

Supplementary Materials

Prediction of fuel properties of torrefied biomass based on back propagation neural network optimized by genetic algorithm

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Table S1. Dataset.

Biomass	Torrefaction condition	Ref.
olive residue, almond shell	N ₂ , 275 °C, 60 min	[1]
olive tree	He, 220~280 °C, 60~360 min	[2]
rice husk	Ar, 220~270 °C, 30~60 min	[3]
coffee grounds	N ₂ , 200~300 °C, 30 min	[4]
banana leaf waste	N ₂ , 220~280 °C, 1 min	[5]
rice straw, rice husk	N ₂ , 200~300 °C, 30 min	[6]
pearl millet, walnut shell	N ₂ , 230~300 °C, 30~90 min	[7]
ash tree, hazelnut shell, refuse-derived fuel	N ₂ , 230~290 °C, 30 min	[8]
garden waste	Ar, 200~300 °C, 30~60 min	[9]
mixture of municipal organic wastes and biomass	N ₂ , 200~275 °C, 30 min	[10]
empty fruit bunches	N ₂ , 225~300 °C, 40 min	[11]
oil palm empty fruit bunch	N ₂ , 250~300 °C, 30 min	[12]
caragana	N ₂ , 225~275 °C, 10~20 min	[13]
pellet consists of 80% larch and 20% oak	anoxic, 200~270 °C, 20~40 min	[14]
rice straw, bamboo dust	N ₂ , 250 °C, 15 min	[15]
pine sawdust	N ₂ , 260~300, 11 min	[16]
ananas comosus peel, annona squamosa peel	N ₂ , 210~300 °C, 30~60 min	[17]
eucalyptus grandis	N ₂ , 230~290 °C, 60 min	[18]
leucaena leucocephala	N ₂ , 260~300 °C, 0~30 min	[19]

Biomass	Torrefaction condition	Ref.
moso bamboo	N ₂ , 200~300 °C, 60~120 min	[20]
rice husk, rice straw	N ₂ , 200~300 °C	[21]
pongamia seed pods	N ₂ , 200~300 °C, 60 min	[22]
rubberwood	N ₂ , 200~300 °C, 20~60 min	[23]
cellulose	N ₂ , 200~290 °C, 30 min	[24]
fruit waste	N ₂ , 210~300 °C, 30~60 min	[25]
empty fruit bunches	N ₂ , 225~300 °C, 20~60 min	[26]
mustard crop residue	N ₂ , 200~300 °C, 30~60 min	[27]
pine, kenaf	N ₂ , 250 °C, 30 min	[28]
prosopis juliflora	N ₂ , 230~270 °C, 30 min	[29]
sugarcane bagasse	N ₂ , 230~280 °C, 30~45 min	[30]
orange peel	N ₂ , 220~280 °C, 30 min	[31]
rice husk, rice straw	N ₂ , 200~300 °C, 60 min	[32]
poplar wood	N ₂ , 200~300 °C, 60 min	[33]
olive kernel	N ₂ , 300 °C, 60 min	[34]
rice husk	oxygen-deficient, 240~280 °C, 0~90 min	[35]
misanthus, hops waste	oxygen-deficient, 250 °C, 60 min	[36]
waste vine shoots	N ₂ , 220~280 °C, 10~60 min	[37]
almond shells, olive stones	N ₂ , 250~300 °C, 45 min	[38]
sugarcane leaves	N ₂ , 225~300 °C, 30 min	[39]
corncob	N ₂ , 210~300 °C, 30 min	[40]
bamboo forest residues	N ₂ , 200~300 °C, 60 min	[41]
leftover rice, leftover cabbage, leftover	Ar, 200~300 °C, 30 min	[42]
pork, watermelon peel		
wooden block	N ₂ , 220~280 °C, 40 min	[43]
sugarcane bagasse	N ₂ , 200~275 °C, 60 min	[44]
sorghum straw	N ₂ , 230~300 °C, 30~108 min	[45]
pigeon pea stalk, eucalyptus	N ₂ , 200~300 °C, 30 min	[46]
sorghum straw	N ₂ , 230~300 °C, 10 min	[47]
rice straw	N ₂ , 200~250 °C, 45 min	[48]
pine wood, rice husk	N ₂ , 210~300 °C, 30 min	[49]
rice husk	N ₂ , 220~300 °C, 30 min	[50]
mixture of waste wood, oak waste wood and sewage sludge	oxygen-deficient, 220~300 °C, 120 min	[51]
corncob, rice husk	N ₂ , 200~300 °C, 30~60 min	[52]
ponkan peel waste	N ₂ , 200~300 °C, 15~60 min	[53]
black alder	N ₂ , 250~300 °C, 30~60 min	[54]
Norway spruce	N ₂ , 225~275 °C, 30~60 min	[55]
sugarcane bagasse	N ₂ , 200~300 °C, 15~60 min	[56]
pigeon pea stalk	N ₂ , 225~275 °C, 15~45 min	[57]
rice husk	N ₂ , 210~300 °C, 30 min	[58]
wood biomass	Ar, 230~290 °C, 60 min	[59]
pine wood	N ₂ , 250~290 °C, 30~60 min	[60]

