Electronic Supplementary Information

LogP values were calculated (ChemAxon) for 55 drug and drug like compounds, including 25 indoleamines and compared to experimental data available in the literature and gave excellent correlation r^2=0.914 (Figure 4). Compounds and data are given in the supplementary data.

Compound	CAS No.	Measured logP	Ref	Calculated logP*
indomethacin	53-86-1	3.52	Avdeef (2003)	3.53
propoanolol	525-66-6	3.48	Avdeef (2003)	2.58
phenol	108-95-2	1.48	Avdeef (2003)	1.67
diclofenac	15307-86-5	4.51	Avdeef (2003)	4.26
benzoic acid	65-85-0	1.96	Avdeef (2003)	1.63
2-aminobenzoic acid	118-92-3	1.26	Avdeef (2003)	1.45
theophyline	58-55-9	0.00	Avdeef (2003)	-0.81
furosemide	54-31-9	2.56	Avdeef (2003)	1.75
thioacetamide	62-55-5	-0.26	Hansh (1995	-0.14
domperidone	57808-66-9	3.90	El Tater (1985)	2.90
acetanilide	103-84-4	1.13	Baena (2005)	1.21
salicyclic acid	69-72-7	2.19	Avdeef (2003)	1.98
acetic acid	64-19-7	-0.30	Avdeef (2003)	-0.22
benzylamine	100-46-9	1.09	Iwasa (1965)	1.10
methylparaben	99-76-3	1.96	Pomana (1987)	1.67
Acetaminophen	103-90-2	0.44	Beana (2004)	0.91
phenacetin	62-44-2	1.48	Beana (2004)	1.41
4-aminophenol	123-30-8	0.04	Hansch (1995)	0.84
caffeine	58-08-2	-0.07	Hansch (1995)	-0.55
clonazepan	1622-61-3	3.02	Avdeef (2003)	3.15
amitryptyline	50-48-6	4.62	Avdeef (2003)	4.81
chloropheniramine	132-22-9	3.39	Avdeef (2003)	3.58
amiloride.HCl	2016-88-8	-0.30	Narasimham (2011)	0.04
ibuprofen	15687-27-1	4.13	Avdeef (2003)	3.84
phenytoin	57-41-0	2.47	Hansch (1995)	1.93
diphenylhydramine. HCl	58-73-1	3.18	Avdeef (2003)	3.65
chloroprozamin.HCl	69-09-0	5.40	Avdeef (2003)	3.93
benzamide	55-21-0	0.64	Sangster (1989)	0.82
cyclohexane	110-82-7	3.44	Sangster (1989)	2.67
cyclohexene	110-83-8	2.86	Sangster (1989)	2.31
serotonin	153-98-0	0.21	Hansch (1995)	0.48
indole	120-72-9	2.14	Sangster (1989)	1.80
1-methylindole	603-76-9	2.71	Sangster (1989)	2.30
2-methylindole	95-20-5	2.53	Sangster (1989)	2.27
3-methylindole	83-34-1	2.63	Sangster (1989)	2.59
5-methylindole	614-96-0	2.68	Sangster (1989)	2.59
1,2-dimethylindole	875-79-6	2.82	Sangster (1989)	2.50
melatonin	73-31-4	1.20	Mor (2004)	1.15
tryptophan	73-22-3	-1.06	Urakami (2003)	-1.09
tryptamine	61-54-1	1.41	Hansch (1995)	1.49

N-acetylserotonin	616-91-1	0.44	Mor (2003)	1.00
5-Methoxytryptamine	608-07-1	1.34	Mor (2004)	1.33
6-hydroxymelatonin	2208-41-5	1.82		0.84
3-indoleacetic acid	87-51-4	1.71	Hansch (1995)	1.1
5-hydroxy-3-indoleacetic acid	54-16-0	2.1	Siren (2004)	1.41
N-acetyltryptamine	1016-47-3	1.34	Mor (2003)	1.31
harmine	442-51-3	2.87	Hansch (1995)	1.85
AFK	Not available	0.74	Harthe (2003)	0.33
AFMK	52450-38-1	0.48	Harthe (2003)	0.34
N-[2-(5-Methyl-1H-indol-2-yl)-ethyl]-acetamide	Not available	2.14	Spadoni (2006)	1.35
N-[2-(5-Fluoro-1H-indol-2-yl)-ethyl]-acetamide	Not available	1.99	Spadoni (2006)	1.29
N-[2-(5-Chloro-1H-indol-2-yl)-ethyl]-acetamide	Not available	2.67	Spadoni (2006)	1.75
5-Hydroxy-N-formylkynurenine	Not available	-2.53	Wishart (2007)	-2.19
6-methoxy-N-acetyltryptamine	Not available	1.28	Mor (2003)	1.15

