

Supporting Information

Synthetic Approach to ABCD ring system of Anticancer Agent Fredericamycin A via Claisen rearrangement and Ring-Closing Metathesis as key steps

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Copies of ^1H , ^{13}C and DEPT135 NMR spectra

Figure S1a: ^1H NMR of Compound 6 (500 MHz, CDCl_3):

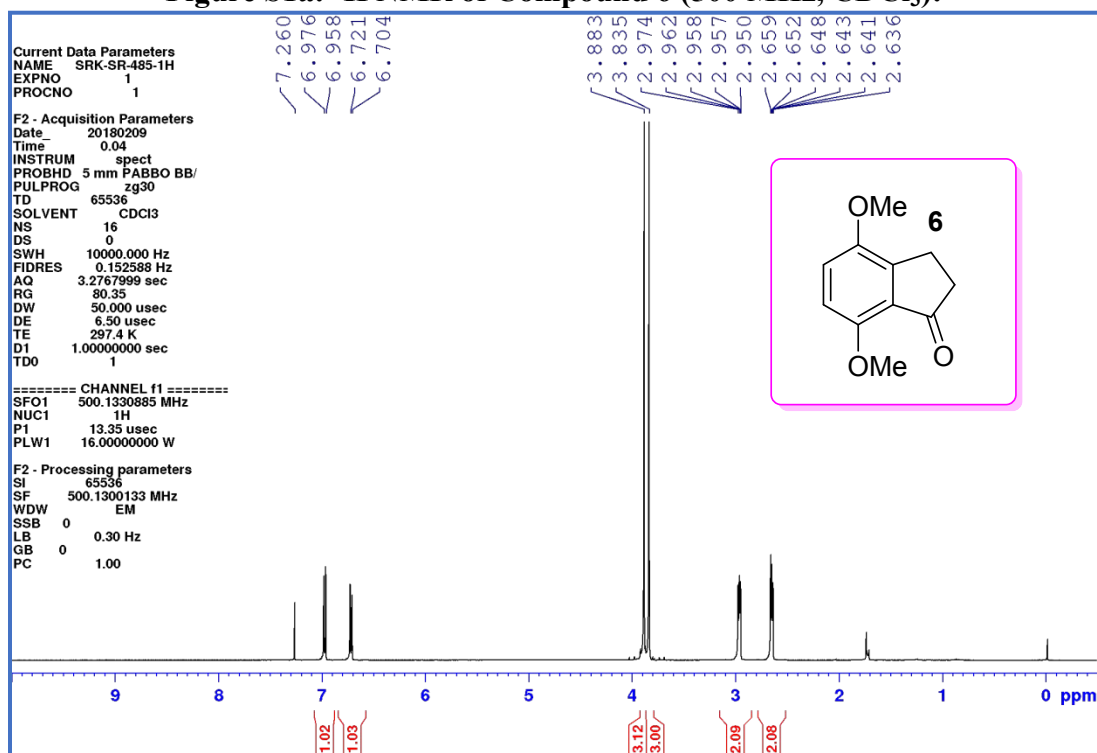


Figure S1b: ^{13}C NMR of Compound 6 (125 MHz, CDCl_3):

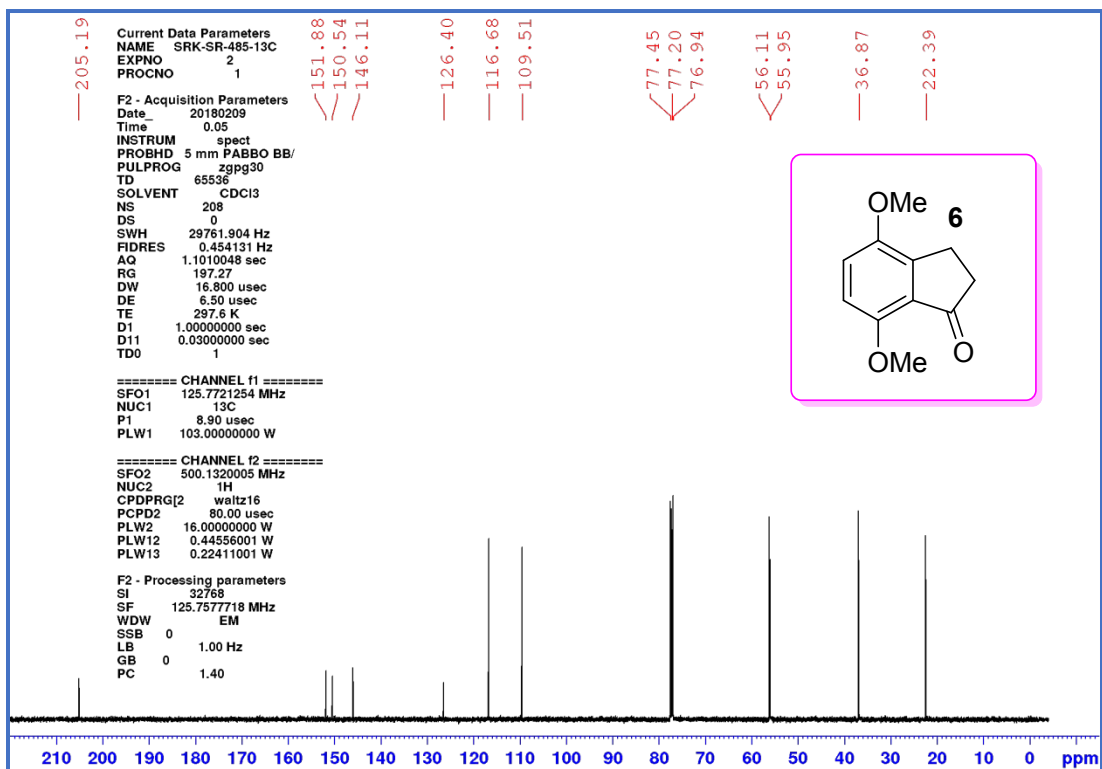


Figure S1c: DEPT 135 NMR of Compound 6 (125 MHz, CDCl₃):

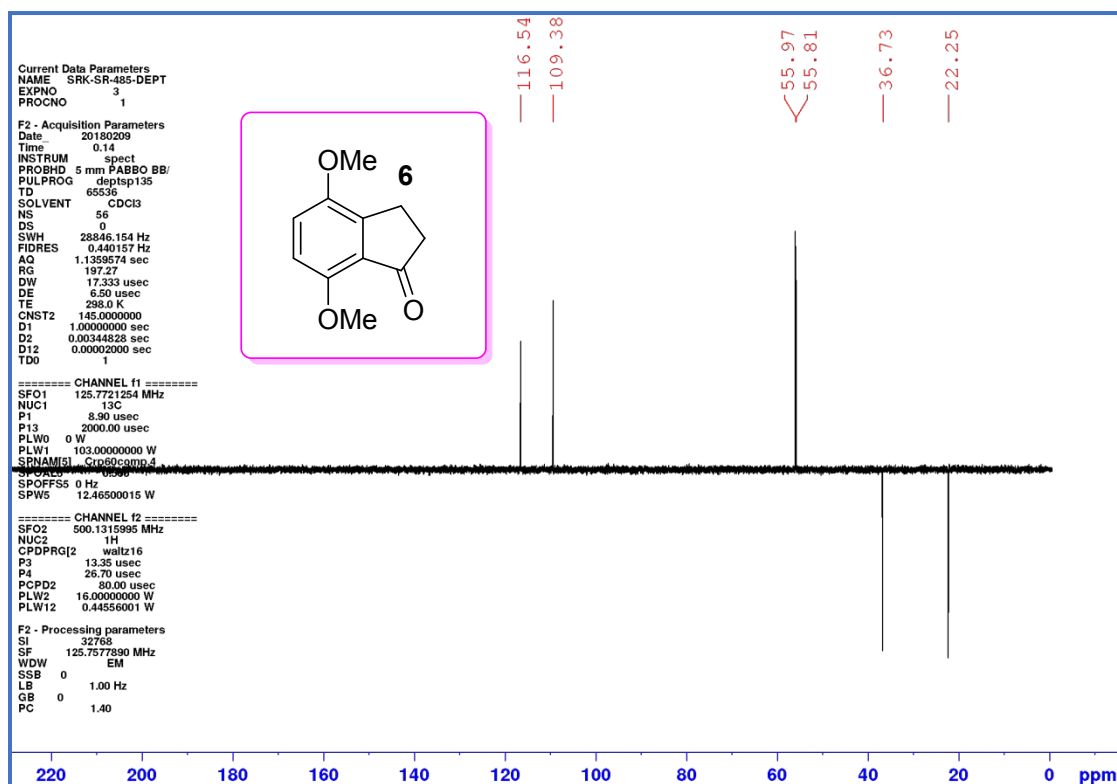


Figure S2a: ¹H NMR of Compound 10 (500 MHz, CDCl₃):

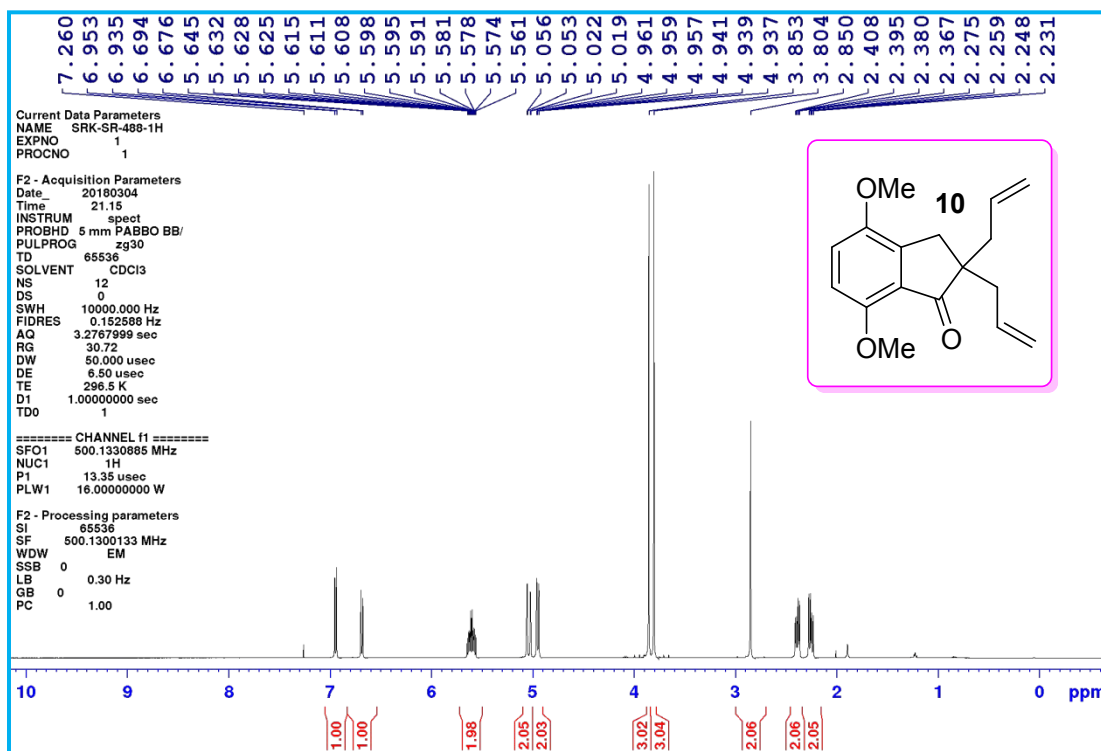


Figure S2b: ^{13}C NMR of Compound 10 (125 MHz, CDCl_3):

