

Electron Spin Resonance spectroscopy suitability for investigating the oxidative stability of non-alcoholic beers

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Supplementary material

Table S1. EC₅₀ values obtained with a sigmoidal fitting (4 parameters) from a graph representing the % of inhibition as a function of log beer concentration expressed as mL beer/mg DPPH.

Beer	EC ₅₀ (mL beer/mg DPPH)	95% CI	R ²
N	1.187	0.972-1.404	0.9690
W	1.656	1.428-1.888	0.9719
B	1.741	1.565-1.920	0.9827
P	0.924	0.827-1.023	0.9835
M	3.164	2.725-3.807	0.9478
C	2.926	2.491-3.455	0.9316
H	1.865	1.694-2.045	0.9790
NO	1.797	1.564-2.034	0.9711
WO	1.609	1.444-1.796	0.9667
BO	2.223	2.054-2.394	0.9839
PO	2.474	2.029-2.962	0.9531
MO	1.802	1.640-1.969	0.9825
CO	2.677	2.300-3.107	0.9422
HO	1.099	0.944-1.253	0.9793

Table S2. EC₅₀ values obtained with a straight-line fitting from a graph representing the % of inhibition as a function of log beer concentration expressed as mL beer/mg DPPH.

Beer	EC ₅₀ (mL beer/mg DPPH)	95% CI	R ²
N	1.285	1.204-1.362	0.9941
W	1.697	1.586-1.807	0.9899
B	1.765	1.638-1.888	0.9865
P	0.896	0.805-0.988	0.9838
M	3.613	3.232-∞	0.9816
C	2.837	2.291-3.667	0.8577
H	1.869	1.703-2.037	0.9699
NO	1.807	1.613-1.994	0.9698
WO	1.607	1.449-1.784	0.9590
BO	2.206	2.041-2.374	0.9755
PO	2.392	1.968-2.903	0.9391
MO	1.814	1.671-1.957	0.9777
CO	2.619	2.231-3.106	0.9172
HO	1.173	1.115-1.228	0.9958

The values reported in Table S2 were used to calculate the β_0 - β_4 values reported in equation 1 and in the graph in Figure 7.

Table S3. EC₅₀ values obtained with a second order polynomial fitting from a graph representing the % of inhibition as a function of beer concentration expressed as mL beer/mg DPPH.

Beer	EC ₅₀ (mL beer/mg DPPH)	95% CI	R ²
N	1.343	1.236-1.458	0.9943
W	1.777	1.584-1.991	0.9882
B	1.953	1.831-2.085	0.9937
P	1.055	0.978-1.133	0.9922
M	3.306	3.004-3.611	0.9803
C	3.145	2.746-3.522	0.9611
H	2.028	1.841-2.237	0.9829
NO	2.028	1.875-2.194	0.9912
WO	1.724	1.550-1.929	0.9798
BO	2.323	2.172-2.483	0.9908
PO	2.787	2.468-3.110	0.9879
MO	1.911	1.767-2.064	0.9913
CO	2.952	2.675-3.224	0.9823
HO	1.230	1.206-1.254	0.9996

Table S4. Pearson correlation coefficients between parameters calculated for lagers and NABs.

Lagers	EtOH	AUC	I ₁₅₀	TPC	EC ₅₀	TBI	DTE	pH	RDS
EtOH	1	0.44	0.44	0.39	-0.87	-0.02	-0.16	0.50	-0.16
AUC	0.44	1	0.96	0.52	-0.57	0.30	-0.50	0.62	0.36
I ₁₅₀	0.44	0.96	1	0.52	-0.59	0.45	-0.48	0.51	0.42
TPC	0.39	0.52	0.52	1	-0.69	0.46	-0.74	0.70	0.71
EC ₅₀	-0.87	-0.57	-0.59	-0.69	1	-0.12	0.25	-0.53	-0.22
TBI	-0.02	0.30	0.45	0.46	-0.12	1	-0.72	0.37	0.78
DTE	-0.16	-0.50	-0.48	-0.74	0.25	-0.72	1	-0.81	-0.68
pH	0.50	0.62	0.51	0.70	-0.53	0.37	-0.81	1	0.47
RDS	-0.16	0.36	0.42	0.71	-0.22	0.78	-0.68	0.47	1

