SUPPORTING INFORMATION 2

High accuracy classification of developmental toxicants by in vitro tests of human neuroepithelial and cardiomyoblast differentiation

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‡ These authors contributed equally to this work.

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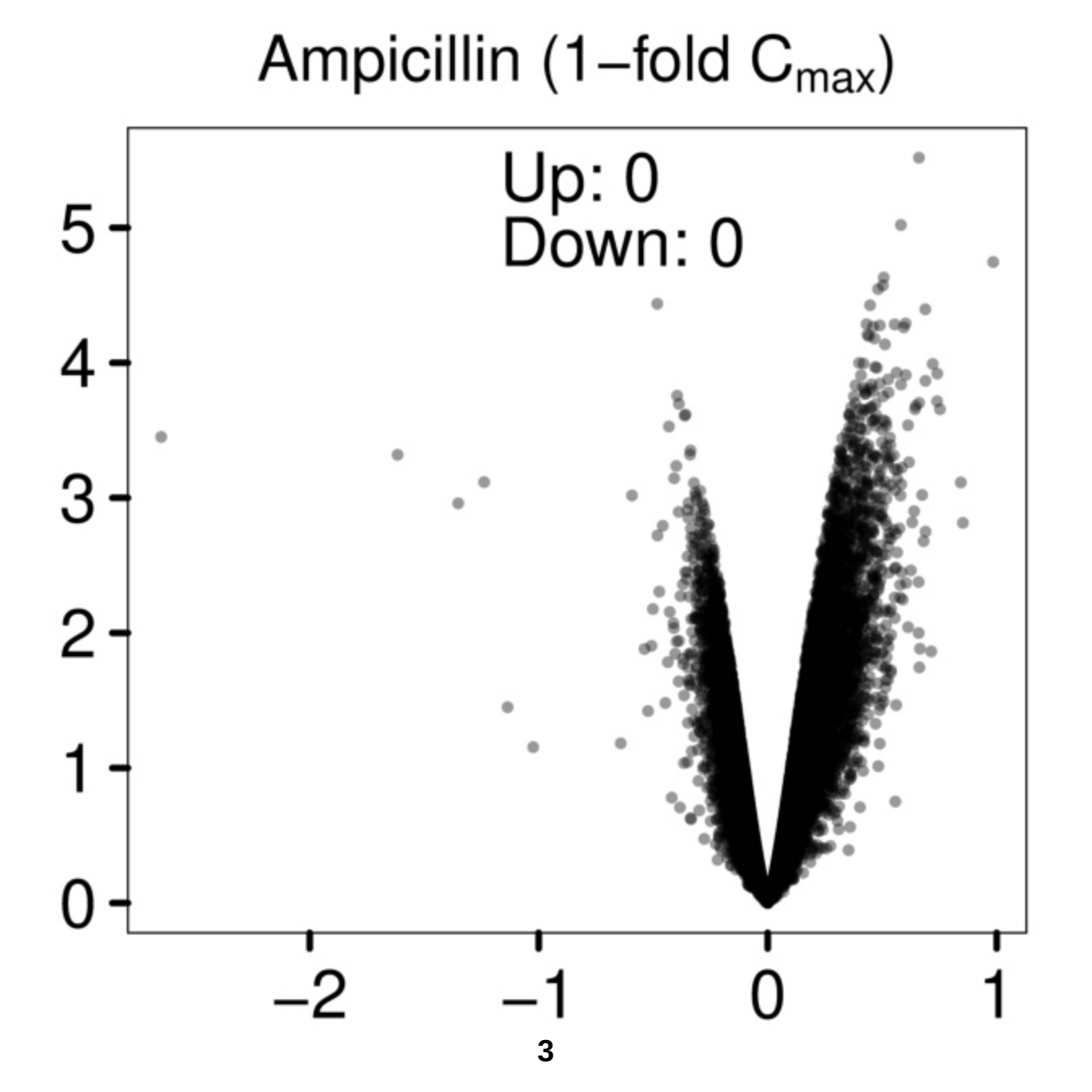
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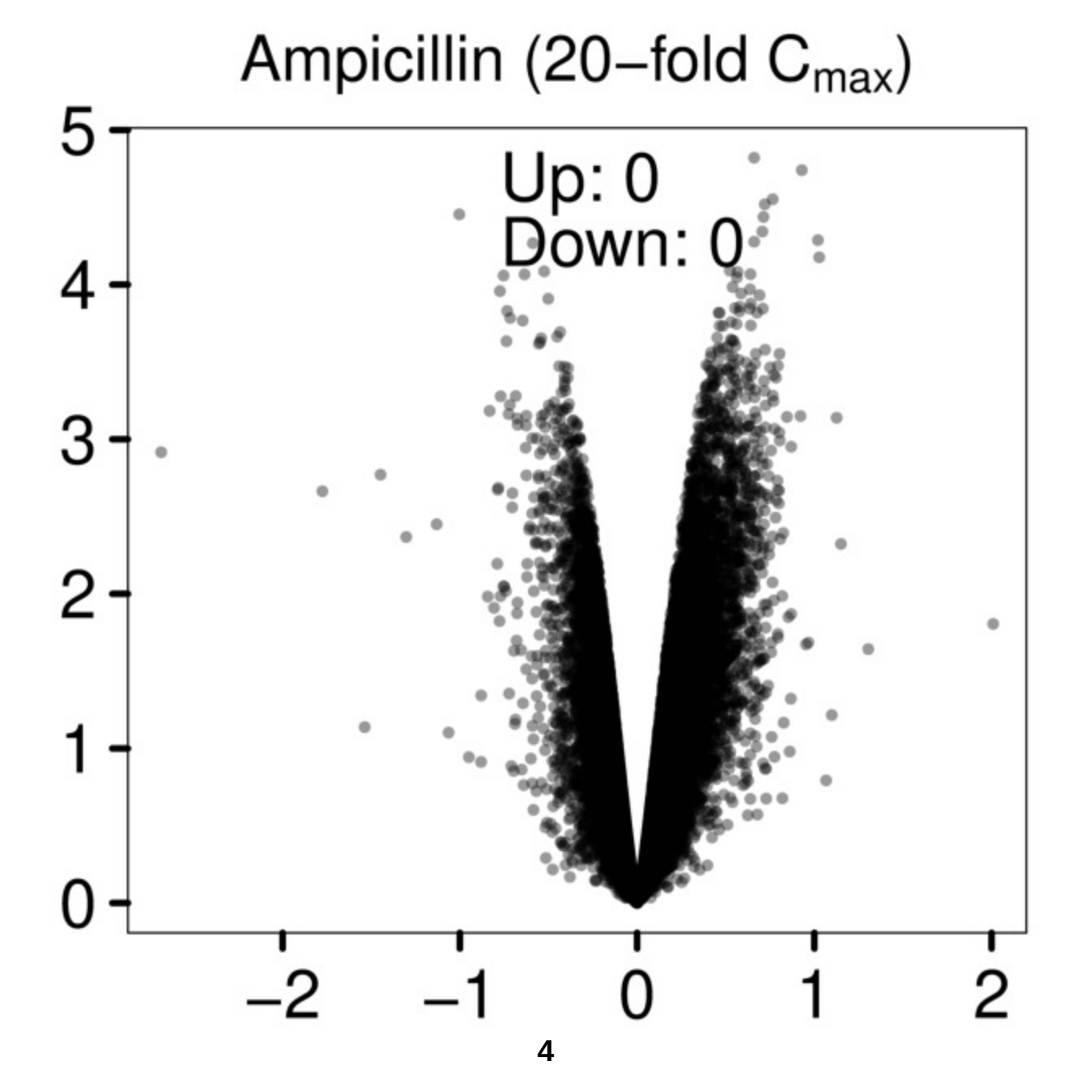
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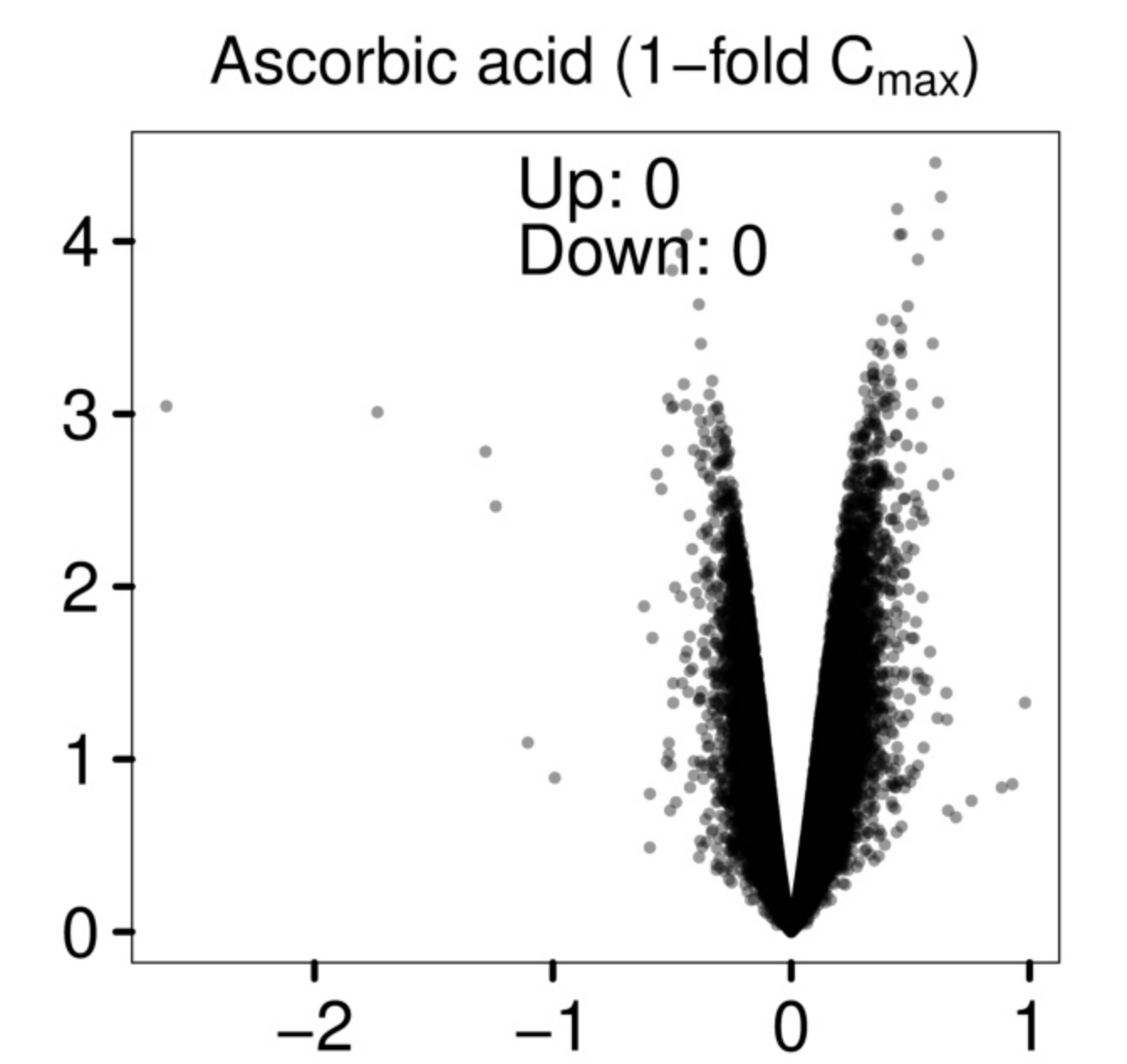
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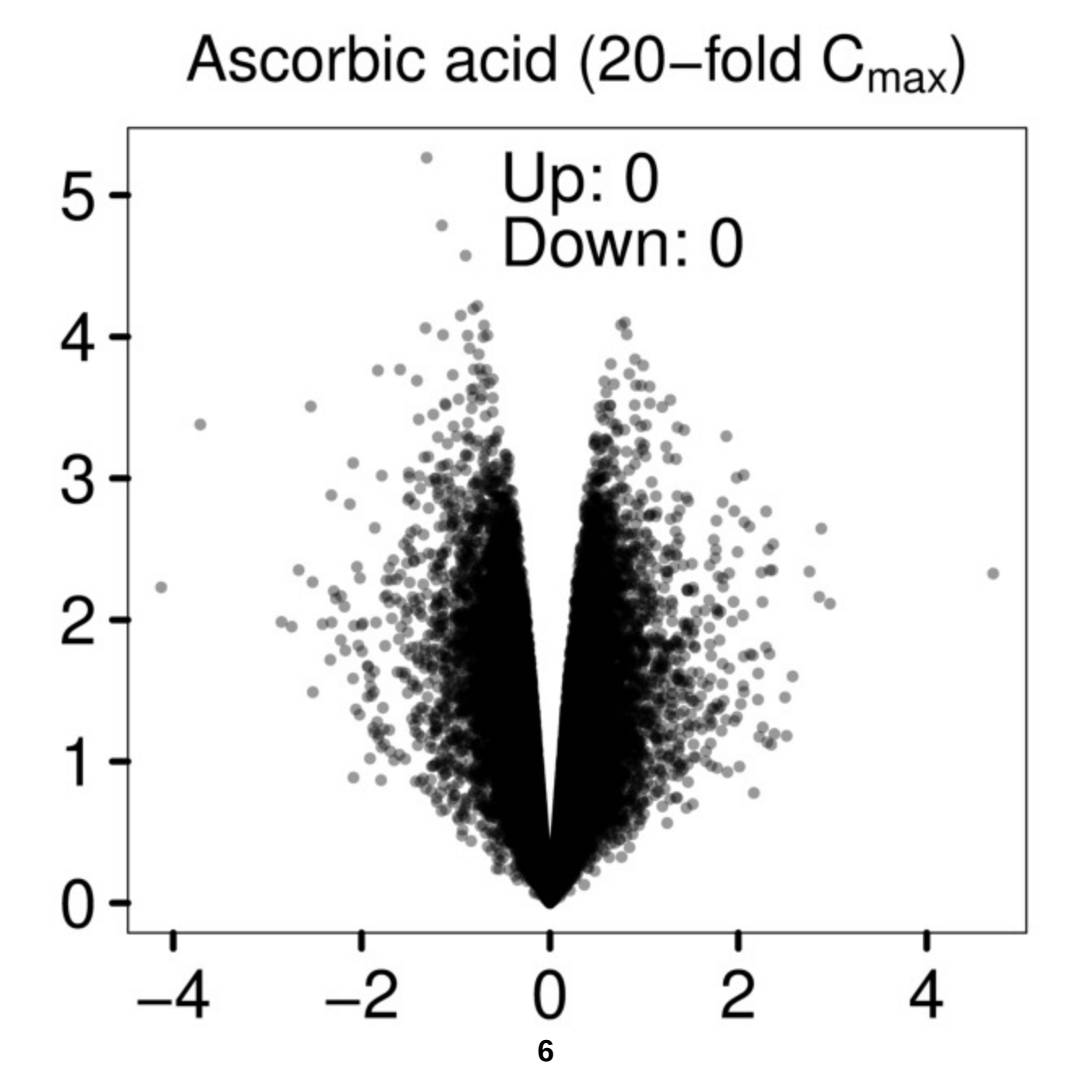
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–2
0
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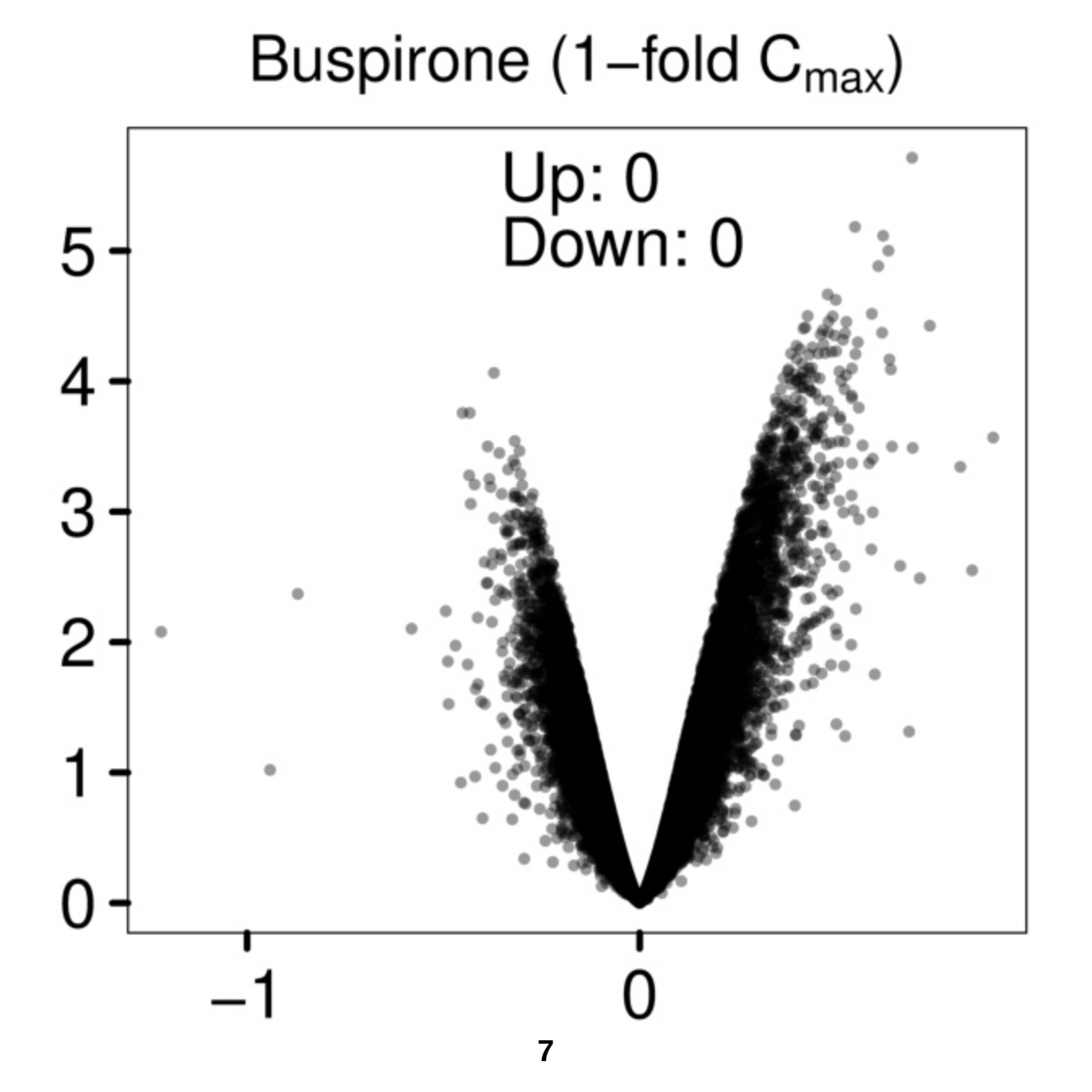
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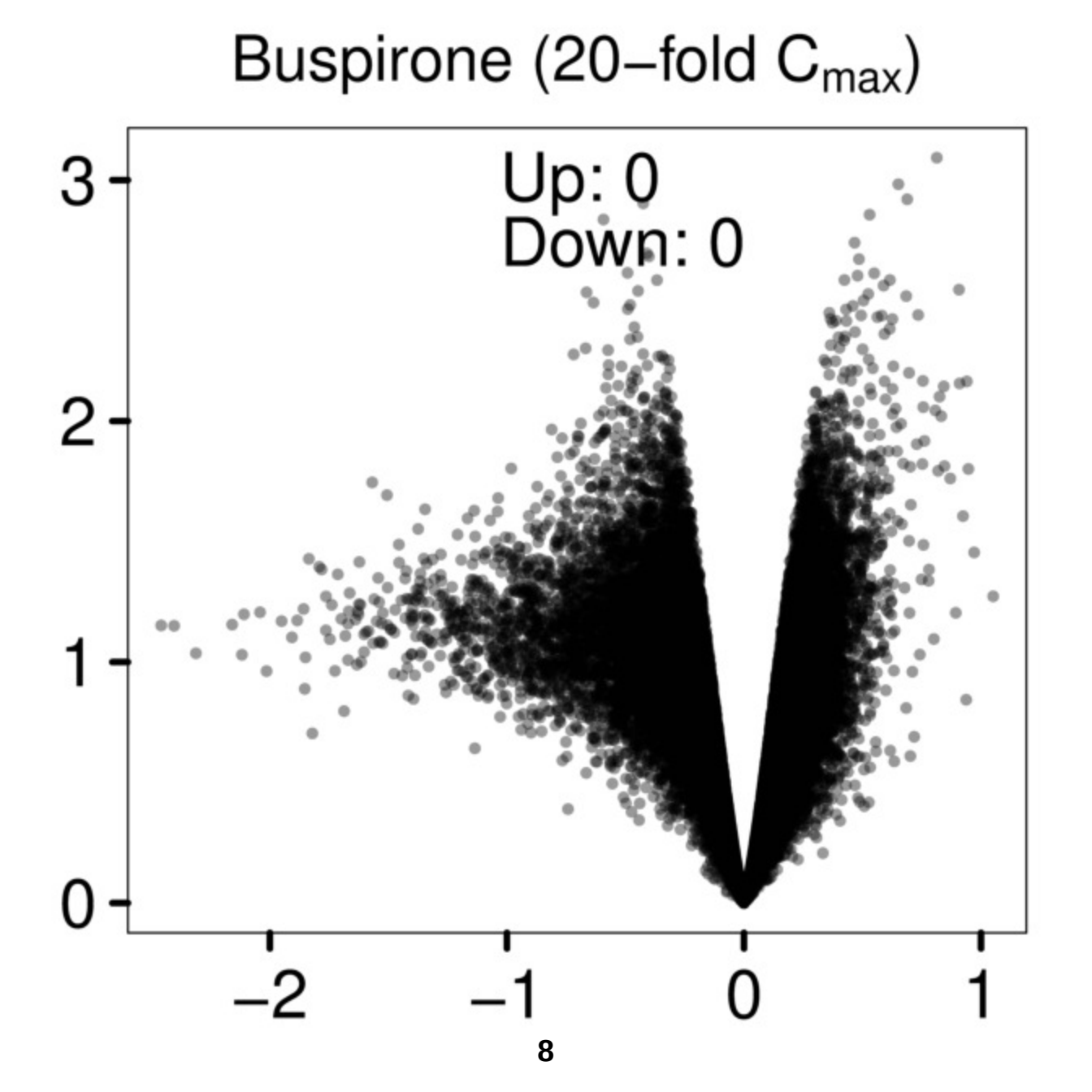
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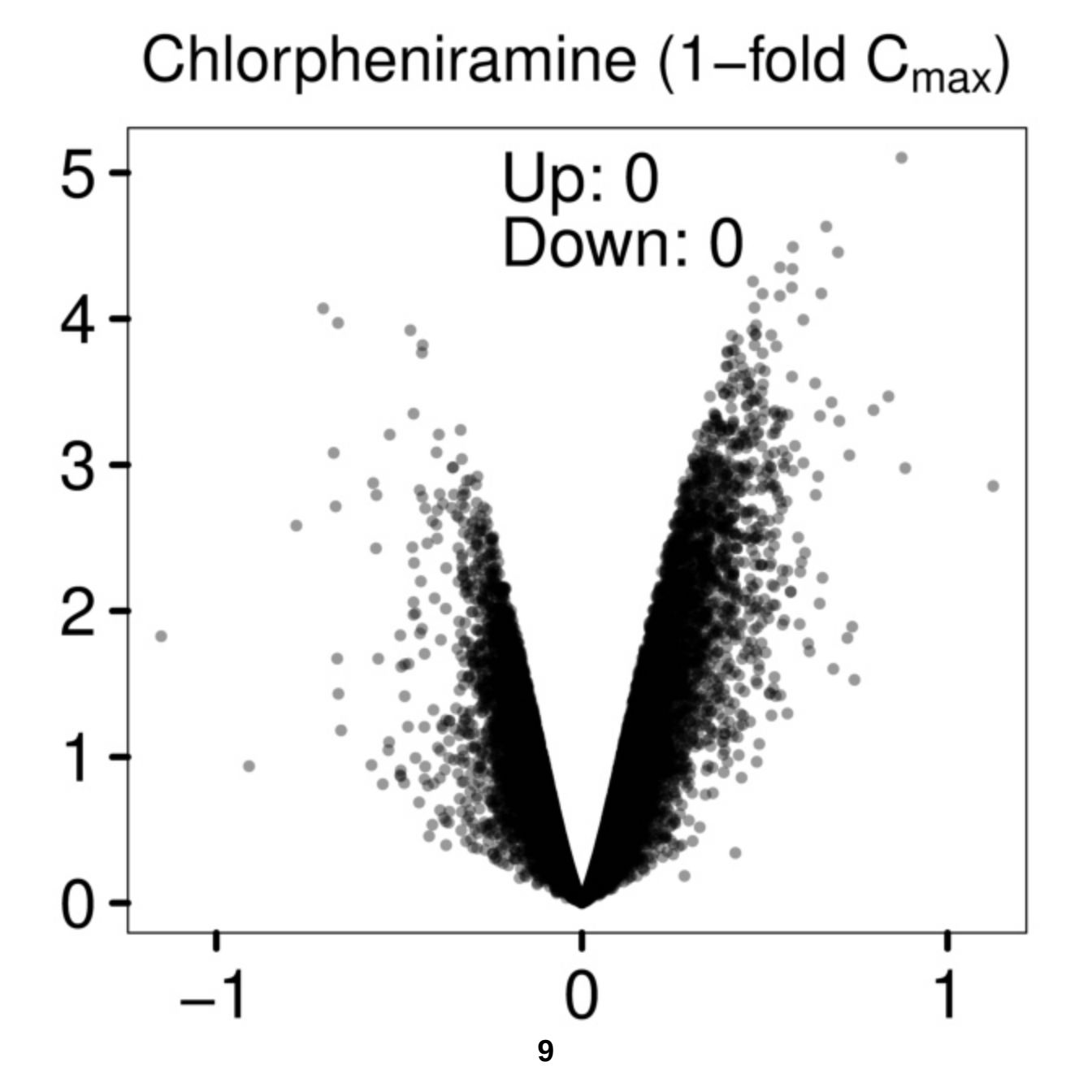
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3
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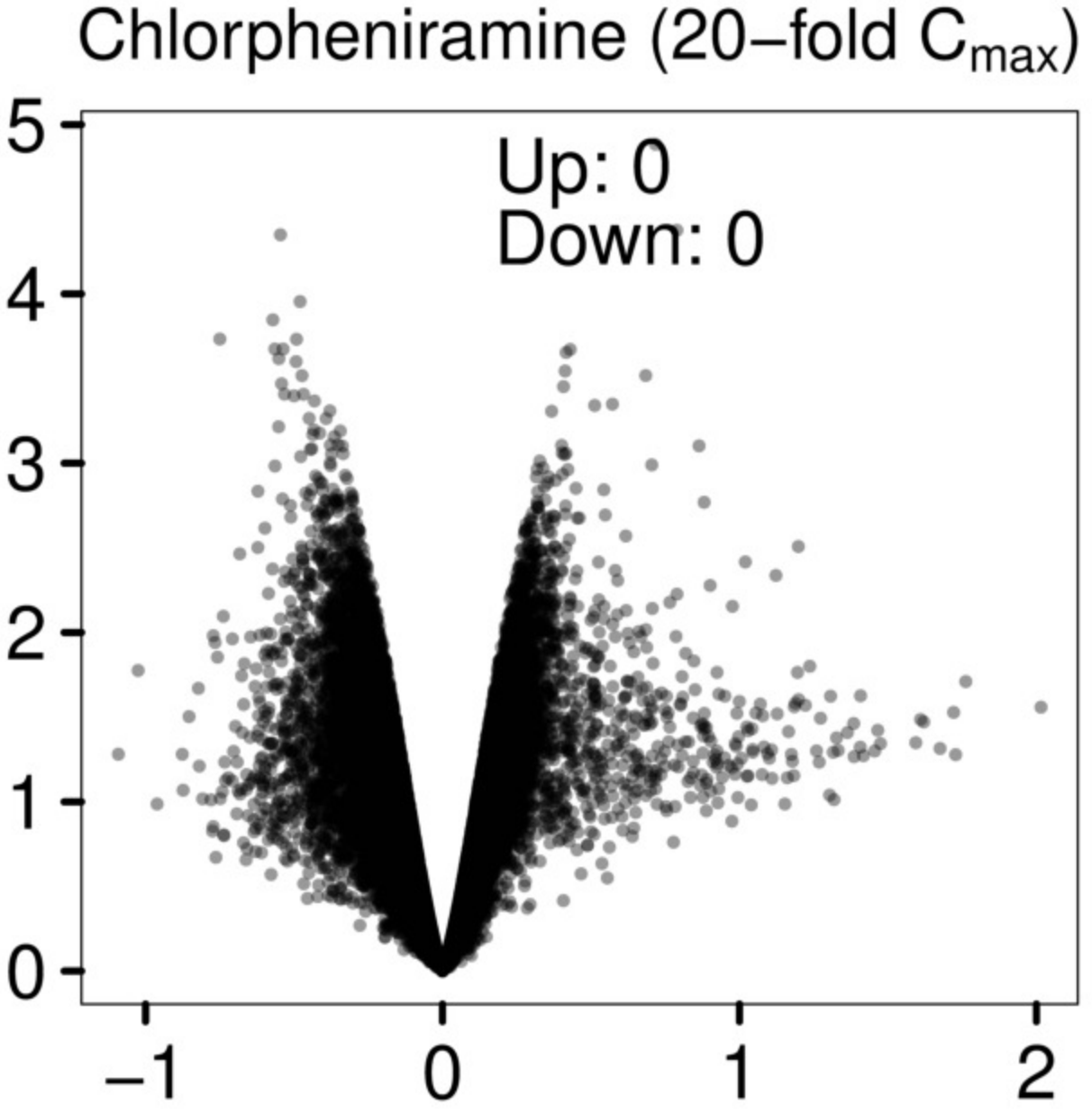
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0
1
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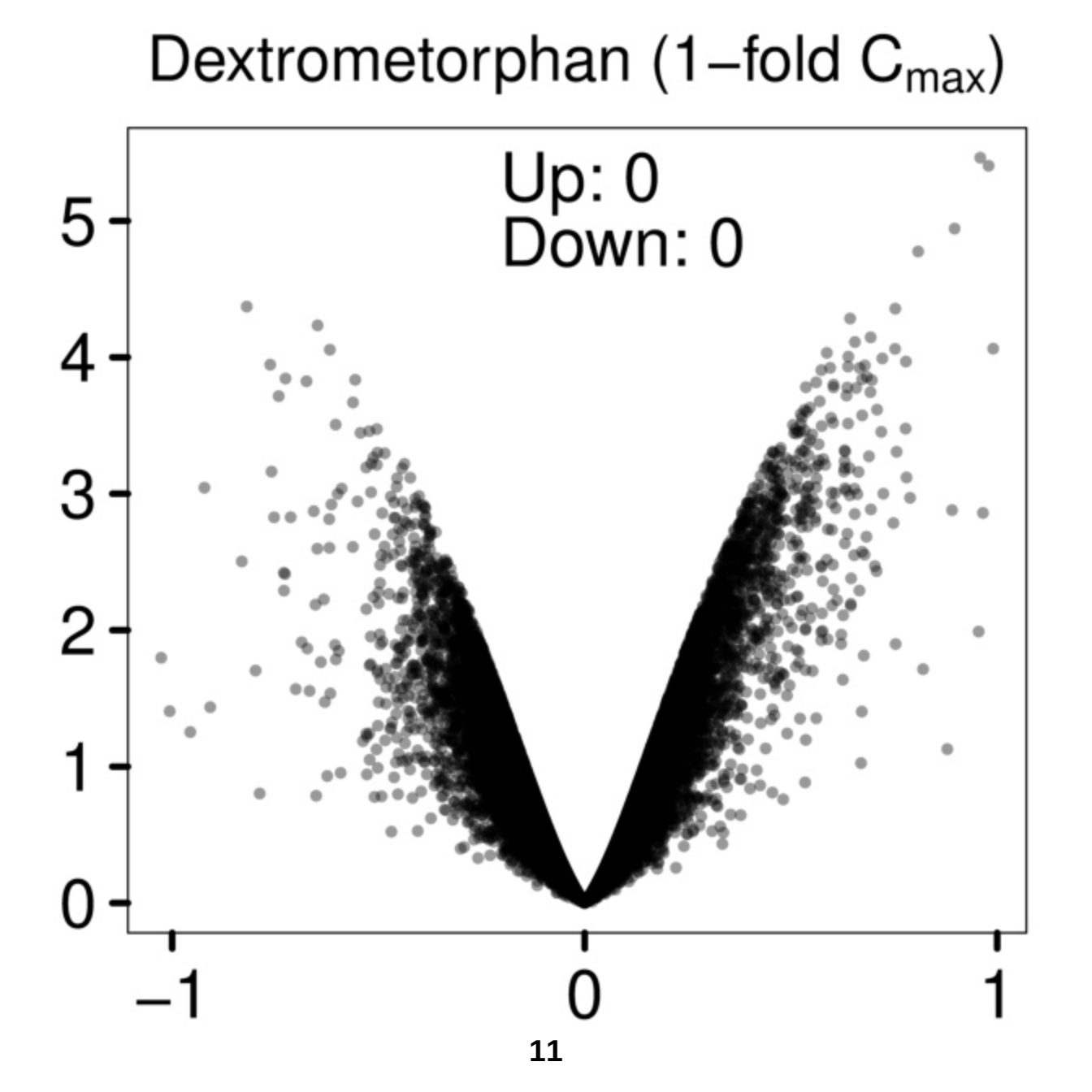
