water

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Supporting Information

Comparative Study of the Oxidative Degradation of Different 4-Aminobenzene Sulfonamides in Aqueous Solution by Sulfite Activation in the Presence of Fe(0), Fe(Ii), Fe(Iii) Or Fe(Vi)

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Table S1. Experimental results obtained for SAs degradation in the system Fe(0)/sulfite. Conditions; $[Sulfonamide]_0 = 5.38 \times 10^{-5}$ M, pH 3, T = 298 K, reaction time 60 min.

Exp. Num.	Sulfonamide	$[Fe(0)]_0$ (M)	$[sulfite]_0$ (M)	% Degraded
1	SMZ	0	5E-03	0.15
2	SMZ	1.79E-02	0	0.05
3	SMZ	5.37E-04	6.25E-05	3.32
4	SMZ	5.37E-04	6.25E-04	17.29
5	SMZ	5.37E-04	3.12E-03	1.93
6	SMZ	1.79E-03	6.25E-05	10
7	SMZ	1.79E-03	2.50E-04	15.27
8	SMZ	1.79E-03	6.25E-04	21.84
9	SMZ	1.79E-03	3.12E-03	25.61
10	SMZ	1.79E-02	5E-03	56.34
11	SDZ	0	5E-03	0.02
12	SDZ	1.79E-02	0	0.18

13	SDZ	5.37E-04	6.25E-05	2.24
14	SDZ	5.37E-04	6.25E-04	21.65
15	SDZ	5.37E-04	3.12E-03	13.71
16	SDZ	1.79E-03	6.25E-05	5.37
17	SDZ	1.79E-03	2.50E-04	18.56
18	SDZ	1.79E-03	6.25E-04	41.37
19	SDZ	1.79E-03	3.12E-03	41.87
20	SDZ	1.79E-02	5E-03	59.14
21	SML	0	5E-03	0.02
22	SML	1.79E-02	0	0.12
23	SML	5.37E-04	6.25E-05	8.59
24	SML	5.37E-04	6.25E-04	21.65
25	SML	5.37E-04	3.12E-03	9.62
26	SML	1.79E-03	6.25E-05	11.83
27	SML	1.79E-03	2.50E-04	18.56
28	SML	1.79E-03	6.25E-04	42.15
29	SML	1.79E-03	3.12E-03	43.17
30	SML	1.79E-02	5E-03	62.11

Table S2. Experimental results obtained for SAs degradation in the system Fe(II)/sulfite. Conditions; $[Sulfonamide]_0 = 5.38 \times 10^{-5}$ M, pH 3, T = 298 K, reaction time 60 min.

Exp. Num.	Sulfonamide	$[Fe(II)]_0$ (M)	$[sulfite]_0$ (M)	% Degraded
31	SMZ	0	5E-03	0.0
32	SMZ	1.79E-02	0	0.96
33	SMZ	5.37E-04	6.25E-05	1.47

34	SMZ	5.37E-04	6.25E-04	18.24
35	SMZ	5.37E-04	3.12E-03	2.3
36	SMZ	1.79E-03	6.25E-05	7.29
37	SMZ	1.79E-03	6.25E-04	17.36
38	SMZ	1.79E-03	3.12E-03	23.25
39	SMZ	1.79E-02	5E-03	42.15
40	SDZ	0	5E-03	0.0
41	SDZ	1.79E-02	0	1.04
42	SDZ	5.37E-04	6.25E-05	2.65
43	SDZ	5.37E-04	6.25E-04	15.14
44	SDZ	5.37E-04	3.12E-03	4.52
45	SDZ	1.79E-03	6.25E-05	7.26
46	SDZ	1.79E-03	6.25E-04	15.15
47	SDZ	1.79E-03	3.12E-03	17.28
48	SDZ	1.79E-02	5E-03	30.23
49	SML	0	5E-03	0.01
50	SML	1.79E-02	0	0.0
51	SML	5.37E-04	6.25E-05	5.28
52	SML	5.37E-04	6.25E-04	18.5
53	SML	5.37E-04	3.12E-03	10.12
54	SML	1.79E-03	6.25E-05	17.54
55	SML	1.79E-03	6.25E-04	45.87
56	SML	1.79E-03	3.12E-03	50.81
57	SML	1.79E-02	5E-03	53.17

Table S3. Experimental results obtained for SAs degradation in the system Fe(III)/sulfite. Conditions; $[Sulfonamide]_0 = 5.38 \times 10^{-5}$ M, pH 3, T = 298 K, reaction time 60 min.

