**Supplementary data to**

**New Coumarin Derivative with Potential Antioxidant Activity: Synthesis, DNA Binding and In silico Studies (Molecular Docking, MD, ADMET).**

Serda Kecel Gunduza\*, Yasemin Budama Kilincb, Bilge Bicaka, Bahar Gokc, Burcu Belmend, Feray Aydogand, Cigdem Yolacand

*aDepartment of Physics, Science Faculty, Istanbul University, 34134, Vezneciler, Istanbul, Turkey*

*bDepartment of Bioengineering, Yildiz Technical University, Davutpasa Campus, 34010 Esenler, Istanbul, Turkey*

*cGraduate School of Natural and Applied Science, Yildiz Technical University, Davutpasa Campus, 34010 Esenler, Istanbul, Turkey*

*dDepartment of Chemistry, Yildiz Technical University, Davutpasa Campus, 34010 Esenler, Istanbul, Turkey*

\*Corresponding author

Serda Kecel Gunduz;

Department of Physics, Science Faculty, Istanbul University, 34134, Vezneciler, Istanbul, Turkey,

e-mail adress: skecel@istanbul.edu.tr

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| **Table S1(a)** Optimized parameters of C3 Bond Lenghts (R)  (Angstroms) | | | | | |
| **R1** | R(1,2) | 1 ,3949 | **R42** | R(32,35) | 1 ,5332 |
| **R2** | R(1,6) | 1 ,3928 | **R43** | R(32,36) | 1 ,0973 |
| **R3** | R(1,7) | 1 ,0842 | **R44** | R(32,37) | 1 ,0974 |
| **R4** | R(2,3) | 1 ,3926 | **R45** | R(35,38) | 1 ,0976 |
| **R5** | R(2,8) | 1 ,0846 | **R46** | R(35,39) | 1 ,0976 |
| **R6** | R(3,4) | 1 ,4011 | **R47** | R(35,40) | 1 ,533 |
| **R7** | R(3,9) | 1 ,0858 | **R48** | R(40,41) | 1 ,5199 |
| **R8** | R(4,5) | 1 ,3988 | **R49** | R(40,42) | 1 ,095 |
| **R9** | R(4,71) | 1 ,5137 | **R50** | R(40,43) | 1 ,095 |
| **R10** | R(5,6) | 1 ,3951 | **R51** | R(41,44) | 1 ,097 |
| **R11** | R(5,10) | 1 ,0856 | **R52** | R(41,45) | 1 ,097 |
| **R12** | R(6,11) | 1 ,0846 | **R53** | R(41,46) | 1 ,4335 |
| **R13** | R(12,13) | 1 ,5432 | **R54** | R(46,47) | 1 ,3561 |
| **R14** | R(12,17) | 1 ,4618 | **R55** | R(47,48) | 1 ,3959 |
| **R15** | R(12,18) | 1 ,0907 | **R56** | R(47,52) | 1 ,406 |
| **R16** | R(12,67) | 1 ,1077 | **R57** | R(48,49) | 1 ,3864 |
| **R17** | R(13,14) | 1 ,545 | **R58** | R(48,53) | 1 ,0819 |
| **R18** | R(13,19) | 1 ,0945 | **R59** | R(49,50) | 1 ,4109 |
| **R19** | R(13,66) | 1 ,0966 | **R60** | R(49,60) | 1 ,3632 |
| **R20** | R(14,15) | 1 ,5328 | **R61** | R(50,51) | 1 ,4033 |
| **R21** | R(14,70) | 1 ,0952 | **R62** | R(50,54) | 1 ,4499 |
| **R22** | R(14,71) | 1 ,5437 | **R63** | R(51,52) | 1 ,387 |
| **R23** | R(15,16) | 1 ,5435 | **R64** | R(51,55) | 1 ,0831 |
| **R24** | R(15,20) | 1 ,0927 | **R65** | R(52,56) | 1 ,0807 |
| **R25** | R(15,69) | 1 ,0969 | **R66** | R(54,57) | 1 ,3563 |
| **R26** | R(16,17) | 1 ,47 | **R67** | R(54,62) | 1 ,5037 |
| **R27** | R(16,21) | 1 ,095 | **R68** | R(57,58) | 1 ,452 |
| **R28** | R(16,68) | 1 ,1064 | **R69** | R(57,59) | 1 ,0823 |
| **R29** | R(17,22) | 1 ,4602 | **R70** | R(58,60) | 1 ,3962 |
| **R30** | R(22,23) | 1 ,5316 | **R71** | R(58,61) | 1 ,2041 |
| **R31** | R(22,24) | 1 ,1085 | **R72** | R(62,63) | 1 ,0901 |
| **R32** | R(22,25) | 1 ,0956 | **R73** | R(62,64) | 1 ,0944 |
| **R33** | R(23,26) | 1 ,5331 | **R74** | R(62,65) | 1 ,0943 |
| **R34** | R(23,27) | 1 ,0956 |  |  |  |
| **R35** | R(23,28) | 1 ,0957 |  |  |  |
| **R36** | R(26,29) | 1 ,0977 |  |  |  |
| **R37** | R(26,30) | 1 ,0976 |  |  |  |
| **R38** | R(26,31) | 1 ,533 |  |  |  |
| **R39** | R(31,32) | 1 ,5325 |  |  |  |
| **R40** | R(31,33) | 1 ,0976 |  |  |  |
| **R41** | R(31,34) | 1 ,0977 |  |  |  |

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| **Table S1(b)** Optimized parameters of C3 Angles (A) (Degrees) | | | | | | | | | | | | | | |
| **A1** | A(2,1,6) | 119 ,4253 | **A16** | A(1,6,5) | 120 ,1408 | **A31** | A(13,14,15) | 108 ,7216 | **A46** | A(17,16,21) | 107 ,6051 | **A61** | A(26,23,27) | 108 ,9272 |
| **A2** | A(2,1,7) | 120 ,2687 | **A17** | A(1,6,11) | 120 ,0831 | **A32** | A(13,14,70) | 107 ,9275 | **A47** | A(17,16,68) | 110 ,9466 | **A62** | A(26,23,28) | 109 ,9875 |
| **A3** | A(6,1,7) | 120 ,3052 | **A18** | A(5,6,11) | 119 ,776 | **A33** | A(13,14,71) | 111 ,1257 | **A48** | A(21,16,68) | 106 ,9147 | **A63** | A(27,23,28) | 106 ,4964 |
| **A4** | A(1,2,3) | 120 ,1663 | **A19** | A(13,12,17) | 110 ,0483 | **A34** | A(15,14,70) | 107 ,7019 | **A49** | A(12,17,16) | 110 ,6529 | **A64** | A(23,26,29) | 109 ,3036 |
| **A5** | A(1,2,8) | 120 ,0236 | **A20** | A(13,12,18) | 109 ,7962 | **A35** | A(15,14,71) | 113 ,2959 | **A50** | A(12,17,22) | 114 ,5547 | **A65** | A(23,26,30) | 109 ,5144 |
| **A6** | A(3,2,8) | 119 ,8093 | **A21** | A(13,12,67) | 110 ,4509 | **A36** | A(70,14,71) | 107 ,8763 | **A51** | A(16,17,22) | 111 ,4089 | **A66** | A(23,26,31) | 113 ,4209 |
| **A7** | A(2,3,4) | 121 ,0976 | **A22** | A(17,12,18) | 109 ,3084 | **A37** | A(14,15,16) | 111 ,1505 | **A52** | A(17,22,23) | 114 ,0697 | **A67** | A(29,26,30) | 106 ,0461 |
| **A8** | A(2,3,9) | 119 ,4485 | **A23** | A(17,12,67) | 110 ,8616 | **A38** | A(14,15,20) | 111 ,0784 | **A53** | A(17,22,24) | 111 ,2064 | **A68** | A(29,26,31) | 109 ,1227 |
| **A9** | A(4,3,9) | 119 ,4531 | **A24** | A(18,12,67) | 106 ,3002 | **A39** | A(14,15,69) | 108 ,5978 | **A54** | A(17,22,25) | 107 ,0879 | **A69** | A(30,26,31) | 109 ,1681 |
| **A10** | A(3,4,5) | 118 ,0575 | **A25** | A(12,13,14) | 111 ,8123 | **A40** | A(16,15,20) | 109 ,4454 | **A55** | A(23,22,24) | 109 ,7749 | **A70** | A(26,31,32) | 113 ,4793 |
| **A11** | A(3,4,71) | 120 ,5527 | **A26** | A(12,13,19) | 110 ,043 | **A41** | A(16,15,69) | 110 ,0142 | **A56** | A(23,22,25) | 108 ,2499 | **A71** | A(26,31,33) | 109 ,2034 |
| **A12** | A(5,4,71) | 121 ,3875 | **A27** | A(12,13,66) | 108 ,9953 | **A42** | A(20,15,69) | 106 ,44 | **A57** | A(24,22,25) | 106 ,0609 | **A72** | A(26,31,34) | 109 ,2534 |
| **A13** | A(4,5,6) | 121 ,1116 | **A28** | A(14,13,19) | 109 ,2508 | **A43** | A(15,16,17) | 111 ,9267 | **A58** | A(22,23,26) | 112 ,5577 | **A73** | A(32,31,33) | 109 ,2939 |
| **A14** | A(4,5,10) | 119 ,3572 | **A29** | A(14,13,66) | 109 ,8176 | **A44** | A(15,16,21) | 110 ,2364 | **A59** | A(22,23,27) | 110 ,3361 | **A74** | A(32,31,34) | 109 ,2759 |
| **A15** | A(6,5,10) | 119 ,5308 | **A30** | A(19,13,66) | 106 ,7934 | **A45** | A(15,16,68) | 109 ,0833 | **A60** | A(22,23,28) | 108 ,3571 | **A75** | A(33,31,34) | 106 ,0686 |
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| **A76** | A(31,32,35) | 113 ,5427 | **A91** | A(41,40,42) | 108,6508 | **A106** | A(49,48,53) | 120 ,1419 | **A121** | A(57,54,62) | 120 ,9654 | **A136** | A(4,71,72) | 109 ,4547 |
| **A77** | A(31,32,36) | 109 ,2897 | **A92** | A(41,40,43) | 108 ,6818 | **A107** | A(48,49,50) | 121 ,9445 | **A122** | A(54,57,58) | 123 ,1547 | **A137** | A(4,71,73) | 109 ,0448 |
| **A78** | A(31,32,37) | 109 ,3187 | **A93** | A(42,40,43) | 106 ,7587 | **A108** | A(48,49,60) | 116 ,5454 | **A123** | A(54,57,59) | 121 ,8408 | **A138** | A(14,71,72) | 109 ,0317 |
| **A79** | A(35,32,36) | 109 ,1555 | **A94** | A(40,41,44) | 110 ,8263 | **A109** | A(50,49,60) | 121 ,5101 | **A124** | A(58,57,59) | 115 ,0046 | **A139** | A(14,71,73) | 108 ,1906 |
| **A80** | A(35,32,37) | 109 ,1892 | **A95** | A(40,41,45) | 110 ,7843 | **A110** | A(49,50,51) | 117 ,1306 | **A125** | A(57,58,60) | 116 ,0783 | **A140** | A(72,71,73) | 106 ,3265 |
| **A81** | A(36,32,37) | 106 ,0748 | **A96** | A(40,41,46) | 107 ,7756 | **A111** | A(49,50,54) | 118 ,162 | **A126** | A(57,58,61) | 126 ,3516 |  |  |  |
| **A82** | A(32,35,38) | 109 ,1713 | **A97** | A(44,41,45) | 108 ,3332 | **A112** | A(51,50,54) | 124 ,7074 | **A127** | A(60,58,61) | 117 ,5701 |  |  |  |
| **A83** | A(32,35,39) | 109 ,1199 | **A98** | A(44,41,46) | 109 ,5216 | **A113** | A(50,51,52) | 121 ,9527 | **A128** | A(49,60,58) | 122 ,3589 |  |  |  |
| **A84** | A(32,35,40) | 113 ,0194 | **A99** | A(45,41,46) | 109 ,5886 | **A114** | A(50,51,55) | 119 ,391 | **A129** | A(54,62,63) | 110 ,8863 |  |  |  |
| **A85** | A(38,35,39) | 106 ,1809 | **A100** | A(41,46,47) | 119 ,596 | **A115** | A(52,51,55) | 118 ,6563 | **A130** | A(54,62,64) | 111 ,0337 |  |  |  |
| **A86** | A(38,35,40) | 109 ,5283 | **A101** | A(46,47,48) | 115 ,6548 | **A116** | A(47,52,51) | 119 ,4614 | **A131** | A(54,62,65) | 111 ,0131 |  |  |  |
| **A87** | A(39,35,40) | 109 ,5901 | **A102** | A(46,47,52) | 124 ,385 | **A117** | A(47,52,56) | 121 ,0196 | **A132** | A(63,62,64) | 108 ,2471 |  |  |  |
| **A88** | A(35,40,41) | 112 ,4383 | **A103** | A(48,47,52) | 119 ,9601 | **A118** | A(51,52,56) | 119 ,519 | **A133** | A(63,62,65) | 108 ,2527 |  |  |  |
| **A89** | A(35,40,42) | 110 ,0525 | **A104** | A(47,48,49) | 119 ,5506 | **A119** | A(50,54,57) | 118 ,7356 | **A134** | A(64,62,65) | 107 ,2699 |  |  |  |
| **A90** | A(35,40,43) | 110 ,0804 | **A105** | A(47,48,53) | 120 ,3074 | **A120** | A(50,54,62) | 120 ,299 | **A135** | A(4,71,14) | 114 ,4735 |  |  |  |

