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Vishnupandi S
Tamil Nadu Agricultural University
Manikanda Boopathi N
nmboopathi@tnau.ac.in

Tamil Nadu Agricultural University
Sathish Kumar Konidala
Vignan's Foundation for Science, Technology and Research
Harsha Sri Kamma
Vignan's Foundation for Science, Technology and Research

Research Article

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In-Silico Screening of Jasmine Volatiles Against Human Serotonin Transporter for Antidepressant Potential

Vishnupandi S[1*], Manikanda Boopathi N[2], Sathish Kumar Konidala [3], Harsha Sri Kamma[4]

[1] Department of Floriculture and Landscape Architecture, Tamil Nadu Agricultural University, Coimbatore, Tamil Nadu, India.
vishnupandisenthilkumar@gmail.com

[1]ORCiD ID: 0009-0005-8275-6841

[2]Department of Plant Biotechnology, Centre for Plant Molecular Biology and Biotechnology, Tamil Nadu Agricultural University, Coimbatore, Tamil Nadu, India.

nmboopathi@tnau.ac.in

[2]ORCiD ID: 0000-0003-3615-3386

[3] Department of Pharmaceutical Sciences, School of Biotechnology and Pharmaceutical Sciences, Vignan's Foundation for Science, Technology and Research, Guntur, Andhra Pradesh, India

sathishkonidala@gmail.com

[3]ORCiD ID: 0000-0001-5326-1499

[4]Department of Pharmaceutical Analysis, Vignan Pharmacy College, Vignan's Foundation for Science, Technology and Research, Guntur, Andhra Pradesh, India

hk186909@gmail.com

[4]ORCiD ID 0009-0009-5329-3162

Abstract

Depression is a major mood disorder associated with impaired monoaminergic neurotransmission, for which current antidepressants often show limited efficacy and adverse side effects. This has intensified interest in plant-derived compounds as safer therapeutic alternatives. *Jasminum sambac* is traditionally recognized for its mood-modulating properties and is rich in volatile organic compounds (VOCs) with potential neuroactive functions. In this study, floral volatiles of *J. sambac* were extracted using Soxhlet extraction, profiled through GC-MS analysis, and subsequently evaluated for their interaction with the human serotonin transporter (SERT) using molecular docking. GC–MS profiling revealed a diverse blend of monoterpenes, sesquiterpenes, benzenoids, and other aromatic derivatives, with key constituents including linalool, benzyl acetate, α-farnesene and germacrene-D. Docking studies

demonstrated that germacrene-D exhibited the strongest binding affinity among jasmine volatiles (-7.9 kcal/mol), closely approaching the standard antidepressant fluoxetine (-8.9 kcal/mol). Hydrophobic interactions dominated the binding mechanism, with Ile172 serving as a conserved interacting residue for most compounds. These results suggested that selected *J. sambac* volatiles possess promising affinity toward SERT, supporting their potential role in modulating serotonergic signalling. Overall, this study provides molecular evidence for the antidepressant potential of jasmine floral metabolites and highlights their suitability for further pharmacological validation.

Keywords: *J. sambac*, Anti-depression, Molecular docking, serotonin transporter, metabolites

Introduction

Depression is a predominant stress-related mood disorder that can occur at any stage of life (Moinuddin et al. 2012). It is characterized by persistent disturbances in normal behavior, including recurrent mood swings, impaired neuro-vegetative functions, cognitive decline, and reduced psychomotor activity (Liang et al. 2022). As a debilitating psychiatric condition, depression causes significant emotional and physiological burdens and is closely linked to dysregulated monoamine neurotransmission and elevated oxidative stress (Shao et al. 2020; Jiang et al. 2022).

Conventional antidepressant classes including tricyclic antidepressants, selective dopamine reuptake inhibitors, selective norepinephrine reuptake inhibitors and selective serotonin reuptake inhibitors (SSRIs) exert their effects largely through modulation of the serotonin transporter (SERT) (Gabrielsen et al. 2012). SERT is a monoamine transporter responsible for reabsorbing serotonin from the synaptic cleft back into the presynaptic neuron, thereby terminating serotonergic signalling. SSRIs enhance serotonergic neurotransmission by inhibiting this reuptake process, allowing increased serotonin availability for synaptic communication (Muszynski et al. 1999).

