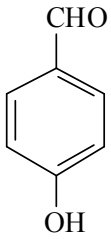
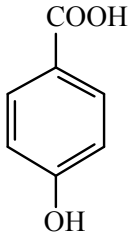
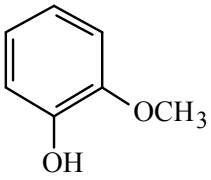
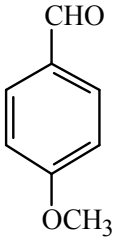
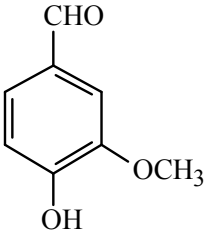
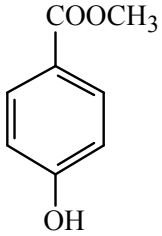
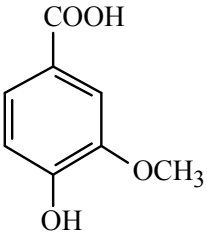
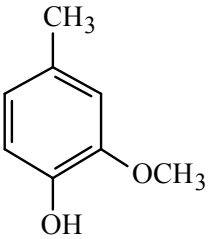
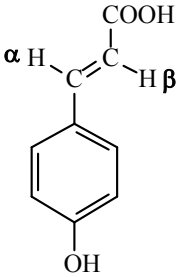
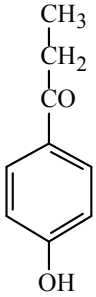
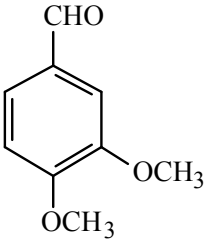
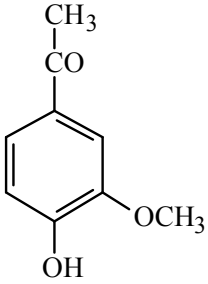
2010-04-13

# Supplementary $^{1}H$ NMR data for lignin models in $CD_3SOCD_3$

| | | |
|---|---|---|
| 1 $C_7H_6O_2$   | 2 $C_7H_6O_3$   | 3 $C_7H_8O_2$   |
| 4 $C_8H_8O_2$   | 5 $C_8H_8O_3$   | 6 $C_8H_8O_3$   |
| 7 $C_8H_8O_4$   | 8 $C_8H_{10}O_2$   | 9 $C_9H_8O_3$   |
| 10 $C_9H_{10}O_2$   | 11 $C_9H_{10}O_3$   | 12 $C_9H_{10}O_3$   |

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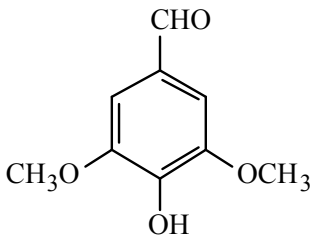
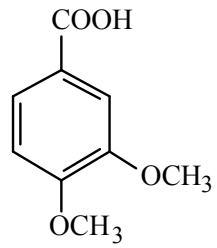
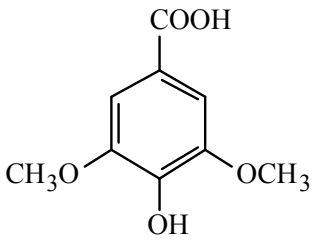
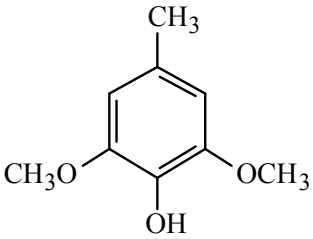
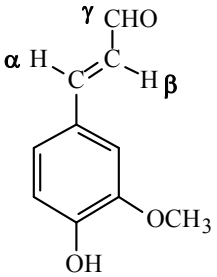
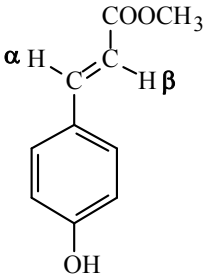
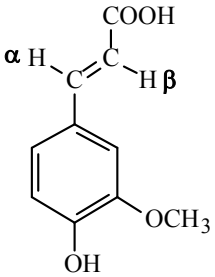
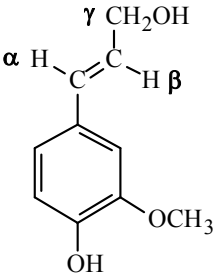
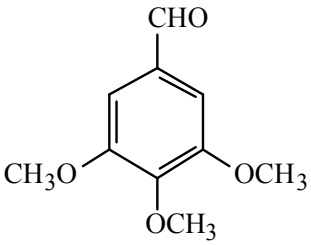
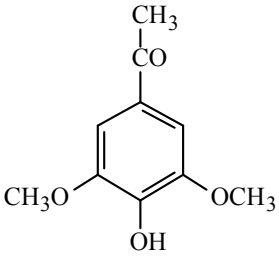
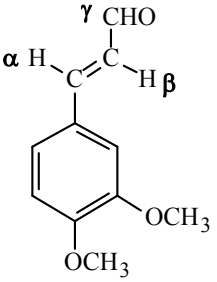
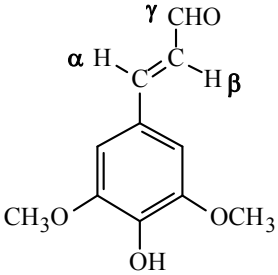
|---|---|---|
| 13 $C_9H_{10}O_4$  | 14 $C_9H_{10}O_4$  | 15 $C_9H_{10}O_5$  |
| 16 $C_9H_{12}O_3$  | 17 $C_{10}H_{10}O_3$  | 18 $C_{10}H_{10}O_3$  |
| 19 $C_{10}H_{10}O_4$  | 20 $C_{10}H_{12}O_3$  | 21 $C_{10}H_{12}O_4$  |
| 22 $C_{10}H_{12}O_4$  | 23 $C_{11}H_{12}O_3$  | 24 $C_{11}H_{12}O_4$  |

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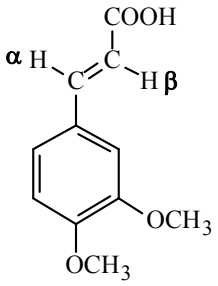
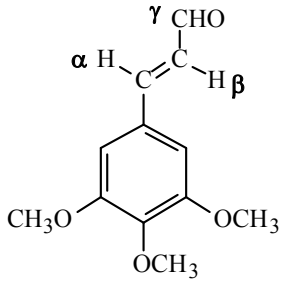
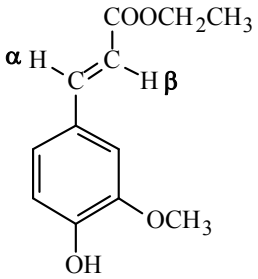
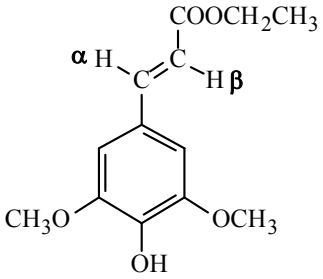
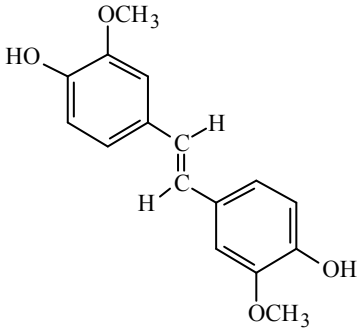
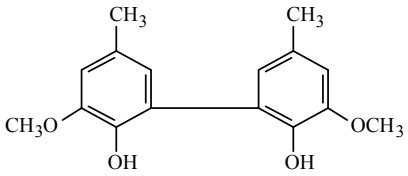
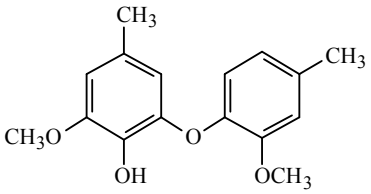
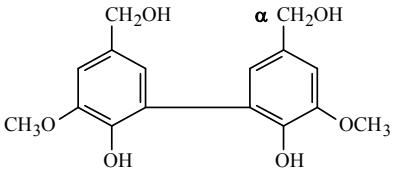
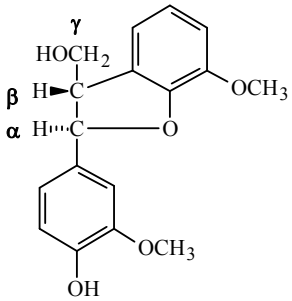
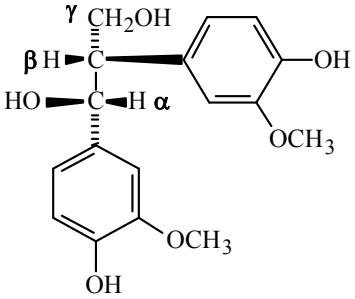
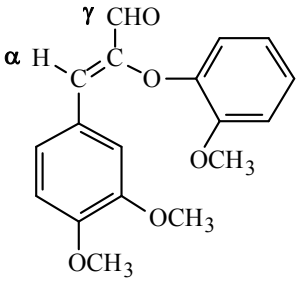
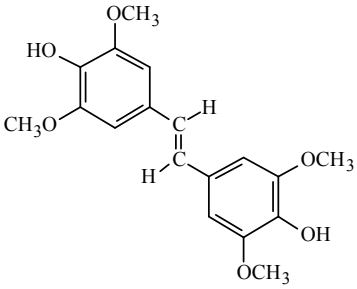
|---|---|---|
| 25 $C_{11}H_{12}O_4$  | 26 $C_{12}H_{14}O_4$  | 27 $C_{12}H_{14}O_4$  |
| 28 $C_{13}H_{16}O_5$  | 29 $C_{16}H_{16}O_4$  | 30 $C_{16}H_{18}O_4$  |
| 31 $C_{16}H_{18}O_4$  | 32 $C_{16}H_{18}O_6$  | 33 $C_{17}H_{18}O_5$  |
| 34 $C_{17}H_{20}O_6$  | 35 $C_{18}H_{18}O_5$  | 36 $C_{18}H_{20}O_6$  |

