

Synthesis and Biological Evaluation of Zeise's Salt Derivatives with Acetylsalicylic Acid Substructure

Alexander Weninger¹, Daniel Baecker¹, Victoria Obermoser¹, Dorothea Egger¹, Klaus Wurst² and Ronald Gust^{1,*}

1 Department of Pharmaceutical Chemistry, Institute of Pharmacy, Center for Molecular Biosciences Innsbruck, University of Innsbruck, CCB – Centrum for Chemistry and Biomedicine, Innrain 80-82, 6020 Innsbruck, Austria; alexander.weninger@uibk.ac.at (A.W.); daniel.baecker@uibk.ac.at (D.B.); victoria.obermoser@gmx.at (V.O.); dorothea.egger@gmx.at (D.E.); ronald.gust@uibk.ac.at (R.G.)

2 Institute of General, Inorganic and Theoretical Chemistry, University of Innsbruck, CCB – Centrum for Chemistry and Biomedicine, Innrain 80-82, 6020 Innsbruck, Austria; klaus.wurst@uibk.ac.at (K.W.)

* Correspondence: ronald.gust@uibk.ac.at; Tel.: +43-512-507-58200

1. HR-ESI-MS

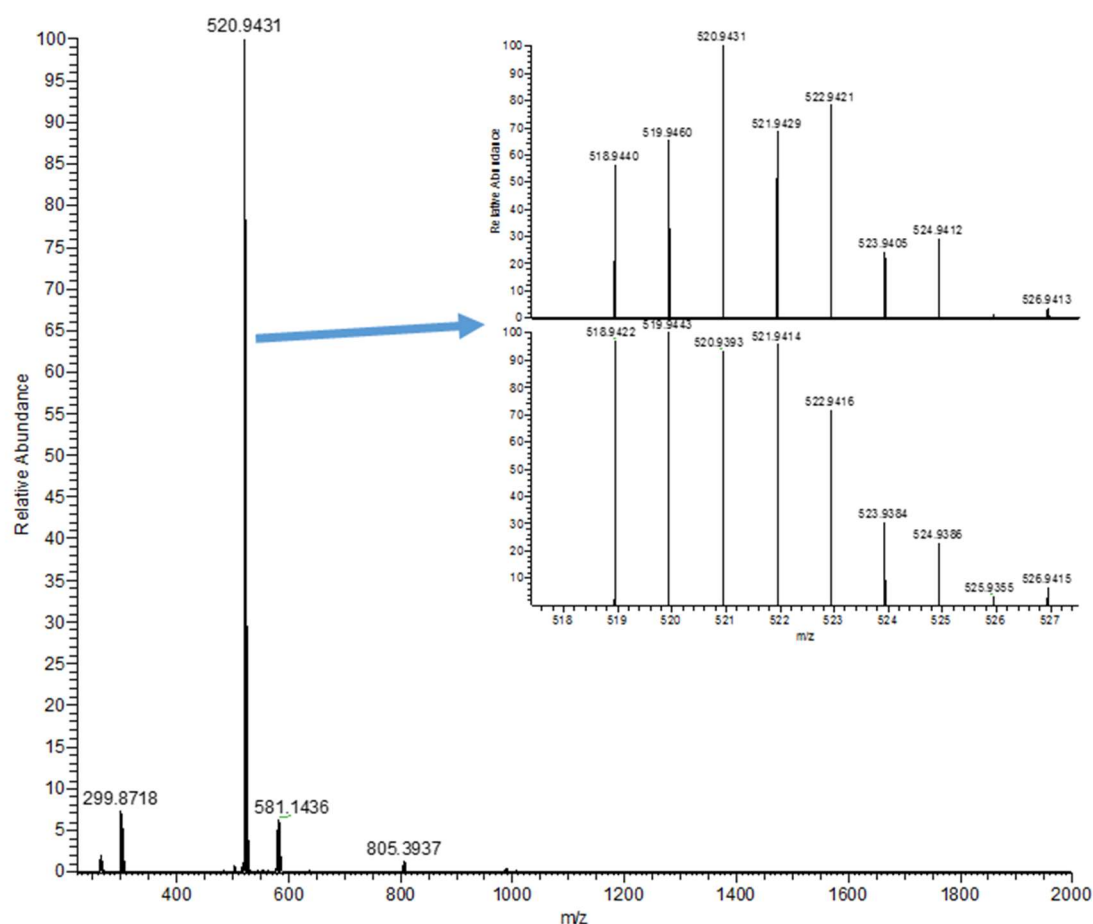


Figure S1. HR-ESI-MS spectrum of Pt-Propene-ASA (**1a**), recorded in negative mode; The inset shows the peak of [**1a**-K] with the characteristic line pattern of the platinum isotopes (top) and the calculated peak (bottom)

2. 1D and 2D NMR spectra

2.1 Propene-ASA (1)

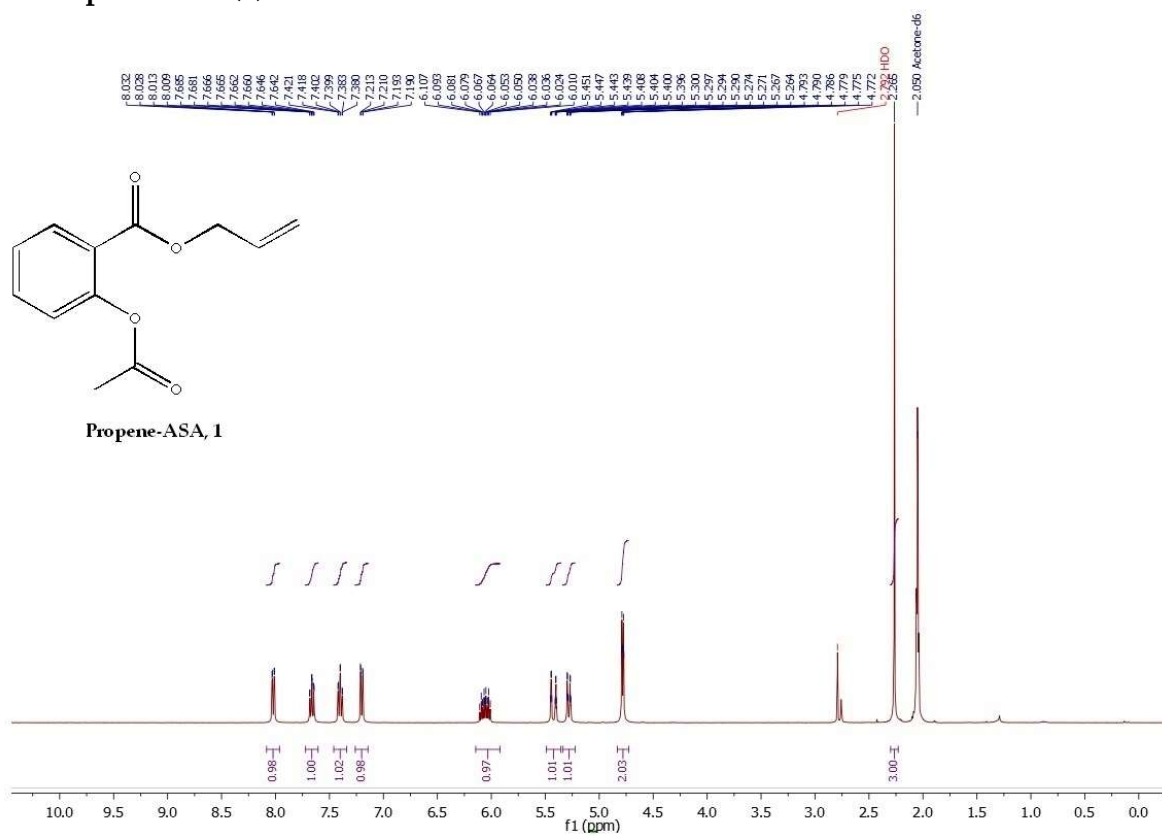


Figure S2. ^1H NMR of Propene-ASA (1) in Acetone- d_6

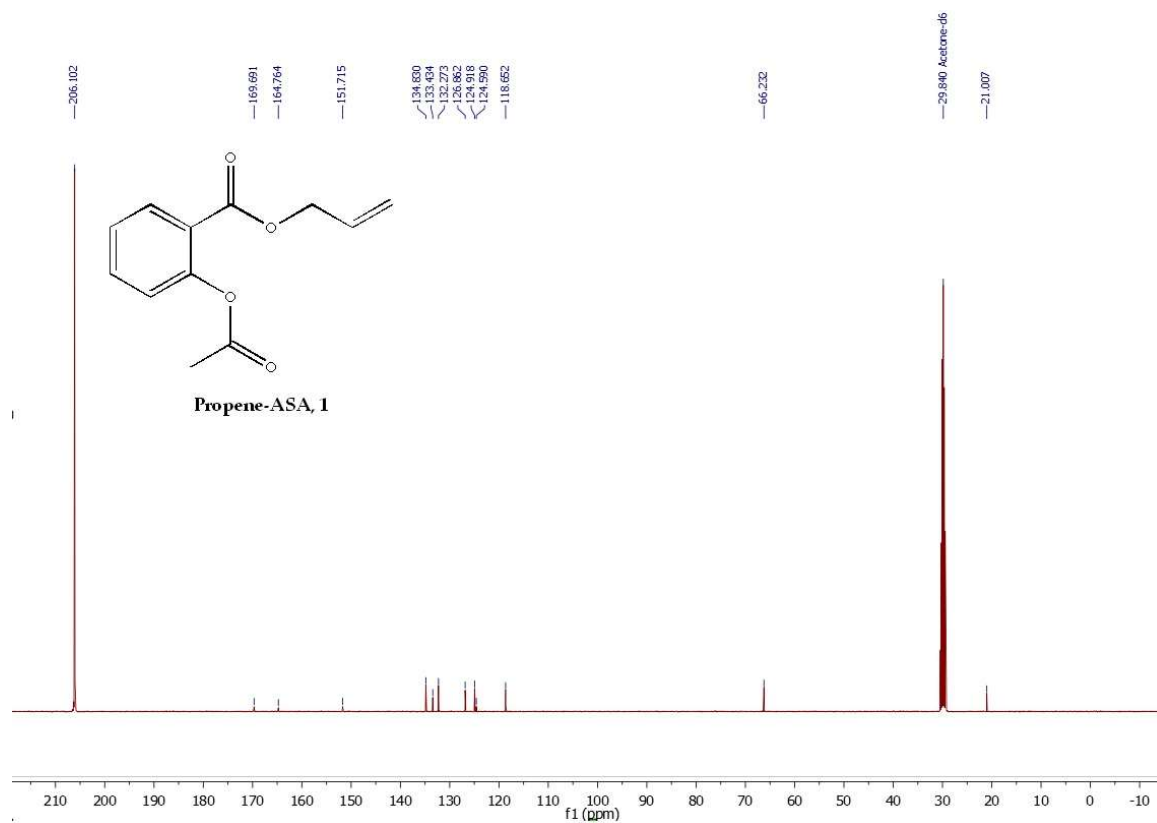
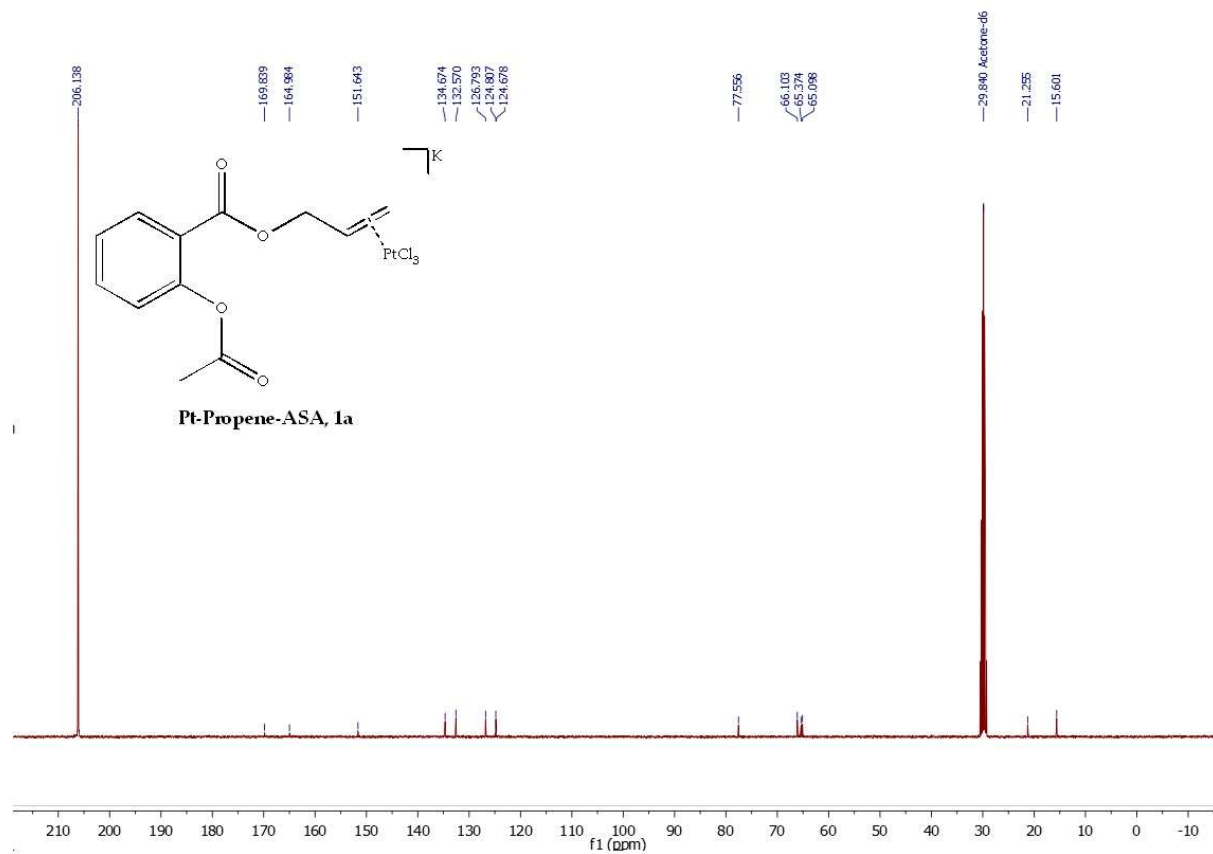
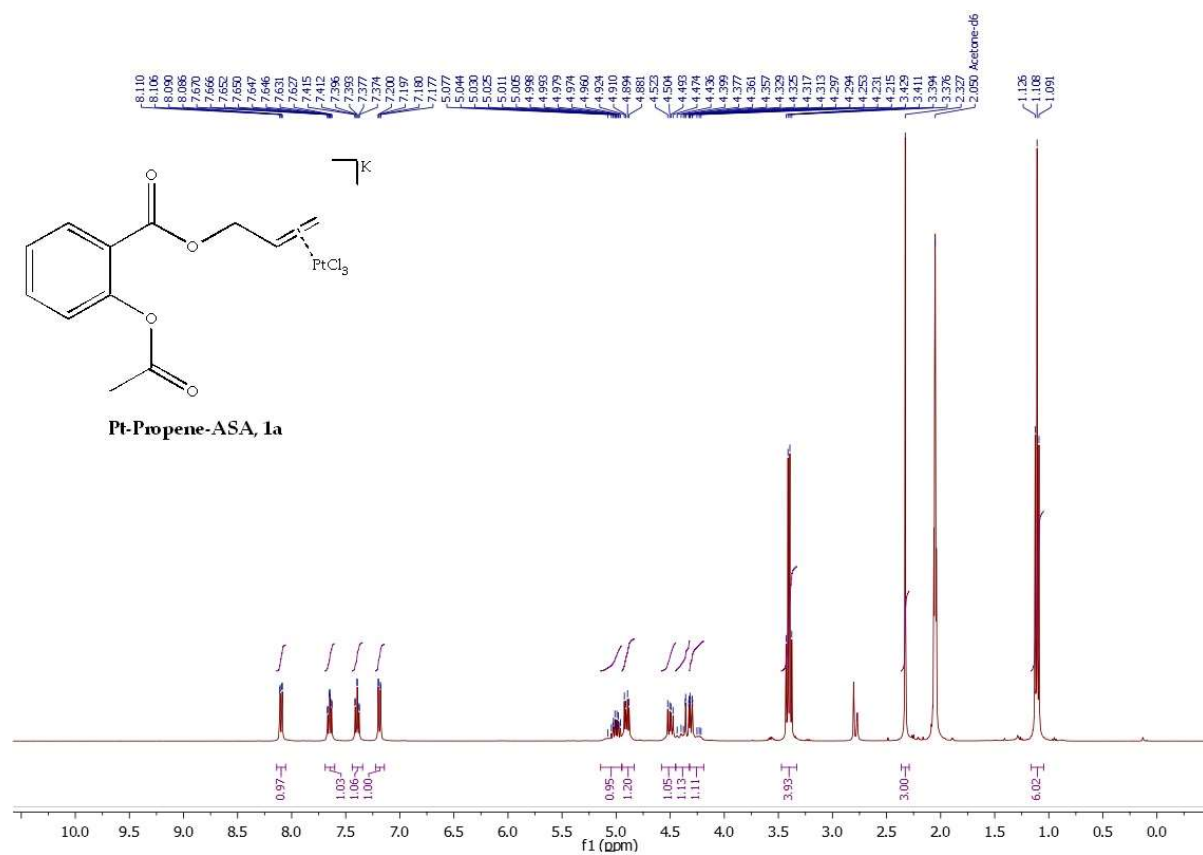


