Supplementary Material (ESI) for Analyst

In Situ detection of Pterins by SERS

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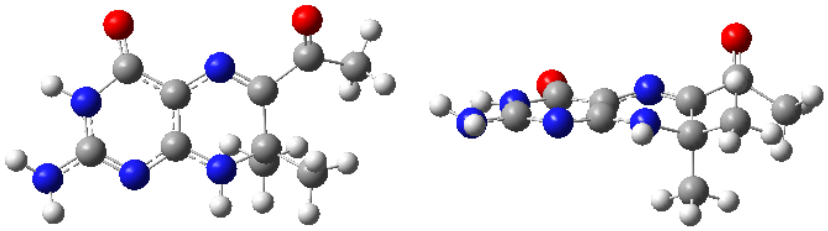
Electronic supplementary information:

1) Dihydropterin

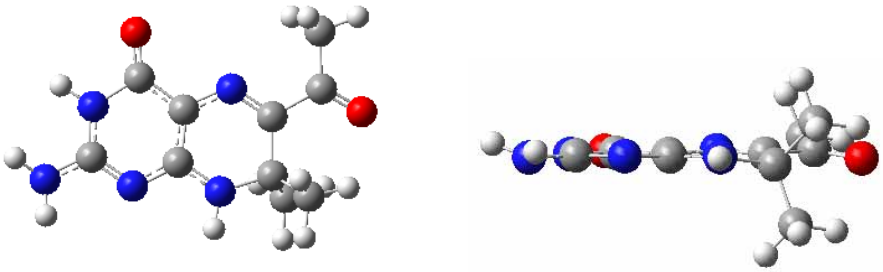
Optimised Geometry:

Two models were constructed (due to two possible ways of arranging the –C(Me)=O group):

Model A



Model B



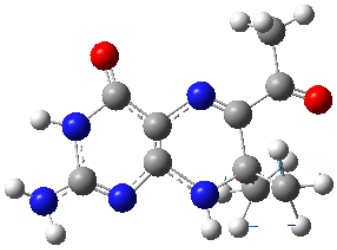
The total energies including the zero-point energy correction term are:

Model A -813.091008 a.u.
Model B -813.112093 a.u.

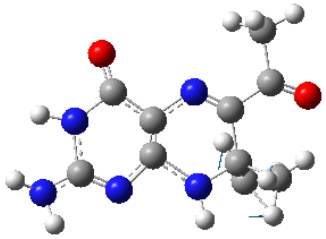
Model B is more stable by 13.2 kcal mol^{-1} and this model was used to report the calculated infra-red and Raman spectra.