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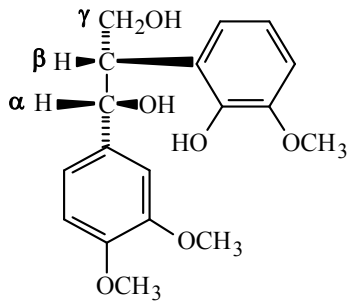
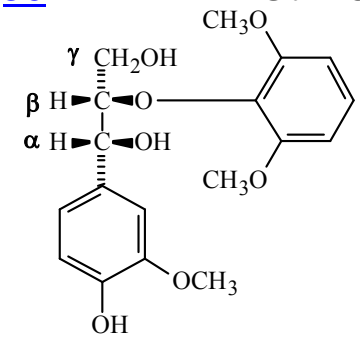
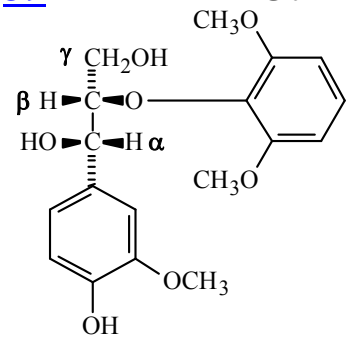
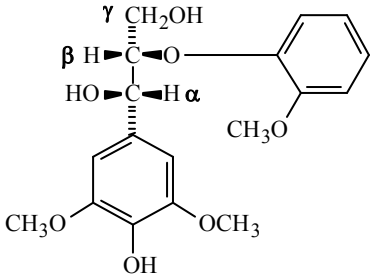
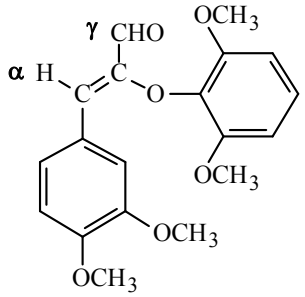
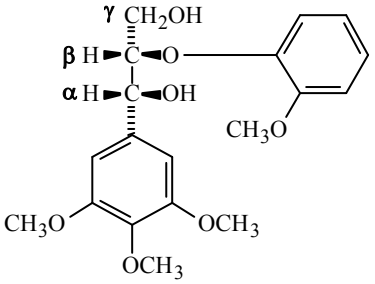
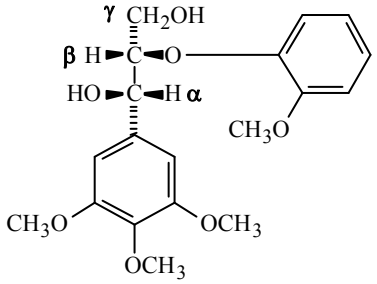
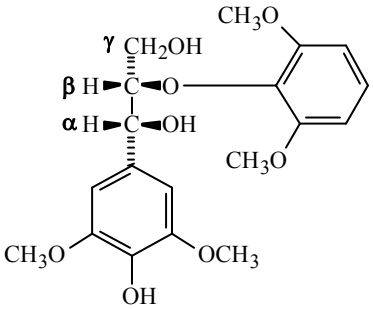
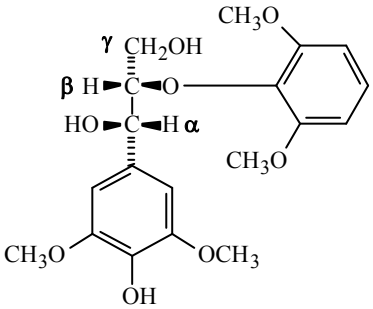
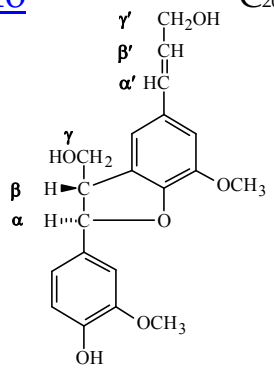
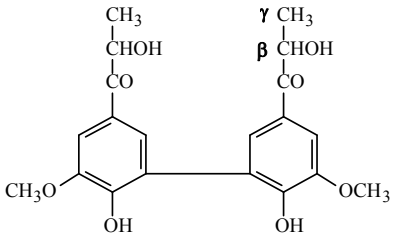
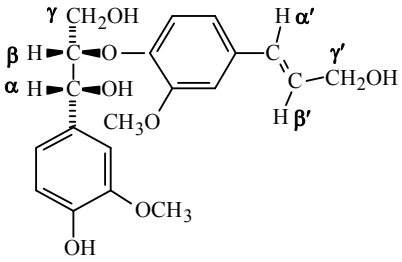
|---|---|---|
| 37 $C_{18}H_{22}O_6$  | 38 $C_{18}H_{22}O_7$  | 39 $C_{18}H_{22}O_7$  |
| 40 $C_{18}H_{22}O_7$  | 41 $C_{19}H_{20}O_6$  | 42 $C_{19}H_{24}O_7$  |
| 43 $C_{19}H_{24}O_7$  | 44 $C_{19}H_{24}O_8$  | 45 $C_{19}H_{24}O_8$  |
| 46 $C_{20}H_{22}O_6$  | 47 $C_{20}H_{22}O_8$  | 48 $C_{20}H_{24}O_7$  |

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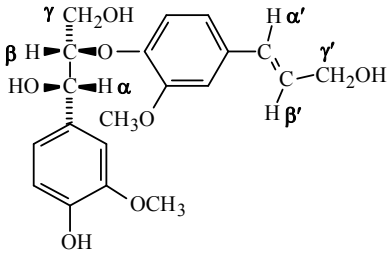
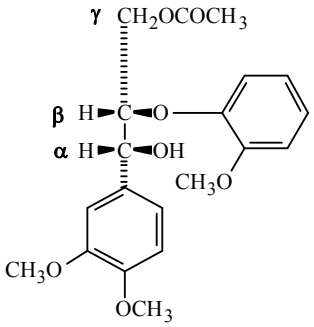
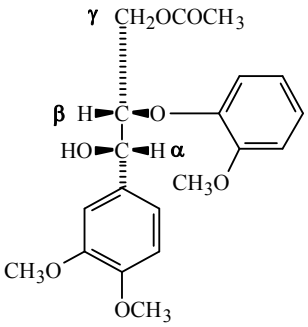
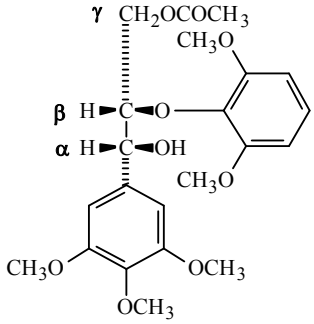
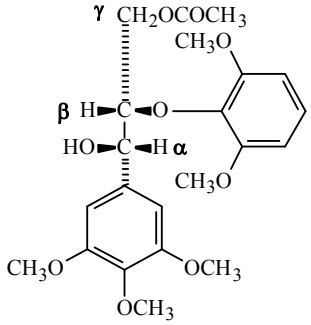
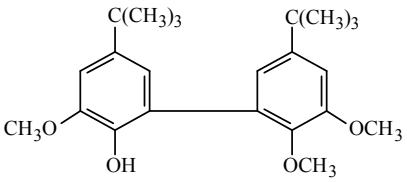
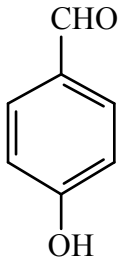
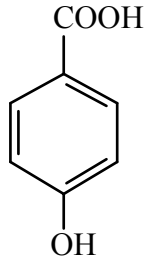
|---|---|---|
| 49 $C_{20}H_{24}O_7$  | 50 $C_{20}H_{24}O_7$  | 51 $C_{20}H_{24}O_7$  |
| 52 $C_{22}H_{28}O_9$  | 53 $C_{22}H_{28}O_9$  | 54 $C_{23}H_{32}O_4$  |

# 1



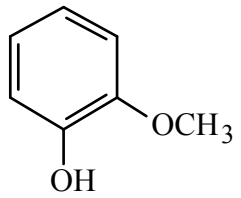

| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 6.94 | 2H, m; H-Ar |
| 7.77 | 2H, m; H-Ar |
| 9.80 | 1H, s; CHO |
| 10.59 | 1H, s; Ar-OH |