NABs	EtOH	AUC	I ₁₅₀	TPC	EC ₅₀	TBI	DTE	pH	RDS
EtOH	1	-0.92	-0.76	-0.56	0.14	-0.61	0.42	-0.47	0.32
AUC	-0.92	1	0.87	0.54	-0.15	0.52	-0.22	0.60	-0.15
I ₁₅₀	-0.76	0.87	1	0.69	-0.03	0.73	0.06	0.42	-0.02
TPC	-0.56	0.54	0.69	1	-0.57	0.40	-0.16	0.42	0.27
EC ₅₀	0.14	-0.15	-0.03	-0.57	1	0.45	0.13	-0.38	-0.44
TBI	-0.61	0.52	0.73	0.40	0.45	1	-0.04	0.08	-0.20
DTE	0.42	-0.22	0.06	-0.16	0.13	-0.04	1	-0.58	0.03
pH	-0.47	0.60	0.42	0.42	-0.38	0.08	-0.58	1	0.52
RDS	0.32	-0.15	-0.02	0.27	-0.44	-0.20	0.03	0.52	1

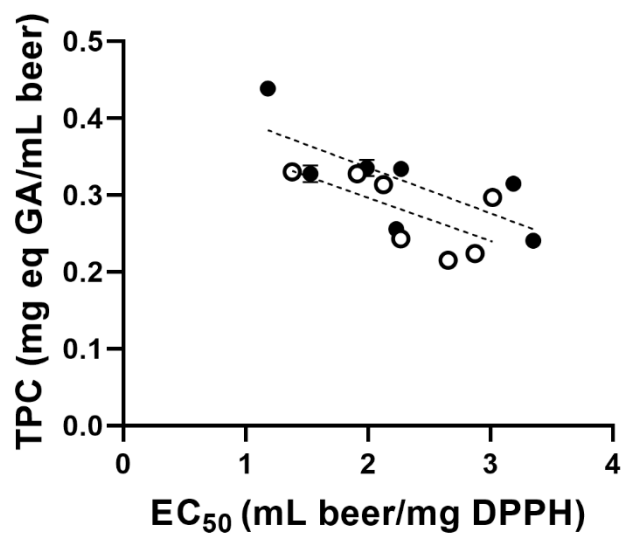


Figure S1. Comparison between the TPC and the EC_{50} values obtained with the DPPH assay. For the alcoholic beers (filled circles) the R^2 value is 0.5394, while for the non-alcoholic beers (empty circles) R^2 is 0.4228.

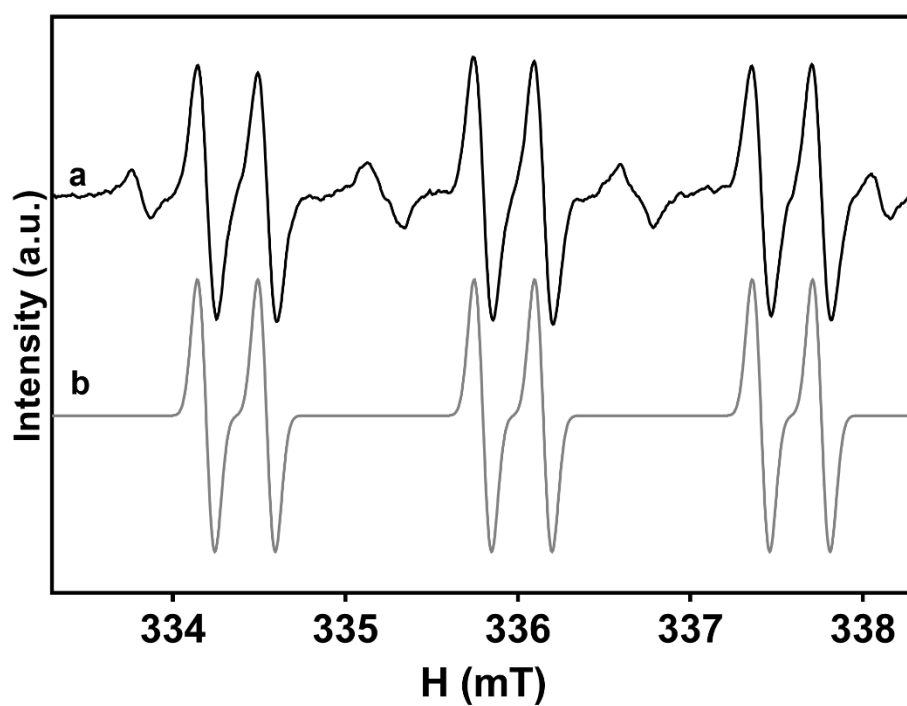


Figure S2. Experimental (a) and simulated (b) spectra of the PBN-1-hydroxyethyl radical adduct detected after 150 mins of thermal treatment at 60 °C of the B beer sample.

