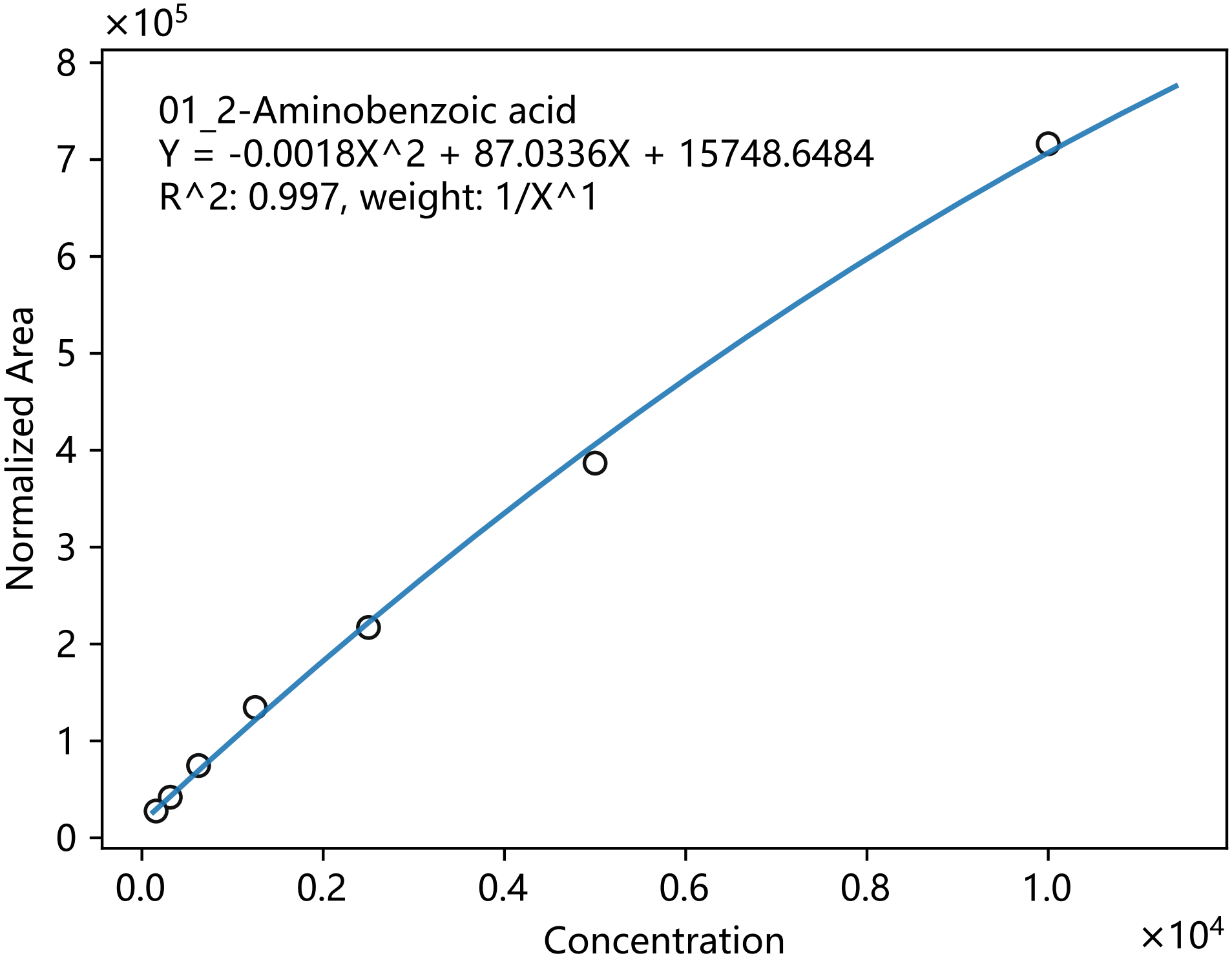
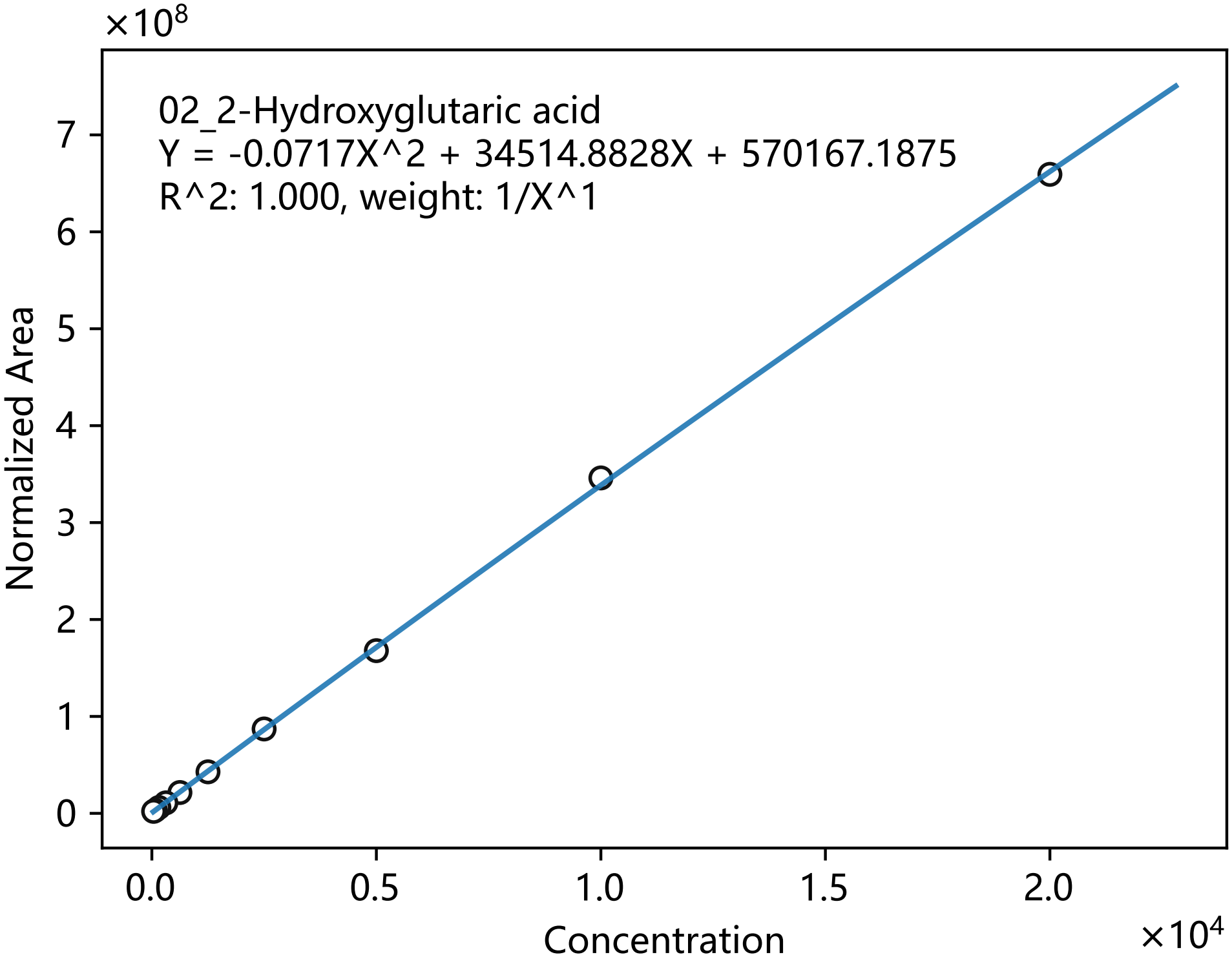
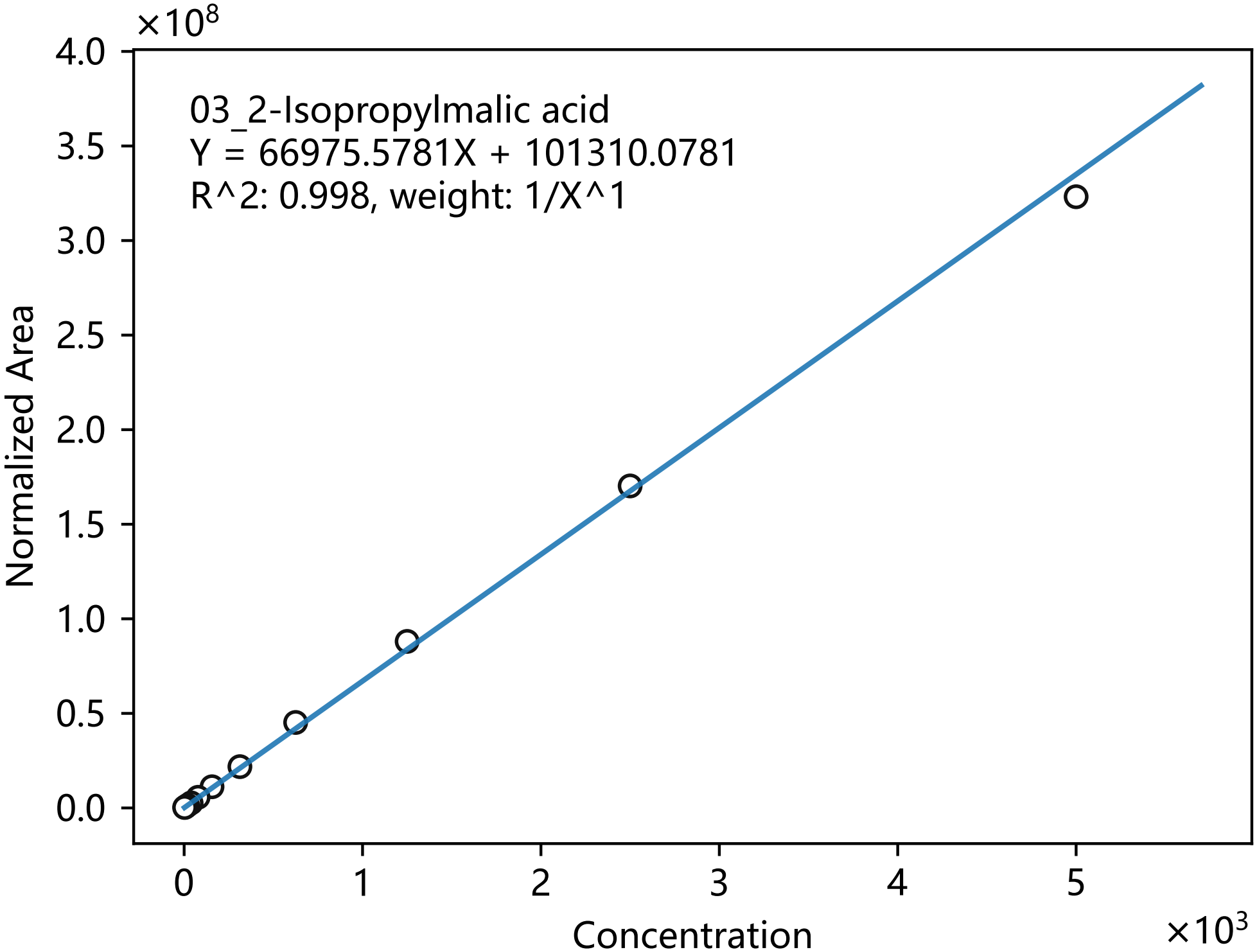
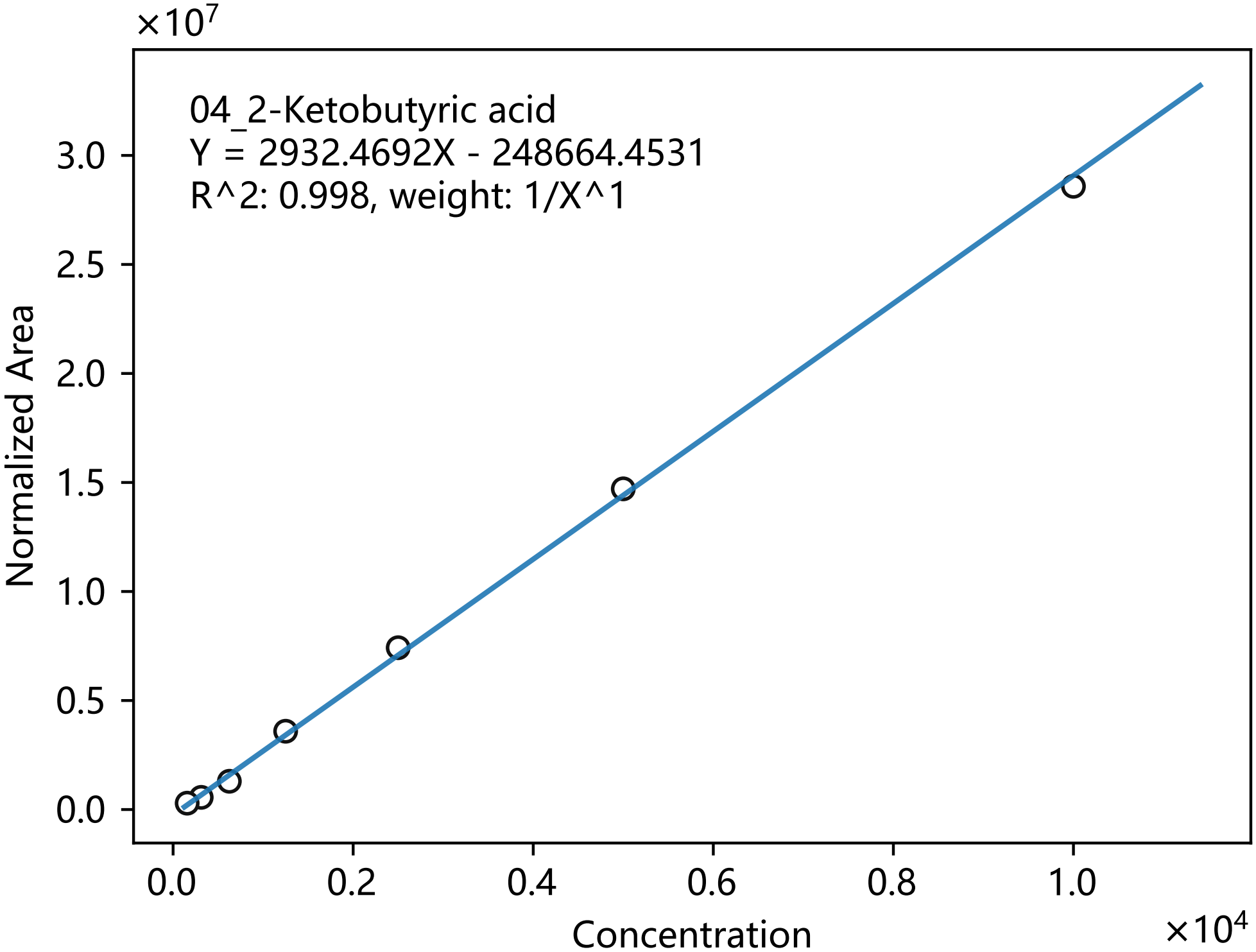
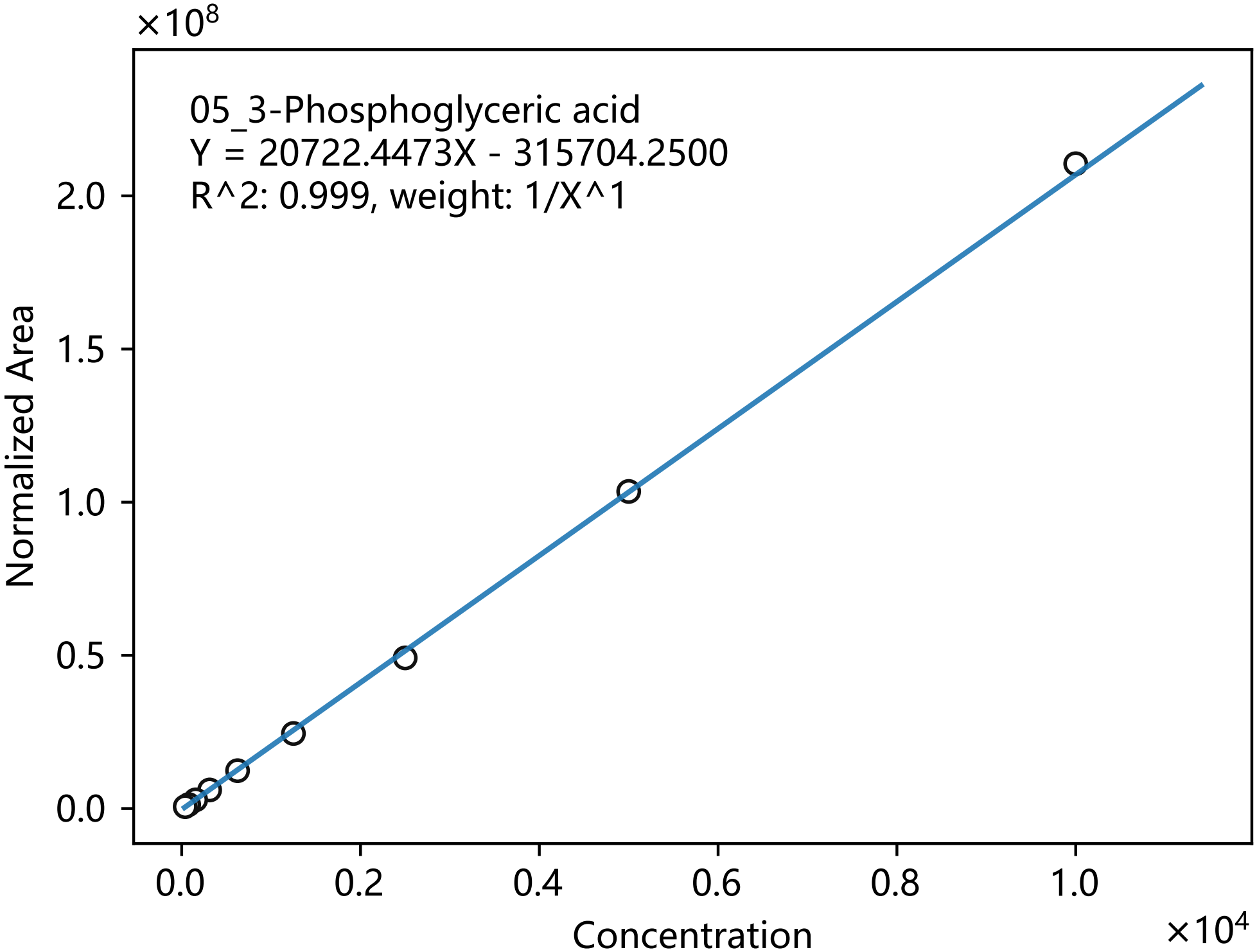
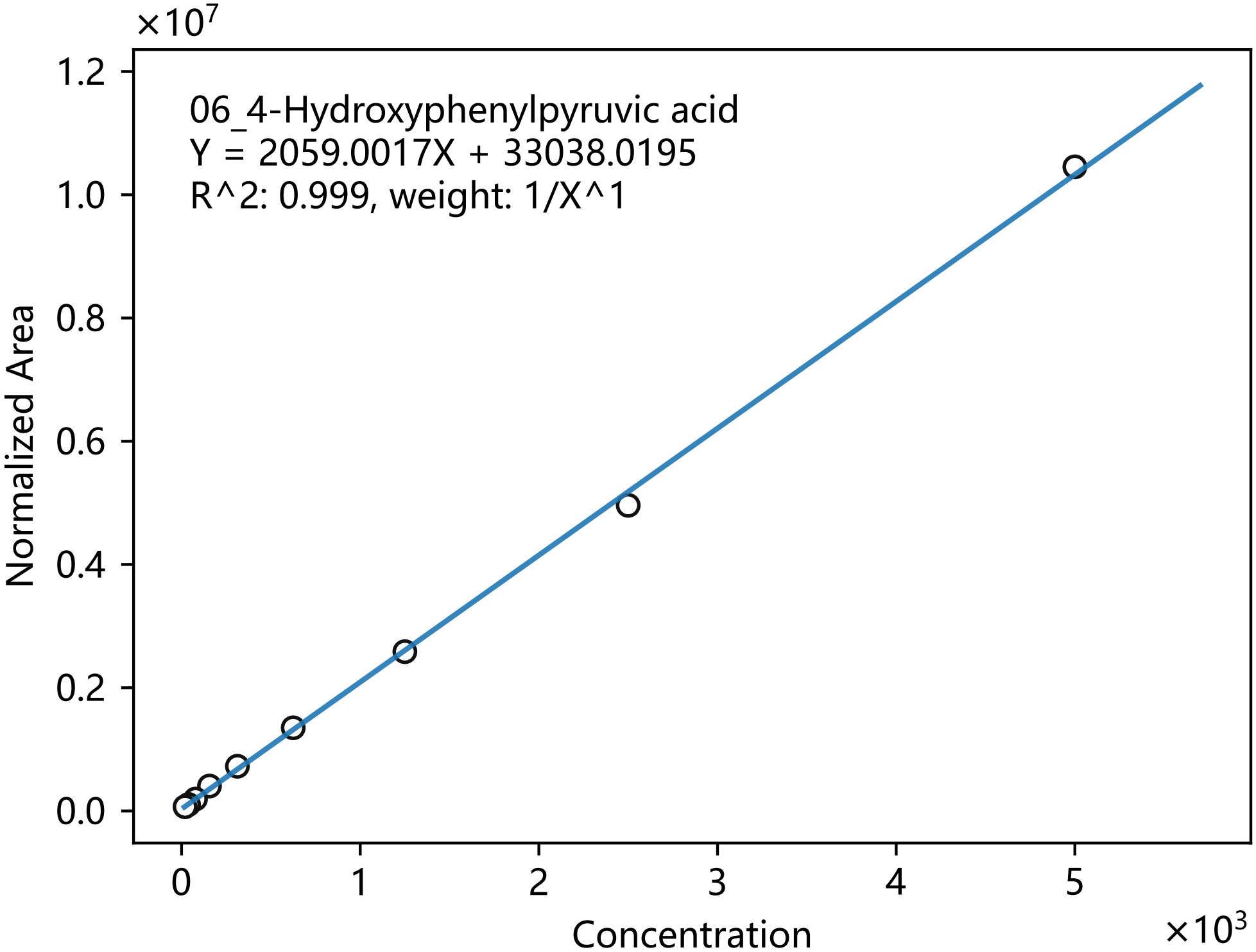

×10^5
8
7
6
5
4
3
2
1
0
01_2-Aminobenzoic acid
Y = -0.0018X^2 + 87.0336X + 15748.6484
R^2: 0.997, weight: 1/X^1
Normalized Area
0.0
0.2
0.4
0.6
0.8
1.0
Concentration
×10^4

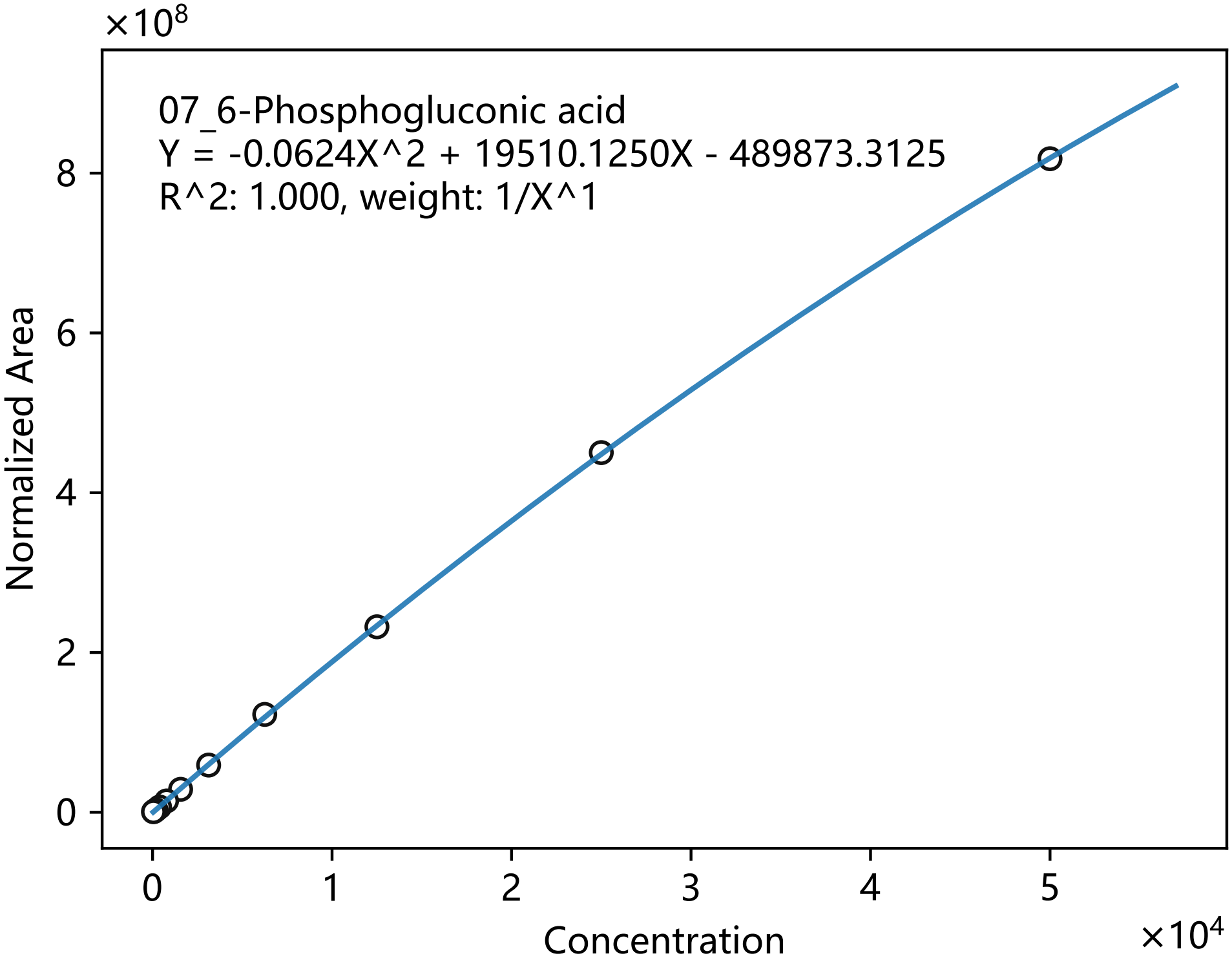

×10^8
02_2-Hydroxyglutaric acid
Y = -0.0717X^2 + 34514.8828X + 570167.1875
R^2: 1.000, weight: 1/X^1
Normalized Area
7
6
5
4
3
2
1
0
0.0
0.5
1.0
1.5
2.0
Concentration
×10^4

