

Supplementary Materials

Evaluating Molecular Properties Involved in Transport of Small Molecules in Stratum Corneum: A Quantitative Structure-Activity Relationship for Skin Permeability

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Table S1. List of compounds applied in development of quantitative structure-activity relationship for skin permeability prediction.

Table S2. List of values estimated for molecular descriptors and skin permeability using quantitative structure-activity relationship developed in this study for compounds applied in model training and validation.

Table S1. List of compounds applied in development of quantitative structure-activity relationship for skin permeability prediction. Relevant information includes the CAS number, chemical name, logarithmic value of experimentally observed skin permeability (observed $\log Kp$), molecular weight (MW), logarithmic value of octanol-water partition coefficient ($\log K_{ow}$), and stage of application in the model development for the 106 compounds included in the training and validation datasets.

CAS No.	Chemical Name	Observed			Modeling Stage
		$\log Kp$ (cm/h)	MW	$\log K_{ow}$	
[71-55-6]	1,1,1-Trichloroethane	-2.35	133.40	2.49	Training
[88-06-2]	2,4,6-Trichlorophenol	-1.23	197.50	3.69	Training
[120-83-2]	2,4-Dichlorophenol	-1.22	163.00	3.06	Training
[99-57-0]	2-Amino-4-nitrophenol	-3.18	154.10	1.26	Training
[95-57-8]	2-Chlorophenol	-1.48	128.60	2.15	Training
[95-48-7]	<i>o</i> -Cresol	-1.80	108.10	1.95	Training
[110-80-5]	2-Ethoxyethanol	-3.60	90.10	-0.32	Training
[5307-14-2]	2-Nitro- <i>p</i> -phenylenediamine	-3.30	153.10	0.53	Validation
[95-54-5]	<i>o</i> -Phenylenediamine	-3.35	108.10	0.15	Training
[60-12-8]	2-Phenylethanol	-1.42	122.20	1.36	Training
[95-65-8]	3,4-Xylenol	-1.44	122.10	2.30	Validation
[108-39-4]	<i>m</i> -Cresol	-1.82	108.10	1.96	Training
[554-84-7]	3-Nitrophenol	-2.25	139.10	2.00	Validation
[119-34-6]	4-Amino-2-nitrophenol	-2.55	154.10	0.96	Validation
[106-41-2]	4-Bromophenol	-1.44	173.00	2.59	Training
[5131-60-2]	4-Chloro- <i>m</i> -phenylenediamine	-2.68	142.60	0.85	Training
[106-48-9]	4-Chlorophenol	-1.44	128.60	2.39	Validation
[106-44-5]	<i>p</i> -Cresol	-1.76	108.10	1.94	Training
[123-07-9]	4-Ethylphenol	-1.46	122.20	2.58	Training
[100-02-7]	4-Nitrophenol	-2.25	139.10	1.91	Training
[106-50-3]	<i>p</i> -Phenylenediamine	-3.62	108.10	-0.30	Training
[52-39-1]	Aldosterone	-5.52	360.40	1.08	Training
[57-43-2]	Amylobarbitol	-2.64	226.30	2.07	Training
[100-66-3]	Anisole	-1.60	108.10	2.11	Training
[51-55-8]	Atropine	-5.07	289.40	1.83	Training
[57-44-3]	Barbital	-3.95	184.20	0.65	Training
[100-52-7]	Benzaldehyde	-0.85	106.10	1.48	Training
[71-43-2]	Benzene	-0.95	78.10	2.13	Validation
[100-51-6]	Benzyl alcohol	-2.22	108.10	1.10	Training
[135-19-3]	<i>b</i> -Naphthol	-1.55	144.20	2.70	Training
[77-28-1]	Butobarbital	-3.72	212.40	1.73	Validation
[107-92-6]	Butyric acid	-3.00	88.11	0.79	Training
[59-50-7]	Chlorocresol	-1.26	142.60	3.10	Training
[88-04-0]	Chloroxylenol	-1.23	156.60	3.27	Training
[132-22-9]	Chlorpheniramine	-2.66	274.80	3.38	Training
[76-57-3]	Codeine	-4.31	299.40	1.19	Training

