Supplementary Material for

Facilitated visual interpretation of scores in principal component analysis by bioactivity-labeling of ^{1}H NMR spectra - metabolomics investigation and identification of a new α-glucosidase inhibitor in Radix Astragali

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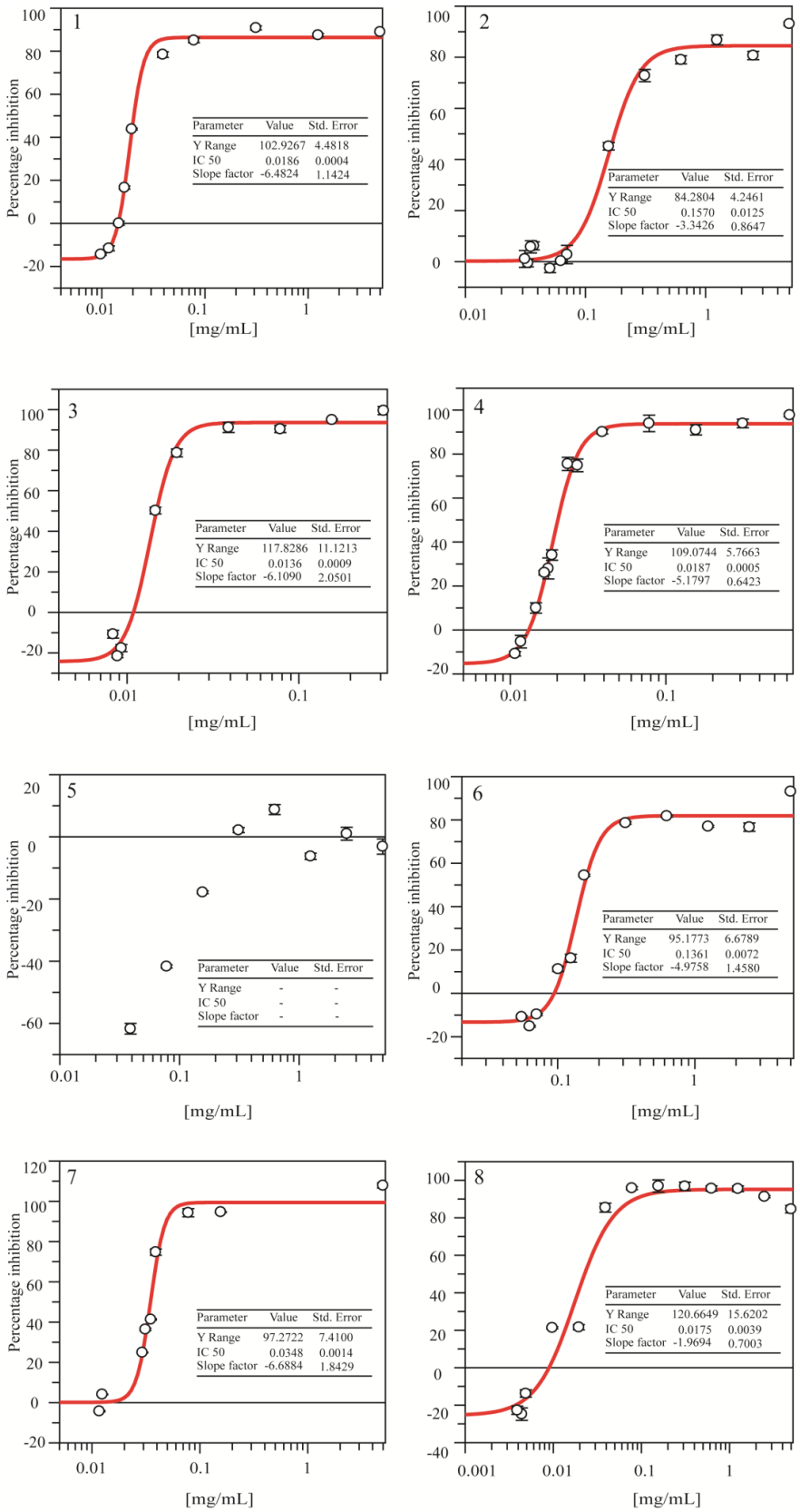

Figure S1. Inhibition curves of the ethyl acetate extracts of 21 samples of Radix Astragali in the α-glucosidase inhibition assay.

