

Optimizing stilbene recovery from cell cultures media: A comprehensive study of the adsorption process

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SUPPLEMENTARY TABLES

Table S1. Physical properties of the tested adsorbents. Sourced from Sigma Aldrich Website. The moisture content was analyzed in the laboratory

Resin	Amberlite XAD-16	Amberlite XAD-4	Amberlite XAD-1180	Amberlite XAD-7	Amberlite FPX66
Chemical nature	SDVB	SDVB	SDVB	Acrylic ester	SDVB
Polarity	Non-polar	Non-polar	Non-polar	Polar	Non-polar
Specific surface area (m ² /g)	900	800	600	450	700
Pore diameter (Å)	100	50	300	90	200–250
Pore volume (mL/g)	1.82	0.98	1.68	1.14	1.4
Moisture content (%)	67.42	62.43	69.81	72.10	70.9

SDVB - Styrene-divinylbenzene

Table S2: Adsorption kinetic models utilized for fitting the experimental data (Adapted from [1,2])

Kinetic model	Pseudo-first order	Pseudo-second order	Intra-particle diffusion
Differential equation	$\frac{dq_{t,i}}{dt} = k_{1,i} \cdot (q_{eq,i} - q_{t,i})$	$\frac{dq_{t,i}}{dt} = k_{2,i} \cdot (q_{eq,i} - q_{t,i})^2$	-
Non-linear form equation	$q_{t,i} = q_{eq,i} \cdot (1 - e^{-k_{1,i}t})$	$q_{t,i} = \frac{k_{2,i} \cdot q_{eq,i}^2 \cdot t}{1 + k_{2,i} \cdot q_{eq,i} \cdot t}$	-
Linear form equation	$\ln(q_{eq,i} - q_{t,i}) = \ln q_{eq,i} - k_{1,i} \cdot t$	$\frac{t}{q_{t,i}} = \frac{1}{k_{2,i} \cdot q_{eq,i}^2} + \frac{t}{q_{eq,i}}$	$q_{t,i} = k_{d,i} \cdot t^{\frac{1}{2}} + C_{d,i}$
Plot (y vs. x)			
Non-linear form	$q_{t,i} \text{ vs. } t$	$q_{t,i} \text{ vs. } t$	-
Linear form	$\ln(q_{eq,i} - q_{t,i}) \text{ vs. } t$	$\frac{t}{q_{t,i}} \text{ vs. } t$	$q_{t,i} \text{ vs. } t^{1/2}$
Plot parameters for linear form	$k_{1,i} = -m$ $q_{eq,i} = \exp(b)$	$q_{eq,i} = m^{-1}$ $k_{2,i} = m^2/b$	$k_{d,i} = m$ $C_{d,i} = b$

m = slope; b = intercept; $q_{t,i}$ = adsorption capacity at time t (mg/g); $k_{1,i}$ = rate constant of PFO model (min^{-1}); $k_{2,i}$ = rate constant of PSO model ($\text{mg} \cdot \text{g}^{-1} \cdot \text{min}^{-1}$); $k_{d,i}$ = rate constant of IPD model ($\text{mg} \cdot \text{g}^{-1} \cdot \text{min}^{-1/2}$); $C_{d,i}$ = constant of IPD model (mg/g); i = stilbene compound.

SUPPLEMENTARY FIGURES

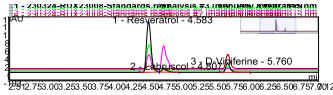


Figure S1: Overlay of the chromatograms of the standard solutions at 315 nm. δ -viniferin, labruscol, leachianol and resveratrol were mixed at different concentration to perform calibration curves

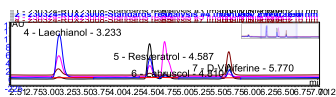


Figure S2: Overlay of the chromatograms of the standard solutions at 210 nm

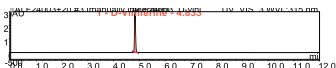


Figure S3: Chromatogram of in-house synthesized and purified δ -viniferin at 315 nm

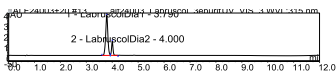


Figure S4: Chromatogram of in-house synthesized and purified labruscol (cis and trans diastereomers) at 315 nm

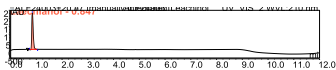


Figure S5: Chromatogram of in-house synthesized and purified leachianol at 210 nm

