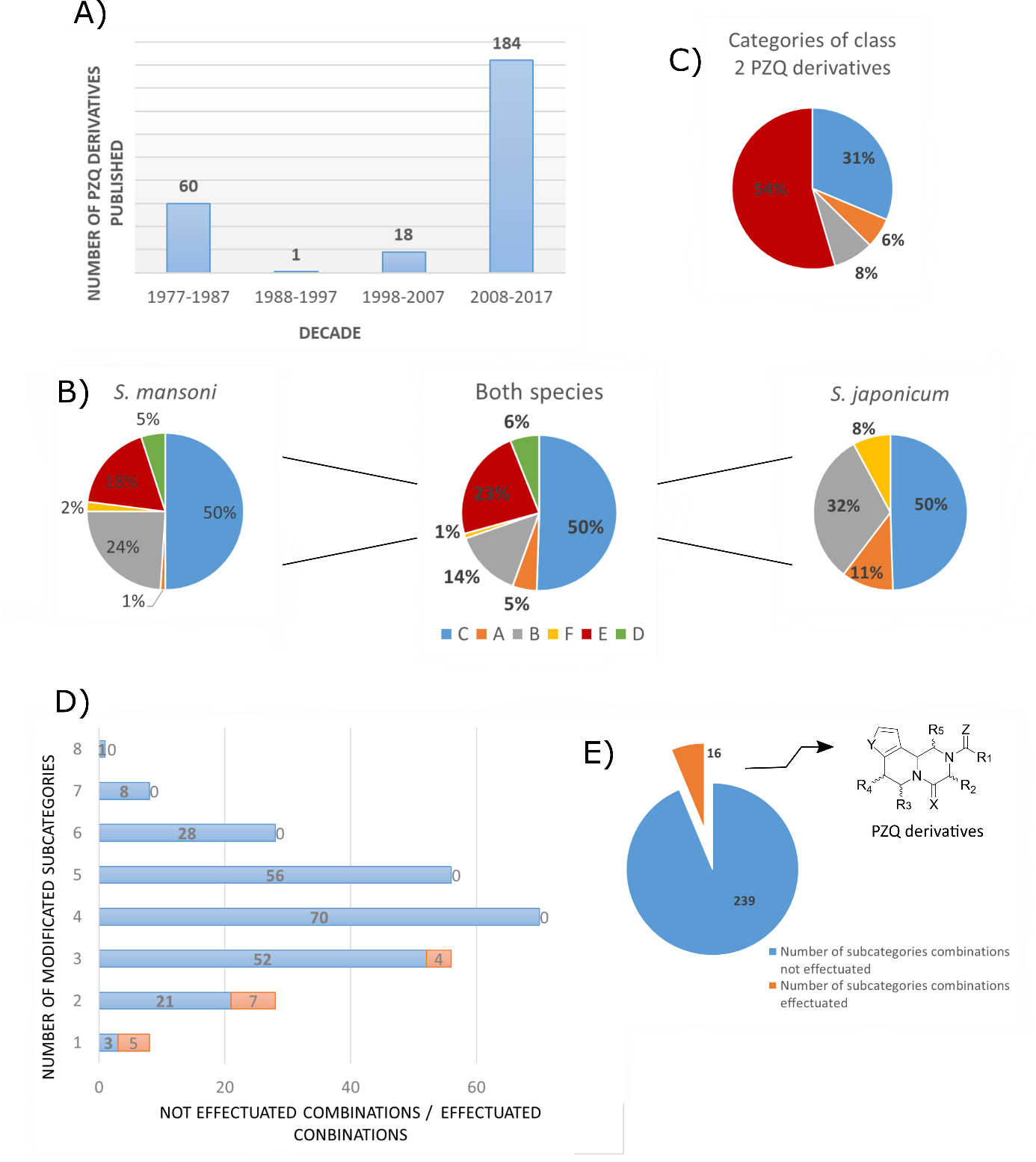
**Could we Expect New Praziquantel Derivatives? A Meta Pharmacometrics/Pharmacoinformatics Analysis of all Antischistosomal Praziquantel Derivatives Found in the Literature**

**SUPPORTING INFORMATION**

Vinícius Barros Ribeiro da Silvaa,b\*, Benjamin Boucherlea, Brice Hoffmanc, Jonathan El Methnid, Anekécia Lauro da Silvae, Antoine Fortunea, Maria Carmo Alves de Limab,Aline Thomasa

