Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary information

In-Depth Investigation on Quantitative Characterization of Pyrolysis Oil by ^{31}P NMR

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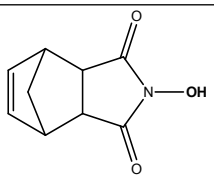
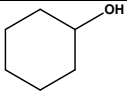
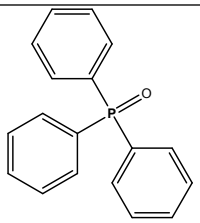
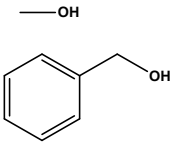
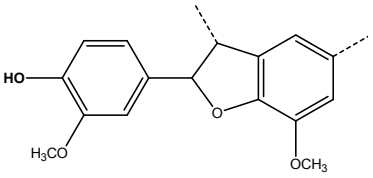
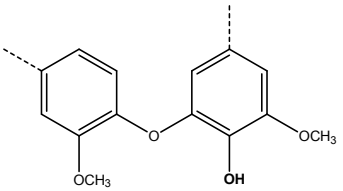
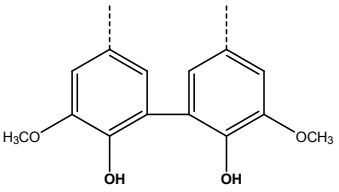
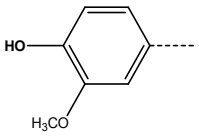
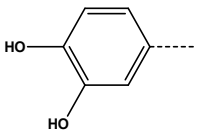
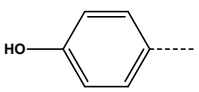
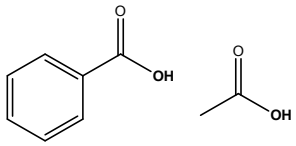
Table S1. Chemical shifts and integration regions for internal standards and functional groups in pyrolysis oil.

Functional group		Integration region (ppm)	Examples
endo-N-hydroxy-5-norbornene-2,3-dicarboximide (NHND, internal standard)		~151.5 ppm	
Cyclohexanol (internal standard)		~145.5 ppm	
Triphenylphosphine oxide (TPPO, ^{31}P atom contained internal standard, which will not need further reaction)		~27.5 ppm	
Aliphatic OH		150.0 - 145.5	
C_5 substituted Condensed phenolic OH	β-5	144.7 - 142.8	
	4-O-5	142.8 - 141.7	
	5-5	141.7 - 140.2	
Guaiacyl phenolic OH		140.2 - 139.0	
Catechol type OH		139.0 - 138.2	
p-hydroxy-phenyl OH		138.2 - 137.3	

Acid OH	136.6 - 133.6	
Water peak	133.1-131.3, 16.9-15.1	

Note: chemical shift provided is for the hydroxyl group in bold and with underline after derivatization with TMDP.

