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Theoretical Prediction of Lipophilicity for Some Drugs Compounds

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ABSTRACT

The theoretical calculations were evaluated for thirty four drug compounds. Many parameters have been calculated theoretically and enter as a model to predicting the best values of practical (Log P). All these compounds were evaluated by semi-empirical (AM1) and Hartree Fock in basis set (HF/STO-3G) using Gaussian 03w. The thermodynamic descriptors like HOMO, LUMO, total energy, Gibbs Free Energy etc were computed and played an important role for predictions the practical lipophilicity values. A linearity was shown when correlated with experimental data. Multiple linear regression analysis was performed to derive quantitative structure activity relationship models which were further evaluated for the predictions.

Keywords: Lipophilicity, HOMO, LUMO, Drug Compounds.

INTRODUCTION

Theoretical calculations have particularly succeeded for ionization potential[1], molecular docking approaches and metabolite of antipyrine. The lipophilicity is measured by the log P, which represents the equilibriumbetween a polar (aqueous) phase and apolar phase (often n-octanol, appropriate for the simulation of[5,6] biological membranes). The lipophilicity of a drug plays a significant role in numerous biological responses.

All the compounds studied have different lipophilicity degree which depends on the substituents[7] involved in its structural chemistry. Using (Log P) parameter by (QSAR) developed for the pharmaceutical,[8-10] biochemical and toxicological. (QSAR) of a series of substituted benzo[a]phenazines, in regard to their anticancer activity, has been studied using the density functional theory (DFT) method, molecular mechanics method (MMC) and statistical method. The Lipophilicity indexes log P, the calculated log P by fragment-based methods) of the[11] molecules were obtained. Electronic, stereochemical, lipophilic and topological descriptors were calculated for biological receptors called peroxisome proliferator-activated receptors (PPARs). Which control the metabolism of[12] carbohydrates and lipids. Dihydrofolate reductase (DHFR) inhibitors have proved to be of value asantibacterial,[13] antimalarial, and antitumor agents. Lipophilicity of the whole molecule (log P) played

an important role. The smaller size of Co^{+2} reduces polarity andincreases the lipophilicity of the bacterial membrane, interrupting normal cellular processes and enhancing theantifungal activity of Co^{+2} complex[14]. *In vitro* and *in vivo* evaluation indicated that the prodrugs were freely soluble, more lipophilic than parent drug. Also, the lipophilicity was determined by normal phase TLC[17], HPLC and QSPR.

MATERIALS AND METHODS

All the calculations have been performed using ChemBio Office (version 11.0.1). The (GAUSSIAN 03W) program was employed for the calculations. The correlation coefficient (R), standard error (SE) and Fisher constant (F) were employed to judge the validity of regression equation. Many sets of drugs were taken which containing (OH-) hydroxy atom on the aliphatic and aromatic compounds.

The physicochemical properties were calculated include thermodynamic parameters ΔG, ΔH, ΔS, steric energy, electronic descriptors [logP, mol refractivity, the highest occupied molecular orbital energy (HOMO) and lowest unoccupied molecular orbital energy (LUMO)].

MM_2 method was used firstly to find the best configuration stable form. The minimization is continued until the root mean square (RMS) gradient value reaches a value smaller than 0.001 kcal/mol Angstrom. Later, (AM1and HF/STO-3G) methods were used to calculate the physical properties of the drugs compounds.

RESULTS AND DISCUSSION

Set one (AM1)

The first set of the drugs was shown in the Table (1) beside the physical parameters which were calculated theoretically using (AM1) method. The relationship between the experimental reported logP values and the computed descriptors was determined using multi-linear regression. At using the enter method in (SPSS), the equation was:

logP = 0.939 + 8.343 (Free Energy) – 0.009 (CV) – 0.006 (S) – 1.082 (HF) – 0.002 (steric) + 9.957 (HOMO) – 5.811 (LUMO) + 0.241 (Mol Ref.) + 5.597 (Part. Coeff.) ------ (1) (No. 34, R = 0.990, St. Error = 0.335, F = 127.442)