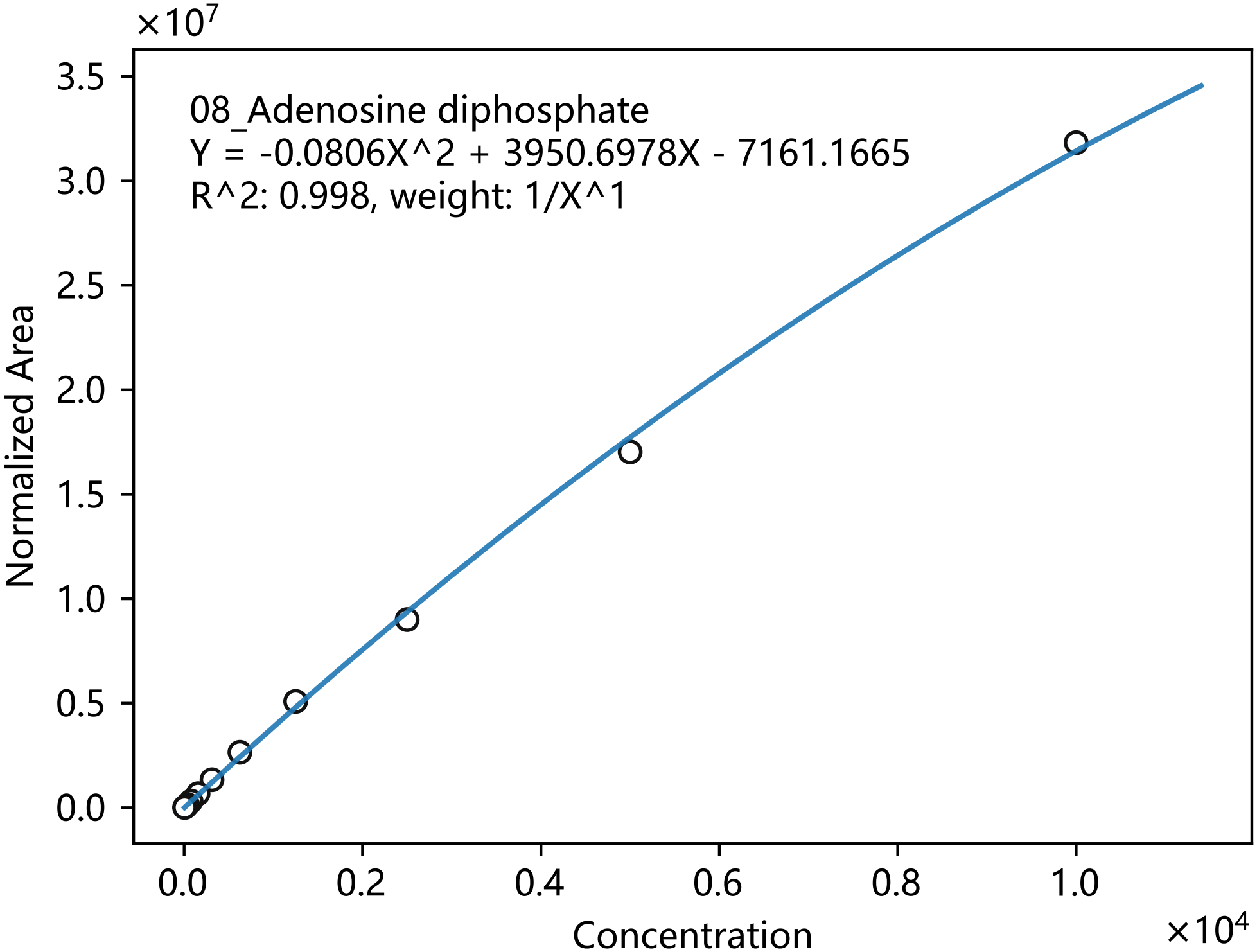

×10^8
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Normalized Area
03_2-Isopropylmalic acid
Y = 66975.5781X + 101310.0781
R^2: 0.998, weight: 1/X^1
0
1
2
3
4
5
Concentration
×10^3

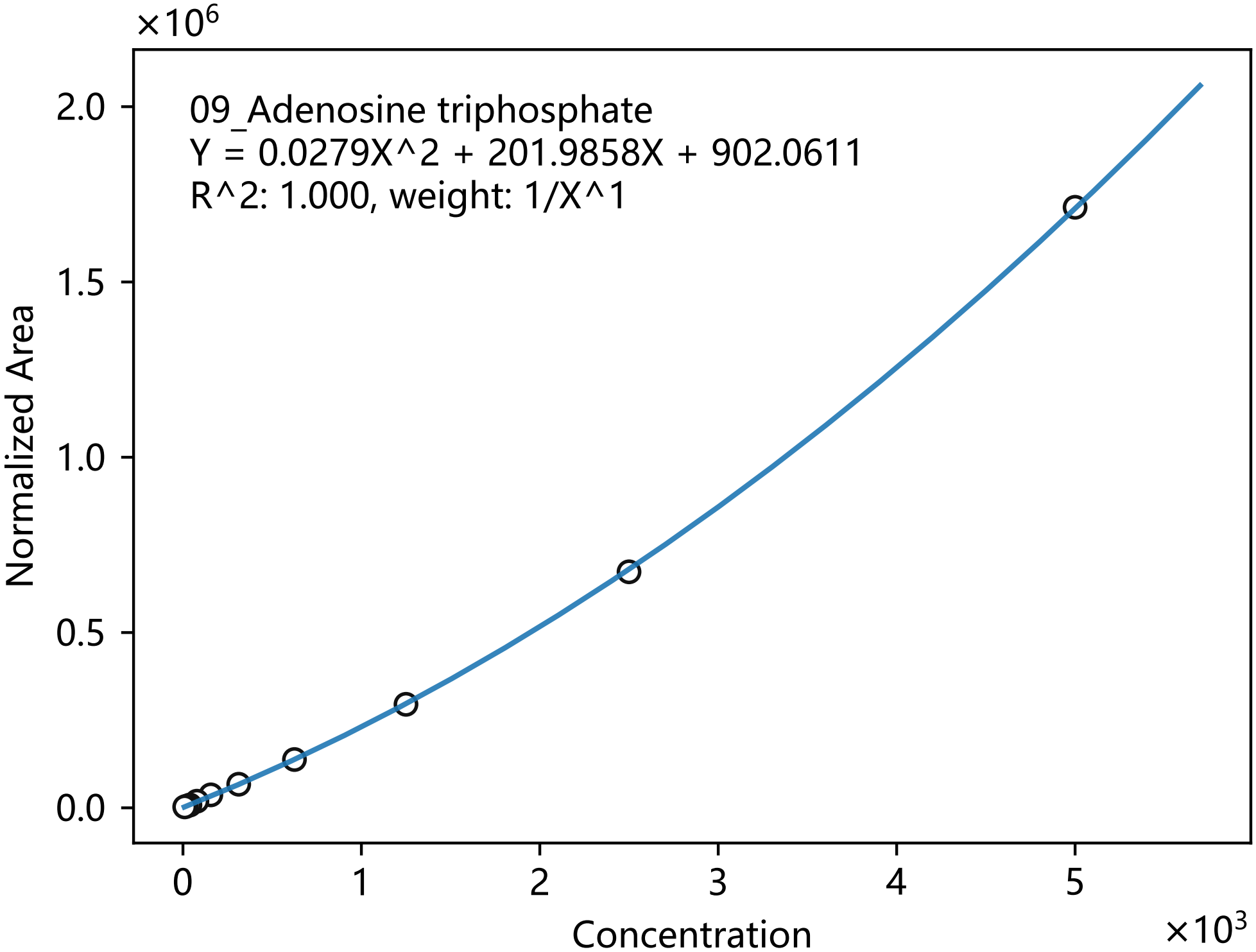

×10^7
04_2-Ketobutyric acid
Y = 2932.4692X - 248664.4531
R^2: 0.998, weight: 1/X^1
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Normalized Area
0.0
0.2
0.4
0.6
0.8
1.0
Concentration
×10^4

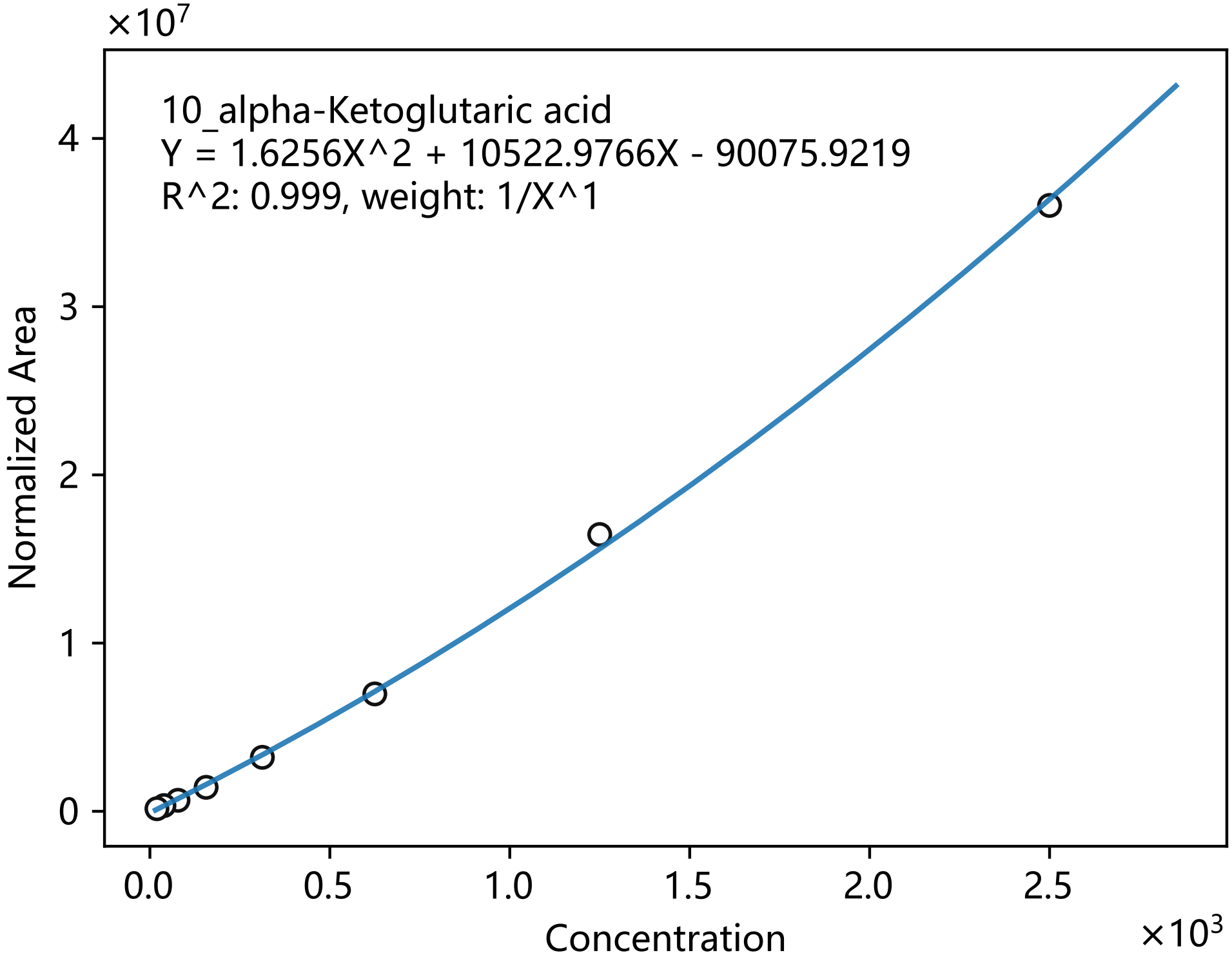

×10^8
05_3-Phosphoglyceric acid
Y = 20722.4473X - 315704.2500
R^2: 0.999, weight: 1/X^1
2.0
1.5
1.0
0.5
0.0
Normalized Area
0.0
0.2
0.4
0.6
0.8
1.0
Concentration
×10^4

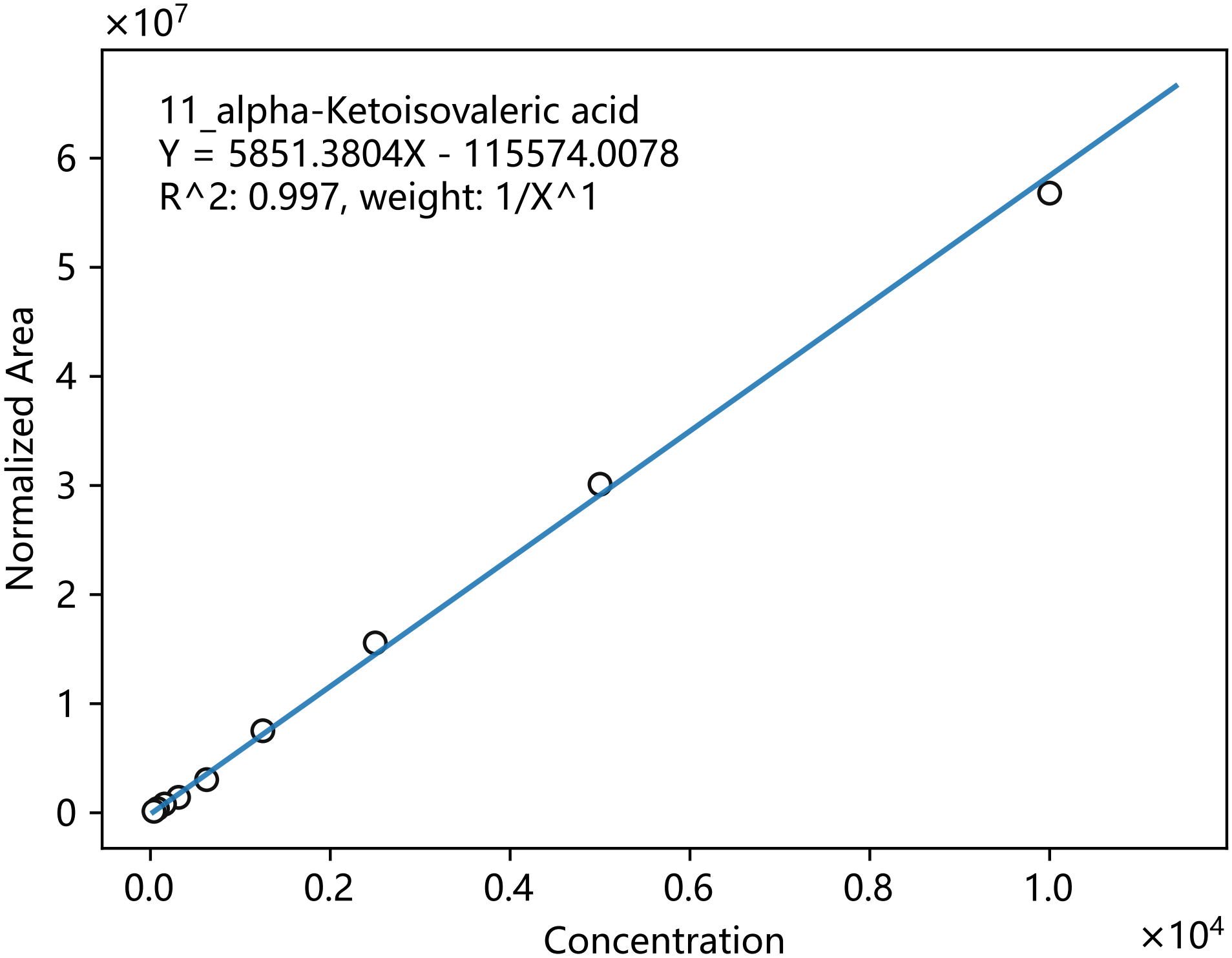

×10^7
1.2
1.0
0.8
0.6
0.4
0.2
0.0
Normalized Area
06_4-Hydroxyphenylpyruvic acid
Y = 2059.0017X + 33038.0195
R^2: 0.999, weight: 1/X^1
0
1
2
3
4
5
Concentration
×10^3

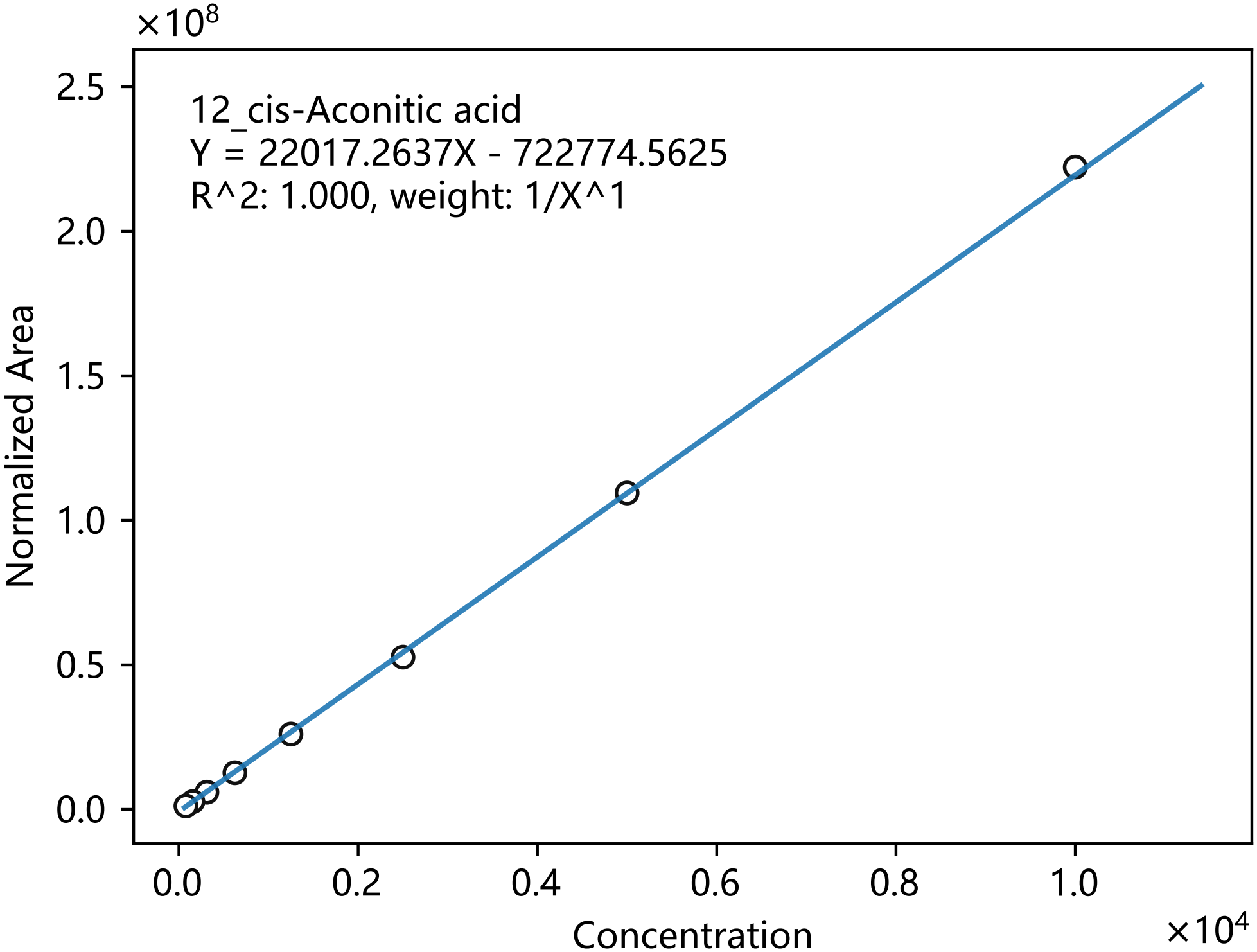

×10^8
07_6-Phosphogluconic acid
Y = -0.0624X^2 + 19510.1250X - 489873.3125
R^2: 1.000, weight: 1/X^1
Normalized Area
8
6
4
2
0
0
1
2
3
4
5
Concentration
×10^4

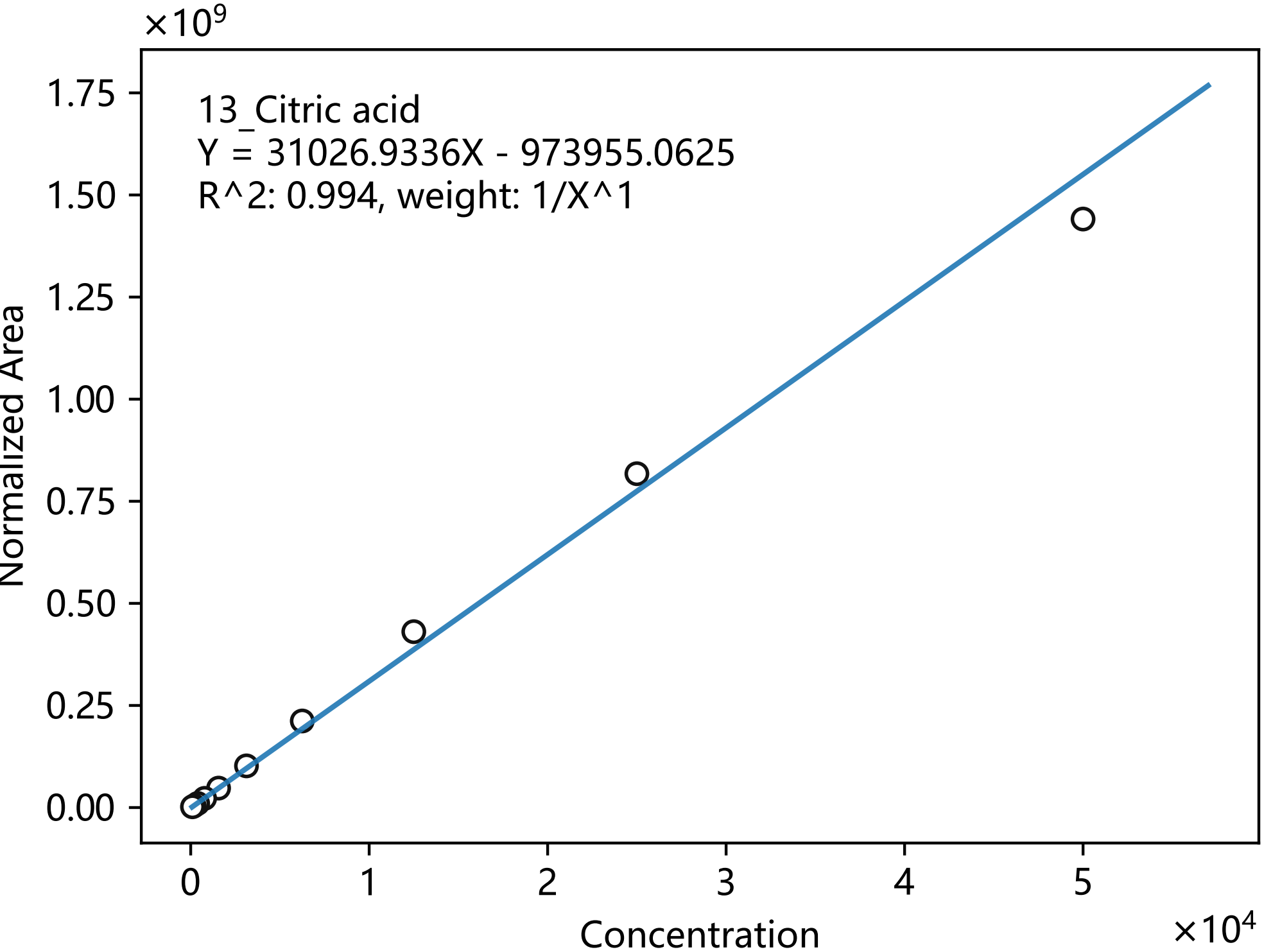

×10^7
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Normalized Area
08_Adenosine diphosphate
Y = -0.0806X^2 + 3950.6978X - 7161.1665
R^2: 0.998, weight: 1/X^1
0.0
0.2
0.4
0.6
0.8
1.0
Concentration
×10^4

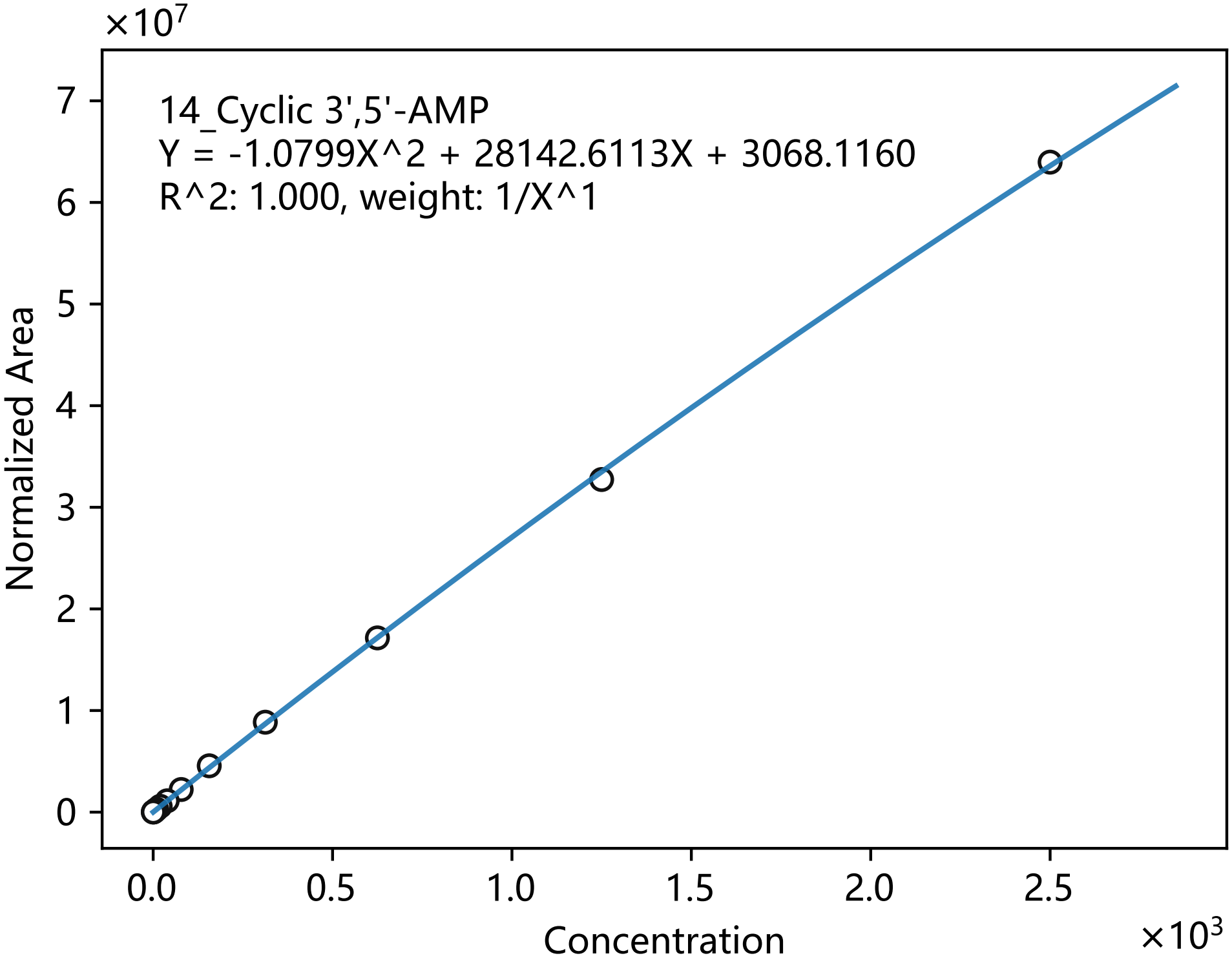

×10^6
09_Adenosine triphosphate
Y = 0.0279X^2 + 201.9858X + 902.0611
R^2: 1.000, weight: 1/X^1
2.0
1.5
1.0
0.5
0.0
Normalized Area
0
1
2
3
4
5
Concentration
×10^3

