

Supporting Information for

Construction of Unique SCF₃-Containing Building Blocks via Allylic Alkylation of Morita-Baylis-Hillman Adducts

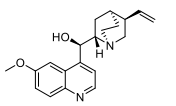
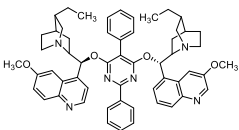
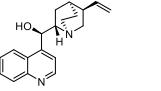
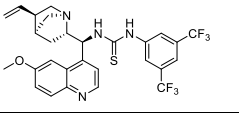
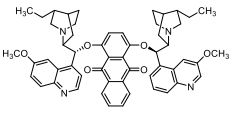
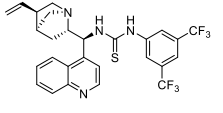
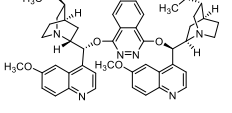
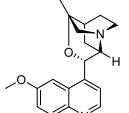
Priyanka Halder,^{a,b} Mahesh D. Pol,^a Milind M. Ahire,^{a,b} and Santosh B. Mhaske*^{a,b}

^aDivision of Organic Chemistry, CSIR-National Chemical Laboratory, Pune - 411008, India

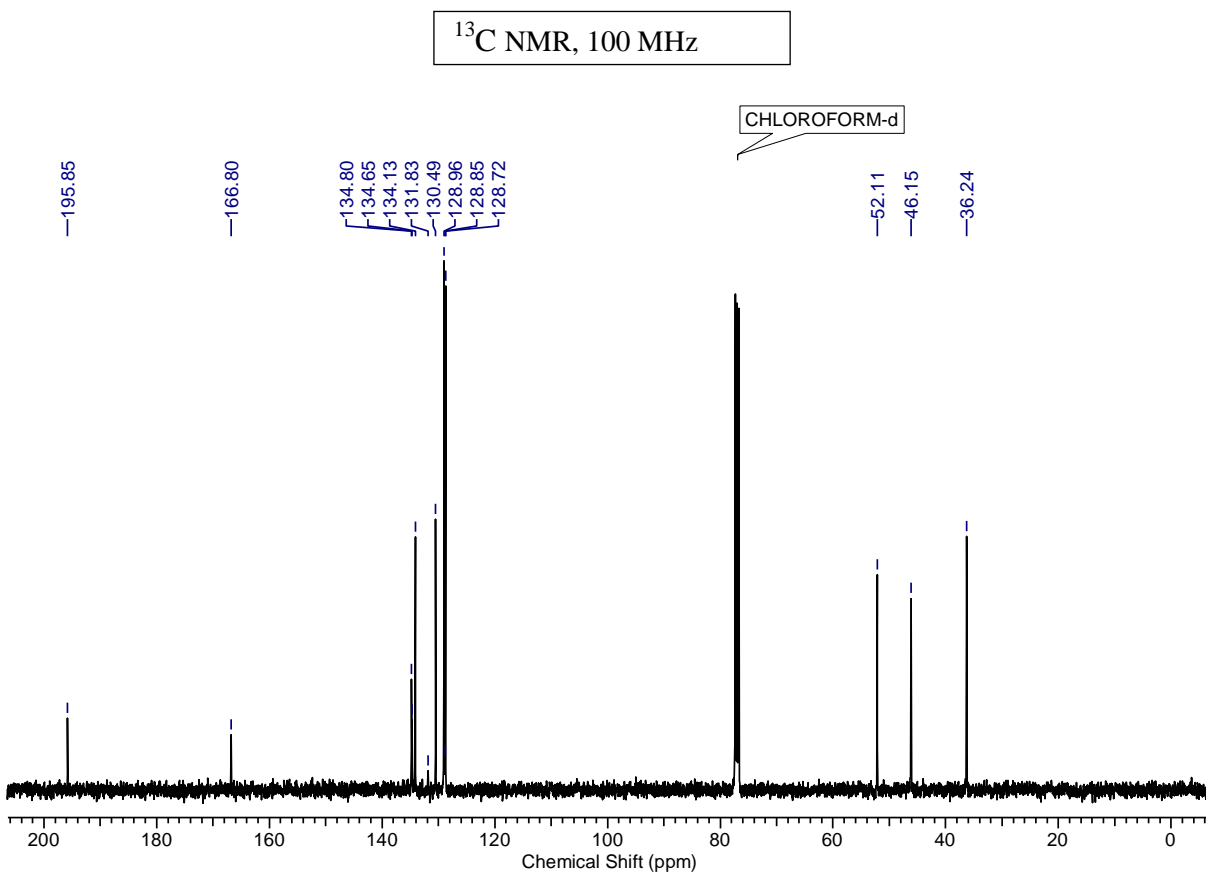
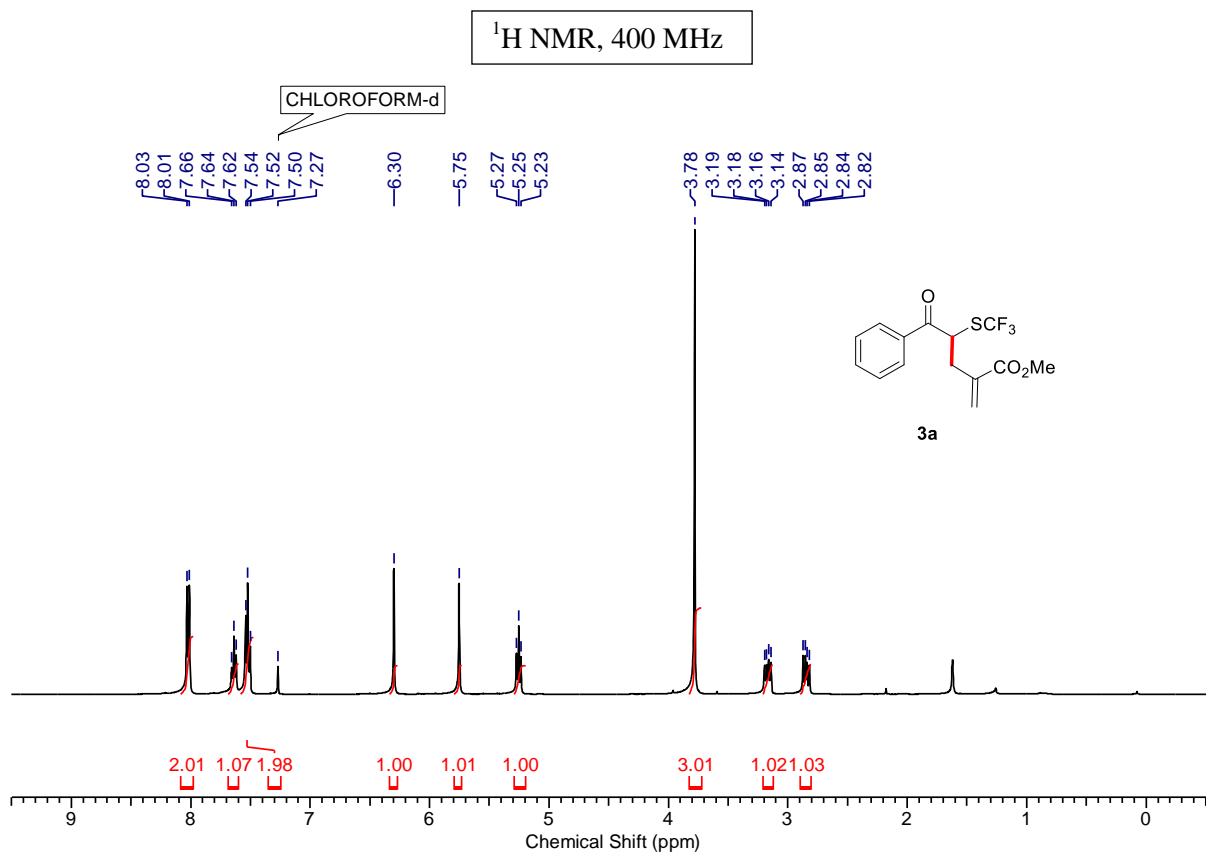
^bAcademy of Scientific and Innovative Research (AcSIR), Ghaziabad - 201002, India

Sr. No.	Index	Page No.
1.	Copies of ¹ H NMR, ¹³ C NMR Spectra, and HRMS Chromatogram	S2-S58

Structures of the catalysts used in Table 2:

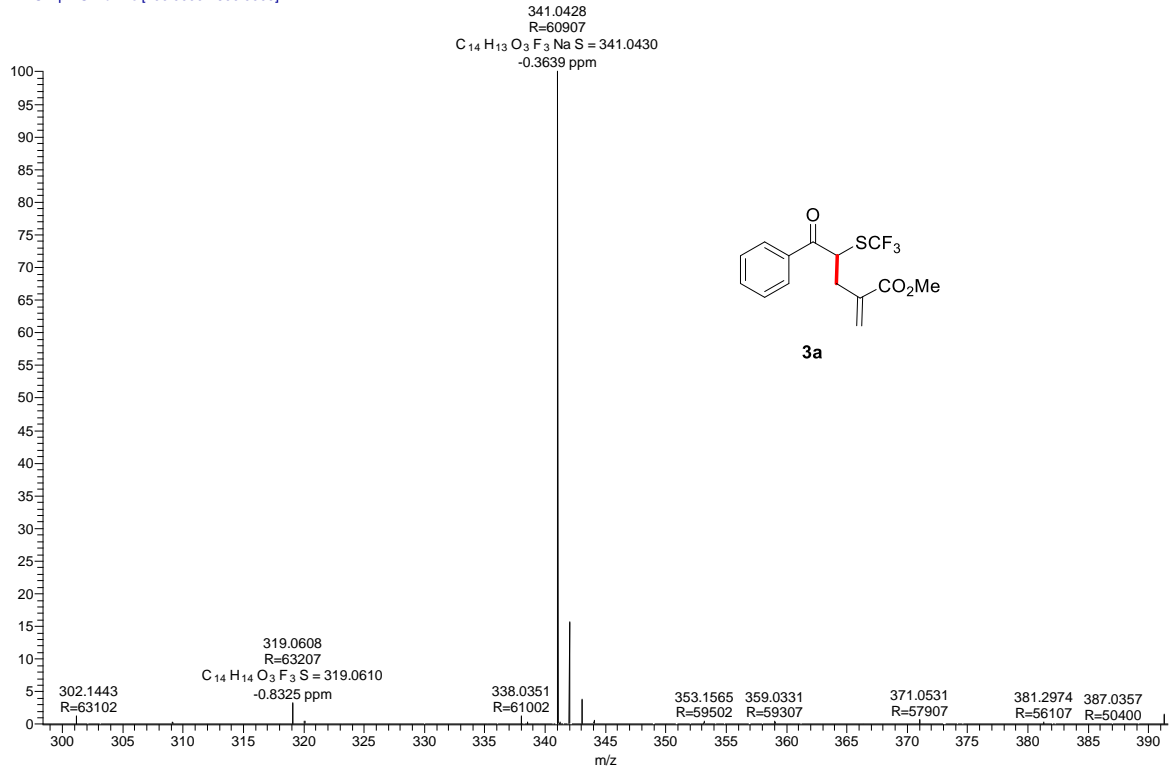
Sr. No.	Base	Structure	Sr. No.	Base	Structure
1.	Quinine		5.	(DHQD) ₂ PYR	
2.	Cinchonidine		6.	Thiourea cat. A	
3.	(DHQ) ₂ AQN		7.	Thiourea cat. B	
4.	(DHQ) ₂ PHAL		8.	β-isocupreidine	

Copies of ^1H NMR, ^{13}C NMR Spectra and HRMS Chromatogram:

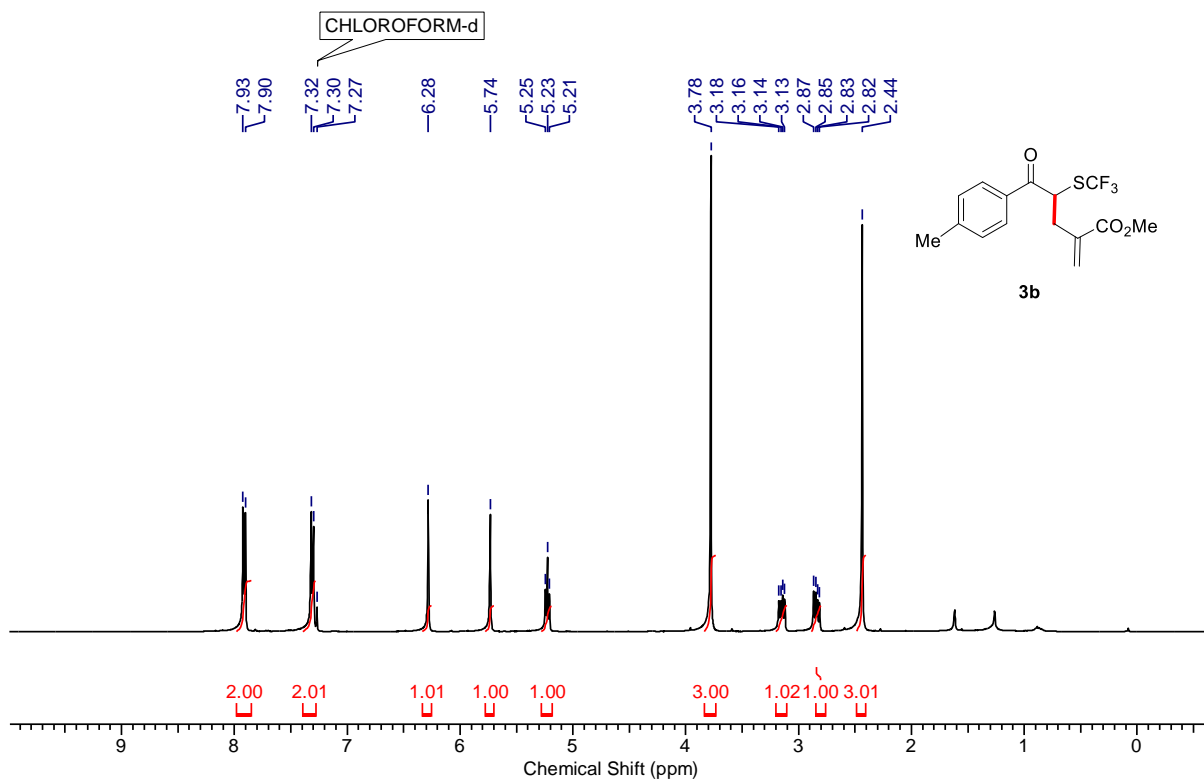


ESI-HRMS

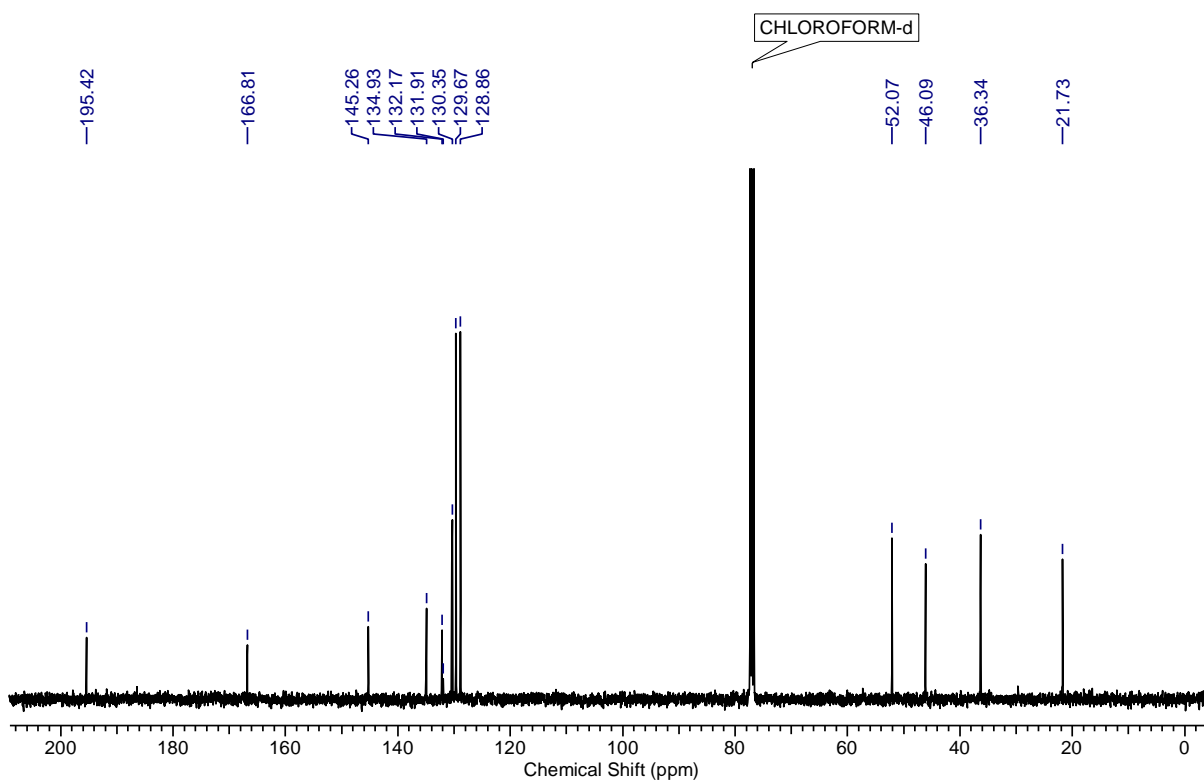
BHA-3 #314 RT: 1.40 AV: 1 NL: 1.22E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]



