

Supporting Information

LC-MS/MS software for screening unknown erectile dysfunction drugs and analogues: artificial neural network classification, peak-count scoring, simple similarity search, and hybrid similarity search algorithms

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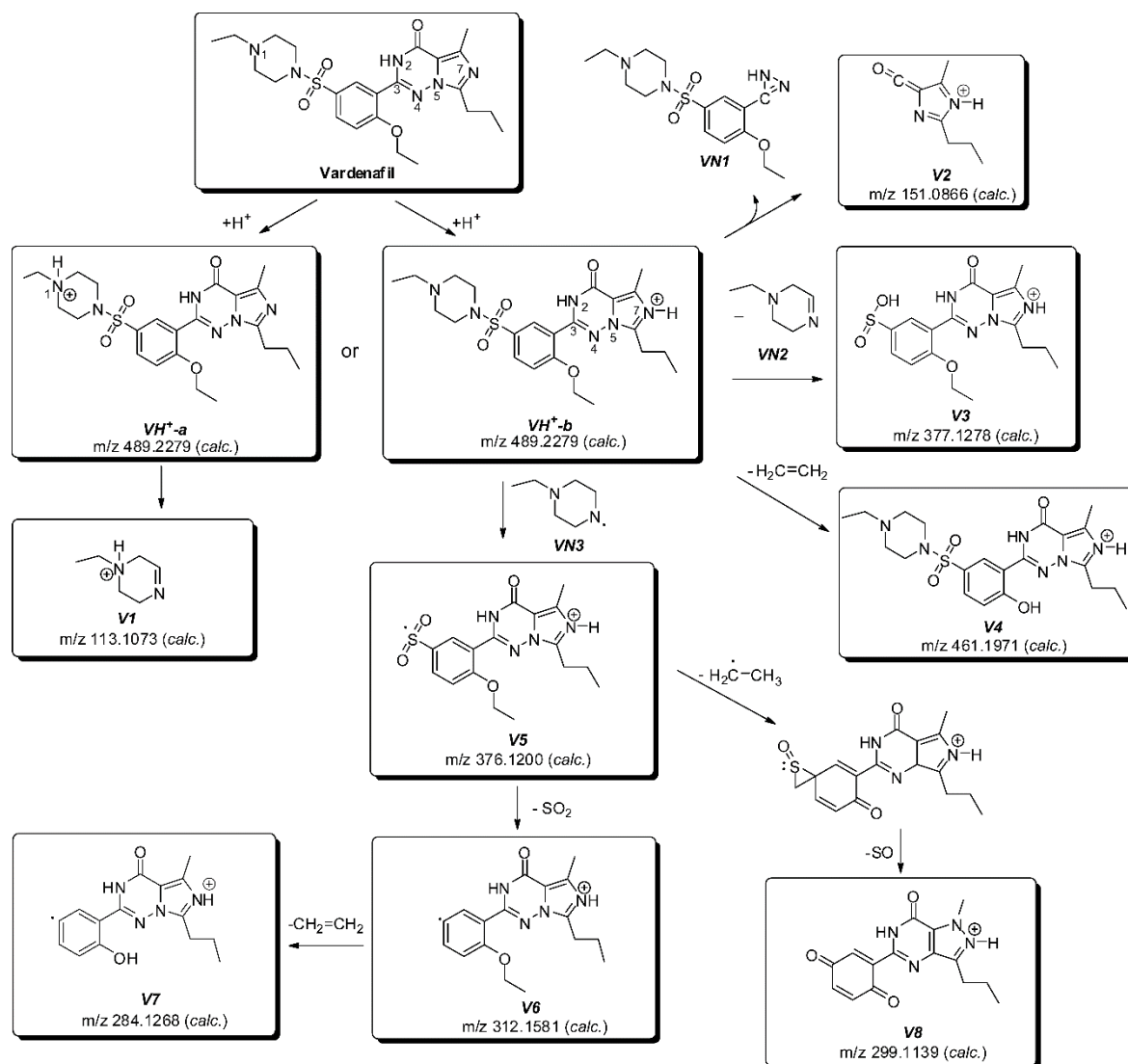
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KEYWORDS: erectile dysfunction (ED) drugs, LC-MS/MS, software, artificial neural network (ANN) modelling, hybrid similarity search (HSS)

