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SUPPLEMENTARY MATERIAL

LC-HRMS AND NMR STUDY OF THE ESTERIFICATION PRODUCTS OF IBUPROFEN WITH SOLKETAL: FORMATION, ISOLATION, AND IDENTIFICATION

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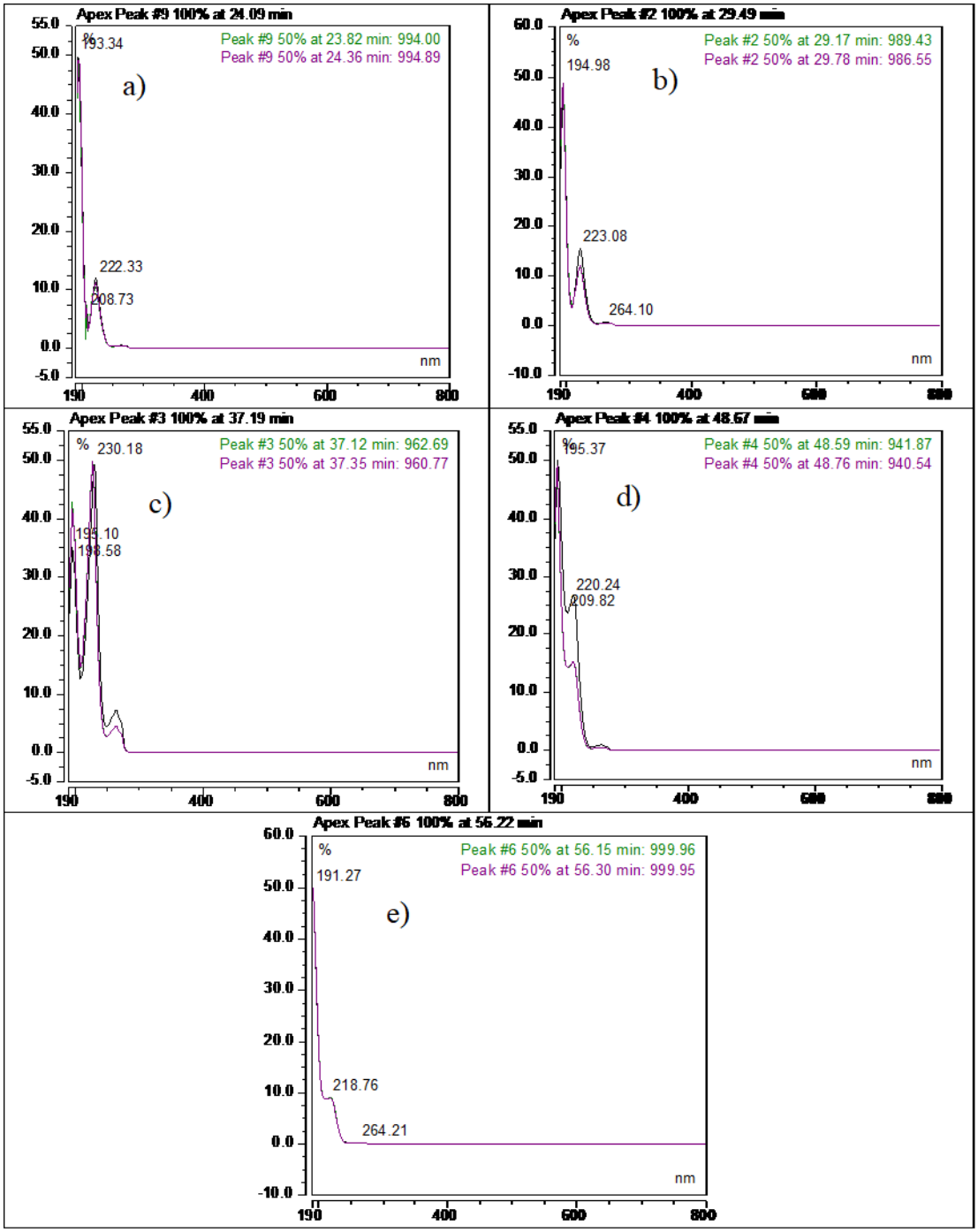


