Electronic Supplementary Material (ESI) for RSC Sustainability.

Supporting Information

Highly Efficient Synthesis of Sustainable Bisphenols from Hydroxycinnamic Acids

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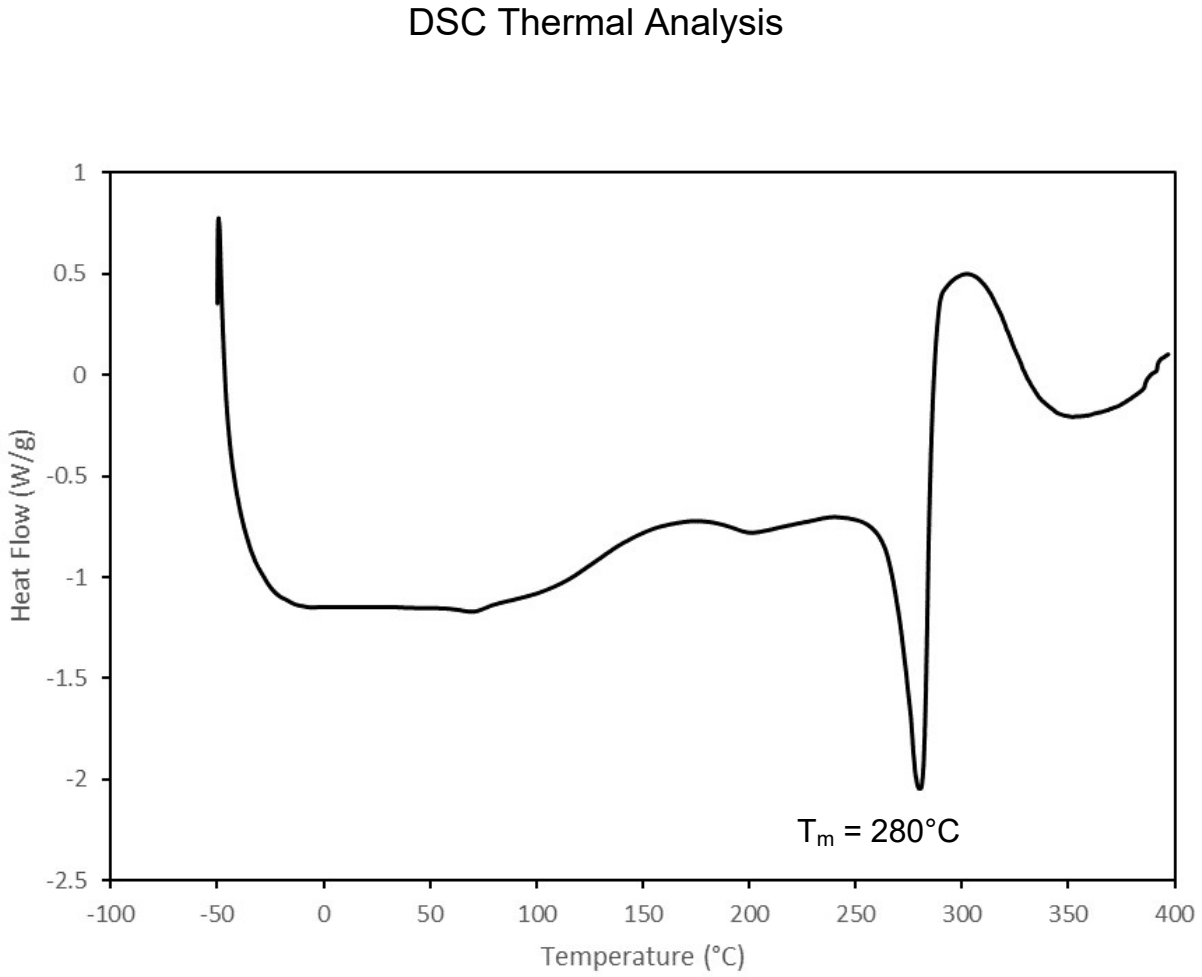


Figure S1. Differential Scanning Calorimetry (DSC) trace of compound **1**.

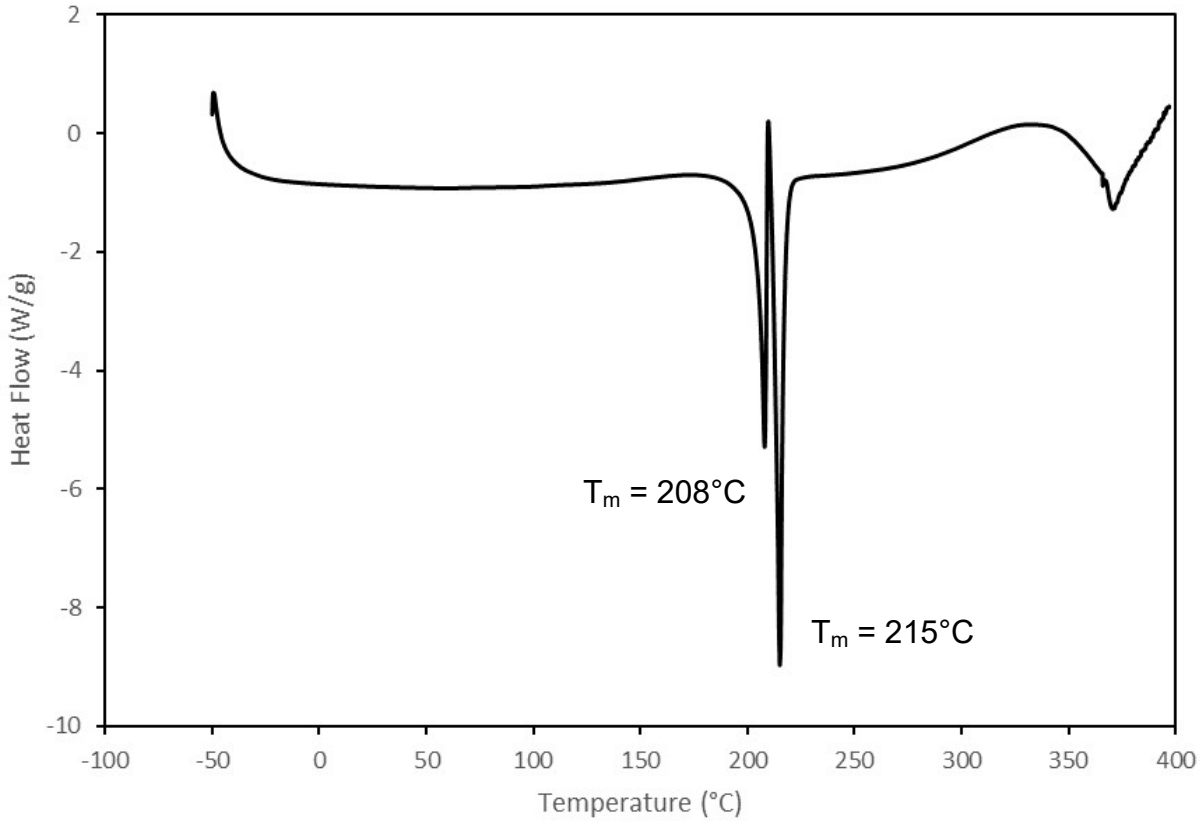


Figure S2. DSC trace of compound **2**.

Figure S3. DSC trace of compound **3**.

