Combined Ambient Ionization Mass Spectrometric and Chemometric Approach for the Differentiation of Hemp and Marijuana Varieties of *Cannabis sativa*

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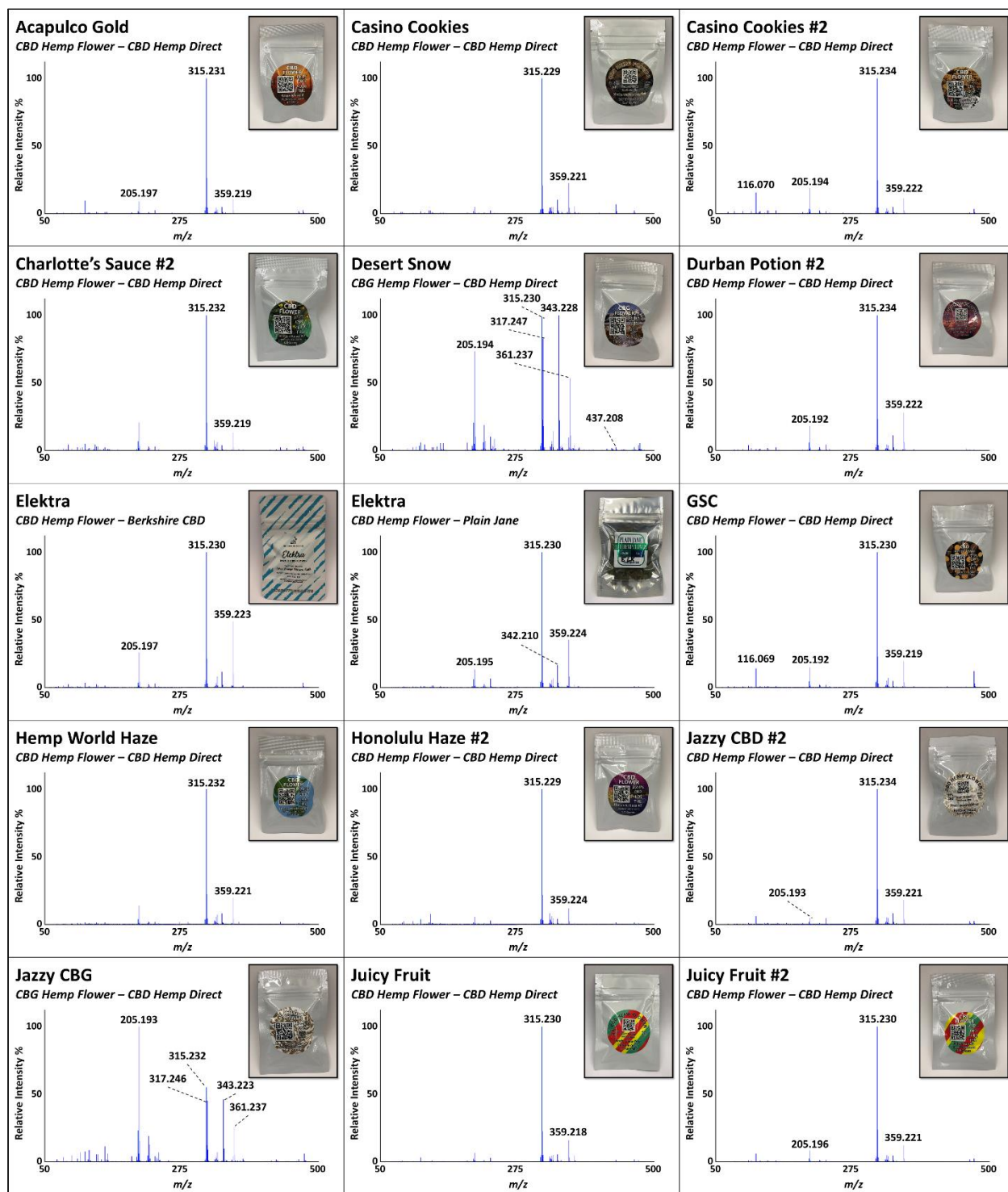**Supporting Information: Mass Spectral Data for *C. sativa* Materials**