¹H NMR, 400 MHz

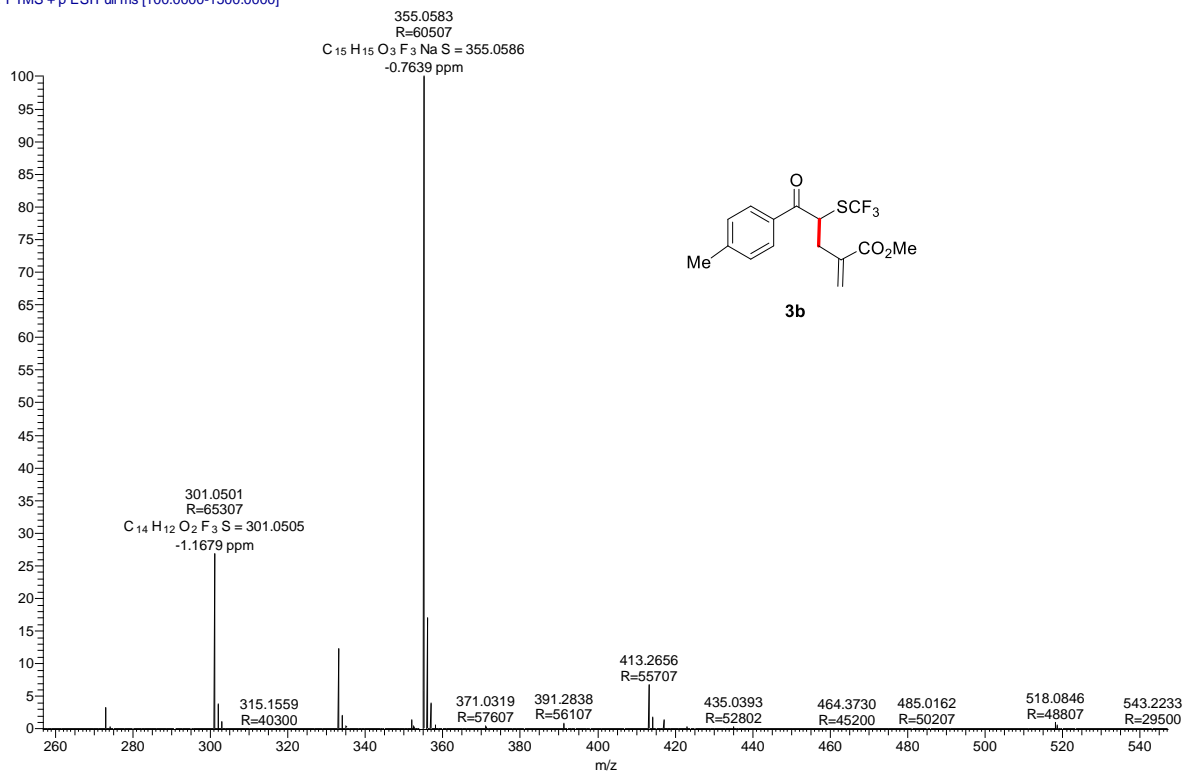


¹³C NMR, 100 MHz

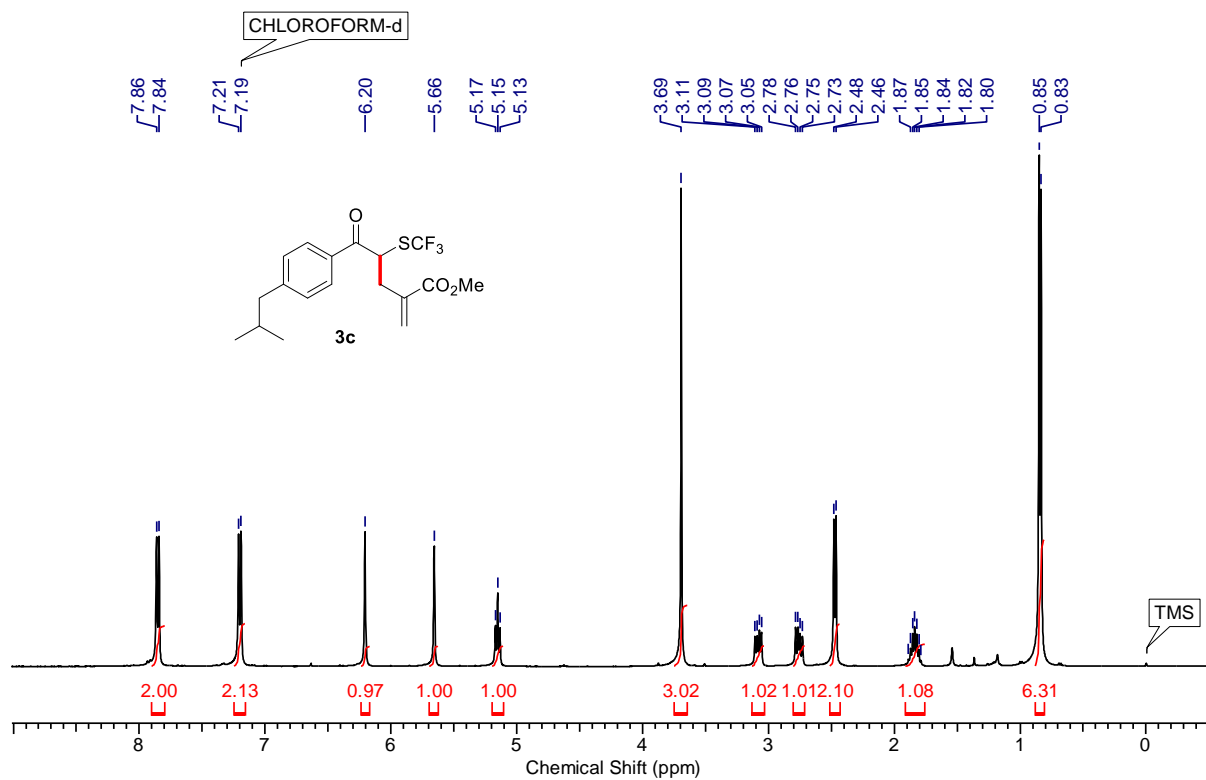


ESI-HRMS

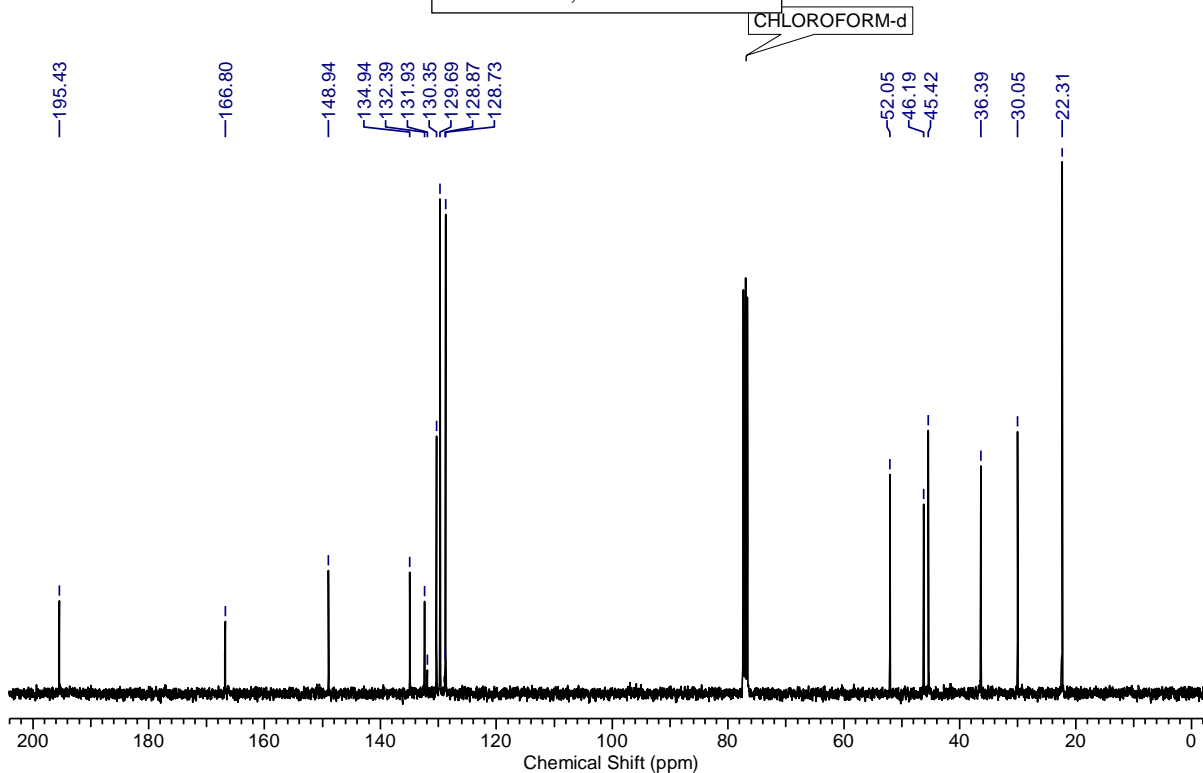
BHA-7_180516154237 #290 RT: 1.29 AV: 1 NL: 2.81E9
T: FTMS + p ESIFull ms [100.0000-1500.0000]



¹H NMR, 400 MHz

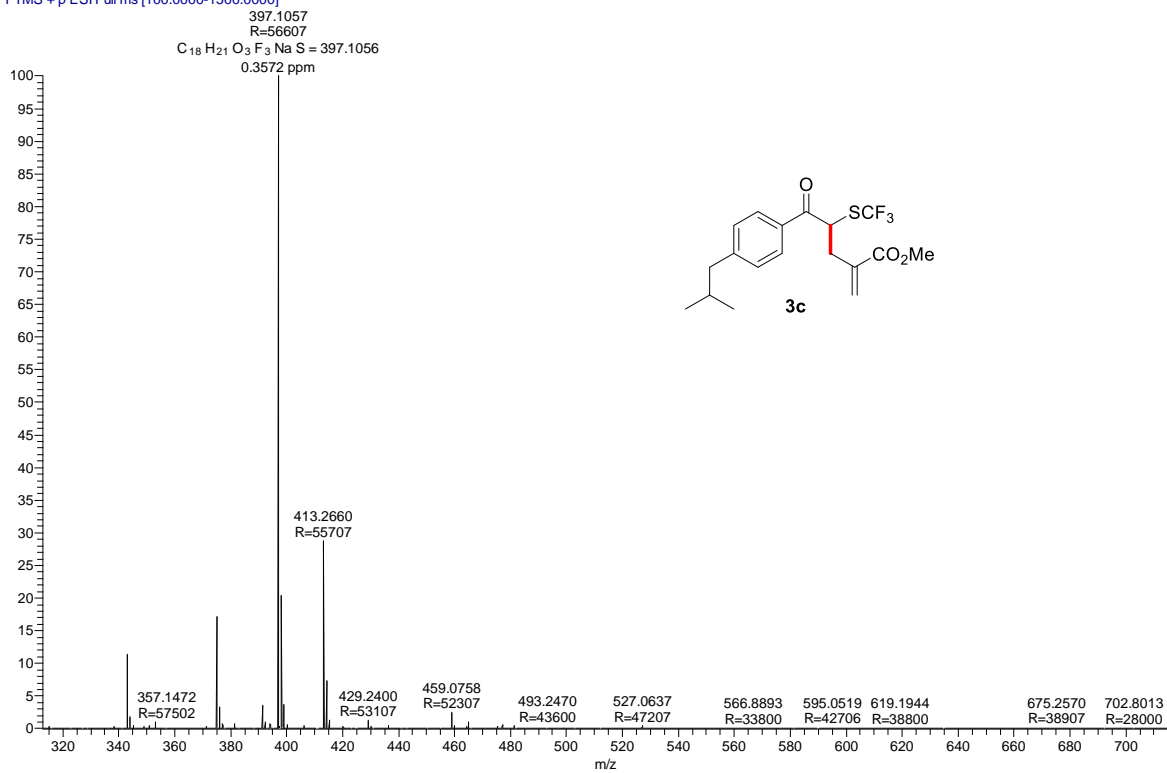


¹³C NMR, 100 MHz

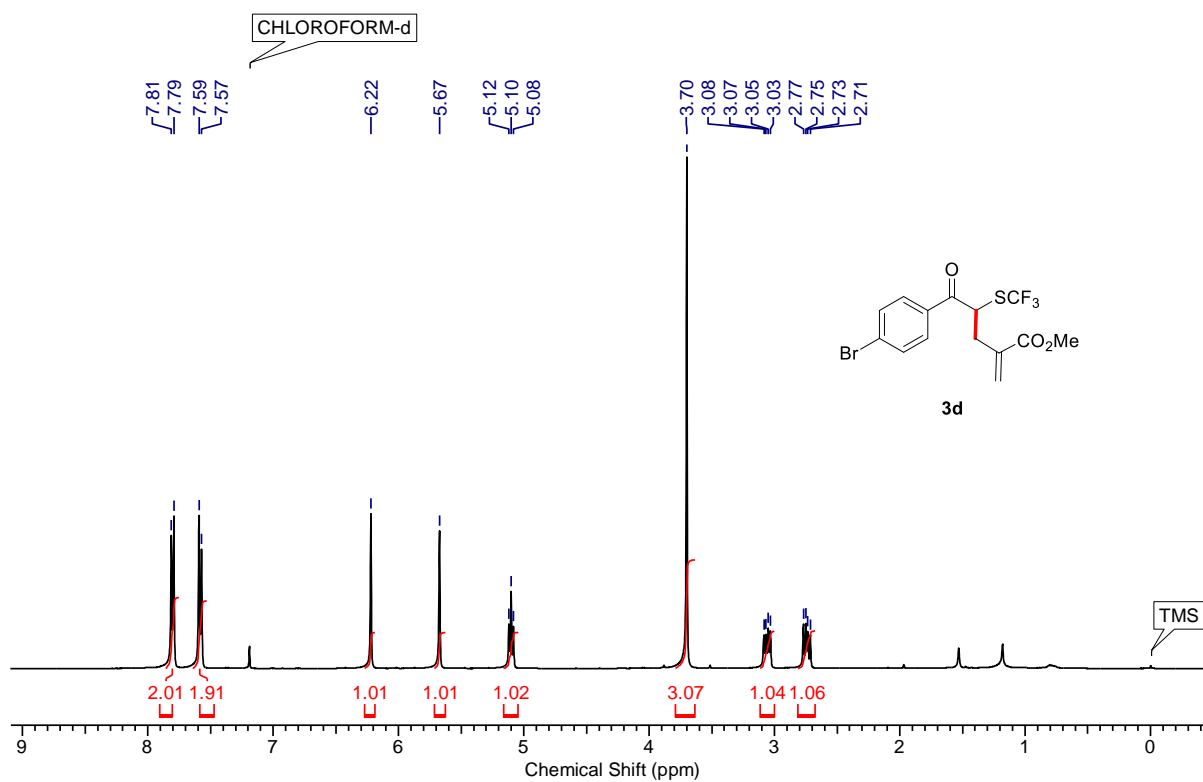


ESI-HRMS

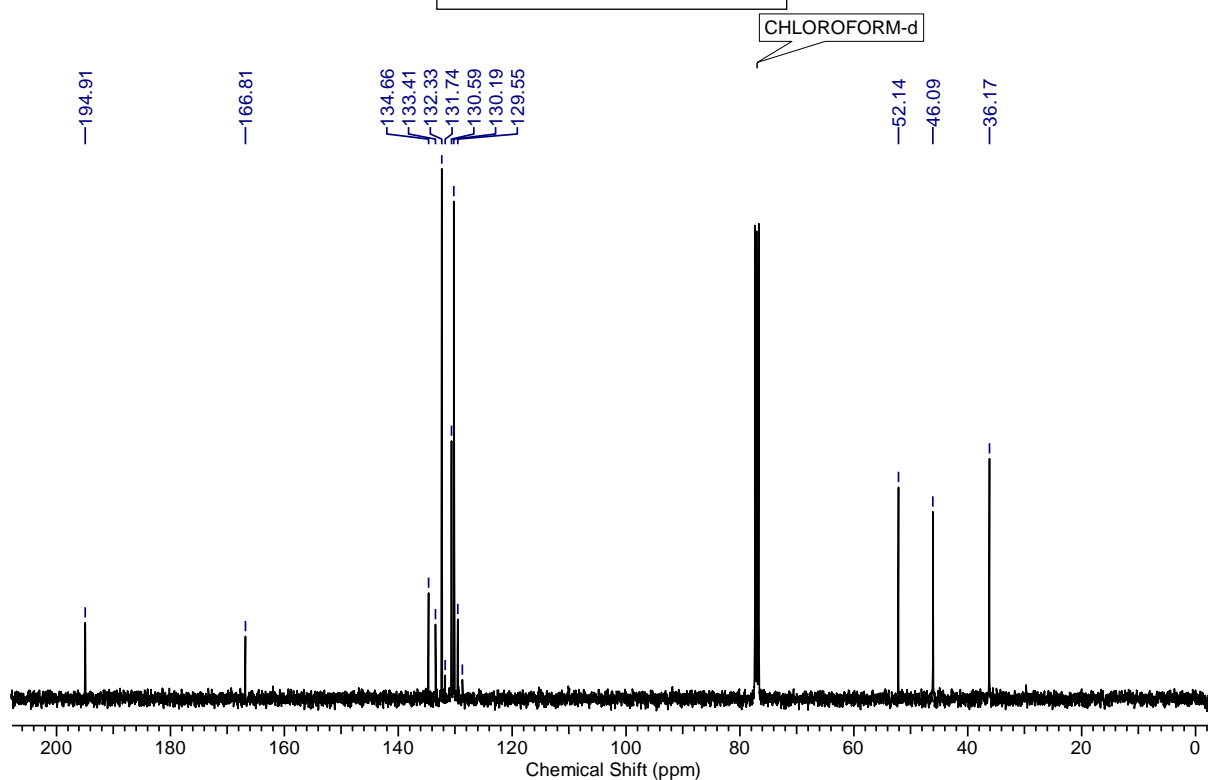
BHA-8 #325 RT: 1.45 AV: 1 NL: 6.37E8
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¹H NMR, 400 MHz

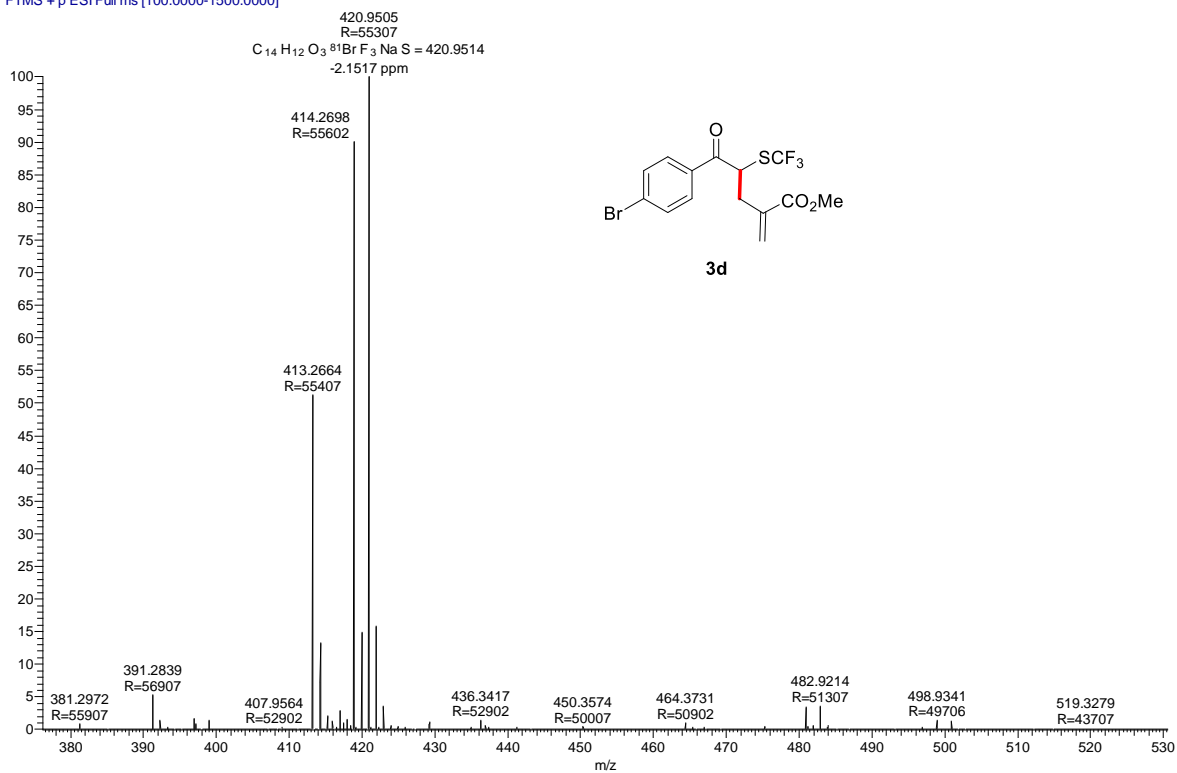


¹³C NMR, 100 MHz

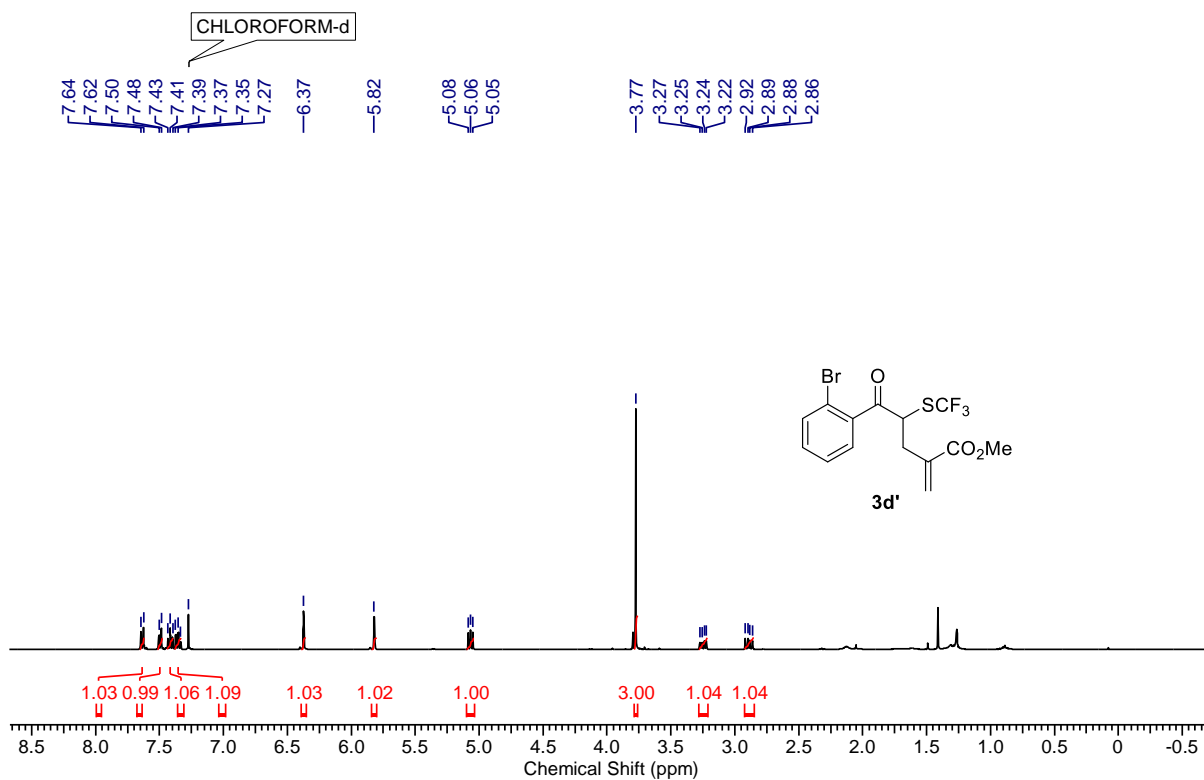


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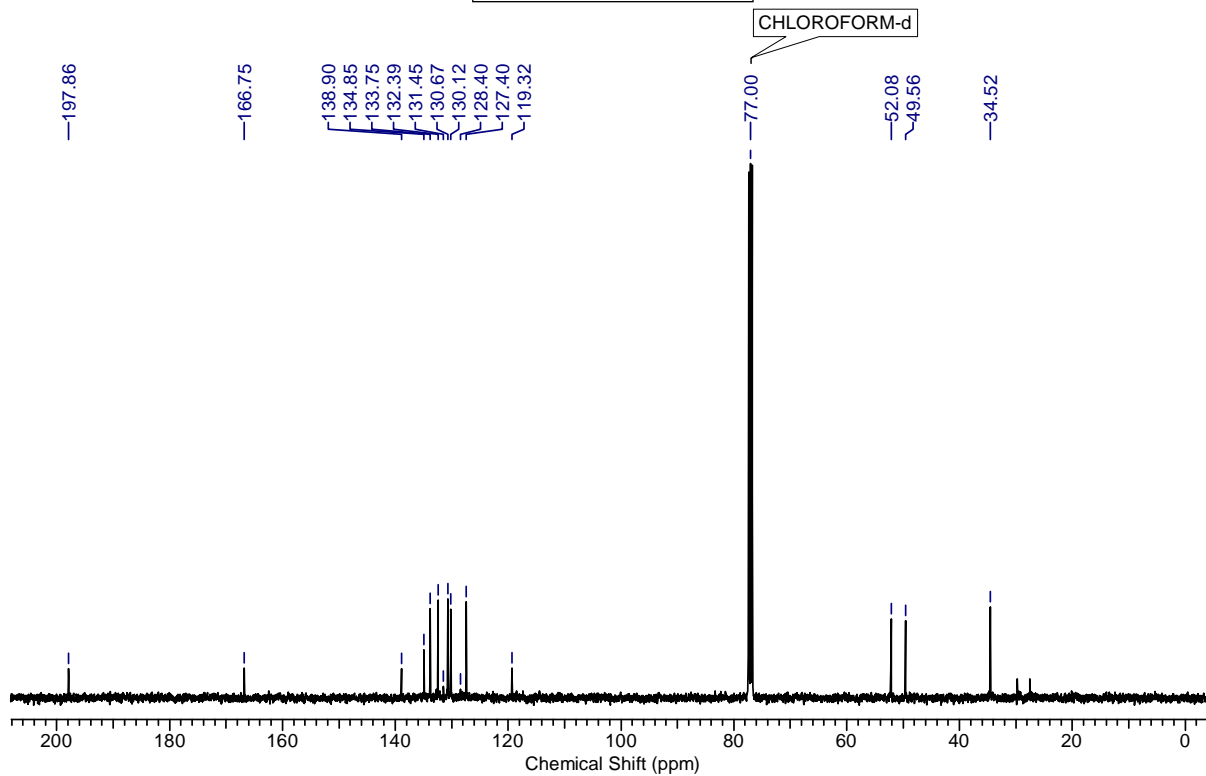
BHA-6_180516153828 #305 RT: 1.36 AV: 1 NL: 4.61E8
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¹H NMR, 400 MHz

