

# MULTIDENTATE ANION RECEPTORS FOR BINDING GLYPHOSATE DIANION: STRUCTURE AND AFFINITY

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Glyphosate is the most widely used herbicide in the EU (and one of the most widely used in the world). This makes it an important analyte to be monitored in the environment. At neutral pH glyphosate exists predominantly as dianion Gly<sup>2-</sup> and a possible monitoring approach would be using anion sensor based on receptor molecules binding Gly<sup>2-</sup>. Such receptors have been proposed.

For the first time relationships between anion receptor structures and their glyphosate dianion (Gly<sup>2-</sup>) binding affinity have been investigated. For this purpose 12 multidentate bisindolocarbazole, bis-urea and bis-carbazole based synthetic receptors were synthesized and their binding affinities towards Gly<sup>2-</sup> were measured in H<sub>2</sub>O:DMSO media (0.5% to 20% of H<sub>2</sub>O).<sup>1</sup> Computational geometries, as well as 1D and 2D NMR experiments were used to elucidate the structures of the complexes formed on binding of Gly<sup>2-</sup>. As expected, binding affinity depends strongly on the spatial position of the binding moieties, which in turn depend on spacer, length and rigidity. However, the relationships are not straightforward and in some cases are counterintuitive. Evidence is presented that with several receptors binding occurs via the phosphonate moiety only. To the best of our knowledge, receptor **17** described here has the strongest affinity towards Gly<sup>2-</sup> ever reported.

## References

1. Kadam, S. A.; Haav, K.; Toom, L.; Pung, A.; Mayeux, C.; Leito, I. *Eur. J. Org. Chem.* **2017**.



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