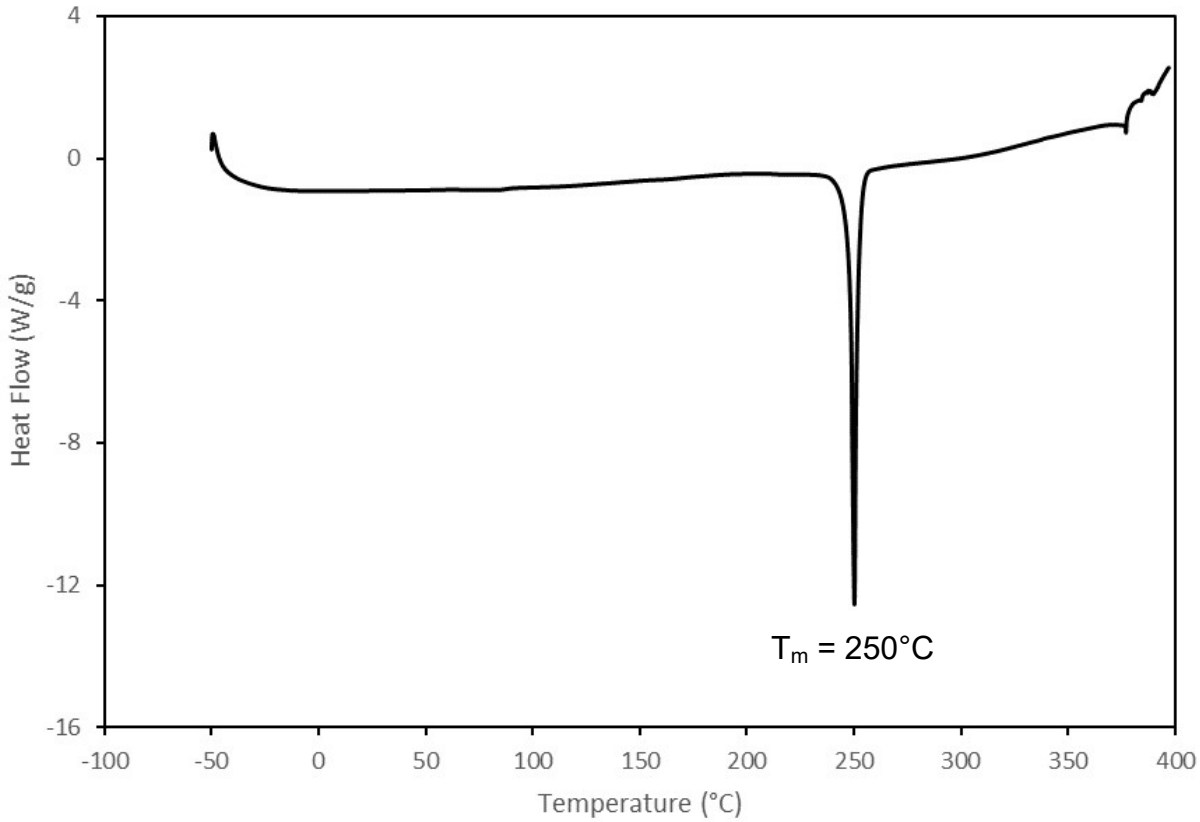


Figure S4. DSC trace of poly(vinylphenol) synthesized from *p*-coumaric acid.

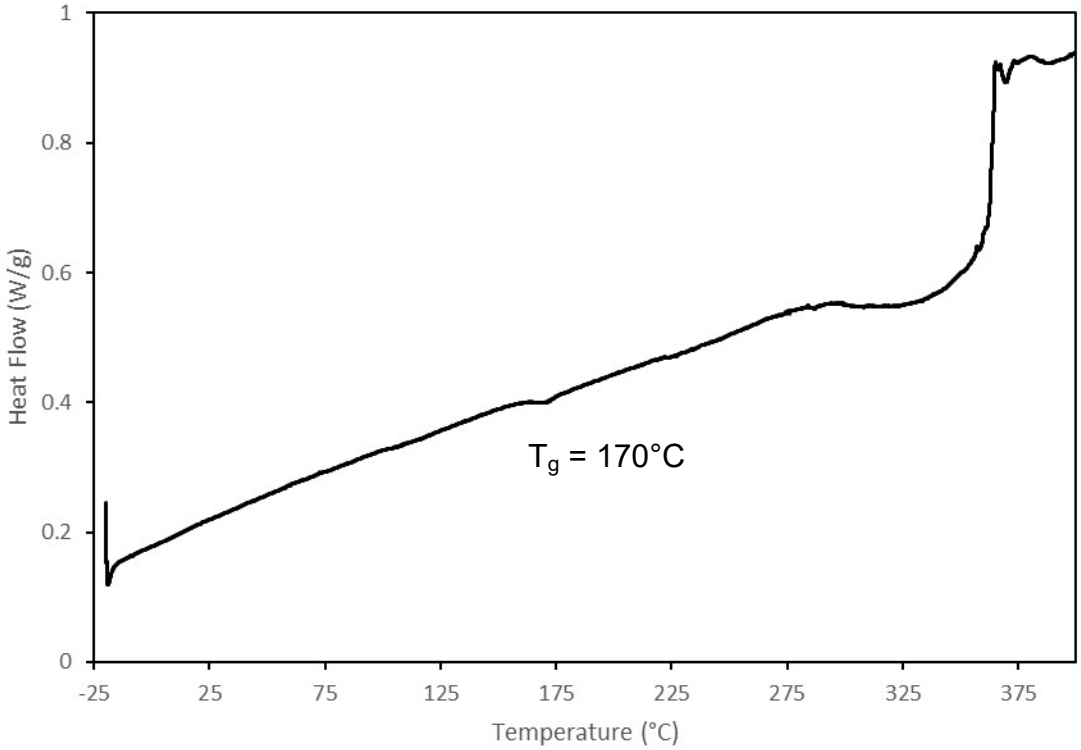
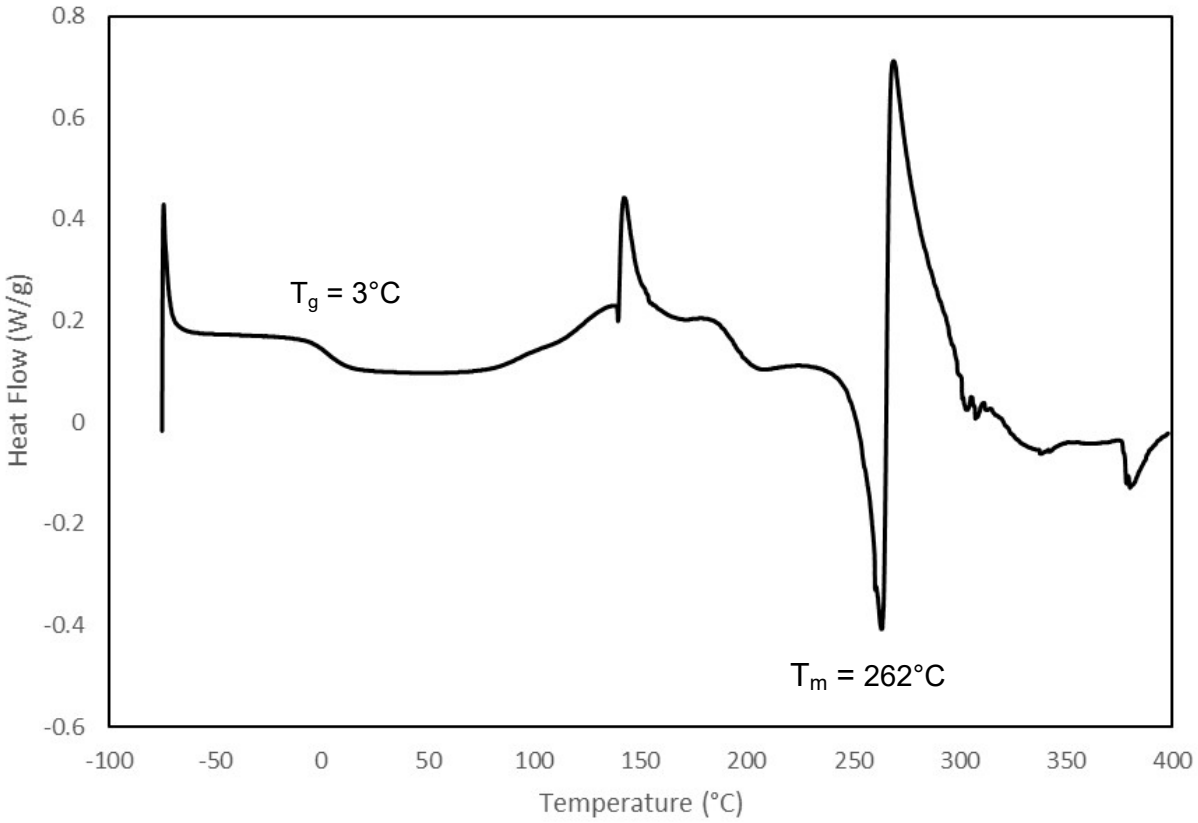
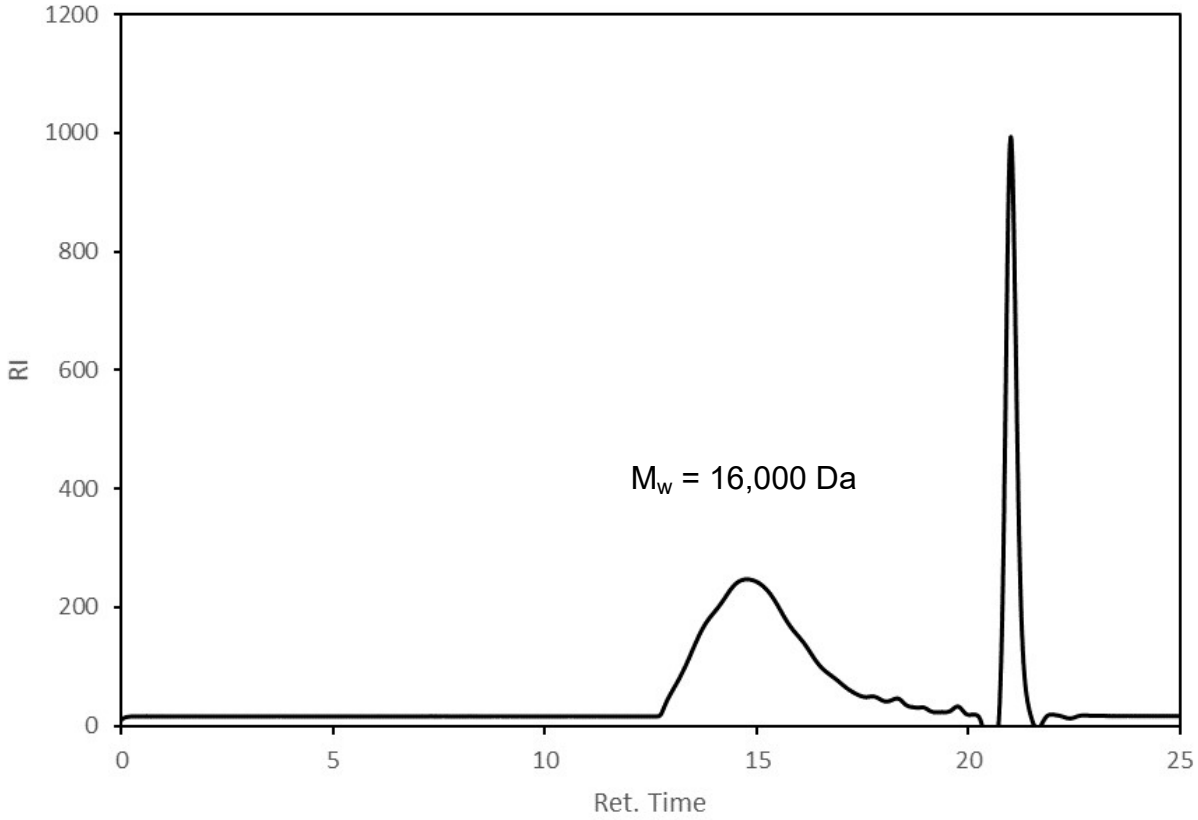


