

Supplementary material:

Supplementary figure 1: Relationship between Yield and Grain density on raw data

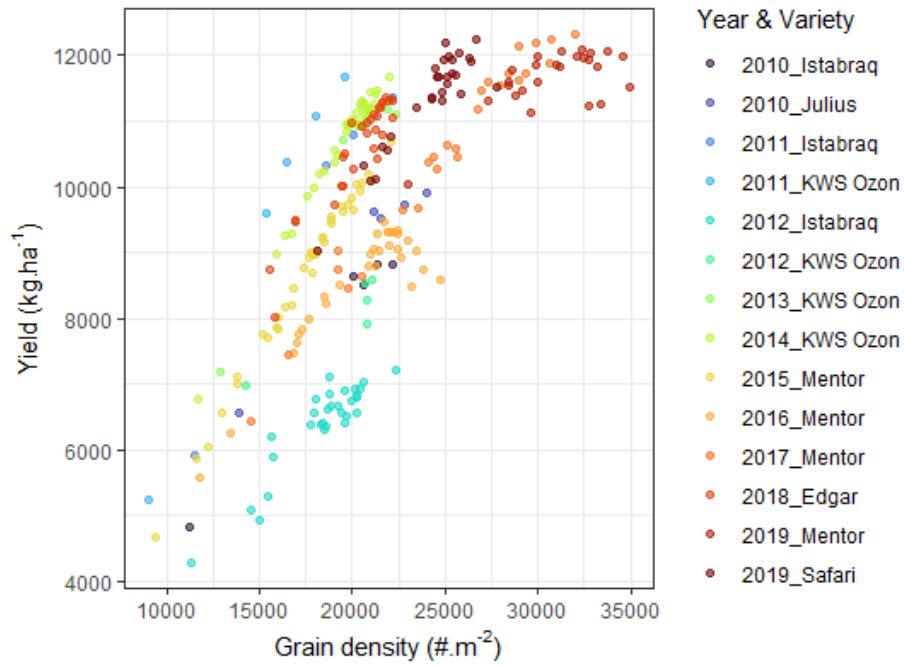


Figure 1: Yield as a function of grain density for each trial (year and variety).

"Year and variety" classification encompass experiment variability due to annual weather, differences in residual soil N available at the end of winter and genotypes.

Supplementary Table 1 : Raw results of observed yield and yield components under the different N fertilization regimes tested each year between 2010 and 2019

