

## **Electronic Supplementary Information 1**

### **Systematic QSAR and iQCCR Modelling of Fused/Non-Fused Aromatic Hydrocarbons (FNFAHs) Carcinogenicity to Rodents: Reduce Unnecessary Chemical Synthesis and Animal Testing**

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Fig. S1

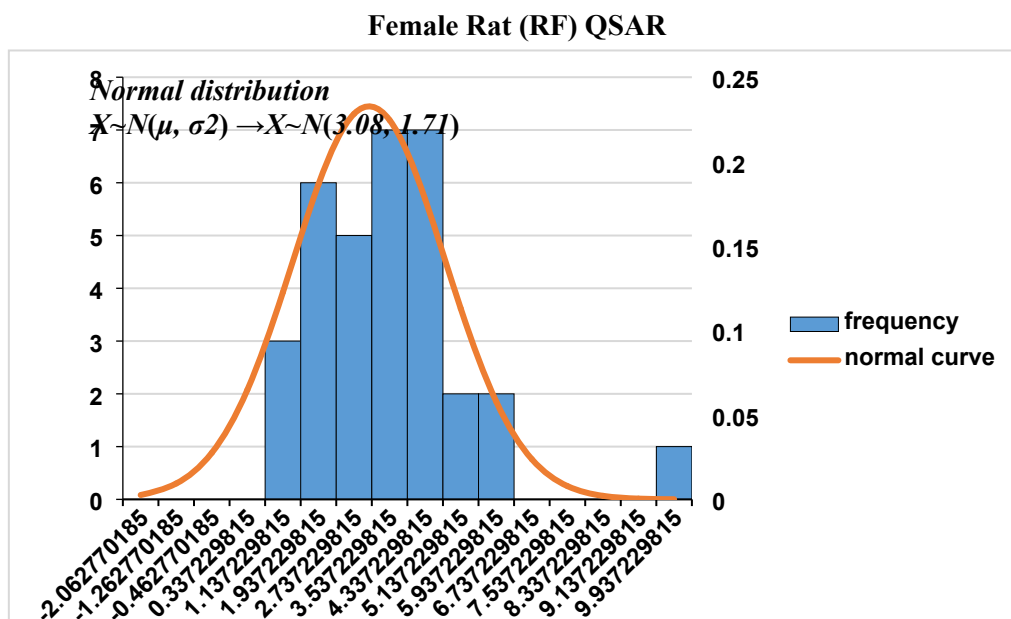


Fig. S1. Carcinogenicity data distribution of FNFAHs used in the female rat dataset.