* Calculated with Chemaxon

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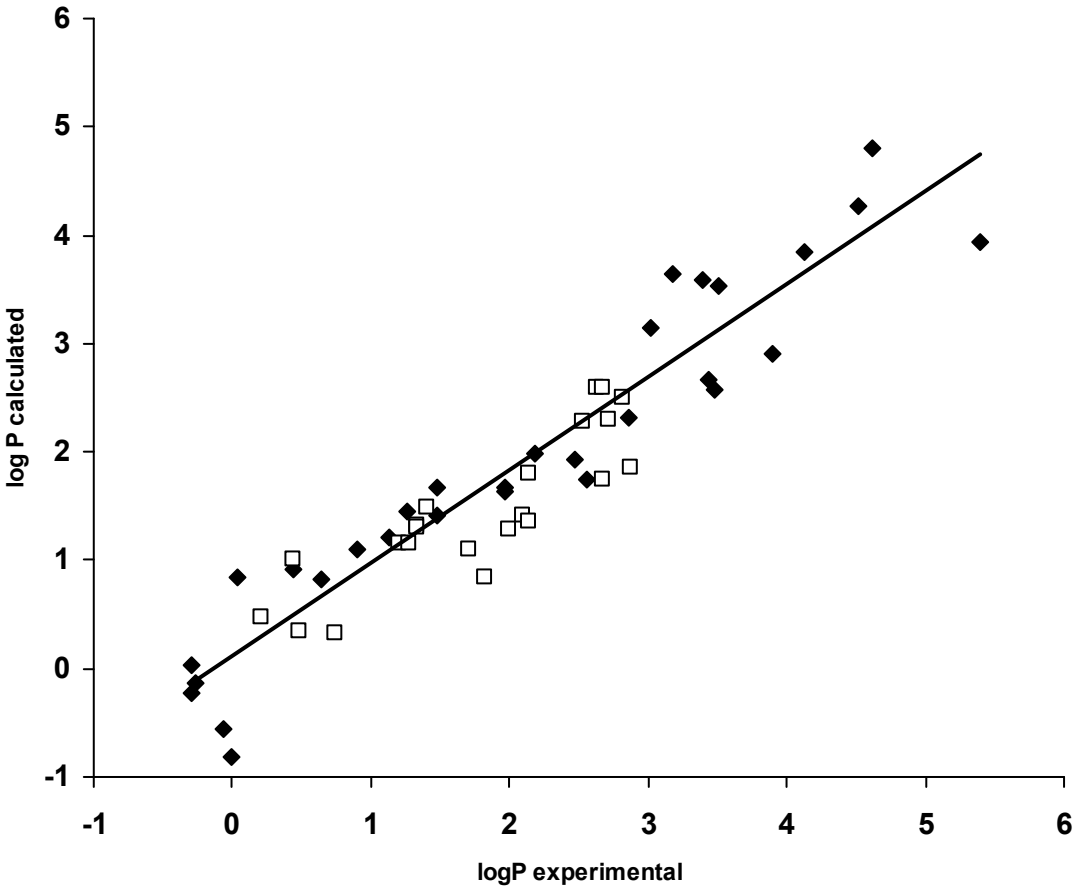
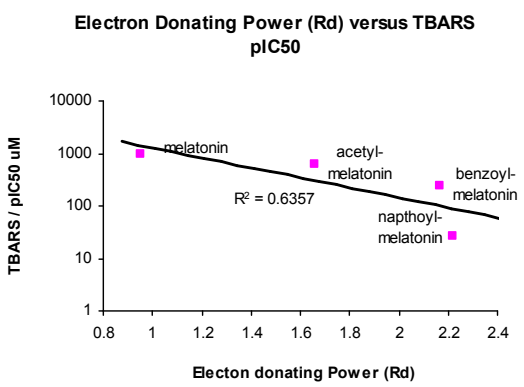
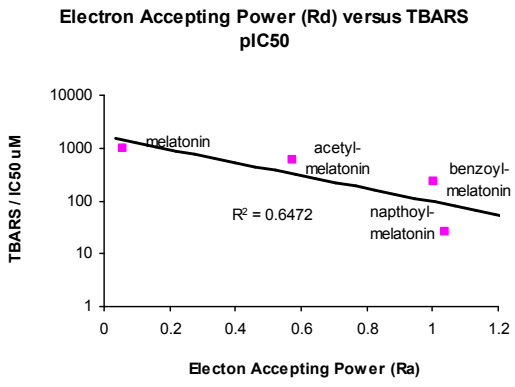
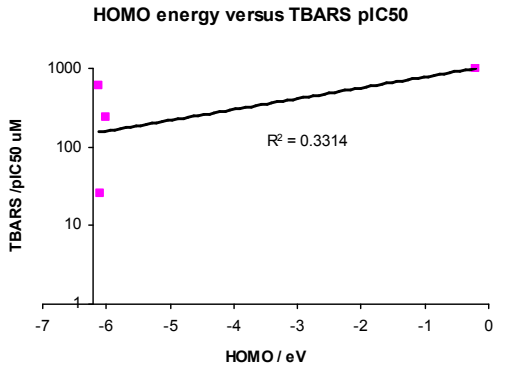
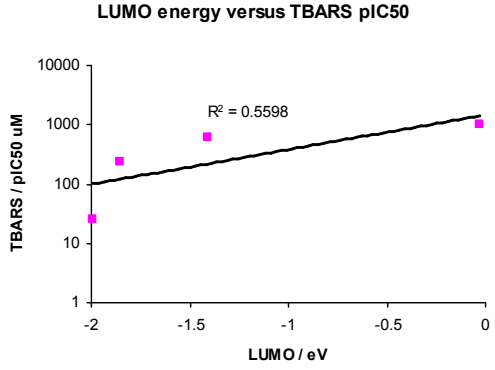


