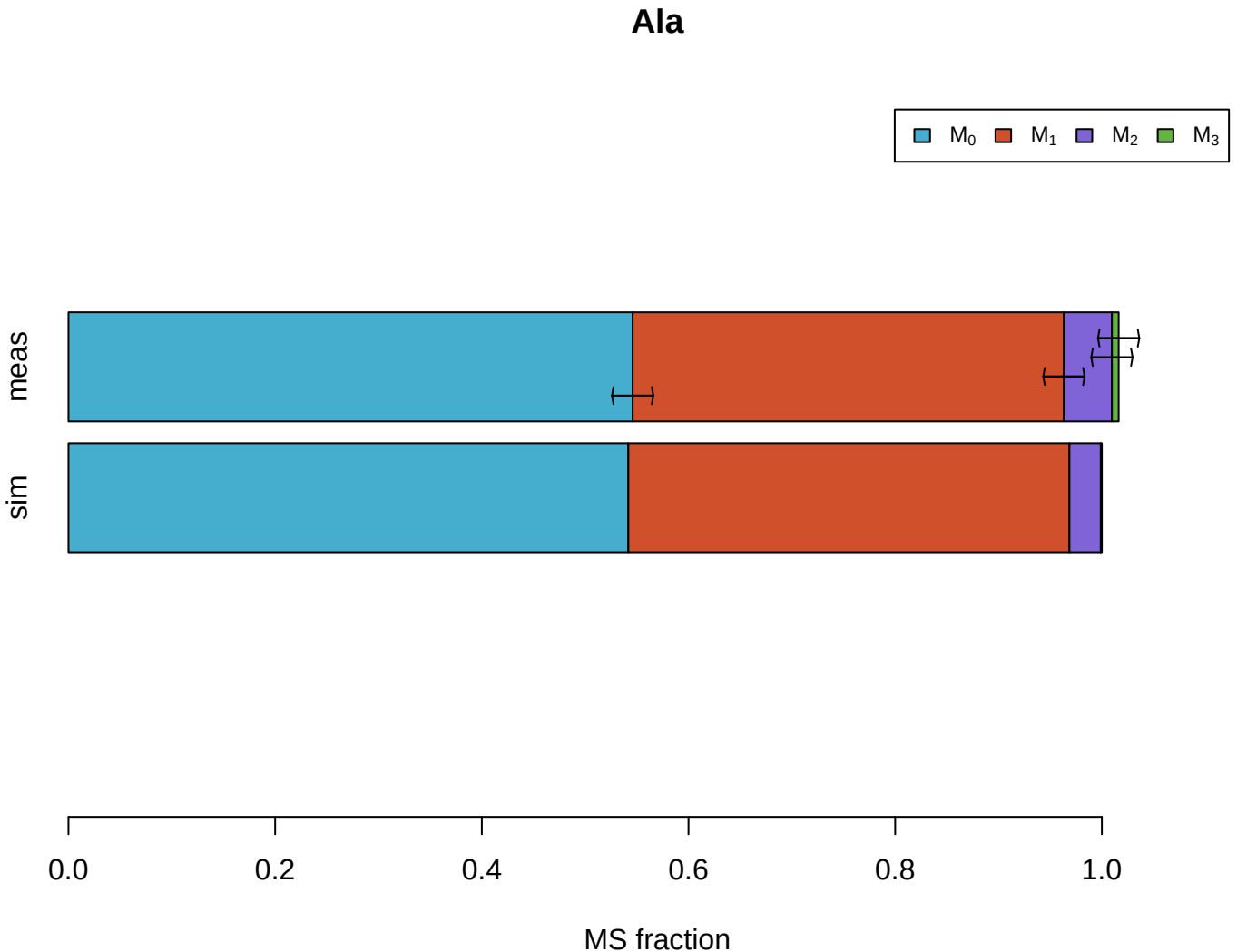
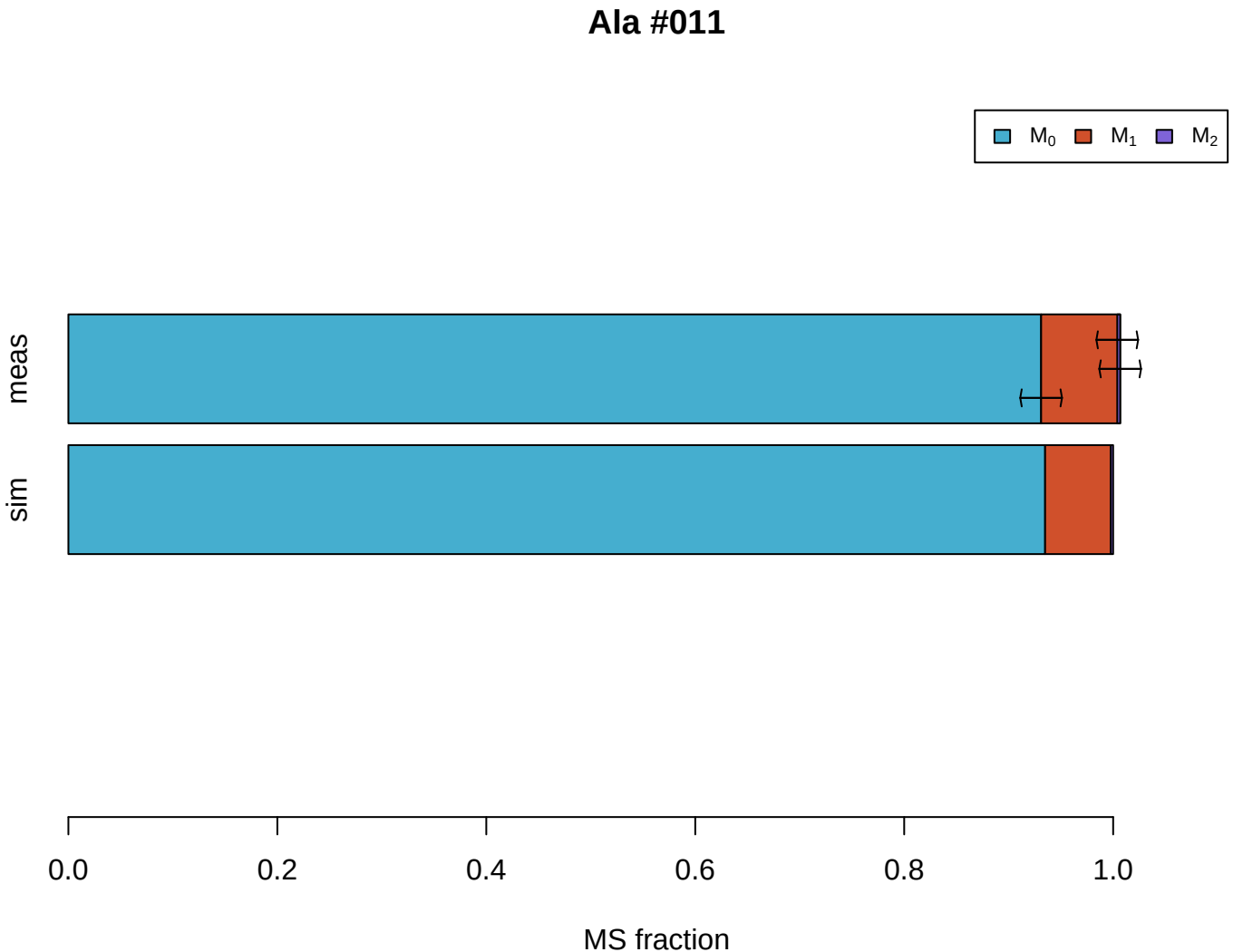
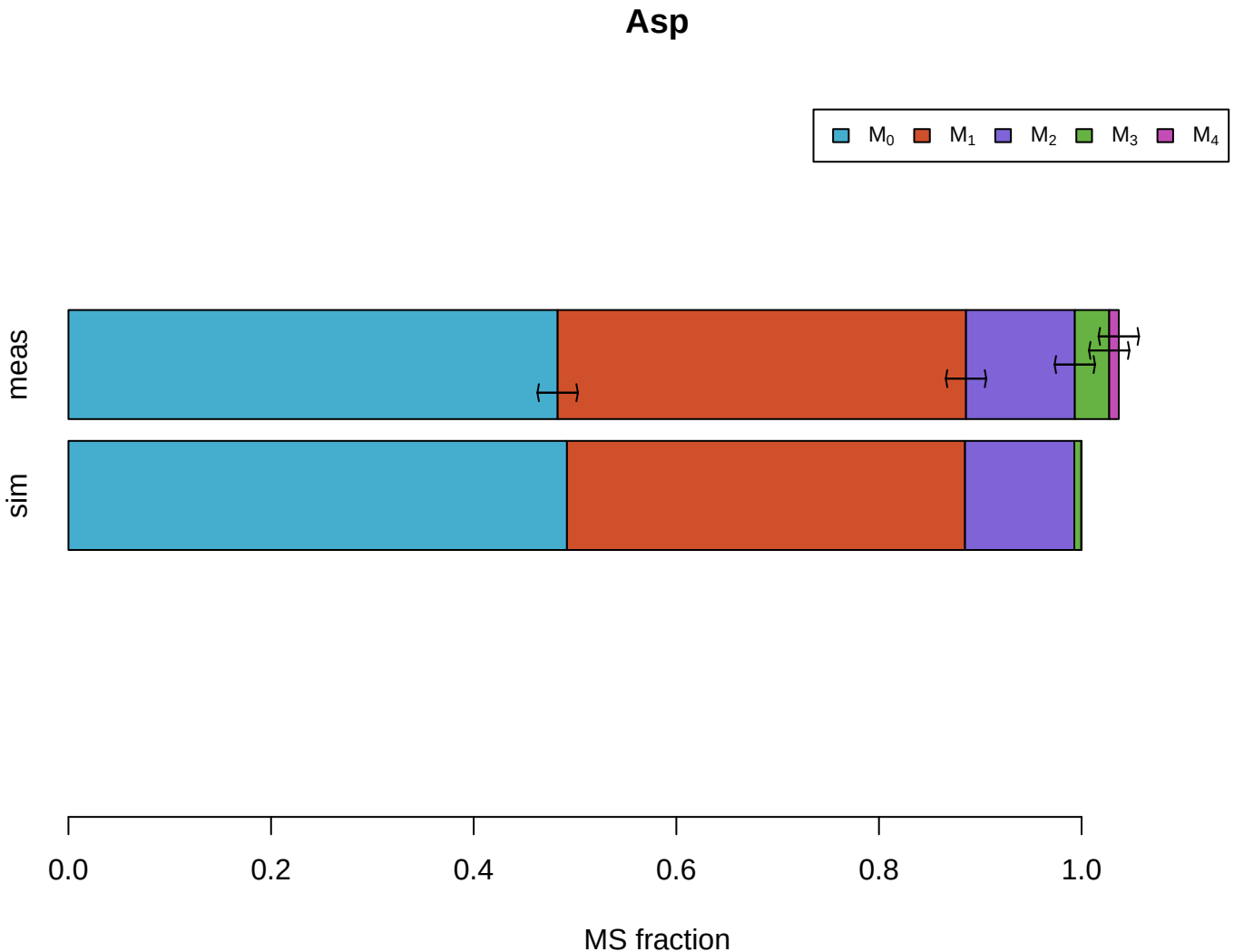
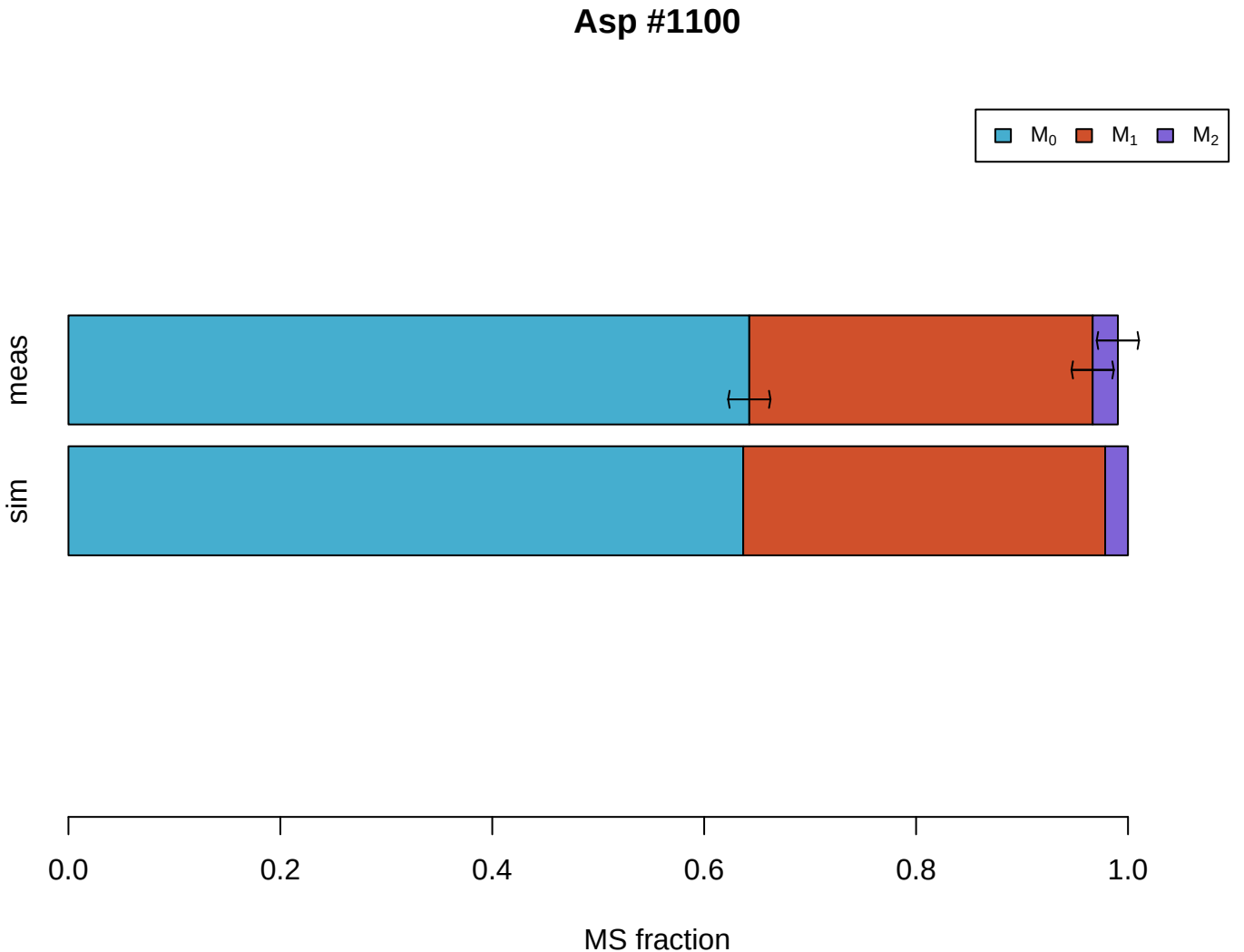
MS measurements
(error bars=±2*dev)


Ala
M0
M1
M2
M3
meas
sim
0.0
0.2
0.4
0.6
0.8
1.0
MS fraction


Ala #011
M0
M1
M2
meas
sim
0.0
0.2
0.4
0.6
0.8
1.0
MS fraction


Asp
M0
M1
M2
M3
M4
meas
sim
0.0
0.2
0.4
0.6
0.8
1.0
MS fraction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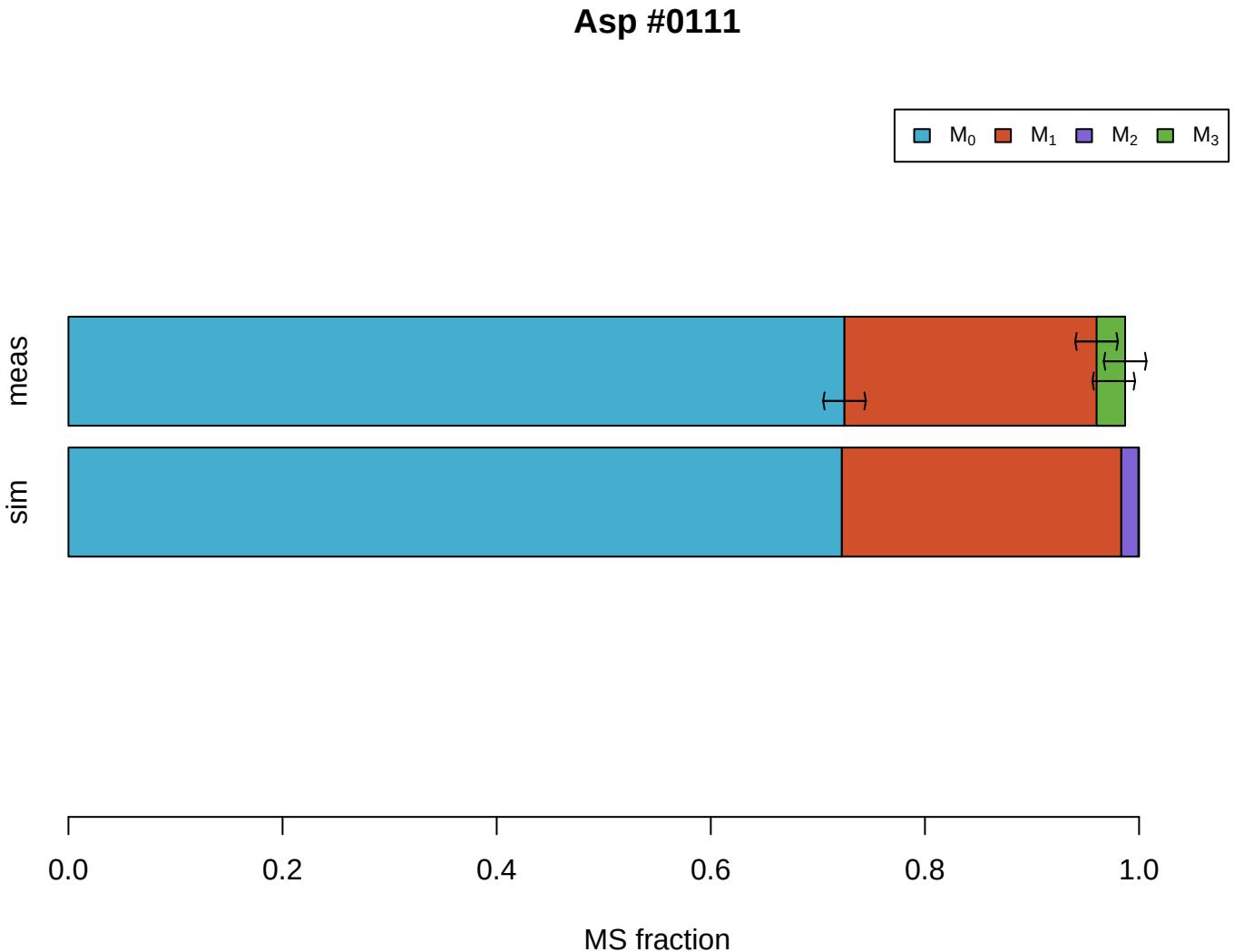
M1
M2
meas
sim
0.0
0.2
0.4
0.6
0.8
1.0
MS fraction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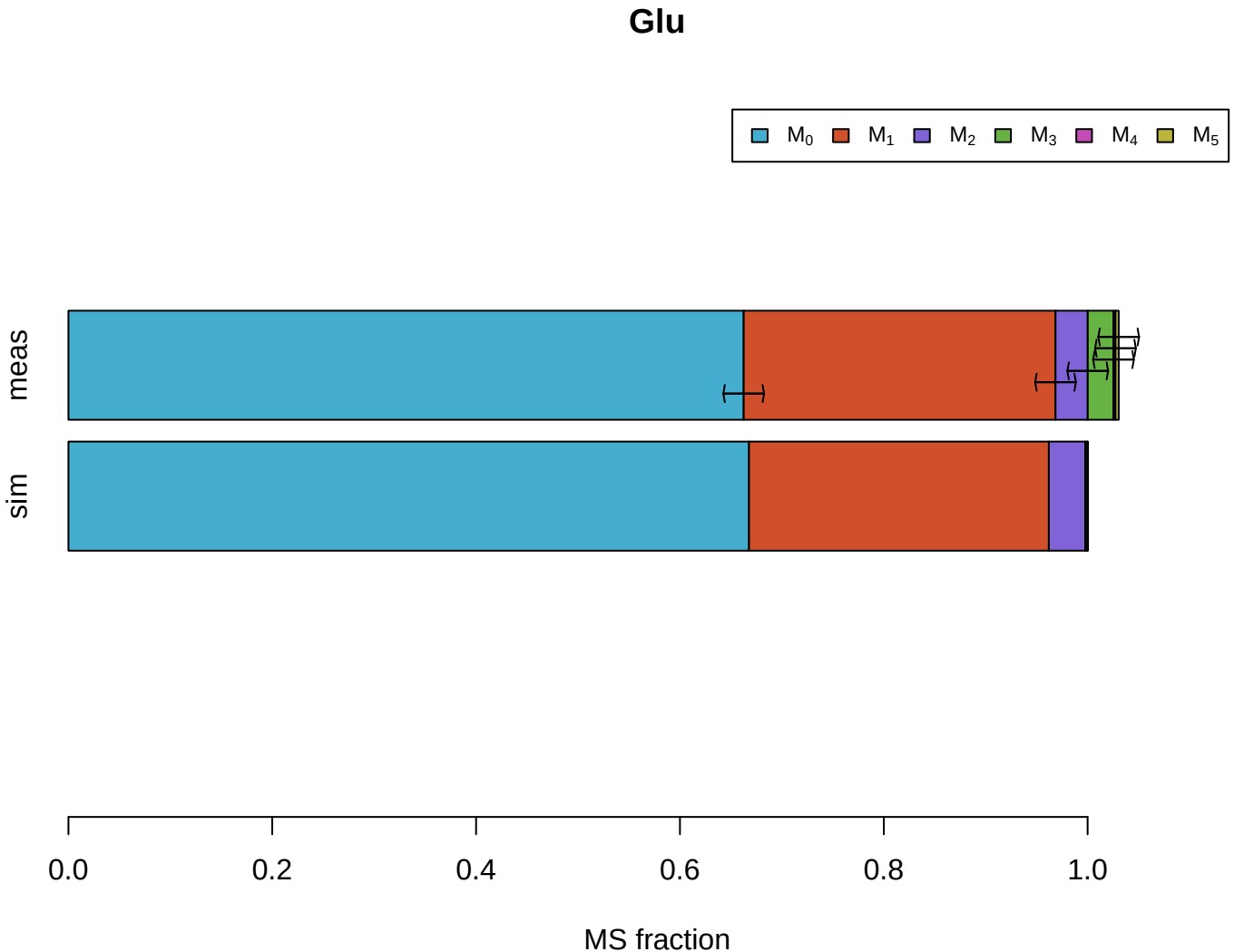
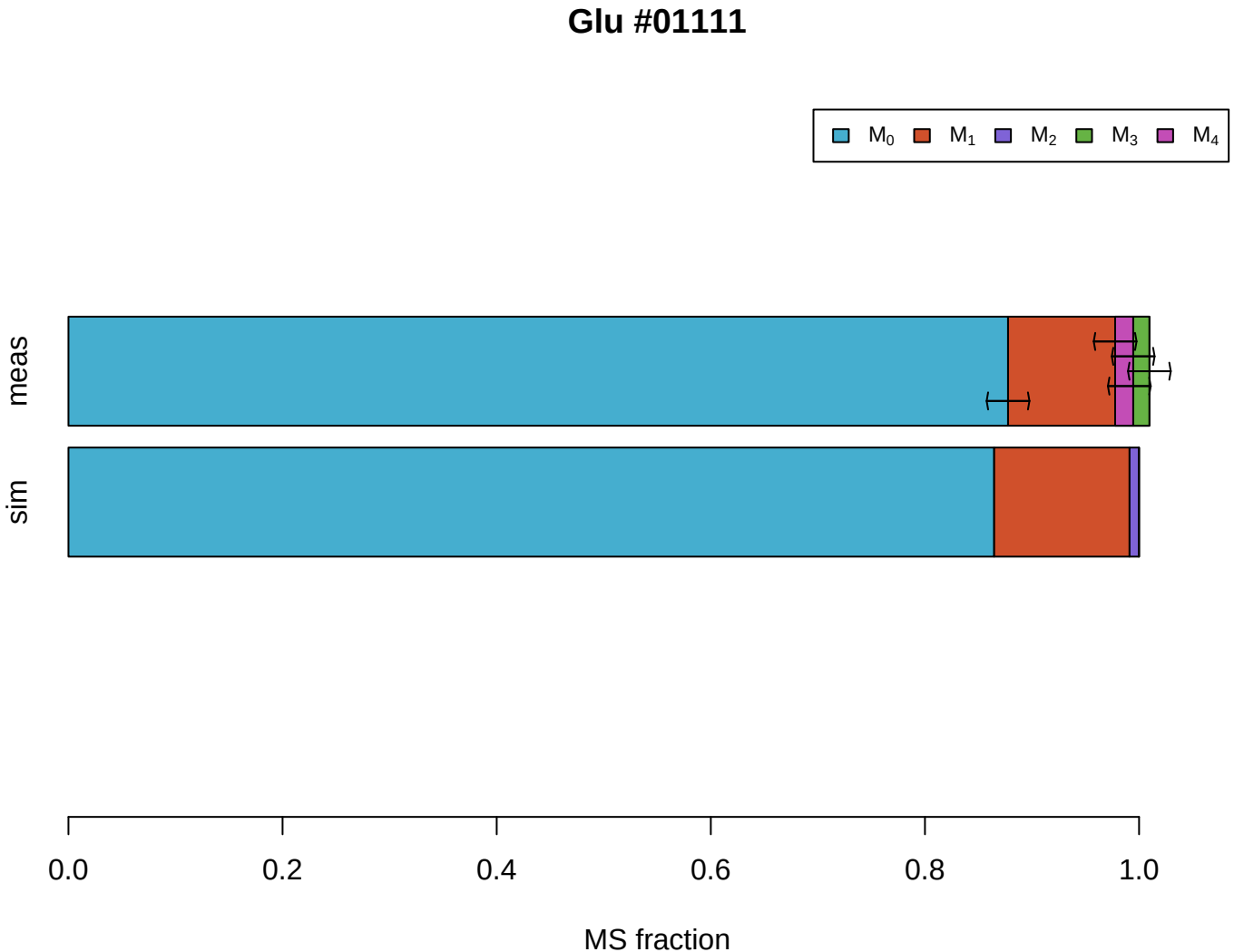
M0
M1
M2
M3
meas
sim
0.0
0.2
0.4
0.6
0.8
1.0
MS fraction