Figure S3. ^{13}C NMR of Propene-ASA (1) in Acetone- d_6

2.2 Pt-Propene-ASA (1a)



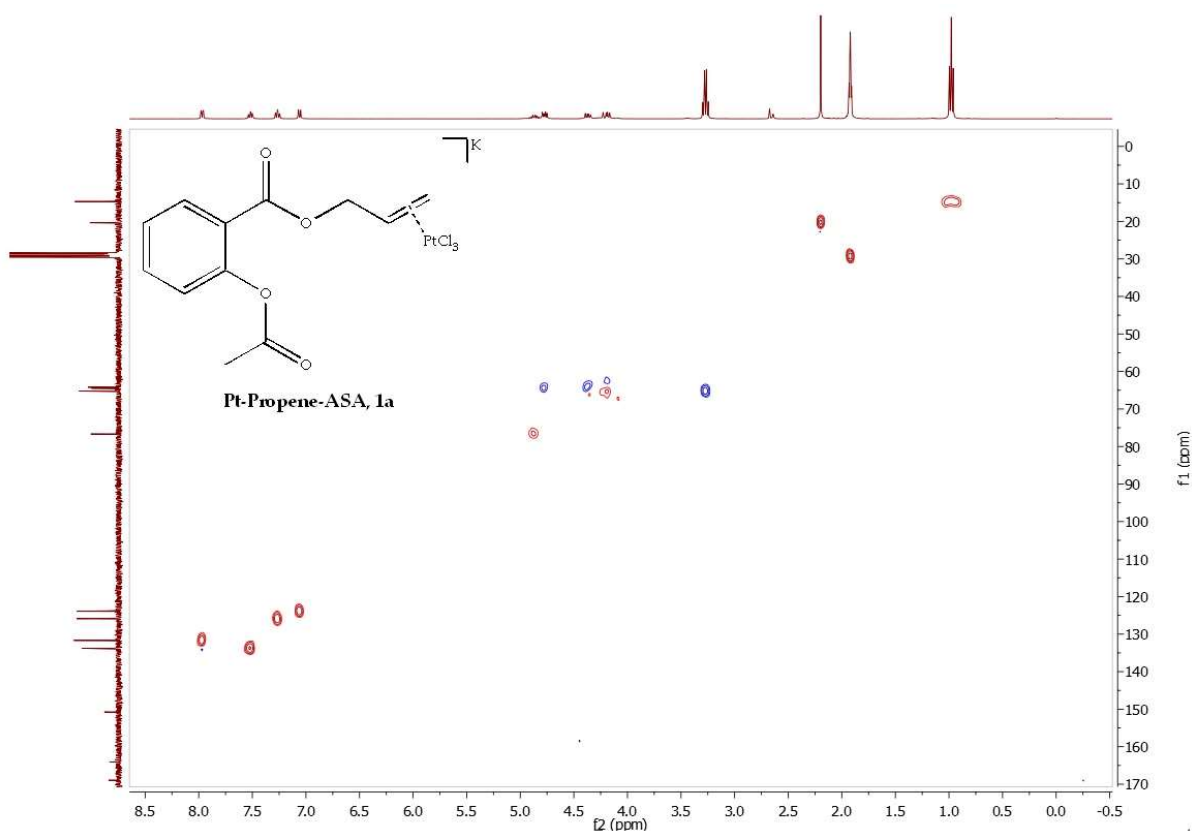


Figure S6. $[^1\text{H}, ^{13}\text{C}]$ -HSQC of Pt-Propene-ASA (1a) in Acetone- d_6

