

**SUPPORTING INFORMATION**

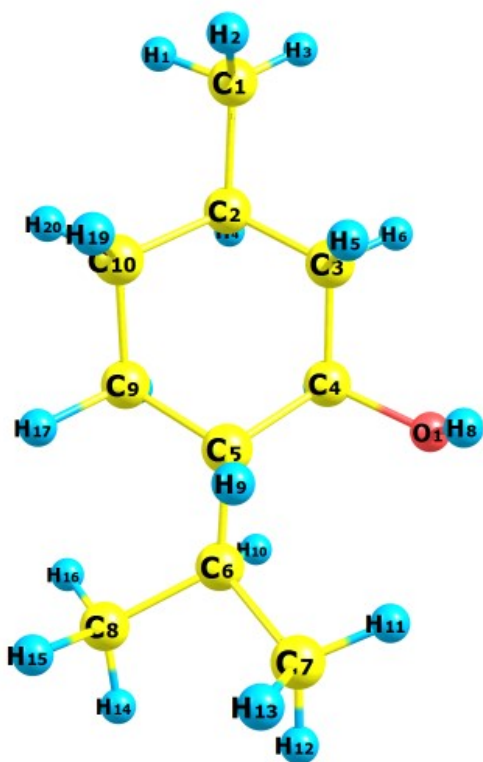
**ATMOSPHERIC DEGRADATION MECHANISM AND KINETICS OF MENTHOL  
INITIATED BY HYDROXYL RADICAL**

**Angappan Mano Priya<sup>1</sup> and Basheer Azaad<sup>2\*</sup>**

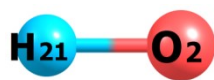
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*<sup>2</sup> Centre for Astrophysics and Space Science, ELTE Eötvös Loránd University, P.O. Box 32, H-1518, Budapest, Hungary*

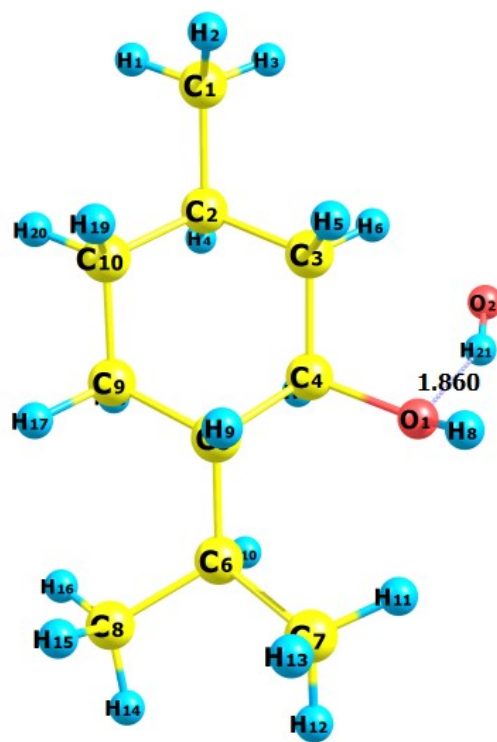
*Corresponding Author: [aazaadb@gmail.com](mailto:aazaadb@gmail.com)*