Glu
M0
M1
M2
M3
M4
M5
meas
sim
0.0
0.2
0.4
0.6
0.8
1.0
MS fraction


Glu #01111
M0
M1
M2
M3
M4
meas
sim
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0.4
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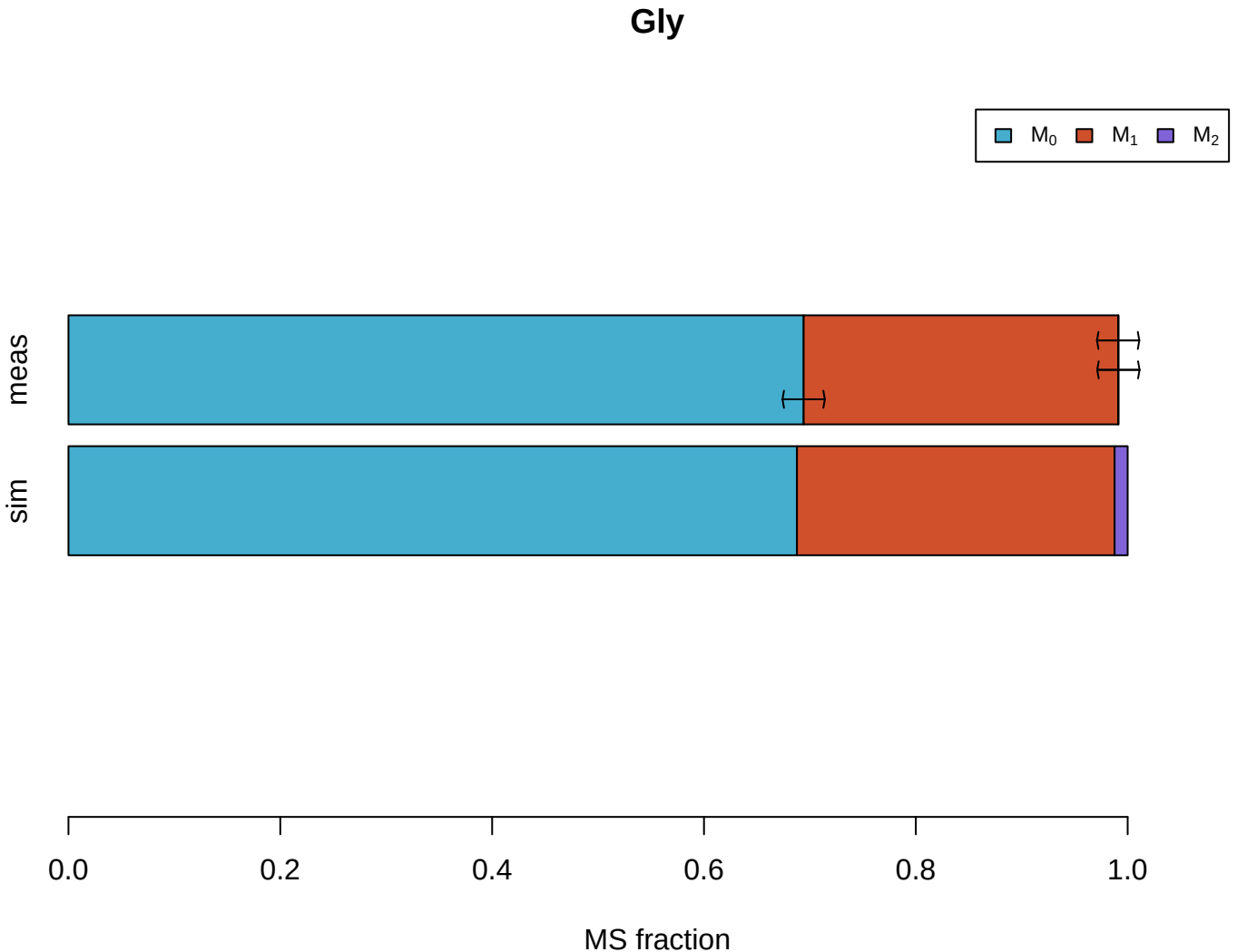
0.8
1.0
MS fraction


Gly
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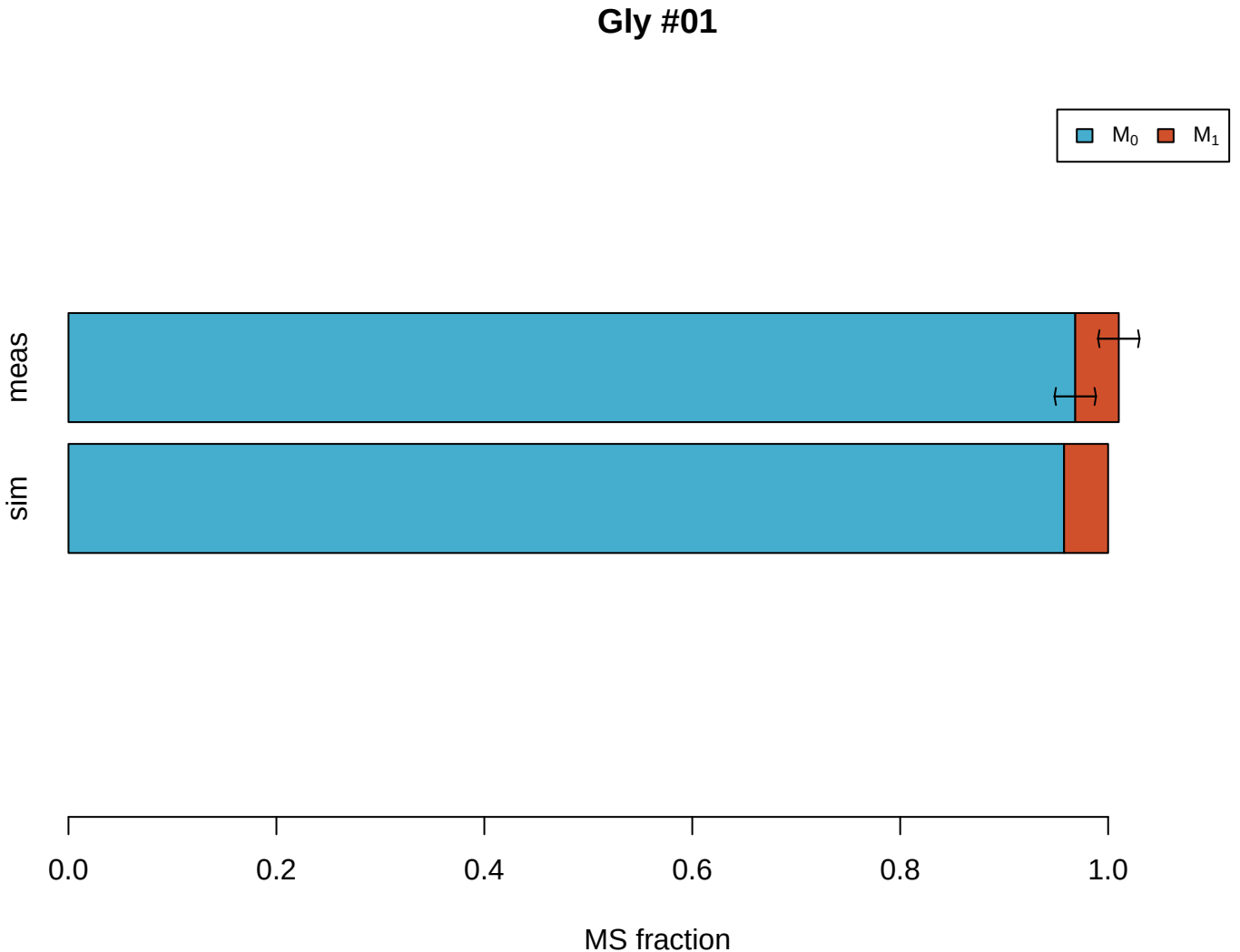
M1
M2
meas
sim
0.0
0.2
0.4
0.6
0.8
1.0
MS fraction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sim
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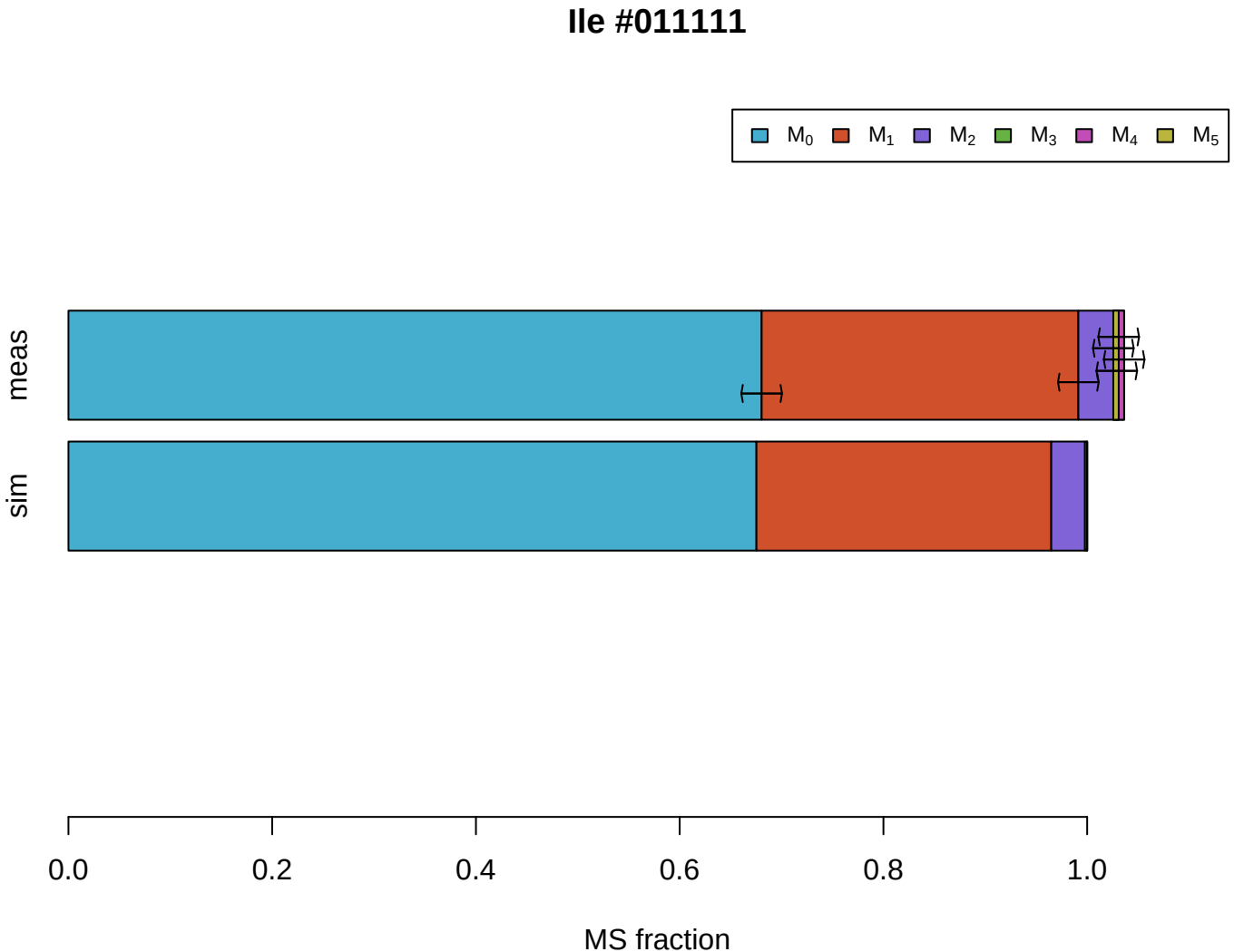
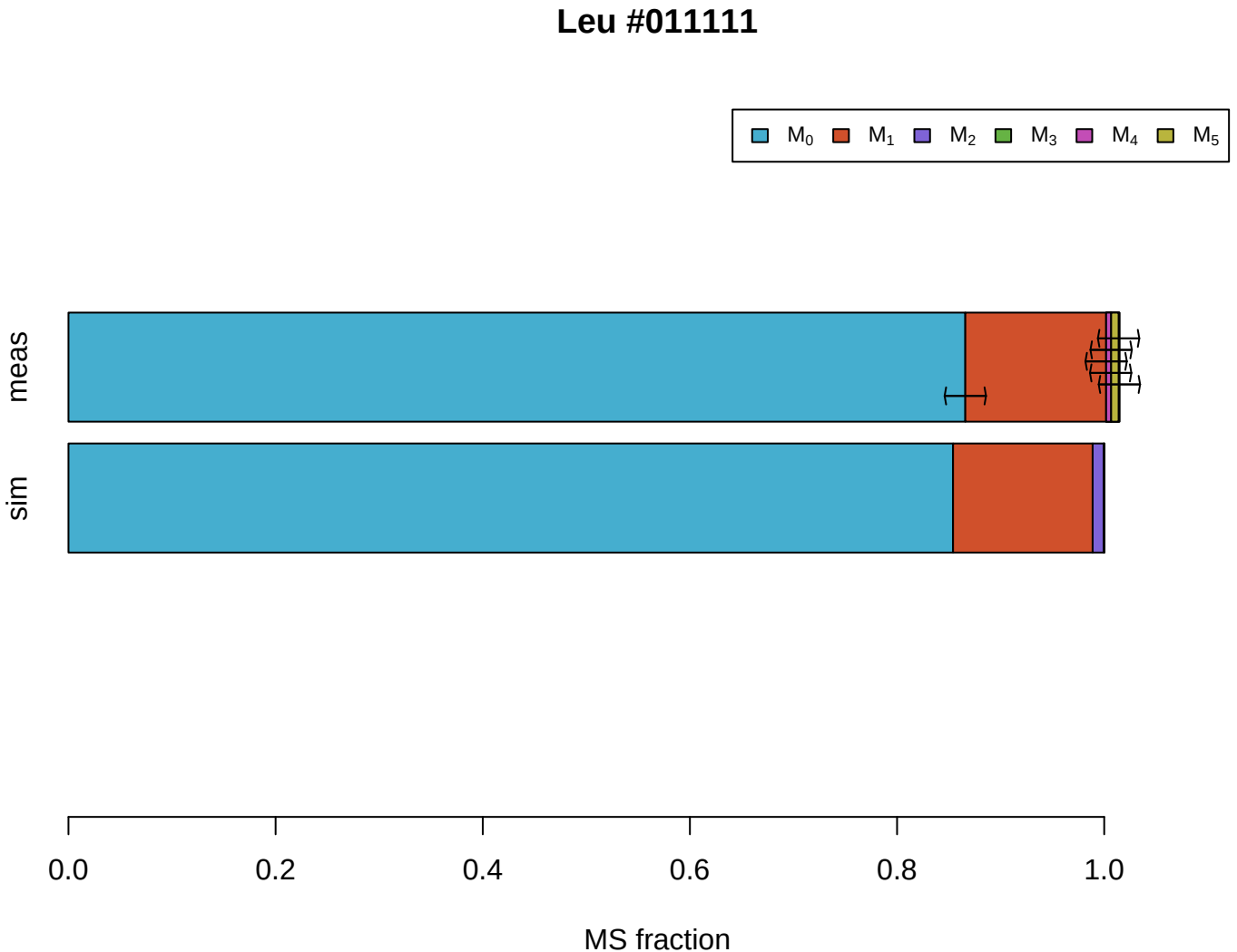
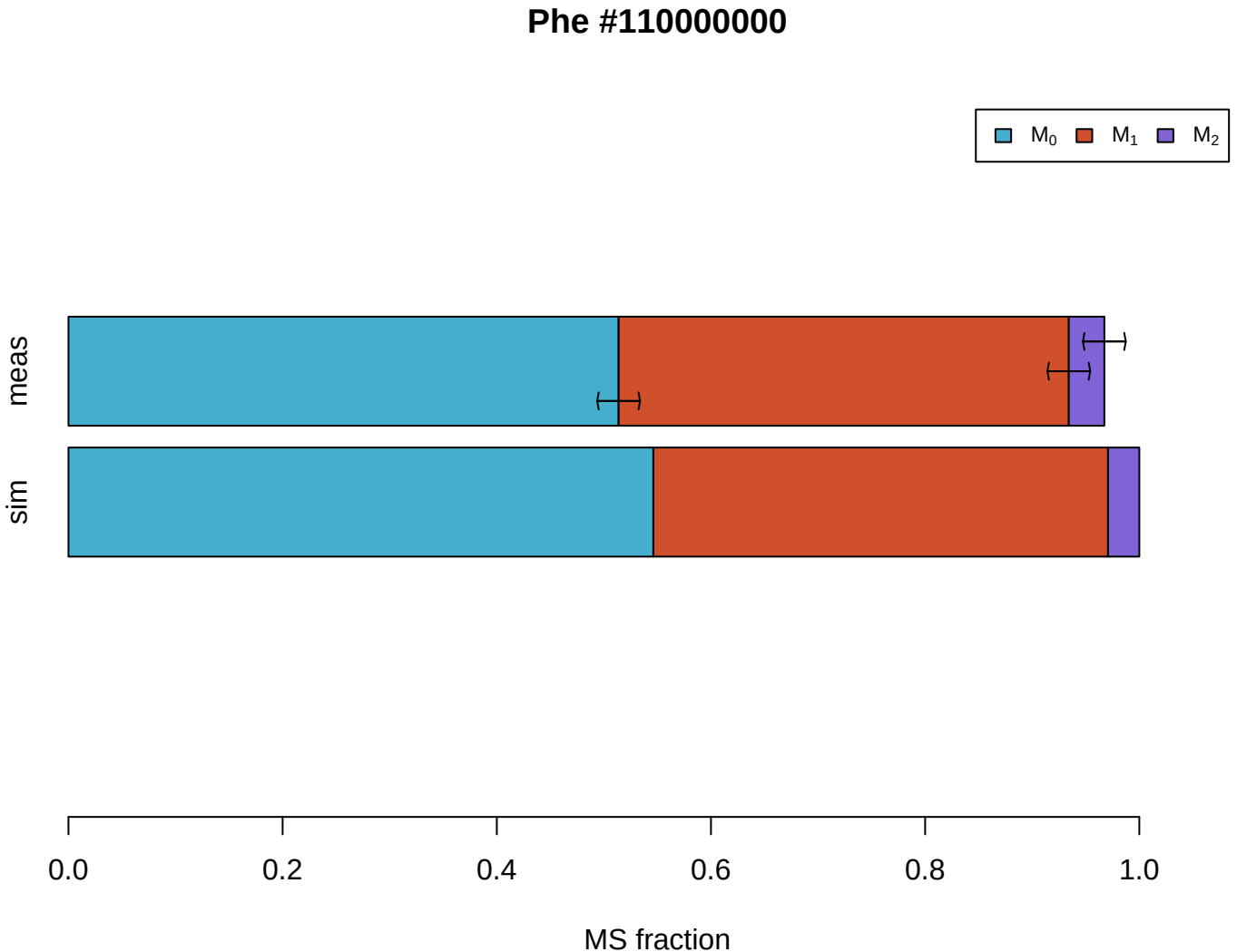
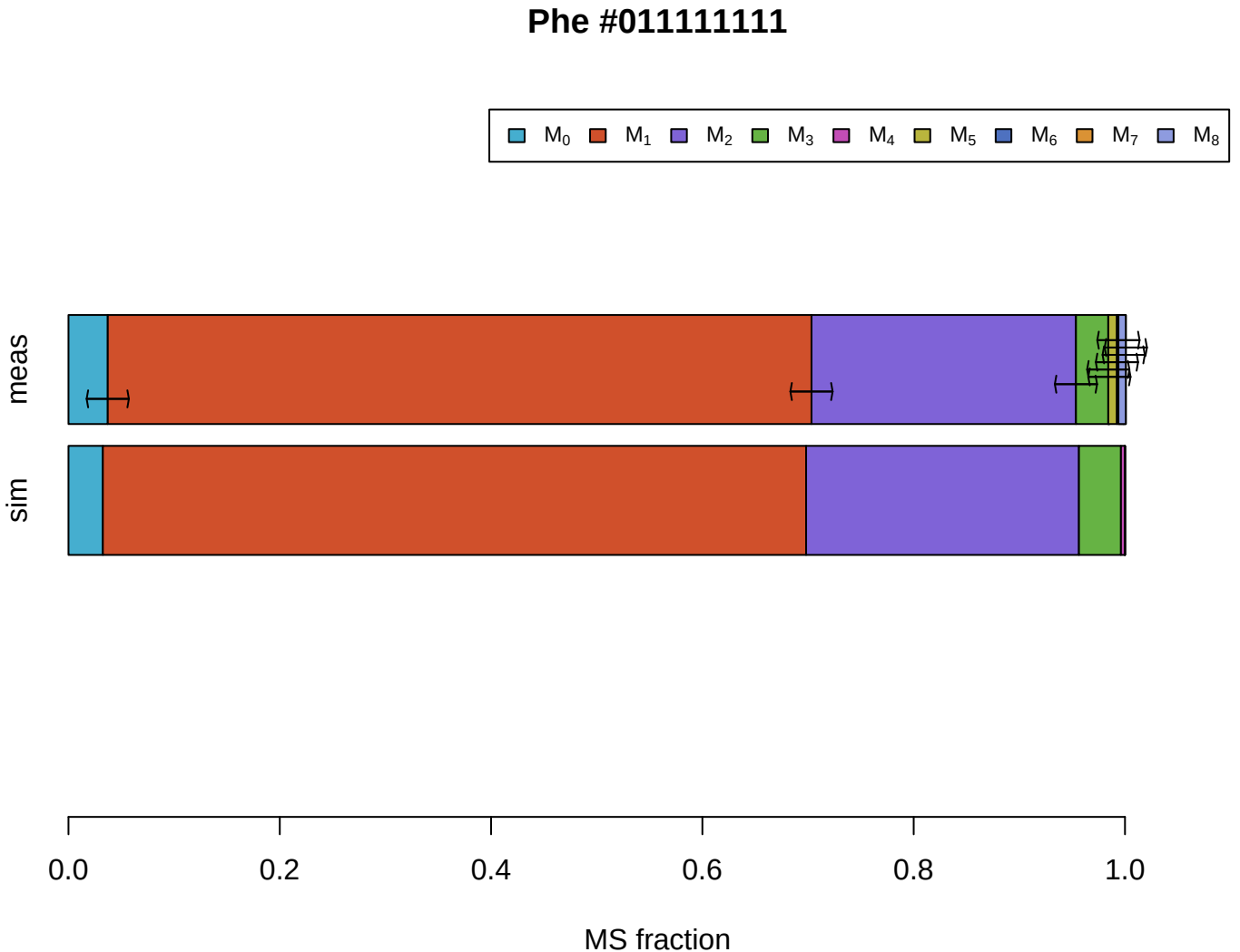
0.4
0.6
0.8
1.0
MS fraction


