

QSAR-3D/CoMFA EM COMPOSTOS IMÍDICOS COM ATIVIDADE ANTINOCICEPTIVA

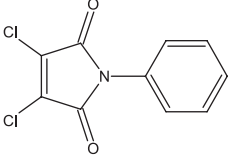
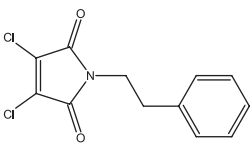
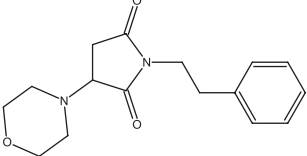
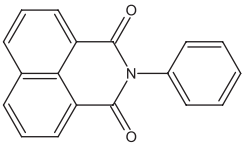
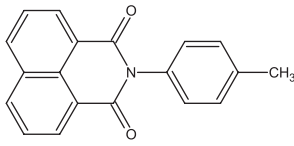
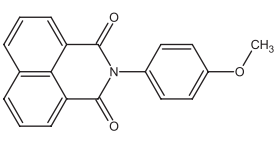
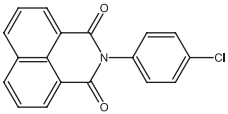
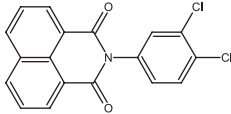
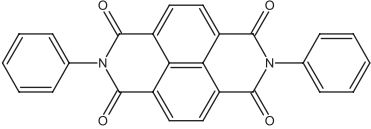
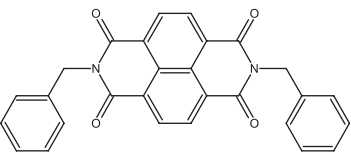
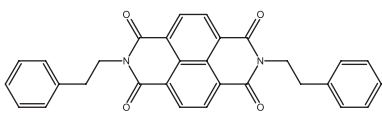
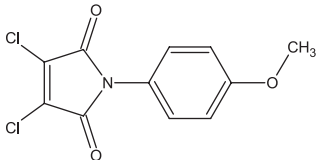
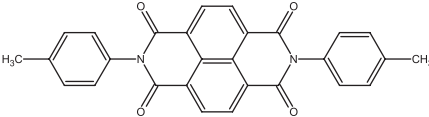
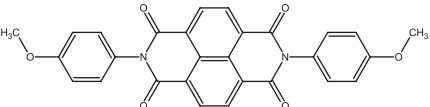
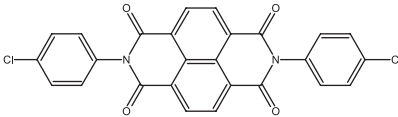
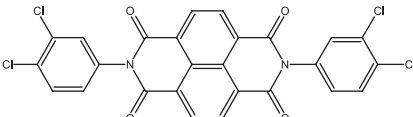
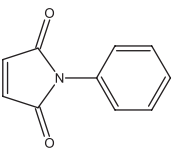
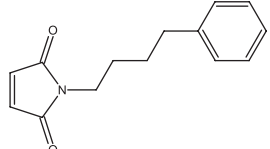
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Tabela 1S. Moléculas constituintes do banco de dados utilizado na QSAR-3D

