Supplementary Information

The use of single particle aerosol mass spectrometry for the automated non-destructive identification of drugs in complex samples

Audrey N. Martin[†‡], George R. Farquar[†*], Paul T. Steele[†], A. Daniel Jones[‡], Matthias Frank[†]

[†]Lawrence Livermore National Laboratory, 7000 East Ave., Livermore, California 94550

[‡]Michigan State University, 212 Biochemistry, East Lansing, Michigan 48824

This supplementary information includes the additional rules trees used to classify the drug samples used in this study.

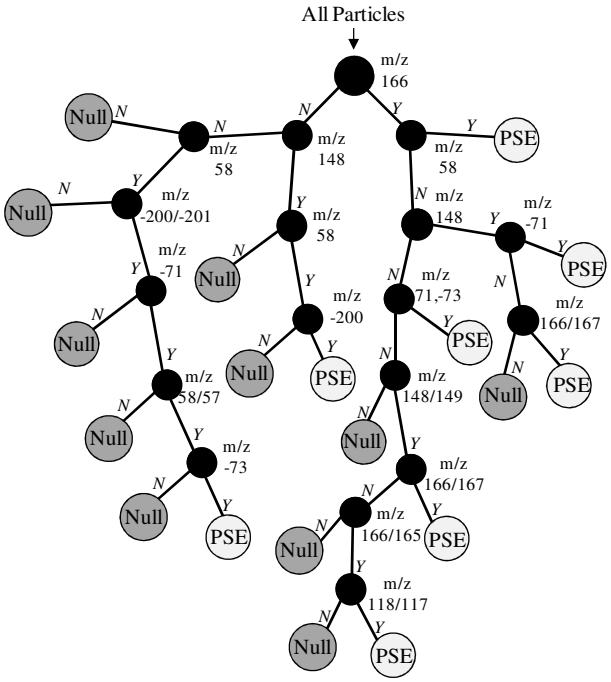

Figure S- 1: Rules tree for classification of pseudoephedrine. The mass vectors probed at each branch division are shown, with 'Y' indicating a positive response and 'N' indicating a negative response. Circles labeled 'PSE' indicate a positive identification for pseudoephedrine; circles labeled 'Null' indicate a negative response.

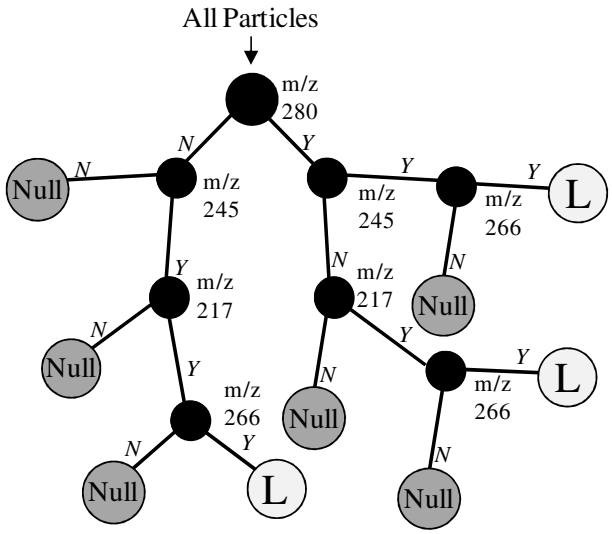

Figure S- 2: Rules tree for classification of loratadine. The mass vectors probed at each branch division are shown, with 'Y' indicating a positive response and 'N' indicating a negative response. Circles labeled 'L' indicate a positive identification for loratadine; circles labeled 'Null' indicate a negative response.