Ile #011111
M0
M1
M2
M3
M4
M5
meas
sim
0.0
0.2
0.4
0.6
0.8
1.0
MS fraction


Leu #011111
M0
M1
M2
M3
M4
M5
meas
sim
0.0
0.2
0.4
0.6
0.8
1.0
MS fraction


Phe #110000000
M0
M1
M2
meas
sim
0.0
0.2
0.4
0.6
0.8
1.0
MS fraction


Phe #011111111
M0
M1
M2
M3
M4
M5
M6
M7
M8
meas
sim
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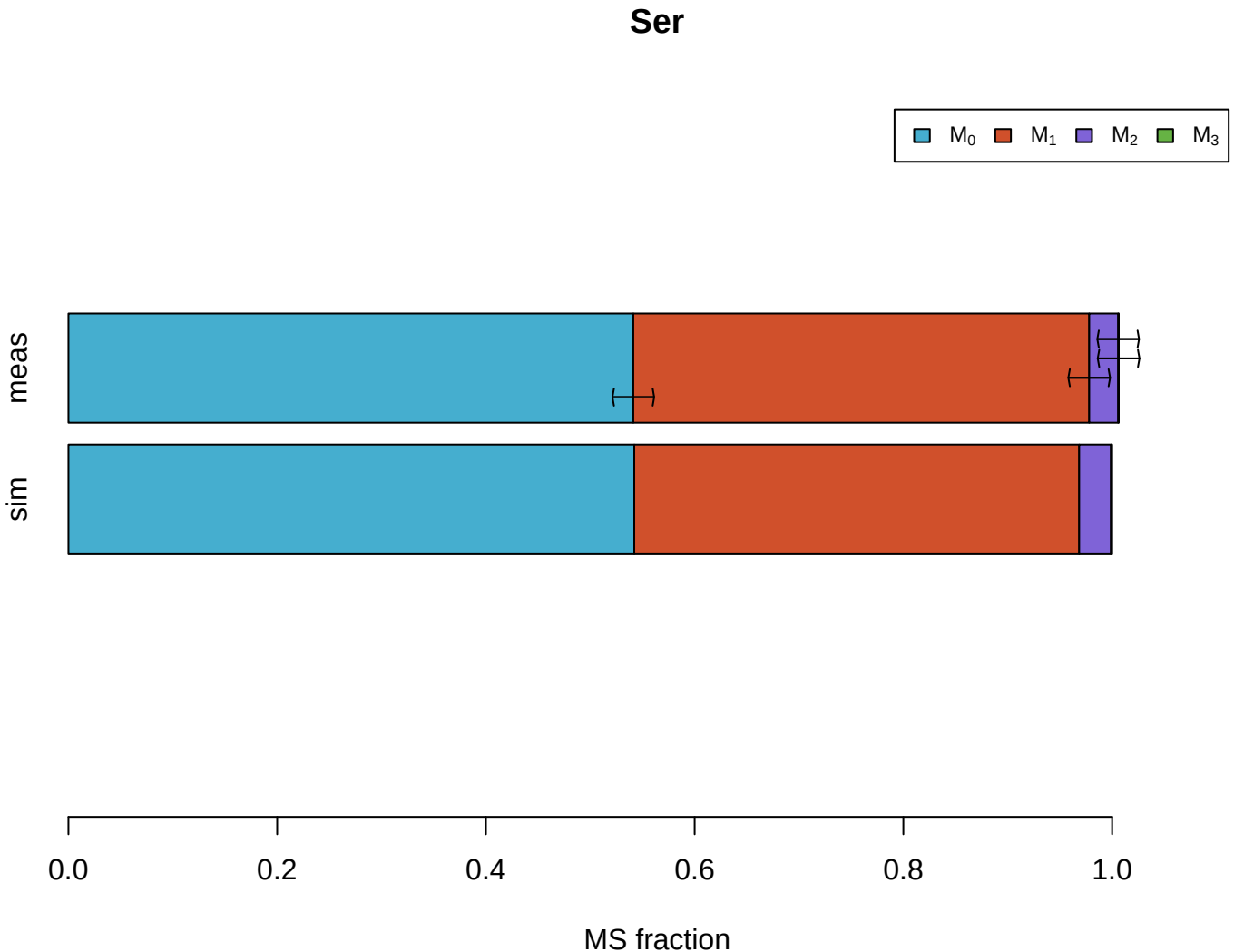
0.2
0.4
0.6
0.8
1.0
MS fraction


Ser
M0
M1
M2
M3
meas
sim
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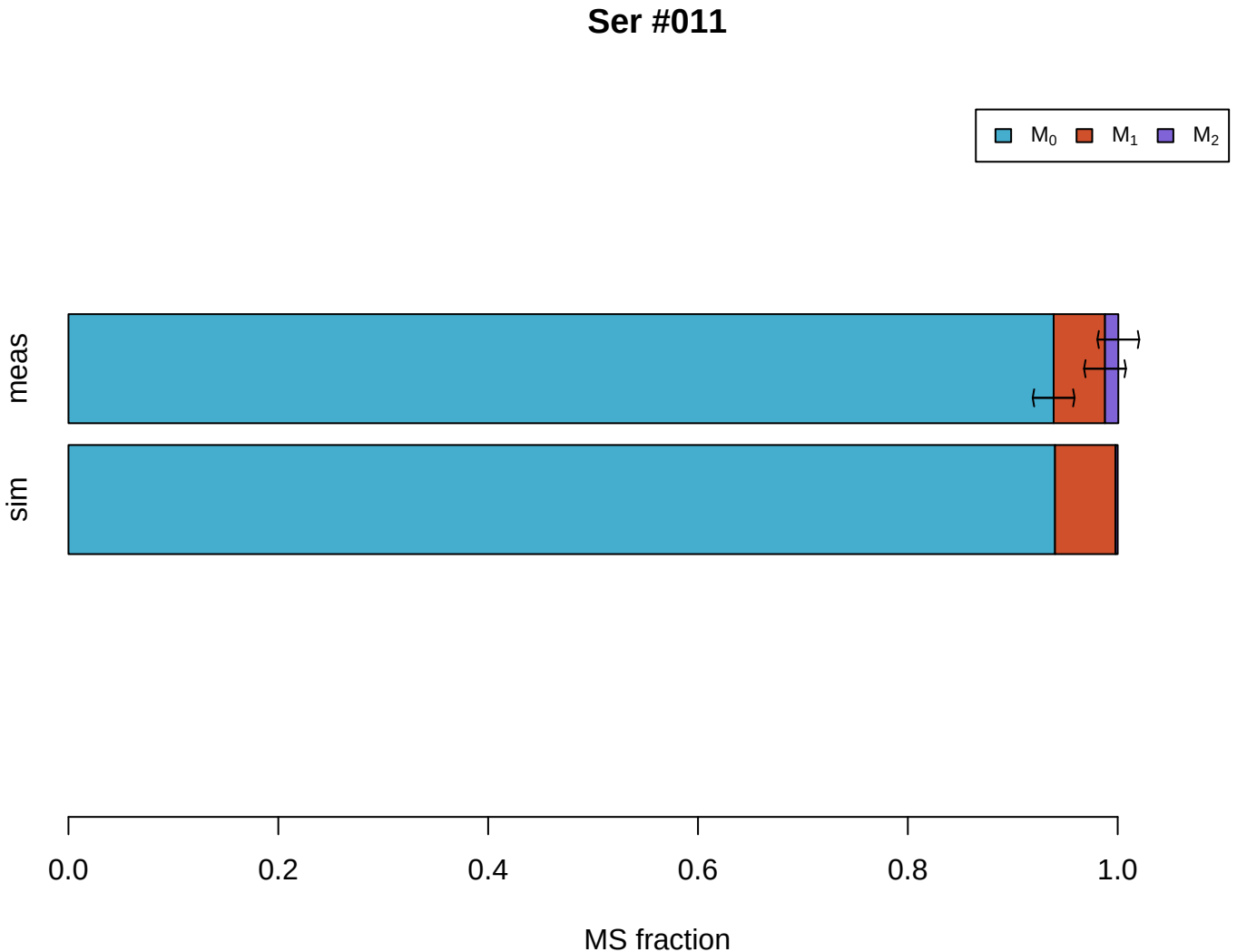
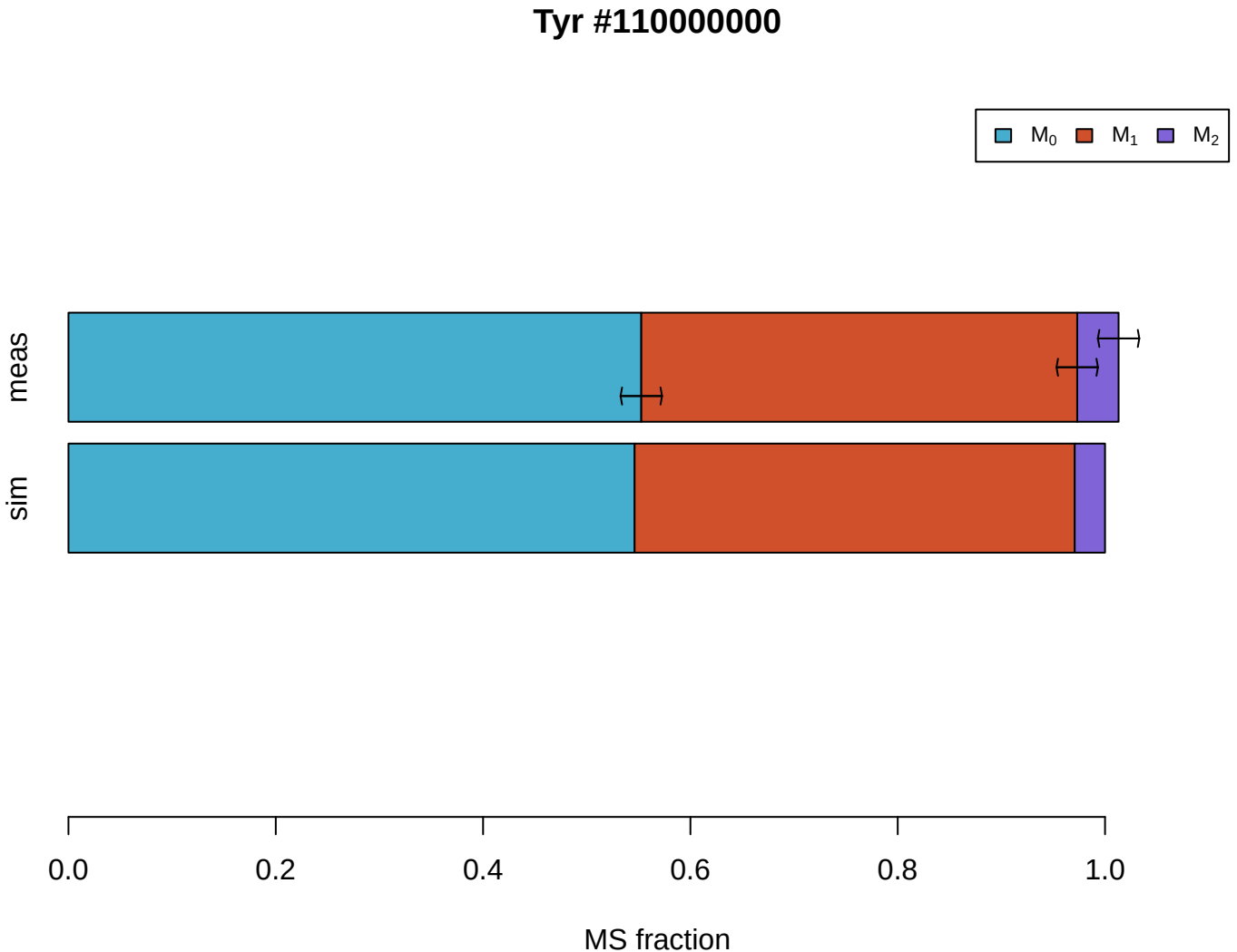
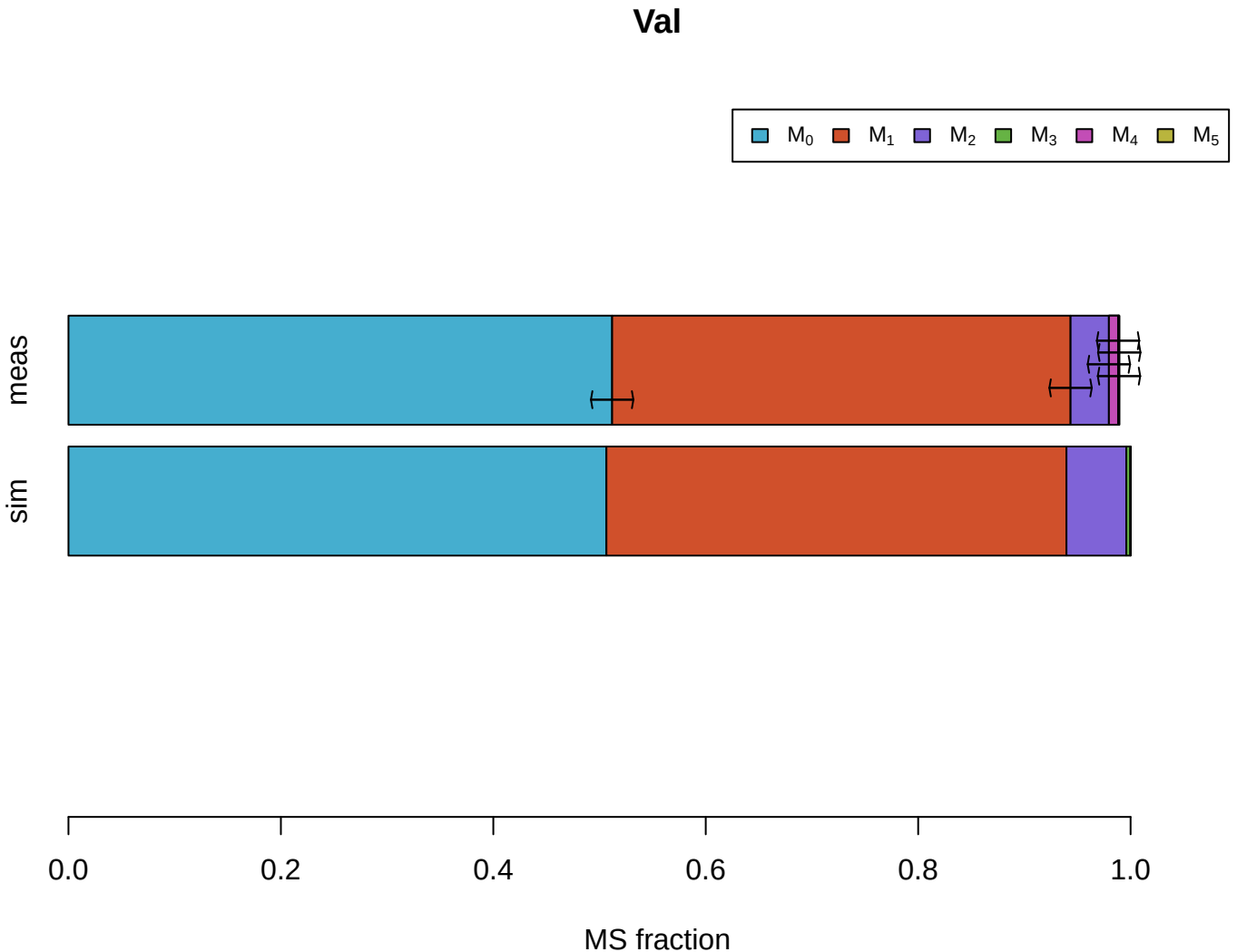
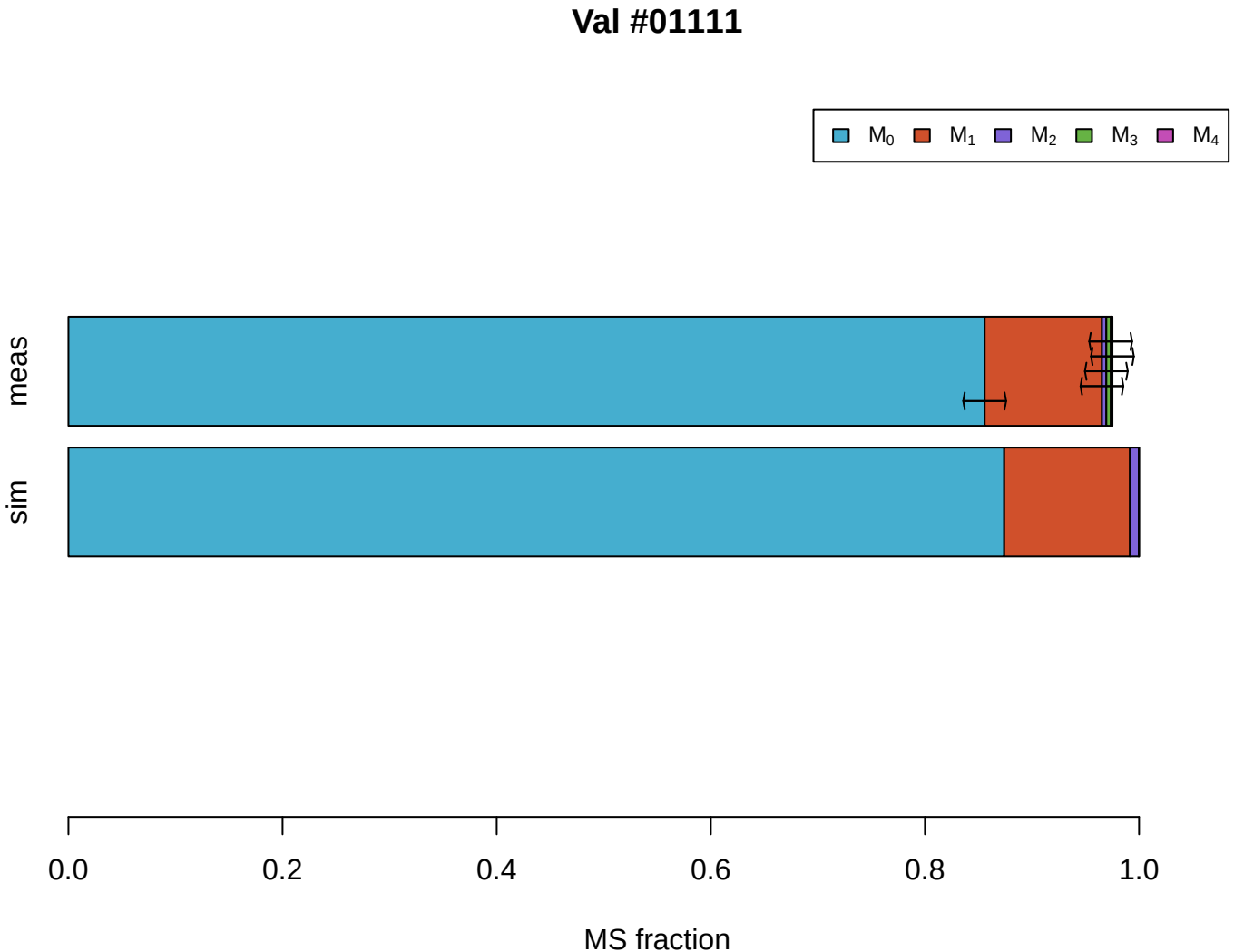
0.2
0.4
0.6
0.8
1.0
MS fraction