Número	pDI ₅₀	Número	pDI ₅₀	Número	pDI ₅₀
01	5,555	02	5,398	03	4,450
					
04	5,764	05	5,660	06	6,161
					
07	5,488	08	6,000	09	6,000
					
10	5,672	11	5,733	12	4,928
					
13	5,921	14	6,337	15	5,775
					
16	5,928	17	4,721	18	5,125
					

*e-mail: melenawalter@gmail.com

Tabela 1S. continuação

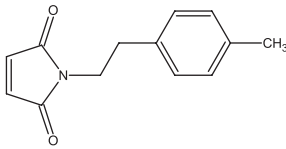
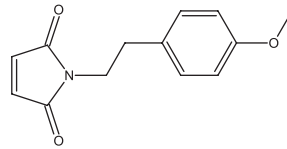
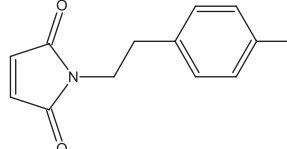
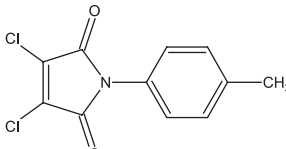
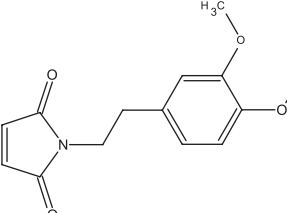
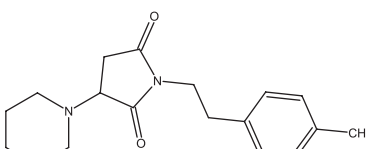
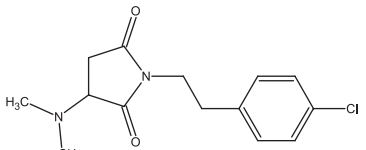
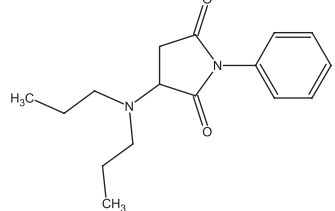
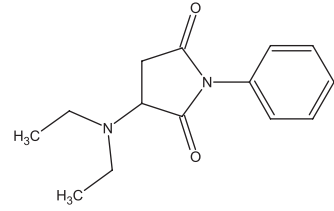
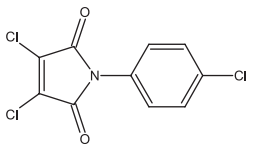
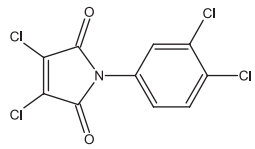
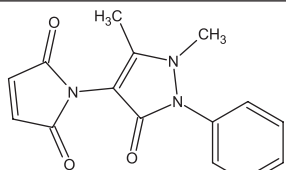
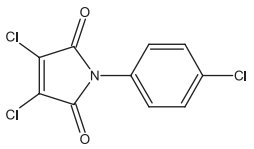
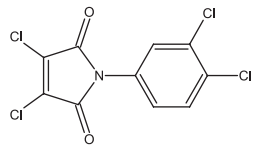
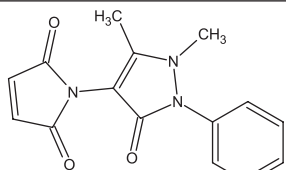
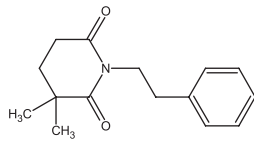
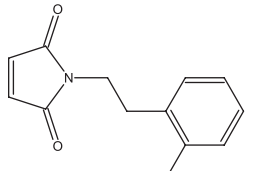
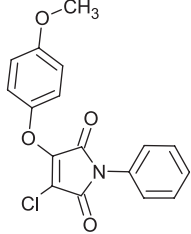
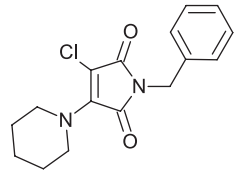
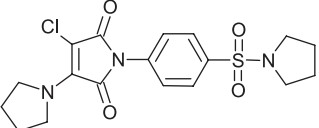
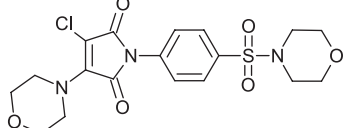
Número	pDI ₅₀	Número	pDI ₅₀	Número	pDI ₅₀
19	5,292	20	5,004	21	4,710
					