Figure S1. Representative DART high-resolution mass spectra of hemp samples used in the training set analyzed in positive-ion mode at 20 V. Images of the corresponding products in their packaging are shown in the insets.
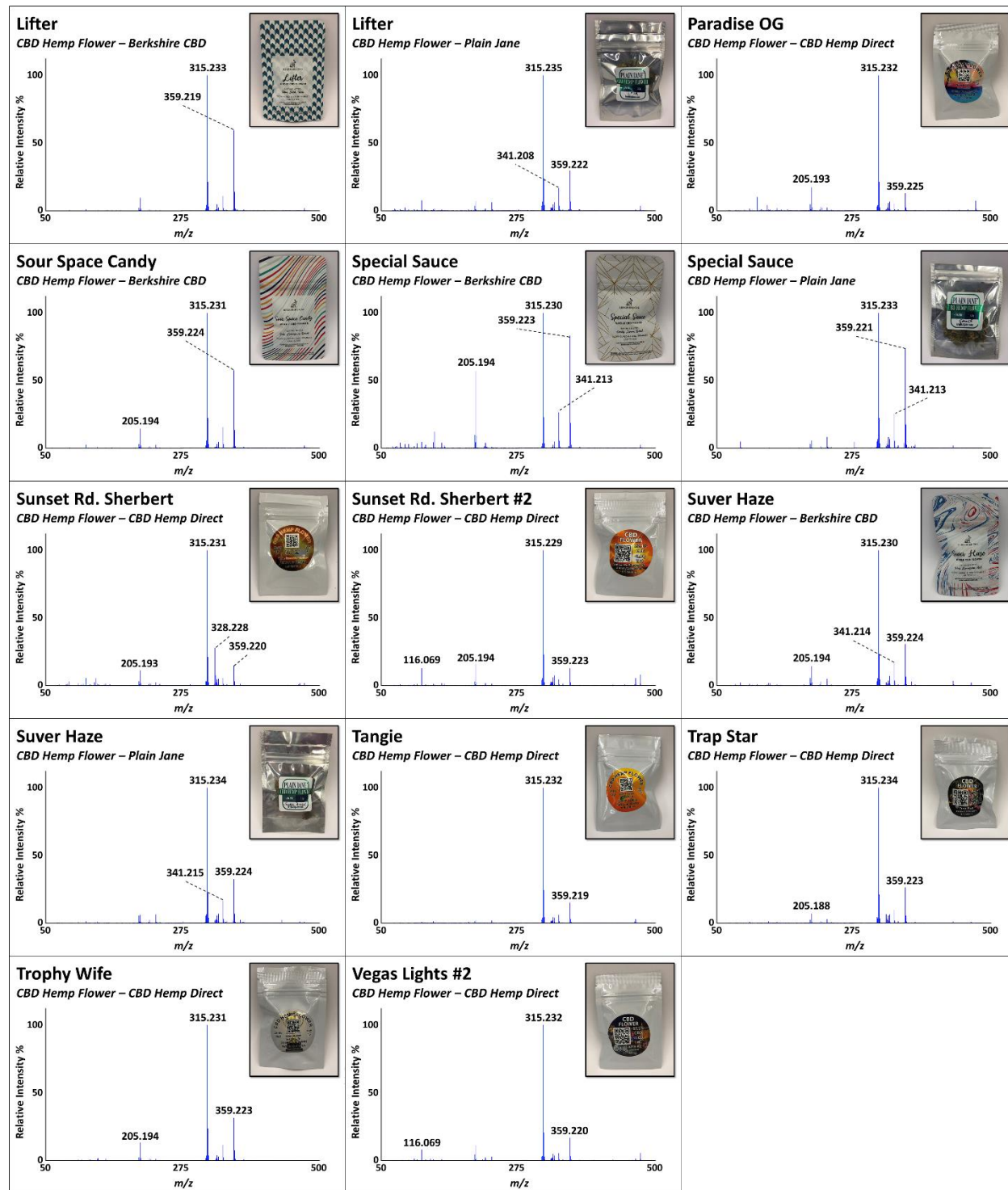
Lifter
CBD Hemp Flower – Berkshire CBD