Despite the availability of several SERT-inhibiting antidepressants (including citalopram, fluoxetine and sertraline), their therapeutic success is often constrained by side effects such as allergic reactions, gastrointestinal disturbances, hepatotoxicity, and in some cases incomplete understanding of their pharmacological mechanisms (Bhat et al. 2019). These limitations emphasize the need for scouting safer and more effective antidepressant agents, motivating interest in plant-derived alternatives known for their chemical diversity, broader therapeutic potential and improved safety profiles.

Traditional plant-based extracts have long been used to treat depression and related disorders (Dubey et al. 2004). More recently, *Jasminum sambac*, a well-known medicinal plant, has attracted attention for its pronounced antidepressant-like effects in experimental models (Krishnaveni et al. 2014; Umukoro et al., 2018; Febrianti et al. 2025). Studies indicate that it can reduce depressive-like behaviours, elevate key neurotransmitters such as serotonin and dopamine, and improve brain antioxidant status, supporting its potential as a complementary therapeutic option.

These species are rich in volatile organic compounds (VOCs) such as linalool, benzyl acetate, indole, and methyl anthranilate, which are known to influence neurological function through olfactory and systemic pathways (Vishnupandi et al. 2024; Rao et al. 2025). While the antidepressant-like effects of jasmine have been observed behaviourally and anecdotally, the molecular basis of these effects remains largely unexplored.

In this study, we employed molecular docking techniques to investigate the interaction of jasmine-derived volatile organic compounds with the human SERT structure. This computational approach aims to identify potential binding affinities and interaction patterns of floral compounds with SERT, providing molecular evidence to support the antidepressant claims associated with jasmine. The findings may contribute to the development of natural, plant-based alternatives or adjuncts to current antidepressant therapies.

Materials and Methods

Fresh plant materials of *Jasminum sambac* were collected and authenticated by Department of Floriculture and Landscape Architecture, Tamil Nadu Agricultural University, Coimbatore, India and provided the voucher specimen number as RG-IFC-3.

Fully opened flowers of *J. sambac* were collected in four replicates from the same plant in the early morning 6.00 AM to maximize the recovery of volatile aromatic compounds (Ghissing et al. 2022). Two hundred grams of fresh flowers are tightly packed into a Soxhlet apparatus and subjected to extraction with n-Hexane for 5 to 6 cycles over several hours at 55 to 60°C. The solvent is then removed from the extracted material using a rotary evaporator to isolate the final concrete product. The extracted concrete is analyzed using Gas Chromatography-Mass Spectrometry (GC-MS) to identify its components. The concrete is first dissolved in hexane, filtered, and centrifuged. A sample of the supernatant is injected into an Agilent Technologies 7890A GC system coupled with a mass spectrometer (specifically using a DB-5 MS capillary column and a NIST 2021 mass spectral database for compound

identification). The GC separates the various components of the sample, which the mass spectrometer then detects and records as spectral peaks. Profiling of floral volatiles from each replicate was carried out and presented in the Table 1. The GC-MS ion chromatogram images were given in the Figure 1.

Molecular docking

A total of 37 volatile constituents were initially identified from jasmine essential oil profiles. Based on fragrance importance and supporting evidence from previous literature, 12 key volatile compounds were shortlisted for subsequent molecular docking analysis. The binding affinities of the selected volatile compounds toward the target protein SERT were evaluated through *in-silico* molecular docking (please see below) along with Fluoxetine as check. The crystal structure of the reference protein SERT (PDB ID**:** 5I6Z) was retrieved from the RCSB Protein Data Bank. The crystallized ligand structure was extracted and prepared in PDBQT format using *Discovery Studio Visualizer 2021*. Structural validation using a Ramachandran plot indicated the presence of minor conformational deviations in the co-crystallized structure.

Protein preparation was carried out in PyRx 0.8, where the AutoDock tool's *Macromolecule* option was used to convert the PDB file into PDBQT format. Ligands were energy-minimized and converted to PDBQT. Docking simulations were performed using VinWizard, selecting the prepared protein and ligand files. A grid box was defined around the binding region corresponding to the co-crystallized ligand to ensure accurate sampling of the active site. After docking, the protein–ligand interactions, including hydrogen bonds and hydrophobic contacts, were analysed and visualized using Discovery Studio Visualizer 2021.