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| **Table S1(c)** Optimized parameters of C3 Dihedrals (D)( Degrees) | | | | | | | | |
| **D1** | D(6,1,2,3) | -0 ,1617 | **D34** | D(18,12,13,14) | -149 ,4557 | **D67** | D(15,14,71,4) | 66 ,3347 |
| **D2** | D(6,1,2,8) | 179 ,5292 | **D35** | D(18,12,13,19) | -27 ,8526 | **D68** | D(15,14,71,72) | -56 ,6291 |
| **D3** | D(7,1,2,3) | -179 ,8393 | **D36** | D(18,12,13,66) | 88 ,9453 | **D69** | D(15,14,71,73) | -171 ,8658 |
| **D4** | D(7,1,2,8) | -0 ,1484 | **D37** | D(67,12,13,14) | 93 ,6341 | **D70** | D(70,14,71,4) | -52 ,7908 |
| **D5** | D(2,1,6,5) | 0 ,1915 | **D38** | D(67,12,13,19) | -144 ,7627 | **D71** | D(70,14,71,72) | -175 ,7547 |
| **D6** | D(2,1,6,11) | -179 ,6708 | **D39** | D(67,12,13,66) | -27 ,9649 | **D72** | D(70,14,71,73) | 69 ,0086 |
| **D7** | D(7,1,6,5) | 179 ,869 | **D40** | D(13,12,17,16) | 69 ,5147 | **D73** | D(14,15,16,17) | -24 ,6002 |
| **D8** | D(7,1,6,11) | 0 ,0067 | **D41** | D(13,12,17,22) | -163 ,5375 | **D74** | D(14,15,16,21) | 95 ,1279 |
| **D9** | D(1,2,3,4) | -0 ,0909 | **D42** | D(18,12,17,16) | -169 ,8305 | **D75** | D(14,15,16,68) | -147 ,7648 |
| **D10** | D(1,2,3,9) | 179 ,586 | **D43** | D(18,12,17,22) | -42 ,8827 | **D76** | D(20,15,16,17) | -147 ,6615 |
| **D11** | D(8,2,3,4) | -179 ,7825 | **D44** | D(67,12,17,16) | -52 ,9724 | **D77** | D(20,15,16,21) | -27 ,9334 |
| **D12** | D(8,2,3,9) | -0 ,1055 | **D45** | D(67,12,17,22) | 73 ,9755 | **D78** | D(20,15,16,68) | 89 ,1739 |
| **D13** | D(2,3,4,5) | 0 ,306 | **D46** | D(12,13,14,15) | -33 ,1213 | **D79** | D(69,15,16,17) | 95 ,7218 |
| **D14** | D(2,3,4,71) | -179 ,15 | **D47** | D(12,13,14,70) | 83 ,435 | **D80** | D(69,15,16,21) | -144 ,5501 |
| **D15** | D(9,3,4,5) | -179 ,3709 | **D48** | D(12,13,14,71) | -158 ,4738 | **D81** | D(69,15,16,68) | -27 ,4428 |
| **D16** | D(9,3,4,71) | 1 ,1731 | **D49** | D(19,13,14,15) | -155 ,18 | **D82** | D(15,16,17,12) | -40 ,1374 |
| **D17** | D(3,4,5,6) | -0 ,2758 | **D50** | D(19,13,14,70) | -38 ,6237 | **D83** | D(15,16,17,22) | -168 ,8051 |
| **D18** | D(3,4,5,10) | 179 ,5142 | **D51** | D(19,13,14,71) | 79 ,4674 | **D84** | D(21,16,17,12) | -161 ,3973 |
| **D19** | D(71,4,5,6) | 179 ,1754 | **D52** | D(66,13,14,15) | 88 ,0025 | **D85** | D(21,16,17,22) | 69 ,935 |
| **D20** | D(71,4,5,10) | -1 ,0346 | **D53** | D(66,13,14,70) | -155 ,4413 | **D86** | D(68,16,17,12) | 81 ,9673 |
| **D21** | D(3,4,71,14) | 71 ,9863 | **D54** | D(66,13,14,71) | -37 ,3501 | **D87** | D(68,16,17,22) | -46 ,7004 |
| **D22** | D(3,4,71,72) | -165 ,2786 | **D55** | D(13,14,15,16) | 61 ,5947 | **D88** | D(12,17,22,23) | 73 ,0012 |
| **D23** | D(3,4,71,73) | -49 ,3448 | **D56** | D(13,14,15,20) | -176 ,2871 | **D89** | D(12,17,22,24) | -51 ,8032 |
| **D24** | D(5,4,71,14) | -107 ,4513 | **D57** | D(13,14,15,69) | -59 ,5618 | **D90** | D(12,17,22,25) | -167 ,2538 |
| **D25** | D(5,4,71,72) | 15 ,2838 | **D58** | D(70,14,15,16) | -55 ,1062 | **D91** | D(16,17,22,23) | -160 ,4402 |
| **D26** | D(5,4,71,73) | 131 ,2176 | **D59** | D(70,14,15,20) | 67 ,0121 | **D92** | D(16,17,22,24) | 74 ,7555 |
| **D27** | D(4,5,6,1) | 0 ,0304 | **D60** | D(70,14,15,69) | -176 ,2626 | **D93** | D(16,17,22,25) | -40 ,6952 |
| **D28** | D(4,5,6,11) | 179 ,8931 | **D61** | D(71,14,15,16) | -174 ,332 | **D94** | D(17,22,23,26) | 175 ,7495 |
| **D29** | D(10,5,6,1) | -179 ,7592 | **D62** | D(71,14,15,20) | -52 ,2137 | **D95** | D(17,22,23,27) | -62 ,3433 |
| **D30** | D(10,5,6,11) | 0 ,1035 | **D63** | D(71,14,15,69) | 64 ,5116 | **D96** | D(17,22,23,28) | 53 ,8915 |
| **D31** | D(17,12,13,14) | -29 ,095 | **D64** | D(13,14,71,4) | -170 ,913 | **D97** | D(24,22,23,26) | -58 ,6873 |
| **D32** | D(17,12,13,19) | 92 ,5081 | **D65** | D(13,14,71,72) | 66 ,1232 | **D98** | D(24,22,23,27) | 63 ,2198 |
| **D33** | D(17,12,13,66) | -150 ,694 | **D66** | D(13,14,71,73) | -49 ,1135 | **D99** | D(24,22,23,28) | 179 ,4546 |
|  |  |  |  |  |  |  |  |  |
| **D100** | D(25,22,23,26) | 56 ,661 | **D124** | D(33,31,32,35) | -57 ,5679 | **D148** | D(35,40,41,44) | -59 ,4266 |
| **D101** | D(25,22,23,27) | 178 ,5681 | **D125** | D(33,31,32,36) | 64 ,5529 | **D149** | D(35,40,41,45) | 60 ,8605 |
| **D102** | D(25,22,23,28) | -65 ,197 | **D126** | D(33,31,32,37) | -179 ,7535 | **D150** | D(35,40,41,46) | -179 ,2545 |
| **D103** | D(22,23,26,29) | -57 ,7221 | **D127** | D(34,31,32,35) | 58 ,0968 | **D151** | D(42,40,41,44) | 62 ,6404 |
| **D104** | D(22,23,26,30) | 58 ,0542 | **D128** | D(34,31,32,36) | -179 ,7824 | **D152** | D(42,40,41,45) | -177 ,0725 |
| **D105** | D(22,23,26,31) | -179 ,7275 | **D129** | D(34,31,32,37) | -64 ,0888 | **D153** | D(42,40,41,46) | -57 ,1875 |
| **D106** | D(27,23,26,29) | 179 ,5759 | **D130** | D(31,32,35,38) | -57 ,5789 | **D154** | D(43,40,41,44) | 178 ,4496 |
| **D107** | D(27,23,26,30) | -64 ,6478 | **D131** | D(31,32,35,39) | 58 ,0657 | **D155** | D(43,40,41,45) | -61 ,2634 |
| **D108** | D(27,23,26,31) | 57 ,5705 | **D132** | D(31,32,35,40) | -179 ,7355 | **D156** | D(43,40,41,46) | 58 ,6217 |
| **D109** | D(28,23,26,29) | 63 ,2069 | **D133** | D(36,32,35,38) | -179 ,7742 | **D157** | D(40,41,46,47) | 179 ,9202 |
| **D110** | D(28,23,26,30) | 178 ,9833 | **D134** | D(36,32,35,39) | -64 ,1296 | **D158** | D(44,41,46,47) | 59 ,27 |
| **D111** | D(28,23,26,31) | -58 ,7985 | **D135** | D(36,32,35,40) | 58 ,0691 | **D159** | D(45,41,46,47) | -59 ,4412 |
| **D112** | D(23,26,31,32) | 179 ,5201 | **D136** | D(37,32,35,38) | 64 ,6784 | **D160** | D(41,46,47,48) | -179 ,3315 |
| **D113** | D(23,26,31,33) | 57 ,3278 | **D137** | D(37,32,35,39) | -179 ,677 | **D161** | D(41,46,47,52) | 0 ,7029 |
| **D114** | D(23,26,31,34) | -58 ,2741 | **D138** | D(37,32,35,40) | -57 ,4782 | **D162** | D(46,47,48,49) | 179 ,9869 |
| **D115** | D(29,26,31,32) | 57 ,4141 | **D139** | D(32,35,40,41) | -179 ,3562 | **D163** | D(46,47,48,53) | 0 ,0488 |
| **D116** | D(29,26,31,33) | -64 ,7782 | **D140** | D(32,35,40,42) | 59 ,375 | **D164** | D(52,47,48,49) | -0 ,0459 |
| **D117** | D(29,26,31,34) | 179 ,6199 | **D141** | D(32,35,40,43) | -58 ,0282 | **D165** | D(52,47,48,53) | -179 ,984 |
| **D118** | D(30,26,31,32) | -58 ,0694 | **D142** | D(38,35,40,41) | 58 ,6873 | **D166** | D(46,47,52,51) | 179 ,9551 |
| **D119** | D(30,26,31,33) | 179 ,7383 | **D143** | D(38,35,40,42) | -62 ,5815 | **D167** | D(46,47,52,56) | -0 ,0119 |
| **D120** | D(30,26,31,34) | 64 ,1364 | **D144** | D(38,35,40,43) | -179 ,9847 | **D168** | D(48,47,52,51) | -0 ,0091 |
| **D121** | D(26,31,32,35) | -179 ,71 | **D145** | D(39,35,40,41) | -57 ,4211 | **D169** | D(48,47,52,56) | -179 ,9761 |
| **D122** | D(26,31,32,36) | -57 ,5891 | **D146** | D(39,35,40,42) | -178 ,6899 | **D170** | D(47,48,49,50) | 0 ,0643 |
| **D123** | D(26,31,32,37) | 58 ,1045 | **D147** | D(39,35,40,43) | 63 ,9069 | **D171** | D(47,48,49,60) | -179 ,8891 |
|  |  |  |  |  |  |  |  |  |
| **D172** | D(53,48,49,50) | -179 ,9975 | **D187** | D(51,50,54,62) | 0 ,1658 | **D200** | D(57,54,62,64) | 120 ,1814 |
| **D173** | D(53,48,49,60) | 0 ,0491 | **D188** | D(50,51,52,47) | 0 ,0483 | **D201** | D(57,54,62,65) | -120 ,5806 |
| **D174** | D(48,49,50,51) | -0 ,0261 | **D189** | D(50,51,52,56) | -179 ,9842 | **D202** | D(54,57,58,60) | -0 ,1242 |
| **D175** | D(48,49,50,54) | -179 ,9901 | **D190** | D(55,51,52,47) | -179 ,9664 | **D203** | D(54,57,58,61) | 179 ,9172 |
| **D176** | D(60,49,50,51) | 179 ,925 | **D191** | D(55,51,52,56) | 0 ,001 | **D204** | D(59,57,58,60) | 179 ,8673 |
| **D177** | D(60,49,50,54) | -0 ,039 | **D192** | D(50,54,57,58) | -0 ,0453 | **D205** | D(59,57,58,61) | -0 ,0913 |
| **D178** | D(48,49,60,58) | 179 ,8116 | **D193** | D(50,54,57,59) | 179 ,9639 | **D206** | D(57,58,60,49) | 0 ,2184 |
| **D179** | D(50,49,60,58) | -0 ,142 | **D194** | D(62,54,57,58) | 179 ,9562 | **D207** | D(61,58,60,49) | -179 ,8192 |
| **D180** | D(49,50,51,52) | -0 ,0308 | **D195** | D(62,54,57,59) | -0 ,0347 |  |  |  |
| **D181** | D(49,50,51,55) | 179 ,984 | **D196** | D(50,54,62,63) | 179 ,7985 |  |  |  |
| **D182** | D(54,50,51,52) | 179 ,9306 | **D197** | D(50,54,62,64) | -59 ,8171 |  |  |  |
| **D183** | D(54,50,51,55) | -0 ,0546 | **D198** | D(50,54,62,65) | 59 ,4208 |  |  |  |
| **D184** | D(49,50,54,57) | 0 ,1282 | **D199** | D(57,54,62,63) | -0 ,203 |  |  |  |
| **D185** | D(49,50,54,62) | -179 ,8732 |  |  |  |  |  |  |
| **D186** | D(51,50,54,57) | -179 ,8328 |  |  |  |  |  |  |

