Supplementary information

Neuro-evolutive modeling of transition temperatures for five-ring bent-core molecules derived from resorcinol

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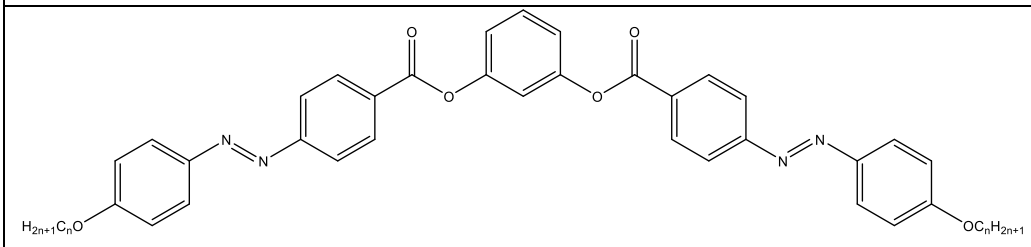
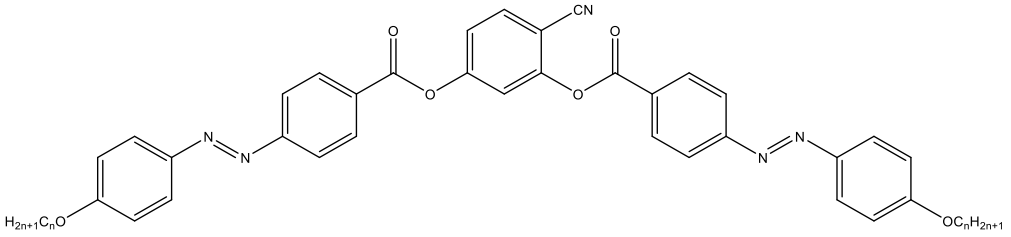
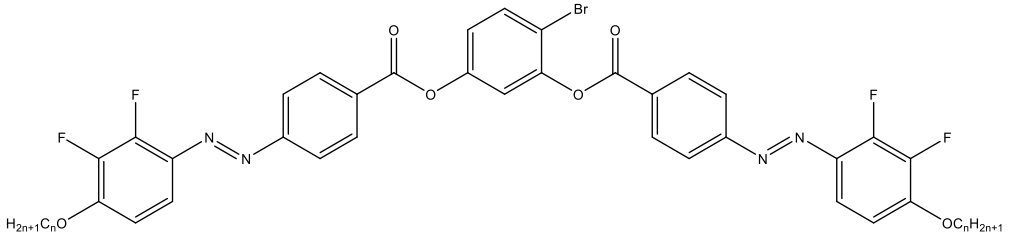
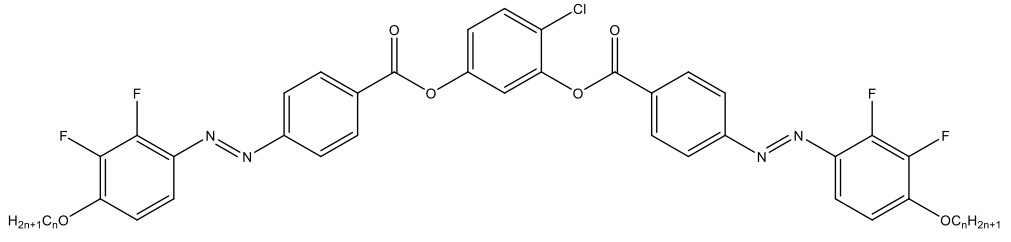
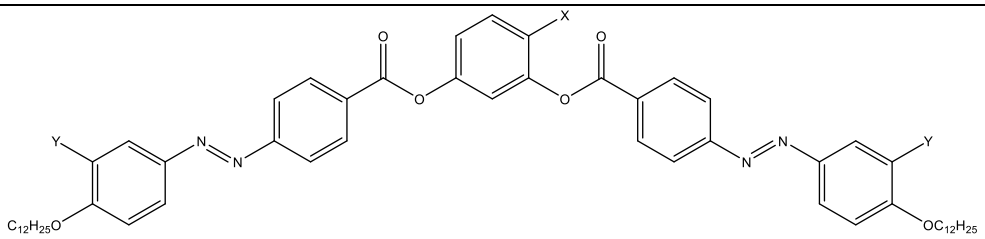
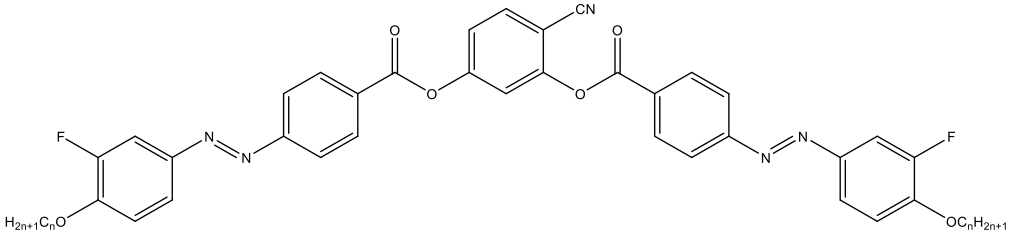
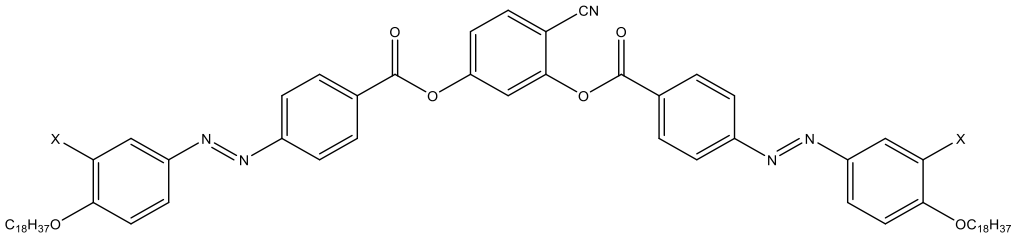
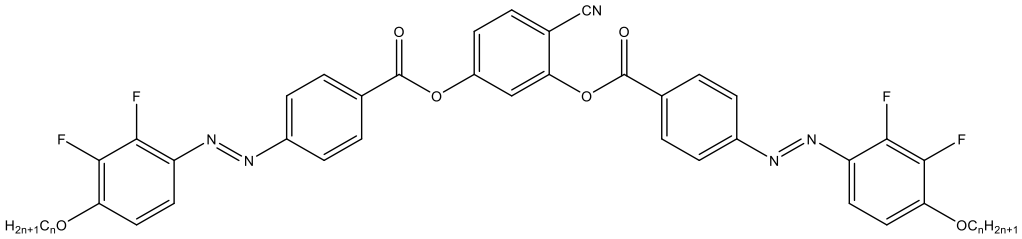
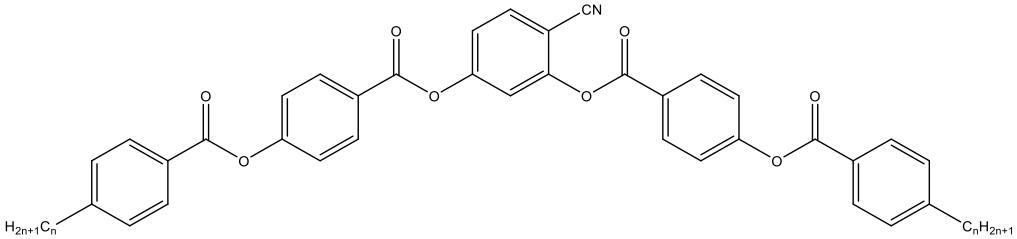
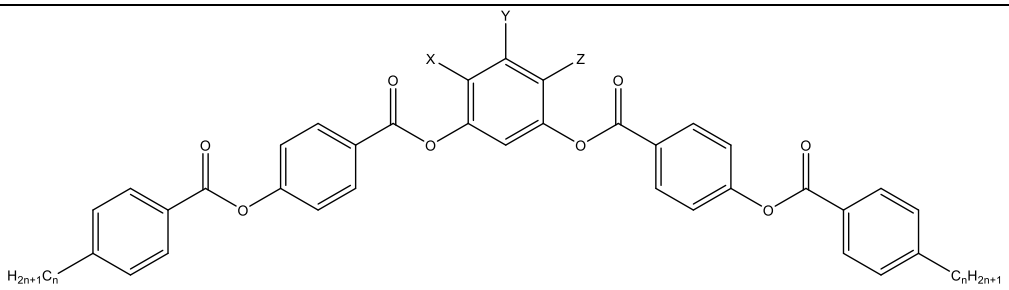
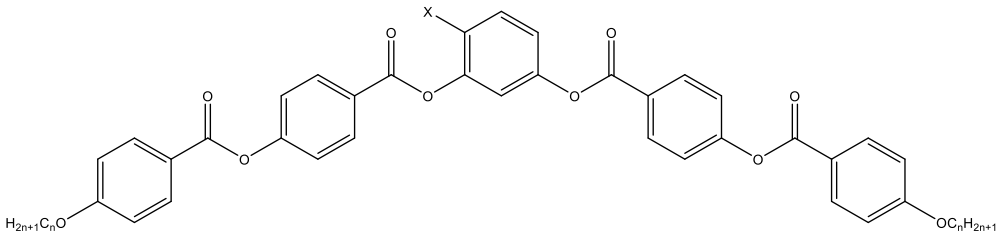
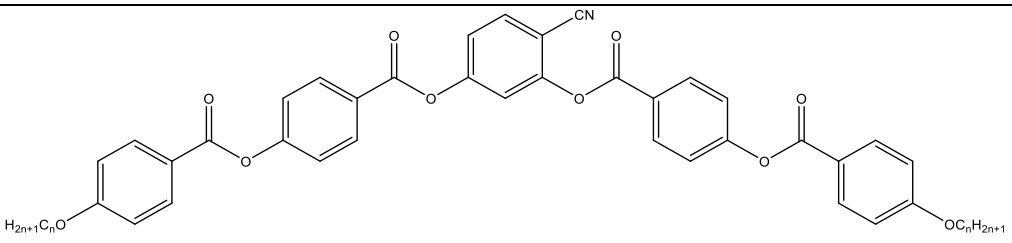
