Rapid characterisation and classification of automotive clear coats by attenuated total reflectance infrared spectroscopy

Mark Maric¹, Wilhelm van Bronswijk¹, Simon W. Lewis¹* and Kari Pitts²

^a 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 ^b ChemCentre, PO Box 1250, Bentley Delivery Centre Western Australia 6983, Australia

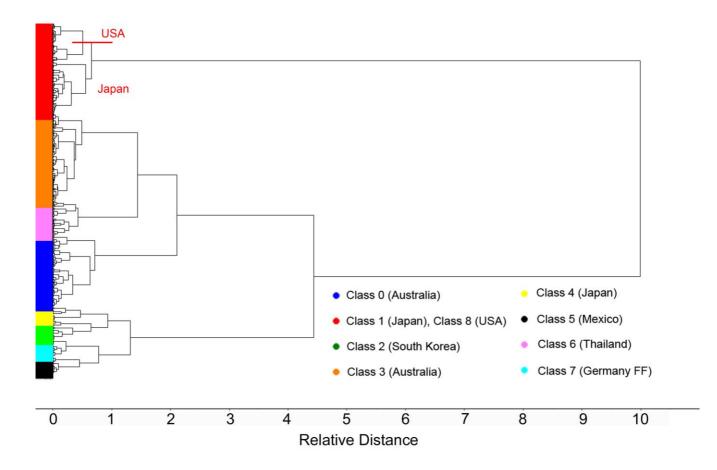


Figure S1: A dendrogram illustrating cluster analysis of the truncated spectral data revealing eight distinct classes. Red line indicates boundary between Class 1 (Japan) and Class 8 (USA) as determined by subsequent PCA.

Table S1 LDA Discriminant Values (DV)											
Sample	0	1	2	3	4	5	6	7	8		
Australia (Class 3)	-26.3	-238.9	-221.7	-3.1	-58.7	-119.7	-17.8	-67.3	-291.6		
Australia (Class 0)	-3.7	-263.2	-256.1	-26.9	-68.0	-145.6	-47.3	-87.4	-317.9		
Spain	-8.3	-227.5	-256.8	-7.5	-53.2	-113.9	-28.4	-58.4	-280.2		
Thailand (Class 6)	-43.4	-219.3	-192.9	-17.6	-46.0	-119.8	-4.2	-39.5	-286.		
UK	-47.2	-228.7	-176.6	-17.0	-56.9	-126.9	-8.1	-51.8	-295.		
Poland	-38.9	-206.9	-185.2	-15.2	-50.5	-114.3	-8.1	-34.2	-276.		
Sweden	-21.7	-174.3	-176.7	-16.8	-31.7	-91.5	-9.5	-29.9	-239.		
	Table S2				PC Sco						
		Sample			2	3					
	Australia (Class 3)			4.7	-1.1	-0.1	_				
	Australia (Class 0)			5.5	1.7	0.4					
		Spain			-0.1	0.5					
		Thailand (Class 6)			-1.1	-0.7					
		UK			-1.4	-0.6					
		Poland			-1.2	-0.5					
		Swed	den	1.7	-0.1	-0.4					

Tables S1 and S2: LDA and PCA data for typical Australian, Spanish, Thai, UK, Polish and Swedish vehicles

Table CALDA Diserinsinent Values (DV)

Well classified vehicles are easily identified from their numerically low discriminant values (DV<5).

The Spanish vehicle is closest to classes 3 (DV=7.5) and 0 (DV=8.3), but not near enough to either to assign it with an acceptable degree of confidence, and is well away from the other classes. Its PC scores confirm it to be near the bisector of groups 3 and 0.

The UK, Polish and Swedish vehicles are closest to class 6 but well away from its centroid (DV>8) in comparison to known class 6 vehicles (DV~4). They cannot be classified as class 6 vehicles with an acceptable level of confidence.

In LDA unknown objects submitted to the model will be classified only in relation to the classes of that model (and the nearness to each class reported as DVs or other proximity measures). It cannot provide an unclassifiable, not encompassed by the model, outcome. The above examples illustrate how the LDA model may describe vehicles that are not encompassed by the calibration set and that discriminant values and PC scores should always be considered before accepting a classification.

Actual/ Predicted	0	1	2	3	4	5	6	7	8	Total	% correct
0	89	0	0	0	0	0	0	0	0	89	100
1	0	105	0	0	0	0	0	0	0	105	100
2	0	0	29	0	0	0	0	0	0	29	100
3	0	0	0	127	0	0	0	0	0	127	100
4	0	0	0	0	33	0	0	0	0	33	100
5	0	0	0	0	0	11	0	0	0	11	100
6	0	0	0	0	0	0	29	0	0	29	100
7	0	0	0	0	0	0	0	25	0	25	100
8	0	0	0	0	0	0	0	0	41	41	100
Total	89	105	29	127	33	11	29	25	41	489	100

Table S3: Confusion matrix displaying the results from LDA of the samples within the calibration set. Overall, the classification accuracy was 100 %.

Table S4: Confusion matrix portraying the test set validation results of the supplemental validation test data from LDA. Overall, the classification accuracy was 100 %.

Actual/ Predicted	0	1	2	3	4	5	6	7	8	Total	% correct
0	56	0	0	0	0	0	0	0	0	56	100
1	0	42	0	0	0	0	0	0	0	42	100
2	0	0	12	0	0	0	0	0	0	12	100
3	0	0	0	49	0	0	0	0	0	49	100
4	0	0	0	0	20	0	0	0	0	20	100
5	0	0	0	0	0	0	0	0	0	0	-
6	0	0	0	0	0	0	25	0	0	25	100
7	0	0	0	0	0	0	0	12	0	12	100
8	0	0	0	0	0	0	0	0	5	5	100
Total	56	42	12	49	20	0	25	12	5	221	100

Table S5: Confusion matrix depicting the additional European paint samples, which were treated as unknowns and assigned an arbitrary class number prior to classification via the model.

Actual/ Predicted	0	1	2	3	4	5	6	7	8	Total	% correct
0	0	0	0	0	0	0	0	0	0	0	-
1	0	0	0	0	0	0	12	0	0	12	0
2	0	0	0	0	0	0	0	0	0	0	-
3	0	0	0	0	0	0	0	0	0	0	-
4	0	0	0	0	0	0	0	0	0	0	-
5	0	0	0	6	0	0	6	0	0	12	0
6	0	0	0	0	0	0	0	0	0	0	-
7	0	0	0	0	0	0	0	0	0	0	-
8	0	0	0	0	0	0	12	0	0	12	0
Total	0	0	0	6	0	0	30	0	0	36	0