

Supporting Information
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Oxidation of eugenol derivatives using KMnO_4 and CrO_3

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- **Eugénoł (1)**

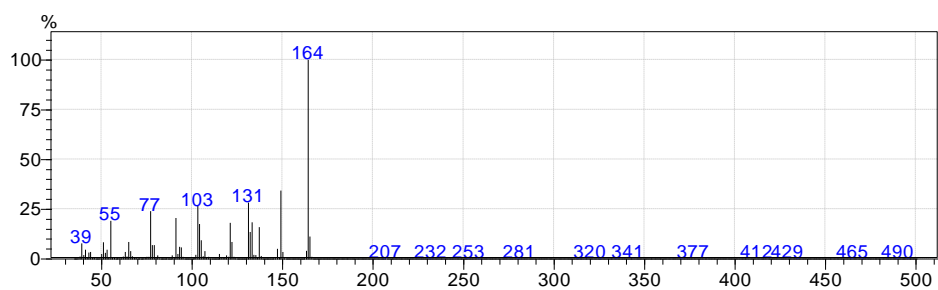


Figure 1. Mass spectrum of eugenol

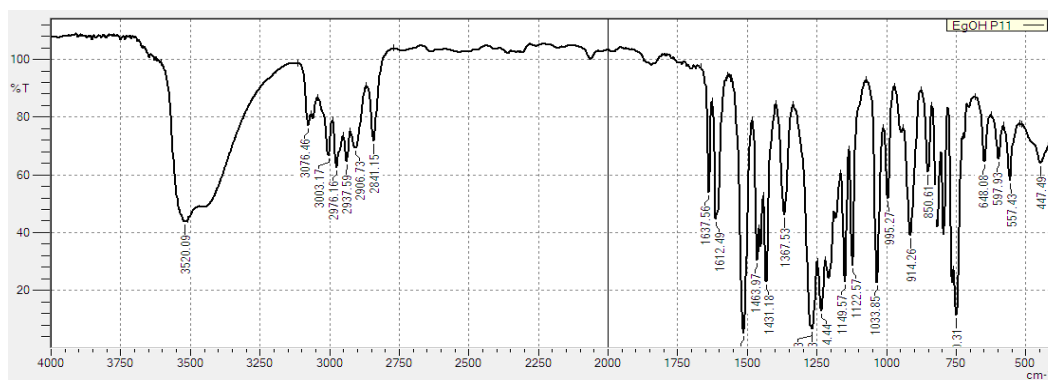


Figure 2. Infra-red spectrum of eugenol

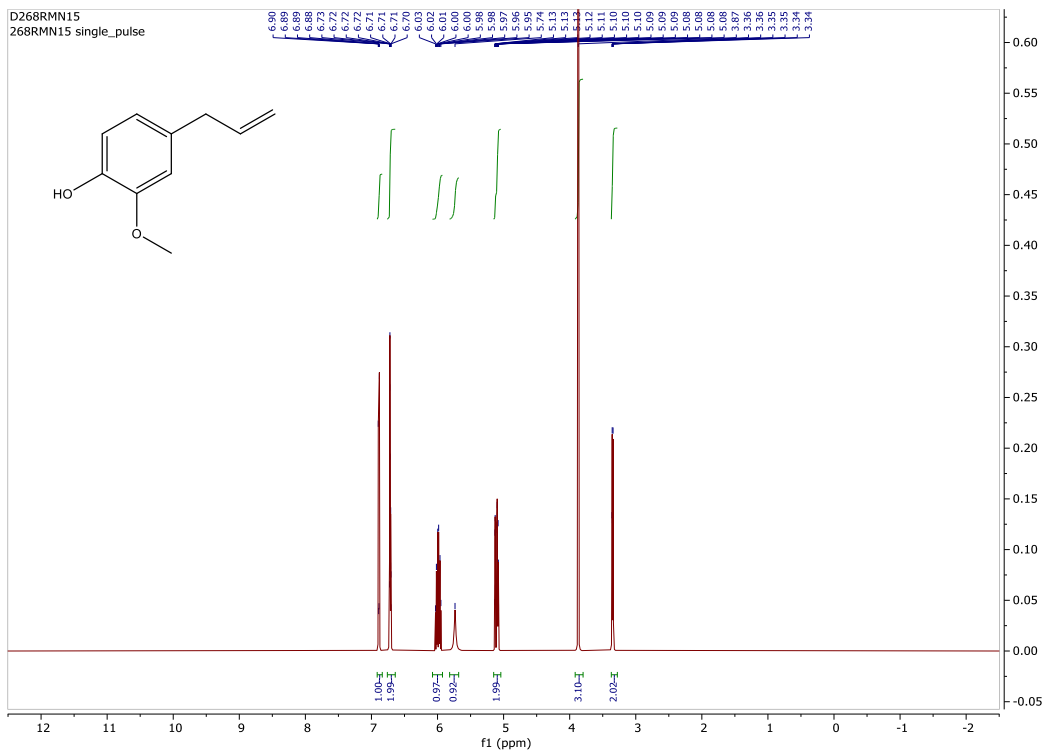


Figure 3. ^1H NMR spectrum of eugenol

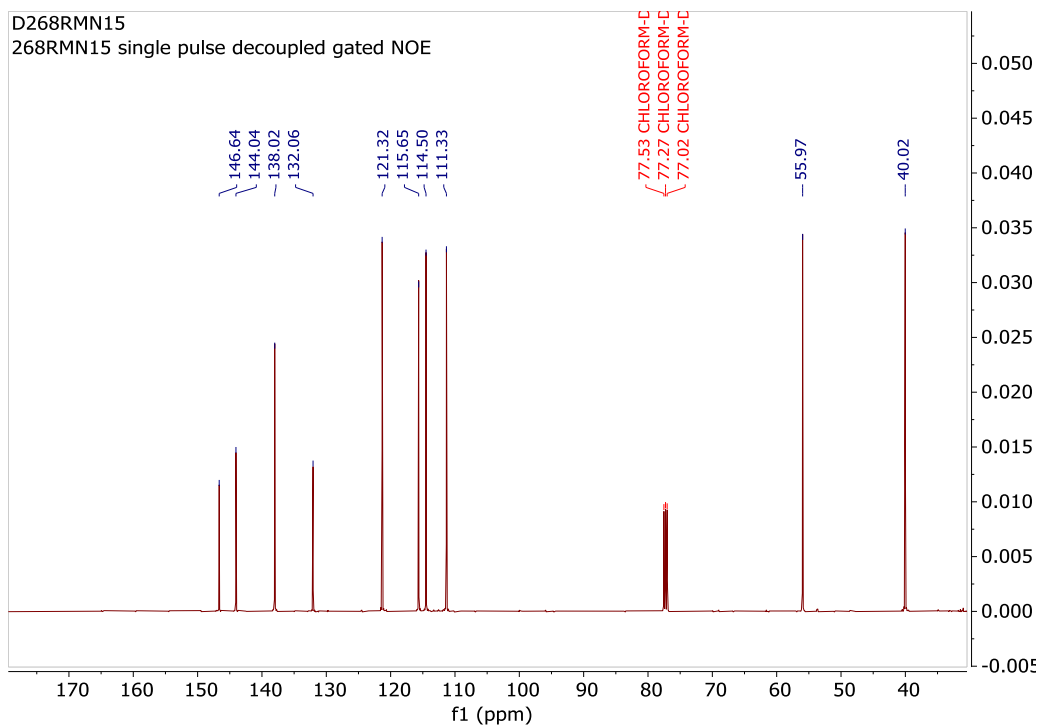


Figure 4. ^{13}C NMR spectrum of eugenol

- Acetyeugenol (2)

