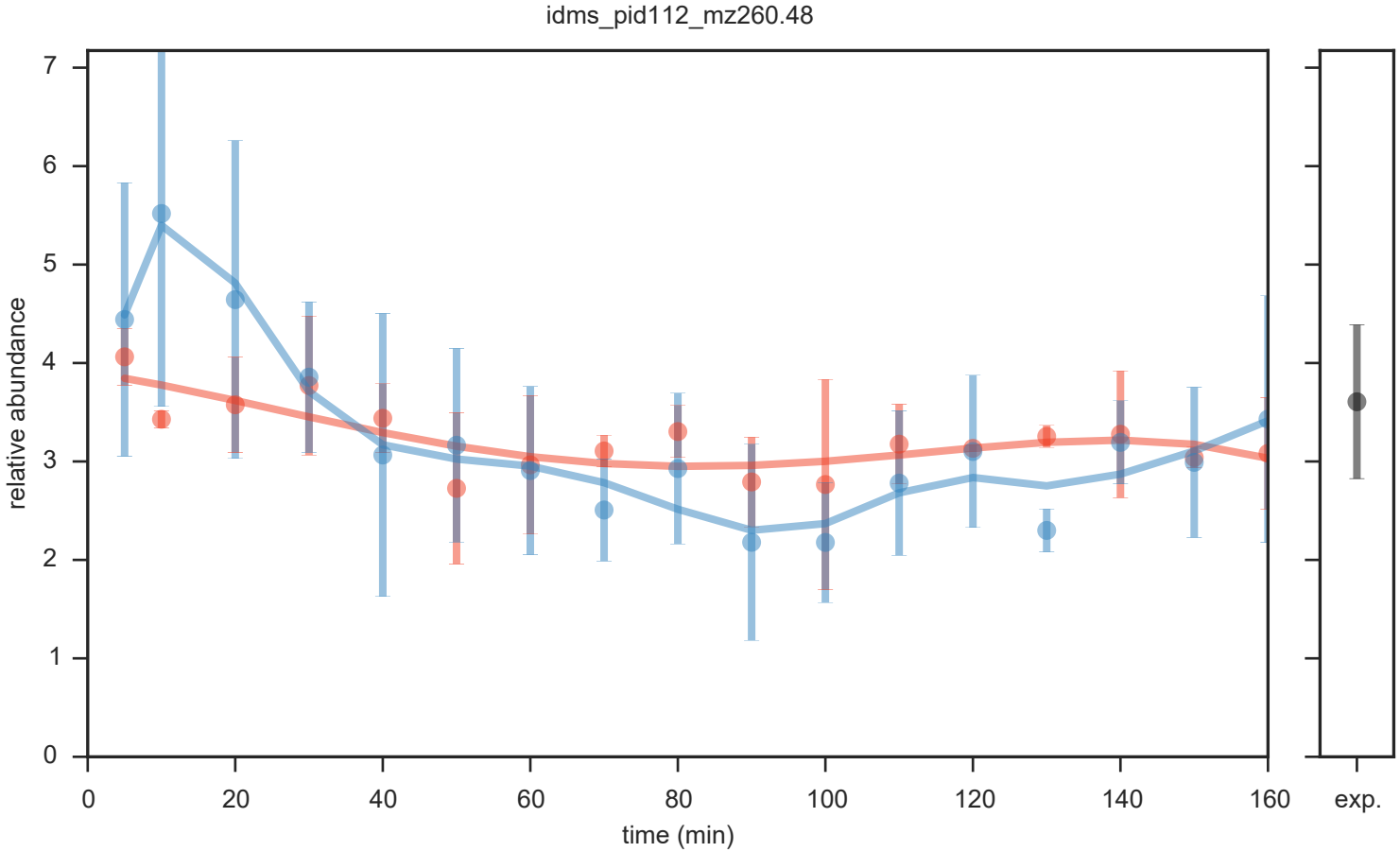
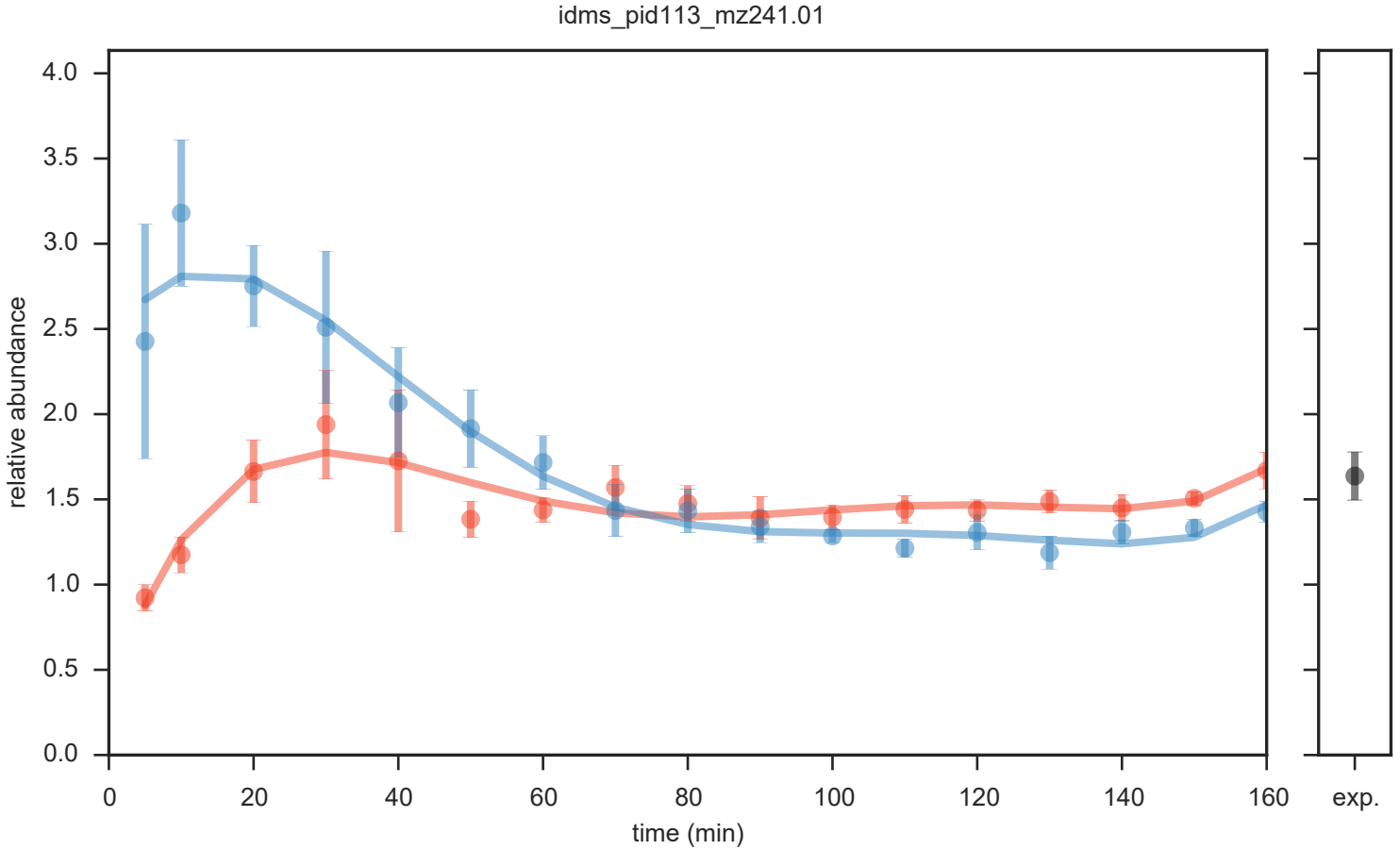
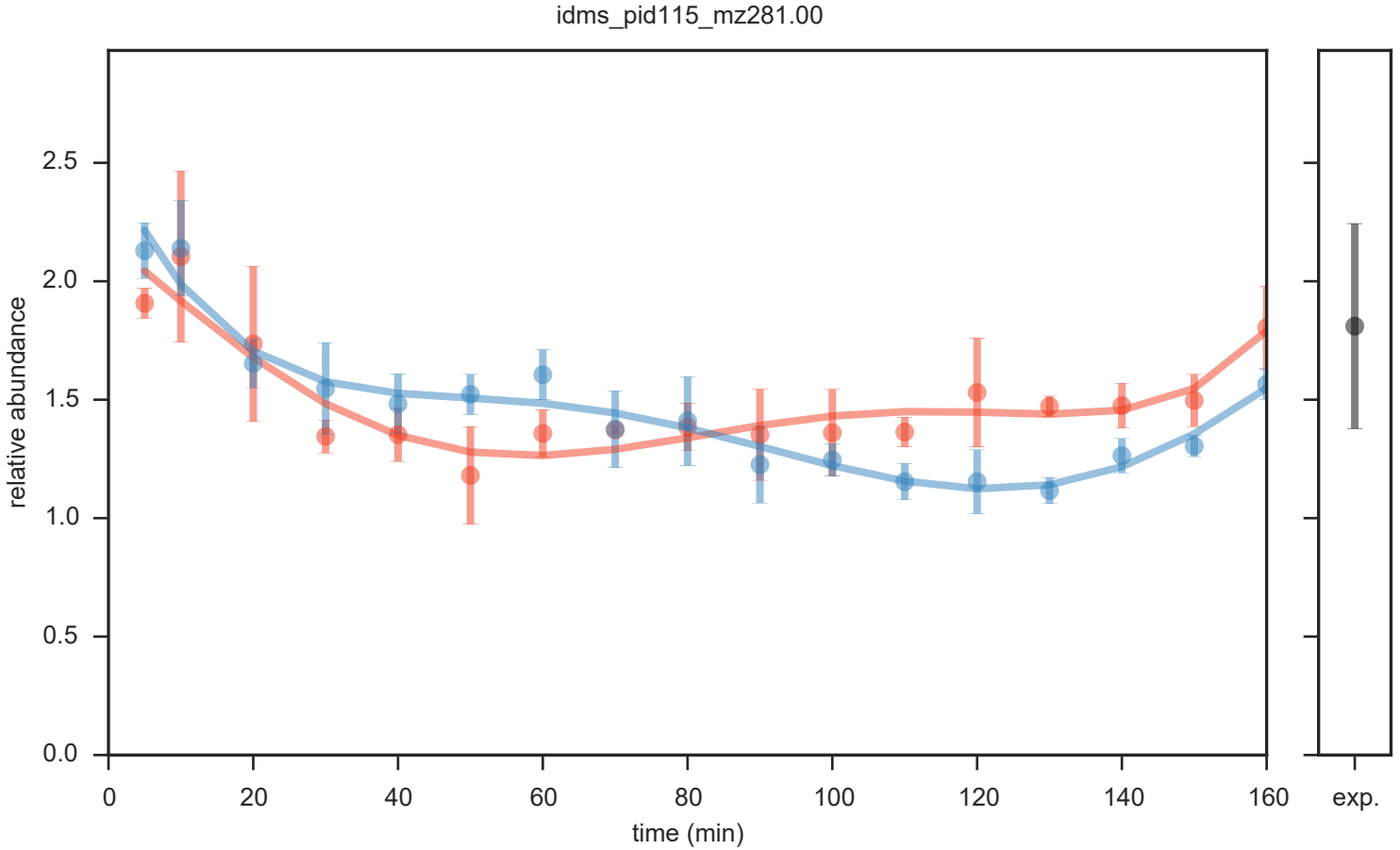
1
2
3
4
0
20
40
60
80
100
120
140
160
time (min)
exp.

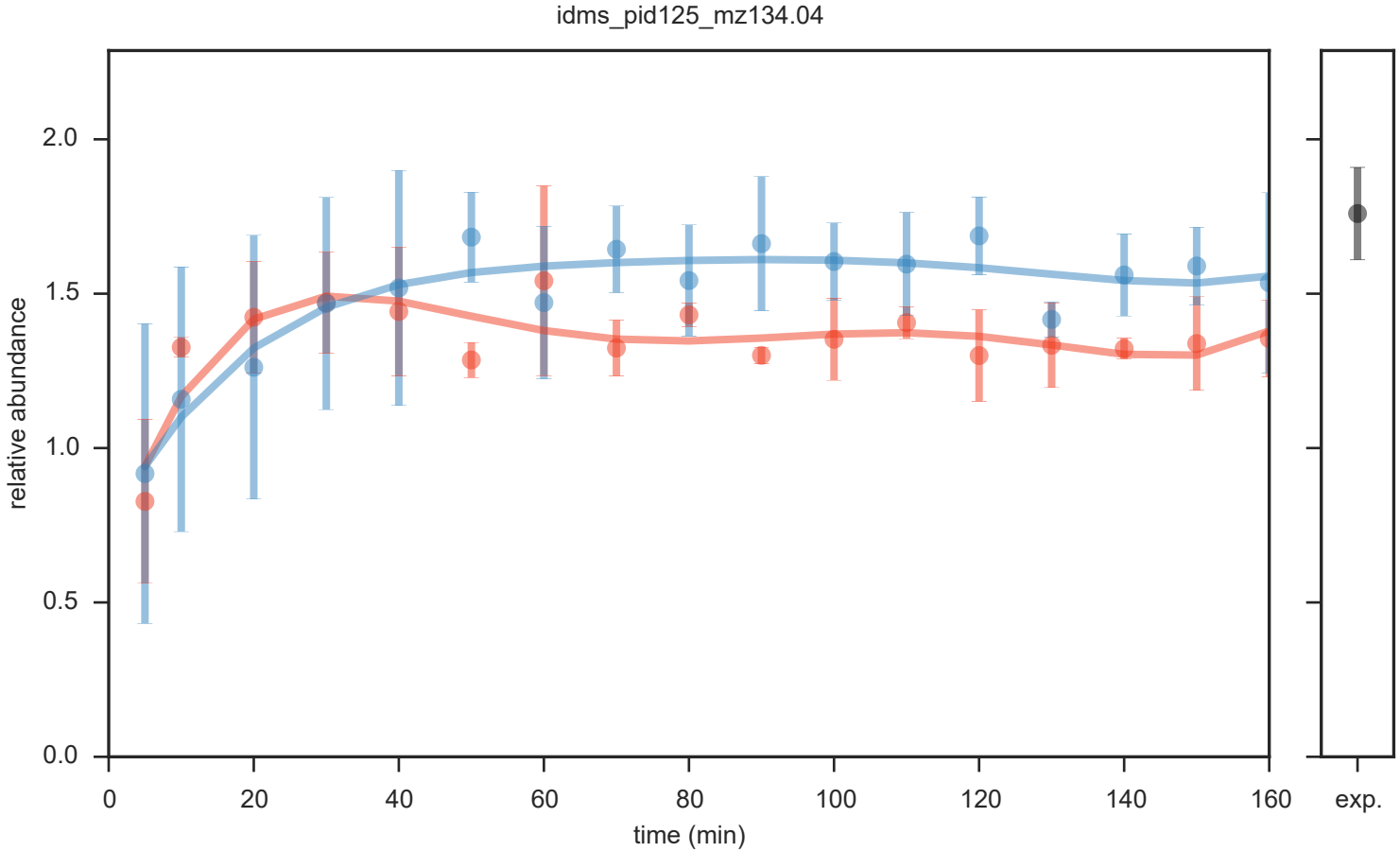

idms_pid97_mz281.02
relative abundance
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
0
20
40
60
80
100
120
140
160
time (min)
exp.

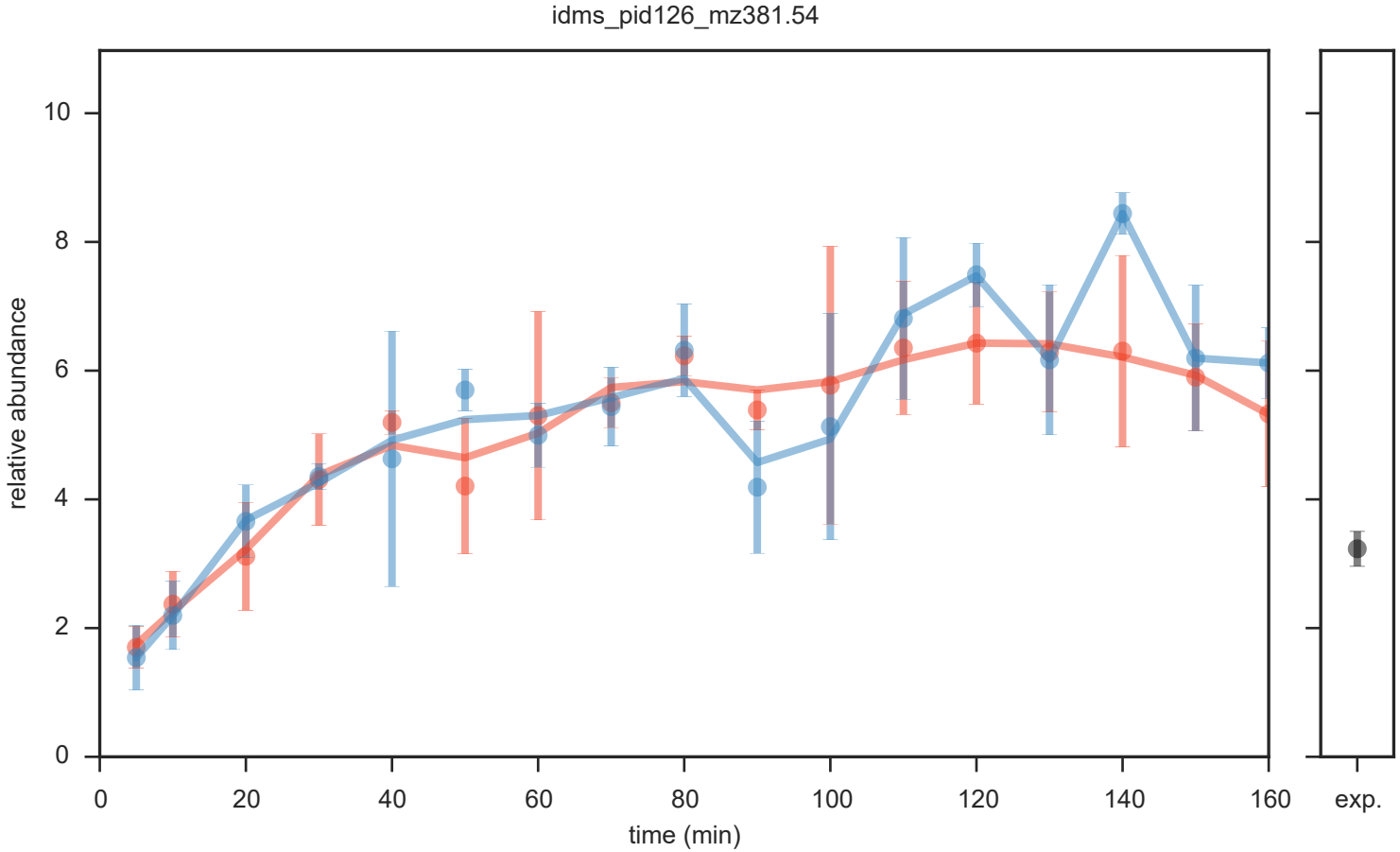

idms_pid105_mz175.05
relative abundance
time (min)
exp.
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
0
20
40
60
80
100
120
140
160

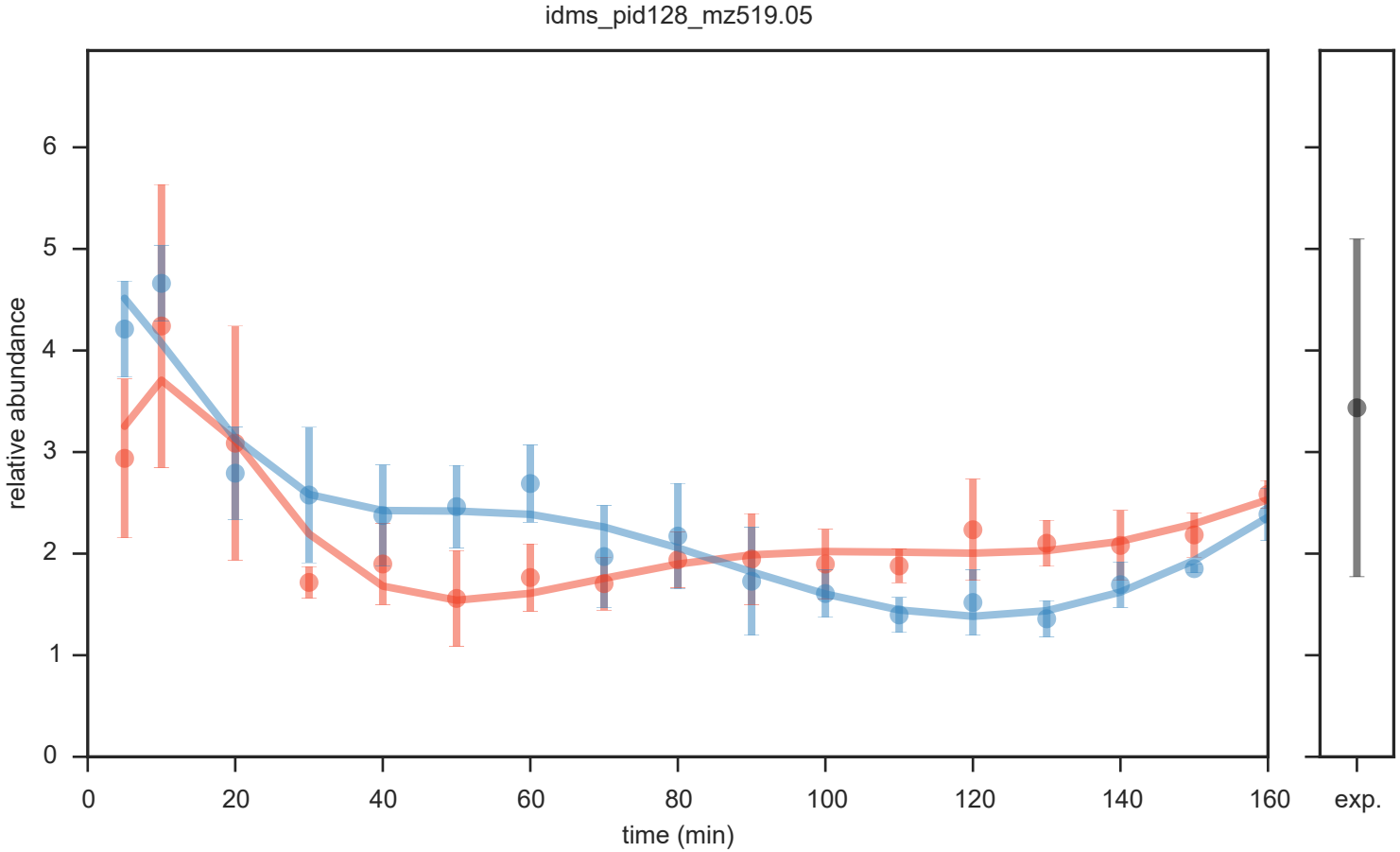

idms_pid112_mz260.48
relative abundance
0
1
2
3
4
5
6
7
0
20
40
60
80
100
120
140
160
time (min)
exp.

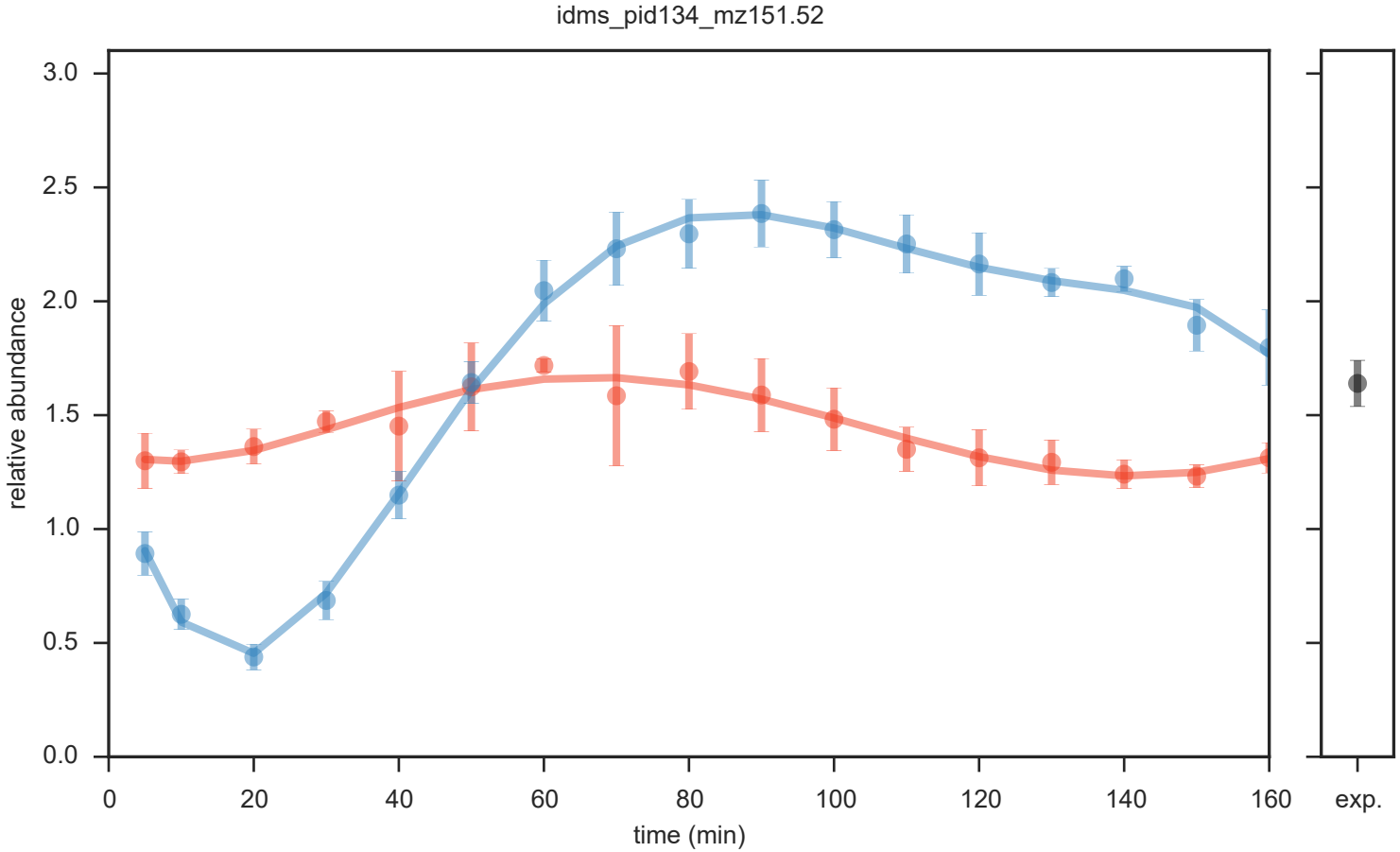

idms_pid113_mz241.01
relative abundance
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

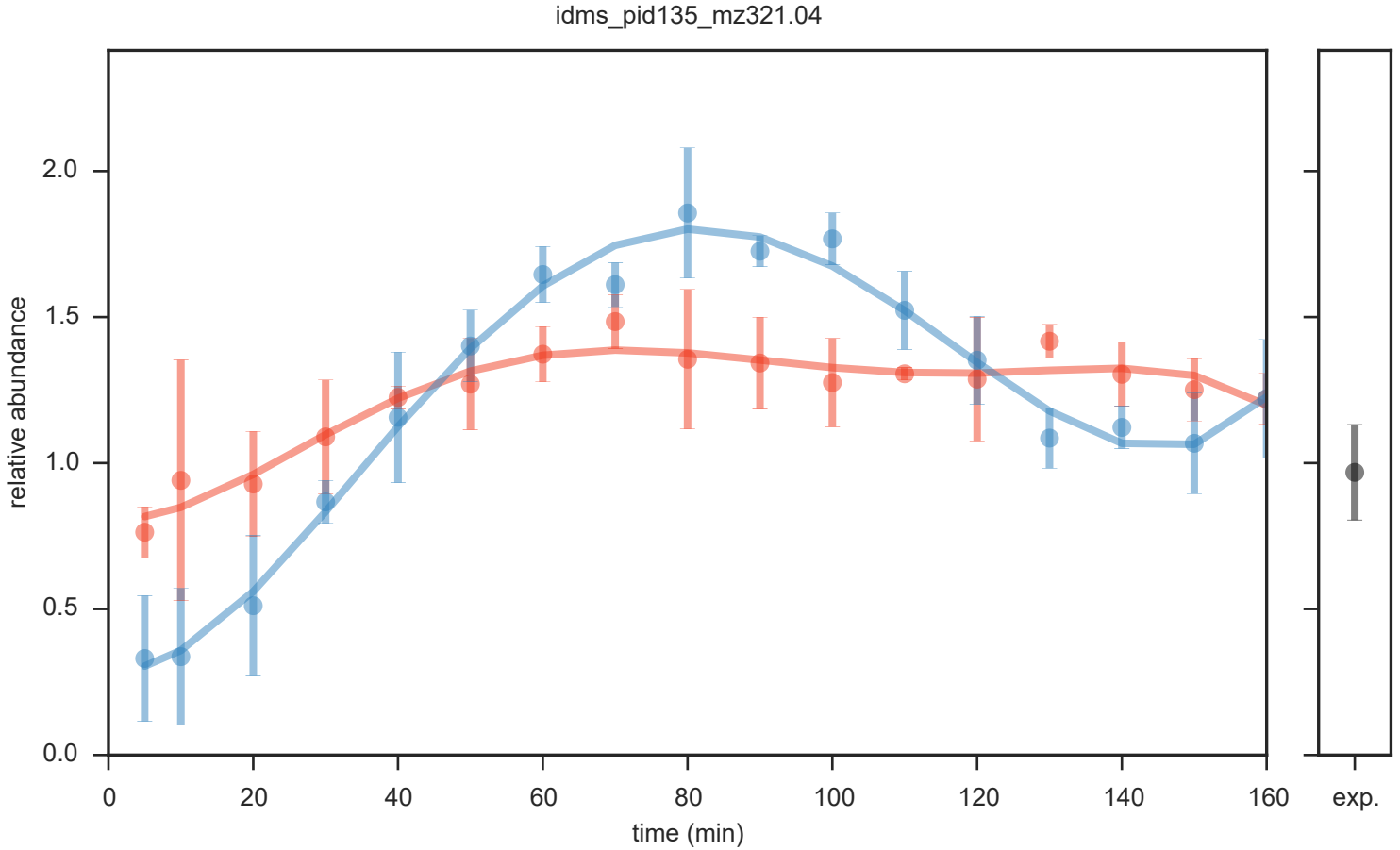

idms_pid115_mz281.00
relative abundance
0.0
0.5
1.0
1.5
2.0
2.5
0
20
40
60
80
100
120
140
160
time (min)
exp.

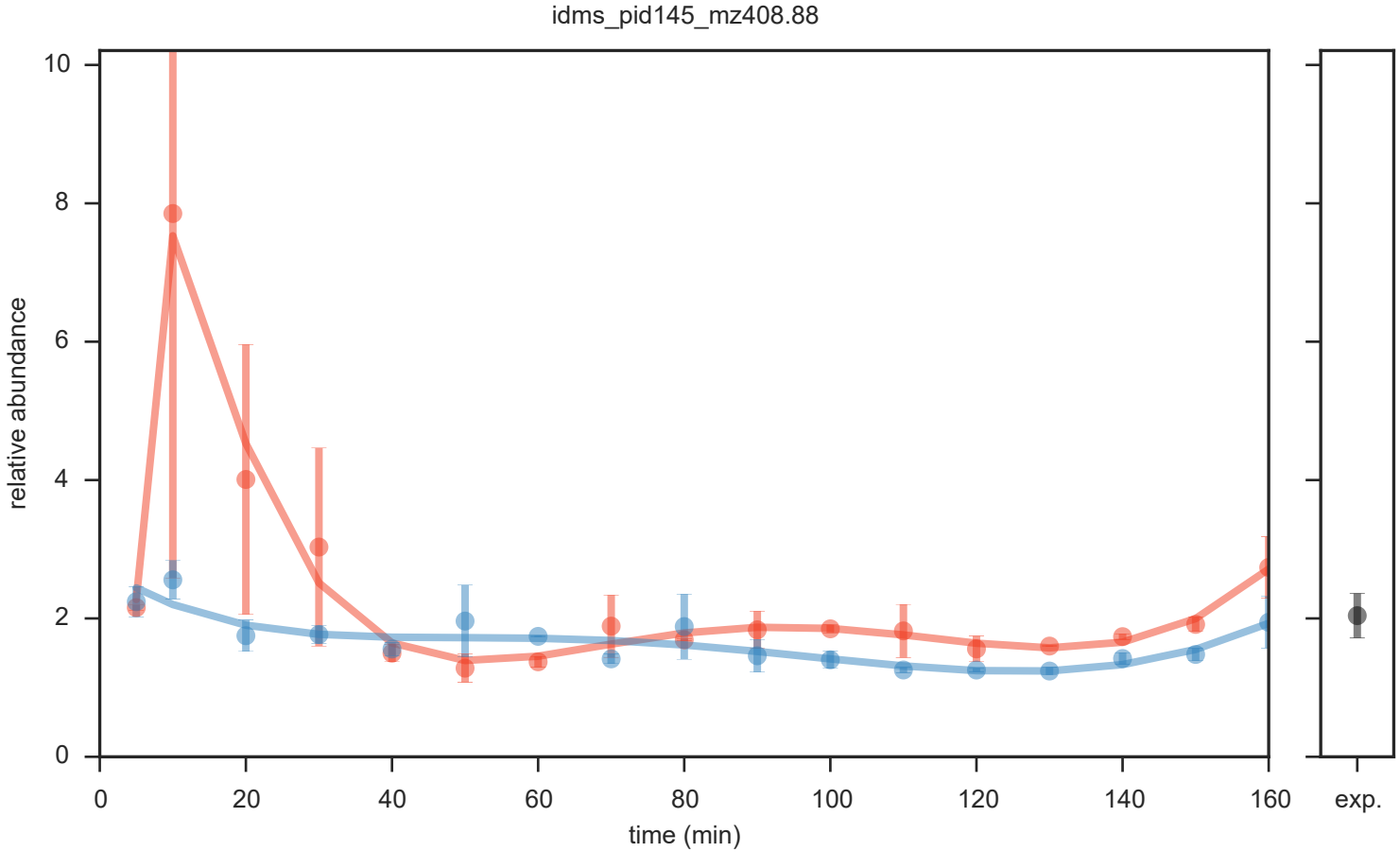

idms_pid125_mz134.04
relative abundance
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

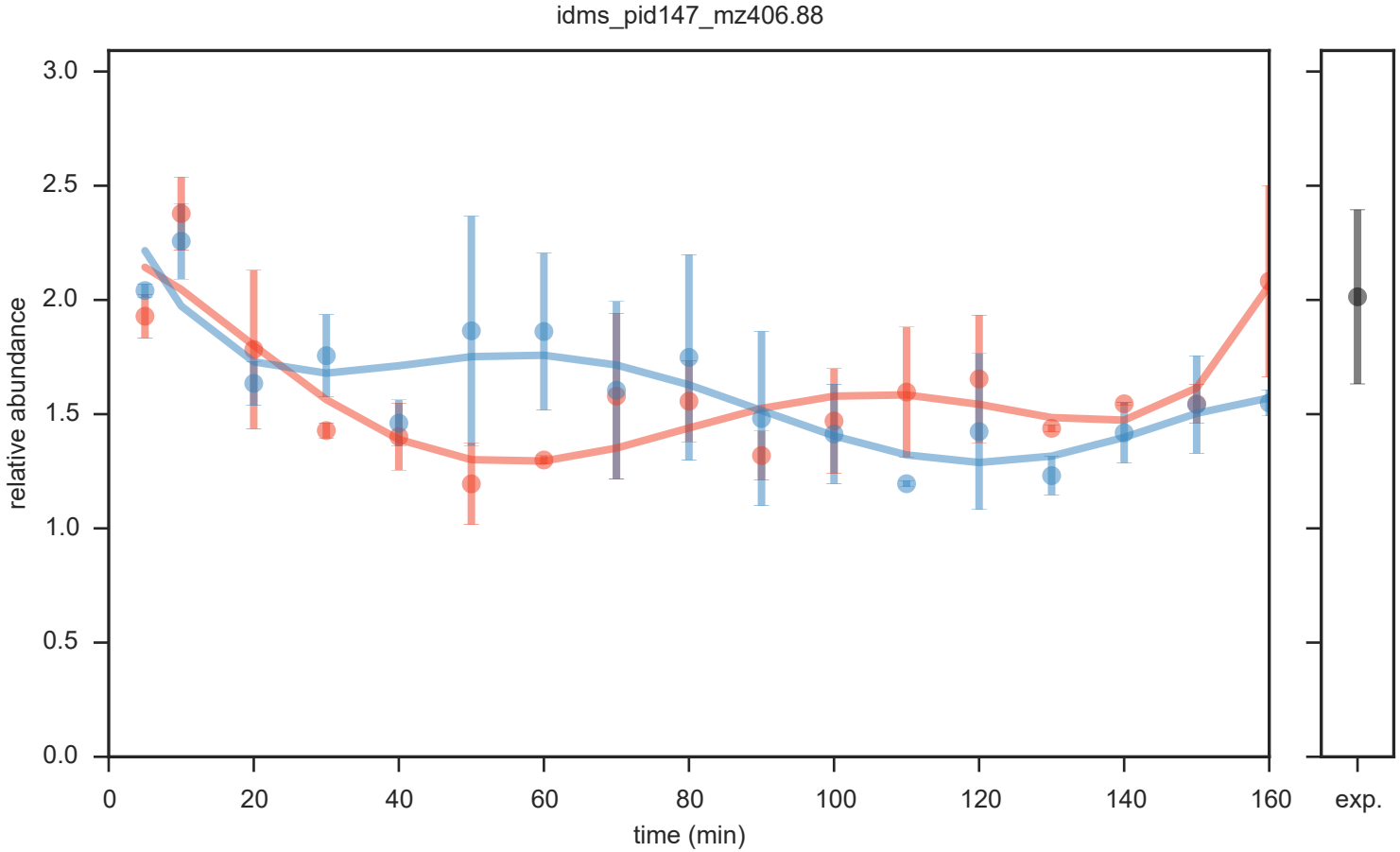

idms_pid126_mz381.54
relative abundance
0
2
4
6
8
10
0
20
40
60
80
100
120
140
160
time (min)
exp.

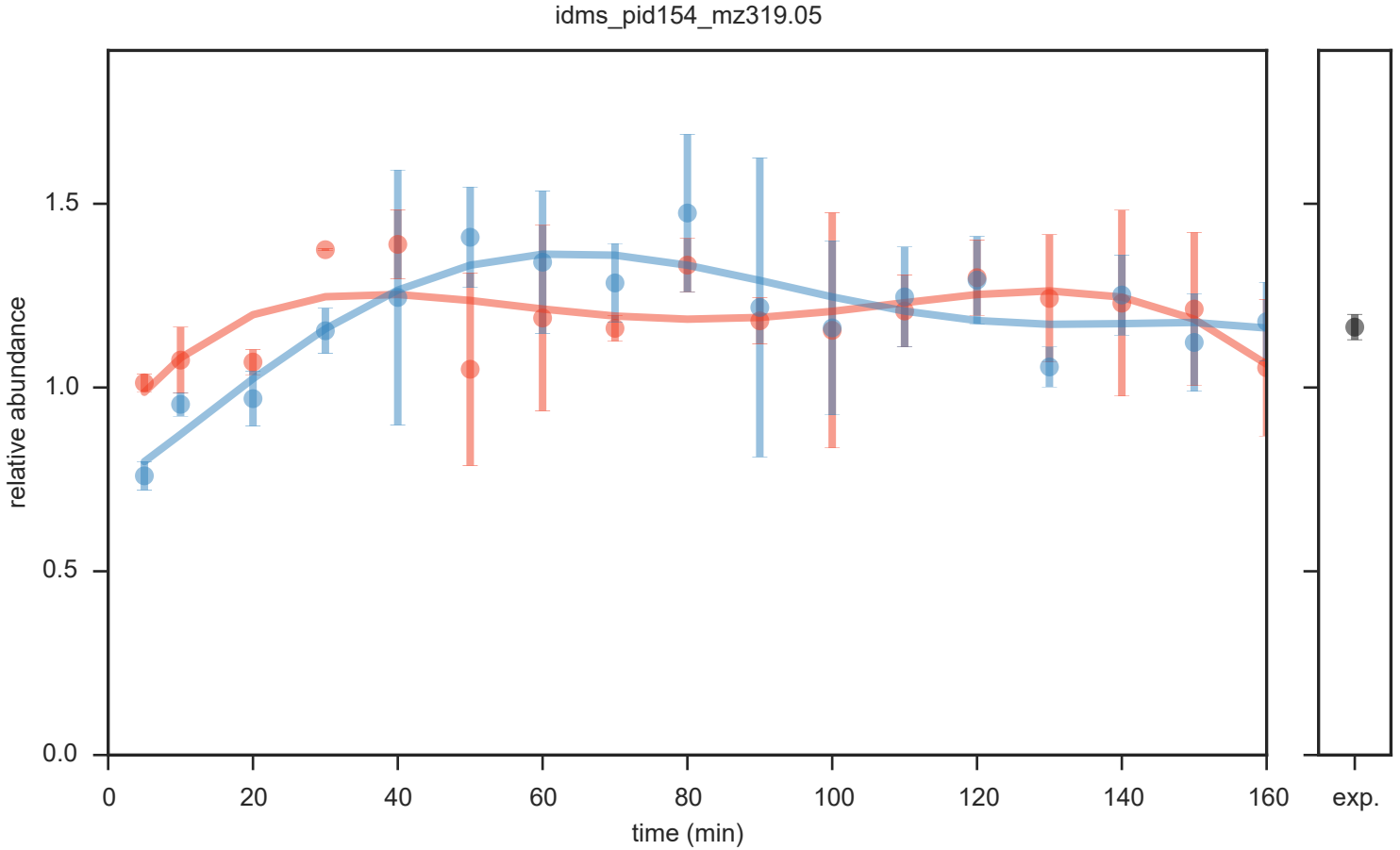

idms_pid128_mz519.05
relative abundance
0
1
2
3
4
5
6
0
20
40
60
80
100
120
140
160
time (min)
exp.

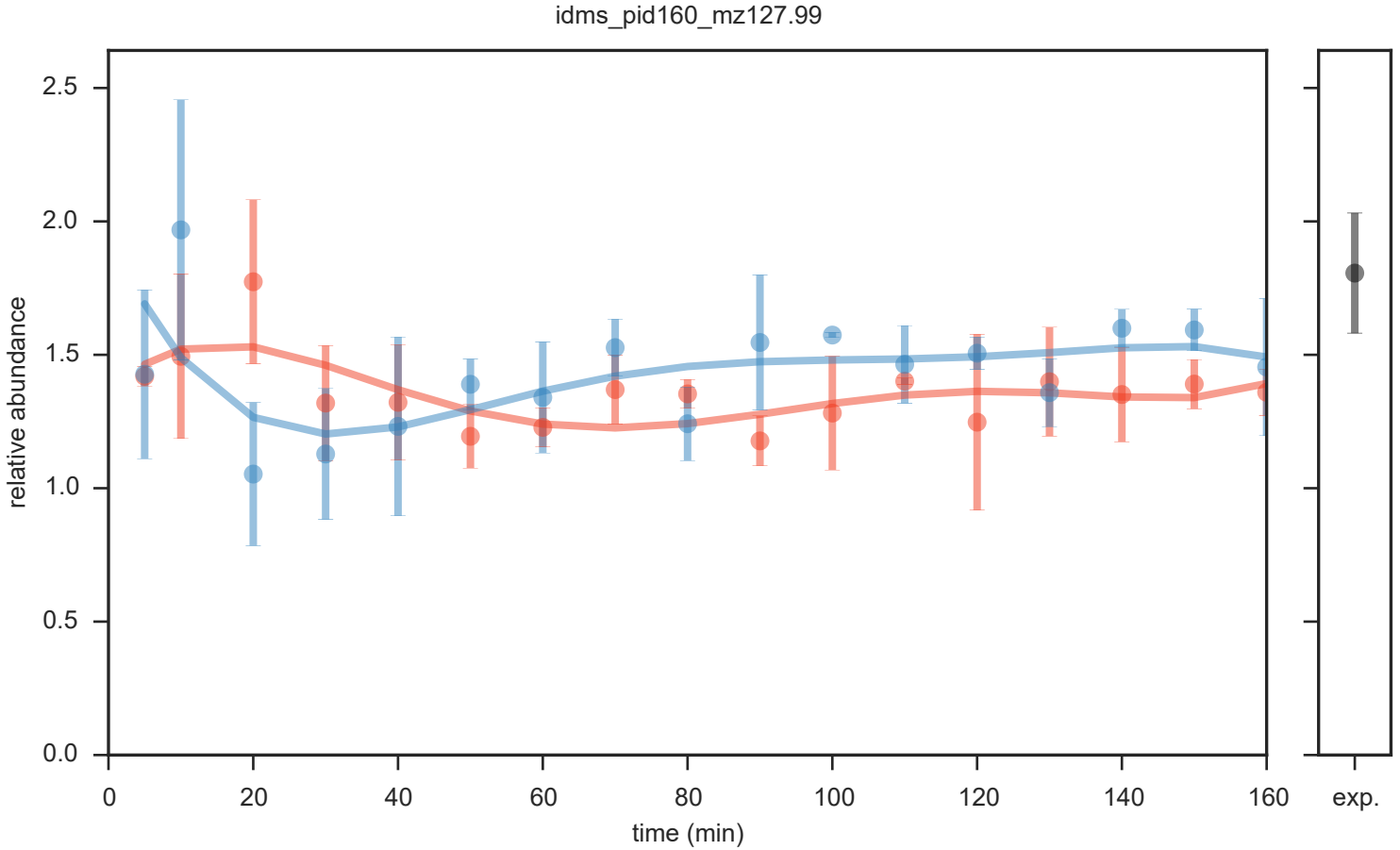

idms_pid134_mz151.52
relative abundance
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

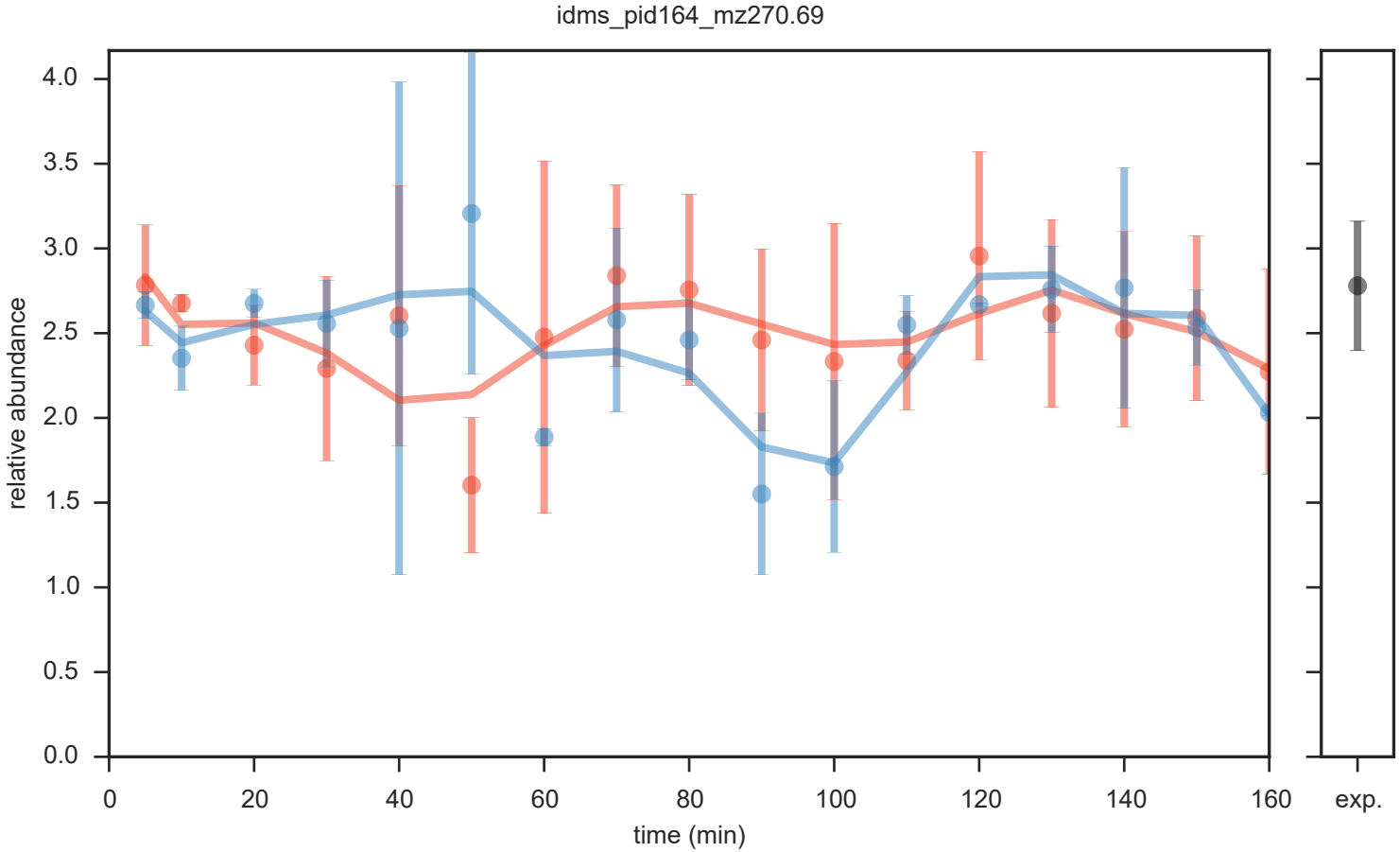

idms_pid135_mz321.04
relative abundance
0.0
0.5
1.0
1.5
2.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

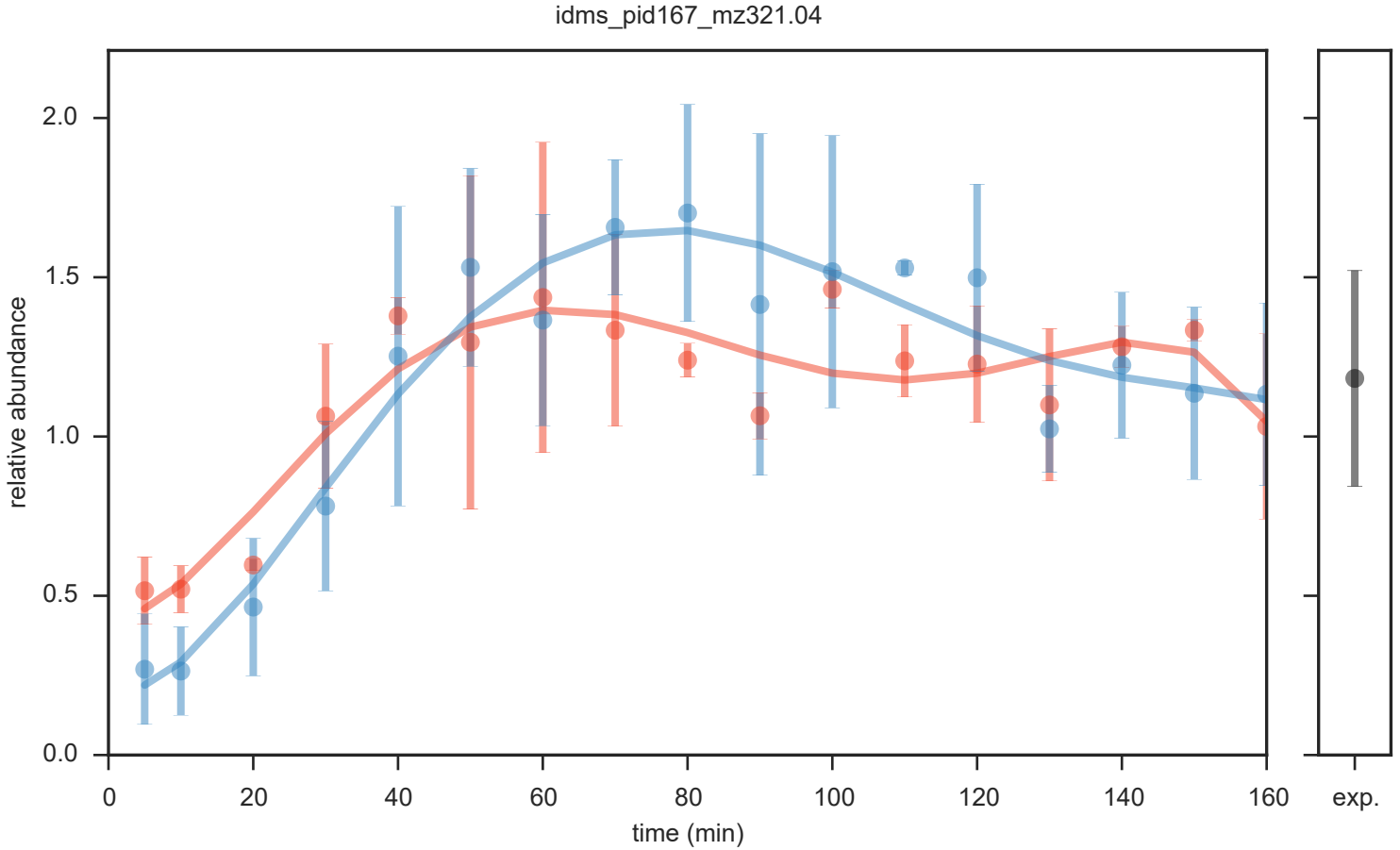

idms_pid145_mz408.88
relative abundance
time (min)
exp.
0
2
4
6
8
10
0
20
40
60
80
100
120
140
160

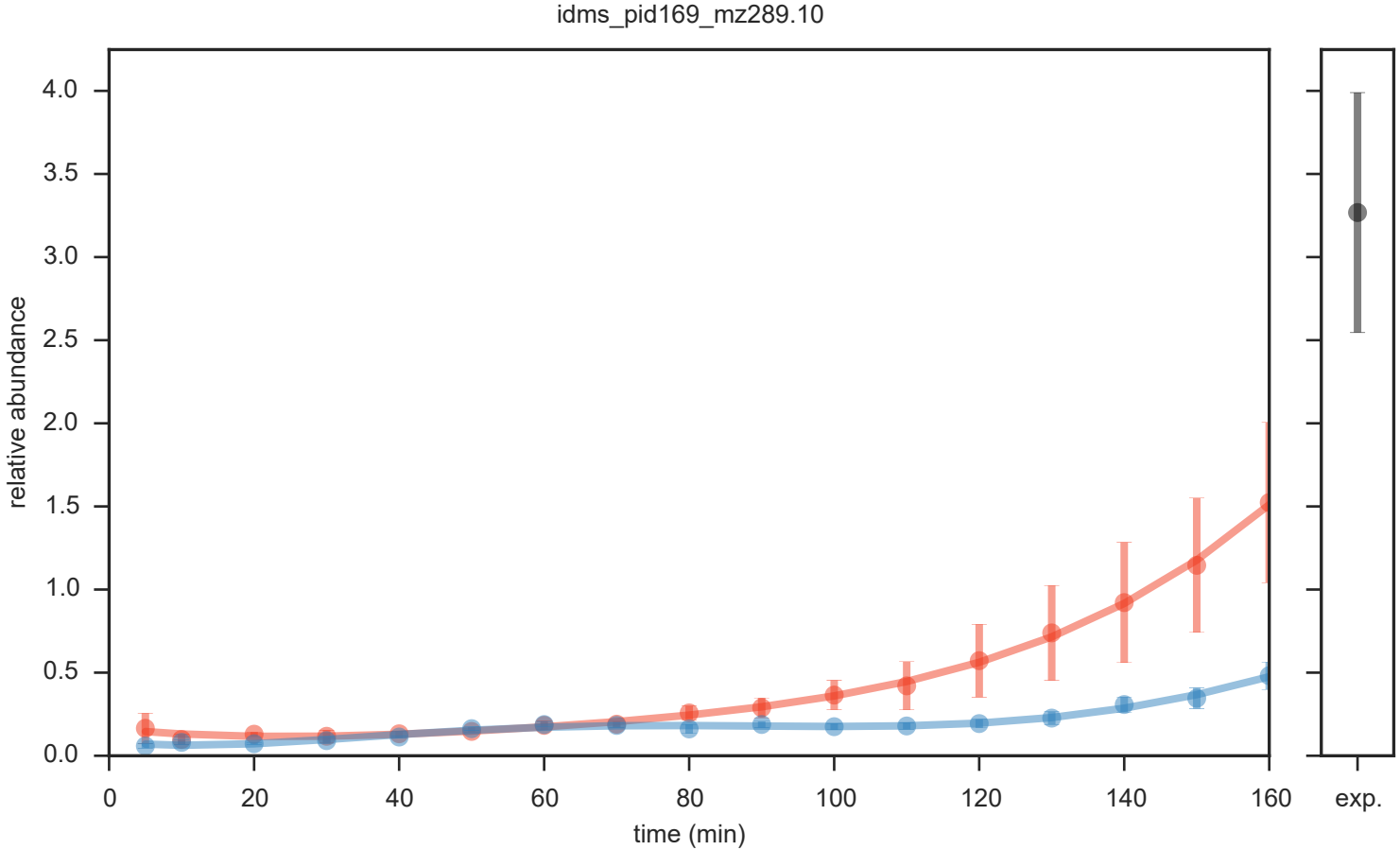

idms_pid147_mz406.88
relative abundance
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

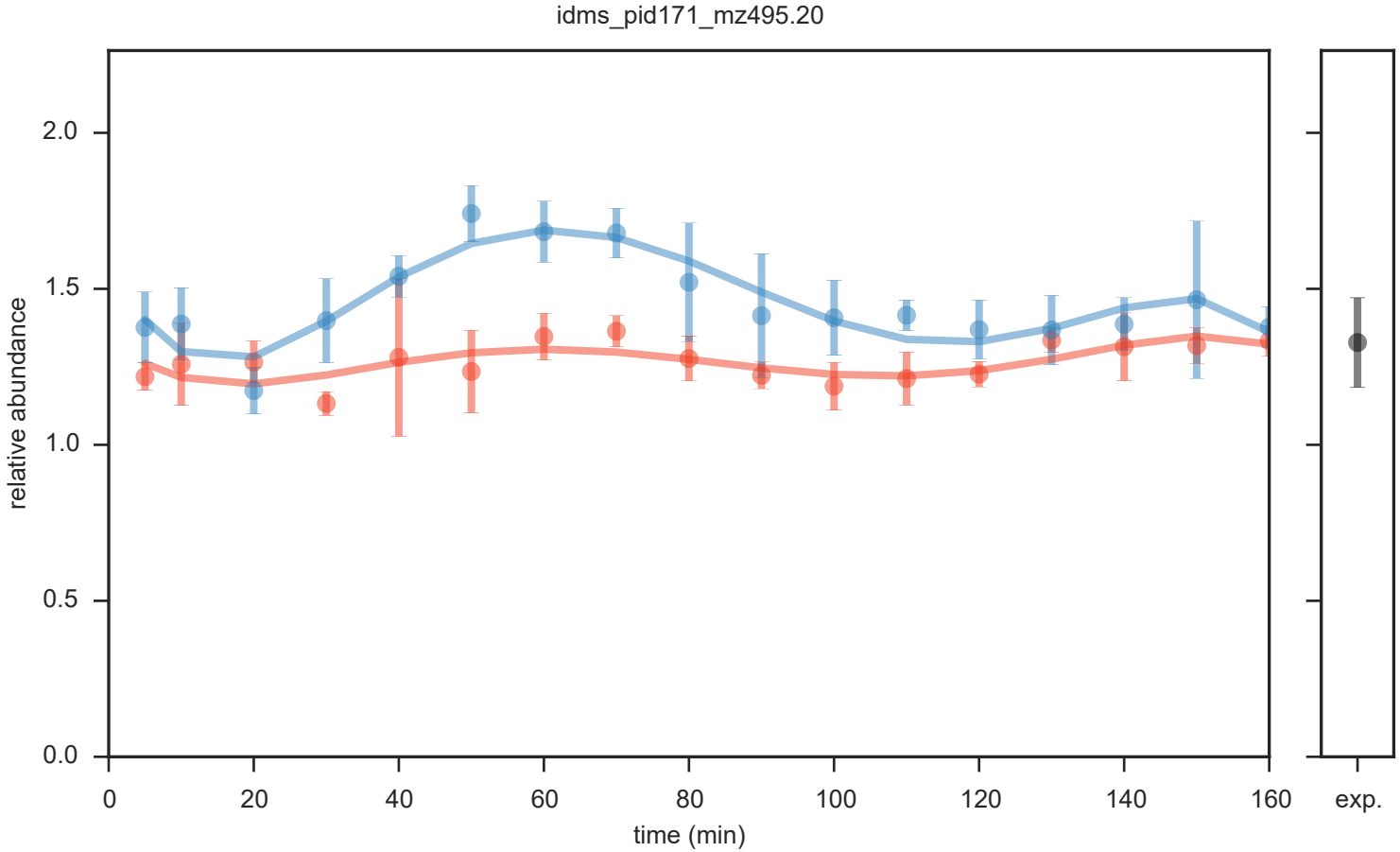

idms_pid154_mz319.05
relative abundance
0.0
0.5
1.0
1.5
0
20
40
60
80
100
120
140
160
time (min)
exp.

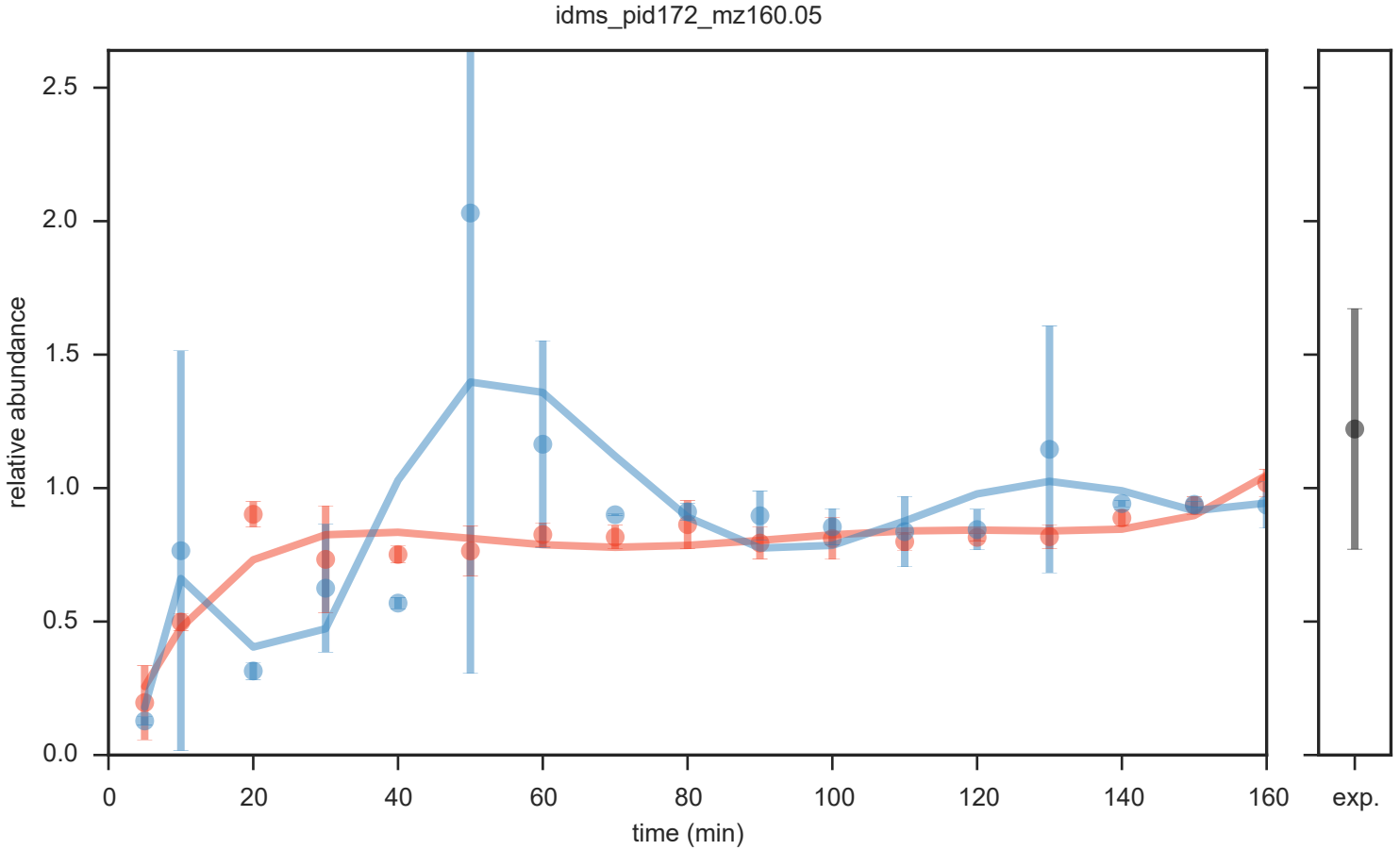

idms_pid160_mz127.99
relative abundance
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

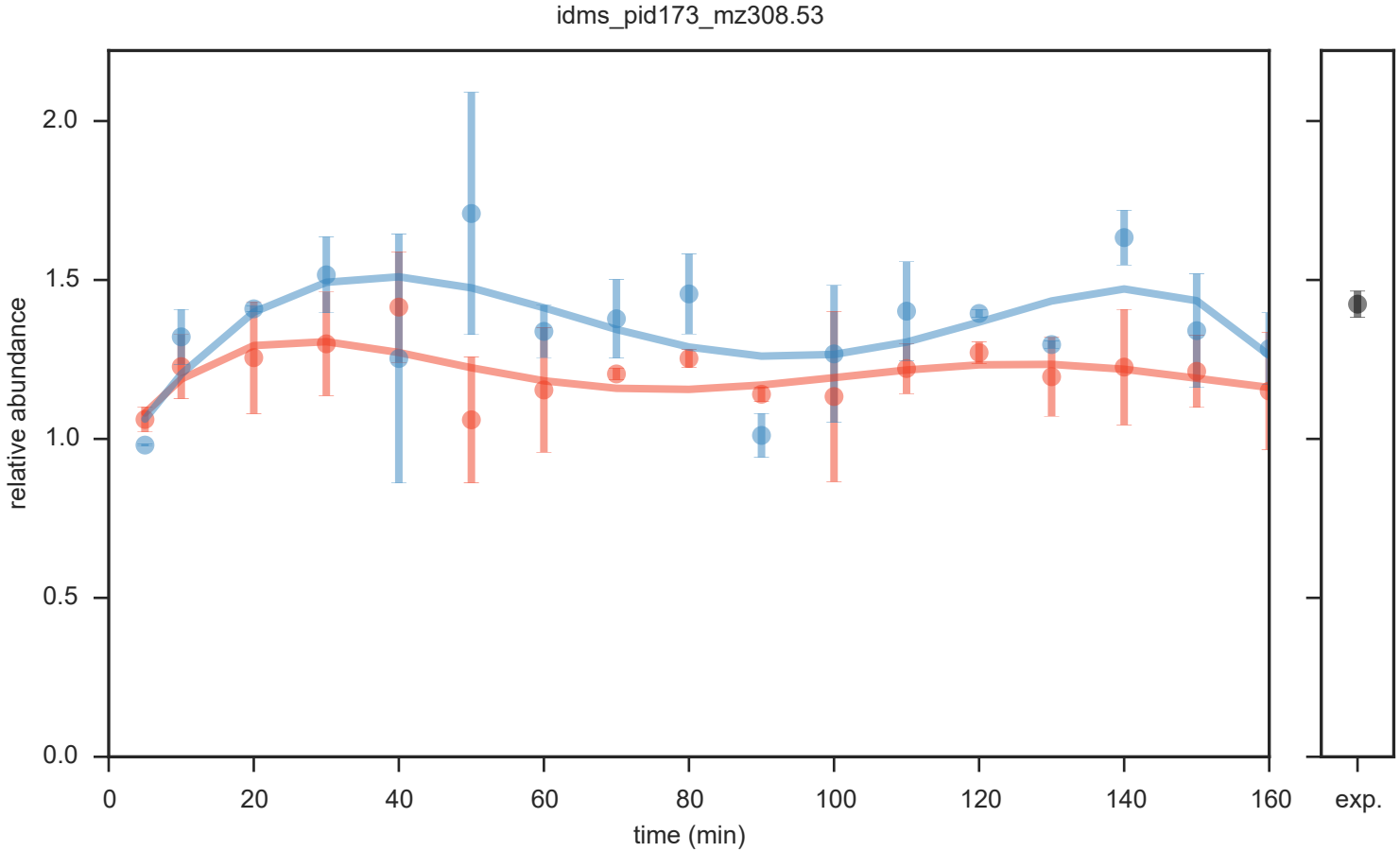

idms_pid164_mz270.69
relative abundance
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

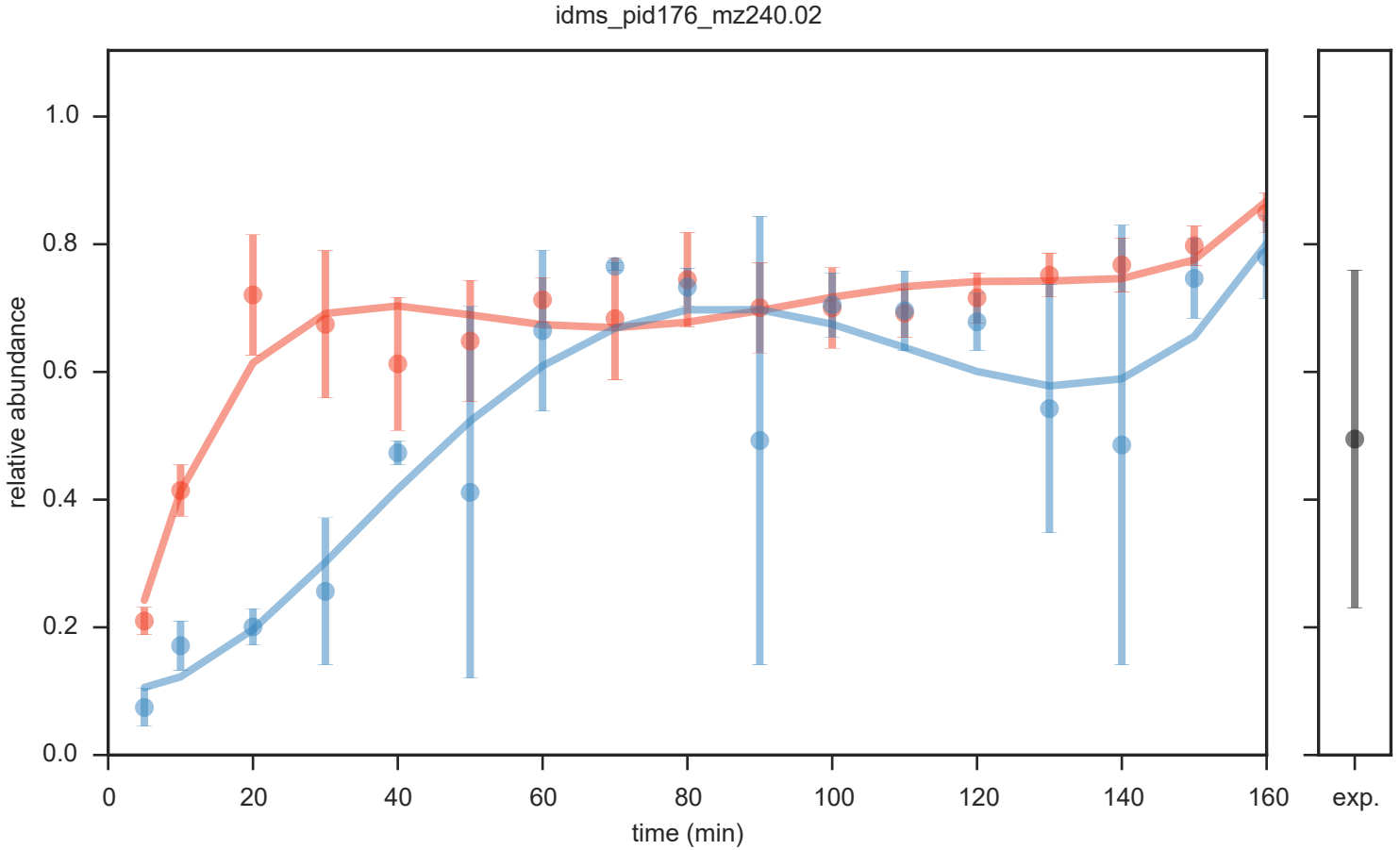

idms_pid167_mz321.04
relative abundance
0.0
0.5
1.0
1.5
2.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

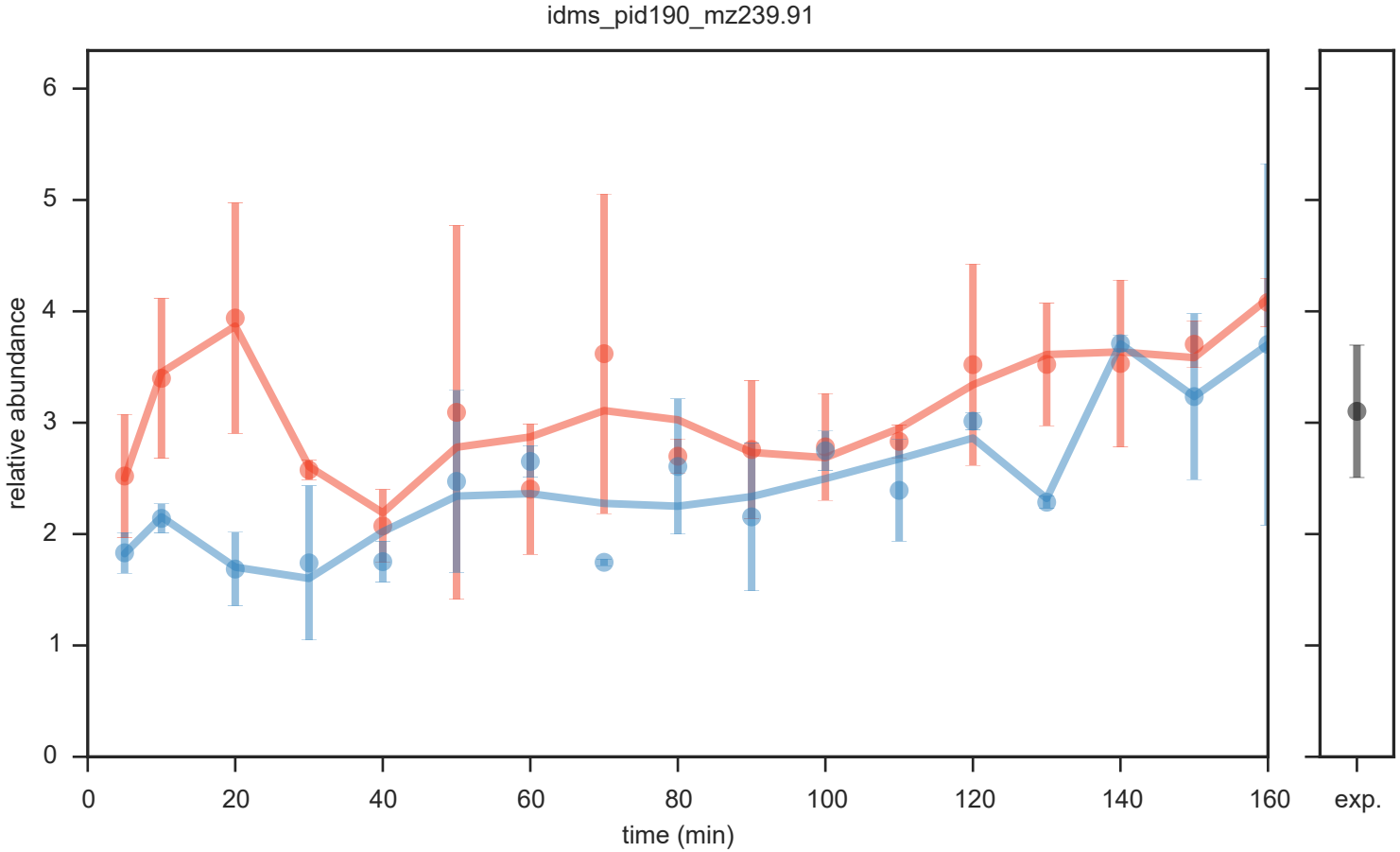

idms_pid169_mz289.10
relative abundance
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

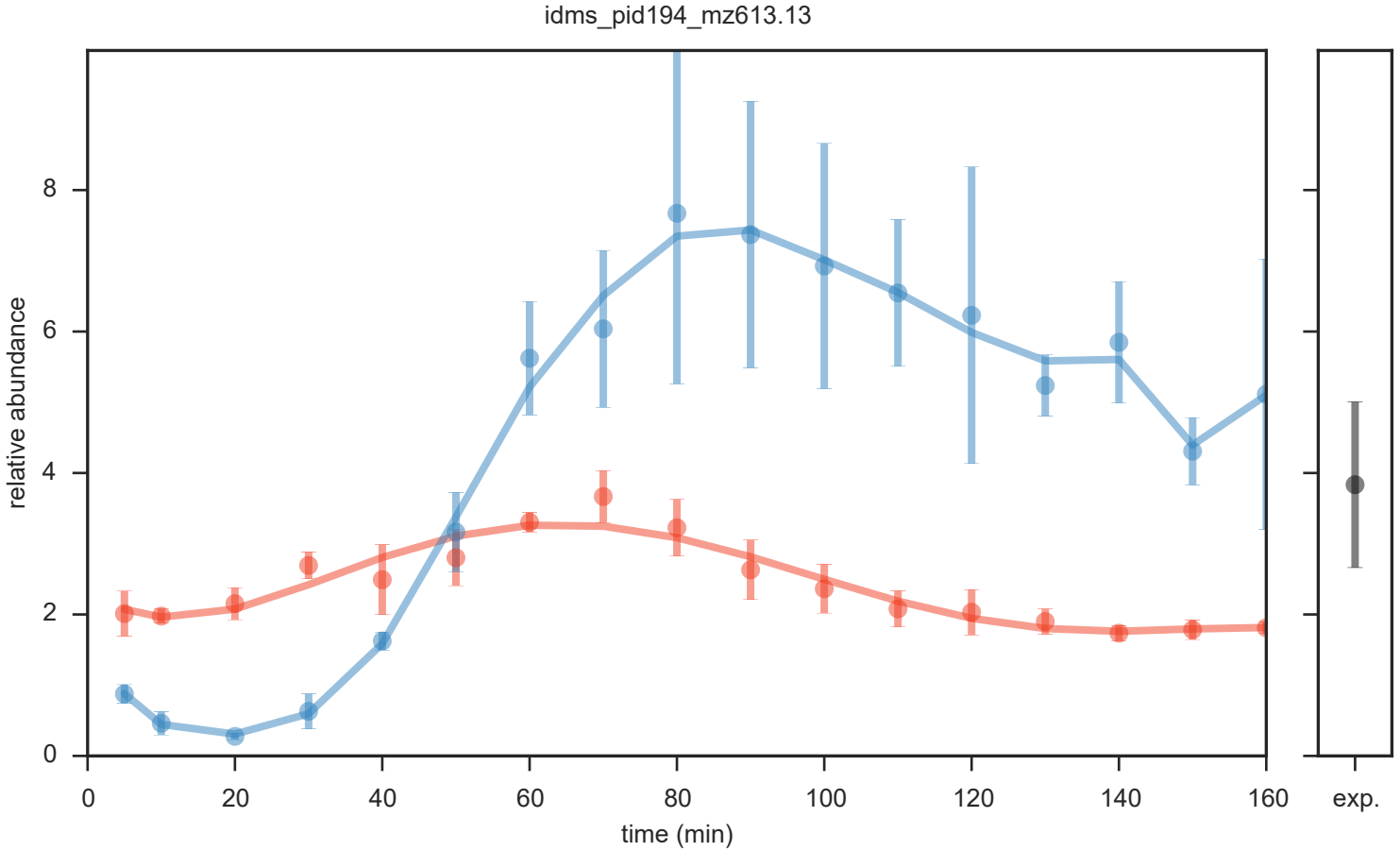

idms_pid171_mz495.20
relative abundance
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

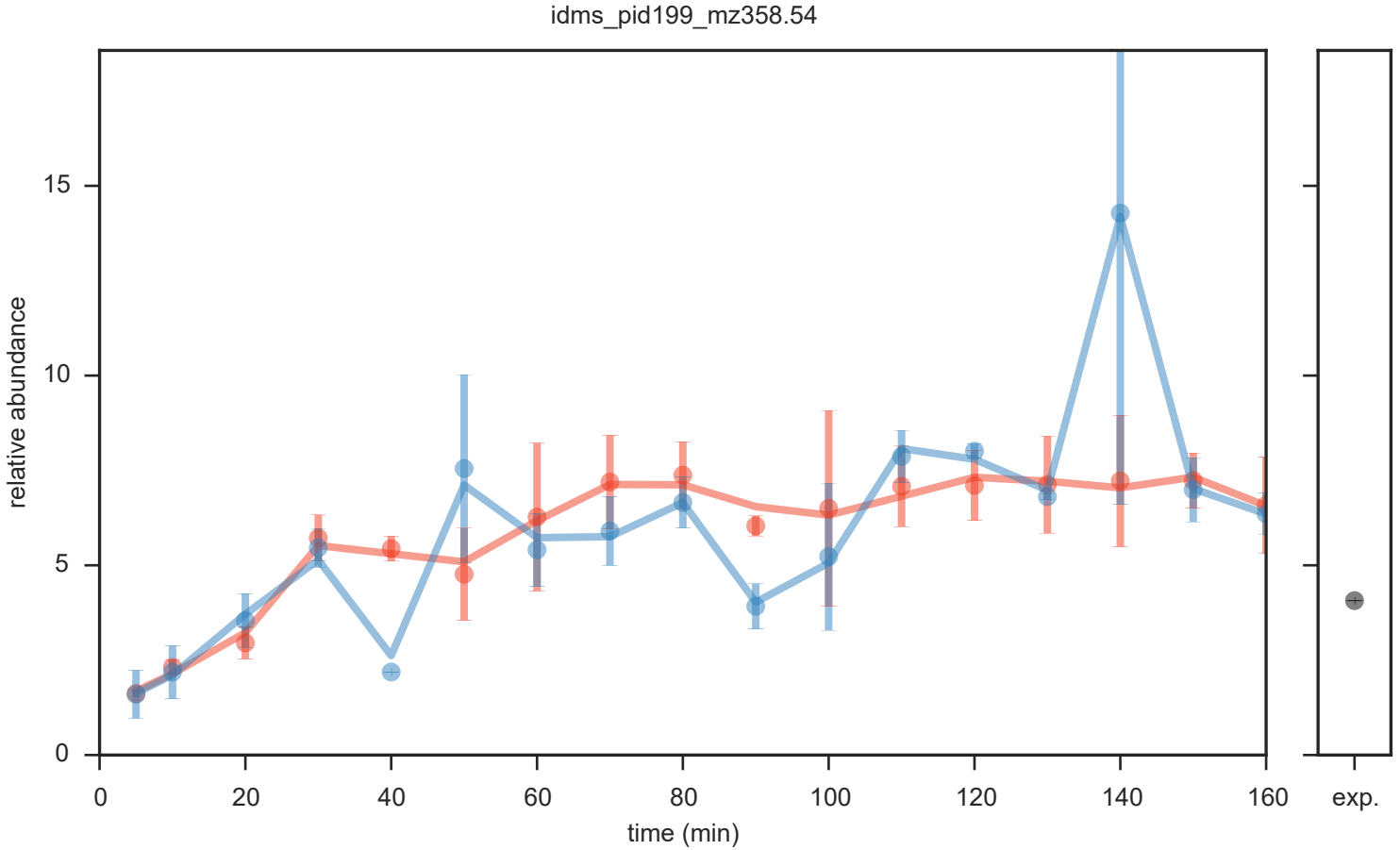

idms_pid172_mz160.05
relative abundance
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

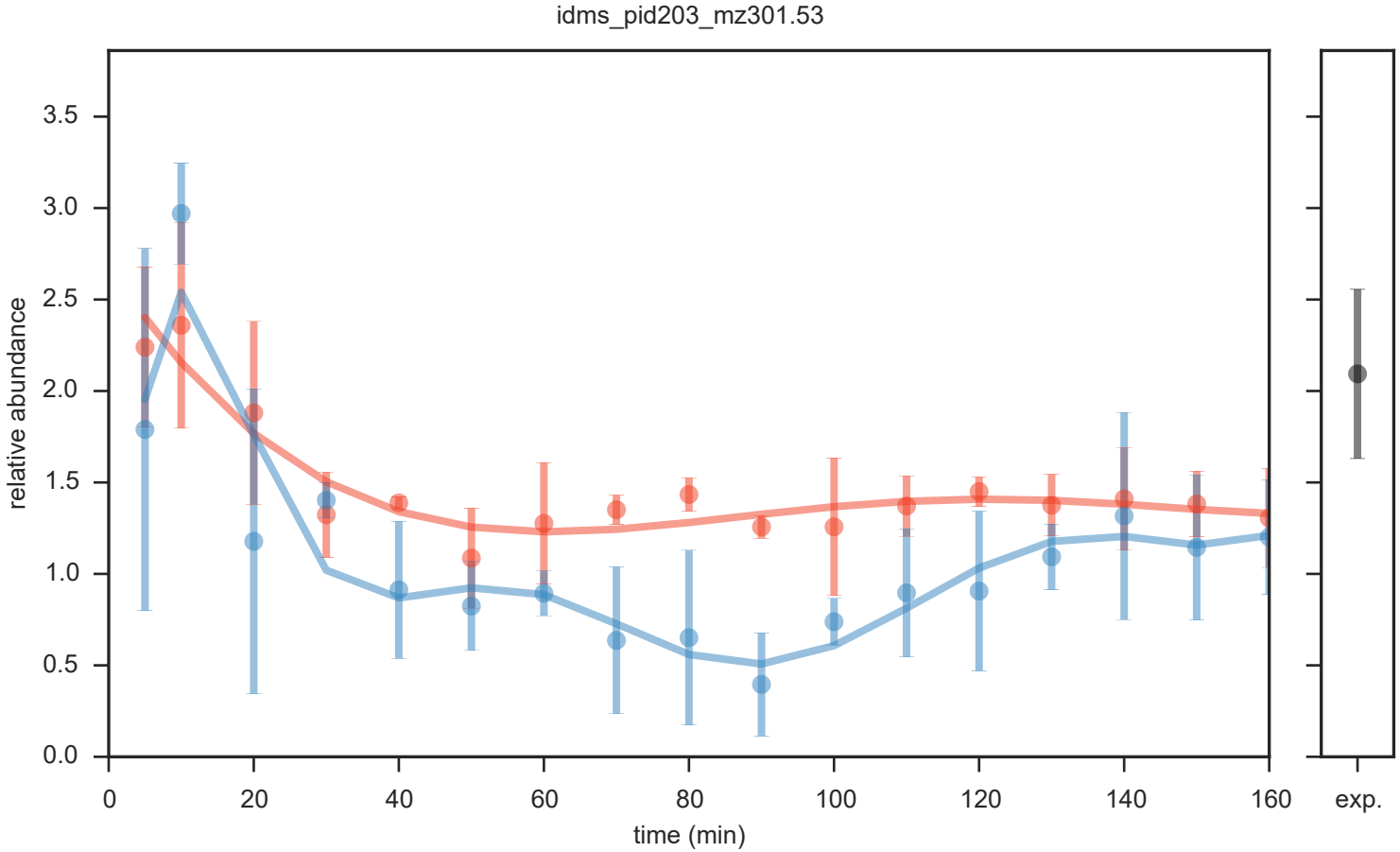

idms_pid173_mz308.53
relative abundance
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

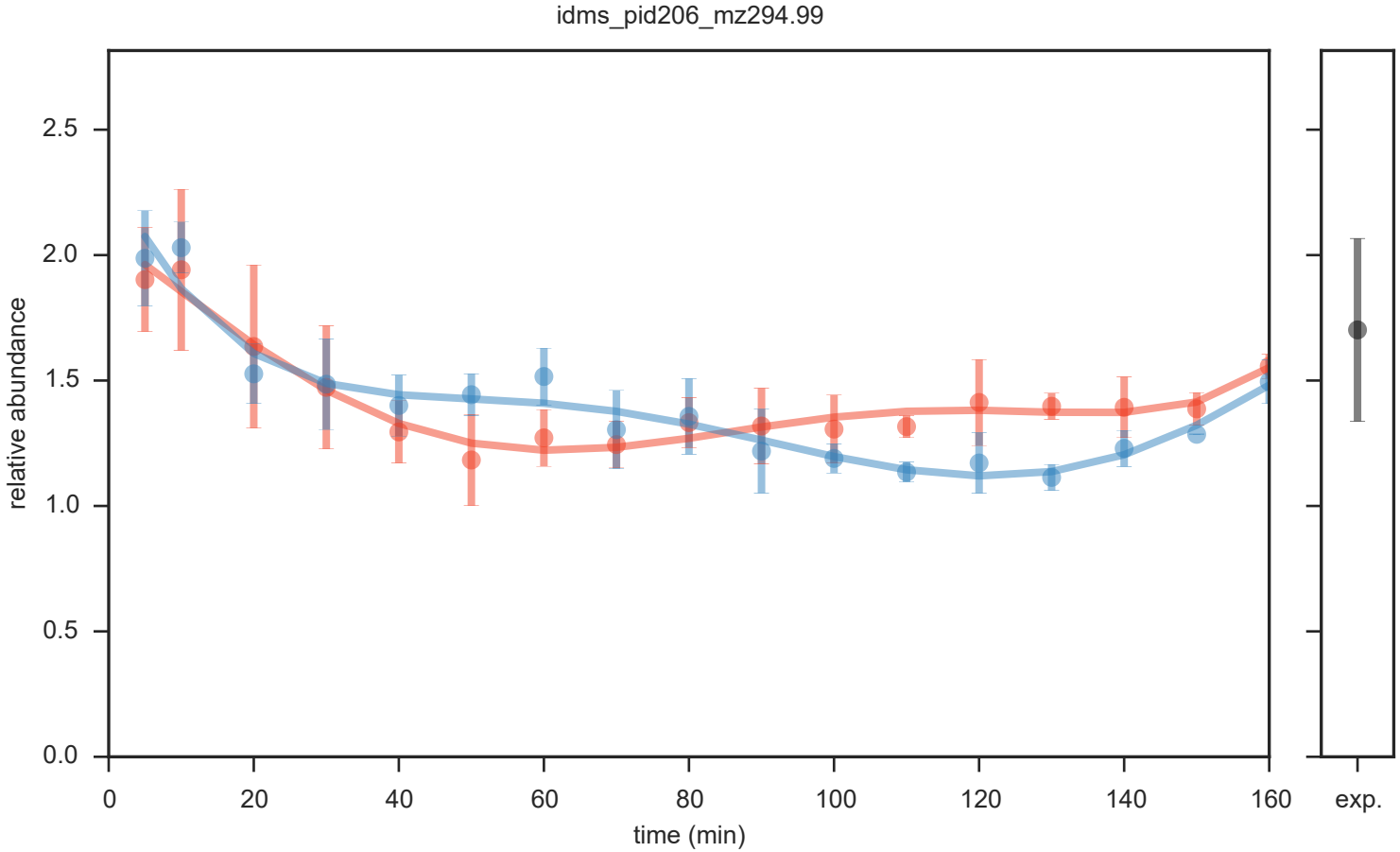

idms_pid176_mz240.02
relative abundance
1.0
0.8
0.6
0.4
0.2
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

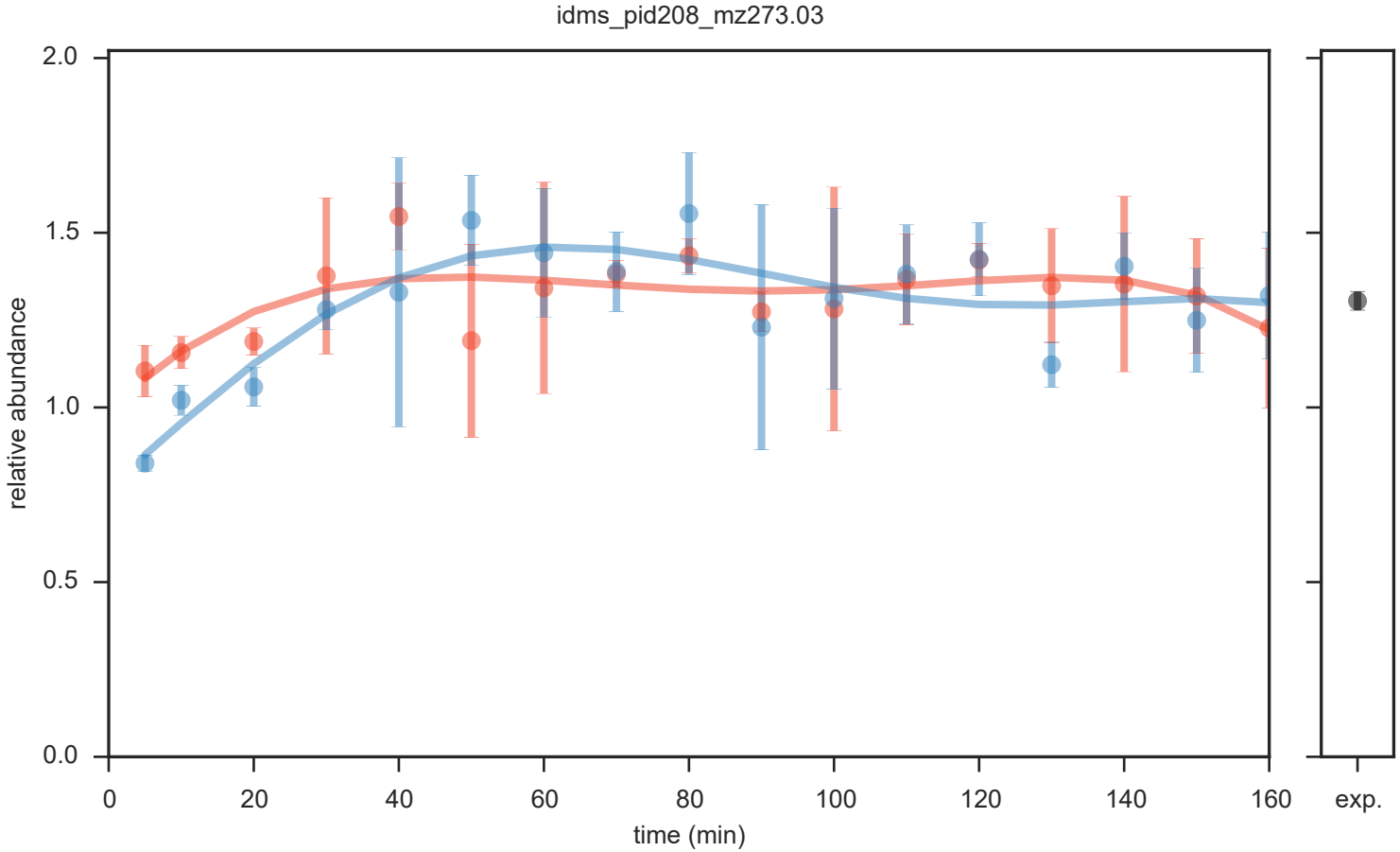

idms_pid190_mz239.91
relative abundance
0
1
2
3
4
5
6
0
20
40
60
80
100
120
140
160
time (min)
exp.

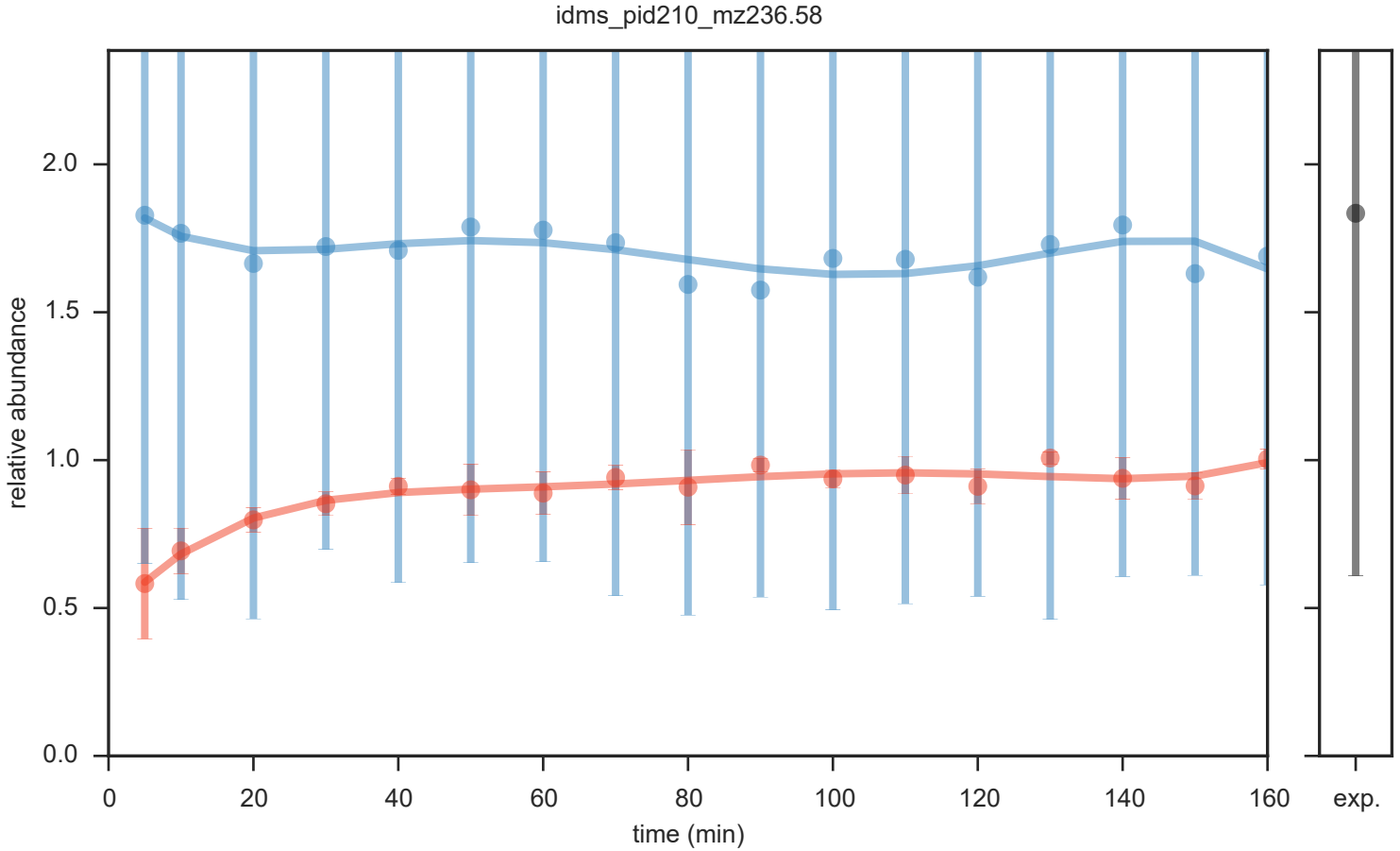

idms_pid194_mz613.13
relative abundance
0
2
4
6
8
0
20
40
60
80
100
120
140
160
time (min)
exp.

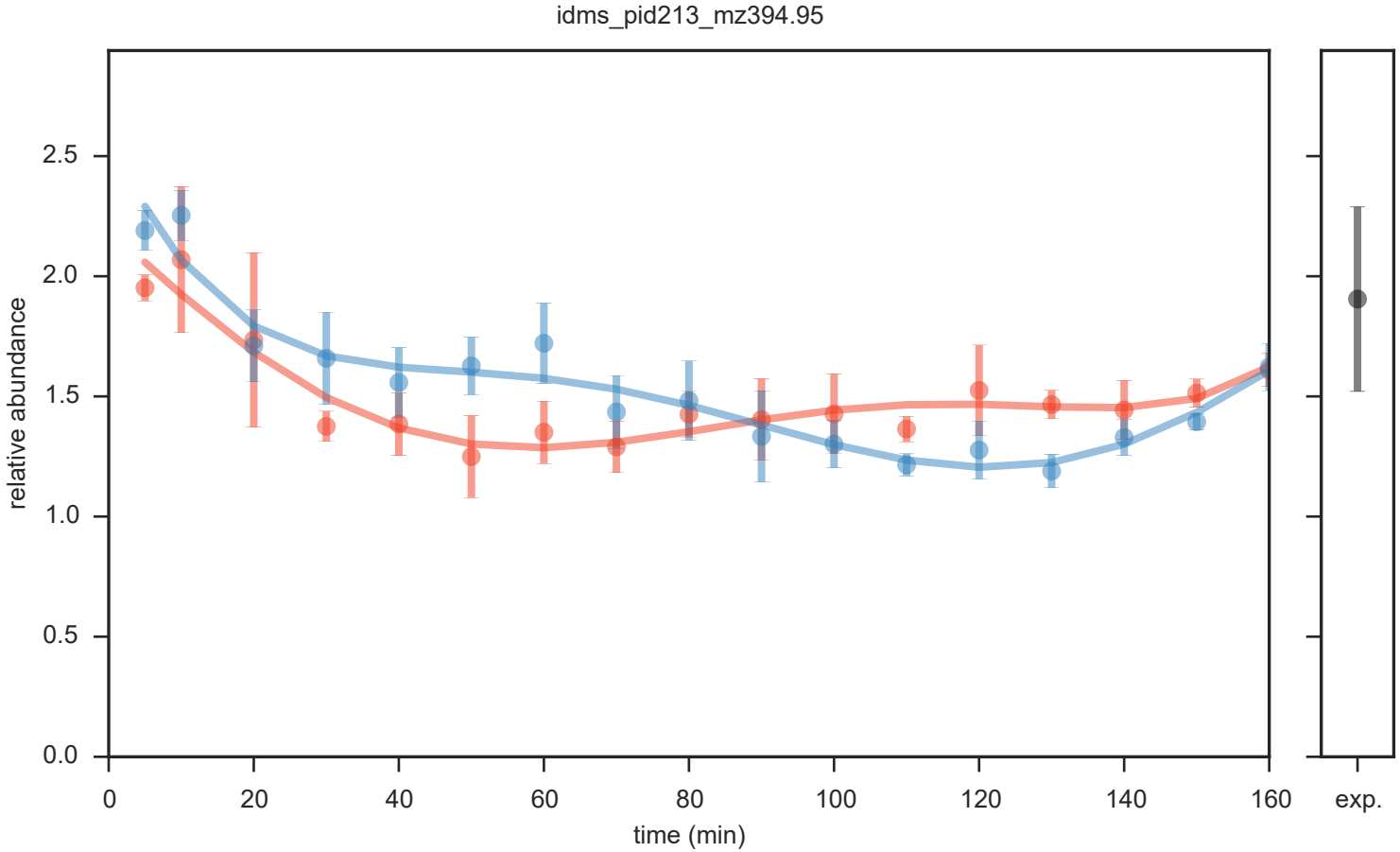

idms_pid199_mz358.54
relative abundance
0
5
10
15
0
20
40
60
80
100
120
140
160
time (min)
exp.

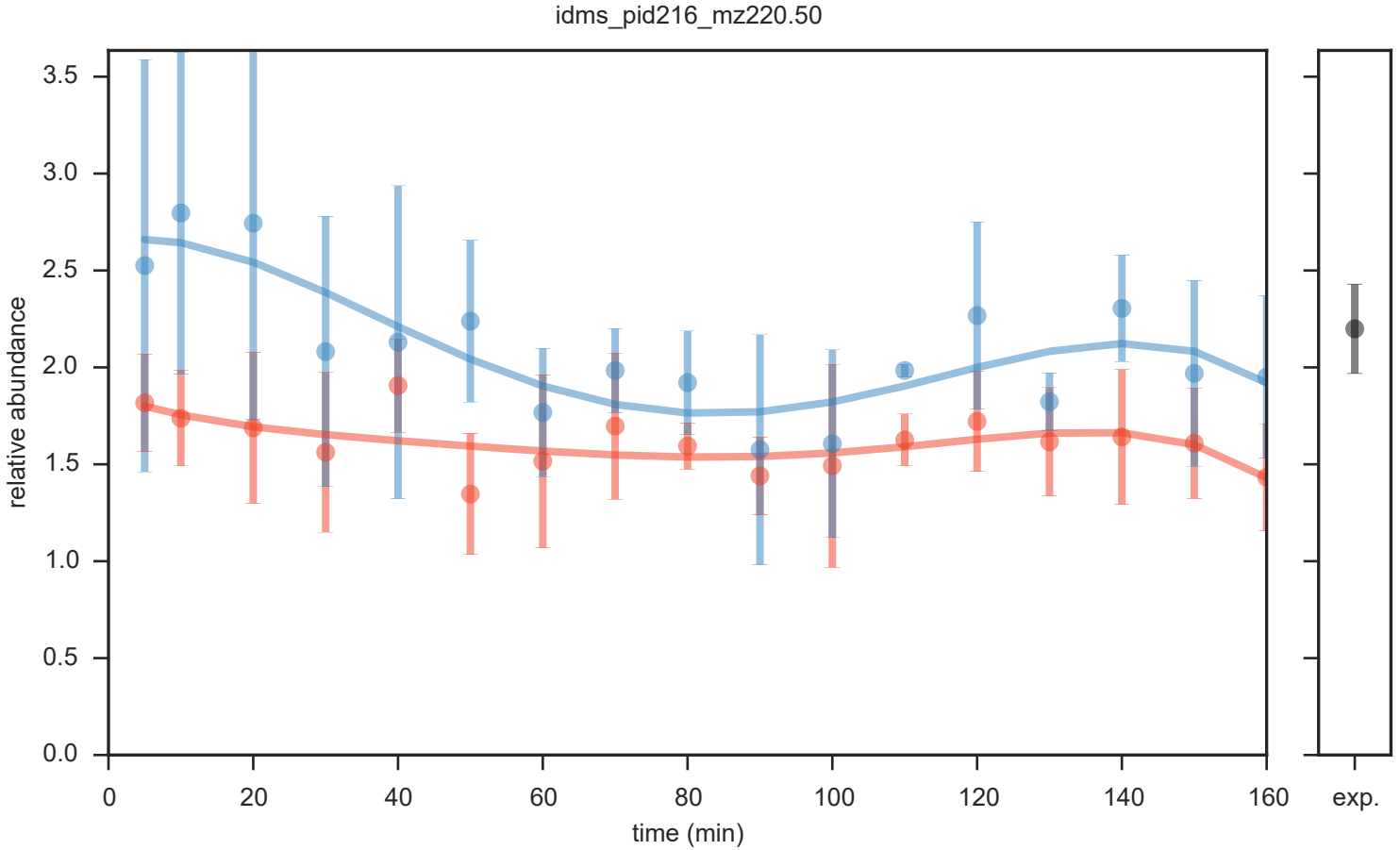

idms_pid203_mz301.53
relative abundance
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
0
20
40
60
80
100
120
140
160
time (min)
exp.

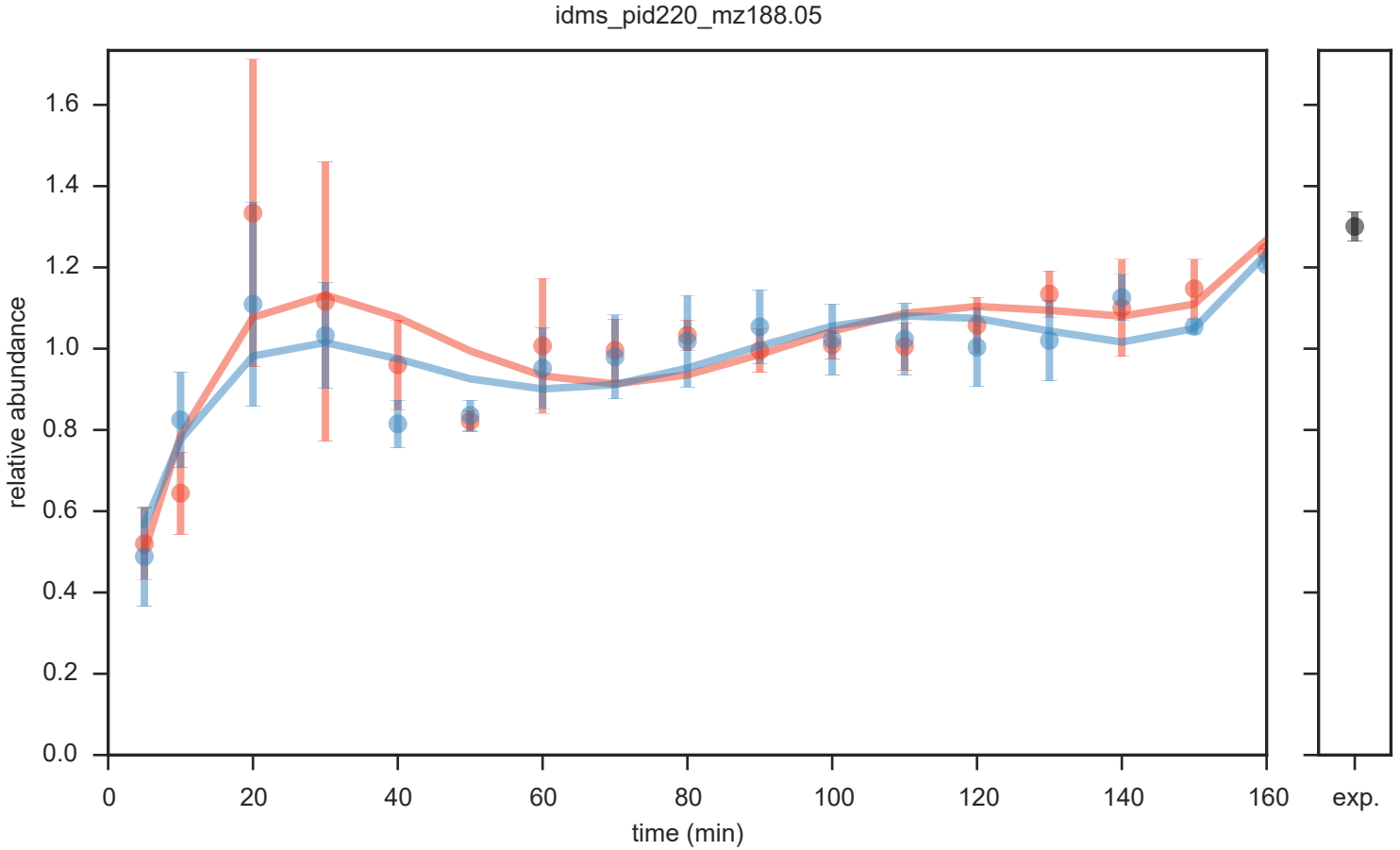

idms_pid206_mz294.99
relative abundance
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

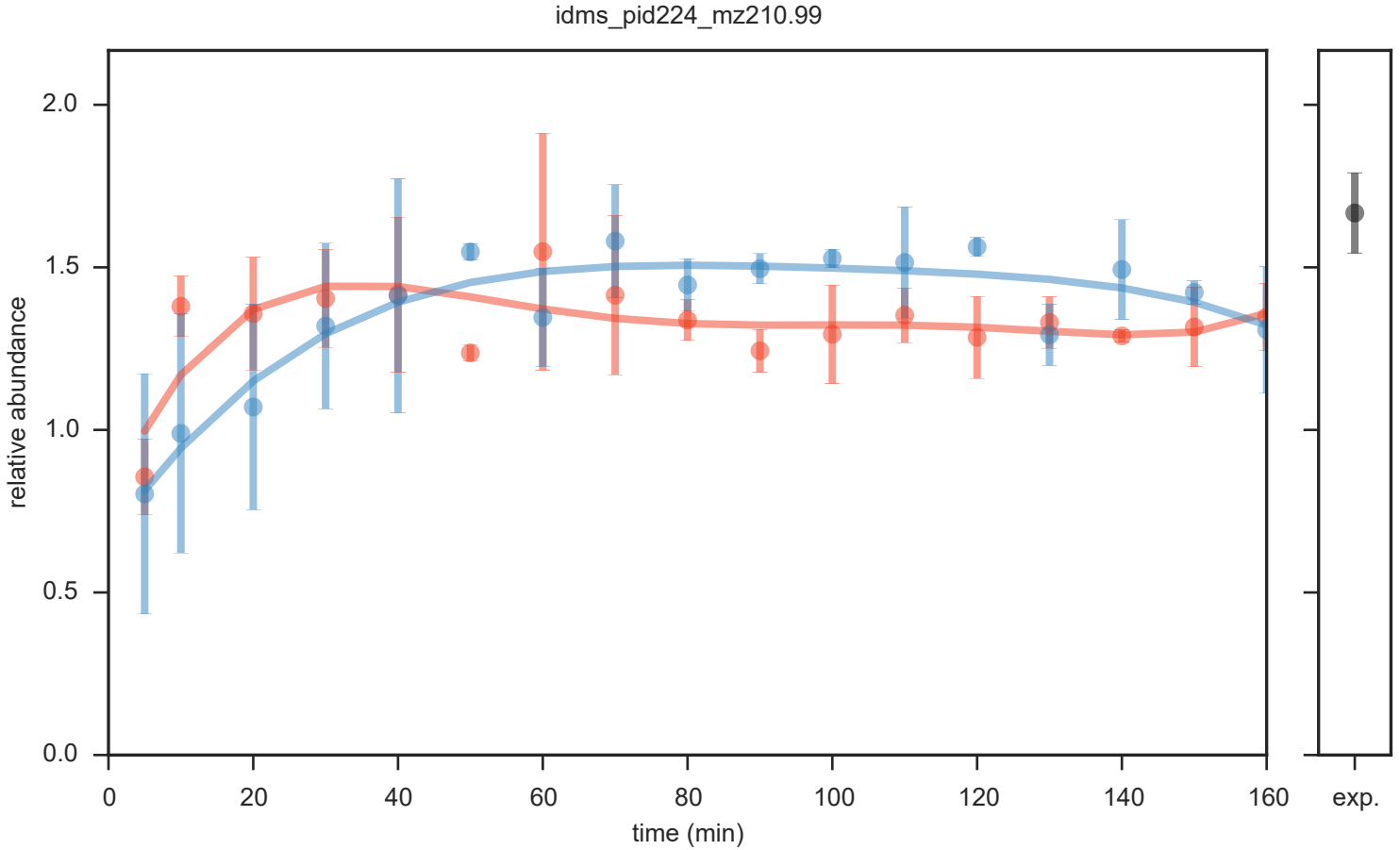

idms_pid208_mz273.03
relative abundance
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

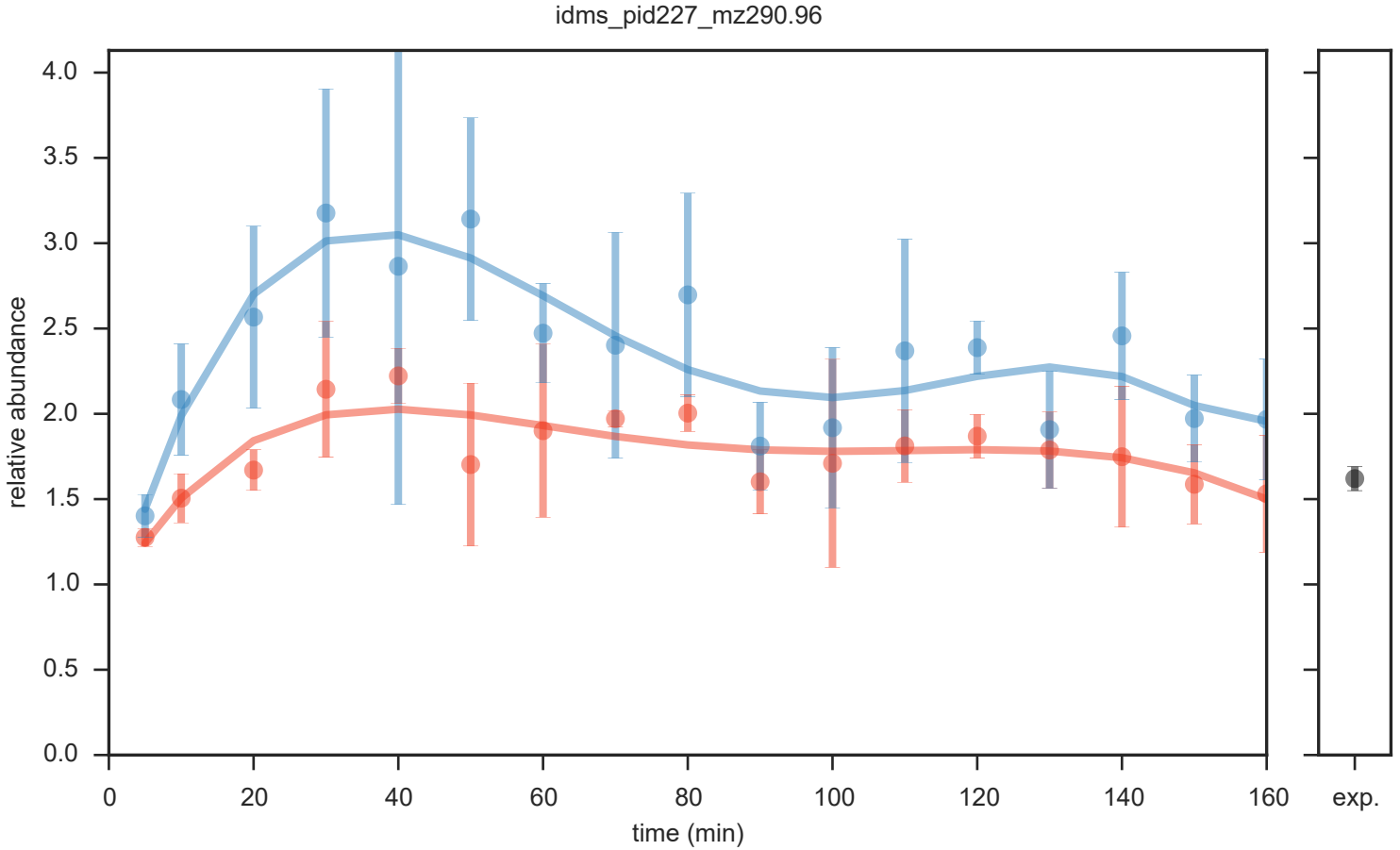

idms_pid210_mz236.58
relative abundance
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

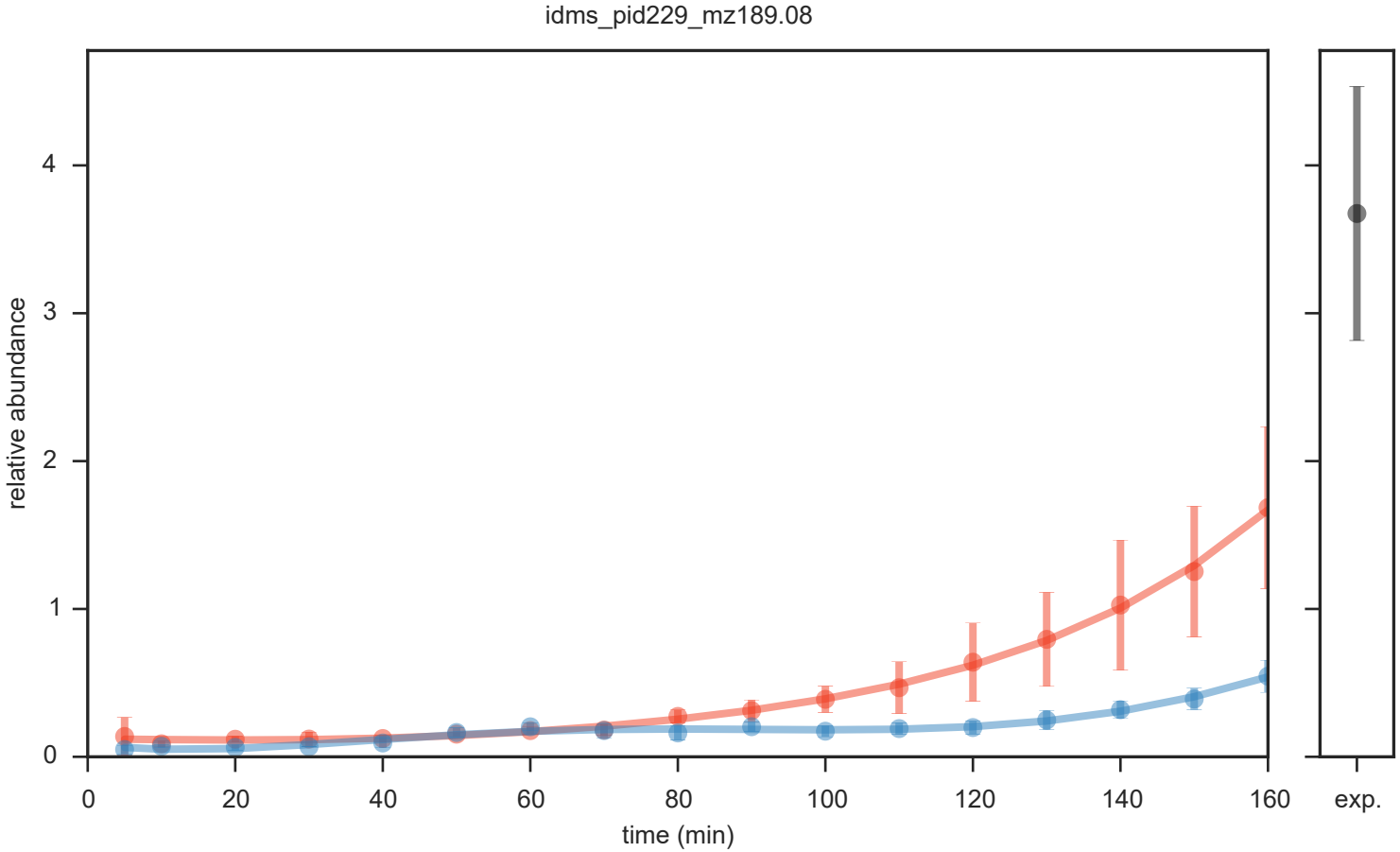

idms_pid213_mz394.95
relative abundance
0.0
0.5
1.0
1.5
2.0
2.5
0
20
40
60
80
100
120
140
160
time (min)
exp.