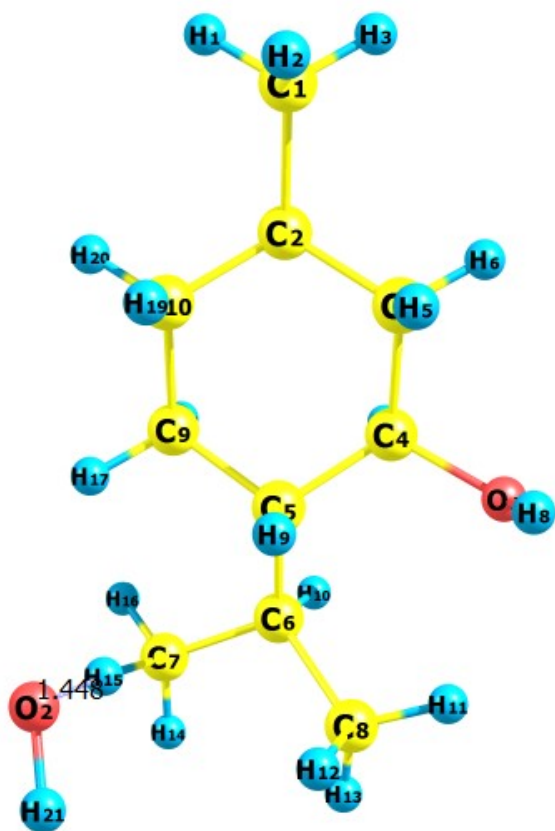
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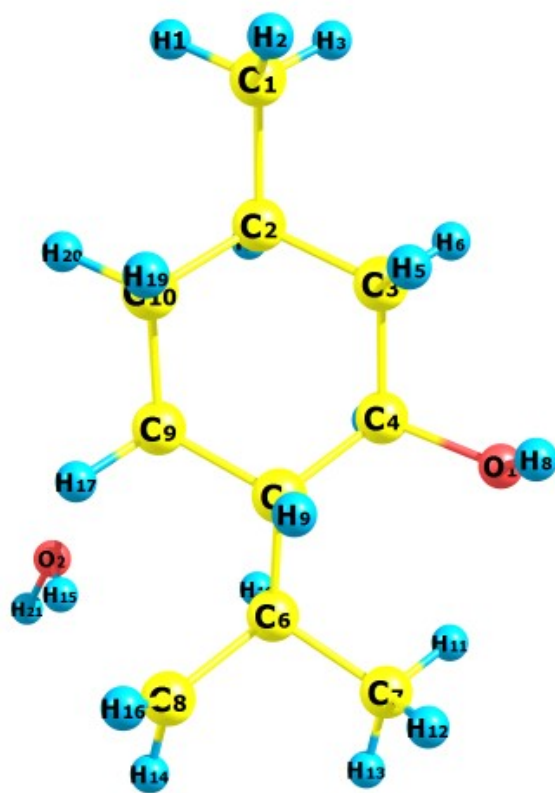
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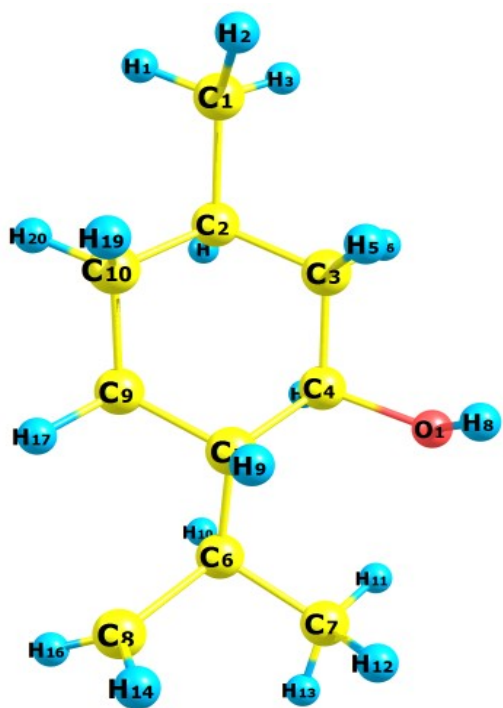
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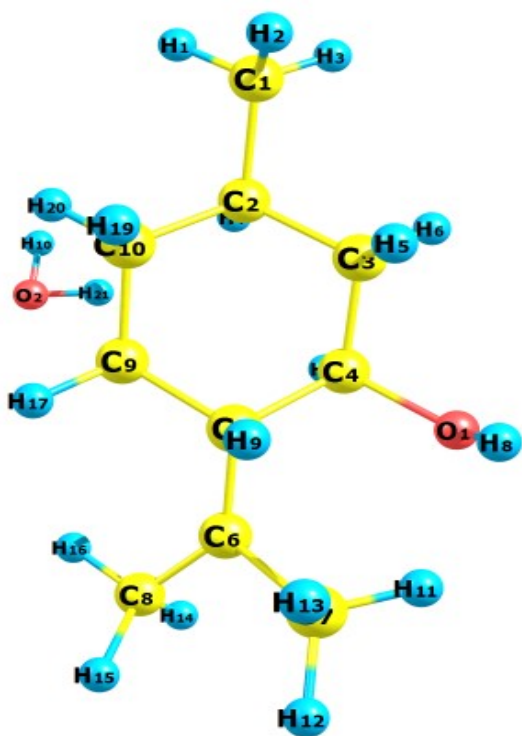
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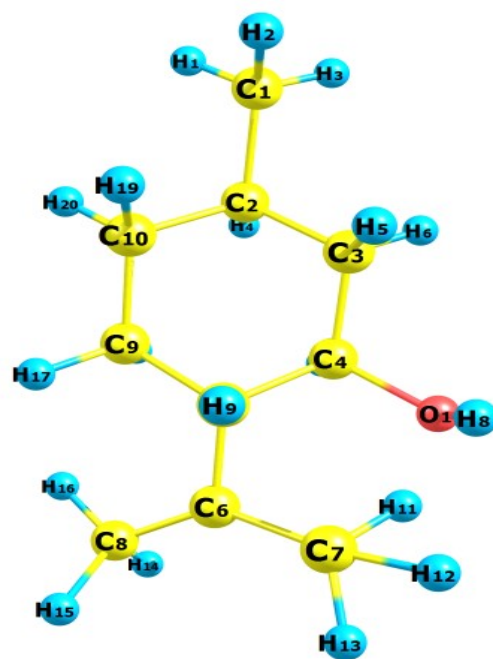
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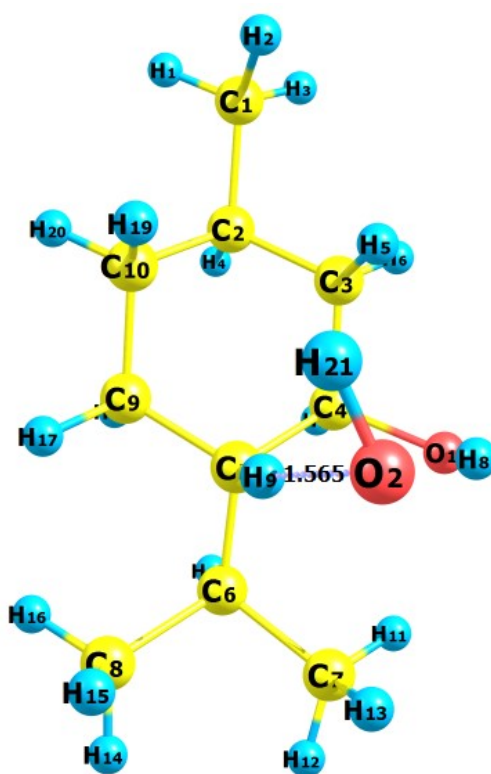
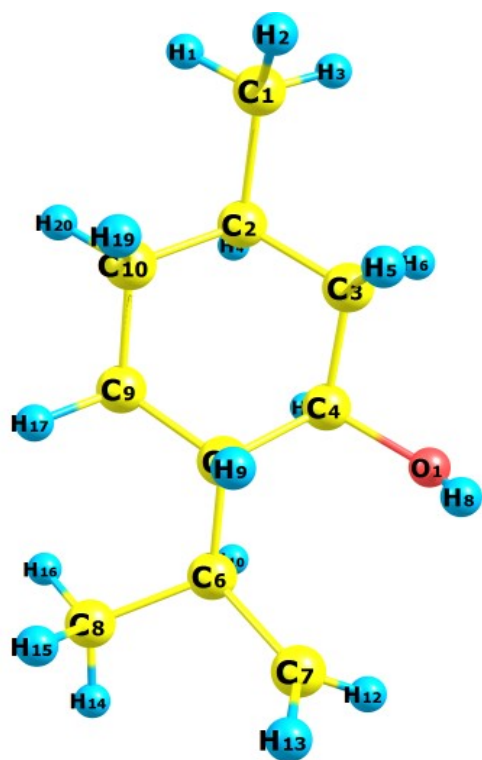
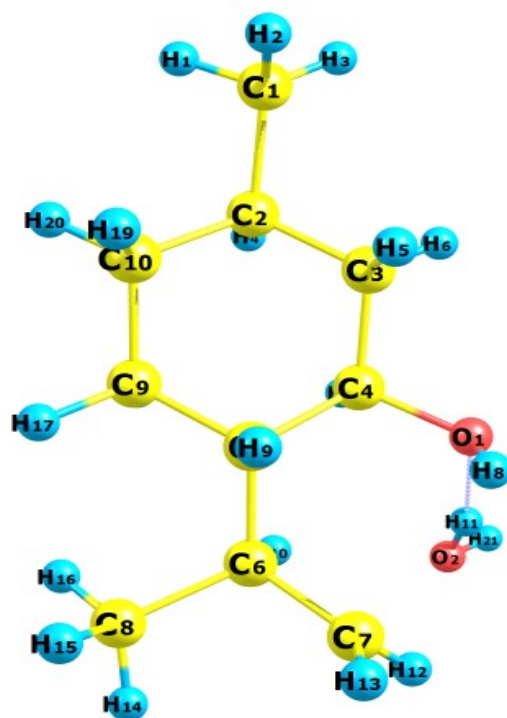
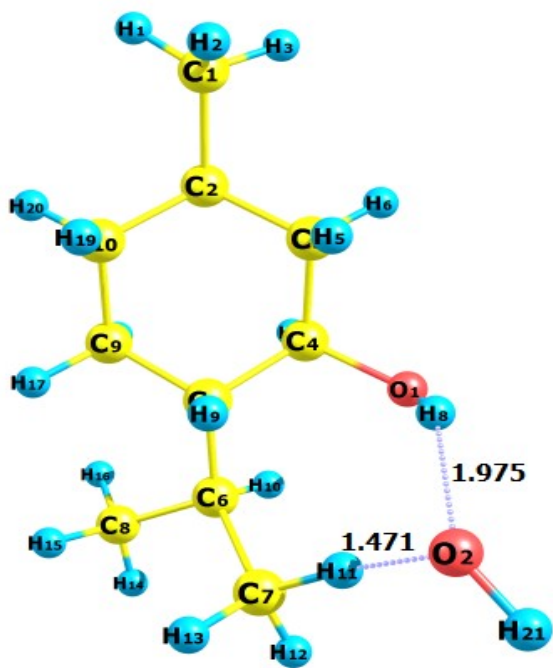
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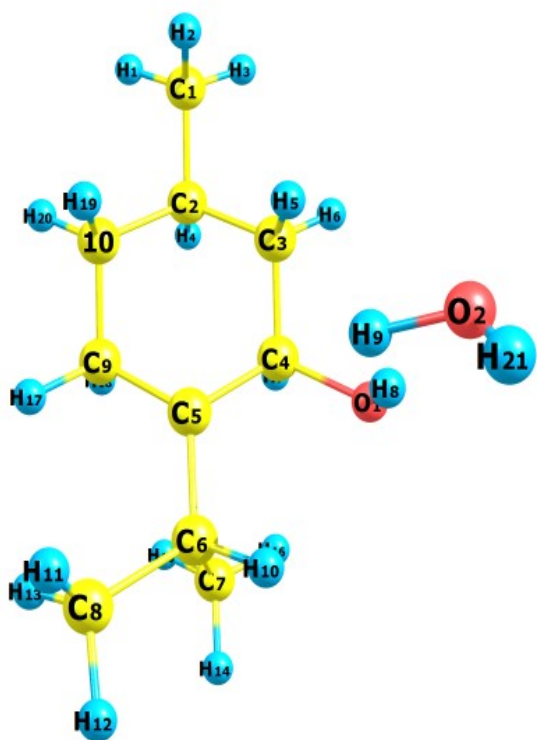