**Table S2** Experimental FT-IR and calculated wavenumbers (cm−1) and the Potential energy distribution (PED %) of the vibrational modes of C3.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | ***Assignment*** | **FT-IR**  **Exp.** | **Ref. Coumarin**  **ring** | **Ref. Piperidine ring** | **Ref. Cyclohexane ring** | **Calculated**  **B3LYP/6-311 ++ G(d,p)** | | **PED Analysis** |
|  |  |  | ***(Bahgat 2006, Arivazhagana et al., 2010, Avdović et al., 2018, Khemakhem et al., 2018, Kiraz et al., 2022, Malacaria et al., 2022)*** | ***(Chandra et al., 2011, Mahalakshmi and Balachandran 2014)*** | ***(Janani et al., 2021)*** | ***Scaling***  ***Wavenumbers*** | ***IR Int.*** | ***GAR2PED PED%*** |
| 1 | νCHcoumarin\_ring | 3085 | 3079 (Bahgat 2006);3071 (Avdović et al., 2018) |  | 3073 (Janani et al., 2021) | 3071 | 7 | νCHcoumarin\_ringsym(99) |
| 2 | νCHcoumarin\_ring |  | 3068 (Bahgat 2006) |  |  | 3067 | 1 | νCHcoumarin\_ring (99) |
| 3 | νCHcoumarin\_ring | 3059 |  |  |  | 3058 | 1 | νCHcoumarin\_ring (99) |
| 4 | νCHcoumarin\_ring |  | 3046 (Bahgat 2006) |  |  | 3044 | 6 | νCHcoumarin\_ringasy,(99) |
| 5 | νCHcyclohexane\_ring |  |  |  | 3039 (Janani et al., 2021) | 3043 | 18 | νCHcyclohexane\_ringsym,(95) |
| 6 | νCHcyclohexane\_ring | 3027 |  |  |  | 3031 | 32 | νCHcyclohexane\_ringasym,(99) |
| 7 | νCHcyclohexane\_ring |  |  |  |  | 3023 | 6 | νCHcyclohexane\_ringasym,(99) |
| 8 | νCHcyclohexane\_ring |  |  |  |  | 3011 | 4 | νCHcyclohexane\_ringasym,(99) |
| 9 | νCHcyclohexane\_ring |  |  |  | 3010 (Janani et al., 2021) | 3009 | 10 | νCHcyclohexane\_ringasym,(99) |
| 10 | νCH-CH3 |  | 2984 (Bahgat 2006) |  | 2983 (Janani et al., 2021) | 2979 | 18 | νCH-CHasym(99) |
| 11 | νCHpiperidine\_ring |  |  |  |  | 2950 | 40 | νCHpiperidine\_ring (91) |
| 12 | νCH-CH3 |  | 2931 (Bahgat 2006); 2933 (Arivazhagana et al., 2010) |  |  | 2939 | 10 | νCH-CH3asym,(100) |
| 13 | νCHpiperidine\_ring |  |  |  |  | 2937 | 107 | νCHpiperidine\_ringasym,(89) |
| 14 | νCH |  |  |  | 2936 (Janani et al., 2021) | 2936 | 21 | νCHasym,(79) |
| 15 | νCH | 2921 |  |  |  | 2924 | 95 | νCHasym,(84) |
| 16 | νCHpiperidine\_ringasy. |  |  | 2922 (Chandra et al., 2011) | 2925 (Janani et al., 2021) | 2920 | 37 | νCHpiperidine\_ringasym,(85) |
| 17 | νCH |  |  |  |  | 2911 | 27 | νCHasym,(97) |
| 18 | νCH, piperidine\_ring |  |  |  | 2909 (Janani et al., 2021) | 2909 | 4 | νCHpiperidine\_ringasym,(92) |
| 19 | νCH |  |  |  |  | 2897 | 22 | νCH,(80) |
| 20 | νCH |  |  |  |  | 2896 | 41 | νCHasym,(90) |
| 21 | νCH |  |  |  |  | 2894 | 40 | νCHsym,(92) |
| 22 | νCH |  |  |  |  | 2894 | 12 | νCH (54) |
| 23 | νCH |  |  |  |  | 2892 | 7 | νCH(74) |
| 24 | νCH-CH3sym, |  |  |  |  | 2892 | 11 | νCH-CH3sym,(100) |
| 25 | νCHpiperidine\_ring |  |  |  |  | 2890 | 9 | νCHpiperidine\_ring (93) |
| 26 | νCHsym, |  |  |  |  | 2883 | 36 | νCHsym,(88) |
| 27 | νCHasym, |  |  |  |  | 2881 | 4 | νCHasym,(89) |
| 28 | νCHpiperidine\_ringsym, |  |  |  |  | 2878 | 62 | νCHpiperidine\_ringsym,(99) |
| 29 | νCHasym, |  |  |  |  | 2875 | 0 | νCHasym,(91) |
| 30 | νCHpiperidine\_ringsym, |  |  |  |  | 2873 | 23 | νCHpiperidine\_ringsym,(86) |
| 31 | νCHsym, |  |  |  |  | 2872 | 68 | νCHsym,(82) |
| 32 | νCHpiperidine\_ringsym, |  |  | 2849 (Chandra et al., 2011) | 2850 (Janani et al., 2021) | 2872 | 10 | νCHpiperidine\_ringsym,(93) |
| 33 | νCHsym, |  |  |  |  | 2864 | 5 | νCHsym,(92) |
| 34 | νCHsym, |  |  |  |  | 2862 | 12 | νCHsym,(96) |
| 35 | νCHsym, |  |  |  |  | 2860 | 7 | νCHsym,(88) |
| 36 | νCHsym, | 2852 |  |  |  | 2858 | 2 | νCHsym,(87) |
| 37 | νCHpiperidine\_ring | 2767 |  |  |  | 2769 | 170 | νCHpiperidine\_ring,(98) |
| 38 | νCHpiperidine\_ring |  |  |  |  | 2755 | 79 | νCHpiperidine\_ring,(99) |
| 39 | νCHpiperidine\_ring |  |  |  |  | 2749 | 26 | νCHpiperidine\_ring,(98) |
| 40 | νC=Ocoumarin\_ring | 1719 | 1718 (Avdović et al., 2018);1727 (Arivazhagana et al., 2010, Kiraz et al., 2022) |  |  | 1724 | 777 | νC=Ocoumarin\_ring (78)+ νCC(9) |
| 41 | νC=Ccoumarin\_ring |  | 1612 (Malacaria et al., 2022);1613 (Kiraz et al., 2022) |  |  | 1618 | 107 | νC=Ccoumarin\_ring (51)+ δCCH (5) |
| 42 | νCCcoumarin\_ring | 1616 | 1617 (Bahgat 2006); 1625 (Arivazhagana et al., 2010) |  |  | 1615 | 498 | νCCcoumarin\_ring (60)+ δCCHring (25) |
| 43 | νCCcyclohexane\_ring |  |  |  |  | 1605 | 10 | νCCcyclohexane\_ring (56)+ δCCHring (23) |
| 44 | νCCcyclohexane\_ring | 1570 | 1566 (Arivazhagana et al., 2010) |  | 1559 (Janani et al., 2021) | 1584 | 1 | νCCcyclohexane\_ring (68)+ δCCHring (18) |
| 45 | νCCcoumarin\_ring | 1556 | 1557 (Bahgat 2006); 1525 (Arivazhagana et al., 2010) |  |  | 1544 | 127 | νCCcoumarin\_ring (70)+ δCCHring (5) |
| 46 | νCCcoumarin\_ring+ δCCHcoumarin\_ring | 1510 |  |  |  | 1500 | 16 | νCCcoumarin\_ring (40)+ δCCHringrock (37) |
| 47 | δCCHcyclohexane\_ring |  |  |  |  | 1490 | 14 | νCCcyclohexane\_ring (34)+ δCCHcyclohexane\_ringrock (58) |
| 48 | δCCHpiperidine\_ringscis, |  |  |  |  | 1490 | 4 | δCCHpiperidine\_ringscis (58) |
| 49 | δCCHscis | 1495 |  |  |  | 1485 | 33 | δCCHscis (82) |
| 50 | δCCHscis | 1477 |  |  |  | 1480 | 9 | δCCHscis (90) |
| 51 | δCCHscis |  |  |  |  | 1474 | 3 | δCCHscis (63)+ δCCHpiperidine\_ringscis (22) |
| 52 | δCCHscis | 1470 |  |  | 1469 (Janani et al., 2021) | 1472 | 5 | δCCHscis (41)+ δCCHpiperidine\_ringscis (43) |
| 53 | δCCHscis |  |  | 1466 (Chandra et al., 2011) |  | 1466 | 2 | δCCHscis (66)+ δCCHpiperidine\_ringscis (21) |
| 54 | δCCHpiperidine\_ringscis |  |  |  |  | 1463 | 2 | δCCHscis (23)+ δCCHpiperidine\_ringscis (61) |
| 55 | δCCHpiperidine\_ringscis |  |  |  |  | 1460 | 6 | δCCHscis (43)+ δCCHpiperidine\_ringscis (49) |
| 56 | δCCHscis |  |  |  |  | 1459 | 1 | δCCHscis (83)+ δCCHpiperidine\_ringscis (5) |
| 57 | δCCHscis |  |  |  |  | 1456 | 0 | δCCHscis (79)+ δCCHringscis (6) |
| 58 | δCCH-CH3-rock | 1452 |  |  |  | 1456 | 7 | δCCH-CH3-rock (86) |
| 59 | δCCHpiperidine\_ringscis |  |  | 1453 (Chandra et al., 2011) |  | 1453 | 3 | δCCHscis (40)+ δCCHpiperidine\_ringscis (35) |
| 60 | δCCHscis |  |  |  |  | 1453 | 0 | δCCHscis (93) |
| 61 | δCCHscis |  |  |  |  | 1452 | 0 | δCCHscis (89) |
| 62 | δCCH-CH3 | 1441 |  |  |  | 1448 | 10 | δCCH-CH3 (100) |
| 63 | δCCH cyclohexane\_ring |  |  |  | 1447 (Janani et al., 2021) | 1447 | 3 | νCC(22)+ δCCHcyclohexane\_ringrock, (53) |
| 64 | νCCcoumarinring+ δCCHcoumarinring | 1427 | 1417 (Arivazhagana et al., 2010) |  |  | 1423 | 16 | νCC(43)+ δCCHcoumarin\_ringrock, (32) |
| 65 | δCNHpiperidine\_ringwag, |  |  |  |  | 1398 | 3 | δCNHpiperidine\_ringwag (25)+ δCNHwag (52) |
| 66 | δCCHwag |  |  |  |  | 1395 | 7 | δCCHwag (67)+ νCC(9) |
| 67 | δCCH-CH3 | 1385 | 1356 (Bahgat 2006); 1373 (Arivazhagana et al., 2010) |  |  | 1384 | 83 | δCCH-CH3 (61)+ νCC(18) |
| 68 | δCNHpiperidineringwag |  |  |  |  | 1375 | 21 | δCNHpiperidine\_ringwag (35)+ δCNHwag (23) |
| 69 | δCCHwag |  |  |  |  | 1372 | 4 | δCCHwag (64)+ νCC(14) |
| 70 | δCCHwag |  |  |  |  | 1368 | 10 | δCCHwag (59)+ δCNHcoumarin\_ringwag (8) |
| 71 | δCCHpiperidine\_ringwag | 1368 |  | 1366 (Chandra et al., 2011);1364 (Mahalakshmi and Balachandran 2014) |  | 1367 | 10 | δCCHpiperidine\_ringwag (44)+ νCC(9)+ δCCHpiperidine\_ringscıss(9)+ δCCHpiperidine\_ringrock,(5) |
| 72 | δCCHcoumarin\_ringwag |  |  |  |  | 1366 | 117 | δCCHcoumarin\_ringwag (31)+ δCCHwag (17) |
| 73 | δCCHpiperidine\_ringwag | 1344 |  | 1340 (Mahalakshmi and Balachandran 2014) |  | 1351 | 20 | δCCHpiperidine\_ringwag (41)+ δCCHwag (16) |
| 74 | δCCHpiperidine\_ringwag |  |  |  |  | 1343 | 3 | δCCHpiperidine\_ringwag (40)+ δCCHpiperidine\_ringscıss (16)+ δCCHpiperidine\_ringtwist (6) |
| 75 | δCCHwag |  |  |  |  | 1338 | 1 | δCCHwag (48)+ δCCHpiperidine\_ringwag (9) |
| 76 | δCCHcyclohexane\_ringrock |  |  |  |  | 1333 | 2 | δCCHcyclohexane\_ringwag (18)+ δCCHwag (10)+ δCCHcyclohexane\_ringrock (31) |
| 77 | νCCcoumarin\_ring | 1325 | 1338 (Bahgat 2006); 1331 (Arivazhagana et al., 2010) |  |  | 1325 | 31 | νCCcoumarin\_ring(80) |
| 78 | δCCHring |  |  |  |  | 1321 | 2 | δCCHwag (16)+ δCCHpiperidine\_ringwag (14)+ δCCHcyclohexane\_ringrock (22) |
| 79 | δCCHring |  |  |  |  | 1317 | 1 | δCCHpiperidine\_ringwag (17)+ δCCHcyclohexane\_ringrock (16)+ νCC(11) |
| 80 | δCCHtwist |  |  |  |  | 1312 | 5 | δCCHtwist(58) |
| 81 | δCCHtwist |  |  |  |  | 1310 | 1 | δCCHtwist(72) |
| 82 | δCCHtwist |  |  |  |  | 1306 | 2 | δCCHtwist(19)+ νCC(12) |
| 83 | δCCHtwist |  |  |  |  | 1300 | 5 | δCCHtwist(10)+ νCC(13) |
| 84 | δCCHtwist+ δCCHwag |  |  |  |  | 1299 | 1 | δCCHtwist(36)+ δCCHwag (35) |
| 85 | δCCHtwist |  |  |  |  | 1295 | 0 | δCCHtwist(62) |
| 86 | δCCHtwist |  |  |  |  | 1289 | 3 | δCCHtwist(43) |
| 87 | νCOcoumarin\_ring | 1295 |  |  |  | 1286 | 370 | νCO(42)+ δCCHcoumarin\_ring(20)+ νCC(6) |
| 88 | δCCHpiperidineringtwist |  |  | 1290 (Mahalakshmi and Balachandran 2014) |  | 1282 | 5 | δCCHpiperidine\_ringtwist(44)+ δCCHpiperidine\_ringwag (5) |
| 89 | δCCHpiperidineringtwist |  |  |  |  | 1280 | 3 | δCCHpiperidine\_ringtwist(22)+ δCCHpiperidine\_ringrock(8)+ δCCHringrock(8)+ δCCHpiperidine\_ringsciss(12) |
| 90 | δCCHring | 1262 |  | 1263 (Mahalakshmi and Balachandran 2014) |  | 1267 | 4 | δCCHtwist(24)+ δCCHwag (12)+ δCCHpiperidine\_ringtwist(7) |
| 91 | δCCHcoumarinringrock |  |  |  |  | 1254 | 20 | δCCHcoumarin\_ringrock(51)+ νCC(17)+ νCO(9) |
| 92 | δCCHtwist+ δCCHwagg |  |  |  |  | 1252 | 1 | δCCHtwist(28)+ δCCHwagg(28)+ δCCHpiperidine\_ringtwist(5) |
| 93 | δCCHwag |  |  |  |  | 1249 | 3 | δCCHwag (20)+ δCCHpiperidine\_ringtwist(10)+ δCCHringwag (9) |
| 94 | δCCHpiperidineringtwist | 1241 |  |  |  | 1242 | 15 | δCCHpiperidine\_ringtwist(52)+ δCCHpiperidine\_ringwag (9) |
| 95 | δCCHtwist |  |  |  |  | 1219 | 1 | δCCHtwist(32)+ δCCHrock(13) |
| 96 | δCCHcoumarinringrock |  |  |  |  | 1217 | 9 | δCCHcoumarin\_ringrock(58)+ νCC(21) |
| 97 | δCCHwag |  |  |  |  | 1208 | 2 | δCCHwag (73) |
| 98 | νCCcyclohexanering |  |  |  |  | 1196 | 2 | νCCring(52)+ δCCCcyclohexane\_ring (14)+ δCCHcyclohexane\_ringrock(12)+ δCCHwag (5) |
| 99 | δCCHrock |  |  |  |  | 1190 | 9 | δCCHrock(12)+ δCCHringrock(6)+ δCCHtwist(5)+ δCCHringtwist(6)+ νCN(16) |
| 100 | δCCHcoumarinringrock | 1205 | 1211 (Bahgat 2006) |  |  | 1186 | 155 | δCCHcoumarin\_ringrock(31)+ νCCcoumarin\_ring(22)+ νCO(28) |
| 101 | δCCHpiperidineringtwist |  |  | 1170 (Chandra et al., 2011);1169 (Mahalakshmi and Balachandran 2014) |  | 1181 | 4 | δCCHtwist(13)+ δCCHpiperidine\_ringtwist(30)+ δCCHpiperidine\_ringrock(12)+ δCCHpiperidine\_ringsciss(7) |
| 102 | δCCHcyclohexaneringrock |  |  |  |  | 1175 | 0 | δCCHcyclohexane\_ringrock(77)+ νCCcyclohexane\_ring(15) |
| 103 | δCCHrock |  |  |  | 1161 (Janani et al., 2021) | 1167 | 1 | δCCHrock(22)+ δCCHpiperidine\_ringtwist(17)+ δCCHtwist(7) |
| 104 | δCCHrock | 1155 |  |  |  | 1159 | 4 | δCCHrock(25)+ δCCHpiperidine\_ringtwist(15)+ νCN(6) |
| 105 | δCCHcyclohexaneringrock |  |  |  |  | 1153 | 0 | δCCHcyclohexane\_ringrock(74)+ νCCcyclohexane\_ring(15) |
| 106 | νCNpiperidinering | 1144 |  | 1143 (Chandra et al., 2011) |  | 1147 | 31 | νCNpiperidine\_ring(35)+ δCCHpiperidine\_ringtwist(24) |
| 107 | δCCHcoumarinringrock |  |  |  |  | 1143 | 157 | δCCHcoumarin\_ringrock(45)+ νCC(17)+ νCN(6) |
| 108 | νCOcoumarinring |  | 1129 (Khemakhem et al., 2018);1131(Arivazhagana et al., 2010, Khemakhem et al., 2018) |  |  | 1124 | 180 | νCCcoumarin\_ring (19)+ νCOcoumarin\_ring (35)+ δCCHcoumarin\_ringrock(6) |
| 109 | δCCHtwist | 1107 |  |  |  | 1115 | 12 | νCC(5)+ νCN(6)+ δCCHtwist(9) |
| 110 | νCC | 1099 |  |  | 1093 (Janani et al., 2021) | 1095 | 43 | νCC(15)+ νCN(9) |
| 111 | νCC |  |  |  |  | 1093 | 4 | νCC(21)+ δCCHpiperidine\_ringrock(7) |
| 112 | νCCpiperidine\_ring |  |  | 1088 (Chandra et al., 2011) |  | 1086 | 16 | νCCpiperidine\_ring (45)+ νCNpiperidine\_ring (24) |
| 113 | νCCcyclohexanering+ δCCHcyclohexaneringrock | 1073 |  |  |  | 1077 | 15 | νCC(35)+ δCCHcyclohexaneringrock(12) |
| 114 | δCCHcoumarinringrock+ νCCcoumarinring | 1058 | 1050 (Arivazhagana et al., 2010) |  |  | 1058 | 118 | νCCcoumarin\_ring (24)+ νCOcoumarin\_ring (15)+ δCCHcoumarin\_ringrock(29) |
| 115 | νCC |  |  |  |  | 1051 | 7 | νCC(56) |
| 116 | νCC |  |  |  |  | 1044 | 1 | νCC(21)+δCCH (11)+δCCHpiperidine\_ring(rock)(5) |
| 117 | νCC |  |  |  |  | 1041 | 0 | νCC(83) |
| 118 | δCCH-CH3 | 1037 |  |  |  | 1035 | 2 | δCCH(70)+ΓCCCCcoumarin\_ring(rock)(12)+ ΓCCCHcoumarin\_ring(7)+δHCH (6) |
| 119 | νCC |  |  |  |  | 1032 | 1 | νCC(78) |
| 120 | νCC |  |  |  |  | 1030 | 5 | νCC(62)+ νCO(7) |
| 121 | νCCcyclohexane\_ring |  |  |  |  | 1026 | 6 | νCCcyclohexane\_ring(52)+ δCCHcyclohexane\_ring(rock)(16)+ δCCCcyclohexane\_ring(12) |
| 122 | νCO | 1025 | 1026 (Arivazhagana et al., 2010) |  |  | 1016 | 47 | νCO(33)+ νCCcoumarin\_ring(13)+ δCCHcoumarin\_ring(rock)(7)+ νCC(6) |
| 123 | δCCH(twist) |  |  |  |  | 1011 | 1 | δCCH(twist)(65)+ δCCH+NCH (6)+ δCCH+OCH (6) |
| 124 | δCCHcoumarin\_ring | 1001 |  |  |  | 1000 | 16 | δCCH(26)+ δCCCcoumarin\_ring(13)+ νCC(7) |
| 125 | νCCpiperidine\_ring |  |  |  |  | 997 | 5 | νCCpiperidine\_ring(20)+ νCC(20)+ δCCH(rock)(13)+ νCN(6) |
| 126 | δCCCcyclohexane\_ring |  |  |  |  | 993 | 0 | δCCCcyclohexane\_ring(62)+ νCCcyclohexane\_ring(30) |
| 127 | νCC |  |  | 983 (Chandra et al., 2011) |  | 981 | 3 | νCC(46)+ νCCpiperidine\_ring(6)+ δCCH+NCHpiperidine\_ring(rock)(6) |
| 128 | ΓCCCHclohexane\_ring |  |  |  |  | 976 | 5 | δCCH+NCHpiperidine\_ring(rock)(11)+ ΓCCCHcyclohexane\_ring(24)+ ΓCCCCcyclohexane\_ring(7)+ νCC(6) |
| 129 | ΓCCCHclohexane\_ring | 978 |  |  |  | 975 | 3 | ΓCCCHcyclohexane\_ring(60)+ ΓCCCCcyclohexane\_ring(11) |
| 130 | νCC | 972 |  | 971 (Chandra et al., 2011) |  | 971 | 2 | νCC(29)+ νCCpiperidine\_ring(24)+ δCCH+NCHpiperidine\_ring(rock)(7) |
| 131 | ΓCCCHclohexane\_ring |  |  |  |  | 959 | 0 | ΓCCCHcyclohexane\_ring(91)+ ΓCCCCcyclohexane\_ring(8) |
| 132 | νCC+ δCCH |  |  |  |  | 951 | 1 | νCCpiperidine\_ring(13)+ δCCH+NCHpiperidine\_ring(rock)(12)+ νCC(9)+ δCCH(rock)(6)+ δCCC+CCH(twist)(6) |
| 133 | νCO | 950 | 926 (Bahgat 2006) |  |  | 950 | 1 | νCO(22)+ νCOcoumarin\_ring(13)+ δCCCcoumarin\_ring(8)+ νCC(6)+ νCCcoumarin\_ring(6)+ δCCH(rock)(6) |
| 134 | δCCH |  |  |  |  | 935 | 0 | δCCH(rock+twist)(49)+ δCCH+OCH(rock)(11)+ δNCH+CCH(rock)(10) |
| 135 | νCCpiperidine\_rin+ νCNpiperidine\_rin+ δCCH | 932 |  | 933 (Chandra et al., 2011) |  | 921 | 10 | νCCpiperidine\_ring(22)+ νCNpiperidine\_ring(10)+ δCCHpiperidine\_ring(twist)(8)+ δCCN+CCCpiperidine\_ring(6) |
| 136 | ΓCCCHcoumarin\_ring |  |  |  |  | 920 | 4 | ΓCCCHcoumarin\_ring(81) |
| 137 | ΓCCCHcyclohexane\_ring | 896 |  |  |  | 903 | 2 | ΓCCCHcyclohexane\_ring(77)+ ΓCCCCcyclohexane\_ring(11) |
| 138 | δCCH piperidine\_ringrock, | 879 |  | 867 (Chandra et al., 2011);894 (Mahalakshmi and Balachandran 2014) |  | 881 | 7 | δCCH(rock) (15)+ δCCHpiperidine\_ring(rock)(11)+ νCNpiperidine\_ring(11)+ δNCH+CCHpiperidine\_ring(rock)(10)+ δCCN+CCCpiperidine\_ring(6) |
| 139 | νCOcoumarin\_ring |  | 872 (Bahgat 2006); 878 (Avdović et al., 2018) |  |  | 855 | 34 | νCOcoumarin\_ring(45)+ νCCcoumarin\_ring(12) |
| 140 | δCCH |  |  |  |  | 854 | 7 | δCCH(rock)(36)+ ΓCCCHcoumarin\_ring(12)+ δNCH+CCH(rock)(11)+ δCCH+OCH(rock)(11) |
| 141 | ΓCCCHcoumarin\_ring | 868 | 867 (Avdović et al., 2018) |  |  | 853 | 18 | ΓCCCHcoumarin\_ring(68)+ ΓCOCOcoumarin\_ring(8) |
| 142 | ΓCCCHcoumarin\_ring | 843 | 845 (Avdović et al., 2018) |  |  | 847 | 37 | ΓCCCHcoumarin\_ring(66)+ ΓCCCCcoumarin\_ring(14)+ ΓCCCOcoumarin\_ring(7) |
| 143 | ΓCCCHcyclohexane\_ring |  |  |  |  | 836 | 0 | ΓCCCHcyclohexane\_ring(58)+ δCCH(rock)(8) |
| 144 | ΓCCCHcyclohexane\_ring | 824 |  | 829 (Chandra et al., 2011) |  | 834 | 0 | ΓCCCHcyclohexane\_ring(43)+ δCCH(rock)(14)+ δNCH+CCHpiperidine\_ring(rock)(5)+ δCCHpiperidine\_ring(rock)(5) |
| 145 | νCC+δCCHcyclohexane\_ring | 803 |  | 803 (Chandra et al., 2011) |  | 806 | 2 | νCC(20)+ δCCHcyclohexane\_ring(18)+ νCCcyclohexane\_ring(16)+ δCCHpiperidine\_ring(rock)(7) |
| 146 | δCCH+ΓCCCH |  |  |  |  | 795 | 2 | δCCH(rock)(30)+ ΓCCCHcoumarin\_ring(20)+ δNCH+CCH(rock)(10)+ δCCH+OCH(rock)(7) |
| 147 | δCCO+CCCcoumarin\_ring |  | 793 (Arivazhagana et al., 2010) |  |  | 789 | 13 | δCCO+CCCcoumarin\_ring(30)+ νCCcoumarin\_ring(18)+ δCCCcoumarin\_ring(16)+ νCO(7)+ δCCO+OCOcoumarin\_ring(rock)(6) |
| 148 | νCC+δCCCpiperidine\_ring |  |  |  |  | 785 | 5 | νCCpiperidine\_ring(23)+ δCCCpiperidine\_ring(rock)(16)+ ΓCCCHcyclohexane\_ring(15)+ δCCH+NCHpiperidine\_ring(rock)(7)+ ΓCCCC(6) |
| 149 | ΓCCCHcoumarin\_ring | 781 |  |  |  | 783 | 16 | ΓCCCHcoumarin\_ring(53)+ ΓCCCO(5) |
| 150 | νCN+δCCH piperidine\_ringrock |  |  |  |  | 778 | 3 | νCN(29)+ δCCHpiperidine\_ring(rock)(24) |
| 151 | δCCH | 749 |  |  |  | 748 | 2 | δCCH(rock)(61)+ δCCH+NCH(rock)(9) |
| 152 | ΓCCCH+ΓCCCCcyclohexane\_ring | 737 |  |  |  | 738 | 28 | ΓCCCHcyclohexane\_ring(31)+ ΓCCCCcyclohexane\_ring(29)+ ΓCCCC(8) |
| 153 | δCCH(rock) |  |  |  |  | 725 | 0 | δCCH(rock)(76) |
| 154 | ΓCCCO+CCCCcoumarin\_ring |  |  |  |  | 721 | 6 | ΓCCCO+CCCCcoumarin\_ring(32)+ ΓCCCCcoumarin\_ring(29)+ ΓCOCO(22)+ ΓCCCC(5) |
| 155 | νCC+δCCCcoumarin\_ring | 725 |  |  |  | 719 | 7 | δCCCcoumarin\_ring(24)+ νCCcoumarin\_ring(24)+ δCCO+CCCcoumarin\_ring(13)+ δCOC(6)+ νCO(5) |
| 156 | δCCH(rock) | 712 |  |  |  | 717 | 4 | δCCH(rock)(79)+ ΓCCCC+CCCH(10) |
| 157 | ΓCCCCcyclohexane\_ring | 697 |  |  | 697, 700 (Janani et al., 2021) | 695 | 43 | ΓCCCCcyclohexane\_ring(58)+ ΓCCCHcyclohexane\_ring(34) |
| 158 | ΓCCCCcoumarin\_ring |  |  |  |  | 688 | 3 | ΓCCCCcoumarin\_ring(44)+ ΓCOCOcoumarin\_ring(29)+ ΓCCCO+CCCCcoumarin\_ring(9)+ ΓCCCO(8) |
| 159 | δCCCcoumarin\_ring |  | 670 (Avdović et al., 2018) |  |  | 679 | 3 | δCCCcoumarin\_ring(45)+ δCCO+CCCcoumarin\_ring(18)+ νCC(11)+ δCCO(5)+ νCOcoumarin\_ring(6) |
| 160 | δCCN+δCCCpiperidine\_ring |  |  |  |  | 640 | 3 | δCCN+CCCpiperidine\_ring(32)+ δCCHpiperidine\_ring(rock)(9)+ δCCH+NCHpiperidine\_ring(rock)(7)+ ΓCCCCcyclohexane\_ring(6)+ δNCC(6) |
| 161 | ΓCCCO+ΓCCCCcoumarin\_ring | 636 | 638 (Bahgat 2006) |  |  | 627 | 4 | ΓCCCO(41)+ ΓCCCCcoumarin\_ring(31)+ ΓCCCO+CCCCcoumarin\_ring(10)+ ΓCCCHcoumarin\_ring(5) |
| 162 | δCCCohexane\_ring | 622 |  |  |  | 622 | 0 | δCCCcyclohexane\_ring(87) |
| 163 | δCCCohexane\_ring | 611 |  |  |  | 586 | 4 | δCCCcyclohexane\_ring(43)+ ΓCCCCcyclohexane\_ring(12)+ δCCC(11) |
| 164 | δCCO+δOCOcoumarin\_ring+  νCCcoumarin\_ring |  |  |  |  | 569 | 14 | δCCO+OCOcoumarin\_ring(rock)(27)+ νCCcoumarin\_ring(20)+ δCCC(10)+ δCCO(8)+ δCOC(5) |
| 165 | δCCC+ δCOCcoumarin\_ring |  | 575 (Bahgat 2006) |  |  | 560 | 22 | δCCCcoumarin\_ring(21)+ δCOC(18)+ δCCO+CCCcoumarin\_ring(10)+ δCCO(10)+ δCCO+OCOcoumarin\_ring(9)+ δCCC(6) |
| 166 | ΓCCCCcoumarin\_ring |  | 552 (Bahgat 2006) |  |  | 536 | 1 | ΓCCCC(41)+ ΓCCCO+CCCCcoumarin\_ring(38)+ δCCH(rock)(6) |
| 167 | ΓCCCC |  |  |  |  | 520 | 5 | ΓCCCC(13)+ δCCN+CCCpiperidine\_ring(8)+ δCCCcyclohexane\_ring(6) |
| 168 | δCCO+CCC |  |  |  |  | 517 | 2 | δCCO+CCCcoumarin\_ring(26)+ δCCN+CCCpiperidine\_ring(5) |
| 169 | δCCN+CCCpiperidine\_ring |  |  | 487 (Chandra et al., 2011) |  | 507 | 2 | δCCN+CCC(52)+ δCNC(rock)(6)+ νCCpiperidine\_ring(5) |
| 170 | δCCC |  |  |  |  | 492 | 6 | δCCC(23)+ ΓCCCCcyclohexane\_ring(14)+ ΓCCCC(10)+ δNCC(9) |
| 171 | δCCC |  |  |  |  | 475 | 2 | δCCC(34)+ δCOC(6)+ δCCO(5)+ ΓCCCCcyclohexane\_ring(5)+ δCCO+CCCcoumarin\_ring(5) |
| 172 | ΓCCCCcoumarin\_ring |  |  |  |  | 450 | 4 | ΓCCCCcoumarin\_ring(54)+ ΓCCCO+CCCCcoumarin\_ring(14)+ ΓCCCO(11)+ ΓCCCHcoumarin\_ring(9) |
| 173 | ΓCCCCcyclohexane\_ring |  |  |  |  | 443 | 2 | ΓCCCCcyclohexane\_ring(22)+ δCCN+CCCpiperidine\_ring(12)+ δCCO+CCCcoumarin\_ring(9)+ ΓCCCC(9) |
| 174 | δCCO+CCCcoumarin\_ring |  |  |  |  | 432 | 3 | δCCO+CCCcoumarin\_ring(55)+ ΓCCCCcyclohexane\_ring(6) |
| 175 | ΓCCCCcyclohexane\_ring |  |  |  |  | 405 | 0 | ΓCCCCcyclohexane\_ring(83) |
| 176 | δCCC |  |  |  |  | 402 | 1 | δCCC(32)+ δCCO(16)+ δCNC(7)+ ΓCCCN(7)+ δNCC(5) |
| 177 | δCCN+CCCpiperidine\_ring |  |  | 395 (Chandra et al., 2011) |  | 394 | 1 | δCCN+CCCpiperidine\_ring(17)+ δCCC+CCH(12) |
| 178 | δCCC+CCH+ΓCCNC+CCCC |  |  |  |  | 377 | 1 | δCCC+CCH(rock)(16)+ ΓCCNC+CCCCpiperidine\_ring(14)+ ΓCCCCcyclohexane\_ring(13) |
| 179 | δCCC |  |  |  |  | 342 | 0 | δCCC(rock)(51)+ ΓCCCC+CCCH(12)+ δCCH(rock)(6) |
| 180 | ΓCCCNpiperidine\_ring |  |  |  |  | 336 | 4 | ΓCCCN(27)+ ΓCCNC+CCCC(14)+ δCCN+CCCpiperidine\_ring(11)+ δCCC(rock)(5) |
| 181 | δCNCpiperidine\_ring (rock) |  |  |  |  | 332 | 1 | δCNC(rock)(13)+ δCCC(rock)(11)+ ΓCCCN(10)+ δCCO+OCOcoumarin\_ring(rock)(8)+ δCCCcoumarin\_ring(5) |
| 182 | δCCCcoumarin\_ring (rock) |  |  |  |  | 314 | 0 | δCCC(rock)(34)+ δCNC(rock)(20)+ δCCO(6) |
| 183 | ΓCCCO+CCCCcoumarin\_ring |  |  |  |  | 280 | 4 | ΓCCCO+CCCCcoumarin\_ring(34)+ ΓCCCCcoumarin\_ring(33)+ ΓCCCC(12) |
| 184 | δCOC+ δCCC |  |  |  |  | 271 | 1 | δCOC(9)+ δCCC(9)+ δNCC(7)+ ΓCCCCcyclohexane\_ring(7)+ δCCC+CCH(twist)(5) |
| 185 | δCCC |  |  |  |  | 265 | 0 | δCCC(21)+ ΓCCCCcyclohexane\_ring(10)+ δCNC(9) |
| 186 | ΓCCCO+CCCCcoumarin\_ring |  |  |  |  | 252 | 1 | ΓCCCO+CCCCcoumarin\_ring(39)+ ΓCCCCcoumarin\_ring(31)+ ΓCCCHcoumarin\_ring(12)+ ΓCCOH(6) |
| 187 | δCCC+CCH(twist)+ ΓCCNC+CCCC |  |  |  |  | 230 | 1 | δCCC+CCH(twist)(16)+ ΓCCNC+CCCCpiperidine\_ring(15)+ δCNC(rock)(8)+ ΓCCCN(5) |
| 188 | δCCC |  |  |  |  | 217 | 0 | δCCC(32)+ ΓCCNC+CCCCpiperidine\_ring(8)+ δCCO(8)+ δNCC(5) |
| 189 | ΓCCCCcyclohexane\_ring |  |  |  |  | 199 | 1 | ΓCCCCcyclohexane\_ring(24)+ δCCC+CCH(twist)(16)+ ΓCCNC+CCCCpiperidine\_ring(9) |
| 190 | ΓCCCHcoumarin\_ring |  |  |  |  | 196 | 1 | ΓCCCH(63)+ ΓCCCO+CCCCcoumarin\_ring(27) |
| 191 | ΓCCCN+CCCCpiperidine\_ring |  |  |  |  | 168 | 1 | ΓCCCN+CCCCpiperidine\_ring(58) |
| 192 | ΓCCCH+CCCC |  |  |  |  | 160 | 0 | ΓCCCH+CCCC(57)+ ΓCCCO+CCCH+OCCH(15) |
| 193 | ΓCCCH+CCCC |  |  |  |  | 158 | 0 | ΓCCCH+CCCC(68)+ ΓCCNC+CNCH(7) |
| 194 | δCCC+ΓCCCN+CCCC |  |  |  |  | 157 | 0 | δCCC(23)+ ΓCCCN+CCCCpiperidine\_ring(18)+ ΓCCCN(7)+ δCCO(6) |
| 195 | ΓCCCHcoumarin\_ring |  |  |  |  | 156 | 0 | ΓCCCH(50)+ ΓCCCO+CCCCcoumarin\_ring(25)+ ΓCCCC(7) |
| 196 | ΓCCCC+CCCH |  |  |  |  | 137 | 1 | ΓCCCC+CCCH(31)+ ΓCCNC+CNCH(20)+ ΓCCOH(9)+ ΓCCNC+CCCCpiperidine\_ring(8)+ ΓCCCH+CCCO+OCCH(6) |
| 197 | ΓCCNC+CCCC |  |  |  |  | 129 | 0 | ΓCCNC+CCCCpiperidine\_ring(17)+ ΓCCCC+CCCH(12)+ ΓCCOH(12)+ ΓCCCH+CCCO+OCCH(10)+ ΓCOCC+COCH(7)+ ΓCCCO+CCCCcoumarin\_ring(7)+ ΓCCCN+NCCH+CCCH(5) |
| 198 | ΓCCCN+CCCC |  |  |  |  | 117 | 0 | ΓCCCN+CCCCpiperidine\_ring(28)+ ΓCOCC+COCH(6)+ δCCC(5) |
| 199 | ΓCCCC+CCCH |  |  |  |  | 109 | 1 | ΓCCCC+CCCH(27)+ ΓCCNC+CNCH(14)+ ΓCCCO+CCCCcoumarin\_ring(12)+ ΓCCOH(10)+ ΓCOCC+COCH(5) |
| 200 | ΓCCCO+CCCC |  |  |  |  | 102 | 0 | ΓCCCO+CCCCcoumarin\_ring(19)+ ΓCCCC+CCCH(8)+ ΓCCOH(6)+ ΓCCCN+NCCH+CCCH(6)+ ΓCCNC+CNCH(5) |
| 201 | ΓCCCO+CCCC |  |  |  |  | 92 | 0 | ΓCCCO+CCCCcoumarin\_ring(16)+ ΓCCCCcoumarin\_ring(16)+ ΓCCCC+CCCH(12) |
| 202 | ΓCCCO+CCCC |  |  |  |  | 85 | 0 | ΓCCCO+CCCCcoumarin\_ring(68)+ ΓCCCCcoumarin\_ring(7) |
| 203 | δCCC |  |  |  |  | 79 | 0 | δCCC(22)+ δCOC(9)+ ΓCCCC+CCCH(6)+ ΓCCNC+CCCCpiperidine\_ring(5) |
| 204 | ΓCCCC+CCCH |  |  |  |  | 62 | 0 | ΓCCCC+CCCH(33)+ ΓCCOH(11)+ ΓCCNC+CNCH(5) |
| 205 | ΓCCNC+CNCH |  |  |  |  | 58 | 0 | ΓCCNC+CNCH(47)+ ΓCCCC+CCCH(7)+ ΓCCCH+CCCO+OCCH(7)+ ΓCOCC+COCH(6) |
| 206 | ΓCCCC+CCCH |  |  |  |  | 50 | 0 | ΓCCCC+CCCH(34)+ ΓCCCC(15)+ δCCC(12) |
| 207 | δCCC |  |  |  |  | 44 | 0 | δCCC(23)+ ΓCCCC+CCCH(14)+ δCOC(15)+ δNCC(7) |
| 208 | ΓCCCC+CCCH |  |  |  |  | 32 | 0 | ΓCCCC+CCCH(24)+ ΓCCOH(14)+ ΓCOCC+COCH(11)+ ΓCCNC+CCCCpiperidine\_ring(15) |
| 209 | ΓCCCC+CCCH |  |  |  |  | 29 | 0 | ΓCCCC+CCCH(39)+ ΓCCNC+CCCC(12) |
| 210 | ΓCCNC+CCCC |  |  |  |  | 18 | 0 | ΓCCNC+CCCCpiperidine\_ring(19)+ ΓCOCC+COCH(11)+ ΓCCOH(10)+ δCCC(13)+ ΓCCNC+CNCH(5)+ δCCO(5) |
| 211 | ΓCCNC+CCCC |  |  |  |  | 14 | 0 | ΓCCNC+CCCCpiperidine\_ring(27)+ ΓCOCC+COCH(19)+ ΓCOCH(8)+ ΓCCCN+NCCH+CCCH(8) |
| 212 | δCCC |  |  |  |  | 10 | 1 | δCCC(25)+ ΓCCNC+CNCH (11)+ ΓCCCN+NCCH+CCCH(8)+ δNCC(8)+ ΓCCCC+CCCH (5) |
| 213 | ΓCOCC+COCH+ ΓCCOH |  |  |  |  | 8 | 1 | ΓCOCC+COCH(25)+ ΓCCOH(22)+ ΓCCCC+CCCH(13)+ ΓCCCO+CCCH+OCCH(11)+ ΓCCCN+NCCH+CCCH(6) |