Figure S5. DSC trace of an 8:2 cis/trans mixture of compound **1**.



GPC of PVP

Figure S6 Gel permeation chromatorgraphy data for poly(vinylphenol) synthesized from *p*-coumaric acid.



Crystallographic Data

Table S1. Crystal data and structure refinement for Compound **3**.

Identification code	Compound 3
Empirical formula	$C_{18}H_{20}O_6$
Formula weight	332.36
Temperature/K	100
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	6.3732(5)
b/Å	9.3953(8)
c/Å	13.6384(12)
α/°	90
β/°	101.205(3)
γ/°	90
Volume/Å^3	801.08(12)
Z	2
ρ_{calc}g/cm^3	1.3778
μ/mm^{-1}	0.103
F(000)	352.2
Crystal size/mm^3	0.316 × 0.198 × 0.152
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	5.3 to 50.68
Index ranges	-7 ≤ h ≤ 7, -11 ≤ k ≤ 11, -16 ≤ l ≤ 16
Reflections collected	9131
Independent reflections	1468 [R_{int} = 0.0340, R_{sigma} = 0.0228]
Data/restraints/parameters	1468/0/113
Goodness-of-fit on F^2	1.064
Final R indexes [I>=2σ (I)]	R_1 = 0.0362, wR_2 = 0.0845
Final R indexes [all data]	R_1 = 0.0411, wR_2 = 0.0877
Largest diff. peak/hole / e Å^{-3}	0.21/-0.20

Table S2. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for Compound **3**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O(001)	2269.2(15)	6907.5(11)	1135.6(7)	22.0(3)
O(002)	8645.7(15)	8548.6(11)	3054.0(7)	24.3(3)
O(003)	5739.4(16)	8531.6(11)	1360.4(7)	24.7(3)
C(004)	4776(2)	5991.4(14)	3742.5(10)	16.9(3)
C(005)	5444(2)	7693.2(14)	2146.1(10)	18.5(3)
C(006)	6622(2)	6822.8(14)	3835.2(10)	17.5(3)
C(007)	3617(2)	6854.9(14)	2049.8(10)	17.6(3)
C(008)	4343(2)	5100.3(14)	4561.6(10)	17.8(3)
C(009)	3282(2)	6015.8(14)	2842.9(10)	18.0(3)
C(00A)	6934(2)	7662.8(14)	3044.8(10)	18.0(3)
C(00B)	162(2)	6358.0(17)	1076.2(11)	25.2(4)
C(00C)	10225(2)	8563.1(17)	3959.4(11)	26.1(4)

Table S3. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for Compound **3**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(001)	20.0(5)	28.5(6)	15.3(5)	-0.7(4)	-2.0(4)	4.9(4)
O(002)	22.0(5)	28.6(6)	20.5(5)	-7.9(4)	0.0(4)	6.5(4)
O(003)	22.1(5)	30.2(6)	20.9(5)	-2.6(4)	2.4(4)	10.9(4)
C(004)	20.5(7)	15.3(7)	15.0(6)	1.4(5)	3.8(5)	-1.8(5)
C(005)	22.1(7)	18.2(7)	15.8(7)	3.1(6)	5.3(5)	3.9(5)
C(006)	19.9(7)	19.0(7)	12.8(6)	1.0(6)	0.9(5)	-0.8(5)
C(007)	19.5(7)	18.2(7)	13.9(7)	4.2(5)	0.5(5)	-0.3(5)
C(008)	19.7(7)	16.6(7)	17.3(7)	-2.8(5)	3.8(5)	-1.5(5)
C(009)	18.4(7)	17.0(7)	18.2(7)	-1.0(5)	2.3(5)	-0.5(5)
C(00A)	17.8(7)	17.0(7)	19.6(7)	0.0(5)	4.3(5)	-1.1(5)
C(00B)	18.5(7)	34.0(8)	20.6(7)	0.6(6)	-2.4(6)	1.4(6)

C(00C)	24.8(8)	30.1(8)	21.0(7)	-9.5(6)	-1.5(6)	1.9(6)

Table S4. Bond Lengths for Compound **3**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O(001)	C(007)	1.3705(15)	C(004)	C(009)	1.3993(18)
O(001)	C(00B)	1.4266(17)	C(005)	C(007)	1.391(2)
O(002)	C(00A)	1.3705(17)	C(005)	C(00A)	1.3972(19)
O(002)	C(00C)	1.4336(16)	C(006)	C(00A)	1.3811(19)
O(003)	C(005)	1.3722(16)	C(007)	C(009)	1.3880(19)
C(004)	C(006)	1.3972(19)	C(008)	C(008)	1.333(3)
C(004)	C(008)	1.4645(18)			

Table S5. Bond Angles for Compound **3**.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C(00B)	O(001)	C(007)	117.08(10)	C(005)	C(007)	O(001)	115.51(12)
C(00C)	O(002)	C(00A)	115.99(11)	C(009)	C(007)	O(001)	124.44(12)
C(008)	C(004)	C(006)	122.05(12)	C(009)	C(007)	C(005)	120.04(12)
C(009)	C(004)	C(006)	119.18(12)	C(008)[1]	C(008)	C(004)	125.90(16)
C(009)	C(004)	C(008)	118.77(12)	C(007)	C(009)	C(004)	120.75(12)
C(007)	C(005)	O(003)	119.39(12)	C(005)	C(00A)	O(002)	113.56(12)
C(00A)	C(005)	O(003)	121.59(12)	C(006)	C(00A)	O(002)	125.10(12)
C(00A)	C(005)	C(007)	119.01(12)	C(006)	C(00A)	C(005)	121.34(12)
C(00A)	C(006)	C(004)	119.68(12)				

Table S6. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for Compound **3**.

Atom	*x*	*y*	*z*	U(eq)

Table S6. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for Compound **3**.