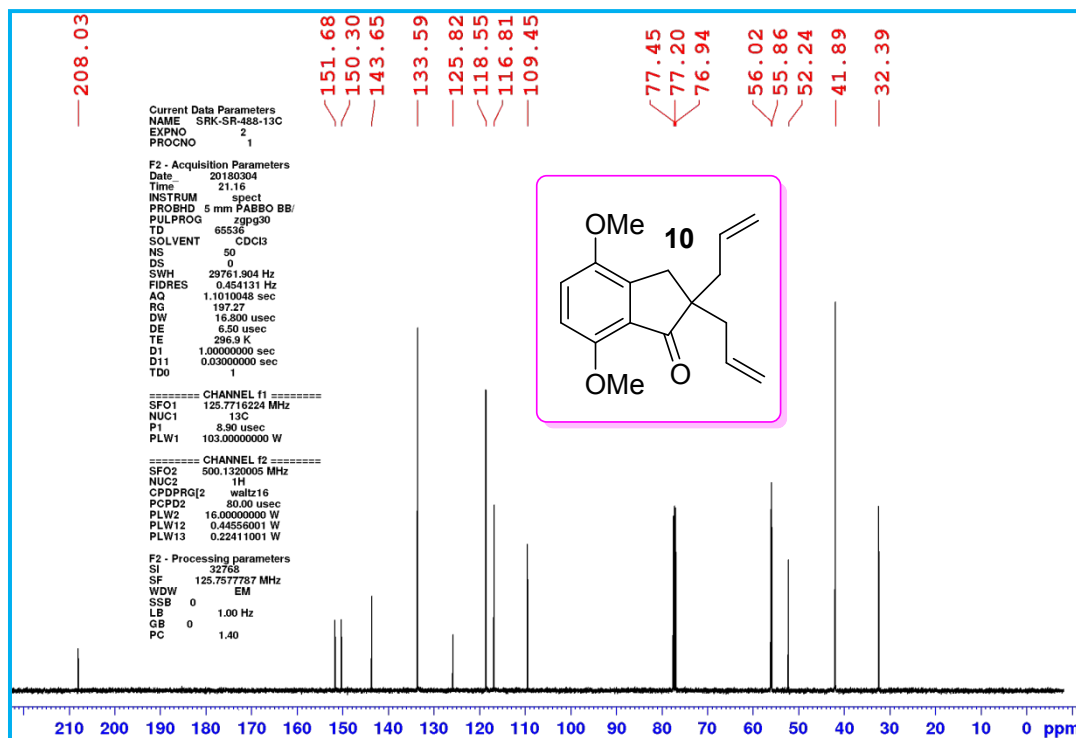


Figure S2c: DEPT 135 NMR of Compound 10 (125 MHz, CDCl_3):

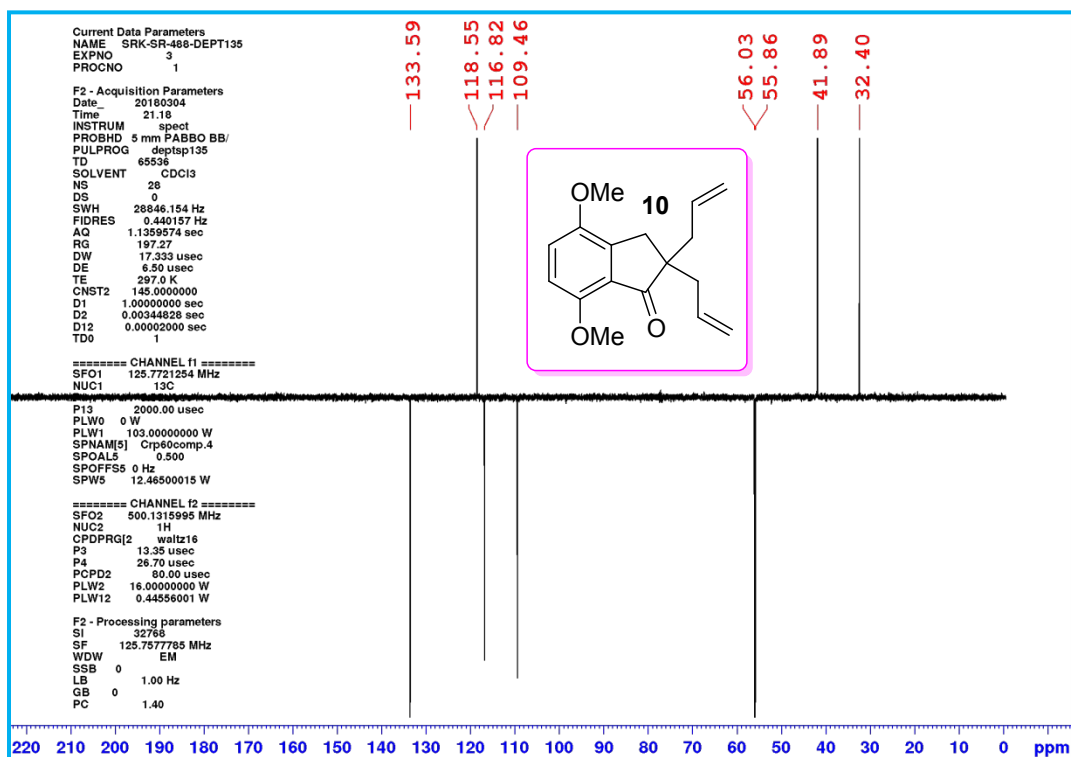


Figure S3a: ^1H NMR of Compound 5 (400 MHz, CDCl_3):

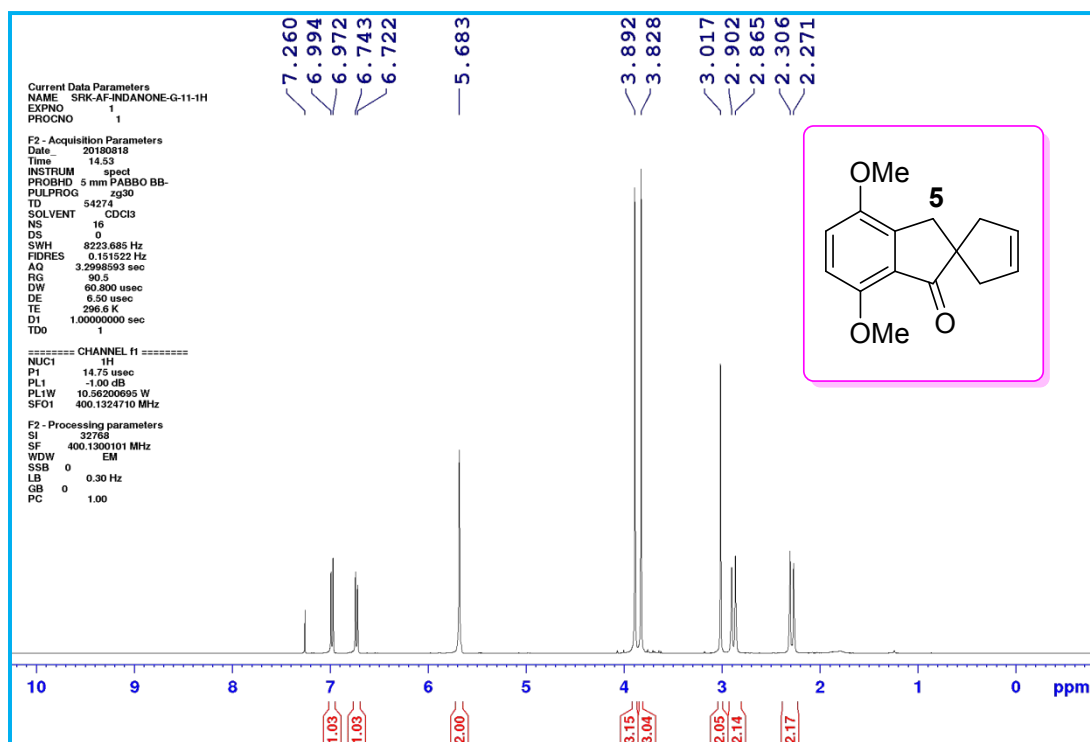


Figure S3b: ^{13}C NMR of Compound 5 (100 MHz, CDCl_3):

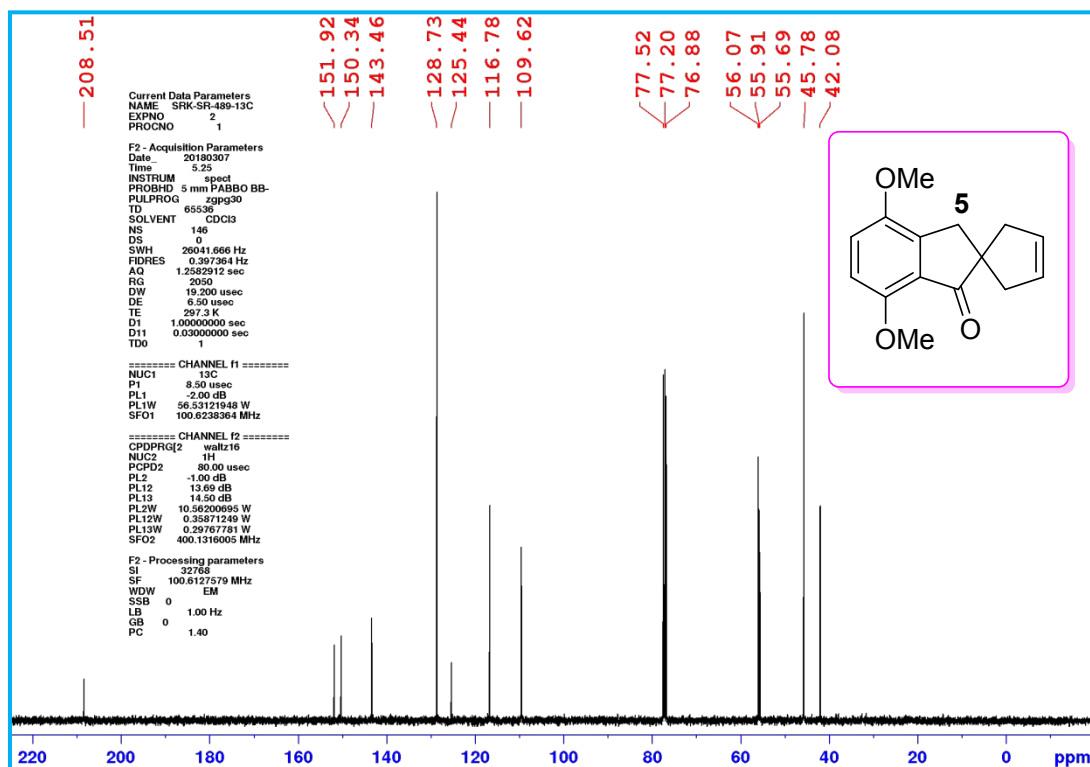


Figure S3c: DEPT 135 NMR of Compound 5 (100 MHz, CDCl₃):

