

Supplementary material

Dihydrotanshinone I inhibits the proliferation and growth of Oxaliplatin-resistant human HCT116 colorectal cancer cells

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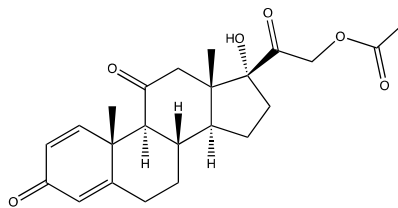
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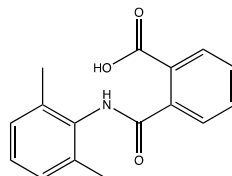
Table S1 Fifteen compounds obtained from LBVS.

| Number | Name | Compound structure |
|--------|---------------------|--------------------|
| 1 | Dihydrotanshinone I | |
| 2 | Chrysin | |
| 3 | Doxycycline hyclate | |
| 4 | Sodium erythorbate | |
| 5 | Luteolin | |
| 6 | Xanthine | |
| 7 | Taxifolin | |

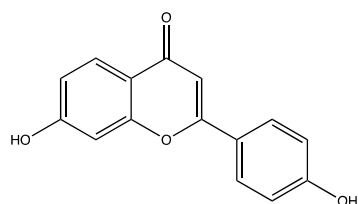
8 Prednisone acetate



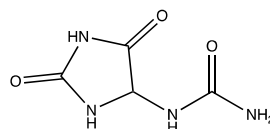
