Supporting Information (SI) for

Structural Analysis of Lignin-Based Furan Resin

Xuhai Zhu[1*], Bardo Bruijnaers[2], Tainise V. Lourençon[1], Mikhail Balakshin[1*]

[1]Department of Bioproducts and Biosystems, School of Chemical Engineering, Aalto University, Vuorimiehentie 1, Espoo, 02150, Finland

[2]Cellulose-Resin Composite Group, Nemho R&D group, Trespa International B.V., Wetering 20, Weert, 6002 SM, The Netherlands

*Mikhail Balakshin – mikhail.balakshin@aalto.fi/Mailing address: PO Box 16300, FI–00076 AALTO, Finland / Phone number: +358–(0)50–308–6570

*Xuhai Zhu –E-mail: zhuxh@dicp.ac.cn/Mailing address: Dalian Institute of Chemical Physics, CAS, 457 Zhongshan Road Dalian, China 116023 / Tel.: +86–0411-8437-9846

ChemNMR ^{1}H Estimation
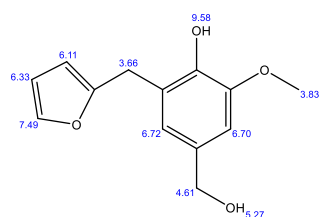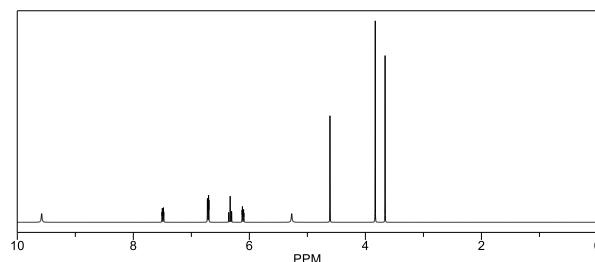
Estimation quality is indicated by color: good, medium, rough


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Protocol of the H-1 NMR Prediction (Lib=SU Solvent=DMSO 300 MHz):

Node      Shift     Base + Inc.    Comment (ppm rel. to TMS)

OH  9.58           4.20      alcohol
                   4.80         1 -C*R
                   0.58         general corrections
OH  5.27           4.20      alcohol
                   1.10         1 -C-C*R
                  -0.03         general corrections
CH  7.49           7.38      2-furan
                  -0.17         1 -C
                   0.28         general corrections
CH  6.11           6.30      2-furan
                  -0.42         1 -C
                   0.23         general corrections
CH  6.33           6.30      2-furan
                  -0.12         1 -C
                   0.15         general corrections
CH  6.70           7.26      1-benzene
                  -0.38         1 -O-C
                  -0.17         1 -O
                  -0.10         1 -CC*R
                   0.00         1 -C-O
                   0.09         general corrections
CH  6.72           7.26      1-benzene
                  -0.32         1 -O-C
                  -0.17         1 -O
                  -0.10         1 -CC*R
                   0.00         1 -C-O
                   0.05         general corrections
CH2 4.61           1.37      methylene
                   1.22         1 alpha -1:C*C*C*C*C*C*1
                   2.20         1 alpha -O
                  -0.18         general corrections
CH3 3.83           0.86      methyl
                   2.87         1 alpha -O-1:C*C*C*C*C*C*1
                   0.10         general corrections
CH2 3.66           1.37      methylene
                   1.22         1 alpha -1:C*C*C*C*C*C*1
                   1.07         1 alpha -1:C-O-C=C-C=1

1H NMR Coupling Constant Prediction

shift   atom index   coupling partner, constant and vector

9.58        7
5.27       17
7.49       14
                 13   7.5   H-C*C-H
                 12   1.5   H-C*CH*C-H
6.11       12
                 13   7.5   H-C*C-H
                 14   1.5   H-C*CH*C-H
6.33       13
                 14   7.5   H-C*C-H
                 12   7.5   H-C*C-H
6.70        5
                  3   1.5   H-C*C*C-H
6.72        3
                  5   1.5   H-C*C*C-H
4.61       16
3.83        9
3.66       10
```
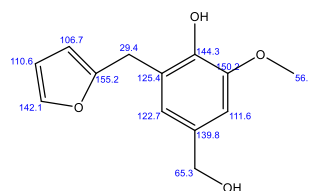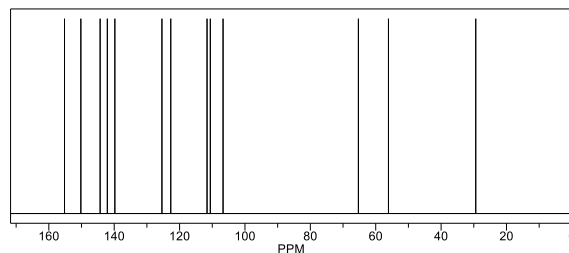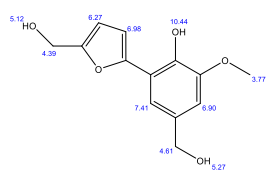
ChemNMR ^{13}C Estimation

Estimation quality is indicated by color: good, medium, rough


```
Protocol of the C-13 NMR Prediction: (Lib=S)

Node      Shift     Base + Inc.    Comment (ppm rel. to TMS)

C   155.2          143.0      2-furan
                     9.5         1 -C
                     2.7         general corrections
CH  142.1          143.0      2-furan
                    -1.8         1 -C
                     0.9         general corrections
CH  106.7          109.9      2-furan
                    -4.2         1 -C
                     1.0         general corrections
CH  110.6          109.9      2-furan
                     0.7         1 -C
                     0.0         general corrections
C   150.2          128.5      1-benzene
                    33.5         1 -O-C
                   -12.8         1 -O
                    -0.1         1 -C
                     0.2         1 -C-O
                     0.9         general corrections
C   144.3          128.5      1-benzene
                   -14.4         1 -O-C
                    28.8         1 -O
                     0.7         1 -C
                    -1.1         1 -C-O
                     1.8         general corrections
C   125.4          128.5      1-benzene
                     1.0         1 -O-C
                   -12.8         1 -O
                     9.2         1 -C
                     0.2         1 -C-O
                    -0.7         general corrections
C   139.8          128.5      1-benzene
                     1.0         1 -O-C
                    -7.4         1 -O
                    -0.1         1 -C
                    12.4         1 -C-O
                     5.4         general corrections
CH  111.6          128.5      1-benzene
                   -14.4         1 -O-C
                     1.4         1 -O
                    -3.0         1 -C
                    -1.2         1 -C-O
                     0.3         general corrections
CH  122.7          128.5      1-benzene
                    -7.7         1 -O-C
                     1.4         1 -O
                     0.7         1 -C
                    -1.2         1 -C-O
                     1.0         general corrections
CH2 65.3            -2.3      aliphatic
                    24.3         1 alpha -1:C*C*C*C*C*C*1
                    49.0         1 alpha -O
                     0.3         1 delta -C
                     0.3         1 delta -O
                    -6.3         general corrections
CH3 56.1            -2.3      aliphatic
                    49.0         1 alpha -O
                     9.3         1 beta -1:C*C*C*C*C*C*1
                     0.3         1 delta -O
                    -0.2         general corrections
CH2 29.4            -2.3      aliphatic
                    24.3         1 alpha -1:C*C*C*C*C*C*1
                    17.0         1 alpha -1:C-O-C=C-C=1
                    -6.2         1 gamma -O
                     0.3         1 delta -C
                     0.3         1 delta -O
                    -4.0         general corrections
```
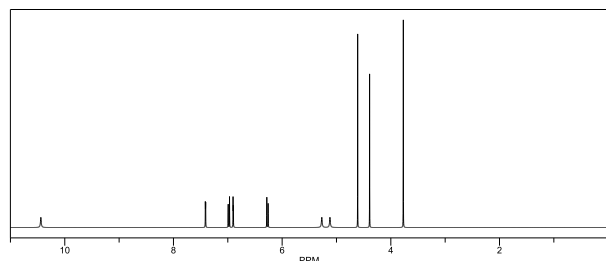
Figure S1. calculated NMR spectra of model **M1**

ChemNMR ^1H Estimation

Estimation quality is indicated by color: good, medium, rough

ChemNMR ^{13}C Estimation

Estimation quality is indicated by color: good, medium, rough
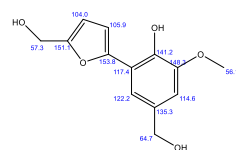

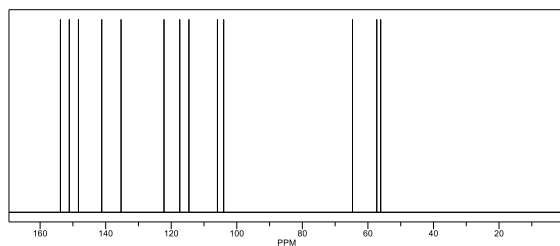Protocol of the H-1 NMR Prediction (Lib=SU Solvent=DMSO 300 MHz):

```
Node      Shift     Base + Inc.    Comment (ppm rel. to TMS)

OH  10.44           4.20      alcohol
                    4.80         1 -C*R
                    1.44         general corrections
OH  5.12            4.20      alcohol
                    1.10         1 -C-C*R
                   -0.18         general corrections
OH  5.27            4.20      alcohol
                    1.10         1 -C-C*R
                   -0.03         general corrections
CH  6.98            6.30      2-furan
                       ?         1 unknown substituent(s)
                   -0.05         1 -C-O
                    0.73         general corrections
CH  6.27            6.30      2-furan
                       ?         1 unknown substituent(s)
                   -0.11         1 -C-O
                    0.08         general corrections
CH  6.90            7.26      1-benzene
                   -0.38         1 -O-C
                   -0.17         1 -O
                    0.10         1 -C*R
                    0.00         1 -C-O
                    0.09         general corrections
CH  7.41            7.26      1-benzene
                   -0.32         1 -O-C
                   -0.17         1 -O
                    0.34         1 -C*R
                    0.00         1 -C-O
                    0.30         general corrections
CH2 4.39            1.37      methylene
                    1.07         1 alpha -1:C-O-C=C-C=1
                    2.20         1 alpha -O
                   -0.25         general corrections
CH2 4.61            1.37      methylene
                    1.22         1 alpha -1:C*C*C*C*C*C*1
                    2.20         1 alpha -O
                   -0.18         general corrections
CH3 3.77            0.86      methyl
                    2.87         1 alpha -O-1:C*C*C*C*C*C*1
                    0.04         general corrections
```

1H NMR Coupling Constant Prediction