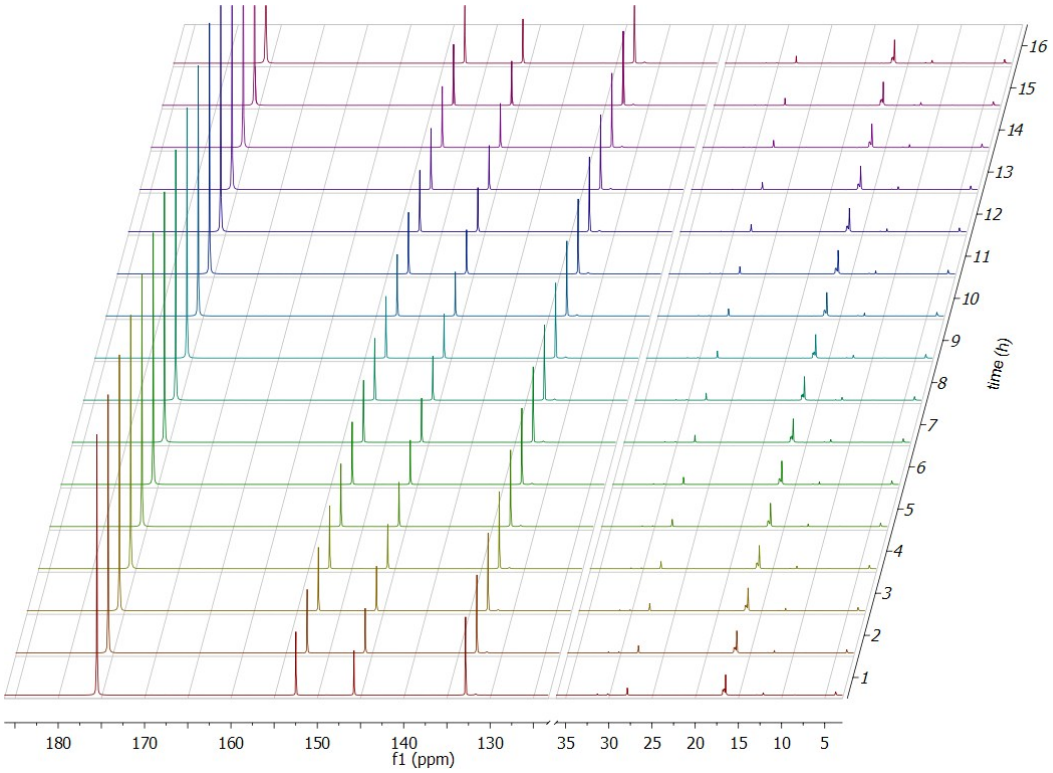


Figure S1. In-situ monitoring for the stability of commonly used internal standards in ^{31}P NMR.

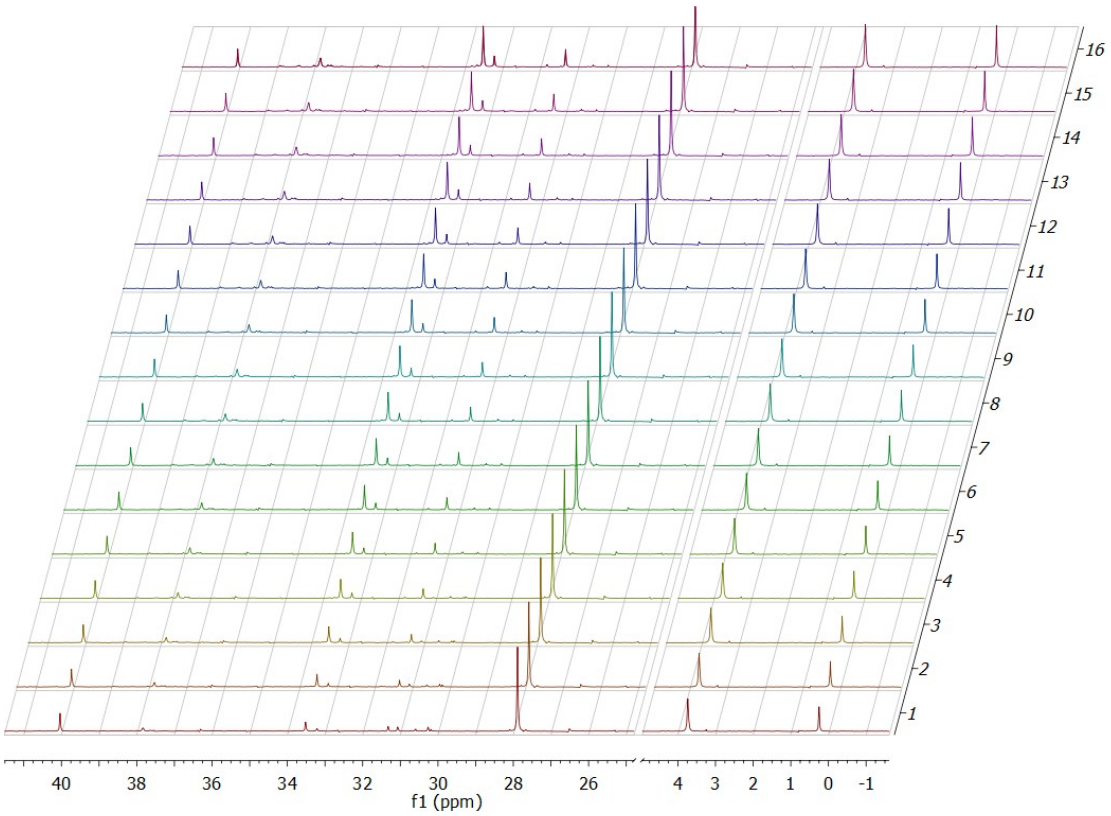


Figure S2. Some growing peaks during the in-situ monitoring of pyrolysis oil in ^{31}P NMR with TPPO as internal standard.