[152-58-9]	Cortexolone	-4.13	346.50	3.08	Training
[64-85-7]	Cortexone	-3.35	330.50	2.88	Training
[50-22-6]	Corticosterone	-4.22	346.50	1.94	Training
[53-06-5]	Cortisone	-5.00	360.50	1.47	Training
[15307-86-5]	Diclofenac	-3.45	318.00	4.51	Training
[90-89-1]	Diethylcarbamazine	-3.89	199.30	0.37	Training
[71-63-6]	Digitoxin	-4.89	764.90	1.85	Training
[509-60-4]	Dihydromorphine	-4.82	287.36	0.93	Training
[299-42-3]	Ephedrine	-2.22	165.20	1.13	Validation
[50-28-2]	Estradiol	-2.28	272.40	4.01	Training
[50-27-1]	Estriol	-4.40	288.40	2.45	Training
[53-16-7]	Estrone	-2.44	270.40	3.13	Training
[64-17-5]	Ethanol	-3.00	46.10	-0.31	Validation
[60-29-7]	Ethyl ether	-2.80	74.10	0.89	Training
[14521-96-1]	Etorphine	-2.44	411.50	2.79	Validation
[437-38-7]	Fentanyl	-2.25	336.50	4.05	Training
[356-12-7]	Fluocinonide	-2.77	494.60	3.19	Training
[111-14-8]	Heptanoic acid	-1.70	130.19	2.42	Training
[53535-33-4]	Heptanol	-1.49	116.20	2.31	Training
[142-62-1]	Hexanoic acid	-1.85	116.16	1.92	Training
[107085-84-7]	Hydrocortisone hemipimelate	-2.75	503.60	3.26	Training
[2203-97-6]	Hydrocortisone hemisuccinate	-3.20	462.50	1.89	Training
[3593-96-2]	Hydrocortisone hexanoate	-1.75	460.60	4.48	Validation
[114593-88-3]	Hydrocortisone hydroxyhexanoate	-3.04	476.60	2.79	Training
[114611-36-8]	Hydrocortisone methylpimelate	-2.27	518.60	3.70	Training
[114593-86-1]	Hydrocortisone methylsuccinate	-3.68	476.60	2.60	Training
[74253-50-2]	Hydrocortisone <i>N,N</i> -dimethylsuccinamate	-4.17	489.60	2.03	Validation
[6678-14-4]	Hydrocortisone octanoate	-1.21	488.70	5.49	Training
[114593-87-2]	Hydrocortisone pimelamate	-3.05	503.60	2.31	Training
[6677-98-1]	Hydrocortisone propionate	-2.47	418.50	2.80	Validation
[114593-85-0]	Hydrocortisone succinamate	-4.59	461.60	1.43	Validation
[50-23-7]	Hydrocortisone	-5.52	362.50	1.61	Validation
[466-99-9]	Hydromorphone	-4.82	285.34	1.60	Training
[12041-98-4]	Hydroxypregnenolone	-3.22	332.50	3.71	Training
[68-96-2]	Hydroxyprogesterone	-3.22	330.50	3.17	Validation
[53-86-1]	Indomethacin	-3.67	357.80	4.27	Training
[119-65-3]	Isoquinoline	-1.78	129.20	2.08	Training
[57-42-1]	Meperidine	-2.43	247.40	2.72	Training
[67-56-1]	Methanol	-3.30	32.00	-0.77	Training
[99-76-3]	Methylhydroxybenzoate	-2.04	152.10	1.96	Training