IC2



I2

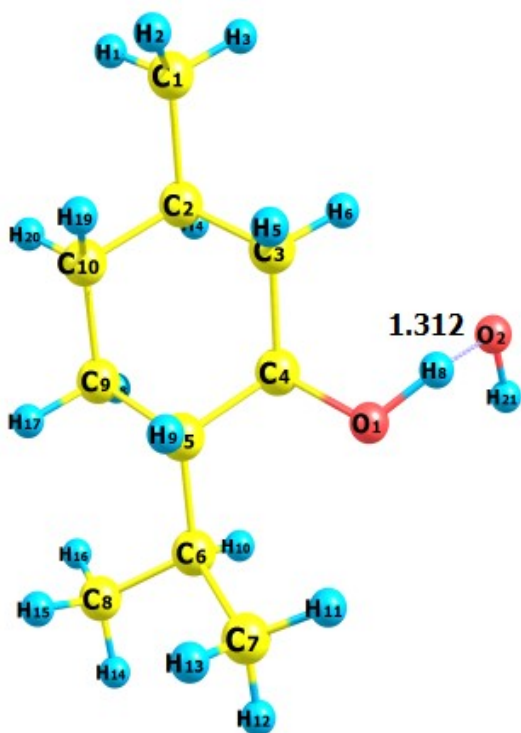




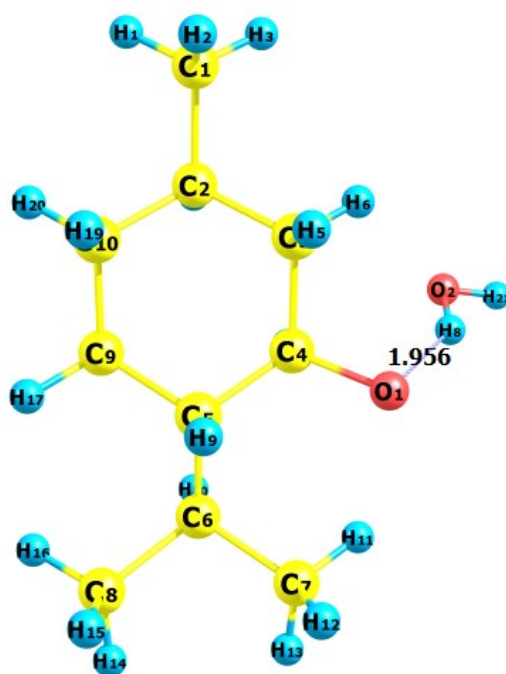
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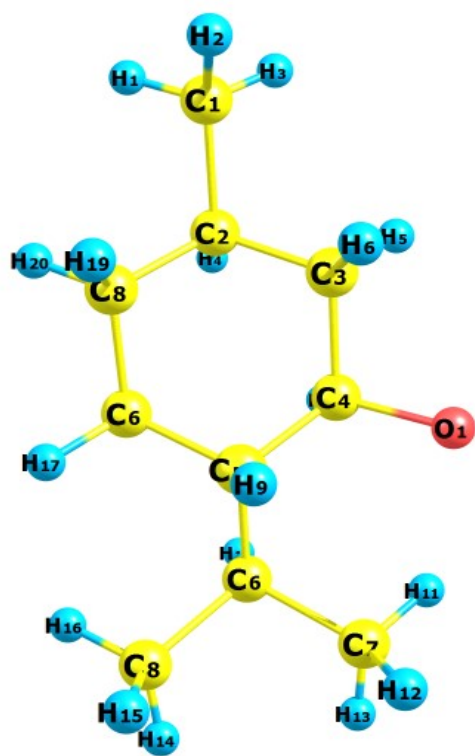
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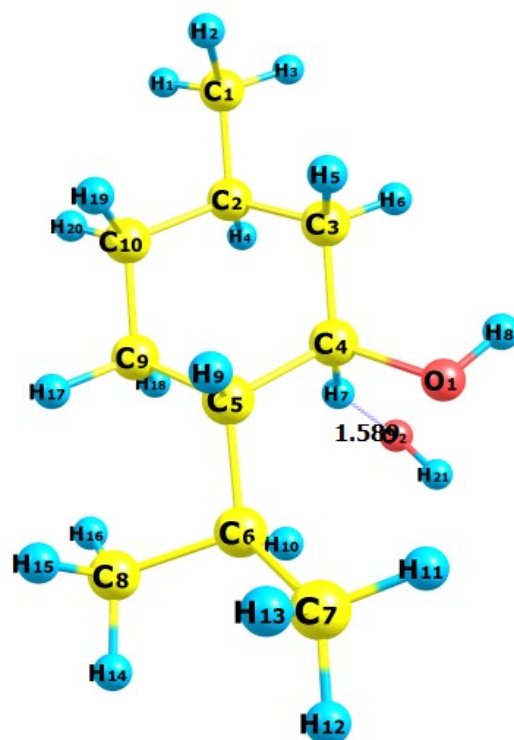
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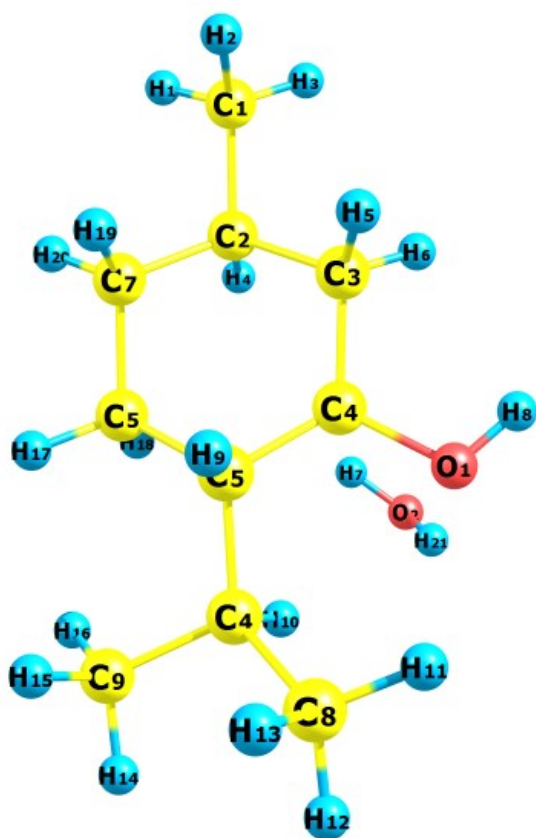
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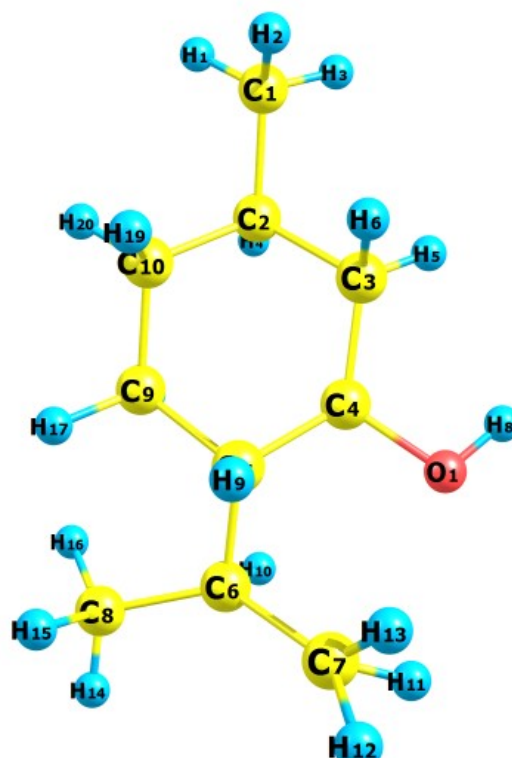
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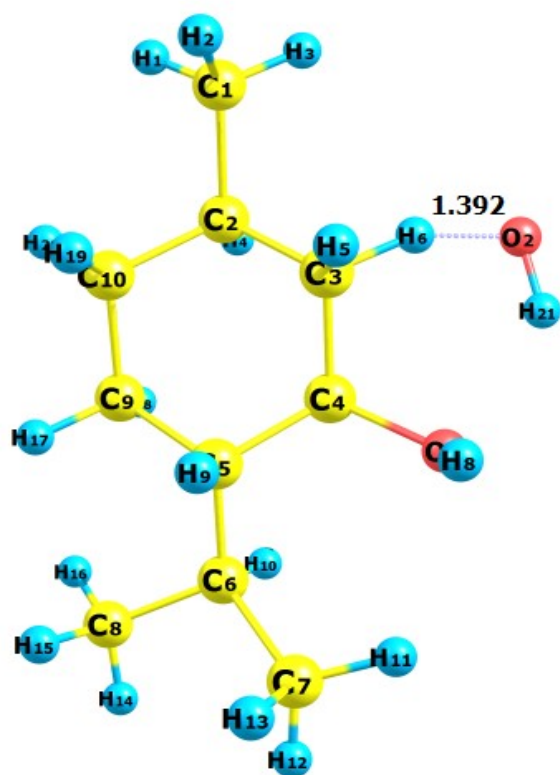
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IC6