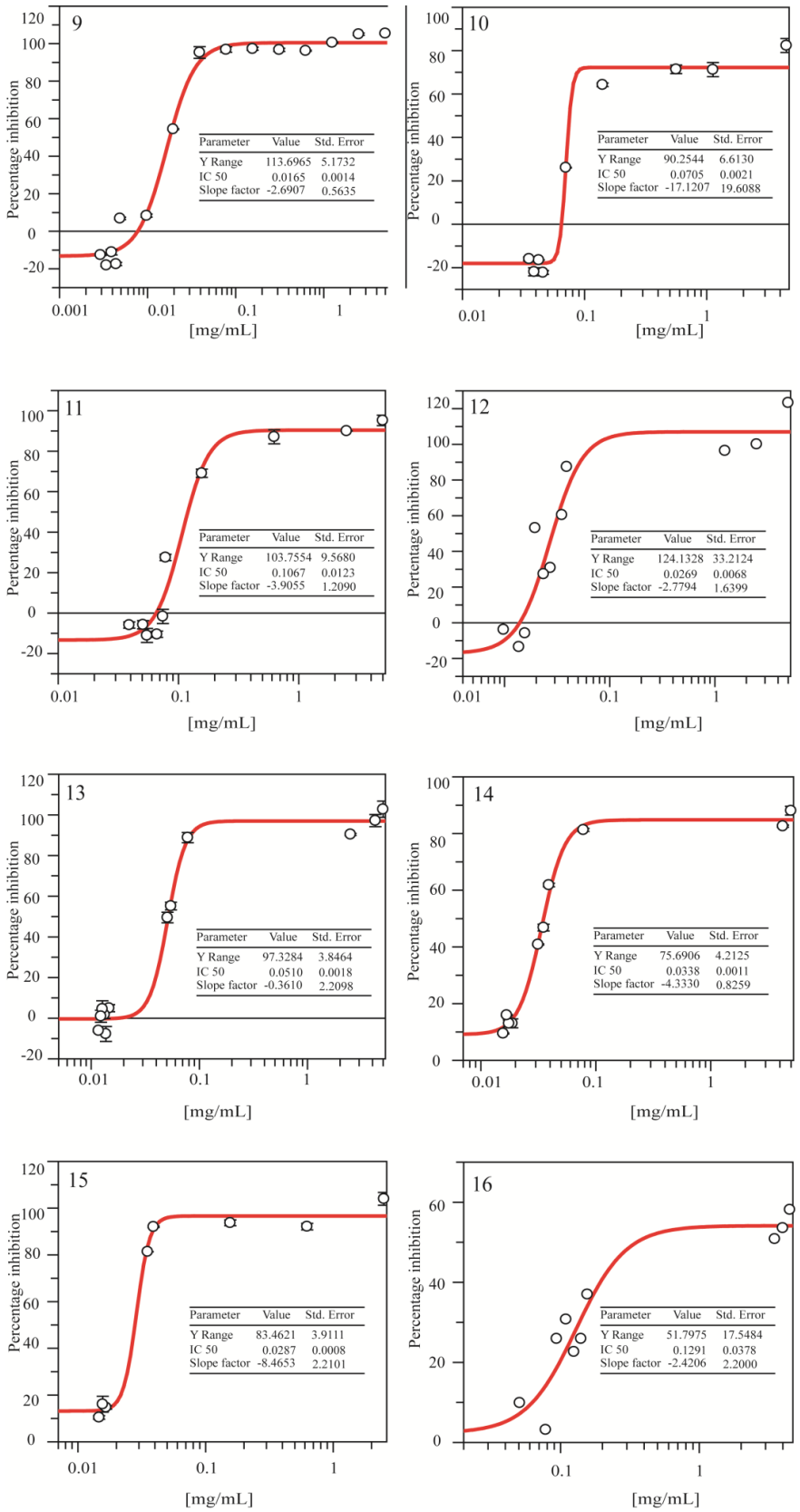

Figure S1 continued. Inhibition curves of the ethyl acetate extracts of 21 samples of Radix Astragali in the α-glucosidase inhibition assay.