[57-27-2]	Morphine	-5.03	285.30	0.89	Training
[22204-53-1]	Naproxen	-3.15	230.30	3.18	Training
[71-36-3]	<i>N</i> -Butanol	-2.52	74.14	0.88	Training
[112-30-1]	<i>N</i> -Decanol	-1.10	158.30	4.57	Training
[111-70-6]	<i>N</i> -Heptanol	-1.50	116.20	2.62	Training
[111-27-3]	<i>N</i> -Hexanol	-1.89	102.20	2.03	Validation
[54-11-5]	Nicotine	-1.72	162.30	1.17	Training
[55-63-0]	Nitroglycerine	-1.96	227.10	1.62	Validation
[1116-54-7]	<i>N</i> -Nitrosodiethanolamine	-5.22	134.13	-1.28	Training
[111-87-5]	<i>N</i> -Octanol	-1.28	130.20	3.00	Training
[143-08-8]	Nonanol	-1.22	144.30	3.77	Training
[71-41-0]	<i>N</i> -Pentanol	-2.22	88.20	1.51	Training
[71-23-8]	<i>N</i> -Propanol	-2.77	60.10	0.25	Training
[124-07-2]	Octanoic acid	-1.60	144.21	3.05	Training
[630-60-4]	Ouabain	-6.11	584.60	-2.00	Training
[109-52-4]	Pentanoic acid	-2.70	102.13	1.39	Validation
[50-06-6]	Phenobarbital	-3.35	232.20	1.47	Training
[108-95-2]	Phenol	-1.71	94.10	1.46	Training
[36322-90-4]	Piroxicam	-3.81	331.40	3.06	Training
[145-13-1]	Pregnenolone	-2.82	316.50	4.22	Training
[57-83-0]	Progesterone	-2.82	314.50	3.87	Training
[69-72-7]	Salicylic acid	-2.20	138.10	2.26	Training
[51-34-3]	Scopolamine	-4.30	303.40	0.98	Training
[100-42-5]	Styrene	-0.19	104.15	2.95	Training
[57-50-1]	Sucrose	-5.28	342.30	-3.07	Training
[56030-54-7]	Sufentanil	-2.26	386.60	3.95	Training
[58-22-0]	Testosterone	-3.40	288.40	3.32	Validation
[89-83-8]	Thymol	-1.28	150.20	3.30	Validation
[57-13-6]	Urea	-3.83	60.60	-2.11	Training
[7732-18-5]	Water	-3.30	18.00	-1.38	Training

Table S2. List of values estimated for molecular descriptors and skin permeability using quantitative structure-activity relationship developed in this study for compounds applied in model training and validation. Relevant information includes the value of molecular descriptors consisting of those for the distance/detour ring index of order 10 (D/Dr10), the sum of topological distances between O..Cl (T(O..Cl)), the Ghose-Crippen octanol-water partition coefficient (ALOGP), and the Ghose-Viswanadhan-Wendoloski antineoplastic-like index at 80% (Neoplastic-80) and the logarithmic value of skin permeability predicted by the model (predicted log *K_p*) for the 106 compounds included in the training and validation datasets.

Chemical Name	Chemical Formula	MW	log <i>K_{ow}</i>	Observed log <i>K_p</i> (cm/h)	D/Dr10	T(O..Cl)	ALOGP	Neoplastic-80	Predicted log <i>K_p</i> (cm/h)
1,1,1-Trichloroethane	C ₂ H ₃ Cl ₃	133.40	2.49	-2.35	0	0	2.029	0	-1.71
2,4,6-Trichlorophenol	C ₆ H ₃ Cl ₃ O	197.50	3.69	-1.23	0	11	3.556	0	-1.21
2,4-Dichlorophenol	C ₆ H ₄ Cl ₂ O	163.00	3.06	-1.22	0	8	2.891	0	-1.51
2-Amino-4-nitrophenol	C ₆ H ₆ N ₂ O ₃	154.10	1.26	-3.18	0	0	0.71	0	-2.61
2-Chlorophenol	C ₆ H ₅ ClO	128.60	2.15	-1.48	0	3	2.227	0	-1.72
<i>o</i> -Cresol	C ₇ H ₈ O	108.10	1.95	-1.80	0	0	2.049	0	-1.69
2-Ethoxyethanol	C ₄ H ₁₀ O ₂	90.10	-0.32	-3.60	0	0	-0.14	0	-3.19
2-Nitro- <i>p</i> -phenylenediamine	C ₆ H ₇ N ₃ O ₂	153.10	0.53	-3.30	0	0	0.231	0	-2.94
<i>o</i> -Phenylenediamine	C ₆ H ₈ N ₂	108.10	0.15	-3.35	0	0	0.337	0	-2.86
2-Phenylethanol	C ₈ H ₁₀ O	122.20	1.36	-1.42	0	0	1.547	0	-2.04
3,4-Xylenol	C ₈ H ₁₀ O	122.10	2.30	-1.44	0	0	2.535	0	-1.36
<i>m</i> -Cresol	C ₇ H ₈ O	108.10	1.96	-1.82	0	0	2.049	0	-1.69
3-Nitrophenol	C ₆ H ₅ NO ₃	139.10	2.00	-2.25	0	0	1.457	0	-2.10
4-Amino-2-nitrophenol	C ₆ H ₆ N ₂ O ₃	154.10	0.96	-2.55	0	0	0.71	0	-2.61
4-Bromophenol	C ₆ H ₅ BrO	173.00	2.59	-1.44	0	0	2.311	0	-1.51
4-Chloro- <i>m</i> -phenylenediamine	C ₆ H ₇ ClN ₂	142.60	0.85	-2.68	0	0	1.001	0	-2.41
4-Chlorophenol	C ₆ H ₅ ClO	128.60	2.39	-1.44	0	5	2.227	0	-1.82
<i>p</i> -Cresol	C ₇ H ₈ O	108.10	1.94	-1.76	0	0	2.049	0	-1.69
4-Ethylphenol	C ₈ H ₁₀ O	122.20	2.58	-1.46	0	0	2.505	0	-1.38
4-Nitrophenol	C ₆ H ₅ NO ₃	139.10	1.91	-2.25	0	0	1.457	0	-2.10
<i>p</i> -Phenylenediamine	C ₆ H ₈ N ₂	108.10	-0.30	-3.62	0	0	0.337	0	-2.86

