

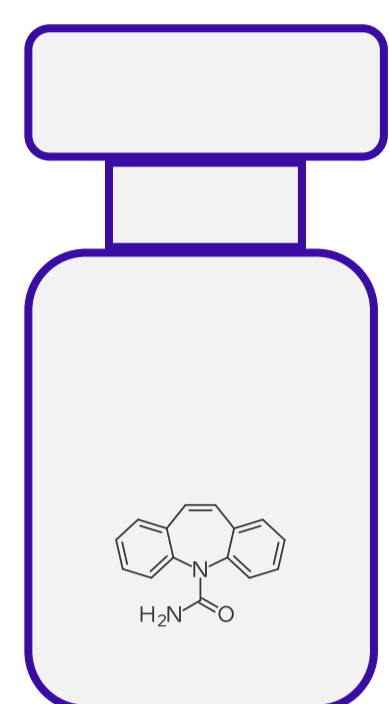
ISOMERS IN NON-TARGET SCREENING

Anneli Kruve,^{a,b} Jaanus Liigand,^c Masoumeh Akhlaqi,^a Wei-Chieh Wang,^a Claudia Möckel^a

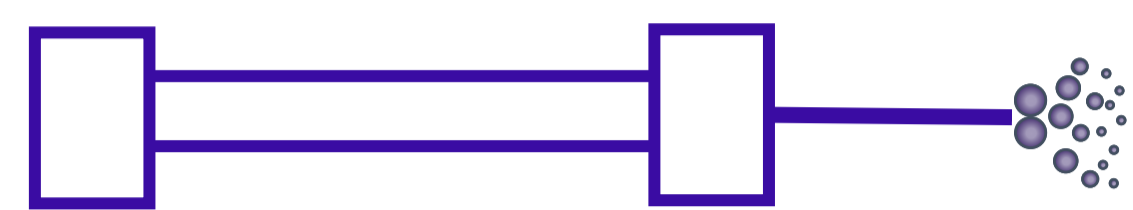
^a Department of Materials and Environmental Chemistry, Stockholm University

