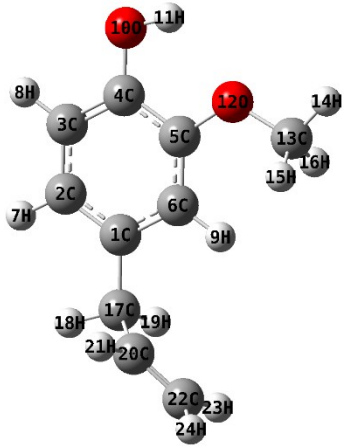
Electronic Supplementary Material (ESI) for RSC Advances.


**Supplementary Table 1.** The optimized molecular structure, Cartesian coordinates, electronic energy added with zero point vibrational energy (ZPVE), ZPVE, and spin multiplicity of **EUG**, **1_a**, **1_b**, **1_b***, **TS1_1**, **1_c**, and **1_d** structures in gas phase environment at B3LYP/6-311+g(d,p) level of theory.

| S. No. | Structure Notation | Structure | x-y-z coordinates | | | | | Electronic Energy with ZPVE | ZPVEs | Spin Multiplicity |
|---|---|---|---|---|---|---|---|---|---|---|
| 1. | **EUG** |  | Tag | Symbol | X | Y | Z | -538.658834 | 0.197726 | 1 |
| | | | 1 | C | 0.921847 | -0.81144 | -0.25298 | | | |
| | | | 2 | C | 0.22401 | -2.00746 | -0.10414 | | | |
| | | | 3 | C | -1.16244 | -2.01827 | 0.071398 | | | |
| | | | 4 | C | -1.86729 | -0.82617 | 0.10102 | | | |
| | | | 5 | C | -1.17351 | 0.38958 | -0.04542 | | | |
| | | | 6 | C | 0.204067 | 0.39514 | -0.21805 | | | |
| | | | 7 | H | 0.76134 | -2.94949 | -0.12717 | | | |
| | | | 8 | H | -1.70675 | -2.94789 | 0.187748 | | | |
| | | | 9 | H | 0.739077 | 1.331006 | -0.31993 | | | |
| | | | 10 | O | -3.22034 | -0.8299 | 0.273338 | | | |
| | | | 11 | H | -3.52022 | 0.088975 | 0.264996 | | | |
| | | | 12 | O | -1.98317 | 1.498768 | 0.00469 | | | |
| | | | 13 | C | -1.38858 | 2.783784 | -0.13284 | | | |
| | | | 14 | H | -2.20475 | 3.501092 | -0.06471 | | | |
| | | | 15 | H | -0.66801 | 2.972635 | 0.669312 | | | |
| | | | 16 | H | -0.8922 | 2.886499 | -1.10326 | | | |
| | | | 17 | C | 2.42711 | -0.79683 | -0.46703 | | | |
| | | | 18 | H | 2.790206 | -1.82936 | -0.40995 | | | |
| | | | 19 | H | 2.660078 | -0.44086 | -1.47759 | | | |
| | | | 20 | C | 3.1732 | 0.042306 | 0.537084 | | | |
| | | | 21 | H | 3.021549 | -0.22728 | 1.5809 | | | |
| | | | 22 | C | 3.97571 | 1.061797 | 0.237507 | | | |
| | | | 23 | H | 4.15119 | 1.364179 | -0.79109 | | | |
| | | | 24 | H | 4.491758 | 1.6249 | 1.007203 | | | |

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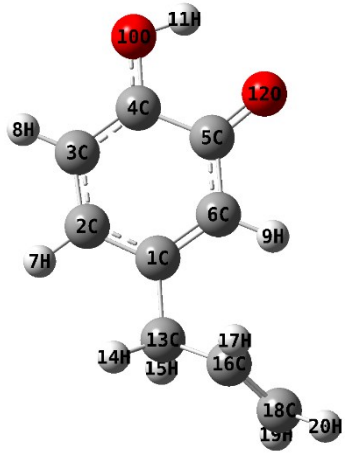
|---|---|---|---|---|---|---|---|---|---|---|
| 2. | **1_a** |  | Tag | Symbol | X | Y | Z | -498.759117 | 0.157271 | 2 |
| | | | 1 | C | -0.68486 | 0.59851 | -0.04708 | | | |
| | | | 2 | C | 0.229393 | 1.696983 | -0.0115 | | | |
| | | | 3 | C | 1.606353 | 1.523583 | 0.011287 | | | |
| | | | 4 | C | 2.114329 | 0.231052 | 0.004996 | | | |
