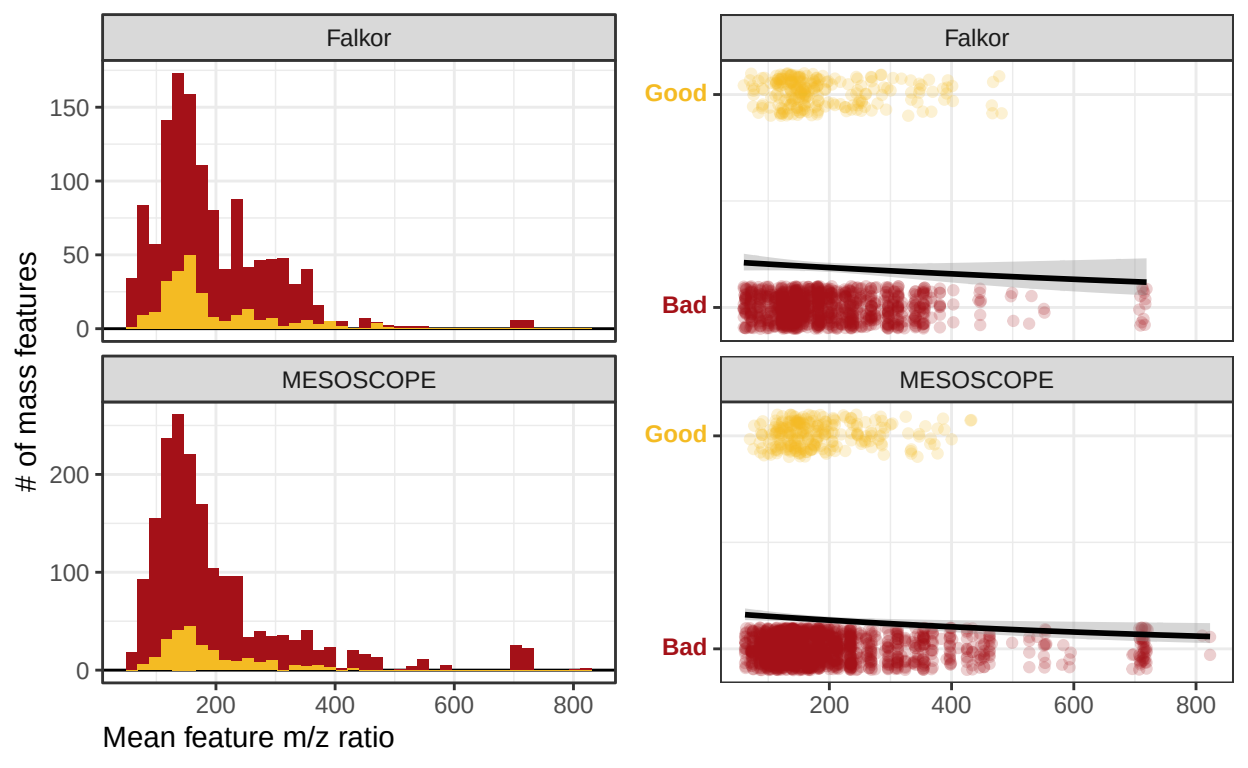
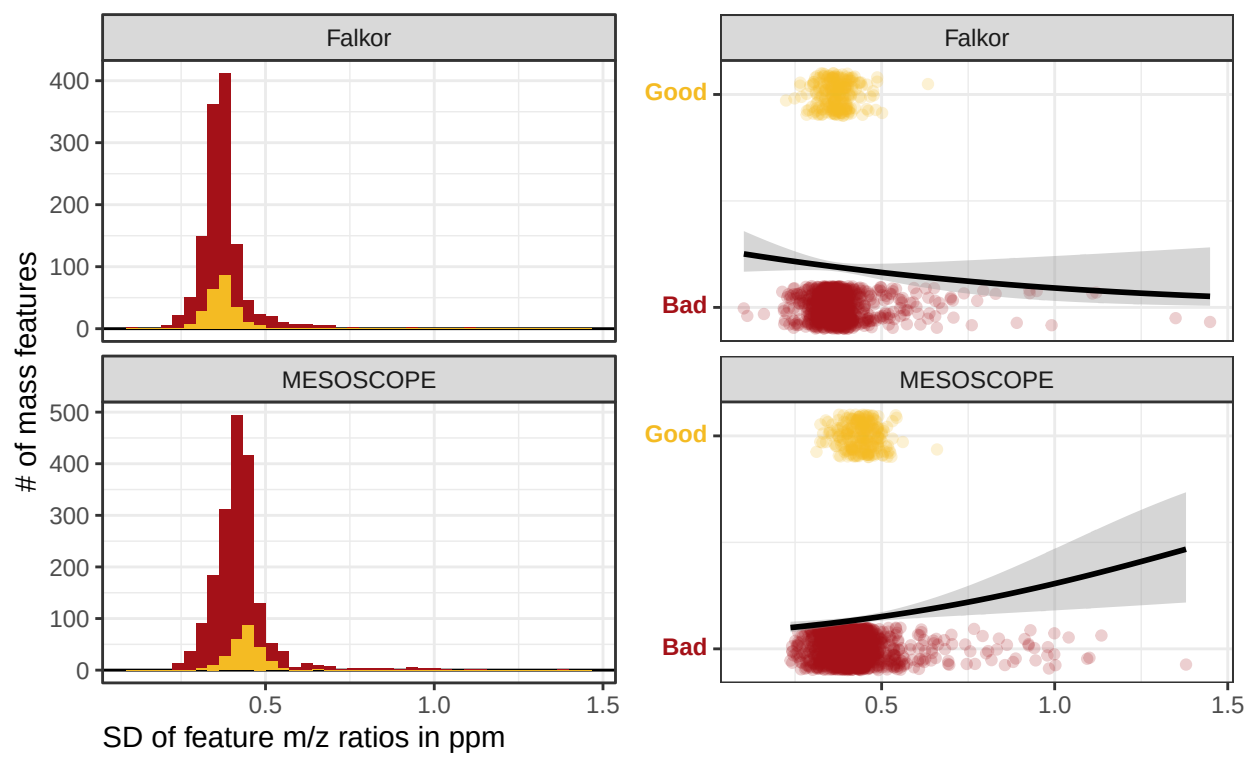
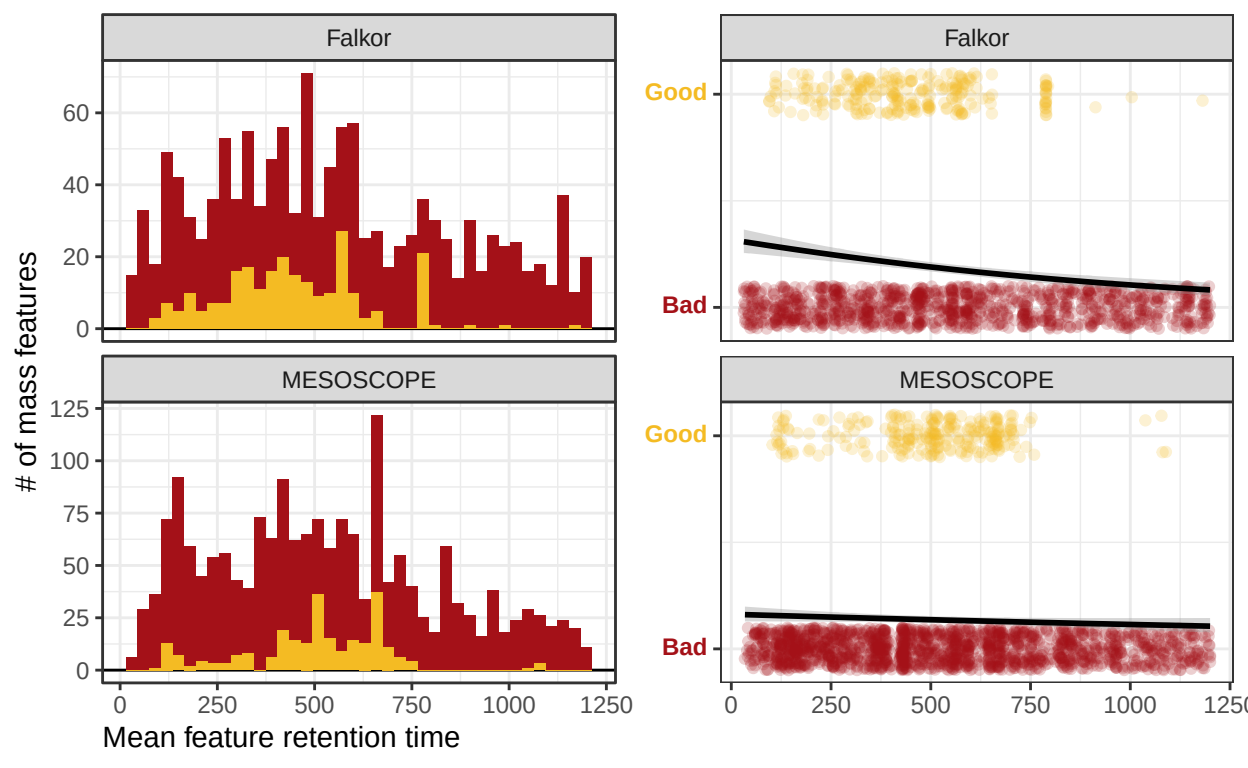
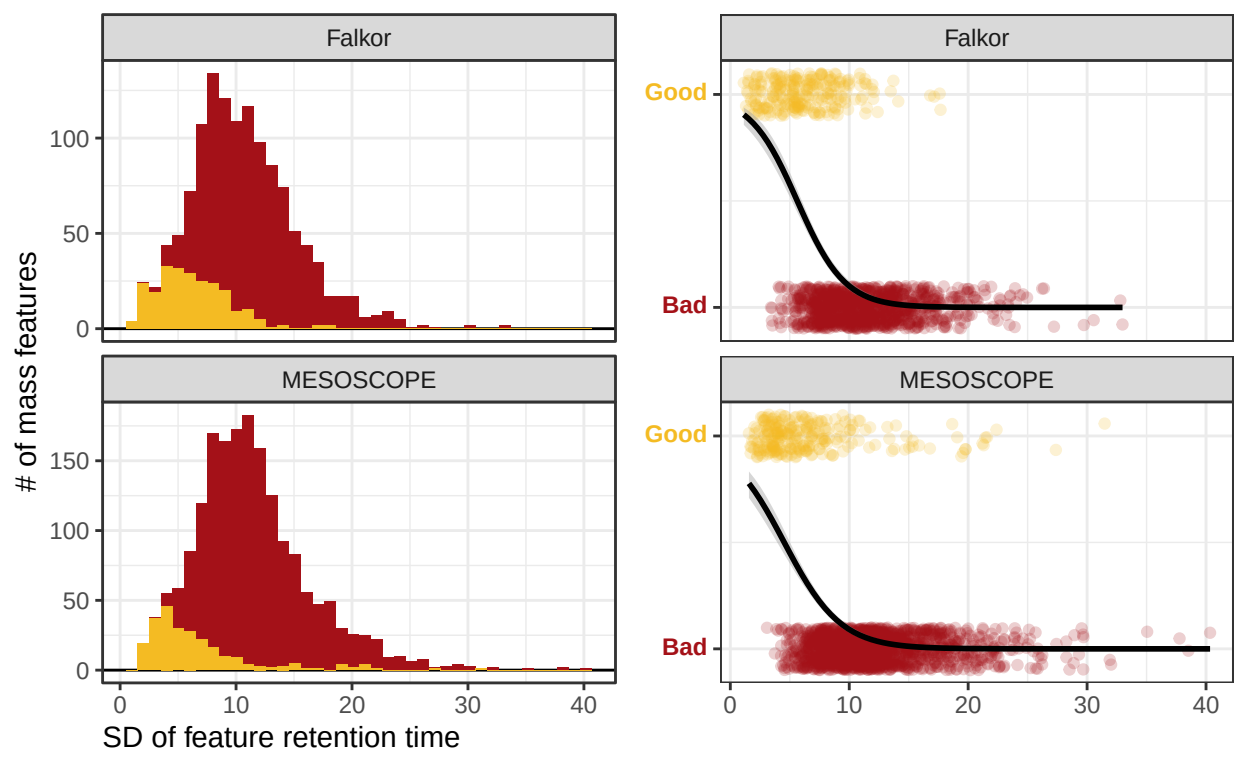
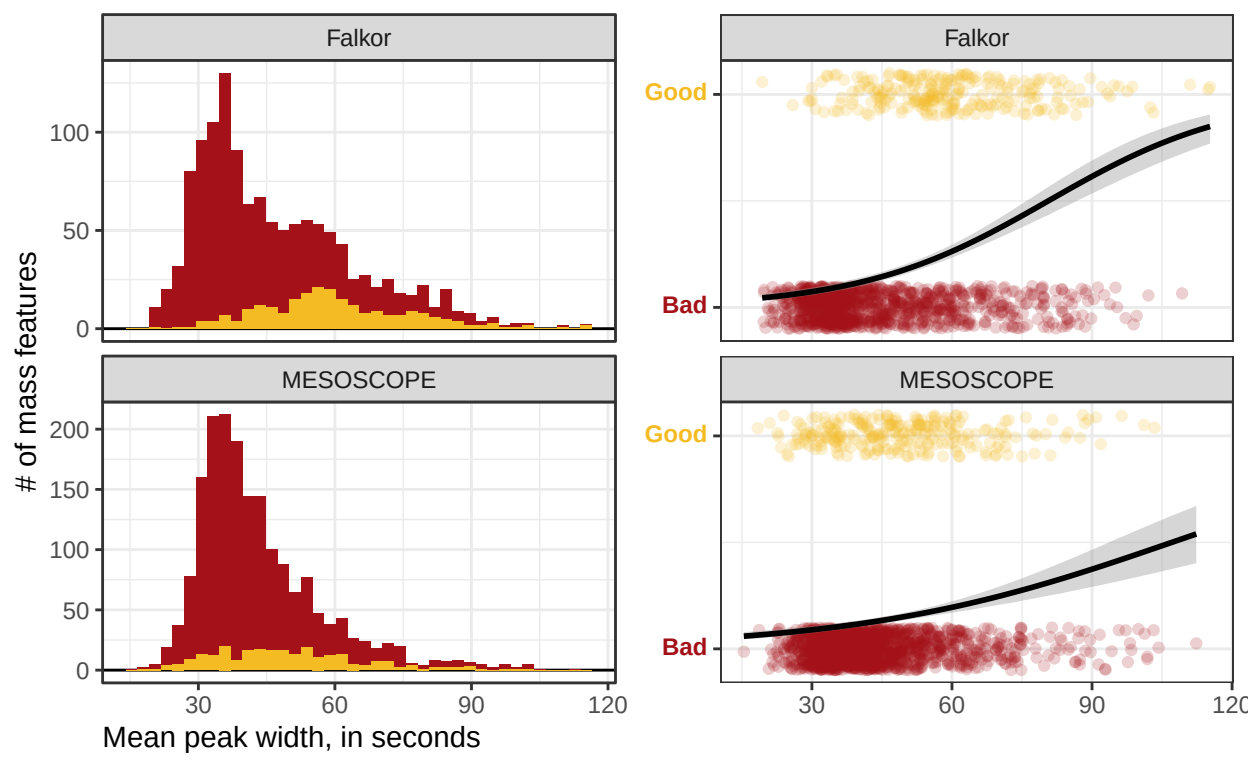
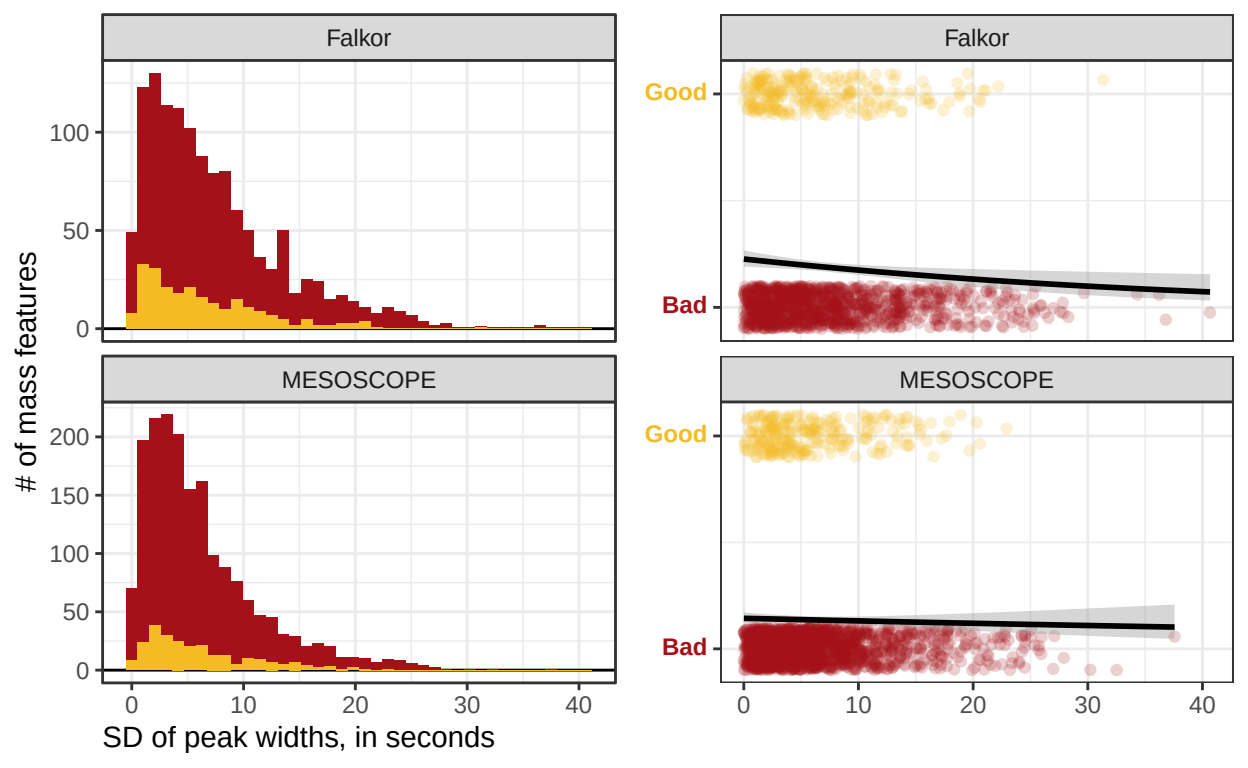