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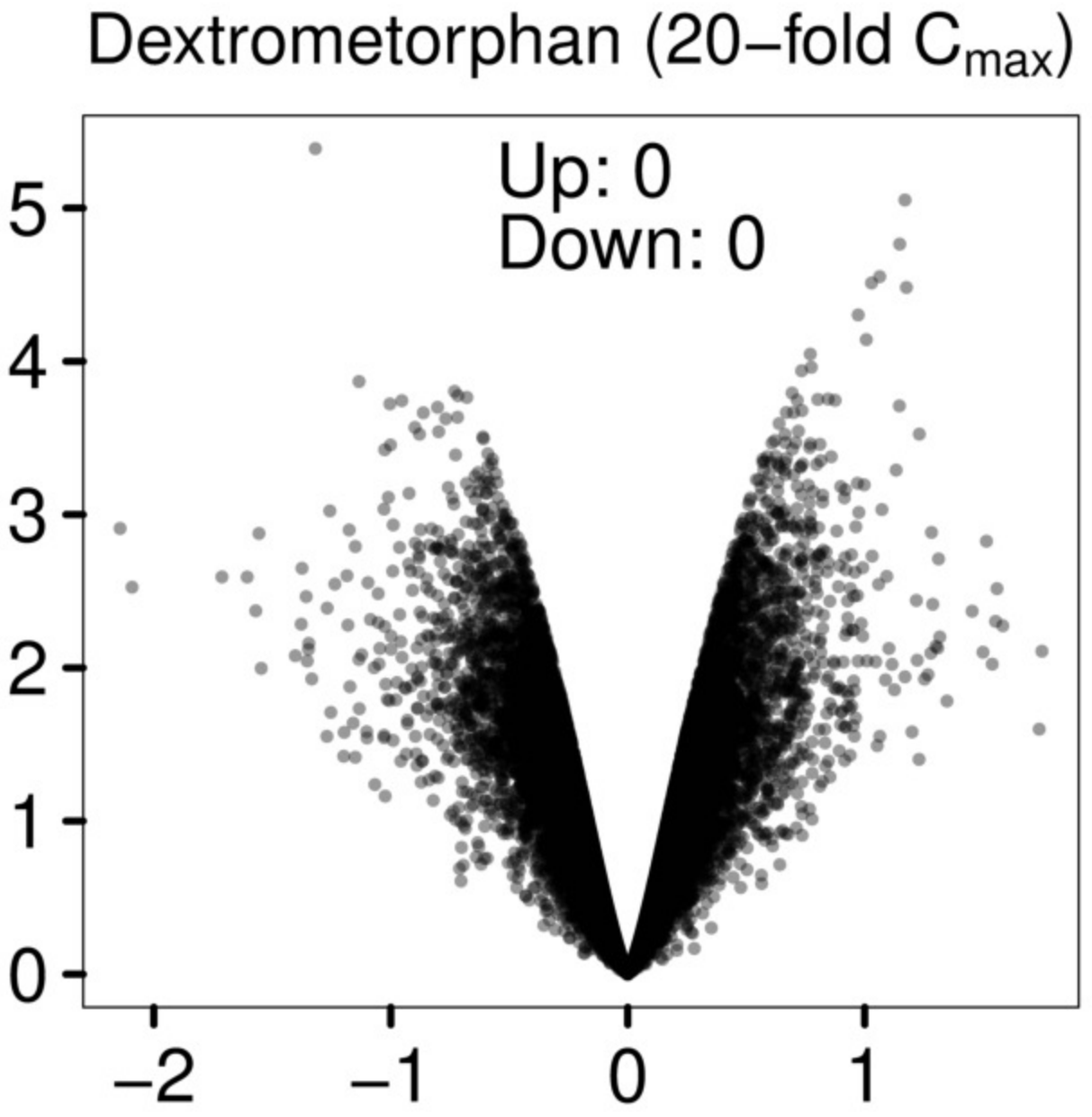
4
3
2
1
0
–1
0
1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Down: 0
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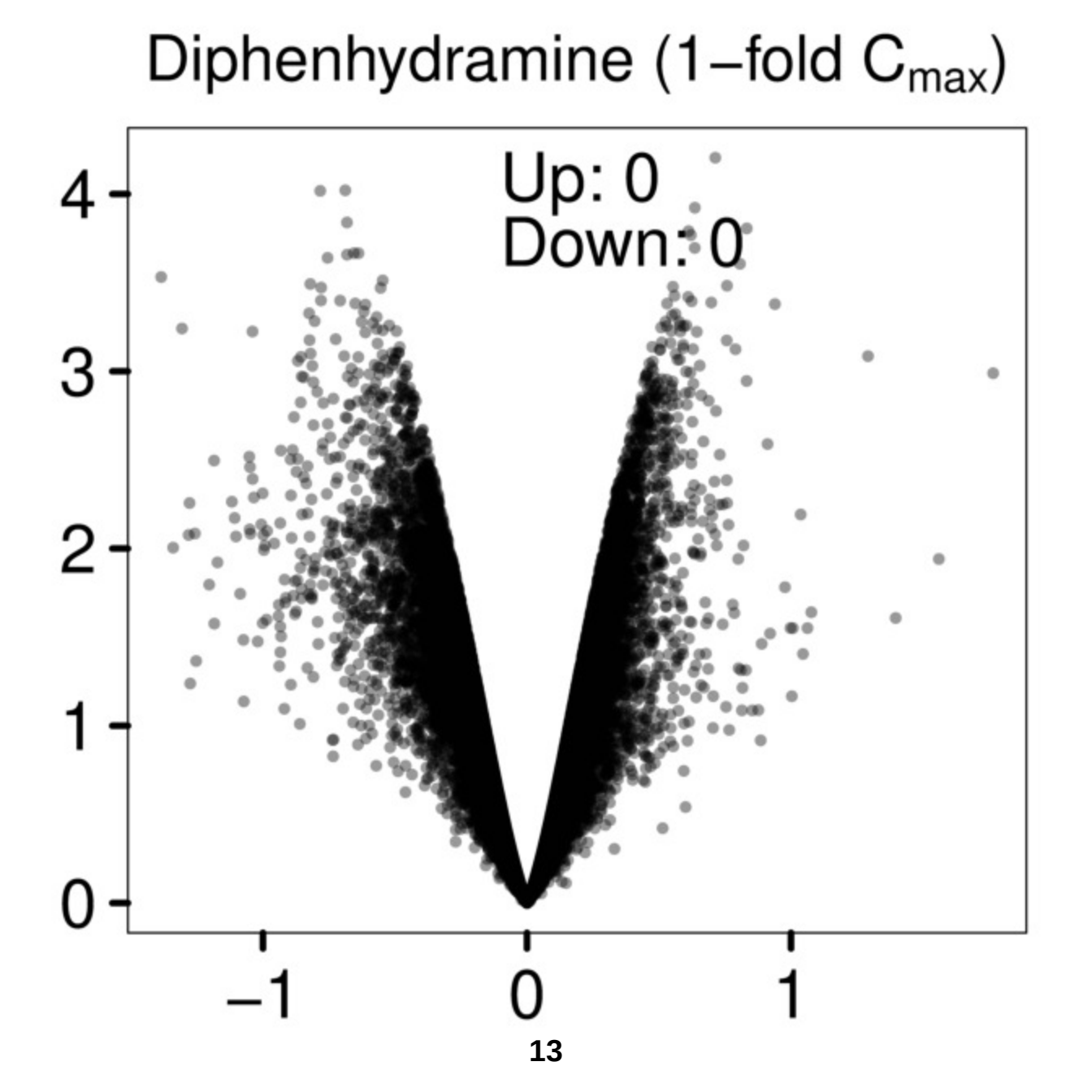
4
3
2
1
0
−2
−1
0
1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Down: 0
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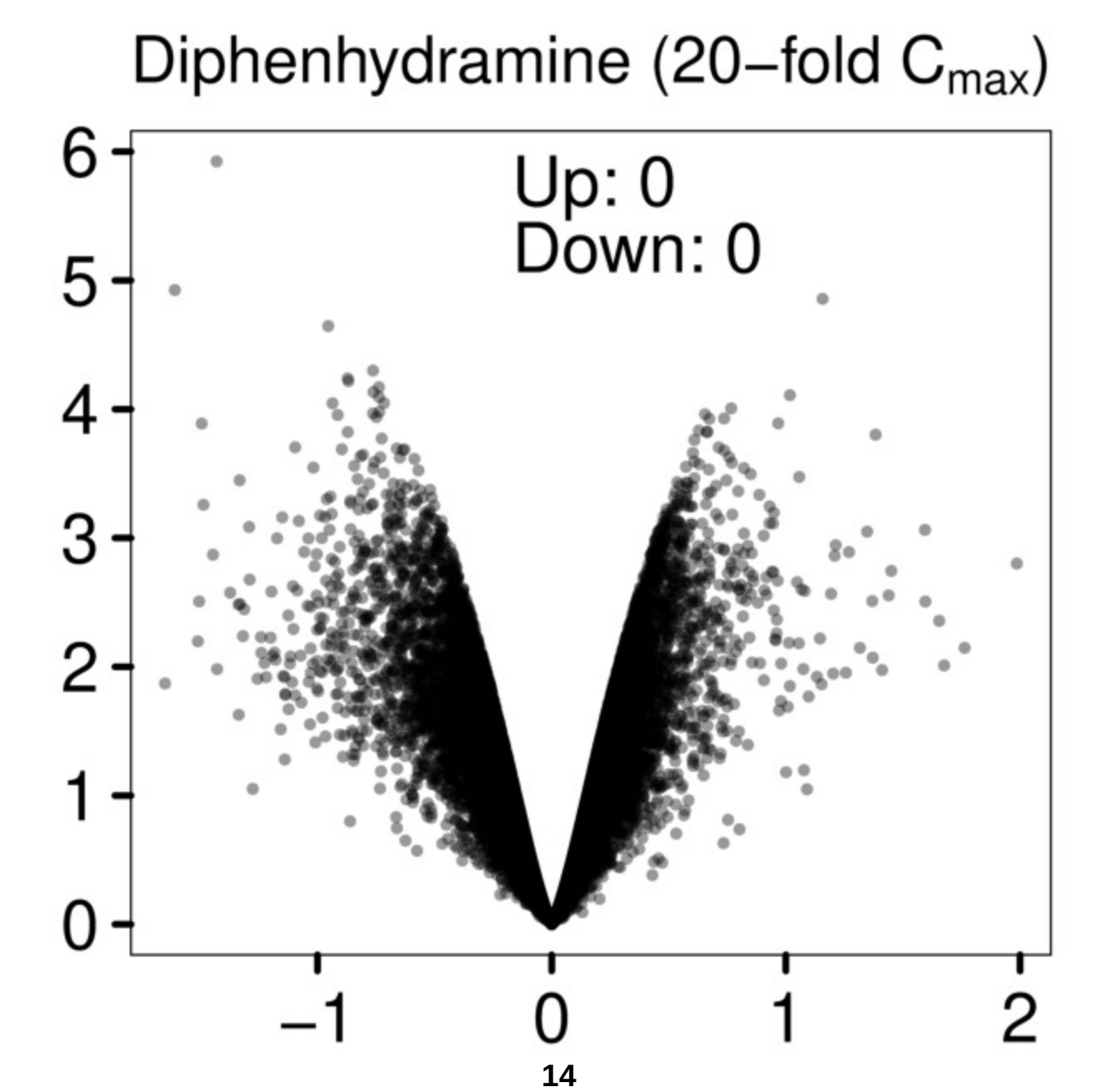
3
2
1
0
−1
0
1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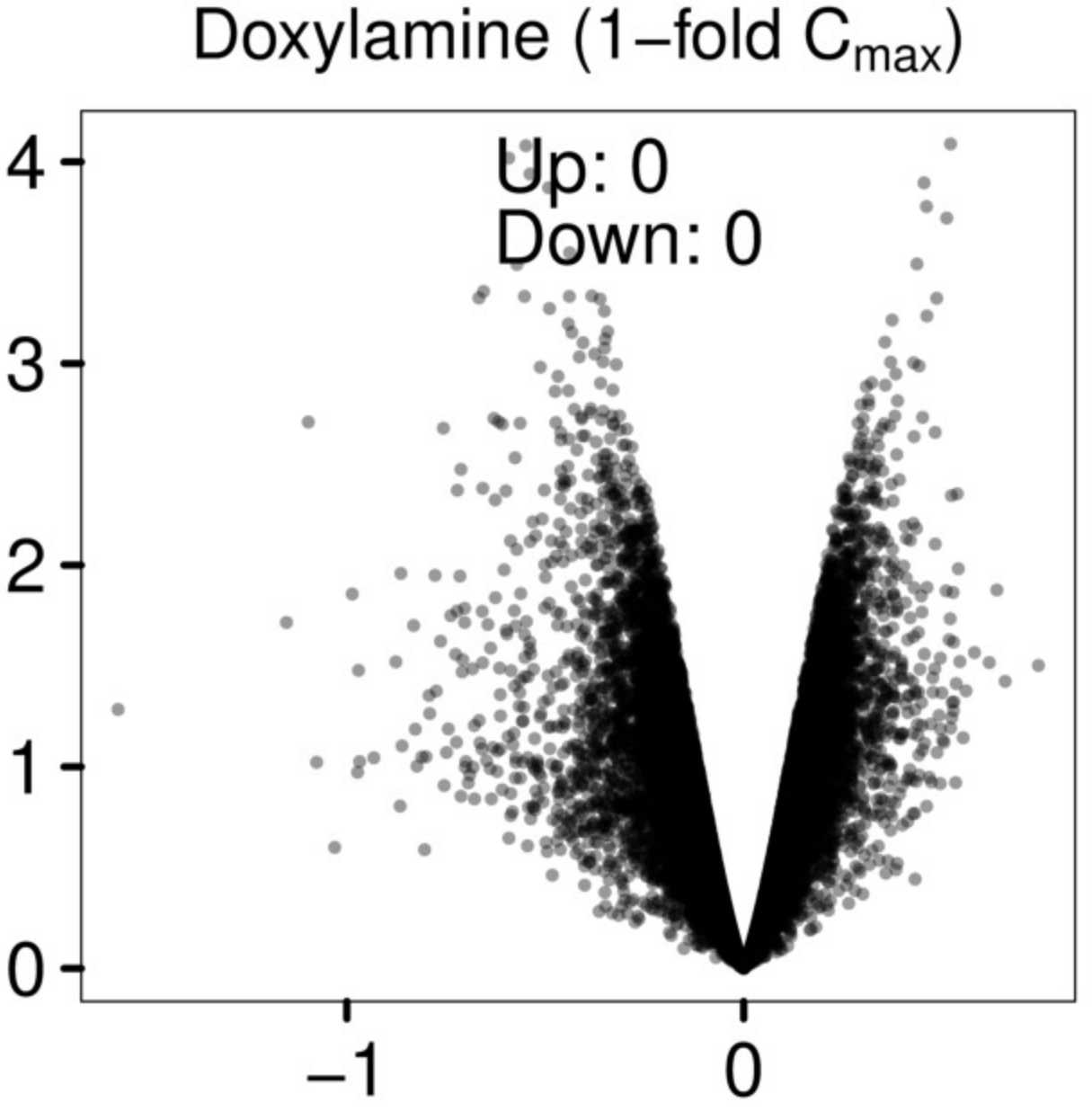
Down: 0
6
5
4
3
2
1
0
−1
0
1
2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2
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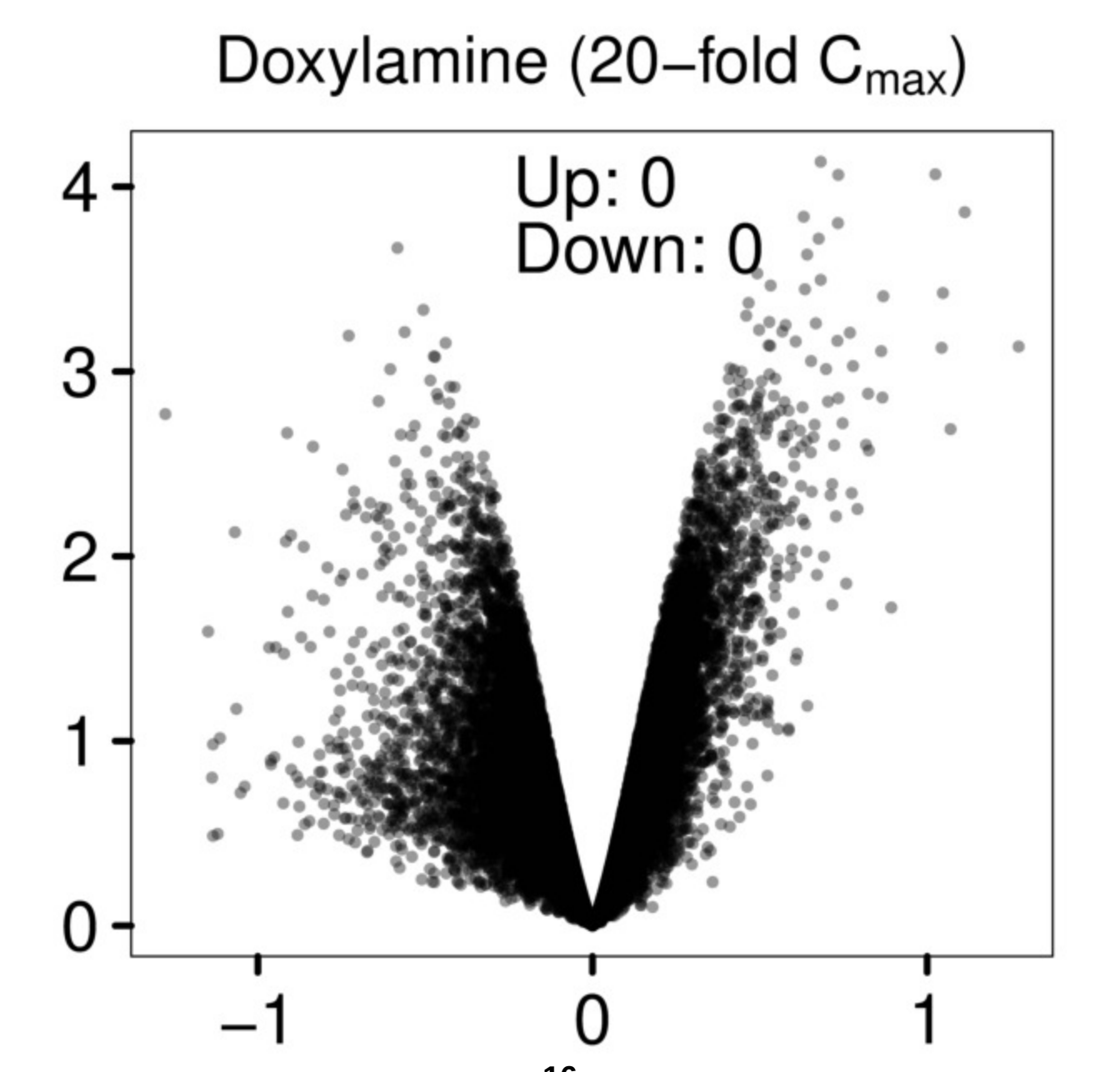
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2
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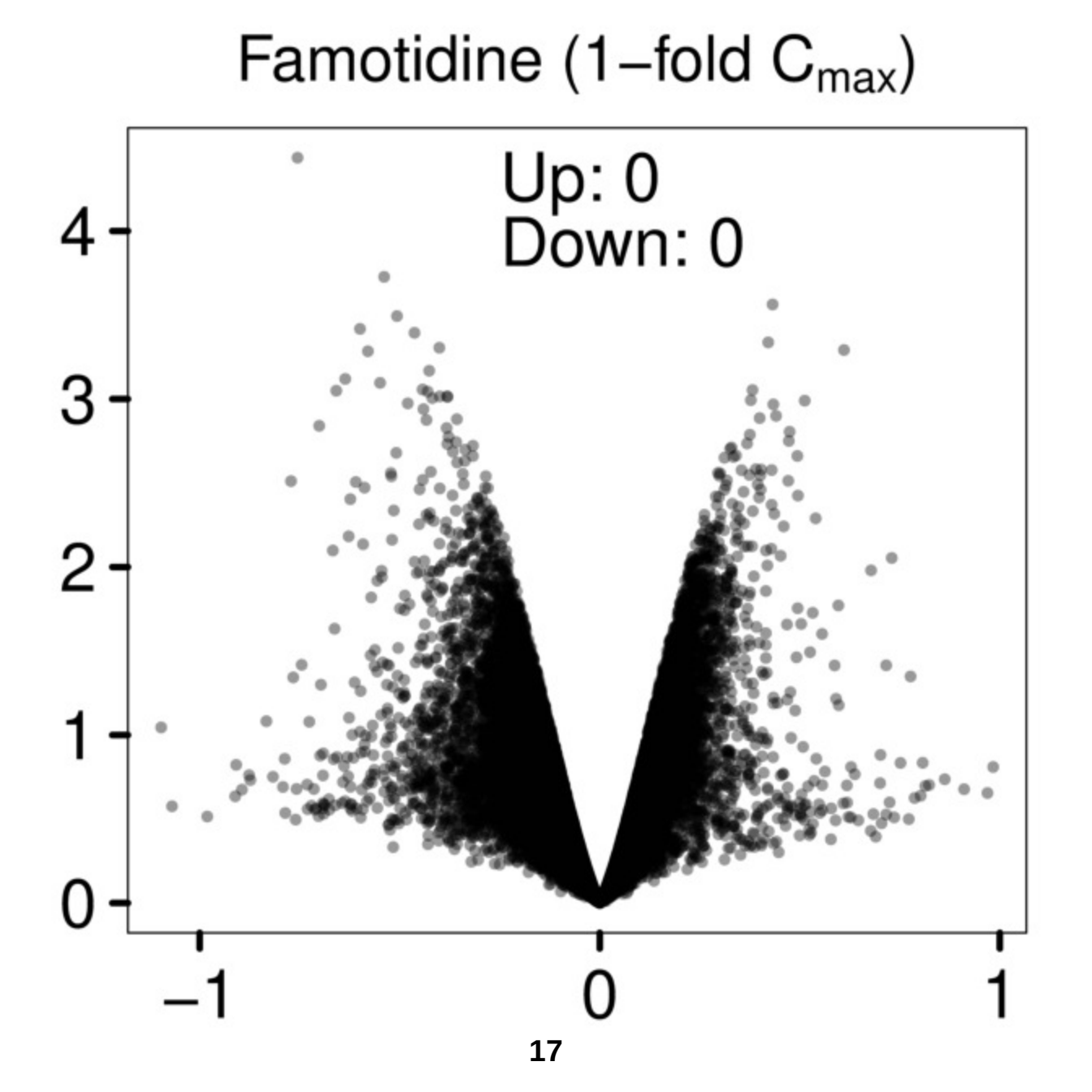
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0
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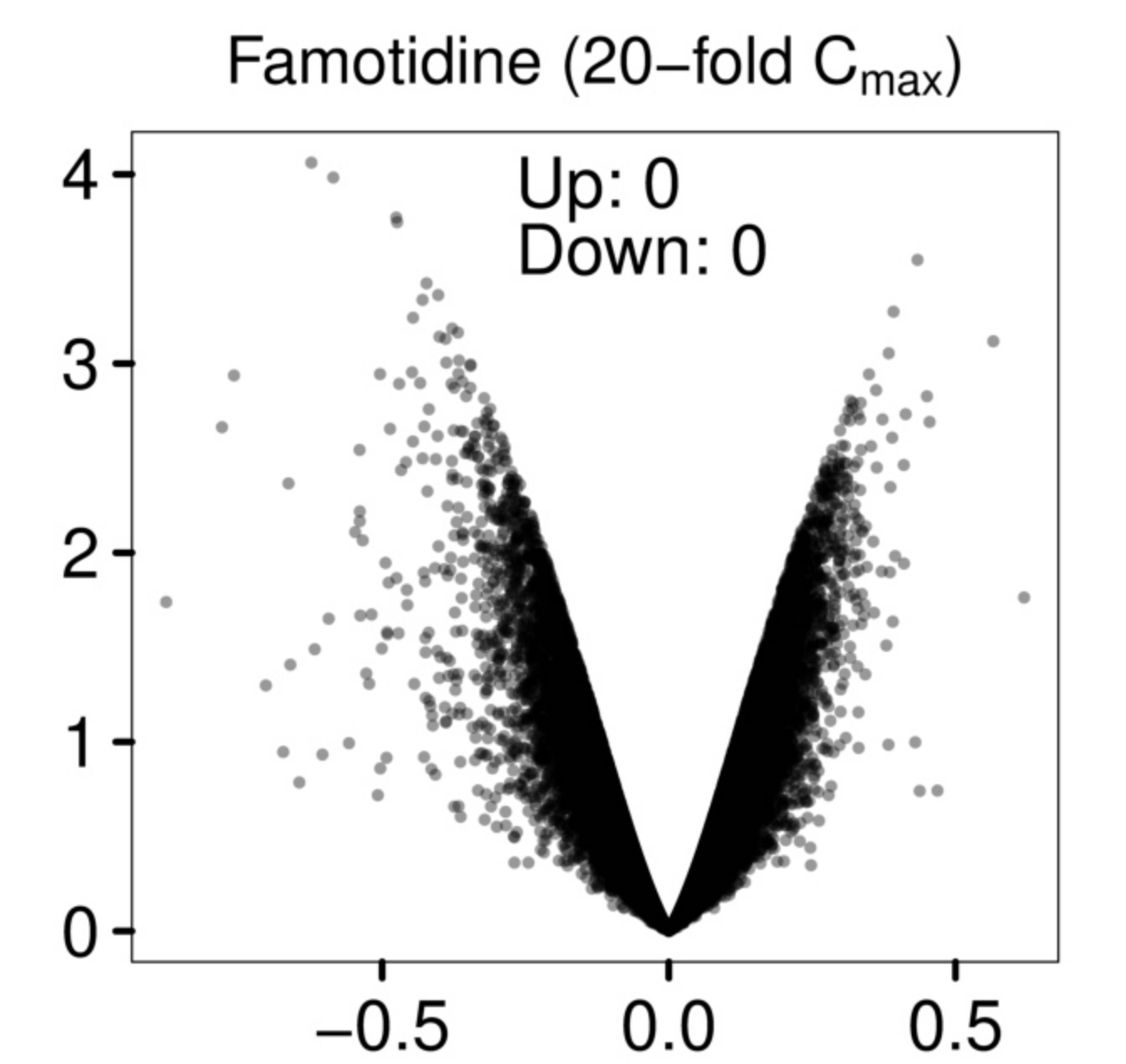
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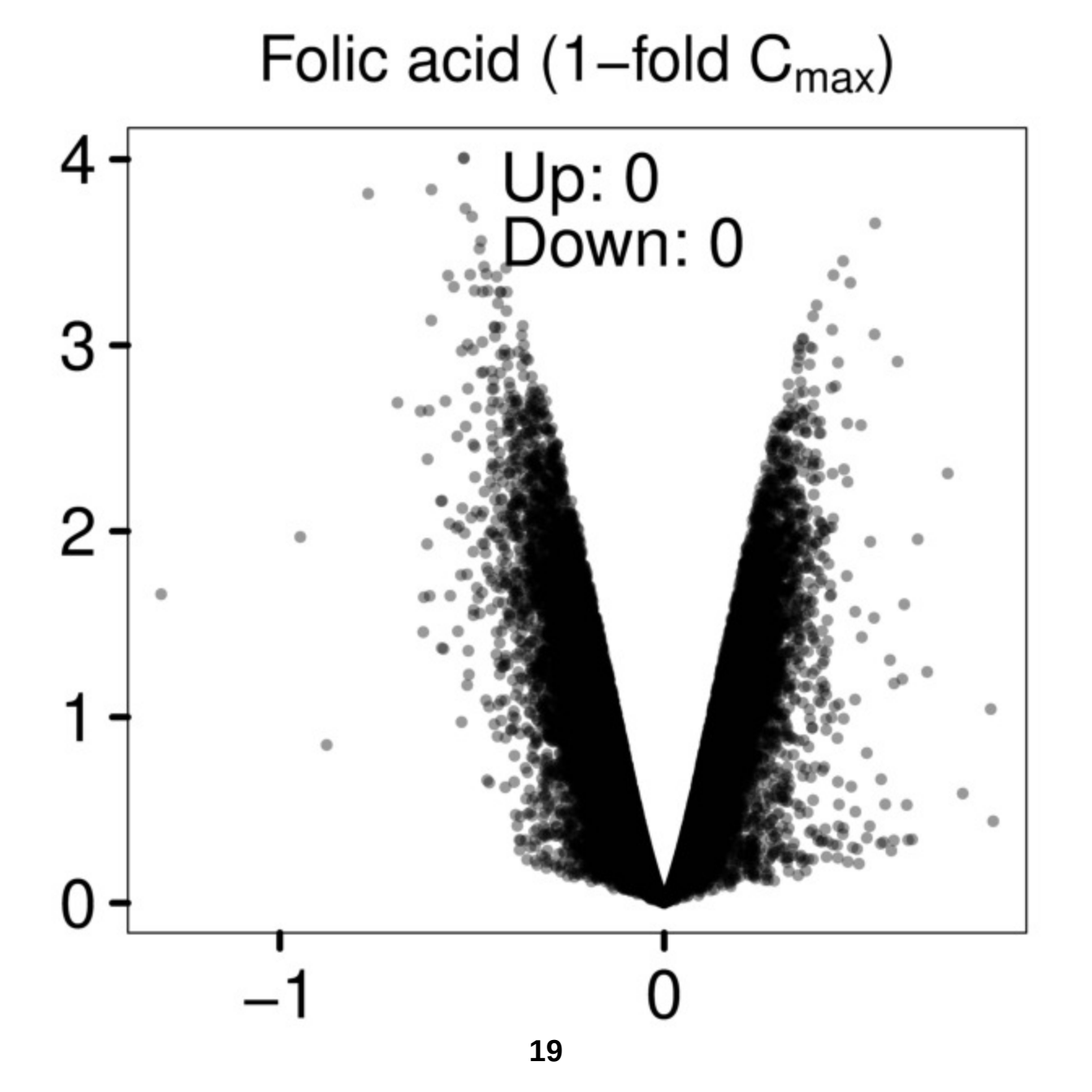
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Up: 0
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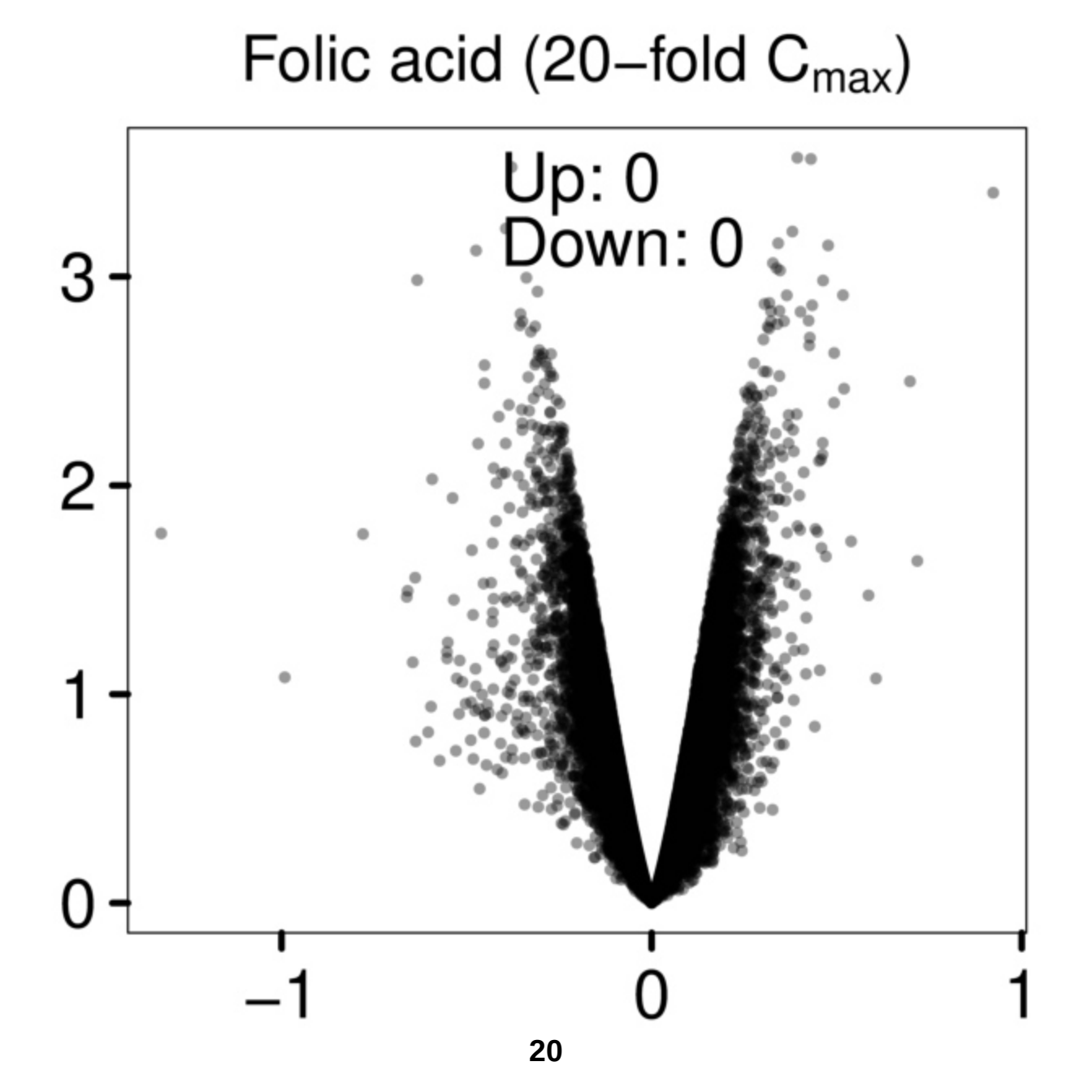
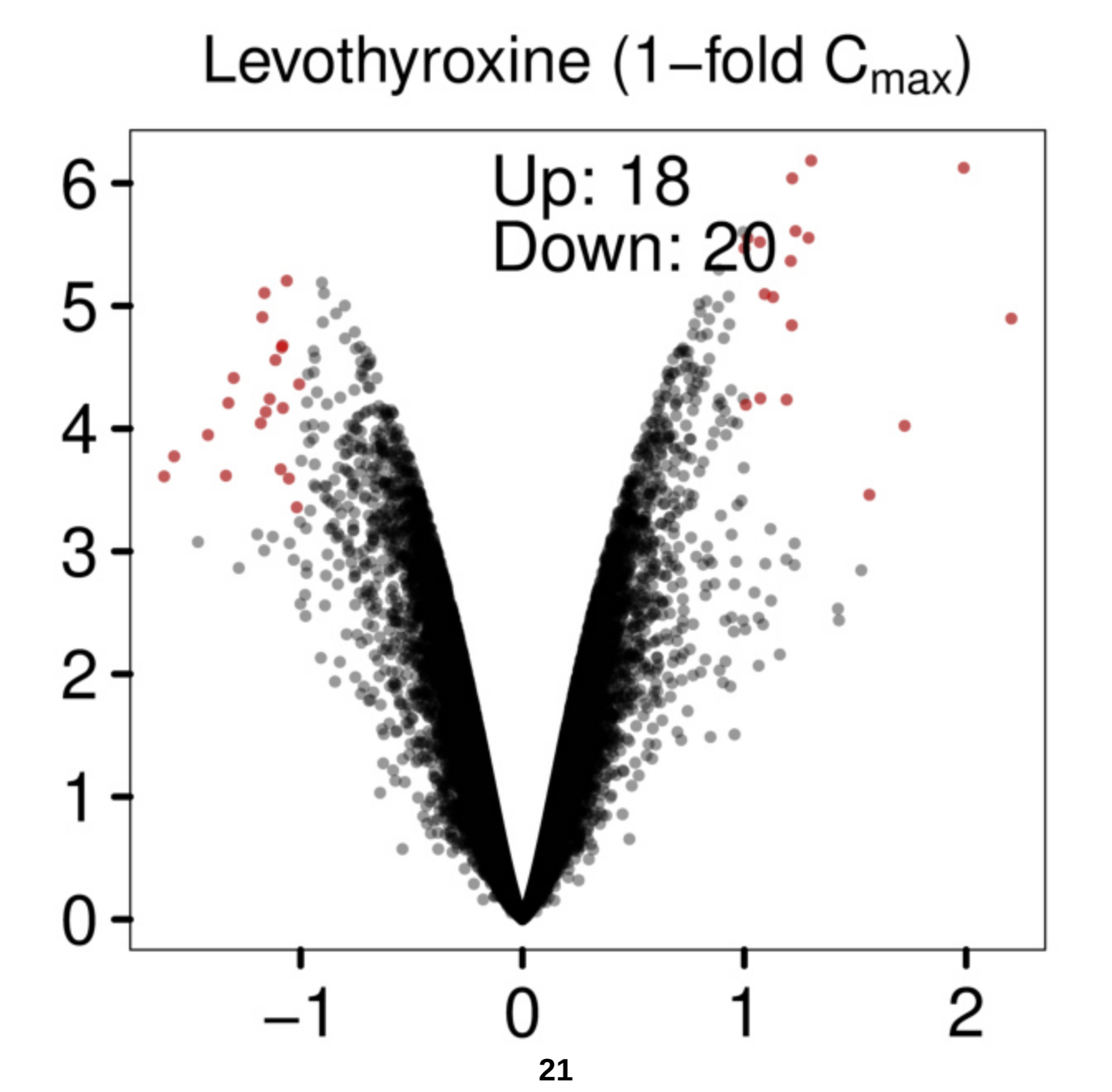
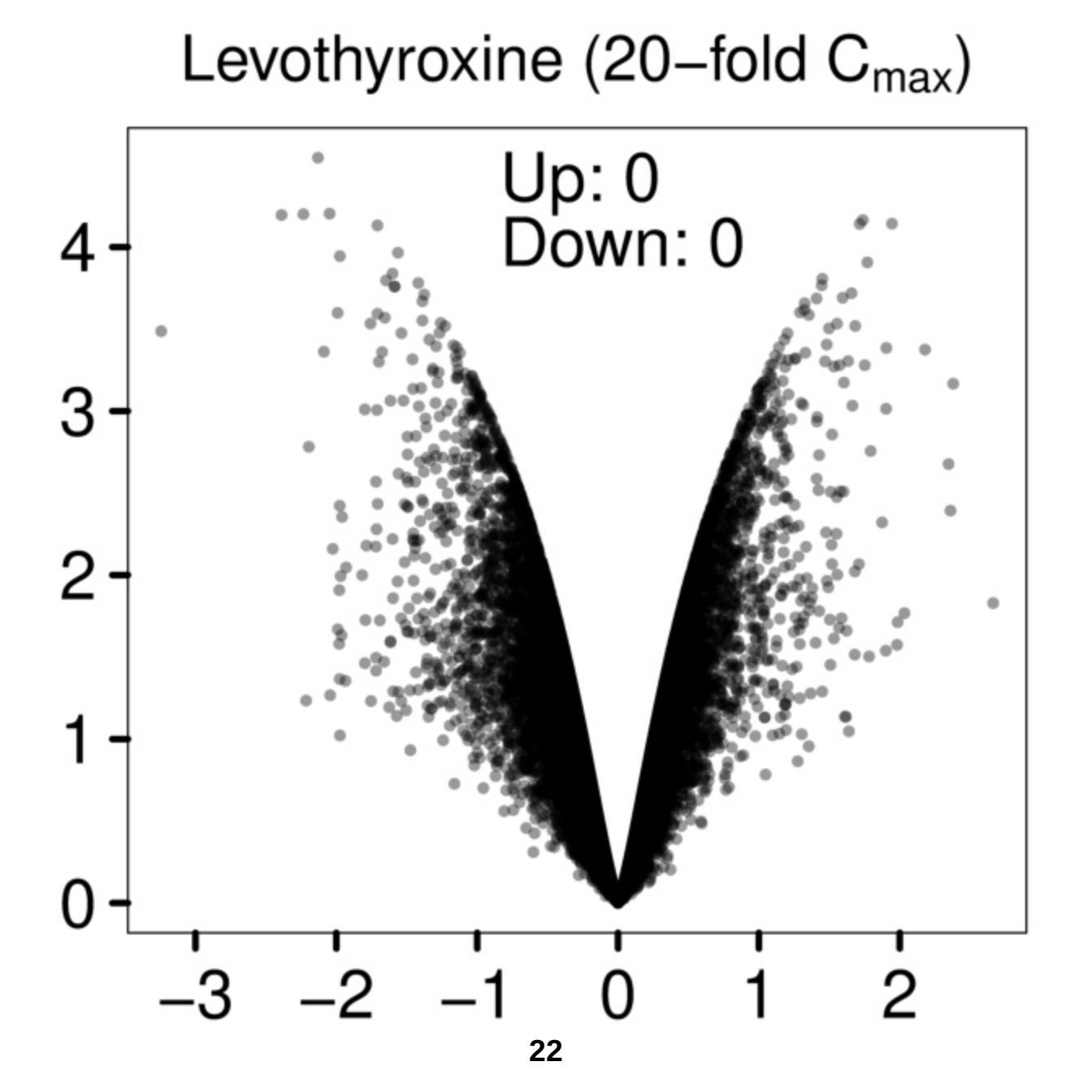
4
3
2
1
0
−1
0