| | | | 5 | C | 1.224657 | -0.93479 | -0.02557 | | | |
| | | | 6 | C | -0.19278 | -0.68272 | -0.05268 | | | |
| | | | 7 | H | -0.17228 | 2.704885 | -0.00183 | | | |
| | | | 8 | H | 2.281876 | 2.370016 | 0.038585 | | | |
| | | | 9 | H | -0.84925 | -1.54415 | -0.0809 | | | |
| | | | 10 | O | 3.421116 | -0.02598 | 0.029748 | | | |
| | | | 11 | H | 3.4886 | -1.00392 | 0.019159 | | | |
| | | | 12 | O | 1.757415 | -2.06844 | -0.02762 | | | |
| | | | 13 | C | -2.1754 | 0.894216 | -0.11333 | | | |
| | | | 14 | H | -2.36004 | 1.837413 | 0.416008 | | | |
| | | | 15 | H | -2.45752 | 1.073696 | -1.15811 | | | |
| | | | 16 | C | -3.05949 | -0.17372 | 0.468736 | | | |
| | | | 17 | H | -2.89631 | -0.40188 | 1.520476 | | | |
| | | | 18 | C | -4.00356 | -0.82999 | -0.20091 | | | |
| | | | 19 | H | -4.19369 | -0.63901 | -1.253 | | | |
| | | | 20 | H | -4.62148 | -1.58053 | 0.278794 | | | |

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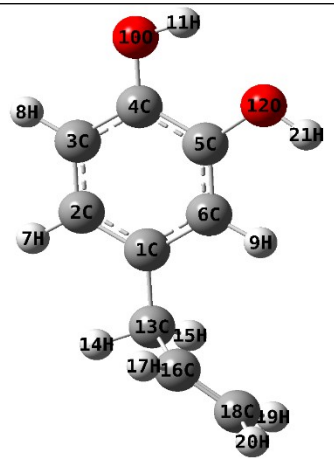
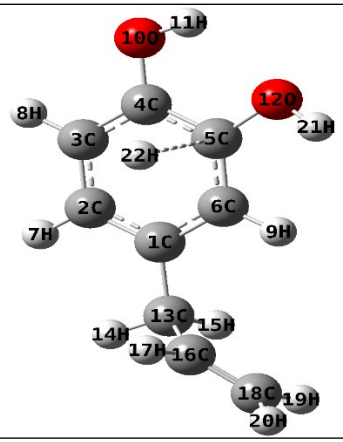
|---|---|---|---|---|---|---|---|---|---|
| 3. | **1_b** |  | Tag Symbol X Y Z<br>1 C 0.724638 -0.62009 -0.23155<br>2 C -0.1155 -1.71922 -0.05049<br>3 C -1.49314 -1.55844 0.105991<br>4 C -2.0546 -0.28928 0.086008<br>5 C -1.21788 0.821235 -0.09265<br>6 C 0.150657 0.658302 -0.24822<br>7 H 0.305142 -2.71872 -0.03236<br>8 H -2.14505 -2.41223 0.247487<br>9 H 0.782834 1.532955 -0.37637<br>10 O -3.40116 -0.1317 0.241846<br>11 H -3.60319 0.812094 0.205421<br>12 O -1.85921 2.04201 -0.09767<br>13 C 2.222518 -0.79174 -0.42573<br>14 H 2.465364 -1.8528 -0.29766<br>15 H 2.500143 -0.53211 -1.45408<br>16 C 3.053458 0.021643 0.531852<br>17 H 2.868631 -0.16195 1.588842<br>18 C 3.965621 0.924398 0.176832<br>19 H 4.177323 1.138867 -0.86687<br>20 H 4.538828 1.47437 0.914856 | -499.377655 | 0.169060 | 1 |
| 4. | **1_b*** |  | Tag Symbol X Y Z<br>1 C 0.73939 -0.63176 -0.20994<br>2 C -0.10165 -1.73097 -0.02759<br>3 C -1.48211 -1.57421 0.098362<br>4 C -2.04776 -0.3077 0.040048<br>5 C -1.21145 0.803628 -0.13994<br>6 C 0.162621 0.643837 -0.26028<br>7 H 0.322147 -2.72843 0.014124<br>8 H -2.13309 -2.42797 0.243621<br>9 H 0.791984 1.51783 -0.40324<br>10 O -3.39712 -0.15171 0.157421<br>11 H -3.59587 0.793178 0.122409 | -499.877902 | 0.170328 | 2 |

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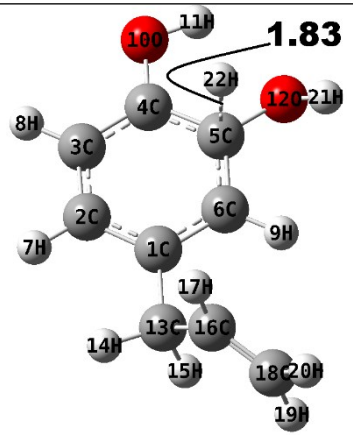
|---|---|---|---|---|---|---|---|---|---|---|
| | | | 12 | O | -1.86381 | 2.01741 | -0.21859 | | | |