Biomass	Torrefaction condition	Ref.
vine pruning, olive tree pruning, corn stalk, poultry litters	N ₂ , 300 °C, 30 min	[61]
rice straw, cotton stalk	N ₂ , 210~290 °C, 20~60 min	[62]
cotton stalk, corn stalk	N ₂ , 200~290 °C, 30 min	[63]
oil palm fiber, Eucalyptus	N ₂ , 250~300 °C, 60 min	[64]
willow, reed canary grass, wheat straw	N ₂ , 230~290 °C, 30 min	[65]
rice straw	N ₂ , 200~300 °C, 60 min	[66]

References:

1. Gürel, K.; Magalhães, D.; Kazanç, F., The effect of torrefaction, slow, and fast pyrolysis on the single particle combustion of agricultural biomass and lignite coal at high heating rates. *Fuel* **2022**, 308, 122054.
2. González-Arias, J.; Gómez, X.; González-Castaño, M.; Sánchez, M.E.; Rosas, J.G.; Cara-Jiménez, J., Insights into the product quality and energy requirements for solid biofuel production: A comparison of hydrothermal carbonization, pyrolysis and torrefaction of olive tree pruning. *Energy* **2022**, 238, 122022.
3. Zhang, L.; Wang, Z.; Ma, J.; Kong, W.; Yuan, P.; Sun, R.; Shen, B., Analysis of functionality distribution and microstructural characteristics of upgraded rice husk after undergoing non-oxidative and oxidative torrefaction. *Fuel* **2022**, 310, 122477.
4. Fu, J.; Liu, J.; Xu, W.; Chen, Z.; Evrendilek, F.; Sun, S., Torrefaction, temperature, and heating rate dependencies of pyrolysis of coffee grounds: Its performances, bio-oils, and emissions. *Bioresource Technol* **2022**, 345, 126346.
5. Alves, J.L.F.; Da Silva, J.C.G.; Sellin, N.; Prá, F.D.B.; Sapelini, C.; Souza, O.; Marangoni, C., Upgrading of banana leaf waste to produce solid biofuel by torrefaction: physicochemical properties, combustion behaviors, and potential emissions. *Environ Sci Pollut R* **2022**, 29, (17), 25733-25747.
6. Chen, C.; Yang, R.; Wang, X.; Qu, B.; Zhang, M.; Ji, G.; Li, A., Effect of in-situ torrefaction and densification on the properties of pellets from rice husk and rice straw. *Chemosphere* **2022**, 289, 133009.
7. Abdullah, I.; Ahmad, N.; Hussain, M.; Ahmed, A.; Ahmed, U.; Park, Y., Conversion of biomass blends (walnut shell and pearl millet) for the production of solid biofuel via torrefaction under different conditions. *Chemosphere* **2022**, 295, 133894.
8. Haykiri-Acma, H.; Yaman, S., Effects of torrefaction after pelleting (TAP) process on strength and fuel characteristics of binderless bio-pellets. *Biomass Convers Bior* **2022**.
9. Grycova, B.; Klemencova, K.; Jezerska, L.; Zidek, M.; Lestinsky, P., Effect of torrefaction on pellet quality parameters. *Biomass Convers Bior* **2022**.
10. Ma, J.; Zhang, Z.; Wang, Z.; Kong, W.; Feng, S.; Shen, B.; Mu, L., Integration of torrefaction and in-situ pelletization for biodried products derived from municipal organic wastes: The influences of temperature on fuel properties and combustion behaviours. *Fuel* **2022**, 313, 122845.
11. Sukiran, M.A.; Wan Daud, W.M.A.; Abnisa, F.; Nasrin, A.B.; Astimar, A.A.; Loh, S.K., Individual torrefaction parameter enhances characteristics of torrefied empty fruit bunches. *Biomass Convers Bior* **2021**, 11, (2), 461-472.
12. Nyakuma, B.B.; Oladokun, O.; Wong, S.L.; Abdullah, T.A.T., Torrefaction of oil palm empty fruit bunch pellets: product yield, distribution and fuel characterisation for enhanced energy recovery. *Biomass Convers Bior* **2021**.