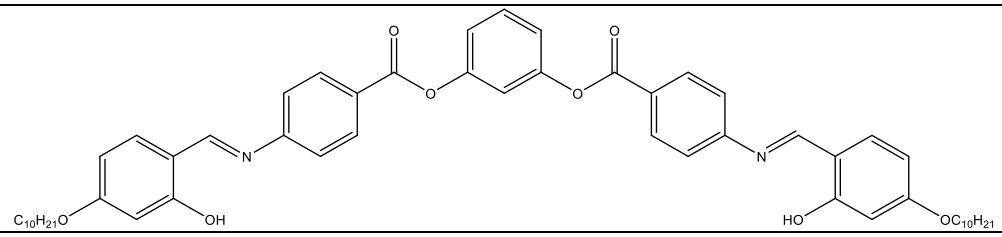
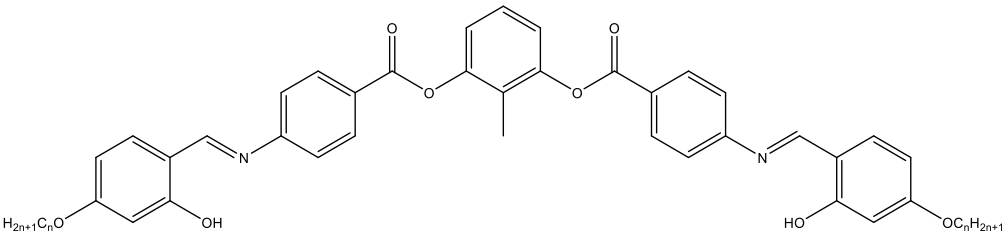
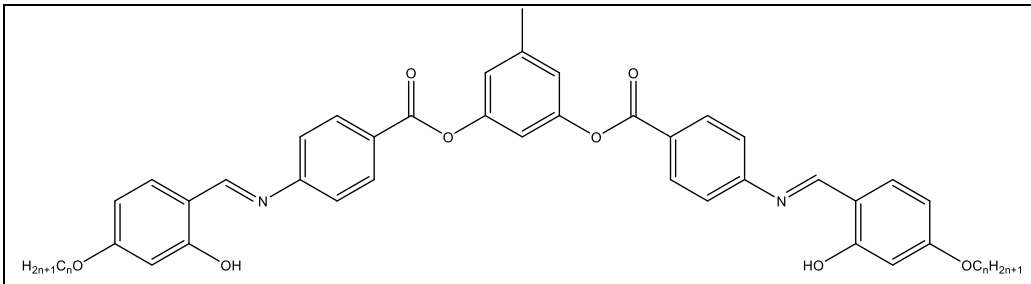
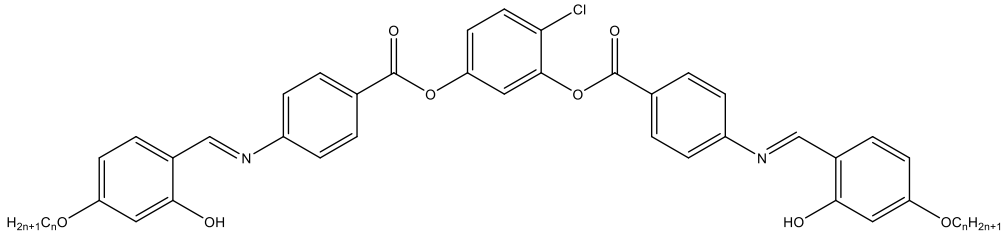
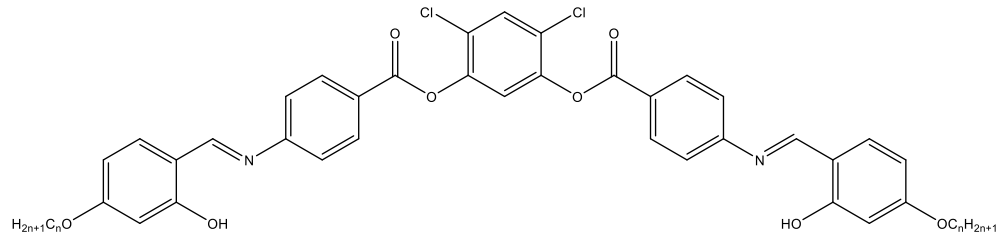
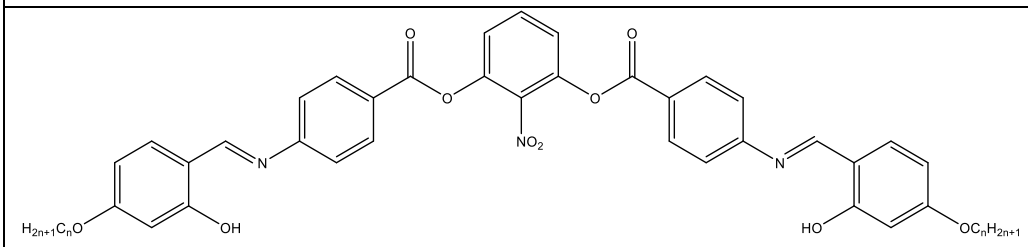
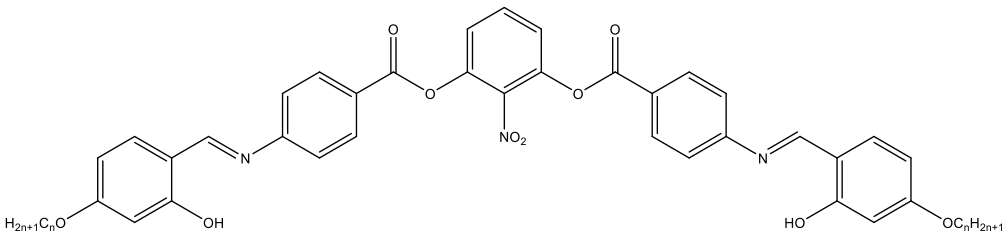
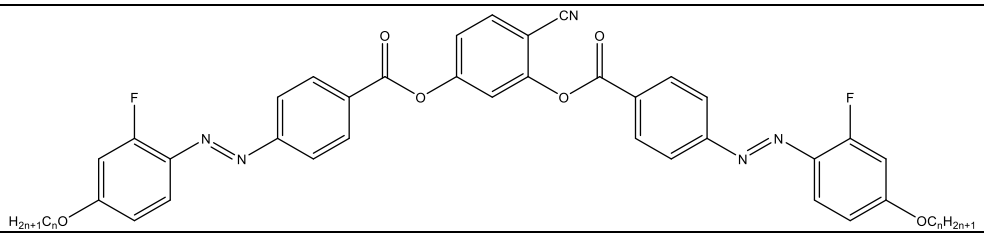
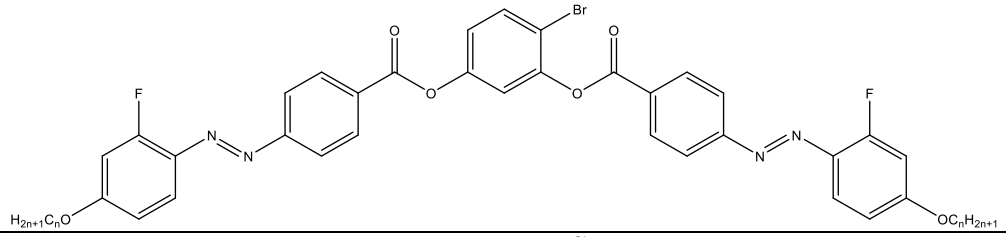
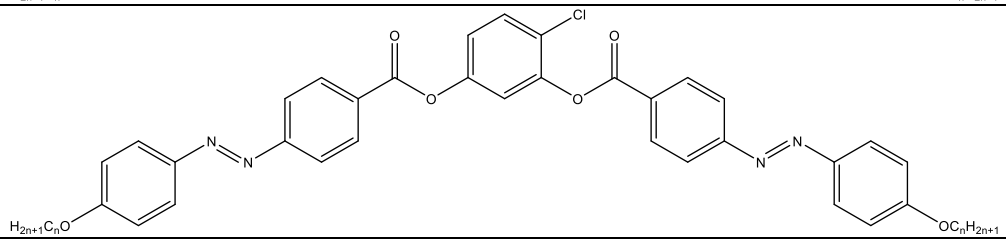
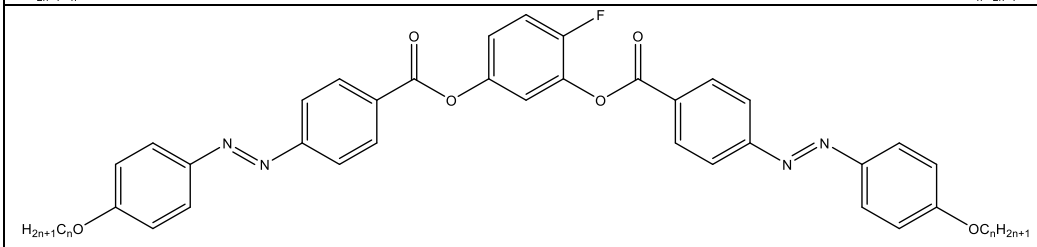
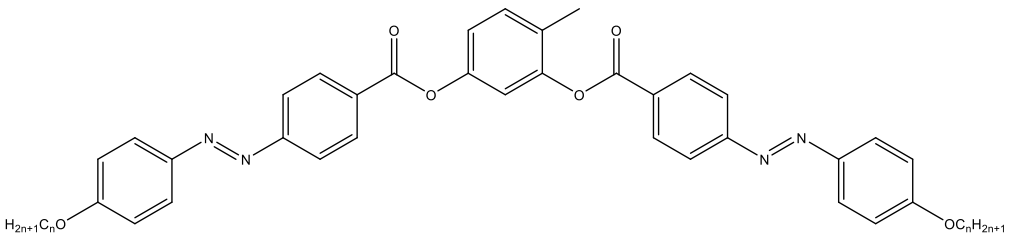
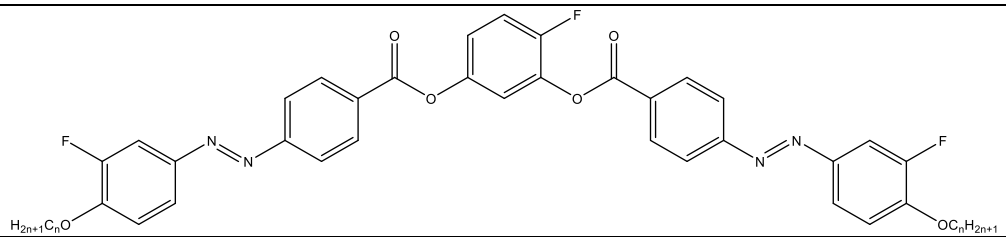
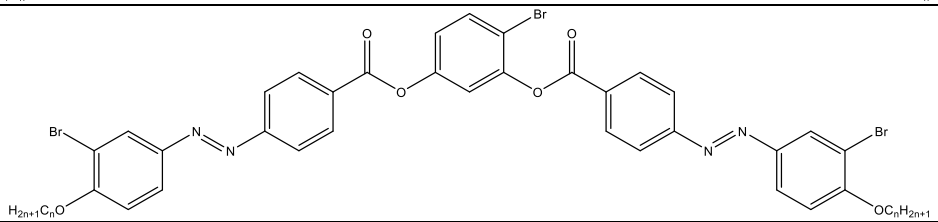
Table S1. The molecular formula of the bent-core compounds included in the database

