Accelerated Aging and Analysis of High Explosives via a Novel Two-Dimensional Gas Chromatography Method

Colleen L. Ray PhD
Chris E. Freye PhD
Q-5 High Explosives Science and Technology

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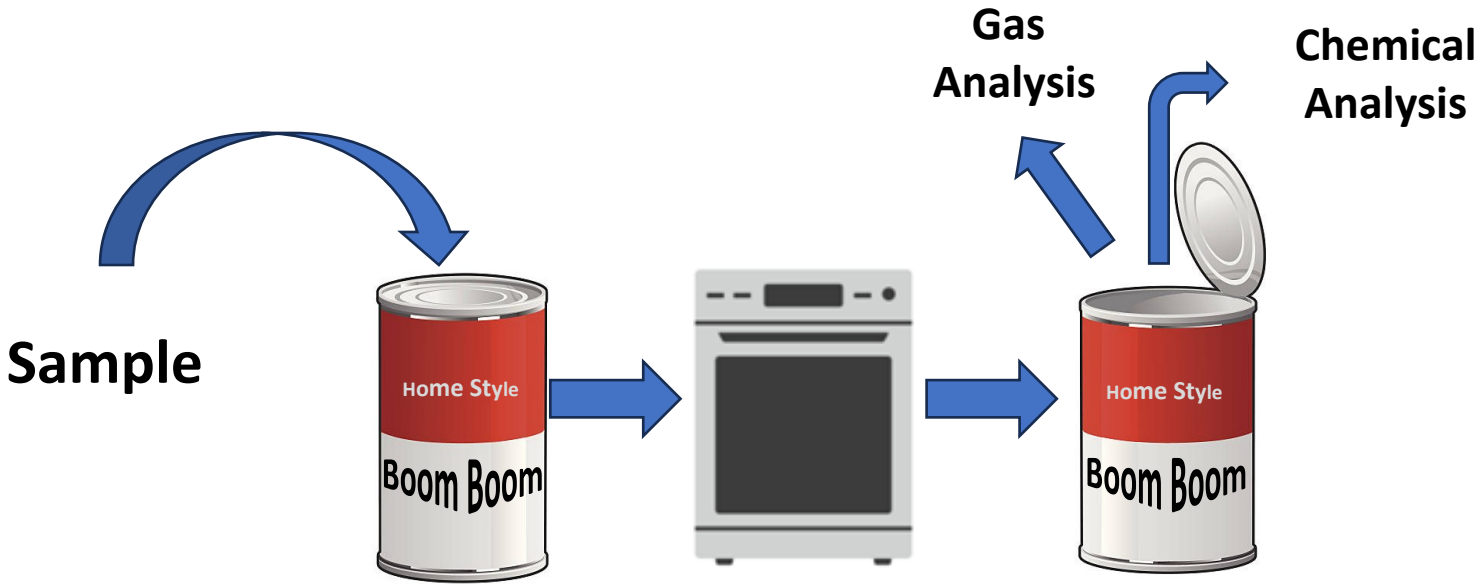
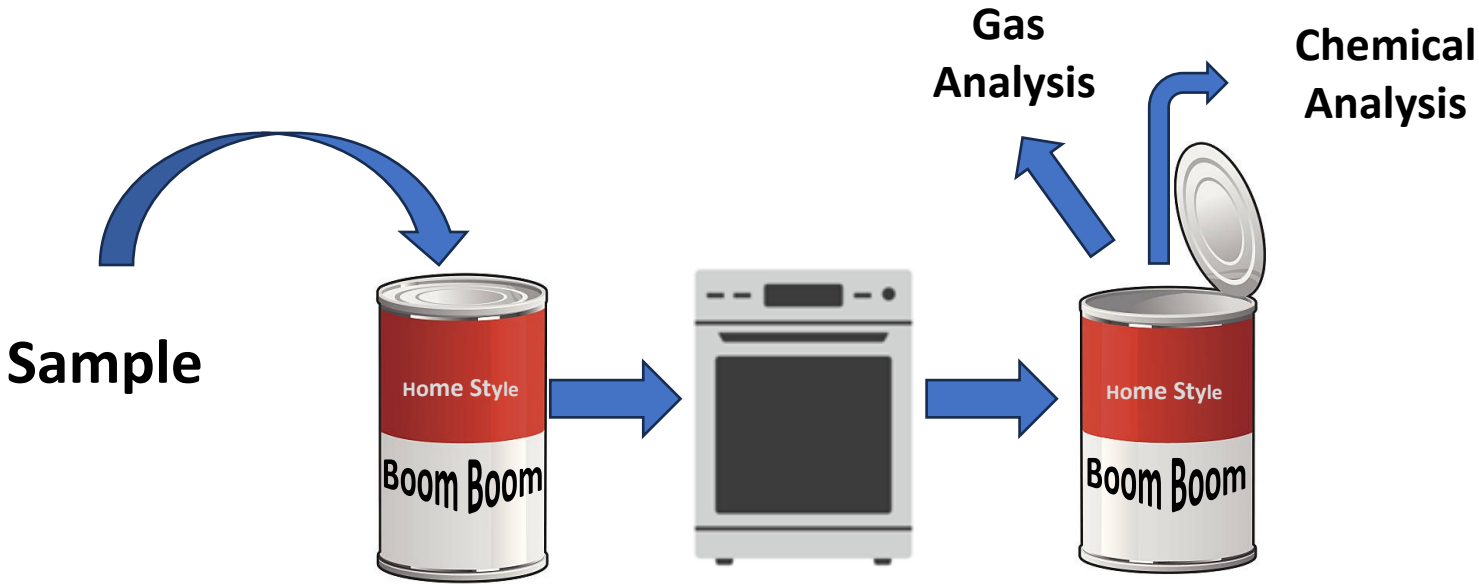
High Explosives Aging Studies