Results and Discussion

GC-MS analysis

The GC–MS profiling of *J. sambac* revealed a complex blend of volatile organic compounds comprising monoterpenes, diterpenes, sesquiterpenes, benzenoids, phenolics, fatty acid derivatives, and long-chain hydrocarbons (Table 1). These classes of compounds collectively contribute to the potential fragrance and bioactive properties of jasmine.

Monoterpenes such as β-myrcene, D-limonene, δ-terpinene, and linalool formed an important fraction of the jasmine VOCs (Croteau & Karp 1991; Knudsen & Gershenzon 2006),

and they were consistently detected across all replicates in relative proportion. Linalool, a classified key monoterpene was present in all samples with slight quantitative variation, representing stable biosynthesis across biological replicates. Furthermore, sesquiterpenes including α-farnesene, germacrene-D, and nerolidol (Knudsen & Gershenzon 2006; Nagegowda et al. 2008) were observed, indicating the metabolic richness and diversity of the jasmine floral volatiles in terpenoid biosynthesis. Among these compounds, α-farnesene showed relatively higher abundance compared to other sesquiterpenes, reflecting its reliable biosynthesis in jasmine flowers. Phenylpropanoid/benzenoid derivatives namely benzyl acetate, methyl anthranilate, indole and cinnamyl benzoate were detected in moderate amounts (Dudareva et al. 1998; Kolosova et al. 2001; Majetic & Sinka 2013), indicating active phenylpropanoid/benzenoid metabolism in jasmine. These compounds were likely involved in the formation of terpenoid-derived volatiles including linalool, β-ocimene, limonene, α-farnesene and nerolidol, suggesting that both phenylpropanoid/benzenoid and terpenoid pathways contribute to the biosynthesis of major floral scent constituents in *J. sambac*. Such phenylpropanoid/benzenoid/terpenoid biosynthetic routes previously characterized in other well-studied scented flowers (Mohd-Hairul et al. 2010).

Earlier studies reported that *J. sambac* flowers are dominated by benzenoid and terpene volatiles, with benzyl acetate, linalool, and α-farnesene identified as the major aroma compounds (Kanlayavattanakul et al., 2013). Another report by Bera et al. (2015) observed that in *J. sambac* flowers, benzyl acetate constituted about 78% of the phenylpropanoid/benzenoid fraction, which formed 54.66% of the total headspace volatiles and monoterpenes contributed 9.12%, with linalool comprising 92% of the group. Sesquiterpenes accounted for 30.31% of the scent profile, dominated by α-farnesene (96%). Trace compounds such as indole contributed an additional 5.91% to the overall volatile emission. Ghissing et al. (2022) reported that *J, sambac* flowers contain a rich blend of benzenoid and terpene volatiles, dominated by benzyl alcohol, benzyl acetate, benzyl benzoate, α-farnesene and linalool. Also added that peak volatile accumulation and emission occurred during nocturnal period, when both phenylpropanoid and terpenoid pathways were highly active.

A notable observation was also noted among long-chain alkanes and fatty acid methyl esters including eicosane, dotriacontane, tetracosanoic acid methyl ester and methyl linolenate. These compounds are typically linked with cuticular wax metabolism rather than direct fragrance contribution in flowers. However, their presence indicates active lipid metabolism

during flower opening and may assist in volatiles stabilization and release dynamics (Ray et al. 2022; Liao et al. 2023).

Molecular docking

The molecular docking studies investigating the binding potential of selected floral volatile compounds found in *J.* sambac with a protein target (PDB ID: 5I6Z) were presented in the Table 2. The docking images (2D & 3D interactions) were depicted in the Figure 2, 3 & 4.

