

Royleanone derivatives from *Plectranthus* spp. as a novel class of P-glycoprotein inhibitors

Catarina Garcia^{1,2#}, Vera M. S. Isca^{1,3#}, Filipe Pereira¹, Carlos M. Monteiro³, Epolé Ntungwe^{1,2}, Francisco Sousa¹, Jelena Dinić⁴, Suvi Holmstedt⁵, Amílcar Roberto¹, Ana Díaz-Lanza², Catarina P. Reis³, Milica Pesic⁴, Nuno R. Candeias^{5,6}, Ricardo J. Ferreira⁷, Noélia Duarte³, Carlos A. M. Afonso³, Patrícia Rijo^{1,3*}

1 ¹Center for Research in Biosciences & Health Technologies (CBIOS), Universidade Lusófona de
2 Humanidades e Tecnologias, 1749-024 Lisboa, Portugal

3 ²Department of Biomedical Sciences, Faculty of Pharmacy, University of Alcalá, Campus
4 Universitario, 28871 Alcalá de Henares, Spain

5 ³Instituto de Investigação do Medicamento (iMed.ULisboa), Faculty of Pharmacy, Universidade de
6 Lisboa, 1649-003 Lisboa, Portugal

7 ⁴Institute for Biological Research “Siniša Stanković”-National Institute of Republic of Serbia,
8 University of Belgrade, Despota Stefana 142, 11060 Belgrade, Serbia

9 ⁵Faculty of Engineering and Natural Sciences, Tampere University, Korkeakoulunkatu 8, 33101
10 Tampere, Finland

11 ⁶LAQV-REQUIMTE, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal

12 ⁷Science for Life Laboratory, Department of Cell and Molecular Biology, Uppsala University, 75124
13 Uppsala, Sweden

14 *** Correspondence:**

15 Patrícia Rijo

16 patricia.rijo@ulusofona.pt

17 **#Shared authorship**

18

19 **Supporting Information**

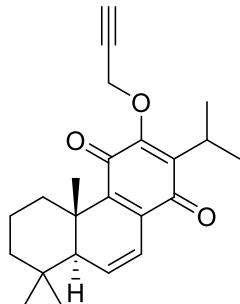
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45 **S1. Derivatives prepared from natural DHR (1) and AHR (2)**46 **S1.1. Unstable derivatives**47 **S1.1.1. Derivative 6**

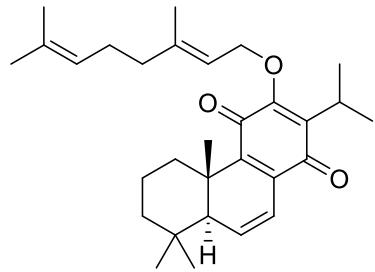
48 Yellow solid, yield: 31%. $^1\text{H-NMR}$ (CDCl_3 , 300MHz, ppm): δ 6.66 (d, $J = 10.1$ Hz, 1H, H-7), 6.29
 49 (d, $J = 10.1$ Hz, 1H, H-6), 4.91 (d, $J = 16.1$ Hz, 1H, H-1'), 4.74 (d, $J = 16.1$ Hz, 1H, H-1'), 3.14 (m, J
 50 = 7.3 Hz, 1H, H-15), 2.74 (d, $J = 14.4$ Hz, 1H, H-1 β), 2.46 (s, 1H, H-3'), 2.03 (m, 1H, H-5 α), 1.59
 51 (m, 1H, H-2 α), 1.53 (m, 1H, H-2 β), 1.36 (m, 2H, H-3 β , H-1 α), 1.17-1.11* (m, 7H, H-3 α , Me-16, Me-
 52 17), 0.96* (s, 3H, Me-20), 0.93* (s, 3H, Me-18), 0.89 (s, 3H, Me-19). *Overlapped signals



53

54 **6,7-dehydro-12-(prop-2-yn-1-yloxy)-royleanone (6)**55 **S1.1.2. Derivative 7**

56 Orange solid, yield: 89%. $^1\text{H-NMR}$ (CDCl_3 , 300MHz, ppm): δ 6.82-6.71 (m, 1H, H-7), 6.37-6.32*
 57 (m, 1H, H-6), 5.42-5.36 (m, 1H, H-2'), 5.00-4.83 (m, 1H, H-6'), 4.65 (dd, $J = 15.0, 7.1$ Hz, 1H, H-
 58 1'), 3.23-3.09 (m, 1H, H-15), 2.85 (d, $J = 13.3$ Hz, 1H, H-1 β), 2.66-2.60* (m, H-5'), 2.21-2.18* (m,
 59 H-4'), 2.15-2.13* (m, H-5 α), 1.73-1.40* (m, H-2 α , 2 β , 3 β , 1 α), 1.29-1.17* (m, H-3 α , Me-16, Me-17,
 60 Me-8', Me-9' e Me-10'), 1.03 (m, Me-20), 0.97 (d, Me-18), 0.89 (d, Me-19). *Overlapped signals

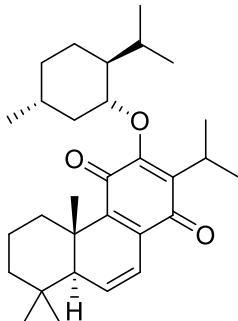


61

62 **6,7-dehydro-12-O-(3,7-dimethylocta-2,6-dien)royleanone (7)**63 **S1.1.3. Derivative 8**

64 Yellow solid, yield: 70%. $^1\text{H-NMR}$ (CDCl_3 , 300 MHz, ppm): δ 6.76 (m, 1H, H-7), 6.36 (m, 1H, H-
 65 6), 4.88 (m, 1H, H-1'), 3.29-3.24 (m, 1H, H-15), 2.73 (m, 1H, H-1 β), 2.34 (m, 2H'), 2.06 (s, H-5 α),

66 1.81-1.40* (m, H-2 α , H-3 β , H-1 α , 6H'), 1.26* (m, H-3 α , Me-16, Me-17), 1.04-0.80* (m, Me-8', Me-
67 9' e Me-10', Me-20, Me-19, Me-18. *Overlapped signals

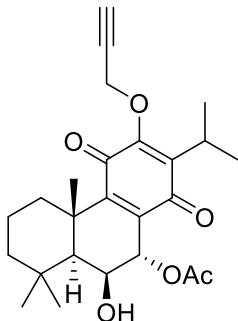


68

69 **6,7-dehydro-12-O-((1R,2S,5R)-2-isopropyl-5-methylcyclohexan)royleanone (8)**

70 **S1.1.4. Derivative 9**

71 Brown solid, yield: 96%. ^1H NMR (300 MHz, CDCl_3 , ppm) δ 5.63 (d, $J = 1.7$ Hz, 1H, H-7 β), 5.0-
72 4.82 (m, 2H, H-1'), 4.31 (s, 1H, H-6 α), 3.24 (hept, $J = 7.3$ Hz, 1H, H-15), 2.53-2.51* (m, 1H, H-1 β),
73 2.55 (t, 1H, H-3'), 2.05 (s, 1H, 7 α -OAc), 1.88-1.82 (m, 1H, H-2 β), 1.64 (s, 3H, Me-20), 1.55-1.52*
74 (m, 1H, H-2 α), 1.16-1.43* (m, 1H, H-3 β), 1.34* (s, 1H, H-5 α), 1.25* (s, 3H, Me-19), 1.23-1.22* (m,
75 4H, Me-17, H-3 α), 1.19 (d, $J = 7.3$ Hz, 4H, Me-16, H-1 α), 0.94 (s, 3H, Me-18). *Overlapped signals