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| **Table S3(a)** The calculated NMR spectra ( SCF GIAO Magnetic shielding)  values for element H only of C3 molecule with RB3LYP/6-311++g(d,p) basis set using methanol solution | | | | | **Table S3(b)** The calculated NMR spectra ( SCF GIAO Magnetic shielding)values for element C only of C3 molecule with  RB3LYP/6-311++g(d,p) basis set using methanol solution | | | | | |
| No References values | | | Reference: TMS B3LYP/6-311+G(2d,p) GIAO  Reference shielding:  31,8821 ppm | | No References values | | | Reference: TMS B3LYP/6311+G(2d,p) GIAO  Reference shielding: 182,466 ppm | | |
| **Atoms** | **Shielding(ppm)** | **Degeneracy** | **Shift (ppm)** | **Degeneracy** | **Atoms** | **Shielding(ppm)** | **Degeneracy** | **Shift (ppm)** | | **Degeneracy** |
| 55-H | 24,0642 | 1 | 7,8179 | 1 | 47-C | 11,8147 | 1 | 170,6509 | 1 | |
| 7-H | 24,2038 | 2 | 7,6783 | 2 | 58-C | 17,4877 | 1 | 164,9779 | 1 | |
| 11-H | 24,2194 | 2 | 7,6627 | 2 | 54-C | 19,2977 | 1 | 163,1679 | 1 | |
| 10-H | 24,3651 | 2 | 7,517 | 2 | 49-C | 19,7004 | 1 | 162,7652 | 1 | |
| 8-H | 24,3933 | 2 | 7,4888 | 2 | 4-C | 33,8463 | 1 | 148,6193 | 1 | |
| 9-H | 24,6831 | 1 | 7,199 | 1 | 5-C | 46,5078 | 1 | 135,9578 | 1 | |
| 56-H | 24,8887 | 1 | 6,9934 | 1 | 3-C | 48,0839 | 1 | 134,3817 | 1 | |
| 53-H | 24,9443 | 1 | 6,9378 | 1 | 2-C | 50,3563 | 1 | 132,1093 | 1 | |
| 59-H | 25,727 | 1 | 6,1551 | 1 | 51-C | 50,6094 | 1 | 131,8562 | 1 | |
| 44-H | 28,0295 | 2 | 3,8526 | 2 | 6-C | 51,6287 | 1 | 130,8369 | 1 | |
| 45-H | 28,0542 | 2 | 3,8279 | 2 | 1-C | 51,7121 | 1 | 130,7535 | 1 | |
| 18-H | 29,1206 | 1 | 2,7615 | 1 | 50-C | 63,3424 | 1 | 119,1232 | 1 | |
| 73-H | 29,1801 | 1 | 2,702 | 1 | 57-C | 68,8001 | 1 | 113,6655 | 1 | |
| 64-H | 29,2974 | 3 | 2,5847 | 3 | 52-C | 71,1775 | 1 | 111,2881 | 1 | |
| 65-H | 29,3103 | 3 | 2,5718 | 3 | 48-C | 74,414 | 1 | 108,0516 | 1 | |
| 21-H | 29,3419 | 3 | 2,5402 | 3 | 41-C | 111,0115 | 1 | 71,4541 | 1 | |
| 70-H | 29,6354 | 1 | 2,2467 | 1 | 22-C | 122,9575 | 1 | 59,5081 | 1 | |
| 25-H | 29,7069 | 4 | 2,1752 | 4 | 16-C | 128,2094 | 1 | 54,2562 | 1 | |
| 19-H | 29,7335 | 4 | 2,1486 | 4 | 12-C | 135,8769 | 1 | 46,5887 | 1 | |
| 68-H | 29,7388 | 4 | 2,1433 | 4 | 71-C | 136,2947 | 1 | 46,1709 | 1 | |
| 63-H | 29,7394 | 4 | 2,1427 | 4 | 14-C | 143,4467 | 1 | 39,0189 | 1 | |
| 67-H | 29,9524 | 1 | 1,9297 | 1 | 31-C | 146,7435 | 1 | 35,7221 | 1 | |
| 24-H | 30,0265 | 4 | 1,8556 | 4 | 32-C | 146,8601 | 1 | 35,6055 | 1 | |
| 72-H | 30,0691 | 4 | 1,813 | 4 | 13-C | 147,2004 | 1 | 35,2652 | 1 | |
| 42-H | 30,0835 | 4 | 1,7986 | 4 | 40-C | 148,3828 | 1 | 34,0828 | 1 | |
| 43-H | 30,0889 | 4 | 1,7932 | 4 | 23-C | 148,8558 | 1 | 33,6098 | 1 | |
| 27-H | 30,2927 | 1 | 1,5894 | 1 | 26-C | 150,1501 | 1 | 32,3155 | 1 | |
| 20-H | 30,5239 | 7 | 1,3582 | 7 | 15-C | 152,1391 | 1 | 30,3265 | 1 | |
| 36-H | 30,5374 | 7 | 1,3447 | 7 | 35-C | 152,7584 | 1 | 29,7072 | 1 | |
| 37-H | 30,55 | 7 | 1,3321 | 7 | 62-C | 161,473 | 1 | 20,9926 | 1 | |
| 33-H | 30,566 | 7 | 1,3161 | 7 |  |  |  |  |  | |
| 34-H | 30,5836 | 7 | 1,2985 | 7 |  |  |  |  |  | |
| 38-H | 30,5896 | 7 | 1,2925 | 7 |  |  |  |  |  | |
| 39-H | 30,5913 | 7 | 1,2908 | 7 |  |  |  |  |  | |
| 28-H | 30,6483 | 1 | 1,2338 | 1 |  |  |  |  |  | |
| 30-H | 30,7011 | 2 | 1,181 | 2 |  |  |  |  |  | |
| 29-H | 30,7113 | 2 | 1,1708 | 2 |  |  |  |  |  | |
| 66-H | 30,8033 | 1 | 1,0788 | 1 |  |  |  |  |  | |
| 69-H | 30,9178 | 1 | 0,9643 | 1 |  |  |  |  |  | |

