

- Raw Data structure
  - 23 formulations
  - Columns -
    - i. Name of the API
    - ii. QTY (mg)
    - iii. Polymer
    - iv. Polymer Qty
    - v. Diluent
    - vi. Diluent Qty
    - vii. Binder
    - viii. Binder Qty
    - ix. Lubricant
    - x. Lubricant Qty
    - xi. Glidant
    - xii. Glidant Qty
    - xiii. Total Weight
    - xiv. Thickness
    - xv. Hardness
    - xvi. Friability
    - xvii. Disintegration time
  - Constant values and range of values-
    - i. Name of the API - Rosuvastatin Calcium [10mg]
    - ii. Polymer - Crosspovidone[ 2 - 4 ]
    - iii. Diluent - Mannitol[ 162.0 - 181.75 ]
    - iv. Binder - MCC[ 5.0 - 20.0 ]
    - v. Lubricant - Magnesium stearate [ 0.25 - 1.0 ]
    - vi. Glidant - Talc[ 1 - 3 ]
    - vii. Total Weight : [ 200 - 200 ]
    - viii. Thickness : [ 2.4 - 3.0 ]
    - ix. Hardness : [ 3.0 - 5.6 ]
    - x. Friability : [ 0.169 - 0.489 ]
    - xi. Disintegration time : [ 7 - 15 ]
  - We have not used the box Behnken method
  
- Models Used -
  1. Extra Tree Regressor
  2. Random Forest
  3. Gradient Boost Regressor
  4. Decision Tree Regressor
  5. SVM Regressor
  6. CART Bagging
  7. kNN Regressor
  8. XGBoost

\*The two tables below can be merged as in similarity to the reference research paper with each model showing both values

\*\*can add the DNN model NRMSE and r2 score to the following tables or can keep them in separate tables.

- NRMSE of models:\*lower is better

	Extra Trees	Random Forest	Gradient Boost	Decision Tree	SVM Regressor	CART Bagging	KNN Regressor	XGBoost
Thickness	<b>0.04</b>	0.06	0.08	0.06	0.05	0.06	0.06	0.06
Hardness	0.03	0.03	<b>0.02</b>	0.06	0.04	0.03	0.04	0.03
Friability	0.05	0.05	<b>0.04</b>	0.08	0.19	0.05	0.09	<b>0.04</b>
Disintegration time	0.06	0.08	0.1	0.08	0.13	<b>0.1</b>	<b>0.1</b>	<b>0.1</b>

- R2 score of Model:\*higher is better

	Extra Trees	Random Forest	Gradient Boost	Decision Tree	SVM Regressor	CART Bagging	KNN Regressor	XGBoost
Thickness	0.81	0.67	0.39	0.62	0.7	0.59	0.66	0.6
Hardness	<b>0.97</b>	0.98	0.99	0.9	0.97	0.98	0.96	<b>0.98</b>
Friability	<b>0.97</b>	0.96	0.98	0.93	0.56	0.97	0.89	<b>0.98</b>
Disintegration time	<b>0.94</b>	0.9	0.82	0.89	0.7	0.84	0.82	0.83

- DNN/ANN model score [NRMSE and R2 score]:

Model	NRMSE	R2
Thickness	0.04	0.89
Hardness	0.02	0.98
Friability	0.03	0.97
Disintegration time	0.3	0.96

- Criteria for best formulation: [\[Reference Barathi Mam\]](#)
  1. Tablet diameter: 8.00 mm
  2. Tablet thickness: 2.4 to 3.0 mm
  3. Tablet Hardness: 3 to 6 kg/cm<sup>2</sup>
  4. DT: 10 to 60 secs
- Sorting criteria for NYJ\_data to get the best 10 formulations:
  1. Lowest Dissolution Time
  2. Lowest absolute difference from ideal thickness value [2.7 mm]
  3. Lowest absolute difference from ideal Hardness value [4.5 kg/cm<sup>2</sup>]

Top 10 formulations:

[+ Sorted\\_formulations\\_NYJ](#) - [click this link for formatted table for better readability](#)

Name of the API	QTY (mg)	Polym er	Polymer Qty	Dil ue nt	Dilu ent Qty	Bi nd er	Bi nd er Qt y	Lubricant	Lubri cant Qty	Gl id an t	Gl id an t Qt y	Tot al We igh t	Thickn ess	Hard ness	Friabi lity	Disintegra tion time
Rosuvasta tin Calcium	10	Cross povid one	3	M an nit ol	170. 7	M C C	13. 31	Magnesi um stearate	0.99	Ta lc	2	20 0	2.69	4.51	0.37	10
Rosuvasta tin Calcium	10	Cross povid one	3	M an nit ol	172. 16	M C C	13. 2	Magnesi um stearate	0.64	Ta lc	1	20 0	2.53	4.47	0.36	10.42
Rosuvasta tin Calcium	10	Cross povid one	3	M an nit ol	171. 77	M C C	13. 94	Magnesi um stearate	0.29	Ta lc	1	20 0	2.46	4.58	0.37	10.26
Rosuvasta tin Calcium	10	Cross povid one	3	M an nit ol	171. 1	M C C	13. 97	Magnesi um stearate	0.94	Ta lc	1	20 0.0 1	2.46	4.58	0.37	10.26
Rosuvasta tin Calcium	10	Cross povid one	2	M an nit ol	171. 58	M C C	13. 93	Magnesi um stearate	0.49	Ta lc	2	20 0	2.51	4.59	0.37	10.15
Rosuvasta tin Calcium	10	Cross povid one	3	M an nit ol	172	M C C	12. 5	Magnesi um stearate	0.5	Ta lc	2	20 0	2.8	4.4	0.358	10
Rosuvasta tin Calcium	10	Cross povid one	4	M an nit ol	169. 5	M C C	12. 5	Magnesi um stearate	1	Ta lc	3	20 0	2.6	4.6	0.366	11
Rosuvasta tin Calcium	10	Cross povid one	2	M an nit ol	171. 75	M C C	15	Magnesi um stearate	0.25	Ta lc	1	20 0	2.4	4.6	0.387	10
Rosuvasta tin Calcium	10	Cross povid one	2	M an nit ol	174. 25	M C C	12. 5	Magnesi um stearate	0.25	Ta lc	1	20 0	2.4	4.4	0.342	11
Rosuvasta tin Calcium	10	Cross povid one	3	M an nit ol	173. 08	M C C	12. 27	Magnesi um stearate	0.65	Ta lc	1	20 0	2.57	4.38	0.34	10.68