While at using (stepwise) method, the equation was shown at the following:

logP = -2.695 + 0.615 (Part. Coeff.) + 8.687 (Thermal Energy) ------ (2) (No. 34, R = 0.988, St. Error = 0.318, F = 632.504)

Table 1(a): Experimental log P and physical parameters using (AM1) method

Drugs	Log P	Zero point Energies Hartree	Thermal Energies Hartree	Enthalpies Hartree	Free Energies Hartree	E(Thermal) Kcal/Mol	CV cal/mol-K
Abacavir	0.72	0.32838	0.34716	0.34811	0.27737	217.848	70.565
Acyclovir	-1.76	0.23925	0.25410	0.25504	0.19589	159.448	54.410
Adenosine	-1.46	0.25538	0.27237	0.27332	0.20836	170.915	62.614
Albuterol	0.02	0.33358	0.35226	0.35320	0.28447	221.046	68.569
Atropine	1.53	0.38692	0.40565	0.40660	0.33719	254.550	72.015
Azacitidine	-1.99	0.23007	0.24585	0.24679	0.18601	154.270	57.956
Carbidopa	-0.19	0.24834	0.26441	0.26536	0.20412	165.920	59.183
Cytarabine	-2.3	0.24291	0.25859	0.25954	0.19869	162.269	58.527
Decitabine	-1.93	0.22512	0.23991	0.24086	0.18207	150.547	54.131
Desvenlafaxine	2.26	0.39517	0.41415	0.41510	0.34679	259.884	72.647
Dobutamine	2.49	0.38899	0.41093	0.41187	0.33115	257.860	81.035
Dyphylline	-1.12	0.25841	0.27588	0.27683	0.21060	173.119	62.450
Floxuridine	-1.2	0.21981	0.23464	0.23558	0.17618	147.238	55.063
Ganciclovir	-2.07	0.24891	0.26584	0.26679	0.20226	166.818	61.578
Homatropine	1.57	0.35820	0.37548	0.37642	0.31073	235.617	67.254
Hydroxychloroquine	3.54	0.42694	0.45075	0.45169	0.36738	282.849	86.496
Isoetharine	1.13	0.33339	0.35212	0.35306	0.28513	220.957	68.544
Isoproterenol	0.25	0.27601	0.29223	0.29318	0.23010	183.379	58.751
Isoxsuprine	2.58	0.38944	0.41082	0.41177	0.33470	257.794	80.003
Lamivudine	-1.02	0.20450	0.21852	0.21946	0.16227	137.123	51.660
Levobunolol	2.86	0.40632	0.42739	0.42833	0.35275	268.191	78.991
Metipranolol	2.67	0.42742	0.45283	0.45377	0.36751	284.155	89.840
Midodrine	-0.32	0.30600	0.32443	0.32538	0.25729	203.585	67.361
Pyridoxine	-1.9	0.18992	0.20219	0.20313	0.15134	126.875	43.813
Risedronic acid	-2.94	0.20154	0.21959	0.22053	0.15486	137.794	65.868
Ritodrin	1.61	0.36055	0.37988	0.38083	0.30928	238.379	73.810
Stavudine	-0.91	0.22577	0.24064	0.24159	0.17852	151.006	53.326
Terbutaline	0.48	0.30482	0.32204	0.32299	0.25716	202.085	63.950
Trihexyphenidyl	5.06	0.48781	0.50820	0.50914	0.43689	318.898	80.508
Tropicamide	1.16	0.34962	0.36833	0.36928	0.29971	231.132	70.344
Vidarabine	-1.46	0.25544	0.27234	0.27328	0.20893	170.895	62.586
Vorinostat	0.86	0.33606	0.35572	0.35666	0.27938	223.216	69.985
Zalcitabine	-1.51	0.23336	0.24698	0.24793	0.19143	154.985	50.659
Zoledronic acid	-2.28	0.18294	0.20023	0.20117	0.13721	125.644	62.757

Table 1(b):

