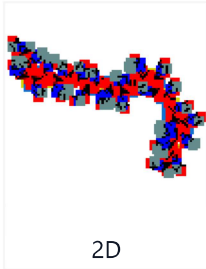
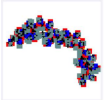
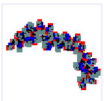



COMPOUND SUMMARY

Agatolimod sodium

PubChem CID	70687254
Structure	 2D
Molecular Formula	$C_{236}H_{280}N_{70}Na_{23}O_{133}P_{23}S_{23}$
Synonyms	Agatolimod sodium Agatolimod tricosasodium salt ChEMBL2103793 CpG-7909 541547-35-7 View More...
Molecular Weight	8204 g/mol <i>Computed by PubChem 2.1 (PubChem release 2021.05.07)</i>
Parent Compound	 CID 70687253 (Pf-3512676 free acid)
Component Compounds	 CID 70687253 (Pf-3512676 free acid)  CID 5360545 (Sodium)
Dates	Create: 2013-02-04 Modify: 2024-07-20

Description

Agatolimod Sodium is the tricosasodium salt of a synthetic 24-mer oligonucleotide containing 3 CpG motifs with potential antineoplastic and immunostimulatory activity. **Agatolimod** selectively targets Toll-like receptor 9 (TLR9), thereby activating dendritic and B cells and stimulating cytotoxic T cell and antibody responses against tumor cells bearing tumor antigens.

▶ [NCI Thesaurus \(NCIt\)](#)

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8 Literature ▼

9 Interactions and Pathways ▼

10 Classification ▼

11 Information Sources

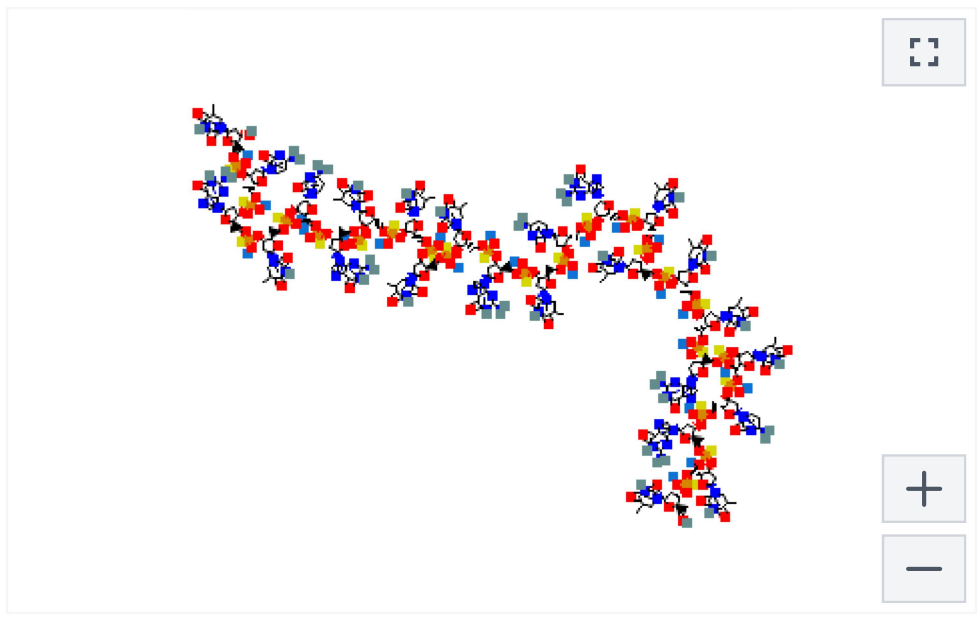
1 Structures



1.1 2D Structure



Chemical Structure Depiction



► [PubChem](#)

1.2 3D Status



Conformer generation is disallowed since too many atoms, MMFF94s unsupported element, too flexible, mixture or salt

► [PubChem](#)

2 Biologic Description



IUPAC Condensed	dThd-sP-dThd-sP-dGuo-sP-dCyd-sP-dThd-sP-dGuo-sP-dThd-sP-dThd-sP-dThd-sP-dThd-sP-dThd-sP-dGuo-sP-dCyd-sP-dThd-sP-dThd-sP-dThd-sP-dThd-sP-dThd-sP-dGuo-sP-dCyd-sP-dThd-sP-dGuo-sP-dCyd-sP-dThd.23Na+
Sequence	TTGCTGTTTTGCTGTTTTGCTGCT
IUPAC	P-thio-thymidylyl-(3'->5')-P-thio-thymidylyl-(3'->5')-2'-deoxy-P-thio-guanylyl-(3'->5')-2'-deoxy-P-thio-cytidylyl-(3'->5')-P-thio-thymidylyl-(3'->5')-2'-deoxy-P-thio-guanylyl-(3'->5')-P-thio-thymidylyl-(3'->5')-P-thio-thymidylyl-(3'->5')-P-thio-thymidylyl-(3'->5')-2'-deoxy-P-thio-guanylyl-(3'->5')-2'-deoxy-P-thio-cytidylyl-(3'->5')-P-thio-thymidylyl-(3'->5')-2'-deoxy-P-thio-guanylyl-(3'->5')-P-thio-thymidylyl-(3'->5')-P-thio-thymidylyl-(3'->5')-P-thio-thymidylyl-(3'->5')-P-thio-thymidylyl-(3'->5')-2'-deoxy-P-thio-guanylyl-(3'->5')-2'-deoxy-P-thio-cytidylyl-(3'->5')-P-thio-thymidylyl-(3'->5')-2'-deoxy-P-thio-guanylyl-(3'->5')-2'-deoxy-P-thio-cytidylyl-(3'->5')-thymidine sodium salt



