

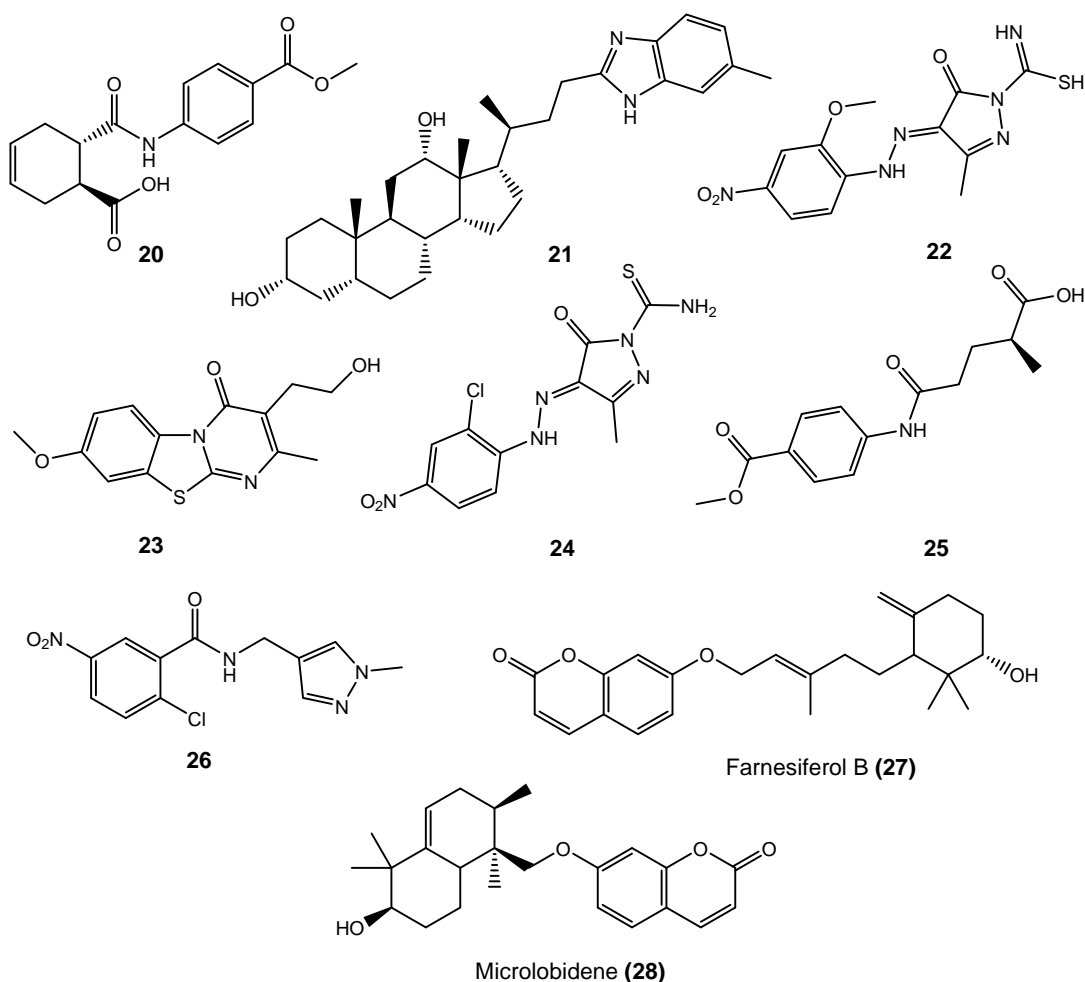
Supplementary Material

IN SILICO WORKFLOW FOR THE DISCOVERY OF NATURAL PRODUCTS ACTIVATING THE G PROTEIN-COUPLED BILE ACID RECEPTOR 1

