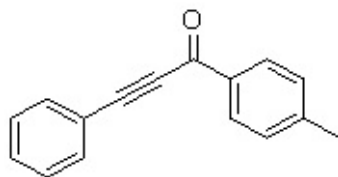


Parameter

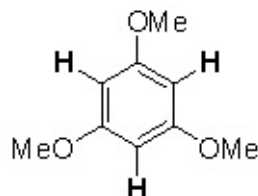
Data File Name // ktclab/ rynnrmrdata/ openuseB/ data/ liyanyao/ nmr/ 3973-0247-qNMR/ 11/ fid
 Title 3973-0247-qNMR.11.fid
 Comment rynnrmr500d h-1, quantitative (d1=60 sec, ns=8)
 Origin Bruker BioSpin GmbH
 Owner ProcessNMR
 Site
 Instrument spect
 Author
 Solvent CDCl3
 Temperature 300.0
 Pulse Sequence zg30
 Experiment 1D
 Probe Z113652_0232 (PA BBO 500S2 BBF-H-D-05 Z SP)

Number of Scans 4
 Receiver Gain 90.5
 Relaxation Delay 60.0000
 Pulse Width 10.6000
 Presaturation Frequency
 Acquisition Time 2.5166
 Acquisition Date 2025-01-14T10:27:56
 Modification Date 2025-01-14T10:28:02
 Class
 Spectrometer Frequency 500.33
 Spectral Width 13020.8
 Lowest Frequency -3432.5
 Nucleus 1H
 Acquired Size 32768
 Spectral Size 131072
 Digital Resolution 0.10

Value 7.69 7.68 7.50 7.48 7.47 7.44 7.42 7.41 7.32 7.31 7.26 6.09



Compound 1



Internal standard = 28.6 mg

Sample = 36.3 mg

%P of standard = 99%

MW of ynone = 220.27

MW of standard = 168.19

Molar ratio = $(1.94/2)/(3/3) = 0.97$

wt% = $(28.6 \times 220.27 \times 0.97 \times 0.99)/(36.3 \times 168.19) \times 100 = \mathbf{99.1\%}$

1.94 1.94 0.97 1.94 1.94 3.00

3.77

2.45

f1 (ppm)