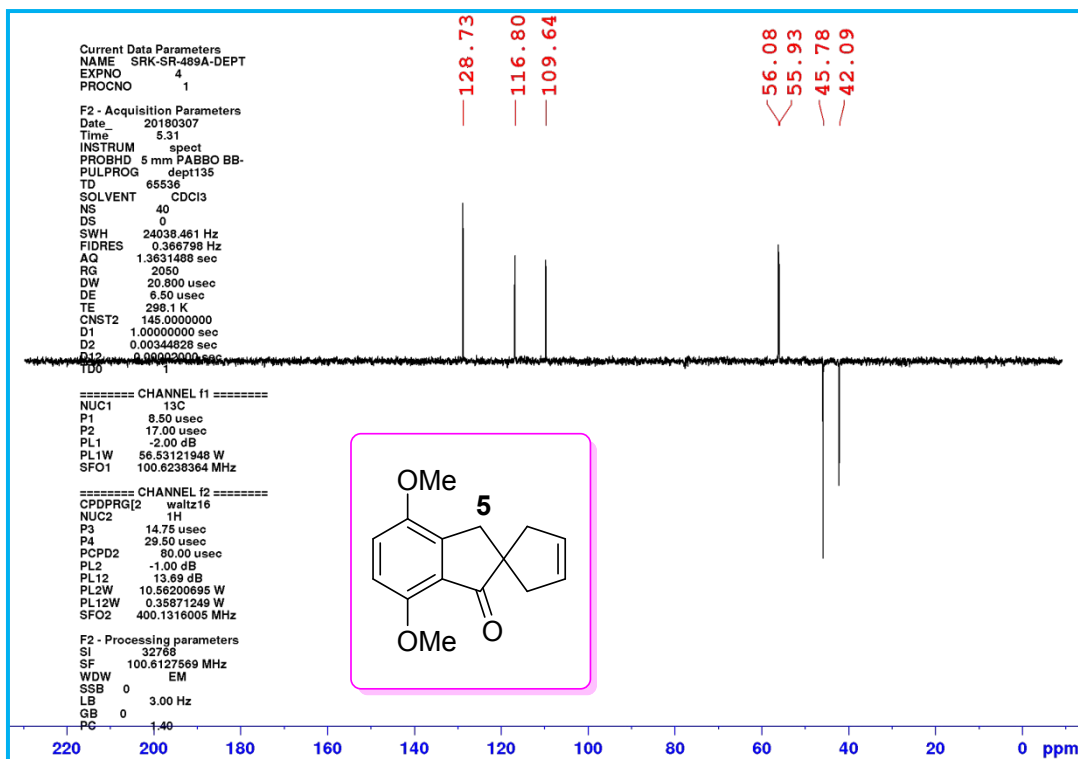


Figure S4a: ¹H NMR of Compound 11 (400 MHz, CDCl₃):

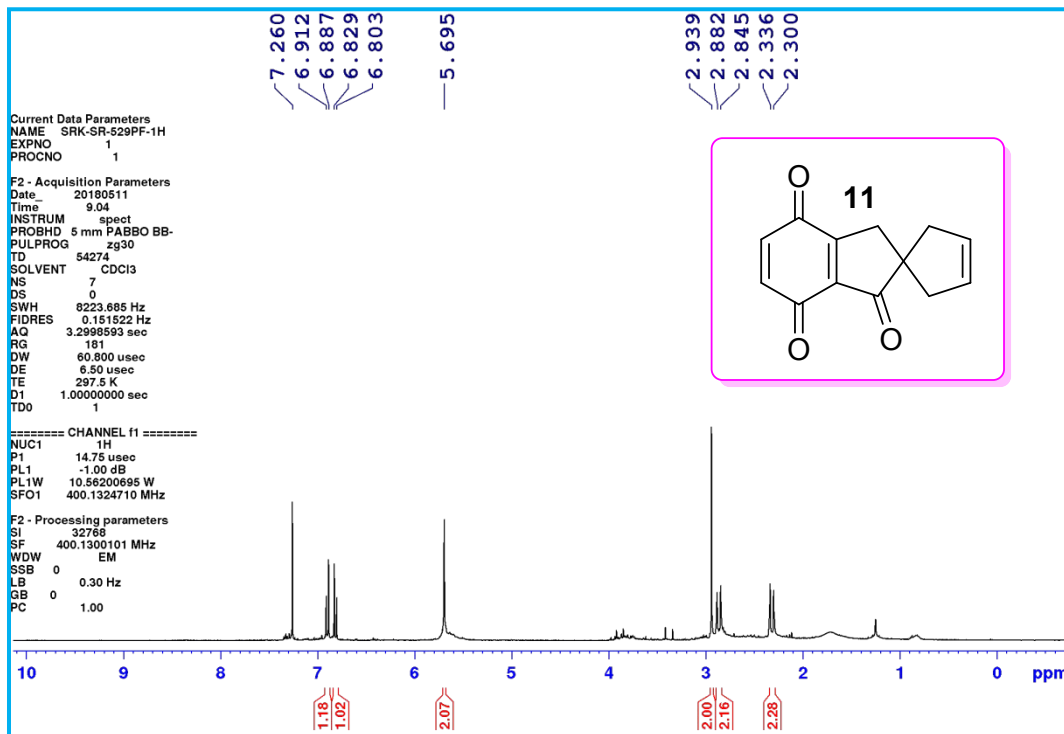


Figure S4b: ^{13}C NMR of Compound 11 (125 MHz, CDCl_3):

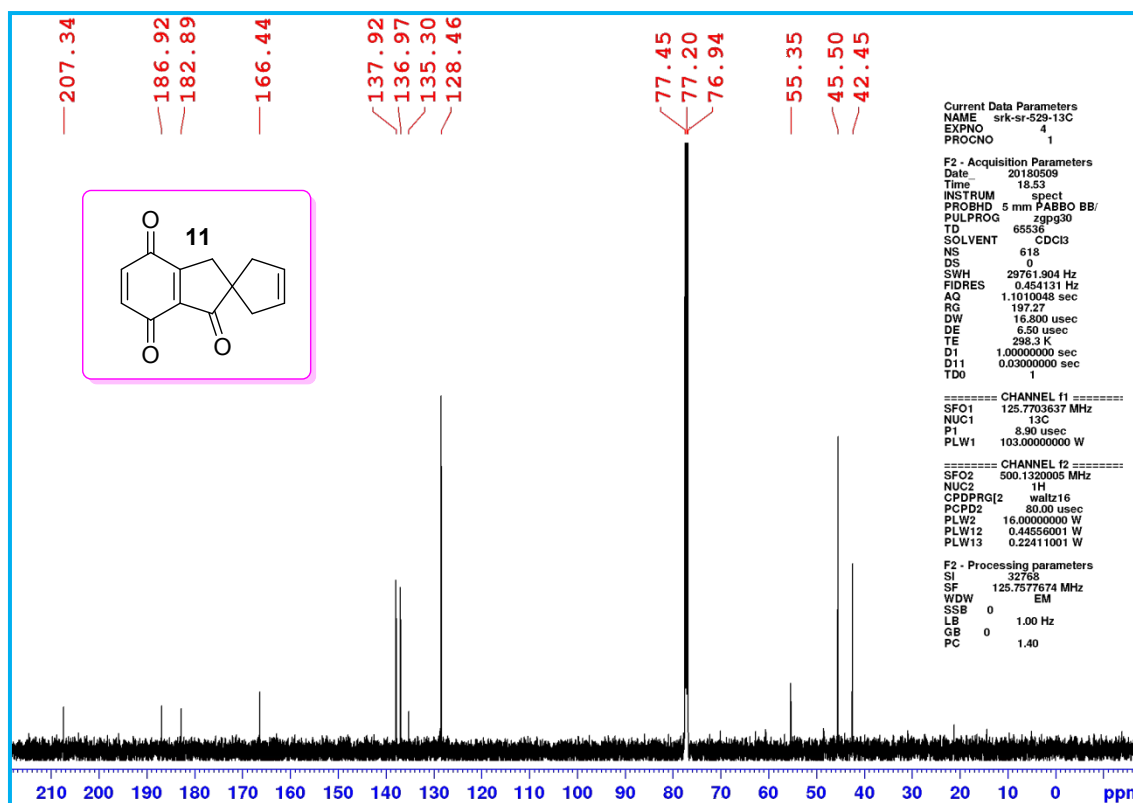


Figure S4c: DEPT 135 NMR of Compound 11 (125 MHz, CDCl_3):