22	4,972	23	4,943	24	3,678
					
25	3,658	26	3,523	27	3,523
					
28	5,031	29	5,503	30	5,602
					
31	3,910	32	4,886	33	4,876
					
34	4,086	35	4,412	36	4,061
					
37	----	38	4,299	39	4,190
					

Tabela 1S. continuação

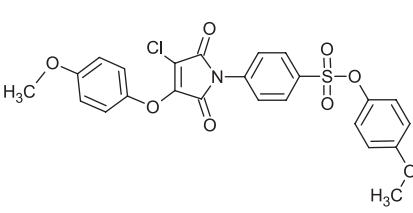
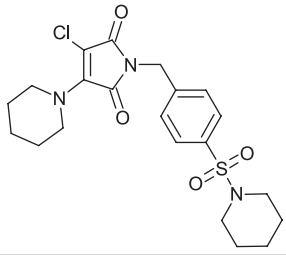
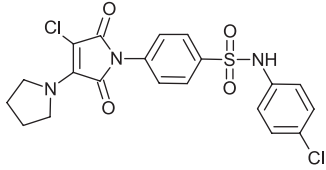
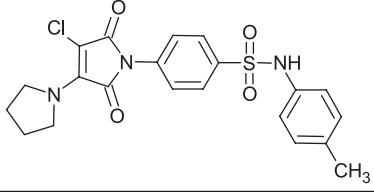
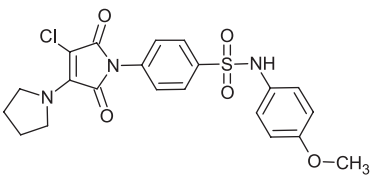
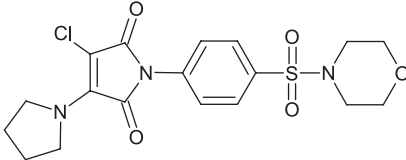
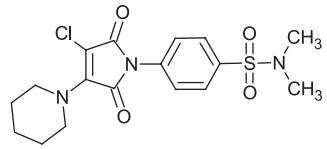
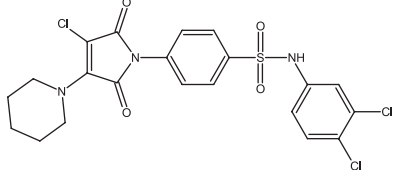
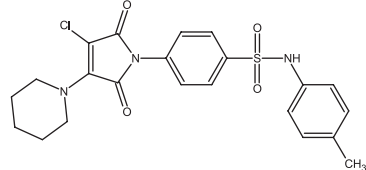
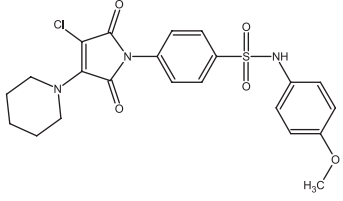
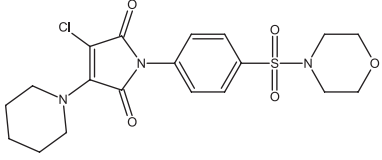
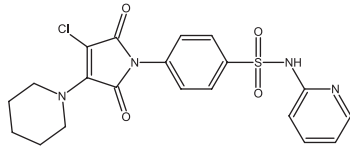
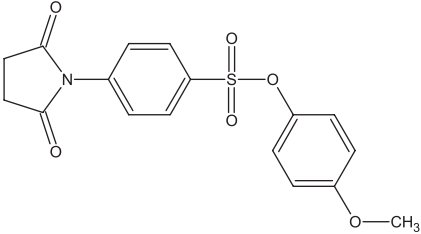
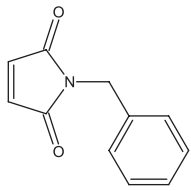
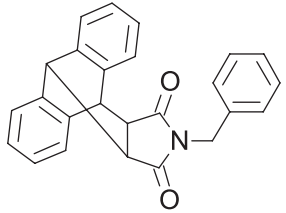
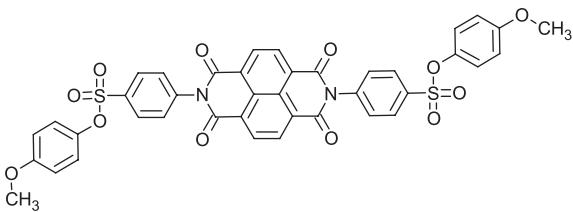
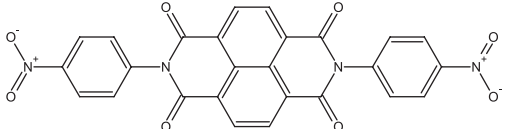
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40	5,130	41	4,855	42	4,580
					