2.3 Butene-ASA (2)

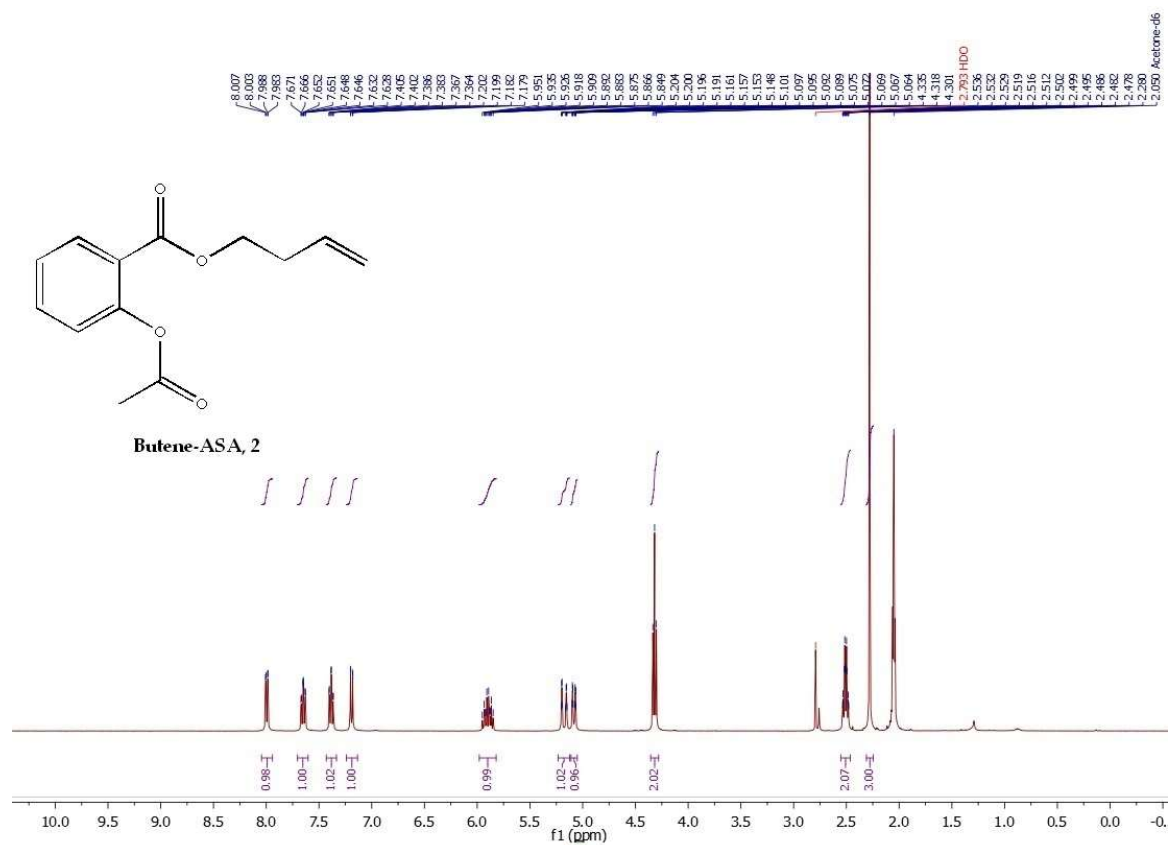


Figure S7. ^1H NMR of Butene-ASA (2) in Acetone- d_6

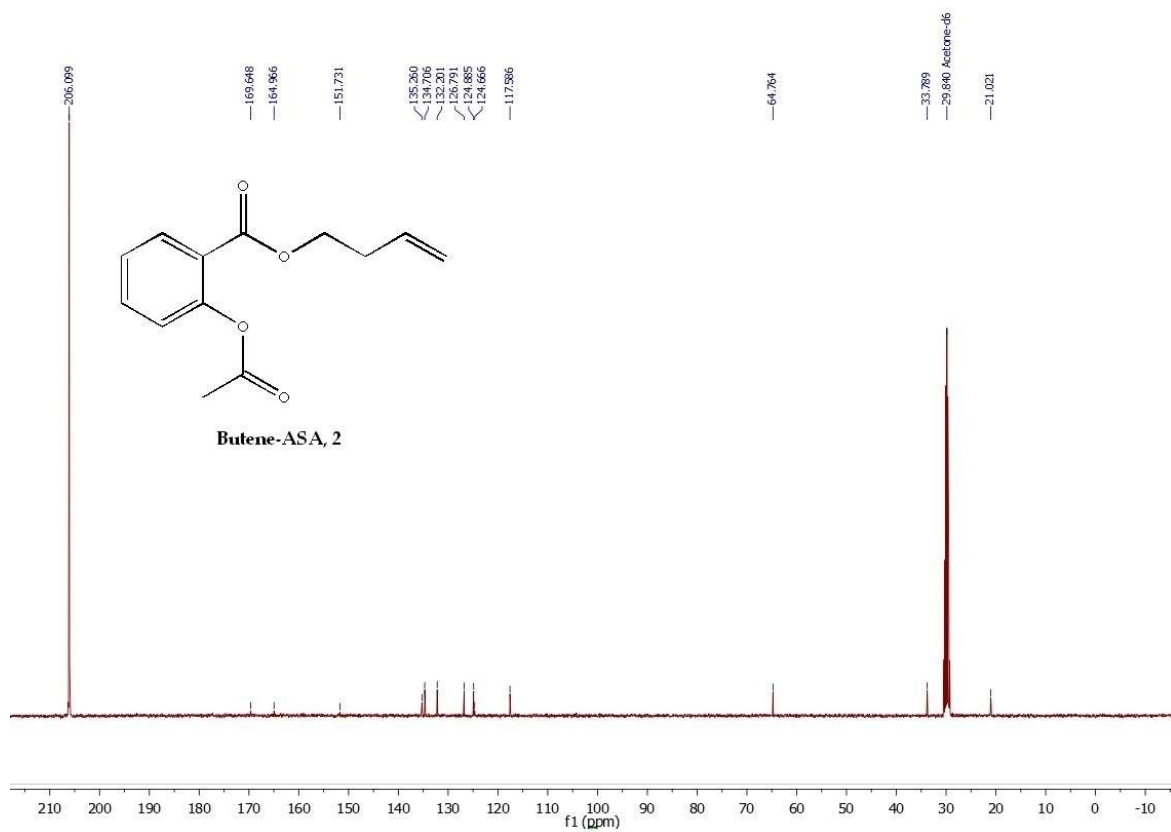


Figure S8. ¹³C NMR of Butene-ASA (2) in Acetone-d₆

2.4 Pt-Butene-ASA (2a)

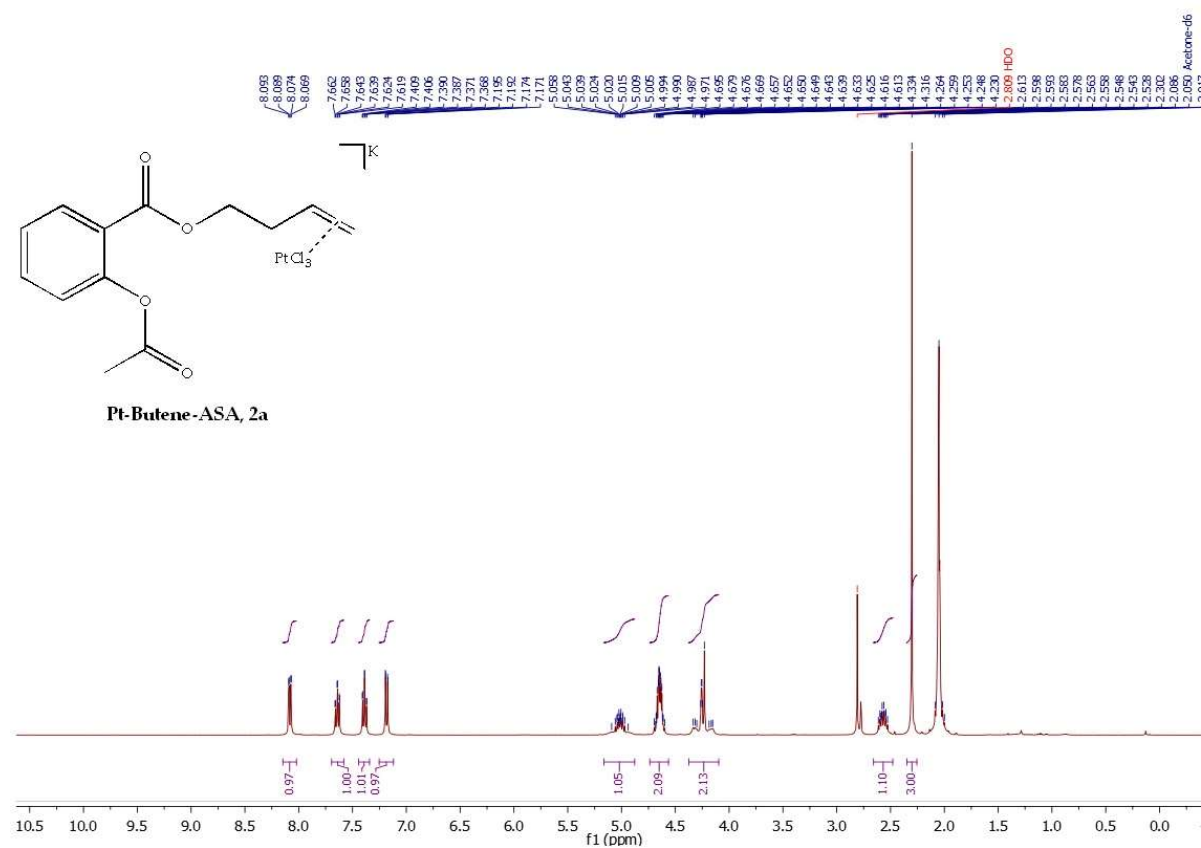


Figure S9. ¹H NMR of Pt-Butene-ASA (2a) in Acetone-d₆

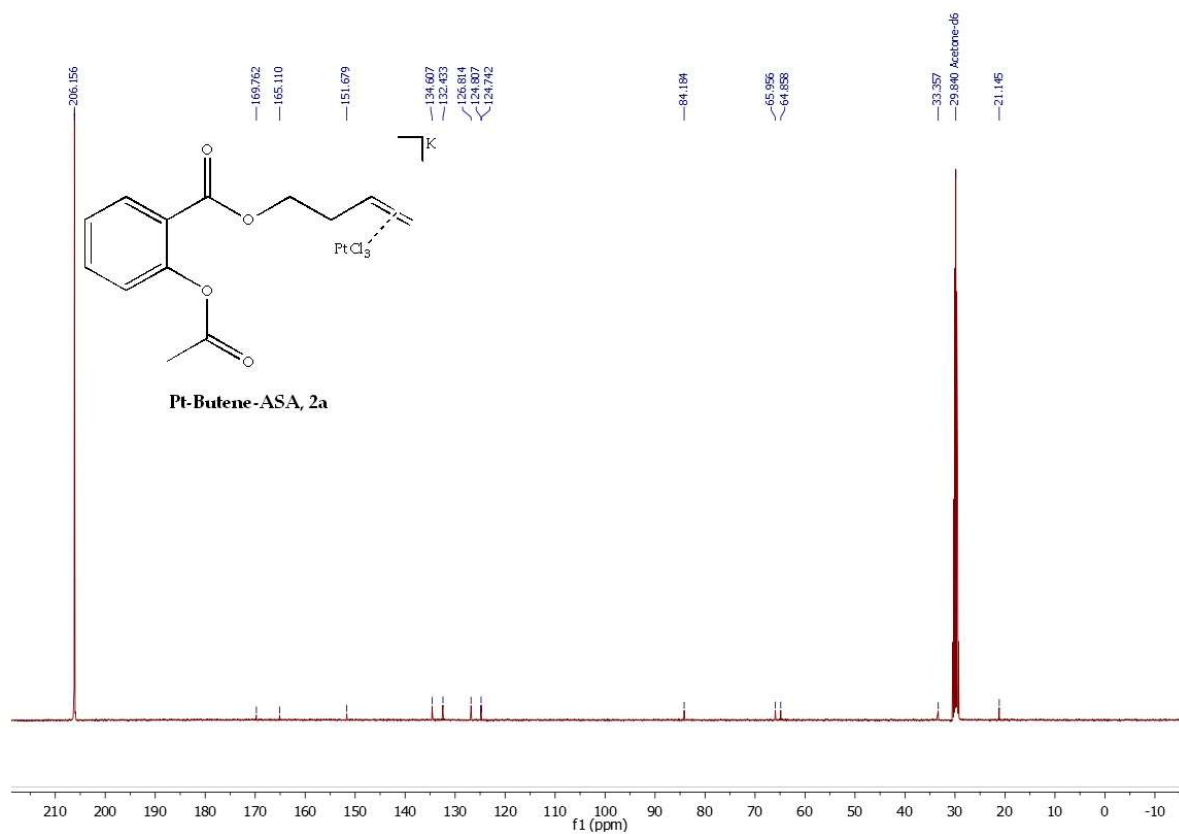


Figure S10. ^{13}C NMR of Pt-Butene-ASA (**2a**) in Acetone- d_6

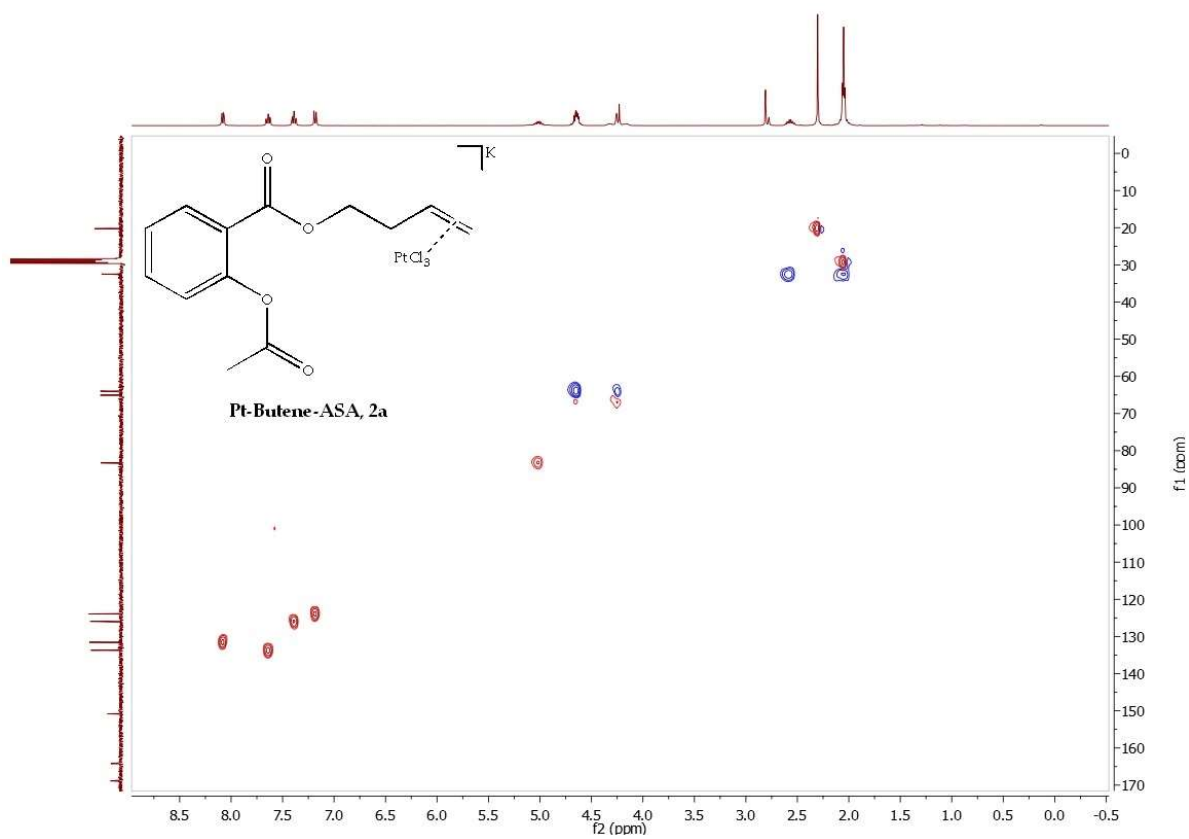