Exp. Num.	Sulfonamide	[Fe(III)]0 (M)	[sulfite]0 (M)	% Degraded
58	SMZ	0	5 E-03	2.1
59	SMZ	1.79E-02	0	1.15
60	SMZ	5.37E-04	6.25E-05	4.28
61	SMZ	5.37E-04	6.25E-04	30.88
62	SMZ	5.37E-04	3.12E-03	8.97
63	SMZ	1.79E-03	6.25E-05	31.34
64	SMZ	1.79E-03	6.25E-04	19.78
65	SMZ	1.79E-03	3.12E-03	28.37
66	SMZ	1.79E-02	5E-03	35.66
67	SDZ	0	5E-03	0.87
68	SDZ	1.79E-02	0	3.1
69	SDZ	5.37E-04	6.25E-05	3.9
70	SDZ	5.37E-04	6.25E-04	28.74
71	SDZ	5.37E-04	3.12E-03	10.58
72	SDZ	1.79E-03	6.25E-05	27.24
73	SDZ	1.79E-03	6.25E-04	20.01
74	SDZ	1.79E-03	3.12E-03	25.14
75	SDZ	1.79E-02	5E-03	27.98
76	SML	0	5E-03	0.00
77	SML	1.79E-02	0	0.0
78	SML	5.37E-04	6.25E-05	5.87
79	SML	5.37E-04	6.25E-04	19.25
80	SML	5.37E-04	3.12E-03	18.24
81	SML	1.79E-03	6.25E-05	20.74

82	SML	1.79E-03	6.25E-04	32.10
83	SML	1.79E-03	3.12E-03	47.19
84	SML	1.79E-02	5E-03	69.17

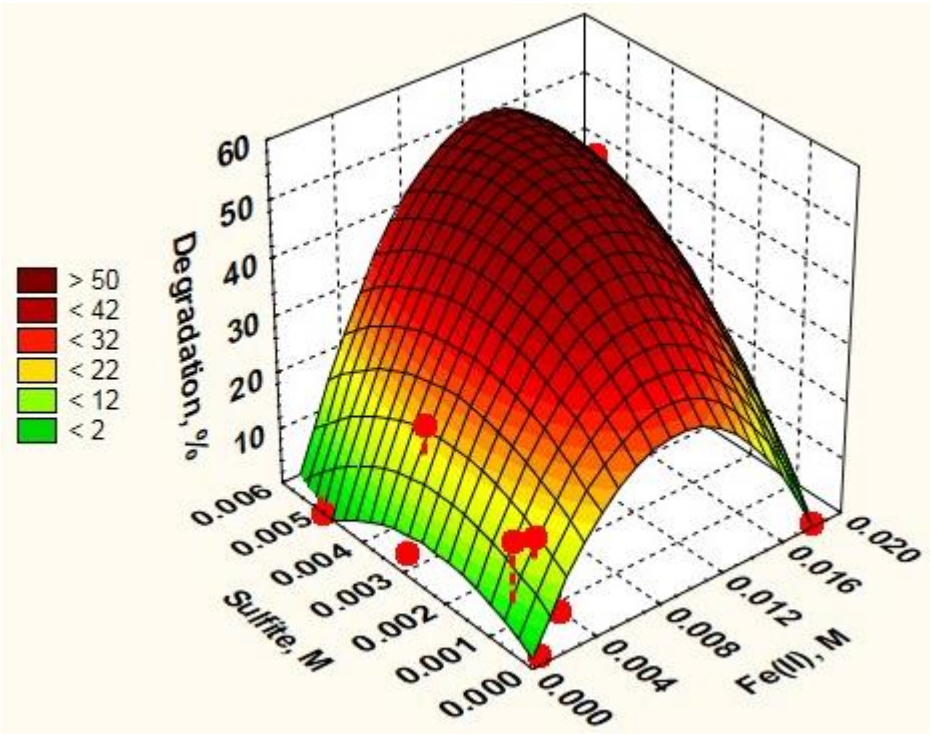
Table S4. Experimental results obtained for SAs degradation in the system Fe(VI)/sulfite. Conditions; $[Sulfonamide]_0 = 5.38 \times 10^{-5}$ M, pH 3, T = 298 K, reaction time 20 min.

