# Elucidating the Reaction Pathways of Veratrylglycero-*β*-guaiacyl Ether Degradation Over Metal-Free Solid Acid Catalysts with Hydrogen

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**Table of Content**

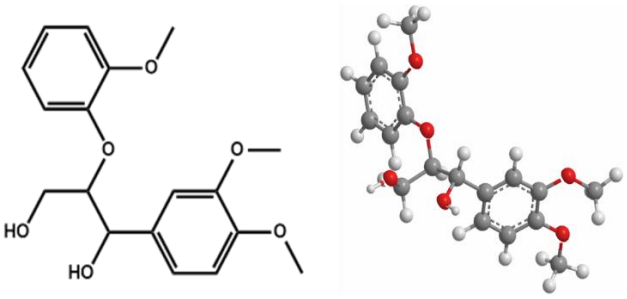



**Figure S1.** 2D and 3D optimized structure of the *β-O-4* model compound (veratrylglycero-β-guaiacyl ether) .

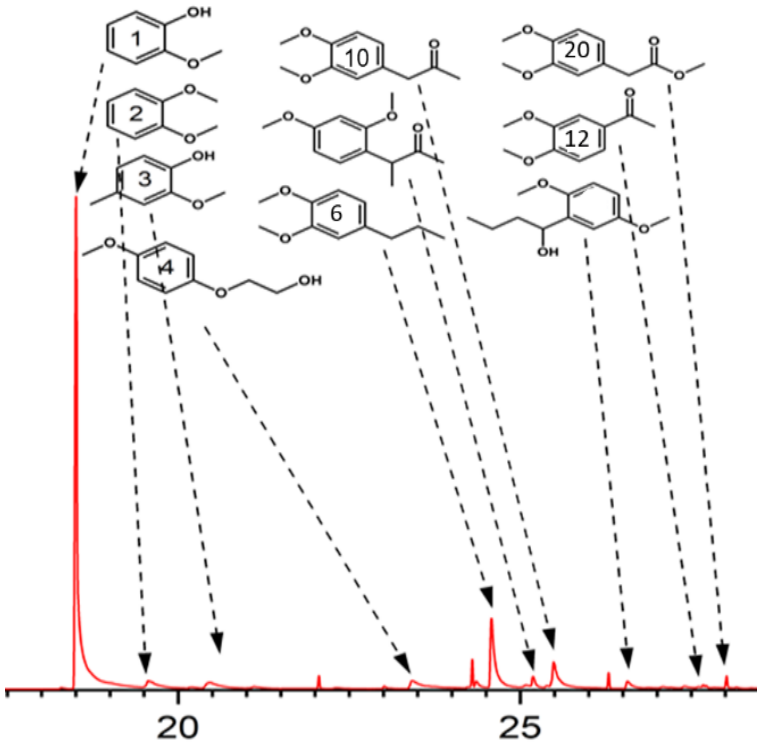


**Figure S2.** GC-MS chromatogram of the products generated during the zeolite cracking of *β-O-4* model compound over CBV 400.