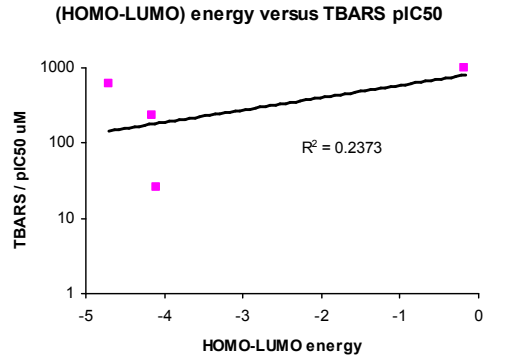
Figure 4. Correlation between experimentally measured logP and logP calculated with Marvin (ChemAxon) Correlation $r^2 = 0.952$, N=54. Indoleamines shown in open squares, other as diamonds.

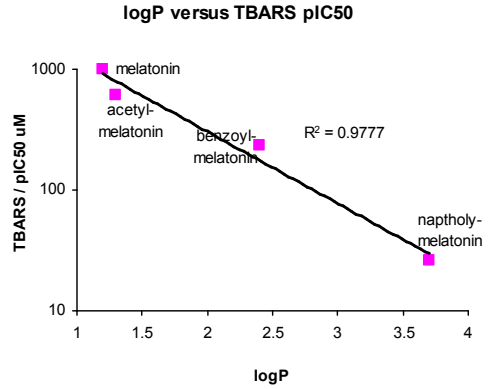

Electron Donating Power (Rd) versus TBARS pIC50
TBARS / pIC50 uM
10000
1000
100
10
1
melatonin
acetyl-melatonin
benzoyl-melatonin
napthoyl-melatonin
R² = 0.6357
0.8
1
1.2
1.4
1.6
1.8
2
2.2
2.4
Electon donating Power (Rd)

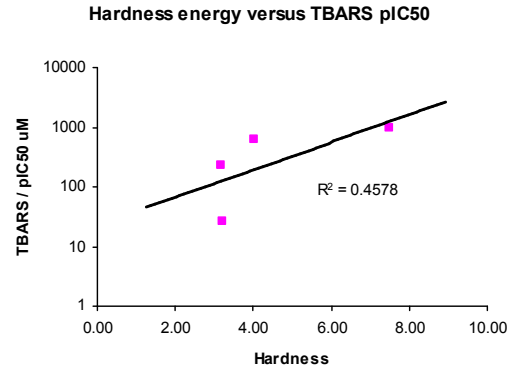

Electron Accepting Power (Rd) versus TBARS pIC50
TBARS / IC50 uM
10000
1000
100
10
1
melatonin
acetyl-melatonin
benzoyl-melatonin
napthoyl-melatonin
R² = 0.6472
0
0.2
0.4
0.6
0.8
1
1.2
Electon Accepting Power (Ra)

