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PROGRAMA CIENTÍFICO

10 nov (segunda-feira/lunes)

	Auditório	Sala I	Sala II	Sala III
09:00				
09:15				
09:30	**Registo**			
09:45				
10:00				
10:15				
10:30	**Abertura/Sesión de apertura**			
10:45				
11:00	**PL1 - Nicola Armaroli** (Auditório)			
11:15				
11:30				
11:45				
12:00	QS1	QP1	QF1	S1
12:15	QS2	QP2	QF2	S2
12:30	QS3	QP3	QF3	S3
12:45	QS4	QP4	QF4	S4
13:00	**Almoço/Comida**			
13:15				
13:30				
13:45				
14:00				
14:15				
14:30	QS5	NN1	BB1	S5
14:45	QS6	NN2	BB2	S6
15:00	QS7	NN3	BB3	S7
15:15	QS8	NN4	BB4	S8
15:30	QS9	NN5	BB5	S9
15:45	QS10	NN6	BB6	S10
16:00	QS11	NN7	BB7	S11
16:15	QS12	NN8	BB8	S12
16:30	**Coffee-Break + Posters**			
16:45				
17:00				
17:15				
17:30	QS13	NN9	ED1	S13
17:45	QS14	NN10	ED2	S14
18:00	QS15	NN11	ED3	S15
18:15	QS16	NN12	ED4	S16
18:30	QS17	NN13	ED5	S17

11 nov (terça-feira/martes)

	Auditório	Sala I	Sala II	Sala III
09:00	QS18	QSU1	QAM1	QAA1
09:15	QS19	QSU2	QAM2	QAA2
09:30	QS20	QSU3	QAM3	QAA3
09:45	QS21	QSU4	QAM4	QAA4
10:00	**PL2 - Pastora Bello Bugallo** (Auditório)			
10:15				
10:30				
10:45				
11:00	**Coffee-Break + Posters**			
11:15				
11:30	QS22	QSU5	QAM5	QAA5
11:45	QS23	QSU6	QAM6	QAA6
12:00	QS24	QSU7	QAM7	QAA7
12:15	QS25	QSU8	QAM8	QAA8
12:30	QS26	QSU9	QAM9	QAA9
12:45	QS27	QSU10	QAM10	QAA10
13:00	**Almoço/Comida**			
13:15				
13:30				
13:45				
14:00				
14:15				
14:30	QS28	QSU11	QAM11	QAA11
14:45	QS29	QSU12	QAM12	QAA12
15:00	QS30	QSU13	QAM13	QAA13
15:15	QS31	QSU14	QAM14	QAA14
15:30	**PL3 - Nuno Mateus** (Auditório)			
15:45				
16:00				
16:15				
16:30	**Coffee-Break + Posters**			
16:45				
17:00				
17:15				
17:30	QS32	QSU15	QAM15	QAA15
17:45	ED6	QSU16	QAM16	QAA16
18:00	ED7	QSU17	QAM17	QAA17
18:15	QT1	QSU18	QAM18	QAA18
20:30	Banquete/Cena de Gala			

12 nov (quarta-feira/miércoles)

	Auditório	Sala I	Sala II	Sala III
09:00	QIE1	QSU19	QI1	QA1
09:15	QIE2	QSU20	QI2	QA2
09:30	QIE3	QSU21	QI3	QA3
09:45	QIE4	QSU22	QI4	QA4
10:00	**PL4 - Antonio Echavarren** (Auditório)			
10:15				
10:30				
10:45				
11:00	**Coffee-Break + Posters**			
11:15				
11:30	QO1	QSU23	QI5	QA5
11:45	QO2	QSU24	QI6	QA6
12:00	QO3	QAM19	QAA19	QA7
12:15	QO4	QAM20	QAA20	QA8
12:30	QO5	QAM21	QAA21	QA9
12:45	QO6	QAM22	NN14	QA10
13:00	**Almoço/Comida**			
13:15				
13:30				
13:45				
14:00				
14:15				
14:30	QO7	CAT1	QIE5	QA11
14:45	QO8	CAT2	QIE6	QA12
15:00	QO9	CAT3	QIE7	QA13
15:15	QO10	CAT4	QIE8	QA14
15:30	QO11	CAT5	QIE9	QA15
15:45		QV1	QA17	QA16
16:00	**PL5 - Verónica Bermudez** (Auditório)			
16:15				
16:30				
16:45				
17:00	**Encerramento/Clausura**			
17:15				