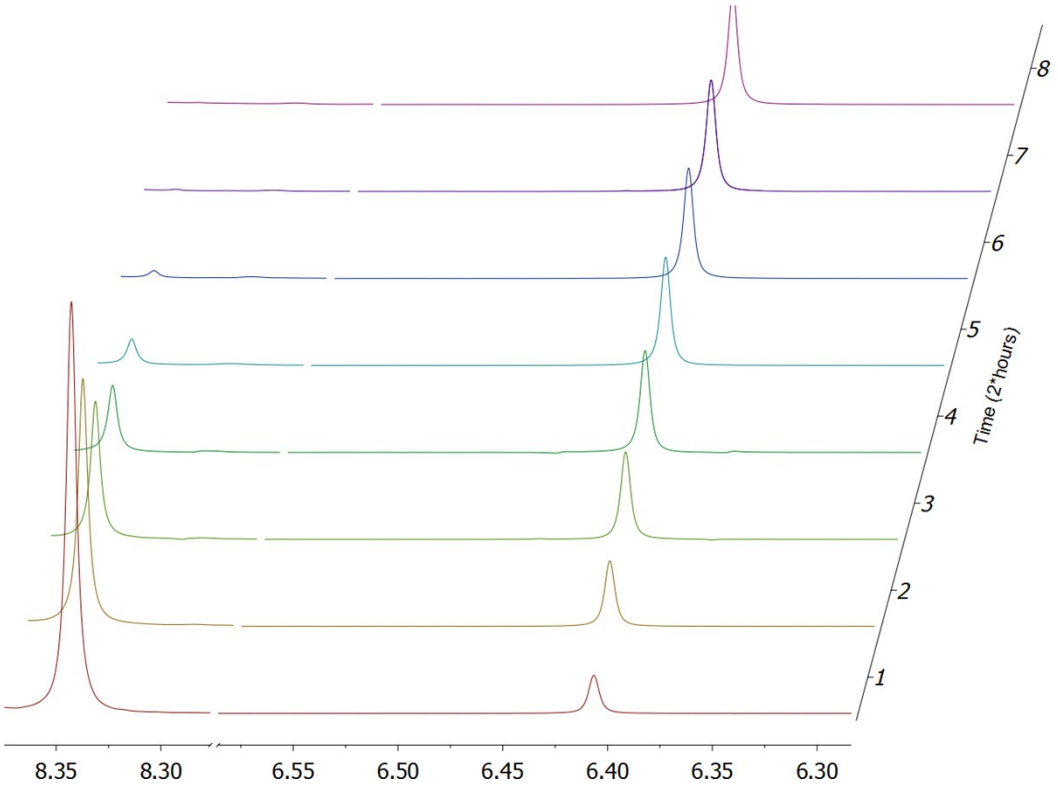


Figure S3. ^{1}H NMR in-situ monitoring for the stability of formic acid in ^{31}P NMR solution.

