

Supplementary Materials

***Thymus satureoides* Oil as Green Corrosion Inhibitor for 316L Stainless Steel in 3% NaCl: Experimental and Theoretical Studies**

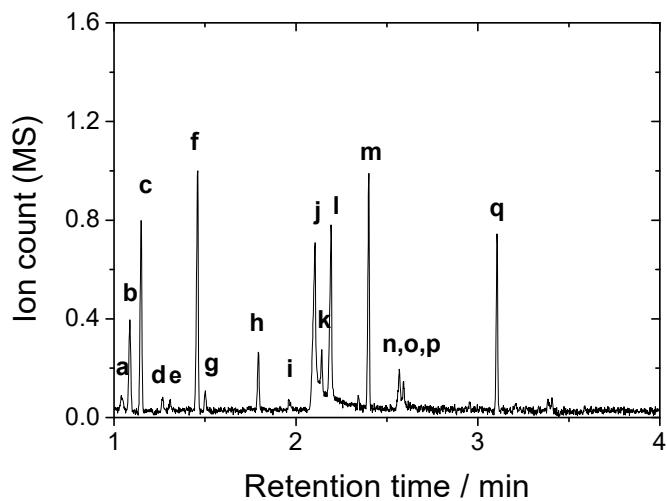


Figure S1. Chromatogram of the *Thymus satureoides* essential oil. Constituents **a,q** are given in SM Table S1.