Relative Intensity %
315.233
359.219
m/z

Lifter
CBD Hemp Flower – Plain Jane

Relative Intensity %
315.235
341.208
359.222
m/z

Paradise OG
CBD Hemp Flower – CBD Hemp Direct

Relative Intensity %
315.232
205.193
359.225
m/z

Sour Space Candy
CBD Hemp Flower – Berkshire CBD

Relative Intensity %
315.231
359.224
205.194
m/z

Special Sauce
CBD Hemp Flower – Berkshire CBD

Relative Intensity %
315.230
359.223
205.194
341.213
m/z

Special Sauce
CBD Hemp Flower – Plain Jane

Relative Intensity %
315.233
359.221
341.213
m/z

Sunset Rd. Sherbert
CBD Hemp Flower – CBD Hemp Direct

Relative Intensity %
315.231
328.228
359.220
205.193
m/z

Sunset Rd. Sherbert #2
CBD Hemp Flower – CBD Hemp Direct

Relative Intensity %
315.229
116.069
205.194
359.223
m/z

Suver Haze
CBD Hemp Flower – Berkshire CBD

Relative Intensity %
315.230
341.214
359.224
205.194
m/z

Suver Haze
CBD Hemp Flower – Plain Jane

Relative Intensity %
315.234
341.215
359.224
m/z

