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Identification of Basic Effector Proteins of Drugs and Vice Versa

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Abstract

This work establishes relationship between drug constitution and its basic effector molecules within the human body. Basic effectors derived from constitutional elements of all the 20 (twenty) drugs were matching with those mentioned in the existing medical literature. Therefore drug and its effects can be identified easily. Retrospectively a drug can also be designed for any given basic effectors within the body.

Keywords: Basic Effectors, Drugs, Anti Cancer Drugs, Designer Drugs.

INTRODUCTION

This is a work, drawing relationship between chemical elements forming a drug compound and the molecular weights of their basic effector proteins in the body that create a biochemical effect(s). This approach can be of use to identify a basic effector protein of a drug compound and vice-versa. A mathematical formula is developed and used for that.

Aim: Identification of molecular weight (s) of basic effectors of drug (s) based on its constituents.

METHOD

Firstly, names of drugs and their chemical formulae are listed.

Next, effector(s) of each of the above mentioned drugs are noted along with their molecular weights in Kilo Daltons are noted. An effector induces biochemical change(s) in the body.

Concepts Used:

Log A/Log B = R (Ratio) = 64.5 /C-H-N-O, Where Log A is Logarithm of molecular weight (elemental atomic weight multiplied by number molecules of that element) of individual element(s) of drug. Log B is Logarithm of molecular weight of similar element(s) of the Deoxy Ribose Nucleic Acid (DNA). C-H-N-O is basic effector. 64.5 kda is the molecular weight of a complex effector molecule.

Atomic weight of the element x number of molecules of the same molecule=Molecular weight of that element in either DNA or Drug.

An effector in this context means, it either carries an element or stimulates or inhibits biochemical reaction(s). In this work, we have assumed a smallest basic effector (One molecule) to be consisting of 1 Carbon, 1 Hydrogen, 1 Oxygen and 1 Nitrogen molecule held together in closed knit group based on their known individual valencies of 4, 1, 2 and 3 respectively. Basic effector molecule(s) could be in multiples of 1 as well. Compared to a basic effector protein group, Haemoglobin is a complex protein molecule which binds to Oxygen (O_2), Carbon (CO_2), Nitrogen (NO), Hydrogen (H_2 O) and Sulphur (SO_2) individually. Carbon, Hydrogen, Nitrogen, Oxygen and Sulphur together in various combinations can form drugs.

The Mathematical Calculation:

Next, the ratio(R) of individual logarithmic values of the molecular weight of elements of a given drug to the logarithmic values of molecular weight of the same element of Deoxy Ribose Nucleic acid (DNA) is obtained. DNA is chosen as denominator, because, it is one of smallest building block protein molecule of human body. So, it was considered for calculating the ratio(R). Therefore, we assume that individual elements of the given drug may interact with "R" times bigger than the smallest basic effector protein moiety(C-H-N-O). The resultant molecular weight(R x Molecular weight of

C-H-N-O) obtained is assumed to be equal to the molecular weight of a complex effector molecule. In this work Haemoglobin is considered as a complex effector. The reason behind this assumption is that haemoglobin interacts with Oxygen (O_2), Carbon (CO_2), Nitrogen (NO), Hydrogen (H_2 O) and Sulphur (SO_2) individually. These elements in different combinations can form different drugs. In this manner we can find out the molecular weight of basic effector protein moiety i.e., C-H-N-O. In this work we have considered 64.5 Kilodaltons as the molecular weight of Haemoglobin. Therefore the derived molecular weights of basic effectors are in Kilo Daltons.

To Sum it up it is: Logarithm of molecular weight (elemental atomic weight multiplied by number molecules of that element) of individual element(s) of drug / Logarithm of molecular weight of similar element(s) of the Deoxy Ribose Nucleic Acid (DNA) = R (Ratio). Using that ratio obtained as the number of times(R) the molecular weight of basic effector protein(s) is equal to 64.5 KILODALTONS –the molecular weight of Haemoglobin.

Therefore, molecular weight of basic effector protein= 64.5/R KILODALTONS (kda).