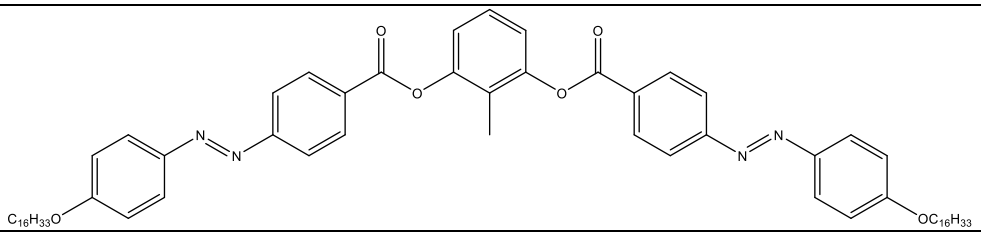
Molecular structure	Code of structure	n	Reference
	S1_1 S1_2 S1_3 S1_4 S1_5 S1_6 S1_7 S1_8 S1_9	6 7 8 9 10 12 14 16 18	[39] [39] [39] [39] [39] [42] [42] [42] [42]
	S2_1 S2_2 S2_3 S2_4 S2_5 S2_6	8 10 12 14 16 18	[40]
	S3_1 S3_2 S3_3 S3_4 S3_5	8 10 12 14 16	[19]
	S4_1 S4_2 S4_3 S4_4 S4_5	8 10 12 14 16	[19]