Fig. S2

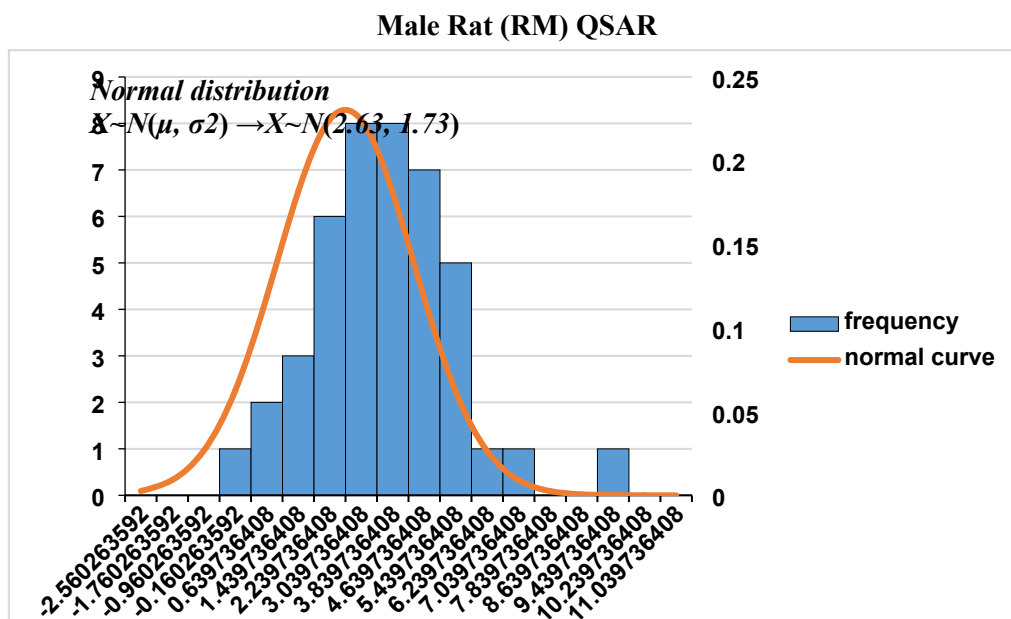


Fig. S2. Carcinogenicity data distribution of FNFAHs used in the male rat dataset.

Fig. S3

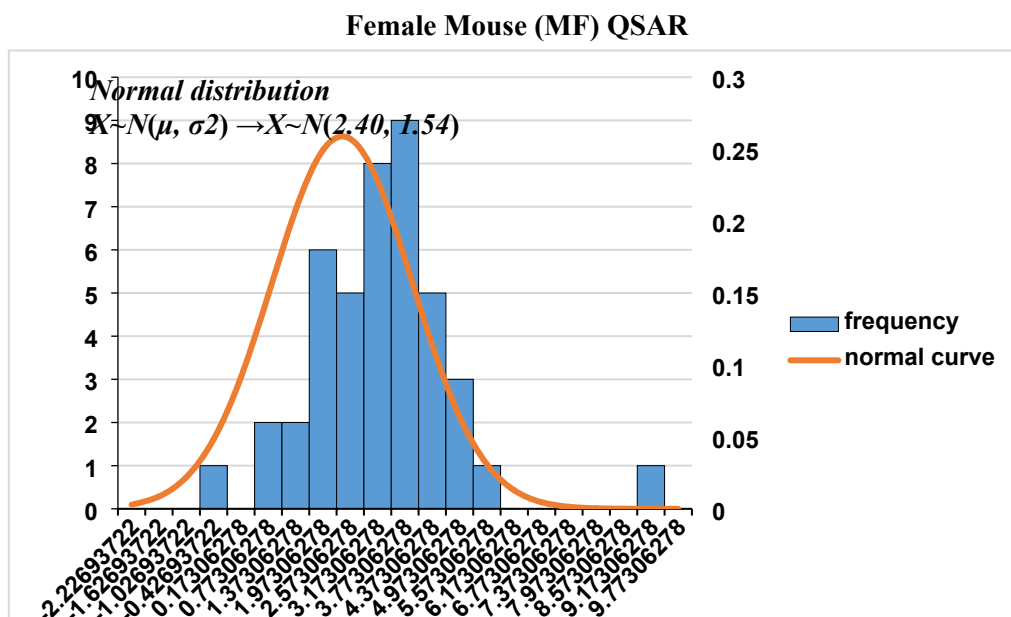


Fig. S3. Carcinogenicity data distribution of FNFAHs used in the female mouse dataset.