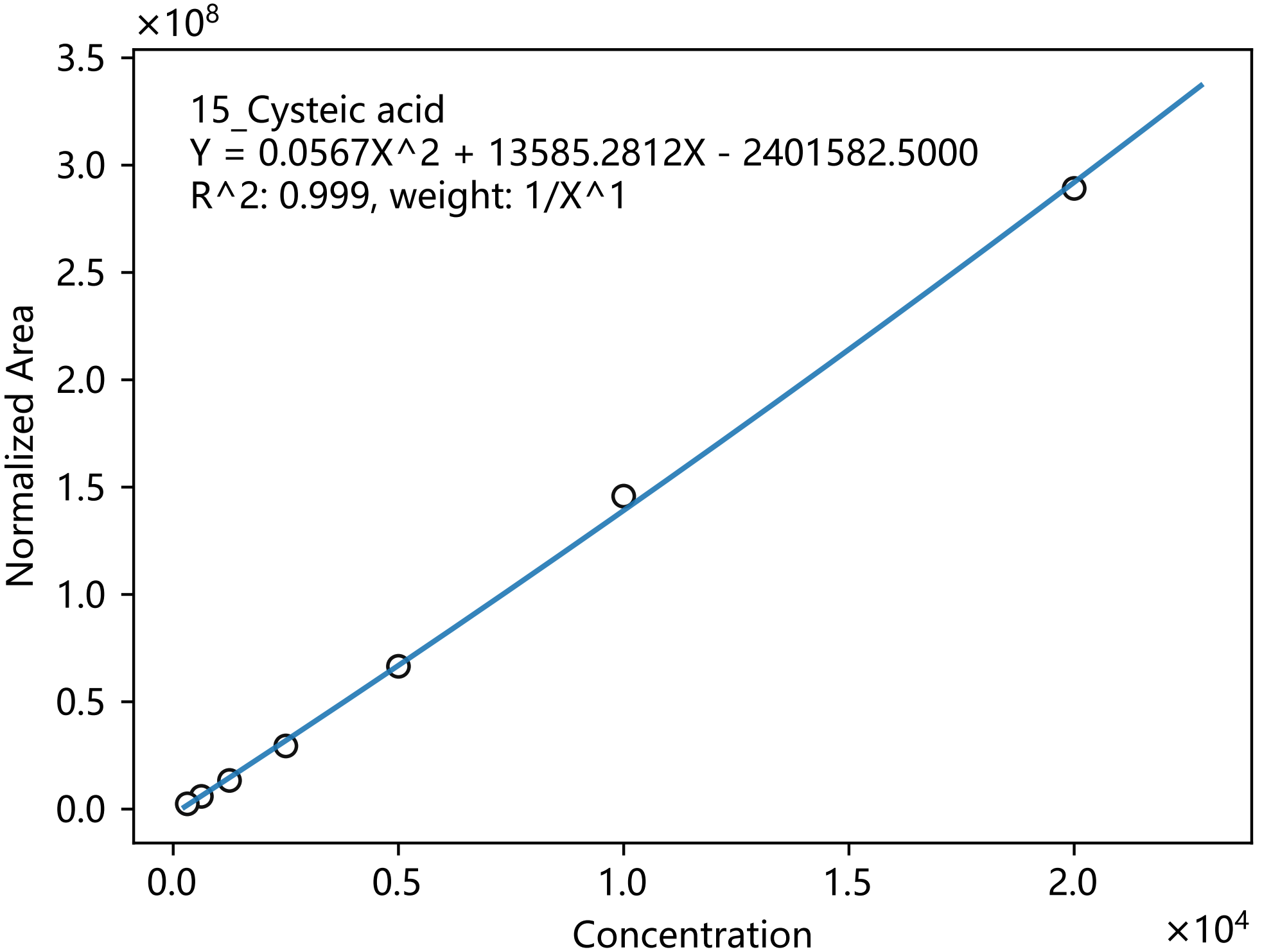

×10^7
10_alpha-Ketoglutaric acid
Y = 1.6256X^2 + 10522.9766X - 90075.9219
R^2: 0.999, weight: 1/X^1
Normalized Area
0
1
2
3
4
0.0
0.5
1.0
1.5
2.0
2.5
Concentration
×10^3

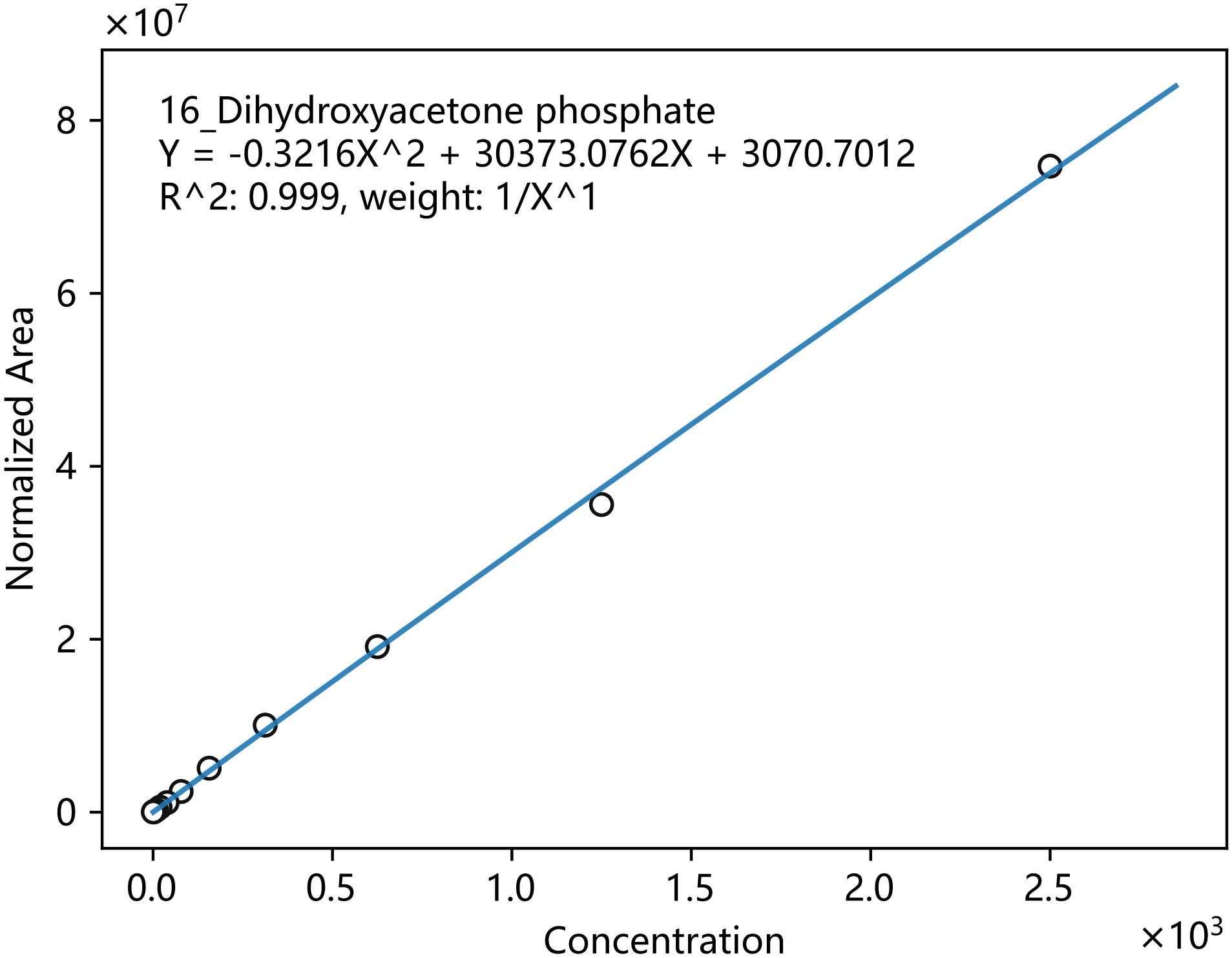

×10^7
11_alpha-Ketoisovaleric acid
Y = 5851.3804X - 115574.0078
R^2: 0.997, weight: 1/X^1
Normalized Area
6
5
4
3
2
1
0
0.0
0.2
0.4
0.6
0.8
1.0
Concentration
×10^4

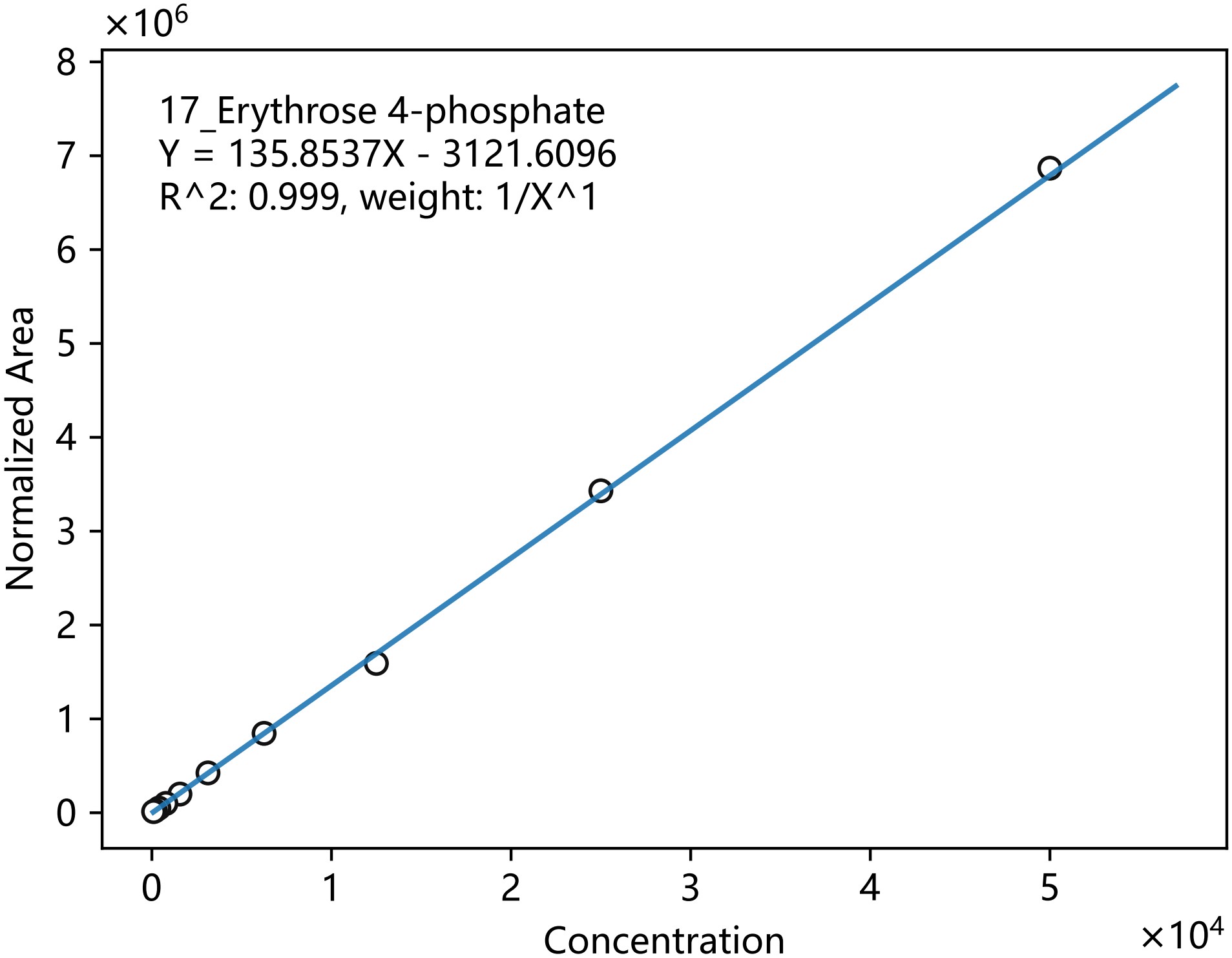

×10^8
2.5
2.0
1.5
1.0
0.5
0.0
Normalized Area
12_cis-Aconitic acid
Y = 22017.2637X - 722774.5625
R^2: 1.000, weight: 1/X^1
0.0
0.2
0.4
0.6
0.8
1.0
Concentration
×10^4

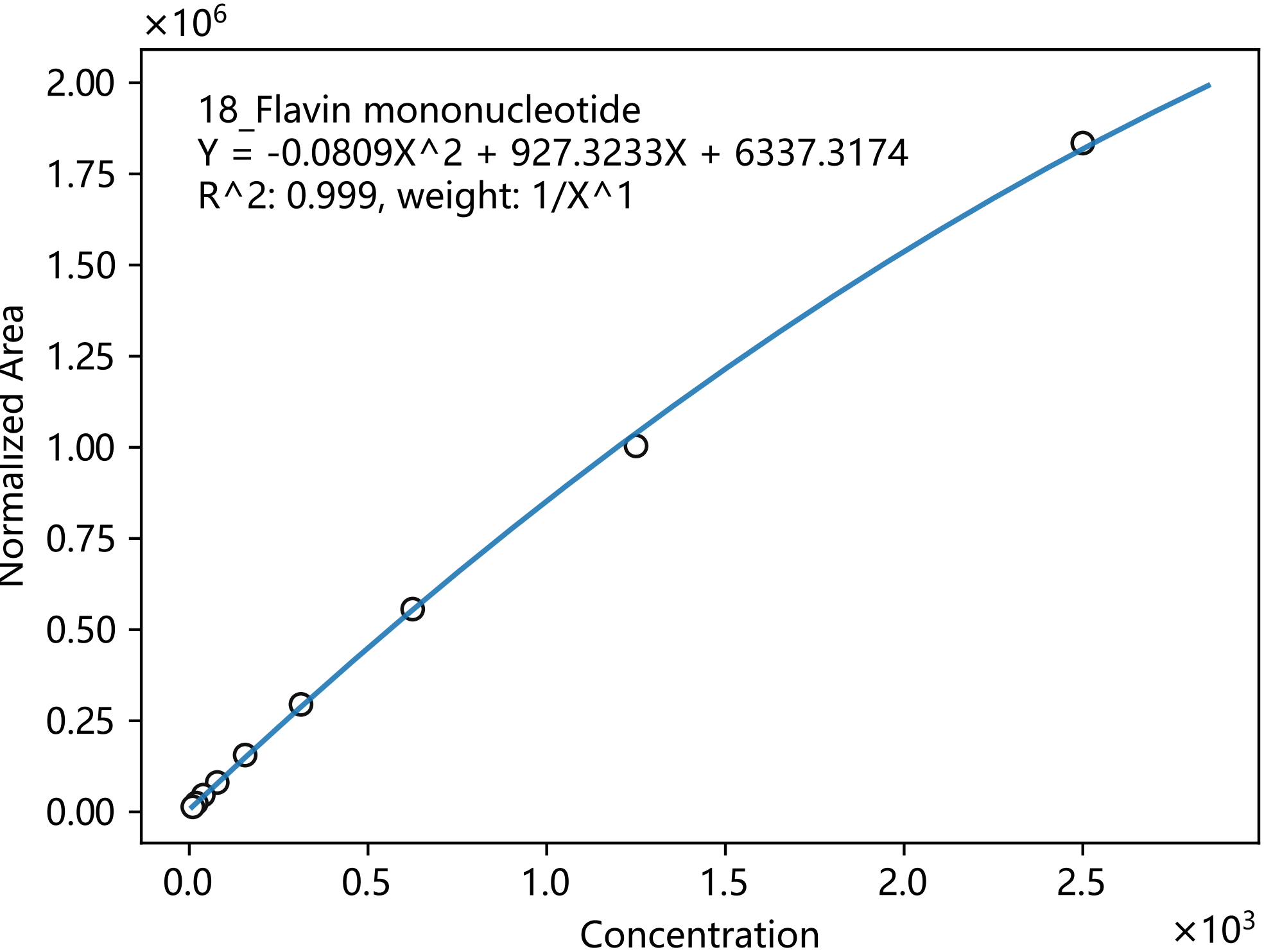

×10^9
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
Normalized Area
13_Citric acid
Y = 31026.9336X - 973955.0625
R^2: 0.994, weight: 1/X^1
0
1
2
3
4
5
Concentration
×10^4

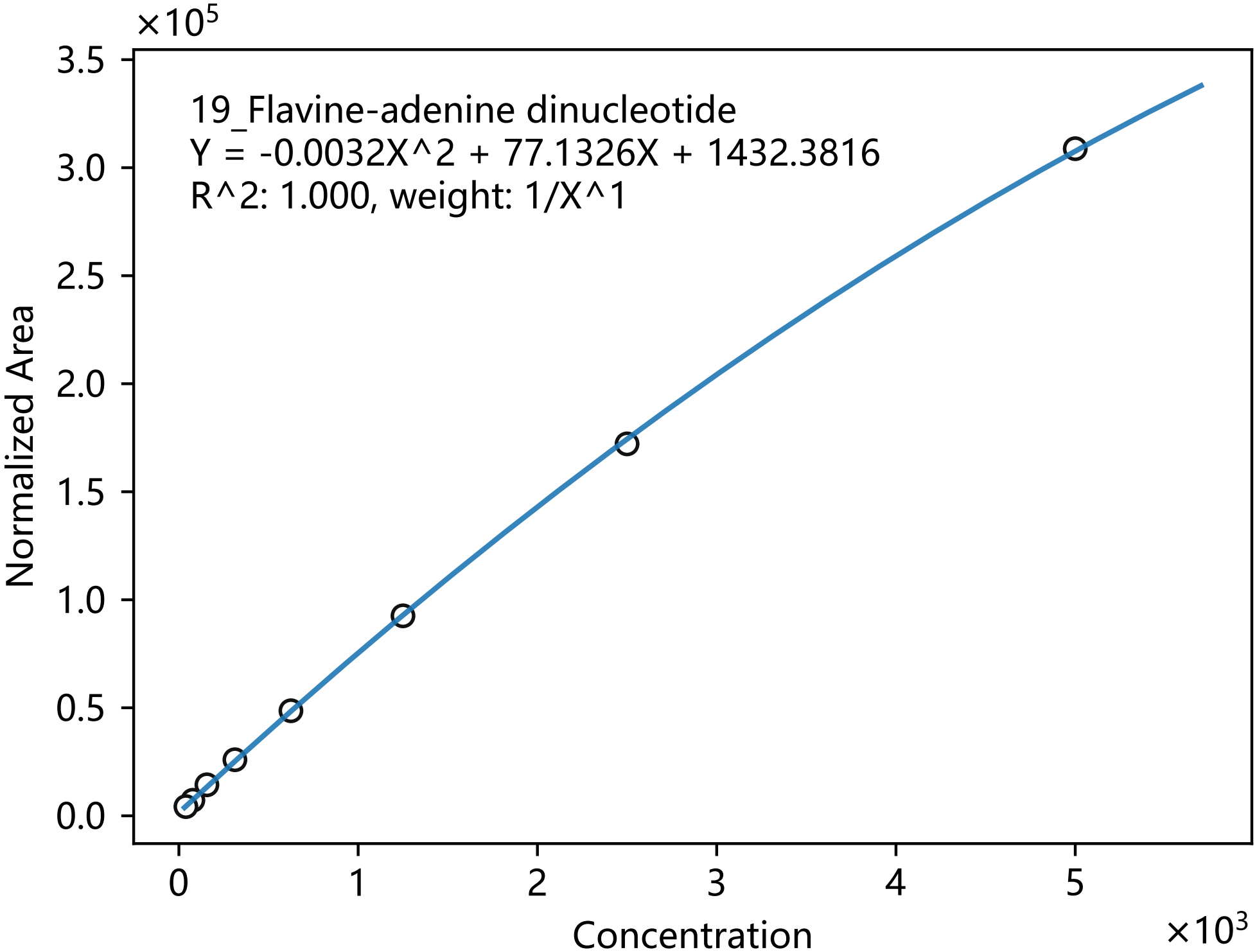

×10^7
14_Cyclic 3',5'-AMP
Y = -1.0799X^2 + 28142.6113X + 3068.1160
R^2: 1.000, weight: 1/X^1
Normalized Area
7
6
5
4
3
2
1
0
0.0
0.5
1.0
1.5
2.0
2.5
Concentration
×10^3

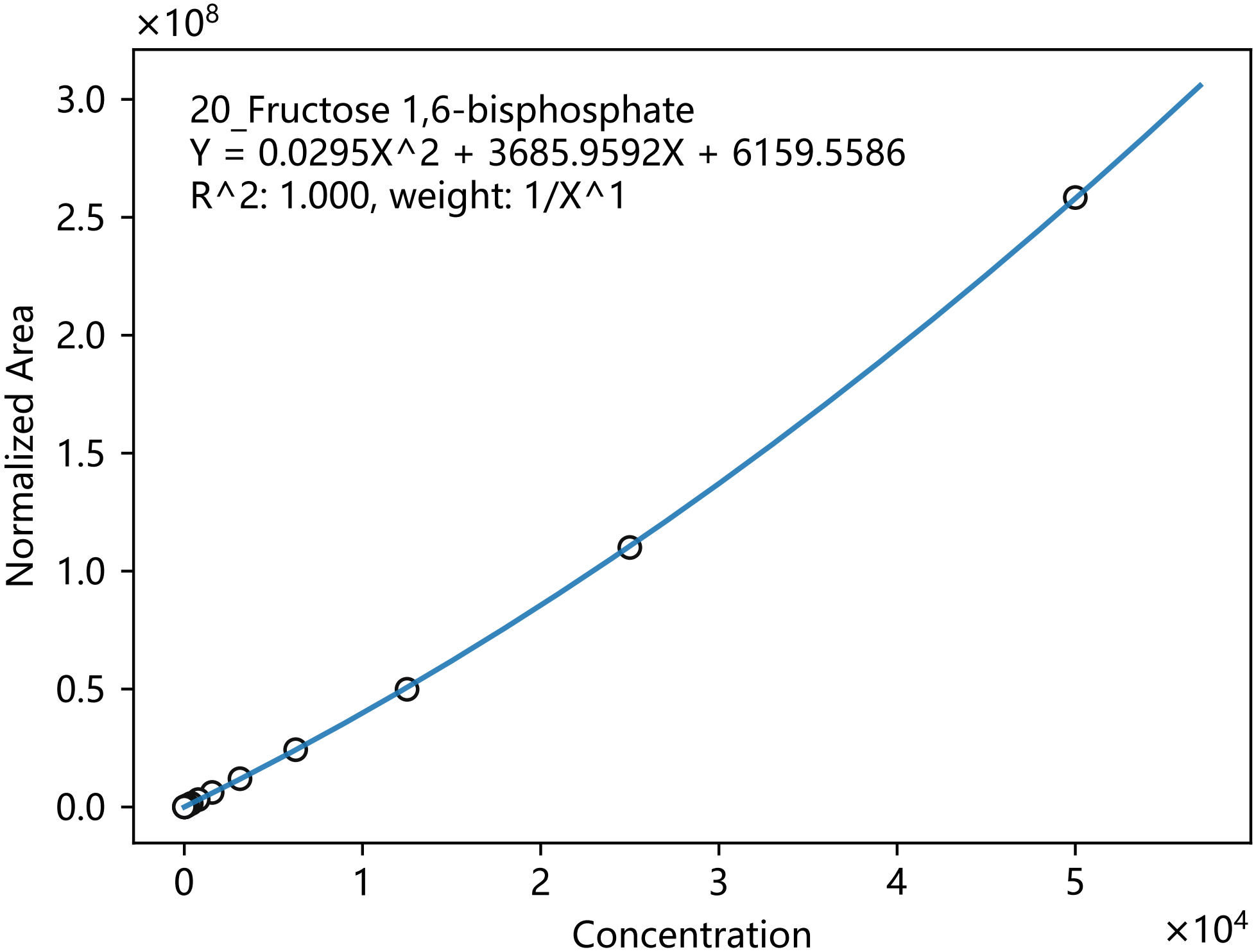

×10^8
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Normalized Area
15_Cysteic acid
Y = 0.0567X^2 + 13585.2812X - 2401582.5000
R^2: 0.999, weight: 1/X^1
0.0
0.5
1.0
1.5
2.0
Concentration
×10^4

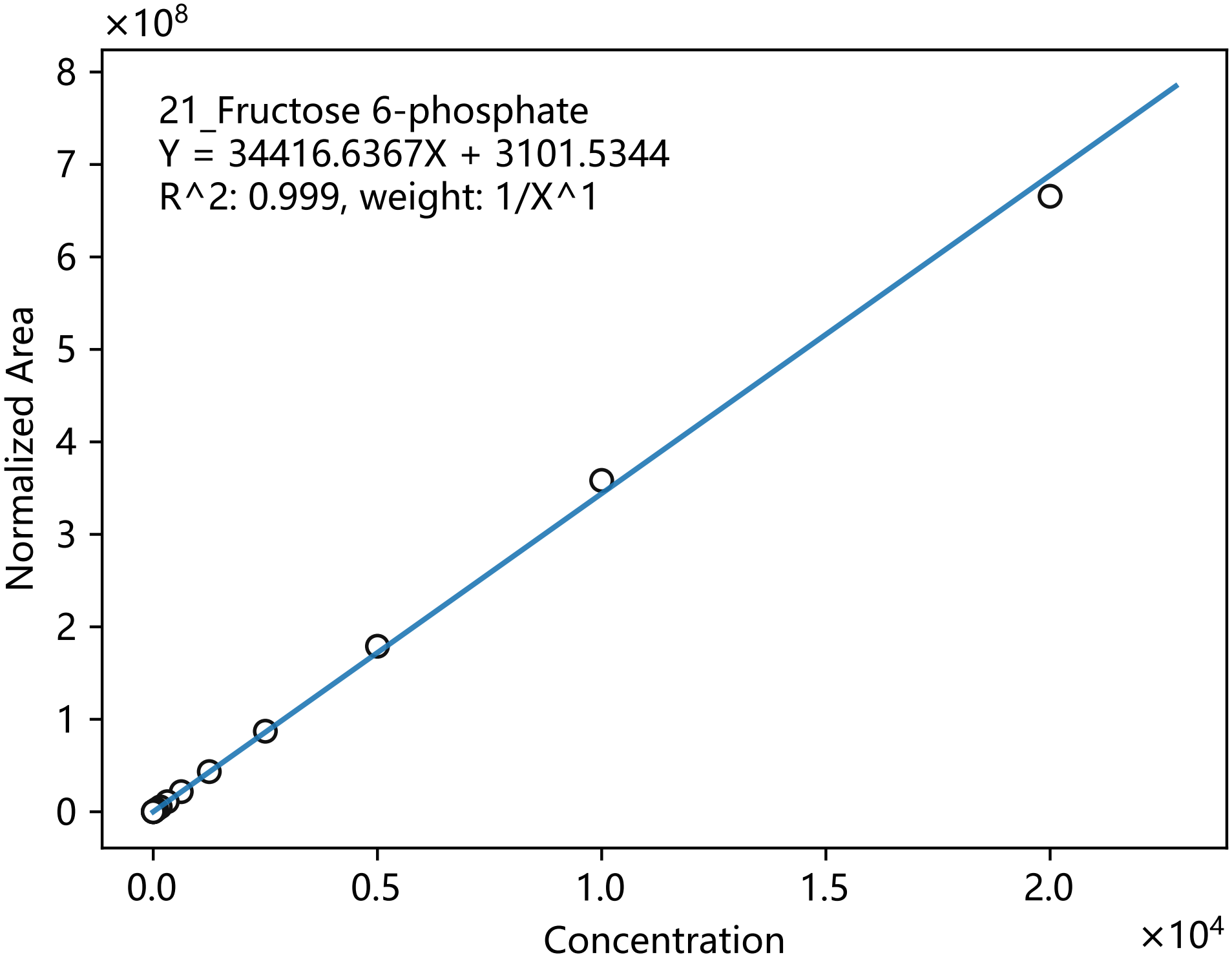

×10^7
16_Dihydroxyacetone phosphate
Y = -0.3216X^2 + 30373.0762X + 3070.7012
R^2: 0.999, weight: 1/X^1
Normalized Area
8
6
4
2
0
0.0
0.5
1.0
1.5
2.0
2.5
Concentration
×10^3