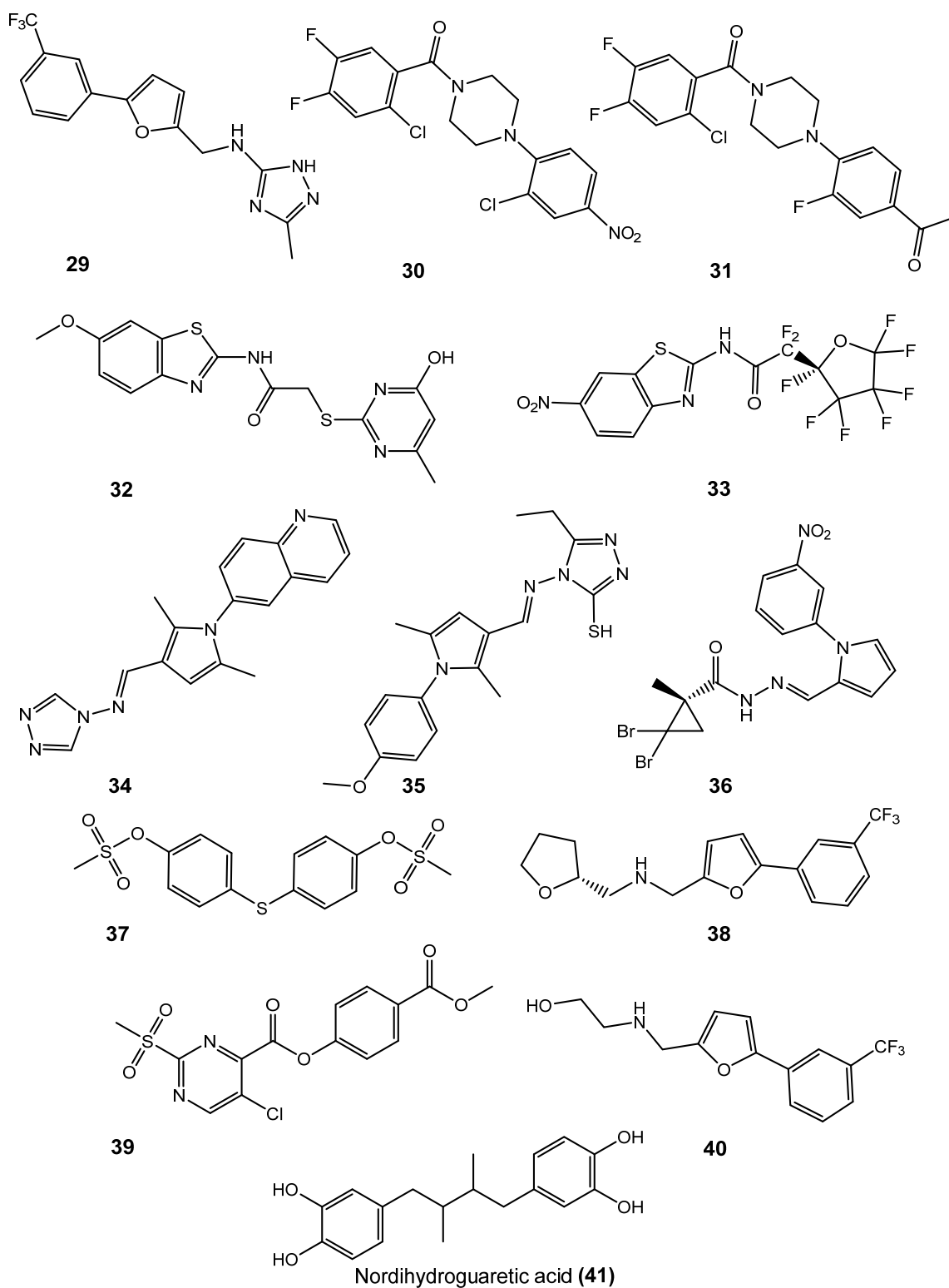
Benjamin Kirchweger, Jadel M. Kratz, Angela Ladurner, Ulrike Grienke, Thierry Langer, Verena M. Dirsch, Judith M. Rollinger*