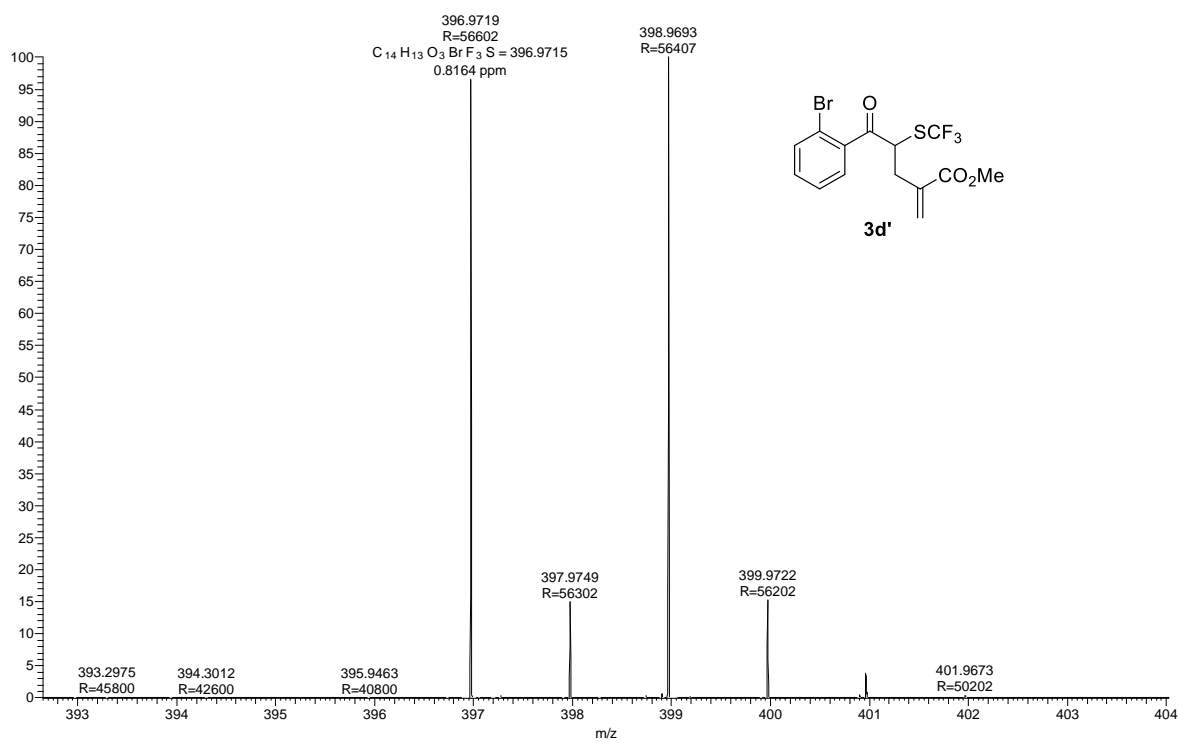


¹³C NMR, 100 MHz

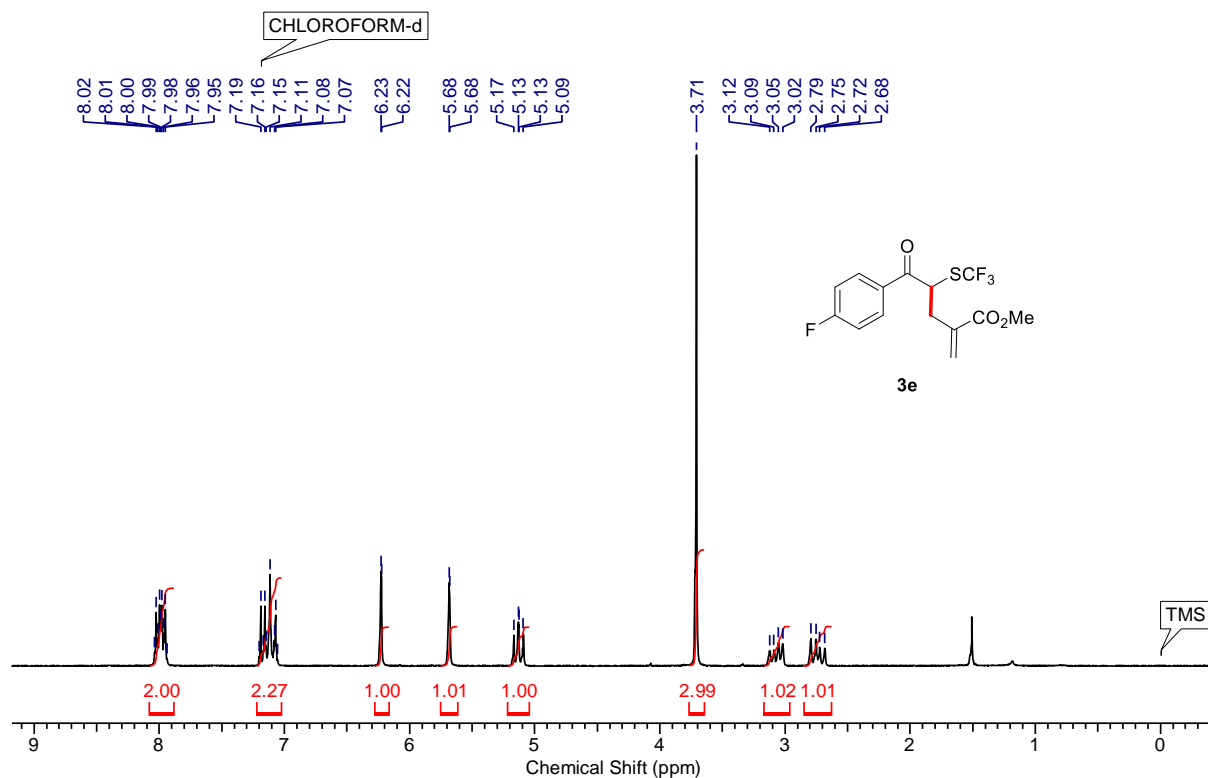


ESI-HRMS

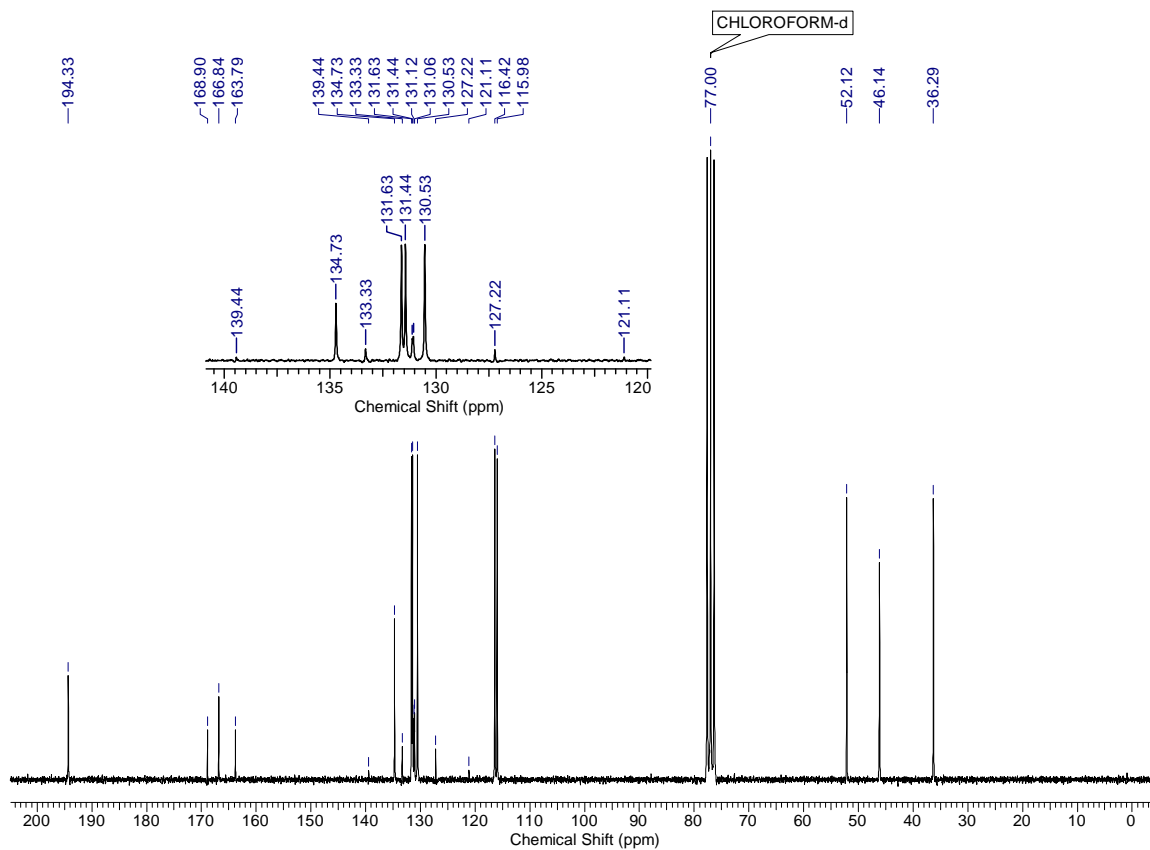
MP_01 #296 RT: 1.71 AV: 1 NL: 1.44E8
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¹H NMR, 200 MHz

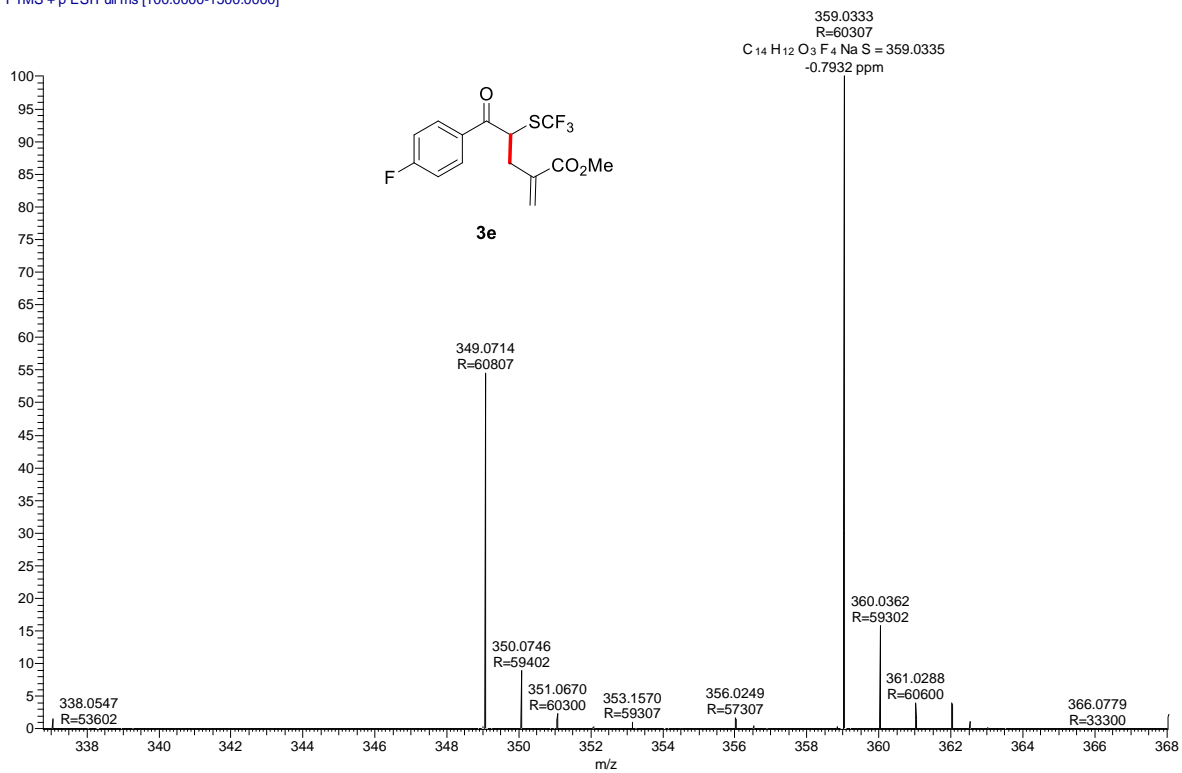


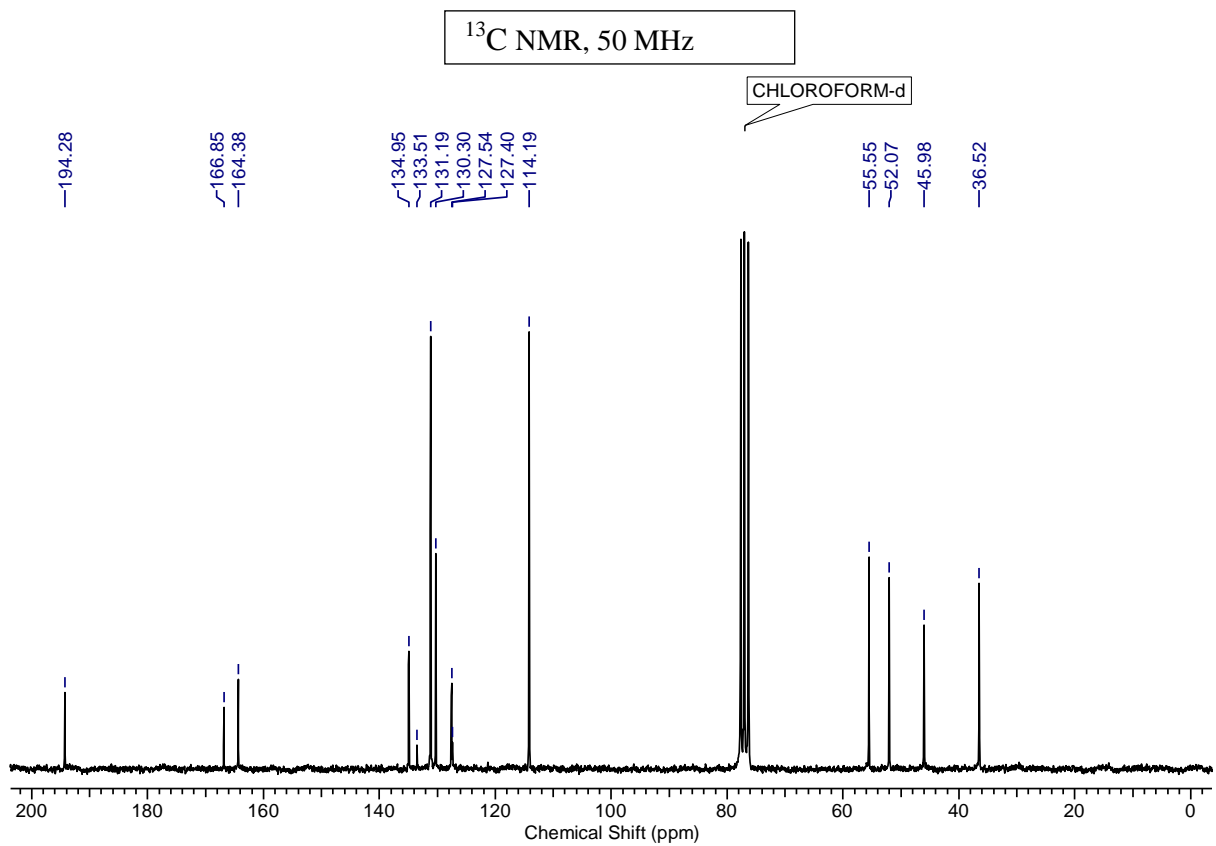
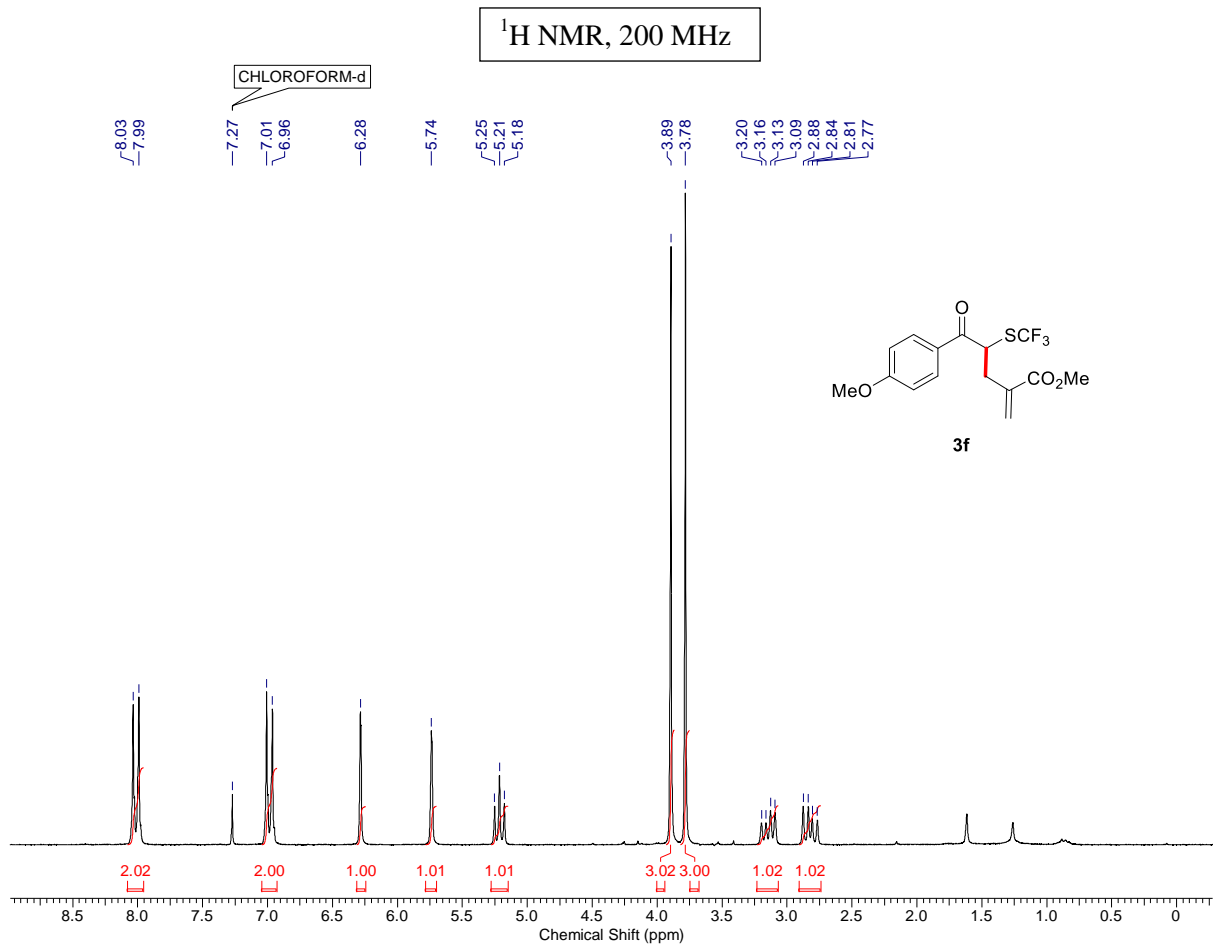
¹³C NMR, 50 MHz