9 Ftaxilide



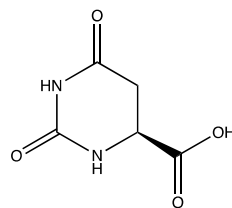
10 7,4'-
dihydroxyflavone



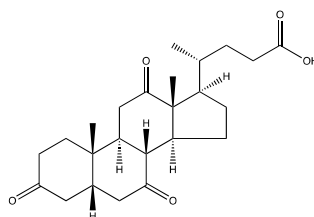
11 Allantoin



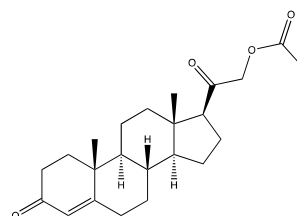
12 L-Dihydroorotic acid



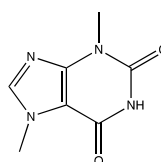
13 Dehydrocholic acid



14 Deoxycorticosterone
acetate



15 Theobromine



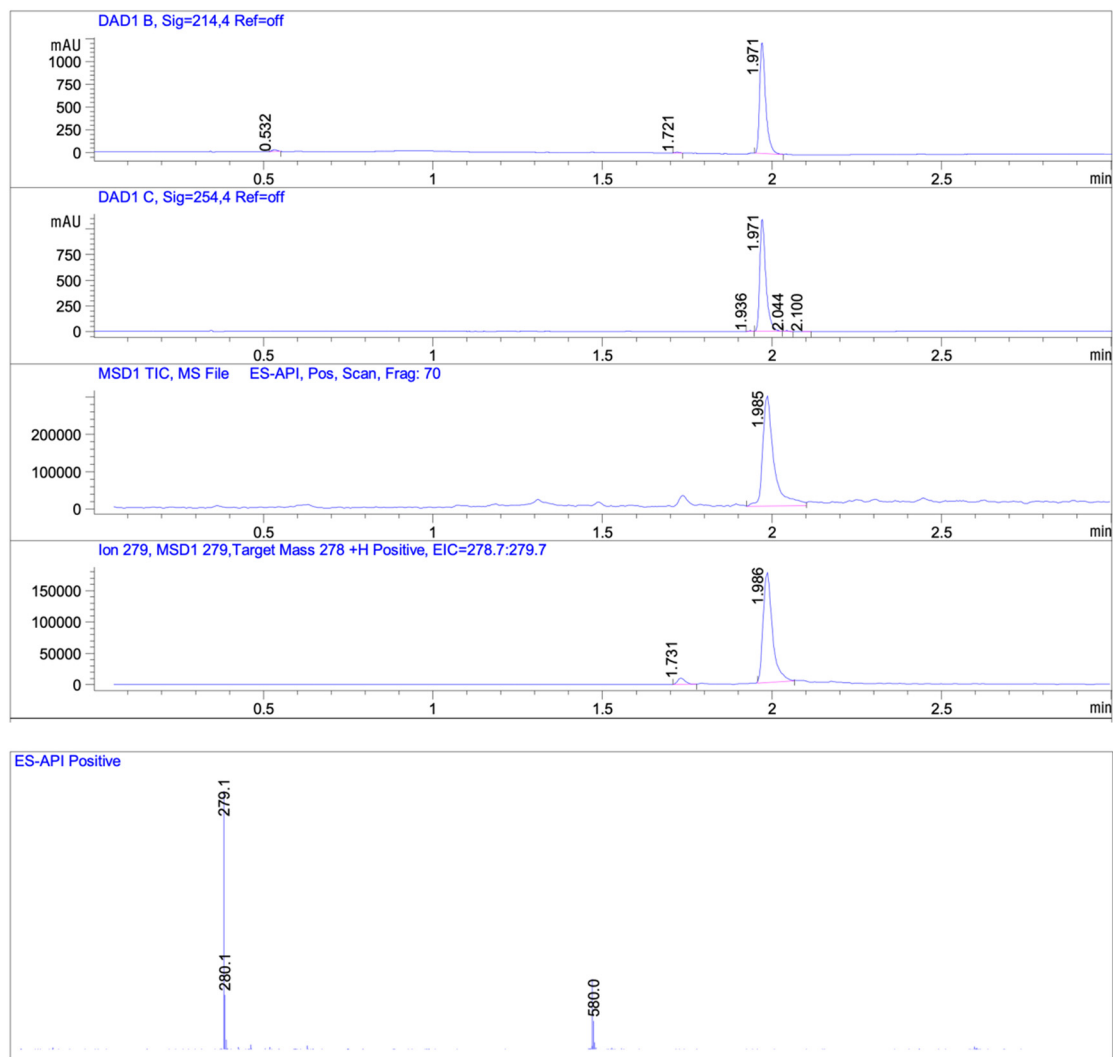
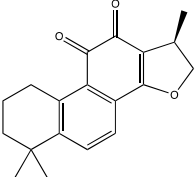
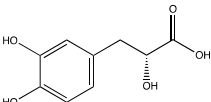
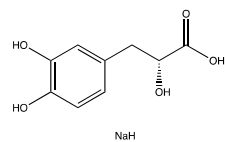


Figure S1 LC-MS of Dihydrotanshinone I

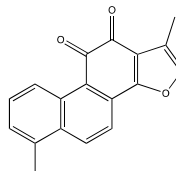
Table S2 Eight compounds from *Salvia miltiorrhiza*.

| Number | Name | Compound structure |
|--------|------------------|--|
| 1 | Cryptotanshinone |  |
| 2 | Danshensu |  |