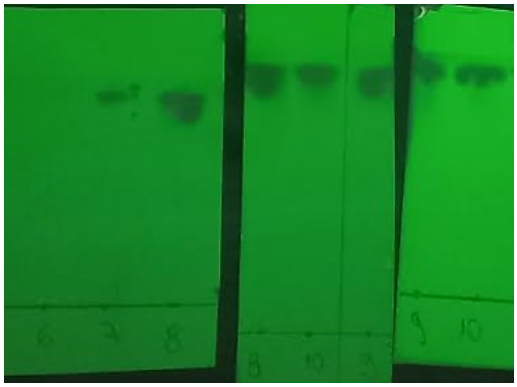
Figure S1. UV spectra of each of the components in the resulting reaction mixture with the following RRTs:

S1a. peak with RRT ~ 0.66;

S1b. peak with RRT = 0.74 (P1);

S1c. peak of Ibuprofen;

S1d. peak with RRT = 1.32 (P2); **3e.** peak with RRT ~1.53

a)  b) 

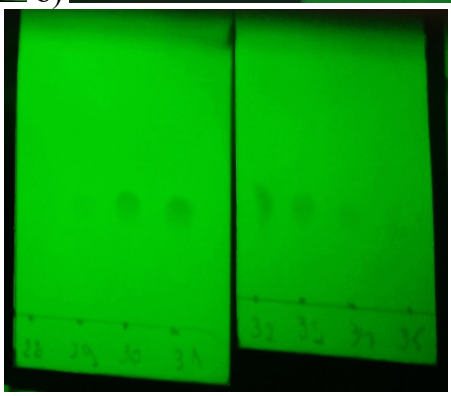
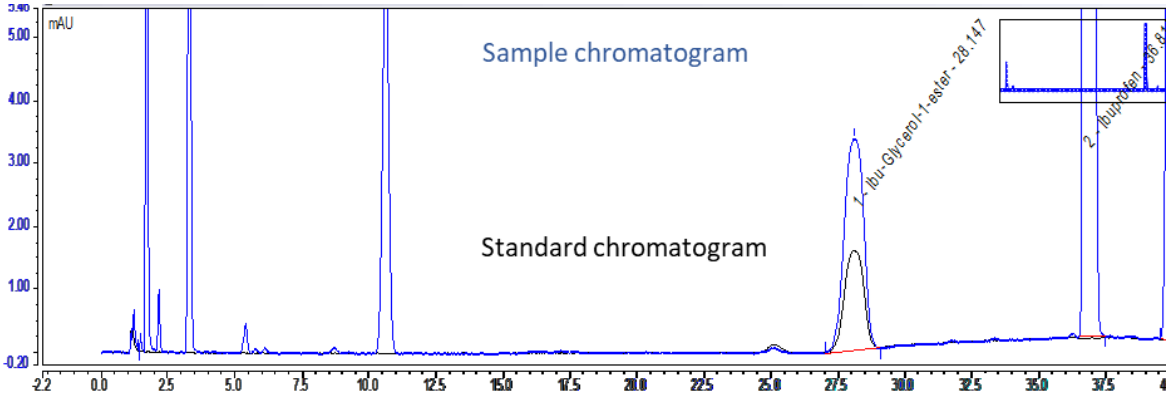
c) 

Figure S2. TLC results before and after the isolation process

S2a. A resulting TLC plate from extraction mixture before the isolation, alongside ibuprofen standard,
S2b. Resulting TLC plates from the application of the fractions labeled with numbers 6-10,
S2c. Resulting TLC plates from the application of the fractions labeled with numbers 29-35

a)

b)


mAU
Sample chromatogram
Standard chromatogram
1 - Ibu-Glycerol-1-ester - 28.147
2 - Ibuprofen - 36.8
5.00
4.00
3.00
2.00
1.00
-0.20
-2.2
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0
22.5
25.0
27.5
30.0
32.5
35.0
37.5

c)

