

Supplementary materials

Synergistic Lipase Inhibition by *Garcinia parvifolia* Metabolites: A ¹H NMR–based Metabolomic Deciphering of Multi-Ligand Interactions

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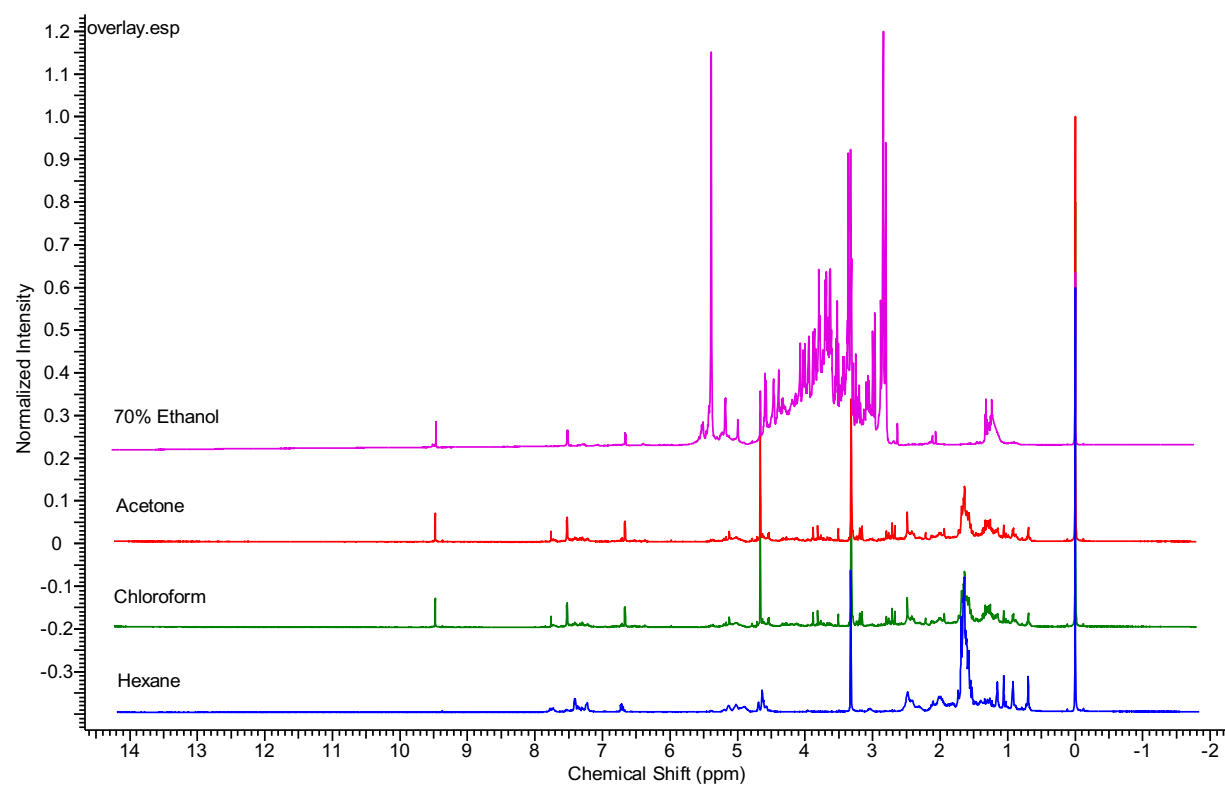
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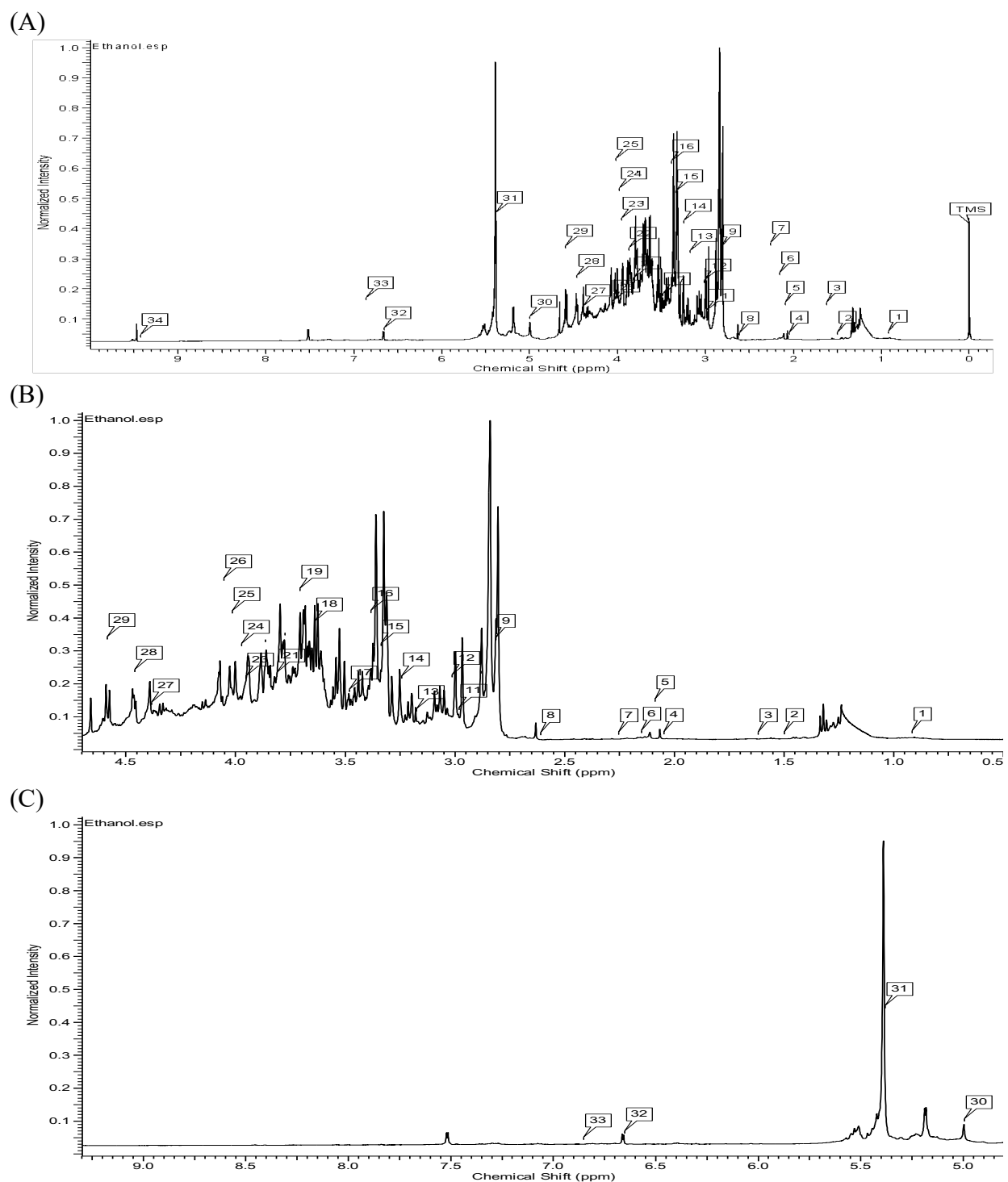
Supplementary Table S1 Extraction yield with different solvents