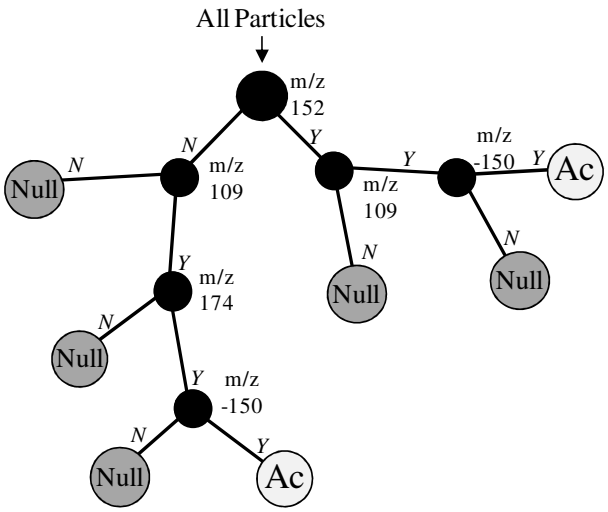

Figure S- 3: Rules tree for classification of acetaminophen. The mass vectors probed at each branch division are shown, with 'Y' indicating a positive response and 'N' indicating a negative response. Circles labeled 'Ac' indicate a positive identification for acetaminophen; circles labeled 'Null' indicate a negative response.

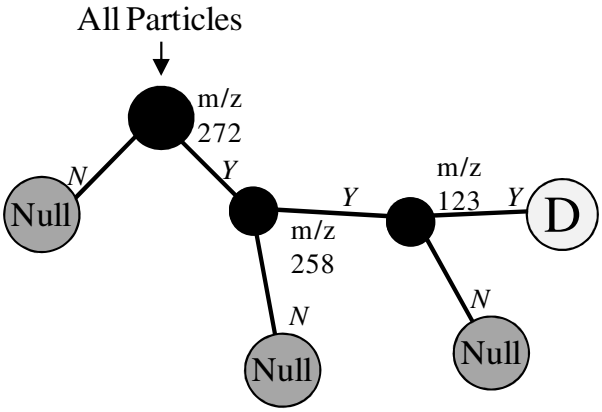

Figure S- 4: Rules tree for classification of dextromethorphan. The mass vectors probed at each branch division are shown, with 'Y' indicating a positive response and 'N' indicating a negative response. Circles labeled 'D' indicate a positive identification for dextromethorphan; circles labeled 'Null' indicate a negative response.

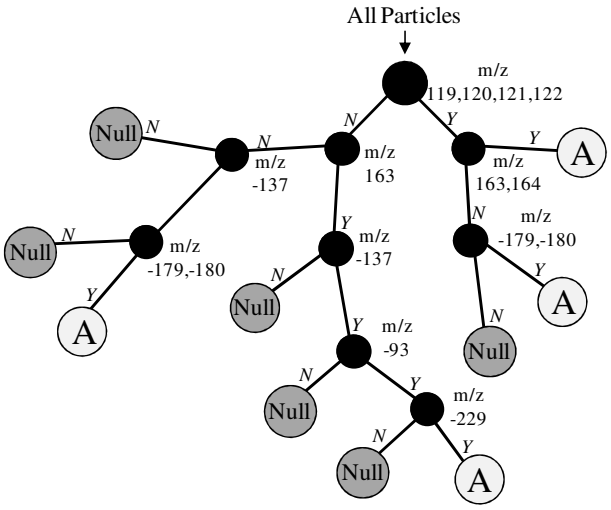

Figure S- 5: Rules tree for classification of aspirin. The mass vectors probed at each branch division are shown, with 'Y' indicating a positive response and 'N' indicating a negative response. Circles labeled 'A' indicate a positive identification for aspirin; circles labeled 'Null' indicate a negative response.

