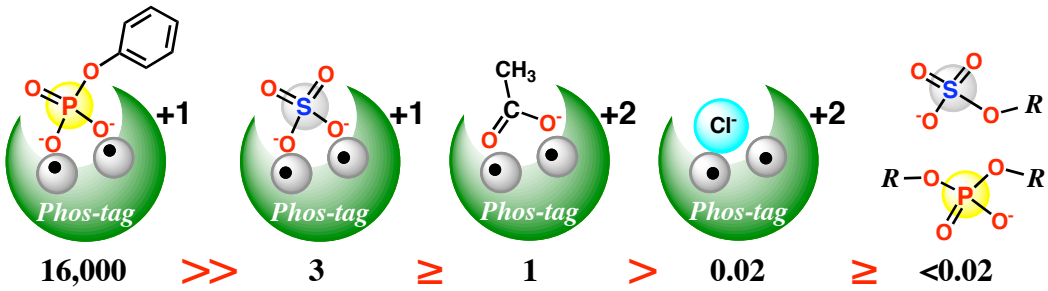
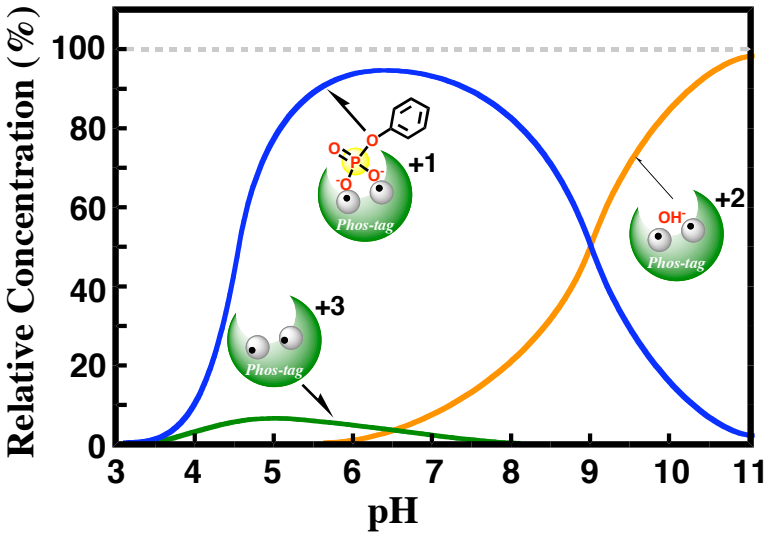
Phos-tag® Chemistry in Solution

1) Anion selectivity indexes of Phos-tag® in H_2O



Phos-tag® 101 series (**+3** ion) selectively captures a phosphomonoester dianion (**–2** ion).
The electric charge of the Phos-tag® 101–phosphomonoester^{2-} complex is **+1**,
which is suitable for MALDI-TOF Mass analysis.
Binding of borate, nitrate, and perchlorate is negligible in H_2O at room temperature.

2) Species distribution of Phos-tag® & phenyl phosphate



Species distribution for an aqueous solution of 10 μM Phos-tag® 101
and 10 μM phenyl phosphate at 25 ˚C with I = 0.10 ($NaNO_3$).

In the low pH region (<3), Phos-tag® 101 series dissociate into two zinc ions and the protonated ligand.
In the high pH region (>9), Phos-tag® 101 series exist almost in hydroxide-bound form.
Monoanionic ROPO$_3$H$^-$ and neutral ROPO$_3$H$_2$ have much less affinity to Phos-tag® 101 series.
At pH >6, phosphomonoesters exist almost in dianionic form (two pK_a values *ca.* 6 and <2).