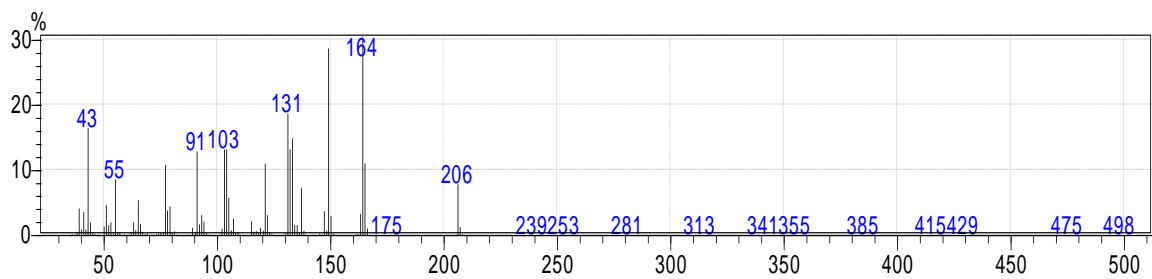


Figure 5. Mass spectrum of acetylugenol

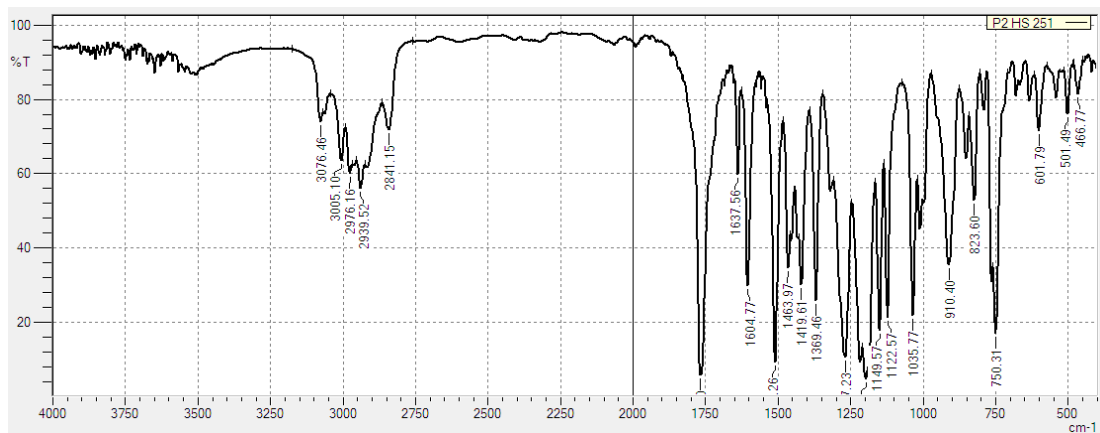


Figure 6. Infra-red spectrum of acetylugenol

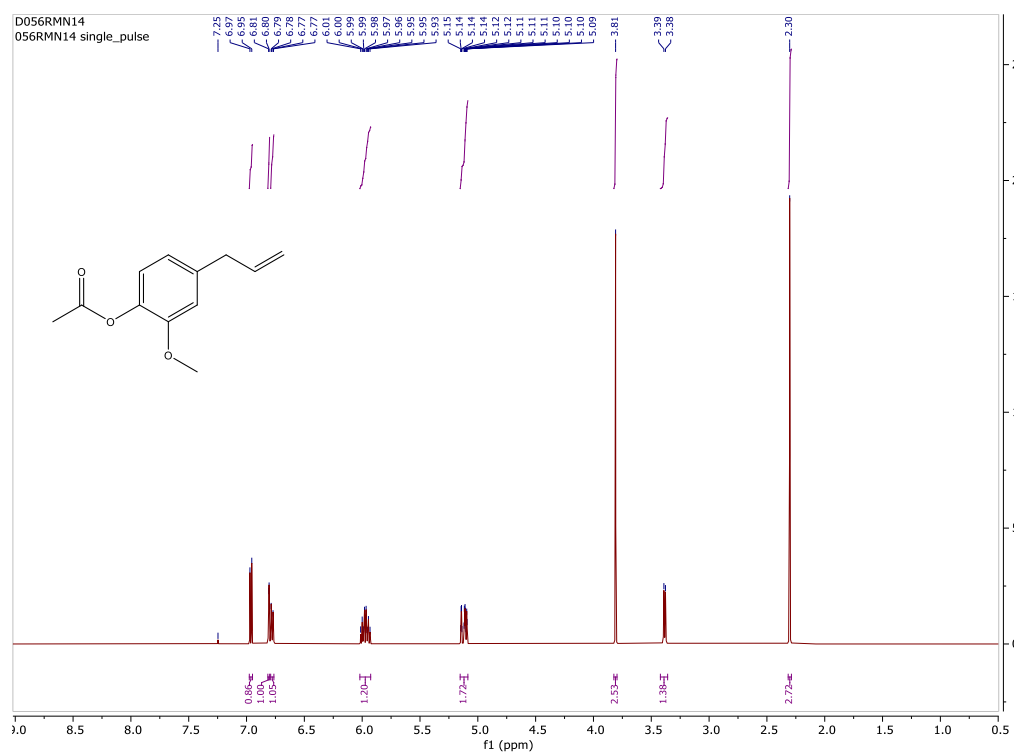


Figure 7. ¹H NMR spectrum of acetylugenol

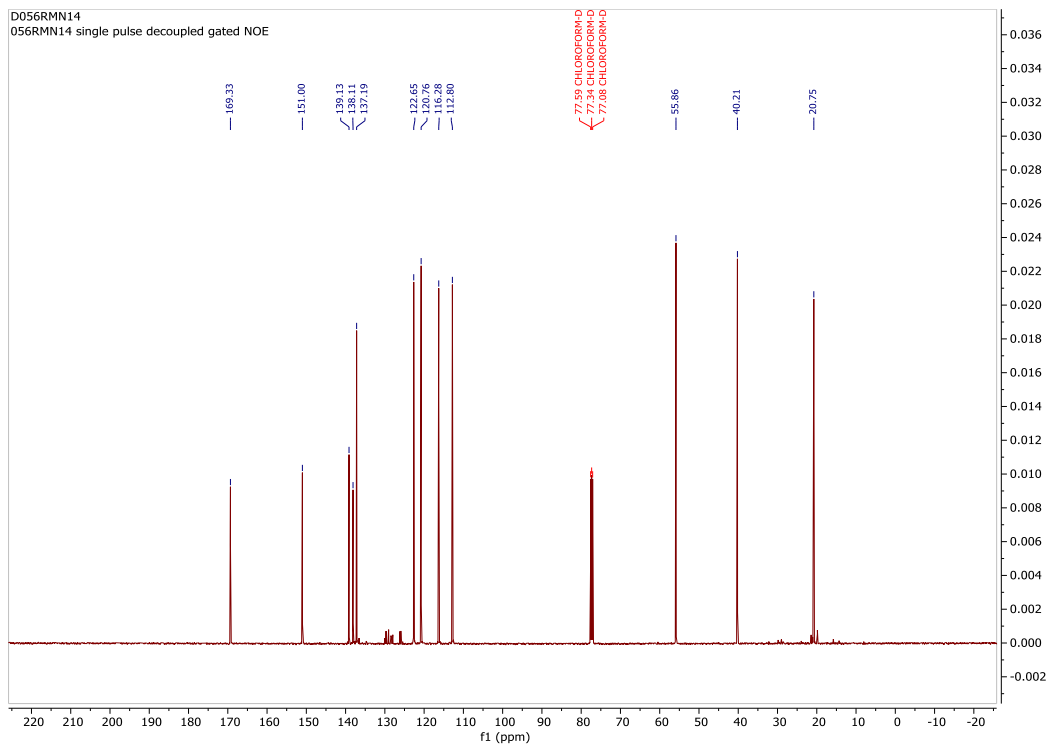


Figure 8. ^{13}C NMR spectrum of acetylugenol

- **Benzyleugenol (3)**

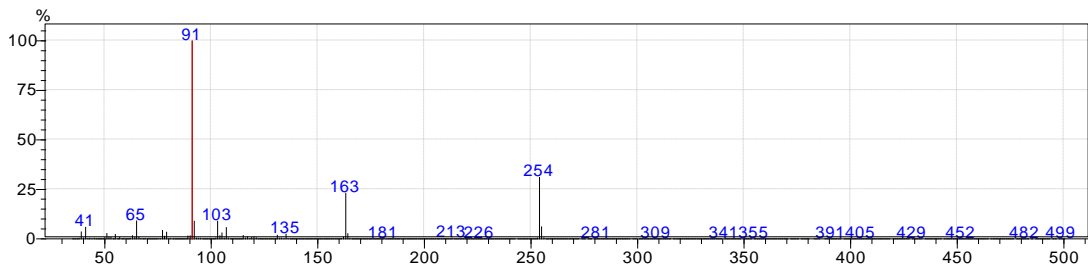


Figure 9. Mass spectrum of benzyleugenol

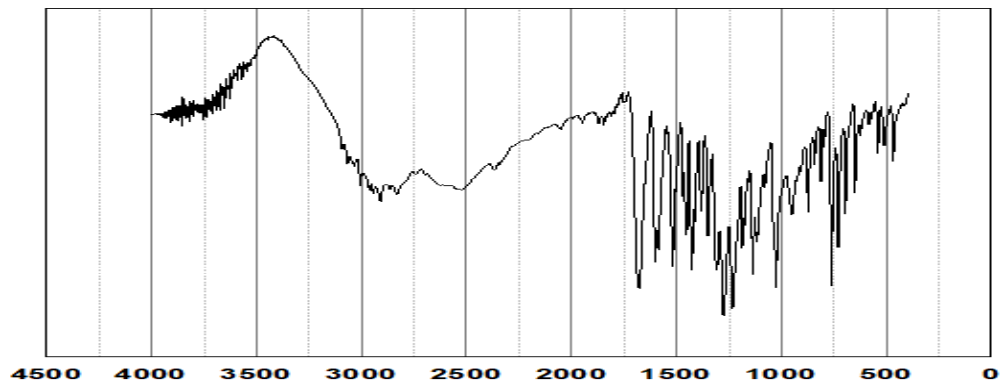


Figure 10. Infra-red spectrum of benzyleugenol

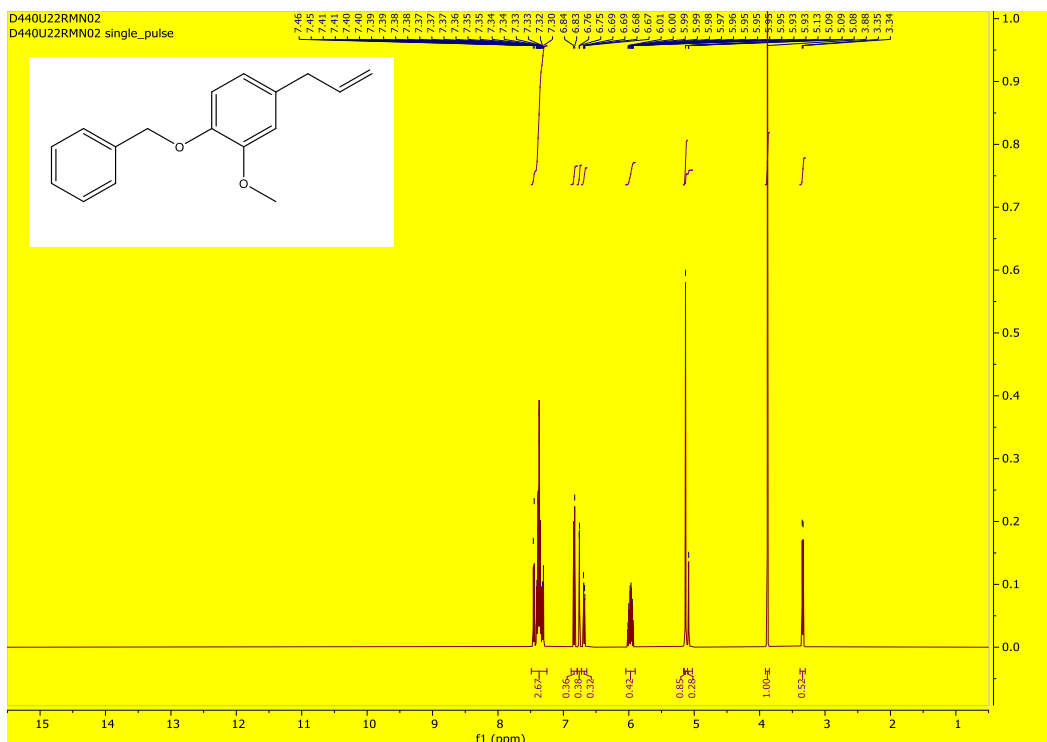


Figure 11. ^1H NMR spectrum of benzyleugenol

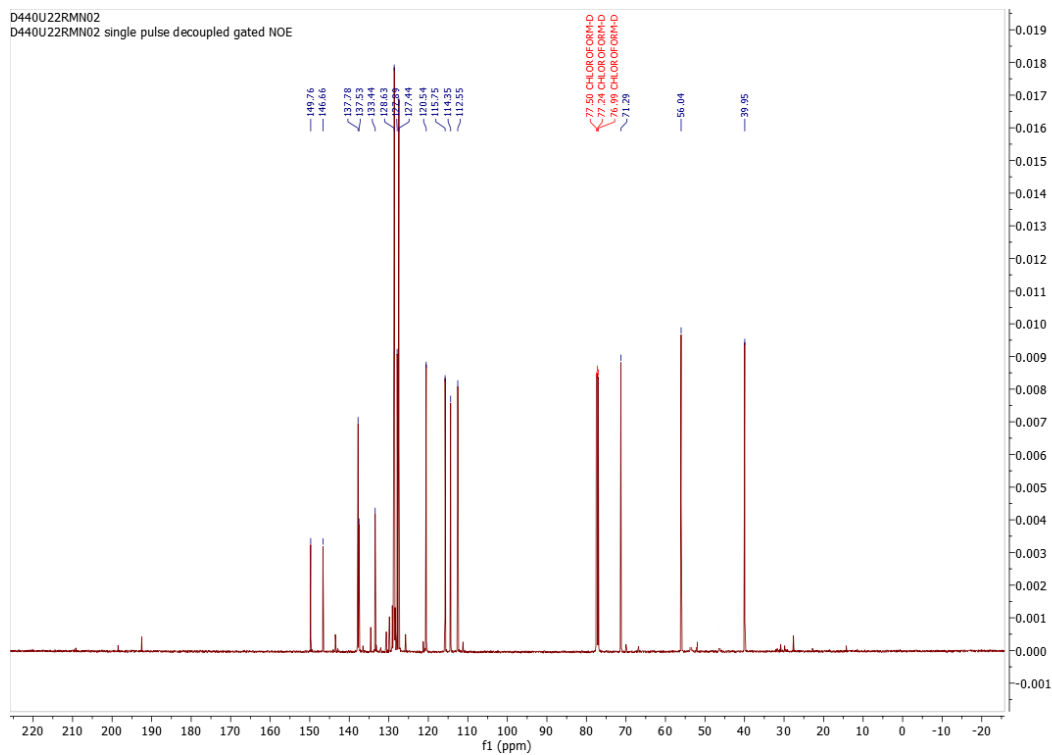


Figure 12. ^{13}C NMR spectrum of benzyleugenol

- Acetylvainillin (4)