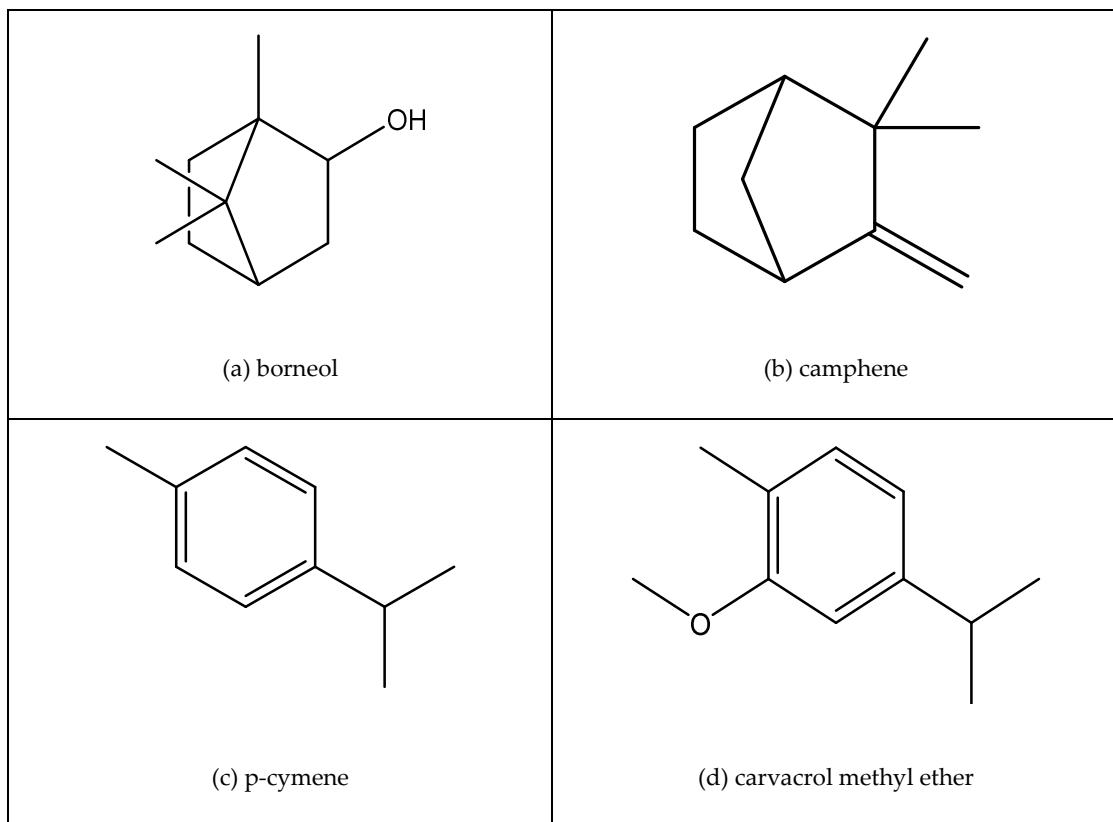


Figure S2. Chemical structure of majority compounds: **a** borneol, **b** camphene, **c** p-cymene and **d** carvacrol methyl ether.

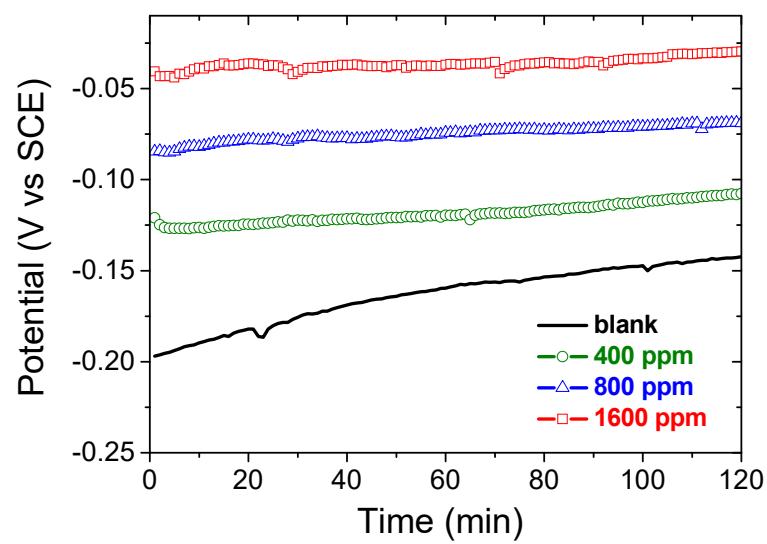
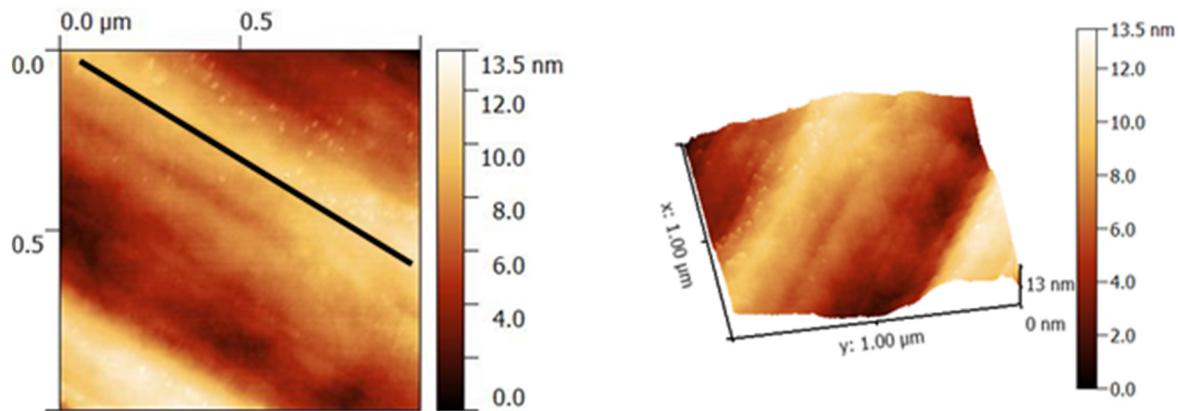
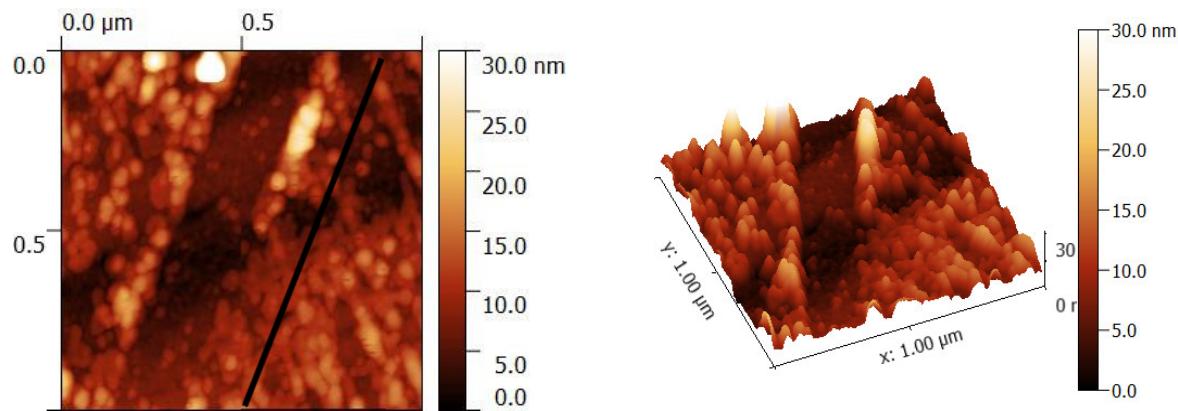