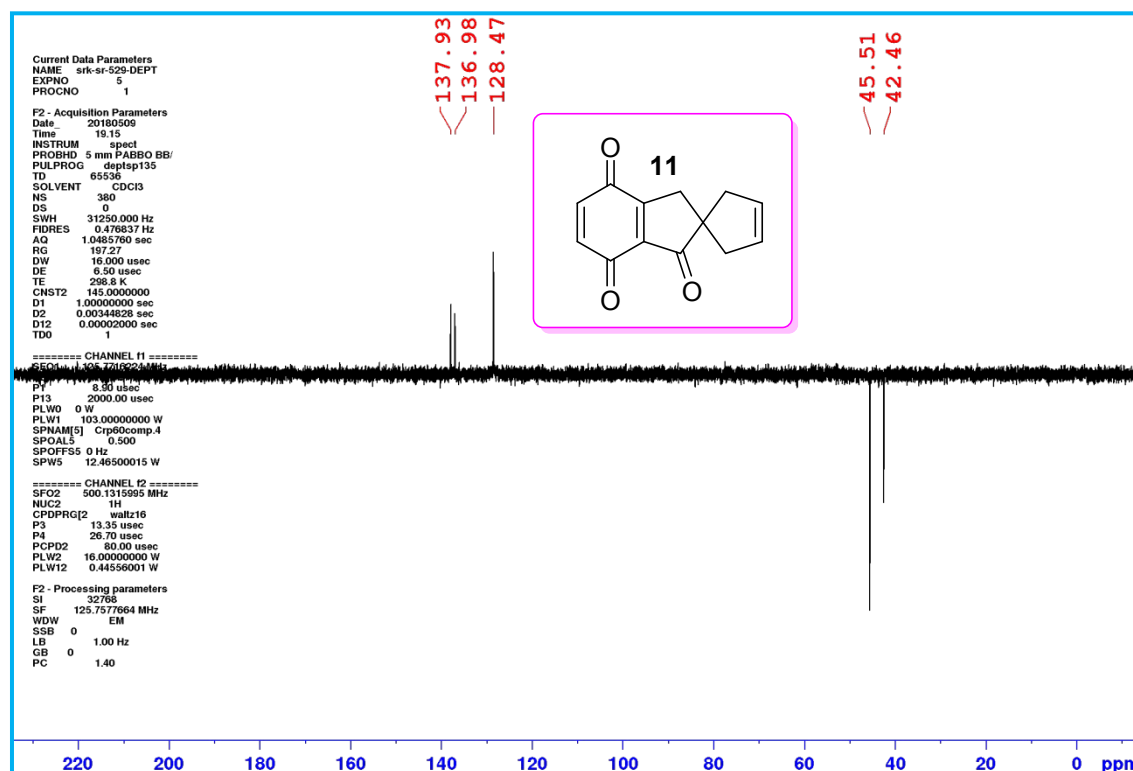


Figure S5a: ^1H NMR of Compound 12 (500 MHz, CDCl_3):

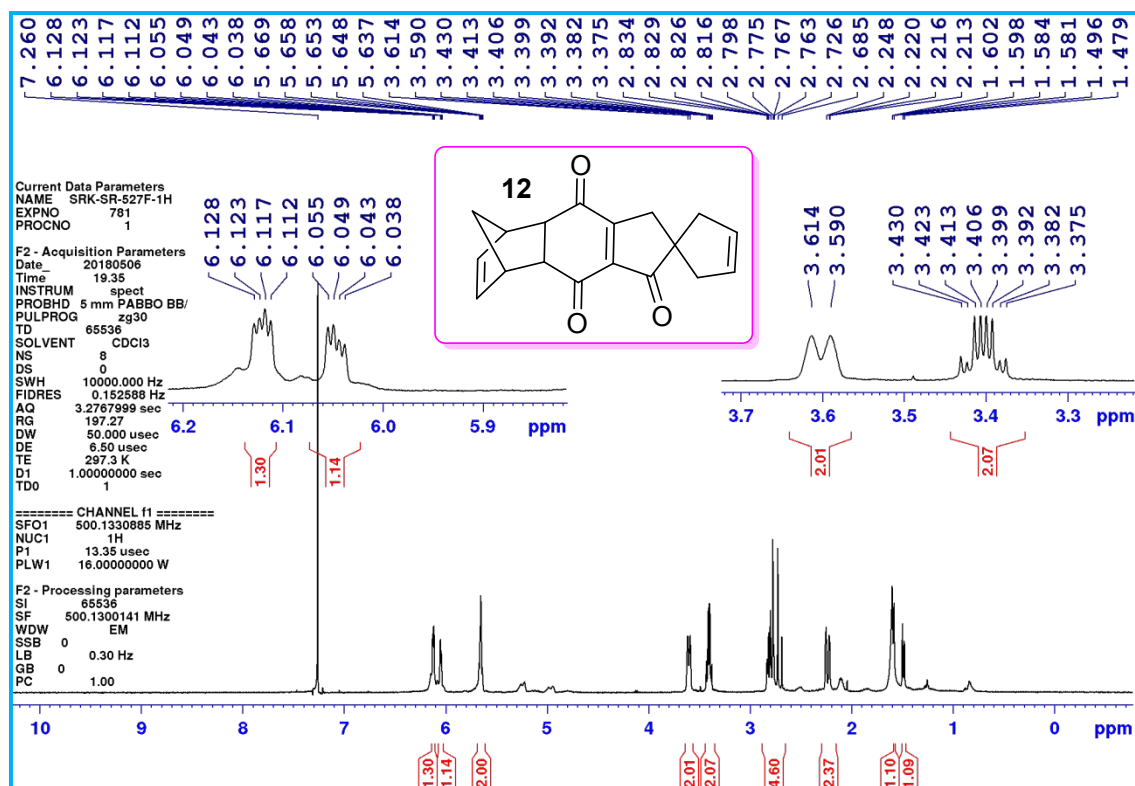


Figure S5b: ^{13}C NMR of Compound 12 (500 MHz, CDCl_3):

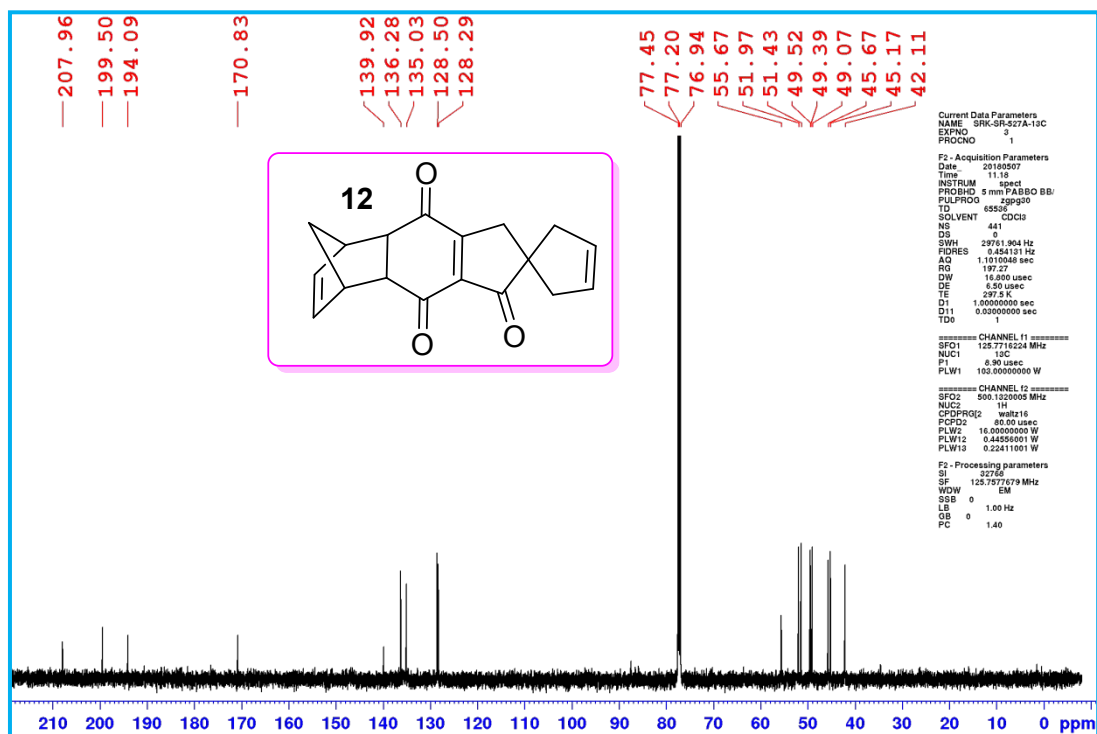


Figure S5c: DEPT 135 NMR of Compound 12 (500 MHz, CDCl₃):

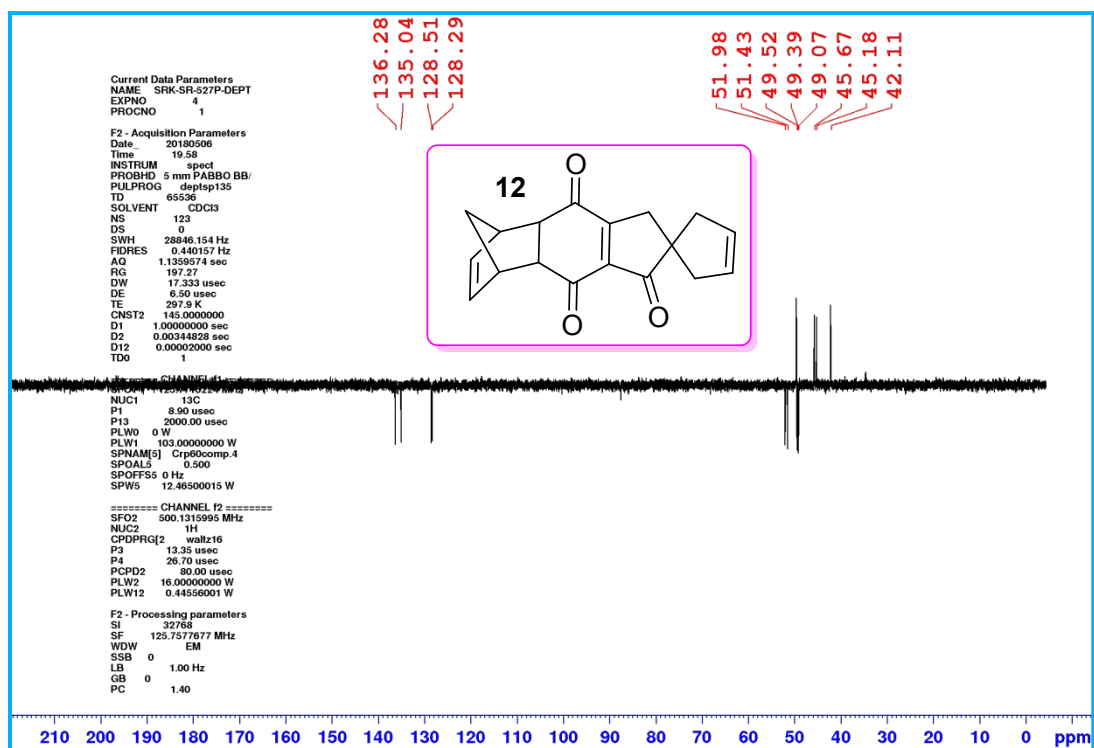


Figure S6a: ¹H NMR of Compound 4 (400 MHz, CDCl₃):

