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Corrigendum

Corrigendum to "Estimating skin permeability from physicochemical characteristics of drugs: A comparison between conventional models and an in vivo-based approach" [Int. J. Pharmaceut. 375 (1–2) (2009) 41–47]

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In page 42, the unit for C_{max} in Eq. (1) should be ml^{-1}.
Values reported in column "S_w" in Table 2, should be revised as shown in the corrected format.

Table 2
Parameters used for flux calculation.

Drug	Active ingredient	MW[a,b]	Log K_{oct}[c,d]	HA[e,f]	HD[f,g]	Expected $A{\cdot}J$ (delivery rate)[h] (ng/h)	$CL^{i}_{transdermal}$ (ml/h)	A^{j} (cm^2)	S_w (ng/ml)	Observed C_{max}[m] (ng/ml)
TD Scop	Scopolamine	303.35	1.24	5	1	5.00E+03	5.00E+04	2.5	6.61E+06	1.00E−01
Oxytrol	Oxybutynin	357	4.3	4	1	1.63E+05	4.28E+04	39	8E+05[b]	3.80E+00
Androderm	Testosteone	288.42	3.32	2	1	1.04E+05	1.98E+04	37	4E+04[k]	5.25E+00
Exelon	Rivastigmine	250.34	1.98	3	0	3.96E+05	5.82E+04	10	5E+07	6.80E+00
Orthoevra-evra	Norelgestromin	327.46	4	3	2	6.25E+03	6.17E+03	20	8.80E+03[k]	1.01E+00
Daytrana	Methylphenidate	233.31	3.65	3	1	3.33E+06	7.17E+04	37.5	1E+05	4.65E+01
EMSAM	Selegiline	187.3	2.7	1	0	2.50E+05	1.40E+05	20	5E+07	1.79E+00
Estraderm	Estradiol	272.39	4.01	2	2	2.08E+03	4.58E+04	18	3.60E+03[k]	4.55E−02
Estradot	Estradiol	272.39	4.01	2	2	4.17E+03	4.12E+04	10	3.60E+03[k]	1.01E−01
Menorest	Estradiol	272.39	4.01	2	2	4.17E+03	3.60E+04	29	3.60E+03[k]	1.02E−01
Menostar	Estradiol	272.39	4.01	2	2	5.83E+02	2.83E+04	3.25	3.60E+03[k]	2.06E−02
Oesclim	Estradiol	272.39	4.01	2	2	4.17E+03	3.57E+04	44	3.60E+03[k]	1.17E−01
Tradelia	Estradiol	272.39	4.01	2	2	2.08E+03	4.34E+04	18	3.60E+03[k]	4.80E−02
Habitrol	Nicotine	162.23	1.17	2	0	8.75E+05	4.17E+04	30	1E+09[l]	21
Nicotine-alza	Nicotine	162.23	1.17	2	0	8.75E+05	4.00E+04	12	1E+09[l]	2.19E+01
Nitroderm	Nitroglycerin	227.11	1.62	9	0	4.00E+05	4.00E+06	20	1.25E+06[b]	1.02E−01
Nitro-Dur	Nitroglycerin	227.11	1.62	9	0	4.00E+05	1.04E+06	20	1.25E+06[b]	1.00E−01
Nitro-Dur-2	Nitroglycerin	227.11	1.62	9	0	4.00E+05	8.58E+05	20	1.25E+06[b]	4.66E−01

[a] Molecular weight.
[b] Data obtained from Budavari (1989).
[c] Logarithmically transformed octanol water partition coefficient.
[d] Data is taken from Hansch et al. (1995).
[e] Number of hydrogen bond acceptor groups on the molecule.
[f] Data compiled from Pubchem.
[g] Number of hydrogen bond donor groups on the molecule.
[h] Labeled delivery rates are cited data of Anonymous (2006).
[i] Transdermal clearance was calculated using labeled delivery rate of transdermal systems and corresponding C_{max} values reported for them.
[j] Patch surface areas obtained from PDR (2006).
[k] Reported by Miura et al. (2006).
[l] Obtained from EPIsuite v.4 (experimental database).
[m] Data obtained from (Farahmand and Maibach, 2009).