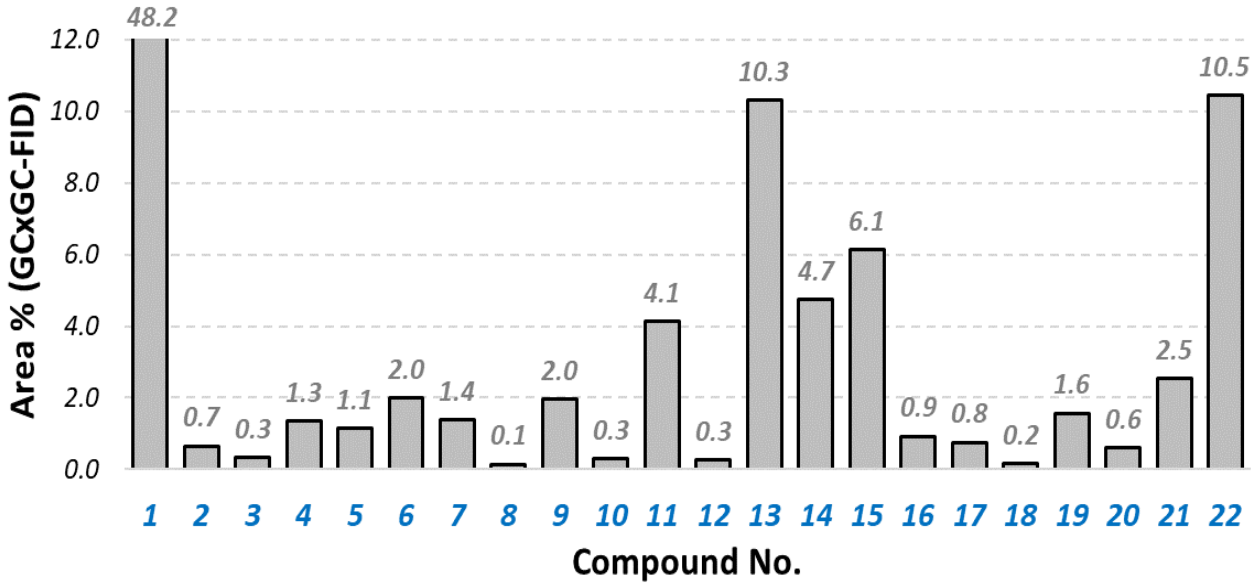
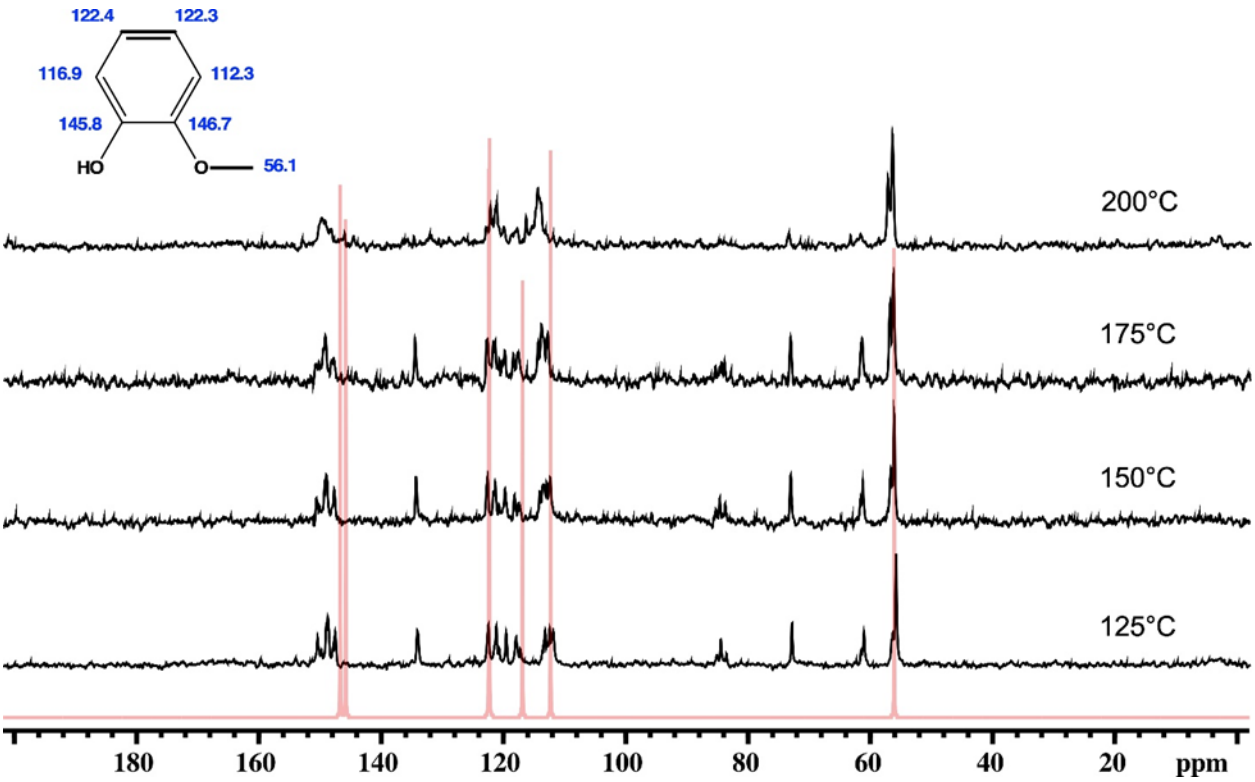



**Figure S3:** Semi-qualitative results of identified products as reported by GC×GC-FID (in area%) from zeolite decomposition of *β-O-4* model compound.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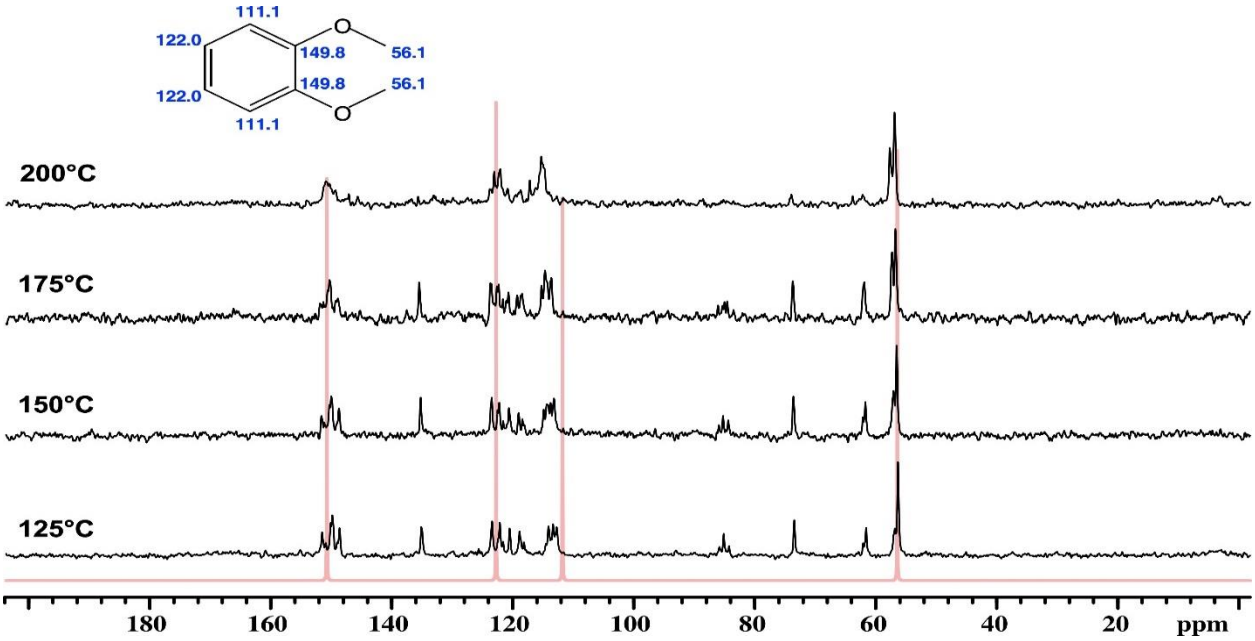
122.3
116.9
112.3
145.8
146.7
HO
O
56.1
200°C
175°C
150°C
125°C
180
160
140
120
100
80
60
40
20