* Correspondence: judith.rollinger@univie.ac.at

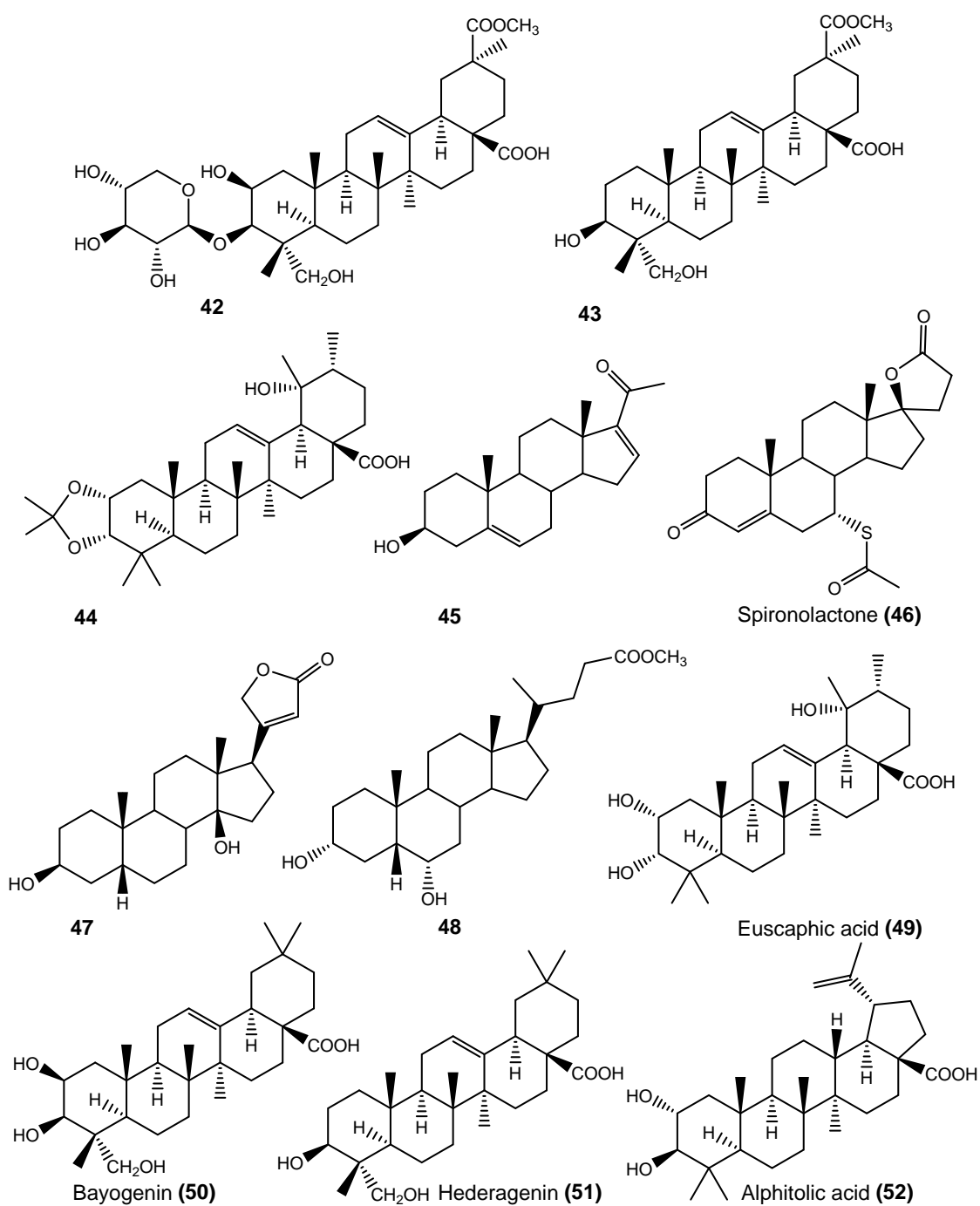
1 Supplementary Figures



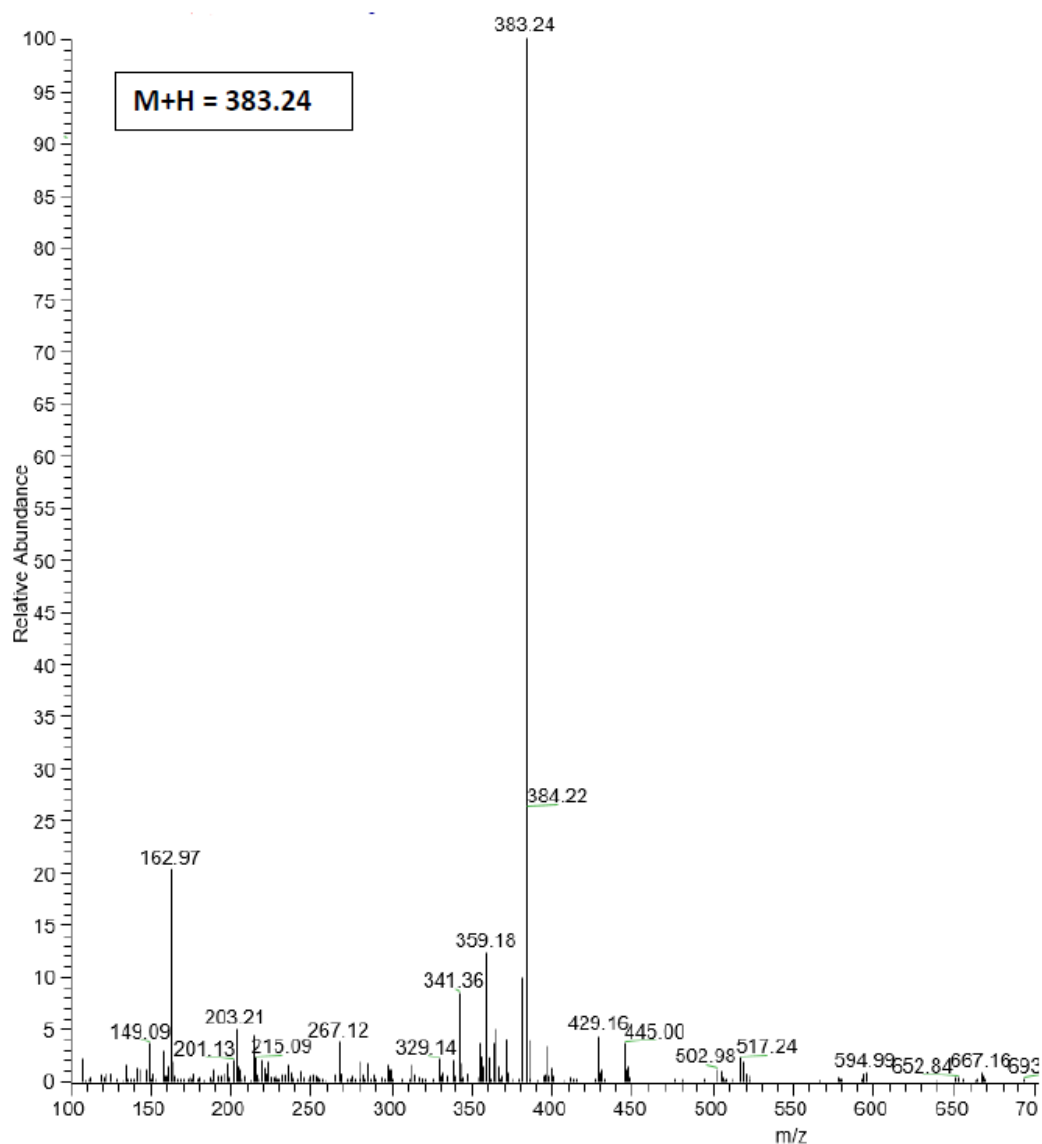
Supplementary Figure 1. Chemical structures of selected virtual hits from group 1; farnesiferol B (27) and microlobidene (28) are secondary plant metabolites, 20-26 are synthetic compounds obtained from SPECS.