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Table**. S1 Structure of all derivatives used in the article; original reference; original name and name used on our paper. Biological activities were measured according to different protocols. Original value of biological activity (**a** = Killing 25 mM 72h by Wang *et al.*, 2013a, **b** = Killing 25 mM 72h by Wang *et al.*, 2013b; **c** = Killing 100 M 24 h by Zheng *et al.*, 2014; **d** = EC50 [M] by Sharma *et al.*, 2014; **e** = EC50 [M] by Liu *et al.*, 2012; **f** = 90% Lethal conc [µM] by Sadhu *et al.*, 2012; **g** = EC50 [M] and EC100 [M] by Kamel *et al.*, 2012; **h** = Mortality single 500 mg/kg dose by Dong *et al.*, 2010; **i** = EC100 [M] by Ronketti *et al.*, 2007; **j** = Mortality single 500 mg/kg dose by Abo-Ghalia and Soliman, 2001; **k** = Mortality single 500 mg/kg dose Abo-Ghalia and Soliman, 2000); class of activity used in our study; specie of the parasite used to test the molecules (J = *Schistosoma japonicum*, M = *Schistoma mansoni*). \*Repeated molecules; \*\* Two times repeated. **ts1** = molecules from training set model 1; **ts2** = molecules from training set model 2. | | | | | | | |
| **Structure** | **Reference** | **Original Name** | | **Name on the Article** | **Biological Activity** | **Class of Activity** | **Specie** |
|  |  | **PZQ** | | **PZQ** | 62.5 % **a**; 100 % **b**; 100 % **c**; 0.5 µM **d**; 0.37 M **e**; 3 M **f**; 0.5< and 10 M **g**; 98 % **h**; 3 µM**i**; 90 % **j. k** | 2 | J and M |
|  | Wang *et al.*. 2013a | **1** | | **1** | 0 % **a** | 0 | J |
|  | Wang *et al.*. 2013a | **2** | | **2\*** | 0 % **a** | 0 | J |
|  | Wang *et al.*. 2013a | **3** | | **3** | 10 %**a** | 1 | J |
|  | Wang *et al.*. 2013a | **4** | | **4\* ts2** | 50 %**a** | 1 | J |
|  | Wang *et al.*. 2013a | **5** | | **5\*** | 0 %**a** | 0 | J |
|  | Wang *et al.*. 2013a | **6** | | **6** | 0 %**a** | 0 | J |
|  | Wang *et al.*. 2013a | **7** | | **7** | 100 %**a** | 2 | J |
|  | Wang *et al.*. 2013a | **8** | | **8** | 0 %**a** | 0 | J |
|  | Wang *et al.*. 2013a | **9** | | **9\*\*** | 87.5 %**a** | 1 | J |
|  | Wang *et al.*. 2013a | **10** | | **10** | 0 %**a** | 0 | J |
|  | Wang *et al.*. 2013a | **11** | | **11** | 62.5 %**a** | 1 | J |
|  | Wang *et al.*. 2013a | **12** | | **12** | 0 %**a** | 0 | J |
|  | Wang *et al.*. 2013a | **13** | | **13** | 0 %**a** | 0 | J |
|  | Wang *et al.*. 2013a | **14** | | **14** | 0 %**a** | 0 | J |
|  | Wang *et al.*. 2013a | **15** | | **15** | 0 %**a** | 0 | J |
|  | Wang *et al.*. 2013a | **16** | | **16** | 0 %**a** | 0 | J |
|  | Wang *et al.*. 2013a | **17** | | **17** | 0 %**a** | 0 | J |
|  | Wang *et al.*. 2013a | **18** | | **18 ts2** | 18.2 %**a** | 1 | J |
|  | Wang *et al.*. 2013a | **19** | | **19** | 57.1 %**a** | 1 | J |
|  | Wang *et al.*. 2013a | **20** | | **20** | 0 %**a** | 0 | J |
|  | Wang *et al.*. 2013a | **21** | | **21** | 0 %**a** | 0 | J |
|  | Wang *et al.*. 2013a | **22** | | **22** | 100 %**a** | 2 | J |
|  | Wang *et al.*. 2013a | **23** | | **23ts1** | 87.5 %**a** | 2 | J |
|  | Wang *et al.*. 2013a | **24** | | **24** | 0 %**a** | 0 | J |
|  | Wang *et al.*. 2013a | **25** | | **25** | 0 %**a** | 0 | J |
|  | Wang *et al.*. 2013a | **26** | | **26** | 0 %**a** | 0 | J |
|  | Wang *et al.*. 2013a | **27** | | **27** | 0 %**a** | 0 | J |
|  | Wang *et al.*. 2013a | **28** | | **28** | 0 %**a** | 0 | J |
|  | Wang *et al.*. 2013a | **29** | | **29** | 0 %**a** | 0 | J |
|  | Wang *et al.*. 2013a | **30** | | **30** | 0 %**a** | 0 | J |
|  | Wang *et al.*. 2013a | **31** | | **31** | 0 %**a** | 0 | J |
|  | Wang *et al.*. 2013a | **32** | | **32** | 0 %**a** | 0 | J |
|  | Wang *et al.*. 2013a | **33** | | **33 ts2** | 100 %**a** | 2 | J |
|  | Wang *et al.*. 2013b | **6a** | **34** | | 87.2 %**b** | 2 | J |
| |  | | --- | |  | | Wang *et al.*. 2013b | **6b** | **35** | | 55 %**b** | 1 | J |
|  | Wang *et al.*. 2013b | **6c** | **36 ts1** | | 50 %**b** | 2 | J |
|  | Wang *et al.*. 2013b | **6d** | **37\*** | | 25 %**b** | 1 | J |
|  | Wang *et al.*. 2013b | **6e** | **38** | | 50 %**b** | 1 | J |
|  | Wang *et al.*. 2013b | **6f** | **39 ts2** | | 54 %**b** | 1 | J |
|  | Wang *et al.*. 2013b | **6g** | **40** | | 33.5 %**b** | 1 | J |
|  | Wang *et al.*. 2013b | **6h** | **41 ts1** | | 37.5 %**b** | 1 | J |
|  | Wang *et al.*. 2013b | **6i** | **42\*** | | 75 %**b** | 2 | J |
| |  | | --- | |  | | Wang *et al.*. 2013b | **6j** | **43** | | 100 %**b** | 2 | J |
|  | Zheng *et al.*. 2014 | **R-1** | **44** | | 0 %**c** | 0 | J |
|  | Zheng *et al.*. 2014 | **R-2** | **45** | | 0%**c** | 0 | J |
|  | Zheng *et al.*. 2014 | **R-3** | **46** | | 60%**c** | 2 | J |
|  | Sharma *et al.*. 2014 | **(R)-3** | **47 ts1, ts2** | | 53.3 µM**d** | 1 | M |
|  | Sharma *et al.*. 2014 | **4** | **48 ts1** | | 132.1 µM**d** | 0 | M |
|  | Sharma *et al.*. 2014 | **5** | **49** | | >300.0 µM**d** | 0 | M |
|  | Liu *et al.*. 2012 | **8b** | **50** | | 0 µM**e** | 0 | M |
|  | Liu *et al.*. 2012 | **8c** | **51** | | 0.9 µM**e** | 2 | M |