Atom	***x***	***y***	***z***	**U(eq)**
H(009)	2025(2)	5451.7(14)	2774.3(10)	21.6(4)
H(006)	7657(2)	6810.5(14)	4439.0(10)	21.0(4)
H(003)	6846(16)	9028(14)	1534(4)	37.0(4)
H(008)	3005(2)	4622.1(14)	4459.0(10)	21.4(4)
H(00a)	-719(5)	6605(10)	427(3)	37.8(5)
H(00b)	227(3)	5321(2)	1150(8)	37.8(5)
H(00c)	-471(6)	6771(8)	1611(5)	37.8(5)
H(00d)	11358(9)	9241(8)	3893(3)	39.2(5)
H(00e)	9556(4)	8848(11)	4518.0(17)	39.2(5)
H(00f)	10842(12)	7609(3)	4086(4)	39.2(5)

Figure S7. Unit Cell of Compound **3**.

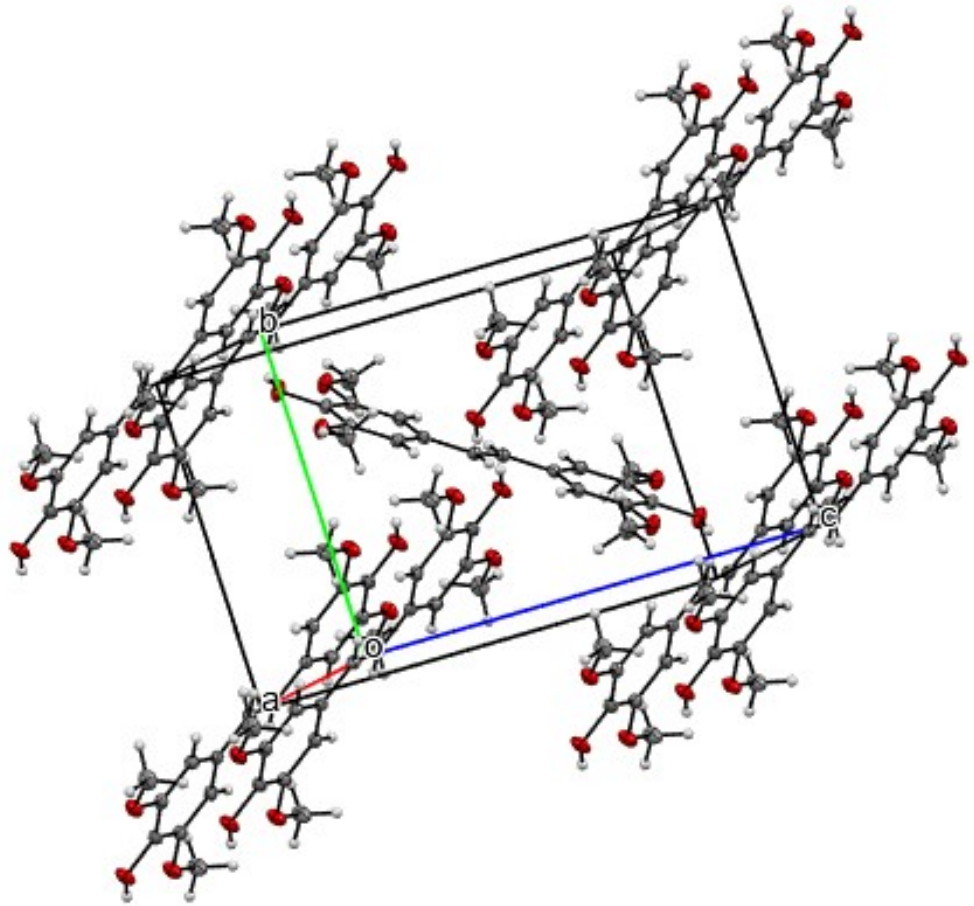


Figure S8. ^{1}H NMR Spectrum of Compound **1**.

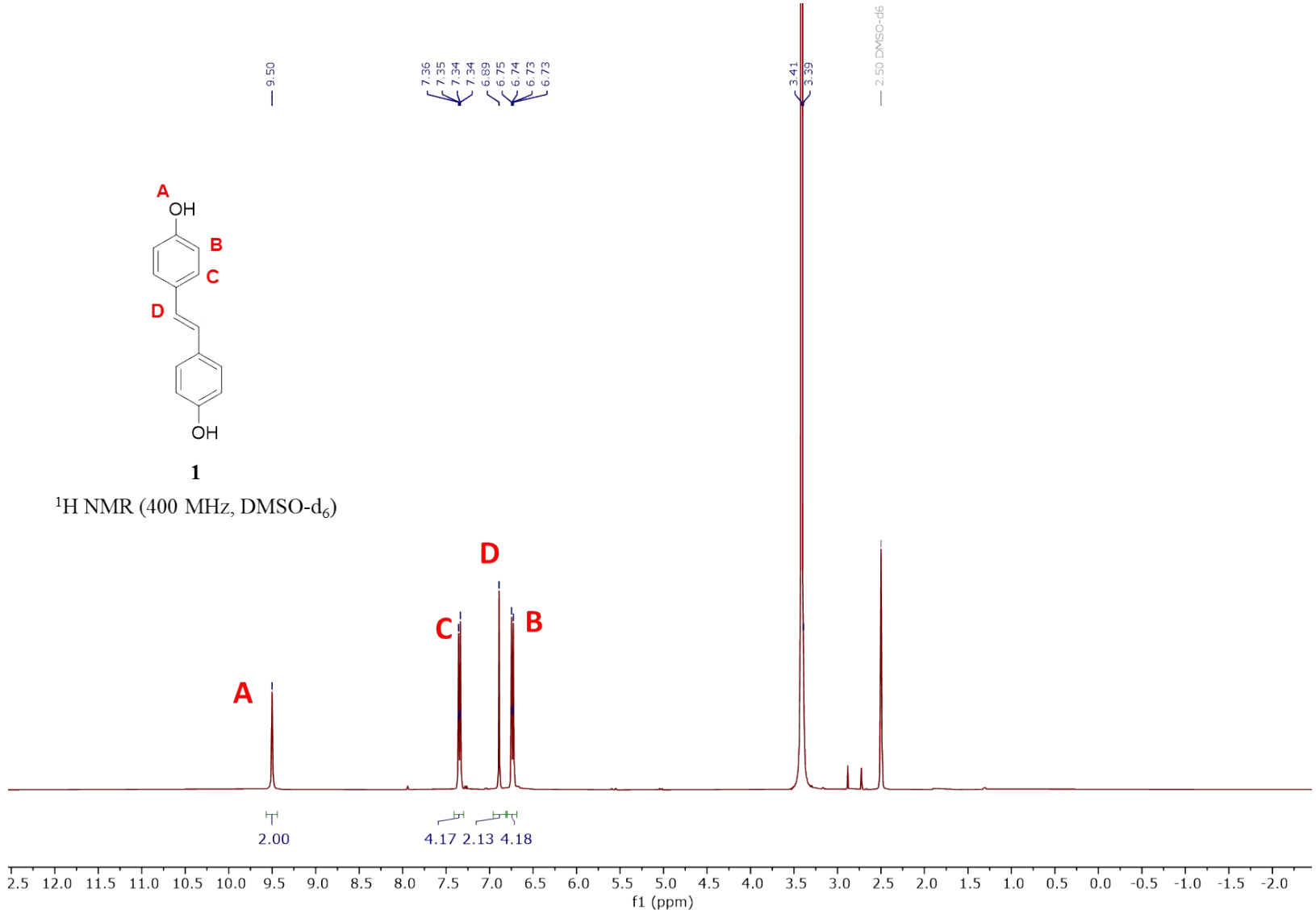


Figure S9. ^{13}C NMR Spectrum of Compound **1**.