13. Yu, Y.; Zhu, Z.; Wang, L.; Wang, G.; Bai, X., Effect of Torrefaction Treatment on Physical and Fuel Properties of Caragana (Caragana korshinskii) Pellets. *Bioenerg Res* **2021**.
14. Oh, K.C.; Kim, J.; Park, S.Y.; Kim, S.J.; Cho, L.H.; Lee, C.G.; Roh, J.; Kim, D.H., Development and validation of torrefaction optimization model applied element content prediction of biomass. *Energy* **2021**, 214, 119027.
15. Sun, Y.; Tong, S.; Li, X.; Wang, F.; Hu, Z.; Dacres, O.D.; Edreis, E.M.A.; Worasuwannarak, N.; Sun, M.; Liu, H.; Hu, H.; Luo, G.; Yao, H., Gas-pressurized torrefaction of biomass wastes: The optimization of pressurization condition and the pyrolysis of torrefied biomass. *Bioresource Technol* **2021**, 319, 124216.
16. Liao, L.; Zheng, J.; Zhang, Y.; Li, C.; Yuan, C., Impact of torrefaction on entrained-flow gasification of pine sawdust: An experimental investigation. *Fuel* **2021**, 289, 119919.
17. Lin, Y.; Zheng, N.; Hsu, C., Torrefaction of fruit peel waste to produce environmentally friendly biofuel. *J Clean Prod* **2021**, 284, 124676.
18. Silveira, E.A.; Luz, S.M.; Leão, R.M.; Rousset, P.; Caldeira-Pires, A., Numerical modeling and experimental assessment of sustainable woody biomass torrefaction via coupled TG-FTIR. *Biomass and Bioenergy* **2021**, 146, 105981.
19. Setkit, N.; Li, X.; Yao, H.; Worasuwannarak, N., Torrefaction behavior of hot-pressed pellets prepared from leucaena wood. *Bioresource Technol* **2021**, 321, 124502.
20. Feng, Z.; Yang, J.; Ni, L.; Gao, Q.; Liu, Z., The chemical and structural transformation of bamboo wastes during torrefaction process. *Environ Prog Sustain* **2021**, 40, (3).
21. Chen, C.; Ji, G.; Mu, L.; Zhang, Y.; Li, A., Comprehensive research on the solid, liquid, and gaseous products of rice husk and rice straw torrefaction. *Sustain Energ Fuels* **2021**, 5, (3), 687-697.
22. Fu, J.; Summers, S.; Turn, S.Q.; Kusch, W., Upgraded pongamia pod via torrefaction for the production of bioenergy. *Fuel* **2021**, 291, 120260.
23. Kongto, P.; Palamanit, A.; Chaiprapat, S.; Tippayawong, N., Enhancing the fuel properties of rubberwood biomass by moving bed torrefaction process for further applications. *Renew Energ* **2021**, 170, 703-713.
24. Cao, X.; Zhang, J.; Cen, K.; Chen, F.; Chen, D.; Li, Y., Investigation of the relevance between thermal degradation behavior and physicochemical property of cellulose under different torrefaction severities. *Biomass and Bioenergy* **2021**, 148, 106061.
25. Lin, Y.; Zheng, N., Torrefaction of fruit waste seed and shells for biofuel production with reduced CO₂ emission. *Energy* **2021**, 225, 120226.
26. Sukiran, M.A.; Wan Daud, W.M.A.; Abnisa, F.; Nasrin, A.B.; Abdul Aziz, A.; Loh, S.K., A comprehensive study on torrefaction of empty fruit bunches: Characterization of solid, liquid and gas products. *Energy* **2021**, 230, 120877.
27. Patidar, K.; Vashishtha, M., Impact of torrefaction conditions on the physicochemical properties of mustard crop residue. *Materials Today: Proceedings* **2021**, 44, 4072-4078.
28. Lee, B.; Sh, L.; Lee, D.; Jeon, C., Effect of torrefaction and ashless process on combustion and NO_x emission behaviors of woody and herbaceous biomass. *Biomass and Bioenergy* **2021**, 151, 106133.
29. Carneiro-Junior, J.A.D.M.; de Oliveira, G.F.D.; Alves, C.T.; Andrade, H.M.C.; Beisl Vieira De Melo, S.A.B.V.; Torres, E.A., Valorization of Prosopis juliflora Woody Biomass in Northeast Brazilian through Dry Torrefaction. *Energies* **2021**, 14, (12), 3465.
30. Pedroso, D.T.; Machin, E.B.; Cabrera-Barjas, G.; Flores, M.; Urra, H.G.; de Carvalho, F.S.; Santos, M.I.S.D.; Machín, A.B.; Canettieri, E.V.; Pérez, N.P.; Teixeira Lacava, P.; Ribeiro Dos Santos, L.;