Tangie
CBD Hemp Flower – CBD Hemp Direct

Relative Intensity %
315.232
359.219
m/z

Trap Star
CBD Hemp Flower – CBD Hemp Direct

Relative Intensity %
315.234
359.223
205.188
m/z

Trophy Wife
CBD Hemp Flower – CBD Hemp Direct

Relative Intensity %
315.231
359.223
205.194
m/z

Vegas Lights #2
CBD Hemp Flower – CBD Hemp Direct

Relative Intensity %
315.232
359.220
116.069
m/z

Figure S1 (continued). Representative DART high-resolution mass spectra of hemp samples used in the training set analyzed in positive-ion mode at 20 V. Images of the corresponding products in their packaging are shown in the insets.
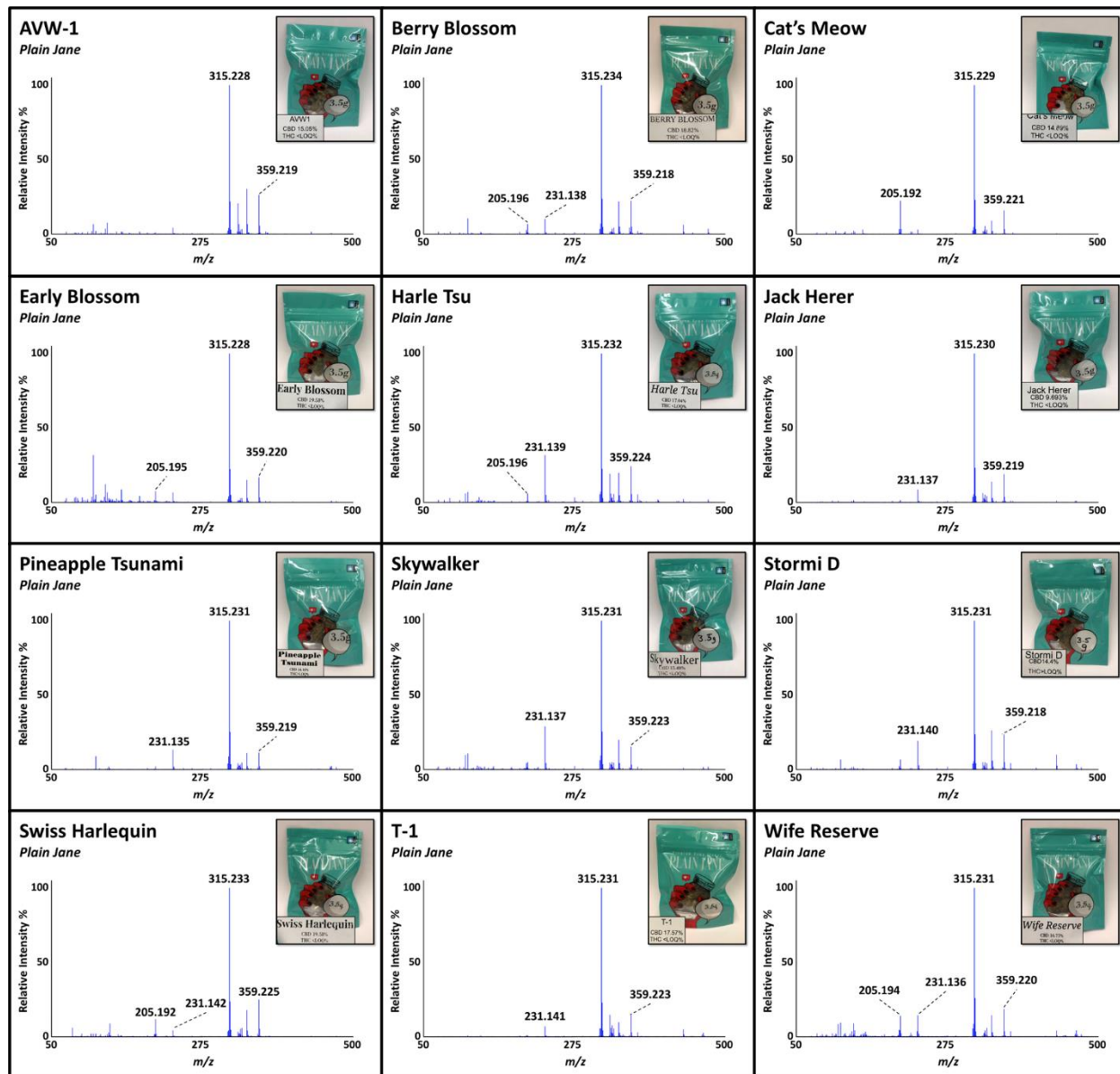
Figure S2. Representative DART high-resolution mass spectra of hemp flower samples from a commercial hemp vendor analyzed in positive-ion mode at 20 V. These samples were used to test the ability of the model to classify "unknowns". Images of the corresponding packaging are shown in the insets.