 X= Br, Y= H (S5_1); X= Br, Y= F (S5_2); X= Cl, Y= H (S5_3); X= Cl, Y= F (S5_4)	S5_1 S5_2 S5_3 S5_4	12 12 12 12	[43] [44] [43] [44]
	S6_1 S6_2 S6_3 S6_4 S6_5 S6_6 S6_7 S6_8 S6_9	4 6 8 10 12 14 16 18 20	[2]
 X= Br (S7_1); X= CH_3 (S7_2)	S7_1 S7_2	18 18	[2]
	S8_1 S8_2 S8_3 S8_4 S8_5	8 10 12 14 16	[2]
	S9_1 S9_2 S9_3 S9_4 S9_5 S9_6 S9_7 S9_8 S9_9 S9_10 S9_11 S9_12	2 3 4 5 6 7 8 9 10 11 12 14	[20]

 X, Z= H and Y=CN (S10_1 and S10_2); X= Cl and Y, Z= H (S10_3); X, Z= Cl and Y= H(S10_4 and S10_5); X, Y= H and Z= CH_3 (S10_6).	S10_1 S10_2 S10_3 S10_4 S10_5 S10_6	6 12 12 6 12 6	[20]
 X= H (S11_1 ÷ S11_4); X= F (S11_5 ÷ S11_8); X= Cl (S11_9 ÷ S11_12); X= CH_3 (S11_13 ÷ S11_16)	S11_1 S11_2 S11_3 S11_4 S11_5 S11_6 S11_7 S11_8 S11_9 S11_10 S11_11 S11_12 S11_13 S11_14 S11_15 S11_16	8 10 12 14 8 10 12 14 8 10 12 14 8 10 12 14	[21]
	S12_1 S12_2 S12_3 S12_4 S12_5 S12_6 S12_7	6 7 8 9 10 12 16	[33]
	S13_1	10	[41]
	S14_1 S14_2 S14_3 S14_4 S14_5 S14_6 S14_7 S14_8 S14_9	7 8 9 10 11 12 16 18 22	[10]

