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Build, Weigh, and Eat Molecules - Scalable Activities Coupled with Breath Analysis Using Direct Analysis in Real Time Mass Spectrometry

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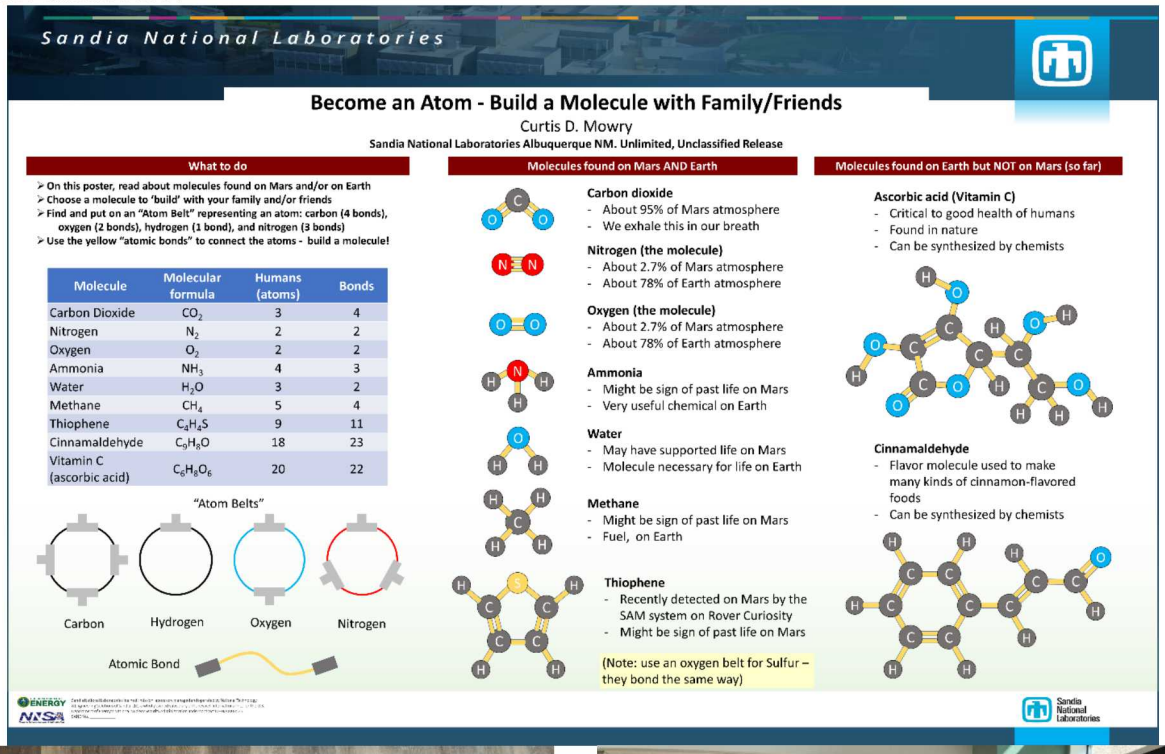
Introduction: Communicating mass spectrometry in relatable and interactive ways can be challenging. Successfully developing audience-appropriate lessons showing mass spectrometry "in action" depends on instrument and time availability, and lab safety. We participate in "Take Our Daughters and Sons to Work Day®", workplace "Family Day", and frequent customer tours that require short demonstrations, high throughput, and adjustable educational language. The typical separation/detection analyses in our lab require too much time or are not sufficiently interactive. We've developed scalable activities that are fun, rapid, and interactive for all ages and education levels: human atom-belts, weigh-a-molecule, and DART-MS breathalyzer. As serial activities, we've hosted a 2.5-hour event for all-ages (~200 visitors) and multiple 6-hour events for 5-12th graders and parents (over 400 visitors each). In these instances, each visitor spends ~30 minutes or less, but interaction and instruction time could easily be increased if less throughput is needed.

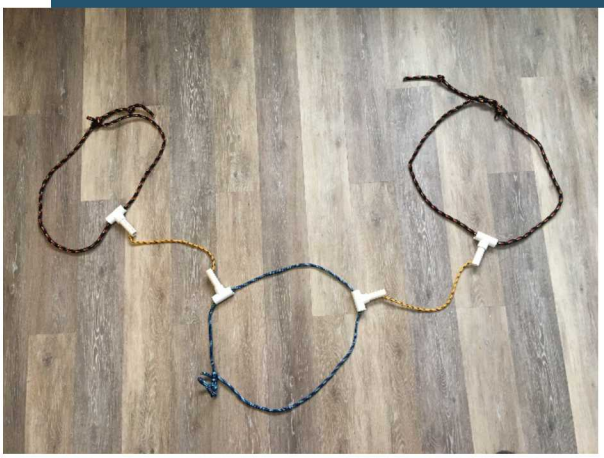
Methods: Each activity has been used as a stand-alone lesson and in series to reinforce concepts. Human atom-belts consist of wearable belts made with ropes and PVC tubing components. With pictorial examples of compounds, each participant "becomes" an atom and bonds with others to form a human-based molecule. Weigh-a-molecule uses 3D-printed molecular models and double-pan balances to introduce and discuss molecular weight concepts by comparison and reference weights. The final activity uses a "breathalyzer" consisting of a Direct Analysis in Real Time (DART-) interfaced Thermo Instruments Velos Pro linear ion trap mass spectrometer (MS). Participants eat candy/gum (unknown to analyst), breathe into the MS source, and the analyst identifies their food choice(s) by the molecules detected – in real time. Level-appropriate information is discussed. Advanced experiments for adult or technical tours are described.