- What are they?
  - Determines the chemical and physical changes high explosives experience over time
- Why do we do it?
  - HE tends to sit around a while
  - Determine performance, safety, etc.
- How do we age it?
  - The all-natural old-fashioned way
    - Not practical
  - Accelerated aging
    - Much more practical but assumptions abound

(some) Traditional Accelerated Aging Studies



(some) Traditional Accelerated Aging Studies

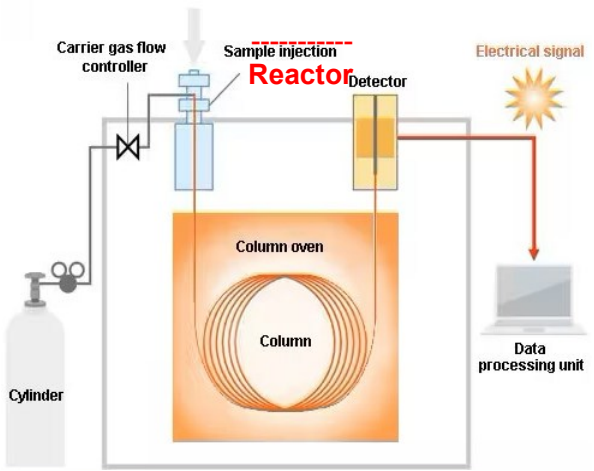


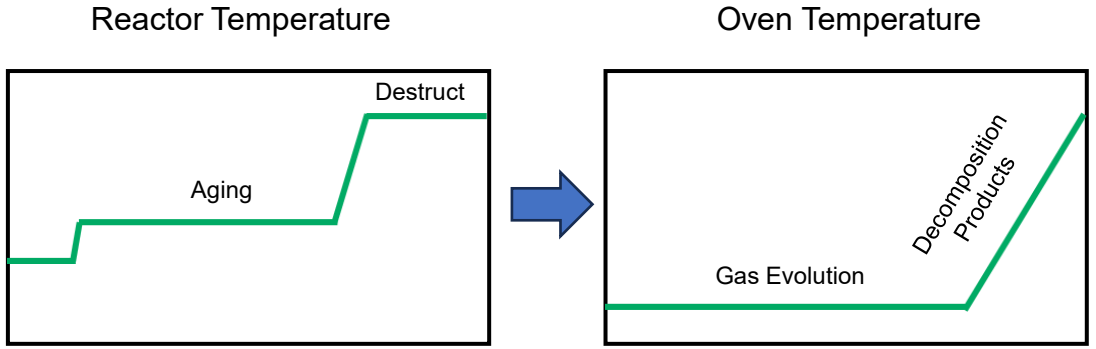
Time investment: YEARS

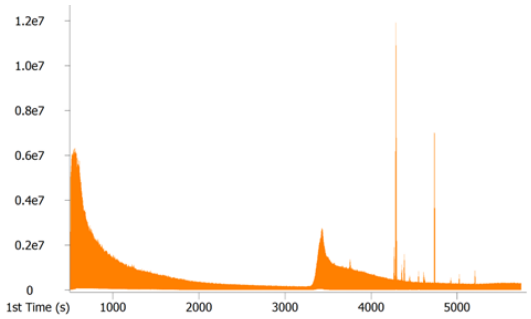
Automated, Rapid, In-Situ Aging of Compound C