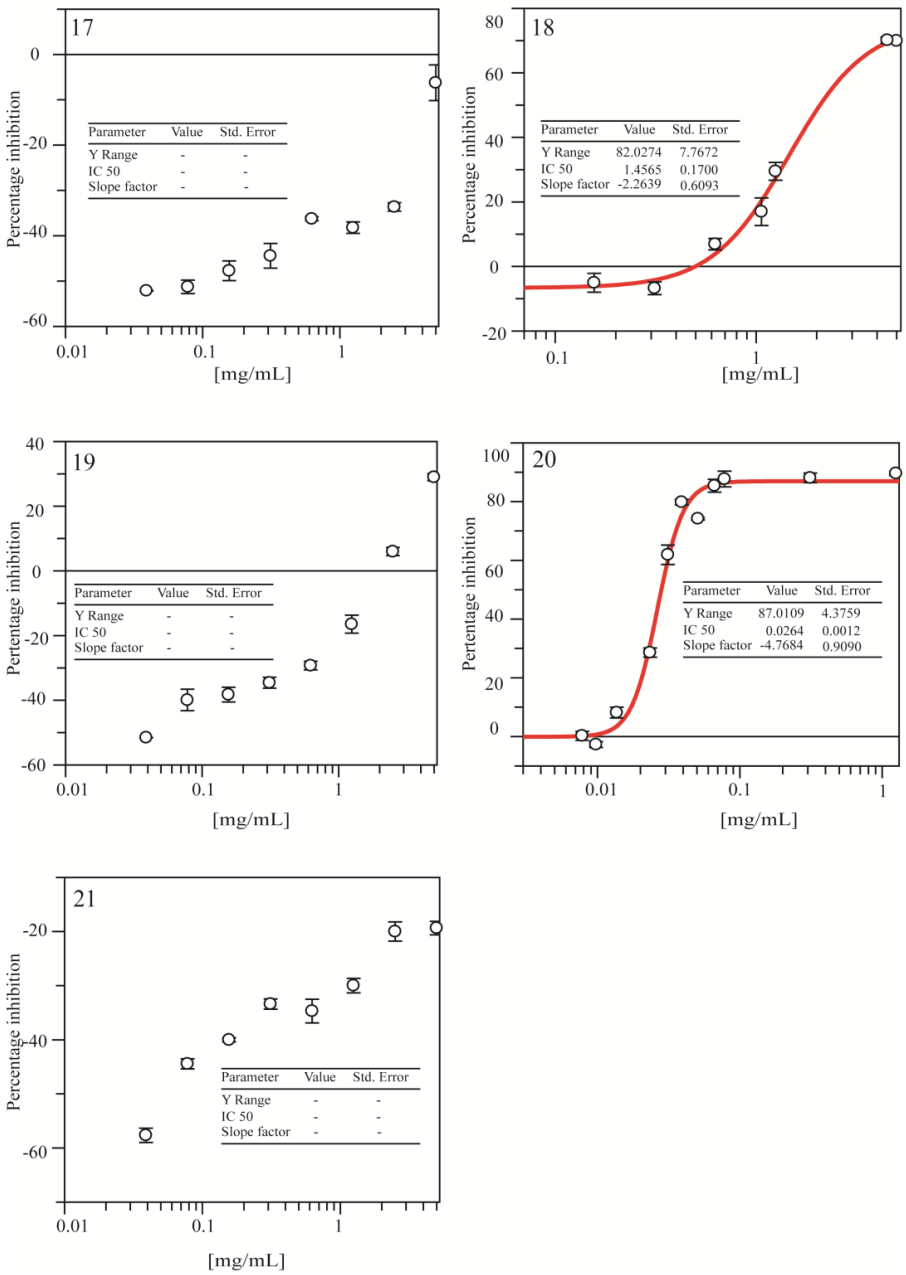

Figure S1 continued. Inhibition curves of the ethyl acetate extracts of 21 samples of Radix Astragali in the α-glucosidase inhibition assay.