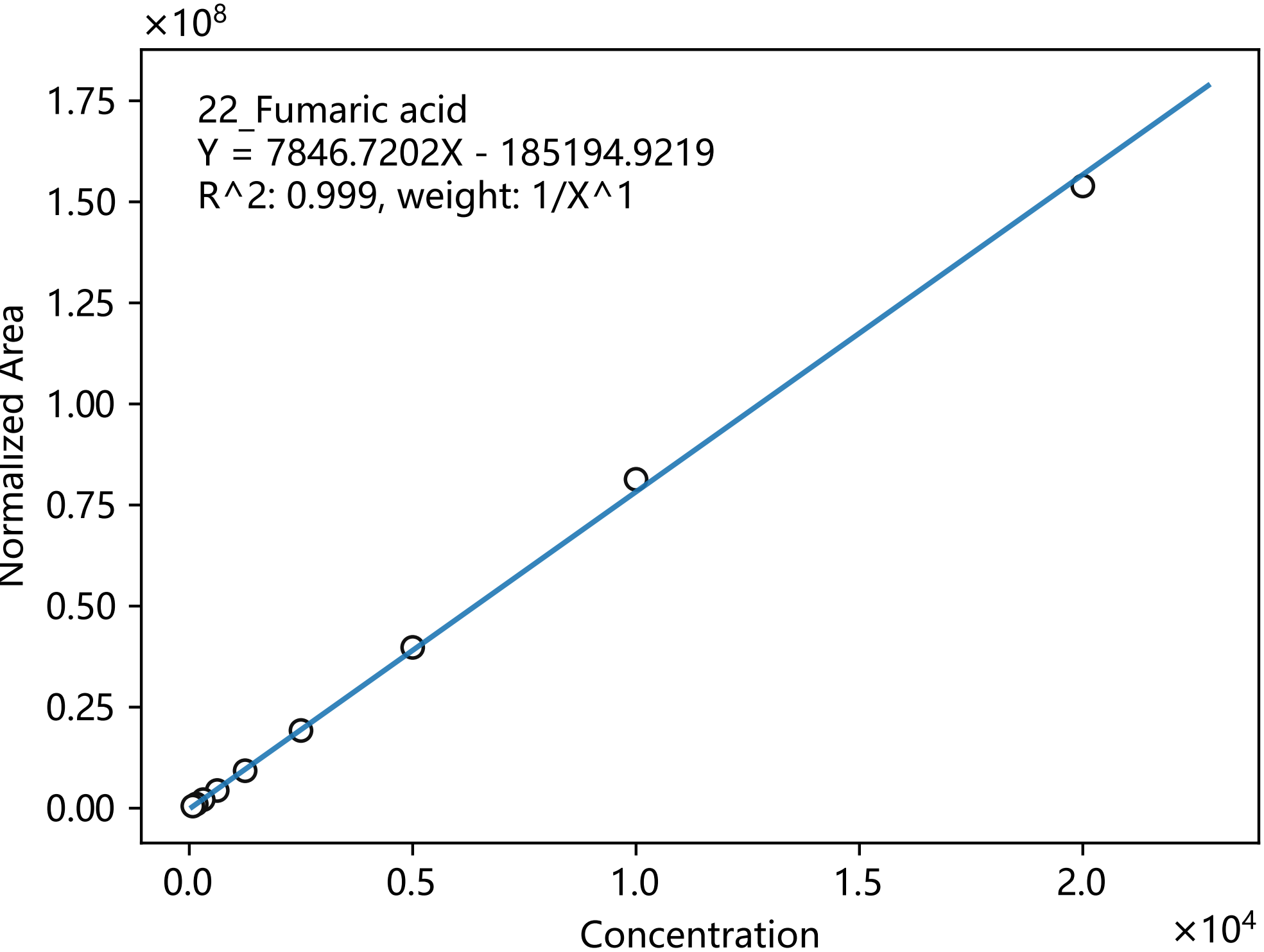

×10^6
8
7
6
5
4
3
2
1
0
17_Erythrose 4-phosphate
Y = 135.8537X - 3121.6096
R^2: 0.999, weight: 1/X^1
Normalized Area
0
1
2
3
4
5
Concentration
×10^4

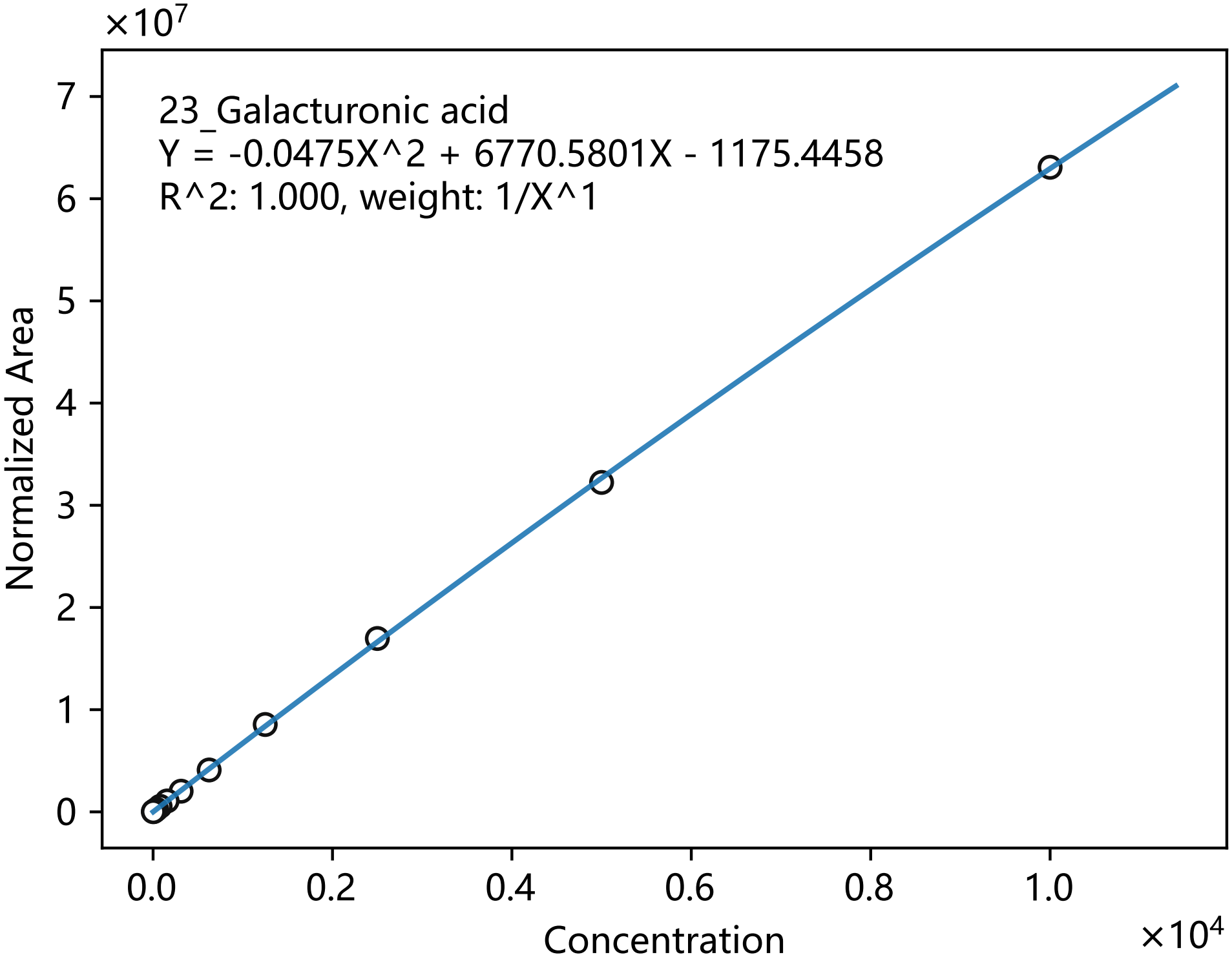

×10^6
2.00
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
Normalized Area
18_Flavin mononucleotide
Y = -0.0809X^2 + 927.3233X + 6337.3174
R^2: 0.999, weight: 1/X^1
0.0
0.5
1.0
1.5
2.0
2.5
Concentration
×10^3

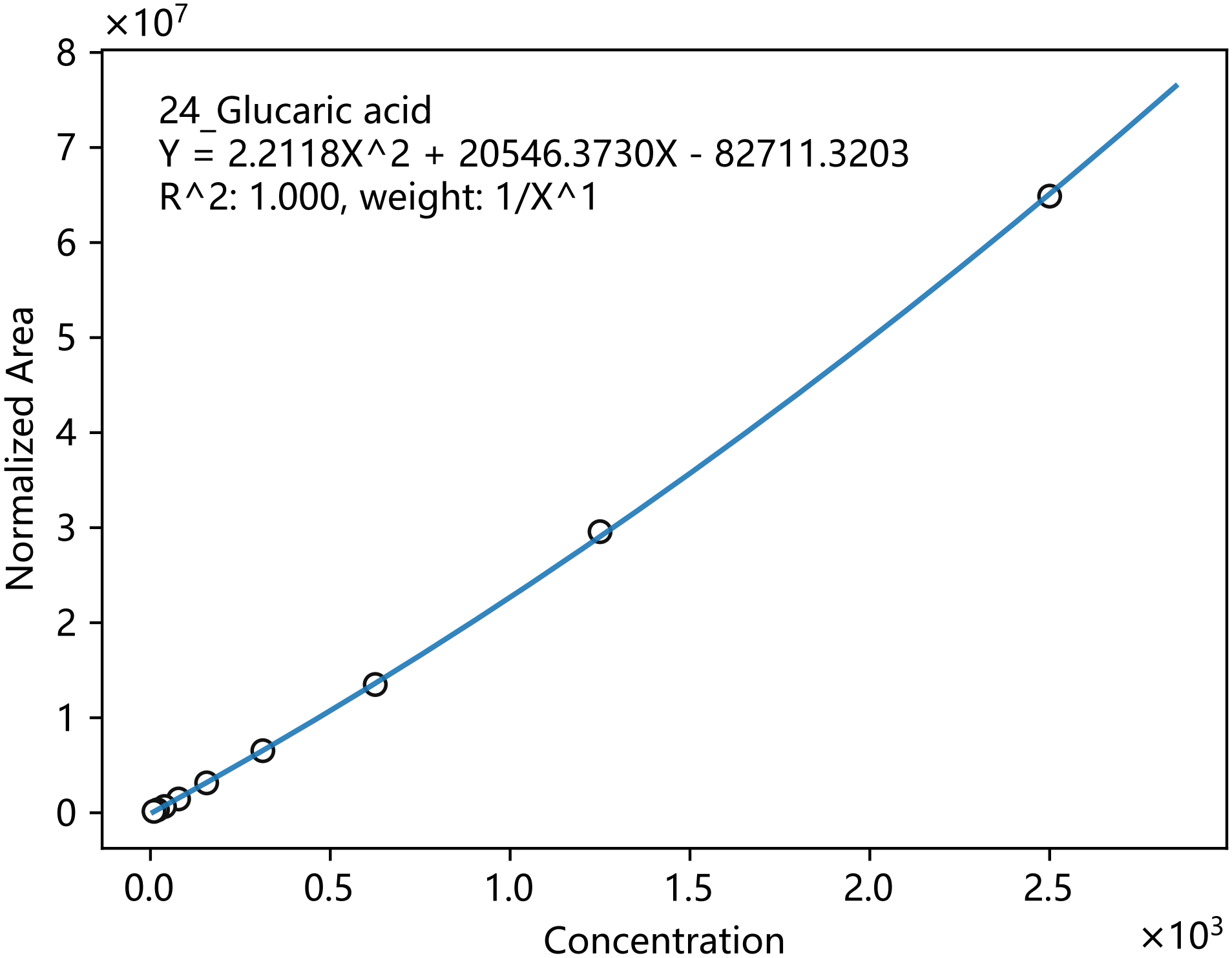

×10^5
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Normalized Area
19_Flavine-adenine dinucleotide
Y = -0.0032X^2 + 77.1326X + 1432.3816
R^2: 1.000, weight: 1/X^1
0
1
2
3
4
5
Concentration
×10^3

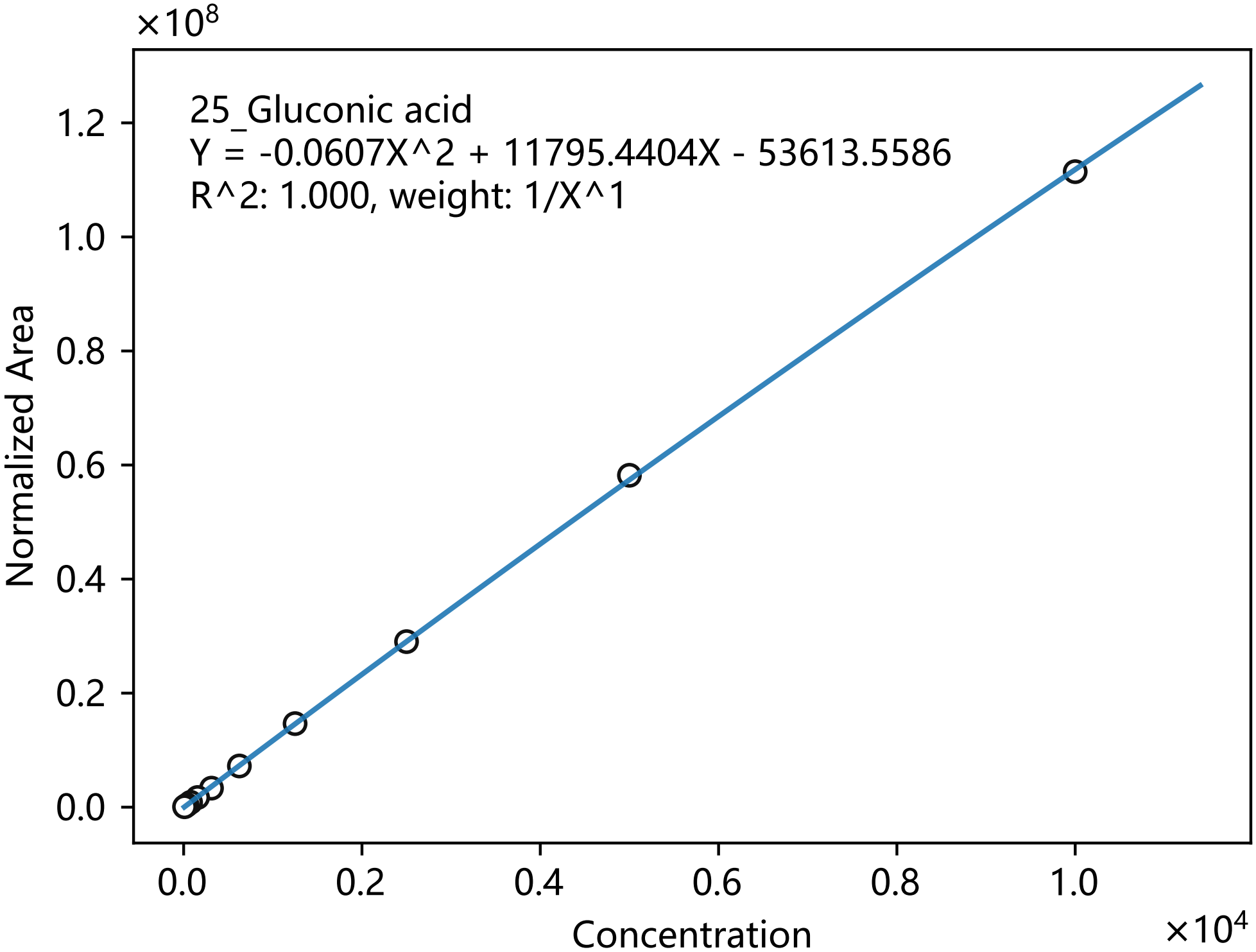

×10^8
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Normalized Area
20_Fructose 1,6-bisphosphate
Y = 0.0295X^2 + 3685.9592X + 6159.5586
R^2: 1.000, weight: 1/X^1
0
1
2
3
4
5
Concentration
×10^4

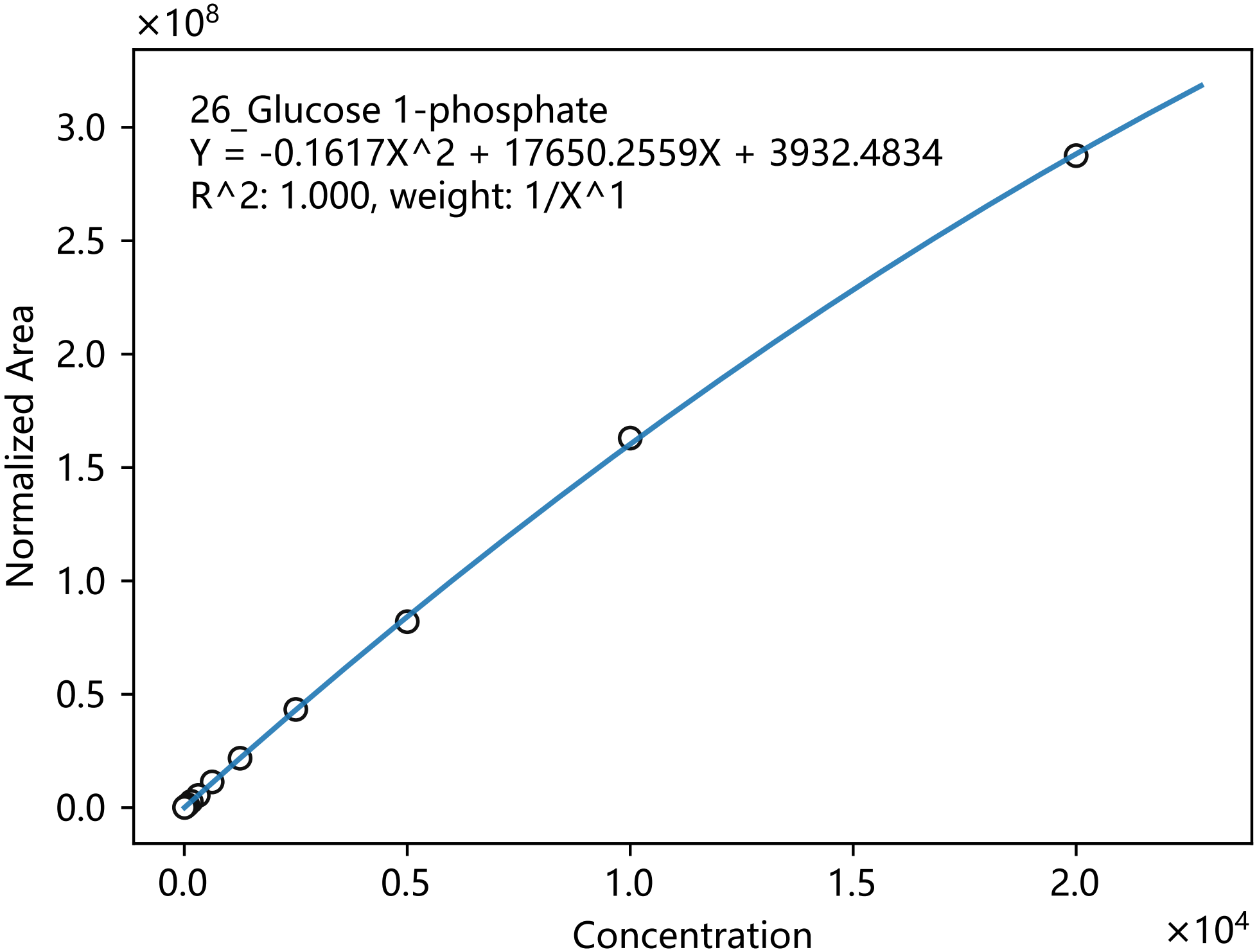

×10^8
8
7
6
5
4
3
2
1
0
21_Fructose 6-phosphate
Y = 34416.6367X + 3101.5344
R^2: 0.999, weight: 1/X^1
Normalized Area
0.0
0.5
1.0
1.5
2.0
Concentration
×10^4

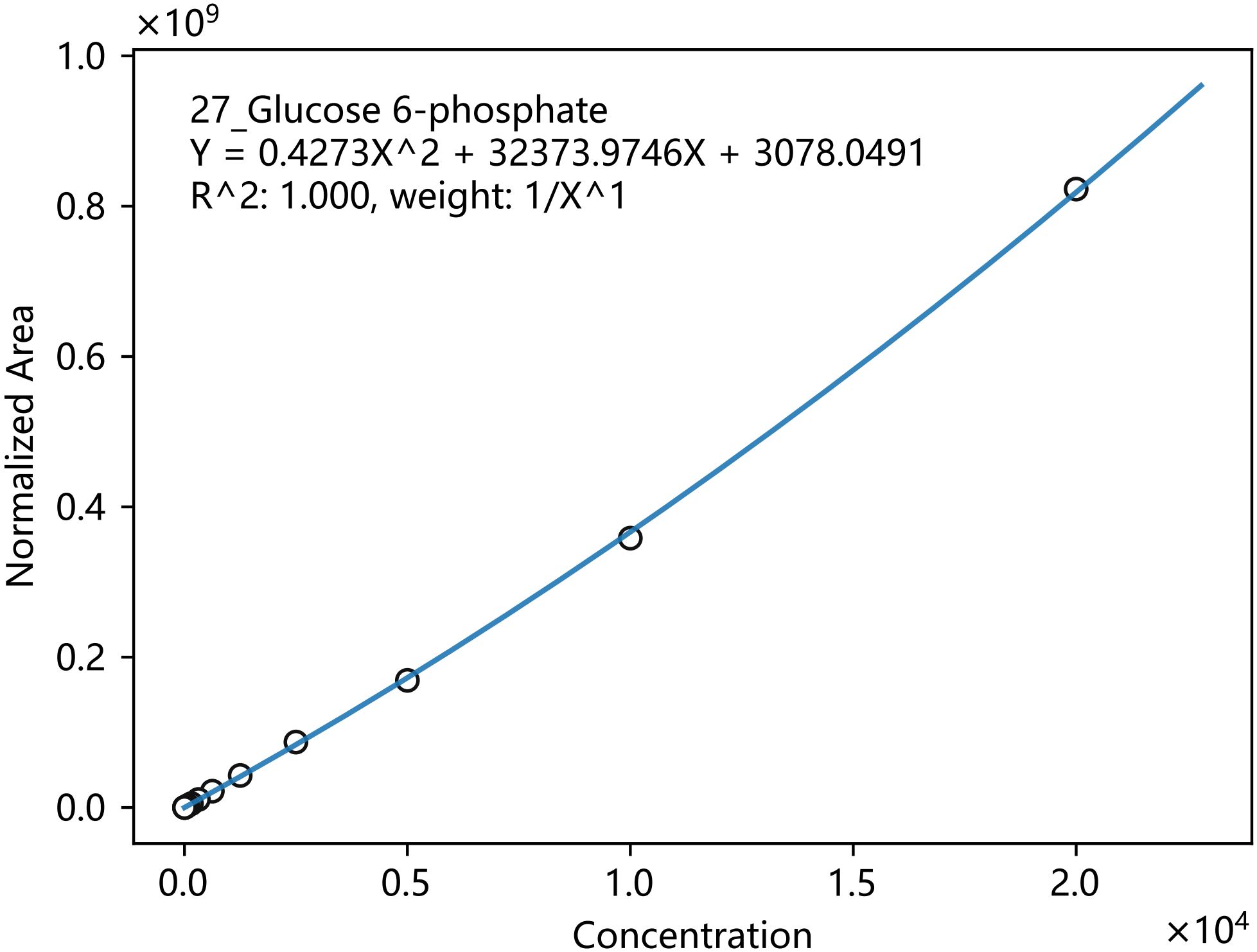

×10^8
22_Fumaric acid
Y = 7846.7202X - 185194.9219
R^2: 0.999, weight: 1/X^1
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
Normalized Area
0.0
0.5
1.0
1.5
2.0
Concentration
×10^4

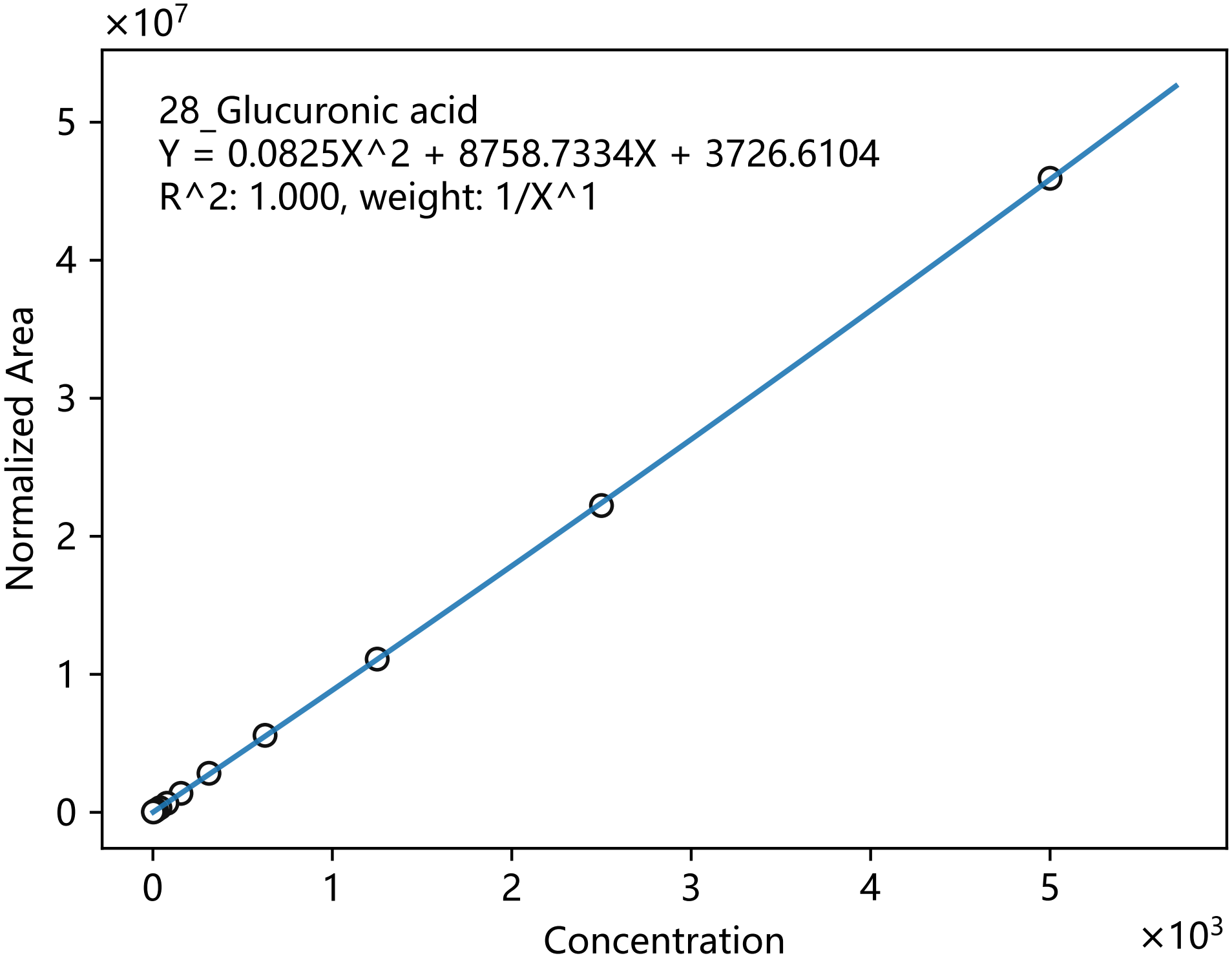

×10^7
23_Galacturonic acid
Y = -0.0475X^2 + 6770.5801X - 1175.4458
R^2: 1.000, weight: 1/X^1
Normalized Area
7
6
5
4
3
2
1
0
0.0
0.2
0.4
0.6
0.8
1.0
Concentration
×10^4

