Electronic Supplementary Material (ESI) for Analytical Methods.


# Computational Design, Synthesis and Utilization of a Magnetic Molecularly Imprinted Polymer on Graphene Oxide Nanosheets for Highly Selective Extraction and Determination of Buprenorphine in Biological Fluids and Tablet

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**Table 1S**
Comparison of the proposed method with other methods applied for extraction and determination of BUP.

| Method | LOD | LOQ | DLR | RSD (%) | Reference |
|---|---|---|---|---|---|
| MMISPE- HPLC-UV | 0.6 | 2.5 | 2.5-500 | < 8.2 | Present work |
| MISPE- HPLC-UV | 3.0 | 10.0 | 10-500 | < 6.5 | [1] |
| EME-CE [a]-UV | 1.0 | 3.0 | 3-700 | < 3.8 | [2] |
| LLE-HPLC-FLD[b] | 1.0 | 3.0 | 3-300 | - | [3] |
| LLE-HPLC-UV | - | 2.0 | 2-50 | < 4.9 | [4] |
| SPE-LC-MS/MS[c] | 0.002 | 0.007 | 0.01-5.0 | < 4.0 | [5] |
| LLE-LC-MS/MS | 0.83 | 5.00 | 5.00-1000 | 6.6 | [6] |

[a] Electro membrane extraction-capillary electrophoresis
[b] Fluorescence detection
[c] liquid chromatography-tandem mass spectrometry
All concentrations are based on μg $L^{-1}$.


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[3] S.T. Ho, J.J. Wang, W. Ho, O.Y.P. Hu, Determination of buprenorphine by high-performance liquid chromatography with fluorescence detection: application to human and rabbit pharmacokinetic studies, J. Chromatogr. B 570 (1991) 339-350.

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[5] A. Ceccato, R. Klinkenberg, P. Hubert, B. Streel, Sensitive determination of buprenorphine and its N-dealkylated metabolite norbuprenorphine in human plasma by liquid

chromatography coupled to tandem mass spectrometry, J. Pharm. Biomed. Anal. 32 (2003) 619-631.

[6] H.R. Lin, C.L. Chen, C.L. Huang, S.T. Chen, A.C. Lua, Simultaneous determination of opiates, methadone, buprenorphine and metabolites in human urine by superficially porous liquid chromatography tandem mass spectrometry, J. Chromatogr. B, 925 (2013) 10-15.

