Supporting Information

In silico screening of comprehensive two-dimensional centrifugal partition chromatography x liquid chromatography for multiple compounds isolation

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Figure S1: HPLC chromatograms of the plant extract (a) LC1: CSH Phenylhexyl column (150 x 4.6 mm i.d., 5 µm), flow-rate at 2 ml/min, gradient elution from 3% to 25% of organic solvent in 17.6 min, detection at 288 nm. (b) LC2: Gemini-NX C18 column (150 x 4.6 mm i.d., 3 µm), flow-rate at 1.5 ml/min, gradient elution from 3% to 25% of organic solvent in 24.2 min, detection at 288 nm.

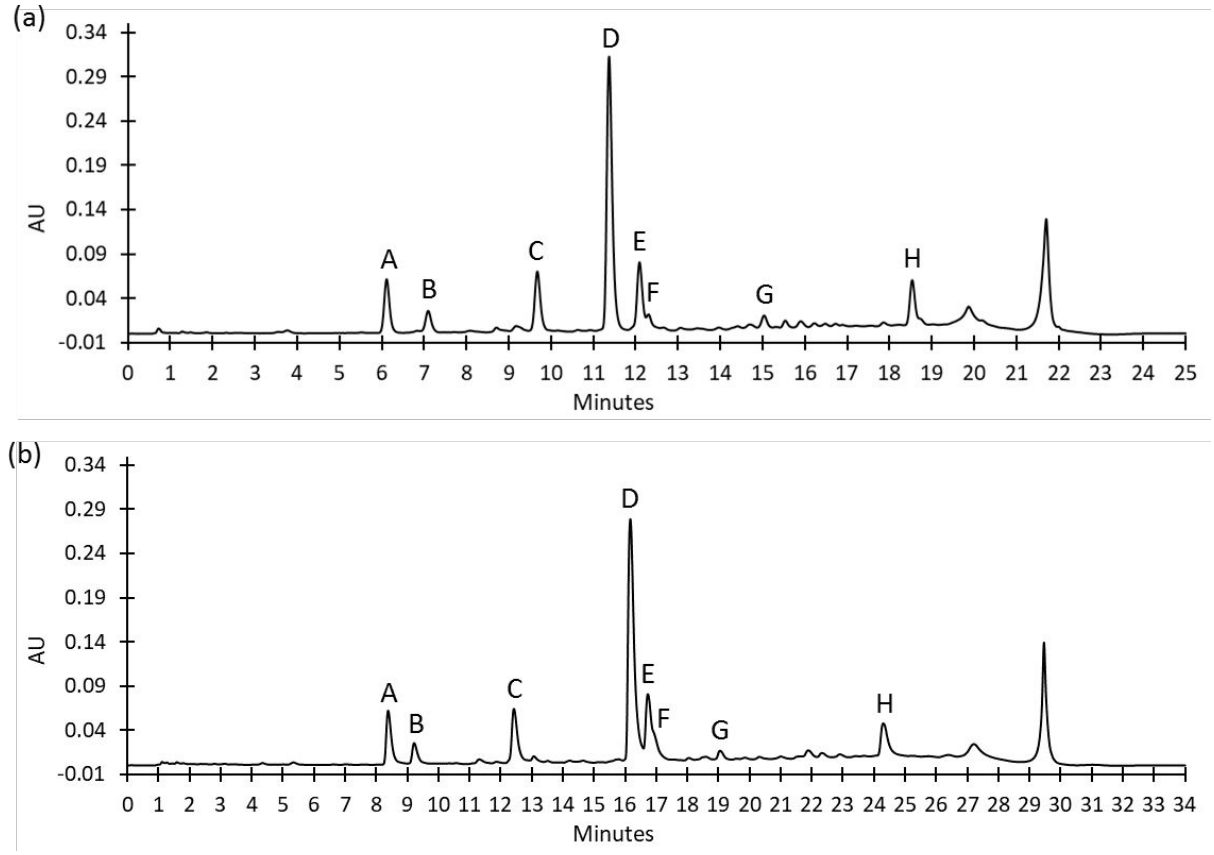

Table S1: Operating conditions for CPC methods

	CPC1	CPC2	CPC3	CPC4
Solvent system	1-Butanol/Water 50/50 (v/v)	1-Butanol/Water 50/50 (v/v)	Ethanol/Ammonium sulfate/Water 22/21/57 (w/w)	Acetonitrile/Sucrose/Water 50/13.3/36.7 (w/w)
Mode	Descending	Ascending	Descending	Ascending
Rotation (rpm)	2500	2500	1500	2300
Flow-rate (ml/min)	8	5	5	3
Temperature	20°C	20°C	15°C	30°C
Stationary phase ratio (*Sf*)	75%	66%	28%	58%
Collection time (min)	0.5	1.0	1.0	1.0
Number of fraction (volume in ml)	45 (4)	36 (5)	36 (5)	60 (3)
Total duration time (min)	22.5	36	36	60

Table S2: K_D-value measurements of compounds in the selected CPC systems.

