Electronic Supplementary Material (ESI) for Digital Discovery.

electronic supplementary information for

A self-driving laboratory designed to accelerate the discovery of adhesive materials

Michael B. Rooney[1,†], Benjamin P. MacLeod[1,2,†], Ryan Oldford[1], Zachary J. Thompson[5], Kolby L. White[5], Justin Tungjunyatham[5], Brian Stankiewicz[5], Curtis P. Berlinguette[1-4,*]

[1]Department of Chemistry, The University of British Columbia, 2036 Main Mall, Vancouver, British Columbia, Canada V6T 1Z1

[2]Stewart Blusson Quantum Matter Institute, The University of British Columbia, 2355 East Mall, Vancouver, British Columbia, Canada V6T 1Z4

[3]Department of Chemical & Biological Engineering, The University of British Columbia, 2360 East Mall, Vancouver, British Columbia, Canada V6T 1Z3

[4]Canadian Institute for Advanced Research (CIFAR), MaRS Innovation Centre, 661 University Ave. Suite 505, Toronto, Ontario, Canada M5G 1M1

[5]3M Company, 3M Center, Maplewood, Minnesota 55144, United States

† : these authors contributed equally to this work

*Email: cberling@chem.ubc.ca

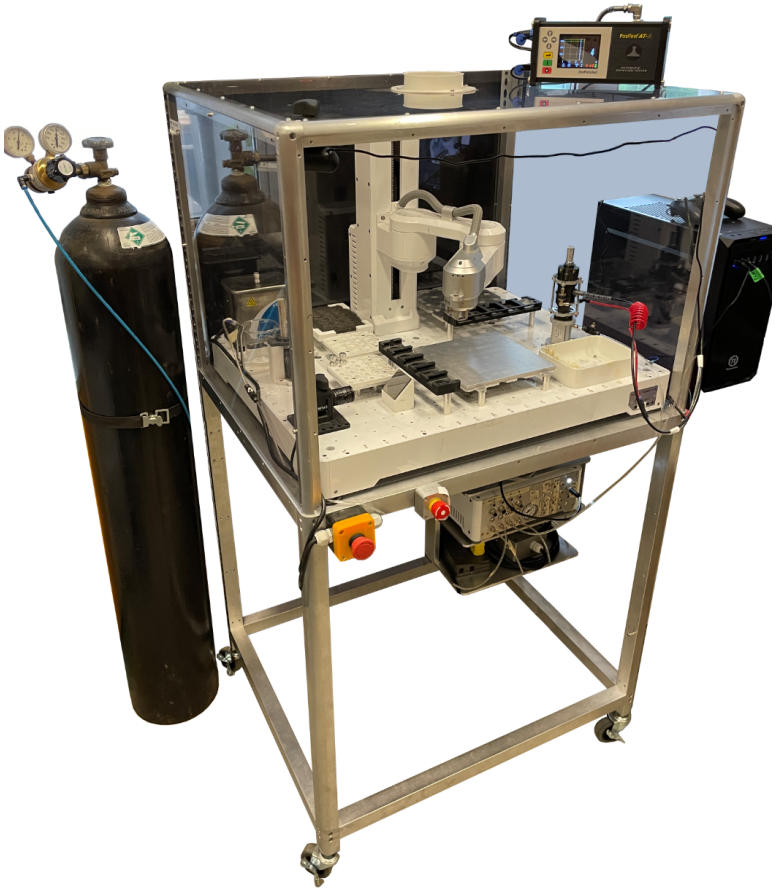


Figure S1 | Photograph of the robotic adhesives testing system

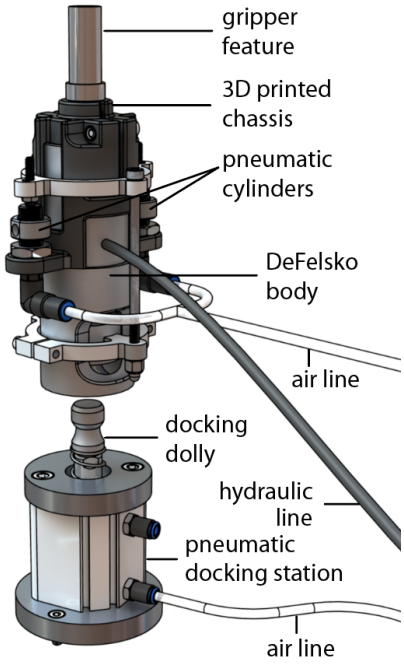
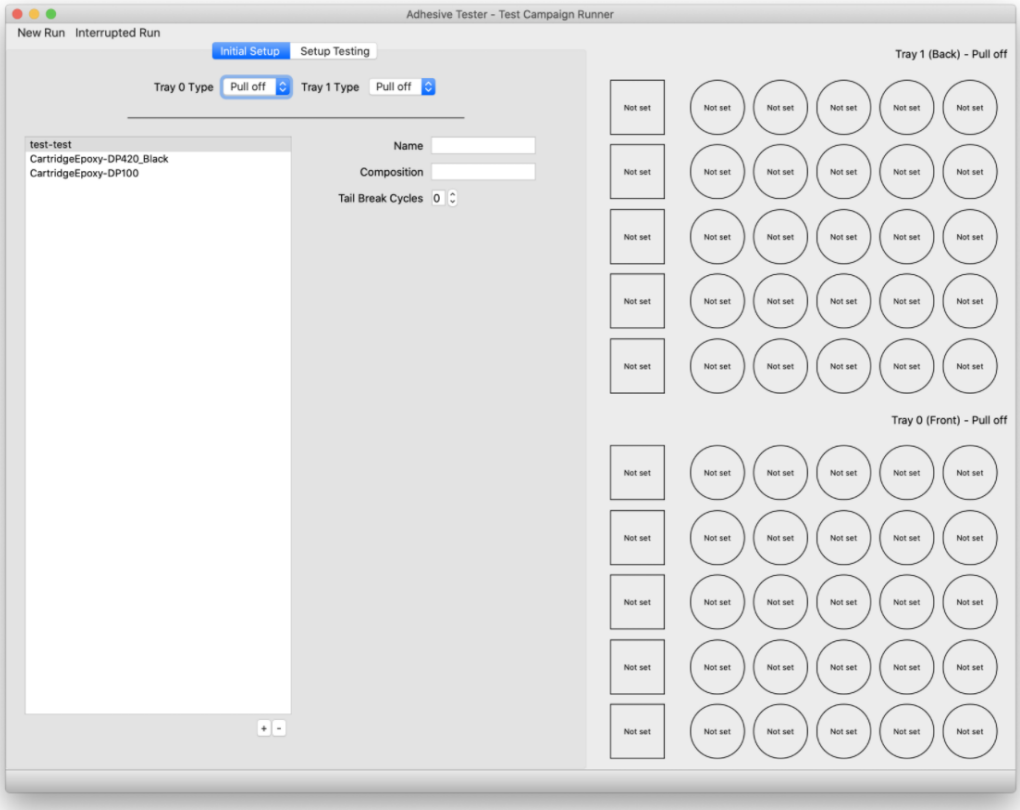