2



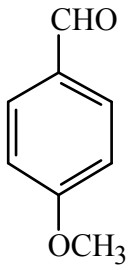

| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 6.83 | 2H, ≈d, *J*=8.4 Hz; H-Ar |
| 7.80 | 2H, ≈d, *J*=8.4 Hz; H-Ar |
| 10.20 | 1H, broad s; Ar-OH |
| 12.39 | 1H, broad s; COOH |

3



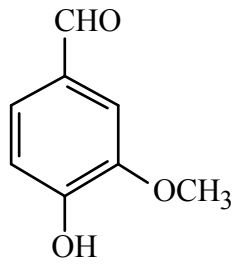

| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 3.75 | 3H, s; $CH_3O$ |
| 6.70-6.94 | 4H, m; H-Ar |
| 8.85 | 1H, s; Ar-OH |

# 4



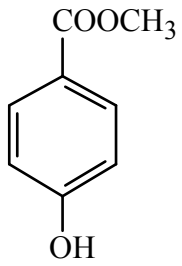

| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 3.87 | 3H, s; $CH_3O$ |
| 7.14 | 2H, m; H-Ar |
| 7.88 | 2H, m; H-Ar |
| 9.88 | 1H, s; CHO |

5



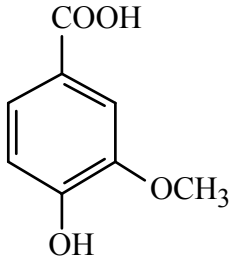

| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 3.85 | 3H, s; $CH_3O$ |
| 6.97 | 1H, d, *J*=8.0 Hz; H-Ar |
| 7.3-7.5 | 2H, m; H-Ar |
| 9.78 | 1H, s; CHO |
| 10.23 | 1H, s; Ar-OH |

# 6



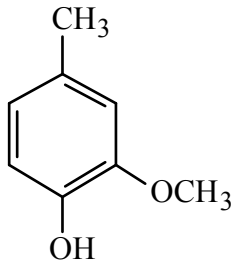

| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 3.79 | 3H, s; $CH_3$ |
| 6.85 | 2H, ≈d, *J*=8.4 Hz; H-Ar |
| 7.81 | 2H, ≈d, *J*=8.8 Hz; H-Ar |
| 10.32 | 1H, broad s; Ar-OH |

7



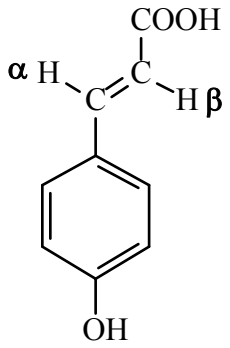

| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 3.81 | 3H, s; $CH_3O$ |
| 6.85 | 1H, d, *J*=8.4 Hz; H-Ar |
| 7.35-7.50 | 2H, m; H-Ar |
| 10.22 | 1H, broad s; Ar-OH |
| 12.42 | 1H, broad s; COOH |

# 8

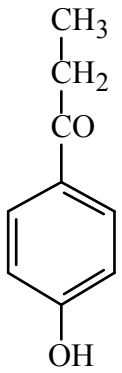



| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 2.19 | 3H, broad s; $CH_3$-Ar |
| 3.73 | 3H, s; $CH_3O$ |
| 6.54 | 1H, ≈dd, *J*=1.2 and 8.0 Hz; H-Ar |
| 6.64 | 1H, d, *J*=8.0 Hz; H-Ar |
| 6.72 | 1H, d, *J*=2.0 Hz; H-Ar |
| 8.59 | 1H, s; Ar-OH |

9

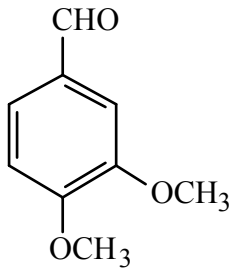



| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 6.28 | 1H, d, *J*=16.0 Hz; $H_\beta$ |
| 6.79 | 2H, ≈d, *J*=8.4 Hz; H-Ar |
| 7.50 | 1H, d, *J*=16.0 Hz; $H_\alpha$ |
| 7.51 | 2H, ≈d, *J*=8.8 Hz; H-Ar |
| 9.94 | 1H, broad s; Ar-OH |
| 12.10 | 1H, broad s; COOH |



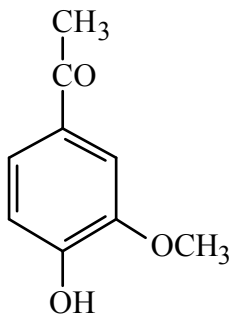

| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 1.06 | 3H, t, *J*=7.6 Hz; $CH_3$ |
| 2.92 | 2H, q, *J*=7.6 Hz; $CH_2$ |
| 6.84 | 2H, ≈d, *J*=8.8 Hz; H-Ar |
| 7.84 | 2H, ≈d, *J*=8.8 Hz; H-Ar |
| 10.28 | 1H, broad s; Ar-OH |

# 11



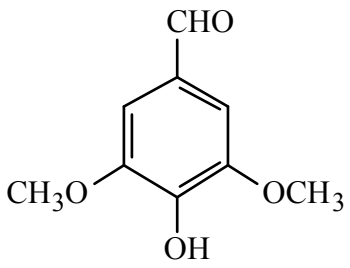

| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 3.84 | 3H, s; $CH_3O$ |
| 3.87 | 3H, s; $CH_3O$ |
| 7.1-7.6 | 3H, m; H-Ar |
| 9.85 | 1H, s; CHO |

# 12



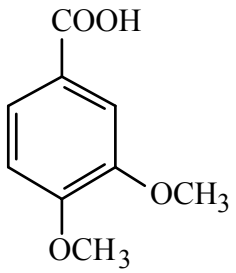

| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 2.49 | 3H, s; $CH_3CO$ |
| 3.83 | 3H, s; $CH_3O$ |
| 6.8-7.6 | 3H, m; H-Ar |
| 9.99 | 1H, broad s; Ar-OH |

13



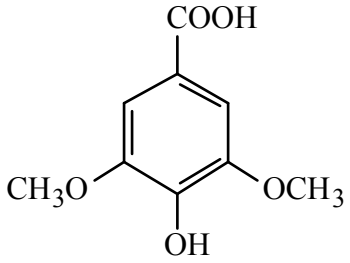

| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 3.85 | 6H, s; $CH_3O$ |
| 7.21 | 2H, s; H-Ar |
| 9.59 | 1H, s; Ar-OH |
| 9.78 | 1H, s; CHO |

# 14

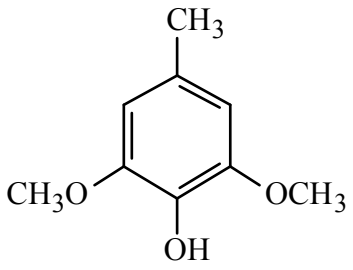



| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 3.80 | 3H, s; $CH_3O$ |
| 3.83 | 3H, s; $CH_3O$ |
| 7.04 | 1H, d, *J*=8.4 Hz; H-Ar |
| 7.44 | 1H, d, *J*=2.0 Hz; H-Ar |
| 7.55-7.60 | 1H, m; H-Ar |
| 12.65 | 1H, broad s; COOH |

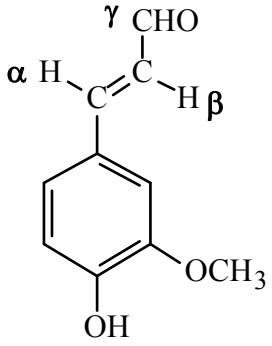
15




| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 3.80 | 6H, s; $CH_3O$ |
| 7.20 | 2H, s; H-Ar |
| 9.18 | 1H, s; Ar-OH |
| 12.58 | 1H, broad s; COOH |

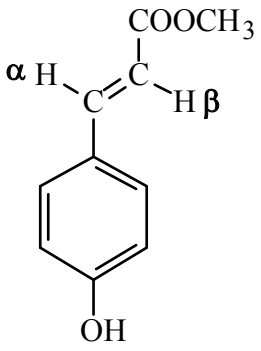



| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 2.21 | 3H, s; $CH_3$-Ar |
| 3.72 | 6H, s; $CH_3O$ |
| 6.41 | 2H, s; H-Ar |
| 7.97 | 1H, s; Ar-OH |

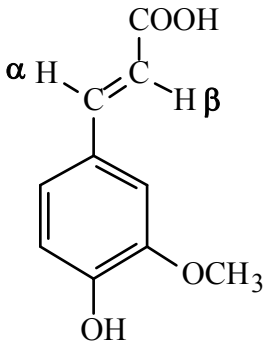



| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 3.83 | 3H, s; $CH_3O$ |
| 6.74 | 1H, dd, *J*=8.0 and 16.0 Hz; $H_\beta$ |
| 6.85 | 1H, d, *J*=8.0 Hz; H-Ar |
| 7.17 | 1H, dd, *J*=2.0 and 8.0 Hz; H-Ar |
| 7.35 | 1H, d, *J*=2.4 Hz; H-Ar |
| 7.60 | 1H, d, *J*=15.6 Hz; $H_\alpha$ |
| 9.59 | 1H, d, *J*=8.0 Hz; $H_\gamma$ |
| 9.79 | 1H, broad s; Ar-OH |