Falkor
MESOSCOPE
# of mass features
Mean feature m/z ratio
Good
Bad

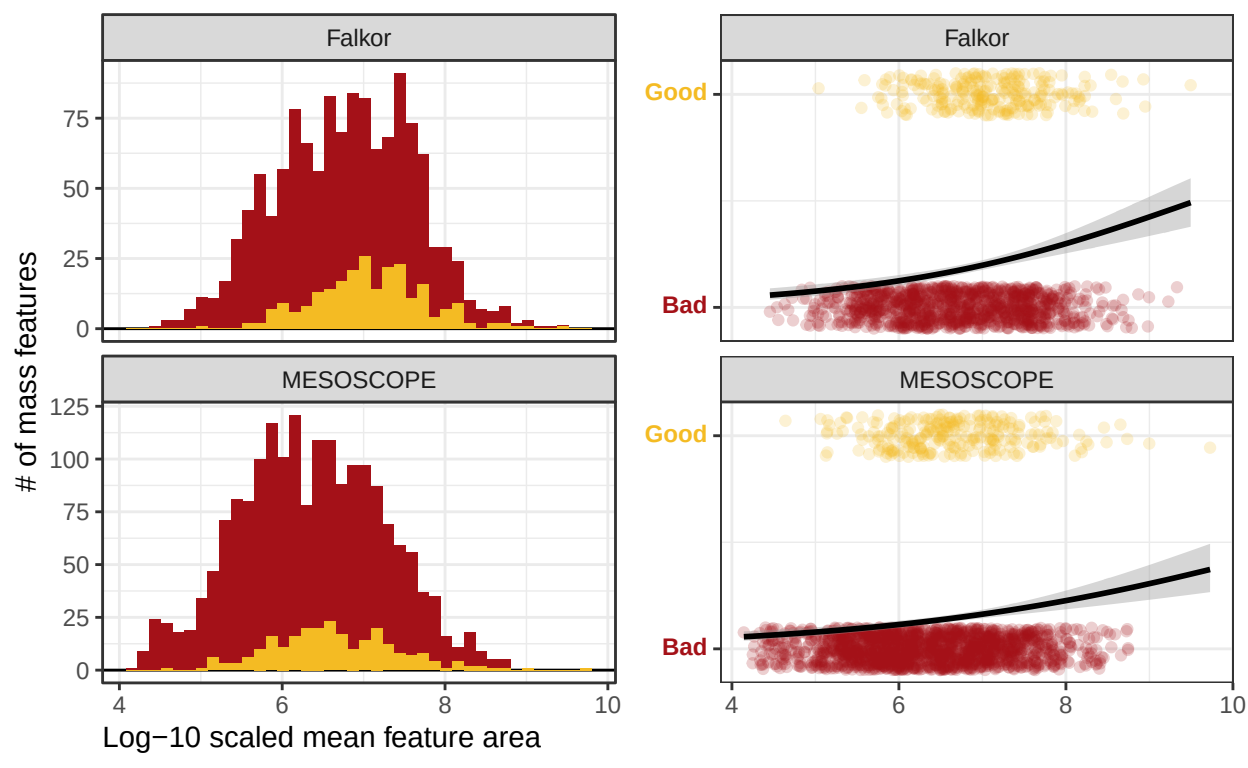

Falkor
MESOSCOPE
# of mass features
SD of feature m/z ratios in ppm
Good
Bad

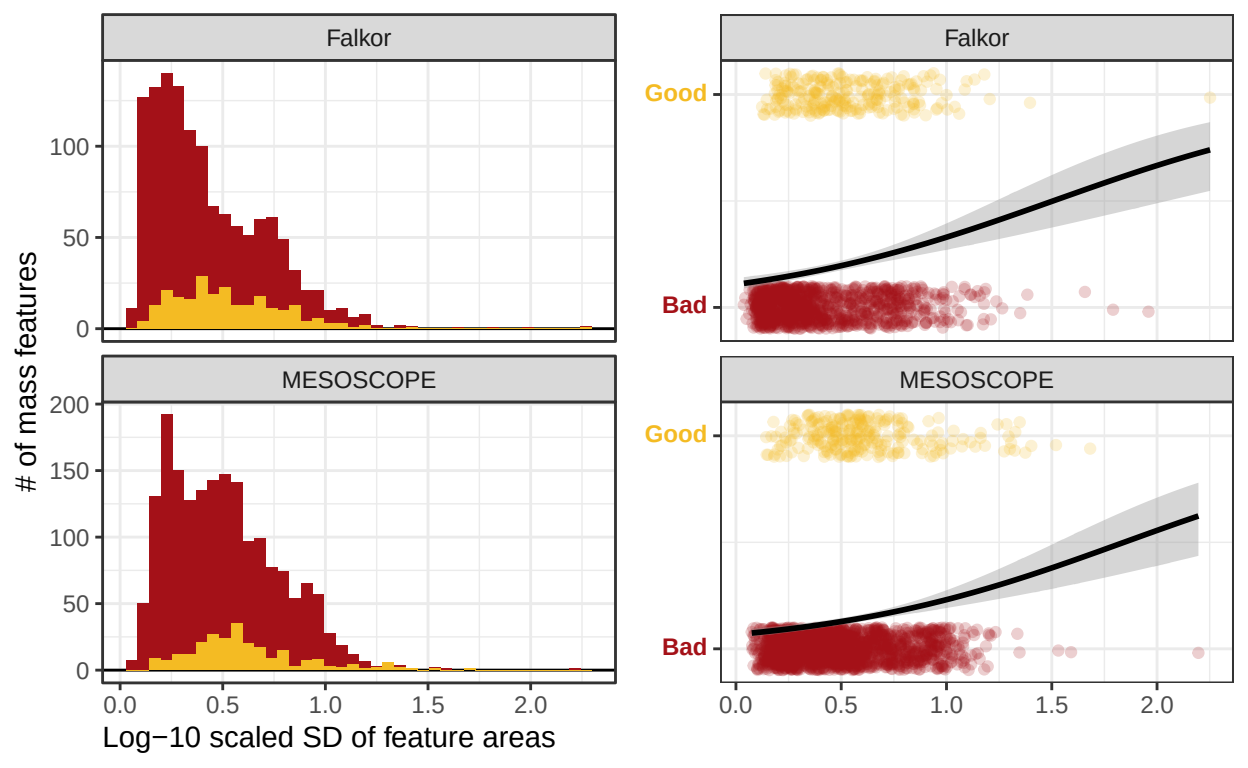

Falkor
MESOSCOPE
# of mass features
Mean feature retention time
0
20
40
60
25
50
75
100
125
250
500
750
1000
1250
Good
Bad