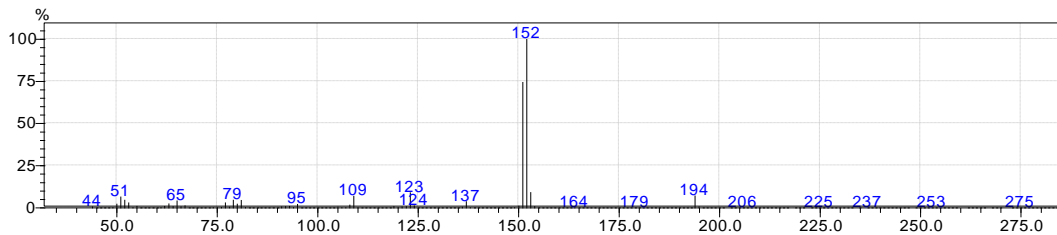


Figure 13. Mass spectrum of acetylvainillin

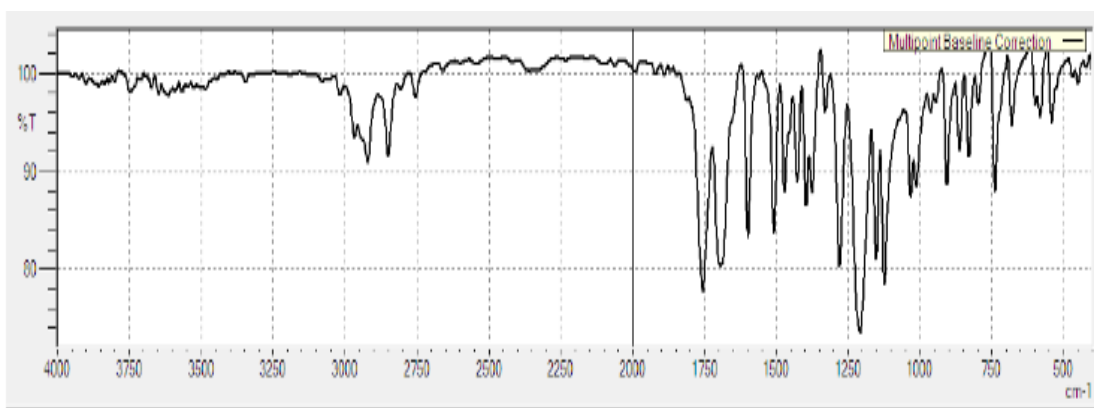


Figure 14. Infra-red spectrum of acetylvainillin

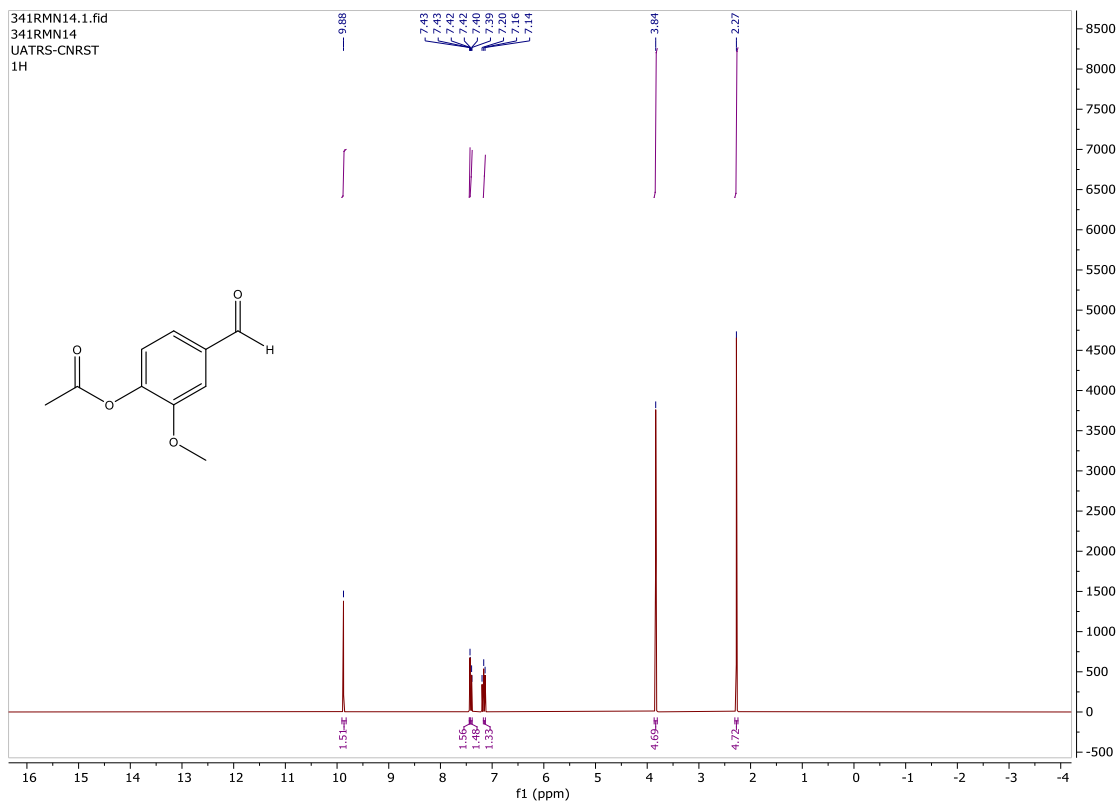


Figure 15. ¹H NMR spectrum of acetylvainillin

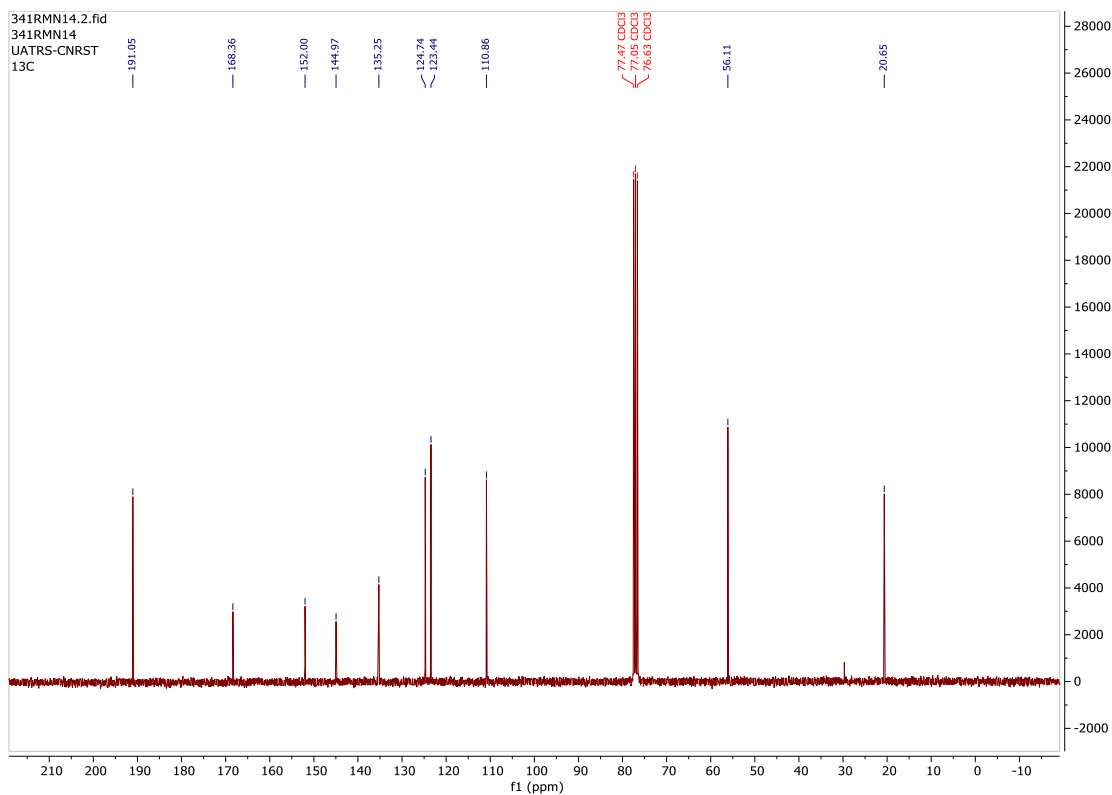


Figure 16. ¹³C NMR spectrum of acetylvainillin

- Acetylvainillic acid (5)