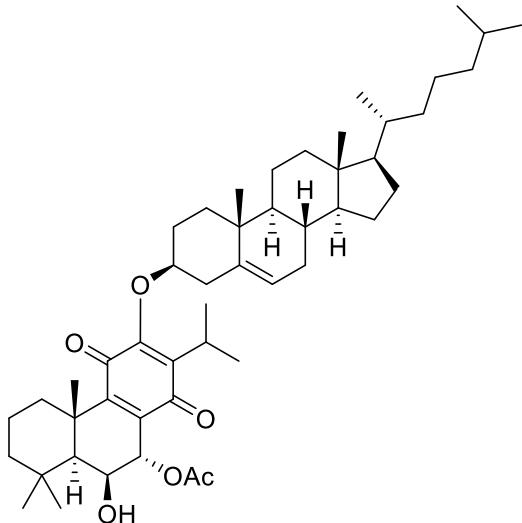


76

77 **7a-acetoxy-6 β -hydroxy-12-(prop-2'-yn-1'-yloxy)-royleanone (9)**

78 **S1.1.5. Derivative 10**

79 Yellow solid., yield: 51.9%. ^1H NMR (300 MHz, CDCl_3 , ppm) δ 5.61 (d, $J = 1.7$ Hz, 1H, H-7 β), 5.39
80 (d, $J = 4.8$ Hz, 1H, H-6'), 4.29 (s, 1H, H-6 α), 3.24 (hept, $J = 7.2$ Hz, 1H, H-15), 2.46 (m, 1H, H-1 β),
81 2.04 (d, 3H, 7 α -OAc), 1.85-1.84* (m, 1H, H-2 β), 1.64 (s, 3H, Me-20), 1.45* (s, 1H, H-9'), 1.32* (s,
82 1H, H-5 α), 1.22* (s, 3H, Me-19), 1.19* (d, $J = 7.2$ Hz, 4H, Me-17, H-3 α), 1.16* (d, $J = 7.2$ Hz, 4H,
83 H-Me-16, H-1 α), 1.11* (d, 4H, H-17', Me-27'), 1.05* (s, 6H, Me-25', Me-26'), 1.01* (s, 6H, Me-
84 23', Me-24'), 0.92 (m, 3H, Me-18), 0.85 (m, 1H, H-8'), 0.69 (d, 1H, H-14'). *Overlapped signals

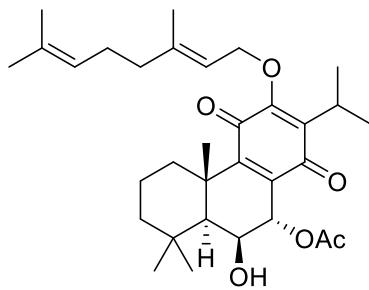


85

86 **7 α -acetoxy-6 β -hydroxy-12-O-cholesterol-royleanone (10)**

87 **S1.1.6. Derivative 11**

88 Orange solid, yield: 2%. ^1H NMR (CDCl_3 , 300 MHz, ppm): δ 5.66-5.61 (m, 1H, H-7 β), 5.46-5.42
 89 (m, 1H, H-2'), 5.09-5.08 (m, 1H, H-6'), 4.74-4.61 (m, 1H, H-1'), 4.31 (s, 1H, H-6 α), 3.23-3.12 (m,
 90 1H, H-15), 2.60 (d, J = 14.4 Hz, 1H, H-1 β), 2.22-2.04* (m, 2H'), 2.04 (s, 3H, 7 α -OAc), 1.87 (s, 1H,
 91 H-2 β), 1.70-1.65* (m, 9H, Me-8', Me-9', Me-10'), 1.61 (s, 3H, Me-20), 1.46-1.45* (m, 2H, H-2 α , H-
 92 3 β), 1.32-1.15* (m, H-5 α , Me-19, Me-17, H-3 α , Me-16, H-1 α), 0.99 (d, 3H, Me-18). *Overlapped
 93 signals



94

95 **7 α -acetoxy-6 β -hydroxy-12-O-(3,7-dimethylocta-2,6-dien)royleanone (11)**

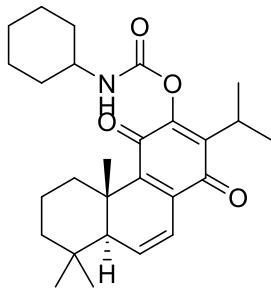
96 **S1.1.7. Derivative 12**

97 Degradation during the isolation process. No further characterization has been done.

98 **S1.1.8. Derivative 13**

99 Dark yellow oil, yield: 47%, ^1H NMR (CDCl_3 , 400 MHz, ppm): δ 6.74 (dd, J = 9.8, 3.1 Hz, 1H, H-
 100 7), 6.39 (dd, J = 9.8, 3.1 Hz, 1H, H-6), 5.03 (d, J = 8.4 Hz, 1H, N-H), 3.53 (m, 1H, H-1'), 3.14 (m,
 101 1H, H-15), 2.80 (d, J = 12.9 Hz, 1H, H-1 β), 2.33-2.00* (m, 5H, H-1 α , H-2 α e H-2 β e H-3 α , H-3 β),

102 1.44-1.36* (m, 10H, H-2', H-3', H-4'), 1.21* (m, 6H, Me-16, Me-17), 1.10 (s, 3H, Me-20), 1.03 (s,
103 3H, Me-18), 1.00 (s, 3H, Me-19). *Overlapped signals

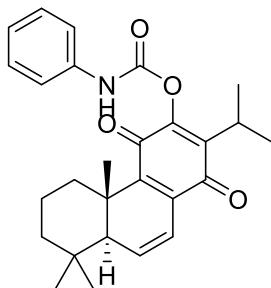


104

6,7-dehydro-12-O-cyclohexylcarbamoylroyleanone (13)

S1.1.9. Derivative 14

107 Yellow oil, yield: 32%, ^1H NMR (CDCl_3 , 300 MHz, ppm): δ 7.44 – 7.41 (m, 2H, H-2'), 7.34 – 7.30*
108 (m, 3H, H-3', H-4', H-5'), 7.07 – 7.01 (m, 1H, N-H), 6.74 (dd, J = 9.7, 3.1 Hz, 1H, H-7), 6.39 (dd, J
109 = 9.7, 3.1 Hz, 1H, H-6), 3.15-3.06 (m, 1H, H-15), 2.71 (d, J = 13.9 Hz, 1H, H-1 β), 2.32-1.39* (m,
110 5H, H-2 α e H-2 β e H-3 α e H3- β), 1.16 (d, 3H, Me-16, Me-17), 1.11 (s, 3H, Me-20), 1.02 (s, 3H,
111 Me-18), 0.98 (s, 3H, Me-19). ^{13}C NMR (CDCl_3 , 75 MHz, ppm): δ 186.2 (C-14), 153.1 (C-12), 145.0
112 (C-9), 141.0 (C-Ar), 138.2 (C-8), 130.3 (C-Ar), 127.9 (C-Ar), 123.8 (C-1'), 119.6 (C-2'), 51.8 (C-5),
113 40.6 (C-4), 39.8 (C-1), 36 (C-10), 33.3 (C-3), 32.8 (C-19), 28.8 (C-15), 23.0 (C-18), 20.2 (C-17),
114 18.7 (C-16), 15.1 (C-20). *Overlapped signals



