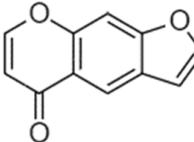
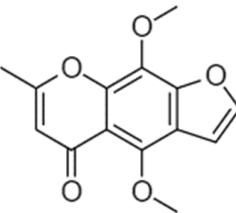
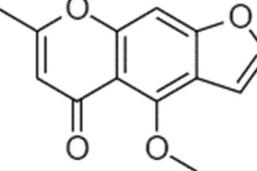


*Supplementary*

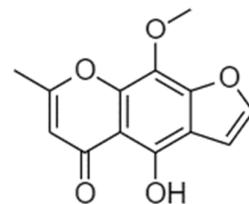
## Transcriptomics, Cheminformatics, and Systems Pharmacology Strategies Unveil the Potential Bioactives to Combat COVID-19

Sivakumar Adarshan<sup>1</sup>, Sakthivel Akassh<sup>2†</sup>, Krishnakumar Avinash<sup>2†</sup>, Mathivanan Bharathkumar<sup>2†</sup>, Pandiyan Muthuramalingam<sup>2,3,4\*</sup>, Hyunsuk Shin<sup>3,4\*</sup>, Venkidasamy Baskar<sup>5</sup>, Jen-Tsung Chen<sup>6\*</sup>, Veluswamy Bhuvaneshwari<sup>7</sup> and Manikandan Ramesh<sup>1</sup>

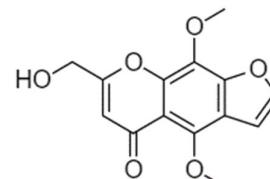
**Table S2:** Bioactive compounds and their canonical SMILES and structures.

S.No.	Compounds	Canonical SMILES	Structure
1	PYR	C1=COC2=CC3=C(C=C21)C(=O)C=CO3	
2	KHE	CC1=CC(=O)C2=C(C3=C(C(=C2O1)OC)OC=C3)OC	
3	VGN	CC1=CC(=O)C2=C(O1)C=C3C(=C2OC)C=CO3	

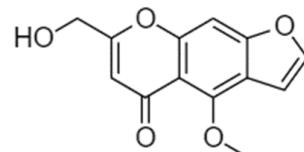
4 KHNOL CC1=CC(=O)C2=C(O1)C(=C3C(=C2O)C=CO3)OC



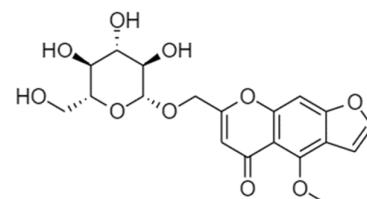
5 AMM COC1=C2C(=O)C=C(OC2=C(C3=C1C=CO3)OC)CO



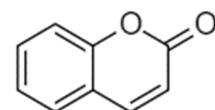
6 KLOL COC1=C2C=CO C2=CC3=C1C(=O)C=C(O3)CO



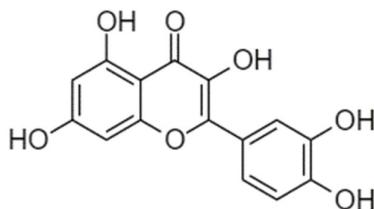
7 KHEL COC1=C2C=CO C2=CC3=C1C(=O)C=C(O3)CO[C@H]4[C@@H]([C@H]([C@@H]([C@H](O4)CO)O)O)O