The binding affinity measured in Kcal/mol, served as the primary metric for evaluating the interaction strength. Among all the tested molecules, the standard drug Fluoxetine showed the lowest (most negative) and thus strongest binding affinity at -8.9 Kcal/mol. Significantly, the volatile compound Germacrene-D exhibited the highest binding affinity among the *Jasminum* constituents, registered -7.9 Kcal/mol, which is notably close to the standard's value. Other compounds with strong to moderate affinities included nerolidol and α- farnesene (both -6.6 Kcal/mol, D-limonene and δ-terpinene (both -6.3 Kcal/mol), and benzyl acetate (-6.2 Kcal/mol). The remaining compounds showed weaker binding, with benzyl alcohol having the weakest affinity at -5.0 Kcal/mol. Analysis of the specific molecular interactions revealed that hydrophobic forces were the primary contributors to the binding stability of the *Jasminum* volatiles. Germacrene-D strong binding is attributed to extensive hydrophobic interactions, specifically seven Pi-Alkyl contacts with multiple residues including Tyr95, Ile172, Phe334, Phe335, Phe341, and Val501. The residue Ile172 was highly conserved in the binding site, participating in hydrophobic interactions for almost all the tested compounds. Although hydrophobic interactions were dominant, benzyl acetate formed a hydrogen bond with Asn177 and geranyl linalool, indole, and linalool formed hydrogen bonds with Ser438. In contrast, Fluoxetine's superior affinity was achieved through a combination of forces, including two conventional H-bonds, a carbon H-bond, various hydrophobic contacts, and unique Fluorine interactions.

Similar interaction patterns have been reported in previous molecular docking studies, where the selected phytochemicals exhibited stable binding within the active site of the target protein through favourable hydrogen bonding and hydrophobic interactions, supporting their potential as effective inhibitors (Elalouf et al. 2024). In another molecular docking (Rahman et al. 2025), GC-MS identified bioactive compounds from Saurauia roxburghii were evaluated against key neuropharmacological targets, including the potassium channel receptor, $GABA_A$

receptor and human serotonin transporter. Among them, 5-(piperidin-1-ylmethyl)-3-pyridin-3-yl-5,6-dihydro-4H-1,2,4-oxadiazine showed the highest binding affinity, suggesting its potential role in the anxiolytic and antidepressant effects of the plant. Molecular docking studies (Ahmad et al. 2023) demonstrated that GC-MS identified compounds from the methanolic leaf extract of *Cestrum nocturnum* bind stably within the active sites of alpha-amylase and acetylcholinesterase with favorable energies, thereby validating their inhibitory potential and provided a molecular basis for their antidiabetic and neuroprotective activities.

Conclusion

The study demonstrates that key volatile compounds from *J. sambac*, particularly germacrene-D, shown strong binding affinity toward the human serotonin transporter, indicating their potential to modulate serotonergic signalling. Combined with the diverse GC-MS profile, these findings provide preliminary molecular evidence supporting the antidepressant potential of jasmine floral metabolites. Further *in vitro* and *in vivo* validation is recommended to confirm their therapeutic relevance.

Statements and Declarations

Competing interests: The authors have no competing interests.

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Author's contributions

Vishnupandi S- Conceptualization, execution and manuscript writing

Manikanda Boopathi N- Revised the manuscript for intellectual content.

Sathish Kumar Konidala - Performed docking protocol validation, visualization of ligand-protein interactions, pharmacological interpretation and critical revision of the *in-silico* results.

Harsha Sri Kamma- Conducted protein and ligand preparation, molecular docking and binding interaction analysis.

Data Availability: All data generated or analysed during this study are included in this published article.

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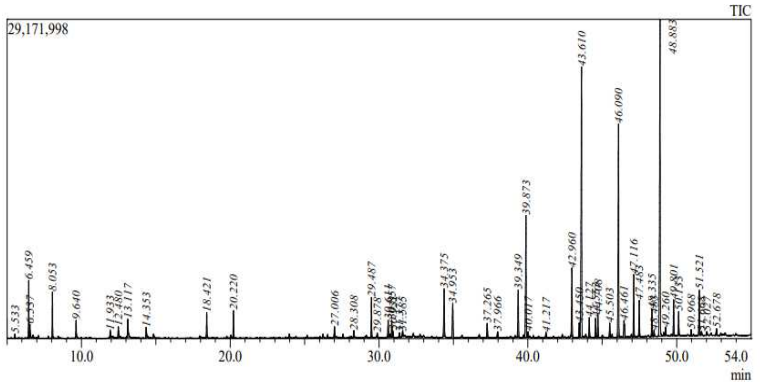
Table 1. GC-MS analysis of *J. sambac*