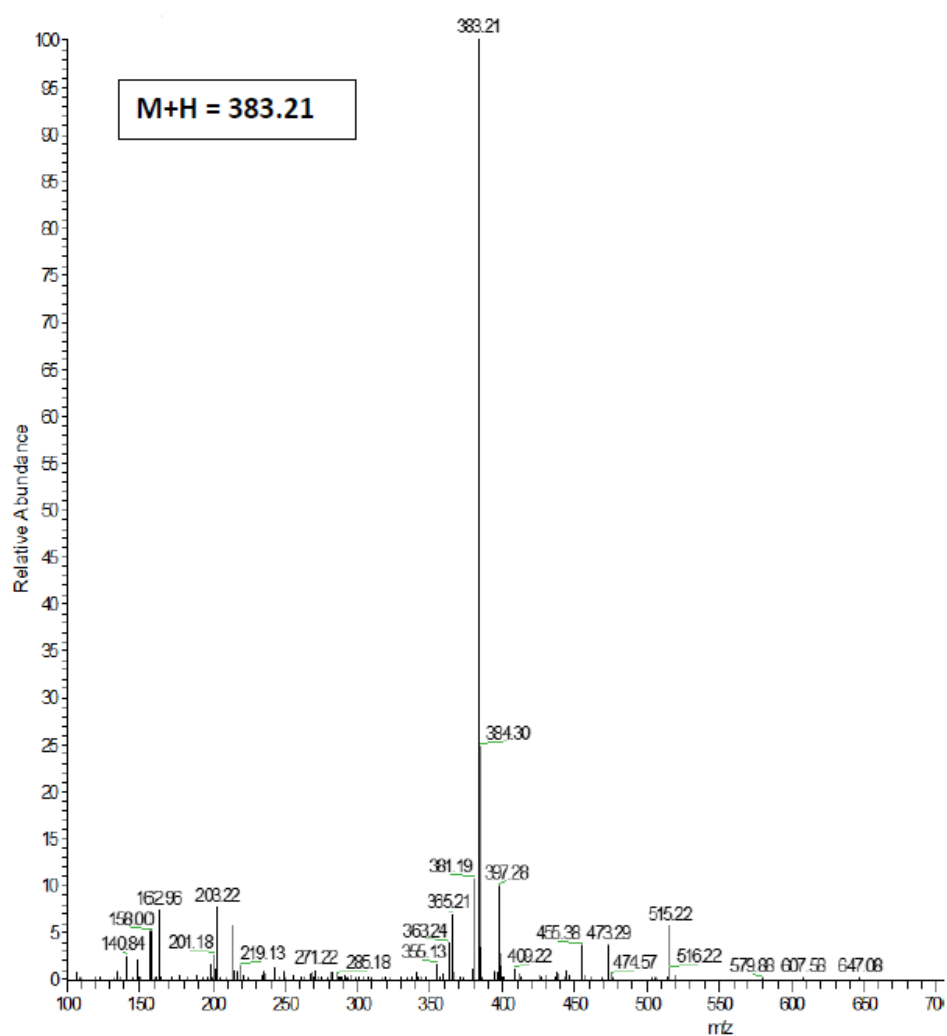
Supplementary Figure 2. Chemical structures of selected virtual hits from group 2; nordihydroguaretic acid (41) is a secondary plant metabolite, 29-40 are synthetic compounds obtained from SPECs.



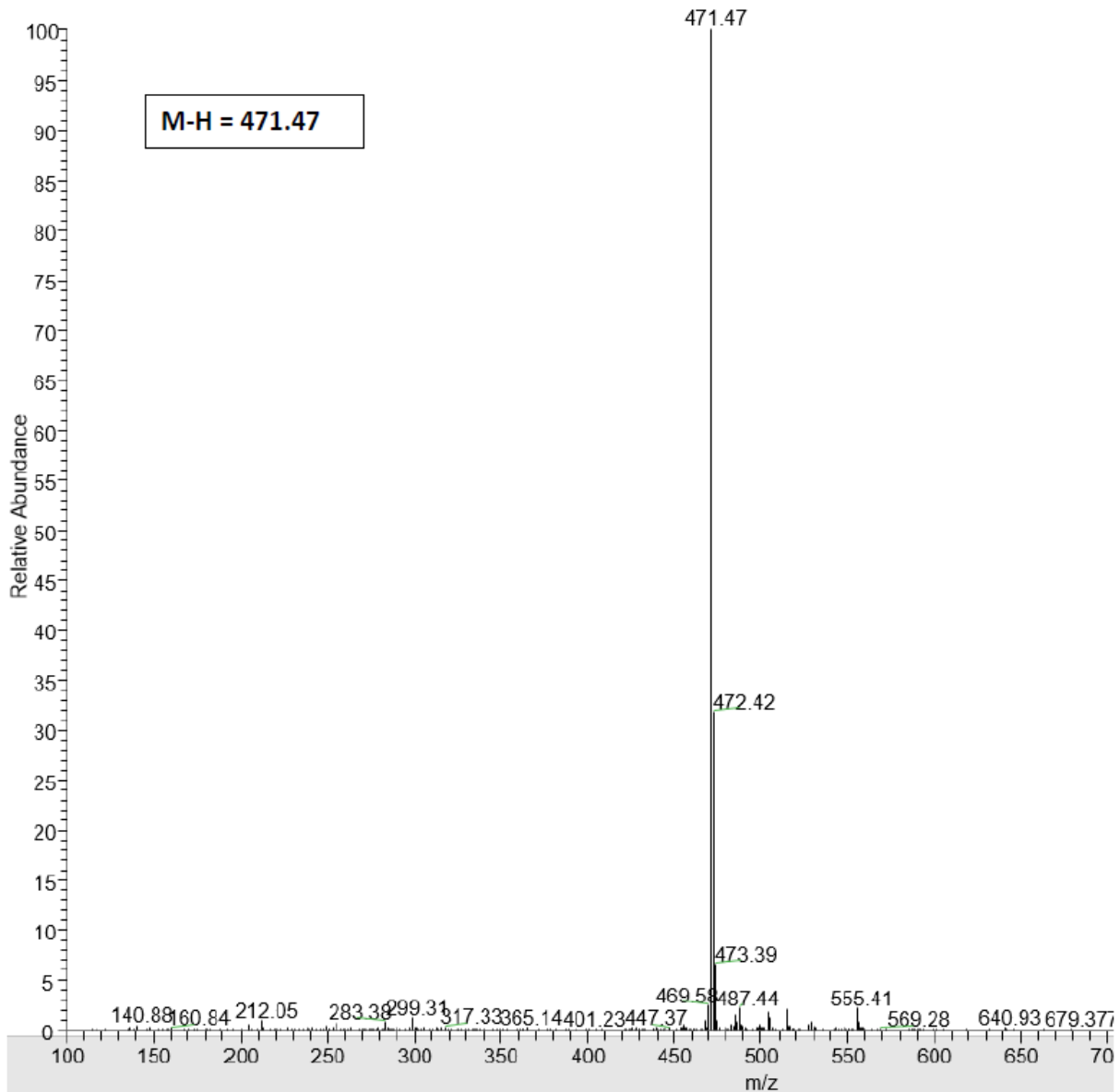
Supplementary Figure 3. Chemical structures of selected virtual hits from groups 4 to 9. Compounds **42** to **44** and **47** to **52** are secondary plant metabolites, **45** is a progesterone derivative and spironolactone (**46**) is an approved drug.



