# An Exploration and Analysis on the Usage of Various Cough Syrups Based on the Role of Active Chemical Ingredient and its Impact Influencing the Consumers

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***Abstract***

*A statistical survey on the behavioral aspects of various cough syrups based on the purchasing pattern, usage and consumption by consumers of different domains and profession were analyzed in depth based on the nature of the cough involved. The frequency of syrup procured along with the mode of purchase pattern, brand, type and the cost were accounted. Role of various cough syrups preferred by the respondents based on the chemically active ingredients (drugs), chemical composition, flavour and emulsifier influencing the purchasing pattern were considered for analysis. Based on the respondent's information, the active chemical ingredients (drugs) in different cough syrups were predominantly Ambroxol, Bromhexine, Chlorpheniramine, Dextromethorphan Diphenhydramine, Guaifenesin, Levodropropizine, Phenylephrine, Salbutamol, Terpin hydrate and Terbutaline. A closer analysis on the existing combination of these active chemical ingredients in cough syrups influencing the medical sector is imparted based on molecular docking of these drugs with serine protease HtrA1. The Mycobacterium Tuberculosis strain ATCC 25618/H37Rv is the major cause of cough*

*emanating through various means. The role of single/double/triple chemically active ingredients in cough syrups certainly influences the pattern of popularity among the various cough syrups and the brand value definitely governs the consumption of the syrups by the respondents. The study clearly illustrates the role of pharmaceutical sector governing the purchasing pattern of syrups on the consumers and the factors influencing the medical field related to disorders/diseases emanating through cough.*

***Keywords:*** *Cough Syrups; active chemical ingredients; drugs; binding affinity; bimolecular interactions*

## 1. Introduction

A comprehensive statistical survey regarding the procurement, consumption and significance of various branded cough syrups consumed by the people in Chennai city (capital of the state of Tamil Nadu, India) were carried out and explored in depth. Purposive sampling method was employed to identify the respondents as some basic understanding of cough syrup (CS) and as a prelude to the study, a survey among the people was conducted for awareness of the active chemical ingredient (ACI) of CS responsible for treating various types of cough. Therefore, all the respondents with a proper knowledge of chemistry involving pharmaceutical chemistry as a topic of study were only provided with a questionnaire, such that the respondents comprised under graduates, post graduates, doctorates and post doctorates in the field of chemistry.

The study was necessary in the following aspects because, the syrups are prescribed by the physicians/doctors predominantly on the brand names prevailing on the geographic demographics of the country. The brand (manufacturers) predominantly influence by marketing executive professionals and excessive advertising through media to promote enhanced trend in sales and exhibit their product across the regional/national level as well as in the global sector. However, the extent of usage and role of cough syrups on the metabolic activity and side effects is lesser known among the consumers since there prevails several types of cough. Further, there exists several combinations of certain ACI that are available either over the counter (OTC) or through valid prescriptions. However they are not procured based on the ACI, but predominantly on the name of the brand.

The study focuses on significance and properties of consumption of these syrups based on their type and chemical composition. Exploration regarding the type of combinations that exist, accessibility and role of CS's on human behavior and conceptions is analyzed. The role of bimolecular interactions of ACI with protein is explored by theoretical studies. The role of single/double/triple combination of ACI in cough syrups influencing the buyers and the importance of brand and its significance on the users is explored. 90% of the respondents were graduates and above, which play a significant factor on the prior knowledge about CS's and ACI present in it. As regard to age, most of the respondents (57%) belong to 21 to 30 years of age. 42% responded that they get cough seasonally and majority of the respondents (72%) follow prescription from the medical practioners or physicians for procuring CS rather than over the counter (OTC) However, significant

number of respondents are influenced through advertisements and social media, which also play a crucial role on the pattern of procurement of the syrups. Interestingly, 43% have certain awareness on the types of CS's existing and 24% of those had awareness about dry as well as wet cough only (apart from other type) which is also a key factor.

An illustrative representation of the awareness by the respondents on various types of cough syrups are provided in Fig 1.

