BULLETIN
OF THE KOREAN CHEMICAL SOCIETY

VOLUME 10, NUMBER 1
FEBRUARY 20, 1989

BKCS 10(1) 1-122 (1989)
ISSN 0523-2964

Estimation of Activity Against Adenocarcinoma CA755 and Toxicity of Purines in Mice Using Physicochemical Parameter and Connectivity Index

Byung-Kak Park, Ho-Soon Kim, Man-Chul Suh[§], Gab-Yong Lee[*†], and U-Hyon Paek[‡]

Department of Chemsitry, Yeungnam University, Kyongsan 713-800
[†]Department of Chemical Education, Hyosung Women's University, Kyongsan 713-702*
[‡]Department of Chemistry, Gyeongsang University, Jinju 660-300. *Received February 27, 1988*

The nonempirical molecular connectivity indexes of a number of mono- and disubstituted purines were calculated. Very good correlations were obtained between anticancer activity (log 1/c) and toxic activity (log $1/LD_{50}$) of these compounds and their molecular connectivity indexes and physicochemical constants. Our structure-activity relationship is discussed briefly in relation to theories of general QSAR.

Introduction

Quantitative structure-activity relationships(QSAR) are currently being used by many synthesis chemists as an aid in the development of new drugs or chemical compounds[1-3]. These QSAR attempt to embody, in a mathematical model, the observed biological activity produced by a series of structurally similar chemical compounds or analogs. Typically, the analogs are generated from a single parent molecule (termed the lead compound) by substituting certain atom(s) (e.g. F, Br, Cl) or molecular substructures (e.g. CH_3, CF_3, $COCl_2$, C_6H_5) at various positions in the parent compound (e.g. on a benzene ring). Since there are usually many available positions for substitution and numerous fragments that could be substituted, the number of analogs that could be generated from any lead compounds are enormous.

As the most commonly used model for QSAR studies, at present, quantum chemical[4-7], physicochemical[8-10], and topological parameters[11-20] have been extensively utilized in the prediction of biological activity of molecules.

The physicochemical model for QSAR studies is the Hansch extrathermodynamic or linear free-energy model[21] and its various modifications[1]. The structure of each substituent is represented by a vector of measurements on its physicochemical properties. These include measures of solubility, lipophilicity (e.g. partition coefficient, P or Hansch $\pi = \log P$), or ionic strength (e.g. Hammett's σ; Swain-Lupton field, F, and resonance, R, constants), and of bulk or steric configuration (e.g. molar refractivity, MR; molecular weight, MW; Taft Es; Verloop constants).

Molecular connectivity as the theoretical approach, the manner in which atoms are connected or branched in a molecule, is a fundamental characteristic of the structure. It is well known that chain isomers of a molecule have varying values of their physical and chemical properties. In addition, molecular connectivity has been successfully used to explain structure-activity relationships with many classes of biological agents.

Purine and purine nucleosides comprise a very important class of potential anticancer agents[22]. Many hundreds of purine analogs have been synthesized[23], and tested for their anticancer properties. Of the purine bases, only mercaptopurine and thioguanine have found general usage in the clinical treatment of cancer[24].

This paper examines the correlation of the molecular connectivity indexes and the physicochemical parameters with the biological activity against adenocarcinoma CA755 and toxicity in mice. The QSAR have been obtained by a multiple regression for relation between the reported biological activity and the theoretical index.

Methods

The structure of a molecule can be reflected by a set of number which we call χ terms[11] and the terms are computed from a hydrogen-suppressed molecular formula.

The simplest term defined ${}^0\chi$ is computed as:

$$ {}^0\chi = \Sigma(\delta_i)^{-1/2} \quad (1) $$

[§]Department of Material Treatment ITTI, Korea Institue of Machinery and Metals, Seoul 150-073.