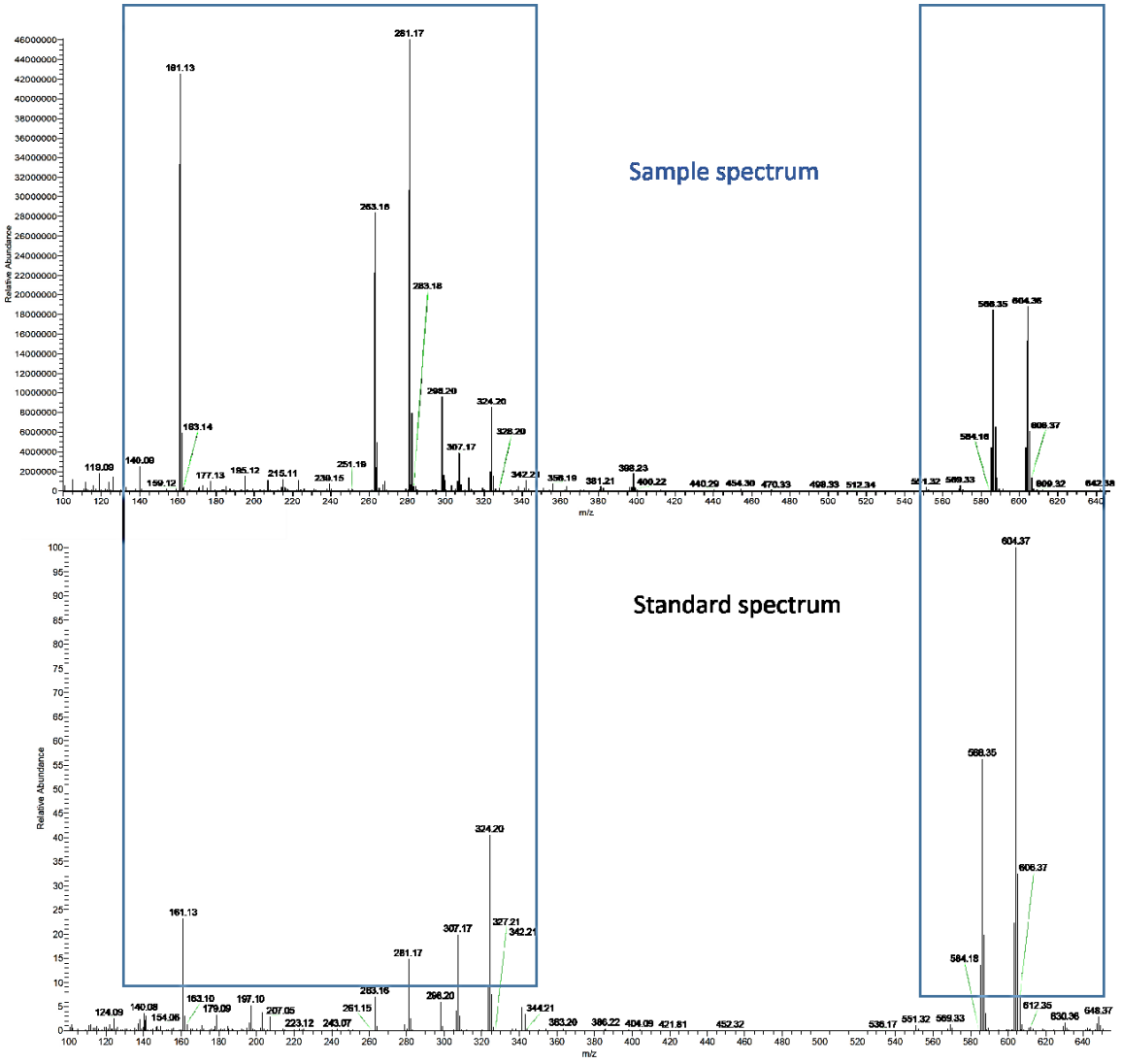