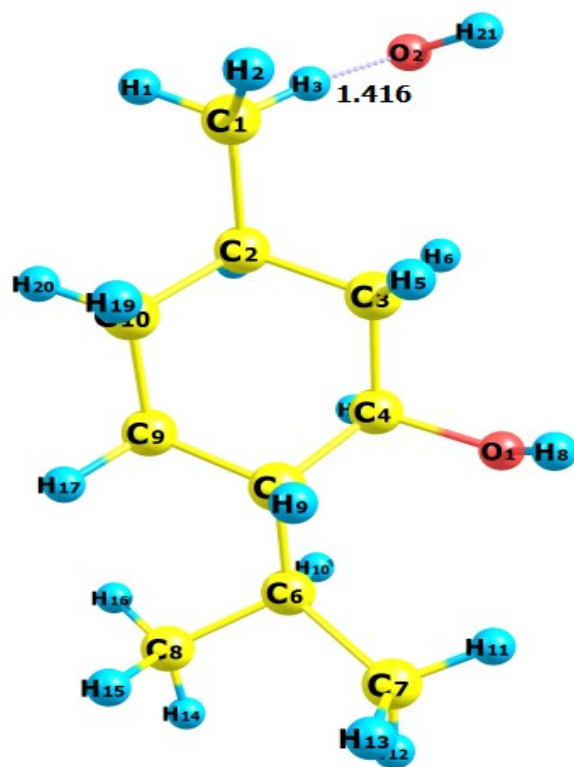
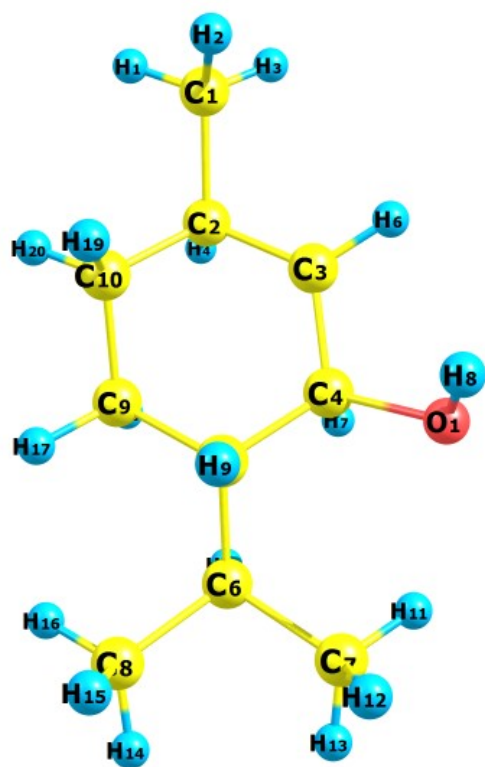
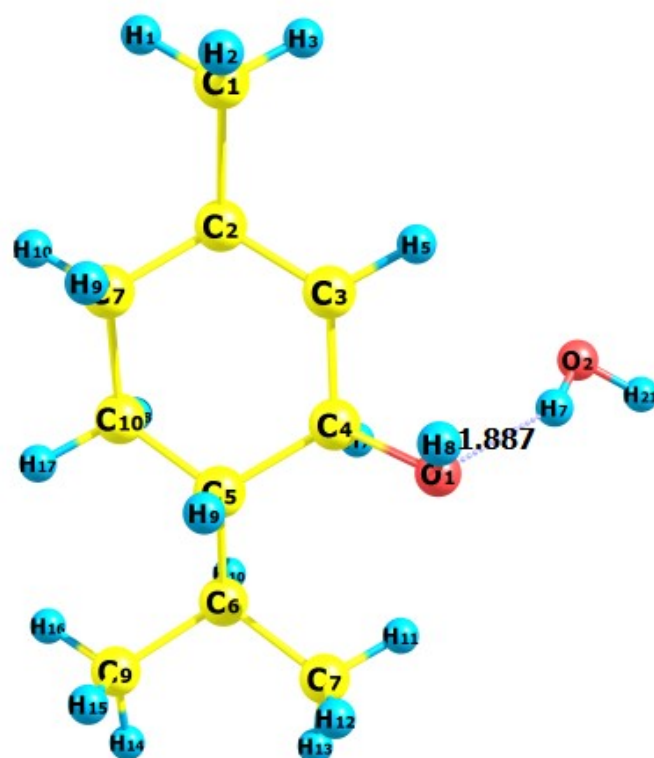


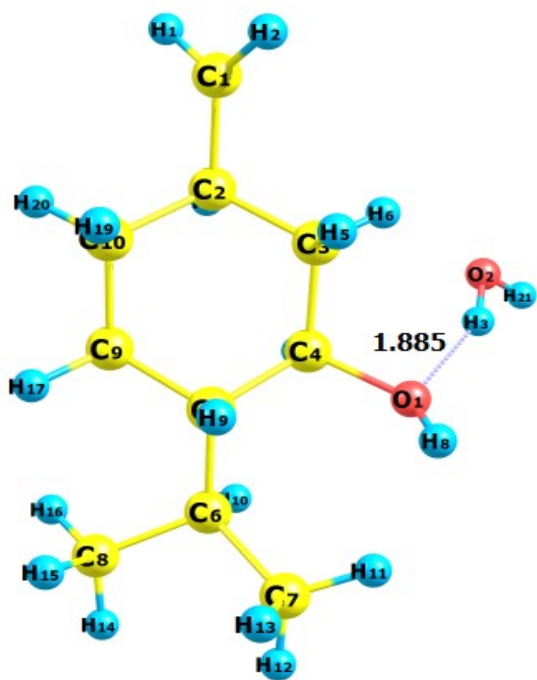
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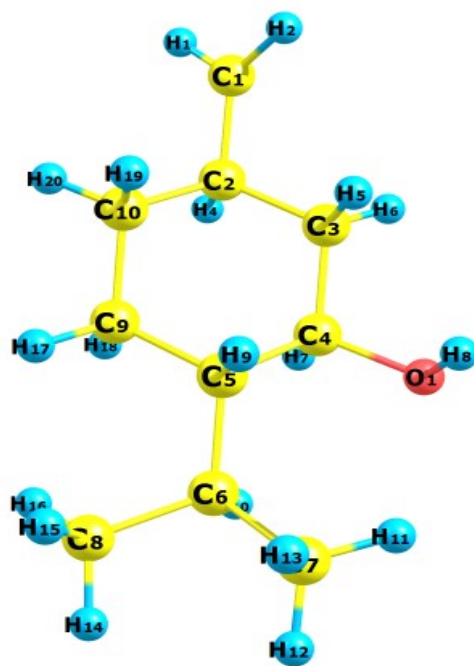
TS7

IC7



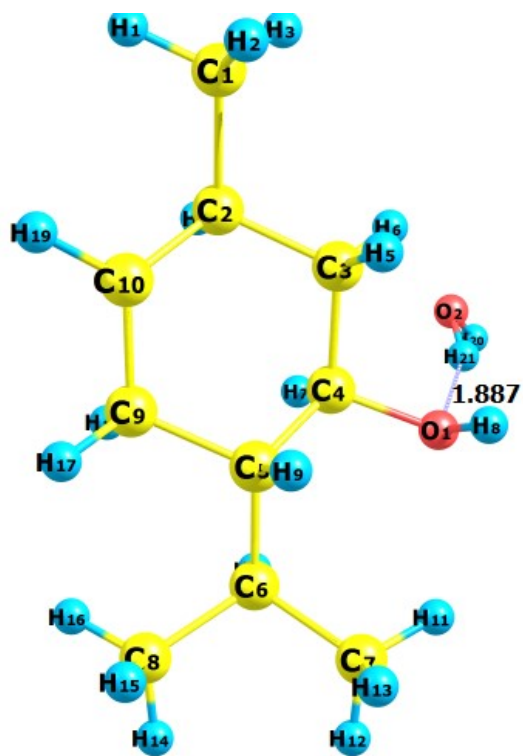
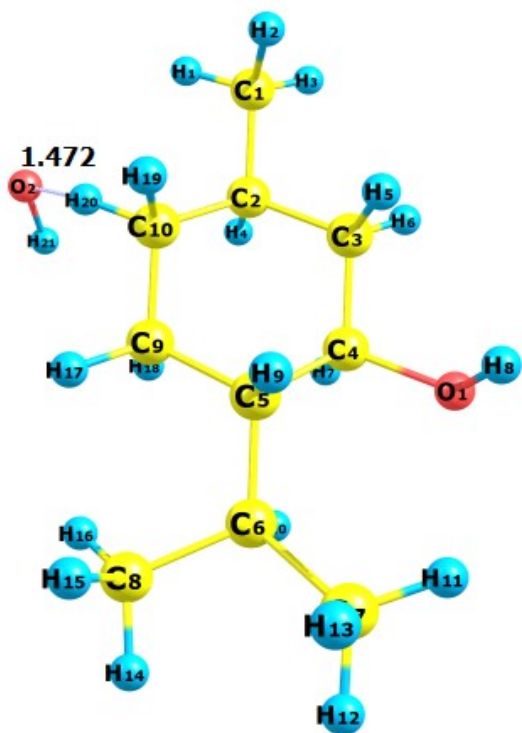