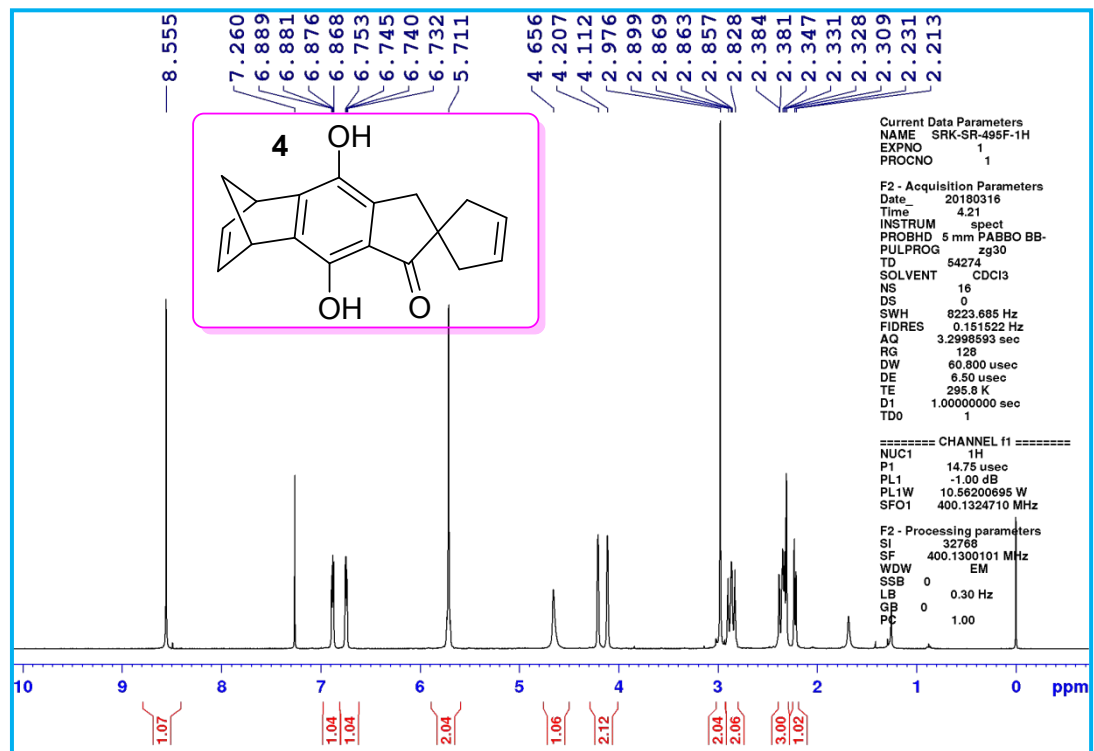


Figure S6b: ^{13}C NMR of Compound 4 (125 MHz, CDCl_3):

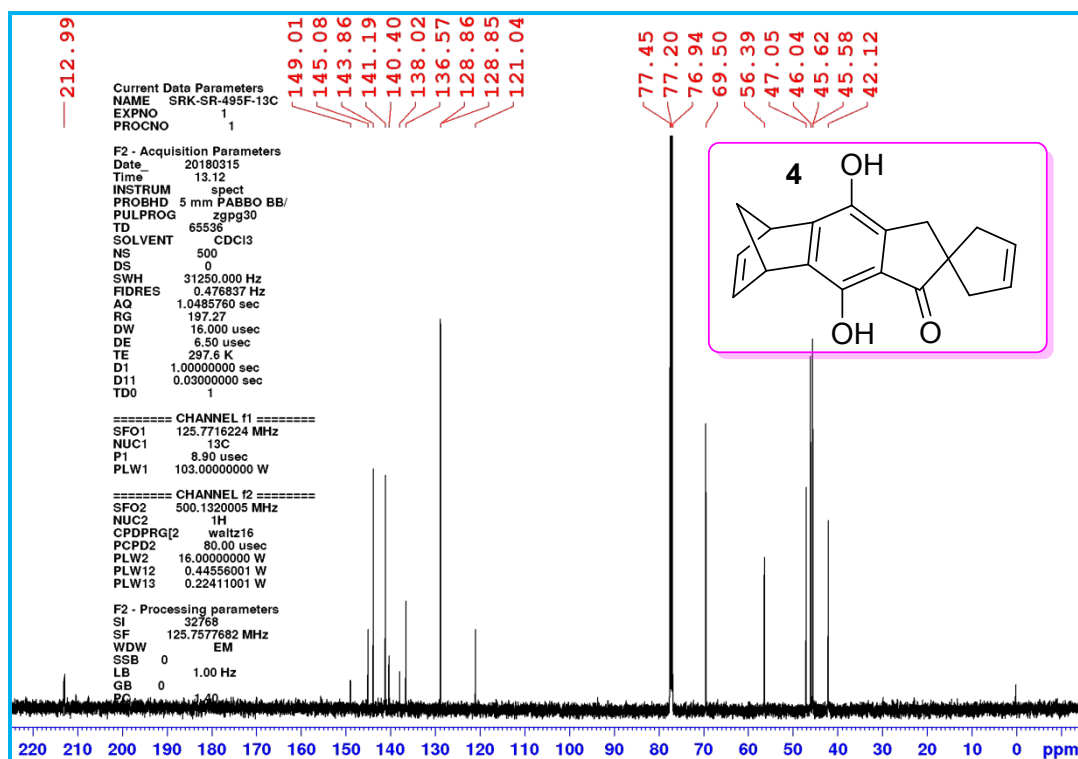


Figure S6c: DEPT 135 NMR of Compound 4 (125 MHz, CDCl_3):

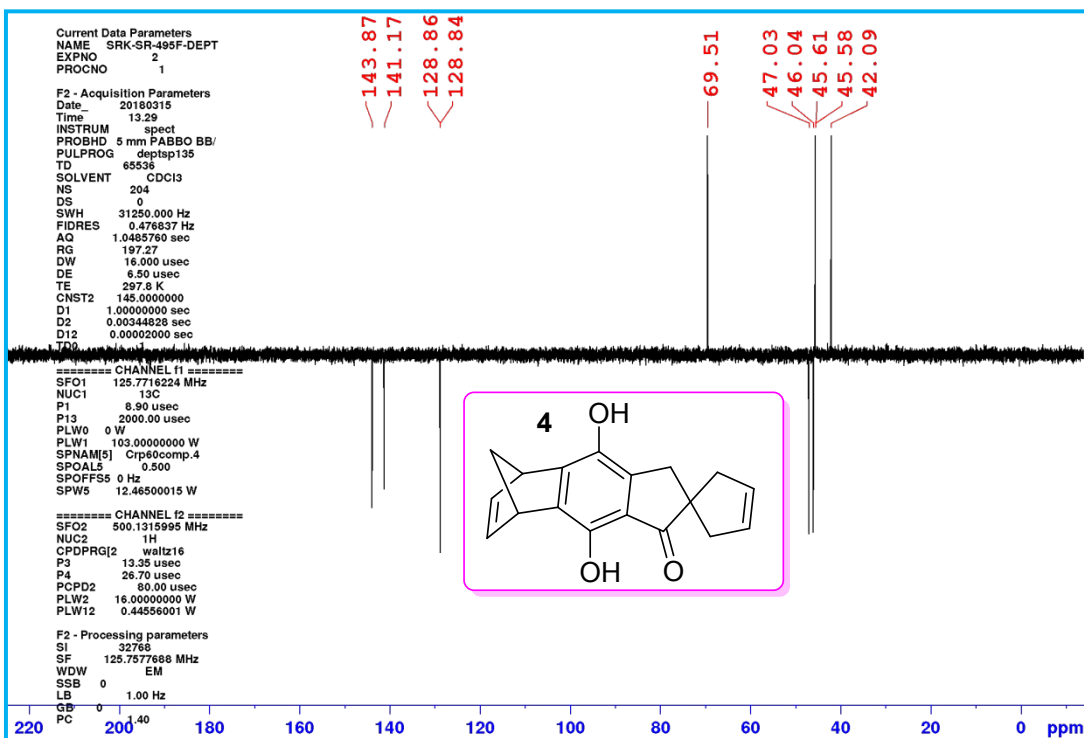


Figure S7a: ^1H NMR of Compound 13 (500 MHz, CDCl_3):

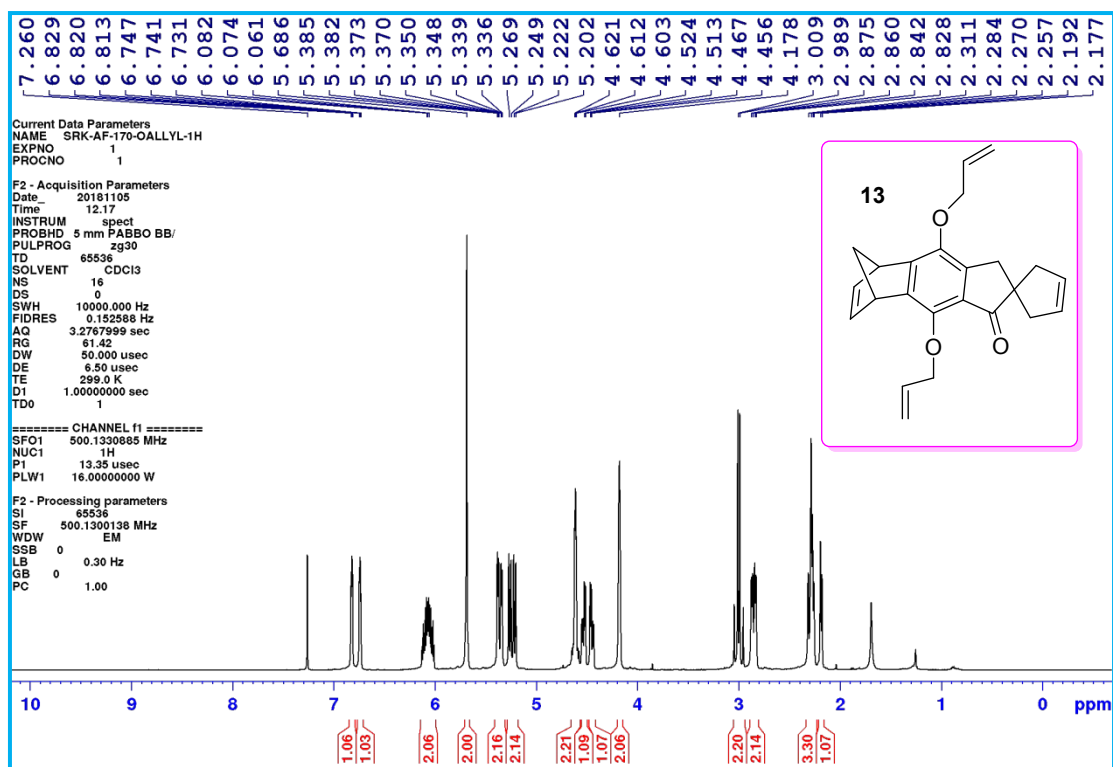


Figure S7b: ^{13}C NMR of Compound 13 (125 MHz, CDCl_3):

