Title of research need: Identifying Potential Isomers of New Emerging Drugs

Keyword(s): Emerging Drugs, Isomer, Chemical Structure, GC-MS, Confirmation

Submitting subcommittee(s): Seized Drug

Date Approved: 03/01/2021

Background Information:

1. Does this research need address a gap(s) in a current or planned standard? (ex.: Field identification system for on scene opioid detection and confirmation)
   Yes, there is a standard in development on new psychoactive substances that may address potential isomers, however without the described research, the burden will be left on each individual FSSP to evaluate every new or emerging drug compound for the existence of potential isomers when establishing an analytical scheme.
   This research need focuses on the prediction of potential isomers of new or emerging drug compounds through computational modelling or other means. Additionally, the ability to predict analytical properties of the potential isomers (e.g., retention behavior, mass spectra, spectroscopic signatures) would be invaluable to the seized drug community.

2. Are you aware of any ongoing research that may address this research need that has not yet been published (e.g., research presented in conference proceedings, studies that you or a colleague have participated in but have yet to be published)?
   No.

   None.

4. Review the annual operational/research needs published by the National Institute of Justice (NIJ) at https://nij.ojp.gov/topics/articles/forensic-science-research-and-development-technology-working-group-operational#latest? Is your research need identified by NIJ?
   No.

5. In what ways would the research results improve current laboratory capabilities?
   Being able to identify whether potential isomers exist for new emerging drugs will allow laboratories to make decisions about the testing and reporting of unknown compounds. The ability to predict retention behavior or spectral information of predicted isomers will provide additional information for the identification, and discrimination, of new emerging drugs.
6. In what ways would the research results improve understanding of the scientific basis for the subcommittee(s)?

The ability to predict the potential for isomers, as well as predict retention behavior or spectral information for emerging drugs would allow the subcommittee to draft guidance on the identification of unknown compounds.

7. In what ways would the research results improve services to the criminal justice system?

The ability to predict potential isomers for new and emerging drugs would assist the criminal justice system by providing preemptive data on what other drugs may be seen on the market based on those currently identified. This type of information could also assist in more rapid scheduling of compounds and would allow forensic laboratories to be more aware of instances where isomeric drug species could be present.

8. Status assessment (I, II, III, or IV):

<table>
<thead>
<tr>
<th>No or limited current research is being conducted</th>
<th>Major gap in current knowledge</th>
<th>Minor gap in current knowledge</th>
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<tbody>
<tr>
<td>Existing current research is being conducted</td>
<td>II</td>
<td>IV</td>
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This research need has been identified by one or more subcommittees of OSAC and is being provided as an informational resource to the community.