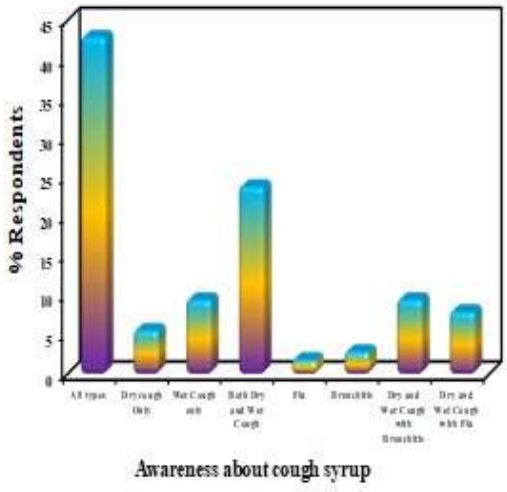


**Fig 1:** Detailed information on the awareness of the various types of cough

65% of respondents felt that pharma companies promote by marketing through doctors/ medical professionals. A detailed illustration and awareness on the knowledge of the composition of cough syrup by respondents and role of brand in accordance prescribed by the physicians are provided in Fig 2a and Fig 2b respectively.

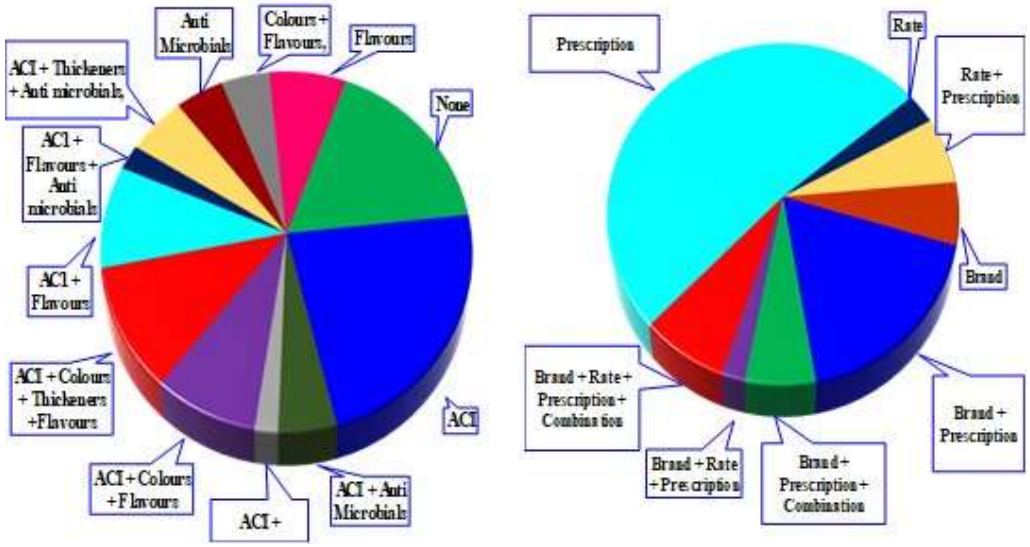


**Fig 2:** (a) Factors influencing the respondent in procuring the cough syrups, (b) Choice of the respondent involved in procuring the cough syrups.

However, 46 % agreed that herbal syrup can be an alternative to allopathic syrup based on factors such as extent of dosage required for treatment, availability and the brand. 51 % also believed that single brand is not localized throughout in the region. One third of the respondents agreed that pharma companies serve the people, however the rest presumably provided information that companies create demand or use promotions to sell their product. Significant number of people (74%) believe that CS is effective, but also mentioned that the quantity of CS involved depends upon the severity of the cough. Interestingly, a few or negligible amount of the respondents are aware of the ACI present in the syrup that are specific for dry/wet, productive, acute, subacute or chronic cough. However, several patterns of cough go away on their own based on the severity and can be treated with home remedies or OTC cough medicines.

The table provides the detailed information regarding the purchase of cough syrups based on the popularity localized in Chennai and its suburbs **(Table 1)**. The table is based on the individual preference of purchase and usage by the respondents and not based on any personal conceptions of the authors. The information procured is based on all seasonal time domain and does not correlate with pre or post COVID-19 scenario. The tabulated syrup has been consumed by several respondents and the name of the cough syrups have been abbreviated as "CS" and that of the manufacturer/Company as "B".