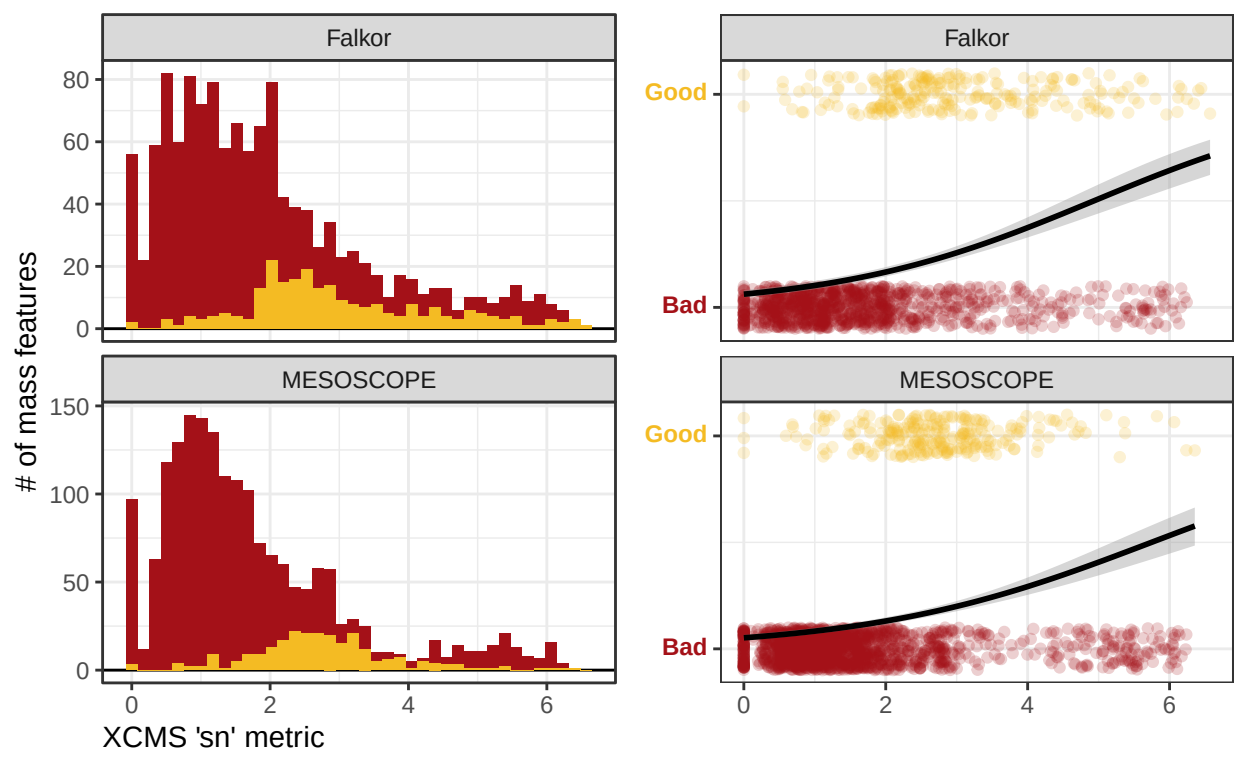

Falkor
MESOSCOPE
# of mass features
SD of feature retention time
Good
Bad

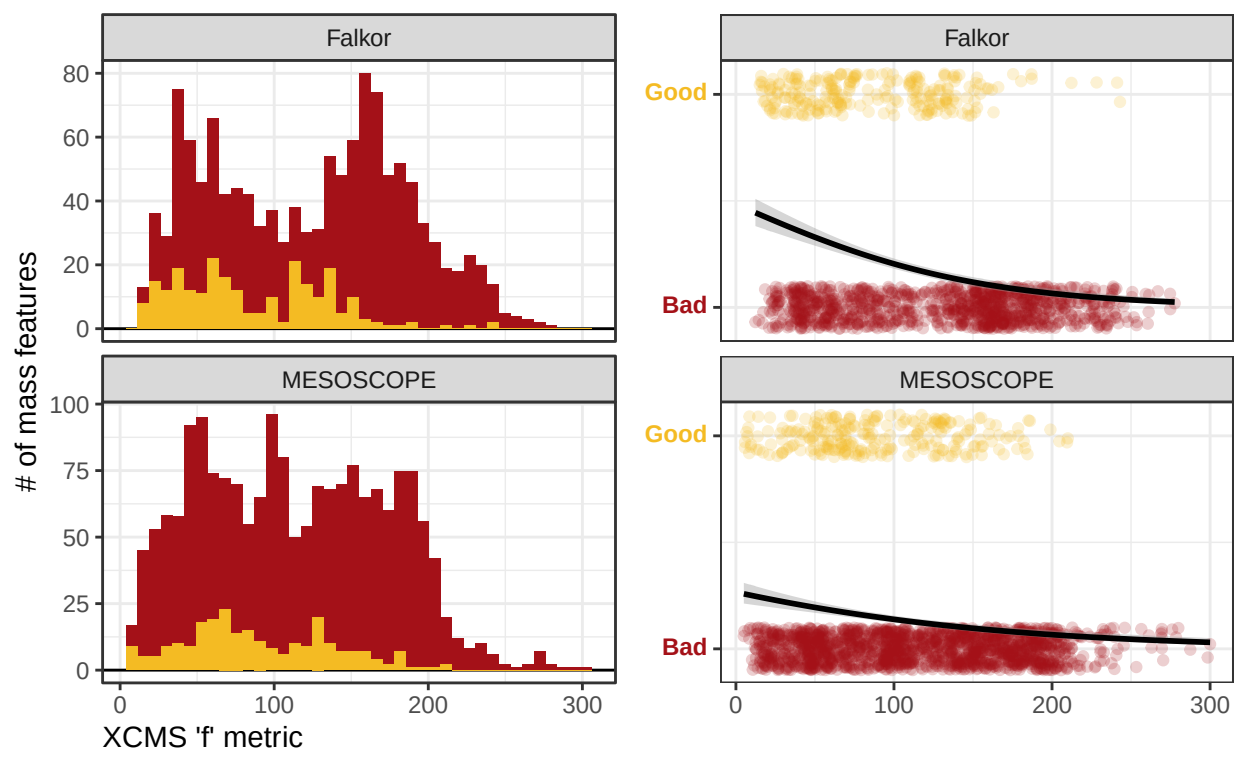

Falkor
MESOSCOPE
# of mass features
Mean peak width, in seconds
Good
Bad

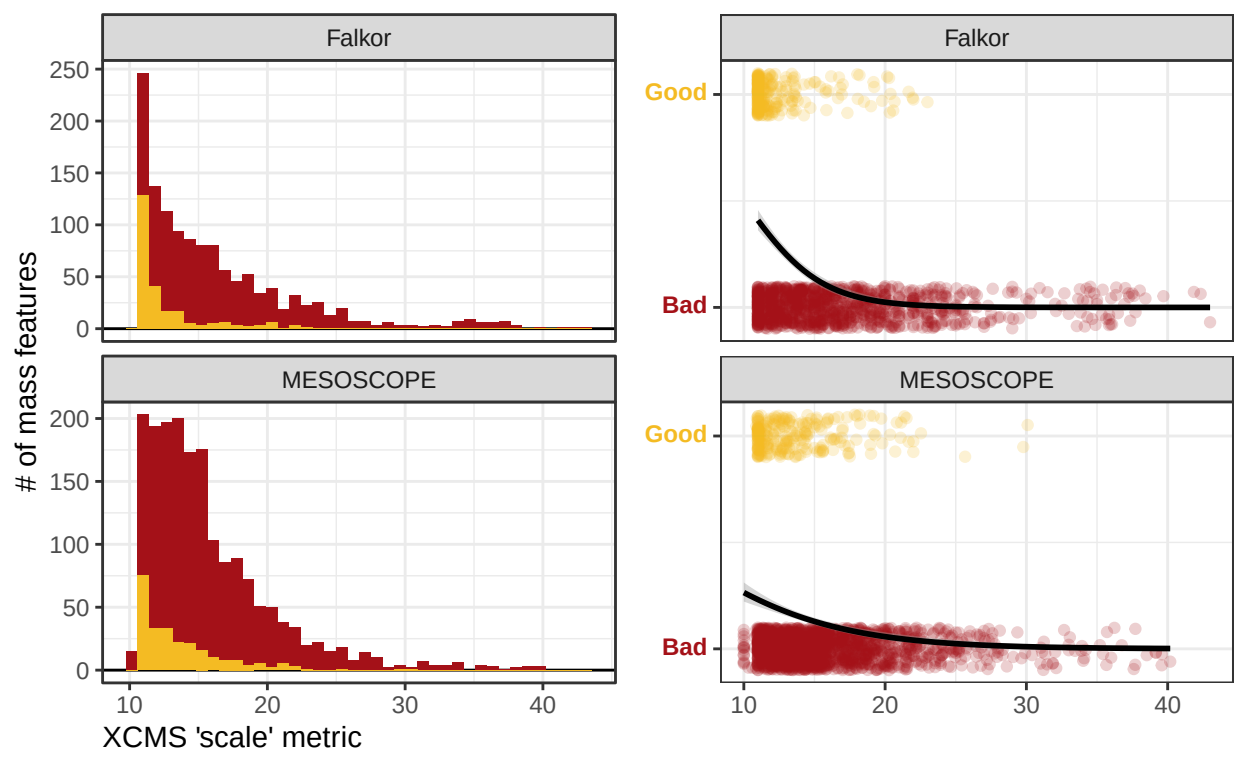

Falkor
MESOSCOPE
# of mass features
SD of peak widths, in seconds
Good
Bad

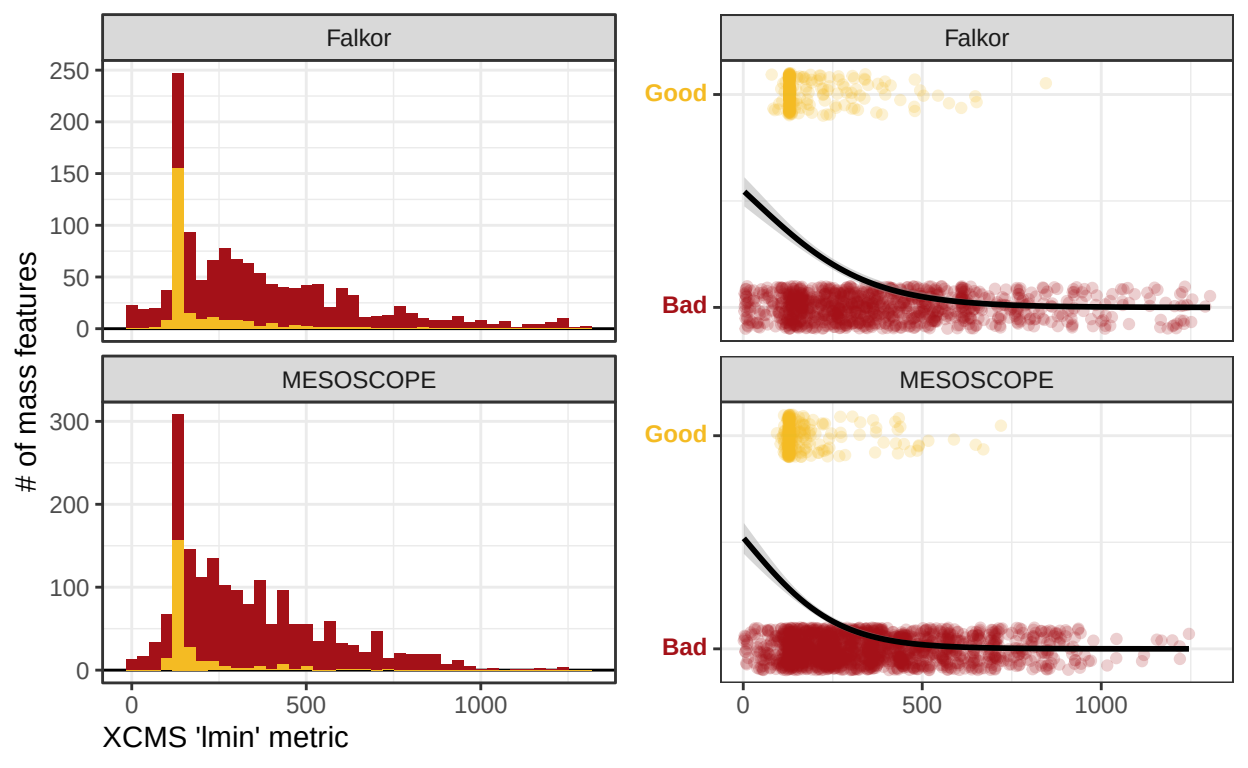

Falkor
MESOSCOPE
# of mass features
0
25
50
75
100