Two strong vibrations are predicted at ~1479 cm^{-1}

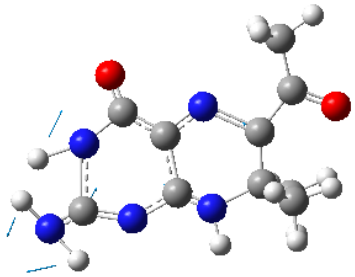
1: 1478.6 cm^{-1}



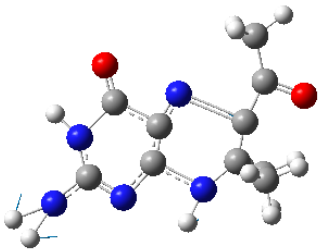
2: 1478.9 cm^{-1}



Vibration at 1567 cm^{-1}



Vibration at 1623 cm^{-1}

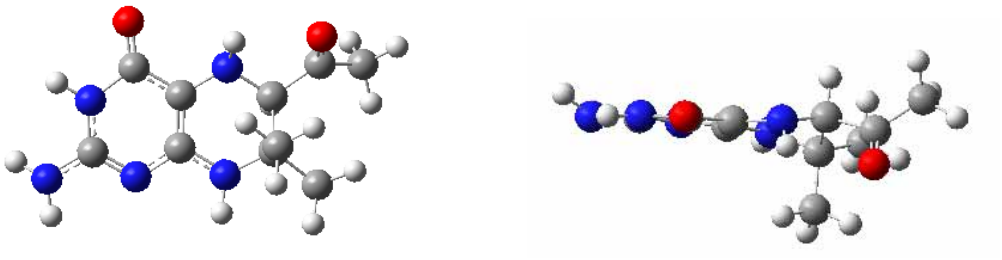


2) Tetrahydropterin

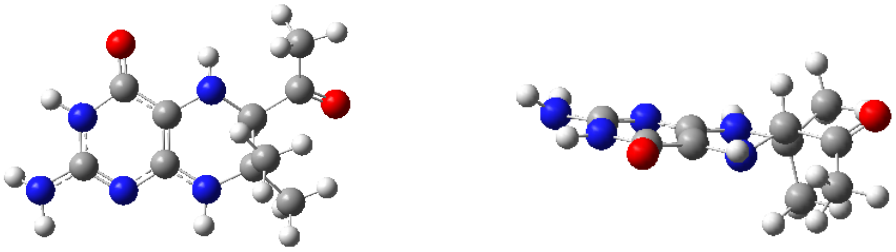
Optimised Geometry:

Four Models were constructed due to possible arrangements of the –C(Me)=O group and the two possible arrangements about the ring chiral carbon atom of the groups a) the –C(Me)=O group and b) the –H.

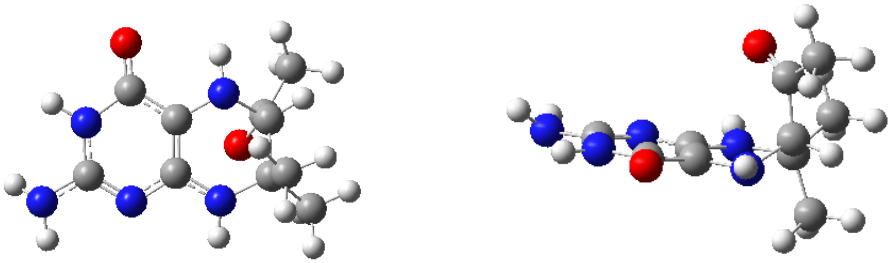
Model A



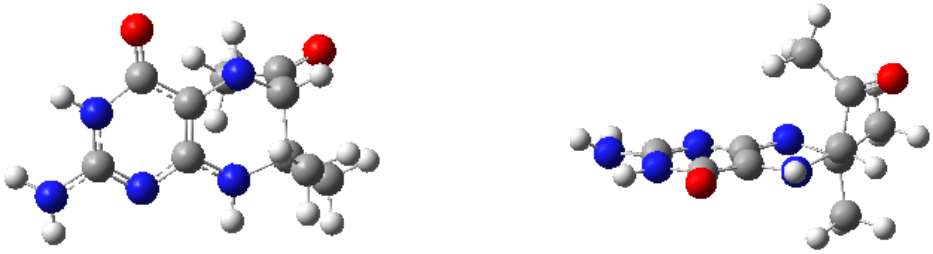
Model B



Model C

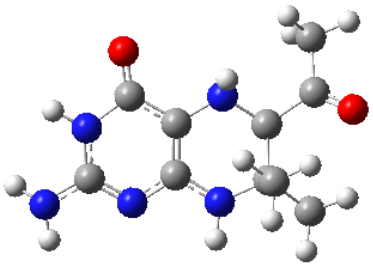


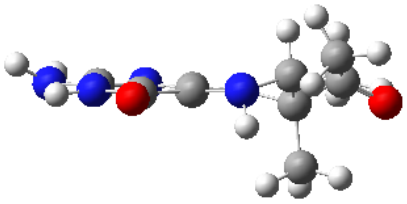
Model D



Model E

Here we took Model B and "inverted" the hydrogen bonded to the N neighbouring the CHC=O(Me) fragment.





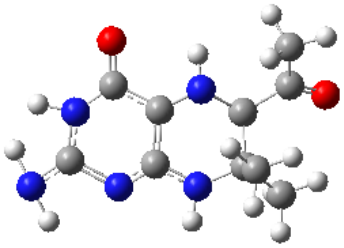
The total energies including the zero-point energy correction term are:

Model A	-814.293011 a.u.	1.79 kcal mol^{-1}
Model B	-814.295865 a.u.	0.00 kcal mol^{-1}
Model C	-814.293951 a.u.	1.20 kcal mol^{-1}
Model D	-814.295169 a.u.	0.44 kcal mol^{-1}
Model E	-814.293081 a.u.	1.75 kcal mol^{-1}

Model B is the most stable by a small amount (1.79 kcal mol^{-1} is the maximum energy difference and so any of the above structures are possible) and this model was used to report the calculated infra-red and Raman spectra.

Two calculated Raman modes of model B

(a) vibration at 1616 cm^{-1}



(b) vibration at 1654 cm^{-1}