Interestingly, most of the CS based on the popularity comprises of either dry or wet cough only. Except for CS13, CS26 and CS29, the price per/100 mL corresponds to less than USD 0.50 and many CS's are around USD 1 and above. Table 1 reveals that except for certain syrups, all other CS's are of uniformly priced, providing competitive scenario of various brands among the pharma companies.

It has been well established that dry cough can be triggered predominantly by smoke generated from automobile, industries and power plants[1-10]. Other major causes of dry cough involve dust, respiratory illnesses (Cold and Flu), Gastroesophageal Reflux Disease (GERD) and through certain medications. However, the productive cough better known as wet cough causes congestion in chest and produces enormous mucus or phlegm that ranges from person to person based on the colour. In general, Pneumonia, Bronchitis, Influenza causes wet cough and the color of the mucus is a better indicator of the severity of the problem.

**Table 1:** Details of the active chemical ingredients (ACI) of the various cough syrup as per the survey from the respondents.

| S. No | Cough Syrup | Active Chemical Ingredients (ACI) | Specification for type of cough | Brand | Rate USD / 100 mL |
|---|---|---|---|---|---|
| 1 | CS1 | Diphenhydramine (DIP) | Dry Chest | B1 | 0.97 |
| 2 | CS2 | Ambroxol (AMB) Guaifenesin (GUA) Salbutamol (SAL) | Dry and Wet Cough | B2 | 1.39 |
| 3 | CS3 | DIP | Dry and Wet Cough | B3 | 0.98 |

| | | | | | |
|---|---|---|---|---|---|
| 4 | CS4 | Chlorpheniramine (CHL) Dextromethorphan (DEX) Phenylephrine (PHE) | Dry and Wet Cough | B4 | 1.19 |
| 5 | CS5 | CHL, DEX | Dry Cough | B5 | 1.39 |
| 6 | CS6 | CHL, DEX | Dry Cough | B6 | 1.82 |
| 7 | CS7 | CHL, DEX, GUA | Dry and Wet Cough | B2 | 1.45 |
| 8 | CS8 | CHL, DEX, PHE | Dry and Wet Cough | B7 | 1.05 |
| 9 | CS9 | CHL, DEX | Dry and Wet Cough | B3 | 0.99 |
| 10 | CS10 | DEX | Dry Cough | B8 | 1.57 |
| 11 | CS11 | AMB, GUA, Terbutaline (TERB) | Dry Cough | B9 | 1.24 |
| 12 | CS12 | CHL, DEX Levodropropizine (LEV) | Dry Cough | B3 | 1.05 |
| 13 | CS13 | SAL | Dry Cough | **B3** | **0.20** |
| 14 | CS14 | AMB | Asthma, COPD | B10 | 2.01 |
| 15 | CS15 | Bromhexine (BRO), GUA, SAL | Cough , Cough with Mucus | B2 | 1.54 |
| 16 | CS16 | Bromhexine (BRO), GUA, SAL | Cough , Cough with Mucus | B11 | 0.69 |
| 17 | CS17 | AMB | Mucolytic | B12 | 0.85 |
| 18 | CS18 | AMB, GUA, TERB | Cough with Mucus | B13 | 1.03 |
| 19 | CS19 | BRO, GUA, TERB | Cough with Mucus | B14 | 1.16 |
| 20 | CS20 | DEX, GUA, Codeine, Pseudo paracetamol | Dry and Wet | B15 | 1.24 |
| 21 | CS21 | AMB, GUA, TERB | Cough with Mucus | B16 | 0.60 |
| 22 | CS22 | CHL, Codeine | Dry | B17 | 1.64 |
| 23 | CS23 | AMB, GUA, TERB | Cough with Mucus | B17 | 0.80 |
| 24 | CS24 | AMB, GUA, TERB | Cough with Mucus | B18 | 1.46 |
| 25 | CS25 | CHL, DEX | Dry | B19 | 1.59 |
| 26 | CS26 | AMB, GUA, TERB | Cough with Mucus | **B8** | **0.47** |
| 27 | CS27 | AMB, GUA, SAL | Asthma, Bronchital | B20 | 0.72 |
| 28 | CS28 | CHL PHE | Cough with Mucus | B21 | 0.98 |
| 29 | CS29 | CHL, DEX, PHE | Cold with Cough | **B22** | **0.35** |