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| **Table S4** Binding energies of docking systems formed with possible receptors of the C3 molecule | | |
| **Docked pose numbers** | **Docking score (kcal/mol)** | |
|  | **(PDB ID:1OG5)** | **(PDB ID:1M17)** |
| 1 | -7.828 | -5.246 |
| 2 | -7.457 | -5.181 |
| 3 | -7.451 | -5.152 |
| 4 | -7.441 | -5.112 |
| 5 | -7.301 | -4.573 |
| 6 | -6.786 | -4.277 |
| 7 | -6.616 | -4.135 |
| 8 | -6.588 | -4.082 |
| 9 | -6.534 | -4.054 |
| 10 | -6.513 | -4.042 |
| 11 | -6.481 | -3.906 |
| 12 | -6.473 | -3.884 |
| 13 | -6.435 | -3.868 |
| 14 | -6.179 | -3.780 |
| 15 | -6.116 | -3.651 |
| 16 | -5.849 | -3.419 |
|  | **Energy (kcalmol)** | |
|  |  |  |
| **Potential Energy-OPLS3** | -1.536.703 | -1.041.490 |
| **RMS Derivative-OPLS3** | 0.114 | 0.081 |
| **Stretch Energy-OPLS3** | 217.454 | 144.083 |
| **Bend Energy-OPLS3** | 1.033.579 | 654.684 |
| **LJ-14 Energy-OPLS3** | 2.235.982 | 1.431.082 |
| **El-14 Energy-OPLS3** | 813.285 | 572.533 |
| **Van der Waals Energy-OPLS3** | -4.382.924 | -2.777.203 |
| **Electrostatic Energy-OPLS3** | -2.496.866 | -1.639.679 |
| **Dihedral Energy-OPLS3** | 893.966 | 486.623 |