```
shift   atom index   coupling partner, constant and vector

10.44        7
5.12        16
5.27        18
6.98        11
                    12   7.5   H-C*C-H
6.27        12
                    11   7.5   H-C*C-H
6.90         5
                     3   1.5   H-C*C*C-H
7.41         3
                     5   1.5   H-C*C*C-H
4.39        15
4.61        17
3.77         9
```
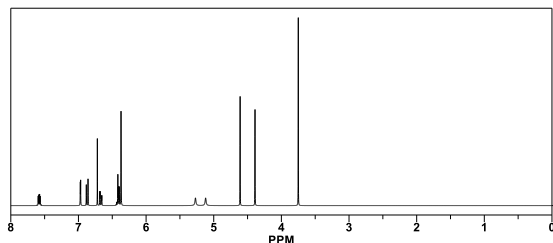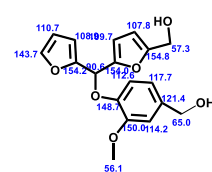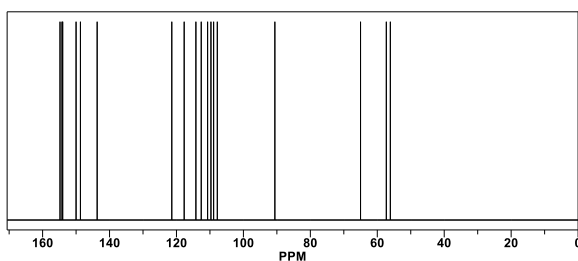
Protocol of the C-13 NMR Prediction: (Lib=S)

```
Node     Shift     Base + Inc.    Comment (ppm rel. to TMS)

C   153.8           143.0      2-furan
                     11.0         1 -1:C*C*C*C*C*C*1
                     -0.2         1 -C-O
                      0.0         general corrections
C   151.1           143.0      2-furan
                     -1.0         1 -1:C*C*C*C*C*C*1
                     11.2         1 -C-O
                     -2.1         general corrections
CH  105.9           109.9      2-furan
                      1.7         1 -1:C*C*C*C*C*C*1
                      0.8         1 -C-O
                     -6.5         general corrections
CH  104.0           109.9      2-furan
                     -4.9         1 -1:C*C*C*C*C*C*1
                     -2.0         1 -C-O
                      1.0         general corrections
C   148.3           128.5      1-benzene
                     33.5         1 -O-C
                    -12.8         1 -O
                      0.5         1 -C*R
                      0.2         1 -C-O
                     -1.6         general corrections
C   141.2           128.5      1-benzene
                    -14.4         1 -O-C
                     28.8         1 -O
                     -1.5         1 -C*R
                     -1.1         1 -C-O
                      0.9         general corrections
C   117.4           128.5      1-benzene
                      1.0         1 -O-C
                    -12.8         1 -O
                      8.0         1 -C*R
                      0.2         1 -C-O
                     -7.5         general corrections
C   135.3           128.5      1-benzene
                      1.0         1 -O-C
                     -7.4         1 -O
                      0.5         1 -C*R
                     12.4         1 -C-O
                      0.3         general corrections
CH  114.6           128.5      1-benzene
                    -14.4         1 -O-C
                      1.4         1 -O
                      0.0         1 -C*R
                     -1.2         1 -C-O
                      0.3         general corrections
CH  122.2           128.5      1-benzene
                     -7.7         1 -O-C
                      1.4         1 -O
                     -1.5         1 -C*R
                     -1.2         1 -C-O
                      2.7         general corrections
CH2 57.3             -2.3      aliphatic
                     17.0         1 alpha -1:C-O-C=C-C=1
                     49.0         1 alpha -O
                      0.3         1 delta -1:C*C*C*C*C*C*1
                     -6.7         general corrections
CH2 64.7             -2.3      aliphatic
                     24.3         1 alpha -1:C*C*C*C*C*C*1
                     49.0         1 alpha -O
                     -0.3         1 delta -1:C-O-C=C-C=1
                      0.3         1 delta -O
                     -6.3         general corrections
CH3 56.1             -2.3      aliphatic
                     49.0         1 alpha -O
                      9.3         1 beta -1:C*C*C*C*C*C*1
                      0.3         1 delta -O
                     -0.2         general corrections
```

Figure S2. calculated NMR spectra of model **M2**

ChemNMR ^{1}H Estimation
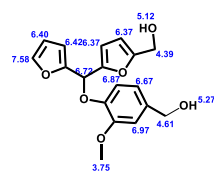
Estimation quality is indicated by color: good, medium, rough

ChemNMR ^{13}C Estimation

Estimation quality is indicated by color: good, medium, rough

Protocol of the H-1 NMR Prediction (Lib=SU Solvent=DMSO 300 MHz):

Node	Shift	Base + Inc.	Comment (ppm rel. to TMS)
OH	5.12	4.20	alcohol
		1.10	1 -C-C*R
		-0.18	general corrections
OH	5.27	4.20	alcohol
		1.10	1 -C-C*R
		-0.03	general corrections
CH	7.58	7.38	2-furan
		-0.08	1 -C-O
		0.28	general corrections
CH	6.37	6.30	2-furan
		-0.11	1 -C-O
		-0.05	1 -C-O
		0.23	general corrections
CH	6.42	6.30	2-furan
		-0.11	1 -C-O
		0.23	general corrections
CH	6.37	6.30	2-furan
		-0.05	1 -C-O
		-0.11	1 -C-O
		0.23	general corrections
CH	6.40	6.30	2-furan
		-0.05	1 -C-O
		0.15	general corrections
CH	6.97	7.26	1-benzene
		0.00	1 -O-C
		-0.38	1 -O-C
		0.00	1 -C-O
		0.09	general corrections
CH	6.87	7.26	1-benzene
		-0.38	1 -O-C
		0.00	1 -O-C
		0.03	1 -C-O
		-0.04	general corrections
CH	6.67	7.26	1-benzene
		0.00	1 -O-C
		-0.32	1 -O-C
		0.00	1 -C-O
		-0.27	general corrections
CH	6.72	1.50	methine
		3.02	2 alpha -1:C*O*C*C*C*1
		2.20	1 alpha -O-1:C*C*C*C*C*C*1
CH2	4.39	1.37	methylene
		1.07	1 alpha -1:C-O-C=C-C=1
		2.20	1 alpha -O
		-0.25	general corrections
CH2	4.61	1.37	methylene
		1.22	1 alpha -1:C*C*C*C*C*1
		2.20	1 alpha -O
		-0.18	general corrections
CH3	3.75	0.86	methyl
		2.87	1 alpha -O-1:C*C*C*C*C*1
		0.02	general corrections

1H NMR Coupling Constant Prediction

shift	atom index	coupling partner, constant and vector
5.12	13	
5.27	24	
7.58	3	
		2 7.5 H-C*C-H
		1 1.5 H-C*CH*C-H
6.37	11	
		10 7.5 H-C*C-H
6.42	1	
		2 7.5 H-C*C-H
		3 1.5 H-C*CH*C-H
6.37	10	
		11 7.5 H-C*C-H
6.40	2	
		3 7.5 H-C*C-H
		1 7.5 H-C*C-H
6.97	17	
		19 1.5 H-C*C*C-H
6.87	20	
		19 7.5 H-C*C-H
6.67	19	
		20 7.5 H-C*C-H
		17 1.5 H-C*C*C-H
6.72	6	
4.39	12	
4.61	23	
3.75	22	

Protocol of the C-13 NMR Prediction: (Lib=S)

Node	Shift	Base + Inc.	Comment (ppm rel. to TMS)
C	154.0	143.0	2-furan
		11.2	1 -C-O
		-0.2	1 -C-O
C	154.2	143.0	2-furan
		11.2	1 -C-O
C	154.8	143.0	2-furan
		-0.2	1 -C-O
		11.2	1 -C-O
		0.8	general corrections
CH	143.7	143.0	2-furan
		-0.2	1 -C-O
		0.9	general corrections
CH	109.7	109.9	2-furan
		-2.0	1 -C-O
		0.8	1 -C-O
		1.0	general corrections
CH	108.9	109.9	2-furan
		-2.0	1 -C-O
		1.0	general corrections
CH	107.8	109.9	2-furan
		0.8	1 -C-O
		-2.0	1 -C-O
		-0.9	general corrections
CH	110.7	109.9	2-furan
		0.8	1 -C-O
		0.0	general corrections
C	148.7	128.5	1-benzene
		33.5	1 -O-C
		-14.4	1 -O-C
		-1.1	1 -C-O
		2.2	general corrections
C	150.0	128.5	1-benzene
		-14.4	1 -O-C
		33.5	1 -O-C
		0.2	1 -C-O
		2.2	general corrections
C	121.4	128.5	1-benzene
		-7.7	1 -O-C
		1.0	1 -O-C
		12.4	1 -C-O
		-12.8	general corrections
CH	114.2	128.5	1-benzene
		1.0	1 -O-C
		-14.4	1 -O-C
		-1.2	1 -C-O
		0.3	general corrections
CH	112.6	128.5	1-benzene
		-14.4	1 -O-C
		1.0	1 -O-C
		0.2	1 -C-O
		-2.7	general corrections
CH	117.7	128.5	1-benzene
		1.0	1 -O-C
		-7.7	1 -O-C
		-1.2	1 -C-O
		-2.9	general corrections
CH	90.6	-2.3	aliphatic
		34.0	2 alpha -1:C-O-C=C-C=1
		49.0	1 alpha -O
		9.3	1 beta -1:C*C*C*C*C*1
		0.3	1 delta -C
		0.3	1 delta -O
CH2	57.3	-2.3	aliphatic
		17.0	1 alpha -1:C-O-C=C-C=1
		49.0	1 alpha -O
		0.3	1 delta -C
		-6.7	general corrections
CH2	65.0	-2.3	aliphatic
		24.3	1 alpha -1:C*C*C*C*C*C*1
		49.0	1 alpha -O
		0.3	1 delta -O
		-6.3	general corrections
CH3	56.1	-2.3	aliphatic
		49.0	1 alpha -O
		9.3	1 beta -1:C*C*C*C*C*C*1
		0.3	1 delta -O
		-0.2	general corrections

Figure S3. calculated NMR spectra of model **M3**

ChemNMR ^{1}H Estimation
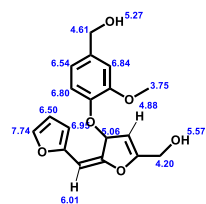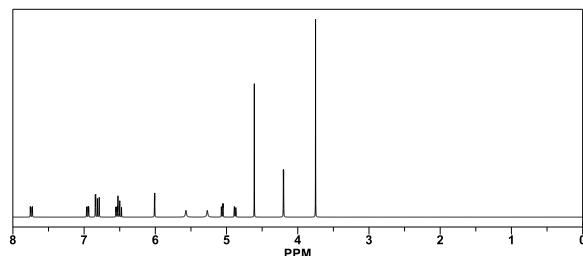
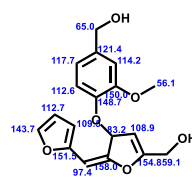Estimation quality is indicated by color: good, medium, rough

ChemNMR ^{13}C Estimation

Estimation quality is indicated by color: good, medium, rough

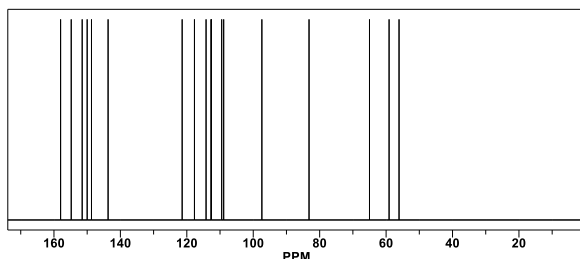Protocol of the H-1 NMR Prediction (Lib=SU Solvent=DMSO 300 MHz):

Node	Shift	Base + Inc.	Comment (ppm rel. to TMS)
OH	5.57	4.20	alcohol
		0.75	1 -CC=C
		0.62	general corrections
OH	5.27	4.20	alcohol
		1.10	1 -C-C*R
		-0.03	general corrections
CH	7.74	7.38	2-furan
		?	1 unknown substituent(s)
		0.36	general corrections
CH	5.06	1.50	methine
		1.36	2 alpha -C=C
		2.20	1 alpha -O-1:C*C*C*C*C*C*1
CH	6.95	6.30	2-furan
		?	1 unknown substituent(s)
		0.65	general corrections
CH	6.50	6.30	2-furan
		?	1 unknown substituent(s)
		0.20	general corrections
CH	6.84	7.26	1-benzene
		-0.13	1 -O-CC=C
		-0.38	1 -O-C
		0.00	1 -C-O
		0.09	general corrections
CH	6.80	7.26	1-benzene
		-0.45	1 -O-CC=C
		0.00	1 -O-C
		0.03	1 -C-O
		-0.04	general corrections
CH	6.54	7.26	1-benzene
		-0.13	1 -O-CC=C
		-0.32	1 -O-C
		0.00	1 -C-O
		-0.27	general corrections
CH2	4.20	1.37	methylene
		0.63	1 alpha -C=C
		2.20	1 alpha -O
CH2	4.61	1.37	methylene
		1.22	1 alpha -1:C*C*C*C*C*1
		2.20	1 alpha -O
		-0.18	general corrections
CH3	3.75	0.86	methyl
		2.87	1 alpha -O-1:C*C*C*C*C*C*1
		0.02	general corrections
H	4.88	5.25	1-ethylene
		-1.00	1 -O-C=C trans
		-0.01	1 -C-O cis
		0.64	1 -C-O gem
H	6.01	5.25	1-ethylene
		-0.60	1 -O-C=C cis
		-0.02	1 -C-O trans
		1.38	1 -C*R gem

1H NMR Coupling Constant Prediction

shift	atom index	coupling partner, constant and vector		
5.57	13			
5.27	24			
7.74	3			
		2	7.5	H-C*C-H
		1	1.5	H-C*CH*C-H
5.06	11			
		25	6.2	H-C-C(sp2)-H
		26	-1.0	H-C>C=C>H
6.95	1			
		2	7.5	H-C*C-H
		3	1.5	H-C*CH*C-H
6.50	2			
		3	7.5	H-C*C-H
		1	7.5	H-C*C-H
6.84	17			
		19	1.5	H-C*C*C-H
6.80	20			
		19	7.5	H-C*C-H
6.54	19			
		20	7.5	H-C*C-H
		17	1.5	H-C*C*C-H
4.20	12			
		25	-1.0	H-CH>C=C<H
4.61	23			
3.75	22			
4.88	25			
		11	6.2	H-C(sp2)-C-H
		12	-1.0	H>C=C<CH-H
6.01	26			
		11	-1.0	H>C=C>C-H

Protocol of the C-13 NMR Prediction: (Lib=S)

Node	Shift	Base + Inc.	Comment (ppm rel. to TMS)
C	154.8	123.3	1-ethylene
		14.2	1 -C-O
		25.5	1 -OC=C
		-8.2	1 -C-O
C	151.5	143.0	2-furan
		12.3	1 -C=C
		-3.8	general corrections
CH	143.7	143.0	2-furan
		2.0	1 -C=C
		-1.3	general corrections
C	158.0	123.3	1-ethylene
		14.2	1 -C-O
		25.5	1 -OC=C
		-5.0	1 -C*R
CH	83.2	-2.3	aliphatic
		39.0	2 alpha -C=C
		49.0	1 alpha -O
		9.3	1 beta -1:C*C*C*C*C*C*1
		10.1	1 beta -O
		-5.0	1 gamma -1:C-O-O=C=C-1
		-2.5	1 gamma -C
		0.6	2 delta -O
		-15.0	general corrections
CH	108.9	123.3	1-ethylene
		-8.2	1 -C-O
		-30.2	1 -OC=C
		14.2	1 -C-O
		9.8	general corrections
CH	109.5	109.9	2-furan
		1.9	1 -C=C
		-2.3	general corrections
CH	112.7	109.9	2-furan
		2.8	1 -C=C
		0.0	general corrections
C	148.7	128.5	1-benzene
		33.5	1 -O-C
		-14.4	1 -O-C
		-1.1	1 -C-O
		2.2	general corrections
C	150.0	128.5	1-benzene
		-14.4	1 -O-C
		33.5	1 -O-C
		0.2	1 -C-O
		2.2	general corrections
C	121.4	128.5	1-benzene
		-7.7	1 -O-C
		1.0	1 -O-C
		12.4	1 -C-O
		-12.8	general corrections
CH	114.2	128.5	1-benzene
		1.0	1 -O-C
		-14.4	1 -O-C
		-1.2	1 -C-O
		0.3	general corrections
CH	112.6	128.5	1-benzene
		-14.4	1 -O-C
		1.0	1 -O-C
		0.2	1 -C-O
		-2.7	general corrections
CH	117.7	128.5	1-benzene
		1.0	1 -O-C
		-7.7	1 -O-C
		-1.2	1 -C-O
		-2.9	general corrections
CH2	59.1	-2.3	aliphatic
		19.5	1 alpha -C=C
		49.0	1 alpha -O
		10.1	1 beta -O
		-2.1	1 gamma -C=C
		-2.5	1 gamma -C
		0.3	1 delta -O
		-12.9	general corrections
CH2	65.0	-2.3	aliphatic
		24.3	1 alpha -1:C*C*C*C*C*C*1
		49.0	1 alpha -O
		0.3	1 delta -O
		-6.3	general corrections
CH3	56.1	-2.3	aliphatic
		49.0	1 alpha -O
		9.3	1 beta -1:C*C*C*C*C*C*1
		0.3	1 delta -O
		-0.2	general corrections
CH	97.4	123.3	1-ethylene
		-8.2	1 -C-O
		-30.2	1 -OC=C
		12.5	1 -C*R

Figure S4. calculated NMR spectra of model **M4**

ChemNMR ¹H Estimation
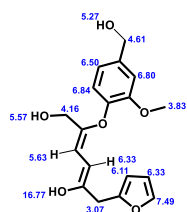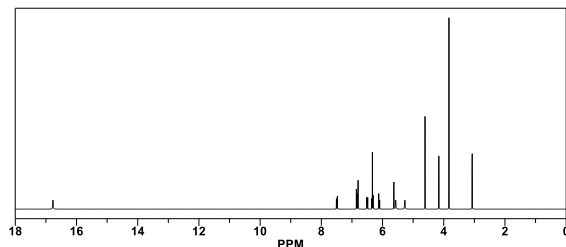
Estimation quality is indicated by color: good, medium, rough

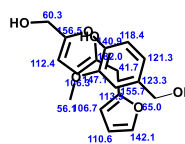Protocol of the H-1 NMR Prediction (Lib=SU Solvent=DMSO 300 MHz):