ppm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122.0
149.8
56.1
149.8
56.1
122.0
111.1
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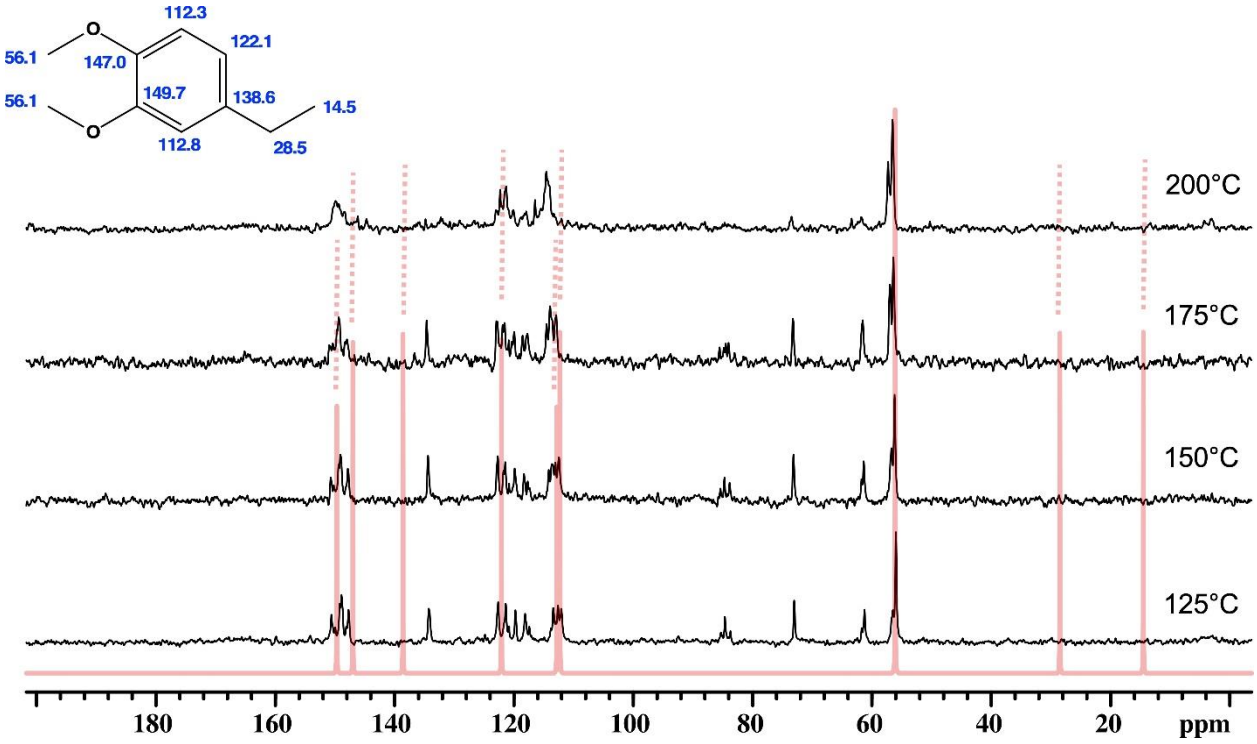
175°C
150°C
125°C
180
160
140
120
100
80
60
40
20
ppm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122.1
56.1
147.0
149.7
138.6
14.5
56.1
112.8
28.5
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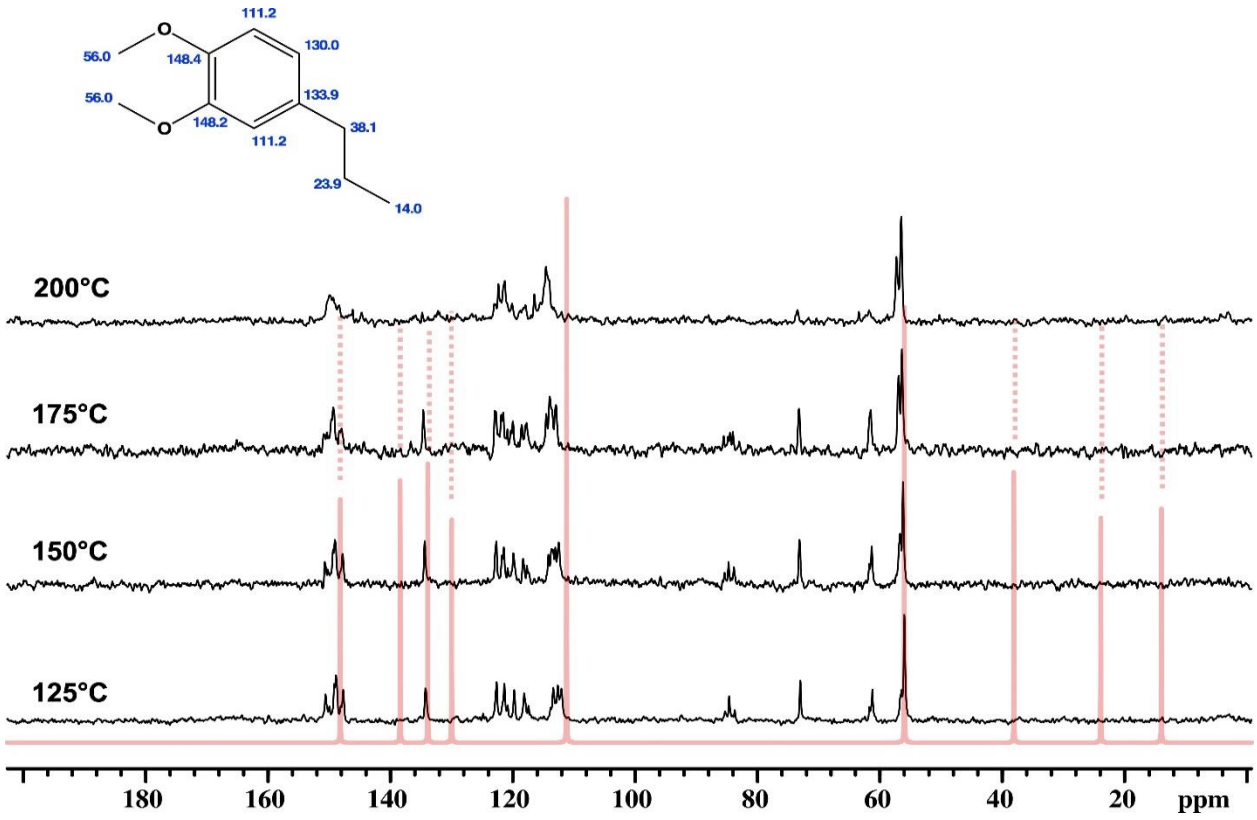
125°C
180
160
140
120
100
80
60
40
20
ppm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56.0