ESI-HRMS

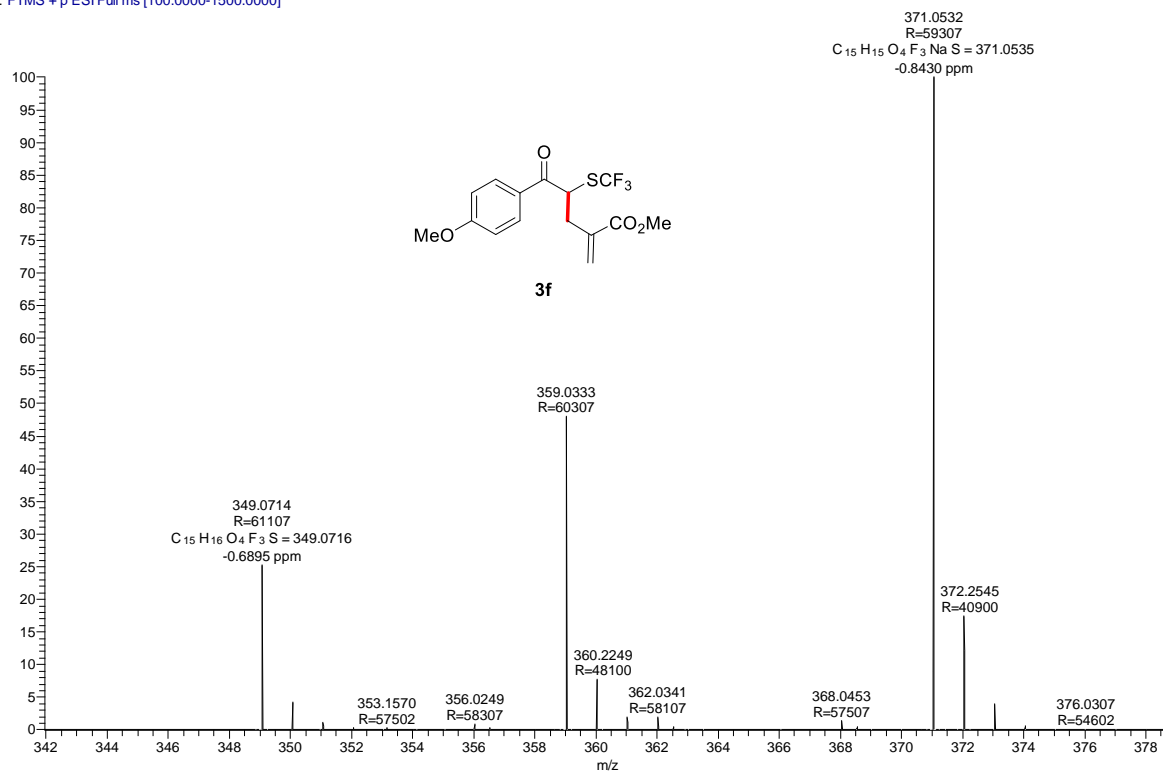
BHA-1 #304 RT: 1.35 AV: 1 NL: 6.19E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



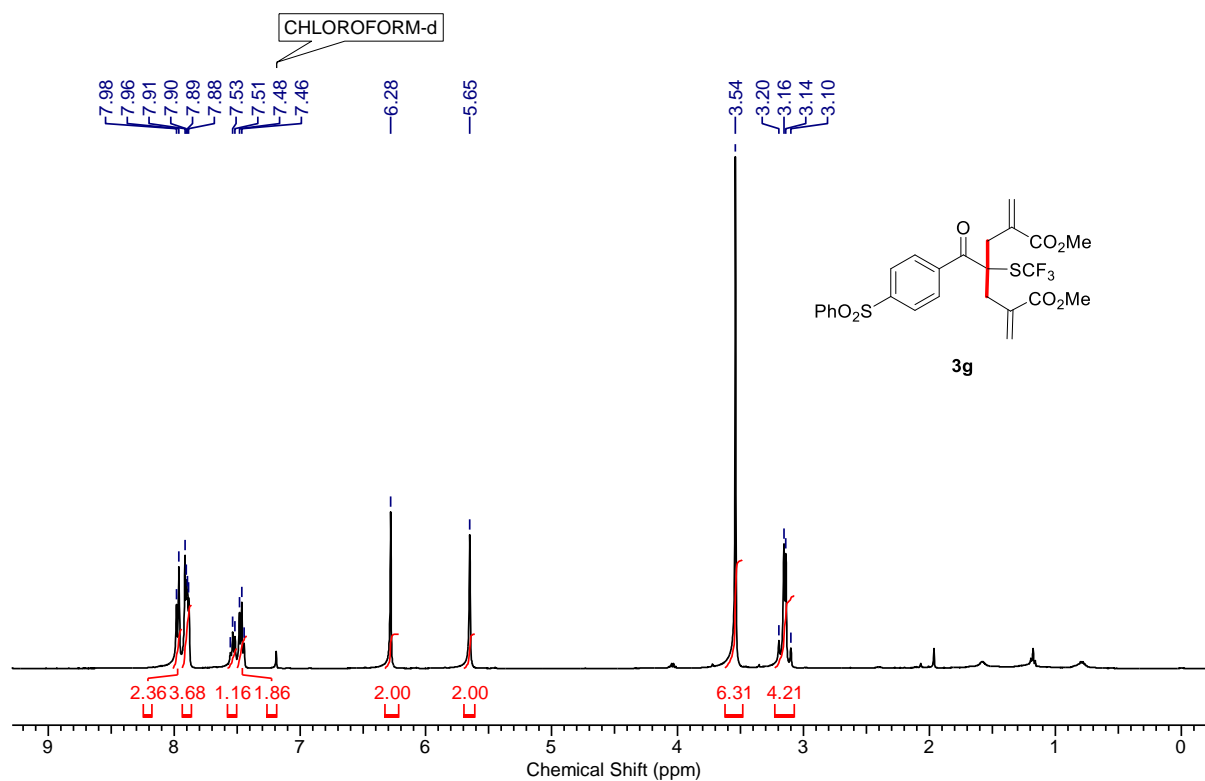


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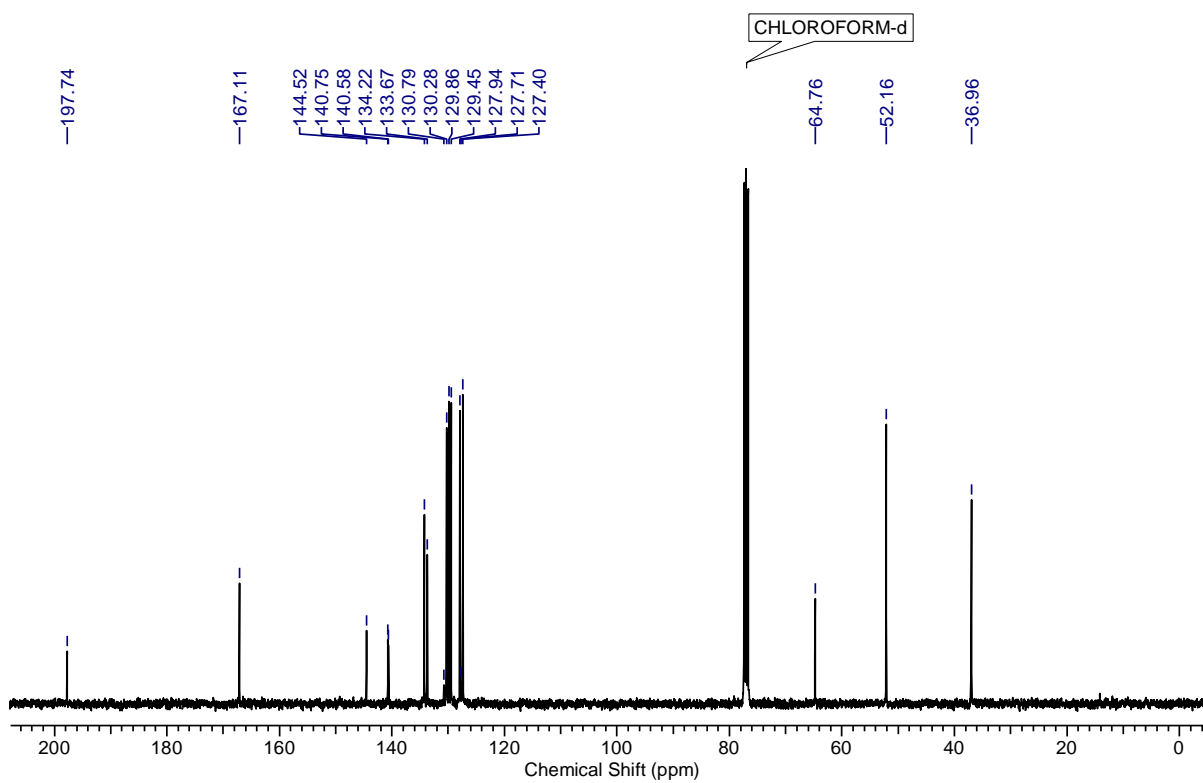
BHA-2 #291 RT: 1.29 AV: 1 NL: 1.84E9
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¹H NMR, 400 MHz

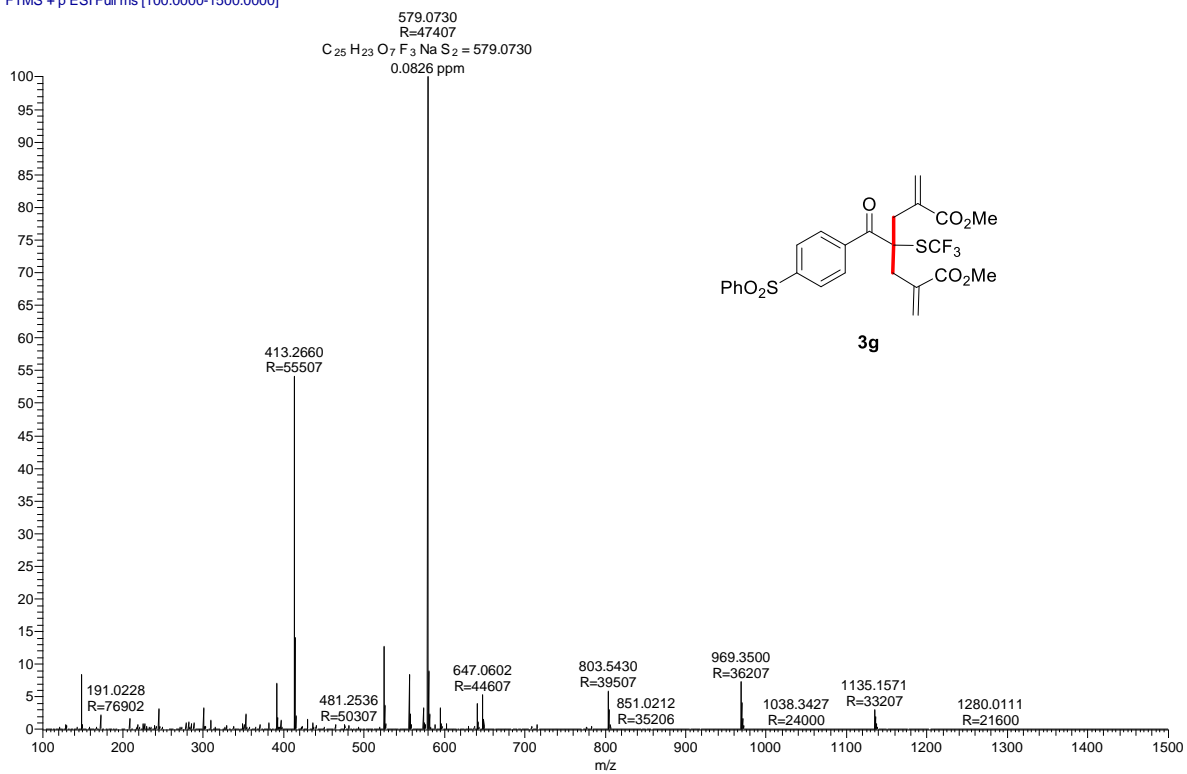


¹³C NMR, 100 MHz

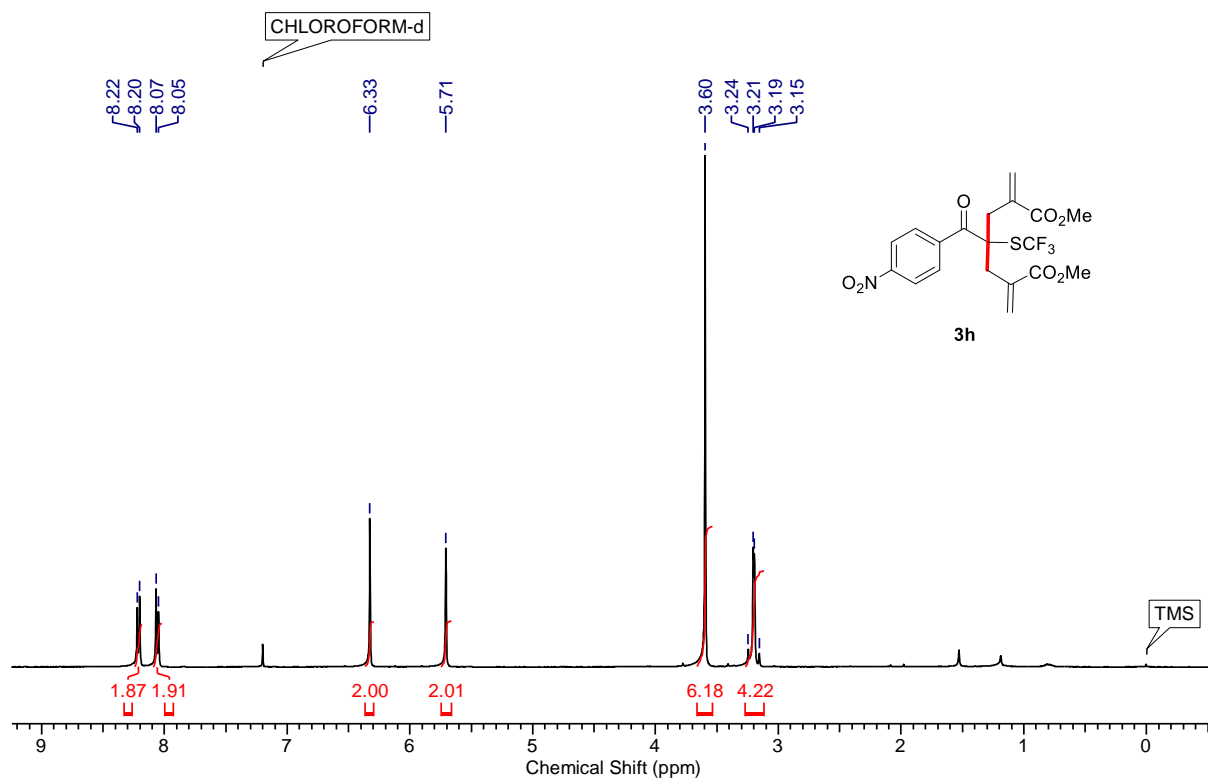


ESI-HRMS

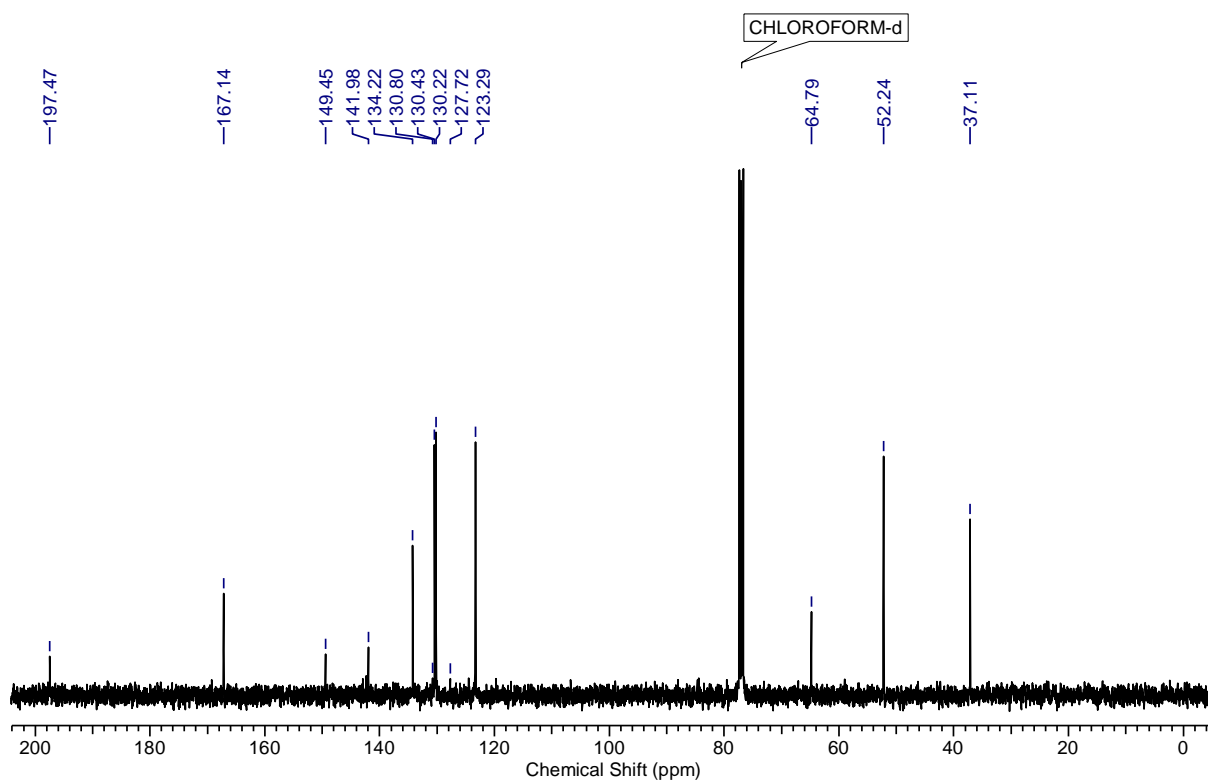
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¹H NMR, 400 MHz

