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Computational studies on the structural variations of MAO-A and MAO-B inhibitors - An *in silico* docking approach

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Supplementary Data

Suppl. Table 1 — Drug-likeness of all the low binding energy variations of Moclobemide

Compound No.	Mass (g/mol)	Log P	Hydrogen Acceptors (in number)	Hydrogen donors (in number)	Molar Refractivity
1	284.74	1.44	4	2	76.29
2	282.77	2.04	3	1	79.23
3	324.85	3.03	3	1	93.54
4	298.77	2.06	3	3	83.07
5	284.74	1.44	4	2	76.29
6	282.77	2.04	3	1	79.23
7	324.85	3.03	3	1	93.54
8	344.84	3.40	3	1	99.70
9	284.74	1.05	4	2	75.43
11	344.84	3.47	3	1	98.75
12	300.74	0.37	5	3	76.59
13	298.77	1.70	5	3	79.68
14	284.74	1.05	4	2	75.43
15	283.75	1.72	4	2	76.97
16	282.77	2.12	3	1	79.07
17	344.84	3.47	3	1	98.75
18	284.74	1.05	4	2	75.43
19	283.75	1.72	4	2	76.97
20	282.77	2.12	3	1	79.07
21	324.85	3.15	3	1	93.23
22	344.84	3.47	3	1	98.75
23	284.74	1.05	4	2	75.43
24	283.75	1.72	4	2	76.97
25	282.77	2.12	3	1	79.07
26	324.85	3.15	3	1	93.23

Suppl. Table 2 — Physicochemical characteristics of all the low binding energy variations of Moclobemide

No.	Topological Polar Surface area (Å^2)	Fraction Csp^3 (saturation)	Log s (solubility)	Bbb*	Number of rotational bonds	Gastro-inestinal absorption	Bio-availability	Pain alerts
1	41.57	0.46	−2.36, Soluble	Y[1]	5	High	0.55	0
2	61.80	0.46	−2.64, Soluble	Y	5	High	0.55	0
3	41.57	0.5	−2.67, Soluble	Y	5	High	0.55	0
4	41.57	0.59	−3.65, Soluble	Y	6	High	0.55	0

5	93.61	0.46	−2.01,Soluble	N[1]	5	High	0.55	0
6	61.80	0.46	−2.23, Soluble	Y	5	High	0.55	0
7	41.57	0.5	−2.67, Soluble	Y	5	High	0.55	0
8	41.57	0.59	−3.65, Soluble	Y	6	High	0.55	0
9	41.57	0.32	−3.92, Soluble	Y	6	High	0.55	0
11	61.80	0.46	−2.12, Soluble	Y	5	High	0.55	0
12	41.57	0.32	−3.85, Soluble	Y	6	High	0.55	0
13	82.03	0.46	−1.88, Very soluble	N	5	High	0.55	0
14	93.61	0.46	−1.55, Very soluble	N	5	High	0.55	0
15	67.59	0.46	−1.95, Very soluble	N	5	High	0.55	0
16	41.57	0.50	−2.71, Soluble	Y	5	High	0.55	0
17	41.57	0.32	−3.85, Soluble	Y	6	High	0.55	0
18	61.80	0.46	−2.12, Soluble	Y	5	High	0.55	0
19	67.59	0.46	−1.95, Very soluble	N	5	High	0.55	0
20	41.57	0.50	−2.71, Soluble	Y	5	High	0.55	0
21	41.57	0.59	−3.73, Soluble	Y	6	High	0.55	0
22	41.57	0.32	−3.85, Soluble	Y	6	High	0.55	0
23	61.80	0.46	−2.12, Soluble	Y	5	High	0.55	0
24	67.59	0.46	−1.95, Very soluble	N	5	High	0.55	0
25	41.57	0.5	−2.71, Soluble	Y	5	High	0.55	0
26	41.57	0.59	−3.73, Soluble	Y	6	High	0.55	0

