

Prediction and evaluation of multiple Output machine learning methods for ethylene oligomerization and aromatization kinetics modeling

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Table S1 Parameters obtained after hyperparametric tuning of three machine learning models

K Nearest Neighbors		Random Forest				Artificial neural network	
Parameters	Value	Parameters	Value	Parameter	Value	Parameter	Value
K	5	n-estimator	120	max_leaf_nodes	None	number of hidden layer	1
Weight function	distance	max_features	auto	Bootstrap	True	number of neurons in the hidden layer	30
		max_depth	3	n_jobs	-1	activation function	Sigmoid
		min-samples-split	2	random_state	1		Relu
		min-samples-leaf	1	criterion	mse	loss	MSE
		min_weight_fraction_leaf	1				

Table S2 Predicted product yields of H-ZSM-5 with Si/Al ratio 25 at temperature of 873 K and space time of 4.1468-18.667gcat·h/mol

Temperature	Space time	Yield of product (%)										
		C_2	C_3	$C_3^=$	$C_4^=$	C_5^o	$C_5^=$	C_6^o	$C_6^=$	C_7^o	$C_7^=$	C_8^o
823K	4.1468	0.33	1.168	28.47	11.08	1.78	3.176	2.876	4.98	5.79	1.132	7.78
	5.334	0.411	2.89	27.88	10.07	1.65	2.71	3.494	3.638	7.57	1.98	9.309
	7.4676	0.59	4.32	24.75	9.85	1.47	2.08	4.413	3.078	10.58	2.97	12.186
	12.443	1.16	7.69	19.25	8.10	1.06	1.17	5.832	2.06	13.24	3.87	18.777
	18.667	1.917	10.82	14.26	6.30	0.85	0.94	6.709	1.083	15.85	4.64	25.899

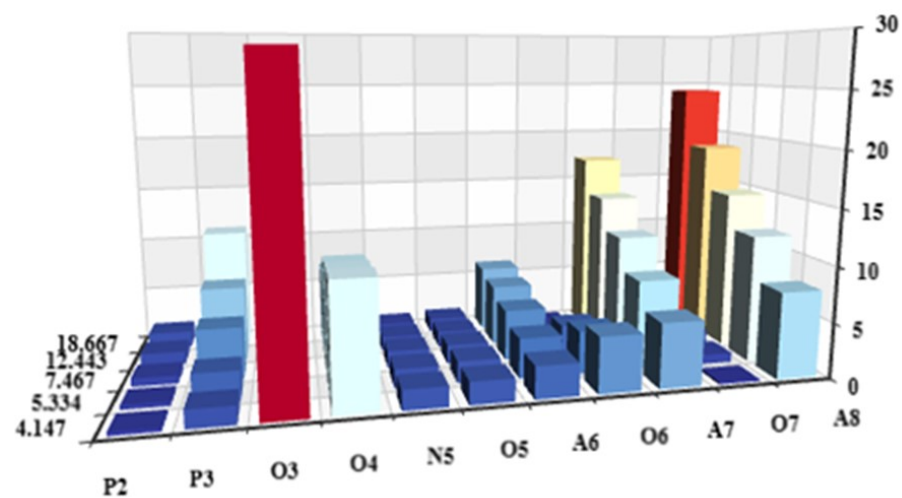
Table S3 Predicted product yields of H-ZSM-5 with Si/Al ratio 19 at temperature of 723 K and space time of 3.23-7.64gcat·h/mol

Temperature	Space time	Yield of product (%)										
		C_2	C_3	$C_3^=$	$C_4^=$	C_5^o	$C_5^=$	C_6^o	$C_6^=$	C_7^o	$C_7^=$	C_8^o
723K	3.23	0.56	0.20	25.00	18.20	2.28	2.63	1.26	7.01	10.66	1.10	14.04
	4.79	0.64	0.32	24.50	17.70	1.75	3.50	1.68	6.76	12.00	2.01	15.12
	7.64	0.88	1.74	23.40	17.00	0.98	4.82	2.26	5.09	13.79	3.10	16.76