BB - Bioquímica e Biotecnologia
CAT - Catálise e Fotocatálise
ED - Educação e Ensino da Química
NN - Nanoquímica e Nanotecnologia
QA - Química Analítica
QAA - Química Agro-Mar-Alimentar
QAM - Química e Ambiente
QF – Química Física
QI - Química Inorgânica
QIE - Química Industrial e Engenharia
QO - Química Orgânica
QP - Química dos Polímeros
QS - Química e Saúde
QSU - Química Sustentável
QT - Química Teórica e Modelação Molecular
QV - Química Verde
S – Simpósio

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Sertraline removal by green-based activated carbons

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Sertraline, an antidepressant, has been detected in Portuguese wastewater treatment plant influents at ng L^{-1} level concentrations [1]. This pharmaceutical compound, commonly prescribed for the treatment of depressive disorders, is characterized by its persistence and limited removal efficiency in conventional treatment processes, constituting a potential environmental hazard as these trace concentrations adversely affect aquatic organisms like bivalves such as *Dreissena rostriformis* [2].

The application of activated carbons is a promising technique for removing sertraline and other emerging pollutants. This study investigates sertraline removal (initial concentration of 3 ppm) using activated carbon derived from olive pits, a lignin-rich and underexploited biomass. The residual sertraline was quantified by HPLC using a mobile phase of 60% acetonitrile and 40% water with 0.01% TFA. A preliminary study compared two carbons produced via chemical activation ($ZnCl_2$ and H_3PO_4) followed by carbonization at 500°C for 1.5 hours, and a char produced by simple carbonization at 800°C for 1 hour without chemical agents. The material produced by simple carbonization was the most effective, achieving 89% sertraline removal within 3 hours.

The influence of pH on adsorption was tested at pH levels 3, 5, 7, 9 and 11, with removal efficiency increasing from 67% to 95%, respectively. The results suggest that non-electrostatic mechanisms, such as π-π stacking and hydrophobic interactions, are dominant [3]. These interactions are enhanced as sertraline (pKa=9.16) becomes more neutral at higher pH values, proving more significant than the electrostatic attraction present when the carbon surface is anionic (pH_{PZC}≈7).

Kinetic assays performed at pH 7 and 11 showed no statistically significant difference, according to an ANOVA test. This is an advantage for wastewater treatment plants, which could apply the process at the pH commonly found in residual waters. The pseudo-second order model best described the adsorption kinetics at pH 7, and the Elovich model at pH 11, these systems are usually used as an indicative of chemisorption processes [3]. Table 1 presents the model applied to each experimental data, the equation of the kinetic models and the values adopted for the constants after the fitting process. The equation symbols have the respective meanings: qt the amount of adsorbate adsorbed by the adsorbent (mg/g); qe the amount of adsorbate adsorbed by the adsorbent at equilibrium (mg/g); k_2 the pseudo-second order rate constant (g/(mg.min)); t the contact time (min); β the desorption constant (mg/g); α initial adsorption rate (mg/(g.min)) [3].

Table 1: Kinetic non-linear fittings for experimental data at pH 7 and 11

Model	Equation	pH	Constants	R^2
Elovich	$q_t = \frac{1}{\beta} ln(1 + \alpha\beta t)$	11	α = 9.7619 ± 3.86 β = 1.1688 ± 0.0839	0.89
Pseudo-second order	$q_t = \frac{q_e^2 k_2 t}{q_2 q_e t + 1}$	7	qe = 6.67 ± 0.25 k_2= 0.01929 ± 0.0046	0.97

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