A0001
Marijuana – NIST

Relative Intensity %

100 — 315.232
50 —
116.069 205.197 359.227
50 — 275 — 500
m/z

A0007
Marijuana – NIST

100 — 161.161
315.233
50 —
205.193
50 — 275 — 500
m/z

A0009
Marijuana – NIST

100 — 315.233
50 —
161.162
50 — 275 — 500
m/z

A0027
Marijuana – NIST

100 — 315.236
50 —
161.165 205.195 359.228
50 — 275 — 500
m/z

A0076
Marijuana – NIST

100 — 315.229
50 —
116.070 161.162 205.194
50 — 275 — 500
m/z

A0096
Marijuana – NIST

100 — 315.234
50 —
161.163
50 — 275 — 500
m/z

A0102
Marijuana – NIST

100 — 315.232
50 —
205.198
50 — 275 — 500
m/z

A0115
Marijuana – NIST

100 — 315.233
50 —
205.195
50 — 275 — 500
m/z

Low THC/Very High CBD
Marijuana – NIH/NIDA

100 — 315.233
341.212
50 — 359.224
106.091 205.194
50 — 275 — 500
m/z

Medium THC/CBD
Marijuana – NIH/NIDA

100 — 315.232
50 —
203.177 341.211 359.222
106.086
50 — 275 — 500
m/z

High THC/Low CBD
Marijuana – NIH/NIDA

100 — 315.231
50 — 359.221
106.091 205.193
50 — 275 — 500
m/z

Very High THC/Low CBD
Marijuana – NIH/NIDA

100 — 315.232
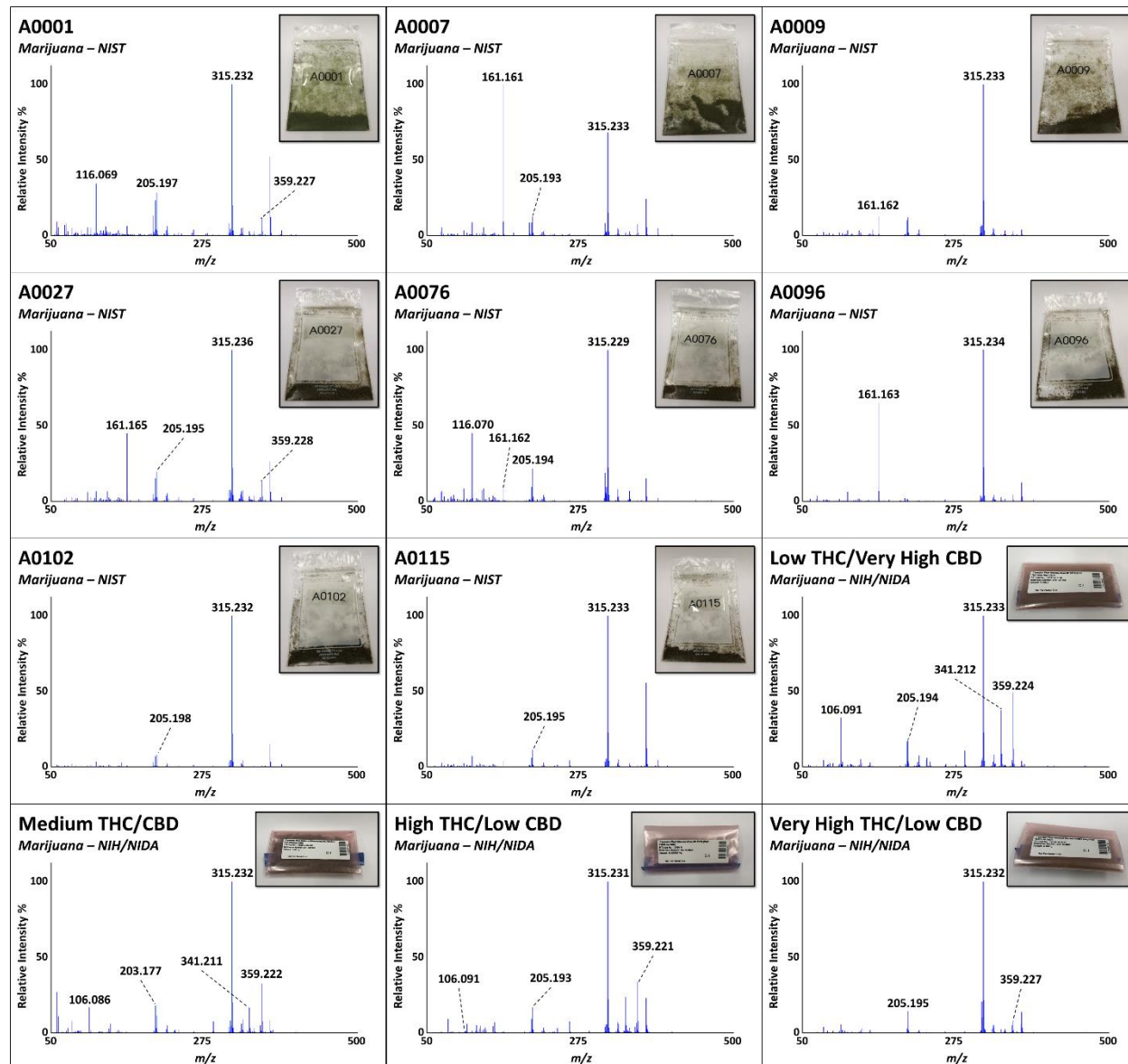50 — 359.227
205.195
50 — 275 — 500
m/z