- GC×GC coupled to LECO Pegasus HRT
  - Separation of complex degradation products
- The inlet on this GC is precisely temperature controlled
  - Let's try that as an aging vessel!
  - Added bonus: high resolution mass spectrometer analyzes aging products in real time
  - Inert atmosphere

Automated, Rapid, In-Situ Aging of Compound C With Gas Chromatography Mass Spectrometry





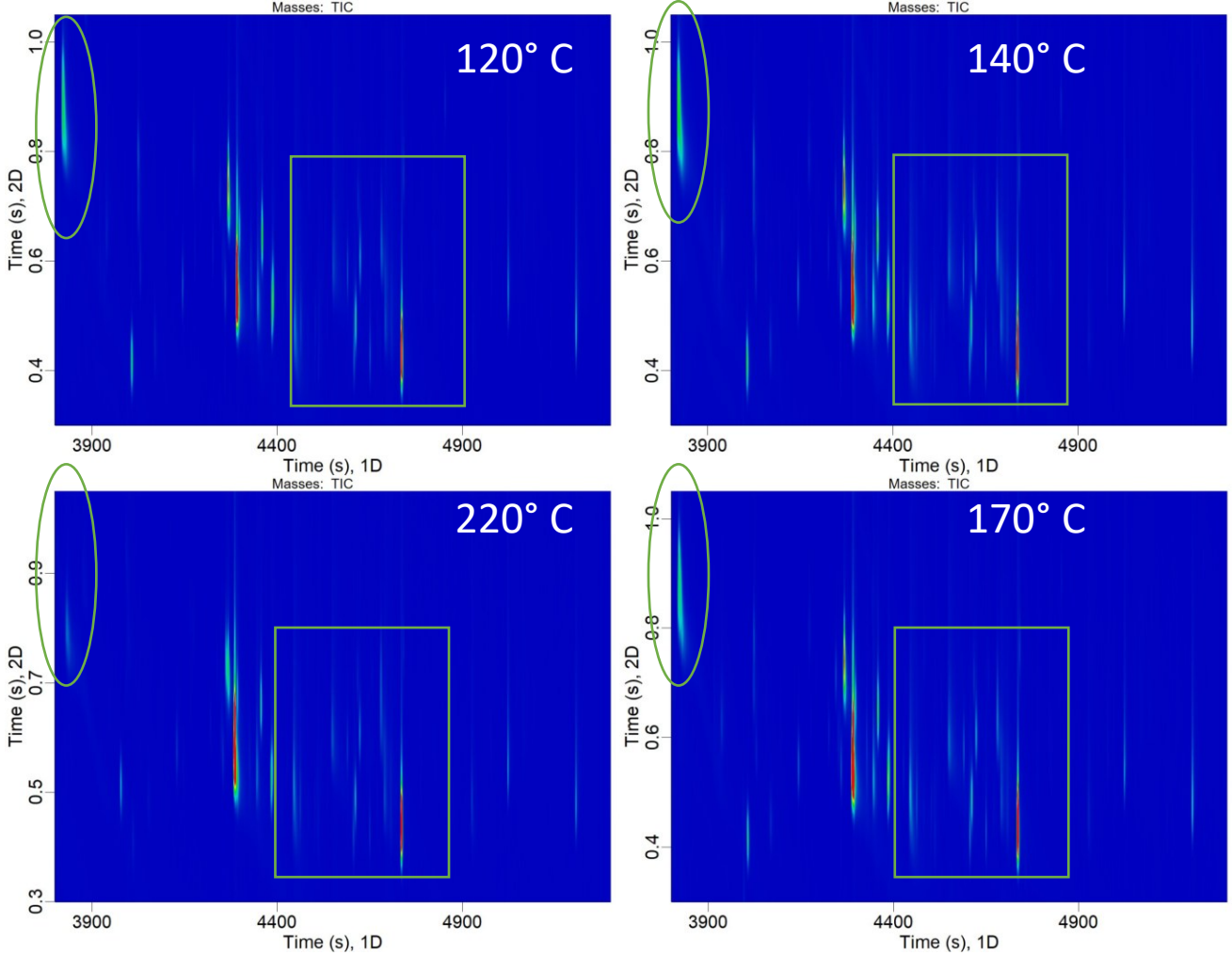


Total Ion Chromatogram (TIC)