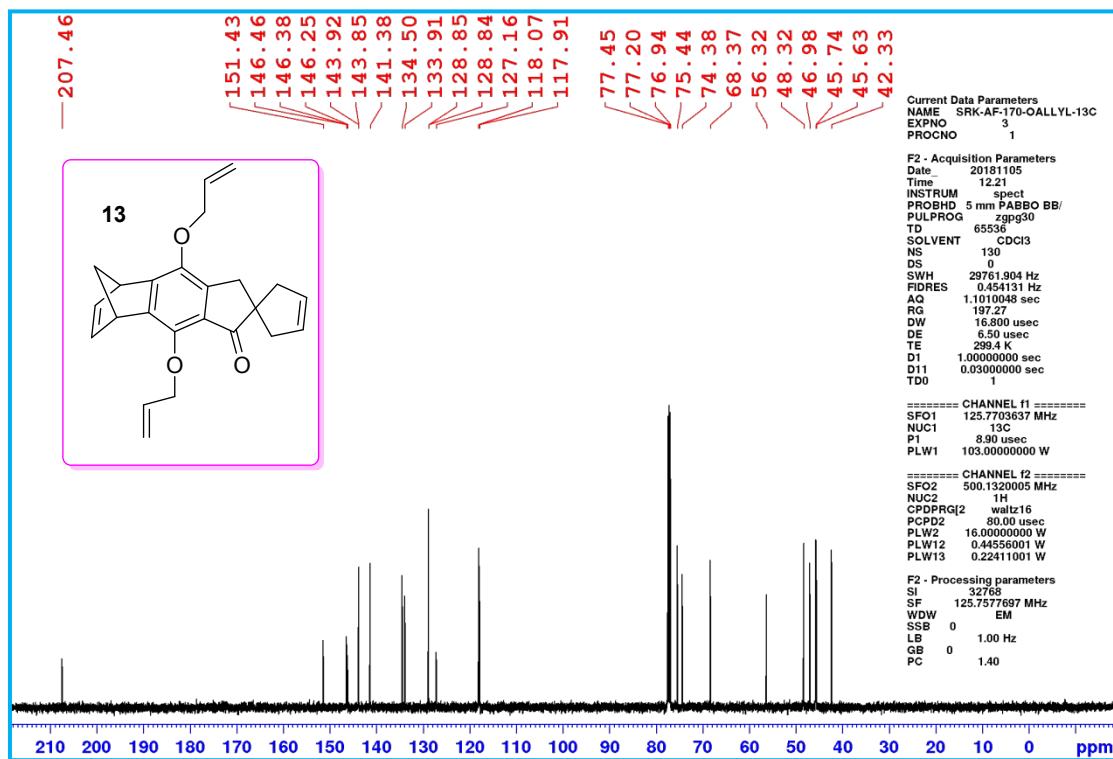


Figure S7c: DEPT 135 NMR of Compound 13 (125 MHz, CDCl₃):

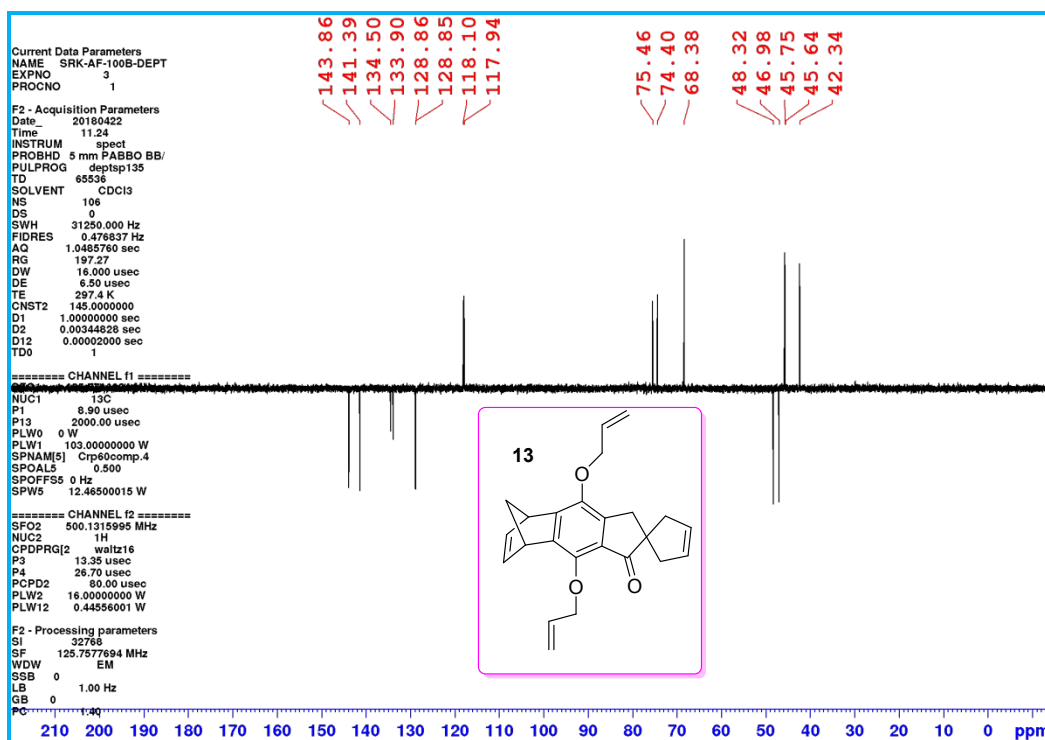


Figure S8a: ¹H NMR of Compound 3 (400 MHz, CDCl₃):

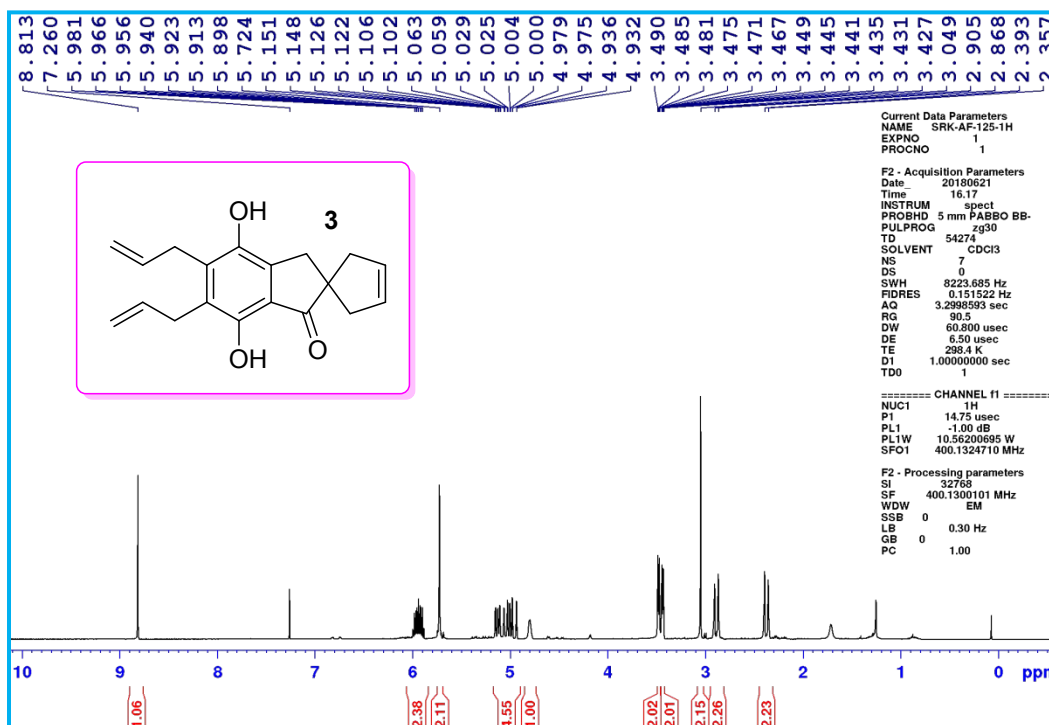


Figure S8b: ^{13}C NMR of Compound 3 (100 MHz, CDCl_3):

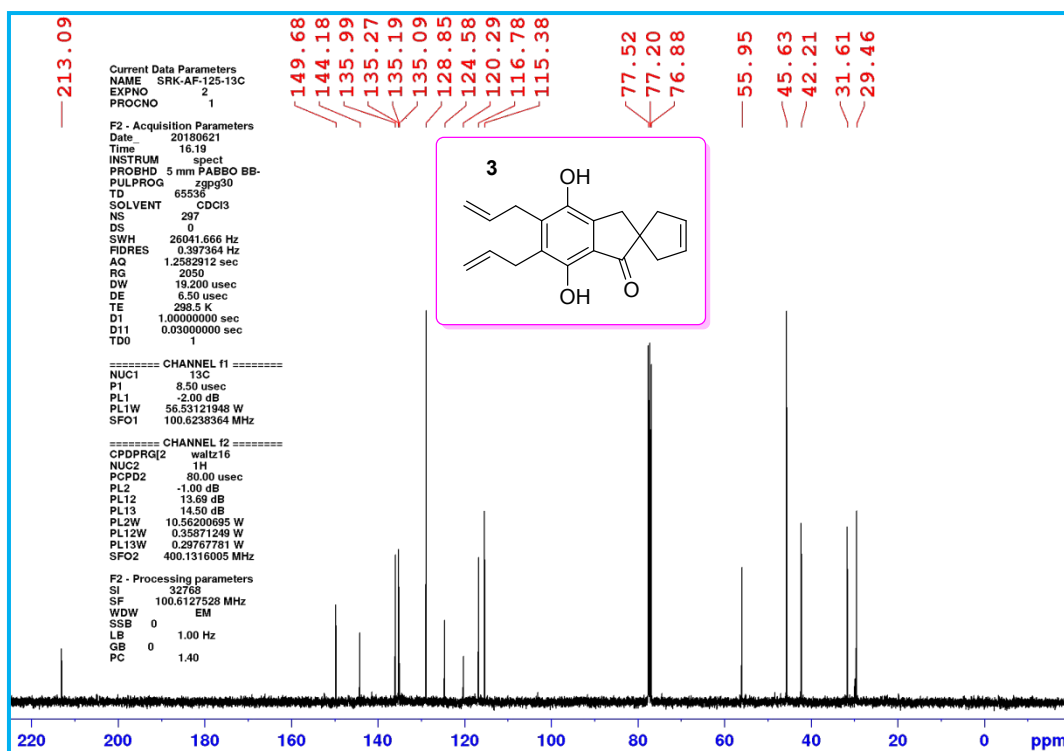


Figure S8c: DEPT 135 NMR of Compound 3 (100 MHz, CDCl_3):