Samples	Yield weight (g)
70% (v/v) Ethanol	9.32±1.15 ^a
Acetone	5.30±0.45 ^b
Chloroform	2.10±0.82 ^c
Hexane	1.37±0.39 ^c

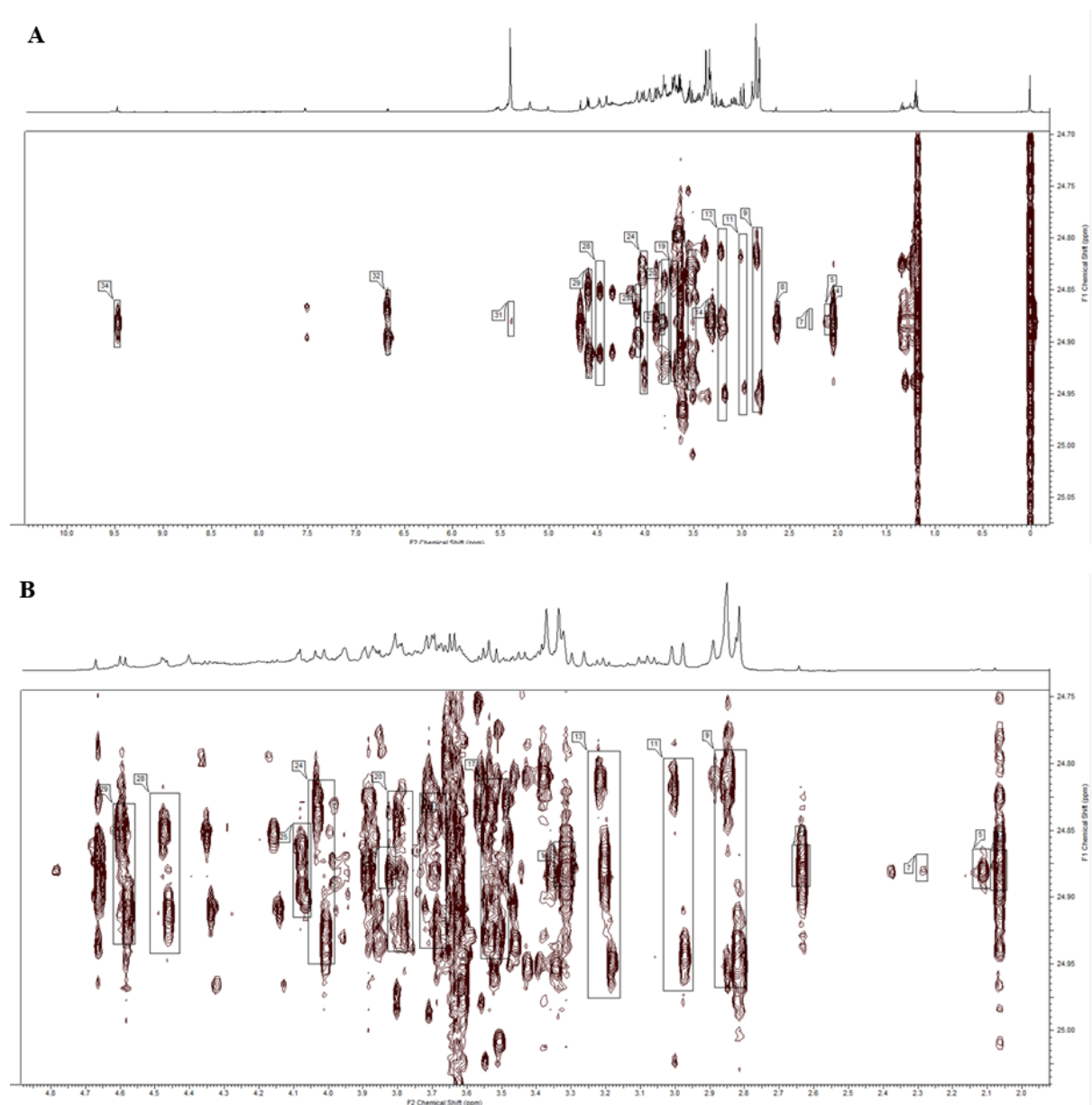
Data are mean ± standard deviation of heptaplicate (n = 7) determination. Values with different superscripts are significantly different at p<0.05.



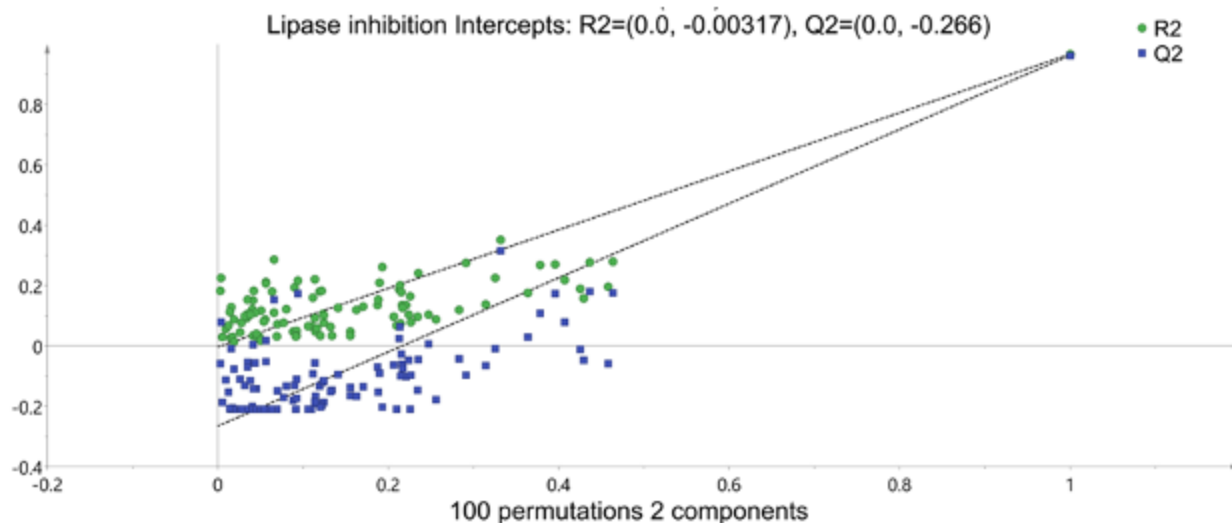
Supplementary Figure S1 Stacked ^1H NMR spectra of the different *G. parvifolia* extracts.