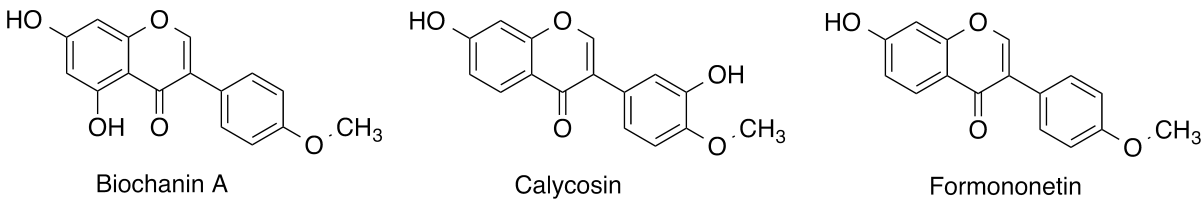

Figure S2. Radix Astragali isoflavones with expected α-glucosidase inhibitory activity.

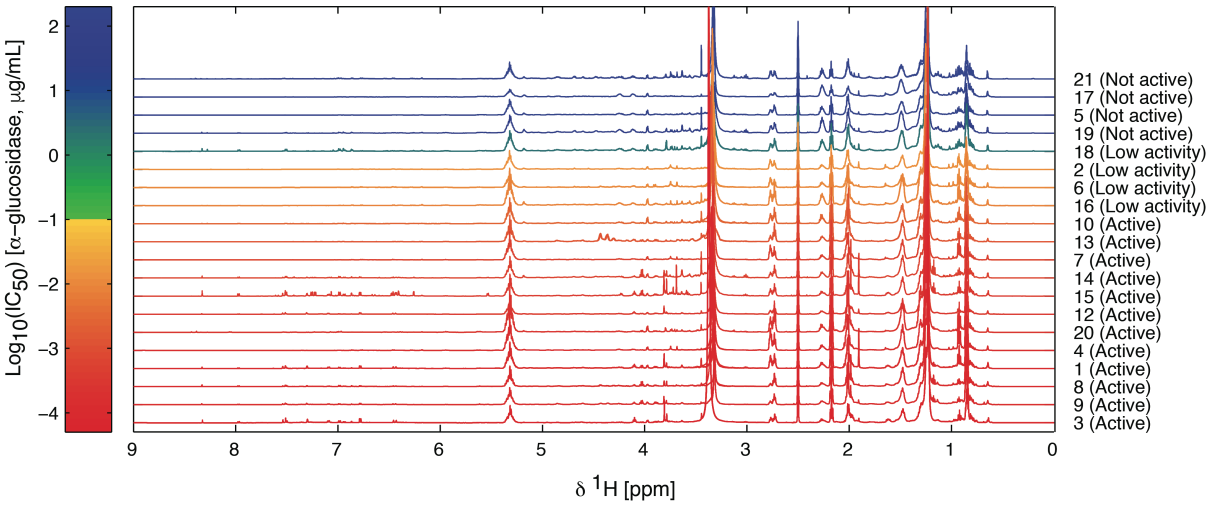

Figure S3. 600 MHz ^{1}H NMR spectra of ethyl acetate extracts of Radix Astragali samples dissolved in DMSO-d_6. The color and order of the spectra reflects the inhibitory activity in the α-glucosidase assay according to the bar to the left. The number to the right gives the number of the sample. Active extracts are those with IC_{50} values < 100 µg/mL and extracts with low activity are those with IC_{50} values ≥ 100 µg/mL. The non-active extract # 19 showed only 30 % inhibition at a concentration of 5 mg/mL and the remaining non-active extracts were arbitrarily set to 10 mg/mL for plotting purposes.