Folic acid (20–fold C_{max})
Up: 0
Down: 0
3
2
1
0
−1
0
1


Levothyroxine (1–fold C_{max})
Up: 18
Down: 20
6
5
4
3
2
1
0
−1
0
1
2


Levothyroxine (20–fold C_{max})
Up: 0
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4
3
2
1
0
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1
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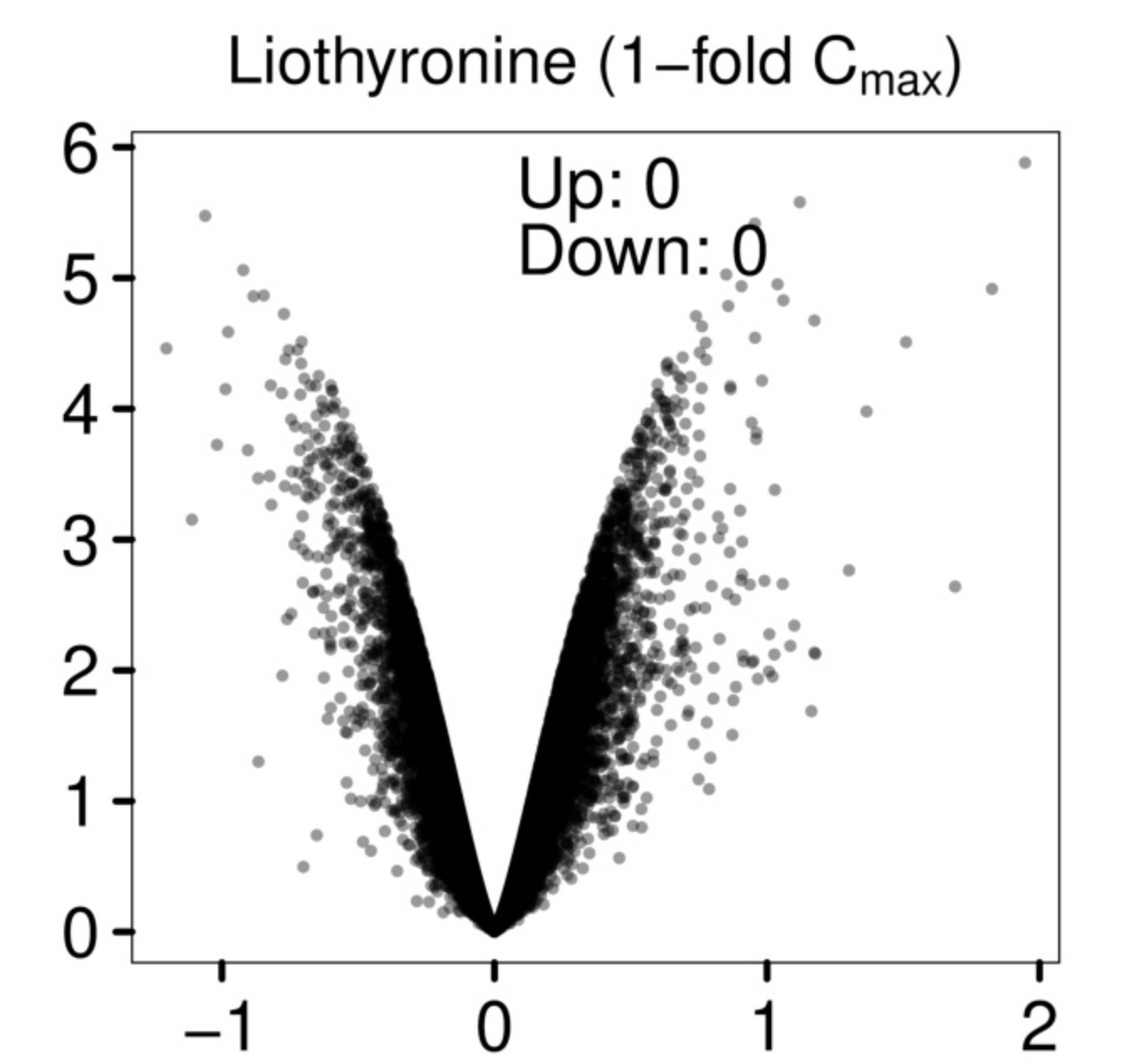
Liothyronine (1–fold C_{max})
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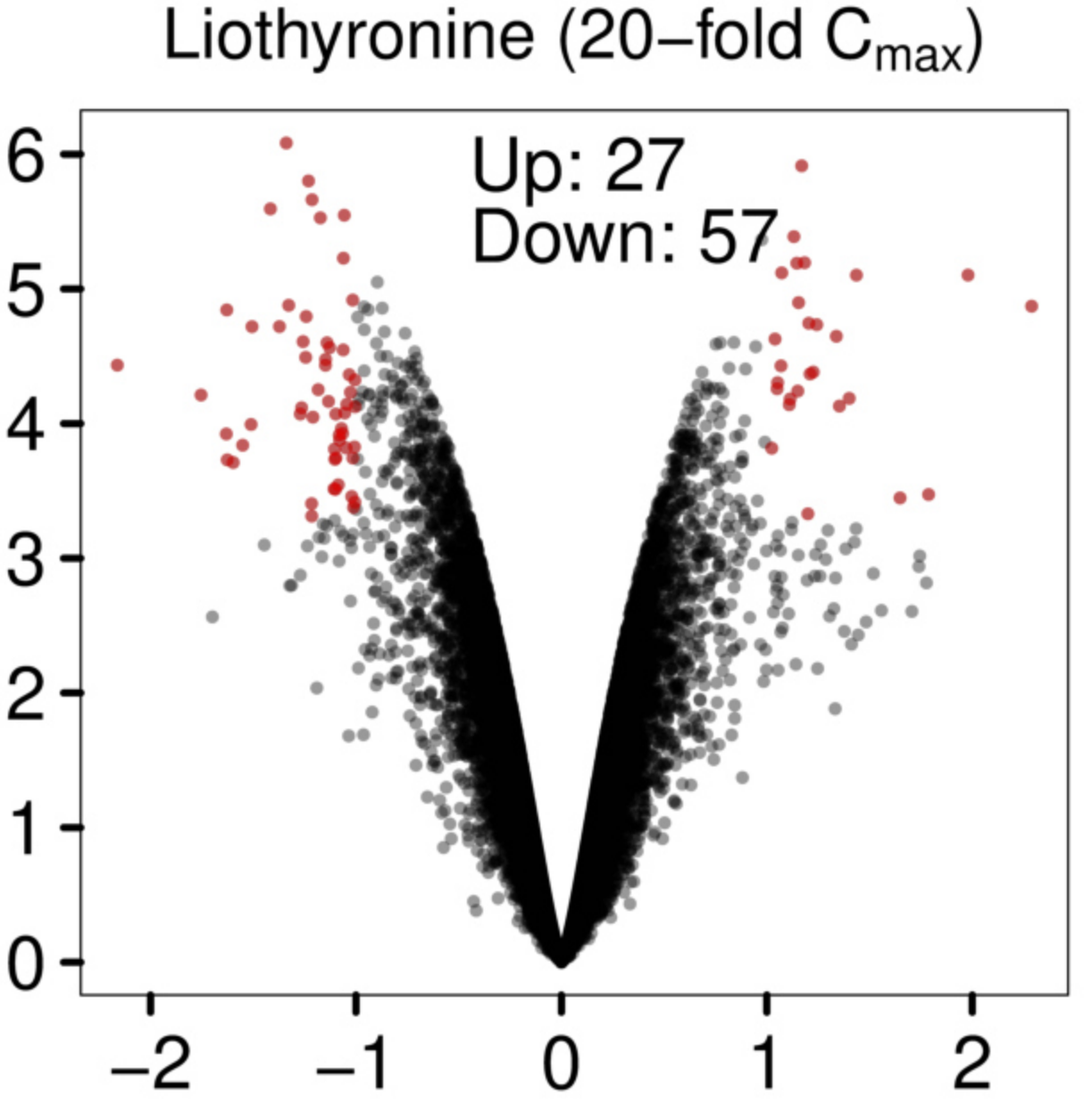
Down: 0
6
5
4
3
2
1
0
−1
0
1
2