```
Node      Shift    Base + Inc.    Comment (ppm rel. to TMS)

OH   5.27         4.20       alcohol
                  1.10         1 -C-C*R
                 -0.03         general corrections
OH   16.77       15.00       enol
                  1.77         general corrections
OH   5.57         4.20       alcohol
                  0.75         1 -CC=C
                  0.62         general corrections
CH   7.49         7.38       2-furan
                 -0.17         1 -C
                  0.28         general corrections
CH   6.11         6.30       2-furan
                 -0.42         1 -C
                  0.23         general corrections
CH   6.33         6.30       2-furan
                 -0.12         1 -C
                  0.15         general corrections
CH   6.80         7.26       1-benzene
                 -0.17         1 -O
                 -0.38         1 -O-C
                  0.00         1 -C-O
                  0.09         general corrections
CH   6.84         7.26       1-benzene
                 -0.53         1 -O
                  0.00         1 -O-C
                  0.03         1 -C-O
                  0.08         general corrections
CH   6.50         7.26       1-benzene
                 -0.17         1 -O
                 -0.32         1 -O-C
                  0.00         1 -C-O
                 -0.27         general corrections
CH2  4.61         1.37       methylene
                  1.22         1 alpha -1:C*C*C*C*C*C*1
                  2.20         1 alpha -O
                 -0.18         general corrections
CH2  4.16         1.37       methylene
                  0.63         1 alpha -C=C
                  2.20         1 alpha -O
                 -0.04         general corrections
CH3  3.83         0.86       methyl
                  2.87         1 alpha -O-1:C*C*C*C*C*C*1
                  0.10         general corrections
CH2  3.07         1.37       methylene
                  1.07         1 alpha -1:C-O-C=C-C=1
                  0.63         1 alpha -C=C
H    5.63         5.25       1-ethylene
                 -0.85         1 -O-1:C*C*C*C*C*C*1 trans
                 -0.01         1 -C-O cis
                  1.24         1 -C=C gem
H    6.33         5.25       1-ethylene
                 -0.22         1 -C cis
                    ?         1 unknown substituent(s)
                  1.24         1 -C=C gem
                  0.06         general corrections
```
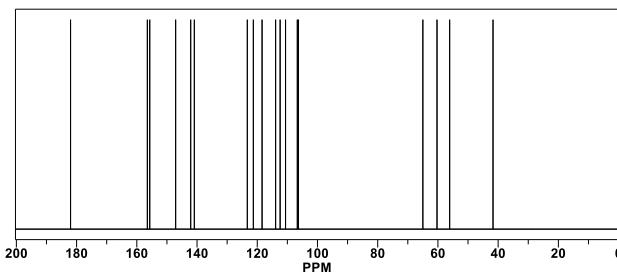
1H NMR Coupling Constant Prediction