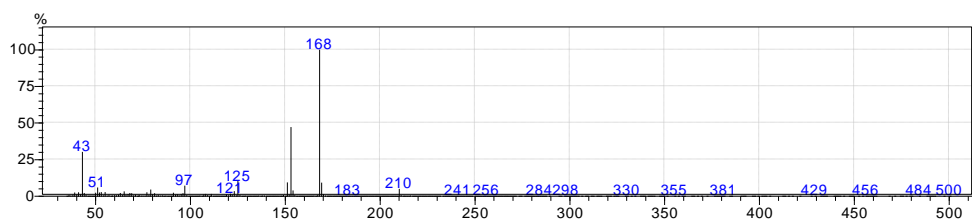


Figure 17. Mass spectrum of acetylvainillic acid

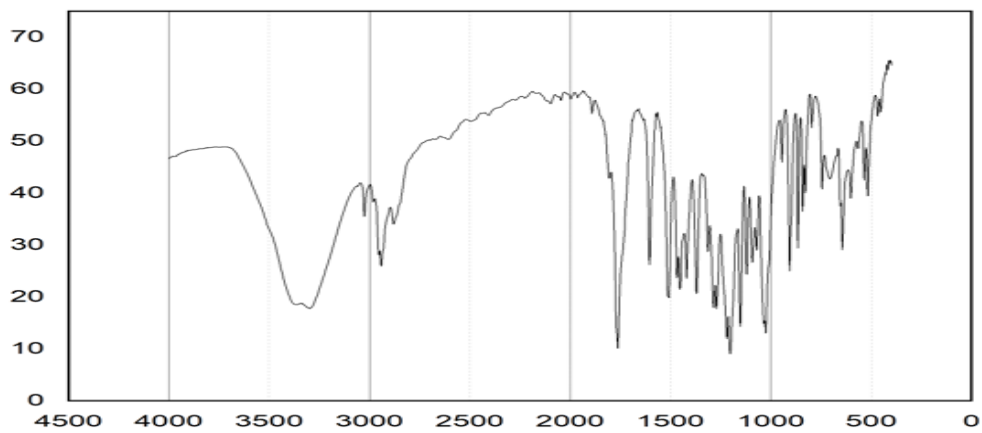


Figure 18. Infra-red spectrum acetylvainillic acid

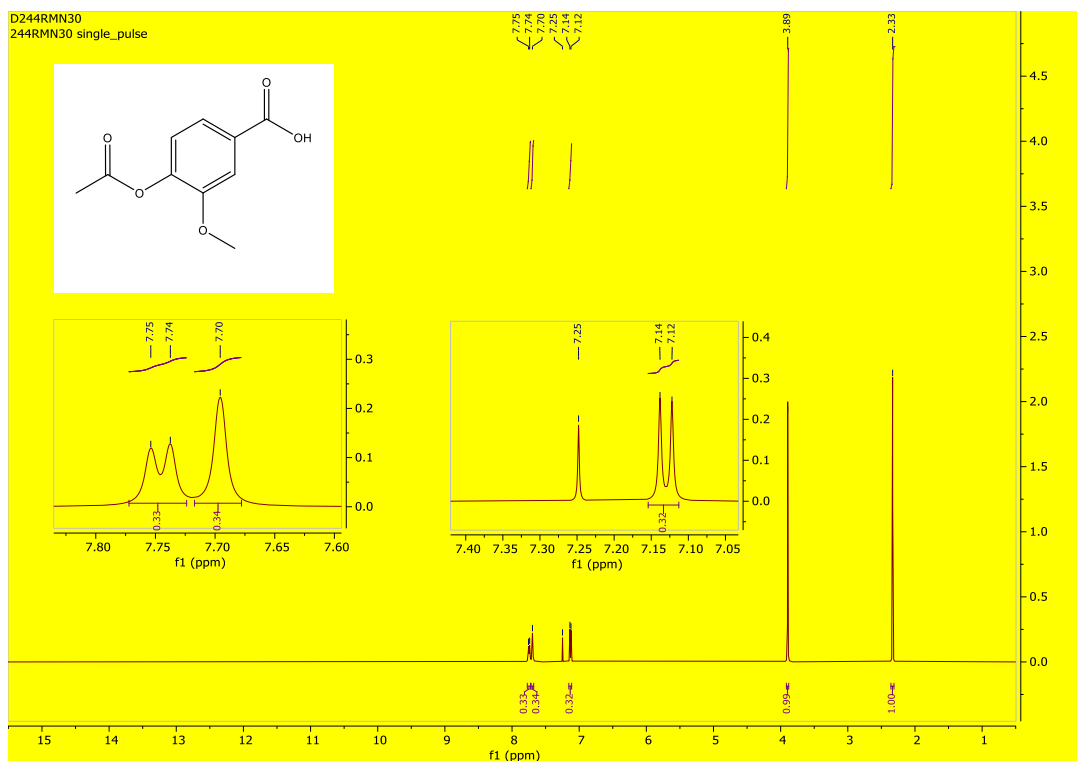


Figure 19. ^1H NMR spectrum of acetylvannillin acid

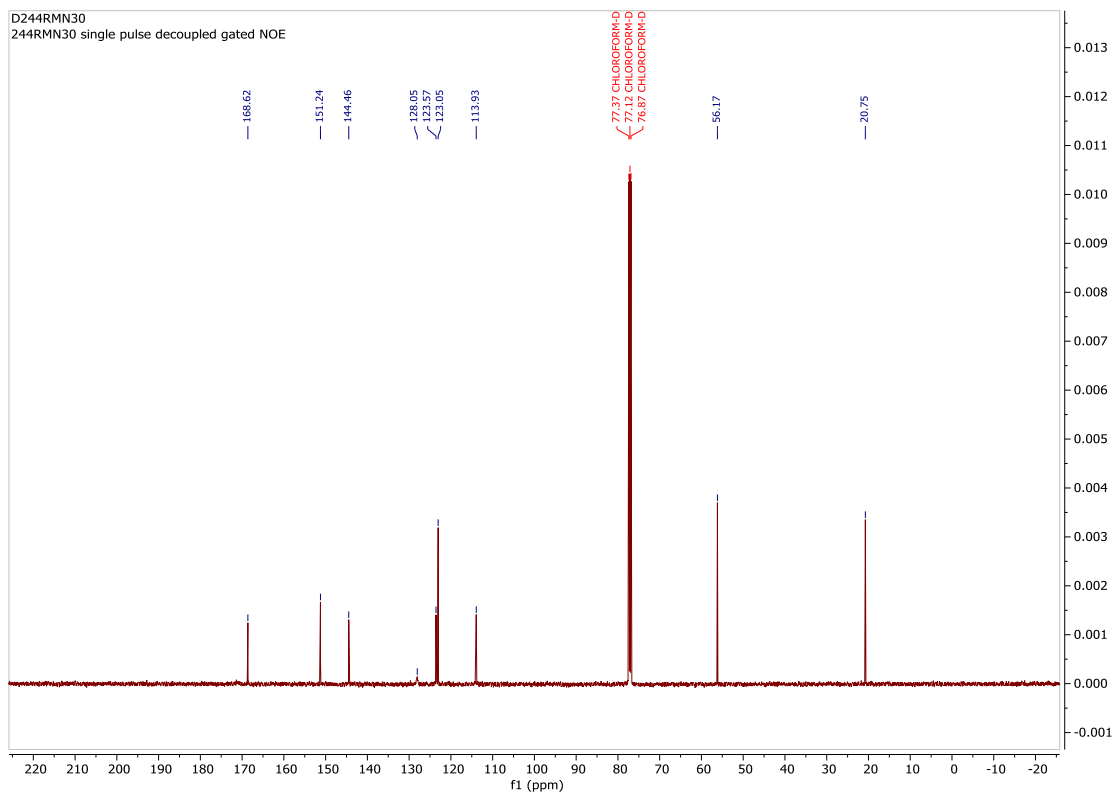


Figure 20. ^{13}C NMR spectrum of acetylvannillin acid

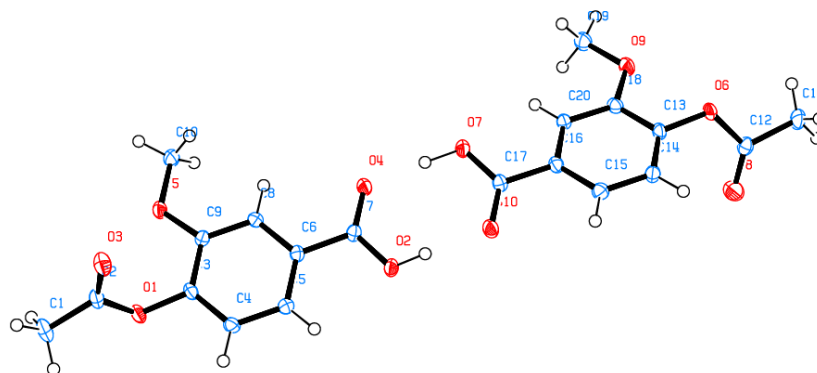


Figure 21. Molecular structure of acetylvainillin acid

- 4-acetoxy-3-methoxyphenylacetic acid (6)

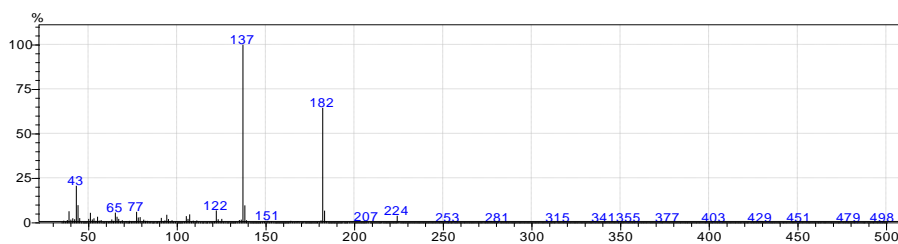


Figure 22. Mass spectrum of 4-acetoxy-3-methoxyphenylacetic acid

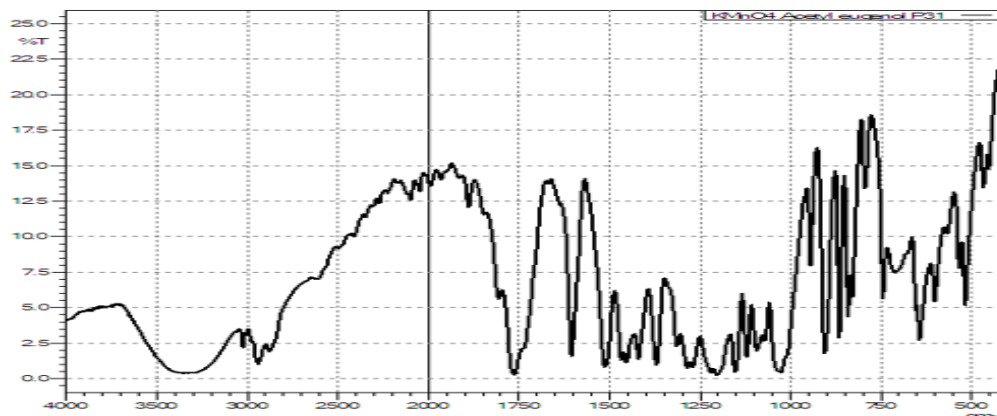


Figure 23. Infra-red spectrum of 4-acetoxy-3-methoxyphenylacetic acid

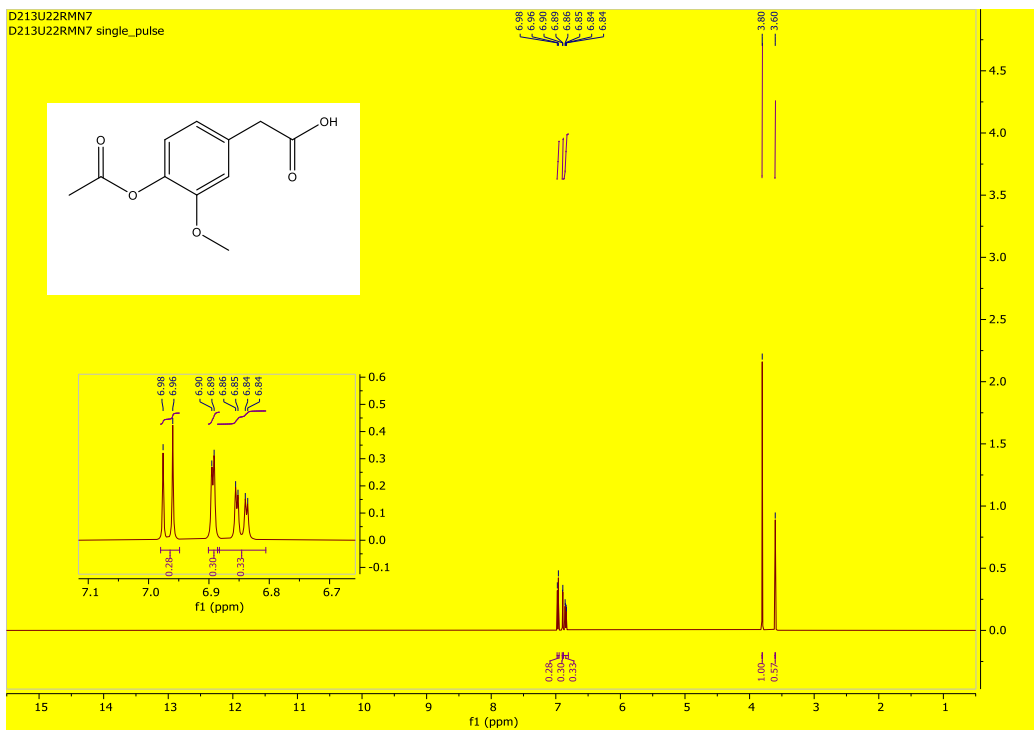


Figure 24. ^1H NMR spectrum of 4-acetoxy-3-methoxyphenylacetic acid

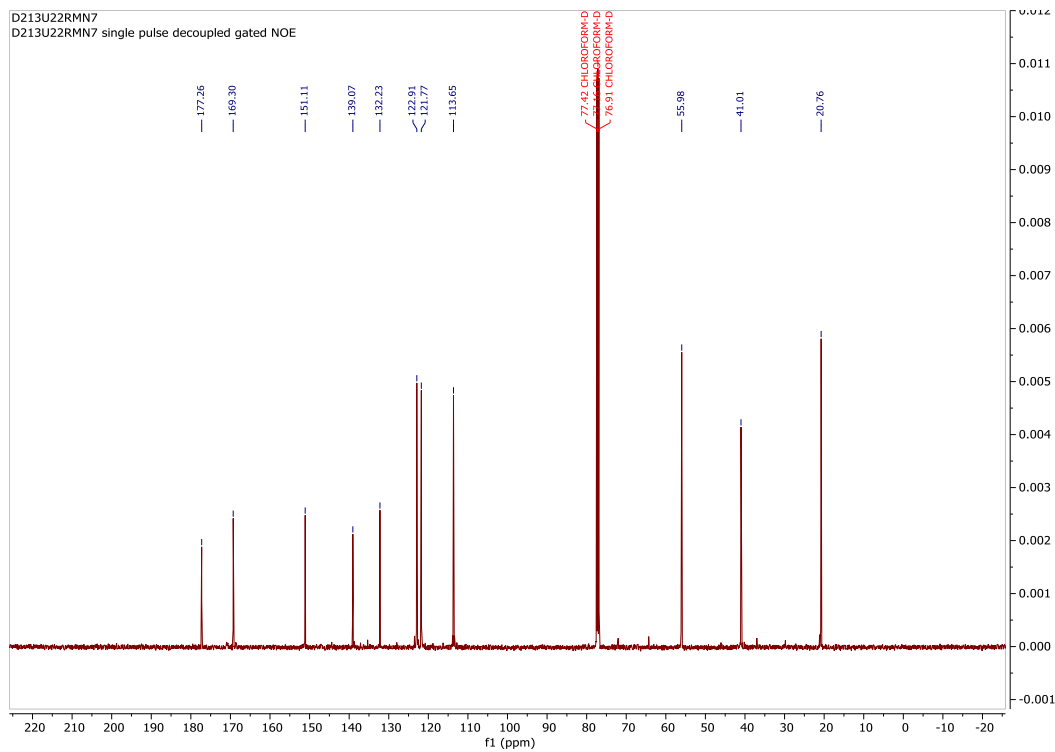


Figure 25. ^{13}C NMR spectrum of 4-acetoxy-3-methoxyphenylacetic acid

- 4-(2,3-dihydroxypropyl)-2-methoxyphenyl acetate (7)