- Andrade De Carvalho Júnior, J., Sugarcane Bagasse Torrefaction for Fluidized Bed Gasification. *Applied Sciences* **2021**, 11, (13), 6105.
- 31. Ullah, H.; Lun, L.; Riaz, L.; Naseem, F.; Shahab, A.; Rashid, A., Physicochemical characteristics and thermal degradation behavior of dry and wet torrefied orange peel obtained by dry/wet torrefaction. *Biomass Convers Bior* **2021**.
 - 32. Chen, C.; Qu, B.; Wang, W.; Wang, W.; Ji, G.; Li, A., Rice husk and rice straw torrefaction: Properties and pyrolysis kinetics of raw and torrefied biomass. *Environmental Technology & Innovation* **2021**, 24, 101872.
 - 33. Li, R.; Wu, C.; Zhu, L.; Hu, Z.; Xu, J.; Yang, Y.; Yang, F.; Ma, Z., Regulation of the elemental distribution in biomass by the torrefaction pretreatment using different atmospheres and its influence on the subsequent pyrolysis behaviors. *Fuel Process Technol* **2021**, 222, 106983.
 - 34. Lampropoulos, A.; Kaklidis, N.; Athanasiou, C.; Montes-Morán, M.A.; Arenillas, A.; Menéndez, J.A.; Binas, V.D.; Konsolakis, M.; Marnellos, G.E., Effect of Olive Kernel thermal treatment (torrefaction vs. slow pyrolysis) on the physicochemical characteristics and the CO₂ or H₂O gasification performance of as-prepared biochars. *Int J Hydrogen Energ* **2021**, 46, (57), 29126-29141.
 - 35. Tsai, W.; Jiang, T.; Tang, M.; Chang, C.; Kuo, T., Enhancement of thermochemical properties on rice husk under a wide range of torrefaction conditions. *Biomass Convers Bior* **2021**.
 - 36. Ivanovski, M.; Petrovic, A.; Ban, I.; Goricanec, D.; Urbanci, D., Determination of the Kinetics and Thermodynamic Parameters of Lignocellulosic Biomass Subjected to the Torrefaction Process. *Materials* **2021**, 14, (24), 7877.
 - 37. Duranay, N.D.; Akkuş, G., Solid fuel production with torrefaction from vineyard pruning waste. *Biomass Convers Bior* **2021**, 11, (6), 2335-2346.
 - 38. Demey, H.; Rodriguez-Alonso, E.; Lacombe, E.; Grateau, M.; Jaricot, N.; Chatroux, A.; Thiery, S.; Marchand, M.; Melkior, T., Upscaling Severe Torrefaction of Agricultural Residues to Produce Sustainable Reducing Agents for Non-Ferrous Metallurgy. *Metals-Basel* **2021**, 11, (12), 1905.
 - 39. Khempila, J.; Kongto, P.; Meena, P., Comparative study of solid biofuels derived from sugarcane leaves with two different thermochemical conversion methods: wet and dry torrefaction. *Bioenerg Res* **2021**.
 - 40. Xiaojie Tiana, L.D.Y.W., Influence of torrefaction pretreatment on corncobs: A study on fundamental characteristics, thermal behavior, and kinetic. *Bioresource Technol* **2020**, (297).
 - 41. Hu, J.; Song, Y.; Liu, J.; Evrendilek, F.; Buyukada, M.; Yan, Y.; Li, L., Combustions of torrefaction-pretreated bamboo forest residues: Physicochemical properties, evolved gases, and kinetic mechanisms. *Bioresource Technol* **2020**, 304, 122960.
 - 42. Huang, J.; Qiao, Y.; Wang, Z.; Liu, H.; Wang, B.; Yu, Y., Valorization of Food Waste via Torrefaction: Effect of Food Waste Type on the Characteristics of Torrefaction Products. *Energ Fuel* **2020**, 34, (5), 6041-6051.
 - 43. Singh, S.; Chakraborty, J.P.; Mondal, M.K., Torrefaction of woody biomass (*Acacia nilotica*): Investigation of fuel and flow properties to study its suitability as a good quality solid fuel. *Renew Energ* **2020**, 153, 711-724.
 - 44. Manatura, K., Inert torrefaction of sugarcane bagasse to improve its fuel properties. *Case Studies in Thermal Engineering* **2020**, 19, 100623.
 - 45. Liu, X.; Yao, Z.; Zhao, L.; Song, J.; Jia, J., Torrefaction of Sorghum Straw Pellets in a Stationary Reactor with a Feeding Screw. *Energ Fuel* **2020**, 34, (5), 5997-6007.
 - 46. Singh, R.K.; Jena, K.; Chakraborty, J.P.; Sarkar, A., Energy and exergy analysis for torrefaction of