Exp. Num.	Sulfonamide	$[Fe(VI)]_0$ (M)	$[sulfite]_0$ (M)	% Degraded
85	SMZ	5 E-05	-	32.72
86	SMZ	1 E-4	-	42.22
87	SMZ	2 E-4	-	53.12
88	SMZ	5 E-05	7.8 E-04	33.99
89	SMZ	5 E-04	5 E-04	44.26
90	SMZ	1 E-04	2 E-04	27.35
91	SMZ	1 E-04	5 E-05	27.91
92	SMZ	1 .79E-02	5 E-03	83.12
93	SMZ	1 .79E-02	1 E-02	100

Table S5. Quadratic equation representing the variation in percentage removal of SAs (f(x,y)) as a function of sulfite (x) and iron-base (y) concentration by different systems. [SAs] = 5.38×10^{-5} M, [Iron-base] = 5.37×10^{-4}—1.79×10^{-2} M, [sulfite] = 6.25×10^{-5}—5.0×10^{-3} M, pH = 3, T = 298 K.

System	Sulfonamide	Quadratic equation
Fe(0)/Sulfite	SMZ	f(x,y) = 1.7873+8222.5935*x+4115.7563*y-4.6514E5*x*x+6.719E5*x*y-9.6766E5*y*y
	SDZ	f(x,y) = -2.6456+11844.4803*x+17401.3848*y-6.5309E5*x*x+6.6884E5*x*y-3.5106E6*y*y
	SML	f(x,y) = 0.5202+12857.1015*x+12609.0029*y-7.201E5*x*x+7.3557E5*x*y-2.6602E6*y*y
Fe(II)/Sulfite	SMZ	f(x,y) = 1.9683+6035.7473*x+5650.1013*y-3.4069E5*x*x+5.0637E5*x*y-1.286E6*y*y
	SDZ	f(x,y) = 3.708+3943.4491*x+4699.7141*y-2.2876E5*x*x+3.8414E5*x*y-1.1442E6*y*y
	SML	f(x,y) = -15.4697+21961.2021*x+46131.8758*y-1.1793E6*x*x+1.6944E6*x*y-1.3147E7*y*y

