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RESEARCH ARTICLE

Molecular docking of gingerol and shogaol for immunomodulatory effect in lupus disease

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Abstract

Background: One of the autoimmune diseases associated with high mortality is lupus or Systemic Lupus Erythematosus (SLE). In addition to symptomatic therapy, the treatment management of this condition includes immunomodulatory therapy. Various studies have been carried out on immunomodulators from natural products. Ginger rhizome (*Zingiber officinale* Roxb.) is a plant with potential immunomodulatory activity. Shogaol, which gives a spicy taste, is a metabolite of gingerol, a marker compound in ginger. Both of these compounds become important components of pharmacological activity. **Objective:** This study aimed to determine the *in silico* immunomodulatory activity of gingerol and shogaol compounds contained in ginger against S100A9, CTLA-4, SRSF1, JAK3, and MYD88 receptors. **Method:** *In silico*, a test was carried out using Pymol and PyRx applications, and receptors were involved in developing the immune system and SLE disease. **Result:** Docking results showed negative binding affinity and an RMSD of 2˚Angstroms. The shogaol, gingerol, and tofacitinib had several amino acid residues in common. **Conclusion:** *In-silico* analysis suggests that shogaol and gingerol could modulate the immune response against lupus. The resulting protein residues were similar between shogaol, gingerol, and the control, supporting their potential for immunomodulatory activity against lupus disease.

Introduction

Immunomodulators are drugs that affect the immune system by improving immune defences to improve the body's response to infections or suppressing abnormal immune responses occurring in immune disorders (Arcusa *et al*., 2022). Autoimmune disease is one of the diseases related to the immune system that can be treated using immunomodulators. The most common autoimmune diseases are RA (rheumatoid arthritis) and SLE (*Systemic Lupus Erythematosus*). In addition to using synthetic drugs as immunomodulator therapies, various studies have been conducted on natural-based immune modulators. These plants include ginger, which contains a gingerol compound (Schoenknecht *et al*., 2016). Shogaol, a metabolite of gingerol, is a dominant spicy constituent (Kemenkes, 2017; Karunakaran & Sadanandan, 2019). Based on *in-vitro* tests, the six-gingerol compound of ginger (*Zingiber officinale*) exhibits immunomodulatory activity (Masniah *et al*., 2021).

The pathophysiological process of SLE can disrupt and damage various cells and tissues. This process is associated with B cell proliferation, overactivation, and differentiation. Several components are altered in patients with SLE, including S1AA8/9, CTLA-4, SRSF 1, JAK 3, and MyD88. The proteins S1AA8 and S1AA9 are part of the S100 protein group that binds calcium and is released as a complex by the phagocytes at the site of inflammation. The calprotectin complex can activate monocytes, amplify cytokine production, regulate the movement of myeloid-derived suppressor cells, and act as a receptor ligand for glycation and TLR4 end products (Lood *et al*., 2011). The CTLA-4 protein, CD152, is expressed in T-cells (Rosenblum *et al*., 2015). CTLA-4 variants are associated with various autoimmune diseases, including SLE, mCTLA-4, and its soluble form,

sCTLA-4 . The JAK-3, SRSF 1, and MYD88 proteins are receptors that induce the production of type 1 IFN, which triggers the formation of macrophage.

Methods

Design

Hardware with Processor Type Intel Core i3-1005G1 CPU specifications @1.20GHz (4 CPUs), 1.2GHz, running the Windows 11 home operating system with 4 GB RAM. Software used includes Pymol, PyRx, ChemDraw, and Discovery Studio 2016. The following are the links to the software used: https://www.rcsb.org/ (protein structure), https://pyrx.sourceforge.io/faq (pyrex), (pymol), https://biosig.lab.uq.edu.au/pkcsm (pkCSM gingerol), https://biosig.lab.uq.edu.au/pkcsm/prediction_single/adme_1699364697.27 (pkCSM shogaol). Proteins S100A9 with code 7QUV, CTLA-4 with code 3OSK, SRSF1 with code 5MY8, JAK3 with code 3LXL, and MYD88 with code 4EO7 were downloaded from the Protein Data Bank website (PDB). Before docking, preparation was performed using the Pymol application to remove water molecules, followed by the docking process using the PyRx application.