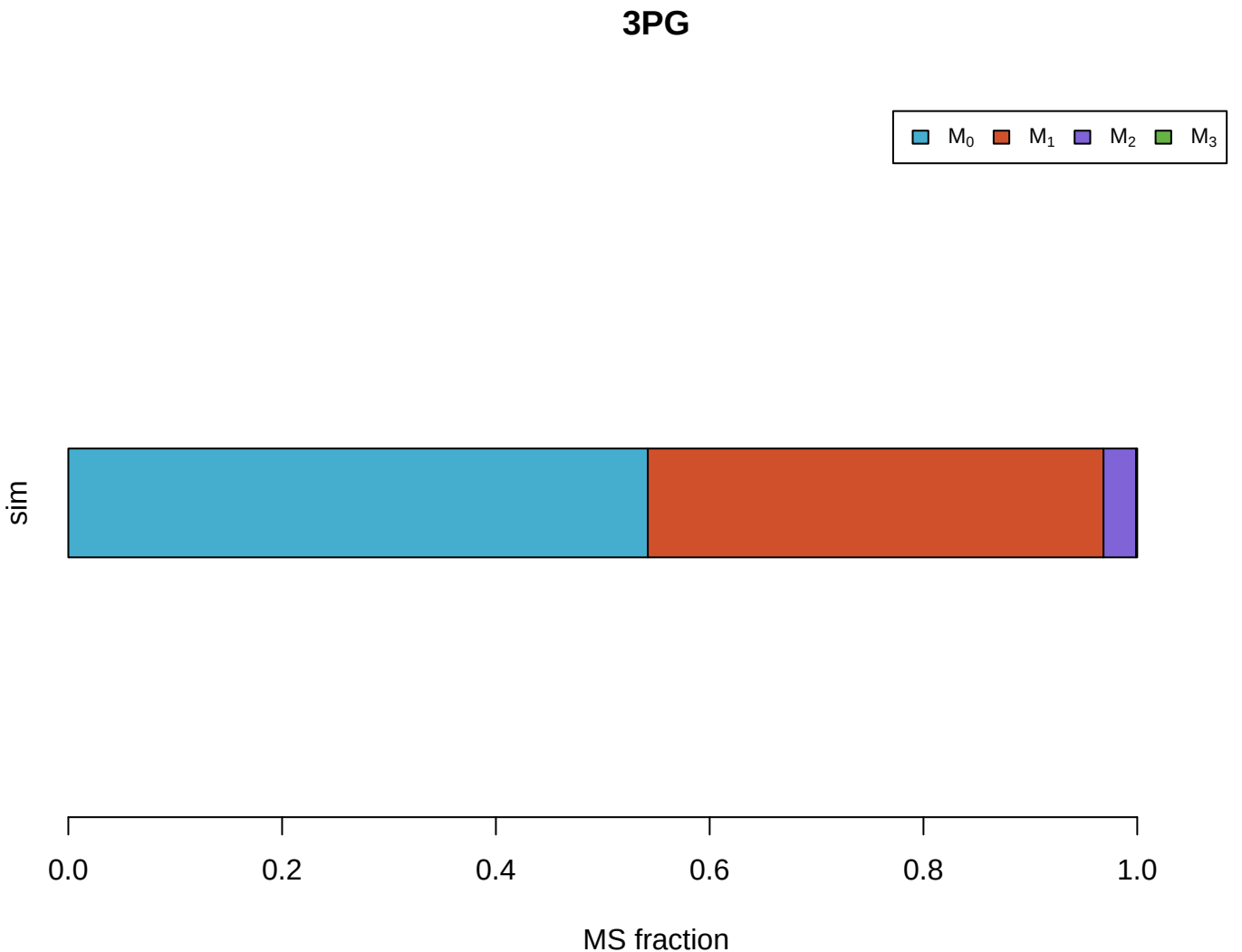

Ser #011
M0
M1
M2
meas
sim
0.0
0.2
0.4
0.6
0.8
1.0
MS fraction

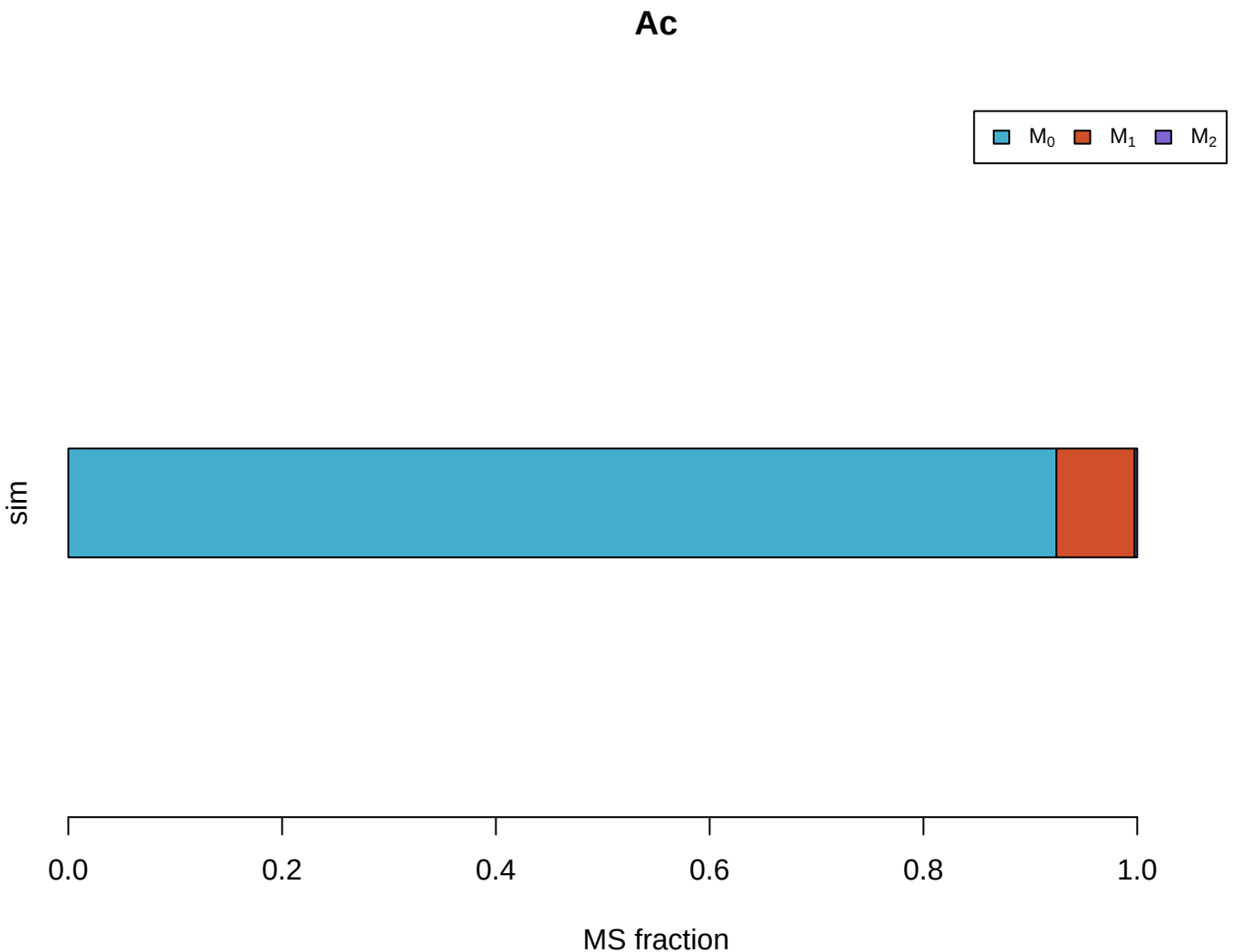

Tyr #110000000
M0
M1
M2
meas
sim
0.0
0.2
0.4
0.6
0.8
1.0
MS fraction

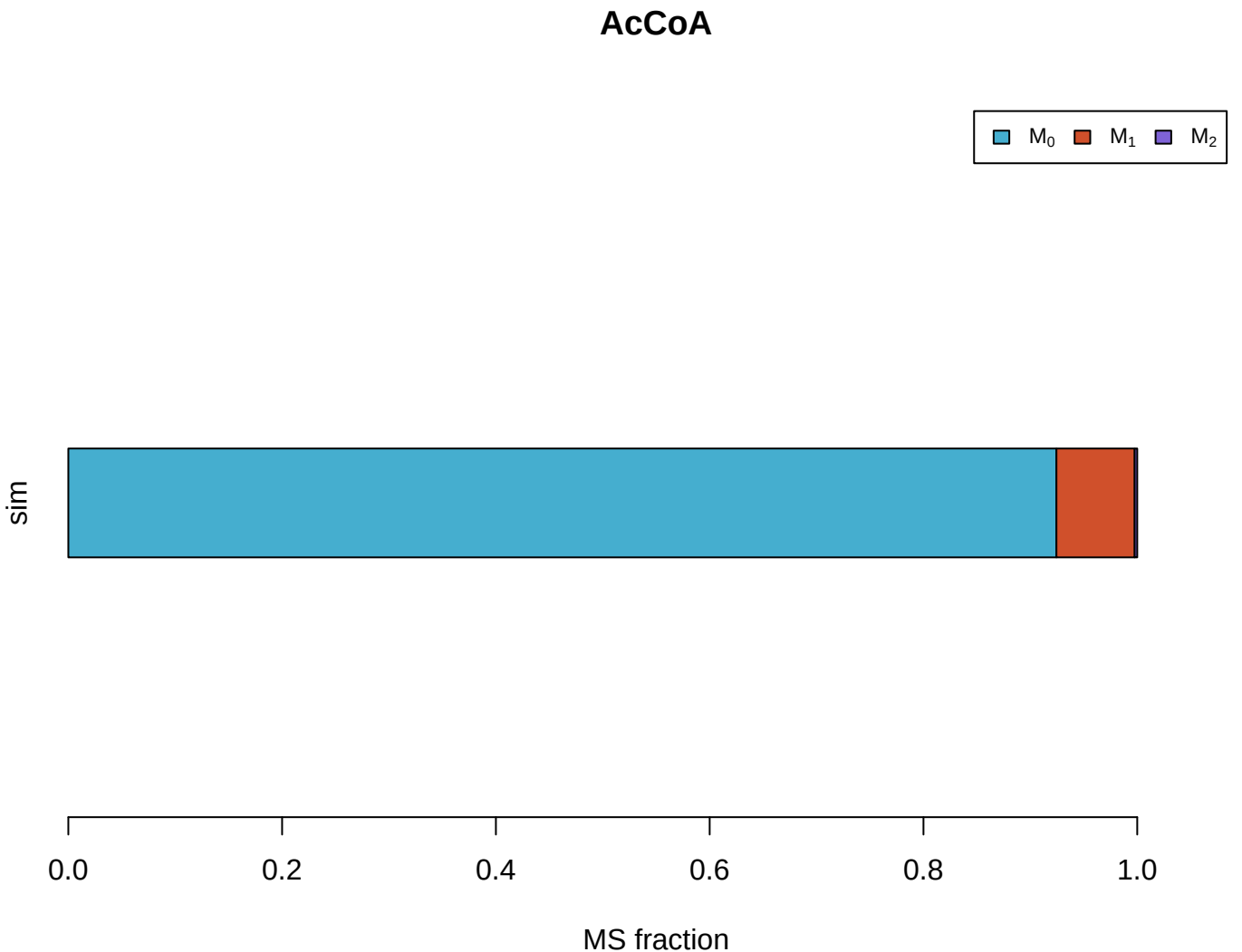

Val
M0
M1
M2
M3
M4
M5
meas
sim
0.0
0.2
0.4
0.6
0.8
1.0
MS fraction

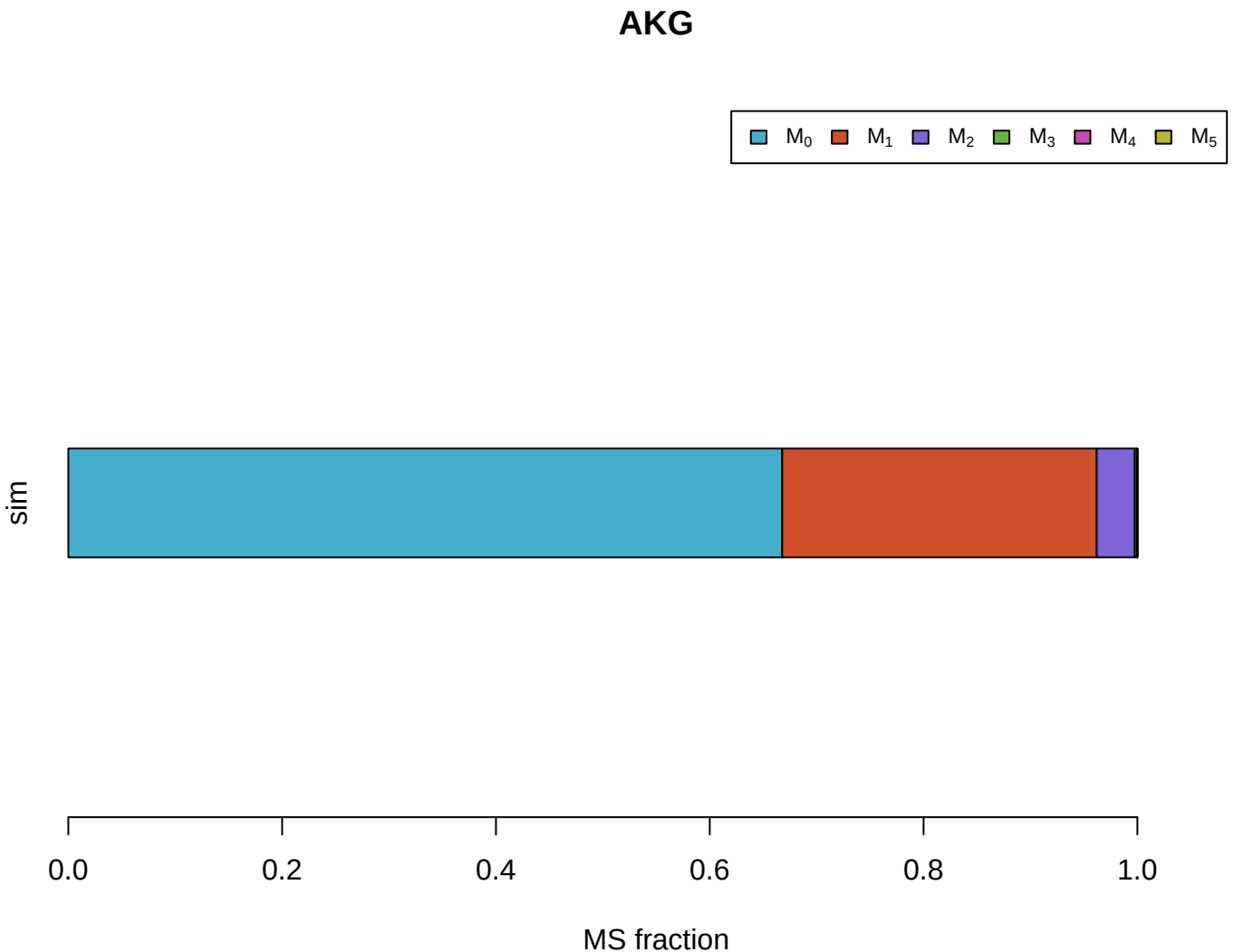

Val #01111
M0
M1
M2
M3
M4
meas
sim
0.0
0.2
0.4
0.6
0.8
1.0
MS fraction

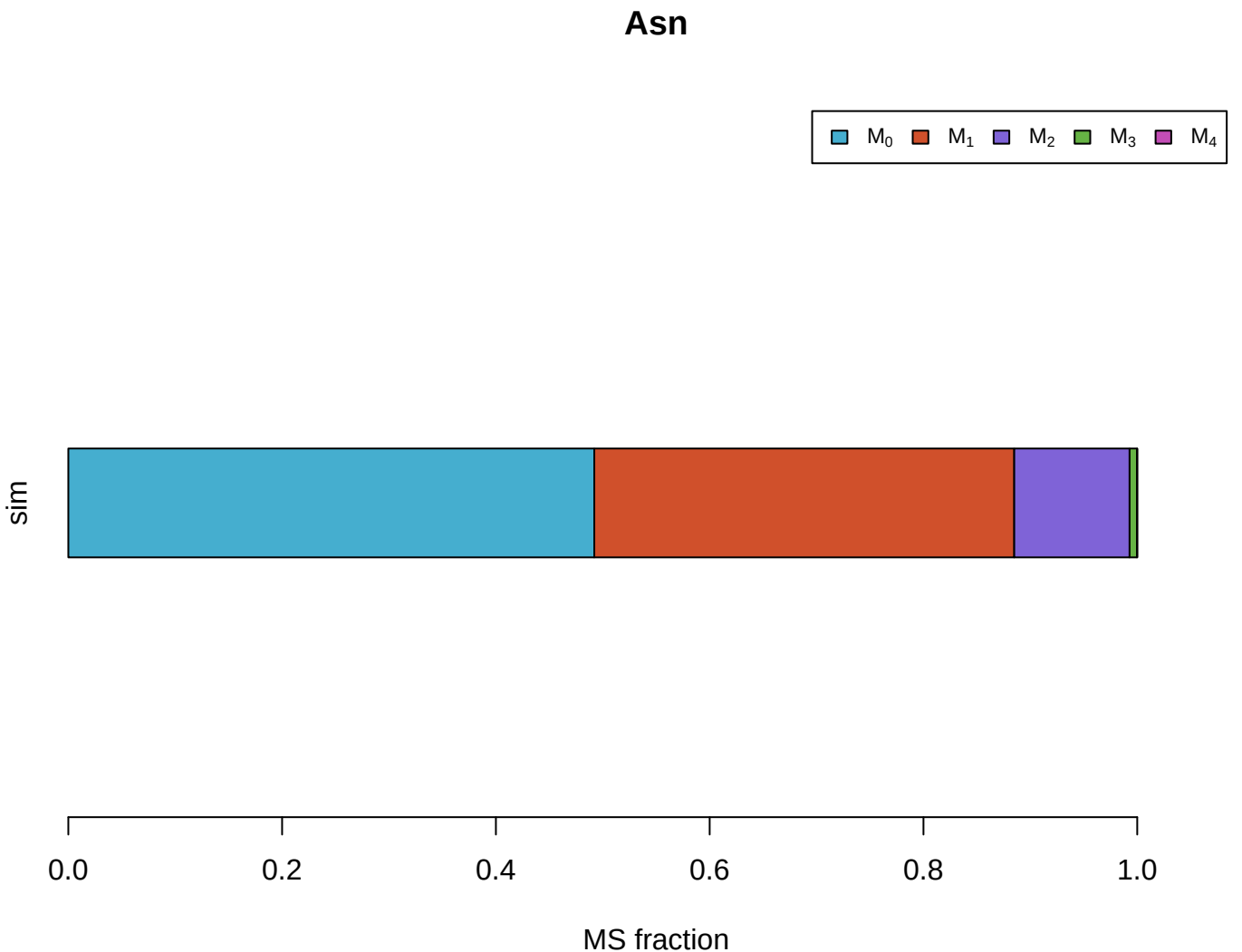
MS simulations

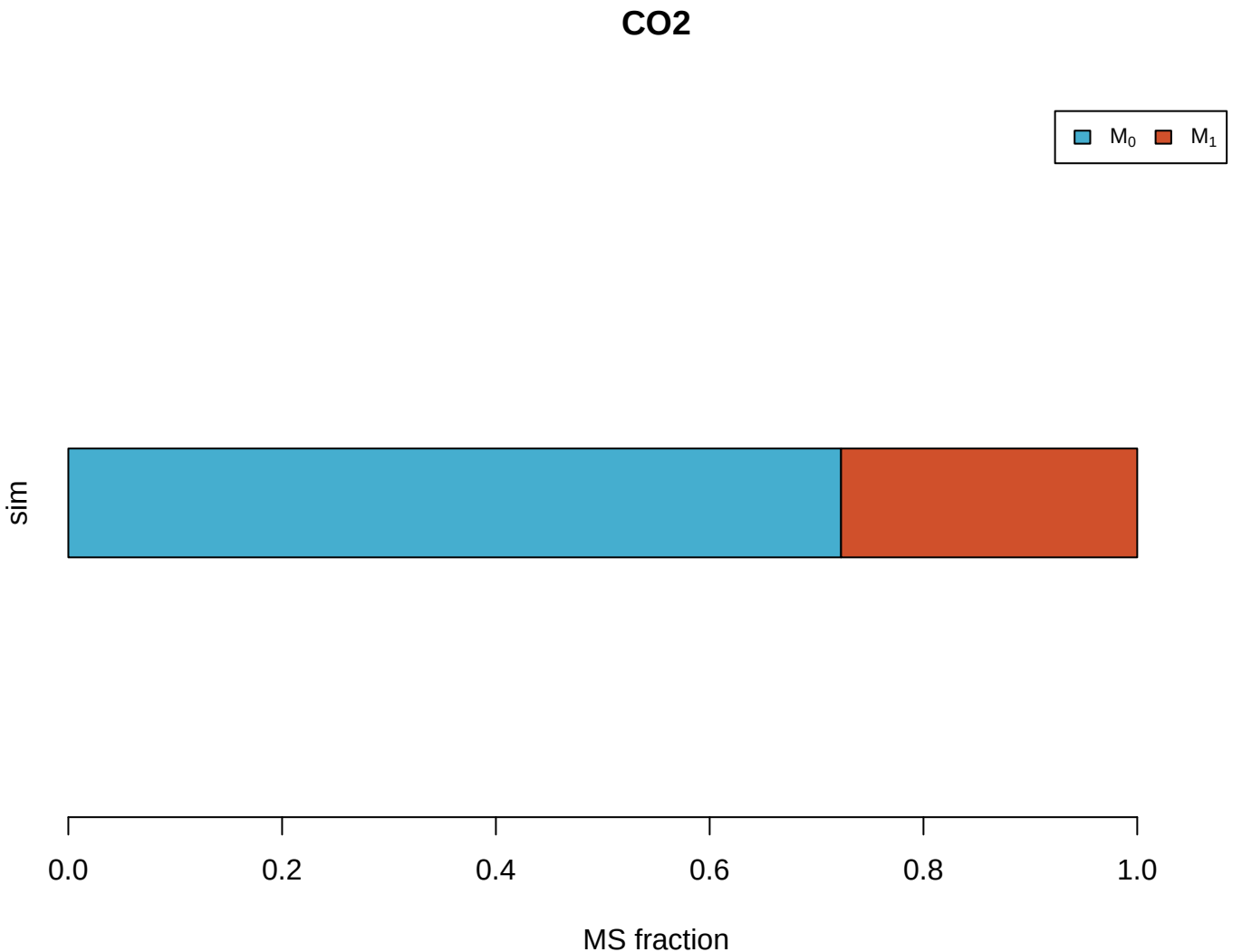

3PG
M0
M1
M2
M3
sim