Suppl. Table 3 — The rat oral LD_{50}, toxicity class number and the accuracy of prediction of ProTox-II server, for all the lower binding energy variations of Moclobemide

Variation number	Rat oral Lethal dose 50% (mg/kg)	Toxicity class number	Accuracy of the prediction (%)
1	707	4	69.26
2	1250	4	70.97
3	1250	4	69.26
4	1250	4	69.26
5	1250	4	69.26
6	1250	4	70.97
7	1250	4	69.26
8	1250	4	69.26
9	1250	4	70.97
11	1250	4	69.26
12	1250	4	69.26
13	1250	4	70.97
14	1250	4	70.97
15	1250	4	70.97
16	1250	4	70.97
17	1250	4	69.26
18	1250	4	69.26
19	1250	4	69.26
20	1250	4	70.97
21	1250	4	69.26
22	1250	4	69.26
23	1250	4	70.97
24	1250	4	70.97
25	1250	4	70.97
26	1250	4	69.26

Suppl. Table 4 — Toxicity analysis (obtained from ProTox-II server and Osiris property explorer) of all the lower binding energy variations of Molcobemide

No	Toxicity Studies					
	ProTox-II server				Osiris Property Explorer	
	Immunotoxicity	Cytotoxicity	Carcinogenicity	Mutagenicty	Irritation	Rep Eff
1	Iav**	Iav	Iav	Iav	Iav	Iav
2	Iav	Iav	Iav	Iav	AC	AC
3	AC	Iav	Iav	Iav	Iav	Iav
4	Iav	Iav	Iav	Iav	Iav	Iav
5	Iav	Iav	Iav	Iav	Iav	Iav
6	Iav	Iav	Iav	Iav	Iav	Iav
7	AC	Iav	Iav	Iav	Iav	Iav
8	Iav	Iav	Iav	Iav	Iav	Iav
9	Iav	Iav	Iav	Iav	Iav	Iav
11	Iav	Iav	Iav	Iav	Iav	Iav
12	Iav	Iav	Iav	Iav	Iav	Iav
13	Iav	Iav	Iav	Iav	Iav	Iav
14	Iav	Iav	Iav	Iav	Iav	Iav
15	Iav	Iav	Iav	Iav	Iav	Iav
16	Iav	Iav	Iav	Iav	Iav	Iav
17	Iav	Iav	Iav	Iav	Iav	Iav
18	Iav	Iav	Iav	Iav	Iav	Iav
19	Iav	Iav	Iav	Iav	Iav	Iav
20	Iav	Iav	Iav	Iav	Iav	Iav
21	Iav	Iav	Iav	Iav	Iav	Iav
22	Iav	Iav	Iav	Iav	Iav	Iav
23	Iav	Iav	Iav	Iav	Iav	Iav
24	Iav	Iav	Iav	Iav	Iav	Iav
25	AC	Iav	Iav	Iav	Iav	Iav
26	Iav	Iav	Iav	Iav	Iav	Iav

Suppl. Table 5 — Drug-likeness of all the low binding energy variations of Toloxatone

Variation No.	Mass (g/mol)	Log P (Lipophilicity)	Hydrogen Acceptors (in number)	Hydrogen donors (in number)	Molar Refractivity
27	223.23	0.70	4	2	60.05
28	222.24	1.36	4	2	61.59
29	225.22	1.67	4	1	58.94
30	221.25	1.77	3	1	63.69
31	263.33	2.79	3	1	77.85
32	283.32	3.12	3	1	83.37
33	223.23	0.70	4	2	60.05
34	222.24	1.36	4	2	61.59
35	225.22	1.67	4	1	58.94
36	221.25	1.77	3	1	63.69
37	263.33	2.79	3	1	77.85
38	283.32	3.12	3	1	83.37
39	289.37	3.33	3	1	85.61
42	225.22	1.52	4	1	58.84
43	221.25	1.69	3	1	63.85
44	263.33	2.68	3	1	78.16
45	221.25	1.69	3	1	63.85
46	263.33	2.68	3	1	78.16
47	283.32	3.04	3	1	84.32
50	225.22	1.52	4	1	58.84
51	221.25	1.69	3	1	63.85