Assessment

Data analysis of the docking result included the calculation of the root mean square deviation (RMSD) value. The affinity of the active ligand compound to the target protein was measured by comparing the energy values of the binding and the type of amino acids that interact with the ligand. This experiment was conducted three times to calculate the average for each compound. The results were presented in the subsequent analysis to make comparisons with ligands, tested compounds, and comparative drugs (Tofacitinib). According to Kotyla *et al*. (2022), tofacitinib is used as a control because it can reduce the development of nephritis disease activity and the occurence of autoantibodies. In addition, it plays a role in reducing pro-inflammatory cytokines, preventing the formation of interferons, and reversing the damage caused by dysfunctional endothelium.

Results

Preparation of 2-dimensional and 3-dimensional structures (ligand and control)

Before conducting *in silico* testing, comparative compounds such as Tofacitinib and ligands like gingerol and shogaol were selected and prepared in a 3D chemically structured format using the Chembio 3D conversion tool. The results for the three-dimensional structures are displayed in Figure 3. For visualising two-dimensional structures, the compounds were drawn using the ChemDraw 19.0.

Preparation of 3-dimensional receptor structures

The PyMOL program, developed by DeLano Scientific, was used to prepare the receptor. This program is capable of generating informative graphics suitable for scientific studies. At this stage, 81 small molecules and the solvent (water) were removed and the natural ligand was transformed into pdbqt format. "*Partial Payment*" was then used to save the file.

Docking validation

The validation procedure for this *in silico* test involved re-docking native ligands obtained from the Protein Data Bank website (https://www.rcsb.org) and some native ligands created using the Discovery Studio Visualiser program. The PyRx-Vina application was used for receptor validation and the process was repeated up to three times.

Ligand-receptor constriction results

Subsequently, PyRx-Vina was employed to assess the compound's interaction with the receptor. PyRx-Vina was chosen due to its cost-effectiveness, user-friendliness, precision, low error rate, and reliability (Allouche, 2012). Among the methods available in the PyRx-Vina program is the Vina method, known for its speed and accuracy in docking compared to other free applications. *In silico* screening or virtual screening, was utilised to predict the binding model of known active ligands, discover new ligands, and forecast the binding affinities of various series of active substances. The PyRx-Vina program is used to upload the generated compounds and receptors. The chemical and receptor are selected, and "*Forward*" is then selected. Finally, the "*Run Vina*" button is clicked to obtain the affinity binding value along with the RMSD after setting the grid box's size and centre.

Molecular docking of gingerol, shogaol and residues with proteins 7QUV, 3OSK, 5MY8, 3LXL and MYD88

The results of the study presented in Table I showed negative affinity binding energy indicating a strong bond formation between the ligand and the receptor. RMSD values reveal variations for each receptor. Figure 1 showed 3-dimensional structure gingerol, shogaol, tofacitinib, crystal structures of S100A9, CTLA-4, SRSF 1, JAK3 and MyD88 receptors in the Protein Data Bank

(Chembio 3D). Table II showed ADMET (Absorption, Distribution, Metabolism, Excretion, Toxicity) gingerol and shogaol.

Table I: Molecular docking of gingerol, shogaol and residues with proteins 7QUV, 3OSK, 5MY8, 3LXL and MYD88