OBSERVATIONS

Chemical Formula of Human DNA: $C_{15} H_{31} N_3 O_{13} P_2$.
Molecular Weight of Haemoglobin: 64.5 KILODALTONS

Table 1:

S. No	Chemical Formula	Logarithmic Value of MOL. WT of Carbon in DNA	Logarithmic Value of MOL. WT of Hydrogen in DNA	Logarithmic Value of MOL. WT of Nitrogen in DNA	Logarithmic Value of MOL. WT of Oxygen in DNA	Logarithmic Value of MOL. WT of Phosphorus in DNA
1	DNA $C_{15}H_{31}N_3O_{13}P_2$	2.255	1.491	1.6232	2.31806	0.301

Table 2:

S. No	Chemical Formula	Logarithmic Value of MOL. WT of Carbon	Logarithmic Value of MOL. WT of Hydrogen	Logarithmic Value of MOL. WT of Nitrogen	Logarithmic Value of MOL. WT of Oxygen
1	MEPOLIZUMAB $C_{66476} H_{10084} N_{1732} O_{2028} S_{46}$	5.9	4	4.38	4.51
2	USTEKINUMAB $C_{6482}H_{10004} N_{1712} O_{2016} S_{46}$	4.89	4	4.37	4.5
3	VINCRISTINE $C_{46}H_{56}N_4O_{10}$	2.74	1.74	1.74	2.2
4	TAXOL $C_{57}H_{51}NO_{14}$	2.83	1.7	1.14	2.35
5	ADALIMUMAB $C_{6428}H_{9512}N_{1694}O_{1987} S_{46}$	4.88	3.97	4.37	4.5
6	TRASTUZUMAB $C_{6470}H_{10012}N_{1726} O_{2013} S_{42}$	4.89	4	4.38	4.5
7	RAMUCIRUMAB $C_{6374} H_{9864} N_{1692} O_{1996} S_{46}$	4.88	3.99	4.37	4.5
8	GOLIMUMAB $C_{6530} H_{10068} N_{1752} O_{2006} S_{44}$	4.89	4	4.38	4.5
9	PANITUMUMAB $C_{6398}H_{9874}N_{1694} O_{2016} S_{48}$	4.88	3.99	4.37	4.50
10	CANAKINUMAB $C_{6452}H_{9958}N_{1722}O_{2010} S_{42}$	4.88	3.99	4.38	4.50
11	DENOSUMAB $C_{6404}H_{9912}N_{1724}O_{2004} S_{50}$	4.88	3.99	4.38	4.50
12	OBINUTUZUMAB $C_{6512}H_{10060}N_{1712} O_{2020} S_{44}$	4.89	4	4.37	4.5
13	TOSITUMOMAB $C_{6416} H_{9874} N_{1688} O_{1987} S_{44}$	4.88	3.99	4.37	4.50
14	POLATUZUMAB $C_{6670} H_{10317} N_{1745} O_{2087} S_{40}$	3.90	4.01	4.38	4.39
15	BEVACIZUMAB $C_{6638} H_{1060} N_{1720} O_{1208} S_{44}$	4.90	3.02	4.38	4.28

16	OFATUMUMAB $C_{6480}\ H_{1022}\ N_{1742}\ O_{2020}\ S_{44}$	4.89	3	4.38	4.5
17	DOSTARLIMAB $C_{6420}\ H_{9832}\ N_{1690}\ O_{2014}\ S_{44}$	4.88	3.99	4.37	4.5
18	IPILIMUMAB $C_{6472}\ H_{9972}\ N_{1732}\ O_{2004}\ S_{40}$	4.89	3.99	4.38	4.5
19	NIVOLUMAB $C_{6362}\ H_{9862}\ N_{1712}\ O_{1995}\ S_{42}$	4.88	3.99	4.37	4.5
20	PERTUZUMAB $C_{17}\ H_{27}\ N\ O_2$	2.3	1.43	1.14	1.5

Table 3:

S. No	Chemical formula	Based on carbon value–molecular weight of basic effector protein (x=64.5 x 1/r)	Based on hydrogen value–molecular weight of basic effector protein (x=64.5 x 1/r)	Based on nitrogen value–molecular weight of basic effector protein (x=64.5 x 1/r)	Based on oxygen value–molecular weight of basic effector protein (x=64.5 x 1/r)	Average molecular weight of basic effector protein
1	MEPOLIZUMAB $C_{66476}\ H_{10084}\ N_{1732}\ O_{2028}\ S_{46}$	25kda	24kda	35kda	33kda	29kda
2	USTEKINUMAB $C_{6482}H_{10004}\ N_{1712}\ O_{2016}\ S_{46}$	30kda	24kda	24kda	33kda	28 kda
3	VINCRISTINE $C_{46}H_{56}N_4O_{10}$	60kda	55kda	60kda	68kda	61kda
4	TAXOL $C_{57}H_{51}NO_{14}$	51kda	56kda	91kda	64kda	66kda
5	ADALIMUMAB $C_{6428}H_{9512}N_{1694}O_{1987}\ S_{46}$	30kda	24kda	24kda	33kda	28kda
6	TRASTUZUMAB $C_{6470}H_{10012}N_{1726}\ O_{2013}\ S_{42}$	30kda	24kda	24kda	33kda	28kda
7	RAMUCIRUMAB $C_{6374}\ H_{9864}\ N_{1692}\ O_{1996}\ S_{46}$	30kda	24kda	24kda	33kda	28kda
8	GOLIMUMAB $C_{6530}\ H_{10068}\ N_{1752}\ O_{2006}\ S_{44}$	30kda	24kda	24kda	33kda	28kda
9	PANITUMUMAB $C_{6398}H_{9874}N_{1694}\ O_{2016}\ S_{48}$	30kda	24kda	24kda	33kda	28kda
10	CANAKINUMAB $C_{6452}H_{9958}N_{1722}O_{2010}\ S_{42}$	30kda	24kda	24kda	33kda	28kda
11	DENOSUMAB $C_{6404}H_{9912}N_{1724}O_{2004}\ S_{50}$	30kda	24kda	24kda	33kda	28kda
12	OBINUTUZUMAB $C_{6512}H_{10060}N_{1712}\ O_{2020}\ S_{44}$	30kda	24kda	24kda	33kda	28kda
13	TOSITUMOMAB $C_{6416}\ H_{9874}\ N_{1688}\ O_{1987}\ S_{44}$	30kda	24kda	24kda	33kda	28kda
14	POLATUZUMAB $C_{6670}\ H_{10317}\ N_{1745}\ O_{2087}\ S_{40}$	37kda	24kda	24kda	34kda	30kda

15	BEVACIZUMAB C_{6638} H_{1060} N $_{1720}$ O_{1208} S_{44}	30kda	32kda	24kda	35kda	30kda
16	OFATUMUMAB C_{6480} H_{1022} N $_{1742}$ O_{2020} S_{44}	30kda	32kda	24kda	33kda	30kda
17	DOSTARLIMAB C_{6420} H_{9832} N $_{1690}$ O_{2014} S_{44}	30kda	24kda	24kda	33kda	28kda
18	IPILIMUMAB C_{6472} H_{9972} N $_{1732}$ O_{2004} S_{40}	30kda	24kda	24kda	33kda	28kda
19	NIVOLUMAB C_{6362} H_{9862} N $_{1712}$ O_{1995} S_{42}	30kda	24kda	24kda	33kda	28kda
20	PERTUZUMAB C_{17} H $_{27}$ N O_2	63kda	67kda	91kda	99kda	80kda

*R(Ratio)=Log (Number of elemental molecular weight in a drug)/ Log (Number of same elemental molecular weight in a DNA molecule)

64.5=64.5 kilo Dalton molecular weight of Haemoglobin.

