

The Halogen Bond and Opioid Detection

- Reference(s):** 1) “Halogen Bonding in DNA Base Pairs”, Anna Parker, John Stewart, Kelling Donald, Carol A. Parish, *J. Am. Chem. Soc.*, **2012**, *134*, 5165-5172;
- 2) “Halogen Bonding Interactions for Aromatic and Nonaromatic Explosive Detection”, Arjun K. A. Jaini, Lillian B. Hughes, Michael M. Klotz, et al., Levin John Ulep, Michael C. Leopold, Carol A. Parish, *ACS Sens.*, **2019**, *4*, 389-397.

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To halt the progression of the opioid crisis, finding new methods of detection is essential. In this study, density functional theory was employed to determine the strength of halogen bonding interactions between a variety of different opioids and the sensor used for detection, 1,4-diodotetrafluorobenzene. The results of this study yielded binding energies between the sigma hole/X-B acceptor on the sensor and the X-B donor on the opioids to be between -3.73 to -16.53 kcal/mol; accordingly, bond lengths between the specified X-B acceptors and the X-B donors ranged from 2.8 Å to 3.3 Å and these bonded complexes were highly directional. Because these values we obtained are characteristic of halogen bonding, theoretically halogen bonding between opioids and the sensor molecule can occur, opening the possibility for halogen bonding to be used as a detection method for a variety of opioids.