Aldosterone	C ₂₁ H ₂₈ O ₅	360.40	1.08	-5.52	140.399	0	1.118	1	-4.85
Amylobarbitol	C ₁₁ H ₁₈ N ₂ O ₃	226.30	2.07	-2.64	0	0	1.909	1	-3.36
Anisole	C ₇ H ₈ O	108.10	2.11	-1.60	0	0	1.814	0	-1.85
Atropine	C ₁₇ H ₂₃ NO ₃	289.40	1.83	-5.07	0	0	1.721	1	-3.49
Barbital	C ₈ H ₁₂ N ₂ O ₃	184.20	0.65	-3.95	0	0	0.745	1	-4.16
Benzaldehyde	C ₇ H ₆ O	106.10	1.48	-0.85	0	0	1.589	0	-2.01
Benzene	C ₆ H ₆	78.10	2.13	-0.95	0	0	1.83	0	-1.84
Benzyl alcohol	C ₇ H ₈ O	108.10	1.10	-2.22	0	0	1.226	0	-2.26
<i>b</i> -Naphthol	C ₁₀ H ₈ O	144.20	2.70	-1.55	34.804	0	2.471	0	-1.64
Butobarbital	C ₁₀ H ₁₆ N ₂ O ₃	212.40	1.73	-3.72	0	0	1.657	1	-3.53
Butyric acid	C ₄ H ₈ O ₂	88.11	0.79	-3.00	0	0	0.893	0	-2.48
Chlorocresol	C ₇ H ₇ ClO	142.60	3.10	-1.26	0	5	2.713	0	-1.49
Chloroxylenol	C ₈ H ₉ ClO	156.60	3.27	-1.23	0	5	3.199	0	-1.15
Chlorpheniramine	C ₁₆ H ₁₉ ClN ₂	274.80	3.38	-2.66	0	0	3.697	1	-2.14
Codeine	C ₁₈ H ₂₁ NO ₃	299.40	1.19	-4.31	135.67	0	1.638	1	-4.46
Cortexolone	C ₂₁ H ₃₀ O ₄	346.50	3.08	-4.13	133.416	0	2.386	1	-3.93
Cortexone	C ₂₁ H ₃₀ O ₃	330.50	2.88	-3.35	126.325	0	3.122	1	-3.38
Corticosterone	C ₂₁ H ₃₀ O ₄	346.50	1.94	-4.22	132.084	0	1.952	1	-4.22
Cortisone	C ₂₁ H ₂₈ O ₅	360.50	1.47	-5.00	139.176	0	1.034	1	-4.89
Diclofenac	C ₁₄ H ₁₁ Cl ₂ NO ₂	318.00	4.51	-3.45	0	32	4.348	1	-3.28
Diethylcarbamazine	C ₁₀ H ₂₁ N ₃ O	199.30	0.37	-3.89	0	0	0.436	1	-4.37
Digitoxin	C ₄₁ H ₆₄ O ₁₃	764.90	1.85	-4.89	427.064	0	3.101	0	-3.85
Dihydromorphine	C ₁₇ H ₂₁ NO ₃	287.36	0.93	-4.82	125.421	0	1.696	1	-4.35
Ephedrine	C ₁₀ H ₁₅ NO	165.20	1.13	-2.22	0	0	1.235	0	-2.25
Estradiol	C ₁₈ H ₂₄ O ₂	272.40	4.01	-2.28	95.835	0	3.813	1	-2.70
Estriol	C ₁₈ H ₂₄ O ₃	288.40	2.45	-4.40	103.496	0	2.846	1	-3.42
Estrone	C ₁₈ H ₂₂ O ₂	270.40	3.13	-2.44	95.835	0	3.773	1	-2.73
Ethanol	C ₂ H ₆ O	46.10	-0.31	-3.00	0	0	-0.009	0	-3.10