```
shift    atom index   coupling partner, constant and vector

5.27      24
16.77     12
5.57      22
7.49       3
                 2   7.5  H-C*C-H
                 1   1.5  H-C*CH*C-H
6.11       1
                 2   7.5  H-C*C-H
                 3   1.5  H-C*CH*C-H
6.33       2
                 3   7.5  H-C*C-H
                 1   7.5  H-C*C-H
6.80      15
                17   1.5  H-C*C*C-H
6.84      18
                17   7.5  H-C*C-H
6.50      17
                18   7.5  H-C*C-H
                15   1.5  H-C*C*C-H
4.61      23
4.16      21
                25  -1.0  H-CH>C=C<H
3.83      20
3.07       6
                26  -1.0  H-CH>C=C<H
5.63      25
                21  -1.0  H>C=C<CH-H
6.33      26
                 6  -1.0  H>C=C<CH-H
```
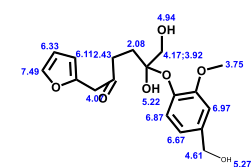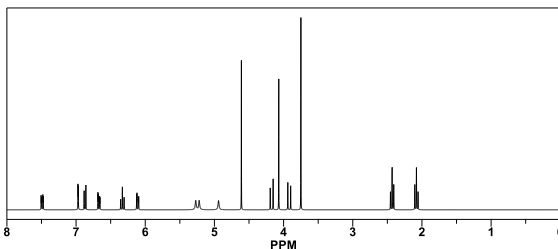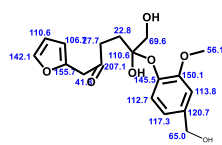
ChemNMR ¹³C Estimation

Estimation quality is indicated by color: good, medium, rough

Protocol of the C-13 NMR Prediction: (Lib=S)

```
Node      Shift    Base + Inc.    Comment (ppm rel. to TMS)

C    155.7        143.0       2-furan
                    9.5         1 -C
                    3.2         general corrections
CH   142.1        143.0       2-furan
                   -1.8         1 -C
                    0.9         general corrections
CH   106.7        109.9       2-furan
                   -4.2         1 -C
                    1.0         general corrections
CH   110.6        109.9       2-furan
                    0.7         1 -C
                    0.0         general corrections
C    140.9        128.5       1-benzene
                   28.2         1 -O-C=C
                  -14.4         1 -O-C
                   -1.1         1 -C-O
                   -0.3         general corrections
C    147.1        128.5       1-benzene
                  -11.5         1 -O-C=C
                   33.5         1 -O-C
                    0.2         1 -C-O
                   -3.6         general corrections
C    123.3        128.5       1-benzene
                   -5.8         1 -O-C=C
                    1.0         1 -O-C
                   12.4         1 -C-O
                  -12.8         general corrections
CH   113.9        128.5       1-benzene
                    0.7         1 -O-C=C
                  -14.4         1 -O-C
                   -1.2         1 -C-O
                    0.3         general corrections
CH   118.4        128.5       1-benzene
                  -11.5         1 -O-C=C
                    1.0         1 -O-C
                    0.2         1 -C-O
                    0.2         general corrections
CH   121.3        128.5       1-benzene
                    0.7         1 -O-C=C
                   -7.7         1 -O-C
                   -1.2         1 -C-O
                    1.0         general corrections
CH2  65.0         -2.3        aliphatic
                   24.3         1 alpha -1:C*C*C*C*C*C*1
                   49.0         1 alpha -O
                    0.3         1 delta -O
                   -6.3         general corrections
C    156.5        123.3       1-ethylene
                   14.2         1 -C-O
                   26.0         1 -O-1:C*C*C*C*C*C*1
                   -7.0         1 -C=C
C    182.0        123.3       1-ethylene
                    9.4         1 -C
                   52.7         1 -O
                   -7.0         1 -C=C
                    3.6         general corrections
CH2  60.3         -2.3        aliphatic
                   19.5         1 alpha -C=C
                   49.0         1 alpha -O
                   10.1         1 beta -O
                   -2.6         1 gamma -1:C*C*C*C*C*C*1
                   -2.1         1 gamma -C=C
                  -11.3         general corrections
CH3  56.1         -2.3        aliphatic
                   49.0         1 alpha -O
                    9.3         1 beta -1:C*C*C*C*C*C*1
                    0.3         1 delta -O
                   -0.2         general corrections
CH2  41.7         -2.3        aliphatic
                   17.0         1 alpha -1:C-O-C=C-C=1
                   19.5         1 alpha -C=C
                   10.1         1 beta -O
                   -2.1         1 gamma -C=C
                   -0.5         general corrections
CH   112.4        123.3       1-ethylene
                   -8.2         1 -C-O
                  -28.4         1 -O-1:C*C*C*C*C*C*1
                   13.6         1 -C=C
                   12.1         general corrections
CH   106.3        123.3       1-ethylene
                   -7.4         1 -C
                  -35.3         1 -O
                   13.6         1 -C=C
                   12.1         general corrections
```

Figure S5. calculated NMR spectra of model **M5**

ChemNMR ¹H Estimation

Estimation quality is indicated by color: good, medium, rough


```
PPM
8   7   6   5   4   3   2   1   0
```

Protocol of the H-1 NMR Prediction (Lib=SU Solvent=DMSO 300 MHz):

```
Node    Shift   Base + Inc.   Comment (ppm rel. to TMS)

OH  5.22        4.20          alcohol
                1.20          1 -CCO
                -0.18         general corrections
OH  5.27        4.20          alcohol
                1.10          1 -C-C*R
                -0.03         general corrections
OH  4.94        4.20          alcohol
                1.20          1 -CCO
                -0.46         general corrections
CH  7.49        7.38          2-furan
                -0.17         1 -C
                0.28          general corrections
CH  6.11        6.30          2-furan
                -0.42         1 -C
                0.23          general corrections
CH  6.33        6.30          2-furan
                -0.12         1 -C
                0.15          general corrections
CH  6.97        7.26          1-benzene
                0.00          1 -O-C
                -0.38         1 -O-C
                0.00          1 -C-O
                0.09          general corrections
CH  6.87        7.26          1-benzene
                -0.38         1 -O-C
                0.00          1 -O-C
                0.03          1 -C-O
                -0.04         general corrections
CH  6.67        7.26          1-benzene
                0.00          1 -O-C
                -0.32         1 -O-C
                0.00          1 -C-O
                -0.27         general corrections
CH2 4.61        1.37          methylene
                1.22          1 alpha -1:C*C*C*C*C*C*1
                2.20          1 alpha -O
                -0.18         general corrections
CH2 4.17,3.915000  1.37       methylene
                2.20          1 alpha -O
                0.38          1 beta -O-1:C*C*C*C*C*C*1
                0.15          1 beta -O
                -0.06         1 beta -C
CH3 3.75        0.86          methyl
                2.87          1 alpha -O-1:C*C*C*C*C*C*1
                0.02          general corrections
CH2 4.07        1.37          methylene
                1.07          1 alpha -1:C-O-C=C-C=1
                1.12          1 alpha -C(=O)-C
                0.51          general corrections
CH2 2.43        1.37          methylene
                1.12          1 alpha -C(=O)-C
                -0.06         1 beta -C
CH2 2.08        1.37          methylene
                0.38          1 beta -O-1:C*C*C*C*C*C*1
                0.15          1 beta -O
                -0.06         1 beta -C
                0.24          1 beta -C(=O)-C
```
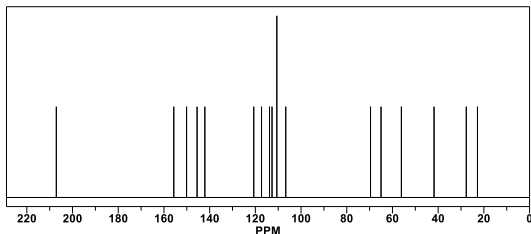
1H NMR Coupling Constant Prediction

```
shift   atom index  coupling partner, constant and vector

5.22    8
5.27    25
4.94    23
7.49    3
                2   7.5  H-C*C-H
                1   1.5  H-C*CH*C-H
6.11    1
                2   7.5  H-C*C-H
                3   1.5  H-C*CH*C-H
6.33    2
                3   7.5  H-C*C-H
                1   7.5  H-C*C-H
6.97    18
                16  1.5  H-C*C*C-H
6.87    15
                16  7.5  H-C*C-H
6.67    16
                15  7.5  H-C*C-H
                18  1.5  H-C*C*C-H
4.61    24
4.04    22 diastereotopic -12.4  H-C-H
3.75    21
4.07    6
2.43    11
                10  7.1  H-CH-CH-H
2.08    10
                11  7.1  H-CH-CH-H
```

ChemNMR ¹³C Estimation

Estimation quality is indicated by color: good, medium, rough


```
PPM
220  200  180  160  140  120  100  80  60  40  20  0
```

Protocol of the C-13 NMR Prediction: (Lib=S)

```
Node    Shift   Base + Inc.   Comment (ppm rel. to TMS)