Liothyronine (20–fold C_{max})
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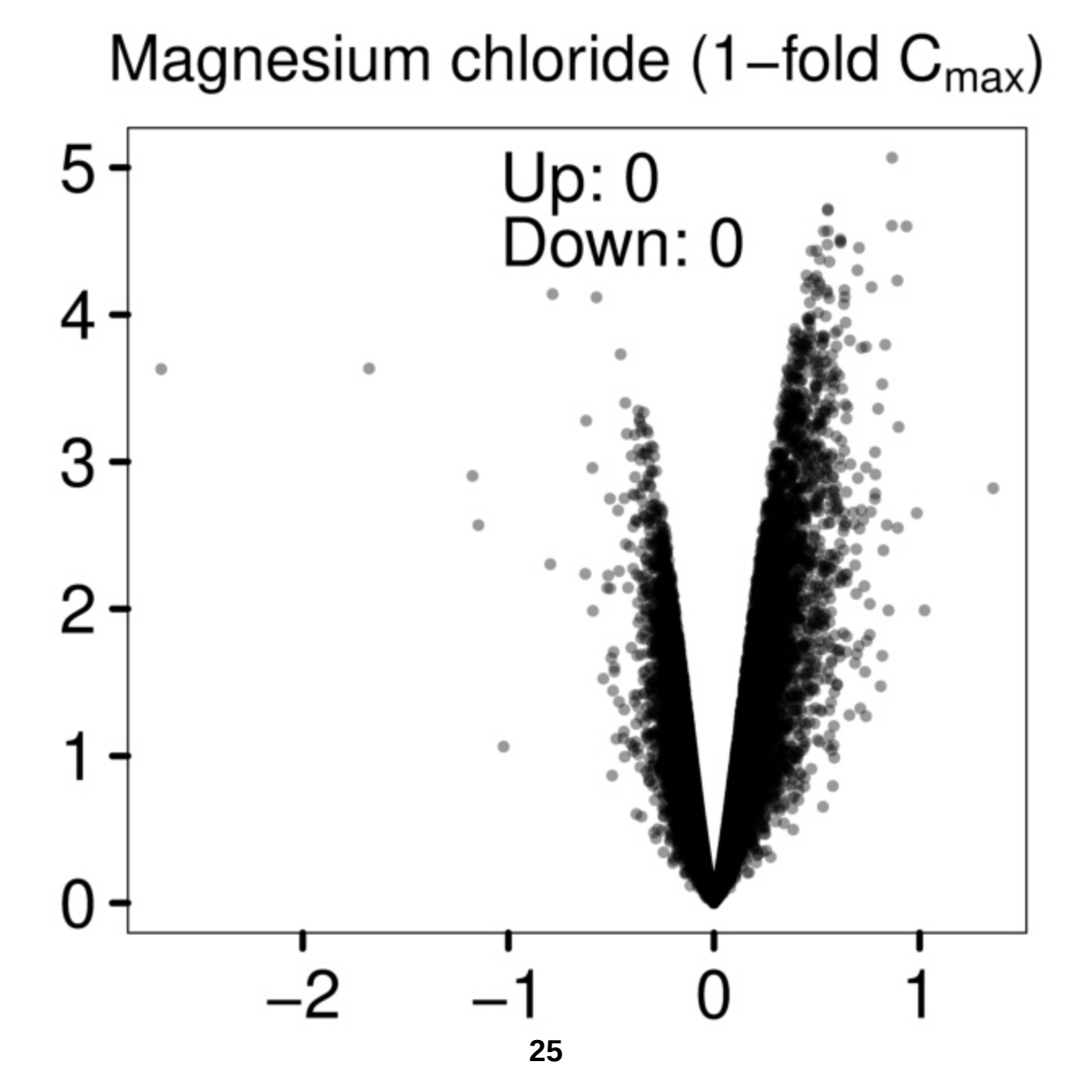
Down: 57
6
5
4
3
2
1
0
−2
−1
0
1
2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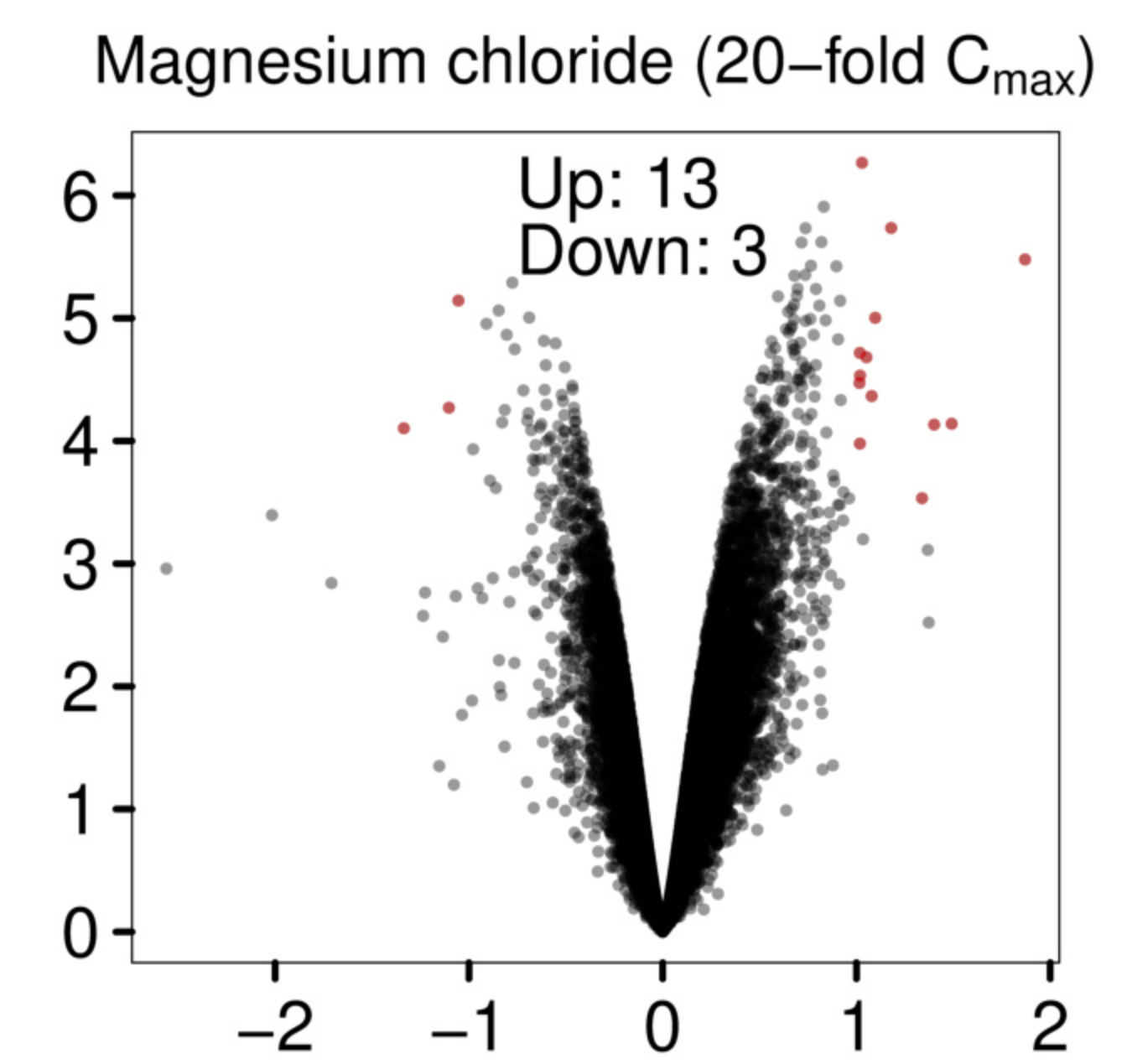
Down: 0
5
4
3
2
1
0
–2
–1
0
1