	S15_1 S15_2 S15_3 S15_4 S15_5 S15_6 S15_7 S15_8 S15_9	7 8 9 10 11 12 16 18 22	[10]
	S16_1 S16_2 S16_3 S16_4 S16_5 S16_6 S16_7 S16_8 S16_9	7 8 9 10 11 12 16 18 22	[10]
	S17_1 S17_2 S17_3 S17_4 S17_5 S17_6 S17_7 S17_8 S17_9	7 8 9 10 11 12 16 18 22	[10]
	S18_1 S18_2 S18_3 S18_4 S18_5 S18_6 S18_7	8 9 10 11 12 16 18	[10]
	S19_1 S19_2 S19_3 S19_4 S19_5 S19_6 S19_7 S19_8	6 7 8 10 11 12 16 18	[10]

	S20_1 S20_2 S20_3 S20_4 S20_5	8 10 12 14 16	[2]
	S21_1 S21_2 S21_3 S21_4 S21_5	8 10 12 14 16	[43]
	S22_1 S22_2 S22_3 S22_4	8 10 14 16	[43]
	S23_1 S23_2 S23_3 S23_4 S23_5	8 10 12 14 16	[43]
	S24_1 S24_2 S24_3 S24_4 S24_5 S24_6 S24_7 S24_8 S24_9 S24_10	6 8 9 10 12 14 16 18 20 22	[32]
	S25_1 S25_2 S25_3	6 14 20	[32]
	S26_1	14	[32]

	S27_1	16	[42]

The accuracy indicators were calculated as follows:

$Mean\ Absolute\ Error\ (MAE)$: $MAE = \frac{1}{n}\sum_{i=1}^{n}\left|y_{actual} - y_{predicted}\right|$ (Equation S1)

$Mean\ Absolute\ Percentage\ Error\ (MAPE)$: $MAPE = \frac{100}{n}\sum_{i=1}^{n}\left|\frac{y_{actual}-y_{predicted}}{y_{actual}}\right|$ (Equation S2)

$Root\ Mean\ Squared\ Error\ (RMSE)$: $RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_{actual} - y_{predicted})^2}$ (Equation S3)

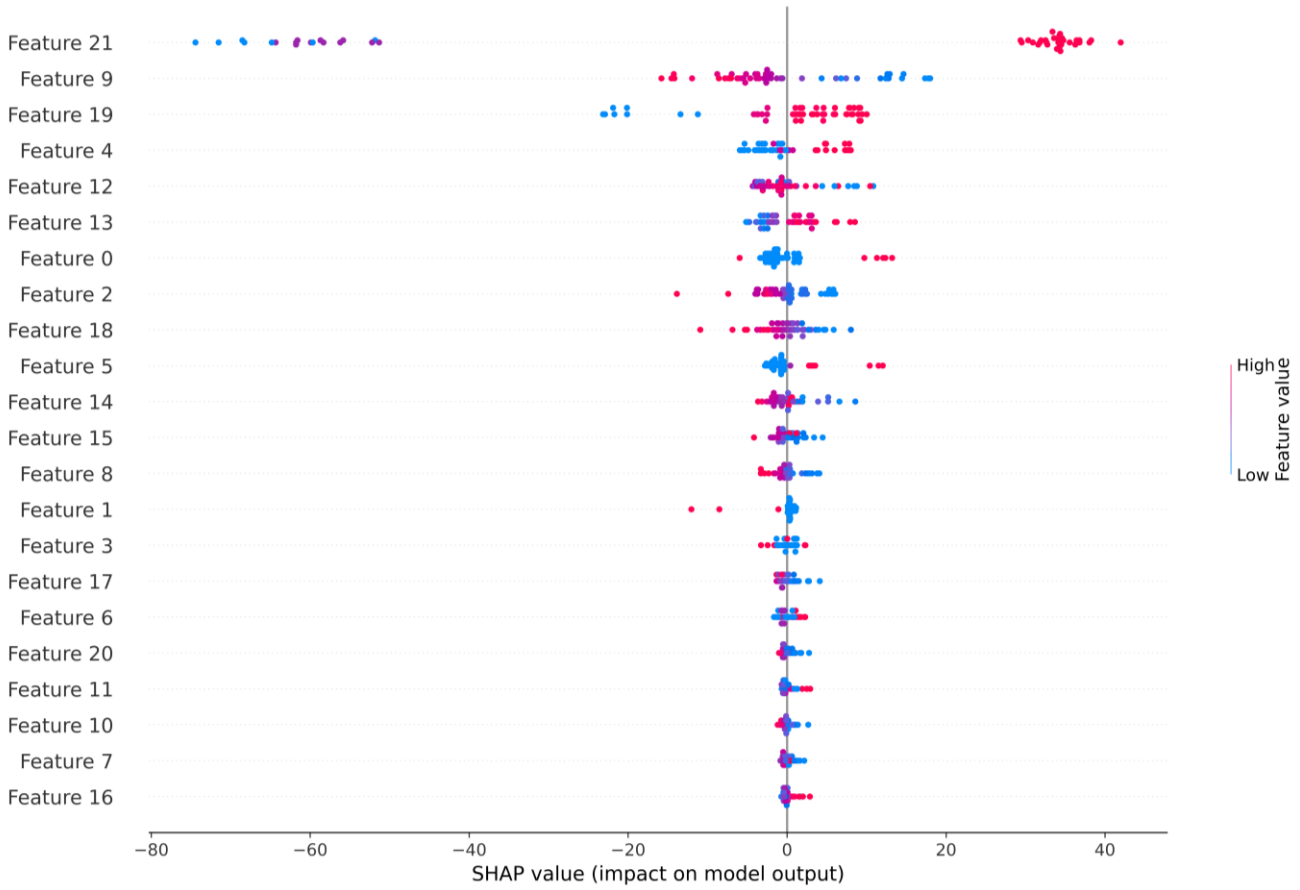


Figure S1- The SHAP values for T1 model.

