# Elucidating the radical C-H functionalization sites on heteroarenes using a radical General-Purpose Reactivity Indicator

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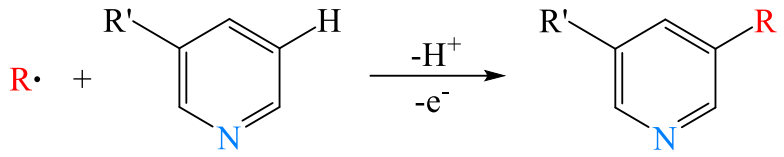
## ABSTRACT

The exploration of radical C-H functionalization on nitrogen heteroarenes has garnered increased to create chemical species with desirable properties [1]. This involves the substitution of C-H bonds with C-R groups within the aromatic ring via radical reactions [2], scheme 1.




**Scheme 1.** Representation of the radical C-H functionalization on heterocycles.

The radical General-Purpose Reactivity Indicator (R-GPRI, $\Xi^0_\alpha$) [3], Equations (1) and (2) has been applied to identify the two most reactive atoms in fourteen nitrogen heteroarenes and compared with the calculated activation barriers for the resulting 140 reactions between 14 heterocycles and 2 radicals,

$$\Xi^0_{nucleophile,\alpha} = (\kappa+1)q^{(0)}_{nucleophile,\alpha} - \Delta N(\kappa-1)f^0_{nucleophile,\alpha} \quad (1)$$

$$\Xi^0_{electrophile,\alpha} = -(\kappa+1)q^{(0)}_{electrophile,\alpha} + \Delta N(\kappa-1)f^0_{electrophile,\alpha} \quad (2)$$

here $q^{(0)}_{nucleophile,\alpha/electrophile,\alpha}$ denotes the atomic charges of each $\alpha$ atom, $f^0_{nucleophile,\alpha/electrophile,\alpha}$ denotes the condensed radical Fukui function, $\kappa$ modulates Equations (1) and (2), and $\Delta N$ is the amount of electron transfer in the reaction.

## References

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