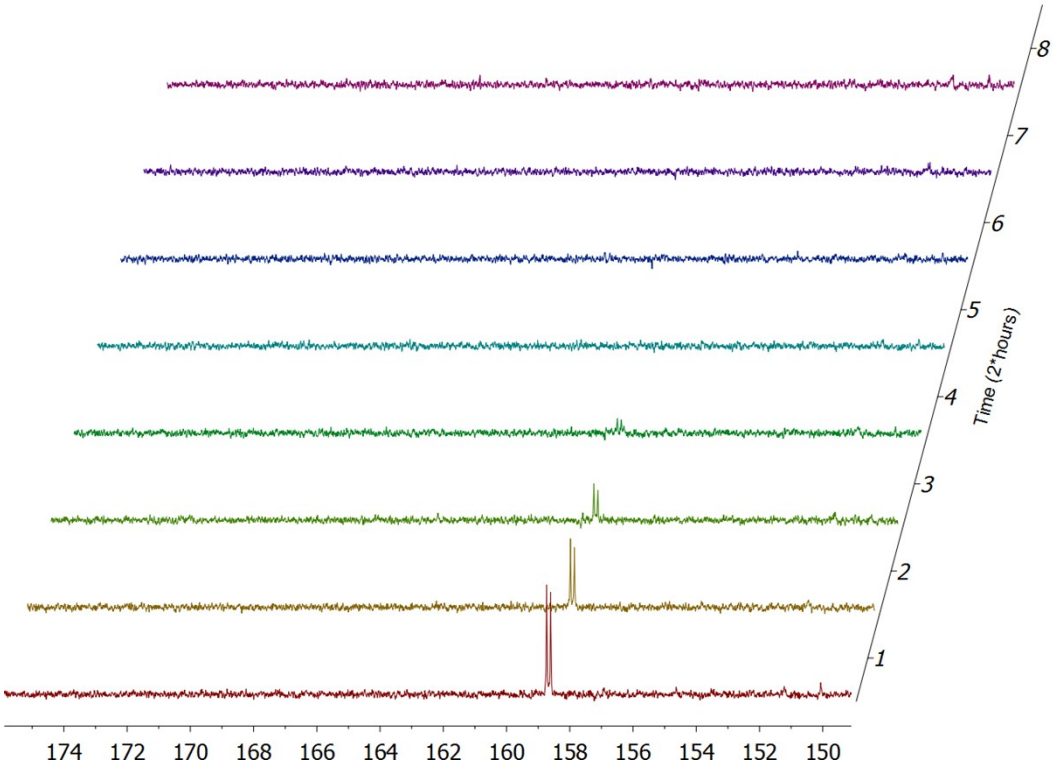


Figure S4. ^{13}C NMR in-situ monitoring for the stability of formic acid in ^{31}P NMR solution.