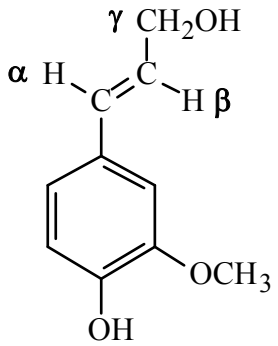
# 18



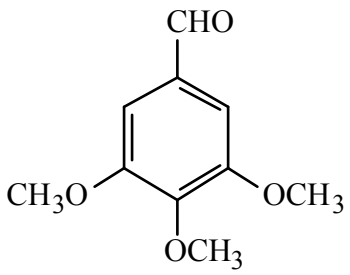

| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 3.69 | 3H, s; $CH_3O$ |
| 6.40 | 1H, d, *J*=16.0 Hz; $H_\beta$ |
| 6.79 | 2H, ≈d, *J*=8.4 Hz; H-Ar |
| 7.55 | 2H, ≈d, *J*=8.4 Hz; H-Ar |
| 7.57 | 1H, d, *J*=16.0 Hz; $H_\alpha$ |
| 10.00 | 1H, s; Ar-OH |




| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 3.82 | 3H, s; $CH_3O$ |
| 6.37 | 1H, d, *J*=16.0 Hz; $H_\beta$ |
| 6.80 | 1H, d, *J*=8.0 Hz; H-Ar |
| 7.09 | 1H, dd, *J*=2.0 and 8.0 Hz; H-Ar |
| 7.28 | 1H, d, *J*=2.0 Hz; H-Ar |
| 7.50 | 1H, d, *J*=16.0 Hz; $H_\alpha$ |
| 9.58 | 1H, broad s; Ar-OH |
| 12.15 | 1H, broad s; COOH |

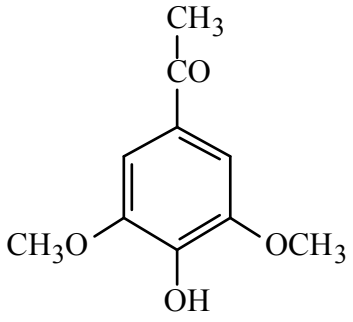



| 400 MHz, $CD_3SOCD_3$, ≈20°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 3.78 | 3H, s; $CH_3O$ |
| 4.08 | 2H, dt, *J*=1.6 and 5.6 Hz; $H_\gamma$ |
| 4.78 | 1H, t, *J*=5.6 Hz; $C_\gamma$-OH |
| 6.18 | 1H, dd, *J*=5.2 and 15.6 Hz; $H_\beta$ |
| 6.42 | 1H, d, *J*=15.6 Hz; $H_\alpha$ |
| 6.70 | 1H, d, *J*=8.1 Hz; H-Ar |
| 6.79 | 1H, dd, *J*=1.8 and 8.1 Hz; H-Ar |
| 7.00 | 1H, d, *J*=1.8 Hz; H-Ar |
| 9.00 | 1H, s; Ar-OH |



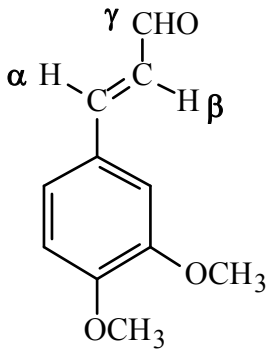

| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 3.88 | 9H, s; $CH_3O$ |
| 7.26 | 2H, s; H-Ar |
| 9.90 | 1H, s; CHO |

22



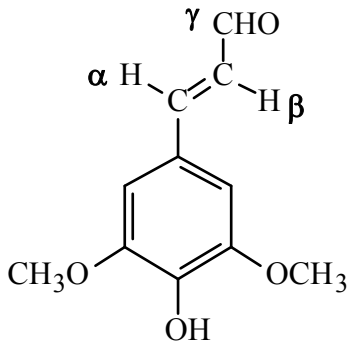

| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 2.53 | 3H, s; $CH_3CO$ |
| 3.83 | 6H, s; $CH_3O$ |
| 7.23 | 2H, s; H-Ar |
| 9.35 | 1H, broad s; Ar-OH |

23

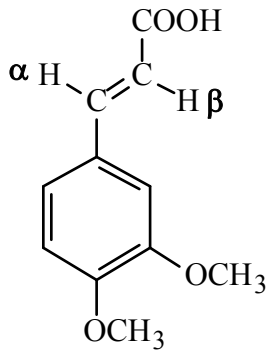



| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 3.83 | 6H, s; $CH_3O$ |
| 6.82 | 1H, dd, *J*=8.0 and 16.0 Hz; $H_\beta$ |
| 7.02-7.42 | 3H, m; H-Ar |
| 7.64 | 1H, d, *J*=15.6 Hz; $H_\alpha$ |
| 9.63 | 1H, d, *J*=8.0 Hz; $H_\gamma$ |

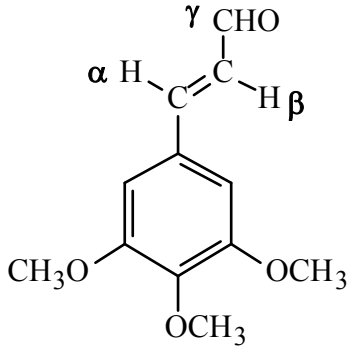
24



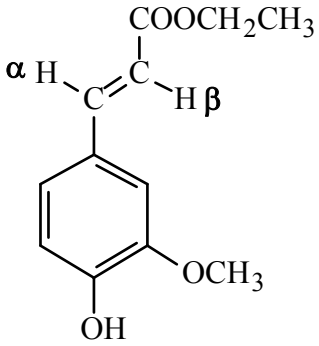

| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 3.82 | 6H, s; $CH_3O$ |
| 6.80 | 1H, dd, *J*=8.0 and 16.0 Hz; $H_\beta$ |
| 7.06 | 2H, s; H-Ar |
| 7.59 | 1H, d, *J*=16.0 Hz; $H_\alpha$ |
| 9.15 | 1H, broad s; Ar-OH |
| 9.60 | 1H, d, *J*=8.0 Hz; $H_\gamma$ |



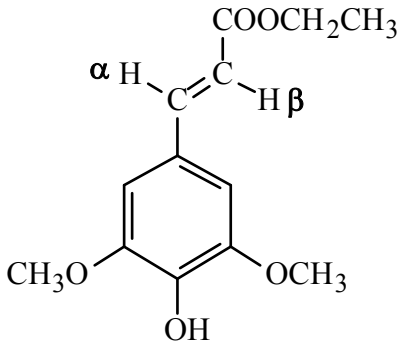

| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 3.79 | 3H, s; $CH_3O$ |
| 3.81 | 3H, s; $CH_3O$ |
| 6.44 | 1H, d, *J*=16.0 Hz; $H_\beta$ |
| 6.98 | 1H, d, *J*=8.4 Hz; H-Ar |
| 7.20 | 1H, dd, *J*=1.6 and 8.0 Hz; H-Ar |
| 7.31 | 1H, d, *J*=1.6 Hz; H-Ar |
| 7.52 | 1H, d, *J*=15.6 Hz; $H_\alpha$ |
| 12.19 | 1H, broad s; COOH |



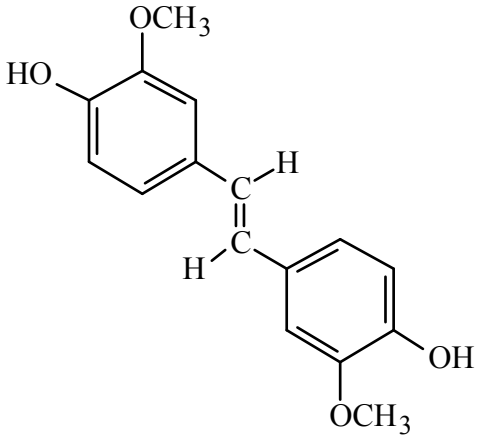

| 400 MHz, $CD_3SOCD_3$, ≈21°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 3.73 | 3H, s; $CH_3O$ |
| 3.84 | 6H, s; $CH_3O$ |
| 6.92 | 1H, dd, *J*=7.6 and 16.0 Hz; $H_\beta$ |
| 7.10 | 2H, s; H-Ar |
| 7.64 | 1H, d, *J*=16.0 Hz; $H_\alpha$ |
| 9.66 | 1H, d, *J*=7.6 Hz; $H_\gamma$ |