- pigeon pea stalk (*cajanus cajan*) and eucalyptus (*eucalyptus tereticornis*). *Int J Hydrogen Energ* **2020**, *45*, (38), 18922-18936.
- 47. Liu, X.; Yao, Z.; Cong, H.; Zhao, L.; Huo, L.; Song, J.; School Of Mechanical Engineering And Automation, N.U.S.C.; Key Laboratory Of Energy Resource Utilization From Agriculture Residue Of Ministry Of Agriculture And Rural Affairs, A.O.A.P.; Institute Of Environment And Sustainable Development In Agriculture, C.A.O.A., Effects of operating conditions and pre-densification on the torrefaction products of sorghum straw. *Int J Agr Biol Eng* **2020**, *13*, (4), 219-225.
 - 48. Kizuka, R.; Ishii, K.; Ochiai, S.; Sato, M.; Yamada, A.; Nishimiya, K., Improvement of Biomass Fuel Properties for Rice Straw Pellets Using Torrefaction and Mixing with Wood Chips. *Waste Biomass Valori* **2020**.
 - 49. Cen, K.; Zhang, J.; Chen, D.; Chen, F.; Zhang, Y.; Ma, H., Comparative study of the fuel quality and torrefaction performance of biomass and its molded pellets: effects of temperature and residence time. *Energy sources. Part A, Recovery, utilization, and environmental effects* **2020**, 1-10.
 - 50. Chen, D.; Chen, F.; Cen, K.; Cao, X.; Zhang, J.; Zhou, J., Upgrading rice husk via oxidative torrefaction: Characterization of solid, liquid, gaseous products and a comparison with non-oxidative torrefaction. *Fuel* **2020**, *275*, 117936.
 - 51. Simonic, M.; Goricanec, D.; Urbanci, D., Impact of torrefaction on biomass properties depending on temperature and operation time. *Sci Total Environ* **2020**, *740*, 140086.
 - 52. Mukhtar, H.; Feroze, N.; Munir, H.M.S.; Javed, F.; Kazmi, M., Torrefaction process optimization of agriwaste for energy densification. *Energy sources. Part A, Recovery, utilization, and environmental effects* **2020**, *42*, (20), 2526-2544.
 - 53. Da Silva, J.C.G.; Pereira, J.L.C.; Andersen, S.L.F.; Moreira, R.D.F.P.; José, H.J., Torrefaction of ponkan peel waste in tubular fixed-bed reactor: In-depth bioenergetic evaluation of torrefaction products. *Energy* **2020**, *210*, 118569.
 - 54. Mokrzycki, J.; Gazińska, M.; Fedyna, M.; Karcz, R.; Lorenc-Grabowska, E.; Rutkowski, P., Pyrolysis and torrefaction of waste wood chips and cone-like flowers derived from black alder (*Alnus glutinosa* L. Gaertn.) for sustainable solid fuel production. *Biomass and Bioenergy* **2020**, *143*, 105842.
 - 55. Wang, L.; Riva, L.; Skreiber, Ø.; Khalil, R.; Bartocci, P.; Yang, Q.; Yang, H.; Wang, X.; Chen, D.; Rudolfsson, M.; Nielsen, H.K., Effect of Torrefaction on Properties of Pellets Produced from Woody Biomass. *Energ Fuel* **2020**, *34*, (12), 15343-15354.
 - 56. Kanwal, S.; Chaudhry, N.; Munir, S.; Sana, H., Effect of torrefaction conditions on the physicochemical characterization of agricultural waste (sugarcane bagasse). *Waste Manage* **2019**, *88*, 280-290.
 - 57. Singh, R.K.; Sarkar, A.; Chakraborty, J.P., Effect of torrefaction on the physicochemical properties of pigeon pea stalk (*Cajanus cajan*) and estimation of kinetic parameters. *Renew Energ* **2019**, *138*, 805-819.
 - 58. Chen, D.; Gao, A.; Ma, Z.; Fei, D.; Chang, Y.; Shen, C., In-depth study of rice husk torrefaction: Characterization of solid, liquid and gaseous products, oxygen migration and energy yield. *Bioresource Technol* **2018**, *253*, 148-153.
 - 59. Aneta Magdziarz, M.W.R.S., Combustion process of torrefied wood biomass. *J Therm Anal Calorim* **2017**, 1339–1349.
 - 60. McNamee, P.; Adams, P.W.R.; McManus, M.C.; Dooley, B.; Darvell, L.I.; Williams, A.; Jones, J.M., An assessment of the torrefaction of North American pine and life cycle greenhouse gas emissions. *Energ Convers Manage* **2016**, *113*, 177-188.