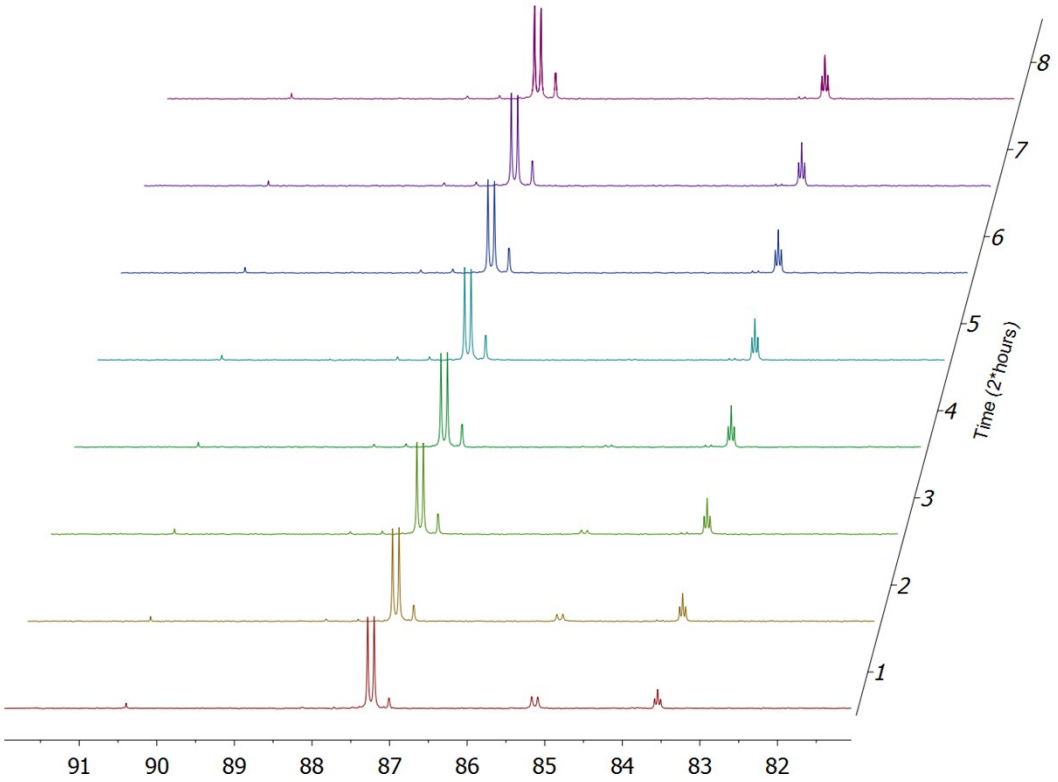


Figure S5. ^{13}C NMR in-situ monitoring for the stability of formic acid in ^{31}P NMR solution.

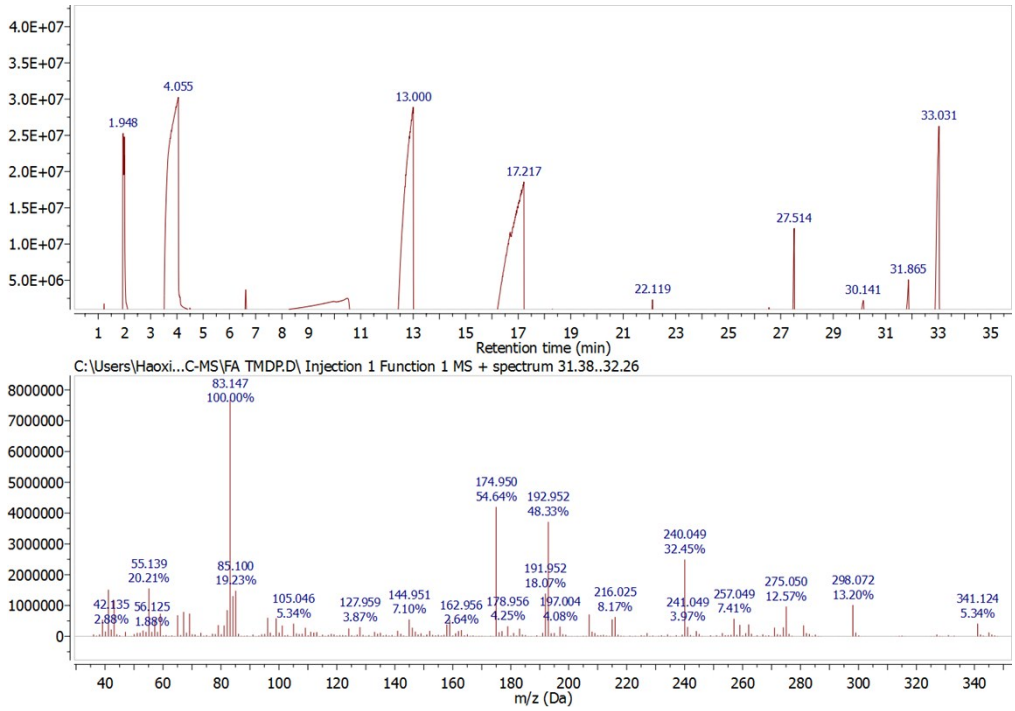


Figure S6. GC-MS data for the formic acid sample after 16 hours of in-situ monitoring in ^{31}P NMR solution. (The peak at 1.948min represents to $CDCl_3$, the peak at 4.055 represents to pyridine, the peak at 13.000 represents to TMDP, the peak at 17.217 represents to two product from water and TMDP, the peak at 27.514 represents to the chromium acetylacetonate, and the peak at 33.031 represents to the TPPO. An Agilent G1530A gas chromatograph (GC) interfaced with a HP 5973 mass spectrometer was used in this study. The GC injector was operated at 300 ^{o}C. A constant He flow of 61.3 ml min^{-1} was maintained in the capillary column (Agilent 190915-433). The GC oven was programmed with the following temperatures: hold at 40 ^{o}C for 3 min then heated up to 142 ^{o}C with a temperature ramp of 6.0 ^{o}C min^{-1} and further heated up to 300 ^{o}C at a rate of 10.0 ^{o}C min^{-1}.)