Fe(III)/Sulfite	SMZ	f(x,y) = 10.5605+10232.1006*x-1166.5745*y-6.0117E5*x*x+4.5193E5*x*y+232.9765*y*y
	SDZ	f(x,y) = 10.5772+8523.559*x-644.7538*y-4.9957E5*x*x+3.1436E5*x*y+128.5625*y*y
	SML	f(x,y) = -0.3557+16567.5905*x+4591.3923*y-9.2501E5*x*x+5.206E5*x*y-918.2642*y*y
Fe(VI)/Sulfite	SMZ	f(x,y) = -41.9111+2.1439E6*x-1.4223E6*y-1.3026E10*x*x+1.0794E10*x*y+1.1336E9*y*y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< 42
< 32
< 22
< 12
< 2
Degradation, %
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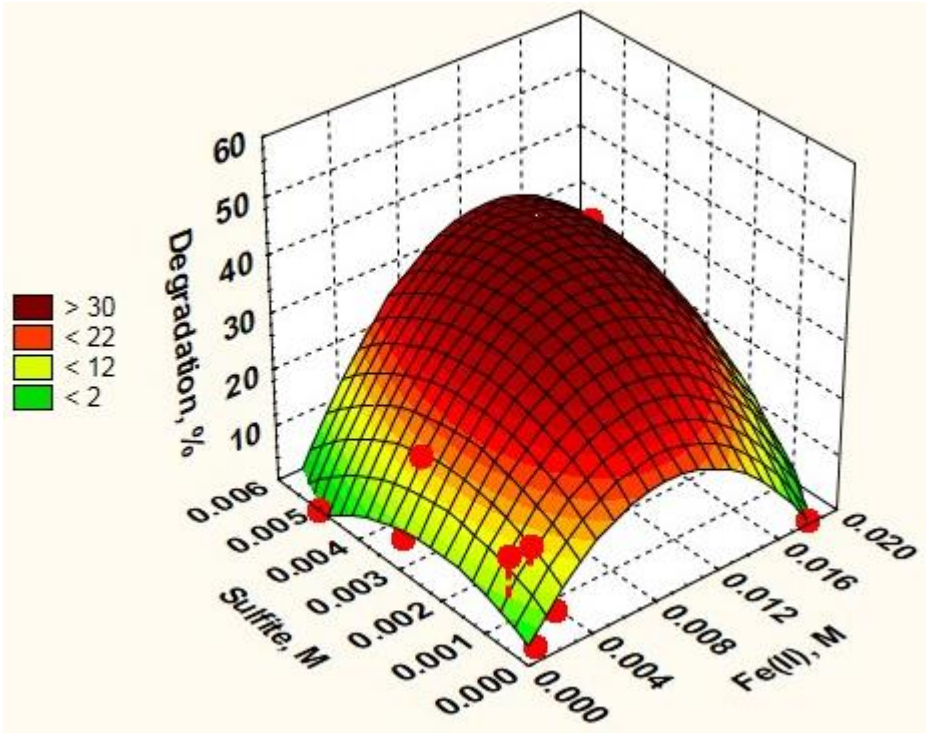
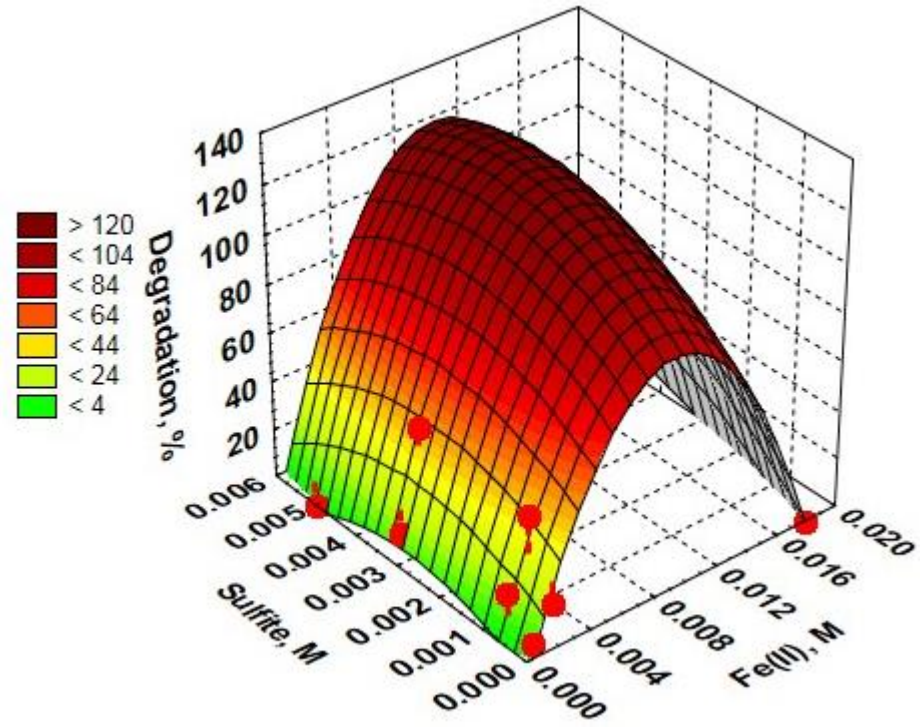
50
40
30
20
10
0.006
0.005
0.004
0.003
0.002
0.001
0.000
Sulfite, M
0.000
0.004
0.008
0.012
0.016
0.020
Fe(III), M

