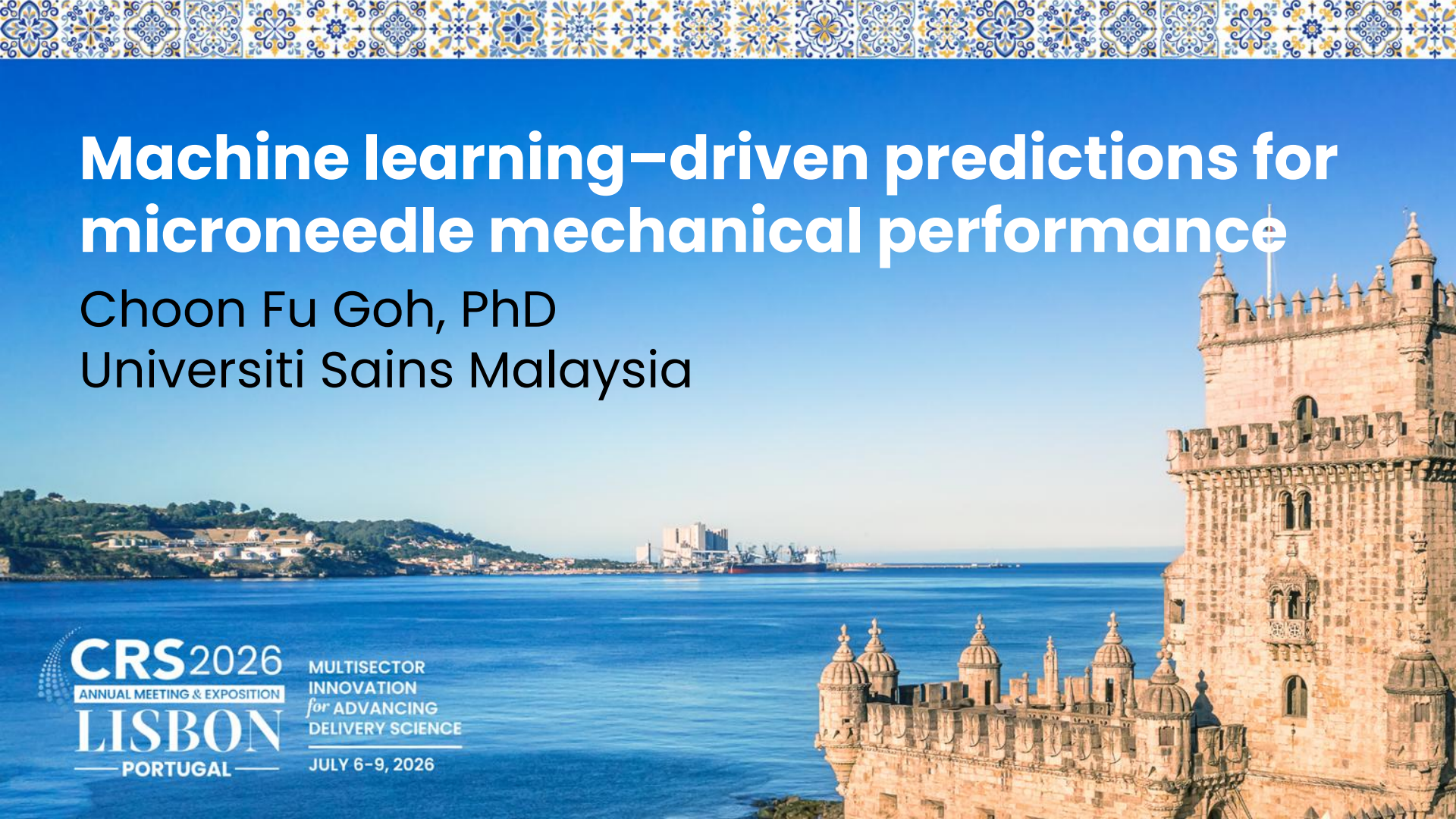




Machine learning–driven predictions for microneedle mechanical performance

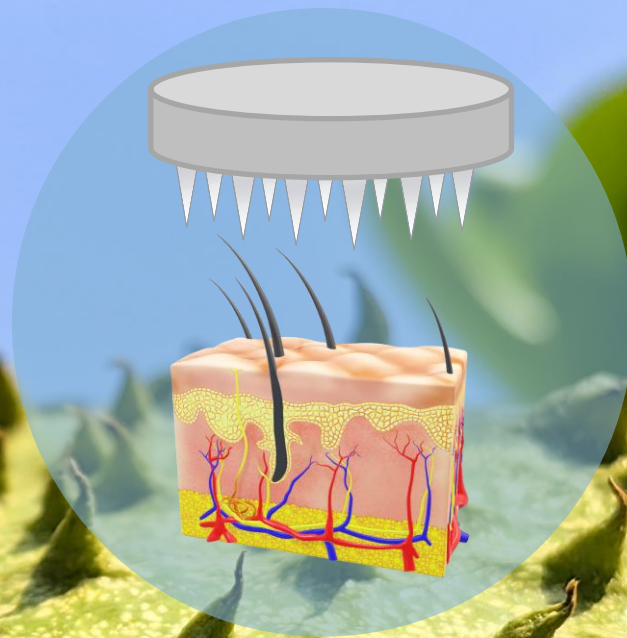
Choon Fu Goh, PhD
Universiti Sains Malaysia



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ANNUAL MEETING & EXPOSITION
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MULTISECTOR
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microneedle



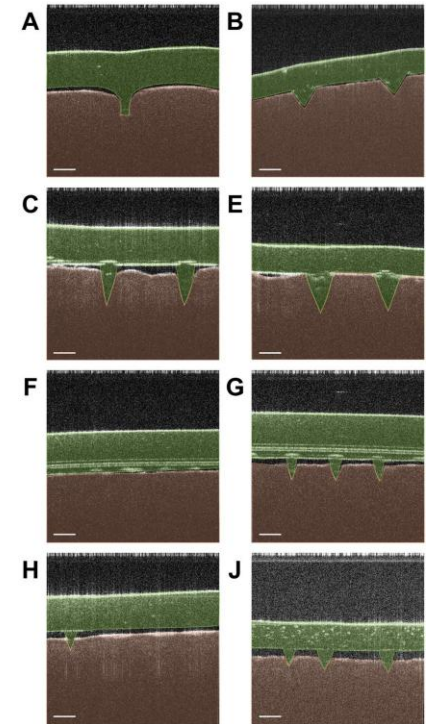
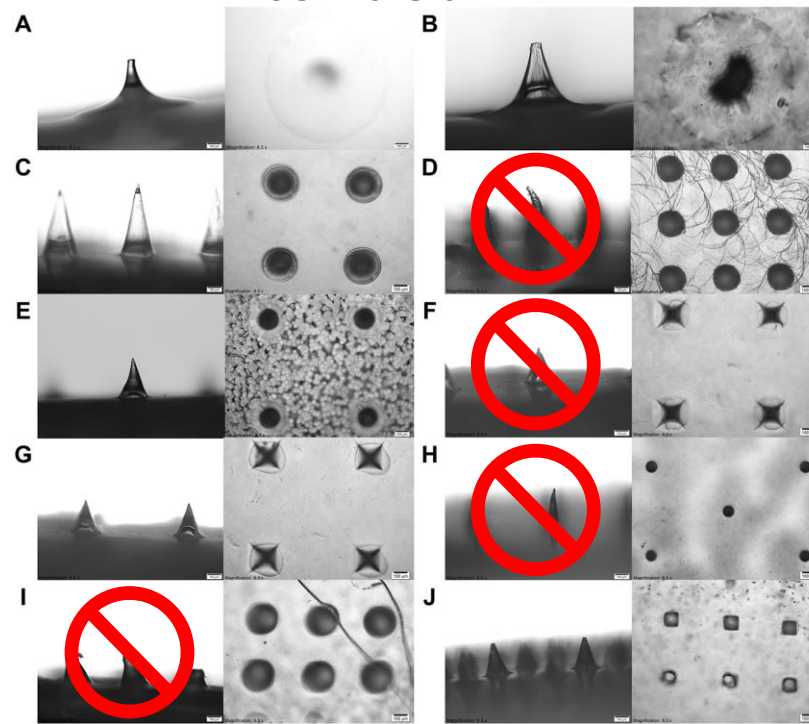
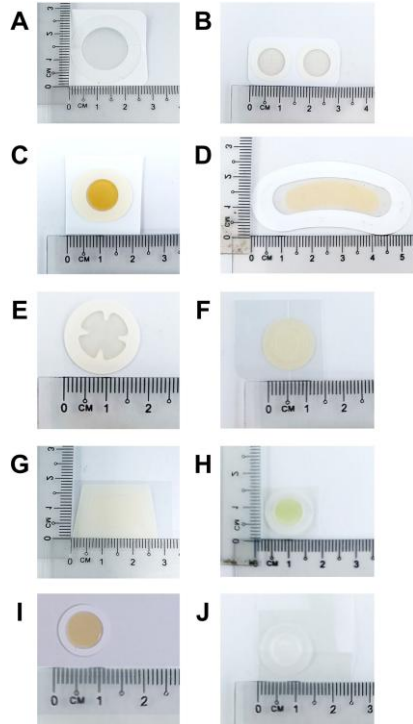
Fortress Hill, Penang



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JULY 6-9, 2026

Do all microneedle array patches* work as intended?