**Fig. 1S:** The most stable structures of (a) BUP-$(AA)_5$-$(EGDMA)_{35}$, (b) GO and GO@$Fe_3O_4$@vinyl.

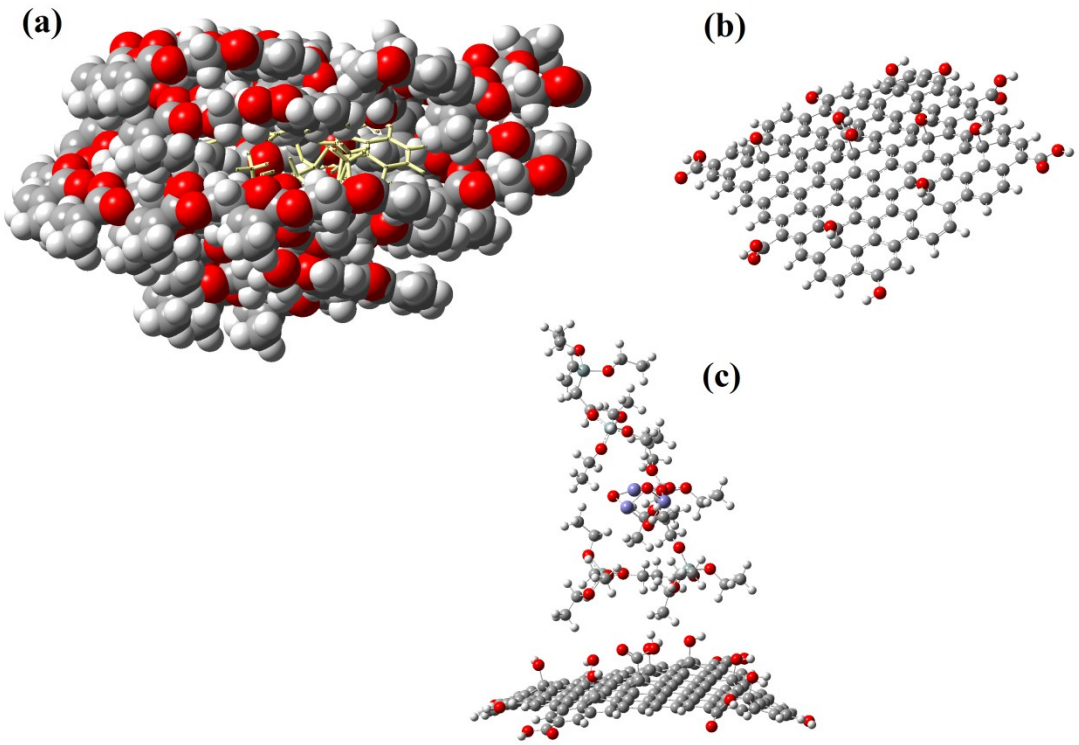
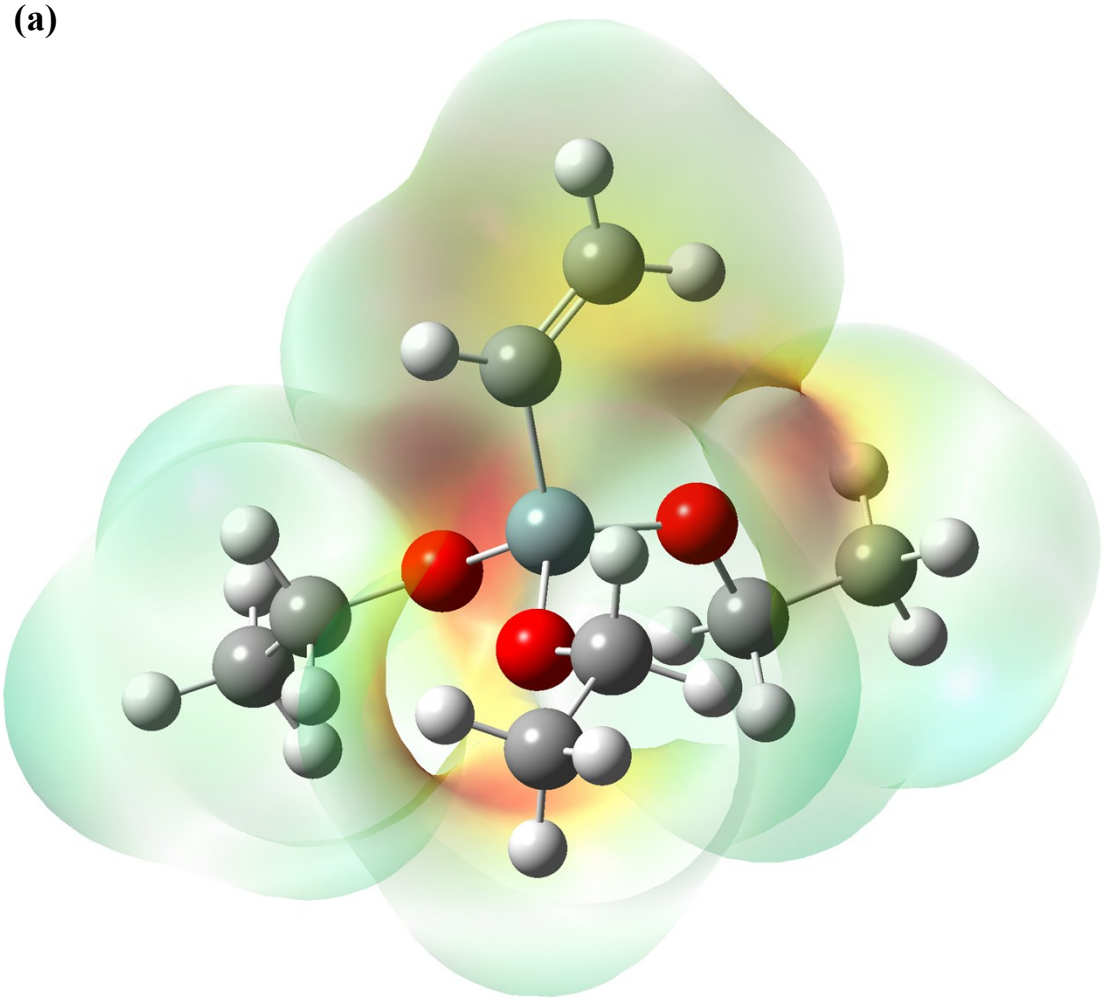
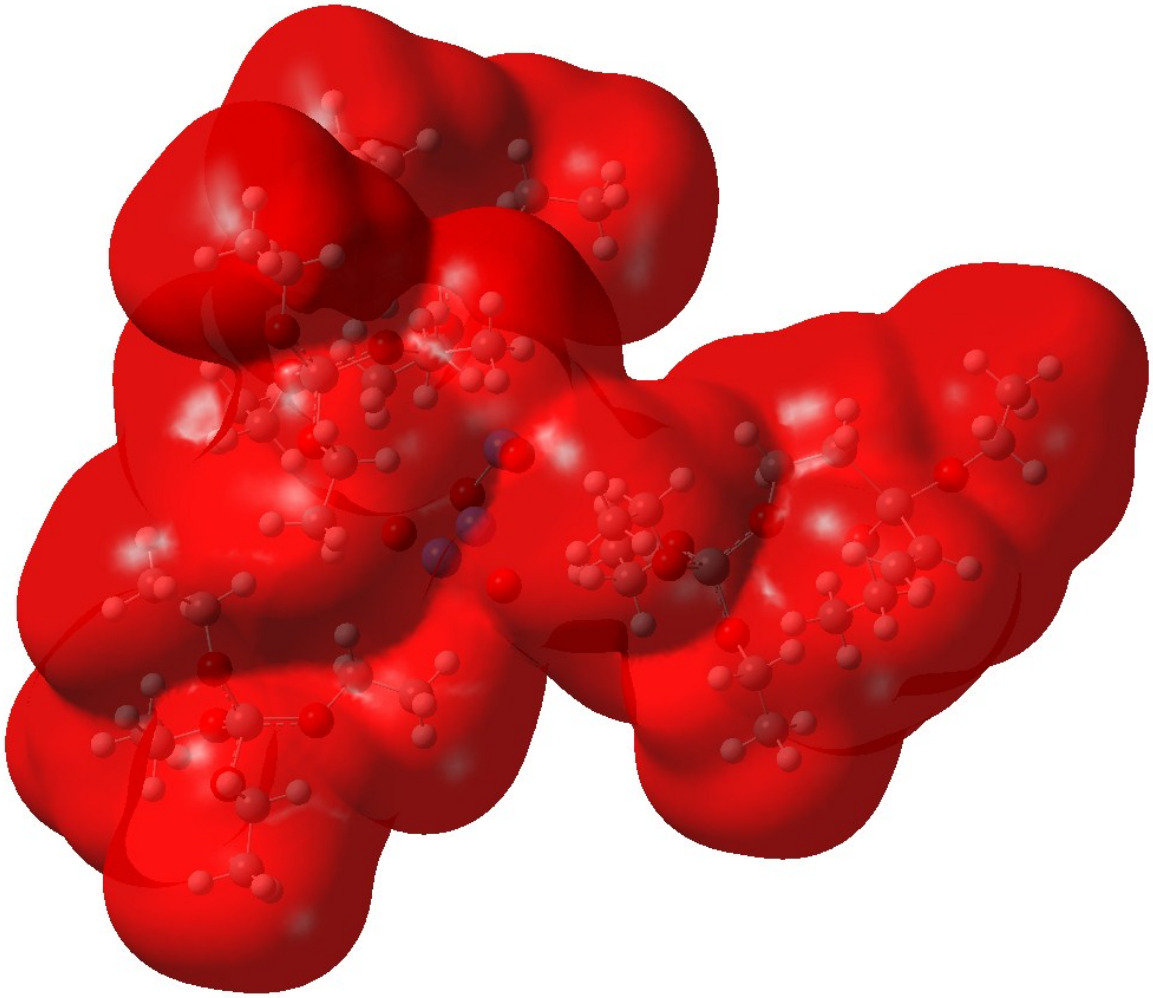