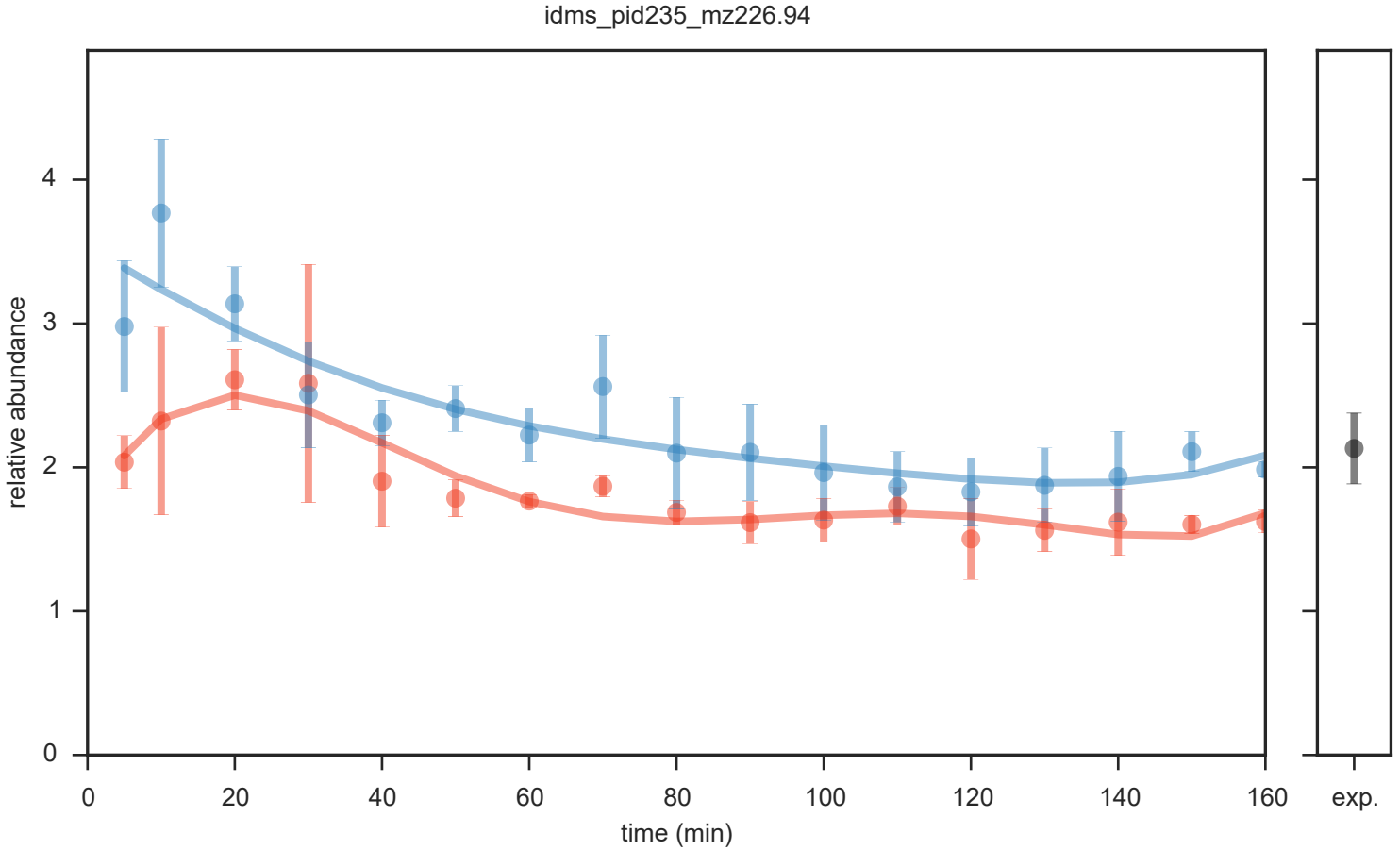

idms_pid216_mz220.50
relative abundance
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

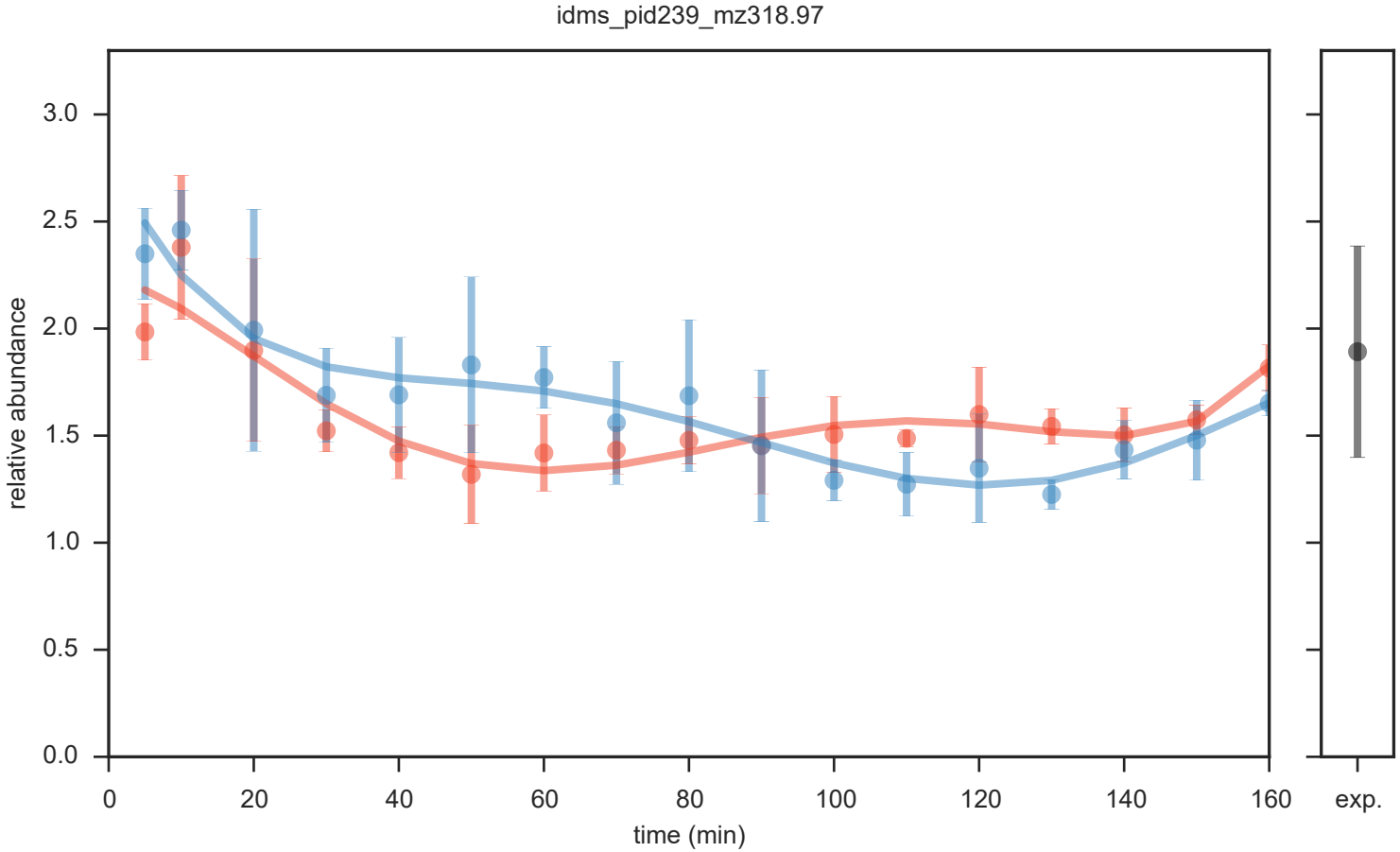

idms_pid220_mz188.05
relative abundance
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
0
20
40
60
80
100
120
140
160
time (min)
exp.

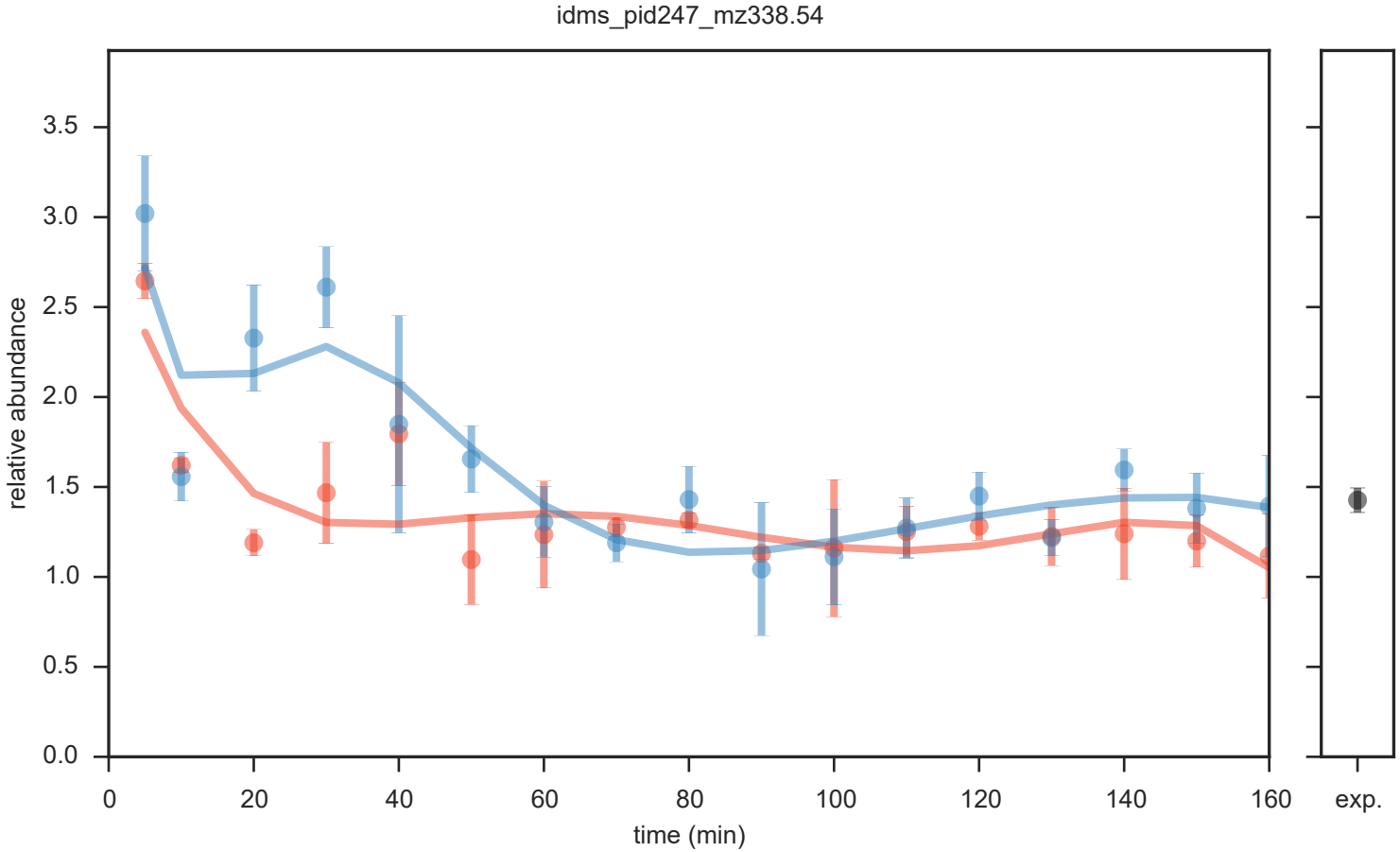

idms_pid224_mz210.99
relative abundance
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

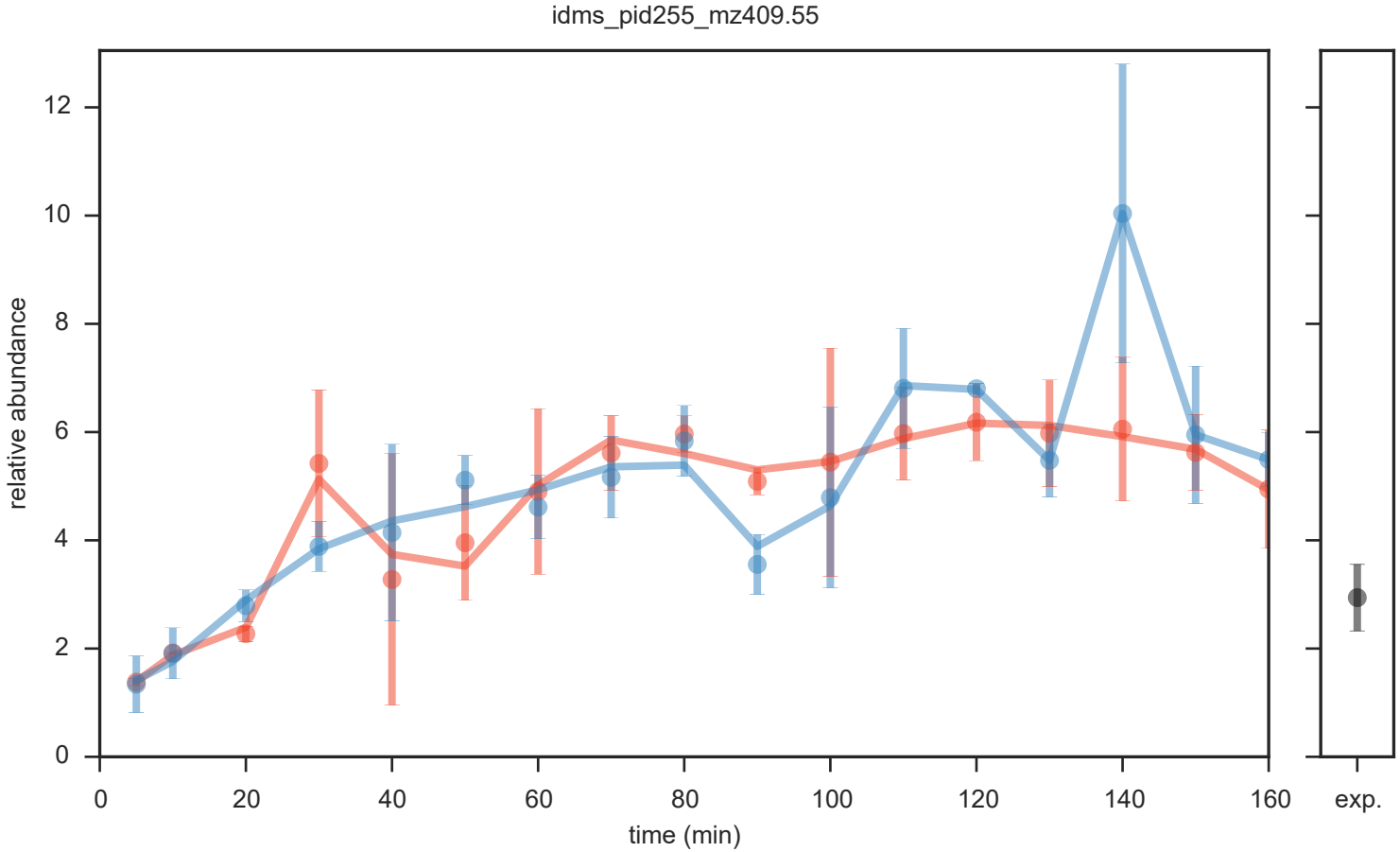

idms_pid227_mz290.96
relative abundance
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

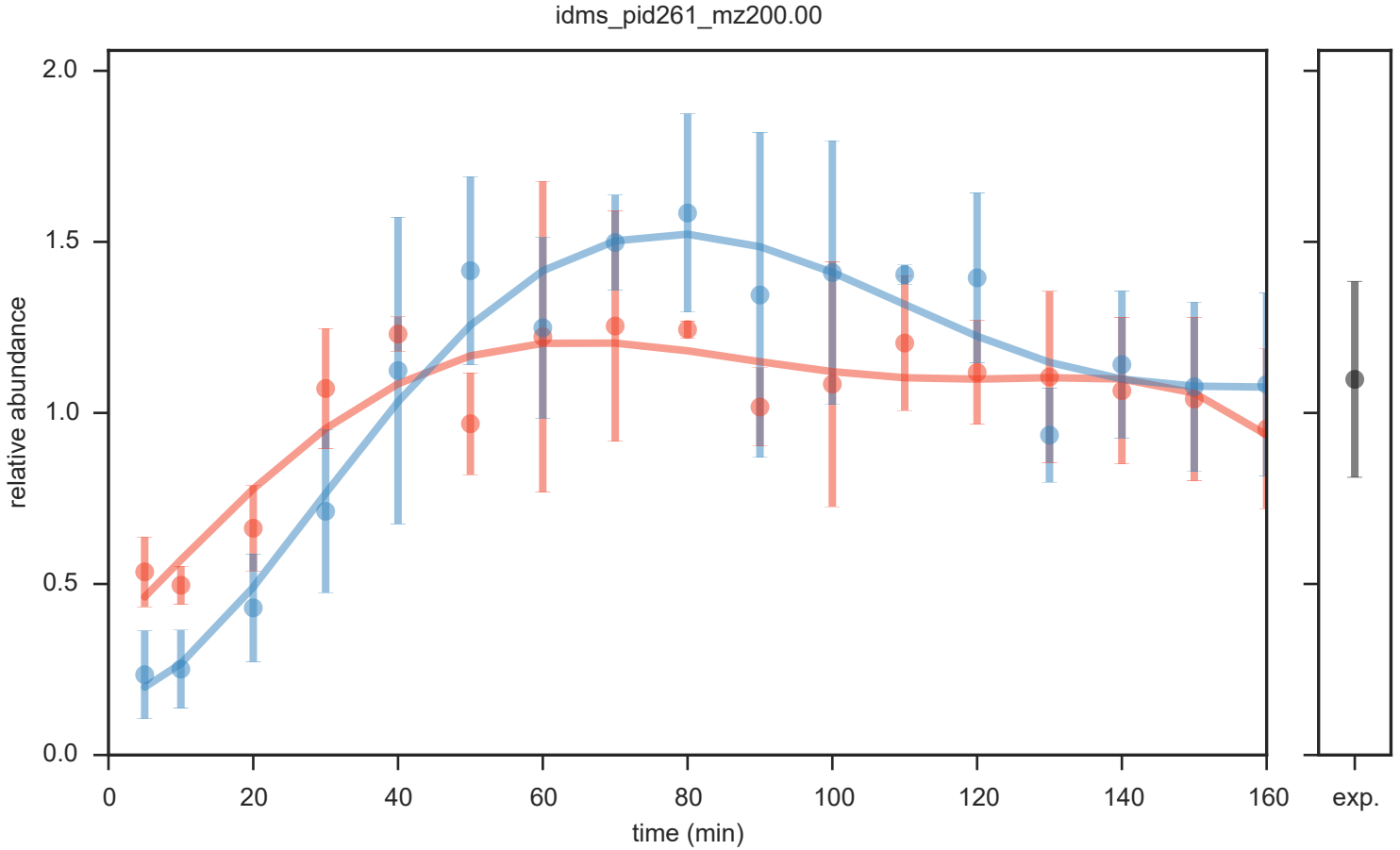

idms_pid229_mz189.08
relative abundance
0
1
2
3
4
0
20
40
60
80
100
120
140
160
time (min)
exp.

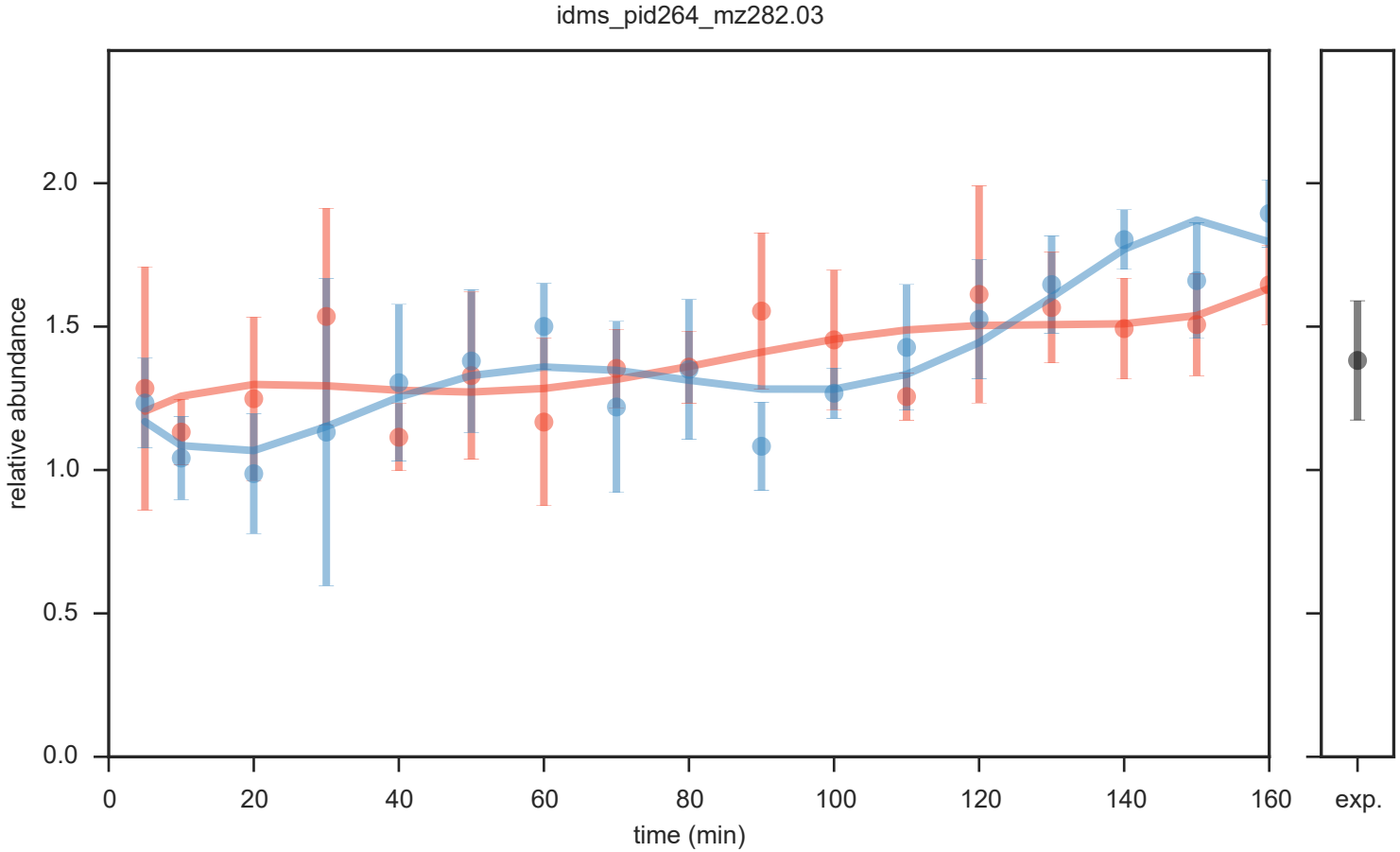

idms_pid235_mz226.94
relative abundance
0
1
2
3
4
0
20
40
60
80
100
120
140
160
time (min)
exp.

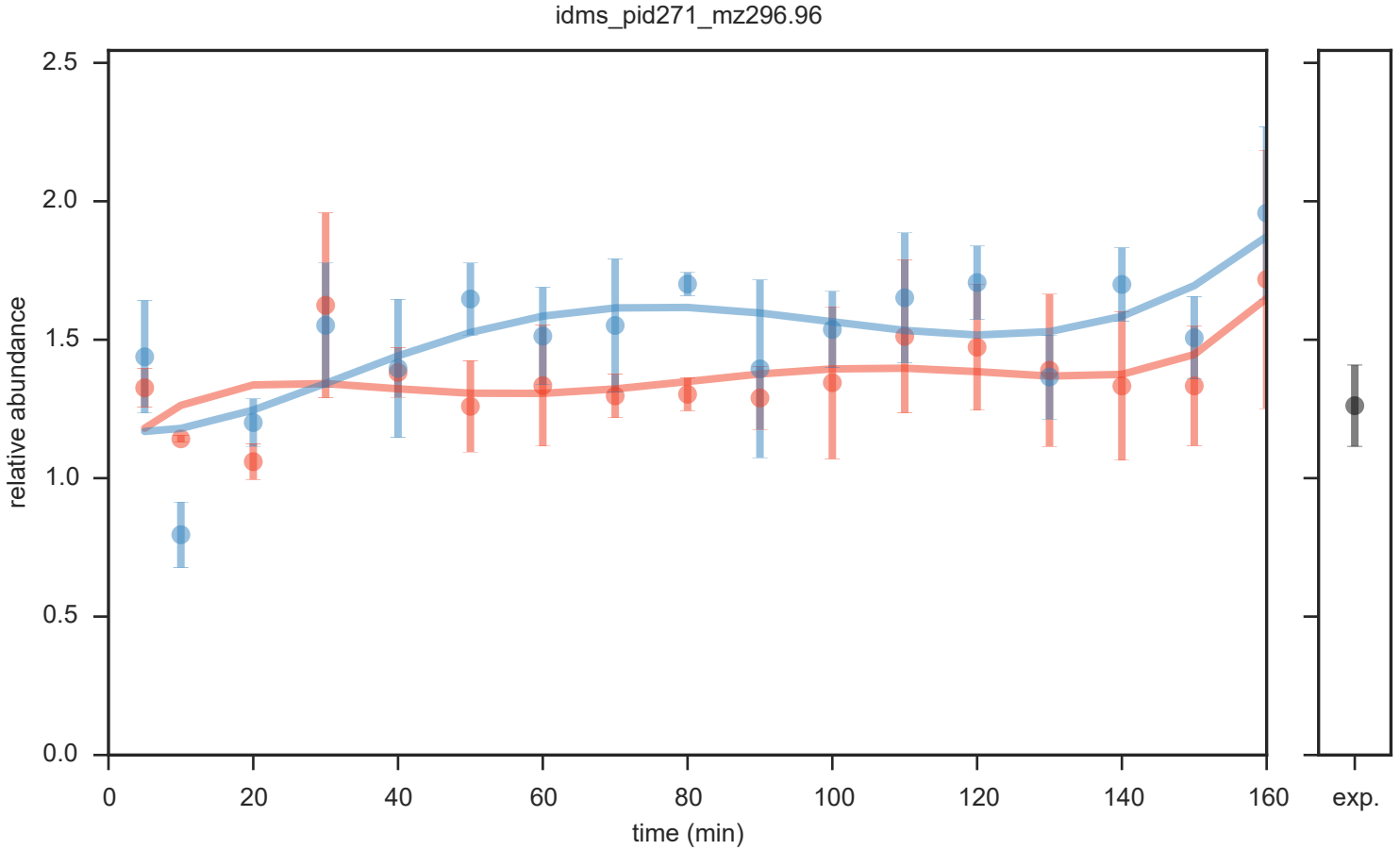

idms_pid239_mz318.97
relative abundance
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

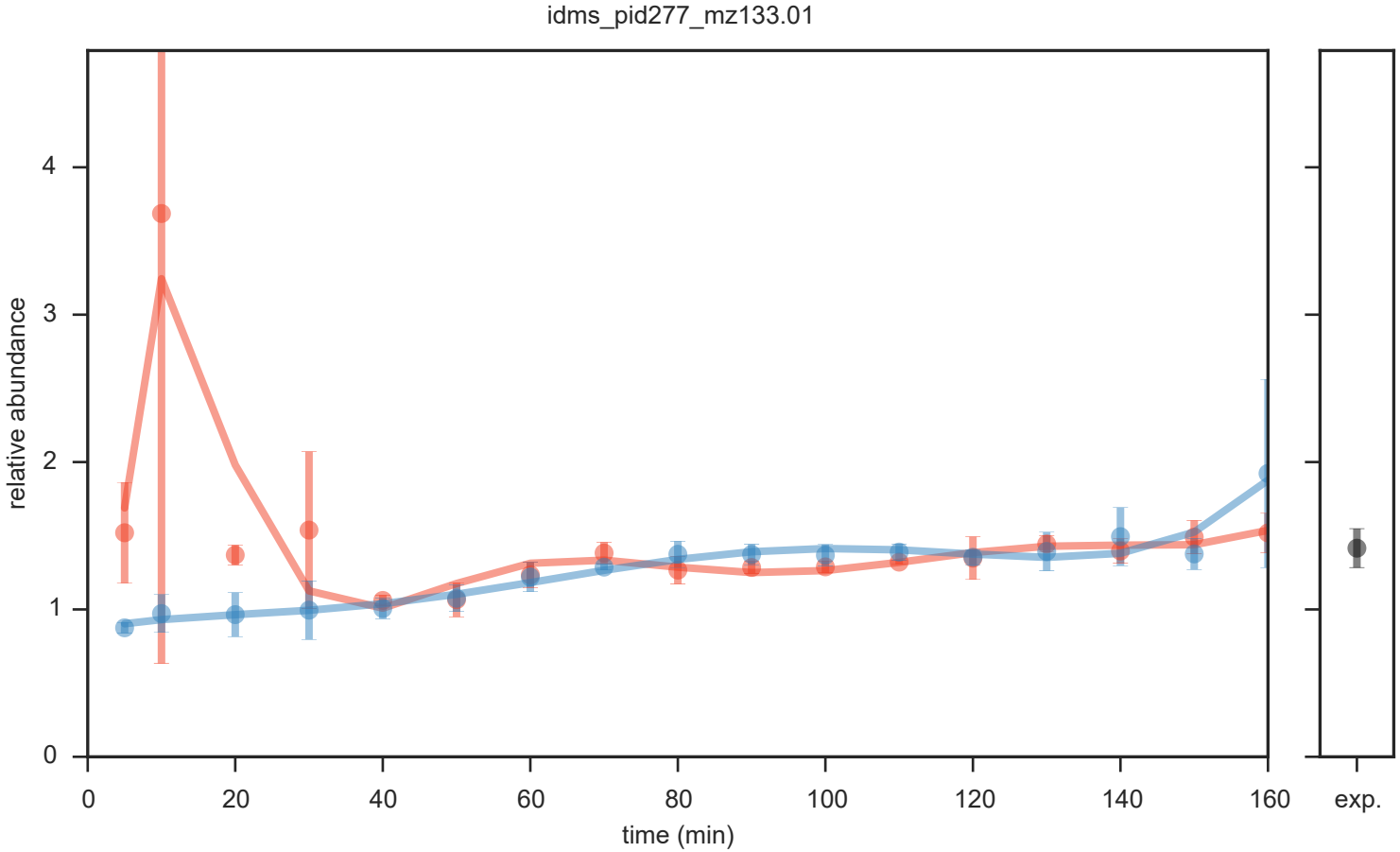

idms_pid247_mz338.54
relative abundance
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
0
20
40
60
80
100
120
140
160
time (min)
exp.

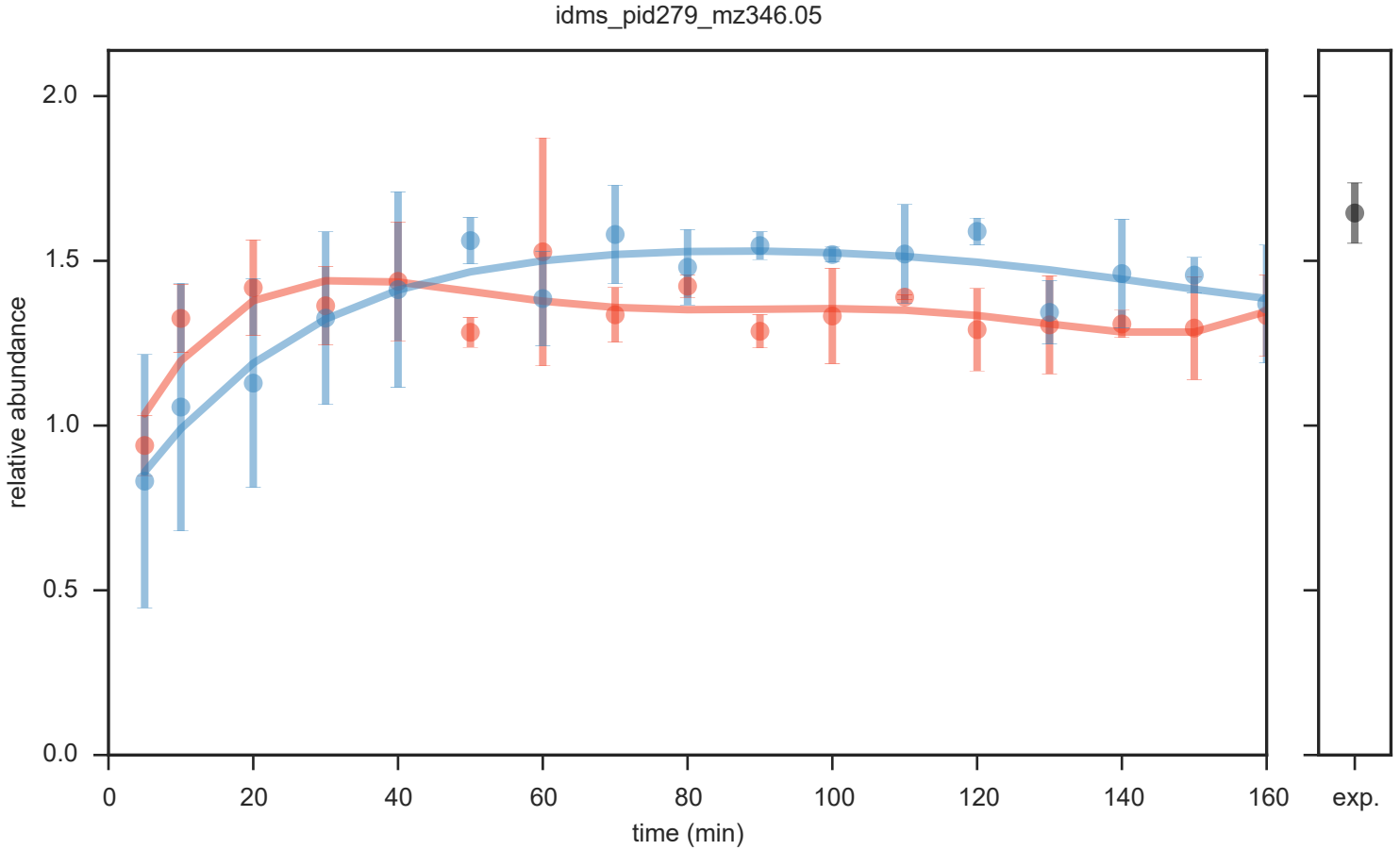

idms_pid255_mz409.55
relative abundance
0
2
4
6
8
10
12
0
20
40
60
80
100
120
140
160
time (min)
exp.

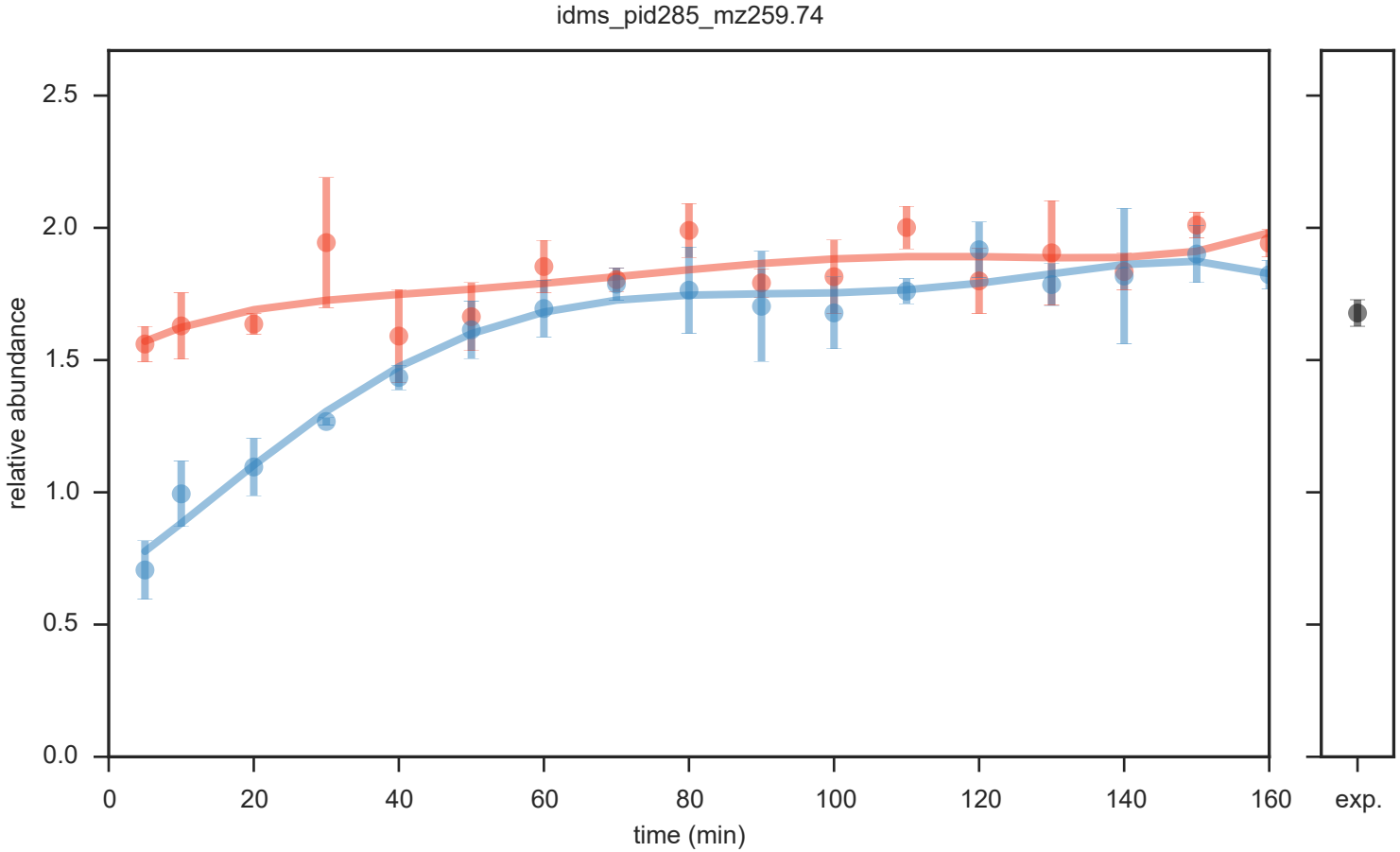

idms_pid261_mz200.00
relative abundance
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

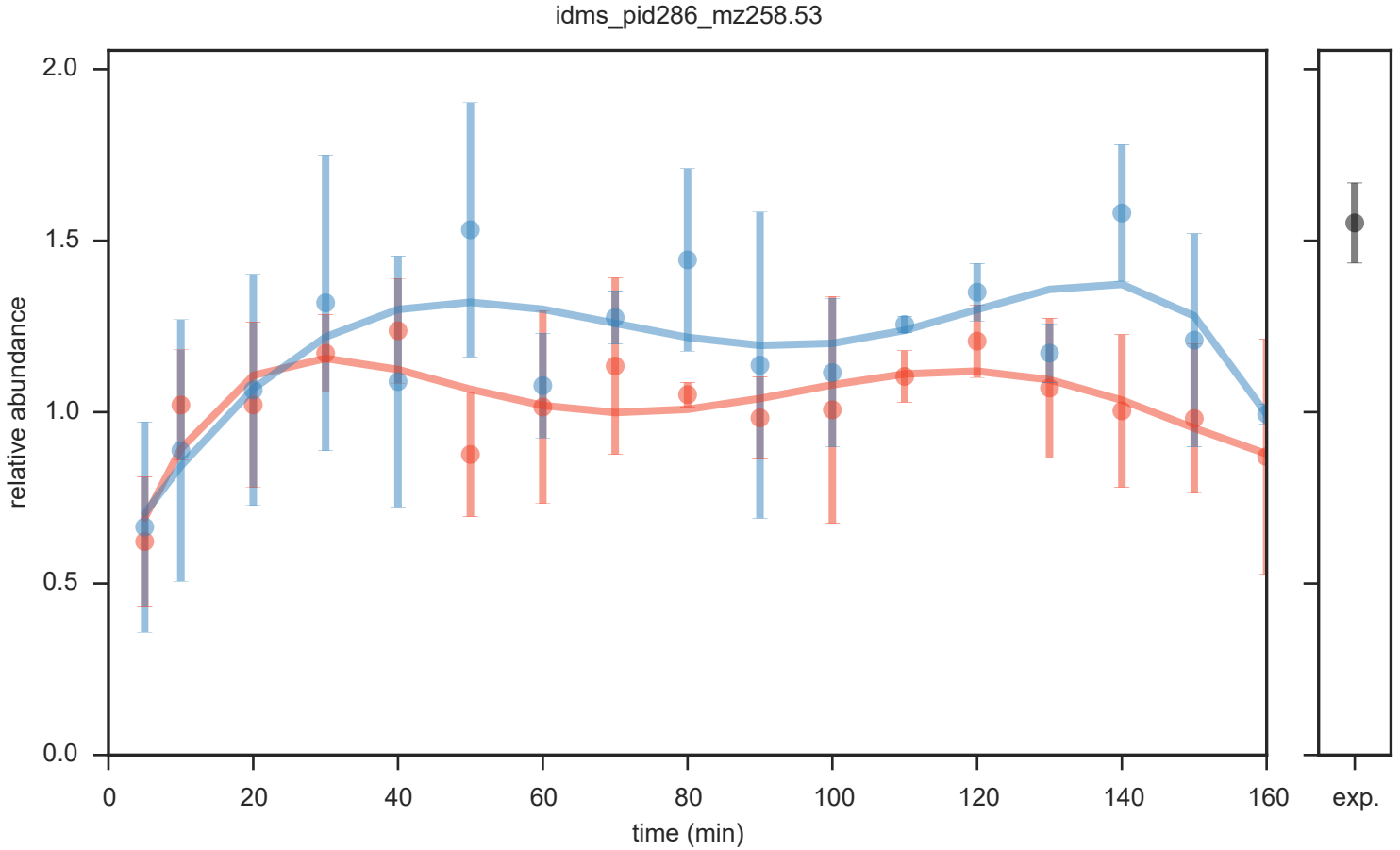

idms_pid264_mz282.03
relative abundance
0.0
0.5
1.0
1.5
2.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

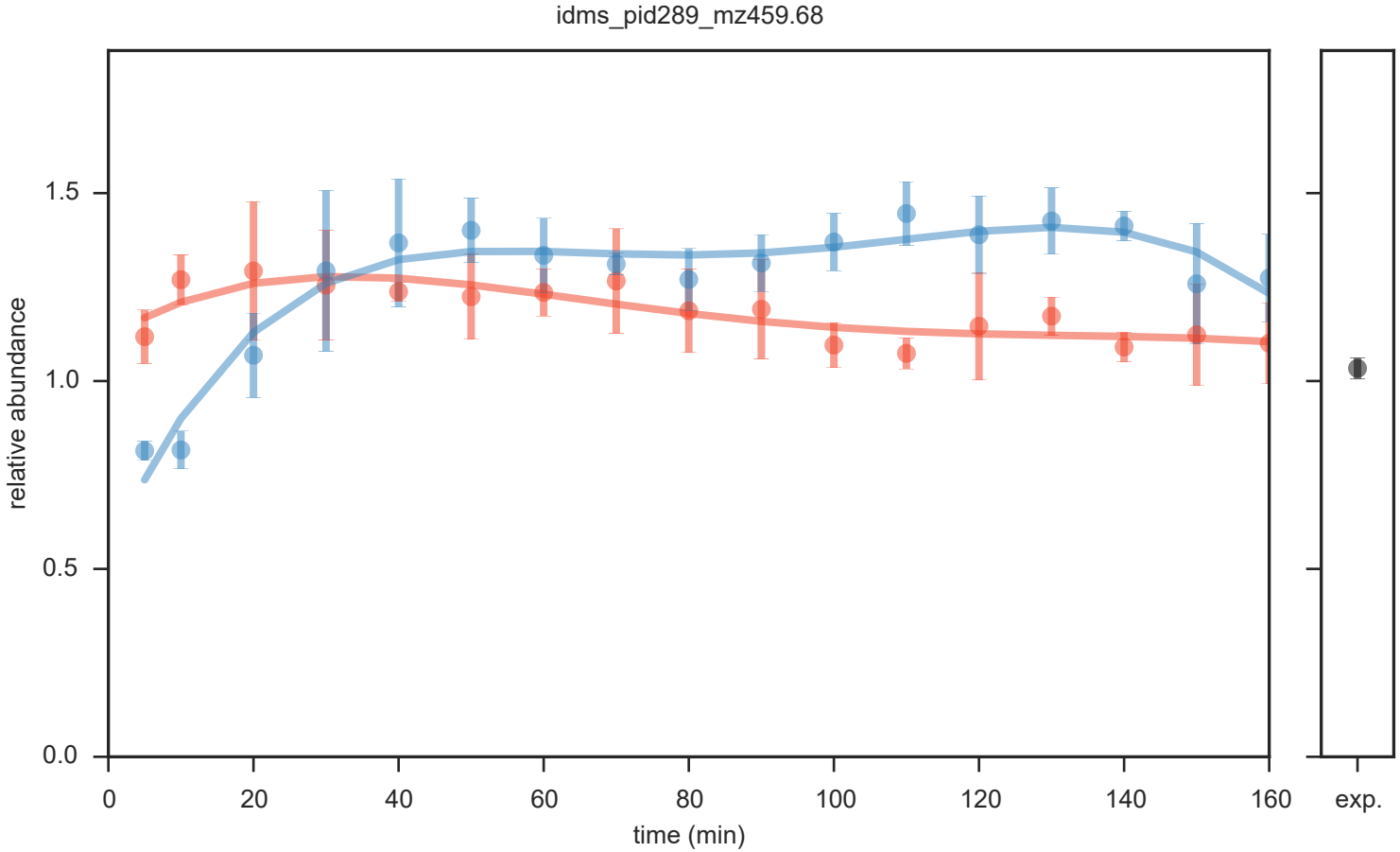

idms_pid271_mz296.96
relative abundance
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

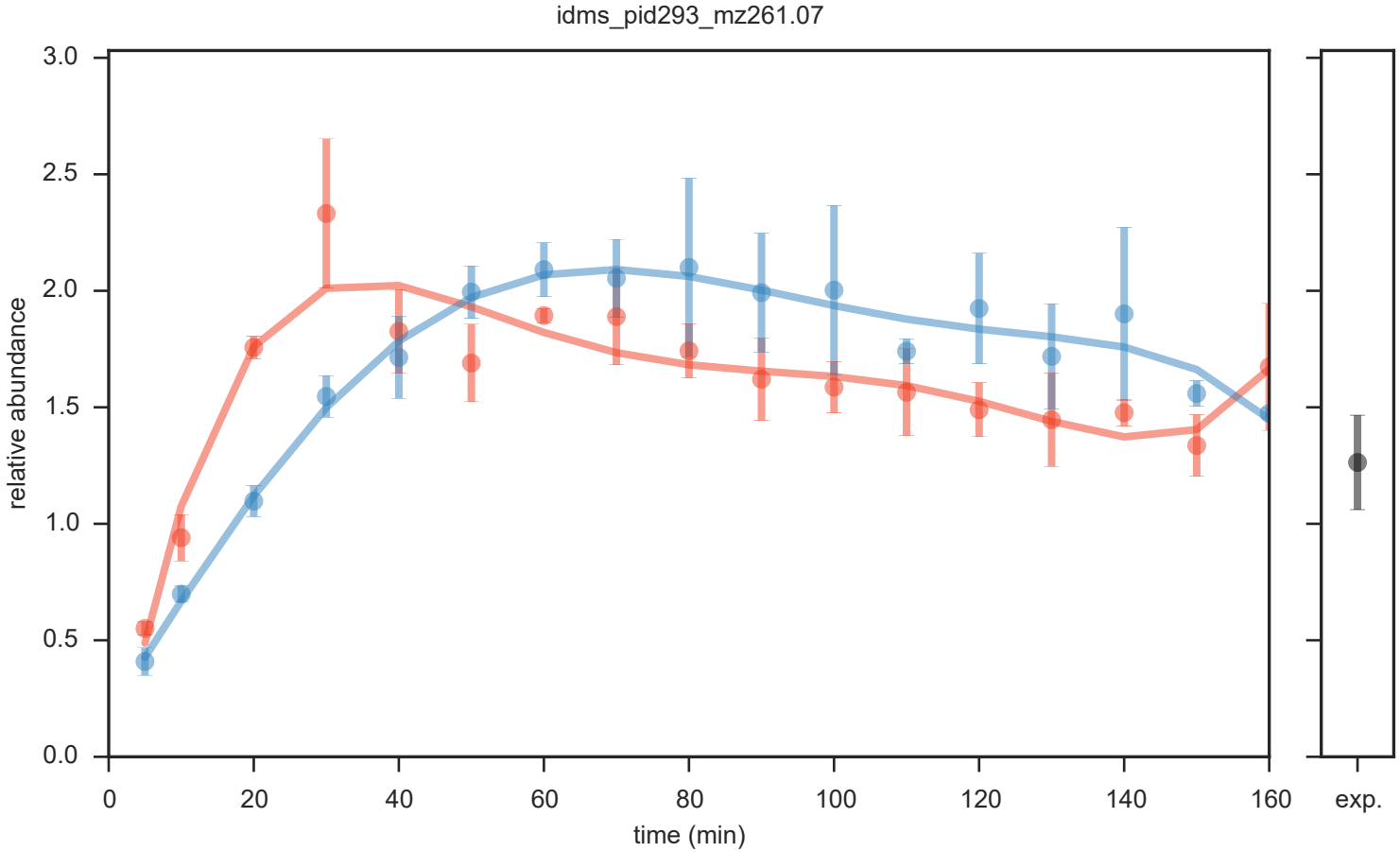

idms_pid277_mz133.01
relative abundance
0
1
2
3
4
0
20
40
60
80
100
120
140
160
time (min)
exp.

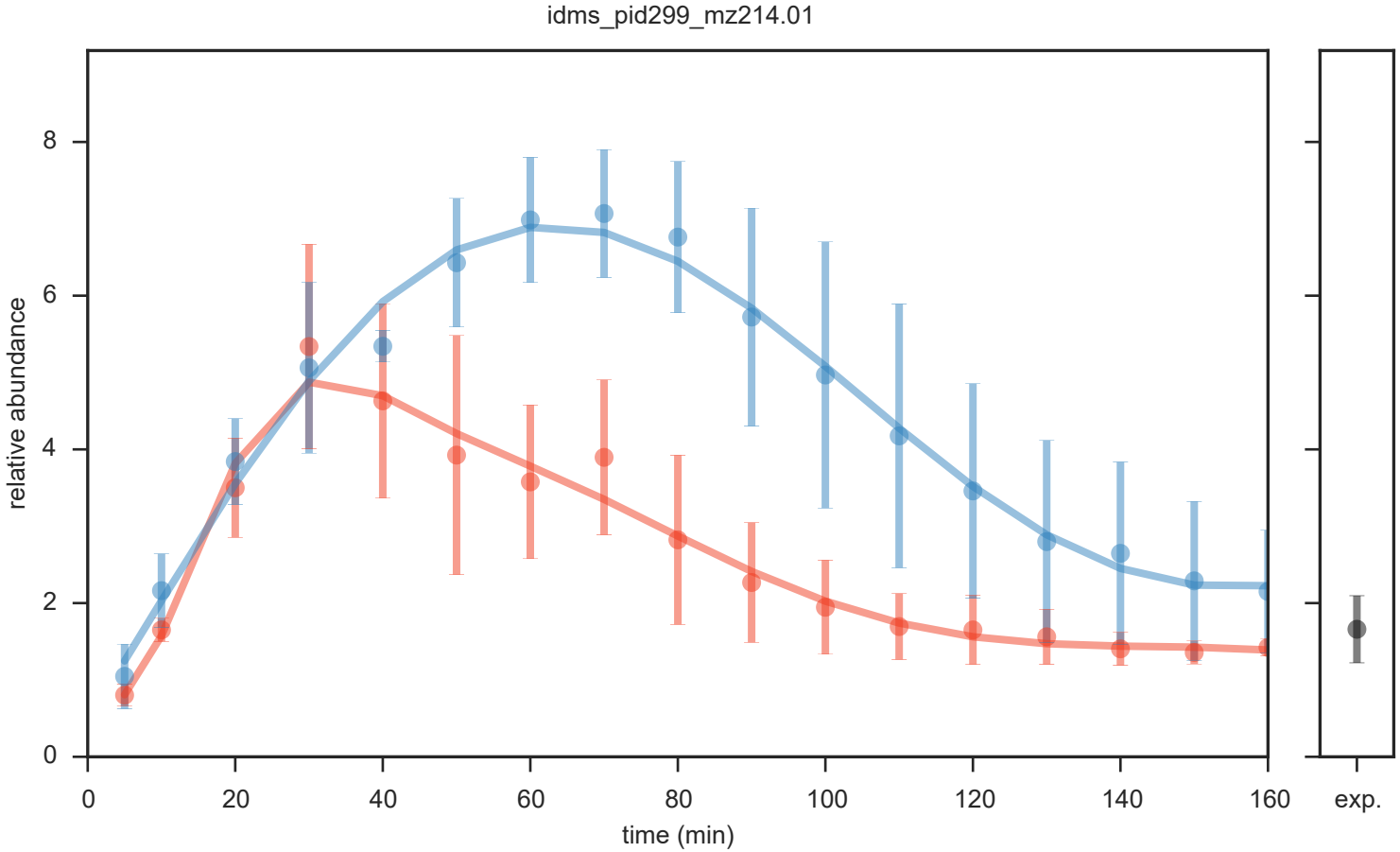

idms_pid279_mz346.05
relative abundance
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

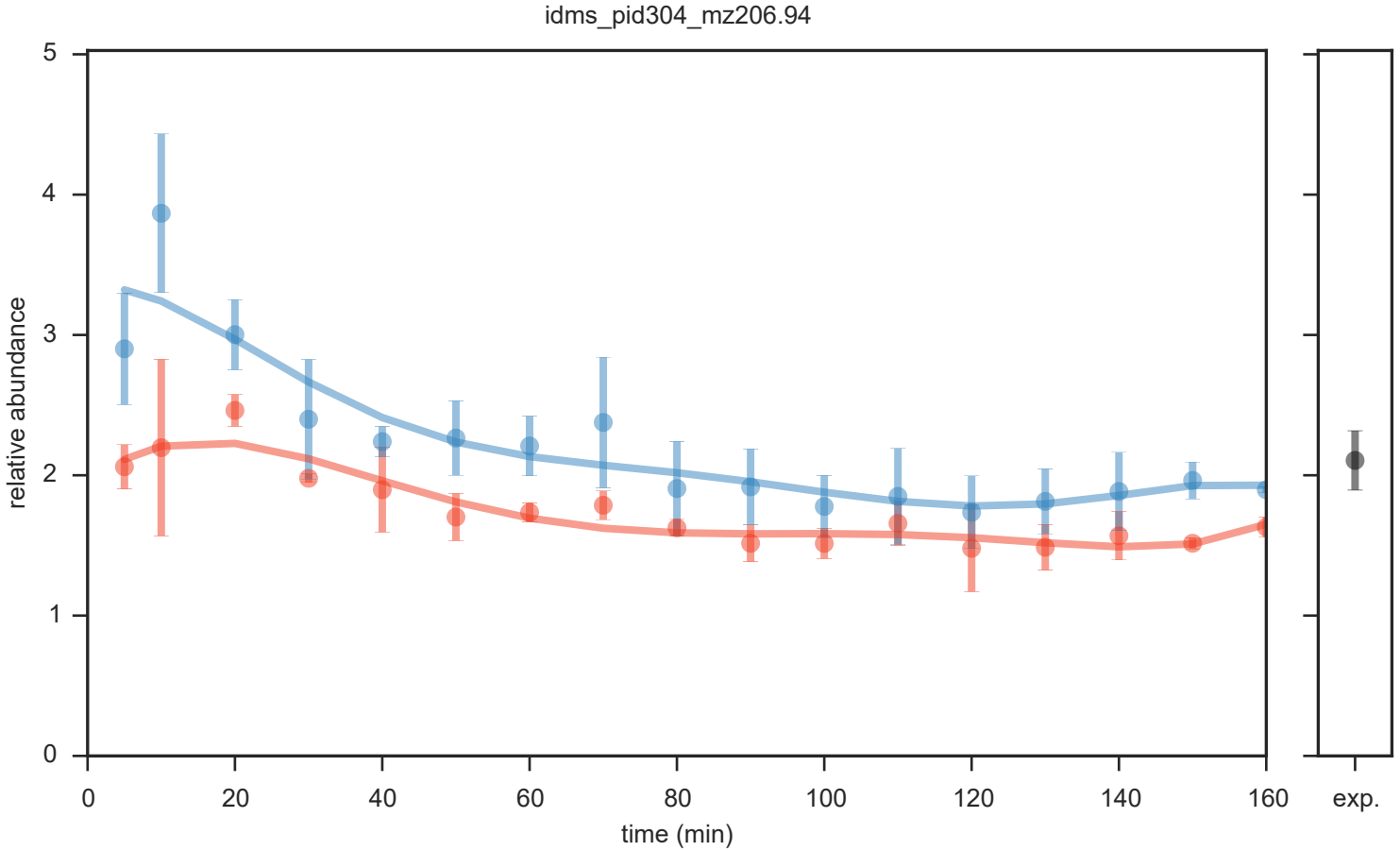

idms_pid285_mz259.74
relative abundance
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

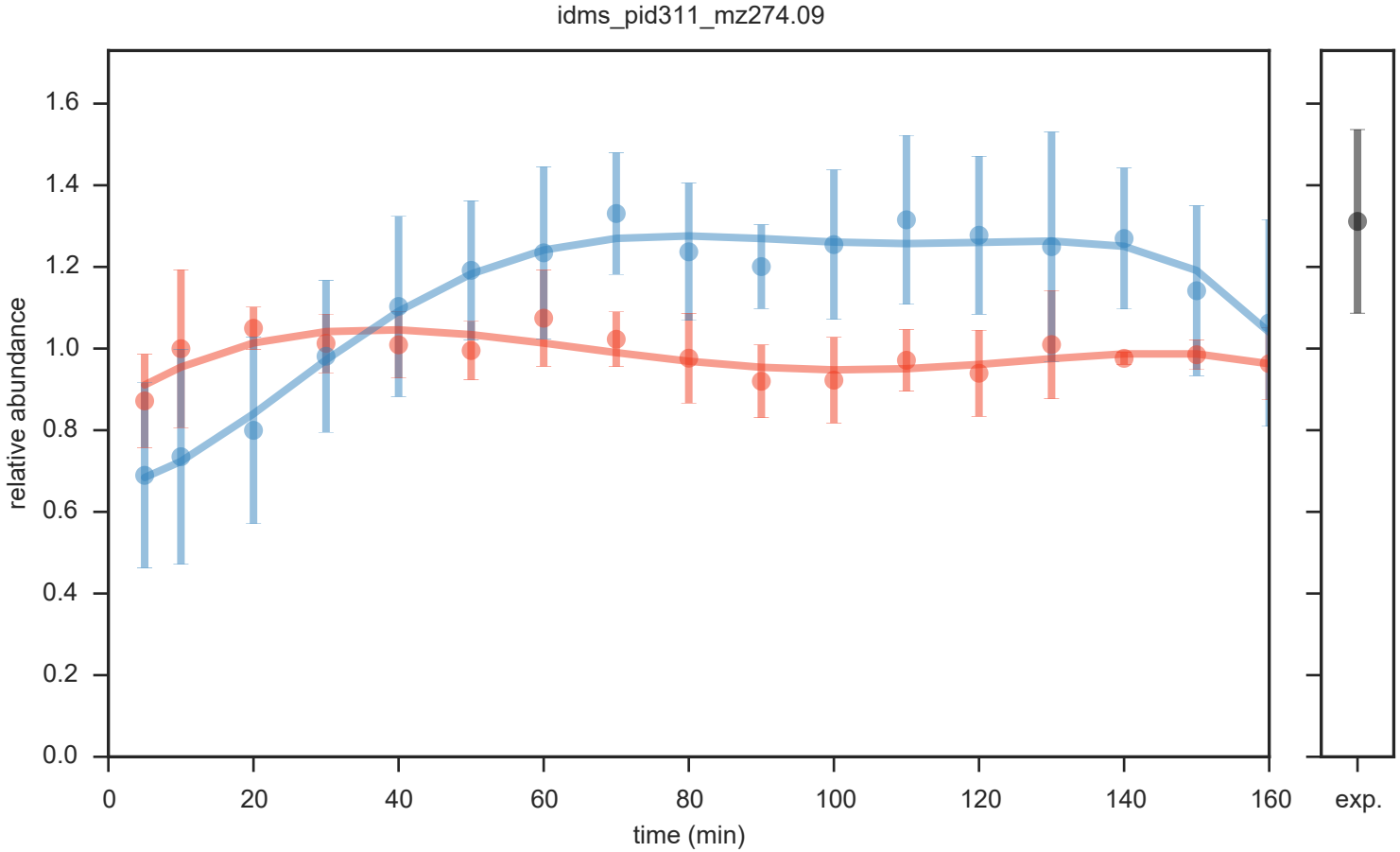

idms_pid286_mz258.53
relative abundance
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

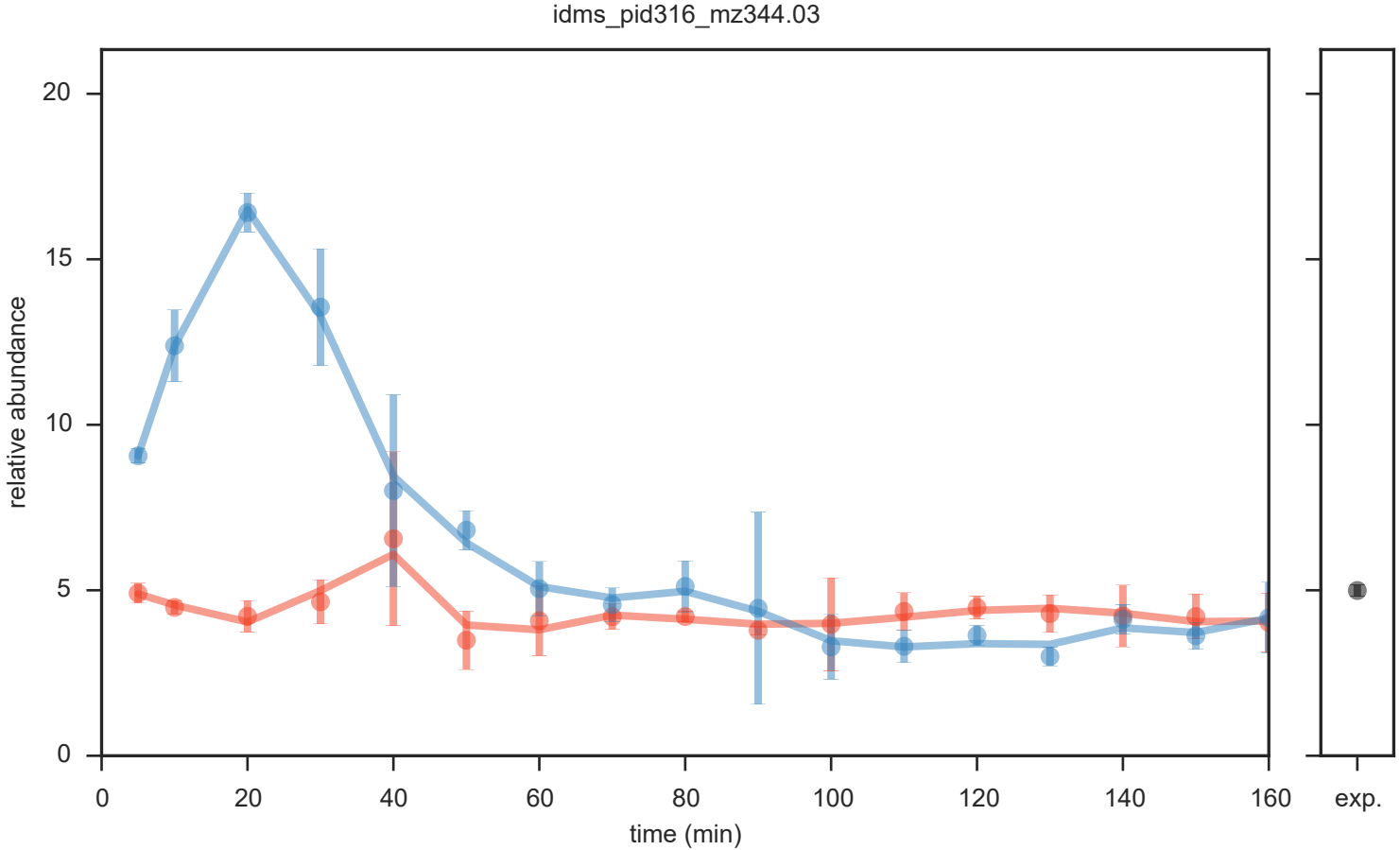

idms_pid289_mz459.68
relative abundance
0.0
0.5
1.0
1.5
0
20
40
60
80
100
120
140
160
time (min)
exp.

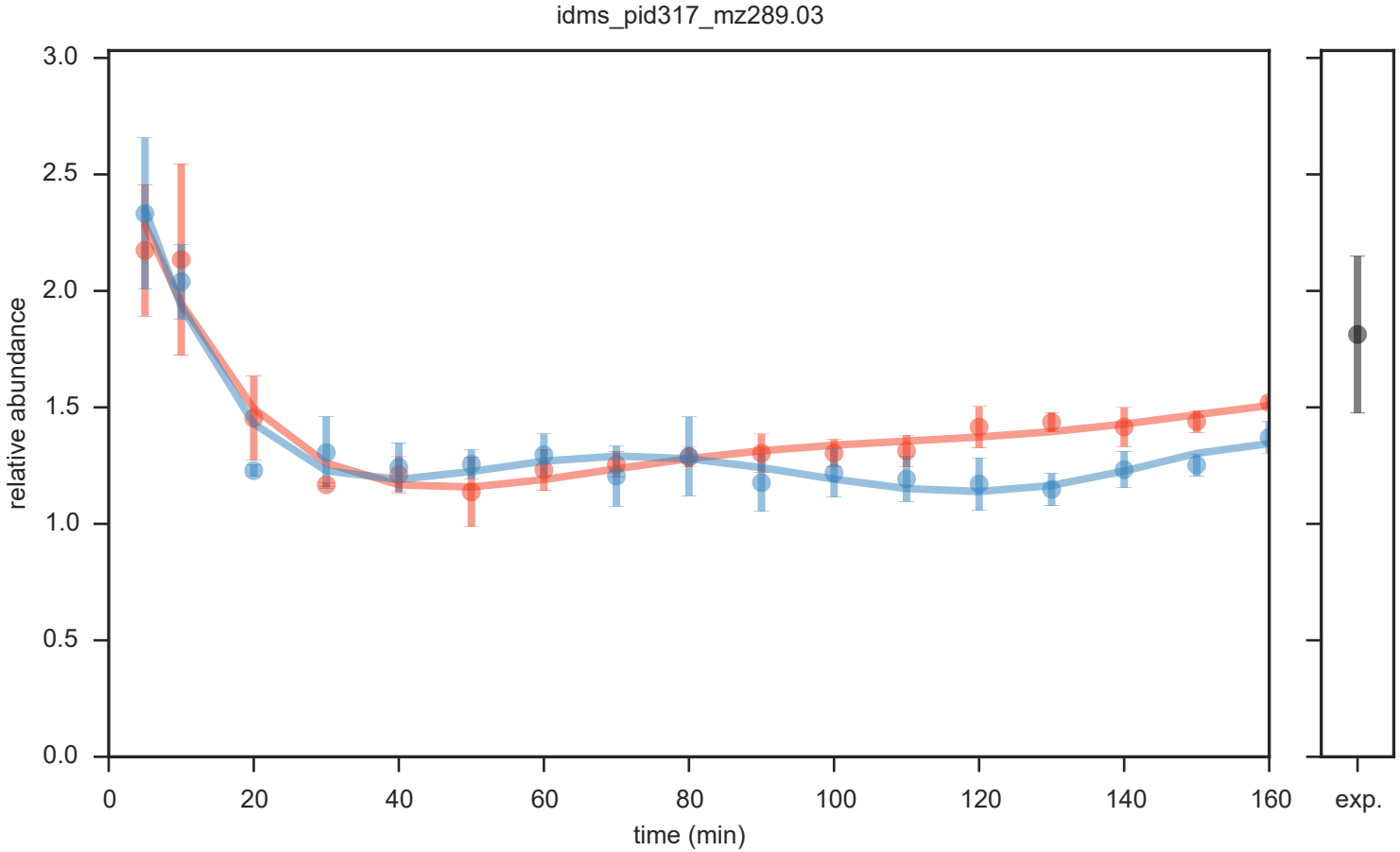

idms_pid293_mz261.07
relative abundance
time (min)
exp.
0.0
0.5
1.0
1.5
2.0
2.5
3.0
0
20
40
60
80
100
120
140
160

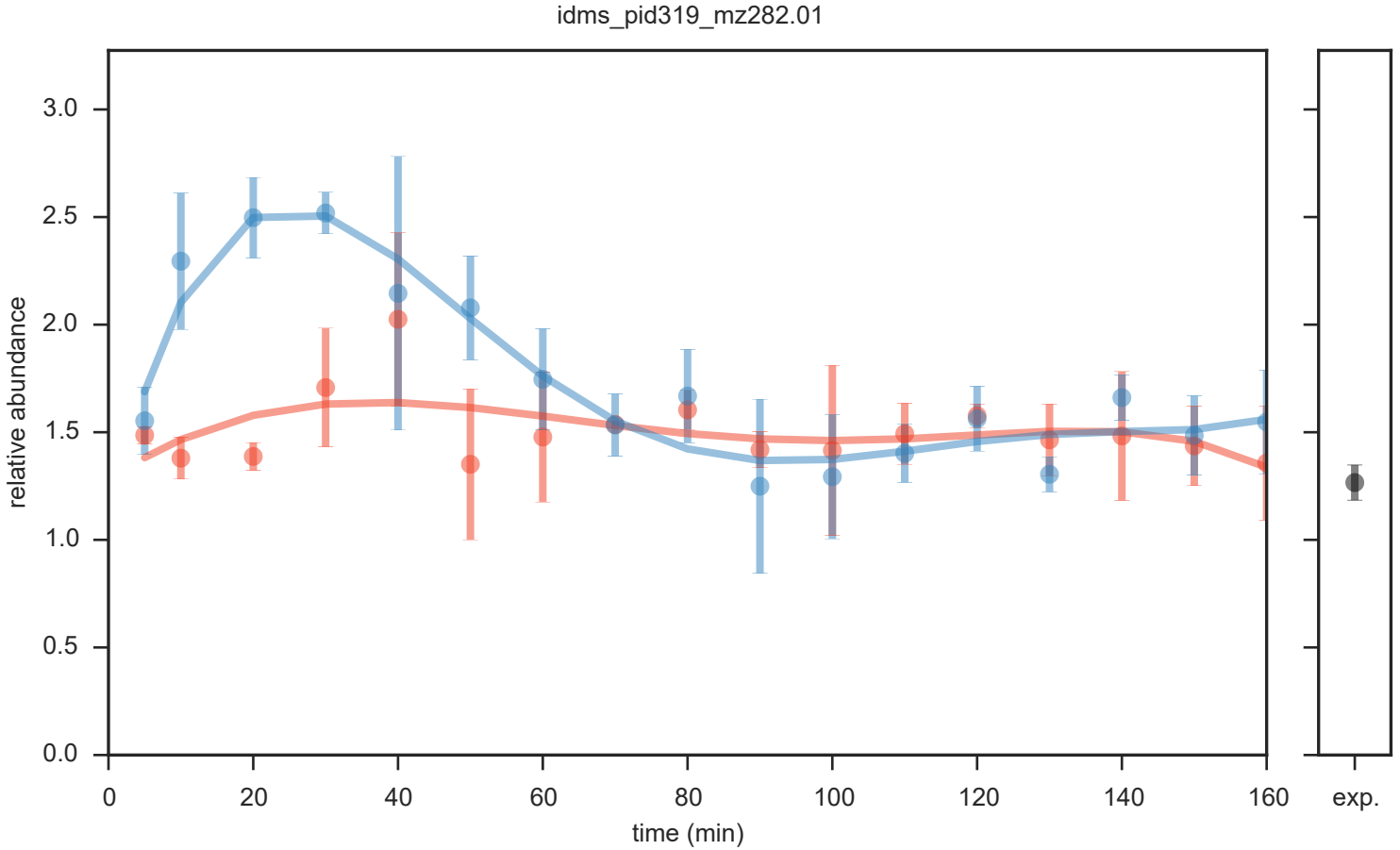

idms_pid299_mz214.01
relative abundance
0
2
4
6
8
0
20
40
60
80
100
120
140
160
time (min)
exp.

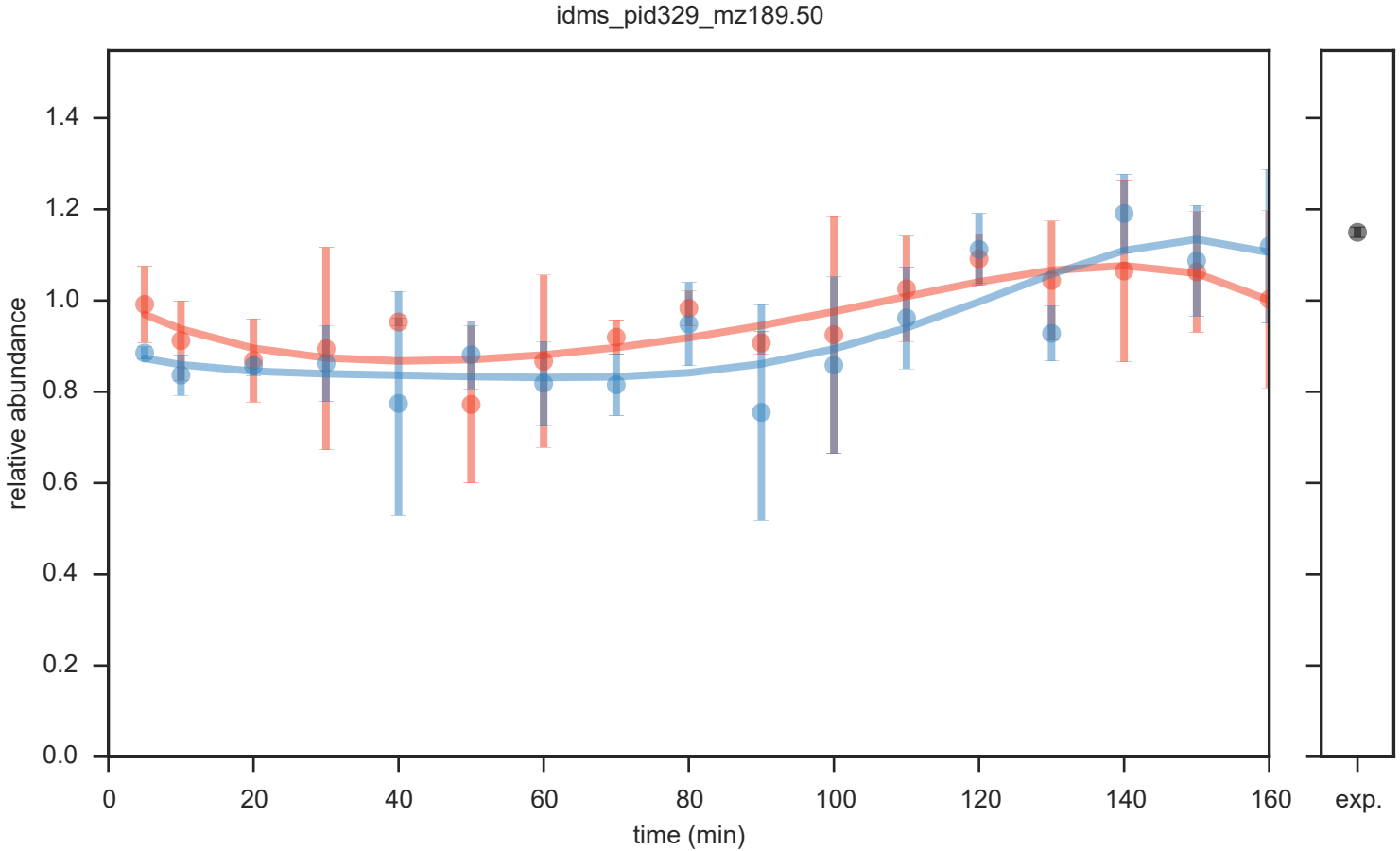

idms_pid304_mz206.94
relative abundance
time (min)
exp.
0
1
2
3
4
5
0
20
40
60
80
100
120
140
160

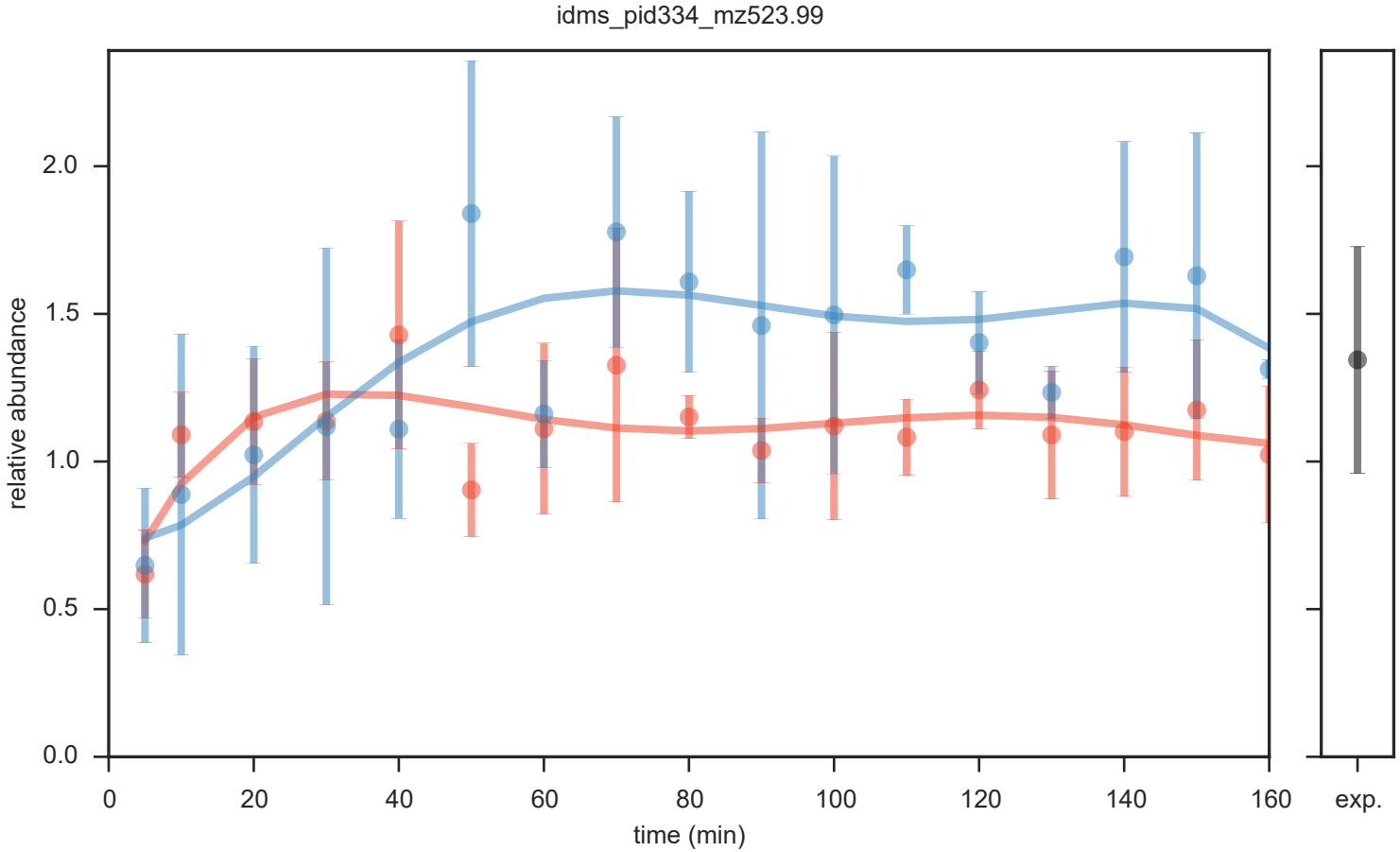

idms_pid311_mz274.09
relative abundance
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
0
20
40
60
80
100
120
140
160
time (min)
exp.

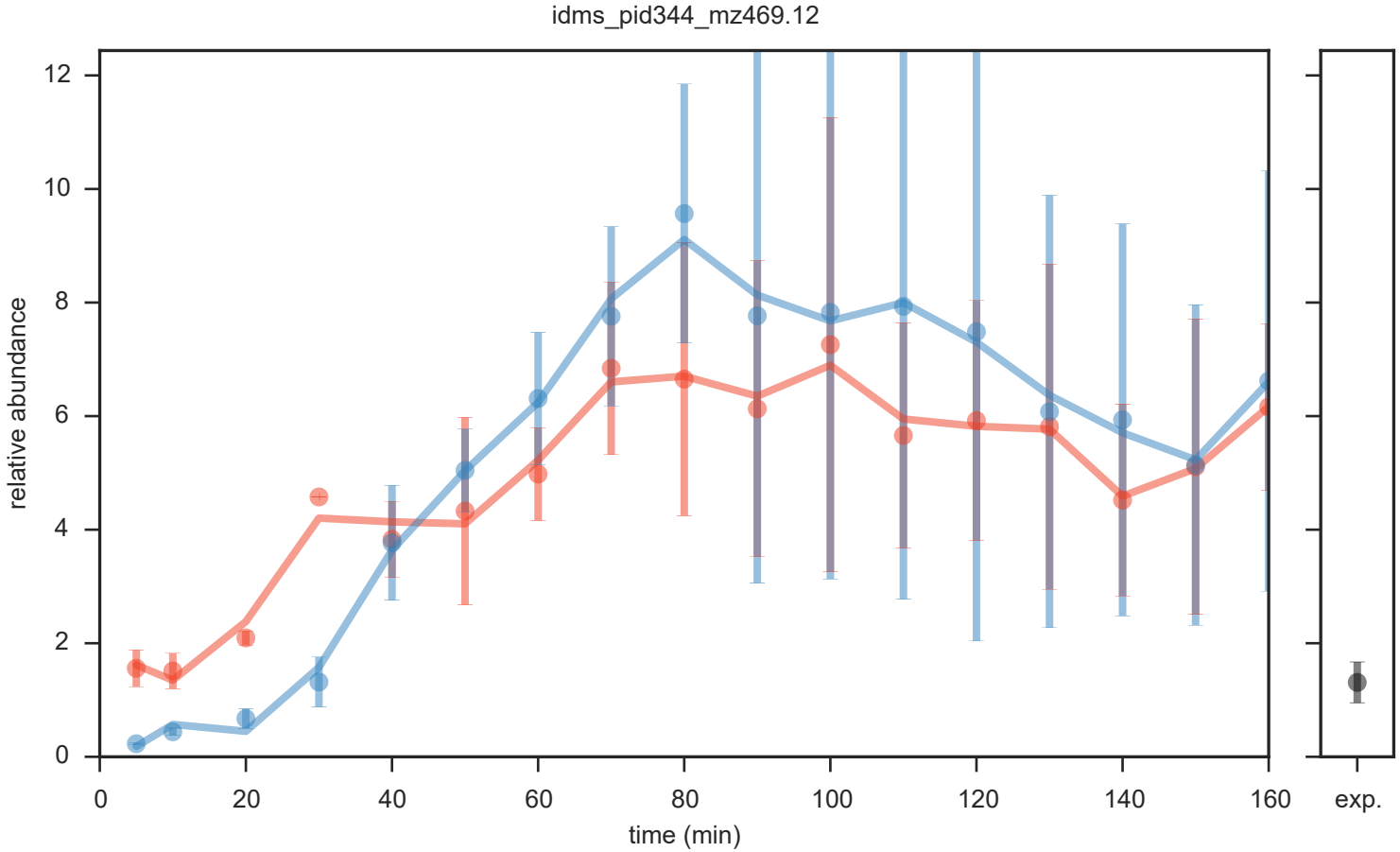

idms_pid316_mz344.03
relative abundance
time (min)
0
5
10
15
20
0
20
40
60
80
100
120
140
160
exp.

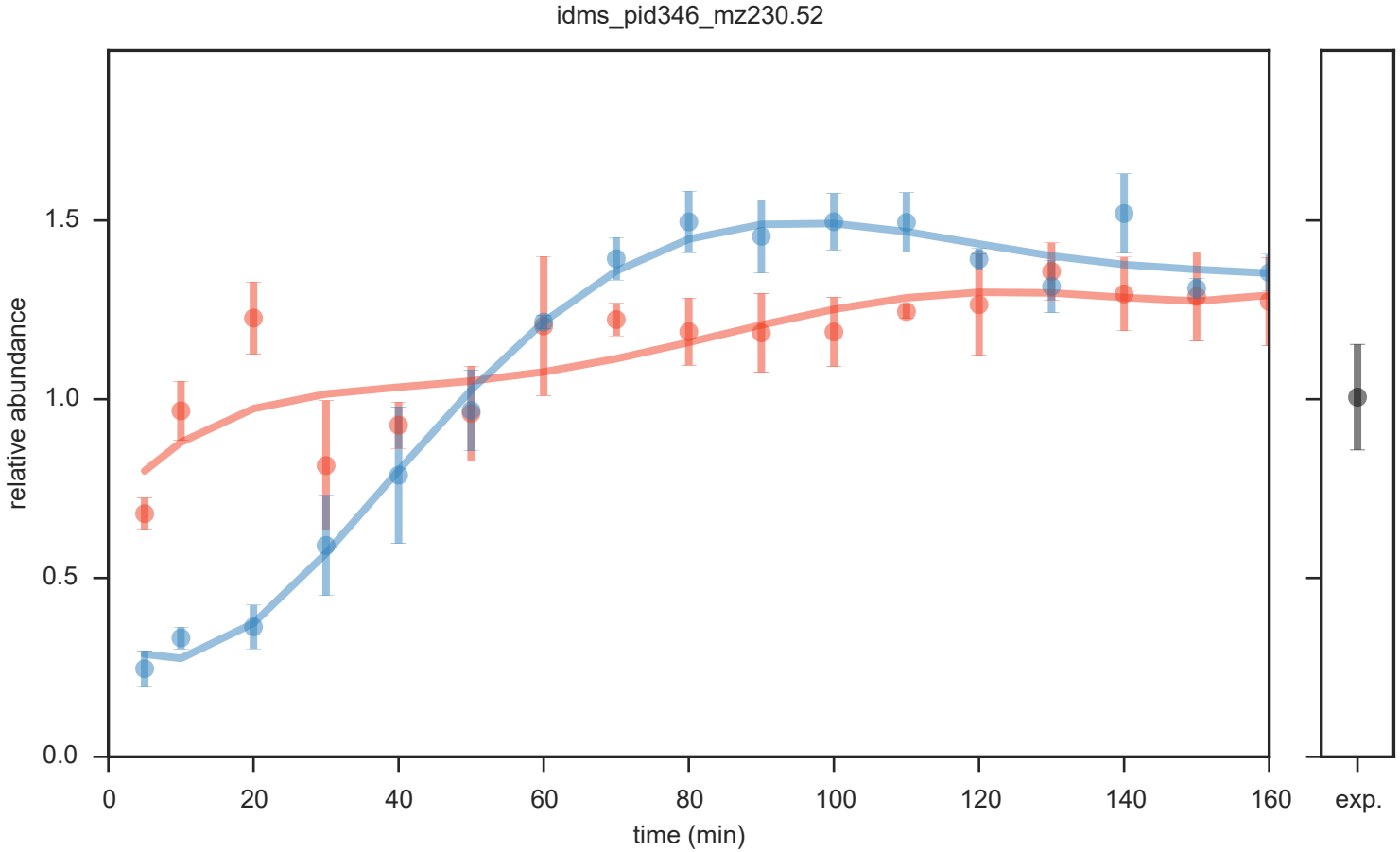

idms_pid317_mz289.03
relative abundance
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

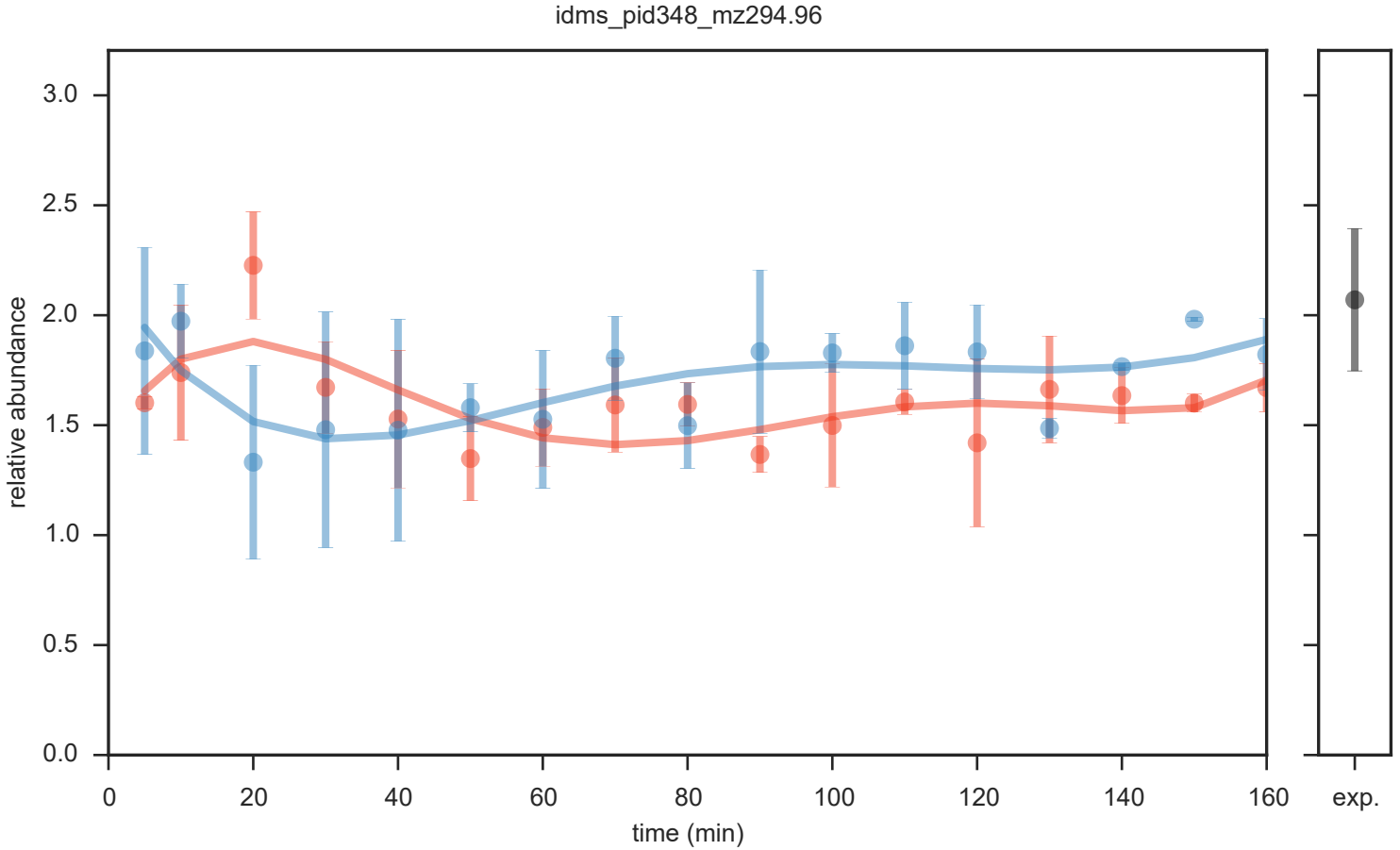

idms_pid319_mz282.01
relative abundance
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

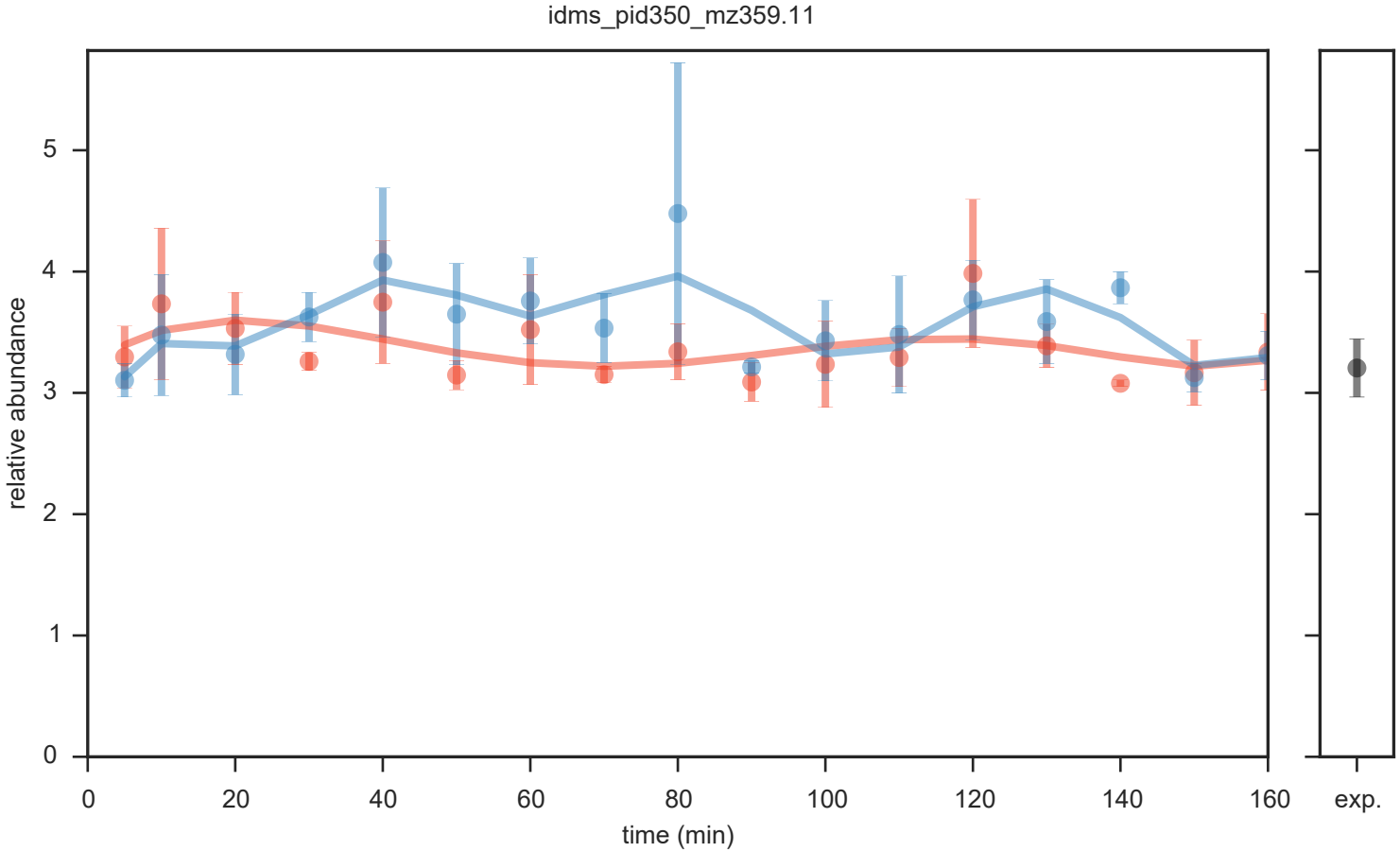

idms_pid329_mz189.50
relative abundance
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
0
20
40
60
80
100
120
140
160
time (min)
exp.

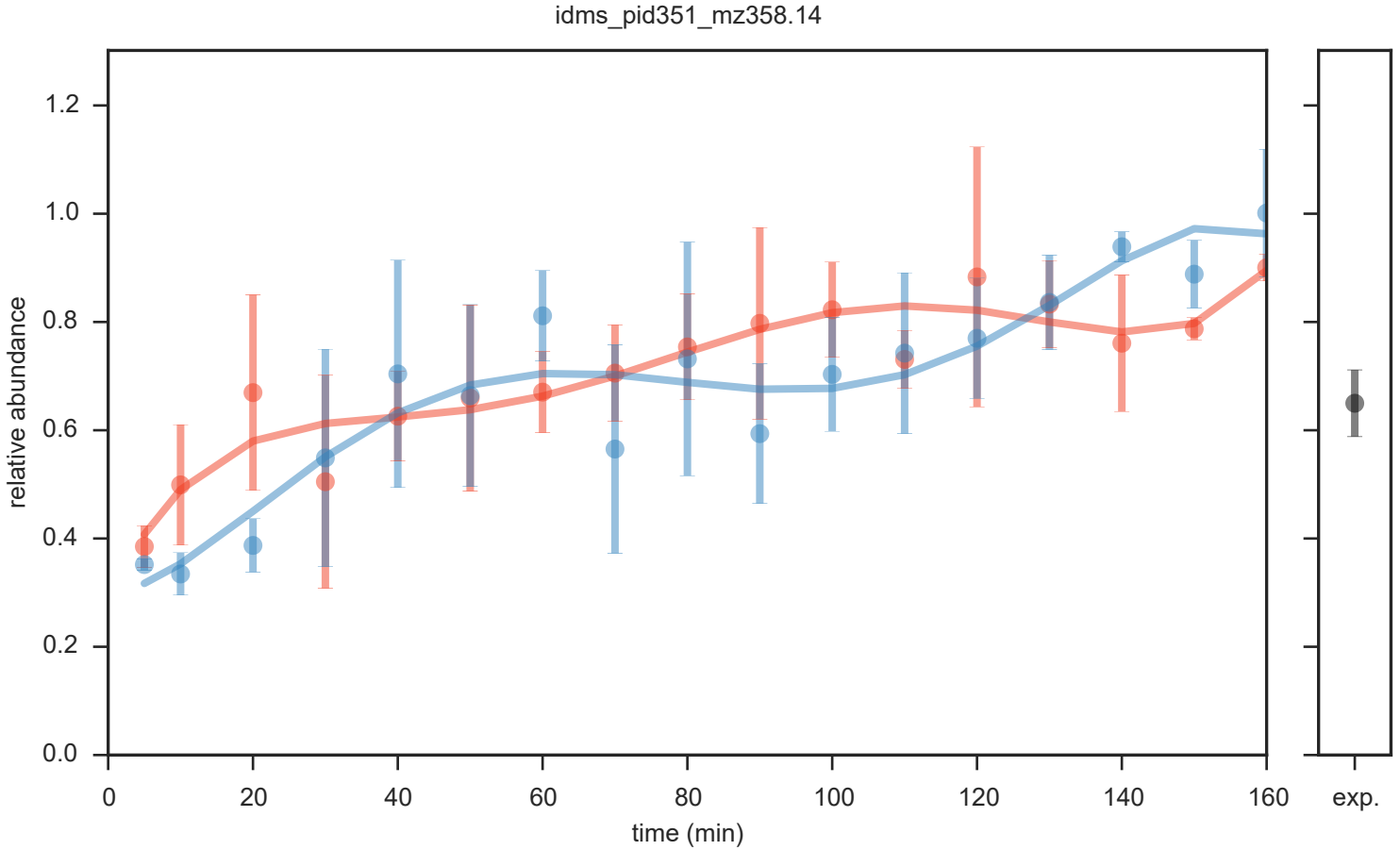

idms_pid334_mz523.99
relative abundance
0.0
0.5
1.0
1.5
2.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

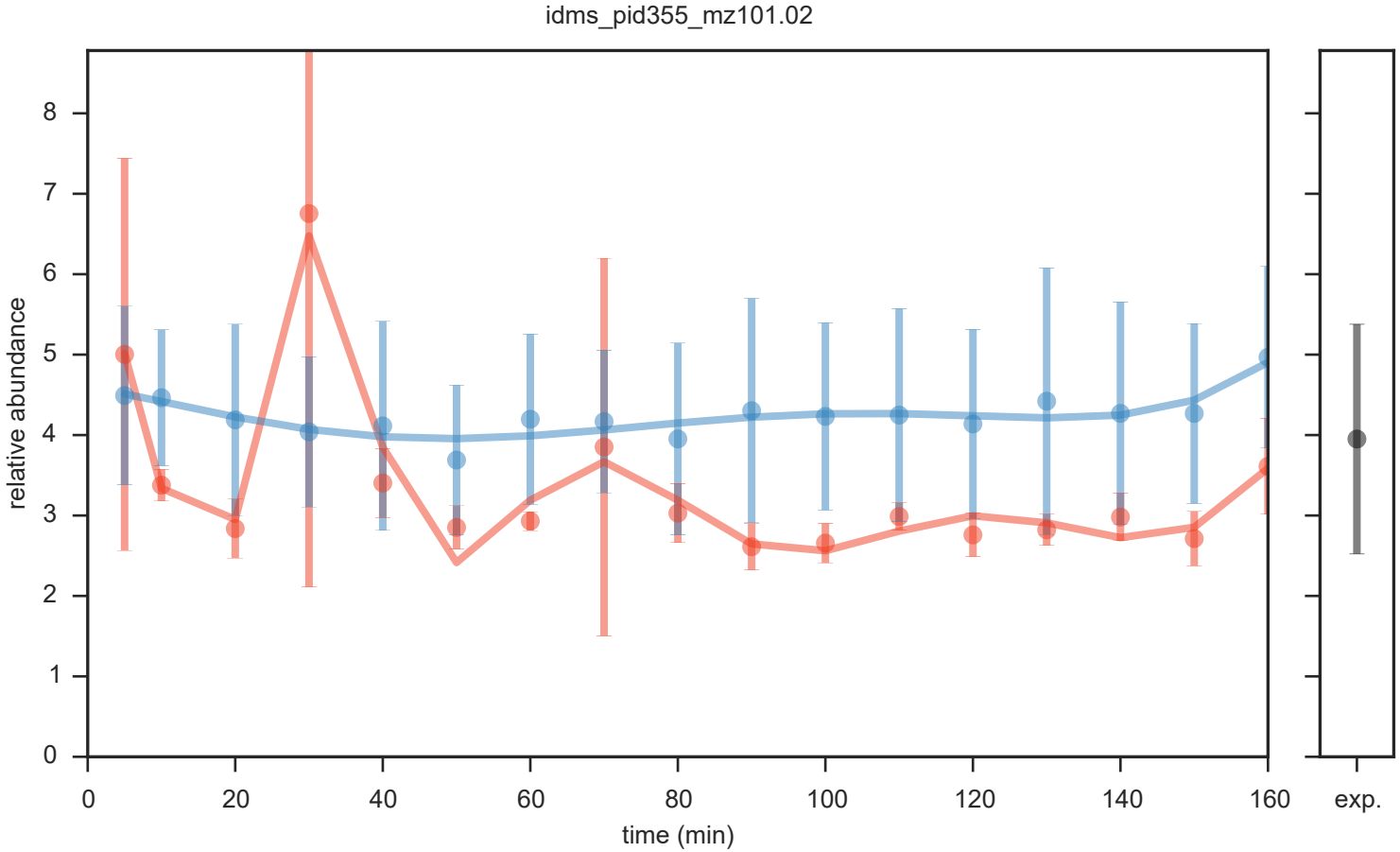

idms_pid344_mz469.12
relative abundance
time (min)
exp.
0
2
4
6
8
10
12
0
20
40
60
80
100
120
140
160

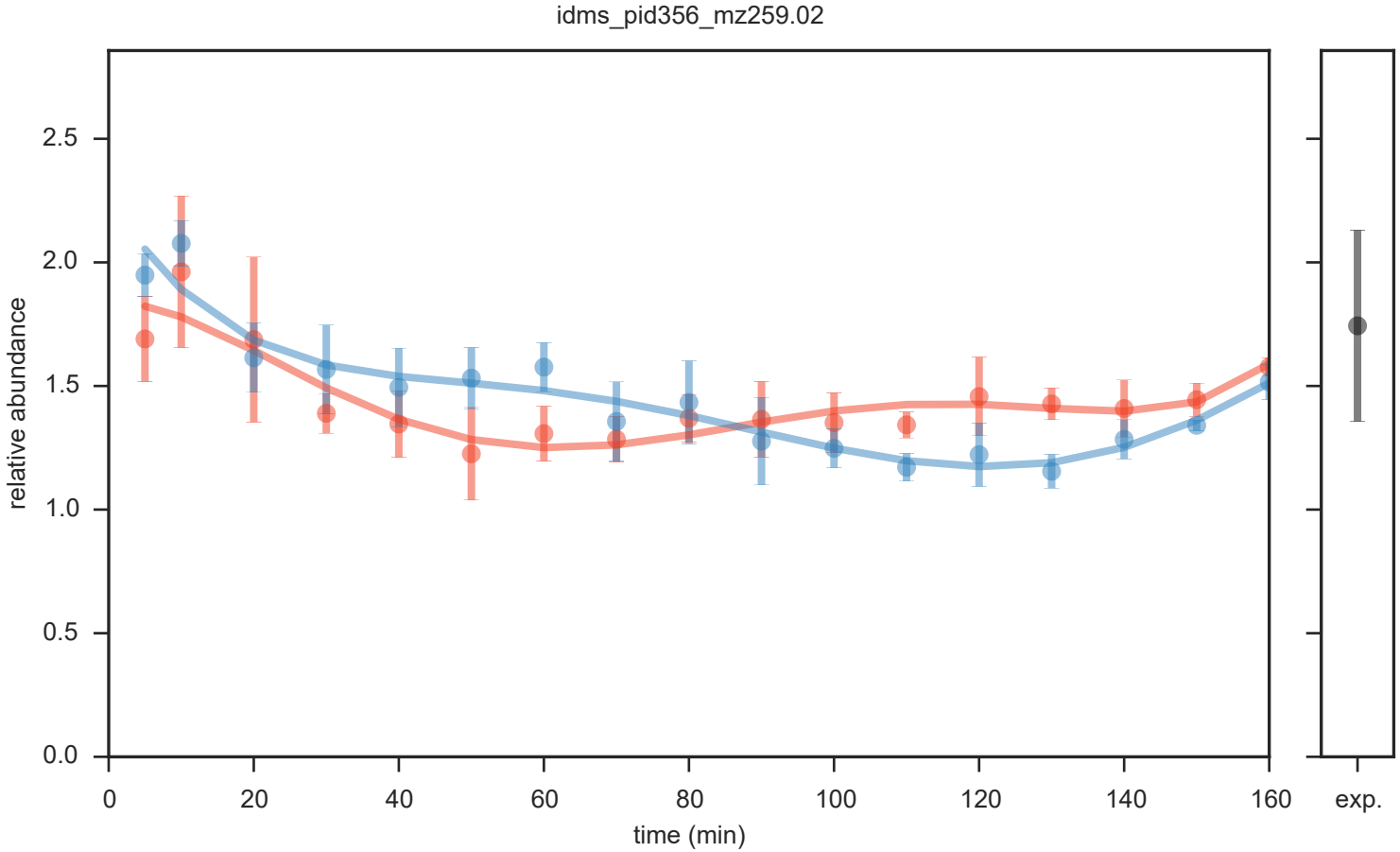

idms_pid346_mz230.52
relative abundance
0.0
0.5
1.0
1.5
0
20
40
60
80
100
120
140
160
time (min)
exp.

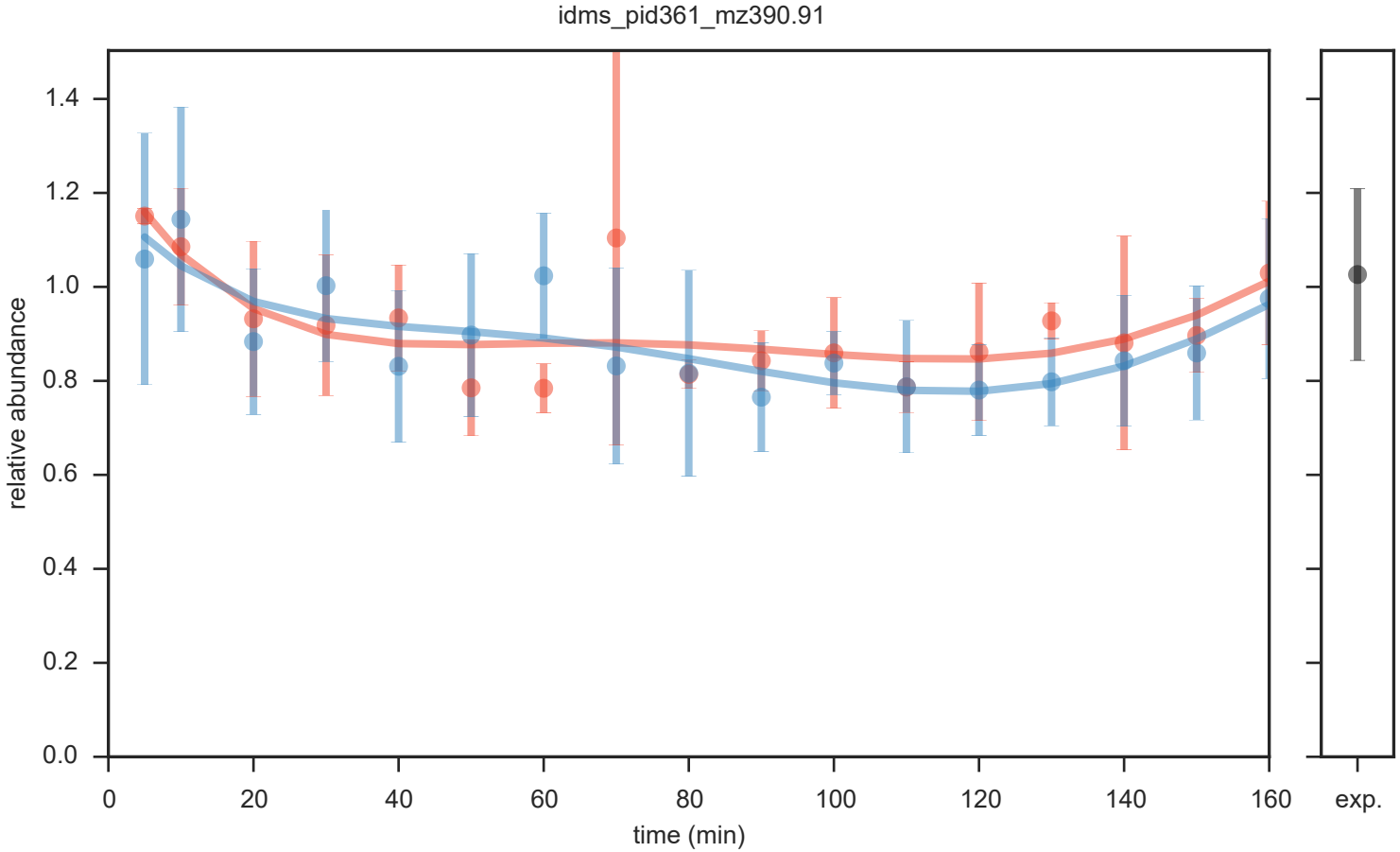

idms_pid348_mz294.96
relative abundance
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

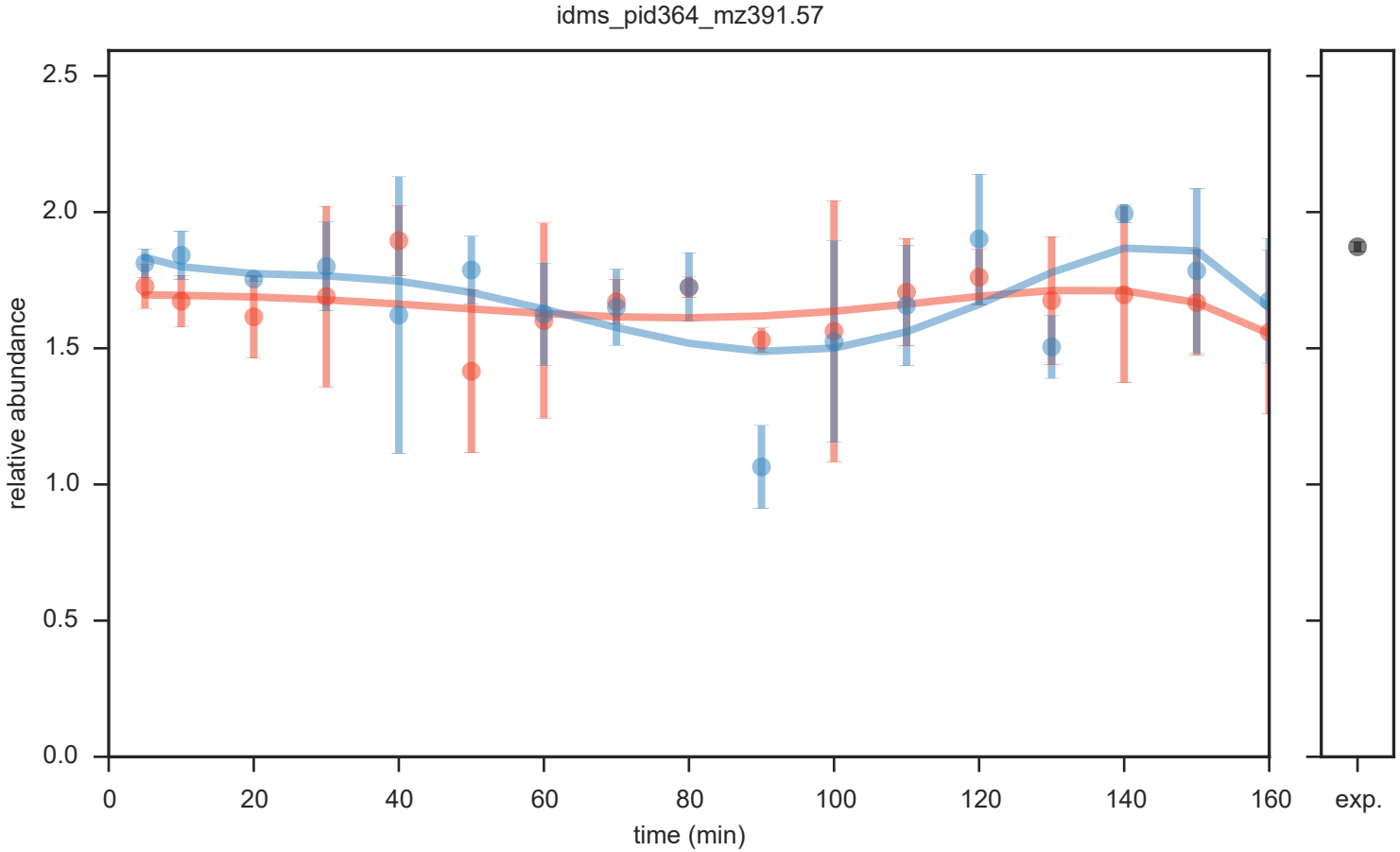

idms_pid350_mz359.11
relative abundance
0
1
2
3
4
5
0
20
40
60
80
100
120
140
160
time (min)
exp.