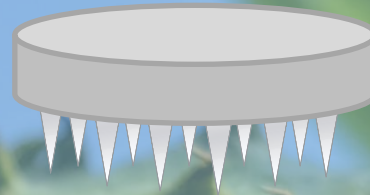
*polymeric microneedle array patches

Drug Deliv Transl Res 2025 15 3986-4003



When ML meets

microneedle

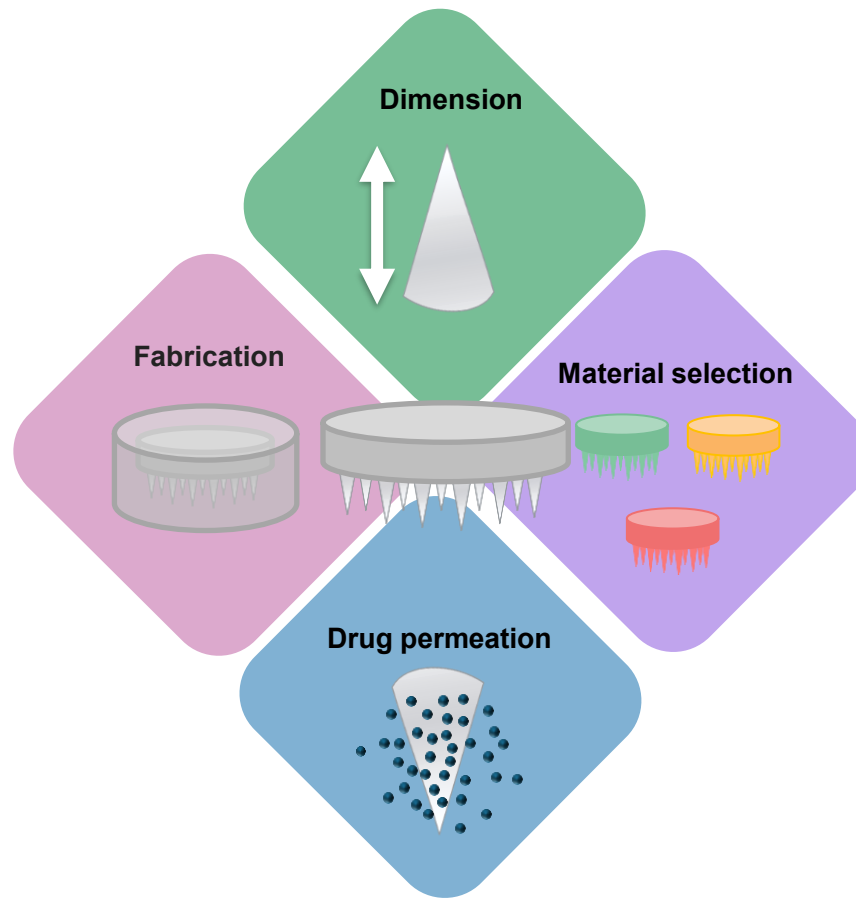


Fortress Hill, Penang



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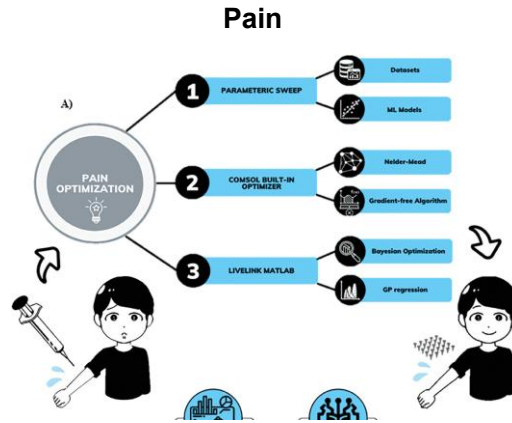
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JULY 6-9, 2026



Biomimetics 2024, 9(8), 469

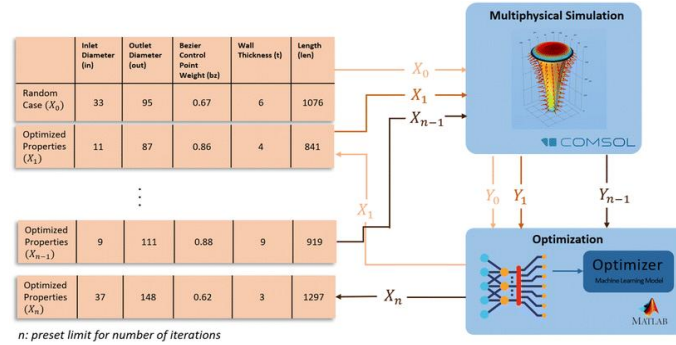


Dimension



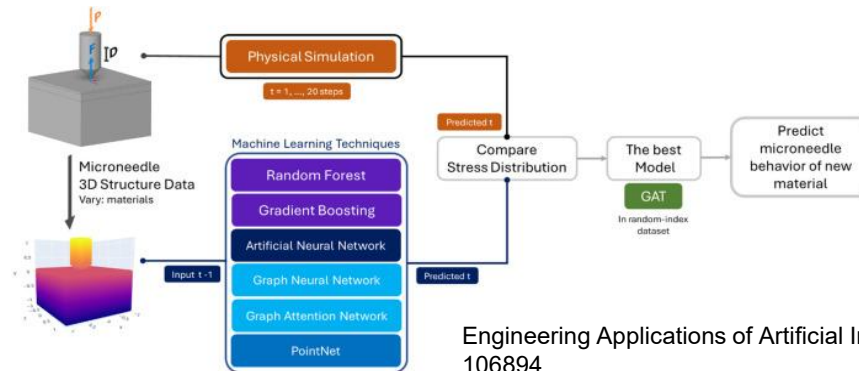
Advanced Sensor Research 2024 3(5)
2300181

Biological fluid sampling (microfluidic)