Fig. S4

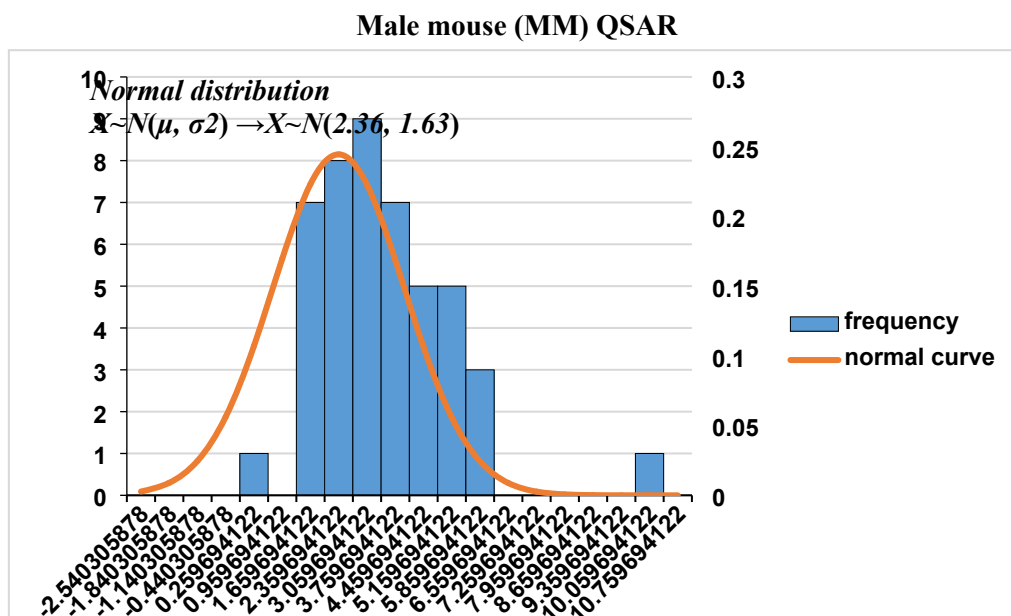


Fig. S4. Carcinogenicity data distribution of FNFAHs used in the male mouse dataset.

Fig. S5

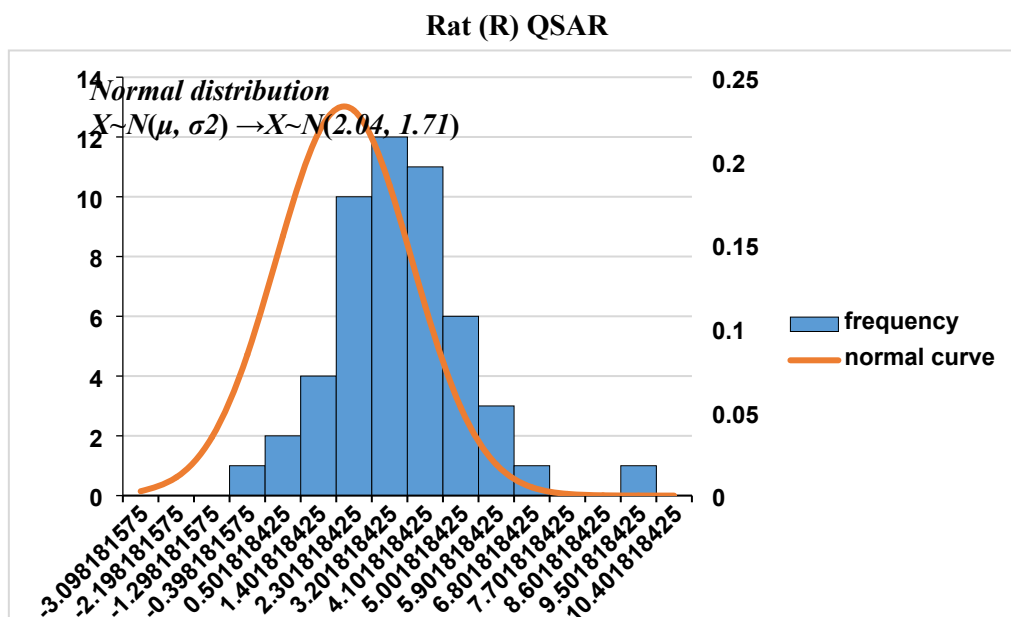


Fig. S5. Carcinogenicity data distribution of FNFAHs used in the rat dataset.