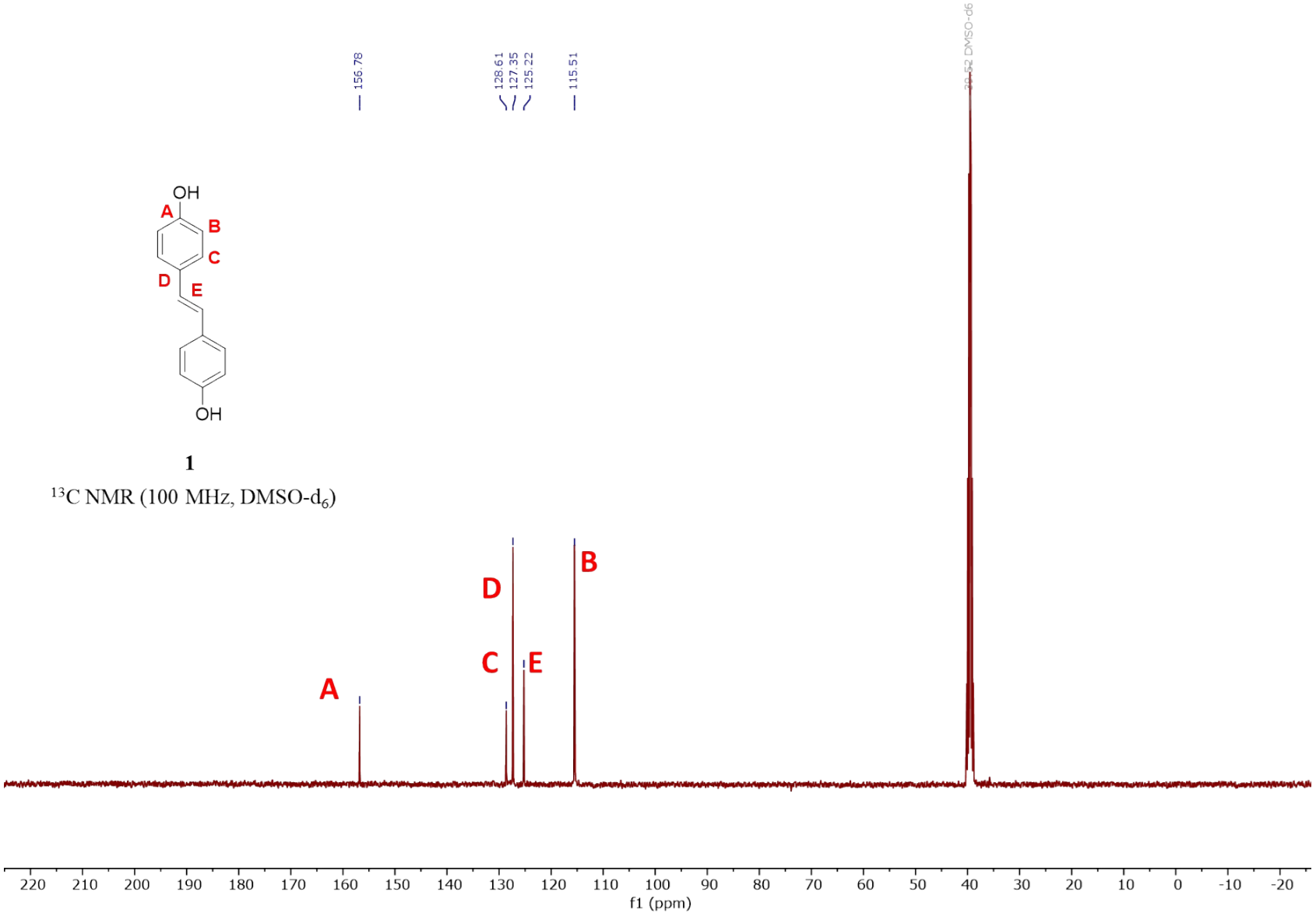


Figure S10. ^{1}H NMR Spectrum of Compound **2**.

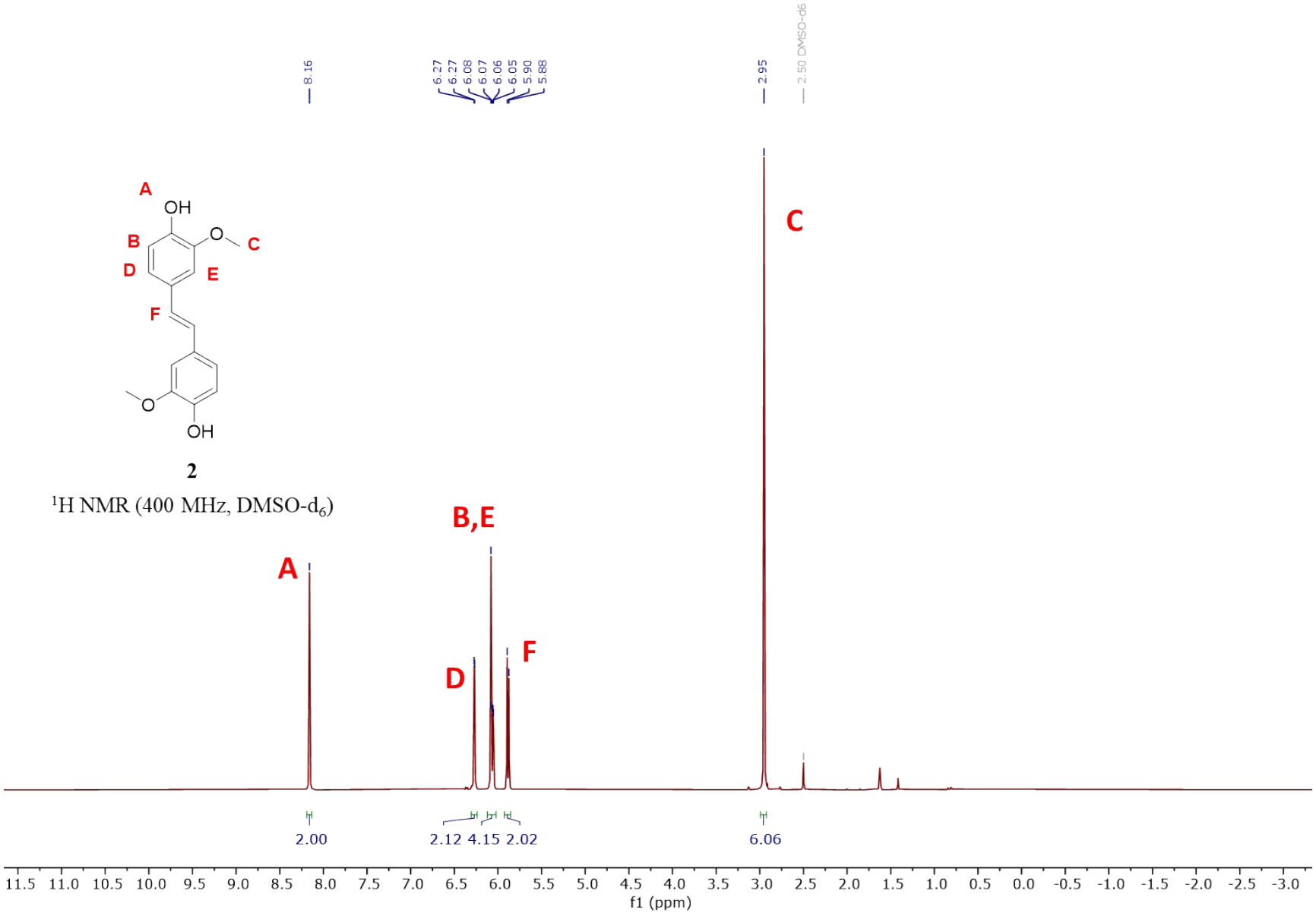


Figure S11 ^{13}C NMR Spectrum of Compound **2**.