I7  
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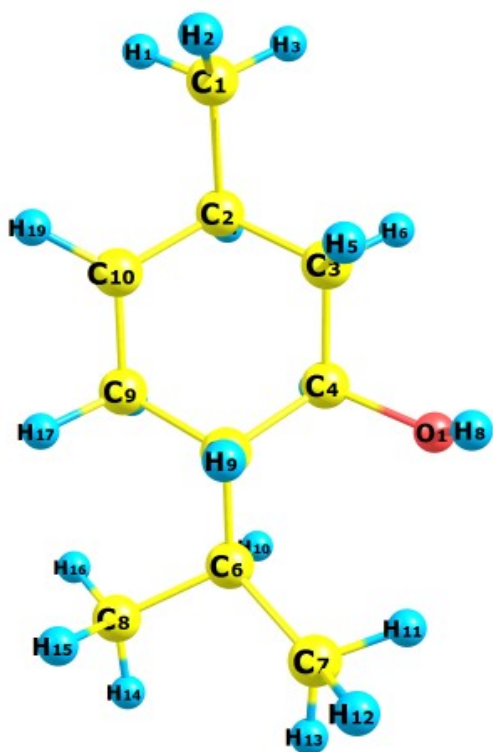
IC8

I8

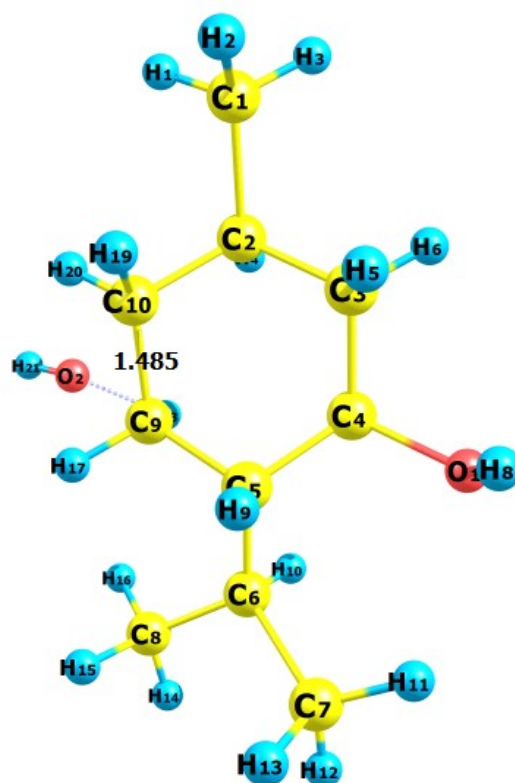




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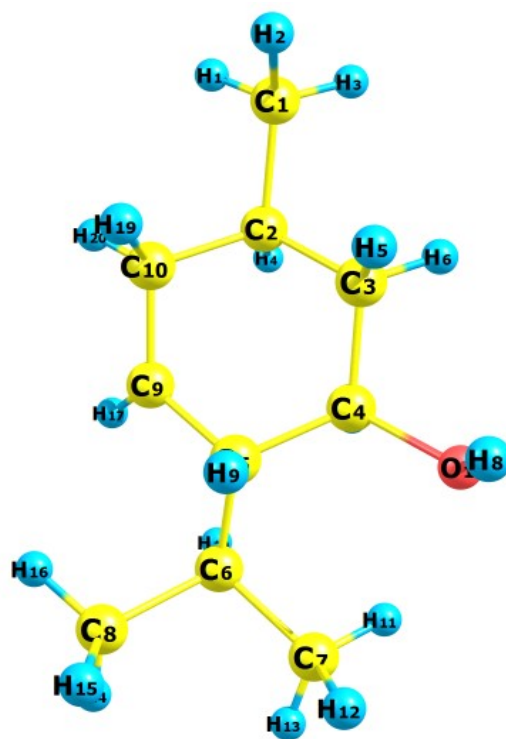
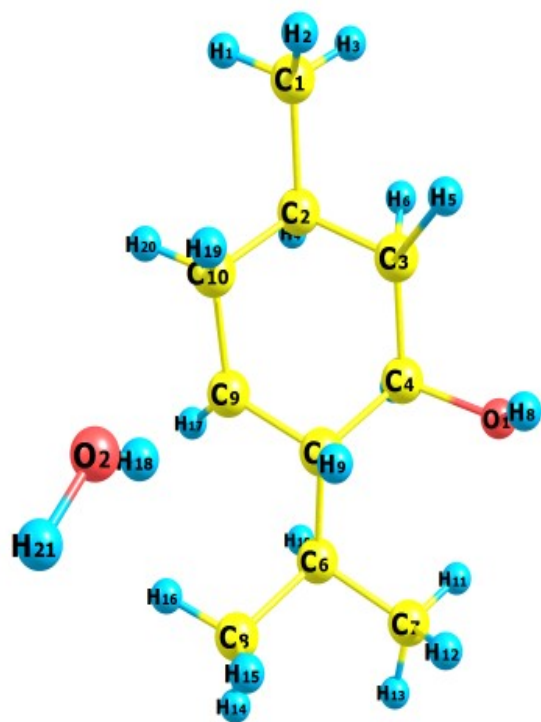


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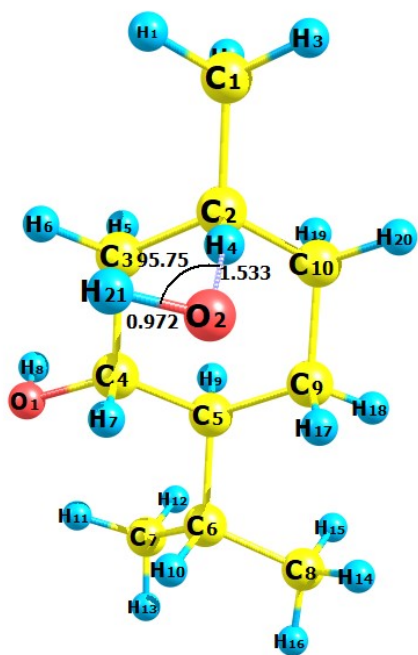
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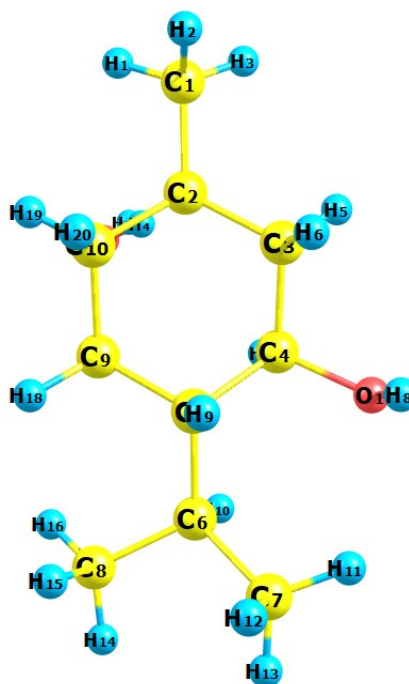


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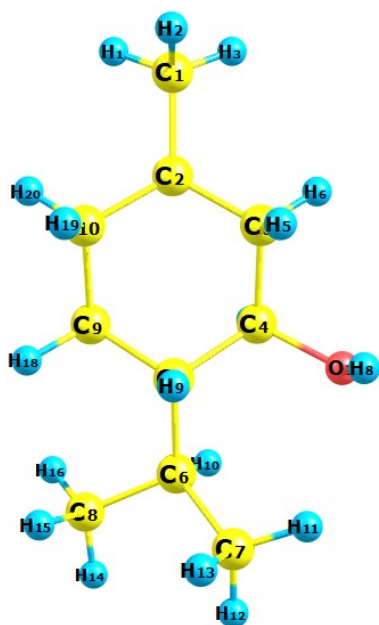
I10