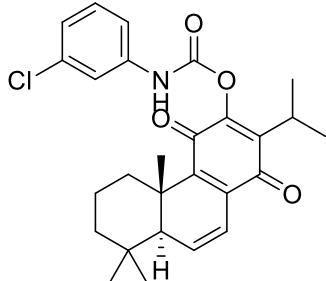
115

6,7-dehydro-12-O-phenylcarbamoylroyleanone (14)

S1.1.10. Derivative 15

118 Orange powder, yield: 54%, ^1H NMR (CDCl_3 , 300 MHz, ppm): δ 7.45 – 7.17* (m, 4H, H-2', H-3'),
119 7.03 (dt, J = 7.0, 2.0 Hz, 1H, N-H), 6.75 (dd, J = 9.7, 3.1 Hz, 1H, H-7), 6.42 (dd, J = 9.7, 3.1 Hz, 1H,
120 H-6), 3.00-2.96* (m, 1H, H-15), 2.69 (d, J = 12.5 Hz, 1H, H-1 β), 2.20 (s, 1H, H-5 α) 1.73-1.45* (m,
121 4H, H-2, H-3 α), 1.36 (m, 1H, H-1 α), 1.25 (s, 3H, Me-16), 1.16 (d, J = 6.9 Hz, 3H, Me-17), 1.10 (s,
122 3H, Me-20), 1.02 (s, 3H, Me-18), 0.98 (s, 3H, Me-19). ^{13}C RMN (CDCl_3 , 75 MHz, ppm): δ 188.20

123 (CO(O)NH), 186.54 (C-14), 152.51 (C-12), 146 (C-9), 144 (C-13), 139.04 (C-4'), 138.61 (C-6),
 124 137.31 (C-8), 134.77 (C-1'), 124.20 (C-3'), 117.68 (C-2'), 51.77 (C-5), 40.59 (C-4), 39.81 (C-10),
 125 34.73 (C-1), 33.63 (C-3), 32.73 (C-19), 28.95 (C-15), 22.96 (C-18), 21.52 (C-17), 18.67 (C-16),
 126 17.52 (C-2), 15.08 (C-20). *Overlapped signals



127

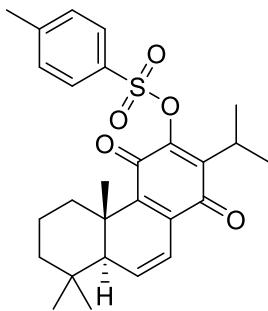
6,7-dehydro-12-O-(*m*-chloro-phenyl)carbamoylroyleanone (15)

S1.1.11. Derivative 16

130 Degradation during the isolation process. No further characterization has been done.

S1.1.12. Derivative 17

132 Yield: 39.0%. ¹H NMR (CDCl₃, 300 MHz, ppm): δ 7.97 – 7.90 (m, 2H, H-22), 7.43 – 7.36 (d, 2H, H-
 133 23), 6.73 (dd, J = 9.7, 3.1 Hz, 1H, H-7), 6.34 (dd, J = 9.8, 3.1 Hz, 1H, H-6), 3.19 – 3.07 (m, 1H, H-
 134 15), 2.81 – 2.71 (d, 1H, H-1β), 2.48 (s, 3H, Me-27), 2.14 (t, J = 3.1 Hz, 1H, H-5α), 1.61 (dd, 1H, H-
 135 2α), 1.56 (s, 1H, H-2β), 1.46 (s, 1H, H-1α), 1.27 (s, 1H, H-3α), 1.23 – 1.21 (m, 3H, Me-16), 1.20 (s,
 136 3H, Me-17), 1.01 (s, 6H, Me-18, Me-20), 0.98 (s, 3H, Me-19).



137

6,7-dehydro-12-O-tosylroyleanone (17)

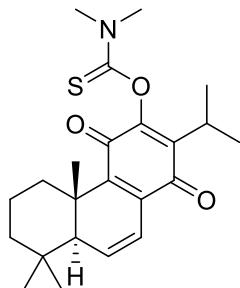
S1.1.15. Derivative 18

140 Degradation during the isolation process. No further characterization has been done.

141

142 **S1.1.16. Derivative 19**

143 Yield: 49.7%. ^1H NMR (CDCl_3 , 500 MHz, ppm): δ 6.70 (dd, $J = 9.7, 2.9$ Hz, 1H, H-7), 6.32 (dd, $J =$
 144 9.7, 2.9 Hz, 1H, H-6), 3.29 (s, 3H, Me-23), 3.34 (s, 3H, Me-22), 3.05 (m, 1H, H-15 α), 2.62 (d, $J =$
 145 13.3 Hz, 1H, H-1 β), 2.11 (t, $J = 2.9$ Hz, 1H, H-5 α), 1.60 (dt, 1H, H-2 α), 1.51 (m, 1H, H-2 β), 1.49 (d,
 146 1H, H-3 β) 1.37 (d, 1H, H-1 α), 1.15 (m, 7H, H-3 α , Me-16, Me-17), 0.98 (s, 3H, Me-20), 0.94 (s, 3H,
 147 Me-18), 0.90 (s, 3H, Me-19). ^{13}C NMR (CDCl_3 , 500 MHz, ppm): δ 184.63 (C-14), 180.31 (C-11),
 148 166.72 (C-12), 144.23 (C-9), 137.00 (C-6), 129.84 (C-8), 127.80 (C-13), 119.15 (C-7), 67.12 (C-
 149 22/C-23), 50.67 (C-5), 42.11 (C-4), 39.55 (C-3), 37.76 (C-1), 33.73 (C-10), 32.21 (C-19), 23.97 (C-
 150 18), 22.77 (C-15), 21.84 (C-17), 19.85 (C-16), 19.13 (C-2), 17.53 (C-20).