52	263.33	2.68	3	1	78.16
53	289.37	3.43	3	1	85.77
54	223.23	1.08	4	2	60.91
56	225.22	1.52	4	1	58.84
57	221.25	1.69	3	1	63.85
59	283.32	3.04	3	1	84.32
60	289.37	3.43	3	1	85.77
61	223.23	1.08	4	2	60.91
63	225.22	1.52	4	1	58.84

Suppl. Table 6 — Physicochemical characteristics of all the low binding energy variations of Toloxatone

No.	Topological Polar Surface area (Å^2)	Fraction Csp^3 (saturation)	Log s (solubility)	Bio-availability	GI absorption	Number of rotational bonds	Blood-brain barrier	Pain alerts
27	70.00	0.36	−2.50, Soluble	0.55	High	2	Y	0
28	75.79	0.36	−1.8, Very soluble	0.55	High	2	N	0
29	49.77	0.36	−1.63, Very soluble	0.55	High	2	N	0
30	49.77	0.36	−2.46, Soluble	0.55	High	2	Y	0
31	49.77	0.42	−2.39,Soluble	0.55	High	2	Y	0
32	49.77	0.53	−3.4, Soluble	0.55	High	3	Y	0
33	70.00	0.24	−3.54, Soluble	0.55	High	3	Y	0
34	75.79	0.36	−2.15, Soluble	0.55	High	2	Y	0
35	49.77	0.36	−1.98, Very soluble	0.55	High	2	N	0
36	49.77	0.36	−2.46, Soluble	0.55	High	2	Y	0
37	49.77	0.42	−2.39, Soluble	0.55	High	2	Y	0
38	49.77	0.53	−3.4, Soluble	0.55	High	3	Y	0
39	49.77	0.24	−3.54, Soluble	0.55	High	3	Y	0
42	49.77	0.36	−2.21, Soluble	0.55	High	4	Y	0
43	49.77	0.42	−2.35, Soluble	0.55	High	3	Y	0
44	49.77	0.53	−3.32, Soluble	0.55	High	3	Y	0
45	49.77	0.42	−2.35, Soluble	0.55	High	3	Y	0
46	49.77	0.50	−2.9, Very soluble	0.55	High	3	Y	0
47	37.00	0.24	−3.60, Soluble	0.55	High	3	Y	0
50	49.77	0.36	−2.21, Soluble	0.55	High	4	Y	0
51	49.77	0.42	−2.35, Soluble	0.55	High	2	Y	0
52	49.77	0.53	−3.32, Soluble	0.55	High	3	Y	0
53	49.77	0.59	−4, Moderately soluble	0.55	High	3	Y	0
54	70.00	0.36	−1.9, Very soluble	0.55	High	4	N	0
56	49.77	0.36	−2.21, Soluble	0.55	High	4	Y	0
57	49.77	0.42	−2.35, Soluble	0.55	High	2	Y	0
59	49.77	0.24	−3.6, Soluble	0.55	High	3	Y	0
60	49.77	0.59	−4, Moderately soluble	0.55	High	3	Y	0
61	70.00	0.36	−1.9, Very soluble	0.55	High	4	N	0
63	49.77	0.36	−2.21, Soluble	0.55	High	4	Y	0

Suppl. Table 7 — The rat oral lethal dose, toxicity class number and the accuracy of prediction of ProTox-II server, for all the low binding energy variations of Toloxatone.