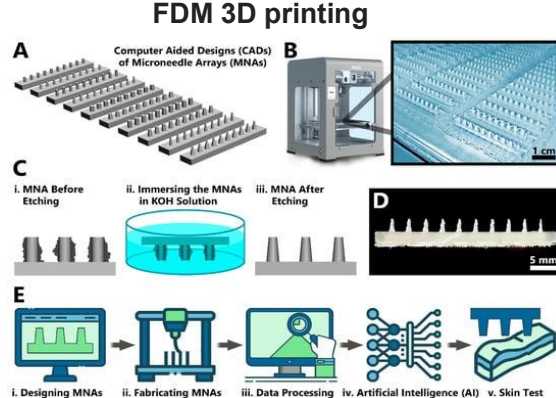
Sensors & Diagnostics 2023 2(4) 858-66

Material selection

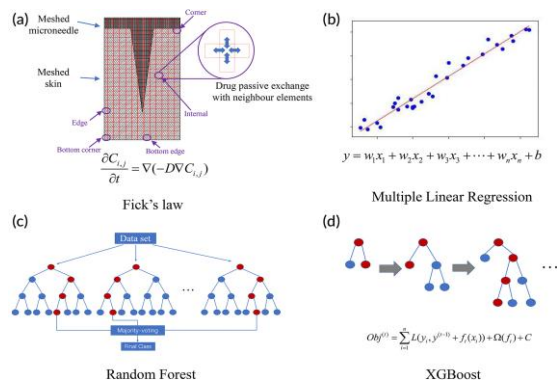


Engineering Applications of Artificial Intelligence 2023 126
106894

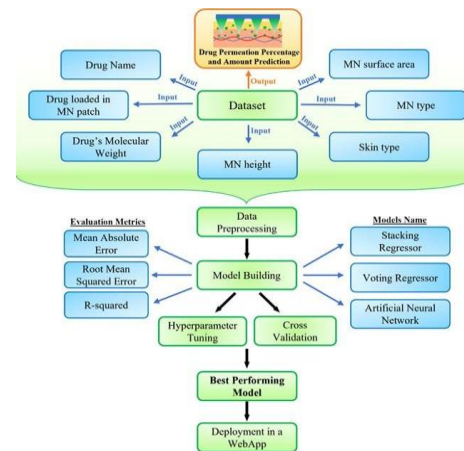
Fabrication



Biosensors 2022 12(7) 491



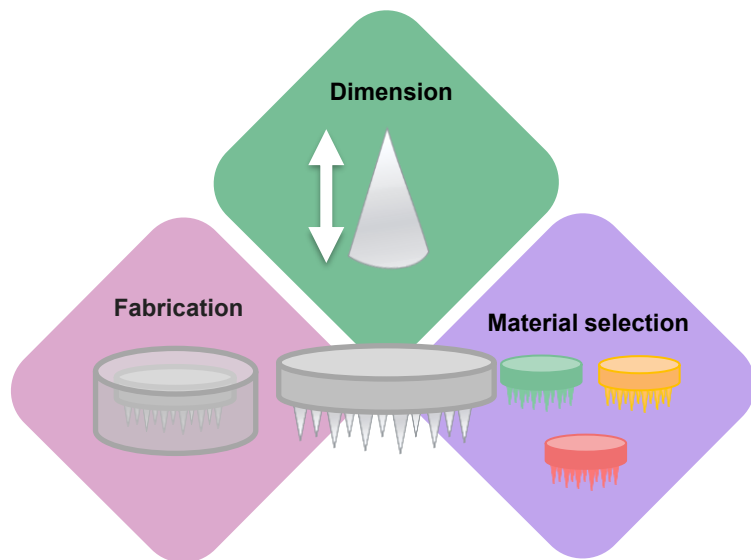
Bioeng Transl Med 2023 8(6) e10512



Eur J Pharm Biopharm 2024 199 114311



Our focus



Microneedle strength

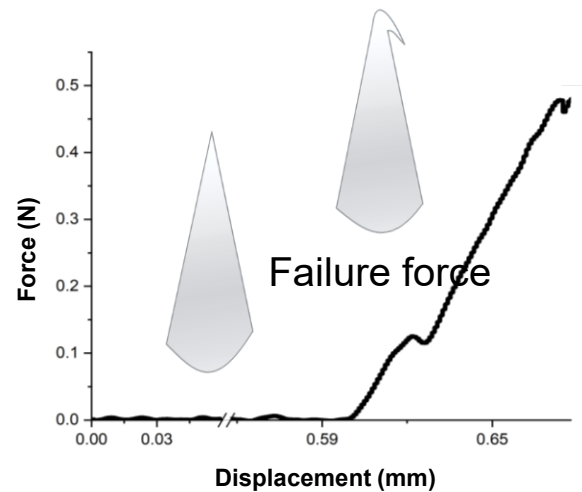


Designed using copilot

Microneedle strength



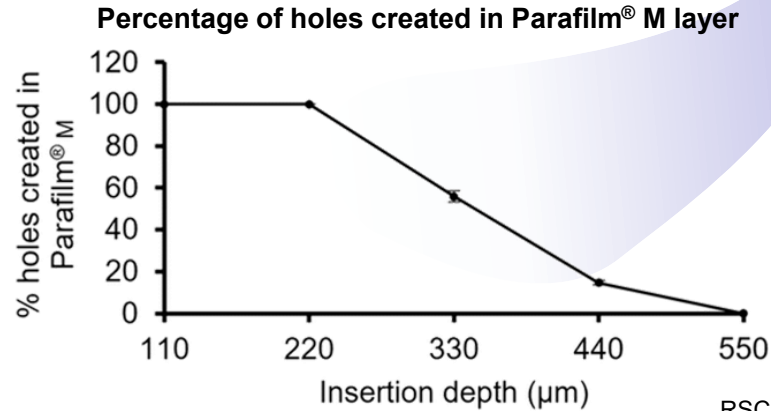
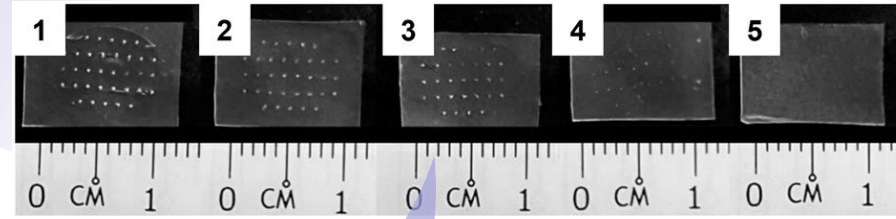
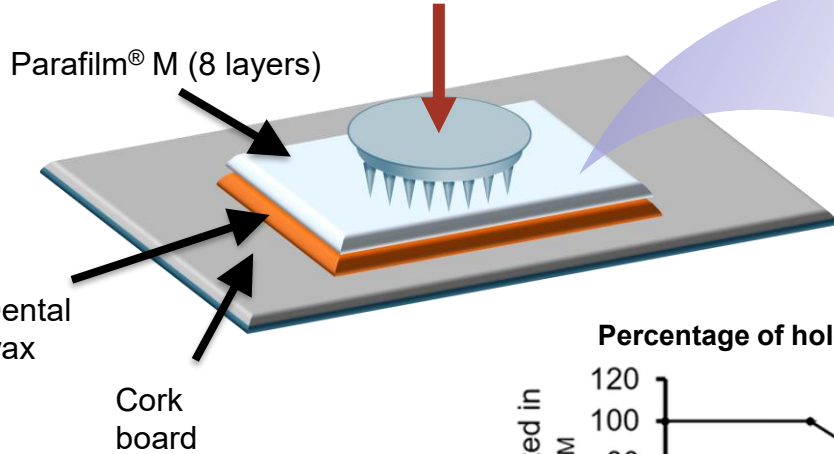
Compression test



RSC Pharm 2024 1 227-233



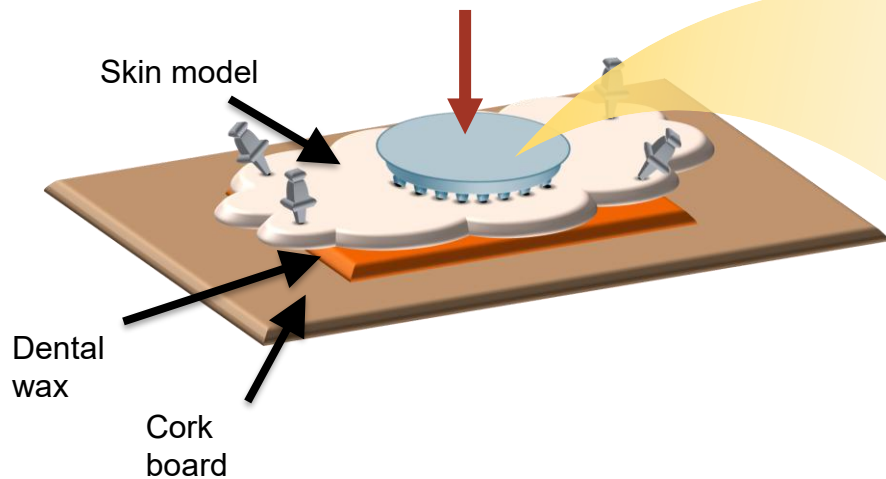
In vitro skin insertion study (Parafilm® M)



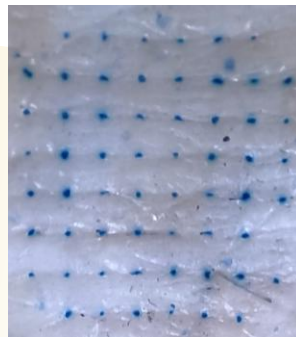
RSC Pharm 2024 1 227-233; Int J Pharm 2014 472(1) 65-73



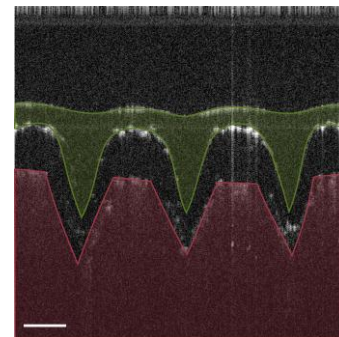
Ex vivo skin insertion study



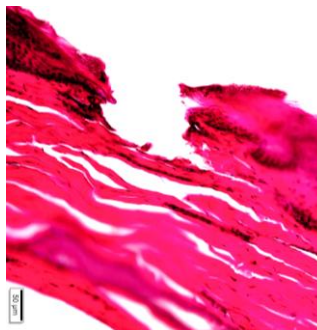
Skin insertion ratio (%)



Penetration depth (optical coherent tomography)



Penetration depth (histology)



J Control Release 2010 147(3) 333-341

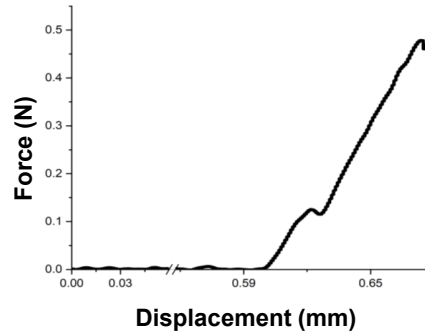


Microneedle dimension

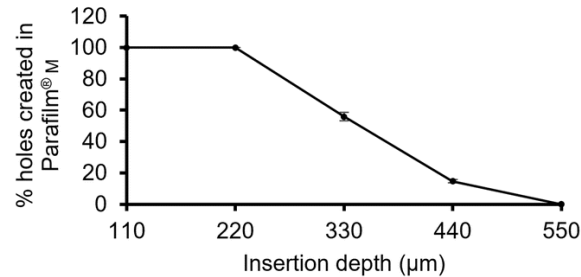
Polymer content

Drug/active content

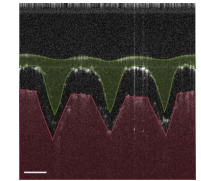
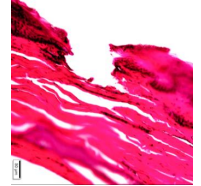
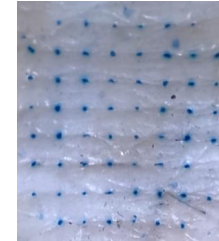
Compression test



***In vitro* skin insertion study
(Parafilm® M)**



***Ex vivo* skin insertion study**



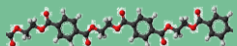
Data mining

Polymer information										Drug information				MN type	MN dimension					MN shape				Compression test		Outcome		
P-Name	P-Single/mixture	P1-Concentration (%)	P2-Concentration (%)	P3-Concentration (%)	P1-MW (Da)	P2-MW (Da)	P3-MW (Da)	D-Name	D-MW	D-log P	D-Concentration (%)	MN-Type	MN Height (um)	MN-Tip radius (um) - sharpness	MN Width (um)	MN Base area (um ²)	MN Aspect ratio (height/width)	MN-Interneedle spacing (um)	MN Volume of single needle (um ³)	MN-Number of needles/patch	MN-Shape	Pyramidal/Obelisk	Cone/tapered cone	Cylinder	Cuboid	Insertion force on the MN to the paraffin (N)	No of layer	% of holes
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	600		350	122500	1.714286	350	24500000	196	pyramidal	1	0	0	0	32	1	98.9
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	600		350	122500	1.714286	350	24500000	196	pyramidal	1	0	0	0	32	2	96.13
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	600		350	122500	1.714286	350	24500000	196	pyramidal	1	0	0	0	32	3	54.14
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	600		350	122500	1.714286	350	24500000	196	pyramidal	1	0	0	0	32	4	13.81
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	600		350	122500	1.714286	350	24500000	196	pyramidal	1	0	0	0	32	5	0
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	600		350	122500	1.714286	350	24500000	196	pyramidal	1	0	0	0	32	6	0
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	600		350	122500	1.714286	350	24500000	196	pyramidal	1	0	0	0	32	7	0
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	600		350	122500	1.714286	350	24500000	196	pyramidal	1	0	0	0	32	8	0
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	600		350	122500	1.714286	350	24500000	196	pyramidal	1	0	0	0	20	1	98.34
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	600		350	122500	1.714286	350	24500000	196	pyramidal	1	0	0	0	20	2	78.59
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	600		350	122500	1.714286	350	24500000	196	pyramidal	1	0	0	0	20	3	37.85
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	600		350	122500	1.714286	350	24500000	196	pyramidal	1	0	0	0	20	4	3.04
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	600		350	122500	1.714286	350	24500000	196	pyramidal	1	0	0	0	20	5	0
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	600		350	122500	1.714286	350	24500000	196	pyramidal	1	0	0	0	20	6	0
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	600		350	122500	1.714286	350	24500000	196	pyramidal	1	0	0	0	20	7	0
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	600		350	122500	1.714286	350	24500000	196	pyramidal	1	0	0	0	20	8	0
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	600		350	122500	1.714286	350	24500000	196	pyramidal	1	0	0	0	10	1	95.44
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	600		350	122500	1.714286	350	24500000	196	pyramidal	1	0	0	0	10	2	49.86
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	600		350	122500	1.714286	350	24500000	196	pyramidal	1	0	0	0	10	3	3.04
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	600		350	122500	1.714286	350	24500000	196	pyramidal	1	0	0	0	10	4	0
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	600		350	122500	1.714286	350	24500000	196	pyramidal	1	0	0	0	10	5	0
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	600		350	122500	1.714286	350	24500000	196	pyramidal	1	0	0	0	10	6	0
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	600		350	122500	1.714286	350	24500000	196	pyramidal	1	0	0	0	10	7	0
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	600		350	122500	1.714286	350	24500000	196	pyramidal	1	0	0	0	10	8	0
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	750		300	90000	2.5	50	22500000	600	pyramidal	1	0	0	0	32	1	97.93
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	750		300	90000	2.5	50	22500000	600	pyramidal	1	0	0	0	32	2	88.81
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	750		300	90000	2.5	50	22500000	600	pyramidal	1	0	0	0	32	3	44.61
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	750		300	90000	2.5	50	22500000	600	pyramidal	1	0	0	0	32	4	6.08
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	750		300	90000	2.5	50	22500000	600	pyramidal	1	0	0	0	32	5	0
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	750		300	90000	2.5	50	22500000	600	pyramidal	1	0	0	0	32	6	0
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	750		300	90000	2.5	50	22500000	600	pyramidal	1	0	0	0	32	7	0
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	750		300	90000	2.5	50	22500000	600	pyramidal	1	0	0	0	32	8	0
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	750		300	90000	2.5	50	22500000	600	pyramidal	1	0	0	0	20	1	94.48
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Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	750		300	90000	2.5	50	22500000	600	pyramidal	1	0	0	0	20	3	4.7
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	750		300	90000	2.5	50	22500000	600	pyramidal	1	0	0	0	20	4	0
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	750		300	90000	2.5	50	22500000	600	pyramidal	1	0	0	0	20	5	0
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	750		300	90000	2.5	50	22500000	600	pyramidal	1	0	0	0	20	6	0
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	750		300	90000	2.5	50	22500000	600	pyramidal	1	0	0	0	20	7	0
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	750		300	90000	2.5	50	22500000	600	pyramidal	1	0	0	0	20	8	0
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	750		300	90000	2.5	50	22500000	600	pyramidal	1	0	0	0	10	1	54.42
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	750		300	90000	2.5	50	22500000	600	pyramidal	1	0	0	0	10	2	26.66
Gantrez® S-97(PVA/MA) / poly(ethylene glycol) mixture	20	7.5	0	0	1500000	10000	0	Ibuprofen s	228.26	3.97	40	hydrogel-formin	750		300	90000	2.5	50	22500000	600	pyramidal	1	0	0	0	10	3	6.35