Drugs	Log P	S cal/mol-K	HF Hartree	Steric energy	HOMO (a.u.)	LUMO (a.u.)	Mol Ref.	Partition Coefficient
Abacavir	0.72	148.877	0.15097	40.67	-0.30382	0.00319	7.8973	0.8057
Acyclovir	-1.76	124.491	-0.08041	15.51	-0.31690	0.00994	5.4966	-2.1354
Adenosine	-1.46	136.720	-0.14181	38.25	-0.32661	-0.00929	6.2955	-2.1577
Albuterol	0.02	144.658	-0.22051	-0.12	-0.33796	0.00395	6.7632	0.0614
Atropine	1.53	146.082	-0.17317	32.90	-0.34748	0.00358	8.1462	1.2992
Azacitidine	-1.99	127.931	-0.25863	12.92	-0.36931	-0.01385	5.3911	-2.1981
Carbidopa	-0.19	128.890	-0.22215	-25.99	-0.32092	0.01247	5.7762	-0.4448
Cytarabine	-2.3	128.064	-0.2743	15.34	-0.33873	-0.00018	5.6022	-2.1951
Decitabine	-1.93	123.727	-0.18278	20.16	-0.36249	-0.00838	5.2380	-1.9012
Desvenlafaxine	2.26	143.772	-0.14428	17.43	-0.32439	0.01927	7.8241	2.6830
Dobutamine	2.49	169.890	-0.1674	1.32	-0.32084	0.00837	8.8106	2.4330
Dyphylline	-1.12	139.395	-0.15661	26.39	-0.33688	-0.02165	6.2242	-1.2861
Floxuridine	-1.2	125.014	-0.36648	22.05	-0.36340	-0.02766	5.3090	-1.4048
Ganciclovir	-2.07	135.806	-0.14534	22.87	-0.31957	-0.01469	6.0691	-2.5448
Homatropine	1.57	138.272	-0.16281	27.30	-0.34750	0.00392	7.6824	1.4274
Hydroxychloroquine	3.54	177.453	-0.02964	24.86	-0.31718	-0.01819	9.7216	4.1159
Isoetharine	1.13	142.972	-0.20758	3.23	-0.32652	0.00245	6.7632	0.9914
Isoproterenol	0.25	132.761	-0.20465	-7.38	-0.32934	0.00299	5.8356	0.1534
Isoxsuprine	2.58	162.193	-0.14145	8.84	-0.32683	0.00385	8.8106	2.6150
Lamivudine	-1.02	120.367	-0.09953	9.64	-0.32222	-0.01616	5.6385	-1.4624
Levobunolol	2.86	159.088	-0.19797	17.93	-0.33775	-0.01415	8.3236	2.2623
Metipranolol	2.67	181.563	-0.26987	19.15	-0.33847	-0.00504	8.6541	2.5454
Midodrine	-0.32	143.306	-0.2255	-5.84	-0.32555	-0.00065	6.7038	-0.4248
Pyridoxine	-1.9	109.014	-0.19064	4.10	-0.34360	-0.00701	4.3282	-0.3450
Risedronic acid	-2.94	138.228	-0.66112	28.74	-0.37478	-0.01503	5.7520	-2.6224
Ritodrin	1.61	150.580	-0.15598	-1.74	-0.32844	0.01275	8.3468	1.6514
Stavudine	-0.91	132.740	-0.1791	7.40	-0.35086	-0.00871	5.5788	-0.4875
Terbutaline	0.48	138.542	-0.20335	0.30	-0.33354	0.01039	6.2994	0.4824
Trihexyphenidyl	5.06	152.058	-0.1029	22.65	-0.33388	0.01885	9.3488	5.1510
Tropicamide	1.16	146.405	-0.05002	4.58	-0.35844	0.00185	8.3290	1.1806
Vidarabine	-1.46	135.449	-0.14293	41.99	-0.31980	-0.00317	6.2955	-2.1577
Vorinostat	0.86	162.648	-0.14613	-8.32	-0.32383	0.01037	7.3609	0.9890
Zalcitabine	-1.51	118.919	-0.14032	15.58	-0.34090	-0.00424	5.2960	-1.2469
Zoledronic acid	-2.28	134.613	-0.61319	41.98	-0.34492	0.00261	5.1815	-3.0656

Table (2) was show the predicted of the (34) drugs using the equation (2). The correlation between the experimental and the predicted values shows an excellent predicted for the drugs (R= 0.988).