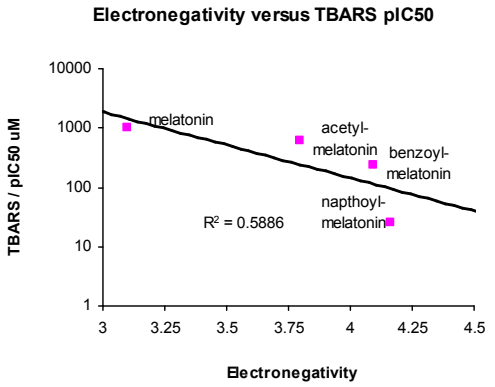

HOMO energy versus TBARS pIC50
TBARS /pIC50 uM
1000
100
10
1
R² = 0.3314
-7
-6
-5
-4
-3
-2
-1
0
HOMO / eV

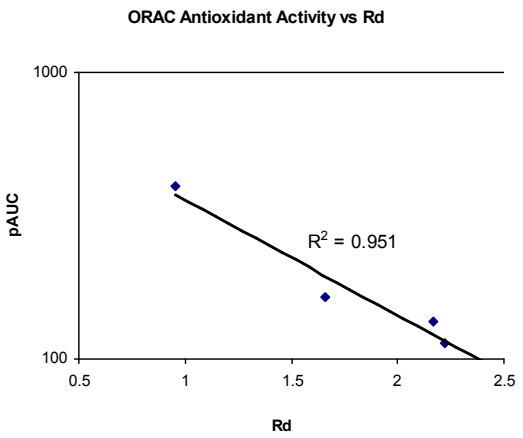

LUMO energy versus TBARS pIC50
TBARS / pIC50 uM
10000
1000
100
10
1
R² = 0.5598
-2
-1.5
-1
-0.5
0
LUMO / eV

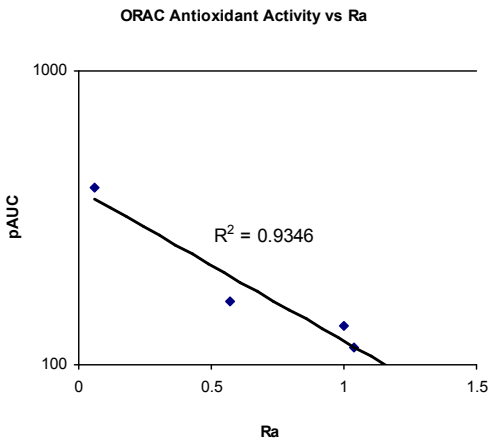

(HOMO-LUMO) energy versus TBARS pIC50
TBARS / pIC50 uM
1000
100
10
1
R² = 0.2373
-5
-4
-3
-2
-1
0
HOMO-LUMO energy

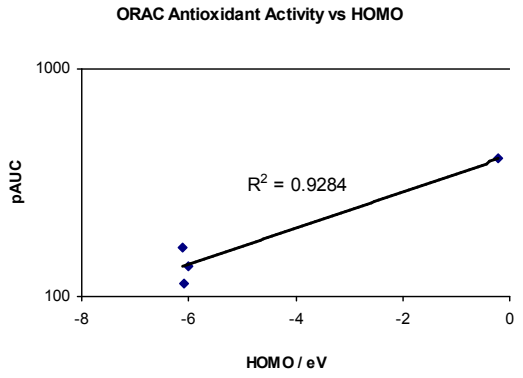

logP versus TBARS pIC50
TBARS / pIC50 uM
1000
100
10
melatonin
acetyl-melatonin
benzoyl-melatonin
napthoyl-melatonin
R² = 0.9777
1
1.5
2
2.5
3
3.5
4
logP

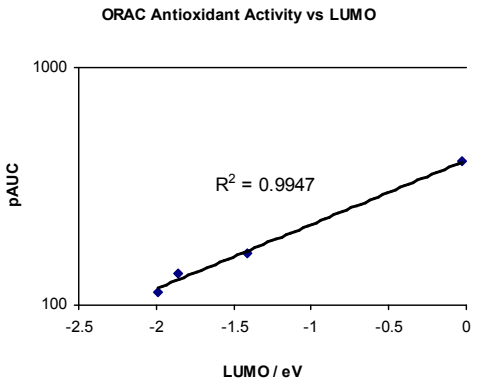

Hardness energy versus TBARS pIC50
TBARS / pIC50 uM
10000
1000
100
10
1
R² = 0.4578
0.00
2.00
4.00
6.00
8.00
10.00
Hardness