125
4
6
8
10
Log−10 scaled mean feature area
Falkor
MESOSCOPE
Good
Bad

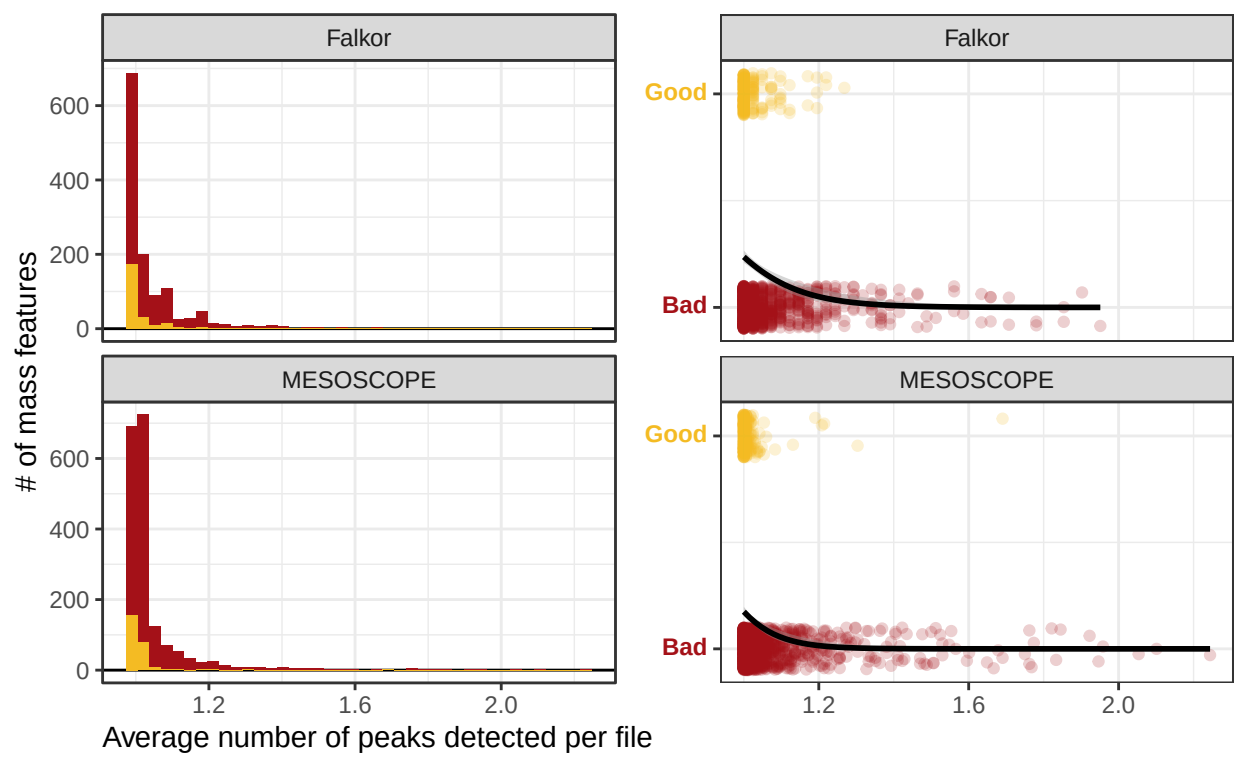

Falkor
MESOSCOPE
# of mass features
Log−10 scaled SD of feature areas
Good
Bad

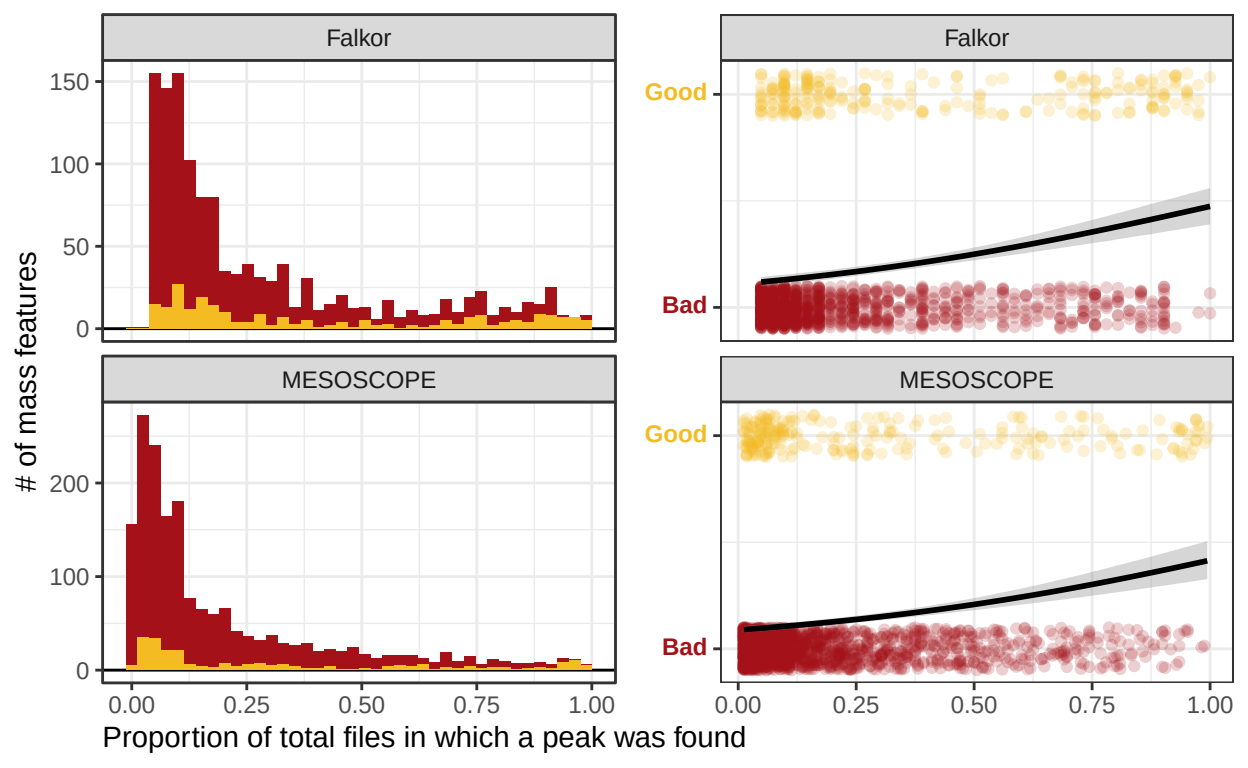

Falkor
MESOSCOPE
# of mass features
XCMS 'sn' metric
Good
Bad

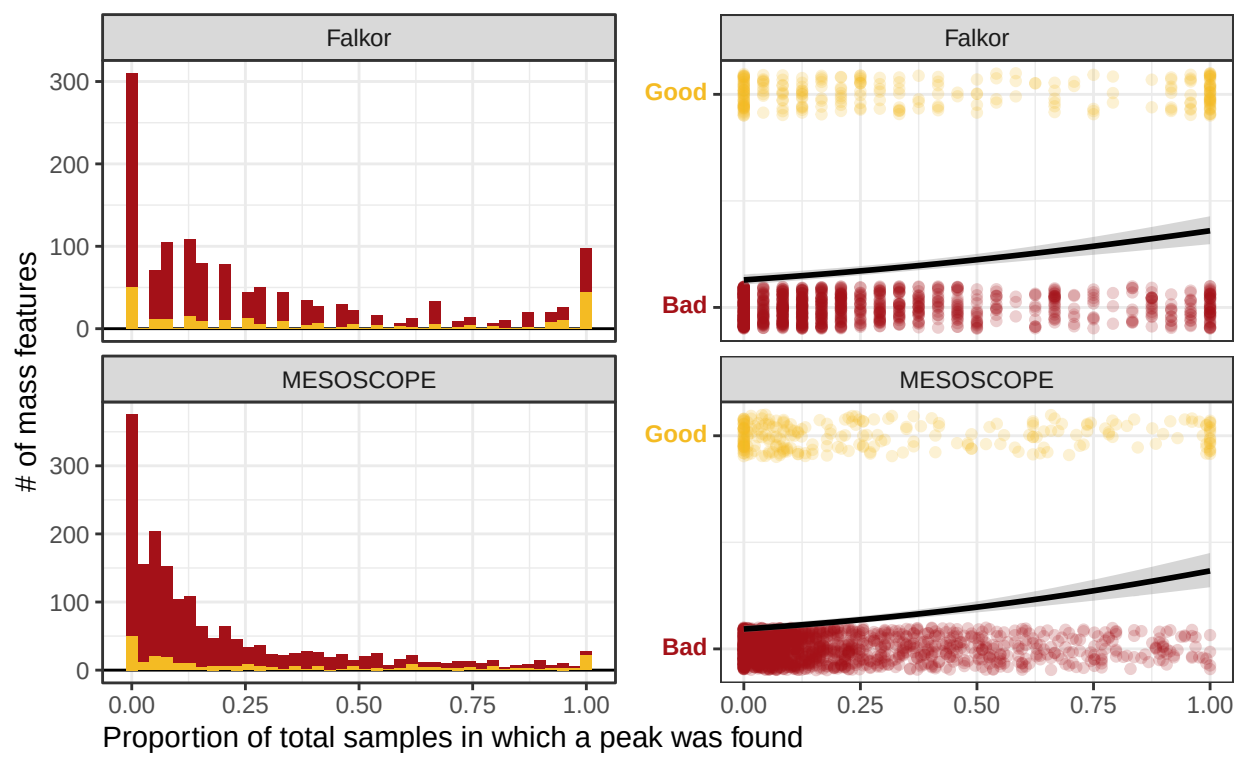

Falkor
MESOSCOPE
# of mass features
XCMS 'f' metric
Good
Bad
0
20
40
60
80
25
50
75
100
0
100
200
300