| | | | 13 | C | 2.236807 | -0.81111 | -0.40305 | | | |
| | | | 14 | H | 2.479308 | -1.86583 | -0.22926 | | | |
| | | | 15 | H | 2.505211 | -0.60034 | -1.44502 | | | |
| | | | 16 | C | 3.08163 | 0.041377 | 0.506095 | | | |
| | | | 17 | H | 2.908031 | -0.09036 | 1.572701 | | | |
| | | | 18 | C | 3.997547 | 0.917642 | 0.098167 | | | |
| | | | 19 | H | 4.198558 | 1.080768 | -0.95685 | | | |
| | | | 20 | H | 4.584259 | 1.496582 | 0.802677 | | | |
| | | | 21 | H | -1.22243 | 2.74877 | -0.09226 | | | |
| | | | 22 | H | -1.0008 | 1.045781 | 2.649219 | | | |
| 5. | **TS1_1** |  | Tag | Symbol | X | Y | Z | -499.871827 | 0.171321 | 2 |
| | | | 1 | C | 0.744804 | -0.62486 | -0.20837 | | | |
| | | | 2 | C | -0.10058 | -1.72957 | -0.02633 | | | |
| | | | 3 | C | -1.48114 | -1.58254 | 0.094366 | | | |
| | | | 4 | C | -2.04813 | -0.31633 | 0.064662 | | | |
| | | | 5 | C | -1.20249 | 0.817547 | -0.01477 | | | |
| | | | 6 | C | 0.17475 | 0.643268 | -0.24548 | | | |
| | | | 7 | H | 0.325856 | -2.72651 | 0.000483 | | | |
| | | | 8 | H | -2.13019 | -2.44298 | 0.202908 | | | |
| | | | 9 | H | 0.794054 | 1.521458 | -0.39549 | | | |
| | | | 10 | O | -3.38964 | -0.15719 | 0.15605 | | | |
| | | | 11 | H | -3.57875 | 0.790621 | 0.099462 | | | |
| | | | 12 | O | -1.86428 | 2.014032 | -0.26087 | | | |
| | | | 13 | C | 2.241632 | -0.80831 | -0.40713 | | | |
| | | | 14 | H | 2.483576 | -1.86363 | -0.23653 | | | |
| | | | 15 | H | 2.50835 | -0.59475 | -1.44867 | | | |
| | | | 16 | C | 3.083351 | 0.043378 | 0.506254 | | | |
| | | | 17 | H | 2.905697 | -0.09006 | 1.571836 | | | |
| | | | 18 | C | 3.998357 | 0.922208 | 0.102536 | | | |
| | | | 19 | H | 4.202475 | 1.087941 | -0.95144 | | | |
| | | | 20 | H | 4.580619 | 1.501695 | 0.810164 | | | |
| | | | 21 | H | -1.41497 | 2.73651 | 0.190594 | | | |

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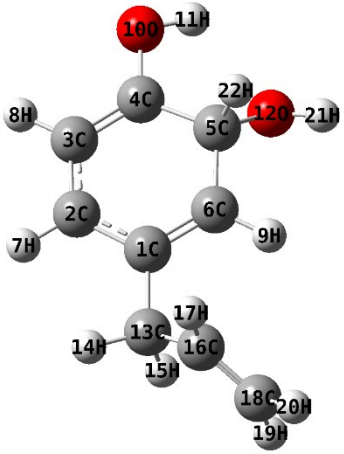
|---|---|---|---|---|---|---|---|---|---|---|
| | | | 22 | H | -1.10865 | 1.036309 | 1.800812 | | | |
| 6. | **1_c** |  | Tag | Symbol | X | Y | Z | -499.911569 | 0.178628 | 2 |
| | | | 1 | C | -0.74144 | 0.59573 | -0.14116 | | | |
| | | | 2 | C | 0.126487 | 1.724622 | -0.12249 | | | |
| | | | 3 | C | 1.520957 | 1.569703 | 0.001149 | | | |
| | | | 4 | C | 2.065985 | 0.325678 | 0.152301 | | | |
| | | | 5 | C | 1.222664 | -0.90262 | 0.313857 | | | |
| | | | 6 | C | -0.22638 | -0.65745 | 0.038498 | | | |
| | | | 7 | H | -0.28762 | 2.717566 | -0.25617 | | | |