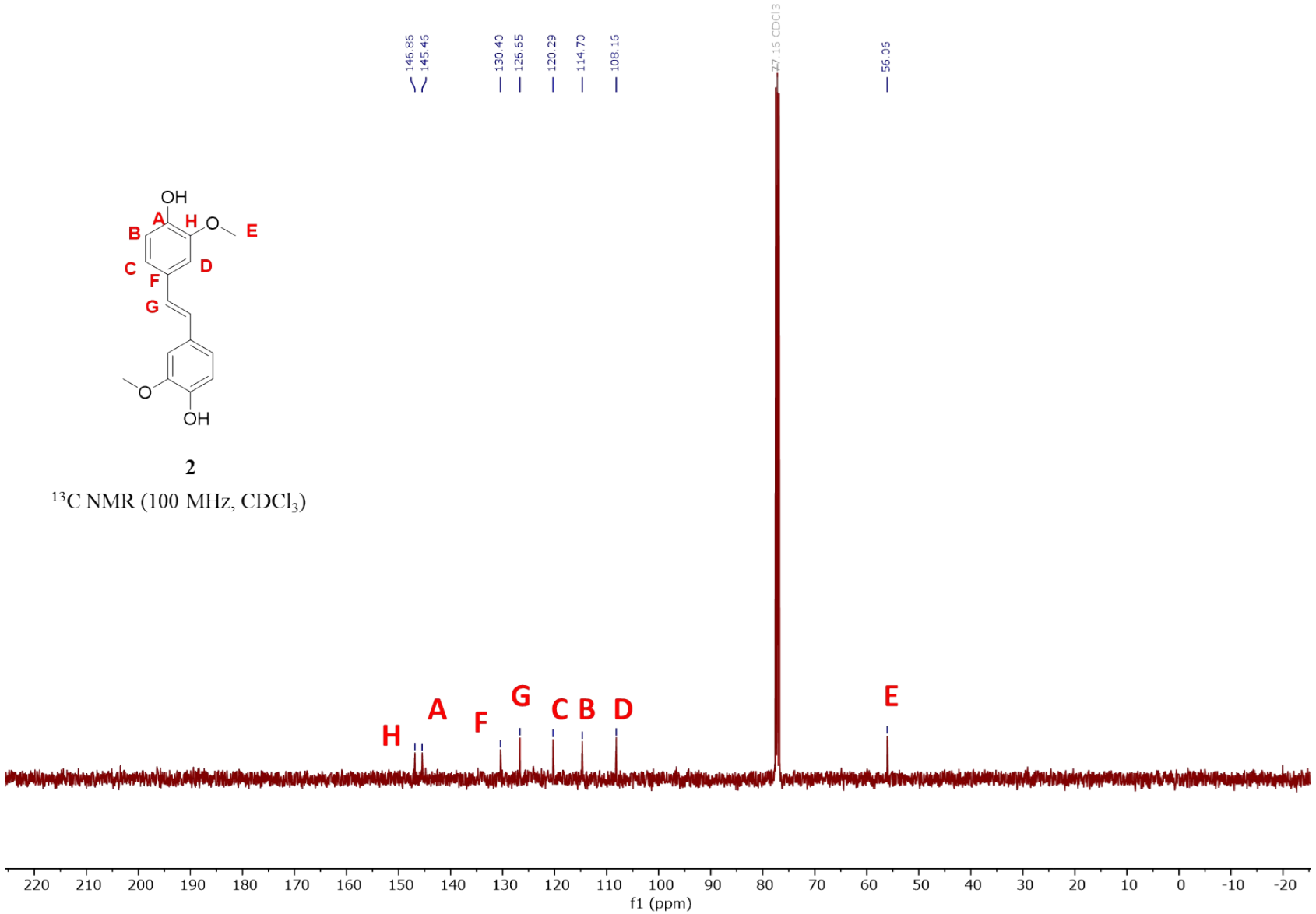


Figure S12. ^{1}H NMR Spectrum of Compound **3**.

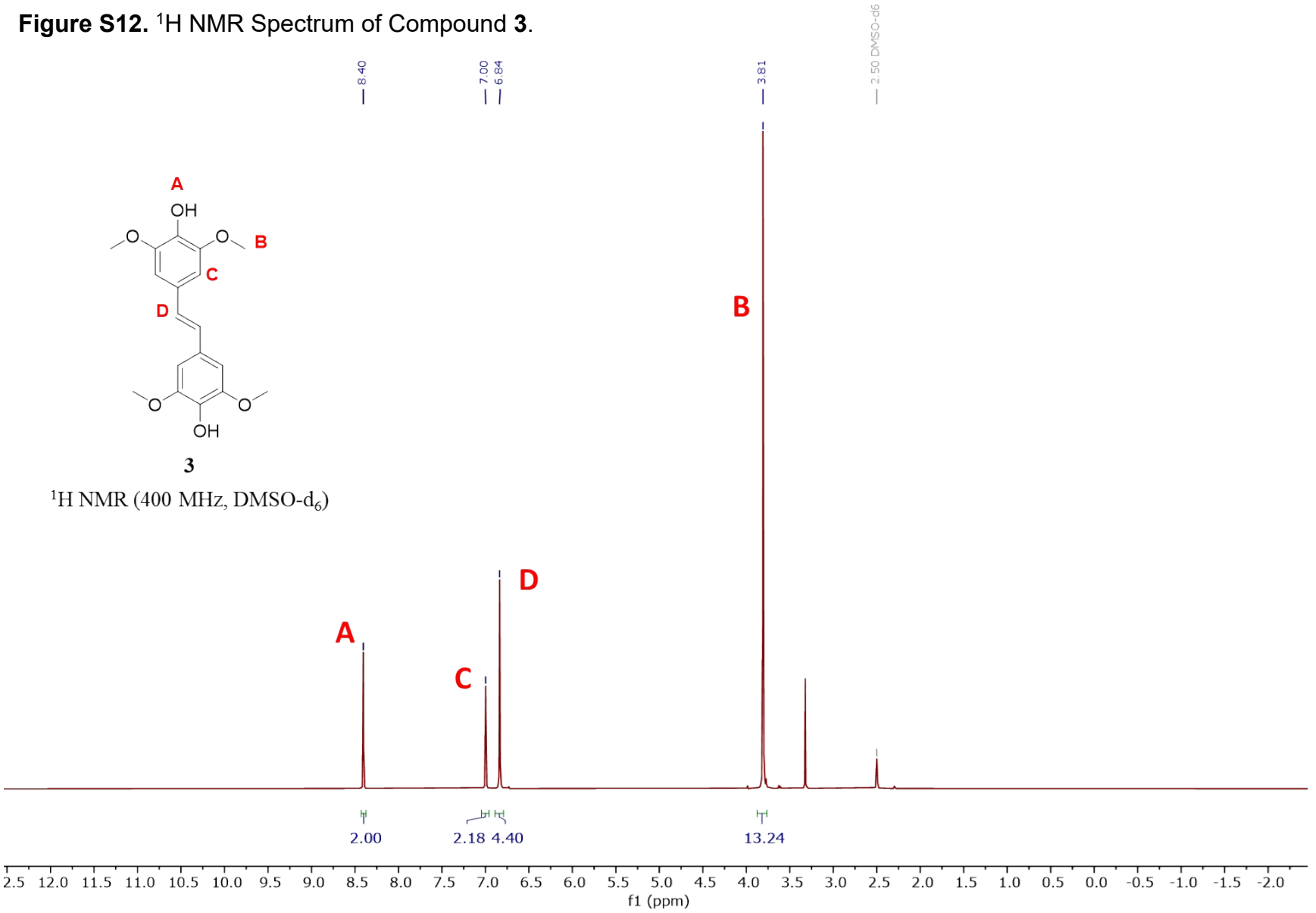
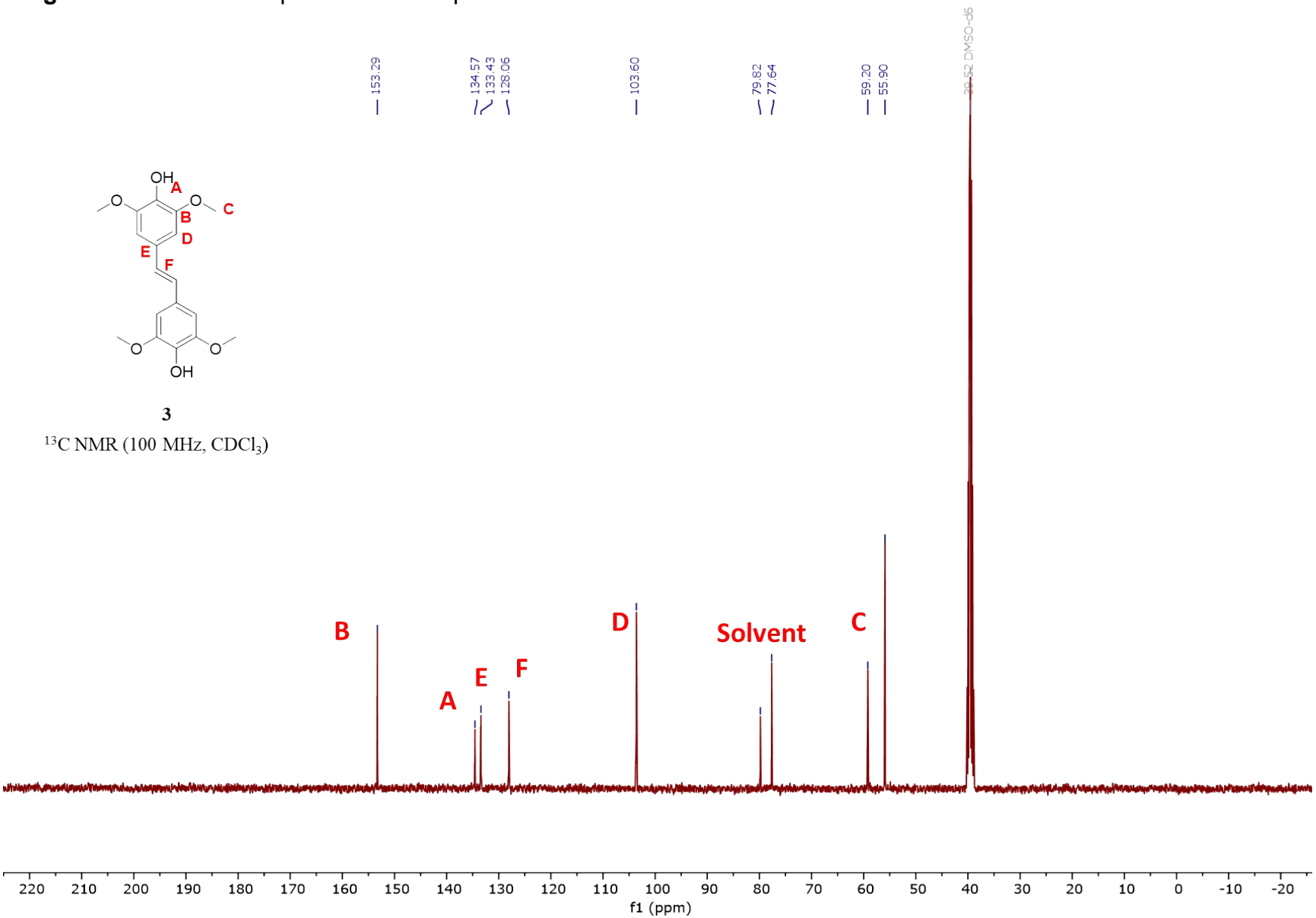


Figure S13. ^{13}C NMR Spectrum of Compound **3**.