C   155.7       143.0         2-furan
                9.5           1 -C
                3.2           general corrections
CH  142.1       143.0         2-furan
                -1.8          1 -C
                0.9           general corrections
CH  106.7       109.9         2-furan
                -4.2          1 -C
                1.0           general corrections
CH  110.6       109.9         2-furan
                0.7           1 -C
                0.0           general corrections
C   145.5       128.5         1-benzene
                30.3          1 -OCC
                -14.4         1 -O-C
                -1.1          1 -C-O
                2.2           general corrections
C   150.1       128.5         1-benzene
                -14.3         1 -OCC
                33.5          1 -O-C
                0.2           1 -C-O
                2.2           general corrections
C   120.7       128.5         1-benzene
                -8.4          1 -OCC
                1.0           1 -O-C
                12.4          1 -C-O
                -12.8         general corrections
CH  113.8       128.5         1-benzene
                0.6           1 -OCC
                -14.4         1 -O-C
                -1.2          1 -C-O
                0.3           general corrections
CH  112.7       128.5         1-benzene
                -14.3         1 -OCC
                1.0           1 -O-C
                0.2           1 -C-O
                -2.7          general corrections
CH  117.3       128.5         1-benzene
                0.6           1 -OCC
                -7.7          1 -O-C
                -1.2          1 -C-O
                -2.9          general corrections
C   207.1       193.0         1-carbonyl
                7.6           1 -C-C
                6.5           1 -C
                0.0           general corrections
C   110.6       -2.3          aliphatic
                18.2          2 alpha -C
                98.0          2 alpha -O
                9.3           1 beta -1:C*C*C*C*C*C*1
                9.4           1 beta -C
                10.1          1 beta -O
                -2.7          1 gamma -C(=O)-C
                0.3           1 delta -O
                -29.7         general corrections
CH2 65.0        -2.3          aliphatic
                24.3          1 alpha -1:C*C*C*C*C*C*1
                49.0          1 alpha -O
                0.3           1 delta -O
                -6.3          general corrections
CH2 69.6        -2.3          aliphatic
                9.1           1 alpha -C
                49.0          1 alpha -O
                9.4           1 beta -C
                20.2          2 beta -O
                -2.6          1 gamma -1:C*C*C*C*C*C*1
                -2.5          1 gamma -C
                0.0           1 delta -C(=O)-C
                -10.7         general corrections
CH3 56.1        -2.3          aliphatic
                49.0          1 alpha -O
                9.3           1 beta -1:C*C*C*C*C*C*1
                0.3           1 delta -O
                -0.2          general corrections
CH2 41.8        -2.3          aliphatic
                17.0          1 alpha -1:C-O-C=C-C=1
                29.3          1 alpha -C(=O)-C
                -2.5          1 gamma -C
                0.3           1 delta -C
CH2 27.7        -2.3          aliphatic
                29.3          1 alpha -C(=O)-C
                9.1           1 alpha -C
                9.4           1 beta -C
                -5.0          1 gamma -1:C-O-C=C-C=1
                -2.5          1 gamma -C
                -12.4         2 gamma -O
                0.3           1 delta -1:C*C*C*C*C*C*1
                0.3           1 delta -O
                1.5           general corrections
CH2 22.8        -2.3          aliphatic
                18.2          2 alpha -C
                0.5           1 beta -C(=O)-C
                9.4           1 beta -C
                20.2          2 beta -O
                -2.6          1 gamma -1:C*C*C*C*C*C*1
                -6.2          1 gamma -O
                -0.3          1 delta -1:C-O-C=C-C=1
                -14.1         general corrections
```

Figure S6. calculated NMR spectra of model **M6**

ChemNMR ^{1}H Estimation
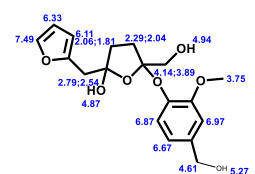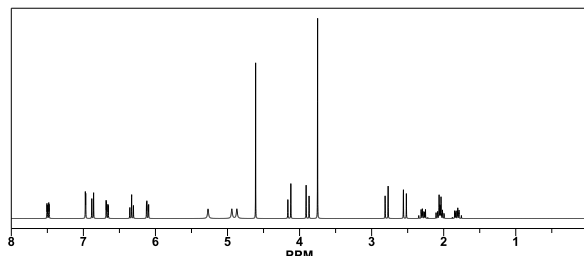
Estimation quality is indicated by color: good, medium, rough

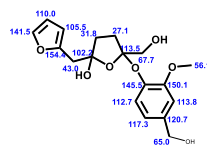Protocol of the H-1 NMR Prediction (Lib=SU Solvent=DMSO 300 MHz):

```
Node      Shift      Base + Inc.    Comment (ppm rel. to TMS)

OH  4.87           4.20        alcohol
                   0.85           1 -CCC*R
                  -0.18           general corrections
OH  4.94           4.20        alcohol
                   1.20           1 -CCO
                  -0.46           general corrections
OH  5.27           4.20        alcohol
                   1.10           1 -C-C*R
                  -0.03           general corrections
CH  7.49           7.38        2-furan
                  -0.17           1 -C
                   0.28           general corrections
CH  6.11           6.30        2-furan
                  -0.42           1 -C
                   0.23           general corrections
CH  6.33           6.30        2-furan
                  -0.12           1 -C
                   0.15           general corrections
CH2 2.29,2.045000  1.85        tetrahydrofuran
                   0.38           1 beta -O-1:C*C*C*C*C*C*1 from methylene
                  -0.06           1 beta -C from methylene
CH2 2.06,1.815000  1.85        tetrahydrofuran
                   0.15           1 beta -O from methylene
                  -0.06           1 beta -C from methylene
CH  6.97           7.26        1-benzene
                   0.00           1 -O-C
                  -0.38           1 -O-C
                   0.00           1 -C-O
                   0.09           general corrections
CH  6.87           7.26        1-benzene
                  -0.38           1 -O-C
                   0.00           1 -O-C
                   0.03           1 -C-O
                  -0.04           general corrections
CH  6.67           7.26        1-benzene
                   0.00           1 -O-C
                  -0.32           1 -O-C
                   0.00           1 -C-O
                  -0.27           general corrections
CH2 4.14,3.895000  1.37        methylene
                   2.20           1 alpha -O
                   0.38           1 beta -O-1:C*C*C*C*C*C*1
                   0.13           1 beta -O-C
                  -0.06           1 beta -C
CH2 4.61           1.37        methylene
                   1.22           1 alpha -1:C*C*C*C*C*C*1
                   2.20           1 alpha -O
                  -0.18           general corrections
CH3 3.75           0.86        methyl
                   2.87           1 alpha -O-1:C*C*C*C*C*C*1
                   0.02           general corrections
CH2 2.79,2.535000  1.37        methylene
                   1.07           1 alpha -1:C-O-C=C-C=1
                   0.13           1 beta -O-C
                   0.15           1 beta -O
                  -0.06           1 beta -C
```

1H NMR Coupling Constant Prediction

```
shift    atom index   coupling partner, constant and vector

4.87        11
4.94        23
5.27        25
7.49         3
                   2    7.5   H-C*C-H
                   1    1.5   H-C*CH*C-H
6.11         1
                   2    7.5   H-C*C-H
                   3    1.5   H-C*CH*C-H
6.33         2
                   3    7.5   H-C*C-H
                   1    7.5   H-C*C-H
2.17         9 diastereotopic -12.4  H-C-H
                  10    7.1   H-CH-CH-H
1.94        10 diastereotopic -12.4  H-C-H
                   9    7.1   H-CH-CH-H
6.97        18
                  16    1.5   H-C*C-H
6.87        15
                  16    7.5   H-C*C-H
6.67        16
                  15    7.5   H-C*C-H
                  18    1.5   H-C*C-H
4.02        22 diastereotopic -12.4  H-C-H
4.61        24
3.75        21
2.66         6 diastereotopic -12.4  H-C-H
```

ChemNMR ^{13}C Estimation

Estimation quality is indicated by color: good, medium, rough
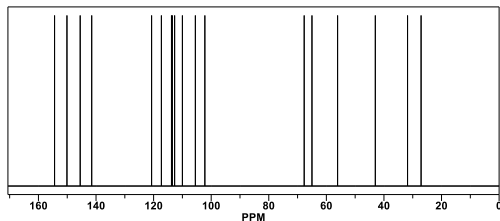
Protocol of the C-13 NMR Prediction: (Lib=S)

```
Node    Shift    Base + Inc.  Comment (ppm rel. to TMS)