Ethyl ether	C ₄ H ₁₀ O	74.10	0.89	-2.80	0	0	0.748	0	-2.58
Etorphine	C ₂₅ H ₃₃ NO ₄	411.50	2.79	-2.44	154.042	0	2.928	0	-2.13
Fentanyl	C ₂₂ H ₂₈ N ₂ O	336.50	4.05	-2.25	0	0	3.839	1	-2.04
Fluocinonide	C ₂₆ H ₃₂ F ₂ O ₇	494.60	3.19	-2.77	185.404	0	1.308	0	-3.45
Heptanoic acid	C ₇ H ₁₄ O ₂	130.19	2.42	-1.70	0	0	2.262	0	-1.55
Heptanol	C ₇ H ₁₆ O	116.20	2.31	-1.49	0	0	2.339	0	-1.49
Hexanoic acid	C ₆ H ₁₂ O ₂	116.16	1.92	-1.85	0	0	1.806	0	-1.86
Hydrocortisone hemipimelate	C ₂₈ H ₄₀ O ₈	503.60	3.26	-2.75	247.224	0	2.784	0	-2.85
Hydrocortisone hemisuccinate	C ₂₅ H ₃₄ O ₈	462.50	1.89	-3.20	210.811	0	1.416	0	-3.54
Hydrocortisone hexanoate	C ₂₇ H ₄₀ O ₆	460.60	4.48	-1.75	211.188	0	3.631	0	-2.03
Hydrocortisone hydroxyhexanoate	C ₂₇ H ₄₀ O ₇	476.60	2.79	-3.04	222.987	0	2.406	0	-2.95
Hydrocortisone methylpimelate	C ₂₉ H ₄₂ O ₈	518.60	3.70	-2.27	259.638	0	3.035	0	-2.77
Hydrocortisone methylsuccinate	C ₂₆ H ₃₆ O ₈	476.60	2.60	-3.68	222.265	0	1.667	0	-3.45
Hydrocortisone <i>N,N</i> -dimethylsuccinamate	C ₂₇ H ₃₉ NO ₇	489.60	2.03	-4.17	233.718	0	1.225	0	-3.83
Hydrocortisone octanoate	C ₂₉ H ₄₄ O ₆	488.70	5.49	-1.21	235.106	0	4.544	0	-1.57
Hydrocortisone pimelamate	C ₂₈ H ₄₁ NO ₇	503.60	2.31	-3.05	247.224	0	2.182	0	-3.27
Hydrocortisone propionate	C ₂₄ H ₃₄ O ₆	418.50	2.80	-2.47	177.992	0	2.263	0	-2.74
Hydrocortisone succinamate	C ₂₅ H ₃₅ NO ₇	461.60	1.43	-4.59	210.811	0	0.814	0	-3.96
Hydrocortisone	C ₂₁ H ₃₀ O ₅	362.50	1.61	-5.52	139.176	0	1.217	1	-4.77
Hydromorphone	C ₁₇ H ₁₉ NO ₃	285.34	1.60	-4.82	125.421	0	1.657	1	-4.38
Hydroxypregnenolone	C ₂₁ H ₃₂ O ₃	332.50	3.71	-3.22	124.851	0	2.577	1	-3.74
Hydroxyprogesterone	C ₂₁ H ₃₀ O ₃	330.50	3.17	-3.22	124.863	0	2.845	1	-3.56
Indomethacin	C ₁₉ H ₁₆ ClNO ₄	357.80	4.27	-3.67	0	39	4.211	1	-3.72
Isoquinoline	C ₉ H ₇ N	129.20	2.08	-1.78	29.717	0	1.588	0	-2.21
Meperidine	C ₁₅ H ₂₁ NO ₂	247.40	2.72	-2.43	0	0	2.446	1	-2.99