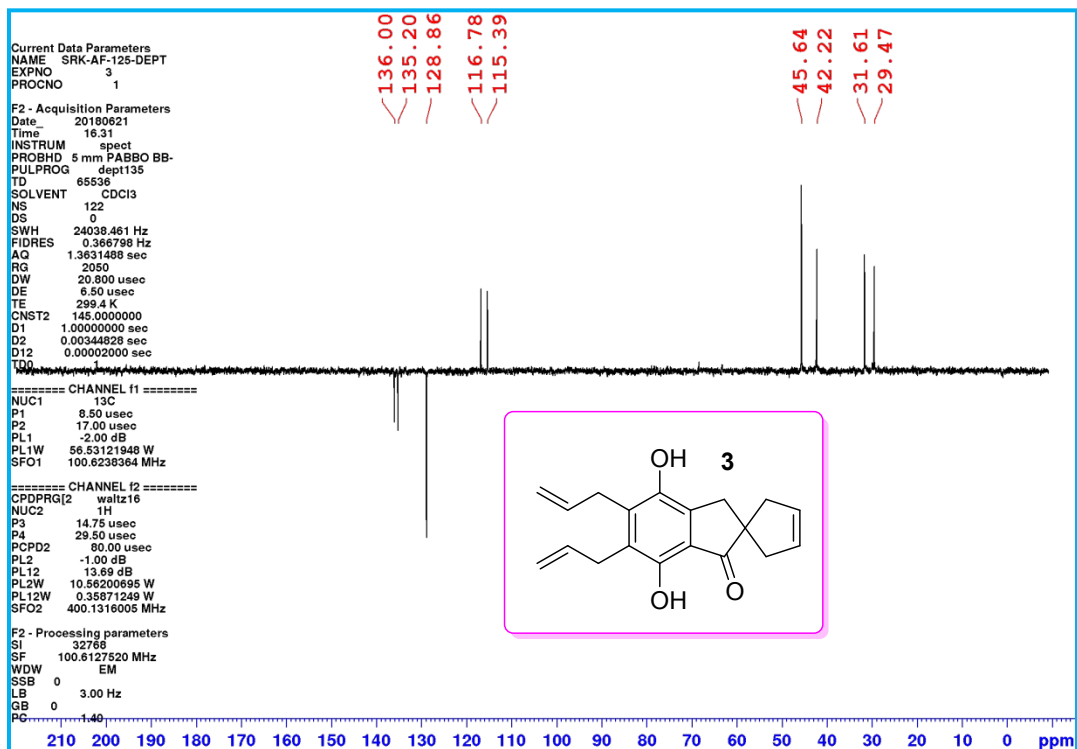


Figure S9a: ^1H NMR of Compound 14 (500 MHz, CDCl_3):

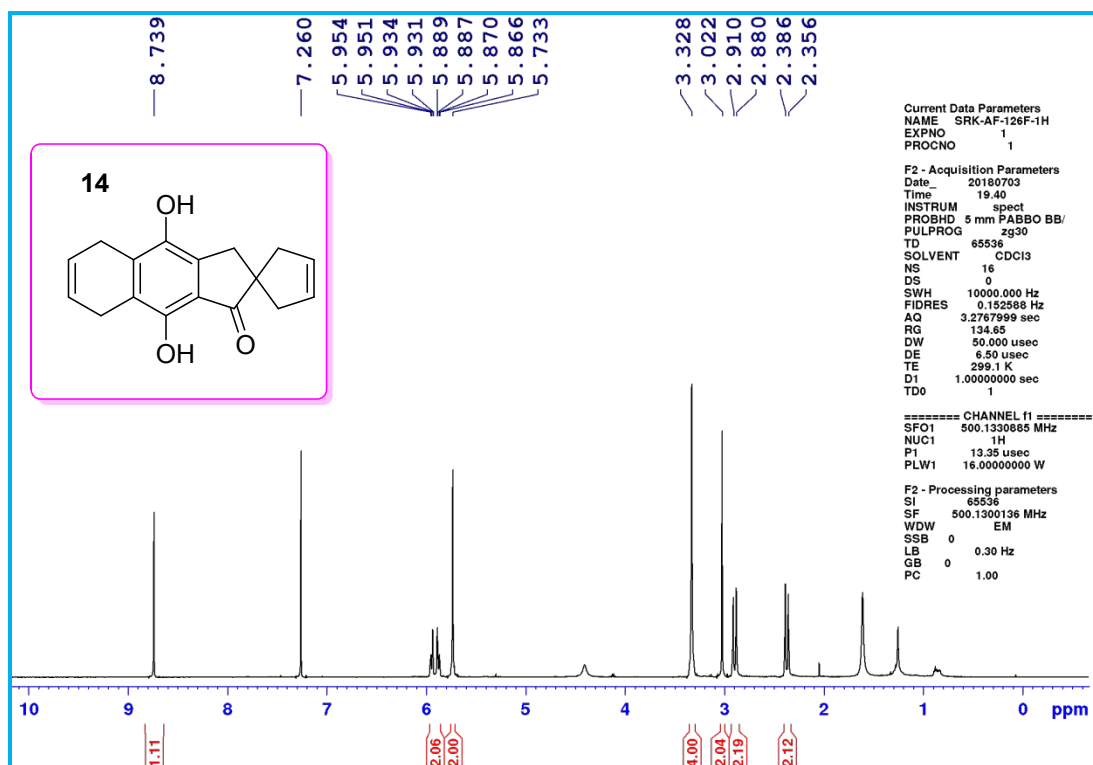


Figure S9b: ^{13}C NMR of Compound 14 (125 MHz, CDCl_3):

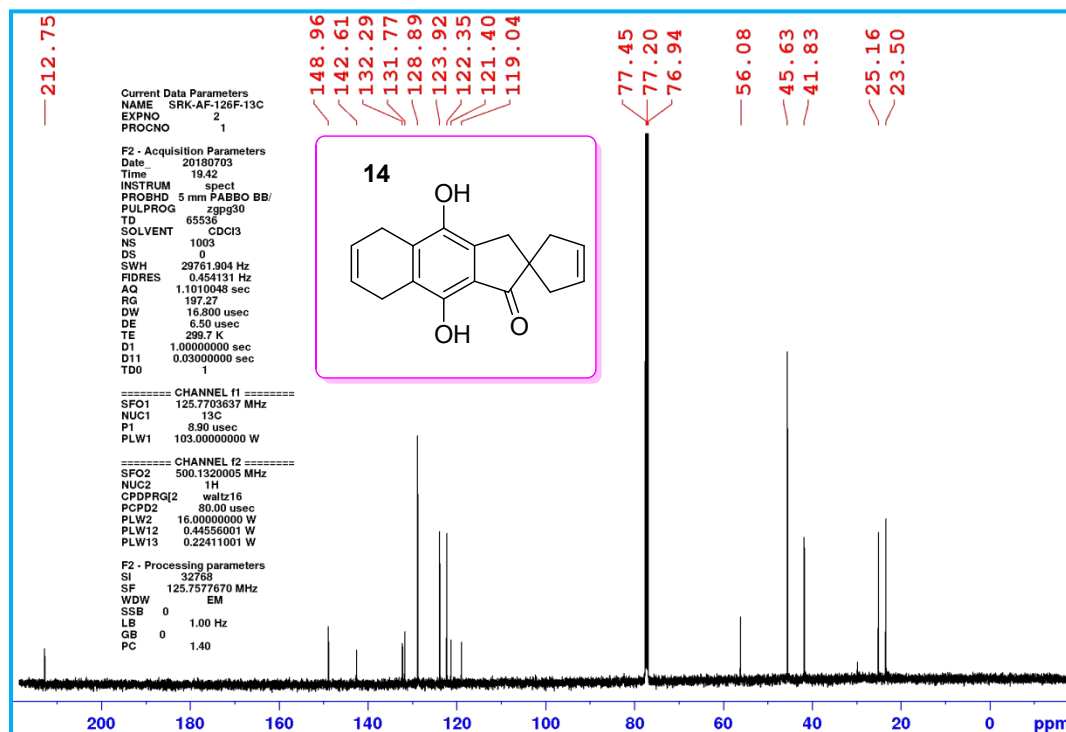


Figure S9c: DEPT 135 NMR of Compound 14 (125 MHz, CDCl₃):

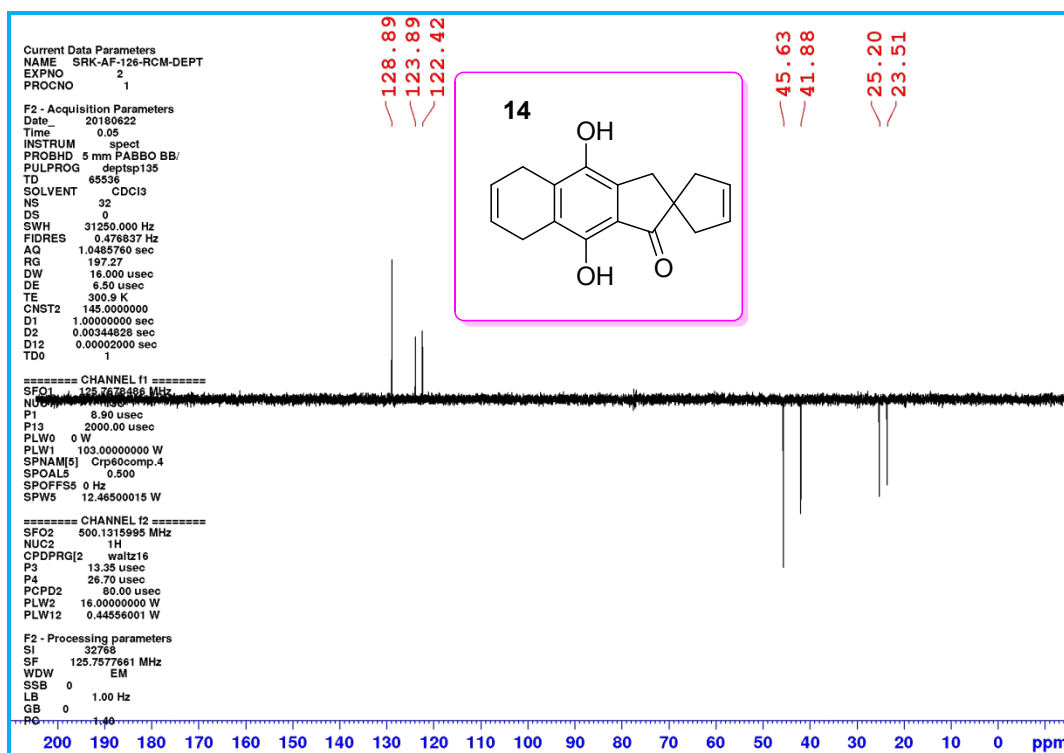


Figure S10a: ¹H NMR of Compound 2 (500 MHz, CDCl₃):