|  | Liu *et al.*. 2012 | **8d** | **52** | | 1000 µM**e** | 0 | M |
|  | Liu *et al.*. 2012 | **8e** | **53** | | 1000 µM**e** | 0 | M |
|  | Liu *et al.*. 2012 | **9a** | **54** | | 1.3 µM**e** | 2 | M |
|  | Liu *et al.*. 2012 | **9b** | **55** | | 1000 µM**e** | 0 | M |
|  | Liu *et al.*. 2012 | **9c** | **56 ts1** | | 0 µM**e** | 0 | M |
|  | Liu *et al.*. 2012 | **9d** | **57** | | 43.7 µM**e** | 1 | M |
|  | Liu *et al.*. 2012 | **9e** | **58 ts1** | | 1000 µM**e** | 0 | M |
|  | Liu *et al.*. 2012 | **9f** | **59** | | 1000 µM**e** | 0 | M |
|  | Liu *et al.*. 2012 | **10c** | **60** | | 46.8 µM**e** | 1 | M |
|  | Liu *et al.*. 2012 | **10d** | **61** | | 9.9 µM**e** | 1 | M |
|  | Liu *et al.*. 2012 | **10e** | **62** | | 1000 µM**e** | 0 | M |
|  | Liu *et al.*. 2012 | **10f** | **63** | | 1000 µM**e** | 0 | M |
|  | Liu *et al.*. 2012 | **10g** | **64** | | 0 µM**e** | 0 | M |
|  | Liu *et al.*. 2012 | **10h** | **65 ts1** | | 0 µM**e** | 0 | M |
|  | Liu *et al.*. 2012 | **11a** | **66** | | 0 µM**e** | 0 | M |
|  | Liu *et al.*. 2012 | **11b** | **67** | | 0 µM**e** | 0 | M |
|  | Liu *et al.*. 2012 | **11c** | **68** | | 0 µM**e** | 0 | M |
|  | Liu *et al.*. 2012 | **11d** | **69** | | 0 µM**e** | 0 | M |
|  | Liu *et al.*. 2012 | **11e** | **70 ts1** | | 0 µM**e** | 0 | M |
|  | Liu *et al.*. 2012 | **11f** | **71 ts1** | | 0 µM**e** | 0 | M |
|  | Liu *et al.*. 2012 | **11g** | **72** | | 0 µM**e** | 0 | M |
|  | Sadhu *et al.*. 2012 | **28** | **73** | | >10 µM**f** | 1 | M |
|  | Sadhu *et al.*. 2012 | **30** | **74** | | 25 µM**f** | 1 | M |
|  | Sadhu *et al.*. 2012 | **31** | **75** | | >100 µM**f** | 0 | M |
|  | Sadhu *et al.*. 2012 | **32** | **76** | | 1000 µM**f** | 0 | M |
|  | Sadhu *et al.*. 2012 | **33** | **77** | | 1000 µM**f** | 0 | M |
|  | Sadhu *et al.*. 2012 | **34** | **78** | | 1000 µM**f** | 0 | M |
|  | Sadhu *et al.*. 2012 | **35** | **79** | | >100 µM**f** | 0 | M |
|  | Sadhu *et al.*. 2012 | **36** | **80** | | 1000 µM**f** | 0 | M |
|  | Sadhu *et al.*. 2012 | **37** | **81** | | 1000 µM**f** | 0 | M |
|  | Sadhu *et al.*. 2012 | **47** | **82** | | 25 µM**f** | 1 | M |
|  | Sadhu *et al.*. 2012 | **48** | **83 ts2** | | 50 µM**f** | 1 | M |
|  | Sadhu *et al.*. 2012 | **49** | **84** | | 25 µM**f** | 1 | M |
|  | Sadhu *et al.*. 2012 | **50** | **85** | | 1000 µM**f** | 0 | M |
|  | Sadhu *et al.*. 2012 | **59** | **86** | | 1000 µM**f** | 0 | M |
|  | Sadhu *et al.*. 2012 | **60** | **87** | | 1000 µM**f** | 0 | M |
|  | Sadhu *et al.*. 2012 | **61** | **88** | | 1000 µM**f** | 0 | M |
|  | Sadhu *et al.*. 2012 | **62** | **89** | | 1000 µM**f** | 0 | M |
|  | Kamel *et al.*. 2012 | **1a** | **90** | | 40 and 70 M**g** | 0 | M |
|  | Kamel *et al.*. 2012 | **1b** | **91** | | 40 and 70 M**g** | 0 | M |
|  | Kamel *et al.*. 2012 | **1c** | **92** | | 20 and 60 M**g** | 1 | M |
|  | Kamel *et al.*. 2012 | **2a** | **93** | | 20 and 50 M**g** | 1 | M |
|  | Kamel *et al.*. 2012 | **2b** | **94** | | 20 and 50 M**g** | 1 | M |
|  | Kamel *et al.*. 2012 | **2c** | **95** | | 10 and 40 M**g** | 1 | M |
|  | Kamel *et al.*. 2012 | **2d** | **96 ts1** | | 5 and 30 M**g** | 1 | M |
|  | Dong *et al.*. 2010 | **2** | **97 ts1** | | 39 %**h** | 1 | M |
| tmpZWNQdc.png | Dong *et al.*. 2010 | **3** | **98** | | 2 %**h** | 0 | M |
| tmpYVs1_r.png | Dong *et al.*. 2010 | **4** | **99** | | 0 %**h** | 0 | M |
|  | Dong *et al.*. 2010 | **5** | **100** | | 9 %**h** | 0 | M |
|  | Dong *et al.*. 2010 | **6** | **101 ts1** | | 0 %**h** | 0 | M |
|  | Dong *et al.*. 2010 | **7** | **102** | | 0 %**h** | 0 | M |
|  | Dong *et al.*. 2010 | **8** | **103 ts2** | | 0 %**h** | 1 | M |
|  | Dong *et al.*. 2010 | **9** | **104** | | 0 %**h** | 0 | M |
|  | Ronketti *et al.*. 2007 | **3** | **105** | | 400 M**i** | 0 | M |
|  | Ronketti *et al.*. 2007 | **4** | **106** | | 28 M**i** | 1 | M |
|  | Ronketti *et al.*. 2007 | **5** | **107** | | 400 M**i** | 0 | M |
|  | Ronketti *et al.*. 2007 | **6** | **108** | | >80 M**i** | 0 | M |
|  | Ronketti *et al.*. 2007 | **7** | **109 ts2** | | 18 M**i** | 1 | M |
|  | Ronketti *et al.*. 2007 | **8** | **110 ts1** | | 200 M**i** | 0 | M |
|  | Ronketti *et al.*. 2007 | **9** | **111** | | 12 M**i** | 1 | M |
|  | Abo-Ghalia and Soliman. 2001 | **b** | **112 ts1** | | 23 % **j** | 1 | M |
|  | Abo-Ghalia and Soliman. 2001 | **c** | **113** | | 12 % **j** | 0 | M |
|  | Abo-Ghalia and Soliman. 2001 | **d** | **114** | | 10 % **j** | 0 | M |
|  | Abo-Ghalia and Soliman. 2001 | **e** | **115 ts2** | | 70 % **j** | 1 | M |
|  | Abo-Ghalia and Soliman. 2001 | **g** | **116** | | 52 % **j** | 1 | M |
|  | Abo-Ghalia and Soliman. 2001 | **h** | **117** | | 55 % **j** | 1 | M |
|  | Abo-Ghalia and Soliman. 2001 | **i** | **118** | | 60 % **j** | 1 | M |
|  | Abo-Ghalia and Soliman. 2001 | **j** | **119\*** | | 75 % **j** | 1 | M |
|  | Abo-Ghalia and Soliman. 2001 | **k** | **120 ts1** | | 68 % **j** | 1 | M |
|  | Abo-Ghalia and Soliman. 2001 | **II** | **121 ts1, ts2** | | 63 % **j** | 1 | M |