Magnesium chloride (20–fold C_{max})
Up: 13
Down: 3
6
5
4
3
2
1
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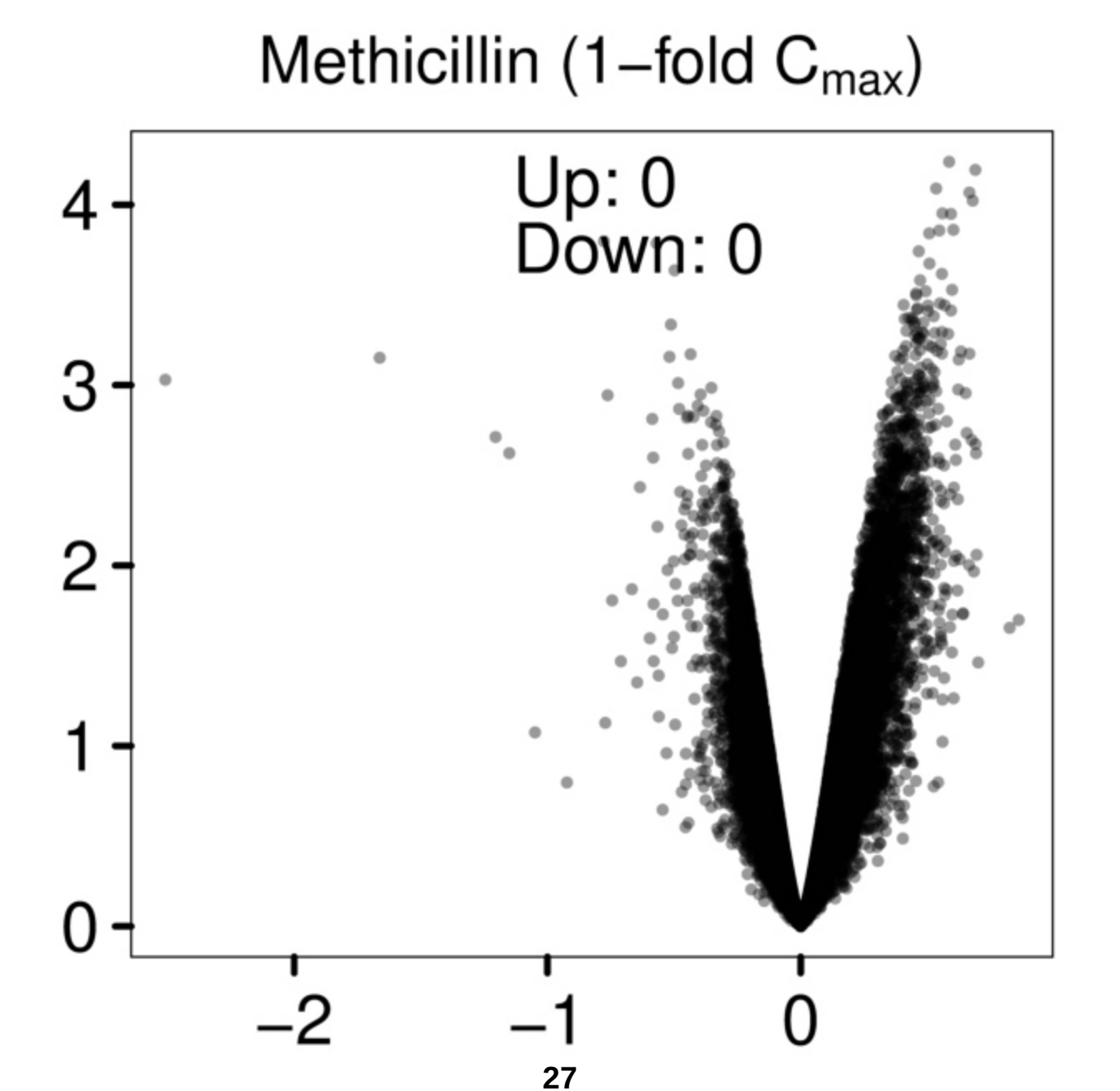
−2
−1
0
1
2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–2
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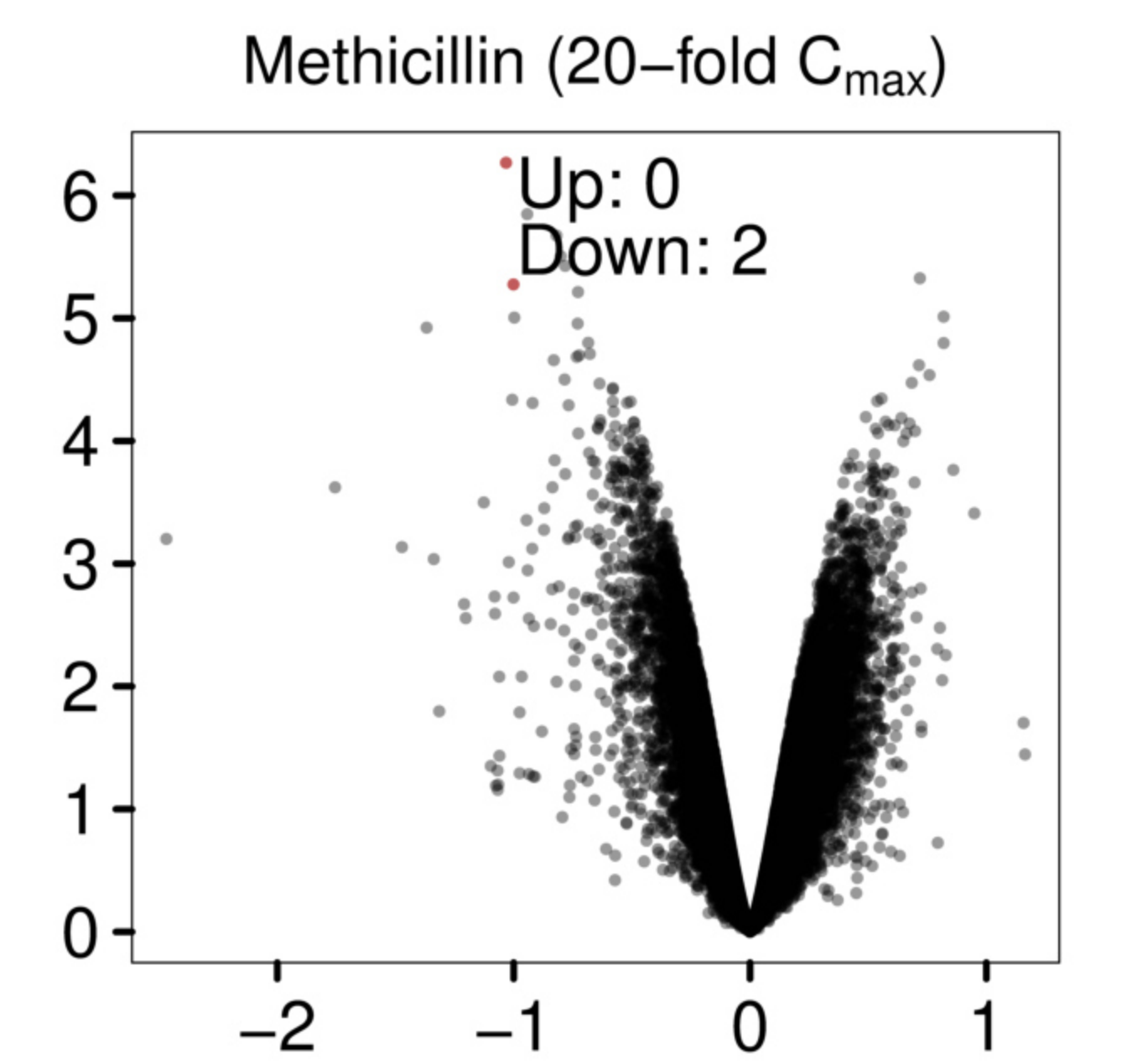
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0
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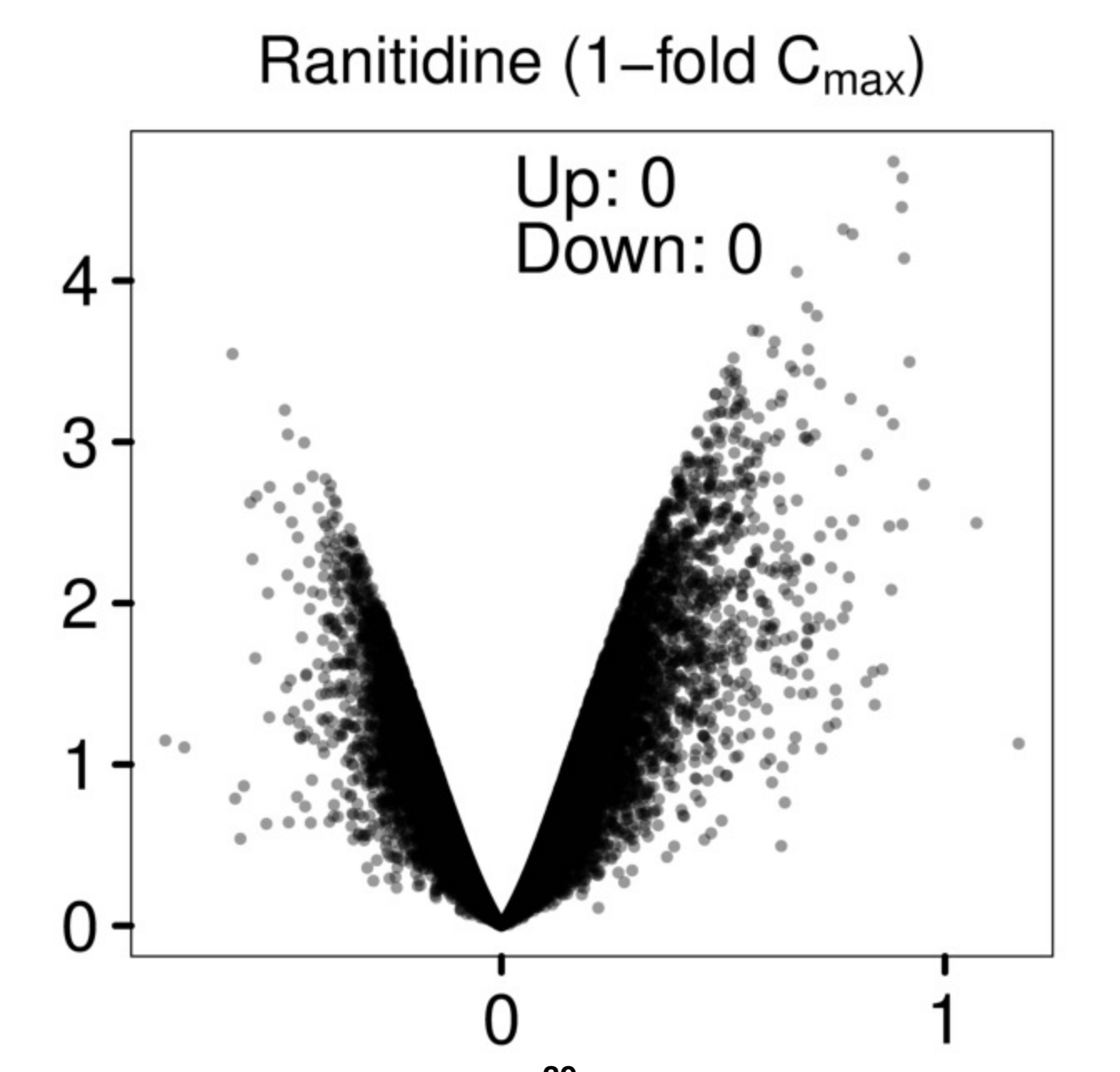
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2
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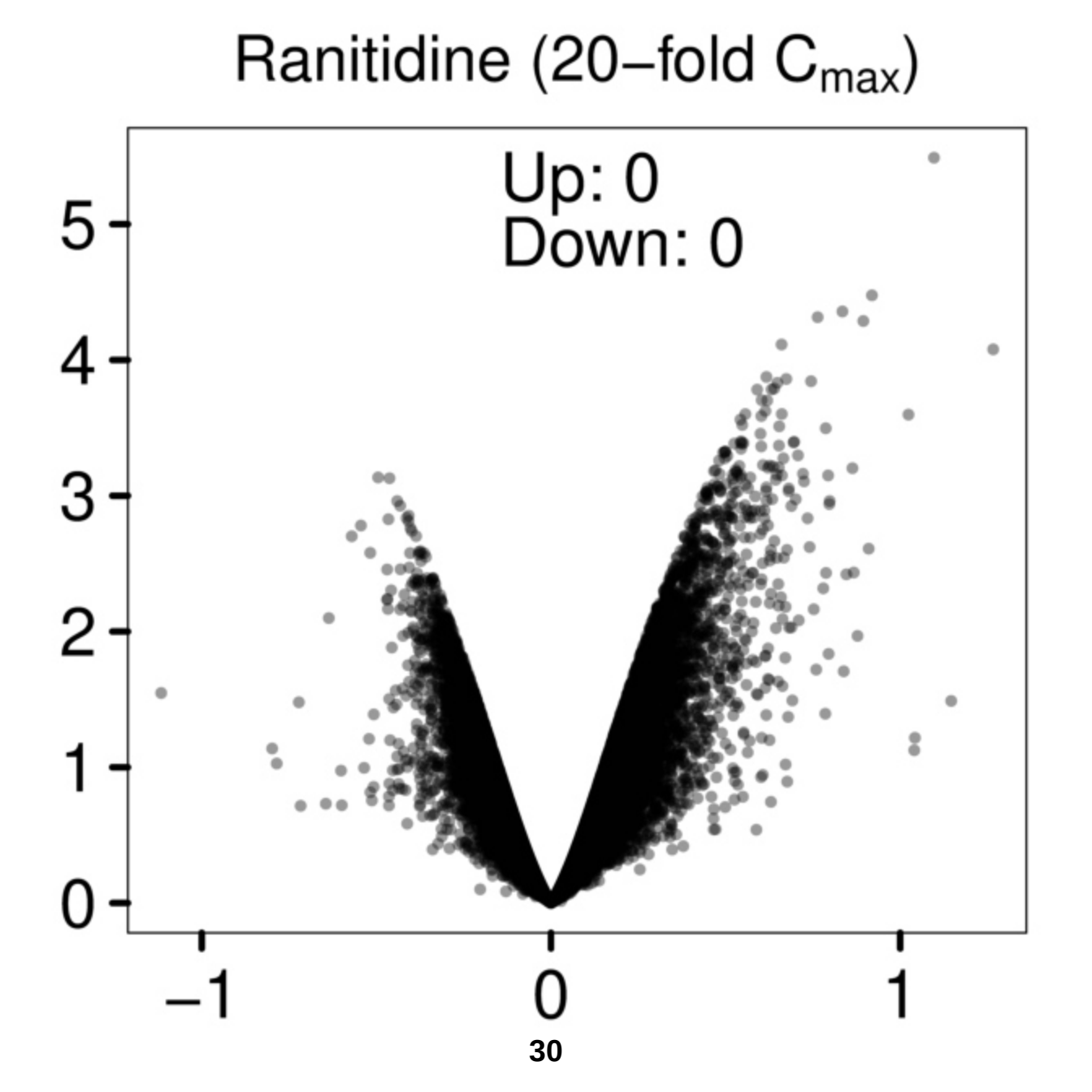
0
0
1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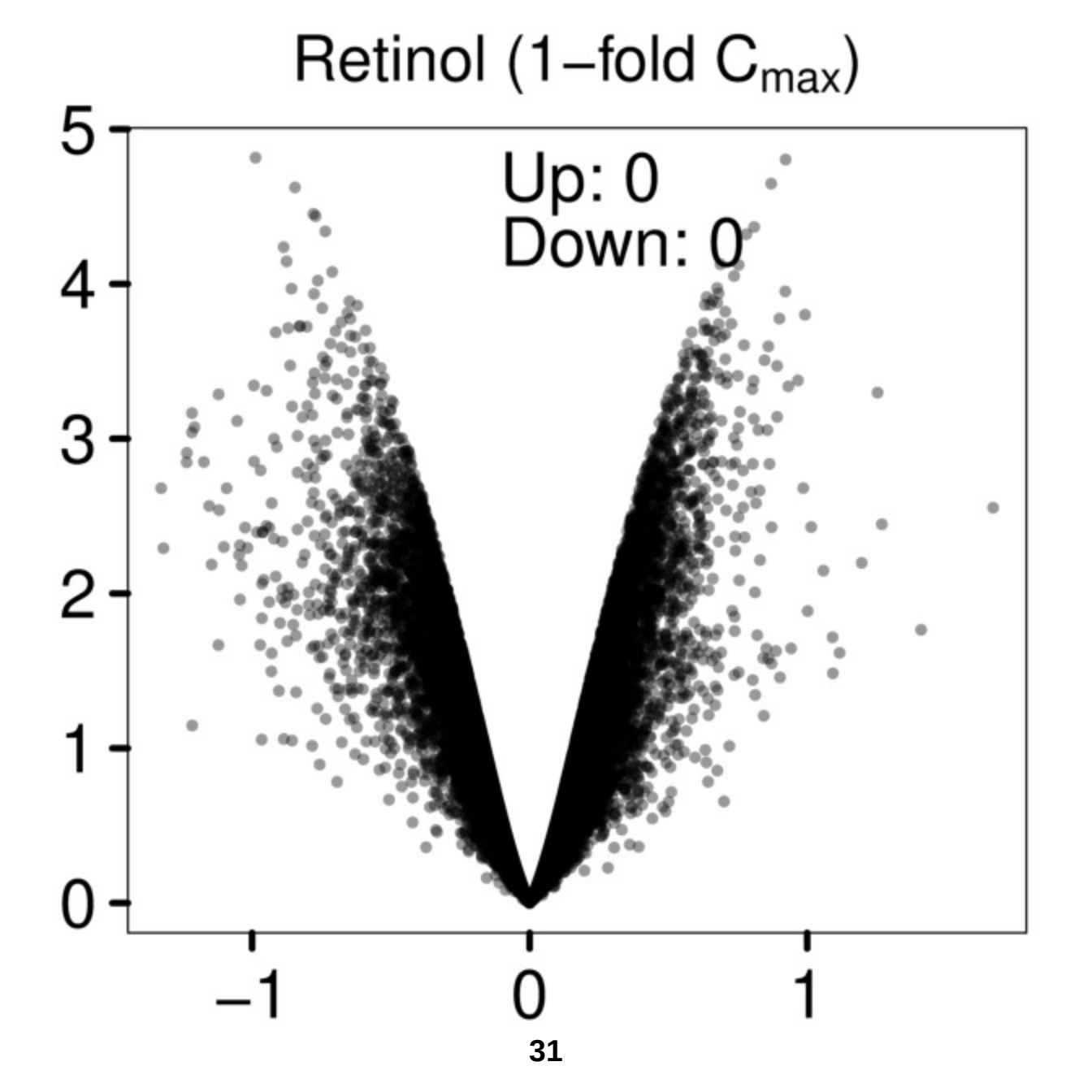
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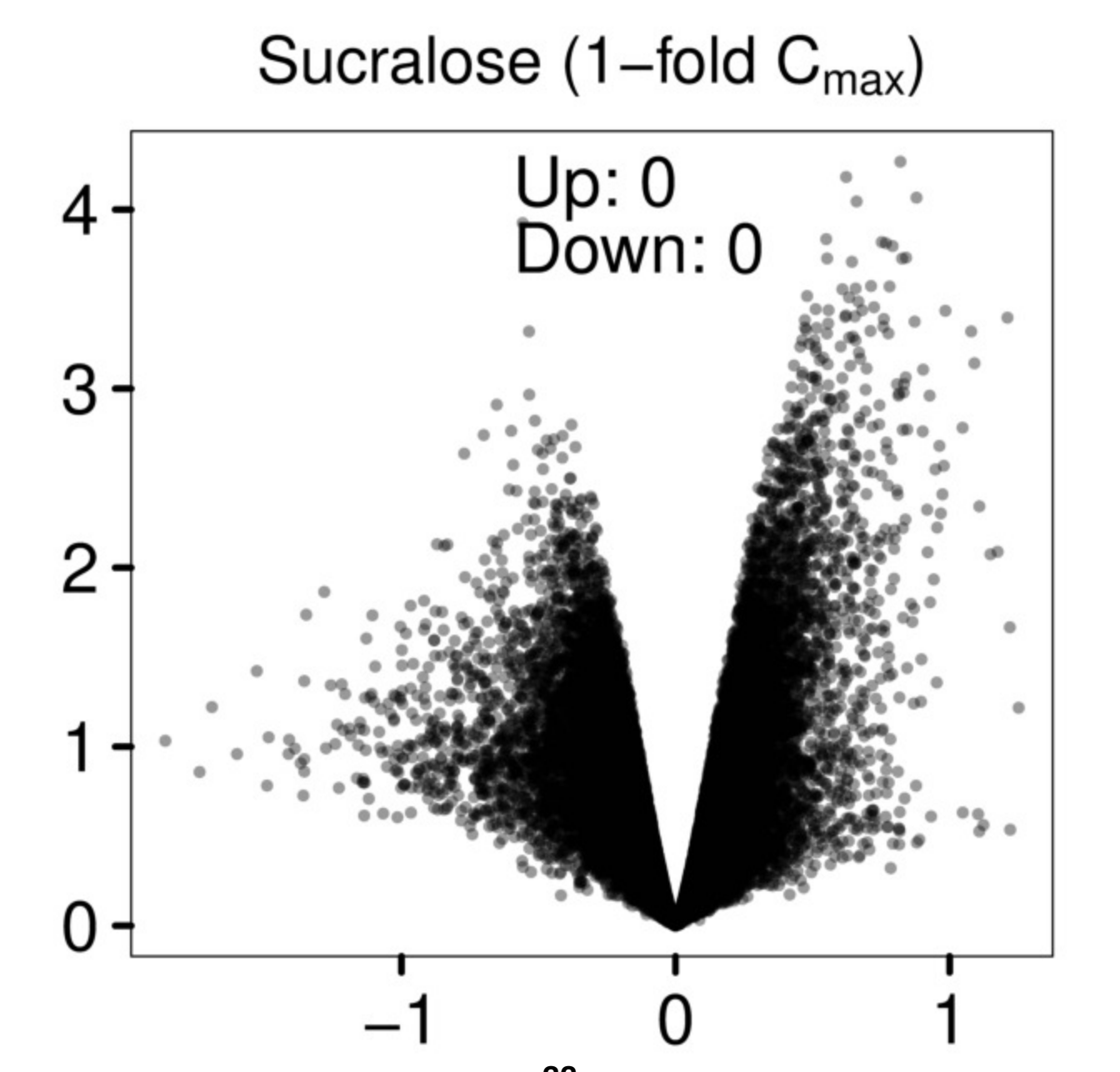
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2
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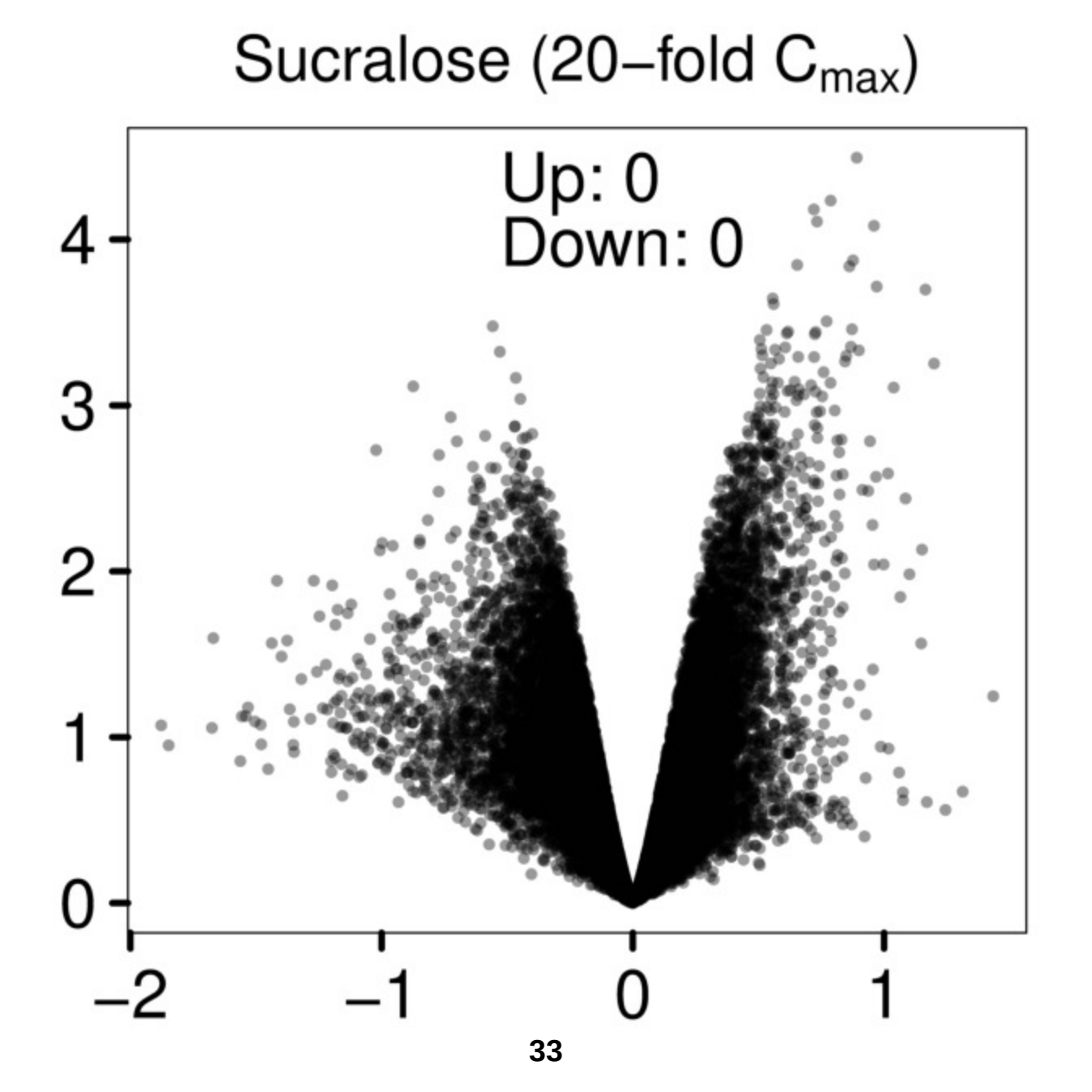
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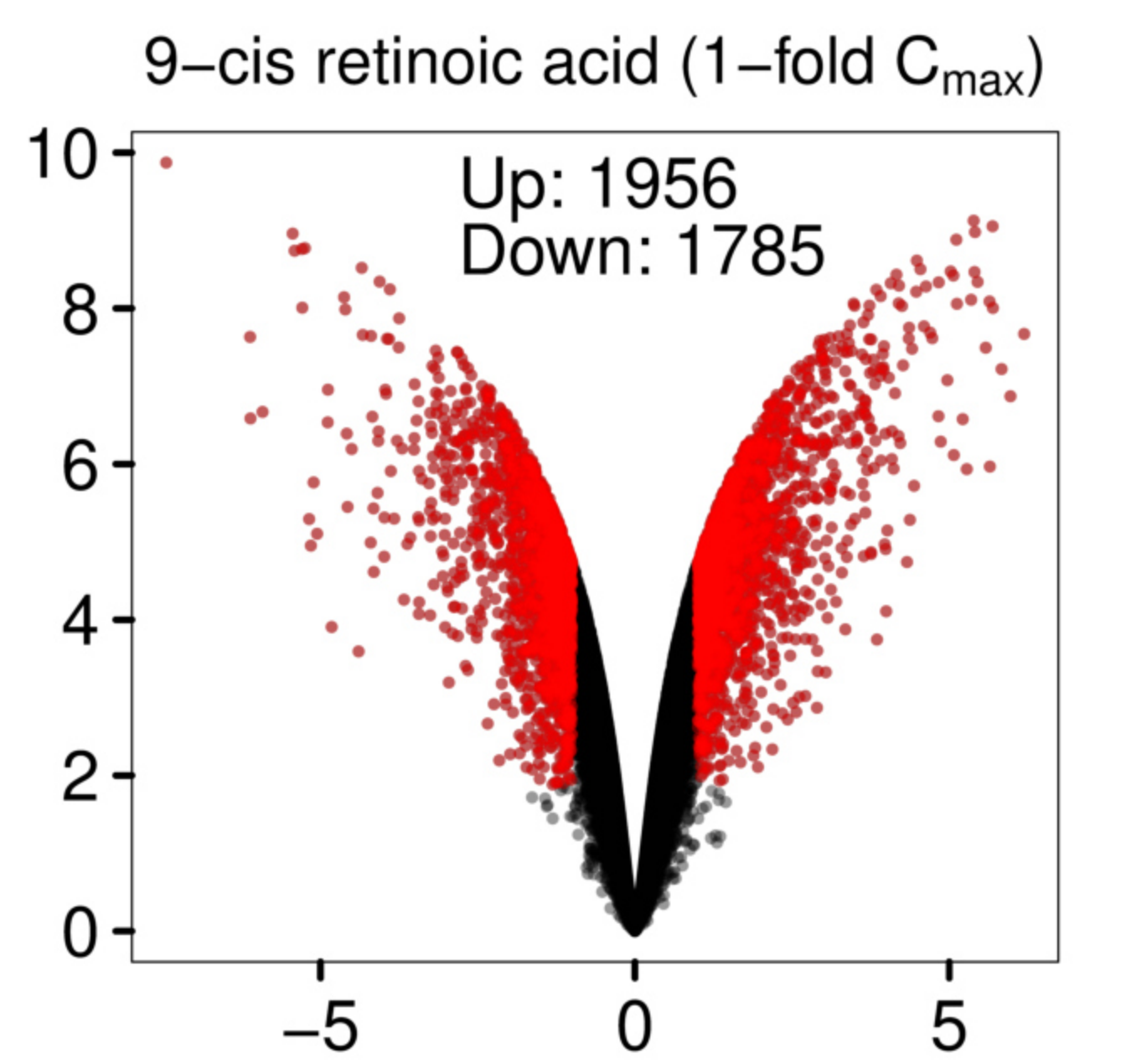
Down: 0
4
3
2
1
0
−2
−1
0
1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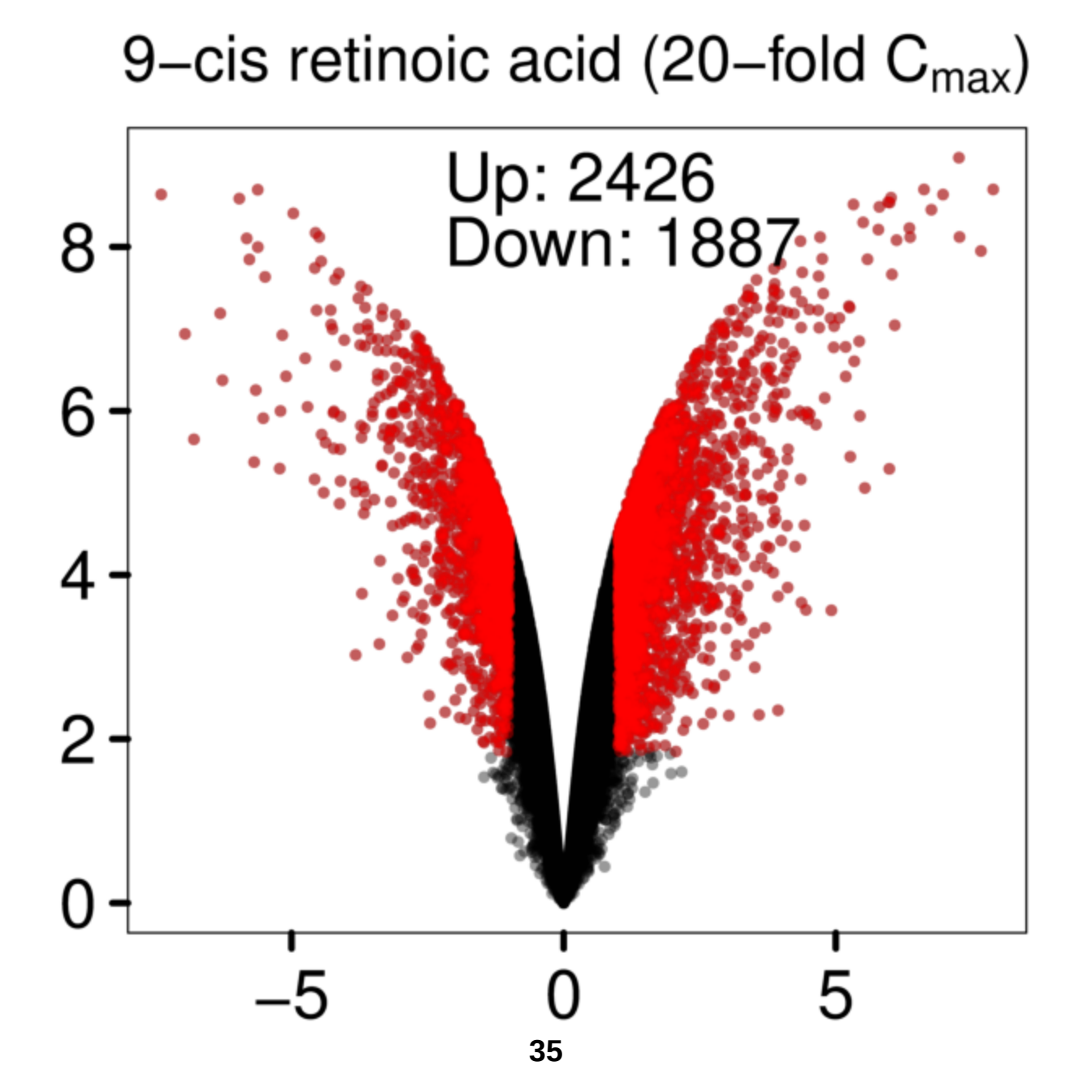
Up: 1956
Down: 1785
10
8
6
4
2
0
–5
0
5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Down: 1887
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6
4
2
0
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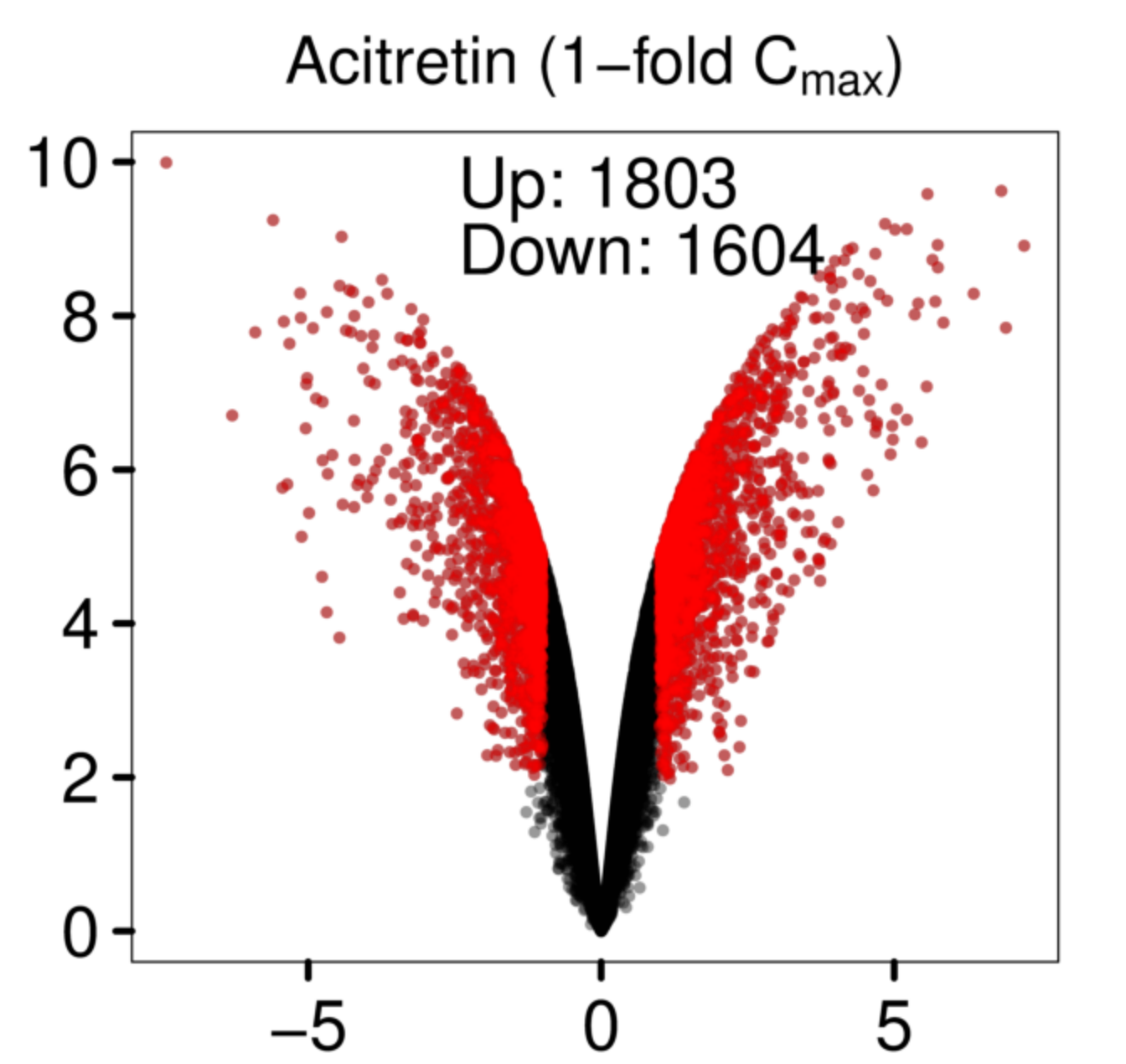
0
5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10
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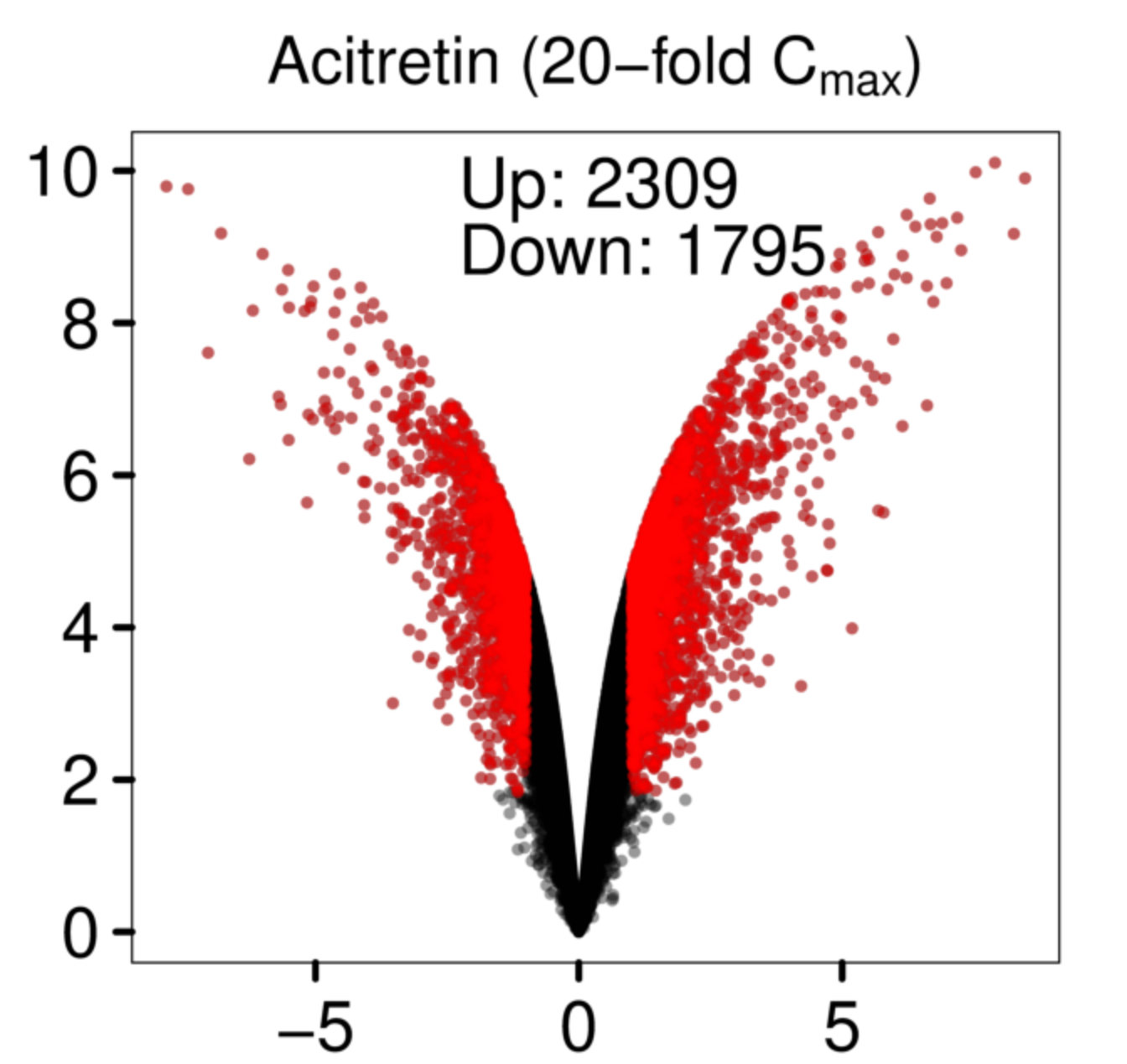
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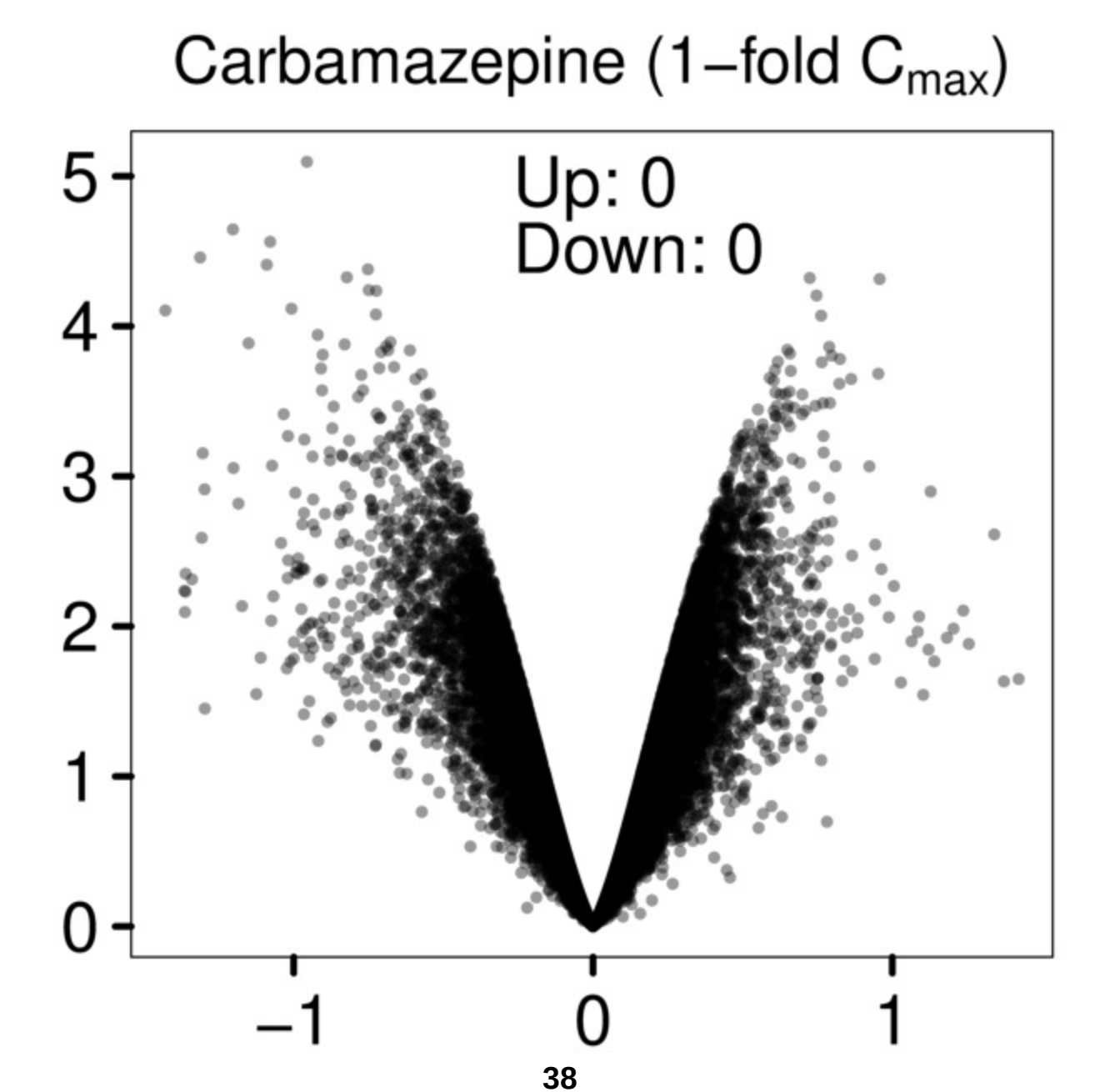
8
6
4
2
0
−5
0
5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Down: 0
5
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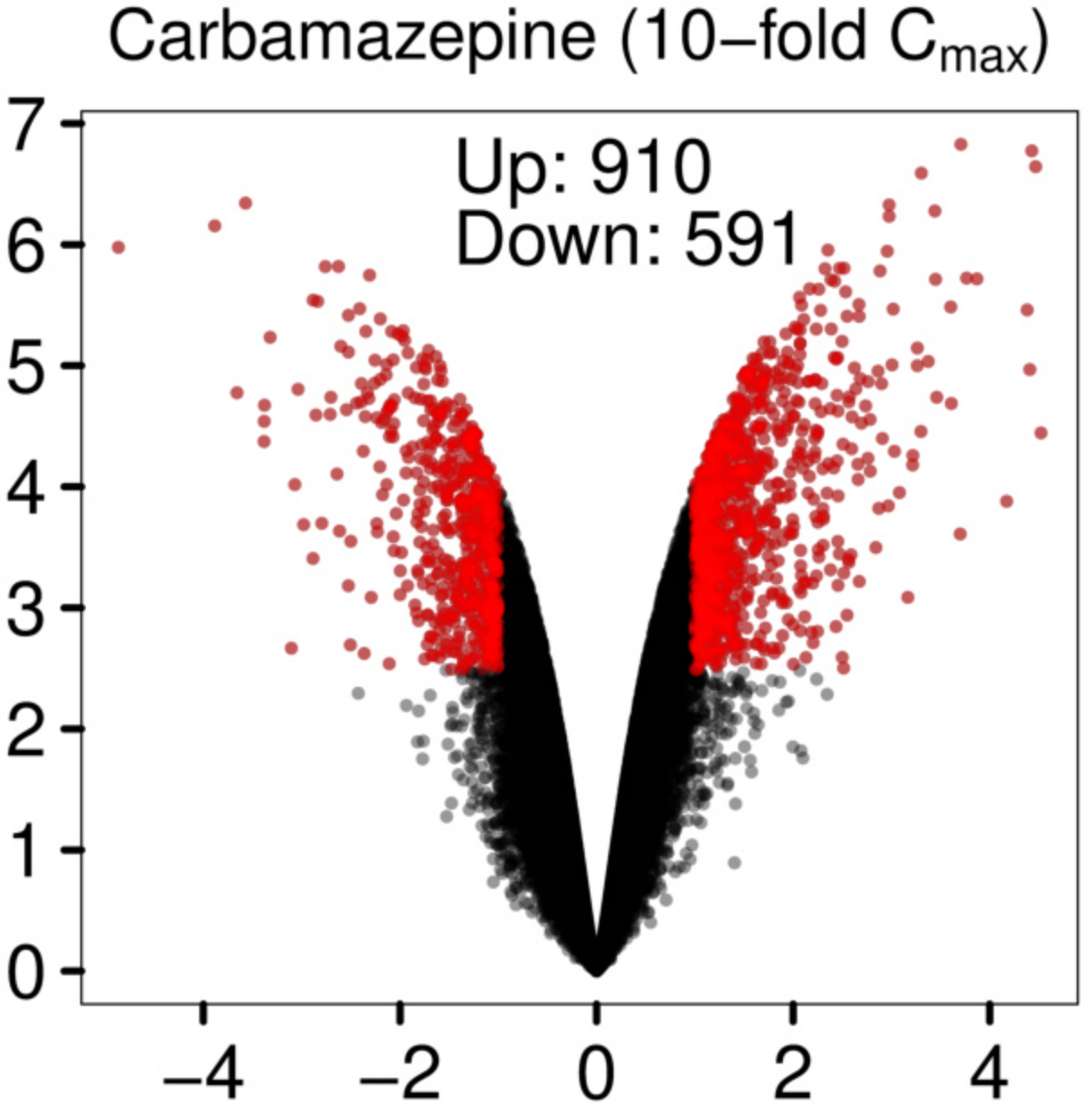
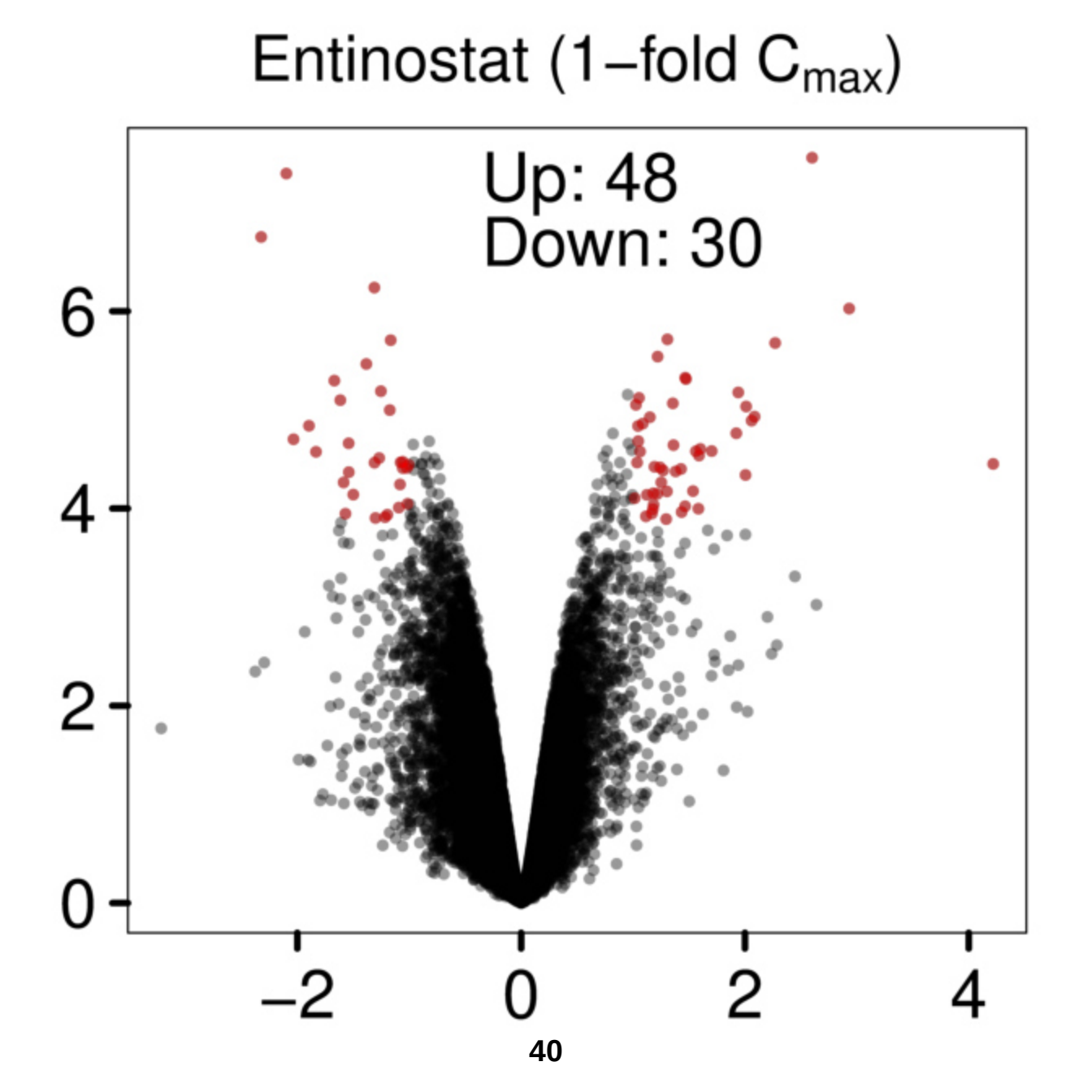
3
2
1
0
–1
0
1


