Please generate the molecular structure (SELFIES) based on the following description. Please think step by step and return the final answer in <answer> </answer> tags. Description:

The molecule is a 3,3'-lysobisphosphatidate obtained by deprotonation of the phosphate OH group of (5,5)-bis-(3-oleoylglycero)-1-phosphate; major species at pH 7.3. It is a conjugate base of a (5,5)-bis-(3-oleoylglycero)-1-phosphate.

(a). Prompt-based Methods

To generate the SELFIES representation, ...\n\n1. **Identify the Base Molecule**:...\n2. **Oleoyl Chain**: ...The oleoyl chain is represented as [C@@H1][C@@H1][C@@H1][C@@H1][C@@H1][C@@H1][C@@H1][C@@H1][C@@H1][C @@H1]...[C@@H1][C@@H1][C@@H1][C@@H1][C@@H1]...[C@@H1][C@@H1][C@@H1] (Repeatd fragments w/o answer format)

<think>\nOkay, so I'm trying to design a SELFIES structure for this molecule... But wait...

but I need to think about the exact arrangement...

but that's not possible...

Wait, perhaps the..., but that's not correct.

CH2-CH2-CH2-CH2-CH2-CH2 (Repetitive self-questioning w/o answer format)

Invalid or Inconsistent Molecule Hallucinations in Reasoning

(b). Fine-tuning Methods without explicit reasoning

[C][C][C][C][C][C][C][C][C][/C][=C][\\C][C][C][C][C][C][C][C][C][E]=Branch1][C][=O][O][C][C@H1][Branch1][O][

C][O][P]... (Lack of Chain-of-Thought)

X Invalid or inconsistent molecules.

(c). MolReasoner

To deduce the molecular structure ...n\n1. **Identify the Core Structure**:...\n\n2. **Understand the Phosphate Group**:...\n\n3. **Incorporate the Oleoyl Groups**: ..., Oleic acid has a straight chain of 18 carbon atoms with a double bond at the 9th position (C9). Therefore, each oleoyl group can be represented as a long hydrocarbon chain (C18) with a double bond.\n\n4. **Construct the Glycerol Backbone**:..., and one hydroxyl group is linked to the phosphate group.\n\n5. **Connect the Components**: \n - Start with the two glycerol molecules. \n - Attach the oleoyl groups to the first and second carbon atoms of each glycerol molecule. \n -... **Use the Provided Fragments**:...\n - The fragment < |CO20| > represents the glycerol backbone.\n - The fragment < CO30|> represents the oleoyl groups. \n\nBy following these steps, we can construct the molecular structure of 3,3'lysobisphosphatidate. \n\nThe final answer is: \n O][C][C@H1][Branch1][C][O][C][O][P][=Branch1][C][=O][Branch1][C][O-

Chemical Knowledge Alignment

[=C][\\C][C][C][C][C][C]</answer>



Structured and Consistent Reasoning