3

^{13}C NMR (100 MHz, $CDCl_3$)

Figure S14. ^{1}H NMR Spectrum of Compound **4**.

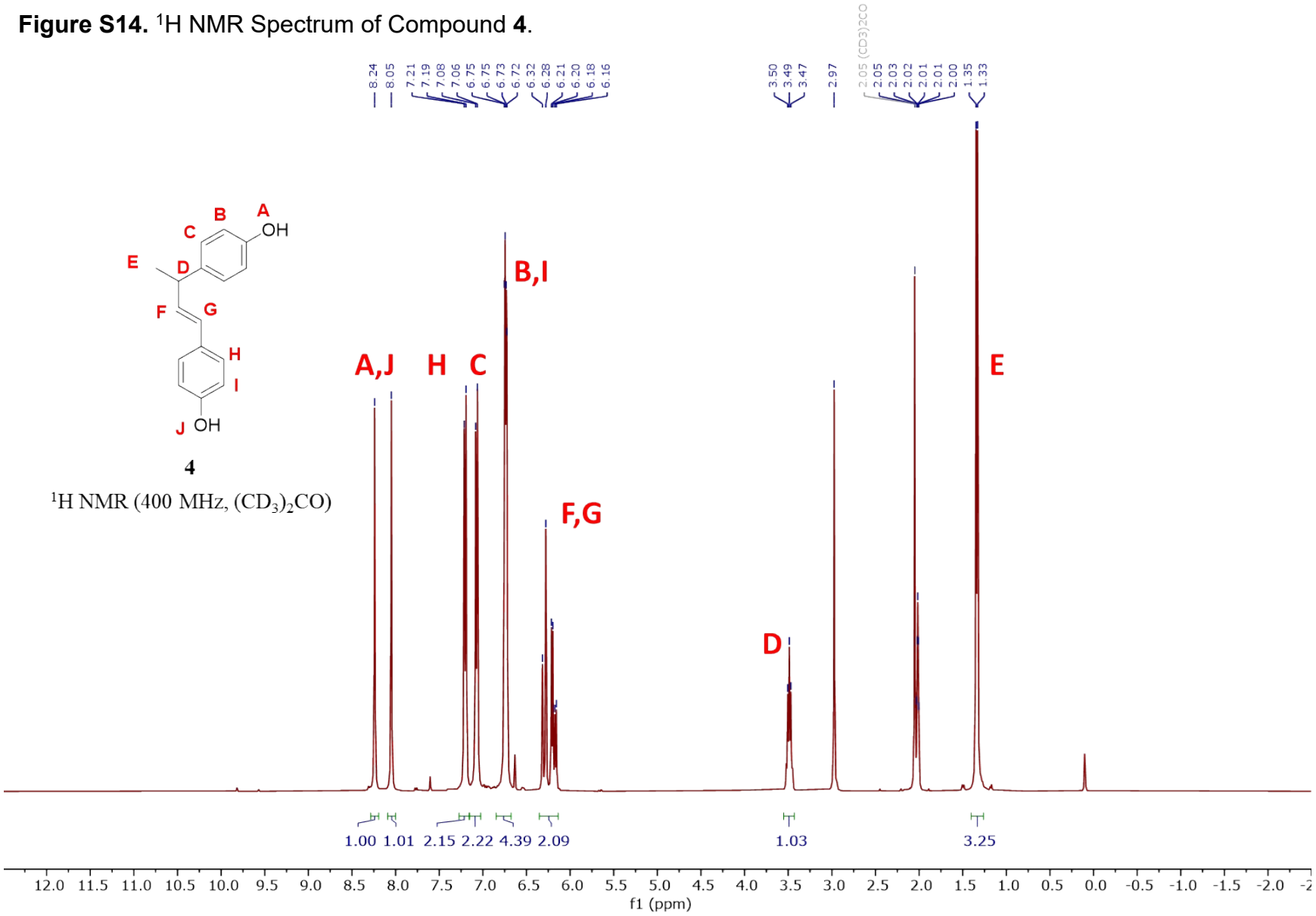


Figure S15. ^{13}C NMR Spectrum of Compound **4**.

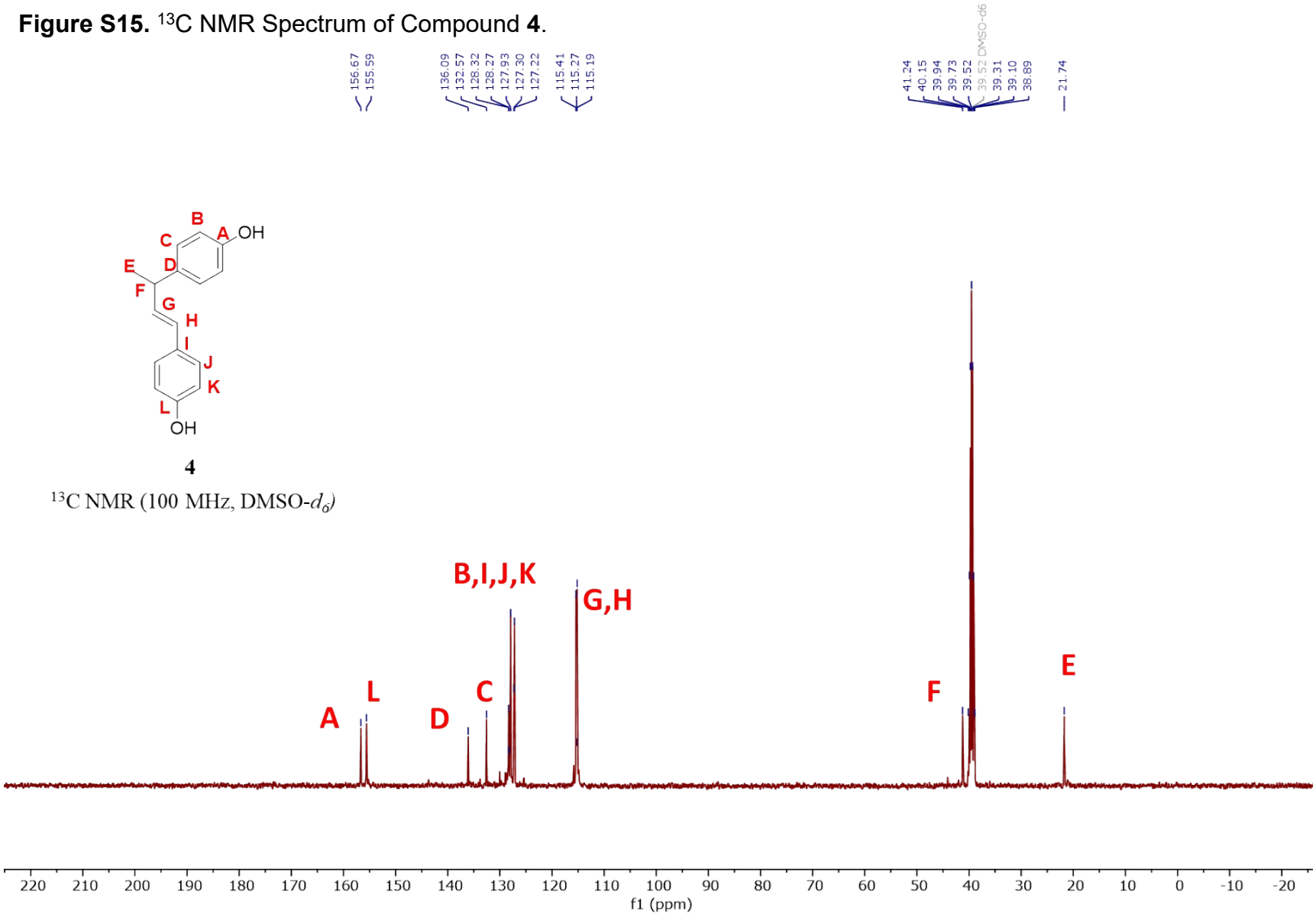


Figure S16. ^{1}H NMR Spectrum of Poly(Vinylphenol)