TIC excluding gaseous species

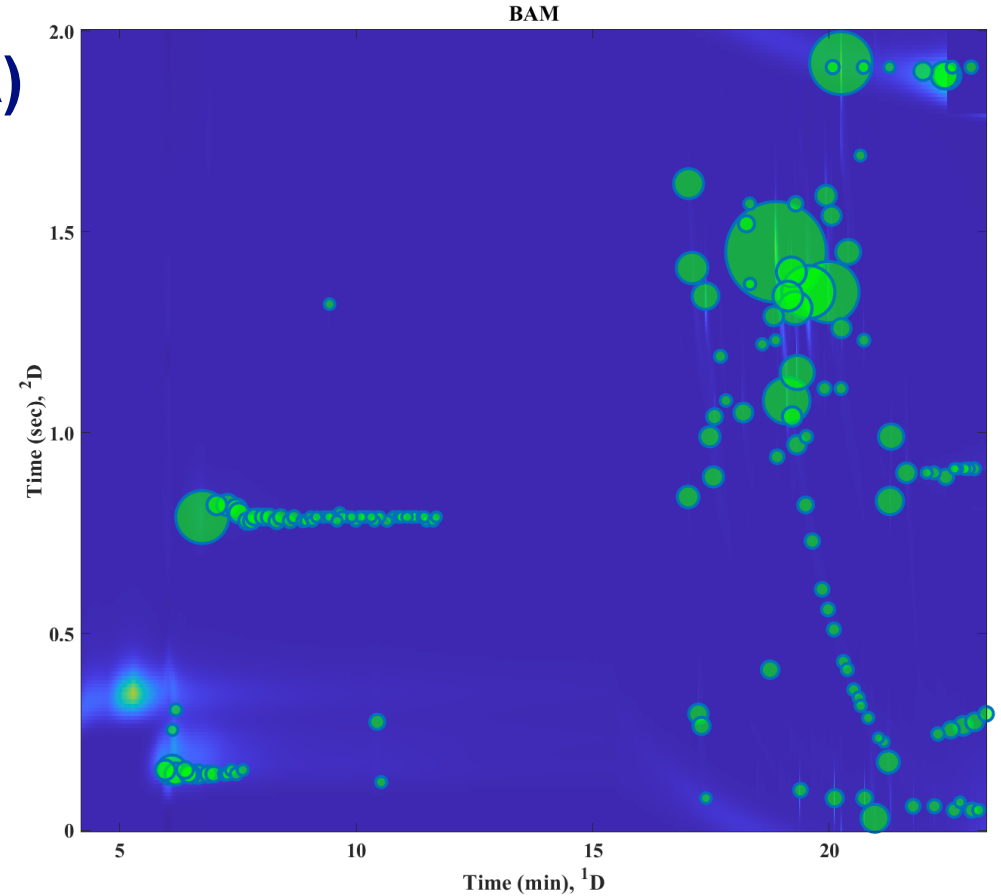
Compound C GC×GC Post-aging

- Dozens of samples
- Gigabytes of data
- Many subtle differences



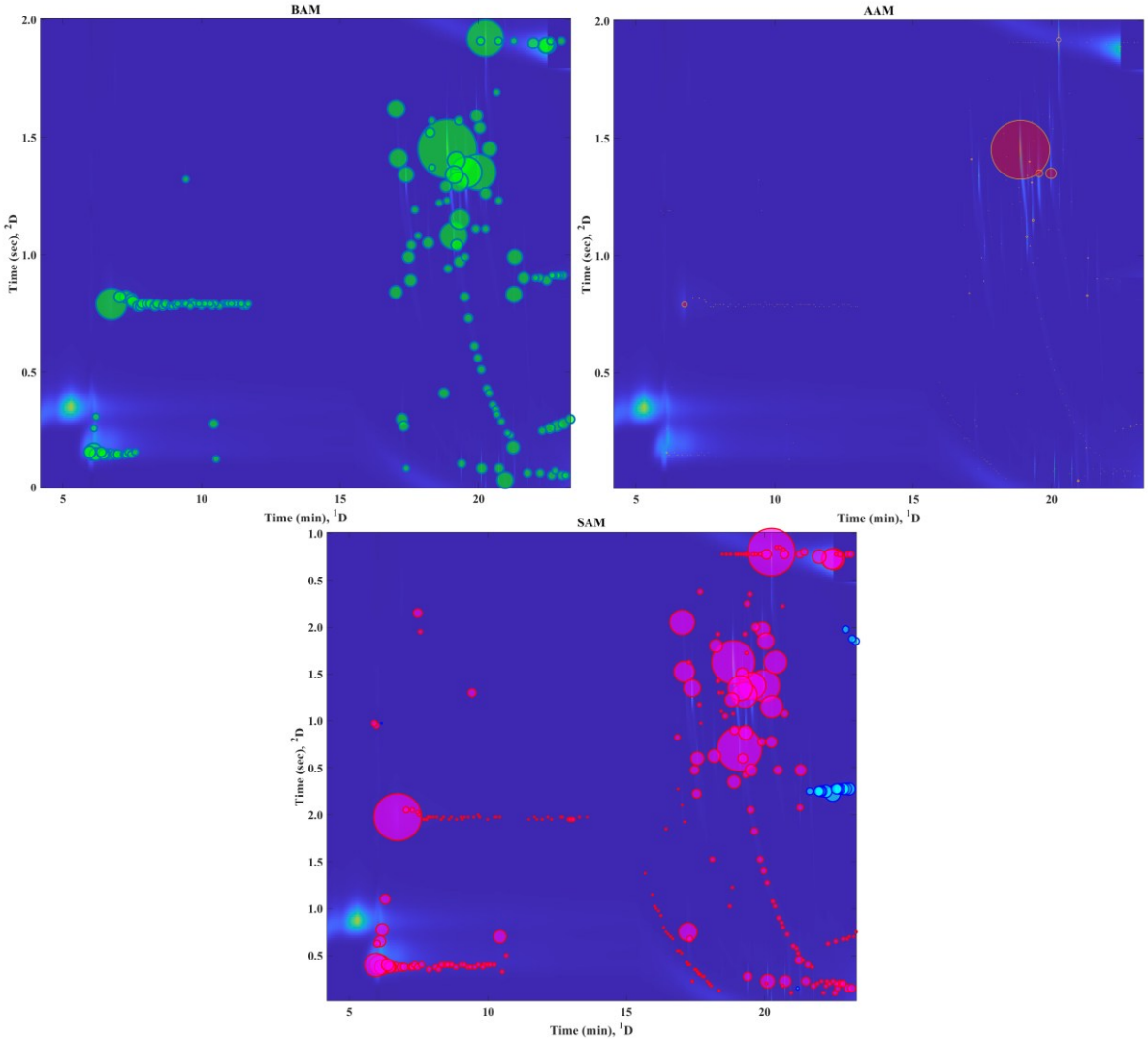
ALteration Analysis (ALA)

- Identifies regions of change across samples
- Processes massive datasets in a matter of minutes
- Basic (BAM), Synchronous (SAM), and Asynchronous (AAM) alteration maps