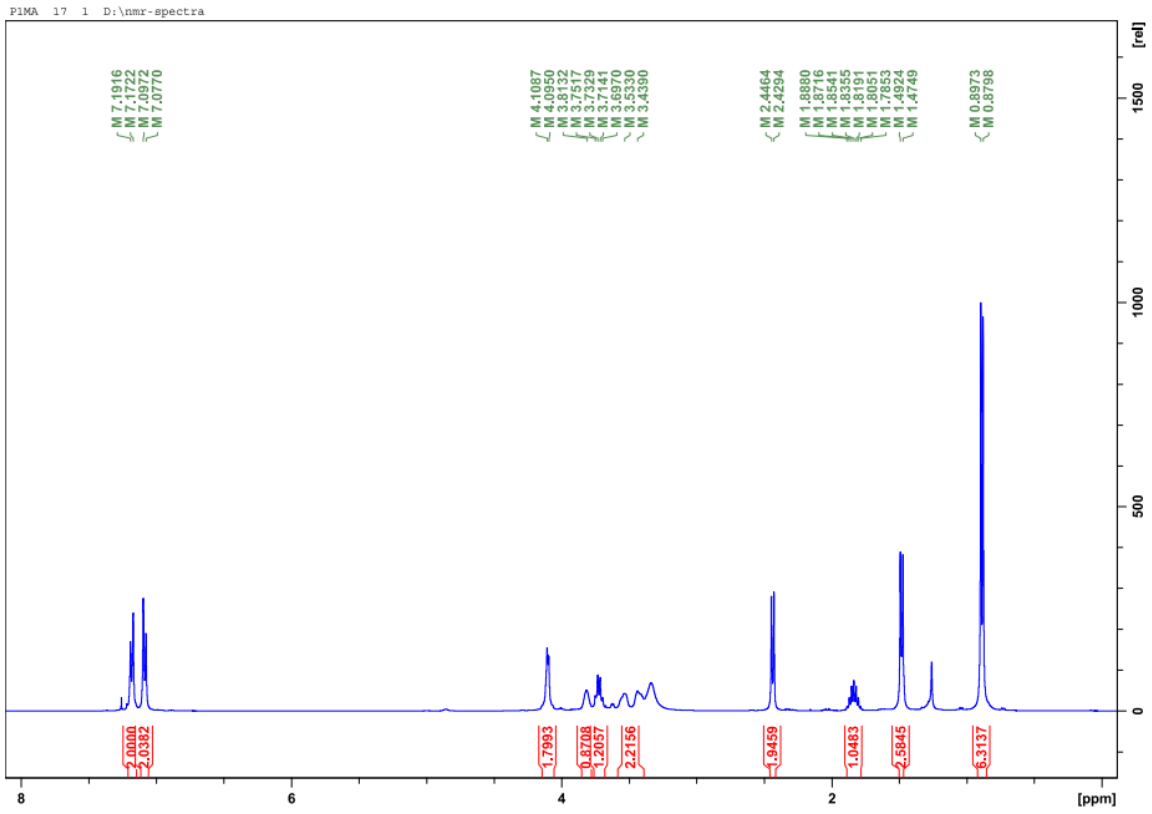