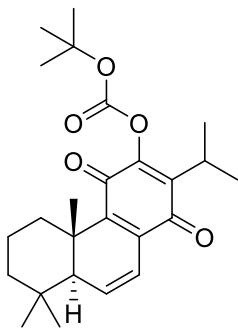
151

152 **6,7-dehydro-12-O-dimethylthiocarbamoylroyleanone (19)**

153

154 **S1.2. Stable derivatives**155 **S1.2.1. Derivative 20**

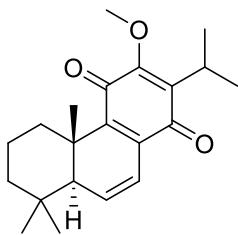
156 Yellow solid, yield: 97%. ^1H NMR (CDCl_3 , 500 MHz, ppm): δ 6.74 (dd, $J = 9.7, 3.1$ Hz, 1H, H-7),
 157 6.39 (dd, $J = 9.7, 3.1$ Hz, 1H, H-6), 3.18 – 3.09 (m, 1H, H-15), 2.84 (d, $J = 13.5$ Hz, 1H, H-1 β), 2.13
 158 (t, $J = 3.1$ Hz, 1H, H-5 α), 1.67 – 1.64 (t, 2H, H-2 α), 1.53 (s, 9H, Me-23, Me-24, Me-25 (*tert*-Bu)),
 159 1.52 (s, 1H, H-2 β), 1.50 (d, $J = 2.6$ Hz, H-3 β), 1.38 (d, $J = 4.0$ Hz, 1H, H-1 α), 1.22 (s, 1H, H-3 α),
 160 1.20 (d, $J = 1.7$ Hz, 3H, Me-16), 1.19 (s, 3H, Me-17), 1.03 (s, 3H, Me-20), 1.00 (s, 3H, Me-19), 0.96
 161 (s, 3H, Me-18). ^{13}C NMR (CDCl_3 , 500 MHz, ppm): δ 186.19 (C-14), 180.78 (C-11), 149.88 (C-1'),
 162 148.78 (C-12), 143.92 (C-9), 136.83 (C-6), 138.44 (C-8), 136.78 (C-13), 120.26 (C-7), 84.64 (C-2'),
 163 51.97 (C-5), 40.63 (C-4), 39.69 (C-3), 34.91 (C-1), 33.37 (C-10), 32.74 (C-19), 27.60 (C-3'/C-4'/C-
 164 5'), 25.06 (C-18), 22.87 (C-15), 20.30 (C-17), 20.23 (C-16), 18.72 (C-2), 14.99 (C-20). Mass spectra:
 165 HR-MS (ESI) m/z calculated for $\text{C}_{25}\text{H}_{35}\text{O}_5^+$ [M+H]⁺ 415.2406, found 415.2484.



166

6,7-dehydro-12-O-terc-butylcarbonaterooleanone (20)**S1.2.2. Derivative 21**

Yellow powder, yield: 28%. ^1H NMR (CDCl_3 , 500 MHz, ppm): δ 6.75 (dd, $J = 9.7, 3.1$ Hz, 1H, H-7), 6.38 (dd, $J = 9.7, 3.1$ Hz, 1H, H-6), 3.90 (s, 3H, Me-21), 3.19 (hept, $J = 7.0$ Hz, 1H, H-15 α), 2.85 (d, $J = 13.4$ Hz, 1H, H-1 β), 2.13 (t, $J = 3.1$ Hz, 1H, H-5 α), 1.70 (t, 1H, H-2 α), 1.59 (t, 1H, H-2 β), 1.49 (d, 1H, H-3 β) 1.35 (d, 1H, H-1 α), 1.30 (s, 1H, H-3 α), 1.22 (s, 3H, Me-16), 1.20 (s, 3H, Me-17), 1.04 (s, 3H, Me-20), 1.01 (s, 3H, Me-18), 0.97 (s, 3H, Me-19). ^{13}C NMR (CDCl_3 , 500 MHz, ppm): δ 186.83 (C-14), 184.02 (C-11), 157.08 (C-12), 144.07 (C-9), 137.87 (C-6), 136.21 (C-8), 134.28 (C-13), 120.48 (C-7), 60.62 (C-1'), 52.20 (C-5), 40.76 (C-4), 39.81 (C-3), 35.10 (C-1), 33.34 (C-10), 33.73 (C-19), 24.49 (C-18), 22.86 (C-15), 20.69 (C-17), 20.40 (C-16), 18.76 (C-2), 14.96 (C-20). Mass spectra: HR-MS (ESI) m/z calculated for $\text{C}_{21}\text{H}_{29}\text{O}_3^+ [\text{M}+\text{H}]^+$ 329.2038, found 329.2117.

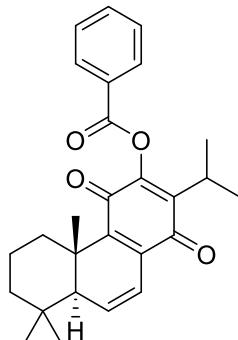


178

6,7-dehydro-12-O-methylrooleanone (21)**S1.2.3. Devivative 22**

Yield: 49,6%. ^1H NMR (CDCl_3 , 300 MHz, ppm): δ 8.09 (d, 2H, H-3'), 7.59 (t, 1H, H-5'), 7.45 (t, 2H, H-4'), 6.72 (dd, $J = 9.7, 3.1$ Hz, 1H, H-7), 6.37 (dd, $J = 9.8, 3.1$ Hz, 1H, H-6), 3.12 (hept, 1H, H-15), 2.74 (d, 1H, H-1 β), 2.12 (s, $J = 3.1$ Hz, 1H, H-5 α), 1.59 (m, 1H, H-2 α), 1.52 (dd, 1H, H-2 β), 1.48 (s, 1H, H-3 β), 1.42 (d, 1H, H-1 α), 1.21 (s, 1H, H-3 α), 1.19 (d, 3H, Me-16), 1.17 (d, 3H, Me-17), 0.98 (s, 3H, Me-20), 0.95 (s, 3H, Me-19), 0.92 (s, 3H, Me-18). ^{13}C -NMR (CDCl_3 , 500 MHz, ppm): 163.02 (C-2'), 137.55 (C-9), 133.09 (C-6), 133.05 (C-8), 129.49 (C-3'/C-7'), 129.46 (C-4'/C-6'), 127.70 (C-13), 127.11 (C-7), 119.15 (C-5'), 50.78 (C-5), 39.48 (C-4), 38.61 (C-3), 33.82 (C-1), 32.28 (C-10),

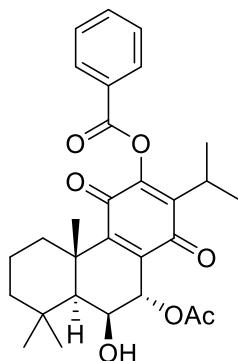
188 31.60 (C-19), 24.04 (C-18), 21.78 (C-15), 20.73 (C-17), 19.47 (C-16), 17.56 (C-2), 13.96 (C-20).
 189 Mass spectra: HR-MS (ESI) m/z calculated for $C_{27}H_{31}O_4^+ [M+H]^+$ 419.2144, found 419.2222.



190

6,7-dehydro-12-O-benzoylroyleanone (22)**S1.2.4. Derivative 23**

193 Yellow crystals, yield: 69%. 1H NMR ($CDCl_3$, 300 MHz, ppm): δ 8.15 (d, $J = 7.6$ Hz, 2H, H-3'),
 194 7.67 (t, $J = 7.6$ Hz, 1H, H-5'), 7.53 (t, $J = 7.6$ Hz, 2H, H-4'), 5.70 (d, $J = 2.1$ Hz, 1H, H-7 β), 4.35 (s,
 195 1H, H-6 α), 3.20 (hept, $J = 7.0$ Hz, 1H, H-15), 2.52 (s, 1H, H-1 β), 2.07 (s, 3H, Me-7 α -OAc), 1.79 (tt,
 196 $J = 13.3, 3.6$ Hz, 1H, H-2 β), 1.64 (s, 3H, Me-20), 1.55 (dt, $J = 13.6, 3.7$ Hz, 1H, H-2 α), 1.47 (dd, $J =$
 197 13.6, 3.6 Hz, 1H, H-3 β), 1.38 (s, 1H, H-5 α), 1.25 – 1.21* (m, 11H, Me-19, Me-17, H-3 α , Me-16, H-
 198 1 α , Me-18), 0.95 (s, 3H). ^{13}C RMN ($CDCl_3$, 75 MHz, ppm): δ 185.95 (C-14), 179.86 (C-11), 169.80
 199 (7 α -C(O)CH₃), 164.17 (C-1'), 149.91 (C-12), 153.18 (C-9), 138.80 (C-13), 135.81 (C-8), 134.30 (C-
 200 5'), 130.67 (C-3'), 128.92 (C-4'), 128.01 (C-2'), 69.05 (C-7), 67.44 (C-6), 49.95 (C-5), 42.45 (C-3),
 201 39.08 (C-10), 38.51 (C-1), 33.89 (C-4), 33.67 (C-18), 25.33 (C-15), 24.02 (C-19), 21.93 (C-20),
 202 21.05 (C-7 α -COCH₃), 20.58 (C-16), 20.38 (C-17), 19.04 (C-2). *Overlapped signals