Apart from the respondent's knowledge on the cough syrups, we have considered certain other CS's (CS14-CS29) that have been well established in the pharma sector in comparison to the top selling syrups (CS1-CS13) as mentioned in table 1. Most of the syrups are combination of two or more ACI, and except for six CS's under study. Interestingly, there exists nine different brands of the top selling cough syrups as listed and in total twenty-one different brands of CS's are localized. The ACI combine of AMB with GUA, and TERB are predominant over other ACI combinations produced in eight different brand names that vary in unit price per 100mL. The study clearly reveals that the respondents are definitely influenced by the brand name even though two ACI namely CHL and DEX are present in 12 different CS's ( CS4 to, CS9, CS12, CS18, CS21, CS23, CS24 and CS26). Based on the respondent's information, molecular docking of active

chemical ingredient present in different types of CS's with serine protease HtrA1 were carried out. More than a century, a bacteria called *Mycobacterium Tuberculosis* (M-TB)[11-14] has resulted havoc in mankind leading millions of deaths and still it continues. The study comprises how these ACI inhibit M-TB and how it interacts with amino acids of the host molecule i.e. protein. The objective of the work was based on the presence of various types of CS's available in the industry upon the perception and view on the educated as well as the uneducated consumers on the purchase of syrups. However, steps have to be well structured and defined in procuring these syrups based on the nature of the cough.

## 2. Results and Discussion

All the drugs obey the Lipinski rule of Five[15]. The Simplified Molecular Input Line Entry System (SMILES) notation of the drugs is provided in detail in table 2 and the structure of the drugs in Figure 3. As per the energetics, binding affinity of the ACI with protein, the following outcome were obtained as shown in Table 3. The AC1 with the largest negative value in $kcalM^{-1}$ when bound to the protein reveals the most active drug in treating the bacterial infection resulting in cough and that of the least negative value as less potent towards the infection.

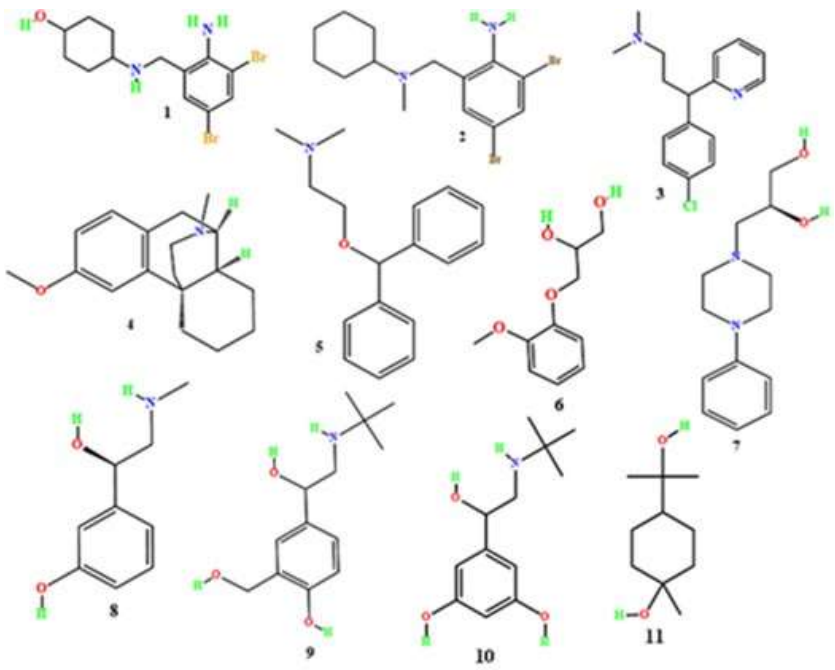

**Fig 3:** Structure of the active ingredients. 1. Ambroxol (**AMB**), 2. Bromhexine (**BRO**), 3. Chlorpheniramine (**CHL**), 4. Dextromethorphan (**DEX**), 5. Diphenhydramine (**DIP**), 6. Guaifenesin (**GUA**), 7. Levodropropizine (**LEV**), 8. Phenylephrine (**PHE**), 9. Salbutamol (**SAL**), 10. Terbutaline (**TERB**) and 11. Terpin hydrate (**TERP**). The hydrogen-bonding acceptor ($HB_a$) and hydrogen-bonding donor ($HB_d$) moieties in the guest molecules are provided for better understanding of the binding mode.