TS11



IC11

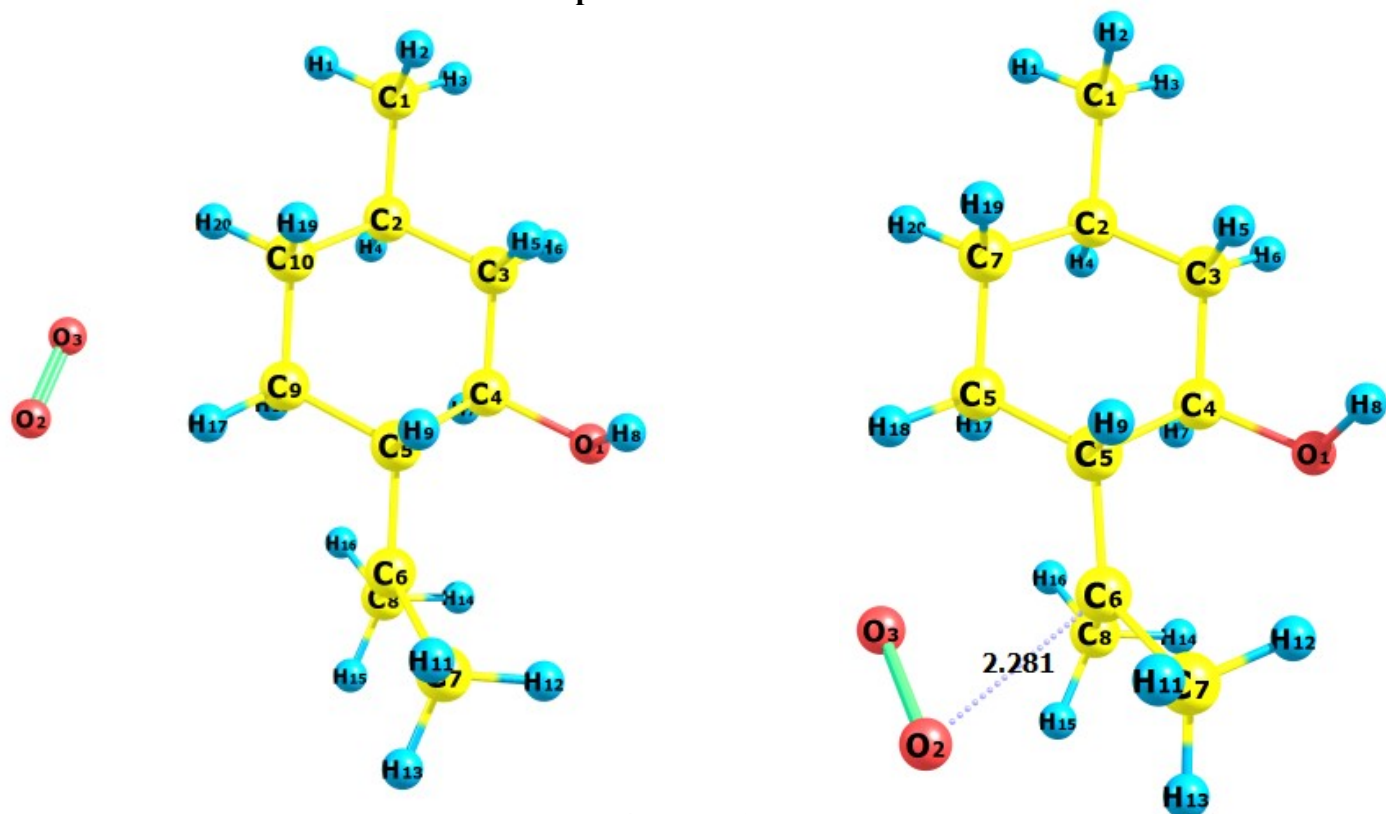


I11



H<sub>2</sub>O

Figure S1 The optimized structures of reactant, reactant complex, transition states, intermediate complexes and



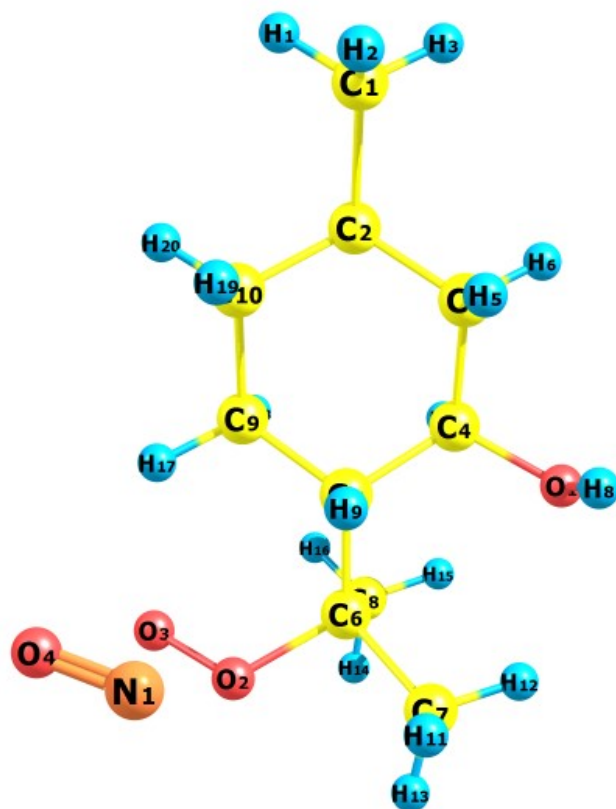
intermediates at M06-2X/6-311+G(d,p)  
level of theory.

I2+O<sub>2</sub>

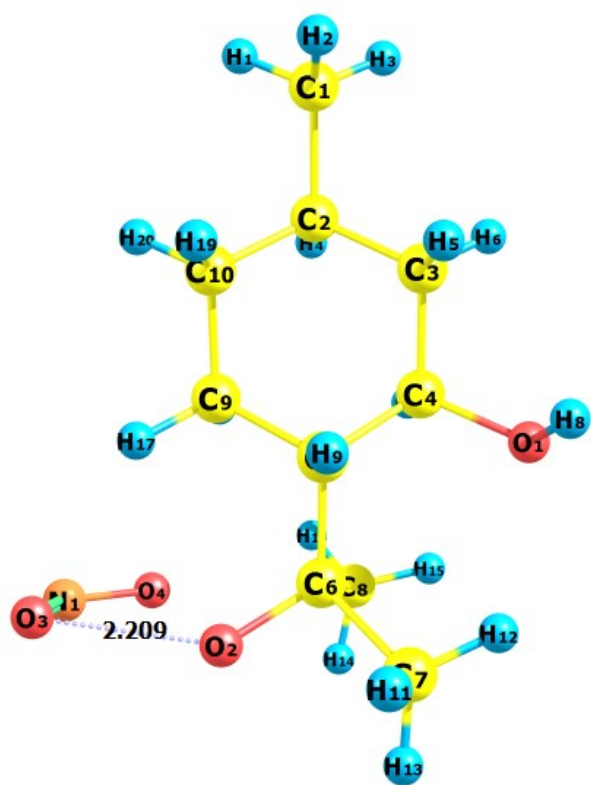


I12

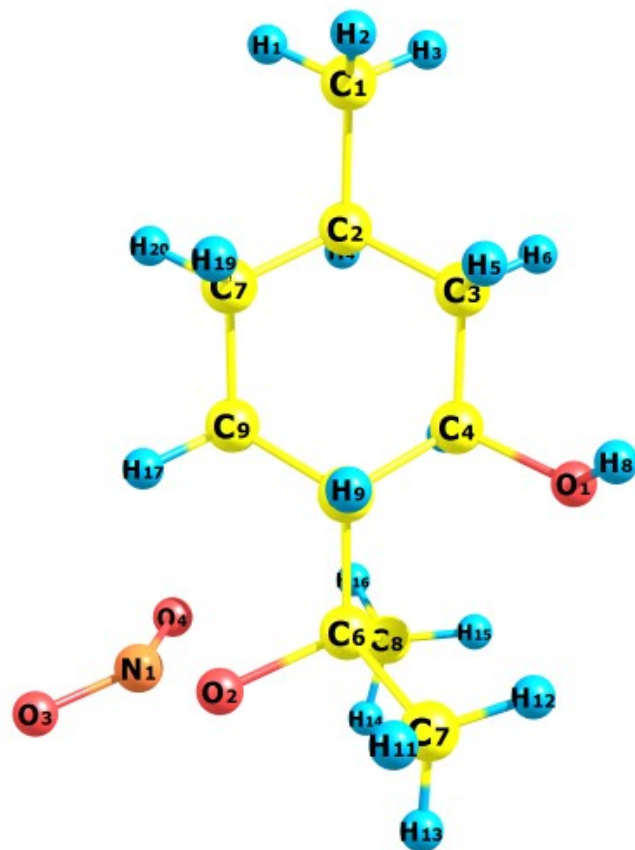
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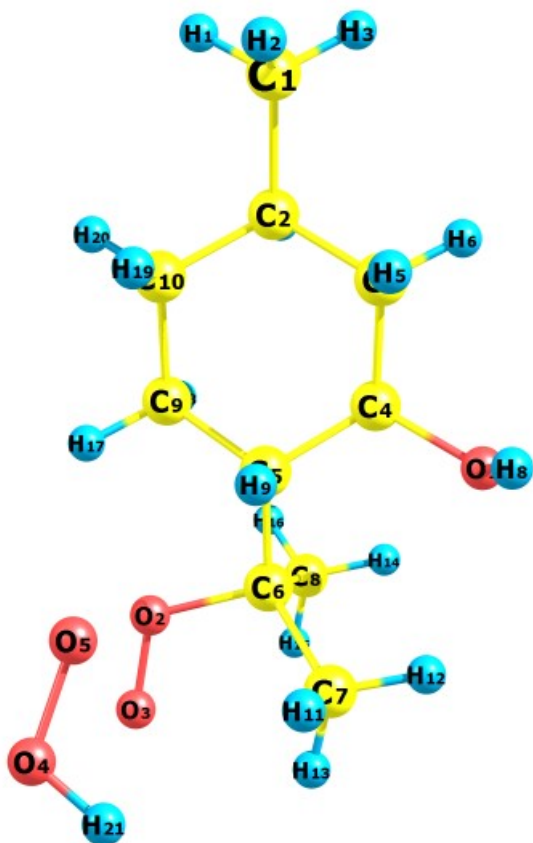
I12+NO