0.0
0.2
0.4
0.6
0.8
1.0
MS fraction


Ac
M0
M1
M2
sim
0.0
0.2
0.4
0.6
0.8
1.0
MS fraction


AcCoA
M0
M1
M2
sim
0.0
0.2
0.4
0.6
0.8
1.0
MS fraction


AKG
M0
M1
M2
M3
M4
M5
sim
0.0
0.2
0.4
0.6
0.8
1.0
MS fraction


Asn
M0
M1
M2
M3
M4
sim
0.0
0.2
0.4
0.6
0.8
1.0
MS fraction


CO2
M0
M1
sim
0.0
0.2
0.4
0.6
0.8
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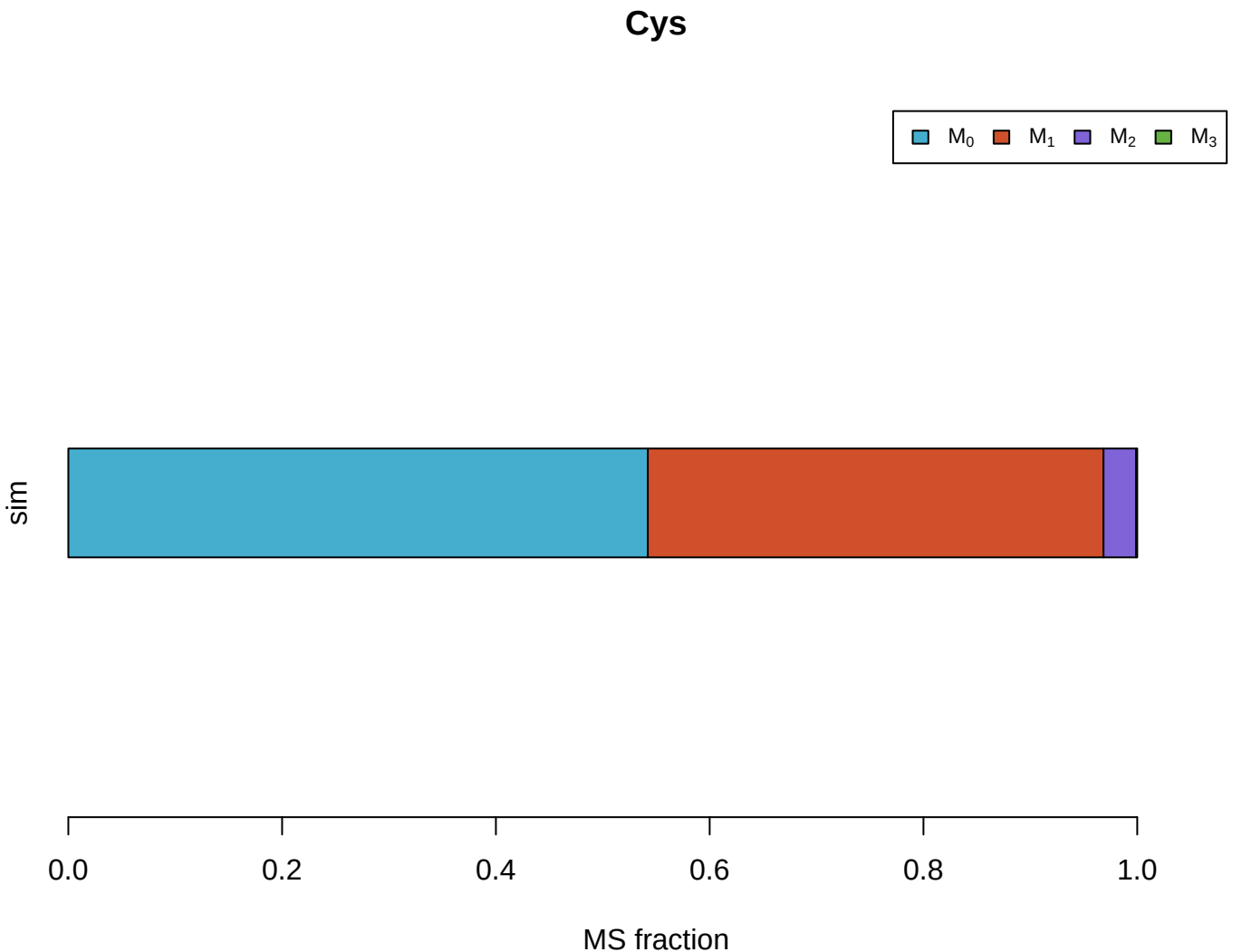
MS fraction


Cys
M0
M1
M2
M3
sim
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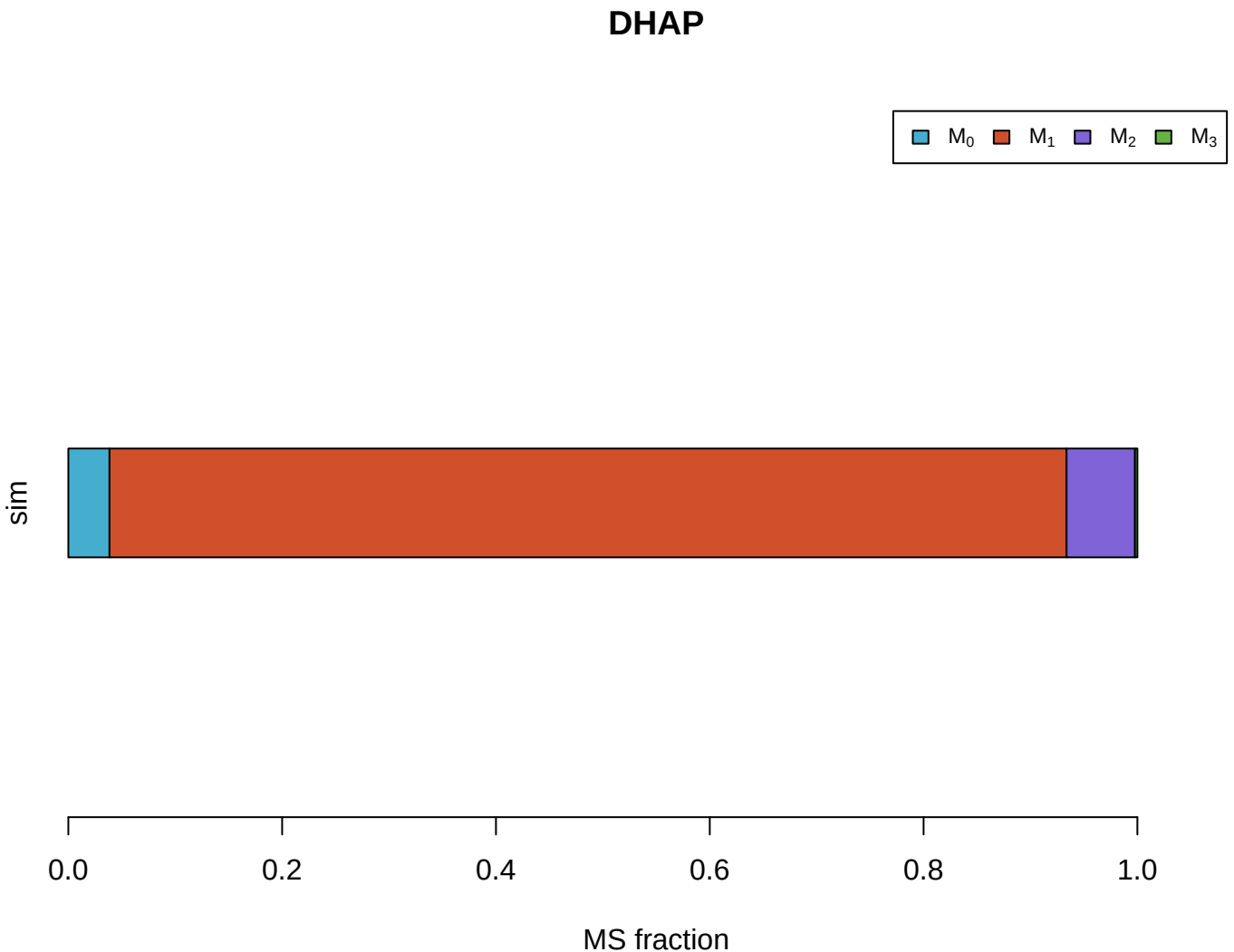
0.2
0.4
0.6
0.8
1.0
MS fraction