**Table 2: SMILES notation of the ACI (drugs)**

| Drug | Name of the Guest molecule (Drug) | Molecular Formula | Mol.wt in $gM^{-1}$ | Heavy atom Count | $HB_a$ | $HB_d$ | Rotatable bonds | Topological Polar Surface Area in $Å^2$ | Lipinski Rule |
|---|---|---|---|---|---|---|---|---|---|
| AMB | Ambroxol | $C_{13}H_{18}Br_2N_2O$ | 378.10 | 18 | 3 | 3 | 3 | 58.3 | Obeys |
| BRO | Bromhexine | $C_{14}H_{20}Br_2N_2$ | 376.13 | 18 | 2 | 1 | 3 | 29.3 | Obeys |
| CHL | Chlorpheniramine | $C_{16}H_{19}ClN_2$ | 274.79 | 19 | 2 | 0 | 5 | 16.1 | Obeys |
| DEX | Dextromethorphan | $C_{18}H_{25}NO$ | 271.4 | 20 | 2 | 0 | 1 | 12.5 | Obeys |
| DIP | Diphenhydramine | $C_{17}H_{21}NO$ | 255.35 | 19 | 2 | 0 | 6 | 12.5 | Obeys |
| GUA | Guaifenesin | $C_{10}H_{14}O_4$ | 198.22 | 14 | 4 | 2 | 5 | 58.9 | Obeys |
| LEV | Levodropropizine | $C_{13}H_{20}N_2O_2$ | 236.31 | 17 | 4 | 2 | 4 | 46.9 | Obeys |
| PHE | Phenylephrine | $C_9H_{13}NO_2$ | 167.20 | 12 | 3 | 3 | 3 | 52.5 | Obeys |
| SAL | Salbutamol | $C_{13}H_{21}NO_3$ | 239.31 | 17 | 4 | 4 | 5 | 72.7 | Obeys |
| TERP | Terpin hydrate | $C_{10}H_{22}O_3$ | 190.28 | 13 | 3 | 3 | 1 | 41.5 | Obeys |
| TERB | Terbutaline | $C_{12}H_{19}NO_3$ | 225.28 | 16 | 4 | 4 | 4 | 72.7 | Obeys |

**Table 3:** Binding energy (BE) in $kcalM^{-1}$ of all the ten conformers of drug-protein complex. C1-C10 refers to the various conformer form of the AC1 binding with the protein.

| | **AMB** | **BRO** | **CHL** | **DEX** | **DIP** | **GUA** | **LEV** | **PHE** | **SAL** | **TERB** | **TERP** |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **C1** | **-7.12** | **-6.48** | **-6.47** | **-7.11** | **-5.64** | **-3.53** | **-5.09** | **-5.51** | **-5.90** | **-5.91** | **-6.34** |
| **C2** | -7.05 | -6.17 | -5.96 | -7.05 | -5.23 | -3.38 | -5.08 | -5.48 | -5.28 | -5.77 | -6.09 |
| **C3** | -6.72 | -6.15 | -5.70 | -7.00 | -5.18 | -3.22 | -5.08 | -5.41 | -4.99 | -5.73 | -6.08 |
| **C4** | -6.51 | -6.10 | -5.57 | -6.89 | -4.97 | -3.09 | -4.85 | -5.30 | -5.06 | -5.65 | -5.98 |
| **C5** | -6.72 | -5.99 | -5.51 | -6.85 | -4.97 | -2.50 | -4.58 | -5.25 | -4.72 | -5.57 | -5.40 |
| **C6** | -6.67 | -5.93 | -5.48 | -6.84 | -4.81 | -2.37 | -4.48 | -5.18 | -4.66 | -5.15 | -5.31 |
| **C7** | -6.66 | -5.84 | -5.43 | -6.83 | -4.49 | -2.13 | -4.38 | -5.00 | -4.51 | -5.07 | -5.22 |
| **C8** | -6.61 | -5.57 | -5.37 | -6.83 | -4.52 | -2.04 | -4.33 | -4.99 | -4.36 | -4.97 | -5.29 |
| **C9** | -6.04 | -5.51 | -5.28 | -6.83 | -4.44 | -1.59 | -4.00 | -4.78 | -3.90 | -4.36 | -5.14 |
| **C10** | -5.99 | -5.42 | -4.74 | -6.69 | -4.36 | -1.47 | -3.82 | -4.58 | -3.66 | -4.22 | -4.91 |