**Fig. 2S:** Electron density surface maps with electrostatic potential surface for (a) 3-VTES, (b) $Fe_3O_4$@vinyl and (c) EGDMA

**(a)**



**(b)**



**(c)**

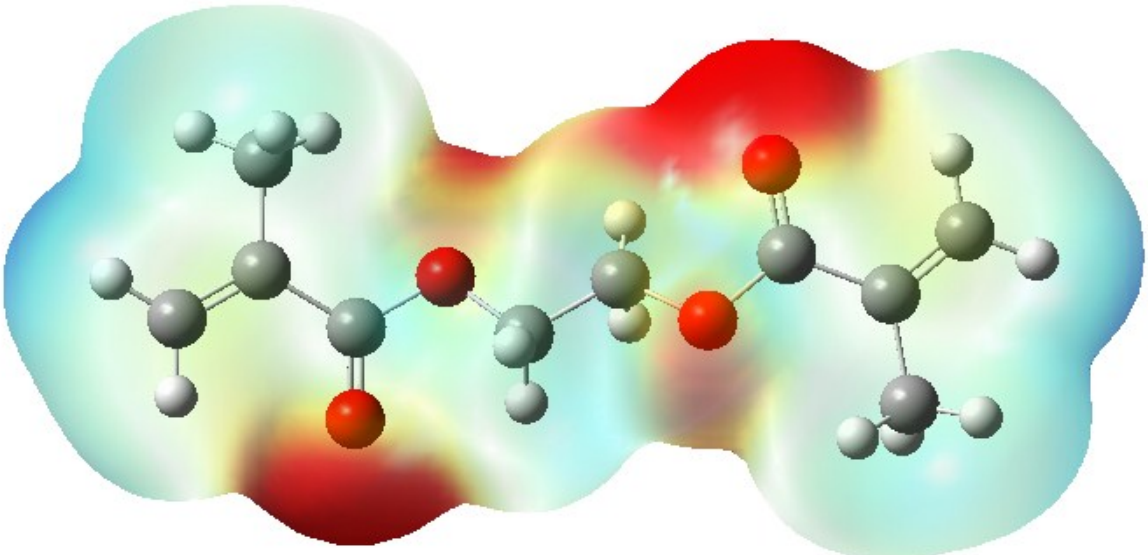