Figure S3. Potential follow-up in open circuit of the stainless steel immersed in 3% NaCl solution without and with the inhibitor.



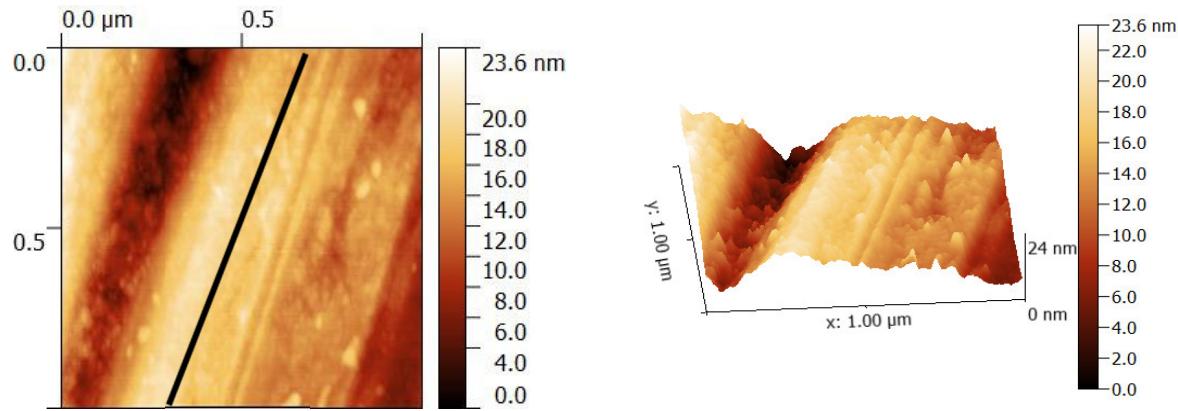
(a)

(a')



(b)

(b')



(c)

(c')

Figure S4. 2D and 3D atomic force micrographs of 316L stainless steel: (a-a') before immersion (polished), (b-b') after immersion in 3% NaCl and (c-c') after immersion in 3% NaCl+1600 ppm during 24 h.

