

Supplementary information

Wavenumbers used for NIR models

Folin Ciocalteu (222 Wavenumbers)

9972 – 9948, 9776, 9772, 9568 – 9560, 9556, 9380, 9376, 9256 – 9244, 9132 – 9116, 9028 – 9020, 9004 – 8996, 8884 – 8796, 8500 – 8492, 8376 – 8360, 8332, 8328, 8312 – 8300, 8212, 8012, 7688, 7272, 7132 – 7032, 7012 – 7004, 6896 – 6884, 6868 – 6832, 6804 – 6672, 6628, 6624, 6164 – 6152, 6092 – 6036, 5992 – 5948, 5852 – 5828, 5684 – 5668, 5640 – 5628, 5256 – 5236, 5024 – 4980, 4860, 4856, 4840 – 4824, 4820, 4744 – 4728, 4724, 4720, 4692 – 4664, 4572, 4568, 4448 – 4416, 4328 – 4320, 4292 – 4276

FRAP (222 Wavenumbers)

9808, 9128 – 9112, 8884, 8880, 7276 – 7268, 7108 – 6608, 6416 – 6408, 6380, 6376, 6120 – 6104, 6092 – 6080, 5992 – 5936, 5804, 5800, 5688 – 5668, 5248 – 5236, 5028 – 4960, 4780 – 4772, 4744 – 4712, 4652 – 4612, 4472 – 4464, 4436 – 4416, 4412, 4292 – 4276, 4164 – 4152

DPPH (513 Wavenumbers)

9940, 9936, 9852 – 9836, 9696 – 9676, 9548 – 9540, 9508 – 9500, 9440 – 9412, 9280 – 9268, 9248 – 9240, 9212 – 9200, 9128 – 9108, 9048 – 9016, 8964 – 8852, 8716, 8412 – 8356, 8316 – 8284, 7924, 7920, 7736 – 7728, 7700 – 7588, 7312 – 7296, 7284 – 7268, 7232 – 6956, 6920 – 6572, 6416 – 6356, 6352 – 6168, 6136 – 6040, 5988 – 5932, 5680 – 5660, 5648 – 5636, 5552 – 5532, 5492 – 5480, 5392, 5388, 5368, 5364, 5272 – 5228, 5208 – 5096, 5004 – 4944, 4876, 4872, 4772 – 4760, 4748 – 4704, 4664 – 4568, 4480 – 4368, 4332, 4296 – 4280, 4260

ABTS (511 Wavenumbers)

9944 – 9936, 9700 – 9692, 9576, 9544, 9280, 9276, 8952, 8408 – 8324, 8308 – 8160, 7880 – 7868, 7680 – 7668, 7620, 7616, 7280 – 7232, 7212 – 7048, 6924 – 6580, 6492 – 6480, 6420 – 6360, 6276 – 6032, 5996 – 5928, 5888 – 5848, 5812 – 5800, 5732 – 5708, 5676 – 5640, 5340 – 5088, 5072 – 5048, 4904 – 4856, 4780 – 4764, 4752 – 4576, 4496 – 4344, 4328 – 4304, 4296 – 4260, 4108 – 4080

CUPRAC (510 Wavenumbers)

9876 – 9860, 9696 – 9680, 9584, 9564, 9424 – 9416, 9324, 9236, 9128 – 9112, 9068 – 9048, 9032 – 9012, 8996 – 8988, 8964 – 8928, 8896 – 8848, 8808, 8600 – 8580, 8548, 8416 – 8400, 8384 – 8324, 8320 – 8284, 8172, 7924, 7920, 7880 – 7868, 7616 – 7592, 7508 – 7496, 7276 – 7264, 7232, 7208 – 7192, 7156 – 6600, 6412 – 6024, 5984 – 5928, 5864 – 5856, 5824 – 5792, 5684 – 5640, 5260 – 5236, 5212 – 5108, 5000 – 4940, 4872 – 4864, 4792 – 4764, 4752 – 4412, 4400 – 4356, 4332 – 4308, 4296 – 4260, 4140 – 4132, 4108 – 4084

Wavenumbers used for ATR-IR models

Folin Ciocalteu (1060 Wavenumbers)

3677 – 3666, 3644 – 3639, 3620 – 3617, 3612 – 3573, 3568 – 3535, 3526 – 3516, 3421 – 3419, 3415 – 3413, 3395 – 3333, 3294 – 3254, 3148 – 3060, 3014, 2982 – 2975, 2921 – 2917, 2889 – 2852, 2851 – 2849, 2808 – 2803, 2792 – 2775, 2769 – 2746, 2740 – 2674, 2668, 2667, 2657 – 2648, 2642 – 2630, 2621 – 2617, 2601 – 2585, 2576 – 2567, 2563 – 2550, 2538 – 2503, 2499 – 2494, 2491 – 2482, 2479 – 2470, 2469 – 2398, 1780 – 1747, 1734 – 1669, 1661, 1655 – 1644, 1631 – 1611,