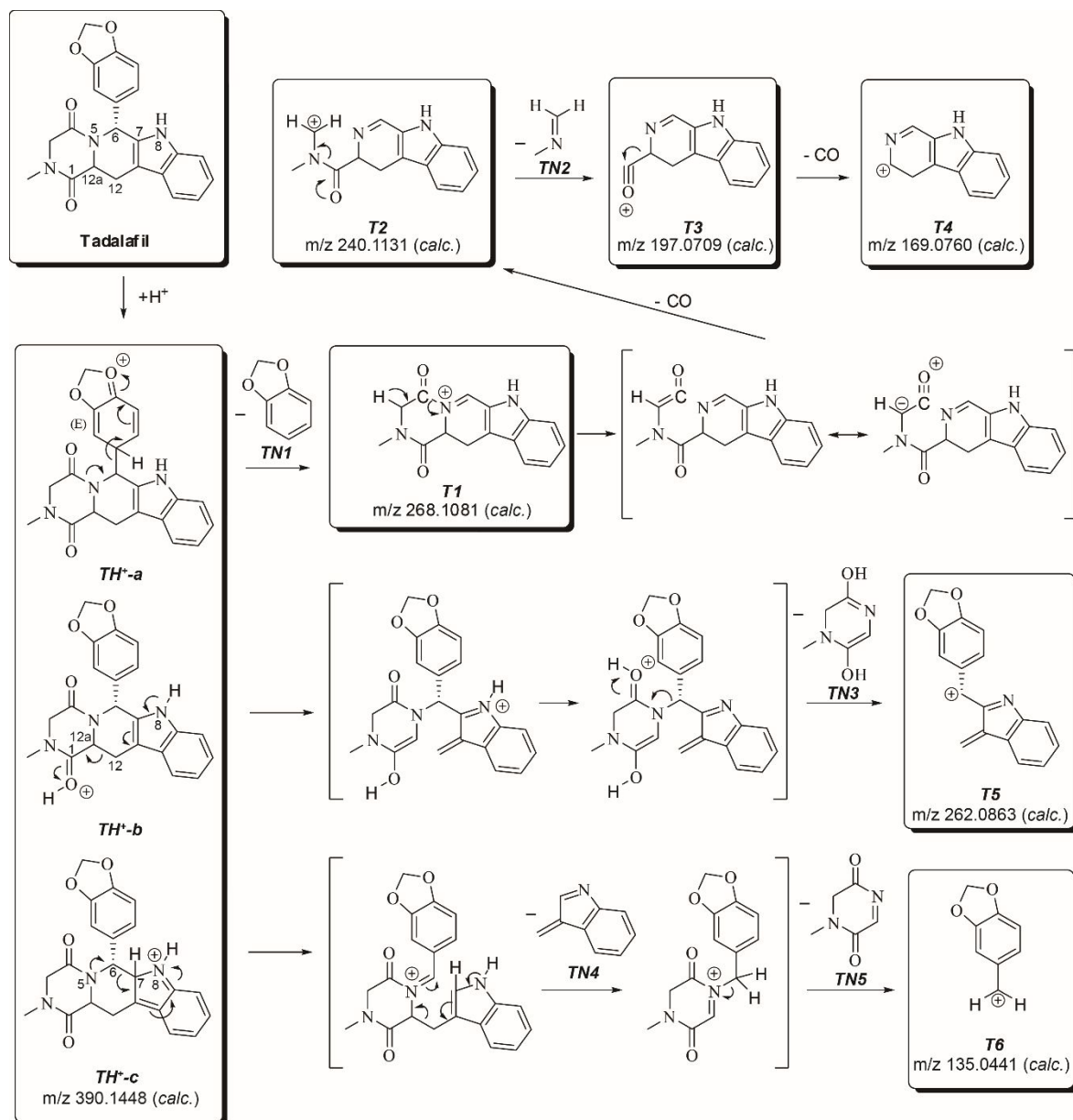
Short title: MS-based software for screening unknown ED drugs and analogues

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Supplementary Scheme S1. A proposed fragmentation mechanism for a protonated vardenafil precursor ion.



Supplementary Scheme S2. A proposed fragmentation mechanism for a protonated tadalafil precursor ion.



Supplementary Table S1. A list of 56 ED drug compounds (34 sildenafil(1–34), 8 vardenafil(35–42), and 14 tadalafil(43–56) family compounds) and 131 other compounds (57–187) for ANN classification modeling. The locations and notations for substituted groups, such as #(*), X(**), R₁, and R₂, can be found in Scheme 1.