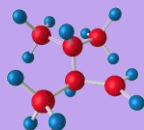
Features

Polymer



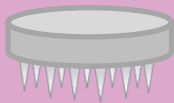
- Molecular weight
- Concentration (individual & total)

Drug



- Molecular weight
- Log P
- Concentration
- Drug content per patch

Microneedle



- Shape
- Needle dimension
- Others*

Target variables

Failure force



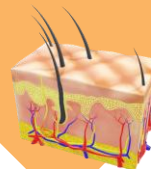
- Rate of force exertion
- Failure force/needle

In vitro insertion



- Insertion force
- Percentage of holes created

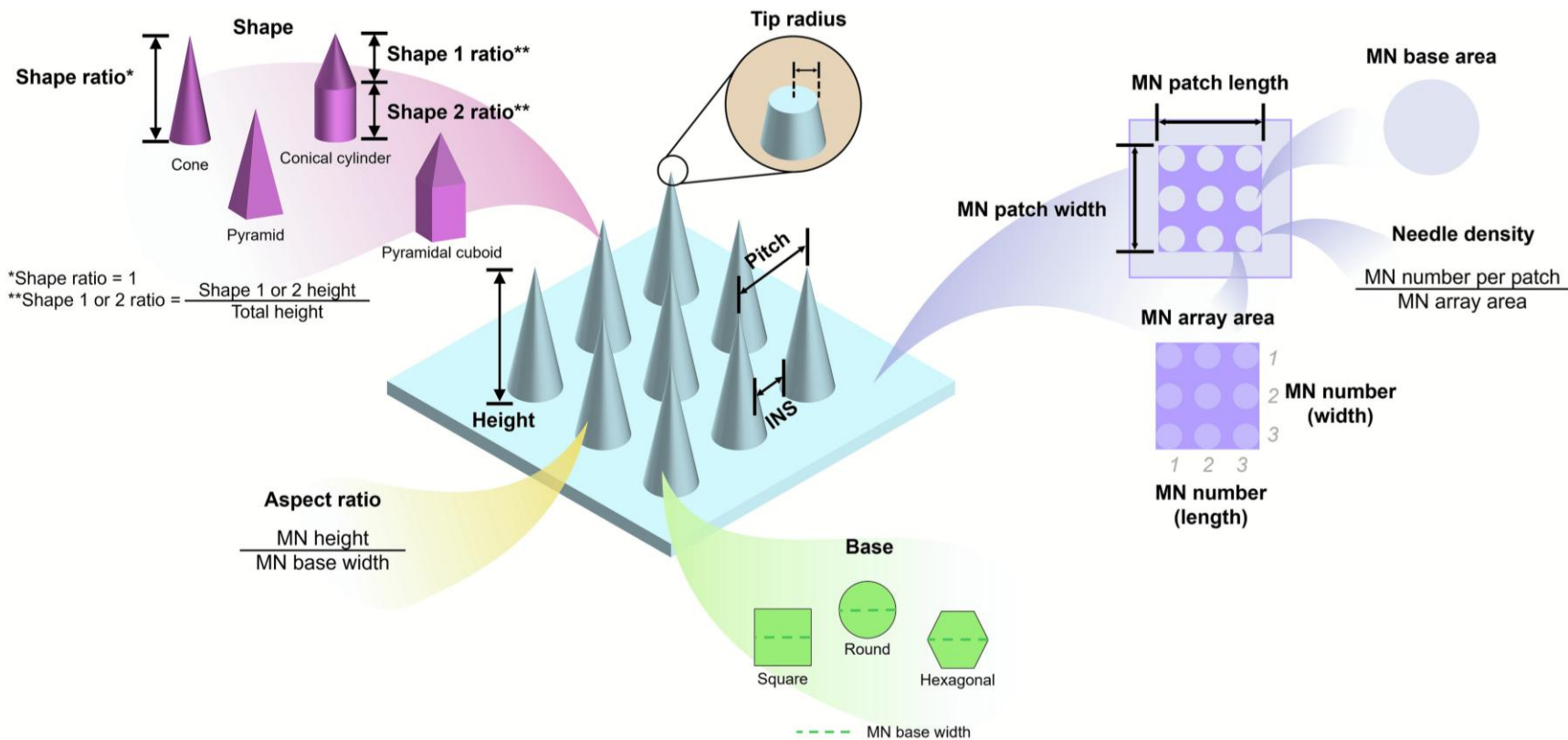
Ex vivo insertion

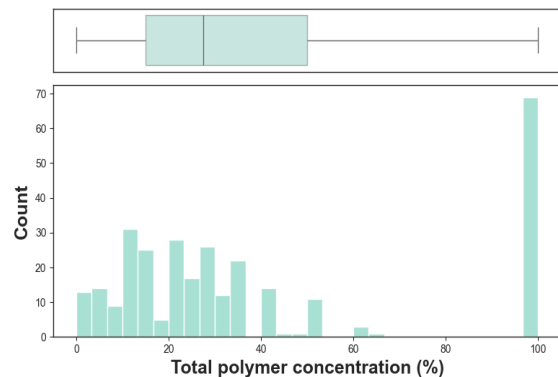


- Skin model
- Skin insertion ratio
- Ex vivo insertion depth

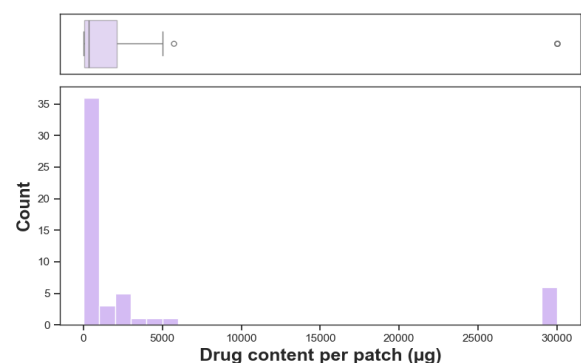
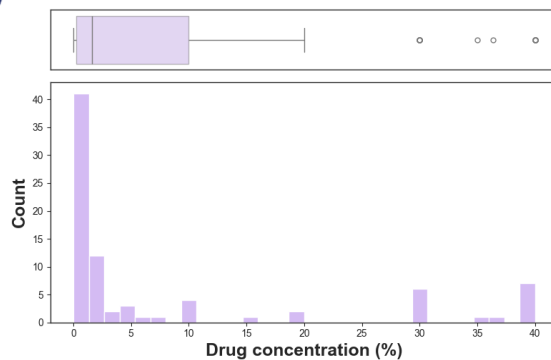
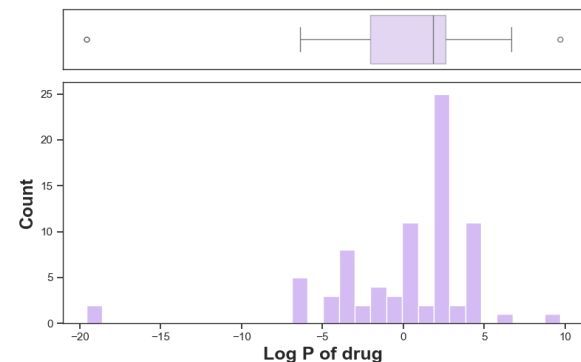
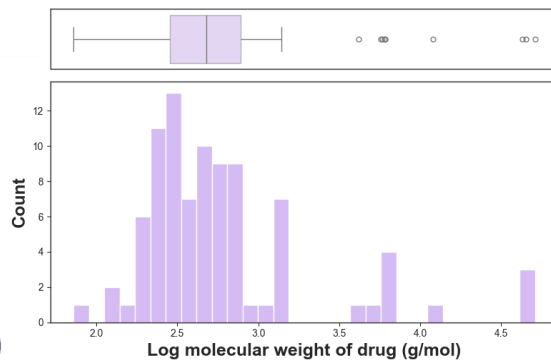
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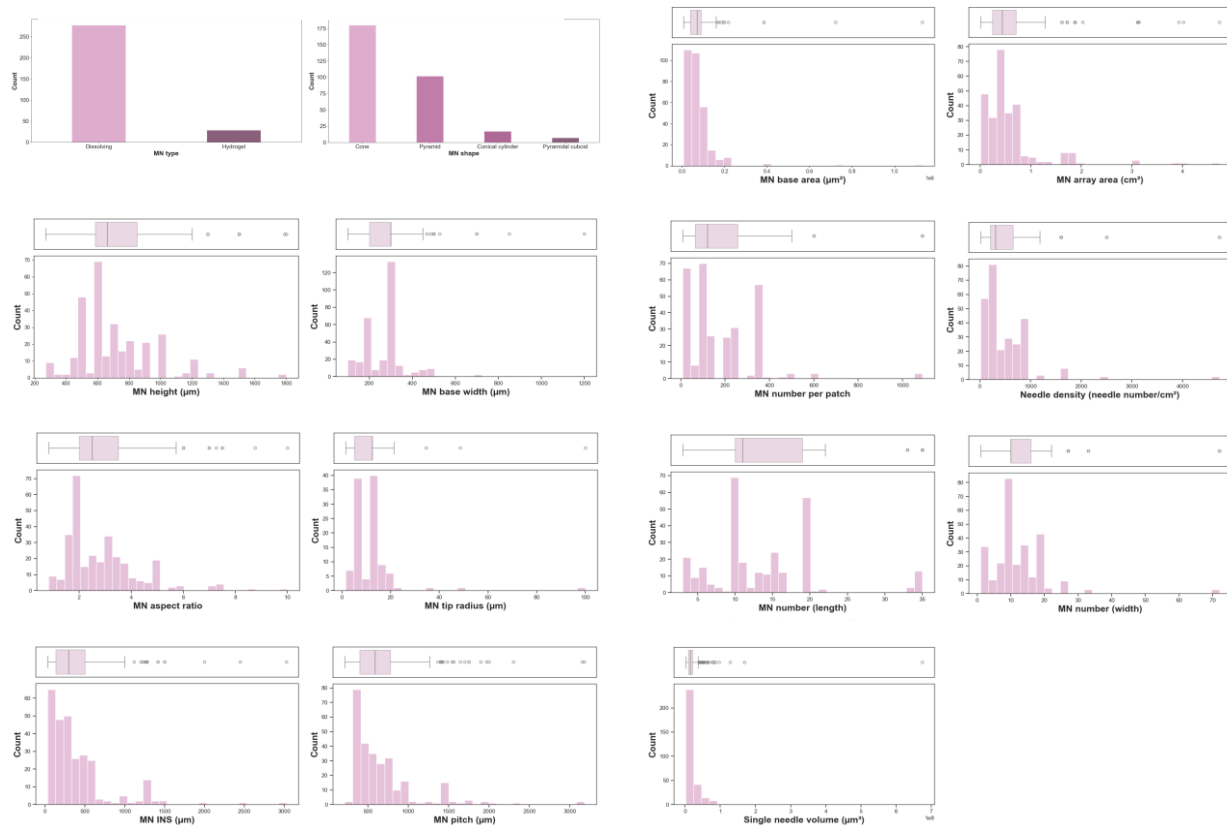