| N Management | | | | Yield (kg ha ⁻¹) | | Grain.dens. (# m ⁻²) | | TKW (g) | | Spike.dens. (# m ⁻²) | | |
|------------------------|---------------------|------------------|------------------|------------------------------|---------|----------------------------------|---------|---------|------|----------------------------------|-------|---------|
| Years | DC ₂₃₋₂₅ | DC ₃₁ | DC ₃₉ | Total N fertilizer supplied | Avg. | Std.dev | Avg. | Std.dev | Avg. | Std.dev | Avg. | Std.dev |
| 2010 -> 2019 | 0 | 0 | 0 | 0 | 6539.5 | 1661 | 13467.9 | 3687 | 49.0 | 5.8 | 285.3 | 43.8 |
| 2012, 2014 -> 2019 | 0 | 0 | 50-70 | 50-70 | 7974.8 | 2176 | 17226.4 | 5634 | 47.1 | 7.9 | 308.9 | 70.8 |
| 2012, 2014 -> 2019 | 0 | 0 | 100+ | 100-120 | 8901.1 | 2178 | 19376.4 | 4708 | 46.2 | 7.4 | 309.0 | 52.2 |
| 2012, 2014 -> 2019 | 0 | 50-70 | 0 | 50-70 | 8737.7 | 1904 | 19031.5 | 4668 | 46.4 | 6.3 | 358.7 | 68.1 |
| 2012, 2014 -> 2019 | 0 | 50-70 | 50-70 | 100-140 | 9612.5 | 1930 | 21014.5 | 4859 | 46.4 | 7.1 | 363.6 | 56.0 |
| 2012 | 0 | 50-70 | 100+ | 150-190 | 6363.2 | 12 | 18453.5 | 226 | 34.5 | 0.5 | 328.0 | 1.9 |
| 2012, 2014 -> 2019 | 0 | 100+ | 0 | 100-120 | 9980.8 | 1533 | 22284.8 | 4153 | 45.3 | 5.6 | 396.3 | 46.7 |
| 2014, 2015 | 0 | 100+ | 50-70 | 150-190 | 9869.3 | 1079 | 18754.3 | 1137 | 52.5 | 3.0 | 392.7 | 75.8 |
| 2012, 2014 -> 2019 | 0 | 100+ | 100+ | 200 | 9963.4 | 1864 | 22122.6 | 4181 | 45.5 | 7.6 | 384.2 | 43.5 |
| 2019 | 30-40 | 30-40 | 30-40 | 90-120 | 10079.3 | - | 20954.9 | - | 48.1 | - | 350.0 | - |
| 2012 -> 2018 | 30-40 | 50-70 | 100+ | 180-230 | 10768.1 | 983 | 24521.8 | 3352 | 44.3 | 5.5 | 388.3 | 19.2 |
| 2016, 2018 | 30-40 | 100+ | 50-70 | 180-230 | 10179.2 | 1625 | 21750.4 | 432 | 46.7 | 6.5 | 407.5 | - |
| 2012, 2014 -> 2019 | 50-70 | 0 | 0 | 50-70 | 8655.7 | 1937 | 18719.1 | 4539 | 46.6 | 5.4 | 369.3 | 46.0 |
| 2012, 2014 -> 2019 | 50-70 | 0 | 50-70 | 100-140 | 9601.7 | 2170 | 20771.3 | 5166 | 46.8 | 6.7 | 377.8 | 53.8 |
| 2012 | 50-70 | 0 | 100+ | 150-190 | 6486.5 | 259 | 18681.8 | 210 | 34.7 | 1.0 | 336.9 | 12.0 |
| 2016 | 50-70 | 30-40 | 100+ | 180-230 | 9473.3 | - | 21702.9 | - | 43.7 | - | 400.8 | - |
| 2012, 2014 -> 2019 | 50-70 | 50-70 | 0 | 100-140 | 9847.8 | 1775 | 22217.6 | 4901 | 44.9 | 6.2 | 413.2 | 38.5 |
| 2010 -> 2019 | 50-70 | 50-70 | 50-70 | 150-210 | 10301.3 | 1440 | 21956.0 | 4813 | 48.1 | 8.3 | 419.0 | 61.9 |
| 2010, 2012 -> 2019 | 50-70 | 50-70 | 100+ | 200-260 | 9782.7 | 1523 | 21290.8 | 3534 | 46.4 | 7.5 | 426.6 | 60.4 |
| 2016 | 50-70 | 100+ | 30-40 | 180-230 | 9044.8 | - | 22421.4 | - | 40.3 | - | 463.3 | - |
| 2011, 2014, 2015, 2019 | 50-70 | 100+ | 50-70 | 200-260 | 10918.5 | 902 | 23115.7 | 5485 | 48.5 | 7.0 | 413.2 | 57.5 |
| 2010, 2012, 2014, 2015 | 50-70 | 100+ | 100+ | 250-310 | 9637.6 | 1741 | 20669.7 | 562 | 46.5 | 7.8 | 415.1 | 64.5 |
| 2016 -> 2019 | 70-90 | 0 | 0 | 70-90 | 10024.2 | 1229 | 22376.4 | 4138 | 45.3 | 4.9 | 429.9 | 31.8 |
| 2014, 2015 | 70-90 | 0 | 50-70 | 120-160 | 9466.1 | 2063 | 17907.1 | 2689 | 52.6 | 3.6 | 369.6 | 31.2 |
| 2012, 2014 -> 2019 | 70-90 | 0 | 70-90 | 140-180 | 10191.9 | 1733 | 21726.0 | 4533 | 47.5 | 6.7 | 401.6 | 47.2 |
| 2016, 2018, 2019 | 70-90 | 30-40 | 50-70 | 150-200 | 10560.3 | 1307 | 22895.2 | 2211 | 46.1 | 3.3 | 444.4 | 34.6 |
| 2016 -> 2019 | 70-90 | 50-70 | 30-40 | 150-200 | 10806.7 | 1316 | 24679.7 | 3562 | 44.1 | 5.5 | 462.5 | 40.5 |
| 2012, 2014 -> 2019 | 70-90 | 70-90 | 0 | 140-180 | 10202.7 | 1736 | 23928.6 | 5025 | 43.3 | 7.2 | 434.9 | 43.8 |
| 2014, 2015, 2018, 2019 | 70-90 | 70-90 | 50-70 | 190-250 | 10887.5 | 867 | 21737.0 | 2417 | 50.3 | 3.3 | 417.8 | 53.1 |
| 2010 -> 2019 | 70-90 | 70-90 | 70-90 | 210-270 | 10398.2 | 1561 | 22902.5 | 4199 | 46.2 | 8.1 | 469.1 | 64.5 |
| 2012, 2014 -> 2019 | 100+ | 0 | 0 | 100-120 | 9806.8 | 1755 | 22230.9 | 4757 | 44.7 | 6.2 | 416.5 | 50.4 |
| 2014, 2015 | 100+ | 0 | 50-70 | 150-190 | 9409.3 | 2173 | 18093.6 | 3040 | 51.7 | 3.3 | 405.8 | 55.4 |
| 2012 -> 2019 | 100+ | 0 | 100+ | 200-240 | 10173.8 | 1980 | 22824.2 | 4938 | 45.3 | 8.3 | 439.6 | 71.1 |
| 2012, 2014 -> 2019 | 100+ | 100+ | 0 | 200-240 | 10351.5 | 1786 | 24479.2 | 4880 | 43.0 | 7.8 | 477.4 | 59.2 |
| 2010 -> 2019 | 100+ | 100+ | 100+ | 300-360 | 10416.7 | 1550 | 24154.9 | 4031 | 43.8 | 8.0 | 490.9 | 54.7 |