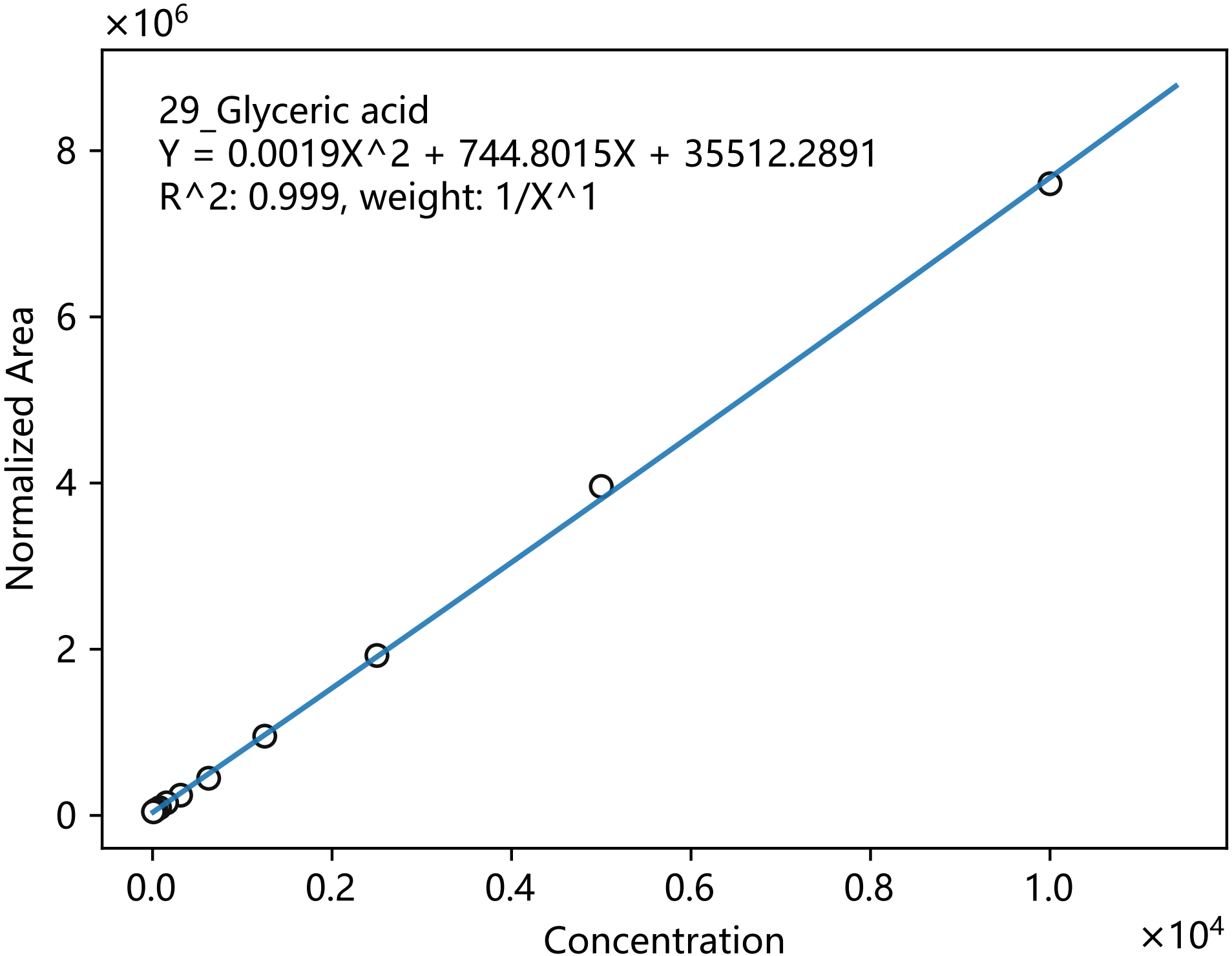

24_Glucaric acid
Y = 2.2118X^2 + 20546.3730X - 82711.3203
R^2: 1.000, weight: 1/X^1
×10^7
8
7
6
5
4
3
2
1
0
Normalized Area
0.0
0.5
1.0
1.5
2.0
2.5
Concentration
×10^3

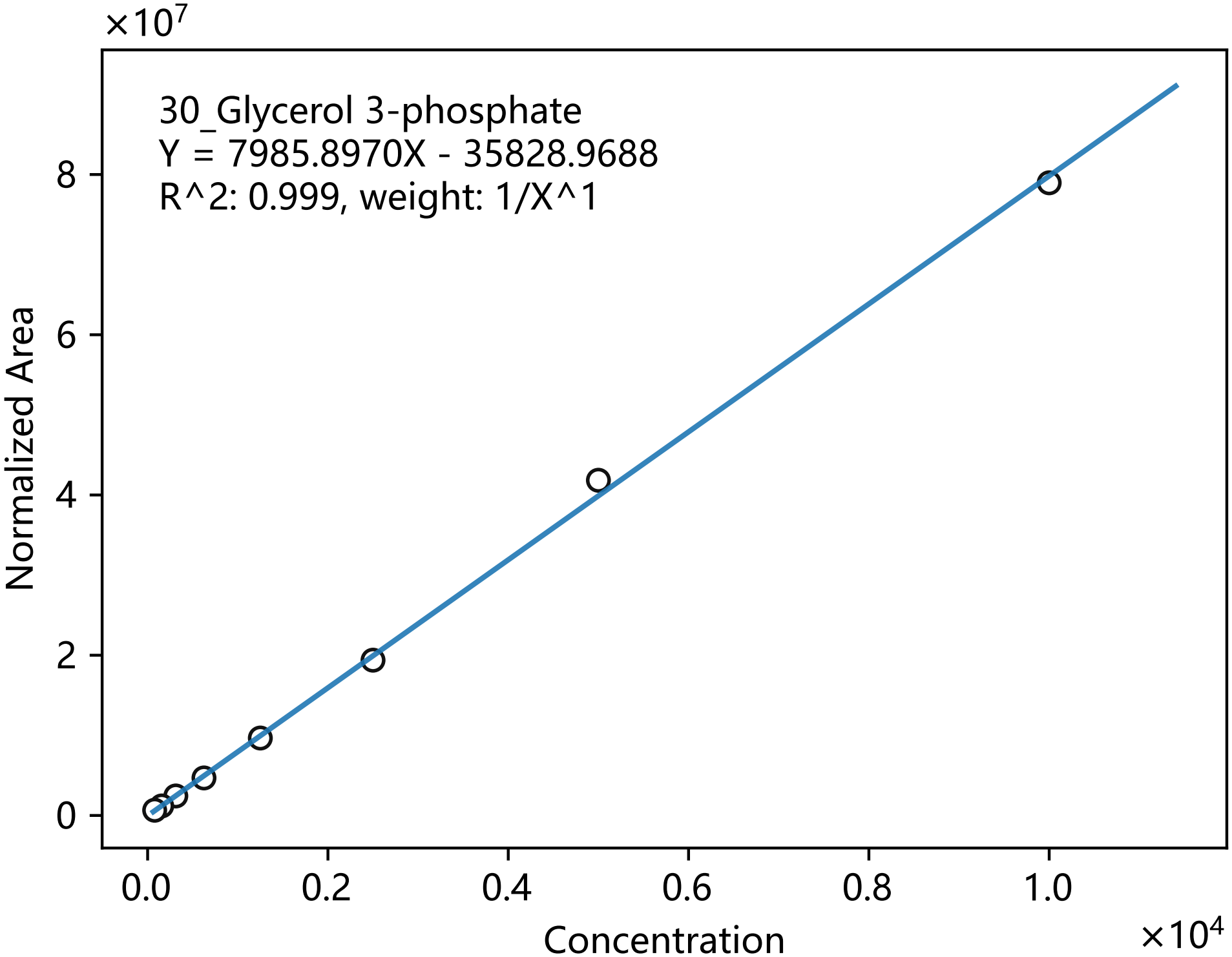

×10^8
25_Gluconic acid
Y = -0.0607X^2 + 11795.4404X - 53613.5586
R^2: 1.000, weight: 1/X^1
Normalized Area
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
Concentration
×10^4

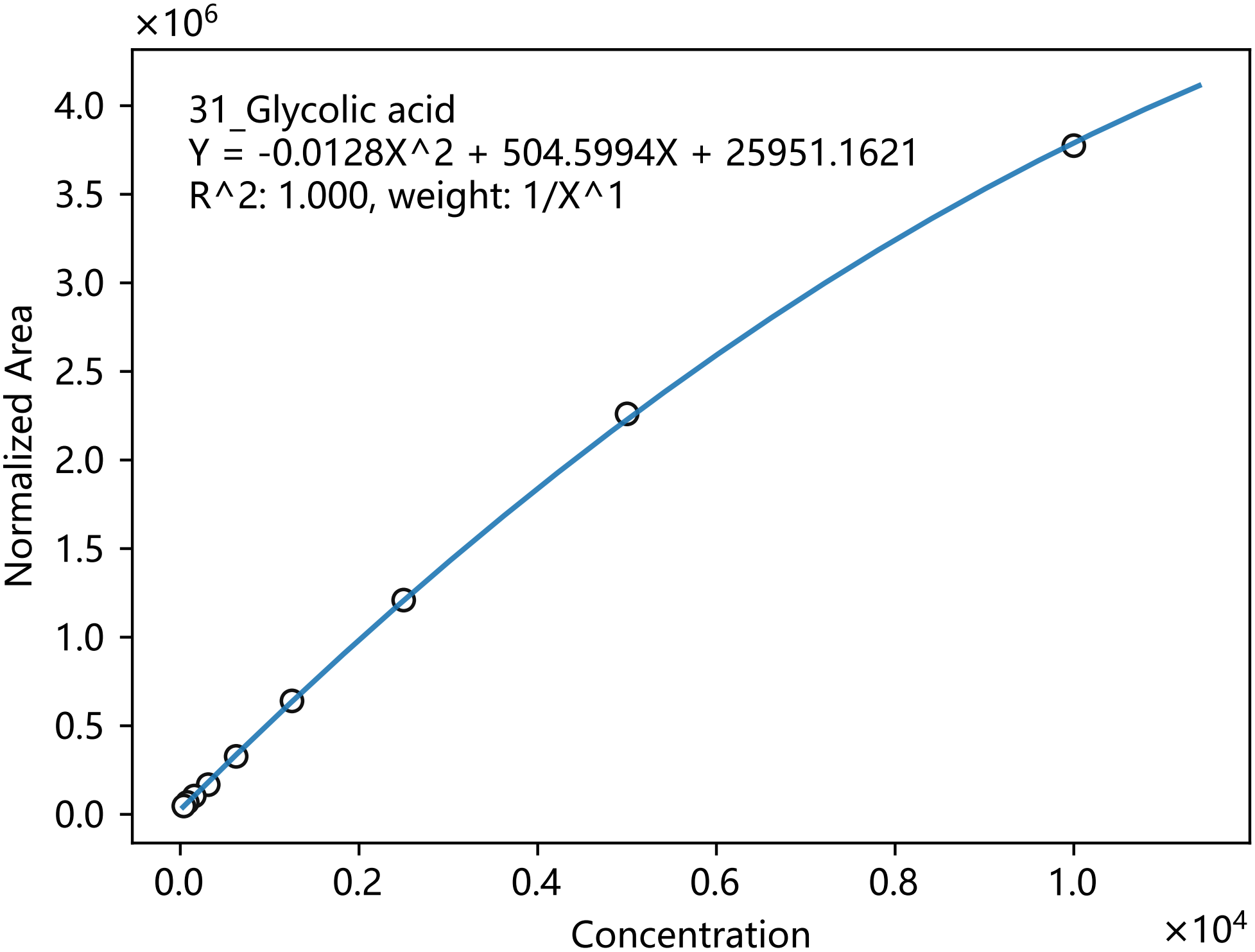

×10^8
26_Glucose 1-phosphate
Y = -0.1617X^2 + 17650.2559X + 3932.4834
R^2: 1.000, weight: 1/X^1
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Normalized Area
0.0
0.5
1.0
1.5
2.0
Concentration
×10^4

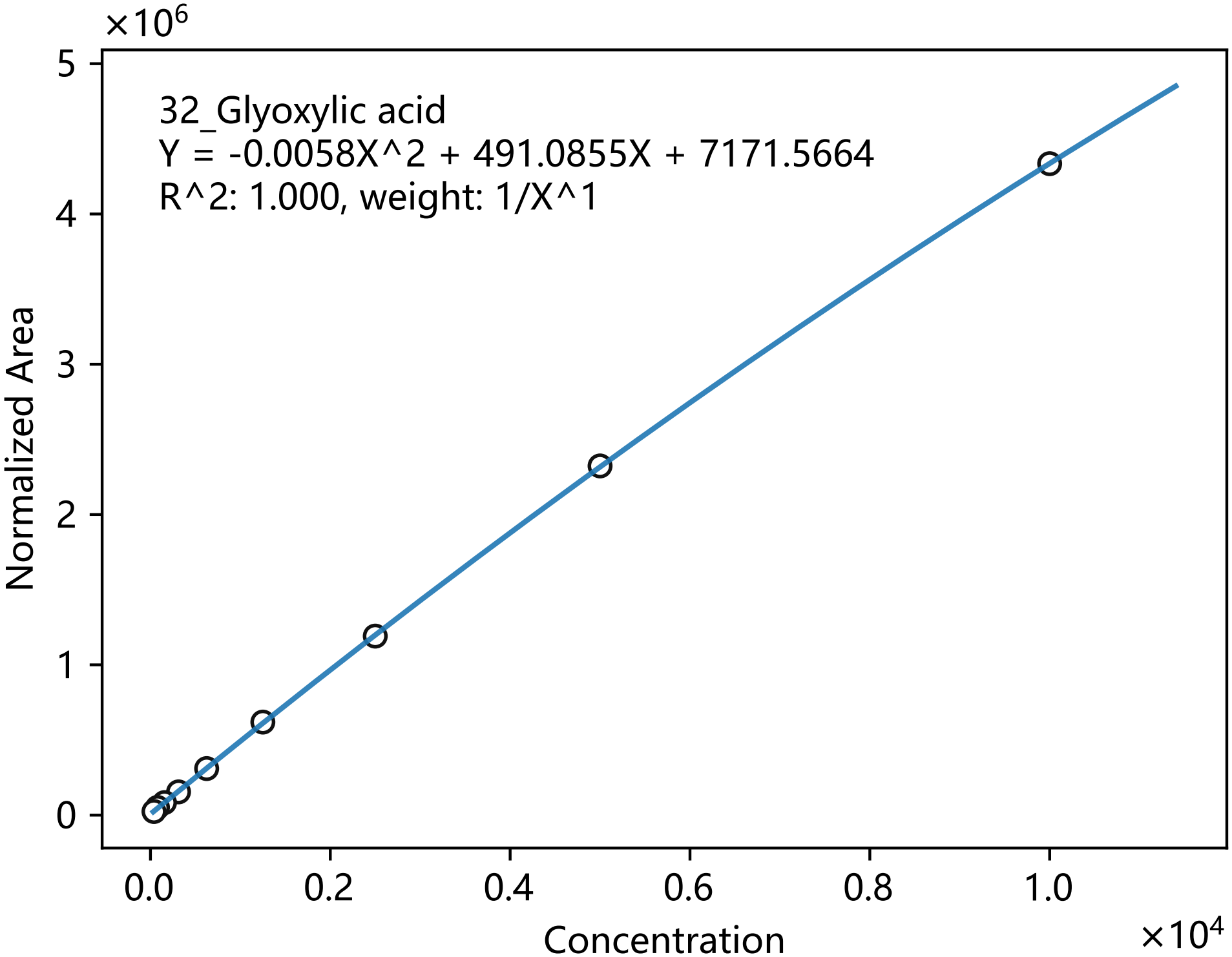

×10^9
1.0
0.8
0.6
0.4
0.2
0.0
Normalized Area
27_Glucose 6-phosphate
Y = 0.4273X^2 + 32373.9746X + 3078.0491
R^2: 1.000, weight: 1/X^1
0.0
0.5
1.0
1.5
2.0
Concentration
×10^4

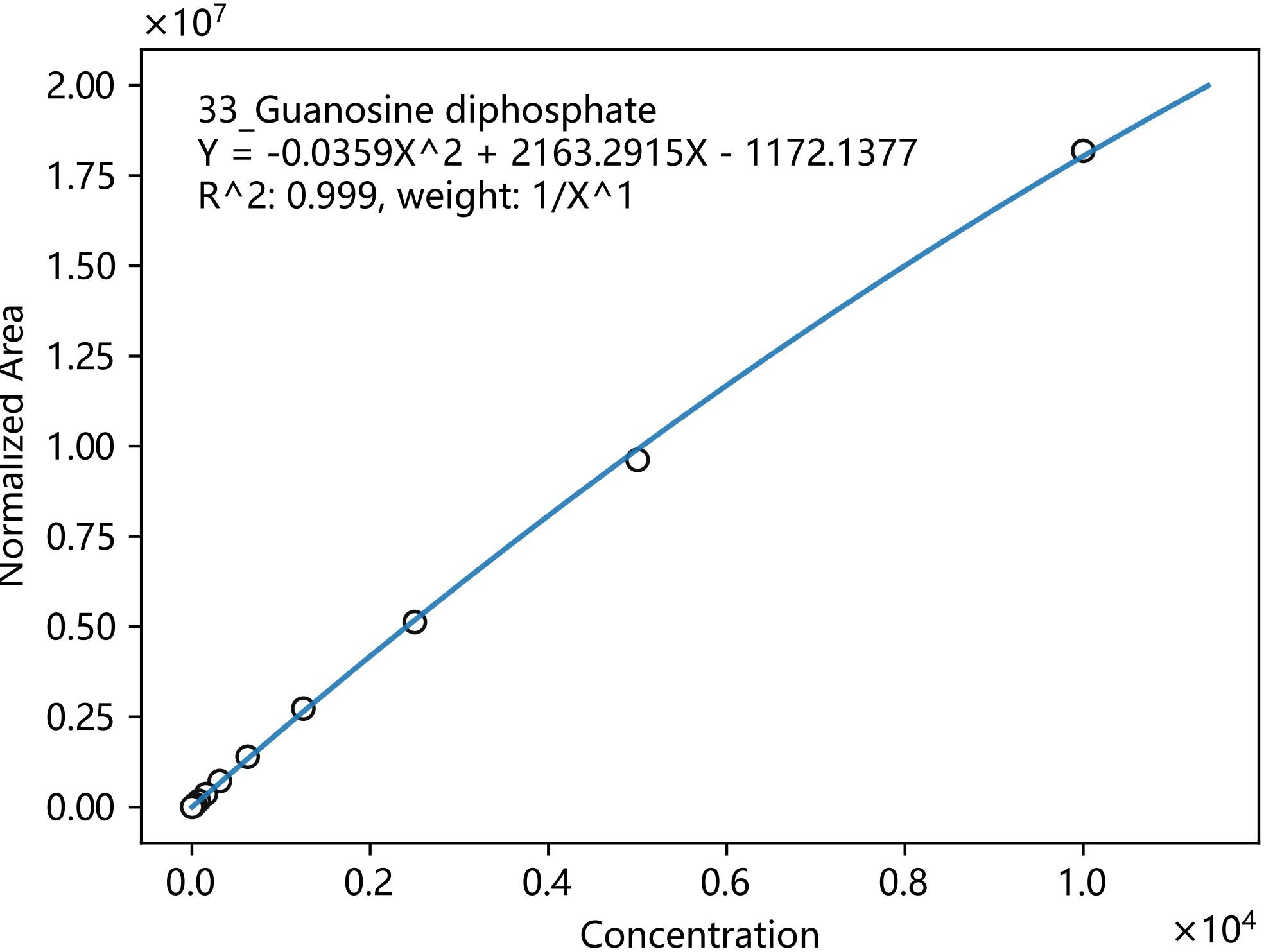

×10^7
28_Glucuronic acid
Y = 0.0825X^2 + 8758.7334X + 3726.6104
R^2: 1.000, weight: 1/X^1
Normalized Area
0
1
2
3
4
5
0
1
2
3
4
5
Concentration
×10^3

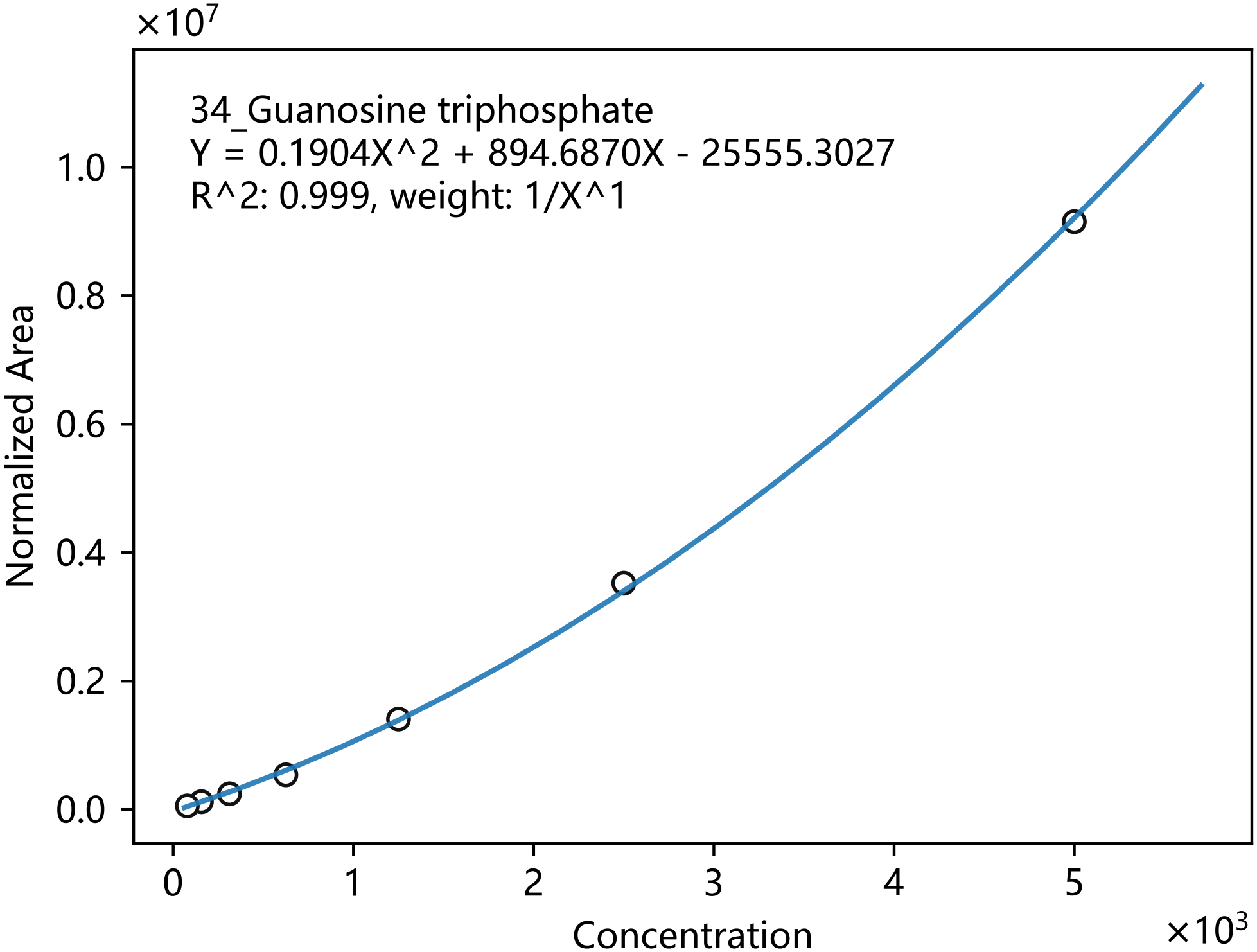

×10^6
29_Glyceric acid
Y = 0.0019X^2 + 744.8015X + 35512.2891
R^2: 0.999, weight: 1/X^1
Normalized Area
8
6
4
2
0
0.0
0.2
0.4
0.6
0.8
1.0
Concentration
×10^4

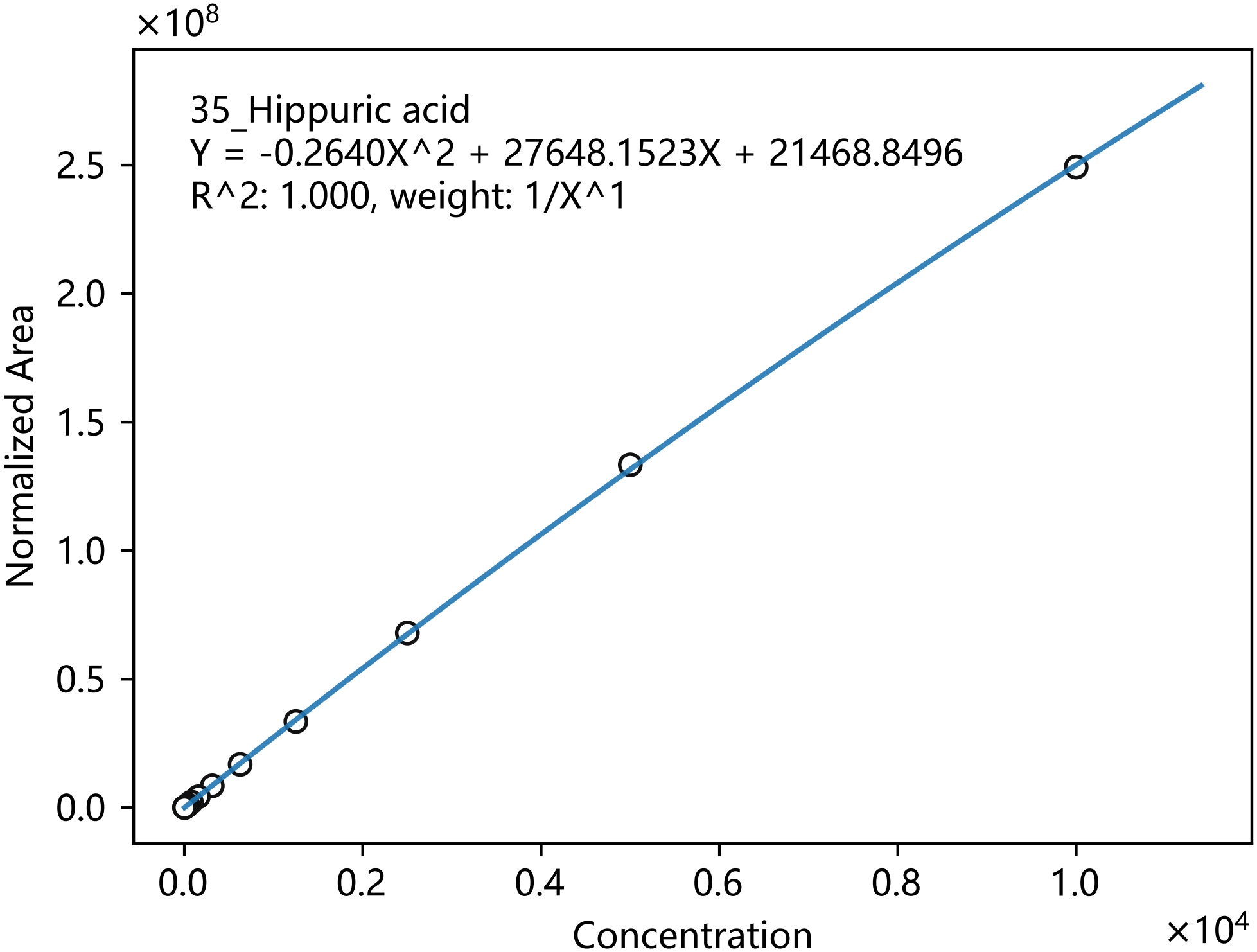

×10^7
30_Glycerol 3-phosphate
Y = 7985.8970X - 35828.9688
R^2: 0.999, weight: 1/X^1
Normalized Area
8
6
4
2
0
0.0
0.2
0.4
0.6
0.8
1.0
Concentration
×10^4