Fig. S6

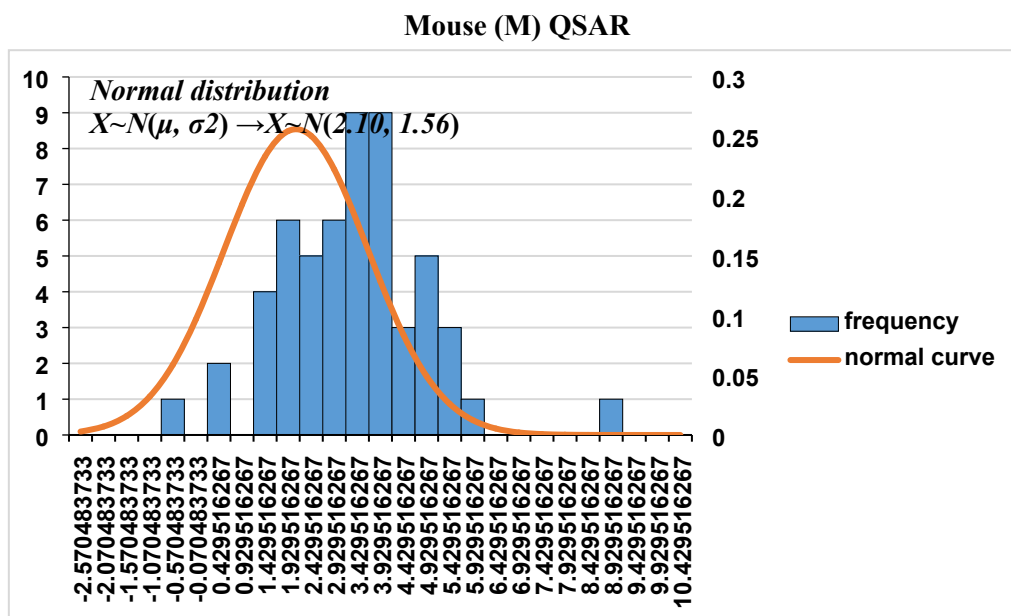


Fig. S6. Carcinogenicity data distribution of FNFAHs used in the mouse dataset.