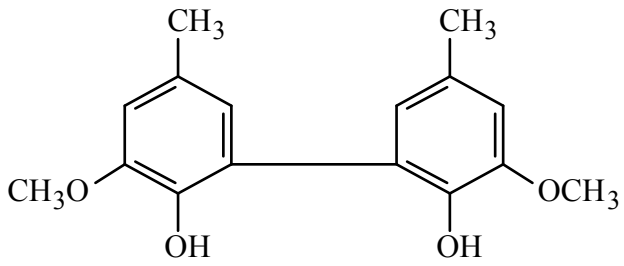

| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 1.26 | 3H, t, *J*=7.2 Hz; $CH_3$-C |
| 3.83 | 3H, s; $CH_3O$ |
| 4.17 | 2H, q, *J*=7.2 Hz; $CH_2$ |
| 6.48 | 1H, d, *J*=16.0 Hz; $H_\beta$ |
| 6.81 | 1H, d, *J*=8.0 Hz; H-Ar |
| 7.12 | 1H, dd, *J*=2.0 and 8.0 Hz; H-Ar |
| 7.33 | 1H, d, *J*=1.6 Hz; H-Ar |
| 7.56 | 1H, d, *J*=16.4 Hz; $H_\alpha$ |
| 9.63 | 1H, broad s; Ar-OH |




| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 1.25 | 3H, t, *J*=7.2 Hz; $CH_3$-C |
| 3.78 | 6H, s; $CH_3O$ |
| 4.17 | 2H, q, *J*=7.2 Hz; $CH_2$ |
| 6.52 | 1H, d, *J*=16.0 Hz; $H_\beta$ |
| 7.03 | 2H, s; H-Ar |
| 7.55 | 1H, d, *J*=16.0 Hz; $H_\alpha$ |
| 8.92 | 1H, broad s; Ar-OH |




| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 3.82 | 6H, s; $CH_3O$ |
| 6.74 | 2H, d, *J*=8.0 Hz; H-Ar |
| 6.93 | 2H, dd, *J*=1.6 and 8.0 Hz; H-Ar |
| 6.95 | 2H, s; vinyl H |
| 7.14 | 2H, d, *J*=1.6 Hz; H-Ar |
| 9.02 | 2H, s; Ar-OH |




| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 2.22 | 6H, s; $CH_3$-C |
| 3.79 | 6H, s; $CH_3O$ |
| 6.5-6.8 | 4H, m; H-Ar |
| 8.06 | 2H, s; Ar-OH |

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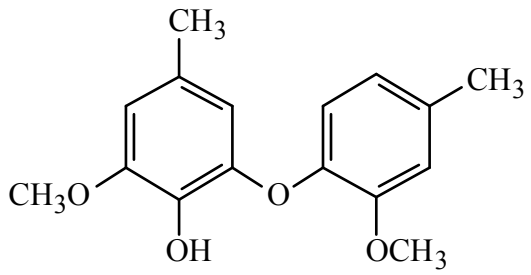
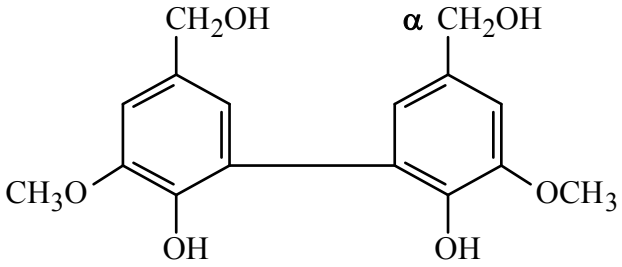
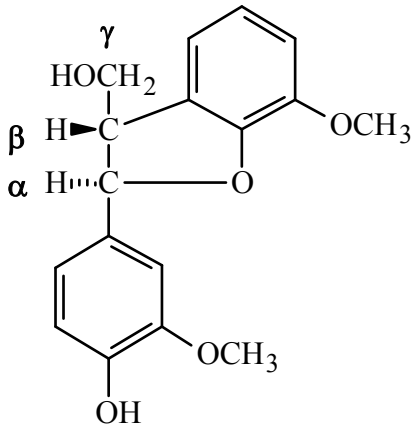


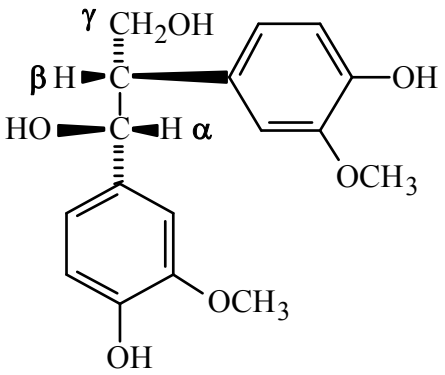

| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 2.12 | 3H, s; $CH_3$-Ar |
| 2.28 | 3H, s; $CH_3$-Ar |
| 3.75 | 3H, s; $CH_3O$ |
| 3.77 | 3H, s; $CH_3O$ |
| 6-7 | 5H, m; H-Ar |
| 8.35 | 1H, s; Ar-OH |



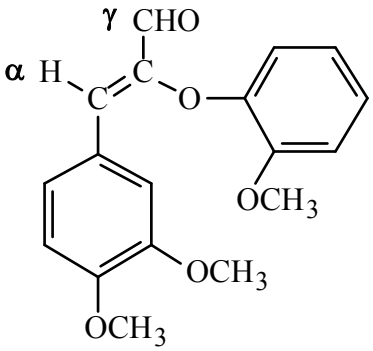

| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 3.81 | 6H, s; $CH_3O$ |
| 4.41 | 4H, d, *J*=5.6 Hz; $H_\alpha$ |
| 5.00 | 2H, t, *J*=5.6 Hz; $C_\alpha$-OH |
| 6.67 | 2H, d, *J*=1.2 Hz; H-Ar |
| 6.88 | 2H, d, *J*=1.6 Hz; H-Ar |
| 8.21 | 2H, s; Ar-OH |



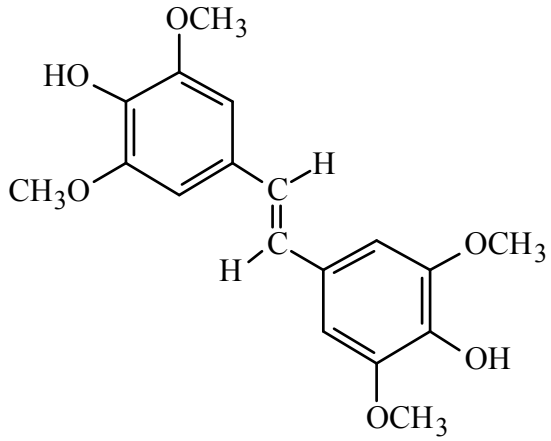

| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 3.45 | 1H, m; $H_\beta$ |
| 3.61 | 1H, m; $H_\gamma$ |
| 3.70 | 1H, m; $H_\gamma$ |
| 3.74 | 3H, s; $CH_3O$ |
| 3.77 | 3H, s; $CH_3O$ |
| 4.99 | 1H, ≈t, *J*=5.4 Hz; $C_\gamma$-OH |
| 5.44 | 1H, d, *J*=6.8 Hz; $H_\alpha$ |
| 6.72-6.94 | 6H, m; H-Ar |
| 8.99 | 1H, s; Ar-OH |



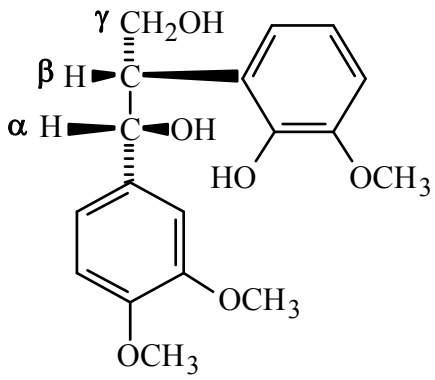

| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 2.72 | 1H, m; $H_\beta$ |
| 3.46 | 1H, m; $H_\gamma$ |
| 3.60 | 3H, s; $CH_3O$ |
| 3.64 | 3H, s; $CH_3O$ |
| 3.65 | 1H, m; $H_\gamma$ |
| 4.35 | 1H, ≈t, *J*=5.0 Hz; $C_\gamma$-OH |
| 4.80 | 1H, ≈t, *J*=4.8 Hz; $H_\alpha$ |
| 4.86 | 1H, d, *J*=4.4 Hz; $C_\alpha$-OH |
| 6.48 | 1H, dd, *J*=2.0 and 8.0 Hz; H-Ar |
| 6.54 | 1H, dd, *J*=2.0 and 8.0 Hz; H-Ar |
| 6.55-6.64 | 4H, m; H-Ar |
| 8.53 | 1H, s; Ar-OH |
| 8.62 | 1H, s; Ar-OH |



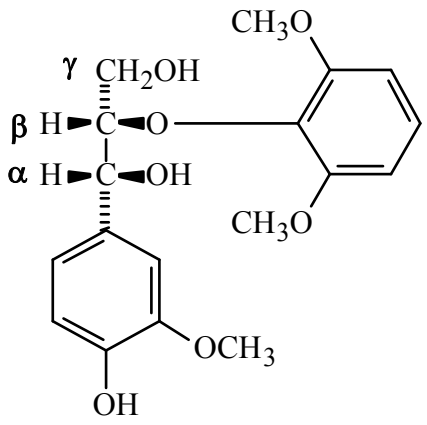

| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 3.64 | 3H, s; $CH_3O$ |
| 3.78 | 3H, s; $CH_3O$ |
| 3.85 | 3H, s; $CH_3O$ |
| 6.67 | 1H, dd, *J*=1.4 and 8.2 Hz; H-Ar |
| 6.76 | 1H, ≈dt, *J*=1.6 and 8.0 Hz; H-Ar |
| 6.97 | 1H, ≈dt, *J*=1.6 and 8.0 Hz; H-Ar |
| 7.04 | 1H, d, *J*=8.4 Hz; H-Ar |
| 7.09 | 1H, dd, *J*=2.0 and 8.4 Hz; H-Ar |
| 7.38 | 1H, dd, *J*=2.0 and 8.4 Hz; H-Ar |
| 7.41 | 1H, s; $H_\alpha$ |
| 7.45 | 1H, d, *J*=2.0 Hz; H-Ar |
| 9.47 | 1H, s; $H_\gamma$ |