No	Class	Compound name	Chemical formula	[M]	[M+H] ⁺	#(*)	X(**)	R ₁	R ₂
1	Sildenafil	Norneosildenafil	C ₂₂ H ₂₉ N ₅ O ₄ S	459.19	460.20	O	SO ₂	Et	a
2	Sildenafil	Sildenafil	C ₂₂ H ₃₀ N ₆ O ₄ S	474.20	475.21	O	SO ₂	Et	b
3	Sildenafil	Homosildenafil	C ₂₃ H ₃₂ N ₆ O ₄ S	488.22	489.23	O	SO ₂	Et	c
4	Sildenafil	Dimethylsildenafil	C ₂₃ H ₃₂ N ₆ O ₄ S	488.22	489.23	O	SO ₂	Et	d
5	Sildenafil	Cyclopentynafil	C ₂₆ H ₃₆ N ₆ O ₄ S	528.25	529.26	O	SO ₂	Et	e
6	Sildenafil	Benzylsildenafil	C ₂₈ H ₃₄ N ₆ O ₄ S	550.24	551.24	O	SO ₂	Et	f
7	Sildenafil	Hydroxyhomosildenafil	C ₂₃ H ₃₂ N ₆ O ₅ S	504.22	505.22	O	SO ₂	Et	g
8	Sildenafil	Methylhydroxyhomosildenafil	C ₂₄ H ₃₄ N ₆ O ₅ S	518.23	519.24	O	SO ₂	Et	g
9	Sildenafil	Mirodenafil	C ₂₆ H ₃₇ N ₅ O ₅ S	531.25	532.26	O	SO ₂	ⁿ Pr	g
10	Sildenafil	Udenafil	C ₂₅ H ₃₆ N ₆ O ₄ S	516.25	517.26	O	SO ₂	ⁿ Pr	h
11	Sildenafil	Propoxyphenylthiosildenafil	C ₂₃ H ₃₂ N ₆ O ₃ S ₂	504.20	505.21	S	SO ₂	ⁿ Pr	b
12	Sildenafil	Thiosildenafil	C ₂₂ H ₃₀ N ₆ O ₃ S ₂	490.18	491.19	S	SO ₂	Et	b
13	Sildenafil	Propoxyphenylthiohomosildenafil	C ₂₄ H ₃₄ N ₆ O ₃ S ₂	518.21	519.22	S	SO ₂	ⁿ Pr	c
14	Sildenafil	Thiohomosildenafil	C ₂₃ H ₃₂ N ₆ O ₃ S ₂	504.20	505.21	S	SO ₂	Et	c
15	Sildenafil	Dimethylthiosildenafil	C ₂₃ H ₃₂ N ₆ O ₃ S ₂	504.20	505.21	S	SO ₂	Et	d
16	Sildenafil	Propoxyphenylthioaildenafil	C ₂₄ H ₃₄ N ₆ O ₃ S ₂	518.21	519.22	S	SO ₂	ⁿ Pr	d
17	Sildenafil	Hydroxythiohomosildenafil	C ₂₃ H ₃₂ N ₆ O ₄ S ₂	520.19	521.20	S	SO ₂	Et	g
18	Sildenafil	Propoxyphenylthiohydroxyhomosildenafil	C ₂₄ H ₃₄ N ₆ O ₄ S ₂	534.21	535.22	S	SO ₂	ⁿ Pr	g
19	Sildenafil	Desmethylcarbodenafil	C ₂₃ H ₃₀ N ₆ O ₃	438.24	439.25	O	CO	Et	b
20	Sildenafil	Carbodenafil	C ₂₄ H ₃₂ N ₆ O ₃	452.25	453.26	O	CO	Et	c