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Table 3
Predicted fluxes (ng/cm^2 h) by different models.

Drug	Active ingredient	Observed in vivo	In vivo model	Model 1	Model 2	Model 3	Model 4	Model 5	Model 6
TD Scop	Scopolamine	1.94E+03	2.13E+03	1.13E+02	3.17E+03	1.55E+03	1.31E+03	5.77E+02	7.32E+02
Oxytrol	Oxybutynin	3.98E+03	3.41E+03	1.24E+03	7.73E+03	9.92E+03	1.23E+04	1.44E+04	2.68E+04
Androderm	Testosteone	2.20E+03	1.76E+03	6.06E+01	2.67E+02	2.86E+02	3.20E+02	1.65E+02	5.75E+02
Exelon	Rivastigmine	5.25E+04	5.72E+04	9.05E+04	1.06E+05	7.74E+04	7.22E+04	2.21E+04	7.17E+04
Orthoevra-evra	Norelgestromin	1.30E+02	5.69E+03	1.72E+01	8.38E+01	1.04E+02	1.24E+02	1.04E+02	2.63E+02
Daytrana	Methylphenidate	9.58E+04	1.03E+05	1.33E+03	1.86E+03	2.58E+03	2.67E+03	1.02E+03	5.94E+03
EMSAM	Selegiline	1.25E+04	2.12E+04	3.67E+05	5.13E+05	5.69E+05	5.58E+05	1.25E+05	1.04E+06
Estraderm	Estradiol	5.51E+01	1.79E+02	3.28E+01	6.54E+01	9.36E+01	1.01E+02	5.67E+01	2.25E+02
Estradot	Estradiol	4.12E+02	6.63E+02	3.28E+01	6.54E+01	9.36E+01	1.01E+02	5.67E+01	2.25E+02
Menorest	Estradiol	1.59E+02	2.28E+02	3.28E+01	6.54E+01	9.36E+01	1.01E+02	5.67E+01	2.25E+02
Menostar	Estradiol	1.79E+02	9.81E+01	3.28E+01	6.54E+01	9.36E+01	1.01E+02	5.67E+01	2.25E+02
Oesclim	Estradiol	7.58E+02	1.825E+03	3.28E+01	6.54E+01	9.36E+01	1.01E+02	5.67E+01	2.25E+02
Tradelia	Estradiol	1.16E+02	1.70E+02	3.28E+01	6.54E+01	9.36E+01	1.01E+02	5.67E+01	2.25E+02
Habitrol	Nicotine	2.92E+04	3.15E+04	7.33E+05	2.24E+06	1.53E+06	1.23E+06	1.90E+05	1.09E+06
Nicotine-alza	Nicotine	7.27E+03	7.55E+03	7.33E+05	2.24E+06	1.53E+06	1.23E+06	1.90E+05	1.09E+06
Nitroderm	Nitroglycerin	4.00E+04	4.26E+04	3.68E+02	2.26E+03	1.54E+03	1.35E+03	3.31E+02	1.20E+03
Nitro-Dur	Nitroglycerin	2.00E+04	2.17E+04	3.68E+02	2.26E+03	1.54E+03	1.35E+03	3.31E+02	1.20E+03
Nitro-Dur-2	Nitroglycerin	1.55e+04	1.466E+04	3.68E+02	2.26E+03	1.54E+03	1.35E+03	3.31E+02	1.20E+03