C  113.5      -8.5      tetrahydrofuran
               18.2       2 alpha -C from aliphatic
               98.0       2 alpha -O from aliphatic
                9.3       1 beta -1:C*C*C*C*C*C*1 from aliphatic
               18.8       2 beta -C from aliphatic
               10.1       1 beta -O from aliphatic
               -2.5       1 gamma -C from aliphatic
               -6.2       1 gamma -O from aliphatic
               -0.3       1 delta -1:C-O-C=C-C=1 from aliphatic
                0.3       1 delta -O from aliphatic
              -23.7       general corrections
C  102.2      -8.5      tetrahydrofuran
               18.2       2 alpha -C from aliphatic
               98.0       2 alpha -O from aliphatic
                7.5       1 beta -1:C-O-C=C-C=1 from aliphatic
               18.8       2 beta -C from aliphatic
               -2.5       1 gamma -C from aliphatic
               -6.2       1 gamma -O from aliphatic
                0.3       1 delta -1:C*C*C*C*C*C*1 from aliphatic
                0.3       1 delta -O from aliphatic
              -23.7       general corrections
C  154.4     143.0      2-furan
               13.6       1 -CCCCC
               -2.2       general corrections
CH 141.5     143.0      2-furan
               -2.4       1 -CCCCC
                0.9       general corrections
CH 105.5     109.9      2-furan
               -5.4       1 -CCCCC
                1.0       general corrections
CH 110.0     109.9      2-furan
                0.1       1 -CCCCC
                0.0       general corrections
CH2 27.1     -11.2      tetrahydrofuran
               18.2       2 alpha -C from aliphatic
               18.8       2 beta -C from aliphatic
               20.2       2 beta -O from aliphatic
               -2.6       1 gamma -1:C*C*C*C*C*C*1 from aliphatic
               -2.5       1 gamma -C from aliphatic
              -12.4       2 gamma -O from aliphatic
               -0.3       1 delta -1:C-O-C=C-C=1 from aliphatic
               -1.1       general corrections
CH2 31.8     -11.2      tetrahydrofuran
               18.2       2 alpha -C from aliphatic
               18.8       2 beta -C from aliphatic
               20.2       2 beta -O from aliphatic
               -5.0       1 gamma -1:C-O-C=C-C=1 from aliphatic
               -2.5       1 gamma -C from aliphatic
               -6.2       1 gamma -O from aliphatic
                0.3       1 delta -1:C*C*C*C*C*C*1 from aliphatic
                0.3       1 delta -O from aliphatic
               -1.1       general corrections
C  145.5     128.5      1-benzene
               30.3       1 -OCC
              -14.4       1 -O-C
               -1.1       1 -C-O
                2.2       general corrections
C  150.1     128.5      1-benzene
              -14.3       1 -OCC
               33.5       1 -O-C
                0.2       1 -C-O
                2.2       general corrections
C  120.7     128.5      1-benzene
               -8.4       1 -OCC
                1.0       1 -O-C
               12.4       1 -C-O
              -12.8       general corrections
CH 113.8     128.5      1-benzene
                0.6       1 -OCC
              -14.4       1 -O-C
               -1.2       1 -C-O
                0.3       general corrections
CH 112.7     128.5      1-benzene
              -14.3       1 -OCC
                1.0       1 -O-C
                0.2       1 -C-O
               -2.7       general corrections
CH 117.3     128.5      1-benzene
                0.6       1 -OCC
               -7.7       1 -O-C
               -1.2       1 -C-O
               -2.9       general corrections
CH2 67.7      -2.3      aliphatic
                9.1       1 alpha -C
               49.0       1 alpha -O
                9.4       1 beta -C
               20.2       2 beta -O
               -2.6       1 gamma -1:C*C*C*C*C*C*1
               -5.0       2 gamma -C
                0.3       1 delta -C
                0.3       1 delta -O
              -10.7       general corrections
CH2 65.0      -2.3      aliphatic
               24.3       1 alpha -1:C*C*C*C*C*C*1
               49.0       1 alpha -O
                0.3       1 delta -O
               -6.3       general corrections
CH3 56.1      -2.3      aliphatic
               49.0       1 alpha -O
                9.3       1 beta -1:C*C*C*C*C*C*1
                0.3       1 delta -O
               -0.2       general corrections
CH2 43.0      -2.3      aliphatic
               17.0       1 alpha -1:C-O-C=C-C=1
                9.1       1 alpha -C
                9.4       1 beta -C
               20.2       2 beta -O
               -5.0       2 gamma -C
                0.3       1 delta -C
                0.3       1 delta -O
               -6.0       general corrections
```

Figure S7. calculated NMR spectra of model **M7**

ChemNMR ¹H Estimation

Estimation quality is indicated by color: good, medium, rough

ChemNMR ¹³C Estimation

Estimation quality is indicated by color: good, medium, rough

Figure S8. calculated NMR spectra of model M8
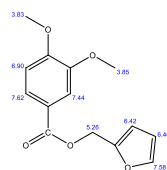
Estimation quality is indicated by color: good, medium, rough

Estimation quality is indicated by color: good, medium, rough
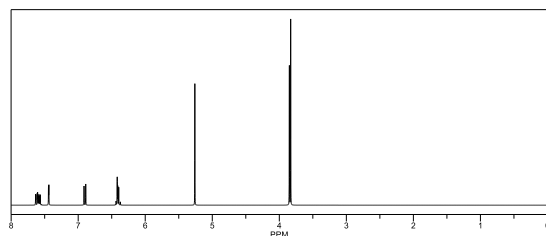
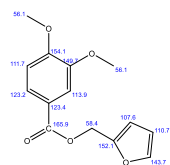

Protocol of the H-1 NMR Prediction (Lib=SU Solvent=DMSO 300 MHz):

```
Node     Shift    Base + Inc.   Comment (ppm rel. to TMS)

CH  7.58           7.38         2-furan
                  -0.08          1 -C-O
                   0.28          general corrections
CH  6.42           6.30         2-furan
                  -0.11          1 -C-O
                   0.23          general corrections
CH  6.40           6.30         2-furan
                  -0.05          1 -C-O
                   0.15          general corrections
CH  7.44           7.26         1-benzene
                  -0.38          1 -O-C
                   0.00          1 -O-C
                   0.71          1 -C(=O)OC
                  -0.15          general corrections
CH  6.90           7.26         1-benzene
                   0.00          1 -O-C
                  -0.38          1 -O-C
                   0.11          1 -C(=O)OC
                  -0.09          general corrections
CH  7.62           7.26         1-benzene
                  -0.32          1 -O-C
                   0.00          1 -O-C
                   0.71          1 -C(=O)OC
                  -0.03          general corrections
CH2 5.26           1.37         methylene
                   1.07          1 alpha -1:C-O-C=C-C=1
                   2.92          1 alpha -OC(=O)-1:C*C*C*C*C*C*1
                  -0.10          general corrections
CH3 3.85           0.86         methyl
                   2.87          1 alpha -O-1:C*C*C*C*C*C*1
                   0.12          general corrections
CH3 3.83           0.86         methyl
                   2.87          1 alpha -O-1:C*C*C*C*C*C*1
                   0.10          general corrections

1H NMR Coupling Constant Prediction

shift   atom index   coupling partner, constant and vector

7.58       16
                17   7.5   H-C*C-H
                18   1.5   H-C*CH*C-H
6.42       18
                17   7.5   H-C*C-H
                16   1.5   H-C*CH*C-H
6.40       17
                16   7.5   H-C*C-H
                18   7.5   H-C*C-H
7.44        5
                 3   1.5   H-C*C*C-H
6.90        2
                 3   7.5   H-C*C-H
7.62        3
                 2   7.5   H-C*C-H
                 5   1.5   H-C*C*C-H
5.26       13
3.85       10
3.83       19
```
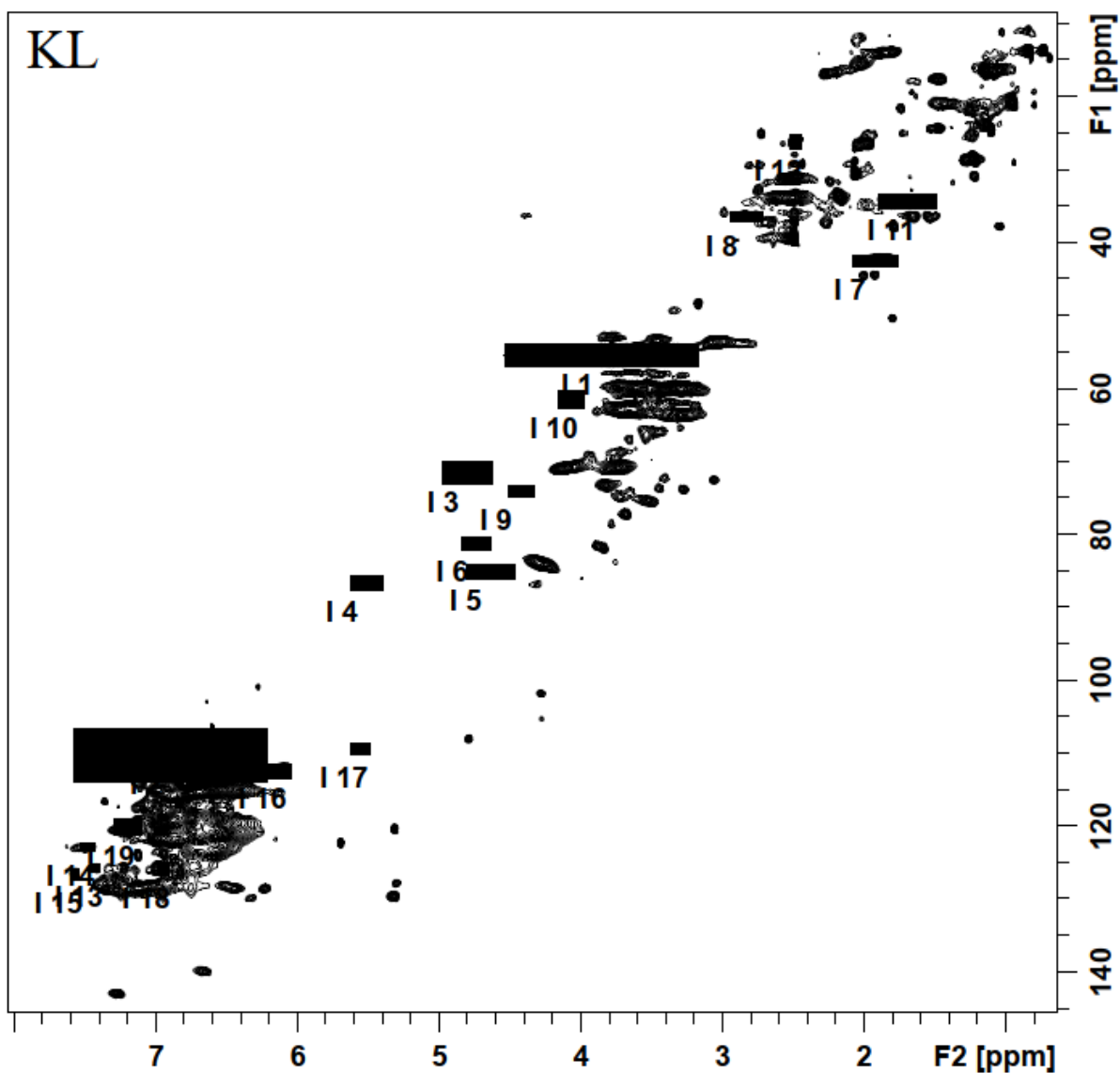
Protocol of the C-13 NMR Prediction: (Lib=S)

```
Node     Shift    Base + Inc.   Comment (ppm rel. to TMS)