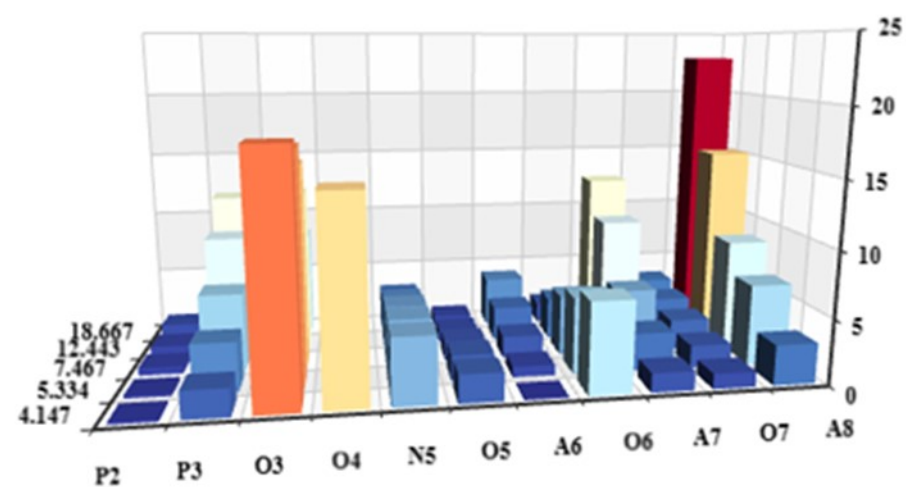
Table S4 Predicted product yields of H-ZSM-5 with Si/Al ratio 19 at temperature of 873 K and space time of 4.6667-18.667gcat·h/mol

Temperature	Space time	Yield of product (%)					
		$C_4^=$	C_6^o	$C_6^=$	C_7^o	$C_7^=$	C_8^o
873K	4.6667	0.30004	8.5659	1.0964	14.3497	1.5497	0.954
	9.3333	0.28953	13.9004	1.5801	19.3084	2.2507	3.085
	18.6667	0.28075	19.68	1.9175	28.5209	3.9116	5.839

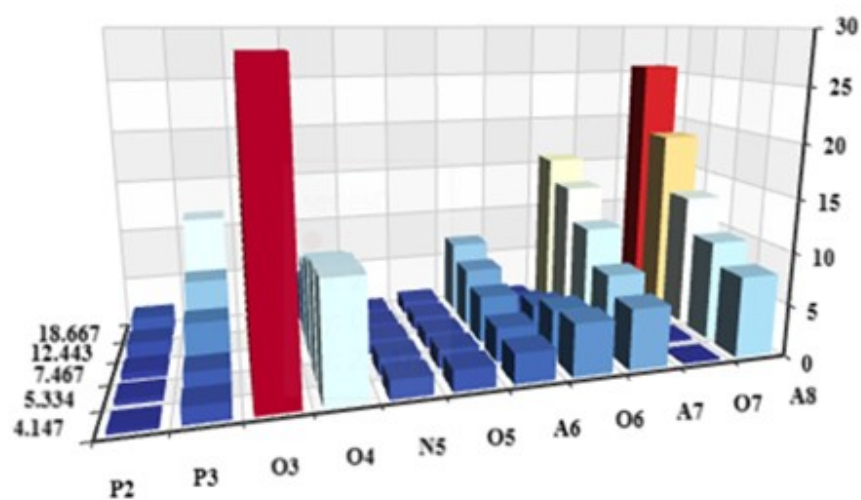
Single-event kinetic model



KNN



RF



ANN

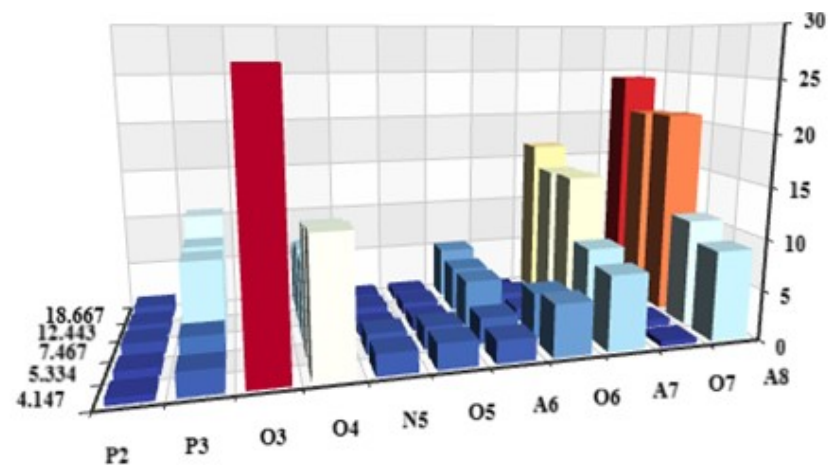


Fig. S1 Comparison of the activity of H-ZSM-5 with a Si/Al ratio of 25 predicted by single-event kinetic model and three machine learning models at temperatures of 823 K and space times of 4.1468-18.667gcat·h/mol