SL. No	Name of the compound	RT	R1	R2	R3	R4	Nature of the compound
			Peak Area %				
1.	β.-Myrcene	5.53	0.21	0.20	0.14	0.21	Monoterpenes
2.	D-Limonene	6.45	2.94	1.50	2.09	1.51	Monoterpenes
3.	Benzyl alcohol	6.54	0.15	0.69	0.64	0.71	Simple phenolic
4.	Eucalyptol	6.53	0.10	-	-	-	Simple phenolic
5.	δ-Terpinene	7.03	0.15	0.14	0.16	0.14	Monoterpenes
6.	Linalool	8.04	1.60	1.60	1.72	2.21	Monoterpenes
7.	Benzyl acetate	9.64	0.43	0.52	0.69	1.33	Benzenoid
8.	Benzene, (isocyanomethyl)	-	-	0.52	0.56	0.63	-
9.	Indole	13.12	0.43	1.05	1.02	1.37	Heteroarene
10.	Methyl anthranilate	14.35	0.41	0.41	0.58	0.66	Phenolic ester
11.	α-Farnesene	18.42	1.08	1.09	1.24	1.40	Sesquiterpenes
12.	Germacrene-D	20.22	0.98	1.02	1.04	1.63	Sesquiterpenes
13.	Nerolidol	27.00	0.36	0.37	0.53	0.48	Sesquiterpenes
14.	Hexadecanoic acid, methyl ester	-	-	-	-	0.22	Ester
15.	n-Hexadecanoic acid	-	-	0.38	0.35	0.27	-
16.	Pentadecanoic acid	28.28	0.20	-	-	-	-
17.	Geranyl Linalool	29.48	1.60	1.60	1.71	1.97	Diterpenes
18.	Palmitic acid	29.87	0.17	0.17	0.19	0.20	Fatty acid
19.	(Z)-Cinnamyl benzoate	30.62	0.66	0.91	1.03	1.03	Benzenoid
20.	Methyl linoleate	-	-	-	-	0.23	Fatty acid
21.	Methyl linolenate	30.85	0.62	1.19	0.88	1.20	Fatty acid
22.	Methyl stearate	31.37	0.26	0.21	0.18	0.26	Fatty acid
23.	α- linolenic acid	-	-	-	0.28	-	Fatty acid
24.	Heptadecane	30.92	0.33	-	-	-	-
25.	9-Tricosene	34.36	2.31	2.29	2.68	3.38	-
26.	1,3,5-triphenyl cyclohexane	37.958	0.20	-	-	-	-
27.	Heneicosane	39.94	2.80	2.29	2.55	2.28	-
28.	Tetracosanoic acid, methyl ester	43.42	0.87	0.72	0.74	0.67	Ester
29.	1,4-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	43.58	16.66	16.54	16.54	16.57	Ester
30.	1-Iodotriacontane	44.116	0.98	-	-	-	
31.	Squalene	44.70	1.14	1.01	1.10	1.08	
32.	Eicosane	46.07	3.97	10.54	11.62	10.78	
33.	Nonacosane	45.49	0.74	-	0.70	-	
34.	Hexacosanoic acid, methyl ester	46.49	0.49	-	-	-	Ester
35.	Tetratetracontane	51.51	2.61	2.29	2.58	2.40	
36.	beta-Sitosterol	51.66	0.21	0.26	-	-	Fatty acid
37.	1-iodo- dotriacontane	52.67	0.41	2.96	2.91	2.79	-

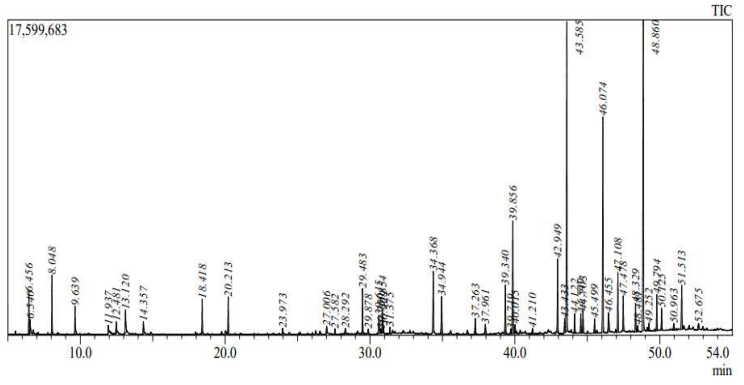
RT- Retention Time, R-Replicates

Table 2. Molecular docking studies of selected volatile organic compounds against SERT