Fig. S7

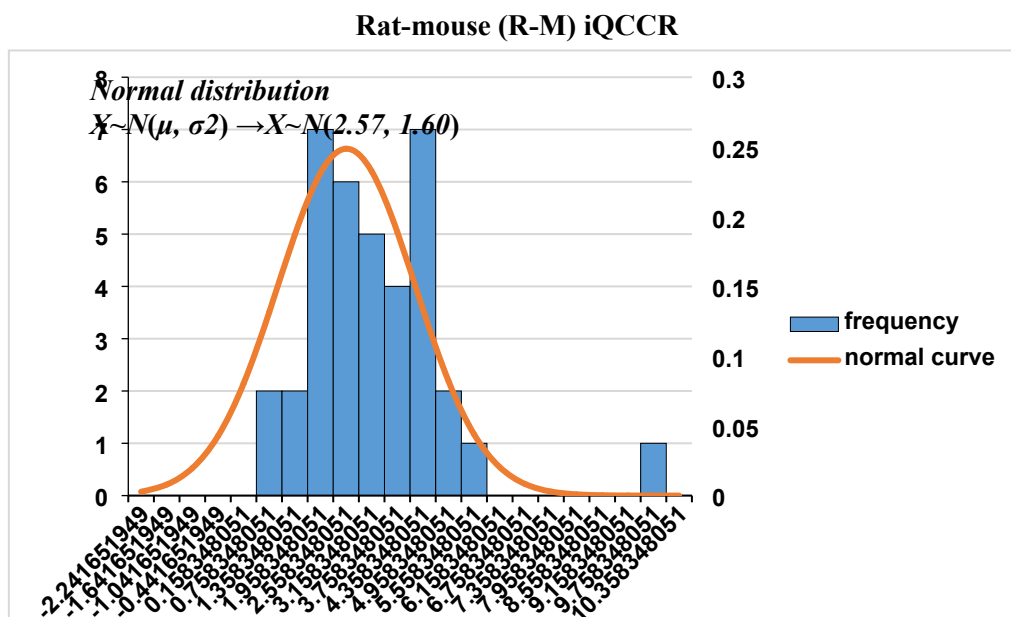
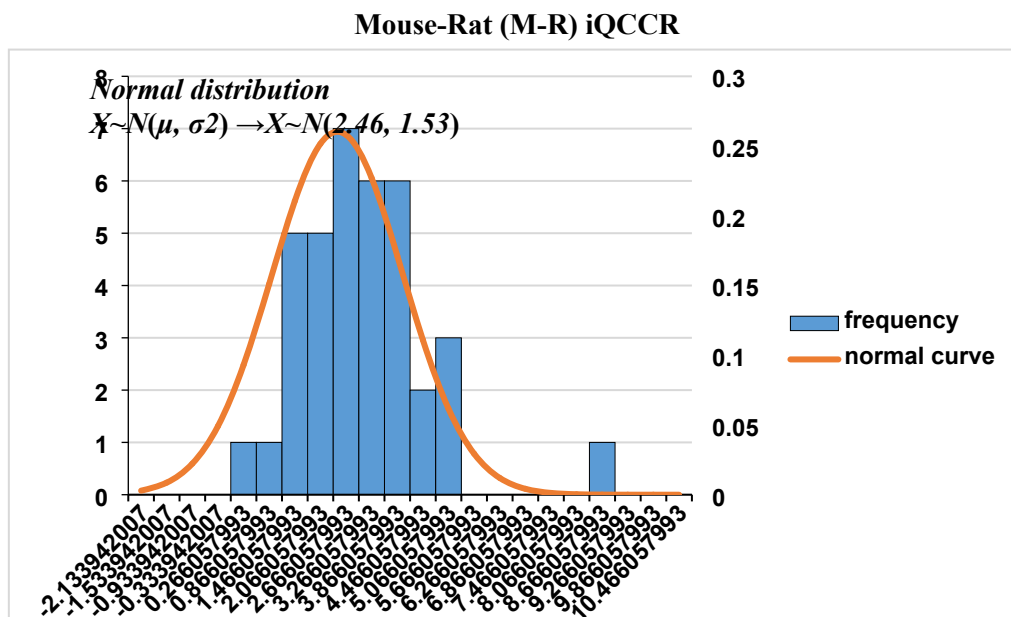
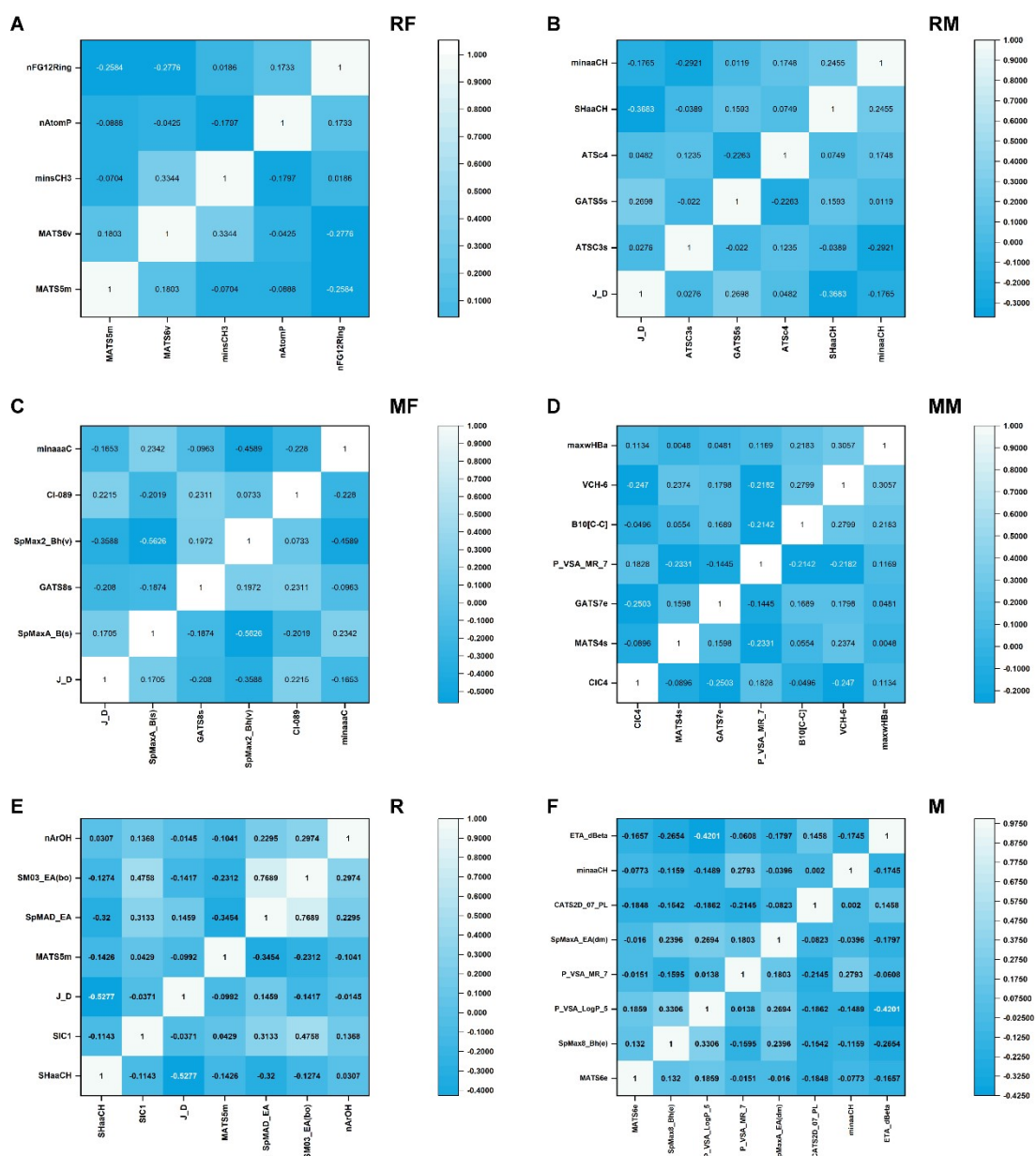