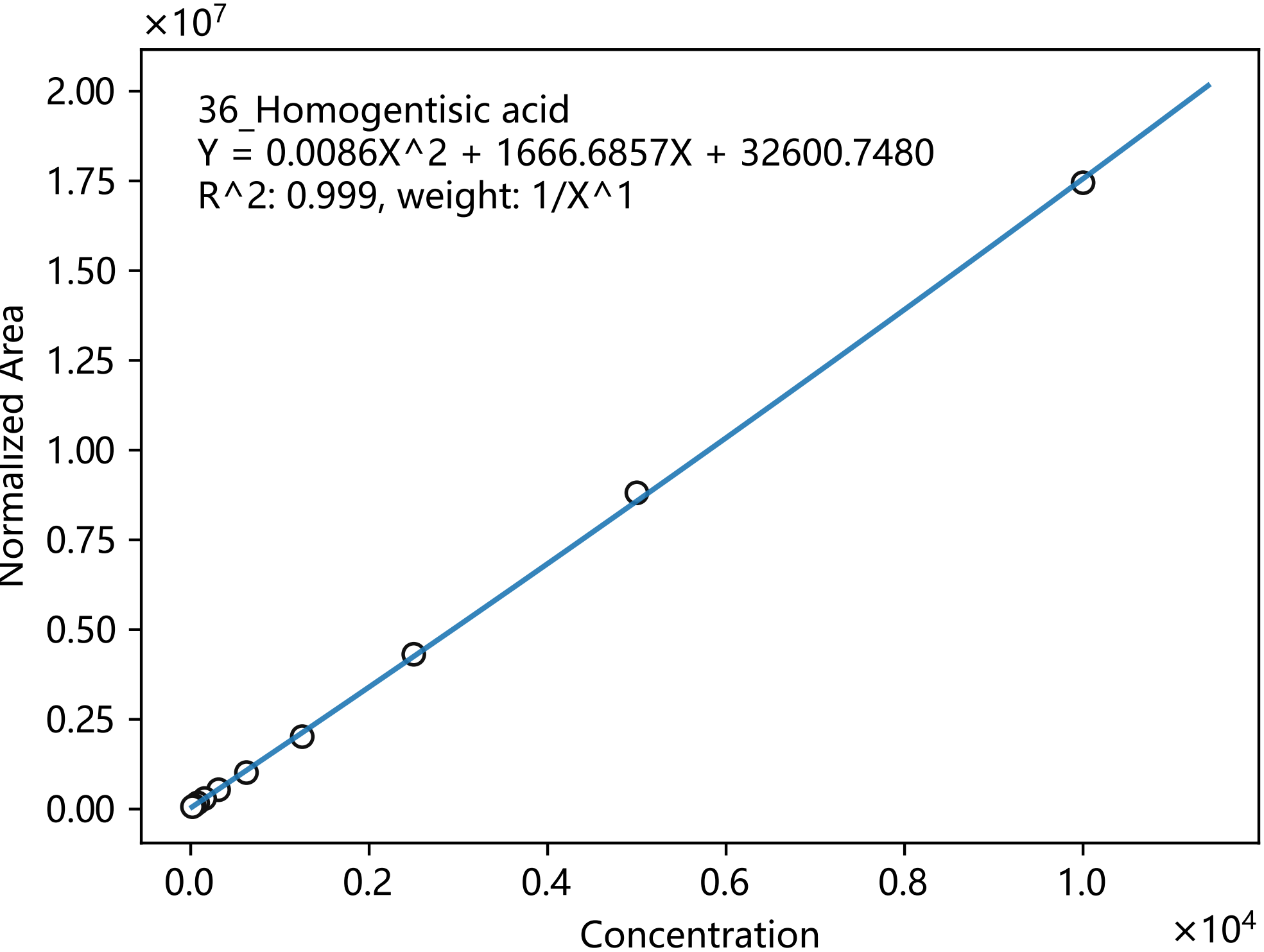

×10^6
31_Glycolic acid
Y = -0.0128X^2 + 504.5994X + 25951.1621
R^2: 1.000, weight: 1/X^1
Normalized Area
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0.0
0.2
0.4
0.6
0.8
1.0
Concentration
×10^4

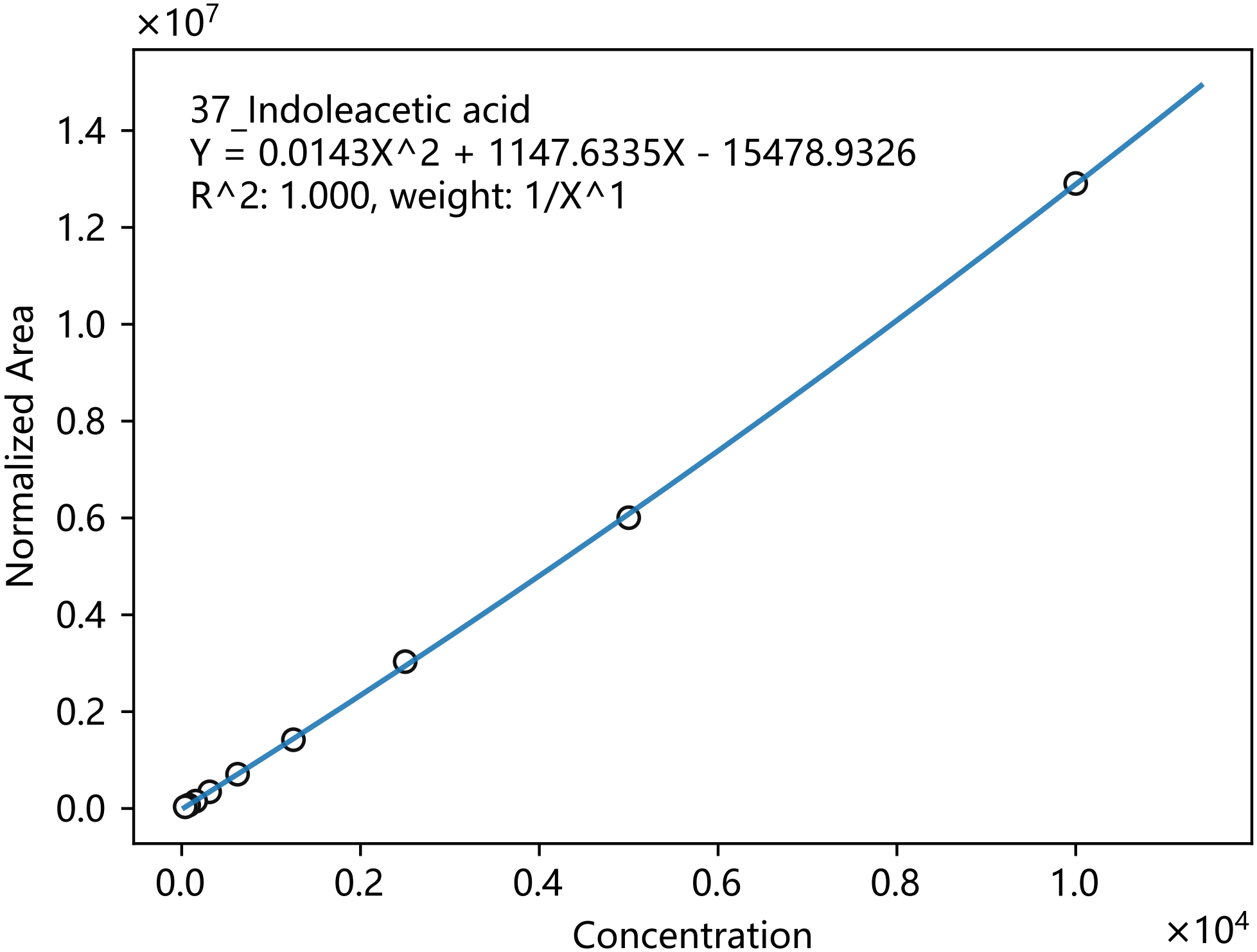

×10^6
5
4
3
2
1
0
32_Glyoxylic acid
Y = -0.0058X^2 + 491.0855X + 7171.5664
R^2: 1.000, weight: 1/X^1
Normalized Area
0.0
0.2
0.4
0.6
0.8
1.0
Concentration
×10^4

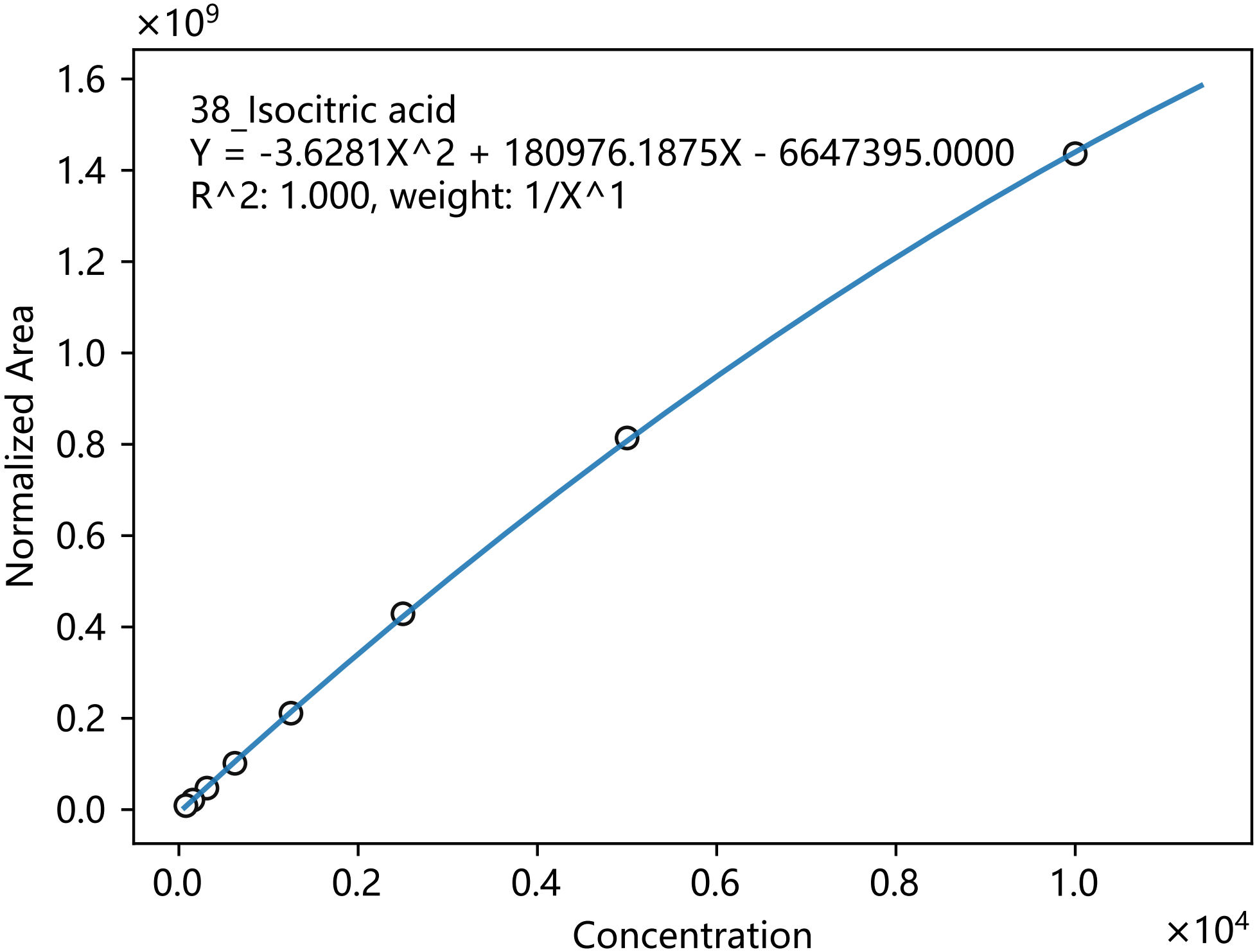

×10^7
2.00
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
Normalized Area
33_Guanosine diphosphate
Y = -0.0359X^2 + 2163.2915X - 1172.1377
R^2: 0.999, weight: 1/X^1
0.0
0.2
0.4
0.6
0.8
1.0
Concentration
×10^4

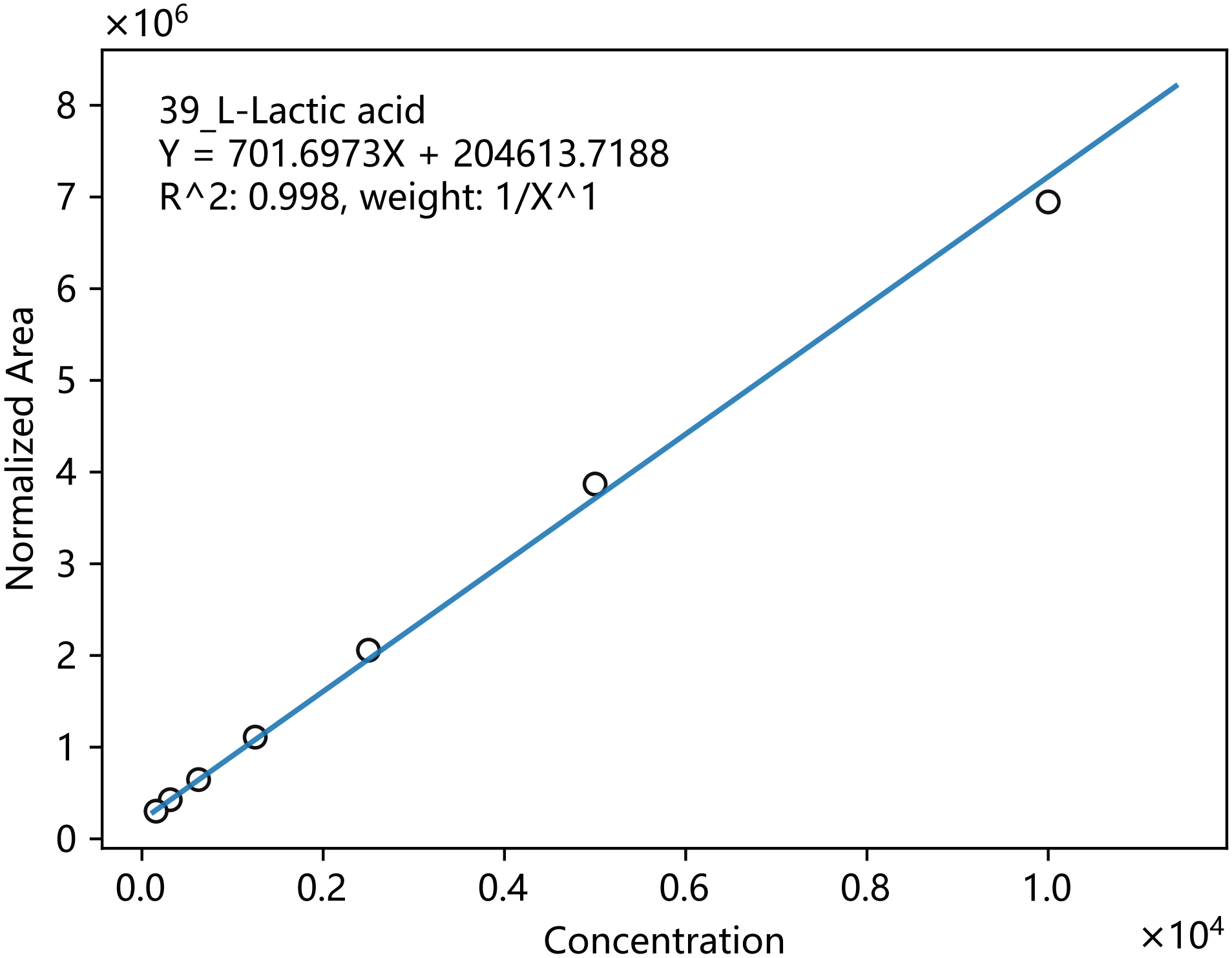

×10^7
34_Guanosine triphosphate
Y = 0.1904X^2 + 894.6870X - 25555.3027
R^2: 0.999, weight: 1/X^1
1.0
0.8
0.6
0.4
0.2
0.0
Normalized Area
0
1
2
3
4
5
Concentration
×10^3

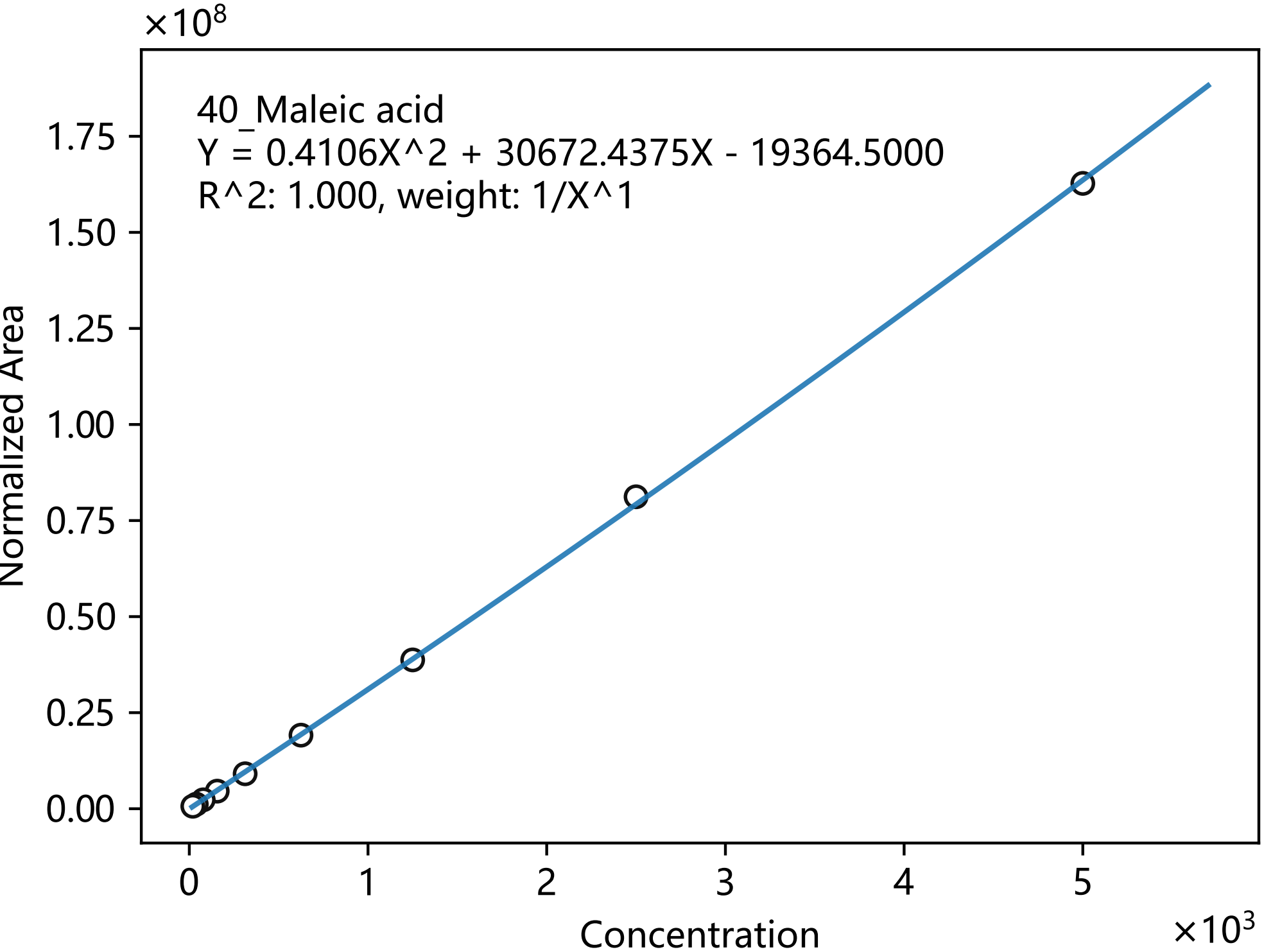

×10^8
35_Hippuric acid
Y = -0.2640X^2 + 27648.1523X + 21468.8496
R^2: 1.000, weight: 1/X^1
2.5
2.0
1.5
1.0
0.5
0.0
Normalized Area
0.0
0.2
0.4
0.6
0.8
1.0
Concentration
×10^4

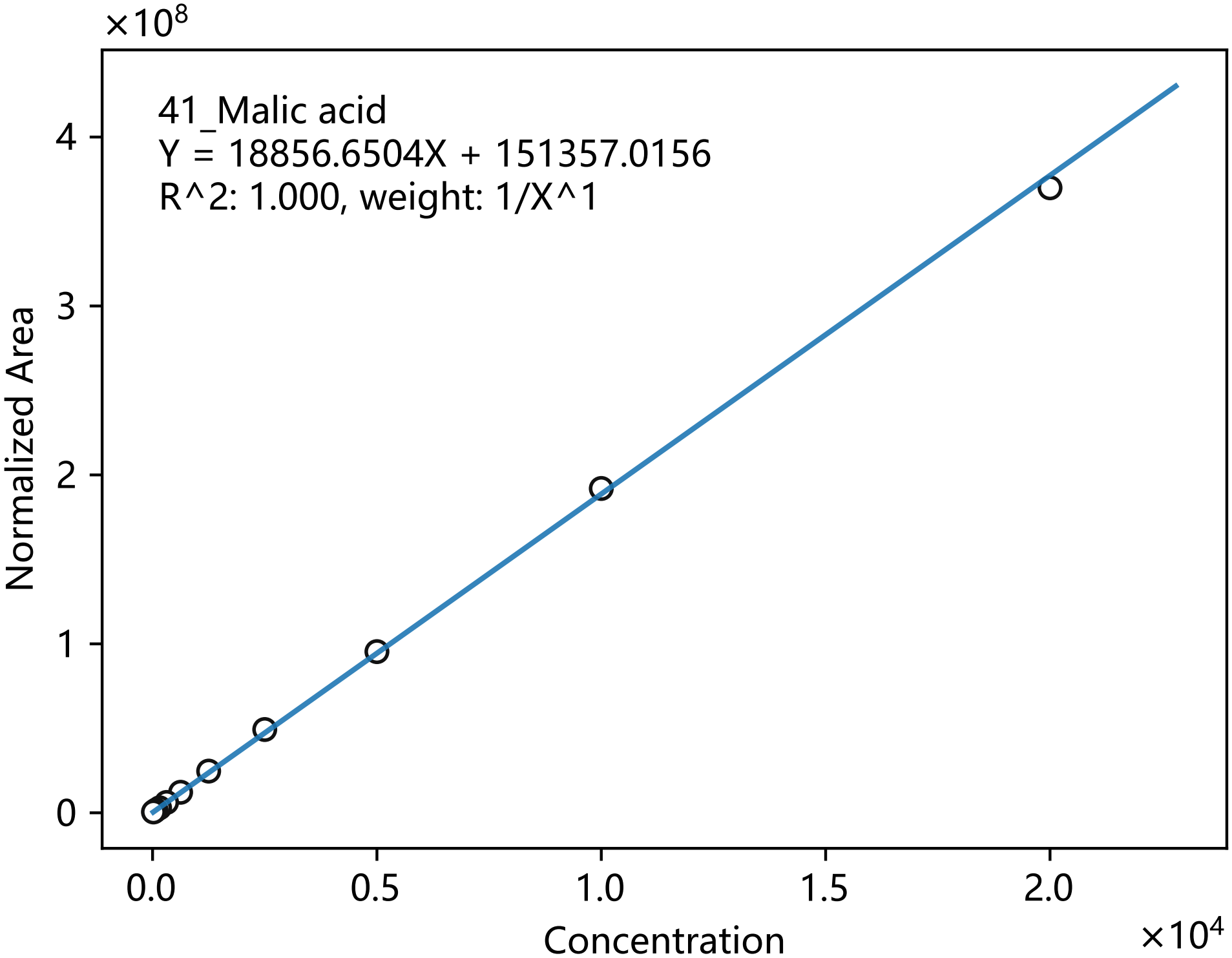

×10^7
36_Homogentisic acid
Y = 0.0086X^2 + 1666.6857X + 32600.7480
R^2: 0.999, weight: 1/X^1
Normalized Area
2.00
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0.0
0.2
0.4
0.6
0.8
1.0
Concentration
×10^4

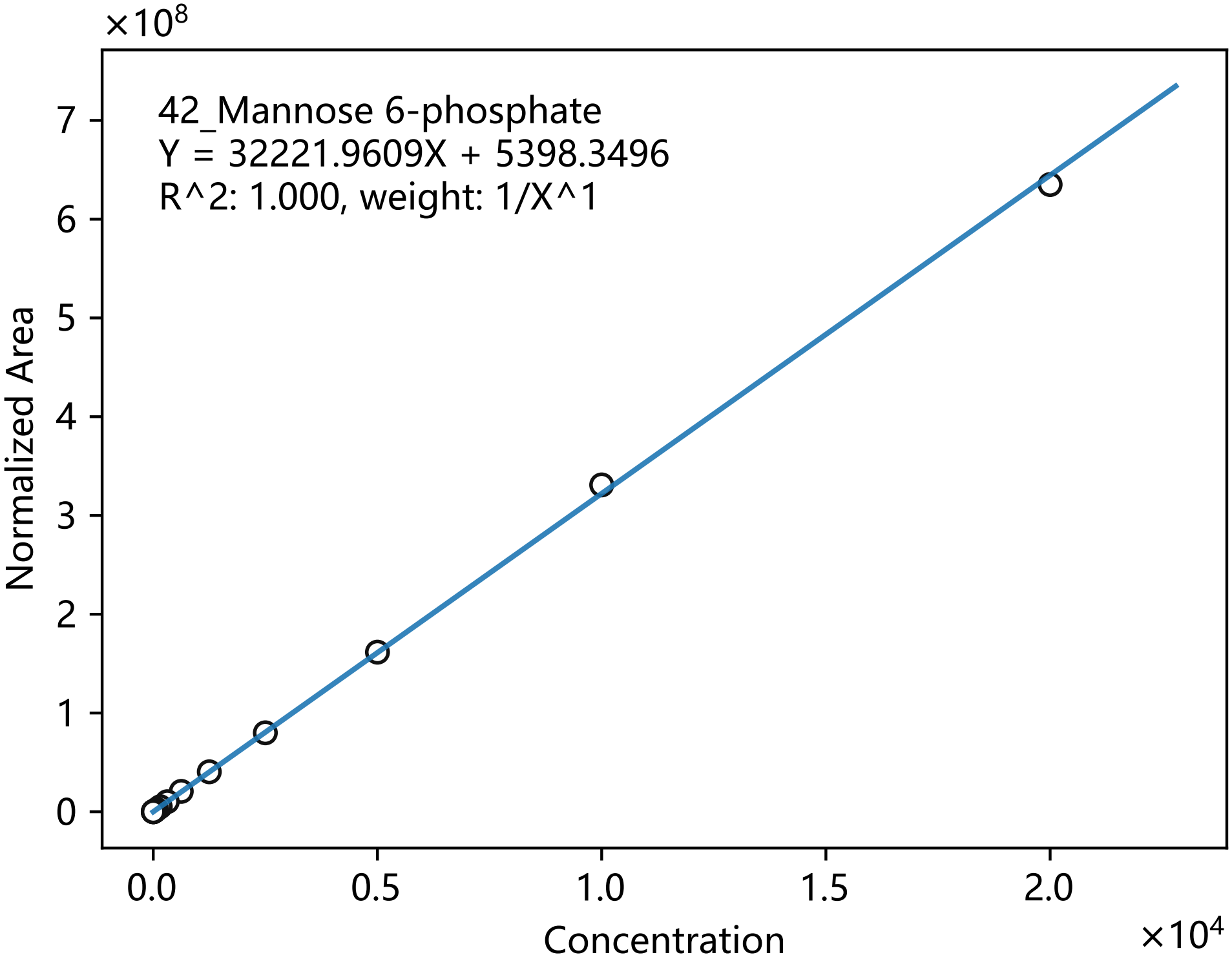

×10^7
37_Indoleacetic acid
Y = 0.0143X^2 + 1147.6335X - 15478.9326
R^2: 1.000, weight: 1/X^1
Normalized Area
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
Concentration
×10^4

