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Supplementary File

Fumarate Based Metal Organic Framework: An Effective Catalyst for the Transesterification of Used Vegetable Oil

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Characterization

The MOF-801 crystalline structure was determined using Bruker D2 Phaser X-ray diffractometer with Cu Kα radiation (λ = 1.5418 Å), with accelerating voltage and current of 30 kV and 10 mA, respectively. FT-IR spectra of MOF-801 was assessed on a Perkin Elmer 1000 FT-IR spectrometer at room temperature. The TGA was performed by heating the samples in N_2 flow using a Perkin-Elmer Thermogravimetric Analyzer 7 with a heating rate of 10 °C/min. The BET surface area and BJH pore volume were measured by N_2 adsorption-desorption isotherm using Micromeritics (Gemini VII, 2390 surface area and porosity USA). MOF-801 sample was degassed at a temperature of 120 °C for 3 h using nitrogen gas. The assessment of transesterification product was carried out by ^{1}H NMR spectroscopy using deuterated chloroform as solvent on a JEOL 400-MHz spectrometer (JEOL, Ltd., Tokyo, Japan) at ambient temperature. The NMR samples were prepared by dissolving 20 mg of the biodiesel product in 2 ml $CDCl_3$ solvent with 0.05% tetramethylsilane (TMS). The surface morphology and elemental composition was carried out using JEOL instrument (JED-2200 Series (Japan)).

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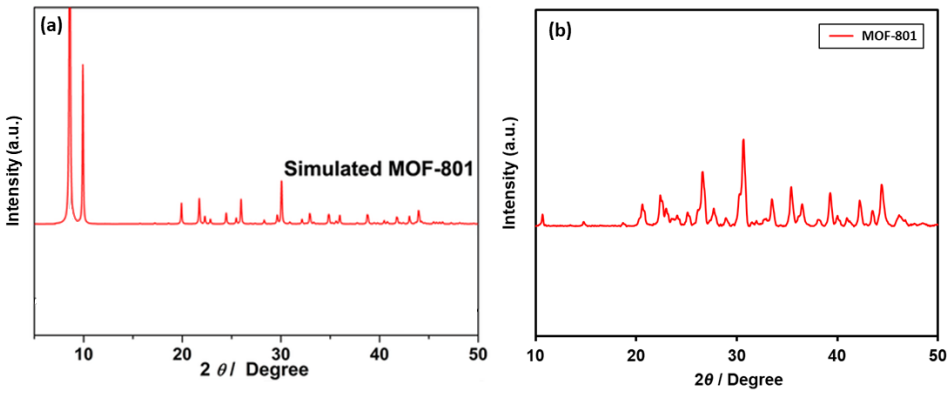

Figure S1: (a) Comparison of the simulated MOF-801 from the previously published data [1] and (b) as-synthesized XRD patterns of MOF-801.

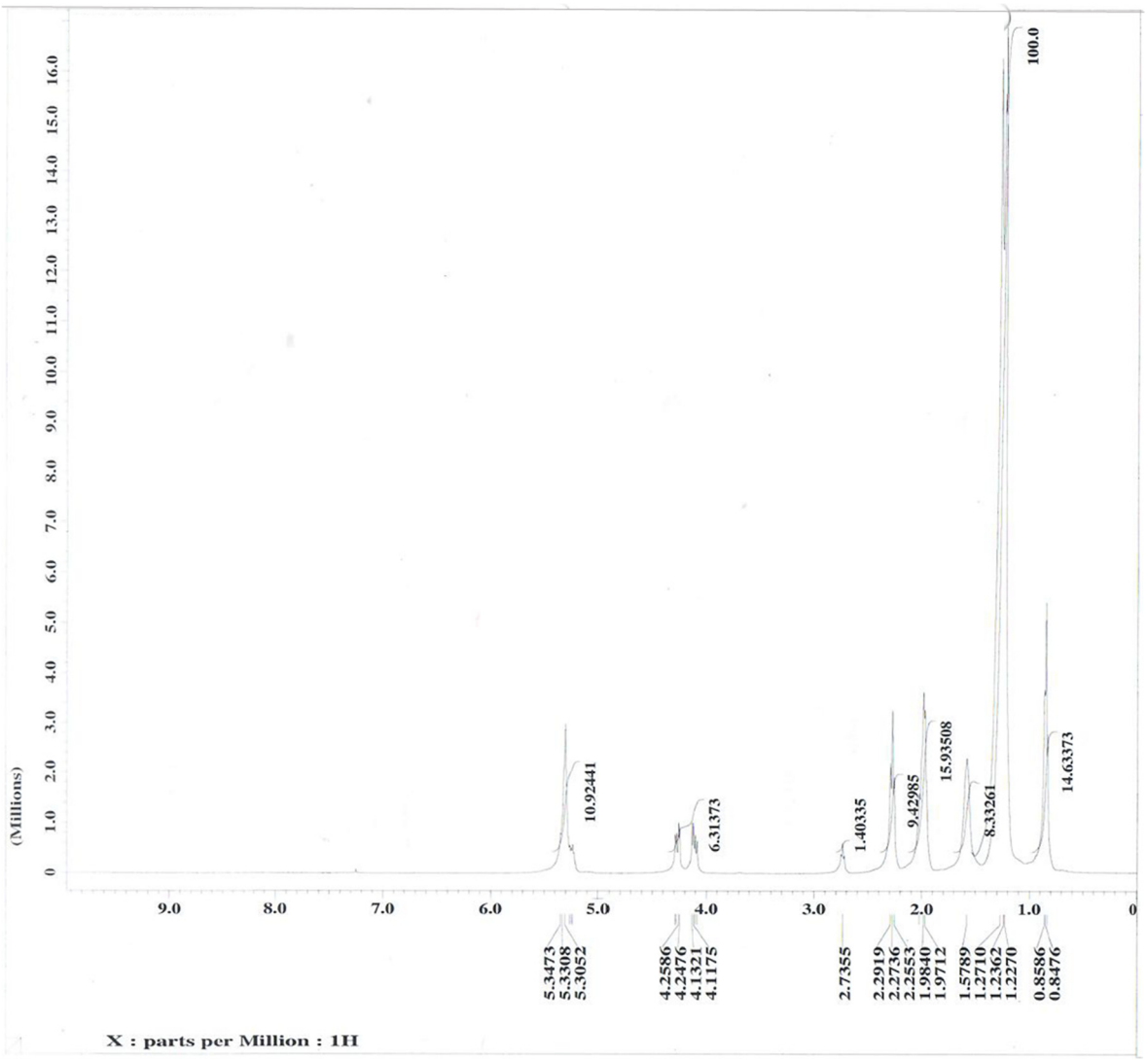

Figure S2: ^{1}H-NMR spectrum of used vegetable oil (UVO).