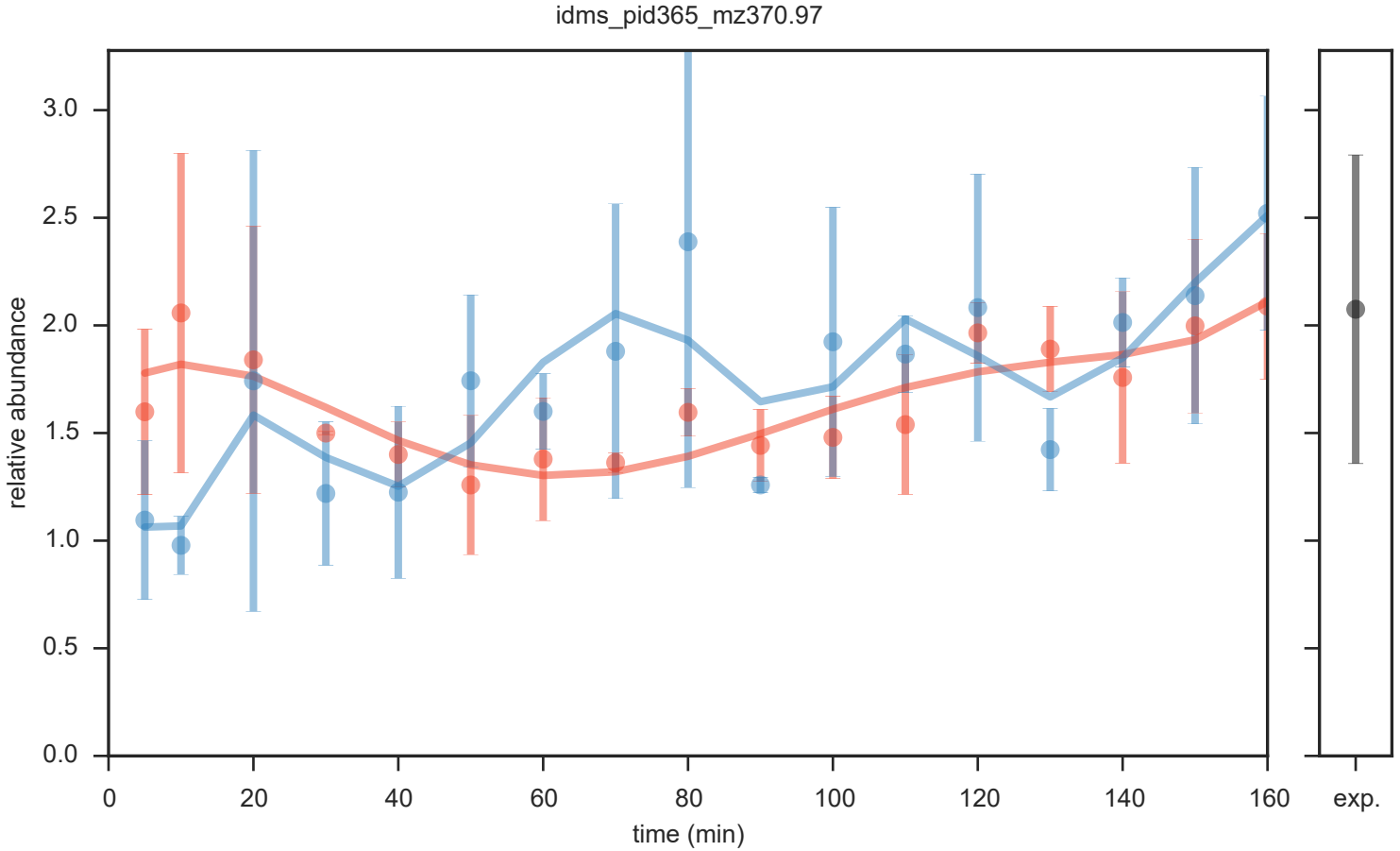

idms_pid351_mz358.14
relative abundance
0.0
0.2
0.4
0.6
0.8
1.0
1.2
0
20
40
60
80
100
120
140
160
time (min)
exp.

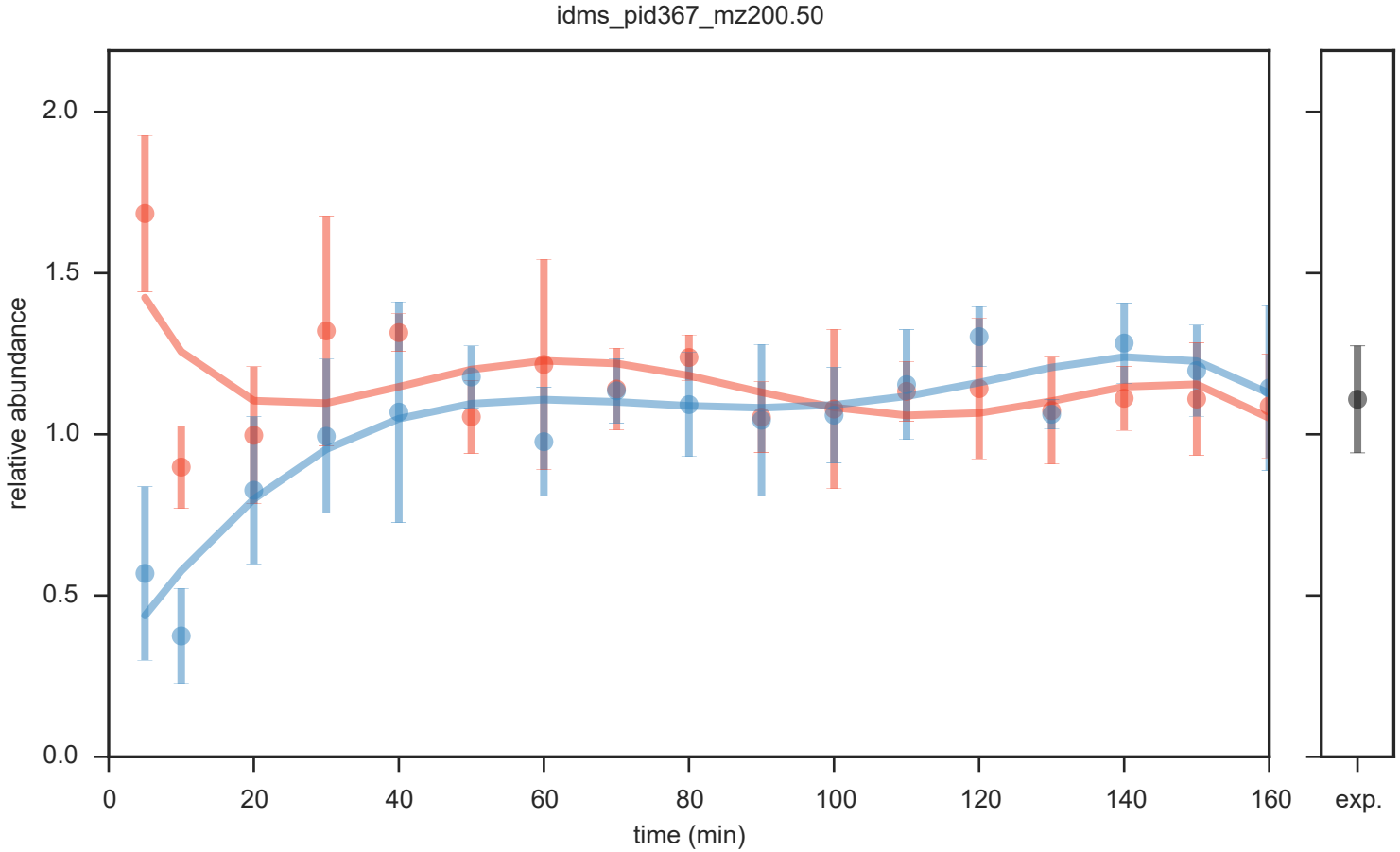

idms_pid355_mz101.02
relative abundance
0
1
2
3
4
5
6
7
8
0
20
40
60
80
100
120
140
160
time (min)
exp.

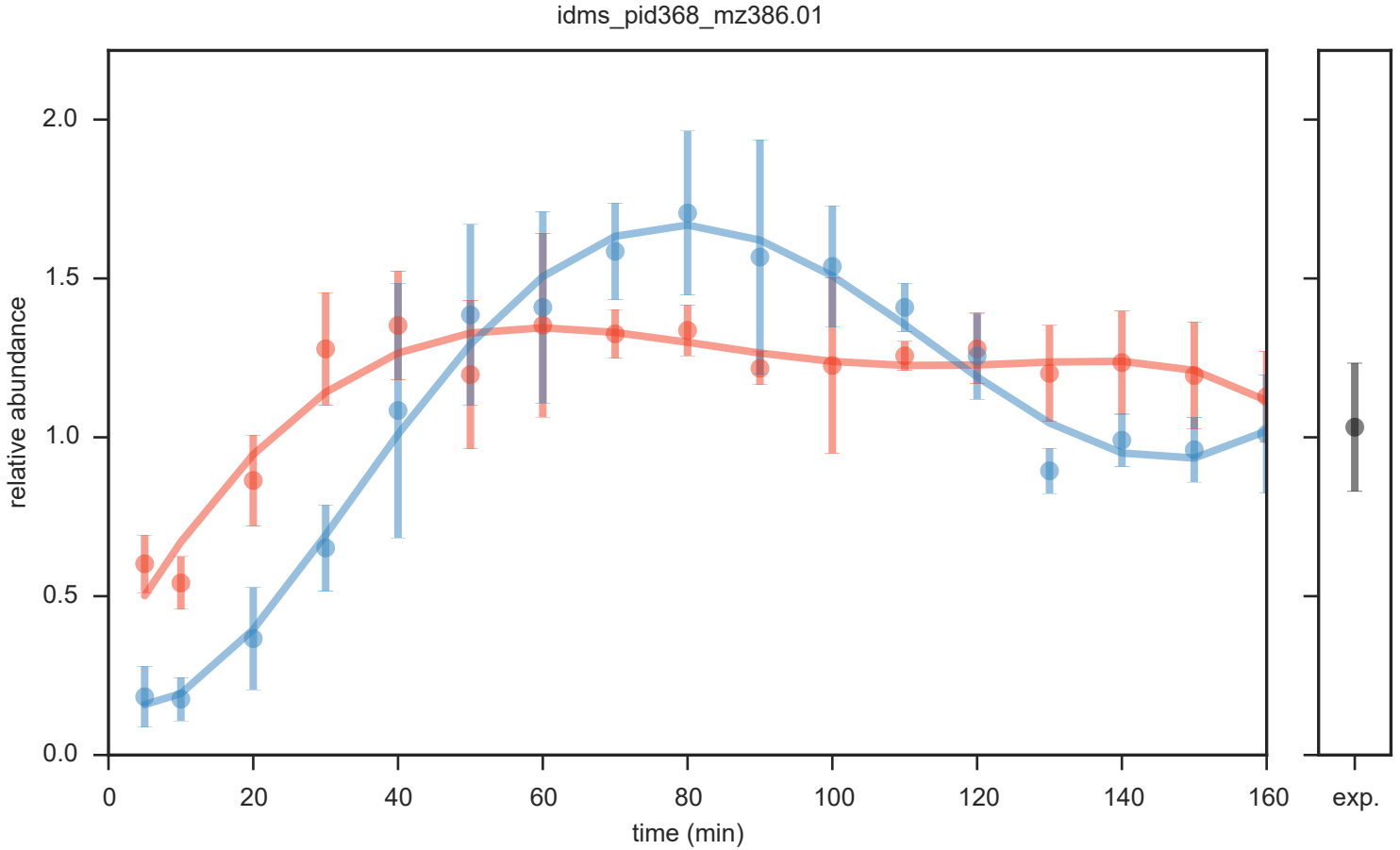

idms_pid356_mz259.02
relative abundance
0.0
0.5
1.0
1.5
2.0
2.5
0
20
40
60
80
100
120
140
160
time (min)
exp.

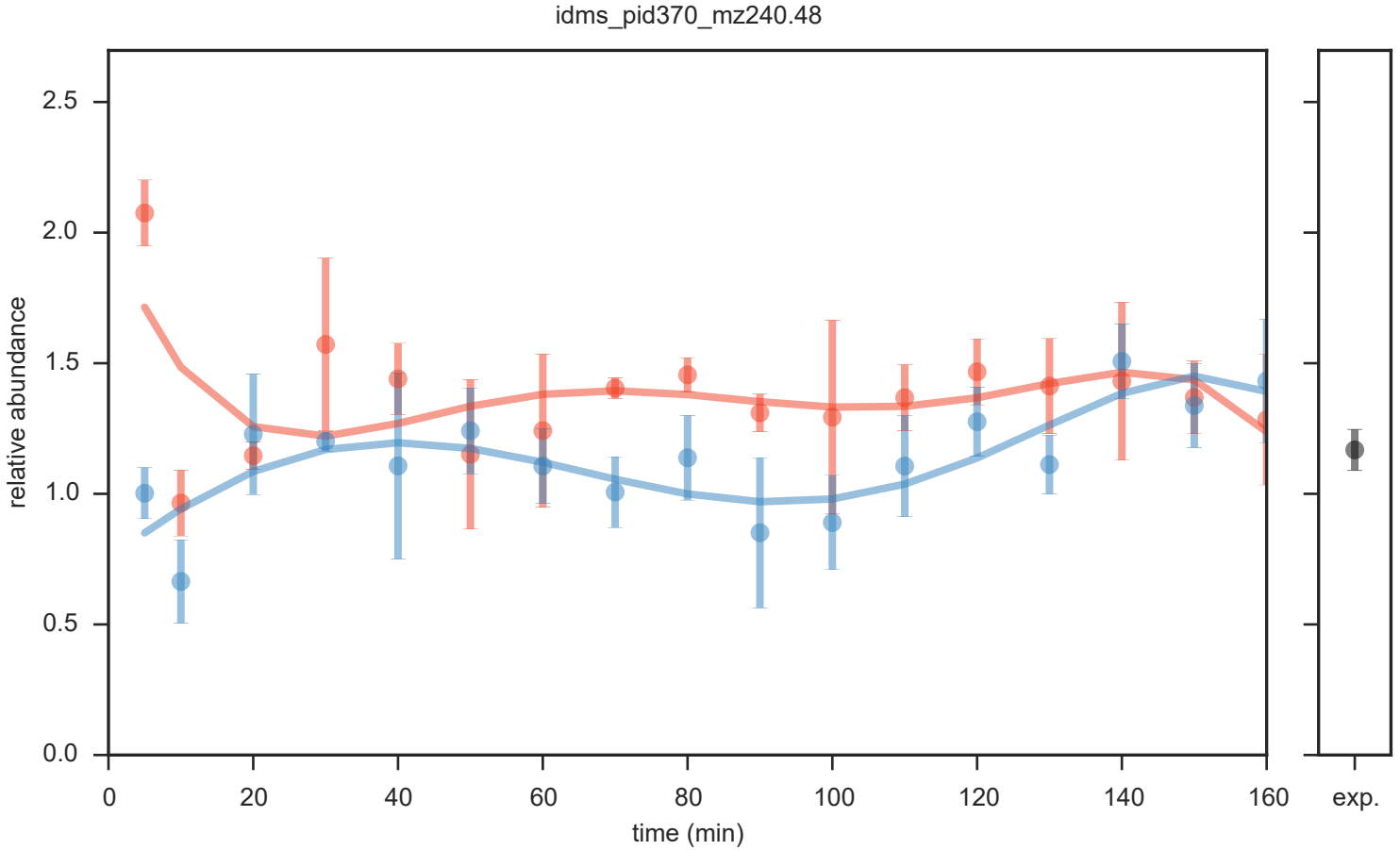

idms_pid361_mz390.91
relative abundance
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
0
20
40
60
80
100
120
140
160
time (min)
exp.

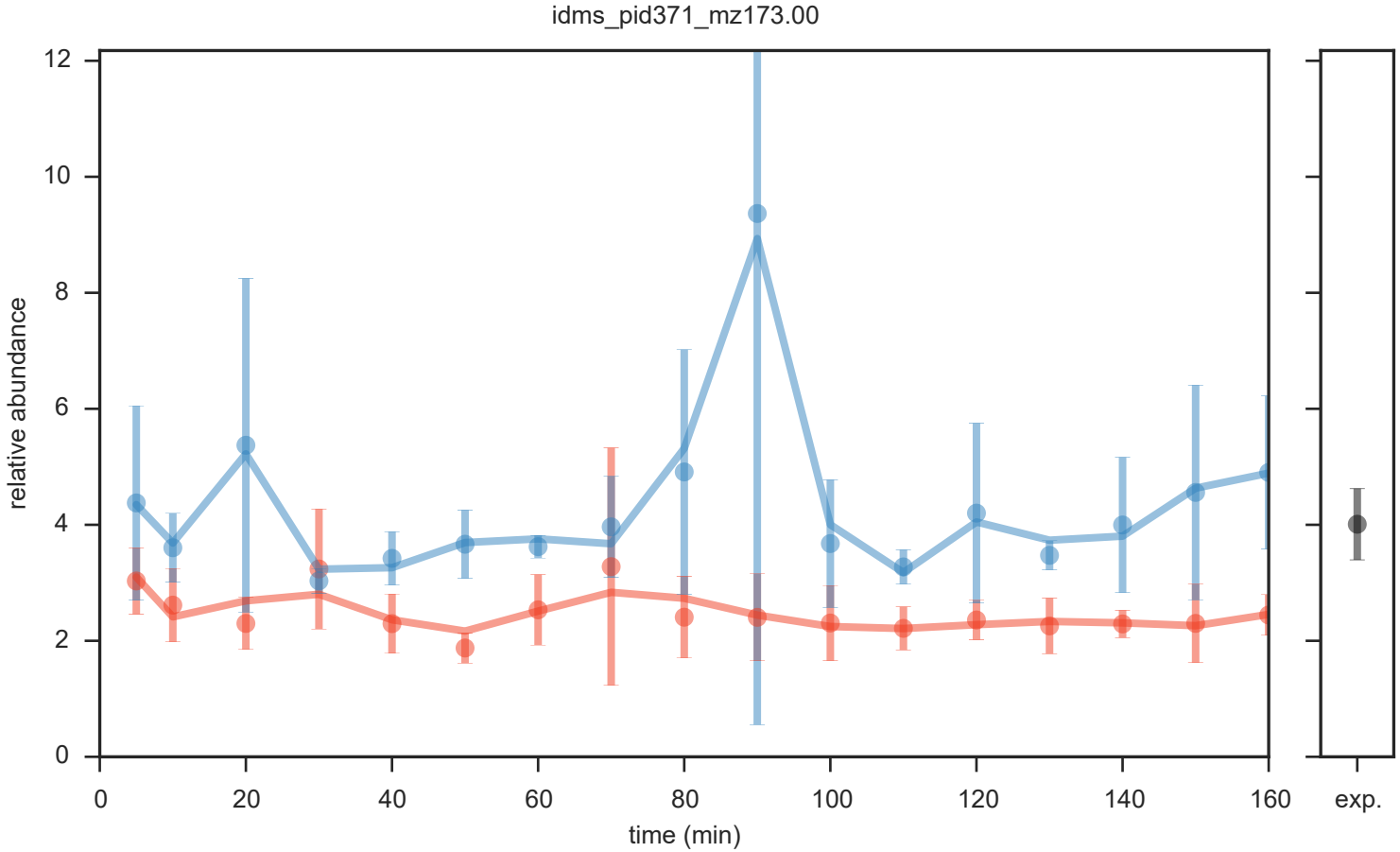

idms_pid364_mz391.57
relative abundance
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

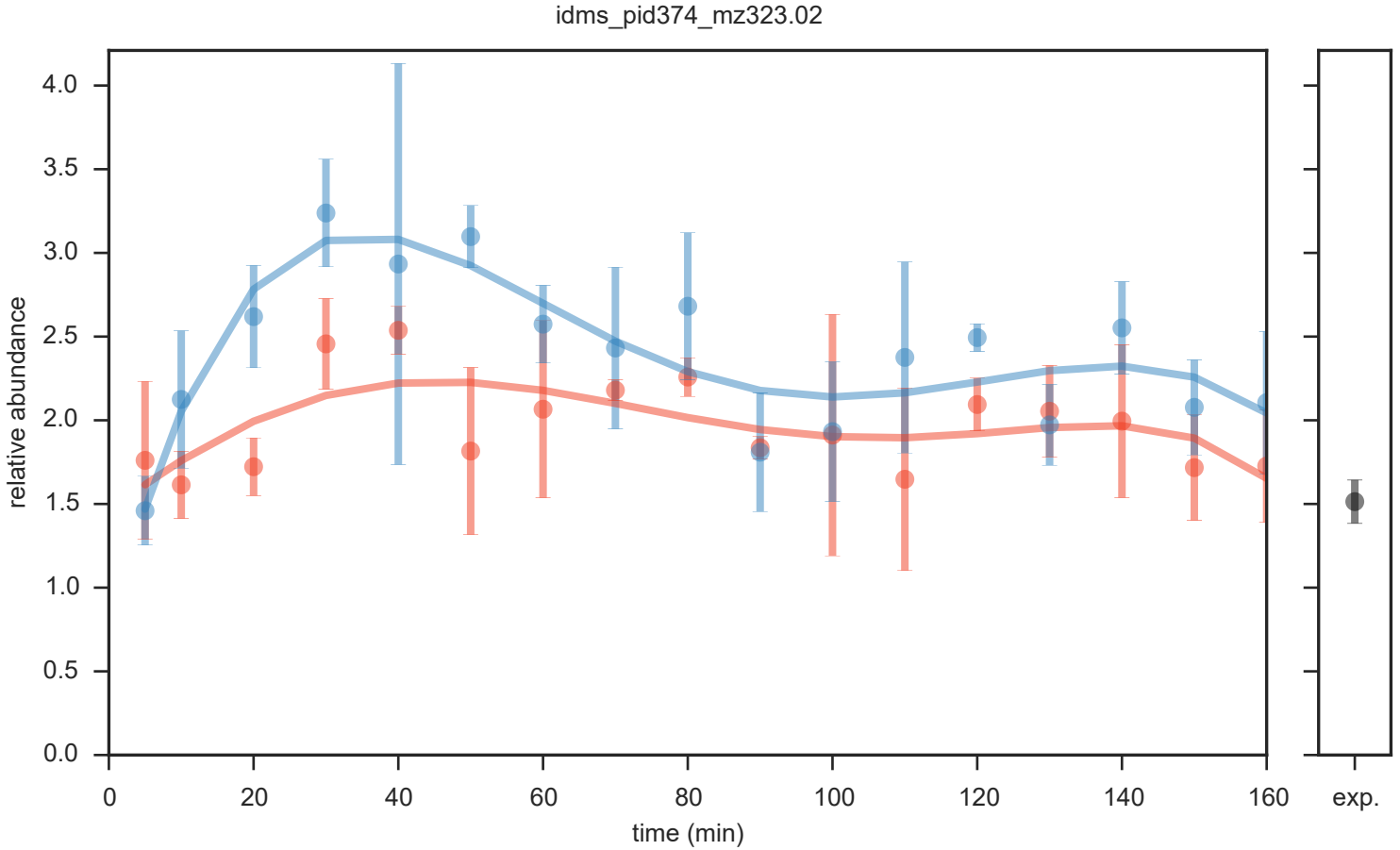

idms_pid365_mz370.97
relative abundance
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

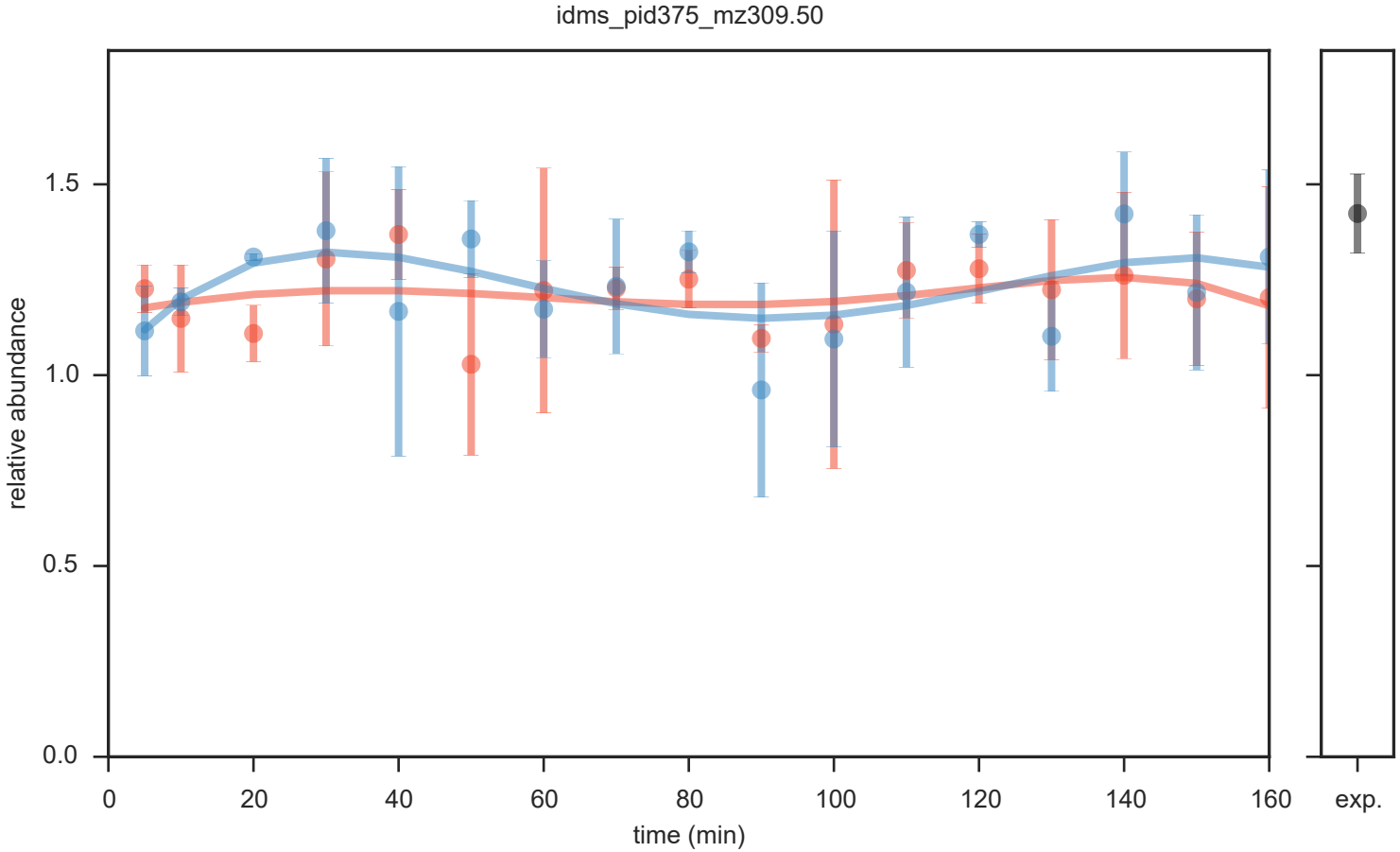

idms_pid367_mz200.50
relative abundance
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

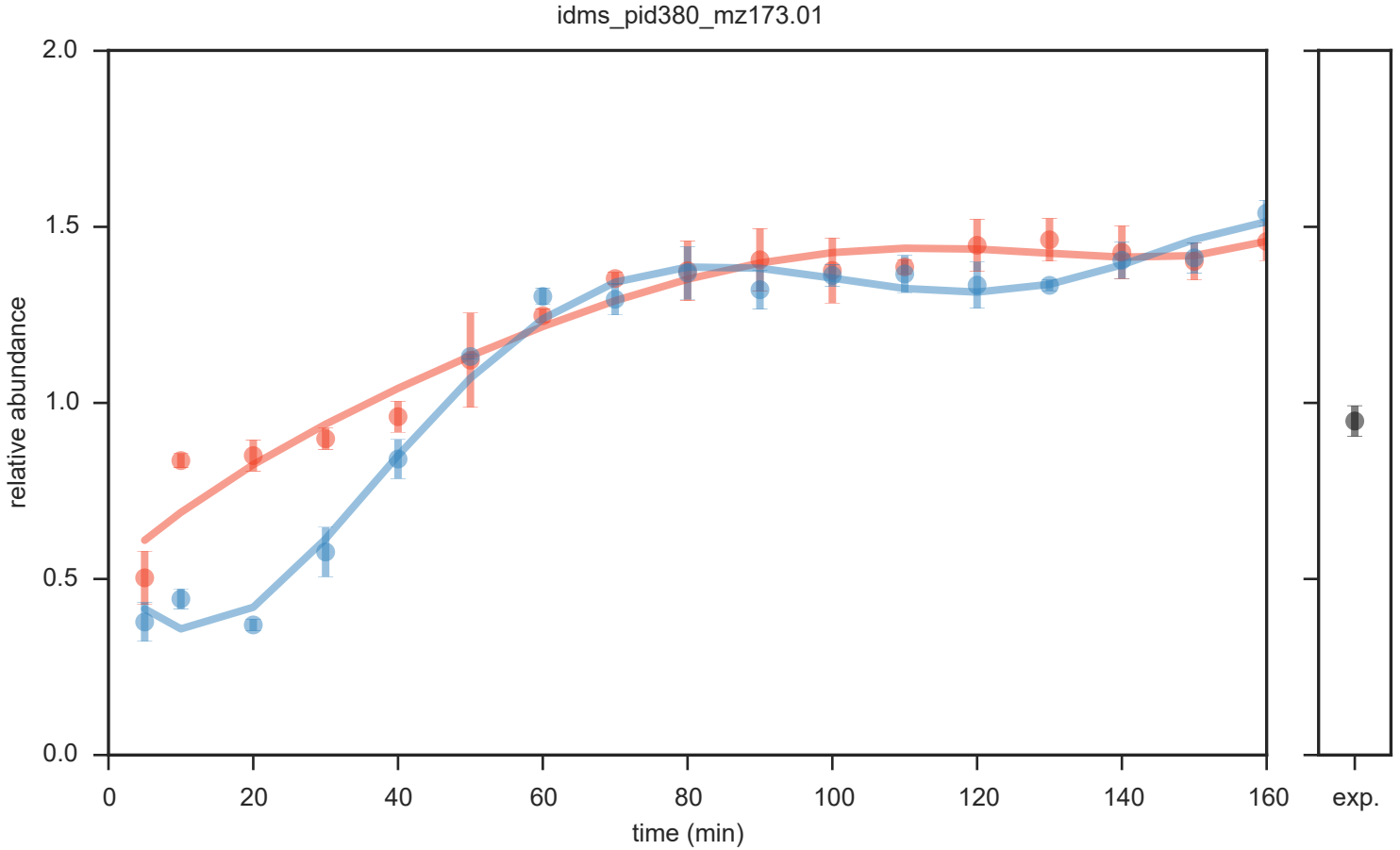

idms_pid368_mz386.01
relative abundance
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

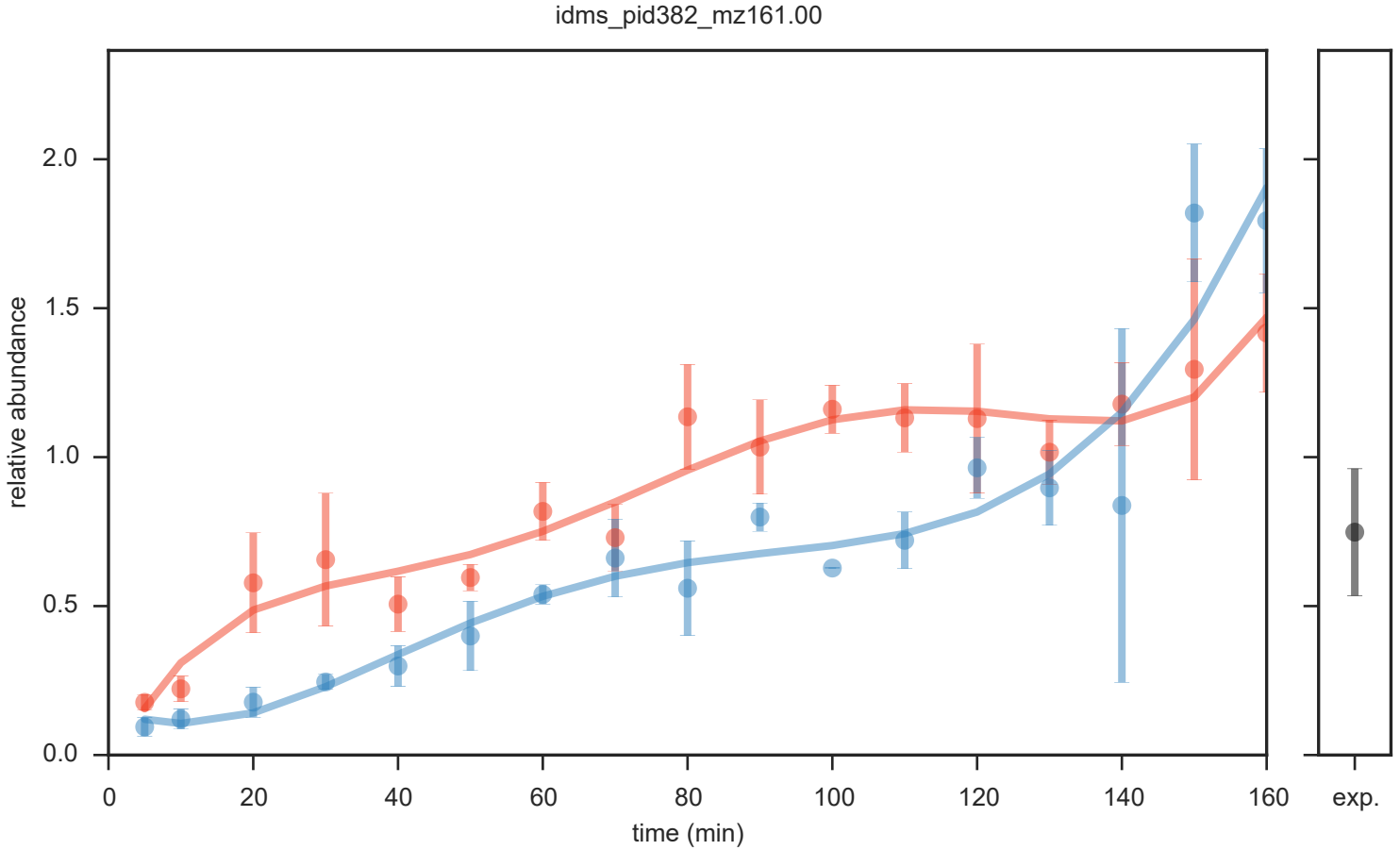

idms_pid370_mz240.48
relative abundance
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

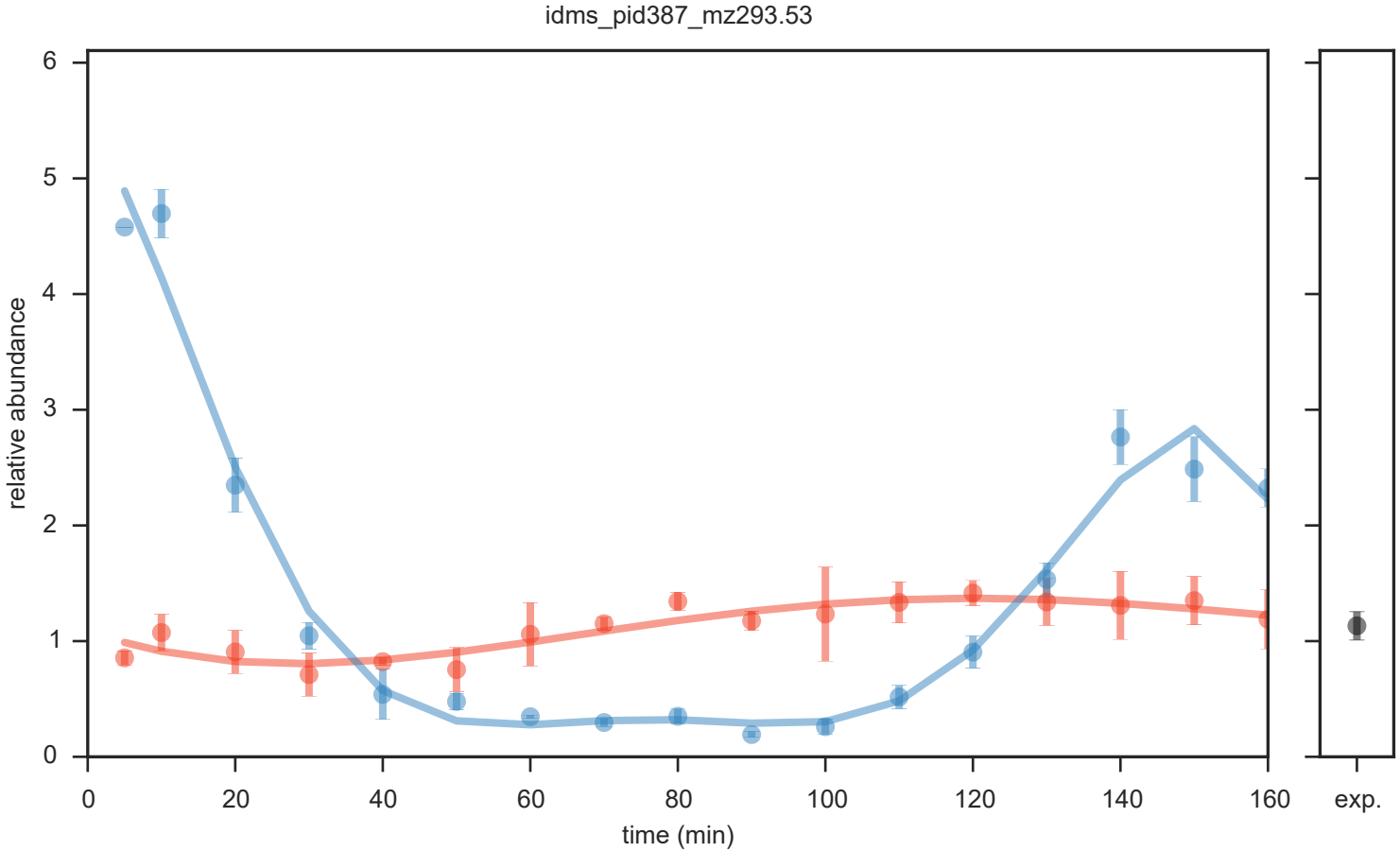

idms_pid371_mz173.00
relative abundance
time (min)
exp.
0
2
4
6
8
10
12
0
20
40
60
80
100
120
140
160

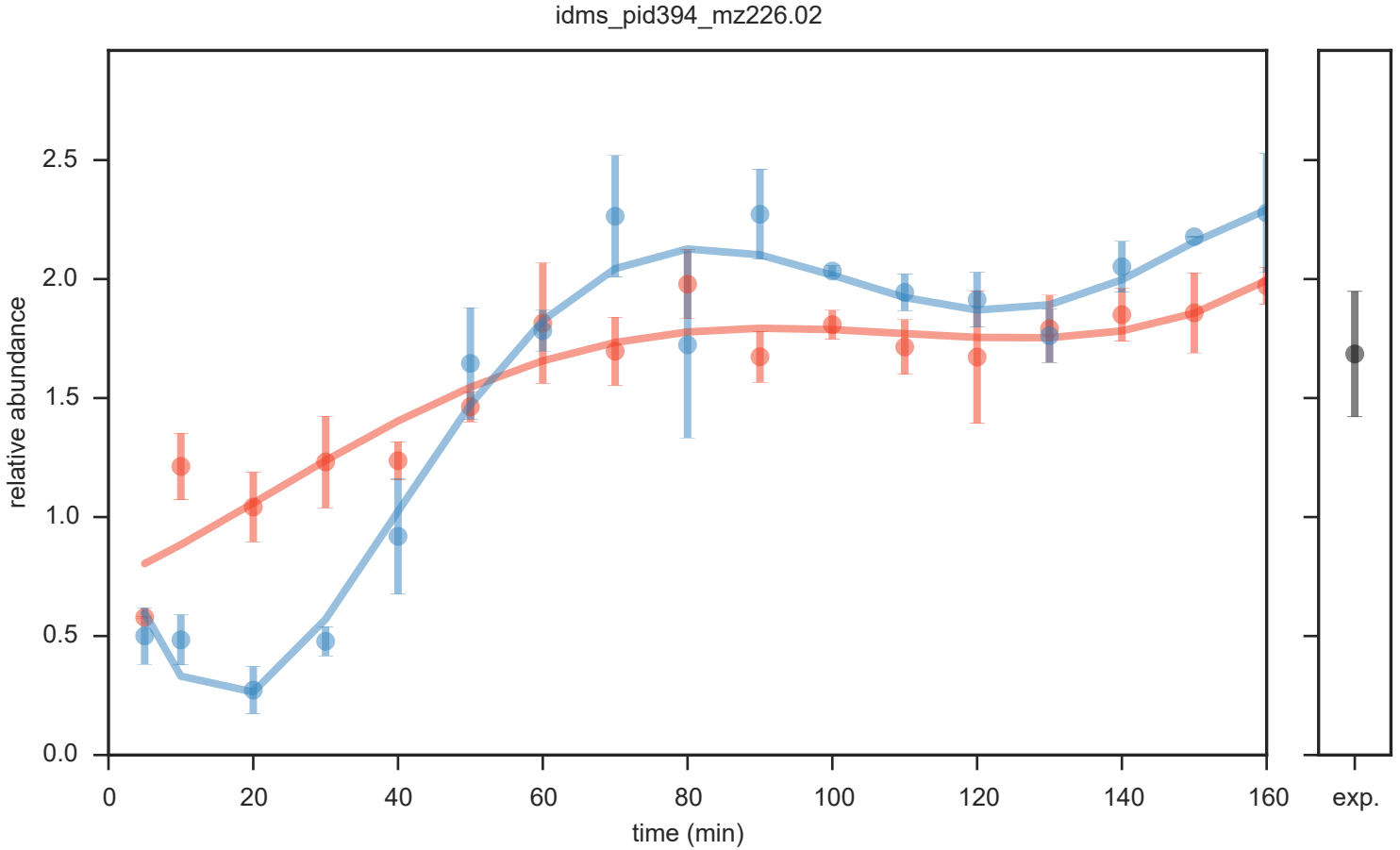

idms_pid374_mz323.02
relative abundance
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

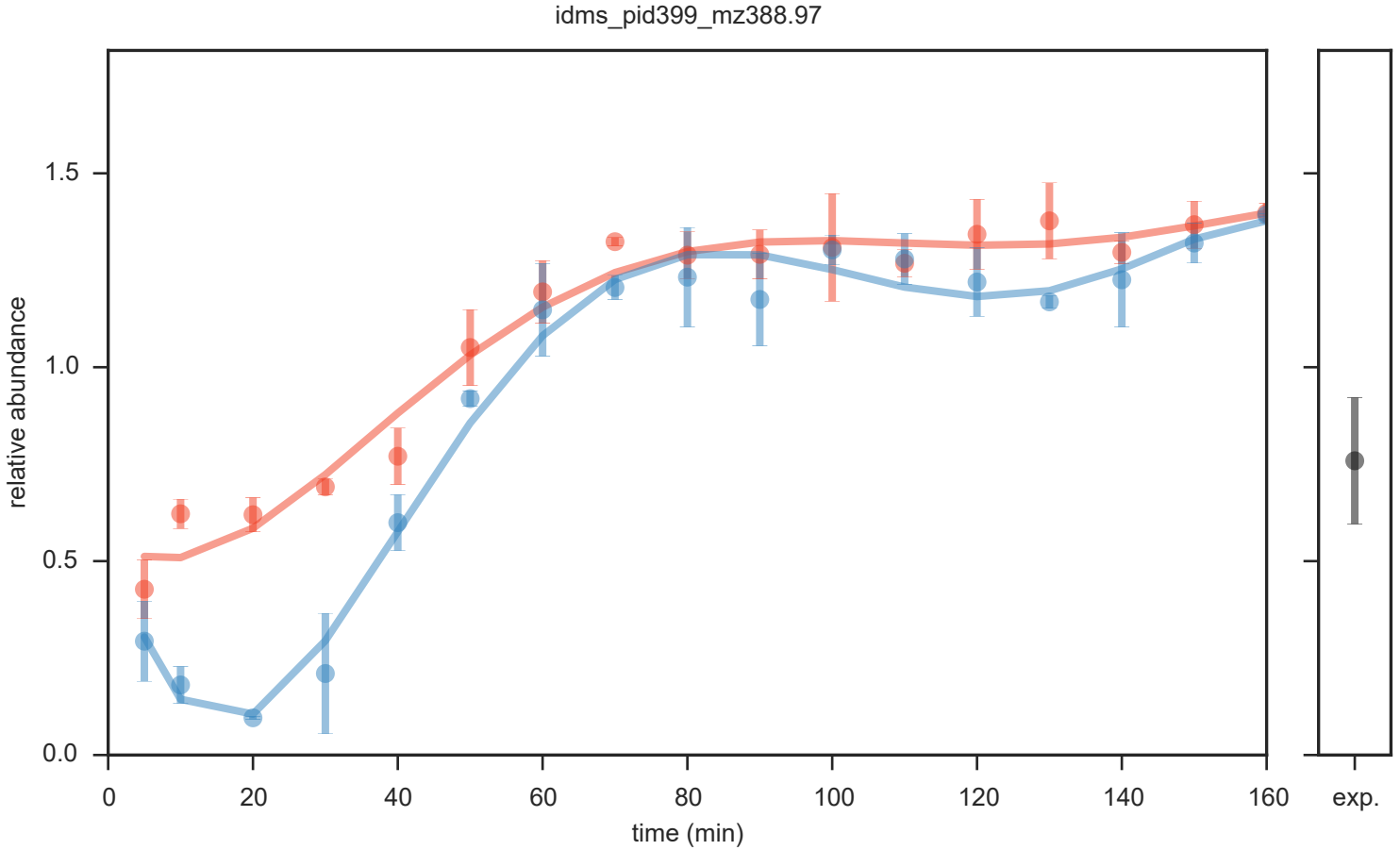

idms_pid375_mz309.50
relative abundance
0.0
0.5
1.0
1.5
0
20
40
60
80
100
120
140
160
time (min)
exp.

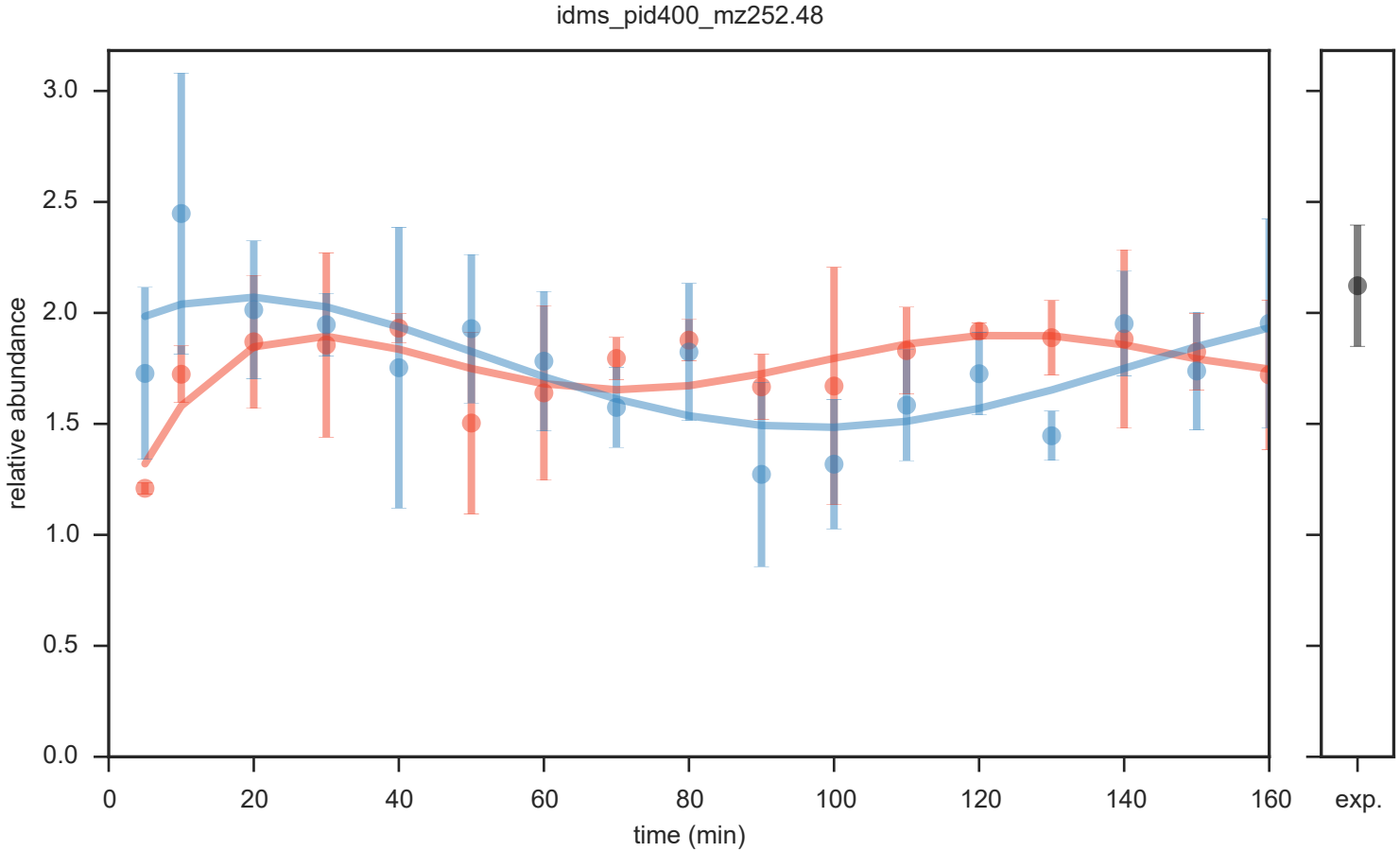

idms_pid380_mz173.01
relative abundance
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

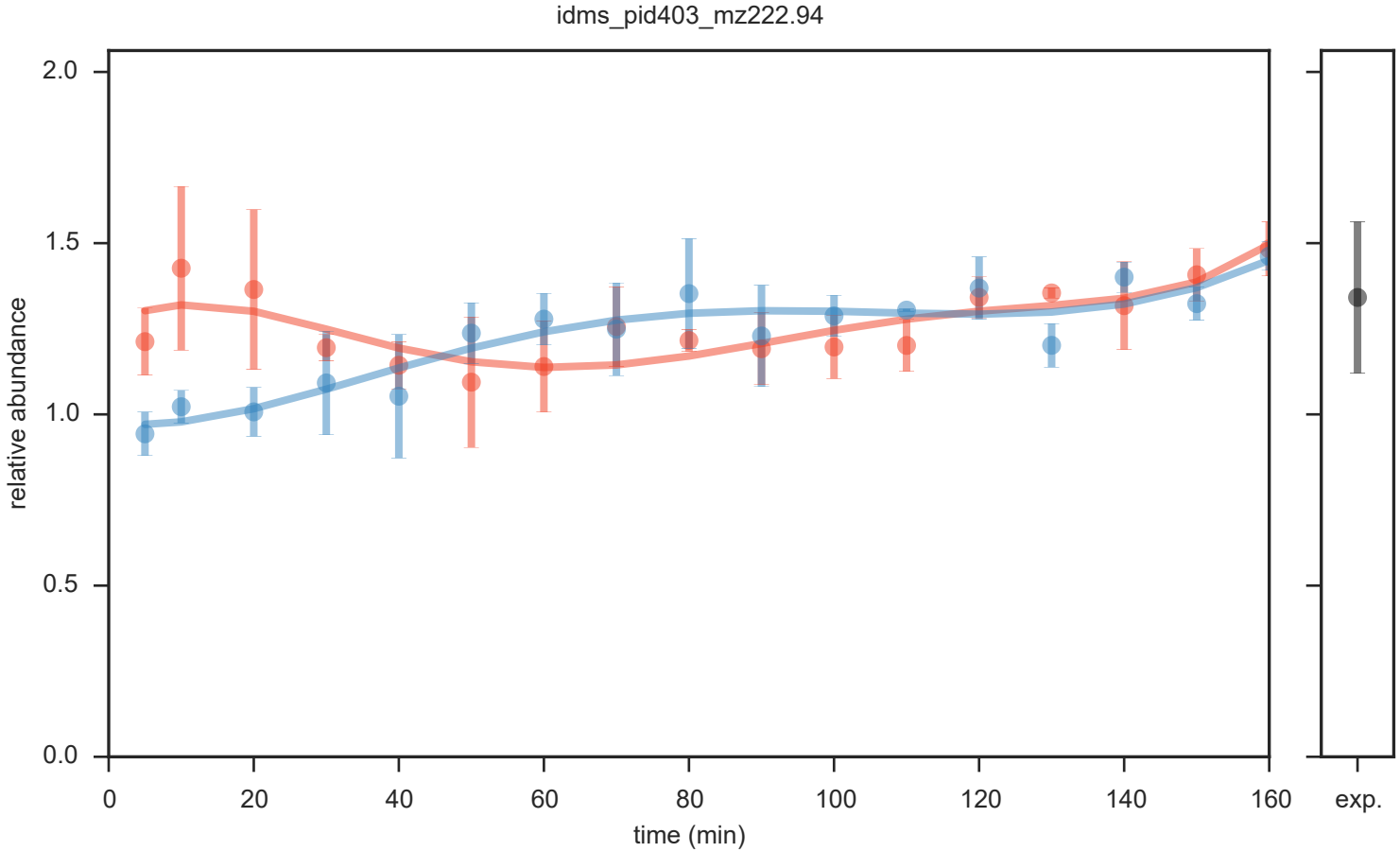

idms_pid382_mz161.00
relative abundance
0.0
0.5
1.0
1.5
2.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

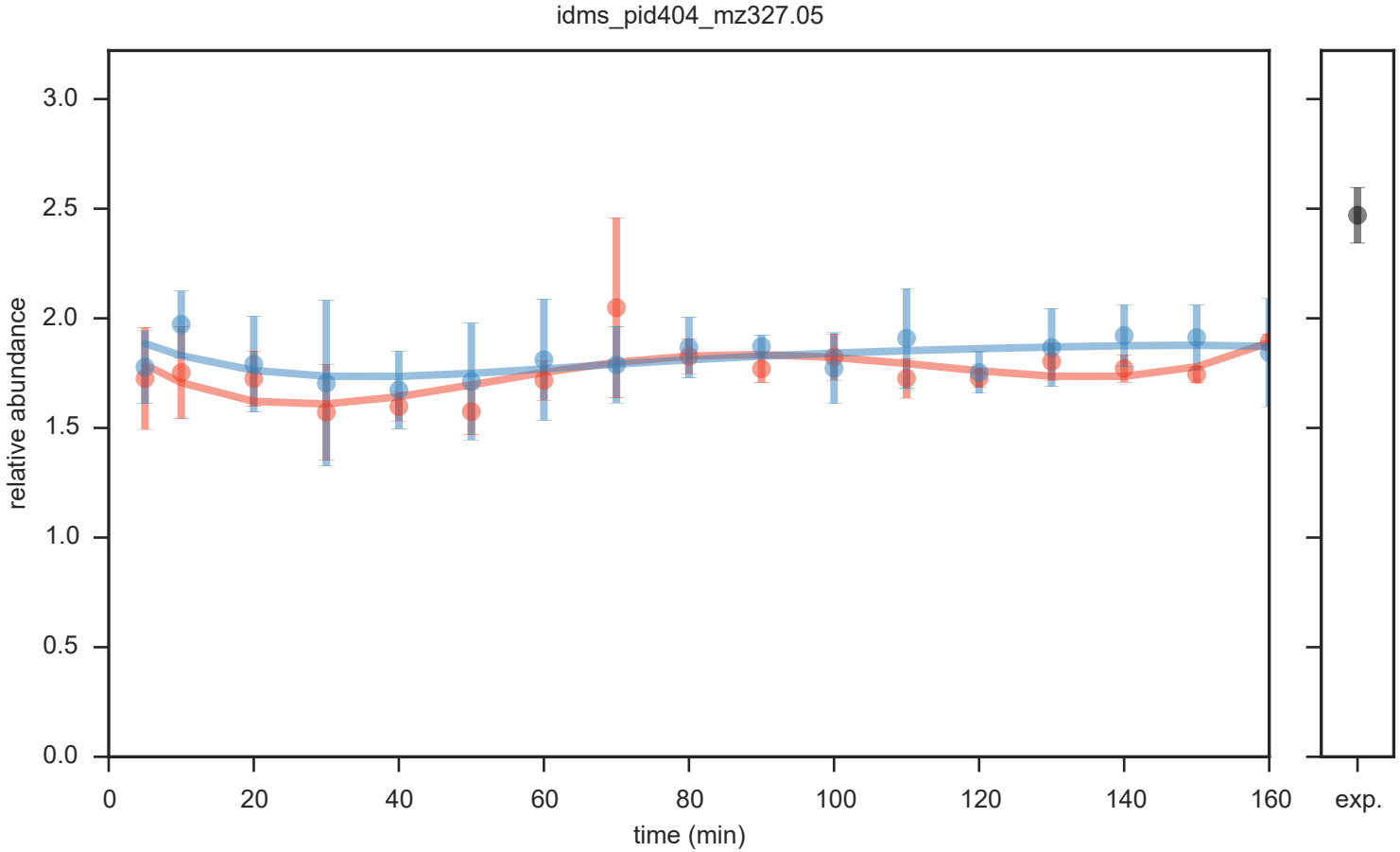

idms_pid387_mz293.53
relative abundance
time (min)
exp.
0
1
2
3
4
5
6
0
20
40
60
80
100
120
140
160

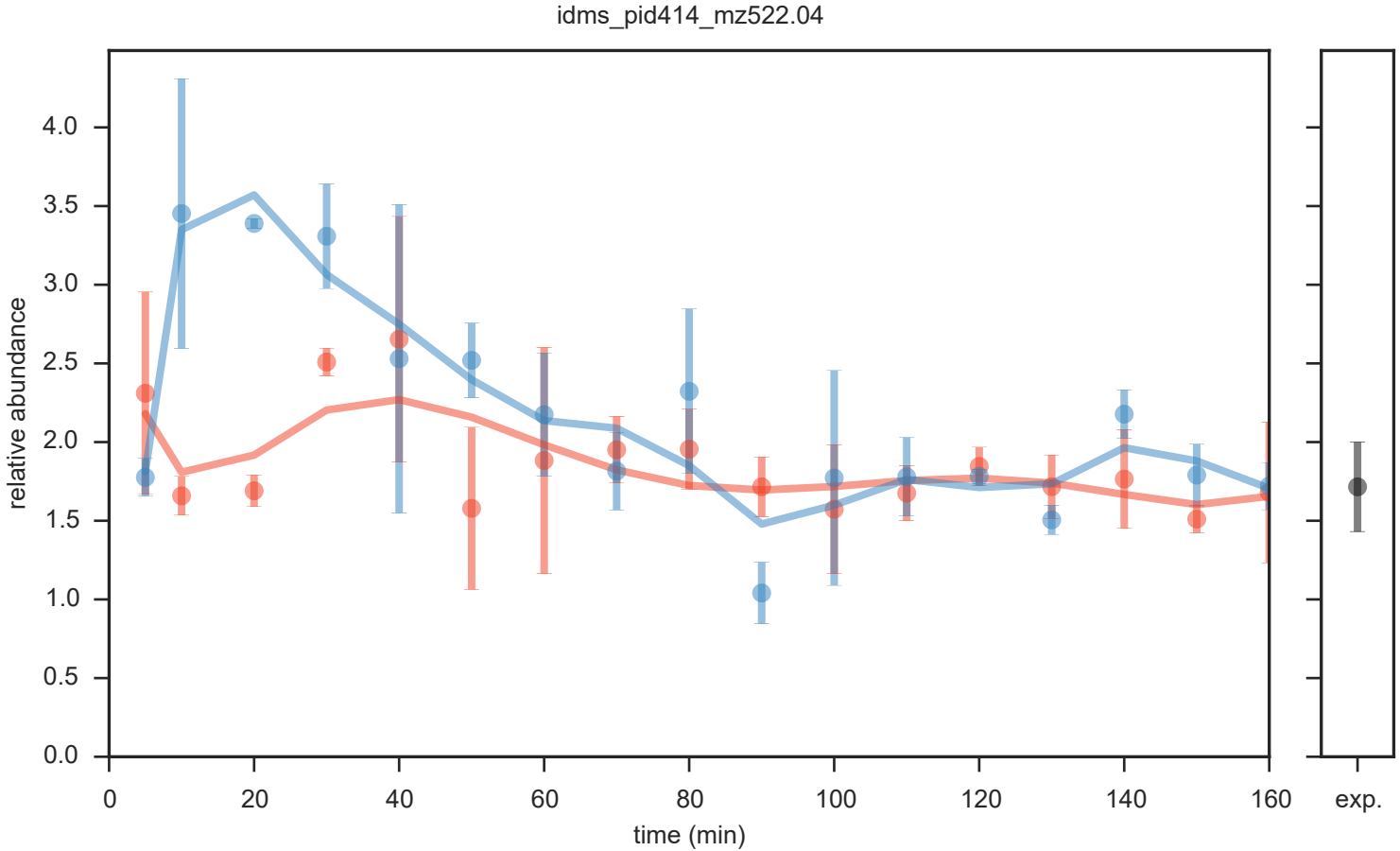

idms_pid394_mz226.02
relative abundance
0.0
0.5
1.0
1.5
2.0
2.5
0
20
40
60
80
100
120
140
160
time (min)
exp.

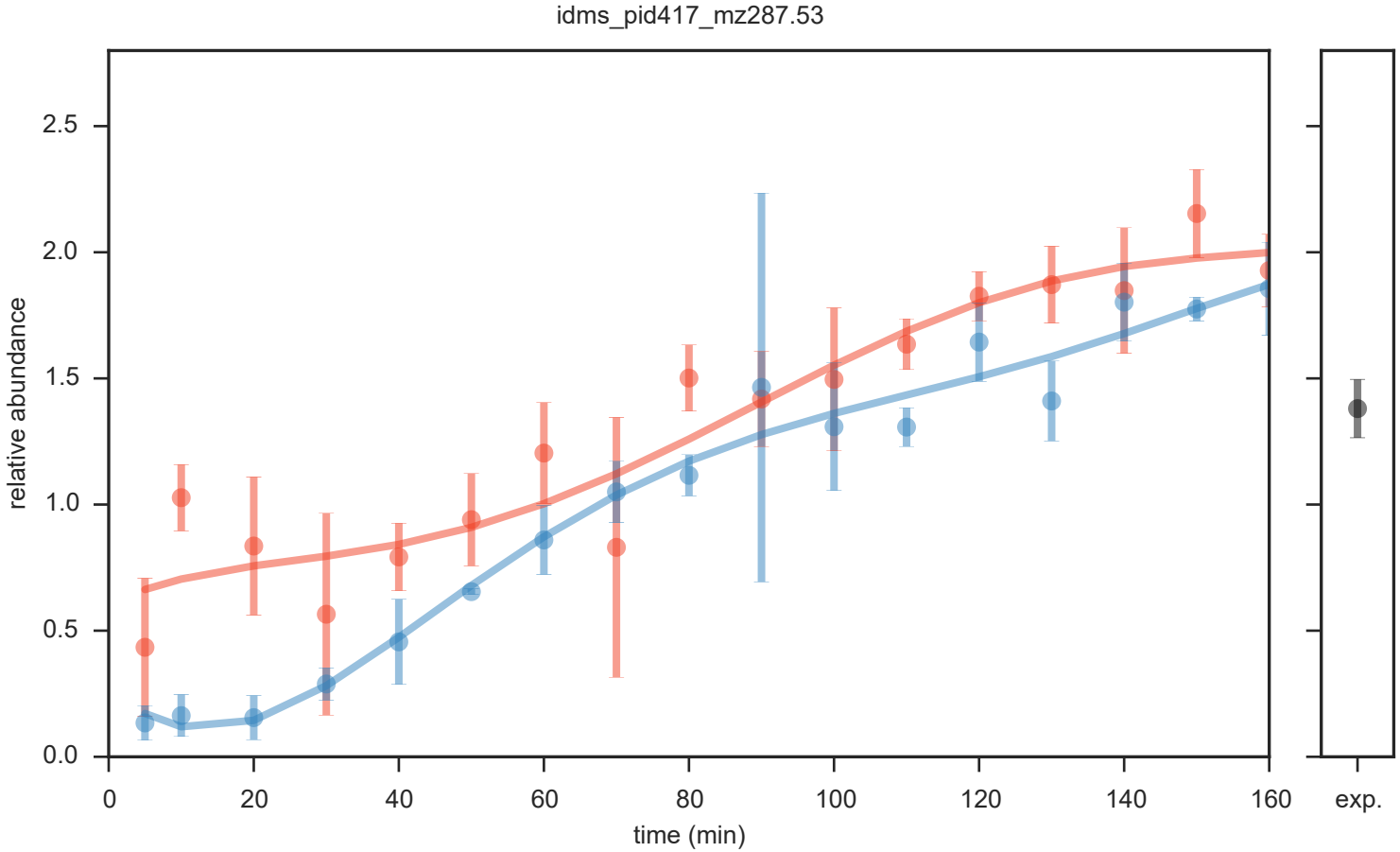

idms_pid399_mz388.97
relative abundance
0.0
0.5
1.0
1.5
0
20
40
60
80
100
120
140
160
time (min)
exp.

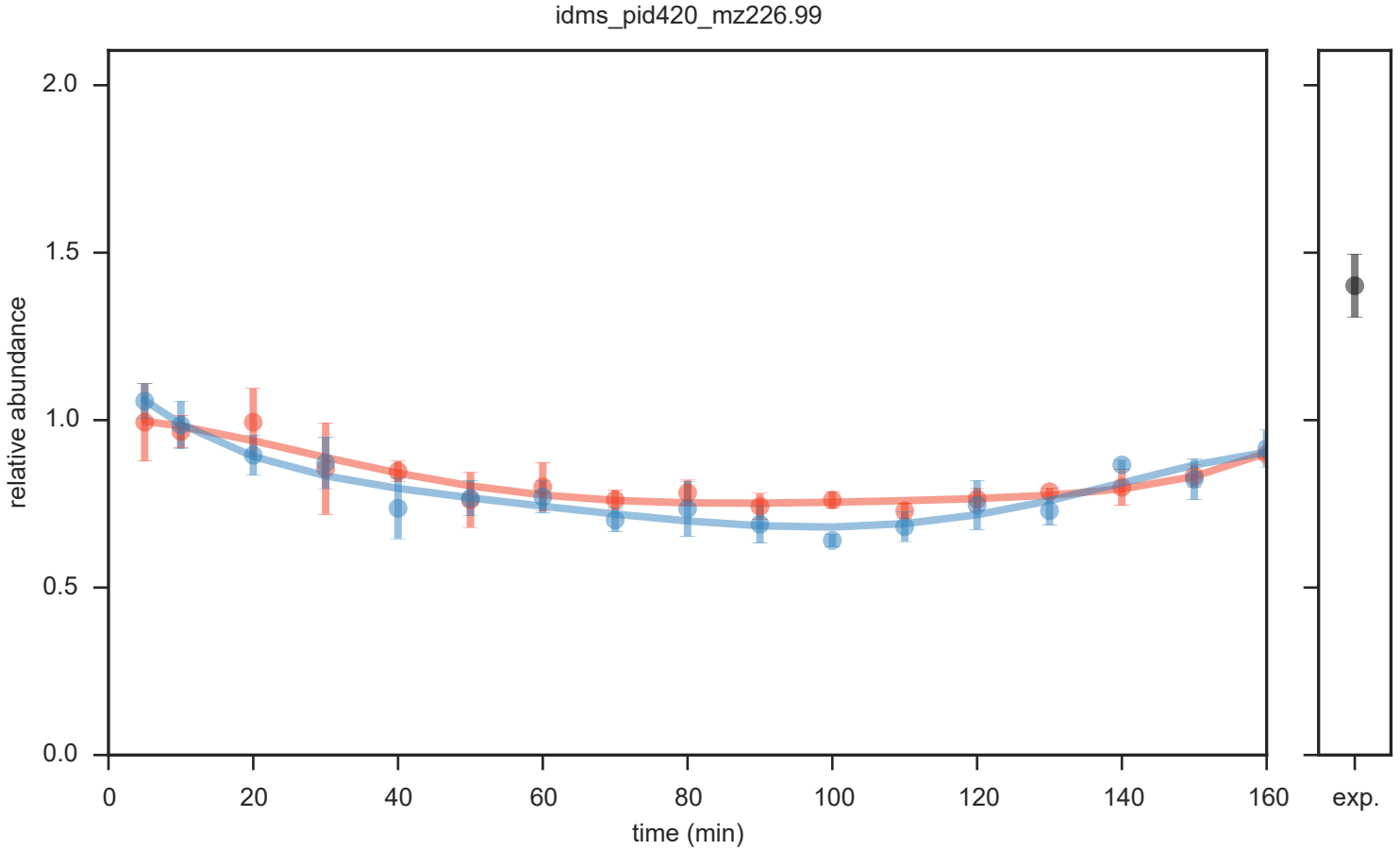

idms_pid400_mz252.48
relative abundance
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

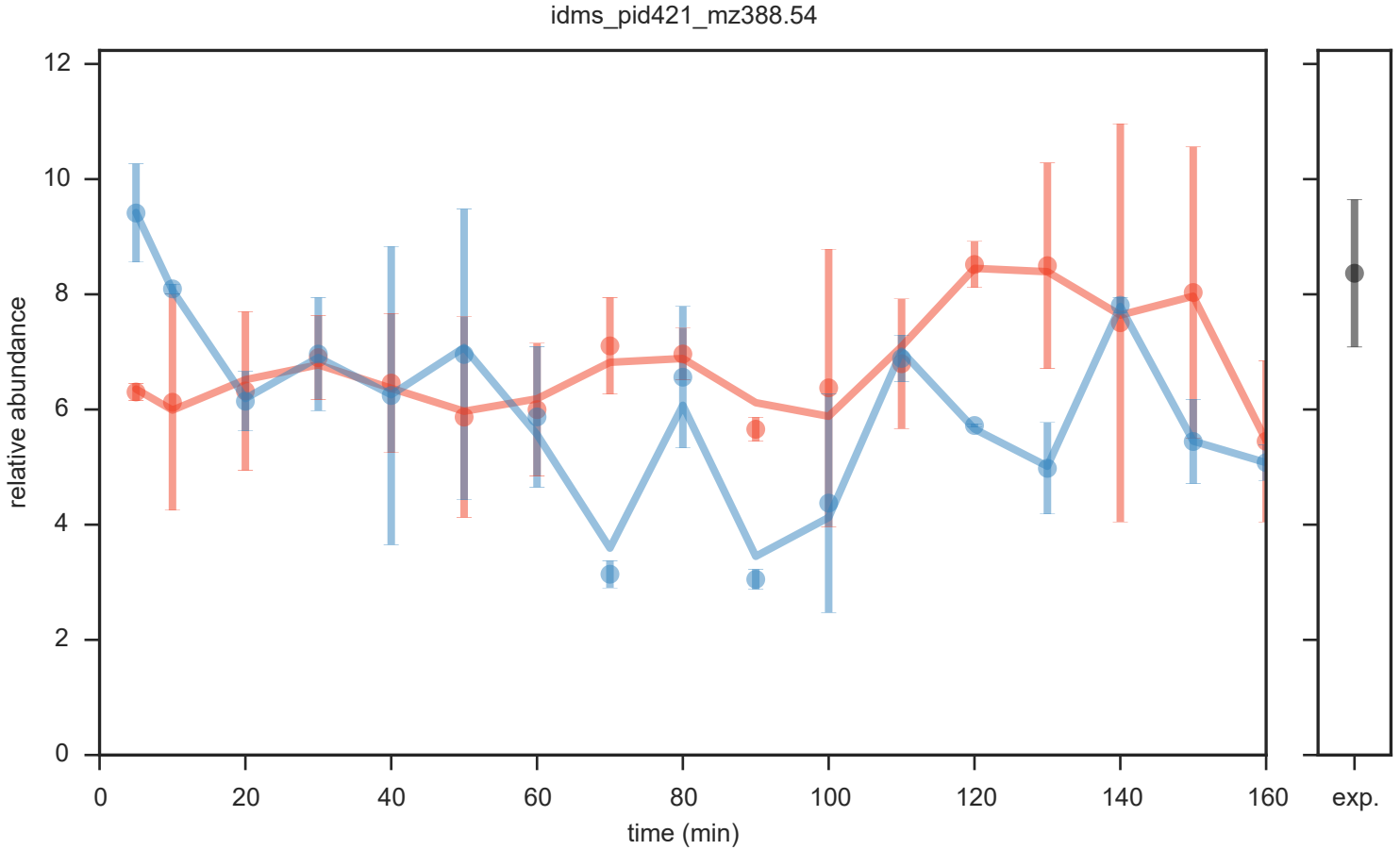

idms_pid403_mz222.94
relative abundance
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

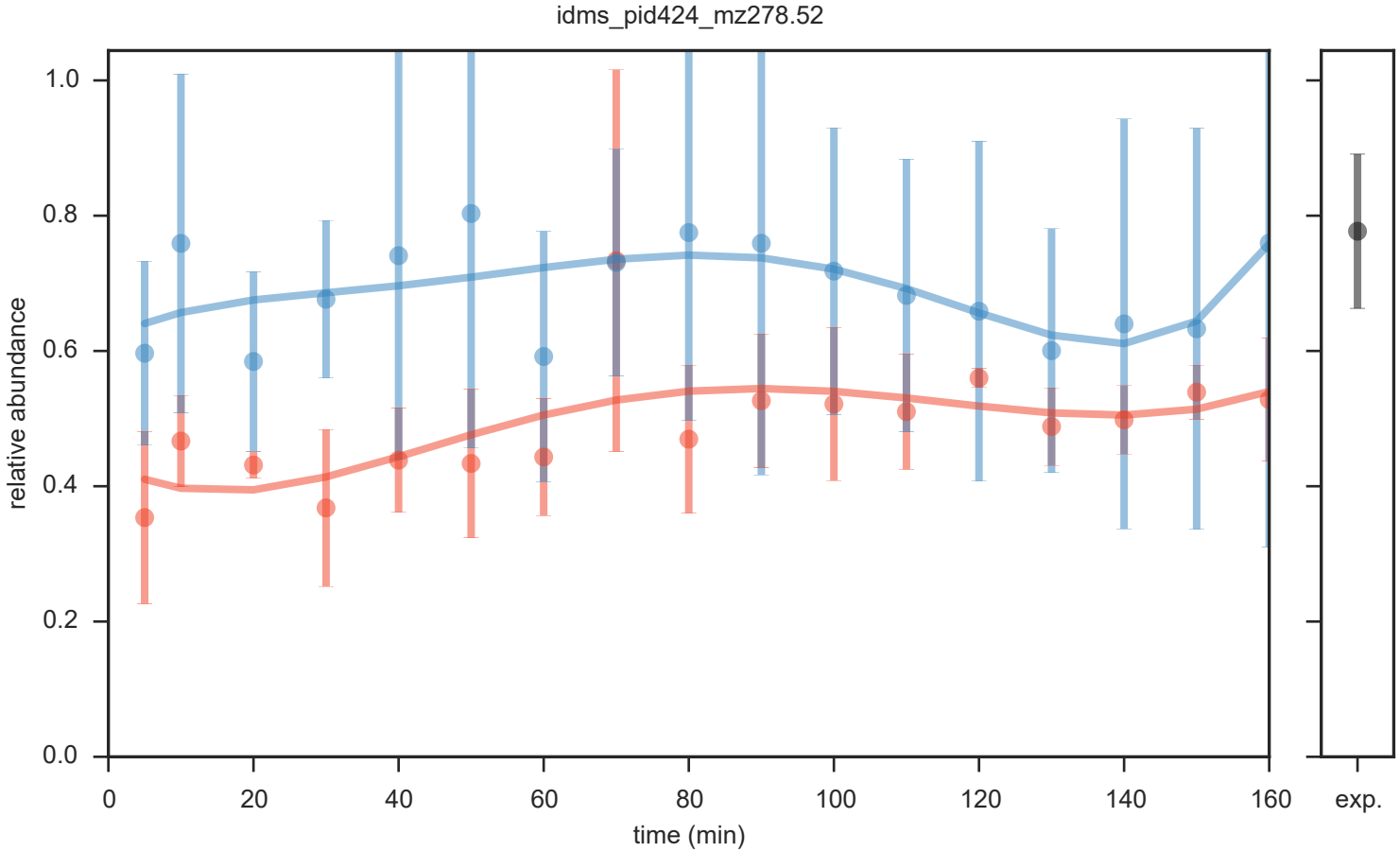

idms_pid404_mz327.05
relative abundance
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

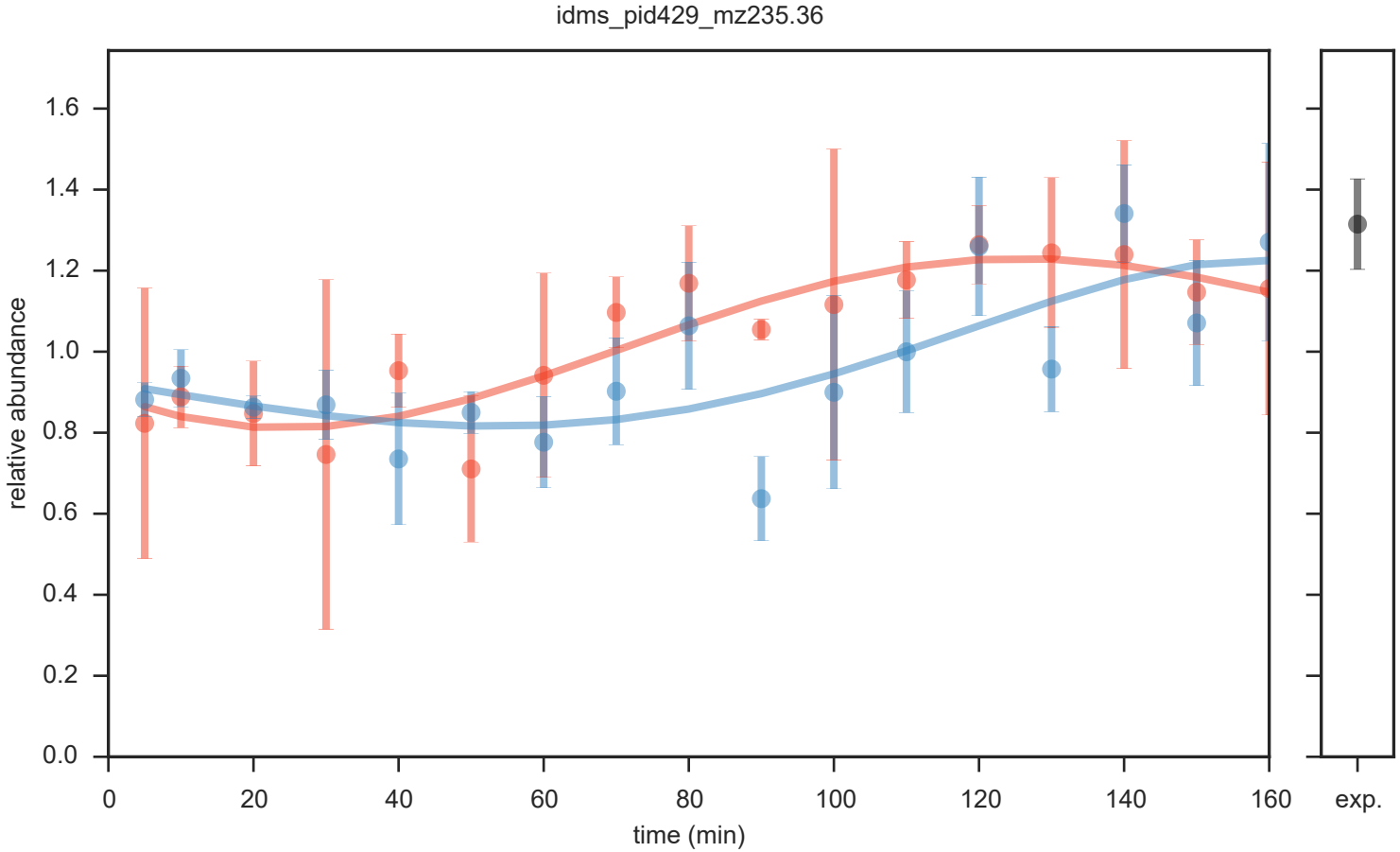

idms_pid414_mz522.04
relative abundance
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

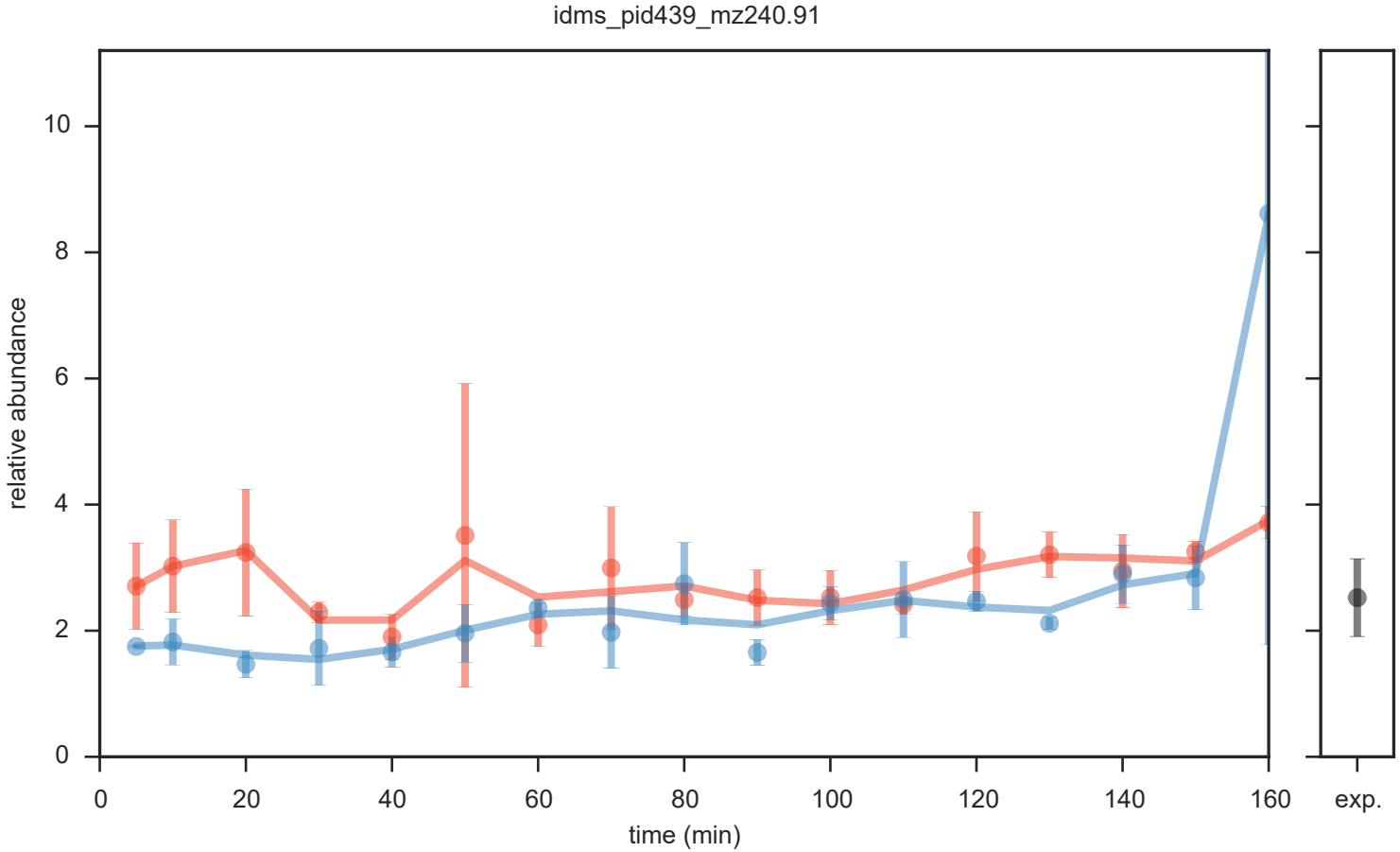

idms_pid417_mz287.53
relative abundance
0.0
0.5
1.0
1.5
2.0
2.5
0
20
40
60
80
100
120
140
160
time (min)
exp.

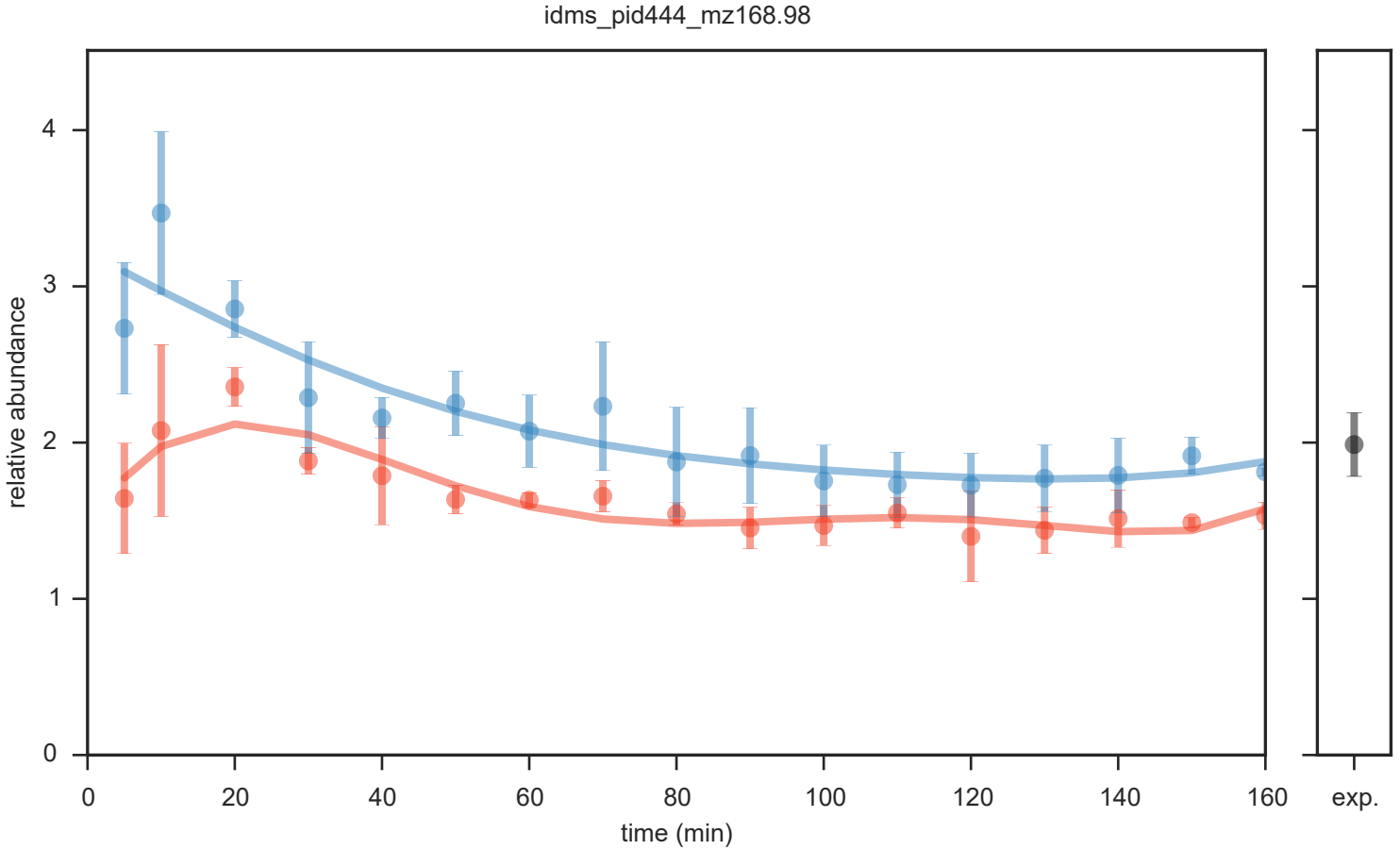

idms_pid420_mz226.99
relative abundance
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

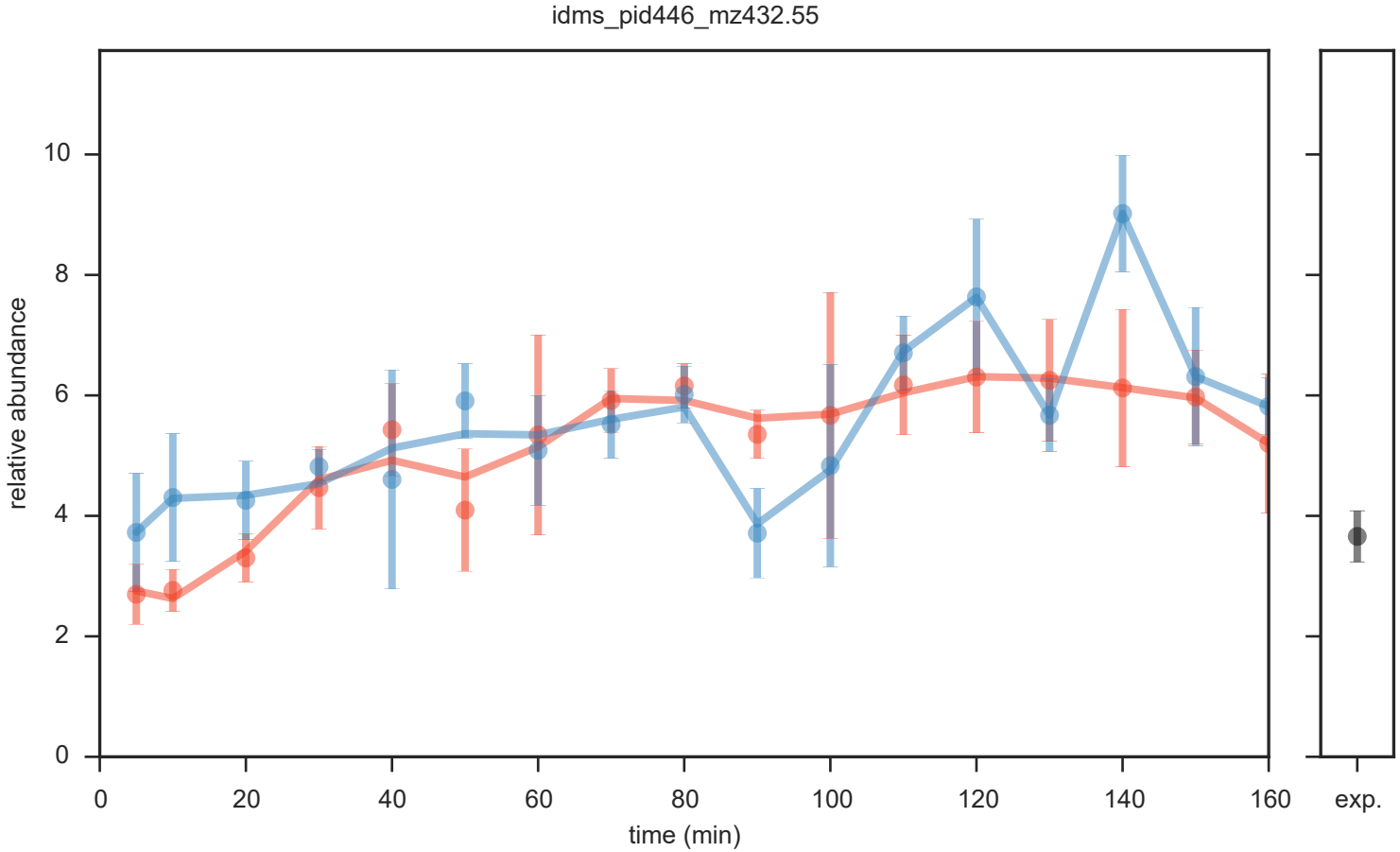

idms_pid421_mz388.54
relative abundance
time (min)
exp.
0
2
4
6
8
10
12
0
20
40
60
80
100
120
140
160

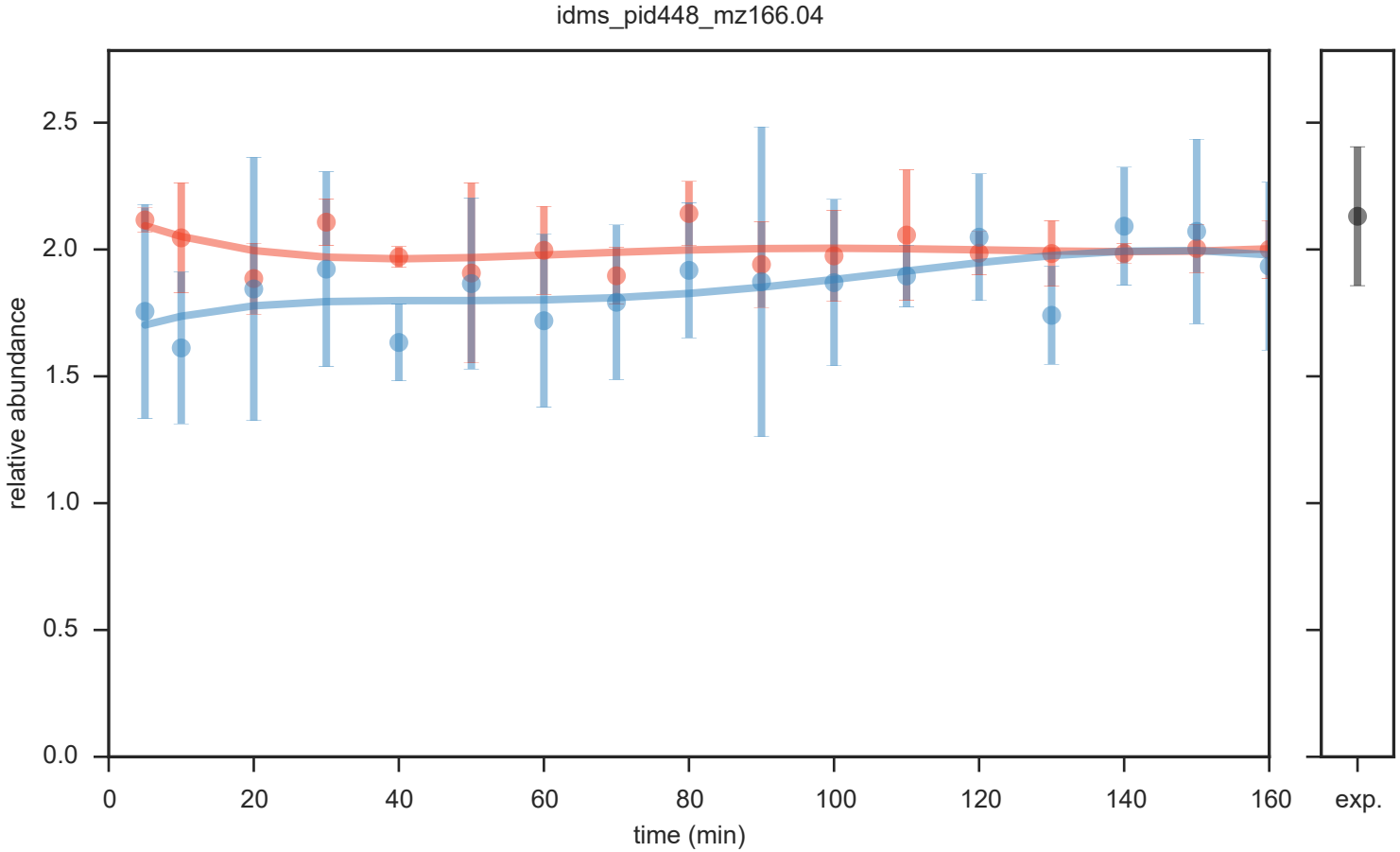

idms_pid424_mz278.52
relative abundance
1.0
0.8
0.6
0.4
0.2
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

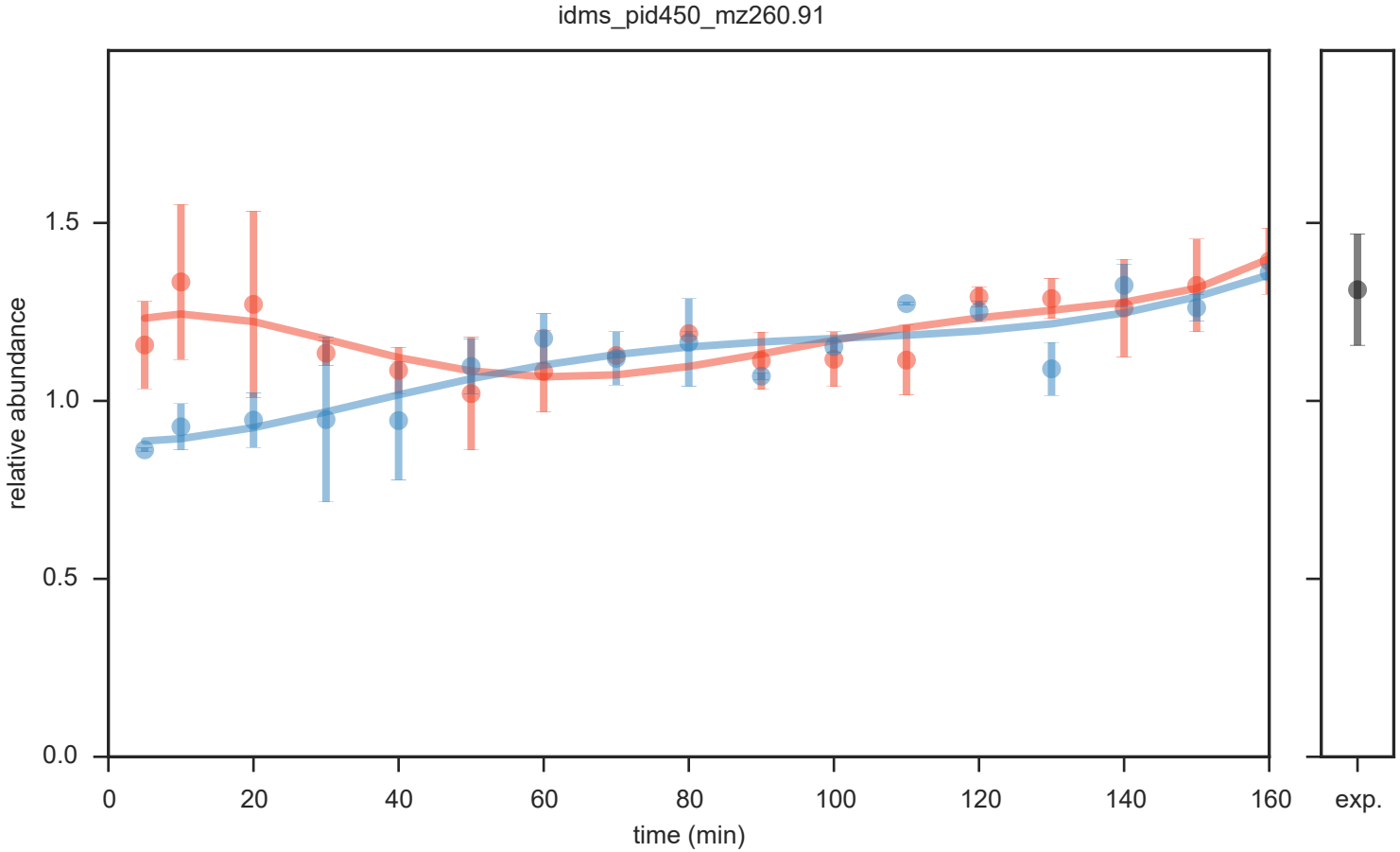

idms_pid429_mz235.36
relative abundance
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
0
20
40
60
80
100
120
140
160
time (min)
exp.

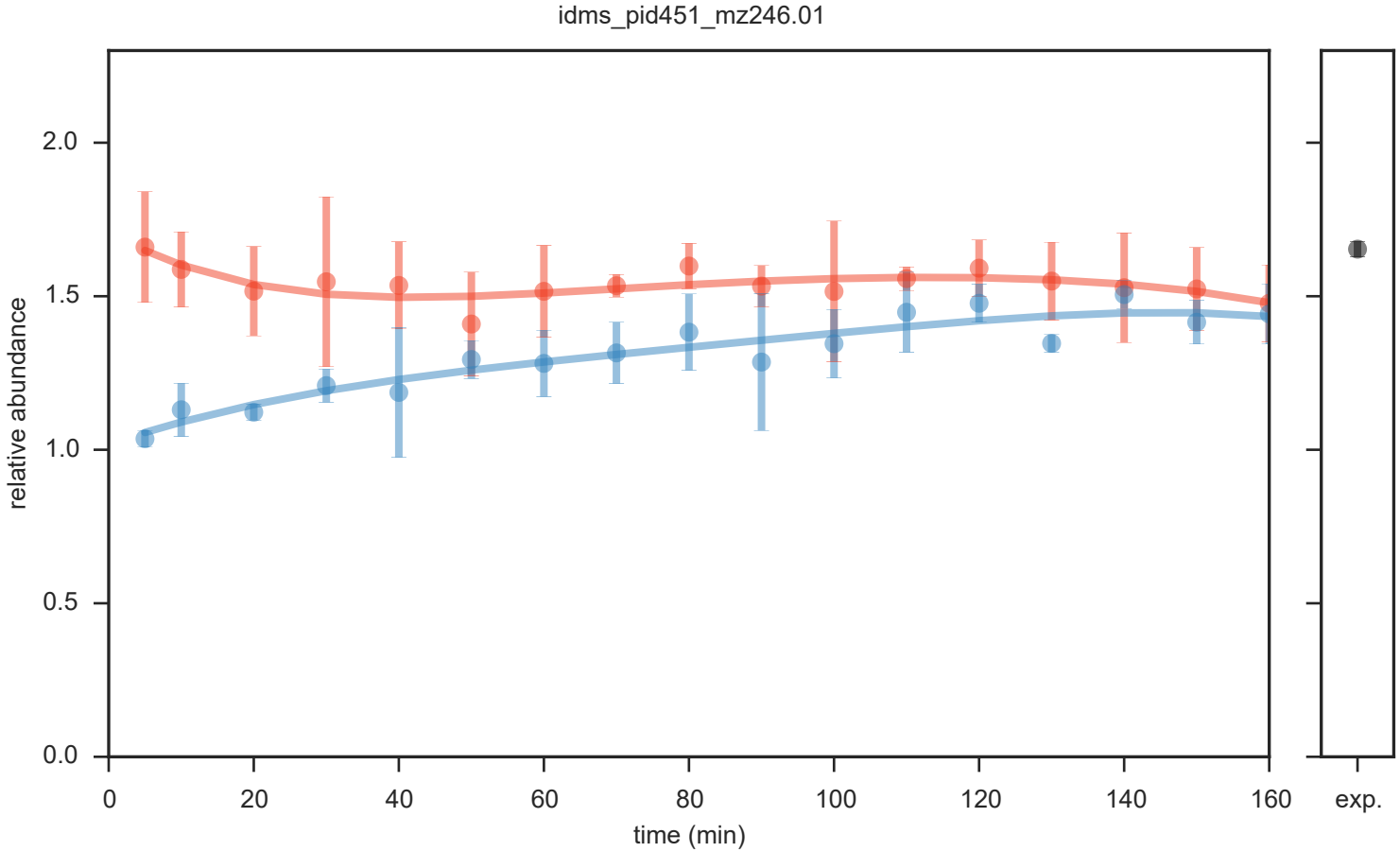

idms_pid439_mz240.91
relative abundance
0
2
4
6
8
10
0
20
40
60
80
100
120
140
160
time (min)
exp.

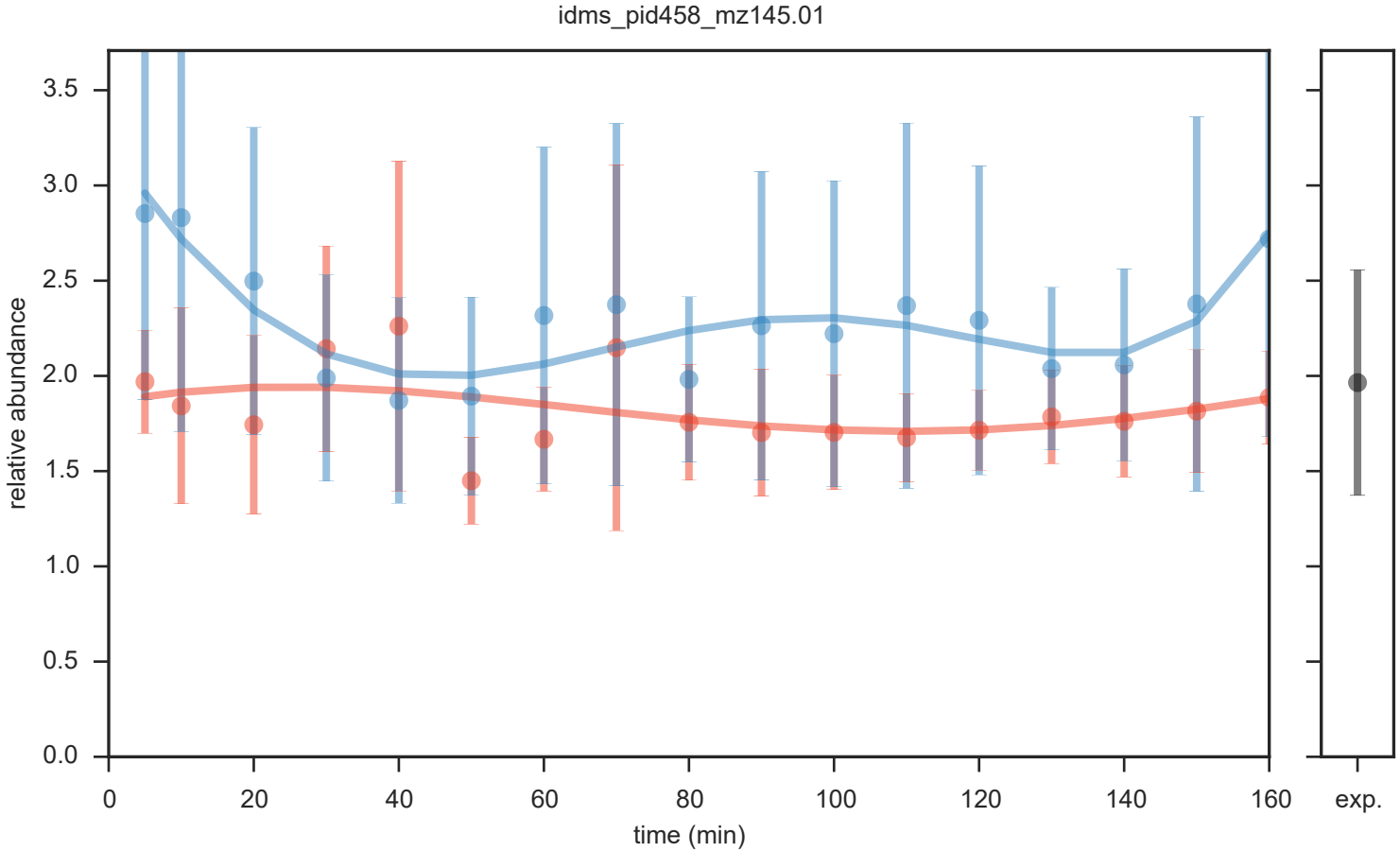

idms_pid444_mz168.98
relative abundance
0
1
2
3
4
0
20
40
60
80
100
120
140
160
time (min)
exp.

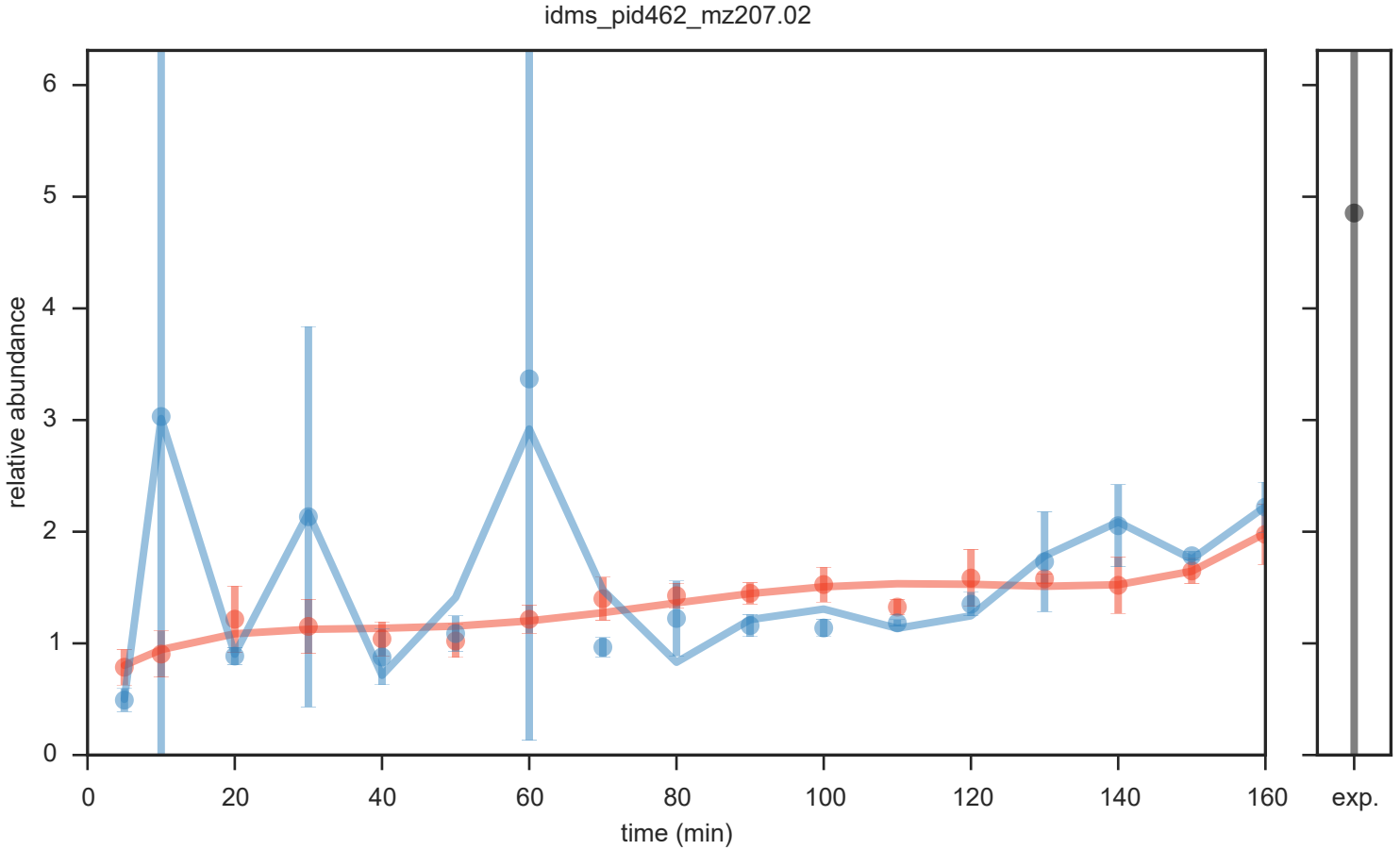

idms_pid446_mz432.55
relative abundance
0
2
4
6
8
10
0
20
40
60
80
100
120
140
160
time (min)
exp.

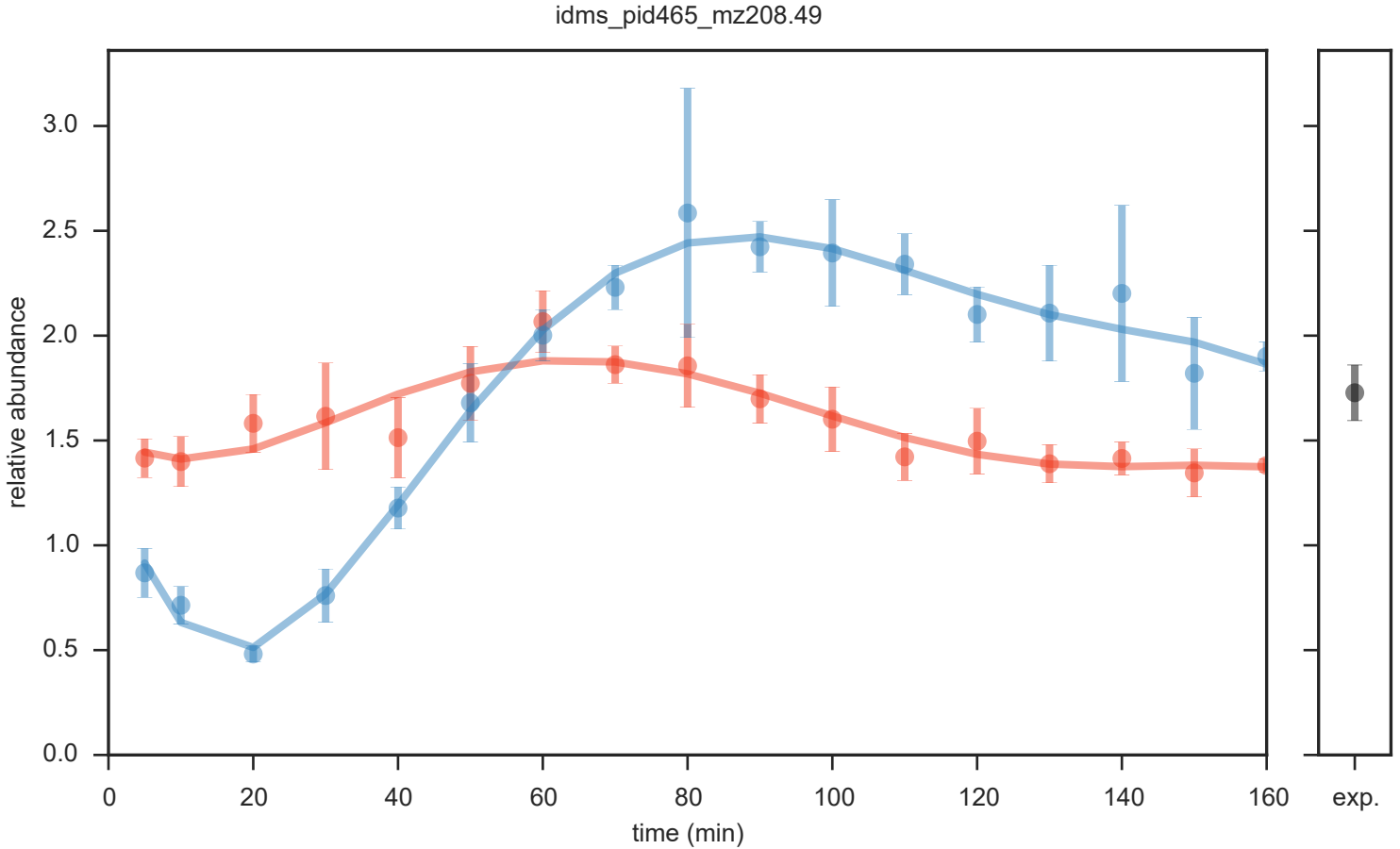

idms_pid448_mz166.04
relative abundance
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

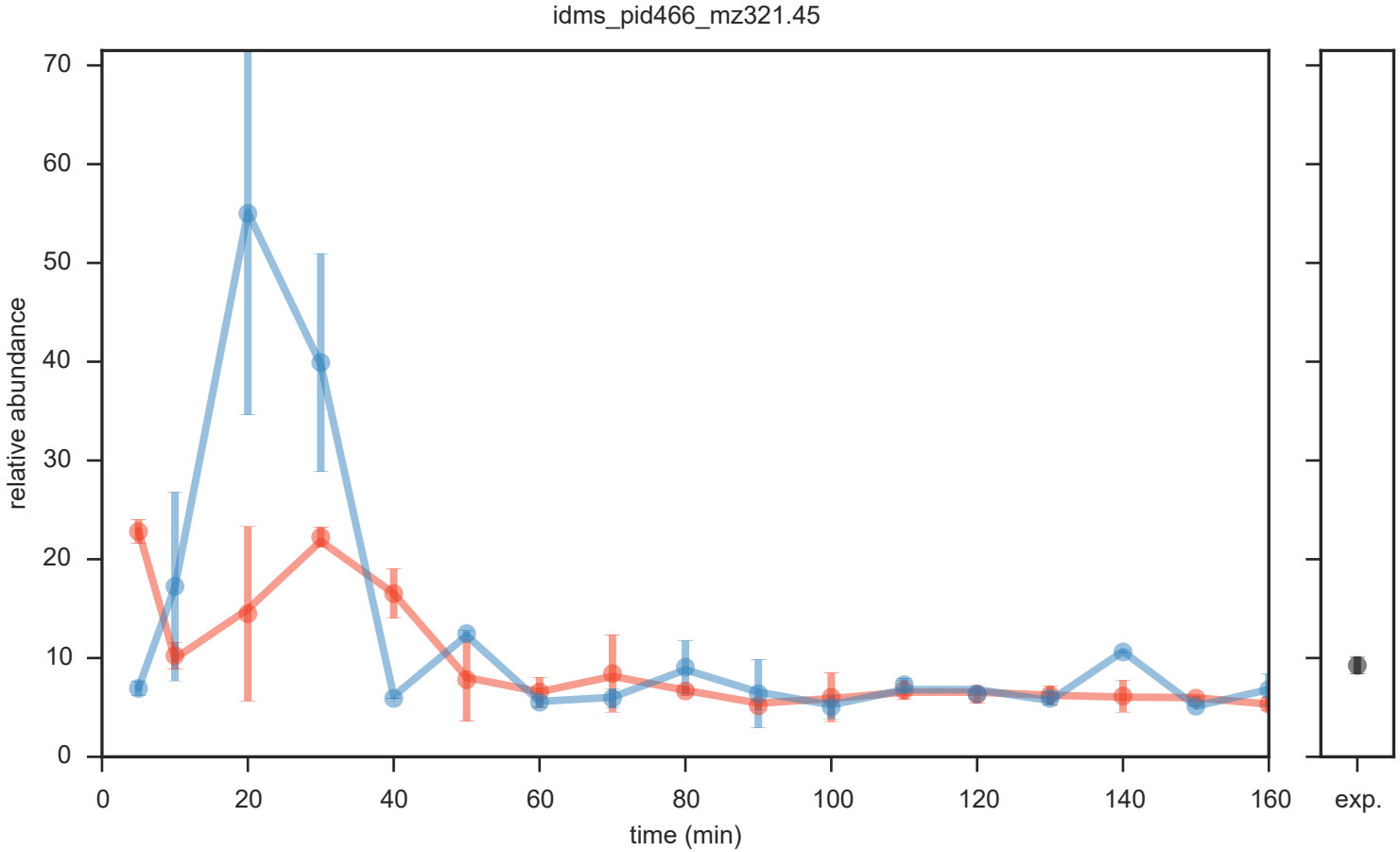

idms_pid450_mz260.91
relative abundance
0.0
0.5
1.0
1.5
0
20
40
60
80
100
120
140
160
time (min)
exp.