Table 2: Experimental and predicted of logP using (AM1) method

No	Drugs	Log P (Practical)	Log P (Predicted)	Residuals	No	Drugs	Log P (Practical)	Log P (Predicted)	Residuals
1	Abacavir	0.72	0.816	0.096	18	Isoproterenol	0.25	-0.062	-0.312
2	Acyclovi	-1.76	-1.801	-0.041	19	Isoxsuprine	2.58	2.482	-0.098
3	Adenosine	-1.46	-1.656	-0.196	20	Lamivudine	-1.02	-1.696	-0.676
4	Albuterol	0.02	0.403	0.383	21	Levobunolol	2.86	2.409	-0.451
5	Atropine	1.53	1.628	0.098	22	Metipranolol	2.67	2.804	0.134
6	Azacitidine	-1.99	-1.911	0.079	23	Midodrine	-0.32	-0.138	0.182
7	Carbidopa	-0.19	-0.672	-0.482	24	Pyridoxine	-1.9	-1.151	0.749
8	Cytarabine	-2.3	-1.799	0.501	25	Risedronic acid	-2.94	-2.4	0.54
9	Decitabine	-1.93	-1.78	0.15	26	Ritodrin	1.61	1.621	0.011
10	Desvenlafaxine	2.26	2.553	0.293	27	Stavudine	-0.91	-0.904	0.006
11	Dobutamine	2.49	2.371	-0.119	28	Terbutaline	0.48	0.399	-0.081
12	Dyphylline	-1.12	-1.089	0.031	29	Trihexyphenidyl	5.06	4.888	-0.172
13	Floxuridine	-1.2	-1.521	-0.321	30	Tropicamide	1.16	1.231	0.071
14	Ganciclovir	-2.07	-1.951	0.119	31	Vidarabine	-1.46	-1.656	-0.196
15	Homatropine	1.57	1.445	-0.125	32	Vorinostat	0.86	1.003	0.143
16	Hydroxychloroquine	3.54	3.752	0.212	33	Zalcitabine	-1.51	-1.316	0.194
17	Isoetharine	1.13	0.974	-0.156	34	Zoledronic acid	-2.28	-2.841	-0.561

In comparison between the predicted and the practical values, we noted that a linear correlation with an excellent correlation coefficient (R = 0.976) as shown in Figure 1.

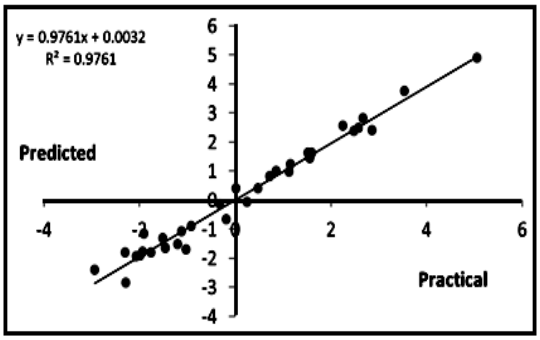

Fig. 1. Correlation between the predicted and the practical of logP for 34 drugs using (AM1)

Set two (HF/STO-3G)

The second set of the drugs was shown in the Table (3) which was calculated theoretically using (HF/STO-3G) method. The relationship between the experimental reported logP values and the computed descriptors was determined using multi-linear regression.