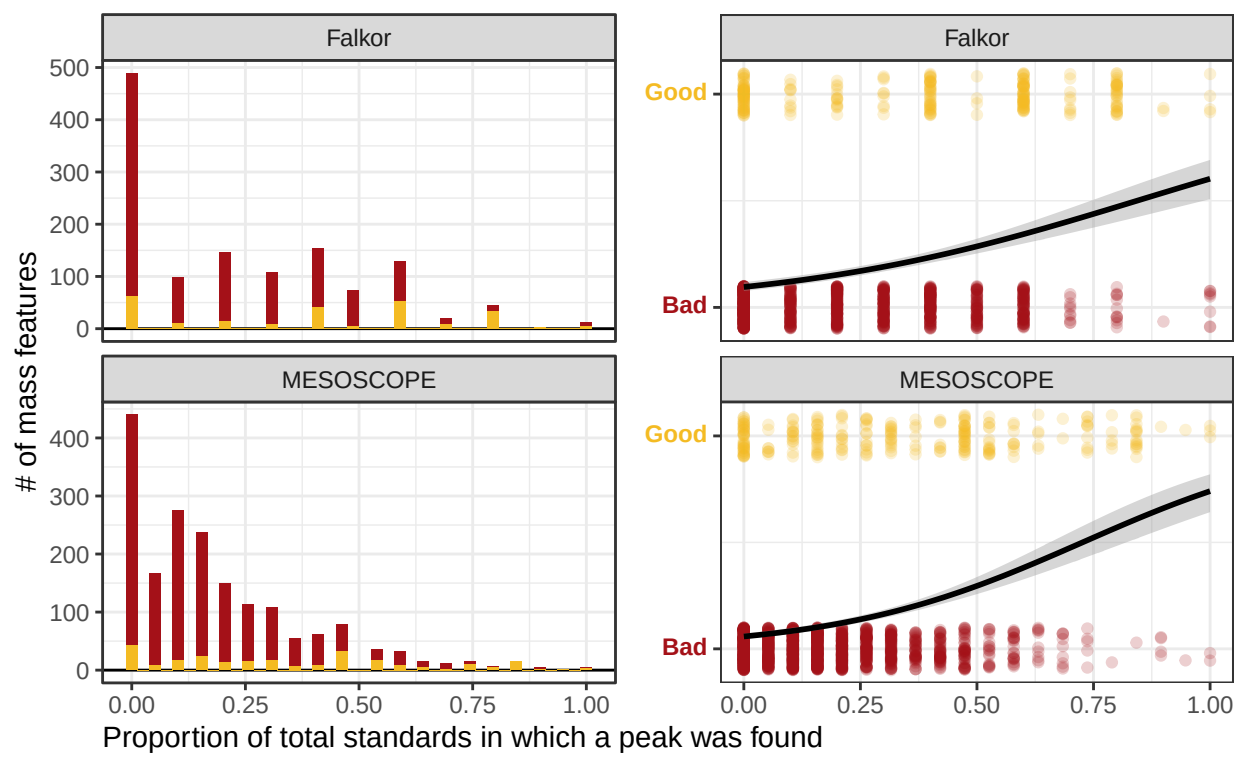

Falkor
MESOSCOPE
# of mass features
XCMS 'scale' metric
Good
Bad

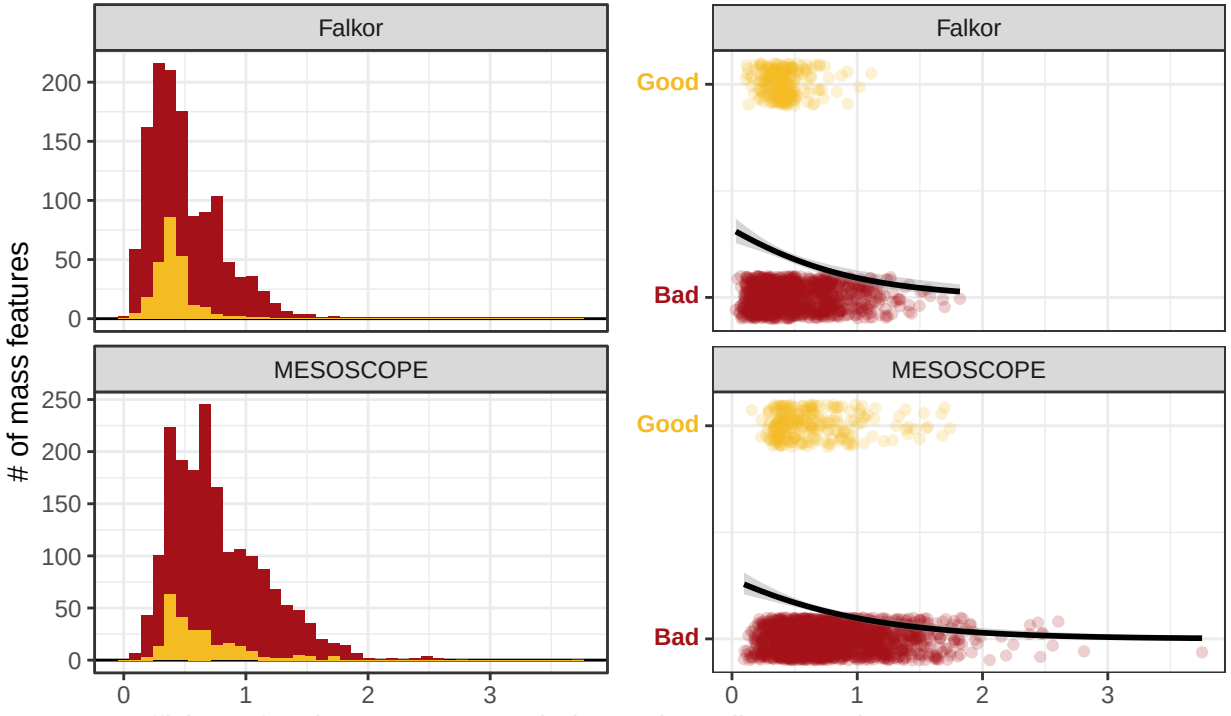

Falkor
MESOSCOPE
# of mass features
XCMS 'lmin' metric
Good
Bad

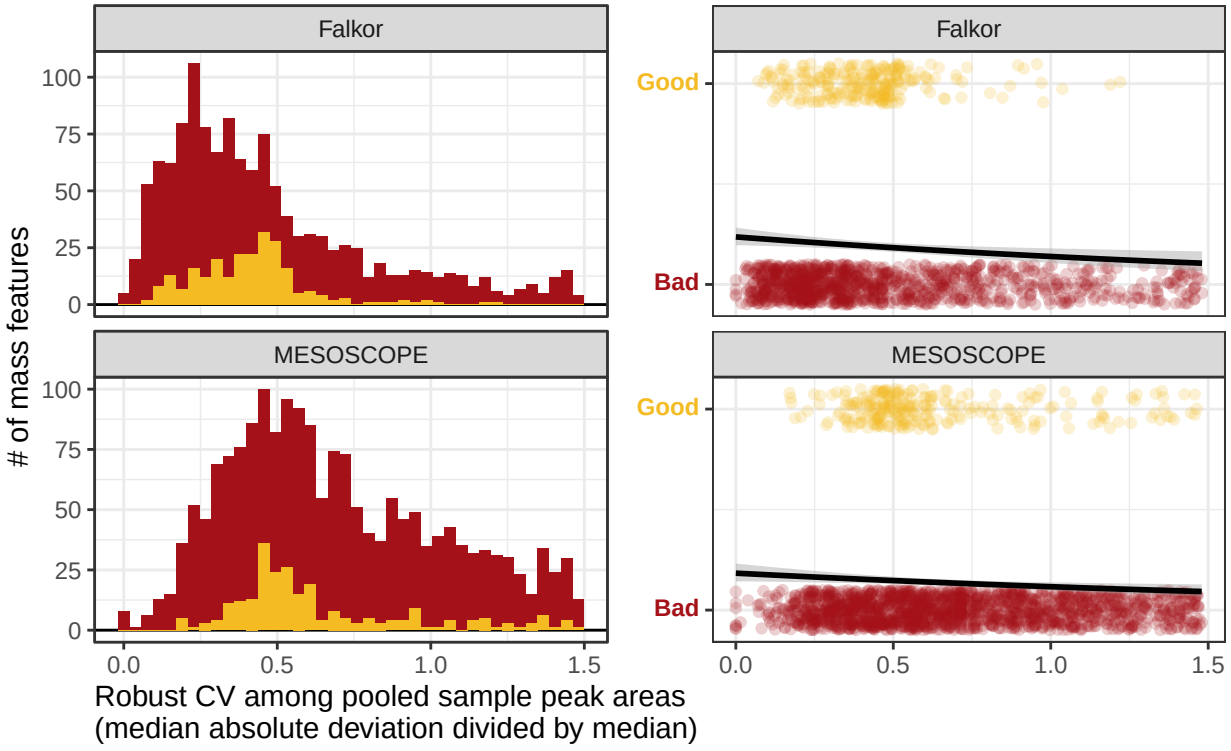

Falkor
MESOSCOPE
# of mass features
600
400
200
0
1.2
1.6
2.0
Average number of peaks detected per file
Good
Bad