Table 1. Valence delta, δ^v, Values for Heteroatoms

Atom	δ^v	Atom	δ^v
$-NH_2$	3	-O-	6
-NH-	4	-C=O	6
>N-	5	O=N-O	6
-C≡N	5	F	7
Pyridine N	5	Cl	0.78
Nitro N	6	Br	0.26
$-N^+<$	6	I	0.16
-S-	0.67	$-SO_2-$	2.67

Where the sum is over all non-hydrogen atoms in the molecule and δ_i is a number assigned to each atoms, reflecting the number of atoms connected to it. The simple connectivity terms does not considere the nature of atom. The first-order $^1\chi$ is computed as:

$$^1\chi=\Sigma(\delta_i\delta_j)^{-1/2} \quad (2)$$

Where the sum is over all connections or edges in the hydrogen-suppressed molecular frame. Atom i and j are formally bonded.

The general extended terms of χ, $^m\chi_p$, $^m\chi_c$, $^m\chi_{pc}$ which indicate linear path(P), cluster(C), path-cluster(PC), respectively, is computed as:

$$^m\chi_t=\sum_{j=1}^{Ns}\left(\prod_{i=1}^{m+1}\delta_i\right)^{-1/2} \quad (3)$$

Where Ns is the number of distinct type with m edges.

Terms describing nonlinear arrangements of bonds, such as clusters of three bonds and circuits (or rings), are computed in a similar way.

The specific treatment of the heteroatoms and the unsaturated substructure require further differentiation of atom connectivity beyond simple adjacency. This level of treatment leads to valence χ terms, χ^v. For this calculation, the valence δ^v values are assigned on the basis of the expression.

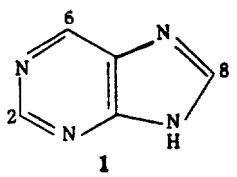
$$\delta^v=Z^v-h_i \quad (4)$$

where Z^v is the number of valence electrons and h_i is the number of attached hydrogen atoms. However, as the atoms of same group have an identical number of valence electrons, this prescription yields same values of δ^v. So we determined empirical parameters of δ^v for the halogens and the sulfur by fitting from QSAR.

The δ^v values for heteroatoms are shown in Table 1.

Results and Discussion

Structure **1** shows molecular structure and numbering of the purine base.



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The substituent constants employed in this study as physicochemical parameter included the hydrophobic parameter (π) and resonance parameter (R) in Table 2[25]. It should be noted that the π values were determined in an aromatic system, *i.e.* from benzene derivatives.

The connectivity terms in Table 3 are selected by stepwise multiple regression analysis.

Table 2. Physicochemical Parameters

Substituent	π	R
Hydrogen	0	0
Methyl	0.56	-0.13
Cyano	-0.57	0.19
Chloro	0.71	-0.15
Bromo	0.86	-0.17
Iodo	1.12	-0.19
Methoxy	-0.02	-0.51
Ethoxy	0.38	-0.44
n-Propoxy	1.05	-0.45
Amino	-1.23	-0.68
Methylamino	-0.47	-0.74
Dimethylamino	0.18	-0.92
Trimethylammonium	-5.96	0
Benzamido	0.49	-0.27
Hydrazino	-0.88	-0.71
Hydroxylamino	-1.34	-0.40
Methylthio	0.61	-
Ethylthio	1.07	-
n-Propylthio	1.57	-
n-Butylthio	2.07	-
iso-Butylthio	2.16	-
sec-Butylthio	2.16	-
2'-Propynylthio	1.01	-
Cyanomethylthio	-0.23	-
Cyclopentylthio	2.25	-
Phenylthio	2.32	-
Thiocyanate	0.41	-
2-Imidazolinthio	0.63	-
1'-Methyl-4'-nitroimidazol-5'-ylthio	0.27	-
Benzylthio	2.57	-
3,4-Dimethylbenzylthio	3.57	-
o-Chlorobenzylthio	3.53	-
o-Fluorobenzylthio	2.96	-
o-Nitrobenzylthio	3.29	-
m-Chlorobenzylthio	3.28	-
p-Fluorobenzylthio	2.96	-
2'-Pyridylmethylthio	1.16	-
Methylsulfonyl	-1.63	0.22
Ethylsulfonyl	-1.13	-
n-Propylsulfonyl	-0.63	-
n-Butylsulfonyl	-0.13	-
Fluorosulfonyl	0.05	0.22
Sulfonamide	-1.82	0.19
N-Methylsulfonamide	-1.32	-
N-n-Propylsulfonamide	-0.32	-
N-iso-Butylsulfonamide	0.23	-
N-3'-Methoxypropylsulfonamide	-0.34	-
N-2'-Ethoxyethylsulfonamide	-0.44	-
N-Benzylsulfonamide	0.19	-