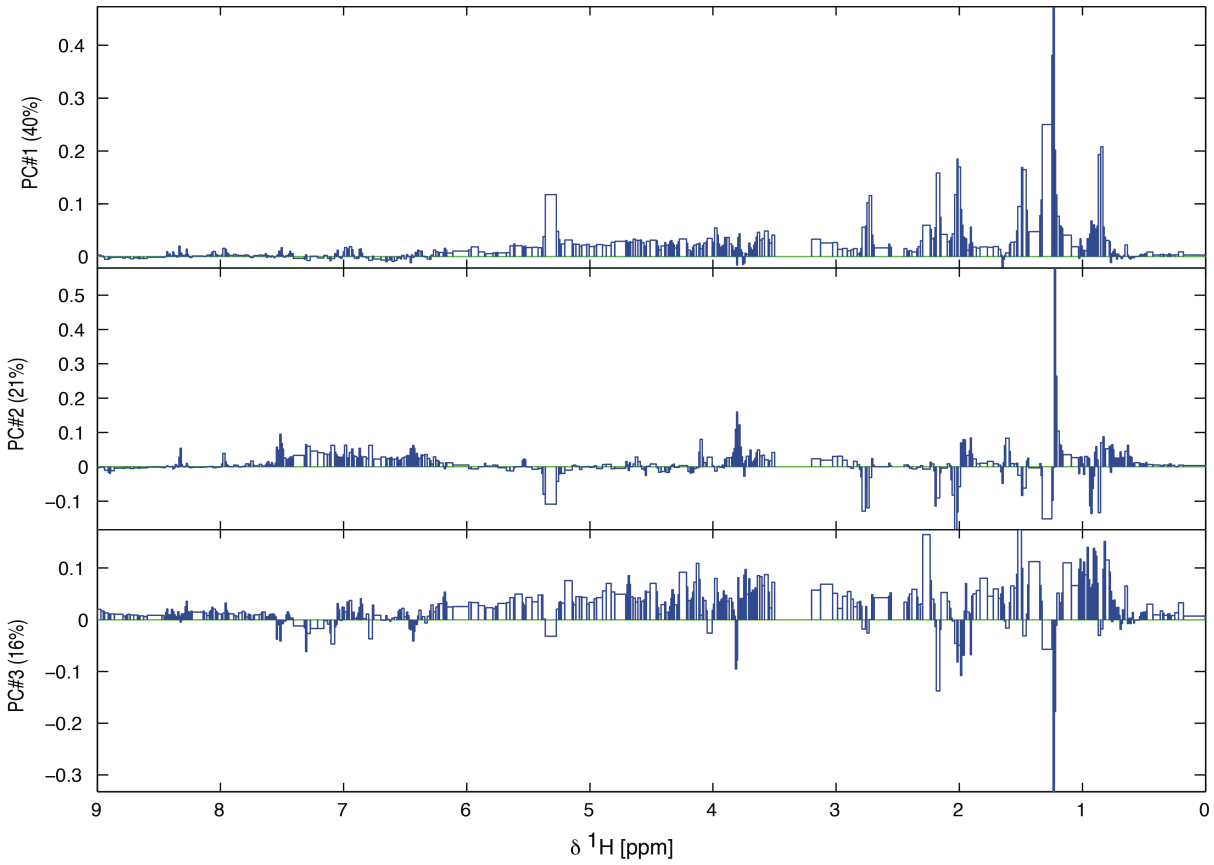

Figure S4. PCA-loading values for components #1, #2 and #3 plotted on the chemical shift axis.

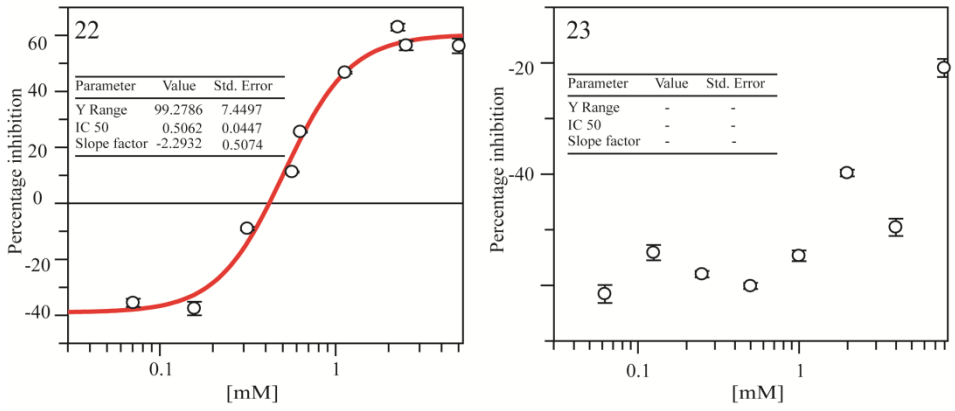

Figure S5. α-Glucosidase inhibition curves: linoleyl ferulate (**1**, sample 22) and hexadecyl ferulate (**2**, sample 23).