SMZ

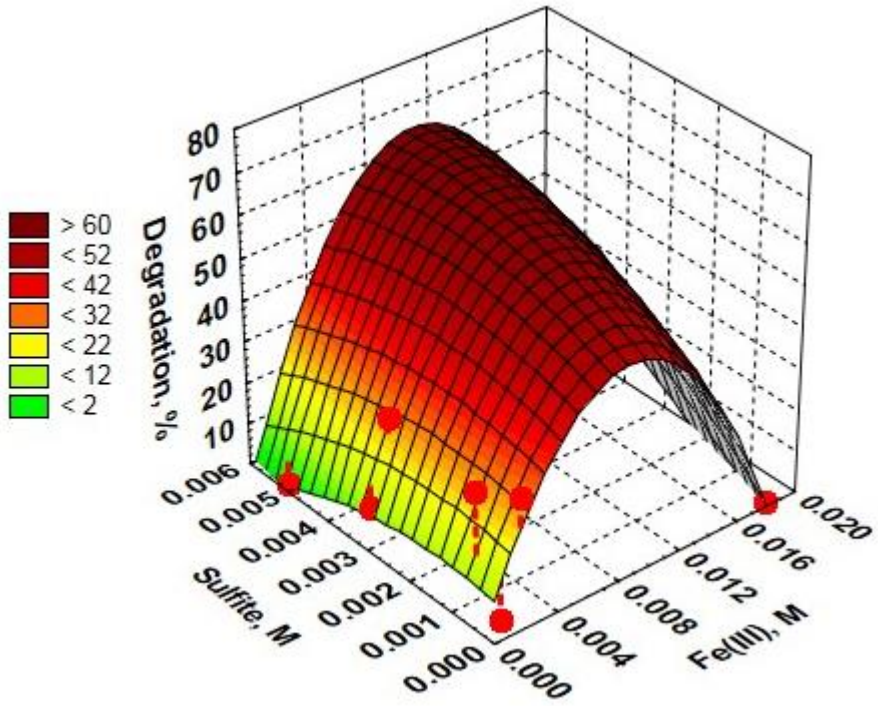

> 30
< 22
< 12
< 2
Degradation, %
60
50
40
30
20
10
0.006
0.005
0.004
0.003
0.002
0.001
0.000
Sulfite, M
0.000
0.004
0.008
0.012
0.016
0.020
Fe(III), M