| | | | 8 | H | 2.182178 | 2.42774 | -0.06352 | | | |
| | | | 9 | H | -0.87867 | -1.52469 | 0.046112 | | | |
| | | | 10 | O | 3.407577 | 0.14409 | 0.218078 | | | |
| | | | 11 | H | 3.580454 | -0.78844 | 0.021511 | | | |
| | | | 12 | O | 1.832417 | -1.92078 | -0.53706 | | | |
| | | | 13 | C | -2.22869 | 0.806972 | -0.39879 | | | |
| | | | 14 | H | -2.45586 | 1.867717 | -0.23949 | | | |
| | | | 15 | H | -2.45015 | 0.599671 | -1.4521 | | | |
| | | | 16 | C | -3.13179 | -0.01841 | 0.47654 | | | |
| | | | 17 | H | -3.01125 | 0.129453 | 1.548533 | | | |
| | | | 18 | C | -4.04085 | -0.8868 | 0.03835 | | | |
| | | | 19 | H | -4.18965 | -1.06818 | -1.0223 | | | |
| | | | 20 | H | -4.67228 | -1.44249 | 0.722704 | | | |
| | | | 21 | H | 1.513968 | -2.78509 | -0.25748 | | | |
| | | | 22 | H | 1.34725 | -1.26429 | 1.354577 | | | |

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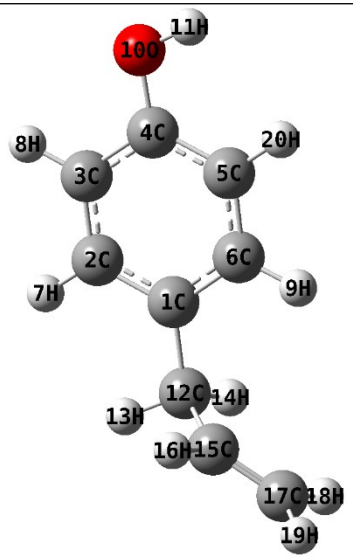
|---|---|---|---|---|---|---|---|---|---|---|
| 7. | **1_d** |  | Tag | Symbol | X | Y | Z | -424.133012 | 0.164921 | 1 |
| | | | 1 | C | -0.48672 | 0.424542 | -0.2363 | | | |
| | | | 2 | C | 0.465985 | 1.423857 | -0.0131 | | | |
| | | | 3 | C | 1.817641 | 1.125561 | 0.133636 | | | |
| | | | 4 | C | 2.242501 | -0.1995 | 0.059562 | | | |
| | | | 5 | C | 1.309117 | -1.21405 | -0.15959 | | | |
| | | | 6 | C | -0.03948 | -0.89837 | -0.30289 | | | |
| | | | 7 | H | 0.147763 | 2.460043 | 0.045306 | | | |
| | | | 8 | H | 2.549389 | 1.90556 | 0.306391 | | | |
| | | | 9 | H | -0.7548 | -1.69785 | -0.46432 | | | |
| | | | 10 | O | 3.58254 | -0.4461 | 0.210474 | | | |
| | | | 11 | H | 3.748277 | -1.39175 | 0.139352 | | | |
| | | | 12 | C | -1.95791 | 0.763258 | -0.41699 | | | |
| | | | 13 | H | -2.08334 | 1.842322 | -0.27009 | | | |
| | | | 14 | H | -2.26785 | 0.552935 | -1.44724 | | | |
| | | | 15 | C | -2.86781 | 0.029143 | 0.53315 | | | |
| | | | 16 | H | -2.6566 | 0.170749 | 1.59165 | | | |
| | | | 17 | C | -3.87664 | -0.76007 | 0.16989 | | | |
| | | | 18 | H | -4.11626 | -0.93177 | -0.87561 | | | |
| | | | 19 | H | -4.50119 | -1.25848 | 0.902808 | | | |
| | | | 20 | H | 1.634253 | -2.24921 | -0.21626 | | | |

**Supplementary Table 2.** The electronic energy added with zero point vibrational energy (ZPVE), ZPVE, and spin multiplicity of each structure involved in all reaction schemes of conversion of eugenol in gas phase environment at B3LYP/6-311+g(d,p) level of theory.