Variation number	Oral rat Lethal dose 50%(mg/kg)	Toxicity class number	Accuracy of the prediction (%)
27	1225	4	72.90
28	1400	4	70.97
29	1400	4	70.97
30	1400	4	70.97

31	1400	4	70.97
32	1400	4	69.26
33	1400	4	72.90
34	1400	4	70.97
35	1400	4	70.97
36	1400	4	72.90
37	1400	4	70.97
38	1225	4	69.26
39	1225	4	69.26
42	2000	4	70.97
43	2000	4	72.90
44	2000	4	70.97
45	2000	4	100
46	1400	4	70.97
47	1225	4	70.97
50	1225	4	72.90
51	1225	4	72.90
52	1400	4	70.97
53	1225	4	70.97
54	1400	4	70.97
56	1500	4	70.97
57	2000	4	72.90
59	2000	4	70.97
60	1225	4	69.26
61	1400	4	70.97
63	2000	4	70.97

Suppl. Table 8 — Toxicity analysis (obtained from ProTox-II server and Osiris property explorer) of all the low binding energy variations of Toloxatone

Variation No.	Toxicity Studies					
	ProTox-II server				Osiris Property Explorer	
	Immunotoxicity	Cytotoxicity	Carcinogenicity	Mutagenicity	Irritation	Rep Eff
27	Iav	Iav	Iav	Iav	Iav	Iav
28	Iav	Iav	Iav	Iav	Iav	Iav
29	Iav	Iav	Iav	Iav	Iav	Iav
30	Iav	Iav	Iav	Iav	Iav	Iav
31	Iav	Iav	Iav	Iav	Iav	AC
32	Iav	Iav	Iav	Iav	AC	Iav
33	Iav	Iav	Iav	Iav	Iav	Iav
34	Iav	Iav	Iav	Iav	Iav	Iav
35	Iav	Iav	Iav	Iav	Iav	Iav
36	Iav	Iav	Iav	Iav	Iav	Iav
37	Iav	Iav	Iav	Iav	Iav	Iav
38	Iav	Iav	Iav	Iav	Iav	Iav
39	Iav	Iav	Iav	Iav	Iav	Iav
42	Iav	Iav	Iav	Iav	Iav	Iav
43	Iav	Iav	Iav	Iav	AC	Iav
44	Iav	Iav	Iav	Iav	AC	Iav
45	Iav	Iav	Iav	Iav	Iav	Iav
46	Iav	Iav	Iav	Iav	Iav	Iav
47	Iav	Iav	Iav	Iav	Iav	Iav
50	Iav	Iav	Iav	Iav	Iav	Iav
51	Iav	Iav	Iav	Iav	Iav	Iav
52	Iav	Iav	Iav	Iav	Iav	Iav

53	Iav	Iav	Iav	Iav	Iav	Iav
54	Iav	Iav	Iav	Iav	Iav	Iav
56	Iav	Iav	Iav	Iav	Iav	Iav
57	Iav	Iav	Iav	Iav	Iav	AC
59	Iav	Iav	Iav	Iav	Iav	Iav
60	Iav	Iav	Iav	Iav	Iav	Iav
61	Iav	Iav	Iav	Iav	Iav	Iav
63	Iav	Iav	Iav	Iav	Iav	Iav

Suppl. Table 9 — Drug-likeness of all the low binding energy variations ofBrofaromine

Variation No.	Drug likeness- Lipinski rule of five				
	Mass (g/mol)	Hydrogen donors (in number)	Hydrogen Acceptors (in number)	Log P (Lipophilicity)	Molar Refractivity
67	366.29	5.30	3	1	98.47
68	386.28	5.67	3	1	104.64
69	342.19	3.41	5	3	83.25
72	324.21	4.31	3	1	84.17
74	386.28	5.67	3	1	104.64
77	386.28	5.39	3	1	103.69
79	366.29	5.41	3	1	98.17
80	352.27	5.02	3	1	93.62
82	325.20	4.16	3	2	83.61
83	324.21	4.31	3	1	84.17
84	386.28	5.67	3	1	104.64
85	352.27	5.12	3	1	93.78
86	338.24	4.56	3	1	88.98
87	328.18	4.14	4	1	79.16
89	326.19	3.10	4	2	80.25
90	324.21	4.17	3	1	83.89