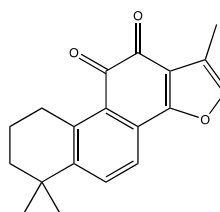
3 Danshensu sodium salt



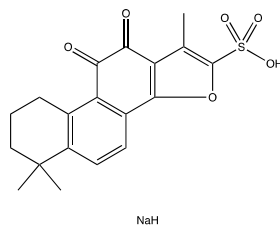
4 Tanshinone I



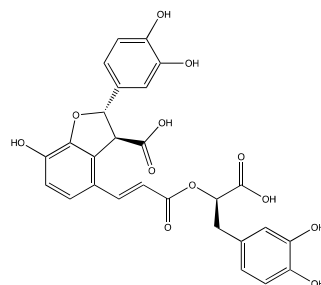
5 Tanshinone IIA



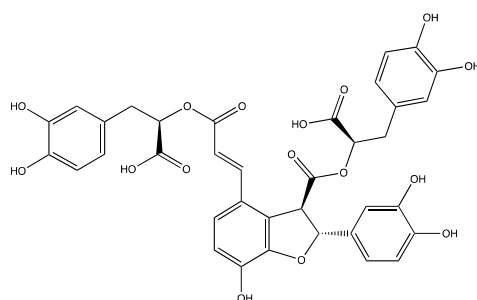
6 Tanshinone IIA sulfonate
sodium



7 Lithospermic acid



8 Salvianolic acid B



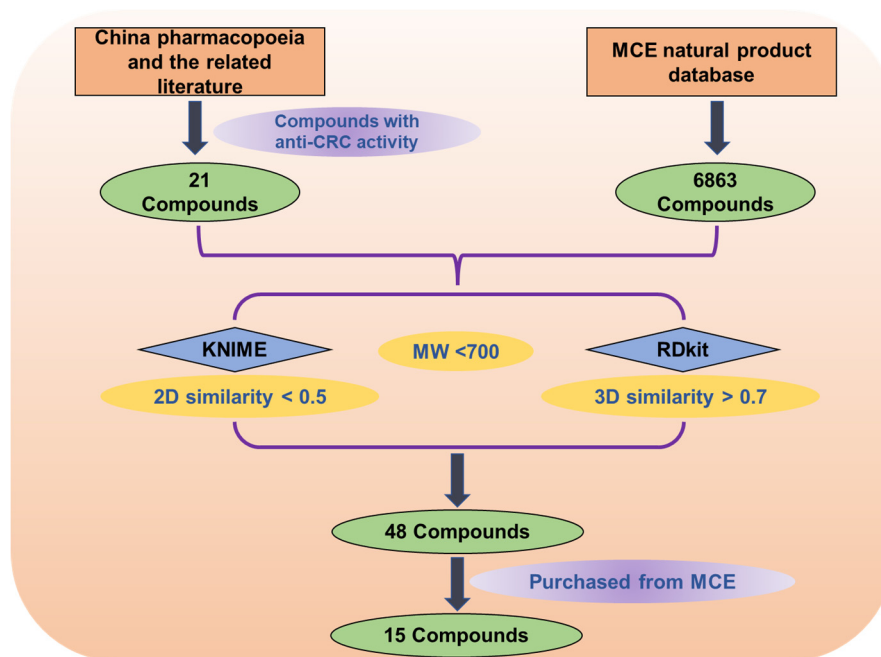
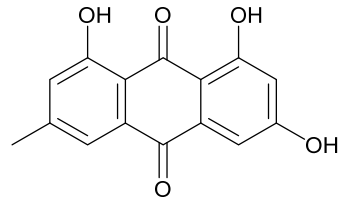


Figure S2 Flow chart of virtual screening. First, 21 natural compounds with anti-CRC activity were selected from the Chinese Pharmacopoeia and related literature. Then, 21 compounds were used as query structures to screen the MCE natural product database (6863 compounds) by 2D and 3D similarity. KNIME was used to compute the 2D similarity between 2D structures. 3D conformations of each compound were generated with ETKDG algorithm in RDkit, then Open3DALIGN algorithm in RDKit was used to compute the 3D similarity between two 3D structures based on the overlap of their pharmacophores and heavy atoms. 48 compounds with 2D similarity less than 0.5 and 3D similarity greater than 0.7 and molecular weight less than 700 were selected. Finally, 15 compounds were purchased from MCE to determine their inhibitory effects on the proliferation of HCT116 cells.