61. Toptas, A.; Yildirim, Y.; Duman, G.; Yanik, J., Combustion behavior of different kinds of torrefied biomass and their blends with lignite. *Bioresource Technol* **2015**, 177, 328-336.
62. Nam, H.; Capareda, S., Experimental investigation of torrefaction of two agricultural wastes of different composition using RSM (response surface methodology). *Energy* **2015**, 91, 507-516.
63. Chen, Y.; Yang, H.; Yang, Q.; Hao, H.; Zhu, B.; Chen, H., Torrefaction of agriculture straws and its application on biomass pyrolysis poly-generation. *Bioresource Technol* **2014**, 156, 70-77.
64. Lu, K.; Lee, W.; Chen, W.; Liu, S.; Lin, T., Torrefaction and low temperature carbonization of oil palm fiber and eucalyptus in nitrogen and air atmospheres. *Bioresource Technol* **2012**, 123, 98-105.
65. Bridgeman, T.G.; Jones, J.M.; Shield, I.; Williams, P.T., Torrefaction of reed canary grass, wheat straw and willow to enhance solid fuel qualities and combustion properties. *Fuel* **2008**, 87, (6), 844-856.
66. Xiaorui, L.; Longji, Y.; Xudong, Y., *Evolution of chemical functional groups during torrefaction of rice straw*. 2021; Vol. 320, p 124328.

Table S2. Parameter values and basic settings of the BPNN-GA model.

Parameters		Values
BPNN	Structure	One hidden layer back propagation
	Hidden neurons	4-14
	Learning ratio	0.01
	Momentum factor	0.01
	Number of data samples	497
	Ratio of training data	0.8
	Ratio of testing data	0.2
GA	Population size	80
	Chromosome length	13X+6
	Maximum generation	300
	Crossover fraction	0.8
	Migration fraction	0.01