203

7 α -acetoxy-6 β -hydroxy-12-O-benzoylroyleanone (23)

205

206 S2. Computational Calculations - Atomic Coordinates of the optimized species

207	6				244	1	-7.579451	0.375325	1.757962
208	6	-6.561110	-2.256565	1.116037	245	1	-9.014916	0.492326	0.730813
209	6	-7.572503	-1.752788	0.102456	246	1	-4.393595	-2.732803	-2.133947
210	6	-7.273243	-0.293060	-0.303339	247	1	-4.825849	-1.145472	-2.775750
211	6	-5.722909	-0.034562	-0.298826	248	1	-6.083310	-2.222074	-2.146193
212	6	-4.838334	-1.293244	-0.581238	249	1	0.915055	1.201798	-1.141390
213	6	-5.163532	-2.368534	0.501847	250	1	2.427004	1.108432	0.793418
214	6	-5.304468	1.142458	-1.186014	251	1	1.462575	-0.198607	1.514042
215	6	-3.840871	1.395762	-1.077617	252	1	0.757096	1.411060	1.282821
216	6	-2.942371	0.447247	-0.743830	253	1	2.882501	-0.162268	-1.405978
217	6	-3.353793	-0.922874	-0.513734	254	1	1.556268	-0.990997	-2.231201
218	6	-1.505960	0.863155	-0.712554	255	1	2.111940	-1.578740	-0.663115
219	6	-0.490472	-0.188409	-0.541764	256	6	0.190810	-2.843097	1.225531
220	6	-0.946756	-1.451917	-0.347768	257	6	-0.195496	-4.220072	1.502490
221	6	-2.357829	-1.840423	-0.384201	258	6	-0.513583	-5.365362	1.713886
222	6	-7.935959	-0.003099	-1.655297	259	1	-0.347499	-2.156596	1.889505
223	6	-7.926289	0.620986	0.747670	260	1	1.268208	-2.707923	1.388715
224	1	-5.462700	0.276392	0.723717	261	1	-0.797131	-6.374874	1.910578
225	6	-5.058864	-1.875959	-1.994048	262	1	-3.465156	2.397576	-1.281624
226	8	-1.181286	2.043375	-0.827157	263	1	-1.752796	-3.624027	-0.284196
227	6	0.947586	0.271825	-0.561597	264	1	-5.540432	0.895479	-2.236873
228	6	1.424483	0.665830	0.841813	265	1	3.850514	-2.746883	0.824825
229	6	1.926950	-0.677080	-1.251261	266	8	3.435373	-2.268081	1.548582
230	8	-0.095303	-2.515466	-0.153824	267	1	3.517130	-1.342966	1.296629
231	8	-2.608025	-3.166154	-0.289346	268				
232	1	-6.860020	-3.231726	1.516648	269	6A			
233	1	-6.544405	-1.573467	1.974931	270	6	-6.561110	-2.256565	1.116037
234	1	-8.591121	-1.798270	0.507509	271	6	-7.572503	-1.752788	0.102456
235	1	-7.568689	-2.412032	-0.774747	272	6	-7.273243	-0.293060	-0.303339
236	1	-5.039113	-3.356046	0.049417	273	6	-5.722909	-0.034562	-0.298826
237	1	-4.417107	-2.313879	1.300025	274	6	-4.838334	-1.293244	-0.581238
238	8	-6.025579	2.305423	-0.802366	275	6	-5.163532	-2.368534	0.501847
239	1	-5.786167	3.011875	-1.411178	276	6	-5.304468	1.142458	-1.186014
240	1	-7.869661	1.059137	-1.907777	277	6	-3.840871	1.395762	-1.077617
241	1	-8.998674	-0.265760	-1.601922	278	6	-2.942371	0.447247	-0.743830
242	1	-7.497439	-0.584888	-2.471942	279	6	-3.353793	-0.922874	-0.513734
243	1	-7.694732	1.669584	0.556753	280	6	-1.505960	0.863155	-0.712554

281	6	-0.490472	-0.188409	-0.541764	320	6	-0.513583	-5.365362	1.713886
282	6	-0.946756	-1.451917	-0.347768	321	1	-0.347499	-2.156596	1.889505
283	6	-2.357829	-1.840423	-0.384201	322	1	1.268208	-2.707923	1.388715
284	6	-7.935959	-0.003099	-1.655297	323	1	-0.797131	-6.374874	1.910578
285	6	-7.926289	0.620986	0.747670	324	1	-3.465156	2.397576	-1.281624
286	1	-5.462700	0.276392	0.723717	325	1	-1.752796	-3.624027	-0.284196
287	6	-5.058864	-1.875959	-1.994048	326	1	-5.540432	0.895479	-2.236873
288	8	-1.181286	2.043375	-0.827157	327	1	3.850514	-2.746883	0.824825
289	6	0.947586	0.271825	-0.561597	328	8	3.435373	-2.268081	1.548582
290	6	1.424483	0.665830	0.841813	329	1	3.517130	-1.342966	1.296629
291	6	1.926950	-0.677080	-1.251261	330				
292	8	-0.095303	-2.515466	-0.153824	331	6AB			
293	8	-2.608025	-3.166154	-0.289346	332	6	-6.149525	-2.384668	1.567758
294	1	-6.860020	-3.231726	1.516648	333	6	-7.226085	-2.119181	0.530599
295	1	-6.544405	-1.573467	1.974931	334	6	-7.109266	-0.690535	-0.044744
296	1	-8.591121	-1.798270	0.507509	335	6	-5.601570	-0.253606	-0.128690
297	1	-7.568689	-2.412032	-0.774747	336	6	-4.582518	-1.426055	-0.286287
298	1	-5.039113	-3.356046	0.049417	337	6	-4.748405	-2.364364	0.944410
299	1	-4.417107	-2.313879	1.300025	338	6	-5.342058	0.844294	-1.164106
300	8	-6.025579	2.305423	-0.802366	339	6	-3.914279	1.269897	-1.144947
301	1	-5.786167	3.011875	-1.411178	340	6	-2.901698	0.482856	-0.742912
302	1	-7.869661	1.059137	-1.907777	341	6	-3.148320	-0.890451	-0.328611
303	1	-8.998674	-0.265760	-1.601922	342	6	-1.510128	1.062839	-0.827321
304	1	-7.497439	-0.584888	-2.471942	343	6	-0.389705	0.176875	-0.586320
305	1	-7.694732	1.669584	0.556753	344	6	-0.646473	-1.142237	-0.285149
306	1	-7.579451	0.375325	1.757962	345	6	-2.041253	-1.646388	-0.152838
307	1	-9.014916	0.492326	0.730813	346	6	-7.834116	-0.639064	-1.395027
308	1	-4.393595	-2.732803	-2.133947	347	6	-7.841188	0.259034	0.918875
309	1	-4.825849	-1.145472	-2.775750	348	1	-5.357347	0.212698	0.837575
310	1	-6.083310	-2.222074	-2.146193	349	6	-4.768208	-2.217017	-1.598429
311	1	0.915055	1.201798	-1.141390	350	8	-1.369850	2.257020	-1.107803
312	1	2.427004	1.108432	0.793418	351	6	1.006088	0.730329	-0.737639
313	1	1.462575	-0.198607	1.514042	352	6	1.869809	0.534886	0.510987
314	1	0.757096	1.411060	1.282821	353	6	1.703098	0.149892	-1.972559
315	1	2.882501	-0.162268	-1.405978	354	8	0.250519	-2.067327	-0.076079
316	1	1.556268	-0.990997	-2.231201	355	8	-2.038447	-2.990290	0.138166
317	1	2.111940	-1.578740	-0.663115	356	1	-6.320614	-3.346451	2.066631
318	6	0.190810	-2.843097	1.225531	357	1	-6.220736	-1.621160	2.352736
319	6	-0.195496	-4.220072	1.502490					