| S. No. | Structure Notation | Electronic Energy with ZPVE | ZPVEs | Spin Multiplicity |
|---|---|---|---|---|
| 1. | **EUG** | -538.658834 | 0.197726 | 1 |
| 2. | **1_a** | -498.759117 | 0.157271 | 2 |
| 3. | **1_b** | -499.377655 | 0.169060 | 1 |
| 4. | **1_b*** | -499.877902 | 0.170328 | 2 |
| 5. | **TS1_1** | -499.871827 | 0.171321 | 2 |
| 6. | **1_c** | -499.911569 | 0.178628 | 2 |
| 7. | **1_d** | -424.133012 | 0.164921 | 1 |
| 8. | **1_d*** | -424.634800 | 0.165335 | 2 |
| 9. | **TS1_2** | -424.624629 | 0.166837 | 2 |
| 10. | **1_e** | -424.663008 | 0.173508 | 2 |
| 11. | **1_f** | -348.890051 | 0.160949 | 1 |
| 12. | **1_g** | -349.452204 | 0.169058 | 2 |
| 13. | **1_h** | -350.103083 | 0.184375 | 1 |
| 14. | **EUG*** | -539.160414 | 0.198056 | 2 |
| 15. | **TS2_1** | -539.154112 | 0.199705 | 2 |
| 16. | **2_a** | -539.194726 | 0.206701 | 2 |
| 17. | **TS2_2** | -539.177942 | 0.204696 | 2 |
| 18. | **2_b*** | -539.209785 | 0.203445 | 2 |
| 19. | **2_a1** | -421.302826 | 0.123870 | 2 |
| 20. | **2_b** | -421.979934 | 0.136977 | 1 |
| 21. | **3_a** | -460.643154 | 0.151096 | 2 |
| 22. | **3_b** | -461.279602 | 0.164046 | 1 |
| 23. | **3_b*** | -461.781254 | 0.164448 | 2 |
| 24. | **TS3_1** | -461.774707 | 0.166127 | 2 |
| 25. | **3_c** | -461.814666 | 0.173332 | 2 |
| 26. | **TS3_2** | -461.799844 | 0.171229 | 2 |
| 27. | **3_d** | -461.811808 | 0.169990 | 2 |
| 28. | **3_d*** | -347.255983 | 0.131660 | 2 |
| 29. | **TS3_3** | -347.245920 | 0.133273 | 2 |
| 30. 3 | **3_e** | -347.284485 | 0.139979 | 2 |
| 31. | **3_f** | -271.511507 | 0.127307 | 1 |
| 32. | **3_c1** | -421.381386 | 0.123813 | 2 |
| 33. | **3_c2** | -421.998469 | 0.135403 | 1 |
| 34. | **3_c2*** | -422.500371 | 0.135748 | 2 |
| 35. | **TS3a_1** | -422.493042 | 0.137746 | 2 |
| 36. | **3_c3** | -422.533349 | 0.145300 | 2 |
| 37. | **4_a** | -423.456925 | 0.152132 | 2 |
| 38. | **4_b** | -424.133012 | 0.164921 | 1 |
| 39. | **4_c** | -424.689183 | 0.173264 | 2 |
| 40. | **4_d** | -425.345861 | 0.188349 | 1 |
| 41. | **EUG*** | -539.160662 | 0.197993 | 2 |
| 42. | **TS4_1** | -539.153523 | 0.199902 | 2 |
| 43. | **4_a1** | -539.193028 | 0.206753 | 2 |
| 44. | **TS4_2** | -539.178042 | 0.204730 | 2 |
| 45. | **4_b*** | -539.190364 | 0.203412 | 2 |
| 46. | **5_a** | -539.220512 | 0.205973 | 2 |