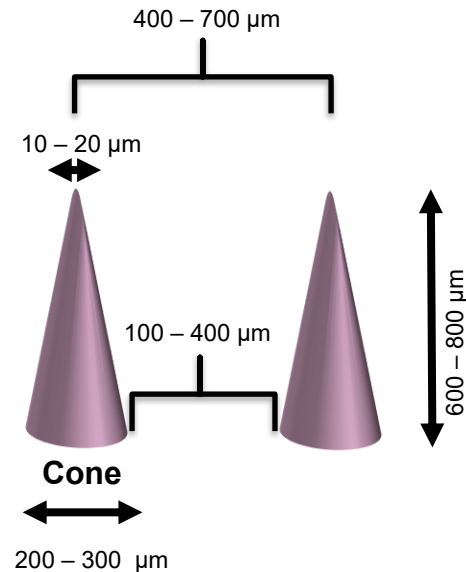
Exploratory data: Actives/drugs



Exploratory data: MN

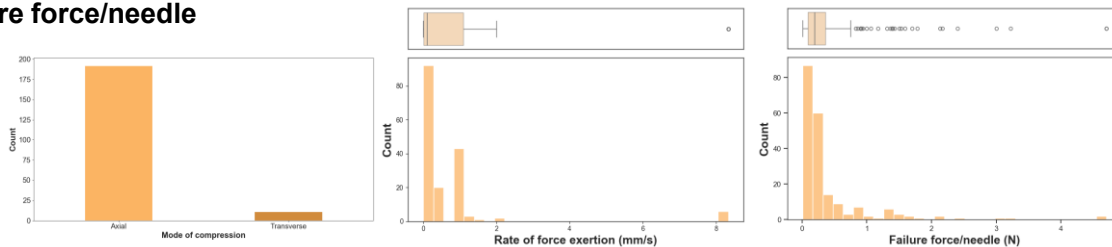


Popular features:

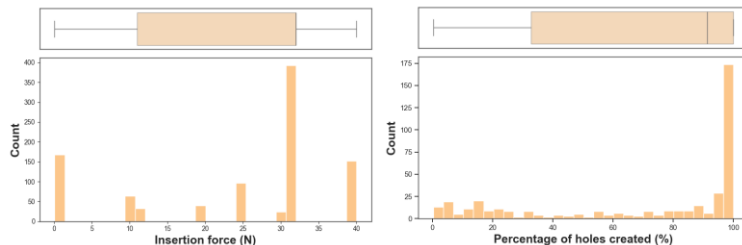


Exploratory data: Target variables

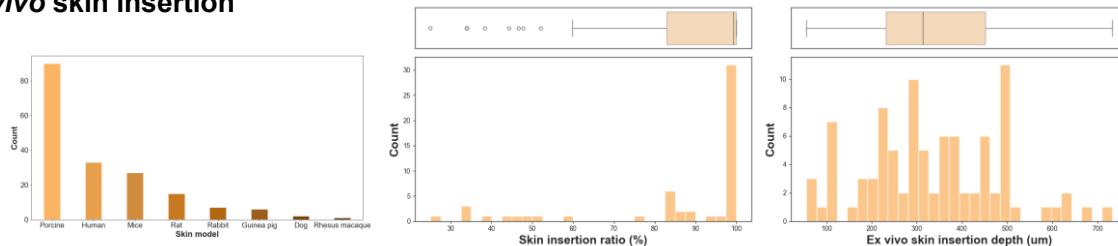
Failure force/needle



In vitro skin insertion



Ex vivo skin insertion



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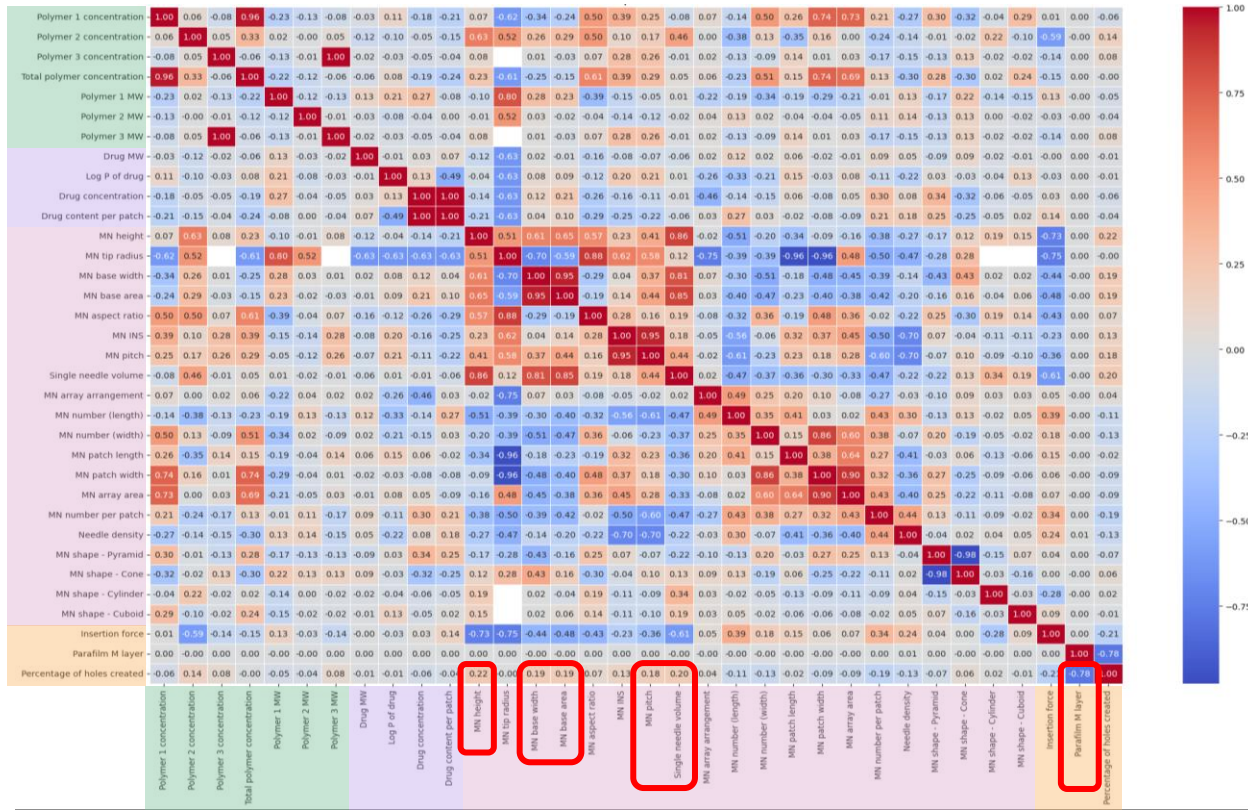
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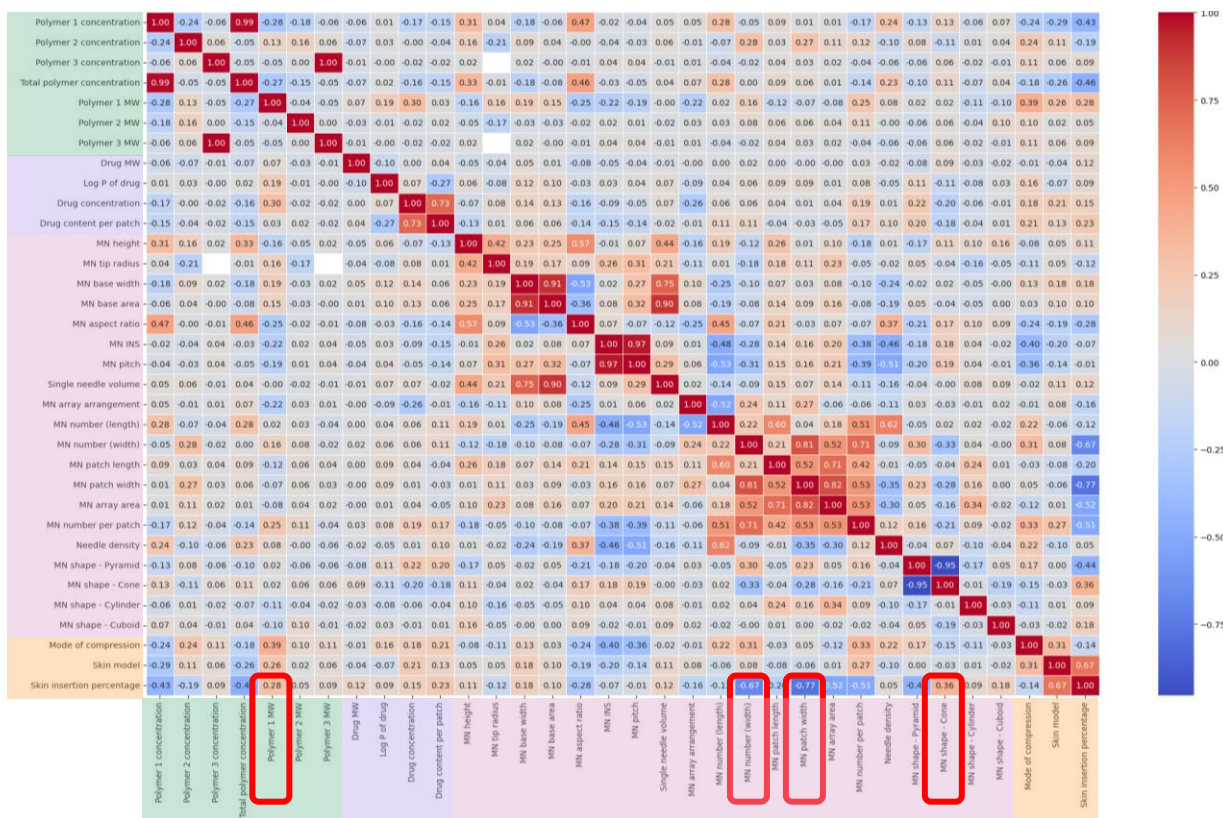
Heatmap: Percentage of holes created