148.4
133.9
56.0
148.2
38.1
111.2
23.9
14.0
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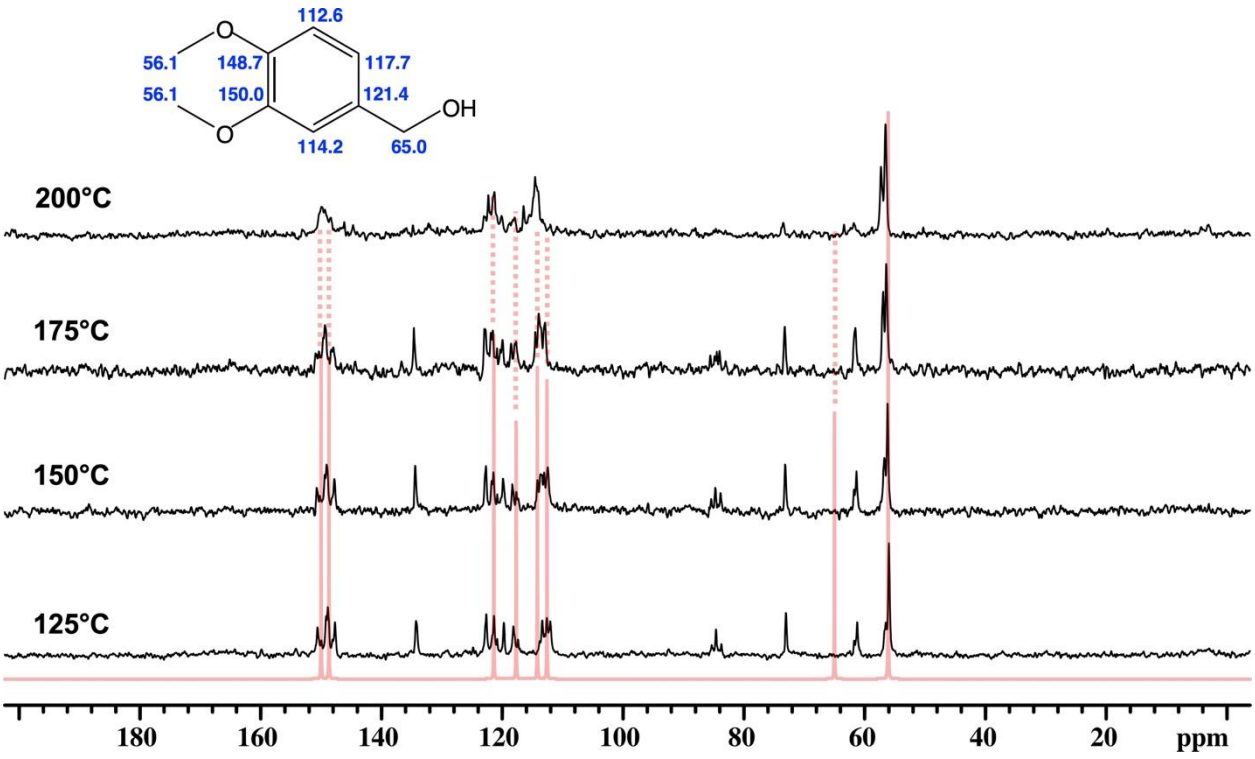
160
140
120
100
80
60
40
20
ppm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148.7
117.7
56.1
150.0
121.4
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114.2
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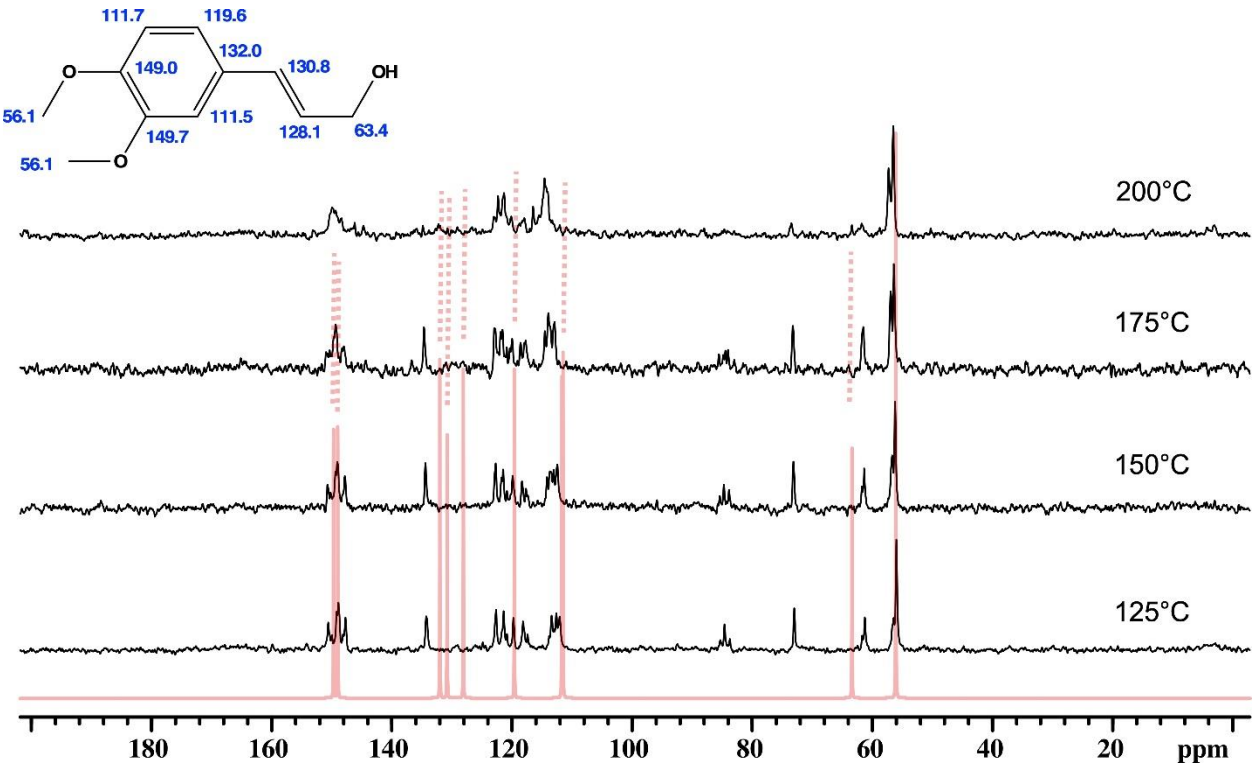
140
120
100
80
60
40
20
ppm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130.8