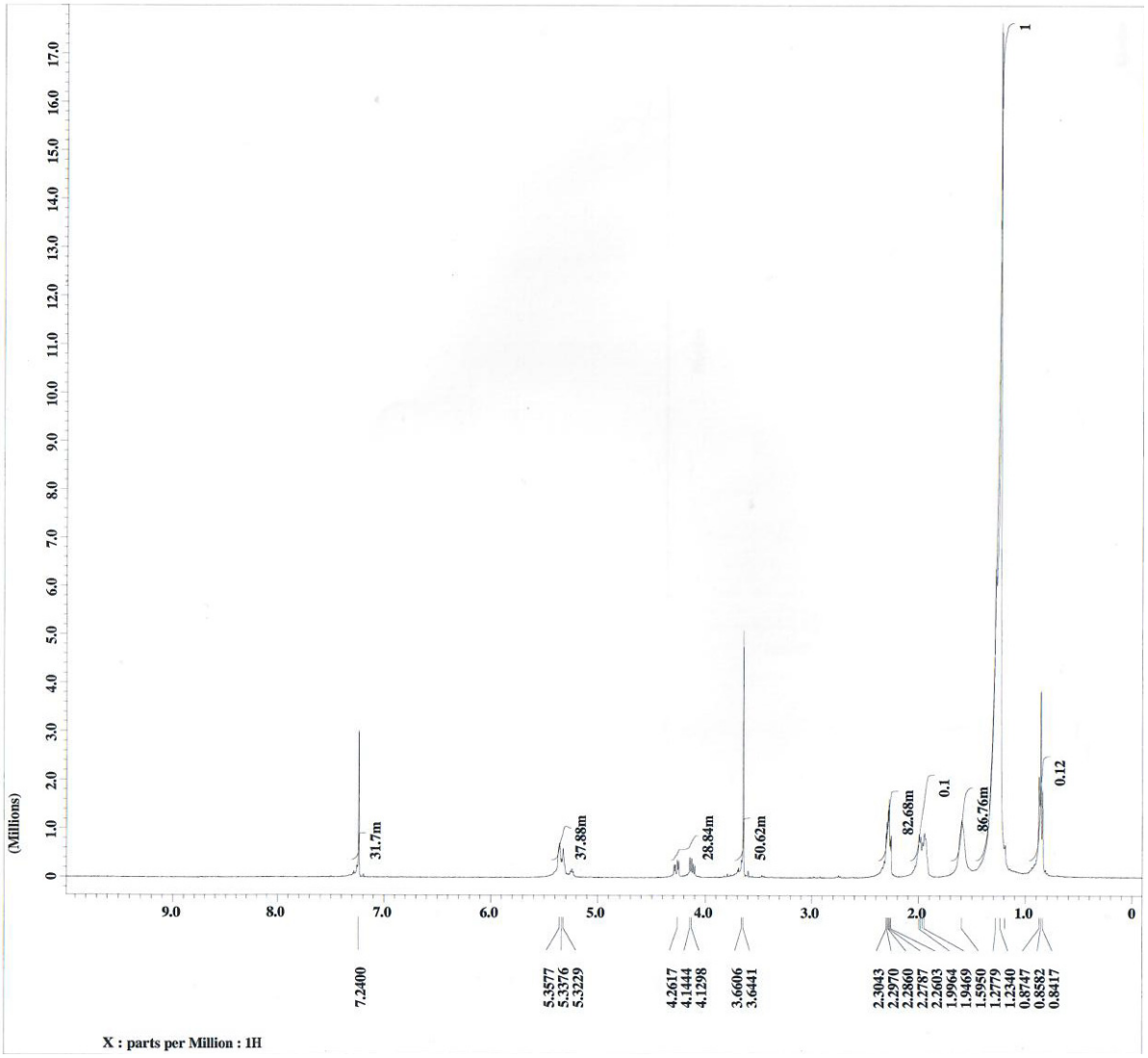

Figure S3: [1]H-NMR spectrum of biodiesel synthesized by transesterification of UVO using MOF-801 catalyst (5 wt.% to oil)at 180 °C in 8 h with methanol to oil 50 wt.%.

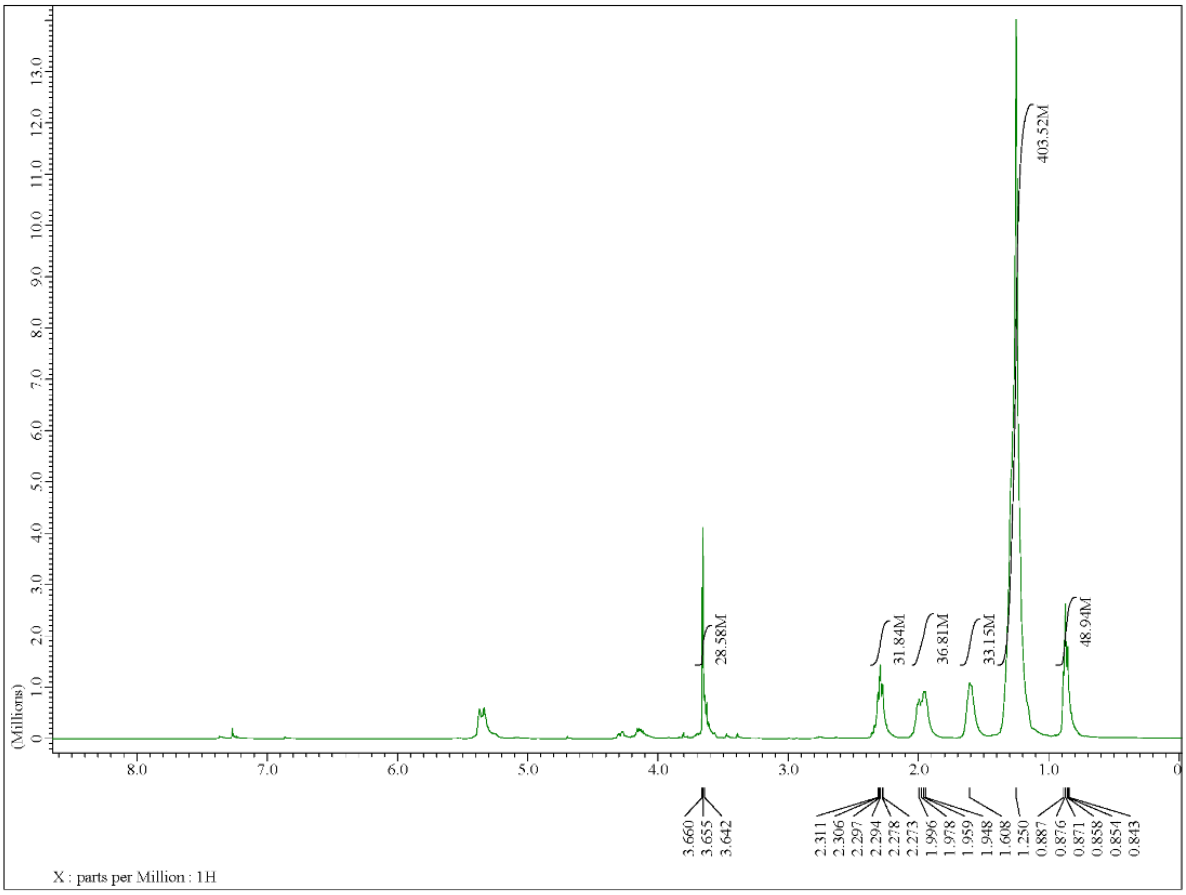

Figure S4: [1]H-NMR spectrum of biodiesel synthesized by transesterification of UVO using MOF-801 catalyst (10 wt.% to oil)at 180 °C in 8 h with methanol to oil 50 wt.%.

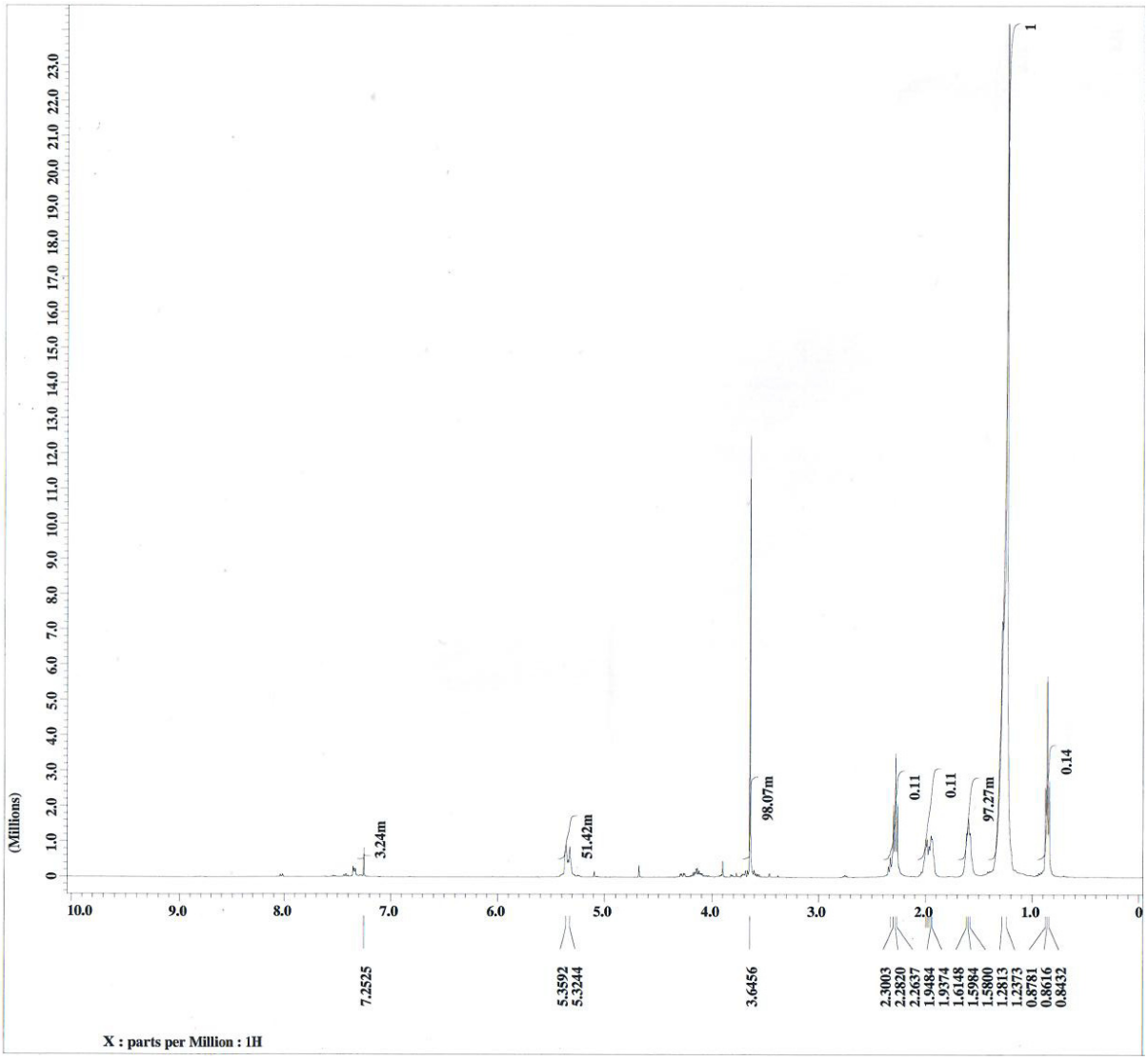

Figure S5: ^{1}H-NMR spectrum of biodiesel synthesized by transesterification of UVO using MOF-801 catalyst (15 wt.% to oil)at 180 °C in 8 h with methanol to oil 50 wt.%.