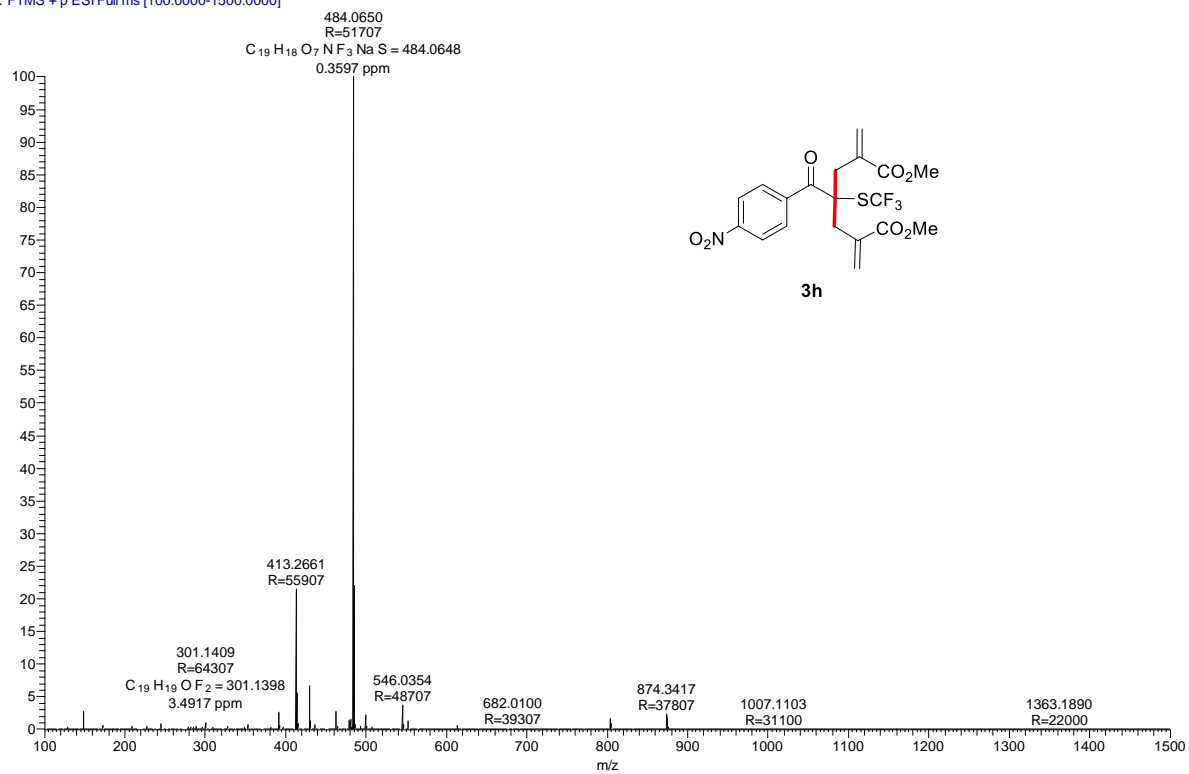


¹³C NMR, 100 MHz



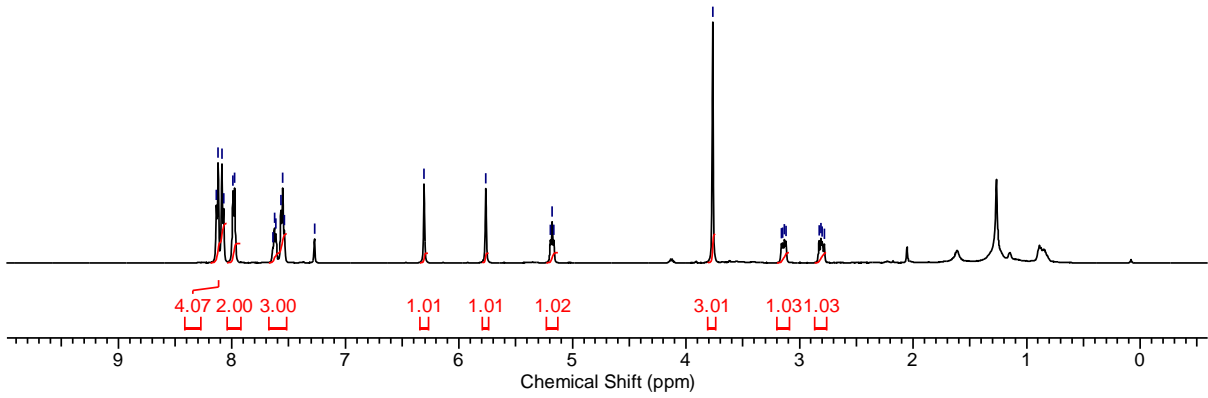
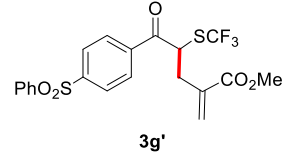
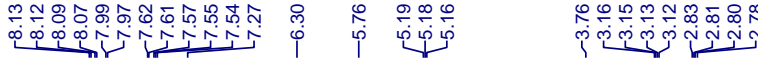
ESI-HRMS

BHA-12 #278 RT: 1.24 AV: 1 NL: 9.44E8
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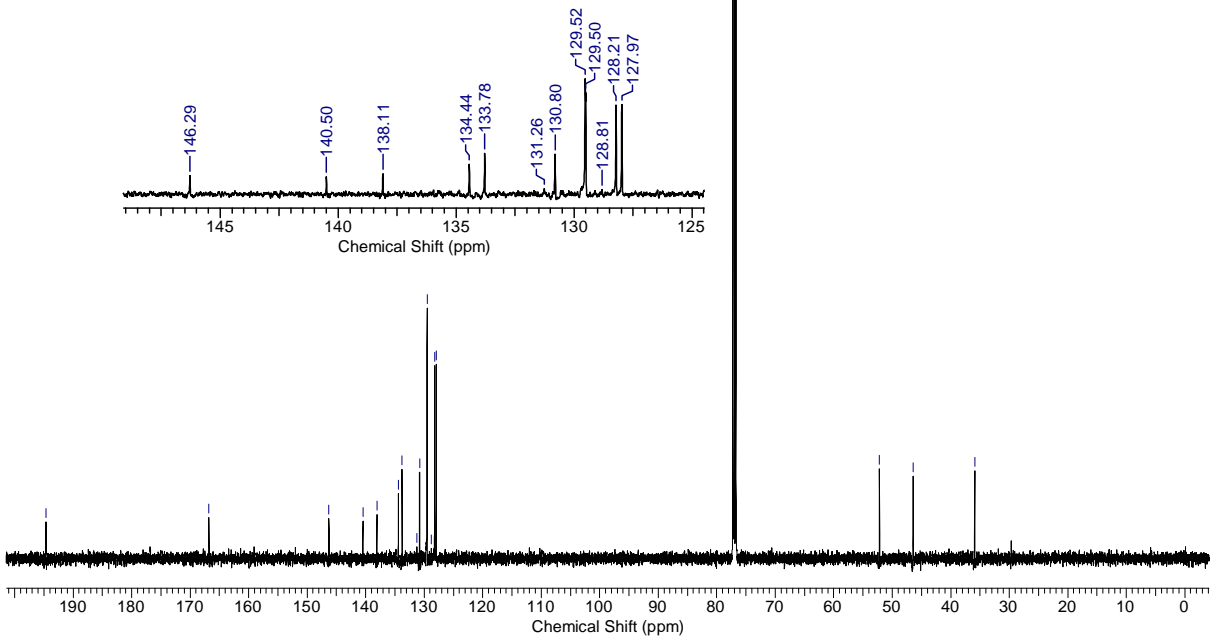
¹H NMR, 500 MHz

CHLOROFORM-d



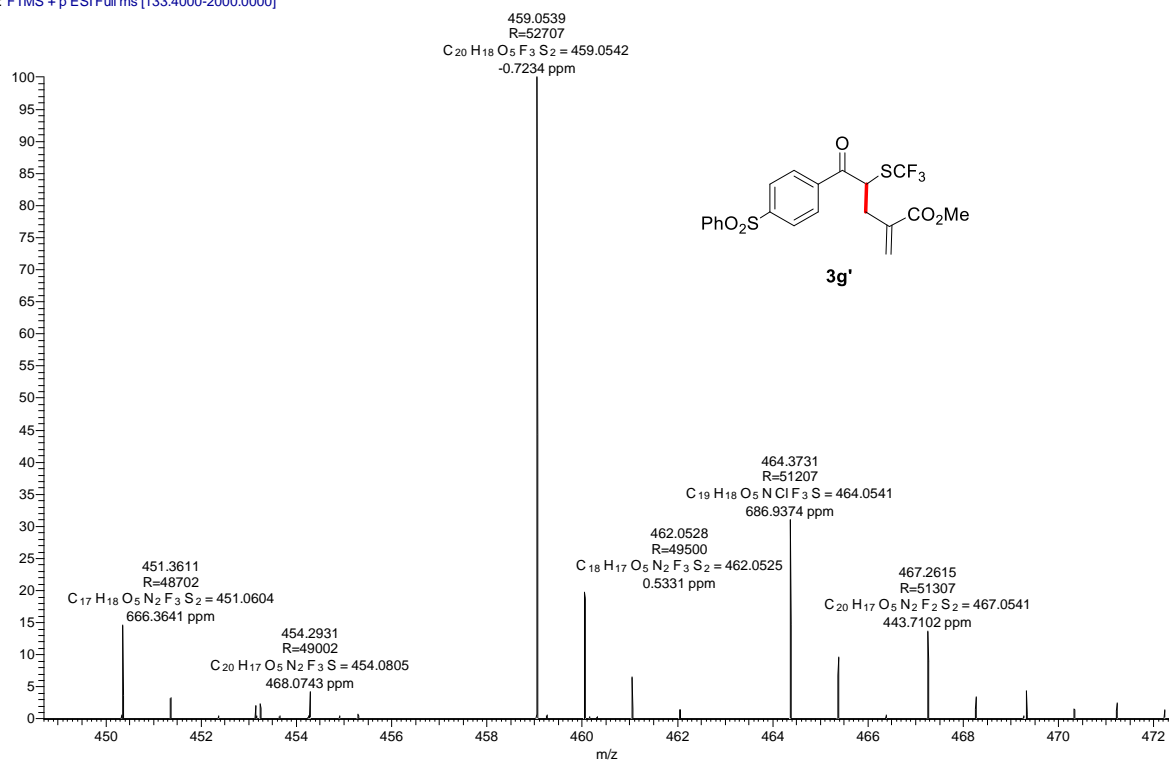
¹³C NMR, 125 MHz

CHLOROFORM-d

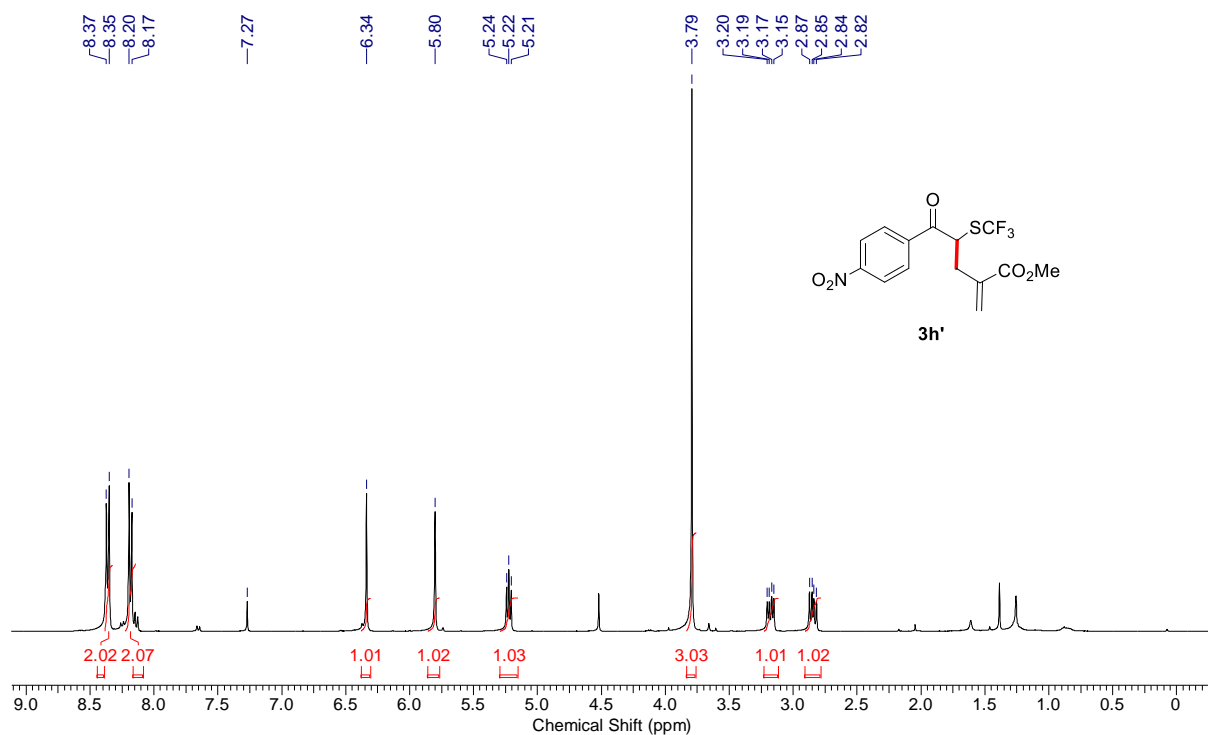


ESI-HRMS

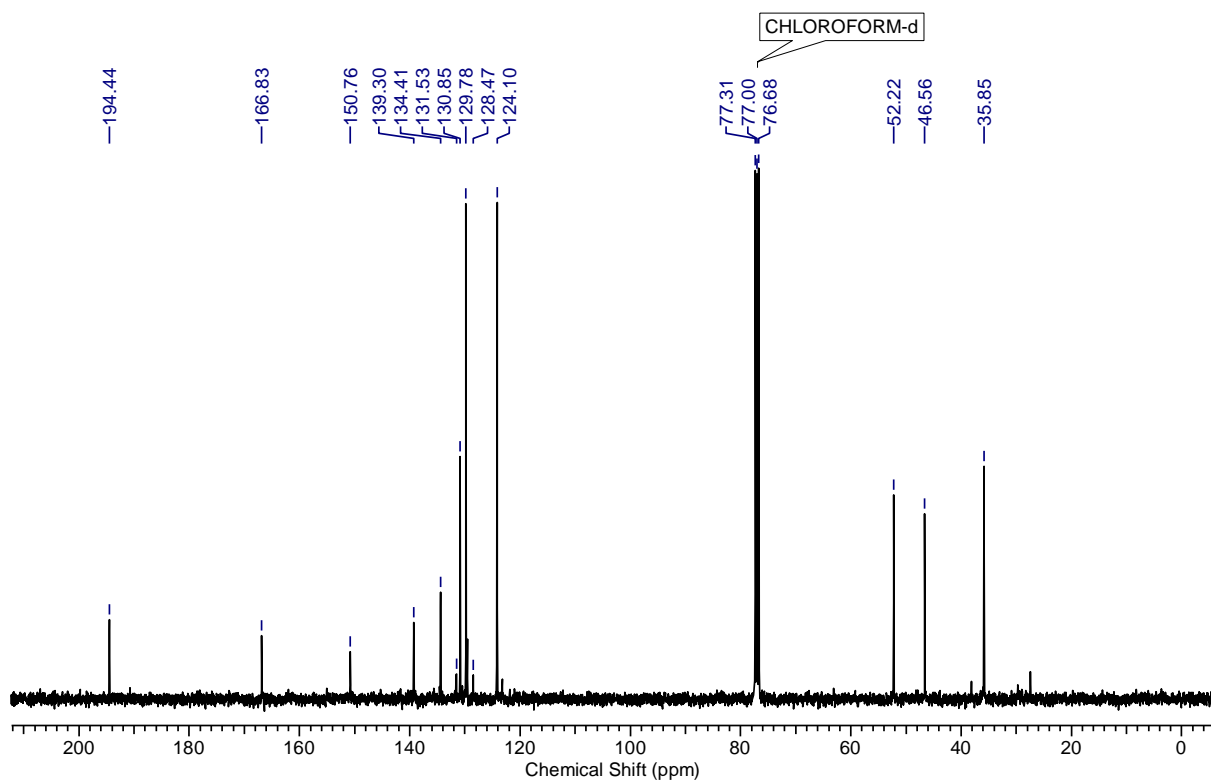
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¹H NMR, 400 MHz

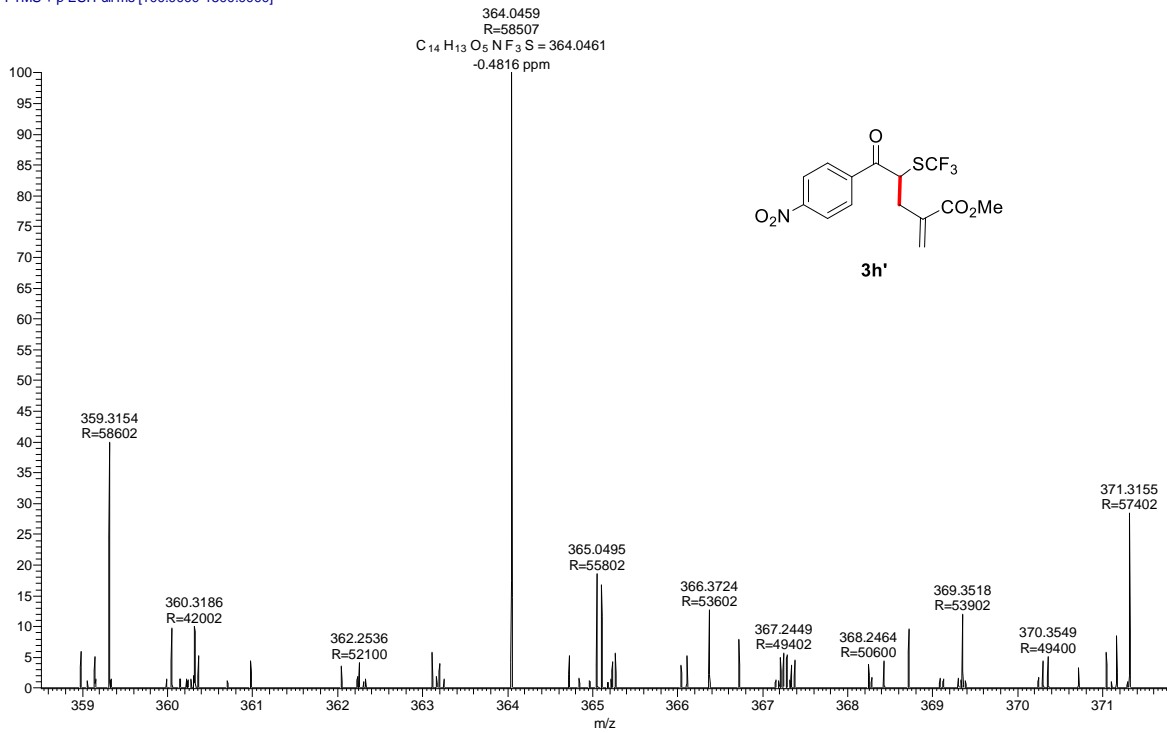


¹³C NMR, 100 MHz

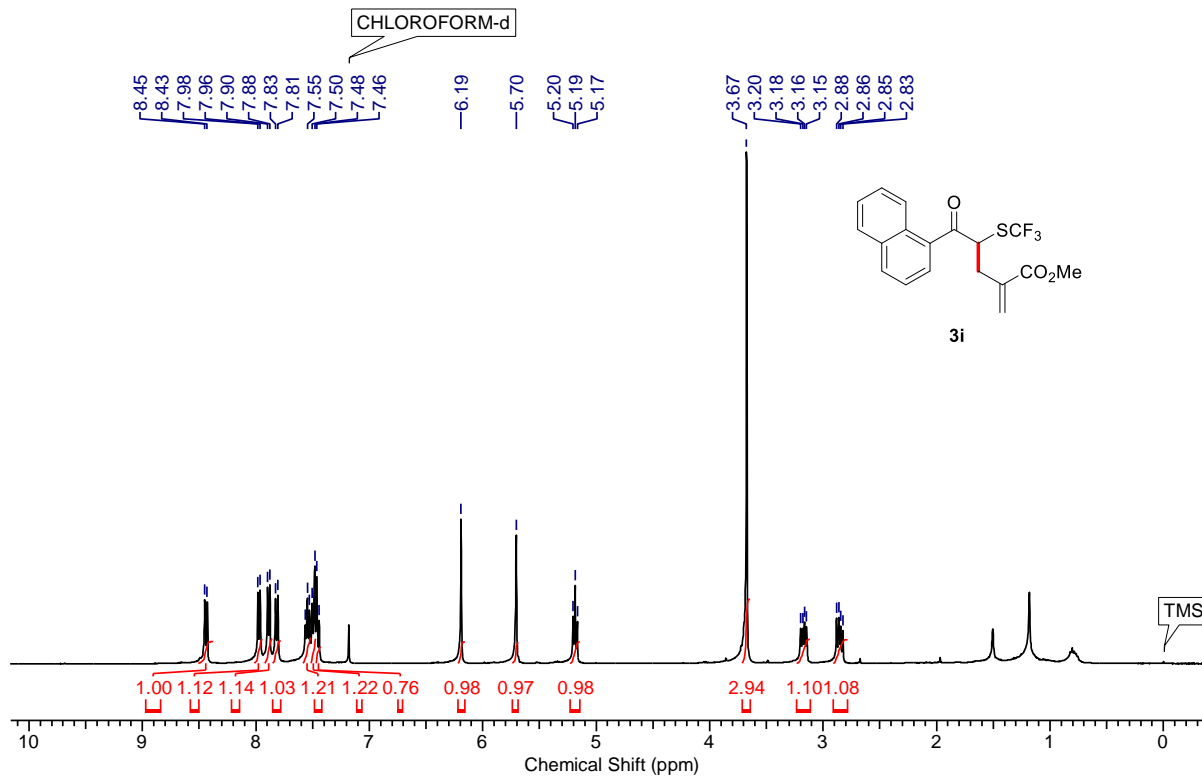


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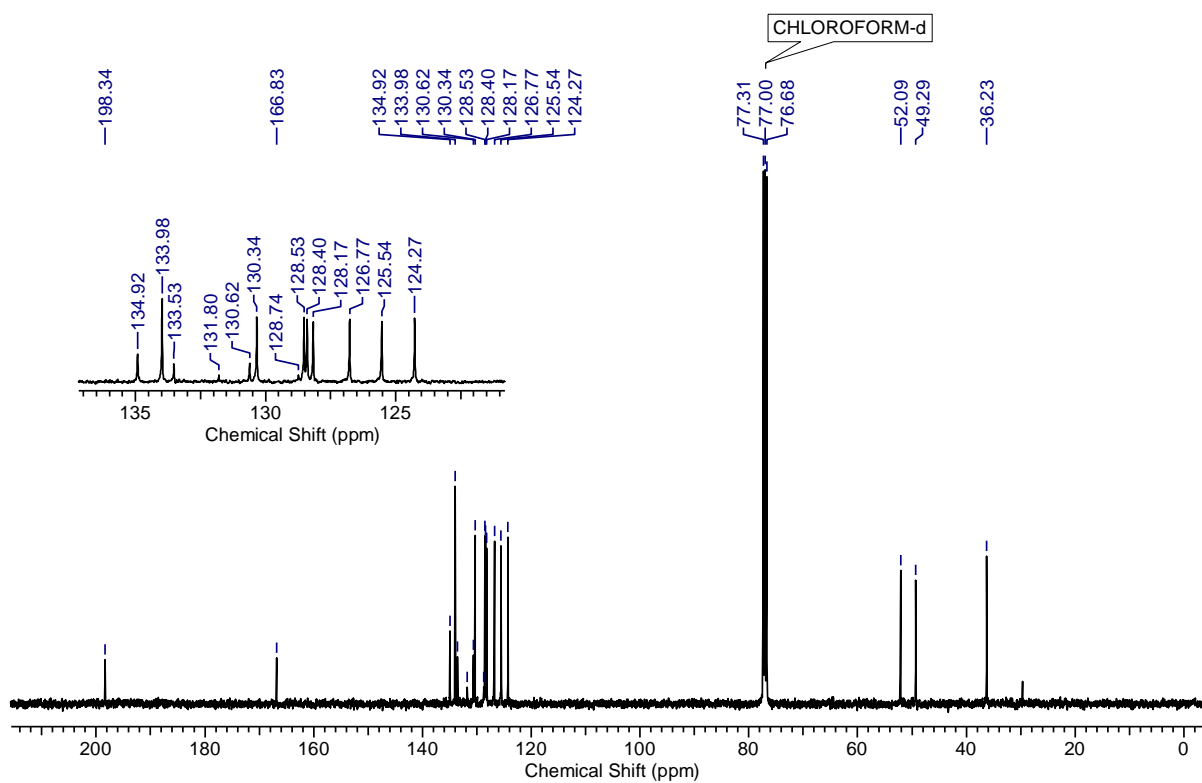
SeF3-1 #280 RT: 1.68 AV: 1 NL: 4.41E5
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¹H NMR, 400 MHz