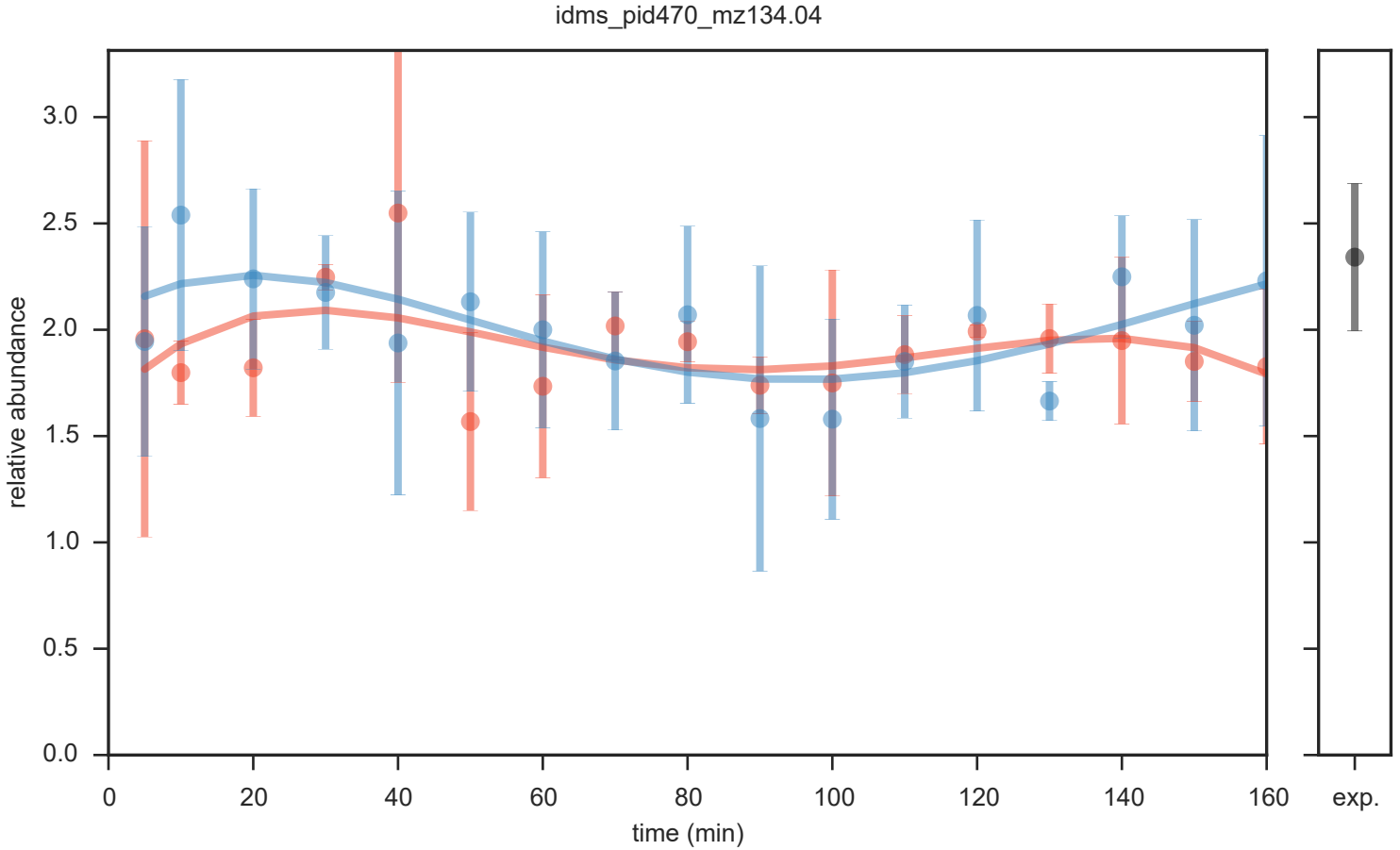

idms_pid451_mz246.01
relative abundance
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

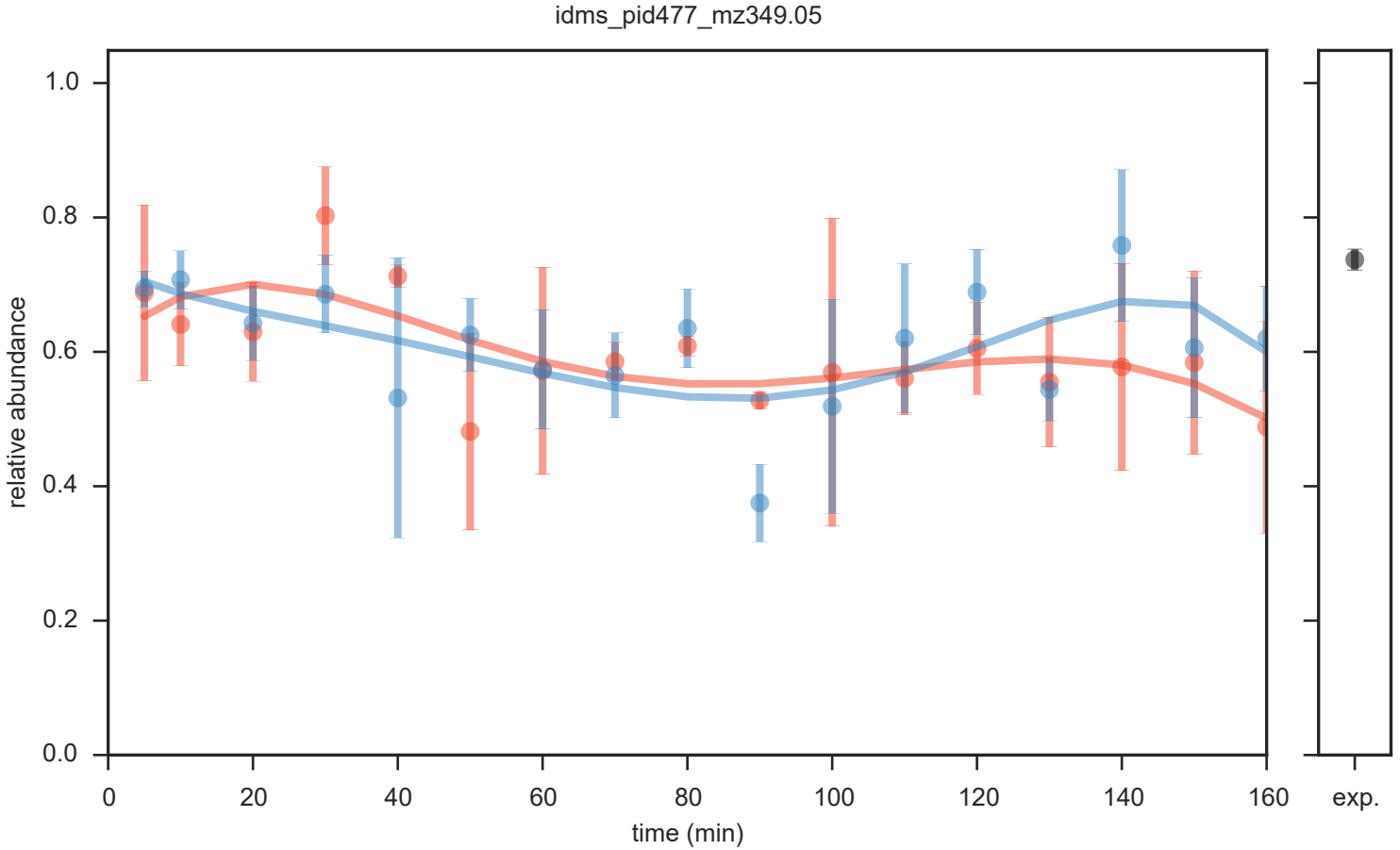

idms_pid458_mz145.01
relative abundance
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

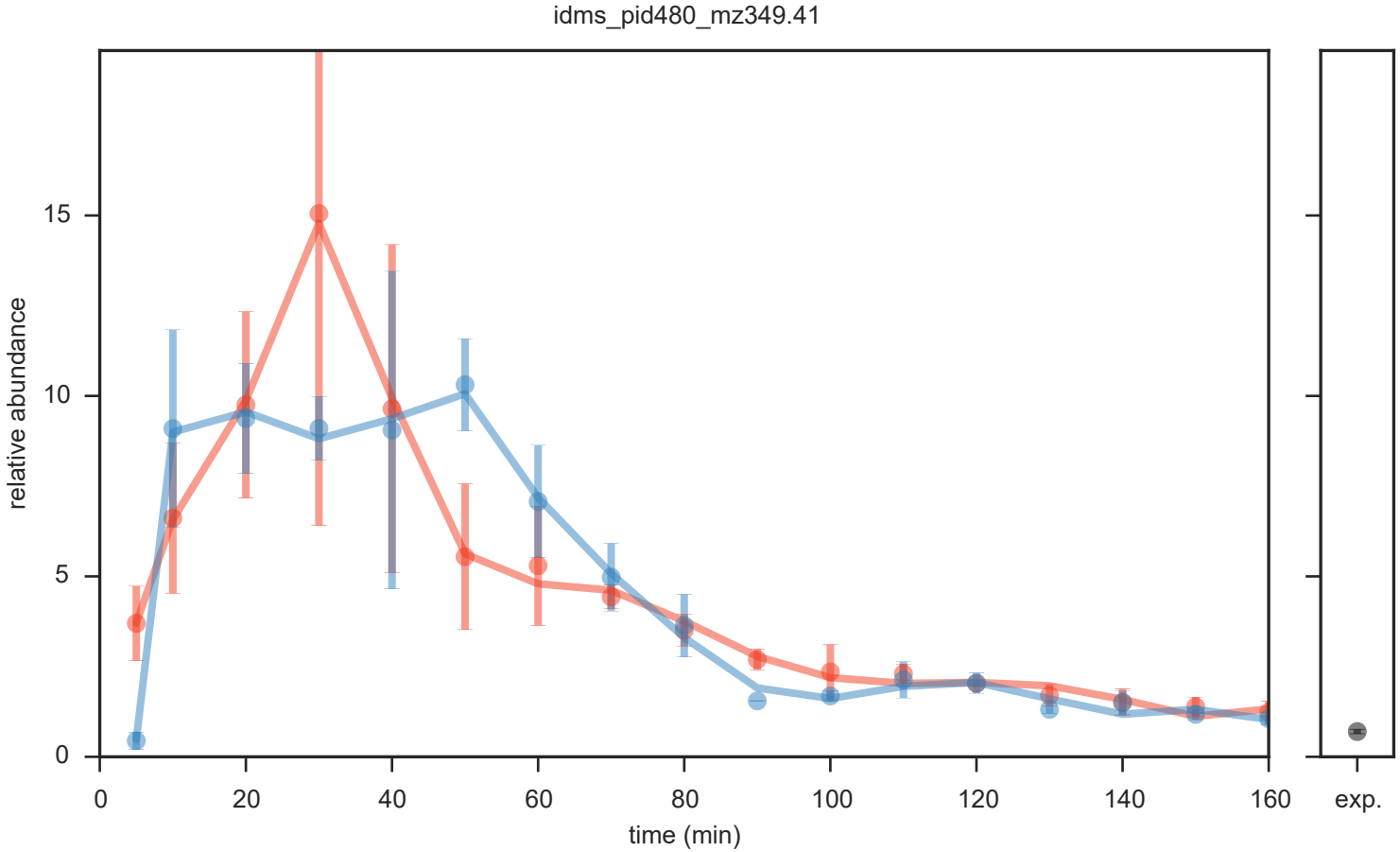

idms_pid462_mz207.02
relative abundance
time (min)
exp.
0
1
2
3
4
5
6
0
20
40
60
80
100
120
140
160

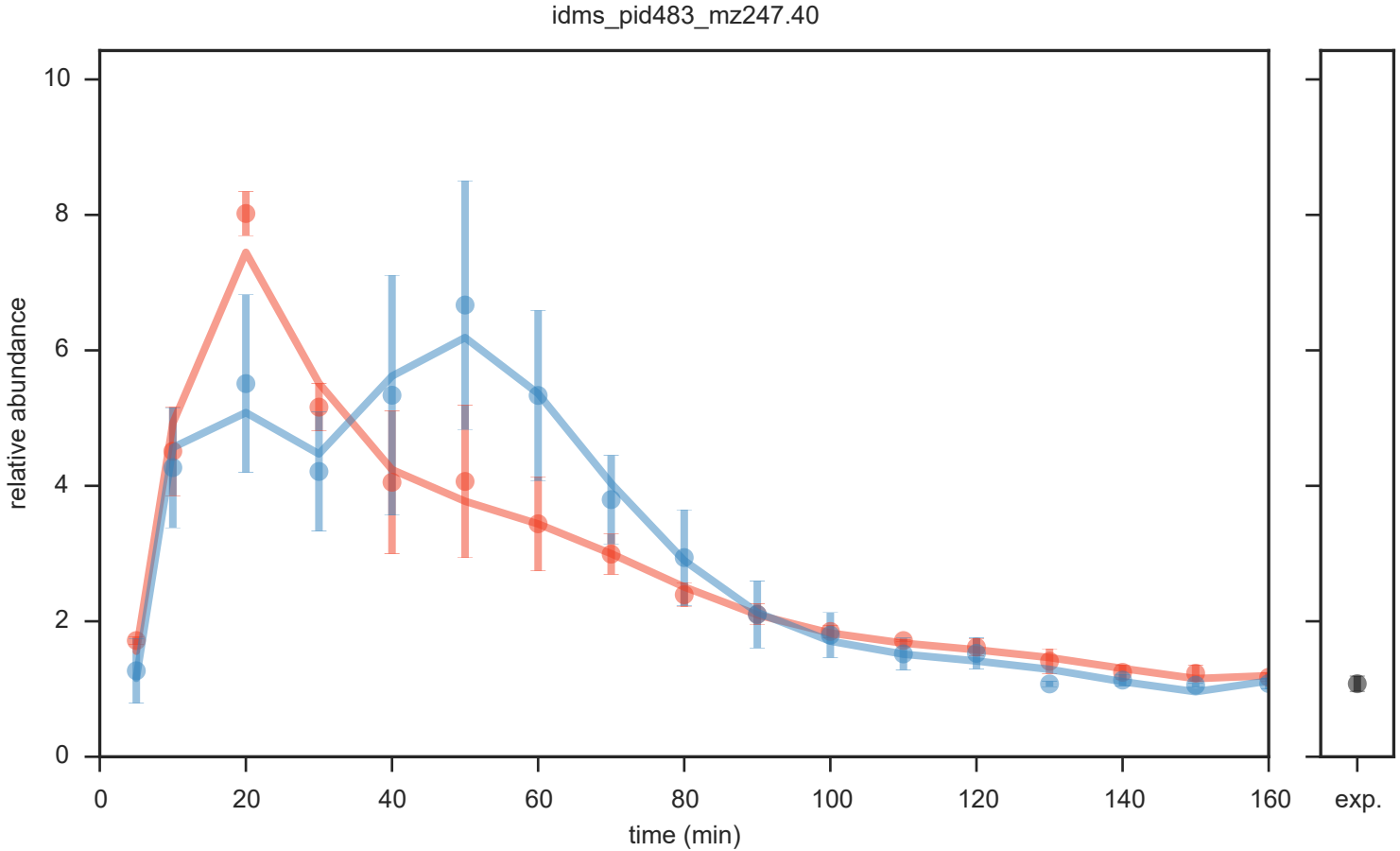

idms_pid465_mz208.49
relative abundance
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

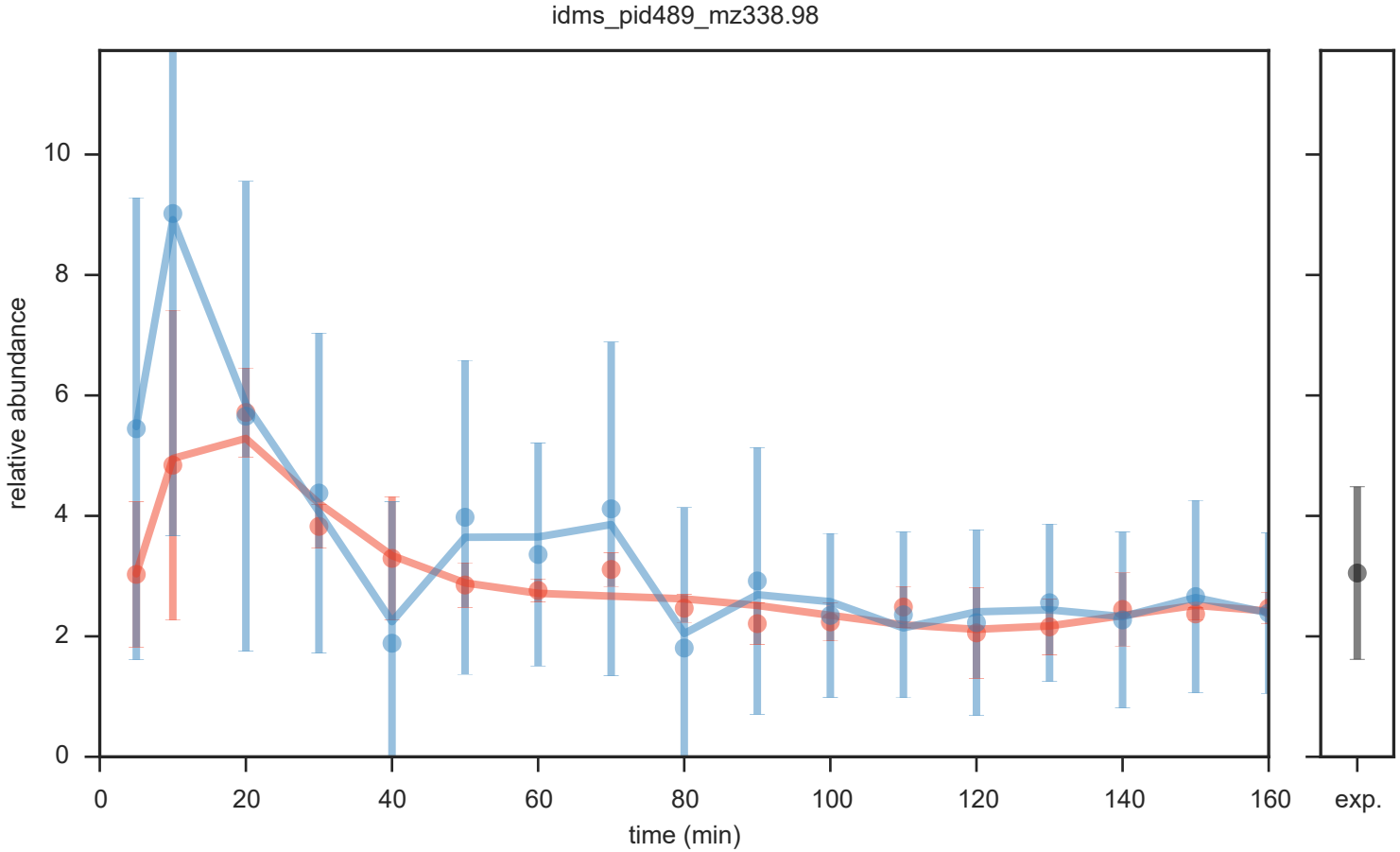

idms_pid466_mz321.45
relative abundance
time (min)
exp.
0
10
20
30
40
50
60
70
0
20
40
60
80
100
120
140
160

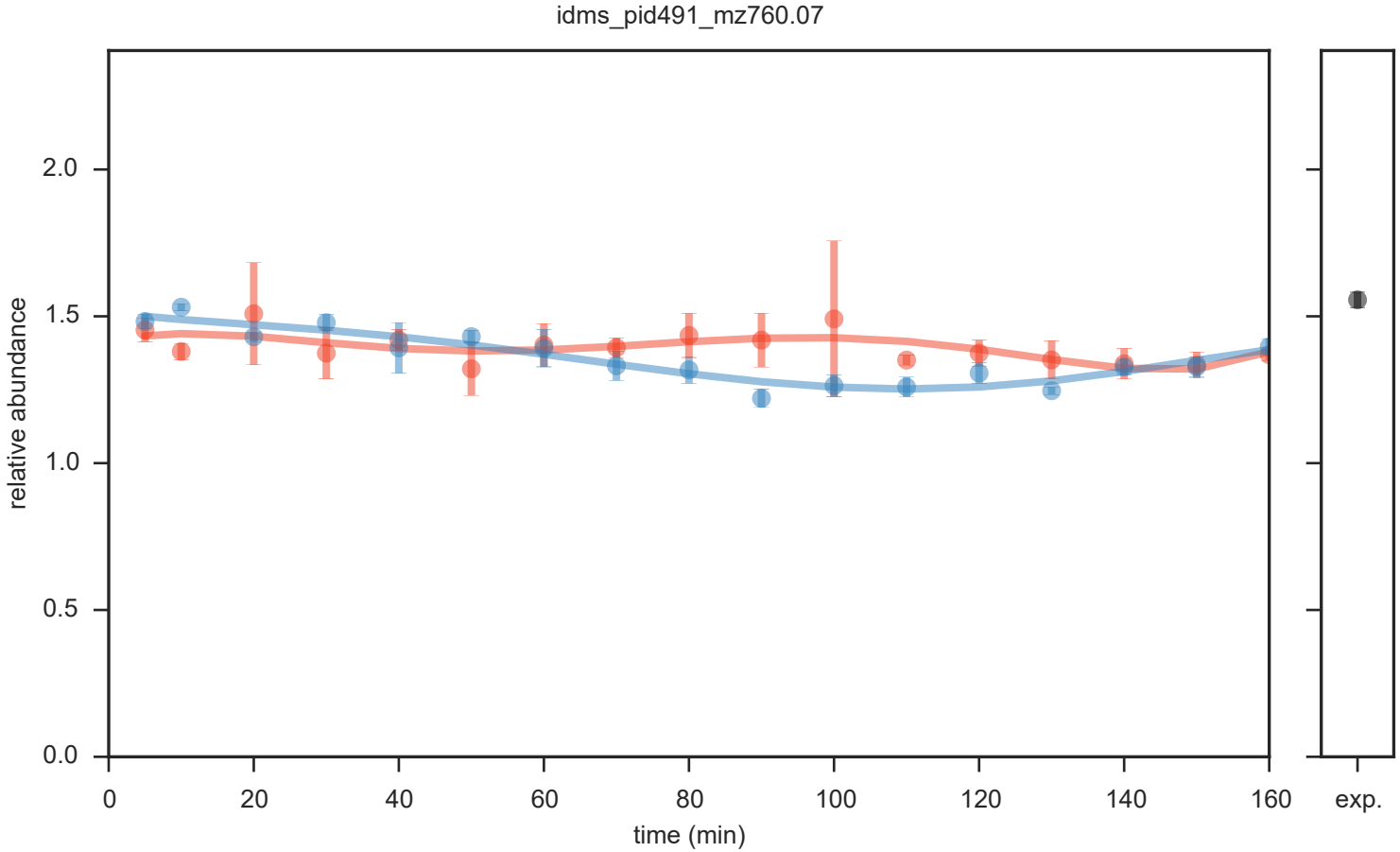

idms_pid470_mz134.04
relative abundance
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

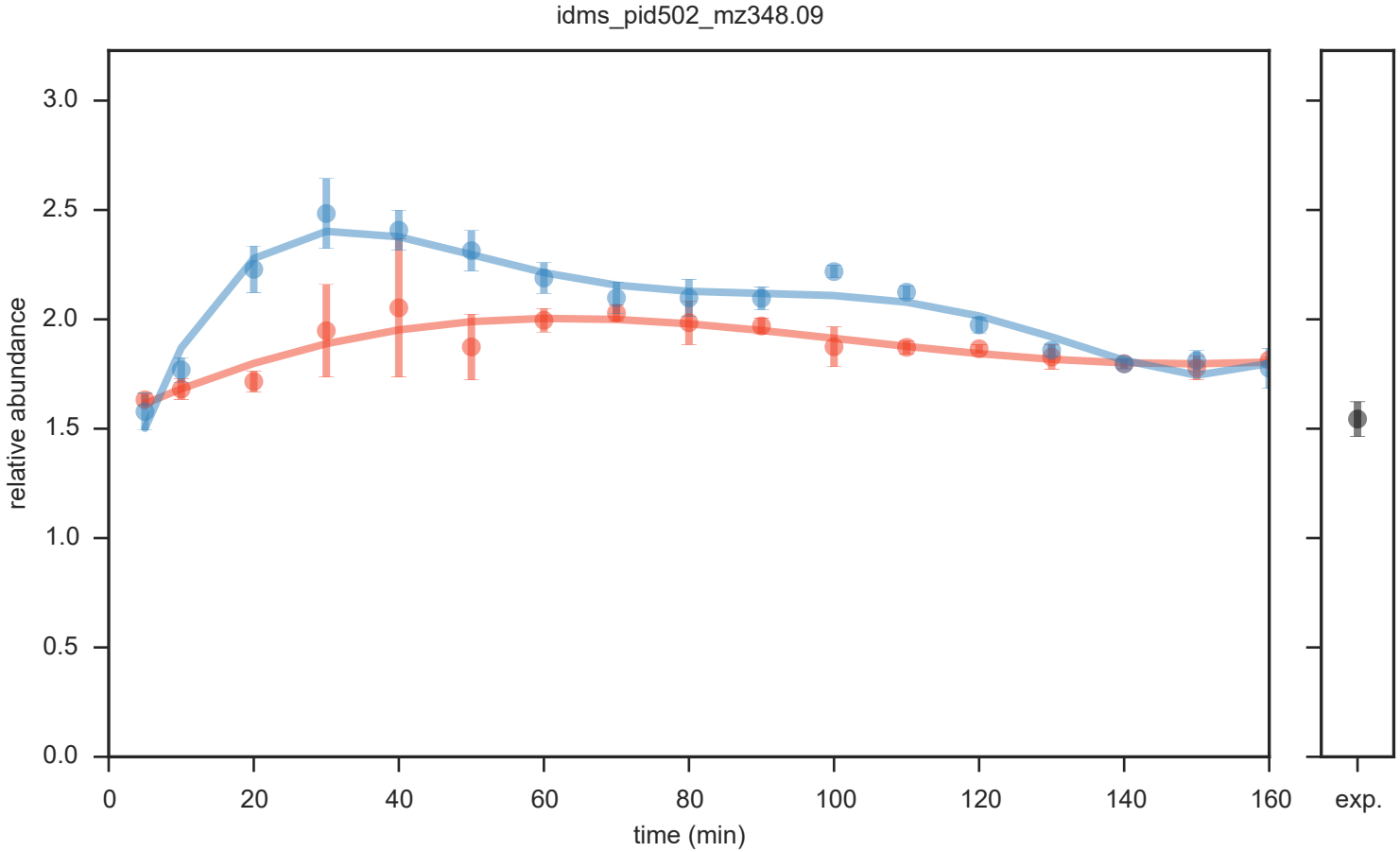

idms_pid477_mz349.05
relative abundance
1.0
0.8
0.6
0.4
0.2
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

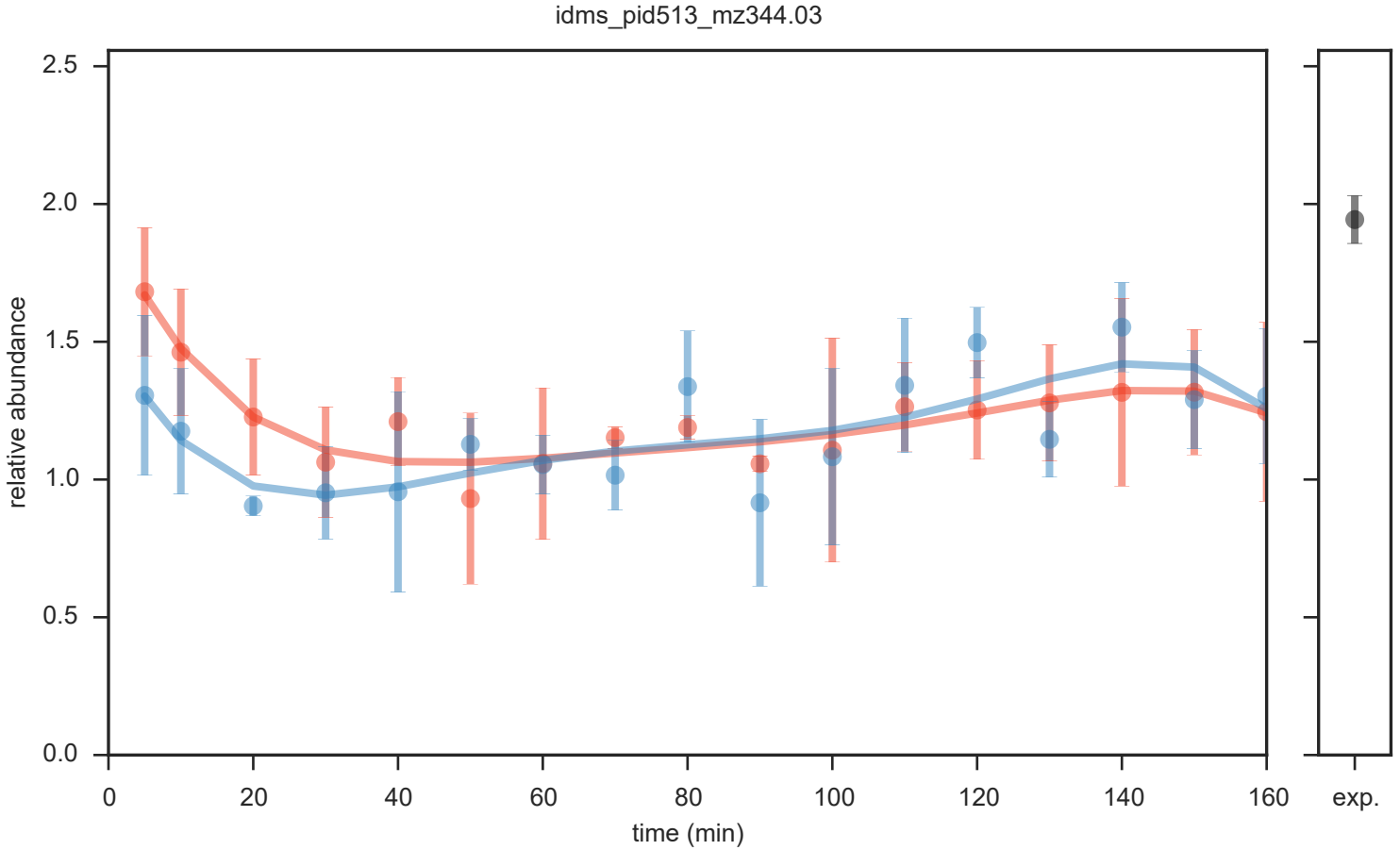

idms_pid480_mz349.41
relative abundance
0
5
10
15
0
20
40
60
80
100
120
140
160
time (min)
exp.

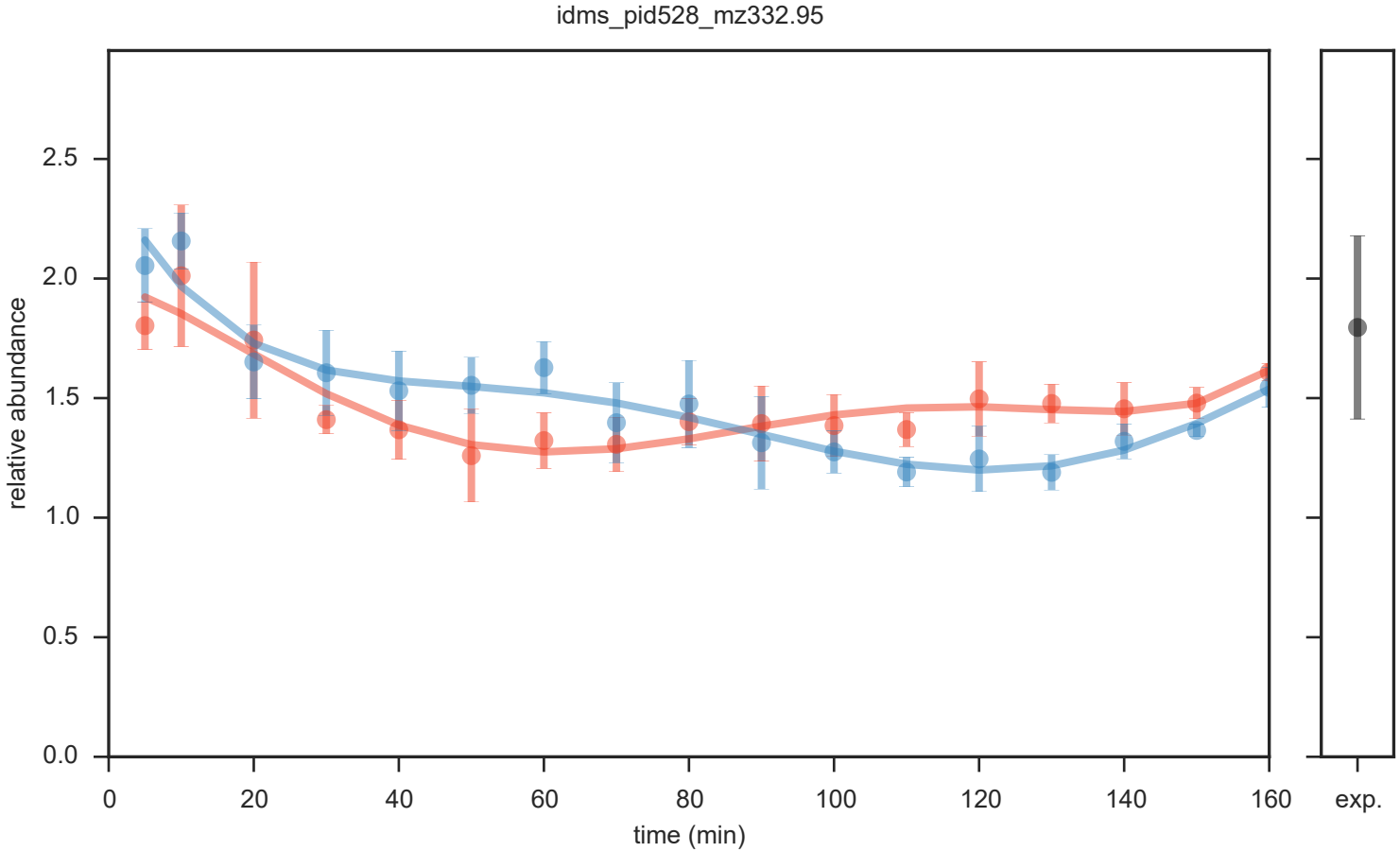

idms_pid483_mz247.40
relative abundance
time (min)
0
2
4
6
8
10
0
20
40
60
80
100
120
140
160
exp.

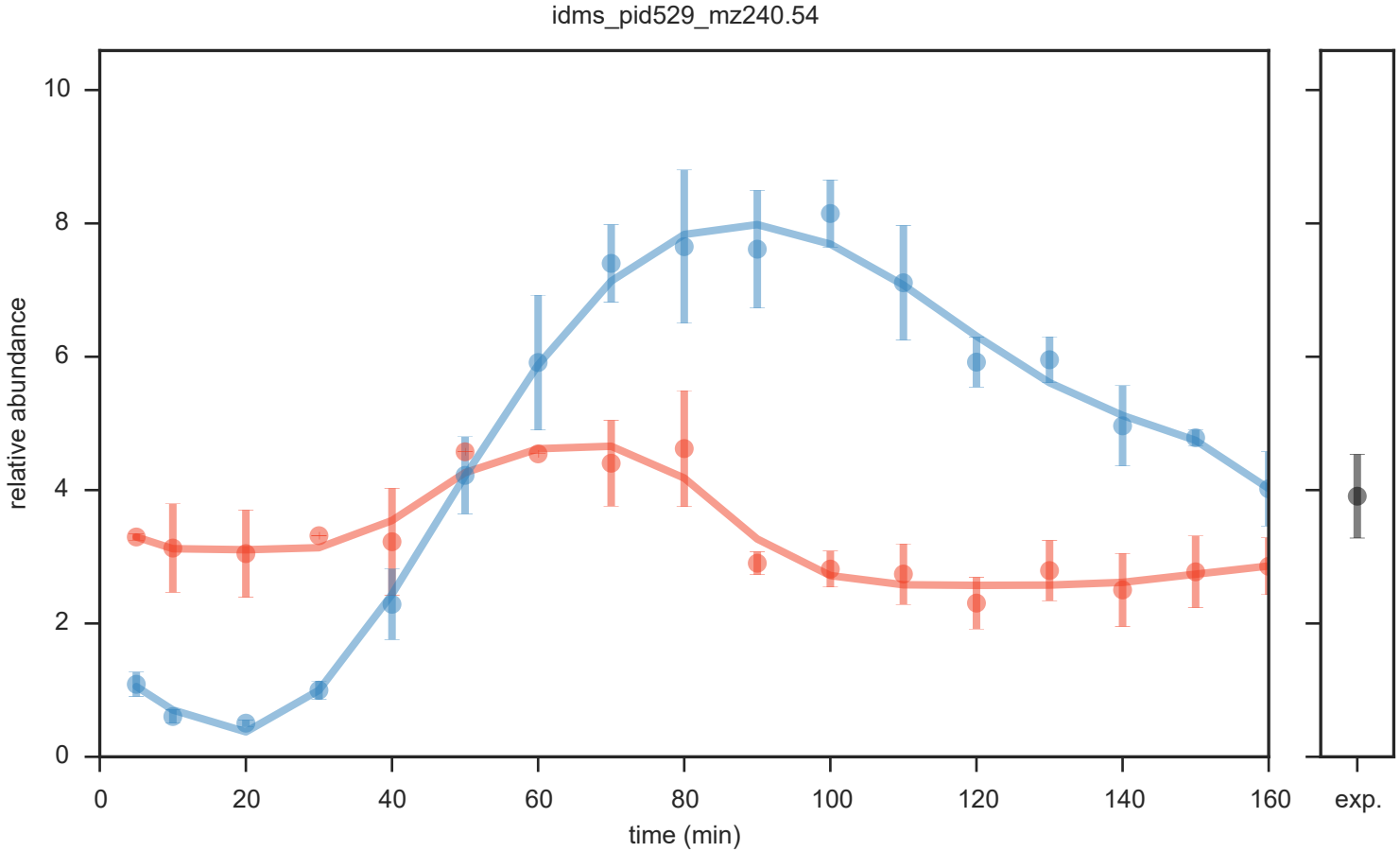

idms_pid489_mz338.98
relative abundance
0
2
4
6
8
10
0
20
40
60
80
100
120
140
160
time (min)
exp.

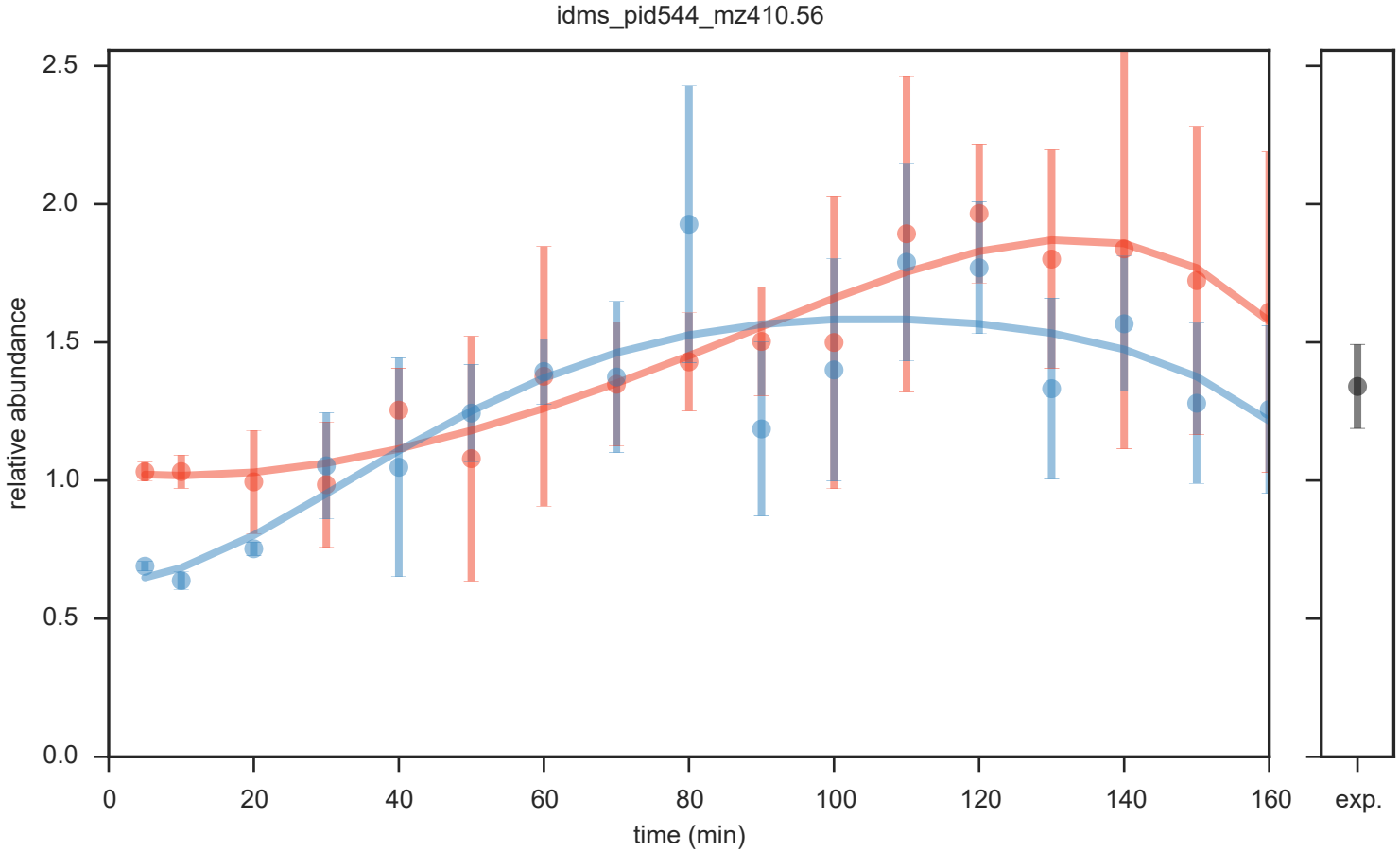

idms_pid491_mz760.07
relative abundance
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

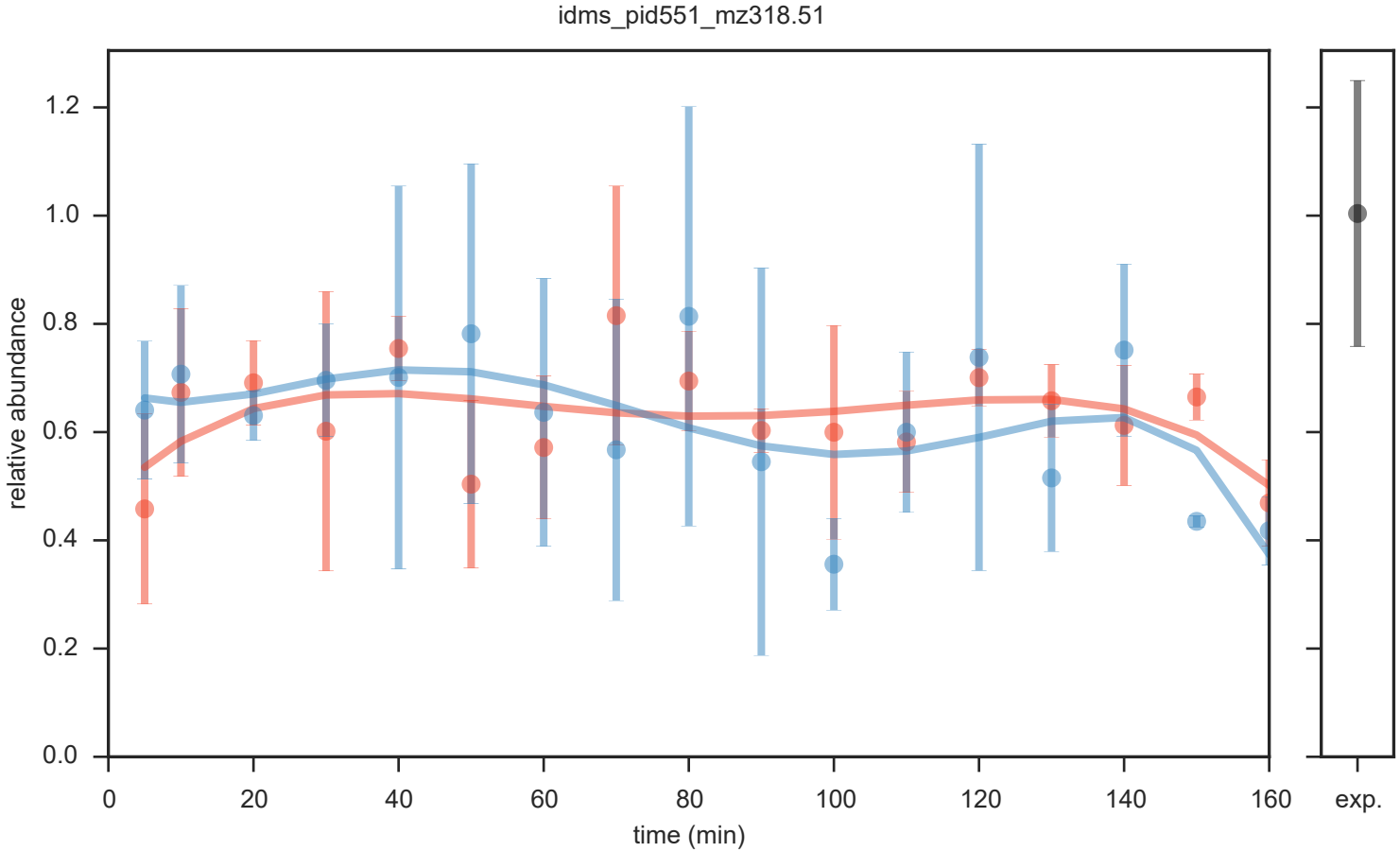

idms_pid502_mz348.09
relative abundance
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

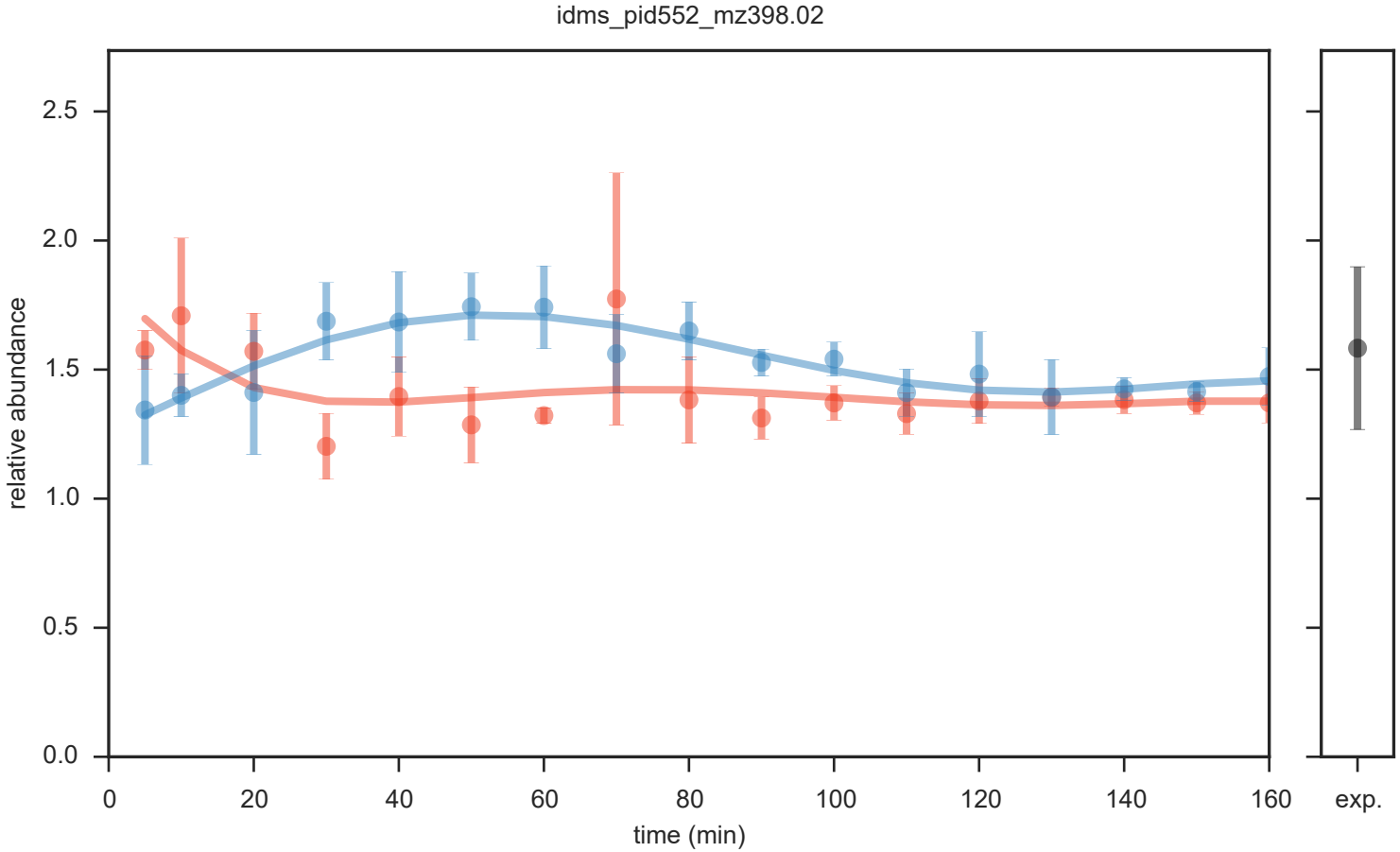

idms_pid513_mz344.03
relative abundance
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

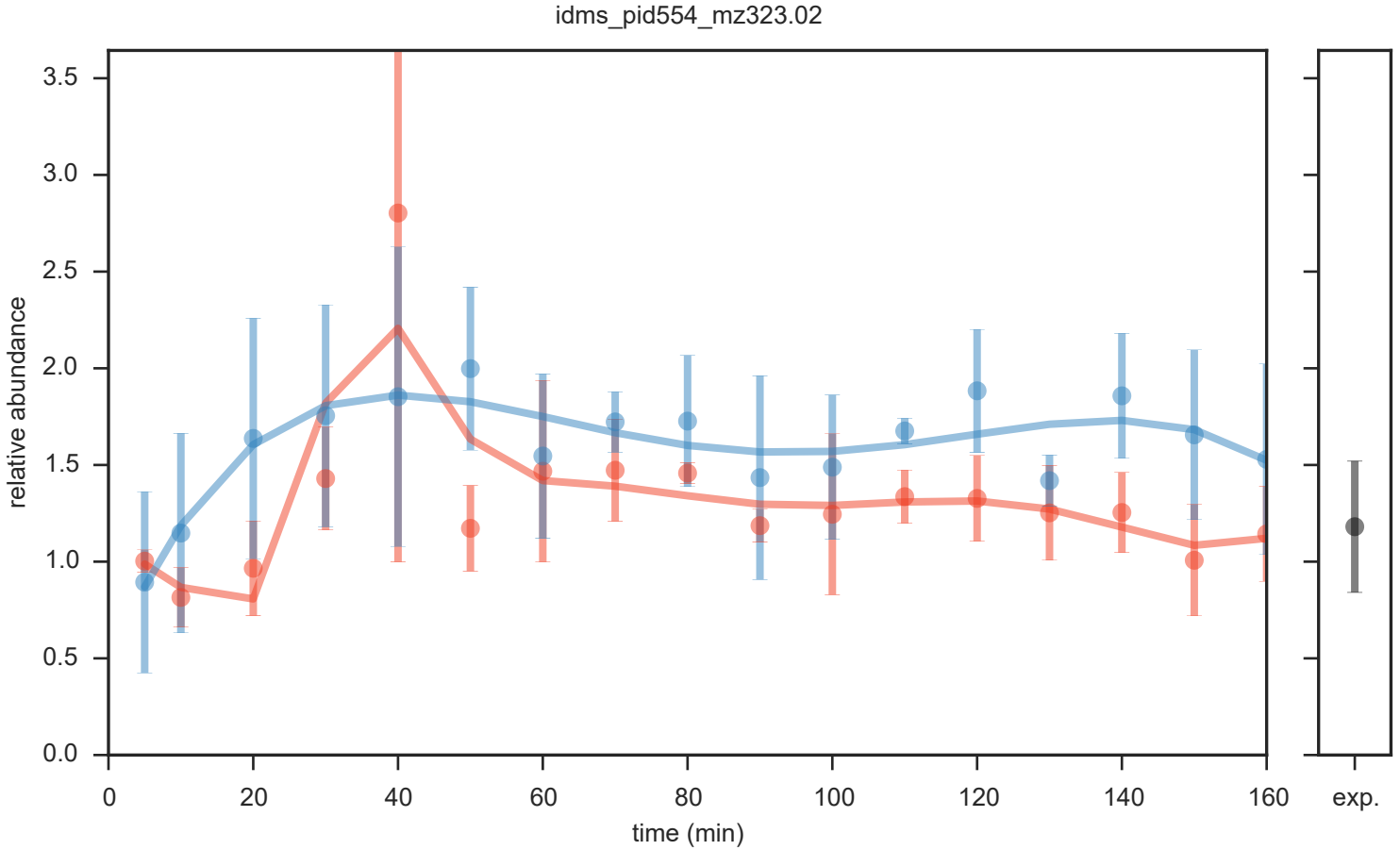

idms_pid528_mz332.95
relative abundance
0.0
0.5
1.0
1.5
2.0
2.5
0
20
40
60
80
100
120
140
160
time (min)
exp.

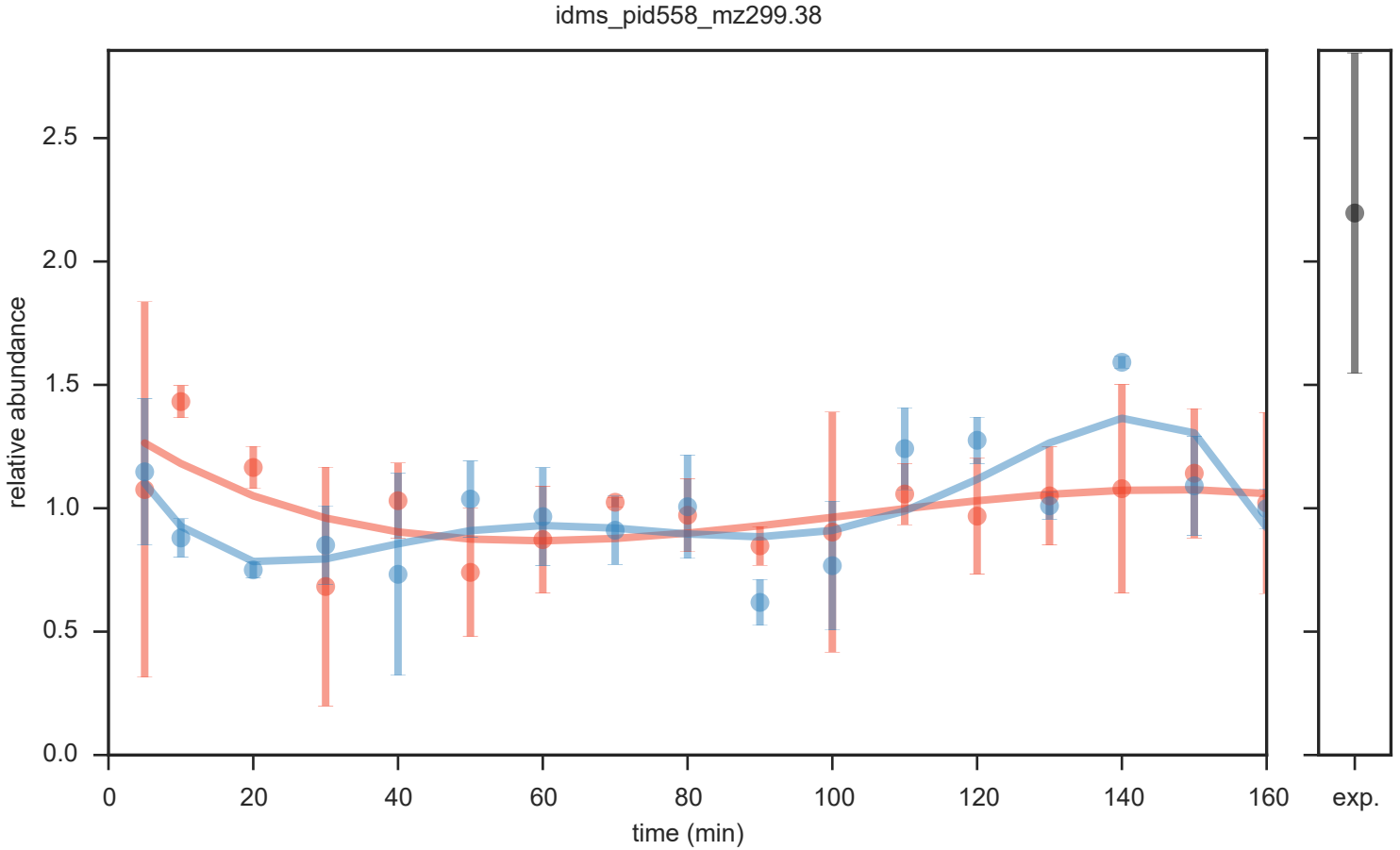

idms_pid529_mz240.54
relative abundance
time (min)
exp.
0
2
4
6
8
10
0
20
40
60
80
100
120
140
160

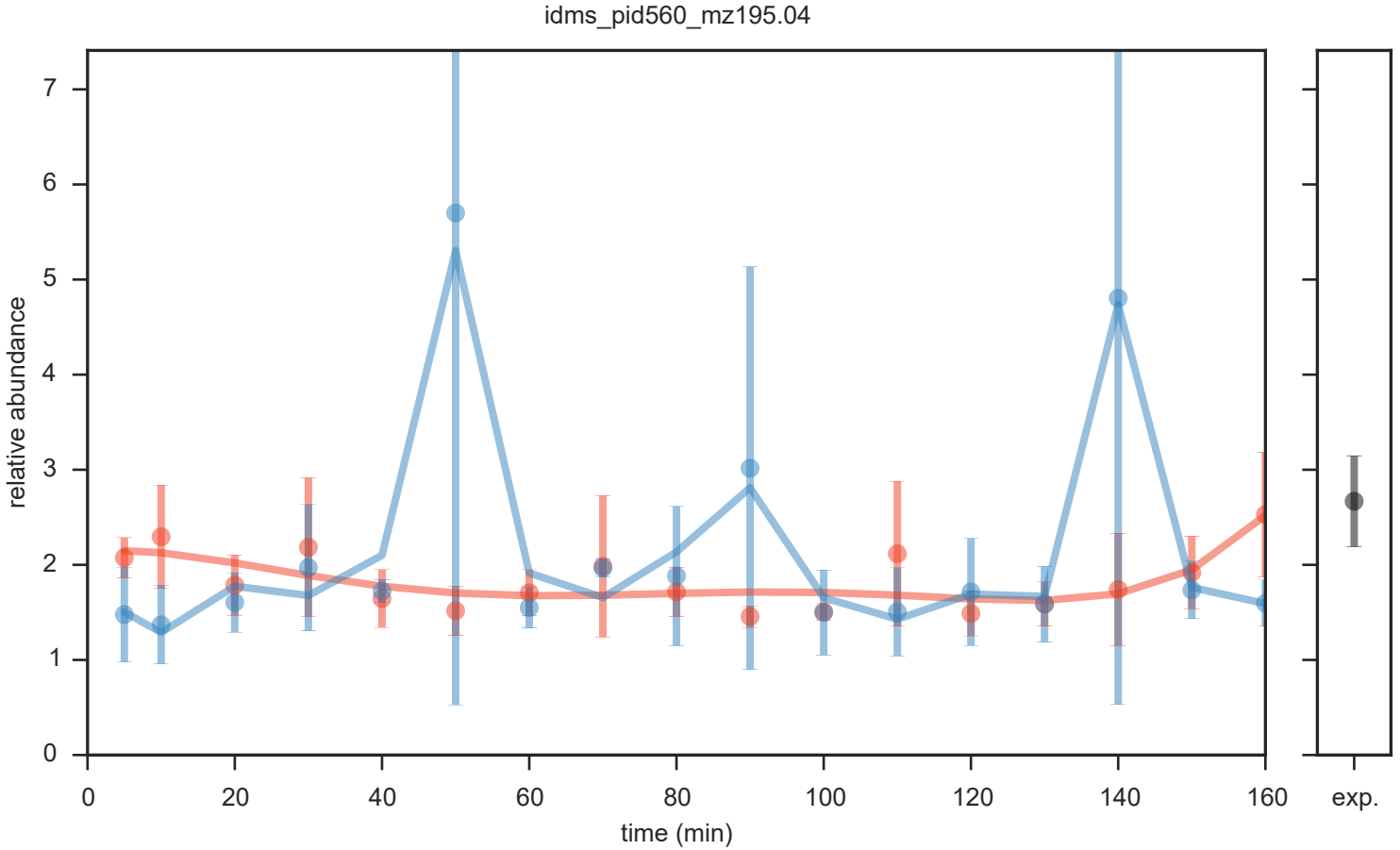

idms_pid544_mz410.56
relative abundance
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

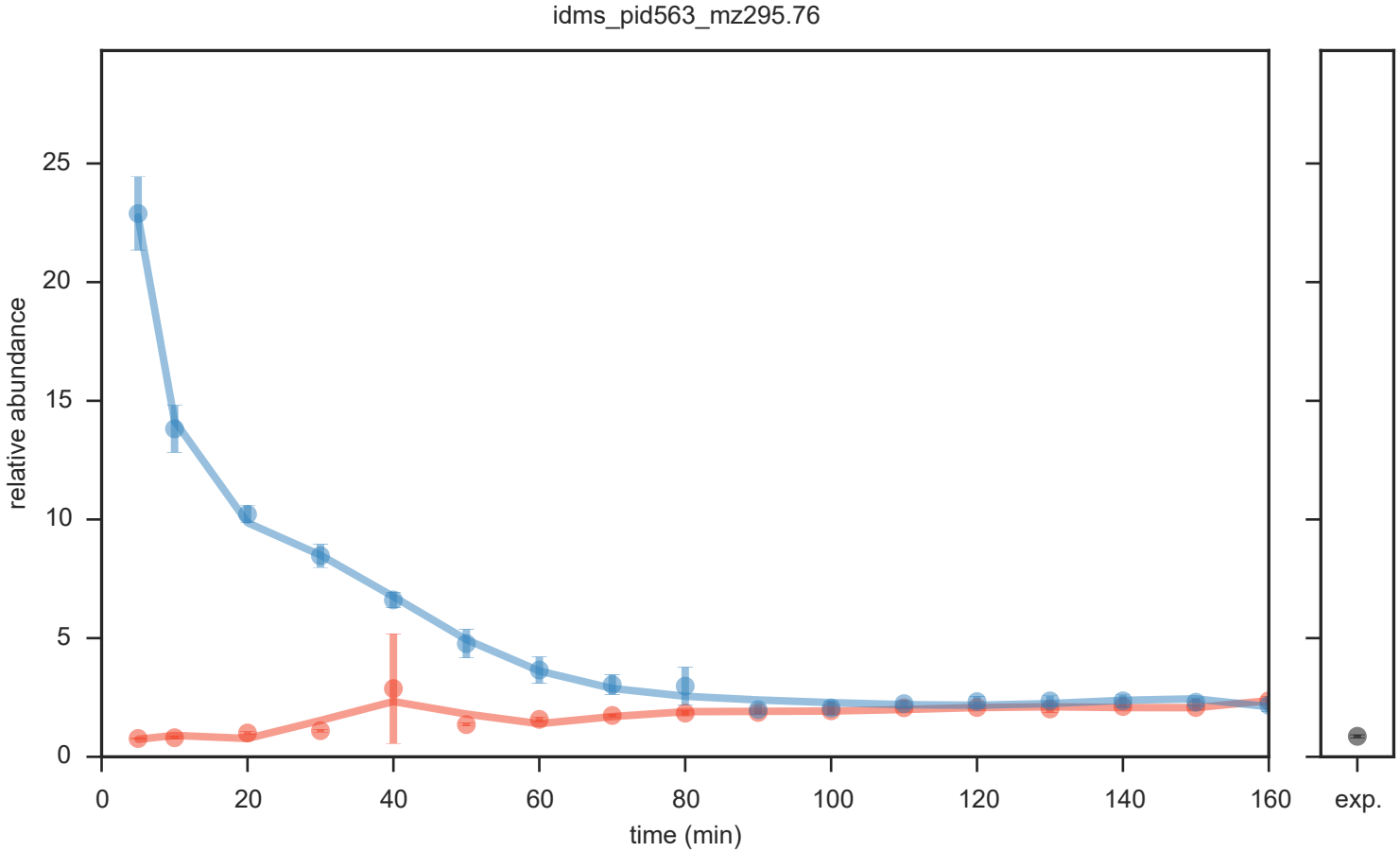

idms_pid551_mz318.51
relative abundance
0.0
0.2
0.4
0.6
0.8
1.0
1.2
0
20
40
60
80
100
120
140
160
time (min)
exp.

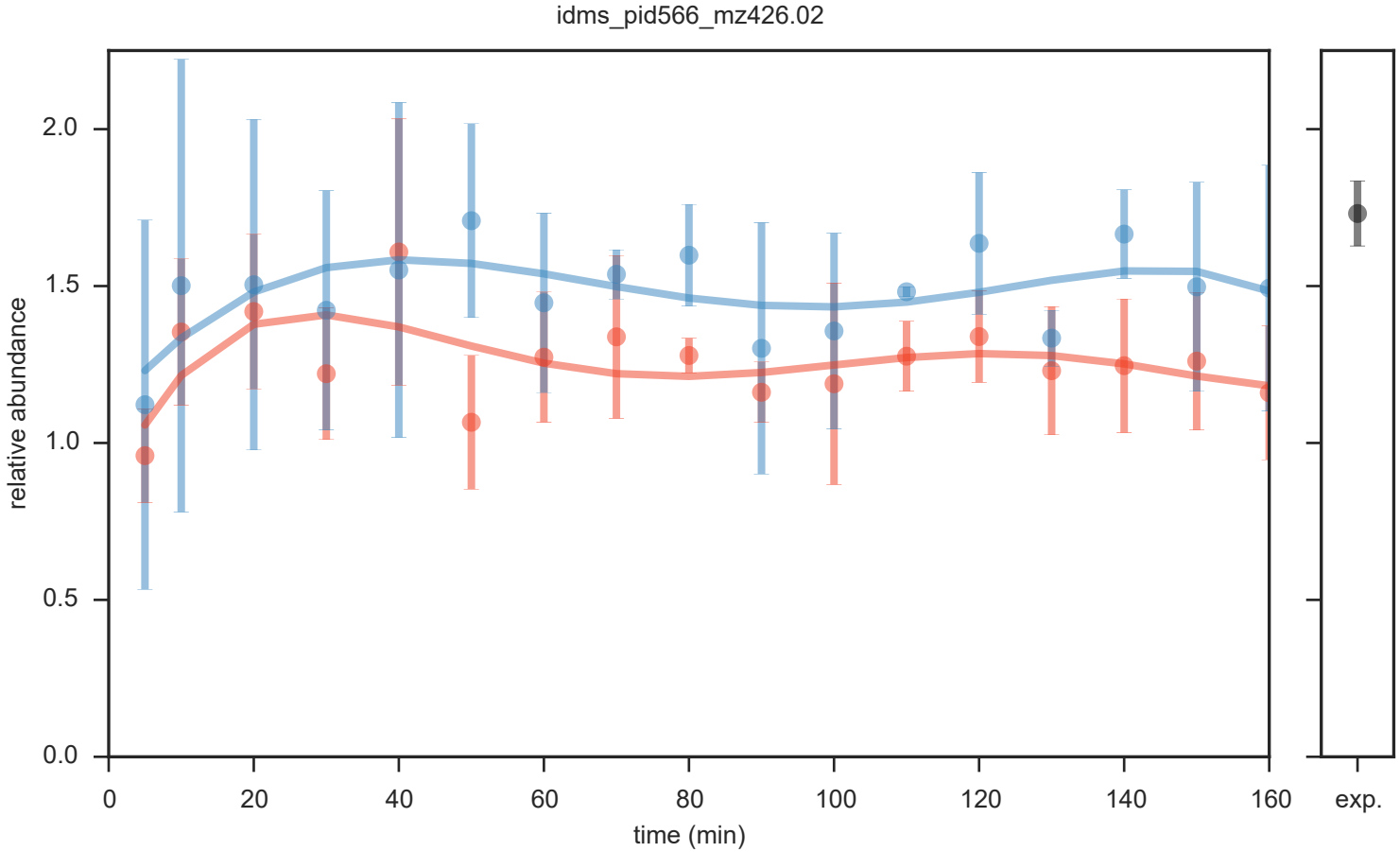

idms_pid552_mz398.02
relative abundance
0.0
0.5
1.0
1.5
2.0
2.5
0
20
40
60
80
100
120
140
160
time (min)
exp.

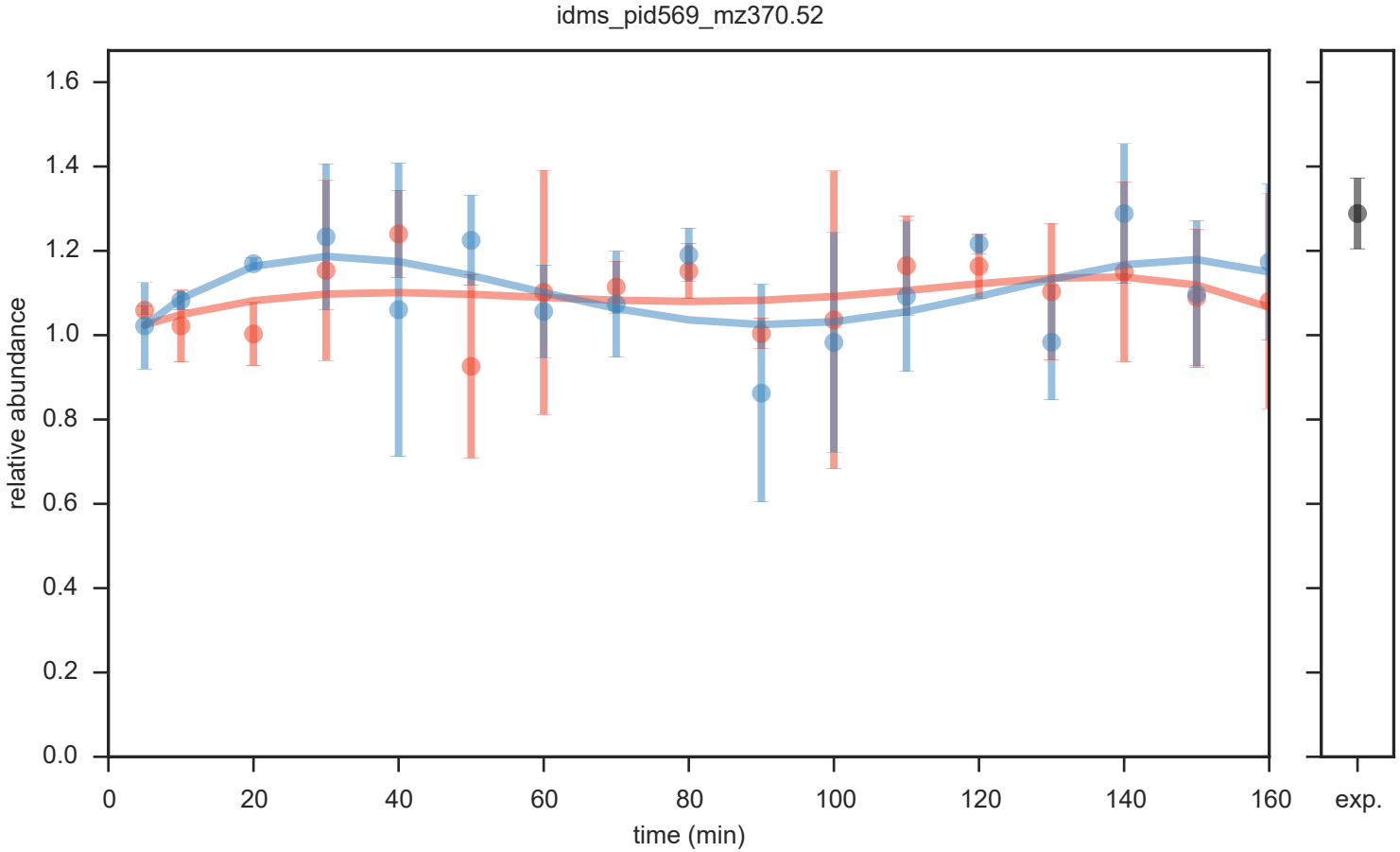

idms_pid554_mz323.02
relative abundance
time (min)
exp.
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
0
20
40
60
80
100
120
140
160

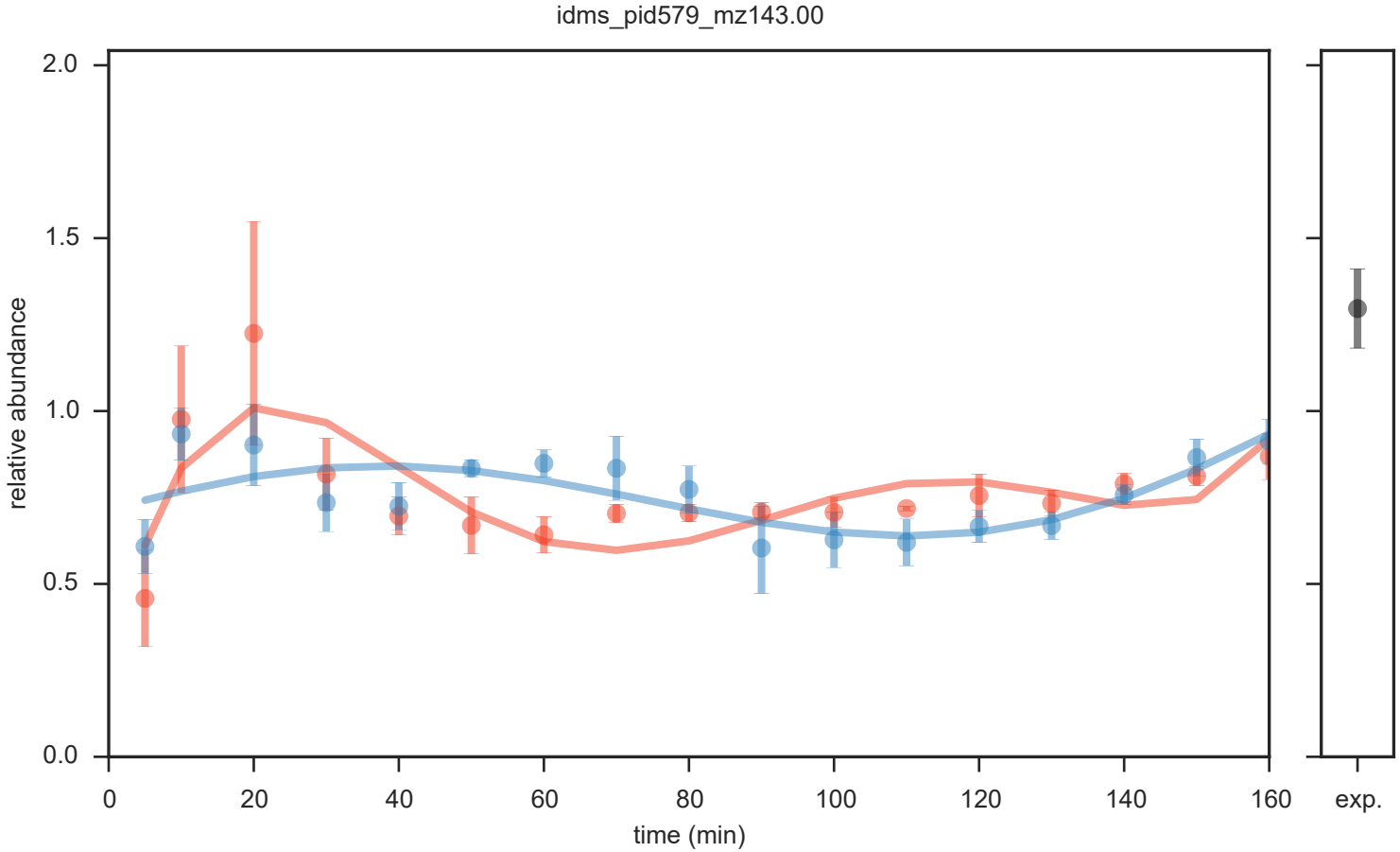

idms_pid558_mz299.38
relative abundance
0.0
0.5
1.0
1.5
2.0
2.5
0
20
40
60
80
100
120
140
160
time (min)
exp.

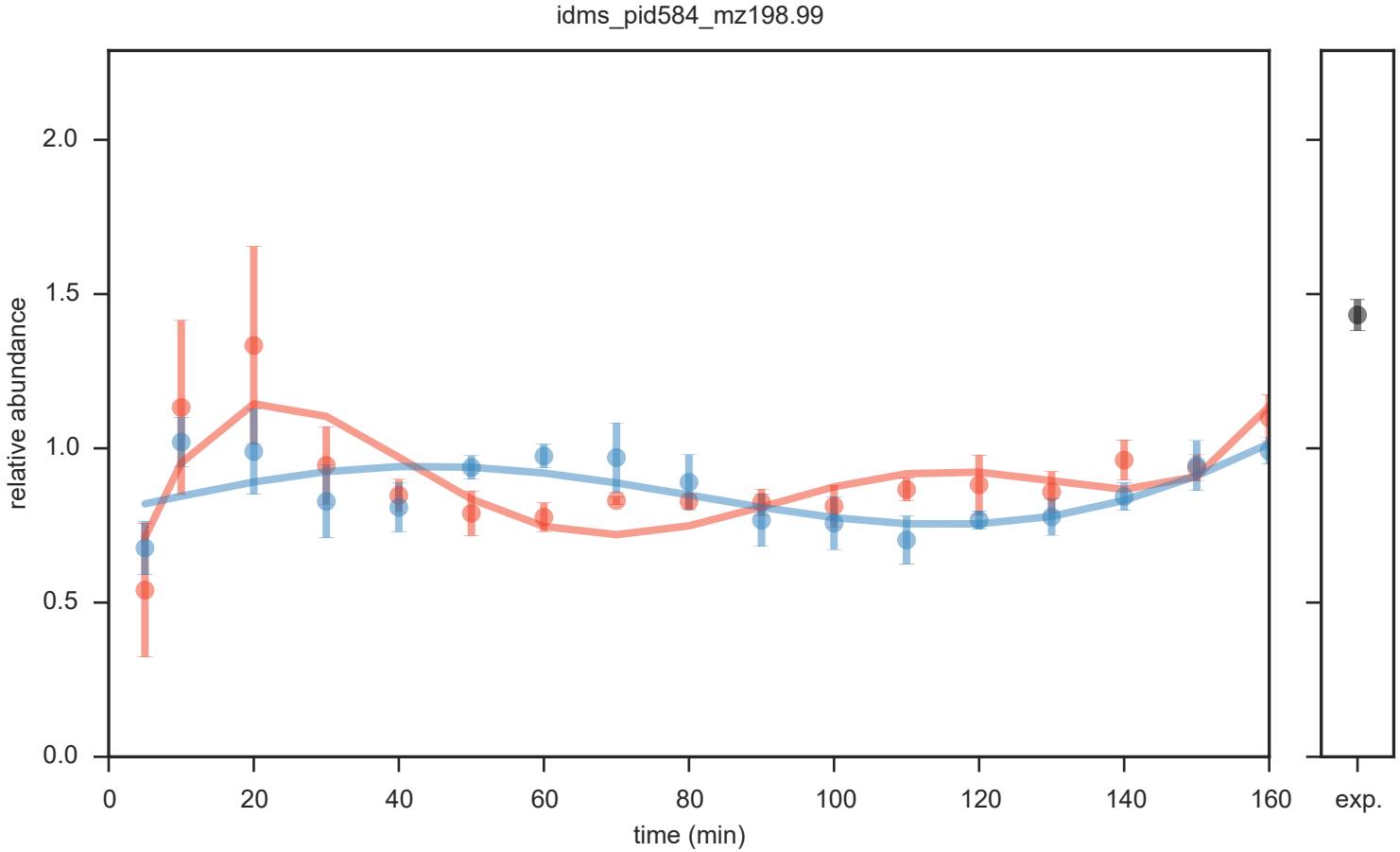

idms_pid560_mz195.04
relative abundance
0
1
2
3
4
5
6
7
0
20
40
60
80
100
120
140
160
time (min)
exp.

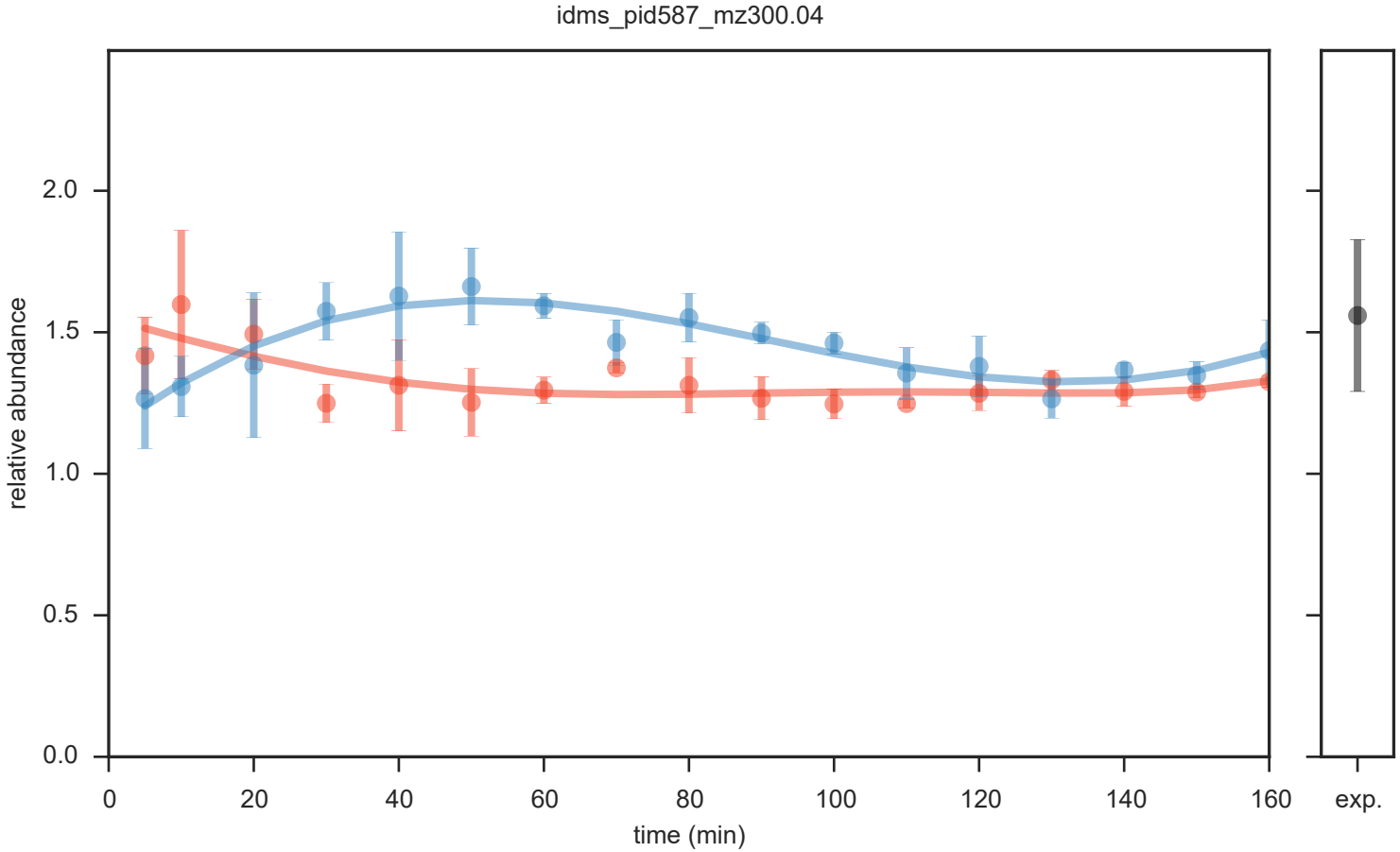

idms_pid563_mz295.76
relative abundance
0
5
10
15
20
25
0
20
40
60
80
100
120
140
160
time (min)
exp.

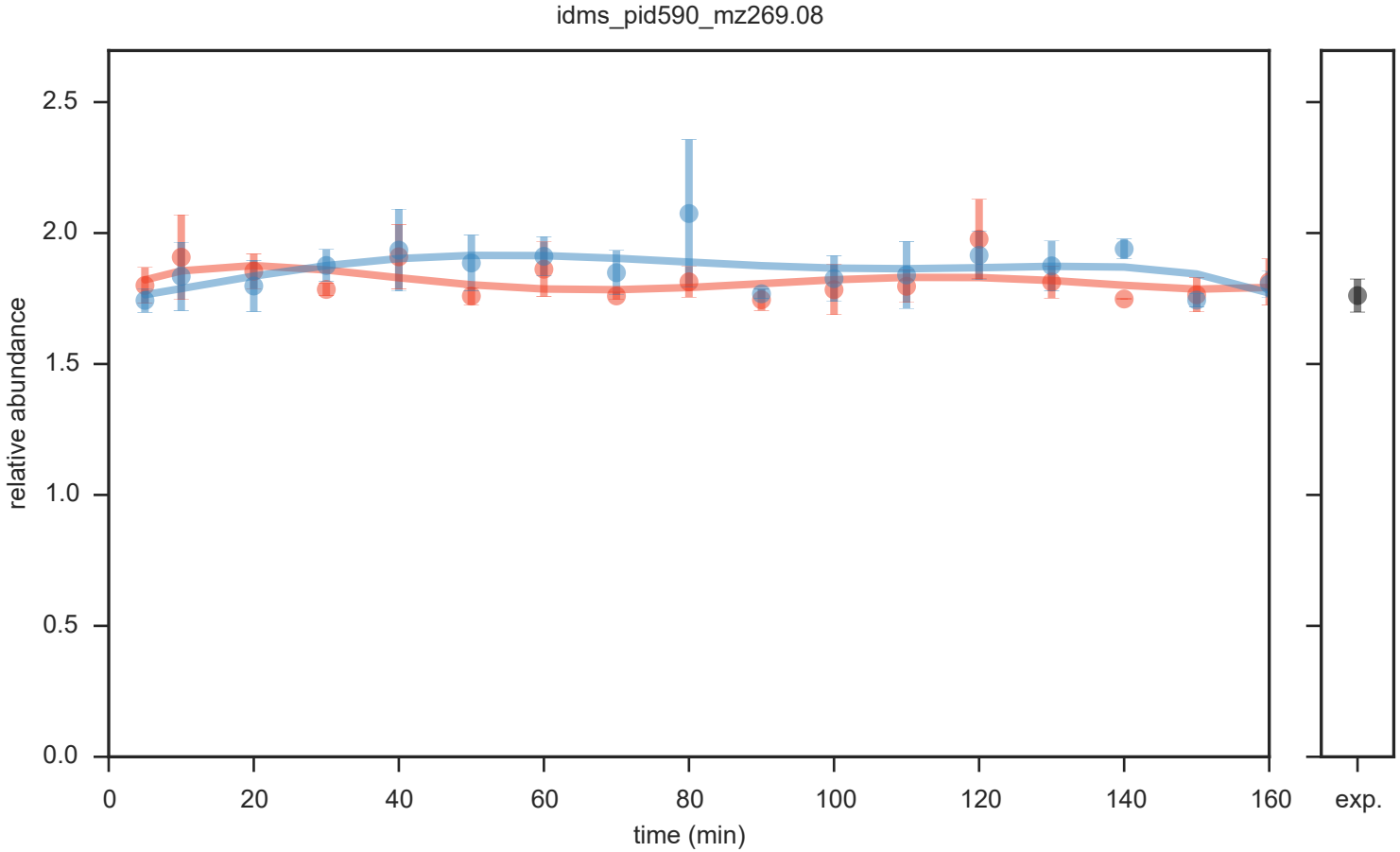

idms_pid566_mz426.02
relative abundance
0.0
0.5
1.0
1.5
2.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

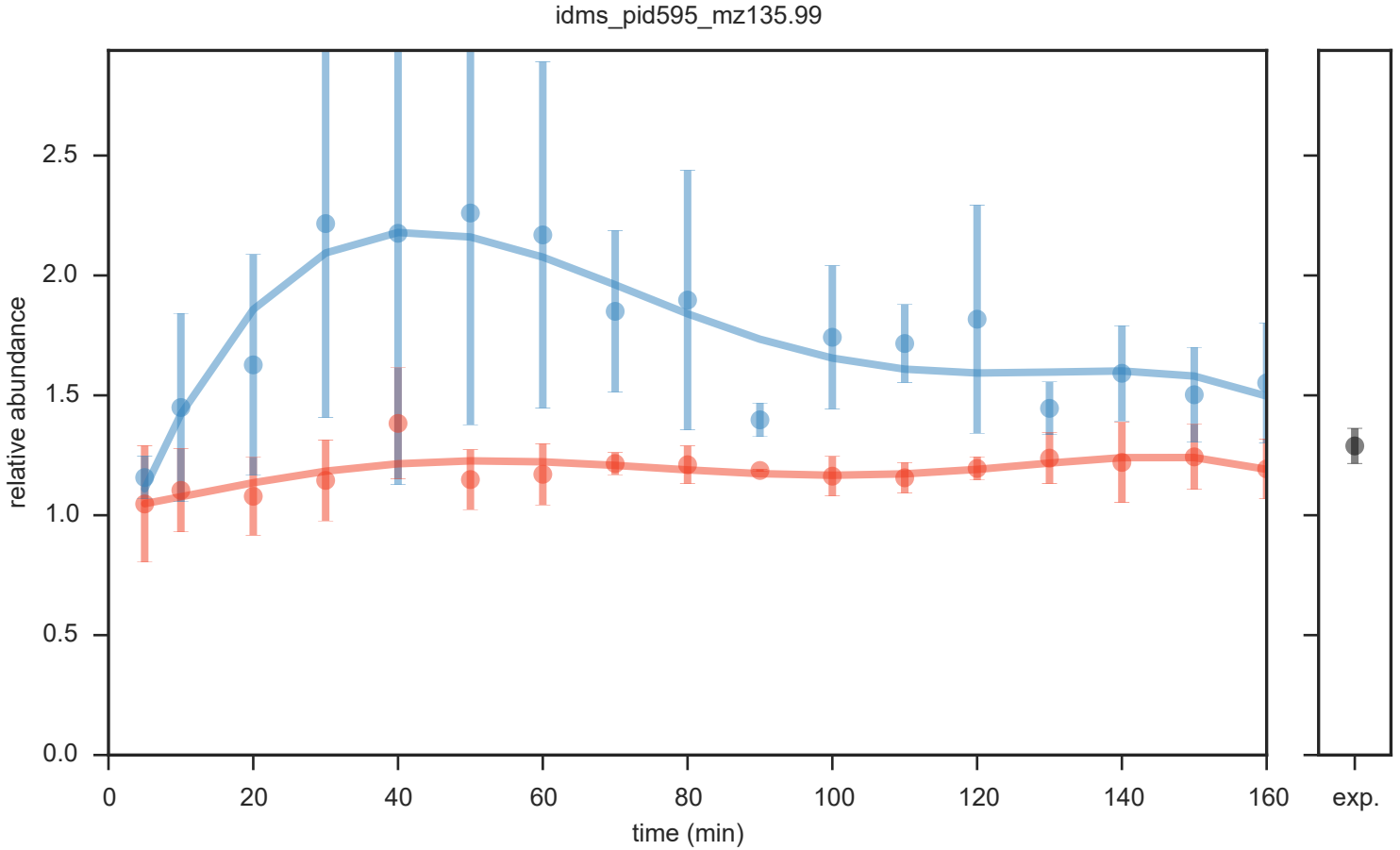

idms_pid569_mz370.52
relative abundance
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

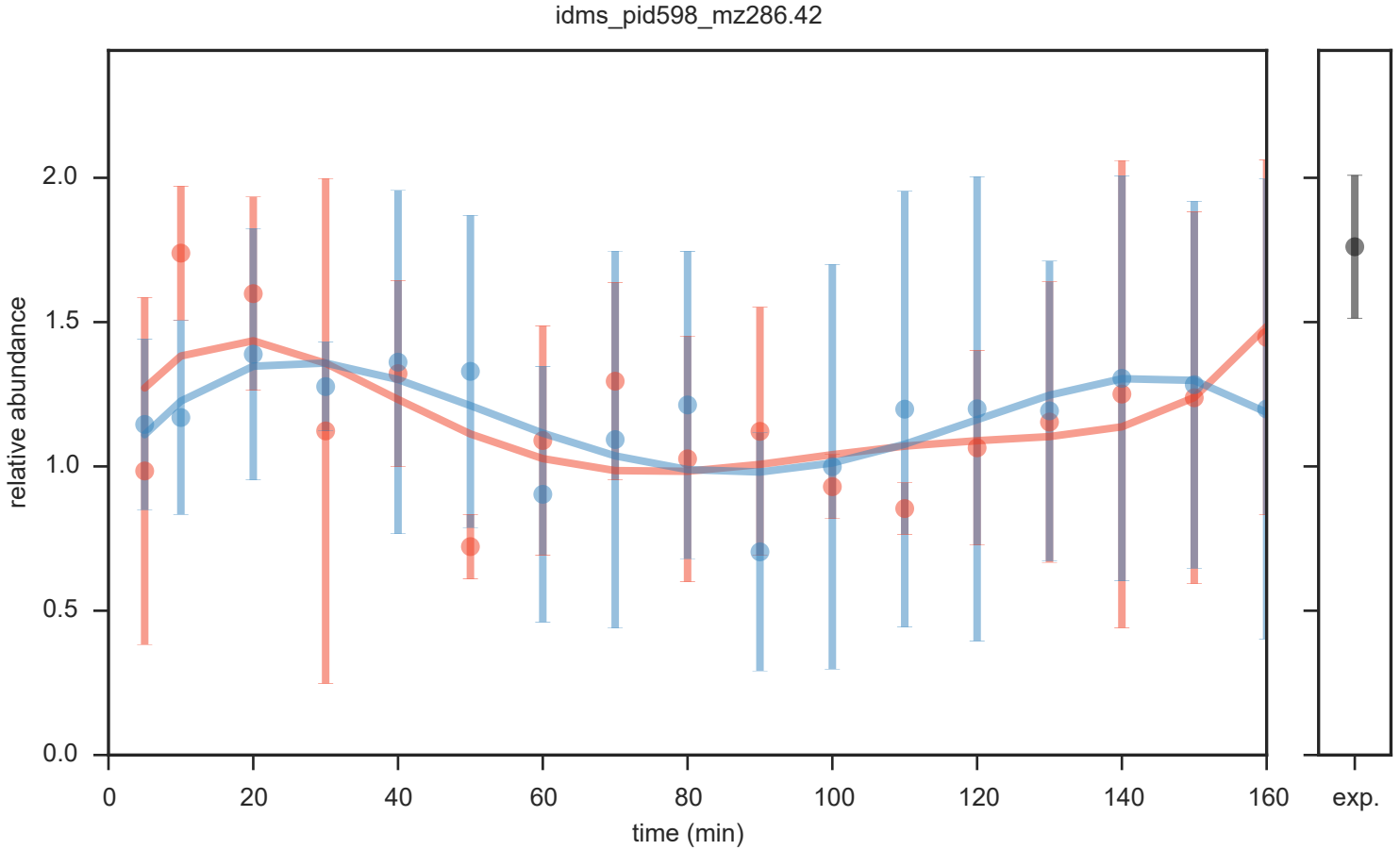

idms_pid579_mz143.00
relative abundance
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

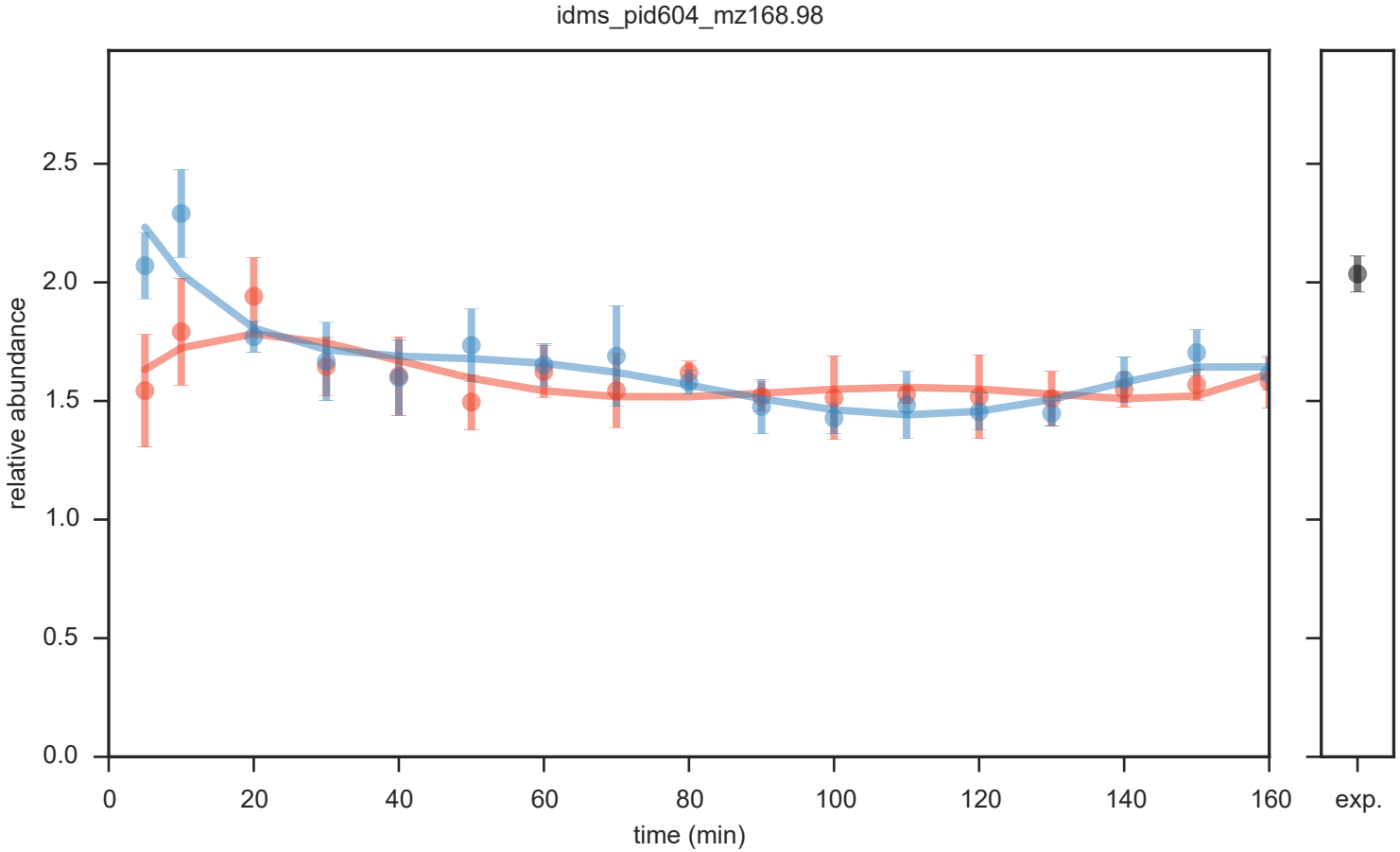

idms_pid584_mz198.99
relative abundance
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

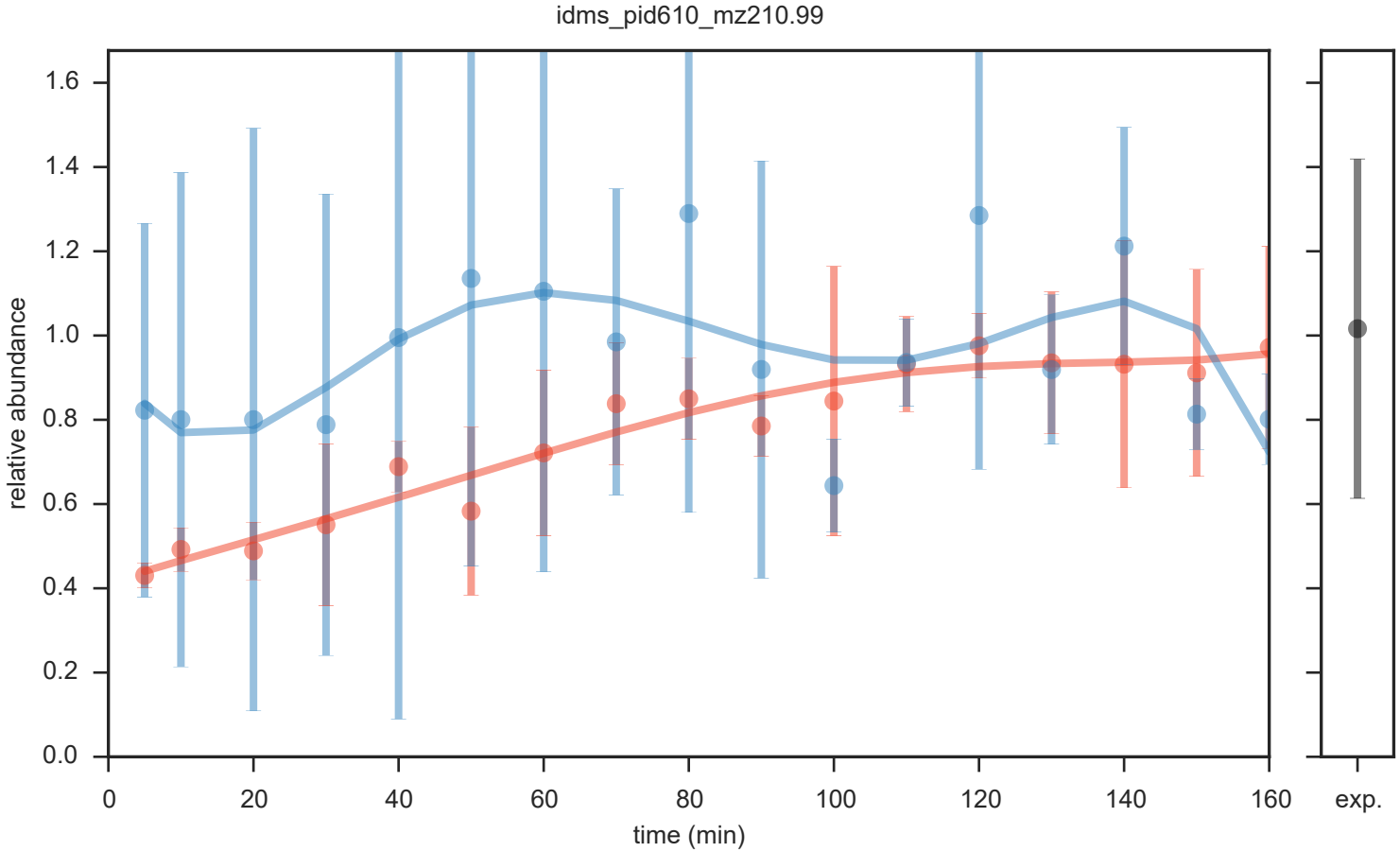

idms_pid587_mz300.04
relative abundance
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

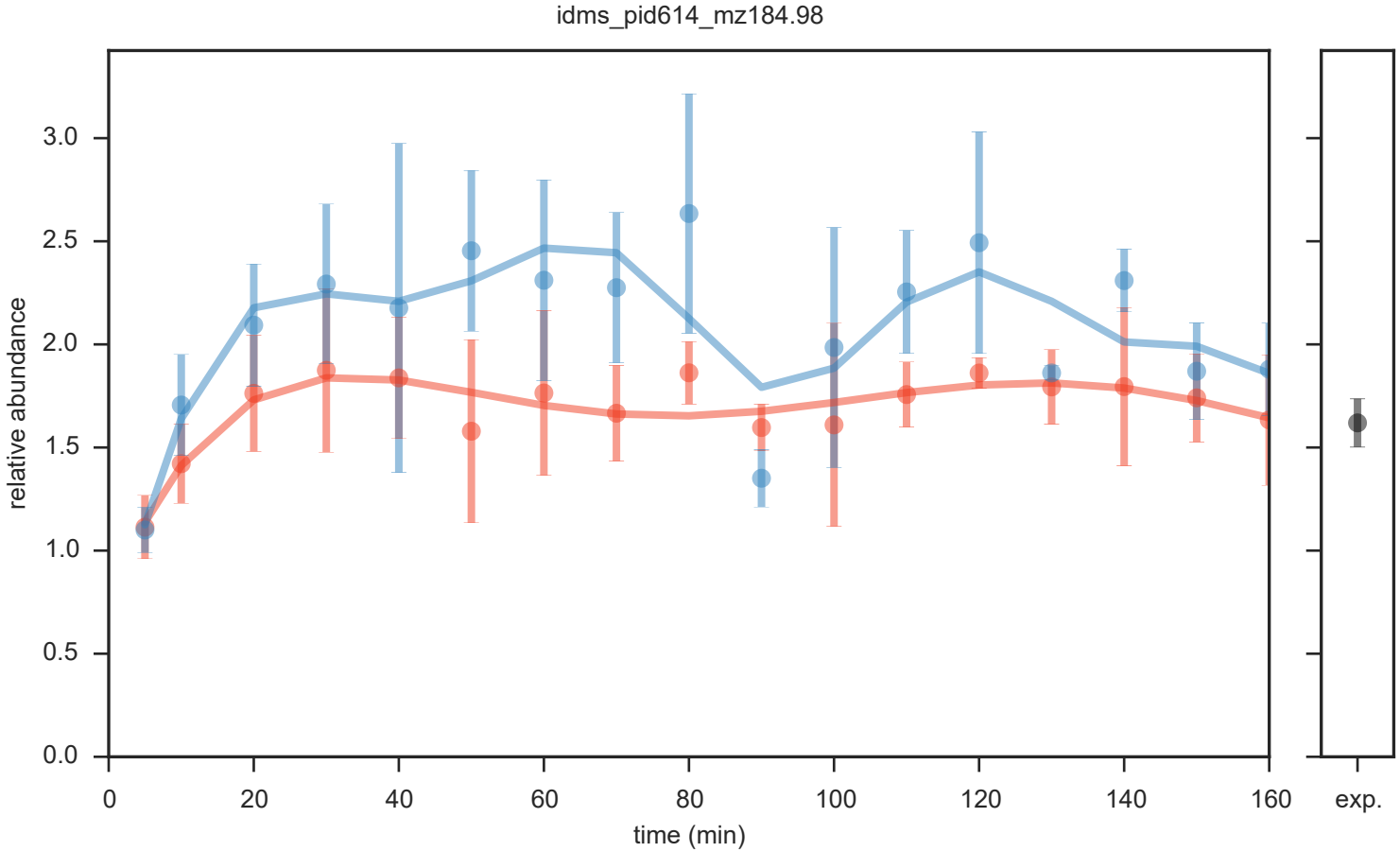

idms_pid590_mz269.08
relative abundance
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

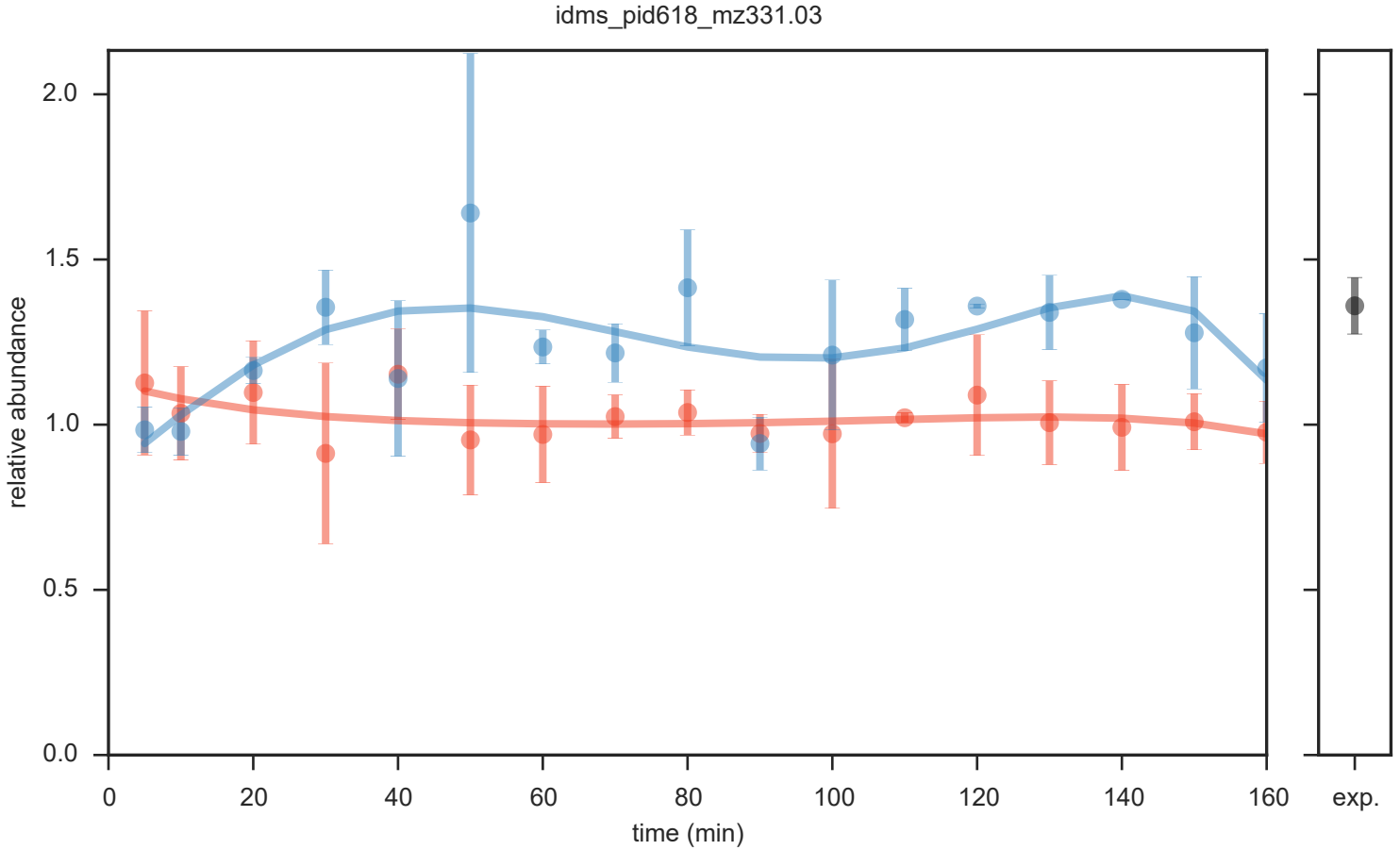

idms_pid595_mz135.99
relative abundance
0.0
0.5
1.0
1.5
2.0
2.5
0
20
40
60
80
100
120
140
160
time (min)
exp.