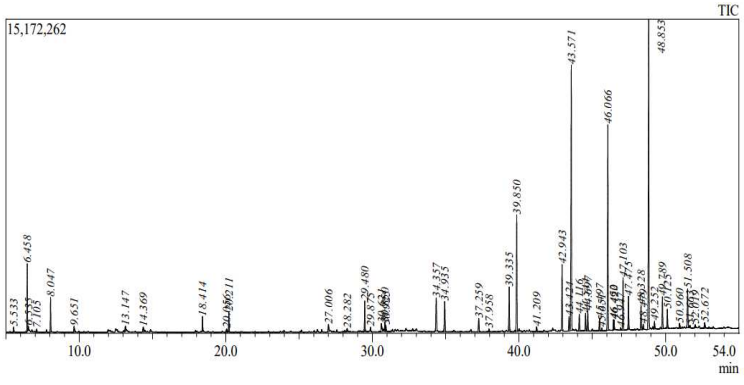
Sl. No	Name of the compound	Protein 5I6Z		
		Binding Affinity (Kcal/mol)	**Conventional H bond**	**Alkyl and pi= alkyl**
1	Benzyl acetate	-6.2	1 (Asn177)	Pi-Sigma: 2 (Tyr176, Ile172) Pi-Pi T Shaped: 2 (Tyr176, Tyr92)
2	Benzyl alcohol	-5.0	-	Pi-Sigma: 1 (Ile172) Pi-Pi T Shaped: 2 (Tyr176, Ser438)
3	D-Limonene	-6.3	-	Pi-Alkyl: 3 (Tyr92, Ile172, Tyr176)
4	Geranyl Linalool	-5.9	1 (Ser438)	Pi-Alkyl: 4 (Ile172, Phe341, Val501)
5	Germacrene-D	-7.9	-	Pi-Alkyl: 7 (Tyr95, Ile172, Phe334, Phe335, Phe341, Val501)
6	Indole	-5.8	1 (Ser438)	Pi-Alkyl: 2 (Ala169, Ala173) Pi-Sigma: 2 (Ile172)
7	Linalool	-5.9	1 (Ser438)	Pi-Alkyl: 4 (Ile172, Phe341, Val501)
8	Methyl anthranilate	-5.6	-	Pi-Alkyl: 2 (Ala169, Ala173) Pi-Sigma: 2 (Ile172, Phe341)
9	Nerolidol	-6.6	Carbon H bond (Ser438)	Pi-Alkyl: 5 (Ile172, Phe341, Phe335, Val501) Pi-Sigma: 1 (Tyr176)
10	α-Farnesene	-6.6	-	Pi-Alkyl: 6 (Ile172, Tyr176, Phe341, Val501)
11	β-Myrcene	-5.7	-	Pi-Alkyl: 10 (Tyr95, Ile172, Tyr176, Phe341, Val501)
12	δ-Terpinene	-6.3	-	Pi-Alkyl: 1 (Tyr95), Pi-Sigma: 1(Ile172), Pi-Pi T Shaped: 1 (Tyr176)
13	Fluoxetine (Std)	-8.9	2 (Asp98, Gly442) Carbon H Bond: 1(Ser336)	Pi-Alkyl: 3 (Ile172, Ala173, Val501) Pi-Sigma: 3 (Tyr95, Ile172) Pi-Pi-T Shaped: 2(Tyr176, Phe341) Fluorine: 3 (Ala169, Ser439, Leu443)



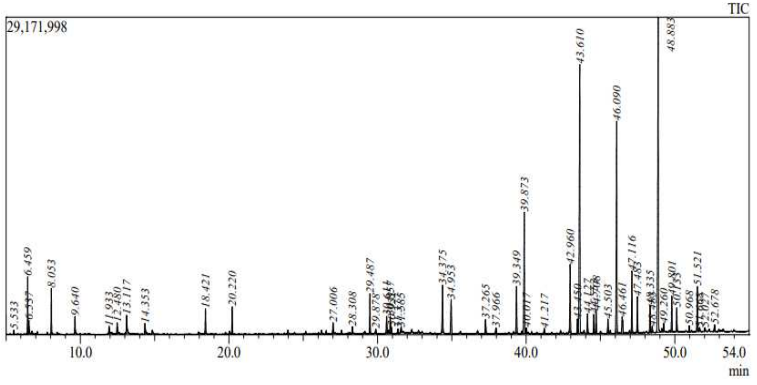
(a) R1



(b) R2



(c) R3



(d) R4

Figure 1. GC-MS total ion chromatogram of volatile organic compounds in flowers of *J. sambac*