Suppl. Table 10 — Physicochemical characteristics of all the low binding energy variations of Brofaromine

No.	Topological Polar Surface area(Å^2)	Log s(solubility)	FractionCsp^3 (saturation)	Number of rotational bonds	Blood-brain barrier	Bio-availability	GI absorption	Pain alerts
67	34.4	−5.25, Moderately soluble	0.56	3	Y	0.55	High	0
68	34.4	−5.5, Moderately soluble	0.30	3	Y	0.55	High	0
69	74.86	−4.04, Moderately soluble	0.43	2	Y	0.55	High	0
72	34.4	−4.27,Moderately soluble	0.47	2	Y	0.55	High	0
74	34.4	−5.5, Moderately soluble	0.30	3	Y	0.55	High	0
77	34.4	−5.35, Moderately soluble	0.30	3	Y	0.55	High	0
79	34.4	−5.35, Moderately soluble	0.56	3	Y	0.55	High	0
80	34.4	−5, Moderately soluble	0.53	3	Y	0.55	High	0
82	60.42	−3.62, Soluble	0.43	2	Y	0.55	High	0
83	34.4	−4.27, Moderately soluble	0.47	2	Y	0.55	High	0
84	34.4	−5.5, Moderately soluble	0.30	3	Y	0.55	High	0
85	34.4	−4.83, Moderately soluble	0.53	3	Y	0.55	High	0
86	34.4	−5.92, Moderately soluble	0.50	3	Y	0.55	High	0
87	34.4	−4.13, Moderately soluble	0.43	2	Y	0.55	High	0
89	54.63	−3.37, Soluble	0.43	2	Y	0.55	High	0
90	34.4	−4.39, Moderately soluble	0.47	2	Y	0.55	High	0

Suppl. Table 11 — The median lethal dose, toxicity class number and the accuracy of prediction of ProTox-II server, for of all the low binding energy variations of Brofaromine

Variation number	Oral Lethal dose50% (mg/kg)	Toxicity class number	Accuracy of the prediction (%)
67	500	4	68.07
68	1195	4	67.38
69	1000	4	68.07
72	2000	4	68.07
74	1170	4	67.38
77	190	3	68.07
79	1000	4	68.07
80	1000	4	68.07
82	1000	4	68.07
83	500	4	68.07
84	500	4	67.38
85	500	4	68.07
86	500	4	67.38
87	1000	4	68.07
89	190	3	68.07
90	190	3	100

Suppl. Table 12 — Toxicity analysis (obtained from ProTox-II server and Osiris property explorer) of all the low binding energy variations of Brofaromine

Variation No.	Toxicity Studies					
	ProTox-II server				Osiris Property Explorer	
	Immunotoxicity	Cytotoxicity	Carcinogenicity	Mutagenty	Irritation	Rep Eff
67	Iav	Iav	Iav	Iav	Iav	Iav
68	Iav	Iav	Iav	Iav	Iav	Iav
69	AC	Iav	Iav	Iav	Iav	Iav
72	Iav	Iav	Iav	Iav	Iav	Iav
74	Iav	Iav	Iav	Iav	Iav	AC
77	Iav	Iav	Iav	Iav	Iav	Iav
79	Iav	Iav	Iav	Iav	Iav	Iav
80	AC	Iav	Iav	Iav	Iav	Iav
82	AC	Iav	AC	AC	Iav	Iav
83	Iav	Iav	Iav	Iav	Iav	Iav
84	AC	Iav	Iav	Iav	Iav	Iav
85	Iav	Iav	Iav	Iav	Iav	Iav
86	Iav	Iav	Iav	Iav	Iav	Iav
87	Iav	Iav	Iav	Iav	Iav	Iav
89	Iav	Iav	Iav	Iav	Iav	Iav
90	Iav	Iav	Iav	Iav	Iav	Iav

Suppl. Table 13 — Drug-likeness of all the low binding energy variations of Selegiline