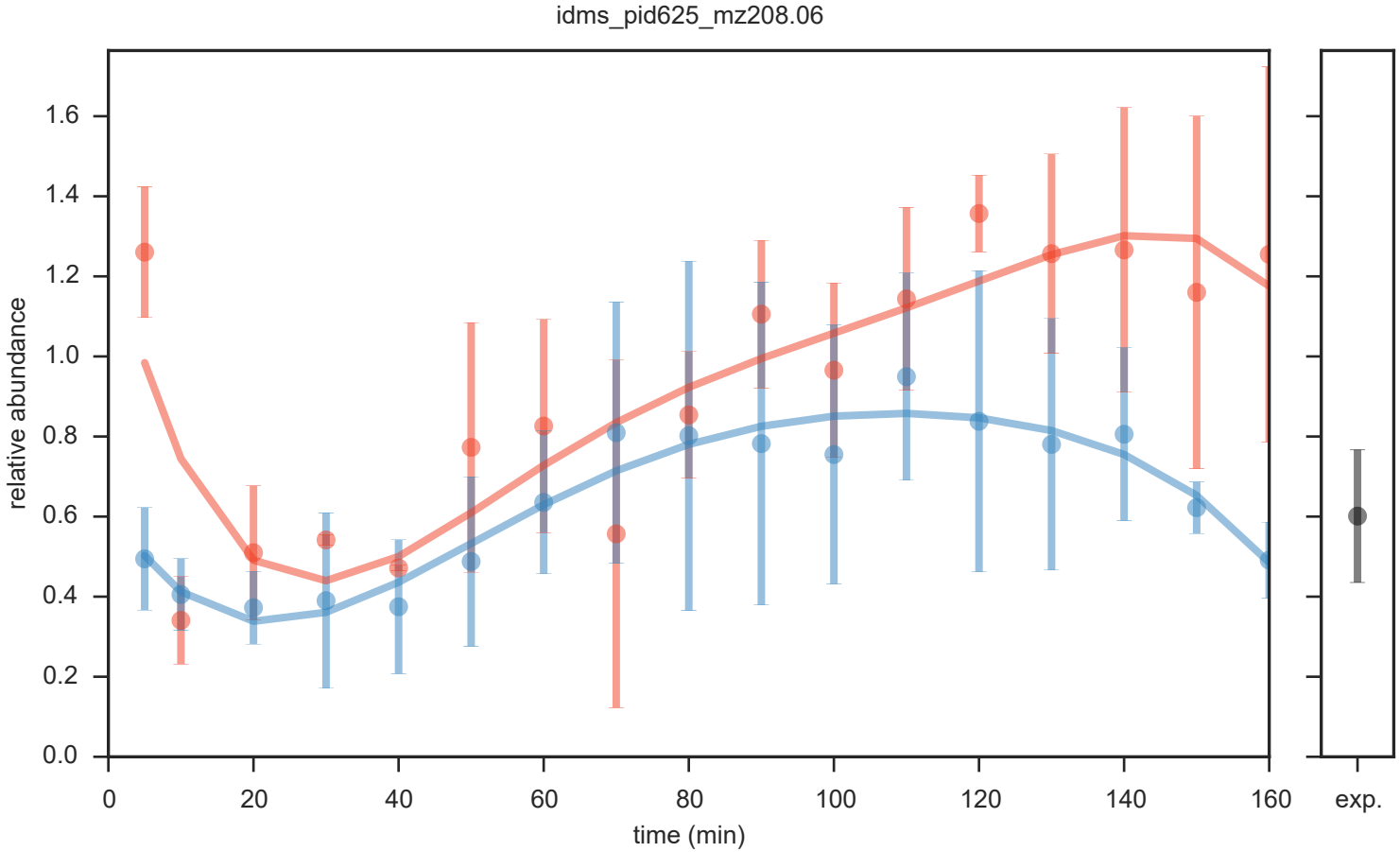

idms_pid598_mz286.42
relative abundance
0.0
0.5
1.0
1.5
2.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

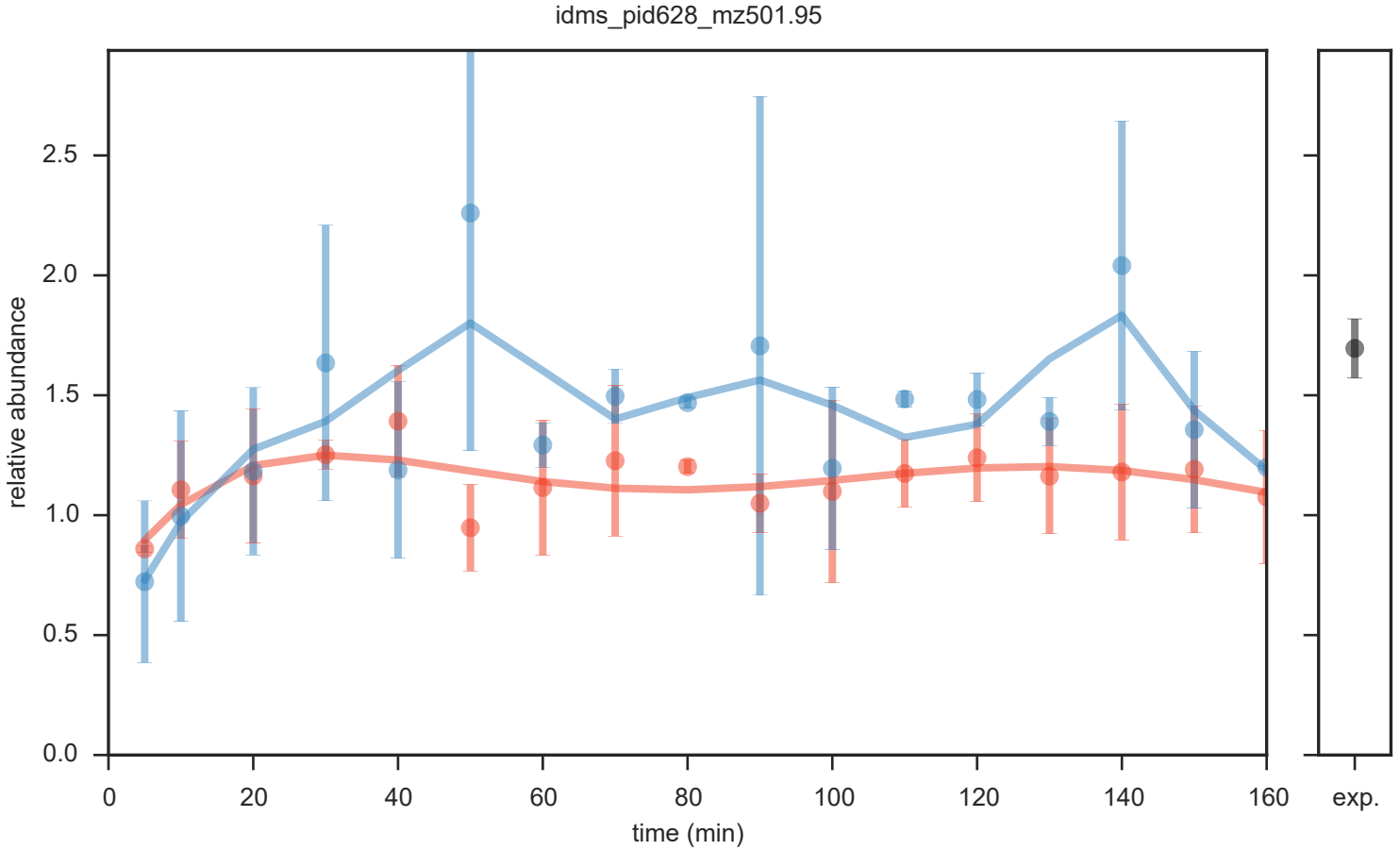

idms_pid604_mz168.98
relative abundance
0.0
0.5
1.0
1.5
2.0
2.5
0
20
40
60
80
100
120
140
160
time (min)
exp.

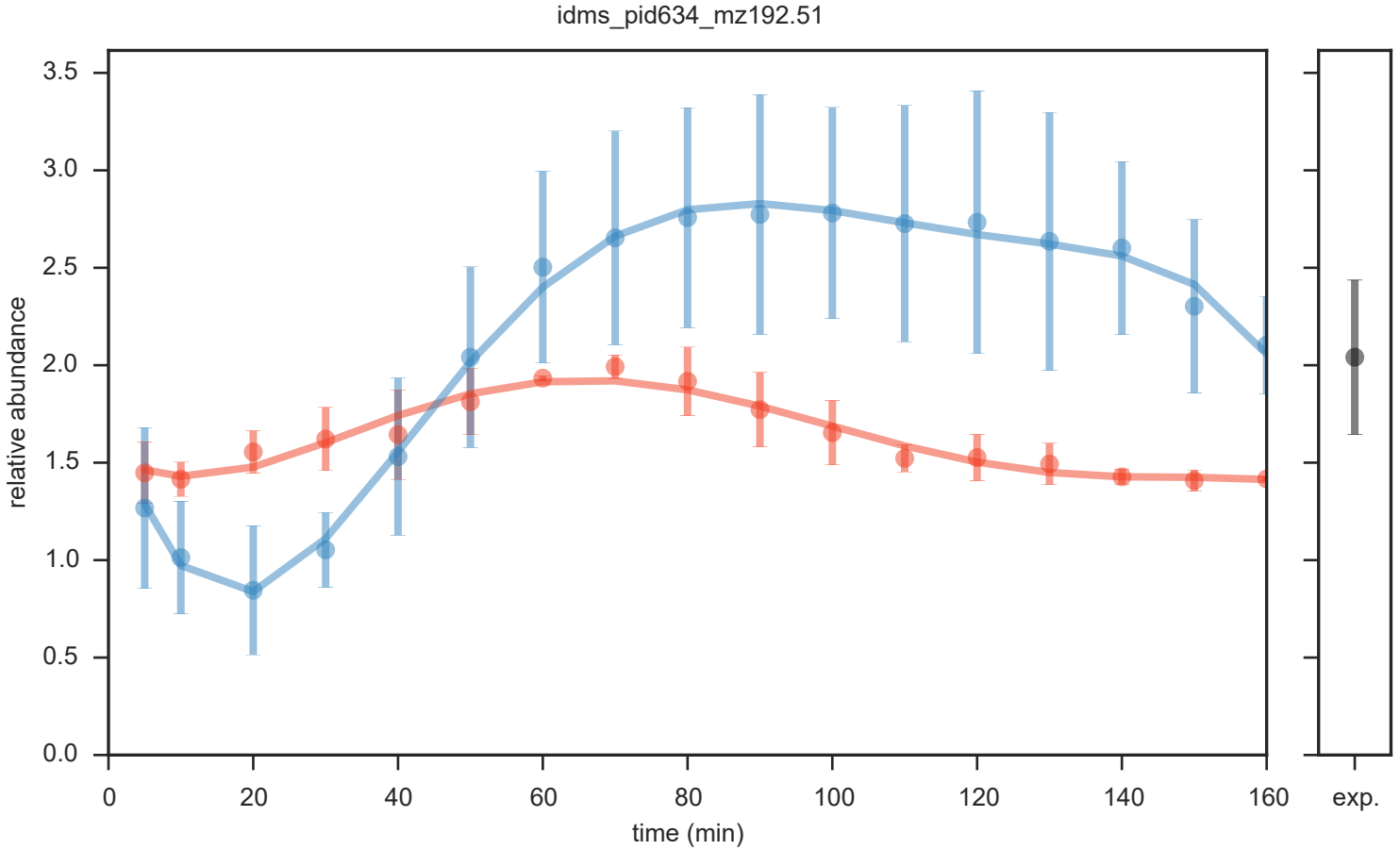

idms_pid610_mz210.99
relative abundance
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
0
20
40
60
80
100
120
140
160
time (min)
exp.

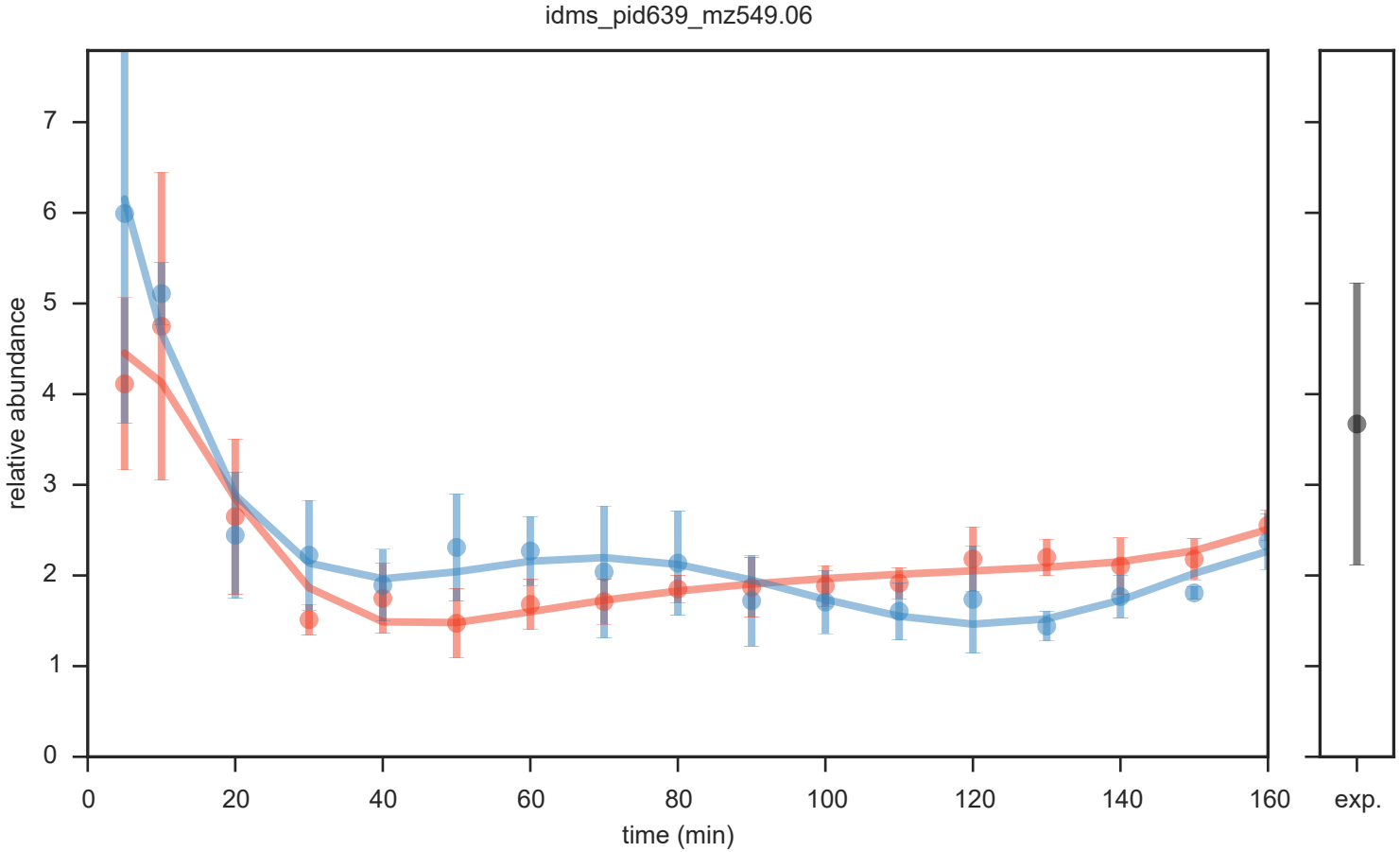

idms_pid614_mz184.98
relative abundance
0.0
0.5
1.0
1.5
2.0
2.5
3.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

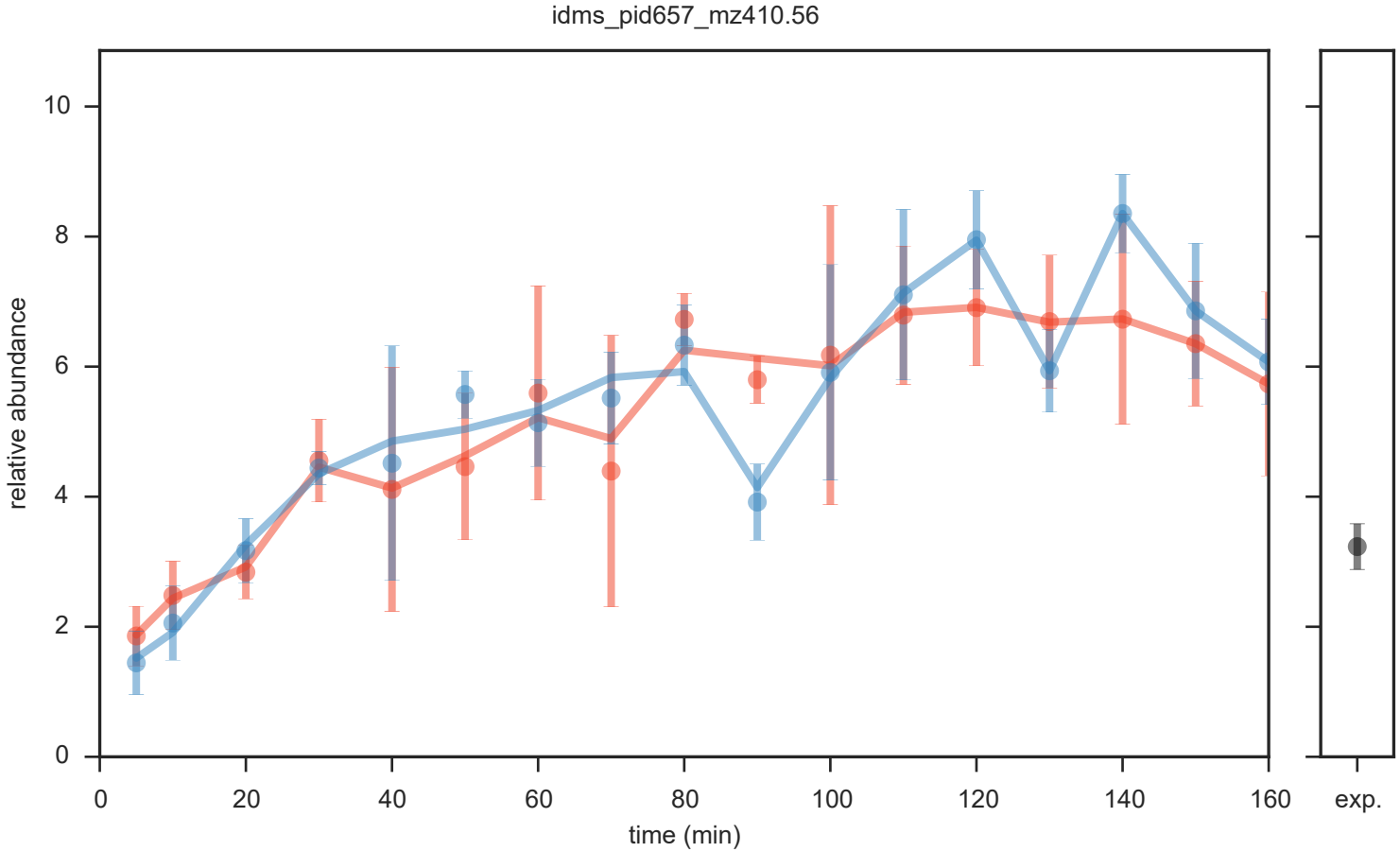

idms_pid618_mz331.03
relative abundance
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

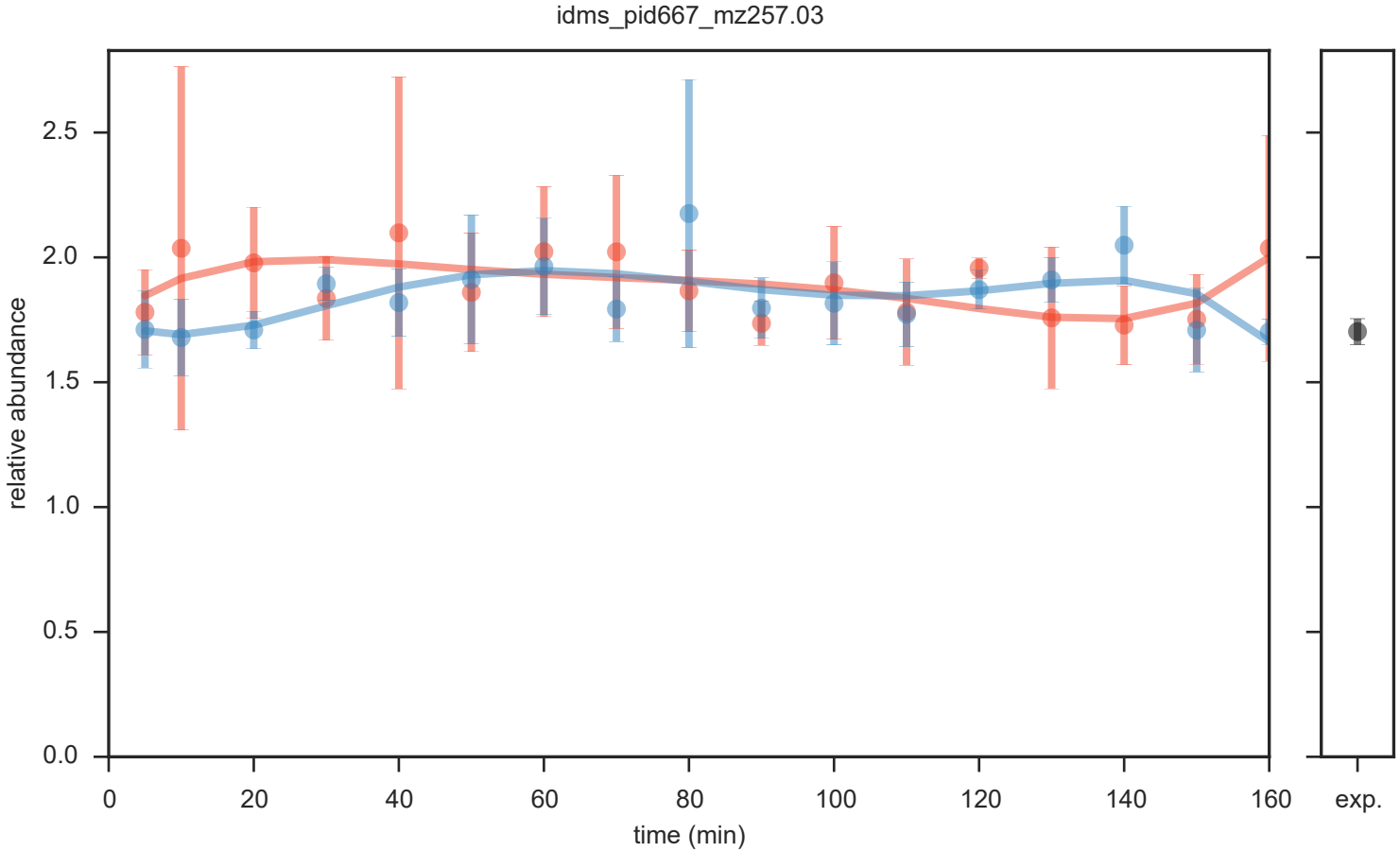

idms_pid625_mz208.06
relative abundance
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
0
20
40
60
80
100
120
140
160
time (min)
exp.

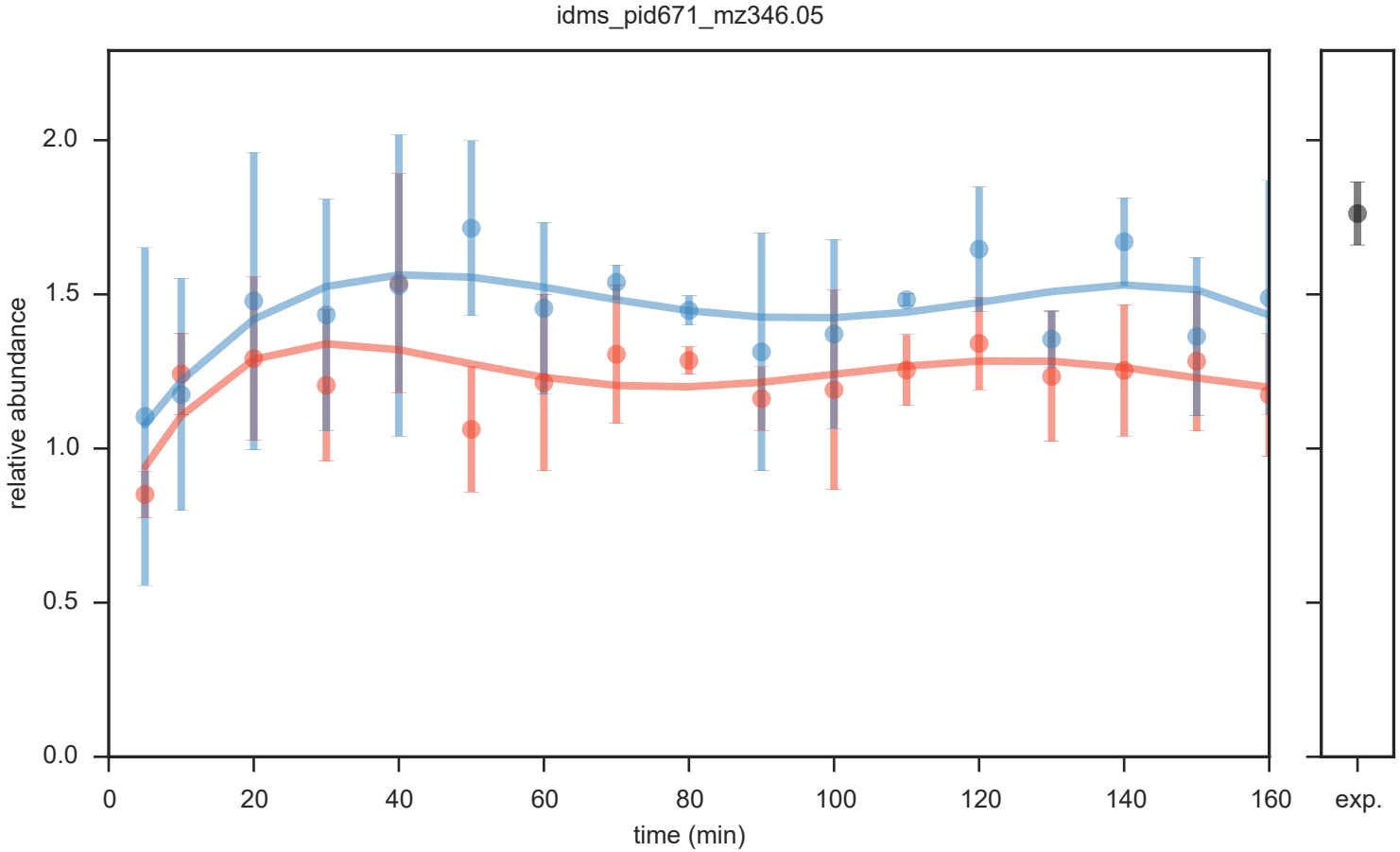

idms_pid628_mz501.95
relative abundance
0.0
0.5
1.0
1.5
2.0
2.5
0
20
40
60
80
100
120
140
160
time (min)
exp.

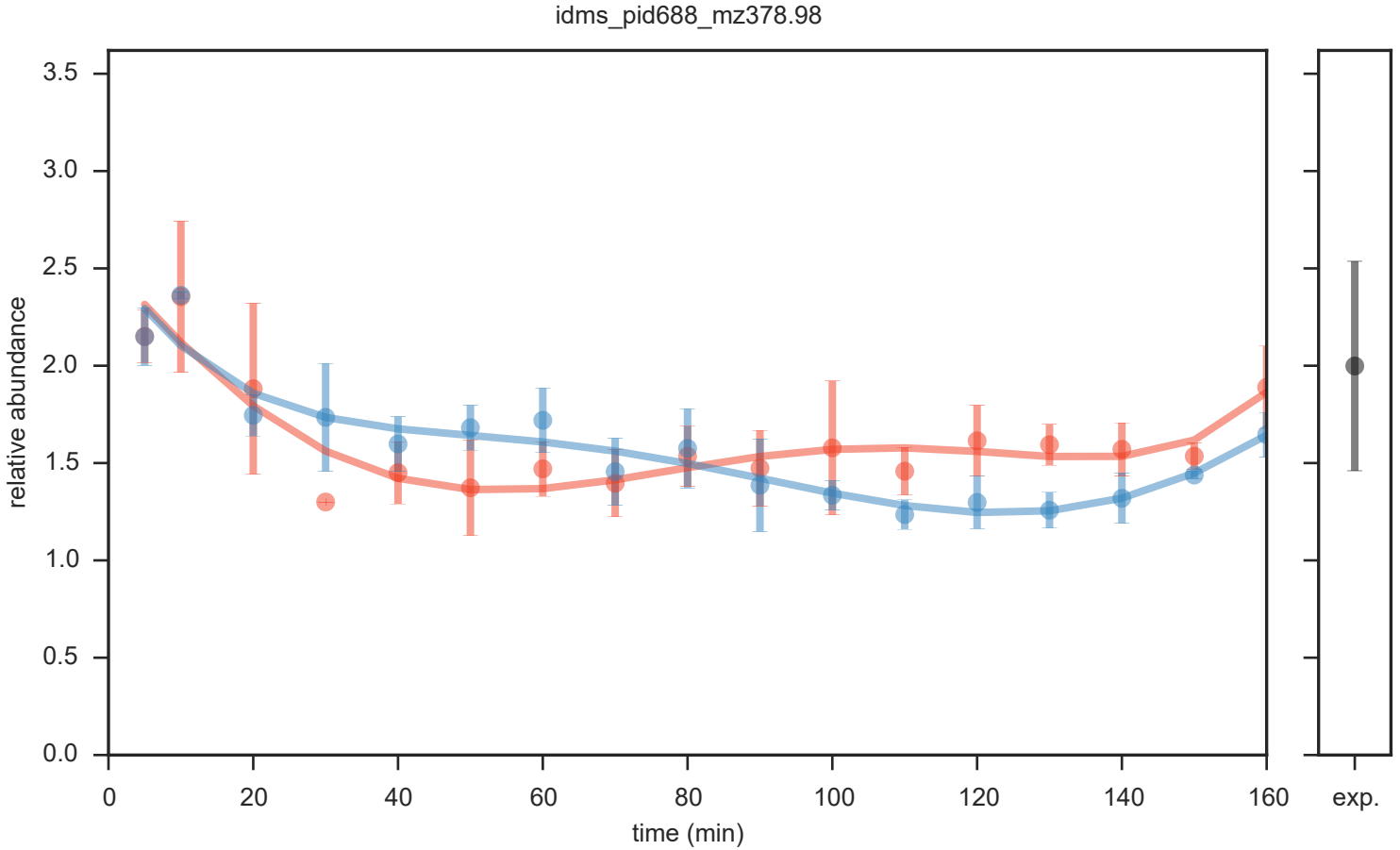

idms_pid634_mz192.51
relative abundance
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

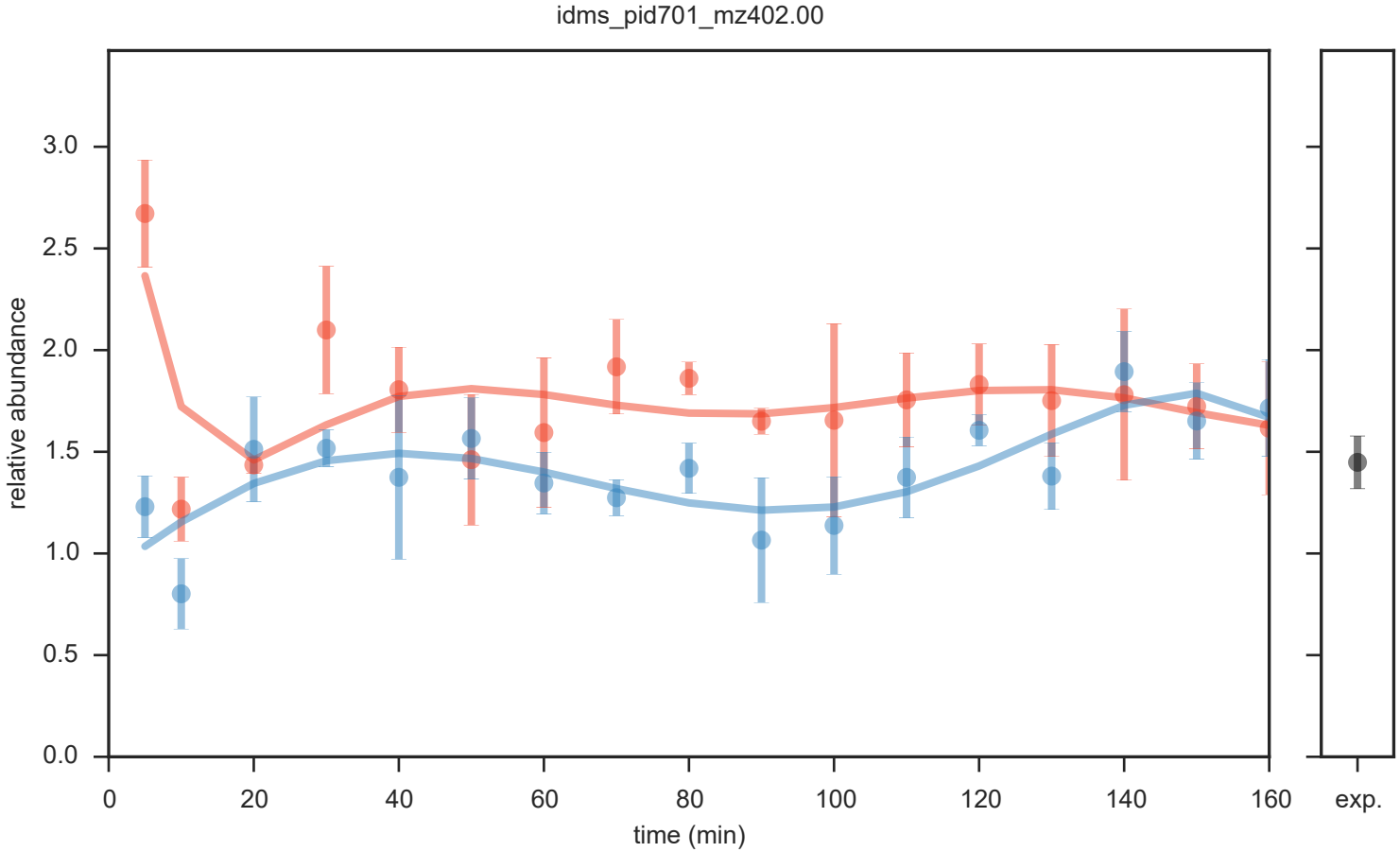

idms_pid639_mz549.06
relative abundance
0
1
2
3
4
5
6
7
0
20
40
60
80
100
120
140
160
time (min)
exp.

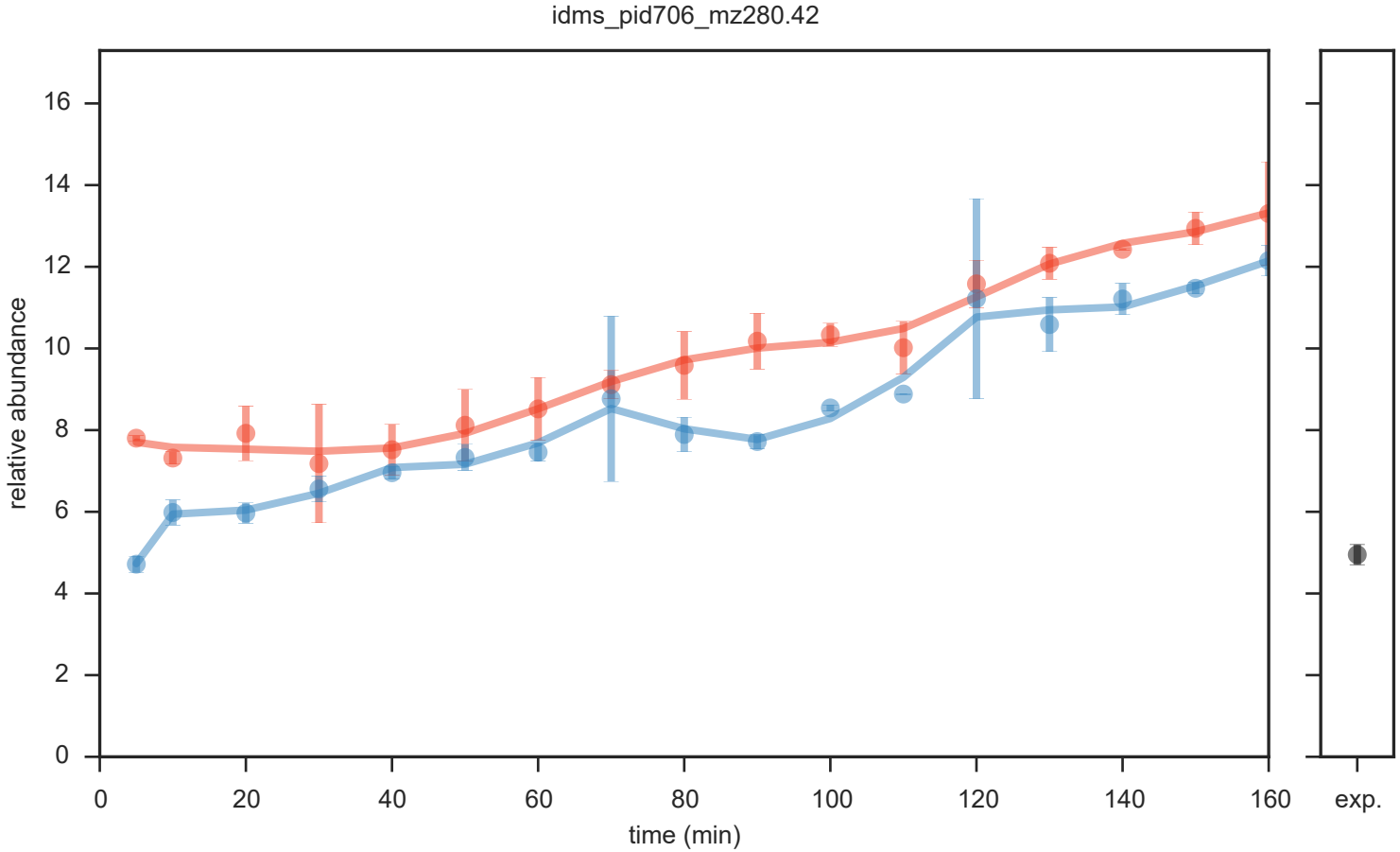

idms_pid657_mz410.56
relative abundance
0
2
4
6
8
10
0
20
40
60
80
100
120
140
160
time (min)
exp.

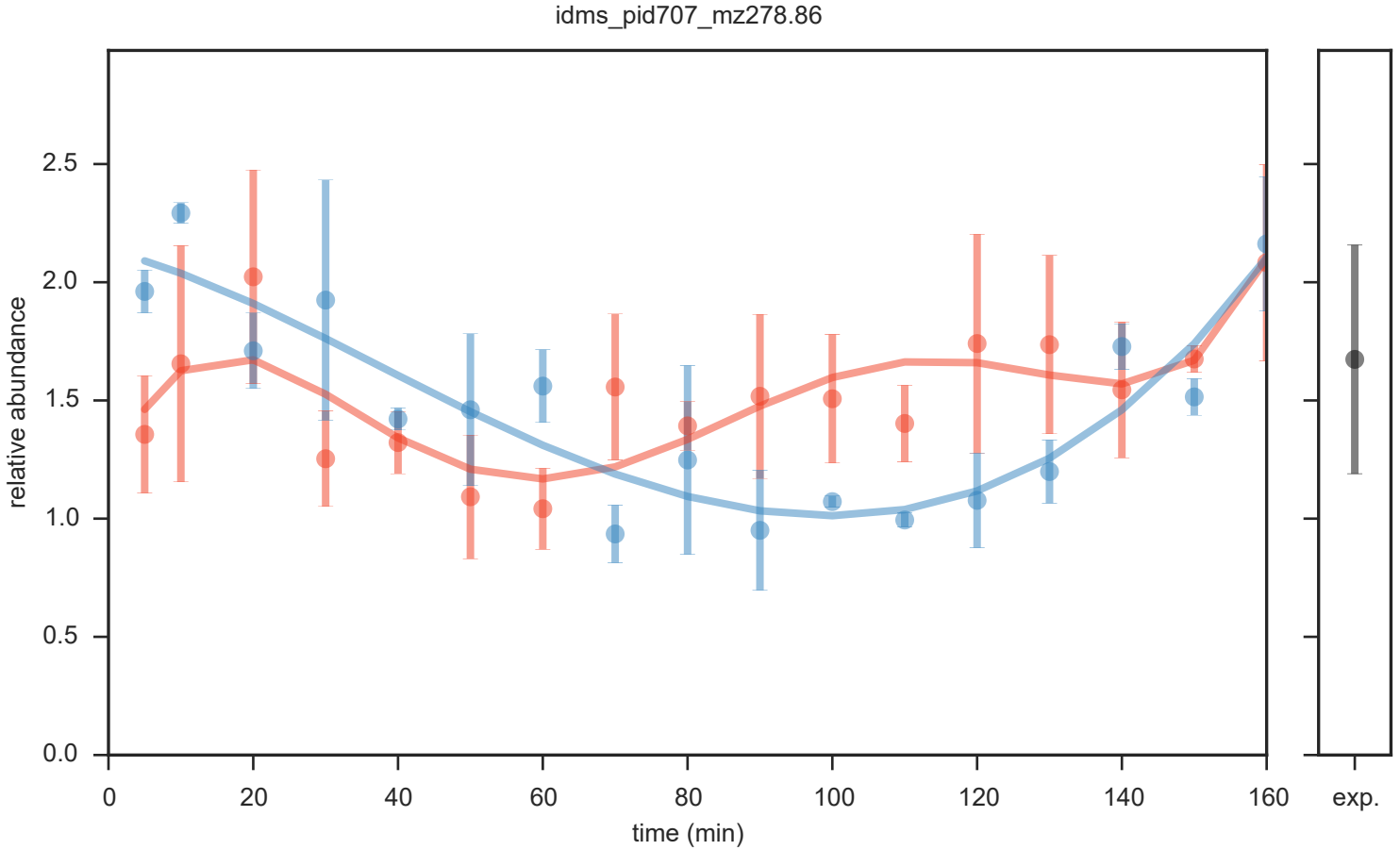

idms_pid667_mz257.03
relative abundance
0.0
0.5
1.0
1.5
2.0
2.5
0
20
40
60
80
100
120
140
160
time (min)
exp.

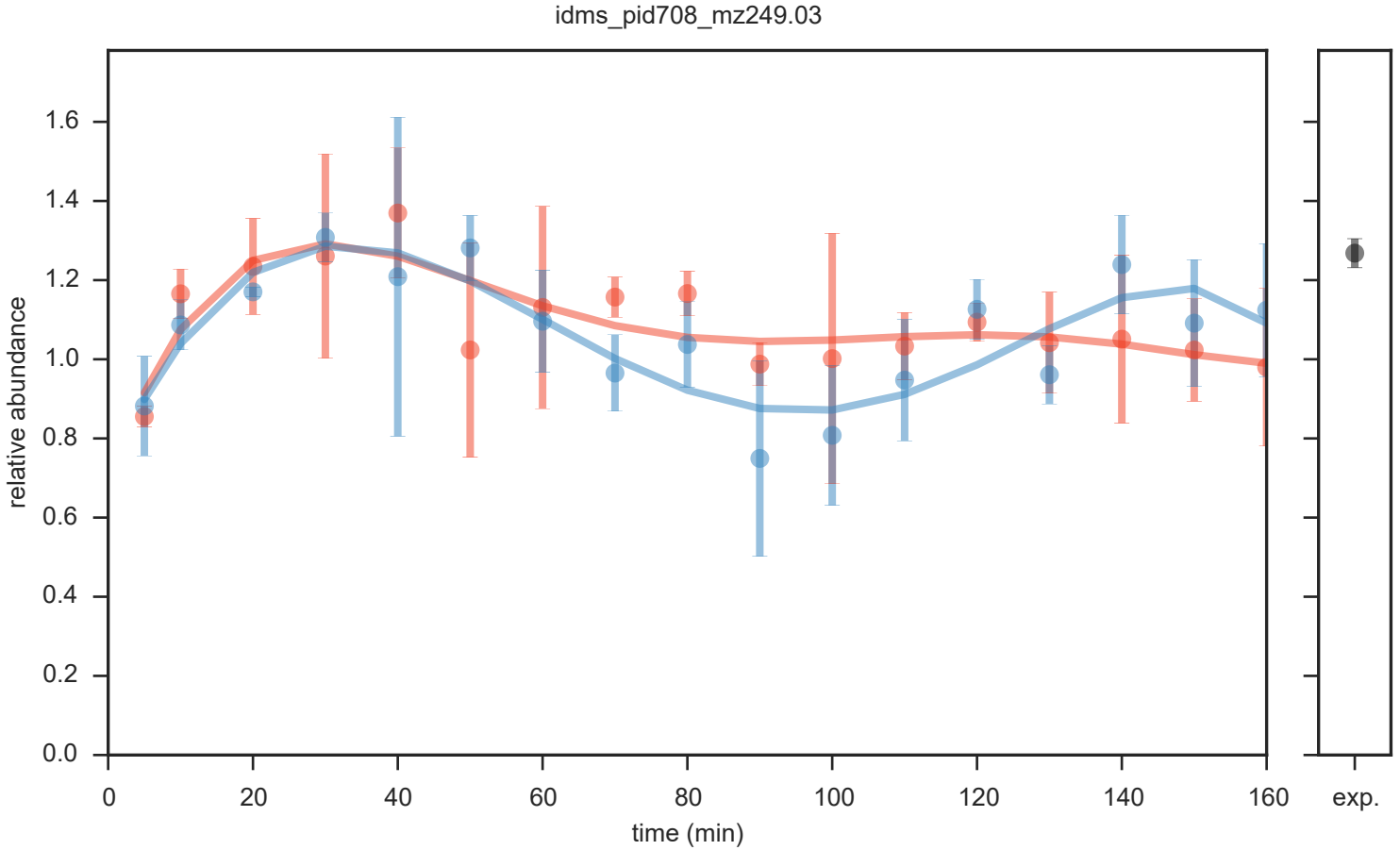

idms_pid671_mz346.05
relative abundance
0.0
0.5
1.0
1.5
2.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

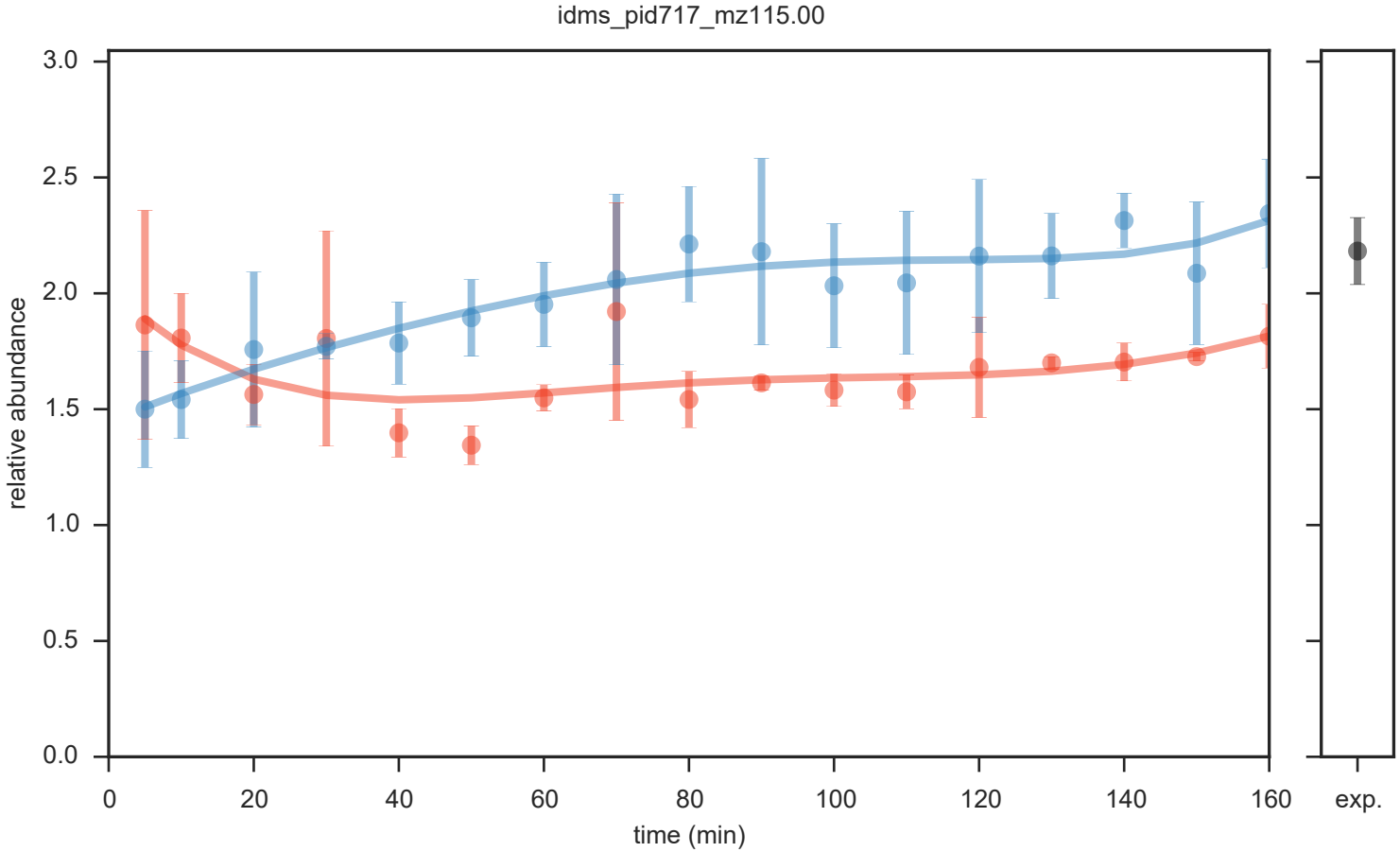

idms_pid688_mz378.98
relative abundance
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

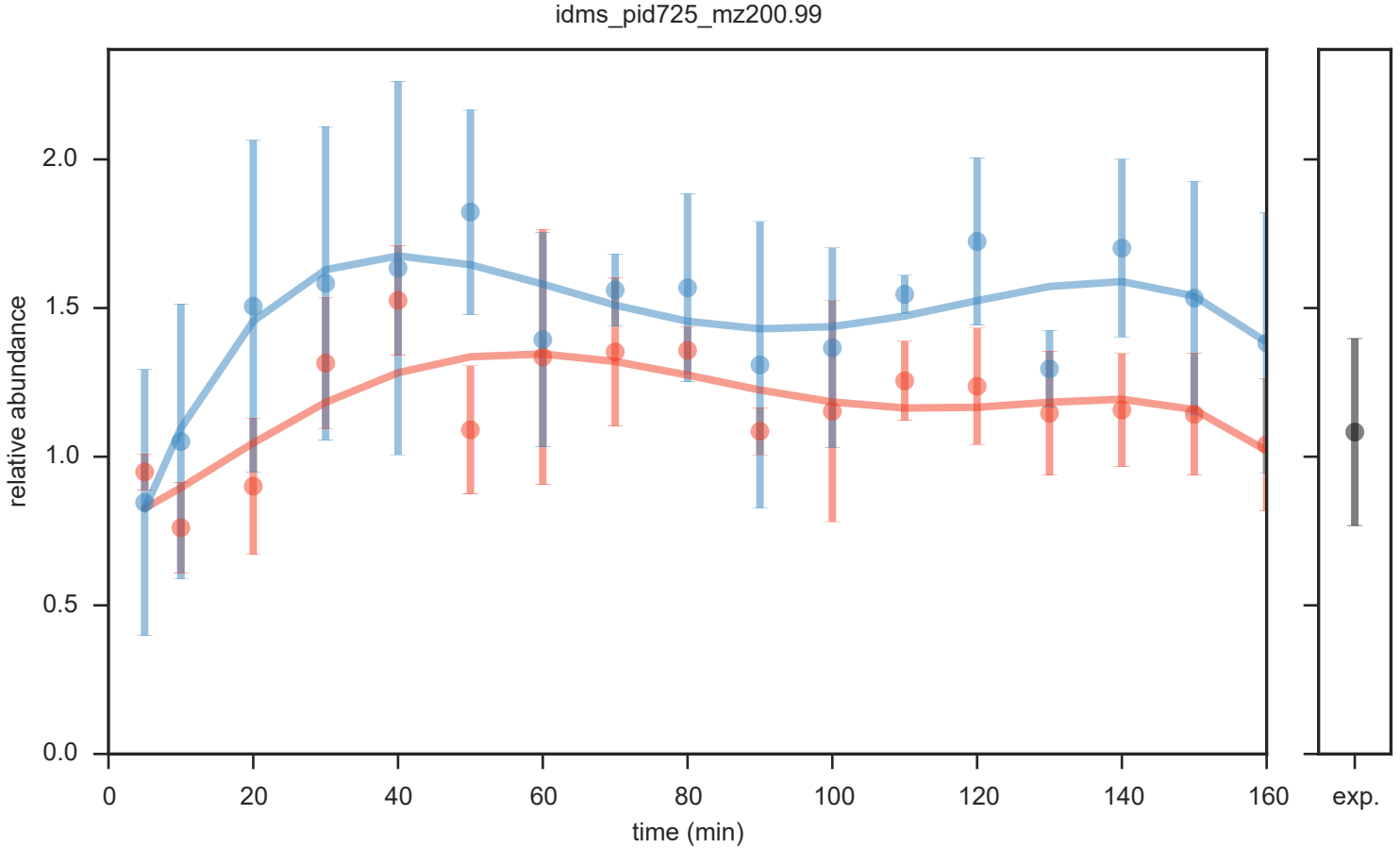

idms_pid701_mz402.00
relative abundance
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid706_mz280.42
relative abundance
0
2
4
6
8
10
12
14
16
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid707_mz278.86
relative abundance
0.0
0.5
1.0
1.5
2.0
2.5
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid708_mz249.03
relative abundance
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid717_mz115.00
relative abundance
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid725_mz200.99
relative abundance
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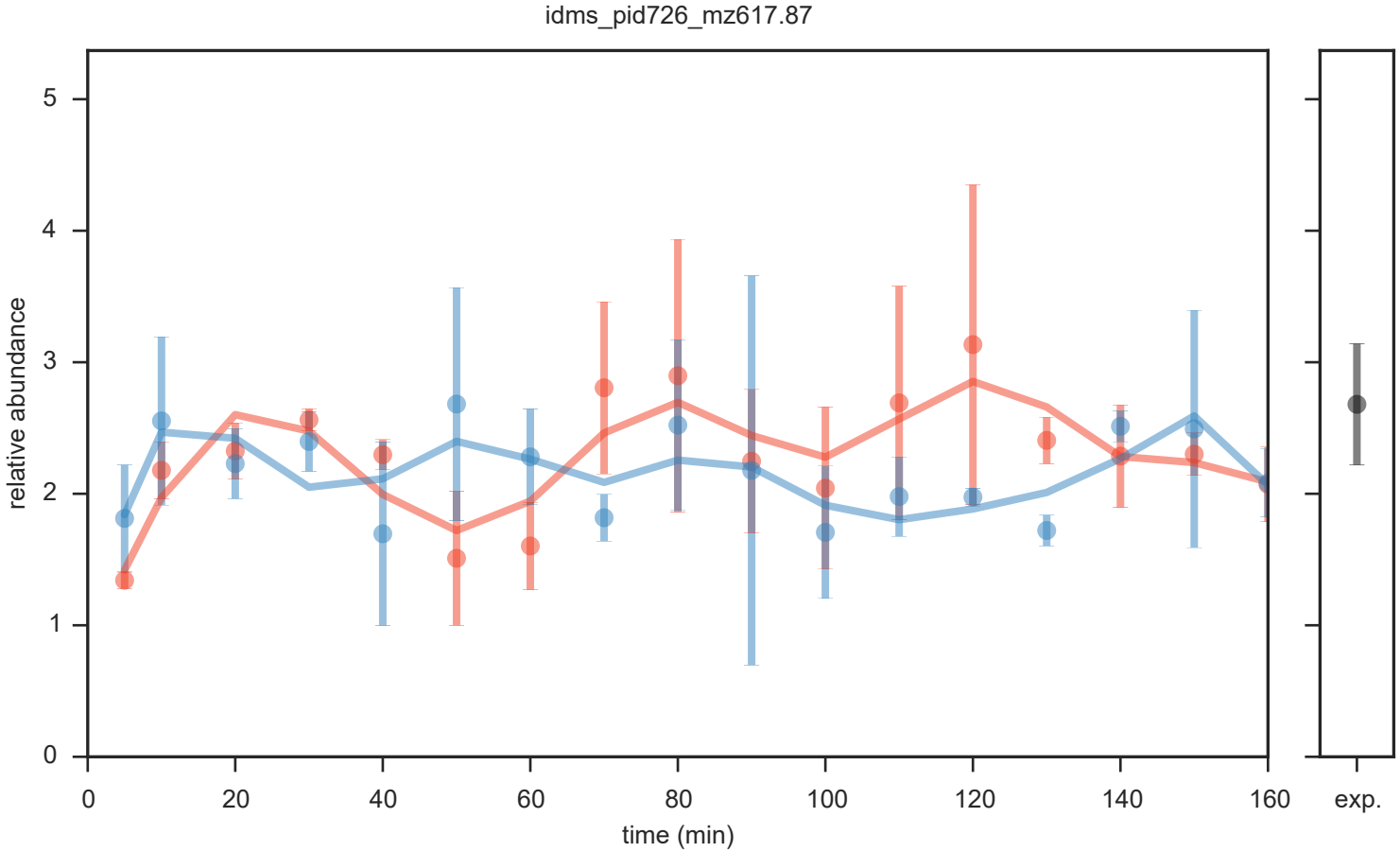
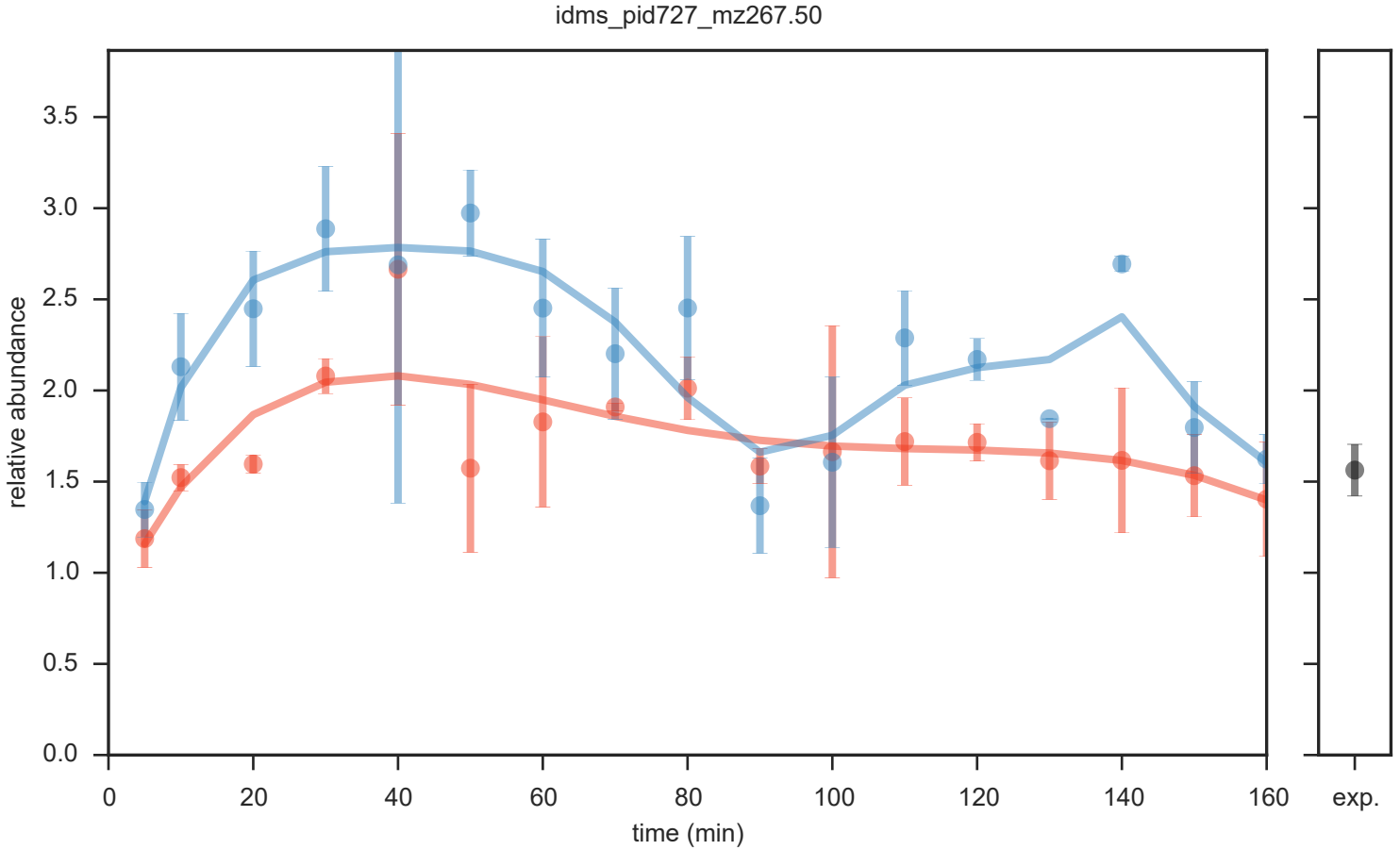
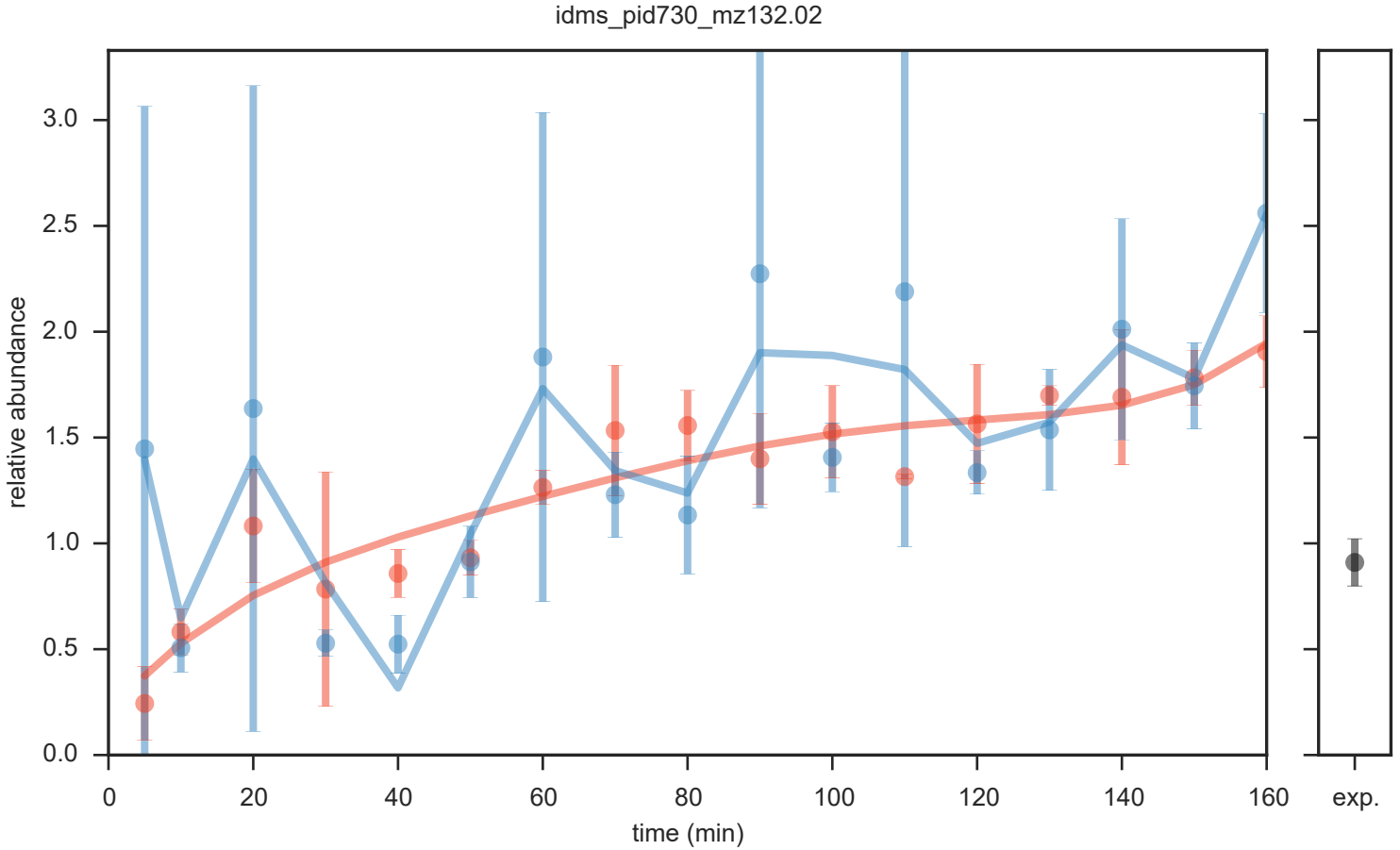
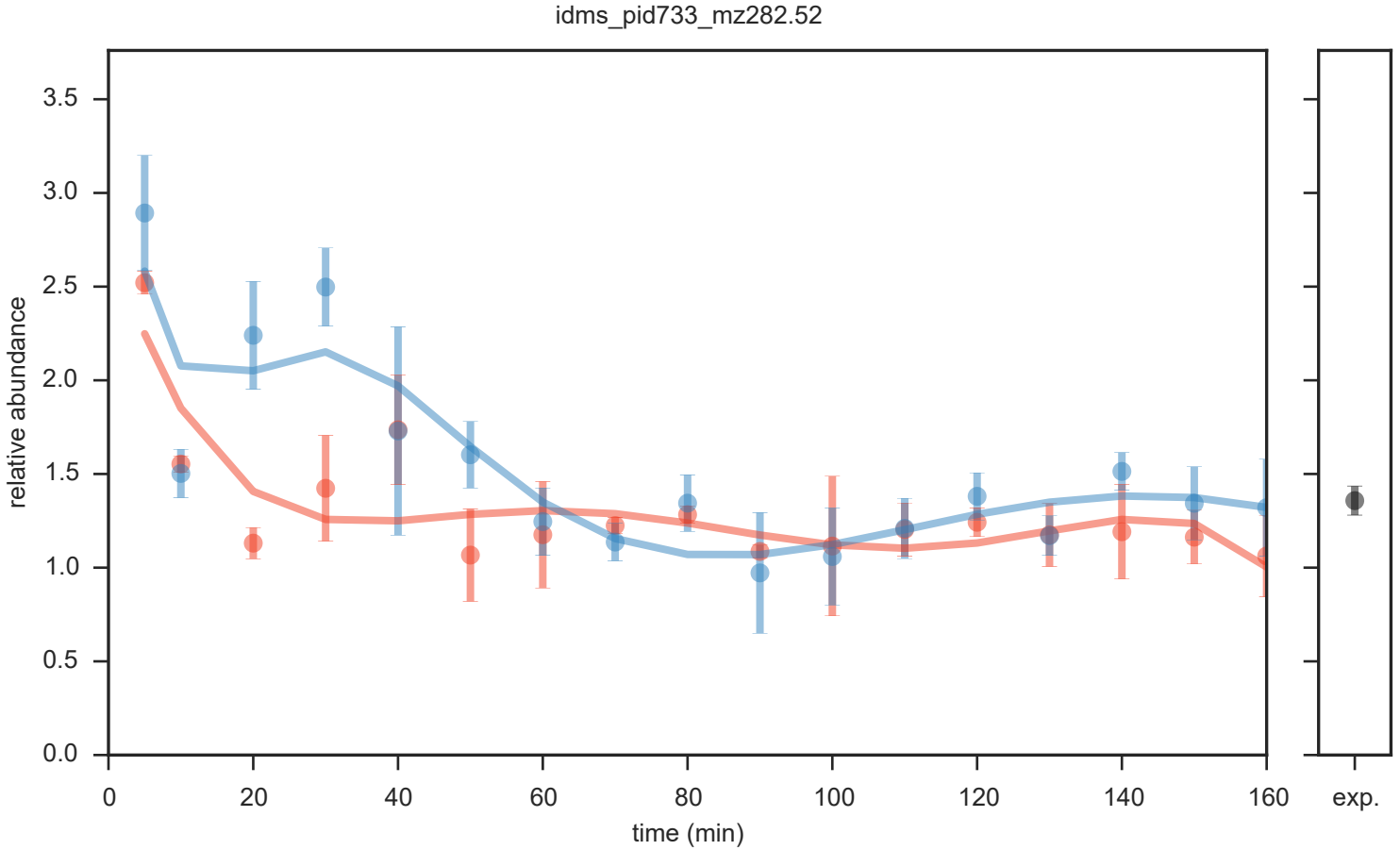
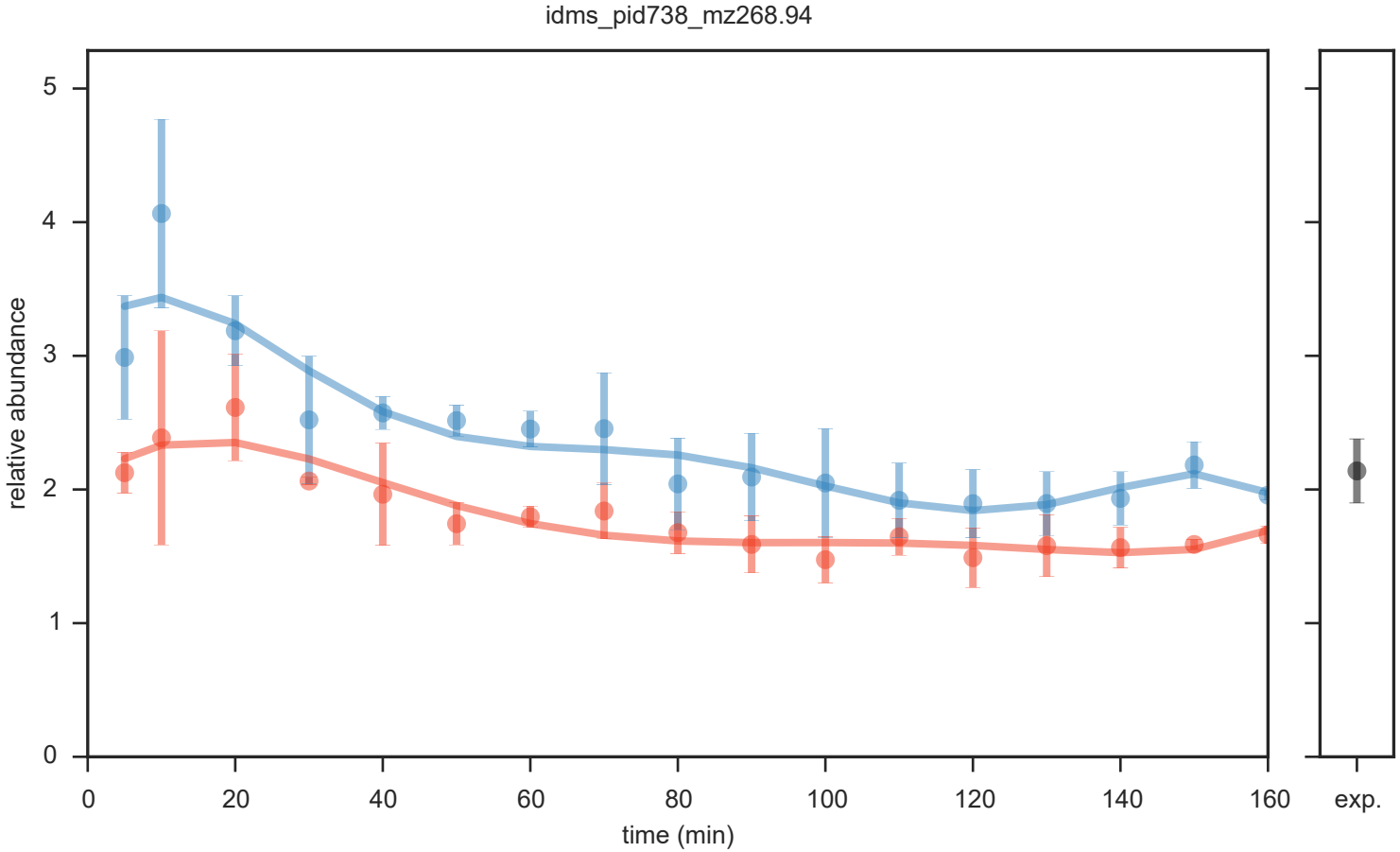
0.5
1.0
1.5
2.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

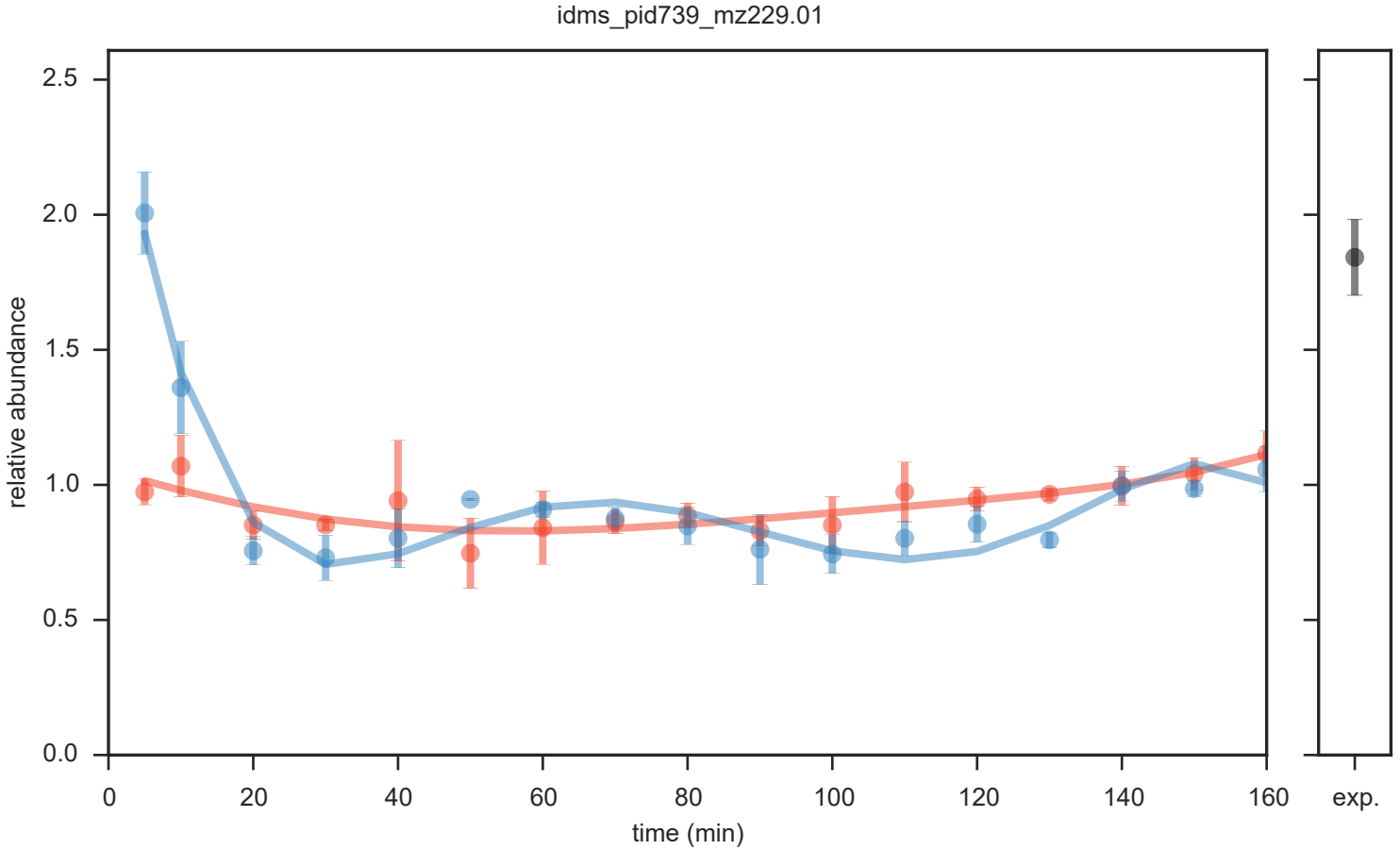

idms_pid726_mz617.87
relative abundance
0
1
2
3
4
5
0
20
40
60
80
100
120
140
160
time (min)
exp.

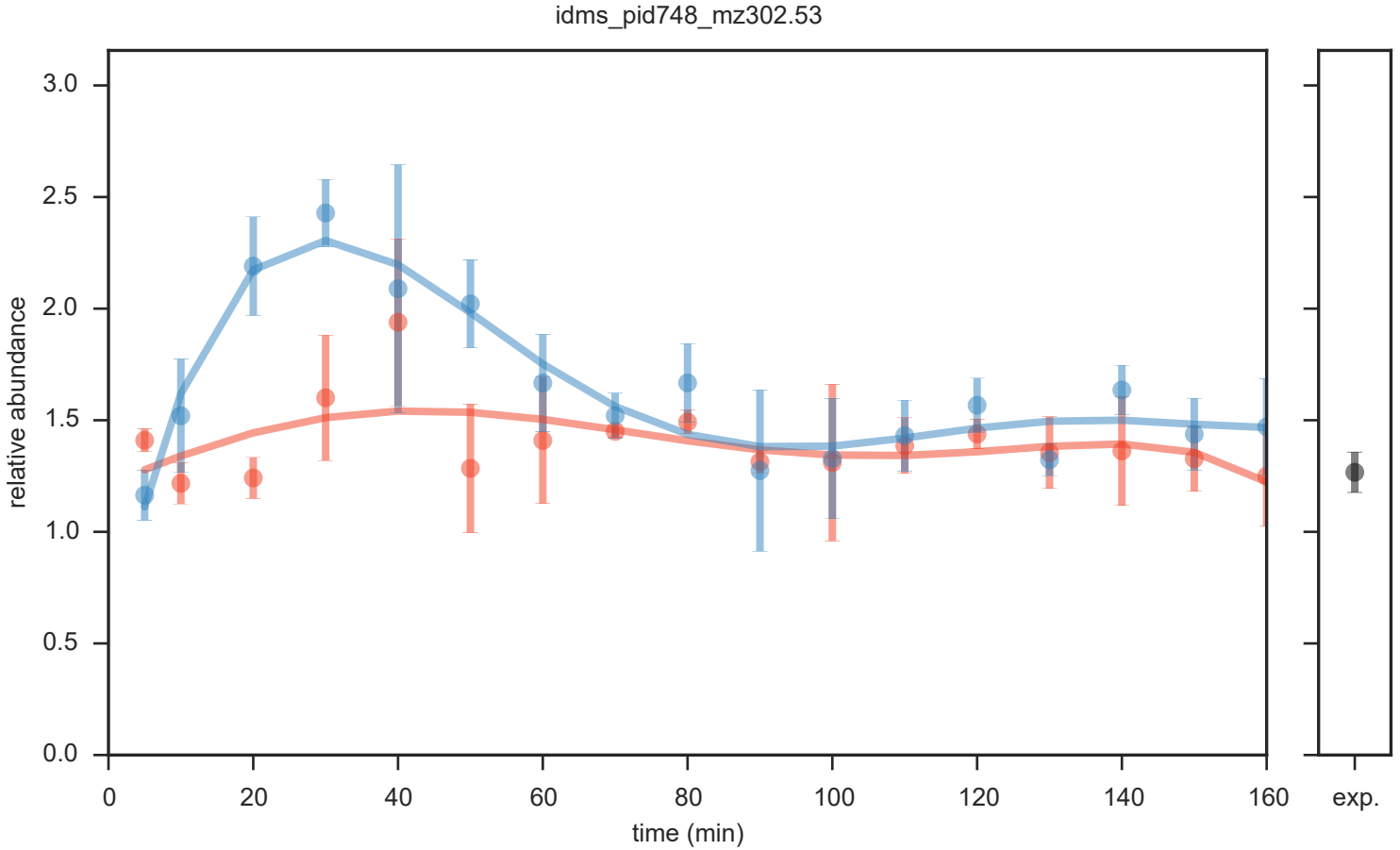

idms_pid727_mz267.50
relative abundance
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
0
20
40
60
80
100
120
140
160
time (min)
exp.

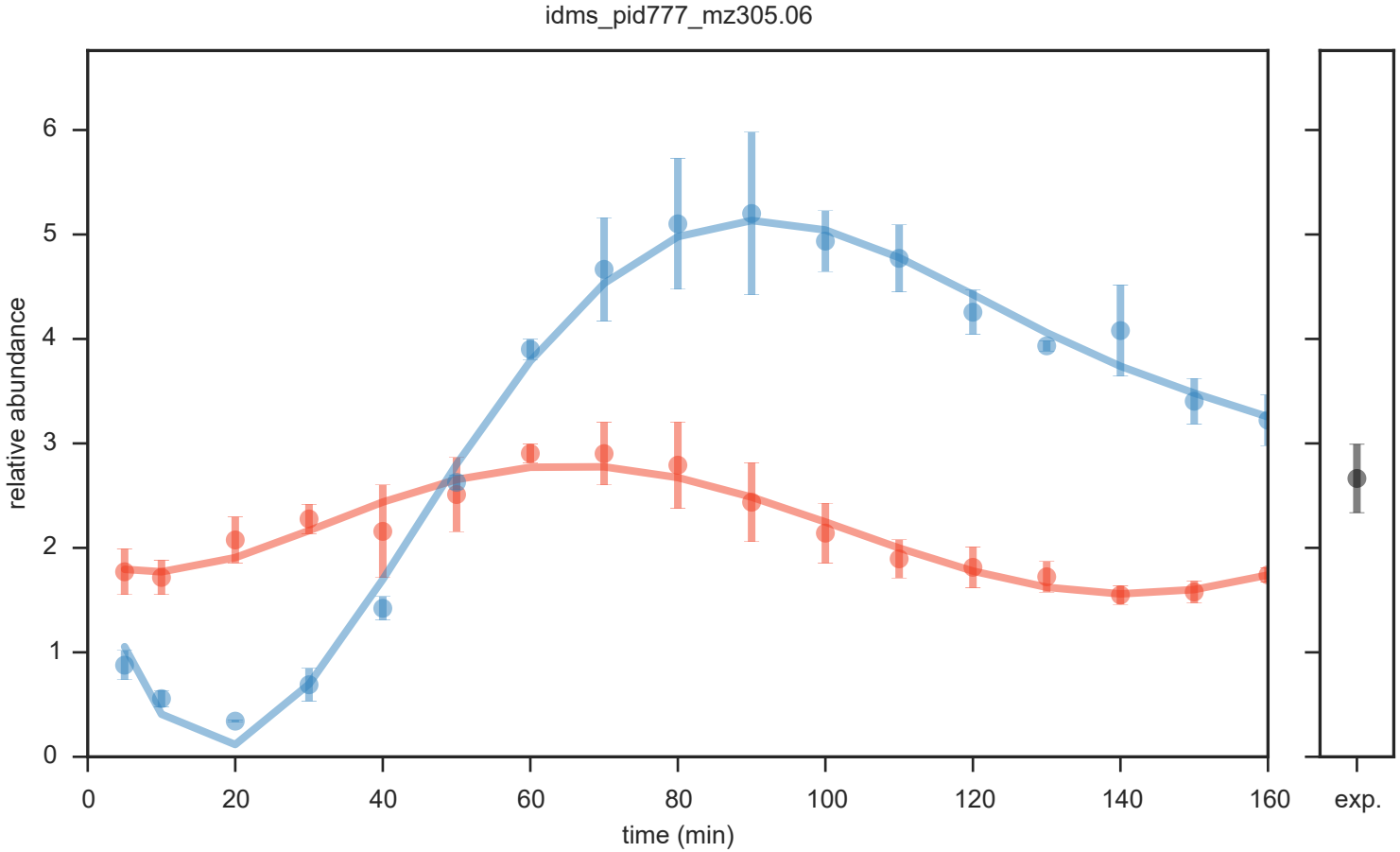

idms_pid730_mz132.02
relative abundance
0.0
0.5
1.0
1.5
2.0
2.5
3.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

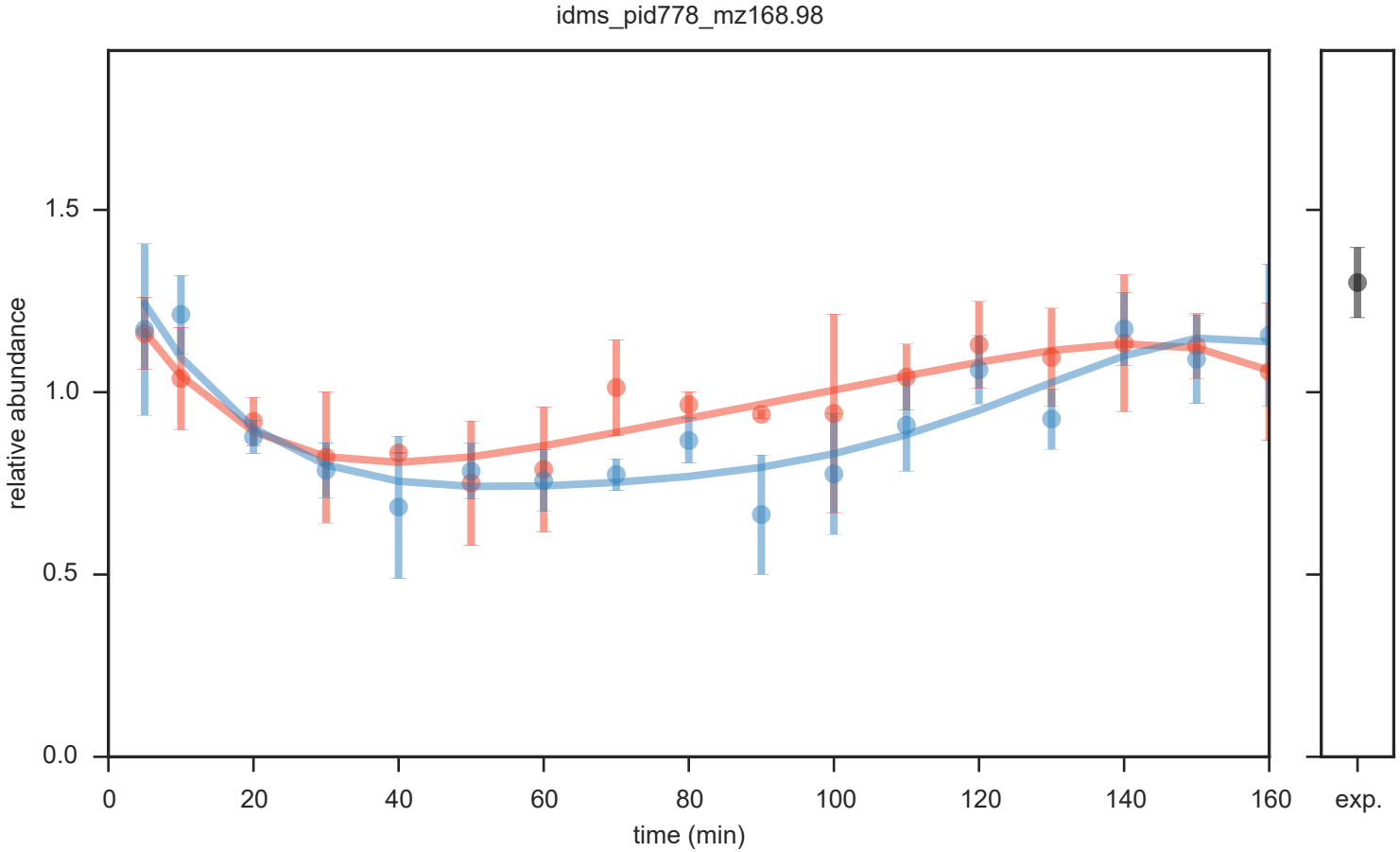

idms_pid733_mz282.52
relative abundance
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

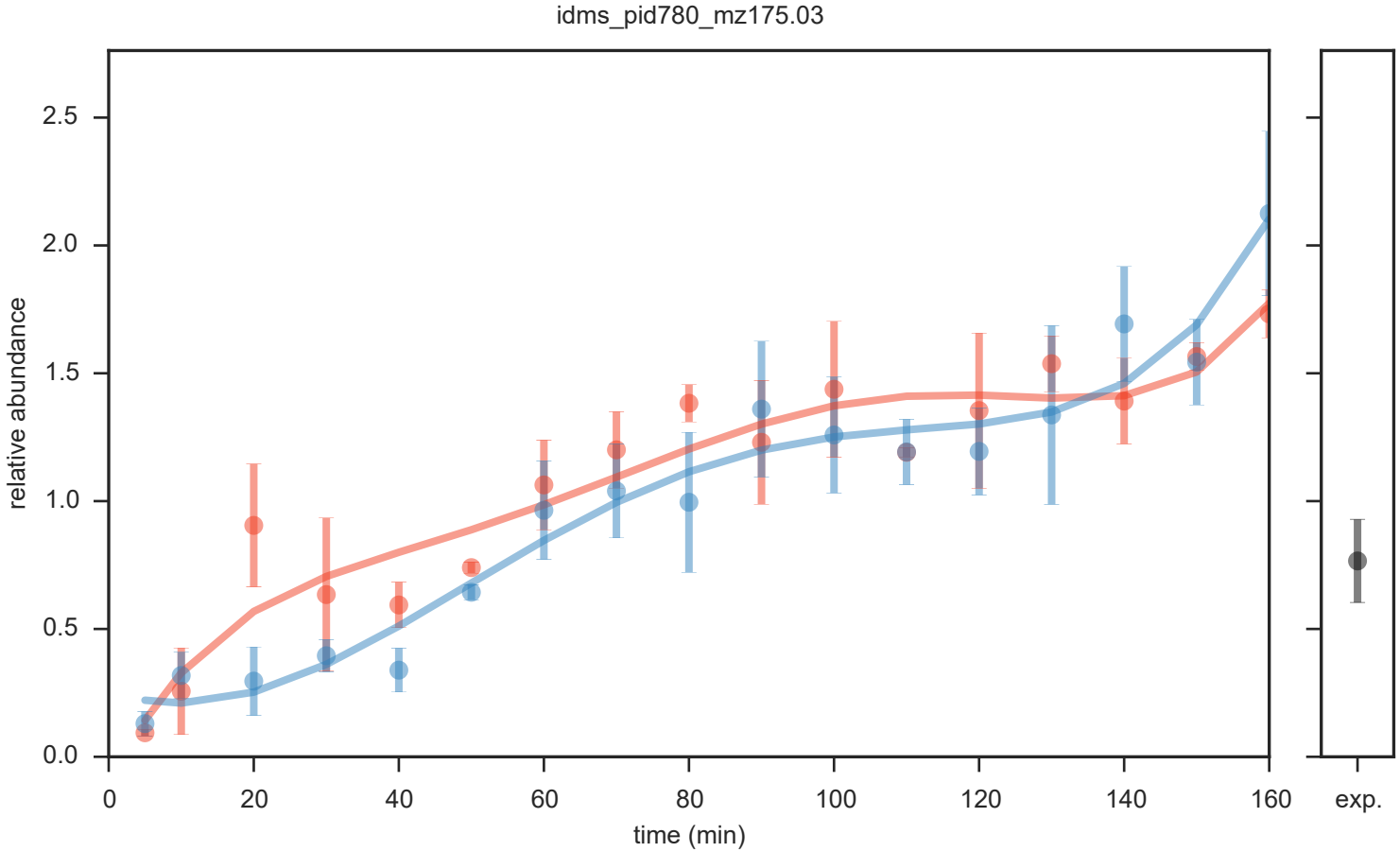

idms_pid738_mz268.94
relative abundance
0
1
2
3
4
5
0
20
40
60
80
100
120
140
160
time (min)
exp.

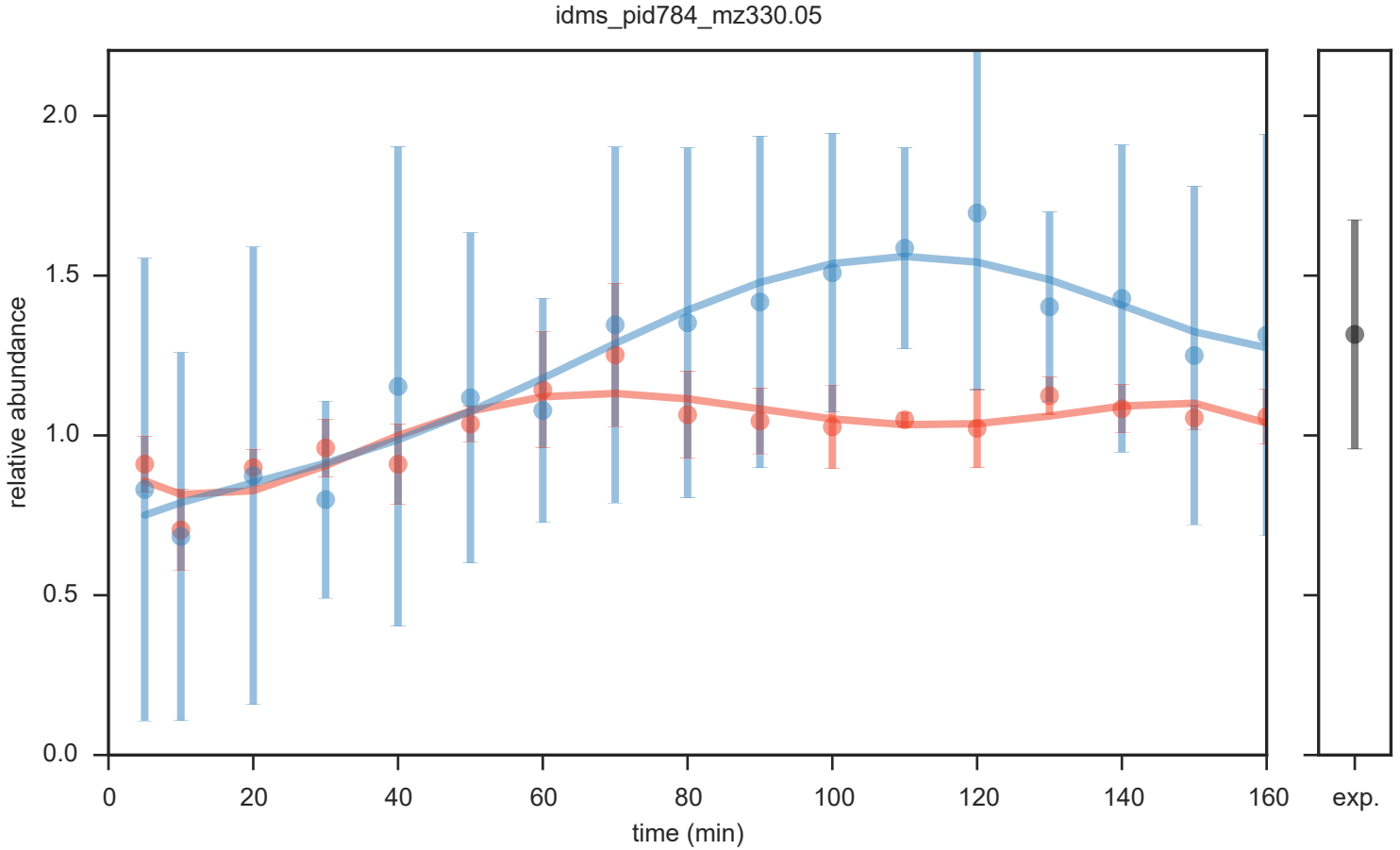

idms_pid739_mz229.01
relative abundance
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

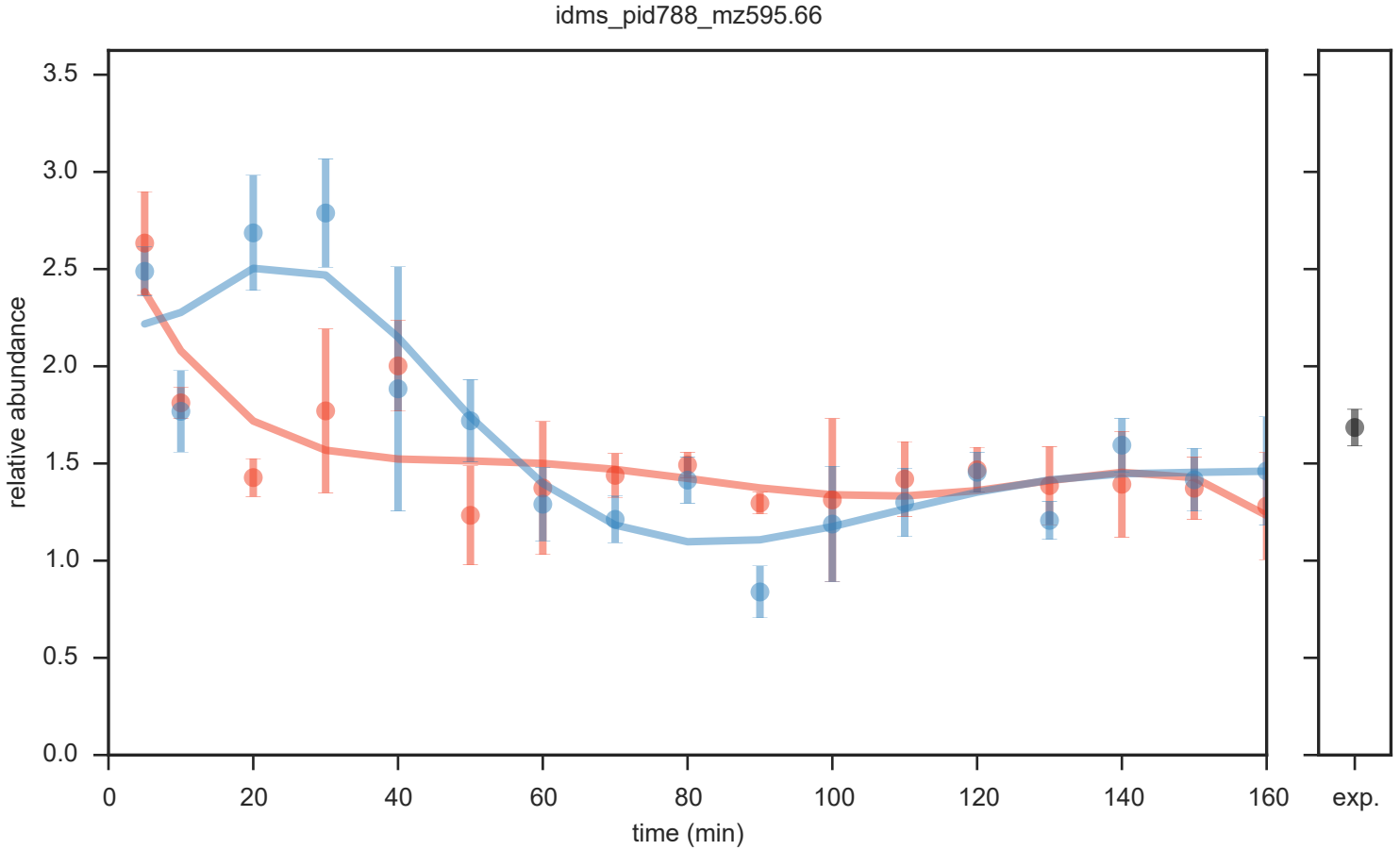

idms_pid748_mz302.53
relative abundance
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

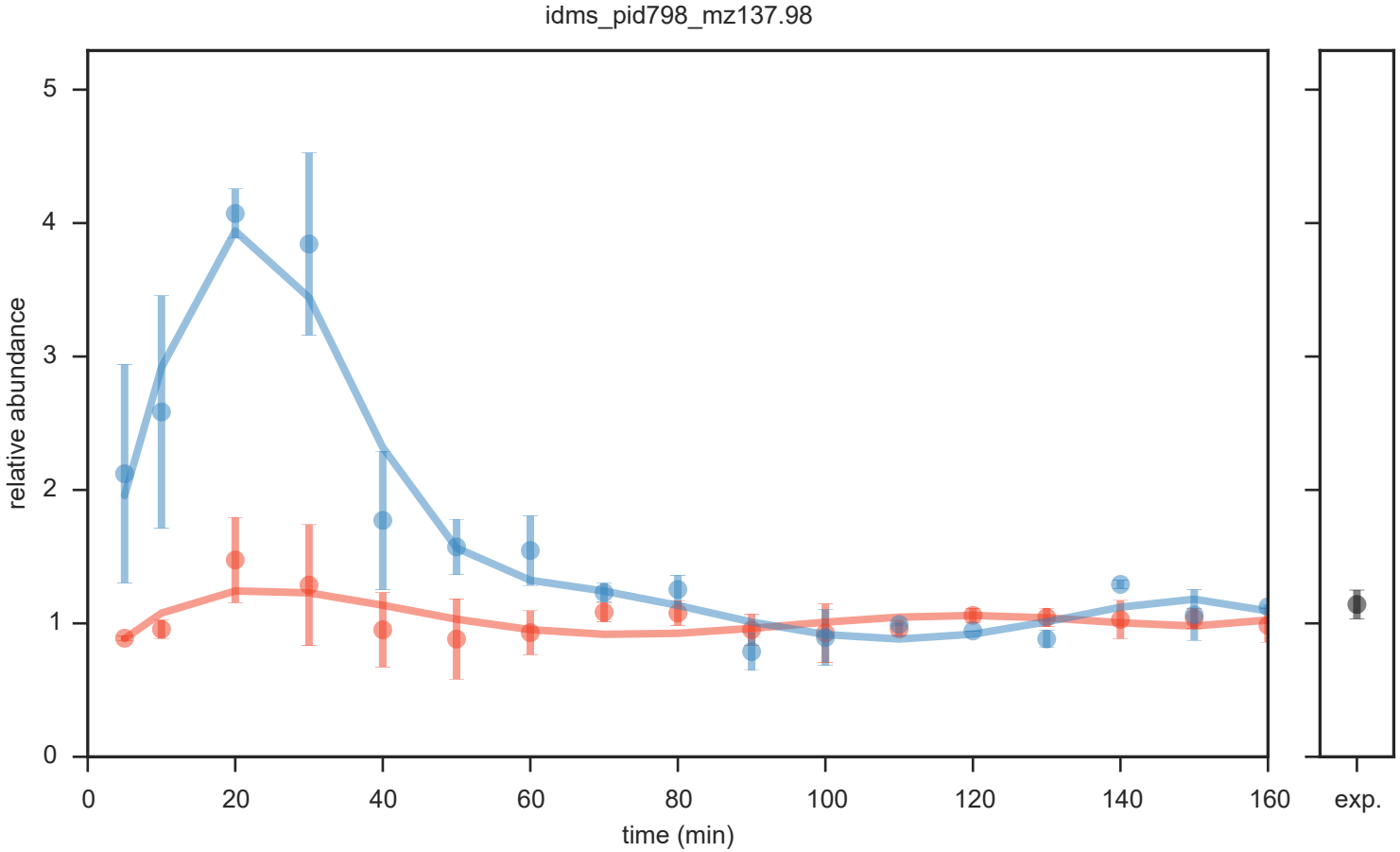

idms_pid777_mz305.06
relative abundance
0
1
2
3
4
5
6
0
20
40
60
80
100
120
140
160
time (min)
exp.

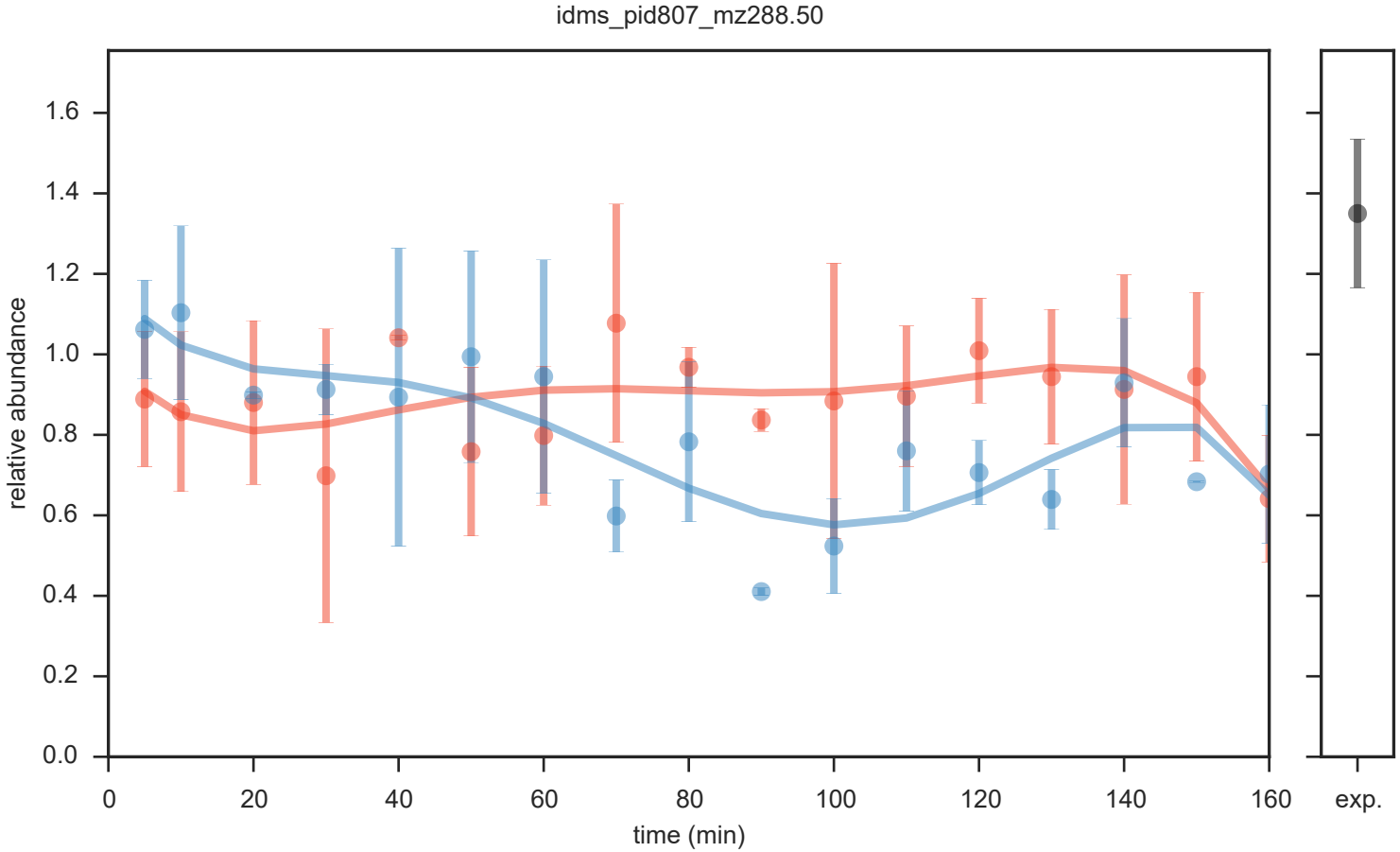

idms_pid778_mz168.98
relative abundance
0.0
0.5
1.0
1.5
0
20
40
60
80
100
120
140
160
time (min)
exp.

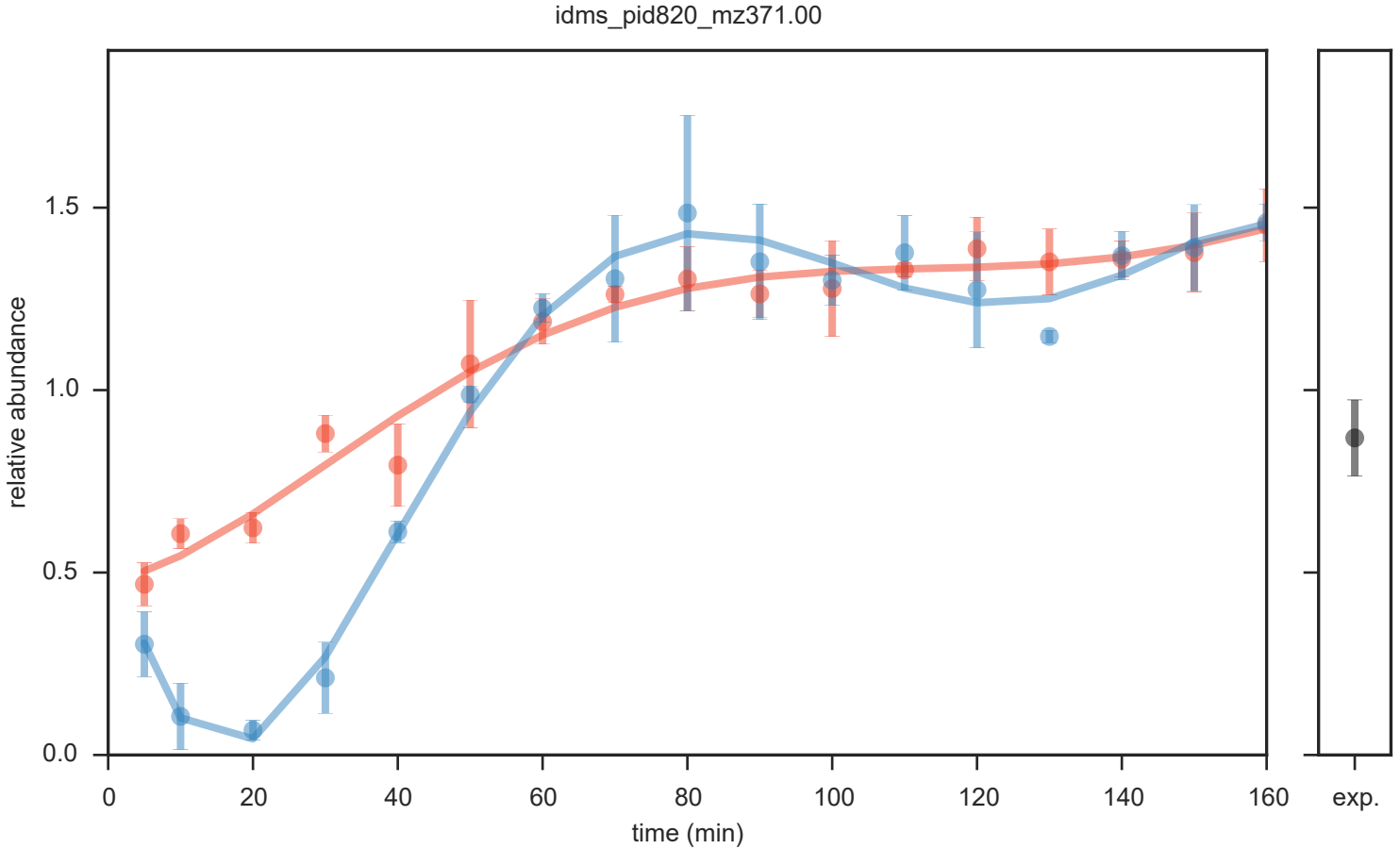

idms_pid780_mz175.03
relative abundance
0.0
0.5
1.0
1.5
2.0
2.5
0
20
40
60
80
100
120
140
160
time (min)
exp.

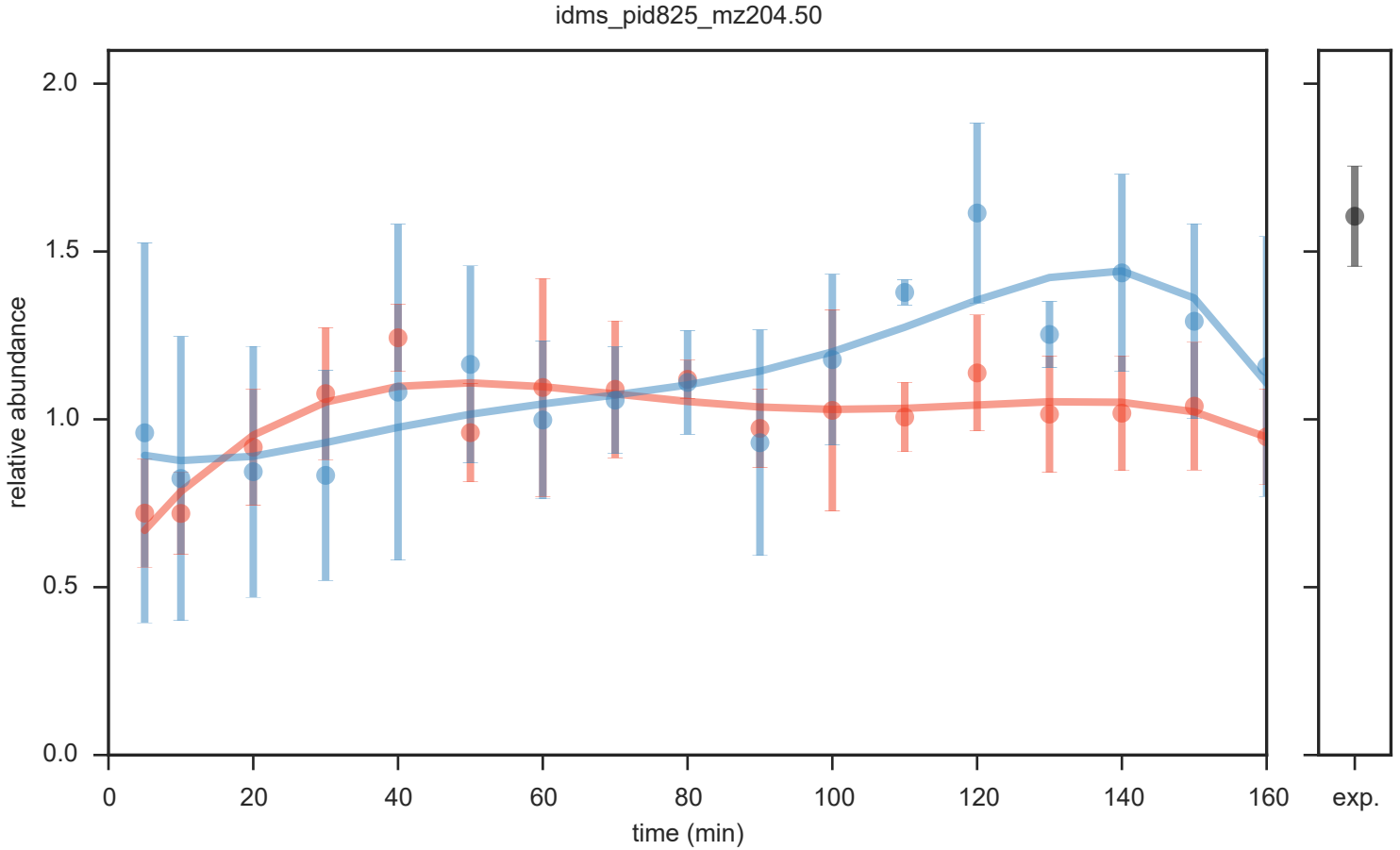

idms_pid784_mz330.05
relative abundance
0.0
0.5
1.0
1.5
2.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

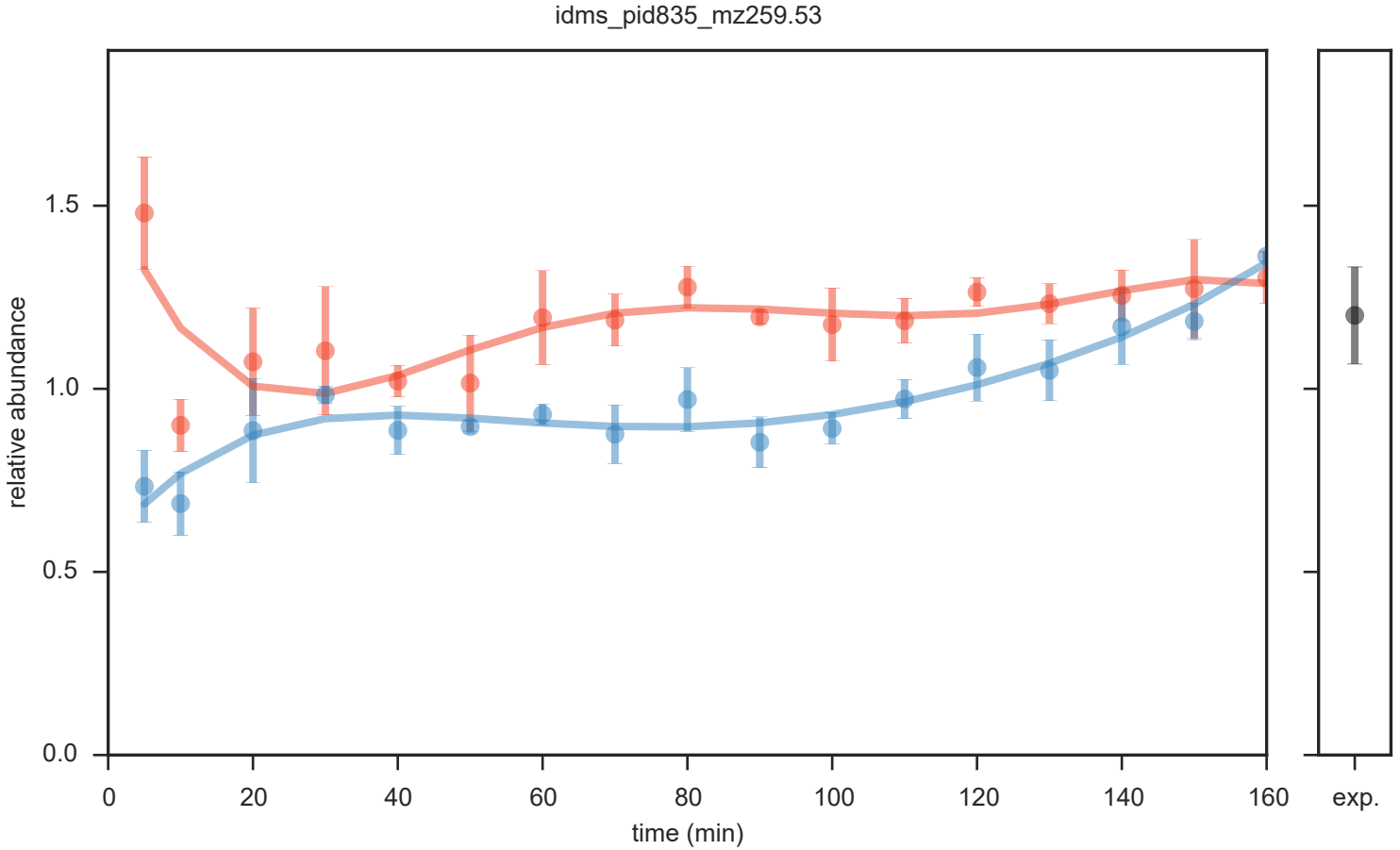

idms_pid788_mz595.66
relative abundance
time (min)
exp.
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
0
20
40
60
80
100
120
140
160

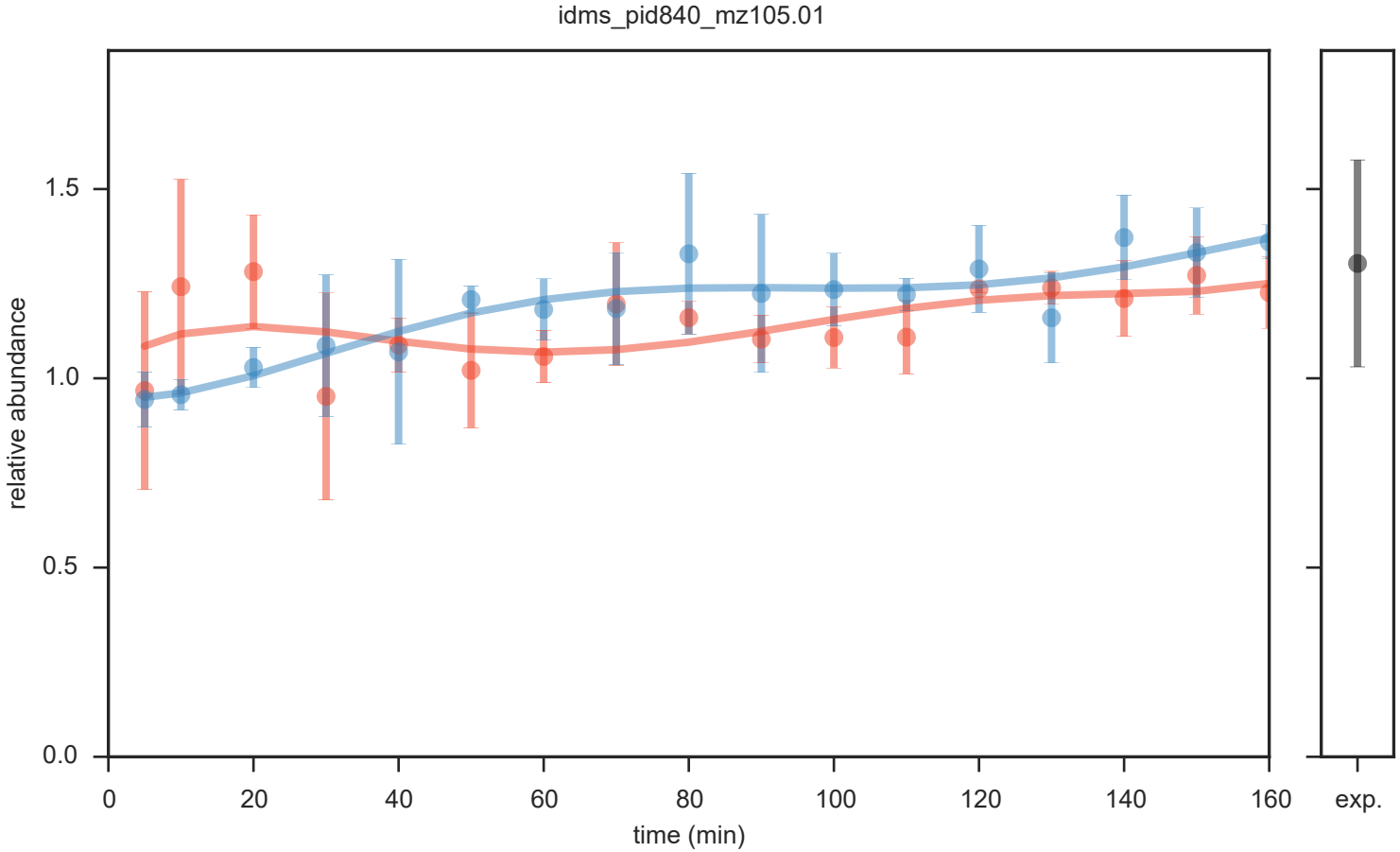

idms_pid798_mz137.98
relative abundance
0
1
2
3
4
5
0
20
40
60
80
100
120
140
160
time (min)
exp.