43	4,984	44	4,300	45	4,893
					
46	4,350	47	4,640	48	4,590
					
49	4,719	50	4,720	51	4,960
					
52	4,757	53	4,610	54	----
					
55	-----			56	-----
					

Tabela 2S. Condições utilizadas na análise de CoMFA para os compostos imídicos (Tabela 1S) com atividade antinociceptiva

Modelo	Minimiza- ção	Sonda	Caixa 1	Caixa 2	Caixa 3
1	GA	N ₃ ⁺¹	X	-	-
2	GA	N ₅ ⁺¹	X	-	-
3	GA	N ₃ ⁺¹	X	-	-
4	GA	Npl ₃ ^{+0,425525}	-	X	-
5	GA	Npl ₃ ⁺¹	-	X	-
6	GA	N ₃ ⁺¹	-	X	-
7	GA	N ₂ ⁺¹	-	X	-
8	GA	N ₂ ⁺¹	-	X	-
9	GA	O ₃ ^{-0,4792}	-	X	-
10	GA	O ₃ ⁻¹	-	X	-
11	GA	O ₃ ⁻¹	-	X	-
12	GA	N ₂ ⁺¹ O ₃ ⁻¹	-	X	-
13	GA	Nam ^{+0,425525}	-	X	-
14	GA	N ₂ ⁺¹	-	-	X
15	GA	Nam ⁺¹	-	-	X
16	AM1	Npl ₃ ^{+0,425525}	-	X	-
17	AM1	Npl ₃ ⁺¹	-	-	X
18	AM1	Nam ⁺¹	-	X	-
19	AM1	Npl ₃ ^{+0,425525}	-	-	X
20	AM1	N ₂ ⁺¹	-	-	X
21	AM1	O ₃ ^{-0,4792}	-	-	X
22	AM1	O ₃ ^{-0,4792}	-	X	-
23	AM1	O ₃ ⁻¹	-	X	-
24	AM1	O ₃ ⁻¹	-	-	X
25	AM1	C ₃ ⁺¹	-	-	X
26	AM1	N ₂ ⁺¹ O ₃ ⁻¹ C ₃ ⁺¹	-	-	X
27	GA	N ₅ ⁺¹	-	-	X
28	GA	N ₃ ⁺¹	-	-	X
29	GA	N ₃ ⁺¹	-	-	X
30	GA	N ₅ ⁺¹	-	-	X
31	GA	N ₃ ⁺¹	-	-	X
32	GA	N ₃ ⁺¹	-	-	X

Tabela 3S. Valores de pDI₅₀ experimentais, previstos pelos modelos 3 e 32 e seus respectivos resíduos e erros %