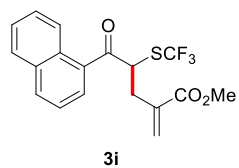
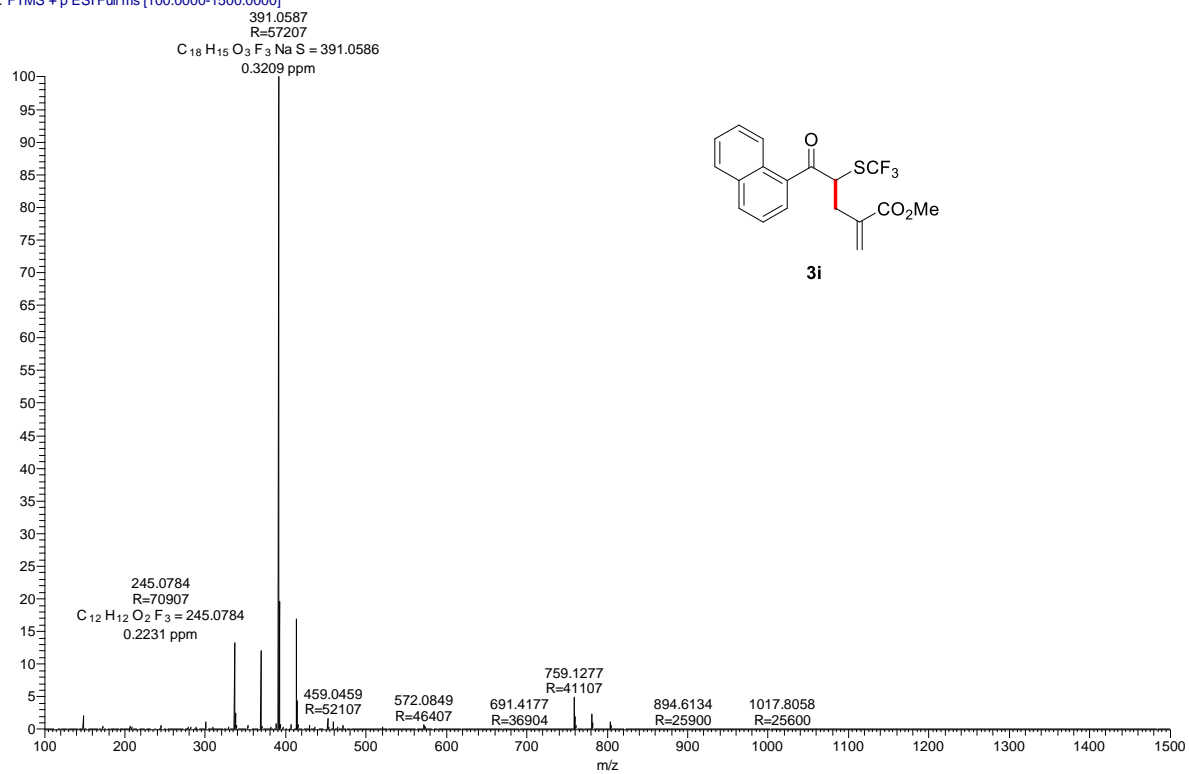


¹³C NMR, 100 MHz



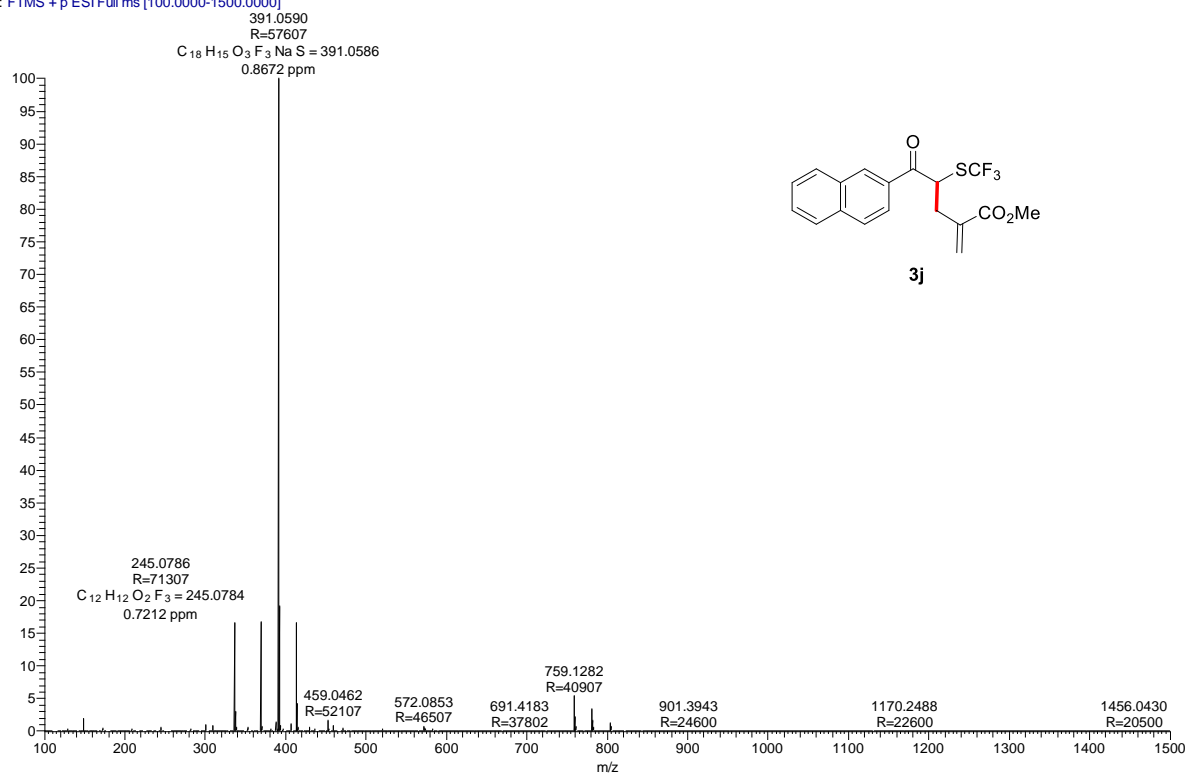
ESI-HRMS

BHA-10 #300 RT: 1.33 AV: 1 NL: 1.35E9
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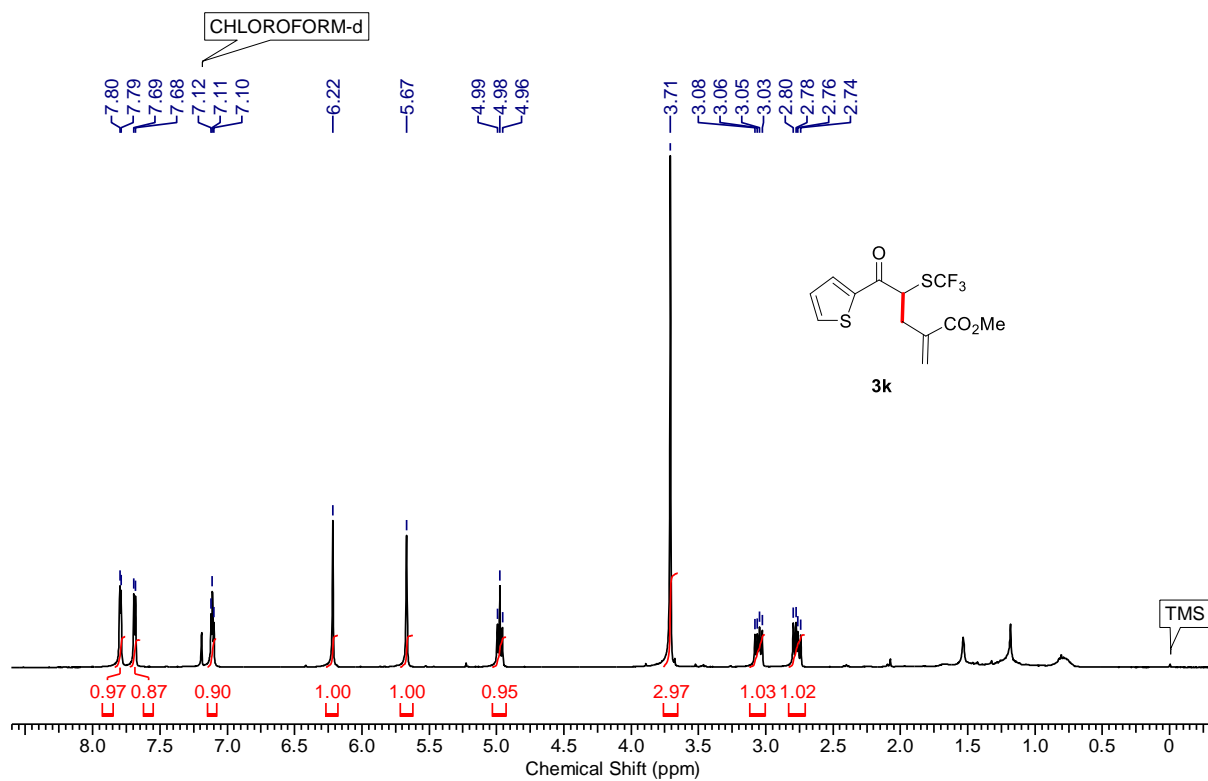


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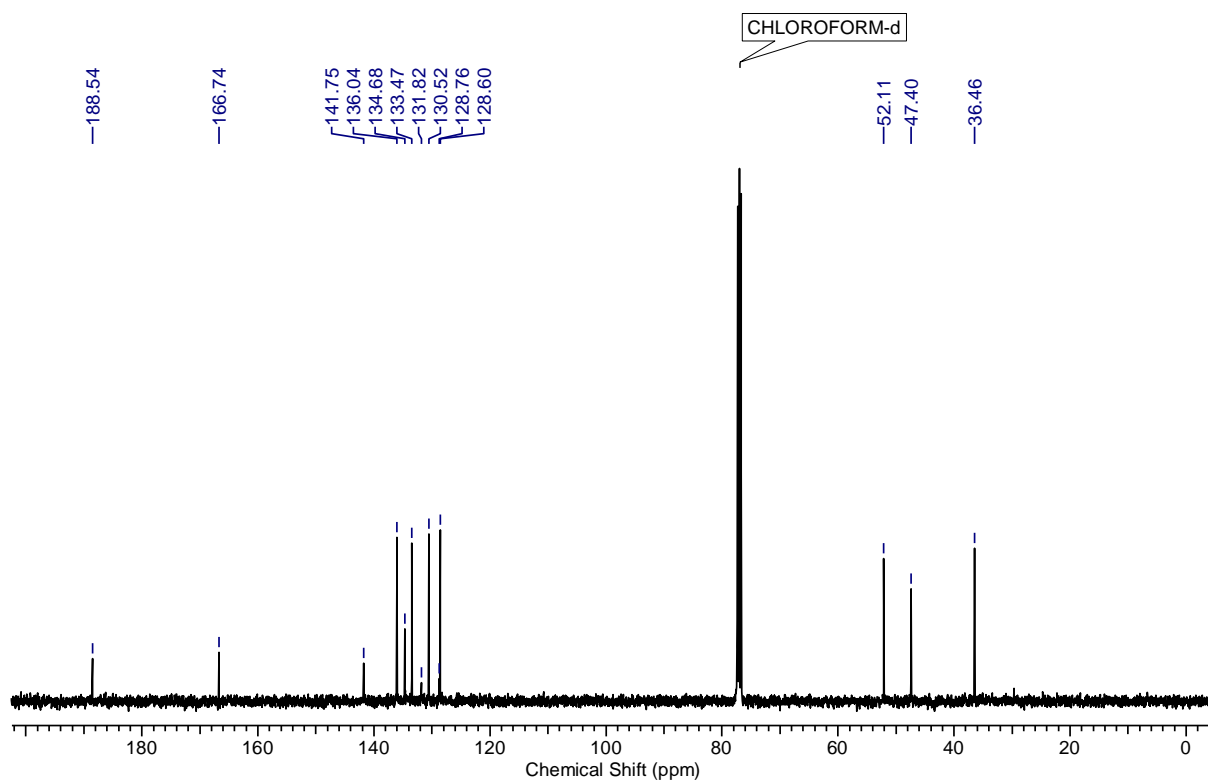
BHA-9 #304 RT: 1.35 AV: 1 NL: 1.34E9
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¹H NMR, 400 MHz

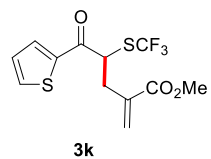
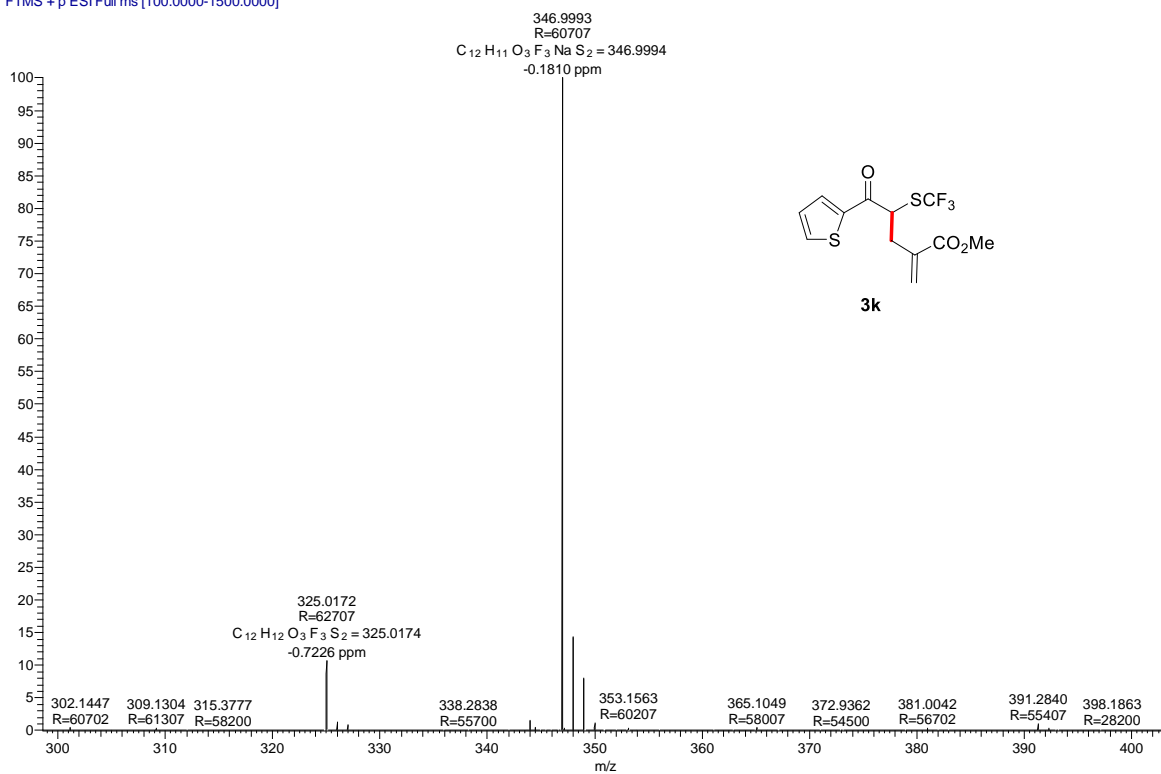