Table 3. χ Terms of Mono- and Disubstituted Purines

Compound	$^3\chi_c$	$^0\chi$	$^1\chi$	$^1\chi^v$
Purine	0.333	6.104	4.466	2.557
6-Chloro	0.538	6.975	4.877	3.050
6-Bromo	0.538	6.975	4.877	3.465
6-Iodo	0.538	6.975	4.877	3.734
6-Methoxy	0.469	7.682	5.415	3.096
6-n-Propoxy	0.469	9.096	6.415	4.184
6-Hydrazino	0.469	7.682	5.415	3.023
6-Trimethylammonium	0.421	9.475	6.089	4.913
6-Methylthio	0.469	7.682	5.415	4.317
6-Ethylthio	0.469	8.389	5.915	4.666
6-Methylsulfonyl	0.421	9.475	6.089	3.902
6-Sulfonamide	0.421	11.052	7.032	4.170
2-Methyl-6-amino	0.827	7.845	5.271	3.204
2-Chloro-6-methylamino	0.758	8.552	5.809	3.731
2-Bromo-6-amino	0.827	7.845	5.271	3.684
2-Amino-6-chloro	0.827	7.845	5.271	3.270
2-Amino-6-bromo	0.827	7.845	5.271	3.684
2-Amino-6-iodo	0.827	7.845	5.271	3.954
2-Amino-6-methyl-sulfonyl	0.709	10.345	6.482	3.871
2-Dimethylamino-6-methylamino	0.636	10.129	6.719	4.283
2,6-Bishydrazino	0.674	9.259	6.347	3.492
2,6-Bis(methyl sulfonyl)	0.565	12.845	7.693	5.250
2-Flurosulfonyl-6-chloro	0.683	10.345	6.482	4.018

Table 4. Observed Predicted CA755 Activity of Mono- and Di-Substituted Purines

Compound	log (1/c)		$\lvert\Delta$log(1/c)$\rvert$
	Observed	Predicted	
Purine	Inactive	4.53	–
6-Chloro	4.23	4.15	0.08
6-Bromo	4.50	4.25	0.25
6-Iodo	4.52	4.30	0.22
6-Methoxy	3.00	3.48	0.47
6-n-Propoxy	3.42	3.68	0.26
6-Hydrazino	3.22	3.12	0.10
6-Trimethylammonium	4.34	4.27	0.06
6-Methylthio	4.51	4.44	0.07
6-Ethylthio	4.45	4.41	0.04
6-Methylsulfonyl	4.04	4.31	0.27
6-Sulfonamide	4.26	3.98	0.28
2-Methyl-6-amino	3.23	2.99	0.23
2-Chloro-6-methylamino	3.37	2.97	0.39
2-Bromo-6-amino	2.56	3.14	0.58
2-Amino-6-chloro	4.05	3.89	0.15
2-Amino-6-bromo	3.91	3.99	0.08
2-Amino-6-iodo	3.91	4.05	0.13
2-Amino-6-methylsulfonyl	4.04	3.97	0.06
2-Dimethylamino-6-methylamino	3.12	2.79	0.33
2,6-Bishydrazino	2.77	2.86	0.09
2,6-Bis(methylsulfonyl)	3.64	3.70	0.06
2-Flurosulfonyl-6-chloro	3.18	3.41	0.23

