AMS vs. NIST Database
Fragmentation Patterns for Pure Organic Molecules

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AMS vs. NIST spectra-Questions

• How comparable are the mass spectra?

• Are there any systematic biases?

• How does it affect analysis of organics?
**Anthracene**

1. 928 941R 38.0P (M) Anthracene
2. 922 936R 29.8P (M) Phenanthrene
3. 893 914R 8.45P (M) Diphenylacetylene
4. 891 894R 7.79P (M) Dibenz[a,e]7,8-diazabicyclo[2.2.2]octa-2,5-diene
5. 887 940R 6.58P (M) 9H-Fluorene, 9-methylene-

**Succinic Acid**

1. 790 937R 66.6P (M) Butanedioic acid
2. 736 763R 13.0P (M) Succinamic acid
3. 736 746R 13.0P (M) Methylmalonic acid
4. 681 689R 2.53P (M) Imidazole, 2-[[beta-carboxy]propionyl]amino-
5. 646 690R 0.63P (M) Dianhydrodulcitol
**Malic Acid**

1. 723 819R 60.8P (M) 3,3-Dimethyl-4-methylamino-butan-2-one
2. 664 708R 11.0P (M) L-Guanidinosuccinimide
3. 639 788R 3.35P (M) Acetaldehyde
62 541 594R 0.07P (M) Malic acid

**Anthracene**

$r = 0.992$
Oleic Acid

\[ r = 0.948 \]

Malic Acid

\[ r = 0.286 \]
# of Carbons in molecule

**m/z 44 Ratio AMS**

**m/z 44 Ratio NIST**

**# of Carbons in molecule**

**Peak Intensity / Total Ratio**

**Oxygen/Carbon Ratio**

- $y = 0.146x$  \( R=0.817 \)
- $y = 0.173x$  \( R=0.805 \)
AMS vs. NIST spectra

What we know

- Aromatic hydrocarbons close agreement

- Some bias towards lower $m/z$ (more fragmentation) for long, aliphatic species

- Oxygenated compounds thermally decompose to $\text{CO}_2/\text{H}_2\text{O}$