Figure S3. Representative DART high-resolution mass spectra of marijuana samples from DEA-registered suppliers analyzed in positive-ion mode at 20 V. Images of the corresponding packaging are shown in the insets.
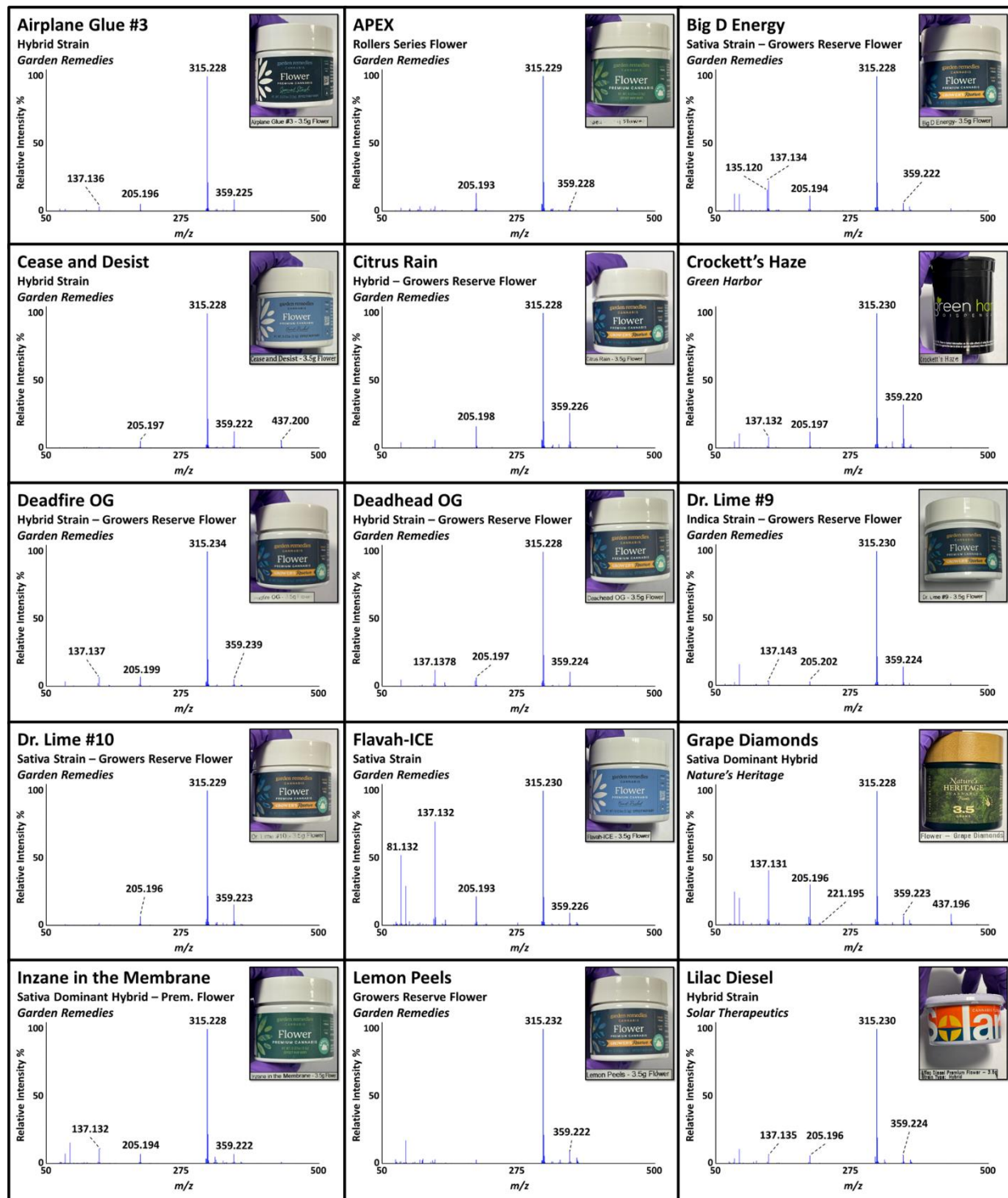
Figure S4. Representative DART high-resolution mass spectra of marijuana flower samples from a recreational *Cannabis* dispensary