Figure S3. Analysis of reference standard of glycerol mono-ester
S2a. Resulting TLC plate from extraction mixture before the isolation, alongside a standard of ibuprofen-glycerol ester;
S2b. HPLC chromatograms at 265 nm;
S2c. MS spectra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M 7.1722
M 7.0972
M 7.0770
M 4.1087
M 4.0950
M 3.8132
M 3.7517
M 3.7329
M 3.7141
M 3.6970
M 3.5330
M 3.4390
M 2.4464
M 2.4294
M 1.8880
M 1.8716
M 1.8541
M 1.8355
M 1.8191
M 1.8051
M 1.7853
M 1.4924
M 1.4749
M 0.8973
M 0.8798
2.0000
2.0382
1.7993
0.8708
1.2057
2.2156
1.9459
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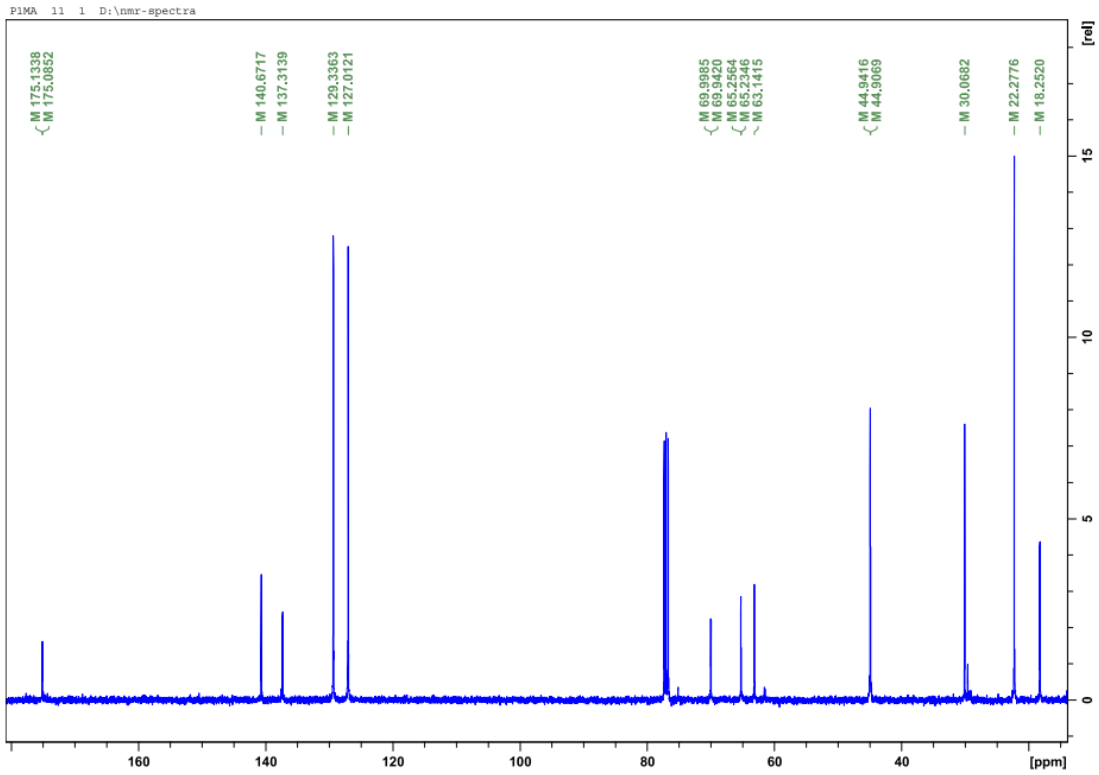
500
0
8
6
4
2
[ppm]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M 63.1415
M 44.9416
M 44.9069
M 30.0682
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10
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0
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140
120
100
80