8 CM C1=CC=C2C(=C1)C=CC(=O)O2



9 QUE C1=CC(=C(C=C1C2=C(C(=O)C3=C(C=C(C3O2)O)O)O)O)O

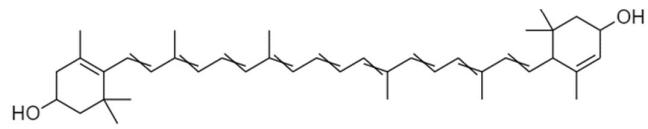




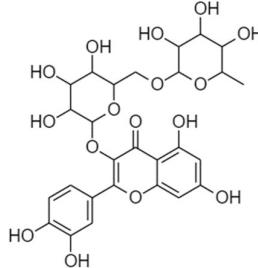
*molecules*



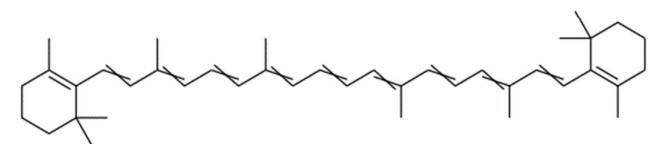
10 LUE CC1=C(C(CC(C1)O)(C)C)C=CC(=CC=CC(=CC=CC=C(C)C=CC=C(C)C=CC2C(=CC(CC2(C)C)O)C)C



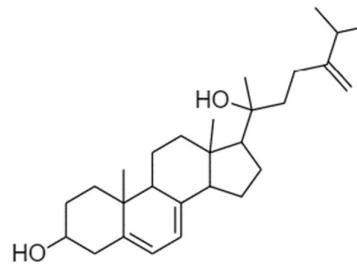
11 RU CC1C(C(C(C(O1)OCC2C(C(C(C(O2)OC3=C(OC4=CC(=CC(=C4C3=O)O)O)C5=CC(=C(C=C5)O)O)O)O)O)O



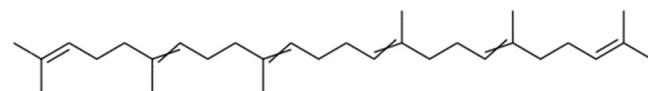
12 BCAR CC1=C(C(CCC1)(C)C)C=CC(=CC=CC(=CC=CC=C(C)C=CC=C(C)C=CC2=C(CC2(C)C)C)C



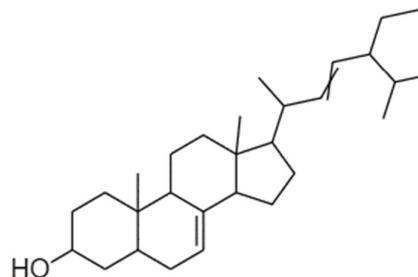
13 AMST CC(C)C(=C)CCC(C)(C1CCC2C1(CCC3C2=CC=C4C3(CCC(C4)O)C)C)O



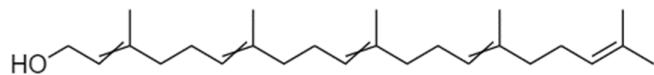
14 SQU CC(=CCCC(=CCCC=C(C)CCC=C(C)CCC=C(C)C)C)C



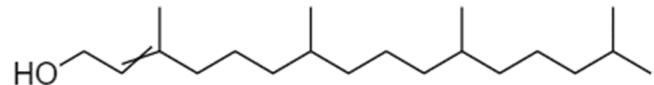
15 SPIN CCC(C=CC(C)C1CCC2C1(CC3C2=CCC4C3(CC(C4)O)C)C)C(C)C



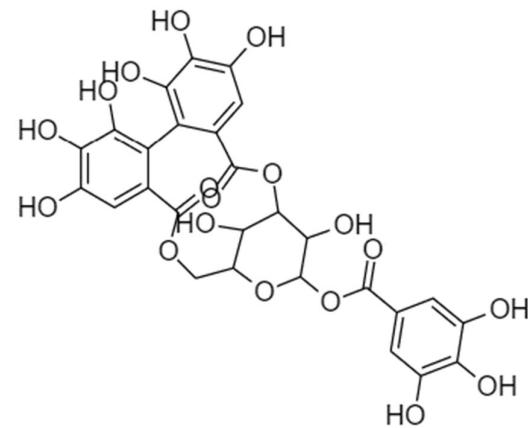
16 POPRE CC(=CCCC(=CCCC(=CCCC(=CCCC(=CCO)C)C)C)C)C