Table S3. Pearson correlation coefficient between any two features

	MO	VM	ASH	FC	Temp	Time	FR	O/C	H/C	HHV	MY	EY
MO	1	-0.03771	-0.09897	-0.37075	-0.03035	-0.04833	0.037311	-0.20386	-0.19213	-0.03871	0.054822	-0.03457
VM	-0.03771	1	-0.34212	-0.61335	0.03735	-0.01406	-0.32559	0.044149	0.148177	-0.01071	-0.01344	0.019636
ASH	-0.09897	-0.34212	1	0.141089	-0.0777	-0.02876	0.192094	0.154517	-0.04417	-0.05151	0.164453	0.007463
FC	-0.37075	-0.61335	0.141089	1	0.054781	0.122013	0.237876	-0.05717	-0.12488	0.055843	-0.00095	-0.01165
Temp	-0.03035	0.03735	-0.0777	0.054781	1	0.002868	0.03945	-0.10698	0.023714	-0.06832	-0.04401	0.10832
Time	-0.04833	-0.01406	-0.02876	0.122013	0.002868	1	0.147655	-0.13014	-0.2308	0.199383	-0.12658	0.00709
FR	0.037311	-0.32559	0.192094	0.237876	0.03945	0.147655	1	-0.22565	-0.26535	-0.05553	-0.01796	-0.06987
O/C	-0.20386	0.044149	0.154517	-0.05717	-0.10698	-0.13014	-0.22565	1	0.235059	-0.01241	0.043467	-0.02176
H/C	-0.19213	0.148177	-0.04417	-0.12488	0.023714	-0.2308	-0.26535	0.235059	1	0.029617	-0.04189	0.096107
HHV	-0.03871	-0.01071	-0.05151	0.055843	-0.06832	0.199383	-0.05553	-0.01241	0.029617	1	-0.09244	-0.13891
MY	0.054822	-0.01344	0.164453	-0.00095	-0.04401	-0.12658	-0.01796	0.043467	-0.04189	-0.09244	1	0.010408
EY	-0.03457	0.019636	0.007463	-0.01165	0.10832	0.00709	-0.06987	-0.02176	0.096107	-0.13891	0.010408	1

Table S4. R² and RMSE results of the training and testing set using BPNN model

	FR	H/C	O/C	HHV	MY	EY
R ² (training)	0.8266	0.7555	0.7783	0.8646	0.8111	0.7201
RMSE (training)	0.161	0.0155	0.1075	1.6033	0.0794	0.0771
R ² (testing)	0.4222	0.6667	0.7203	0.8145	0.7146	0.6487
RMSE (testing)	0.1782	0.0127	0.2444	1.8196	0.1467	0.0926

Figure S1. Comparison of BPNN predicted and experimental data of training set.

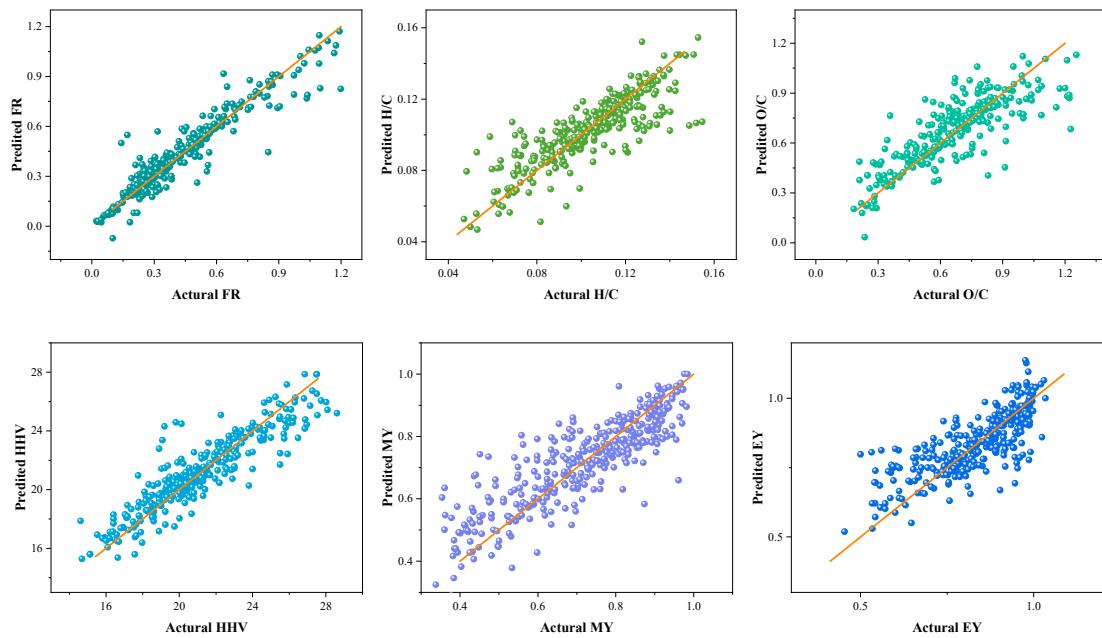


Figure S2. Comparison of BPNN predicted and experimental data of testing set.