Figure S11. ^1H , ^{13}C -HSQC of Pt-Butene-ASA (**2a**) in Acetone- d_6

2.5 Pentene-ASA (3)

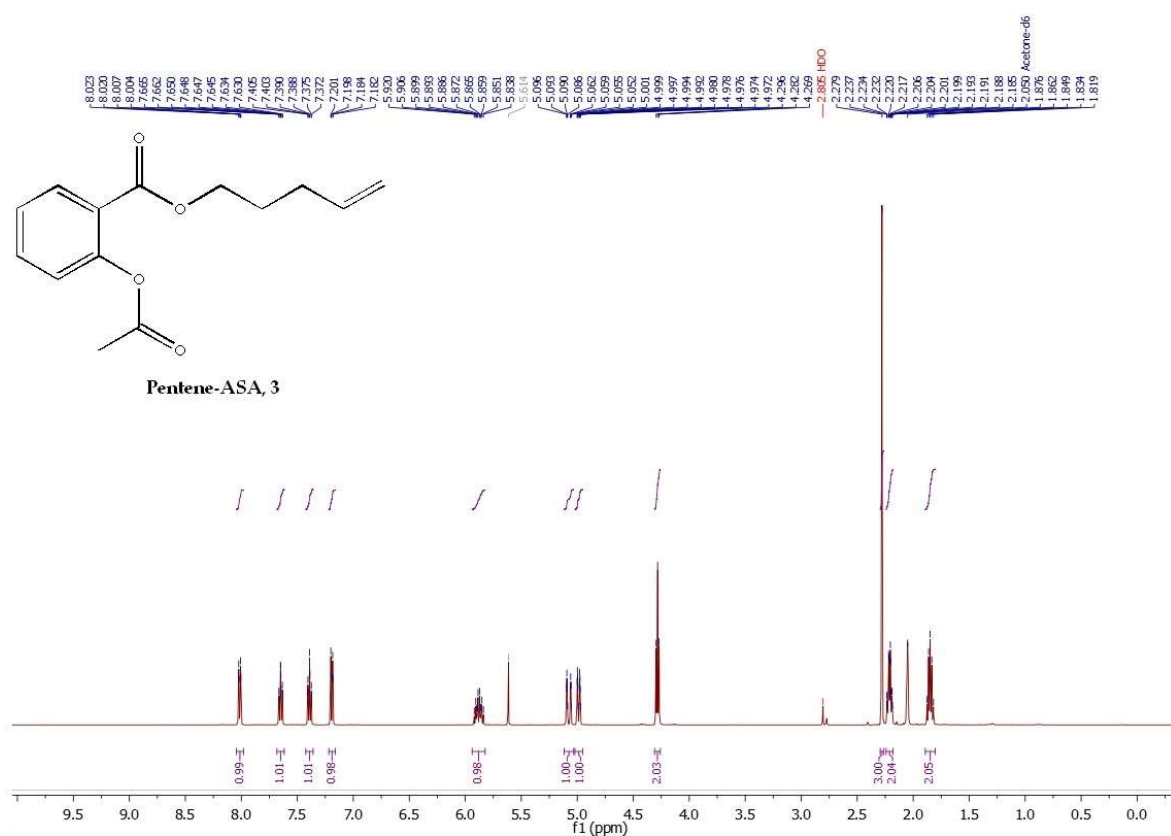


Figure S12. ¹H NMR of Pentene-ASA (3) in Acetone-*d*₆

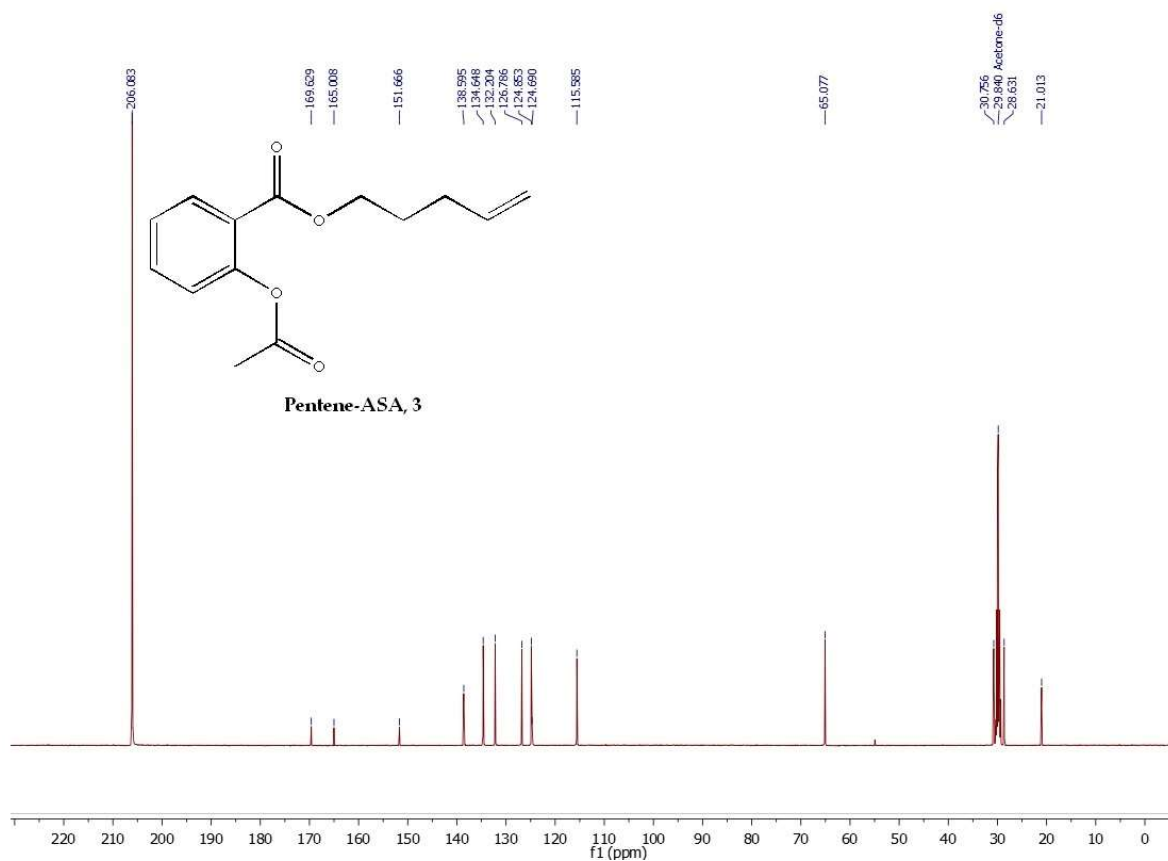


Figure S13. ¹³C NMR of Pentene-ASA (3) in Acetone-*d*₆

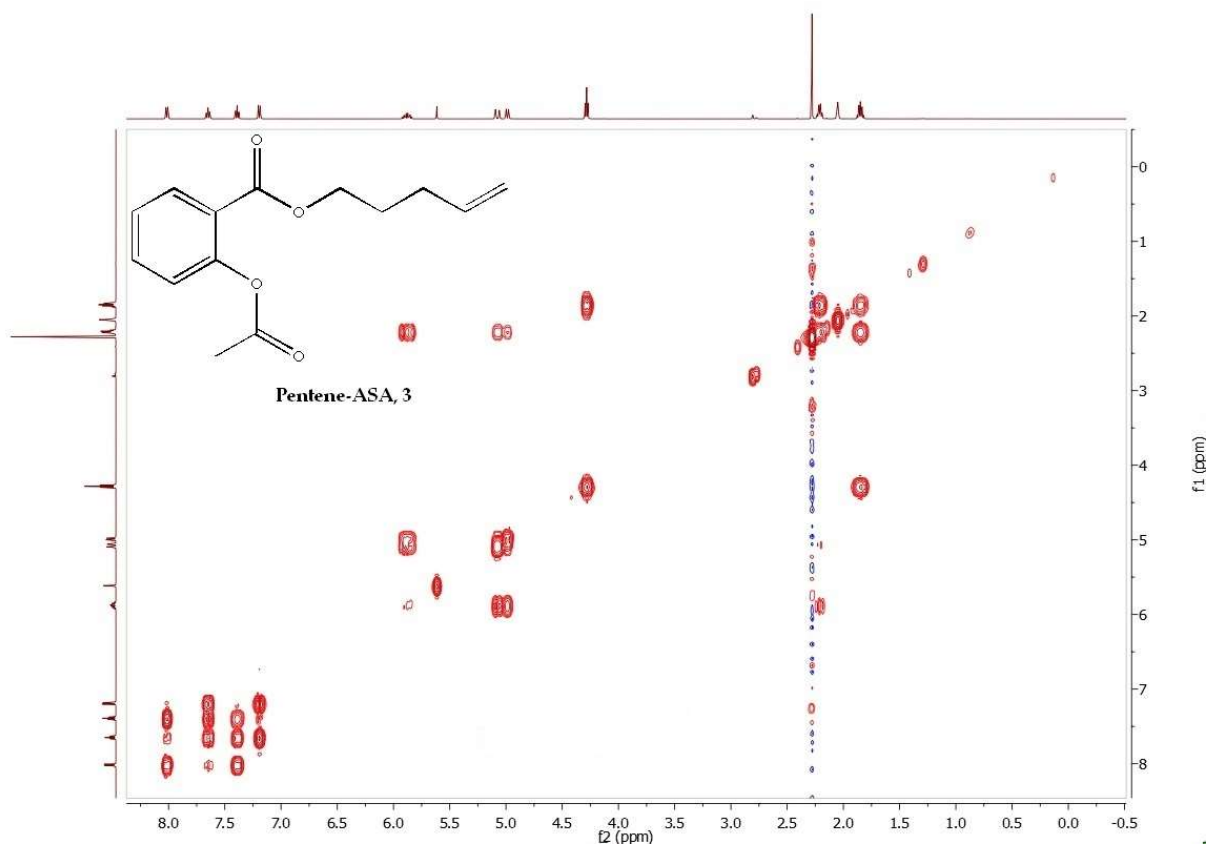


Figure S14. $[^1\text{H},^1\text{H}]$ -COSY of Pentene-ASA (3) in Acetone- d_6

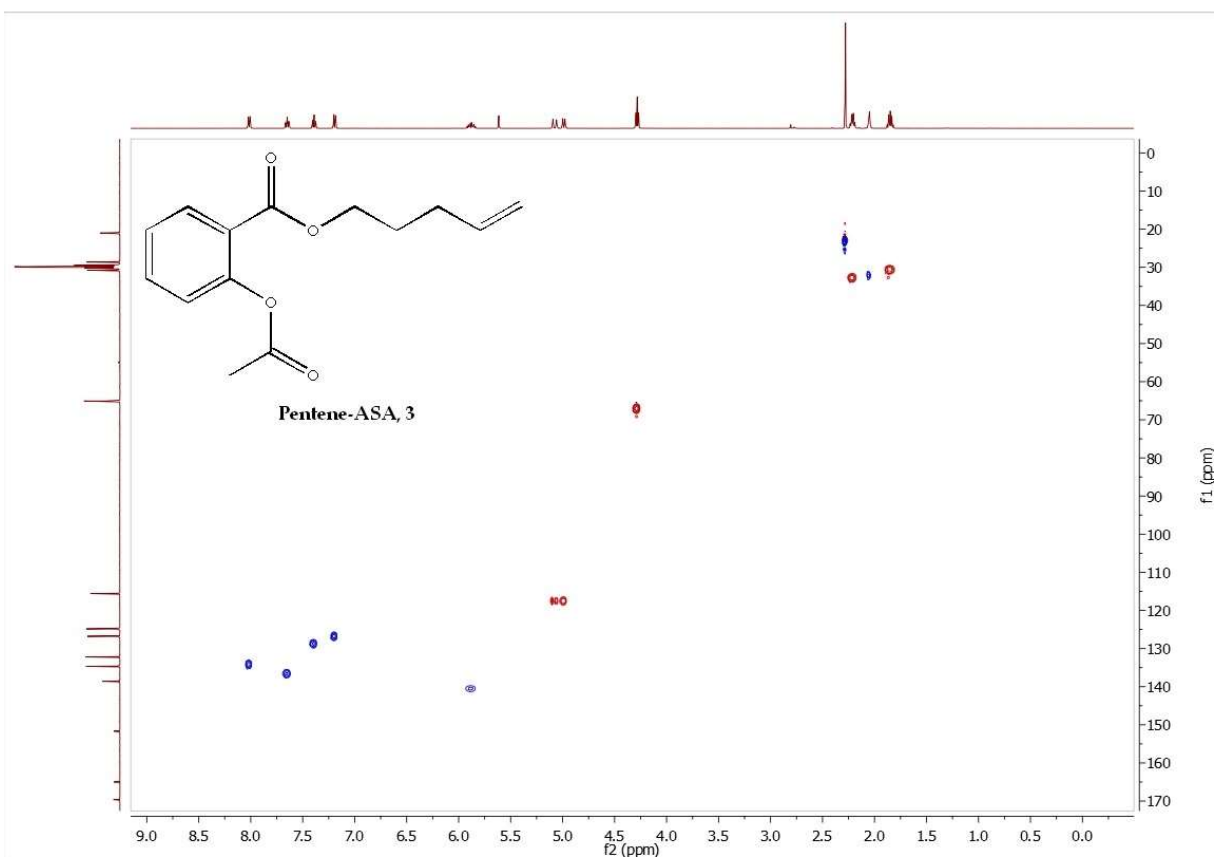


Figure S15. $[^1\text{H},^{13}\text{C}]$ -HSQC of Pentene-ASA (3) in Acetone- d_6