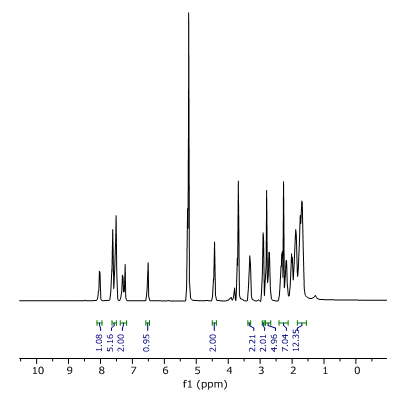
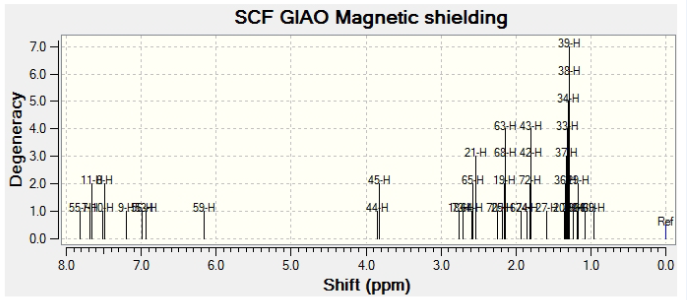
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| --- | --- | --- | --- |
| **Table S5** Virtual screening of synthesized C3 showing drug-likeliness by Molinspiration and Swissadme servers | | | |
| ***Molinspiration*** | | | |
| **Molinspiration property engine** | | **Molinspiration bioactivity score** | |
| **miLogP** | 8.33 | **GPCR ligand** | 0.20 |
| **TPSA** | 38.78 | **Ion channel modulator** | 0.09 |
| **natoms** | 34 | **Kinase inhibitor** | -0.16 |
| **MW** | 473.74 | **Nuclear receptor ligand** | 0.35 |
| **nON** | 4 | **Protease inhibitor** | 0.22 |
| **nOHNH** | 0 | **Enzyme inhibitor** | 0.28 |
| **nviolations** | **1** |  |  |
| **nrotb** | 12 |  |  |
| **volume** | 499.96 |  |  |
| ***SwissADME properties*** | | | |
| **Physicochemical Properties** | | **Lipophilicity** | |
| **Polar surface area** | 38.77 Å² | **LogPO/W(iLOGP)** | 5.97 |
| **No. of H-bond acceptors** | 4 | **LogPO/W(XLOGP3)** | 7.79 |
| **No. of H-bond donors** | 0 | **LogPO/W(WLOGP)** | 6.69 |
| **Molar refractivity** | 146.58 | **LogPO/W(MLOGP)** | 4.97 |
| **Rotatable bond count** | 12 | **LogPO/W(SILICOS-IT)** | 6.60 |
| **Heavy atom count** | 34 | **Consensus LogPO/W** | 6.40 |
| **Aromatic Heavy atom count** | 0 | **Water Solubility** | |
| **Lipinski's rule of five** | 1 | **Log S (ESOL)** | -6.89 |
| **Bioavailability** | 0.55 | **Log S (Ali)** | -8.45 |
| **MW** | 473.73 g/mol | **Log S (SILICOS-IT)** | -6.62 |
|  |  |  |  |
| **Pharmacokinetics** | | **Druglikeness** | |
| **GI absoption** | High | **Lipinski** | **Yes; 1 violation: MLOGP>4.15** |
| **BBBpermeant** | No | **Ghose** | No; 3 violations: WLOGP>5.6, MR>130, #atoms>70 |
| **CYP3A4 inhibitor** | Yes | **Veber** | No; 1 violation: Rotors>10 |
| **Log KP (SKİN PERMEATION)** | -3.66 cm/s | **Muegge** | No; 1 violation: XLOGP3>5 |
|  |  | **Bioavailability Score** | **0.55** |