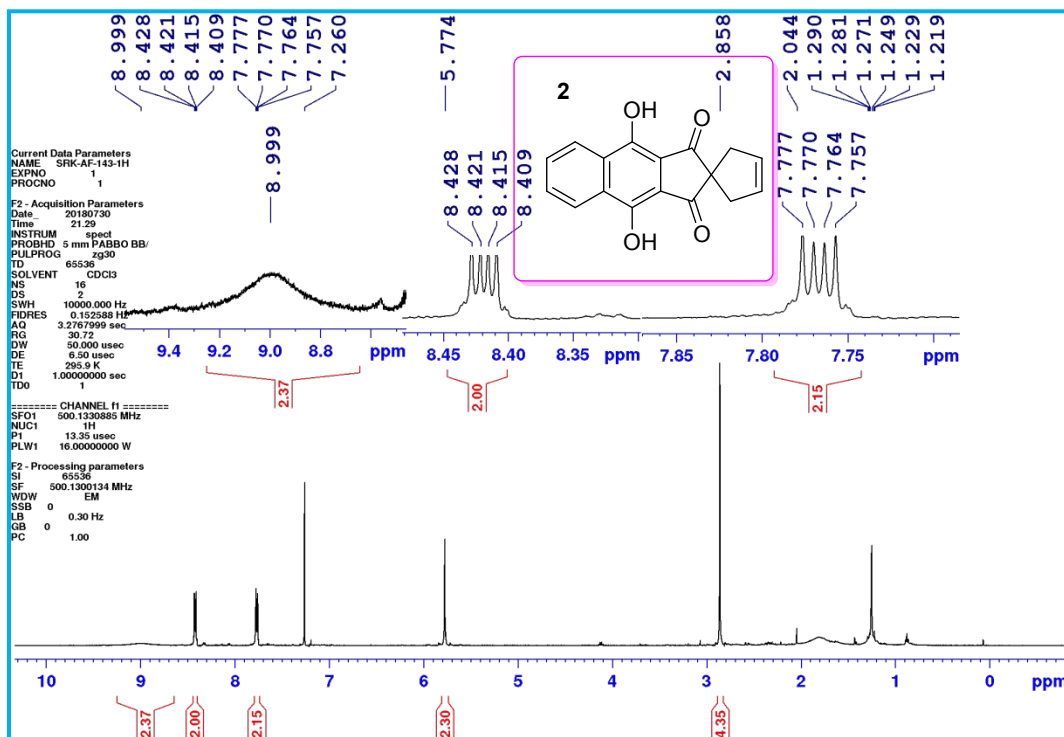
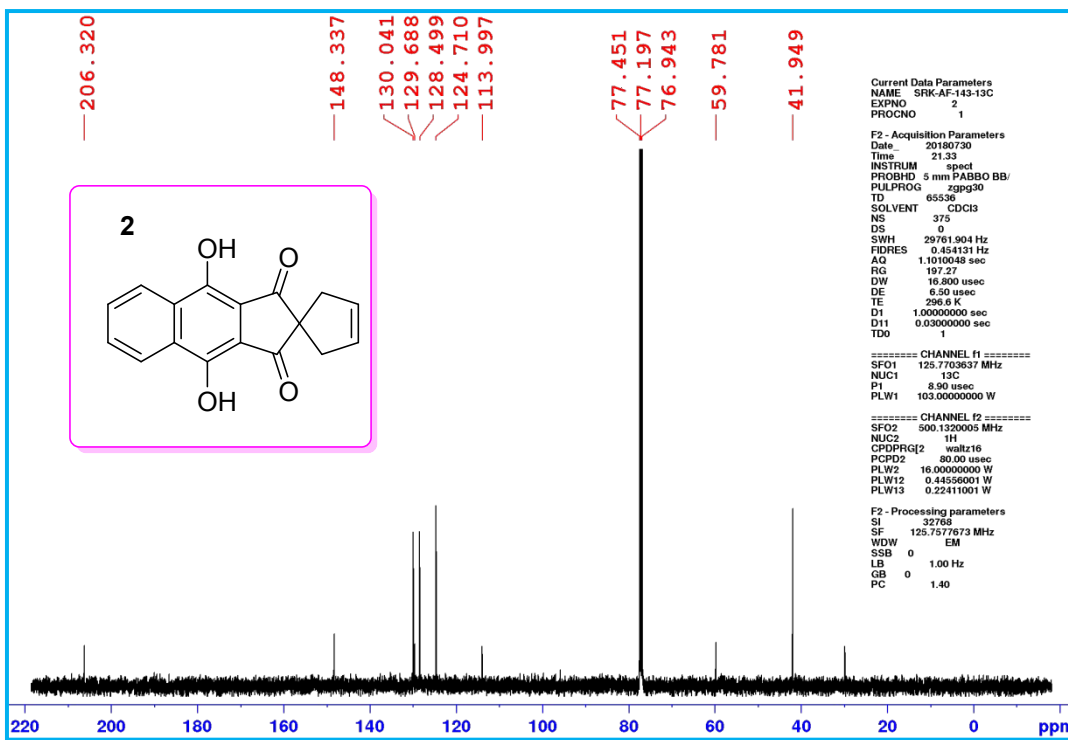


Figure S10b: ^{13}C NMR of Compound 2 (125 MHz, CDCl_3):



HRMS data for compound 3F

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Analysis Info

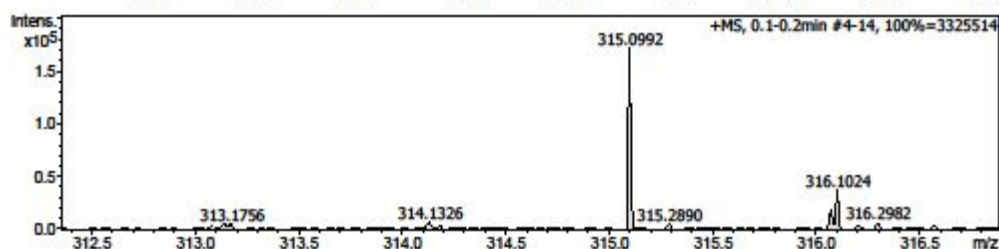
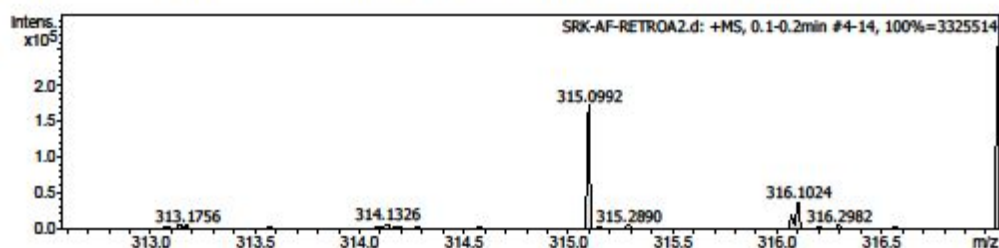
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Sample Name SRK-AF-RETROA2
Comment C19H18O3

Acquisition Date 7/17/2019 8:06:16 PM

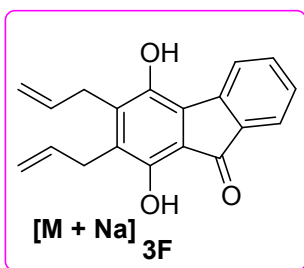
Operator kpk
Instrument maXis impact 282001.00081

Acquisition Parameter

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Scan End	1000 m/z	Set Collision Cell RF	1200.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e ⁻ Conf	N-Rule
315.0992	1	C19H16NaO3	315.0992	0.0	15.8	1	100.00	11.5	even	ok



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Analysis Info

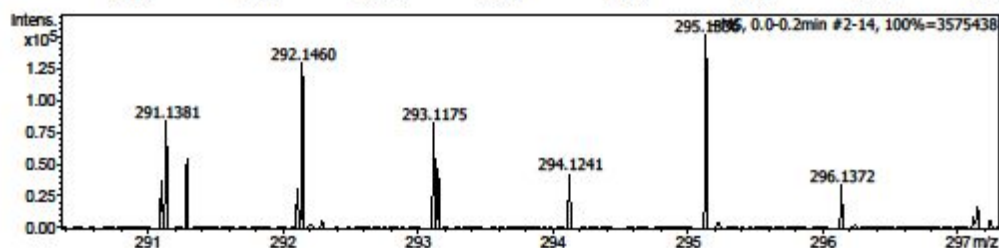
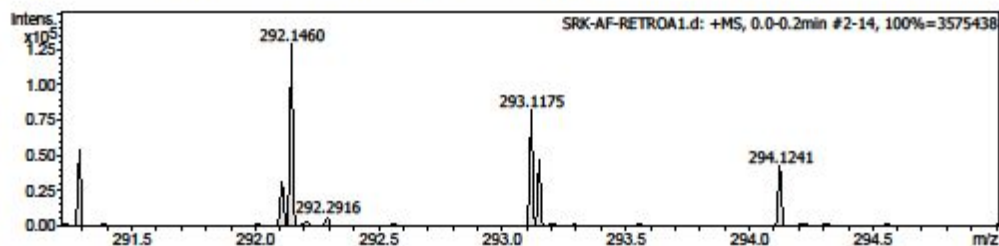
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Comment C19H16O3

Acquisition Date 7/17/2019 7:58:25 PM

Operator kpk
Instrument maXis impact 282001.00081

Acquisition Parameter

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Scan End	1000 m/z	Set Collision Cell RF	1200.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e ⁻ Conf	N-Rule
293.1175	1	C19H17O3	293.1172	-1.0	176.3	1	100.00	11.5	even	ok