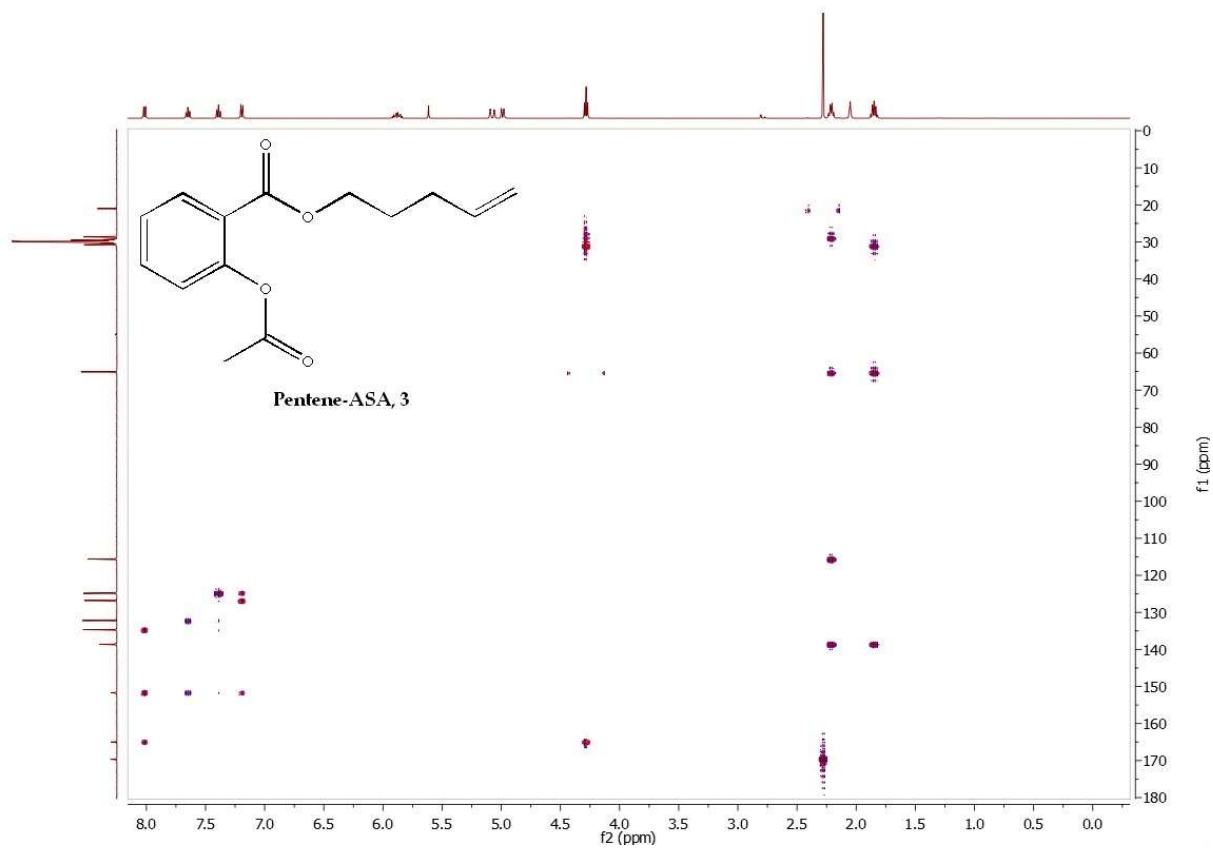


Figure S16. $^1\text{H},^{13}\text{C}$ -HMBC of Pentene-ASA (3) in Acetone- d_6

2.6 Pt-Pentene-ASA (3a)

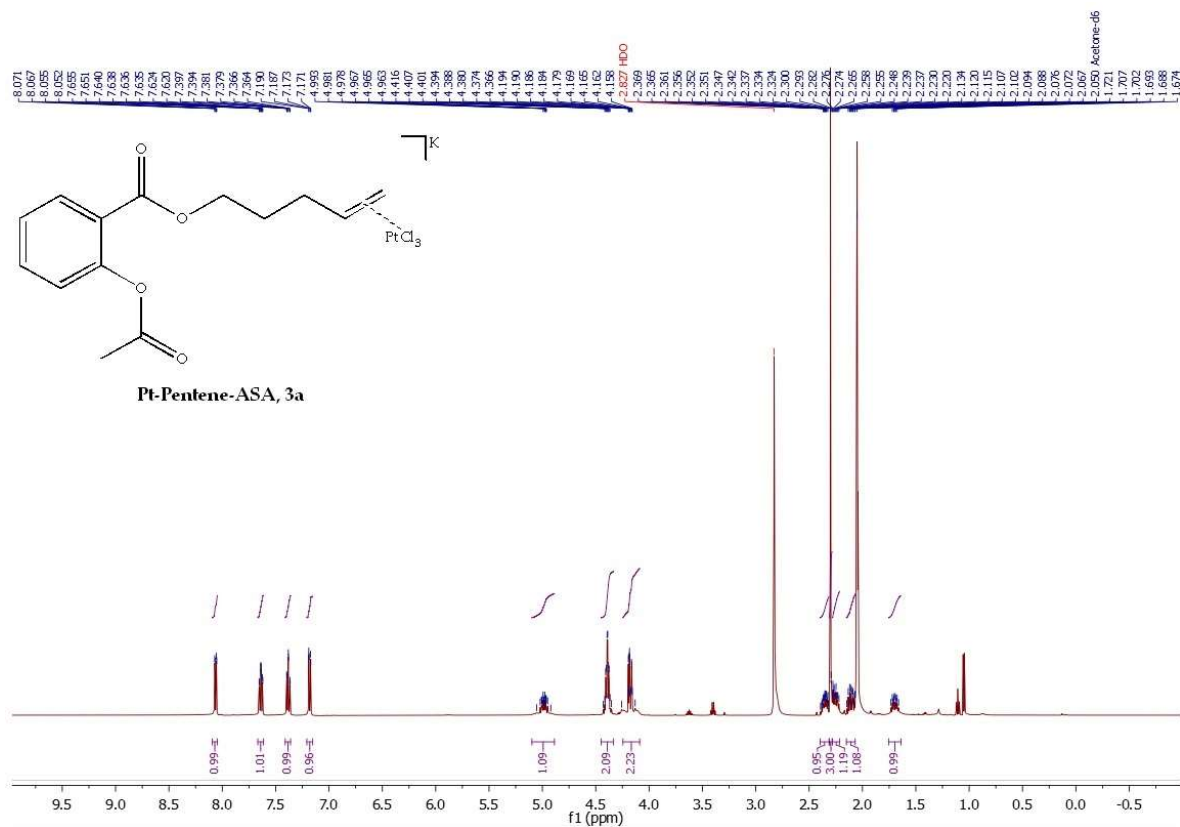


Figure S17. ^1H NMR of Pt-Pentene-ASA (3a) in Acetone- d_6

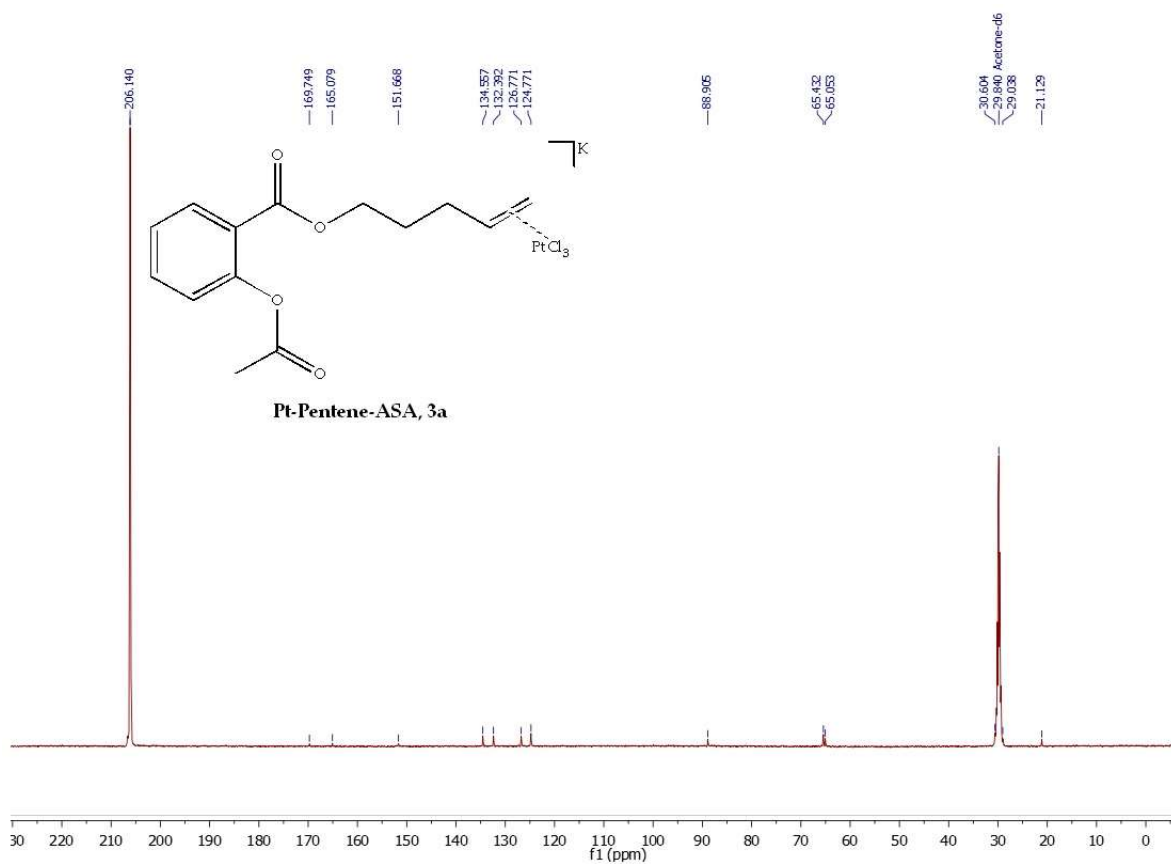


Figure S18. ¹³C NMR of Pt-Pentene-ASA (3a) in Acetone-*d*₆

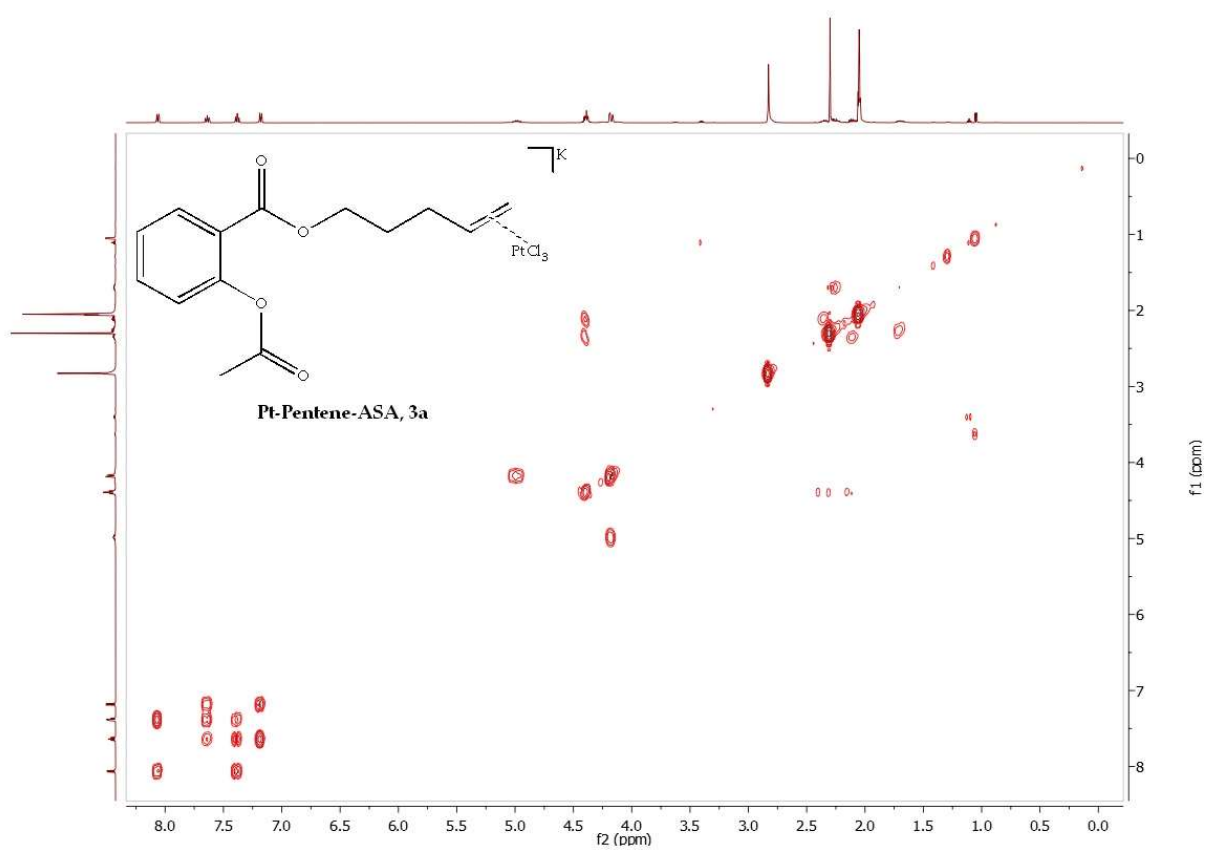


Figure S19. [¹H, ¹H]-COSY of Pt-Pentene-ASA (3a) in Acetone-*d*₆

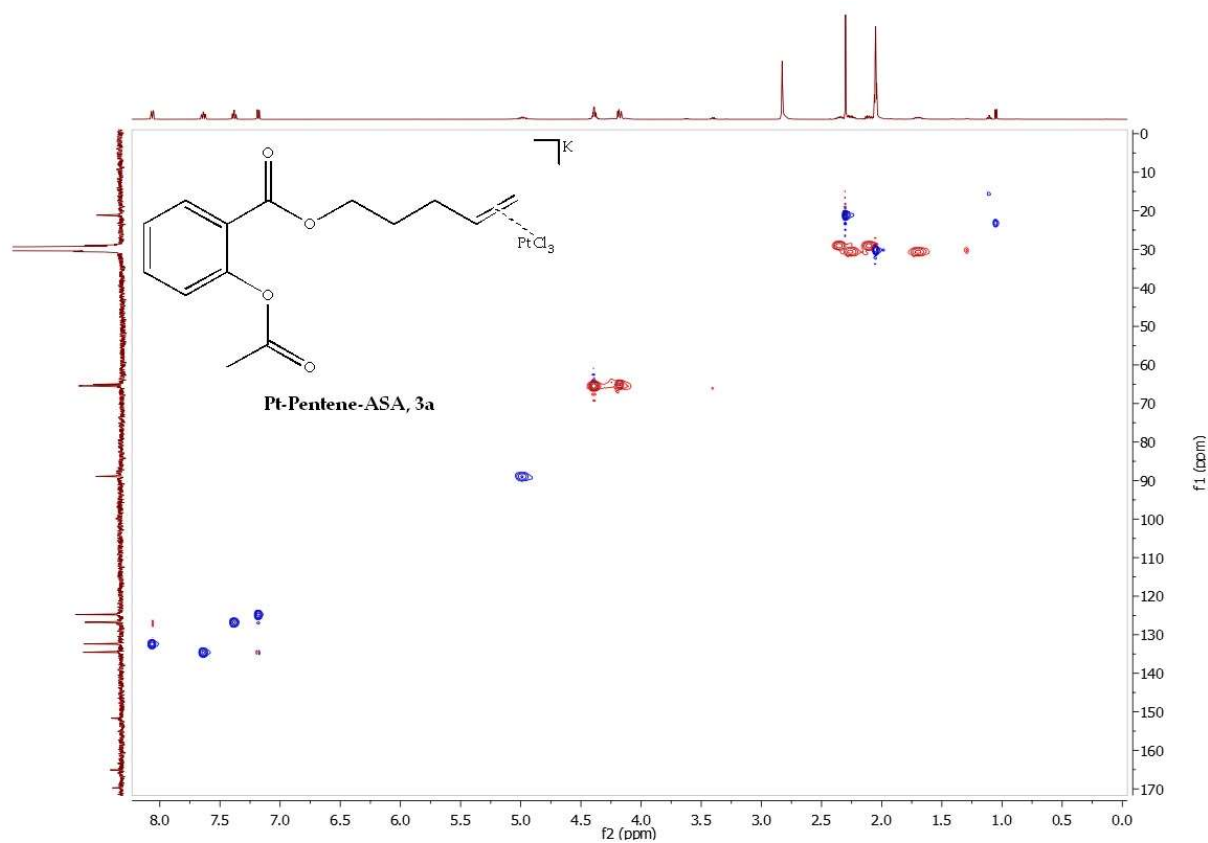


Figure S20. $[^1\text{H},^{13}\text{C}]$ -HSQC of Pt-Pentene-ASA (3a) in Acetone- d_6