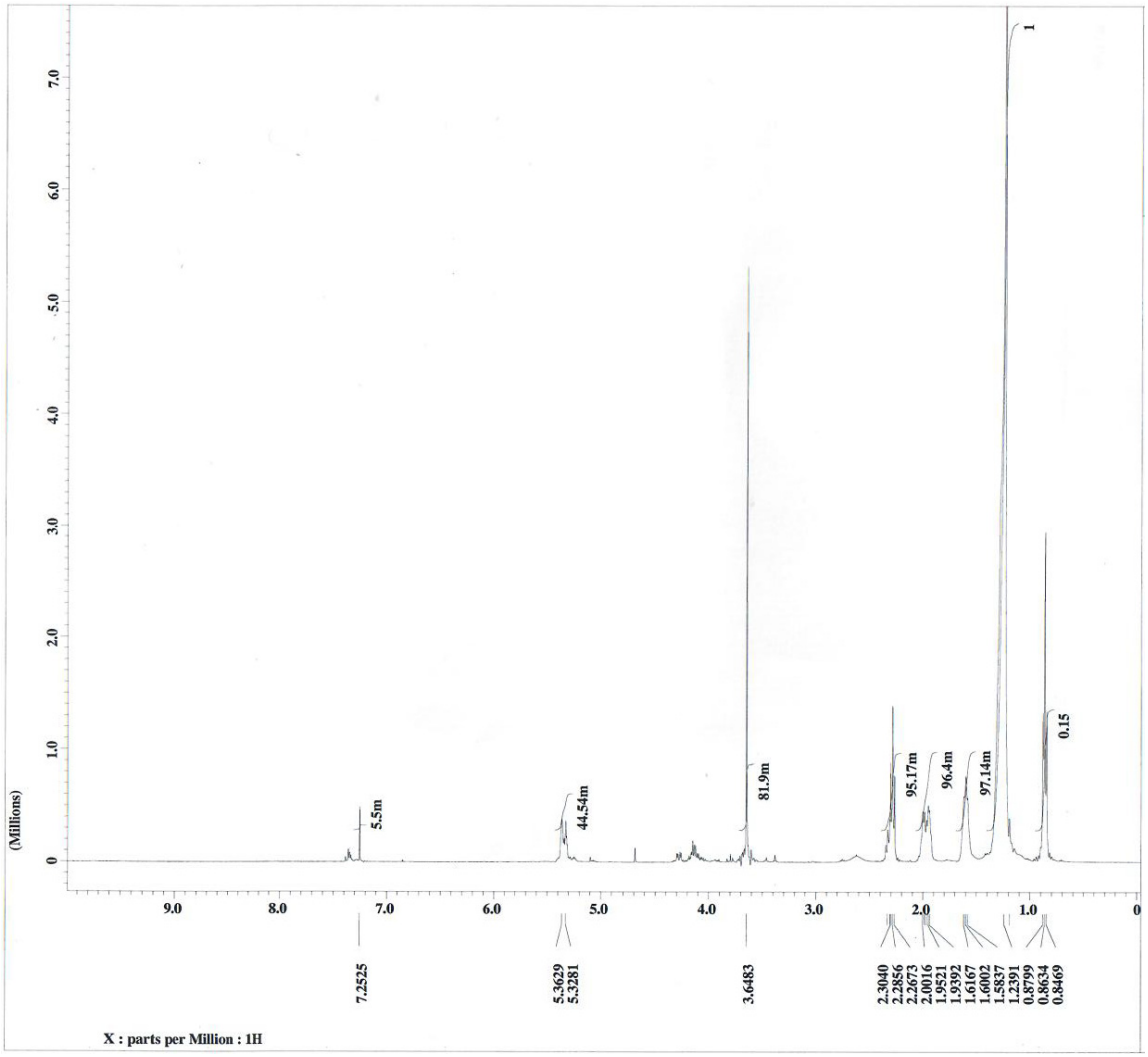

Figure S6: ^{1}H-NMR spectrum of biodiesel synthesized by transesterification of UVO using MOF-801 catalyst (20 wt.% to oil)at 180 °C in 8 h with methanol to oil 50 wt.%.

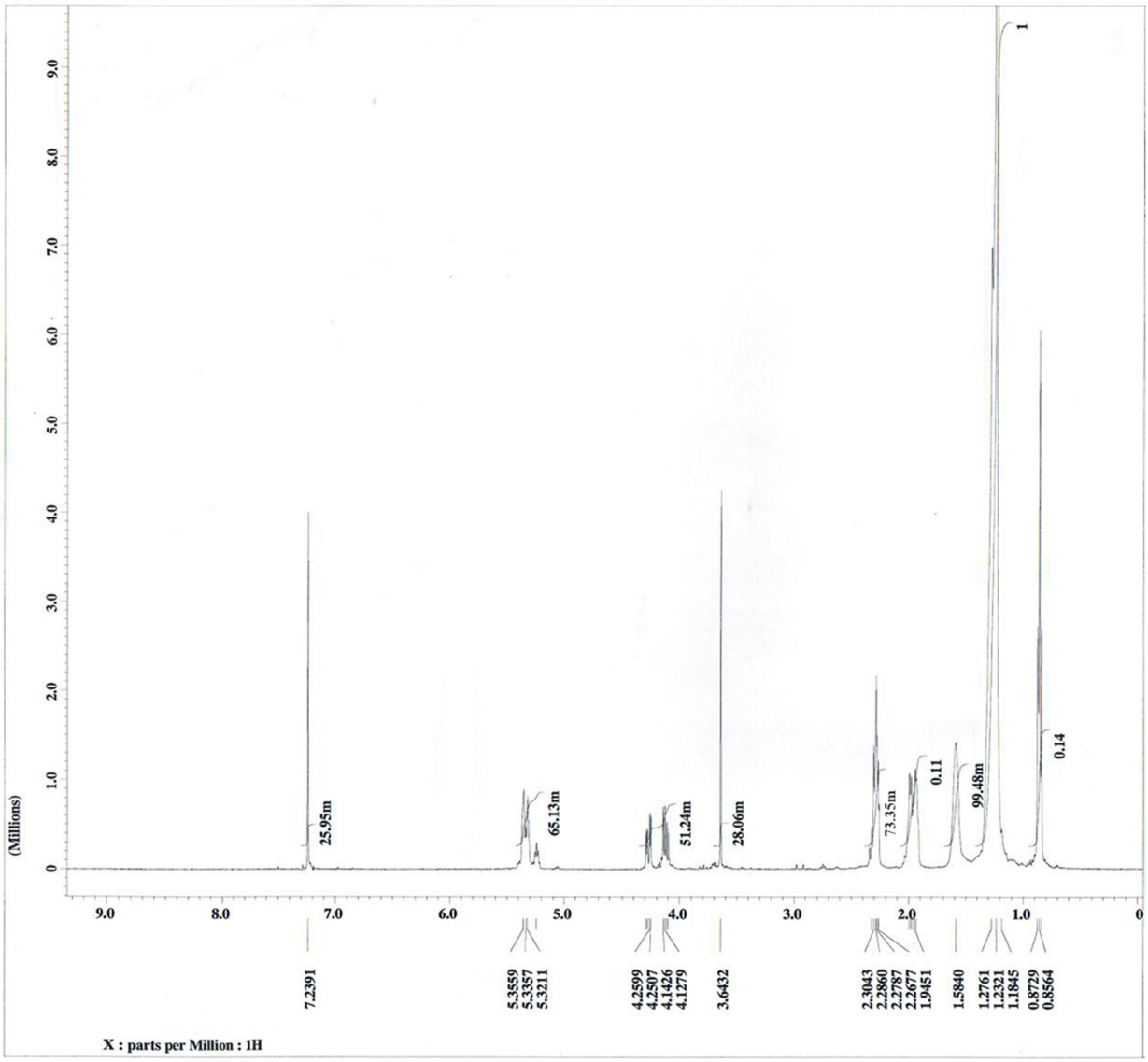

Figure S7: ^{1}H-NMR spectrum of biodiesel synthesized by transesterification of UVO using MOF-801 catalyst (10 wt.% to oil)at 180 °C in 8 h with methanol to oil 30 wt.%.