1593 - 1529, 1528 - 1519, 1487 - 1475, 1466 - 1442, 1435 - 1401, 1390 - 1370, 1300 - 1287, 1260 - 1232, 1175 - 1163, 1141 - 1125, 1046 - 1016, 983, 972 - 924, 851 - 822, 800, 799, 792 - 777, 747 - 729, 682 - 676

FRAP (725 Wavenumbers)

3677 - 3666, 3644 - 3639, 3620 - 3617, 3612 - 3573, 3568 - 3535, 3526 - 3516, 3421 - 3419, 3415 - 3413, 3395 - 3355, 3344 - 3333, 3294 - 3275, 3274 - 3269, 3259 - 3254, 3148 - 3060, 3014, 2982 - 2975, 2921 - 2917, 2889 - 2880, 2852 - 2849, 2808 - 2803, 2792 - 2775, 2769 - 2746, 2740 - 2674, 2668, 2667, 2657 - 2648, 2642 - 2630, 2621 - 2617, 2601 - 2585, 2576 - 2567, 2563 - 2550, 2538 - 2521, 2515 - 2503, 2499 - 2494, 2491 - 2482, 2479 - 2475, 2470 - 2432, 2428 - 2418, 2410 - 2398, 1780 - 1747, 1734 - 1669, 1661, 1655 - 1644, 1631 - 1611, 1593 - 1586, 1529 - 1519, 1487 - 1475, 1466 - 1442, 1435 - 1401, 1390 - 1370, 1300 - 1287, 1260 - 1232, 1175 - 1163, 1141 - 1125, 1046 - 1044, 1024 - 1016, 983, 972 - 948, 940 - 924, 851 - 834, 833 - 830, 824 - 822, 800, 799, 792 - 777, 747 - 729, 682 - 676

DPPH (805 Wavenumbers)

3680 - 3669, 3661 - 3629, 3622 - 3596, 3592 - 3574, 3568 - 3513, 3502 - 3358, 3342 - 3278, 3150 - 3054, 3046 - 3037, 2920, 2919, 2885 - 2880, 2783 - 2765, 2763 - 2751, 2738 - 2727, 2723 - 2620, 2465 - 2463, 2445 - 2443, 2427 - 2425, 2402 - 2399, 2398, 1780 - 1750, 1732 - 1702, 1698 - 1659, 1636 - 1611, 1606, 1597 - 1587, 1571, 1541, 1540, 1531 - 1522, 1486 - 1478, 1465 - 1442, 1433 - 1400, 1386 - 1372, 1360 - 1351, 1298 - 1292, 1260 - 1253, 1240 - 1236, 1188 - 1180, 1173 - 1160, 1137 - 1124, 1105 - 1103, 1065 - 1059, 1021 - 1018, 975 - 961, 956, 954, 939 - 924, 887 - 830, 823 - 819, 807 - 799, 793 - 777, 743 742 - 731, 678 - 675, 670, 669

ABTS (360 Wavenumbers)

3675 - 3673, 3658 - 3655, 3650, 3649, 3638 - 3630, 3417 - 3414, 3391 - 3362, 3337 - 3333, 3320 - 3318, 3302 - 3300, 3235 - 3229, 3208 - 3204, 2996 - 2778, 2761 - 2746, 2731 - 2711, 2689, 2668, 2667, 2638, 2623 - 2619, 2601, 2600, 2446, 2445, 1729, 1726, 1702, 1696, 1694, 1687 - 1663, 1652 - 1648, 1628 - 1612, 1500 - 1497, 1485 - 1414, 1386 - 1374, 1167 - 1163, 1108 - 1102, 1086 - 1082, 911 - 905, 885 - 879, 850 - 847, 821 - 818, 807 - 801, 793 - 789, 788 - 778, 747 - 738, 710 - 700

Cuprac (1601 Wavenumbers)

3680 - 3520, 3514, 3513, 3470, 3469 - 3455, 3429 - 3352, 3344 - 3328, 3240 - 3184, 3141 - 3049, 3048 - 3013, 2996 - 2967, 2926 - 2922, 2886 - 2877, 2829 - 2694, 2688 - 2590, 2577 - 2573, 2559 - 2554, 2504 - 2460, 2452 - 2420, 2403 - 2396, 1780 - 1749, 1736 - 1656, 1645 - 1546, 1542 - 1539, 1532 - 1521, 1514, 1489 - 1477, 1465 - 1439, 1436 - 1371, 1360 - 1340, 1321 - 1308, 1301 - 1286, 1270 - 1268, 1262 - 1236, 1230 - 1200, 1192 - 1179, 1174 - 1147, 1142 - 1109, 1099 - 1068, 1046 - 1041, 1025 - 1007, 1003 - 992, 986 - 980, 975 - 943, 936 - 920, 905 - 891, 887 - 881, 866