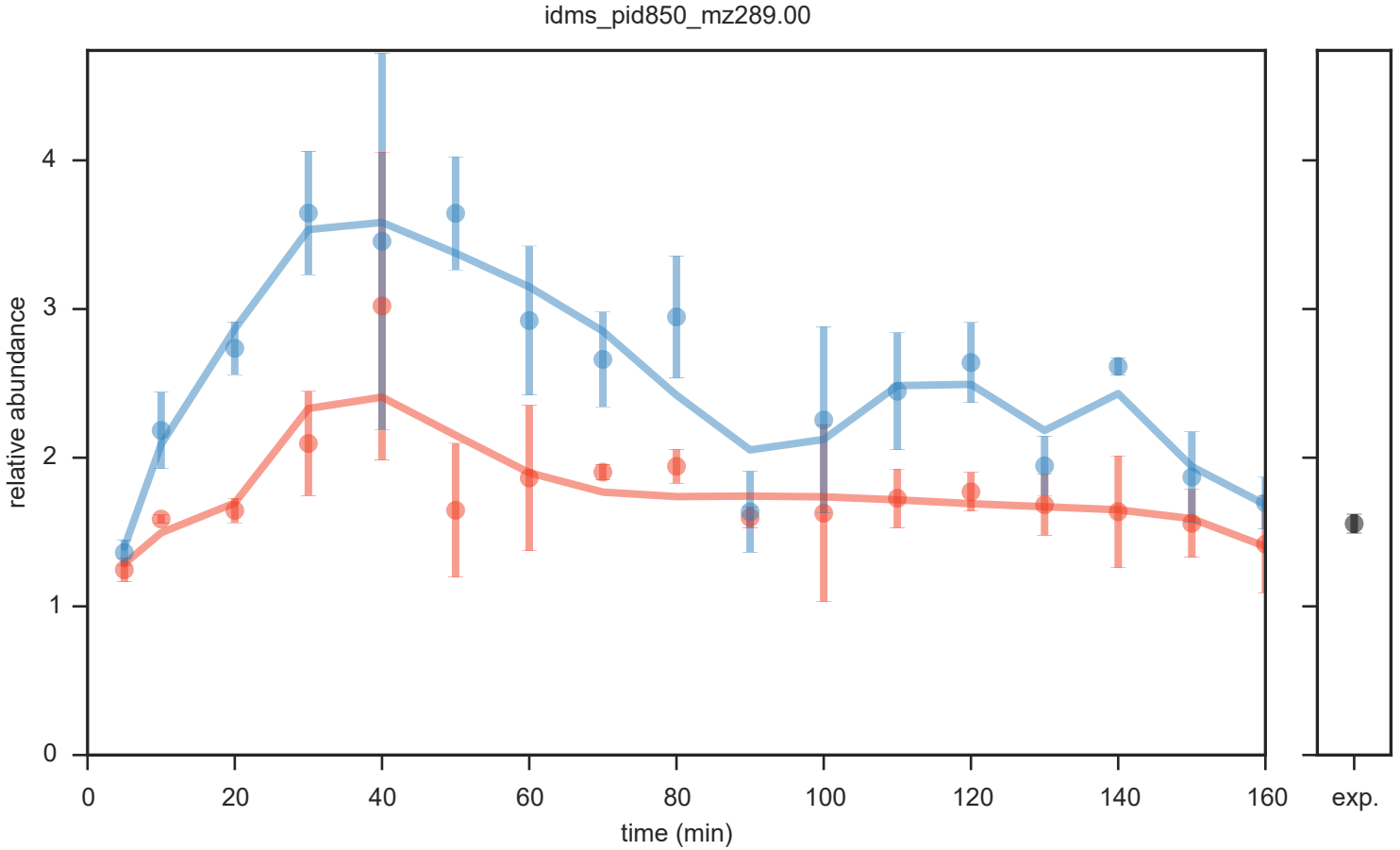

idms_pid807_mz288.50
relative abundance
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid820_mz371.00
relative abundance
0.0
0.5
1.0
1.5
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid825_mz204.50
relative abundance
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid835_mz259.53
relative abundance
0.0
0.5
1.0
1.5
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid840_mz105.01
relative abundance
0.0
0.5
1.0
1.5
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid850_mz289.00
relative abundance
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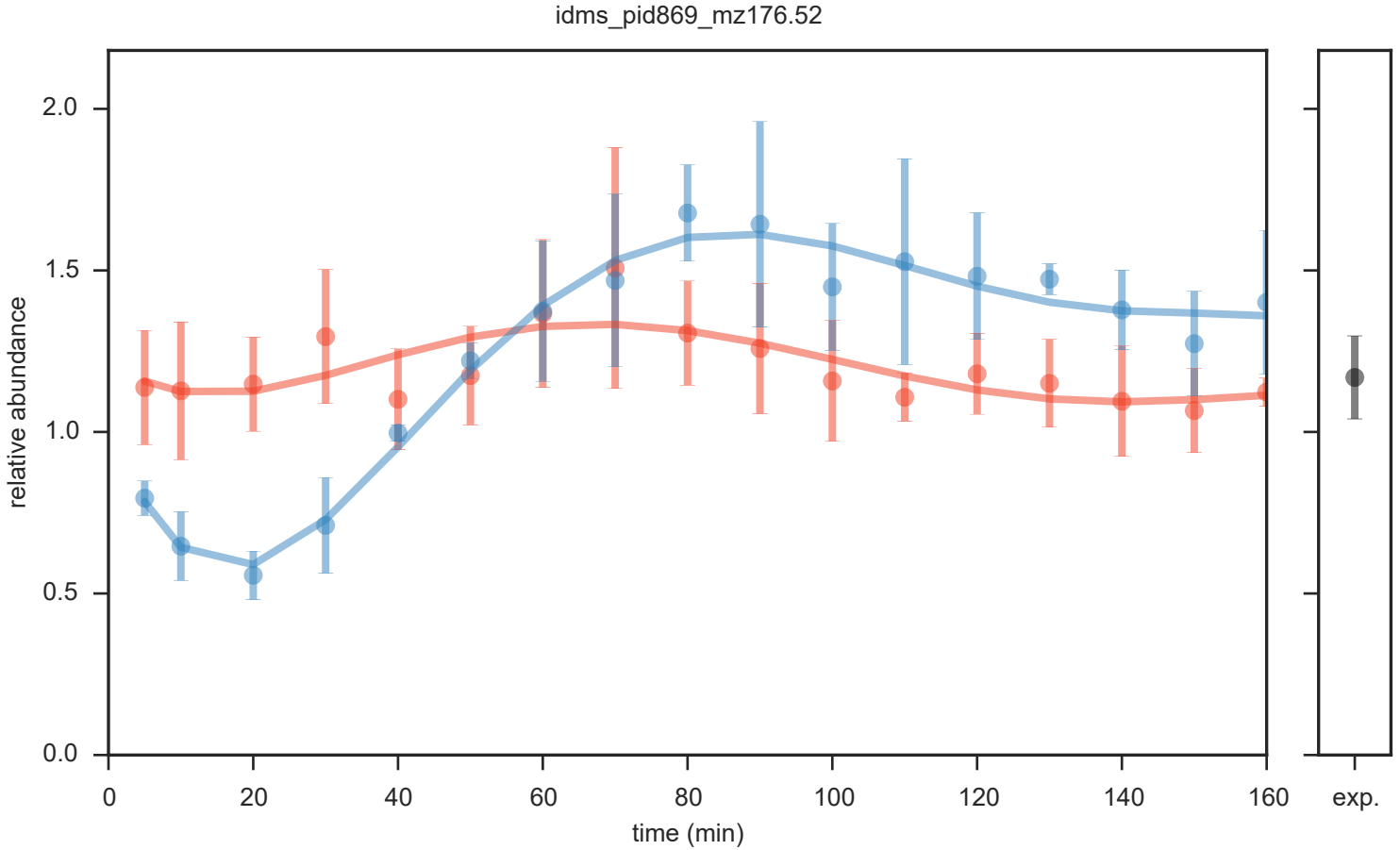
1
2
3
4
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid869_mz176.52
relative abundance
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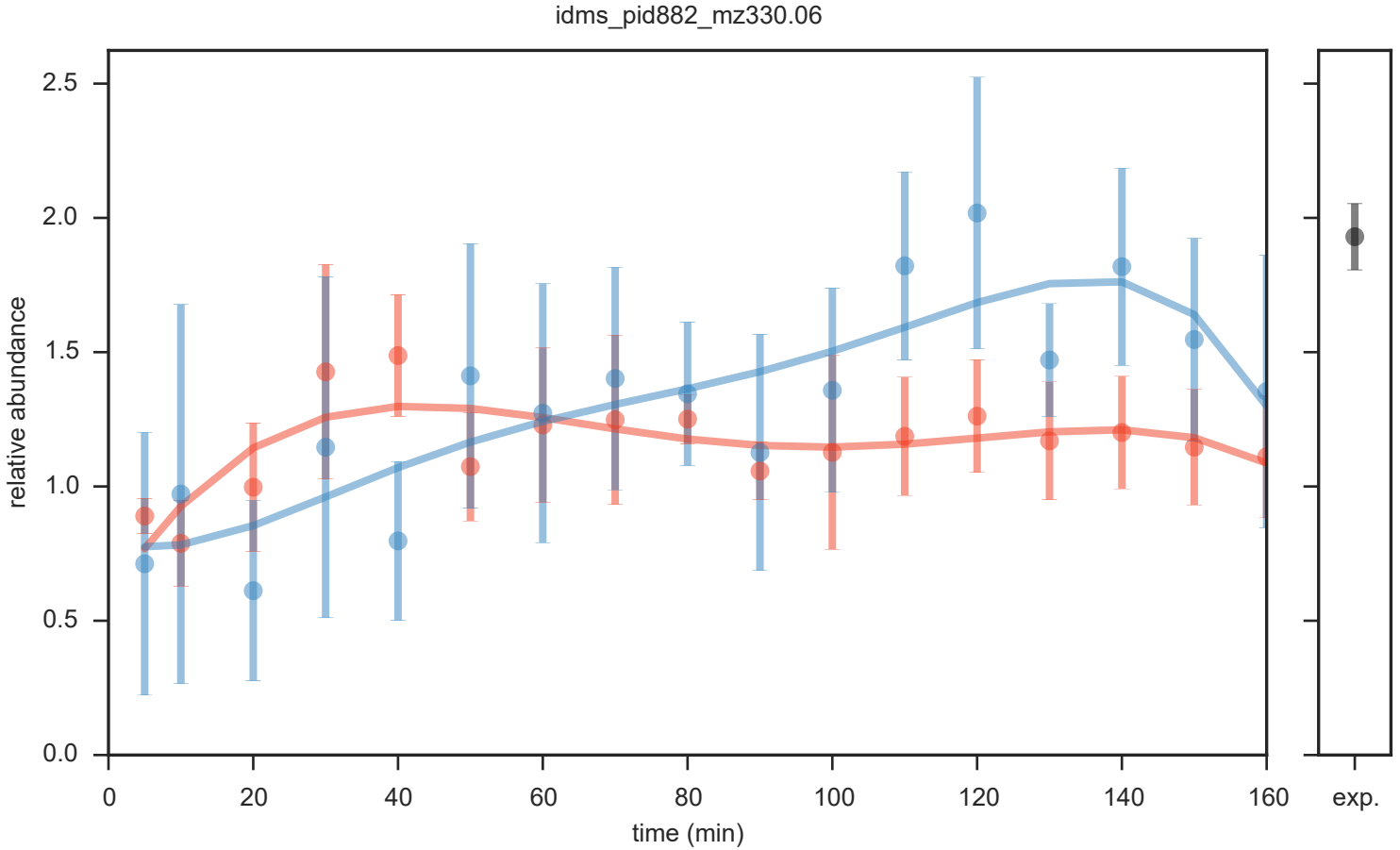
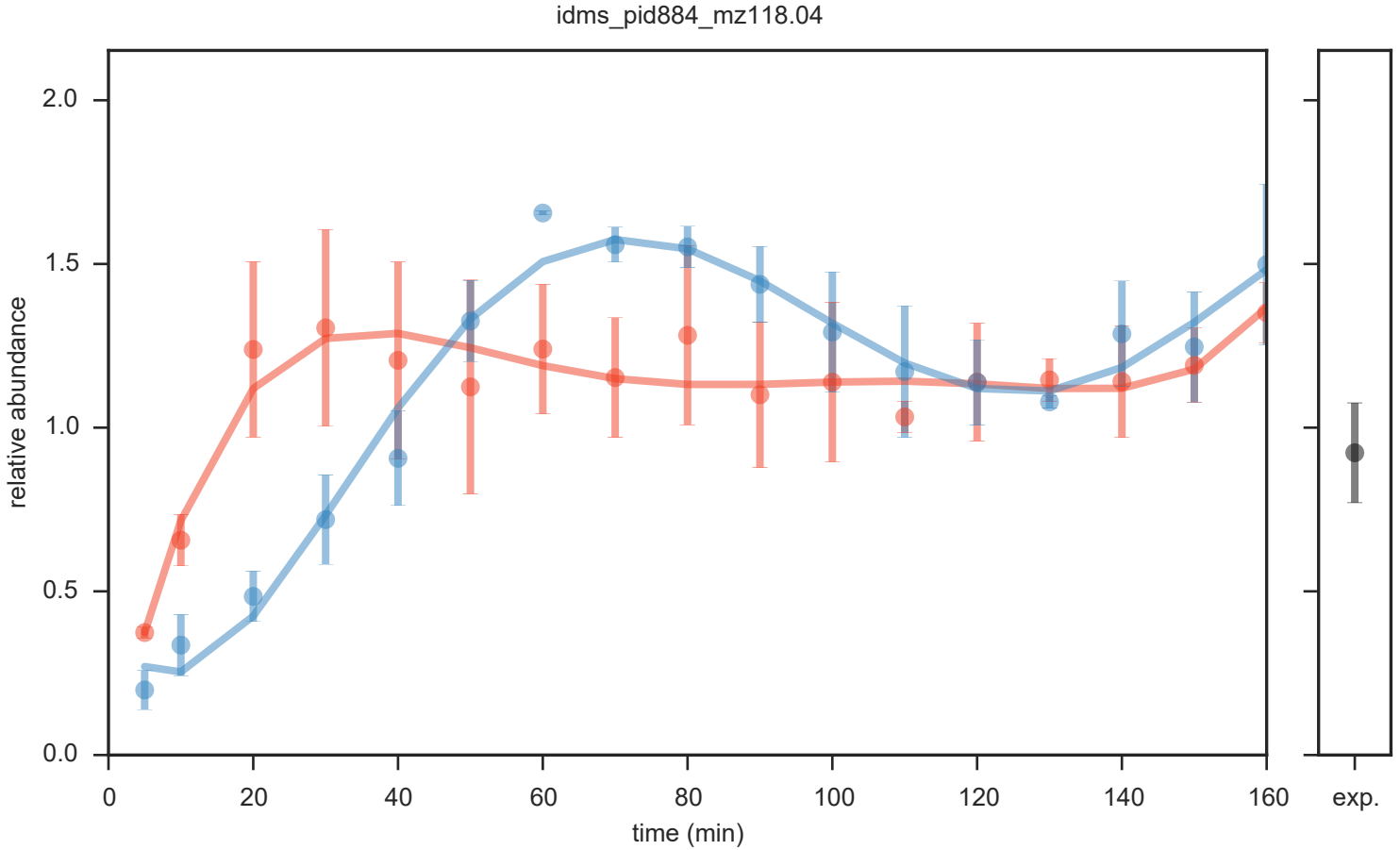
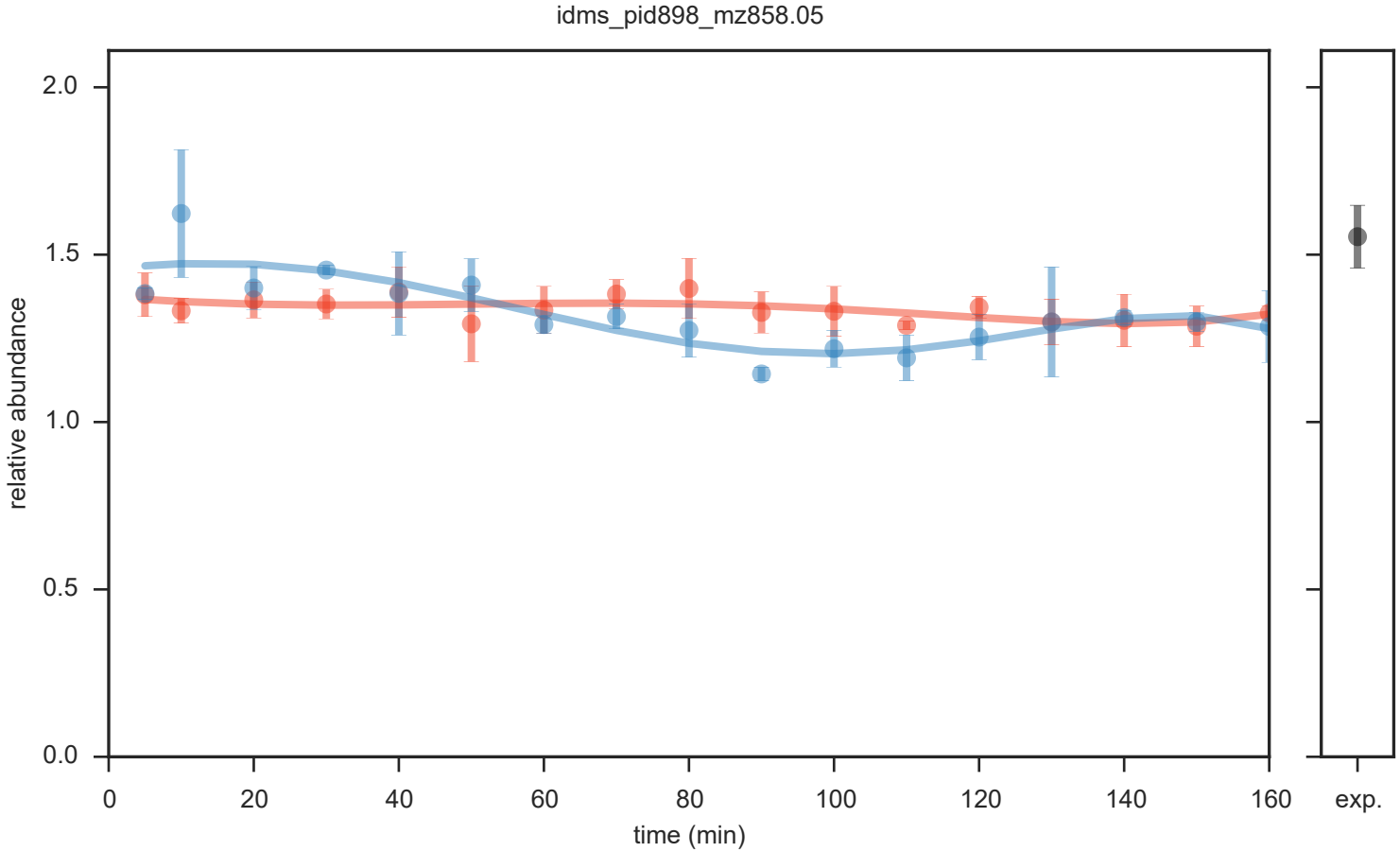
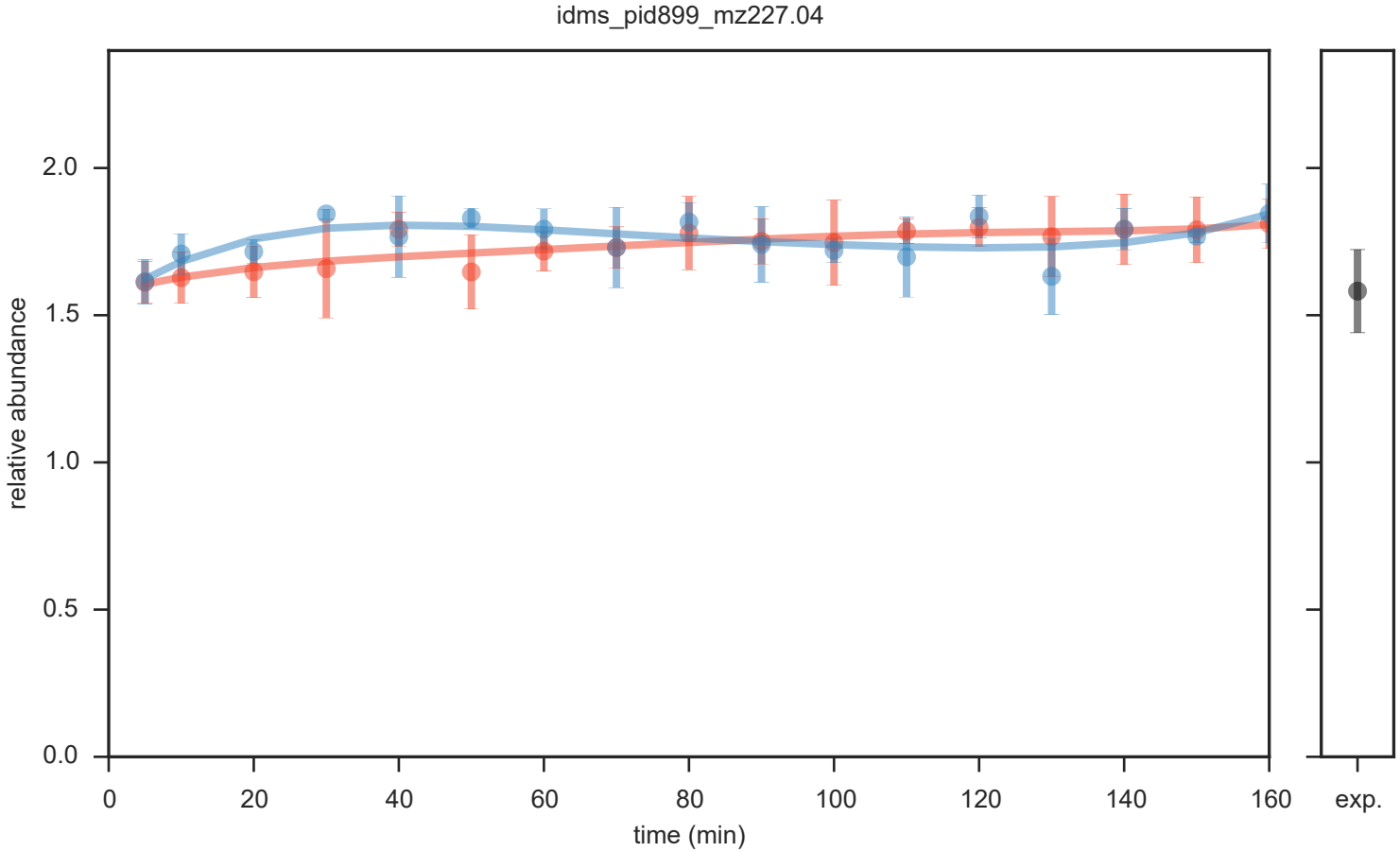
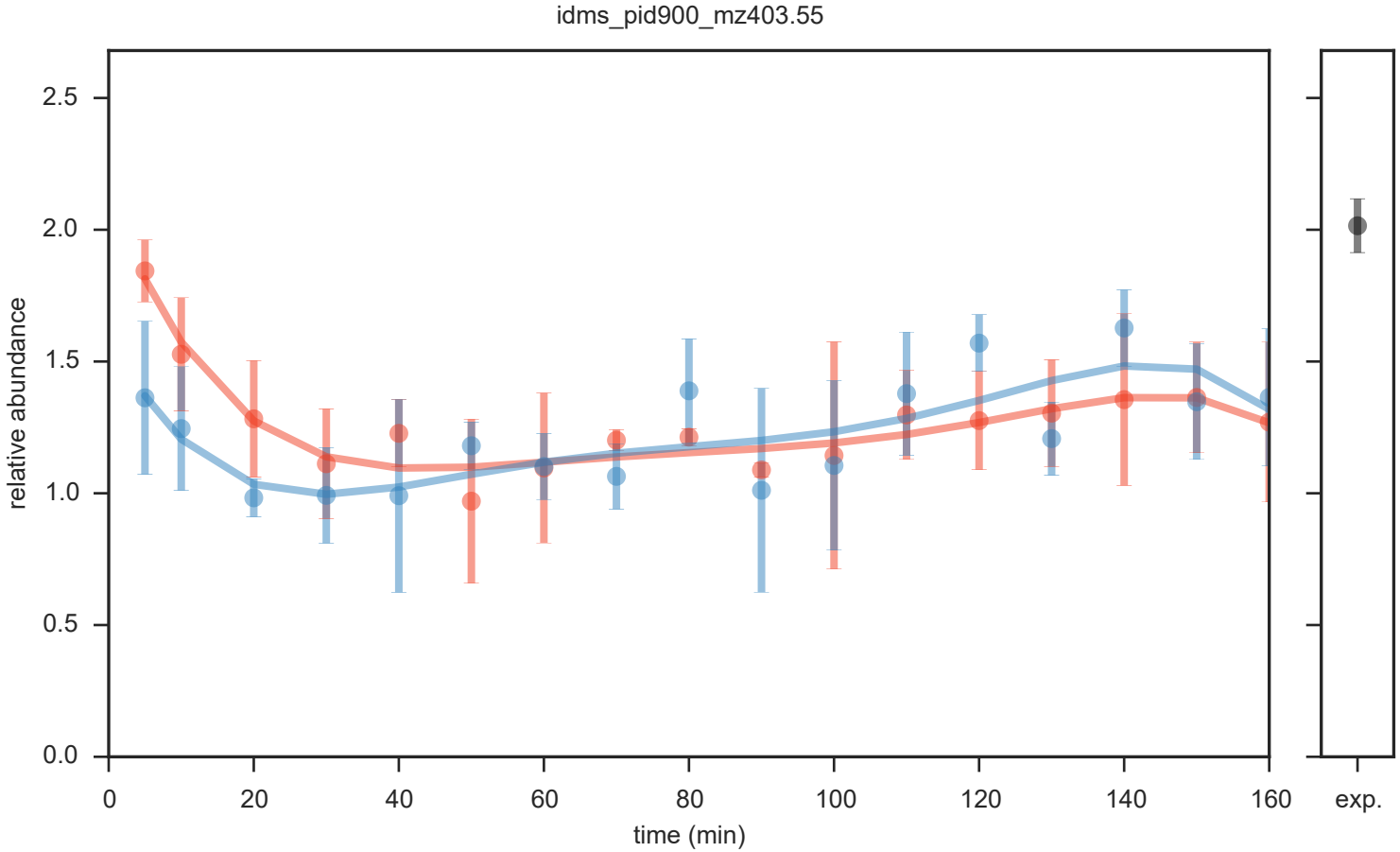
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

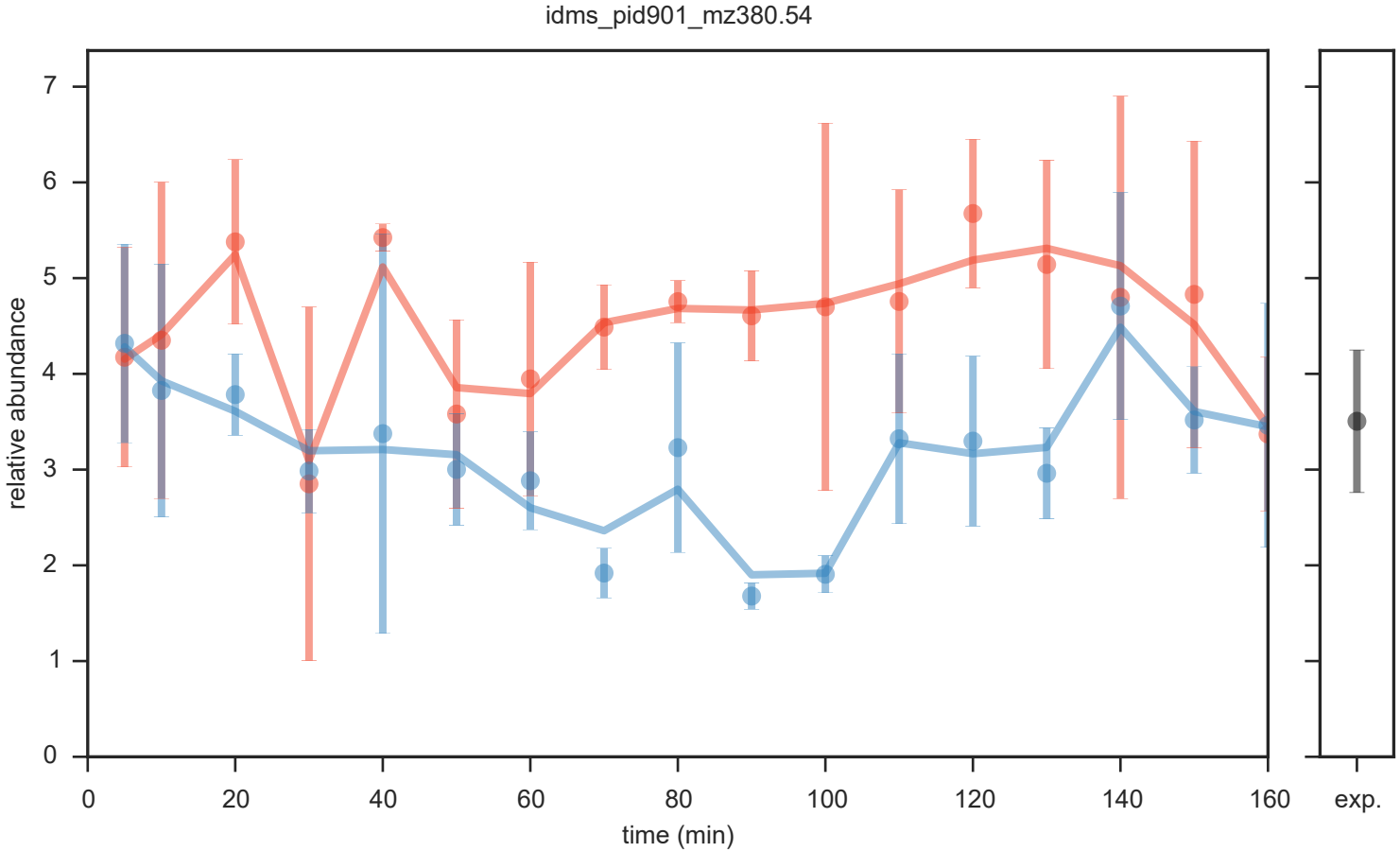

idms_pid882_mz330.06
relative abundance
0.0
0.5
1.0
1.5
2.0
2.5
0
20
40
60
80
100
120
140
160
time (min)
exp.

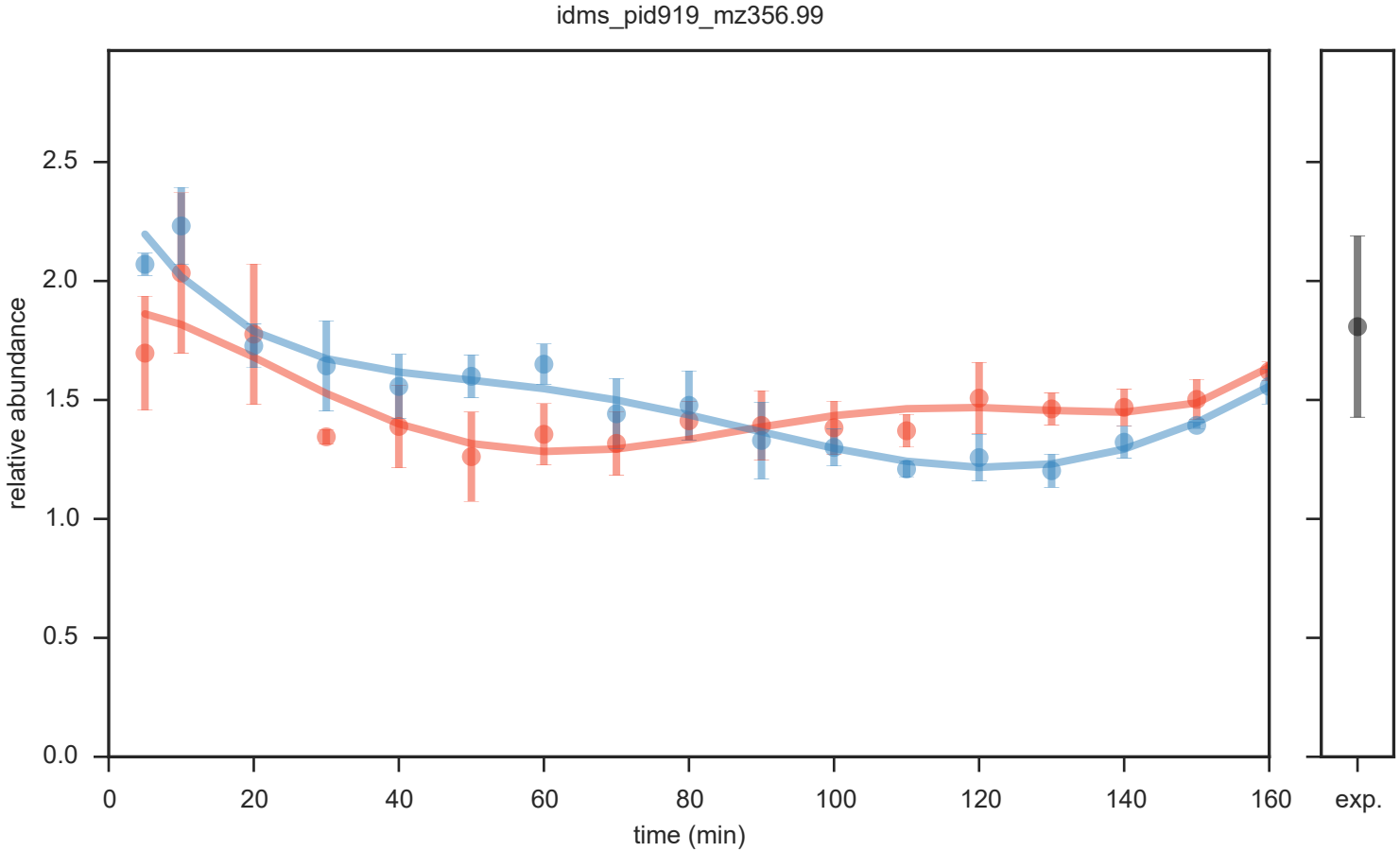

idms_pid884_mz118.04
relative abundance
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

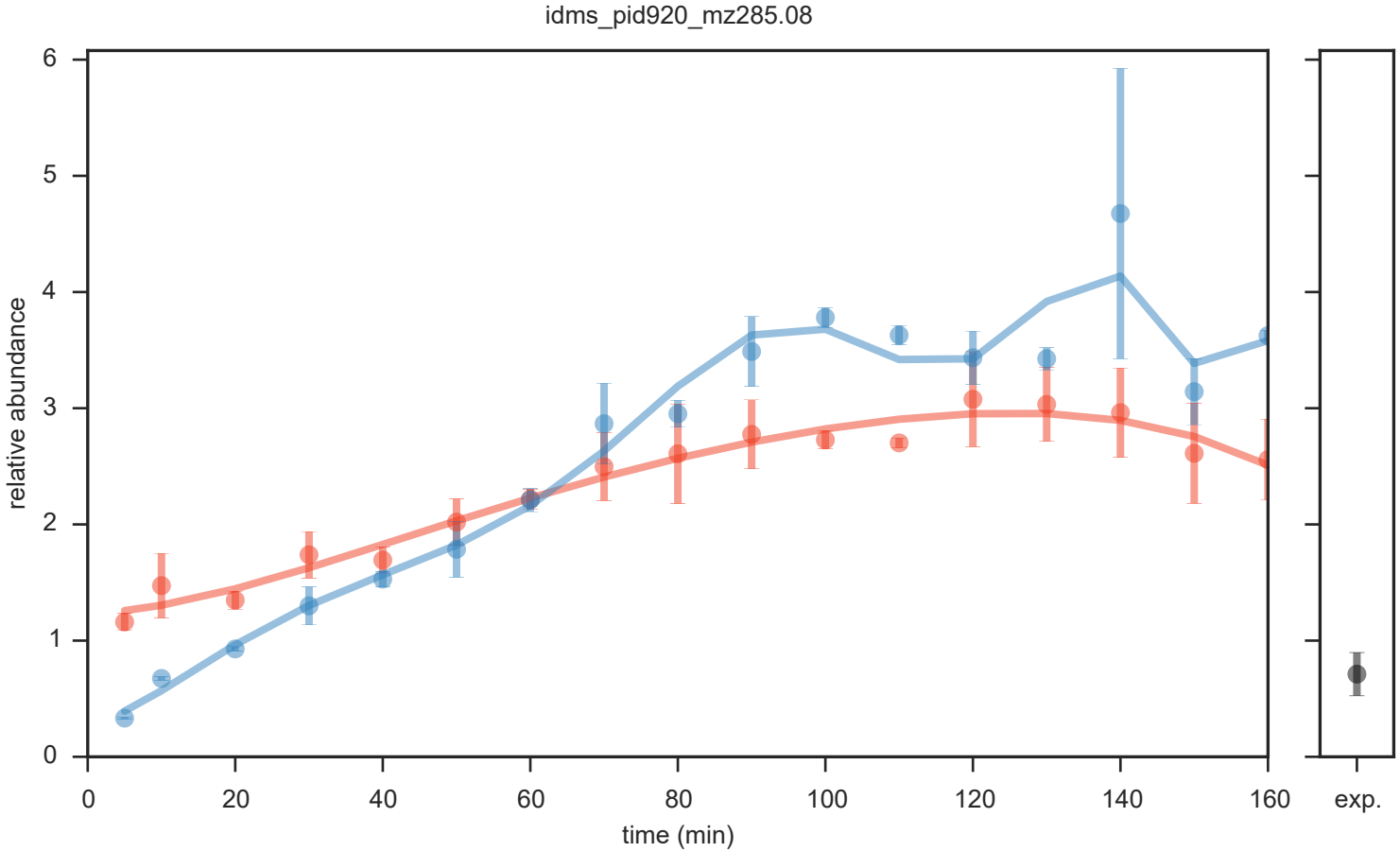

idms_pid898_mz858.05
relative abundance
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

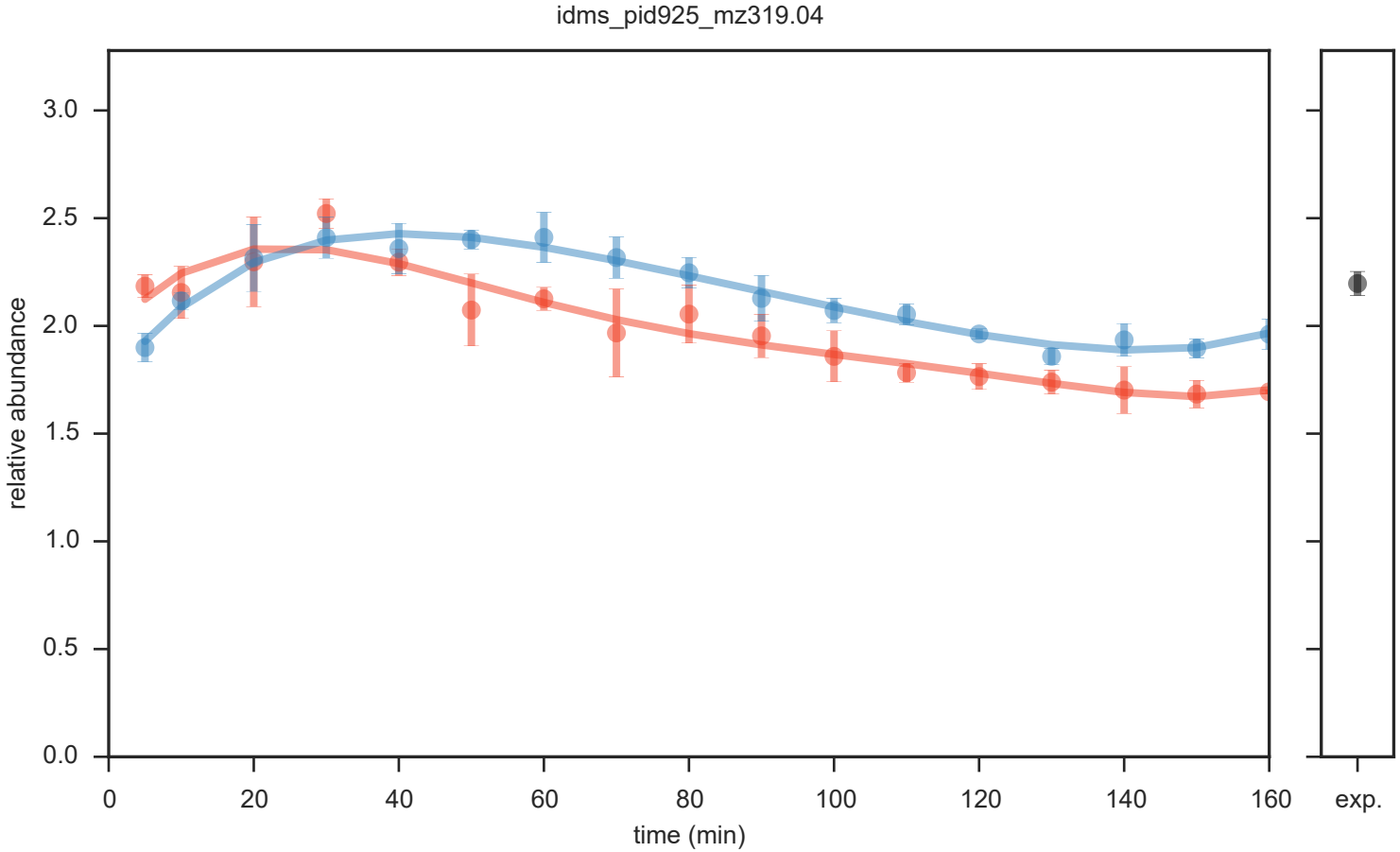

idms_pid899_mz227.04
relative abundance
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

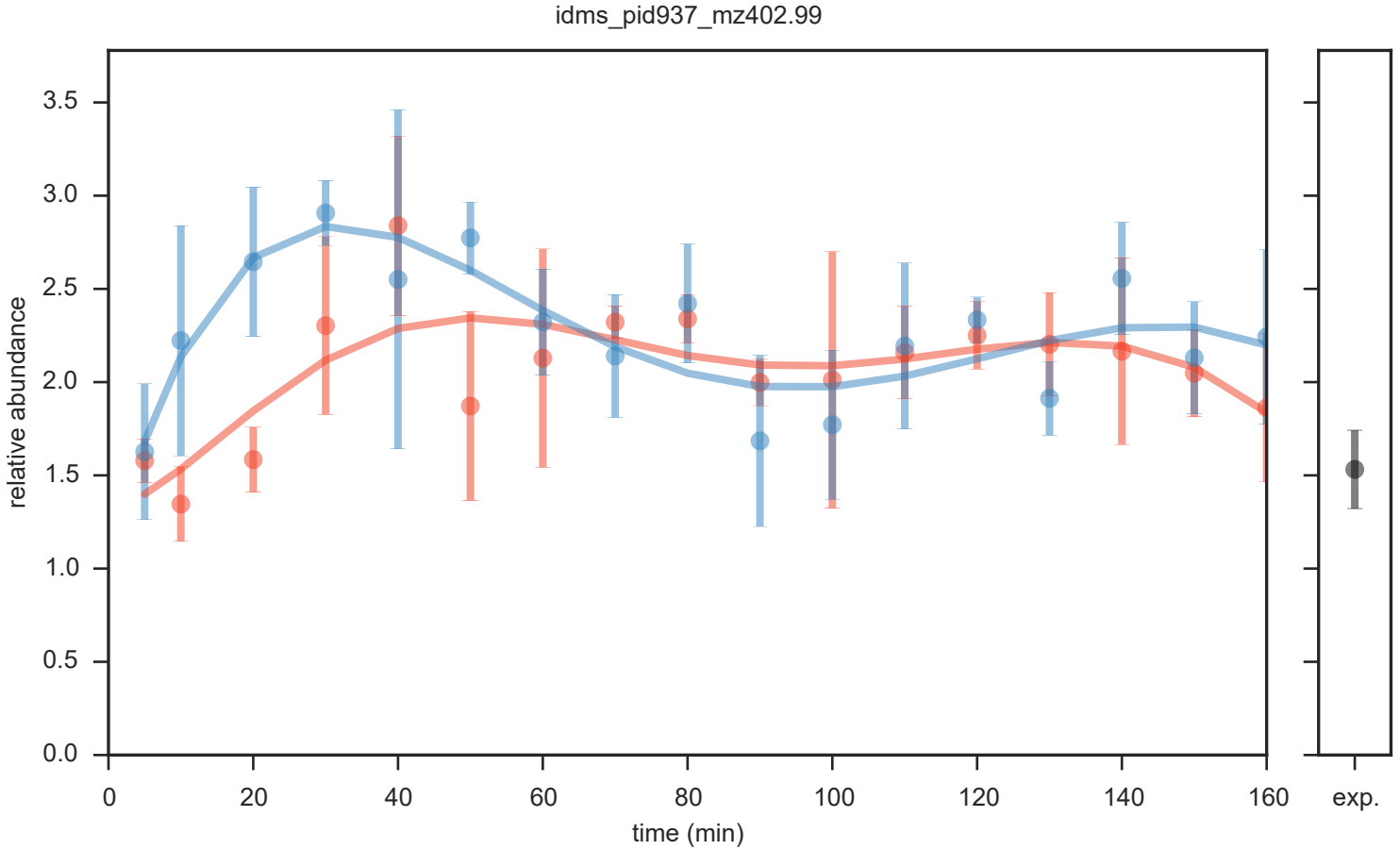

idms_pid900_mz403.55
relative abundance
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

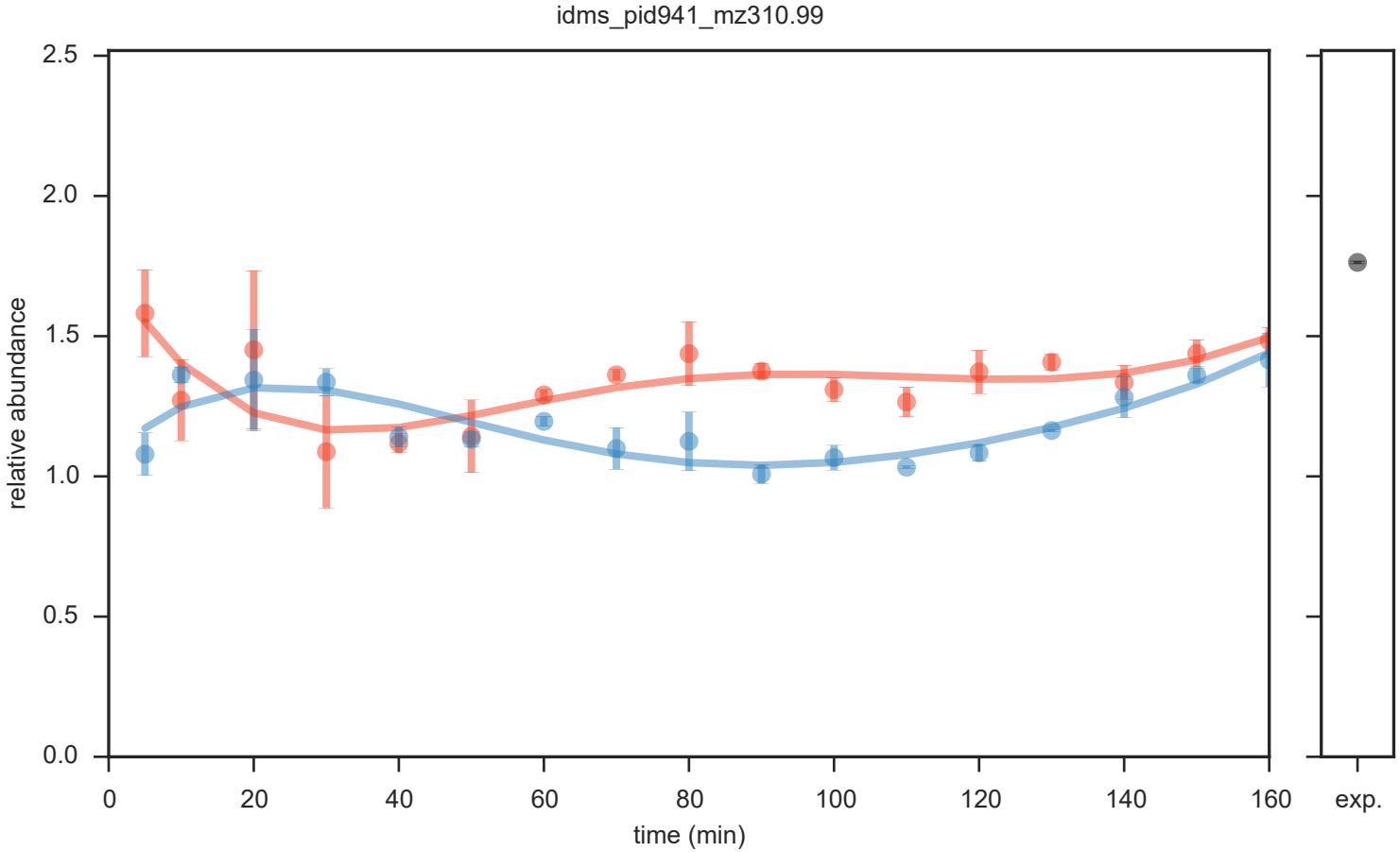

idms_pid901_mz380.54
relative abundance
0
1
2
3
4
5
6
7
0
20
40
60
80
100
120
140
160
time (min)
exp.

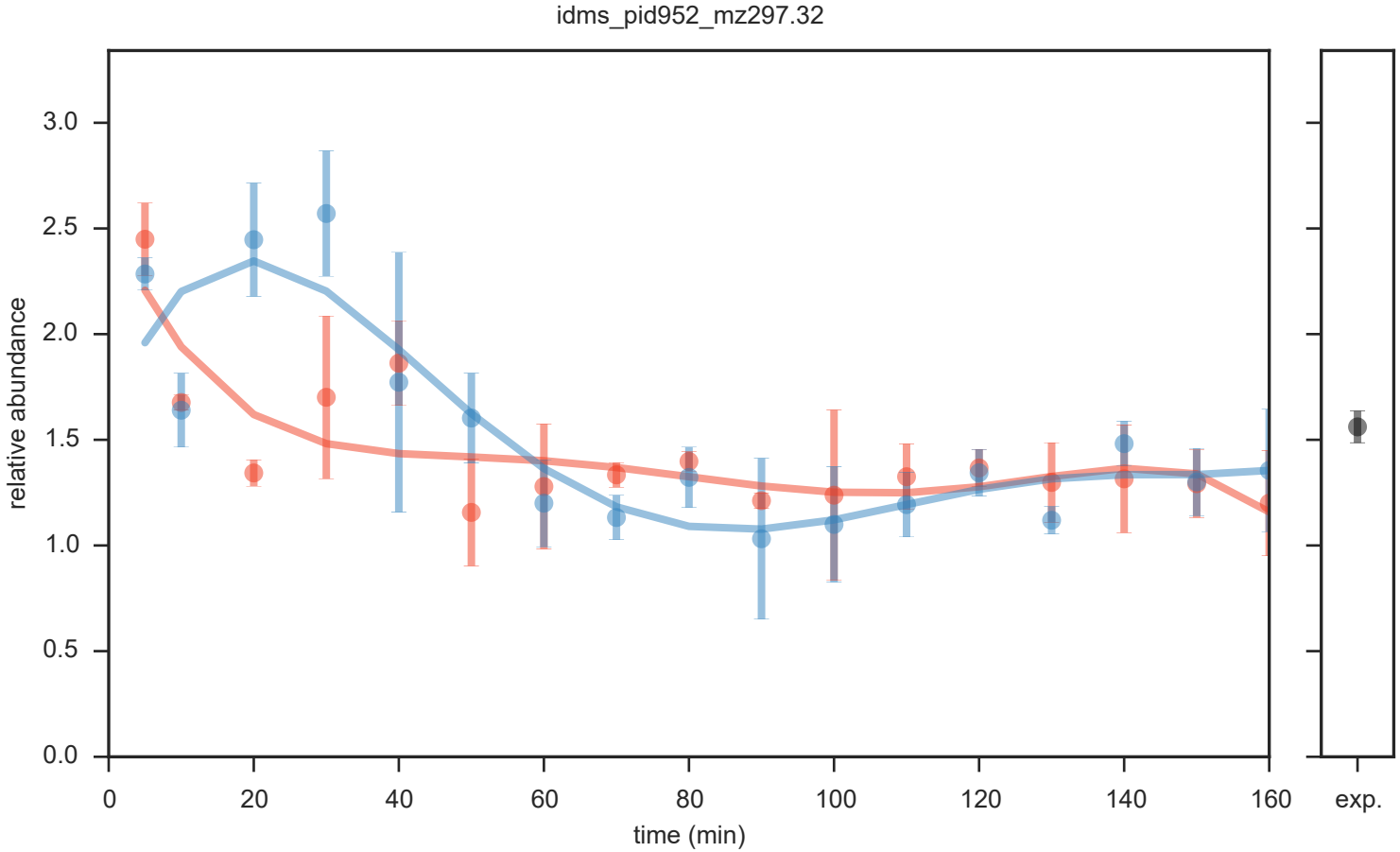

idms_pid919_mz356.99
relative abundance
0.0
0.5
1.0
1.5
2.0
2.5
0
20
40
60
80
100
120
140
160
time (min)
exp.

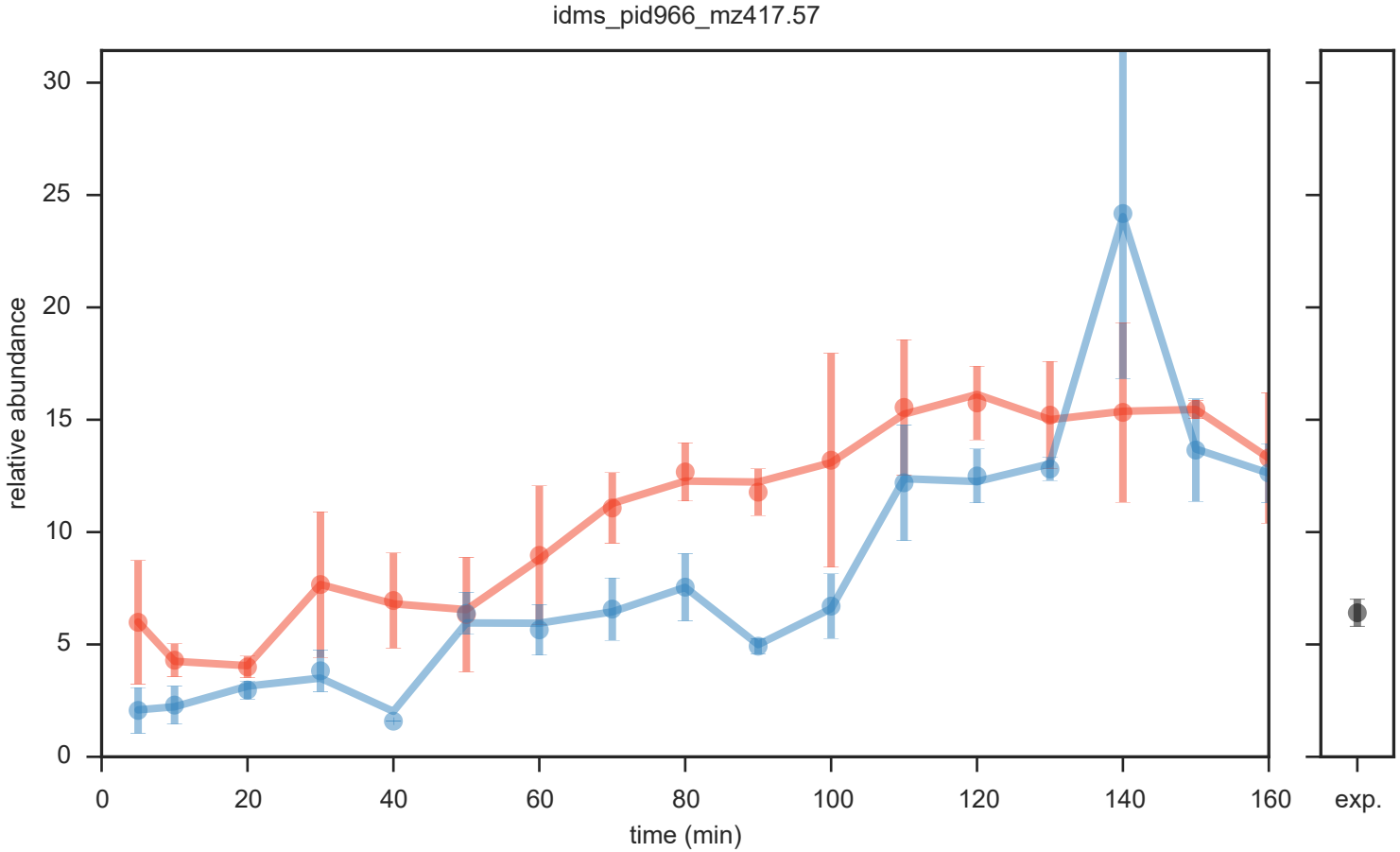

idms_pid920_mz285.08
relative abundance
time (min)
exp.
0
1
2
3
4
5
6
0
20
40
60
80
100
120
140
160

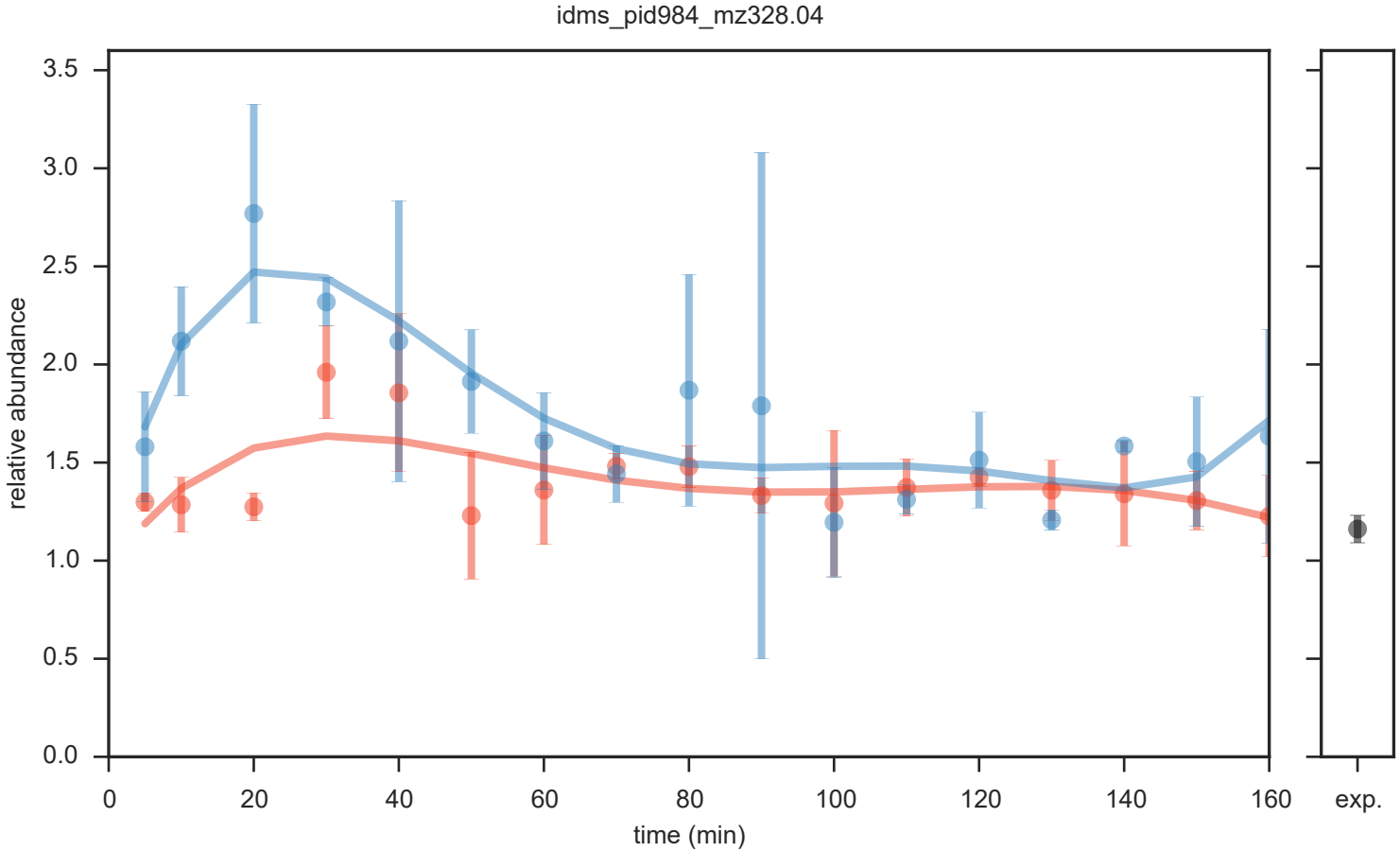

idms_pid925_mz319.04
relative abundance
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

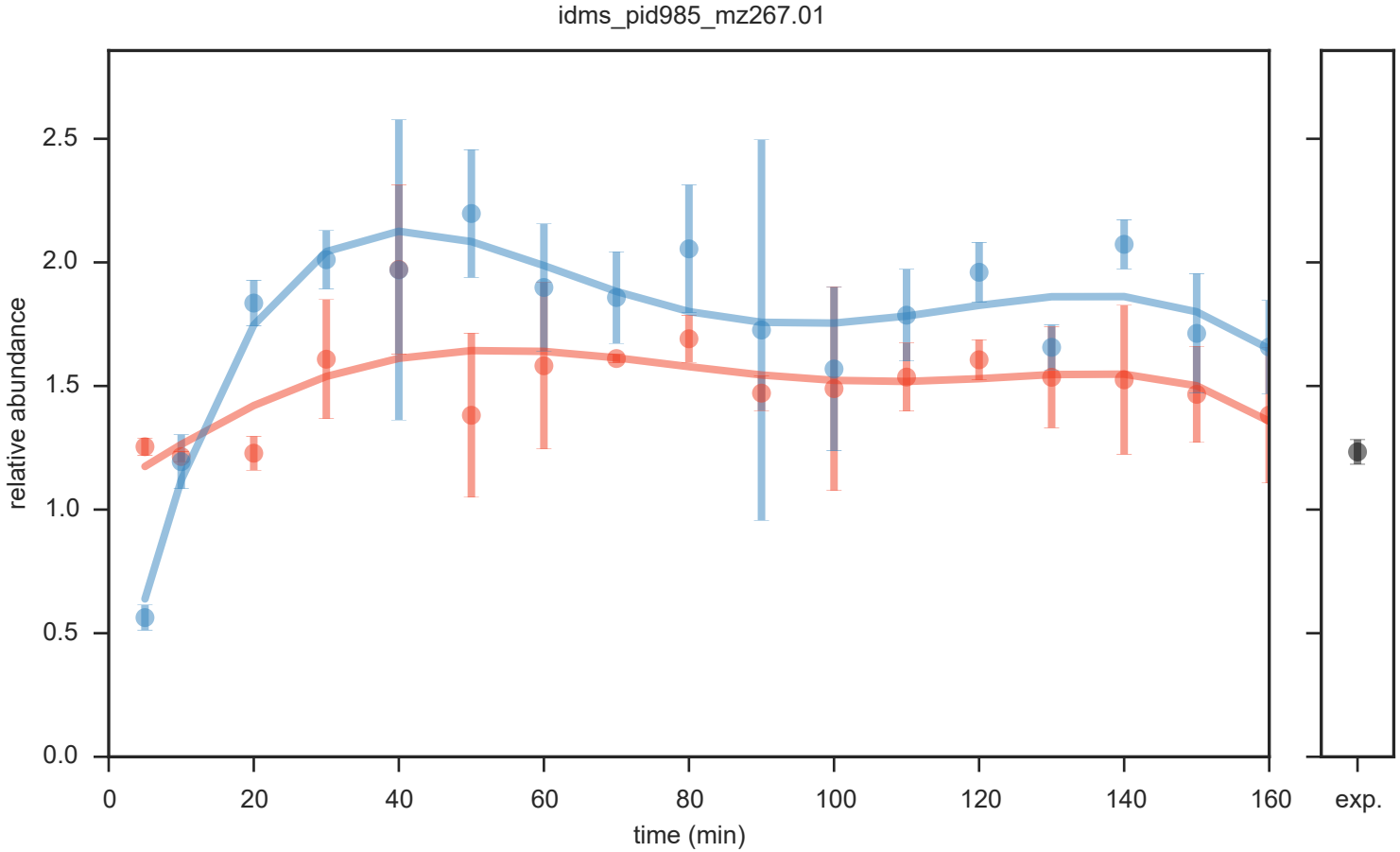

idms_pid937_mz402.99
relative abundance
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
0
20
40
60
80
100
120
140
160
time (min)
exp.

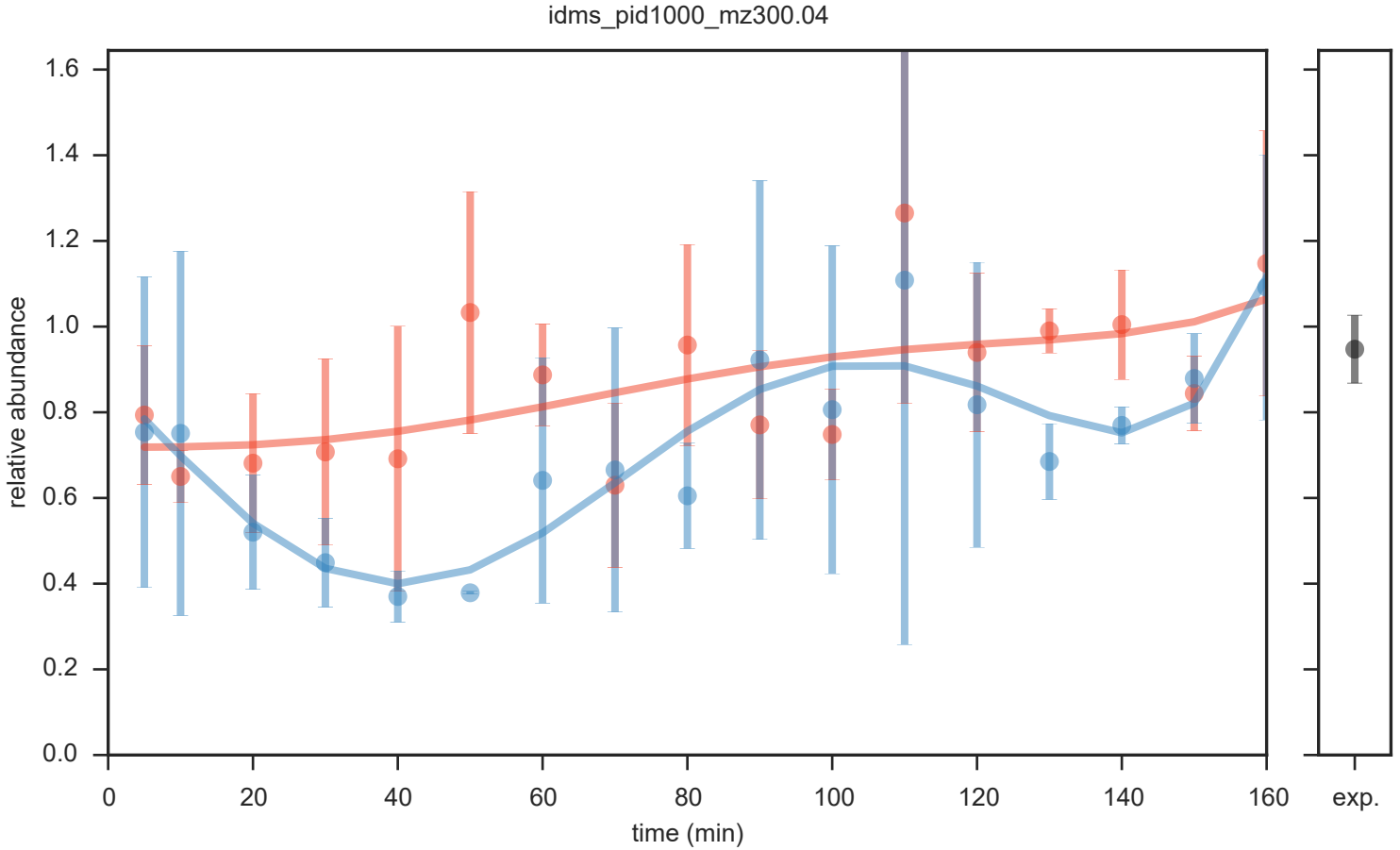

idms_pid941_mz310.99
relative abundance
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

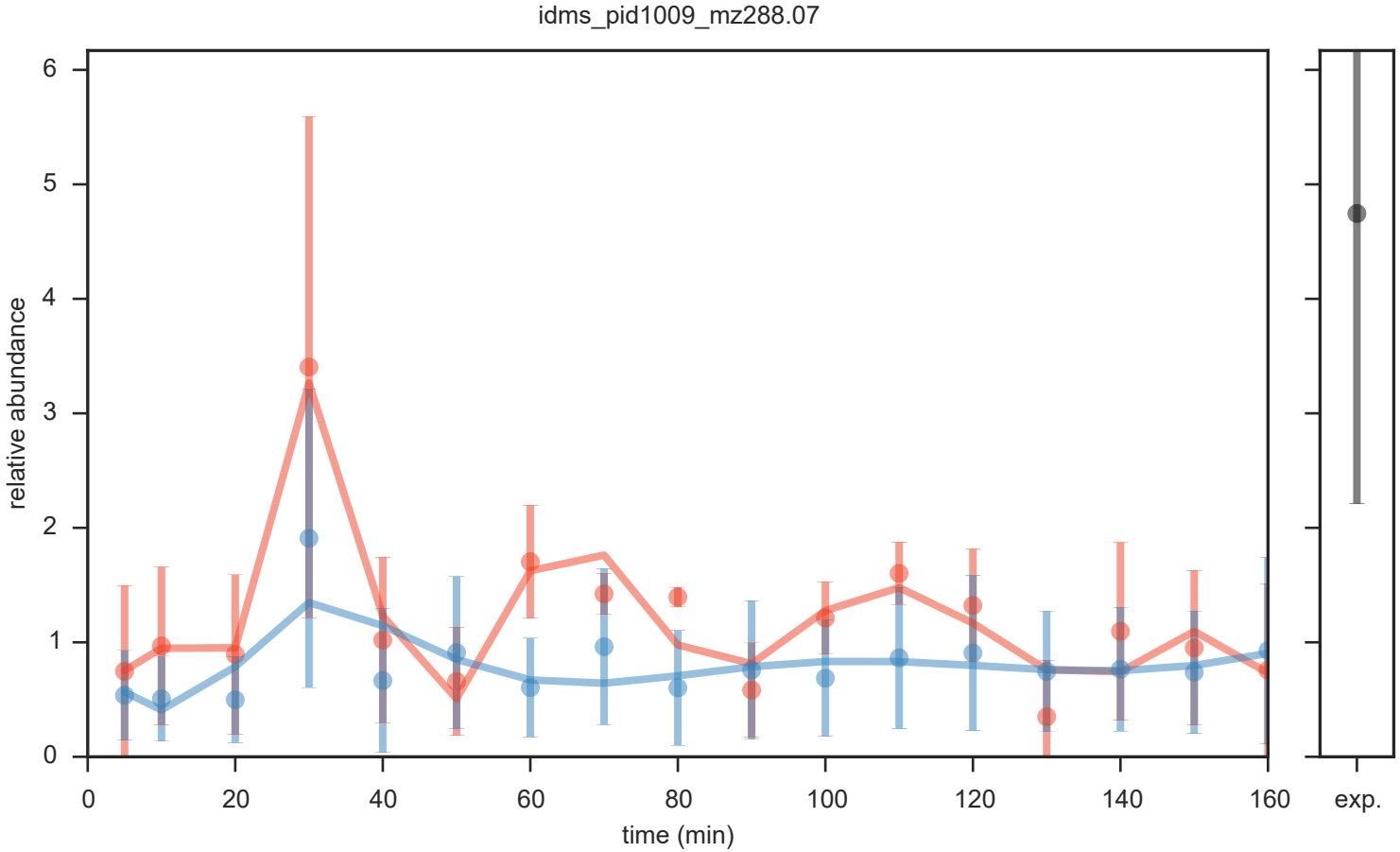

idms_pid952_mz297.32
relative abundance
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

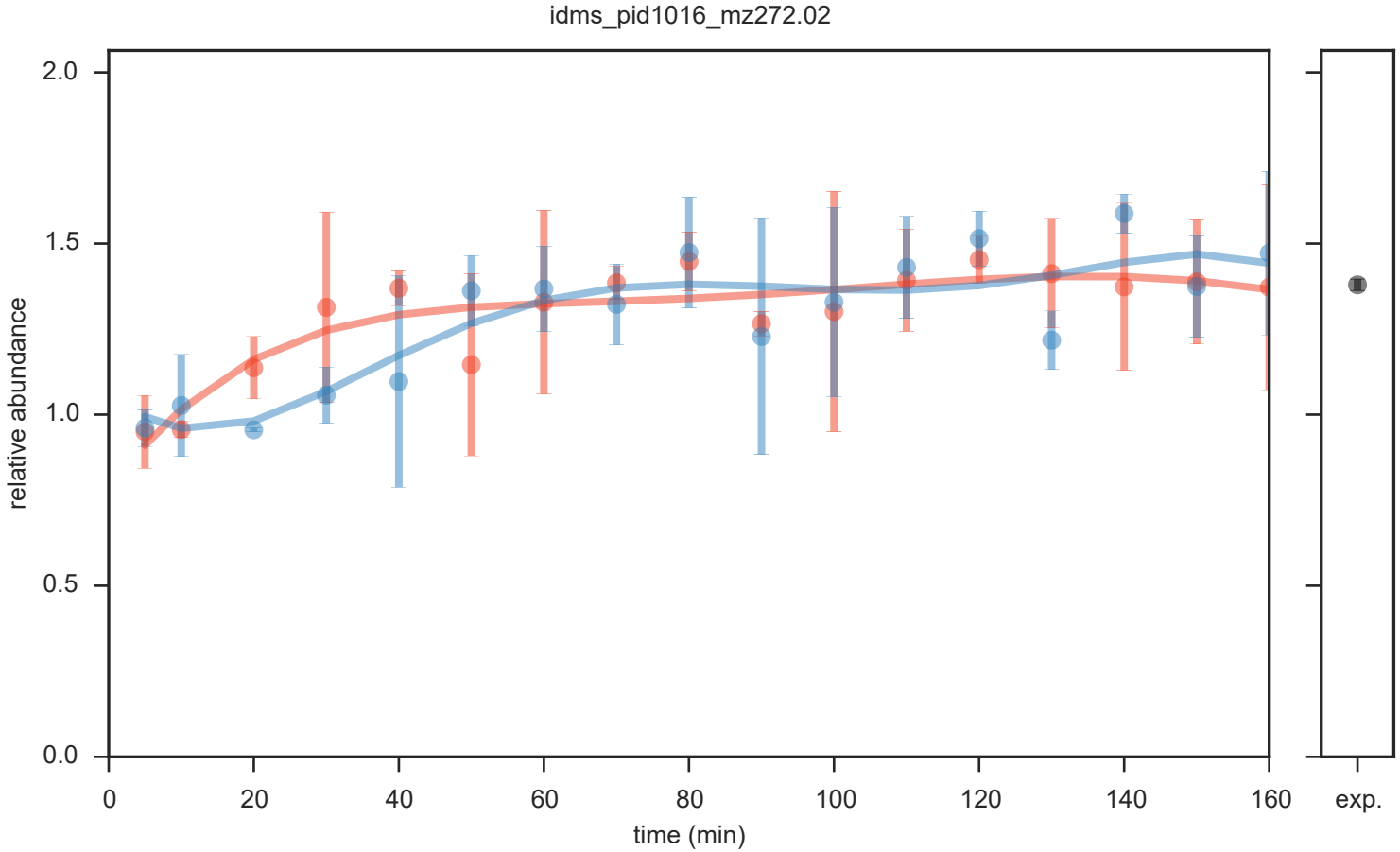

idms_pid966_mz417.57
relative abundance
time (min)
exp.
0
5
10
15
20
25
30
0
20
40
60
80
100
120
140
160

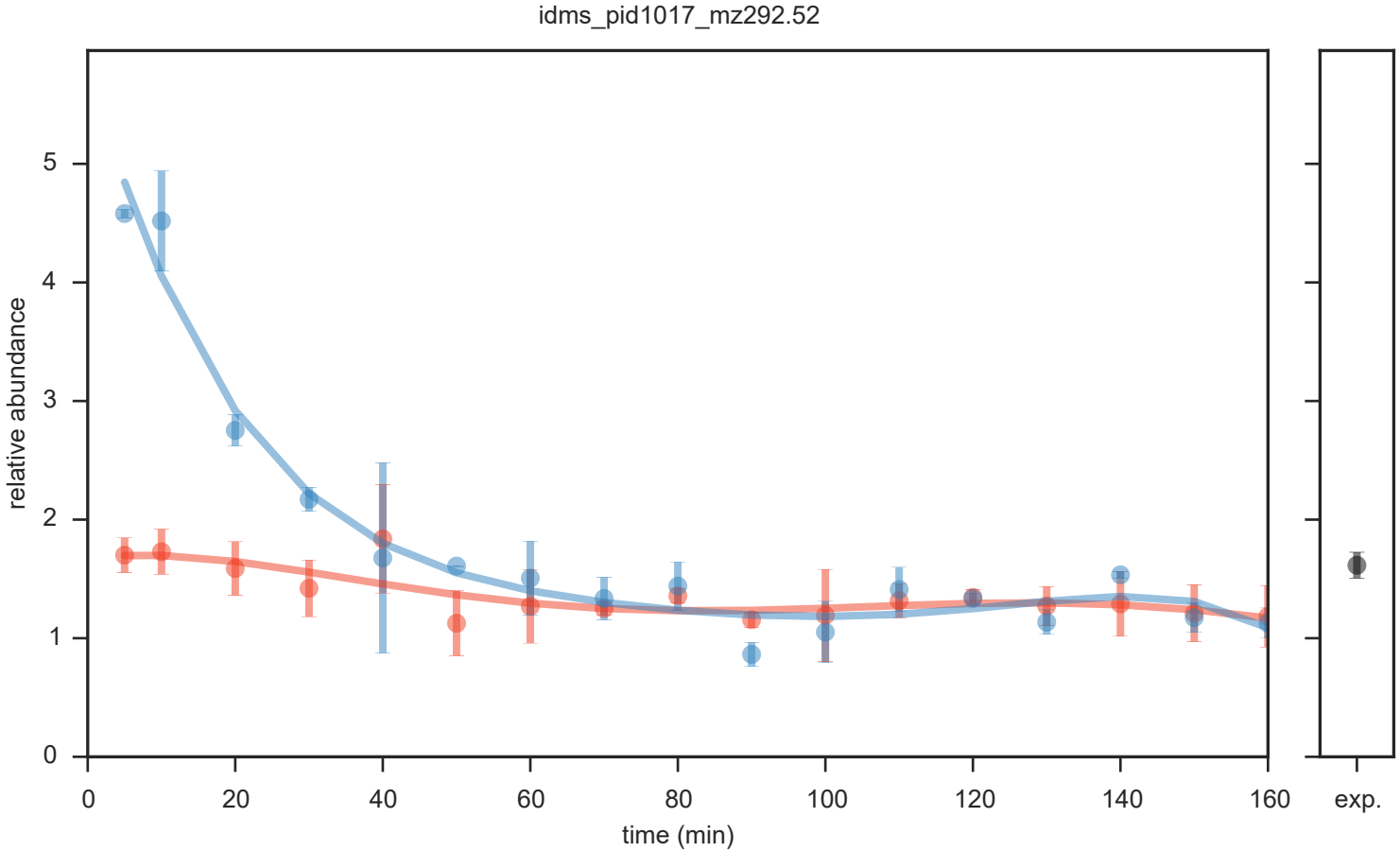

idms_pid984_mz328.04
relative abundance
time (min)
exp.
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
0
20
40
60
80
100
120
140
160

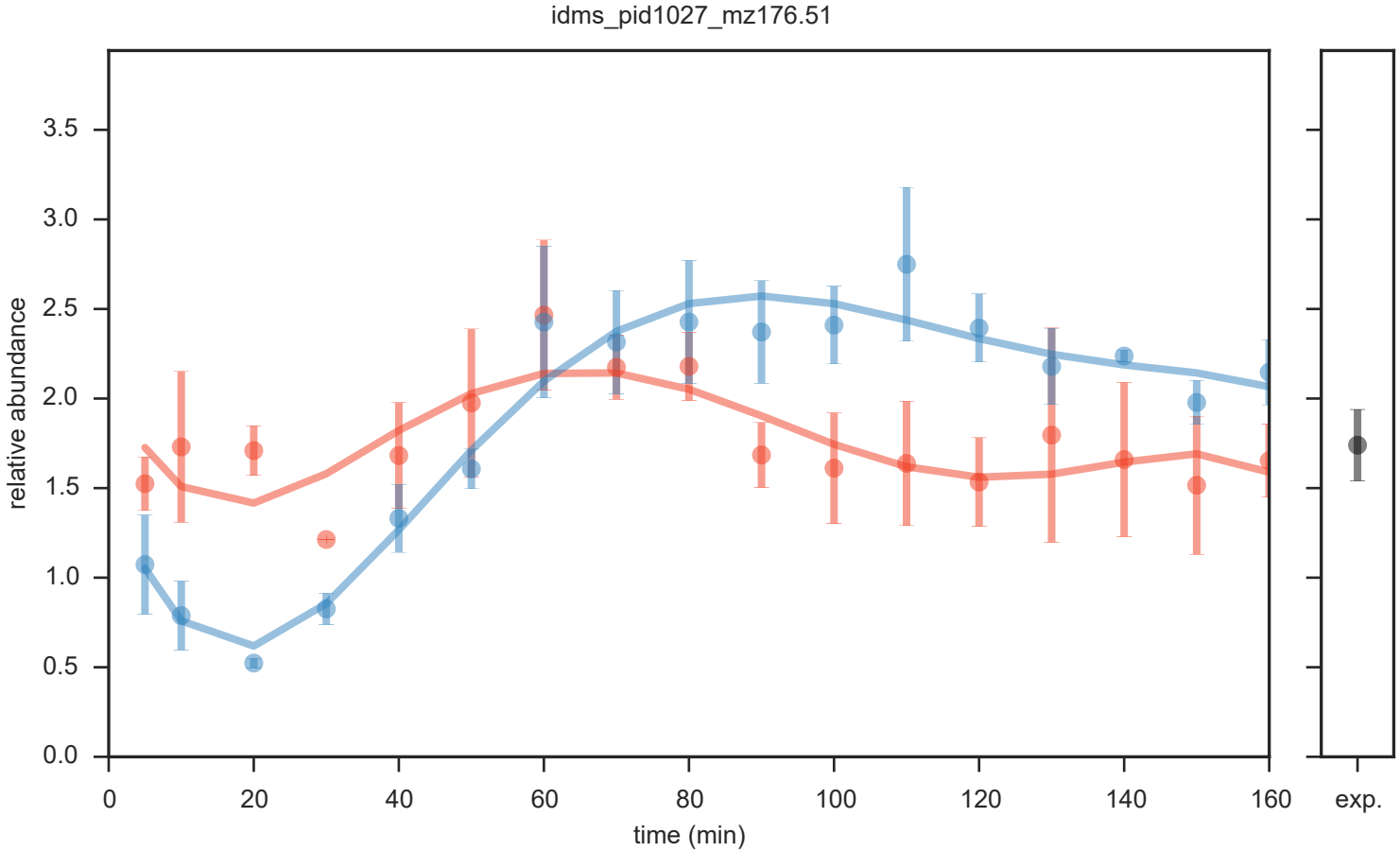

idms_pid985_mz267.01
relative abundance
0.0
0.5
1.0
1.5
2.0
2.5
0
20
40
60
80
100
120
140
160
time (min)
exp.

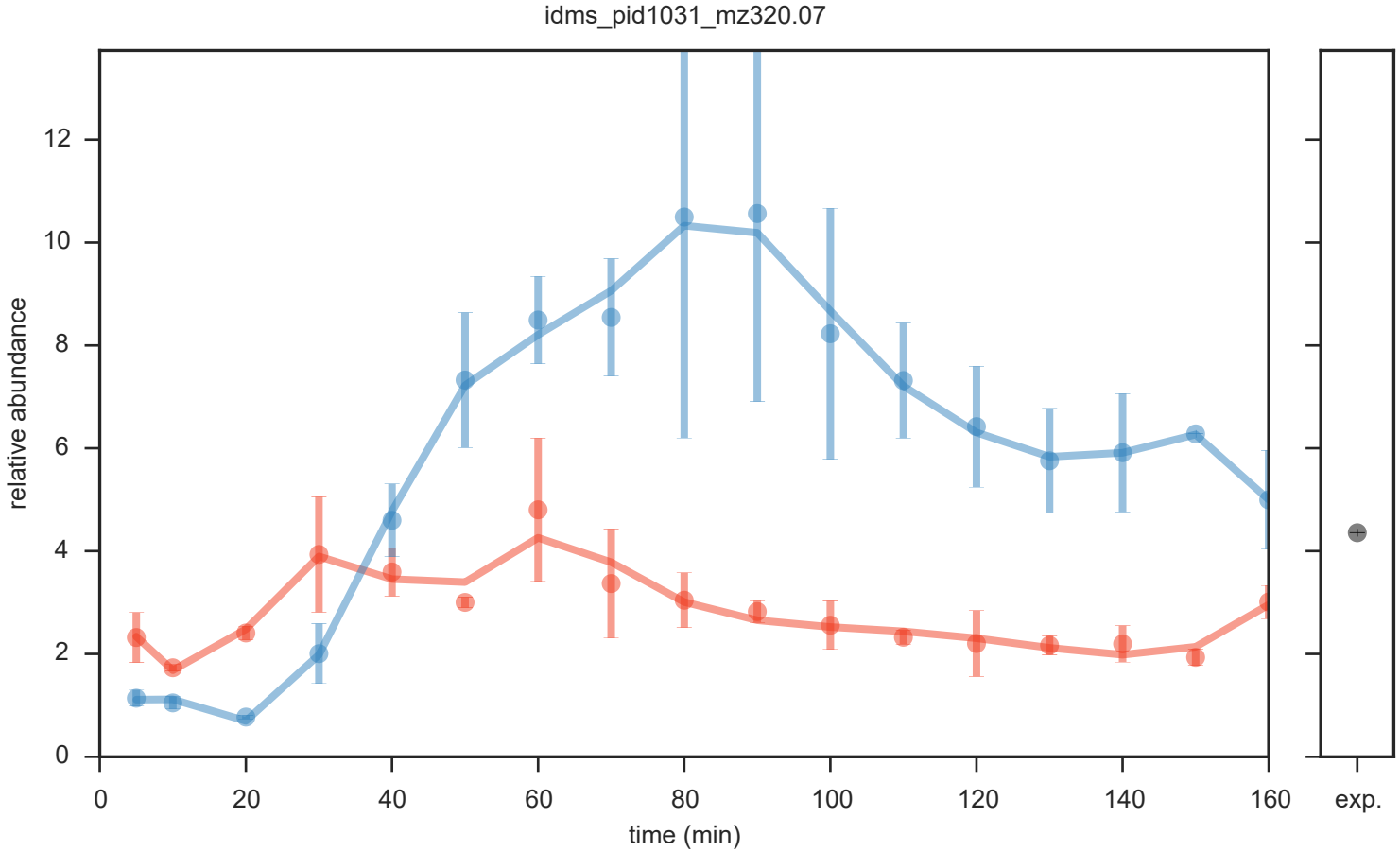

idms_pid1000_mz300.04
relative abundance
time (min)
exp.
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
0
20
40
60
80
100
120
140
160

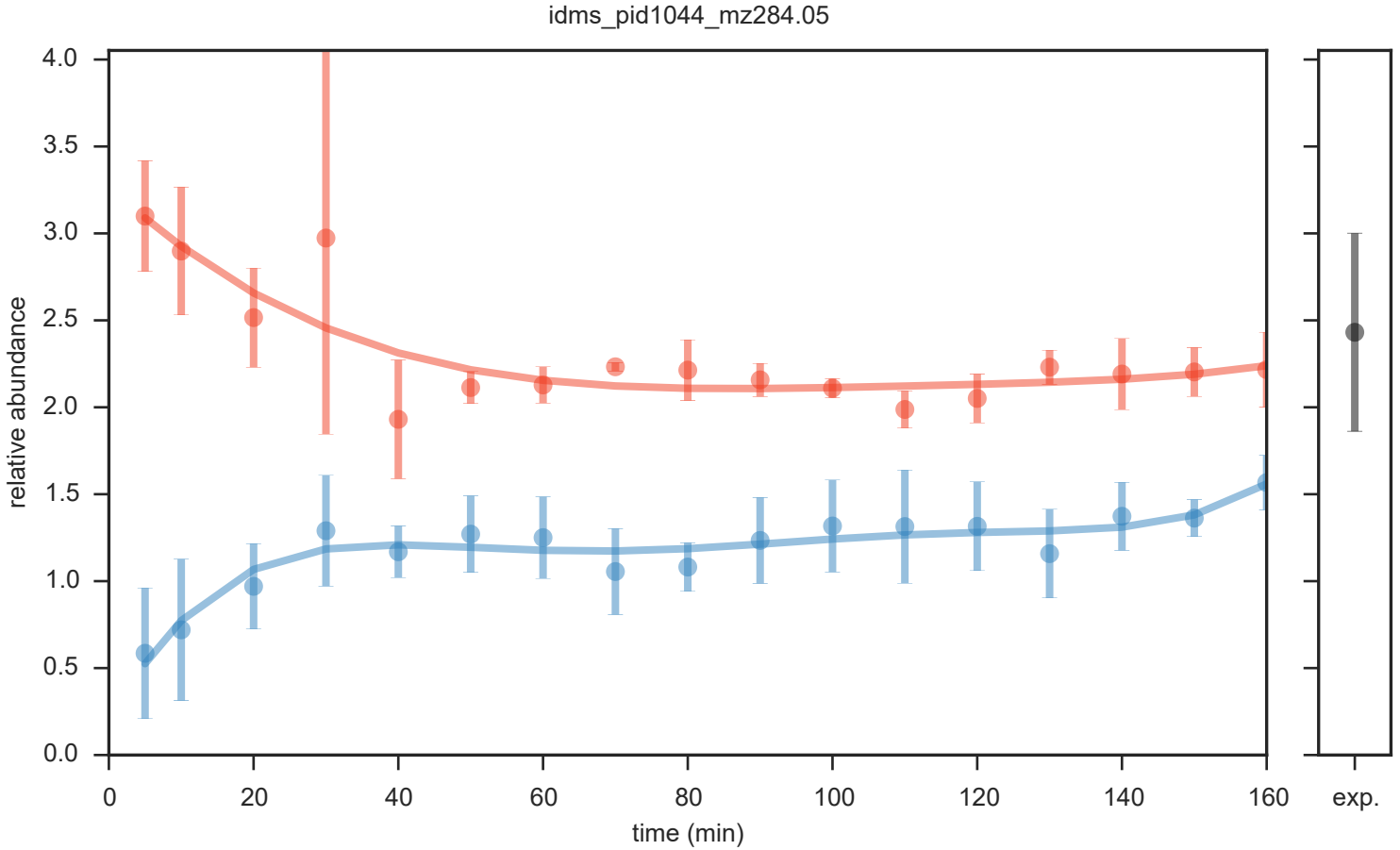

idms_pid1009_mz288.07
relative abundance
time (min)
exp.
0
1
2
3
4
5
6
0
20
40
60
80
100
120
140
160

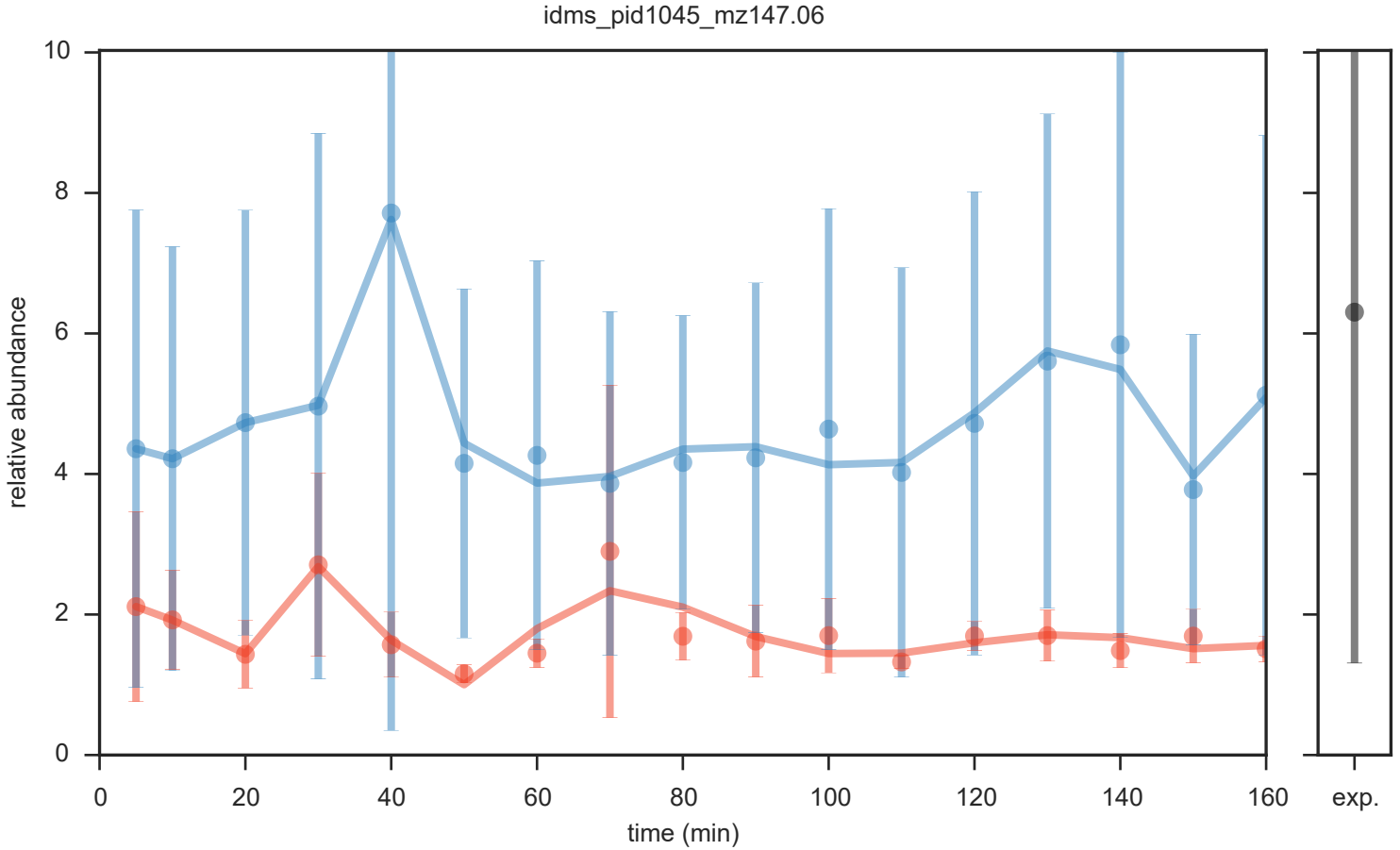

idms_pid1016_mz272.02
relative abundance
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

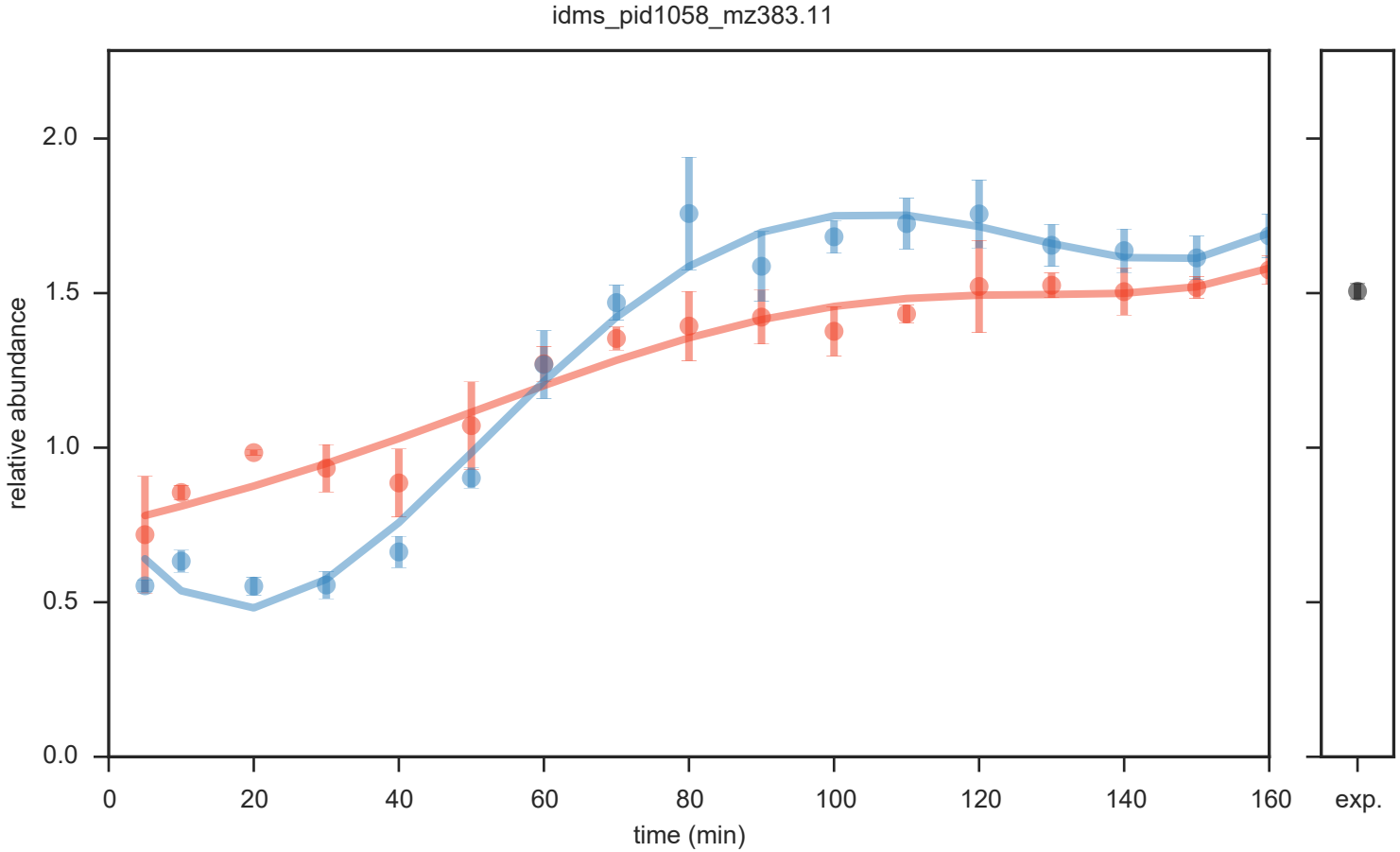

idms_pid1017_mz292.52
relative abundance
0
1
2
3
4
5
0
20
40
60
80
100
120
140
160
time (min)
exp.

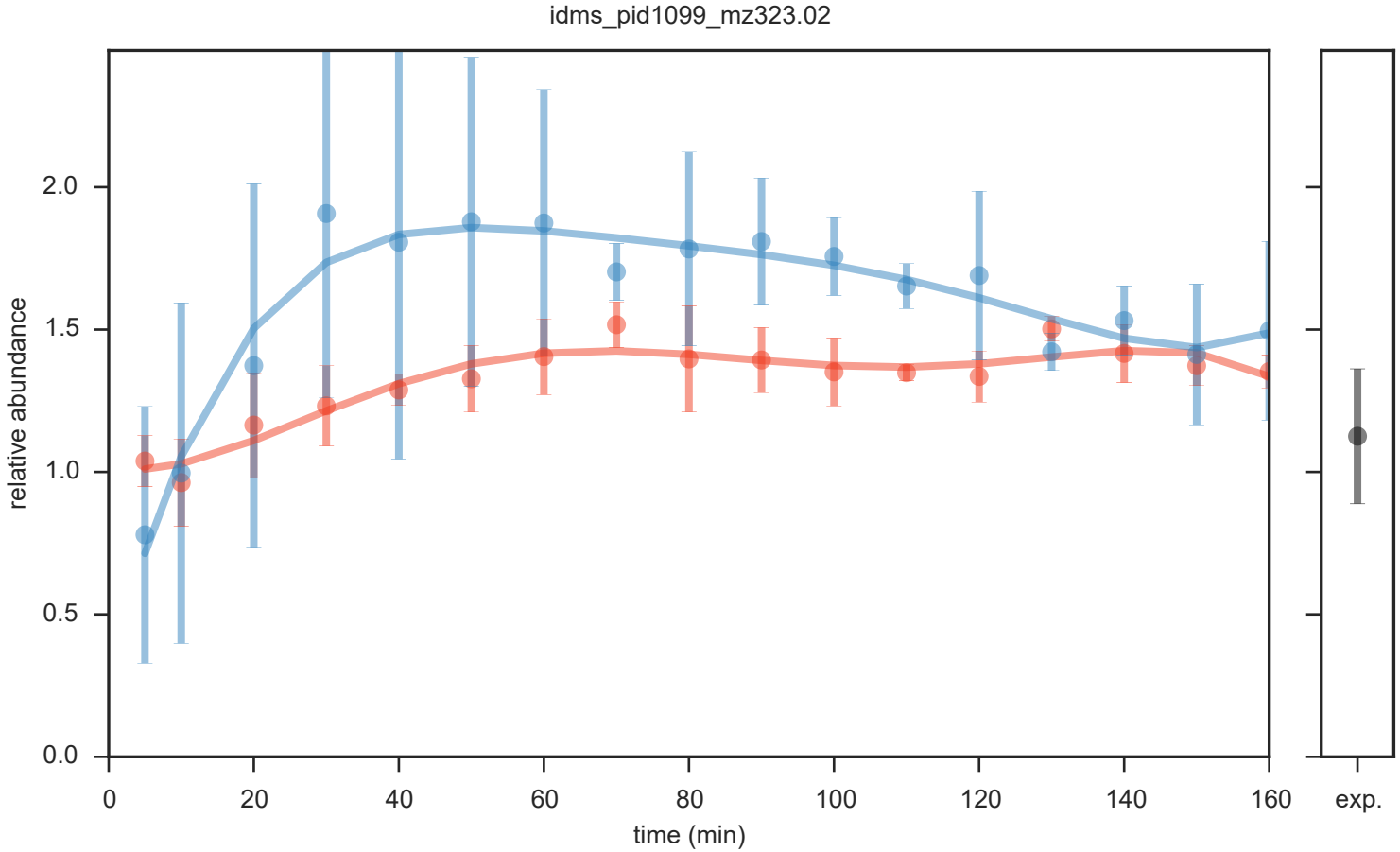

idms_pid1027_mz176.51
relative abundance
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
0
20
40
60
80
100
120
140
160
time (min)
exp.

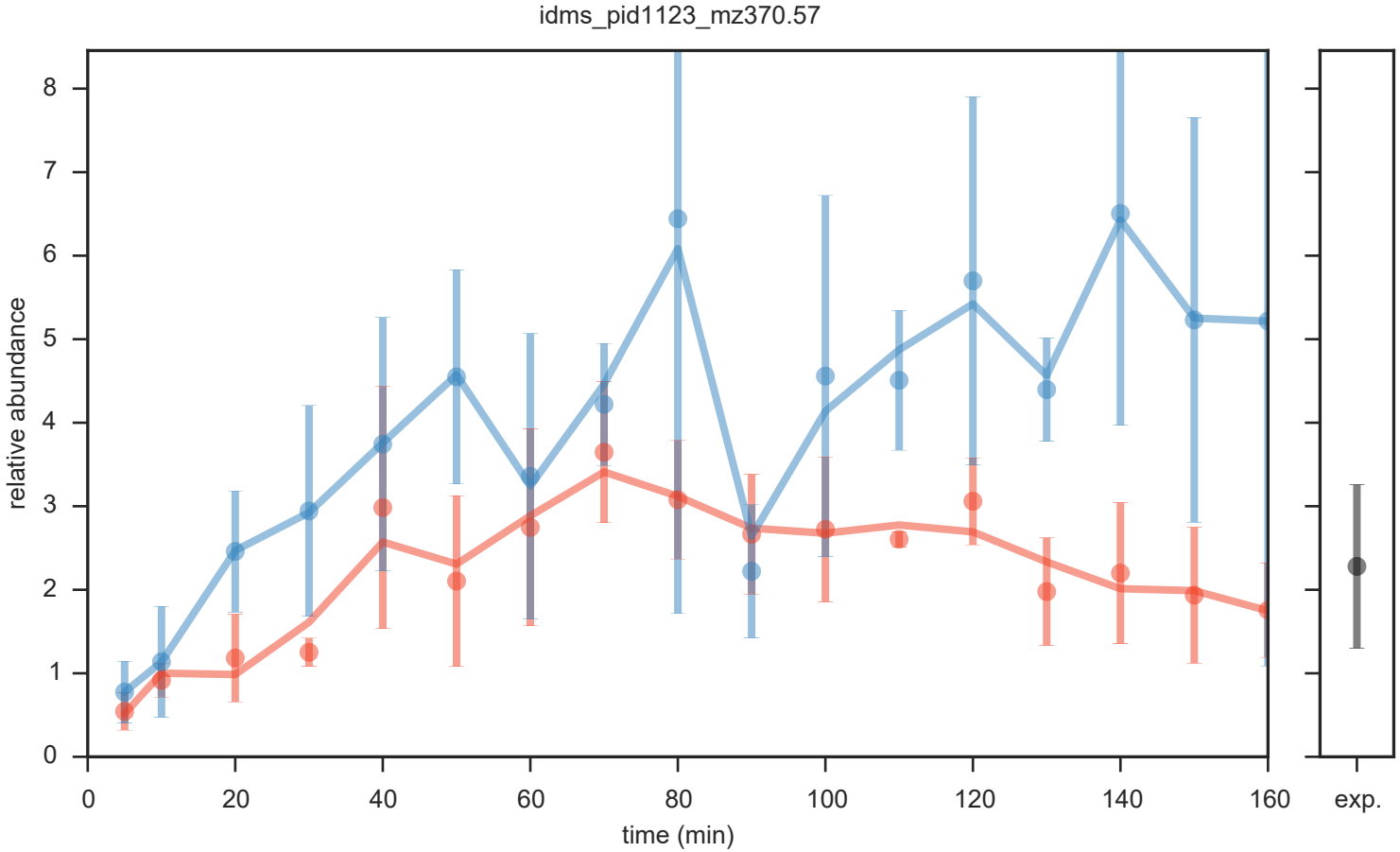

idms_pid1031_mz320.07
relative abundance
0
2
4
6
8
10
12
0
20
40
60
80
100
120
140
160
time (min)
exp.