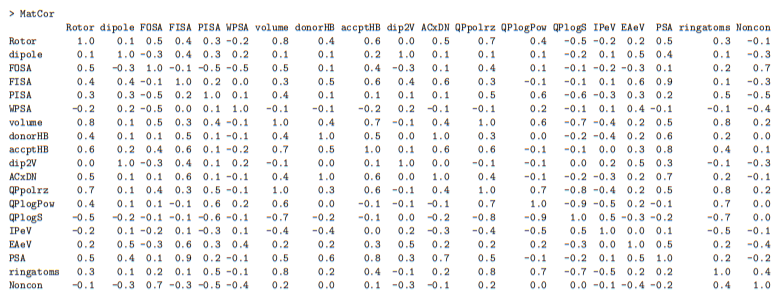
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**Figure S1** **A**) Number of PZQ derivatives used in our study *versus* the decades (1977 till 2017); **B**) Proportion of derivatives subcategory according to the worm species in which they were tested; **C**) Subcategories proportion of class 2 compounds. **D**) Histogram of number of modified subcategories vs not effectuated combinations (orange)/ effectuated combinations (blue); **E**) Sector graph of the total number of modifications, not performed modifications (blue) and performed modifications (orange);

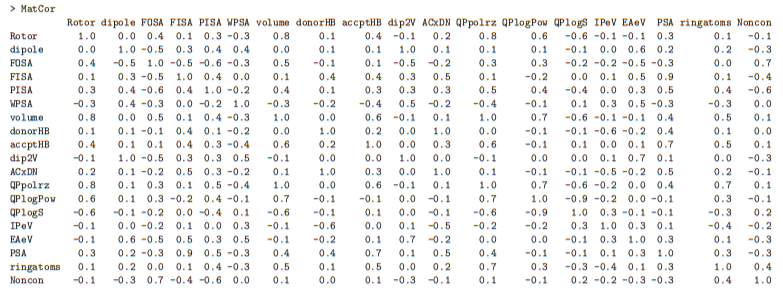
|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | | | | | | | |
| **Table. S2** Phase scores of the derivatives. \* = Derivatives that do not match the model. | | | | | | | |
| **Name** | **Vector Score** | **Volume Score** | **Num. Sites Matched** | **Matched Ligand Site** | **Fitness** | **Align Score** | | |
| **PZQ** | 0.991302 | 0.913960 | 4 | A(1) H(3) H(4) R(6) | 2.817619 | 0.105171 | | |
| **1** | \* | \* | \* | \* | \* | \* | | |
| **2** | 0.995679748 | 0.854227255 | 4 | A(1) H(5) H(4) R(6) | 2.785305396 | 0.077521928 | | |
| **3** | 0.992072696 | 0.870822384 | 4 | A(1) H(5) H(4) R(6) | 2.779185426 | 0.100451585 | | |
| **4** | 0.991903321 | 0.897502474 | 4 | A(1) H(5) H(4) R(6) | 2.805726097 | 0.100415638 | | |
| **5** | 0.992161391 | 0.776488745 | 4 | A(1) H(3) H(4) R(5) | 2.685102406 | 0.100257276 | | |
| **6** | 0.993691872 | 0.763930116 | 4 | A(1) H(3) H(4) R(5) | 2.682633388 | 0.089986321 | | |
| **7** | 0.994258807 | 0.788029777 | 4 | A(2) H(4) H(5) R(6) | 2.707508191 | 0.089736472 | | |
| **8** | 0.994141392 | 0.753222038 | 4 | A(2) H(4) H(5) R(6) | 2.671871037 | 0.090590872 | | |
| **9** | 0.993342266 | 0.767584016 | 4 | A(1) H(3) H(4) R(5) | 2.684993689 | 0.091119111 | | |
| **10** | 0.993184882 | 0.767067361 | 4 | A(2) H(4) H(5) R(6) | 2.682822752 | 0.092915389 | | |
| **11** | 0.994629497 | 0.698686686 | 4 | A(2) H(3) H(4) R(6) | 2.621301016 | 0.086418201 | | |
| **12** | 0.99465519 | 0.818379644 | 4 | A(1) H(5) H(4) R(7) | 2.742894035 | 0.08416896 | | |
| **13** | \* | \* | \* | \* | \* | \* | | |
| **14** | \* | \* | \* | \* | \* | \* | | |
| **15** | \* | \* | \* | \* | \* | \* | | |
| **16** | \* | \* | \* | \* | \* | \* | | |
| **17** | 0.793695956 | 0.459670387 | 4 | A(1) H(3) H(4) R(5) | 1.347643657 | 1.086867224 | | |
| **18** | 0.838905816 | 0.428571808 | 4 | A(1) H(3) H(4) R(5) | 1.298287185 | 1.163028527 | | |
| **19** | 0.797472603 | 0.413913933 | 4 | A(1) H(2) H(4) R(5) | 1.240942612 | 1.164532709 | | |
| **20** | 0.847309355 | 0.409850985 | 4 | A(1) H(2) H(3) R(5) | 1.288195222 | 1.162758142 | | |
| **21** | 0.8441528 | 0.421562997 | 4 | A(1) H(2) H(3) R(5) | 1.304520011 | 1.153434944 | | |
| **22** | 0.992430237 | 0.873513785 | 4 | A(2) H(5) H(6) R(8) | 2.784898899 | 0.925479075 | | |
| **23** | 0.997194793 | 0.737346214 | 4 | A(1) H(4) H(3) R(6) | 2.643717083 | 0.108988709 | | |
| **24** | \* | \* | \* | \* | \* | \* | | |
| **25** | 0.997166343 | 0.722976413 | 4 | A(1) H(4) H(5) R(6) | 2.628975524 | 0.109400678 | | |
| **26** | 0.997010043 | 0.729170128 | 4 | A(1) H(4) H(5) R(6) | 2.634283242 | 0.110276314 | | |
| **27** | 0.997388912 | 0.749683236 | 4 | A(1) H(4) H(5) R(6) | 2.656868418 | 0.108244475 | | |
| **28** | 0.997780779 | 0.825090374 | 4 | A(1) H(4) H(3) R(5) | 2.73413329 | 0.106485435 | | |
| **29** | 0.996428339 | 0.739391881 | 4 | A(1) H(4) H(3) R(5) | 2.641756002 | 0.112877062 | | |
| **30** | 0.997027419 | 0.655315858 | 4 | A(1) H(4) H(3) R(5) | 2.560902307 | 0.109729165 | | |
| **31** | 0.998177729 | 0.679658181 | 4 | A(2) H(4) H(3) R(6) | 2.59155274 | 0.103539803 | | |
| **32** | 0.998121011 | 0.67814052 | 4 | A(1) H(4) H(5) R(6) | 2.590415238 | 0.103015551 | | |
| **33** | 0.997848832 | 0.769511235 | 4 | A(2) H(5) H(4) R(6) | 2.678443053 | 0.106700417 | | |
| **34** | 0.99080235 | 0.86823273 | 4 | A(2) H(5) H(6) R(8) | 2.7682049 | 0.10899622 | | |
| **35** | 0.93784188 | 0.79221637 | 4 | A(1) H(5) H(4) R(7) | 2.71032862 | 0.02367555 | | |
| **36** | 0.93474144 | 0.72960607 | 4 | A(1) H(5) H(4) R(7) | 2.64286109 | 0.02578371 | | |
| **37** | 0.99197893 | 0.87346442 | 4 | A(2) H(5) H(6) R(8) | 2.78160133 | 0.10061043 | | |
| **38** | 0.99353304 | 0.72846801 | 4 | A(1) H(5) H(4) R(7) | 2.64740339 | 0.0895172 | | |
| **39** | 0.99185822 | 0.89973239 | 4 | A(1) H(4) H(5) R(7) | 2.80778215 | 0.10057015 | | |
| **40** | 0.99163511 | 0.90073972 | 4 | A(1) H(4) H(5) R(7) | 2.80738034 | 0.10199338 | | |
| **41** | 0.99107932 | 0.89817031 | 4 | A(1) H(4) H(5) R(7) | 2.80121524 | 0.10564127 | | |
| **42** | 0.99243044 | 0.87351636 | 4 | A(2) H(5) H(6) R(8) | 2.7848989 | 0.09725748 | | |
| **43** | 0.99289574 | 0.81043423 | 4 | A(2) H(5) H(6) R(8) | 2.72567865 | 0.09318158 | | |
| **44** | 0.99165545 | 0.83745316 | 4 | A(1) H(5) H(4) R(6) | 2.74400652 | 0.1021225 | | |
| **45** | 0.99115206 | 0.8791445 | 4 | A(1) H(5) H(4) R(6) | 2.78234364 | 0.1055435 | | |
| **46** | 0.99122912 | 0.89822233 | 4 | A(1) H(4) H(5) R(7) | 2.80174691 | 0.10524546 | | |
| **47** | 0.99580915 | 0.53041765 | 4 | A(2) H(9) H(10) R(13) | 2.49083404 | 0.04247131 | | |
| **48** | 0.9974709 | 0.39478094 | 4 | A(3) H(6) H(7) R(12) | 2.3413913 | 0.06103265 | | |
| **49** | 0.81138981 | 0.28171286 | 4 | A(3) H(12) H(11) R(15) | 1.59171477 | 0.60166549 | | |
| **50** | 0.99257338 | 0.82963332 | 4 | A(3) H(7) H(8) R(10) | 2.73959477 | 0.09913432 | | |
| **51** | 0.99725041 | 0.73735659 | 4 | A(1) H(4) H(3) R(6) | 2.64383545 | 0.10892586 | | |
| **52** | 0.99872743 | 0.64983988 | 4 | A(2) H(5) H(6) R(8) | 2.60940635 | 0.04699314 | | |
| **53** | 0.99981923 | 0.59073892 | 4 | A(2) H(7) H(6) R(9) | 2.48757625 | 0.12357829 | | |
| **54** | 0.99897444 | 0.88245725 | 4 | A(1) H(4) H(5) R(7) | 2.8461441 | 0.04234511 | | |
| **55** | 0.99859265 | 0.67915644 | 4 | A(1) H(5) H(4) R(7) | 2.63719996 | 0.04865895 | | |
| **56** | 0.99981938 | 0.67795739 | 4 | A(1) H(3) H(4) R(7) | 2.66524257 | 0.01504104 | | |