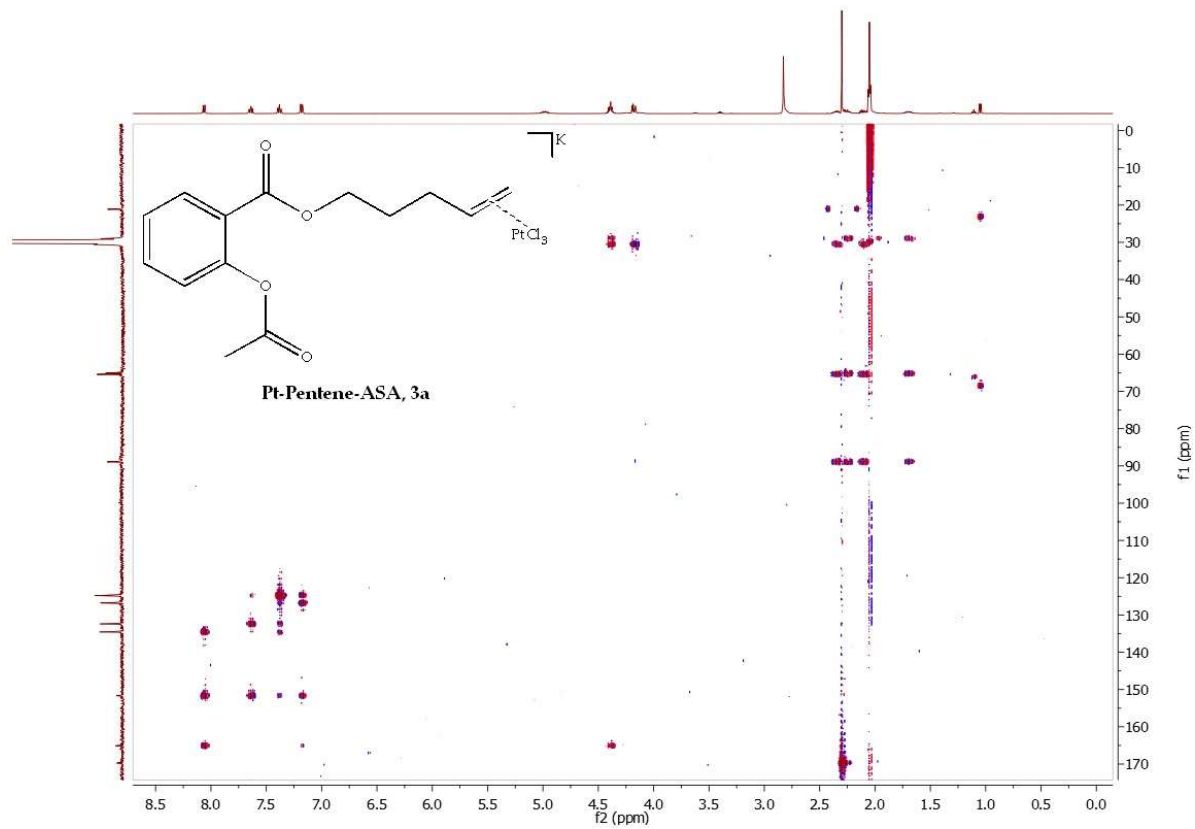
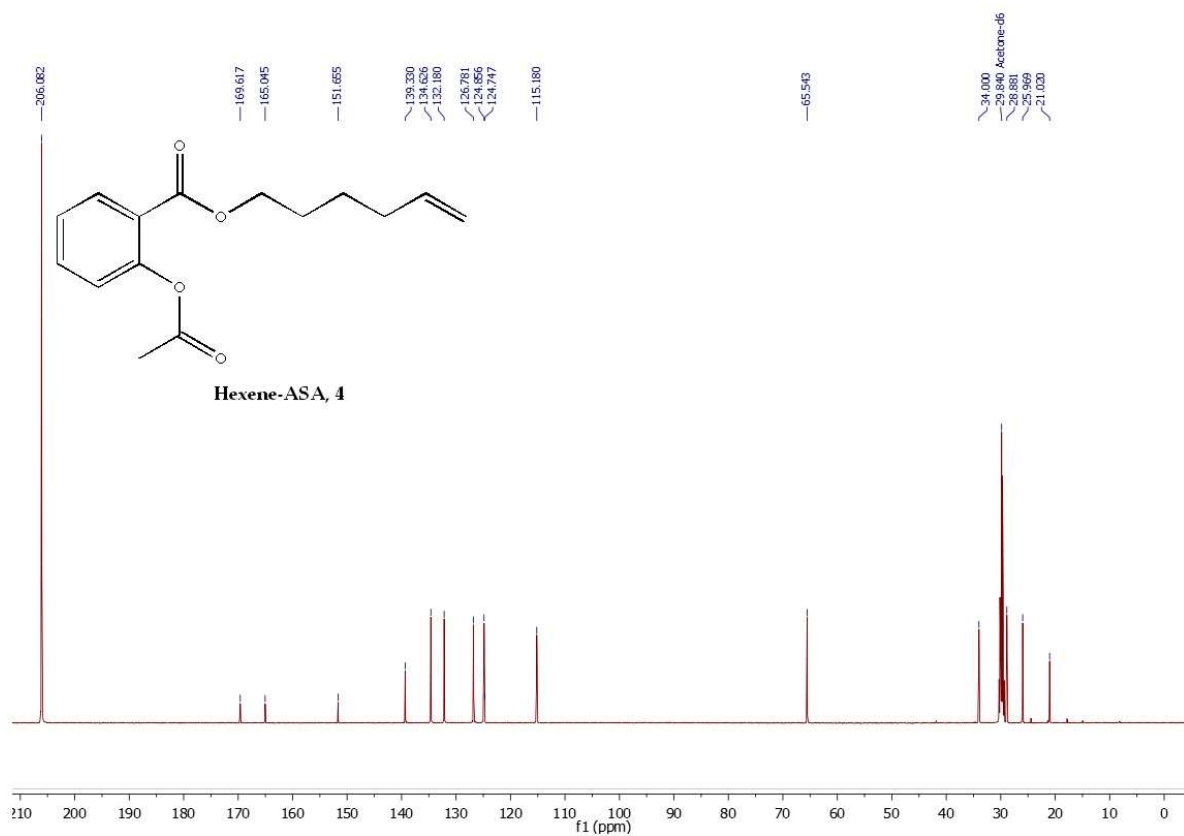
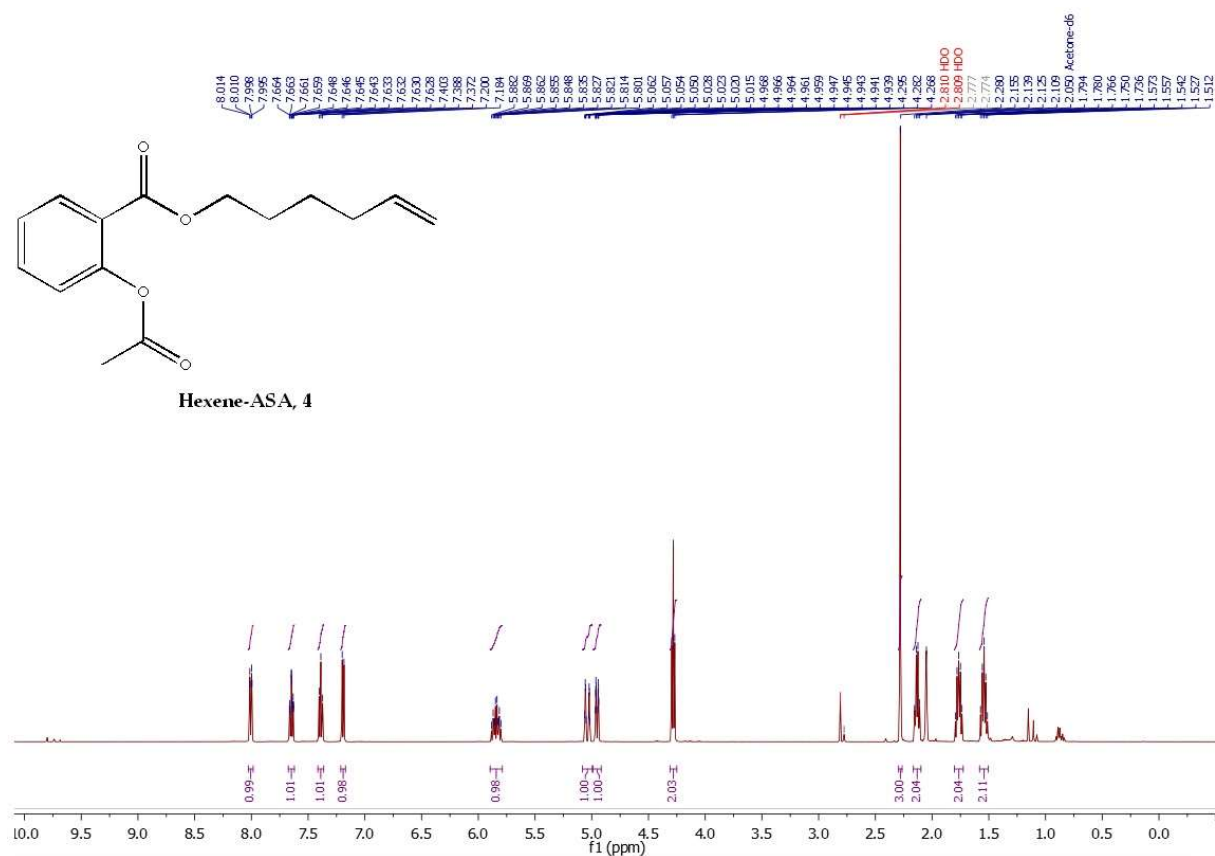


Figure S21. $[^1\text{H},^{13}\text{C}]$ -HMBC of Pt-Pentene-ASA (3a) in Acetone- d_6