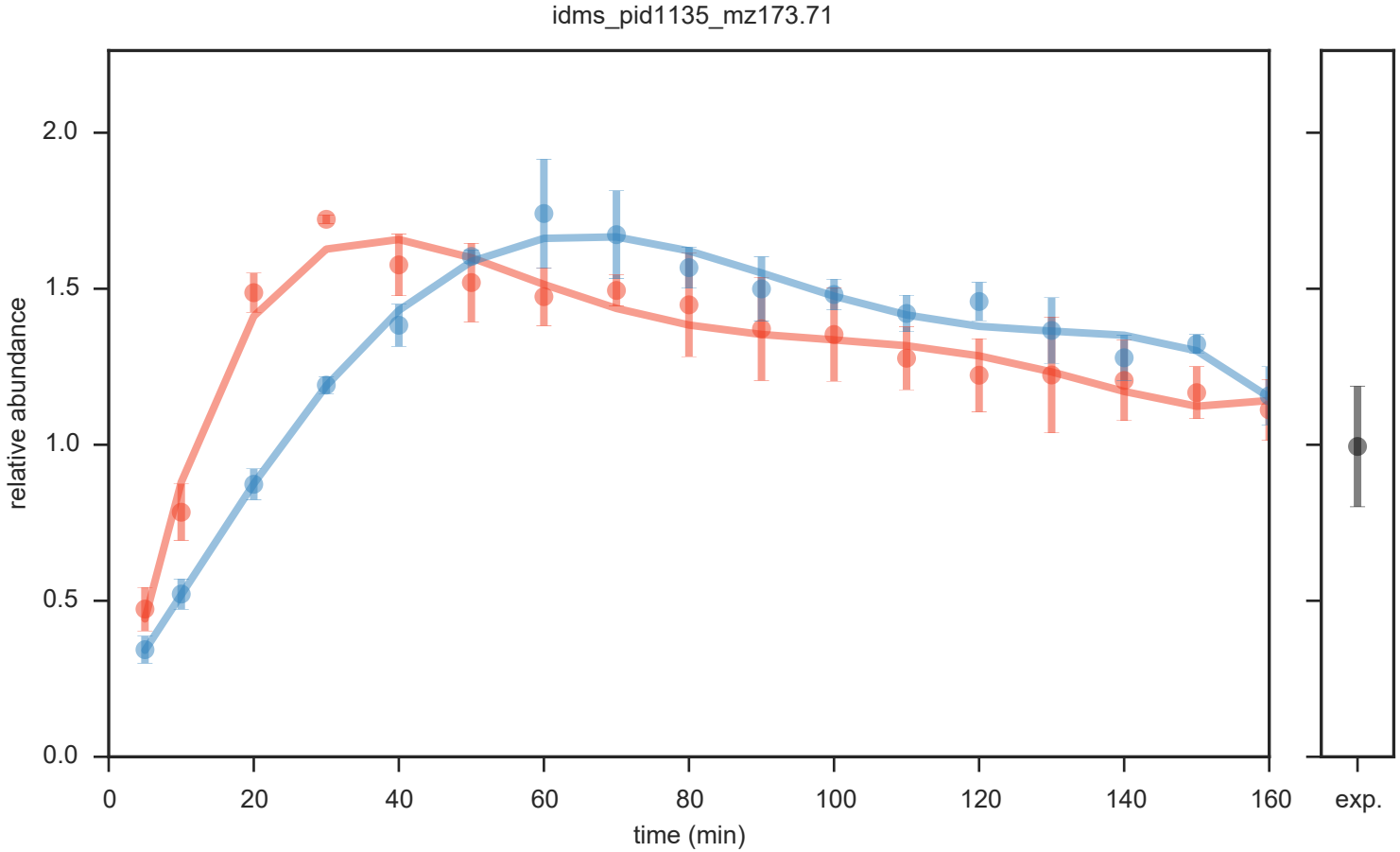

idms_pid1044_mz284.05
relative abundance
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

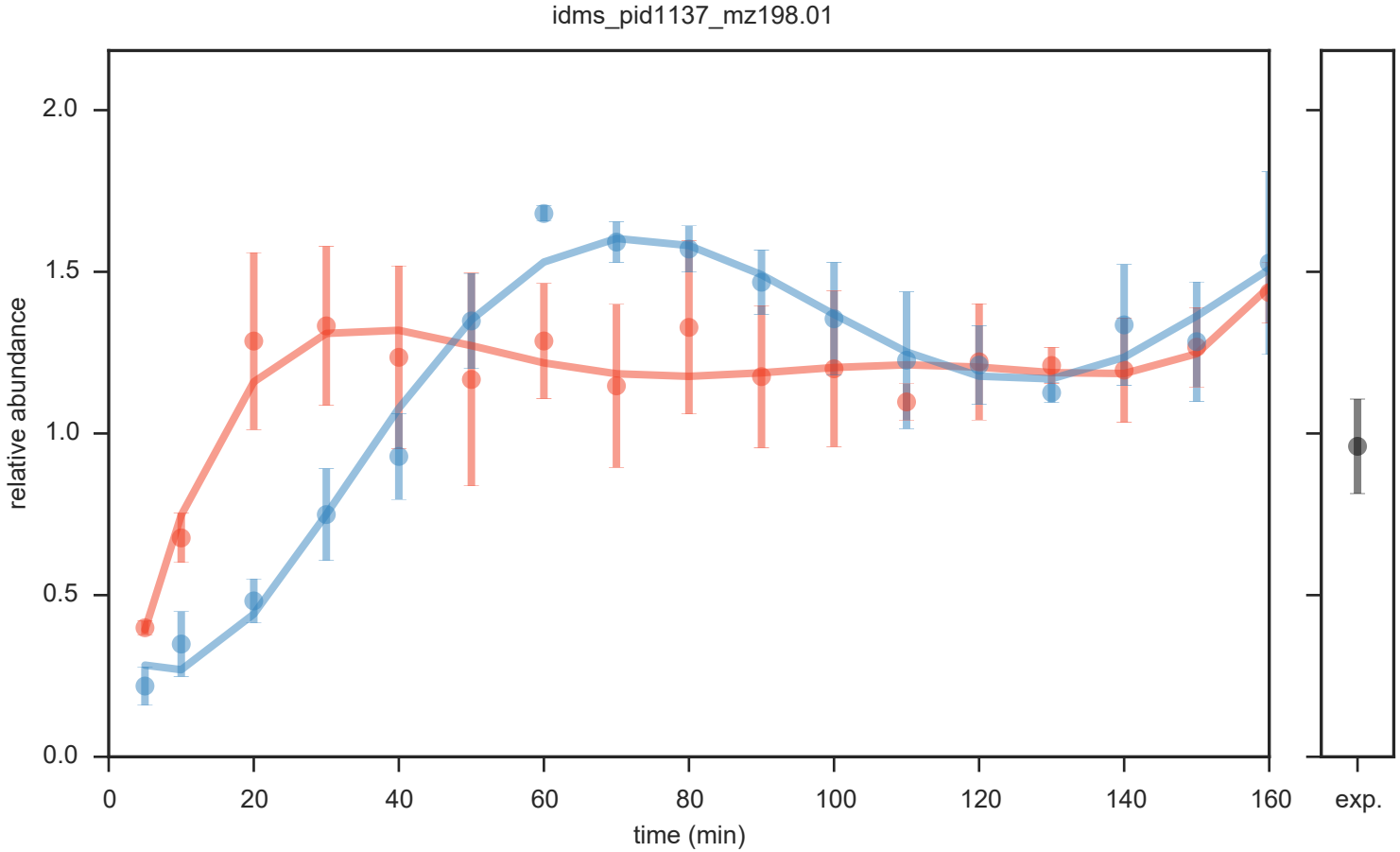

idms_pid1045_mz147.06
relative abundance
time (min)
exp.
0
2
4
6
8
10
0
20
40
60
80
100
120
140
160

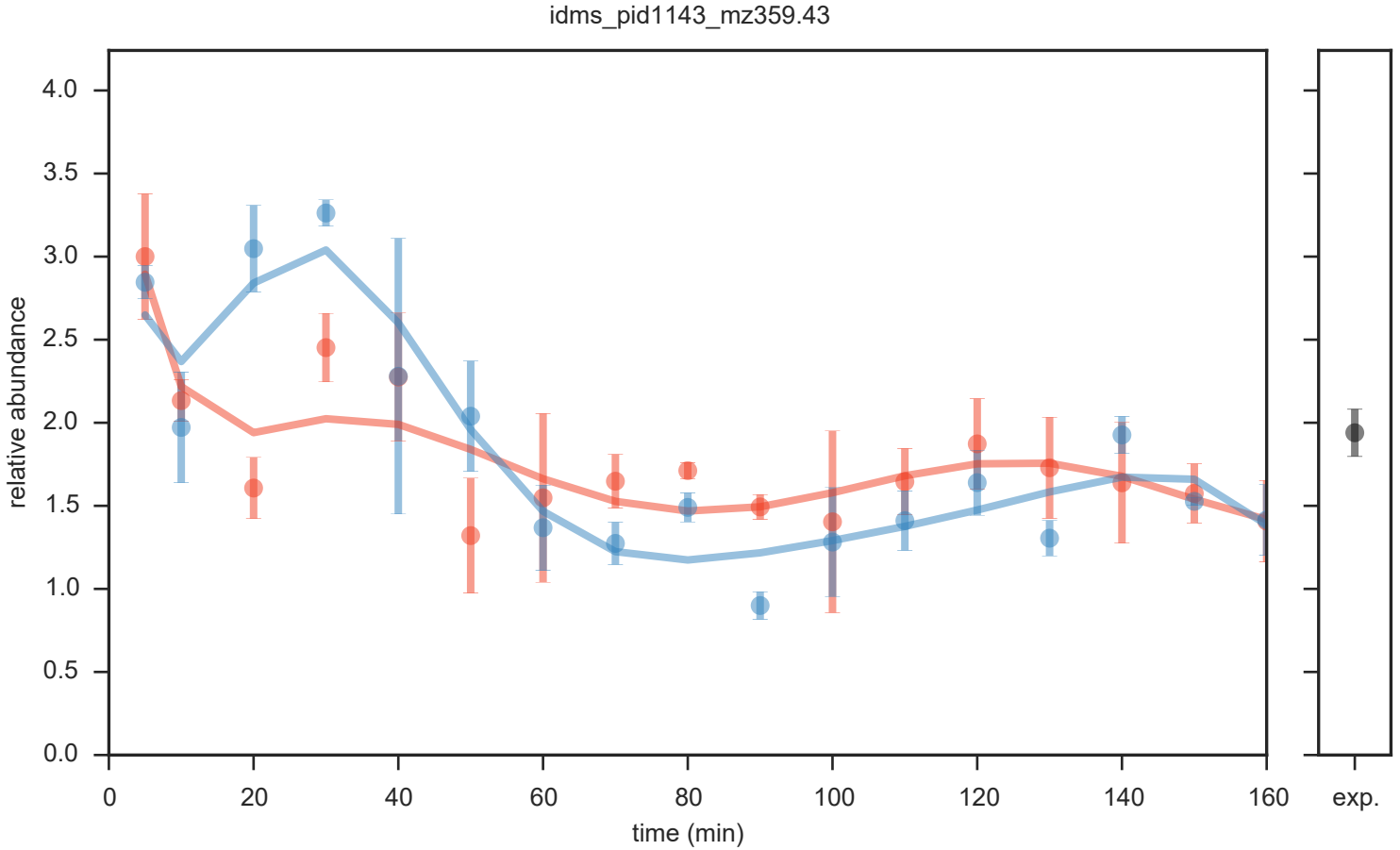

idms_pid1058_mz383.11
relative abundance
0.0
0.5
1.0
1.5
2.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

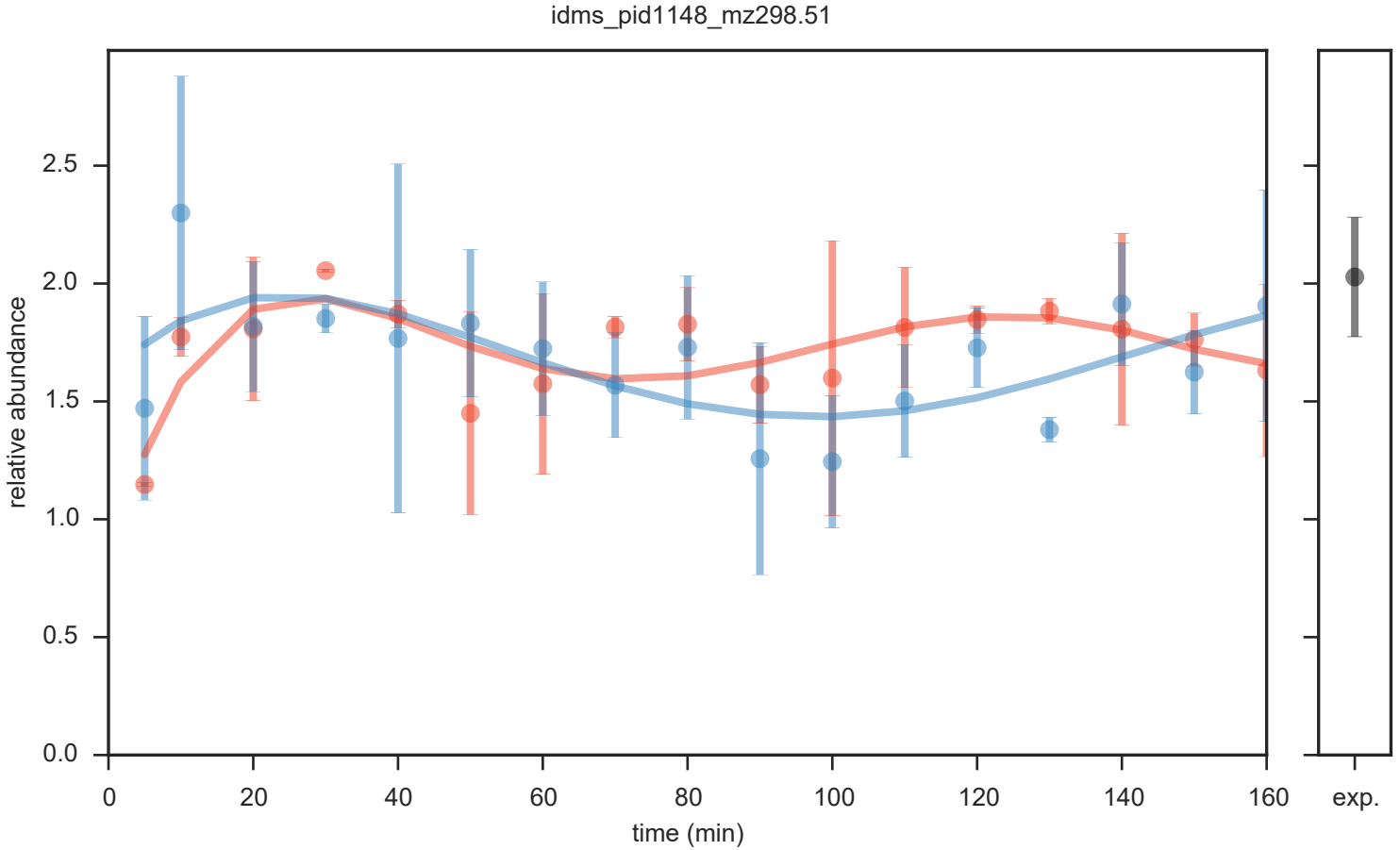

idms_pid1099_mz323.02
relative abundance
0.0
0.5
1.0
1.5
2.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

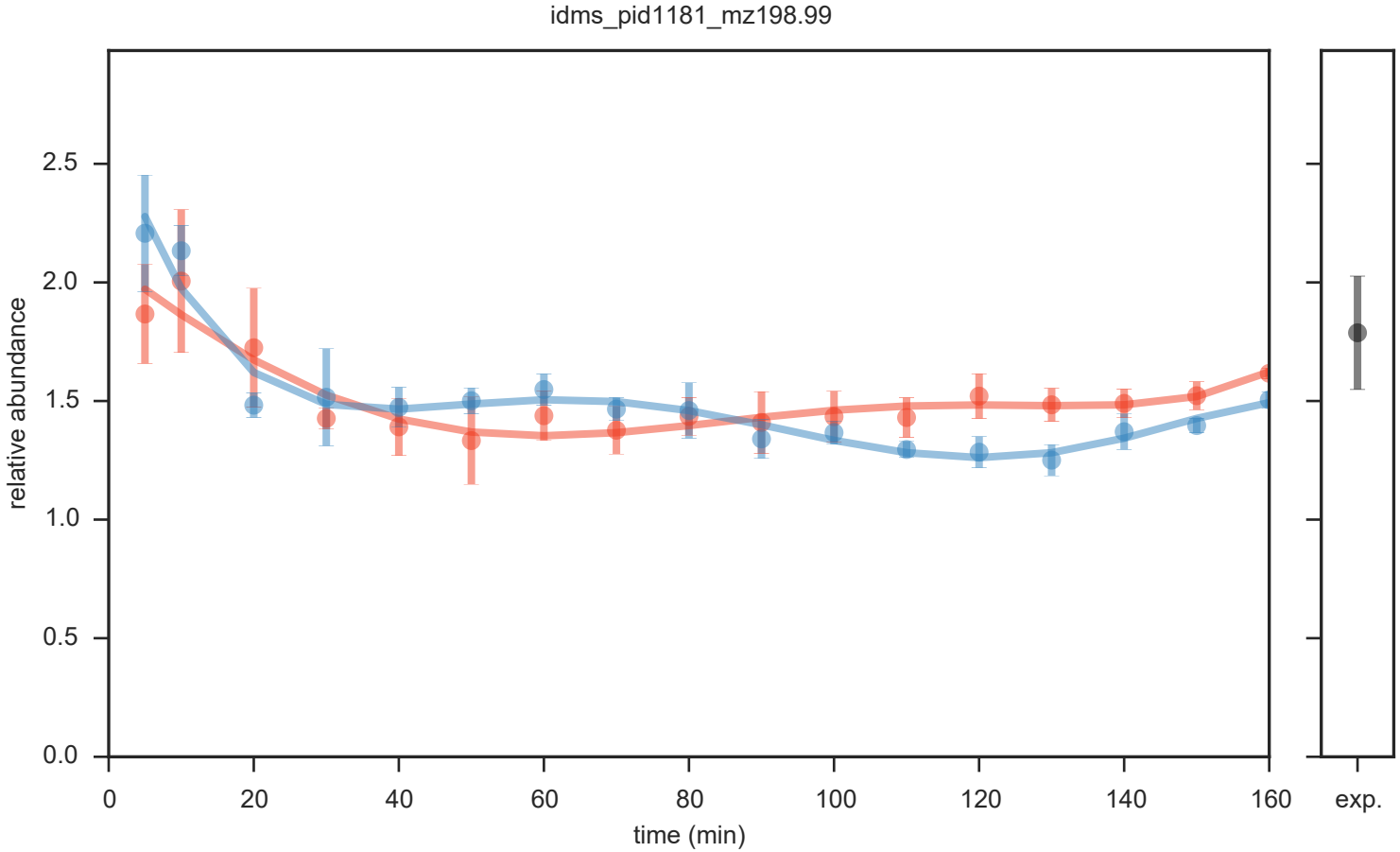

idms_pid1123_mz370.57
relative abundance
0
1
2
3
4
5
6
7
8
0
20
40
60
80
100
120
140
160
time (min)
exp.

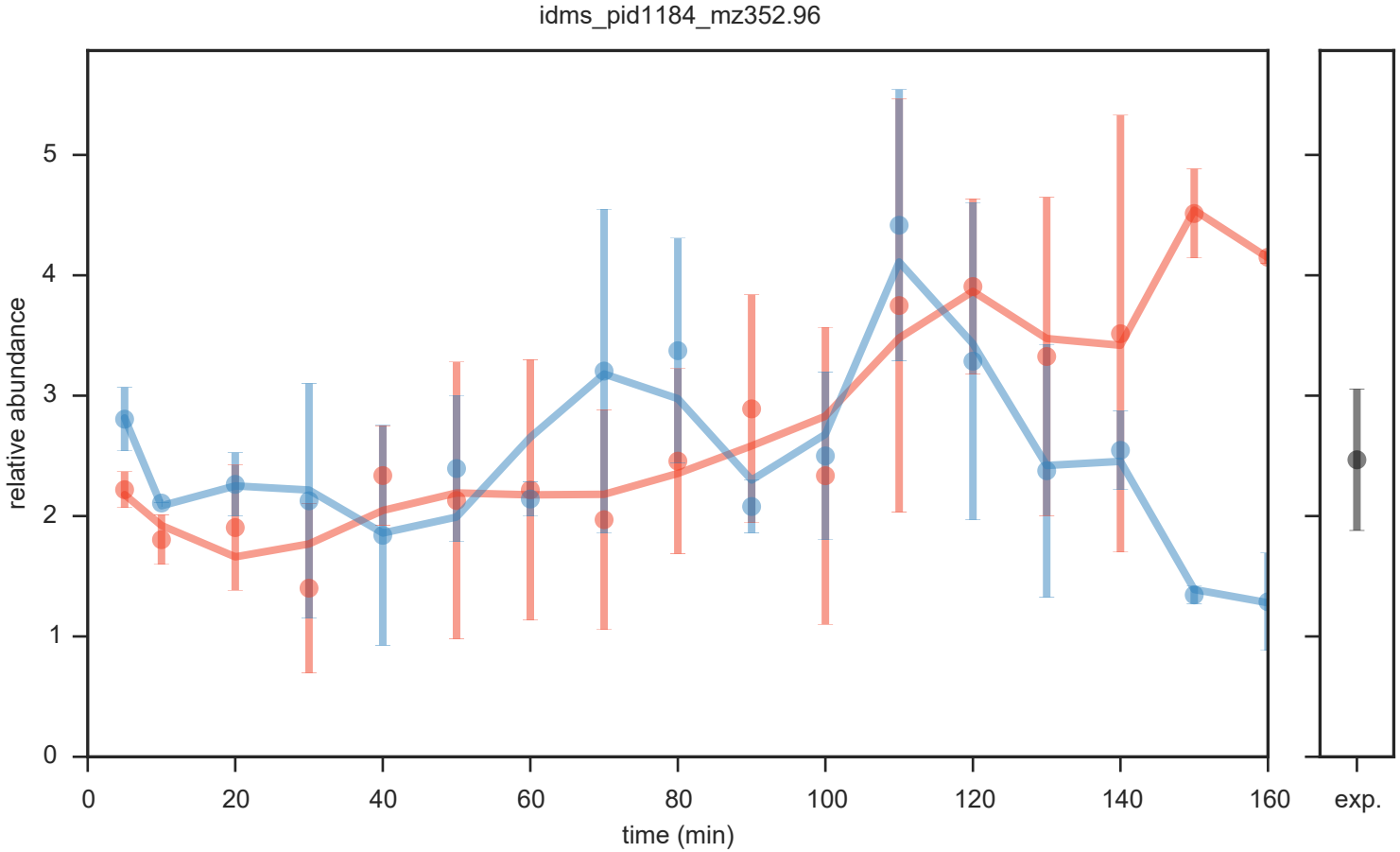

idms_pid1135_mz173.71
relative abundance
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

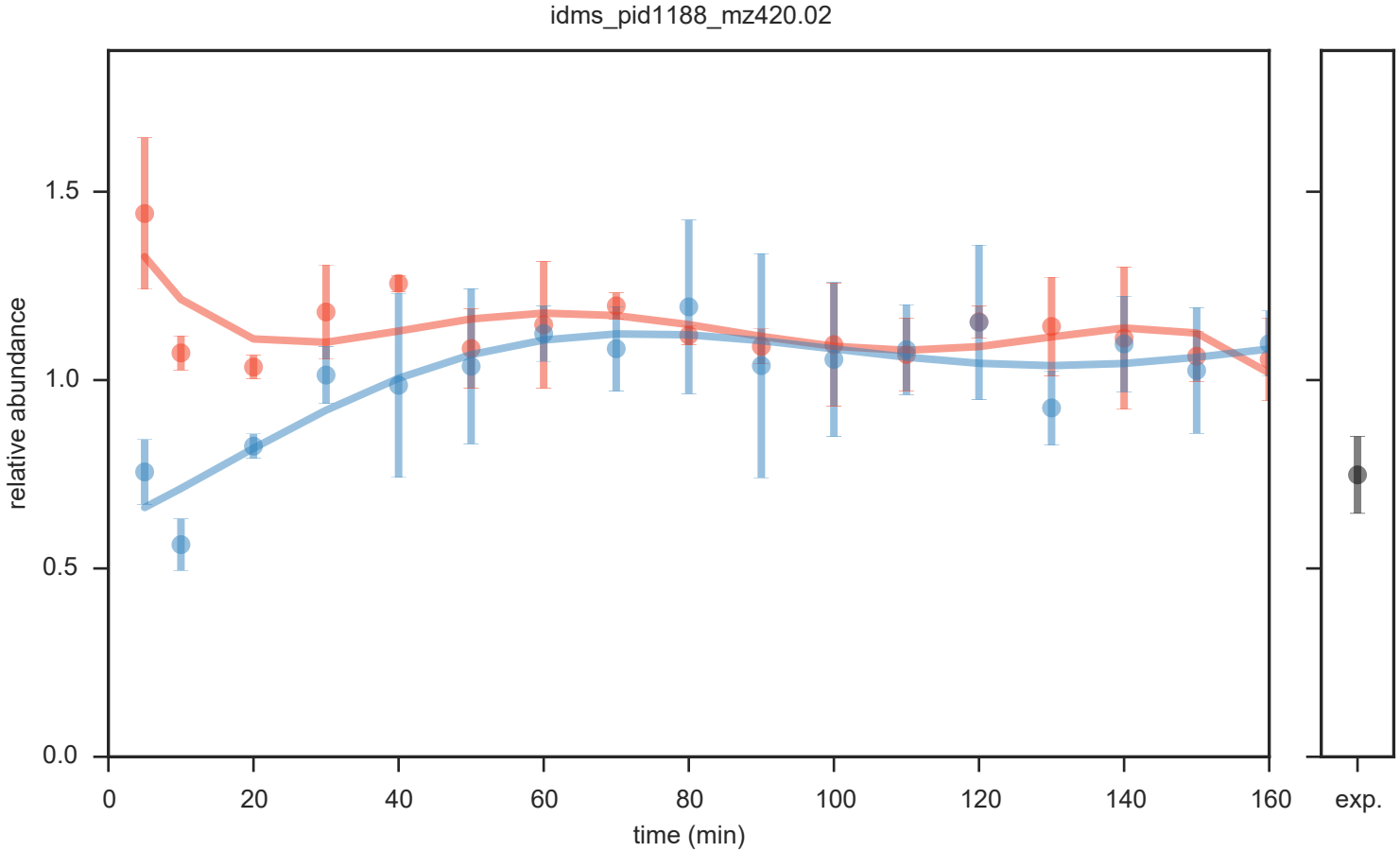

idms_pid1137_mz198.01
relative abundance
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

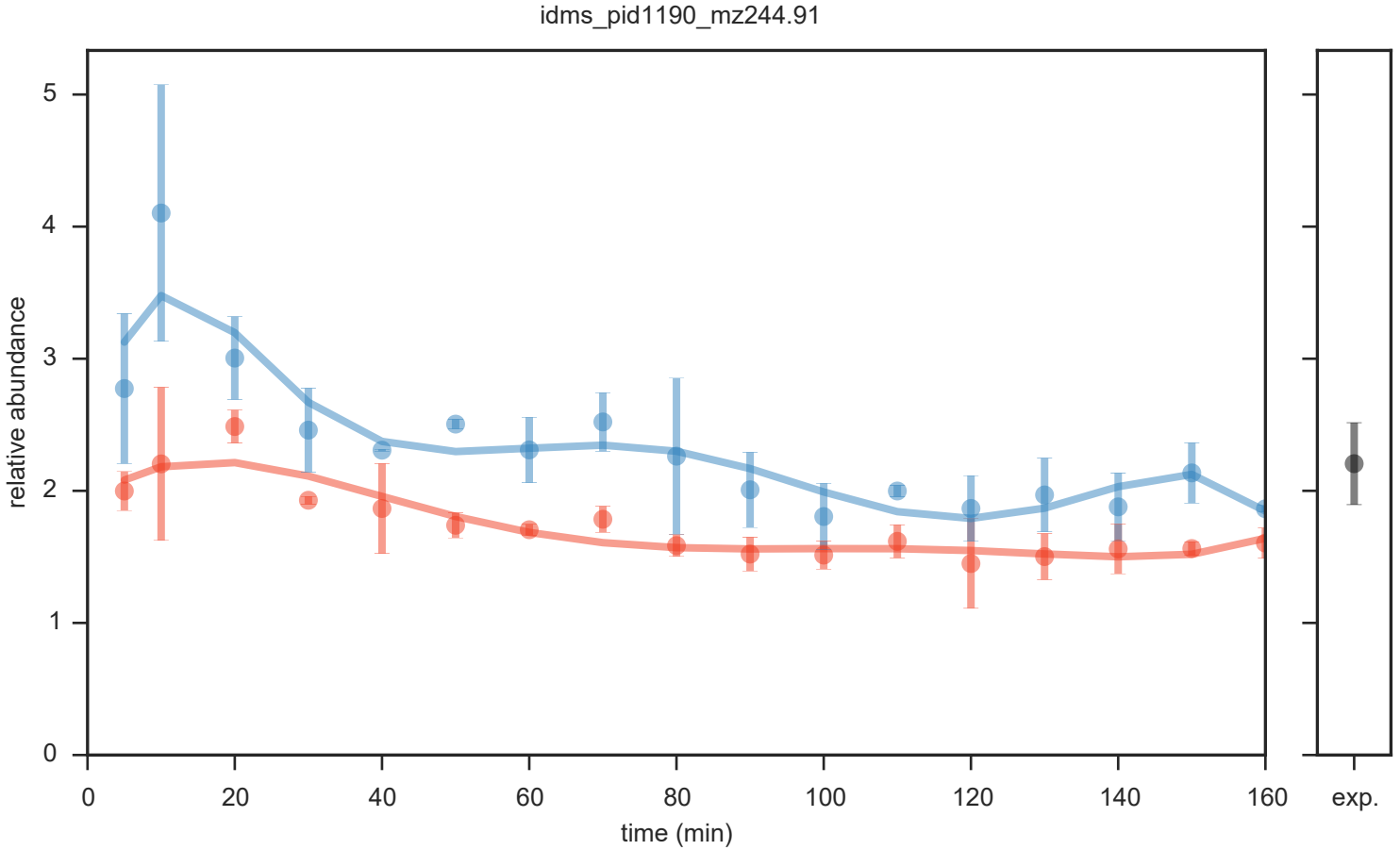

idms_pid1143_mz359.43
relative abundance
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

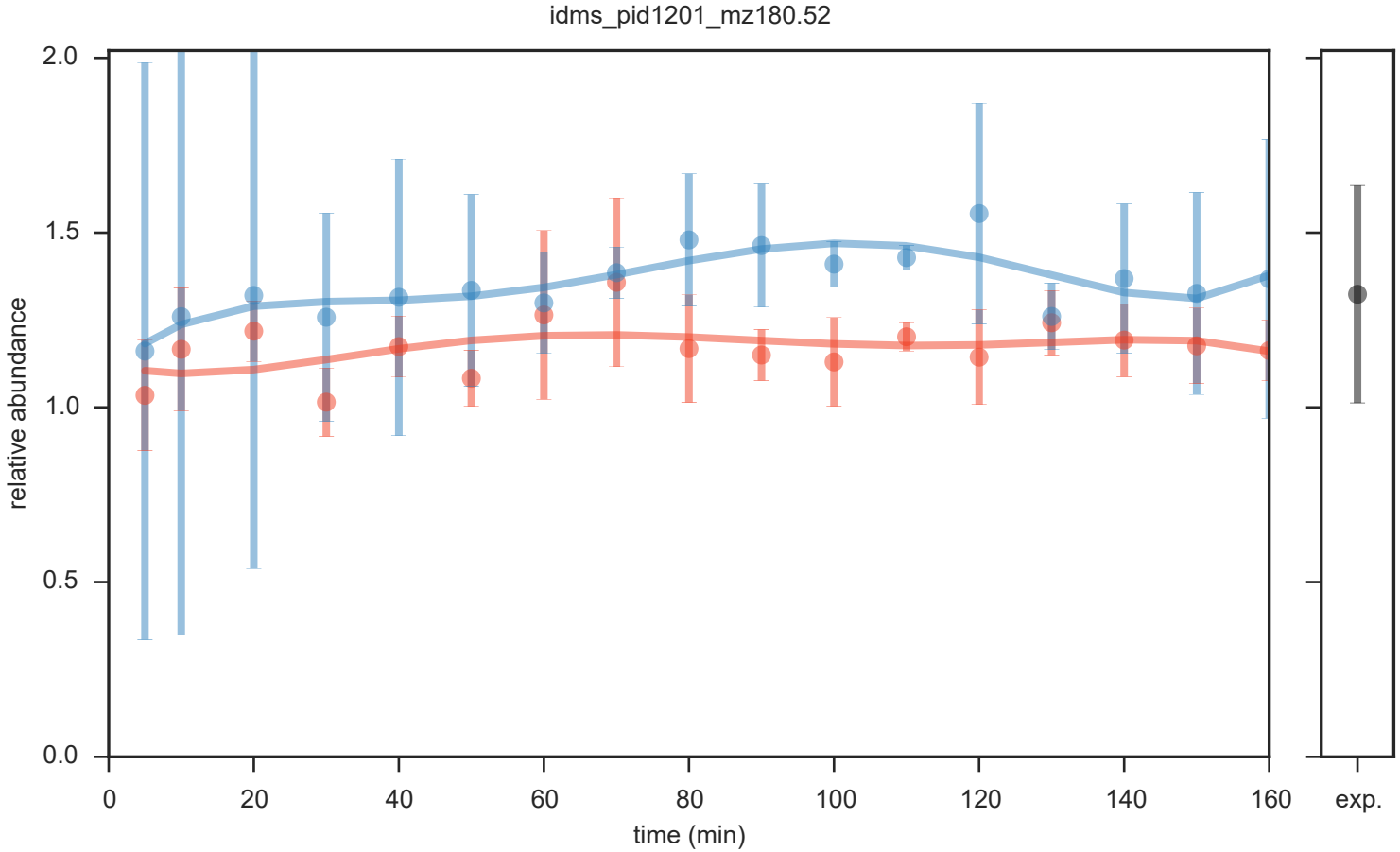

idms_pid1148_mz298.51
relative abundance
0.0
0.5
1.0
1.5
2.0
2.5
0
20
40
60
80
100
120
140
160
time (min)
exp.

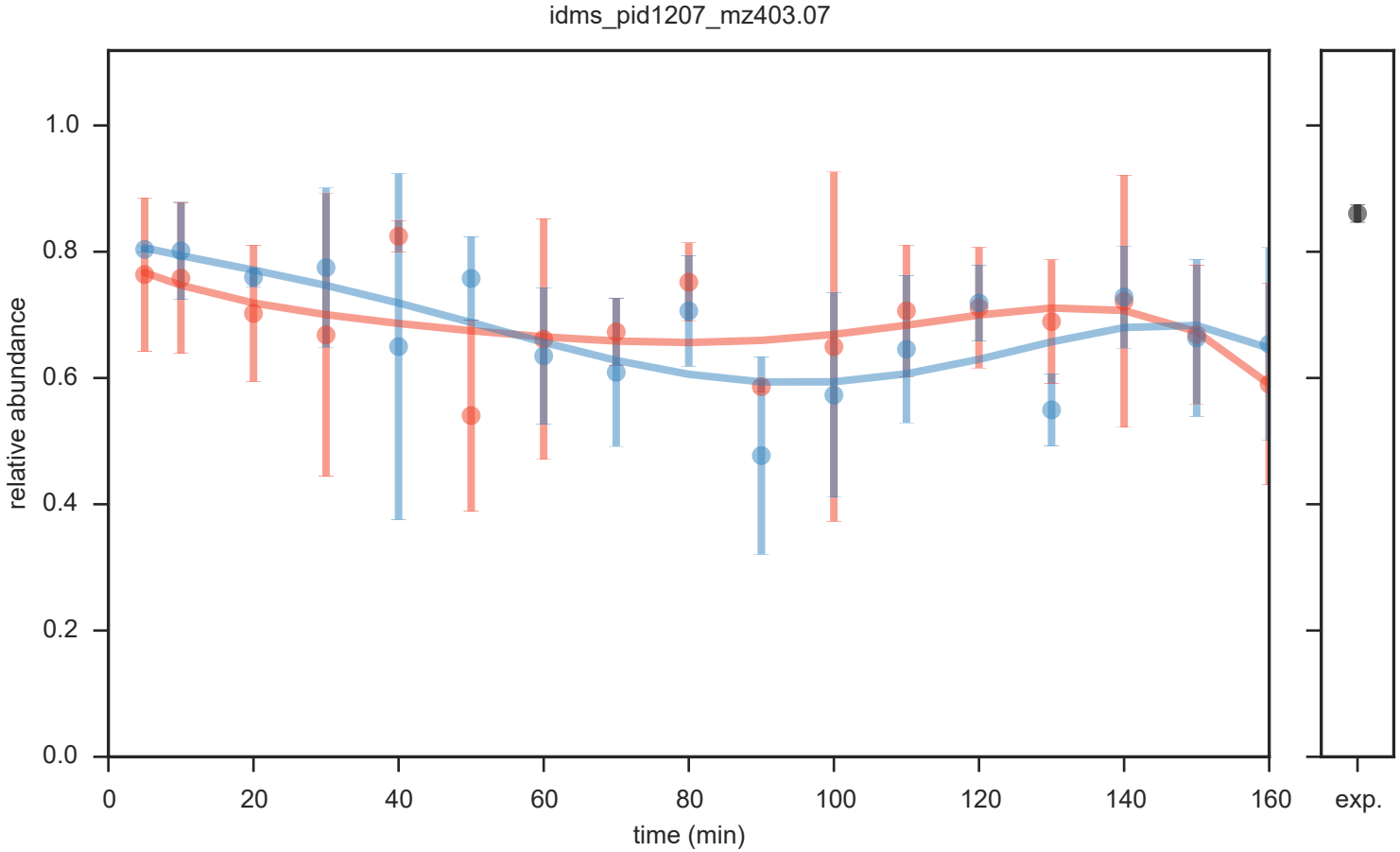

idms_pid1181_mz198.99
relative abundance
0.0
0.5
1.0
1.5
2.0
2.5
0
20
40
60
80
100
120
140
160
time (min)
exp.

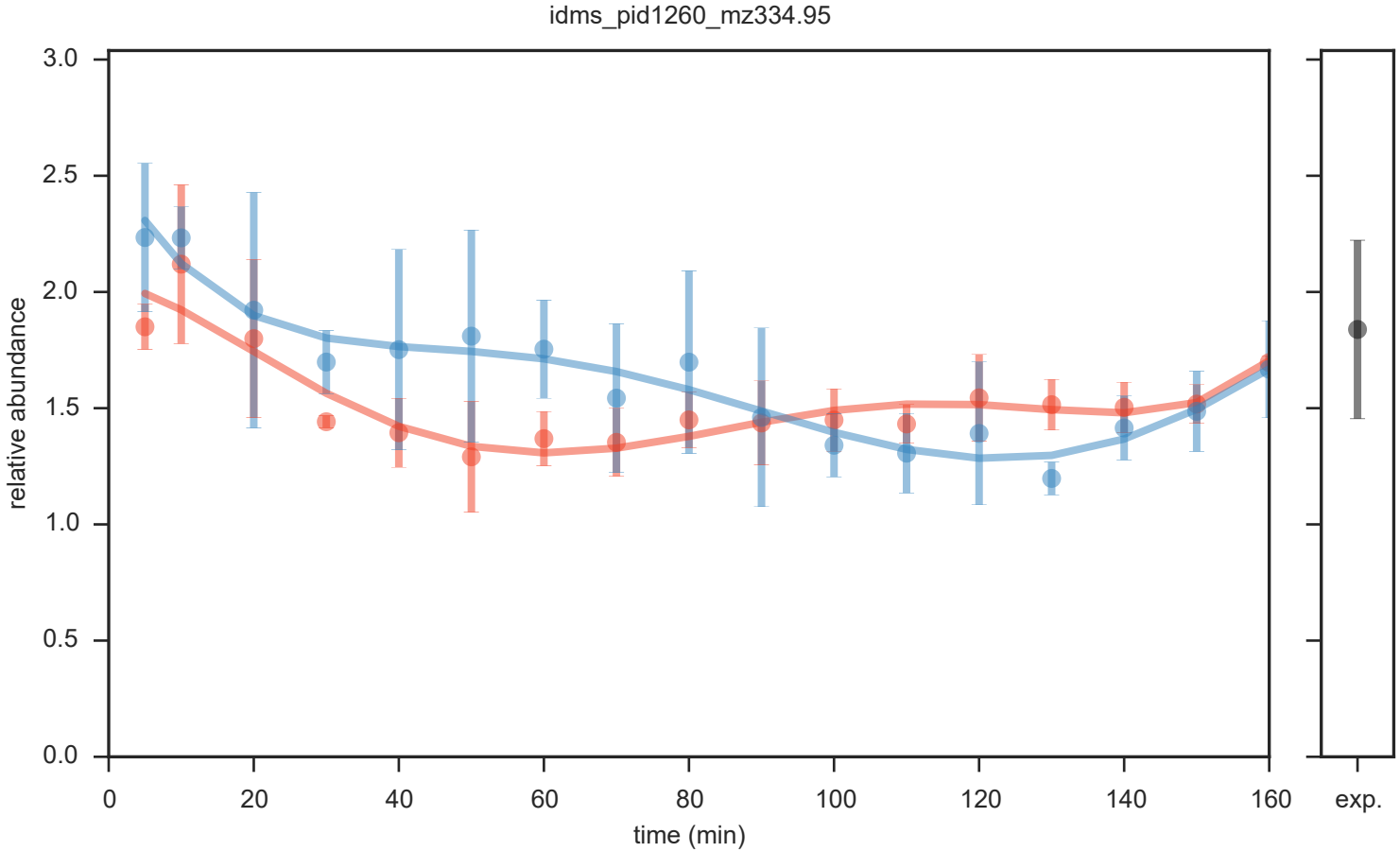

idms_pid1184_mz352.96
relative abundance
0
1
2
3
4
5
0
20
40
60
80
100
120
140
160
time (min)
exp.

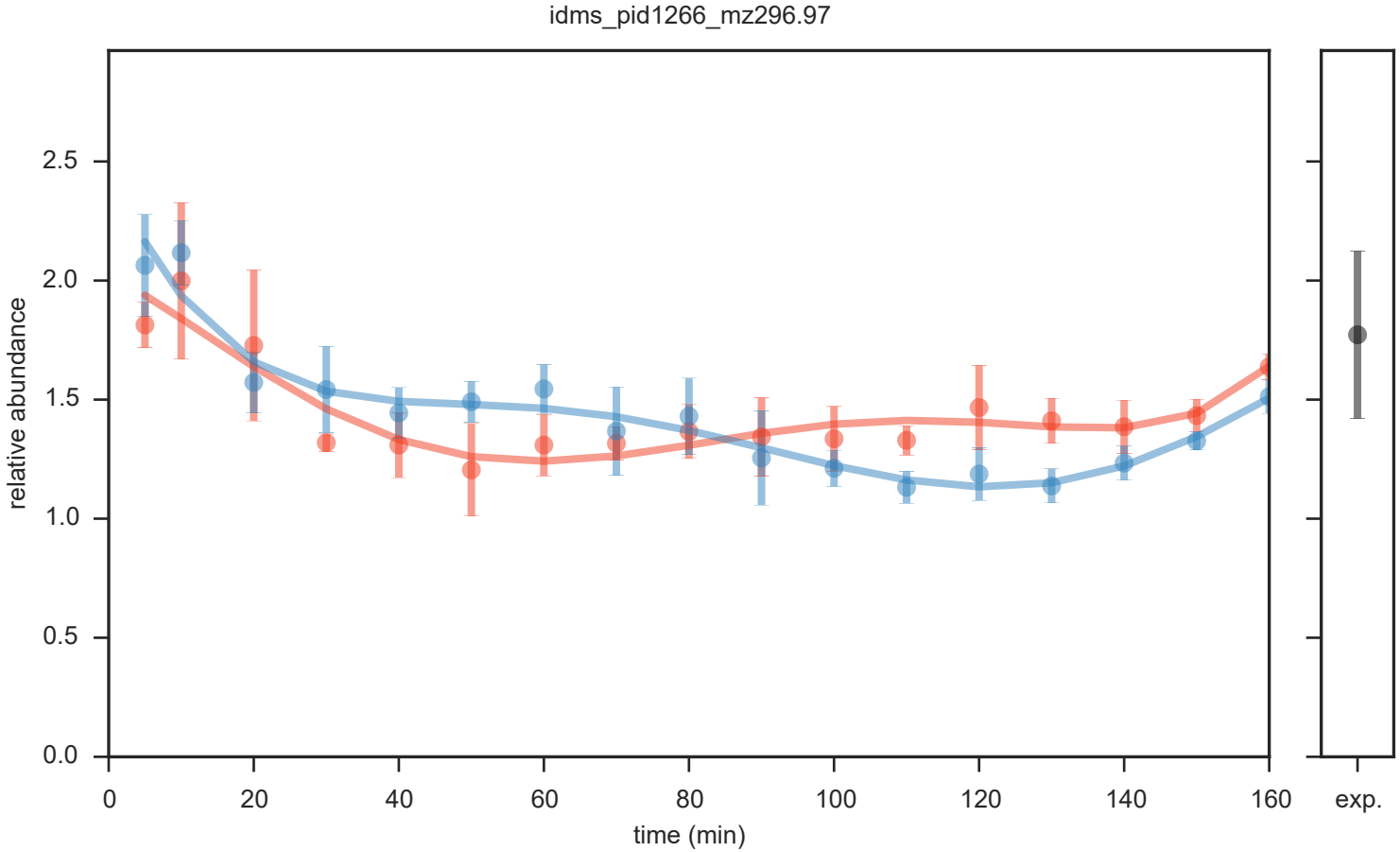

idms_pid1188_mz420.02
relative abundance
0.0
0.5
1.0
1.5
0
20
40
60
80
100
120
140
160
time (min)
exp.

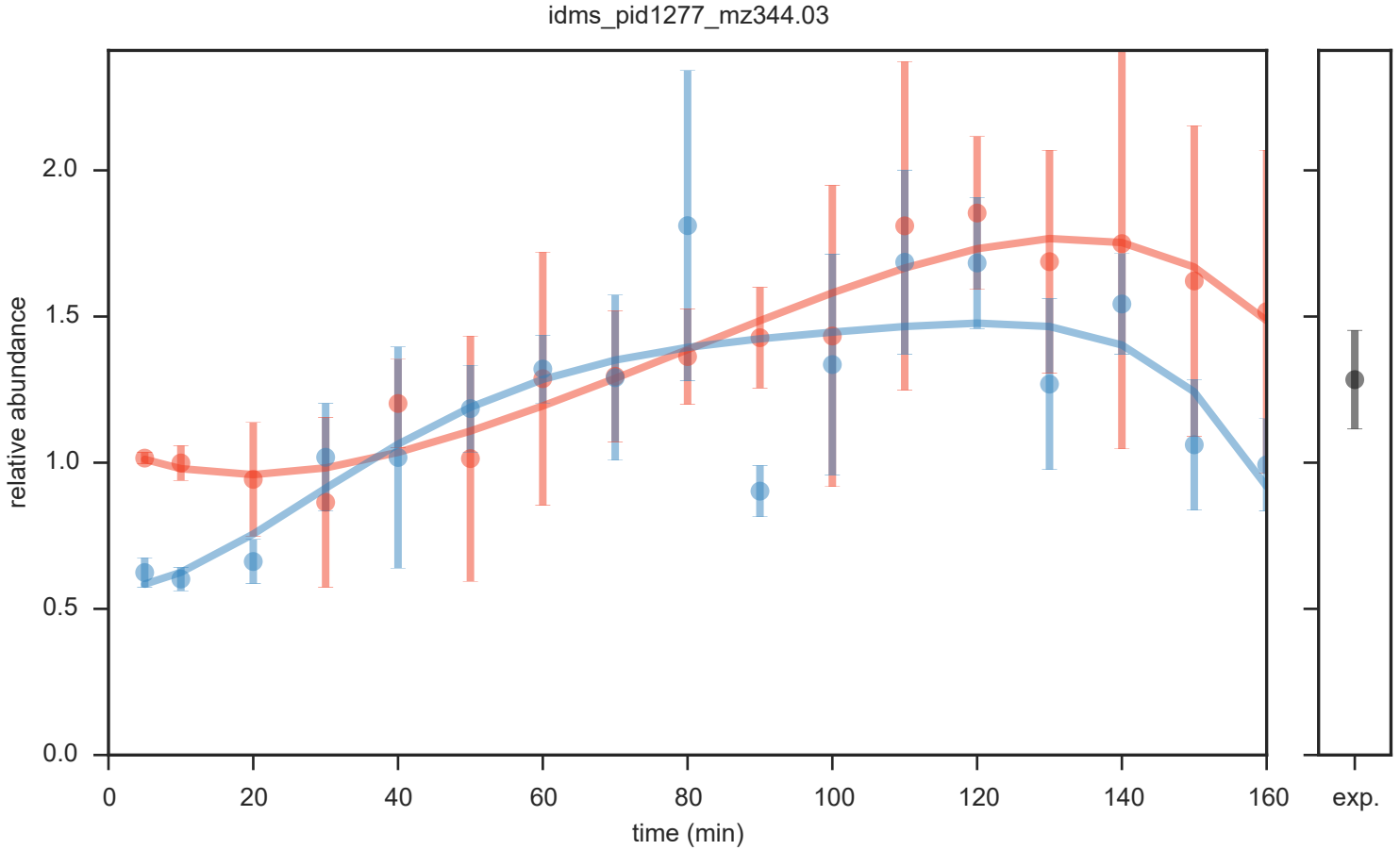

idms_pid1190_mz244.91
relative abundance
0
1
2
3
4
5
0
20
40
60
80
100
120
140
160
time (min)
exp.

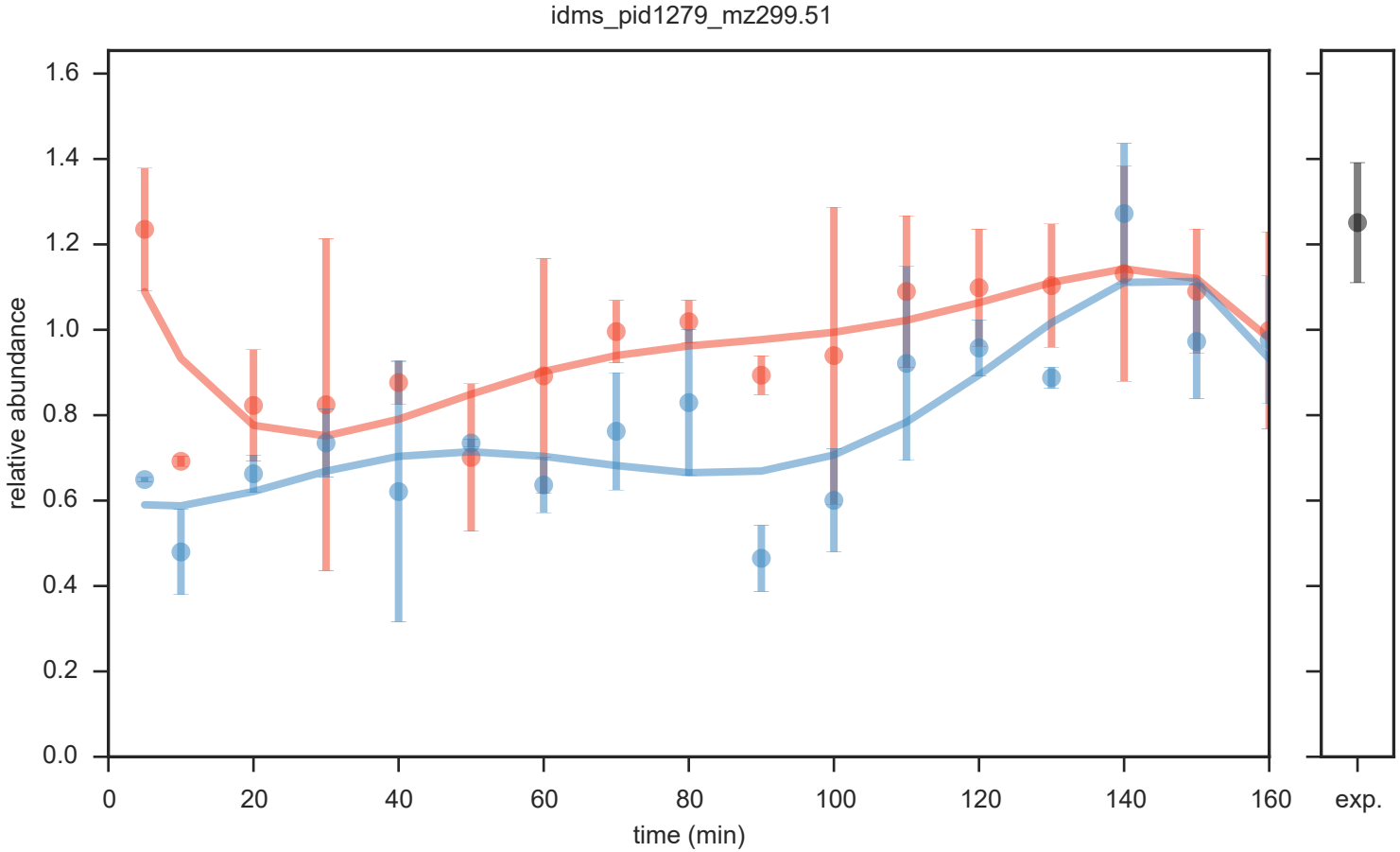

idms_pid1201_mz180.52
relative abundance
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

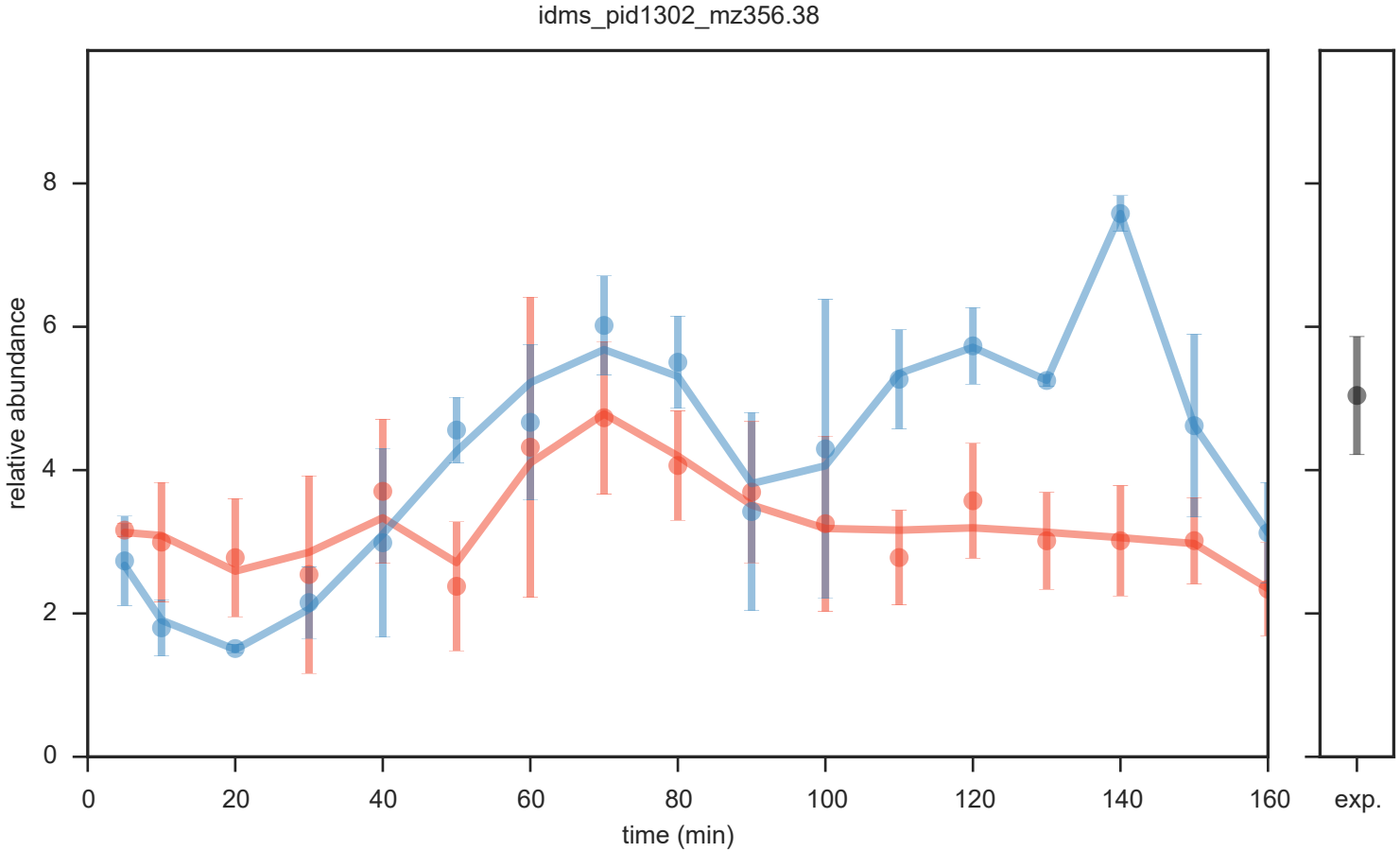

idms_pid1207_mz403.07
relative abundance
1.0
0.8
0.6
0.4
0.2
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

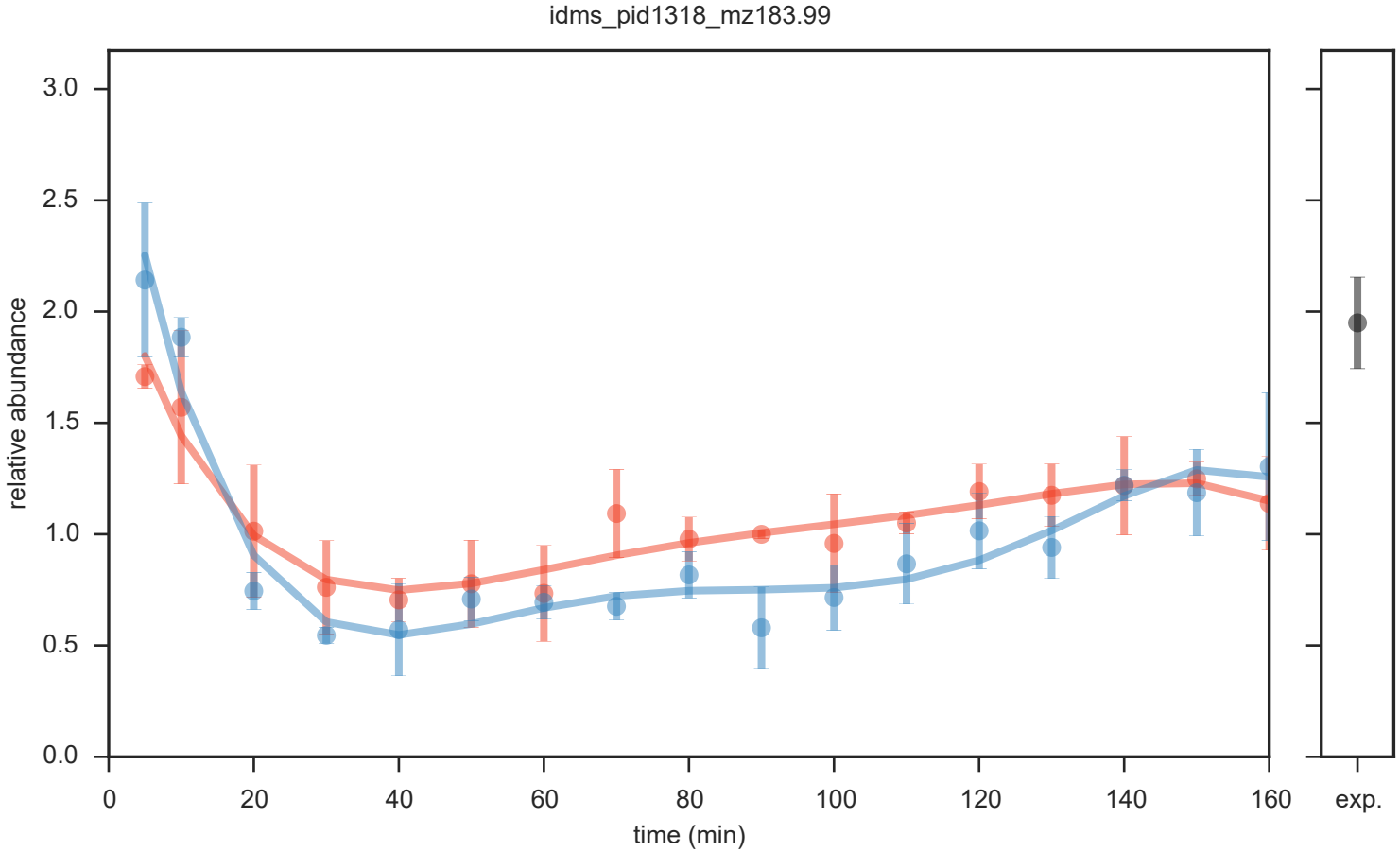

idms_pid1260_mz334.95
relative abundance
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

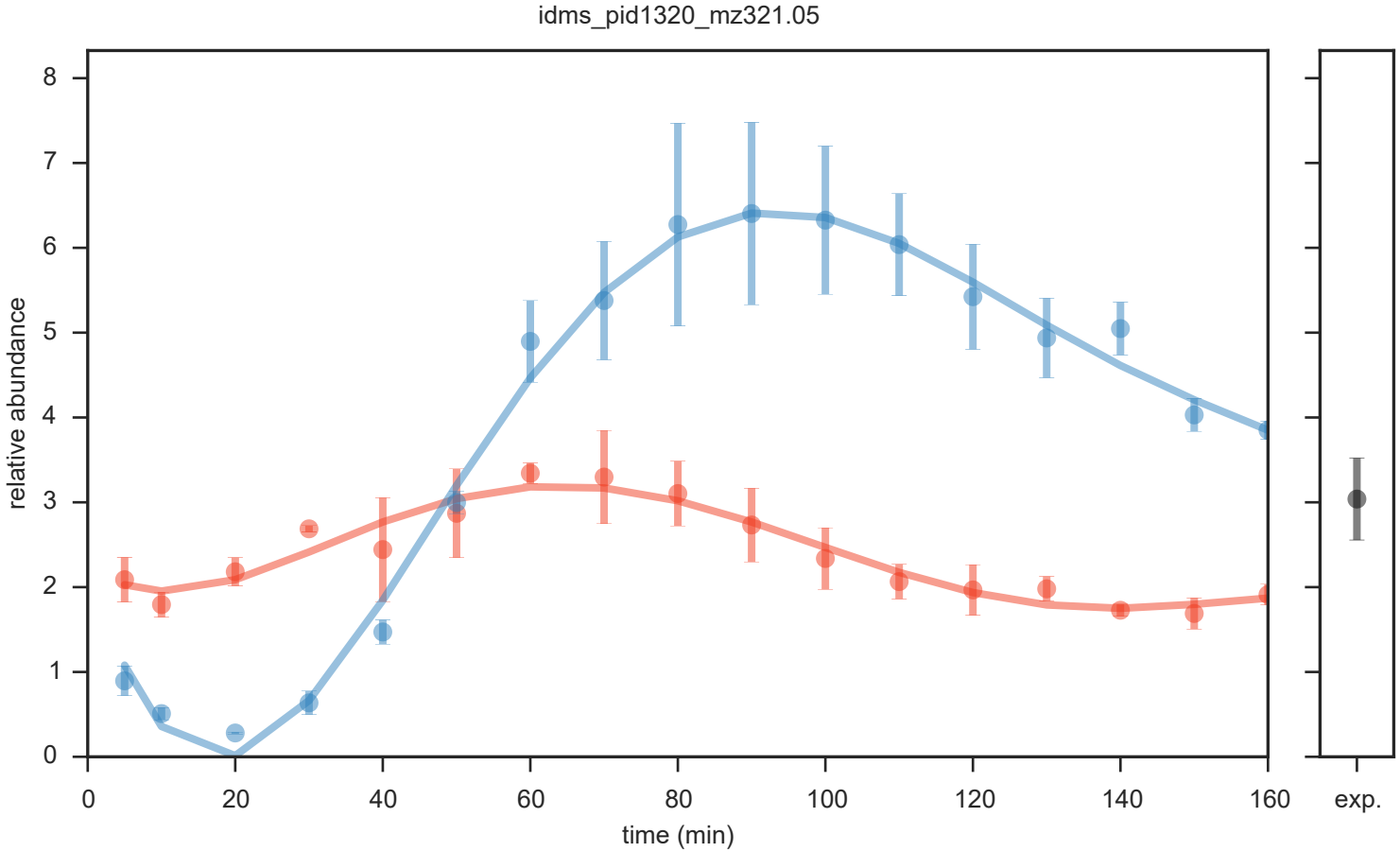

idms_pid1266_mz296.97
relative abundance
0.0
0.5
1.0
1.5
2.0
2.5
0
20
40
60
80
100
120
140
160
time (min)
exp.

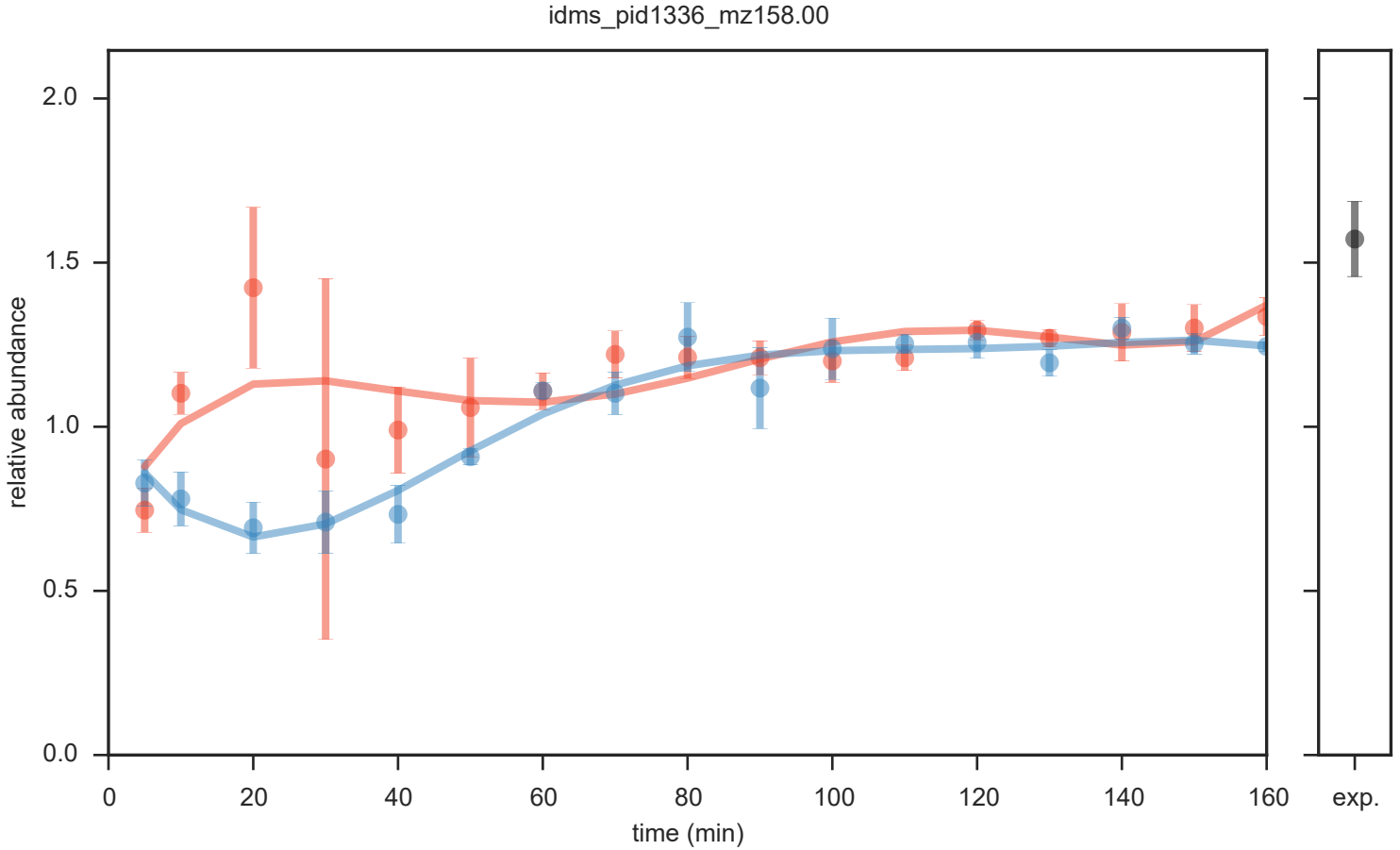

idms_pid1277_mz344.03
relative abundance
0.0
0.5
1.0
1.5
2.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

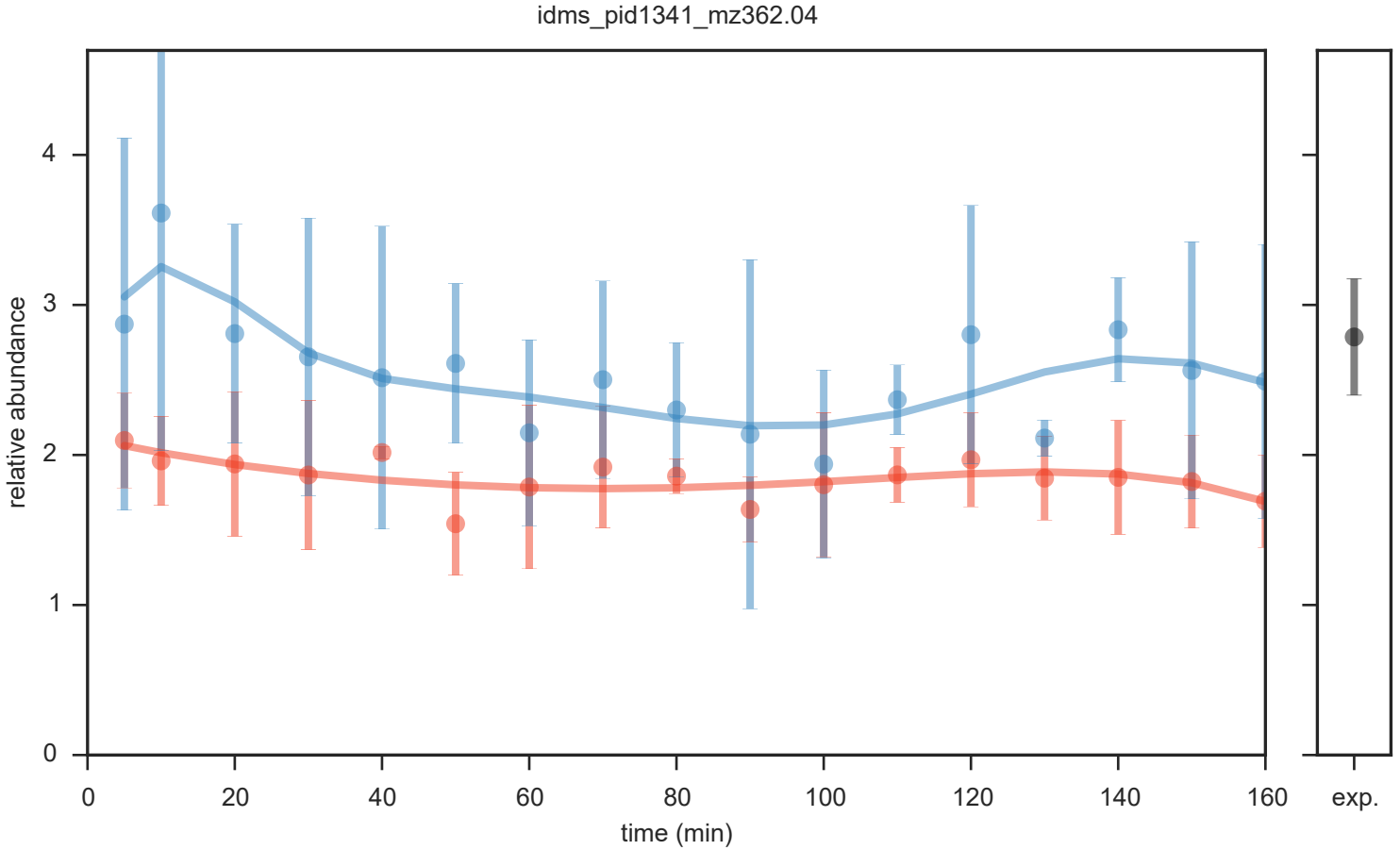

idms_pid1279_mz299.51
relative abundance
time (min)
exp.
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
0
20
40
60
80
100
120
140
160

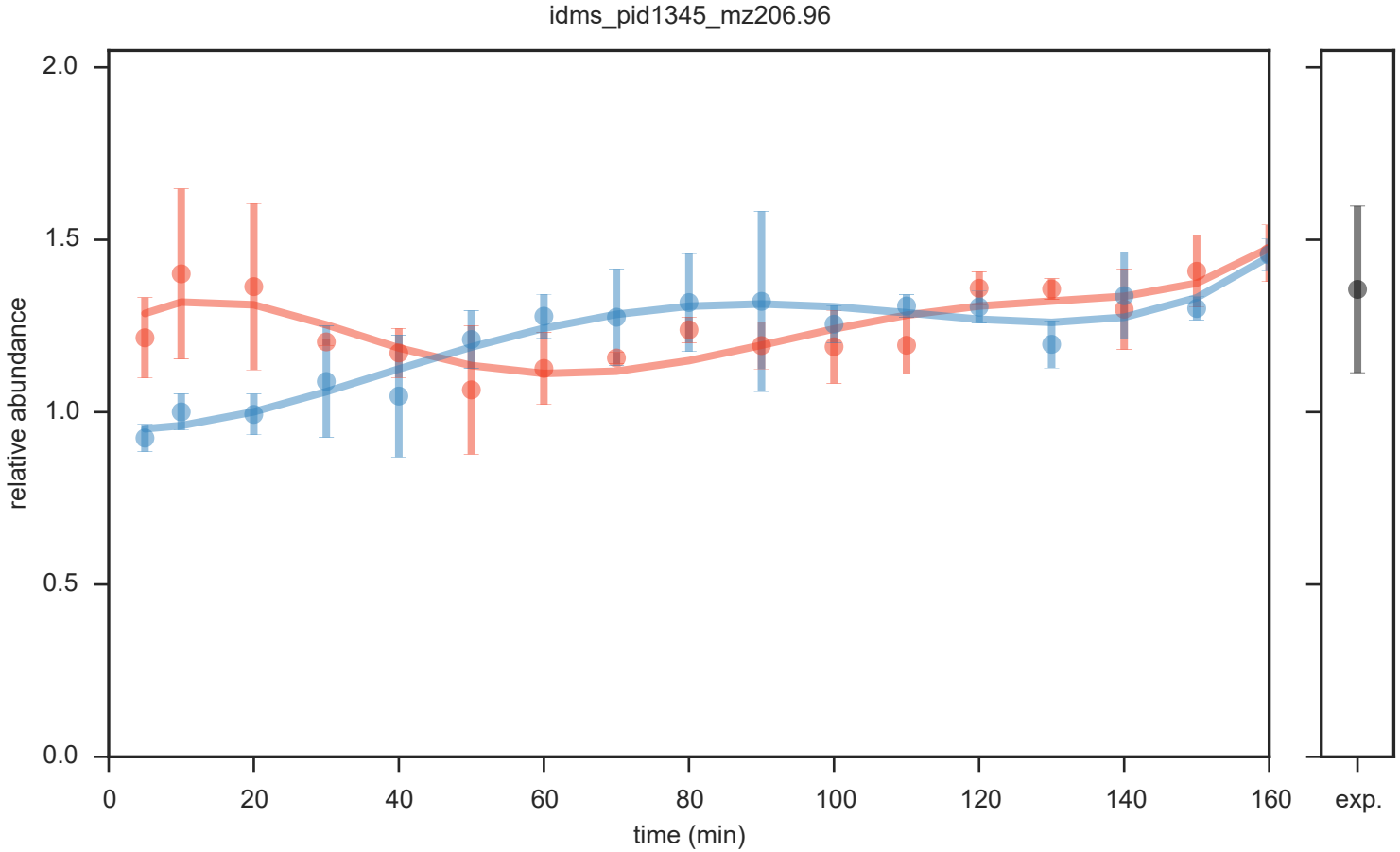

idms_pid1302_mz356.38
relative abundance
0
2
4
6
8
0
20
40
60
80
100
120
140
160
time (min)
exp.

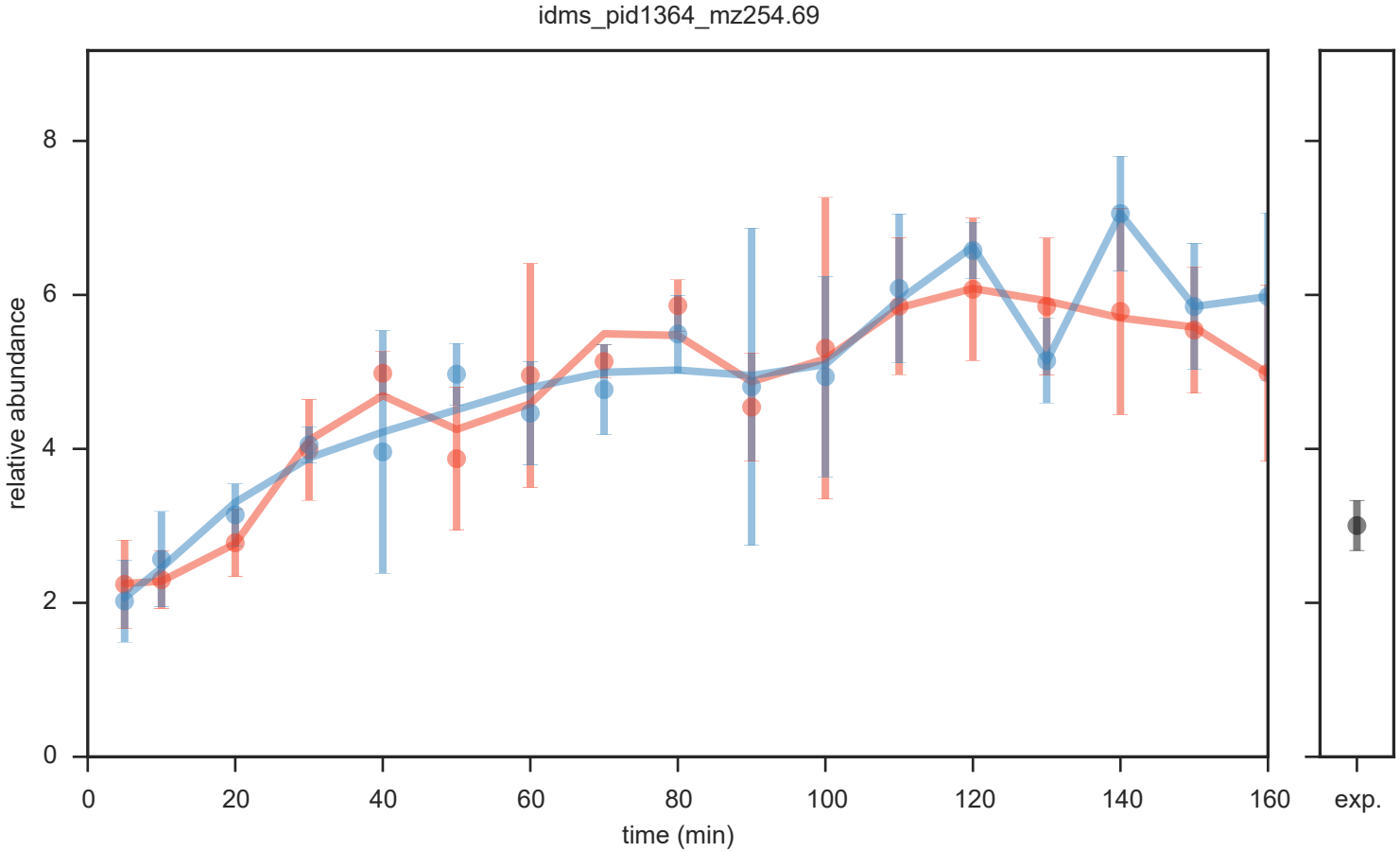

idms_pid1318_mz183.99
relative abundance
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

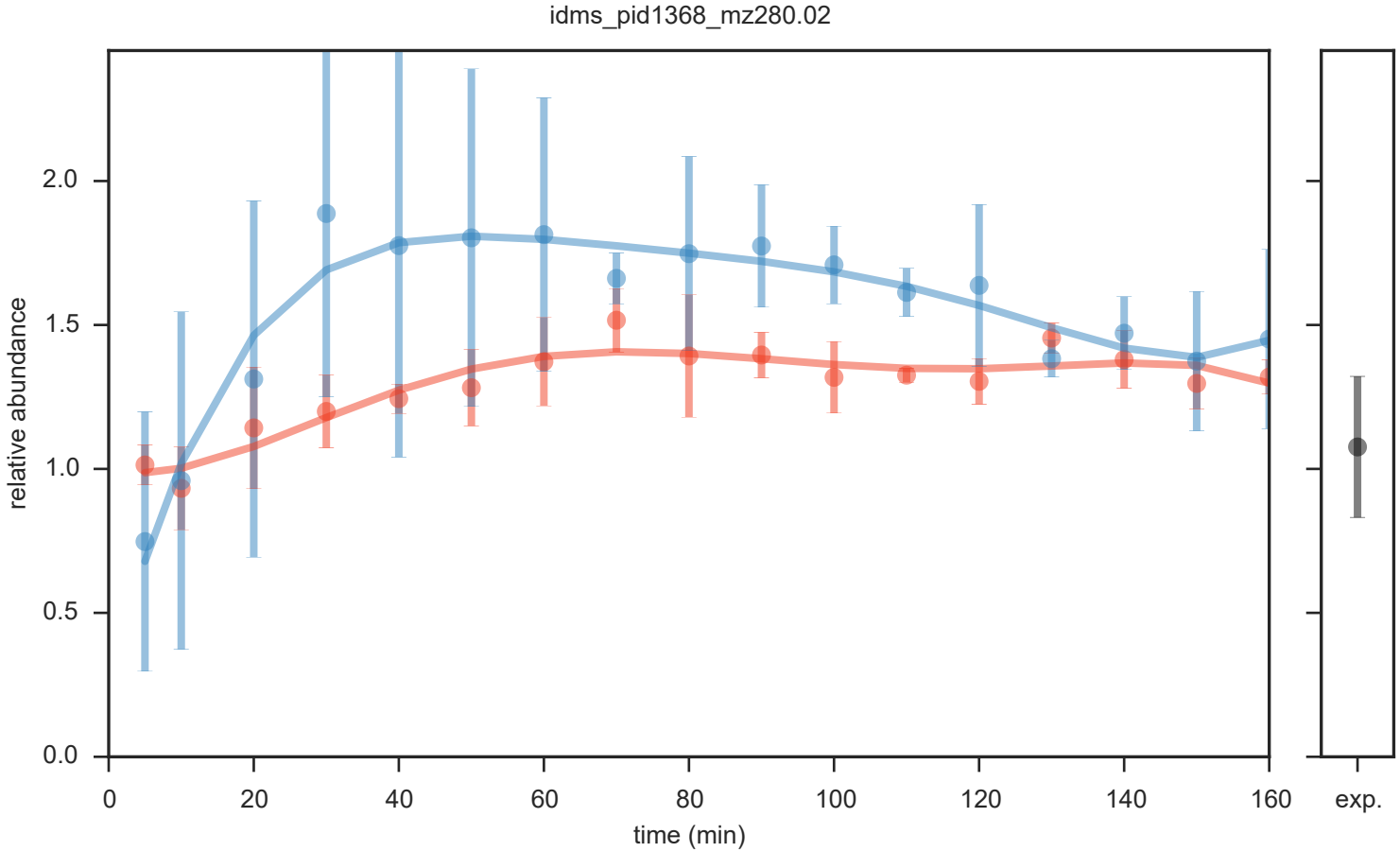

idms_pid1320_mz321.05
relative abundance
0
1
2
3
4
5
6
7
8
0
20
40
60
80
100
120
140
160
time (min)
exp.

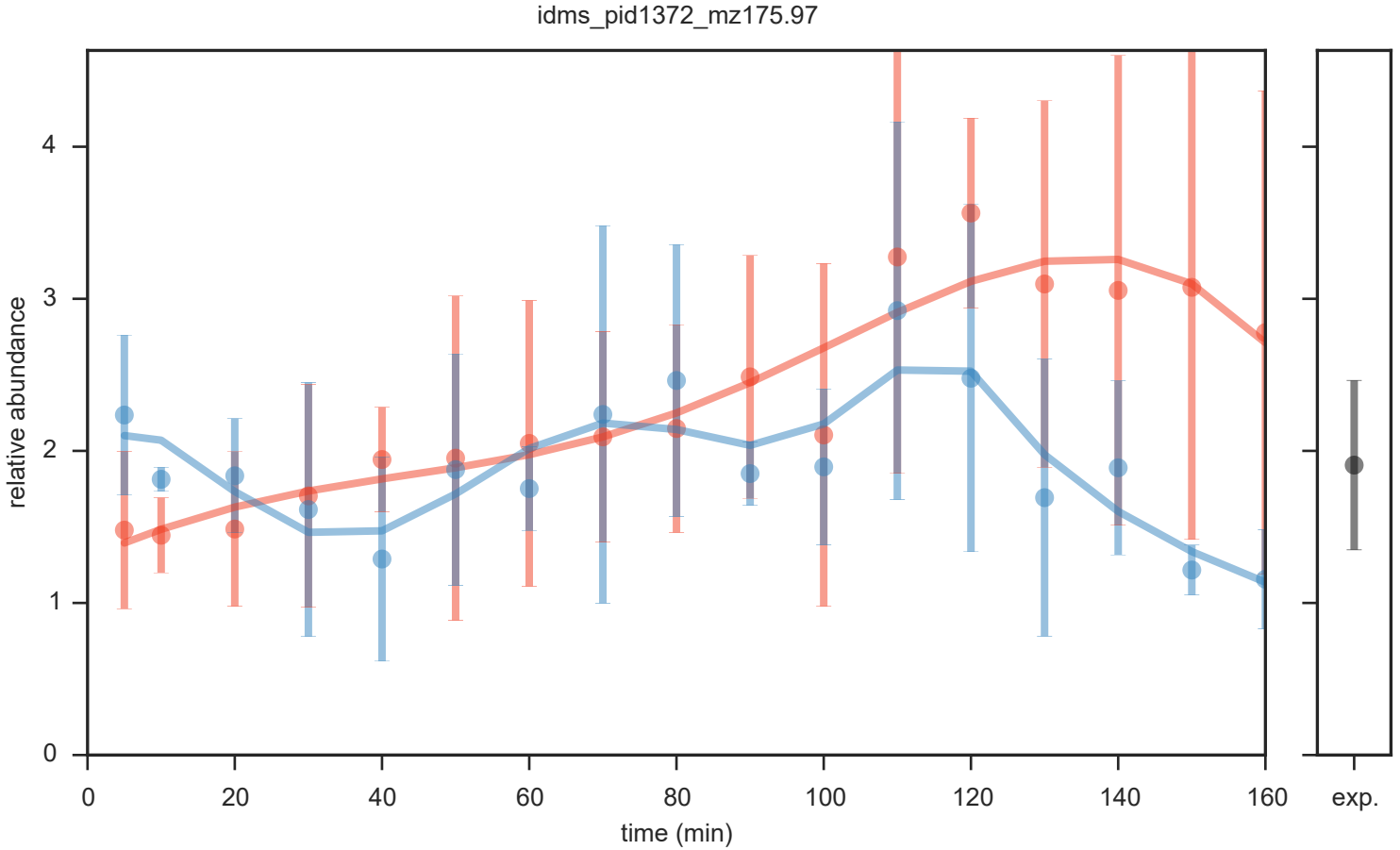

idms_pid1336_mz158.00
relative abundance
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

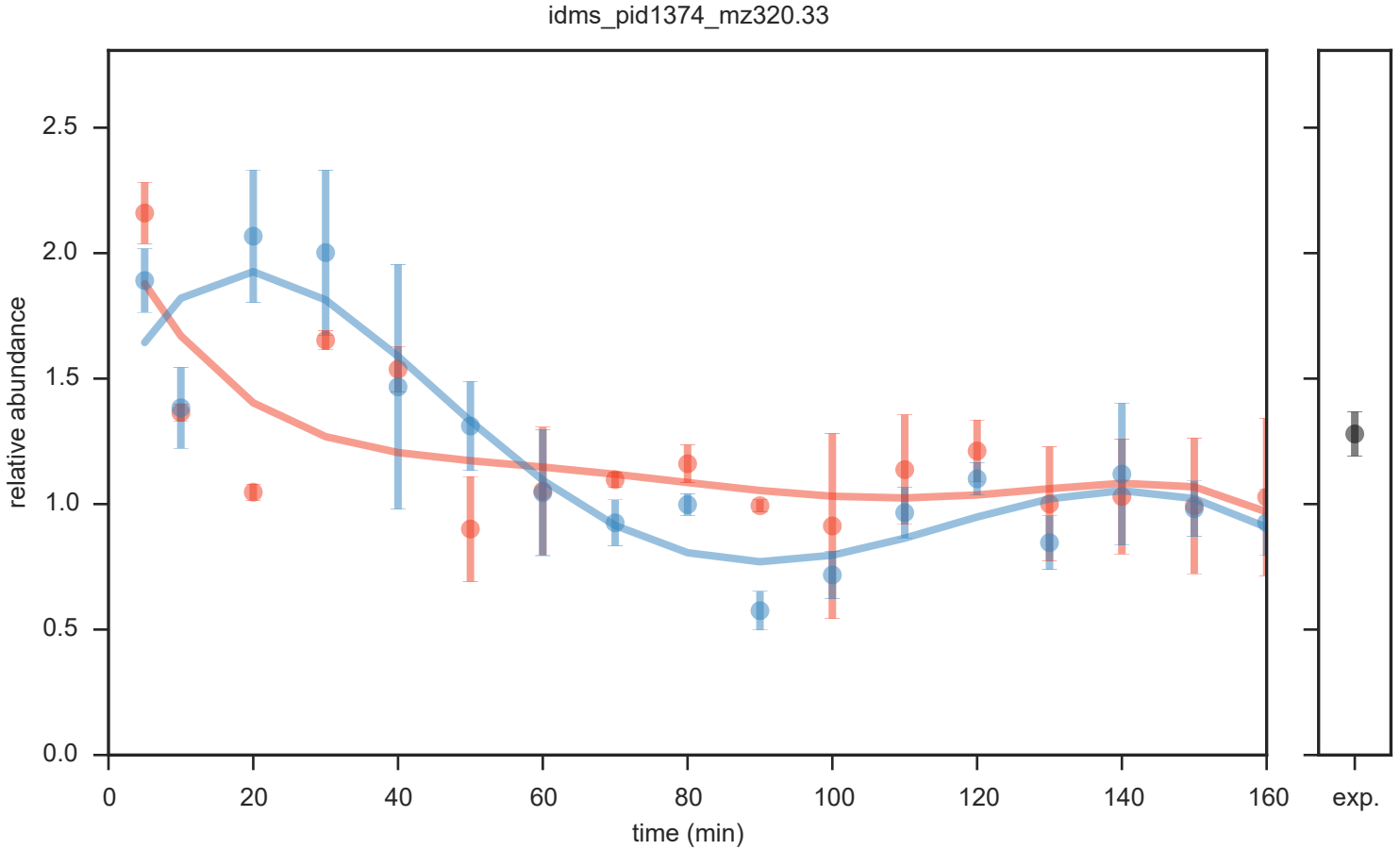

idms_pid1341_mz362.04
relative abundance
0
1
2
3
4
0
20
40
60
80
100
120
140
160
time (min)
exp.

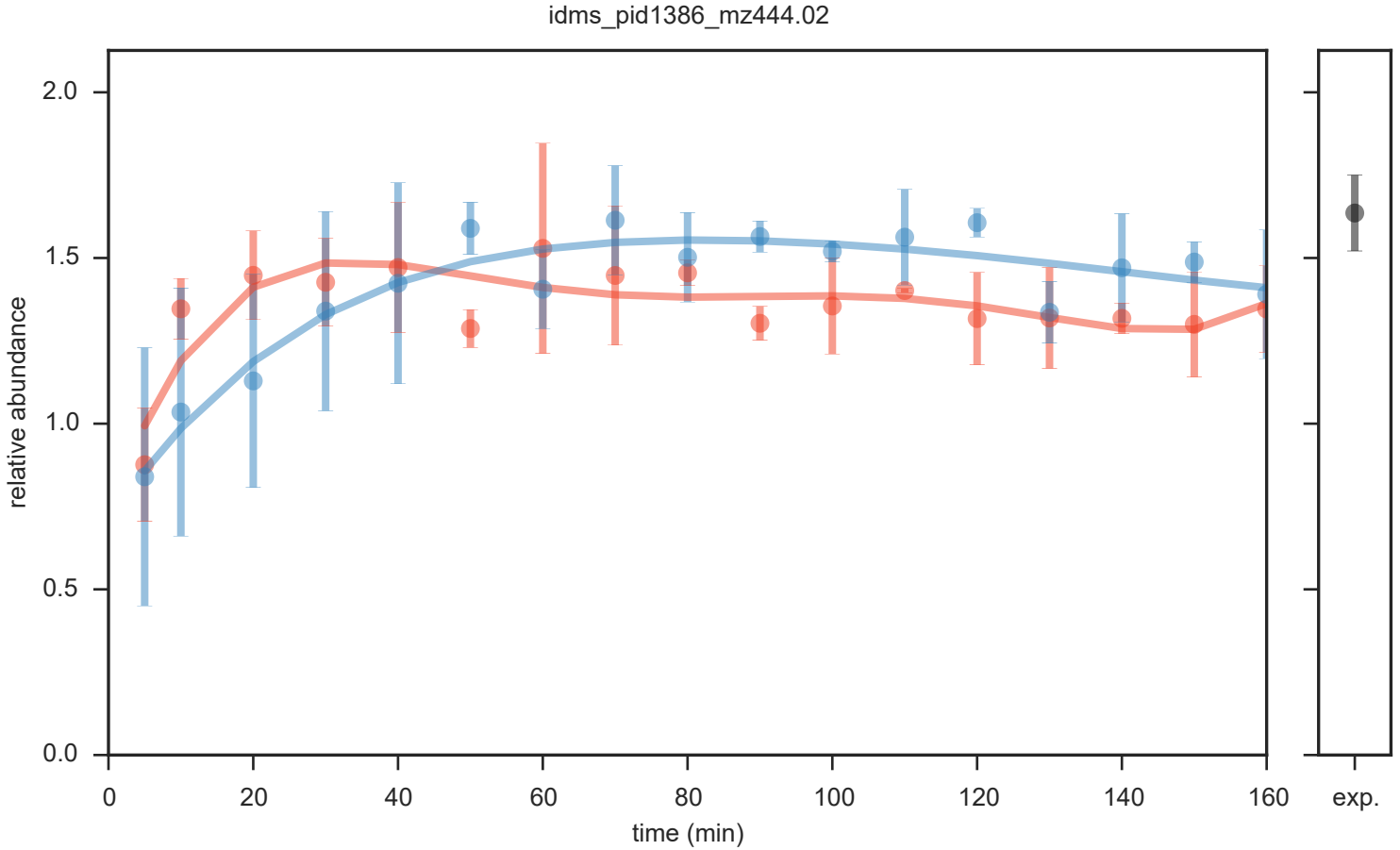

idms_pid1345_mz206.96
relative abundance
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

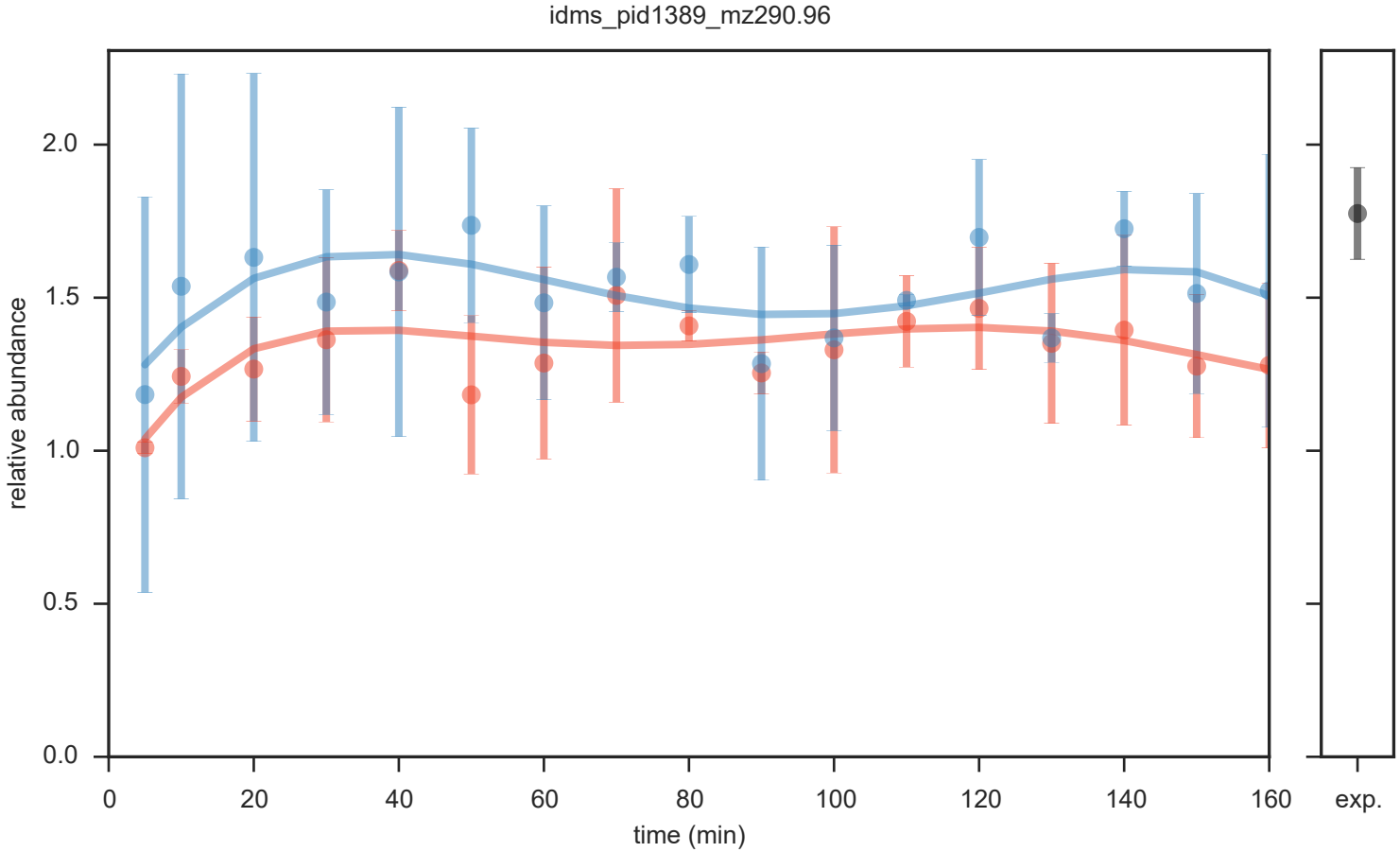

idms_pid1364_mz254.69
relative abundance
0
2
4
6
8
0
20
40
60
80
100
120
140
160
time (min)
exp.

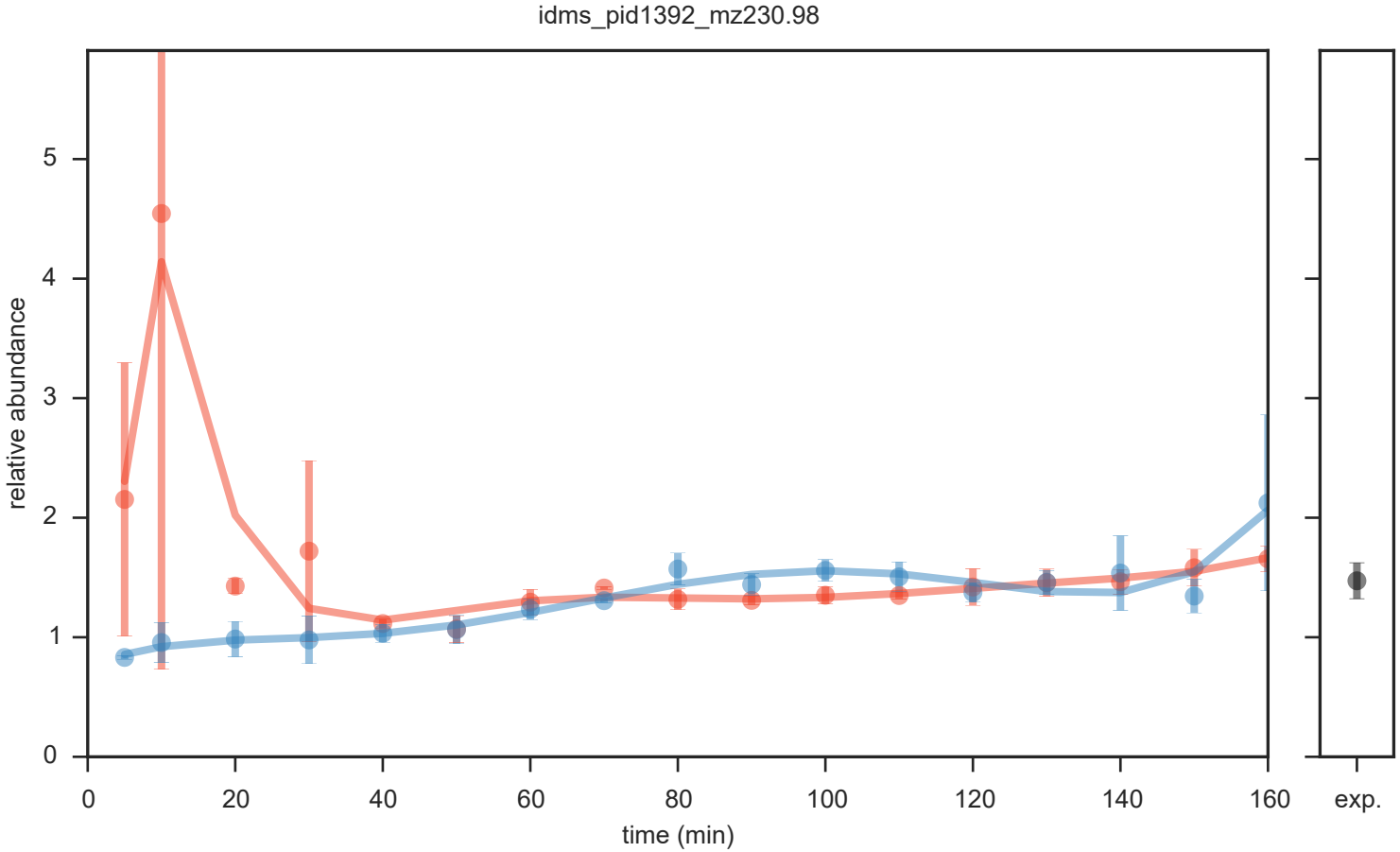

idms_pid1368_mz280.02
relative abundance
0.0
0.5
1.0
1.5
2.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

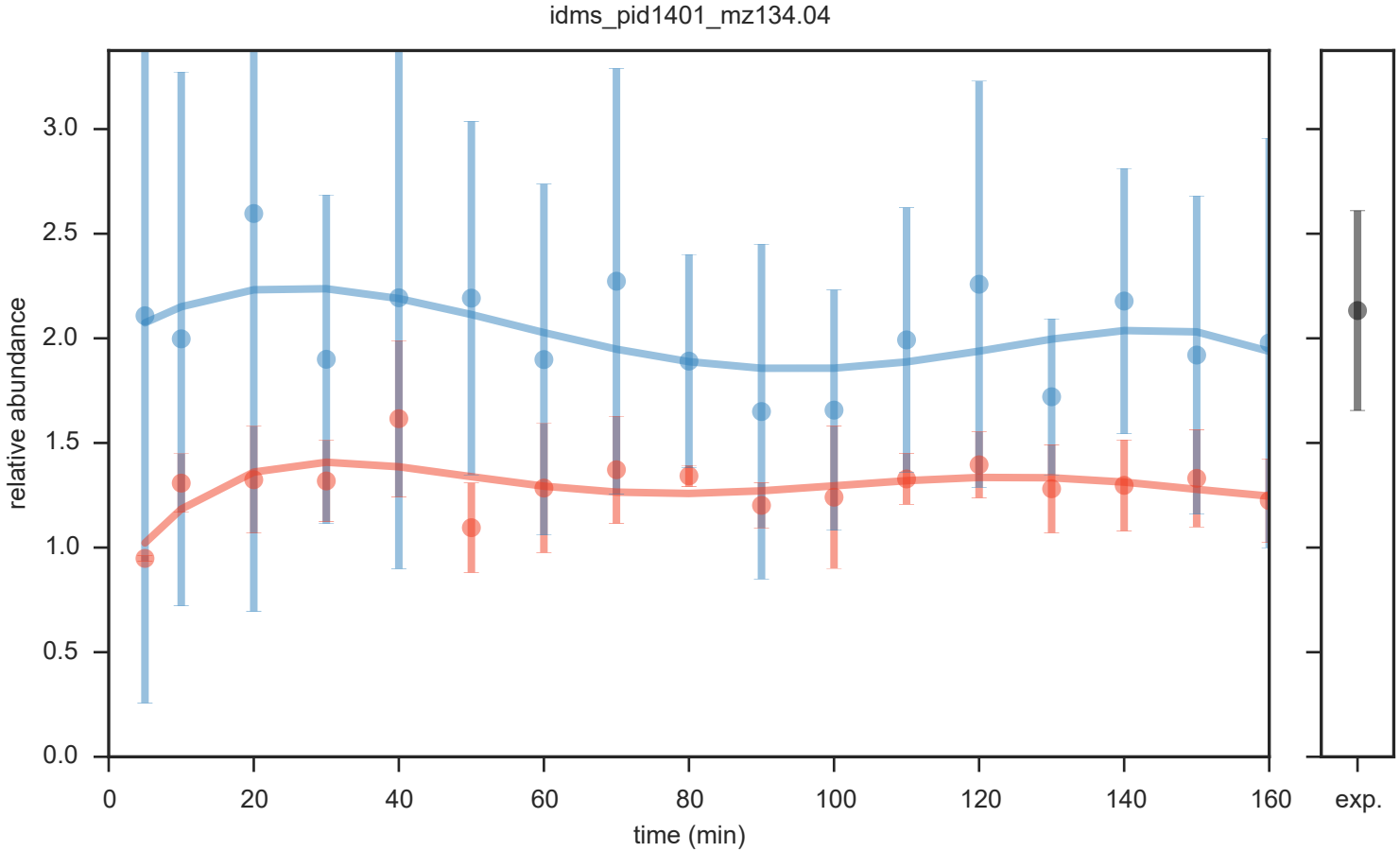

idms_pid1372_mz175.97
relative abundance
0
1
2
3
4
0
20
40
60
80
100
120
140
160
time (min)
exp.

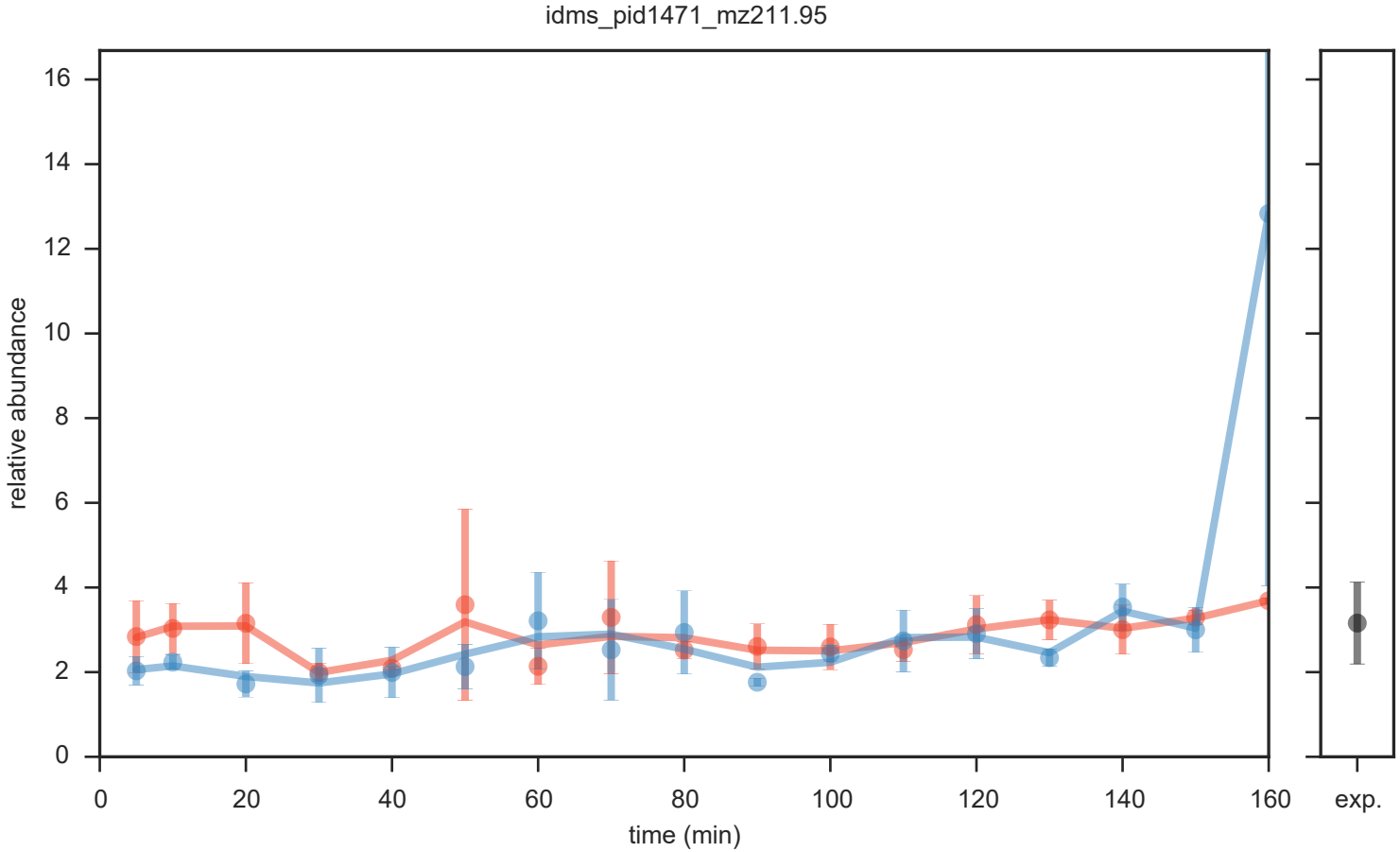

idms_pid1374_mz320.33
relative abundance
0.0
0.5
1.0
1.5
2.0
2.5
0
20
40
60
80
100
120
140
160
time (min)
exp.

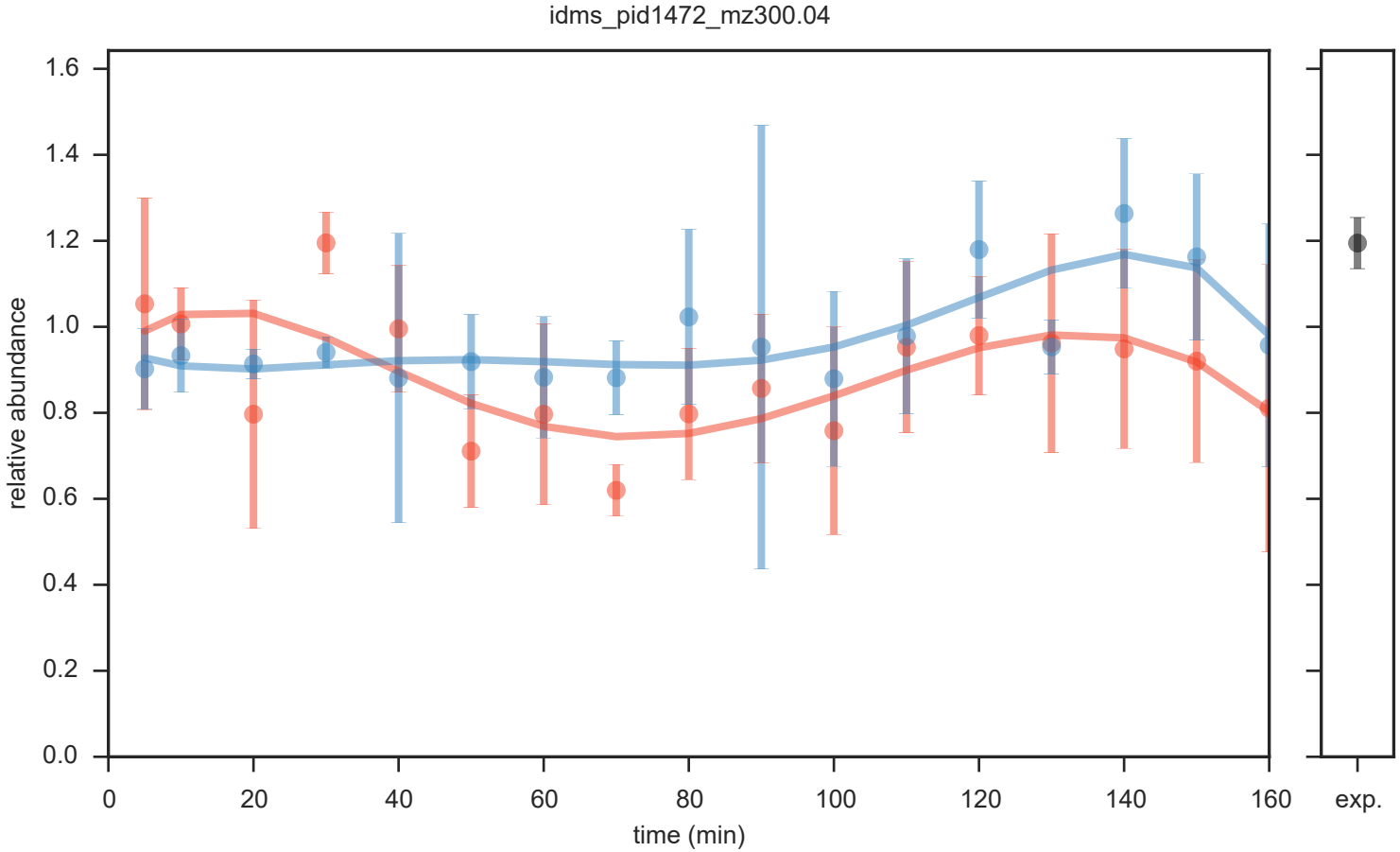

idms_pid1386_mz444.02
relative abundance
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

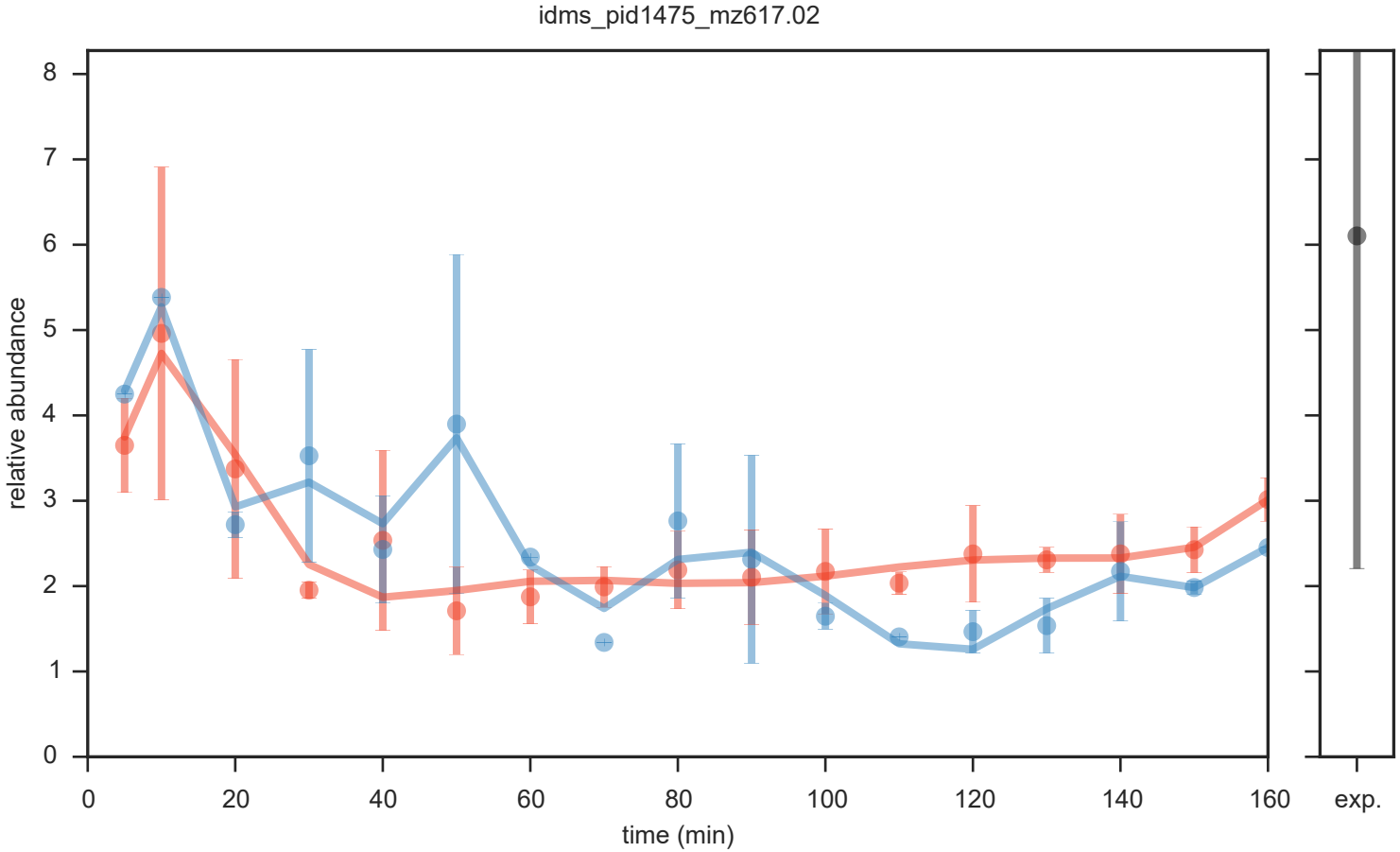

idms_pid1389_mz290.96
relative abundance
0.0
0.5
1.0
1.5
2.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

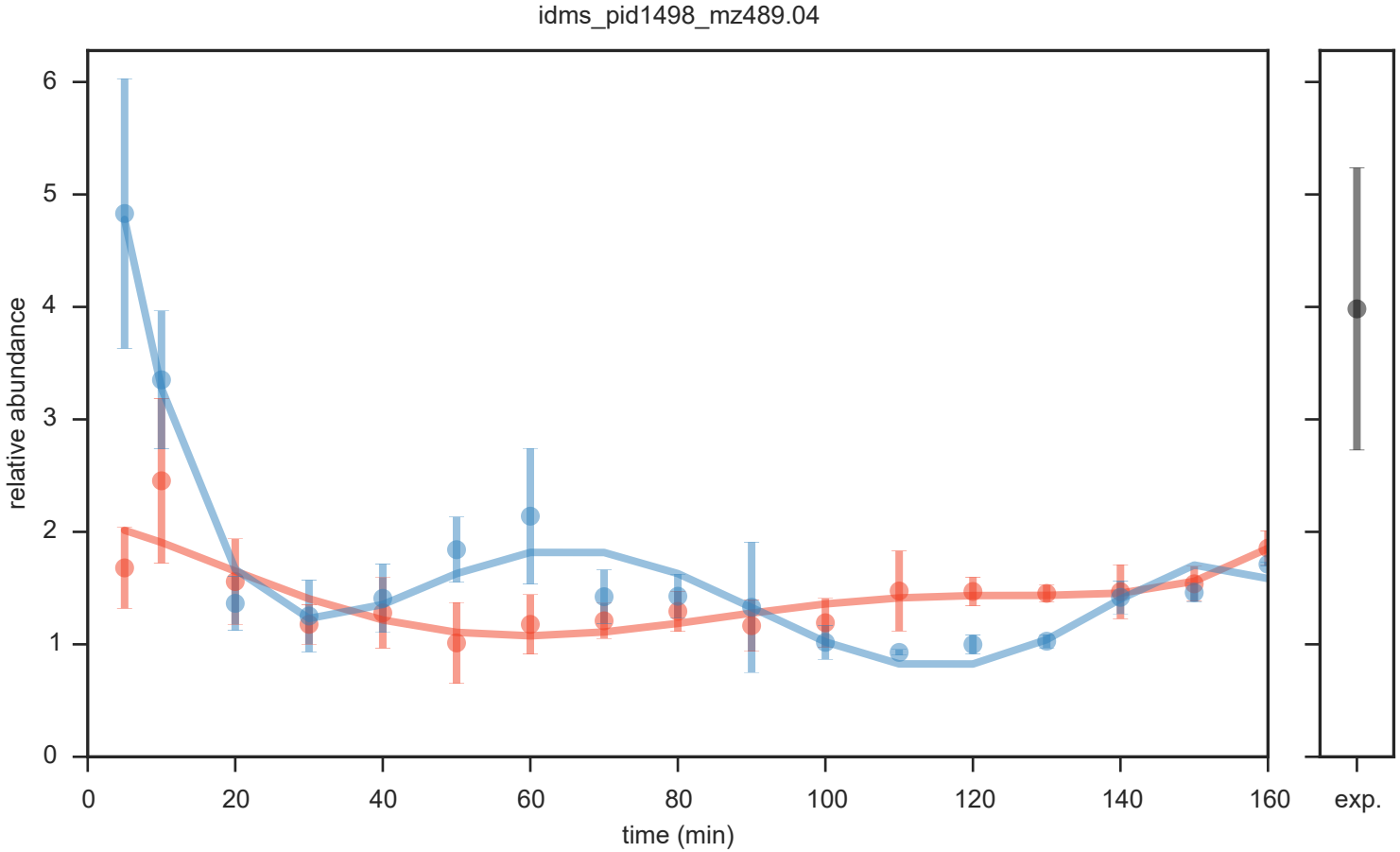

idms_pid1392_mz230.98
relative abundance
0
1
2
3
4
5
0
20
40
60
80
100
120
140
160
time (min)
exp.