Protein	Test compound	Average binding energy	Average RMSD lower (A°)	Average RMSD upper (A°)	Residues protein
7QUV	Natif ligan	-6.5	0.41	0.72	Val 17 (A), Ile 14 (A)
	Gingerol	-4.5	1.49	3.15	Val 77 (A), Met 80 (A), Ile 14 (A), Glu 43 (A)
	Shgogaol	-4.9	1.20	2.36	Val 77 (A), Val 17 (A), Met 80 (A), Ile 14 (A), Ala 84 (A), Ser 13 (A)
	Tofacitinib	-5.1	2.80	3.70	Val 77 (A), Val 17 (A), Ile 14 (A), Glu 43 (A), Ser 13 (A)
3OSK	Natif ligan	-4.6	1.71	2.96	Thr 80 (A), Ser 20 (A)
	Gingerol	-4.3	1.49	2.67	Val 49 (A), Tyr 92 (A), Ile 67 (A), Glu 48 (A), Arg 40 (A)
	Shgogaol	-4.3	1.62	3.09	Val 49 (A), Tyr 92 (A), Ile 67 (A)Arg 40 (A)
	Tofacitinib	-4.8	5.60	9.12	Ile 18 (A), Thr 80 (A), Ser 20 (A)
5MY8	Natif ligan	-6.5	0.41	0.72	Val 223 (A), Val 167 (A), Val 145 (A), Val 94 (A), Ala 107 (A), Leu 168 (A), Leu 86 (A), Gly 169 (A), His 170 (A), Ile 228 (A)
	Gingerol	-4.5	1.49	3.15	Val 223 (A), Val 167 (A), Val 94 (A), Tyr 227 (A), Leu 220 (A), Leu 168 (A), Leu 86 (A), Glu 166 (A), Gly 169 (A), His 171 (A), His 170 (A), Ala 107 (A)
	Shgogaol	-4.9	1.20	2.36	Val 223 (A), Val 145 (A), Val 94 (A), Tyr 227 (A), Leu 168 (A), Leu 86 (A), Glu 166 (A), His 170 (A), Lys 109 (A), Phe 165 (A)
	Tofacitinib	-5.1	2.80	3.70	Val 145 (A), Leu 220 (A), His 211 (A), Phe 165 (A)
3LXL	Natif ligan	-4.6	1.71	2.96	Val 836 (A), Ala 966 (A), Leu 95 (A), Leu 905 (A), Leu 828 (A), Met 902 (A)
	Gingerol	-4.3	1.49	2.67	Val 836 (A), Leu 956 (A), Leu 905 (A), Leu 828 (A), Met 902 (A), Lys 830 (A), Ala 966 (A), Asp 967 (A)
	Shgogaol	-4.3	1.62	3.09	Val 836 (A), Leu 956 (A), Leu 828 (A), Lys 855 (A), Tyr 904 (A), Ala 966 (A), Ala 853 (A), Asp 967 (A), Asn 954 (A), Glu 871 (A)
	Tofacitinib	-4.8	5.60	9.12	Val 836 (A), Leu 956 (A), Leu 828 (A), Lys 855 (A), Ala 966 (A), Ala 853 (A), Cys 909 (A)
MYD88	Natif ligan	-5.6	1.62	1.97	Trp 205 (A), Leu 189 (A)
	Gingerol	-5.7	1.46	1.85	Val 198 (A), Tyr 167 (A), Ser 209 (A), Cys 166 (A)
	Shgogaol	-5.0	1.79	2.09	Tyr 167 (A), Ser 194 (A), Asp 195 (A), Glu 232 (A), Phe 235 (A), Phe164 (A)
	Tofacitinib	-5.4	1.62	1.97	Ala 292 (A), Cys 274 (A)

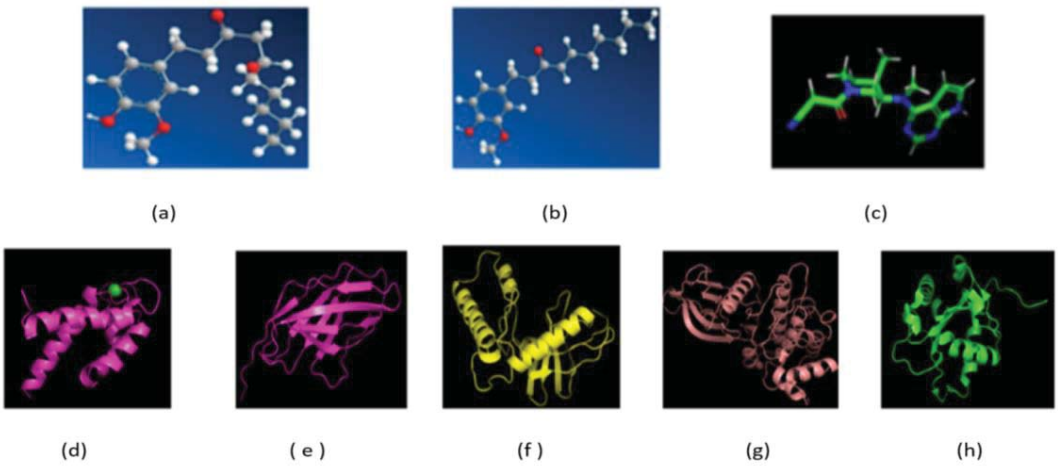

Figure 1: 3-dimensional structure (upper) of (a) Gingerol, (b) Shogaol and (c) Tofacitinib, Crystal structures (lower) of S100A9 (d), CTLA-4 (e), SRSF 1 (f), JAK3 (g) and MyD88 (h) receptors in the Protein Data Bank (Chembio 3D)