	Solvent system	Mode	Predictive K_D							
			A	B	C	D	E	F	G	H
CPC1	1-Butanol/water 50/50 (v/v)	Descending	0.1	0.6	1.6	4.1	3.9	0.8	2.7	2.5
CPC2	1-Butanol/water 50/50 (v/v)	Ascending	8.9	1.8	0.6	0.2	0.3	1.2	0.4	0.4
CPC3	Ethanol/Ammonium sulfate/Water 22/21/57 (w/w)	Descending	2.0	2.8	4.7	6.9	6.5	5.2	9.3	15.7
CPC4	Acetonitrile/Sucrose/Water 50/13.3/36.7 (w/w)	Ascending	8.6	2.9	1.6	2.3	1.9	7.8	2.4	1.1

Here can be found the ternary diagram of CPC 3 and CPC4: Liu et al., Journal of chromatography A, 1356 (2014) 157-162; de Brito Cardoso, Separation and purification technology, 104 (2013) 106-113.

Equations: calculation of the harmonic mean $\overline{H}$ and the arithmetic mean $\overline{A}$ of the nearest-neighbor distances

$$\overline{H} = \frac{n-1}{\sum_{i=1}^{n-1} \frac{1}{di}} \qquad \textit{Equation 1}$$

$$\overline{A} = \frac{\sum_{i=1}^{n-1} di}{n-1} \qquad \textit{Equation 2}$$

with n number of components and di nearest-neighbor distance for compound *i*

Figure S2: 2D-contour plots of off-line comprehensive CPC1xLC1 separations (system #1) at different sample loads. (a) Injection of 350 µl of a sample extract at a concentration of 27 mg/ml; (b) Injection of 1.5 ml of a sample extract at a concentration of 27 mg/ml. To be compared with Figure 4a in manuscript.

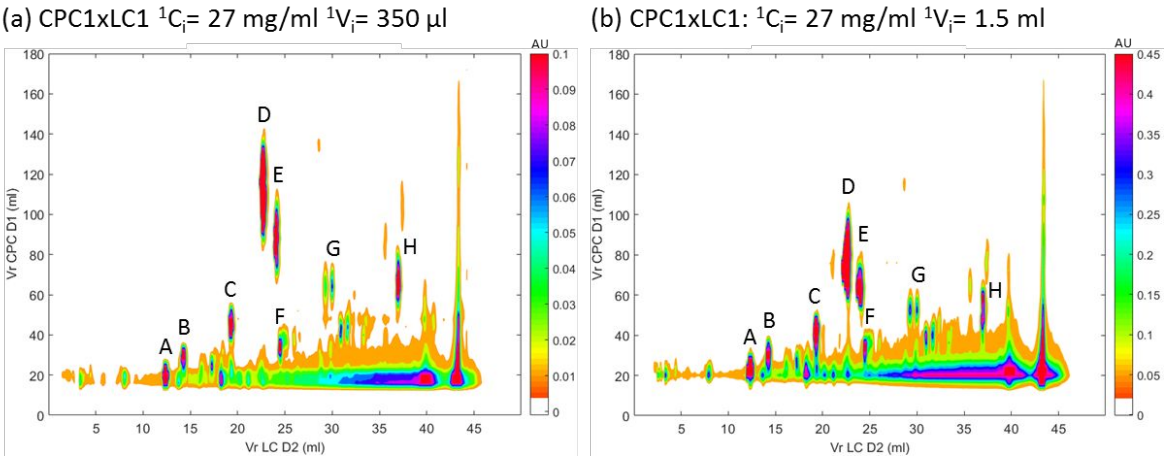

Figure S3: Evolution of (a) system homogeneity, (b) minimal distance between peaks in function of stationary phase retention rate in ^{1}D-CPC for the 2D systems using LC1 method as second dimension.