Introduction and Discussion

This study examines the retention of organophosphate and phosphothioate pesticides (OPs) by gas chromatography-mass spectrometry (GCMS) using a BPX90 capillary column (Table 1). Chromatographic characteristics are compared with retention on a non-polar column (BPX) under identical conditions.

The isothermal elution of OPs from BPX5 and BPX90 columns shows no significant correlation (Fig 1). Notable changes in retention characteristics are observed for desorption and OPs carrying a substituent with an extended π-electron system. Retention by BPX5 shows a strong correlation with molecular weight (Fig 2). Barriers to forming a continuous π-electron system over a large π-domain bridge the OP population with planar analytes eluted later than those of similar molecular weight that are out of plane of the ligand.

The same influence on retention is not observed for BPX90. The shift in OP retention between BPX5 and BPX90 shows structure-dependent correlation with the octanol-water partition coefficient (Kow) (Fig 3). Kow is a useful measure of partitioning as it gauges the surface chemistry of the analyte by measuring interactions in a polar environment. The correlation is linear for planar and out of plane conformations.

The out of plane group is further divided with unsaturated and aromatic OPs showing different shifts in retention to those OPs having aliphatic substituents. Rotation of each series away from the vertical (i.e. no difference between phases) to horizontal (i.e. orthogonal retention that is independent of Kow) is a measure of phase orthogonality.

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Conclusion

Retention on a BPX90 column is determined by steric access to the π-electron structure, the presence of hard or soft double bonds (e.g. phosphates and phosphothioates), planar, free rotation and polar nature (Fig 4). In contrast, non-polar retention shows a clear association between molecular weight and, where identical conditions, is attributable to both conventional Henry’s Law behavior and to analytic mobility.

Non-polar retention of OPs may be subdivided on the basis of intramolecular mobility (free rotational barriers and the possibility of through conjugation). In contrast, retention of OPs by the same BPX90 column is complex and influenced by functionality rather than molecular size.

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