By using the enter method in (SPSS), the equation was:

logP = -2.365 + 4.621 (Free Energy) + 0. 028(CV)– 0.015 (S) – 5.241x10 (HF) - 0.001(steric) + 0.859 (HOMO) + 1.647(LUMO) + 0.178(Mol Ref.) + 0.612 (Part. Coeff.) ------ (3) (No. 34, R= 0.989, St. Error = 0.345, F = 119.98)

While using (stepwise) method, the equation was shown at the following:

logP = -2.328 + 0.605(Part. Coeff.) + 8.042 (Free Energy) ------ (4) (No. 34, R= 0.988, St. Error = 0.322, F = 616.499)

Table 3(a): Experimental logP and physical parameters using (HF/STO-3G) method

Drugs	Log P	Zero point Energies Hartree	Thermal Energies Hartree	Enthalpies Hartree	Free Energies Hartree	E (Thermal) Kcal/Mol	CV cal/mol-K
Abacavir	0.72	0.37352	0.39093	0.39187	0.32474	245.31	64.588
Acyclovir	-1.76	0.2714	0.28555	0.2865	0.22735	179.186	50.91
Adenosine	-1.46	0.28947	0.30476	0.3057	0.24538	191.239	57.578
Albuterol	0.02	0.38573	0.40321	0.40416	0.33831	253.02	63.88
Atropine	1.53	0.44721	0.46466	0.46561	0.3991	291.579	65.601
Azacitidine	-1.99	0.26076	0.27533	0.27627	0.21763	172.772	53.965
Carbidopa	-0.19	0.28136	0.2965	0.29744	0.23826	186.055	56.079
Cytarabine	-2.3	0.27636	0.29067	0.29161	0.2333	182.396	53.56
Decitabine	-1.93	0.25572	0.26946	0.2704	0.21401	169.088	50.524
Desvenlafaxine	2.26	0.46089	0.47835	0.47929	0.41456	300.166	66.313
Dobutamine	2.49	0.44697	0.46707	0.46802	0.39306	293.091	74.416
Dyphylline	-1.12	0.29614	0.31262	0.31357	0.25072	196.172	58.583
Floxuridine	-1.2	0.24764	0.26201	0.26296	0.20423	164.416	52.43
Ganciclovir	-2.07	0.28219	0.29772	0.29866	0.23837	186.82	57.471
Homatropine	1.57	0.41303	0.42914	0.43009	0.36652	269.291	61.264
Hydroxychloroquine	3.54	0.49412	0.51629	0.51723	0.43768	323.974	80.054
Isoetharine	1.13	0.38678	0.40402	0.40496	0.34088	253.526	63.548
Isoproterenol	0.25	0.31845	0.33343	0.33437	0.27475	209.23	54.579
Isoxsuprine	2.58	0.44623	0.46602	0.46697	0.39408	292.434	73.455
Lamivudine	-1.02	0.23432	0.24699	0.24793	0.19375	154.987	46.733
Levobunolol	2.86	0.47037	0.49011	0.49105	0.41912	307.546	73.209
Metipranolol	2.67	0.49681	0.52077	0.52171	0.44015	326.787	84.358
Midodrine	-0.32	0.35155	0.36815	0.36909	0.30607	231.016	61.076
Pyridoxine	-1.9	0.21706	0.22835	0.2293	0.17993	143.295	41.21
Risedronic acid	-2.94	0.22605	0.24189	0.24283	0.18111	151.785	57.845
Ritodrin	1.61	0.4131	0.43153	0.43247	0.36262	270.787	69.127
Stavudine	-0.91	0.25561	0.2698	0.27075	0.21246	169.302	50.613
Terbutaline	0.48	0.3519	0.36782	0.36876	0.30706	230.809	59.622
Trihexyphenidyl	5.06	0.57023	0.58908	0.59002	0.52086	369.651	72.354
Tropicamide	1.16	0.39934	0.41767	0.41862	0.34913	262.094	66.491
Vidarabine	-1.46	0.28837	0.3041	0.30505	0.24273	190.828	58.486
Vorinostat	0.86	0.38499	0.40377	0.40471	0.33164	253.366	65.257
Zalcitabine	-1.51	0.26585	0.27889	0.27983	0.22371	175.005	47.116
Zoledronic acid	-2.28	0.20696	0.22332	0.22427	0.16305	140.138	59.832

Table 3(b):

