

PCR Output Statistics

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Yield

The absolute mass concentration of newly synthesised amplicons.

Initially, all 1kb amplicons are part of larger 5kb plasmids. 1 amplicon per plasmid. The molar concentration of newly synthesised free-floating amplicons (linear dsDNA, not in plasmids) is thus given by:

$$[amplicon*] = [amplicon]_{final} - [amplicon]_0$$

The mass concentration of newly synthesised amplicons is:

$$y = f_2([amplicon*], bp_{amplicon})$$

$$y \geq 0$$

Where $[amplicon*]$ is in nanomolar.

Note: The amplicons that are in the plasmids will not migrate at the same time on the gel as the newly synthesised amplicons.

Times Amplification

How many times the molar concentration of the amplicon has been amplified from the initial condition.

$$a = \frac{[amplicon]_{final}}{[amplicon]_0}$$

$$a \geq 0$$

This measure uses the final amplicon molar conc (free floating amplicons+amplicons in plasmids) divided by the initial amplicon molar conc (amplicons in plasmids). $a = 1$ if no new amplicons are synthesised. a can be less than 1, if the dsDNA plasmids separate and then bind with primers, so that they cannot reassociate.

If based on mass concentration instead, this measure would give the same result.

Purity

How dominant the newly synthesised amplicon species is, with respect to other species which are not primers, dNTPs, or initial plasmid.

Purity (in terms of % of nt in the reaction mix converted to new amplicons)

How dominant the newly synthesised amplicon species is, with respect to other species which are not primers, dNTPs, or initial plasmid.

The number of single nucleotide bases in newly synthesised amplicons divided by $N_A V$ is:

$$N_{amplicon} = 2bp_{amplicon}[amplicon*]$$

The total number of single nucleotides in the system (calculated from the initial condition of the simulation where only plasmids, primers, dNTPs and polymerase exist) divided by $N_A V$ is:

$$N_{system} = 2bp_{plasmid}[amplicon]_0 + bp_{primer}([p_T]_0 + [p_B]_0) + [dntp]_0$$

Purity is:

$$p = \frac{N_{amplicon}}{N_{system}}$$

$$0 \leq p < 1$$

Purity approaches 1 as all of the nucleotides in the system are converted into amplicons. However p is always less than 1 because not all nucleotides in the initial plasmids can be converted into free-floating amplicons.