

## Supplementary Materials

### Stereoselective separation, configuration determination, and quantification of flavanone glycosides in Citrus using chiral HPLC-UV in combination with CD spectra

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Fig S1

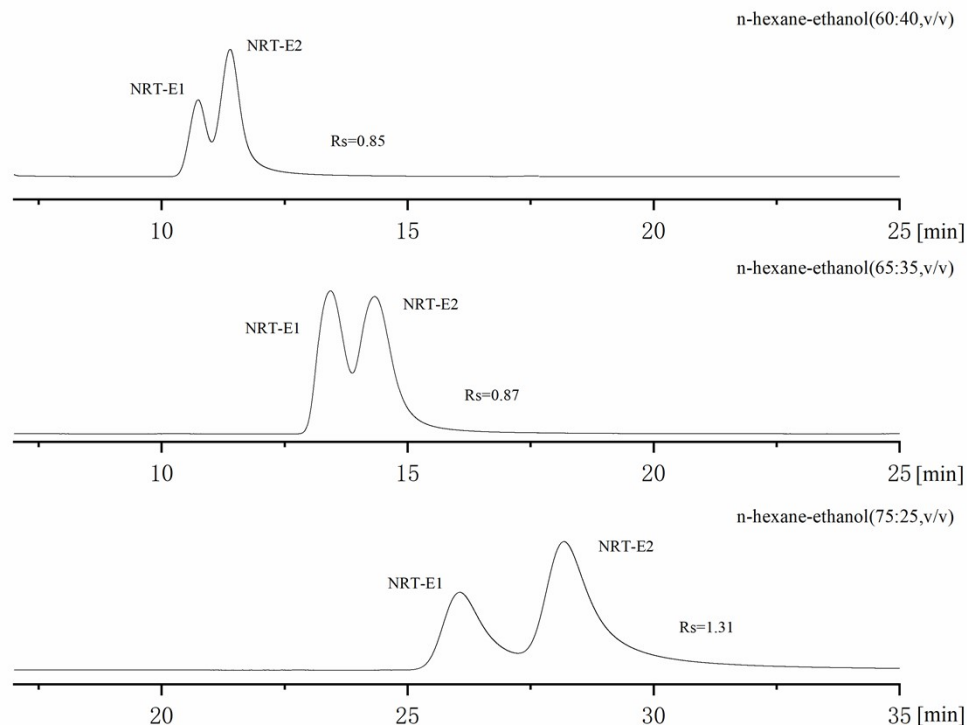


Fig. S1 Chromatograms of Narirutin with various mobile phases on Chiral INC column.

**Table S1**

Analytes	Detection instrument	Mobile phase	Rs	Extraction recovery (%)	RSD (%)	Ref
naringin, neohesperidin	Chiral-LC-CD	n-hexane-CHCl <sub>3</sub> -ethano	-	-	-	[16]
naringin, neohesperidin, narirutin, hesperidin	DM-β-CD	0.1 M borate buffer	≤0.54 ≤2.48 ≤0.65 -	-	-	[23]
naringin, neohesperidin	Chiral-LC-CD	n-hexane-ethanol	≤9.2 ≤4.1	-	-	[24]
naringin, hesperidin	nano-LC-UV	MeOH-IPA	≤2.25 -	-	-	[14]
naringin	Chiral-SFC	ethanol-methanol	≤5.1	-	2.6-2.7	[15]

23. N. Gel-Moreto, R. Streich and R. Galensa, *Journal of Chromatography A*, 2001, **925**, 279–289.

24. S. Caccamese and R. Chillemi, *J Chromatogr A*, 2010, **1217**, 1089-1093.

Comparison with other methods.

**Table 1 naringin-1s-no-sugar-energies-blin**

Conf ID	Energy (Hartree)	ΔE (Hartree)	Boltzmann Factor	Population (%)
1	-994.0833458	0	1	15.50
2	-994.0833449	8.94E-07	0.999053998	15.49
3	-994.0832688	7.7065E-05	0.921653204	14.29
4	-994.0831747	0.00017109	0.834327181	12.94
5	-994.0831743	0.00017154	0.833933333	12.93
6	-994.083107	0.00023884	0.776586685	12.04
7	-994.0831069	0.00023892	0.776513518	12.04
8	-994.0817981	0.00154774	0.194262665	3.01
9	-994.0799827	0.0033631	0.028427257	0.44
10	-994.0798523	0.00349353	0.024761019	0.38

11	-994.0797297	0.00361616	0.02174617	0.34
12	-994.0796223	0.00372349	0.019410455	0.30
13	-994.079621	0.00372484	0.019382898	0.30

Table 2 neohesperidin-1s-no-sugar-energies-blin

Conf ID	Energy (Hartree)	$\Delta E$ (Hartree)	Boltzmann Factor	Population (%)
1	-1108.597349	0	1	19.17
2	-1108.597092	0.00025627	0.762384021	14.61
3	-1108.596927	0.00042188	0.639779996	12.26
4	-1108.596925	0.00042404	0.638318668	12.24
5	-1108.59692	0.00042833	0.635426198	12.18
6	-1108.596807	0.00054169	0.563566496	10.80
7	-1108.59666	0.00068881	0.482284444	9.24
8	-1108.596607	0.00074138	0.456176542	8.74
9	-1108.593785	0.00356408	0.022978921	0.44
10	-1108.593456	0.00389261	0.016228567	0.31