

Correction

Correction to: “Experimental, DFT and QSAR models for the discovery of new pyrazines corrosion inhibitors for steel in oilfield acidizing environment” [Int. J. Electrochem. Sci., 15 (2020) 9066 – 9080; doi: 10.20964/2020.09.72]

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The authors regret that there were errors in the original published version.

Tables 3-7 were missing in the original published version. They are provided below:

Table 3. Linear regression model of the various descriptors.

Parameters	Coefficient	t-value	p-value	F-value	Significance
Energy (au)	0.00	0.03	0.98	0.00	no
E _{HOMO} (eV)	-16.72	-1.26	0.25	1.59	no
E _{LUMO} (eV)	-35.60	-3.35	0.02	11.19	yes
ΔE (eV)	-14.82	-0.75	0.48	0.56	no
η	-29.63	-0.75	0.48	0.56	no
s	349.42	0.69	0.52	0.48	no
μ	-28.79	-2.19	0.07	4.79	no
χ	28.79	2.19	0.07	4.79	no
ω	20.88	3.06	0.02	9.39	yes
ΔN	-123.12	-1.82	0.12	3.33	no
Dipole Moment (D)	8.69	4.07	0.01	16.54	yes
LogP	-10.42	-2.47	0.05	6.09	no
Polarizability	-3.83	-1.37	0.22	1.89	no
Molecular Volume (Å ³)	-0.31	-1.40	0.21	1.96	no
Molecular Area (Å ²)	-0.29	-1.35	0.22	1.83	no

Table 4. Multiple Linear regression model using two descriptors

Parameters	Coefficient	t-value	p-value	F-value	R squared	R squared Adjusted	Significance
Dipole Moment	8.69	3.71	0.01	6.89	0.73	0.63	no
Energy (au)	0.00	0.00	1.00				
Dipole Moment	8.03	3.51	0.02	8.46	0.77	0.68	no
E _{HOMO} (eV)	-7.52	-0.91	0.40				
Dipole Moment	5.97	3.19	0.02	19.26	0.89	0.84	yes
E _{LUMO} (eV)	-20.86	-2.57	0.05				
Dipole Moment	8.45	3.61	0.02	7.37	0.75	0.65	no
ΔE (eV)	-5.89	-0.50	0.64				
Dipole Moment	8.45	3.61	0.02	7.37	0.75	0.65	no
η	-11.79	-0.50	0.64				
Dipole Moment	8.48	3.64	0.01	7.36	0.75	0.65	no
s	148.03	0.50	0.64				
Dipole Moment	7.08	3.29	0.02	11.75	0.82	0.75	no
μ	-14.72	-1.61	0.17				
Dipole Moment	7.08	3.29	0.02	11.75	0.82	0.75	no
χ	14.72	1.61	0.17				
Dipole Moment	6.22	3.21	0.02	17.09	0.87	0.82	no
ω	11.90	2.33	0.07				
Dipole Moment	7.47	3.35	0.02	10.09	0.80	0.72	no
ΔN	-59.14	-1.31	0.25				
Dipole Moment	6.78	3.11	0.03	12.26	0.83	0.76	no
LogP	-5.34	-1.69	0.15				
Dipole Moment	8.00	4.22	0.01	12.50	0.83	0.77	no
Polarizability	-2.53	-1.73	0.14				
Dipole Moment	7.98	4.22	0.01	12.60	0.83	0.77	no
M V (Å ³)	-0.20	-1.74	0.14				
Dipole Moment	8.02	4.19	0.01	12.24	0.83	0.76	no
M Area (Å ²)	-0.19	-1.69	0.15				

Table 5. Multiple Linear regression model using three descriptors

Parameters	Coefficient	t-value	p-value	F-value	R squared	R squared Adjusted	Significance
Dipole Moment	5.81	2.85	0.05	11.16	0.89	0.81	no
ELUMO	-20.57	-2.34	0.08				
ΔE	-4.71	-0.55	0.61				
Dipole Moment	5.81	2.85	0.05	11.16	0.89	0.81	no
ELUMO	-20.57	-2.34	0.08				
η	-9.42	-0.55	0.61				
Dipole Moment	5.81	2.87	0.05	11.31	0.89	0.82	no
ELUMO	-20.65	-2.37	0.08				
s	127.74	0.60	0.58				
Dipole Moment	5.81	2.85	0.05	11.16	0.89	0.81	no
ELUMO	-29.99	-1.60	0.18				
μ	9.42	0.55	0.61				
Dipole Moment	5.81	2.85	0.05	11.16	0.89	0.81	no
ELUMO	-29.99	-1.60	0.18				
χ	-9.42	-0.55	0.61				
Dipole Moment	5.61	2.83	0.05	12.22	0.90	0.83	no
ELUMO	-82.49	-1.09	0.34				
ω	-36.97	-0.82	0.46				
Dipole Moment	5.80	2.87	0.05	11.35	0.89	0.82	no
ELUMO	-28.34	-1.89	0.13				
ΔN	38.86	0.61	0.57				
Dipole Moment	5.90	2.82	0.05	10.47	0.89	0.80	no
ELUMO	-18.40	-1.41	0.23				
LogP	-1.09	-0.26	0.81				
Dipole Moment	6.19	3.19	0.03	12.35	0.90	0.83	no
ELUMO	-16.53	-1.69	0.17				
Polarizability	-1.24	-0.85	0.44				
Dipole Moment	6.18	3.20	0.03	12.46	0.90	0.83	yes
ELUMO	-16.46	-1.69	0.17				
Molecular Vol	-0.10	-0.87	0.43				
Dipole Moment	6.18	3.19	0.03	12.38	0.90	0.83	no
ELUMO	-16.70	-1.73	0.16				
Molecular Area	-0.09	-0.85	0.44				
Dipole Moment	5.93	2.86	0.05	10.54	0.89	0.80	no
ELUMO	-21.21	-2.34	0.08				
Energy	0.00	-0.30	0.78				

Table 6. Experimental and predicted corrosion inhibition efficiencies of the pyrazine molecules.

Molecule	Experimental %IE	Predicted %IE	Standard Deviation
A	22.63	24.51	1.33
B	32.22	38.64	4.54
C	48.08	51.33	2.30
D	42.11	39.15	2.09
E	64.72	65.27	0.39
F	55.24	52.72	1.78
G	43.62	35.12	6.01
H	24.35	26.14	1.27

Table 7. Quantum Chemical Descriptors for Pyrazine Test Set with predicted inhibition efficiencies

Parameters	TEST A	TEST B	TEST C	TEST D
Energy (au)	-756.01	-492.23	-395.90	-547.59
E_{HOMO} (eV)	-6.15	-7.19	-6.25	-5.86
E_{LUMO} (eV)	-2.22	-1.79	-1.35	-1.86
$(\Delta E = E_{\text{HOMO}} - E_{\text{LUMO}})$ (eV)	3.93	5.40	4.90	4.00
Dipole Moment (D)	6.63	6.24	4.88	6.20
LogP	-0.75	-0.72	0.41	-0.45
Polarizability	50.78	50.79	50.03	52.22
Molecular Volume (\AA^3)	127.44	131.85	121.05	145.35
Molecular Area (\AA^2)	149.59	152.20	137.40	171.95
Predicted % IE	78.85	68.90	54.35	68.43