Figure S2 | Details of the modified strength testing tool and docking station



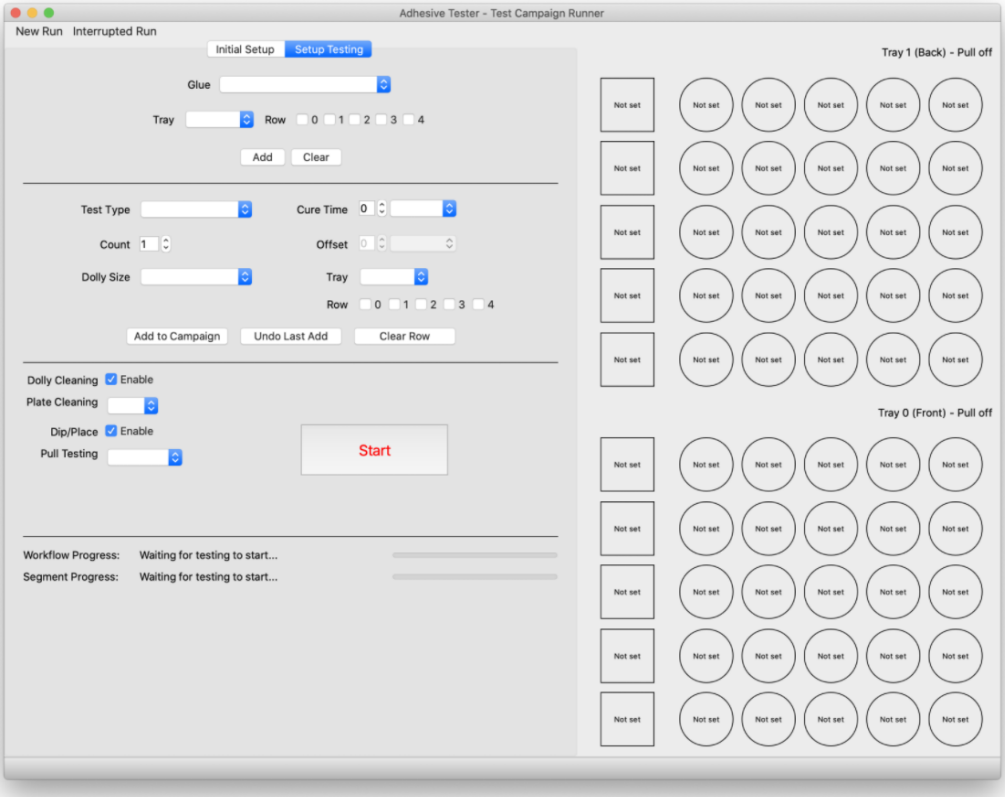


Figure S3 | Graphical user interface screenshots

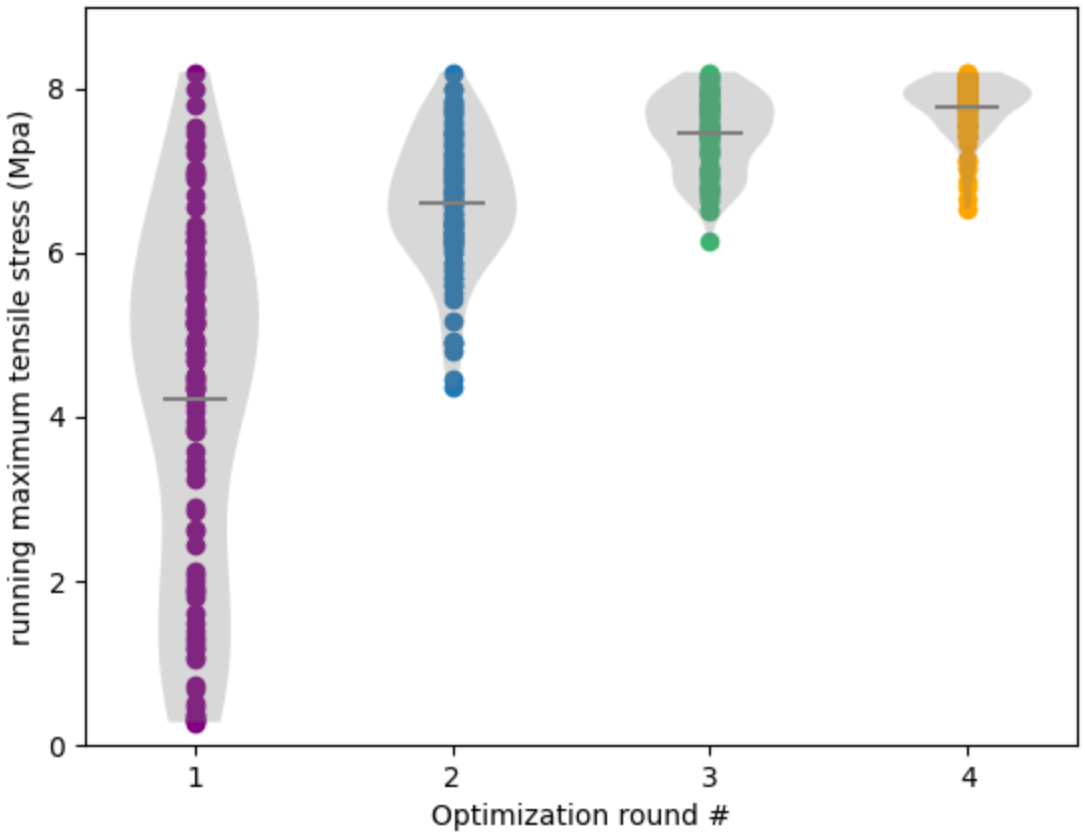


Figure S4 | Simulated optimization campaigns using the same optimizer configuration described in the manuscript. The experiment was emulated using a noisy approximation to the experimental data given by $S = 0.2 + 8\,(0.7 + 0.3\,U_{[0,1]})exp(-\frac{1}{2}(\frac{R-0.4}{0.05})^2)$ where *S* is the maximum recorded tensile stress (in Mpa), *R* is the resin fraction and $U_{[0,1]}$ indicates a sample drawn from the uniform random distribution over the interval [0,1]. 100 replicate optimization campaigns were simulated. After the completion of each simulated optimization round, the running maximum tensile stress observed across all completed rounds was recorded. For each round, the mean of the running maxima across all fifty replicates is indicated by the grey bar. The violin plot shows a kernel density estimate computed from the running maxima across all fifty replicates. The Python code for executing and plotting these simulations can be found at https://github.com/berlinguette/ada

Table S1 | DP420 pull-off data. Dollies with a 20-mm diameter bond area were used for these experiments.

Cure time (h)		2	3	5	6
Sample strength (N) (reported from DeFelsko Head)	*replicate 1*	250	1470	5081	6424
	replicate 2	309	1186	4789	5552
	replicate 3	no data[a]	1460	5072	4543