Supplementary panel 1: Model fitting procedure for the prediction of grain density with spike density and spike fertility

The following models were compared to evaluate the fit improvement using generalized additive model (GAM) over linear model.

$$\text{Linear} : E(y_i) = \beta_0 + \beta_1 x_i + \beta_2 z_i + \epsilon$$

$$\text{GAM_1} : g(E(y_i)) = \beta_0 + \beta_1 x_i + f_2(z_i) + \epsilon$$

$$\text{GAM_2} : g(E(y_i)) = \beta_0 + f_1(x_i) + f_2(z_i) + \epsilon$$

$$\text{GAM_3} : g(E(y_i)) = \beta_0 + f_1(x_i) + f_2(z_i) + f_3(x_i, z_i) + \epsilon$$

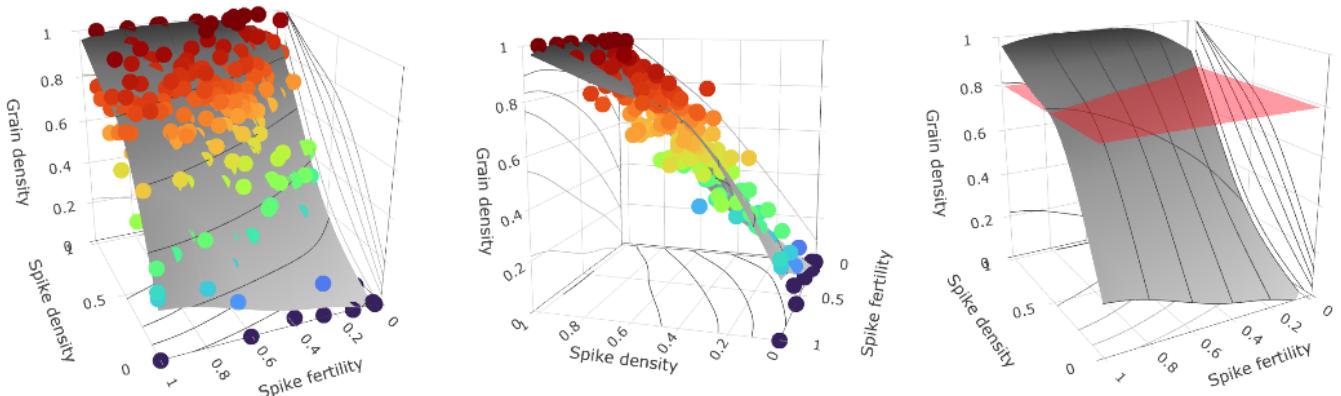
where y is the response variable, here the normalized grain density, β_0 is the intercept, β_1 and β_2 are the parameters of x and y in linear mode. X is the normalized spike density and z is the normalized spike fertility. The functions f_1, f_2 refer to a smooth function when f_3 refers to a tensor product interaction.

Restricted maximum likelihood (REML) was used to fit models individually to the data.