Variation No.	Drug-likeness- Lipinski rule of five				
	Mass(g/mol)	Hydrogen donors (in numbers)	Hydrogen Acceptors (in numbers)	Log P (Lipophilicity)	Molar Refractivity
93	263.38	0	1	3.85	86.74
94	269.42	0	1	4.23	88.20
96	277.40	0	1	3.77	90.76

99	277.40	0	1	3.77	90.76
100	263.38	0	1	3.85	86.74
101	269.42	0	1	4.23	88.20
104	243.39	0	1	3.48	80.58
105	263.38	0	1	3.85	86.74
106	269.42	0	1	4.23	88.20
108	277.40	0	1	3.77	90.76
115	263.38	0	1	3.92	85.79
116	269.42	0	1	4.13	88.04
117	277.40	0	1	3.79	90.60

Suppl. Table 14 — Physicochemical characteristics of all the low binding energy variations of Selegiline

No.	Topological Polar Surface area ((Å^2))	Log s (solubility)	Fraction Csp^3 (saturation)	Number of rotational bonds	bbb	Bio-availability	GI absorption	Pain alerts
93	3.24	−4.44, Moderately soluble	0.26	5	Y	0.55	High	0
94	3.24	−4.74, Moderately soluble	0.58	5	Y	0.55	High	0
96	3.24	−4.62, Moderately soluble	0.30	6	Y	0.55	High	0
99	3.24	−4.62, Moderately soluble	0.30	6	Y	0.55	High	0
100	3.24	−4.44, Moderately soluble	0.26	5	Y	0.55	High	0
101	3.24	−4.82, Moderately soluble	0.58	5	Y	0.55	High	0
104	3.24	−4.14, Moderately soluble	0.53	5	Y	0.55	High	0
105	3.24	−4.44, Moderately soluble	0.26	5	Y	0.55	High	0
106	3.24	−4.82, Moderately soluble	0.58	5	Y	0.55	High	0
108	3.24	−4.62, Moderately soluble	0.30	6	Y	0.55	High	0
115	3.24	−4.4, Moderately soluble	0.26	5	Y	0.55	High	0
116	3.24	−4.66, Moderately soluble	0.58	5	Y	0.55	High	0
117	3.24	−4.59, Moderately soluble	0.30	6	Y	0.55	High	0

Suppl. Table 15 — The oral rat median lethal dose, toxicity class number and the accuracy of prediction of ProTox-II server, for all the low binding energy variations of Selegiline.

Variation number	Oral rat Lethal dose 50% (mg/kg)	Toxicity class number	Accuracy of the prediction (%)
93	385	4	68.07
94	267	3	69.26
96	385	4	54.26
99	385	4	69.26
100	385	4	69.26
101	385	4	69.26
104	385	4	72.90

105	75	3	69.26
106	385	4	69.26
108	75	3	69.26
115	225	3	70.97
116	95	3	69.26
117	385	4	69.26

Suppl. Table 16 — Toxicity analysis (obtained from ProTox-II server and Osiris property explorer) of all the low binding energy variations of Selegiline.

Variation No.	Toxicity Studies					
	Protox-II server				Osiris Property Explorer	
	Immunotoxicity	Cytotoxicity	Carcinogenicity	Mutagenicity	Irritation	Rep Eff[#]
93	Iav	Iav	Iav	Iav	Iav	Iav
94	Iav	Iav	Iav	Iav	Iav	Iav
96	Iav	Iav	Iav	Iav	Iav	Iav
99	Iav	Iav	Iav	Iav	Iav	Iav
100	Iav	Iav	Iav	Iav	Iav	Iav
101	Iav	Iav	Iav	Iav	Iav	Iav
104	Iav	Iav	Iav	Iav	AC	AC
105	Iav	Iav	Iav	Iav	Iav	Iav
106	Iav	Iav	Iav	Iav	Iav	Iav
108	Iav	Iav	Iav	Iav	Iav	Iav
115	Iav	Iav	Iav	Iav	Iav	Iav
116	Iav	Iav	Iav	Iav	Iav	Iav
117	Iav	Iav	Iav	Iav	Iav	Iav