21	Sildenafil	Chlorodenafil	C ₁₉ H ₂₁ ClN ₄ O ₃	388.13	389.14	O	CO	Et	CH ₂ Cl
22	Sildenafil	Gendenafil	C ₁₉ H ₂₂ N ₄ O ₃	354.17	355.18	O	CO	Et	CH ₃
23	Sildenafil	Acetil acid	C ₁₈ H ₂₀ N ₄ O ₄	356.15	357.16	O	CO	Et	OH
24	Sildenafil	Piperidinohongdenafil	C ₂₄ H ₃₁ N ₅ O ₃	437.24	438.25	O	COCH ₂	Et	a
25	Sildenafil	Dimethylhongdenafil	C ₂₄ H ₃₂ N ₆ O ₃	452.25	453.26	O	COCH ₂	Et	b
26	Sildenafil	Hongdenafil	C ₂₅ H ₃₄ N ₆ O ₃	466.27	467.28	O	COCH ₂	Et	c
27	Sildenafil	Dimethylacetildenafil	C ₂₅ H ₃₄ N ₆ O ₃	466.27	467.28	O	COCH ₂	Et	d
28	Sildenafil	Hydroxyhongdenafil	C ₂₅ H ₃₄ N ₆ O ₄	482.26	483.27	O	COCH ₂	Et	g
29	Sildenafil	Cinnamylidenafil	C ₂₃ H ₃₈ N ₆ O ₃	554.30	555.31	O	COCH ₂	Et	i
30	Sildenafil	Oxohongdenafil	C ₂₅ H ₃₂ N ₆ O ₄	480.25	481.26	O	COCH ₂	Et	j
31	Sildenafil	Hydroxychlorodenafil	C ₁₉ H ₂₃ ClN ₄ O ₃	390.15	391.15	O	COH	Et	CH ₂ Cl
32	Sildenafil	Nitrodenafil	C ₁₇ H ₁₉ N ₅ O ₄	357.14	358.15	O	-	Et	NO ₂
33	Sildenafil	Dichlorodenafil	C ₁₉ H ₂₀ Cl ₂ N ₄ O ₂	406.10	407.10	O	-	Et	k
34	Sildenafil	Imidazosagatriazinone	C ₁₇ H ₂₀ N ₄ O ₂	312.16	313.17	O	-	Et	-
35	Vardenafil	Acetylvardenafil	C ₂₅ H ₃₄ N ₆ O ₃	466.27	467.28	O	COCH ₂	Et	c
36	Vardenafil	Desulfovardenafil	C ₁₇ H ₂₀ N ₄ O ₂	312.16	313.17	O	-	Et	-
37	Vardenafil	Hydroxyvardenafil	C ₂₃ H ₃₂ N ₆ O ₅ S	504.22	505.22	O	SO ₂	Et	g
38	Vardenafil	Norneovardenafil	C ₁₈ H ₂₀ N ₄ O ₄	356.15	357.16	O	CO	Et	OH
39	Vardenafil	Pseudovardenafil	C ₂₂ H ₂₉ N ₅ O ₄ S	459.19	460.20	O	SO ₂	Et	a
40	Vardenafil	Vardenafil	C ₂₃ H ₃₂ N ₆ O ₄ S	488.22	489.23	O	SO ₂	Et	c
41	Vardenafil	N-Desethyl vardenafil	C ₂₁ H ₂₈ N ₆ O ₄ S	460.19	461.20	O	SO ₂	Et	l
42	Vardenafil	Hydroxythiovardenafil	C ₂₃ H ₃₂ N ₆ O ₄ S ₂	520.19	521.20	S	SO ₂	Et	g
43	Tadalafil	2-Hydroxypropyl nortadalafil	C ₂₄ H ₂₃ N ₃ O ₅	433.16	434.17	R	R	CH ₂ CH(OH)CH ₃	
44	Tadalafil	Acetaminotadalafil	C ₂₃ H ₂₀ N ₄ O ₅	432.14	433.15	R	R	NHC(O)CH ₃	

45	Tadalafil	Aminotadalafil	C ₂₁ H ₁₈ N ₄ O ₄	390.13	391.14	R	R	NH ₂
46	Tadalafil	cis-Cyclopentyltadalafil	C ₂₆ H ₂₅ N ₃ O ₄	443.18	444.19	R	R	cyclopentyl
47	Tadalafil	Nortadalafil	C ₂₁ H ₁₇ N ₃ O ₄	375.12	376.13	S	S	H
48	Tadalafil	Epi-Aminotadalafil	C ₂₁ H ₁₈ N ₄ O ₄	390.13	391.14	S	R	NH ₂
49	Tadalafil	Homotadalafil	C ₂₃ H ₂₁ N ₃ O ₄	403.15	404.16	R	R	CH ₂ CH ₃
50	Tadalafil	N-Butyltadalafil	C ₂₅ H ₂₅ N ₃ O ₄	431.18	432.19	R	R	(CH ₂) ₃ CH ₃
51	Tadalafil	Octylnortadalafil	C ₂₉ H ₃₃ N ₃ O ₄	487.25	488.25	R	R	(CH ₂) ₇ CH ₃
52	Tadalafil	Tadalafil	C ₂₂ H ₁₉ N ₃ O ₄	389.14	390.14	R	R	CH ₃
53	Tadalafil	Tadalafil impurity E	C ₂₂ H ₁₉ N ₃ O ₄	389.14	390.14	S	S	CH ₃
54	Tadalafil	Chloropretadalafil	C ₂₂ H ₁₉ ClN ₂ O ₅	426.10	427.11	R	R	OCH ₃
55	Tadalafil	Tadalafil impurity A	C ₂₀ H ₁₉ N ₃ O ₃	349.14	350.15	S	R	NHCH ₃
56	Tadalafil	Tadalafil impurity D	C ₂₂ H ₂₀ ClN ₃ O ₄	425.11	426.12	R	R	NHCH ₃
57	Others	Amiloride	C ₆ H ₈ ClN ₇ O	229.05	230.06			
58	Others	Bumetanide	C ₁₇ H ₂₀ N ₂ O ₅ S	364.11	365.12			
59	Others	Clopamide	C ₁₄ H ₂₀ ClN ₃ O ₃ S	345.09	346.10			
60	Others	Methazolamide	C ₅ H ₈ N ₄ O ₃ S ₂	236.00	237.01			
61	Others	Quinethazone	C ₁₀ H ₁₂ ClN ₃ O ₃ S	289.03	290.04			
62	Others	Avanafil	C ₂₃ H ₂₆ ClN ₇ O ₃	483.18	484.19			
63	Others	Dapoxetine	C ₂₁ H ₂₃ NO	305.18	306.19			
64	Others	Icariin	C ₃₃ H ₄₀ O ₁₅	676.24	677.24			
65	Others	Thioquinapiperifil	C ₂₄ H ₂₈ N ₆ OS	448.20	449.21			
66	Others	Xanthoanthrafil	C ₁₉ H ₂₃ N ₃ O ₆	389.16	390.17			
67	Others	Yohimbin	C ₂₁ H ₂₆ N ₂ O ₃	354.19	355.20			
68	Others	4-Dimethylaminoantipyrine	C ₁₃ H ₁₇ N ₃ O	231.14	232.14			