Results and Discussion: We have performed the first two activities, human atom-belts and weigh-a-molecule, in elementary school classrooms individually. Here we used them in series as flow-control prior to the breathalyzer demonstration for a large 2.5-hour Family Day event with approximately 200 attendees ranging from 5 to 85 years old. Human atom-belts were prepared from rope and PVC tees to create bonding sites. Bonds consisted of PVC tubing and short lengths of rope. Volunteers and a poster guided the free form building of molecules such as water, CO_2, and cinnamaldehyde.

The following materials can be used to make a minimum of 24 atom-belts and 22 bonds: 200 ft of 3/8 in. diameter rope (~$24), two 15-packs of PVC tees (~$10), 10 ft. of 2 in. diameter PVC pipe (~$2). Bonds are made using a 2.5 in. length of PVC pipe with a hole drilled to accept the rope, and 18-24 in. of rope knotted at ends to retain the

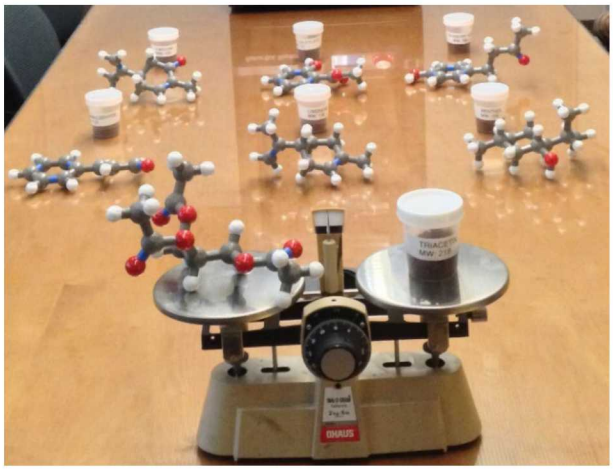
PVC. Atom belts are made with a 66 in. (5.5 ft.) length of rope – adjustability created with a taught-line knot. The loose end of the belt has either a figure-eight or a bow-line knot to prevent the belt from being deconstructed, and knots are secured with a small dab of hot-glue. The photos show completed ropes and volunteers demonstrating a water molecule.

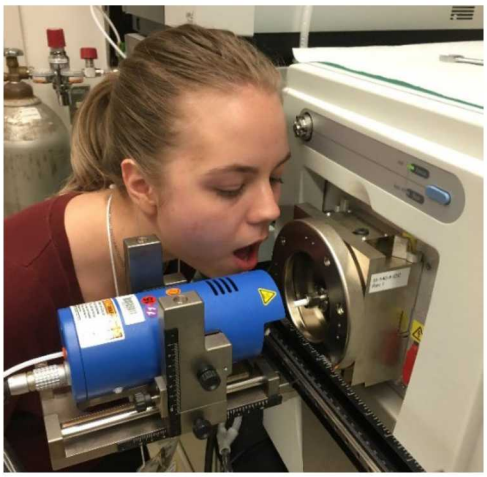




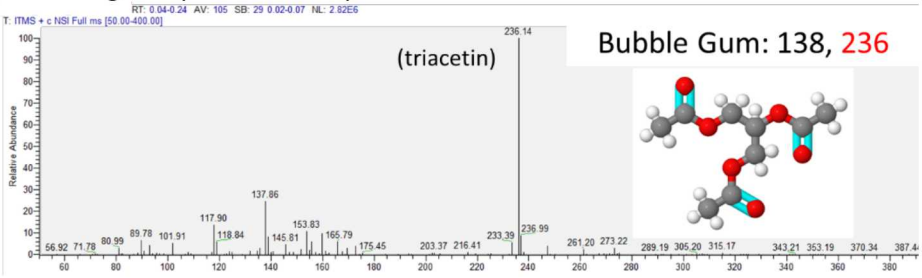
While building molecules, groups (~15 people) were assigned and escorted to the weigh-a-molecule demonstration. Multiple 3D-printed molecules (corresponding to those detected later in the breathalyzer) and double-pan balances were available. Other types of models could be utilized. Volunteers discussed how atomic weights lead to molecular weights. Plastic cups with sand were used as calibration weights to compare the models and thus identify the molecules. Double-pan balances were specifically used to focus on "more atoms equals a heavier molecule", *i.e.,* relative weights are used to avoid confusion with respect to <u>model</u> weight versus <u>molecule</u> weight.

On a 10-15 minute cycle (depending on visitor load) groups were then escorted to the lab for a breathalyzer experiment. Food items (eaten prior to entering the lab) included cinnamon or root-beer flavored candy, bubble gum, cherry cough drops, or breath mints. Upon breathing into the MS source, soft ionization produced m/z peaks from each breath, *e.g.*, protonated methyl salicylate (m/z 153 – root beer candy), menthol (m/z 156 - mint), and cinnamaldehyde (m/z 133 – cinnamon gum/candy) were detected. Multiple-candy "spoof" attempts were detected. Chosen candies enabled rapid identification with a high success rate (>90%). "Advanced" groups were shown MS/MS revealing cocaine and/or methamphetamine on their paper currency.





Ammoniated triacetin in bubble gum (not a flavor) was also detected.



The activities are flexible, allowing for different topics (food chemistry, forensics, etc.), and different educational levels. It is important to pre-test candy available at your site as sometimes formulations and availability change! We utilized an ion trap but other analyzers (quadrupole, triple quadrupole) could be used. We have also used various themes such as: "food is chemistry", "bubblegum CSI", "did you eat a molecule today?".

Novel Aspect: Scalable activities for a rapid, fun, and interactive mass spectrometry instructional event adjustable to different educational levels.

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