Supplementary Table 2: Performance parameters of the tested models during the fitting procedure

| | Adjusted R ² | REML | AIC |
|--------|-------------------------|--------|--------|
| Linear | 0.860 | -230.4 | -472.8 |
| GAM_1 | 0.864 | -231.2 | -476.9 |
| GAM_2 | 0.872 | -235.8 | -489.9 |
| GAM_3 | 0.904 | -260.2 | -548.9 |

Supplementary Figure 2: Visualization of the fitted Generalized Additive Model



3D representation of the generalized additive model and the normalized values of grain density over spike fertility and spike density. Points colors represent the level of grain density, blue being the lowest values while red being the highest grain densities. The red surface on the 3rd panel represents the grain density_n = 0.8.

Supplementary Table 3 : Linear regressions of normalized grain density, spike density and spike fertility and the influence of total N fertilizer. Normalization procedures correspond to equation 5 in Material & Method.

| Linear regression of grain density and spike density by level of spike fertility | | | Linear regression of grain density and spike fertility by level of spike density | | | Linear regression of spike density and N supply (DC 25 & DC 30) by level of spike fertility | | | Linear regression of spike fertility and N supply (DC 39) by level of spike density | | |
|--|----------------|---------|--|----------------|---------|---|----------------|---------|---|----------------|---------|
| Spike fertility | R ² | p-value | Spike density | R ² | p-value | Spike fertility | R ² | p-value | Spike density | R ² | p-value |
| 0 | 0.883 | 0.00005 | 0 | 0.584 | 0.0770 | 0 | 0.905 | 0.00002 | 0 | 0.205 | 0.367 |
| 0.1 | 0.869 | 0.00676 | 0.1 | 0.724 | 0.0674 | 0.1 | 0.841 | 0.01 | 0.1 | 0.771 | 0.0502 |
| 0.2 | 0.917 | 0 | 0.2 | 0.581 | 0.0464 | 0.2 | 0.708 | 0.00001 | 0.2 | 0.0669 | 0.575 |
| 0.3 | 0.828 | 0 | 0.3 | 0.687 | 0.00013 | 0.3 | 0.622 | 0 | 0.3 | 0.427 | 0.00824 |
| 0.4 | 0.826 | 0 | 0.4 | 0.678 | 0 | 0.4 | 0.651 | 0 | 0.4 | 0.664 | 0 |
| 0.5 | 0.675 | 0 | 0.5 | 0.753 | 0 | 0.5 | 0.374 | 0.0002 | 0.5 | 0.608 | 0 |
| 0.6 | 0.769 | 0 | 0.6 | 0.556 | 0 | 0.6 | 0.875 | 0 | 0.6 | 0.448 | 0 |
| 0.7 | 0.821 | 0 | 0.7 | 0.407 | 0.00003 | 0.7 | 0.593 | 0.00001 | 0.7 | 0.416 | 0.00002 |
| 0.8 | 0.893 | 0 | 0.8 | 0.394 | 0.00303 | 0.8 | 0.77 | 0 | 0.8 | 0.173 | 0.0681 |
| 0.9 | 0.651 | 0.00003 | 0.9 | 0.519 | 0.0285 | 0.9 | 0.457 | 0.00148 | 0.9 | 0.0104 | 0.794 |
| 1 | 0.728 | 0.00001 | 1 | 0.294 | 0.0200 | 1 | 0.679 | 0.00005 | 1 | 0.00646 | 0.751 |

Supplementary Table 4 : Linear regressions of normalized spike density and different fertilizer N supplies. Normalization procedures correspond to Eq. 5 in Material & Method.

| Spike fertility levels | Linear regression of spike density and N supply at DC 25 | | Linear regression of spike density and N supply at DC 30 | | Linear regression of spike density and total N supply | |
|------------------------|--|---------|--|---------|---|---------|
| | R ² | p-value | R ² | p-value | R ² | p-value |
| 0 | 0.805 | 0.0000 | 0.508 | 0.0009 | 0.822 | 0.0000 |
| 0.1 | 0.744 | 0.0125 | 0.498 | 0.0765 | 0.879 | 0.0018 |
| 0.2 | 0.554 | 0.0004 | 0.701 | 0.0000 | 0.817 | 0.0000 |
| 0.3 | 0.326 | 0.0029 | 0.170 | 0.0403 | 0.597 | 0.0000 |
| 0.4 | 0.185 | 0.0112 | 0.237 | 0.0035 | 0.617 | 0.0000 |
| 0.5 | 0.228 | 0.0058 | 0.082 | 0.1124 | 0.493 | 0.0000 |
| 0.6 | 0.490 | 0.0001 | 0.203 | 0.0183 | 0.656 | 0.0000 |
| 0.7 | 0.351 | 0.0018 | 0.128 | 0.0791 | 0.618 | 0.0000 |
| 0.8 | 0.519 | 0.0002 | 0.423 | 0.0011 | 0.781 | 0.0000 |
| 0.9 | 0.390 | 0.0043 | 0.066 | 0.2888 | 0.609 | 0.0001 |
| 1 | 0.406 | 0.0025 | 0.556 | 0.0002 | 0.903 | 0.0000 |