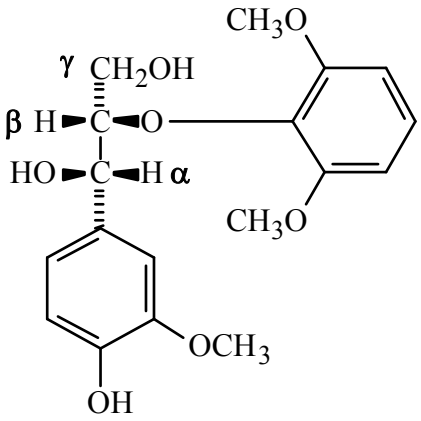

| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 3.81 | 6H, s; $CH_3O$ |
| 6.83 | 4H, s; H-Ar |
| 6.99 | 2H, s; vinyl H |
| 8.40 | 2H, s; Ar-OH |



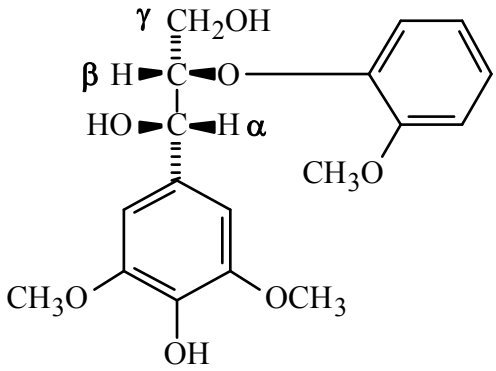

| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 3.40 | 1H, m; $H_\beta$ |
| 3.61 | 3H, s; $CH_3O$ |
| 3.65 | 3H, s; $CH_3O$ |
| 3.71 | 3H, s; $CH_3O$ |
| 3.81 | 2H, t, *J*=5.4 Hz; $H_\gamma$ |
| 4.58 | 1H, ≈t, *J*=5.2 Hz; $C_\gamma$-OH |
| 4.90 | 1H, dd, *J*=4.2 and 8.0 Hz; $H_\alpha$ |
| 5.37 | 1H, d, *J*=4.2 Hz; $C_\alpha$-OH |
| 6.53-6.77 | 6H, m; H-Ar |
| 8.42 | 1H, s; Ar-OH |



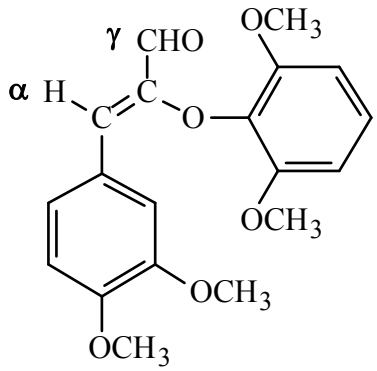

| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 3.40 | 1H, m; $H_\gamma$ |
| ≈3.71 | 1H, m; $H_\gamma$ |
| 3.75 | 6H, s; $CH_3O$ |
| 3.78 | 3H, s; $CH_3O$ |
| 3.99 | 1H, ≈t, *J*=6.0 Hz; $C_\gamma$-OH |
| 4.12 | 1H, m; $H_\beta$ |
| 4.80 | 1H, ≈t, *J*=4.8 Hz; $H_\alpha$ |
| 5.08 | 1H, d, *J*=4.8 Hz; $C_\alpha$-OH |
| 6.66 | 2H, d, *J*=8.4 Hz; H-Ar |
| 6.67-6.74 | 2H, m; H-Ar |
| 6.93 | 1H, d, *J*=1.8 Hz; H-Ar |
| 6.97 | 1H, t, *J*=8.4 Hz; H-Ar |
| 8.73 | 1H, s; Ar-OH |



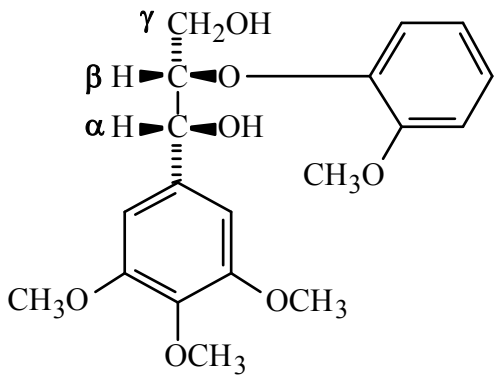

| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 3.21 | 1H, m; $H_\gamma$ |
| 3.63 | 1H, m; $H_\gamma$ |
| 3.73 | 3H, s; $CH_3O$ |
| 3.74 | 6H, s; $CH_3O$ |
| 4.00 | 1H, m; $H_\beta$ |
| 4.24 | 1H, ≈t, *J*=5.6 Hz; $C_\gamma$-OH |
| 4.86 | 1H, m; $H_\alpha$ |
| 4.86 | 1H, m; $C_\alpha$-OH |
| 6.66 | 2H, d, *J*=8.4 Hz; H-Ar |
| 6.69 | 1H, d, *J*=8.0 Hz; H-Ar |
| 6.80 | 1H, dd, *J*=1.8 and 8.0 Hz; H-Ar |
| 6.97 | 1H, t, *J*=8.4 Hz; H-Ar |
| 6.98 | 1H, d, *J*=1.8 Hz; H-Ar |
| 8.72 | 1H, s; Ar-OH |



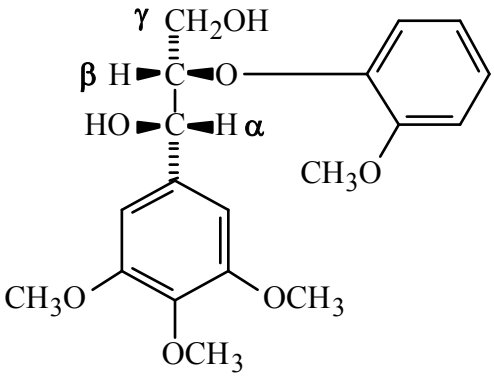

| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 3.26 | 1H, m; $H_\gamma$ |
| 3.59 | 1H, m; $H_\gamma$ |
| 3.71 | 6H, s; $CH_3O$ |
| 3.76 | 3H, s; $CH_3O$ |
| 4.29 | 1H, m; $H_\beta$ |
| 4.63 | 1H, ≈t, *J*=5.6 Hz; $C_\gamma$-OH |
| 4.72 | 1H, ≈t, *J*=4.4 Hz; $H_\alpha$ |
| 5.29 | 1H, d, *J*=4.4 Hz; $C_\alpha$-OH |
| 6.66 | 2H, s; H-Ar |
| 6.80-6.90 | 2H, m; H-Ar |
| 6.96 | 1H, dd, *J*=1.8 and 7.6 Hz; H-Ar |
| 7.03 | 1H, dd, *J*=2.2 and 8.0 Hz; H-Ar |
| 8.12 | 1H, s; Ar-OH |



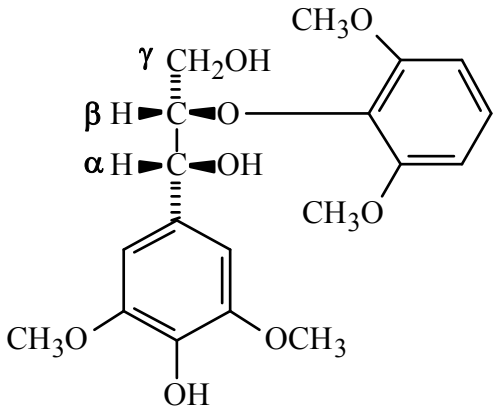

| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 3.70 | 6H, s; $CH_3O$ |
| 3.73 | 3H, s; $CH_3O$ |
| 3.80 | 3H, s; $CH_3O$ |
| 6.68 | 2H, d, *J*=8.4 Hz; H-Ar |
| 6.77 | 1H, s; $H_\alpha$ |
| 7.00 | 1H, t, *J*=8.4 Hz; H-Ar |
| 7.05 | 1H, d, *J*=8.4 Hz; H-Ar |
| 7.44-7.52 | 2H, m; H-Ar |
| 9.23 | 1H, s; $H_\gamma$ |