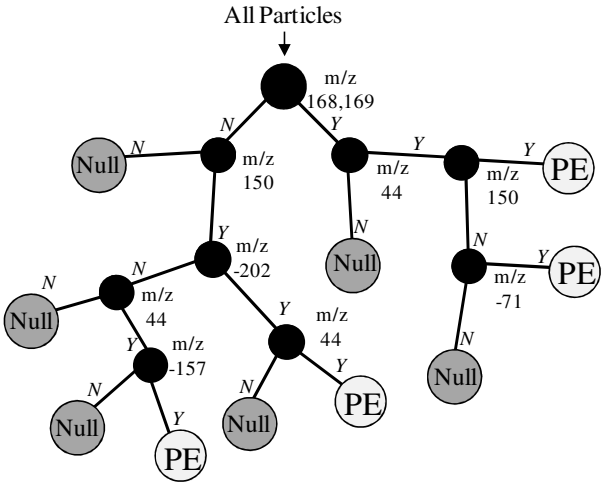

Figure S- 6: Rules tree for classification of phenylephrine. The mass vectors probed at each branch division are shown, with 'Y' indicating a positive response and 'N' indicating a negative response. Circles labeled 'PE' indicate a positive identification for

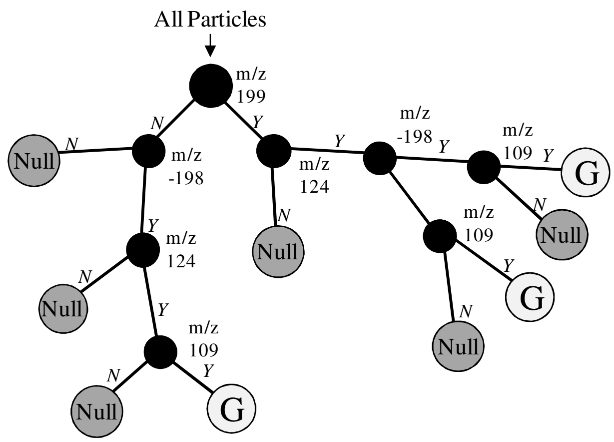

Figure S- 7: Rules tree for classification of guaifenesin. The mass vectors probed at each branch division are shown, with 'Y' indicating a positive response and 'N' indicating a negative response. Circles labeled 'A' indicate a positive identification for aspirin; circles labeled 'Null' indicate a negative response.

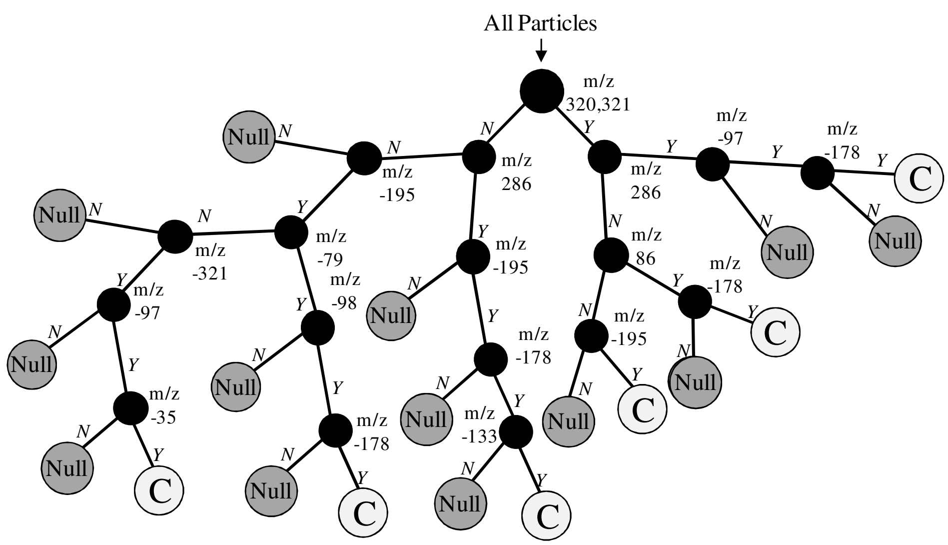

Figure S- 8: Rules tree for classification of chloroquine. The mass vectors probed at each branch division are shown, with 'Y' indicating a positive response and 'N' indicating a negative response. Circles labeled 'A' indicate a positive identification for aspirin; circles labeled 'Null' indicate a negative response.