**Fig. 3S:** Hydrogen bonding between GO@$Fe_3O_4$@vinyl and EGDMA.

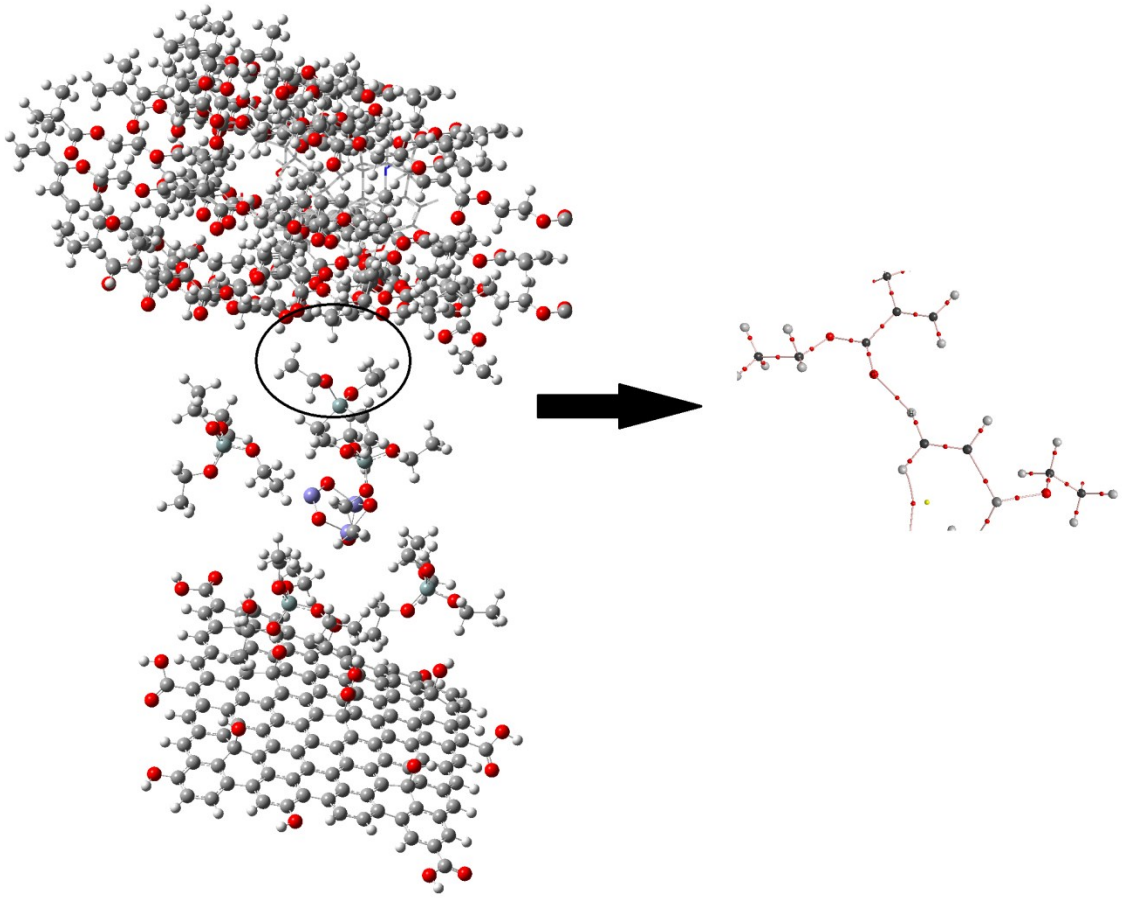
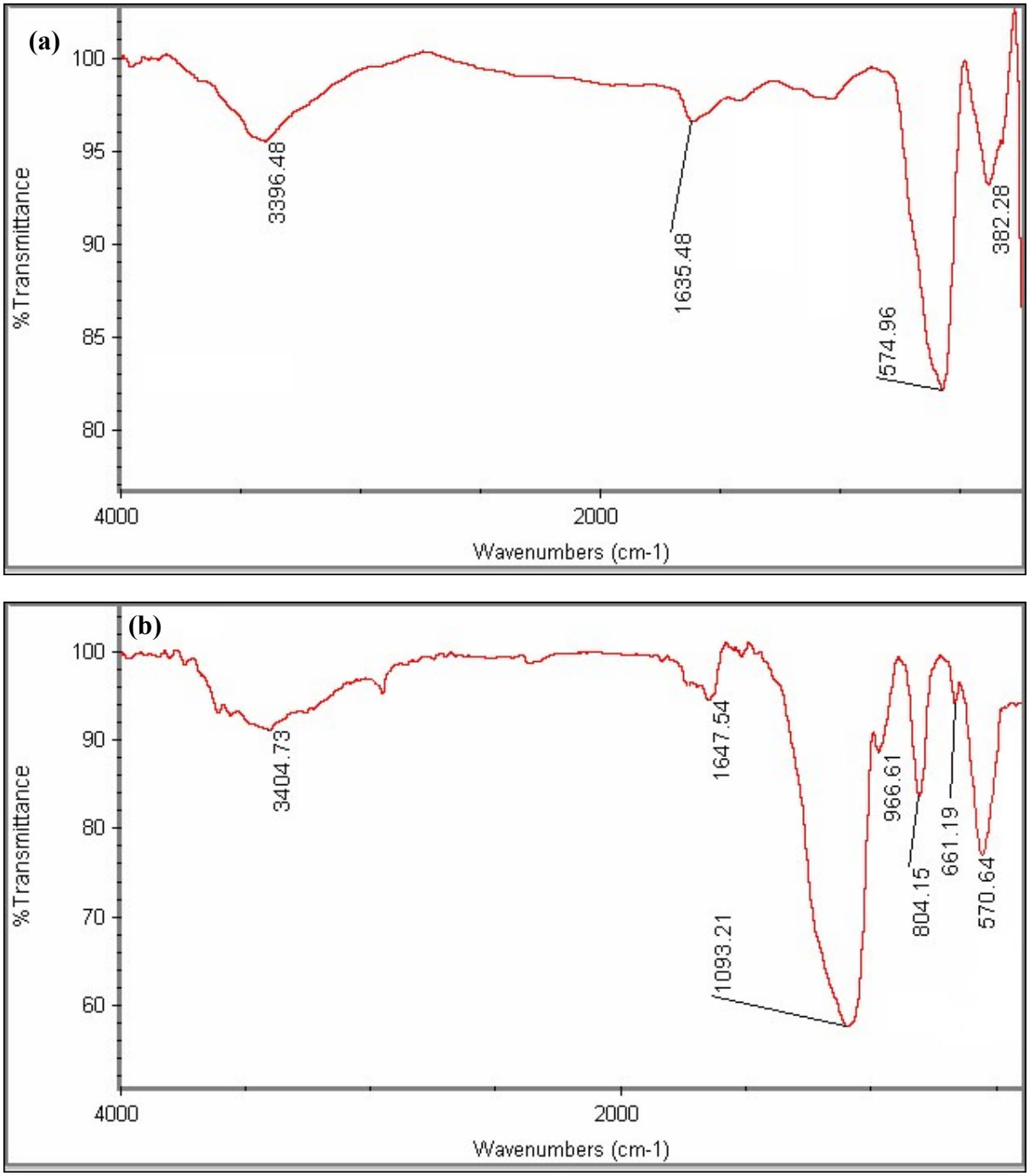
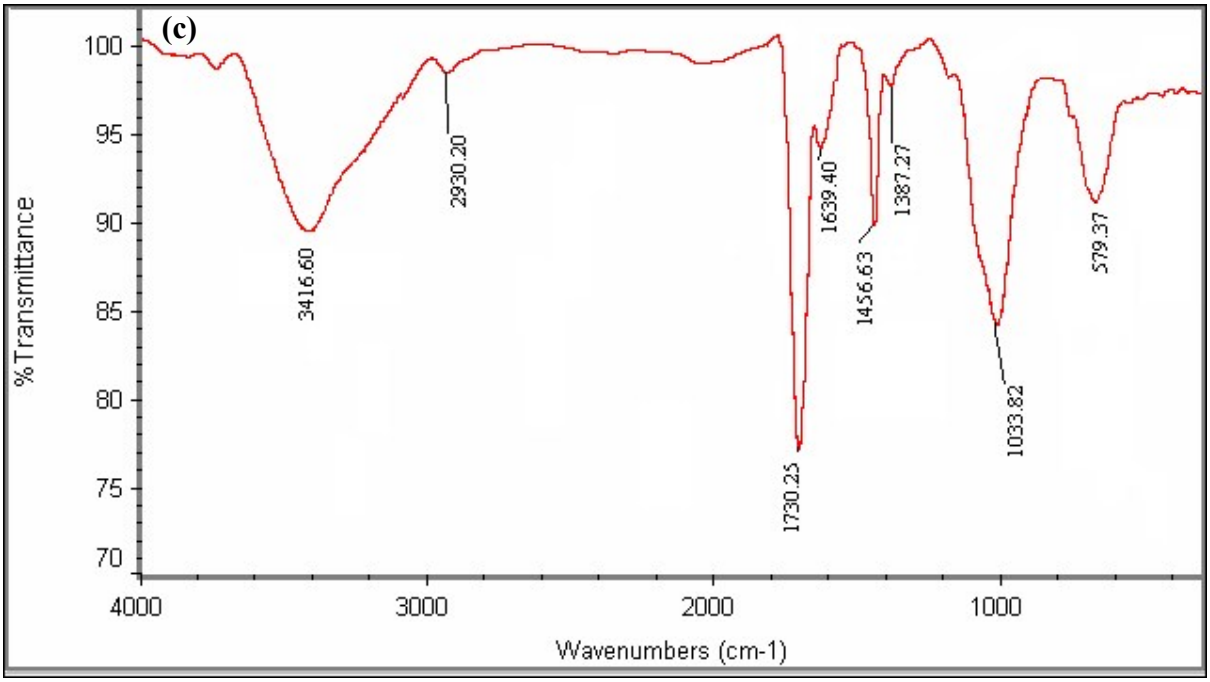


**Fig. 4S:** FT-IR spectra of (a) GO@$Fe_3O_4$, (b) GO@$Fe_3O_4$@3-VTES and (c) MMIP composites.




(c)
100
95
90
85
80
75
70
% Transmittance
3416.60
2930.20
1730.25
1639.40
1456.63
1387.27
1033.82
579.37
4000
3000
2000
1000
Wavenumbers (cm-1)