

## Product Information

### 2-O-hexadecanoyl-3-O-(2,4S,6S-trimethyl-2E-docosenoyl)-6-O-(2R,4S,6S-trimethyl-3R-hydroxy-tetracosanoyl)-2'-O-(2,4S,6S-trimethyl-2E-docosenoyl)-4'-O-(

**Cat. No.:** X26-02-ZQ4844

**Size:** 1 mg; 10 mg; 25 mg; 100 mg

**Compound CID:** 52929959

**Synonym:**

PAT16(22:1(2E)(2Me,4Me[S],6Me[S])/24:0(2Me[R],3OH[R],4Me[S],6Me[S])/22:1(2E)(2Me,4Me[S],6Me[S])/22:1(2E)(2Me,4Me[S],6Me[S]))

**This product is for research use only and is not intended for diagnostic use.**

#### Product Information

<b>Description</b>	This penta-acylated trehalose features a 3R-hydroxy-tetracosanoyl chain at the 6-position combined with multiple C22 phthienoic acid branches. It is used to study how site-specific hydroxylation affects the molecular recognition of mycobacterial lipids by host receptors.
<b>Molecular Weight</b>	2077.3
<b>Molecular Formula</b>	C <sub>130</sub> H <sub>242</sub> O <sub>17</sub>
<b>IUPAC Name</b>	[(3R,5R,6R)-5-hexadecanoyloxy-3-hydroxy-6-[(2R,3S,5S)-4-hydroxy-6-(hydroxymethyl)-3,5-bis[(E,4S,6S)-2,4,6-trimethyldocos-2-enoyl]oxy]oxan-2-yl]oxy-4-[(E,4S,6S)-2,4,6-trimethyldocos-2-enoyl]oxyoxan-2-yl)methyl (2S,3S,4S,6S)-3-hydroxy-2,4,6-trimethyltetracosanoate
<b>InChI</b>	InChI=1S/C130H242O17/c1-18-23-28-33-38-43-48-53-57-58-63-67-72-77-82-87-92-106(9)97-110(13)118(133)114(17)128(139)140-102-116-119(134)122(145-126(137)112(15)99-108(11)95-104(7)90-85-80-75-70-65-61-55-50-45-40-35-30-25-20-3)124(143-117(132)93-88-83-78-73-68-59-52-47-42-37-32-27-22-5)130(142-116)147-129-123(146-127(138)113(16)100-109(12)96-105(8)91-86-81-76-71-66-62-56-51-46-41-36-31-26-21-4)120(135)121(115(101-131)141-129)144-125(136)111(14)98-107(10)94-103(6)89-84-79-74-69-64-60-54-49-44-39-34-29-24-19-2/h98-100,103-110,114-116,118-124,129-131,133-135H,18-97,101-102H2,1-17H3/b111-98+,112-99+,113-100+/t103-,104-,105-,106-,107-,108-,109-,110-,114-,115?,116?,118-,119+,120?,121+,122?,123-,124+,129+,130+/m0/s1
<b>InChI Key</b>	BXXANTUABTYJSH-NVCYORSTSA-N
<b>Canonical SMILES</b>	CCCCCCCCCCCCCCCC[C@H](C)C[C@H](C)[C@@H]([C@H](C)C(=O)OCC1[C@H](C([C@H]([C@H](O1)O)[C@@H]2[C@H](C([C@@H](C(O2)CO)OC(=O)/C(=C/[C@@H](C)C[C@@H](C)CCCCCCCCCCCCC)/C)O)OC(=O)/C(=C/[C@@H](C)C[C@@H](C)CCCCCCCCCCCCC)/C)O



C(=O)CCCCCCCCCCCCCCC)OC(=O)/C=C/[C@@H](C)C[C@@H](C)CCCCCCCCCCCCCCC)/C)O)O

<b>Source</b>	Chemical synthesis
<b>Form</b>	Solid or liquid
<b>Purity</b>	≥90%
<b>Identity</b>	Confirmed by NMR/HPLC/MS.
<b>Stability</b>	The product is stable for one year when stored at the recommended temperature in lyophilized powder.
<b>Quality Level</b>	Research level
<b>Applications</b>	2- <i>O</i> -hexadecanoyl-3- <i>O</i> -(2,4 <i>S</i> ,6 <i>S</i> -trimethyl-2 <i>E</i> -docosenoyl)-6- <i>O</i> -(2 <i>R</i> ,4 <i>S</i> ,6 <i>S</i> -trimethyl-3 <i>R</i> -hydroxy-tetracosanoyl)-2'- <i>O</i> -(2,4 <i>S</i> ,6 <i>S</i> -trimethyl-2 <i>E</i> -docosenoyl)-4'- <i>O</i> -(2,4 <i>S</i> ,6 <i>S</i> -trimethyl-2 <i>E</i> -docosenoyl)- $\alpha$ , $\alpha$ -trehalose can be used to study the biophysical impact of a 3-hydroxy substitution on the thermodynamic stability of docosenoyl-rich trehalose lipids.
<b>Storage</b>	Store at -20°C.