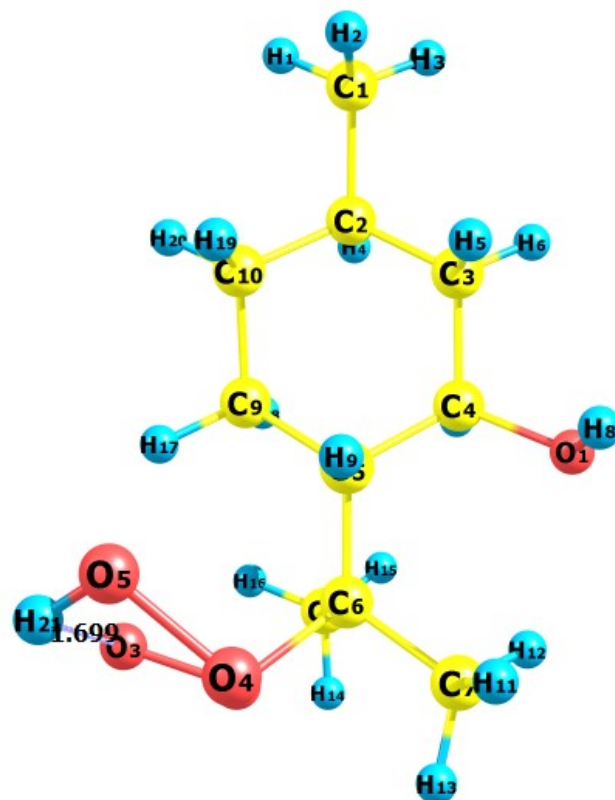
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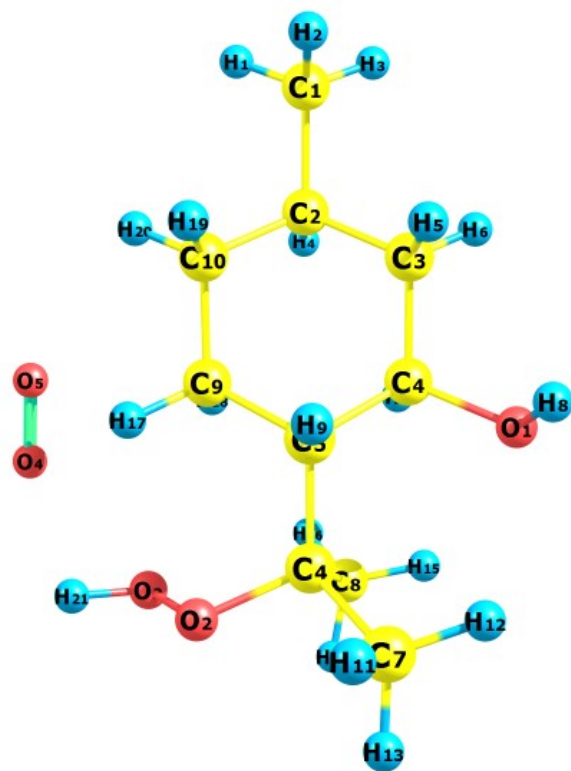
I13



I12+HO<sub>2</sub>

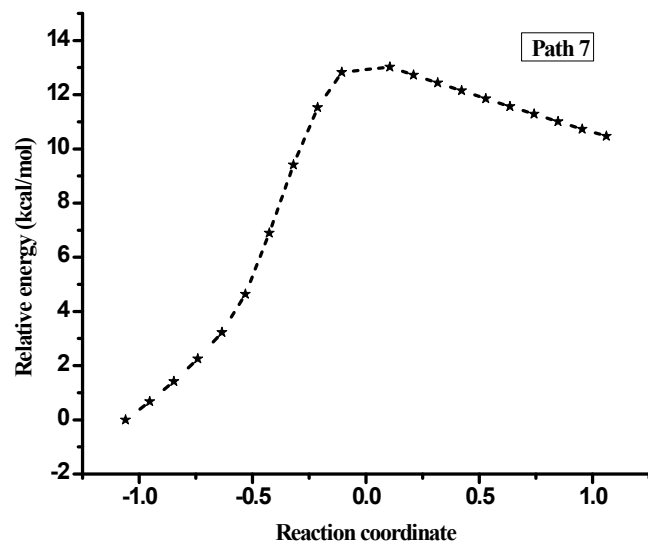
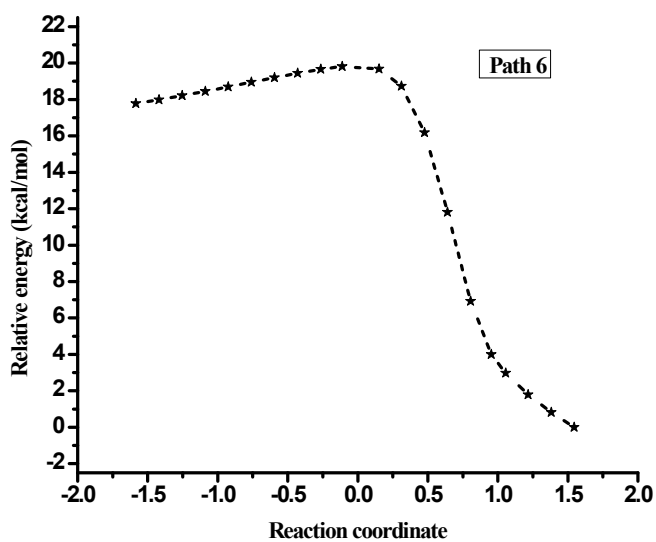
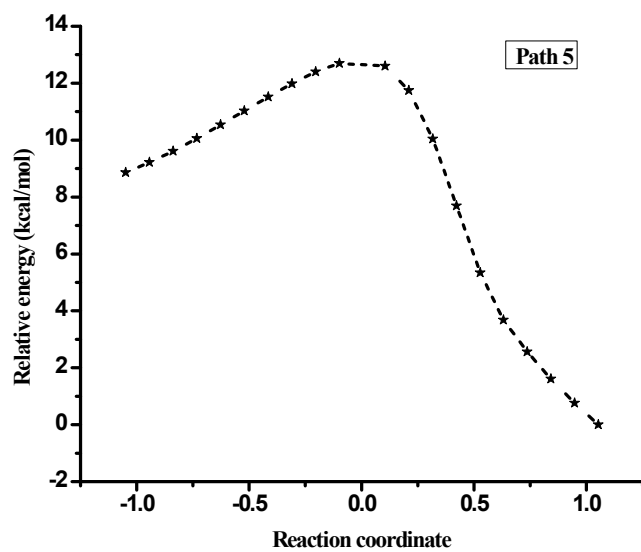
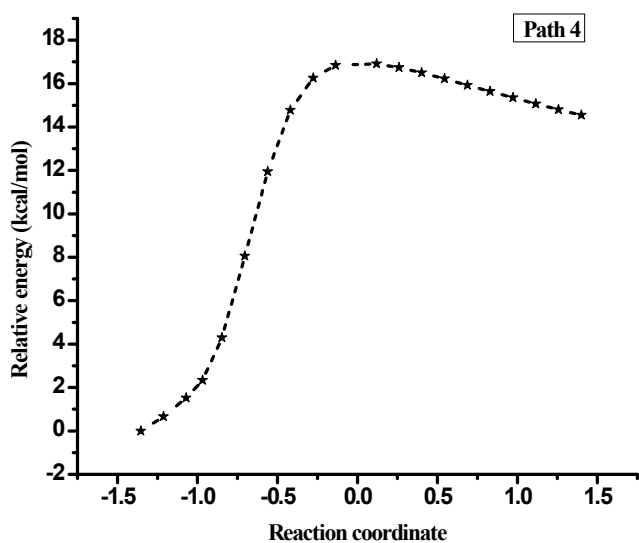
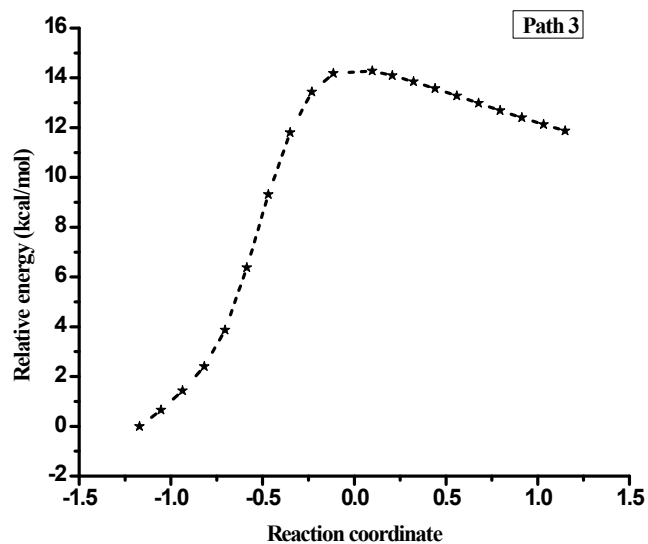
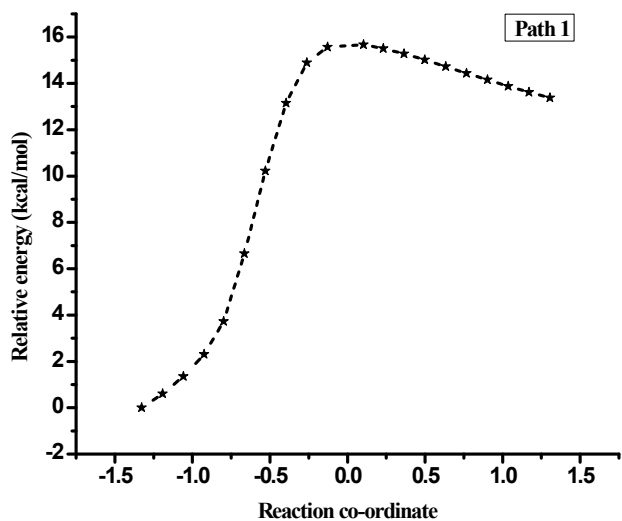