60
40
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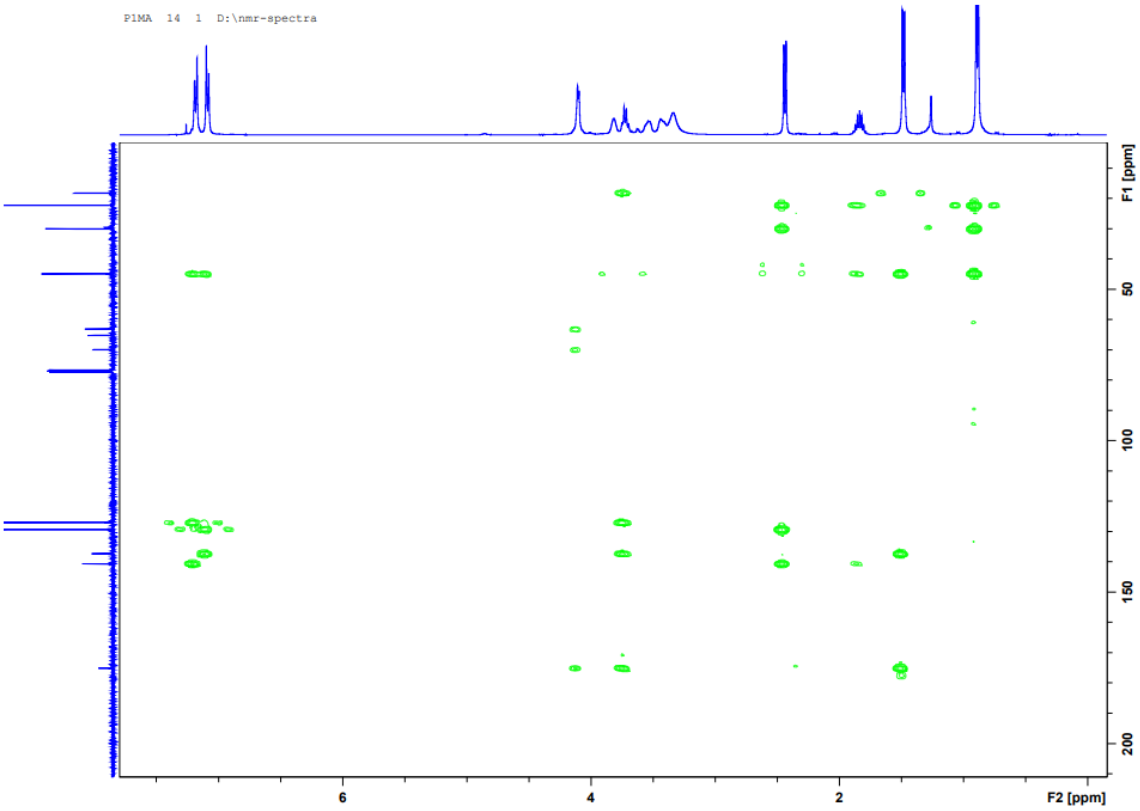
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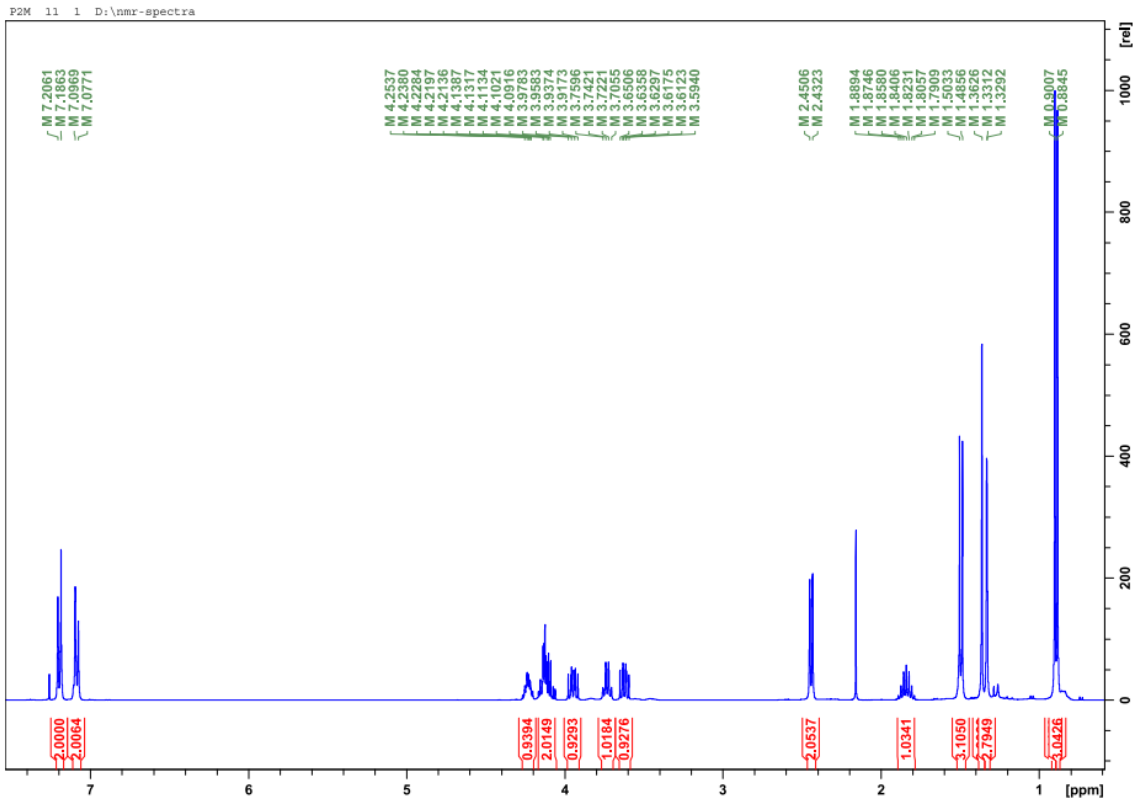
100
150
200
6
4
2
F2 [ppm]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M 1.5033
M 1.4856
M 1.3526
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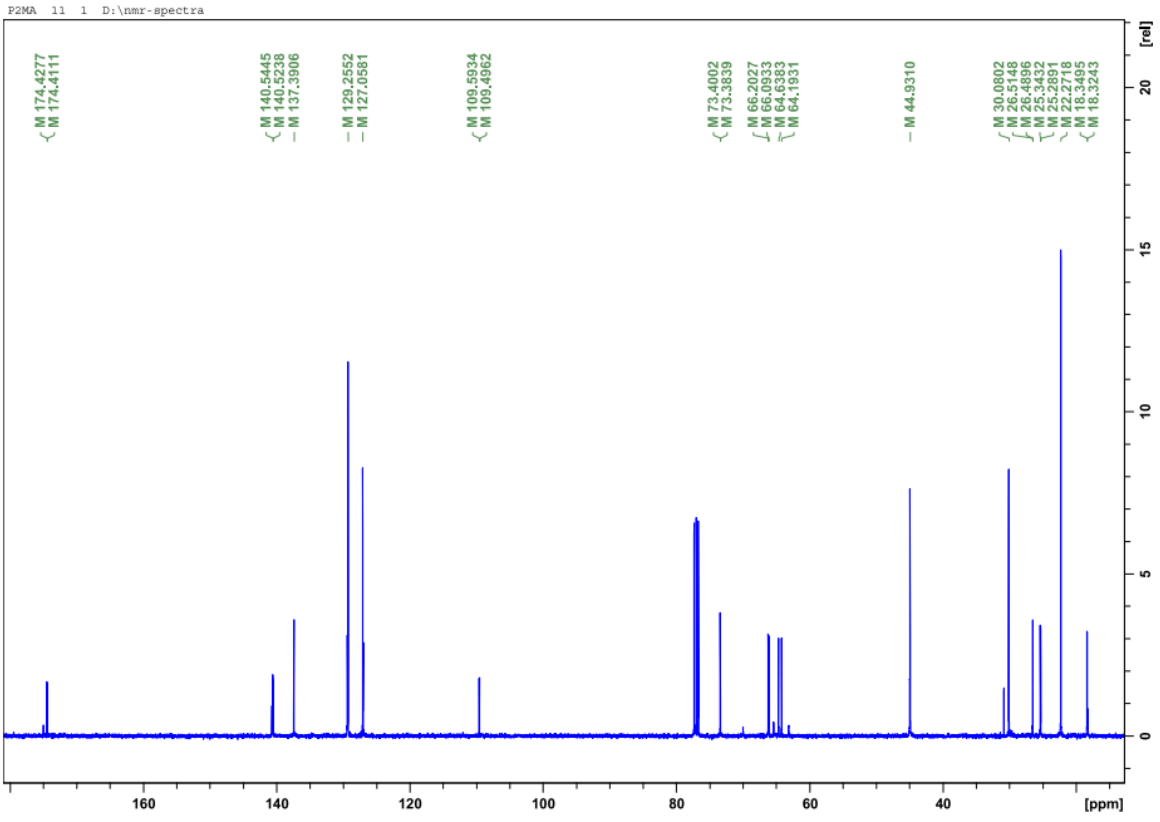
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M 73.4002
M 73.3839
M 66.2027