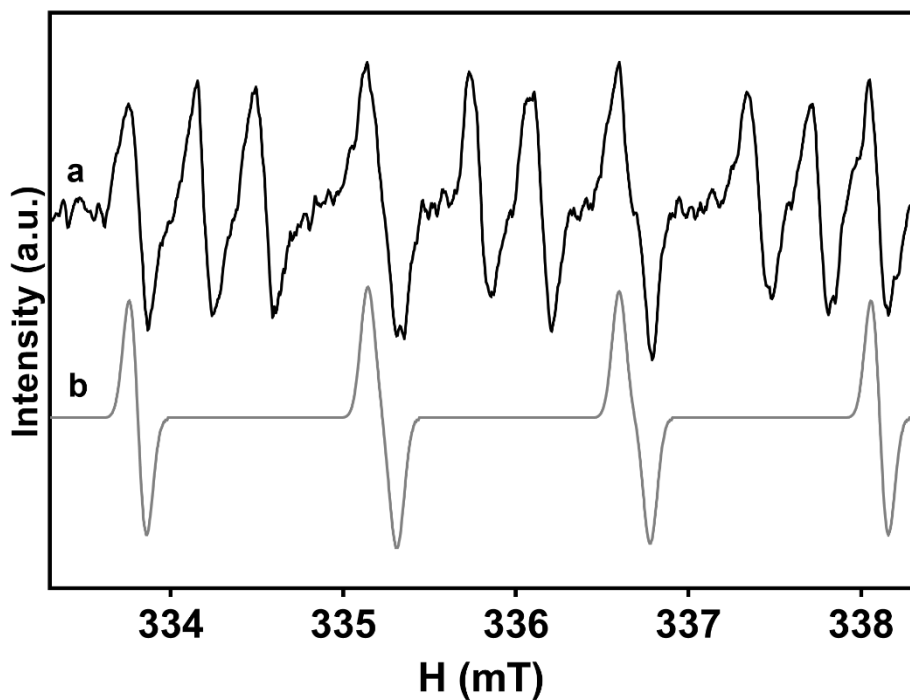


Figure S3. Experimental (a) and simulated (b) spectra of the *tert*-butyl aminoxyl radical detected after 150 mins of thermal treatment at 60 °C of the B0 beer sample.

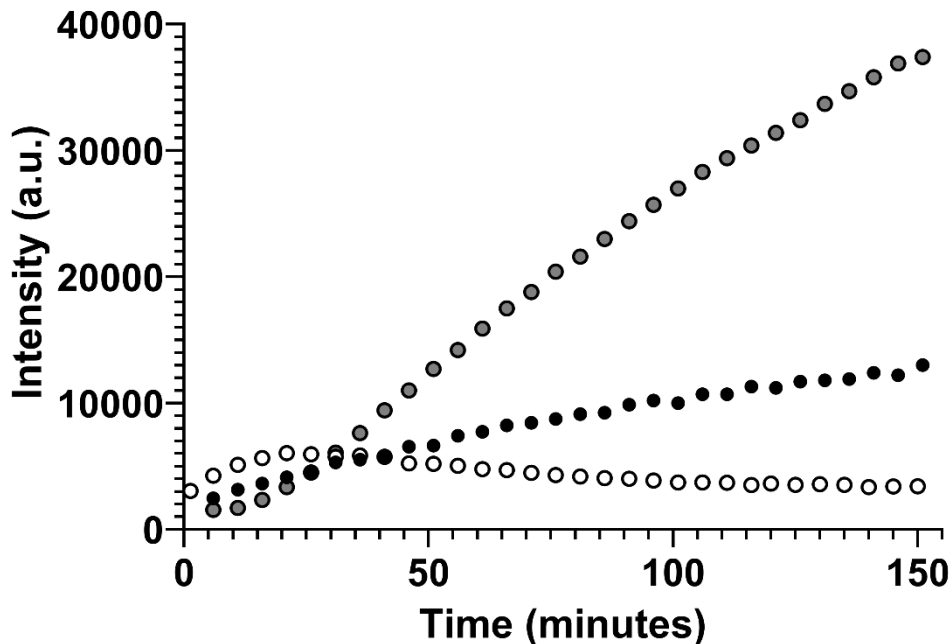


Figure S4. Kinetic curves of the intensity of the PBN-1-hydroxyethyl radical adduct as a function of time for the alcoholic H beer (black filled circles), for the NAB H0 (empty circles), and for the H0 beer added with EtOH to reach the same % of H, all subjected to thermal treatment at 60 °C.