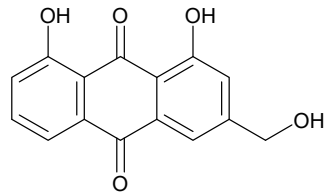
Table S3 Twenty-one known natural compounds with anti-CRC effects.

| Number | Name | Compound structure |
|--------|------|--------------------|
|--------|------|--------------------|

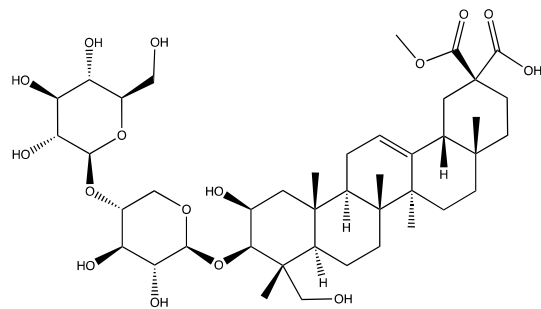
1 Frangula emodin



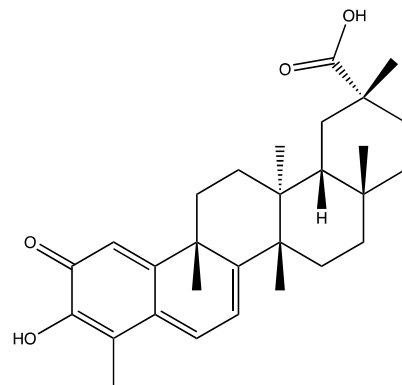
2 Rhabarberone



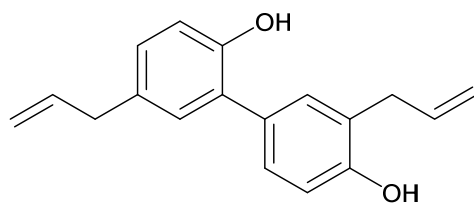
3 Esculentoside A



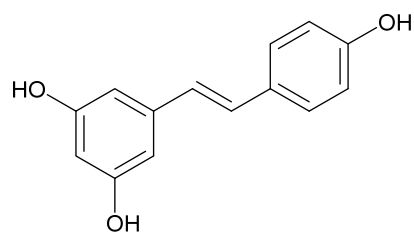
4 Tripterin (Celastrol)