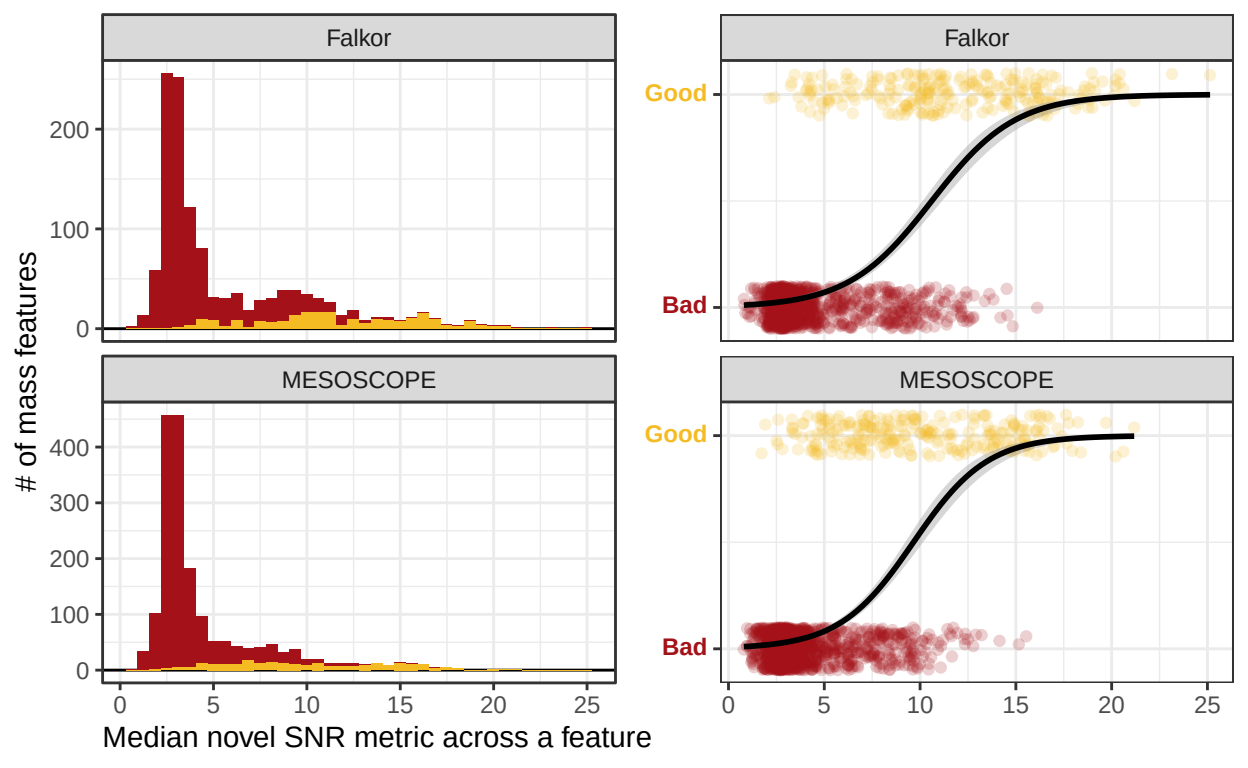

Falkor
MESOSCOPE
# of mass features
150
100
50
0
200
100
0
0.00
0.25
0.50
0.75
1.00
Proportion of total files in which a peak was found
Good
Bad

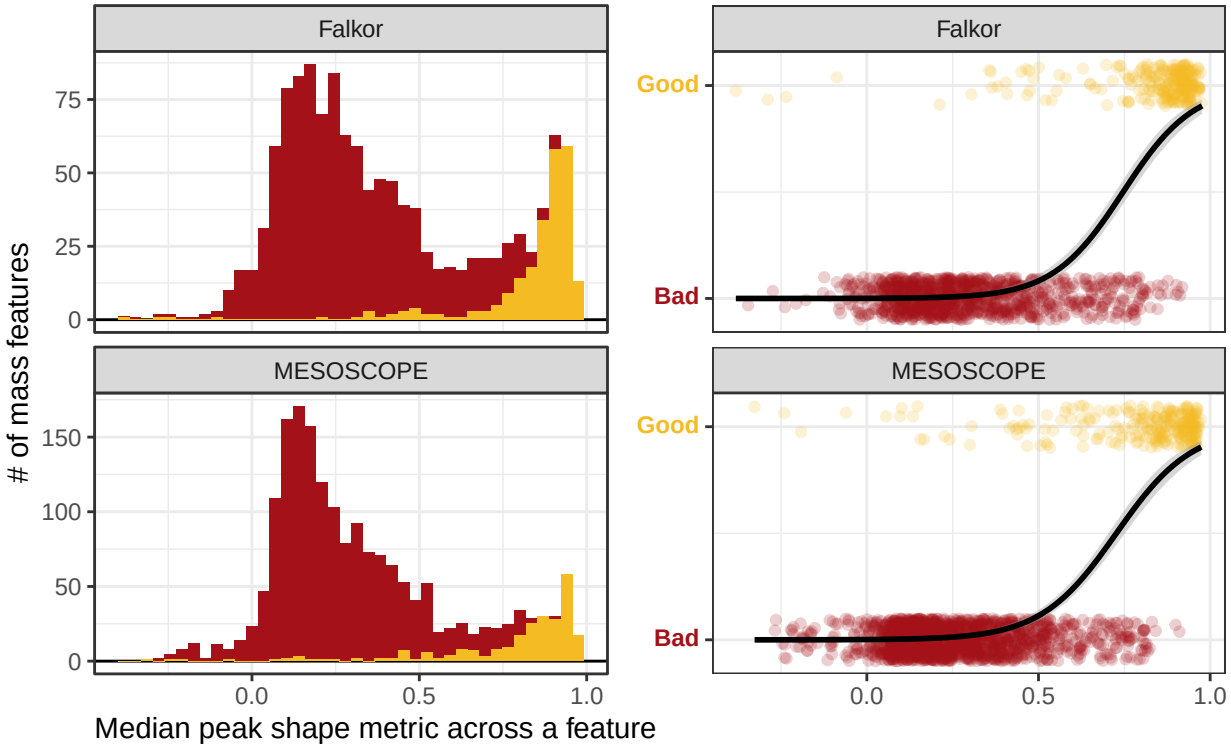

Falkor
MESOSCOPE
# of mass features
300
200
100
0
0.00
0.25
0.50
0.75
1.00
Proportion of total samples in which a peak was found
Good
Bad

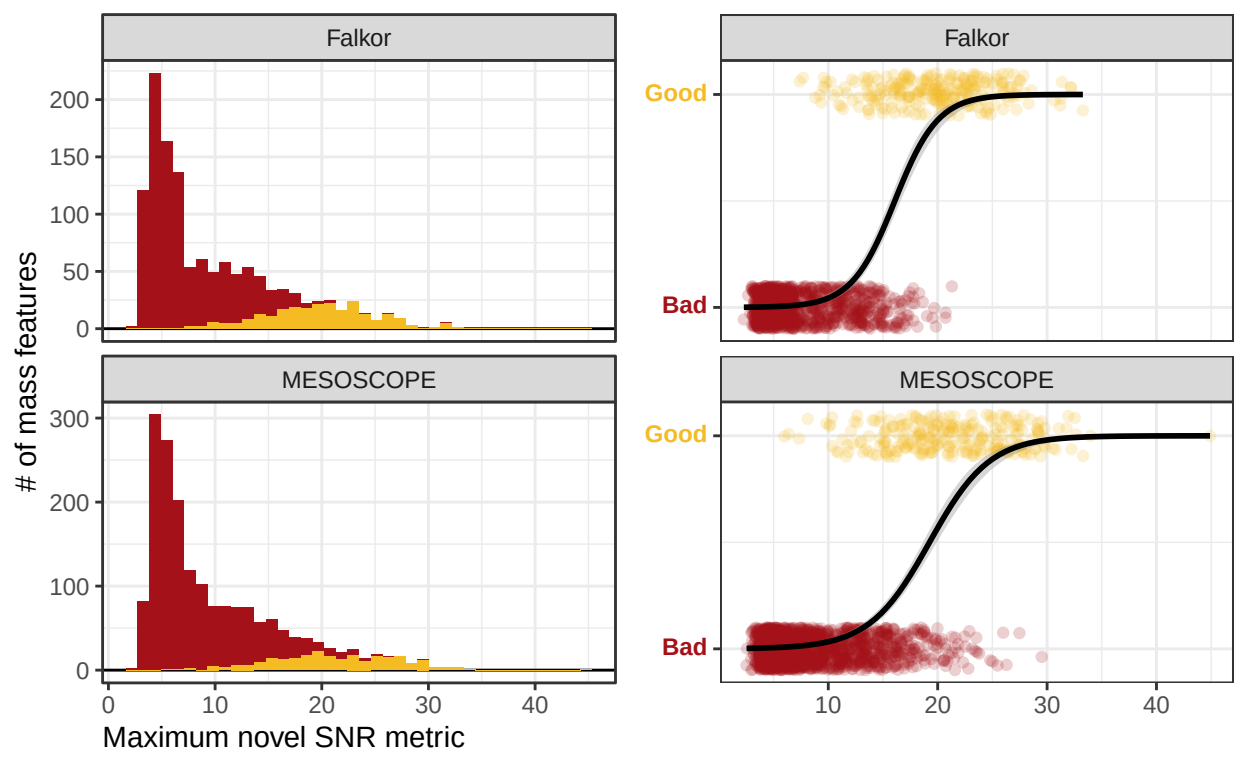

Falkor
MESOSCOPE
# of mass features
Proportion of total standards in which a peak was found
Good
Bad
0.00
0.25
0.50
0.75
1.00

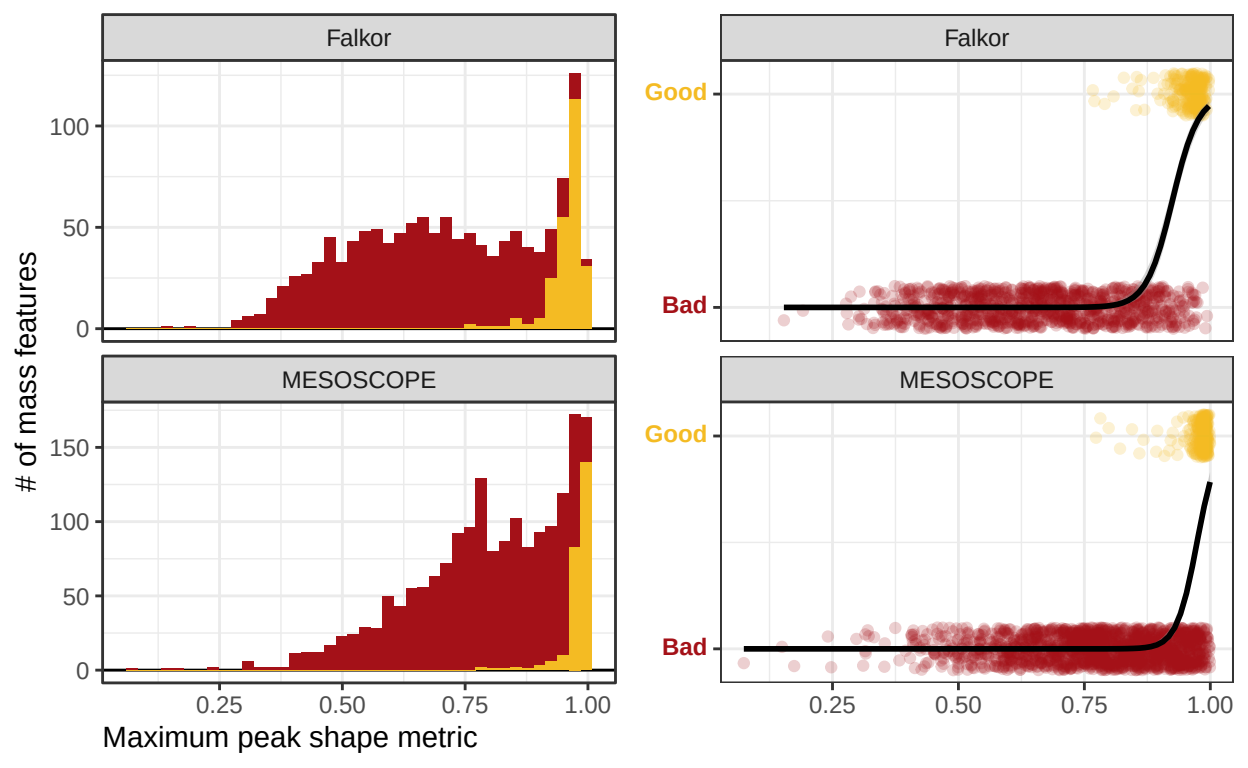

Falkor
MESOSCOPE
# of mass features
Coefficient of variance among pooled sample replicate peak areas
Good
Bad