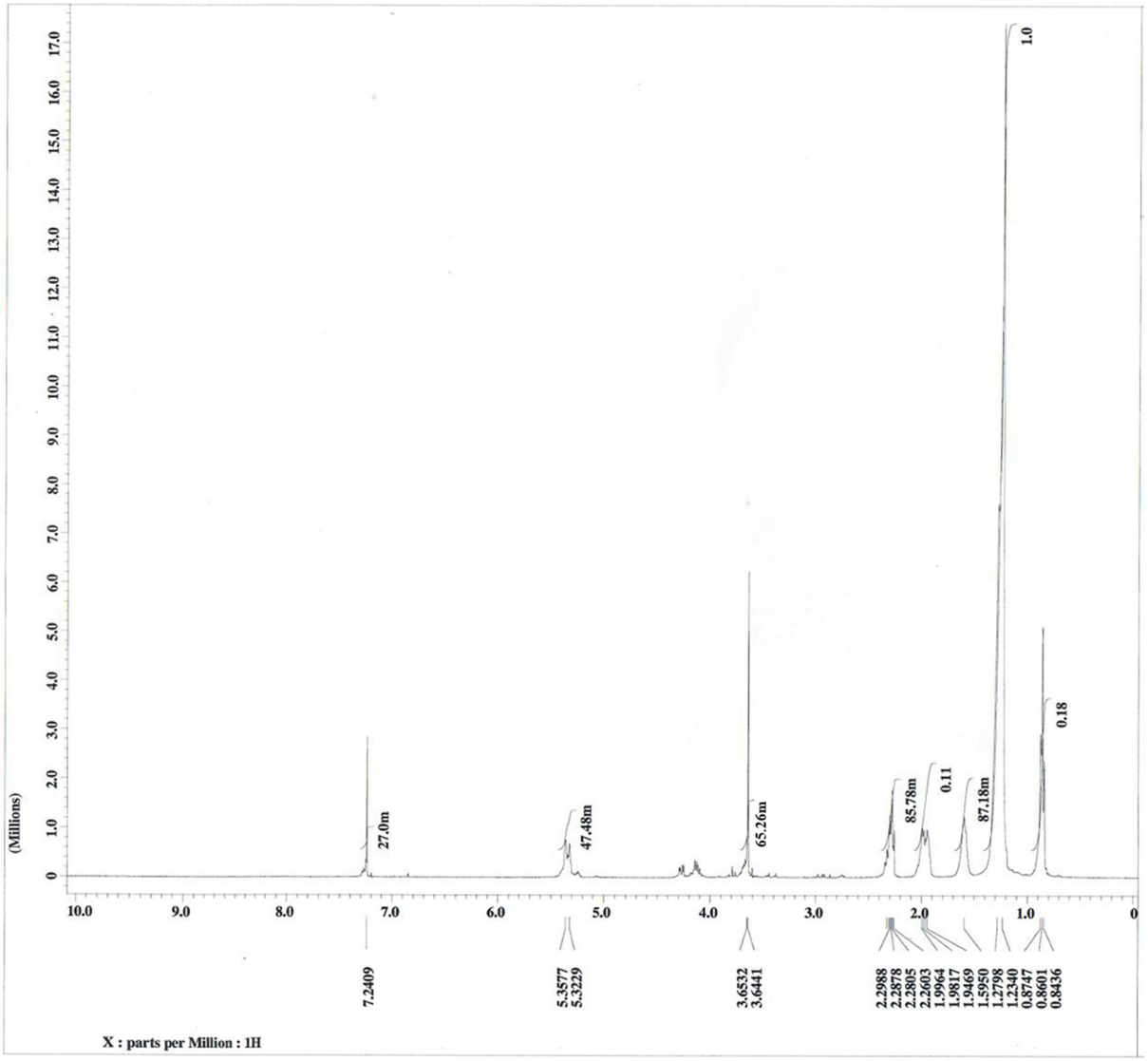

Figure S8: [1]H-NMR spectrum of biodiesel synthesized by transesterification of UVO using MOF-801 catalyst (10 wt.% to oil)at 180 °C in 8 h with methanol to oil 40 wt.%.

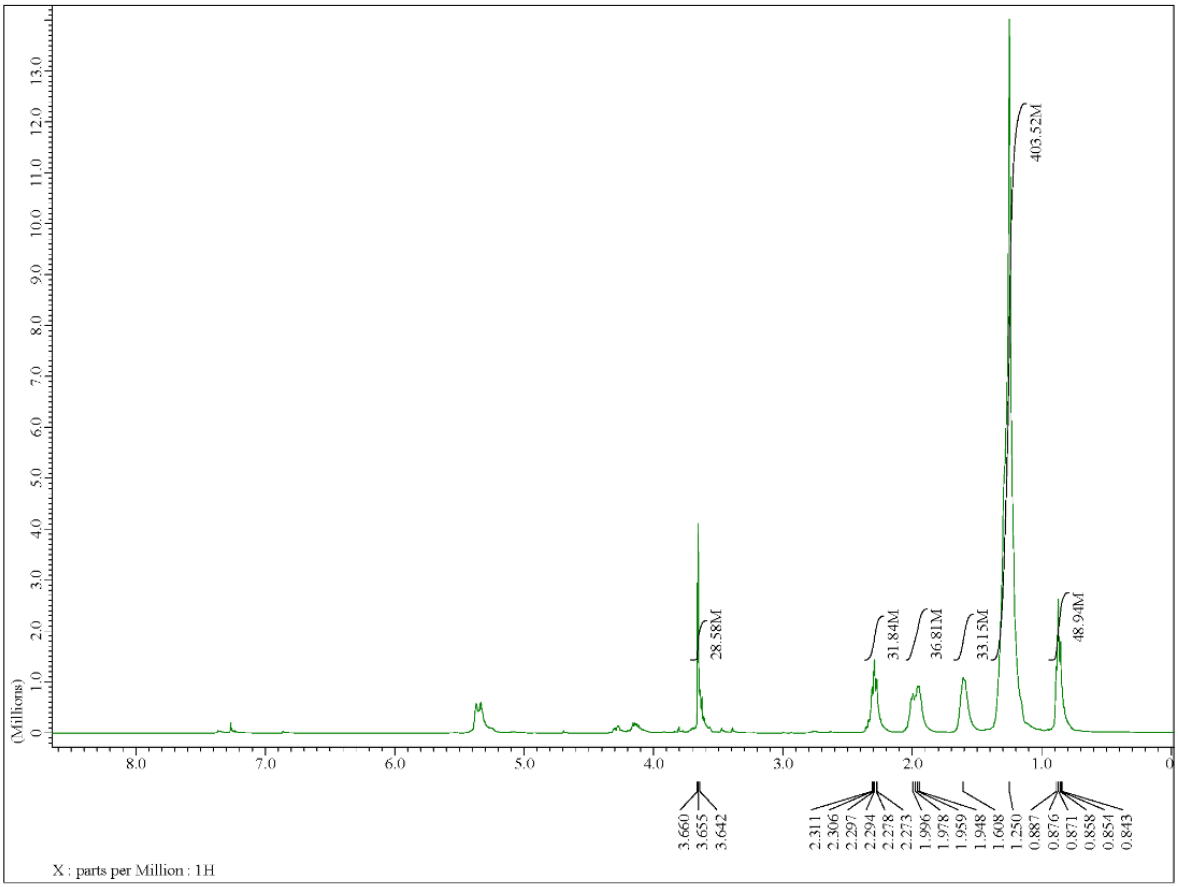

Figure S9: [1]H-NMR spectrum of biodiesel synthesized by transesterification of UVO using MOF-801 catalyst (10 wt.% to oil)at 180 °C in 8 h with methanol to oil 50 wt.%.