SDZ

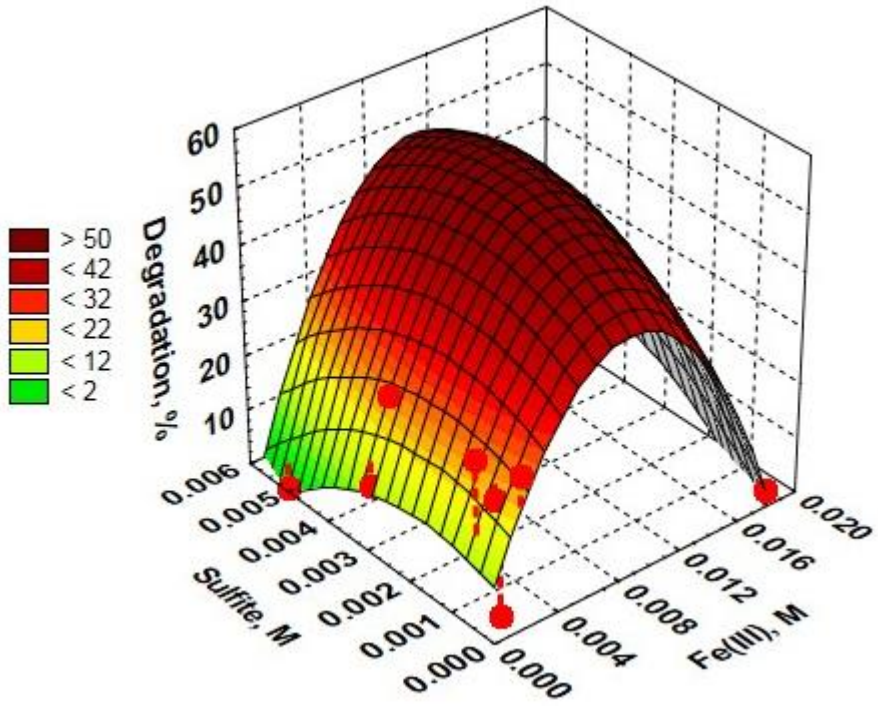


SML

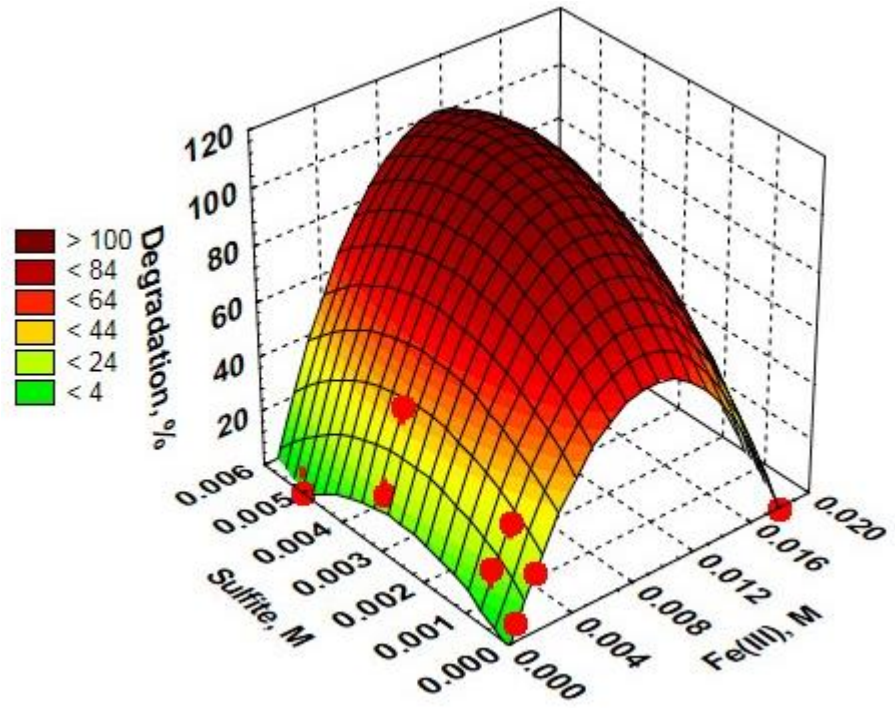
Figure S1. Response surface obtained for the degradation of SAs as a function of Fe(II) and sulfite concentrations. [SAs] = 5.38 × 10^{-5} M, [Fe(II)] = 5.37 × 10^{-4}—1.79 × 10^{-2} M, [sulfite] = 6.25 × 10^{-5}—5.0 × 10^{-3} M, pH 3, T = 298 K.


> 60
< 52
< 42
< 32
< 22
< 12
< 2
Degradation, %
80
70
60
50
40
30
20
10
0.006
0.005
0.004
0.003
0.002
0.001
0.000
Sulfite, M
0.000
0.004
0.008
0.012
0.016
0.020
Fe(III), M