C   152.1         143.0         2-furan
                   11.2          1 -C-O
                   -2.1          general corrections
CH  143.7         143.0         2-furan
                   -0.2          1 -C-O
                    0.9          general corrections
CH  107.6         109.9         2-furan
                   -2.0          1 -C-O
                   -0.3          general corrections
CH  110.7         109.9         2-furan
                    0.8          1 -C-O
                    0.0          general corrections
C   149.7         128.5         1-benzene
                   33.5          1 -O-C
                  -14.4          1 -O-C
                   -0.1          1 -C(=O)-O-C
                    2.2          general corrections
C   154.1         128.5         1-benzene
                  -14.4          1 -O-C
                   33.5          1 -O-C
                    4.3          1 -C(=O)-O-C
                    2.2          general corrections
C   123.4         128.5         1-benzene
                    1.0          1 -O-C
                   -7.7          1 -O-C
                    2.0          1 -C(=O)-O-C
                   -0.4          general corrections
CH  113.9         128.5         1-benzene
                  -14.4          1 -O-C
                    1.0          1 -O-C
                    1.2          1 -C(=O)-O-C
                   -2.4          general corrections
CH  111.7         128.5         1-benzene
                    1.0          1 -O-C
                  -14.4          1 -O-C
                   -0.1          1 -C(=O)-O-C
                   -3.3          general corrections
CH  123.2         128.5         1-benzene
                   -7.7          1 -O-C
                    1.0          1 -O-C
                    1.2          1 -C(=O)-O-C
                    0.2          general corrections
C   165.9         166.0         1-carboxyl
                    6.0          1 -1:C*C*C*C*C*C*1
                   -5.0          1 -C from O-carboxyl
                   -1.1          general corrections
CH2 58.4           -2.3         aliphatic
                   17.0          1 alpha -1:C-O-C=C-C=1
                   54.9          1 alpha -O-C=O
                   -2.6          1 gamma -1:C*C*C*C*C*C*1
                   -8.6          general corrections
CH3 56.1           -2.3         aliphatic
                   49.0          1 alpha -O
                    9.3          1 beta -1:C*C*C*C*C*C*1
                    0.3          1 delta -O
                   -0.2          general corrections
CH3 56.1           -2.3         aliphatic
                   49.0          1 alpha -O
                    9.3          1 beta -1:C*C*C*C*C*C*1
                    0.3          1 delta -O
                   -0.2          general corrections
```

Figure S9. calculated NMR spectra of model **M9**

Figure S10. integral of typical structures in KL (nlev = 50, lev0 = 20, toplev = 100 %)

Detailed data set for Figure S10:

Name = KL   xzc12-4   ExpNo =   2   ProcNo =   1

Baseline = 0   Noise = 0

#	SI_F1	row1	row2	row1(ppm)	row2(ppm)	abs. Int.	Integral	norm. Int.	Mode
	SI_F2	col1	col2	col1(ppm)	col2(ppm)				
Methoxyl (I1)	1024	739	754	56.87234	53.74060	7.4108e+13	7.0675e+07	**300**	**a**
	1024	578	706	4.53892	3.17355				
G2(I2)	1024	468	503	113.83346	106.57680	2.2984e+13	2.1919e+07	**93.043**	**a**
	1024	294	421	7.57623	6.21993				
Aα(I3)	1024	663	677	72.88113	70.01336	1.7135e+12	1.6341e+06	**6.9364**	**a**
	1024	537	570	4.98152	4.62657				

Bα(I4)   1024   593   603   87.71448   85.63781   5.2104e+11   4.969e+05   **2.1092   a**

   1024   476   498   5.63634   5.39155

Cα(I5)   1024   601   610   86.03336   84.05559   8.9228e+11   8.5095e+05   **3.6121   a**

   1024   553   584   4.80405   4.47970

C'α(I6)   1024   620   628   81.97892   80.19892   3.2991e+11   3.1463e+05   **1.3355   a**

   1024   550   569   4.84076   4.63881

SRβ(I7)   1024   804   812   43.21573   41.53674   1.2648e+12   1.2062e+06   **5.1202   a**

   1024   807   837   2.08733   1.76134

Arα(I8)   1024   834   840   37.01077   35.76978   3.9495e+11   3.7666e+05   **1.5988   a**

   1024   727   748   2.94367   2.71499

AGα(I9)   1024   654   662   74.79440   73.24104   2.9683e+11   2.8307e+05   **1.2016   a**

   1024   580   597   4.51274   4.33490

Dγ(I10)   1024   712   723   62.53218   60.29508   7.1084e+11   6.7791e+05   **2.8776   a**

   1024   613   630   4.16823   3.97984

DHCAβ(I11)   1024   842   852   35.36743   33.23687   2.0074e+12   1.9144e+06   **8.1264   a**

   1024   825   863   1.89965   1.48361

AVβ(I12)   1024   881   890   27.05822   25.14071   2.3597e+11   2.2504e+05   **0.95525   a**

   1024   766   773   2.52763   2.44913

V6(I13)   1024   408   416   126.53445   124.84582   2.1618e+11   2.0616e+05   **0.87512   a**

   1024   302   313   7.49588   7.37565

VA6(I14)   1024   423   428   123.44588   122.30872   1.6251e+11   1.5498e+05   **0.65786   a**

   1024   298   307   7.53416   7.43899

Bi6(I16)   1024   405   411   127.04691   125.78339   1.6579e+11   1.5811e+05   **0.67115   a**

   1024   292   297   7.60157   7.55002

E-EEα(I17)   1024   471   480   113.33772   111.31609   5.9059e+11   5.6323e+05   **2.3908   a**

   1024   421   437   6.21767   6.05112

Z-EEα(I18)   1024   486   493   110.05257   108.59953   2.5104e+11   2.3941e+05   **1.0162   a**

   1024   477   489   5.61890   5.49201

SB1α(I19)   1024   407   416   126.73103   124.83575   7.7581e+11   7.3987e+05   **3.1406   a**

   1024   349   356   6.99091   6.91557

SB5β(I20)   1024   433   444   121.17155   118.96039   1.3081e+12   1.2475e+06   **5.2952   a**

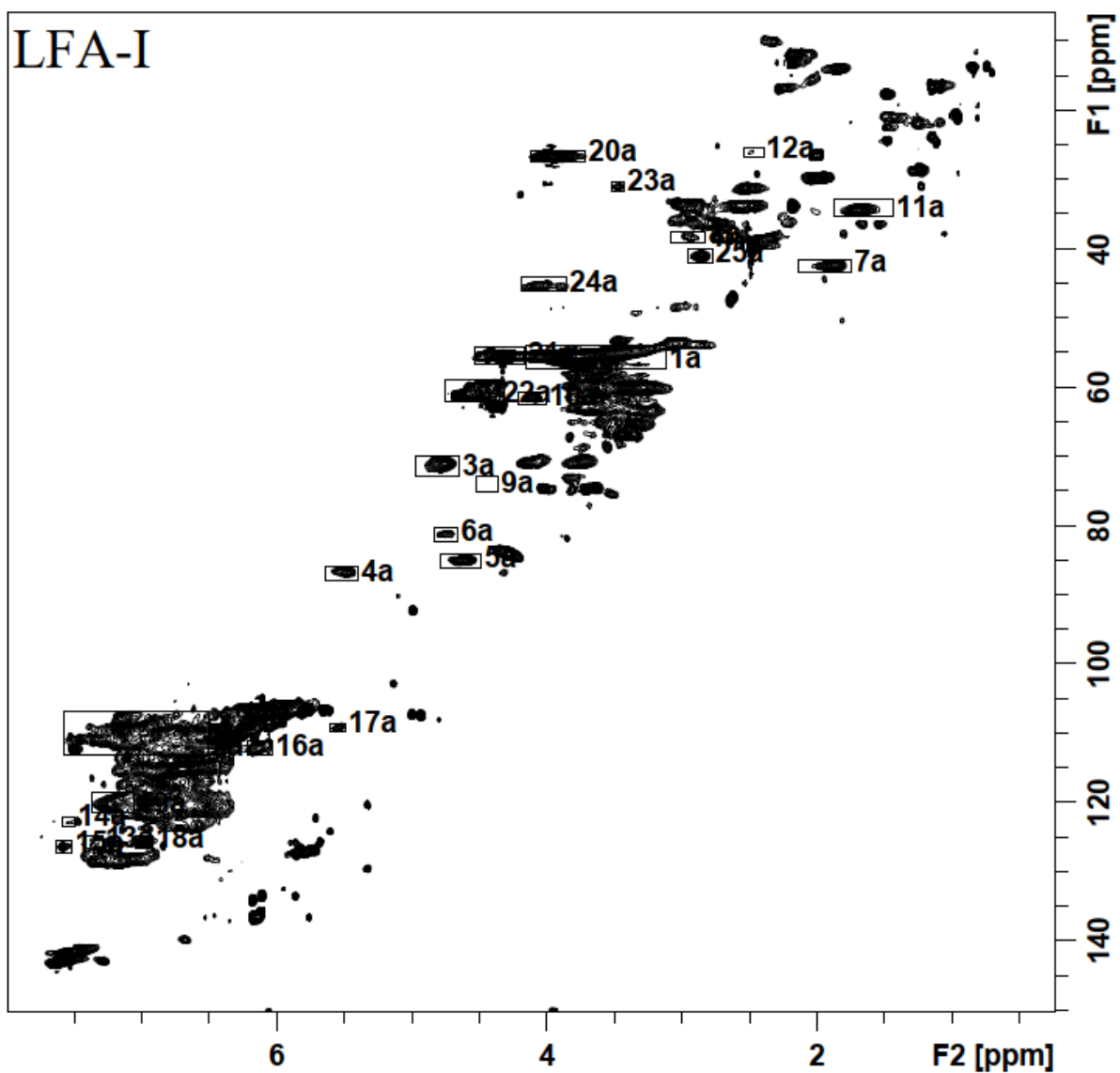   1024   320   338   7.30020   7.10987

Figure S11. integral of typical aromatic units in LFA-I (nlev = 50, lev0 = 20, toplev = 100 %)

Detailed data set for Figure S11:

Name = LFA-I   xzc33-S ExpNo =   2 ProcNo =   1

Baseline = 0   Noise = 0

 # SI_F1 row1 row2 row1(ppm) row2(ppm) abs. Int.   Integral norm. Int. Mode

   SI_F2 col1 col2 col1(ppm) col2(ppm)