Carbamazepine (10–fold C_{max})
Up: 910
Down: 591
7
6
5
4
3
2
1
0
−4
−2
0
2
4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Up: 48
Down: 30
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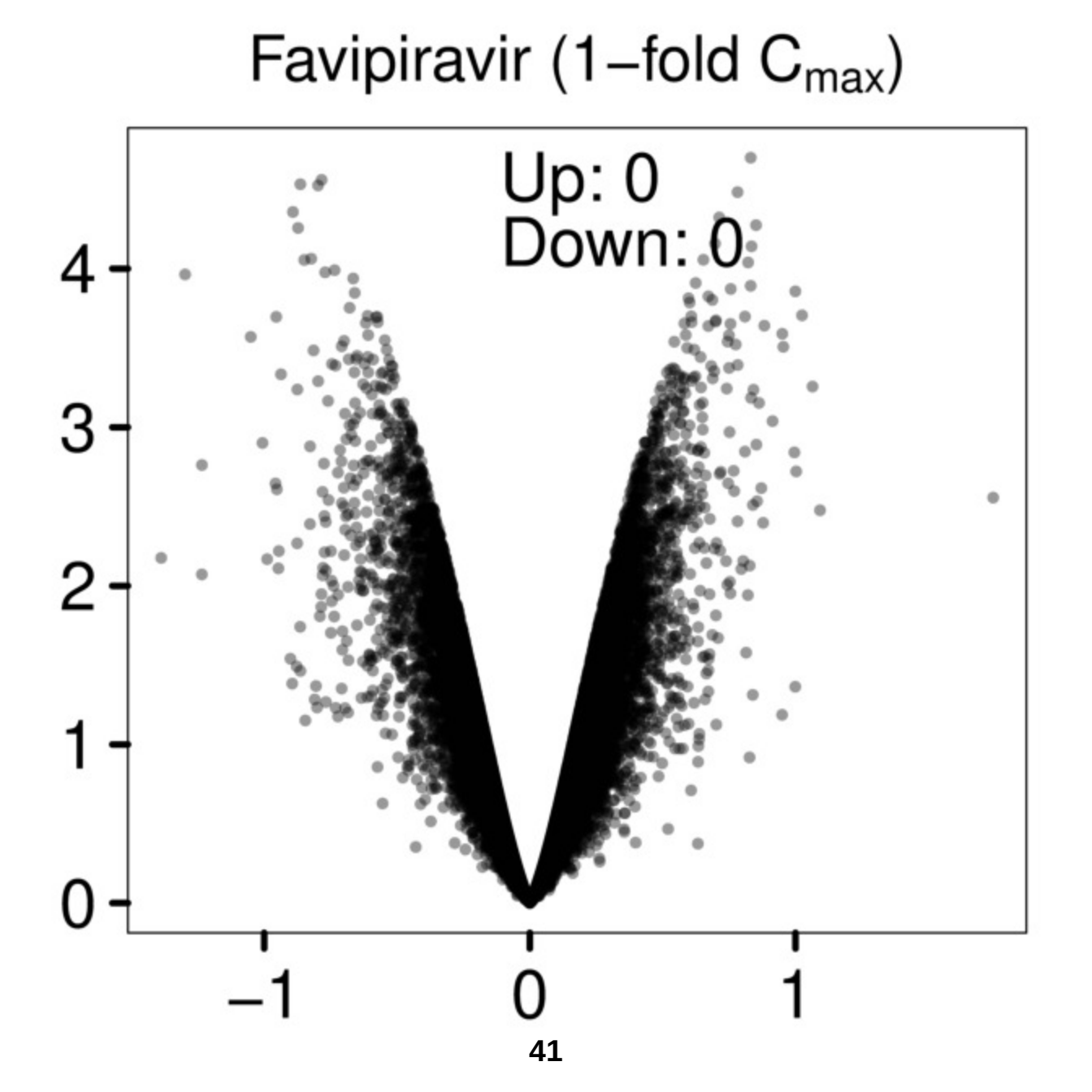
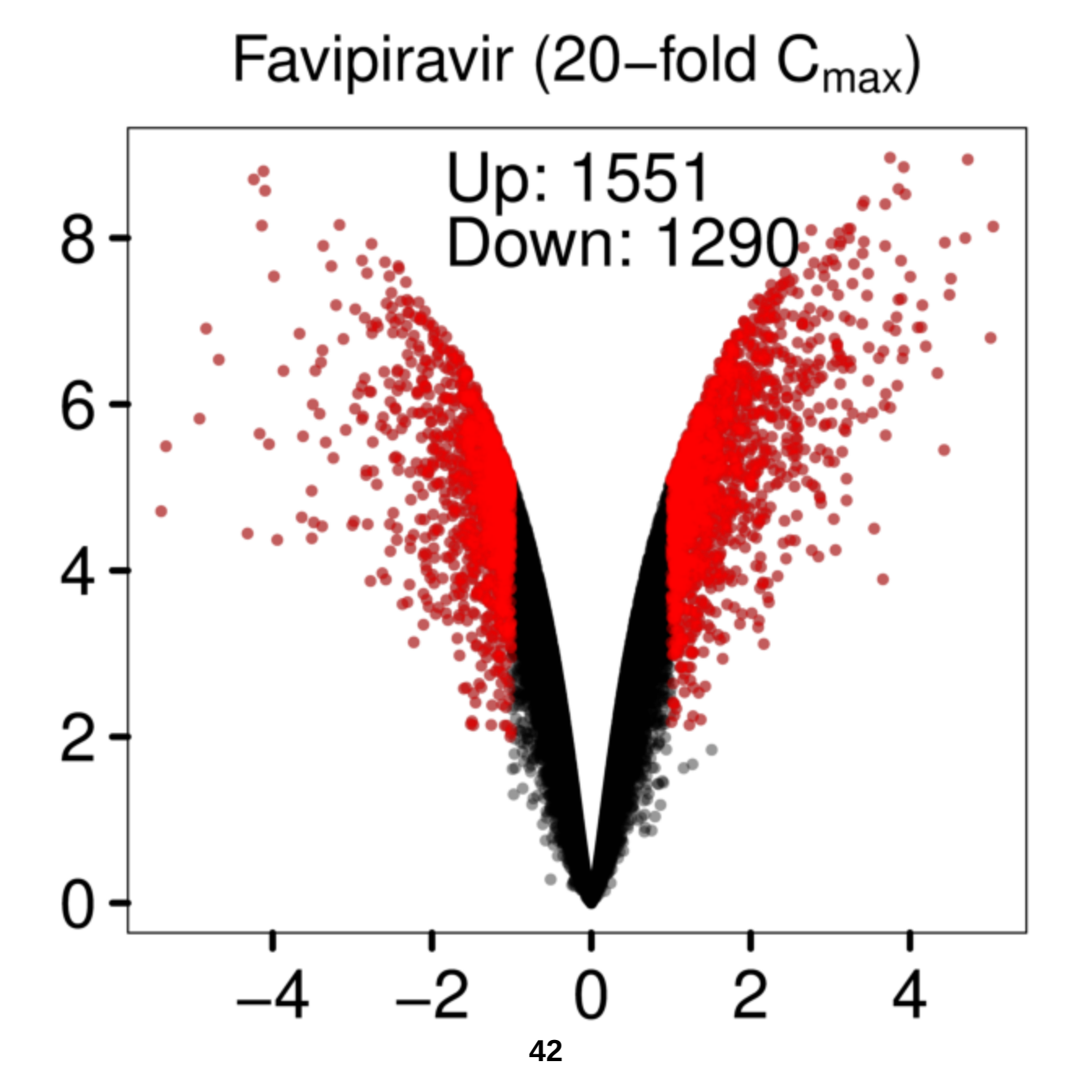
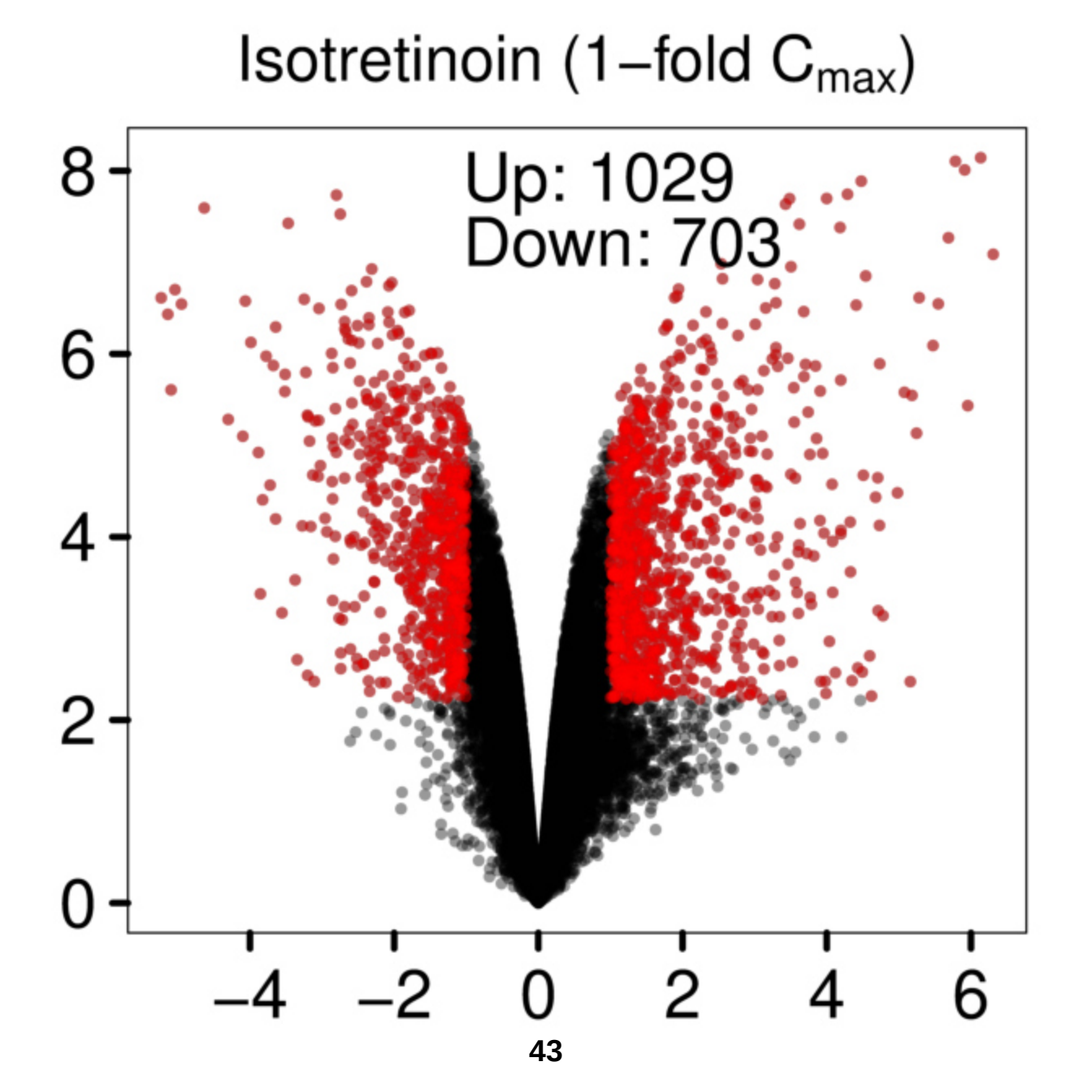
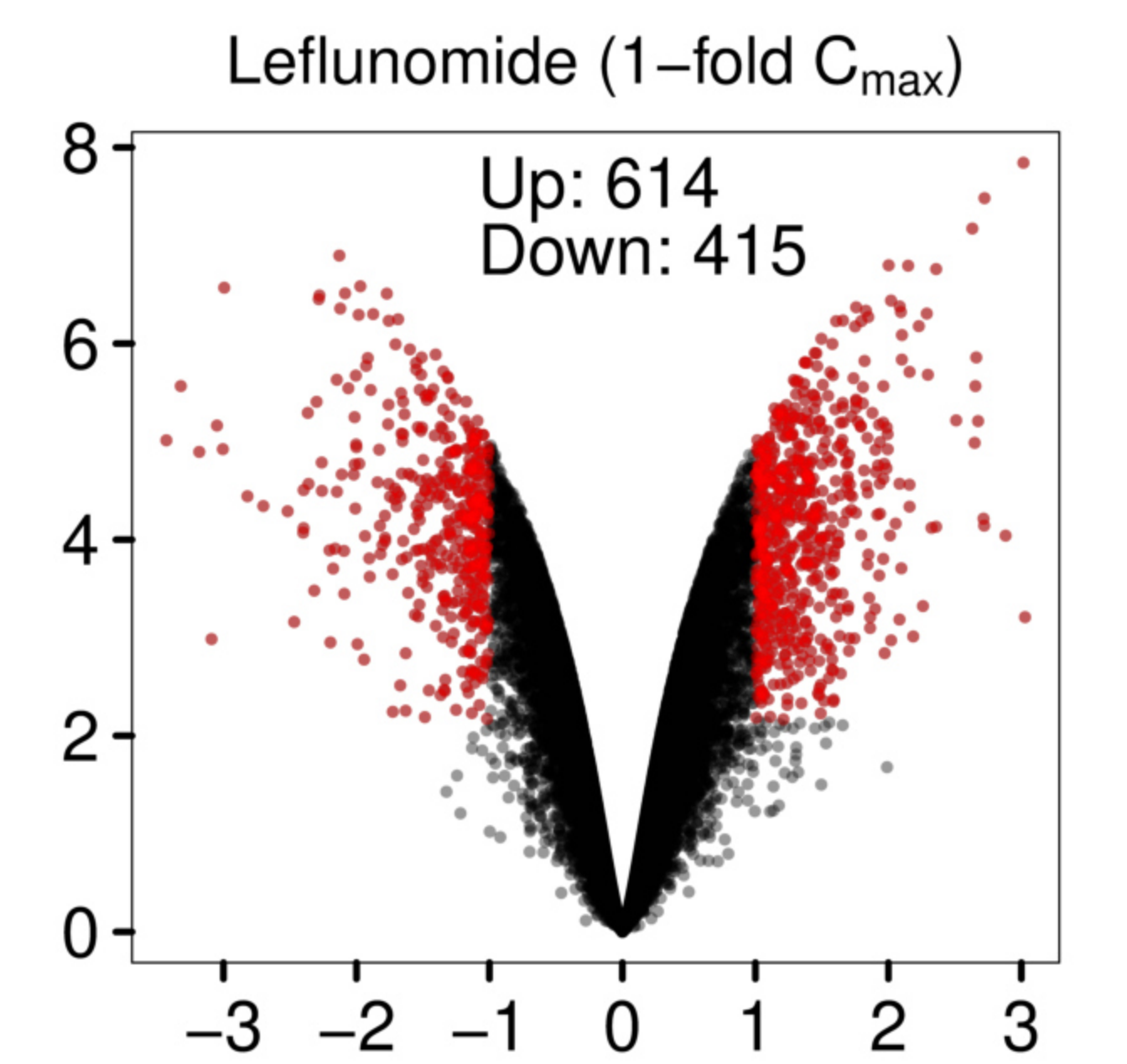
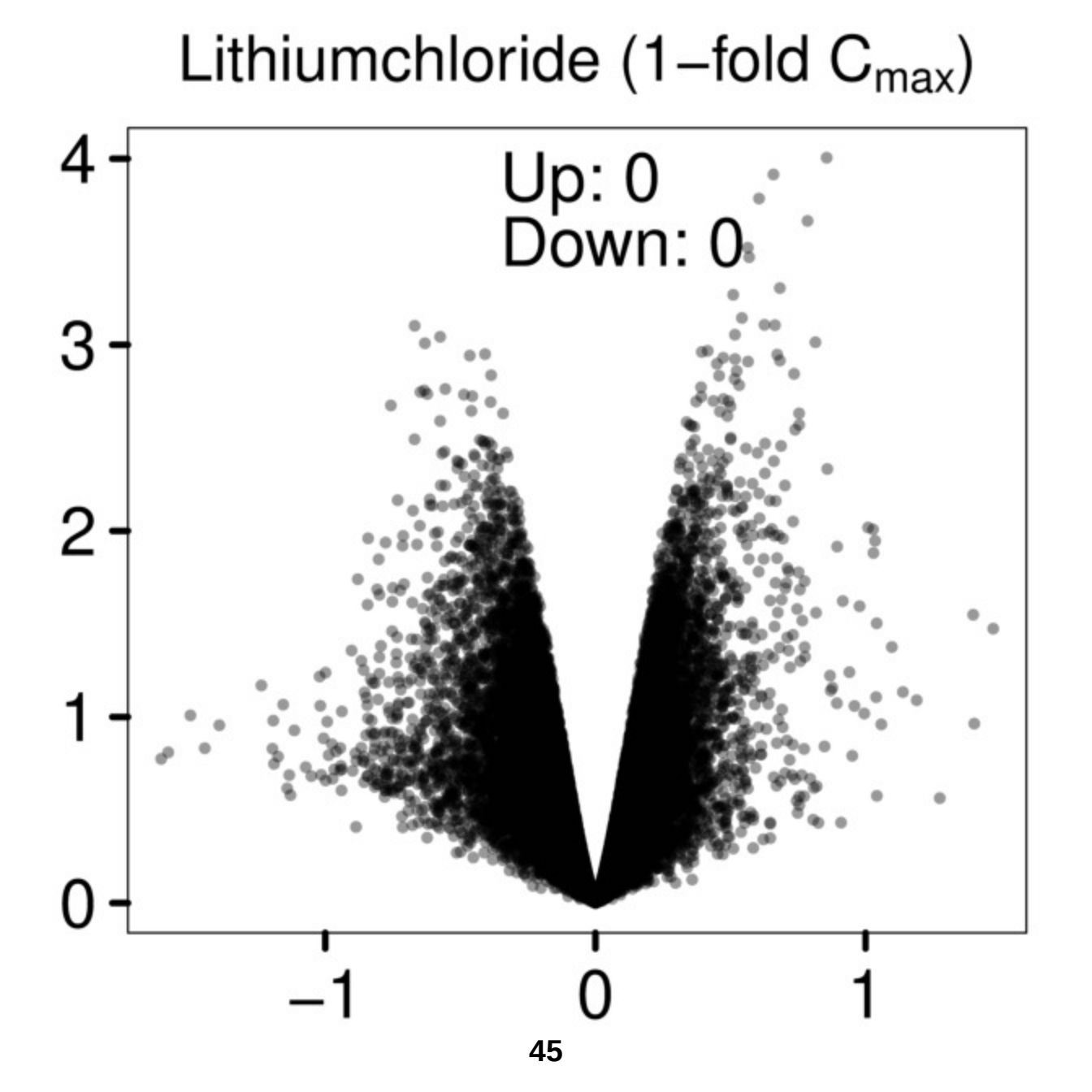
4
2
0
–2
0
2
4