Drugs	Log P	S cal/mol-K	HF Hartree	Steric energy	HOMO (a.u.)	LUMO (a.u.)	Mol Ref.	Partition Coefficient
Abacavir	0.72	141.283	-930.423	40.67	-0.22696	0.23407	7.8973	0.8057
Acyclovir	-1.76	124.488	-797.035	15.51	-0.24613	0.25526	5.4966	-2.1354
Adenosine	-1.46	126.954	-945.719	38.25	-0.26515	0.20221	6.2955	-2.1577
Albuterol	0.02	138.585	-773.769	-0.12	-0.24819	0.25947	6.7632	0.0614
Atropine	1.53	139.978	-924.621	32.9	-0.27591	0.25418	8.1462	1.2992
Azacitidine	-1.99	123.426	-890.403	12.92	-0.2811	0.19989	5.3911	-2.1981
Carbidopa	-0.19	124.55	-785.01	-25.99	-0.22639	0.27185	5.7762	-0.4448
Cytarabine	-2.3	122.733	-874.641	15.34	-0.23293	0.23022	5.6022	-2.1951
Decitabine	-1.93	118.694	-816.563	20.16	-0.25619	0.22355	5.238	-1.9012
Desvenlafaxine	2.26	136.238	-814.521	17.43	-0.23635	0.2732	7.8241	2.683
Dobutamine	2.49	157.761	-961.953	1.32	-0.22866	0.26586	8.8106	2.433
Dyphylline	-1.12	132.268	-892.562	26.39	-0.24286	0.2083	6.2242	-1.2861
Floxuridine	-1.2	123.596	-917.797	22.05	-0.26909	0.21977	5.309	-1.4048
Ganciclovir	-2.07	126.899	-908.288	22.87	-0.23465	0.22866	6.0691	-2.5448
Homatropine	1.57	133.784	-886.045	27.3	-0.27023	0.26006	7.6824	1.4274
Hydroxychloroquine	3.54	167.434	-1378.101	24.86	-0.2403	0.19039	9.7216	4.1159
Isoetharine	1.13	134.875	-773.767	3.23	-0.2359	0.25814	6.7632	0.9914
Isoproterenol	0.25	125.495	-696.621	-7.38	-0.23569	0.26197	5.8356	0.1534
Isoxsuprine	2.58	153.415	-961.943	8.84	-0.24279	0.2591	8.8106	2.615
Lamivudine	-1.02	114.034	-1081.576	9.64	-0.25192	0.21027	5.6385	-1.4624
Levobunolol	2.86	151.39	-925.775	17.93	-0.24973	0.21819	8.3236	2.2623
Metipranolol	2.67	171.661	-1000.77	19.15	-0.24192	0.25486	8.6541	2.5454
Midodrine	-0.32	132.648	-862.173	-5.84	-0.25357	0.24625	6.7038	-0.4248
Pyridoxine	-1.9	103.915	-580.886	4.1	-0.26614	0.23528	4.3282	-0.345
Risedronic acid	-2.94	129.899	-1512.527	28.74	-0.27302	0.23132	5.752	-2.6224
Ritodrin	1.61	147.012	-923.369	-1.74	-0.23984	0.26814	8.3468	1.6514
Stavudine	-0.91	122.678	-783.873	7.4	-0.25559	0.24349	5.5788	-0.4875
Terbutaline	0.48	129.866	-735.199	0.3	-0.24374	0.26658	6.2994	0.4824
Trihexyphenidyl	5.06	145.56	-893.856	22.65	-0.26466	0.27298	9.3488	5.151
Tropicamide	1.16	146.255	-902.671	4.58	-0.27912	0.24359	8.329	1.1806
Vidarabine	-1.46	131.163	-945.712	41.99	-0.25192	0.21998	6.2955	-2.1577
Vorinostat	0.86	153.782	-864.299	-8.32	-0.23188	0.26625	7.3609	0.989
Zalcitabine	-1.51	118.12	-726.977	15.58	-0.24261	0.22045	5.296	-1.2469
Zoledronic acid	-2.28	128.837	-1490.837	41.98	-0.26986	0.28835	5.1815	-3.0656

Table (4) showed the predicted of the (34) drugs using the equation (4). The correlation between the experimental and the predicted values shows an excellent predicted for the drugs (R= 0.988) as shown in Figure 2.