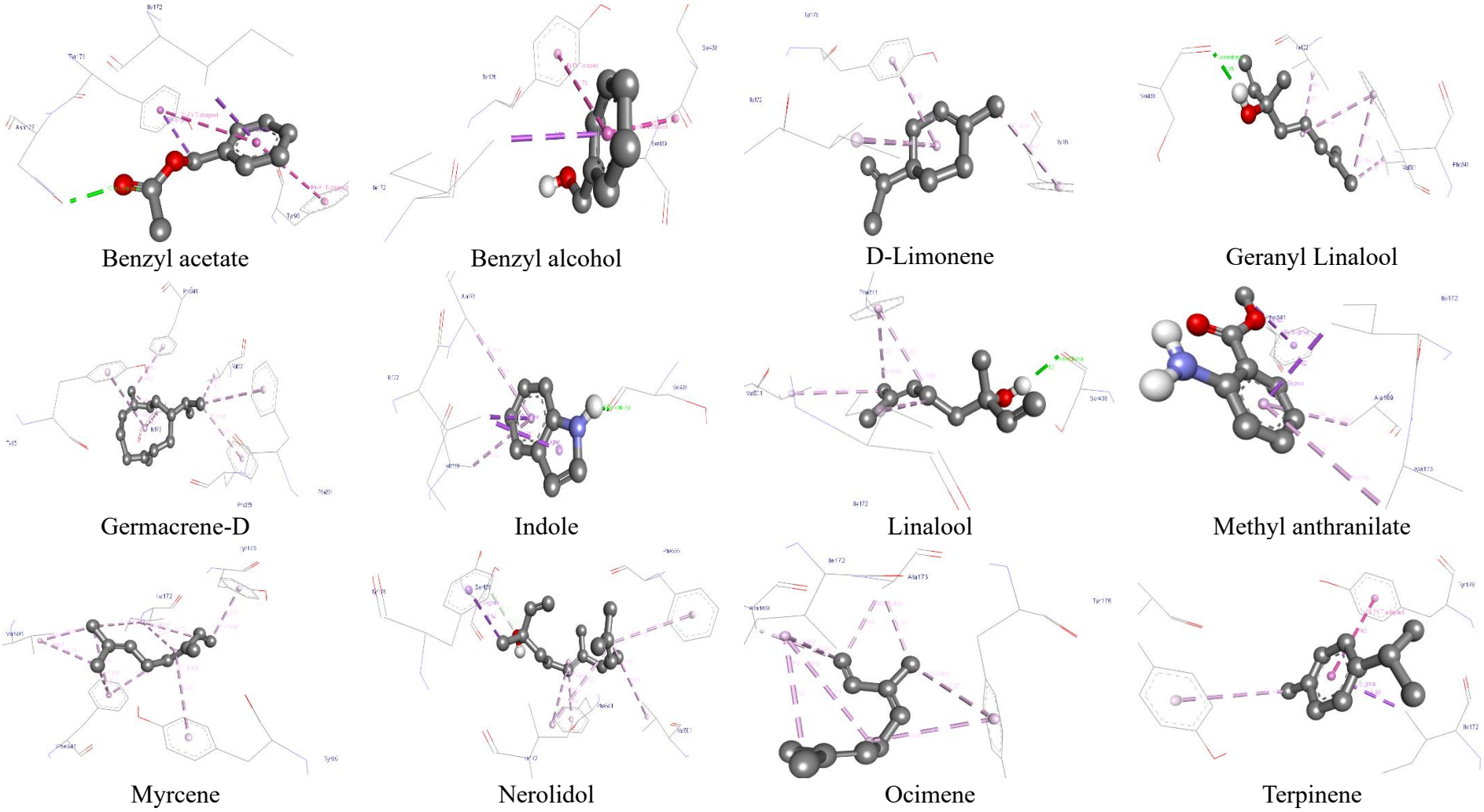


Figure 2. 2D interactions of volatiles againt SERT Protein

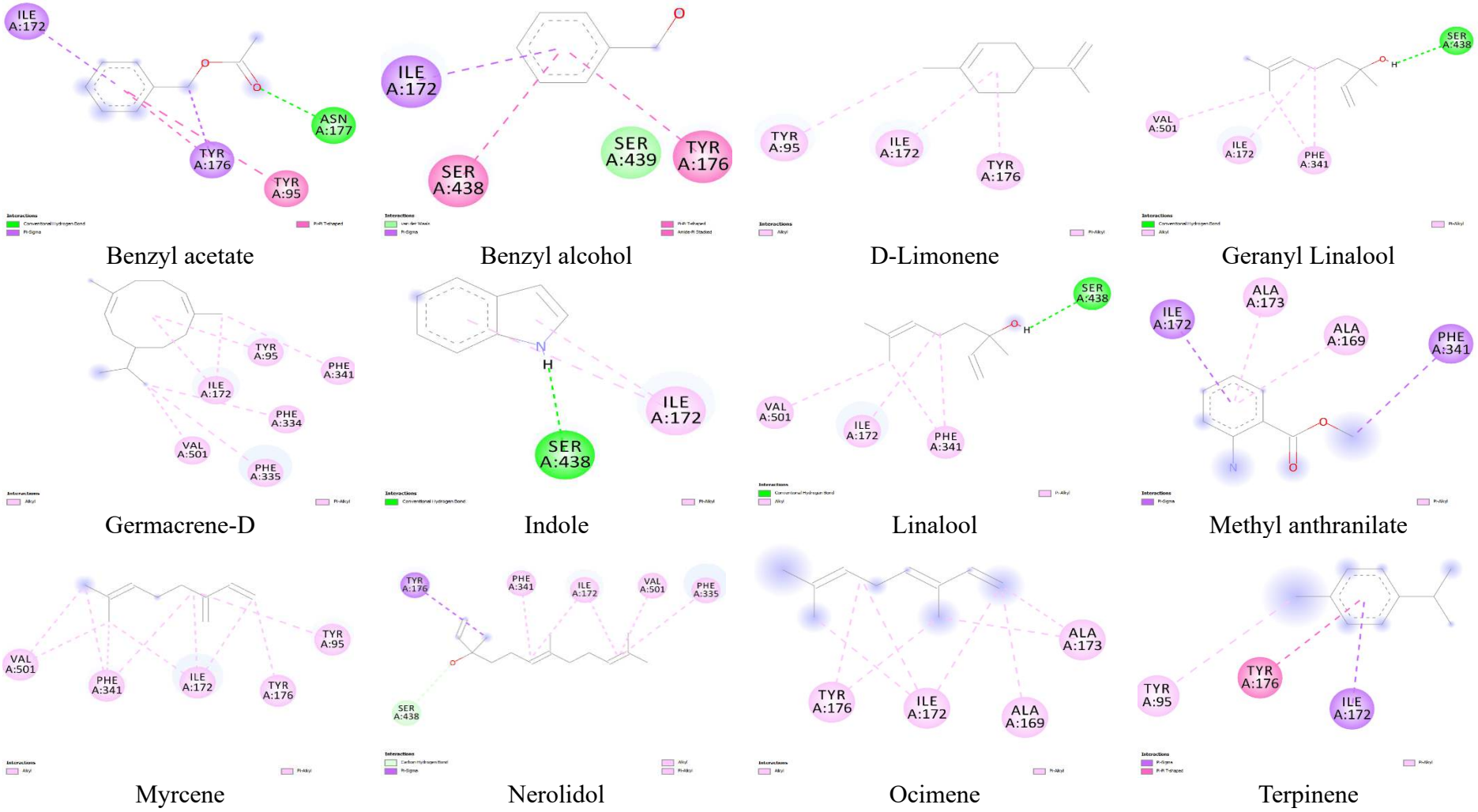


Figure 3. 3D interactions of volatiles againt SERT Protein

Figure 4. 2D & 3D interactions of Fluoxetine againt SERT Protein