| **57** | 0.99918171 | 0.81434706 | 4 | A(1) H(3) H(4) R(7) | 2.79162222 | 0.02628787 | | |
| **58** | 0.99963406 | 0.78600815 | 4 | A(1) H(3) H(4) R(7) | 2.77487526 | 0.01292035 | | |
| **59** | 0.99968009 | 0.54725676 | 4 | A(1) H(4) H(5) R(8) | 2.52834965 | 0.02230464 | | |
| **60** | 0.9927379 | 0.73248446 | 4 | A(1) H(5) H(6) R(7) | 2.64470566 | 0.09662004 | | |
| **61** | 0.99438805 | 0.58436014 | 4 | A(2) H(4) H(5) R(7) | 2.50492124 | 0.08859233 | | |
| **62** | 0.99390764 | 0.62875651 | 4 | A(3) H(6) H(7) R(8) | 2.55016877 | 0.08699446 | | |
| **63** | 0.99426994 | 0.53464649 | 4 | A(3) H(4) H(5) R(9) | 2.4541889 | 0.08967304 | | |
| **64** | 0.99470259 | 0.6575604 | 4 | A(3) H(4) H(5) R(8) | 2.60948408 | 0.0513347 | | |
| **65** | 0.9919963 | 0.70213353 | 4 | A(1) H(4) H(5) R(6) | 2.61086455 | 0.09991834 | | |
| **66** | 0.9957749 | 0.85422725 | 4 | A(1) H(5) H(4) R(6) | 2.7853054 | 0.07752193 | | |
| **67** | 0.99931375 | 0.78195025 | 4 | A(2) H(6) H(7) R(9) | 2.7538099 | 0.03294492 | | |
| **68** | 0.9974709 | 0.39478094 | 4 | A(3) H(6) H(7) R(12) | 2.3413913 | 0.06103265 | | |
| **69** | 0.94343647 | 0.71475413 | 4 | A(1) H(2) H(4) R(5) | 2.64103137 | 0.02059108 | | |
| **70** | 0.98274913 | 0.73898233 | 4 | A(1) H(4) H(5) R(7) | 2.81740076 | 0.01837455 | | |
| **71** | 0.9925537 | 0.80928676 | 4 | A(1) H(5) H(6) R(8) | 2.8573649 | 0.09627551 | | |
| **72** | 0.99660046 | 0.40731533 | 4 | A(3) H(10) H(11) R(12) | 2.36485383 | 0.04687435 | | |
| **73** | 0.97442913 | 0.76498233 | 4 | A(1) H(2) H(4) R(5) | 2.64103137 | 0.10252193 | | |
| **74** | 0.99398082 | 0.77718301 | 4 | A(3) H(9) H(8) R(10) | 2.696864 | 0.08915979 | | |
| **75** | 0.9925537 | 0.80928676 | 4 | A(2) H(5) H(6) R(8) | 2.7138989 | 0.60166549 | | |
| **76** | 0.99509723 | 0.54192815 | 4 | A(4) H(8) H(9) R(11) | 2.46784335 | 0.08301843 | | |
| **77** | 0.99745376 | 0.62656567 | 4 | A(2) H(4) H(5) R(7) | 2.58620876 | 0.0453728 | | |
| **78** | 0.99772056 | 0.62891551 | 4 | A(2) H(6) H(5) R(7) | 2.59080865 | 0.0429929 | | |
| **79** | 0.92746207 | 0.6823847 | 4 | A(1) H(3) H(4) R(7) | 2.47264226 | 0.06837458 | | |
| **80** | 0.99787199 | 0.53243824 | 4 | A(3) H(5) H(6) R(8) | 2.49522162 | 0.04210634 | | |
| **81** | 0.99957118 | 0.78025537 | 4 | A(2) H(4) H(5) R(7) | 2.76342468 | 0.01968224 | | |
| **82** | 0.87288725 | 0.57084155 | 4 | A(1) H(5) H(4) R(7) | 2.32363356 | 0.14411428 | | |
| **83** | 0.87185618 | 0.55762016 | 4 | A(2) H(5) H(6) R(7) | 2.31375636 | 0.13886397 | | |
| **84** | 0.84420582 | 0.47920976 | 4 | A(1) H(4) H(3) R(6) | 2.20593827 | 0.14097277 | | |
| **85** | 0.83537959 | 0.47535008 | 4 | A(2) H(4) H(5) R(6) | 2.20884106 | 0.12226633 | | |
| **86** | 0.8326067 | 0.44117705 | 4 | A(2) H(6) H(4) R(7) | 2.1721827 | 0.12192125 | | |
| **87** | 0.84770362 | 0.42600477 | 4 | A(2) H(5) H(6) R(7) | 2.16934337 | 0.12523802 | | |
| **88** | 0.85202792 | 0.48621099 | 4 | A(3) H(5) H(6) R(7) | 2.23737566 | 0.12103589 | | |
| **89** | 0.92359361 | 0.50838094 | 4 | A(2) H(6) H(4) R(7) | 2.33917239 | 0.11136258 | | |
| **90** | 0.9941965 | 0.63792451 | 4 | A(1) H(3) H(4) R(6) | 2.55393923 | 0.09381814 | | |
| **91** | 0.99851825 | 0.62000475 | 4 | A(2) H(5) H(6) R(8) | 2.58834319 | 0.03621576 | | |
| **92** | 0.99670689 | 0.58272327 | 4 | A(1) H(3) H(4) R(7) | 2.52256608 | 0.06823689 | | |
| **93** | 0.99942719 | 0.6946888 | 4 | A(1) H(4) H(5) R(8) | 2.67012524 | 0.02878889 | | |
| **94** | 0.99983372 | 0.69267161 | 4 | A(1) H(4) H(5) R(8) | 2.67925718 | 0.01589778 | | |
| **95** | 0.99955574 | 0.59472296 | 4 | A(1) H(3) H(4) R(8) | 2.57452342 | 0.02370634 | | |
| **96** | 0.99931375 | 0.78195025 | 4 | A(2) H(6) H(7) R(9) | 2.7538099 | 0.03294492 | | |
| **97** | 0.99514897 | 0.68706955 | 4 | A(2) H(6) H(7) R(8) | 2.61252964 | 0.08362665 | | |
| **98** | 0.99111327 | 0.80665062 | 4 | A(1) H(3) H(4) R(8) | 2.71042267 | 0.10480946 | | |
| **99** | 0.9906532 | 0.66647503 | 4 | A(1) H(3) H(4) R(8) | 2.56889146 | 0.10588412 | | |
| **100** | 0.99403123 | 0.81421571 | 4 | A(1) H(3) H(4) R(6) | 2.73488682 | 0.08803214 | | |
| **101** | 0.99418415 | 0.81376407 | 4 | A(2) H(4) H(5) R(7) | 2.7362518 | 0.08603571 | | |
| **102** | 0.99432714 | 0.89077737 | 4 | A(1) H(4) H(5) R(6) | 2.81440786 | 0.08483598 | | |
| **103** | 0.99439812 | 0.69508422 | 4 | A(2) H(6) H(7) R(8) | 2.61582231 | 0.08839204 | | |
| **104** | 0.99150066 | 0.59580335 | 4 | A(4) H(8) H(6) R(12) | 2.50171197 | 0.10271045 | | |
| **105** | 0.99131594 | 0.83382812 | 4 | A(1) H(4) H(3) R(6) | 2.7401802 | 0.10195663 | | |
| **106** | 0.99236609 | 0.90094882 | 4 | A(1) H(5) H(6) R(8) | 2.81154627 | 0.09812237 | | |
| **107** | 0.9925537 | 0.80928676 | 4 | A(1) H(5) H(6) R(8) | 2.72161086 | 0.09627551 | | |
| **108** | 0.99280578 | 0.38811519 | 4 | A(1) H(6) H(7) R(12) | 2.29964841 | 0.09752708 | | |
| **109** | 0.9931434 | 0.73847555 | 4 | A(1) H(5) H(6) R(7) | 2.65502212 | 0.09191619 | | |
| **110** | 0.99131888 | 0.89505022 | 4 | A(2) H(5) H(6) R(8) | 2.79938861 | 0.10437658 | | |
| **111** | 0.99389096 | 0.74209202 | 4 | A(1) H(5) H(6) R(7) | 2.66213469 | 0.08861795 | | |
| **112** | 0.99123764 | 0.80531328 | 4 | A(1) H(3) H(4) R(5) | 2.71129097 | 0.10231195 | | |
| **113** | 0.99334827 | 0.61365242 | 4 | A(2) H(8) H(9) R(11) | 2.52963654 | 0.09283698 | | |
| **114** | 0.9936078 | 0.6429614 | 4 | A(1) H(7) H(8) R(10) | 2.56085114 | 0.09086167 | | |
| **115** | 0.99417833 | 0.66568373 | 4 | A(2) H(4) H(5) R(6) | 2.58592032 | 0.08873009 | | |
| **116** | 0.99373865 | 0.63799089 | 4 | A(1) H(5) H(6) R(7) | 2.55795291 | 0.08853195 | | |
| **117** | 0.99430294 | 0.55842529 | 4 | A(1) H(5) H(6) R(7) | 2.47929738 | 0.08811702 | | |
| **118** | 0.99253863 | 0.52382452 | 4 | A(2) H(8) H(9) R(10) | 2.43583197 | 0.09663741 |
| **119** | 0.99406678 | 0.77047214 | 4 | A(2) H(4) H(5) R(6) | 2.69201684 | 0.08702649 |
| **120** | 0.9941281 | 0.6647981 | 4 | A(1) H(2) H(3) R(5) | 2.58230362 | 0.09194711 |
| **121** | 0.9970197 | 0.57971653 | 4 | A(1) H(3) H(4) R(9) | 2.54610229 | 0.03676074 |