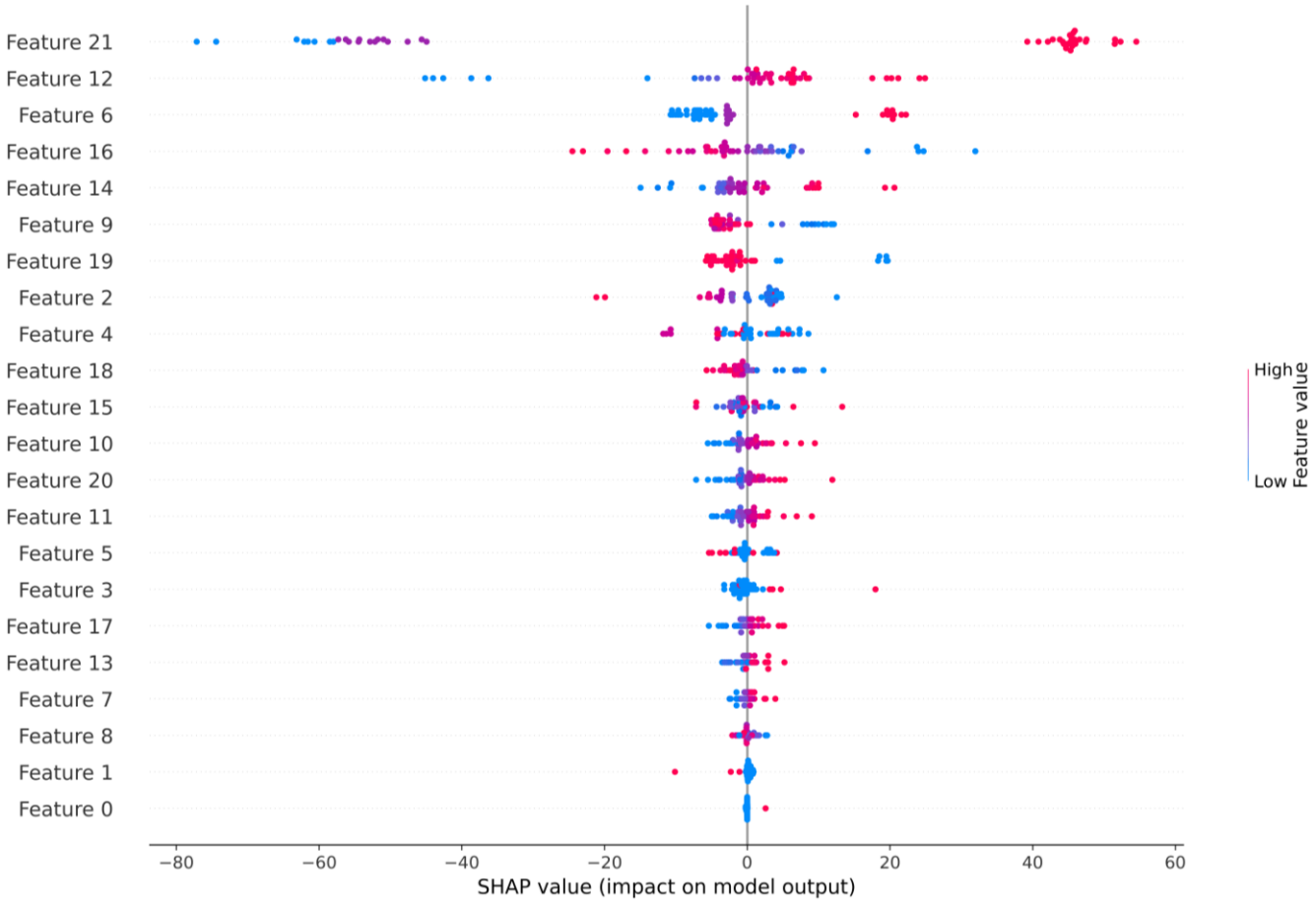


Figure S2- The SHAP values for T2 model.