Compostos	pDI ₅₀ experimental	Modelo 3			Modelo 32		
		pDI ₅₀ previsto	Resíduo	Erro %	pDI ₅₀ previsto	Resíduo	Erro %
1	5,555	4,256	1,299	<u>23,39</u>	4,567	0,988	17,78
2	5,398	5,364	0,034	0,62	5,182	0,216	4,01
3	4,456	4,438	0,018	0,40	4,212	0,244	5,47
4	5,764	5,709	0,055	0,96	6,489	-0,725	12,59
5	5,660	5,743	-0,083	1,46	5,868	-0,208	3,68
6	6,161	5,712	0,449	7,29	6,189	-0,028	0,46
7	5,488	5,639	-0,151	2,74	5,533	-0,045	0,81
8	6,000	5,703	0,297	4,96	6,095	-0,095	1,59
9	6,000	5,981	0,019	0,31	5,743	0,257	4,28
10	5,672	5,469	0,203	3,58	5,952	-0,280	4,93
11	5,733	5,691	0,042	0,73	6,094	-0,361	6,30
12	4,928	4,706	0,222	4,51	4,949	-0,021	0,43
13	5,921	6,013	-0,092	1,55	5,806	0,115	1,93
14	6,337	6,445	-0,108	1,70	6,025	0,312	4,92
15	5,775	5,778	-0,003	0,05	5,852	-0,077	1,33
16	5,928	5,006	0,922	15,55	6,474	-0,546	9,20
17	4,726	4,731	-0,005	0,11	5,615	-0,889	18,81
18	5,125	4,997	0,128	2,50	4,748	0,377	7,36
19	5,292	5,150	0,142	2,69	4,737	0,555	10,49
20	5,004	5,063	-0,059	1,18	4,769	0,235	4,70
21	4,710	4,972	-0,262	5,56	4,813	-0,103	2,19
22	4,972	4,331	0,641	12,89	6,076	-1,104	<u>22,21</u>
23	4,943	4,984	-0,041	0,83	5,331	-0,388	7,85
24	3,678	3,577	0,101	2,75	3,713	-0,035	0,95
25	3,658	3,520	0,138	3,78	3,751	-0,093	2,55
26	3,523	3,367	0,156	4,42	3,727	-0,204	5,79
27	3,523	3,535	-0,012	0,34	3,771	-0,248	7,03
28	5,031	3,990	1,041	<u>20,69</u>	4,270	0,761	15,13
29	5,503	3,976	1,527	<u>27,74</u>	4,127	1,376	<u>25,01</u>
30	5,602	5,588	0,014	0,25	5,069	0,533	9,51
31	3,910	4,120	-0,210	5,37	3,884	0,026	0,68
32	4,886	4,382	0,504	10,32	4,344	0,542	11,09
33	4,876	4,937	-0,062	1,26	4,602	0,274	5,63
34	4,086	5,308	-1,222	<u>29,91</u>	4,246	-0,160	3,91
35	4,412	5,340	-0,928	<u>21,04</u>	3,964	0,448	10,15
36	4,061	5,308	-1,247	<u>30,71</u>	3,877	0,184	4,52
37	-	4,563	-	-	4,401	-	-
38	4,299	7,336	-3,037	<u>70,65</u>	4,605	-0,306	7,12
39	4,187	4,207	-0,020	0,47	4,385	-0,197	4,71
40	5,130	7,816	-2,686	<u>52,37</u>	5,054	0,076	1,48
41	4,855	6,474	-1,619	<u>33,34</u>	4,476	0,379	7,81
42	4,580	7,871	-3,291	<u>71,85</u>	4,771	-0,191	4,18
43	4,984	8,347	-3,363	<u>67,49</u>	5,065	-0,081	1,62
44	4,295	6,503	-2,207	<u>51,39</u>	4,299	-0,004	0,09
45	4,893	2,800	2,093	<u>42,78</u>	4,674	0,219	4,48
46	4,350	7,964	-3,614	<u>83,09</u>	4,424	-0,074	1,70
47	4,640	6,867	-2,227	<u>48,00</u>	4,523	0,117	2,53
48	4,590	6,503	-1,913	<u>41,68</u>	4,415	0,175	3,82
49	4,719	7,101	-2,382	<u>50,49</u>	4,871	-0,152	3,22
50	4,720	7,237	-2,517	<u>53,32</u>	4,794	-0,074	1,57
51	4,962	7,981	-3,019	<u>60,84</u>	5,040	-0,078	1,57
52	4,757	5,918	-1,161	<u>24,41</u>	5,026	-	-
53	4,610	4,850	-0,240	5,20	4,786	-0,176	3,83
54	-	4,662	-	-	4,445	-	-
55	-	7,487	-	-	6,518	-	-
56	-	8,689	-	-	6,240	-	-