Table 4:

S. No	Chemical formula	Molecular weight(s) of basic effector(s) In existing medical literature (KDA)	Matching (within +7 to -7 kda) molecular weights of individual basic effector of table-3 (yes/no)	Matching average molecular weights of invidual basic effectors of table -3 (yes/not known)
1	MEPOLIZUMAB C_{66476} H_{10084} N_{1732} O_{2028} S_{46}	IL-5[1]- ≈ 26.5 [2]	YES	YES
2	USTEKINUMAB $C_{6482}H_{10004}N_{1712}O_{2016}S_{46}$	P40 SUBUNIT[3] OF IL-12 & IL-23-≈ 34.6 [4]	YES	YES
3	VINCRISTINE $C_{46}H_{56}N_4O_{10}$	BETA SUBUNIT OF TUBULIN[5]-≈ 55 [6]	YES	YES
4	TAXOL $C_{57}H_{51}NO_{14}$	BETA SUBUNIT OF TUBULIN[7] -≈ 55[6]	YES	NO
5	ADALIMUMAB $C_{6428}H_{9512}N_{1694}O_{1987}S_{46}$	TANSMEMBRANE[8] TNF α-≈26 [9]	YES	YES
6	TRASTUZUMAB $C_{6470}H_{10012}N_{1726}O_{2013}S_{42}$	ECD IV OF HER2[11]-≈17.1 [10,14]	YES	NO
7	RAMUCIRUMAB C_{6374} H $_{9864}$ N $_{1692}$ O $_{1996}$ S $_{46}$	HUMAN VEGF [17]-≈21 [16]	YES	YES
8	GOLIMUMAB C_{6530} H $_{10068}$ N $_{1752}$ O $_{2006}$ S $_{44}$	TRANSMEMBRANE [12] TNF α-≈26 [9]	YES	YES
9	PANITUMUMAB $C_{6398}H_{9874}N_{1694}O_{2016}S_{48}$	ECD III OF EGFR [15]-≈22.9 [13]	YES	YES
10	CANAKINUMAB $C_{6452}H_{9958}N_{1722}O_{2010}S_{42}$	IL-1β [18]-≈31 [19]	YES	YES
11	DENOSUMAB $C_{6404}H_{9912}N_{1724}O_{2004}S_{50}$	HUMAN RANKL [20]-≈20 [21]	YES	NO
12	OBINUTUZUMAB $C_{6512}H_{10060}N_{1712}O_{2020}S_{44}$	CD 20 [24]-≈33 [25]	YES	YES
13	TOSITUMOMAB C_{6416} H_{9874} N $_{1688}$ O_{1987} S $_{44}$	CD 20 [26]-≈33 [25]	YES	YES
14	POLATUZUMAB C_{6670} H $_{10317}$ N $_{1745}$ O $_{2087}$ S $_{40}$	CD79B [27]-≈33 [28]	YES	YES
15	BEVACIZUMAB C_{6638} H_{1060} N $_{1720}$ O_{1208} S_{44}	VEGF [29]-≈21 [16, 30]	YES	NO
16	OFATUMUMAB C_{6480} H_{1022} N $_{1742}$ O_{2020} S_{44}	CD 20 [31]-≈33 [25]	YES	YES

17	DOSTARLIMAB C_{6420} H_{9832} N $_{1690}$ O_{2014} S_{44}	PD-1 [32]-≈32 [33]	YES	YES
18	IPILIMUMAB C_{6472} H_{9972} N $_{1732}$ O_{2004} S_{40}	CTLA 4 [34]-≈33 [35]	YES	YES
19	NIVOLUMAB C_{6362} H_{9862} N $_{1712}$ O_{1995} S_{42}	PD-1 [36]-≈32 [33]	YES	YES
20	PERTUZUMAB C_{17} H $_{27}$ N O_2	ECD II OF HER2 [22]-≈105 [23]	YES	NO

DISCUSSION

Individual molecular weights of derived basic effector(s) of all the 20 (twenty) drugs mentioned in this study coincides with that mentioned in existing medical literature.

This approach can be used to identify potential basic effector(s) of a drug, within human body. Retrospectively, a drug can also be created for a particular basic effector.

CONCLUSION

In this the individually derived molecular weights of basic effector of all 20 drugs mentioned above matches with that mentioned in existing literature. So this above approach can be of use in identifying potential basic effector(s) of a drug. It can be also be used to design a drug for a potential basic effector.

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