OH
56.1
111.5
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128.1
63.4
56.1
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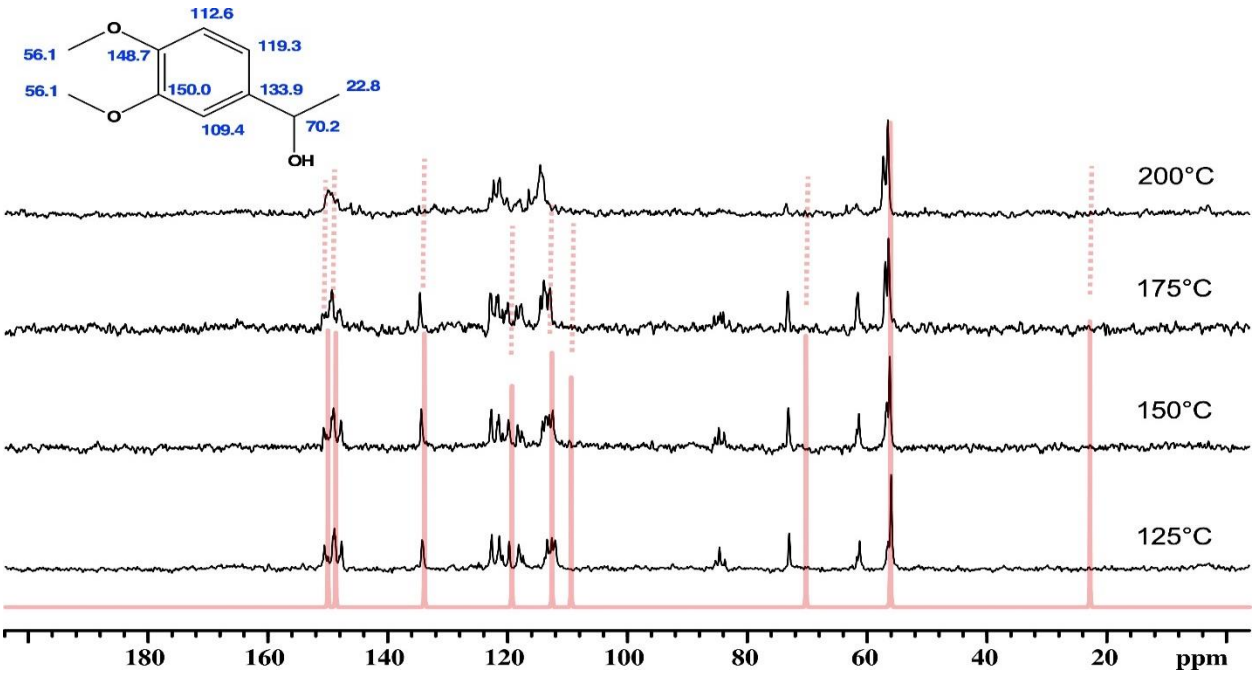
150°C
125°C
180
160
140
120
100
80
60
40
20
ppm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119.3
56.1
150.0
133.9
22.8
109.4
70.2
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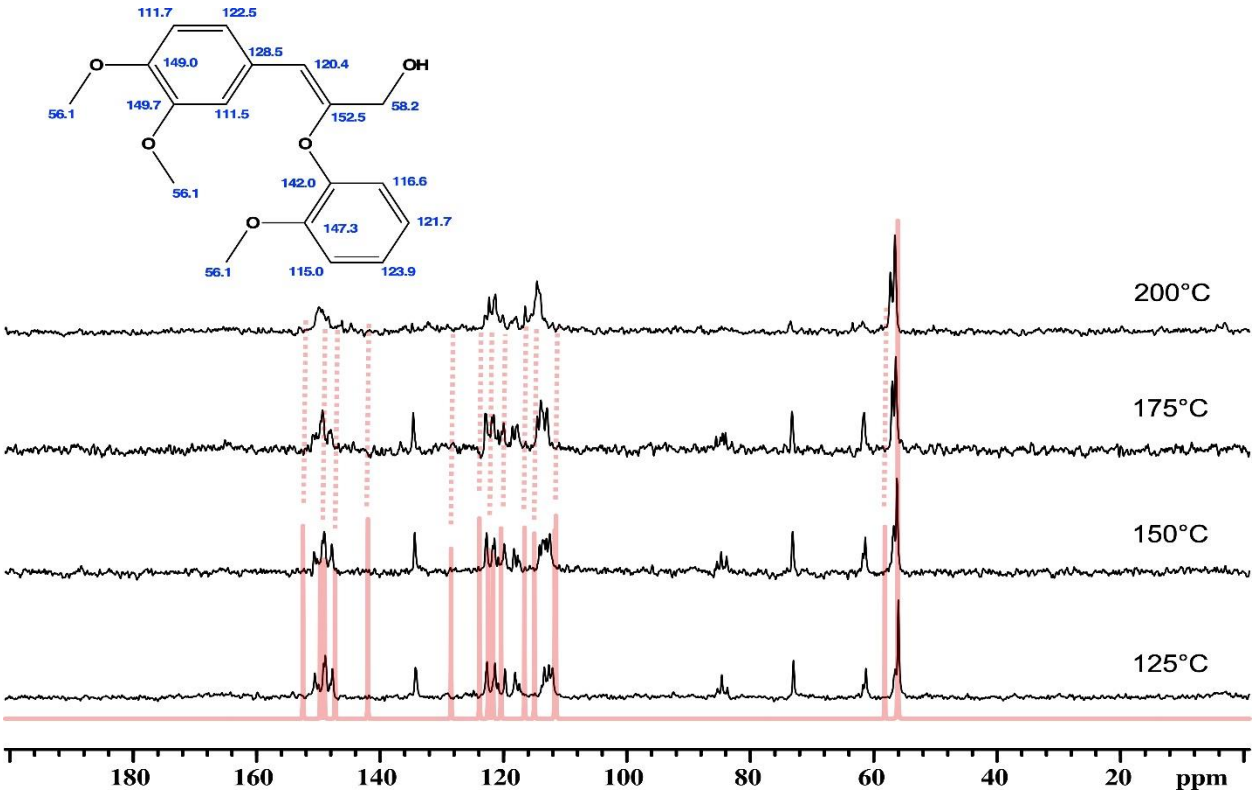
125°C
180
160
140
120
100
80
60
40
20