AMB and DEX resulted in BE of -7.12 kcal/mol of the most stable conformer (C1) which were found to have the highest tendency in effective binding with the protein. AMB and DEX are present in CS17 and CS10 respectively in the absence of any combined ACI in the CS was found to be effective in binding with M-TB, thereby decreasing its potency. BRO and CHL resulted in BE of -6.48 kcal/mol. But these two drugs are always in combined form with one or two other ACI's present in various CS's. TERB and SAL resulted in BE of -5.91 kcal/mol of which SAL alone exists as a single ACI in CS13,

produced by B3. The order of docking score of these drugs with protein is as follows AMB ≈ DEX > BRO ≈ CHL > TERP > TERB ≈ SAL > DIP > PHE > LEV > GUA.The drug that possesses the least BE is GUA and the most are AMB and DEX.

The outcome of the studies provides interesting aspects regarding the presence of several cough syrups manufactured by various companies (Brand) with modification on the colour, flavour, emulsifier .Among the drugs present in **CS**, AMB (**CS 14** and **17)** SAL **(CS13)** CHL **(CS22)** , DIP **(CS1** and **CS3)** and DEX **(CS10)** exist as the single ACI. These CS's are available as a single ACI in the cough syrups apart from stabilizers and additives. Among the energetics of the conformers, SAL exhibits vast variation in the conformer energies and they are present as an active ingredient in **CS13** syrup, which is the most economical syrup available in the market produced by the pharma company **B3. CS13** from **B3** is one of the top selling CS accounts for the top three CS's apart from **CS13**, and they are **CS3** and **CS12.**

Interestingly, the combination of drugs provides interesting results such that AMB and DEX is not present as combined ACI in any of the CS even though both possesses similar binding affinity based on the energetics. This is presumably attributed to the structural characteristics involving functional groups that are involved in bimolecular interactions. Similarly, BRO and CHL are not present as combined ACI in any of the CS's even though both are equally potential in treating the cough. Interestingly, TERB and SAL does not exist as combined active ingredient.

Though CHL and DEX differ in their structure, but they form effective combination and are present in several top selling CS's syrups such as **CS5, CS6, CS9, CS12** and **CS25** which play a major role in the medical field. Based on the binding energies, the following outcomes supported the combinations that never arises among the CS's .

**3.Outcomes on combination of ACI based on energetics.**

AMB + BRO + CHL combination does not arise in any of the syrups as listed. Similarly, the combination of BRO + CHL + DEX does not exist to the best of our knowledge, though the above mentioned ACI have a better affinity towards the bacterial infection. TERB, BRO, DEX, LEV, GUA, PHE and TERP has not been as the single ACI in any of the CS's such that these ACI's always exist in certain combinations only. Among the ACI, DIP do not form combinations with any other ACI but it is found to be effective when it exists as single ACI in syrups like **CS1** and **CS3.** The double ACI combination are obtained in two set of distinguishable formulation of CS's. They are CHL + DEX, which are found in **CS5, CS6** and **CS12,** CHL + PHE in **CS28.** However, the triple ACI combinations widely obtained in the market are obtained in six different CS's (Table 3) They are AMB + GUA + SAL **in CS2** and **CS27**. AMB + GUA + TERB **(CS11, CS18, CS21, CS23, CS24** and **CS26)**. CHL + DEX **+** PHE **(CS4, CS8 and CS29)**. CHL + DEX + GU **(CS7).** BRO + GUA + SAL **(CS15** and **CS16)**. BRO + GUA + TERB **( CS19)**.