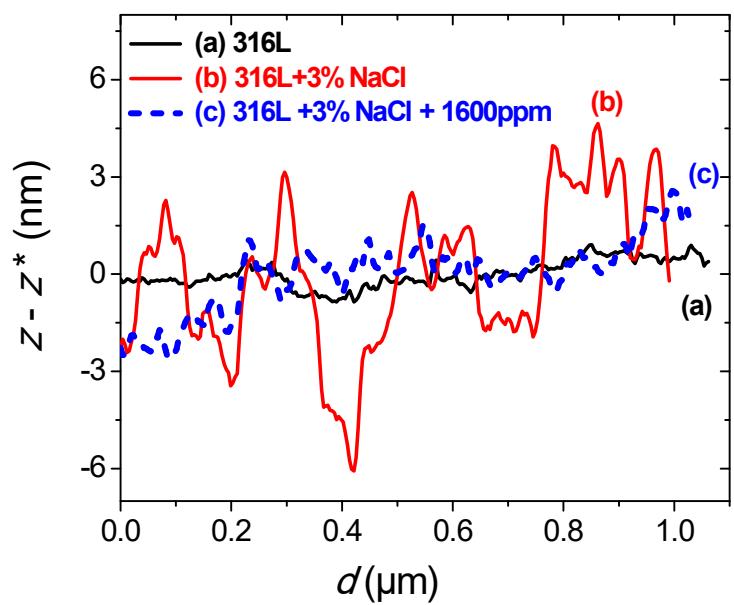
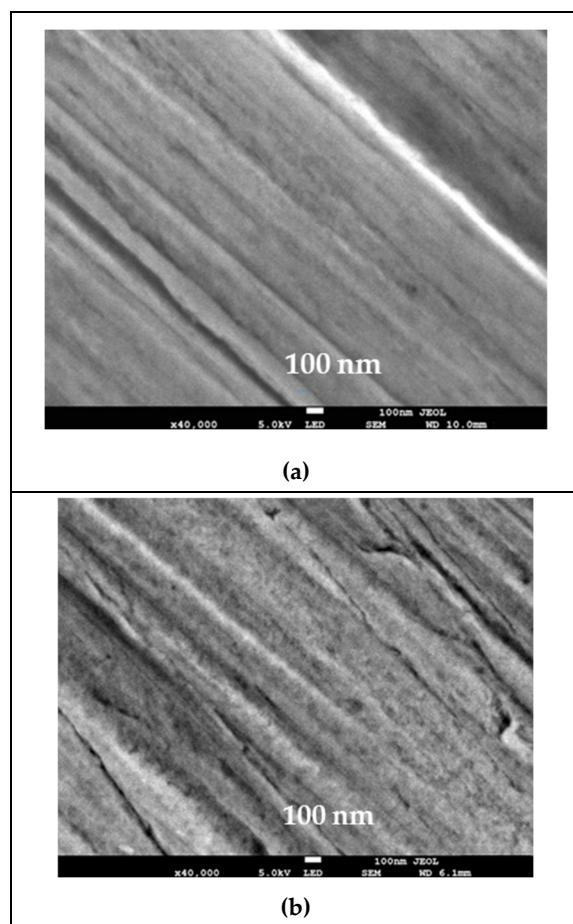


Figure S5. Calculated roughness ($z - z^*$) factor for 316L stainless steel: (a) before immersion (polished), (b) after immersion in 3% NaCl and c after immersion in 3% NaCl+1600 ppm inhibitor during 24 h.



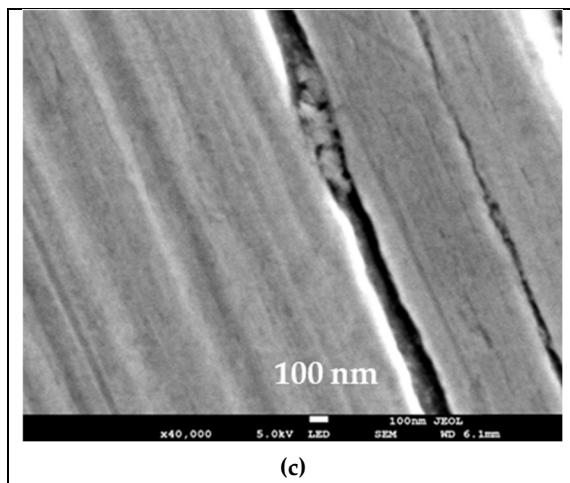


Figure S6. SEM image of 316L stainless steel: **a** before immersion (polished), **b** after immersion in 3% NaCl and **c** after immersion in 3% NaCl+1600 ppm inhibitor during 24 h.