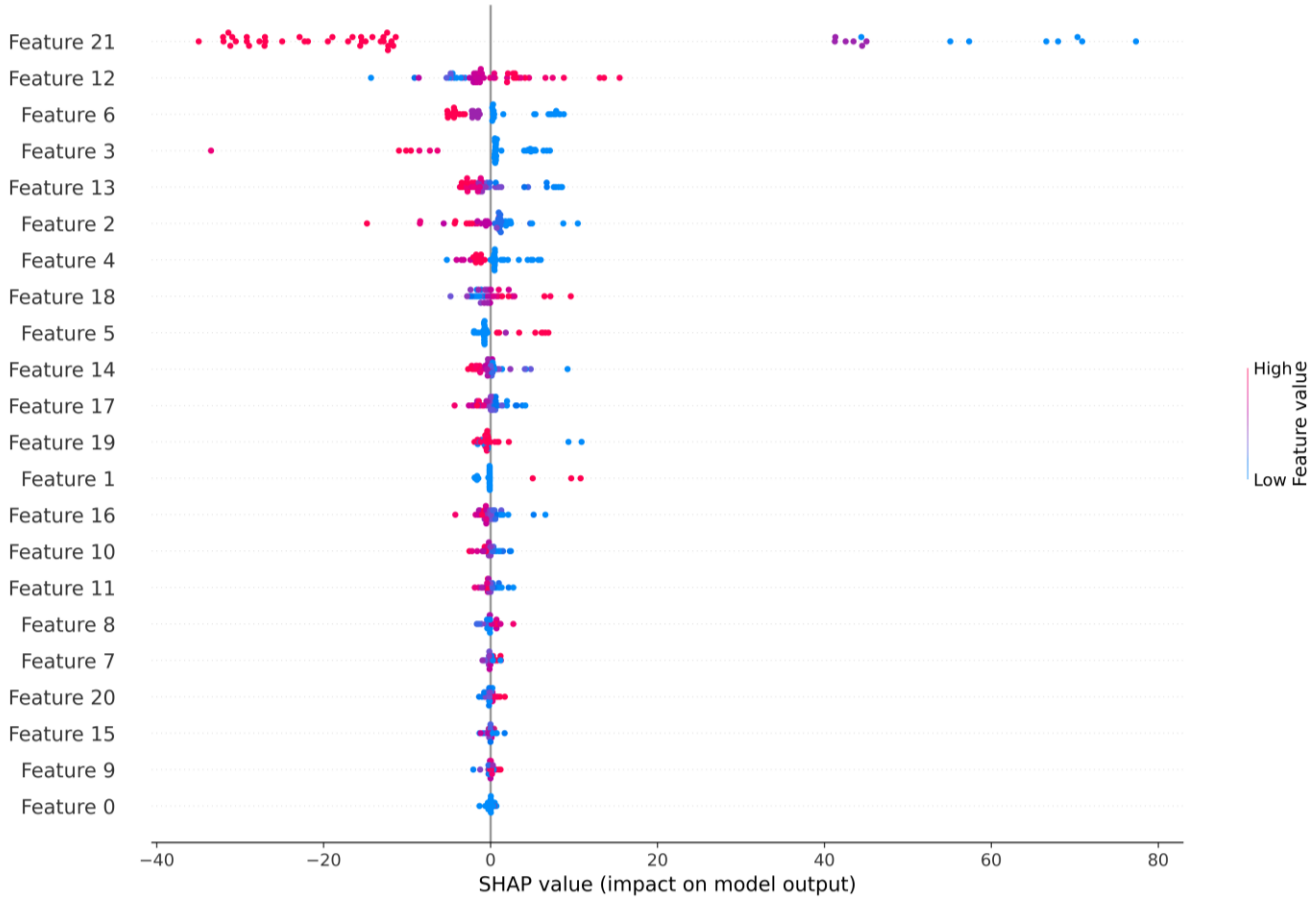


Figure S3- The SHAP values for T3 model.

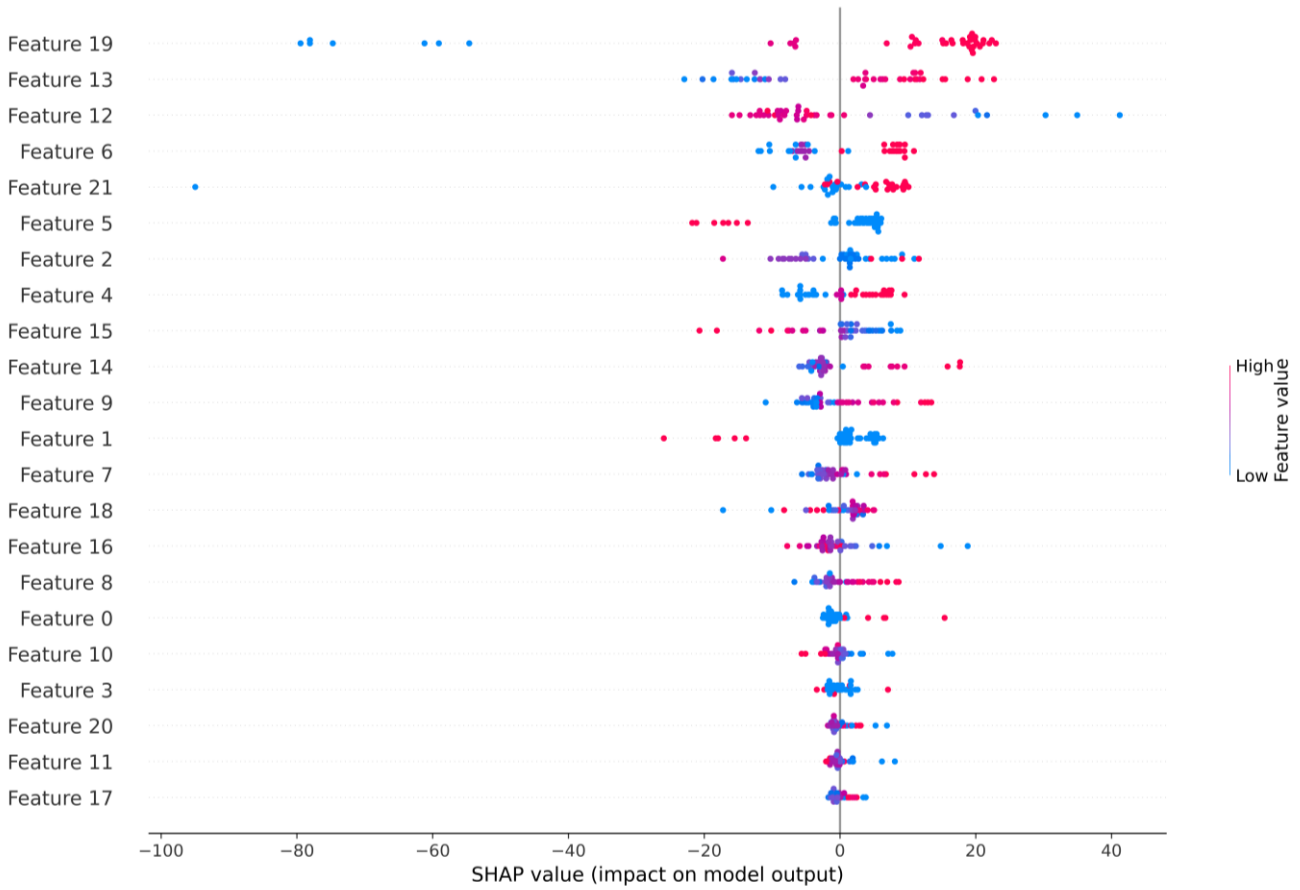


Figure S4- The SHAP values for T4 model.