DHAP
M0
M1
M2
M3
sim
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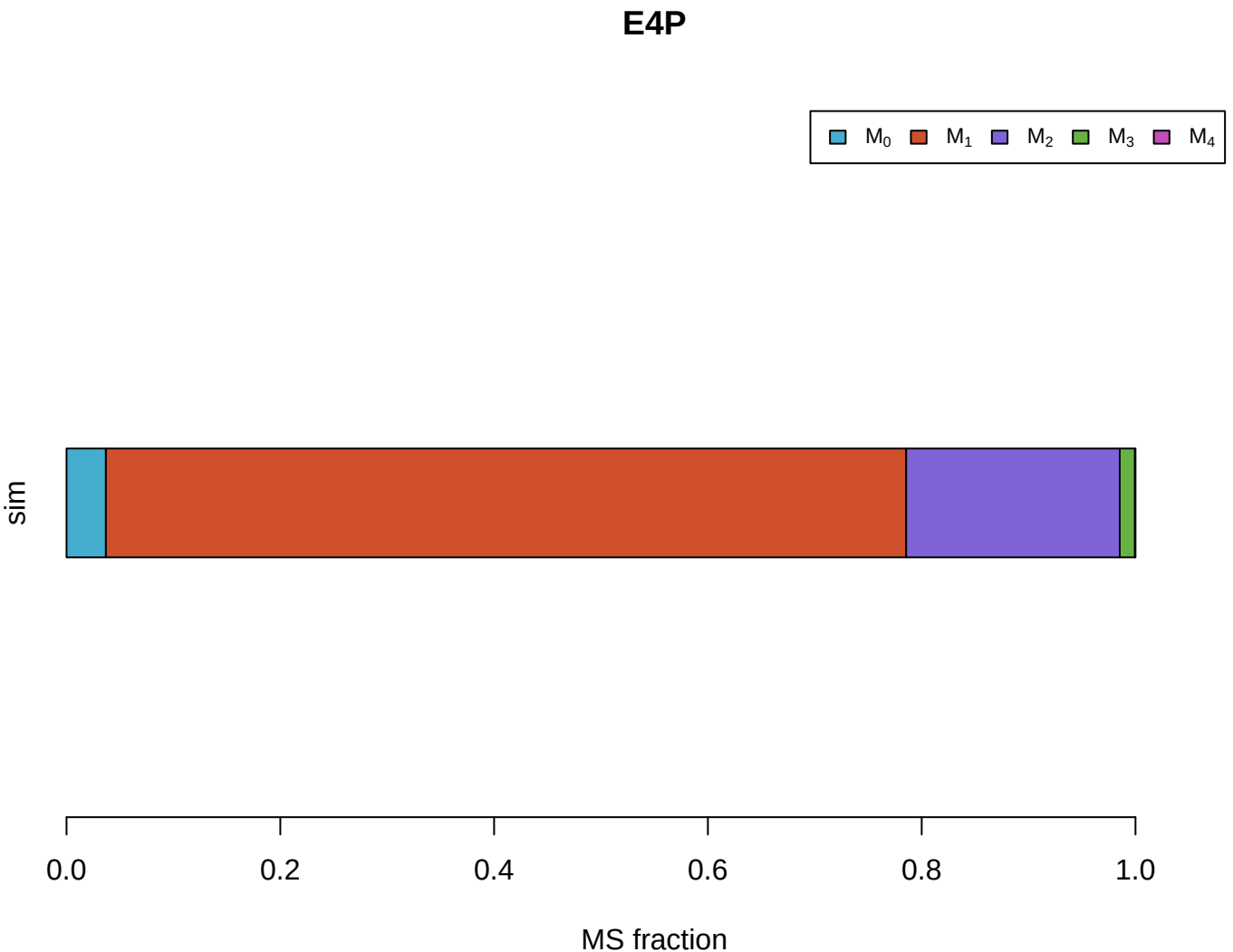
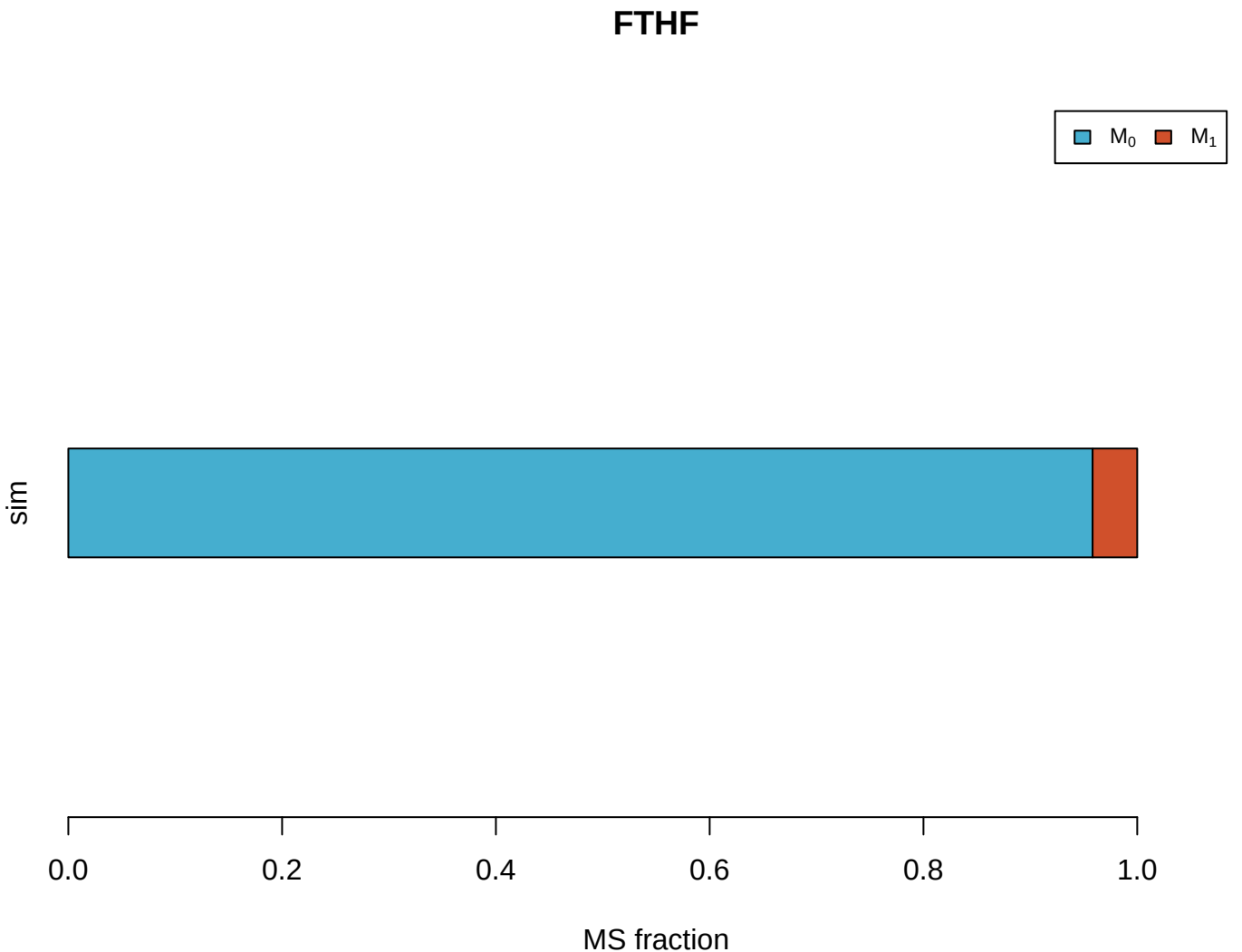
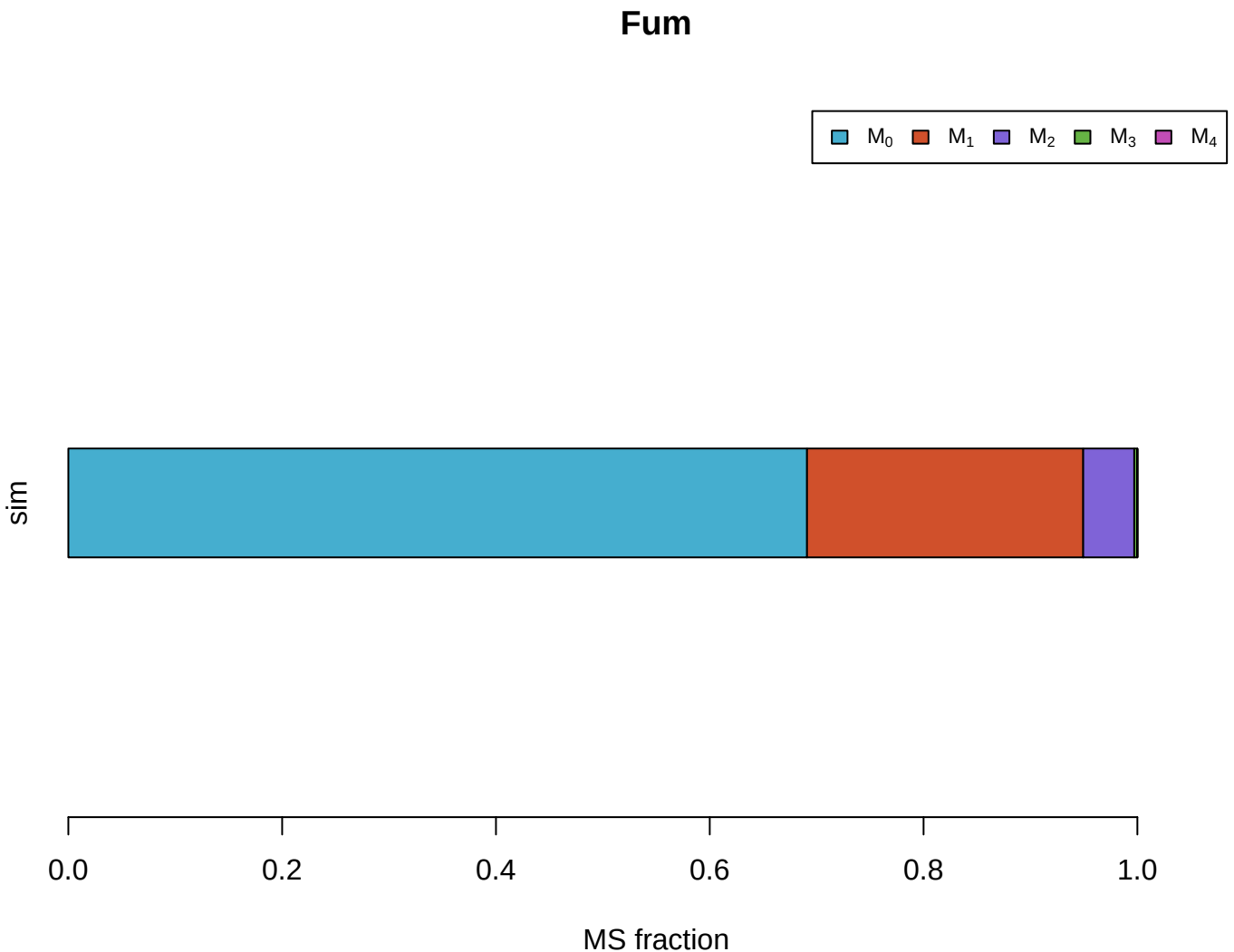
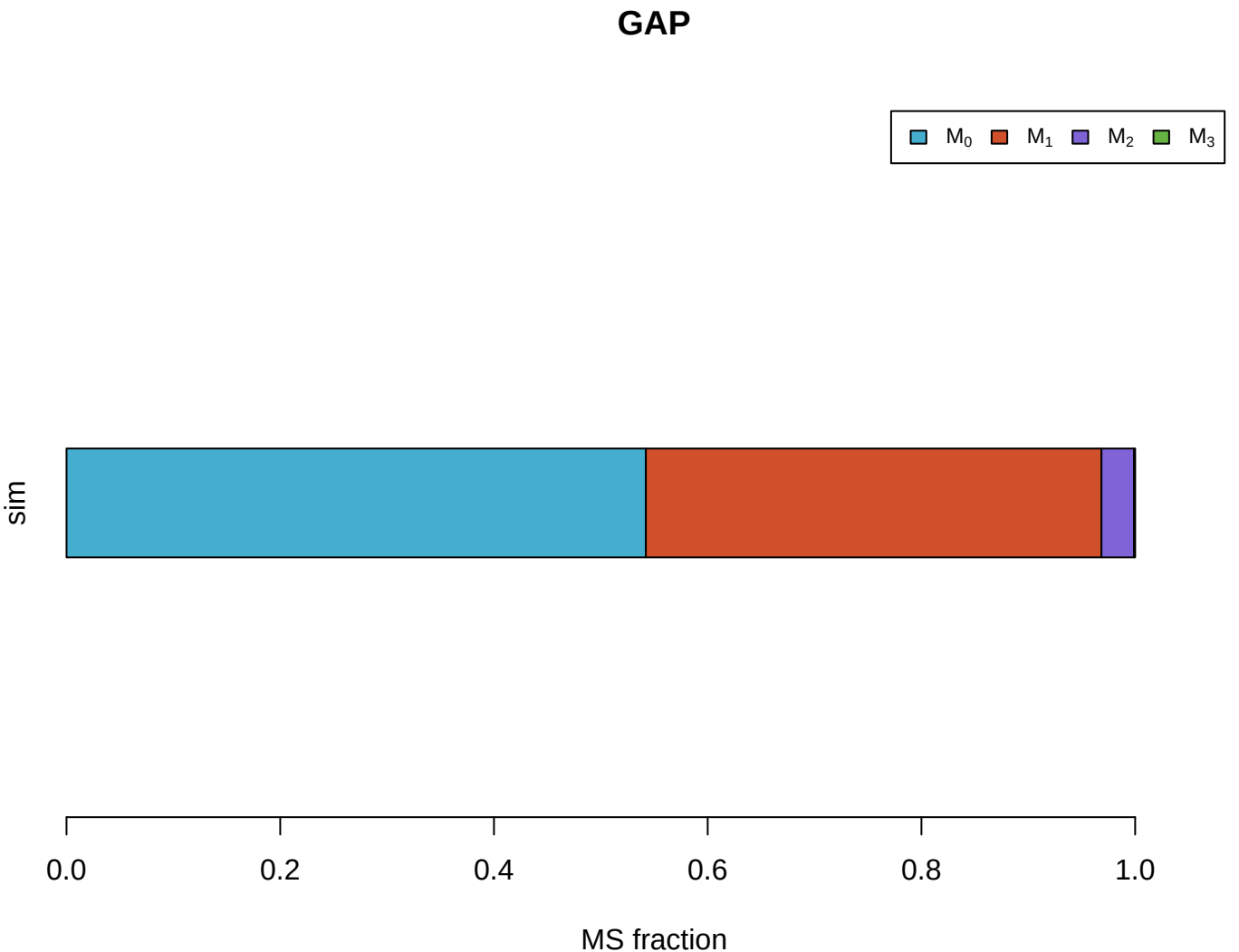
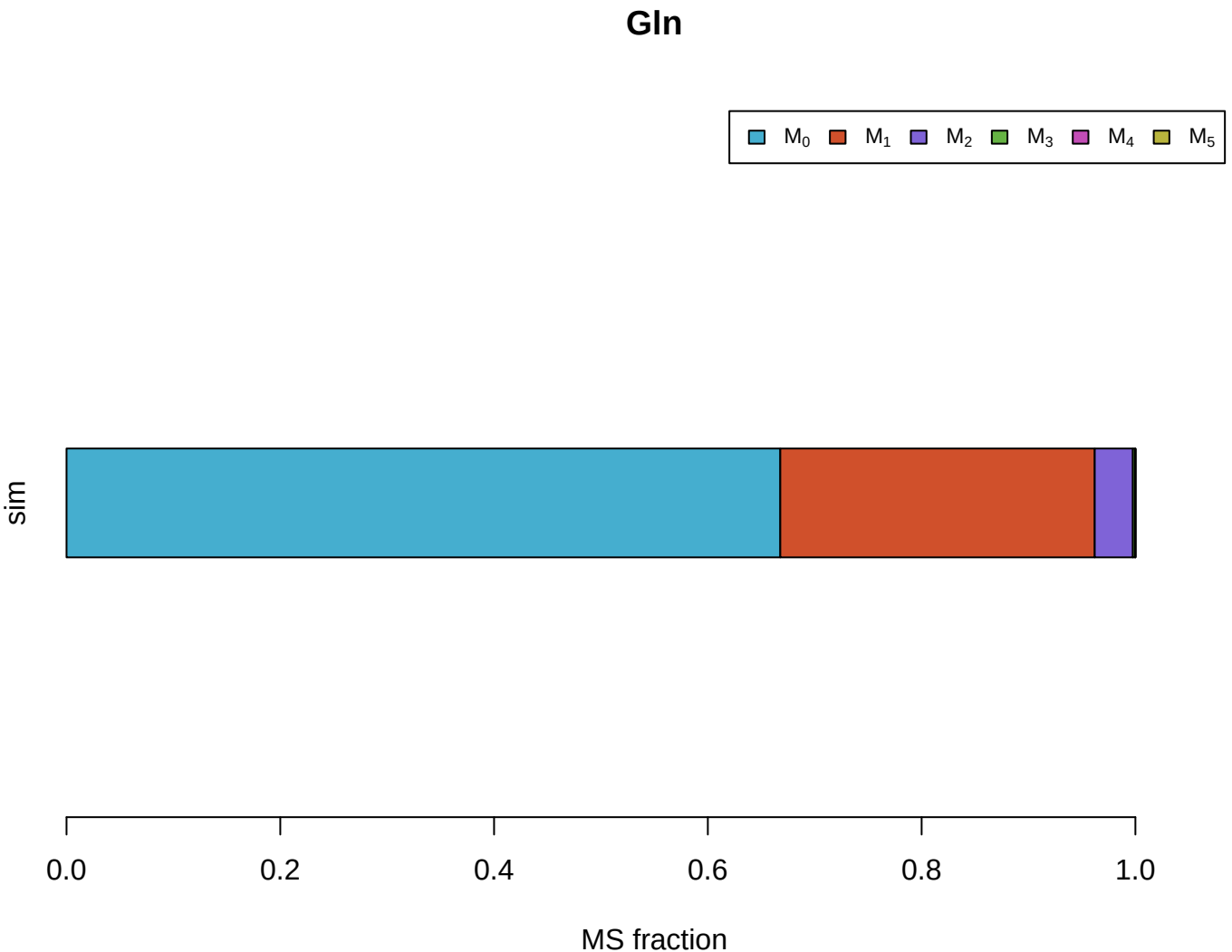
0.2
0.4
0.6
0.8
1.0
MS fraction