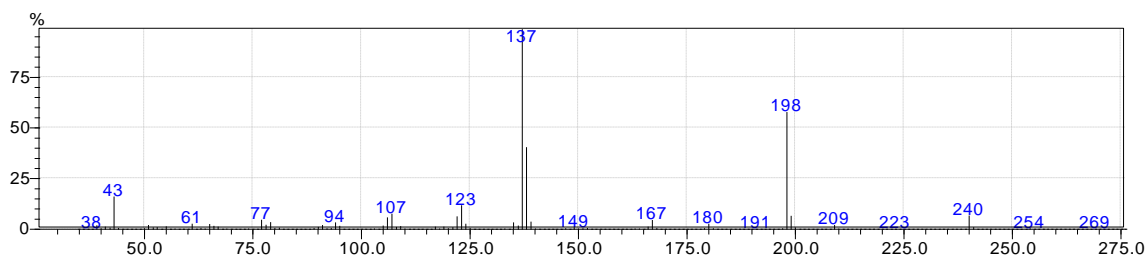


Figure 26. Mass spectrum of 4-(2,3-dihydroxypropyl)-2-methoxyphenyl acetate

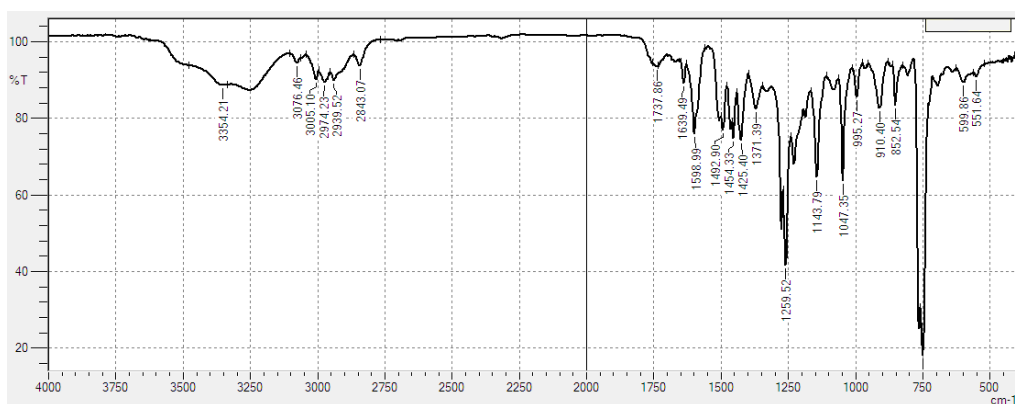


Figure 27. Infra-red spectrum of 4-(2,3-dihydroxypropyl)-2-methoxyphenyl acetate

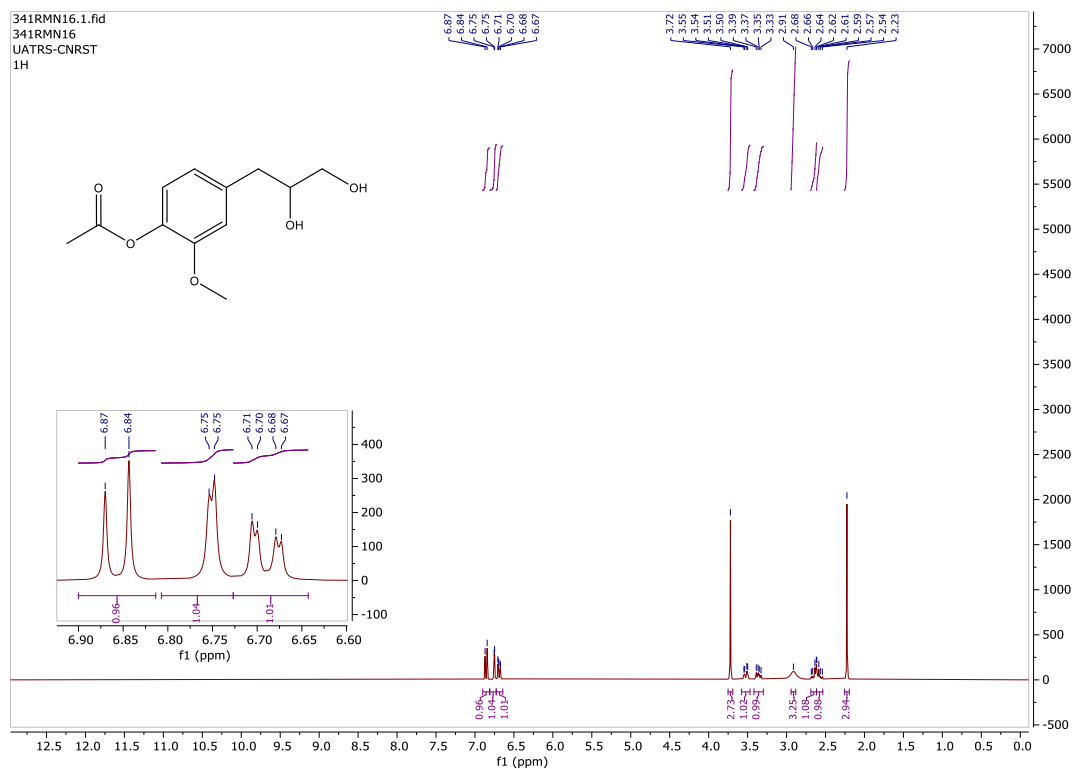


Figure 28. ¹H NMR spectrum of 4-(2,3-dihydroxypropyl)-2-methoxyphenyl acetate

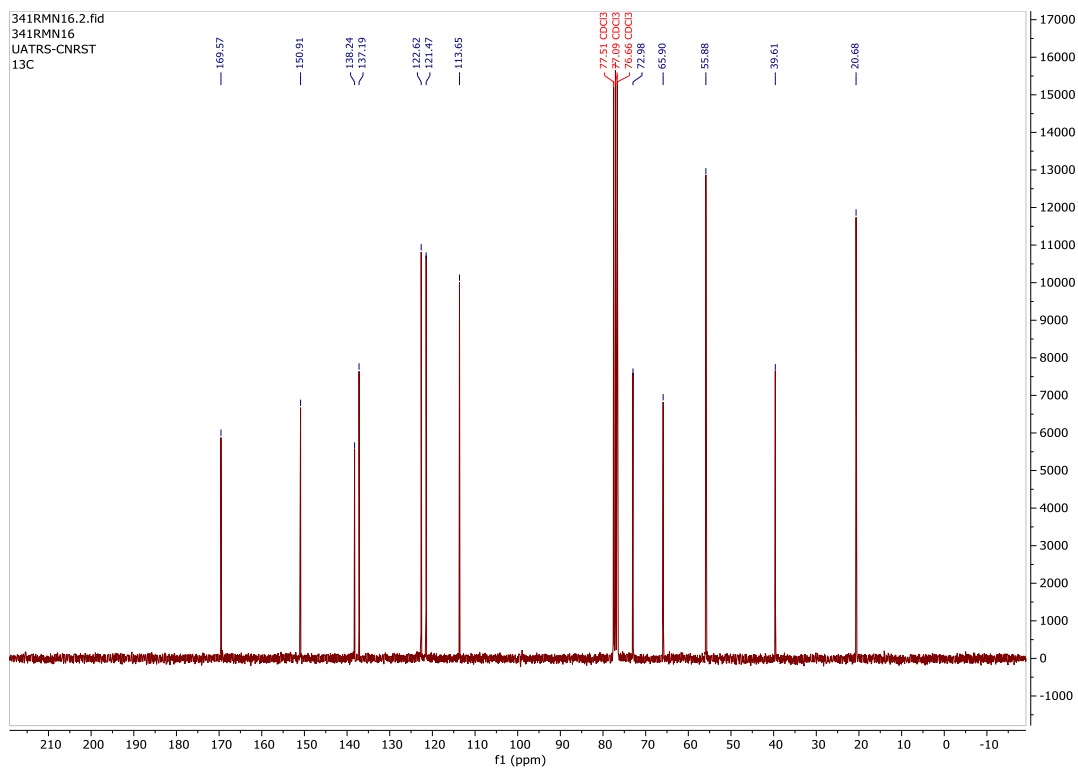


Figure 29. ^{13}C NMR spectrum of 4-(2,3-dihydroxypropyl)-2-methoxyphenyl acetate