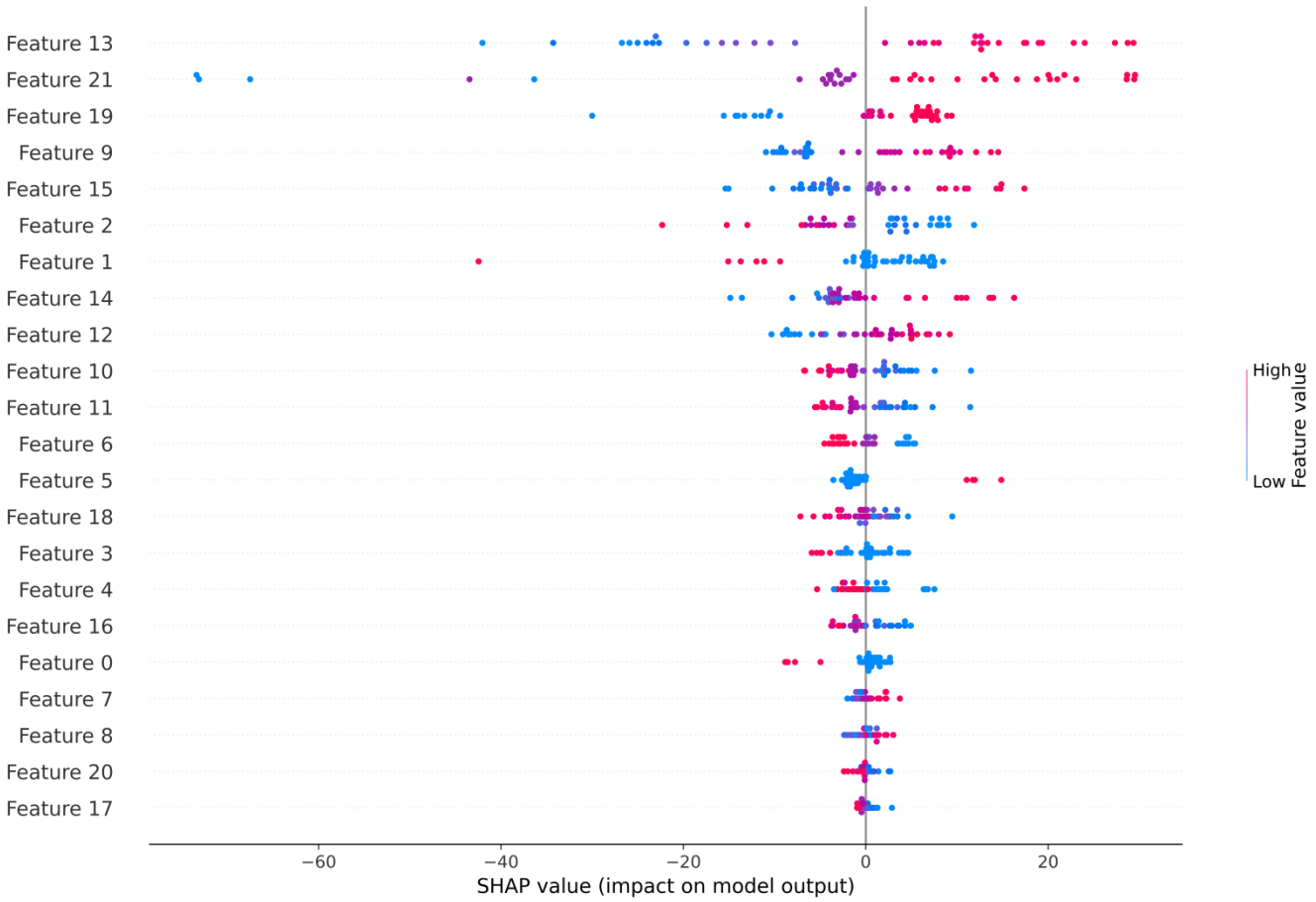


Figure S5- The SHAP values for T5 model.

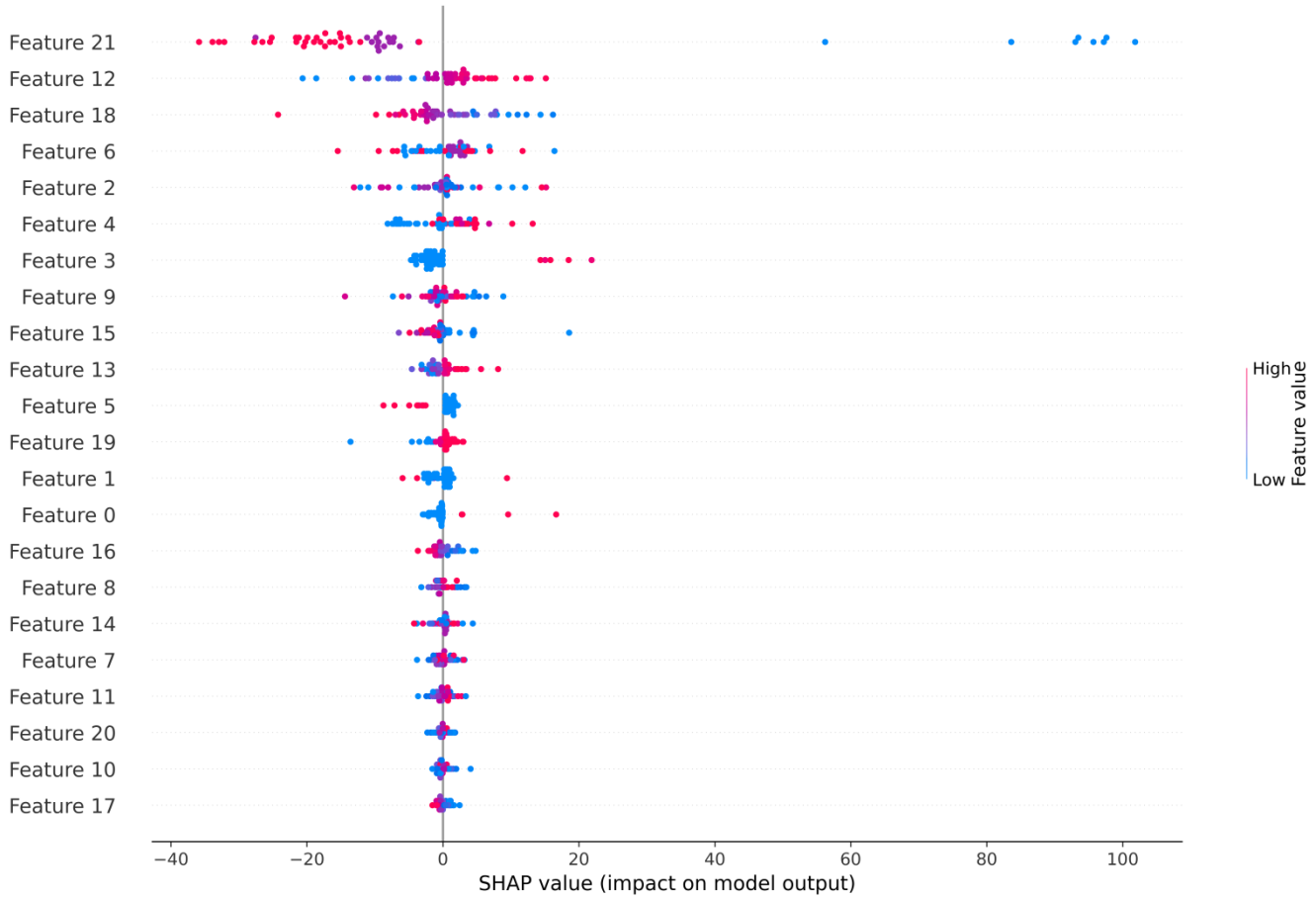


Figure S6- The SHAP values for T6 model.