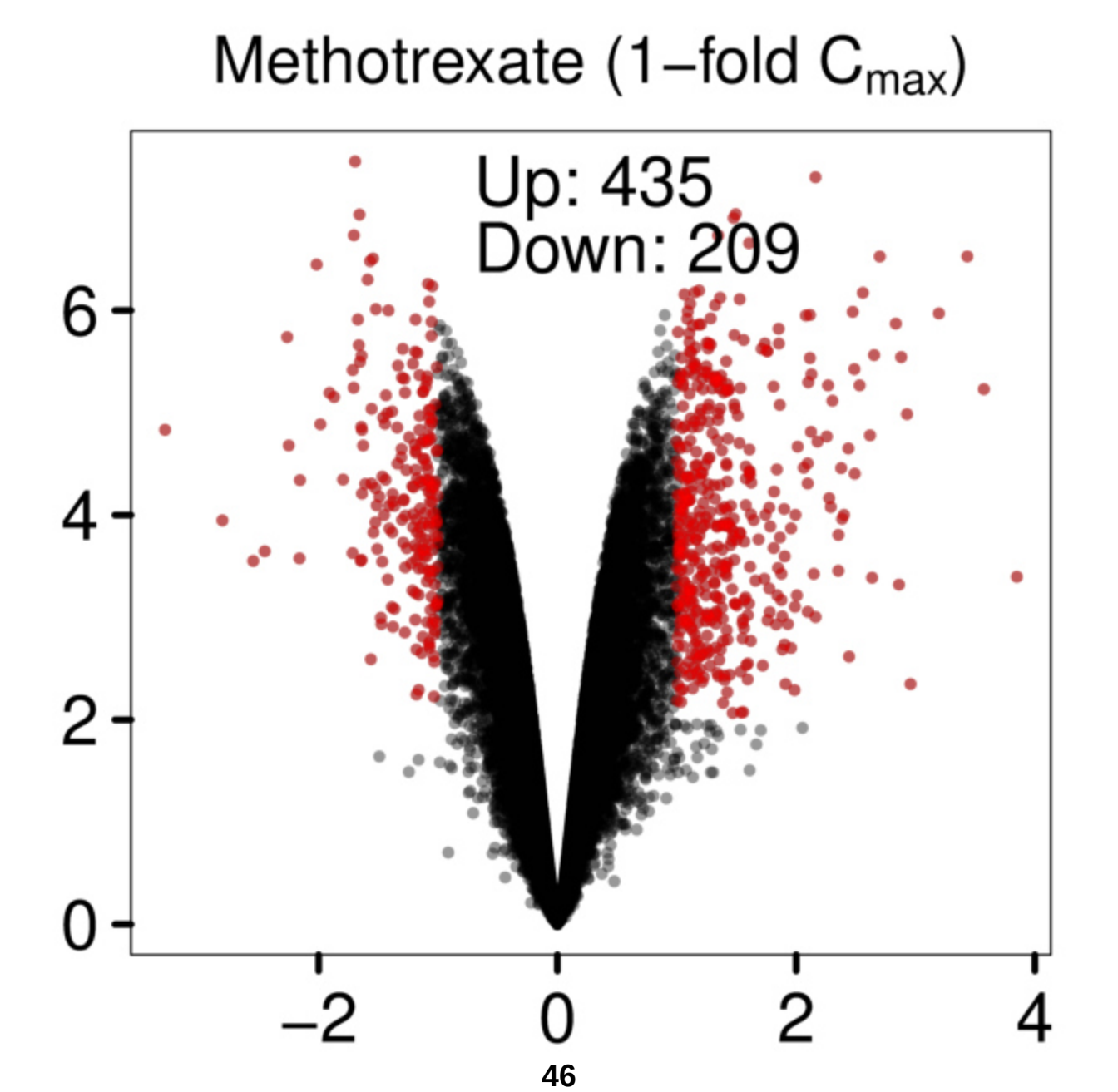

Favipiravir (1–fold C_{max})
Up: 0
Down: 0
4
3
2
1
0
−1
0
1

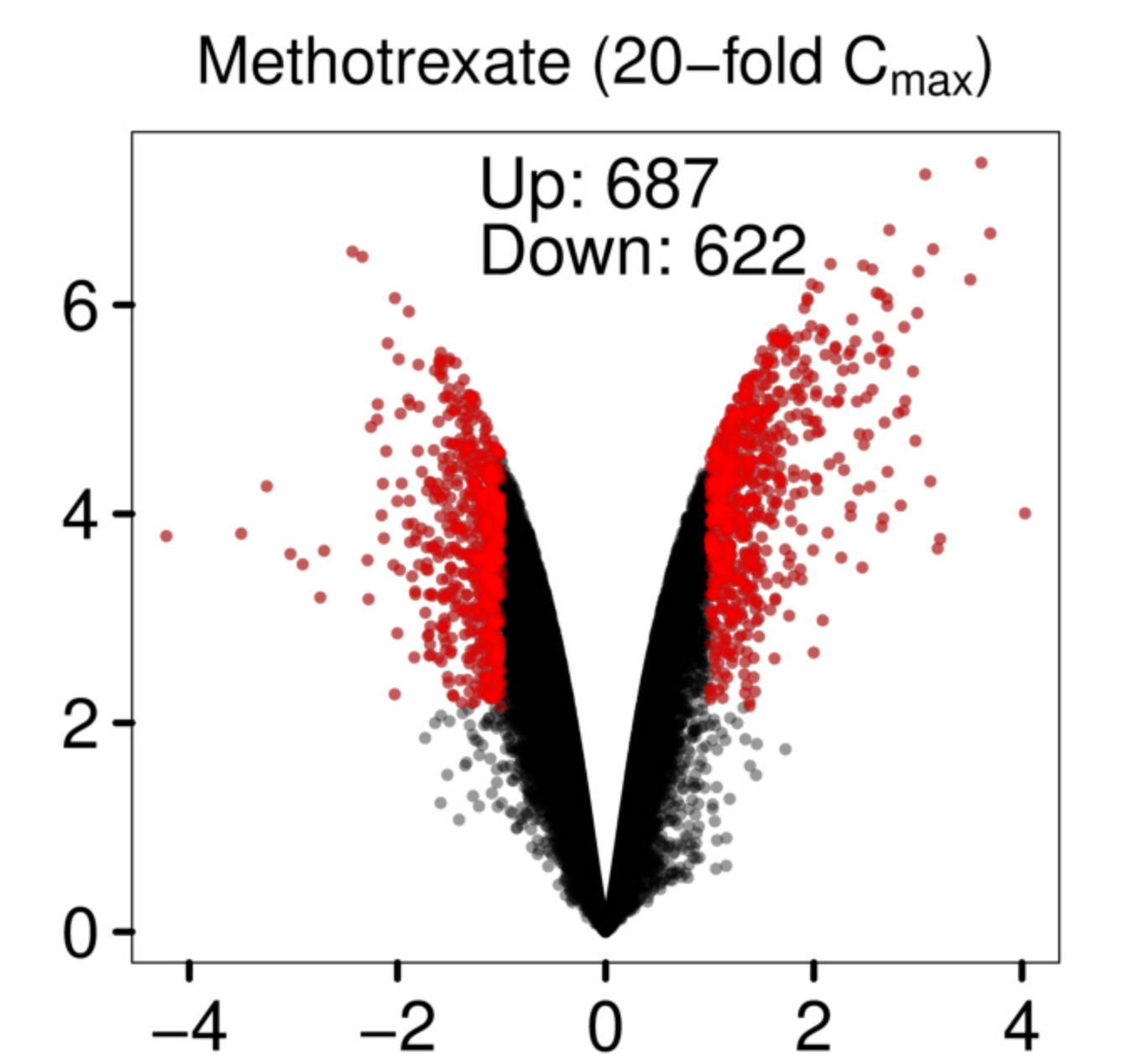

Favipiravir (20–fold C_{max})
Up: 1551
Down: 1290
8
6
4
2
0
−4
−2
0
2
4

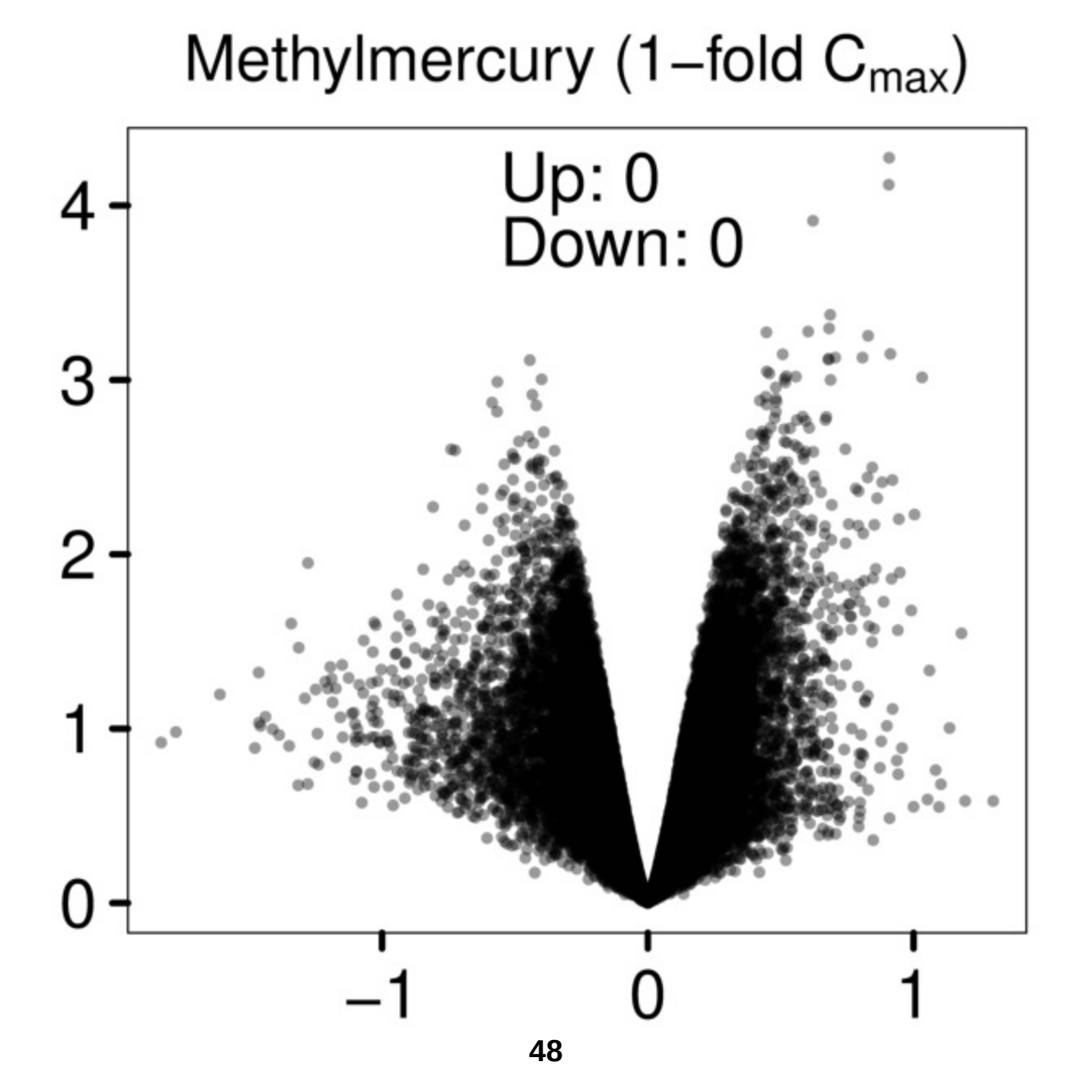

Isotretinoin (1–fold C_{max})
Up: 1029
Down: 703
8
6
4
2
0
−4
−2
0
2
4
6

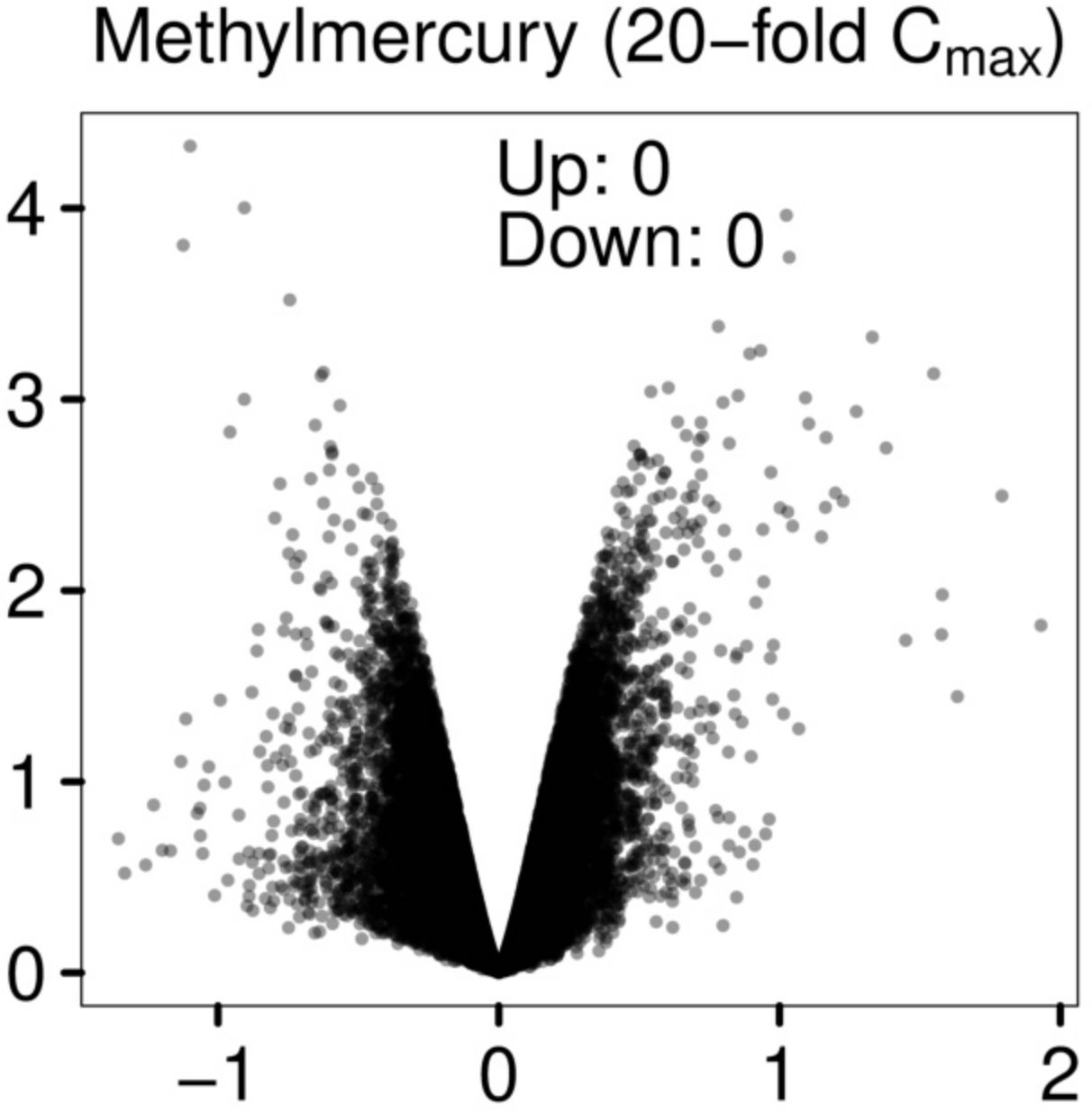

Leflunomide (1–fold C_{max})
Up: 614
Down: 415
8
6
4
2
0
−3
−2
−1
0
1
2
3

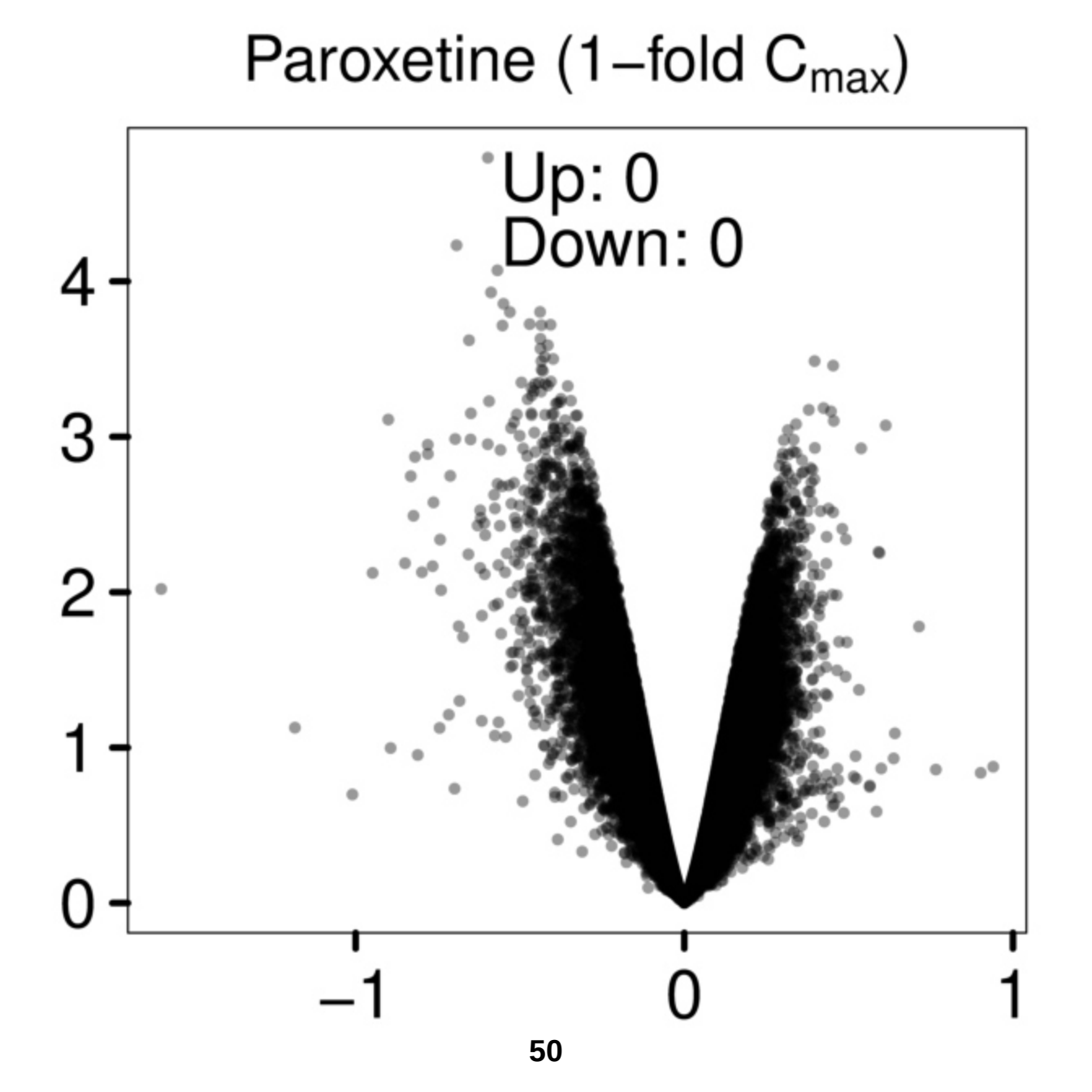

Lithiumchloride (1–fold C_{max})
Up: 0
Down: 0
4
3
2
1
0
−1
0
1

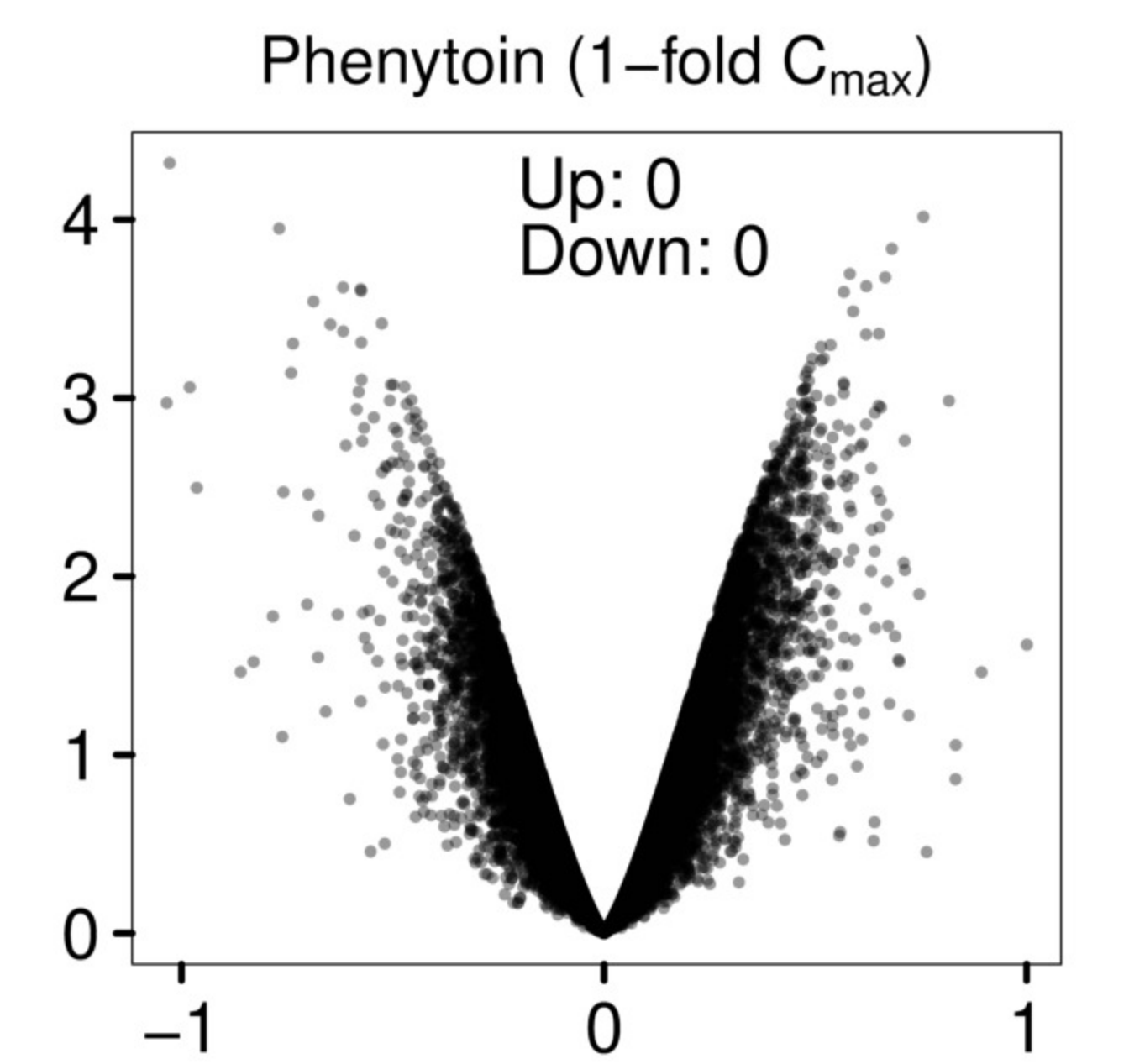

Methotrexate (1–fold C_{max})
Up: 435
Down: 209
6
4
2
0
−2
0
2
4

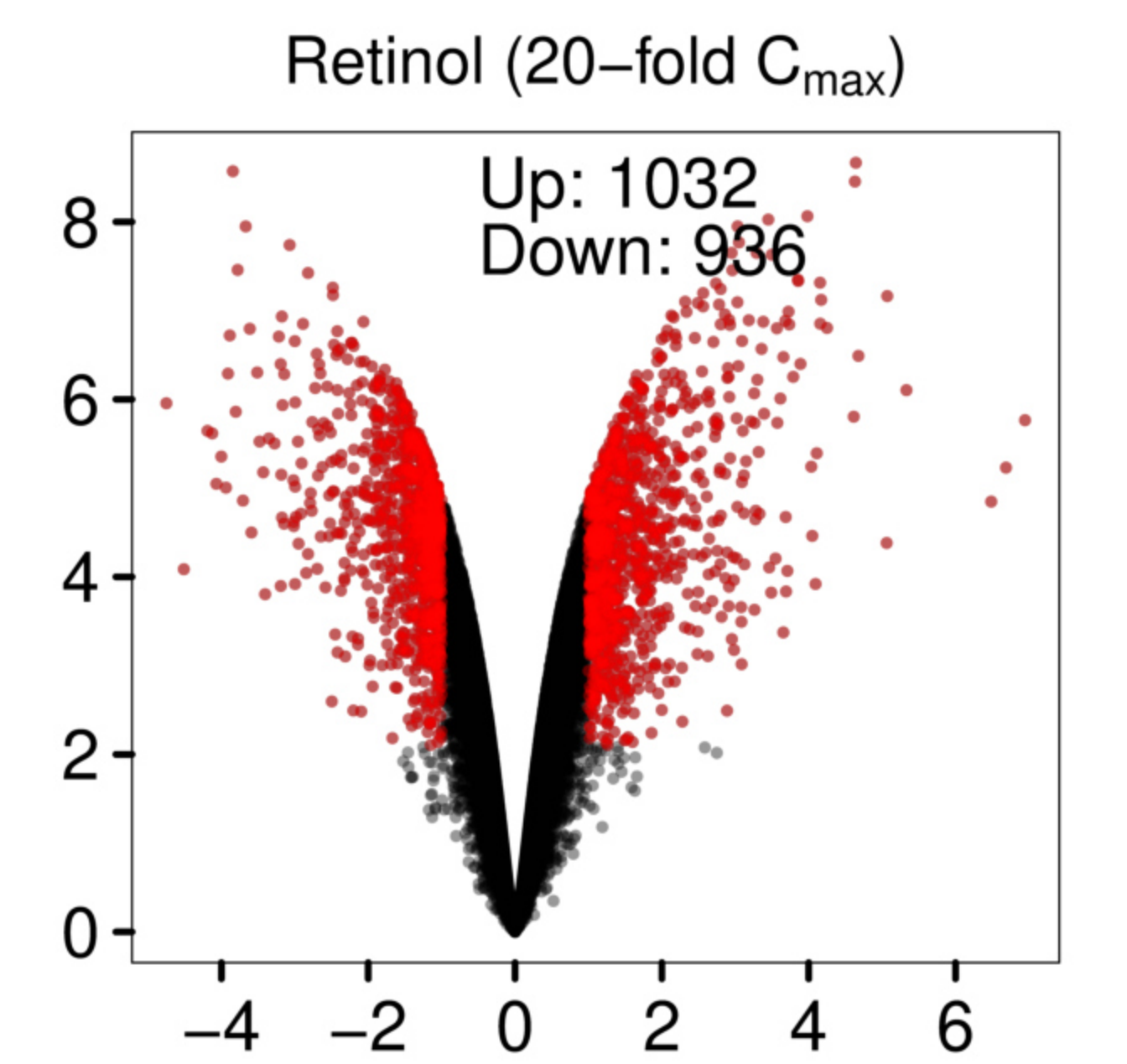

Methotrexate (20–fold C_{max})
Up: 687
Down: 622
6
4
2
0
–4
–2
0
2
4

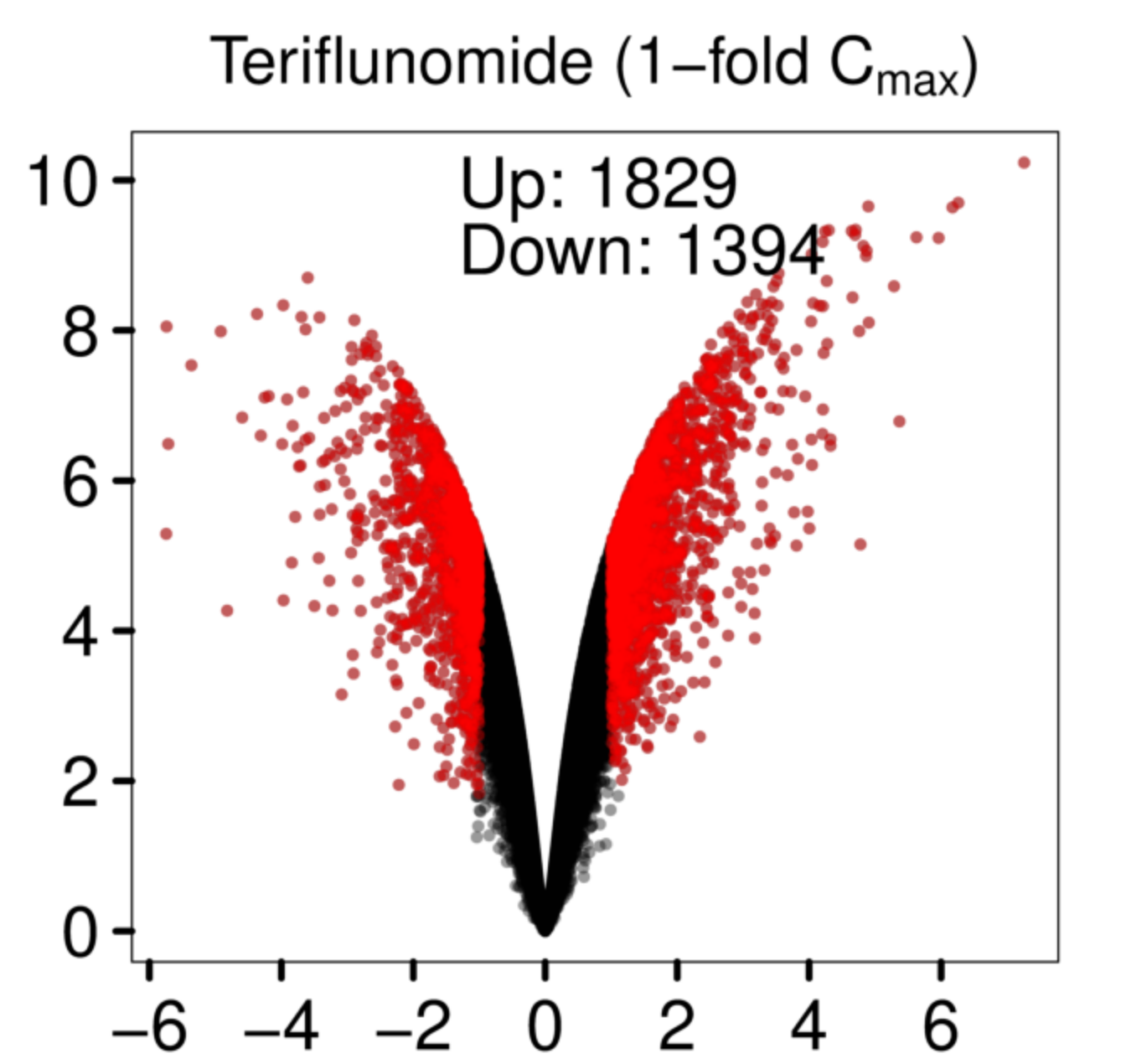

Methylmercury (1–fold C_{max})
Up: 0
Down: 0
4
3
2
1
0
–1
0
1

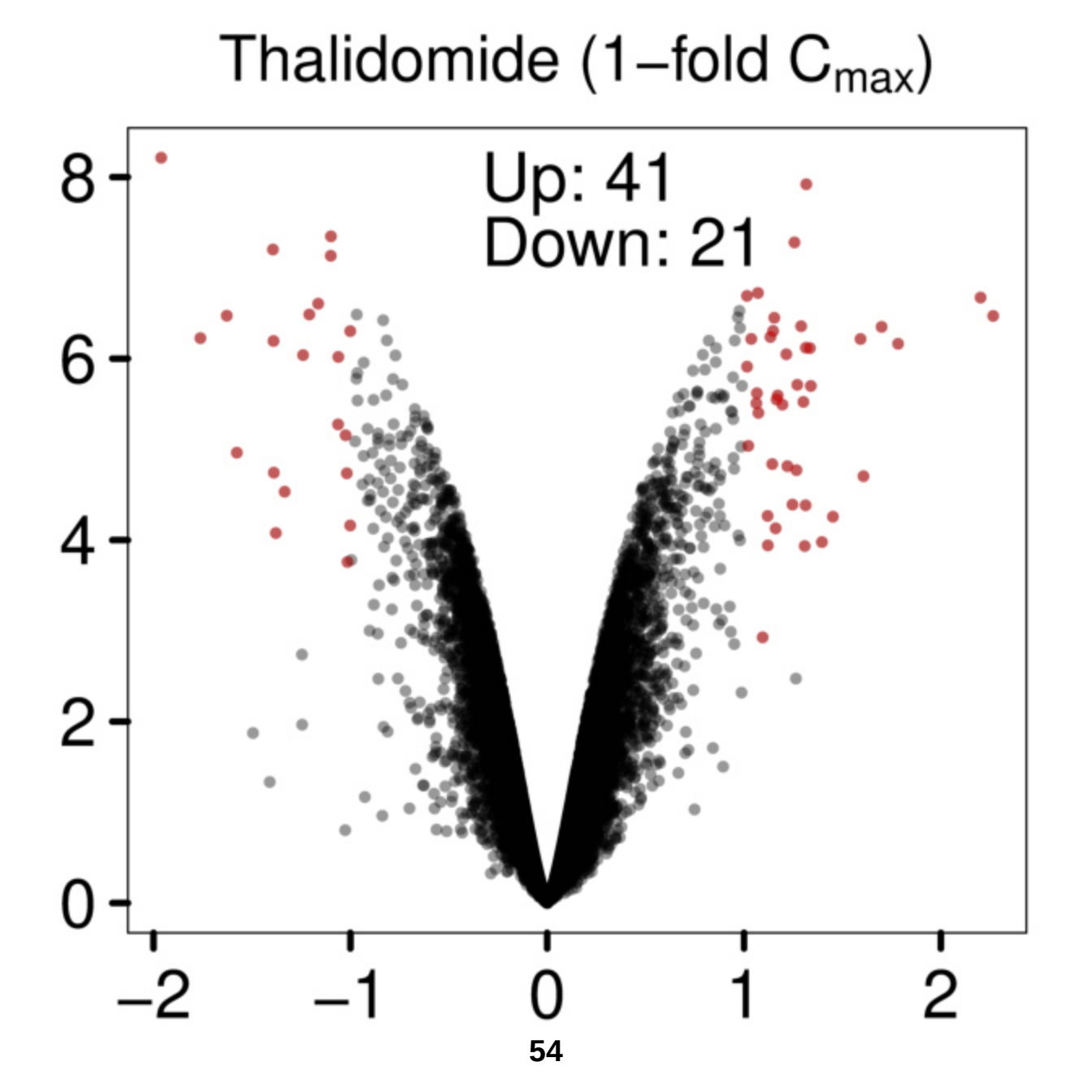

Methylmercury (20–fold C_{max})