In vitro



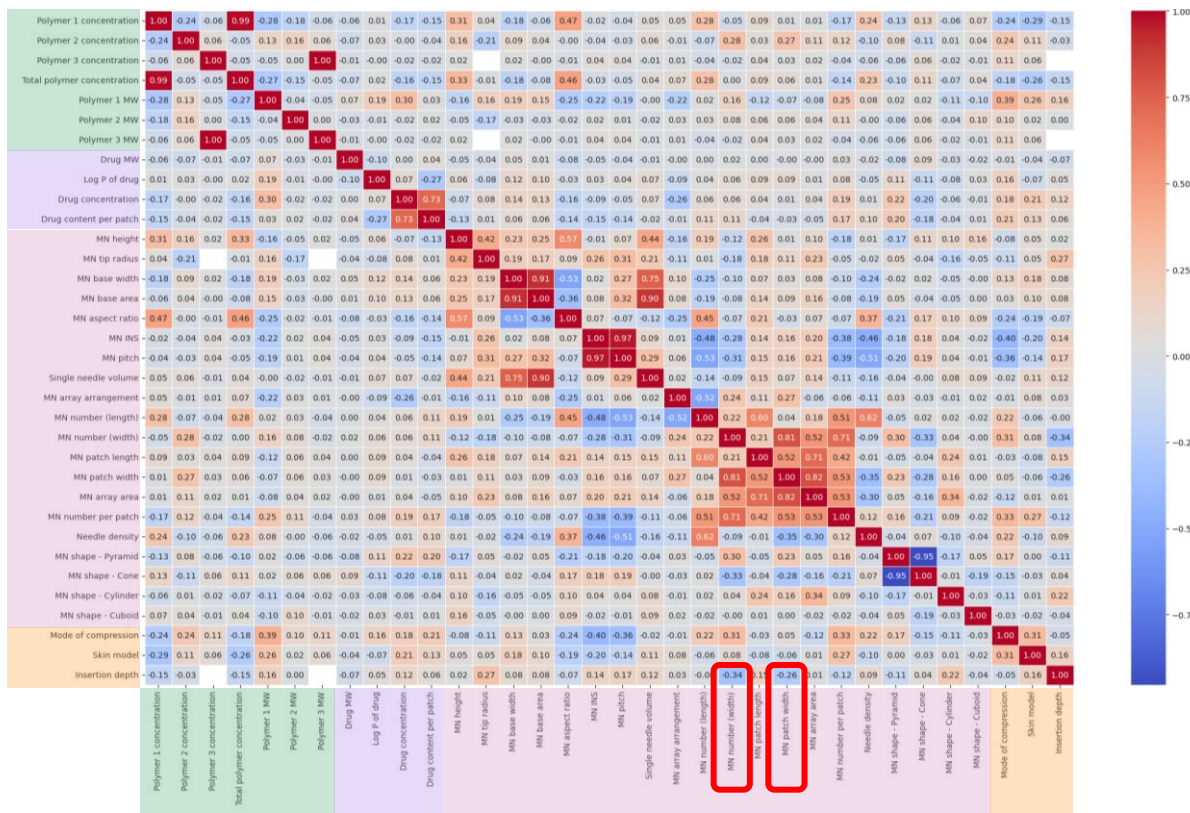
Heatmap: Skin insertion ratio

Ex vivo



Heatmap: Insertion depth

Ex vivo



Model development

Failure force



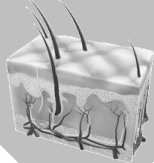
- Rate of force exertion
- Failure force/needle

In vitro insertion



- Insertion force
- Percentage of holes created

Ex vivo insertion



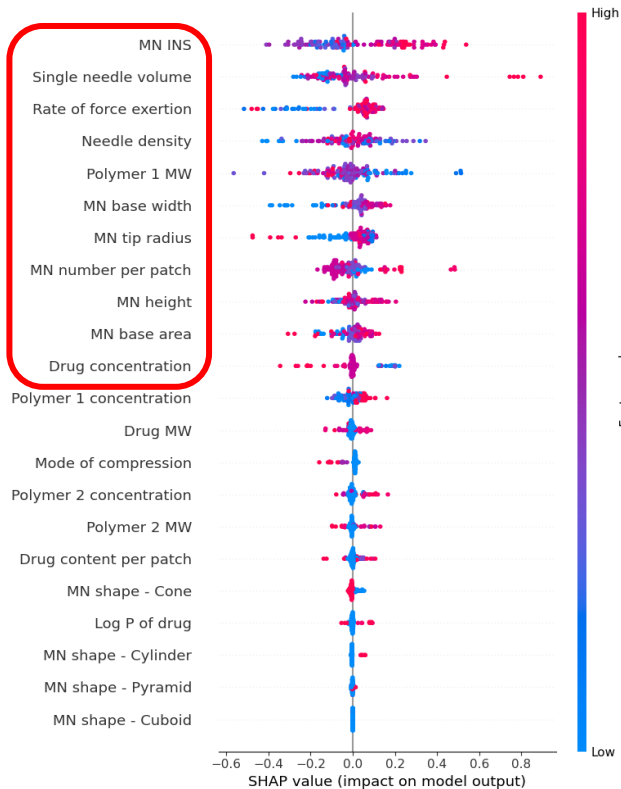
- Skin model
- Skin insertion ratio
- Ex vivo insertion depth