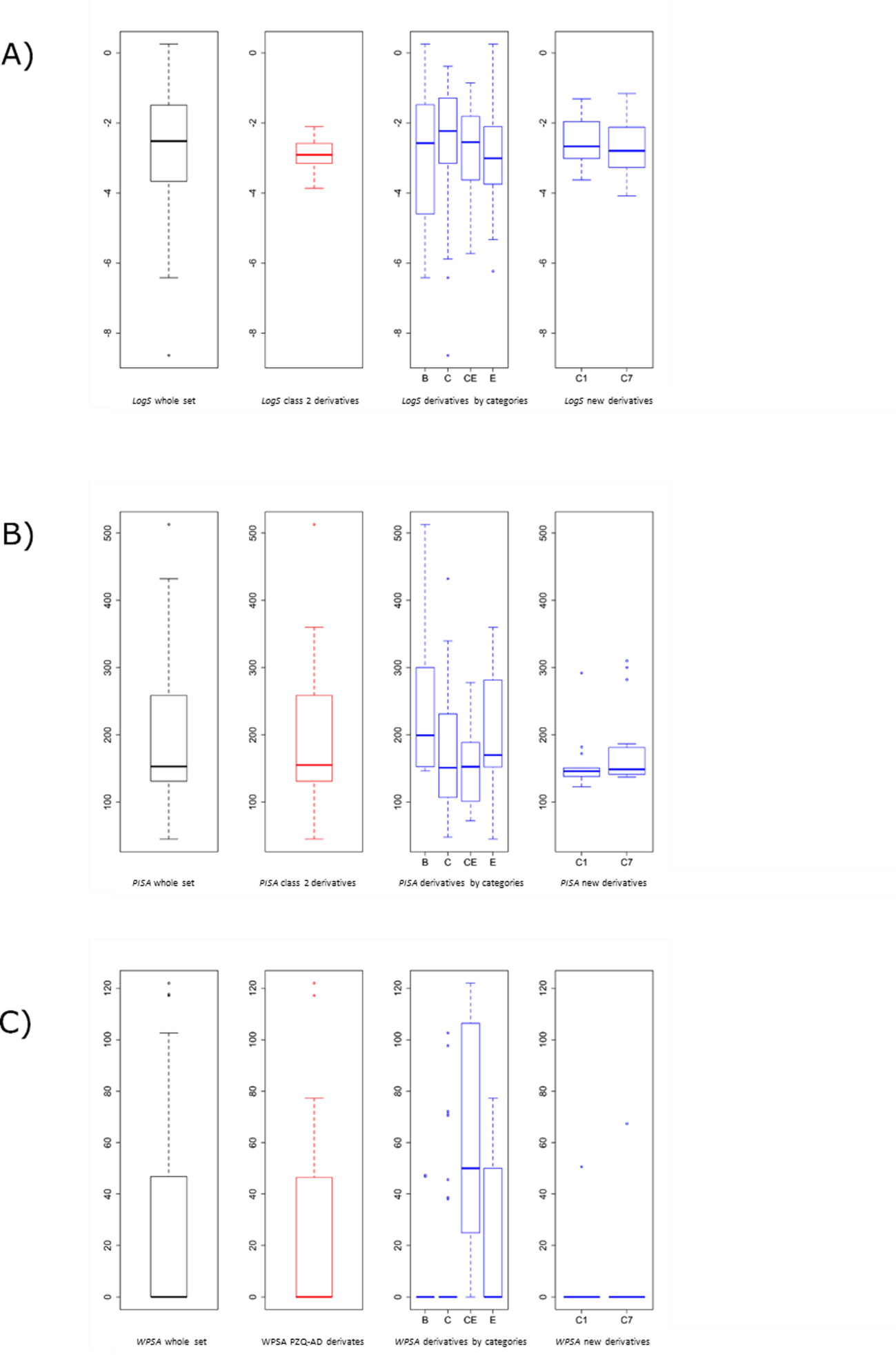
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| **Table. S3** Physico-chemical parameters calculated to the derivatives matching with the pharmacophore using the software QikProp from Schrodinger. \* = Derivatives that do not match the pharmacophore model. | | | | | | |
| **Name** | **Category** | **WPSA** | **EA(eV)** | **PISA** | **LogS** | **IP** |
| **PZQ** |  | 0 | 0.125 | 152.95 | -2.555 | 9.515 |
| **1** | C. D | \* | \* | \* | \* | \* |
| **2** | C | 0 | 0.021 | 149.33 | -0.622 | 9.686 |
| **3** | C | 0 | 0.035 | 154.739 | -0.776 | 9.51 |
| **4** | C | 0 | 0.033 | 85.001 | -2.099 | 9.545 |
| **5** | C | 0 | 0.14 | 83.453 | -0.603 | 9.732 |
| **6** | C | 0 | 0.289 | 105.508 | -2.17 | 9.326 |
| **7** | C | 72.2 | 0.296 | 112.372 | -2.589 | 9.569 |
| **8** | C | 97.667 | 0.302 | 99.203 | -2.076 | 9.298 |
| **9** | C | 0 | 0.284 | 94.884 | -2.094 | 9.606 |
| **10** | C | 0 | 0.678 | 154.256 | -0.954 | 9.647 |
| **11** | C | 45.596 | 0.951 | 48.156 | -0.934 | 9.573 |
| **12** | C | 0 | 0.414 | 129.985 | -2.298 | 9.561 |
| **13** | D | \* | \* | \* | \* | \* |
| **14** | C | \* | \* | \* | \* | \* |
| **15** | C. D | \* | \* | \* | \* | \* |
| **16** | A. C. D | \* | \* | \* | \* | \* |
| **17** | A. C | 0 | -0.263 | 154.261 | -1.895 | 9.535 |
| **18** | A. C | 0 | -0.279 | 152.753 | -1.329 | 9.511 |
| **19** | A | 0 | -0.293 | 152.765 | -1.818 | 9.51 |
| **20** | A. C | 0 | 0.127 | 339.985 | -2.443 | 9.481 |
| **21** | A. C | 44.225 | 0.881 | 277.045 | -2.429 | 9.56 |
| **22** | A. C | 73.239 | 0.145 | 155.821 | -2.139 | 9.192 |
| **23** | F | 49.984 | 0.861 | 154.838 | -2.391 | 9.178 |
| **24** | C. D. F | \* | \* | \* | \* | \* |
| **25** | C. F | 49.983 | 0.863 | 104.876 | -2.957 | 9.608 |
| **26** | C. F | 49.785 | 0.792 | 152.753 | -1.329 | 9.511 |
| **27** | C. F | 49.981 | 0.859 | 72.576 | -1.851 | 9.579 |
| **28** | C. F | 49.99 | 0.754 | 98.33 | -2.513 | 9.507 |
| **29** | C. F | 49.755 | 0.774 | 98.321 | -2.519 | 9.471 |
| **30** | C. F | 49.745 | 0.75 | 113.715 | -2.388 | 9.499 |
| **31** | C. F | 95.567 | 0.967 | 122.522 | -5.735 | 9.524 |
| **32** | C. F | 49.989 | 0.866 | 156.048 | -3.664 | 9.598 |
| **33** | C. F | 121.965 | 0.873 | 229.721 | -3.482 | 9.524 |
| **34** | F | 0 | 0.152 | 258.595 | -2.88 | 9.841 |
| **35** | F | 77.373 | 0.488 | 263.524 | -1.961 | 9.165 |
| **36** | F | 68.16 | 0.579 | 45.101 | -2.111 | 8.844 |
| **37** | F | 0 | 0.035 | 183.86 | -3.423 | 8.523 |
| **38** | F | 70.955 | 0.51 | 302.295 | -5.335 | 8.454 |
| **39** | F | 0 | 0.089 | 302.22 | -4.216 | 8.493 |
| **40** | F | 0 | 0.109 | 281.418 | -6.235 | 8.763 |
| **41** | F | 0 | 0.08 | 156.094 | 0.251 | 9.266 |
| **42** | F | 0 | 0.145 | 131.397 | -2.735 | 9.098 |
| **43** | F | 0 | 0.374 | 155.768 | -3.139 | 8.881 |
| **44** | C | 0 | 0.13 | 153.186 | -1.428 | 9.381 |
| **45** | C | 0 | 0.114 | 152.994 | -2.602 | 9.677 |
| **46** | C | 0 | 0.205 | 149.708 | -2.942 | 9.588 |
| **47** | C | 0 | -0.134 | 108.473 | -2.345 | 8.335 |
| **48** | C | 102.637 | 1.791 | 294.242 | -2.913 | 8.383 |
| **49** | C | 0 | 0.565 | 293.6 | -2.882 | 8.331 |
| **50** | F | 0 | 0.052 | 140.893 | -1.496 | 9.363 |
| **51** | F | 47.238 | 0.716 | 360.187 | -3.16 | 9.593 |
| **52** | B | 0 | 0.253 | 350.603 | -2.577 | 9.646 |
| **53** | B. F | 0 | 0.343 | 498.176 | -4.187 | 9.47 |
| **54** | B | 0 | -0.007 | 512.964 | -3.87 | 9.675 |
| **55** | B | 0 | 0.241 | 304.441 | -1.488 | 9.563 |
| **56** | B | 0 | 0.247 | 146.225 | -5.778 | 8.575 |
| **57** | B | 0 | 0.129 | 153.144 | -6.415 | 9.533 |