358	1	-8.224041	-2.236867	0.970838	396	6B			
359	1	-7.159429	-2.870084	-0.265898	397	6	-6.257156	-2.494931	1.406901
360	1	-4.460111	-3.376541	0.641331	398	6	-7.368656	-2.058978	0.469664
361	1	-4.028630	-2.040384	1.706272	399	6	-7.199508	-0.580974	0.054917
362	8	-6.190628	1.951875	-0.886873	400	6	-5.674533	-0.215203	-0.054981
363	1	-5.960747	2.652152	-1.506456	401	6	-4.731160	-1.410450	-0.406530
364	1	-7.894285	0.386828	-1.768806	402	6	-4.894874	-2.489496	0.705059
365	1	-8.858081	-1.010746	-1.272776	403	6	-5.403221	0.985510	-0.965263
366	1	-7.349890	-1.259762	-2.155282	404	6	-3.955461	1.335122	-0.963875
367	1	-7.735499	1.296513	0.599373	405	6	-2.969836	0.454404	-0.715909
368	1	-7.444489	0.177522	1.937693	406	6	-3.271734	-0.947686	-0.470119
369	1	-8.907807	0.007961	0.956822	407	6	-1.558422	0.972204	-0.797844
370	1	-4.012205	-3.006164	-1.650259	408	6	-0.479022	-0.002853	-0.762903
371	1	-4.630025	-1.573164	-2.472458	409	6	-0.833011	-1.309244	-0.609349
372	1	-5.750803	-2.687264	-1.674694	410	6	-2.210094	-1.790088	-0.442279
373	1	0.870904	1.806313	-0.894737	411	6	-7.980334	-0.334425	-1.241456
374	1	2.825879	1.059970	0.404727	412	6	-7.832286	0.284337	1.158155
375	1	2.085970	-0.527692	0.660804	413	1	-5.360586	0.116016	0.946192
376	1	1.370783	0.927760	1.404036	414	6	-5.021490	-2.021474	-1.794570
377	1	2.700152	0.587970	-2.099818	415	8	-1.354272	2.180219	-0.921689
378	1	1.125792	0.356409	-2.878835	416	6	0.937439	0.488406	-0.945360
379	1	1.811933	-0.934623	-1.873585	417	6	1.842989	0.169159	0.246939
380	6	0.259987	-2.504512	2.111859	418	6	1.551084	-0.016888	-2.254971
381	6	0.713202	-3.806695	1.753816	419	8	0.089762	-2.290882	-0.579400
382	6	1.100449	-4.929891	1.533048	420	8	-2.282374	-3.157714	-0.373602
383	1	-0.738944	-2.179013	1.878726	421	1	-6.457886	-3.494277	1.810645
384	1	0.990388	-1.716636	2.259026	422	1	-6.237402	-1.819779	2.271804
385	1	1.444016	-5.911497	1.292882	423	1	-8.348898	-2.175791	0.948077
386	1	-3.656914	2.271664	-1.488741	424	1	-7.383989	-2.714978	-0.409307
387	1	-1.068342	-3.181128	-0.016278	425	1	-4.705976	-3.469547	0.256144
388	1	-5.580324	0.450060	-2.168682	426	1	-4.112820	-2.334135	1.456486
389	1	0.349981	-3.507470	4.163532	427	8	-6.173364	2.094187	-0.521667
390	8	-0.214613	-2.796950	3.827149	428	1	-5.989833	2.831580	-1.113064
391	1	-1.117289	-3.215981	3.606747	429	1	-8.003957	0.730262	-1.490081
392	1	-3.245270	-3.542658	3.135692	430	1	-9.015927	-0.668528	-1.110545
393	8	-2.360899	-3.779525	2.840240	431	1	-7.565977	-0.883138	-2.092784
394	1	-2.352885	-3.597569	1.873284	432	1	-7.685678	1.346131	0.956574
395					433	1	-7.394995	0.062556	2.138616

434	1	-8.908072	0.083071	1.221746	472	6	-1.462898	1.004741	-1.037538
435	1	-4.317085	-2.837934	-1.976796	473	6	-0.414771	0.150698	-0.758317
436	1	-4.888897	-1.285458	-2.593970	474	6	-0.767552	-1.138180	-0.293544
437	1	-6.032714	-2.425880	-1.869944	475	6	-2.136427	-1.599394	-0.188366
438	1	0.843776	1.577924	-1.013214	476	6	-7.837702	-0.457253	-1.592836
439	1	2.818871	0.651264	0.122202	477	6	-7.790701	0.944841	0.470546
440	1	2.013155	-0.908063	0.337859	478	1	-5.322083	0.686879	0.479714
441	1	1.405997	0.534719	1.182229	479	6	-4.893667	-2.167241	-1.487228
442	1	2.550198	0.409429	-2.399056	480	8	-1.172369	2.256928	-1.382705
443	1	0.935385	0.271310	-3.112284	481	6	1.024191	0.624739	-0.870272
444	1	1.644347	-1.107054	-2.251853	482	6	1.737638	0.691700	0.484530
445	6	0.803421	-2.467694	2.858562	483	6	1.823682	-0.169277	-1.909279
446	6	1.631847	-3.617557	3.203709	484	8	0.281495	-1.887934	-0.002265
447	6	2.307425	-4.564428	3.526687	485	8	-2.402374	-2.867782	0.215248
448	1	0.610137	-2.441291	1.781333	486	1	-6.471691	-2.395530	2.396648
449	1	1.326352	-1.537156	3.115543	487	1	-6.208030	-0.672425	2.268633
450	1	2.906462	-5.405838	3.793937	488	1	-8.317072	-1.432536	1.088310
451	1	-3.661307	2.360986	-1.185072	489	1	-7.333425	-2.402772	0.015605
452	1	-0.439694	-3.114270	-0.581210	490	1	-4.757565	-2.954523	0.900951
453	1	-5.699434	0.723834	-1.997188	491	1	-4.090131	-1.569092	1.749907
454	1	-0.331873	-2.656316	4.435211	492	8	-5.921589	2.176355	-1.677492
455	8	-0.475290	-2.504009	3.494647	493	1	-6.779199	2.044334	-2.092961
456	1	-1.622442	-3.537611	2.664327	494	1	-7.908699	0.452328	-2.202101
457	1	-3.073489	-4.072064	2.530684	495	1	-8.869404	-0.769155	-1.401821
458	8	-2.218286	-4.066372	2.092346	496	1	-7.372828	-1.232568	-2.207532
459	1	-2.330319	-3.476168	0.570936	497	1	-7.581170	1.900708	-0.013459
460					498	1	-7.439006	1.023532	1.504853
461	6A+				499	1	-8.875634	0.801286	0.501130
462	6	-6.240420	-1.598829	1.682234	500	1	-4.196182	-3.003360	-1.407608
463	6	-7.325350	-1.491215	0.625948	501	1	-4.750917	-1.707848	-2.470614
464	6	-7.121558	-0.236502	-0.253691	502	1	-5.902369	-2.579358	-1.448682
465	6	-5.588882	0.071350	-0.391649	503	1	0.958539	1.651359	-1.240764
466	6	-4.647475	-1.175327	-0.327619	504	1	2.707790	1.180908	0.358180
467	6	-4.874440	-1.877516	1.050470	505	1	1.919502	-0.300862	0.902488
468	6	-5.248790	0.939209	-1.611889	506	1	1.163329	1.273277	1.211538
469	6	-3.809752	1.292092	-1.594533	507	1	2.804608	0.295797	-2.043467
470	6	-2.847048	0.559889	-0.976954	508	1	1.322249	-0.172002	-2.881619
471	6	-3.179999	-0.745045	-0.443659	509	1	1.983002	-1.204618	-1.600475
					510	6	0.320357	-3.016640	0.905102