ppm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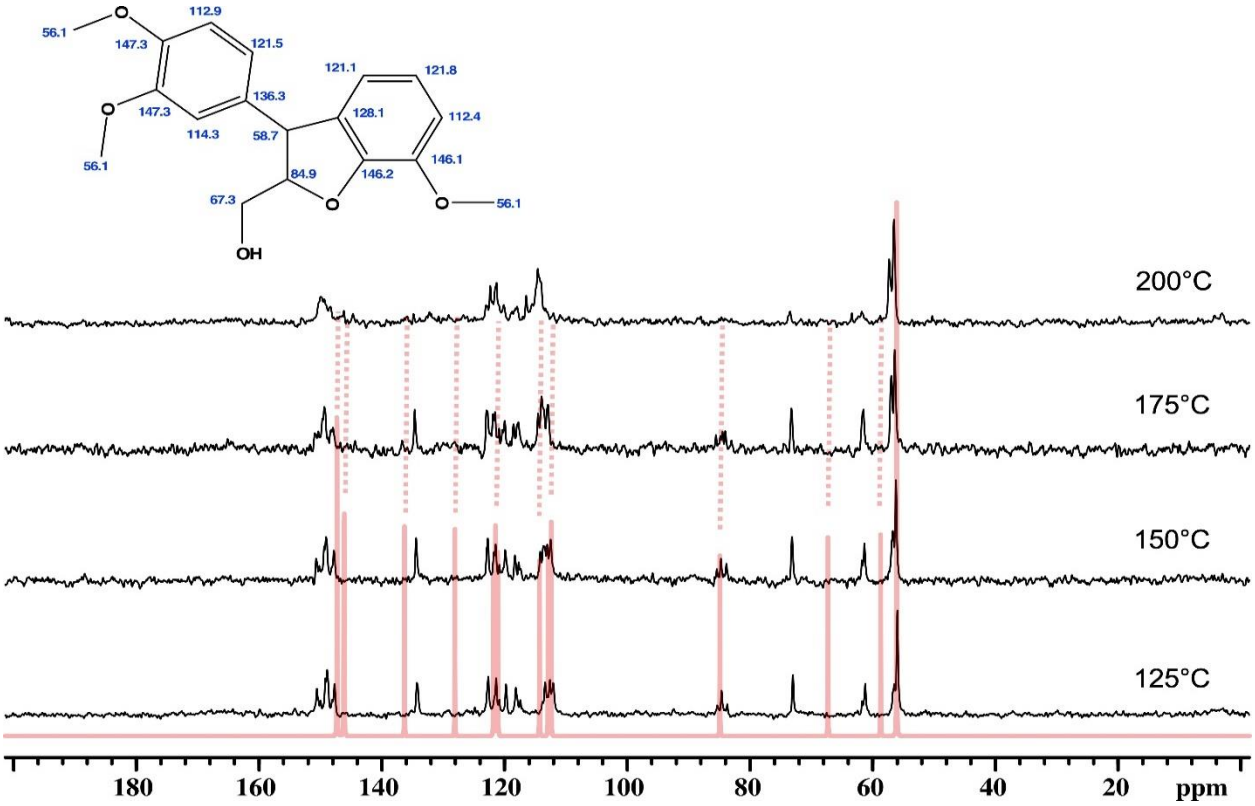
128.5
149.0
120.4
OH
56.1
149.7
111.5
152.5
58.2
56.1
142.0
116.6
147.3
121.7
56.1
115.0
123.9
200°C
175°C
150°C
125°C
180
160
140
120
100
80
60
40
20
ppm


56.1
112.9
147.3
121.5
121.1
121.8
136.3
147.3
128.1
112.4
114.3
58.7
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56.1
84.9
146.2
67.3
56.1
OH
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175°C
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125°C