Suppl. Table 17 — Drug-likeness of all the low binding energy variations of Rasagiline

Variation No.	Drug likeliness- Lipinski rule of five				
	Mass (g/mol)	Hydrogen donors (in numbers)	Hydrogen Acceptors (in numbers)	Log P (Lipophilicity)	Molar Refractivity
120	247.33	1	1	3.95	79.89
121	253.38	1	1	4.34	81.34
123	186.25	2	1	2.45	58.86
124	185.26	1	1	2.60	59.42
125	227.34	1	1	3.59	73.72
126	247.33	1	1	3.95	79.89
127	253.38	1	1	4.34	81.34
130	227.34	1	1	3.59	73.72
131	199.29	1	1	2.85	64.22
132	247.33	1	1	3.95	79.89
133	253.38	1	1	4.34	81.34
139	247.33	1	1	3.95	79.89
140	253.38	1	1	4.34	81.34
141	187.24	2	2	1.99	56.47
142	186.25	2	1	2.45	58.86
143	199.29	1	1	3.24	64.07
144	247.33	1	1	3.88	78.94
145	253.38	1	1	4.41	81.18
147	186.25	2	2	2.45	57.16
148	187.24	2	2	1.26	55.61
150	189.23	1	2	2.24	54.5
151	247.33	1	1	3.68	78.94
152	227.34	1	1	3.56	73.42

153	199.29	1	1	2.92	64.07
154	187.24	2	2	1.61	55.61
155	186.25	2	2	2.27	57.16
156	227.34	1	1	3.70	73.42
157	199.29	1	1	3.07	64.07
158	247.33	1	1	4.03	78.94

Suppl. Table 18 — Physicochemical characteristics of all the low binding energy variations of Rasagiline

No.	Topological Polar Surface area(Å^2)	Log s (solubility)	Fraction Csp^3 (saturation)	Number of rotational bonds	bbb	Bio-availability	GI absorption	Pain alerts
120	12.03	−3.82, Soluble	0.22	3	Y	0.55	High	0
121	12.03	−4.2, Moderately soluble	0.56	3	Y	0.55	High	0
123	38.05	−1.9, Very soluble	0.33	2	Y	0.55	High	0
124	12.03	−3.11, Soluble	0.47	3	Y	0.55	High	0
125	12.03	−3.52, Soluble	0.5	3	Y	0.55	High	0
126	12.03	−3.82, Soluble	0.22	3	Y	0.55	High	0
127	12.03	−4.2, Moderately soluble	0.56	3	Y	0.55	High	0
130	12.03	−3.52, Soluble	0.5	3	Y	0.55	High	0
131	12.03	−2.83, Soluble	0.43	3	Y	0.55	High	0
132	12.03	−3.82, Soluble	0.22	3	Y	0.55	High	0
133	12.03	−4.2, Moderately soluble	0.56	3	Y	0.55	High	0
139	12.03	−3.82, Soluble	0.22	3	Y	0.55	High	0
140	12.03	−4.2, Moderately soluble	0.56	3	Y	0.55	High	0
141	32.26	−2.12, Soluble	0.33	2	Y	0.55	High	0
142	38.05	−1.9, Very soluble	0.33	2	Y	0.55	High	0
143	12.03	−2.87, Soluble	0.43	3	Y	0.55	High	0
144	12.03	−3.71, Soluble	0.22	3	Y	0.55	High	0
145	12.03	−4.19, Moderately soluble	0.56	3	Y	0.55	High	0
147	38.05	−1.47, Very soluble	0.33	2	Y	0.55	High	0
148	32.26	−1.73, Very soluble	0.33	2	Y	0.55	High	0
150	12.03	−2.38, Soluble	0.33	2	Y	0.55	High	0
151	12.03	−3.67, Soluble	0.22	3	Y	0.55	High	0
152	12.03	−3.49, Soluble	0.5	3	Y	0.55	High	0
153	12.03	−2.82, Soluble	0.43	3	Y	0.55	High	0
154	32.26	−1.99, Very soluble	0.33	2	Y	0.55	High	0
155	38.05	−1.82, very soluble	0.33	2	Y	0.55	High	0
156	12.03	−3.26, Soluble	0.47	3	Y	0.55	High	0
157	12.03	−2.91, Soluble	0.43	3	Y	0.55	High	0
158	12.03	−3.87, Soluble	0.22	3	Y	0.55	High	0