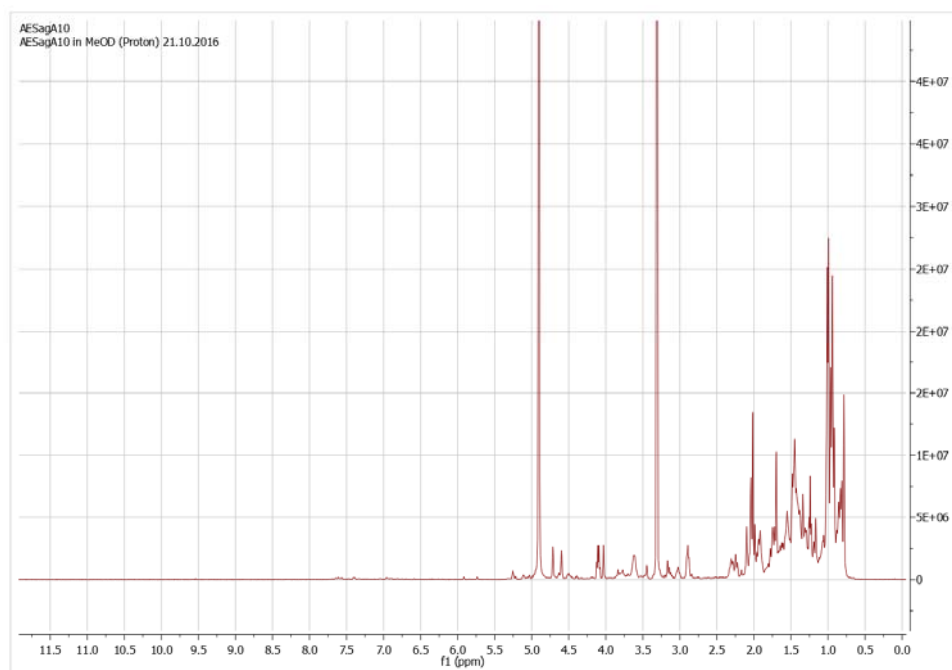
Supplementary Figure 4. MS data of microlobidene (**28**) (ThermoLTQiontrap; HESI; 275°C Capillary Temp; 300°C Source Heater Temp; Sheath Gas Flow 40.00; Aux Gas Flow 10.00; Sweep Gas Flow 10.00; Positive Source Voltage 3.70 kV; 100.00 uA Source Current; 18.00 V Capillary Voltage; 90.00 V Tube Lens)