Table II: ADMET (Absorption, Distribution, Metabolism, Excretion, Toxicity) gingerol and shogaol

Property value	Model name	Gingerol		Shogaol	
		Predicted	Unit	Predicted	Unit
Absoption	Water solubility	**-3.164**	Numeric (log mol/L)	**-3.941**	Numeric (log mol/L)
Absoption	Caco2 permeability	**0.94**	Num (log Papp in 10^{-6} cm/s)	**1.391**	Num (log Papp in 10^{-6} cm/s)
Absoption	Intestinal absorption (human)	**92.416**	Numeric (% Absorbed)	**92.686**	Numeric (% Absorbed)
Absoption	Skin Permeability	**-2.817**	Numeric (log Kp)	**-2.584**	Numeric (log Kp)
Absoption	P-glycoprotein substrate	**Yes**	Categorical (Yes/No)	**No**	Categorical (Yes/No)
Absoption	P-glycoprotein I inhibitor	**No**	Categorical (Yes/No)	**Yes**	Categorical (Yes/No)
Absoption	P-glycoprotein II inhibitor	**No**	Categorical (Yes/No)	**No**	Categorical (Yes/No)
Distribution	VDss (human)	**0.524**	Numeric (log L/kg)	**0.501**	Numeric (log L/kg)
Distribution	Fraction unbound (human)	**0.258**	Numeric (Fu)	**0.147**	Numeric (Fu)
Distribution	BBB permeability	**-0.727**	Numeric (log BB)	**-0.197**	Numeric (log BB)
Distribution	CNS permeability	**-2.788**	Numeric (log PS)	**-1.777**	Numeric (log PS)
Metabolism	CYP2D6 substrate	**No**	Categorical (Yes/No)	**No**	Categorical (Yes/No)
Metabolism	CYP3A4 substrate	**No**	Categorical (Yes/No)	**Yes**	Categorical (Yes/No)
Metabolism	CYP1A2, CYP2C19 & 9 inhibitior	**Yes**	Categorical (Yes/No)	**Yes**	Categorical (Yes/No)
Metabolism	CYP2D6, CYP3A4 inhibitior	**No**	Categorical (Yes/No)	**No**	Categorical (Yes/No)
Excretion	Total Clearance	**1.339**	Numeric (log ml/min/kg)	**1.44**	Num (log ml/min/kg)
Excretion	Renal OCT2 substrate	**No**	Categorical (Yes/No)	**No**	Categorical (Yes/No)
Toxicity	AMES toxicity	**No**	Categorical (Yes/No)	**No**	Categorical (Yes/No)
Toxicity	Max. tolerated dose (human)	**0.635**	Numeric (log mg/kg/day)	**0.759**	Numeric (log mg/kg/day)
Toxicity	hERG I inhibitor	**No**	Categorical (Yes/No)	**No**	Categorical (Yes/No)
Toxicity	hERG II inhibitor	**No**	Categorical (Yes/No)	**Yes**	Categorical (Yes/No)
Toxicity	Oral Rat Acute Toxicity (LD50)	**1.958**	Numeric (mol/kg)	**2.081**	Numeric (mol/kg)
Toxicity	Oral Rat Chronic Toxicity	**1.631**	Num (log mg/kg_bw/day)	**2.159**	Num (log mg/kg_bw/day)
Toxicity	Hepatotoxicity	**No**	Categorical (Yes/No)	**No**	Categorical (Yes/No)
Toxicity	Skin Sensitisation	**No**	Categorical (Yes/No)	**Yes**	Categorical (Yes/No)
Toxicity	*T. Pyriformis* toxicity	**1.487**	Numeric (log ug/L)	**2.475**	Numeric (log ug/L)
Toxicity	Minnow toxicity	**0.966**	Numeric (log mM)	**0.15**	Numeric (log mM)