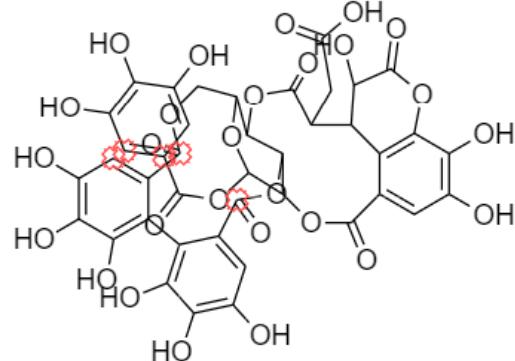
17 PHY CC(C)CCCC(C)CCCC(C)CCCC(=CCO)C



18 COR C1C2C(C(C(C(O2)OC(=O)C3=CC(=C(C(=C3)O)O)O)O)OC(=O)C4=CC(=C(C(=C4C5=C(C(=C(C=C5C(=O)O1)O)O)O)O)O) O)O

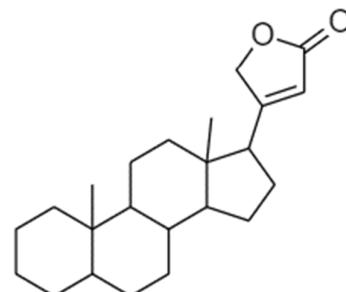


19 CHA C1C2C3C(C(C(O2)OC(=O)C4=CC(=C(C(=C4)O)O)O)OC(=O)C5=CC(=C(C6=C5C(C(C(=O)O3)CC(=O)O)C(C(=O)O6)O)O)OC(=O)C7=CC(=C(C(=C7C8=C(C(=C(C=C8C(=O)O1)O)O)O)O)O

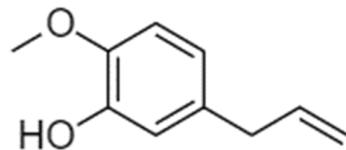


20 GALLO NA  
21 CARD CC1CCCC1CCC3C2CCC4(C3CCC4C5=CC(=O)OC5)C

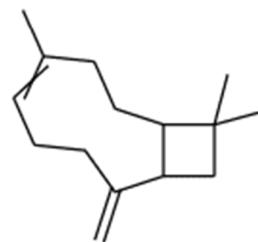
NA



22 CHAVI CO C1=C(C=C(C=C1)CC=C)O

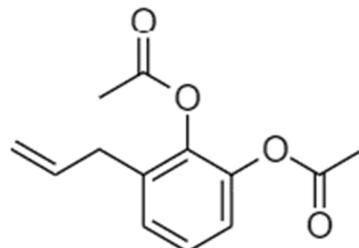


23 CAPH CC1=CCCC(=C)C2CC(C2CC1)(C)C

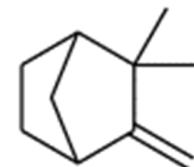


24	CHAVIA	NA		
25	ALYD	CC(=O)OC1=CC=CC(=C1OC(=O)C)CC=C		
26	CHAVIME	NA		
27	CAPE	CC1(C2CCC(C2)C1=C)C		
28	FPIN	NA		
29	EU	COC1=C(C=CC(=C1)CC=)O		
30	LIME	NA		
31	PIN	CC1=CCC2CC1C2(C)C		
32	CIN	CC1(C2CCC(O1)(CC2)C)C		
33	SPRO	NA		

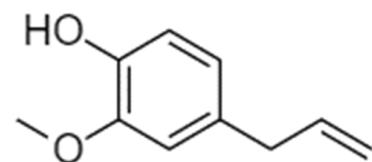
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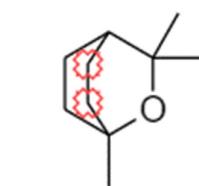
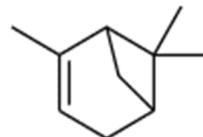
NA



NA



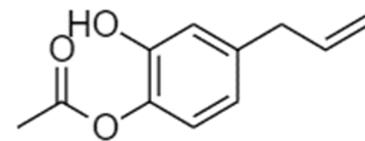
NA



NA

34 ALYM

CC(=O)OC1=C(C=C(C=C1)CC=CC=O)



NA: Not Available