| 47. | **5_b** | -539.871120 | 0.221206 | 1 |
| 48. | **5_c** | -540.405965 | 0.230285 | 2 |
| 49. | **5_d** | -541.012206 | 0.243041 | 1 |
| 50. | **5_e** | -541.594193 | 0.253311 | 2 |
| 51. | **5_f** | -542.214157 | 0.267127 | 1 |
| 52. | **5_g** | -542.771374 | 0.276054 | 2 |
| 53. | **5_h** | -543.424235 | 0.291066 | 1 |
| 54. | **5_i** | -503.484356 | 0.248808 | 2 |

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|---|---|---|---|---|
| 55. | **5_j** | -504.142135 | 0.263336 | 1 |
| 56. | **5_k** | -428.247798 | 0.243915 | 2 |
| 57. | **5_l** | -428.901154 | 0.258419 | 1 |
| 58. | **5_m** | -353.010545 | 0.239324 | 2 |
| 59. | **5_n** | -353.661810 | 0.254001 | 1 |
| 60. | **6_a** | -537.998589 | 0.182327 | 2 |
| 61. | **TS6_1** | -537.975149 | 0.182017 | 2 |
| 62. | **6_b** | -537.987833 | 0.183597 | 2 |
| 63. | **TS6_2** | -537.987874 | 0.183307 | 2 |
| 64. | **6_c** | -538.007079 | 0.185344 | 2 |
| 65. | **6_d** | -538.669829 | 0.198951 | 1 |
| 66. | **TS6_3** | -538.618426 | 0.194057 | 1 |
| 67. | **6_d*** | -538.642892 | 0.193868 | 1 |
| 68. | **6_e** | -462.202890 | 0.169101 | 1 |
| 69. | **6_f** | -462.794800 | 0.178760 | 2 |
| 70. | **TS6_4** | -462.750589 | 0.175054 | 2 |
| 71. | **6_g** | -462.806842 | 0.179364 | 2 |
| 72. | **6_h** | -463.432998 | 0.192219 | 1 |
| 73. | **6_i** | -463.994855 | 0.200445 | 2 |
| 74. | **6_j** | -464.645785 | 0.215587 | 1 |
| 75. | **7_a** | -462.734921 | 0.180287 | 2 |
| 76. | **7_b** | -463.414376 | 0.193206 | 1 |
| 77. | **7_b*** | -463.916336 | 0.193360 | 2 |
| 78. | **TS7_1** | -463.906415 | 0.195133 | 2 |
| 79. | **7_c** | -463.943189 | 0.201646 | 2 |
| 80. | **TS7_2** | -463.927136 | 0.199816 | 2 |
| 81. | **7_d*** | -463.943624 | 0.198085 | 2 |
| 82. | **EUG^** | -539.160628 | 0.198124 | 2 |
| 83. | **TS7_1a** | -539.152390 | 0.199804 | 2 |
| 84. | **7_a1** | -539.193406 | 0.206814 | 2 |
| 85. | **7_c1** | -423.501339 | 0.151856 | 2 |
| 86. | **7_c2** | -424.133844 | 0.164943 | 1 |
| 87. | **7_c2*** | -424.635615 | 0.165376 | 2 |
| 88. | **TS7_2a** | -424.624885 | 0.166928 | 2 |
| 89. | **7_c3** | -424.661703 | 0.173569 | 2 |
| 90. | **7_d** | -348.890051 | 0.160949 | 1 |
| 91. | **8_a** | -538.043309 | 0.184551 | 2 |
| 92. | **8_b** | -538.668635 | 0.197246 | 1 |