|  |  |  |  |
| --- | --- | --- | --- |
| **Table S6** Virtual screening of synthesized C3 showing ADME,Drug-likeliness, Toxicity by PreADMET server | | | |
| ***ADME*** | | | |
| **AlogP98 value** | 7.444900 | **AmolRef** | 141.322700 |
| **BBB** | 11.9686 | **HIA** | 97.943746 |
| **Buffer\_solubility\_mg\_L** | 1.05034 | **MDCK** | 55.5294\* |
| **Caco2** | 56.4028 | **Pgp\_inhibition** | Inhibitor |
| **CYP\_2C19\_inhibition** | Non | **Plasma\_Protein\_Binding** | 90.136011 |
| **CYP\_2C9\_inhibition** | Non | **Pure\_water\_solubility\_mg\_L** | 0.344103 |
| **CYP\_2D6\_inhibition** | Inhibitor | **Skin\_Permeability** | -2.42711 |
| **CYP\_2D6\_substrate** | Substrate | **Solvation Free Energy** | -10.030000 |
| **CYP\_3A4\_inhibition** | Non |  |  |
| **CYP\_3A4\_substrate** | Substrate |  |  |
|  |  |  |  |
|  | | | |
| ***Druglikeness*** | | | |
| **CMC\_like\_Rule** | Not qualified | **MDDR\_like\_Rule** | **Drug-like** |
| **CMC\_like\_Rule\_Violation\_Fields** | AlopP98\_value, AMolRef, No\_Total\_atoms | **MDDR\_like\_Rule\_Violation\_Fields** | - |
| **CMC\_like\_Rule\_Violations** | 3 | **MDDR\_like\_Rule\_Violations** | 0 |
| **Lead-like\_Rule\_Violation\_Fields** | Molecular\_weight, AlopP98\_value | **Rule\_of\_Five** | **Suitable** |
| **Lead\_like\_Rule** | Violated | **Rule\_of\_Five\_Violation\_Fields** | AlopP98\_value |
| **Lead-like\_Rule\_Violation** | 2 |  |  |
| **WDI\_like\_Rule** | Out of 90% cutoff | **Rule\_of\_Five\_Violations** | **1** |
| **WDI\_like\_Rule\_Violation\_Fields** | AlopP98\_value, AMolRef, Kier\_flexibility, Kier\_alpha\_01, Kier\_alpha\_02, Kier\_alpha\_03, VChi\_00, VChi\_01, VChi\_02, VChi\_03\_path, Wiener\_index |  | |
| **WDI\_like\_Rule\_Violations** | 11 |  |  |
|  | | | |
| **Toxicity** | | | |
| **algae\_at** | 0.00156005 | **medaka\_at** | 5.4668e-006 |
| **Ames\_test** | **non-mutagen** | **minnow\_at** | 6.3585e-006 |
| **Carcino\_Mouse** | **negative** | **TA100\_10RLI** | negative |
| **Carcino\_Rat** | **negative** | **TA100\_NA** | negative |
| **daphnia\_at** | 0.00155476 | **TA1535\_10RLI** | negative |
| **hERG\_inhibition** | medium\_risk | **TA1535\_NA** | negative |
|  |  |  |  |

|  |  |  |  |
| --- | --- | --- | --- |
| **Table S7** Pharmacokinetic Properties of synthesized C3 showing **ADME and Toxicity** by pkCSM server | | | |
| ***Absoption*** | **Descriptor** | **C3** | **Unit** |
| **Water Solubility** | **-5.965** | Numeric  (log mol/L) |
| **Caco2 permeability** | **1.147** | Numeric  (log Papp in 10-6 cm/s) |
| **Intestinal absorption (human)** | **90.036** | Numeric (% Absorbed) |
| **Skin Permeability** | **-2.811** | Numeric (log Kp) |
| **P-glycoprotein substrate** | **Yes** | Categorical (Yes/No) |
| **P-glycoprotein I inhibitor** | **Yes** | Categorical (Yes/No) |
| **P-glycoprotein II inhibitor** | **Yes** | Categorical (Yes/No) |
| ***Distribution*** | **VDss (human)** | **0.658** | Numeric (log L/kg) |
| **Fraction unbound (human)** | **0** | Numeric (Fu) |
| **BBB permeability** | **0.839** | Numeric (log BB) |
| **CNS permeability** | **-2.009** | Numeric (log PS) |
| ***Metabolism*** | **CYP2D6 substrate** | **Yes** | Categorical (Yes/No) |
| **CYP3A4 substrate** | **Yes** | Categorical (Yes/No) |
| **CYP1A2 inhibitior** | **No** | Categorical (Yes/No) |
| **CYP2C19 inhibitior** | **No** | Categorical (Yes/No) |
| **CYP2C9 inhibitior** | **No** | Categorical (Yes/No) |
| **CYP2D6 inhibitior** | **No** | Categorical (Yes/No) |
| **CYP3A4 inhibitior** | **No** | Categorical (Yes/No) |
| ***Excretion*** | **Total Clearance** | **1.287** | Numeric (log ml/min/kg) |
| **Renal OCT2 substrate** | **Yes** | Categorical (Yes/No) |
| ***Toxicity*** | **AMES toxicity** | **No** | Categorical (Yes/No) |
| **Max. tolerated dose (human)** | **-0.418** | Numeric (log mg/kg/day) |
| **hERG I inhibitor** | **No** | Categorical (Yes/No) |
| **hERG II inhibitor** | **Yes** | Categorical (Yes/No) |
| **Oral Rat Acute Toxicity (LD50)** | **2.902** | Numeric (mol/kg) |
| **Oral Rat Chronic Toxicity (LOAEL)** | **1.96** | Numeric (log mg/kg\_bw/day) |
| **Skin Sensitisation** | **No** | Categorical (Yes/No) |
| ***T.Pyriformis* toxicity** | **0.545** | Numeric (log ug/L) |
| ***Minnow toxicity*** | **-0.843** | Numeric (log mM) |

|  |  |  |
| --- | --- | --- |
| **Table S8.** The hydrogen bonding interactions of C3 bounded by B-DNA dodecamer. | | |
| **Donor Atom** | **Acceptor Atom** | **Bond Length (Å)** |
| H7 of DA5 (chain A) | O55 of C3 | 2.6 |
| H61 of DA6 (chain A) | O55 of C3 | 2.3 |
| H7 of DG16 (chain B) | O74 of C3 | 3.1 |
| H61 of DA17 (chain B) | O74 of C3 | 1.8 |
| H7 of DA17 (chain B) | O74 of C3 | 2.2 |
| H61 of DA17 (chain B) | O61 of C3 | 3.0 |
| H62 of DA18 (chain B) | O61 of C3 | 2.9 |
| H61 of DA18 (chain B) | O61 of C3 | 3.0 |

|  |  |  |  |
| --- | --- | --- | --- |
| **TableS9:** The affinity energies and RMSD values of C3 bounded by B-DNA dodecamer**.** | | | |
|  | | | |
| **Mode** | **Affinity (kcal/mol)** | **Dist from rmsd l.b.** | **Best mode rmsd l.b.** |
| 1 | -5.5 | 0.000 | 0.000 |
| 2 | -5.2 | 2.744 | 6.884 |
| 3 | -5.1 | 2.417 | 5.106 |
| 4 | -5.1 | 3.292 | 7.025 |
| 5 | -5.1 | 2.522 | 3.994 |
| 6 | -5.1 | 2.768 | 6.125 |
| 7 | -5.0 | 2.474 | 7.091 |
| 8 | -5.0 | 1.510 | 2.131 |
| 9 | -5.0 | 1.862 | 4.110 |

