Supporting information:

Molecular structure recognition by blob detection

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Comparison of different blob detection methods:

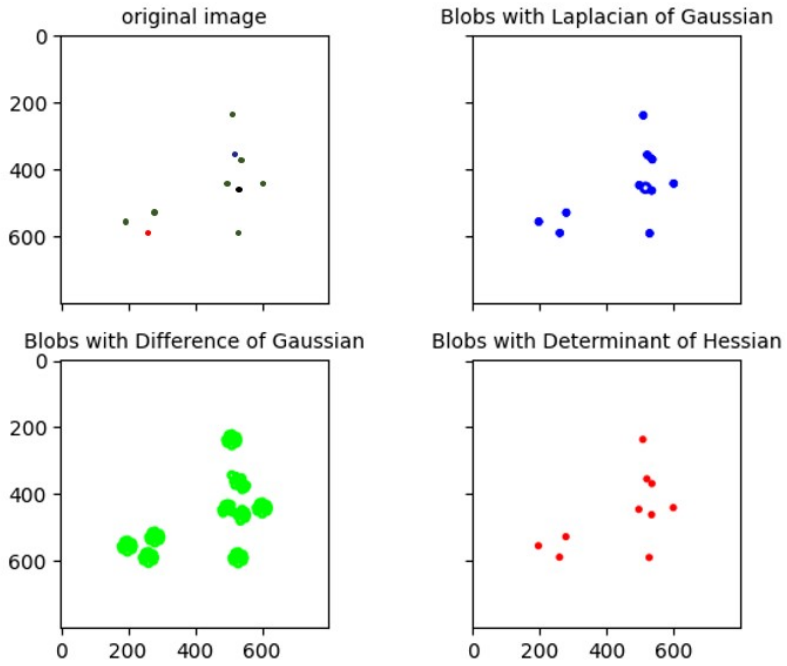

Figure S1. a) the original image of H_2O-CH_3NH_2 molecule; b) the blobs detected by the Laplacian of Gaussian method; c) the blobs detected by the Difference of Gaussian method; d) the blobs detected by the Determinant of Hessian method. The parameter of max_sigma is set to 10 and the parameter of threshold is set to 0.03.

Figure S1 shows the comparison of different blob detection method together with the original molecule. The max_sigma stands for the maximum standard deviation for Gaussian kernel, which can be approximately viewed as the radius of the blob. The threshold represents the absolute lower bound for detecting blobs.

It can be seen that for the Laplacian of Gaussian (LOG) method and the Difference of Gaussian (DOG) method, the number of blobs cannot be correctly detected. On a contrary, Bay's Determinant of Hessian (DOH) method can detect the correct number of blobs.

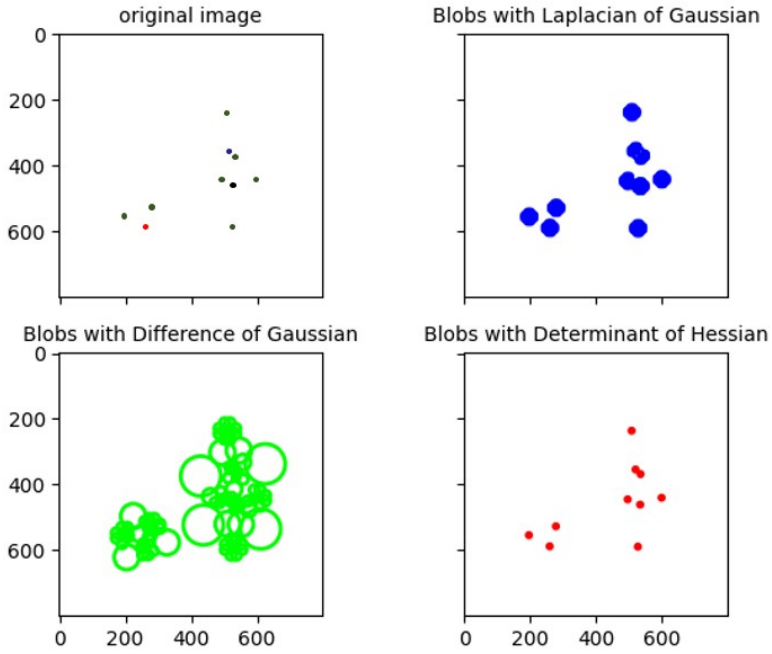

Figure S2. a) the original image of H_2O-CH_3NH_2 molecule; b) the blobs detected by the Laplacian of Gaussian method; c) the blobs detected by the Difference of Gaussian method; d) the blobs detected by the Determinant of Hessian method. The parameter of max_sigma is set to 50 and the parameter of threshold is set to 0.03.

Figure S2 shows the comparison with max_sigma being 50 and threshold being 0.03. It can be seen that Bay's Determinant of Hessian (DOH) method is stable to detect the correct number of blobs.

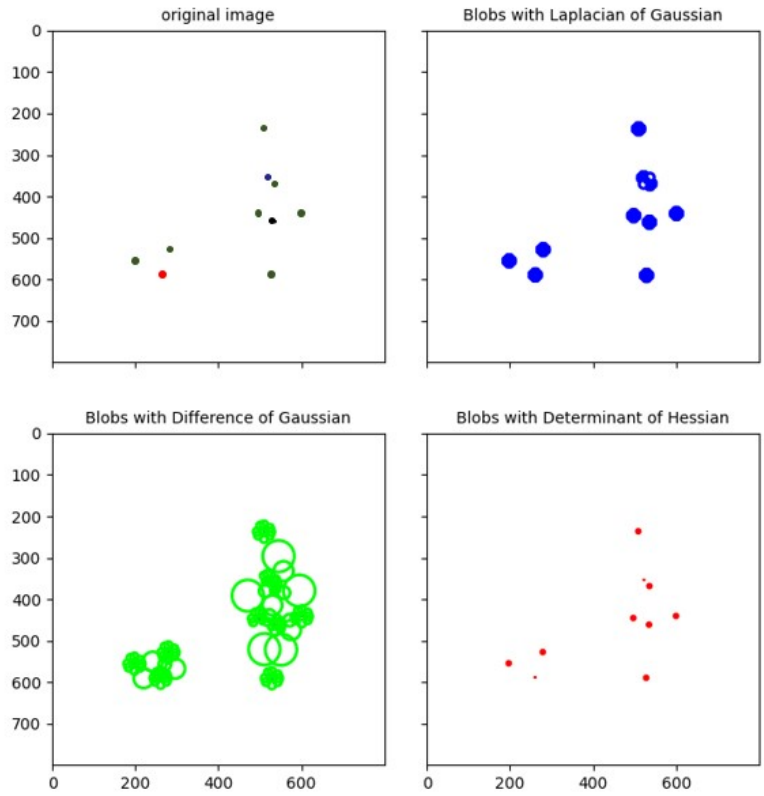

Figure S3. a) the original image of H_2O-CH_3NH_2 molecule; b) the blobs detected by the Laplacian of Gaussian method; c) the blobs detected by the Difference of Gaussian method; d) the blobs detected by the Determinant of Hessian method. The parameter of max_sigma is set to 30 and the parameter of threshold is set to 0.05.

Figure S3 shows the comparison with max_sigma being 30 and threshold being 0.05. It can be seen that the DOH method can detect the correct number of blobs as well. However, in Fig. S3d, the detected blobs are of different size. This is because the atoms are assigned with different colors, as shown in Fig. S3a. When converted to gray-scale, the different shades of gray atoms would have different radius due to numerical roundup. Eventually, the detected blobs appear with different size.