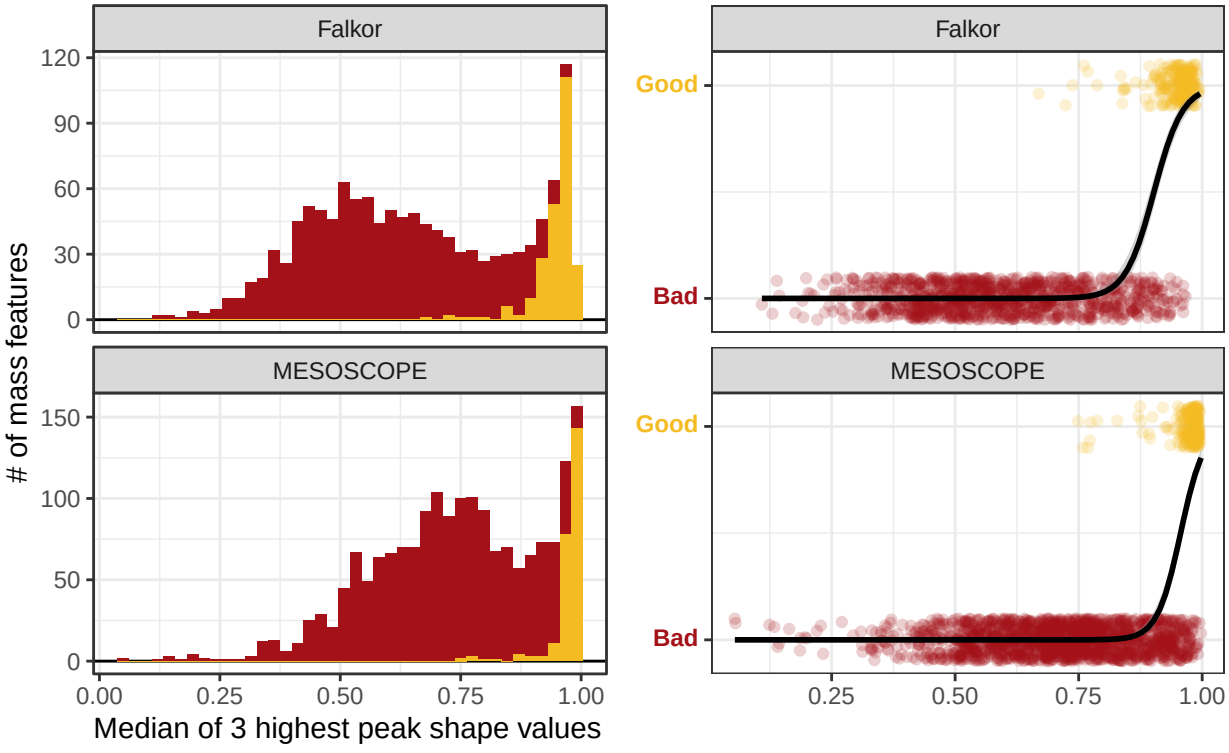

Falkor
MESOSCOPE
# of mass features
100
75
50
25
0
0.0
0.5
1.0
1.5
Good
Bad
Robust CV among pooled sample peak areas
(median absolute deviation divided by median)

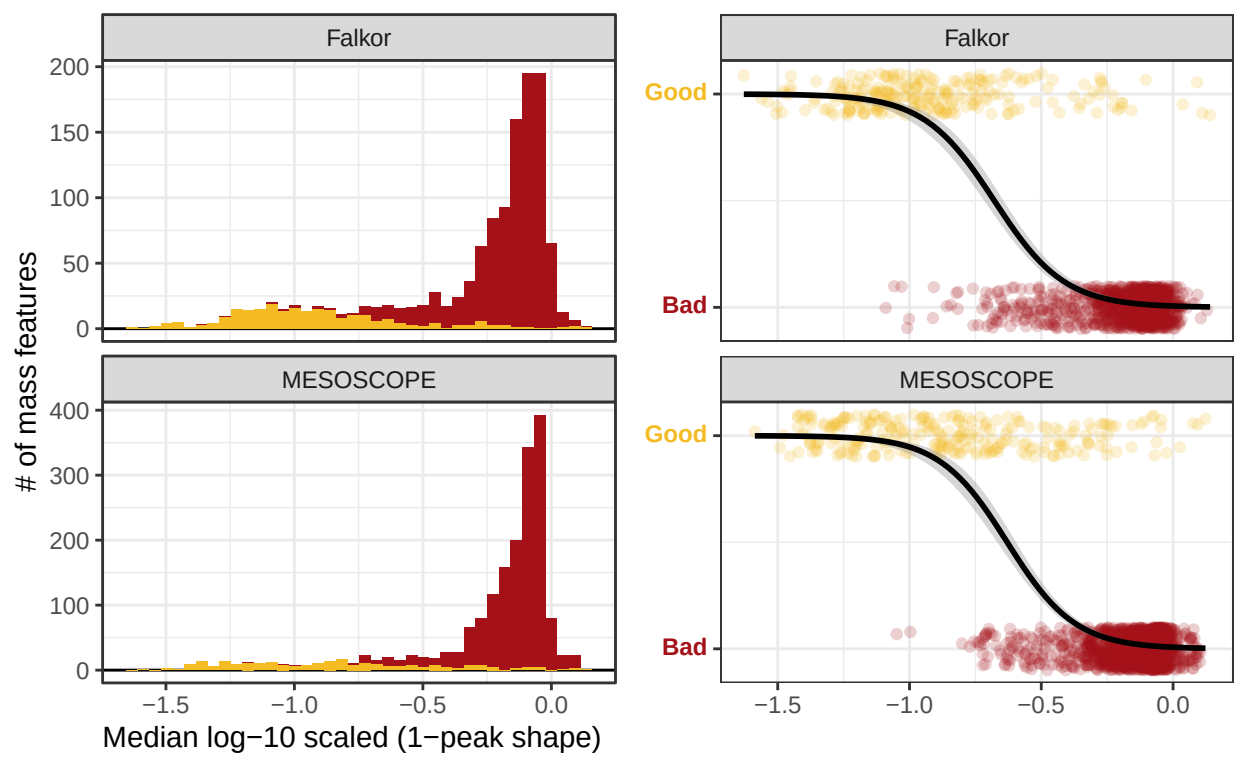

Falkor
MESOSCOPE
# of mass features
Median novel SNR metric across a feature
Good
Bad

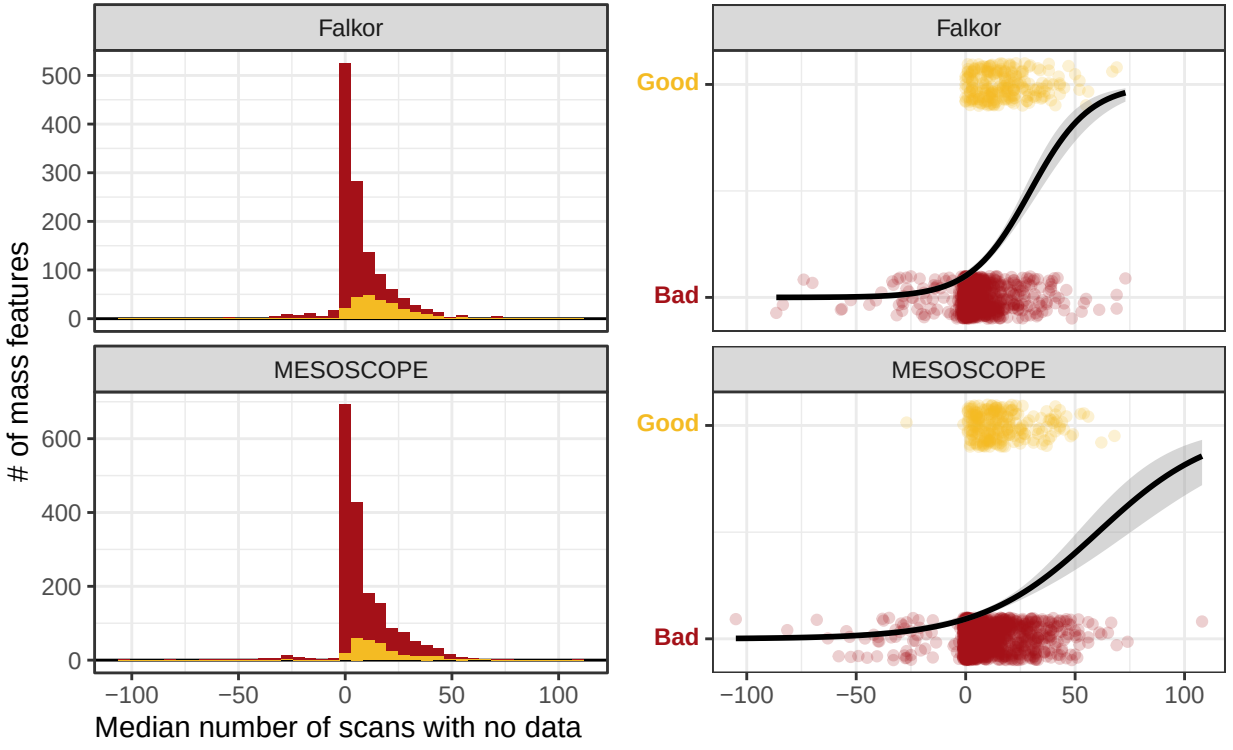

Falkor
MESOSCOPE
# of mass features
75
50
25
0
150
100
50
0
0.0
0.5
1.0
Median peak shape metric across a feature
Falkor
MESOSCOPE
Good
Bad
Good
Bad
0.0
0.5
1.0