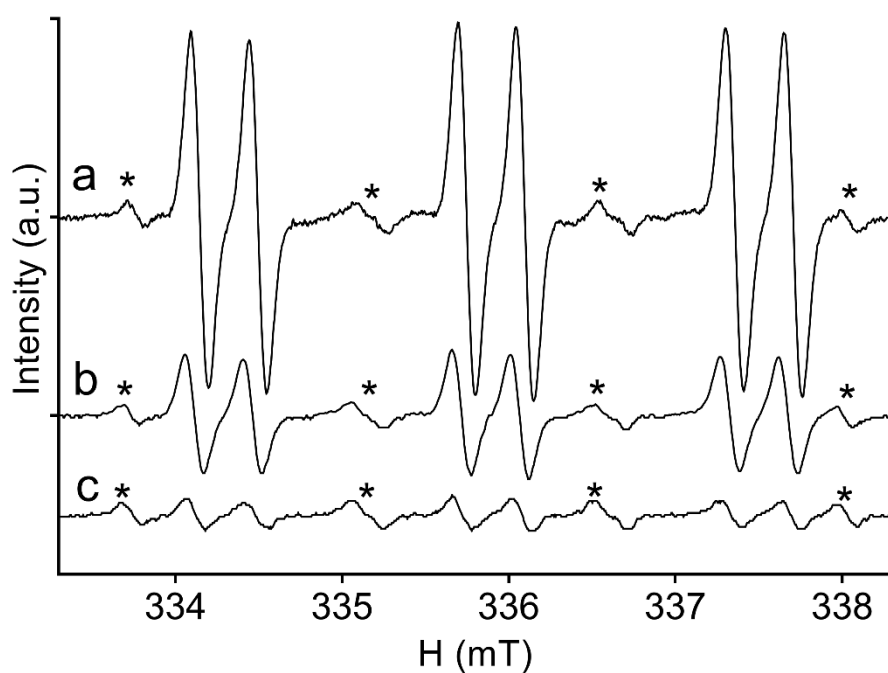


Figure S5. Experimental ESR spectra recorder after 150 min for: a) the H0 beer added with EtOH to reach the same % of H; b) the alcoholic H beer; and c) the NAB H0, all subjected to thermal treatment at 60 °C. The intensity of the signals indicated by the asterisk (*tert*-butyl aminoxy radical) is comparable in the three spectra.

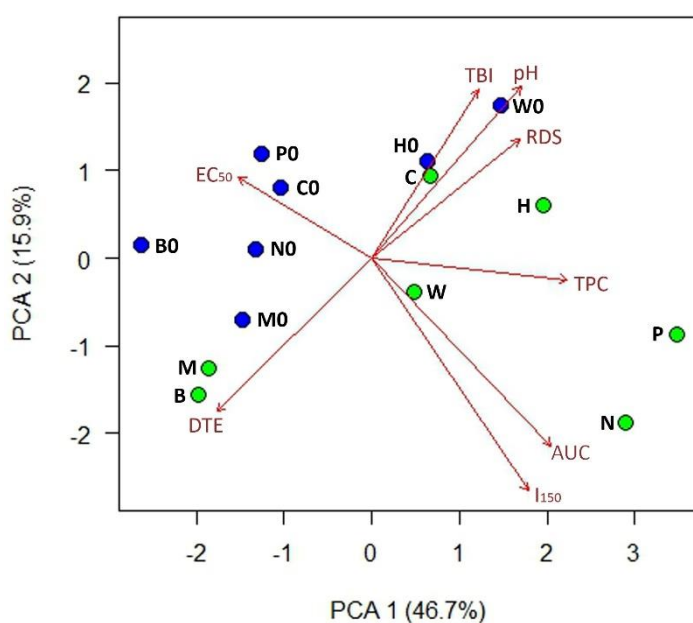


Figure S6. Principal component analysis applied to all the beers studied in this work. Lagers are indicated by green circles, NABs by blue circles. All the variables are considered except EtOH concentration.