**Crystal structures of new ivermectin pseudopolymorphs**

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**1. Atomic cartesian coordinates for ivermectin B1a from DFT**

# atomic number x y z

1 8 5.4985317889 4.7382474150 26.3264189615

2 8 -2.1290580797 5.9686302255 28.5412351518

3 8 -3.3211098625 4.0191329156 27.9937655972

4 8 6.5709229587 2.4759172439 23.6336834899

5 8 3.3309046002 5.0879550488 25.4628712442

6 8 -2.6783399403 5.2095024956 21.3033023581

7 1 -1.8666549078 5.0558326070 20.7987920226

8 8 -2.8239881803 8.7326715107 20.5232140023

9 8 -4.5729741726 4.9647120711 23.8254347139

10 8 -3.1919152906 6.6045786428 24.5641064163

11 8 4.4890543788 0.9539934518 24.9278559319

12 8 8.4997630313 1.2123390226 24.1182083708

13 8 10.5849044035 2.4044052691 21.2978935638

14 1 10.5646069118 2.4326667136 20.1755279960

15 8 -4.6277531087 8.3400388055 18.5784554244

16 1 -4.4246643228 9.1224865809 19.1129527805

17 8 8.4187026759 1.1313993485 19.9423762167

18 6 -1.5803699326 7.3317530179 21.9472503905

19 6 2.2382463203 6.9454051842 26.6819294629

20 6 4.5470824544 2.3784711324 24.9829588192

21 1 4.0428476780 2.8004802267 24.1009110986

22 6 -2.8220005900 6.6058211997 21.4557617720

23 6 9.4826420237 2.0046352246 23.4327782722

24 1 9.1679082719 3.0588536094 23.4455336419

25 6 -3.4037277935 5.4268097168 28.1877980998

26 6 -3.0283705299 7.3710431337 20.1280539037

27 1 -2.2316974007 7.0724806715 19.4242804524

28 6 3.2534804829 6.5122146100 25.6226345112

29 1 4.2468490470 6.8824688159 25.9154776043

30 6 -0.5655889466 6.7259310519 22.5816023653

31 1 -0.6950887376 5.6648130589 22.7930658532

32 6 4.1283275675 4.4159405913 26.4311856154

33 1 3.8484772344 4.7520363054 27.4358420540

34 6 2.9258227513 7.1169759513 24.2254774630

35 1 2.8389941573 8.2012692787 24.3632968773

36 6 -1.1046511650 5.7688736619 27.5546674022

37 1 -0.9772962846 4.6894580838 27.3923220494

38 6 1.6189625620 6.5920683596 23.6913698208

39 1 1.4637089639 5.5200599310 23.8098099618

40 6 0.2044424274 6.3317804512 28.1272641772

41 1 0.0685801996 7.3960193872 28.3419798355

42 1 0.3840854221 5.8330911175 29.0899652820

43 6 1.3437586486 6.0768247246 27.1747204818

44 1 1.4041639480 5.0547054318 26.8036855057

45 6 -3.9898280645 6.0095944436 23.6474824563

46 6 -4.0553257157 6.8638828322 22.3831531649

47 1 -3.9730385573 7.9055087952 22.7156371440

48 6 -5.3668078435 6.6909664318 21.6588748734

49 1 -6.2156511482 6.4042607771 22.2745344336

50 6 -4.3825852769 7.2175755177 19.4257018073

51 1 -4.2921797538 6.3637349179 18.7397022757

52 6 -1.7081495120 8.7511649319 21.4394766523

53 1 -1.9370412258 9.4797799873 22.2265068512

54 1 -0.7998216256 9.0875610445 20.9195886408

55 6 -2.9058653827 3.2454694393 29.1402286367

56 1 -1.9234023056 3.6174961414 29.4721340650

57 6 0.6725691584 7.3150690122 23.0651225164

58 1 0.8162221905 8.3873608445 22.9332834067

59 6 6.0226211707 2.7929272259 24.9180644472

60 1 6.5831559467 2.2750898816 25.7078170366

61 6 6.1536994210 4.3168225705 25.1152592338

62 1 5.6733920136 4.8003589934 24.2563523128

63 6 3.8973134493 2.9152504765 26.2668017621

64 1 2.8235599597 2.7053687821 26.2822096284

65 1 4.3498291873 2.4037857148 27.1231573863

66 6 9.6198653087 1.5902839481 21.9524918340