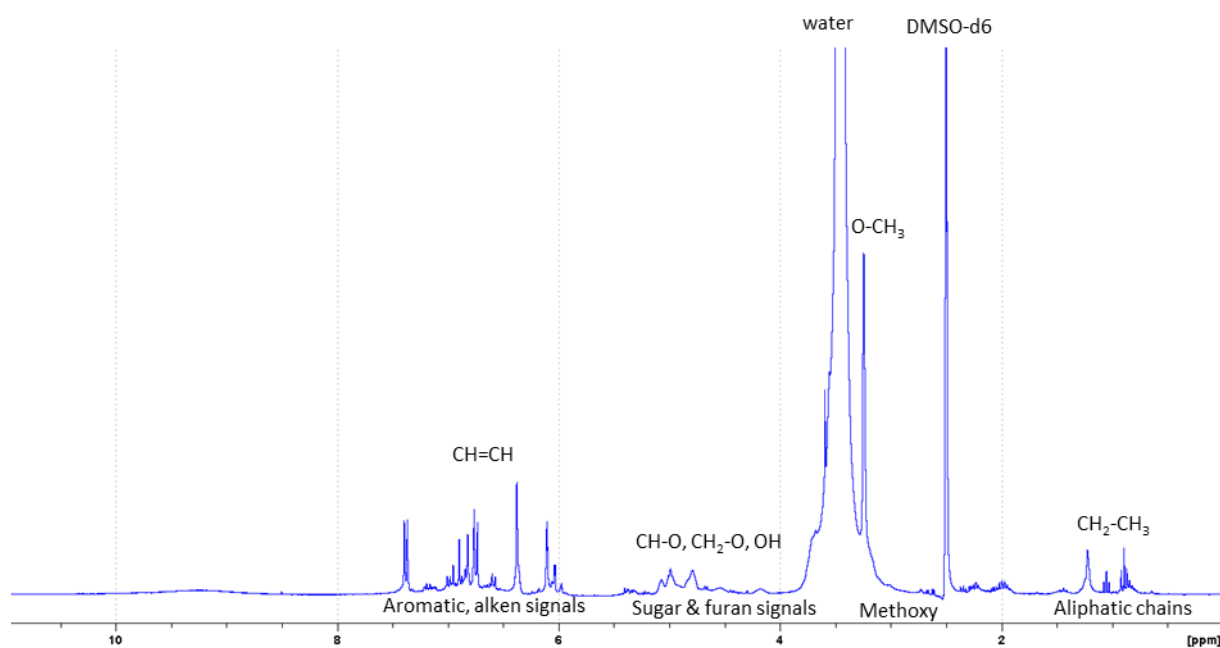


Figure S 6 : ^1H NMR spectrum of the extract concentrated in stilbens

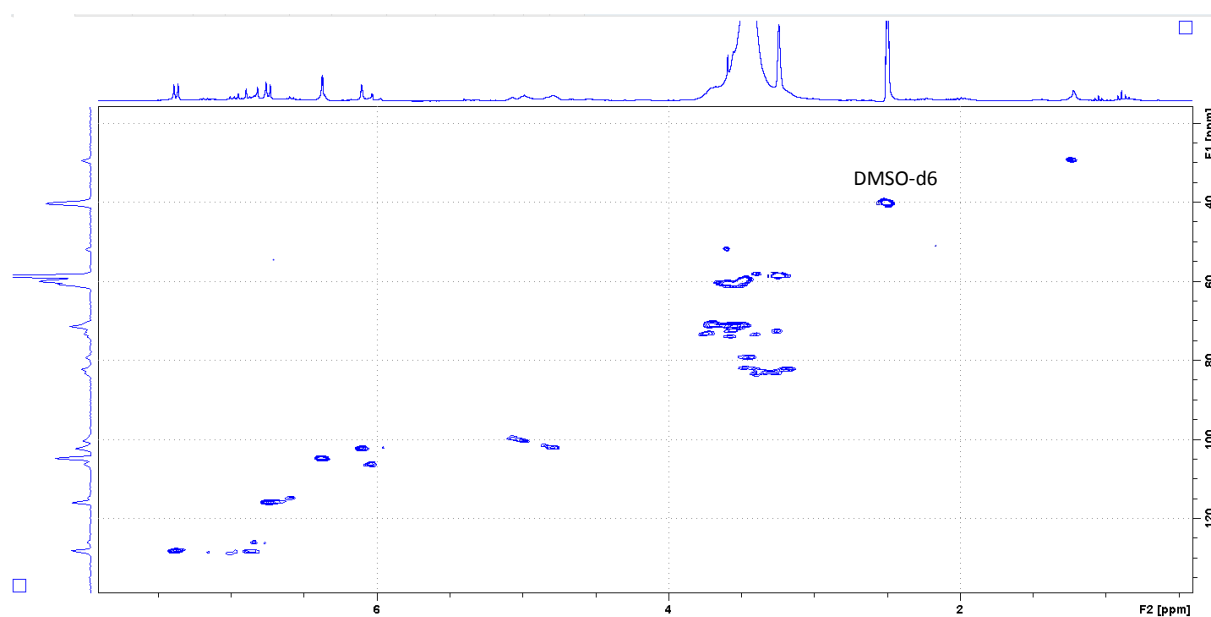


Figure S7: HSQC spectrum of the extract concentrated in stilbens

Few fatty chains are registered in NMR with signals between 0.5 and 1.5 ppm correlated with carbon below 30 ppm. The singlet at 3.24 ppm that correlated at 56.0 ppm is typical from methoxy group on aromatic ring, thus could be attributed to pterostilbene but more probably to lignin derived products such hydroxycinnamic acids and/or lignans. Under the peak of water, the HSQC reveals numerous correlations with peaks between 50-85 ppm. In addition of peaks from labruscol coupling and benzofuran rings of δ - and ϵ -viniferin, these signals are with high probability link to sugar moieties. Indeed, this assumption is reinforced by the correlated signals around 5 ppm and 100 ppm typical of anomeric peaks. Upper that 6 and 100 ppm, the peaks are characteristics of aromatic signals and fully consistent with an extract rich in stilbens.

References

- [1] E.D. Revellame, D.L. Fortela, W. Sharp, R. Hernandez, M.E. Zappi, Adsorption kinetic modeling using pseudo-first order and pseudo-second order rate laws: A review, *Clean. Eng. Technol.* 1 (2020) 100032. <https://doi.org/10.1016/j.clet.2020.100032>.
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