>70% missing data

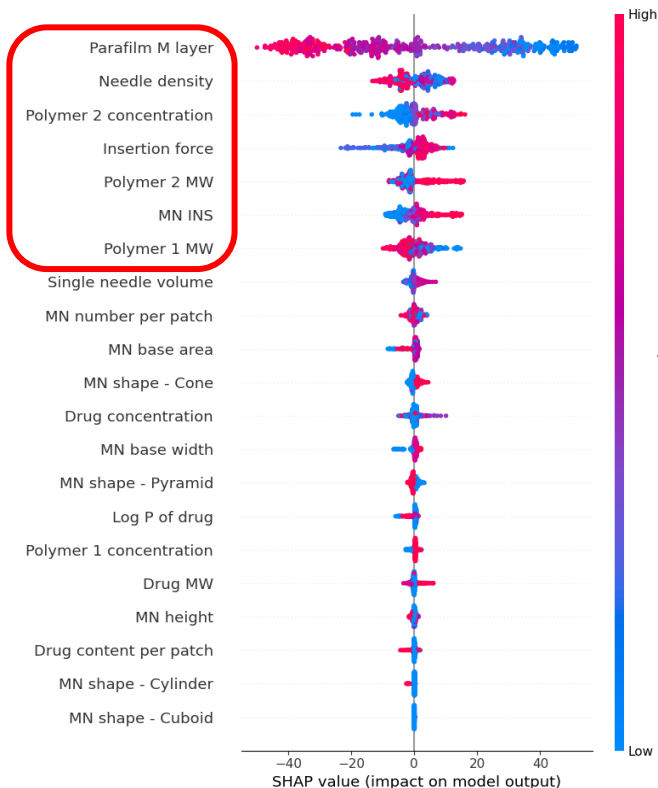


SHAP analysis

Failure force

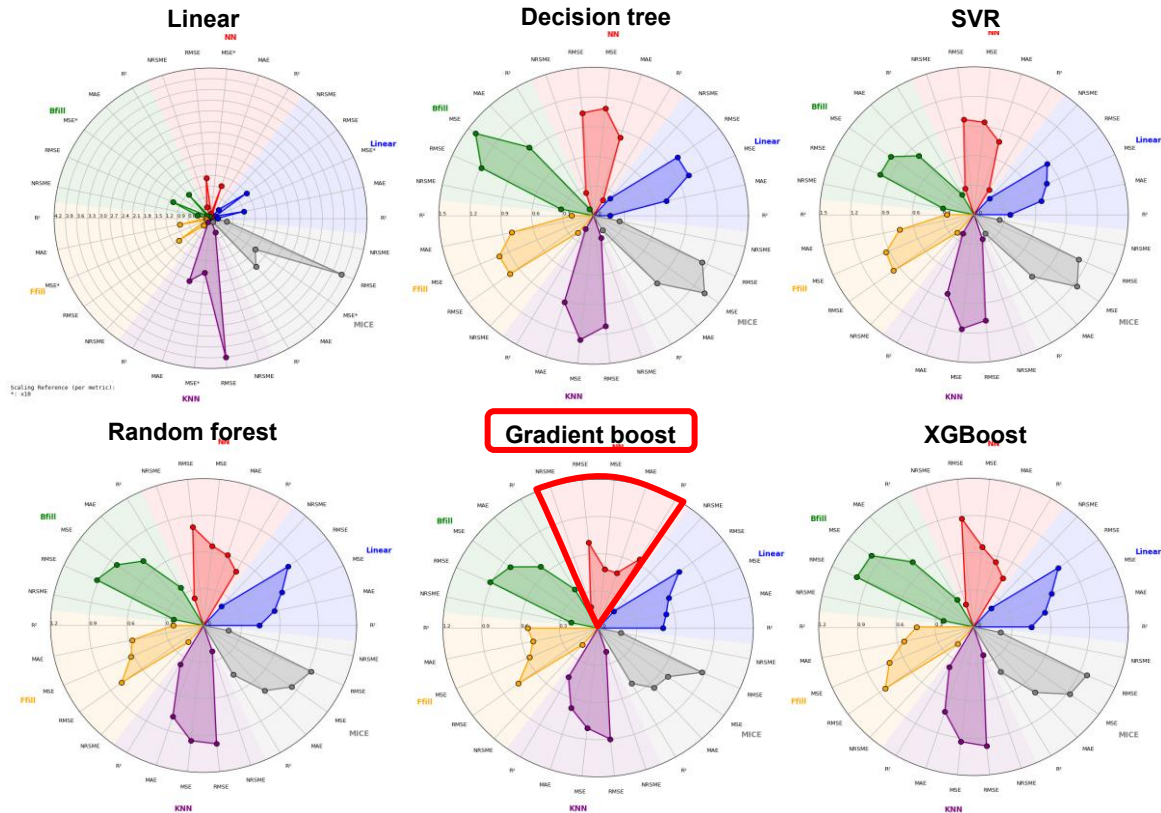


Percentage of holes created



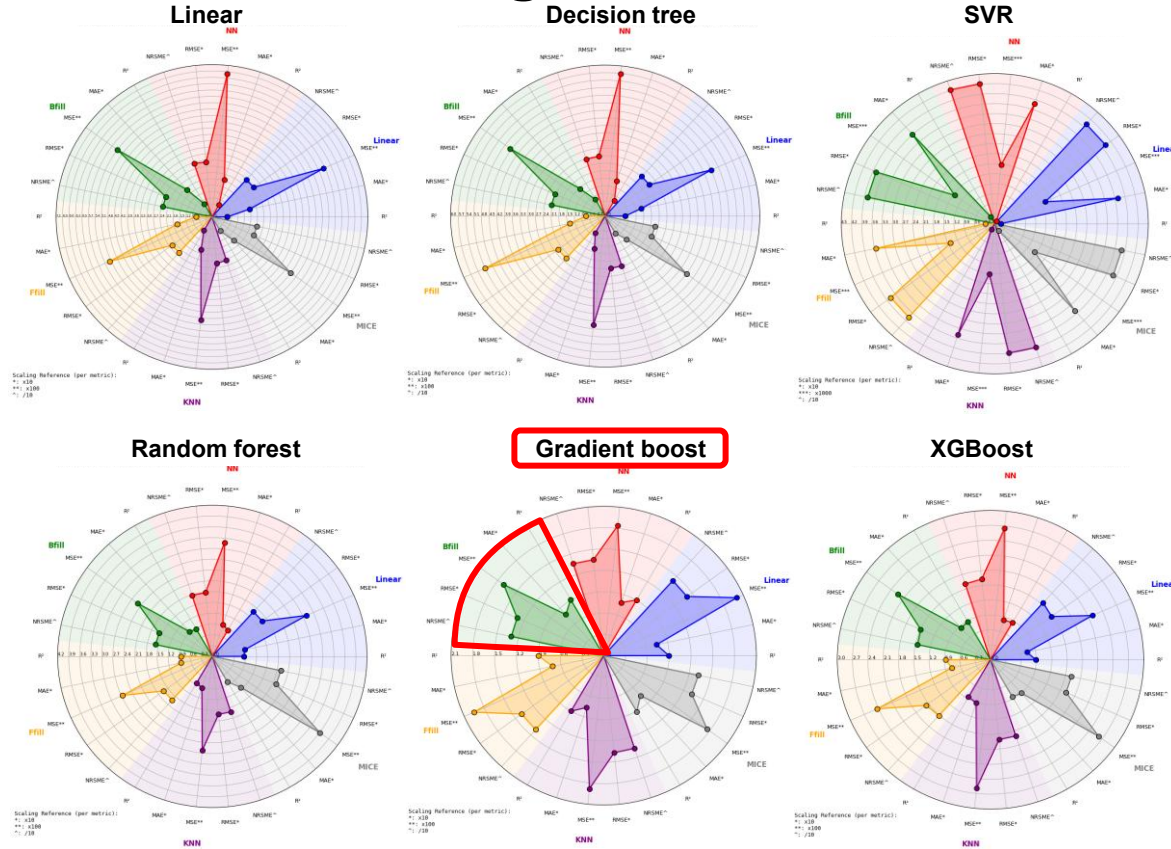
Data imputation: Failure force

*Hyperparameter tuning with Bayesian optimisation



Data imputation: Percentage of holes created

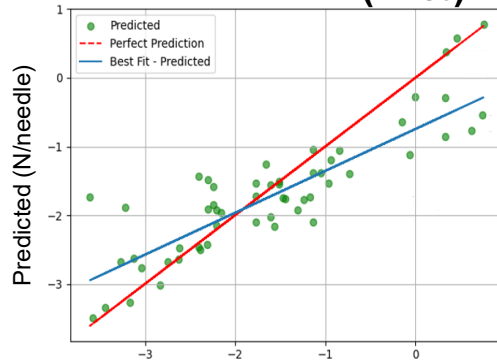
*Hyperparameter tuning with Bayesian optimisation



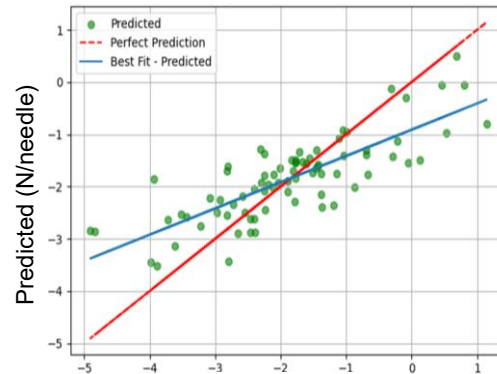
Data augmentation

*Synthetic Minority Over-Sampling Technique for Gaussian Noise

Failure force (20%)

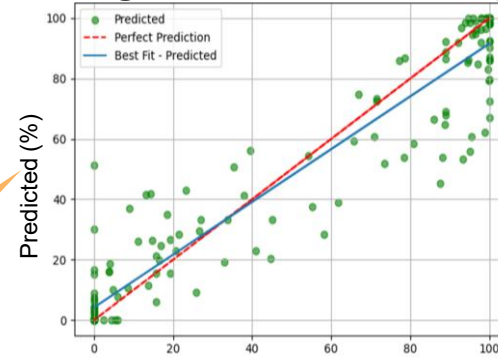


Actual (N/needle)

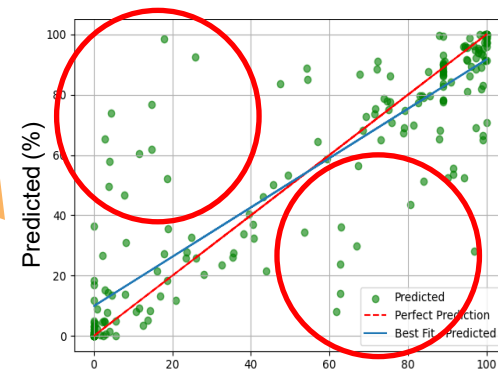


Actual (N/needle)

Percentage of holes created (16%)



Actual (%)



Actual (%)

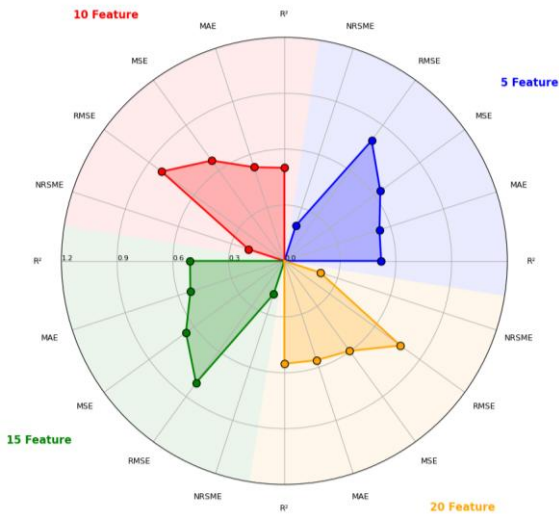
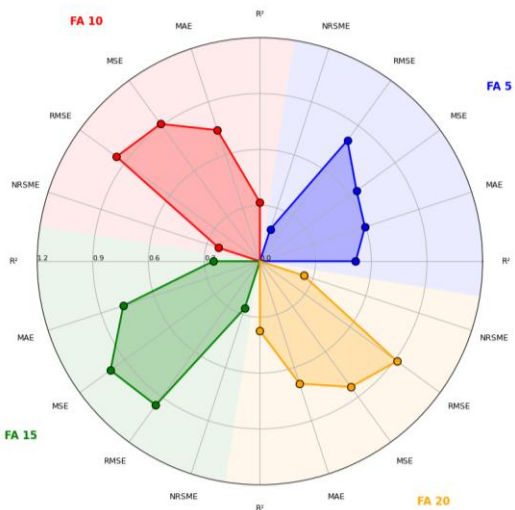
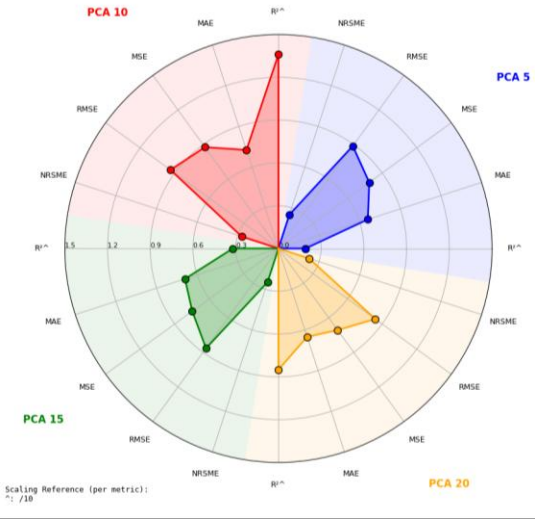