69	Others	Aceclofenac	C ₁₆ H ₁₃ Cl ₂ NO ₄	353.02	354.03
70	Others	Acetaminophen	C ₈ H ₉ NO ₂	151.06	152.07
71	Others	Diclofenac	C ₁₄ H ₁₁ Cl ₂ NO ₂	295.02	296.02
72	Others	Ketoprofen	C ₁₆ H ₁₄ O ₃	254.09	255.10
73	Others	Meclofenamate	C ₁₄ H ₁₁ Cl ₂ NO ₂	295.02	296.02
74	Others	Mefenamic acid	C ₁₅ H ₁₅ NO ₂	241.11	242.12
75	Others	Meloxicam	C ₁₄ H ₁₃ N ₃ O ₄ S ₂	351.03	352.04
76	Others	Oxyphenbutazone	C ₁₉ H ₂₀ N ₂ O ₃	324.15	325.15
77	Others	Piroxicam	C ₁₅ H ₁₃ N ₃ O ₄ S	331.06	332.07
78	Others	Desmethylsibutramine	C ₁₆ H ₂₄ ClN	265.16	266.17
79	Others	Didesmethylsibutramine	C ₁₅ H ₂₂ ClN	251.14	252.15
80	Others	Atenolol	C ₁₄ H ₂₂ N ₂ O ₃	266.16	267.17
81	Others	Benzylsibutramine	C ₂₀ H ₂₄ ClN	313.16	314.17
82	Others	Bisacodyl	C ₂₂ H ₁₉ NO ₄	361.13	362.14
83	Others	Bupropion	C ₁₃ H ₁₈ ClNO	239.11	240.12
84	Others	Caffeine	C ₈ H ₁₀ N ₄ O ₂	194.08	195.09
85	Others	Diethylpropion	C ₁₃ H ₁₉ NO	205.15	206.16
86	Others	Fenfluramine	C ₁₂ H ₁₆ F ₃ N	231.12	232.13
87	Others	Naltrexone	C ₂₀ H ₂₃ NO ₄	341.16	342.17
88	Others	Orlistat	C ₂₉ H ₅₃ NO ₅	495.39	496.40
89	Others	Paroxetine	C ₁₉ H ₂₀ FNO ₃	329.14	330.15
90	Others	Phendimetrazine	C ₁₂ H ₁₇ NO	191.13	192.14
91	Others	Phenolphthalein	C ₂₀ H ₁₄ O ₄	318.09	319.10
92	Others	Propranolol	C ₁₆ H ₂₁ NO ₂	259.16	260.16

93	Others	Rimonabant	C ₂₂ H ₂₁ Cl ₃ N ₄ O	462.08	463.09
94	Others	Sertraline	C ₁₇ H ₁₇ Cl ₂ N	305.07	306.08
95	Others	Sibutramine	C ₁₇ H ₂₆ ClN	279.18	280.18
96	Others	Levothyroxine	C ₁₅ H ₁₁ I ₄ NO ₄	776.69	777.69
97	Others	Liothyronine	C ₁₅ H ₁₂ I ₃ NO ₄	650.79	651.80
98	Others	(-)-Cotinine	C ₁₀ H ₁₃ N ₂ O	176.10	177.10
99	Others	1-(Methoxymethyl)-1H-benzotriazole	C ₈ H ₉ N ₃ O	163.07	164.08
100	Others	4(or 5)-Methyl-1H-Benzotriazole	C ₇ H ₇ N ₃	133.06	134.07
101	Others	2',2'-Difluoro-2'-deoxyuridine	C ₉ H ₁₀ F ₂ N ₂ O ₅	264.06	265.06
102	Others	Methyl 2-(aminosulfonyl)benzoate	C ₈ H ₉ NO ₄ S	215.03	216.03
103	Others	<i>o</i> -Toluenesulfonamide	C ₇ H ₉ NO ₂ S	171.04	172.04
104	Others	4,4'-Thiodianiline	C ₁₂ H ₁₂ N ₂ S	216.07	217.08
105	Others	4-Aminoantipyrine	C ₁₁ H ₁₃ N ₃ O	203.11	204.11
106	Others	4'-Hydroxy-5,7-dimethoxyflavanone	C ₁₇ H ₁₆ O ₅	300.10	301.11
107	Others	6-Methylcoumarin	C ₁₀ H ₈ O ₂	160.05	161.06
108	Others	7-Aminoflunitrazepam	C ₁₆ H ₁₄ FN ₃ O	283.11	284.12
109	Others	Acemetacin	C ₂₁ H ₁₈ ClNO ₆	415.08	416.09
110	Others	Ajmalicine	C ₂₁ H ₂₄ N ₂ O ₃	352.18	353.19
111	Others	Alachlor	C ₁₄ H ₂₀ ClNO ₂	269.12	270.13
112	Others	Allopurinol	C ₅ H ₄ N ₄ O	136.04	137.05
113	Others	Ametryn	C ₉ H ₁₇ N ₅ S	227.12	228.13
114	Others	Atrazine-desethyl	C ₆ H ₁₀ ClN ₅	187.06	188.07
115	Others	Atropine	C ₁₇ H ₂₃ NO ₃	289.17	290.18
116	Others	Azoxystrobin (free acid)	C ₂₁ H ₁₅ N ₃ O ₅	389.10	390.11