Table 5. χ Terms of 6-Substituted Purines

Compound	$^3\chi_c$	$^3\chi_c^v$	$^1\chi$	$^1\chi^v$	$^0\chi^v$
Purine	0.333	0.120	4.466	2.557	4.574
Chloro	0.538	0.238	4.877	3.050	5.629
Bromo	0.538	0.331	4.877	3.465	6.457
Iodo	0.538	0.391	4.877	3.734	6.996
Methylthio	0.469	0.248	5.415	4.317	6.718
Ethylthio	0.469	0.248	5.915	4.666	7.425
Cyano	0.469	0.168	5.415	2.958	5.443
Ethoxy	0.469	0.157	5.915	3.684	6.611
Amino	0.469	0.176	4.877	2.773	5.073
Hydrazino	0.469	0.168	5.415	3.023	5.573
n-Propylthio	0.469	0.248	6.415	5.166	8.132
n-Butylthio	0.469	0.248	6.915	5.666	8.839
iso-Butylthio	0.878	0.657	6.771	5.522	9.002
sec-Butylthio	0.758	0.747	6.401	5.493	9.002
2′-Propynylthio	0.469	0.248	6.415	4.812	7.925
Cyanomethylthio	0.469	0.248	6.415	4.536	7.372
Cyclopentylthio	0.674	0.601	7.433	5.617	9.123
Phenylthio	0.674	0.452	7.933	5.616	9.104
2′-Imidazolinylthio	0.674	0.425	7.433	2.585	8.709
1′-Methyl-4′-nitro-imidazol-5′-ylthio	1.311	0.680	9.165	6.183	10.569
Benzylthio	0.674	0.366	8.433	6.223	9.812
3′,4′-Dimethylbenzylthio	1.145	0.655	8.904	7.050	11.657
o-Chlorobenzylthio	0.872	0.514	8.844	6.456	10.866
o-Fluorobenzylthio	0.872	0.514	8.844	6.329	10.112
o-Nitrobenzylthio	1.105	0.443	9.755	6.677	10.959
m-Chlorobenzylthio	0.962	0.555	8.827	6.700	10.866
p-Fluorobenzylthio	0.962	0.429	8.827	6.323	10.112
2′-Pyridylmethylthio	0.874	0.340	8.433	6.083	9.681
Ethylsulfonyl	1.182	0.480	6.649	4.430	7.632
n-Propylsulfonyl	1.182	0.480	7.149	4.930	8.339
n-Butylsulfonyl	1.182	0.480	7.649	5.430	9.046
N-Methylsulfonamide	1.247	0.470	7.570	4.550	8.333
N-n-Propylsulfonamide	1.247	0.470	8.570	5.610	9.747
N-iso-Butylsulfonamide	1.655	0.878	8.926	5.966	10.617
N-3′-Methoxypropyl-sulfonamide	1.247	0.470	9.570	6.100	10.863
N-2′-Ethoxyethyl-sulfonamide	1.274	0.470	9.570	6.188	10.863
N-Benzylsulfonamide	1.451	0.587	10.588	6.668	11.427

The CA755 activity (log 1/c) and toxicity (log $1/LD_{50}$) of the compounds studied are those of Neiman and Quinn[25].

From Table 2 and 3, the relationship with CA755 activity is:

$$\log(1/C) = -0.1789(\pm 0.0223)\,{}^3\chi_c + 1.6539(\pm 0.3570)\,R(6) - 0.5665(\pm 0.0926)\,{}^0\chi + 0.5554(\pm 0.2295)\,{}^1\chi + 0.3234(\pm 0.2021)\,{}^1\chi^v + 4.7453(\pm 1.2925) \quad (5)$$

$$N=20 \qquad r=0.9027 \qquad S=0.3131$$

In this case, the structural characteristics influencing the electron-receptor role of the substituent are best quantified by the combination of the simple connectivity ($^3\chi_c$, $^0\chi$, $^1\chi$), the