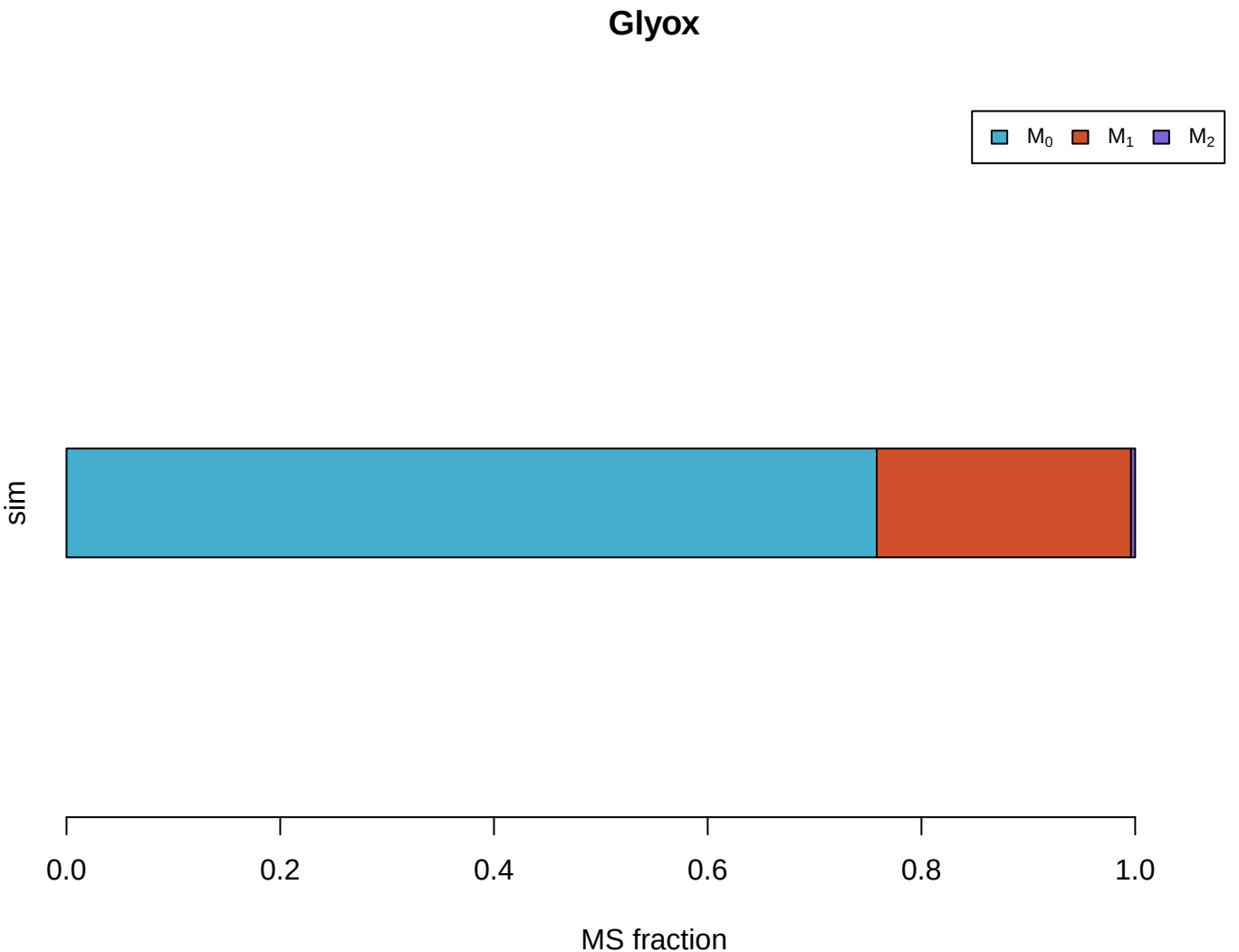

E4P
M0
M1
M2
M3
M4
sim
0.0
0.2
0.4
0.6
0.8
1.0
MS fraction

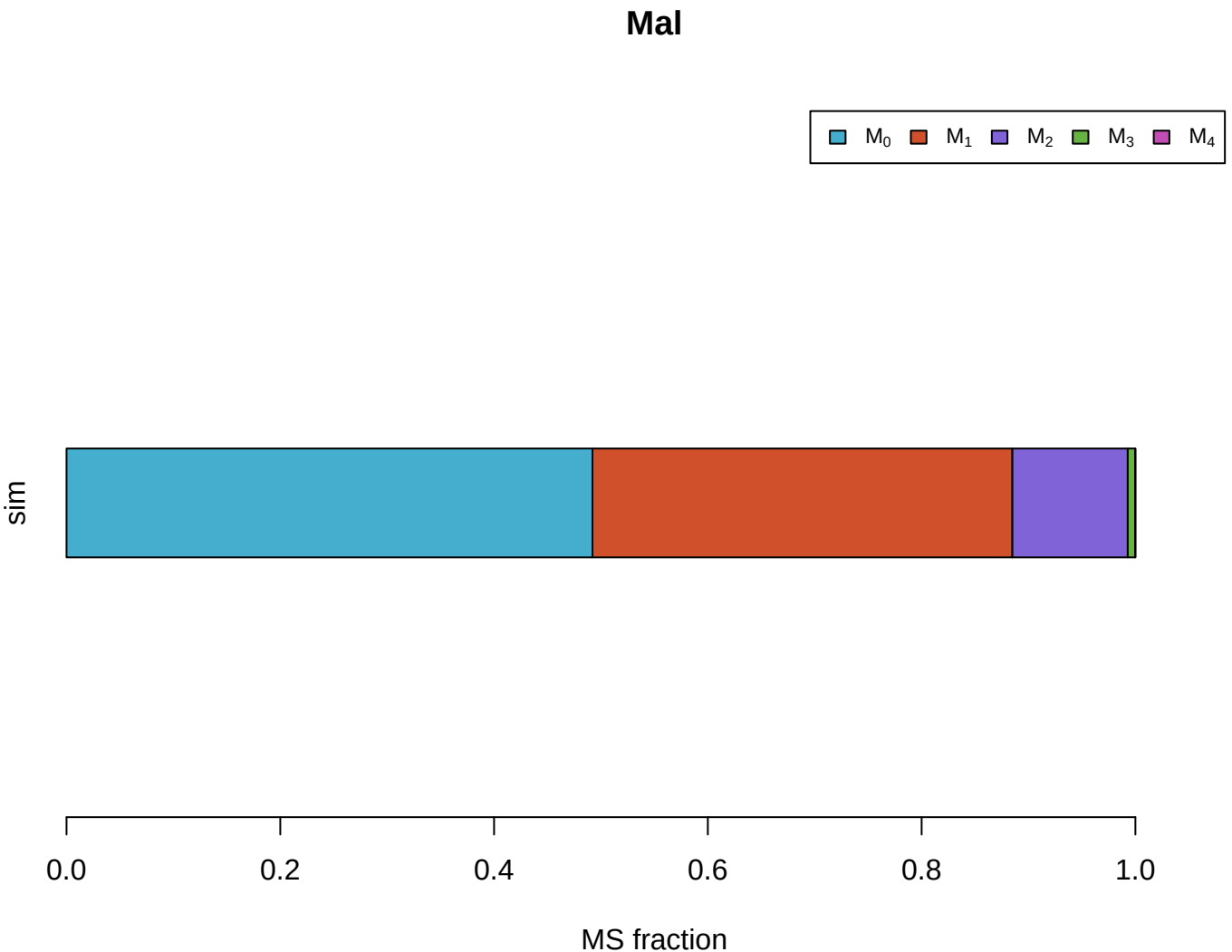

FTHF
M0
M1
sim
0.0
0.2
0.4
0.6
0.8
1.0
MS fraction

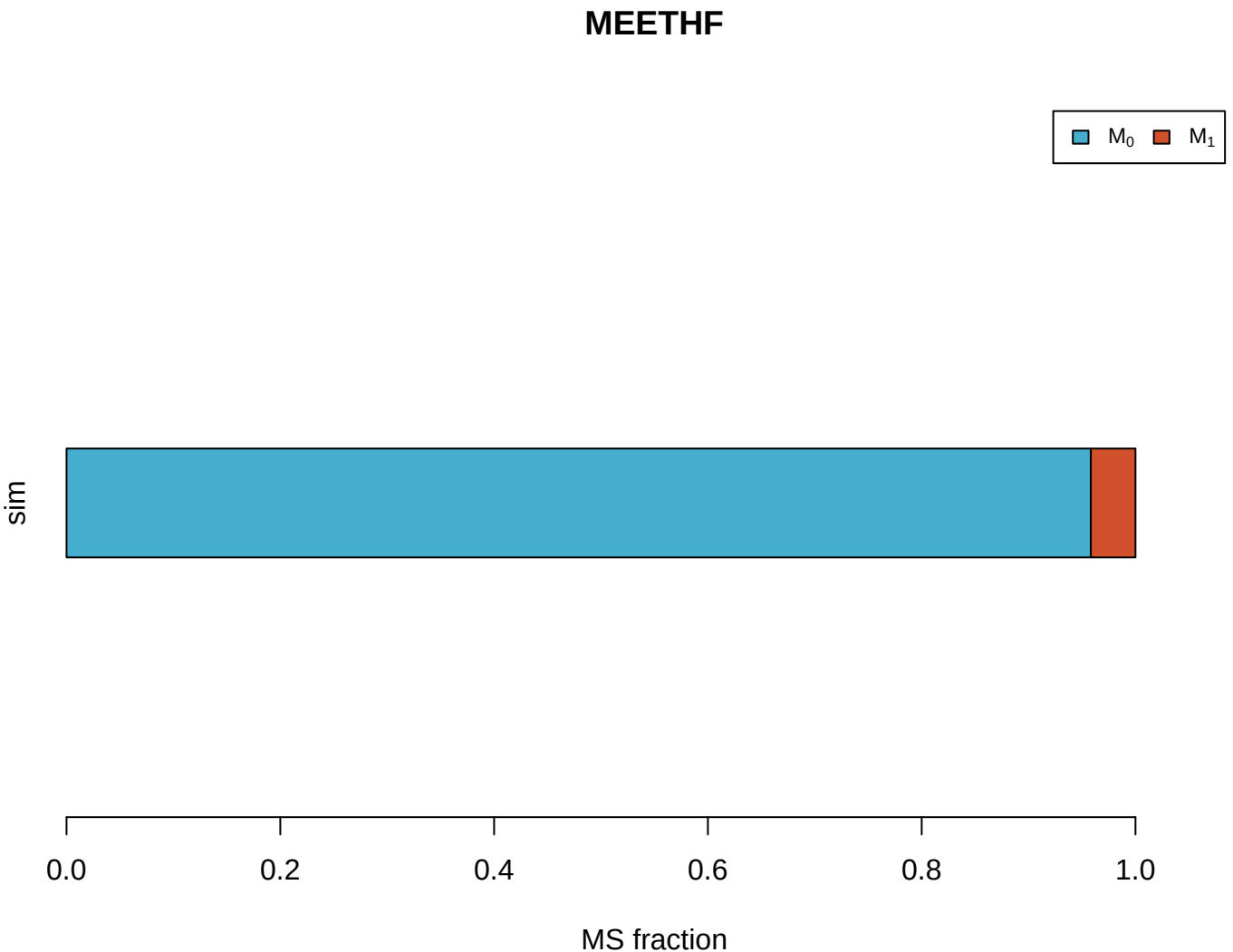

Fum
M0
M1
M2
M3
M4
sim
0.0
0.2
0.4
0.6
0.8
1.0
MS fraction

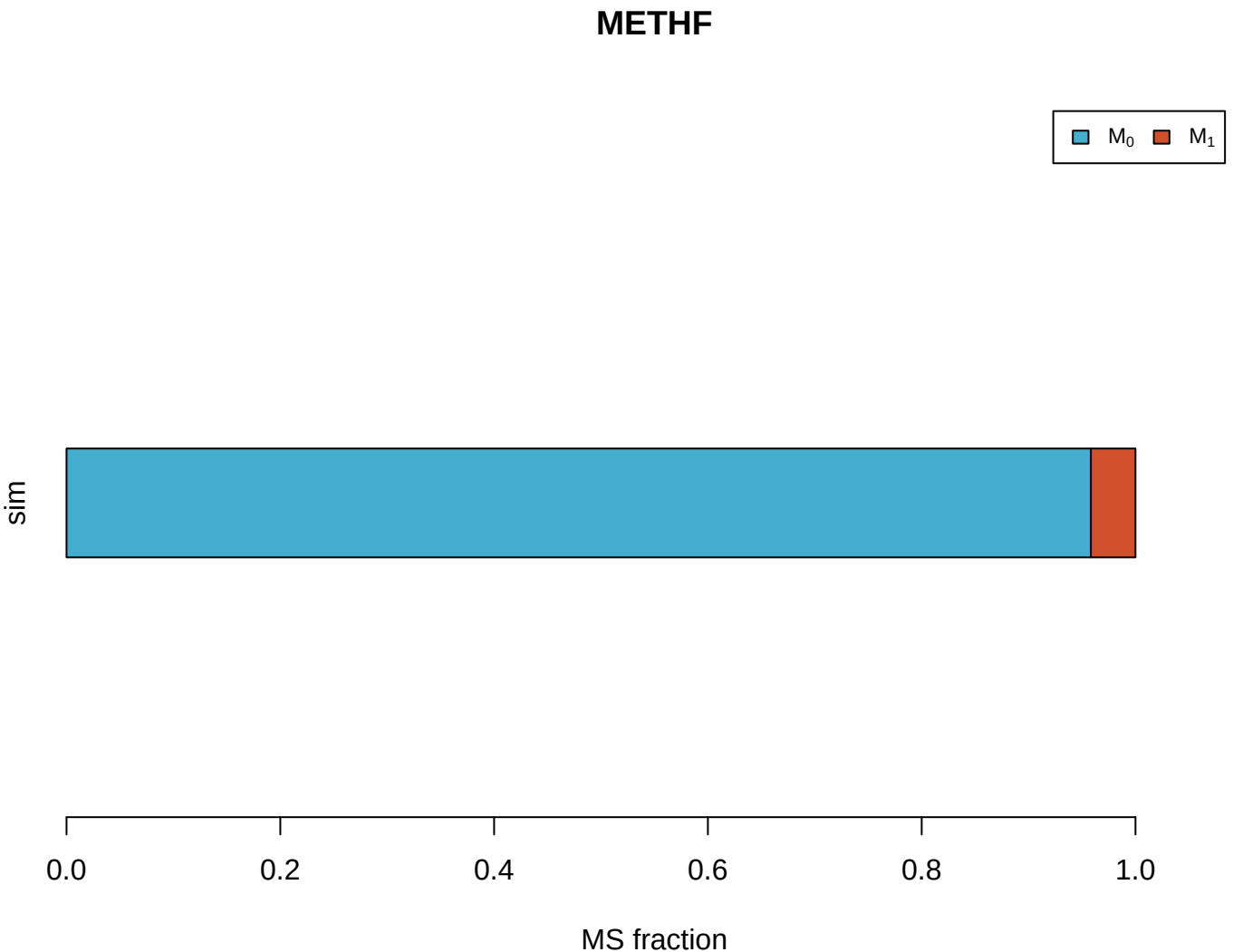

GAP
M0
M1
M2
M3
sim
0.0
0.2
0.4
0.6
0.8
1.0
MS fraction

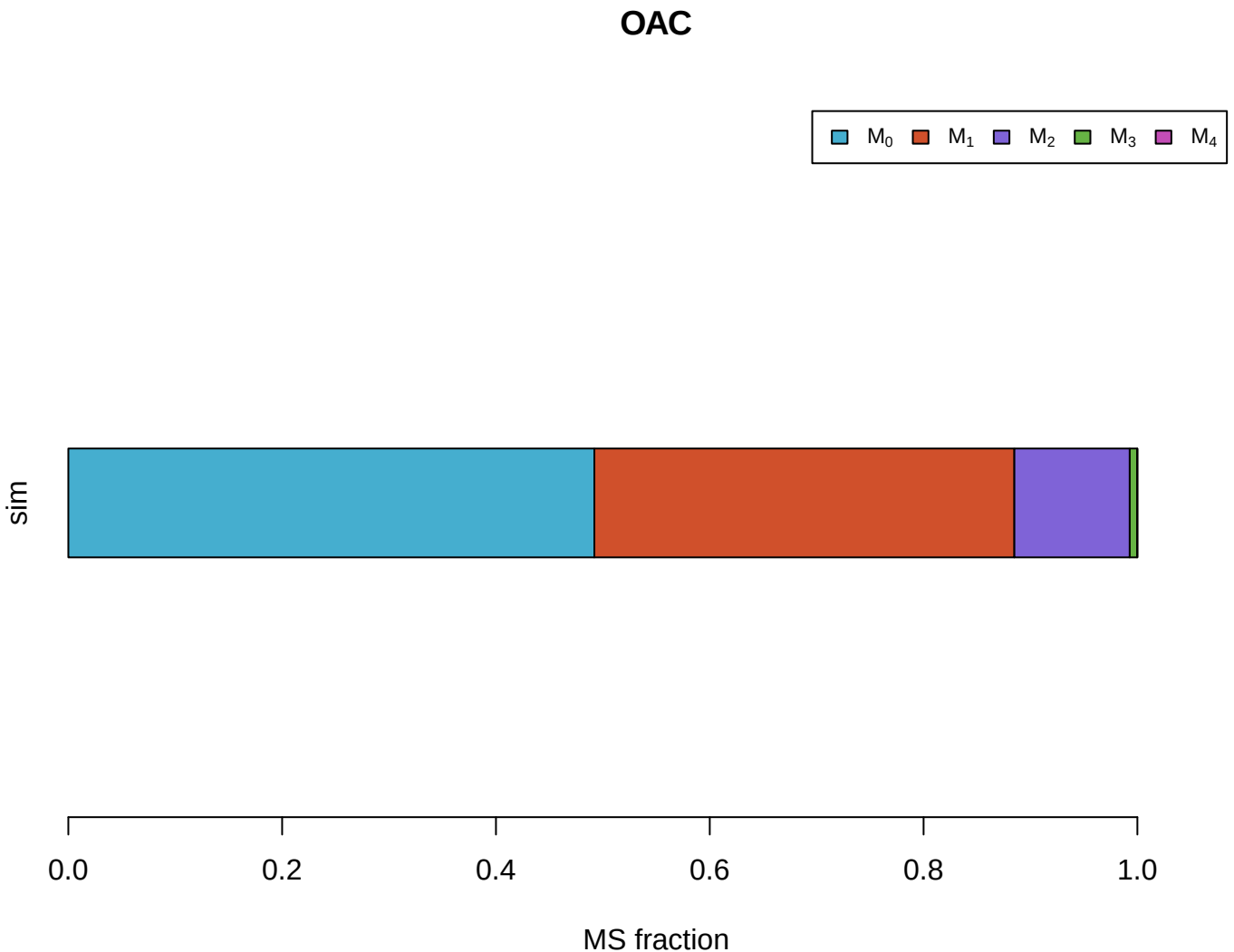

Gln
M0
M1
M2
M3
M4
M5
sim
0.0
0.2
0.4
0.6
0.8
1.0
MS fraction

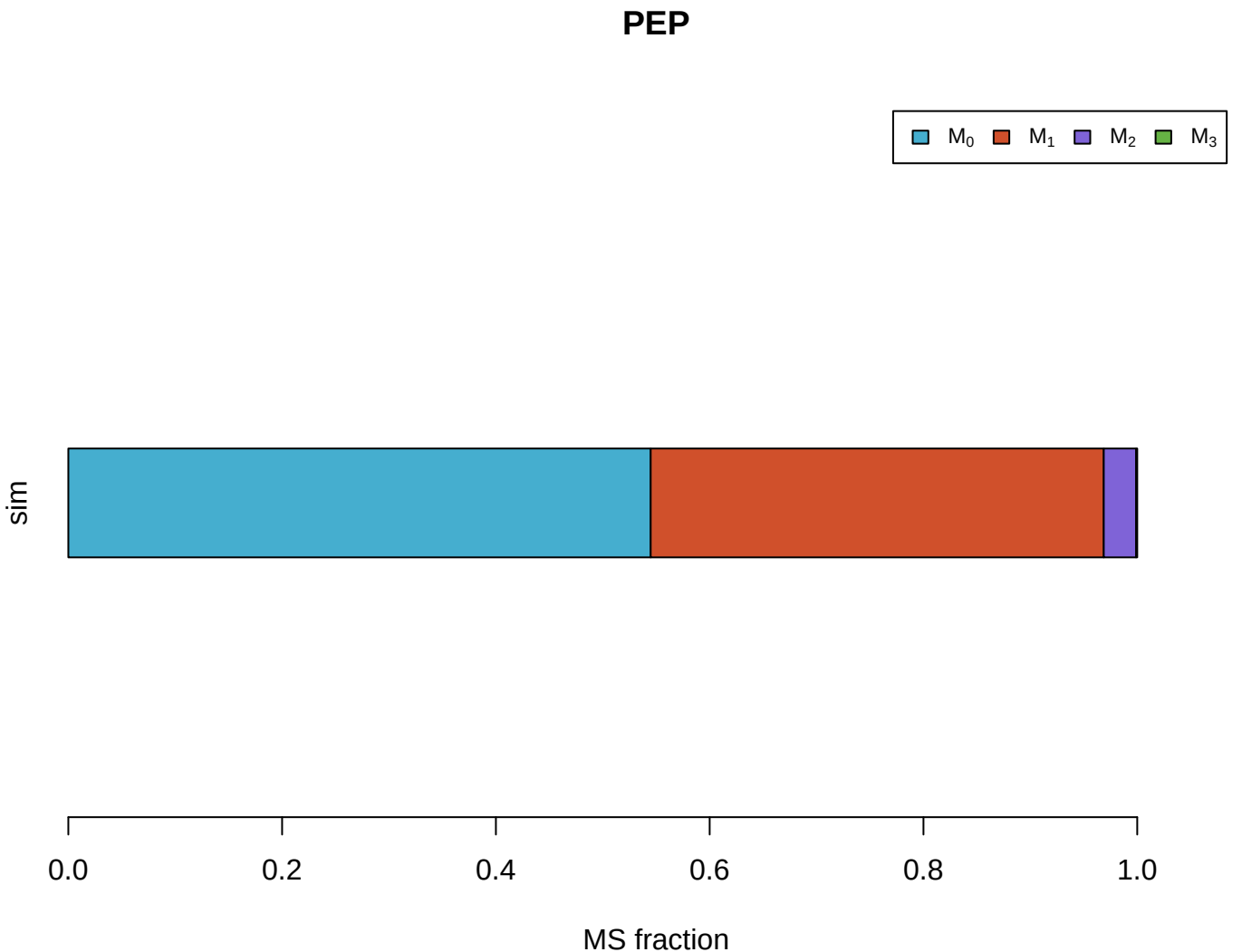

Glyox
M0
M1
M2
sim
0.0
0.2
0.4
0.6
0.8
1.0
MS fraction

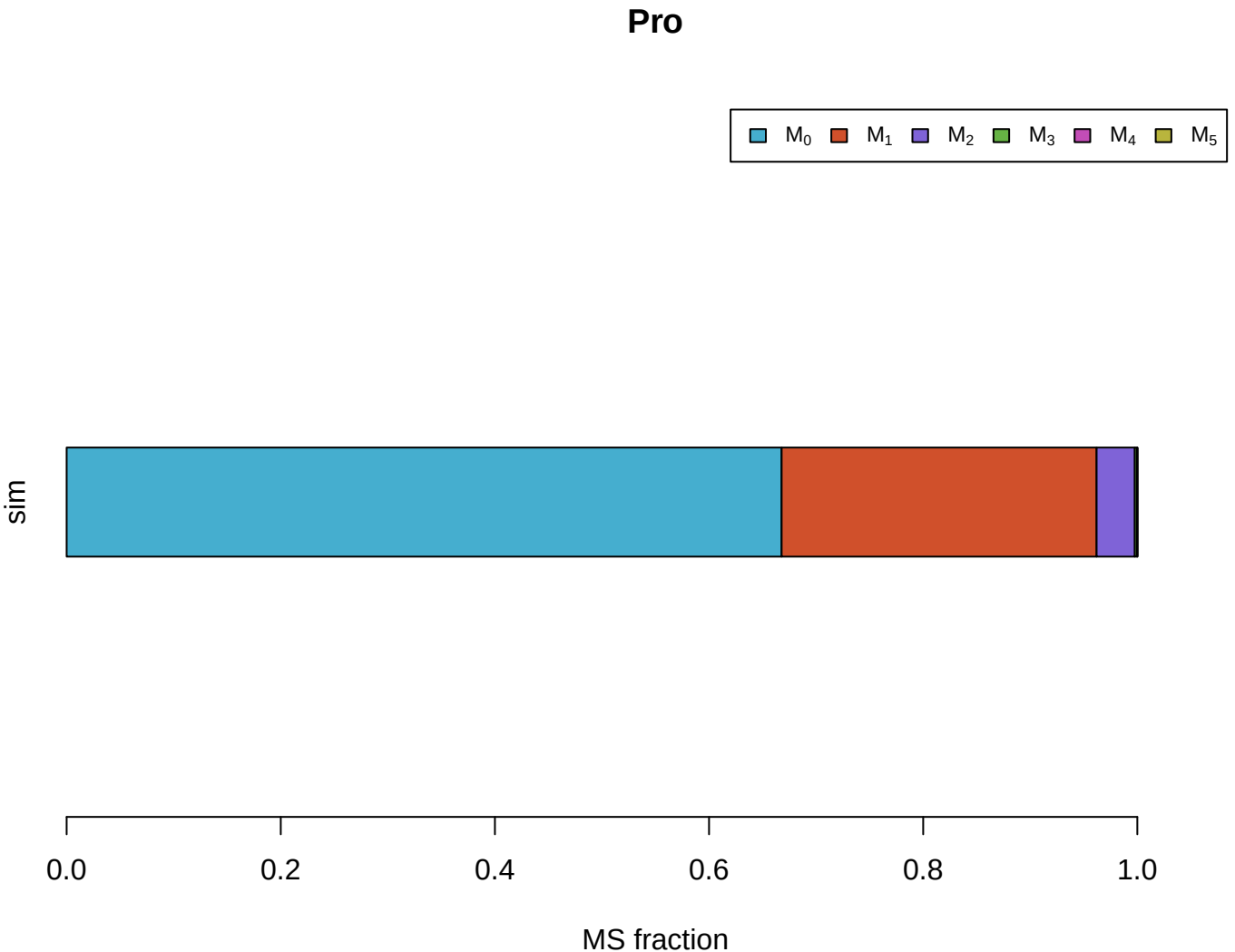

Mal
M0
M1
M2
M3
M4
sim
0.0
0.2
0.4
0.6
0.8
1.0
MS fraction

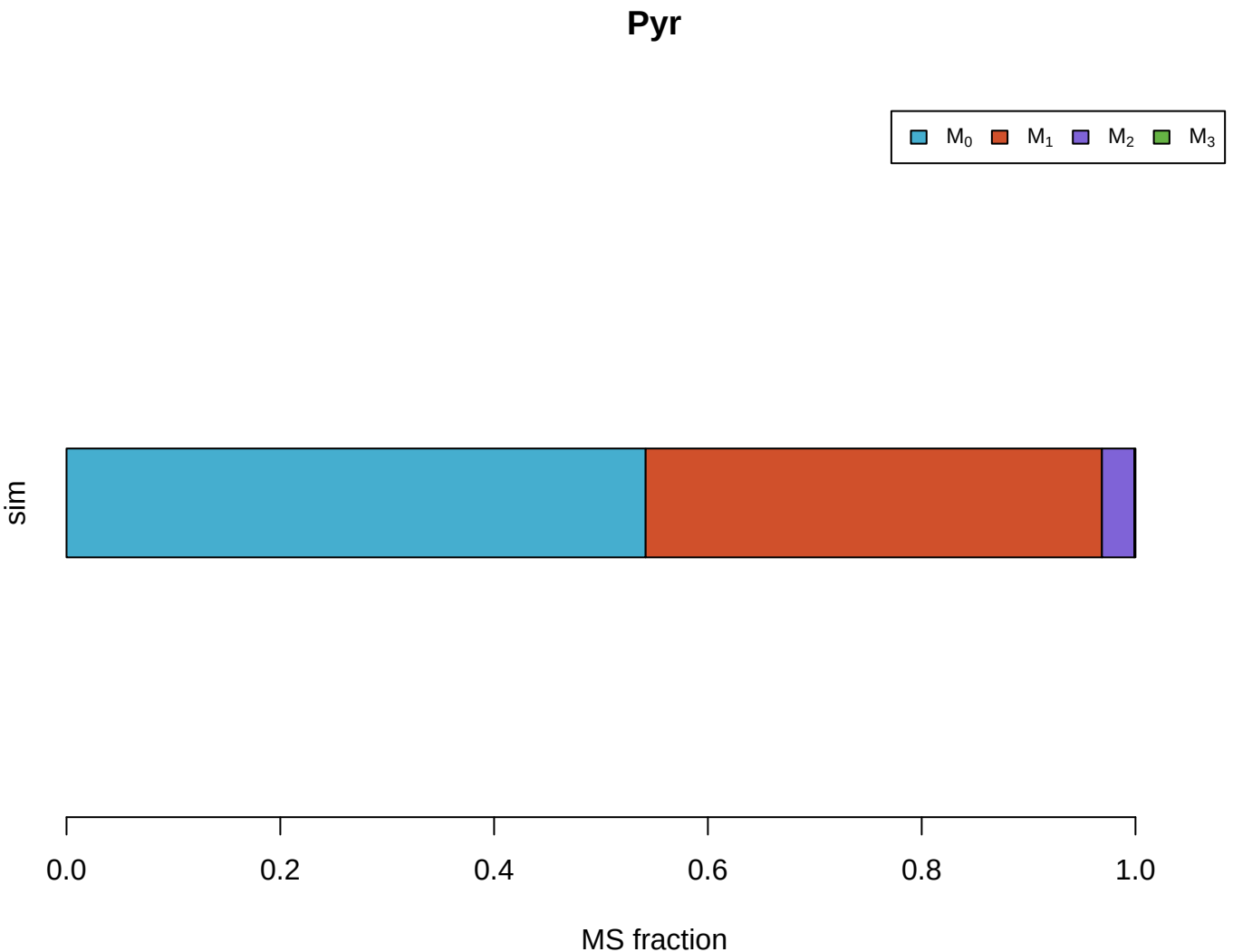

MEETHF
M0
M1
sim
0.0
0.2
0.4
0.6
0.8
1.0
MS fraction