| **58** | B | 0 | 0.13 | 152.75 | -0.936 | 9.492 |
| **59** | B | 46.822 | 0.293 | 154.027 | 0.253 | 9.548 |
| **60** | C | 0 | 0.188 | 154.8 | -1.041 | 9.519 |
| **61** | C | 38.656 | 1.492 | 146.755 | -0.38 | 9.775 |
| **62** | C | 0 | 1.095 | 304.672 | -1.515 | 9.59 |
| **63** | C | 0 | 0.608 | 297.64 | -1.508 | 9.472 |
| **64** | C | 38.056 | 0.982 | 136.287 | -1.543 | 9.241 |
| **65** | C | 0 | 0.803 | 339.866 | -2.827 | 9.186 |
| **66** | C. H | 0 | 0.388 | 277.955 | -2.584 | 9.185 |
| **67** | C. H | 0 | 0.394 | 84.855 | -1.783 | 9.532 |
| **68** | C | 0 | 1.929 | 82.013 | -1.065 | 9.589 |
| **69** | C | 0 | 1.95 | 84.834 | -0.933 | 9.545 |
| **70** | C | 0 | 2.028 | 85.745 | -0.823 | 9.575 |
| **71** | C | 0 | 2.091 | 77.126 | -0.918 | 9.547 |
| **72** | C | 0 | 2.052 | 256.977 | -2.093 | 9.59 |
| **73** | C. D | 0 | 0.9 | 207.332 | -2.309 | 9.589 |
| **74** | C. F | 0 | -0.001 | 221.003 | -1.478 | 9.555 |
| **75** | C. D. F | 0 | 0.904 | 152.69 | -0.355 | 9.649 |
| **76** | C. F | 117.659 | 0.887 | 152.672 | -0.863 | 9.634 |
| **77** | B | 0 | 0.403 | 321.099 | -5.455 | 9.676 |
| **78** | B. C | 0 | 0.405 | 247.963 | -3.955 | 9.59 |
| **79** | B. C. D | 0.576 | 1.178 | 46.893 | -2.326 | 8.899 |
| **80** | B. C | 117.917 | 1.176 | 151.017 | -2.636 | 9.693 |
| **81** | B. C | 0 | 0.517 | 157.321 | -3.961 | 8.638 |
| **82** | F | 0 | 0.305 | 152.314 | -3.749 | 9.52 |
| **83** | C. F | 117.169 | 0.978 | 154.501 | -3.59 | 9.506 |
| **84** | C. F | 0 | 0.299 | 155.575 | -3.823 | 9.571 |
| **85** | C. F | 117.166 | 0.986 | 273.029 | -4.612 | 9.489 |
| **86** | B. C. F | 0 | 0.441 | 351.151 | -3.459 | 8.908 |
| **87** | B. C. F | 0 | 0.441 | 312.841 | -3.142 | 8.727 |
| **88** | B. C. F | 117.704 | 1.027 | 249.15 | 0.008 | 9.375 |
| **89** | B. C. F | 0 | 0.507 | 339.994 | -1.866 | 9.703 |
| **90** | B | 0 | 0.567 | 149.866 | -1.475 | 9.462 |
| **91** | B | 0 | 0.51 | 146.972 | -0.599 | 9.453 |
| **92** | B | 47.352 | 0.656 | 211.741 | -4.587 | 9.297 |
| **93** | B | 0 | 0.146 | 211.741 | -4.068 | 9.353 |
| **94** | B | 0 | -0.064 | 199.546 | -2.425 | 9.744 |
| **95** | B | 0 | 0.258 | 295.867 | -4.602 | 8.475 |
| **96** | B | 0 | 0.059 | 189.243 | -2.128 | 9.361 |
| **97** | C | 70.512 | 0.369 | 205.394 | -2.011 | 9.058 |
| **98** | C | 0 | 0.12 | 166.962 | -4.351 | 9.134 |
| **99** | C | 0 | -0.217 | 147.206 | -3.97 | 9.835 |
| **100** | C | 0 | -0.034 | 146.295 | -3.522 | 9.836 |
| **101** | C | 0 | 0.016 | 269.338 | -3.361 | 9.76 |
| **102** | C | 0 | -0.012 | 269.564 | -5.23 | 9.94 |
| **103** | C | 71.186 | 0.195 | 134.374 | -4.081 | 9.9 |
| **104** | C | 0 | 0.142 | 432.218 | -6.417 | 8.404 |
| **105** | F | 0 | 1.453 | 321.944 | -6.63 | 8.592 |
| **106** | F | 0 | -0.081 | 318.391 | -6.267 | 8.595 |
| **107** | F | 0 | 0.281 | 431.069 | -7.958 | 8.586 |
| **108** | F | 0 | 1.102 | 286.772 | -6.408 | 8.53 |
| **109** | C | 0 | -0.043 | 334.363 | -5.722 | 9.062 |
| **110** | C | 0 | 0.146 | 279.286 | -5.888 | 8.864 |
| **111** | C | 0 | 0.113 | 154.09 | -2.782 | 9.516 |
| **112** | C | 0 | -0.216 | 142.647 | -3.238 | 9.363 |
| **113** | C | 0 | 0.27 | 152.77 | -2.515 | 9.282 |
| **114** | C | 0 | 0.117 | 152.775 | -1.28 | 9.406 |
| **115** | C | 0 | 0.239 | 152.618 | -1.297 | 9.257 |
| **116** | C | 0 | 0.281 | 154.22 | -4.564 | 9.568 |
| **117** | C | 0 | 0.394 | 93.647 | -1.99 | 9.918 |
| **118** | C | 0 | 0.395 | 94.004 | -3.062 | 9.026 |
| **119** | C | 0 | 0.645 | 316.595 | -8.635 | 8.091 |
| **120** | A. D | 118.871 | 1.225 | 154.258 | -1.949 | 9.559 |
| **121** | C | 0 | 0.043 | 149.866 | -2.87 | 9.426 |