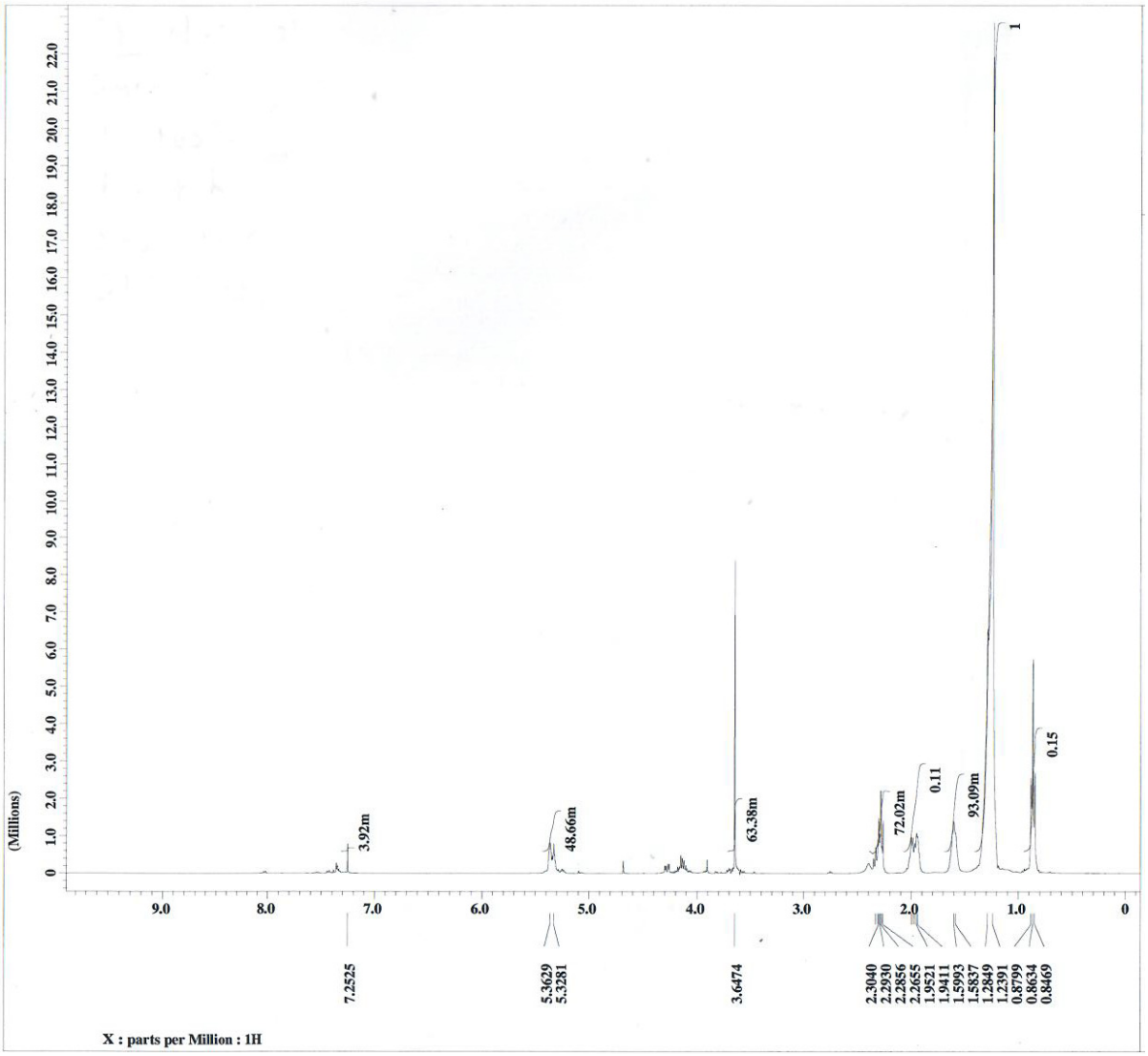

Figure S10: [1]H-NMR spectrum of biodiesel synthesized by transesterification of UVO using MOF-801 catalyst (10 wt.% to oil)at 180 °C in 8 h with methanol to oil 60 wt.%.

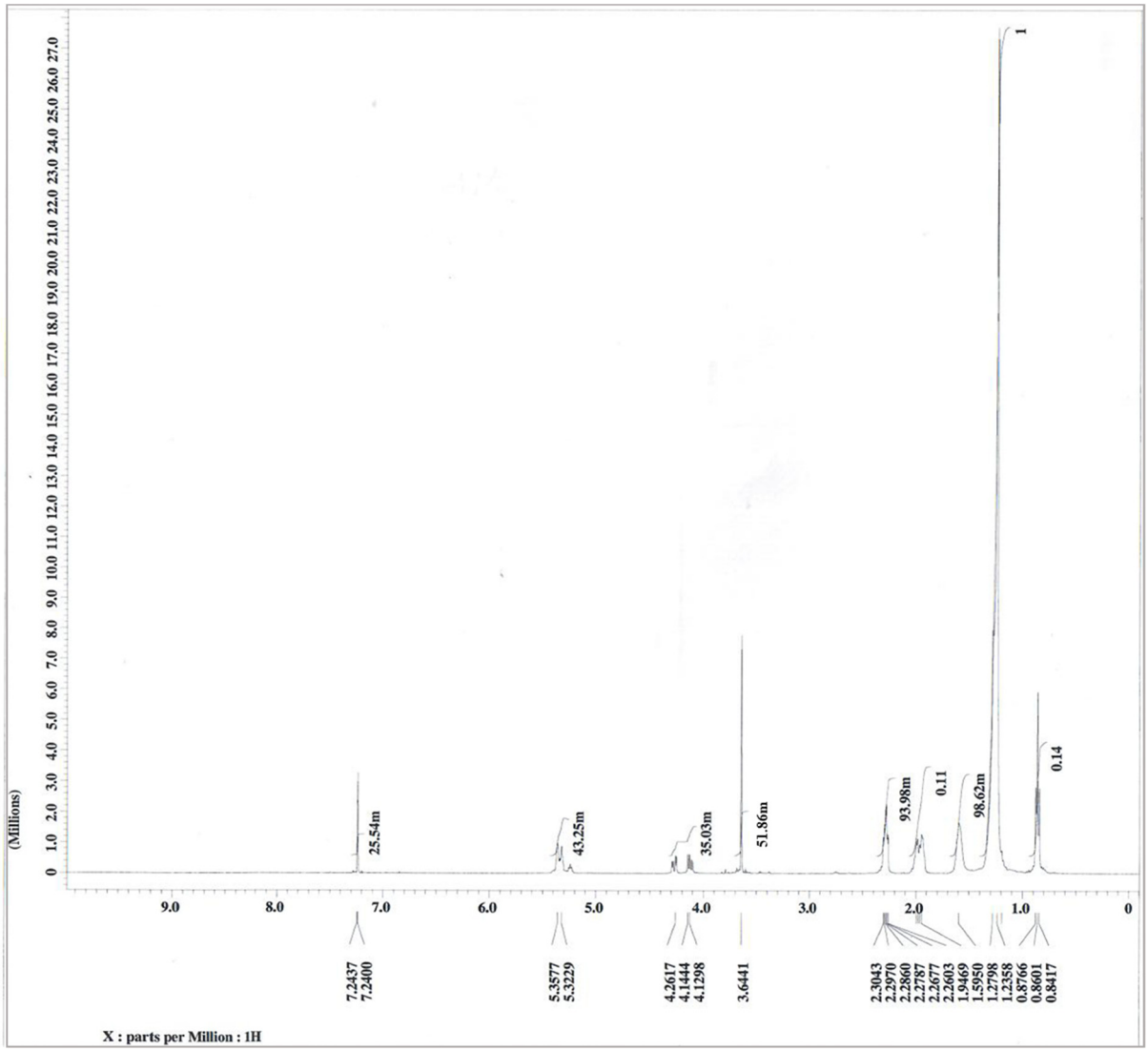

Figure S11: ^{1}H-NMR spectrum of biodiesel synthesized by transesterification of UVO using MOF-801 catalyst (10 wt.% to oil)at 180 °C in 2 h with methanol to oil 50 wt.%.