- **Vanillin (8)**

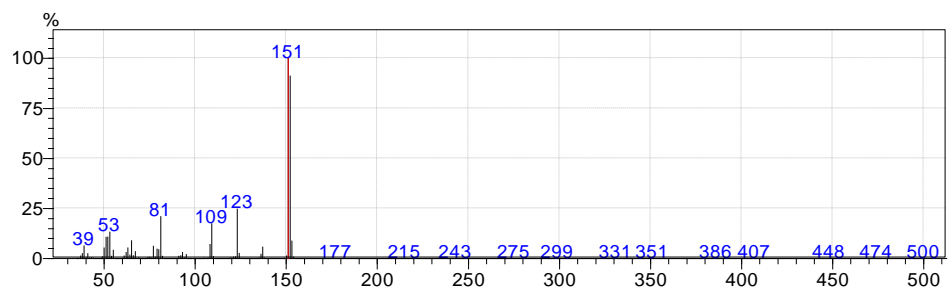


Figure 30. Mass spectrum of vanillin

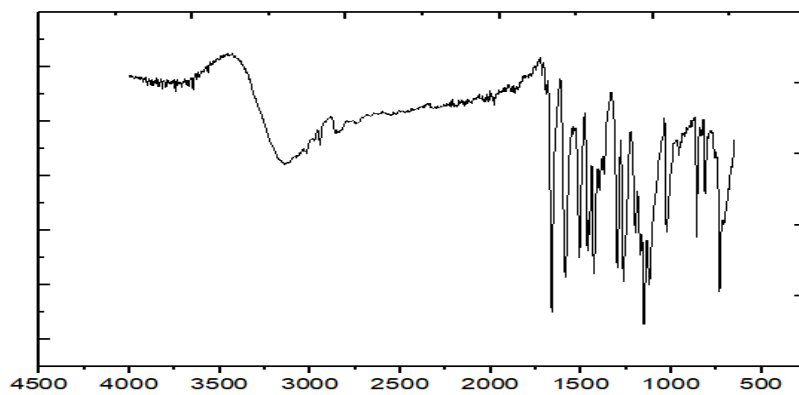


Figure 31. Infra-red spectrum of vanillin

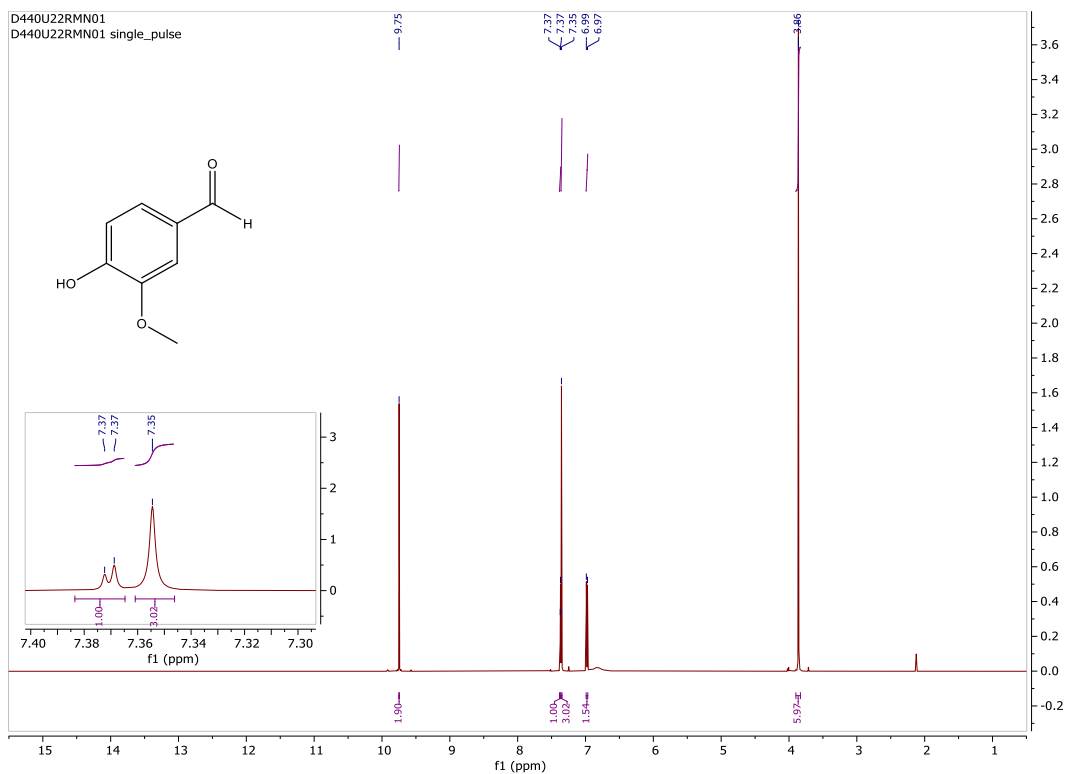


Figure 32. ^1H NMR spectrum of vanillin

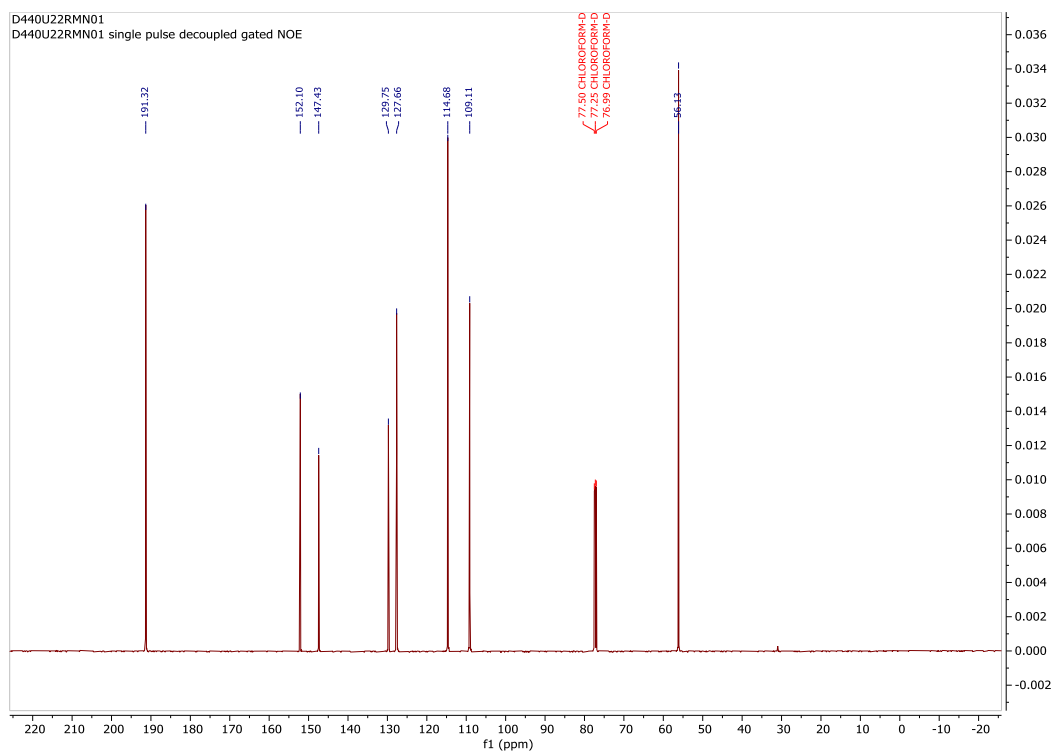


Figure 33. ^{13}C NMR spectrum of vanillin

- Vanillin oxime (9)