Fig. S7. Carcinogenicity data distribution of FNFAHs used in the rat-mouse iQCCR dataset.

Fig. S8

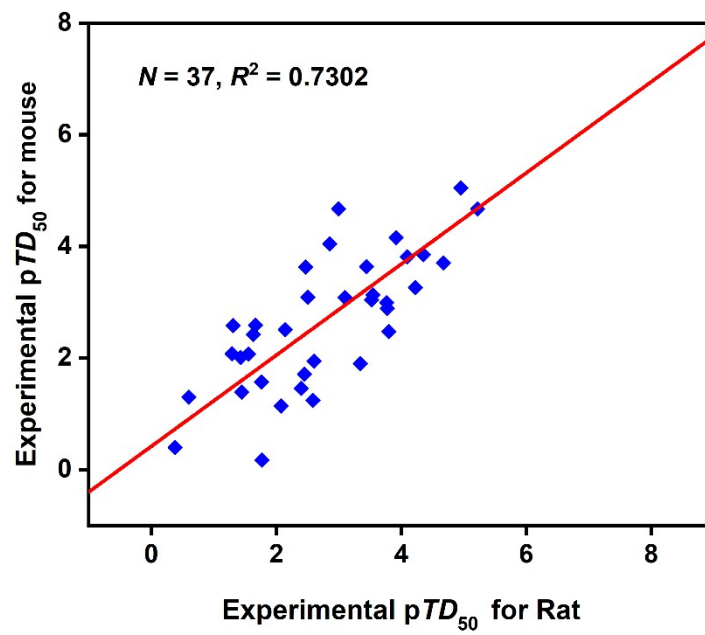


**Fig. S9**



**Fig. S9.** Inter-correlation plots of molecular descriptors appearing in the best QSAR model. (A) Female rat model; (B) Male rat model; (C) Female mouse model; (D) Male mouse model; (E) Rat model; (F) Mouse model.

**Fig. S10**



**Fig. S10.** Linear regression analysis plot based the experimental pTD<sub>50</sub> values for rat versus the experimental pTD<sub>50</sub> values for mouse.