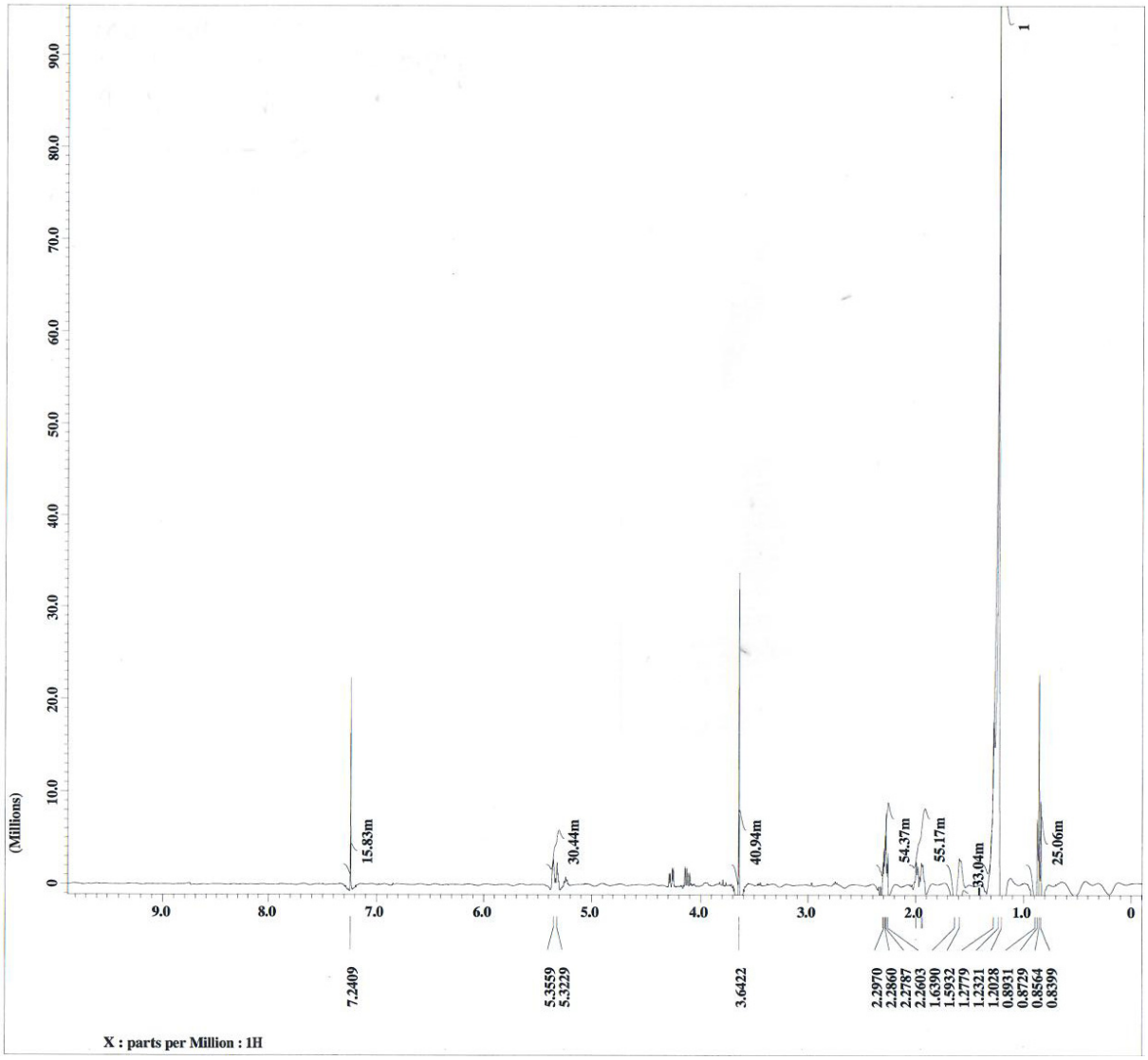

Figure S12: ^{1}H-NMR spectrum of biodiesel synthesized by transesterification of UVO using MOF-801 catalyst (10 wt.% to oil)at 180 °C in 4 h with methanol to oil 50 wt.%.

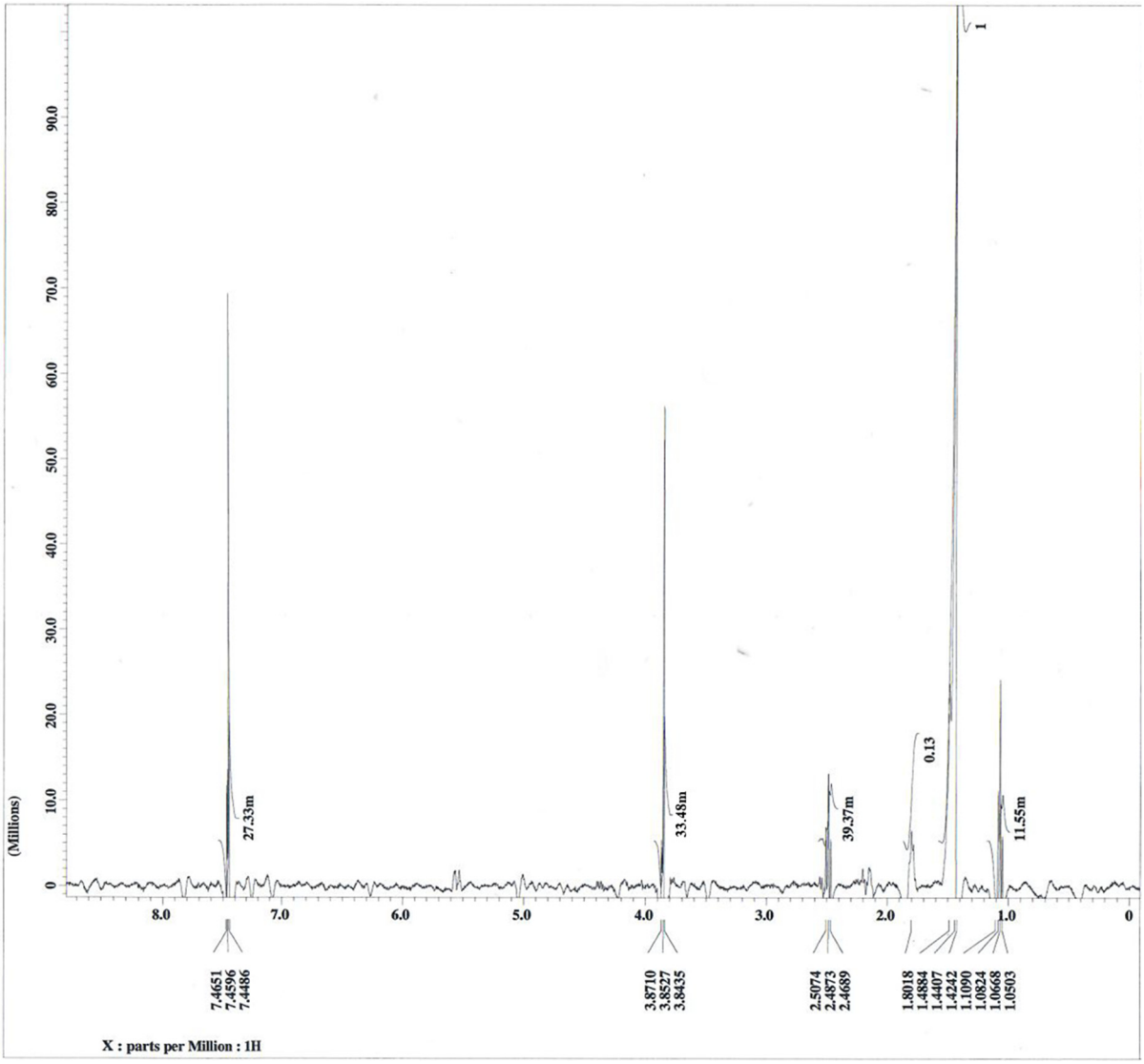

Figure S13: ^{1}H-NMR spectrum of biodiesel synthesized by transesterification of UVO using MOF-801 catalyst (10 wt.% to oil)at 180 °C in 6 h with methanol to oil 50 wt.%.