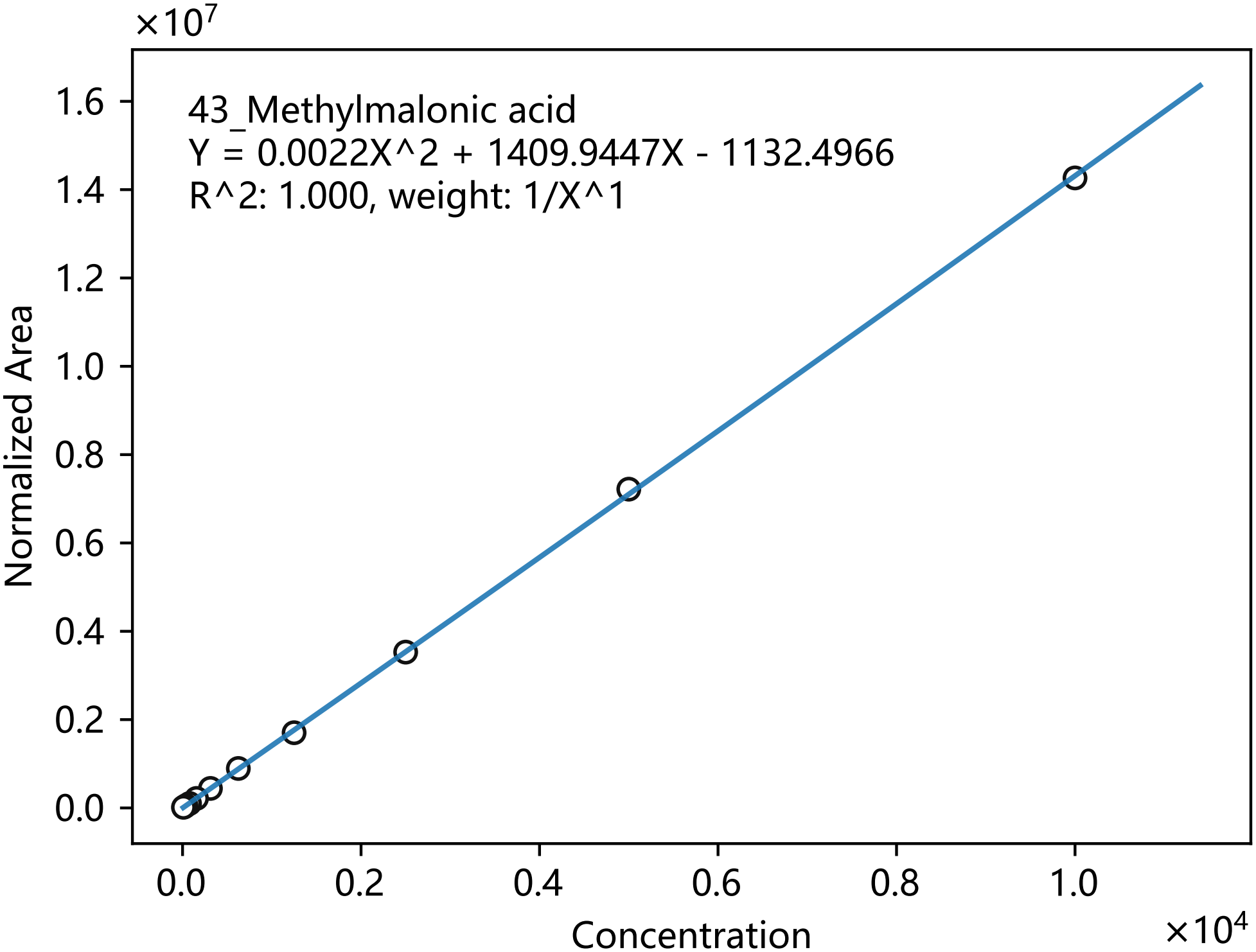

×10^9
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
Normalized Area
38_Isocitric acid
Y = -3.6281X^2 + 180976.1875X - 6647395.0000
R^2: 1.000, weight: 1/X^1
0.0
0.2
0.4
0.6
0.8
1.0
Concentration
×10^4

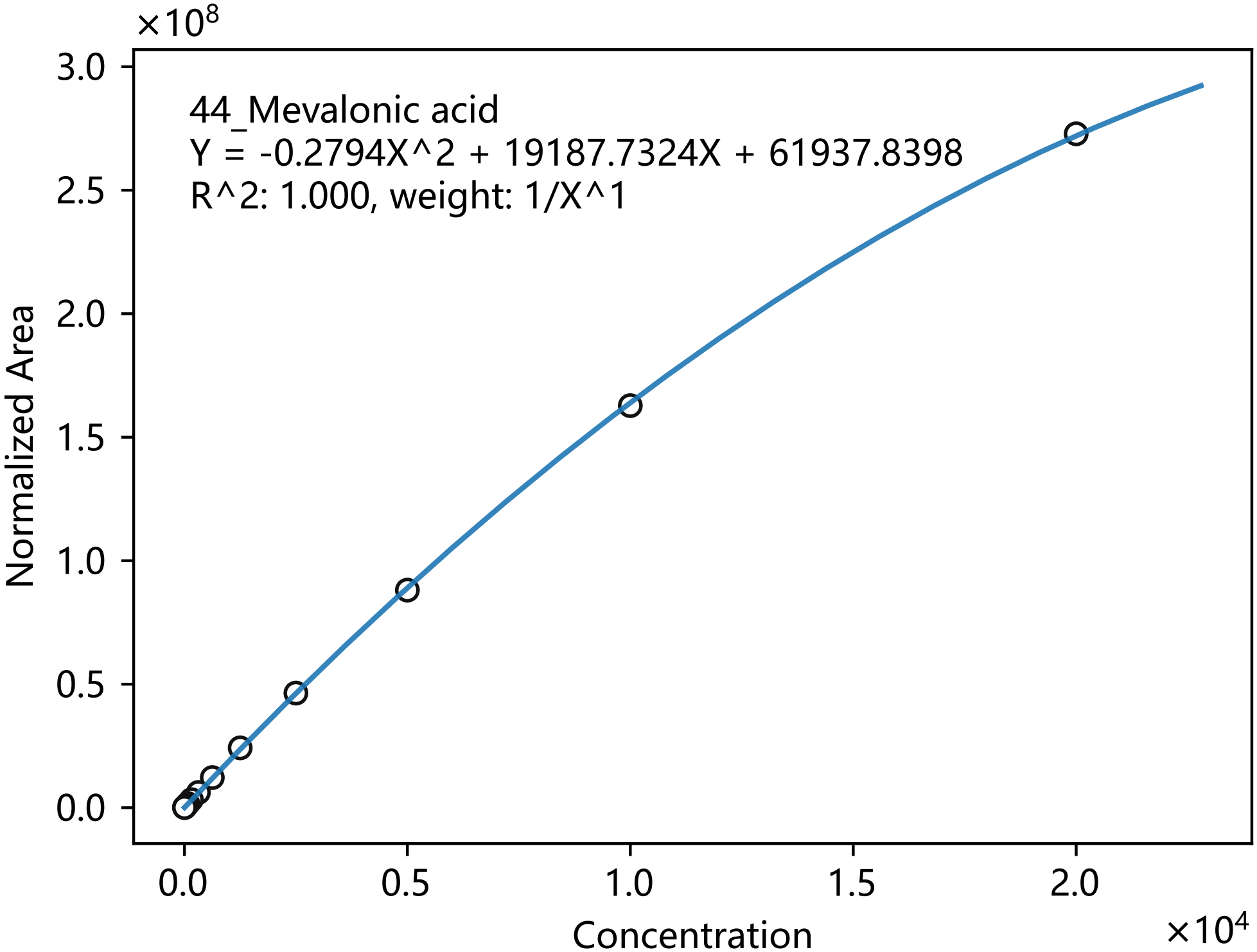

×10^6
39_L-Lactic acid
Y = 701.6973X + 204613.7188
R^2: 0.998, weight: 1/X^1
Normalized Area
0
1
2
3
4
5
6
7
8
0.0
0.2
0.4
0.6
0.8
1.0
Concentration
×10^4

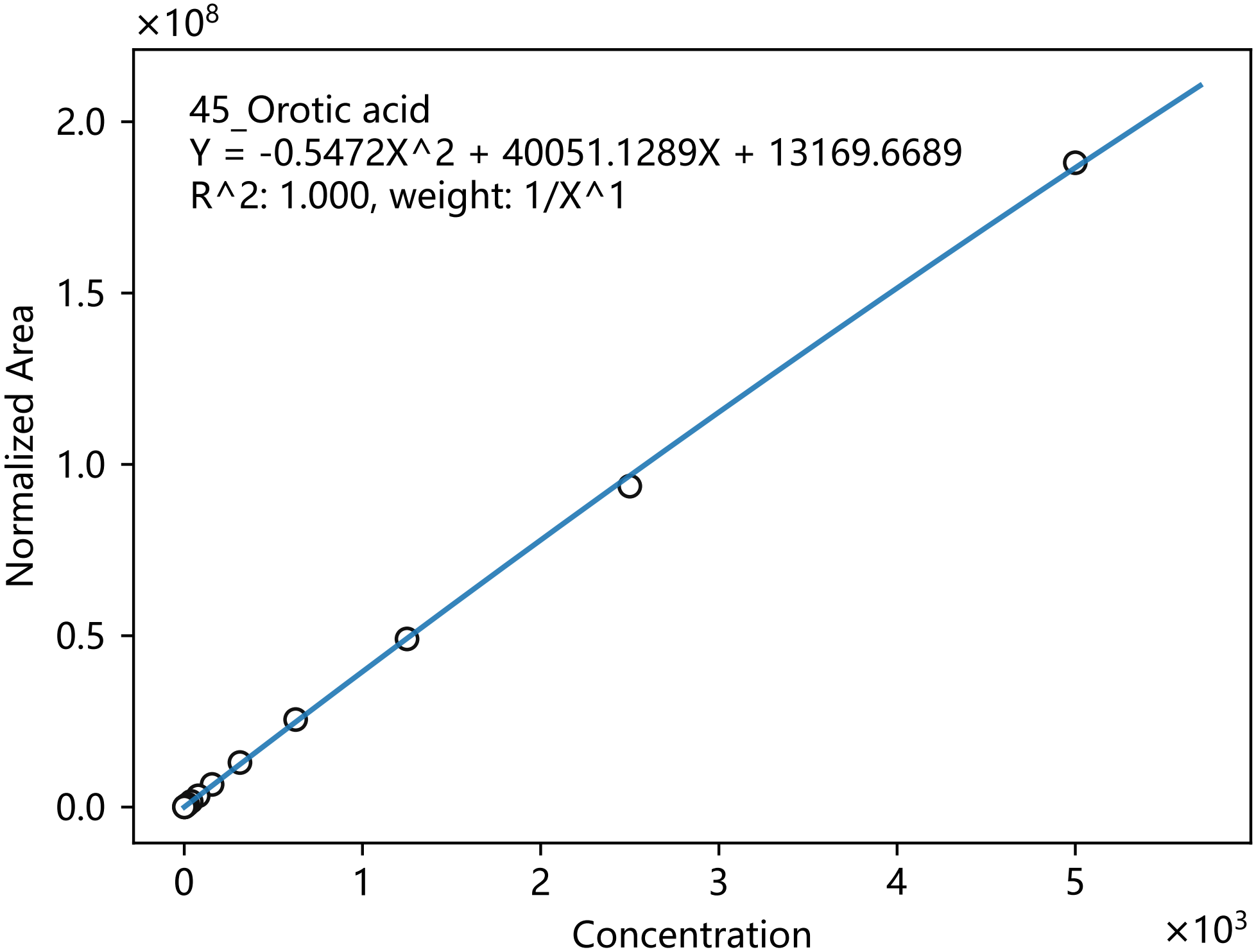

×10^8
40_Maleic acid
Y = 0.4106X^2 + 30672.4375X - 19364.5000
R^2: 1.000, weight: 1/X^1
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
Normalized Area
0
1
2
3
4
5
Concentration
×10^3

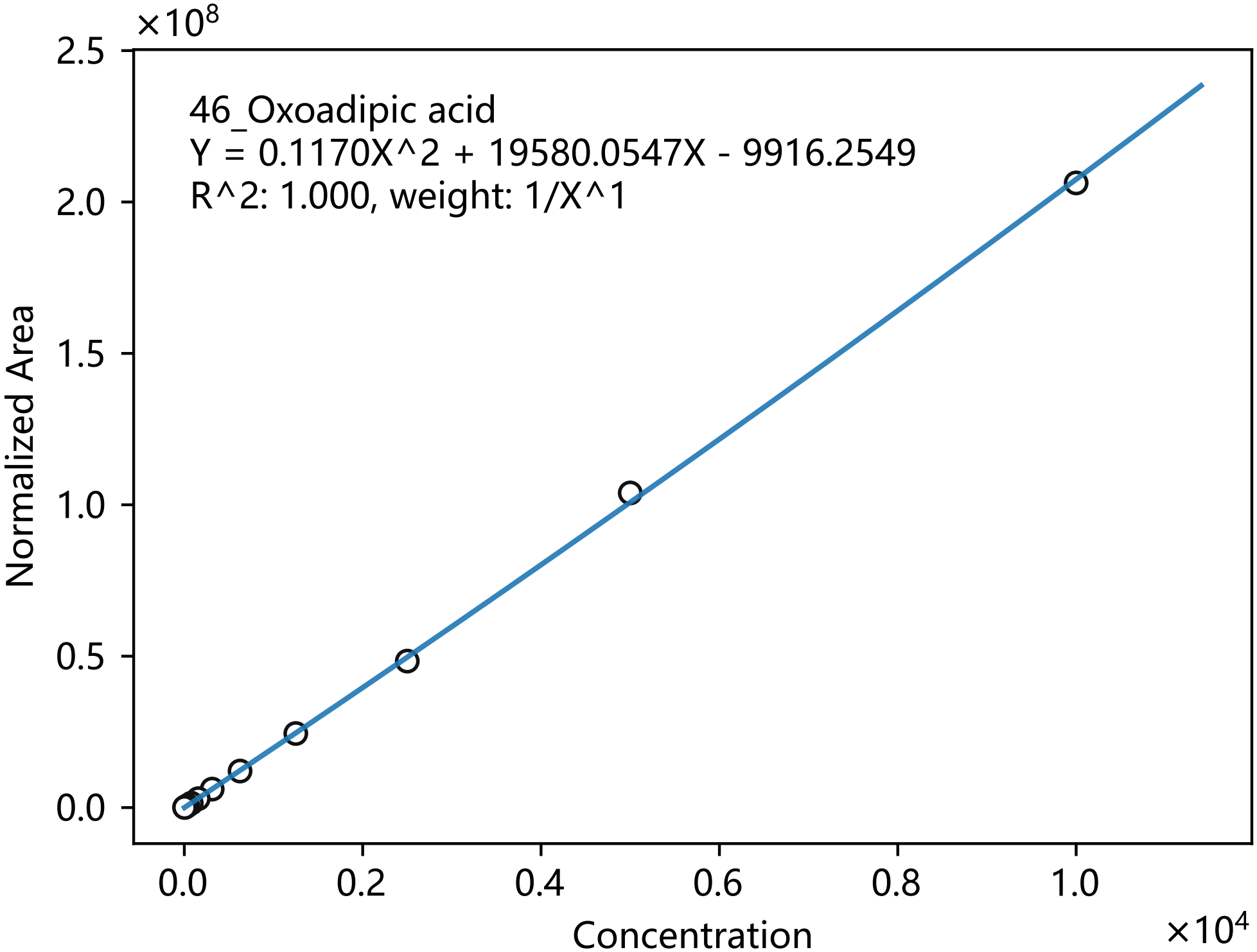

×10^8
41_Malic acid
Y = 18856.6504X + 151357.0156
R^2: 1.000, weight: 1/X^1
Normalized Area
4
3
2
1
0
0.0
0.5
1.0
1.5
2.0
Concentration
×10^4

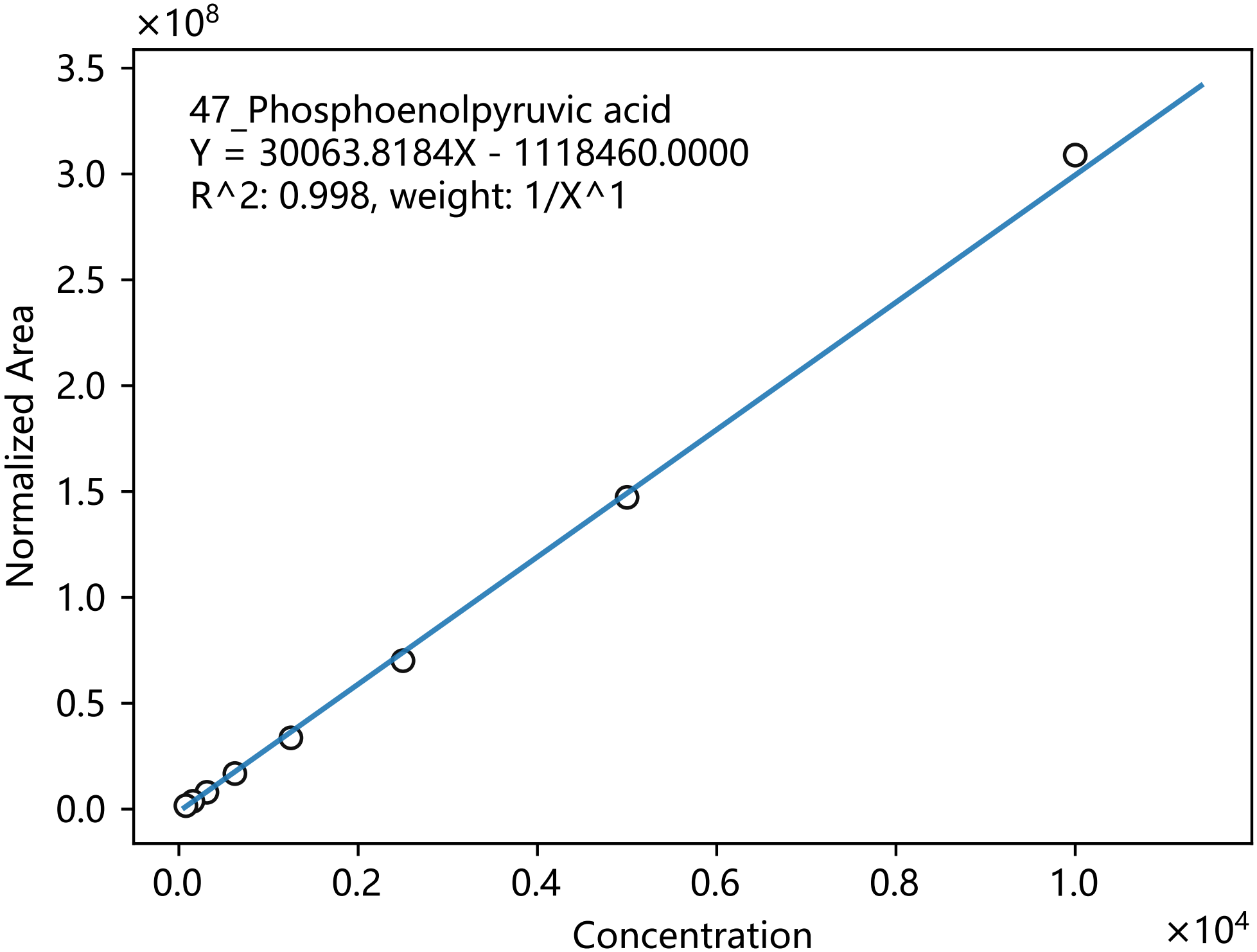

×10^8
42_Mannose 6-phosphate
Y = 32221.9609X + 5398.3496
R^2: 1.000, weight: 1/X^1
Normalized Area
7
6
5
4
3
2
1
0
0.0
0.5
1.0
1.5
2.0
Concentration
×10^4

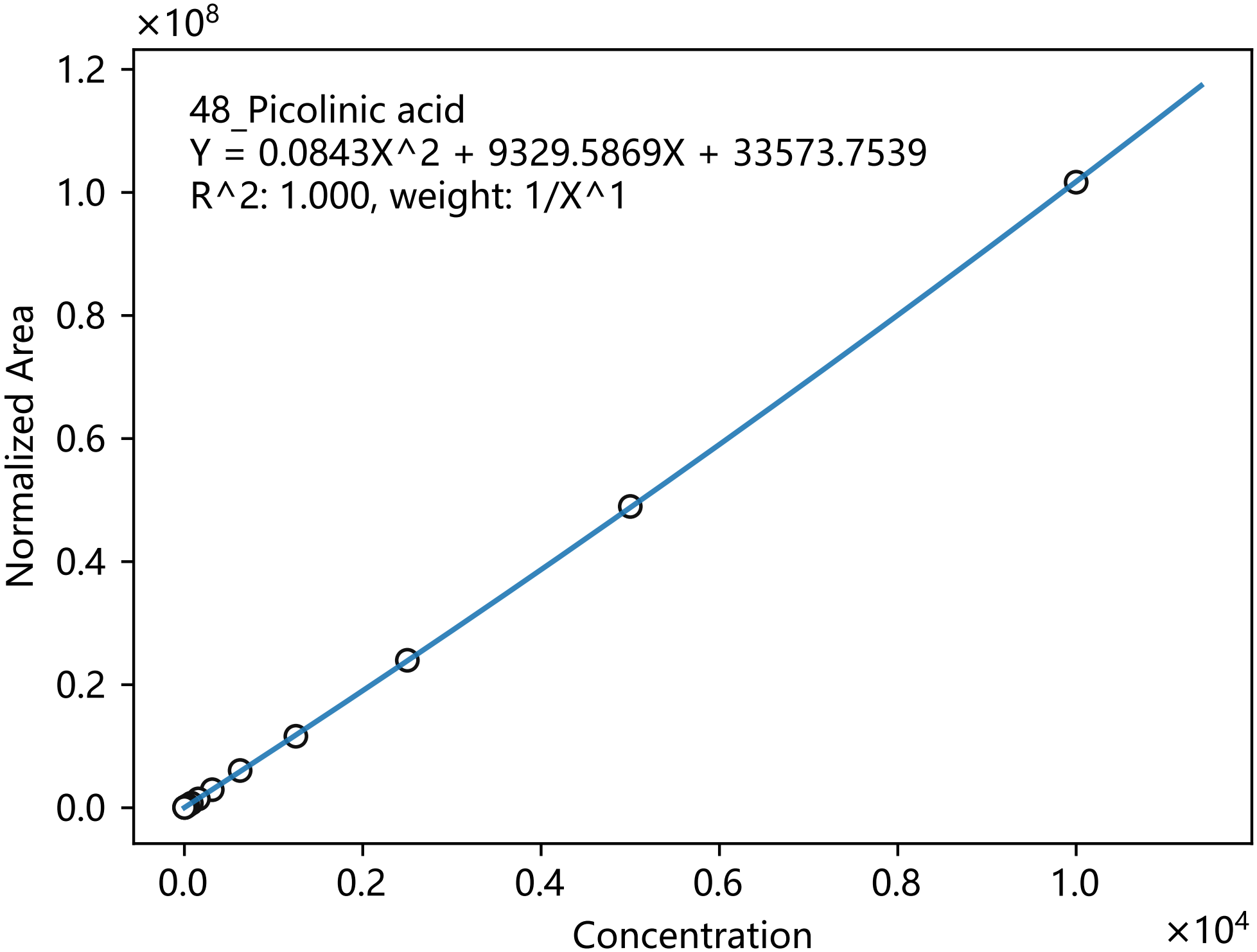

×10^7
43_Methylmalonic acid
Y = 0.0022X^2 + 1409.9447X - 1132.4966
R^2: 1.000, weight: 1/X^1
Normalized Area
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
Concentration
×10^4

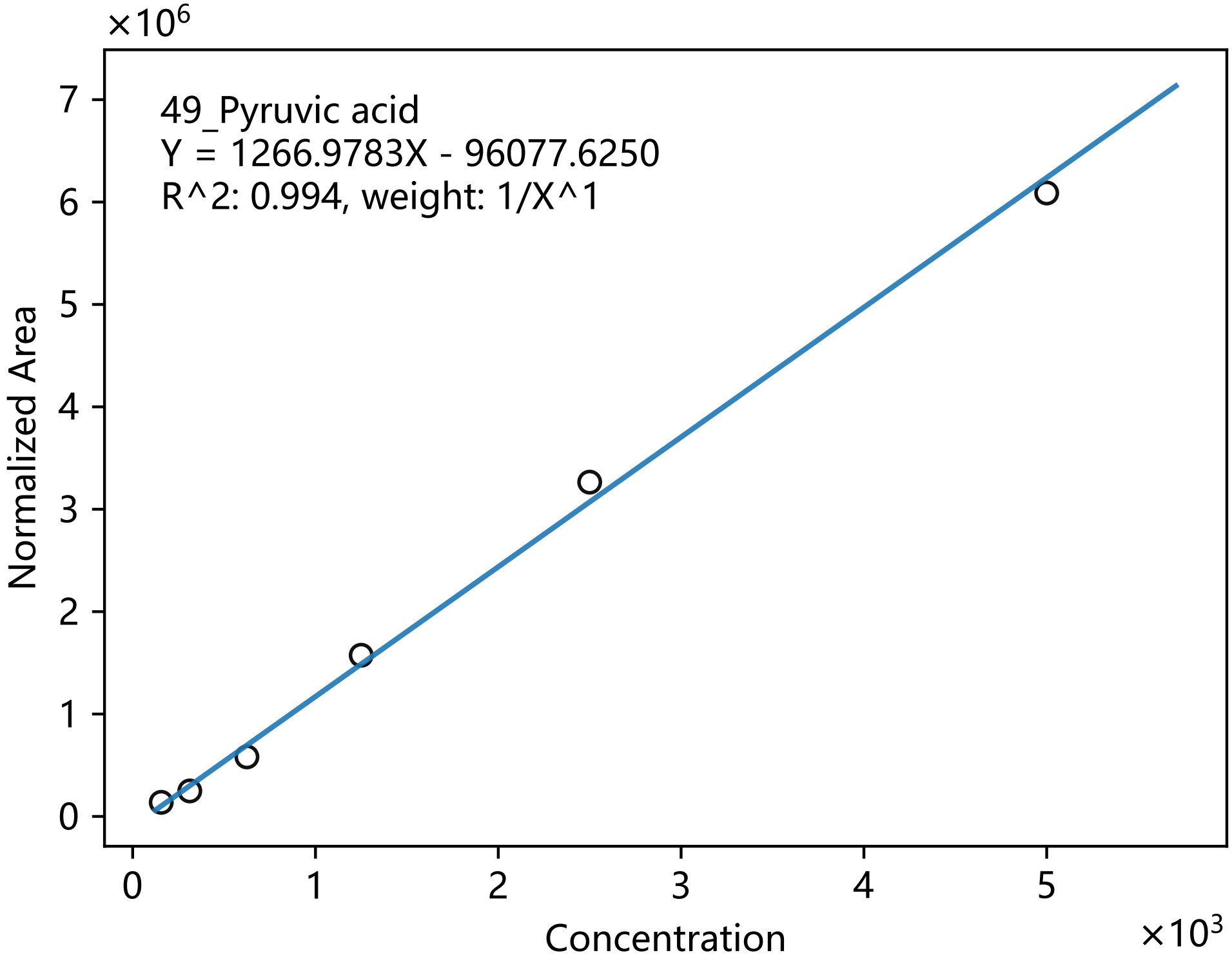

×10^8
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Normalized Area
44_Mevalonic acid
Y = -0.2794X^2 + 19187.7324X + 61937.8398
R^2: 1.000, weight: 1/X^1
0.0
0.5
1.0
1.5
2.0
Concentration
×10^4

