

SUPPLEMENTARY

Table S1 The top hits from the NADI virtual screen, grouped according to the associated plants source

| PLANT | NADI CODE | Docking score (kcal/mol) | COMPOUND |
|------------------------|-----------|--------------------------|---|
| Endiandra kingiana | MSC3673 | -13.10 | Kingianin B |
| | MSC3676 | -12.90 | Kingianin E |
| | MSC3684 | -12.80 | Kingianin M |
| | MSC3683 | -12.80 | Kingianin L |
| | MSC3675 | -12.70 | Kingianin D |
| | MSC3678 | -12.50 | Kingianin G |
| | MSC3680 | -12.30 | Kingianin I |
| | MSC3679 | -12.20 | Kingianin H |
| | MSC3685 | -11.90 | Kingianin N |
| | MSC3681 | -11.90 | Kingianin J |
| Calophyllum inophyllum | MSC3469 | -12.50 | Epifriedelanol |
| | MSC429 | -12.50 | Friedelin |
| | MSC3471 | -12.30 | Canophyllol |
| | MSC3485 | -12.20 | Friedelan-3-one |
| | MSC3462 | -12.10 | Pyranojacareubin |
| | MSC3470 | -12.00 | Canophyllal |
| | MSC3473 | -11.90 | 3-oxo-Friedelan-28-oic acid |
| | MSC3472 | -11.90 | Canophyllic acid |
| | MSC3486 | -11.90 | Calaustralin |
| Boesenbergia rotunda | MSC2076 | -12.20 | Panduratin F |
| | MSC2067 | -12.20 | Panduratin B1 |
| | MSC2068 | -12.10 | Panduratin B2 |
| | MSC2101 | -11.90 | Rotundol |
| | MSC2111 | -11.90 | (2S)-7,8-Dihydro-5-hydroxy-2-methyl-2-(4"-methyl-3"-pentenyl)-8-phenyl-2H,6H-benzo[1,2-b:5,4-b']dipyran-6-one |
| | MSC2075 | -11.90 | Panduratin E |
| | MSC513 | -12.50 | Centellasaponin D |
| | MSC515 | -12.100 | Sceffoleoside A |

| | | | |
|-------------------|---------|--------|--|
| Centella asiatica | MSC502 | -12.00 | Madecassoside |
| | MSC514 | -12.00 | Asiaticoside |
| | MSC518 | -12.00 | 11,12-dehydrousolic acid Lactone |
| Manilkara zapota | MSC3016 | -14.60 | Lupeol benzoate |
| | MSC3018 | -13.00 | beta-Amyrin benzoate |
| | MSC3020 | -12.30 | alpha-Spinasterol benzoate/(3b,5a,22E)-Stigmasta-7,22-dien-3-ol benzoate |
| | MSC3017 | -12.30 | beta-Amyrin acetate |
| | MSC3029 | -12.10 | Lup-20(29)-en-3.23-diol |
| Psidium guajava | MSC2125 | -12.50 | Guavacoumaric acid |
| | MSC2126 | -12.20 | Guavin B |
| | MSC2124 | -12.20 | Ilelatifol D |
| | MSC2136 | -12.10 | 2alpha-Hydroxy-3beta-para-E-coumaroyloxyurs-12,18-dien-28-oic acid |
| | MSC2121 | -11.90 | Jacoumaric acid |

Table S2 Physicochemical properties of the compounds

| DRUG/COMPOUND | Everolimus | Asiaticoside | Asiatic acid |
|--------------------------------------|------------|--------------|--------------|
| MW (g/mol) | 958.2 | 959.12 | 488.699 |
| LogP | 5.9 | 2.33 | 5.44 |
| H-Bond Donor | 3 | 12 | 4 |
| H-Bond Acceptor | 14 | 19 | 5 |
| Rotatable bond | 9 | 10 | 2 |
| Polar surface area (Å ²) | 204.66 | 315.21 | 97.99 |