Table S1. Main constituents of the *Thymus satureoides* essential oil.

	Compound	% FID	
a	α-thujene	1%	
b	α-pinene	7%	
c	camphene	12%	
d	α-pinene	1%	
e	myrcene	1%	
f	p-cymene	12%	
g	limonene	1%	
h	α-terpinene	5%	
i	borneol	13%	
j	unknown terpene	5%	m/z: 119-121-136-134-93-91-77
k	unknown terpene	15%	m/z: 68-67-93-91-121-136-107-132
l	thymol methyl ether	1%	
m	carvacrol methyl ether	10%	
n	thymol	3%	
o	carvacrol	1%	
p	isobornyl acetate	1%	
q	caryophyllene	9%	

Table S2. Electrochemical parameters (corrosion potential (E_{corr}), corrosion current density (i_{corr}), passivation current density (i_{pass}), pitting corrosion (E_{pit})) of 316L in 3% NaCl without inhibitor at different temperatures.

Temperature (°C)	E_{corr} (V vs SCE)	I_{corr} ($\mu A/cm^2$)	I_{pass} ($\mu A/cm^2$)	E_{pit} (V vs SCE)
25	- 0.383	3.38	7.74	0.290
40	- 0.386	6.38	23.33	0.134
60	- 0.407	10.89	32.21	0.077
80	- 0.420	13.59	68.23	0.019

Table S3. Electrochemical parameters (corrosion potential (E_{corr}), corrosion current density (i_{corr}), passivation current density (i_{pass}), pitting corrosion (E_{pit})) of 316L stainless steel in 3% NaCl with 1600 ppm inhibitor at different temperatures.

Tempera- ture (°C)	E_{corr} (V vs SCE)	i_{corr} ($\mu A/cm^2$)	i_{pass} ($\mu A/cm^2$)	E_{pit} (V vs SCE)	EI (%)
25	-0.287	0.62	5.55	0.380	82
40	-0.292	2.06	20.09	0.227	68
60	-0.364	4.31	21.52	0.099	60
80	-0.369	5.53	36.14	0.027	60

Table S4. The activation parameters values (activation enthalpy (ΔH^*), activation entropy (ΔS^*) and activation free energy (ΔG^*)) of 316L stainless steel in 3% NaCl without and with 1600 ppm of the Thymus satureoides oil.

Inhibitor	ΔH^* (kJ/mol)	ΔS^* (J/mol.K)	ΔG^* (kJ/mol)
Blank	19.6	-168.6	69.8
1600 ppm	31.7	-140.6	73.6

Table S5. Energies of the HOMO (Highest Occupied Molecular Orbital) and the LUMO (Lowest Unoccupied Molecular Orbital) of the two oxygenated compounds in water with one H₂O molecule. ΔE is the energy gap HOMO-LUMO.

Molecule / Functional	E_{HOMO} (eV)	E_{LUMO} (eV)	ΔE (eV)
Borneol			
B3LYP	-7.57	-0.38	7.19
BMK	-8.55	0.37	8.92
M062X	-9.15	-0.09	9.06
Carvacrol methyl ether			
B3LYP	-6.25	-0.42	5.83
BMK	-7.02	0.35	7.37
M062X	-7.58	-0.14	7.44

Table S6. B3LYP dipole moment (in Debye) for the four majority compounds in gaseous phase.

Molecule	B3LYP	BMK	M062X
Borneol	1.49	1.50	1.49
Camphene	0.66	0.66	0.65
Carvacrol methyl ether	1.40	1.43	1.39
p-cymene	0.05	0.05	(0.04)*

*We have not obtained a geometry corresponding to a strict energy minimum. It remains one small imaginary frequency which we have not been able to remove.