117	Others	Chrysin	C ₁₅ H ₁₀ O ₄	254.06	255.07
118	Others	Diazinon	C ₁₂ H ₂₁ N ₂ O ₃ PS	304.10	305.11
119	Others	Dimethachlor ESA	C ₁₃ H ₁₉ NO ₅ S	301.10	302.11
120	Others	Dimethenamid-ESA	C ₁₂ H ₁₉ NO ₅ S ₂	321.07	322.08
121	Others	Dinotefuran	C ₇ H ₁₄ N ₄ O ₃	202.11	203.11
122	Others	Diuron	C ₉ H ₁₀ Cl ₂ N ₂ O	232.02	233.02
123	Others	Desmethyldiuron	C ₈ H ₈ Cl ₂ N ₂ O	218.00	219.01
124	Others	Doxepine	C ₁₉ H ₂₁ NO	279.16	280.17
125	Others	Ecgonine-methyl-ester (EME)	C ₁₀ H ₁₇ NO ₃	199.12	200.13
126	Others	Fenpropidin	C ₁₉ H ₃₁ N	273.25	274.25
127	Others	Fipronil-sulfide	C ₁₂ H ₄ Cl ₂ F ₆ N ₄ S	419.94	420.95
128	Others	Flurazepam	C ₂₁ H ₂₃ ClFN ₃ O	387.15	388.16
129	Others	Fluroxypyr	C ₇ H ₅ Cl ₂ FN ₂ O ₃	253.97	254.97
130	Others	Fosthiazate	C ₉ H ₁₈ NO ₃ PS ₂	283.05	284.05
131	Others	Gabapentin	C ₉ H ₁₇ NO ₂	171.13	172.13
132	Others	Haloperidol	C ₂₁ H ₂₃ ClFNO ₂	375.14	376.15
133	Others	Harmine	C ₁₃ H ₁₂ N ₂ O	212.10	213.10
134	Others	Heptenophos	C ₉ H ₁₂ ClO ₄ P	250.02	251.02
135	Others	Imidacloprid-urea	C ₉ H ₁₀ ClN ₃ O	211.05	212.06
136	Others	Imipramine	C ₁₉ H ₂₄ N ₂	280.19	281.20
137	Others	Isorhamnetin-3-Galactoside-6"-Rhamnoside	C ₂₈ H ₃₂ O ₁₆	624.17	625.18
138	Others	Kaempferol-7-neohesperidoside	C ₂₇ H ₃₀ O ₁₅	594.16	595.17
139	Others	L-(+)-Lysine	C ₆ H ₁₄ N ₂ O ₂	146.11	147.11
140	Others	Lacosamide	C ₁₃ H ₁₈ N ₂ O ₃	250.13	251.14