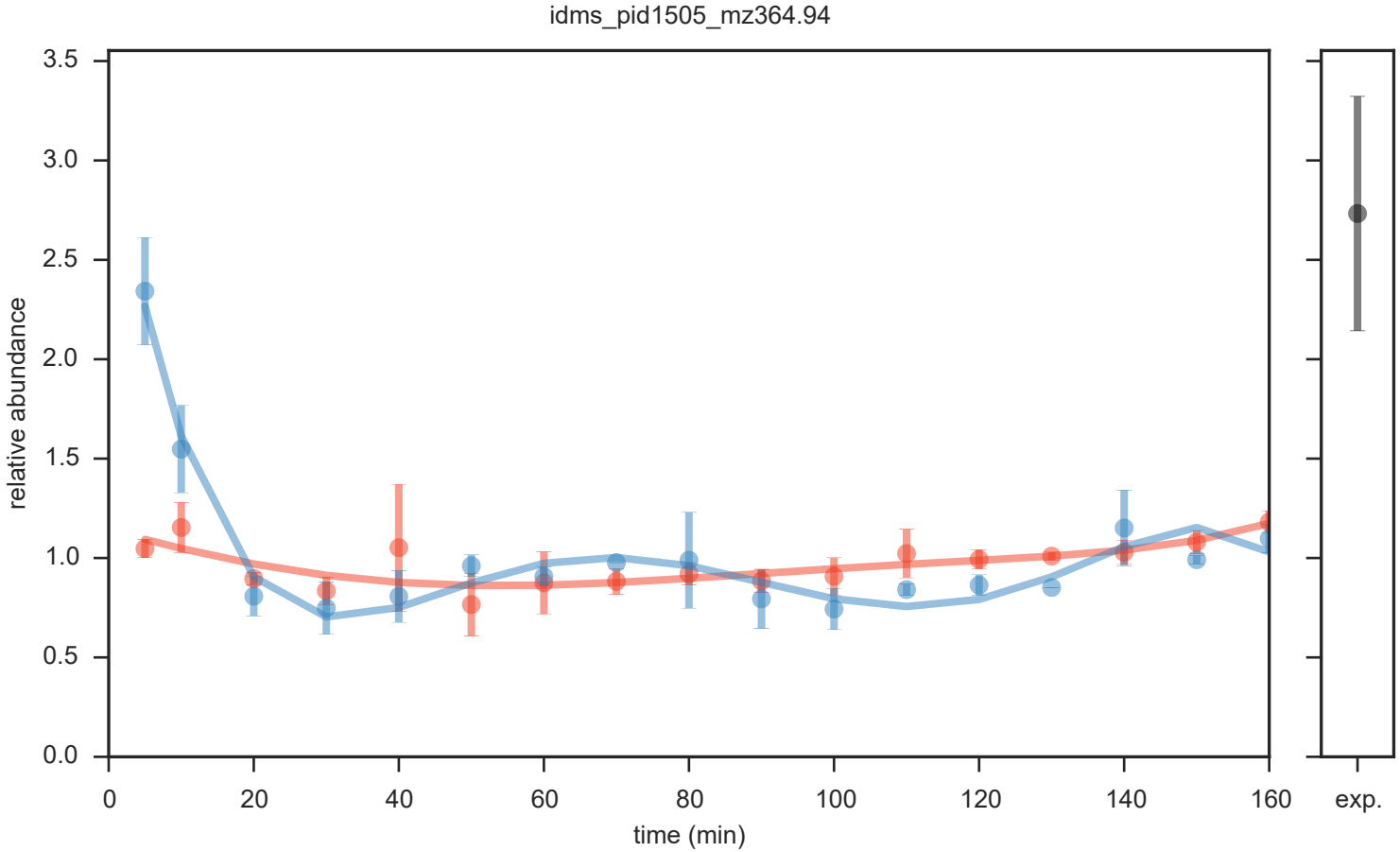

idms_pid1401_mz134.04
relative abundance
0.0
0.5
1.0
1.5
2.0
2.5
3.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

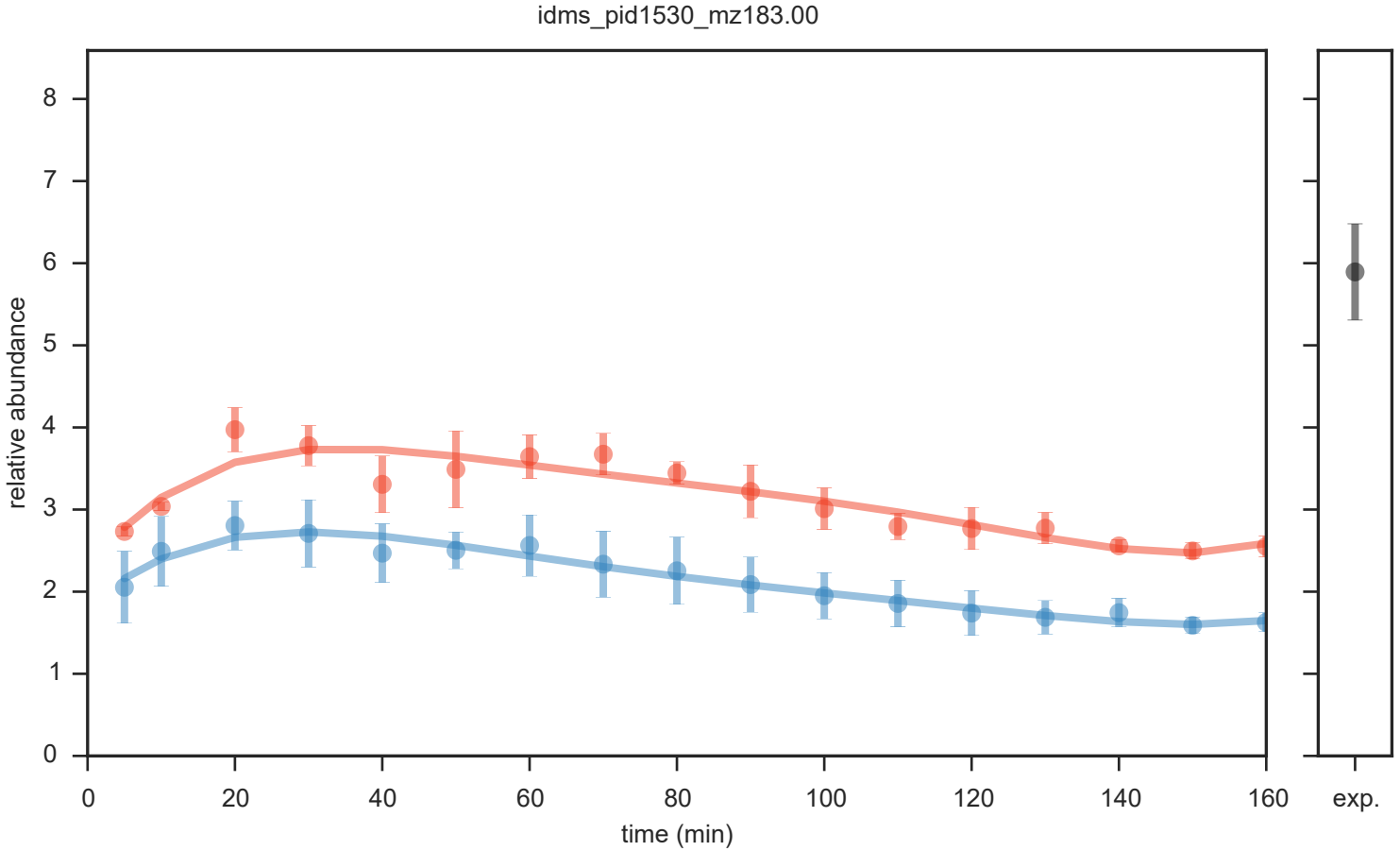

idms_pid1471_mz211.95
relative abundance
0
2
4
6
8
10
12
14
16
0
20
40
60
80
100
120
140
160
time (min)
exp.

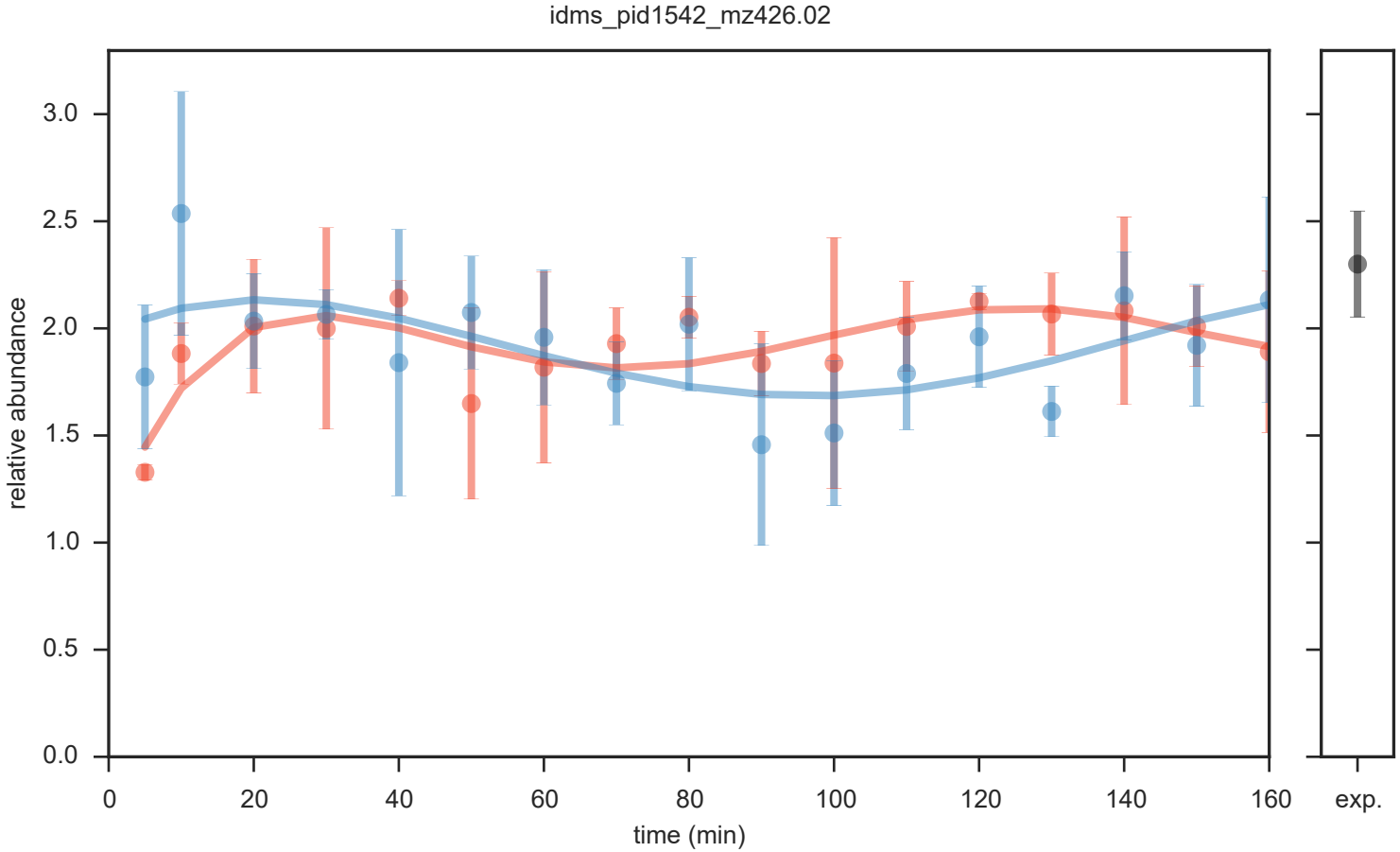

idms_pid1472_mz300.04
relative abundance
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

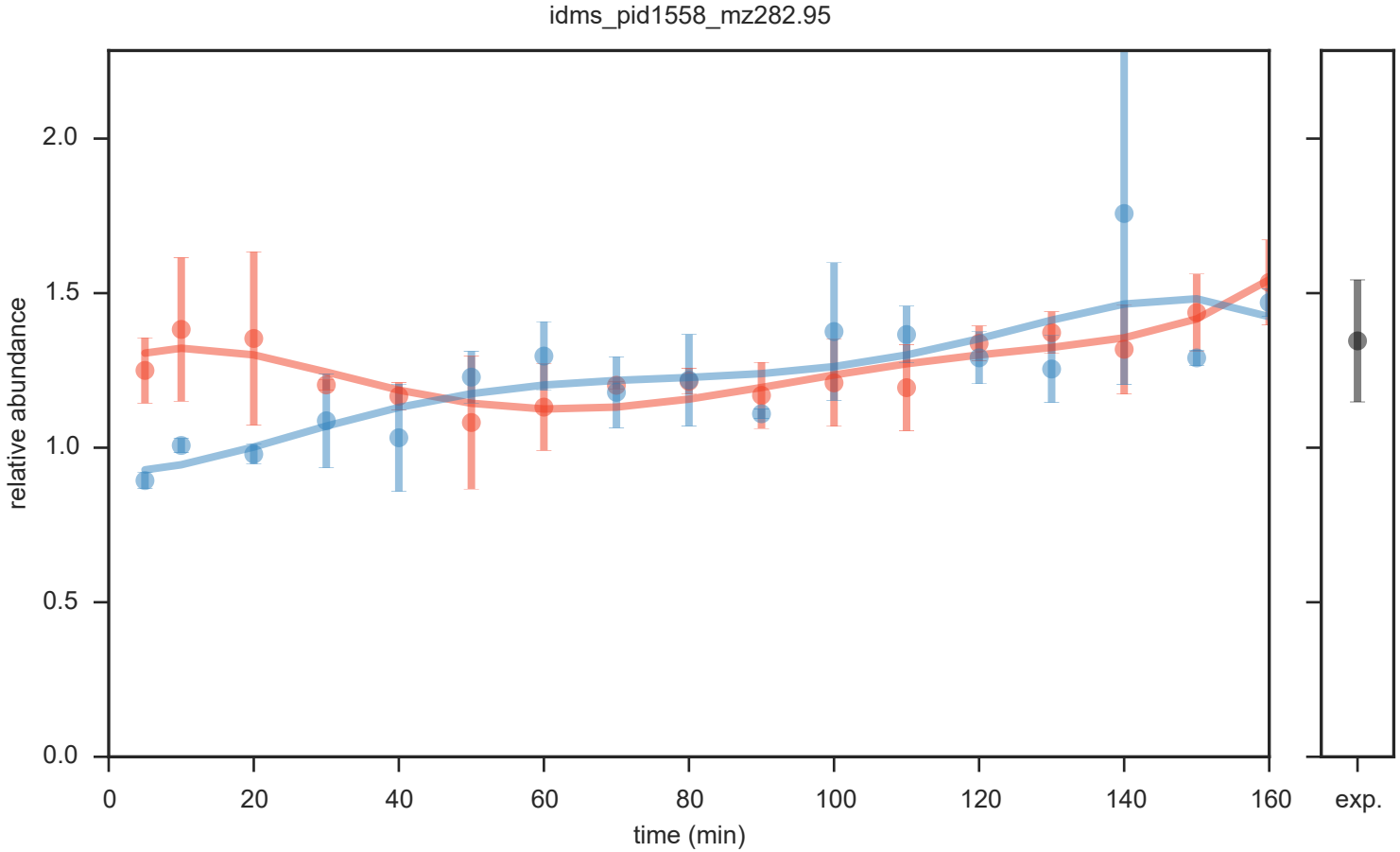

idms_pid1475_mz617.02
relative abundance
time (min)
exp.
0
1
2
3
4
5
6
7
8
0
20
40
60
80
100
120
140
160


idms_pid1498_mz489.04
relative abundance
0
1
2
3
4
5
6
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid1505_mz364.94
relative abundance
time (min)
exp.
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
0
20
40
60
80
100
120
140
160


idms_pid1530_mz183.00
relative abundance
0
1
2
3
4
5
6
7
8
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid1542_mz426.02
relative abundance
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid1558_mz282.95
relative abundance
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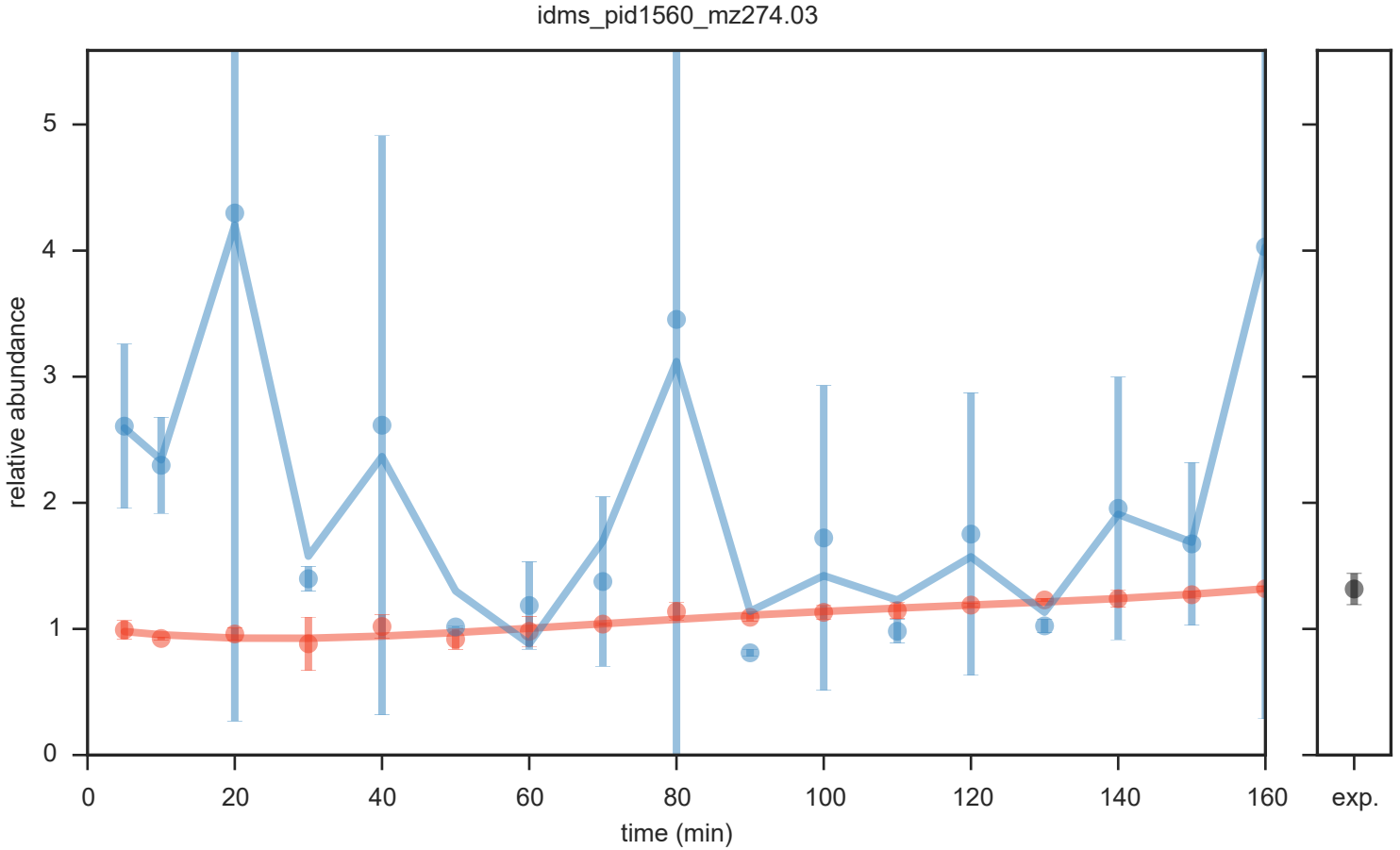
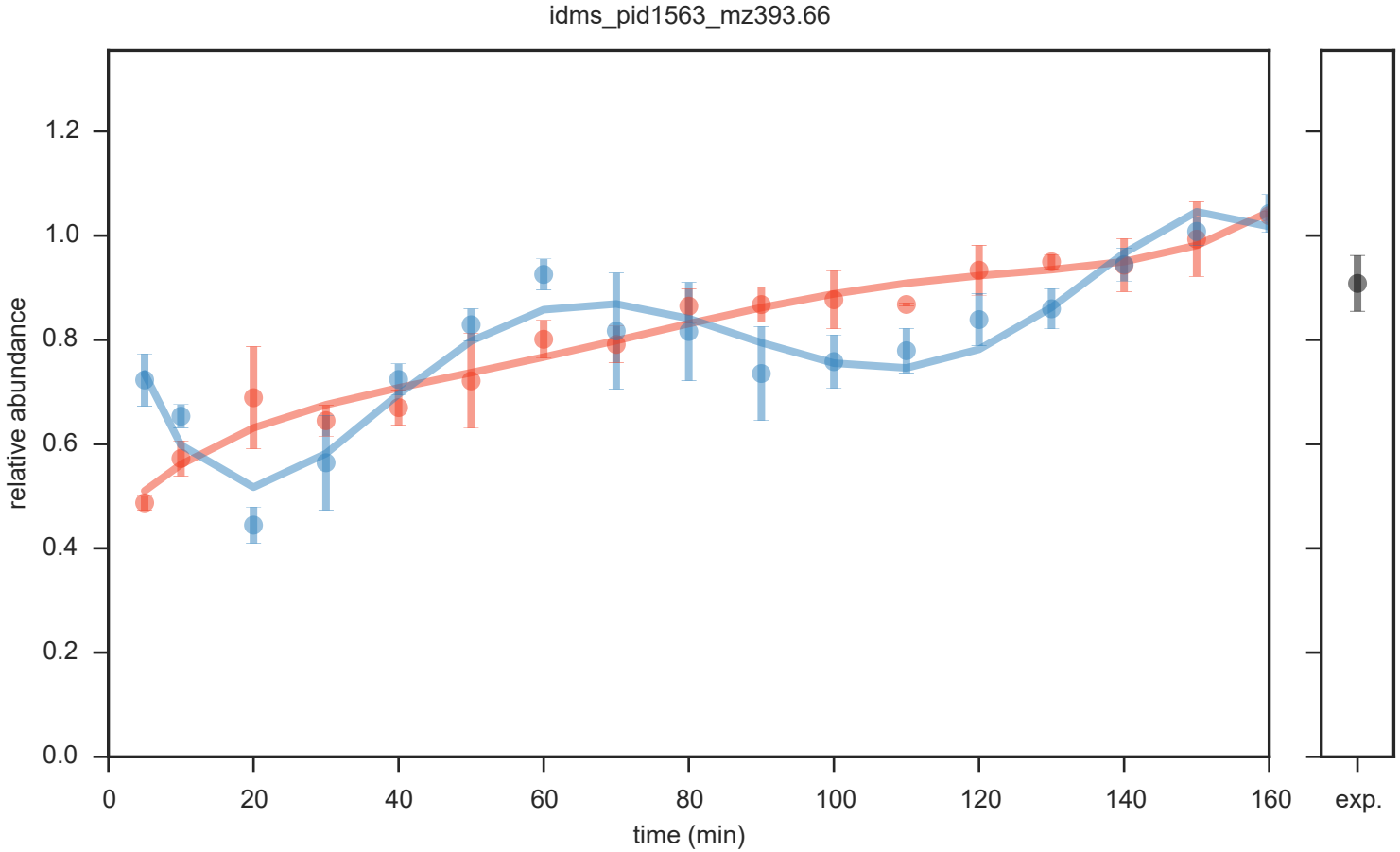
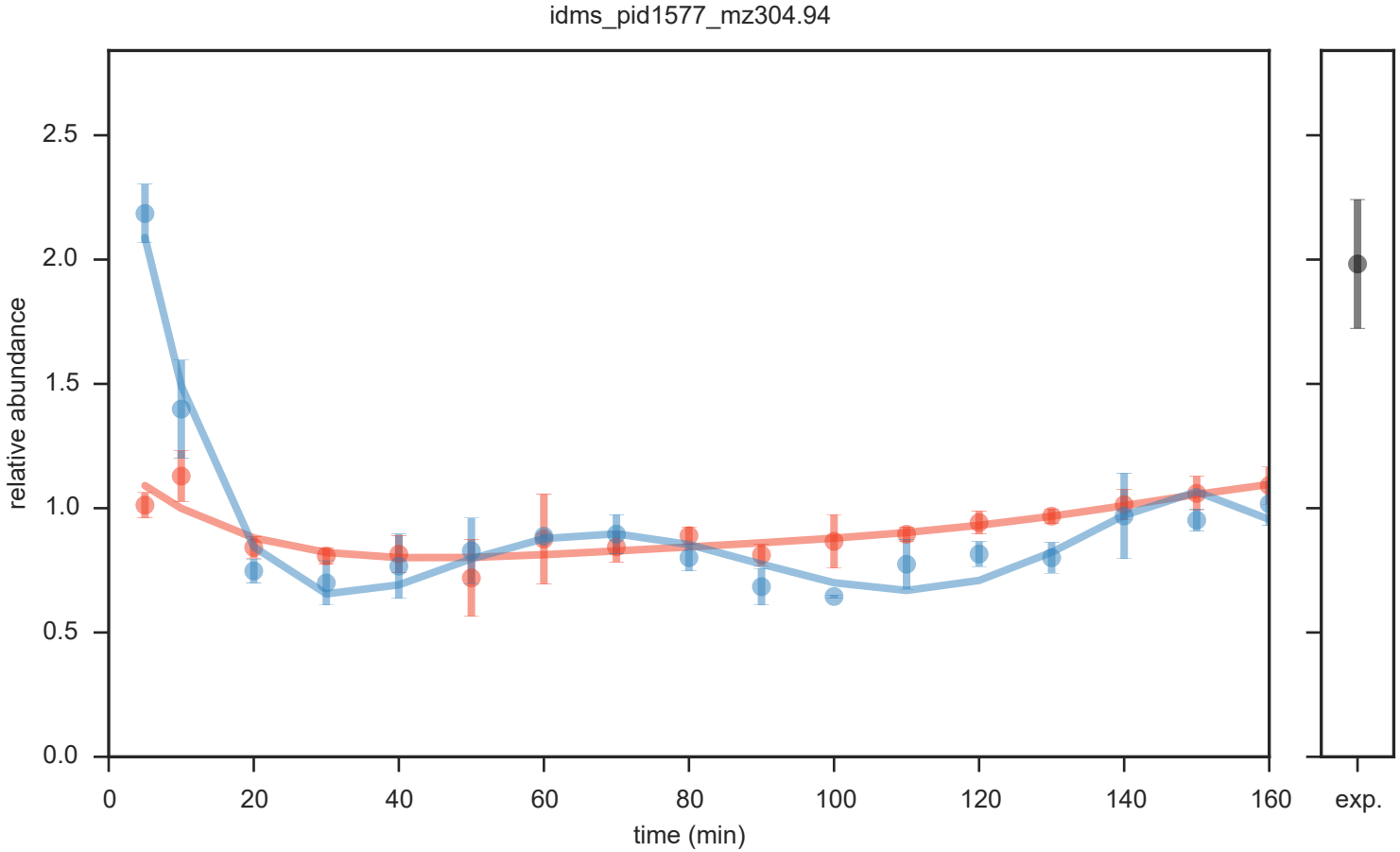
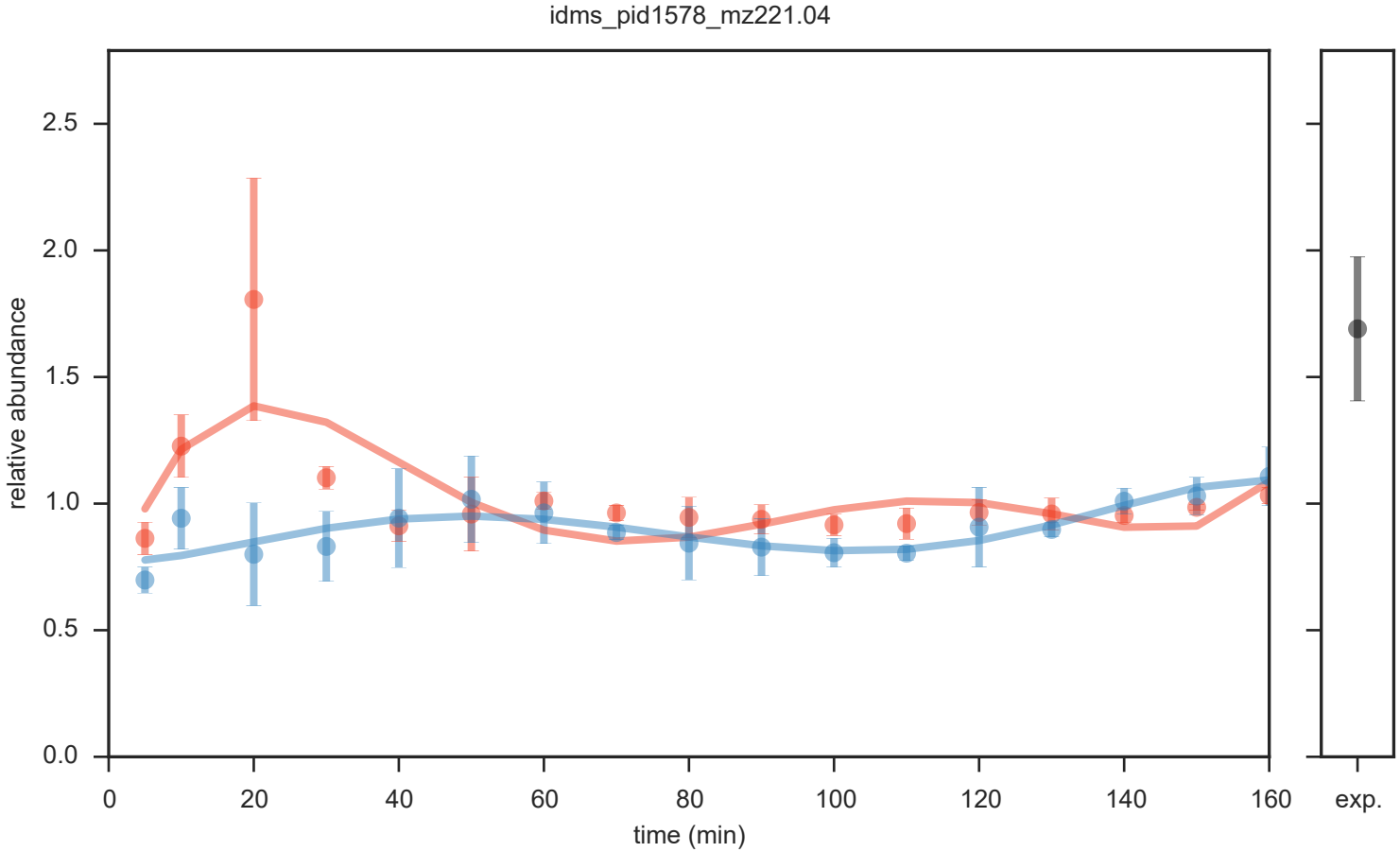
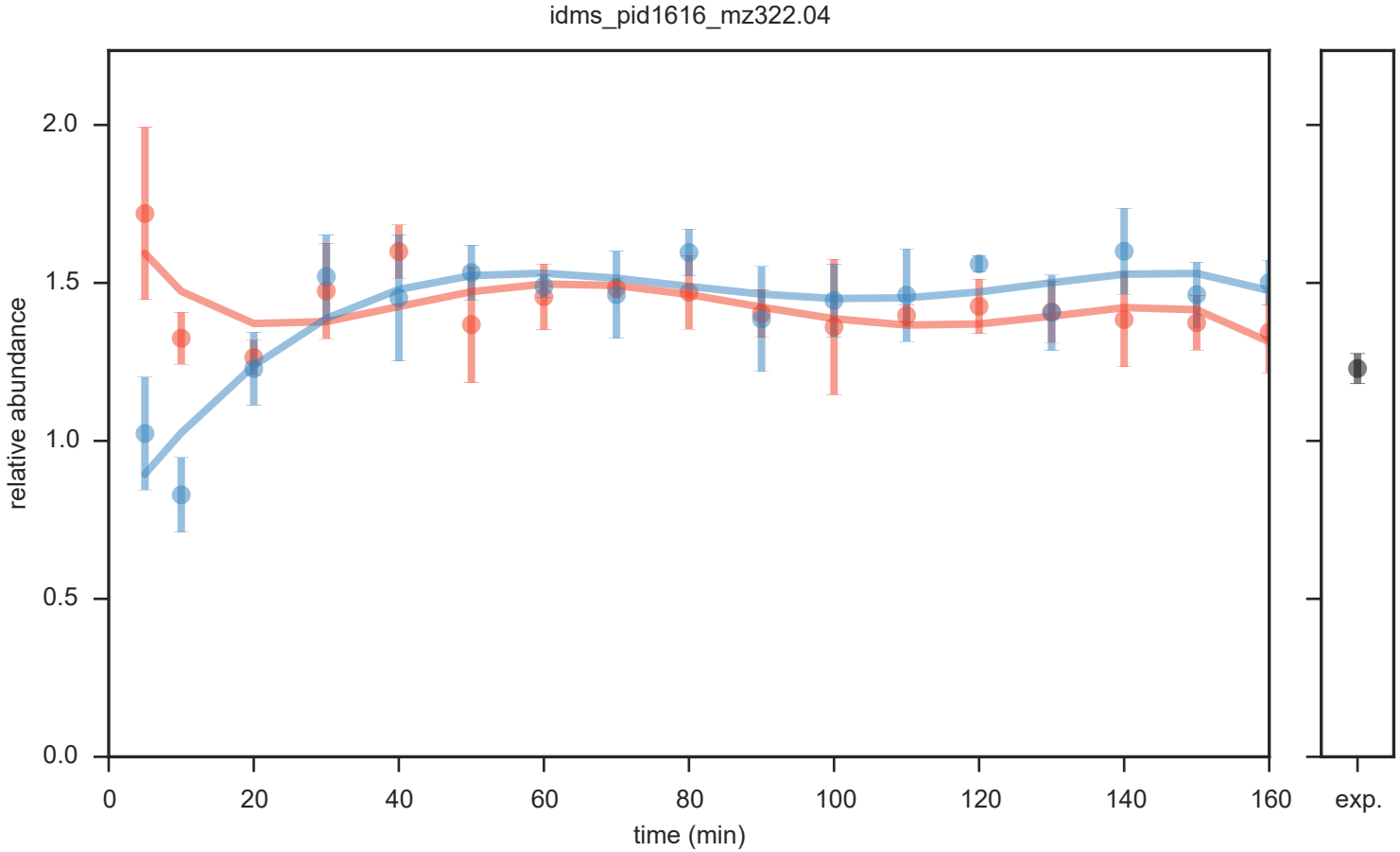
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

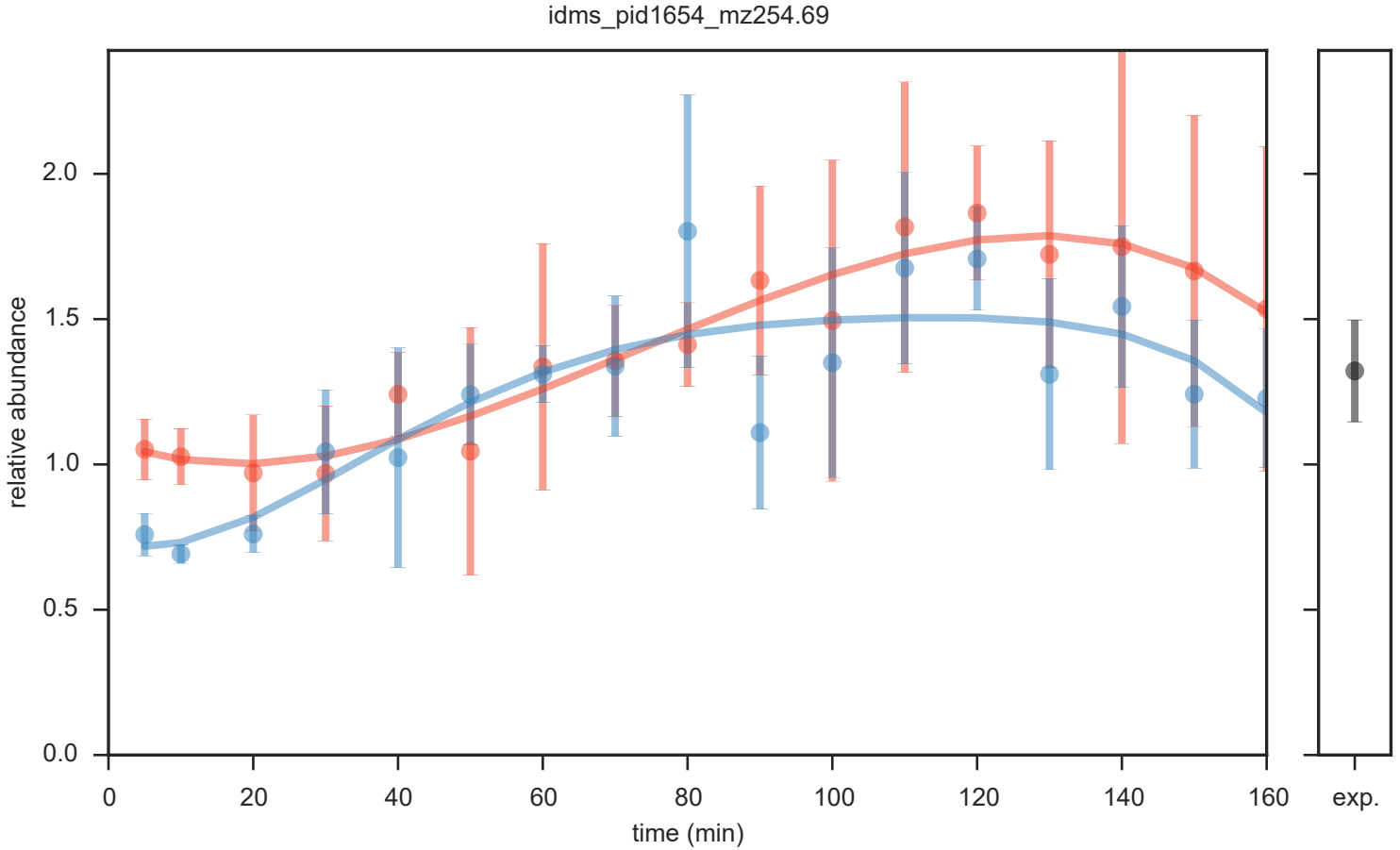

idms_pid1560_mz274.03
relative abundance
0
1
2
3
4
5
0
20
40
60
80
100
120
140
160
time (min)
exp.

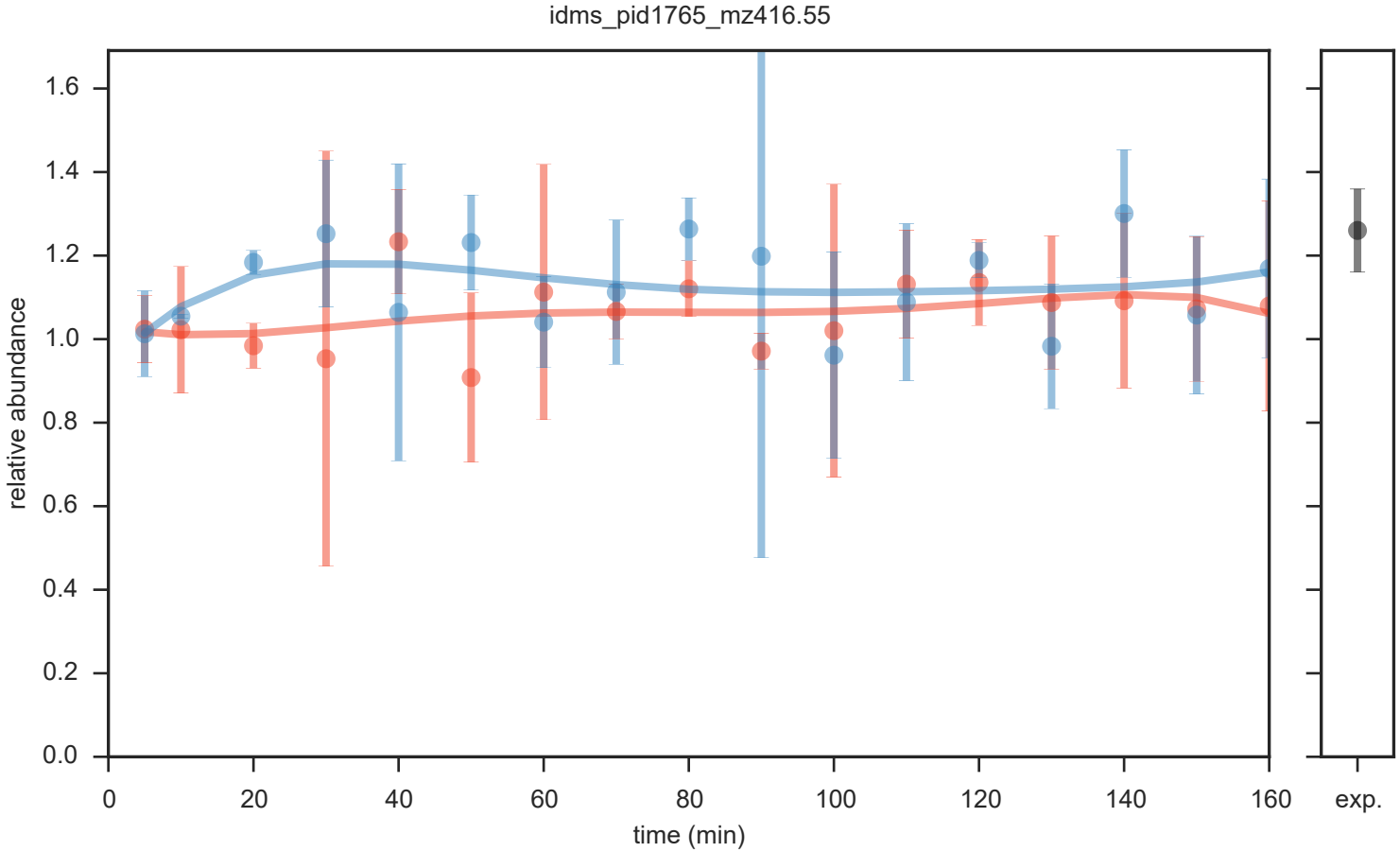

idms_pid1563_mz393.66
relative abundance
0.0
0.2
0.4
0.6
0.8
1.0
1.2
0
20
40
60
80
100
120
140
160
time (min)
exp.

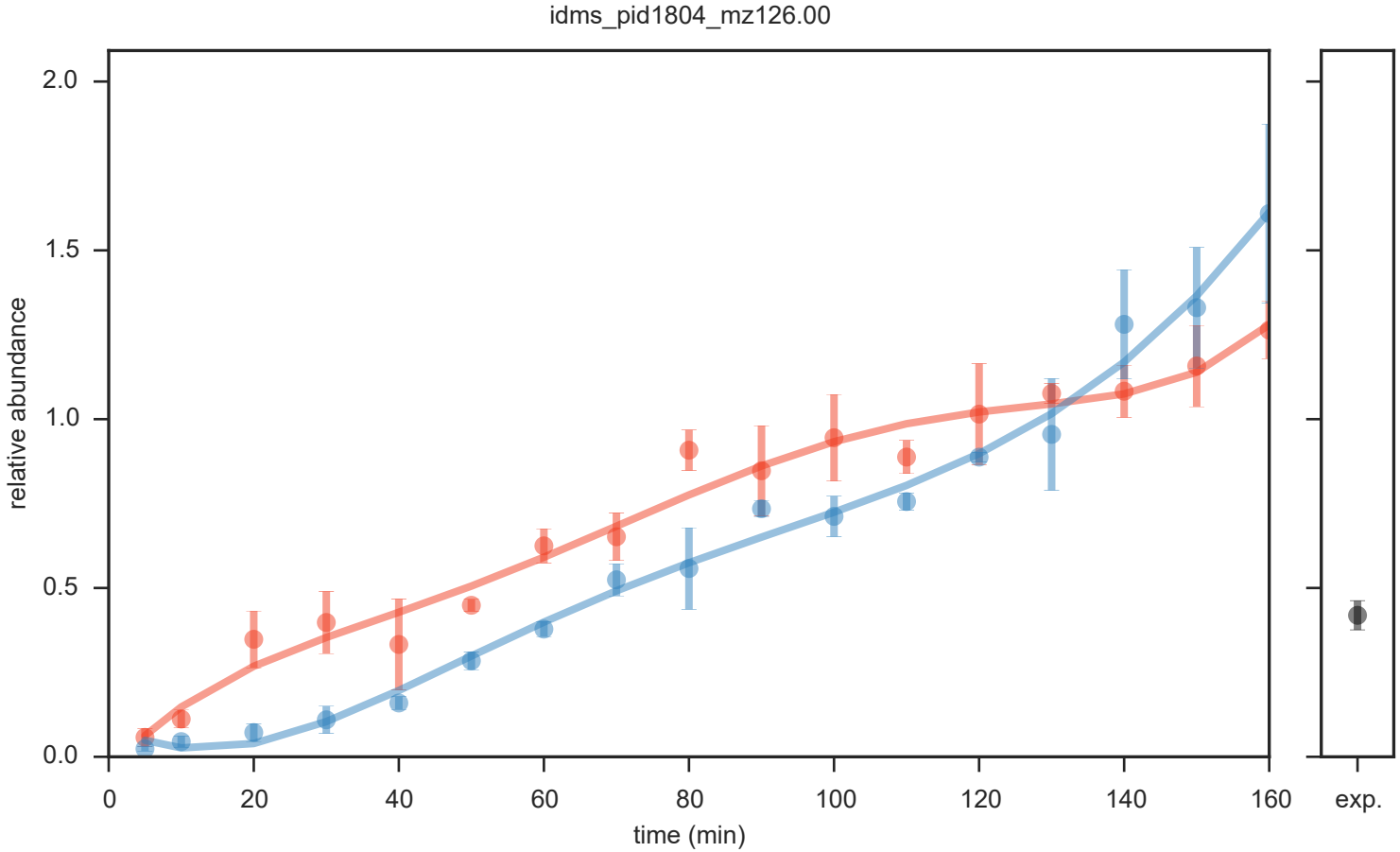

idms_pid1577_mz304.94
relative abundance
0.0
0.5
1.0
1.5
2.0
2.5
0
20
40
60
80
100
120
140
160
time (min)
exp.

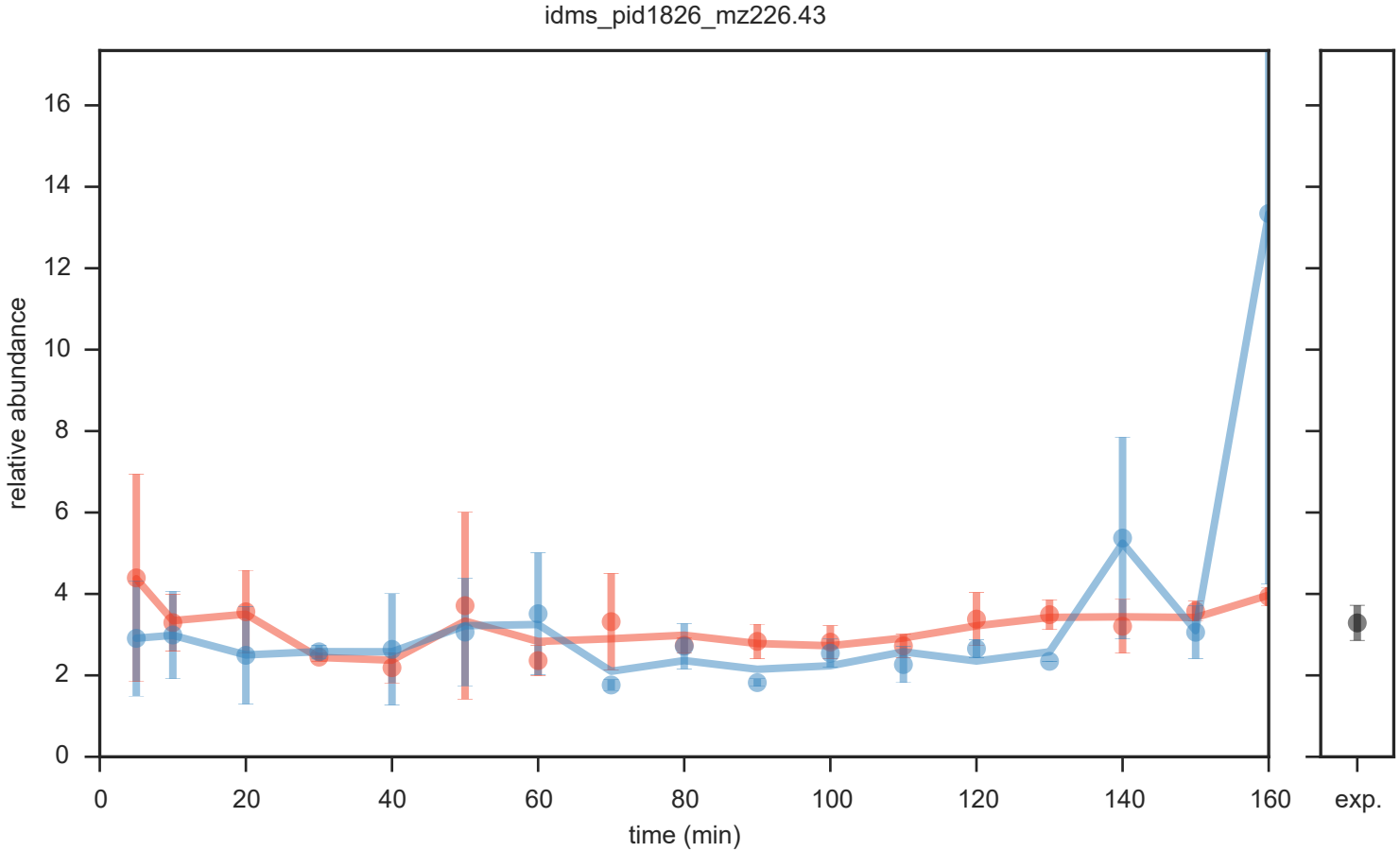

idms_pid1578_mz221.04
relative abundance
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

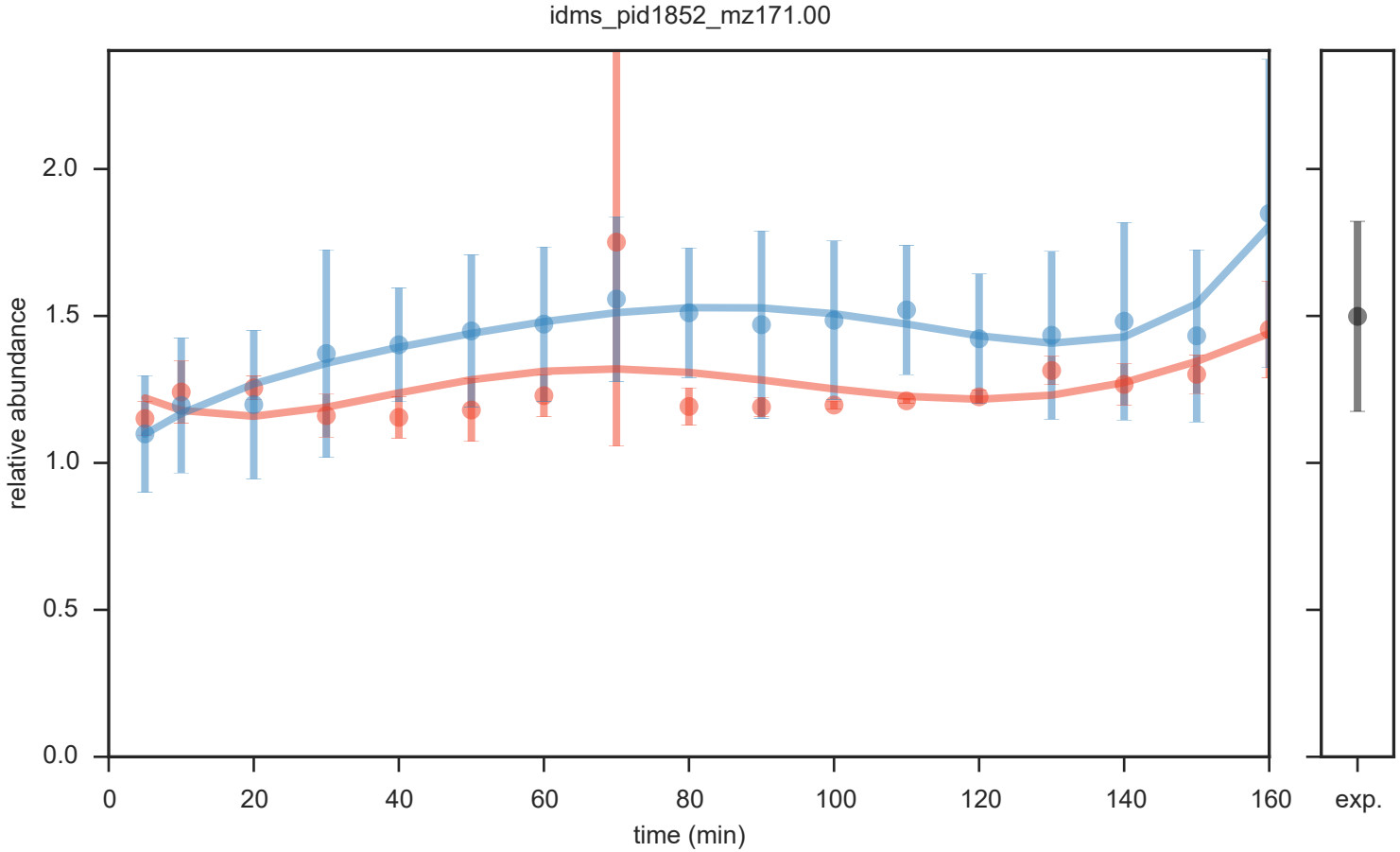

idms_pid1616_mz322.04
relative abundance
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

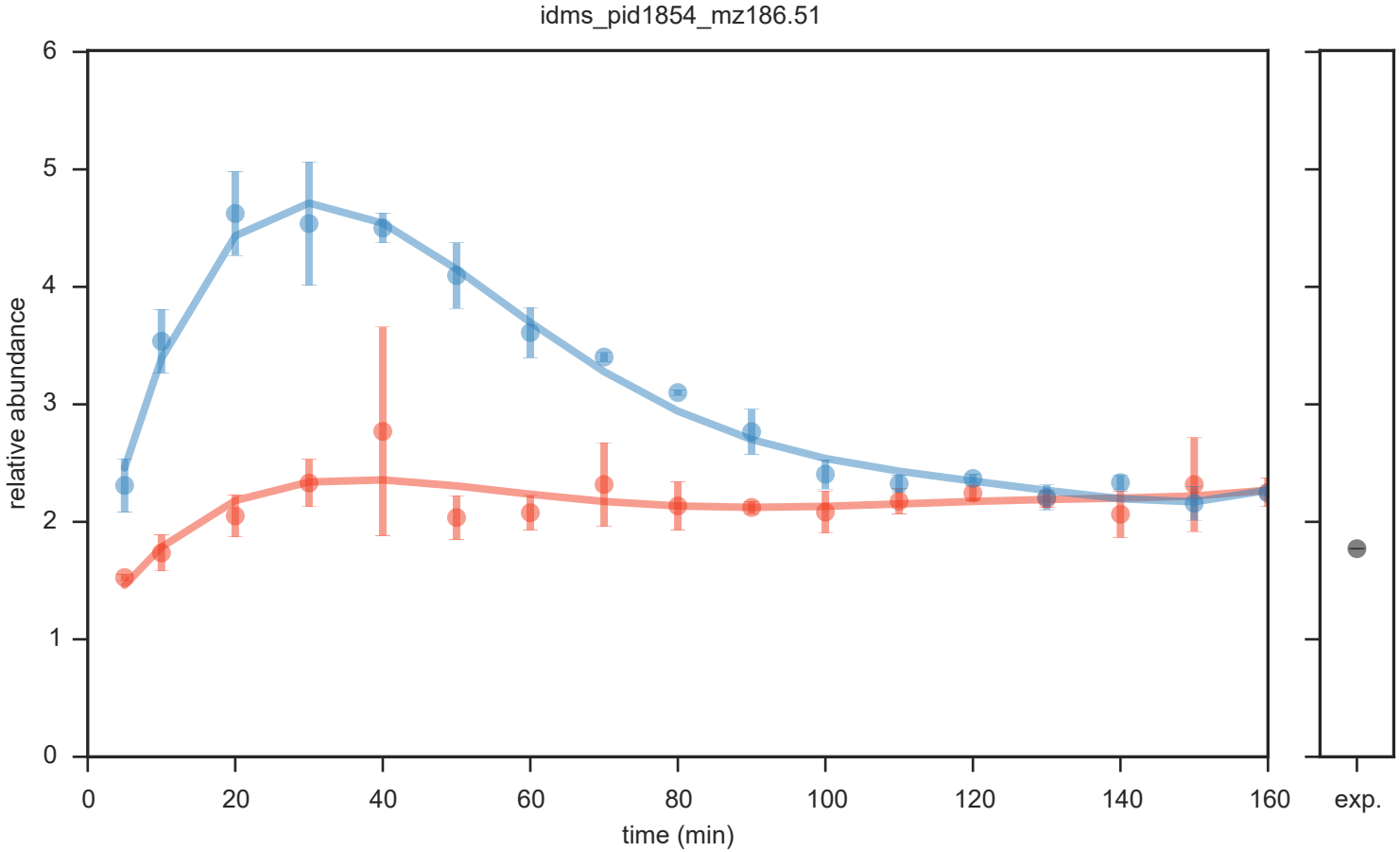

idms_pid1654_mz254.69
relative abundance
0.0
0.5
1.0
1.5
2.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

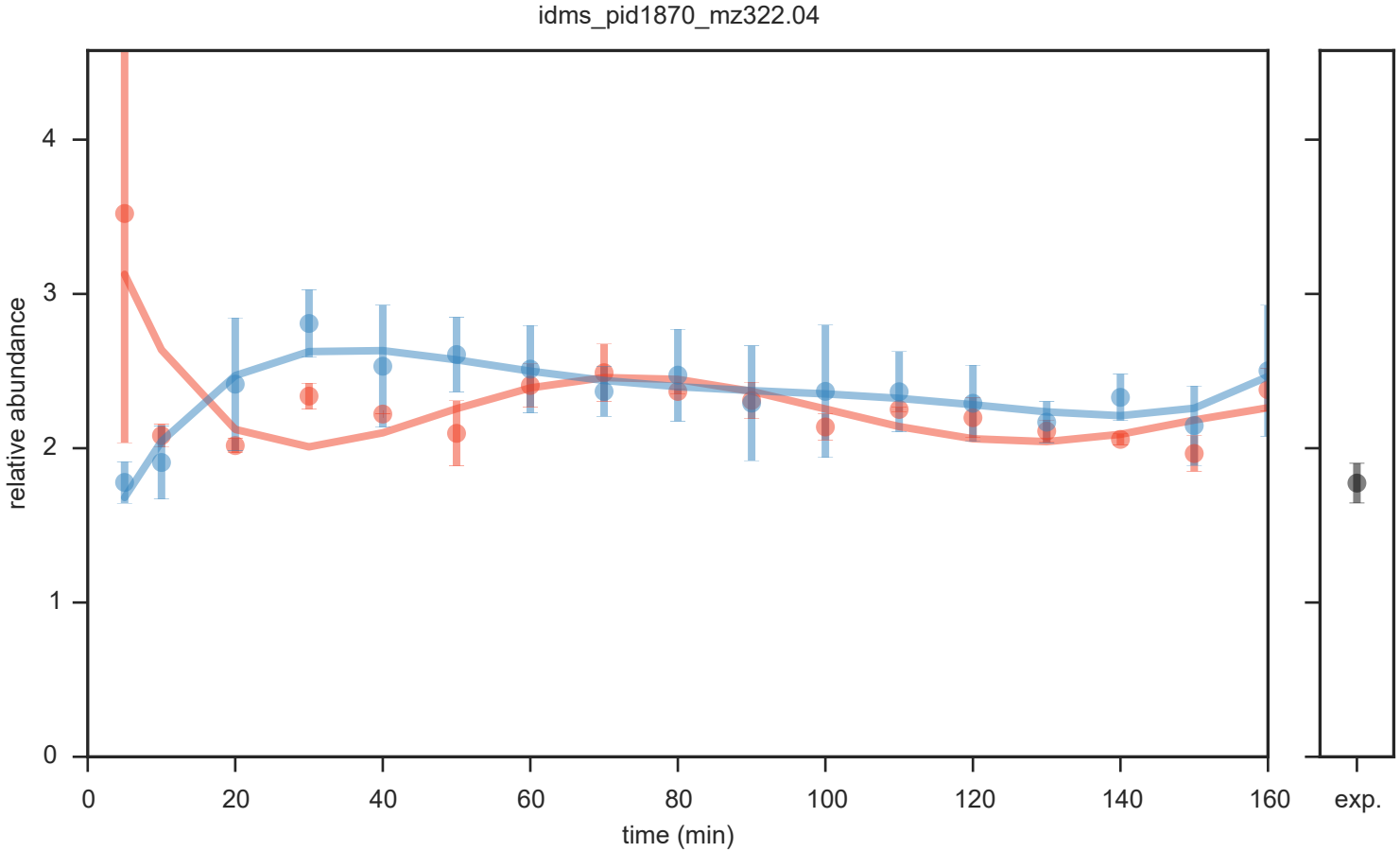

idms_pid1765_mz416.55
relative abundance
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
0
20
40
60
80
100
120
140
160
time (min)
exp.

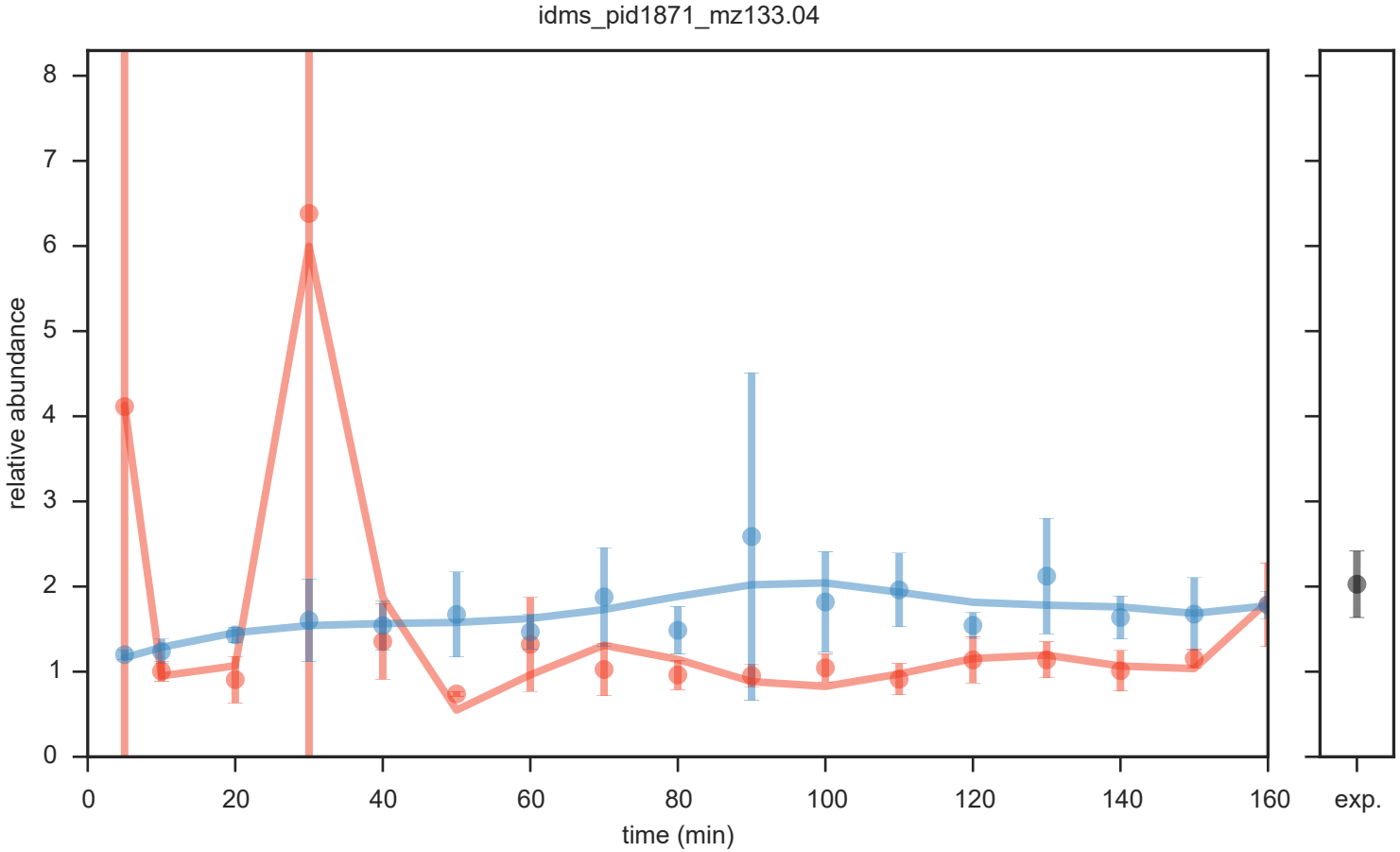

idms_pid1804_mz126.00
relative abundance
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

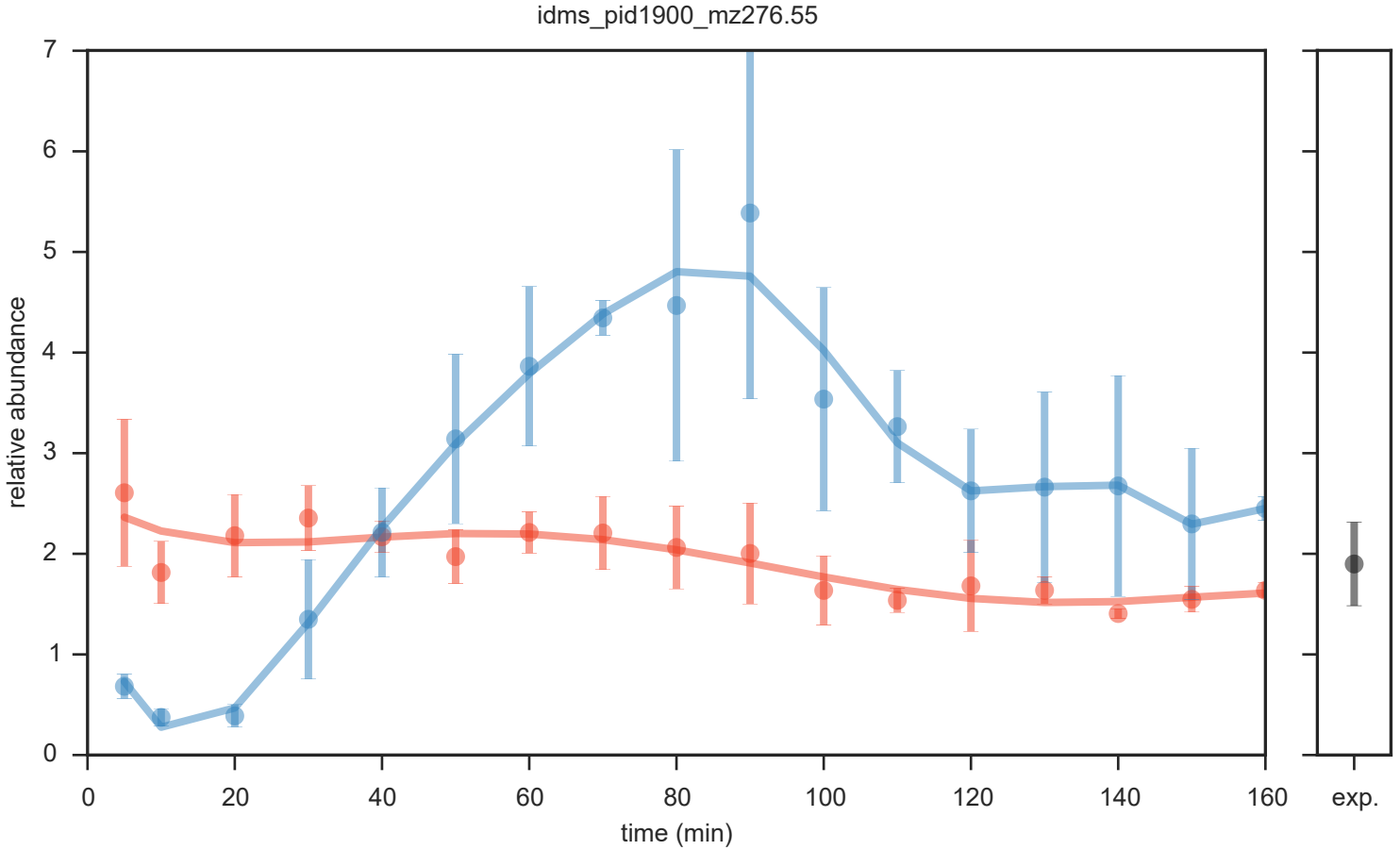

idms_pid1826_mz226.43
relative abundance
0
2
4
6
8
10
12
14
16
0
20
40
60
80
100
120
140
160
time (min)
exp.

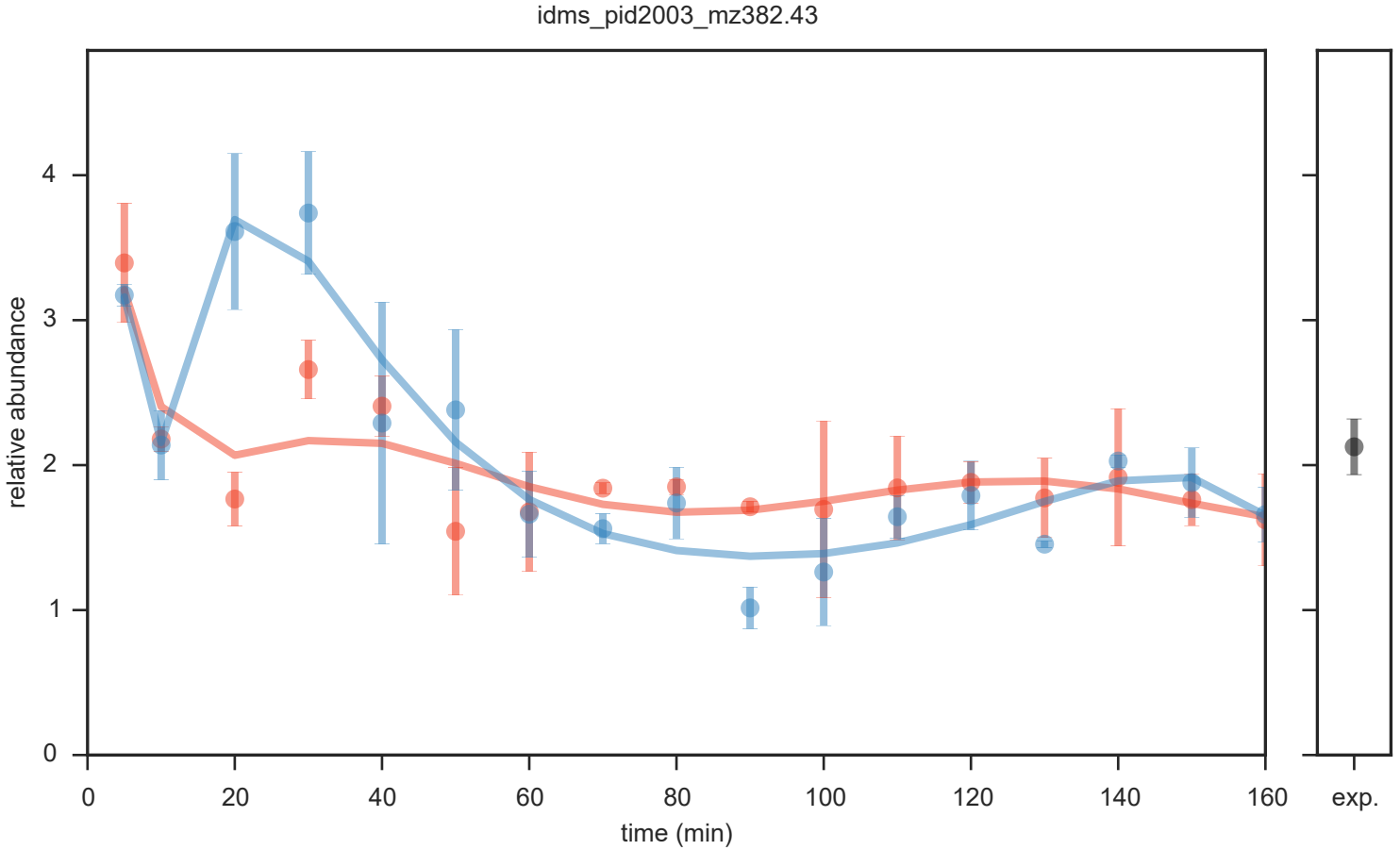

idms_pid1852_mz171.00
relative abundance
0.0
0.5
1.0
1.5
2.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

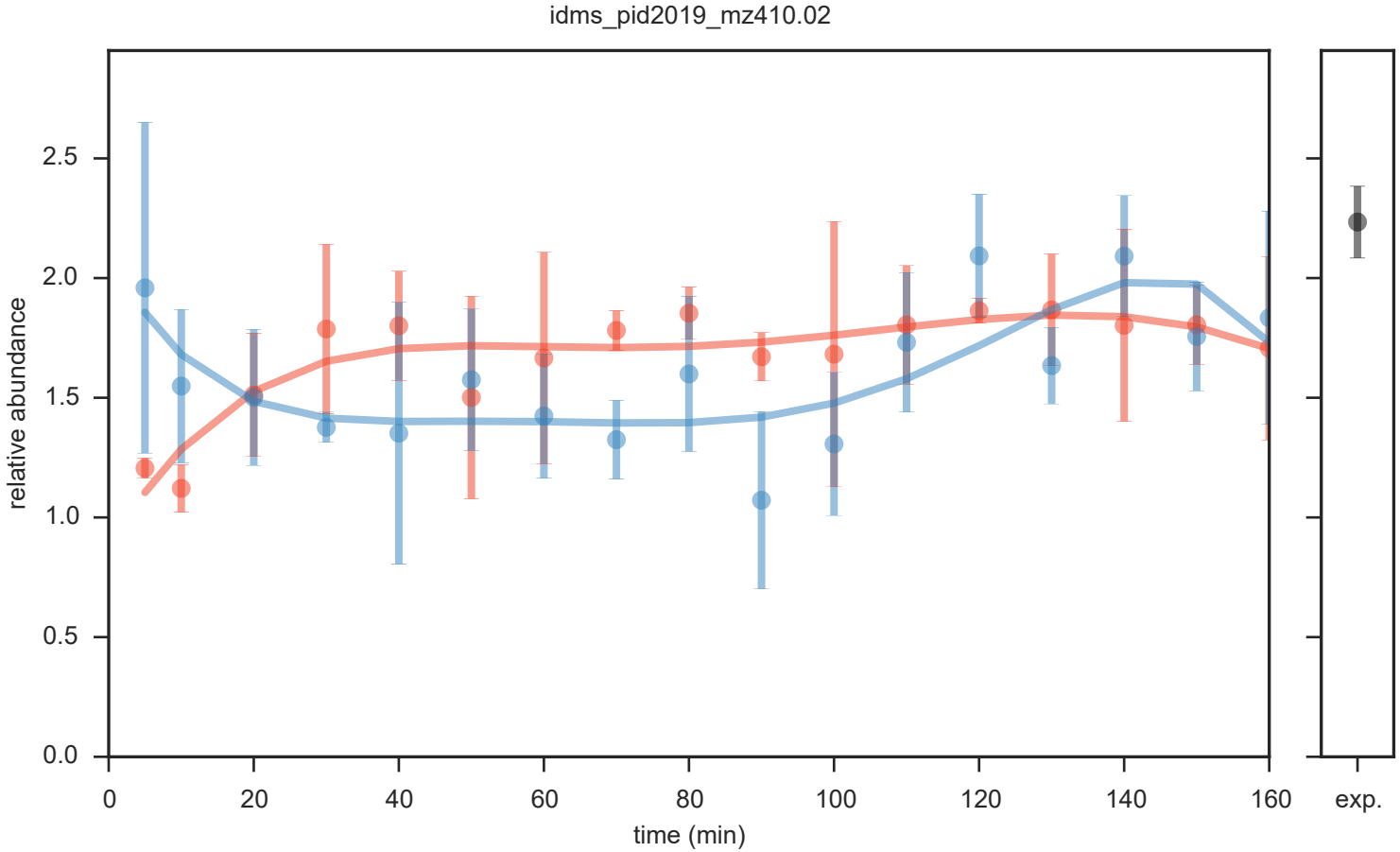

idms_pid1854_mz186.51
relative abundance
time (min)
exp.
0
1
2
3
4
5
6
0
20
40
60
80
100
120
140
160

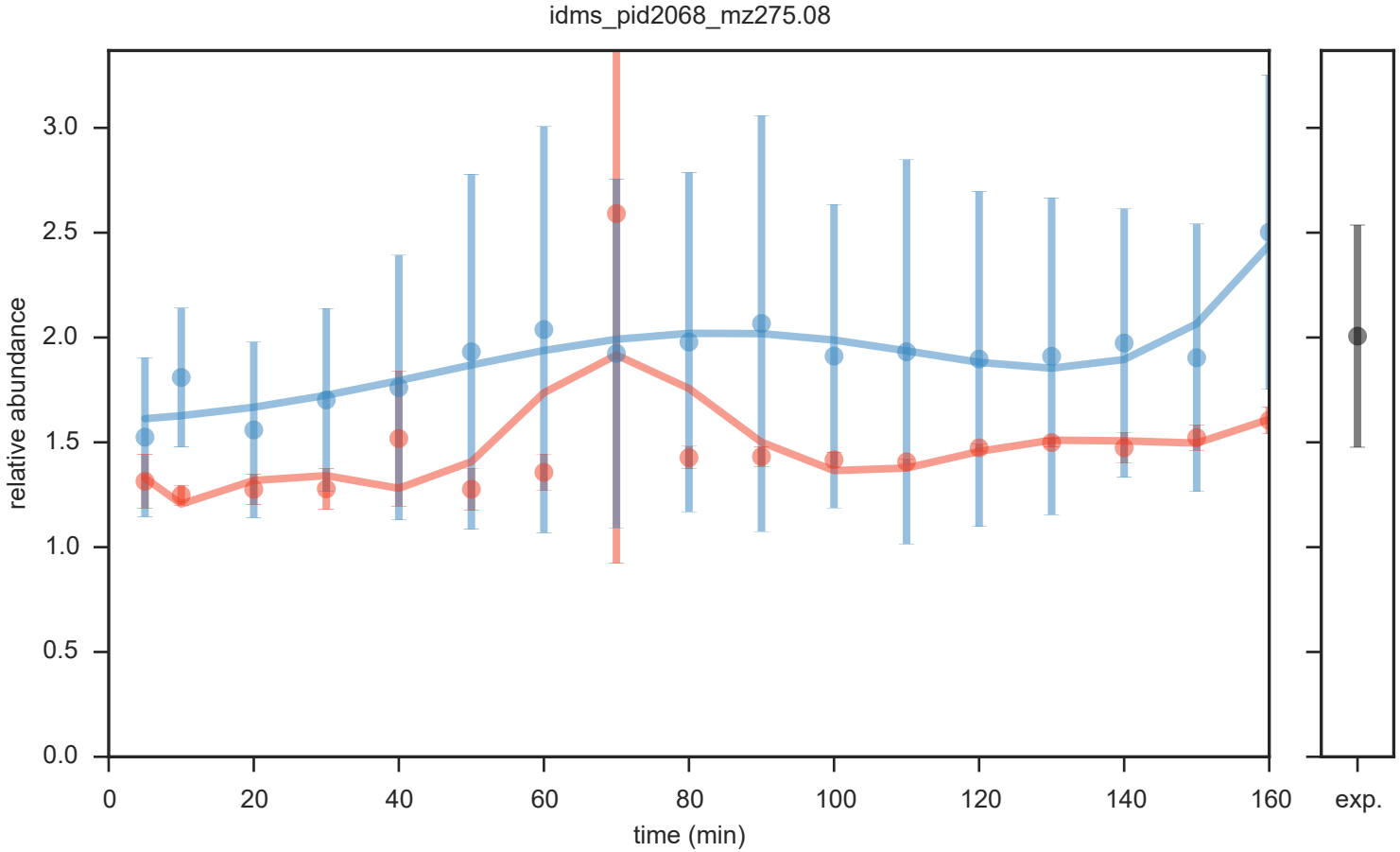

idms_pid1870_mz322.04
relative abundance
0
1
2
3
4
0
20
40
60
80
100
120
140
160
time (min)
exp.

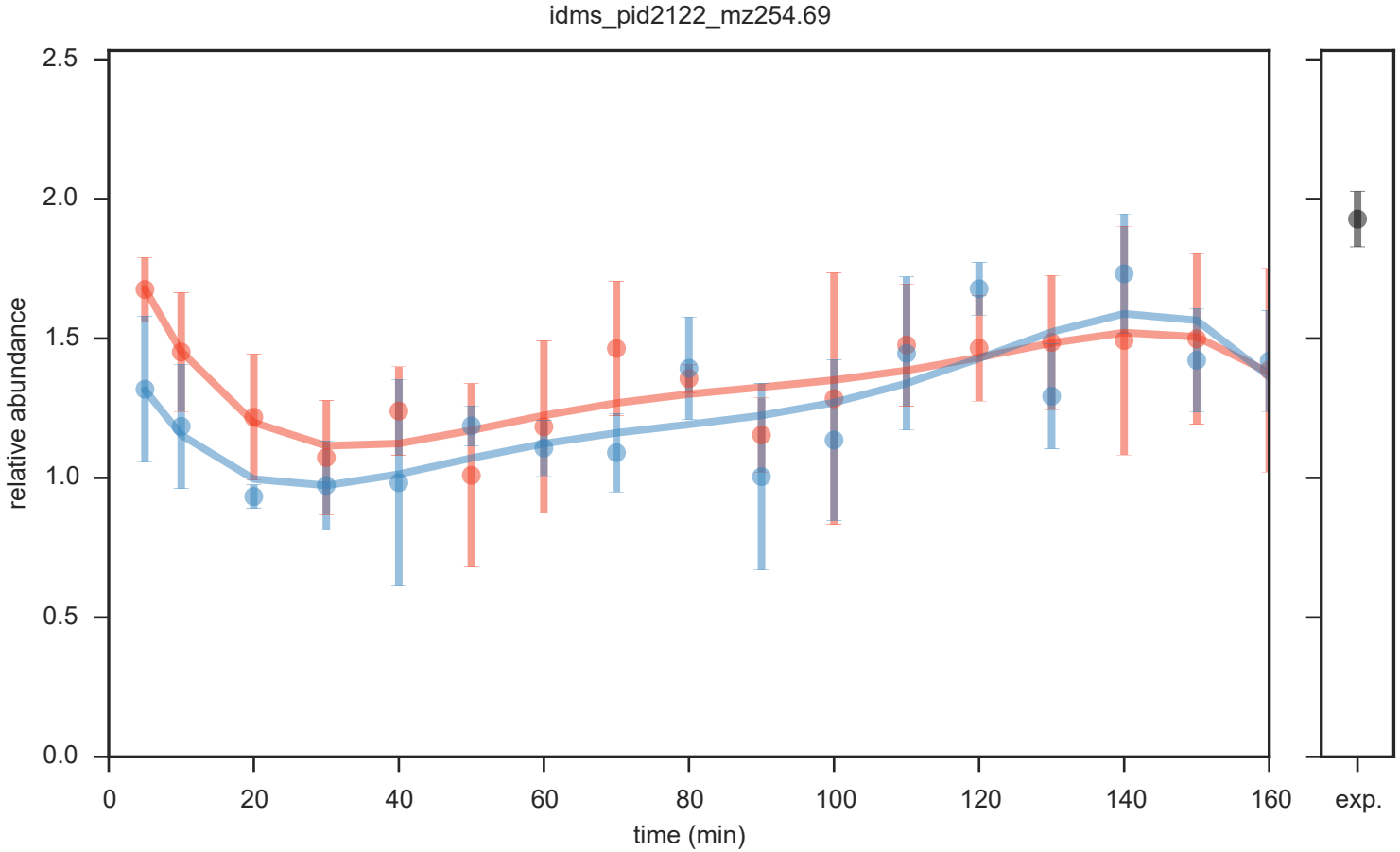

idms_pid1871_mz133.04
relative abundance
0
1
2
3
4
5
6
7
8
0
20
40
60
80
100
120
140
160
time (min)
exp.

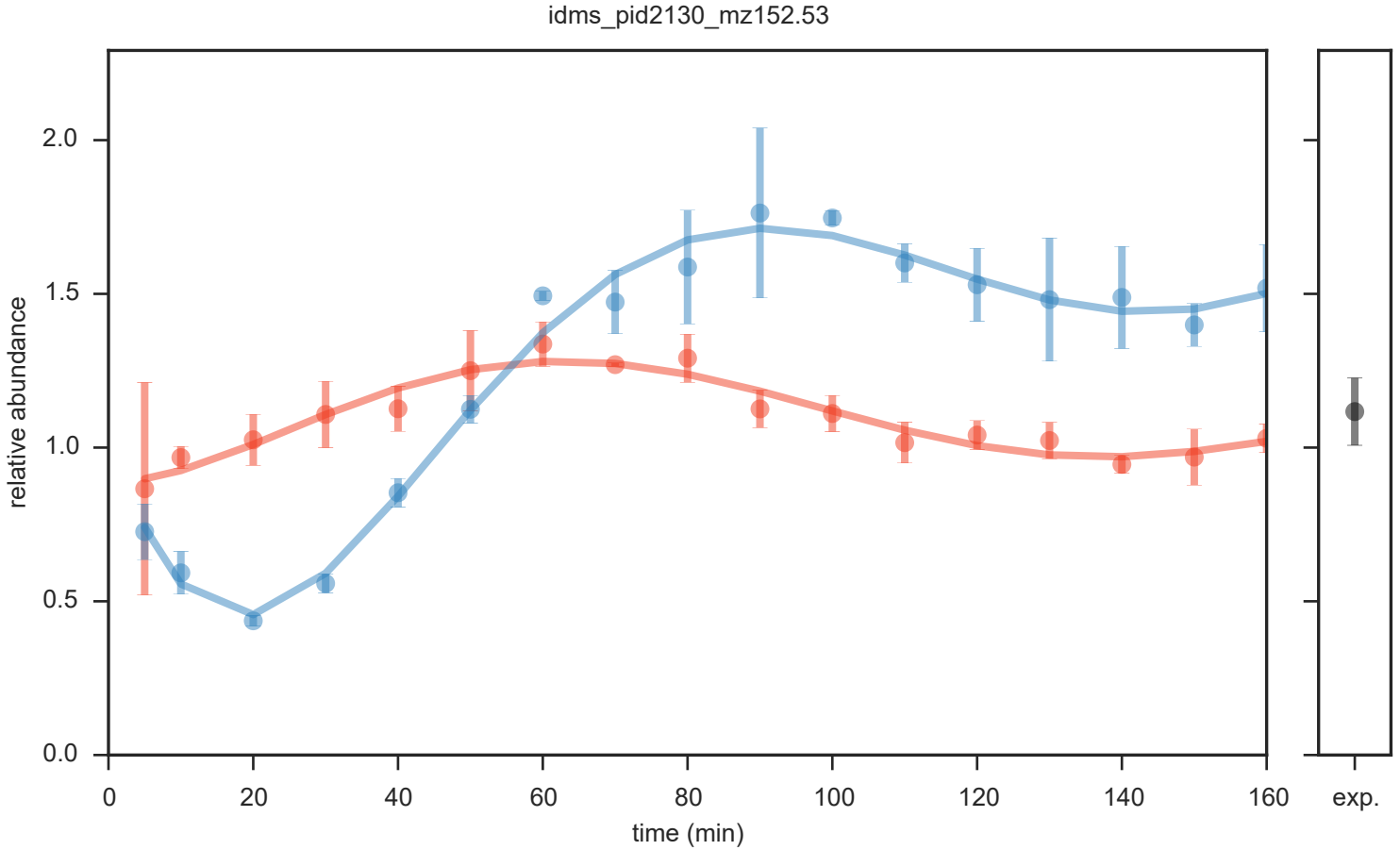

idms_pid1900_mz276.55
relative abundance
time (min)
exp.
0
1
2
3
4
5
6
7
0
20
40
60
80
100
120
140
160

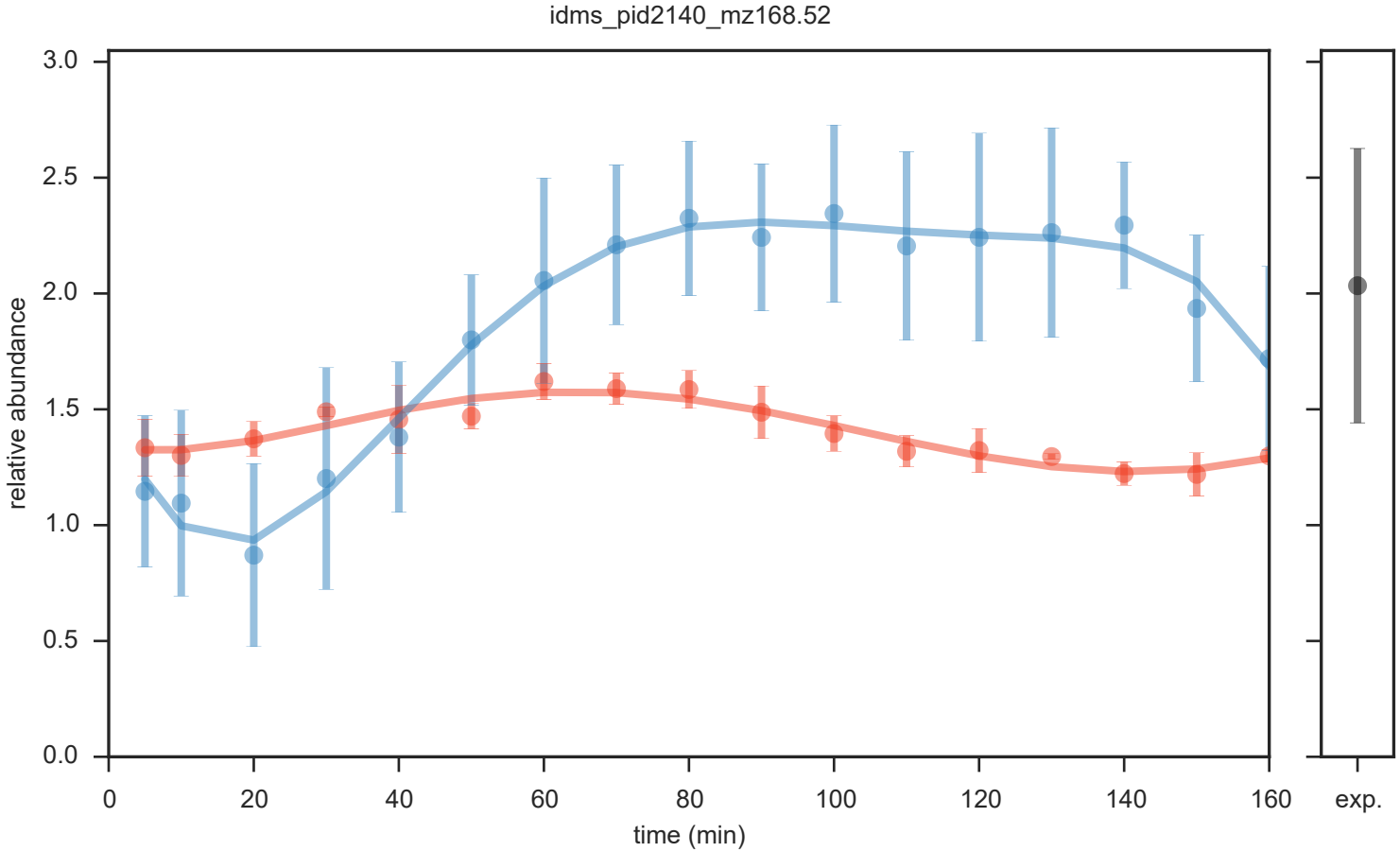

idms_pid2003_mz382.43
relative abundance
0
1
2
3
4
0
20
40
60
80
100
120
140
160
time (min)
exp.

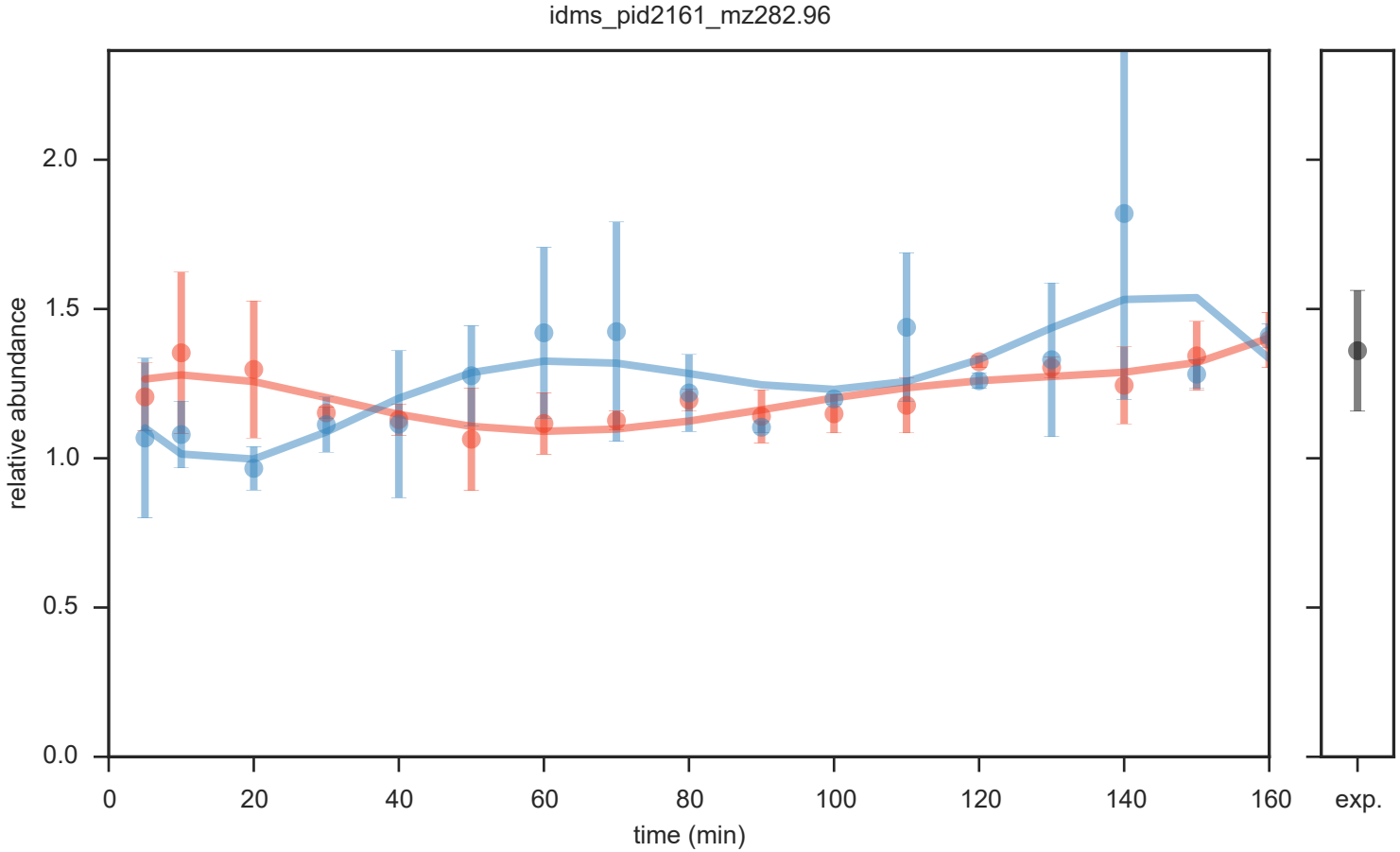

idms_pid2019_mz410.02
relative abundance
0.0
0.5
1.0
1.5
2.0
2.5
0
20
40
60
80
100
120
140
160
time (min)
exp.

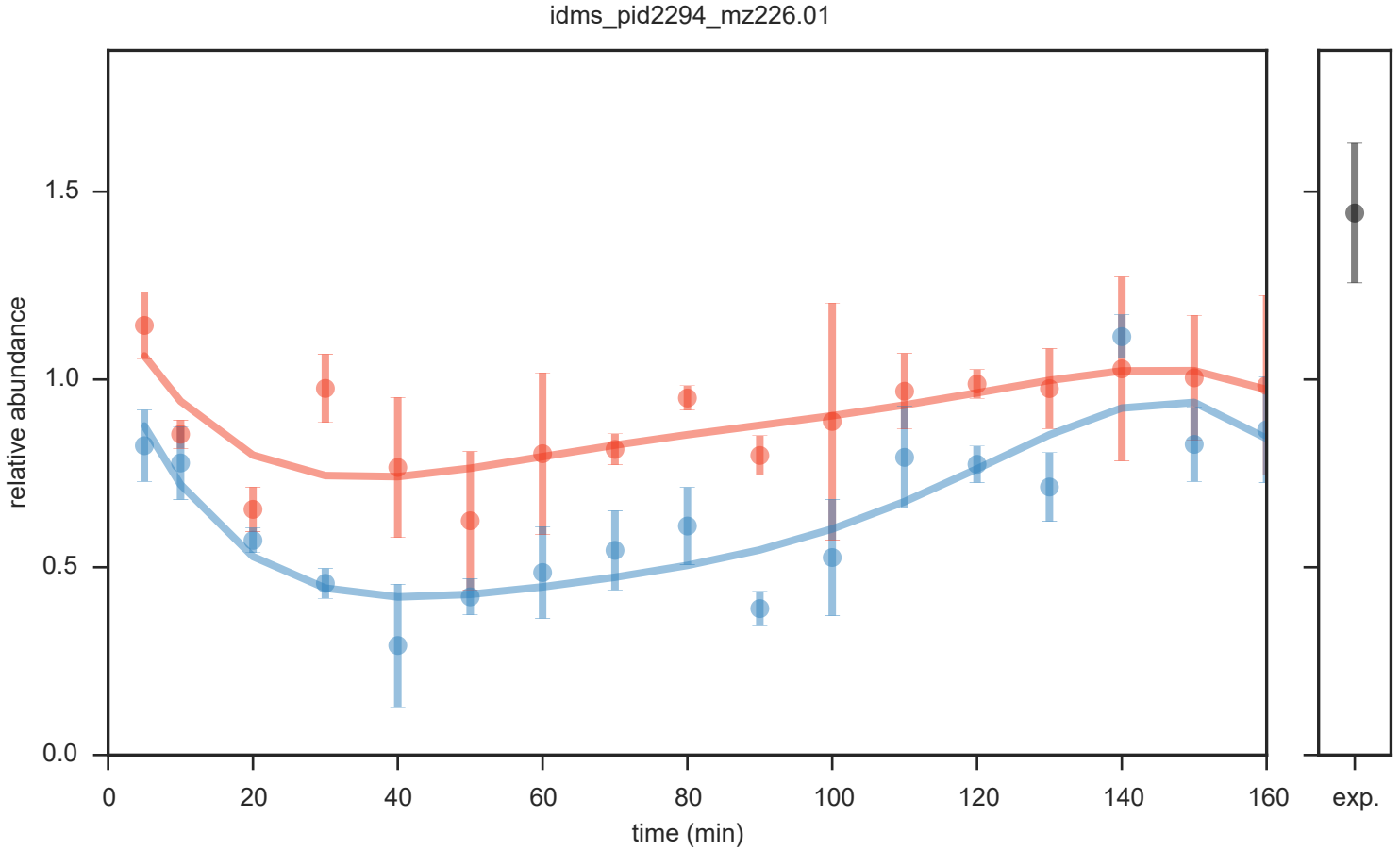

idms_pid2068_mz275.08
relative abundance
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

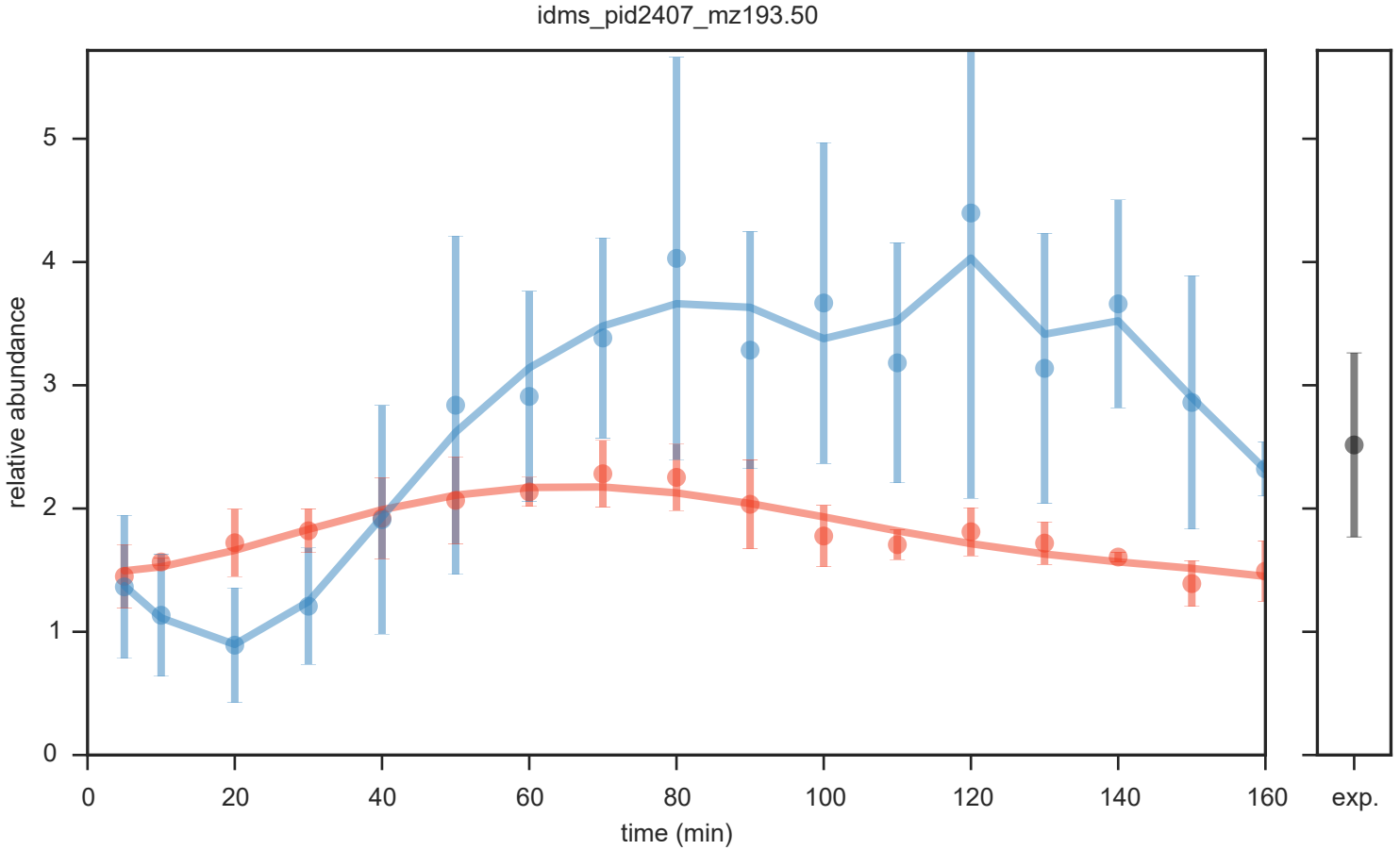

idms_pid2122_mz254.69
relative abundance
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

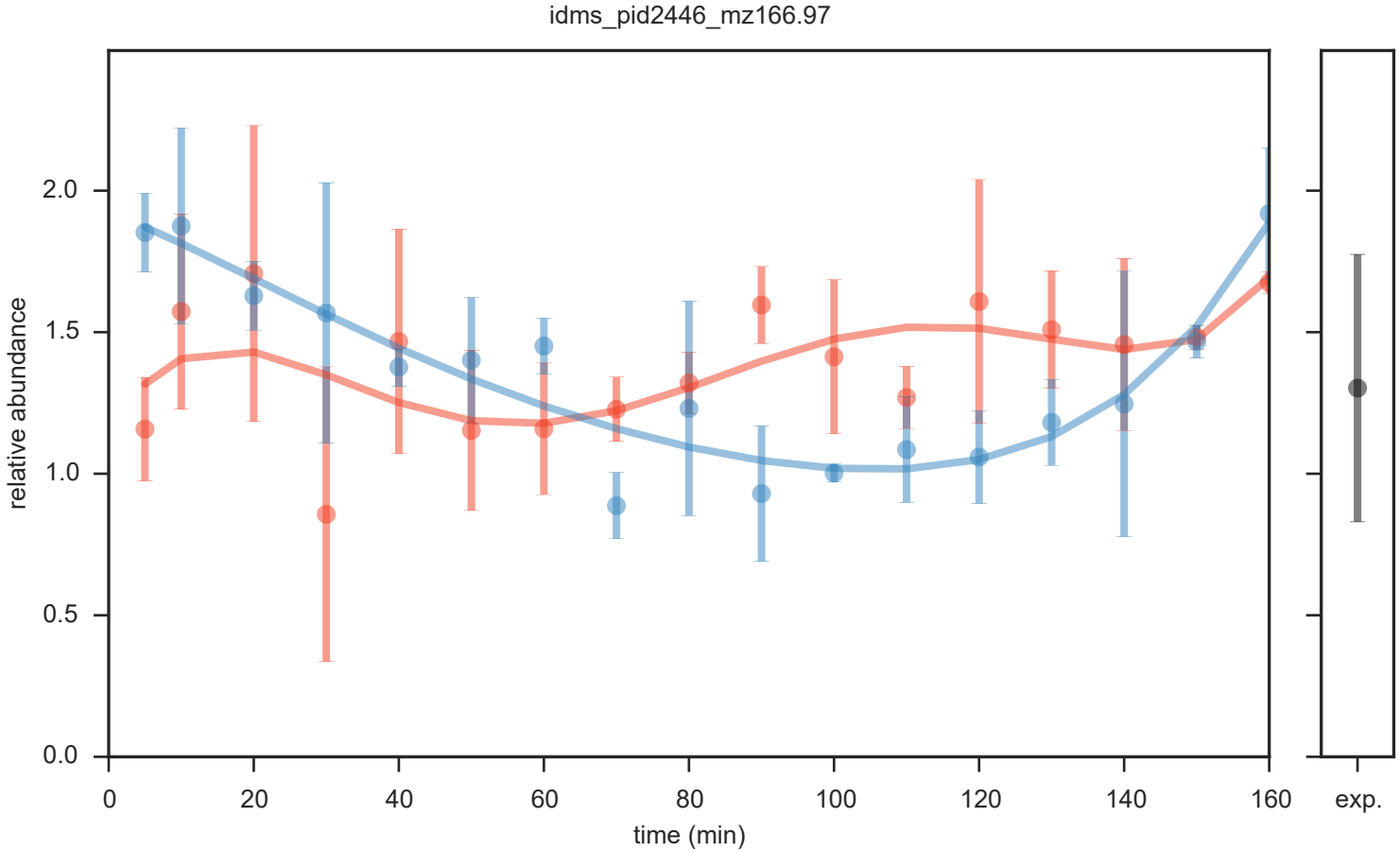

idms_pid2130_mz152.53
relative abundance
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

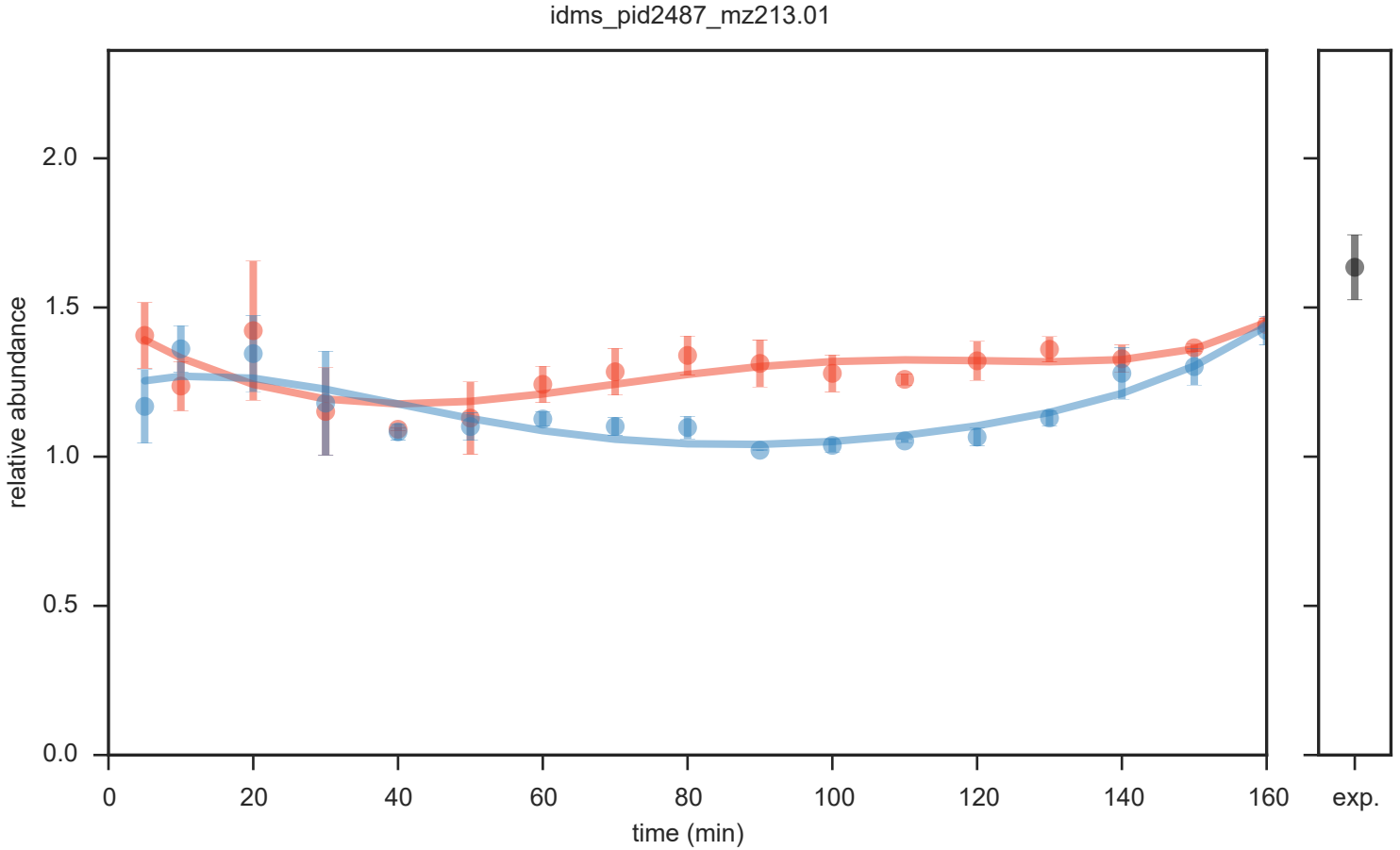

idms_pid2140_mz168.52
relative abundance
time (min)
exp.
0.0
0.5
1.0
1.5
2.0
2.5
3.0
0
20
40
60
80
100
120
140
160

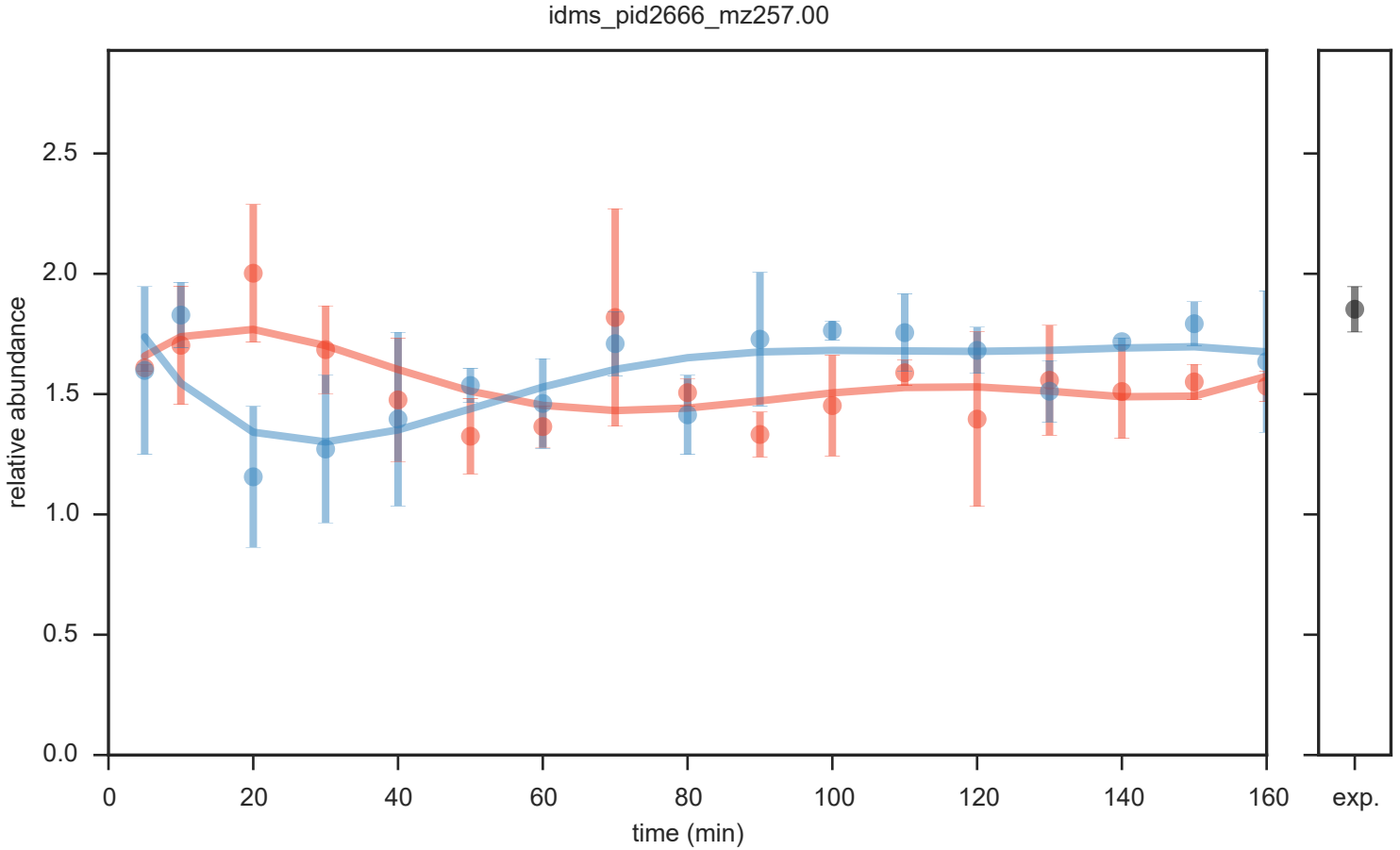

idms_pid2161_mz282.96
relative abundance
0.0
0.5
1.0
1.5
2.0
0
20
40
60
80
100
120
140
160
time (min)
exp.

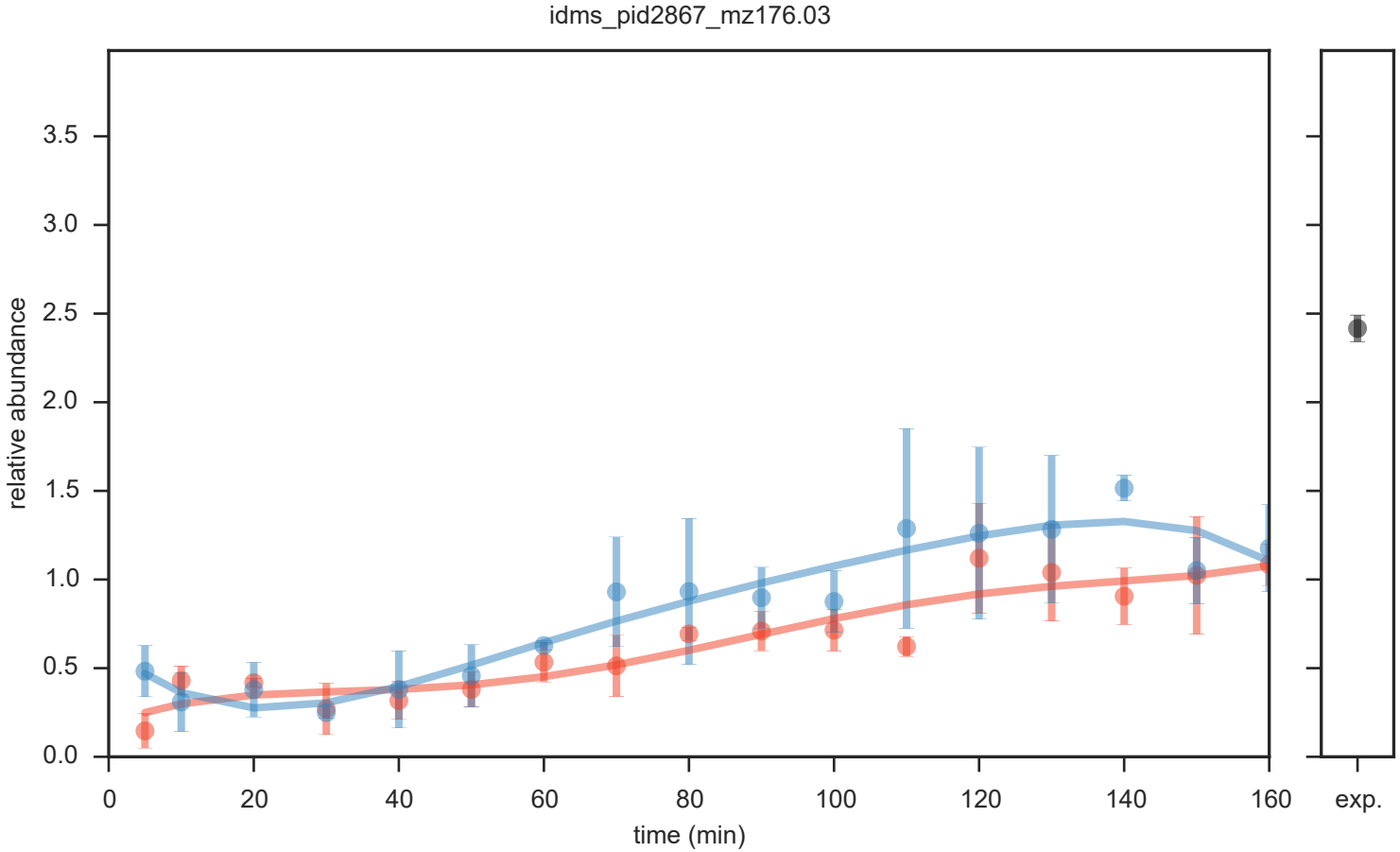

idms_pid2294_mz226.01
relative abundance
0.0
0.5
1.0
1.5
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid2407_mz193.50
relative abundance
0
1
2
3
4
5
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid2446_mz166.97
relative abundance
0.0
0.5
1.0
1.5
2.0
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid2487_mz213.01
relative abundance
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid2666_mz257.00
relative abundance
0.0
0.5
1.0
1.5
2.0
2.5
0
20
40
60
80
100
120
140
160
time (min)
exp.


idms_pid2867_mz176.03
relative abundance
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
0
20
40
60
80
100
120
140
160
time (min)
exp.