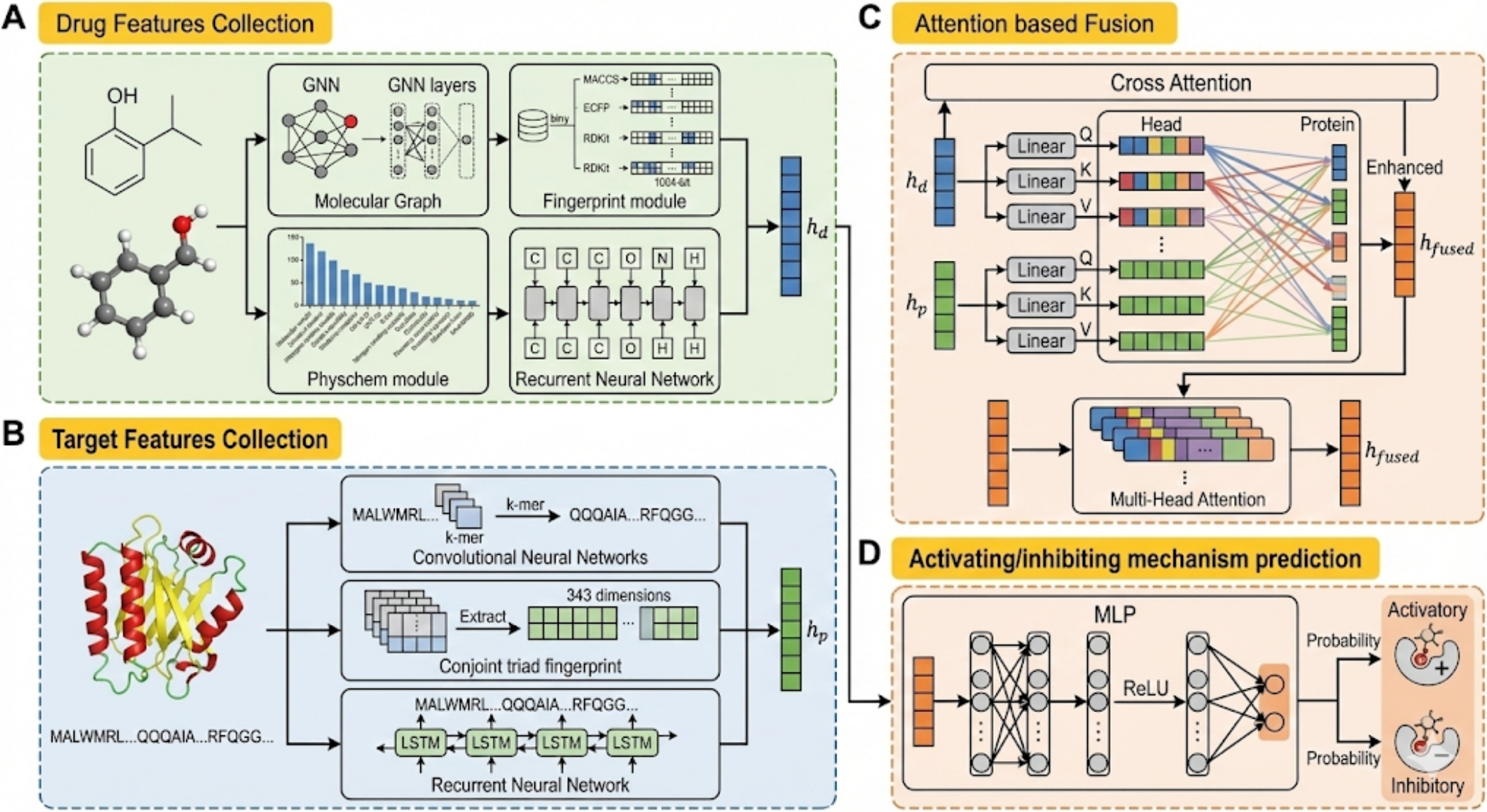
A
Drug Features Collection
OH
GNN
GNN layers
Molecular Graph
MACCS
ECFP
RDKit
RDKit
1004-bit
Fingerprint module
Physchem module
C C C O N H
C C C O H H
Recurrent Neural Network
h_d
B
Target Features Collection
MALWMRL...QQQAIA...RFQGG...
MALWMRL...
k-mer
k-mer
QQQAIA...RFQGG...
Convolutional Neural Networks
343 dimensions
Extract
Conjoint triad fingerprint
MALWMRL...QQQAIA...RFQGG...
LSTM
LSTM
LSTM
LSTM
Recurrent Neural Network
h_p
C
Attention based Fusion
Cross Attention
Head
Protein
Linear
Q
K
V
Enhanced
h_{fused}
Multi-Head Attention
D
Activating/inhibiting mechanism prediction
MLP
ReLU
Probability
Probability
Activatory
Inhibitory