¹³C NMR, 100 MHz

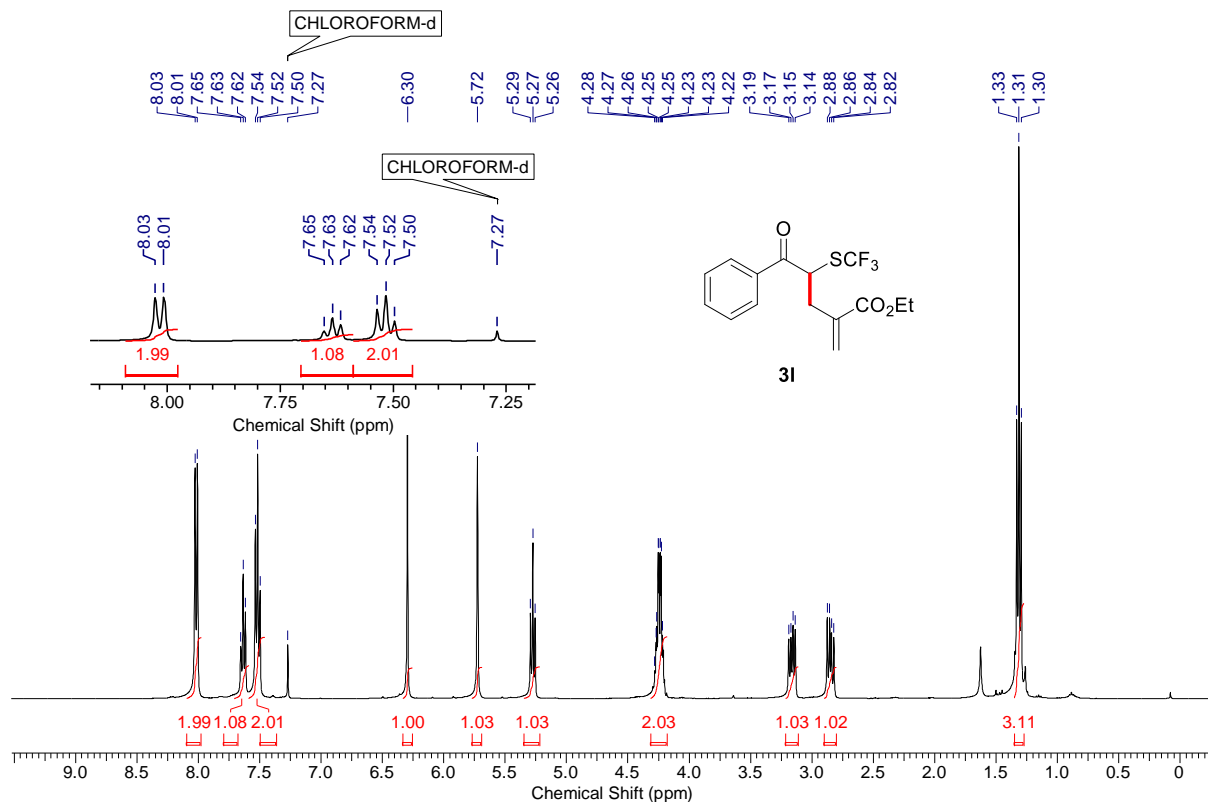


ESI-HRMS

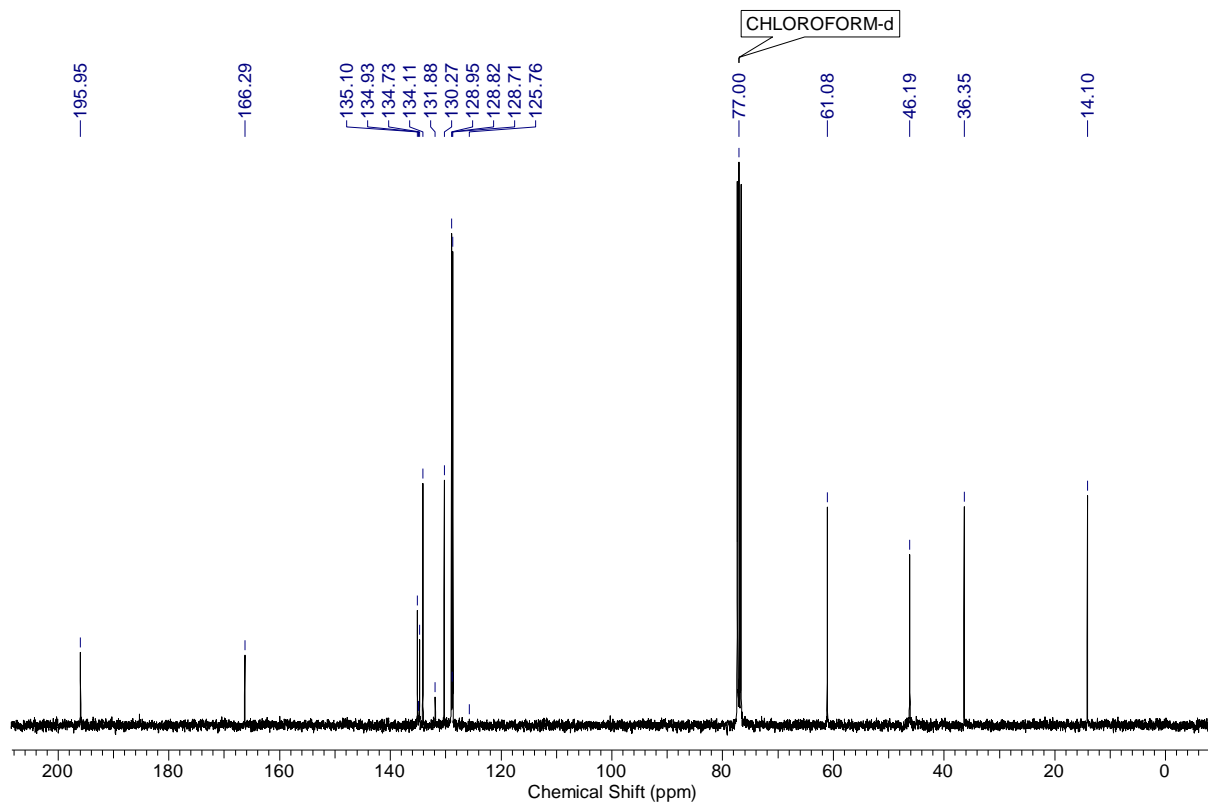
BHA-5 #280 RT: 1.25 AV: 1 NL: 1.84E9
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¹H NMR, 400 MHz

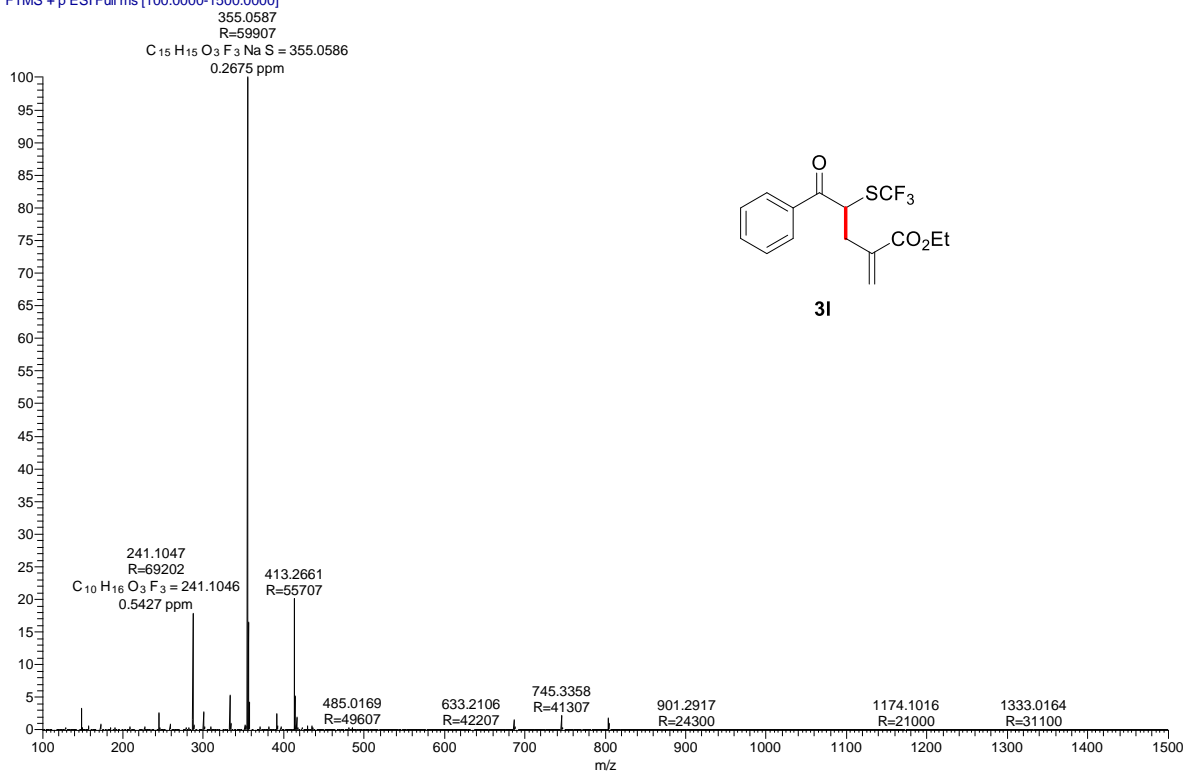


¹³C NMR, 100 MHz

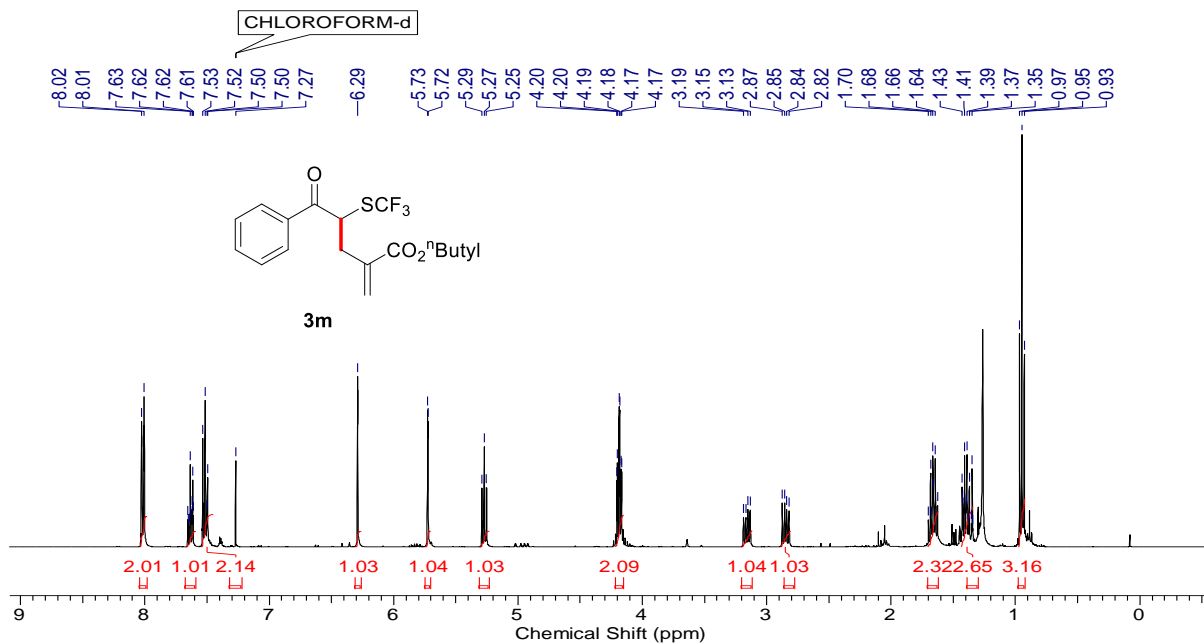


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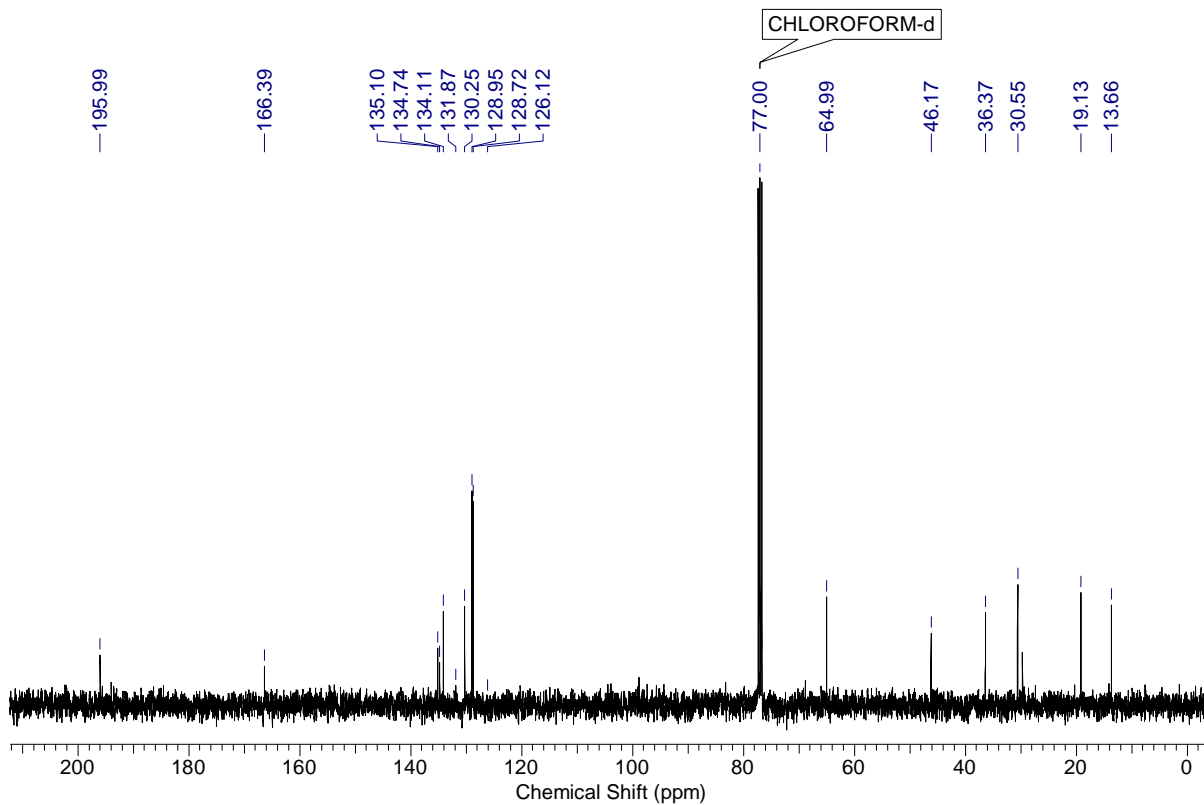
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¹H NMR, 400 MHz

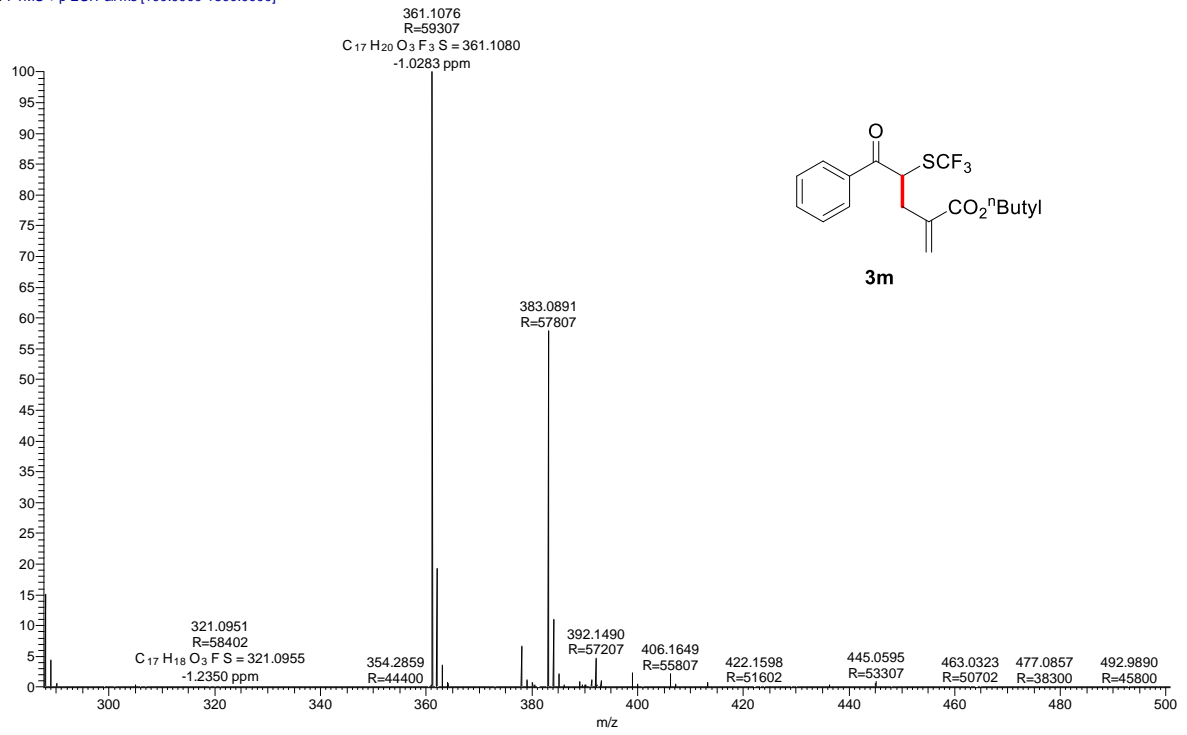


¹³C NMR, 100 MHz

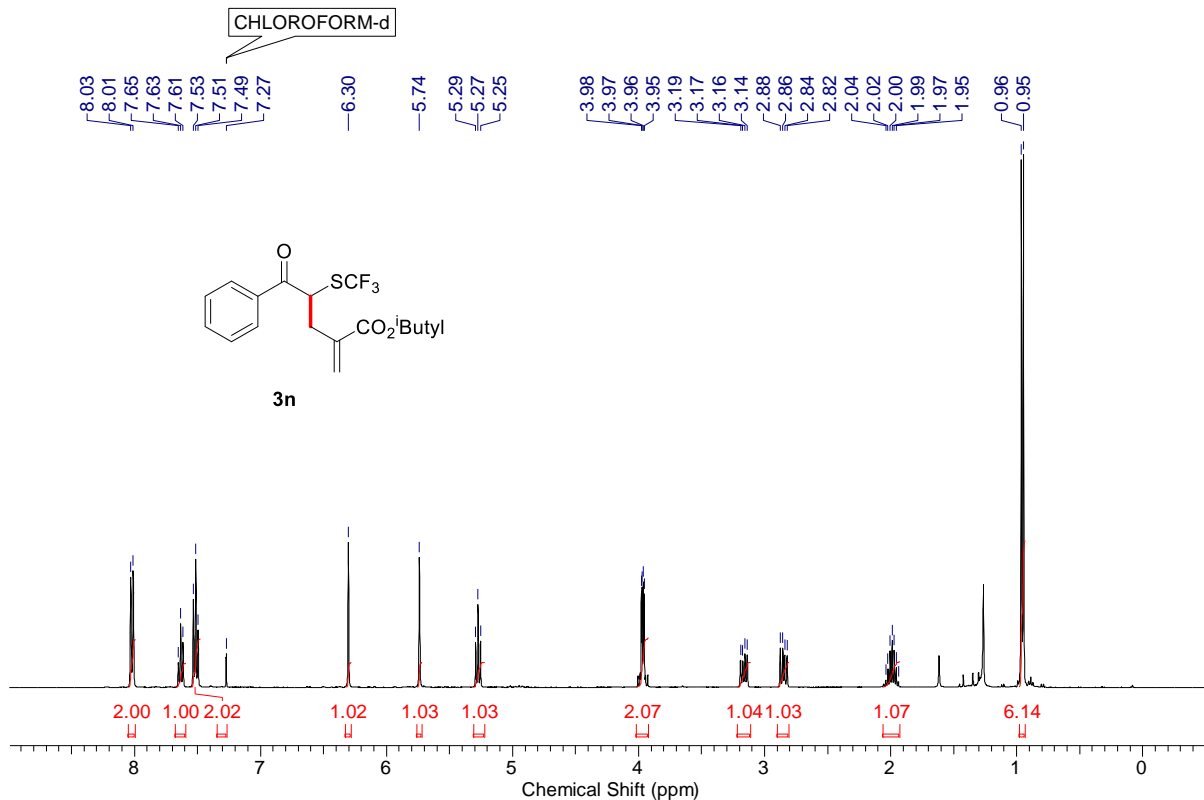


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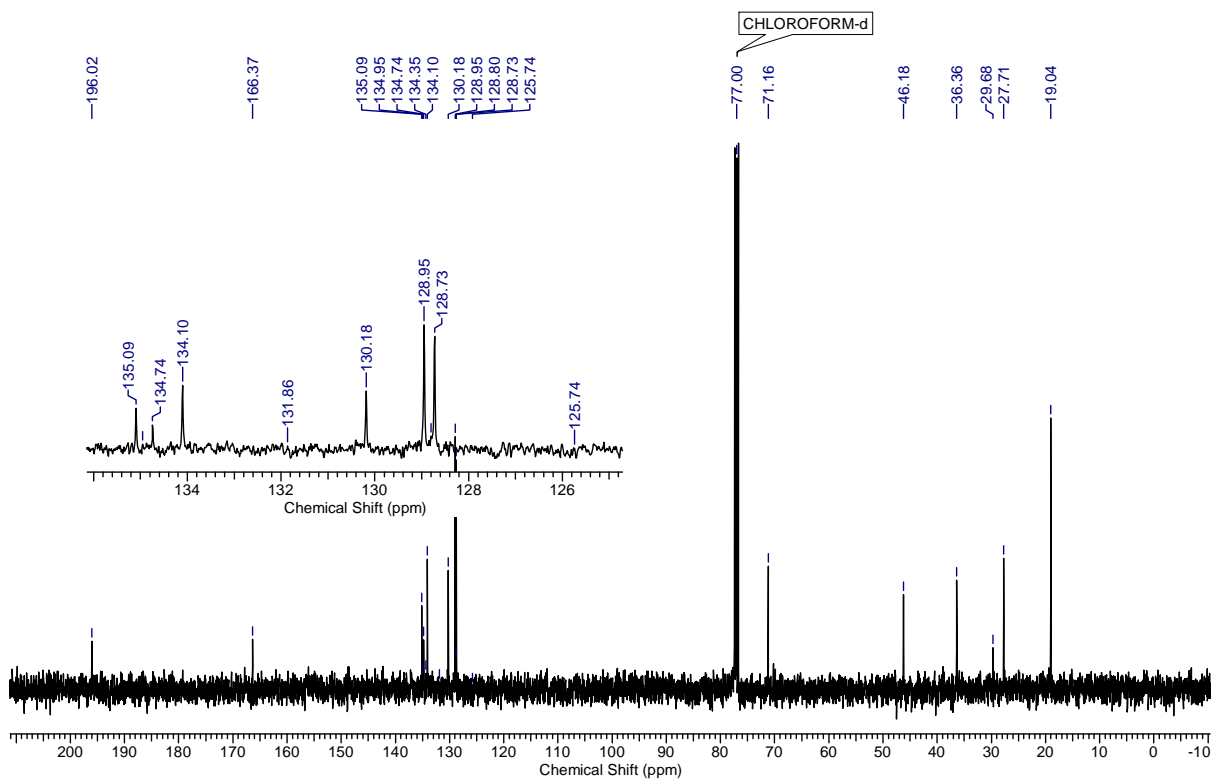
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¹H NMR, 400 MHz