Table 6. Observed and Predicted Toxicities of 6-Substituted Purines

Substituent	log(1/LD$_{50}$)		$\lvert\Delta$log(1/LD$_{50}$)$\rvert$
	Observed	Predicted	
Purine	Nontoxic	2.82	–
Chloro	2.73	2.94	0.21
Bromo	2.79	2.90	0.11
Iodo	2.96	2.85	0.11
Methylthio	3.16	3.12	0.04
Ethylthio	3.04	3.10	0.06
Cyano	3.26	3.17	0.09
Ethoxy	3.24	3.08	0.16
Amino	3.10	3.18	0.08
Hydrazino	3.24	3.19	0.05
n-Propylthio	3.21	3.10	0.11
n-Butylthio	3.06	3.10	0.04
iso-Butylthio	3.15	3.12	0.03
sec-Butylthio	3.02	3.10	0.08
2′-Propynylthio	3.12	3.13	0.01
Cyanomethylthio	3.35	3.30	0.05
Cyclopentylthio	3.23	3.22	0.01
Phenylthio	3.32	3.24	0.08
2′-Imidazolinylthio	3.38	3.40	0.02
1′-Methyl-4′-nitro-imidazol-5′-ylthio	3.60	3.55	0.05
Benzylthio	3.13	3.27	0.14
3′-4′-Dimethylbenzylthio	3.20	3.14	0.06
o-Chlorobenzylthio	3.04	3.13	0.09
o-Fluorobenzylthio	3.31	3.25	0.06
o-Nitrobenzylthio	3.42	3.39	0.03
m-Fluorobenzylthio	3.22	3.20	0.02
p-Fluorobenzylthio	3.28	3.25	0.03
2′-Pyridylmethylthio	3.38	3.41	0.03
Ethylsulfonyl	3.30	3.39	0.09
n-Propylsulfonyl	3.39	3.39	0.00
n-Butylsulfonyl	3.43	3.40	0.03
N-Methylsulfonamide	3.53	3.45	0.08
N-n-Propylsulfonamide	3.43	3.47	0.04
N-iso-Butylsulfonamide	3.58	3.50	0.08
N-3′-Methoxypropyl-sulfonamide	3.48	3.54	0.06
N-2′-Ethoxyethyl-sulfonamide	3.57	3.57	0.00
N-Benzylsulfonamide	3.58	3.69	0.11

valence connectivity ($^1\chi^v$), and the resonance constant ($R(6)$) as effects of substituents at position 6. This result indicates that both a connectivity structural characteristic and an electronic influence contribute to the activity within the series.

Equation 5 relates the CA 755 antitumor potency of mono- and disubstituted purines to the connectivity indexes of substituents at positions and the resonance constant R at position 6. It accounts for 81% of the variance in the biological data ($r^2 = 0.81$). The predicted values are shown in Table 4.

Equation 6, a toxicity correlation, was derived from the data in Table 2 and Table 5.

$$\log\left(\frac{1}{LD_{50}}\right) = -0.1095\,(\pm 0.1456)\,{}^3\chi_c + 0.3784\,(\pm 0.2046)\,{}^3\chi_c^v - 0.1101\,(\pm 0.0216)\,\pi(6) + 0.1654\,(\pm 0.0445)\,{}^1\chi^c + 0.1993\,(\pm 0.0803)\,{}^1\chi^v - 0.1736\,(\pm 0.0706)\,{}^0\chi^v + 2.5509\,(\pm 0.1096) \quad (6)$$

$N=36 \qquad r=0.9257 \qquad s=0.0878$

The predicted values using equation 6 are shown in Table 6. These results are in reasonable agreement with the observed toxicities of 6-substituted purines.

In each case, a meaningful correlation has been obtained between a quantitative activity and selected connectivity terms or physicochemical parameters. This approach will contribute to obtaining direct structural information in order to permit the familiar iterative process: Experimental observation-Theoretical consideration-Experimental observation-Clinical treatment.

