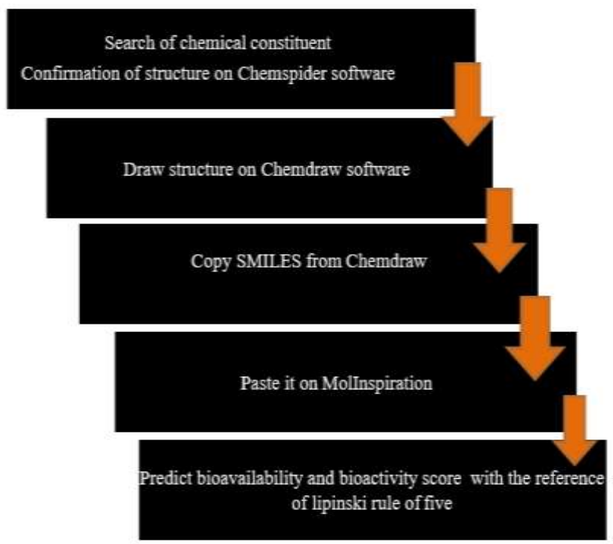
DRUG REPURPOSING IN DRUG DISCOVERY

RESEARCH BACKGROUND:

Cymbopogon, also known as **lemongrass**, barbed wire grass, silky heads, Cochin grass, Malabar grass, oily heads or fever grass, is a genus of Asian, African, Australian, and tropical island plants in the grass family. Some species (particularly *Cymbopogon citratus*) are commonly cultivated as culinary and medicinal herbs because of their scent, resembling that of lemons (Citrus limon).

PROCESS:



RESULTS AND DISCUSSIONS:

Drug likeness score for compounds:

Sr. No.	Compounds	milog P	TPSA	n atoms	MW	n ON	N OHNH	n violations	n rotb	volume
1.	**Citral**	3.65	17.07	11	152.24	1	0	0	4	169.74
2.	**Geranial(alpha-citral)**	3.65	17.07	11	154.25	1	0	0	4	169.74
3.	**Neral (beta-citral)**	3.65	17.07	11	152.23	1	0	0	4	169.74
4.	**Myracene**	3.99	0.00	10	136.24	0	0	0	4	162.24
5.	**Geraniol**	3.20	20.23	11	154.25	1	1	0	4	175.57
6.	**Nerol**	3.20	20.23	11	153.23	1	1	0	4	175.57
7.	**Citronellol**	3.15	20.23	11	156.27	1	1	0	5	181.79
8.	**Limonene**	3.62	0.00	10	136.24	0	0	0	1	157.30
9.	**Alpha-Terpinolene**	2.60	20.23	11	154.25	1	1	0	1	170.65
10.	**Geranyl acetate**	3.91	26.30	14	196.29	2	0	0	6	212.09

Biological activity of taken compounds with the reference of receptor mechanism:

Sr. No.	Compounds	GPCR ligand	Ion channel modulator	Kinase inhibitor	Nuclear receptor ligand	Protease inhibitor	Enzyme inhibitor
1.	**Citral**	-0.86	-0.25	-1.29	-0.42	-0.57	0.02
2.	**Geranial(alpha-citral)**	-0.86	-0.25	-1.29	-0.42	-0.57	0.02
3.	**Neral (beta-citral)**	-0.86	-0.25	-1.29	-0.42	-0.57	0.02
4.	**Myracene**	-1.11	-0.33	-1.51	-0.45	-1.31	-0.07
5.	**Geraniol**	-0.60	0.07	-1.32	-0.20	-1.03	0.28
6.	**Nerol**	-0.60	0.07	-1.32	-0.20	-1.03	0.28
7.	**Citronellol**	-0.81	-0.24	-1.16	-0.61	-0.83	-0.12
8.	**Limonene**	-0.91	-0.27	-2.01	-0.34	-1.38	-0.21
9.	**Alpha-Terpineol**	-0.51	0.15	-1.45	-0.02	-0.78	0.14
10.	**Geranyl acetate**	-0.50	0.04	-1.11	-0.12	-0.80	0.21

Evaluation of drug likeliness

The drug likeness was calculated and discussed on the basis of Lipinski's rule and its component for all prepared compounds using Molinspiration software.

The physicochemical properties including:

- An octanol-water partition coefficient (Milog P) < 5 that means these shows good permeability across cell membrane,
- polar surface area (TPSA) < 160 Å2 which shown to be a very good descriptor characterizing drug absorption,
- number of violation (n violations) =1 or < 0 it means compound easily bind to receptor
- molecular weight (MW) < 500 required for characterizing drug absorption
- number of rotatable bonds (n rotb) < 10 this measures molecular flexibility
- number hydrogen bond donors (n OHNH) ≤ 5 (The sum of OHs and NHs)
- total molecular polar surface area (TPSA) > 160Ao2
- hydrogen bond acceptors (nON) > 7

From the results reveal that these compounds are orally bioactive because they possess groups which act as substrate for transporter.

Potency of compounds according to obtained data

Number of violations

In all the 10 compounds that are more important which have least number or no violations observed.

Molecular weight

All constituents of data passes the Lipinski rule of five for molecular weight.

Conclusion

The Phytochemical screening and Pharmacognostical evaluation parameters of *Cymbopogon citratus* were performed and it showed the presence of many pharmacological active phyto- constituents. Further study into the absorption, distribution, metabolism, excretion, toxicity (ADMET) of these lead compounds in addition to in vitro and in vivo experiments are needed to validate utilization and sourcing of various therapeutic interventions from these plants.

Effective formulations to be developed using indigenous medicinal plants, With proper pharmacological experiments and clinical trials.