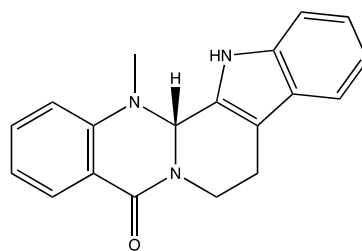
5 Honokiol



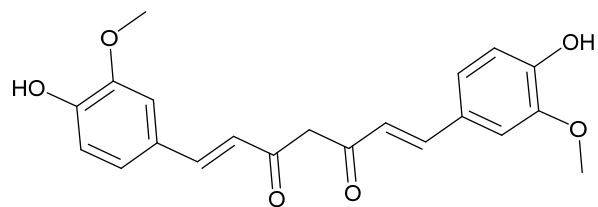
6 Resveratrol



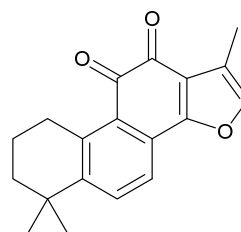
7 Evodiamine



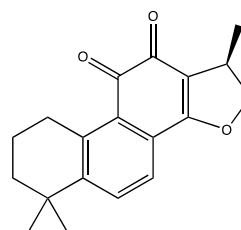
8 Octahydrocurcumin



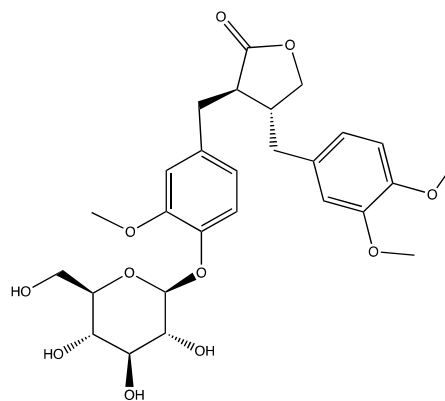
9 Tanshinone IIA



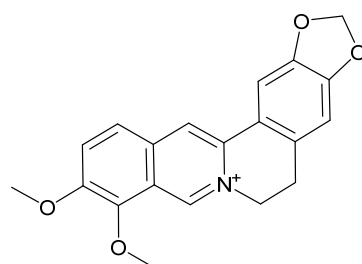
10 Cryptotanshinone



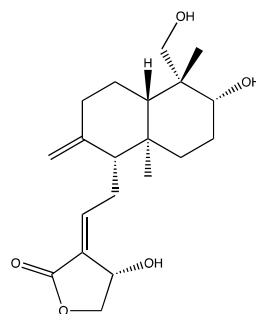
11 Arctiin



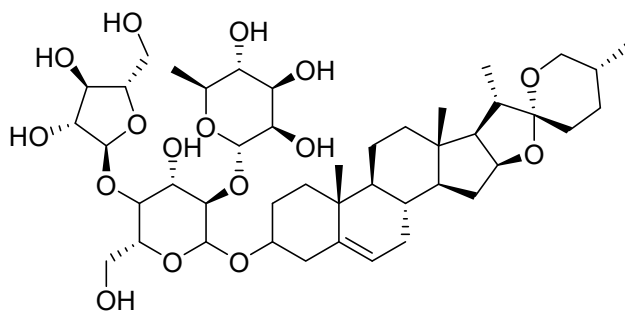
12 Berberine



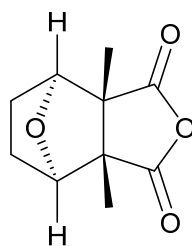
13 Andrographolide



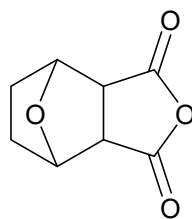
14 Polyphyllin I



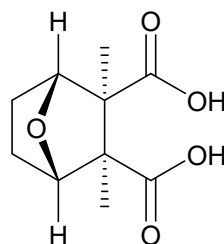
15 cantharidin



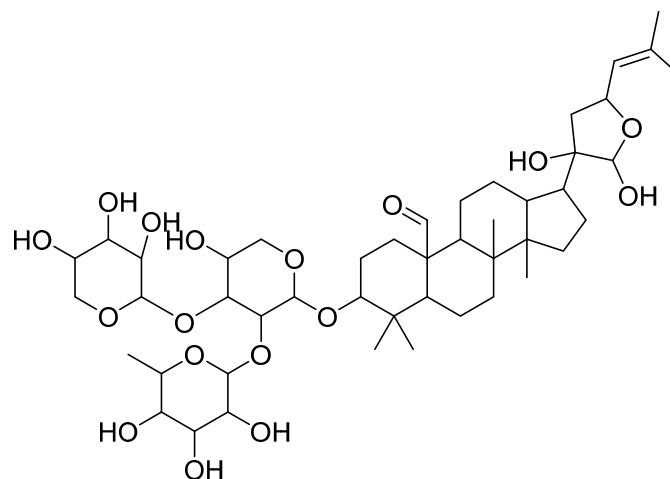
16 Norcantharidin



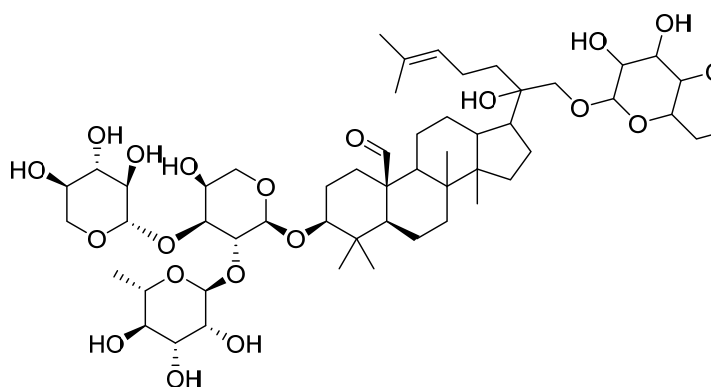
17 Sodium
Cantharidinate For
Injection



18 GypenosideA



19 GypenosideXLIX



20 GypenosideXLVI