2.7 Hexene-ASA (4)



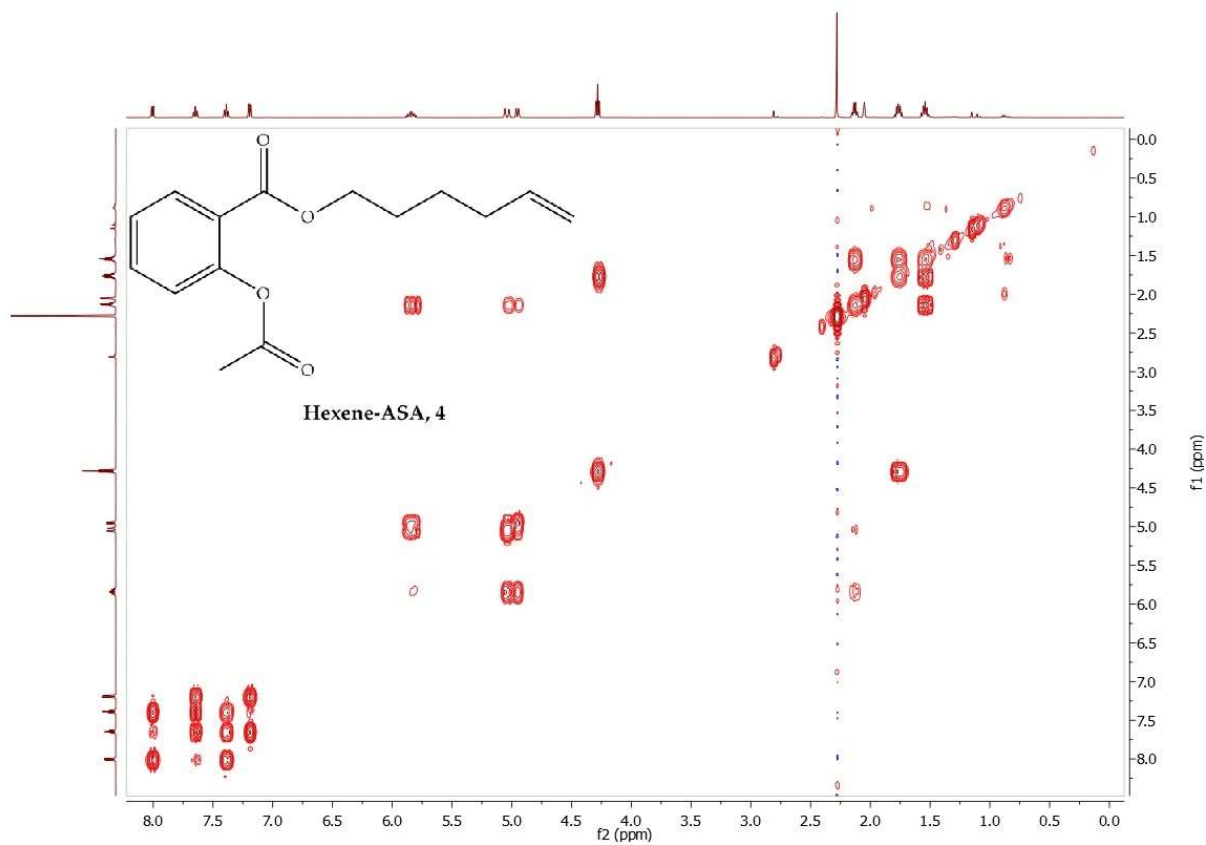


Figure S24. $[^1\text{H}, ^1\text{H}]$ -COSY of Hexene-ASA (4) in Acetone- d_6

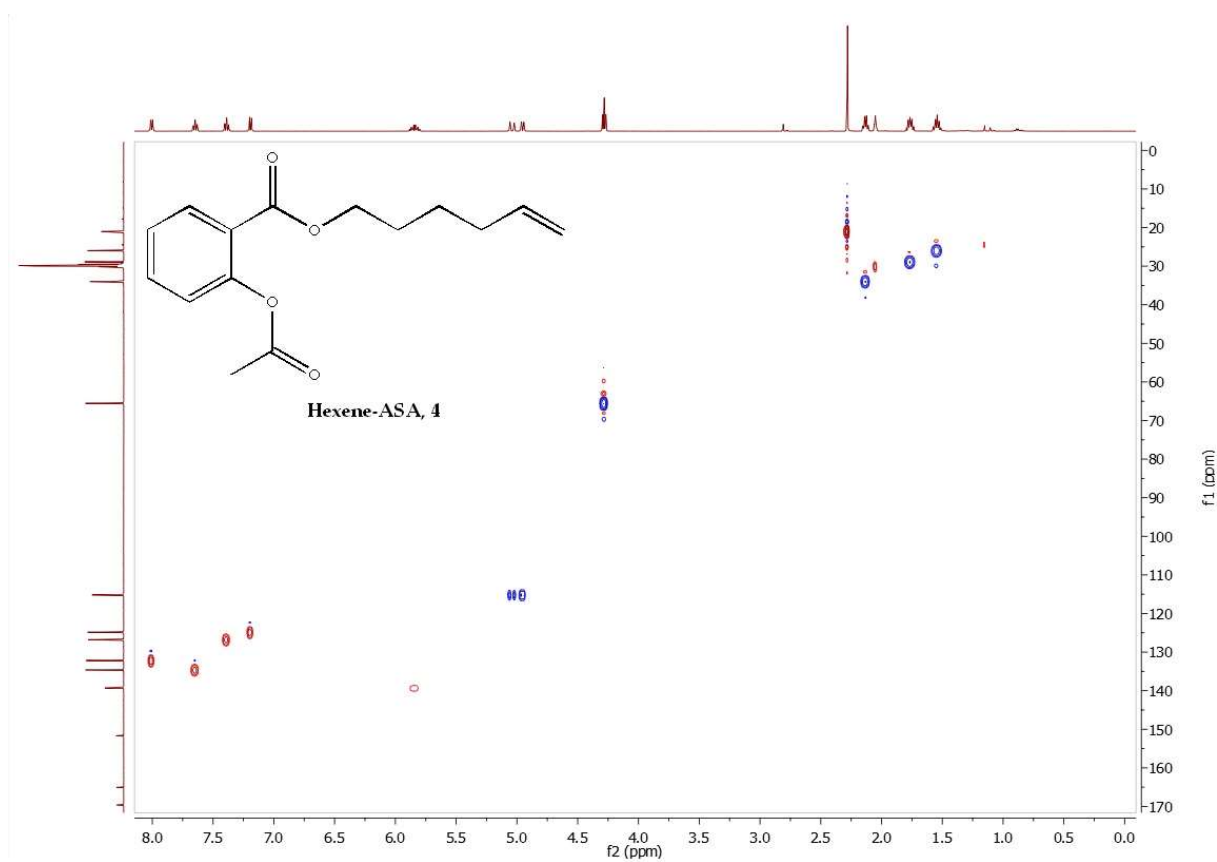


Figure S25. $[^1\text{H}, ^{13}\text{C}]$ -HSQC of Hexene-ASA (4) in Acetone- d_6