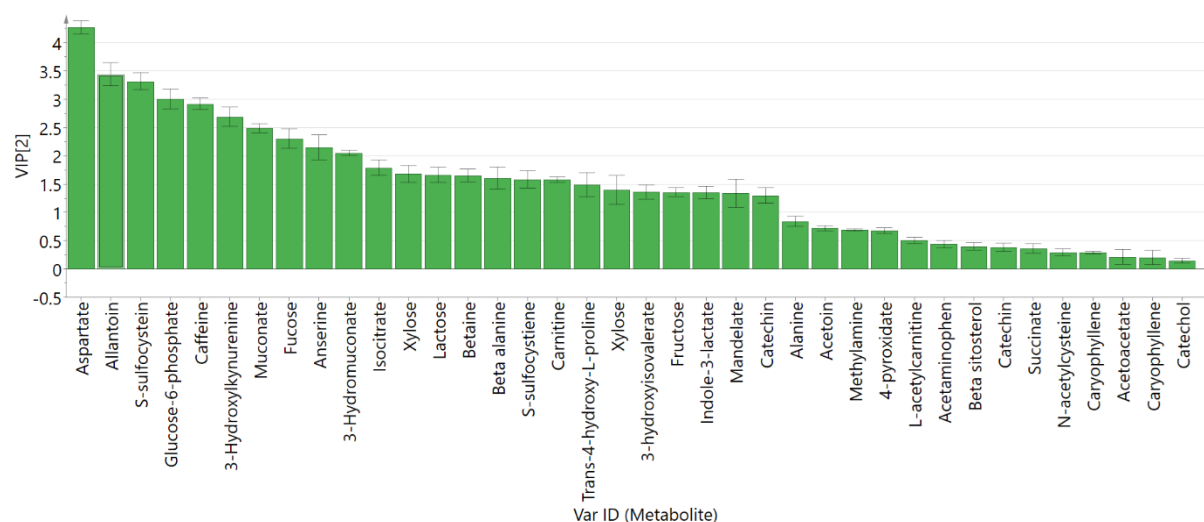
Supplementary Figure S2 (A) ^1H NMR spectrum of *G. parvifolia* extract. (B) An expanded ^1H NMR spectrum between δ 0.50 and δ 4.70. (C) An expanded ^1H NMR spectrum between δ 4.80 and δ 9.30. For the interpretation of the numbers assigned to the metabolites, refer to Table 2.



Supplementary Figure S3 2D J-resolved experiments of *G. parvifolia* extract: (A) in the region from δ -0.20 to 10.04; (B) in the region from δ 1.30 to 4.60; Refer Table 2 for metabolite number interpretation



Supplementary Figure S4 The permutation plots of the developed PLS model developed for the lipase inhibition activity of *G. parvifolia* extracts



Supplementary Figure S5 Partial least squares (PLS) variable importance in projection (VIP) plot of *G. parvifolia* extract, highlighting key metabolites and their corresponding chemical shifts (δ , ppm): aspartate (δ 2.82), allantoin (δ 5.38), S-sulfocystein (δ 3.66), glucose-6-phosphate (δ 3.78), caffeine (δ 3.34), 3-hydroxykynurenine (δ 3.7), muconate (δ 2.86), fucose (δ 3.86), anserine (δ 3.82), 3-hydromuconate (δ 2.98), isocitrate (δ 4.06), xylose (δ 4.58), lactose (δ 4.46), betaine (δ 3.26), β -alanine (δ 3.18), S-sulfocystiene (δ 4.02), carnitine (δ 3.22), trans-4-hydroxy-L-proline (δ 3.46), xylose (δ 5.18), 3-hydroxyisovalerate (δ 1.26), fructose (δ 3.9), indole-3-lactate (δ 4.34), mandelate (δ 5.02), catechin (δ 4.54, δ 6.66), alanine (δ 1.54), acetoin (δ 2.18), methylamine (δ 2.62), 4-pyroxidate (δ 2.46), L-acetylcarnitine (δ 2.1), acetaminophen (δ 2.14), β -sitosterol (δ 0.9), succinate (δ 2.34), N-acetylcysteine (δ 2.06), caryophyllene (δ 4.9, δ 0.98), acetoacetate (δ 2.26), and catechol (δ 6.86).

Supplementary Table S2 Docking score of catechin, β -sitosterol, β -caryophyllene and reference standard orlistat with of Human Pancreatic Lipase (PDB ID: 1LPB).

Ligand	Docking Score(kcal/mol)
Orlistat	-5.528
Catechin	-6.09
β -sitosterol	-6.336
β -caryophyllene	-5.188