Suppl. Table 19 — The oral rat lethal dose, toxicity class number and the accuracy of prediction of ProTox-II server, for all the low binding energy variations of Rasagiline

Variation number	Oral rat Lethal dose 50%(mg/kg)	Toxicity class number	Accuracy of the prediction (%)
120	753	4	68.07
121	753	4	69.26
123	250	3	68.07
124	2500	5	70.97
125	2500	5	70.97
126	2500	5	69.26
127	753	4	69.26
130	2500	5	69.26
131	2500	5	69.26

132	2500	5	69.26
133	753	4	69.26
139	753	4	68.07
140	753	4	68.07
141	347	4	69.26
142	250	3	68.07
143	753	4	69.26
144	250	3	70.97
145	753	4	69.26
147	250	3	69.26
148	753	4	69.26
150	250	3	69.26
151	753	4	69.26
152	250	3	72.9
153	250	3	72.9
154	370	4	69.26
155	250	3	69.26
156	753	4	70.97
157	753	4	70.97
158	250	3	69.26

Suppl. Table 20 — Toxicity analysis (obtained from ProTox-II server and Osiris property explorer) of all the low binding energy variations of Rasagiline.

Variation No	Toxicity Studies					
	ProTox-II server				Osiris Property Explorer	
	Immunotoxicity	Cytotoxicity	Carcinogenicity	Mutagenicity	Irritation	Rep Eff
120	Iav	Iav	Iav	AC	Iav	Iav
121	Iav	Iav	Iav	Iav	Iav	Iav
123	Iav	Iav	Iav	Iav	Iav	Iav
124	Iav	Iav	Iav	Iav	Iav	Iav
125	Iav	Iav	Iav	Iav	Iav	Iav
126	Iav	Iav	Iav	AC	Iav	Iav
127	Iav	Iav	Iav	Iav	Iav	Iav
130	Iav	Iav	Iav	Iav	Iav	Iav
131	Iav	Iav	Iav	Iav	Iav	Iav
132	Iav	Iav	Iav	AC	Iav	Iav
133	Iav	Iav	Iav	Iav	Iav	Iav
139	Iav	Iav	Iav	AC	Iav	Iav
140	Iav	Iav	Iav	Iav	Iav	Iav
141	Iav	Iav	Iav	Iav	Iav	Iav
142	Iav	Iav	Iav	Iav	Iav	Iav
143	Iav	Iav	Iav	Iav	Iav	Iav
144	Iav	Iav	Iav	Iav	Iav	Iav
145	Iav	Iav	Iav	Iav	Iav	Iav
147	Iav	Iav	Iav	Iav	Iav	Iav
148	Iav	Iav	Iav	Iav	Iav	Iav
150	Iav	Iav	Iav	Iav	Iav	Iav
151	Iav	Iav	Iav	Iav	Iav	Iav
152	Iav	Iav	Iav	Iav	Iav	Iav
153	Iav	Iav	Iav	Iav	Iav	Iav
154	Iav	Iav	Iav	Iav	Iav	Iav
155	Iav	Iav	Iav	Iav	Iav	Iav
156	Iav	Iav	Iav	Iav	Iav	Iav
157	Iav	Iav	Iav	Iav	Iav	Iav

158	Iav	Iav	Iav	AC	Iav	Iav