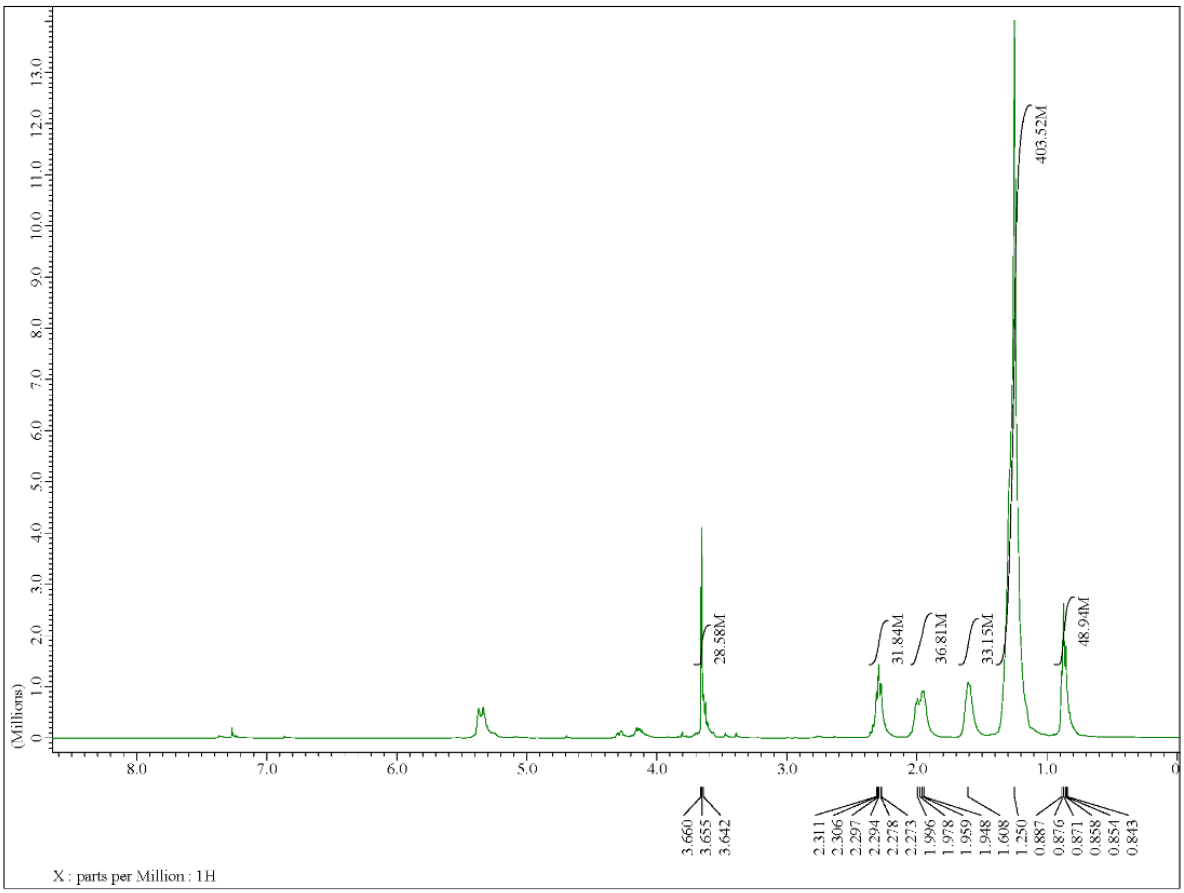

Figure S14: [1]H-NMR spectrum of biodiesel synthesized by transesterification of UVO using MOF-801 catalyst (10 wt.% to oil)at 180 °C in 8 h with methanol to oil 50 wt.%.

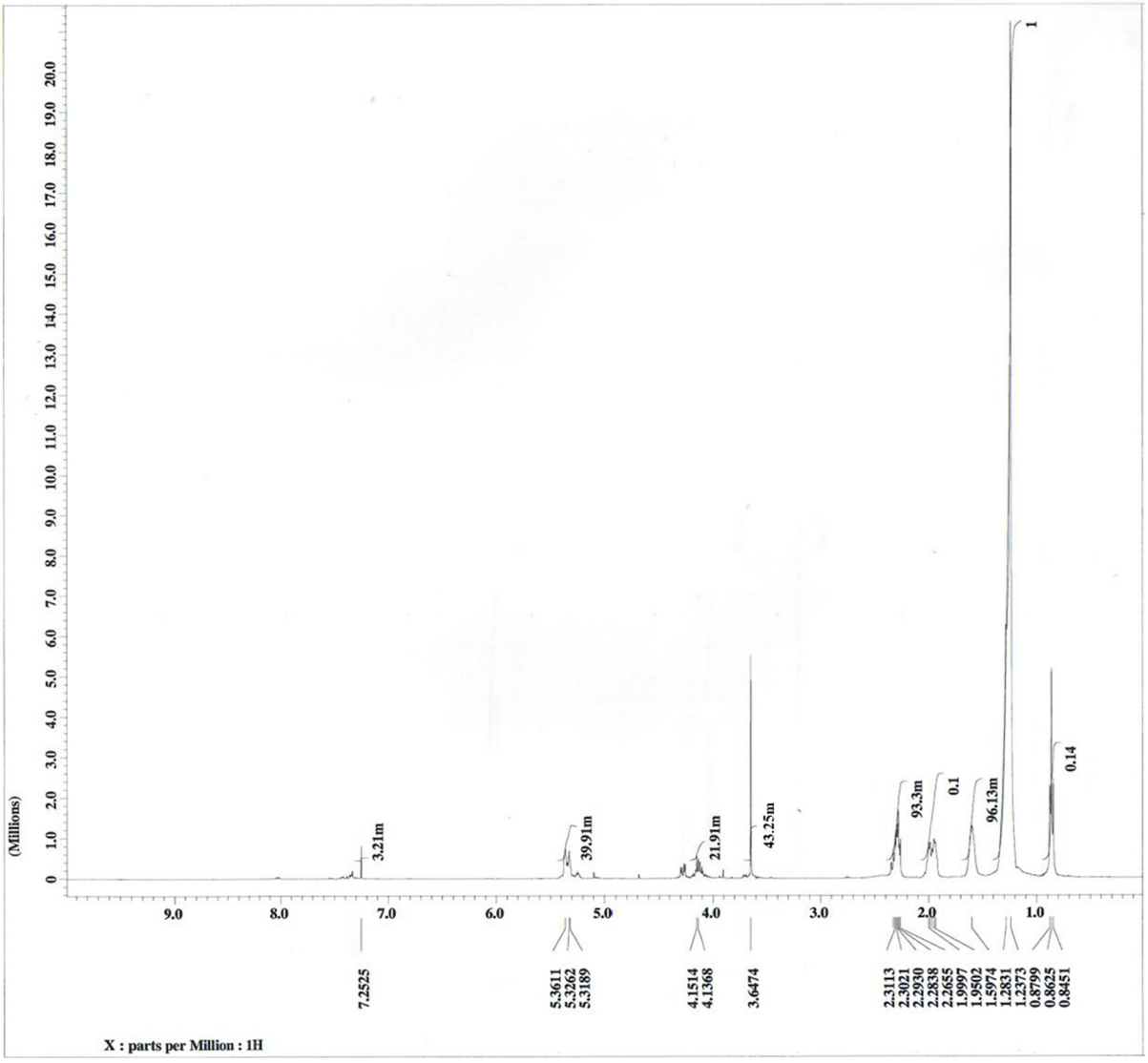

Figure S15: ^{1}H-NMR spectrum of biodiesel synthesized by transesterification of UVO using MOF-801 catalyst (10 wt.% to oil)at 140 °C in 8 h with methanol to oil 50 wt.%.

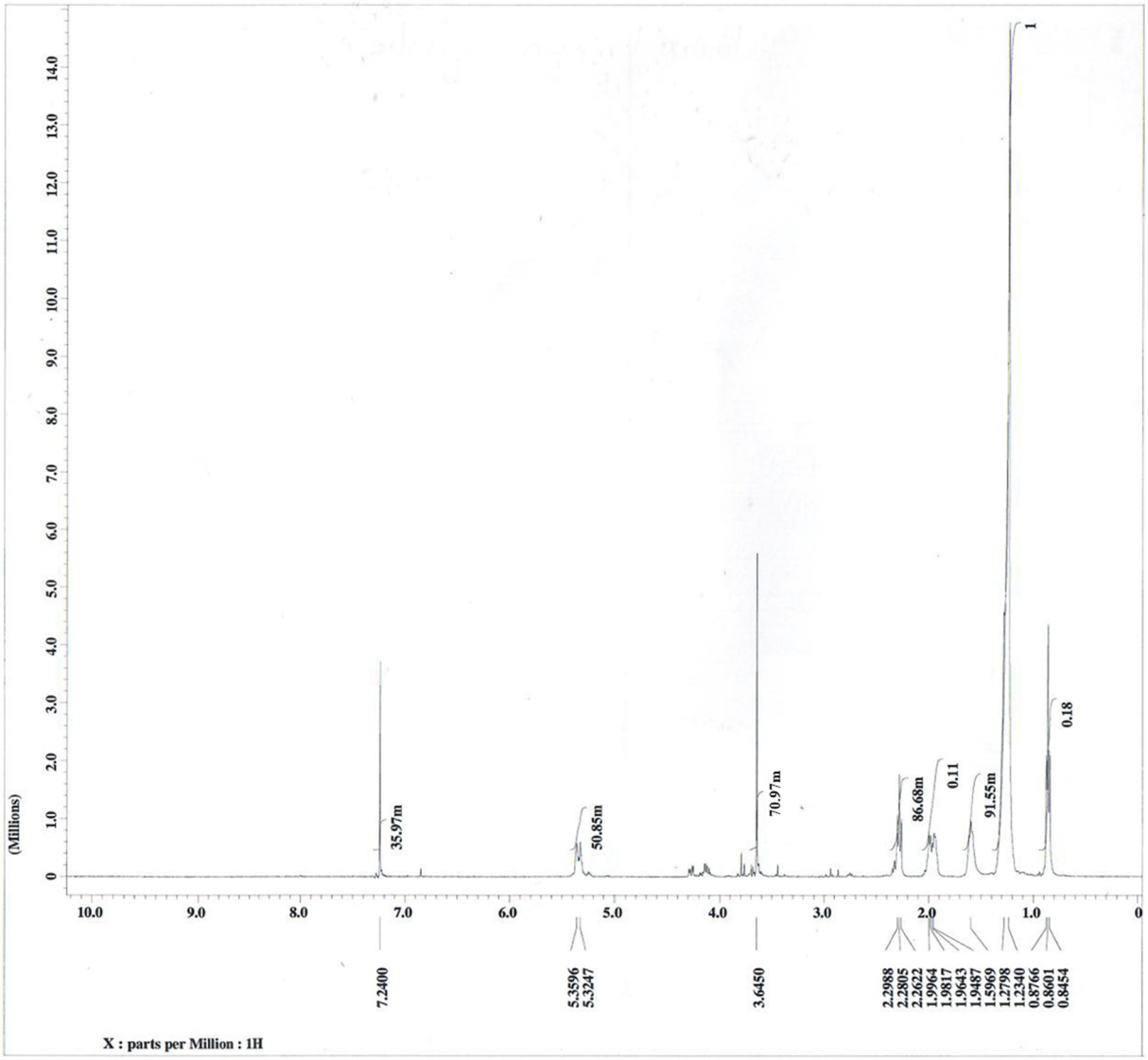

Figure S16: ^{1}H-NMR spectrum of biodiesel synthesized by transesterification of UVO using MOF-801 catalyst (10 wt.% to oil)at 160 °C in 8 h with methanol to oil 50 wt.%.