**Table 4**: The available effective combination of ACI in top selling Cough syrups in Chennai.

| S.No | Single ingredient | Double ingredients | Triple ingredients |
|---|---|---|---|
| 1. | Ambroxol | Chlropheniramine + Dextromethorphan | Ambroxol + Guaifenesin + Salbutamol |
| 2. | Diphenhydramine | Chlrophenaramine + Phenylephrine | Ambroxol + Guaifenesin + Terbutaliene |
| 3. | Dextromethorphan | | Chlropheniramine + Dextromethorphan + Phenylephrine |
| 4. | Salbutamol | | Chlropheniramine + Dextromethoprhan + Guaifenesin |
| 5. | | | Bromhexine + Guaifenesin + Salbutamol |
| 6. | | | Bromhexine + Guaifenesin + Terbutaliene |

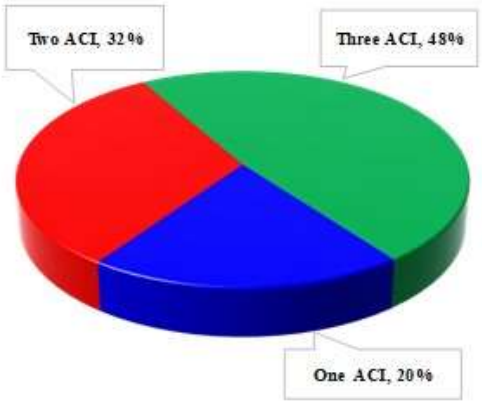


**Fig 4:** Availability of the ACI combination in Cough syrups

The stability of the binding pattern based on the energetics is complimented by the nature of the bimolecular interactions which is an important concept in host-guest chemistry where the protein molecule is considered as host and the drug as guest. The bimolecular interactions involve conventional hydrogen bonding (cHB), non-conventional hydrogen bonding (NcHB), hydrophobic interactions, weaker forces of interactions and unfavorable interaction if exists. In general presence of multiple bimolecular interactions results in destabilization of the host guest complex. All the drugs exhibit HB and hydrophobic interactions. The energetically more stable drug AMB possess more HB interactions than any other interactions. Interestingly, DEX which is energetically equally stable is governed predominantly by hydrophobic interactions. In several drugs, bonding with protein molecule, HB interaction predominates over other interactions except in the

case of DEX and TERP. As shown in the table 5, information on the bimolecular interaction existing between various drugs and the protein of the stable conformer is provided. Interestingly, there exists a large variation in the ratio of HB: Hydrophobic interactions as well with that of other interactions in all the CS's. The above fact established that, all the AC1 being different play a key role in binding with the protein in different aspects, thereby initiating their action on the cough.

**Table 5:** The hydrogen bonding, hydrophobic, Van der waals, Polar amino acids and Non-Polar amino acids.

| Drug | Hydrogen Bonding (HB) (i) | Hydrophobic interactions (ii) | van der Waals interaction (iii) | Other interactions | Ratio of (i: ii) | Ratio of (i+ii) /iii | Polar amino acids involved in bimolecular interaction | Non polar amino acids involved in bimolecular interaction |
|---|---|---|---|---|---|---|---|---|
| AMB | **4** | **2** | **5** | 1 | **2** | **1.2** | 4 | 4 |
| BRO | **3** | **2** | **3** | 0 | **1.5** | **1.67** | 4 | 4 |
| CHL | **2** | **2** | **11** | 0 | **1** | **0.36** | 5 | 4 |
| DEX | **2** | **9** | **5** | 0 | **0.22** | **2.2** | 3 | 4 |
| DIP | **6** | **2** | **4** | 0 | **3** | **2** | 6 | 3 |
| GUA | **7** | **2** | **4** | 0 | **3.5** | **2.2** | 4 | 5 |
| LEV | **3** | **3** | **7** | 0 | **1** | **0.85** | 3 | 5 |
| PHE | **5** | **3** | **2** | 0 | **1.67** | **4** | 4 | 3 |
| SAL | **4** | **5** | **6** | 0 | **0.8** | **1.5** | 5 | 5 |
| TERP | **5** | **1** | **5** | 0 | **5** | **1.2** | 5 | 3 |
| TERB | **5** | **8** | **1** | 0 | **0.63** | **13** | 4 | 6 |

The survey questionnaire had the choices where the people were brought about how they procure the cough syrups and they were given options based on the brand of the pharmaceutical companies, doctor's prescription, combination of drugs and also based on the price of the cough syrup. The data revealed that the respondents predominantly prefer the syrups which the medical practioners prescribe without any hesitation. Moreover, in turn, the pharma companies promote their brand through various means like advertisements, supplying more of their brands in the market and justify their brands to medical practioners through various methods by sales representatives, exhibitions and workshops (Figure 5).