Supplementary Table 5 : Games - Howell test. Results of the Games-Howell post-hoc test on (a) grain density and (b) TKW. both variables being normalized between their trial's minimal and maximal values

a

| strategies | Normalized Grain density | | | | | | |
|---------------|--------------------------|---------------|---------------|---------------|---------------|---------------|---------------|
| | 2 N1-_N2-_N3+ | 3 N1-_N2+_N3- | 4 N1-_N2+_N3+ | 5 N1+_N2-_N3- | 6 N1+_N2-_N3+ | 7 N1+_N2+_N3- | 8 N1+_N2+_N3+ |
| 1 N1-_N2-_N3- | ns | *** | **** | ** | **** | **** | **** |
| 2 N1-_N2-_N3+ | | ns | **** | ns | *** | **** | **** |
| 3 N1-_N2+_N3- | | | * | ns | * | *** | **** |
| 4 N1-_N2+_N3+ | | | | * | ns | ns | **** |
| 5 N1+_N2-_N3- | | | | | * | *** | **** |
| 6 N1+_N2-_N3+ | | | | | | ns | **** |
| 7 N1+_N2+_N3- | | | | | | | ** |

b

| strategies | Normalized TKW | | | | | | |
|---------------|----------------|---------------|---------------|---------------|---------------|---------------|---------------|
| | 2 N1-_N2-_N3+ | 3 N1-_N2+_N3- | 4 N1-_N2+_N3+ | 5 N1+_N2-_N3- | 6 N1+_N2-_N3+ | 7 N1+_N2+_N3- | 8 N1+_N2+_N3+ |
| 1 N1-_N2-_N3- | ns | * | *** | ** | *** | *** | **** |
| 2 N1-_N2-_N3+ | | ns | ns | ns | ns | ** | ** |
| 3 N1-_N2+_N3- | | | ns | ns | ns | *** | ** |
| 4 N1-_N2+_N3+ | | | | ns | ns | * | * |
| 5 N1+_N2-_N3- | | | | | ns | ** | ** |
| 6 N1+_N2-_N3+ | | | | | | * | ns |
| 7 N1+_N2+_N3- | | | | | | | ns |

Supplementary Table 6 : Games - Howell test including the impact of N_{SRW}. Results of the Games-Howel post-hoc test on (a) grain density and (b) TKW, both variables being normalized between their trial's minimal and maximal values

a.

| | | Normalized grain density | | | | | | |
|---------------------------------|---------------|--------------------------|---------------|---------------|---------------|---------------|---------------|---------------|
| N _{SRW} | Strategies | 2 N1- N2- N3+ | 3 N1- N2+ N3- | 4 N1- N2+ N3+ | 5 N1+ N2- N3- | 6 N1+ N2- N3+ | 7 N1+ N2+ N3- | 8 N1+ N2+ N3+ |
| Under 46 kg ha ⁻¹ | 1 N1- N2- N3- | ns | ** | **** | * | *** | *** | **** |
| | 2 N1- N2- N3+ | | ns | ** | ns | ** | *** | **** |
| | 3 N1- N2+ N3- | | | ns | ns | ns | * | *** |
| | 4 N1- N2+ N3+ | | | | ns | ns | ns | **** |
| | 5 N1+ N2- N3- | | | | | ns | ns | ** |
| | 6 N1+ N2- N3+ | | | | | | ns | ** |
| | 7 N1+ N2+ N3- | | | | | | | ns |
| Above 46 kg ha ⁻¹ | 1 N1- N2- N3- | ns | ns | * | ns | * | ** | *** |
| | 2 N1- N2- N3+ | | ns | ns | ns | ns | * | ** |
| | 3 N1- N2+ N3- | | | ns | ns | ns | * | *** |
| | 4 N1- N2+ N3+ | | | | ns | ns | ns | ** |
| | 5 N1+ N2- N3- | | | | | ns | * | ** |
| | 6 N1+ N2- N3+ | | | | | | ns | * |
| | 7 N1+ N2+ N3- | | | | | | | * |

b.