SMZ

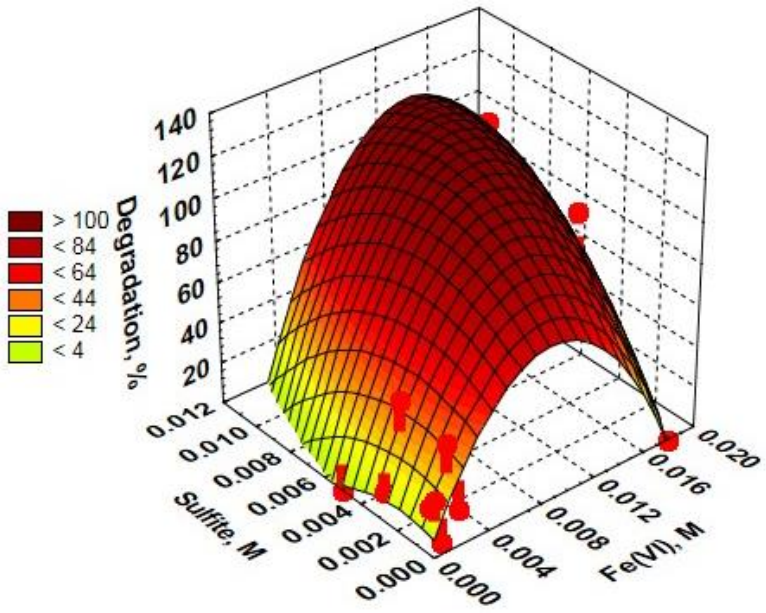

> 50
< 42
< 32
< 22
< 12
< 2
Degradation, %
60
50
40
30
20
10
0.006
0.005
0.004
0.003
0.002
0.001
0.000
Sulfite, M
0.000
0.004
0.008
0.012
0.016
0.020
Fe(III), M

SDZ



SML

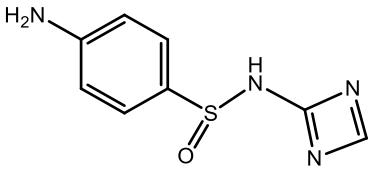
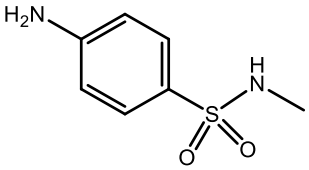
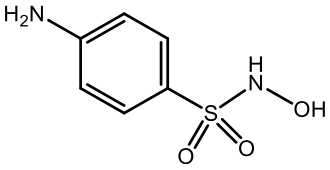
Figure S2. Response surface obtained for the degradation of SAs as a function of Fe(III) and sulfite concentrations. [SAs] = 5.38 × 10^{-5} M, [Fe(III)] = 5.37 × 10^{-4}—1.79 × 10^{-2} M, [sulfite] = 6.25 × 10^{-5}—5.0 × 10^{-3} M, pH 3, T = 298 K.

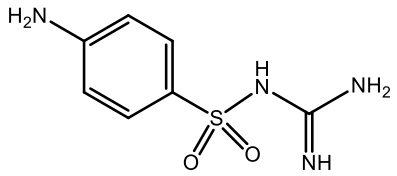
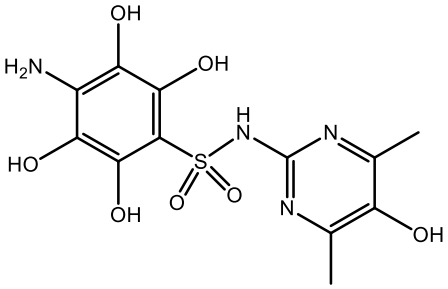


SMZ

Figure S3. Response surface obtained for the degradation of SMZ as a function of Fe(VI) and sulfite concentrations. [SAs] = 5.38 × 10^{-5} M, [Fe(VI)] = 5.37 × 10^{-4}—1.79 × 10^{-2} M, [sulfite] = 6.25 × 10^{-5}—5.0 × 10^{-3} M, pH 3, T = 298 K.

Table S6. Proposed degradation byproducts by retention time from the different sulfonamide derivatives

Sulfonamide Iron-based/sulfite system	Retention time (min)	Detected Mass m/z ($M+H^+$) (Calc. mass)	Chemical formula	Proposed molecular structure
SDZ Fe(0), Fe(II), Fe(VI)	1.14	209.0780 (208.2355)	$C_6H_{12}N_2O_4S$	
SDZ Fe(0), Fe(II)	1.90	187.0974 (186.2132)	$C_{10}H_{10}N_4$	
SDZ Fe(0), Fe(III)	3.48	189.1124 (188.2291)	$C_{10}H_{12}N_4$	

SMZ Fe(0), Fe(II), Fe(III)	3.53	215.1283 (214.2664)	$C_{12}H_{14}N_4$	
SMZ Fe(VI)	3.94	359.0470 (358.3934)	$C_{12}H_{14}N_4O_5S_2$	
SML Fe(0), Fe(II), Fe(VI)	5.63	301.0067 (300.3142)	$C_9H_8N_4O_4S_2$