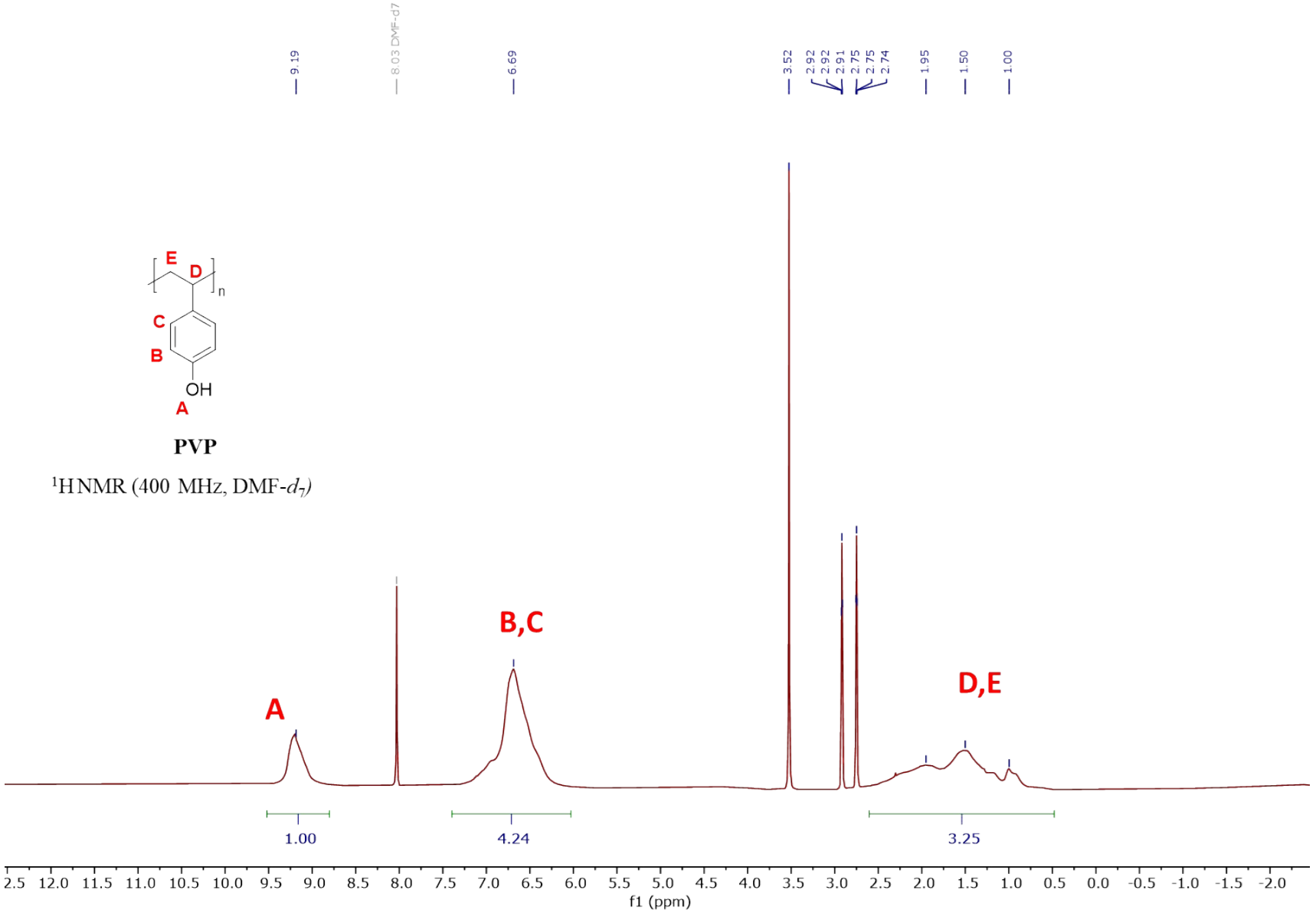


Figure S17. ^{13}C NMR Spectrum of Poly(Vinylphenol).

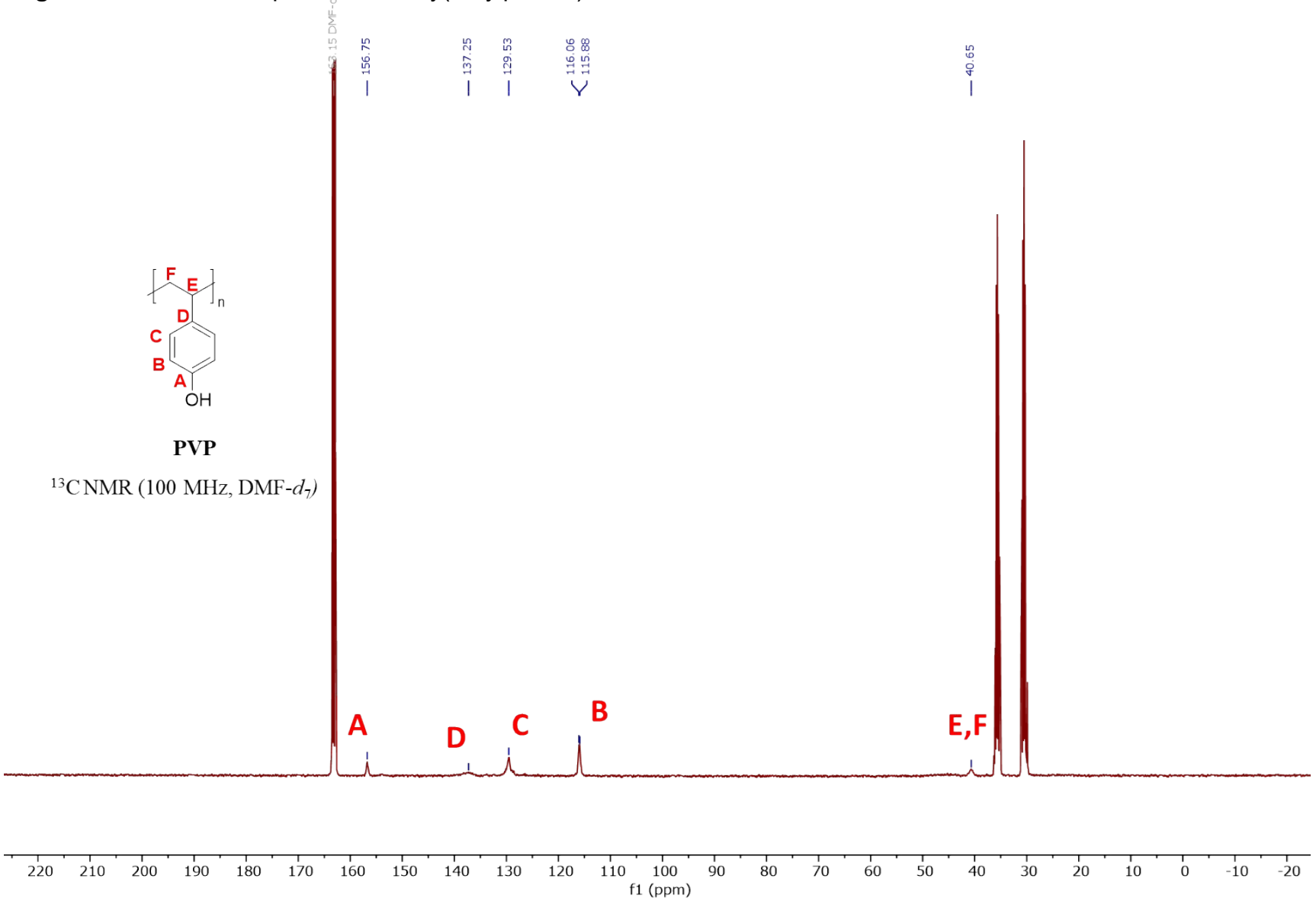


Figure S18. ^{1}H NMR of Cis/Trans Mixture of Compound **1**.