Table 4: Experimental and predicted of logP using (HF/STO-3G) method

No.	Drugs	Log P	Log P (Practical)	Residuals (Predicted)	No.	Drugs	Log P (Practical)	Log P (Predicted)	Residuals
1	Abacavir	0.72	0.771	0.051	18	Isoproterenol	0.25	-0.026	-0.276
2	Acyclovi	-1.76	-1.792	-0.032	19	Isoxsuprine	2.58	2.423	-0.157
3	Adenosine	-1.46	-1.66	-0.2	20	Lamivudine	-1.02	-1.655	-0.635
4	Albuterol	0.02	0.43	0.41	21	Levobunolol	2.86	2.411	-0.449
5	Atropine	1.53	1.668	0.138	22	Metipranolol	2.67	2.752	0.082
6	Azacitidine	-1.99	-1.908	0.082	23	Midodrine	-0.32	-0.124	0.196
7	Carbidopa	-0.19	-0.681	-0.491	24	Pyridoxine	-1.9	-1.09	0.81
8	Cytarabine	-2.3	-1.78	0.52	25	Risedronic acid	-2.94	-2.458	0.482
9	Decitabine	-1.93	-1.757	0.173	26	Ritodrin	1.61	1.587	-0.023
10	Desvenlafaxine	2.26	2.629	0.369	27	Stavudine	-0.91	-0.914	-0.004
11	Dobutamine	2.49	2.305	-0.185	28	Terbutaline	0.48	0.433	-0.047
12	Dyphylline	-1.12	-1.09	0.03	29	Trihexyphenidyl	5.06	4.977	-0.083
13	Floxuridine	-1.2	-1.535	-0.335	30	Tropicamide	1.16	1.194	0.034
14	Ganciclovir	-2.07	-1.951	0.119	31	Vidarabine	-1.46	-1.681	-0.221
15	Homatropine	1.57	1.483	-0.087	32	Vorinostat	0.86	0.937	0.077
16	Hydroxychloroquine	3.54	3.682	0.142	33	Zalcitabine	-1.51	-1.283	0.227
17	Isoetharine	1.13	1.013	-0.117	34	Zoledronic acid	-2.28	-2.871	-0.591

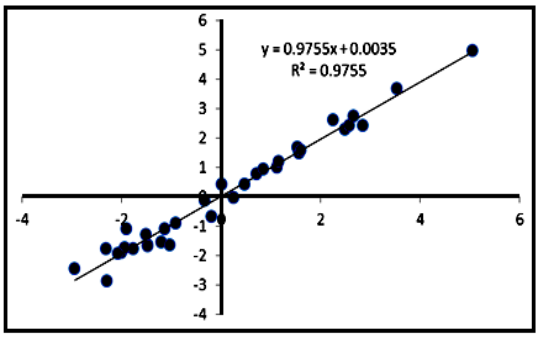

Fig. 2. Correlation between the predicted and the practical of for 34 drugs using (HF/STO-3G)

CONCLUSION

The theoretical calculations plays a significant role in the description of the practical parameters like (log P). The results of the theoretical calculated at Table 3 of drugs showed a perfect exploration for descriptors. These results have been showed an excellent correlation between the practical values with predicted as shown in Fig.1 and Fig. 2. This mean that the physicochemical parameters is very useful to give us an information about our system and sometimes help to predicted the practical values before determine them. There is no difference in correlation coefficient about (R = 0.988) for the two methods (AM1) and (HF/STO-3G). Also, no large difference in the standard error about (0.318) to (0.322). But the Fisher value about (632.5) in (AM1) method at equation (2) compare to (HF/STO-3G) about (616.499) at equation (4).

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Conflicts of interest

There is no conflict of interest for all authors.

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