analyzed in positive-ion mode at 20 V. Images of the corresponding packaging are shown in the insets.
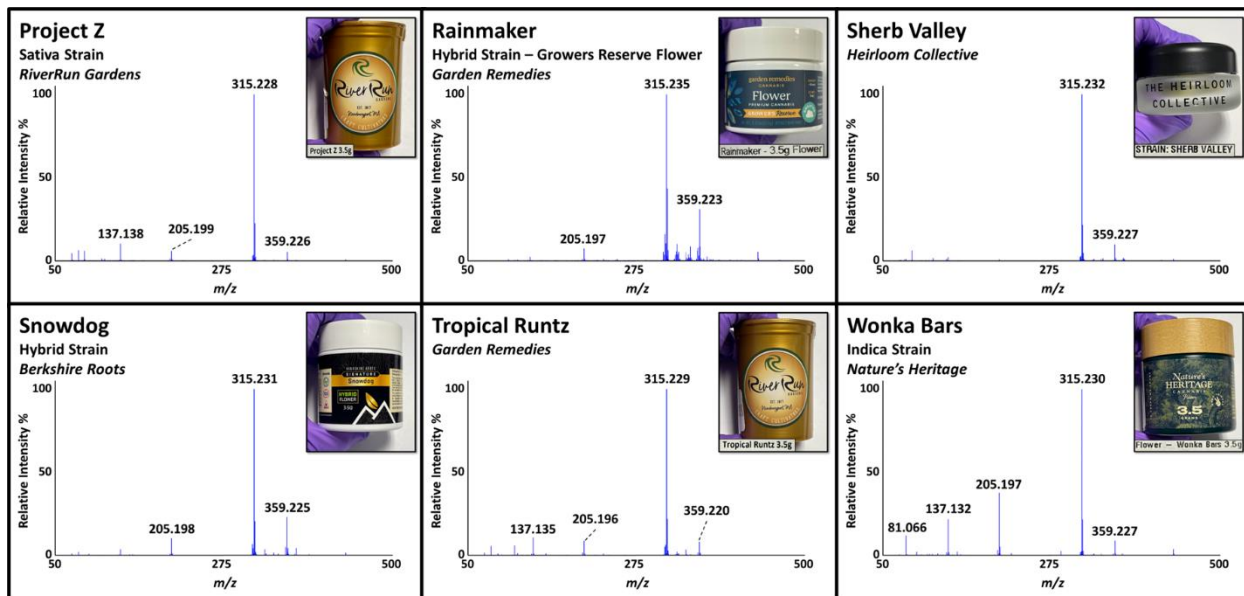
Figure S4 (continued). Representative DART high-resolution mass spectra of marijuana flower samples from a recreational *Cannabis* dispensary analyzed in positive-ion mode at 20 V. Images of the corresponding packaging are shown in the insets.