^b Department of Environmental Science, Stockholm University

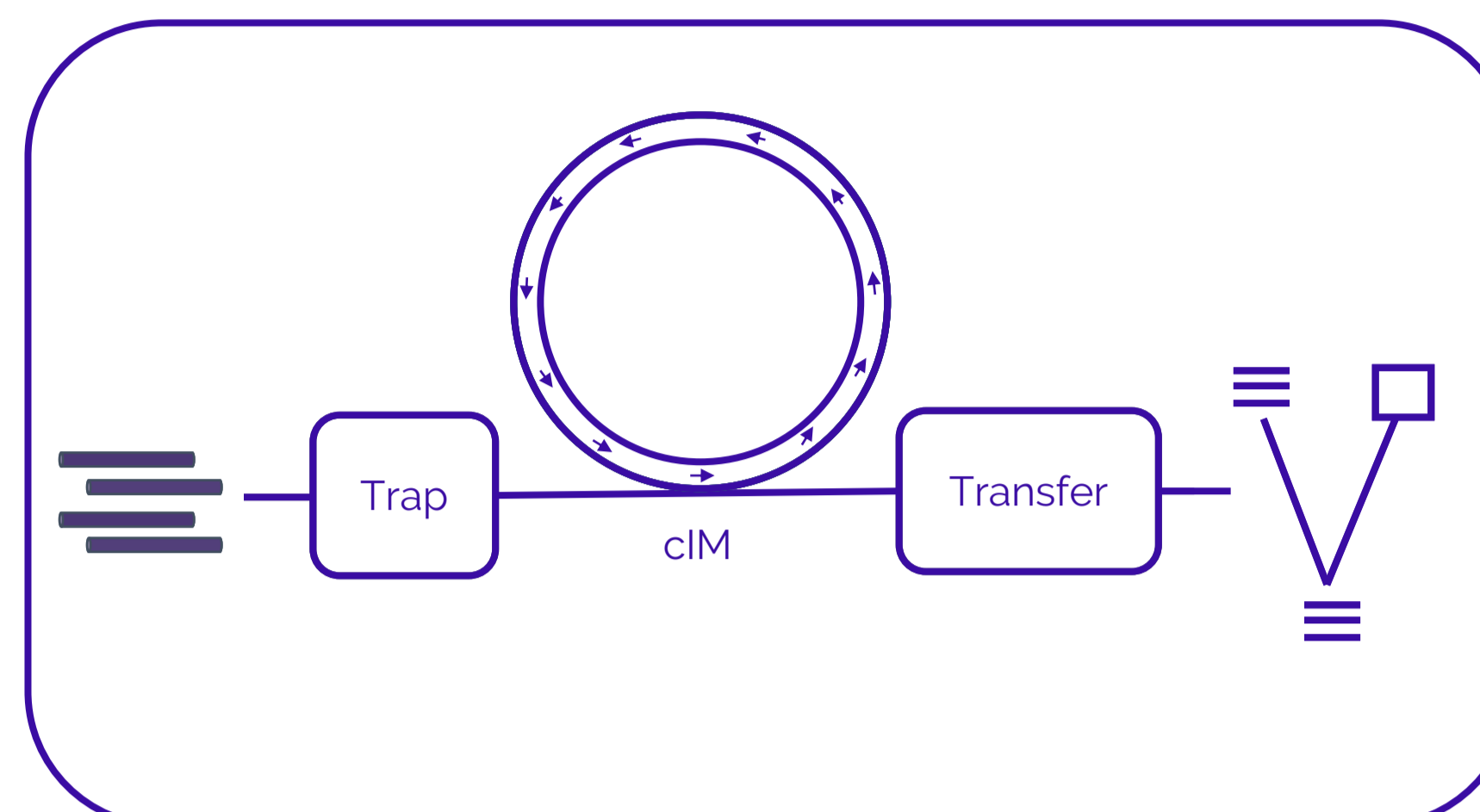
^c Quantem Analytics



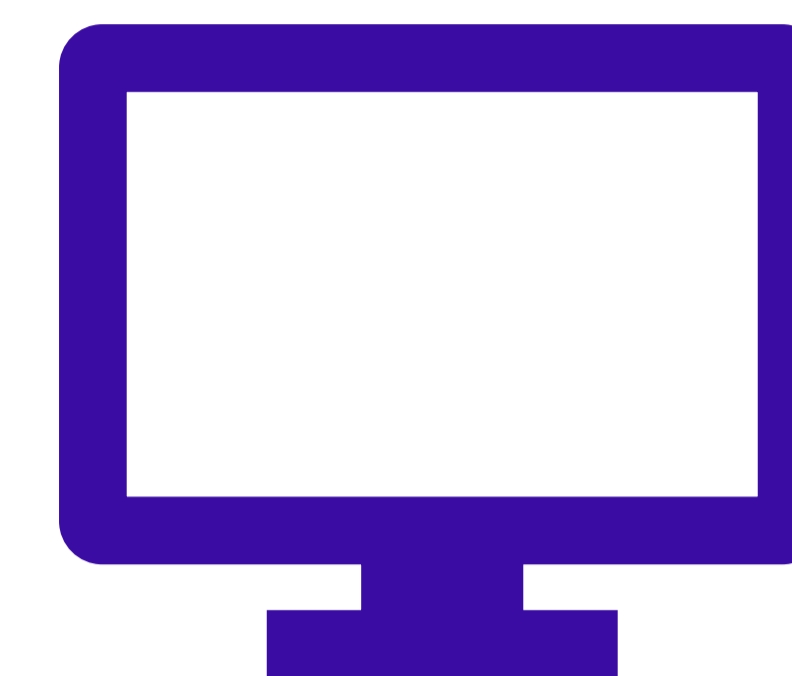
14
isomeric
chemicals



C18 150 × 3.0 mm
0.1% formic acid & MeCN
5 to 100% in 20 min

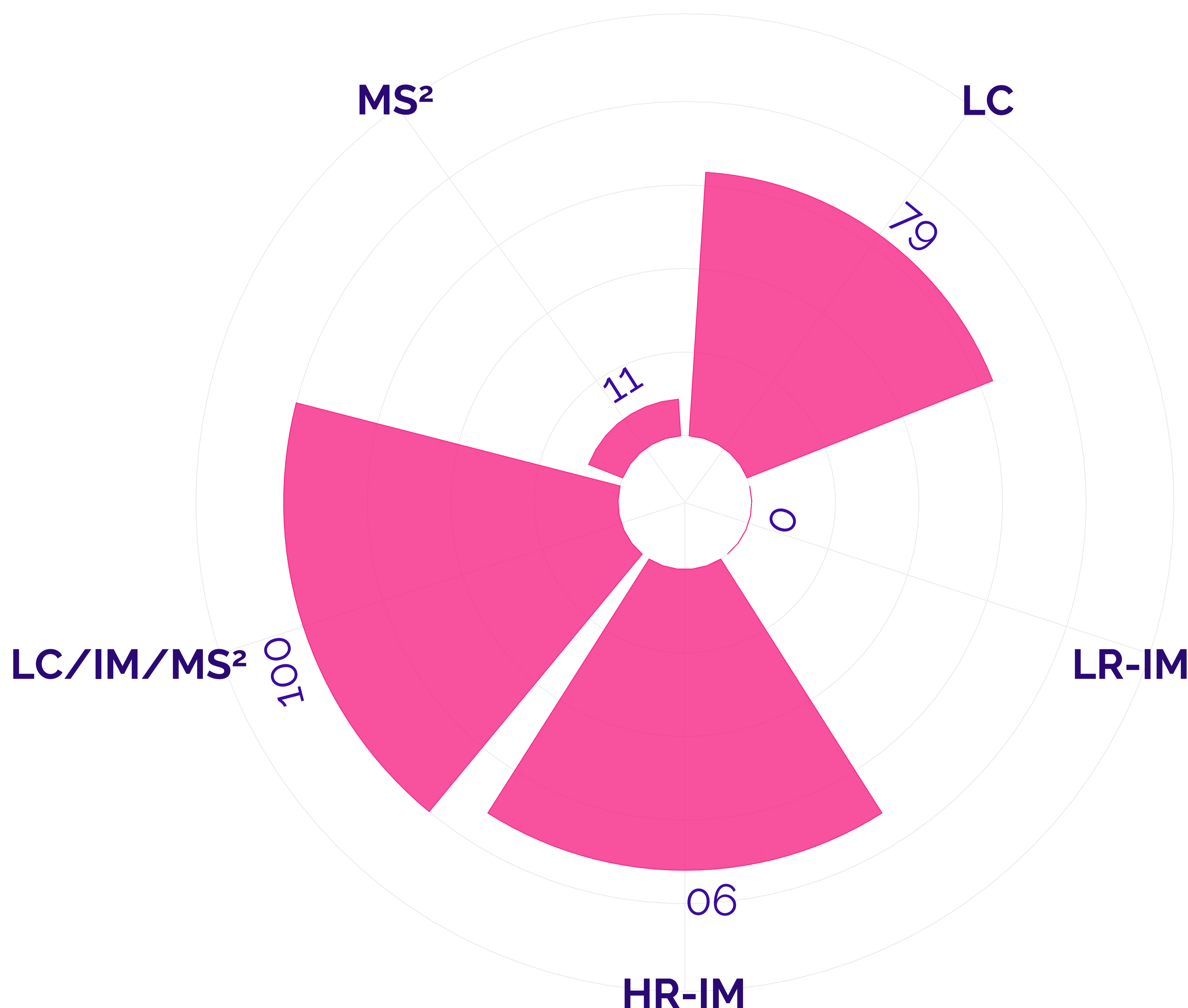


Q Exactive Orbitrap
DDA, inclusion list
&
Cyclic IMS
LR-IM: single pass
HR-IM: multiple pass



SIRIUS+CSI:FingerID
&
CFM-ID

none of the pairs of isomeric candidate structures could be distinguished with *in-silico* methods



retention time and high resolution ion mobility were most efficient in distinguishing pairs of isomeric candidate structures if analytical standards were available