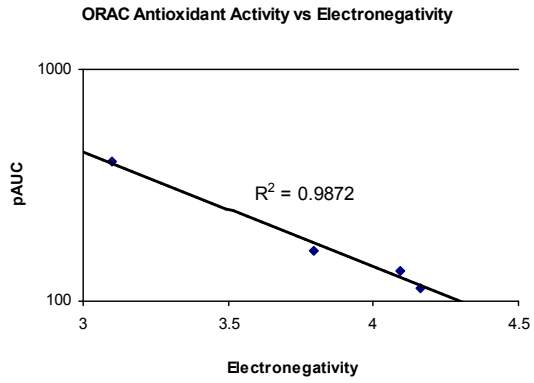

Electronegativity versus TBARS pIC50
TBARS / pIC50 uM
10000
1000
100
10
1
melatonin
acetyl-melatonin
benzoyl-melatonin
napthoyl-melatonin
R² = 0.5886
3
3.25
3.5
3.75
4
4.25
4.5
Electronegativity

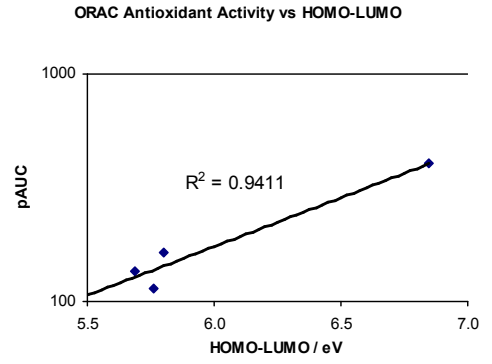

ORAC Antioxidant Activity vs Rd
1000
100
pAUC
R2 = 0.951
0.5
1
1.5
2
2.5
Rd

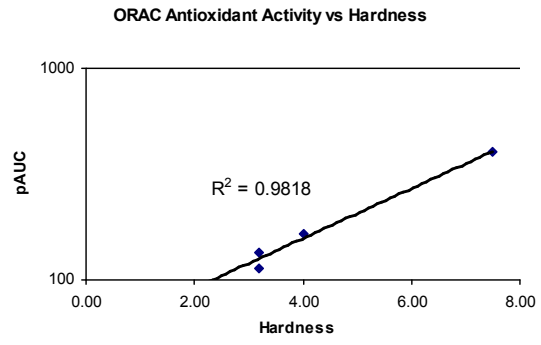

ORAC Antioxidant Activity vs Ra
1000
100
pAUC
R2 = 0.9346
0
0.5
1
1.5
Ra

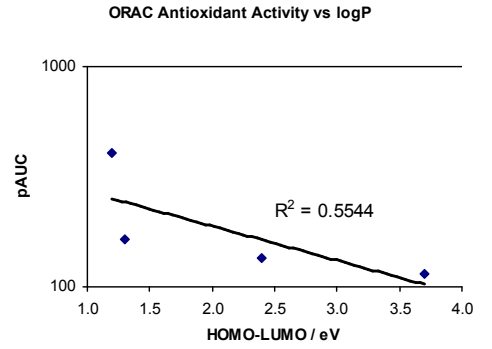

ORAC Antioxidant Activity vs HOMO
1000
100
pAUC
R2 = 0.9284
-8
-6
-4
-2
0
HOMO / eV


ORAC Antioxidant Activity vs LUMO
1000
100
pAUC
R2 = 0.9947
-2.5
-2
-1.5
-1
-0.5
0
LUMO / eV


ORAC Antioxidant Activity vs Electronegativity
1000
100
pAUC
R2 = 0.9872
3
3.5
4
4.5
Electronegativity


ORAC Antioxidant Activity vs HOMO-LUMO
1000
100
pAUC
R2 = 0.9411
5.5
6.0
6.5
7.0
HOMO-LUMO / eV


ORAC Antioxidant Activity vs Hardness
1000
100
pAUC
R2 = 0.9818
0.00
2.00
4.00
6.00
8.00
Hardness


ORAC Antioxidant Activity vs logP
1000
100
pAUC
R2 = 0.5544
1.0
1.5
2.0
2.5
3.0
3.5
4.0
HOMO-LUMO / eV