Sample stress (MPa) (computed from strength and dolly bond area)	*replicate 1*	0.80	4.68	16.17	20.45
	replicate 2	0.98	3.78	15.24	17.67
	replicate 3	no data[a]	4.65	16.14	14.46
Mean stress across replicates (MPa)		0.89	4.37	15.85	17.53
Standard deviation across replicates (MPa)		0.13	0.51	0.53	3.00

[a]No data was obtained for the third replicate sample for the 2h cure time due to an instrumentation error

Table S2 | DP190 pull-off data. Dollies with a 10-mm diameter bond area were used for these experiments.

Cure time (d)		1	2	5
Sample strength (N) (reported from DeFelsko Head)	*replicate 1*	1089	1423	1629
	replicate 2	815	1441	1703
	replicate 3	1063	1377	1678
Sample stress (MPa) (computed from strength and dolly bond area)	*replicate 1*	13.87	18.12	20.74
	replicate 2	10.38	18.35	21.68
	replicate 3	13.53	17.53	21.36
Mean stress across replicates (MPa)		12.59	18.00	21.26
Standard deviation across replicates (MPa)		1.93	0.42	0.48

Table S3 | DP190 lap shear data. Lap-shear specimens with a 0.5 in^2 bond area were used for these experiments.

Cure time (d)		1	2	5
Sample strength (lbf) (reported from universal tester)	*replicate 1*	537.8	651.8	789.6
	replicate 2	484.7	703.3	777.5
	replicate 3	531.1	654.5	815.2
Sample stress (MPa)	*replicate 1*	7.42	8.99	10.89
	replicate 2	6.68	9.70	10.72
	replicate 3	7.32	9.03	11.24
Mean stress across replicates (MPa)		7.14	9.24	10.95
Standard deviation across replicates (MPa)		0.40	0.40	0.27

Table S4| optimization pull-off tests (round 1). Dollies with a 20-mm diameter bond area were used for these experiments.