Descriptor Value: Gingerol= Molecular weight 276.367, LogP 4.039, #RotatableBonds=9, #Acceptors=3, #Donor=1; Surface area=120.825;
Shogaol : Moleckular weight 262.349, LogP 3.6489, #Rotatable Bonds 8, #Acceptors 3, #Donor1; Surface Area 11 4.461

Discussion

This study used binding affinity and RMSD validation as the methods. Binding affinity, as defined by Kastritis & Bonvin, (2013), is the interaction force between two or more molecules that are reversibly bound. The score, as an indicator of the strength with which the test ligand binds to the receptor. The score (minus) decreases with the stability of the ligand-protein interaction (Hardjono, 2016).

The atomic positions between the experimental structure and the protein structure being docked were compared using RMSD, a two-position measurement procedure (Lestari, Nasrudin, & Rahmanpiu, 2020). The method was considered valid when the resulting RMSD value was 2 Å. A smaller RMSD value indicates a better-predicted ligand poses, as they closely resemble the native ligand conformation. Conversely, a larger RMSD value implies a higher error in predicting the ligand-protein interaction due to the greater differences in conformation between the predicted ligands.

The two RMSDs produced by PyRx-Vina are lower and higher. However, since the lower RMSD is obtained by searching for all potential atoms in symmetrical molecules, only the value of the lower RMSD was examined (Bell & Zhang, 2019). Therefore, the lower RMSD value is more accurate (Meli & Biggin, 2020). To

continue using the methods in the next stage of the research, this validation process ensures that these methods are effective and validated. In both ligan-receptor interactions in native ligands, test and control compounds exhibited a type of binding with various amino acids.

On the protein S100A9, the same amino acid interactions were observed among the four groups of compounds, namely, the native ligan, shogaol, gingerol, and control. The compounds were located at the same site on the calprotectin S100A9 protein, suggesting that gingerol and shogaol have the potential to participate in positive feedback mechanisms involving increased leukocyte recruitment and pro-inflammatory cytokine release from tenocytes, thus mitigating the inflammatory response in the early stages of the disease (Kim *et al*., 2015).

The CTLA-4 protein also exhibited similar interactions with the four groups of compounds. CTLA-4 protein played a role in inhibiting the activity of T-lymphocytes. This inhibition resulted in a decrease in the immunosuppressive response, an uncontrolled increase in the immune response, and a decrease in the T- regulator lymphocytes (suppressing the working of T-cells so as not to exaggerate), which failed the homeostasis of the immune system (Destiawan *et al*., 2021). CTLA-4, also known as CD152, is a protein receptor mainly expressed in T-cells. Human CTLA-4 variants are associated with various autoimmune diseases, including SLE, RA, T1DM, GD, and MS (Ren *et al.*, 2021).

SRSF1 is a multifunctional protein that contributes to the activation of IL-2 transcription. Levels of SRSF1 decrease in the T-cells of SLE patients, and excess expression of SRSF1 in the T-cells of SLE patients enhance IL-2 production (Katsuyama & Moulton, 2021). SRSF1, a splicing factor Serine/Arginine member 1 (SRSF1), is abundantly expressed in most tissues and acts as the primary controller of T-cell activity and is involved in the immune regulation of SLE (Su & Huang, 2021). Similar interactions observed among the four groups of compounds suggest that the compound binds to the same site in the SRSF1 protein.

JAK kinase receptors directly activate the PI3K/AKT signalling pathway, and phosphorylated JAK activates PI3C. The JAK/STAT pathway is negatively regulated by various mechanisms to limit cytokine signalling and reduce cytokine response. Many cytokines play a role in SLE pathogenesis, either by acting directly on effector cells or creating a pro-inflammatory environment. Since JAK kinase can be effectively blocked by small synthetic compounds, they are promising targets to control cytokine signaling and restore immune balance. JAK belongs to the tyrosine kinase family and there are currently four identified JAKs: JAK1, JAK2, JAK3, and TYK2 (Kotyla *et al*., 2022).