M 66.0933
M 64.5533
M 64.1931
M 44.9310
M 30.0802
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M 25.3432
M 25.2891
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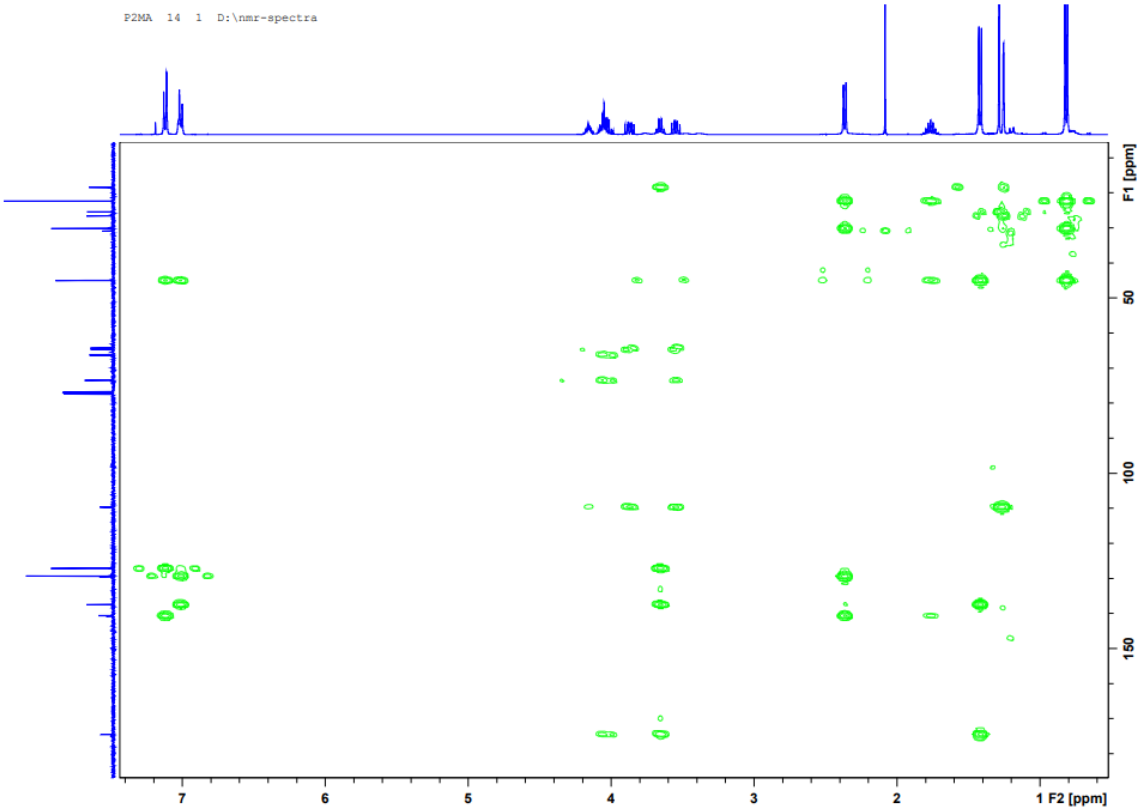

Figure S4. ^{1}H and ^{13}C NMR spectra of isolated products P1 and P2:
S4a. ^{1}H NMR spectra of P1
S4b. ^{13}C NMR spectra of P1
S4c. HMBC 2D NMR spectra of P1
S4d. ^{1}H NMR spectra of P2
S4e. ^{13}C NMR spectra of P2
S4f. HMBC 2D NMR spectra of P2