Methanol	CH ₄ O	32.00	-0.77	-3.30	0	0	-0.358	0	-3.34
Methylhydroxybenzoate	C ₈ H ₈ O ₃	152.10	1.96	-2.04	0	0	1.418	0	-2.12
Morphine	C ₁₇ H ₁₉ NO ₃	285.30	0.89	-5.03	125.421	0	0.381	1	-5.25
Naproxen	C ₁₄ H ₁₄ O ₃	230.30	3.18	-3.15	68.623	0	2.824	1	-3.20
N-Butanol	C ₄ H ₁₀ O	74.14	0.88	-2.52	0	0	0.971	0	-2.43
N-Decanol	C ₁₀ H ₂₂ O	158.30	4.57	-1.10	0	0	3.708	0	-0.56
N-Heptanol	C ₇ H ₁₆ O	116.20	2.62	-1.50	0	0	2.339	0	-1.49
N-Hexanol	C ₆ H ₁₄ O	102.20	2.03	-1.89	0	0	1.883	0	-1.81
Nicotine	C ₁₀ H ₁₄ N ₂	162.30	1.17	-1.72	0	0	1.243	0	-2.24
Nitroglycerine	C ₃ H ₅ N ₃ O ₉	227.10	1.62	-1.96	0	0	0.078	0	-3.04
N-Nitrosodiethanolamine	C ₄ H ₁₀ N ₂ O ₃	134.13	-1.28	-5.22	0	0	-0.988	0	-3.77
N-Octanol	C ₈ H ₁₈ O	130.20	3.00	-1.28	0	0	2.796	0	-1.18
Nonanol	C ₉ H ₂₀ O	144.30	3.77	-1.22	0	0	3.252	0	-0.87
N-Pentanol	C ₅ H ₁₂ O	88.20	1.51	-2.22	0	0	1.427	0	-2.12
N-Propanol	C ₃ H ₈ O	60.10	0.25	-2.77	0	0	0.515	0	-2.74
Octanoic acid	C ₈ H ₁₆ O ₂	144.21	3.05	-1.60	0	0	2.718	0	-1.24
Ouabain	C ₂₉ H ₄₄ O ₁₂	584.60	-2.00	-6.11	252.634	0	-2.171	0	-6.28
Pentanoic acid	C ₅ H ₁₀ O ₂	102.13	1.39	-2.70	0	0	1.349	0	-2.17
Phenobarbital	C ₁₂ H ₁₂ N ₂ O ₃	232.20	1.47	-3.35	0	0	1.321	1	-3.76
Phenol	C ₆ H ₆ O	94.10	1.46	-1.71	0	0	1.563	0	-2.03
Piroxicam	C ₁₅ H ₁₃ N ₃ O ₄ S	331.40	3.06	-3.81	97.236	0	1	1	-4.64
Pregnenolone	C ₂₁ H ₃₂ O ₂	316.50	4.22	-2.82	117.771	0	3.485	1	-3.07
Progesterone	C ₂₁ H ₃₀ O ₂	314.50	3.87	-2.82	117.771	0	3.58	1	-3.01
Salicylic acid	C ₇ H ₆ O ₃	138.10	2.26	-2.20	0	0	1.167	0	-2.30
Scopolamine	C ₁₇ H ₂₁ NO ₄	303.40	0.98	-4.30	0	0	0.824	1	-4.10
Styrene	C ₈ H ₈	104.15	2.95	-0.19	0	0	2.382	0	-1.47
Sucrose	C ₁₂ H ₂₂ O ₁₁	342.30	-3.07	-5.28	0	0	-4.311	0	-6.04
Sufentanil	C ₂₂ H ₃₀ N ₂ O ₂ S	386.60	3.95	-2.26	0	0	3.231	1	-2.46

Testosterone	$C_{19}H_{28}O_2$	288.40	3.32	-3.40	102.038	0	3.333	1	-3.07
Thymol	$C_{10}H_{14}O$	150.20	3.30	-1.28	0	0	3.243	0	-0.88
Urea	CH_4N_2O	60.60	-2.11	-3.83	0	0	-1.042	0	-3.81
Water	H_2O	18.00	-1.38	-3.30	0	0	-0.564	0	-3.48