Round	Resin/Total Epoxy Fraction	Replicate	Pull-Off Test Force (N)	Pull-Off Test Force (KN)	Pull-Off Stress (MPa)
1	0.0891	1	82.0	0.082	0.26
		2	87.0	0.087	0.28
		3	0.0	0.000	0.00
	0.7500	1	0.0	0.000	0.00
		2	0.0	0.000	0.00
		3	0.0	0.000	0.00
	0.5905	1	479.0	0.479	1.52
		2	319.0	0.319	1.02
		3	315.0	0.315	1.00
	0.4059	1	2115.0	2.115	6.73
		2	2115.0	2.115	6.73
		3	2117.0	2.117	6.74
	0.4095	1	2418.0	2.418	7.70
		2	2424.0	2.424	7.72
		3	2729.0	2.729	8.69

Table S5| optimization pull-off tests (round 2). Dollies with a 20-mm diameter bond area were used for these experiments.

Round	Resin/Total Epoxy Fraction	Replicate	Pull-Off Test Force (N)	Pull-Off Test Force (KN)	Pull-Off Stress (MPa)
2	0.3305	1	766.0	0.766	2.44
		2	819.0	0.819	2.61
		3	1017.0	1.017	3.24
	1.0000	1	0.0	0.000	0.00
		2	79.0	0.079	0.25
		3	65.0	0.065	0.21
	0.4369	1	1156.0	1.156	3.68
		2	1122.0	1.122	3.57
		3	1169.0	1.169	3.72
	0.3719	1	1109.0	1.109	3.53
		2	1367.0	1.367	4.35
		3	1596.0	1.596	5.08
	0.2762	1	385.0	0.385	1.23
		2	441.0	0.441	1.40
		3	450.0	0.450	1.43

Table S6| optimization pull-off tests (round 3). Dollies with a 20-mm diameter bond area were used for these experiments.

Round	Resin/Total Epoxy Fraction	Replicate	Pull-Off Test Force (N)	Pull-Off Test Force (KN)	Pull-Off Stress (MPa)
3	0.4340	1	1341.0	1.341	4.27
		2	1215.0	1.215	3.87
		3	1242.0	1.242	3.95
	0.0000	1	71.0	0.071	0.23
		2	71.0	0.071	0.23
		3	70.0	0.070	0.22
	0.5500	1	643.0	0.643	2.05
		2	613.0	0.613	1.95
		3	604.0	0.604	1.92
	0.4257	1	1898.0	1.898	6.04
		2	1910.0	1.910	6.08
		3	1991.0	1.991	6.34
	0.3725	1	1957.0	1.957	6.23
		2	1725.0	1.725	5.49
		3	1975.0	1.975	6.29

Table S7| optimization pull-off tests (round 4). Dollies with a 20-mm diameter bond area were used for these experiments.

Round	Resin/Total Epoxy Fraction	Replicate	Pull-Off Test Force (N)	Pull-Off Test Force (KN)	Pull-Off Stress (MPa)
4	0.3892	1	1249.0	1.249	3.98
		2	1273.0	1.273	4.05
		3	1367.0	1.367	4.35
	0.4594	1	1220.0	1.220	3.88
		2	1241.0	1.241	3.95
		3	1300.0	1.300	4.14
	0.4633	1	1326.0	1.326	4.22
		2	1612.0	1.612	5.13
		3	1597.0	1.597	5.08
	0.8848	1	0.0	0.000	0.00
		2	96.0	0.096	0.31
		3	0.0	0.000	0.00
	0.3666	1	1674.0	1.674	5.33
		2	1951.0	1.951	6.21
		3	2226.0	2.226	7.09

Video S1 | Video of the robotic workflow

A video showing the robotic workflow can be found at https://youtu.be/LxWiLR13hkc