141	Others	Lamotrigine	C ₉ H ₇ Cl ₂ N ₅	255.01	256.02
142	Others	Lenacil	C ₁₃ H ₁₈ N ₂ O ₂	234.14	235.14
143	Others	Linuron	C ₉ H ₁₀ Cl ₂ N ₂ O ₂	248.01	249.02
144	Others	Litracen	C ₂₀ H ₂₃ N	277.18	278.19
145	Others	Mabuterol	C ₁₃ H ₁₈ ClF ₃ N ₂ O	310.11	311.11
146	Others	Meperidine	C ₁₅ H ₂₁ NO ₂	247.16	248.16
147	Others	Metamitron	C ₁₀ H ₁₀ N ₄ O	202.09	203.09
148	Others	Metamitron-desamino	C ₁₀ H ₉ N ₃ O	187.07	188.08
149	Others	Metazachlor	C ₁₄ H ₁₆ ClN ₃ O	277.10	278.11
150	Others	Metazachlor OXA	C ₁₄ H ₁₅ N ₃ O ₃	273.11	274.12
151	Others	Myricitrin	C ₂₁ H ₂₀ O ₁₂	464.10	465.10
152	Others	N,N-Diethyl-m-toluamide	C ₁₂ H ₁₇ NO	191.13	192.14
153	Others	N-Acetyl-DL-aspartic acid	C ₆ H ₉ NO ₅	175.05	176.06
154	Others	Naringenin	C ₁₅ H ₁₂ O ₅	272.07	273.08
155	Others	N-Bisdesmethyl Tramadol	C ₁₄ H ₂₁ NO ₂	235.16	236.16
156	Others	N-desmethylpheniramine	C ₁₅ H ₁₈ N ₂	226.15	227.15
157	Others	N-Isopropyl-N-phenyl-p-phenylenediamine	C ₁₅ H ₁₈ N ₂	226.15	227.15
158	Others	Norephedrine	C ₉ H ₁₃ NO	151.10	152.11
159	Others	O-Acetyl-L-serine	C ₅ H ₉ NO ₄	147.05	148.06
160	Others	Omethoate	C ₅ H ₁₂ NO ₄ PS	213.02	214.03
161	Others	<i>o</i> -Chlorophenylpiperazine	C ₁₀ H ₁₃ ClN ₂	196.08	197.08
162	Others	Oxadiazon	C ₁₅ H ₁₈ Cl ₂ N ₂ O ₃	344.07	345.08
163	Others	Oxprenolol	C ₁₅ H ₂₃ NO ₃	265.17	266.18
164	Others	Oxycodone	C ₁₈ H ₂₁ NO ₄	315.15	316.15

165	Others	Palatinose	C ₁₂ H ₂₂ O ₁₁	342.12	343.12
166	Others	Pindolol	C ₁₄ H ₂₀ N ₂ O ₂	248.15	249.16
167	Others	Pioglitazone	C ₁₉ H ₂₀ N ₂ O ₃ S	356.12	357.13
168	Others	Plumericin	C ₁₅ H ₁₄ O ₆	290.08	291.09
169	Others	Praziquantel	C ₁₉ H ₂₄ N ₂ O ₂	312.18	313.19
170	Others	Prometon	C ₁₀ H ₁₉ N ₅ O	225.16	226.17
171	Others	Propachlor-ESA	C ₁₁ H ₁₅ NO ₄ S	257.07	258.08
172	Others	Propazine-2-hydroxy	C ₉ H ₁₇ N ₅ O	211.14	212.15
173	Others	Protopine	C ₂₀ H ₁₉ NO ₅	353.13	354.13
174	Others	Pymetrozine	C ₁₀ H ₁₁ N ₅ O	217.10	218.10
175	Others	Pyrimethamine	C ₁₂ H ₁₃ ClN ₄	248.08	249.09
176	Others	Ranitidine	C ₁₃ H ₂₂ N ₄ O ₃ S	314.14	315.15
177	Others	Repaglinide	C ₂₇ H ₃₆ N ₂ O ₄	452.27	453.27
178	Others	Secbumeton	C ₁₀ H ₁₉ N ₅ O	225.16	226.17
179	Others	Sulfadimethoxine	C ₁₂ H ₁₄ N ₄ O ₄ S	310.07	311.08
180	Others	Sulfaguanidine	C ₇ H ₁₀ N ₄ O ₂ S	214.05	215.06
181	Others	Sulfathiazole	C ₉ H ₉ N ₃ O ₂ S ₂	255.01	256.02
182	Others	Thifensulfuron-methyl	C ₁₂ H ₁₃ N ₅ O ₆ S ₂	387.03	388.04
183	Others	trans-Zeatin riboside	C ₁₅ H ₂₁ N ₅ O ₅	351.15	352.37
184	Others	Triclocarban	C ₁₃ H ₉ Cl ₃ N ₂ O	313.98	314.99
185	Others	Trinexapac-ethyl	C ₁₃ H ₁₆ O ₅	252.10	253.11
186	Others	Tyramine	C ₈ H ₁₁ NO	137.08	138.09
187	Others	Velutin	C ₁₇ H ₁₄ O ₆	314.08	315.09

Supplementary Table S2. Function keys in AI-SIDA.