3.1.2 InChI

InChI=1S/C236H303N70O133P23S23.23Na/c1-91-47-287(223(333)269-193(91)309)157-23-105(308)130(394-157)62-370-440(347,463)418-107-25-158(283-19-15-153(237)253-219(283)329)395-131(107)63-372-457(364,480)434-123-41-175(301-85-247-181-187(301)257-213(241)263-207(181)323)412-148(123)80-388-452(359,475)429-118-36-170(296-56-100(10)202(318)278-232(296)342)400-136(118)68-376-442(349,465)419-109-27-160(285-21-17-155(239)255-221(285)331)397-133(109)65-374-459(366,482)436-125-43-177(303-87-249-183-189(303)259-215(243)265-209(183)325)413-149(125)81-389-455(362,478)432-121-39-173(299-59-103(13)205(321)281-235(299)345)407-143(121)75-383-447(354,470)424-114-32-166(292-52-96(6)198(314)274-228(292)338)403-139(114)71-379-445(352,468)422-113-31-165(291-51-95(5)197(313)273-227(291)337)406-142(113)74-382-450(357,473)427-117-35-169(295-55-99(9)201(317)277-231(295)341)410-146(117)78-386-462(369,485)439-128-46-180(306-90-252-186-192(306)262-218(246)268-212(186)328)416-152(128)84-392-454(361,477)431-120-38-172(298-58-102(12)204(320)280-234(298)344)402-138(120)70-378-444(351,467)421-110-28-161(286-22-18-156(240)256-222(286)332)398-134(110)66-375-460(367,483)437-126-44-178(304-88-250-184-190(304)260-216(244)266-210(184)326)414-150(126)82-390-456(363,479)433-122-40-174(300-60-104(14)206(322)282-236(300)346)408-144(122)76-384-448(355,471)425-115-33-167(293-53-97(7)199(315)275-229(293)339)404-140(115)72-380-446(353,469)423-112-30-164(290-50-94(4)196(312)272-226(290)336)405-141(112)73-381-449(356,472)426-116-34-168(294-54-98(8)200(316)276-230(294)340)409-145(116)77-385-461(368,484)438-127-45-179(305-89-251-185-191(305)261-217(245)267-211(185)327)415-151(127)83-391-453(360,476)430-119-37-171(297-57-101(11)203(319)279-233(297)343)401-137(119)69-377-443(350,466)420-108-26-159(284-20-16-154(238)254-220(284)330)396-132(108)64-373-458(365,481)435-124-42-176(302-86-248-182-188(302)258-214(242)264-208(182)324)411-147(124)79-387-451(358,474)428-111-29-163(289-49-93(3)195(311)271-225(289)335)399-135(111)67-371-441(348,464)417-106-24-162(393-129(106)61-307)288-48-92(2)194(310)270-224(288)334;...../h15-22,47-60,85-90,105-152,157-180,307-308H,23-46,61-84H2,1-14H3,(H,347,463)(H,348,464)(H,349,465)(H,350,466)(H,351,467)(H,352,468)(H,353,469)(H,354,470)(H,355,471)(H,356,472)(H,357,473)(H,358,474)(H,359,475)(H,360,476)(H,361,477)(H,362,478)(H,363,479)(H,364,480)(H,365,481)(H,366,482)(H,367,483)(H,368,484)(H,369,485)(H2,237,253,329)(H2,238,254,330)(H2,239,255,331)(H2,240,256,332)(H,269,309,333)(H,270,310,334)(H,271,311,335)(H,272,312,336)(H,273,313,337)(H,274,314,338)(H,275,315,339)(H,276,316,340)(H,277,317,341)(H,278,318,342)(H,279,319,343)(H,280,320,344)(H,281,321,345)(H,282,322,346)(H3,241,257,263,323)(H3,242,258,264,324)(H3,243,259,265,325)(H3,244,260,266,326)(H3,245,261,267,327)(H3,246,262,268,328);...../q;23*+1/p-23/t105-,106-,107-,108-,109-,110-,111-,112-,113-,114-,115-,116-,117-,118-,119-,120-,121-,122-,123-,124-,125-,126-,127-,128-,129+,130+,131+,132+,133+,134+,135+,136+,137+,138+,139+,140+,141+,142+,143+,144+,145+,146+,147+,148+,149+,150+,151+,152+,157+,158+,159+,16