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140
120
100
80
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20
ppm

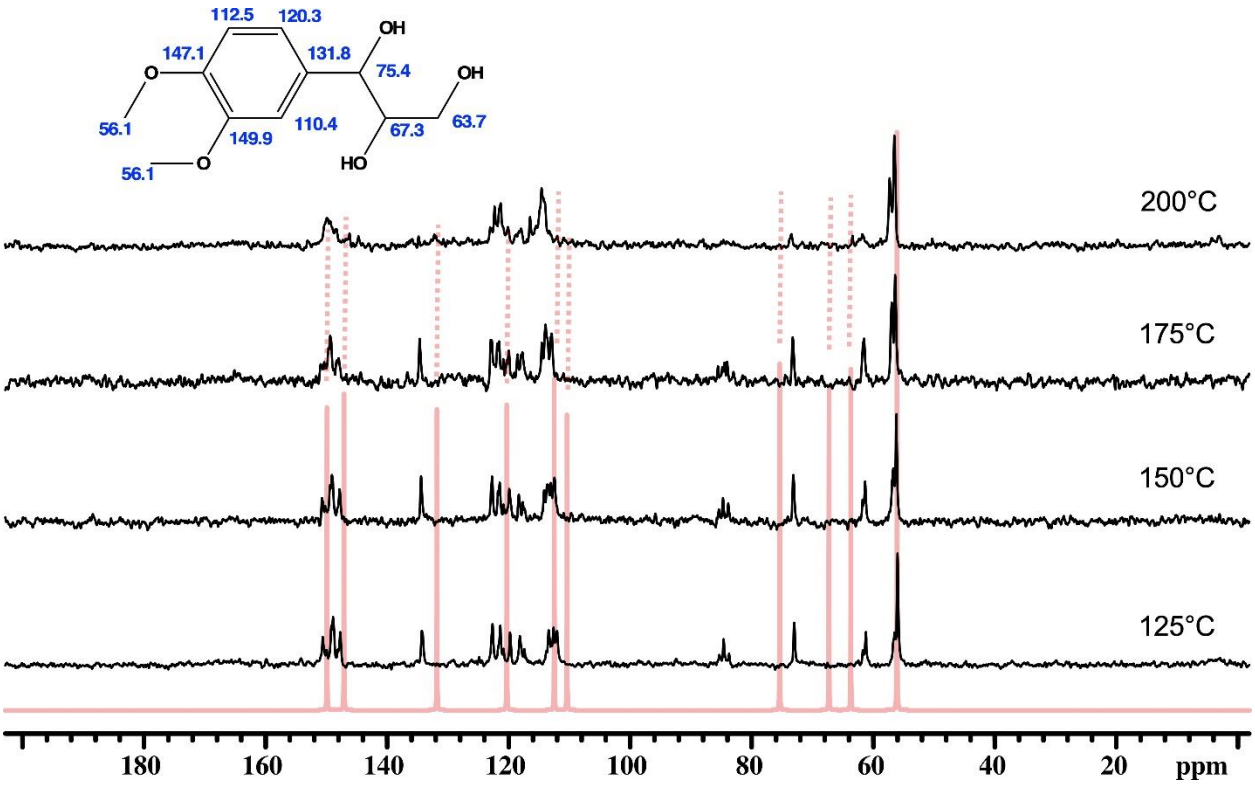
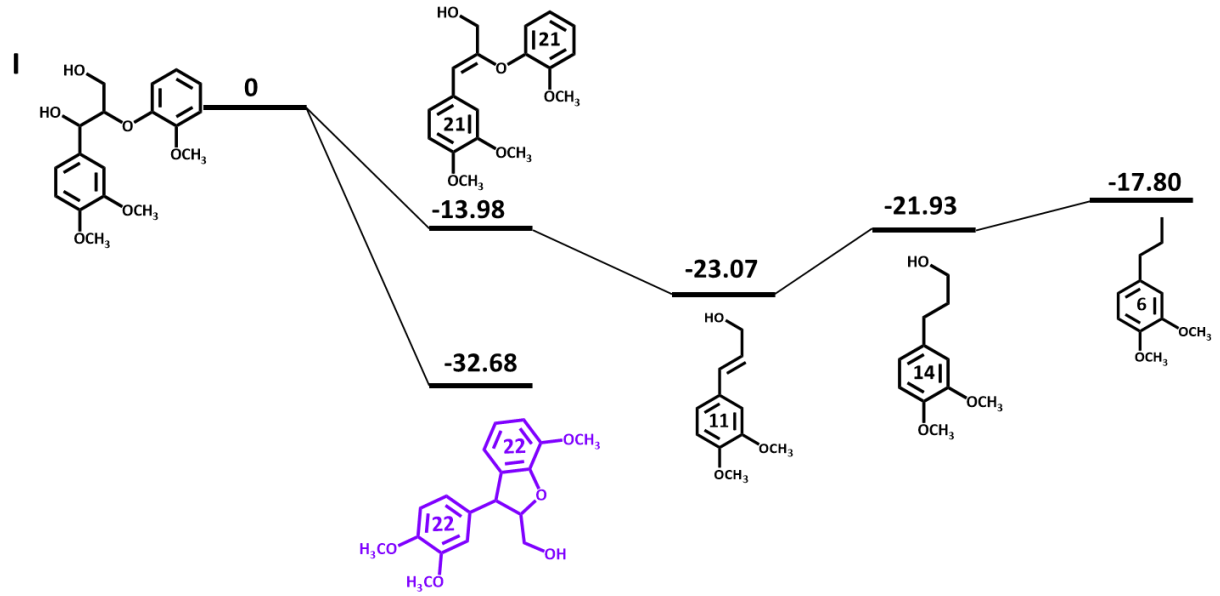



**Figure S4:** Identification of product and intermediates based on $^{13}$C NMR profile with *in-situ* recorded spectra. Red verticle lines show the ChemDraw 19.0 (© PerkinElmer Infomatics) predicted $^{13}$C NMR of compounds (**1**, **2**, **5**, **6**, **7**, **11**, **13**, **21**, **22**, **26**).



