

# Preliminary studies into the effect of environmental degradation on the characterisation of automotive clear coats by attenuated total reflectance infrared spectroscopy

Georgina Sauzier,<sup>a</sup> Mark Maric,<sup>a</sup> Wilhelm van Bronswijk,<sup>a</sup> and Simon W. Lewis<sup>a\*</sup>

<sup>a</sup> Department of Chemistry, Curtin University, GPO Box U1987, Perth, Western Australia 6845, Australia, E-mail: S.Lewis@curtin.edu.au; Tel: +61 8 9266 2484

## Supporting Information

**Table S1:** Discriminant values of samples exposed to Western Australian environmental conditions, averaged over an eight-month exposure period.

Sample	0	1	2	3	4	5	6	7	8
MMM001	-245.8	<b>-6.0</b>	-306.2	-249.4	-90.9	-50.9	-203.0	-157.0	-30.5
MMM031	-117.5	-127.7	-384.2	-108.7	-58.8	-95.9	-81.5	<b>-4.8</b>	-206.5
MMM397	-13.7	-194.5	-256.8	<b>-4.9</b>	-42.3	-143.1	-17.8	-77.2	-260.4

**Table S2:** Discriminant values of a test sample taken from a Suzuki Swift vehicle, averaged from six replicates.

Sample	0	1	2	3	4	5	6	7	8
Suzuki Swift	-96.1	-57.4	-243.5	-102.4	<b>-20.2</b>	-75.0	-73.6	-60.3	-117.9

**Table S3:** Discriminant values of test samples with post-manufacture (respray) coatings, averaged from six replicates.

Sample	0	1	2	3	4	5	6	7	8
Mitsubishi Verada	-968.3	-955.2	<b>-259.9</b>	-942.9	-914.4	-1188.2	-906.3	-1102.1	-1124.8
Holden VZ Commodore Executive	-937.3	-856.5	<b>-218.3</b>	-916.1	-856.9	-1082.3	-873.6	-1085.7	-990.7
Ford Telstar	-894.0	-841.2	<b>-208.8</b>	-874.3	-822.6	-1063.9	-835.5	-1037.6	-984.2
Ford Falcon	-960.5	-921.8	<b>-248.0</b>	-937.2	-890.4	-1153.8	-892.2	-1091.7	-1081.2
Mazda 323 Astina	-967.4	-933.4	<b>-253.7</b>	-944.0	-905.1	-1169.5	-903.7	-1094.7	-1099.4
Holden Commodore SS (1)	-917.2	-840.0	<b>-213.2</b>	-899.0	-839.2	-1067.2	-856.6	-1049.9	-982.4
Holden Commodore SS (2)	-426.4	-258.2	<b>-105.8</b>	-419.1	-302.7	-399.3	-377.7	-467.3	-331.4

**Table S4:** Discriminant values of four test samples taken from a Daewoo Lanos vehicle, averaged from six replicates.

Sample	0	1	2	3	4	5	6	7	8
Bonnet	<b>-14.2</b>	-222.0	-335.0	-53.6	-64.4	-166.9	-63.4	-132.4	-271.2
Left Door	<b>-10.0</b>	-196.1	-147.1	-34.9	-43.1	-147.1	-38.0	-101.9	-250.1
Right-Side Bonnet	<b>-10.4</b>	-199.4	-315.5	-40.1	-47.1	-149.1	-42.4	-110.1	-250.8
Right Rear Bumper	<b>-8.8</b>	-197.8	-303.0	-35.7	-44.7	-149.2	-37.8	-103.6	-252.7

Bolded values signify the smallest magnitude discriminant value achieved for each sample across all classes, with samples assigned to the class yielding the smallest discriminant value. Samples that exhibit numerically low discriminant values ( $DV < 7$ ) are considered to be well classified.

In LDA, all unknown samples are assigned to one of the pre-established classes of the model, based upon their distance to each class (as determined by their discriminant values). This does not consider the possibility of atypical samples that are not yet encompassed by the model. The above examples illustrate the importance of considering discriminant values before accepting classifications given using LDA.