| | | Normalized TKW | | | | | | |
|---------------------------------|---------------|----------------|---------------|---------------|---------------|---------------|---------------|---------------|
| N _{SRW} | Strategies | 2 N1- N2- N3+ | 3 N1- N2+ N3- | 4 N1- N2+ N3+ | 5 N1+ N2- N3- | 6 N1+ N2- N3+ | 7 N1+ N2+ N3- | 8 N1+ N2+ N3+ |
| Under 46 kg ha ⁻¹ | 1 N1- N2- N3- | ns | ns | * | ns | ns | ** | * |
| | 2 N1- N2- N3+ | | ns | ns | ns | ns | ns | ns |
| | 3 N1- N2+ N3- | | | ns | ns | ns | * | ns |
| | 4 N1- N2+ N3+ | | | | ns | ns | ns | ns |
| | 5 N1+ N2- N3- | | | | | ns | ns | ns |
| | 6 N1+ N2- N3+ | | | | | | ns | ns |
| | 7 N1+ N2+ N3- | | | | | | | ns |
| Above 46 kg ha ⁻¹ | 1 N1- N2- N3- | ns | ns | ns | ns | ns | *** | **** |
| | 2 N1- N2- N3+ | | ns | ns | ns | ns | ** | *** |
| | 3 N1- N2+ N3- | | | ns | ns | ns | ns | ** |
| | 4 N1- N2+ N3+ | | | | ns | ns | ns | * |
| | 5 N1+ N2- N3- | | | | | ns | ns | ** |
| | 6 N1+ N2- N3+ | | | | | | ns | * |
| | 7 N1+ N2+ N3- | | | | | | | ns |

Supplementary Table 7 : Median, 1st and 3rd quantiles of normalized yield components values per strategies of N fertilization. Normalization procedure corresponds to Eq. 5 of the material & method.

| N fertilization strategies | Normalized spike density | Normalized spike fertility | Normalized grain density | Normalized thousand Kernel Weight | Yield |
|----------------------------|--------------------------|----------------------------|--------------------------|-----------------------------------|--------------------|
| 1 N1-_N2-_N3- | 0.36 [0.01 ; 0.54] | 0.39 [0.24 ; 0.72] | 0.41 [0.00 ; 0.61] | 0.71 [0.49 ; 0.95] | 0.51 [0.00 ; 0.73] |
| 2 N1-_N2-_N3+ | 0.29 [0.13 ; 0.46] | 0.77 [0.65 ; 0.89] | 0.51 [0.32 ; 0.68] | 0.62 [0.38 ; 0.86] | 0.67 [0.43 ; 0.79] |
| 3 N1-_N2+_N3- | 0.48 [0.44 ; 0.66] | 0.40 [0.29 ; 0.63] | 0.62 [0.52 ; 0.70] | 0.57 [0.42 ; 0.68] | 0.71 [0.65 ; 0.81] |
| 4 N1-_N2+_N3+ | 0.56 [0.44 ; 0.65] | 0.66 [0.51 ; 0.84] | 0.78 [0.71 ; 0.82] | 0.53 [0.35 ; 0.58] | 0.88 [0.83 ; 0.93] |
| 5 N1+_N2-_N3- | 0.58 [0.49 ; 0.68] | 0.34 [0.19 ; 0.46] | 0.55 [0.50 ; 0.71] | 0.51 [0.39 ; 0.61] | 0.68 [0.54 ; 0.85] |
| 6 N1+_N2-_N3+ | 0.62 [0.52 ; 0.69] | 0.54 [0.36 ; 0.64] | 0.77 [0.69 ; 0.87] | 0.51 [0.41 ; 0.63] | 0.91 [0.79 ; 0.95] |
| 7 N1+_N2+_N3- | 0.73 [0.63 ; 0.82] | 0.41 [0.21 ; 0.61] | 0.84 [0.79 ; 0.86] | 0.30 [0.20 ; 0.41] | 0.87 [0.82 ; 0.90] |
| 8 N1+_N2+_N3+ | 0.90 [0.75 ; 1.00] | 0.45 [0.25 ; 0.71] | 0.92 [0.85 ; 1.00] | 0.22 [0.02 ; 0.35] | 0.92 [0.84 ; 1.00] |

Supplementary figure 3: Distribution of normalized yield within each N strategy. Each yield level is colored with the total amount of N provided. The vertical dotted line corresponds to a normalized yield value of 0.9.