Drug	Active ingredient	Model 7	Model 8	Model 9	Model 10	Model 11	Model 12
TD Scop	Scopolamine	1.35E+03	7.76E+02	2.38E+03	9.07E+01	2.89E+03	2.78E+03
Oxytrol	Oxybutynin	1.14E+04	3.17E+04	5.24E+03	3.66E+06	8.23E+03	8.26E+03
Androderm	Testosteone	3.02E+02	4.25E+02	1.66E+02	4.71E+05	2.43E+02	2.47E+02
Exelon	Rivastigmine	7.21E+04	4.52E+04	6.90E+04	1.80E−08	8.75E+04	8.81E+04
Orthoevra-evra	Norelgestromin	1.17E+02	2.62E+02	5.38E+01	3.95E+04	8.35E+01	8.46E+01
Daytrana	Methylphenidate	2.81E+03	4.79E+03	1.05E+03	1.22E+06	1.52E+03	1.60E+03
EMSAM	Selegiline	5.67E+05	5.13E+05	3.09E+05	2.48E+09	3.76E+05	3.98E+05
Estraderm	Estradiol	1.05E+02	2.32E+02	3.76E+01	4.25E+04	5.82E+01	6.06E+01
Estradot	Estradiol	1.05E+02	2.32E+02	3.76E+01	4.25E+04	5.82E+01	6.06E+01
Menorest	Estradiol	1.05E+02	2.32E+02	3.76E+01	4.25E+04	5.82E+01	6.06E+01
Menostar	Estradiol	1.05E+02	2.32E+02	3.76E+01	4.25E+04	5.82E+01	6.06E+01
Oesclim	Estradiol	1.05E+02	2.32E+02	3.76E+01	4.25E+04	5.82E+01	6.06E+01
Tradelia	Estradiol	1.05E+02	2.32E+02	3.76E+01	4.25E+04	5.82E+01	6.06E+01
Habitrol	Nicotine	1.32E+06	7.29E+05	1.55E+06	4.68E+09	1.52E+06	1.58E+06
Nicotine-alza	Nicotine	1.32E+06	7.29E+05	1.55E+06	4.68E+09	1.52E+06	1.58E+06
Nitroderm	Nitroglycerin	1.39E+03	7.68E+02	1.48E+03	7.92E+04	1.77E+03	1.79E+03
Nitro-Dur	Nitroglycerin	1.39E+03	7.68E+02	1.48E+03	7.92E+04	1.77E+03	1.79E+03
Nitro-Dur-2	Nitroglycerin	1.39E+03	7.68E+02	1.48E+03	7.92E+04	1.77E+03	1.79E+03

Table 4
Correlation of models with observed in vivo data, and the in vivo model[a,b].

Model no.	Correlation with observed in vivo data Spearman rank correlation coefficient	Correlation with in vivo model Spearman rank correlation coefficient
Model 1	0.83	0.66
Model 2	0.71	0.67
Model 3	0.76	0.71
Model 4	0.80	0.75
Model 5	0.76	0.71
Model 6	0.80	0.75
Model 7	0.80	0.75
Model 8	0.76	0.71
Model 9	0.71	0.67
Model 10	0.46	0.30
Model 11	0.71	0.67
Model 12	0.71	0.67

[a] n (total number of data points) = 18.
[b] All correlations were significant (p-value < 0.005) except for the correlations of model 10 with the observed in vivo data and the in vivo model.

In page 43, the last sentence in the Results section should be omitted, since the observation was based on an erroneous specification of water solubility for two of the compounds in Table 2: "The discrepancy between data and the prediction reaches the maximum (1000–10,000-fold underestimation) for nicotine (with the smallest molecular weight and log K_{oct}), nitroglycerin (with the largest number of hydrogen bond acceptor groups), and for oxybutynin (with the largest molecular weight and log K_{oct}) where the flux was overestimated by around 1000-fold."

Some values reported in Tables 3 and 4 should be as presented in corrected version.

Two of the data points representing nicotine and oxybutynin should be changed in Figure 1, as shown here.

In page 45, the last sentence of the 3rd paragraph should be omitted, as it was based on a wrong water solubility value for nicotine: "Nevertheless, flux for the smallest molecule with a low log K_{oct}, nicotine, has been largely underestimated by most in vitro-based equations."

Corrected Figure 1 legend: Comparison of different models predictive power according to the observed in vivo data; correlations with physicochemical parameters (a) molecular weight, (b) logarithmically transformed octanol water partition coefficient, and (c) number of hydrogen bond acceptor groups on the molecule.