67 1 10.0102162245 0.5671245782 21.8965558423

68 6 -1.5116318527 6.4206258197 26.2334212579

69 1 -1.6134811630 7.5035567456 26.3818252384

70 1 -0.7372278873 6.2663198057 25.4788255435

71 6 -5.5415574261 6.9094553624 20.3524914245

72 6 -3.9027892360 6.0050948325 26.8489751845

73 1 -4.8253856321 5.4977904454 26.5578405687

74 1 -4.1191509950 7.0698517039 26.9931312534

75 6 -2.8429578572 5.8545953505 25.7582643508

76 1 -2.7540902560 4.8016257573 25.4794588467

77 6 8.2535085641 1.6265491262 21.2631188597

78 1 7.9116373125 2.6773832096 21.2248962045

79 6 -2.7188083539 1.7941659527 28.6506458249

80 1 -2.3880636450 1.2186243828 29.5267118167

81 6 2.3246929696 8.4012301998 27.0759204448

82 1 3.3668133666 8.6972977956 27.2480540851

83 1 1.7655166993 8.6154794636 27.9881487208

84 1 1.9351580711 9.0598501566 26.2892043760

85 6 4.0631438519 6.8677649642 23.2147720526

86 1 5.0258012226 7.2070594996 23.6137643577

87 1 3.8688727673 7.4108197128 22.2854667719

88 1 4.1461682732 5.8055280220 22.9720961603

89 6 -3.8909750075 3.4516348165 30.3082596704

90 1 -4.8817267663 3.1095237332 29.9792250640

91 6 -4.3441992256 5.7596631633 29.3512322378

92 1 -4.3030429091 6.8365897805 29.5435858058

93 1 -5.3648927941 5.5183441125 29.0315382281

94 6 -3.9866782924 4.9597995206 30.6081768619

95 1 -4.7347840493 5.1381377316 31.3900504471

96 1 -3.0250543314 5.3116833976 31.0022877380

97 6 -1.5811260336 1.7189665271 27.6082544723

98 1 -1.9061411907 2.2202991017 26.6893522958

99 1 -0.7247657309 2.2939855052 27.9874299504

100 6 7.2087485065 1.2033840965 23.5443718487

101 1 6.6480254764 0.4756139751 24.1335195361

102 6 10.7833741423 1.8573933110 24.2053844084

103 1 10.6647686085 2.2285386896 25.2270665565

104 1 11.5770122089 2.4185231274 23.7077530445

105 1 11.0757691839 0.8037716305 24.2549078583

106 6 7.2439127964 0.7985734907 22.0710573599

107 1 6.2358894305 0.8840286783 21.6555370292

108 1 7.5434870690 -0.2535242998 22.0113507907

109 6 -3.4877671460 2.6682269342 31.5640811597

110 1 -3.5503809409 1.5858799475 31.4179347211

111 1 -4.1437868882 2.9247761026 32.4027843687

112 1 -2.4605583616 2.9070581034 31.8662133220

113 6 3.2561202804 0.4304842473 24.4689961507

114 1 2.9995179848 0.8140943539 23.4701510266

115 1 2.4232657741 0.6550726269 25.1504620641

116 1 3.3726409498 -0.6543663150 24.4122114668

117 6 7.5893381082 4.8024647014 25.2331135154

118 1 7.5970012083 5.8757090023 25.4425690375

119 1 8.1305506637 4.6248158299 24.3029234837

120 1 8.1085451657 4.2900572063 26.0489099660

121 6 -6.8827123259 6.7791106229 19.6823855701

122 1 -6.8683433268 5.9787015550 18.9307649702

123 1 -7.1390182690 7.7003041734 19.1502989007

124 1 -7.6709985030 6.5537160027 20.4050641925

125 6 -4.0238954580 1.1754313075 28.1265135510

126 1 -4.7976647004 1.1453460289 28.8997962828

127 1 -3.8665193051 0.1464803680 27.7906746069

128 1 -4.4119258401 1.7547349830 27.2838634465

129 6 7.3883028907 1.4896462216 19.0439668391

130 1 7.6802619764 1.1138171199 18.0602157375

131 1 7.2639084802 2.5824190194 18.9818442109

132 1 6.4164358628 1.0488276490 19.3101686154

133 6 -1.1053023615 0.2985942149 27.2837777619

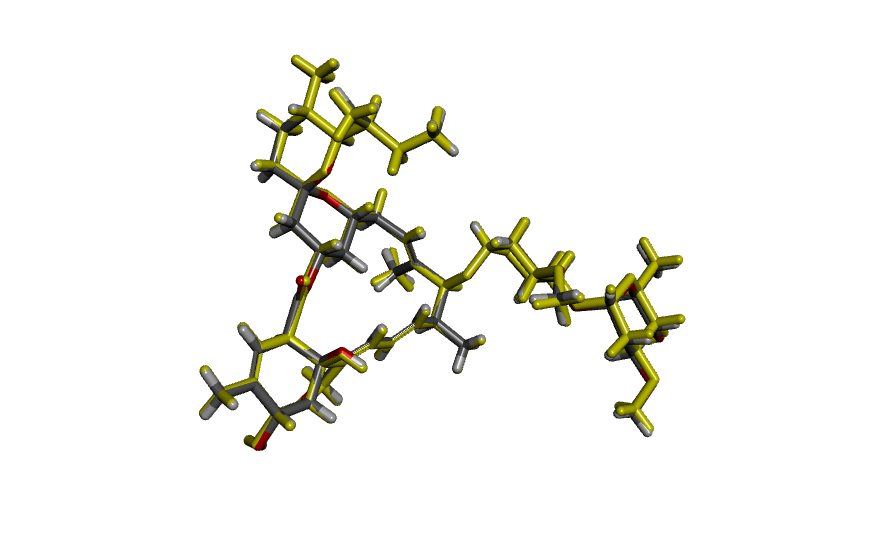
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135 1 -1.8894359405 -0.3032699460 26.8142656088