Methoxyl(I1)   1024 738 753 57.07990 54.00709 5.9417e+13 5.6665e+07   **300 a**

   1024 614 710   4.15006   3.12031

G2(I2)   1024   472 501 113.11025 106.89172 1.8077e+13 1.7239e+07   **91.27 a**

   1024 294 393   7.57550   6.51197

Aα(I3)   1024   664   677   72.67445   70.06174   1.2703e+12 1.2115e+06   **6.414   a**

     1024   537   567   4.96677   4.65019

Bα(I4)   1024   592   601   87.80064   85.94424   4.7693e+11 4.5483e+05   **2.408   a**

     1024   475   497   5.63108   5.39754

Cα(I5)   1024   601   609   85.94424   84.22535   7.5991e+11 7.2471e+05   **3.8368   a**

     1024   555   582   4.77474   4.49449

C'α(I6)   1024   619   627   82.09393   80.51256   2.6982e+11 2.5732e+05   **1.3624   a**

     1024   550   566   4.83183   4.66576

SRβ(I7)   1024   804   812   43.29043   41.63521   9.814e+11 9.3594e+05   **4.9551   a**

     1024   802   838   2.13209   1.75063

Arα(I8)   1024   824   831   39.02505   37.68814   3.7038e+11 3.5322e+05   **1.87   a**

     1024   714   737   3.07212   2.83371

AGα(I9)   1024   653   663   75.12163   73.01823   2.1066e+11 2.009e+05   **1.0636   a**

     1024   579   594   4.51650   4.36076

Dγ(I10)   1024   713   721   62.42607   60.77340   4.6521e+11 4.4366e+05   **2.3489   a**

     1024   609   627   4.19903   4.00735

DHCAβ(I11)   1024   842   854   35.33900   32.87951   1.6852e+12 1.6071e+06   **8.5086   a**

     1024   821   867   1.92651   1.43658

AVβ(I12)   1024   883   889   26.74288   25.40851   1.2242e+11 1.1675e+05   **0.6181   a**

     1024   765   777   2.53260   2.40511

V6(I13)   1024   409   415   126.34295   125.13434   1.8565e+11 1.7705e+05   **0.93733   a**

     1024   309   320   7.41127   7.29067

VA6(I14)   1024   423   428   123.42866   122.40794   9.5628e+10   91198   **0.48283   a**

     1024   293   301   7.58153   7.49676

Bi6(I15)   1024   405   412   127.11896   125.62713   1.9833e+11 1.8914e+05   **1.0014   a**

     1024   289   299   7.62921   7.51795

E-EEα(I16)   1024   472   481   113.06442   111.18002   6.0827e+11 5.8009e+05   **3.0712   a**

     1024   421   438   6.21463   6.02920

Z-EEα(I17)   1024   488   493   109.76671   108.58895   1.5602e+11 1.4879e+05   **0.78776   a**

     1024   478   488   5.60535   5.49939

SB1α(I18)   1024   408   416   126.49082   124.92048   5.5834e+11 5.3247e+05   **2.8191   a**

     1024   344   355   7.03583   6.91927

SB5β(I19) 1024 433 445 121.18516 118.70278 1.2164e+12 1.1601e+06   **6.1417 a**

   1024 305 332 7.45604   7.16186

CH2 in pFA(I20) 1024 880 887 27.37992 25.91314 1.4712e+13 1.403e+07   **74.28 a**

   1024 617 654 4.11856   3.72374

CH2OH in pFA(I21) 1024 741 752 56.59333 54.14869 8.2265e+12 7.8454e+06   **41.536 a**

   1024 578 612 4.52887   4.17275

CH2OCH2 in pFA(I22) 1024 715 729 61.97152 59.16019 4.1691e+12 3.9759e+06   **21.05 a**

   1024 558 595 4.74564   4.35081

New peak 2(I23)   1024 860 865 31.53580 30.43572 1.1151e+11 1.0635e+05   **0.56303 a**

   1024 673 681 3.51471   3.42955

New peak 3(I24) 1024 791 800 45.95916 44.24791 5.7779e+11 5.5102e+05   **2.9173 a**

   1024 611 641 4.18050   3.85535

New peak 4(I25) 1024 811 819 41.92551 40.09203   4.84e+11 4.6157e+05   **2.4437 a**
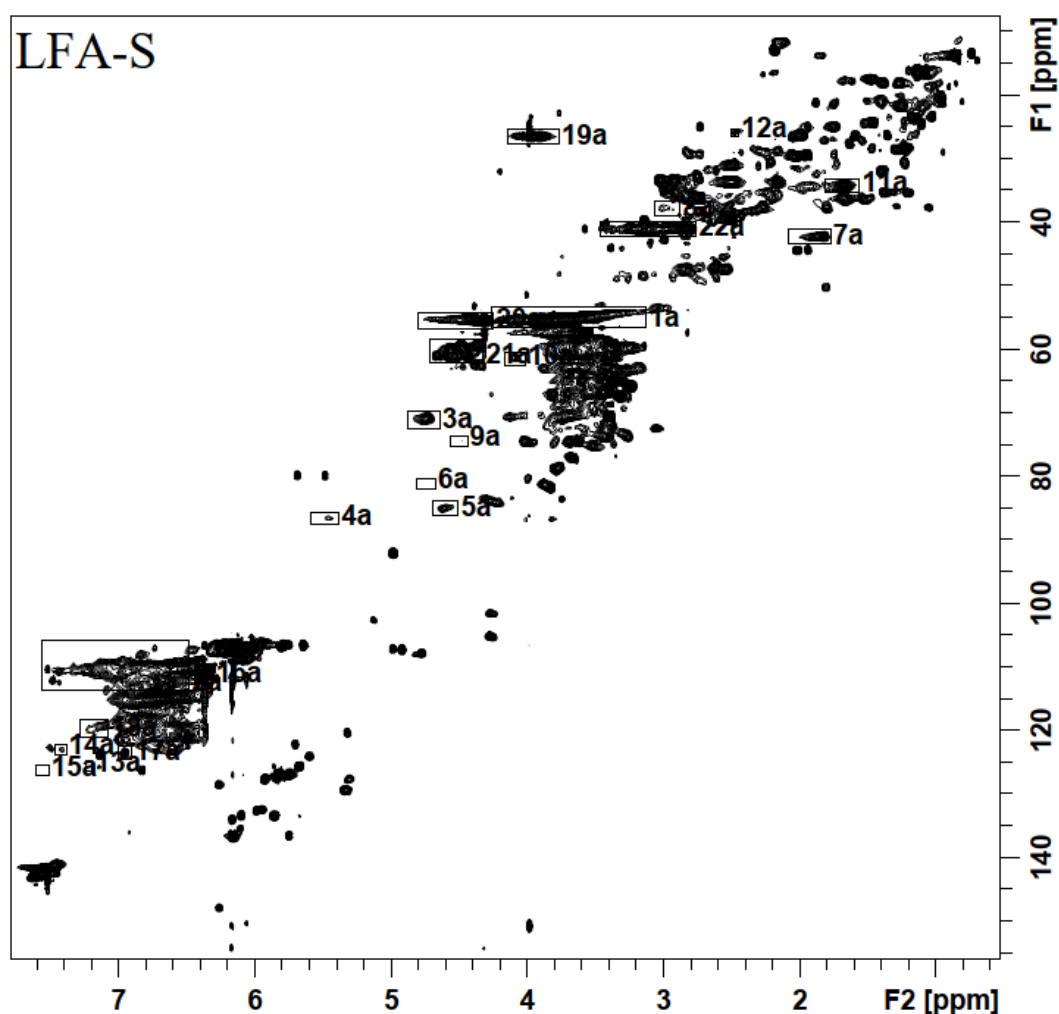
   1024 726 742 2.94957   2.77926

Detailed data set for Figure S12:

 Name = LFA-S   xzc33-L   ExpNo =   2   ProcNo =   1

Baseline = 0   Noise = 0

 # SI_F1 row1 row2 row1(ppm) row2(ppm) abs. Int.   Integral norm. Int. Mode
   SI_F2 col1 col2 col1(ppm) col2(ppm)

Methoxyl(I1) 1024 741 755 56.33739 53.46749 3.4298e+13 3.271e+07   300 a
   1024 604 709   4.24803   3.12895

G2(I2) 1024 472 497 112.91586 107.64885 1.0506e+13 1.0019e+07   91.892 a
   1024 296 384   7.54531   6.60333

Aα(I3) 1024 665 677 72.34975 69.77652 6.9156e+11 6.5953e+05   6.0489 a
   1024 546 567   4.87054   4.64776

Bα(I4) 1024 592 601 87.63552 85.69382 2.2353e+11 2.1317e+05   1.9551 a
   1024 477 499   5.61500   5.37349

Cα(I5) 1024 600 611 86.08216 83.62267 4.1166e+11 3.9259e+05   3.6007 a
   1024 553 583   4.79992   4.47539

C'α(I6) 1024 618 626 82.14528 80.59537 1.487e+11 1.4181e+05   1.3006 a
   1024 552 568   4.80493   4.63447

SRβ(I7) 1024 804 814 43.11005 41.08134 7.1584e+11 6.8268e+05   6.2613 a
   1024 816 834   1.98494   1.78934

Arα(I8) 1024 825 832 38.70461 37.15125 2.5115e+11 2.3951e+05   2.1967 a
   1024 716 729   3.04900   2.91316

AGα(I9) 1024 652 658 75.17170 73.89760 1.0919e+11 1.0413e+05   0.95505 a
   1024 575 586   4.55936   4.43995

Dγ(I10) 1024 712 721 62.36367 60.55312 2.6153e+11 2.4941e+05   2.2875 a
   1024 613 626   4.15770   4.02201

DHCAβ(I11) 1024 843 850 34.99521 33.37225 9.0064e+11 8.5892e+05   7.8777 a
   1024 834 854   1.78934   1.57925

AVβ(I12) 1024 885 890 26.14826 25.11269 6.6369e+10   63295 0.58051 a
   1024 771 776   2.46033   2.41505

V6(I13) 1024   408   415 126.43388 124.90428 1.0777e+11 1.0277e+05   **0.9426 a**

1024 322 330   7.27053   7.18673

VA6(I14) 1024 422 427 123.45518 122.28786 8.1289e+10   77524 **0.71102 a**

1024 305 311   7.45824   7.38785

Bi6(I15) 1024 405 412 126.89611 125.41914 9.0653e+10   86453 **0.79292 a**

1024 291 299   7.59788   7.51748

E-EEα(I16) 1024 475 479 112.34071 111.42860 3.8079e+11 3.6315e+05   **3.3307 a**

1024 400 413   6.43551   6.29877

SB1α(I17) 1024 417 427 124.42645 122.44919 3.2148e+11 3.0659e+05   **2.8119 a**

1024 345 356   7.01968   6.91093

SB5β(I18) 1024 430 444 121.77834 118.70651 6.6448e+11 6.337e+05   **5.8121 a**

1024 320 341   7.29651   7.06912

CH2 in pFA(I19) 1024 878 888 27.48687 25.41445 1.7224e+13 1.6426e+07   **150.66 a**

1024 615 649   4.13779   3.76692

CH2OH in pFA(I20)   1024 740 751 56.50079 54.21022 2.1092e+13 2.0115e+07   **184.49 a**

1024 553 604   4.80005   4.25434

CH2OCH2 in pFA(I21)   1024 714 731 62.06361 58.57322 5.8616e+12 5.5901e+06 **51.27 a**

1024 561 597   4.70998   4.32852

New peak 7(I22) 1024 809 819 41.99383 40.03048 1.1442e+13 1.0912e+07   **100.08 a**

1024 678 743   3.45964   2.76029