Table. S4 Matrix correlation to model 1 calculated using the software R.



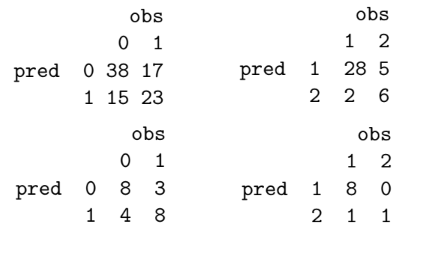
**Table. S5** Matrix correlation to model 2 calculated using the software R.





**Figure S2.** Boxplots representing the variability of physico-chemical properties. In black the whole set; in red only the active derivatives (PZQ-AD or Class 2), in blue the already synthetized derivatives divided by categories and the new proposed derivatives from categories C1 and C7.; A) LogS (Min. = -2.59; 1st Qu. =-2.12; Median = -1.99; Mean = -1.6; 3rd Qu. = -0.9; Max. = -0.6; var = 0.56; sd = 0.75); B) PISA (Min. = 48.16; 1st Qu. =92.41; Median = 108.94; Mean = 114.26; 3rd Qu. = 150.56; Max. = 154.74; var = 1197.52; sd = 34.61); C) WPSA (Min. = 0.00; 1st Qu. =0.00; Median = 23.62; Mean = 36.07; 3rd Qu. = 69.17; Max. = 121.97; var = 1747.2; sd = 41.8).

|  |  |  |
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| **Tab. S6.** Physico-chemical parameters and their interval values to distinguish the active molecules from the inactive ones. \* Description of the physico-chemical parameter and algorithms used to generate the values were extracted from Schrödinger QikProp manual (Schrödinger. 2017c). | | |
| **Parameters** | **Description\*** | **Coefficient** |
| ***EA (eV)*** | PM3 calculated electron affinity | - 2.44 |
| ***WPSA*** | Weakly polar component of the total solvent accessible surface area (SASA) in square angstroms using a probe with a 1.4 Å radius (halogens. P. and S). | + 0.015 |
| ***PISA*** | π (carbon and attached hydrogen) component of the SASA | - 0.03 |
| ***LogS*** | Predicted aqueous solubility. log S. S in mol dm–3 is the concentration of the solute in a saturated solution that is in equilibrium with the crystalline solid | + 1.01 |
| ***IP (eV)*** | PM3 calculated ionization potential | + 6.1 |

****

**C**)

**A**)

**D**)

**B**)

**Figure S3. A**) Confusion matrix for model 1 training set, class PZQ-AD *vs* Class 0; **B)** Confusion matrix for model 1 test set, PZQ-AD *vs* Class 0. **C**) Confusion matrix for model 1 training set, class PZQ-AD *vs* Class 0; **B** Confusion matrix for model 1 test set, class 1 *vs* Class 2.

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**Figure S4.** Structure of all new active derivatives proposed by our work.

**Table. S7.** Names, categories, calculated physico-chemical parameters and the probability to belong to class PZQ-AD and 2 to the new proposed derivatives. When the probability is bigger or equal to 50% the derivative is classified on Class PZQ-AD or 2.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Name** | **Category** | **WPSA** | **EA(eV)** | **PISA** | **LogS** | **IP** | **Prob. Class PZQ-AD** | **Prob. Class 2** |
| C1 1 | C1 | 0 | 0.078 | 148.145 | -2.117 | 9.551 | 56% | 27% |
| C1 2 | C1 | 0 | 0.082 | 147.944 | -2.709 | 9.538 | 56% | 14% |
| C1 3 | C1 | 0 | 0.106 | 143.261 | -3.169 | 9.493 | 55% | 8% |
| C1 4 | C1 | 0 | 0.07 | 146.061 | -1.668 | 9.433 | 57% | 24% |
| C1 5 | C1 | 0 | 0.074 | 137.217 | -2.672 | 9.515 | 56% | 17% |
| C1 6 | C1 | 0 | 0.144 | 122.782 | -1.963 | 9.617 | 52% | 59% |
| C1 7 | C1 | 0 | 0.125 | 292.110 | -3.628 | 9.441 | 54% | 0% |
| C1 8 | C1 | 0 | 0.094 | 282.326 | -3.693 | 9.484 | 55% | 0% |
| C1 9 | C1 | 0 | 0.144 | 148.864 | -2.429 | 9.374 | 52% | 7% |
| C1 10 | C1 | 0 | 0.21 | 150.980 | -3.301 | 9.783 | 49% | 26% |
| C1 11 | C1 | 50.632 | 1.903 | 138.216 | -3.014 | 9.318 | 4% | 4% |
| C1 12 | C1 | 0 | 0.004 | 172.128 | -2.577 | 9.623 | 60% | 14% |
| C1 13 | C1 | 0 | 0.061 | 138.163 | -1.313 | 9.633 | 57% | 68% |
| C1 14 | C7 | 0 | 0.079 | 136.957 | -1.459 | 9.679 | 56% | 72% |
| C1 15 | C7 | 0 | 0.045 | 182.136 | -2.973 | 9.668 | 58% | 9% |
| C7 1 | C7 | 0 | 0.265 | 138.438 | -2.435 | 9.525 | 45% | 22% |
| C7 2 | C7 | 0 | 0.266 | 137.944 | -2.800 | 9.521 | 45% | 15% |
| C7 3 | C7 | 0 | 0.265 | 138.476 | -3.403 | 9.502 | 45% | 7% |
| C7 4 | C7 | 0 | 0.116 | 137.217 | -3.141 | 9.495 | 54% | 9% |
| C7 5 | C7 | 0 | 0.116 | 300.256 | -4.030 | 9.525 | 54% | 0% |
| C7 6 | C7 | 0 | 0.263 | 310.183 | -4.084 | 9.532 | 45% | 0% |
| C7 7 | C7 | 0 | 0.557 | 175.719 | -2.215 | 9.511 | 29% | 10% |
| C7 8 | C7 | 0 | 0.801 | 151.027 | -1.164 | 9.785 | 19% | 82% |
| C7 9 | C7 | 67.359 | 2.116 | 147.046 | -2.028 | 9.146 | 3% | 3% |
| C7 10 | C7 | 0 | 0.273 | 171.955 | -2.884 | 9.508 | 45% | 5% |
| C7 11 | C7 | 0 | 0.42 | 144.486 | -1.197 | 9.559 | 37% | 56% |
| C7 12 | C7 | 0 | 0.403 | 145.513 | -2.044 | 9.597 | 37% | 37% |
| C7 13 | C7 | 0 | 0.324 | 186.726 | -3.087 | 9.561 | 42% | 4% |