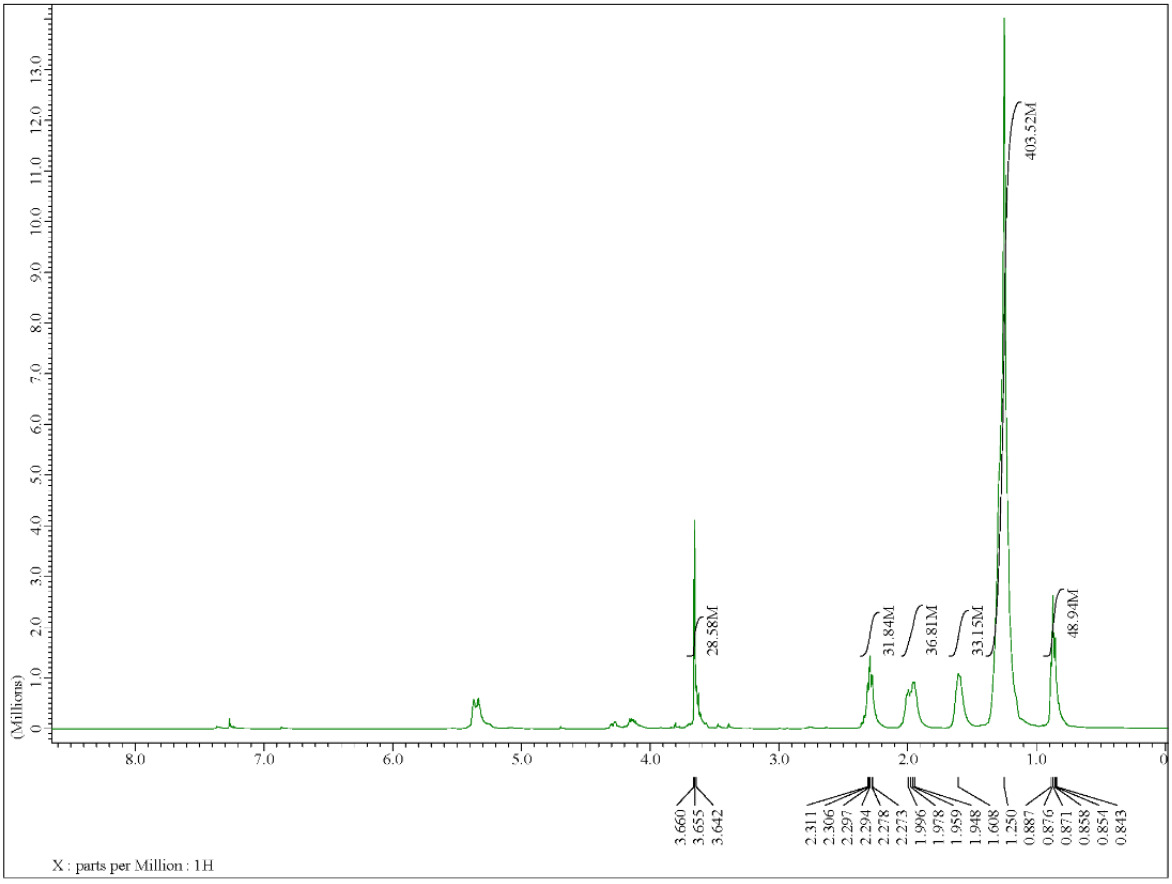

Figure S17: ^{1}H-NMR spectrum of biodiesel synthesized by transesterification of UVO using MOF-801 catalyst (10 wt.% to oil)at 180 °C in 8 h with methanol to oil 50 wt.%.

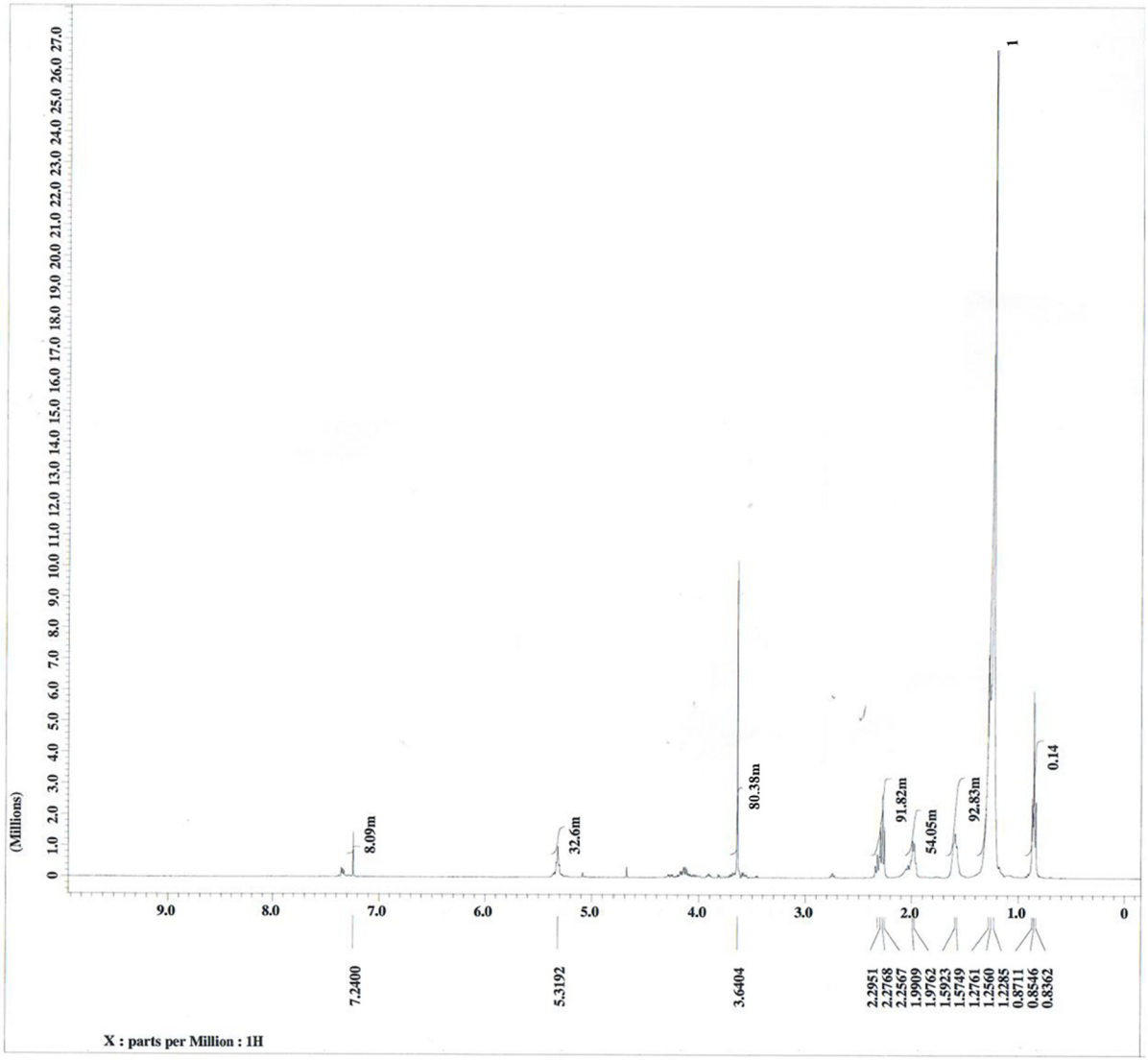

Figure S18: ^{1}H-NMR spectrum of biodiesel synthesized by transesterification of UVO using MOF-801 catalyst (10 wt.% to oil)at 200 °C in 8 h with methanol to oil 50 wt.%.

References:

[1] Ke, F.; Peng, C.; Zhang, T.; Zhang, M.; Zhou, C.; Cai, H.; Zhu, J.; Wan, X. Fumarate-based metal-organic frameworks as a new platform for highly selective removal of fluoride from brick tea. Scientific Reports 2018, 8, 939.