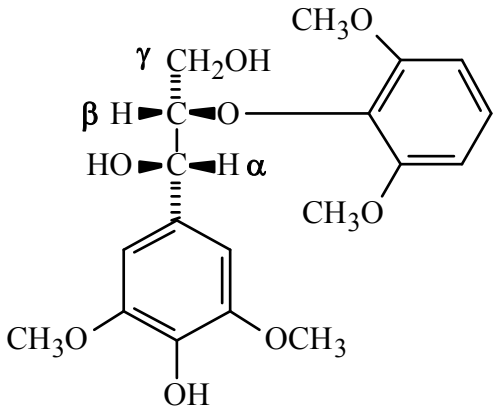

| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| ≈3.64 | 2H, m; $H_\gamma$ |
| 3.61 | 3H, s; $CH_3O$ |
| 3.69 | 3H, s; $CH_3O$ |
| 3.73 | 6H, s; $CH_3O$ |
| 4.32 | 1H, m; $H_\beta$ |
| 4.64 | 1H, d, *J*=5.8 Hz; $C_\gamma$-OH |
| 4.74 | 1H, ≈t, *J*=5.0 Hz; $H_\alpha$ |
| 5.44 | 1H, d, *J*=4.8 Hz; $C_\alpha$-OH |
| 6.71 | 2H, s; H-Ar |
| 6.76-6.99 | 4H, m; H-Ar |



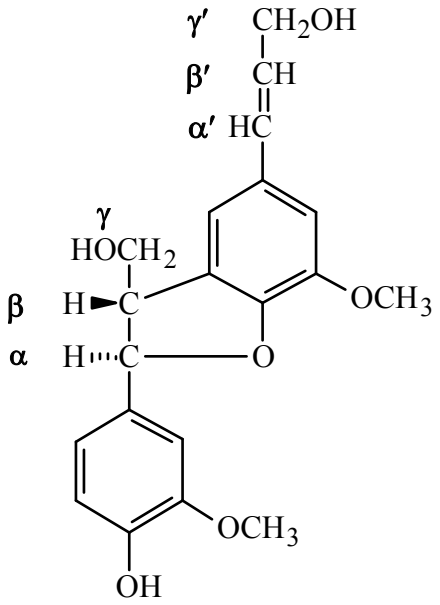

| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 3.27 | 1H, m; $H_\gamma$ |
| ≈3.62 | 1H, m; $H_\gamma$ |
| 3.62 | 3H, s; $CH_3O$ |
| 3.74 | 6H, s; $CH_3O$ |
| 3.75 | 3H, s; $CH_3O$ |
| 4.33 | 1H, m; $H_\beta$ |
| 4.67 | 1H, d, *J*=5.4 Hz; $C_\gamma$-OH |
| 4.77 | 1H, ≈t, *J*=4.4 Hz; $H_\alpha$ |
| 5.42 | 1H, d, *J*=5.2 Hz; $C_\alpha$-OH |
| 6.72 | 2H, s; H-Ar |
| 6.80-7.04 | 4H, m; H-Ar |



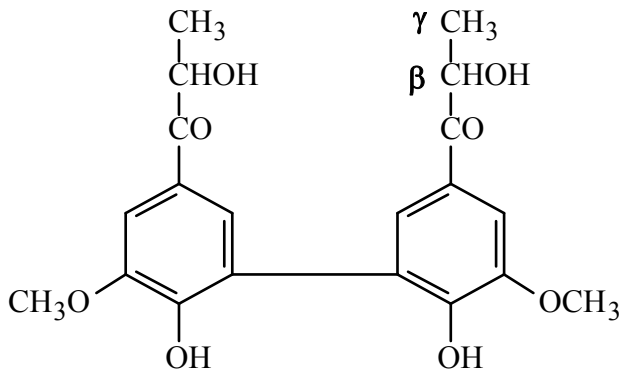

| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 3.41 | 1H, m; $H_\gamma$ |
| 3.71 | 1H, m; $H_\gamma$ |
| 3.73 | 6H, s; $CH_3O$ |
| 3.75 | 6H, s; $CH_3O$ |
| 3.99 | 1H, ≈t, *J*=6.0 Hz; $C_\gamma$-OH |
| 4.14 | 1H, m; $H_\beta$ |
| 4.82 | 1H, ≈t, *J*=4.8 Hz; $H_\alpha$ |
| 5.12 | 1H, d, *J*=5.2 Hz; $C_\alpha$-OH |
| 6.61 | 2H, s; H-Ar |
| 6.67 | 2H, d, *J*=8.2 Hz; H-Ar |
| 6.97 | 1H, t, *J*=8.2 Hz; H-Ar |
| 8.12 | 1H, s; Ar-OH |



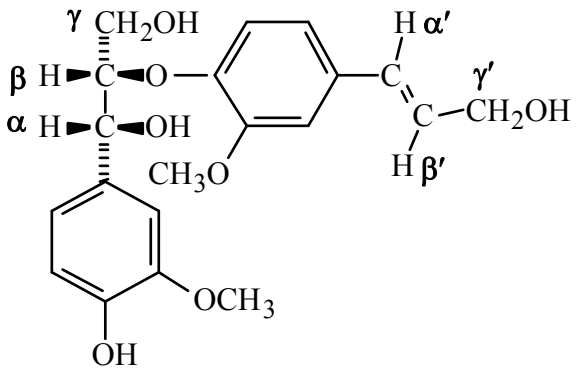

| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 3.24 | 1H, m; $H_\gamma$ |
| 3.64 | 1H, m; $H_\gamma$ |
| 3.72 | 6H, s; $CH_3O$ |
| 3.74 | 6H, s; $CH_3O$ |
| 4.05 | 1H, m; $H_\beta$ |
| 4.28 | 1H, ≈t, *J*=5.6 Hz; $C_\gamma$-OH |
| 4.85 | 1H, ≈t, *J*=5.0 Hz; $H_\alpha$ |
| 4.90 | 1H, d, *J*=5.2 Hz; $C_\alpha$-OH |
| 6.66 | 2H, d, *J*=8.2 Hz; H-Ar |
| 6.69 | 2H, s; H-Ar |
| 6.97 | 1H, t, *J*=8.2 Hz; H-Ar |
| 8.11 | 1H, s; Ar-OH |



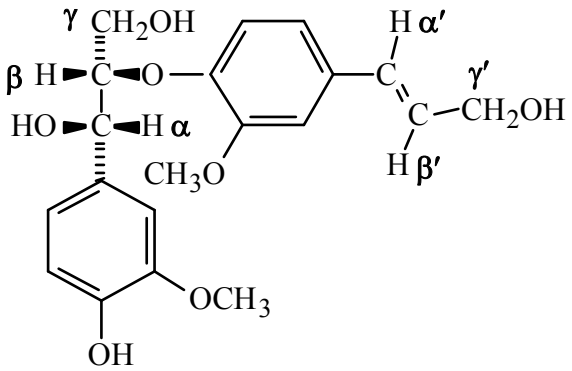

| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 3.44 | 1H, m; $H_\beta$ |
| 3.62 | 1H, m; $H_\gamma$ |
| 3.70 | 1H, m; $H_\gamma$ |
| 3.74 | 3H, s; $CH_3O$ |
| 3.79 | 3H, s; $CH_3O$ |
| 4.08 | 2H, dt, *J*=1.2 and 5.4 Hz; $H_{\gamma'}$ |
| 4.76 | 1H, ≈t, *J*=5.4 Hz; $C_{\gamma'}$-OH |
| 5.01 | 1H, ≈t, *J*=5.2 Hz; $C_\gamma$-OH |
| 5.45 | 1H, d, *J*=6.4 Hz; $H_\alpha$ |
| 6.21 | 1H, td, *J*=5.4 and 15.6 Hz; $H_{\beta'}$ |
| 6.46 | 1H, ≈t, *J*=15.6 Hz; $H_{\alpha'}$ |
| 6.70-6.98 | 5H, m; H-Ar |
| 9.00 | 1H, s; Ar-OH |



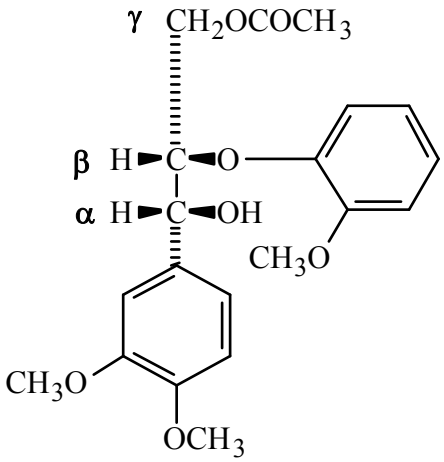

| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 1.29 | 6H, d, *J*=6.4 Hz; $H_\gamma$ |
| 3.91 | 6H, s; $CH_3O$ |
| 5.03 | 2H, m; $H_\beta$ |
| 5.12 | 2H, d, *J*=6.4 Hz; $C_\beta$-OH |
| 7.52 | 2H, d, *J*=2.2 Hz; H-Ar |
| 7.54 | 2H, d, *J*=2.2 Hz; H-Ar |
| 9.59 | 2H, broad s; Ar-OH |