Up: 0
Down: 0
4
3
2
1
0
−1
0
1
2

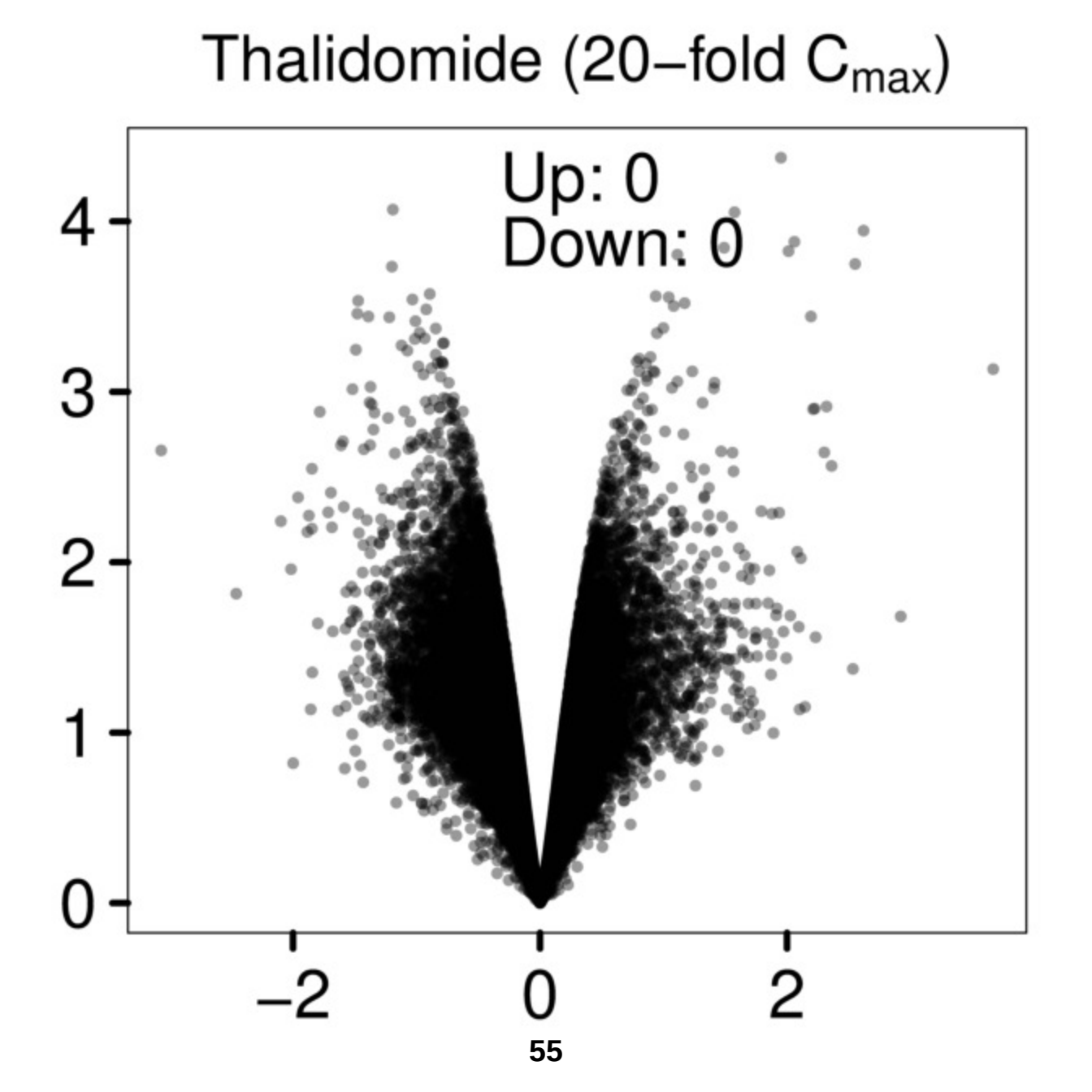

Paroxetine (1–fold C_{max})
Up: 0
Down: 0
4
3
2
1
0
−1
0
1

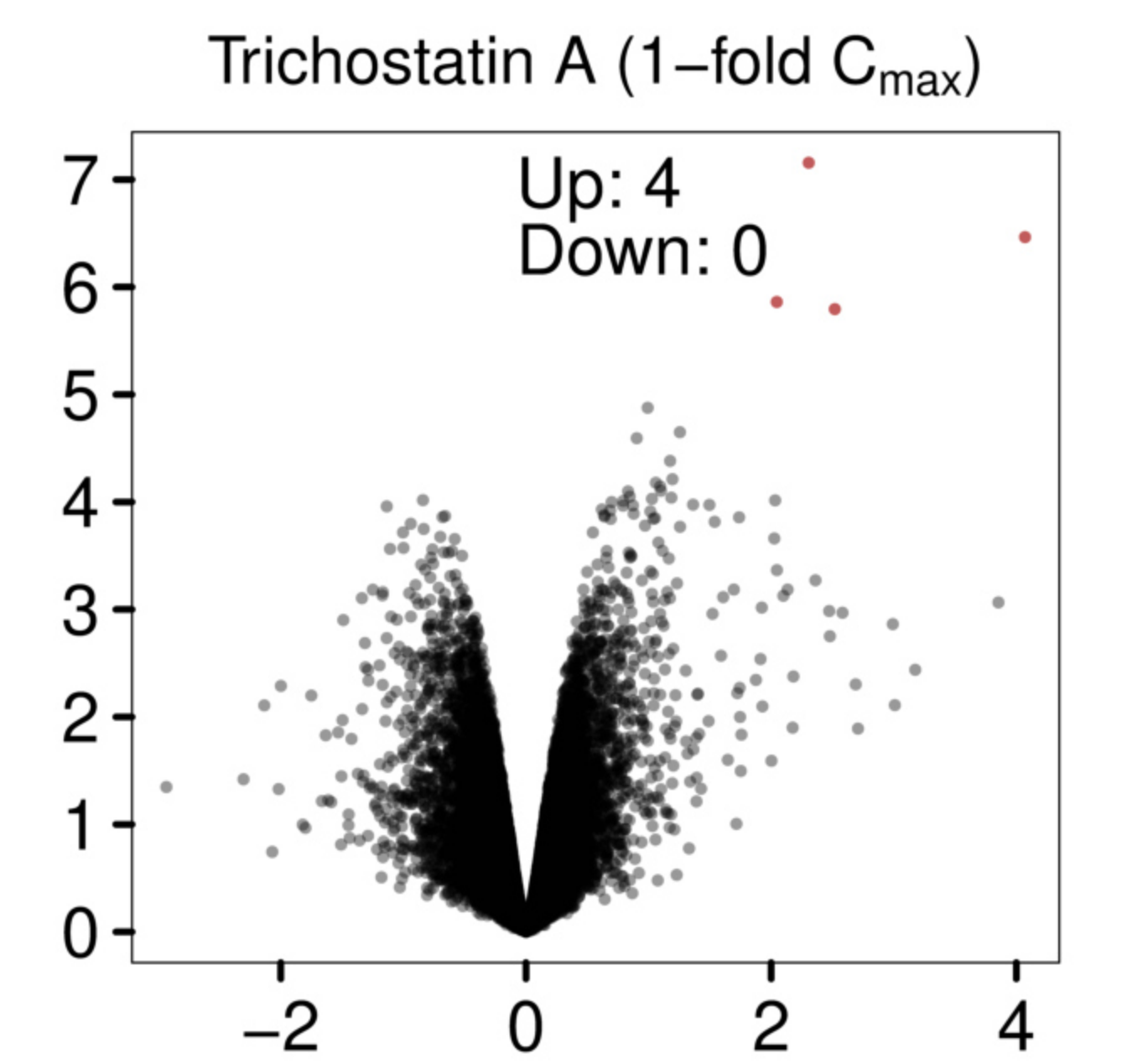

Phenytoin (1–fold C_{max})
Up: 0
Down: 0
4
3
2
1
0
–1
0
1

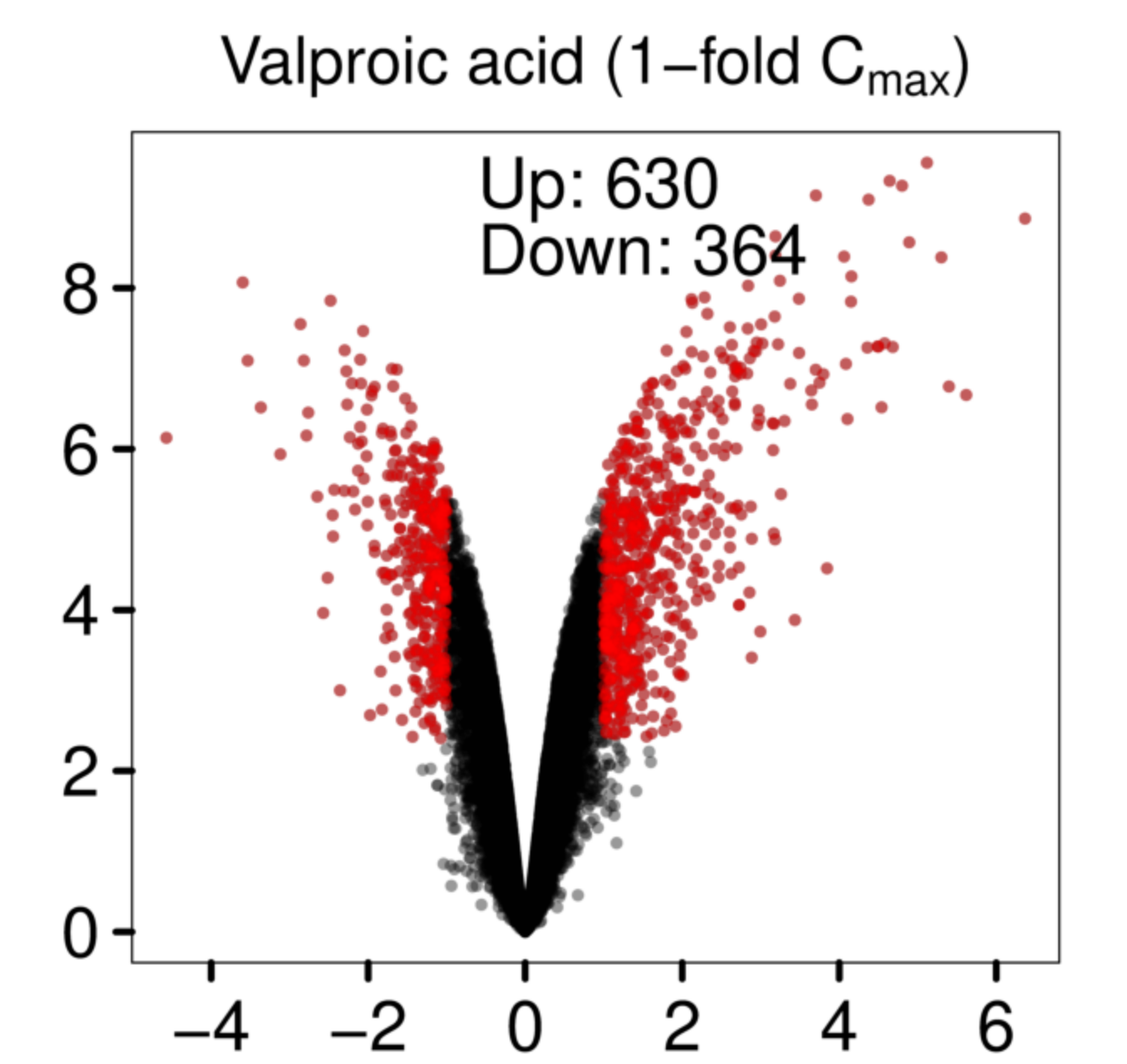

Retinol (20–fold C_{max})
Up: 1032
Down: 936
8
6
4
2
0
−4
−2
0
2
4
6

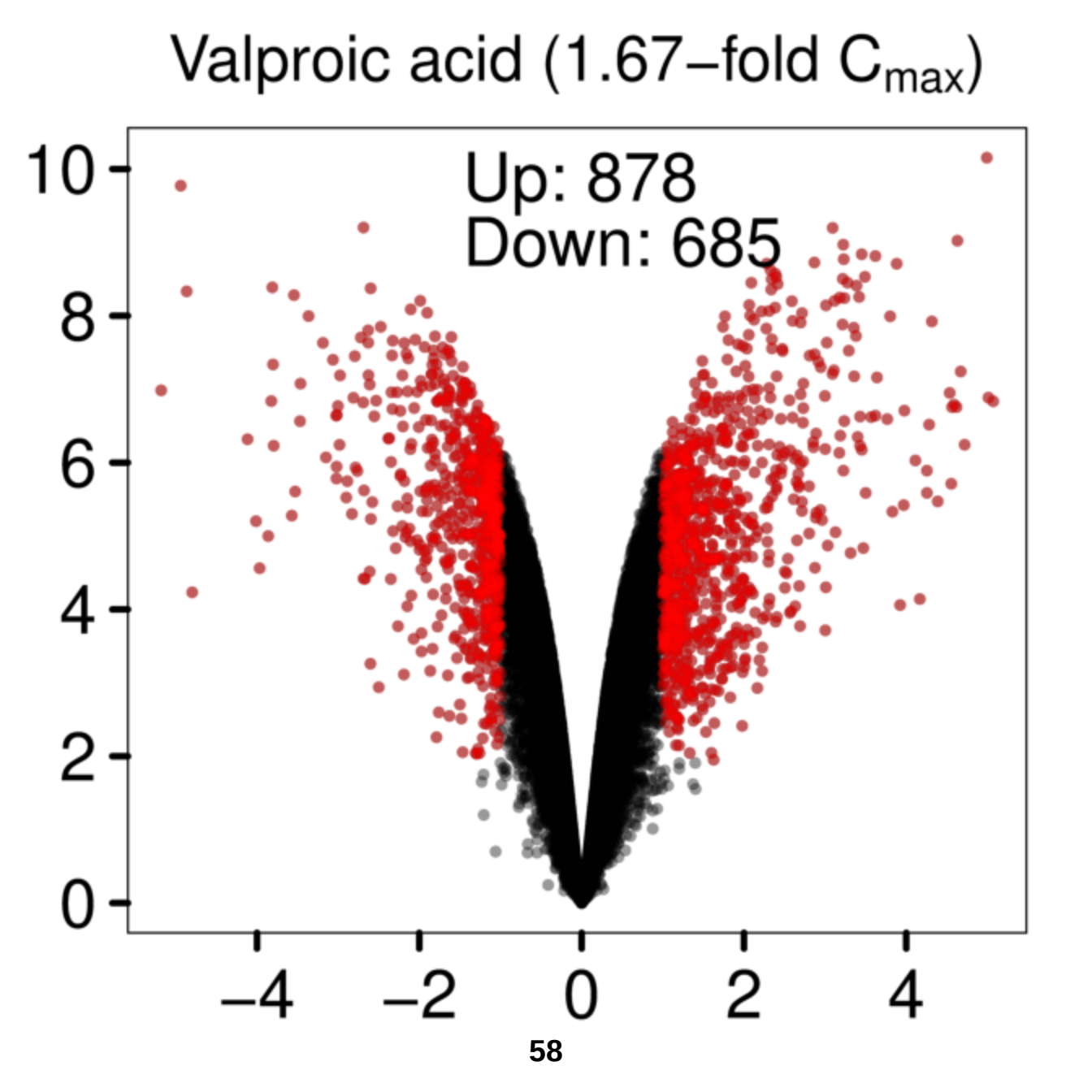

Teriflunomide (1–fold C_{max})
Up: 1829
Down: 1394
10
8
6
4
2
0
−6
−4
−2
0
2
4
6

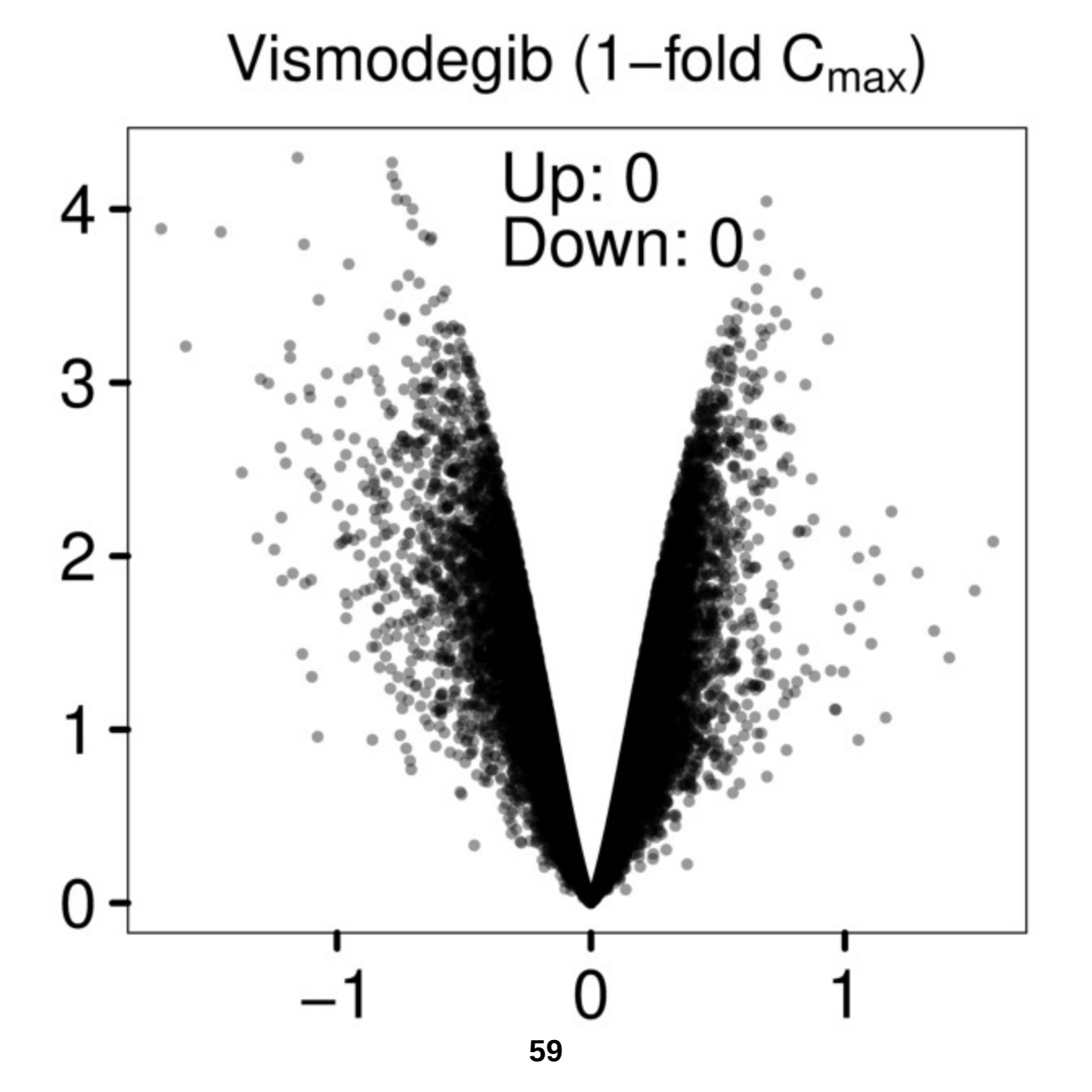

Thalidomide (1–fold C_{max})
Up: 41
Down: 21
8
6
4
2
0
−2
−1
0
1
2


Thalidomide (20–fold C_{max})
Up: 0
Down: 0
4
3
2
1
0
–2
0
2


Trichostatin A (1–fold C_{max})
Up: 4
Down: 0
7
6
5
4
3
2
1
0
–2
0
2
4


Valproic acid (1–fold C_{max})
Up: 630
Down: 364
8
6
4
2
0
−4
−2
0
2
4
6


Valproic acid (1.67–fold C_{max})
Up: 878
Down: 685
10
8
6
4
2
0
−4
−2
0
2
4


Vismodegib (1–fold C_{max})
Up: 0
Down: 0
4
3
2
1
0
−1
0
1