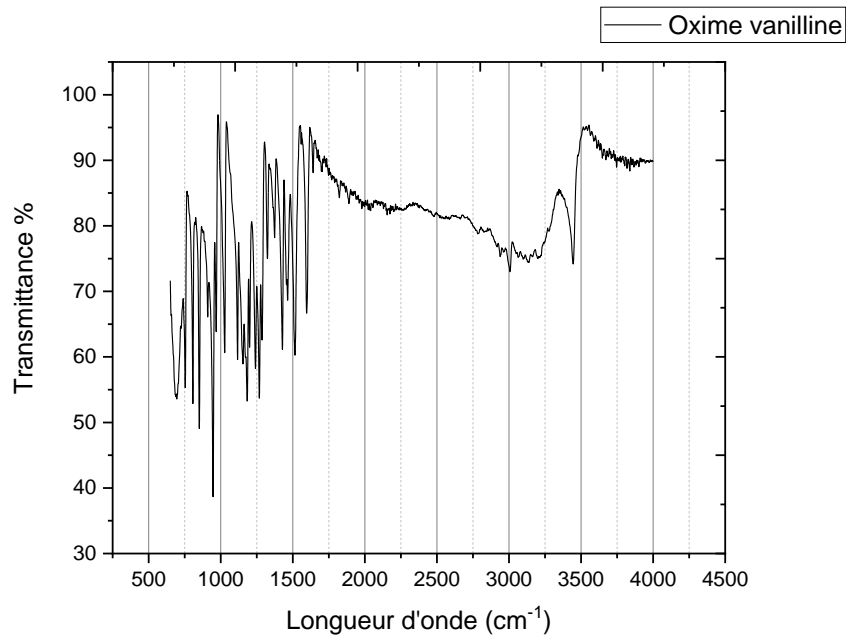


Figure 34. Infra-red spectrum of vanillin oxime

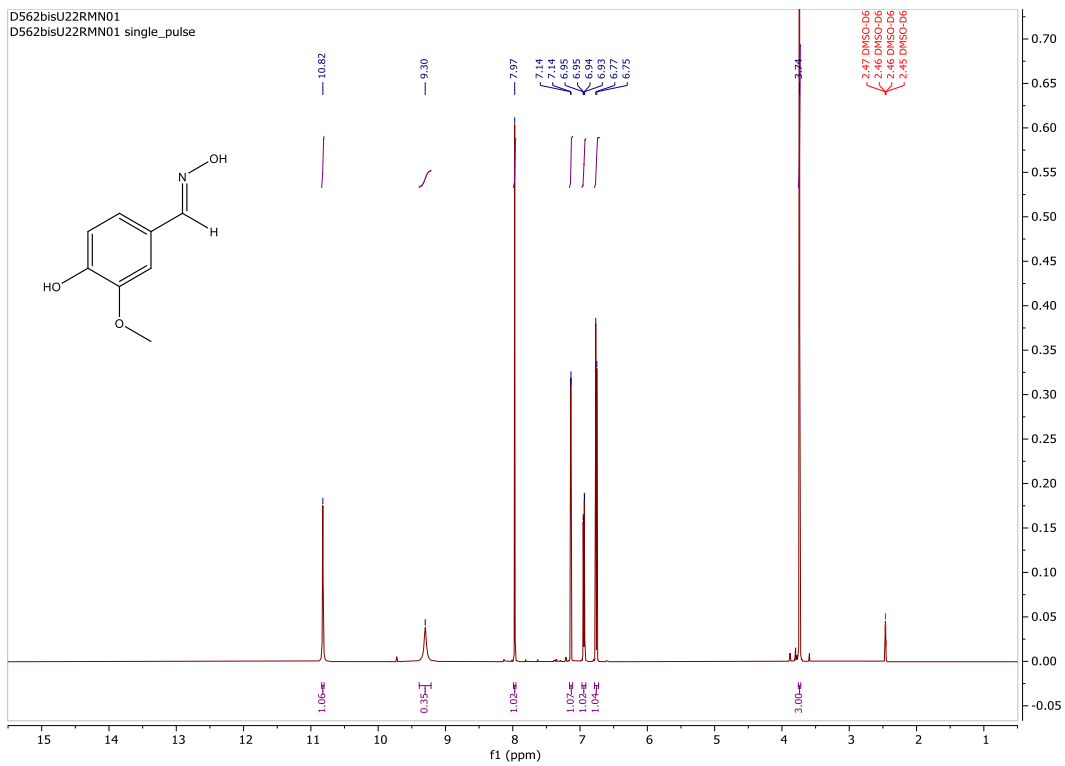


Figure 35. ¹H NMR spectrum of vanillin oxime

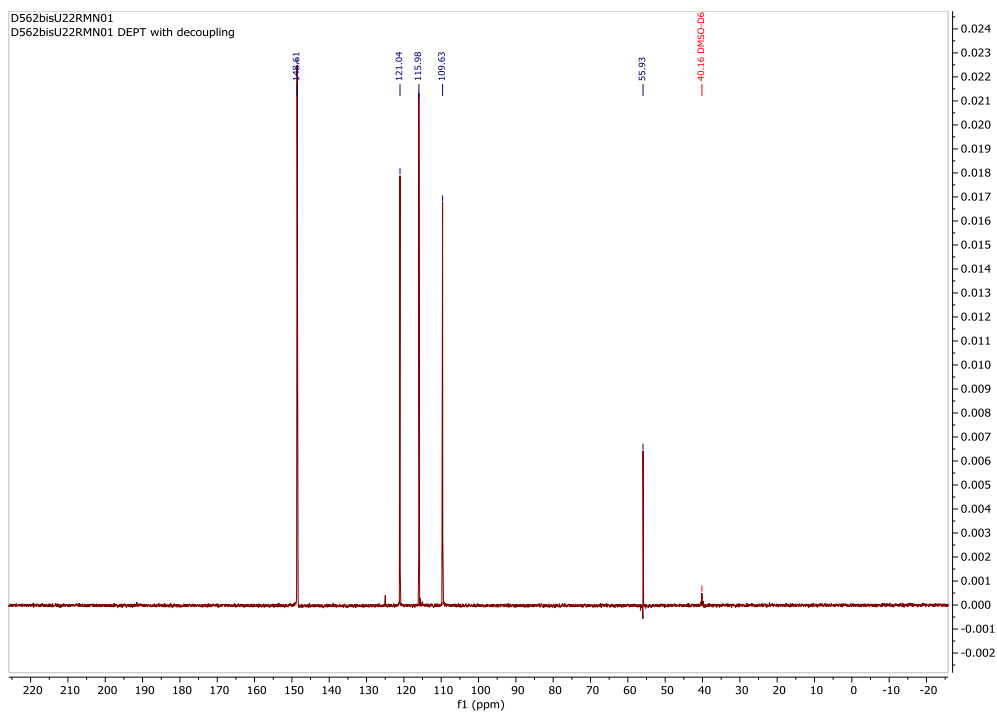


Figure 36. ^{13}C NMR spectrum of vanillin oxime

- **Methyl 4-hydroxy-3-methoxybenzoate (10)**

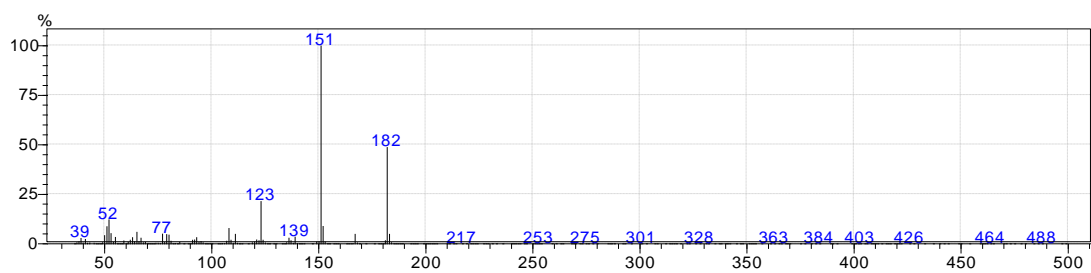


Figure 37. Mass spectrum of methyl 4-hydroxy-3-methoxybenzoate

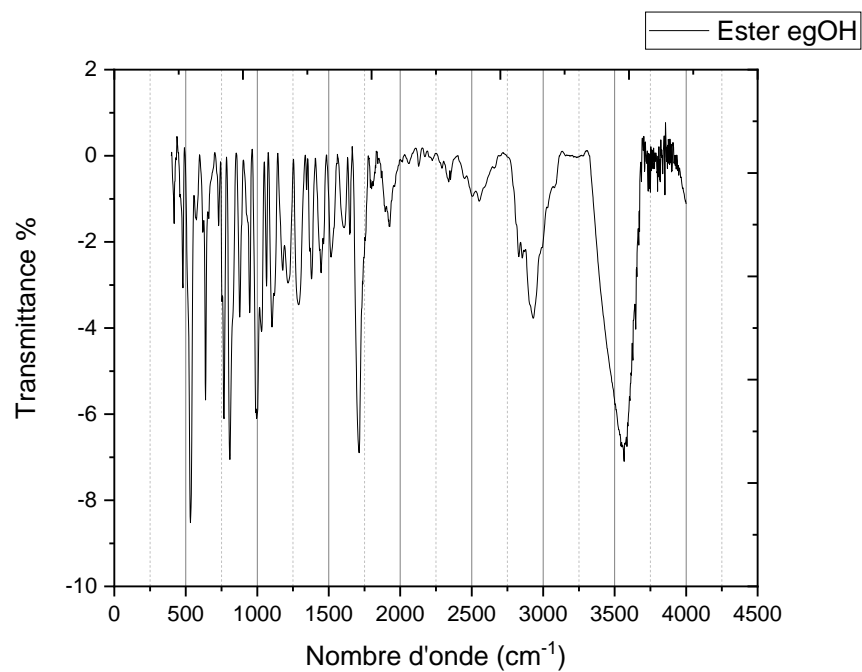


Figure 38. Infra-red spectrum of methyl 4-hydroxy-3-methoxybenzoate

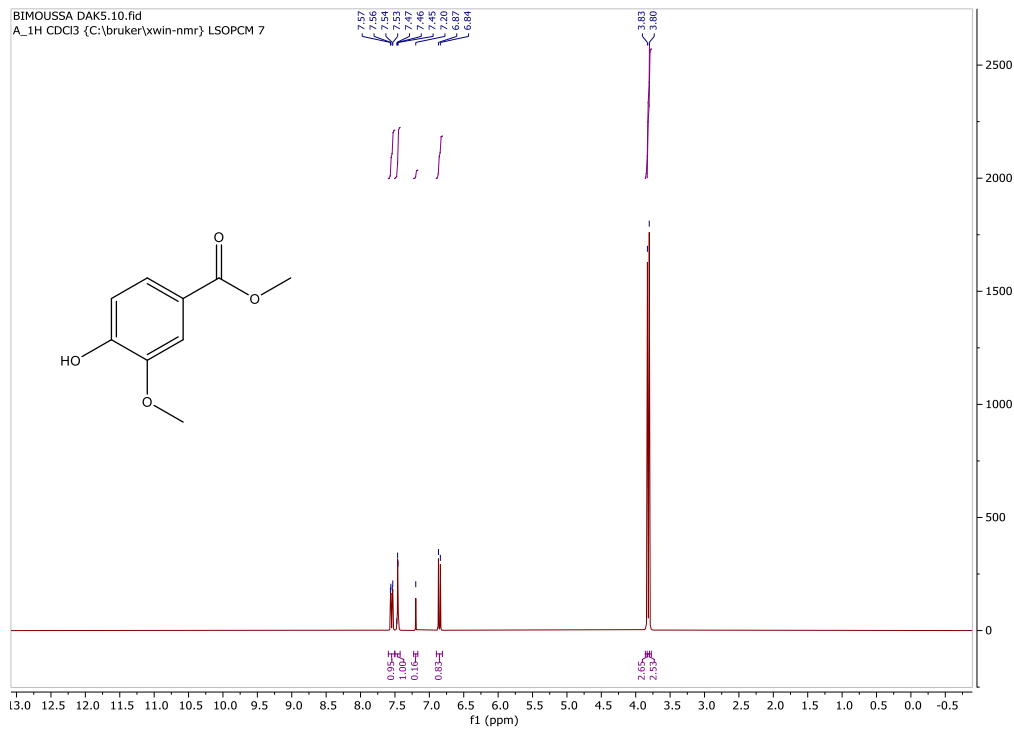


Figure 39. ¹H NMR spectrum of methyl 4-hydroxy-3-methoxybenzoate

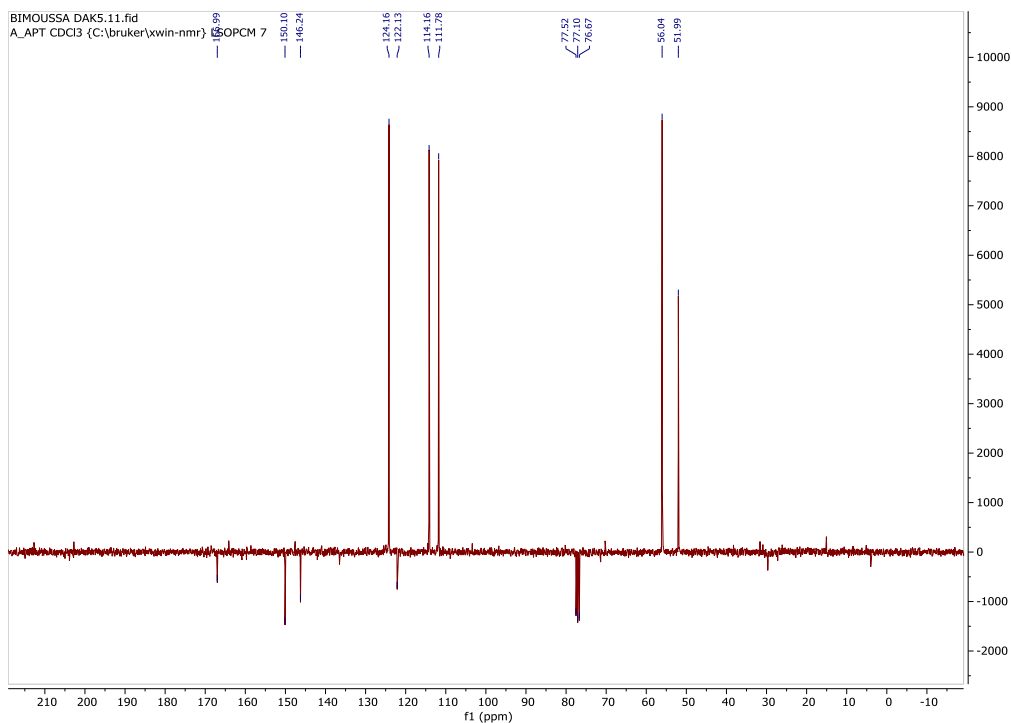


Figure 40. ^{13}C NMR spectrum of methyl 4-hydroxy-3-methoxybenzoate

- **Vanillic acid (11)**

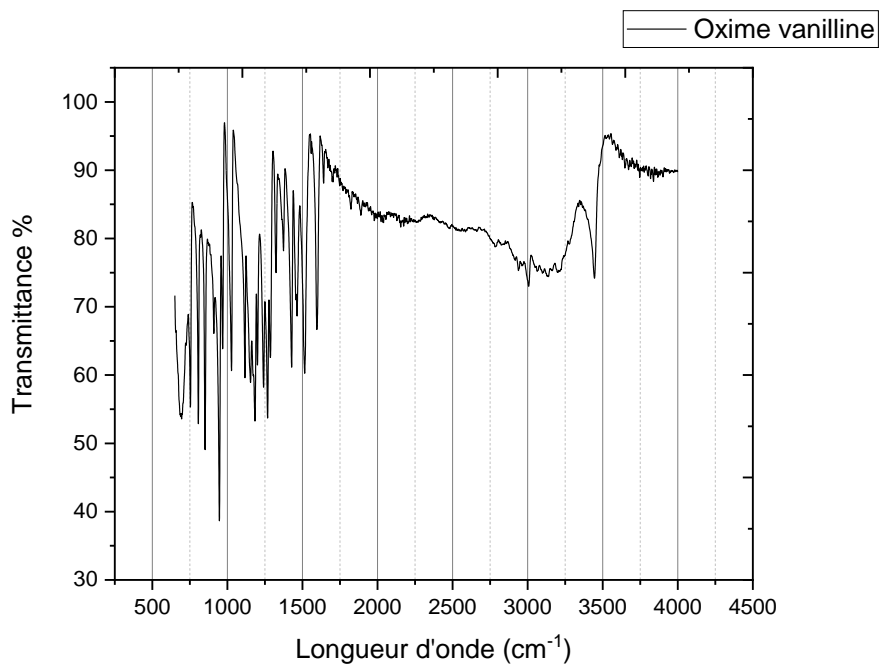


Figure 41. Infra-red spectrum of vanillic acid

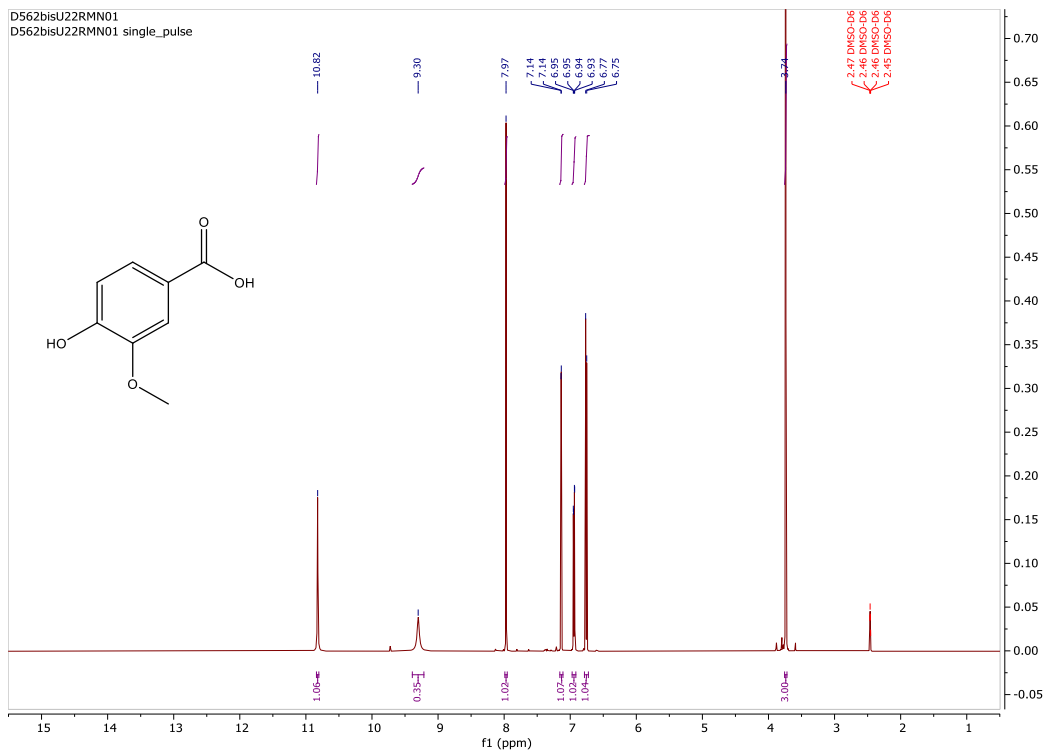


Figure 42. ^1H NMR spectrum of vanillic acid

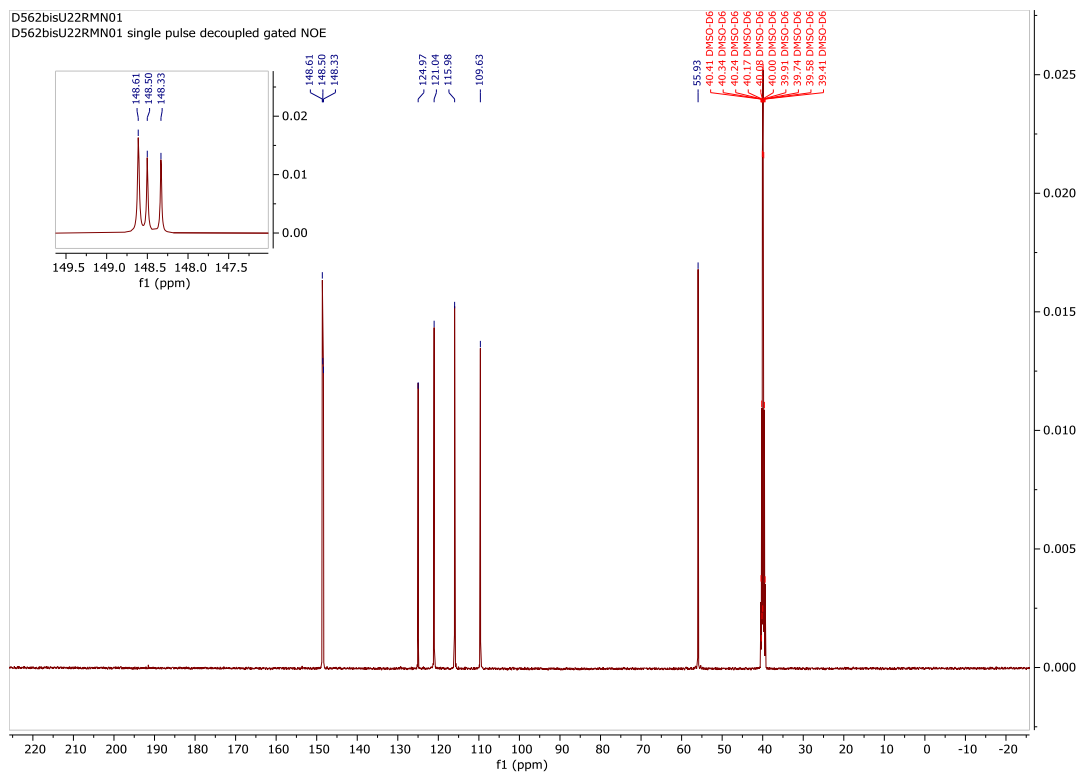


Figure 43. Spectre RMN ^{13}C de de vanillic acid

- 4-(benzyloxy)-3-methoxybenzoic acid (12)