Acknowledgement. We thank the Korea Science and Engineering Foundation for financial support.

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Studies on the Paramagnetic Impurity Y_2BaCuO_5 in Superconducting $YBa_2Cu_3O_{7-\delta}$ Phase

Jin-Ho Choy* and Sung-Ho Chun

Department of Chemistry, Seoul National University, Seoul 151-742. *Received May 20, 1988*

Conventional ceramic method has been used to prepare the green phase, Y_2BaCuO_5, commonly observed in 90-K superconductor $YBa_2Cu_3O_{7-\delta}$ as an impurity phase. The powder X-ray diffraction analysis indicates that Y_2BaCuO_5 has an orthorhombic symmetry with lattice parameter of a = 12.2 Å, b = 5.61 Å, and c = 7.14 Å. The average g-value 2.13 observed in ESR spectrum is attributable to Cu^{2+} stabilized in C_{4v} field. From the magnetic susceptibility (μ_{eff} = 2.29 BM) and the ESR measurements, it is confirmed that Cu(II) $3d^9$ electrons in Y_2BaCuO_5 are localized and can be characterized by Curie-Weiss behavior. Optical reflectance spectrum shows a broad absorption peak around 680 nm due to $dxy \rightarrow dx^2\text{-}y^2$ eletronic transition.

Introduction

Since the discovery of high Tc superconductor by Bednorz and Müller[1], and Wu *et al*[2], numerous studies on this system have been performed with various scientific and technological points of view.

Recently some efforts have been made to prepare the pure $YBa_2Cu_3O_{7-\delta}$ phase not by conventional ceramic processing and fabricating methods but by chemical precursor ones[3,4], because a green insulator Y_2BaCuO_5 is very often detected in the polycrystalline superconductor $YBa_2Cu_3O_{7-\delta}$ as an impurity phase.

The purpose of this work is to investigate physicochemical properties of the green phase Y_2BaCuO_5, which might suppress the superconducting behavior, and to differentiate its spectroscopic properties from the superconducting phase.

In this work, preparation, structure, magnetic susceptibility measurement, electron spin resonance, and optical reflectance spectroscopic studies have been systematically carried out on Y_2BaCuO_5.

Experimental

Y_2BaCuO_5 was prepared by two steps: at first a mixture of 1:1:1 mole ratio of Y_2O_3, $BaCO_3$, and CuO powders has been pelletized and preheated at 900 °C for 18 hours and then the sample was reground, repelletized, and finally heated at 940 °C in oxygen atmosphere for 24 hours. Color of the obtained product was green.

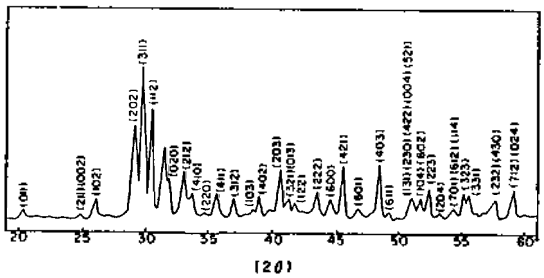

Figure 1. XRD pattern of Y_2BaCuO_5.

X-ray diffraction patterns were recorded with Ni-filtered Cu-K_α radiation (λ = 1.5418 Å) on Jeol diffractometer. Electron spin resonance spectra were obtained from 10 K to 300 K with a Bruker Et 200tt X-band spectrometer. Magnetic susceptibility measurement was carried out with a Faraday type magnetobalance from 77 to 300 K. Optical reflectance spectrum was obtained at room temperature with a Carry 16 spectrometer.

Results and Discussion

According to the X-ray powder diffraction analysis, a single phase of Y_2BaCuO_5 has been identified as an orthorhombic crystal system. Its space group is P_{nma} or P_{na2_1} with the lattice parameters a = 12.2 Å, b = 5.61 Å, and c = 7.14 Å