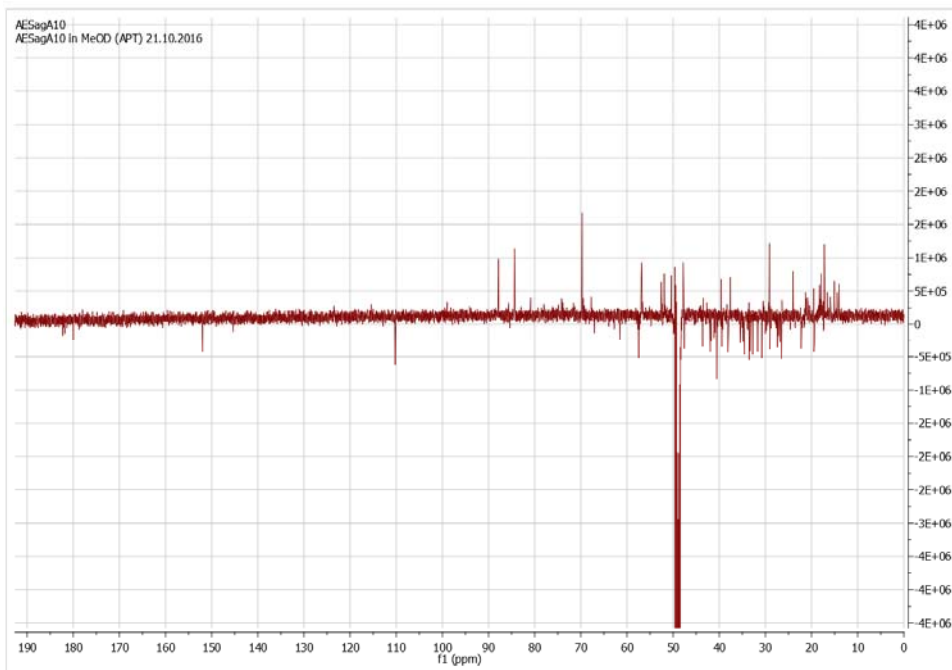
Supplementary Figure 5. MS data of farnesiferol B (**27**) (ThermoLTQiontrap; HESI; 275°C Capillary Temp; 300°C Source Heater Temp; Sheath Gas Flow 40.00; Aux Gas Flow 10.00; Sweep Gas Flow 10.00; Positive Source Voltage 3.70 kV; 100.00 uA Source Current; 18.00 V Capillary Voltage; 90.00 V Tube Lens)



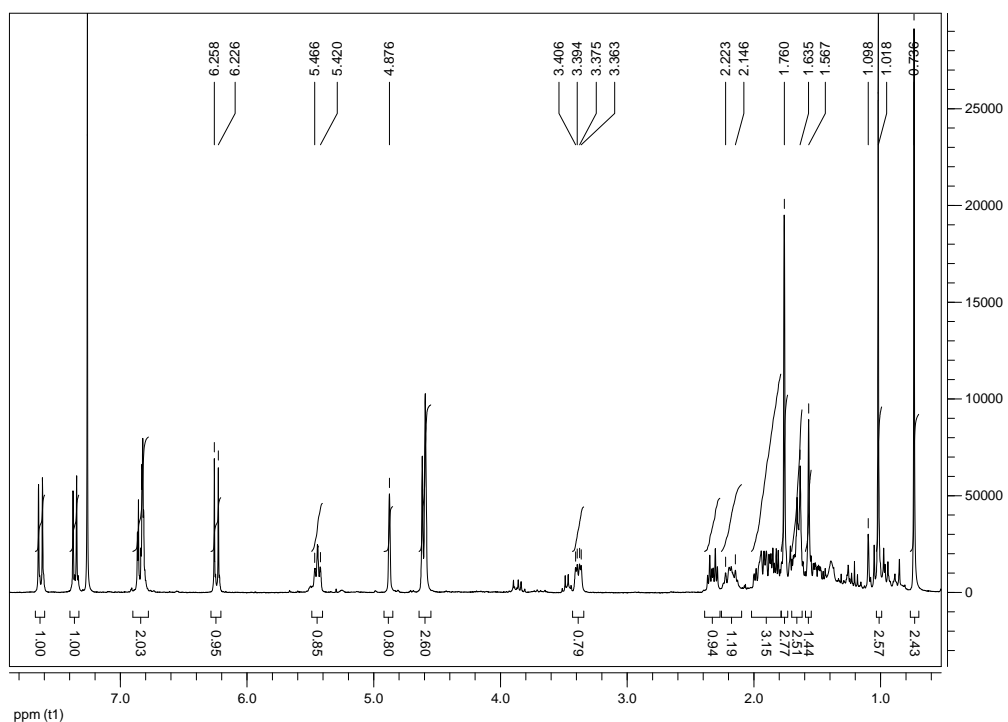
Supplementary Figure 6. MS data of alphitolic acid (**52**) (ThermoLTQiontrap; HESI; 275°C Capillary Temp; 300°C Source Heater Temp; Sheath Gas Flow 40.00; Aux Gas Flow 10.00; Sweep Gas Flow 10.00; Positive Source Voltage 3.70 kV; 100.00 uA Source Current; -30.00 V Capillary Voltage; -110.00 V Tube Lens)