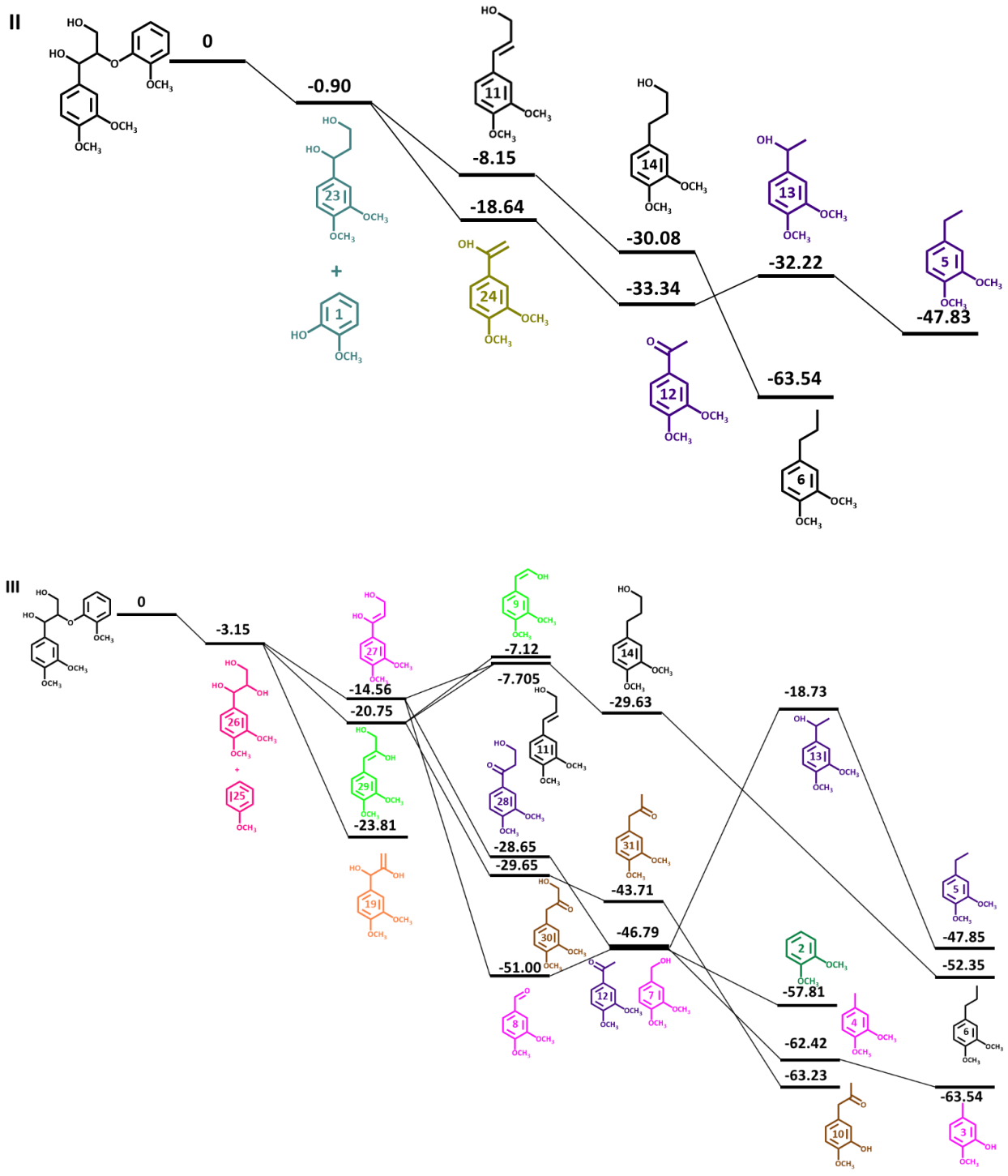
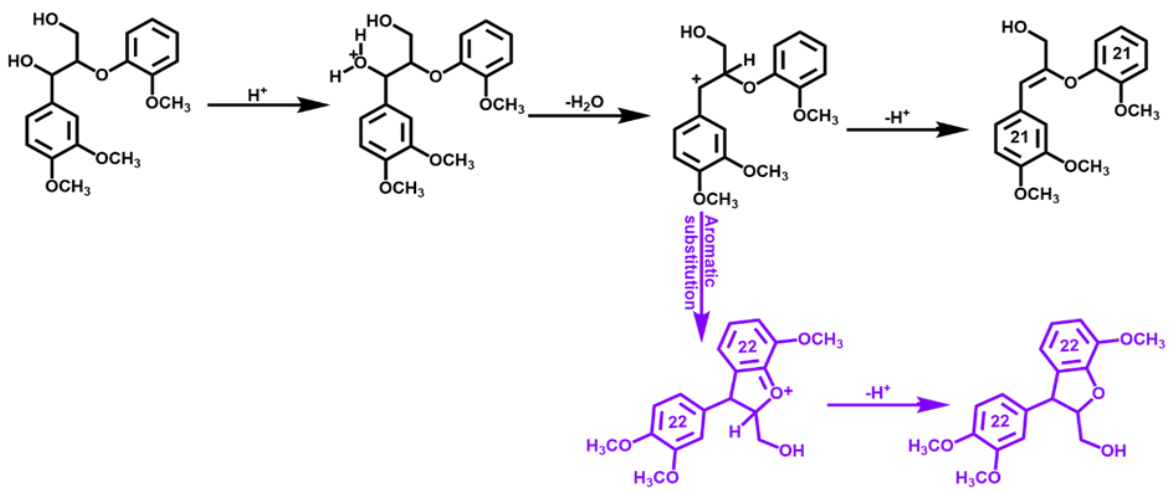



**Figure S5.** The calculated energy profiles of three main pathways shown in Figure 4. Unit of the energy is kcal/mol.




**Scheme S1:** Primary ion mechanism of *β-O-4* acidolysis over zeolite.