No.	Function
1	Setting for a chromatogram
2	Browse LC-MS (LC-MS/MS) data
3	Save the peak list
4	Chromatogram
5	Classification in the 2 nd layer and search in the 3 rd layer using the MS/MS peak list
6	Information for MS (MS/MS) spectrum
7	Mass spectrum
8	Scan filter parameters
9	Browse MS/MS spectra file
10	MS/MS peak list and setting for threshold
11	The row number and file name of descriptors in the descriptor table
12	Conversion of spectra to descriptors
13	Deletion of descriptors
14	MS/MS spectrum
15	Browse descriptor files
16	Browse a trained ANN model
17	Descriptors
18	Prediction of the ED-type using the trained ANN model
19	Save the table of descriptors or predicted classes
20	Predicted ED types
21	Setting for intensity threshold
22	MS/MS peak list
23	Browse a database
24	Browse the peak list of MS/MS spectrum
25	Option for search engines
26	Selecting a search engine
27	Save the table of the searched results
28	List for the searched candidate compounds
29	View the selected candidate compound
30	Parameter of MS/MS spectrum
31	MS/MS spectra for a query compound (above) and hit compound (below)

Supplementary Table S3. ED drug compounds used as query compounds

No.	Compound name	Chemical formula	[M]	[M+H] ⁺
1	Norneosildenafil	C ₂₂ H ₂₉ N ₅ O ₄ S	459.19	460.20
2	Homosildenafil	C ₂₃ H ₃₂ N ₆ O ₄ S	488.22	489.23
3	Dimethylsildenafil	C ₂₃ H ₃₂ N ₆ O ₄ S	488.22	489.23
4	Hydroxythiohomosildenafil	C ₂₃ H ₃₂ N ₆ O ₄ S ₂	520.19	521.20
5	Methylhydroxyhomosildenafil	C ₂₄ H ₃₄ N ₆ O ₅ S	518.23	519.24
6	Thiohomosildenafil	C ₂₃ H ₃₂ N ₆ O ₃ S ₂	504.20	505.21
7	Dimethylthiosildenafil	C ₂₃ H ₃₂ N ₆ O ₃ S ₂	504.20	505.21
8	Propoxyphenylthioaildenafil	C ₂₄ H ₃₄ N ₆ O ₃ S ₂	518.21	519.22
9	Propoxyphenylthiohomosildenafil	C ₂₄ H ₃₄ N ₆ O ₃ S ₂	518.21	519.22
10	Propoxyphenylthiohydroxyhomosildenafil	C ₂₄ H ₃₄ N ₆ O ₄ S ₂	534.21	535.22
11	Dimethylhongdenafil	C ₂₄ H ₃₂ N ₆ O ₃	452.25	453.26
12	Piperidinohongdenafil	C ₂₄ H ₃₁ N ₅ O ₃	437.24	438.25
13	Dimethylacetildenafil	C ₂₅ H ₃₄ N ₆ O ₃	466.27	467.28
14	Hydroxyhongdenafil	C ₂₅ H ₃₄ N ₆ O ₄	482.26	483.27
15	Desmethylcarbodenafil	C ₂₃ H ₃₀ N ₆ O ₃	438.24	439.25
16	Chlorodenafil	C ₁₉ H ₂₁ ClN ₄ O ₃	388.13	389.14
17	Gendenafil	C ₁₉ H ₂₂ N ₄ O ₃	354.17	355.18
18	Acetil acid	C ₁₈ H ₂₀ N ₄ O ₄	356.15	357.16
19	Nitrodenafil	C ₁₇ H ₁₉ N ₅ O ₄	357.14	358.15
20	Dichlorodenafil	C ₁₉ H ₂₀ Cl ₂ N ₄ O ₂	406.10	407.10
21	Pseudovardenafil	C ₂₂ H ₂₉ N ₅ O ₄ S	459.19	460.20
22	Hydroxyvaridenafil	C ₂₃ H ₃₂ N ₆ O ₅ S	504.22	505.22
23	Acetylvaridenafil	C ₂₅ H ₃₄ N ₆ O ₃	466.27	467.28
24	Norneovardenafil	C ₁₈ H ₂₀ N ₄ O ₄	356.15	357.16
25	Tadalafil	C ₂₂ H ₁₉ N ₃ O ₄	389.14	390.14
26	Homotadalafil	C ₂₃ H ₂₁ N ₃ O ₄	403.15	404.16
27	N-Butyltadalafil	C ₂₅ H ₂₅ N ₃ O ₄	431.18	432.19
28	Octylnortadalafil	C ₂₉ H ₃₃ N ₃ O ₄	487.25	488.25
29	cis-Cyclopentyltadalafil	C ₂₆ H ₂₅ N ₃ O ₄	443.18	444.19
30	Aminotadalafil	C ₂₁ H ₁₈ N ₄ O ₄	390.13	391.14
31	Acetaminotadalafil	C ₂₃ H ₂₀ N ₄ O ₅	432.14	433.15

Supplementary Figure S1. PCS search results for sulfamethoxazole. Upper panel: LC-MS/MS spectrum acquired for sulfamethoxazole at collision energy 29.9 eV. Lower panel: library LC-MS/MS spectrum acquired for sulfamethoxazole at collision energy 35 eV. The PCS rank score was calculated to be 690.