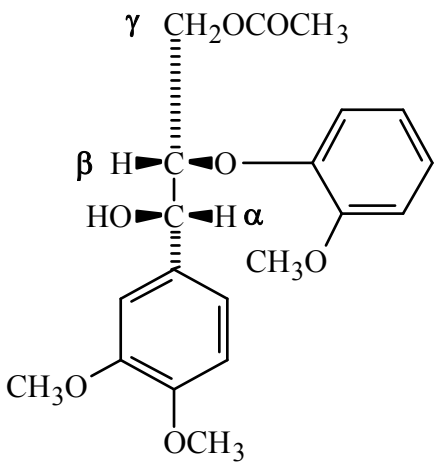

| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 3.59 | 2H, m; $H_\gamma$ |
| 3.73 | 3H, s; $CH_3O$ |
| 3.73 | 3H, s; $CH_3O$ |
| 4.08 | 2H, ≈dt, *J*=0.2 and 5.2 Hz; $H_{\gamma'}$ |
| 4.30 | 1H, m; $H_\beta$ |
| 4.60 | 1H, ≈t, *J*=5.6 Hz; $C_\gamma$-OH |
| 4.70 | 1H, ≈t, *J*=5.0 Hz; $H_\alpha$ |
| 4.79 | 1H, ≈t, *J*=5.6 Hz; $C_{\gamma'}$-OH |
| 5.30 | 1H, d, *J*=4.4 Hz; $C_\alpha$-OH |
| 6.22 | 1H, dt, *J*=15.9 and 5.2 Hz; $H_{\beta'}$ |
| 6.43 | 1H, broad d, *J*=15.9 Hz; $H_{\alpha'}$ |
| 6.67 | 1H, d, *J*=7.6 Hz; H-Ar |
| 6.77 | 1H, dd, *J*=1.8 and 8.2 Hz; H-Ar |
| 6.84 | 1H, dd, *J*=2.0 and 8.4 Hz; H-Ar |
| 6.92 | 1H, d, *J*=8.4 Hz; H-Ar |
| ≈6.99 | 2H, m; H-Ar |
| 8.74 | 1H, s; Ar-OH |



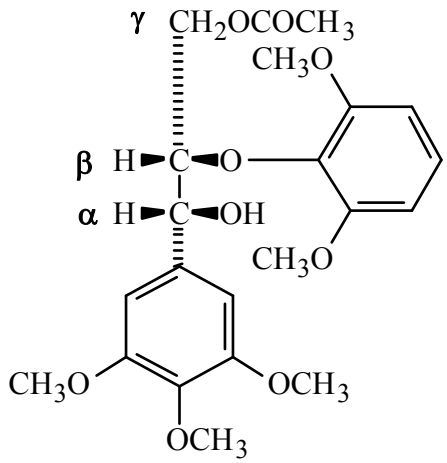

| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 3.25 | 1H, m; $H_\gamma$ |
| 3.58 | 1H, m; $H_\gamma$ |
| 3.72 | 3H, s; $CH_3O$ |
| 3.79 | 3H, s; $CH_3O$ |
| 4.09 | 2H, ≈dt, *J*=1,2 and 5.2 Hz; $H_{\gamma'}$ |
| 4.26 | 1H, m; $H_\beta$ |
| 4.62 | 1H, ≈t, *J*=5.4 Hz; $C_\gamma$-OH |
| 4.71 | 1H, ≈t, *J*=4.6 Hz; $H_\alpha$ |
| 4.79 | 1H, ≈t, *J*=5.4 Hz; $C_{\gamma'}$-OH |
| 5.24 | 1H, d, *J*=4.4 Hz; $C_\alpha$-OH |
| 6.24 | 1H, dt, *J*=15.9 and 5.2 Hz; $H_{\beta'}$ |
| 6.45 | 1H, broad d, *J*=15.9 Hz; $H_{\alpha'}$ |
| 6.68 | 1H, d, *J*=8.2 Hz; H-Ar |
| 6.76 | 1H, dd, *J*=2.0 and 8.2 Hz; H-Ar |
| 6.86 | 1H, dd, *J*=2.0 and 8.4 Hz; H-Ar |
| 6.94-6.98 | 2H, m; H-Ar |
| 7.04 | 1H, d, J=2.0 Hz; H-Ar |
| 8.75 | 1H, s; Ar-OH |



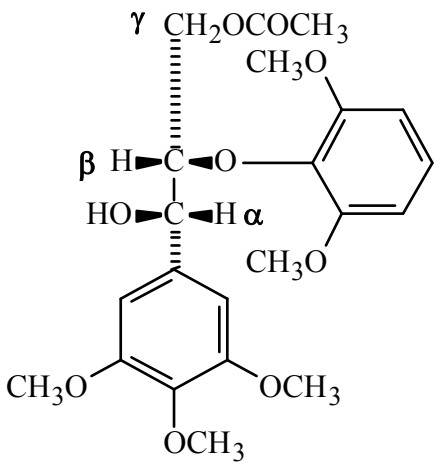

| 400 MHz, $CD_3SOCD_3$, 20°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 1.89 | 3H, s; $CH_3CO$ |
| 3.71 | 3H, s; $CH_3O$ |
| 3.71 | 3H, s; $CH_3O$ |
| 3.72 | 3H, s; $CH_3O$ |
| 4.22 | 1H, dd, *J*=3.3 and 11.9 Hz; $H_\gamma$ |
| 4.27 | 1H, dd, *J*=5.9 and 11.9 Hz; $H_\gamma$ |
| 4.53 | 1H, ddd, *J*=3.3, 5.9 and 5.9 Hz; $H_\beta$ |
| 4.78 | 1H, dd, *J*=4.6 and 5.9 Hz; $H_\alpha$ |
| 5.64 | 1H, d, *J*=4.6 Hz; OH |
| 6.77-7.03 | 7H, m; H-Ar |



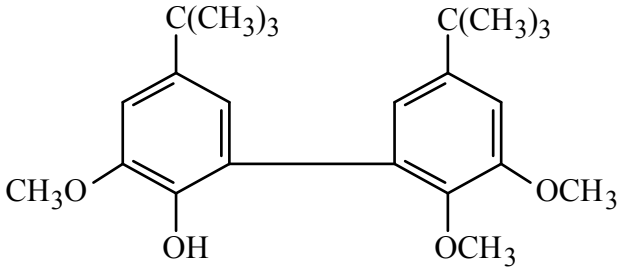

| 400 MHz, $CD_3SOCD_3$, 20°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 1.91 | 3H, s; $CH_3CO$ |
| 3.72 | 3H, s; $CH_3O$ |
| 3.73 | 3H, s; $CH_3O$ |
| 3.76 | 3H, s; $CH_3O$ |
| 3.82 | 1H, dd, *J*=7.1 and 11.9 Hz; $H_\gamma$ |
| 4.11 | 1H, dd, *J*=3.2 and 11.9 Hz; $H_\gamma$ |
| 4.56 | 1H, ddd, *J*=3.2, 4.9 and 7.1 Hz; $H_\beta$ |
| 4.80 | 1H, dd, *J*=4.6 and 4.9 Hz; $H_\alpha$ |
| 5.62 | 1H, d, *J*=4.6 Hz; OH |
| 6.82-7.06 | 7H, m; H-Ar |




| 400 MHz, $CD_3SOCD_3$, 20°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 1.77 | 3H, s; $CH_3CO$ |
| 3.63 | 3H, s; $CH_3O$ |
| 3.73 | 6H, s; $CH_3O$ |
| 3.76 | 6H, s; $CH_3O$ |
| 4.05 | 1H, dd, *J*=2.5 and 11.6 Hz; $H_\gamma$ |
| 4.30 | 1H, dd, *J*=6.4 and 11.6 Hz; $H_\gamma$ |
| 4.36 | 1H, ddd, *J*=2.5, 4.6 and 6.4 Hz; $H_\beta$ |
| 4.93 | 1H, dd, *J*=4.6 and 4.8 Hz; $H_\alpha$ |
| 5.57 | 1H, d, *J*=4.8 Hz; OH |
| 6.64 | 2H, d, *J*=8.4 Hz; H-Ar |
| 6.65 | 2H, s; H-Ar |
| 6.97 | 1H, t, *J*=8.4 Hz; H-Ar |




| 400 MHz, $CD_3SOCD_3$, 20°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 1.85 | 3H, s; $CH_3CO$ |
| 3.65 | 3H, s; $CH_3O$ |
| 3.73 | 6H, s; $CH_3O$ |
| 3.75 | 6H, s; $CH_3O$ |
| 3.86 | 1H, dd, *J*=6.3 and 11.8 Hz; $H_\gamma$ |
| 4.07 | 1H, dd, *J*=3.5 and 11.8 Hz; $H_\gamma$ |
| 4.34 | 1H, ddd, *J*=3.5, 4.5 and 6.3 Hz; $H_\beta$ |
| 4.84 | 1H, dd, *J*=4.5 and 4.5 Hz; $H_\alpha$ |
| 5.42 | 1H, d, *J*=4.5 Hz; OH |
| 6.66 | 2H, d, *J*=8.4 Hz; H-Ar |
| 6.80 | 2H, s; H-Ar |
| 6.99 | 1H, t, *J*=8.4 Hz; H-Ar |




| 400 MHz, $CD_3SOCD_3$, 28°C, $(CH_3)_4Si$ | |
|---|---|
| **δ (ppm)** | |
| 1.27 | 9H, s; $C(CH_3)_3$ |
| 1.28 | 9H, s; $C(CH_3)_3$ |
| 3.55 | 3H, s; $CH_3O$ |
| 3.83 | 6H, s; $CH_3O$ |
| 6.6-7.0 | 4H, m; H-Ar |
| 8.09 | 1H, s; Ar-OH |