Feature abstraction & selection: Failure force

Principal component analysis

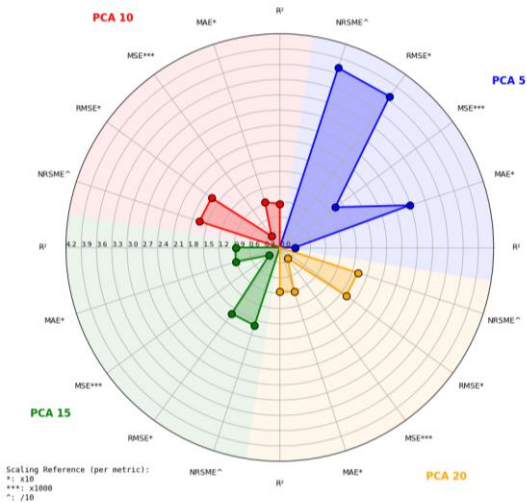
Factor analysis

Forward selection

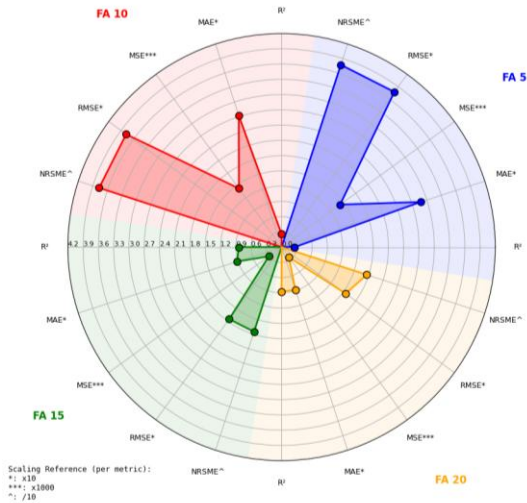


Feature abstraction & selection: Percentage of holes created

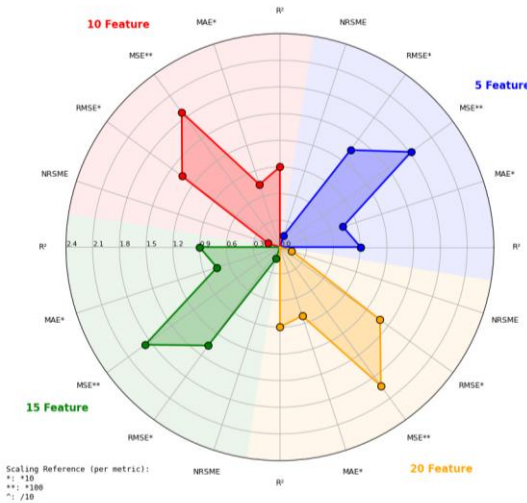
Principal component analysis



Factor analysis

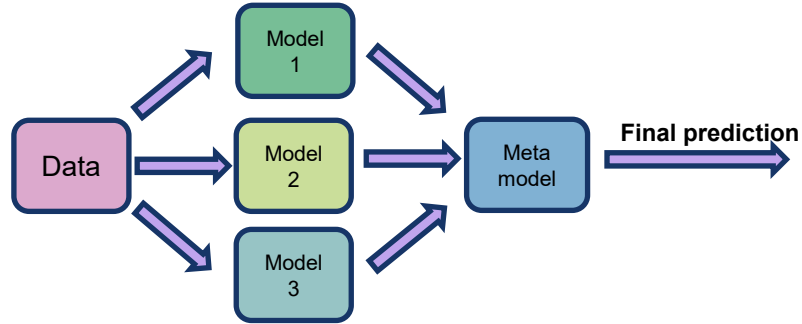


Forward selection

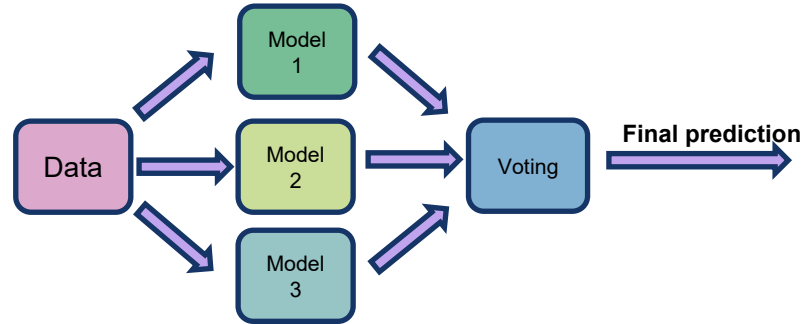


Model selection – ensemble method

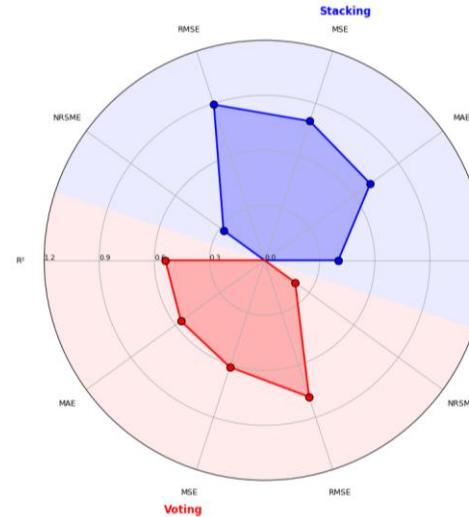
Stacking model



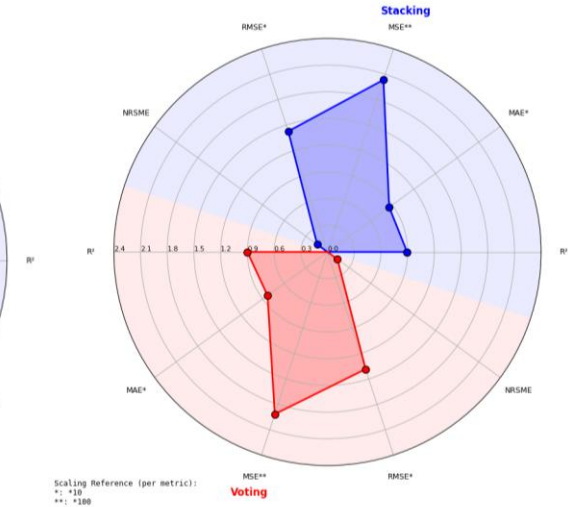
Voting model



Failure force



Percentage of holes created



Conclusion

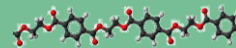
In vitro mechanical performances relies on the **polymer** composition, **drug** content and **microneedle** design.

Data augmentation is beneficial in solving low data set.

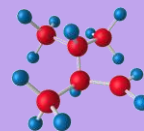
Gradient boosting regression is a robust model for MN mechanical prediction.

Future more clinically relevant prediction on **ex vivo** skin insertion is warranted.

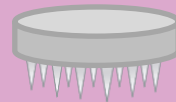
Polymer



Drug



Microneedle



GUI development

Graphical user interface



*Python (3.12.4) with Visual Studio Code

µMech v1.0

Polymer info

Polymer 1-molecular weight (g/mol): 10000

Polymer 1-concentration (%): 90

Polymer 2-molecular weight (g/mol): 12000

Polymer 2-concentration (%): 10

Drug info

Drug molecular weight (g/mol): 5000

Drug concentration (%): 2

Drug log P: 1

Drug content per patch (mg): 10

Compression test:

Mode of compression: Axial

Rate of force exertion (mm/s): 10

Microneedle (MN) dimension info

MN base width (µm): 1000

MN height (µm): 1100

MN number per patch: 100

MN inter-needle spacing (µm): 100

MN tip radius (µm): 20

Needle density: 12

MN base area (µm²): 1100000

Single needle volume (µm³): 1100000000

In vitro skin insertion test:

Insertion force (N): 110

Extra Information:

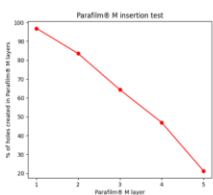
MN aspect ratio: 0.91

Suggestion best fitness:

Buttons: Suggestion, Clear, Predict

Compression test:
Predicted failure force/needle (N): 0.43

Parafilm® M insertion test:
% of holes created in Parafilm® M layer 1: 56.9%
% of holes created in Parafilm® M layer 3: 83.5%
% of holes created in Parafilm® M layer 4: 47.0%
% of holes created in Parafilm® M layer 5: 23.3%



µMech v1.0

Polymer info

Polymer 1-molecular weight (g/mol):

Polymer 1-concentration (%): %

Polymer 2-molecular weight (g/mol):

Polymer 2-concentration (%): %

Drug info

Drug molecular weight (g/mol):

Drug concentration (%): %

Drug log P:

Drug content per patch (mg):

Compression test:

Mode of compression: Axial

Rate of force exertion (mm/s):

Microneedle (MN) dimension info

MN base width (µm):

MN height (µm):

MN number per patch:

MN inter-needle spacing (µm):

MN tip radius (µm):

Needle density:

MN base area (µm²):

Single needle volume (µm³):

In vitro skin insertion test:

Insertion force (N):

Extra Information:

MN aspect ratio:

Suggestion best fitness:

Buttons: Suggestion, Clear, Predict

Shape 1 ratio:

Shape 2 ratio (Optional):

Select MN shape:

User Manual:
Press "Predict" to predict Force and holes %
Use Case 1:
Fill in all info, press "Predict" to predict Force and holes %
Use Case 2:
Fill in "Rate of Force" = 0, press "Predict" to predict holes % only
Use Case 3:
Fill in "Insertion Force" = 0, press "Predict" to predict Failure Force only
Additional Features:
Press "Suggest" to auto fill best options for specific columns (Empowered by Genetic Algo)



Parafilm® M layer	% of isolates created in Parafilm® M layers
1	85
2	78
3	62
4	52
5	5

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Machine learning-driven insights into the mechanical performance of polymeric microneedle array patches ☆

Xue Yao Liew ^{a,1}, Jing Yi Lee ^{b,1}, Jia Yee Ong ^b, Ying Ying Tham ^b, Eik Den Yeoh ^c,
Mohd Azam Osman ^a, Choon Fu Goh ^b  

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Abstract

With growing interest in microneedle technology for enhancing transdermal drug delivery, the current body of literature provides a valuable data reservoir for understanding and predicting mechanical performance — a critical prerequisite for microneedle array patches (MAP) to effectively breach the skin barrier. The integration

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Acknowledgements



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