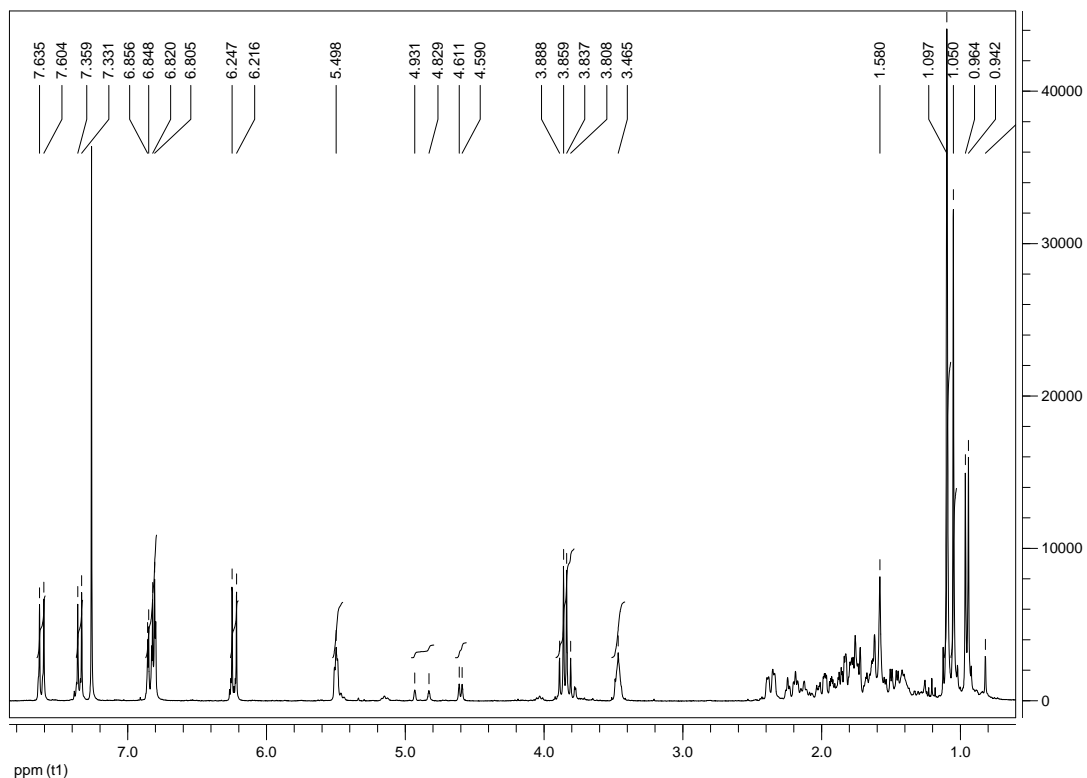
Supplementary Figure 7. $^1\text{H-NMR}$ spectrum of 52 (CD_3OD , ref.: δH 3.31 ppm, 500 MHz NMR, ~ 2 mg)



Supplementary Figure 8. $^{13}\text{C-APT}$ spectrum of 52 (CD_3OD , ref.: δC 49.00 ppm, 500 MHz NMR, ~ 2 mg)



Supplementary Figure 9. ¹H-NMR of **27** (CDCl₃, ref.: δH 7.26 ppm, 300 MHz NMR, 5.6mg)



Supplementary Figure 10. ¹H-NMR of **28** (CDCl₃, ref.: δH 7.26 ppm, 300 MHz NMR, 5.6mg)