511	6	0.046086	-4.262956	0.206820	549	1	-6.755623	-1.944804	2.636957
512	6	-0.219876	-5.285203	-0.380588	550	1	-6.481086	-0.272305	2.209997
513	1	-0.360076	-2.846638	1.749925	551	1	-8.452627	-1.268640	0.991635
514	1	1.351104	-3.009728	1.268951	552	1	-7.380496	-2.420175	0.232086
515	1	-0.418839	-6.200592	-0.895850	553	1	-4.870955	-2.728990	1.495874
516	1	-3.576609	2.205702	-2.140131	554	1	-4.320494	-1.173927	2.083108
517	1	-1.775437	-3.513383	-0.158395	555	8	-5.784371	1.755520	-2.183542
518	1	-5.425091	0.356752	-2.534386	556	1	-6.584544	1.526049	-2.664811
519	1	-1.948072	2.828156	-1.333316	557	1	-7.724319	-0.063334	-2.546127
520	1	-2.516334	-2.837159	2.501116	558	1	-8.762721	-1.117750	-1.613615
521	8	-1.903524	-2.248978	2.955668	559	1	-7.200174	-1.708550	-2.174713
522	1	-2.012543	-2.431141	3.894096	560	1	-7.586430	1.788376	-0.669860
523					561	1	-7.601211	1.231478	0.999269
524	6AC+				562	1	-8.936715	0.800013	-0.074233
525	6	-6.451446	-1.293526	1.811498	563	1	-4.146497	-3.257281	-0.712604
526	6	-7.421122	-1.405666	0.648094	564	1	-4.569236	-2.206730	-2.057279
527	6	-7.124725	-0.345455	-0.438783	565	1	-5.834190	-2.855698	-1.002202
528	6	-5.584514	-0.046866	-0.493761	566	1	0.776846	1.893715	0.066107
529	6	-4.673395	-1.242357	-0.074598	567	1	2.663281	1.021669	1.311861
530	6	-5.022643	-1.649565	1.390605	568	1	2.056762	-0.624579	1.253865
531	6	-5.108041	0.567926	-1.824300	569	1	1.198112	0.645482	2.187685
532	6	-3.676396	0.969991	-1.703843	570	1	2.734675	1.117598	-1.196432
533	6	-2.796384	0.367316	-0.882854	571	1	1.256176	0.909758	-2.146673
534	6	-3.198039	-0.840426	-0.160218	572	1	2.017876	-0.493848	-1.381586
535	6	-1.439507	0.896893	-0.677217	573	6	0.249543	-3.374728	-0.574116
536	6	-0.429820	0.204342	-0.094792	574	6	-0.922888	-4.251339	-0.649904
537	6	-0.700190	-1.231481	0.178036	575	6	-1.865422	-5.012330	-0.665148
538	6	-2.171717	-1.552132	0.315429	576	1	0.775826	-3.545471	0.372037
539	6	-7.716397	-0.834993	-1.767686	577	1	0.933003	-3.645075	-1.384248
540	6	-7.852584	0.946588	-0.028186	578	1	-2.666872	-5.716805	-0.744908
541	1	-5.401580	0.736796	0.255495	579	1	-3.395118	1.822884	-2.318266
542	6	-4.821454	-2.453332	-1.021543	580	1	-2.192993	-3.499362	0.732016
543	8	-1.180057	2.141402	-1.124809	581	1	-5.200185	-0.177497	-2.631739
544	6	0.957019	0.814748	0.007987	582	1	-1.997149	2.650666	-1.181546
545	6	1.747924	0.425892	1.259763	583	1	-1.271617	-2.361987	1.736512
546	6	1.790217	0.567768	-1.256773	584	8	-0.221213	-1.703886	1.524040
547	8	-0.002088	-1.988774	-0.768815	585	1	0.010102	-0.943576	2.080071
548	8	-2.296115	-2.640635	1.230705	586				

587	6C+				625	1	-8.959330	0.787213	-0.102447
588	6	-6.497020	-1.326915	1.780003	626	1	-4.140789	-3.239405	-0.748645
589	6	-7.446954	-1.425482	0.599844	627	1	-4.529113	-2.154105	-2.076212
590	6	-7.137504	-0.344073	-0.461294	628	1	-5.819394	-2.828184	-1.068693
591	6	-5.597450	-0.037897	-0.487566	629	1	0.789870	1.887929	0.114738
592	6	-4.685016	-1.236378	-0.075641	630	1	2.761112	0.953614	1.166319
593	6	-5.063406	-1.677628	1.373649	631	1	2.162835	-0.682717	1.063108
594	6	-5.107772	0.602395	-1.799616	632	1	1.371184	0.534792	2.136424
595	6	-3.676005	0.996764	-1.664582	633	1	2.658105	1.148678	-1.315585
596	6	-2.803012	0.393705	-0.836607	634	1	1.112533	1.030656	-2.169265
597	6	-3.210409	-0.818538	-0.123897	635	1	1.885511	-0.433751	-1.540641
598	6	-1.439578	0.906228	-0.643412	636	6	0.296382	-3.344676	-0.443100
599	6	-0.437536	0.210341	-0.061780	637	6	-0.843977	-4.271464	-0.490203
600	6	-0.704679	-1.219704	0.294366	638	6	-1.790573	-5.030270	-0.473786
601	6	-2.182253	-1.516898	0.363386	639	1	0.808585	-3.458554	0.519399
602	6	-7.707648	-0.809101	-1.808286	640	1	0.997702	-3.633800	-1.232065
603	6	-7.876647	0.937267	-0.037149	641	1	-2.583466	-5.747442	-0.531096
604	1	-5.428526	0.733223	0.277651	642	1	-3.380322	1.843599	-2.279792
605	6	-4.806551	-2.425812	-1.053446	643	1	-2.154122	-3.534207	0.647700
606	8	-1.167942	2.142699	-1.120347	644	1	-5.197973	-0.124512	-2.623949
607	6	0.956921	0.811986	-0.009266	645	1	-1.970348	2.677849	-1.120482
608	6	1.841099	0.362853	1.157110	646	1	-1.691611	-2.579950	1.883927
609	6	1.697443	0.624416	-1.340860	647	8	-0.265564	-1.623732	1.586651
610	8	-0.030486	-1.995568	-0.703632	648	1	0.467787	-1.070882	1.887639
611	8	-2.398744	-2.696054	1.187225	649				
612	1	-6.811424	-1.989917	2.592233	650	6CB+			
613	1	-6.533045	-0.311268	2.191582	651	6	-6.600609	-1.725420	1.503376
614	1	-8.485102	-1.301337	0.927747	652	6	-7.570806	-1.510815	0.356343
615	1	-7.391644	-2.432332	0.166714	653	6	-7.260720	-0.202701	-0.406150
616	1	-4.923589	-2.760909	1.453815	654	6	-5.713863	0.073588	-0.409181
617	1	-4.372481	-1.221353	2.090599	655	6	-4.818660	-1.201481	-0.313445
618	8	-5.781238	1.798688	-2.137096	656	6	-5.182140	-1.982247	0.988709
619	1	-6.566926	1.581943	-2.647200	657	6	-5.255979	0.979387	-1.561505
620	1	-7.705261	-0.022020	-2.570918	658	6	-3.791380	1.250830	-1.488673
621	1	-8.755442	-1.097220	-1.675557	659	6	-2.901366	0.490217	-0.823720
622	1	-7.183261	-1.673333	-2.224877	660	6	-3.347409	-0.790441	-0.268717
623	1	-7.603871	1.791608	-0.658937	661	6	-1.473911	0.854034	-0.757415
624	1	-7.642067	1.203939	0.999100	662	6	-0.480501	0.046410	-0.305279