136 1 -0.7778633929 -0.2282990827 28.1879081791

**Table 1s.** Selected torsion angles for **I**.

|  |  |  |
| --- | --- | --- |
| Torsion angle (°) | X-ray analysis | DFT |
| C14−O41−C42−O43 | −54.3(5) | −66.82 |
| O51−C50−O49−C45 | −67.8(5) | −77.86 |
| O23−C22−C4−C9 | −90.2(5) | −98.49 |
| O1−C8−C7−O39 | 34.2(5) | 39.51 |
| O49−C45−C46−O60 | 64.3(6) | 67.17 |
| O27−C28−C32−C35 | −65.4(7) | −62.42 |
| O41−C14−C13−C40 | −63.4(6) | −64.42 |

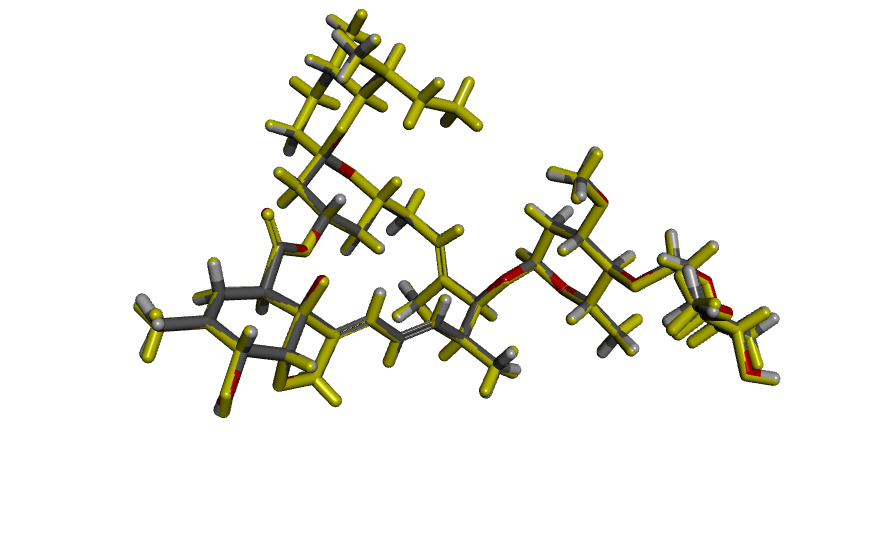


**Figure S1.** Overlay of IVM molecules present in **I** and BIFYOF.

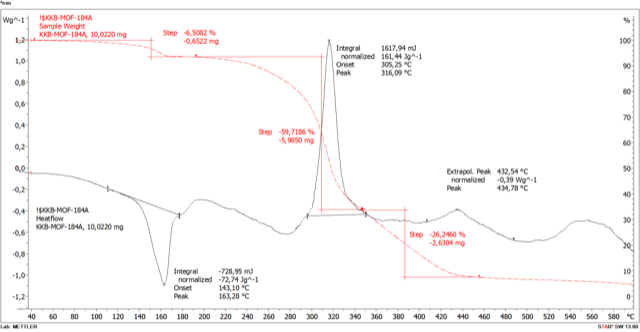
A picture containing diagram

Description automatically generated

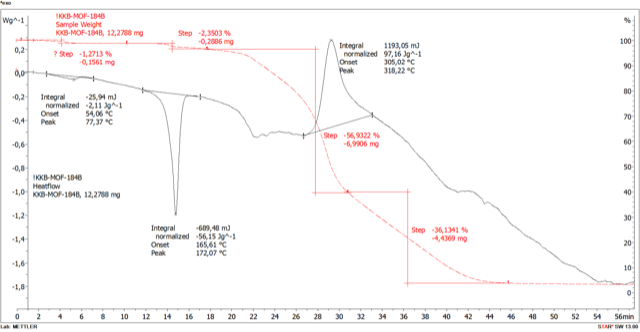
**Figure S2.** Overlay of the first kind of symmetrically unique IVM molecules present in **II** and **III**.



**Figure S3.** Overlay of the second kind of symmetrically unique IVM molecules present in **II** and **III**.

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**Figure S4.** Processed DSC and TGA data for **I**.

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**Figure S5.** Processed DSC and TGA data for **II**.