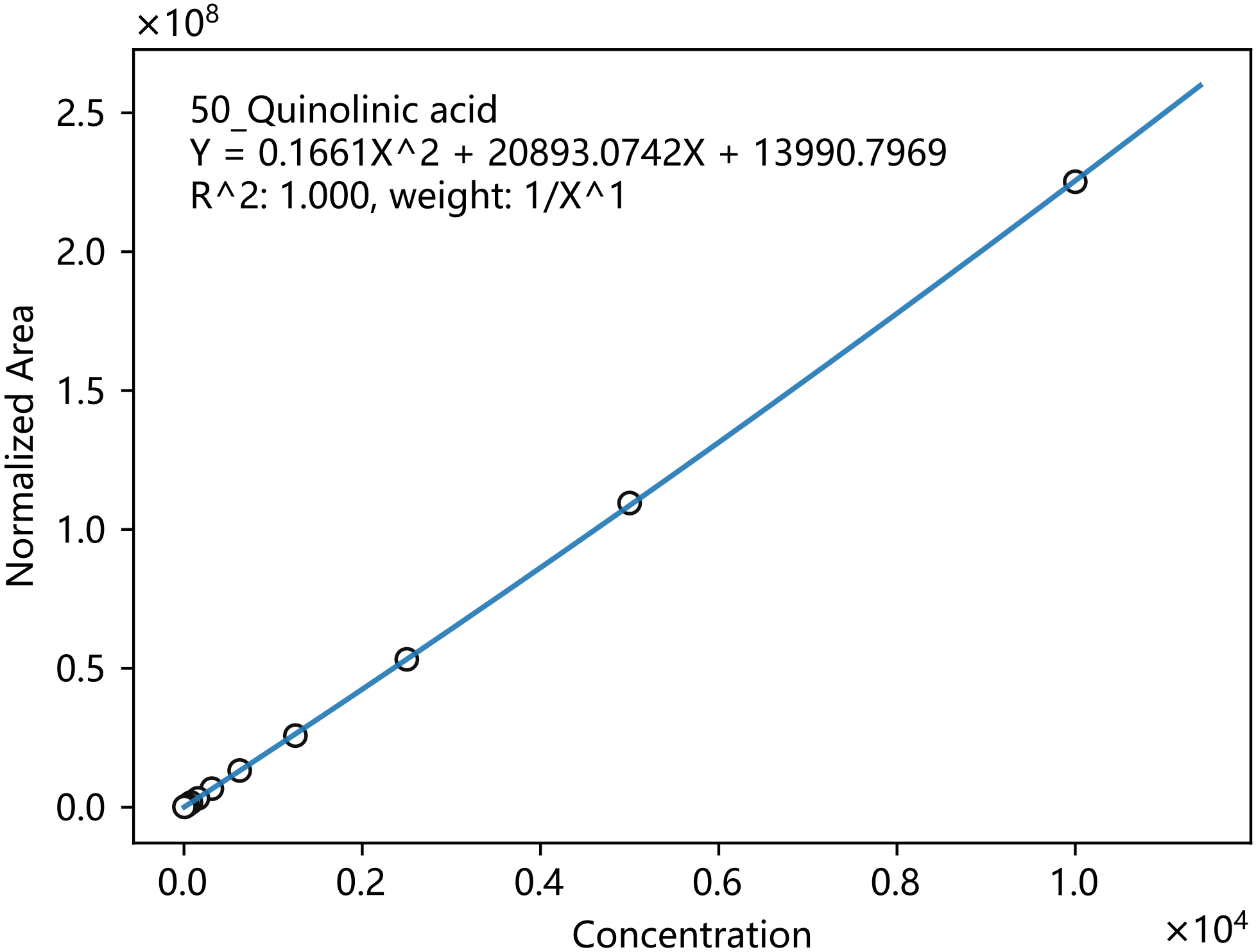

×10^8
45_Orotic acid
Y = -0.5472X^2 + 40051.1289X + 13169.6689
R^2: 1.000, weight: 1/X^1
2.0
1.5
1.0
0.5
0.0
Normalized Area
0
1
2
3
4
5
Concentration
×10^3

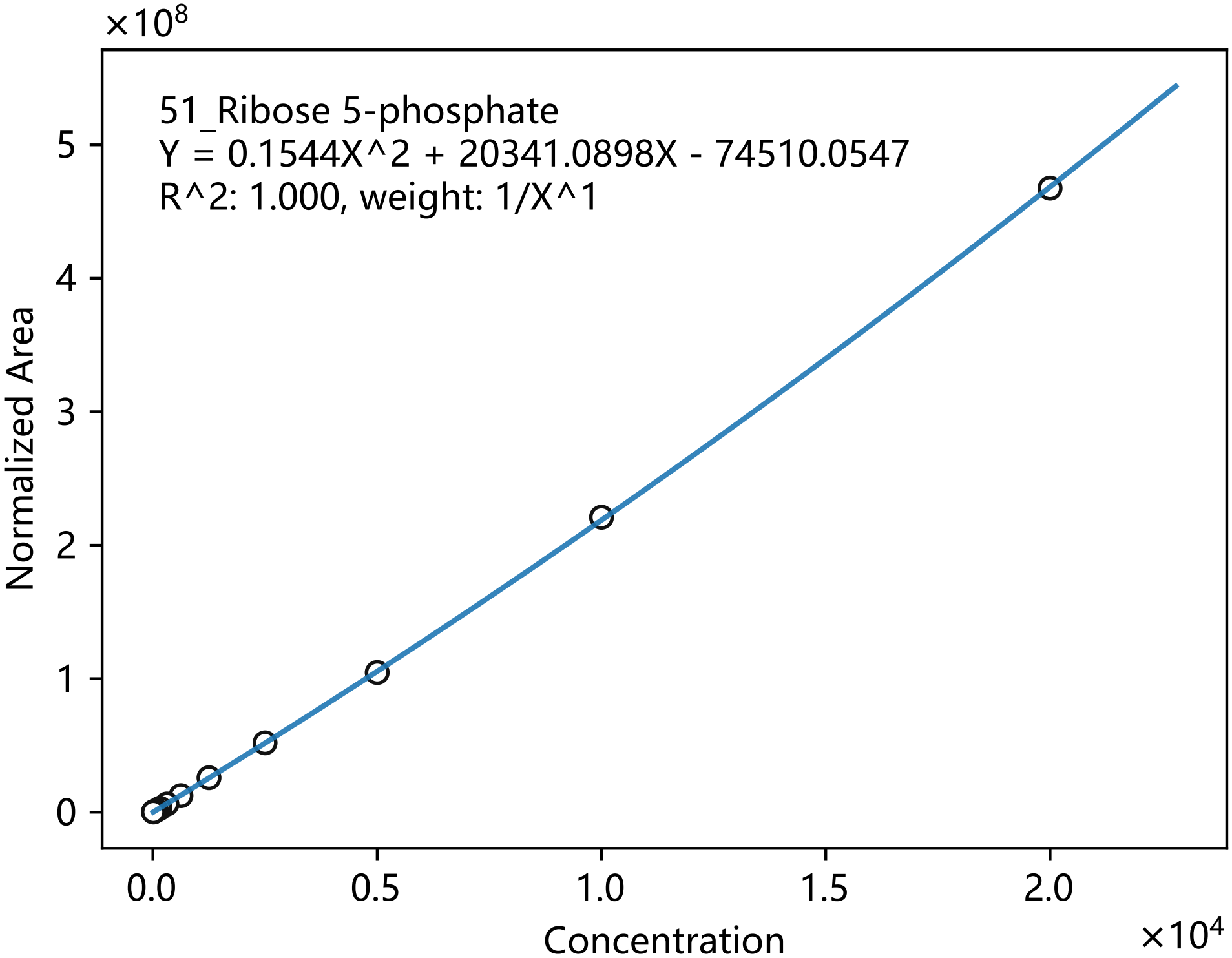

46_Oxoadipic acid
Y = 0.1170X^2 + 19580.0547X - 9916.2549
R^2: 1.000, weight: 1/X^1
×10^8
2.5
2.0
1.5
1.0
0.5
0.0
Normalized Area
0.0
0.2
0.4
0.6
0.8
1.0
×10^4
Concentration

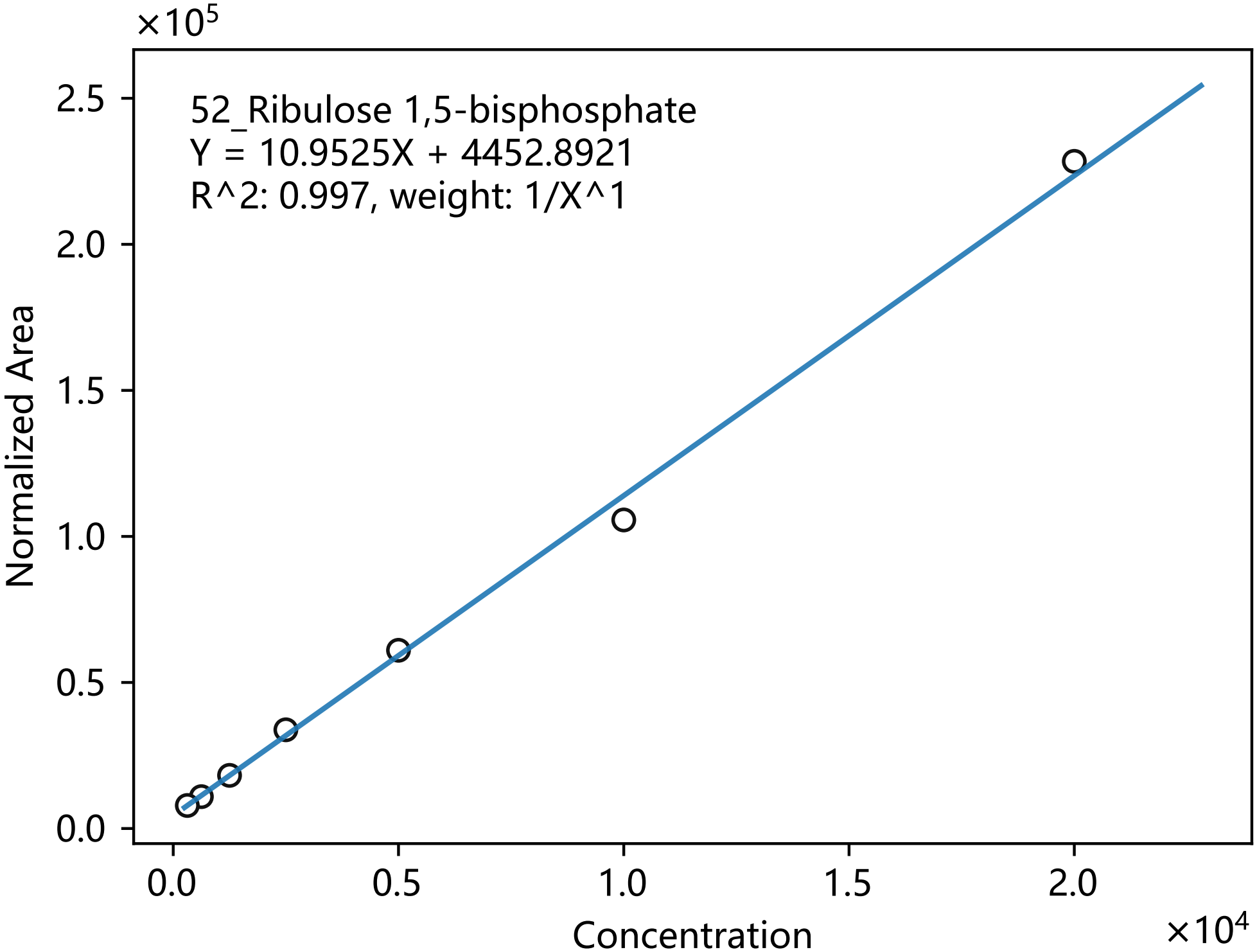

×10^8
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
47_Phosphoenolpyruvic acid
Y = 30063.8184X - 1118460.0000
R^2: 0.998, weight: 1/X^1
Normalized Area
0.0
0.2
0.4
0.6
0.8
1.0
Concentration
×10^4

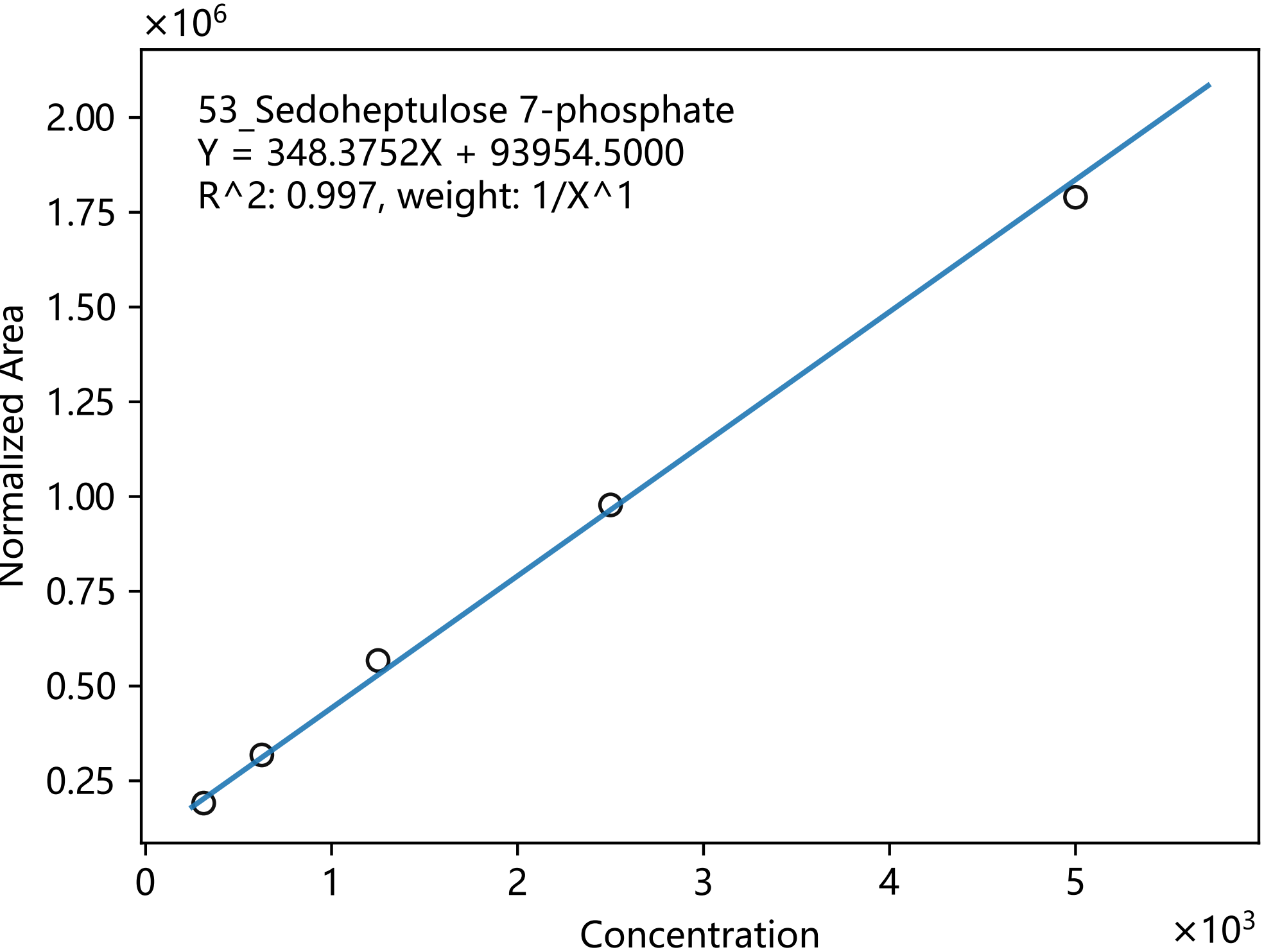

×10^8
1.2
1.0
0.8
0.6
0.4
0.2
0.0
48_Picolinic acid
Y = 0.0843X^2 + 9329.5869X + 33573.7539
R^2: 1.000, weight: 1/X^1
Normalized Area
0.0
0.2
0.4
0.6
0.8
1.0
Concentration
×10^4

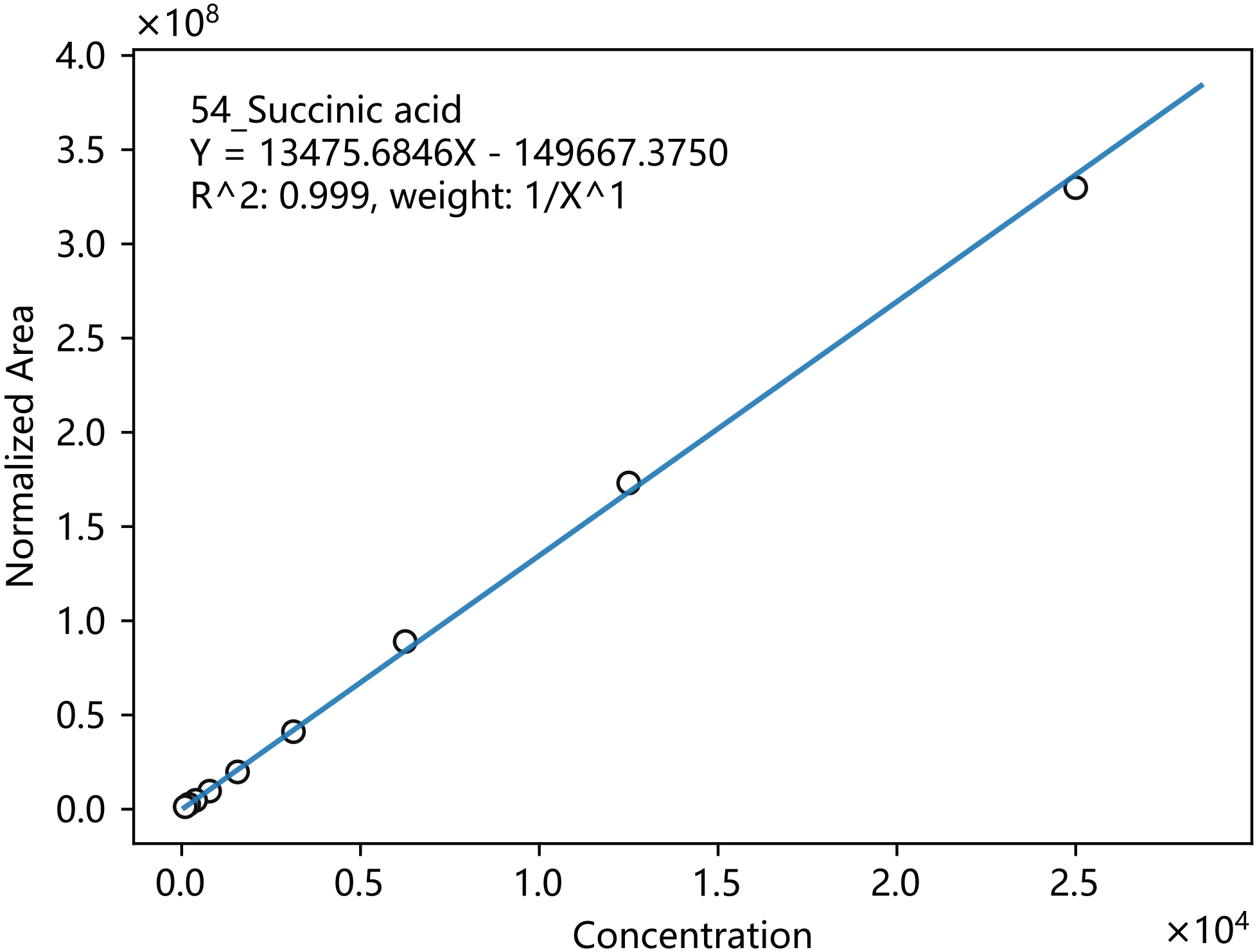

×10^6
49_Pyruvic acid
Y = 1266.9783X - 96077.6250
R^2: 0.994, weight: 1/X^1
Normalized Area
0
1
2
3
4
5
6
7
0
1
2
3
4
5
Concentration
×10^3

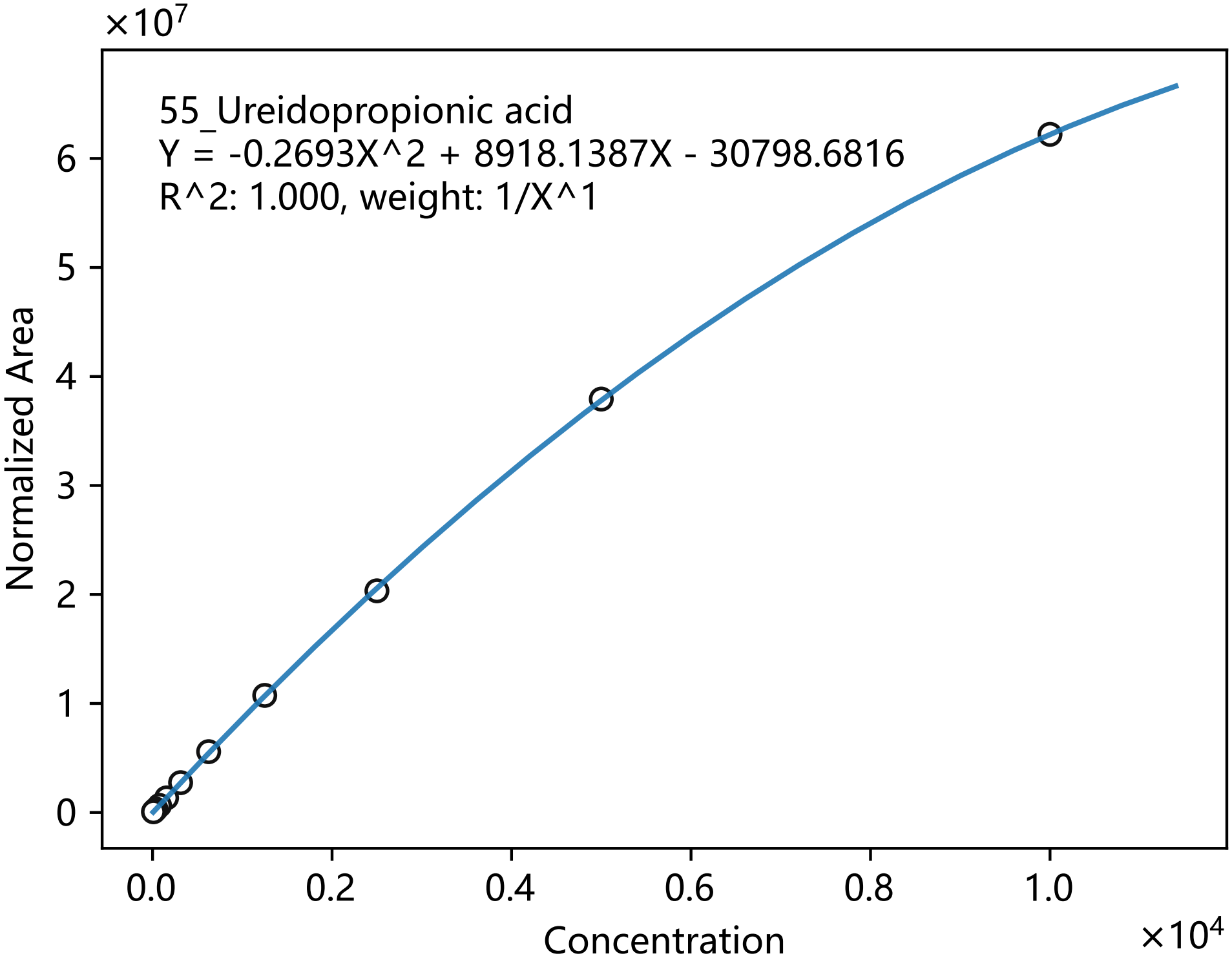

×10^8
50_Quinolinic acid
Y = 0.1661X^2 + 20893.0742X + 13990.7969
R^2: 1.000, weight: 1/X^1
2.5
2.0
1.5
1.0
0.5
0.0
Normalized Area
0.0
0.2
0.4
0.6
0.8
1.0
Concentration
×10^4

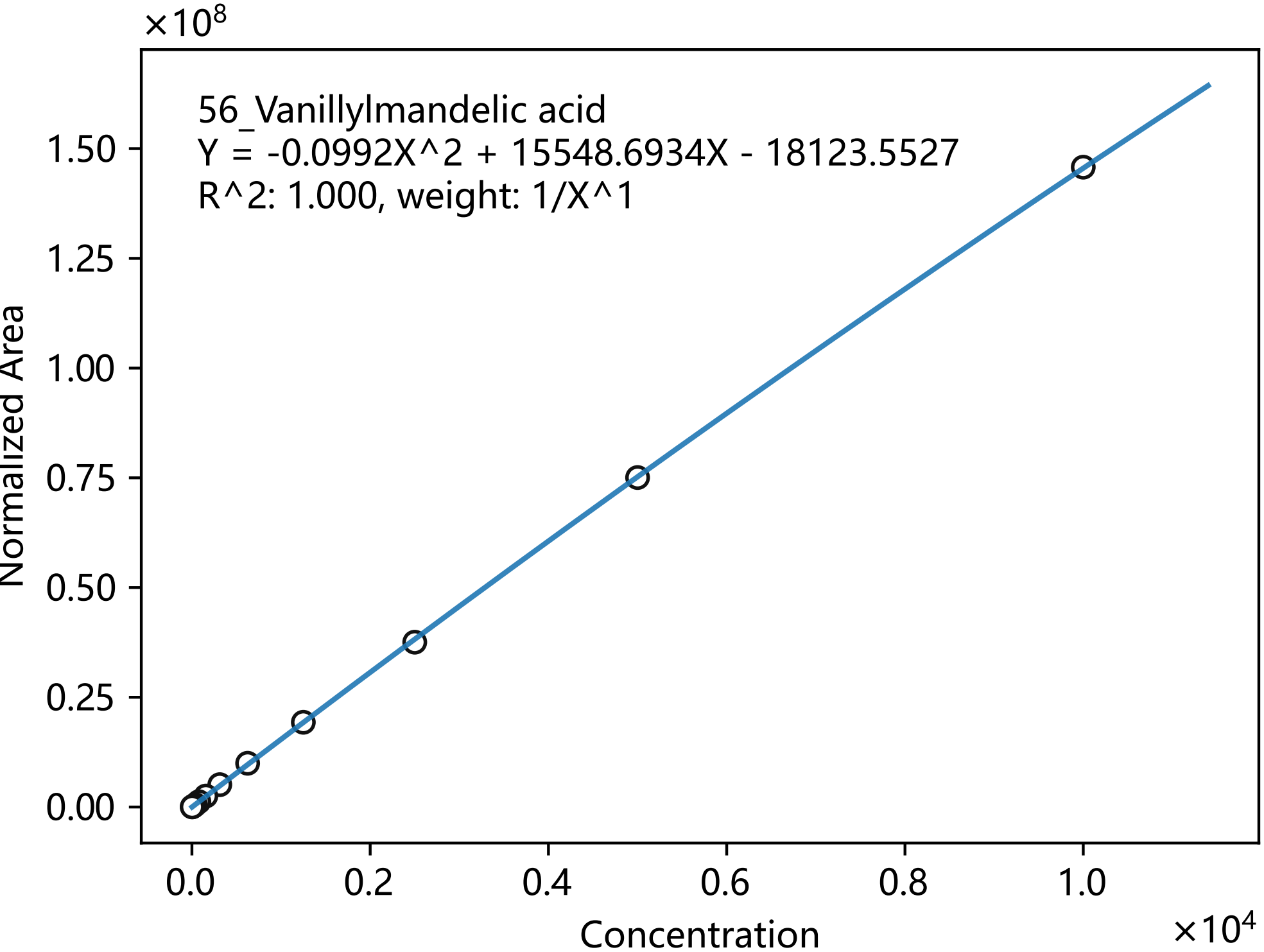

×10^8
51_Ribose 5-phosphate
Y = 0.1544X^2 + 20341.0898X - 74510.0547
R^2: 1.000, weight: 1/X^1
Normalized Area
5
4
3
2
1
0
0.0
0.5
1.0
1.5
2.0
Concentration
×10^4


×10^5
52_Ribulose 1,5-bisphosphate
Y = 10.9525X + 4452.8921
R^2: 0.997, weight: 1/X^1
Normalized Area
2.5
2.0
1.5
1.0
0.5
0.0
0.0
0.5
1.0
1.5
2.0
Concentration
×10^4


×10^6
53_Sedoheptulose 7-phosphate
Y = 348.3752X + 93954.5000
R^2: 0.997, weight: 1/X^1
2.00
1.75
1.50
1.25
1.00
0.75
0.50
0.25
Normalized Area
0
1
2
3
4
5
Concentration
×10^3


×10^8
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Normalized Area
54_Succinic acid
Y = 13475.6846X - 149667.3750
R^2: 0.999, weight: 1/X^1
0.0
0.5
1.0
1.5
2.0
2.5
Concentration
×10^4


×10^7
55_Ureidopropionic acid
Y = -0.2693X^2 + 8918.1387X - 30798.6816
R^2: 1.000, weight: 1/X^1
Normalized Area
6
5
4
3
2
1
0
0.0
0.2
0.4
0.6
0.8
1.0
Concentration
×10^4


×10^8
56_Vanillylmandelic acid
Y = -0.0992X^2 + 15548.6934X - 18123.5527
R^2: 1.000, weight: 1/X^1
1.50
1.25
1.00
0.75
0.50
0.25
0.00
Normalized Area
0.0
0.2
0.4
0.6
0.8
1.0
Concentration
×10^4