For the MyD88 protein, there were no similar interaction between native ligands with gingerol, shogaol, or tofacitinib. The only similarity is the amino acid Tyr 167, suggesting that gingerol shogaol, and tofacitinib do not share significant similarities with the MyD88, which acts as an adapter to connect signals received from outside and signals transferred to the inside of the cell (Su & Huang, 2021). The binding between the activated TLR and MyD88 is mediated by the C-terminal domain of the Toll-interleukin 1 receptor (IL-1R) (TIR) of their respective cytoplasms, which allows myddosome assembly (Olson *et al*., 2019). MyD88 is a central immune adaptor protein that regulates the pathogenesis of disease in SLE and works at the back of a TLR, a well-known disease mediator in SLE. Several components of the MyD88/TLR signalling pathway have been identified as risk factors in patients with SLE, including TLR7-TLR9, IRAK1, IRAK 4, OPN, and ACP1 (Wu *et al*., 2015).

Gingerol has a negative solubility value. It is a very soluble compound in water, well-absorbed but toxic. Has a small distribution in the body. Gingerol tends to be metabolised by the P450 enzyme. Have a fairly high MTD (Maximum Tolerated Dose). Shogaol is a compound that is soluble in water, has good permeability, and increases the body's ability to absorb Has a large therapeutic range but has no high mutagenic or toxic properties. Gingerol and shogaol have the potential to be developed as immunomodulators. More in-depth research needs to be done both *in silico*, *in vitro*, and *in vivo* as a preclinical study. This is to promote the development of ginger-based products in the community and to encourage the establishment of standardised medicines.

Conclusion

Based on the results of the research, it is evident that gingerol and shogaol compounds have the potential to act as immunomodulators in the treatment of lupus disease, functioning as immunosuppressants. The docking results using the PyRx application against Calprotectin S100A9 receptors, SRSF Protein Kinase 1, and Tyrosine Protein Kinase JAK3 revealed favourable binding affinity value so it was used as a drug as well as an RMSD value of 2 angstroms. Additionally, these compounds shared similar amino acid residues with gingerol and shogaol.

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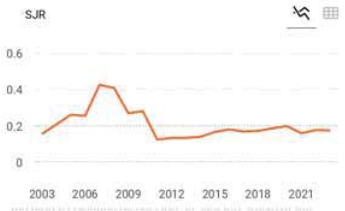

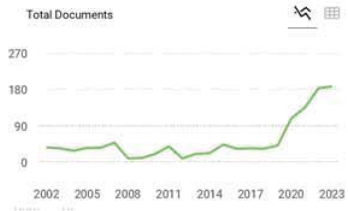

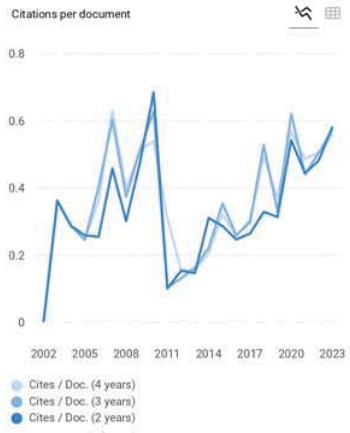

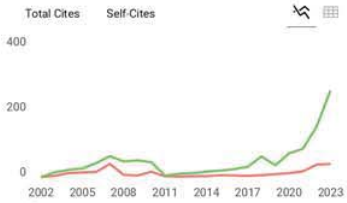

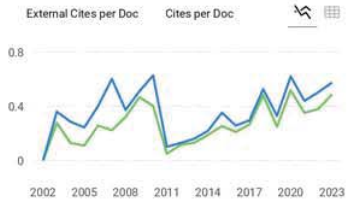

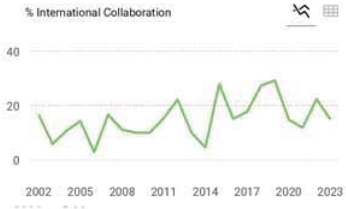

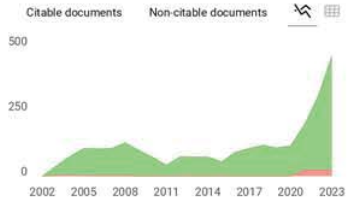

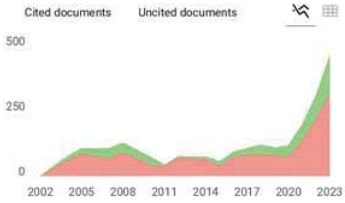

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