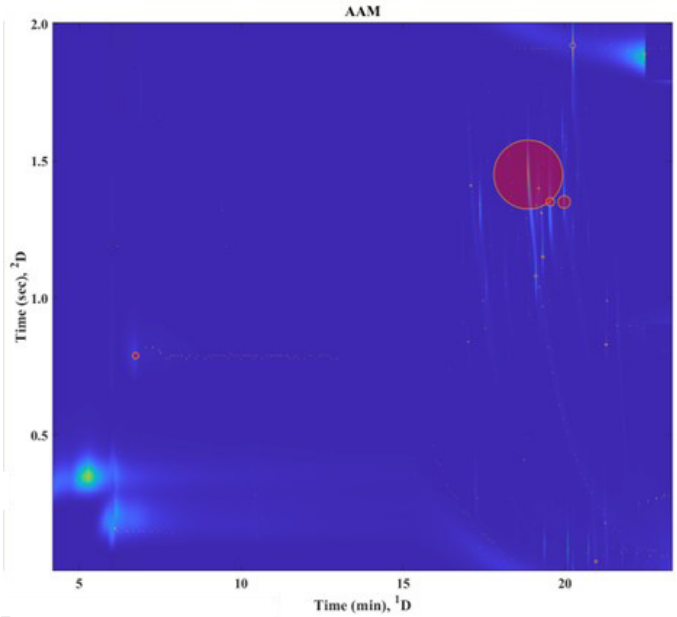
ALA Continued

- Alteration maps reveal both the location and nature of change



Hit List

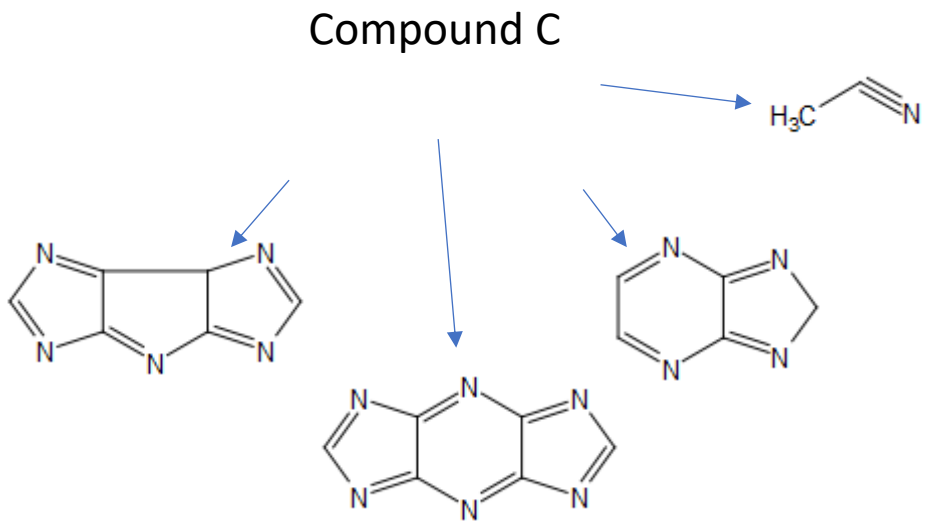
- The generated hit list gives relevant information in numerical format
  - Location
  - ALA scores
  - m/z responsible for the score



'Pin2d'	'Pin1d'	'BAM'	'SAM'	'AAM'	'Tile 1D'	'Tile 2D'	'Grid #'	'Wraparound'	'Top mz BAM'	'Top mz SAM'	'Top mz AAM'	'Num m/z BAM'	BAM	SAM	AAM
145	1765	1	0.540583	1	295	7	4	0	74	74	74	448	120	120	120
192	1930	0.393451	0.643305	-0.00511	322	10	3	0	99	99	99	448	145	145	145
135	1898	0.372611	0.289032	0.032622	317	7	3	0	74	74	74	448	120	120	120
135	1847	0.279036	0.211473	0.015398	308	7	4	0	68	68	68	448	114	114	114
79	309	0.278014	0.644761	0.008143	52	4	4	0	35	35	35	448	81	81	81
108	1792	0.21715	0.564924	-0.00117	299	6	2	0	75	75	75	448	121	121	121
1	2764	0.139557	-0.11647	0.000293	461	1	3	0	74	74	47	448	120	120	93
115	1819	0.116094	0.057304	0.001277	304	6	3	0	114	114	114	448	160	160	160
131	1814	0.109801	0.185426	-0.00051	303	7	3	0	35	35	35	448	81	81	81
141	1552	0.098207	0.123683	0.000545	259	7	1	0	50	50	50	448	96	96	96

Identification of Important Products

- Alteration map allows the analyst to focus on important compounds
  - Look at what changes
  - Then, what *doesn't* change
- In this case dozens of products were identified
  - Purine-like bicyclics
  - A variety of tricyclics
  - The world's most expensive ACN



Future Work

- More explosives!
  - Compare data to existing aging study data
- Compatibility of HE with other materials
  - Binding agents
  - Packaging materials
- Compatibility of inert materials

Questions?

Thanks to:

Aging and Lifetimes

High Explosives & Energetics