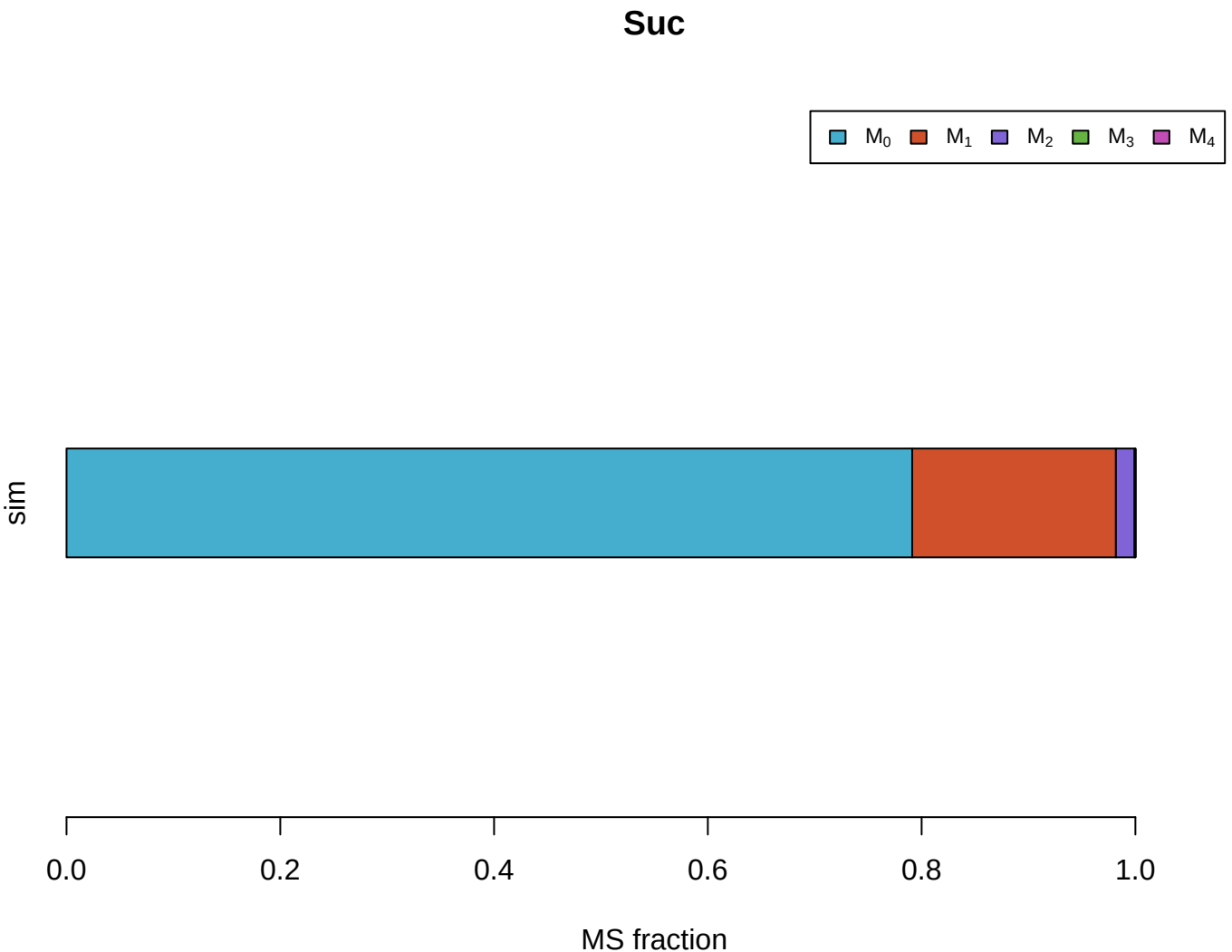

METHF
M0
M1
sim
0.0
0.2
0.4
0.6
0.8
1.0
MS fraction

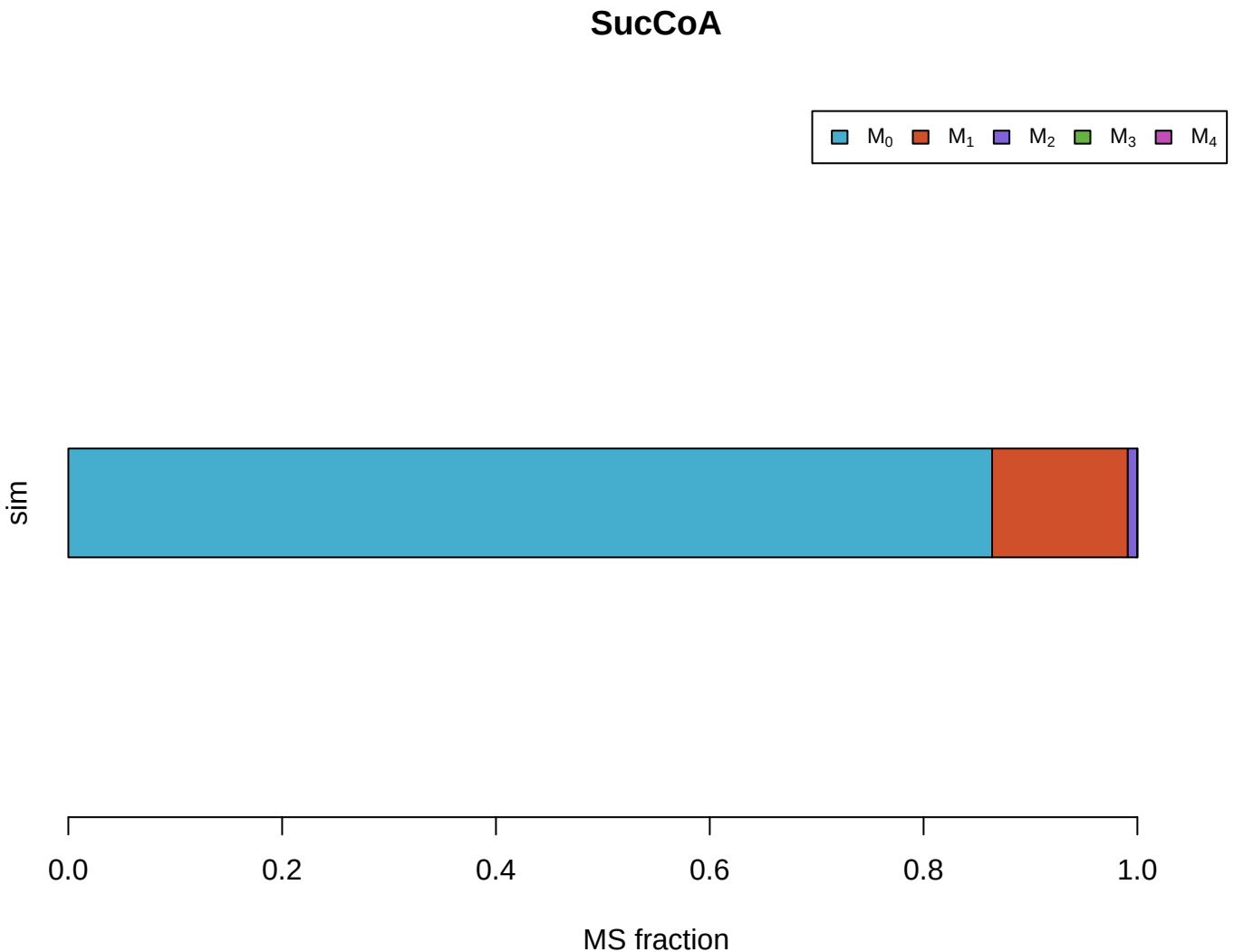

OAC
M0
M1
M2
M3
M4
sim
0.0
0.2
0.4
0.6
0.8
1.0
MS fraction

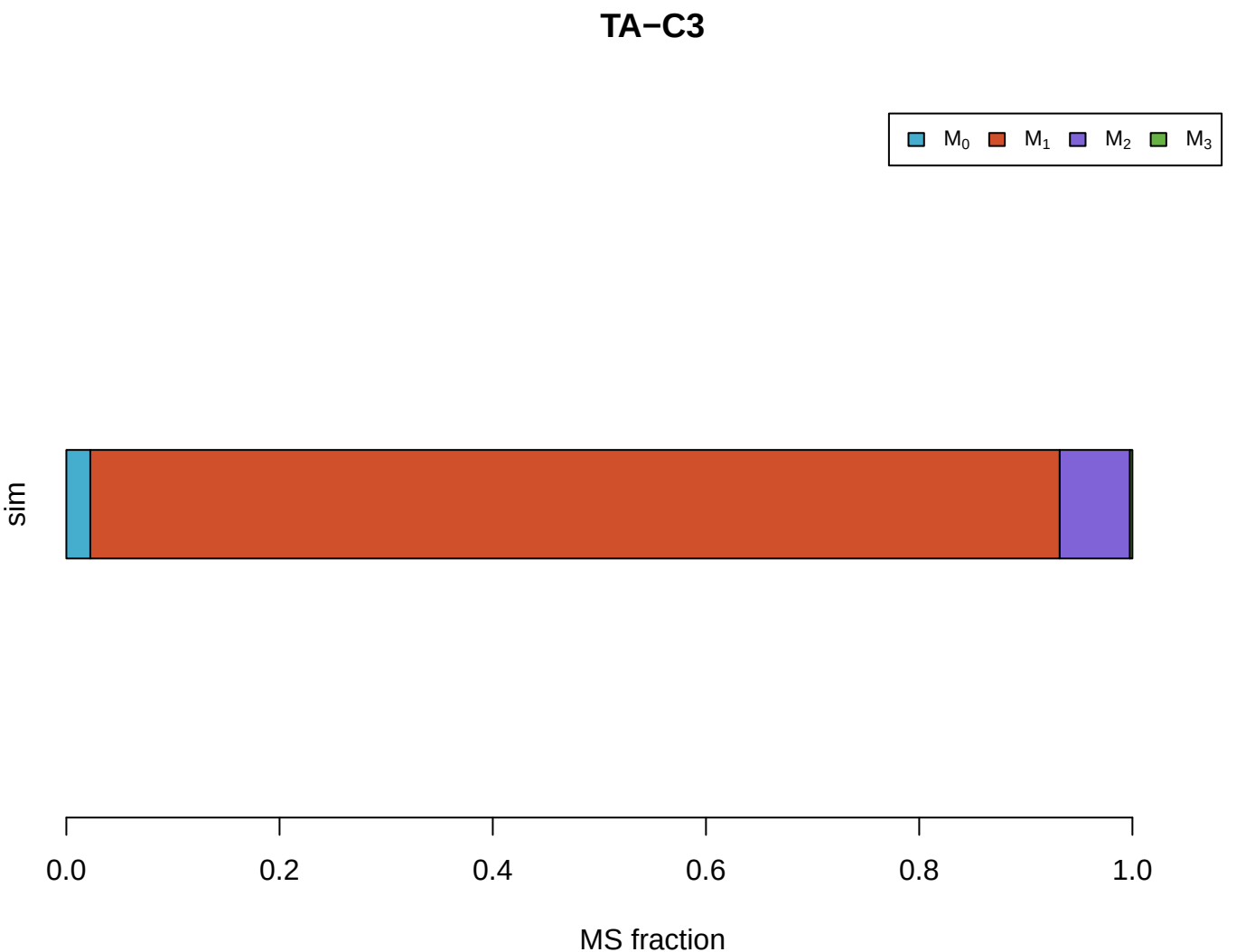

PEP
M0
M1
M2
M3
sim
0.0
0.2
0.4
0.6
0.8
1.0
MS fraction

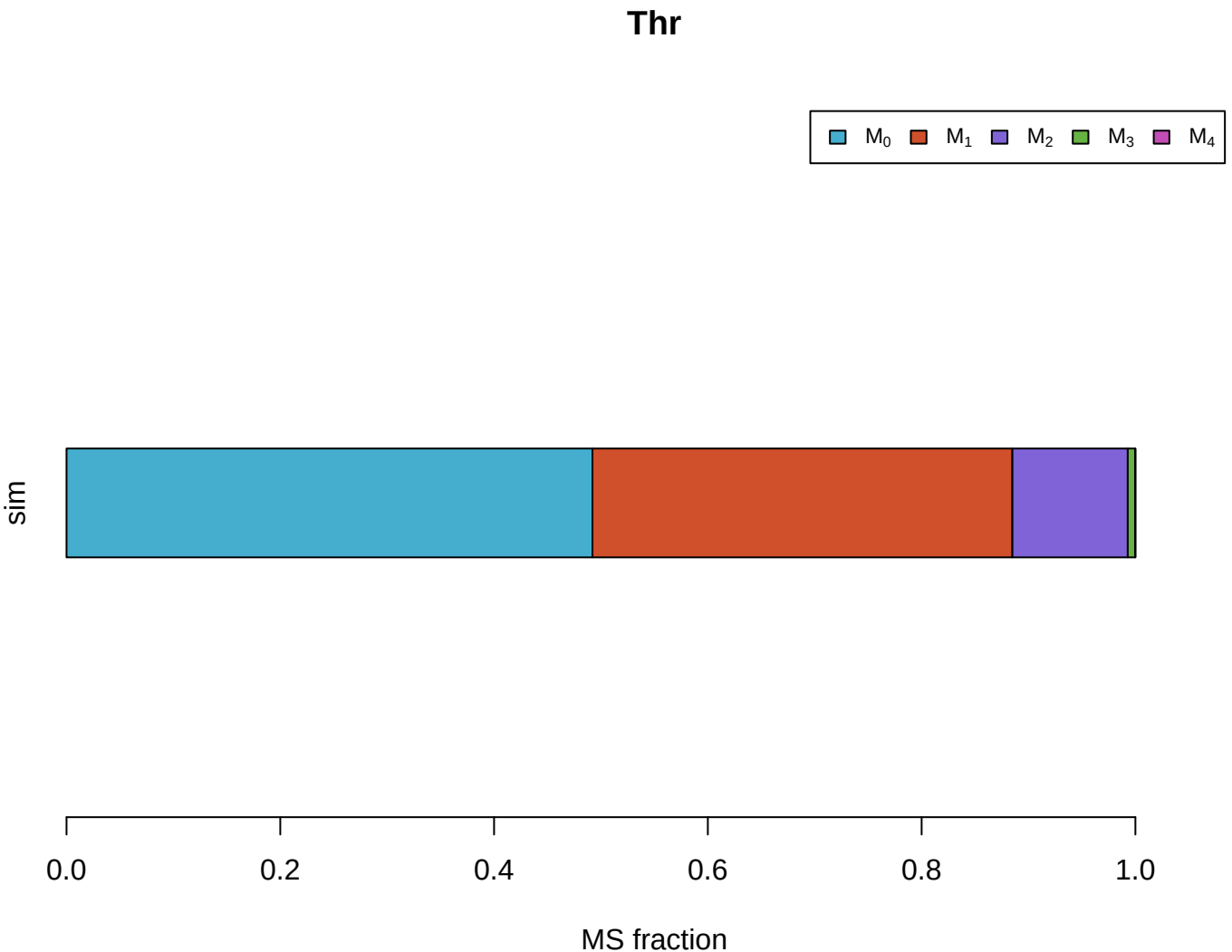

Pro
M0
M1
M2
M3
M4
M5
sim
0.0
0.2
0.4
0.6
0.8
1.0
MS fraction

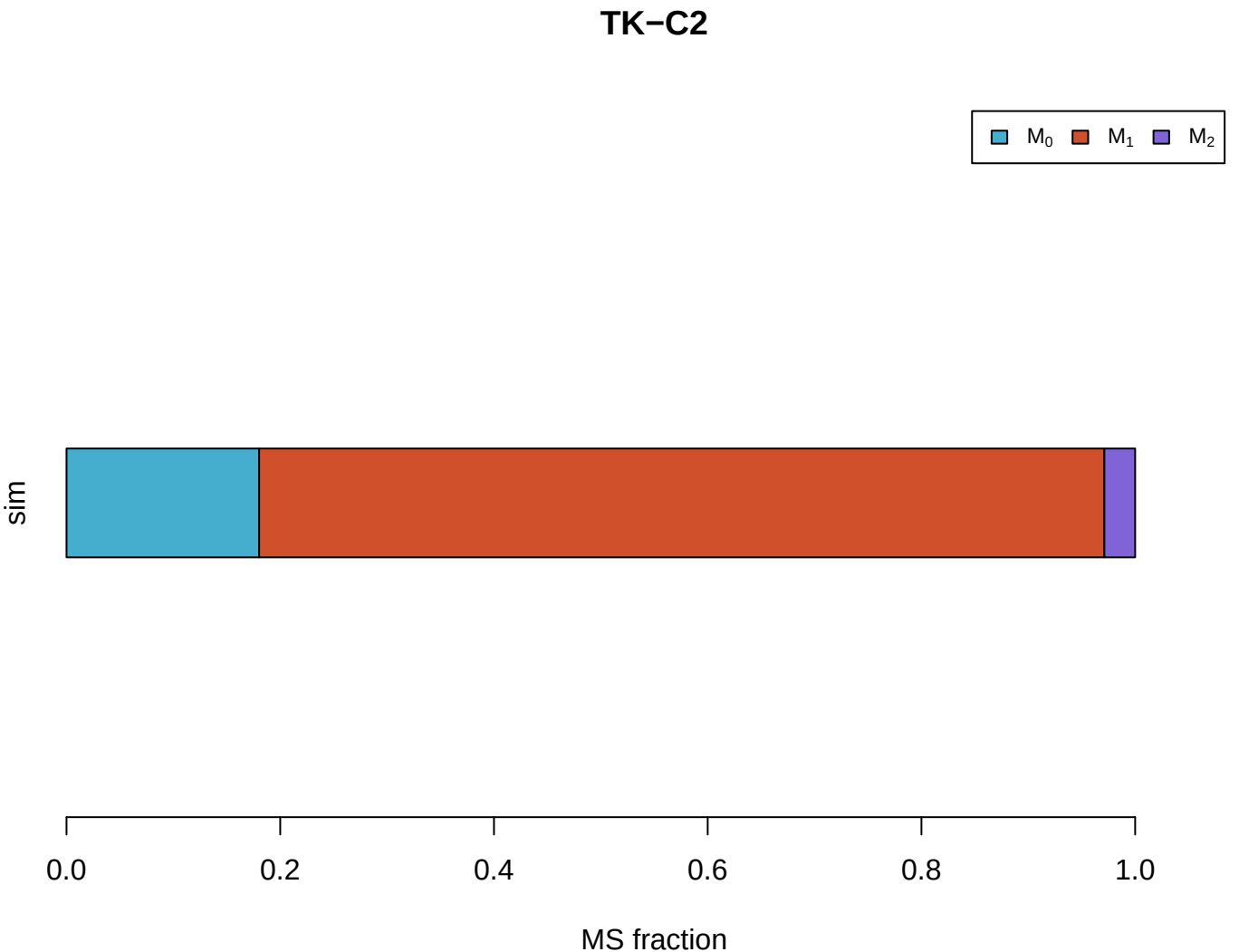

Pyr
M0
M1
M2
M3
sim
0.0
0.2
0.4
0.6
0.8
1.0
MS fraction


Suc
M0
M1
M2
M3
M4
sim
0.0
0.2
0.4
0.6
0.8
1.0
MS fraction


SucCoA
M0
M1
M2
M3
M4
sim
0.0
0.2
0.4
0.6
0.8
1.0
MS fraction


TA−C3
M0
M1
M2
M3
sim
0.0
0.2
0.4
0.6
0.8
1.0
MS fraction


Thr
M0
M1
M2
M3
M4
sim
0.0
0.2
0.4
0.6
0.8
1.0
MS fraction


TK−C2
M0
M1
M2
sim
0.0
0.2
0.4
0.6
0.8
1.0
MS fraction