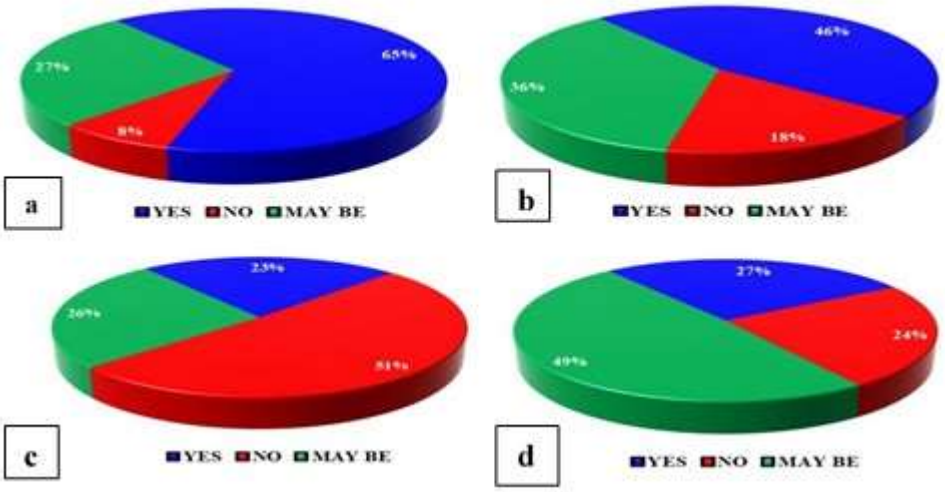


**Fig 5** a) Promotion of Cough syrups through advertisements, medical professionalism, doctors or through pharmacists. b) Respondents considering their options towards herbal syrups from allopathic cough syrups. c) Localization of single brand cough syrups throughout the country. c) Representation of pharma companies on serving the people at subsidized prices

The major findings on the nature of active chemical ingredients and the cough syrups Brand B2 and B3 account for 1/4$^{th}$ of the popular cough syrups across the city. Similarly, nearly 10 brands market their cough syrup by two AC1 combination comprising CHL+ DEX only. Predominantly, 3 ACI were procured and consumed by the respondents of which AMB+ GUA was branded by 8 different brands, and BRO+ GUA by 3 brands. This clearly reveals that GUA is found to be the important active chemical ingredients in syrups containing 3 active chemical ingredients.

Altogether, the people are influenced by the company's promotion and the results were the clear indication based on the responses in the survey. Interestingly, people localized in an area gradually have the mindset of shifting to herbal medicines than allopathic medicine post COVID-19 pandemic. The respondents revealed better results by using ayurvedic cough syrups, which was found to be an interesting pattern. There are many brands which have the same composition of cough syrups but for their marketing strategies and localization of their company, they sell their brands throughout the country. This information collected through our survey provides the mindset of the customers. Further, the effectiveness of the cough syrup, when taken into the account was not encouraging and it was found to be less prominent in treatment of cough

## 4. Conclusion

A Comparison on the binding stability upon complex formation between host (protein)-guest (active chemical ingredients) through docking approach provides a complete analysis on the factors influencing the energetics and nature of the bimolecular interactions for which the ligand favoring the biomolecule. The structural aspects and the presence of hydrogen-bonding acceptor and donor moieties in the drug impart a key role

on the binding with the amino acids of protein. The theoretically calculated docking score of host-guest provides an important elucidation on the combination of the active ingredients in the cough syrup, which play a vital role on health and metabolism. Both hydrogen bonding and hydrophobic interactions operate together in stabilizing the drug-protein complex irrespective on the structural aspects of the drug. The influence of multiple active ingredients is of utmost importance in the case of role of various established cough syrups present in the market.

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