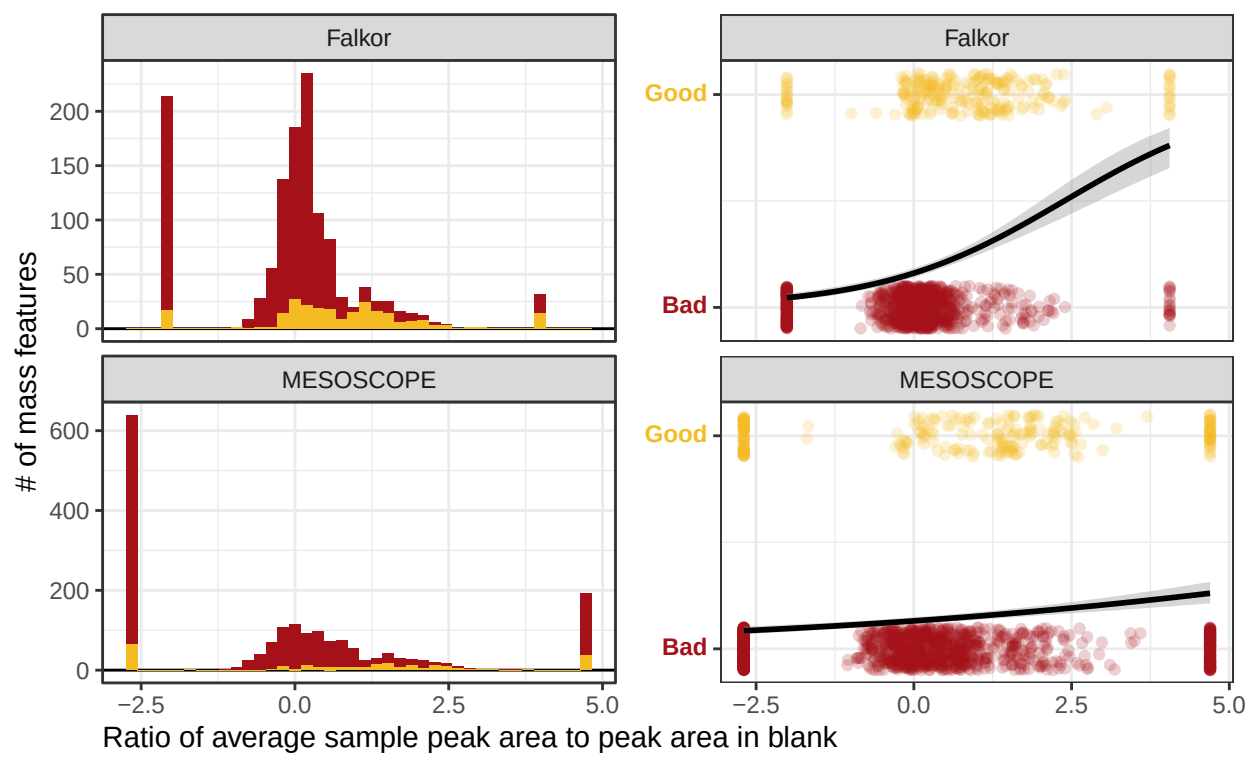

Falkor
MESOSCOPE
# of mass features
Maximum novel SNR metric
Good
Bad

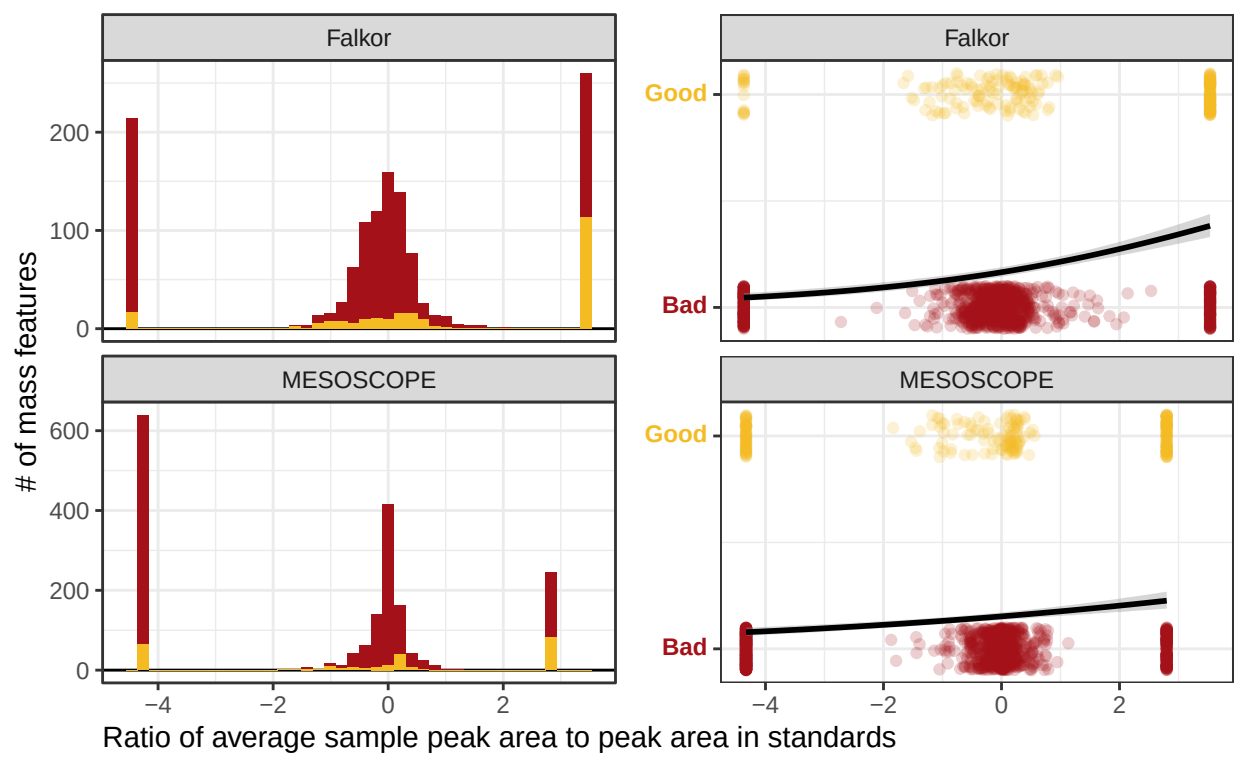

Falkor
MESOSCOPE
# of mass features
100
50
0
150
0.25
0.50
0.75
1.00
Maximum peak shape metric
Good
Bad

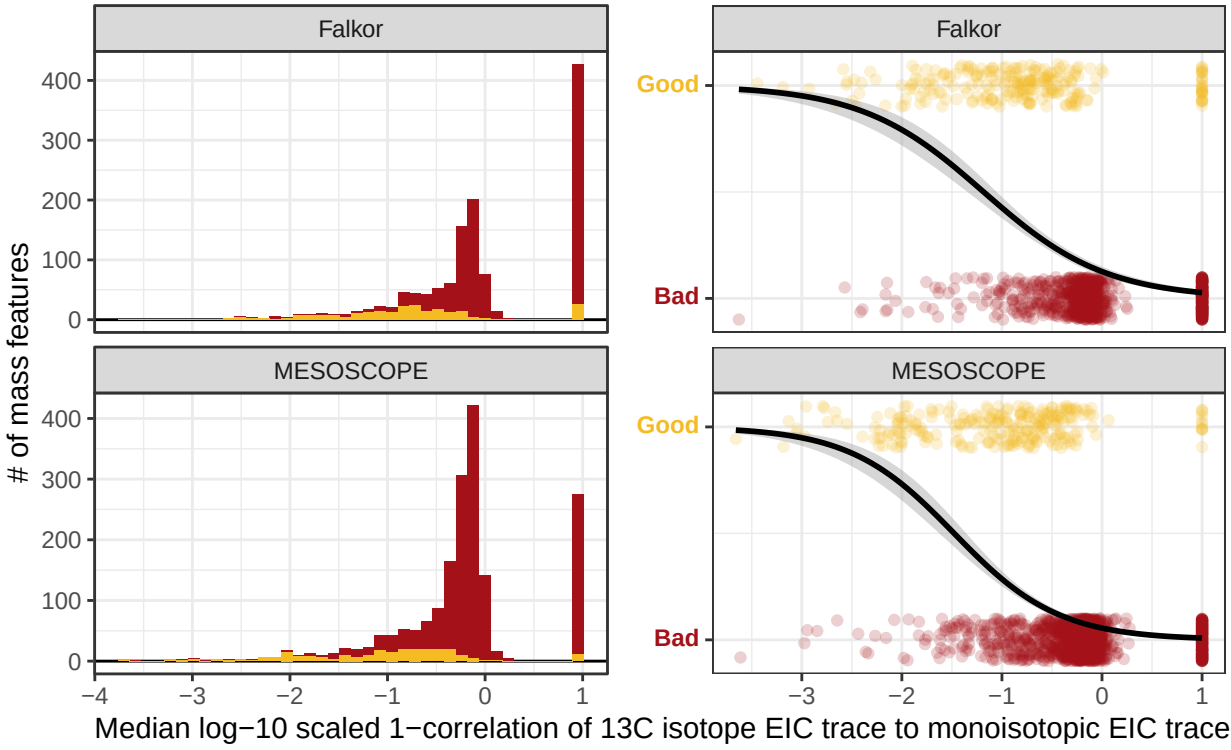

Falkor
MESOSCOPE
# of mass features
Median of 3 highest peak shape values
Good
Bad

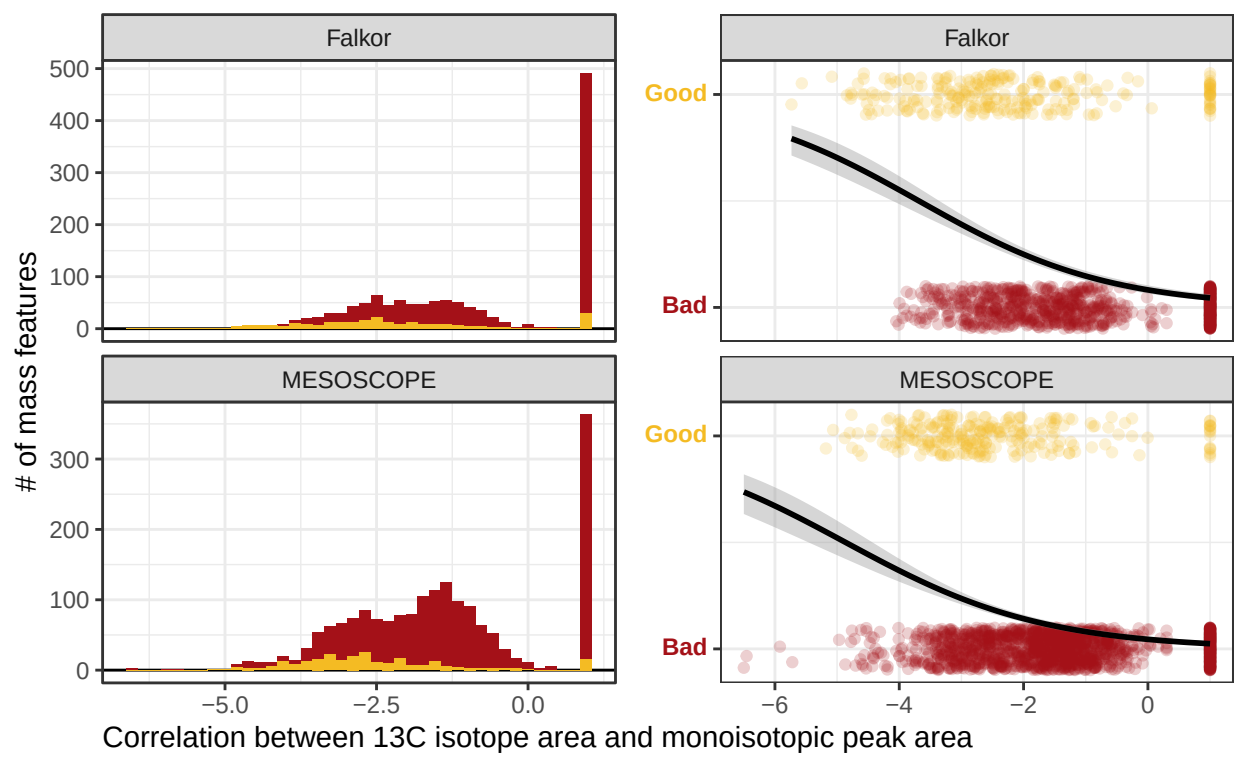

Falkor
MESOSCOPE
# of mass features
Median log−10 scaled (1−peak shape)
Good
Bad


Falkor
MESOSCOPE
# of mass features
500
400
300
200
100
0
600
400
200
0
−100
−50
0
50
100
Median number of scans with no data
Falkor
MESOSCOPE
Good
Bad
Good
Bad
−100
−50
0
50
100


Falkor
MESOSCOPE
# of mass features
0
50
100
150
200
400
600
Good
Bad
−2.5
0.0
2.5
5.0
Ratio of average sample peak area to peak area in blank


Falkor
MESOSCOPE
# of mass features
200
100
0
600
400
200
0
Good
Bad
−4
−2
0
2
Ratio of average sample peak area to peak area in standards


Falkor
MESOSCOPE
# of mass features
400
300
200
100
0
−4
−3
−2
−1
0
1
Good
Bad
Median log−10 scaled 1−correlation of 13C isotope EIC trace to monoisotopic EIC trace


Falkor
MESOSCOPE
# of mass features
500
400
300
200
100
0
−5.0
−2.5
0.0
Good
Bad
−6
−4
−2
Correlation between 13C isotope area and monoisotopic peak area