TS14



P1

Figure S2 The structures of secondary reactions of intermediates (I2) optimized at M06-2X/6-311+G(d,p) level of theory.



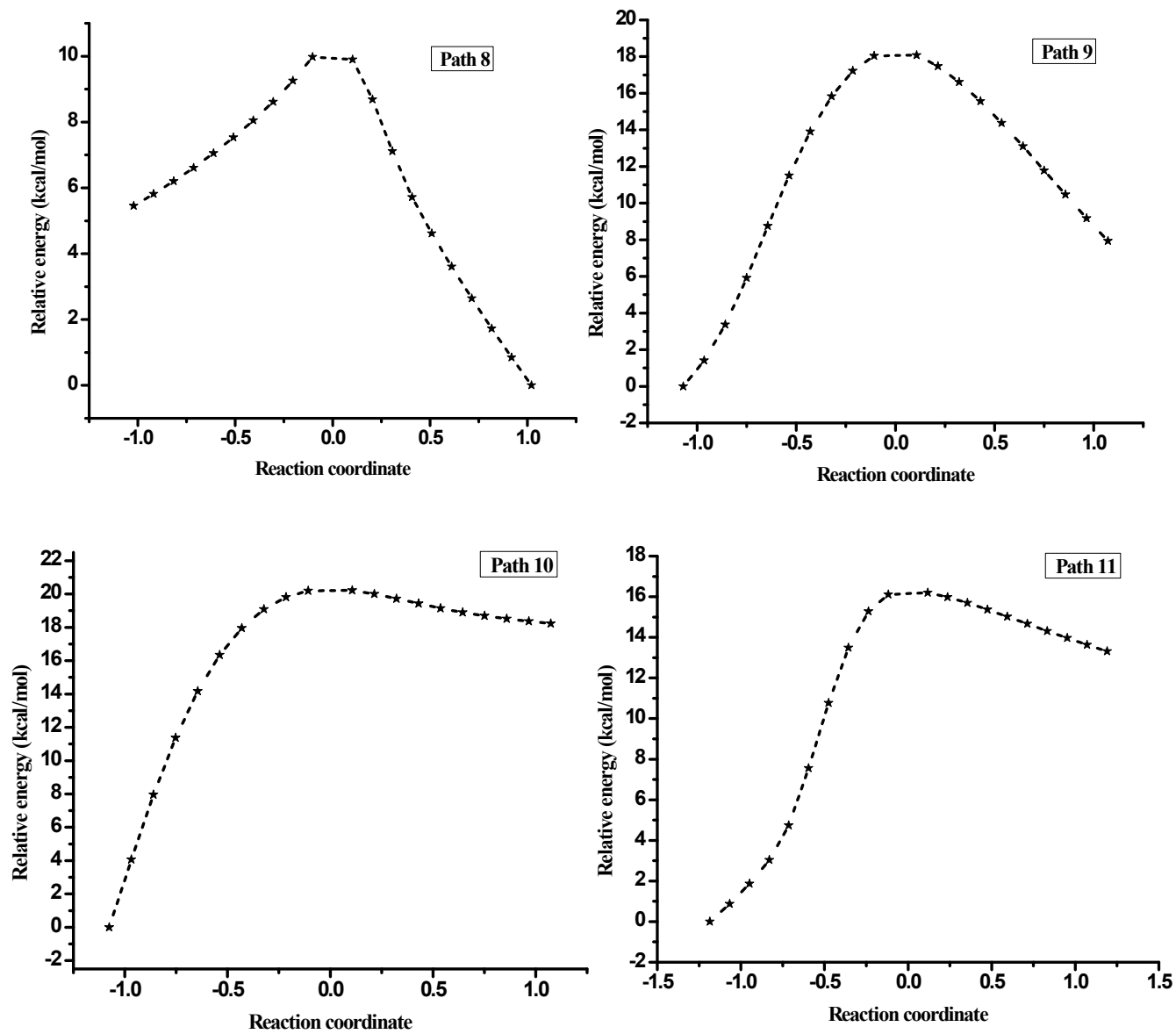


Figure S3 The intrinsic reaction coordinate (IRC) profile of all initial reactions optimized at M06-2X/6-311+G(d,p) level of theory.



**Table S1 Wigner tunneling factor of H-atom abstraction of Menthol with OH radical calculated at M06-2X/6-311+g(d,p) level of theory.**

| <b>T (K)</b> | <b>k<sub>I1</sub></b> | <b>k<sub>I2</sub></b> | <b>k<sub>I3</sub></b> | <b>k<sub>I4</sub></b> | <b>k<sub>I5</sub></b> | <b>k<sub>I6</sub></b> | <b>k<sub>I7</sub></b> | <b>k<sub>I8</sub></b> | <b>k<sub>I9</sub></b> | <b>k<sub>I0</sub></b> | <b>k<sub>I11</sub></b> |
|--------------|-----------------------|-----------------------|-----------------------|-----------------------|-----------------------|-----------------------|-----------------------|-----------------------|-----------------------|-----------------------|------------------------|
| <b>278</b>   | 1.61                  | 1.47                  | 1.54                  | 1.25                  | 2.68                  | 1.22                  | 1.97                  | 1.68                  | 1.51                  | 1.45                  | 1.21                   |
| <b>288</b>   | 1.57                  | 1.44                  | 1.50                  | 1.23                  | 2.57                  | 1.20                  | 1.90                  | 1.63                  | 1.48                  | 1.42                  | 1.20                   |
| <b>298</b>   | 1.53                  | 1.41                  | 1.47                  | 1.22                  | 2.46                  | 1.19                  | 1.84                  | 1.59                  | 1.45                  | 1.39                  | 1.19                   |
| <b>300</b>   | 1.53                  | 1.41                  | 1.46                  | 1.21                  | 2.44                  | 1.19                  | 1.83                  | 1.58                  | 1.44                  | 1.39                  | 1.18                   |
| <b>400</b>   | 1.30                  | 1.23                  | 1.26                  | 1.12                  | 1.81                  | 1.10                  | 1.47                  | 1.33                  | 1.25                  | 1.22                  | 1.10                   |
| <b>500</b>   | 1.19                  | 1.15                  | 1.17                  | 1.08                  | 1.52                  | 1.07                  | 1.30                  | 1.21                  | 1.16                  | 1.14                  | 1.07                   |