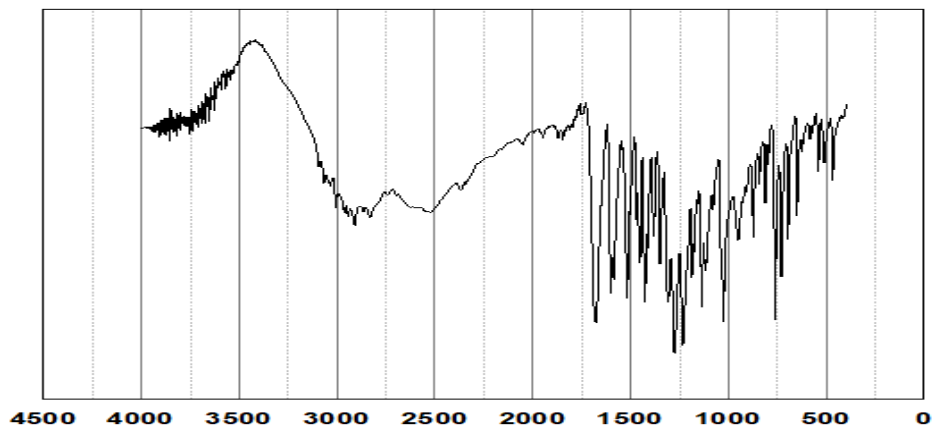


Figure 44. Infra-red spectrum of 4-(benzyloxy)-3-methoxybenzoic acid

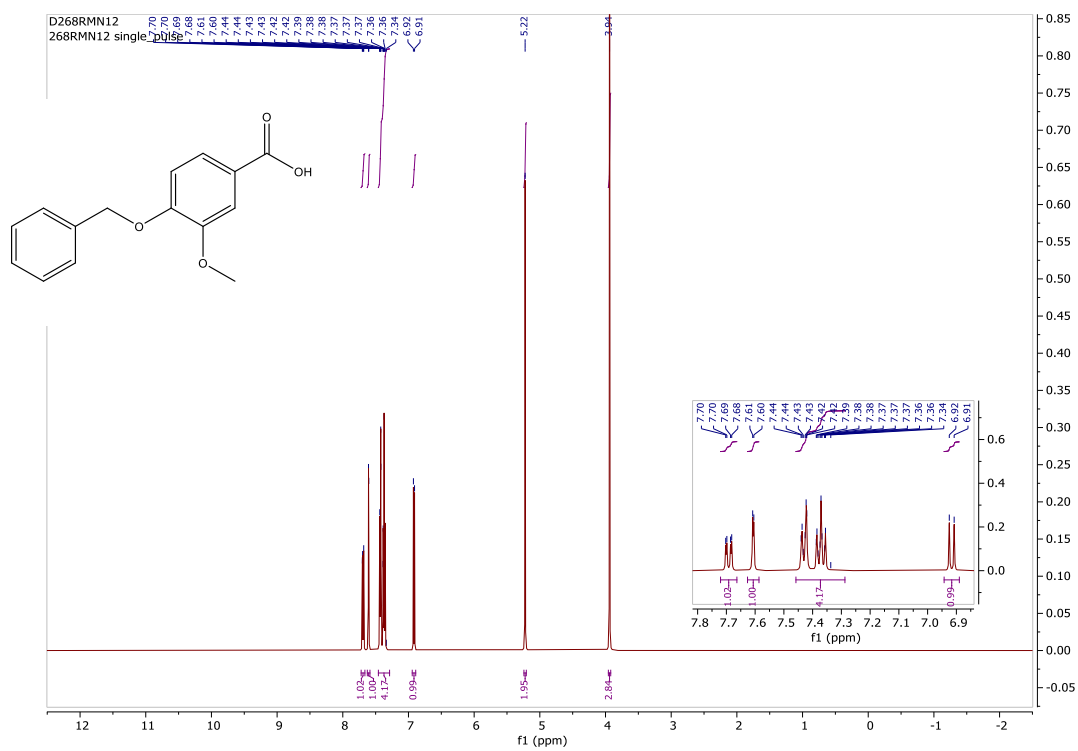


Figure 45. ¹H NMR spectrum of 4-(benzyloxy)-3-methoxybenzoic acid

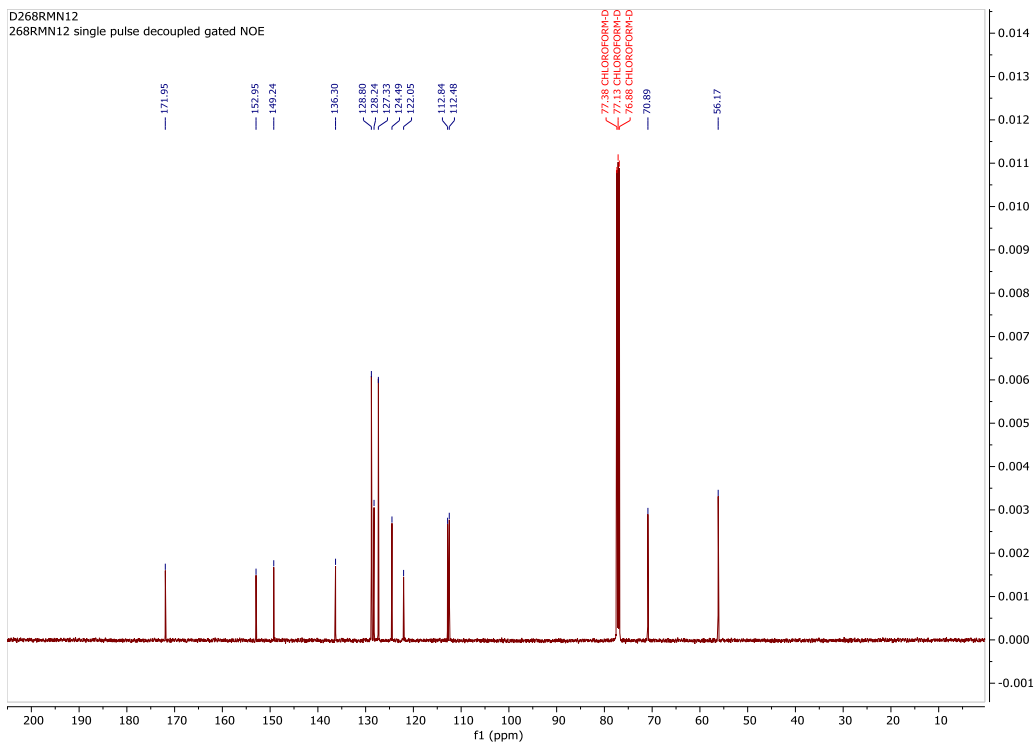


Figure 46. ^{13}C NMR spectrum of 4-(benzyloxy)-3-methoxybenzoic acid

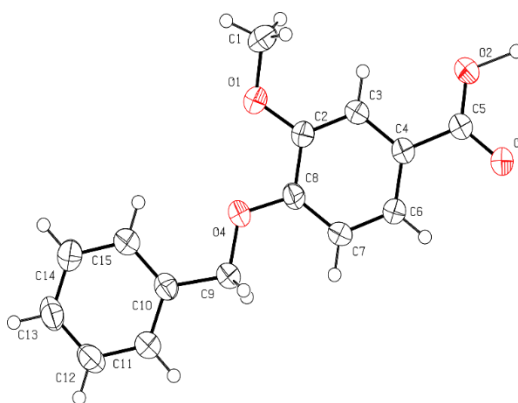


Figure 47. Molecular structure of 4-(benzyloxy)-3-methoxybenzoic acid

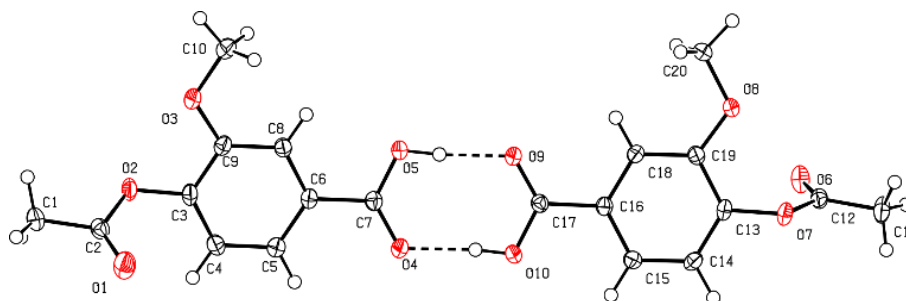


Figure 48. Molecular structure of Acetylvainillin acid

Table 1. Crystallographic data of acetylvanillin acid and 4-(benzyloxy)-3-methoxybenzoic acid

Experiments were carried out with Cu *K* α radiation using a Bruker D8 Venture diffractometer. Absorption was corrected for by numerical methods, *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., *J. Appl. Cryst.* 48 (2015) 3-10. H atoms were treated by a mixture of independent and constrained refinement.

	Acetylvanillin acid	4-(benzyloxy)-3-methoxybenzoic acid
Chemical formula	C ₁₀ H ₁₀ O ₅	C ₁₅ H ₁₄ O ₄
M_r	210.18	258.26
Crystal system, space group	Monoclinic, $P2_1/n$	Triclinic, $P\bar{1}$
Temperature (K)	100	296
a, b, c (Å)	5.2172 (7), 12.2478 (8), 30.949 (5)	5.0827 (1), 8.1994 (2), 15.3955 (3)
a, b, γ (°)	90, 95.428 (9), 90	90.573 (1), 97.623 (1), 96.311 (1)
V (Å ³)	1968.7 (4)	631.89 (2)
Z	8	2
μ (mm ⁻¹)	0.99	0.82
Crystal size (mm)	0.26 × 0.13 × 0.12	0.33 × 0.13 × 0.04
T_{\min}, T_{\max}	0.786, 1.000	0.792, 1.000
No. of measured, independent and observed [$I > 2s(I)$] reflections	54371, 3880, 3853	25655, 2471, 2247
R_{int}	0.029	0.044
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.618	0.619
$R[F^2 > 2s(F^2)], wR(F^2), S$	0.033, 0.088, 1.08	0.042, 0.113, 1.05
No. of reflections	3880	2471
No. of parameters	281	176
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e ⁻ ·Å ⁻³)	0.23, -0.26	0.19, -0.28
CCDC deposition number	2350395	2350396