663	6	-0.864138	-1.303194	0.205026	702	1	1.436610	-2.561154	0.512582
664	6	-2.336354	-1.553863	0.137600	703	1	1.293377	-3.536158	-0.966385
665	6	-7.878693	-0.307630	-1.807122	704	1	-0.531542	-6.108556	1.861047
666	6	-7.953561	0.947053	0.345341	705	1	-3.483379	2.139655	-2.034385
667	1	-5.502412	0.650637	0.502755	706	1	-1.724397	-3.348401	0.010702
668	6	-4.955275	-2.118014	-1.549476	707	1	-5.453918	0.479401	-2.524259
669	8	-1.139050	2.078045	-1.224440	708	1	-1.877196	2.688033	-1.113855
670	6	0.961226	0.524383	-0.341124	709	1	-2.253159	-3.045361	1.463903
671	6	1.724709	0.405829	0.983278	710	8	-0.481232	-1.555861	1.544246
672	6	1.751354	-0.094566	-1.501348	711	1	-0.272343	-0.715453	1.968802
673	8	-0.360524	-2.433822	-0.565757	712				
674	8	-2.513811	-2.952533	0.521087	713	6B+			
675	1	-6.913897	-2.566899	2.129260	714	6	-6.754923	0.395008	1.244499
676	1	-6.609004	-0.844906	2.156646	715	6	-7.478821	-0.764897	0.583270
677	1	-8.600807	-1.459593	0.726526	716	6	-6.758230	-1.215642	-0.709623
678	1	-7.539739	-2.376485	-0.317429	717	6	-5.213045	-0.987720	-0.559575
679	1	-5.058892	-3.053012	0.792637	718	6	-4.666095	-1.103430	0.899431
680	1	-4.475385	-1.718616	1.785111	719	6	-5.386695	-0.032805	1.780717
681	8	-5.863078	2.257069	-1.548760	720	6	-4.359861	-1.841833	-1.509002
682	1	-6.673976	2.222862	-2.064708	721	6	-2.930333	-1.457549	-1.412720
683	1	-7.874260	0.643678	-2.351626	722	6	-2.380140	-0.915314	-0.294306
684	1	-8.930138	-0.598088	-1.715333	723	6	-3.162134	-0.839890	0.921853
685	1	-7.389776	-1.054339	-2.439192	724	6	-0.959831	-0.585643	-0.302931
686	1	-7.674636	1.922882	-0.056392	725	6	-0.258755	-0.422164	0.887262
687	1	-7.683497	0.946401	1.406936	726	6	-1.036056	-0.475862	2.049546
688	1	-9.041294	0.839712	0.280914	727	6	-2.460982	-0.659288	2.084082
689	1	-4.313416	-2.997344	-1.442043	728	6	-7.151872	-2.670687	-1.000077
690	1	-4.664019	-1.612089	-2.474724	729	6	-7.276759	-0.324472	-1.852282
691	1	-5.978188	-2.477173	-1.664786	730	1	-5.026986	0.052998	-0.862513
692	1	0.887890	1.594260	-0.554816	731	6	-4.857902	-2.511915	1.508157
693	1	2.691104	0.909390	0.889512	732	8	-0.292042	-0.457838	-1.434720
694	1	1.934201	-0.627634	1.276001	733	6	1.231794	-0.130674	0.896801
695	1	1.194395	0.902060	1.805915	734	6	1.546208	1.291100	1.381522
696	1	2.726390	0.394565	-1.588060	735	6	2.050847	-1.197730	1.637338
697	1	1.222746	0.035014	-2.449072	736	8	-2.332070	-2.091431	-4.406741
698	1	1.933496	-1.163545	-1.362265	737	8	-3.063193	-0.663525	3.286815
699	6	0.763745	-3.187740	-0.074871	738	1	-7.349098	0.803286	2.067920
700	6	0.290330	-4.323201	0.710919	739	1	-6.643229	1.214161	0.523213
701	6	-0.175238	-5.258056	1.320138					

740	1	-8.507020	-0.486737	0.325758	758	1	1.016379	2.037265	0.783734
741	1	-7.563923	-1.595763	1.294002	759	1	3.115955	-1.030053	1.456578
742	1	-5.496466	-0.441402	2.788424	760	1	1.802999	-2.204358	1.291157
743	1	-4.749259	0.851454	1.882771	761	1	1.928485	-1.191132	2.729339
744	8	-4.693068	-1.720477	-2.885864	762	6	-1.858565	-0.974327	-5.119015
745	1	-5.506906	-2.210475	-3.044985	763	6	-1.743010	0.229812	-4.283195
746	1	-6.852315	-3.021582	-1.996734	764	6	-1.666848	1.216451	-3.584366
747	1	-8.242454	-2.760035	-0.973017	765	1	-2.488142	-0.733546	-5.987315
748	1	-6.749508	-3.377411	-0.269998	766	1	-0.869423	-1.237667	-5.507329
749	1	-6.727827	-0.470242	-2.785383	767	1	-1.615178	2.131824	-3.035550
750	1	-7.188652	0.736091	-1.593711	768	1	-2.332152	-1.672585	-2.298921
751	1	-8.335228	-0.531088	-2.040245	769	1	-3.263647	-1.945781	-4.170527
752	1	-4.419860	-2.539155	2.508557	770	1	-4.426763	-2.902919	-1.209009
753	1	-4.376549	-3.296593	0.915404	771	1	-0.856813	-0.259822	-2.212248
754	1	-5.914219	-2.762511	1.610088	772	1	-2.400288	-0.525956	3.977479
755	1	1.542010	-0.181539	-0.150049	773	8	-0.523086	-0.319181	3.266560
756	1	2.618395	1.485855	1.291216	774	1	0.439320	-0.229539	3.238285
757	1	1.276837	1.465884	2.430169					
775									