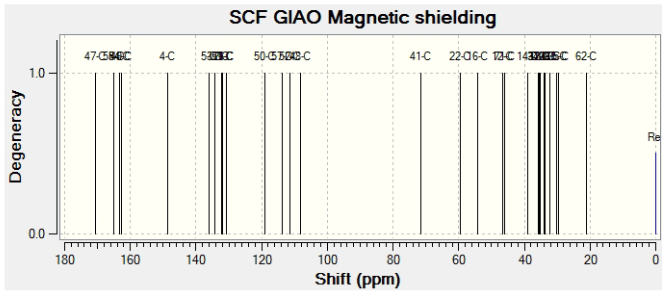


**(b)**

**(a)**

**Fig. S1** The experimental(a) and calculated(b) 1H-NMR spectra of C3

**Fig. S1** The experimental(a) and calculated(b) 1H-NMR spectra of C3



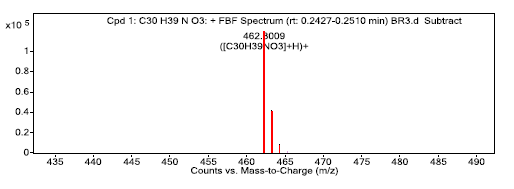
**(b)**

**(a)**

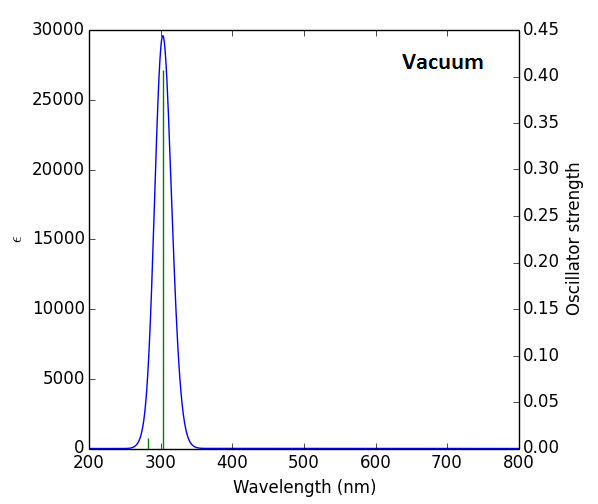
**Fig. S2** The experimental(a) and calculated(b) 13C-NMR spectra of C3

metin içeren bir resim

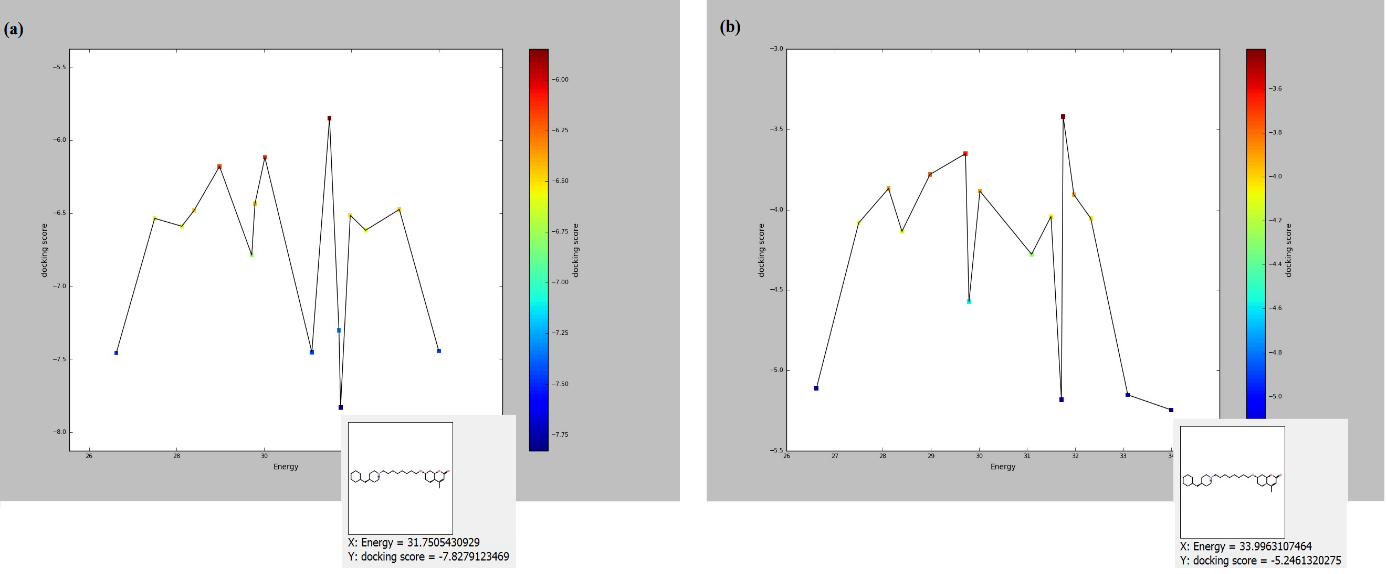
Açıklama otomatik olarak oluşturuldu



**Fig. S3** The LC-MS (ESI-QTOF) spectra of C3



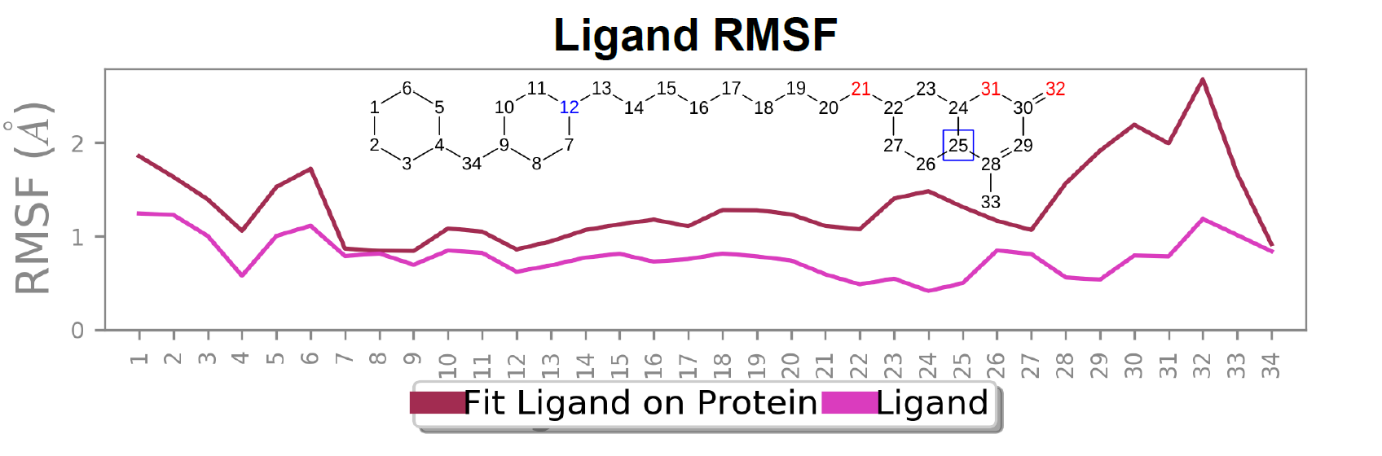
**Fig. S4** The calculated UV spectra of C3 in vacuum

**Fig. S5** The energy of the possible binding poses and docking score between C3 and target receptors CYP450 (a), EGFR (b)

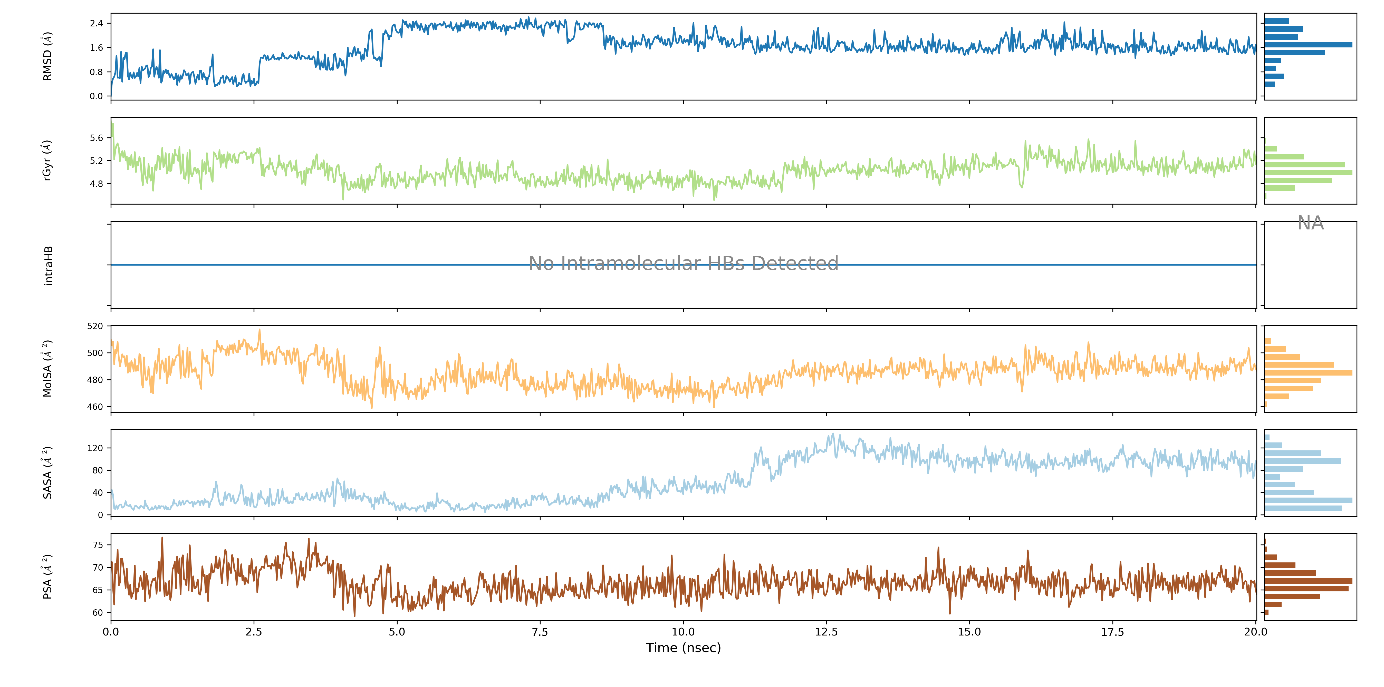
metin, iç mekan, ekran, elektronik eşyalar içeren bir resim

Açıklama otomatik olarak oluşturuldu

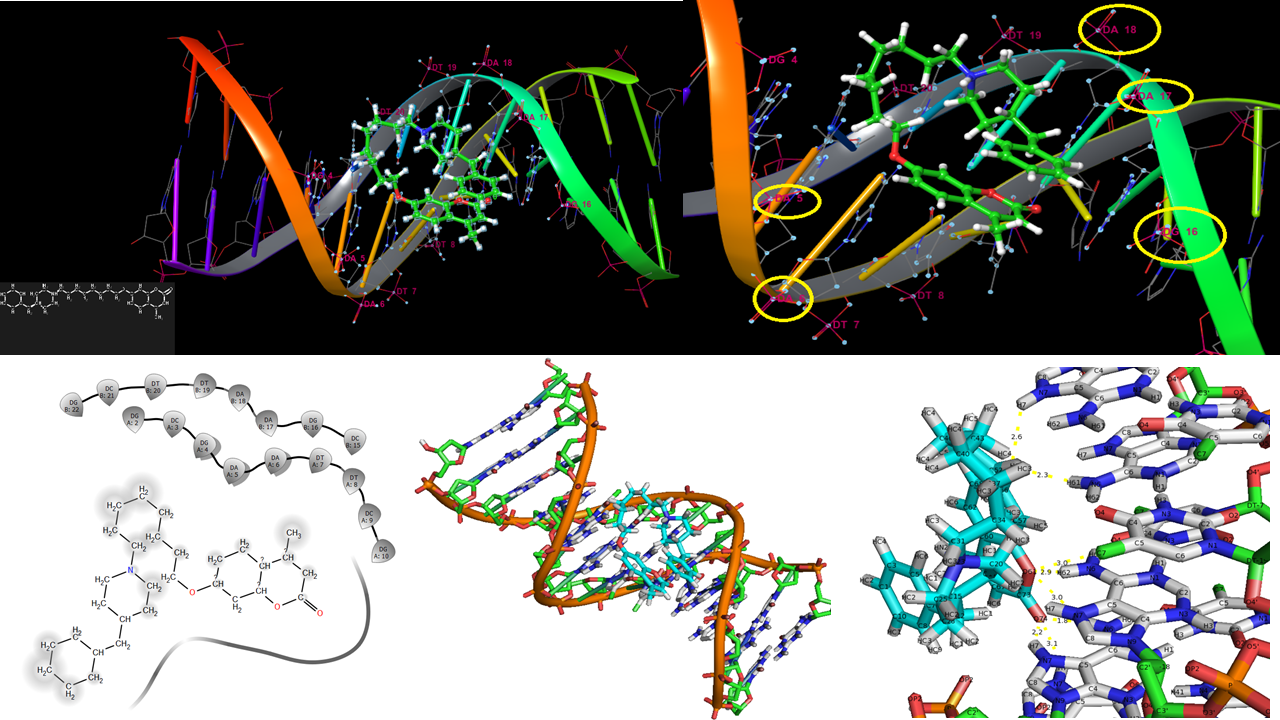
**Fig. S6** The MD system for C3 and CyP450 enzyme with 13740 water molecules, 42 Cl- and 38 Na+ ions

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**Fig. S7** The Ligand Root Mean Square Fluctuation (L-RMSF) of C3 in the MD system

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**Fig. S8** The RMSD, radius of gyration, intramolecular hydrogen bonds, molecular surface area, solvent accessible surface area and polar surface area (PSA) of C3 in the MD system for 20ns



**Fig. S9** The best docked pose, close interaction, and hydrogen bonding interaction between C3 and the B-DNA



**Fig. S10a.** Emission spectra of the DNA-EB system in the presence of C3. DNA=50 µM, EB=5 µM and C3=5–22.5 µM.

*C:\Users\isikk\Downloads\C3 EB deneyi (1).tif*

**Fig. S10b.** Emission spectra of the DNA-EB system in the presence of C3. DNA=50 µM, EB=5 µM and C3=5–22.5 µM. The arrow shows the emission intensity changes upon increasing C3 concentration.