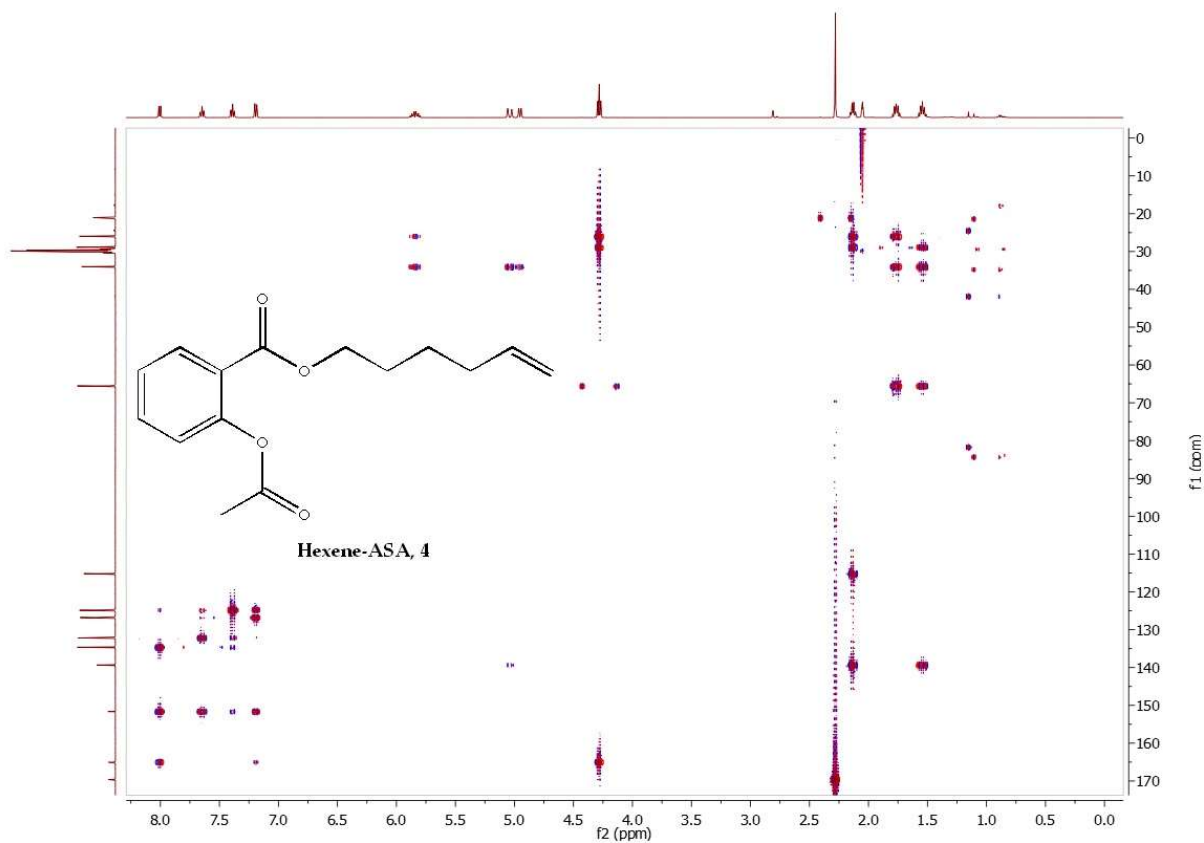


Figure S26. $[^1\text{H},^{13}\text{C}]$ -HMBC of Hexene-ASA (4) in Acetone- d_6

2.8 Pt-Hexene-ASA (4a)

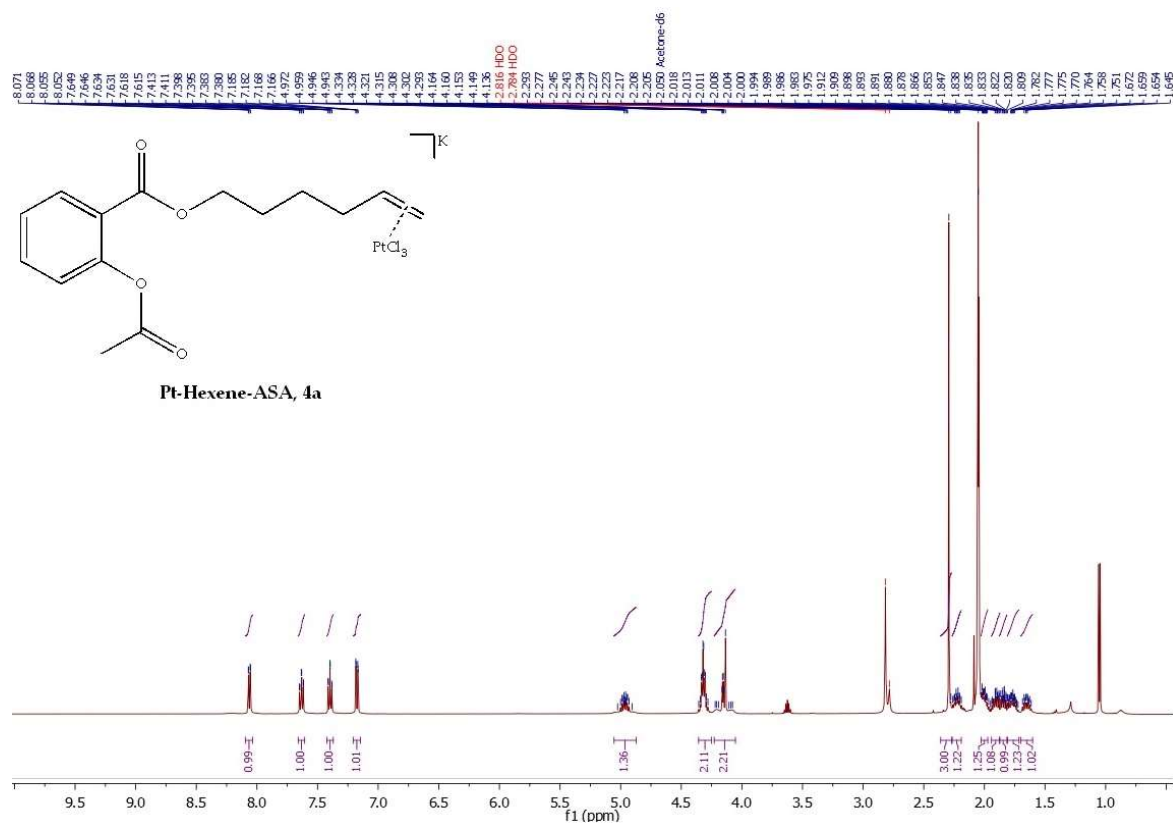


Figure S27. ^1H NMR of Pt-Hexene-ASA (4a) in Acetone- d_6

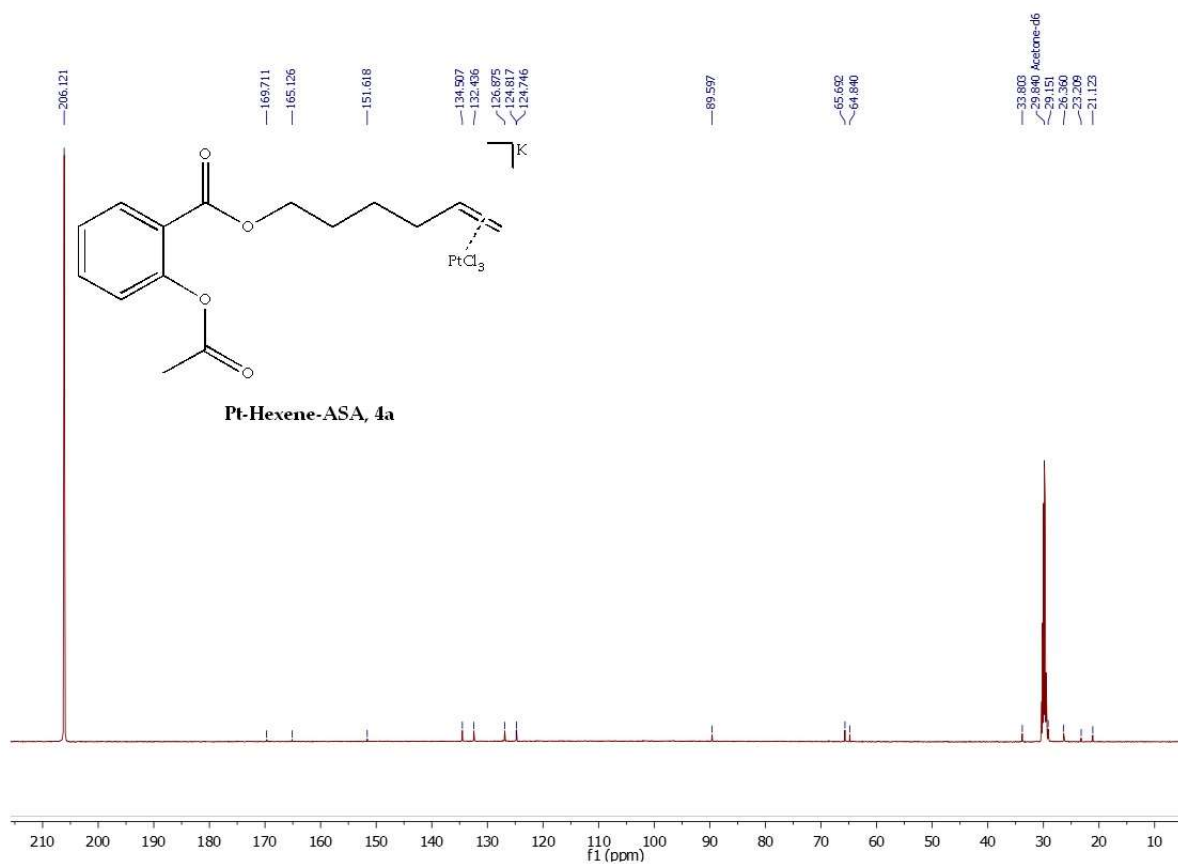


Figure S28. ^{13}C NMR of Pt-Hexene-ASA (4a) in Acetone- d_6

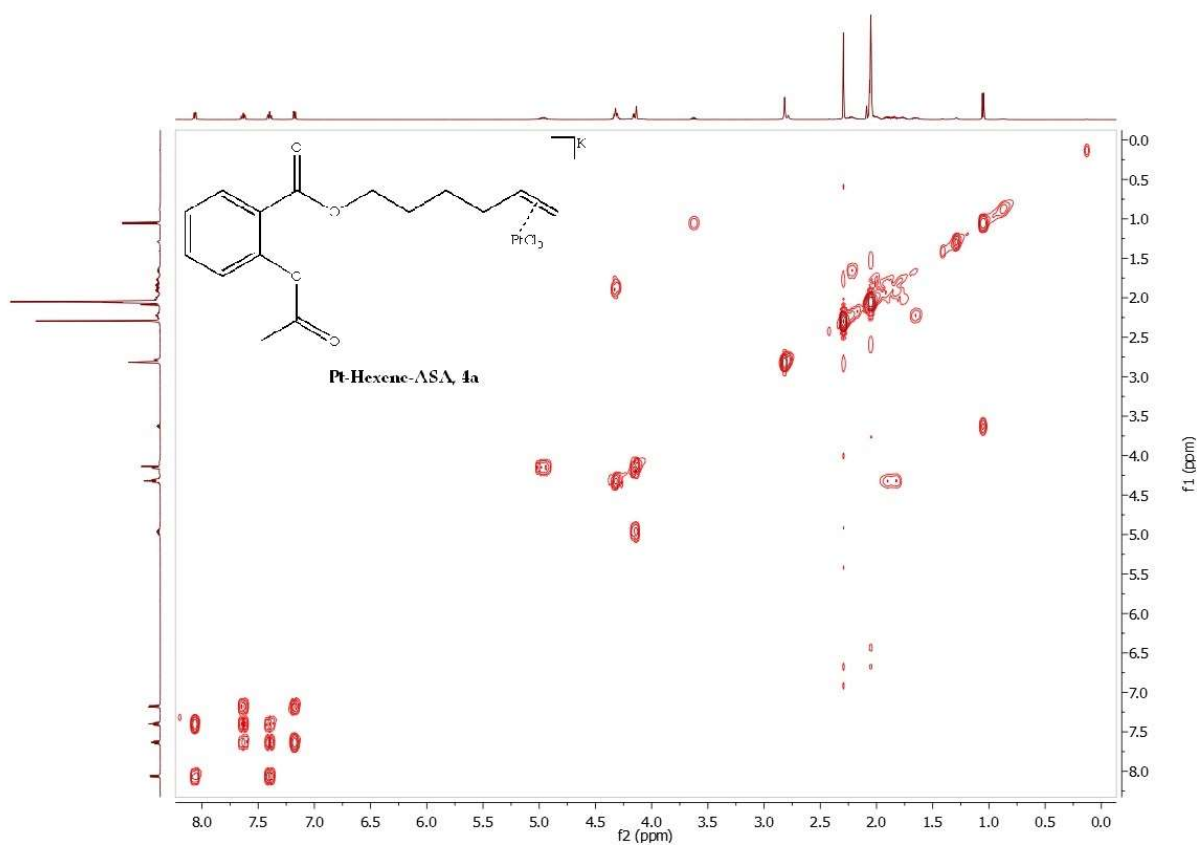


Figure S29. $[^1\text{H}, ^1\text{H}]$ -COSY of Pt-Hexene-ASA (4a) in Acetone- d_6

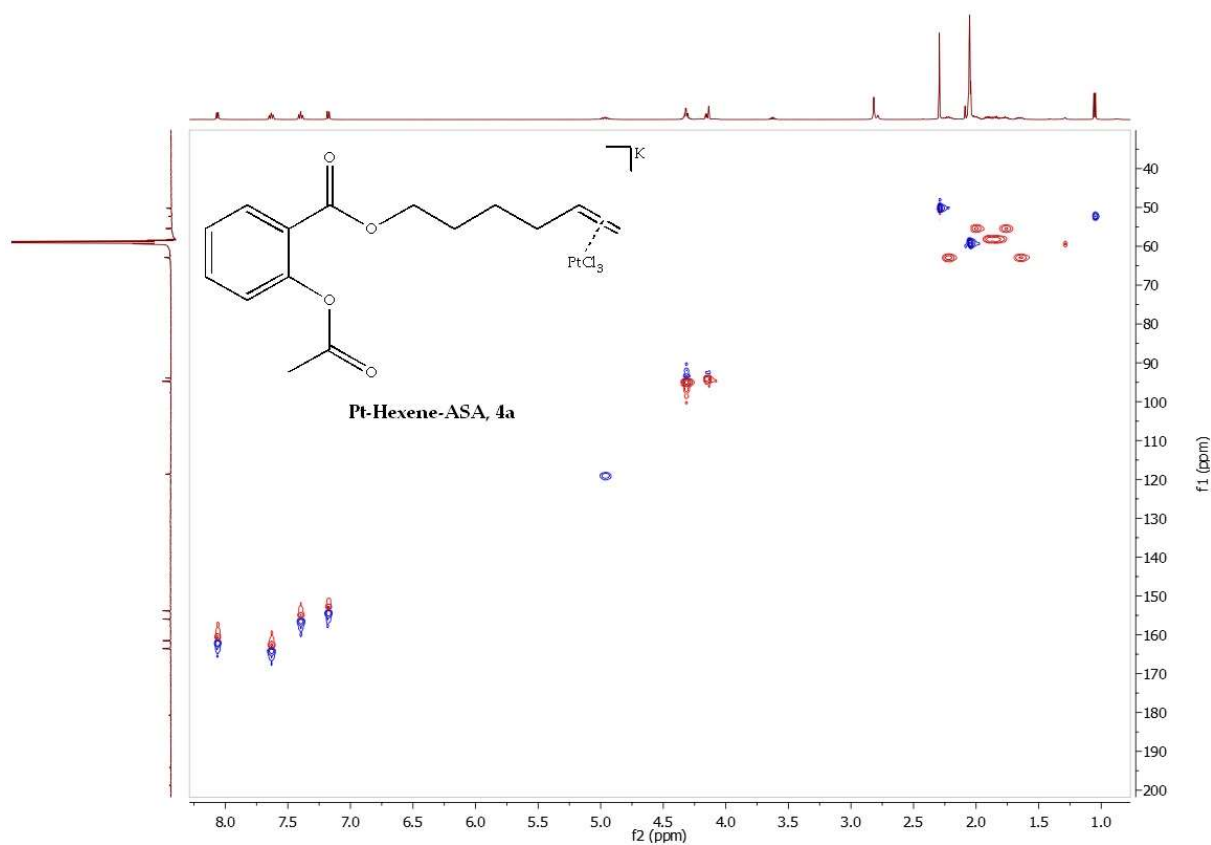


Figure S30. ^1H , ^{13}C -HSQC of Pt-Hexene-ASA (**4a**) in Acetone- d_6

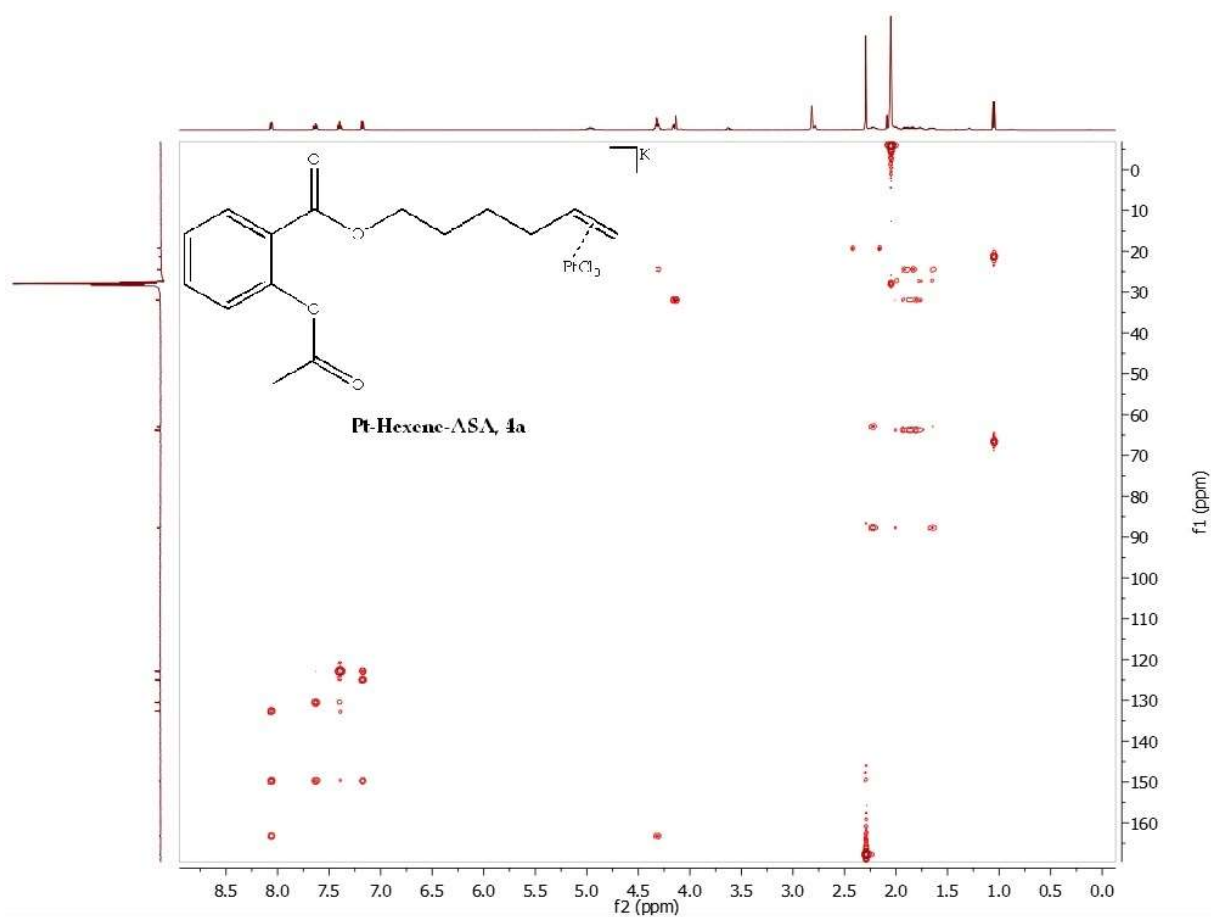


Figure S31. ^1H , ^{13}C -HMBC of Pt-Hexene-ASA (**4a**) in Acetone- d_6

3. Crystal Data

Supplementary Table T1. Crystal Data and structure refinement for **1a**

Empirical formula	C ₁₆ H ₂₂ Cl ₃ KO ₅ Pt	
Formula weight	634.87	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /c (no. 14)	
Unit cell dimensions	a = 8.3367(3) Å	$\alpha = 90^\circ$
	b = 12.4677(5) Å	$\beta = 92.7060(10)^\circ$
	c = 20.8667(9) Å	$\gamma = 90^\circ$
Volume	2166.46(15) Å ³	
Z	4	
Density (calculated)	1.946 Mg/m ³	
Absorption coefficient	7.061 mm ⁻¹	
F(000)	1224	
Crystal size	0.220 x 0.110 x 0.070 mm ³	
Theta range for data collection	2.446 to 25.997°	
Index ranges	-10<=h<=9, -15<=k<=15, -25<=l<=25	
Reflections collected	53983	
Independent reflections	4266 [R(int) = 0.0473]	
Completeness to theta = 25.242°	99.9%	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.862 and 0.598	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	4266 / 3 / 248	
Goodness-of-fit on F ²	1.089	
Final R indices [I>2sigma(I)]	R1 = 0.0186, wR2 = 0.0408	
R indices (all data)	R1 = 0.0234, wR2 = 0.0420	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.946 and -1.446 e.Å ⁻³	