Novel Fluorine-containing Energetic Materials: How Potential Are They? A Computational Evaluation Various Performance Study

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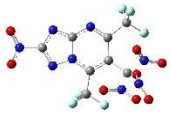
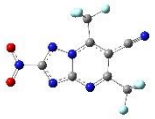
LIST OF SUPPORTING INFORMATION

Fig. SI-1. Optimized structures of 28 derivatives based on 2-nitro-[1,2,4]triazolo[1,5-a]pyrimidine at the B3LYP/6-31+G(d,p) level.



A_1

A_2



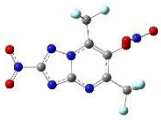
A_3

A_4

A_5

A_6

A_7



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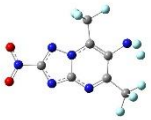

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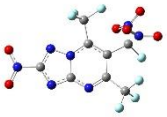

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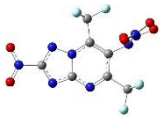
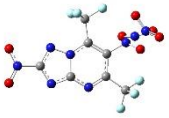


A_{11}

A_{12}



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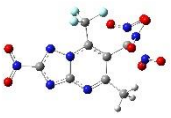

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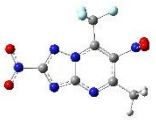

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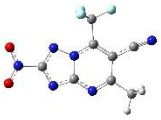

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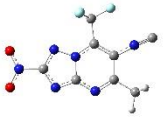

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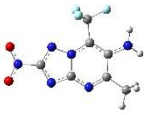

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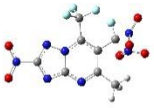
B_9



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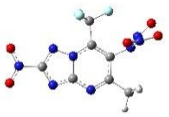

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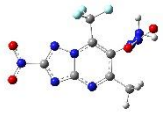

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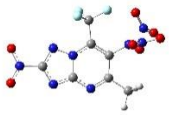

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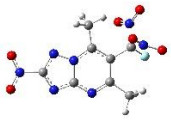
C_1



C_2

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