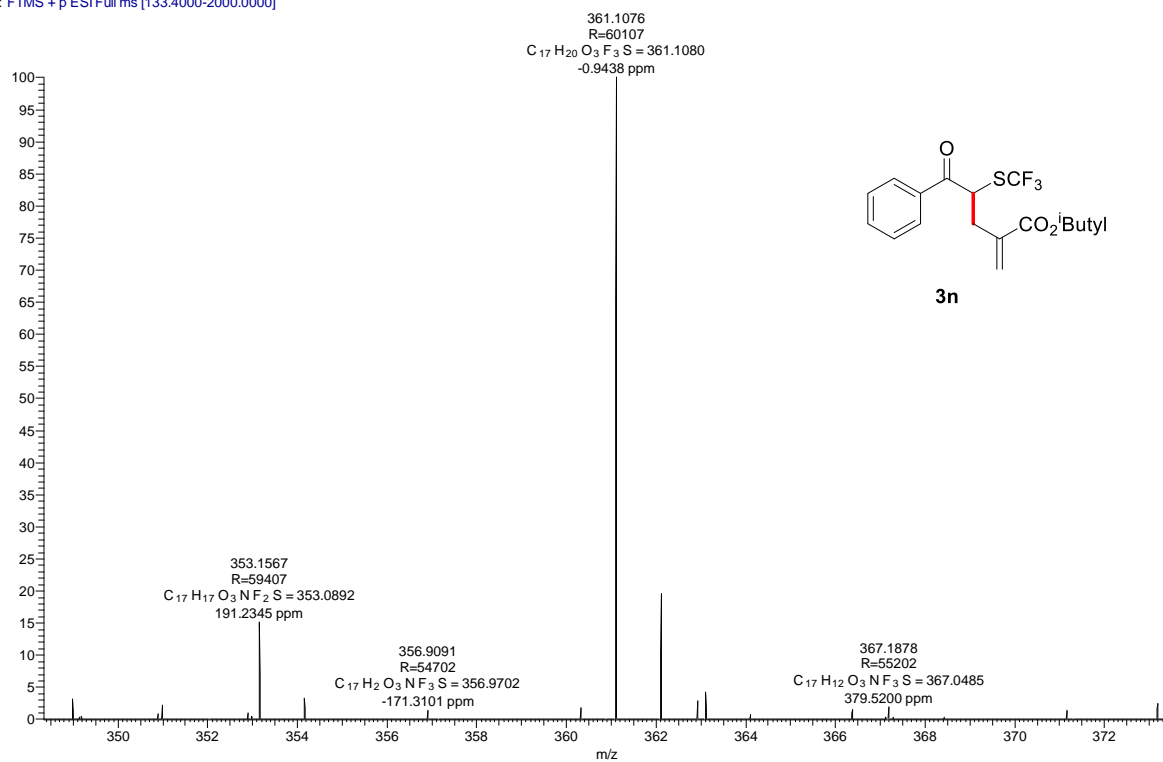


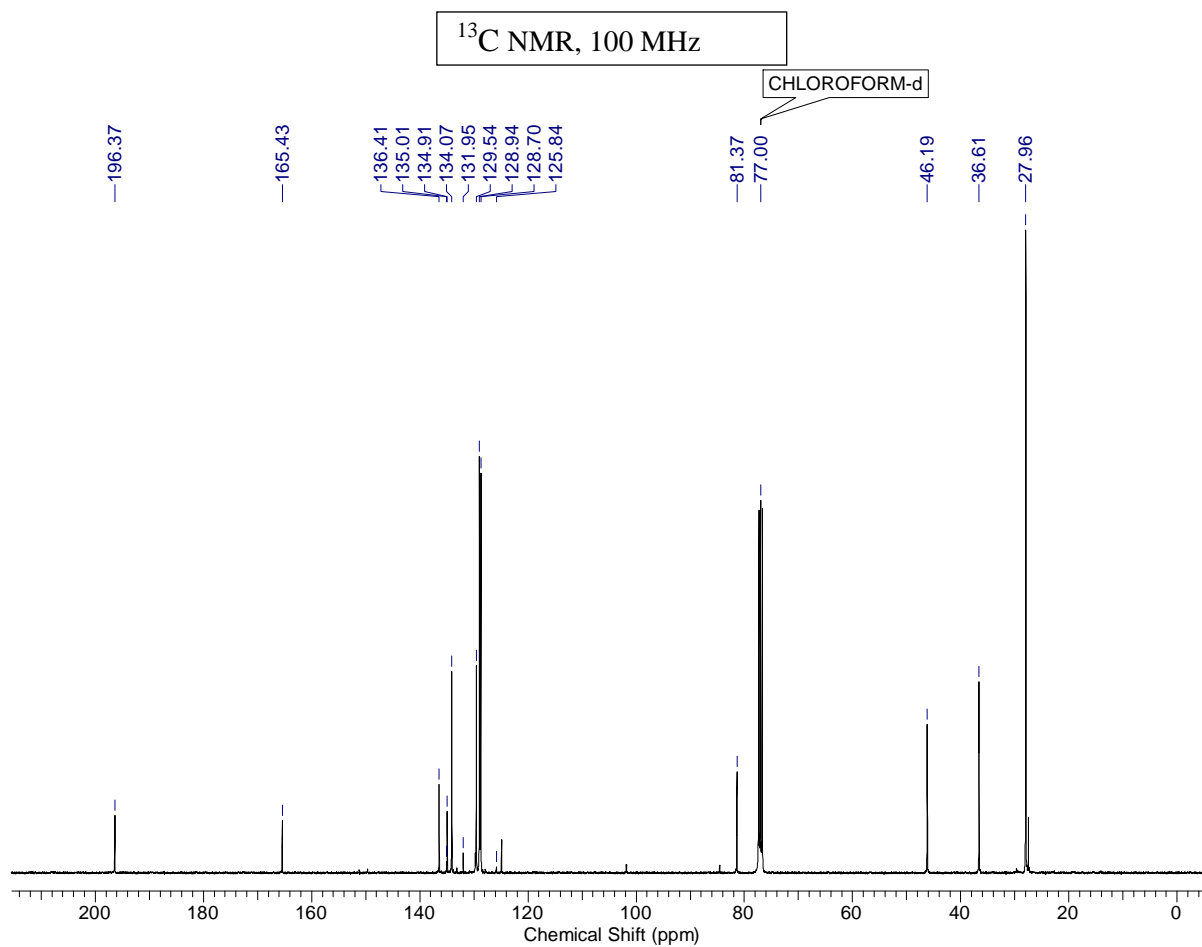
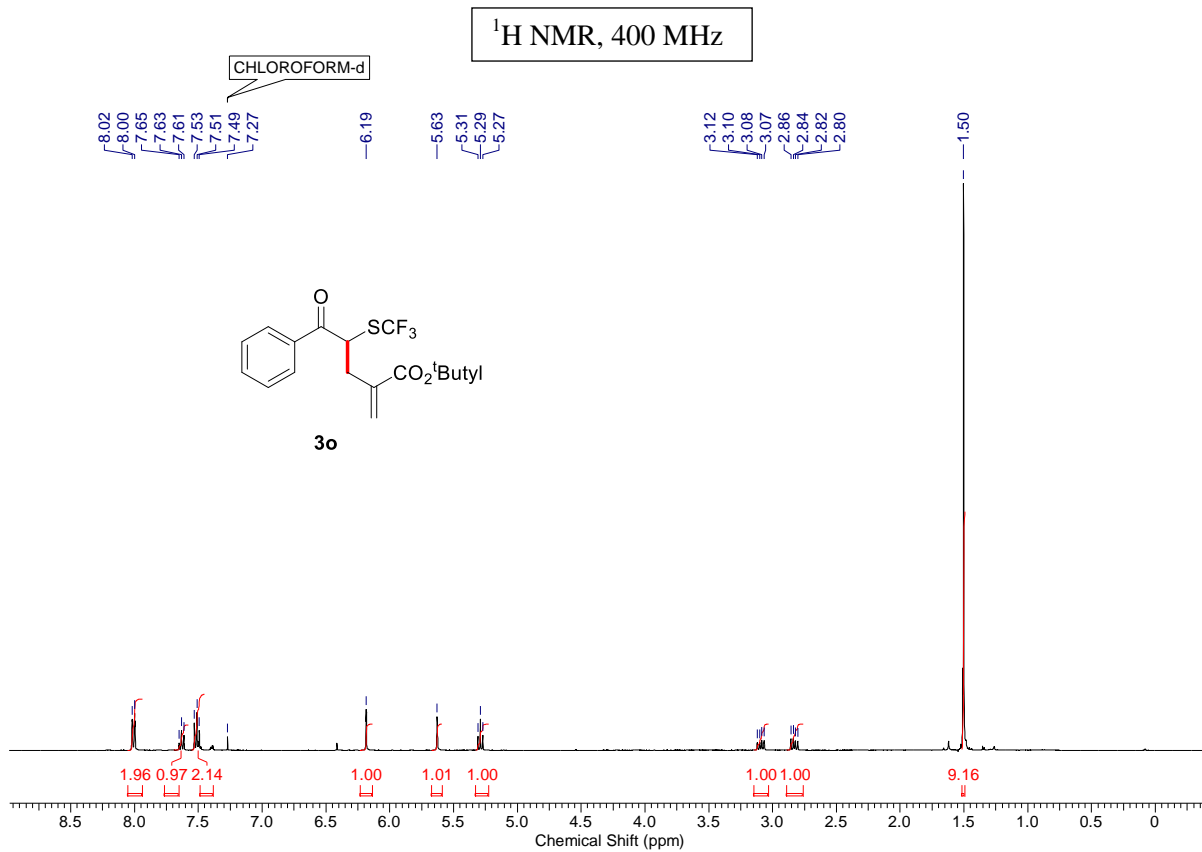
¹³C NMR, 100 MHz



ESI-HRMS

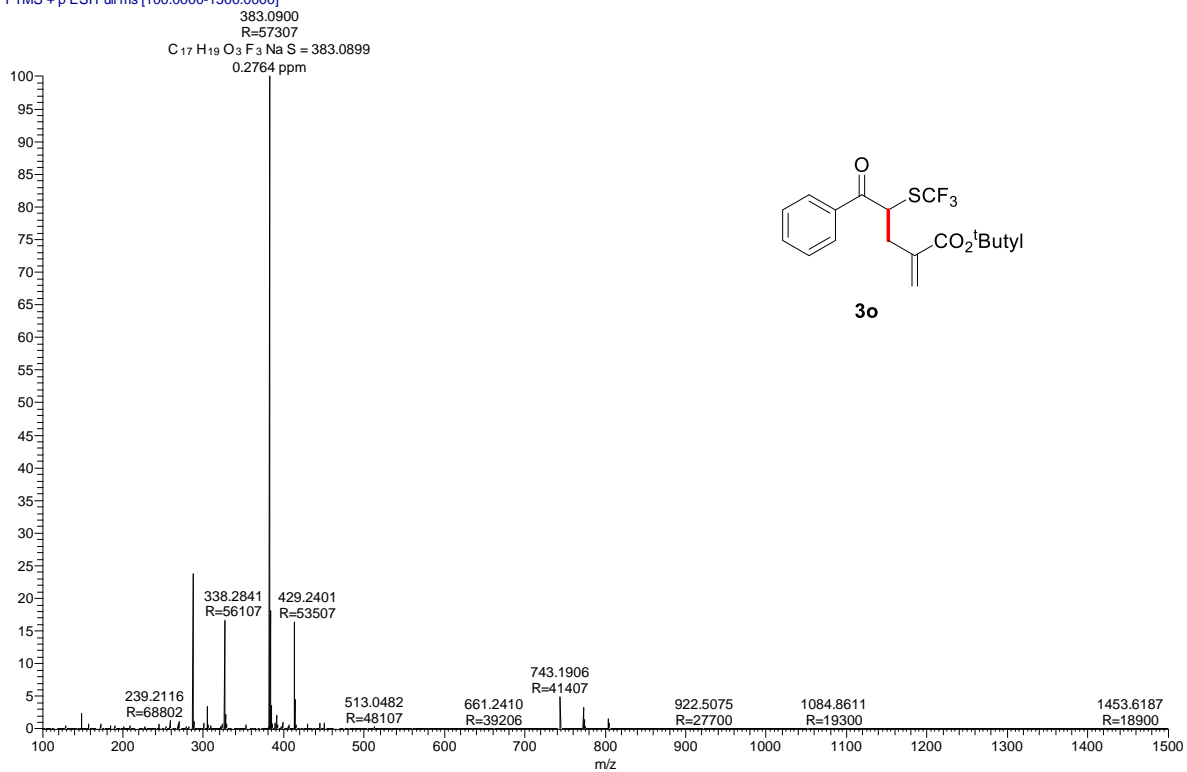
SEF3-16 #300 RT: 1.33 AV: 1 NL: 5.59E7
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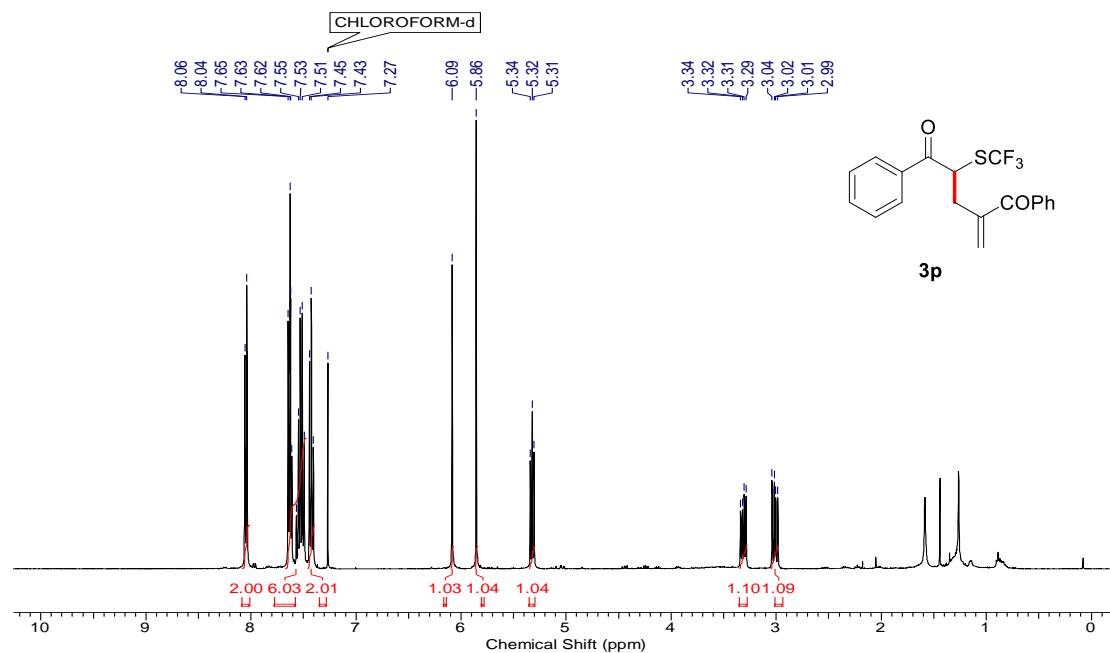


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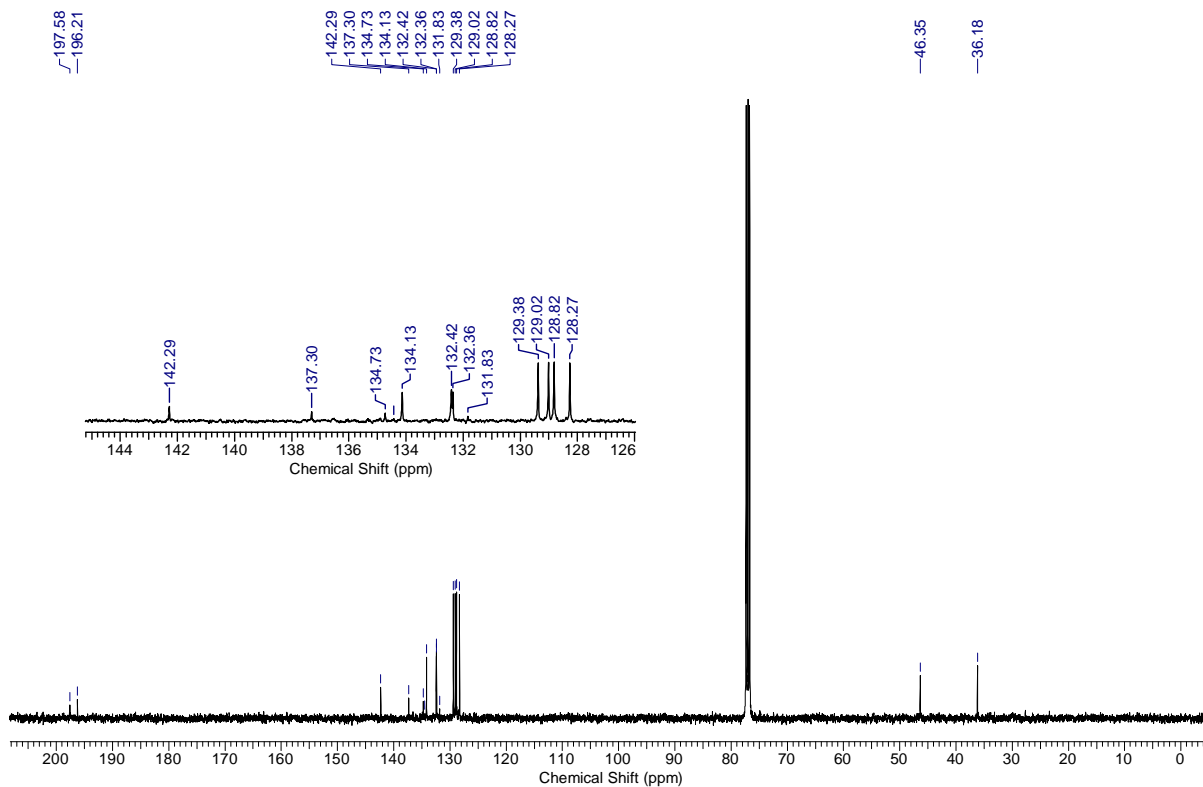
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¹H NMR, 400 MHz

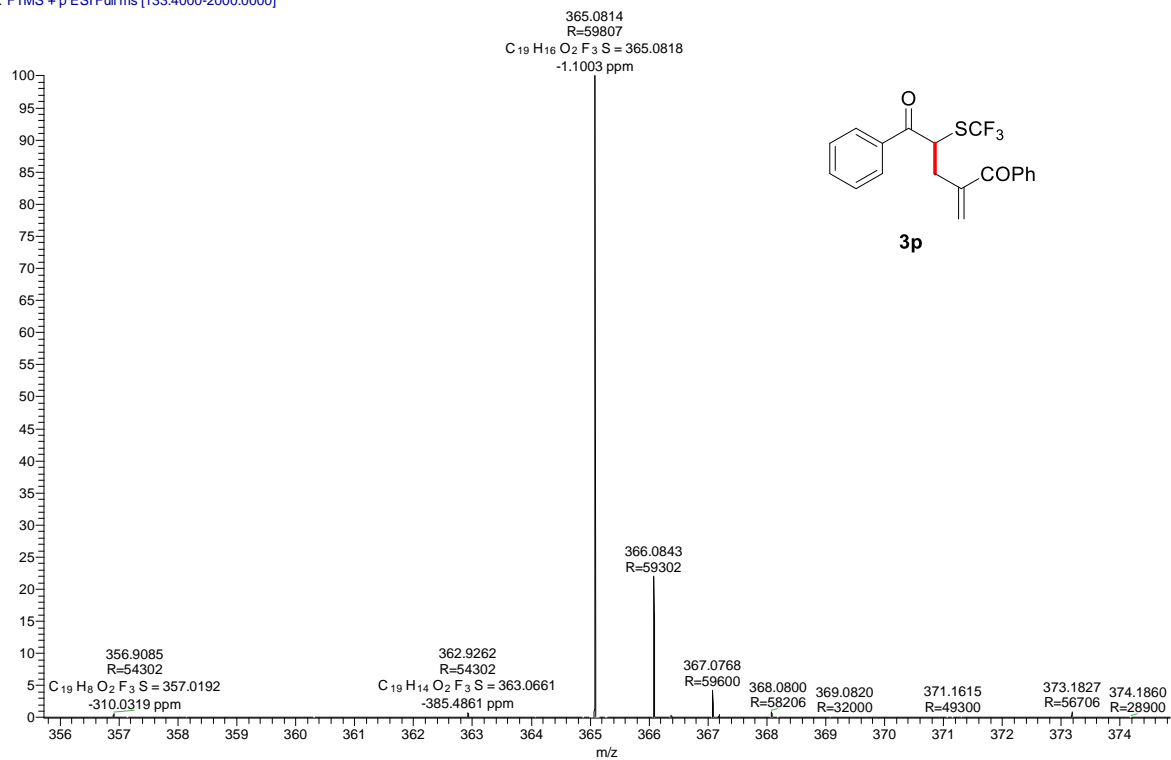


¹³C NMR, 100 MHz

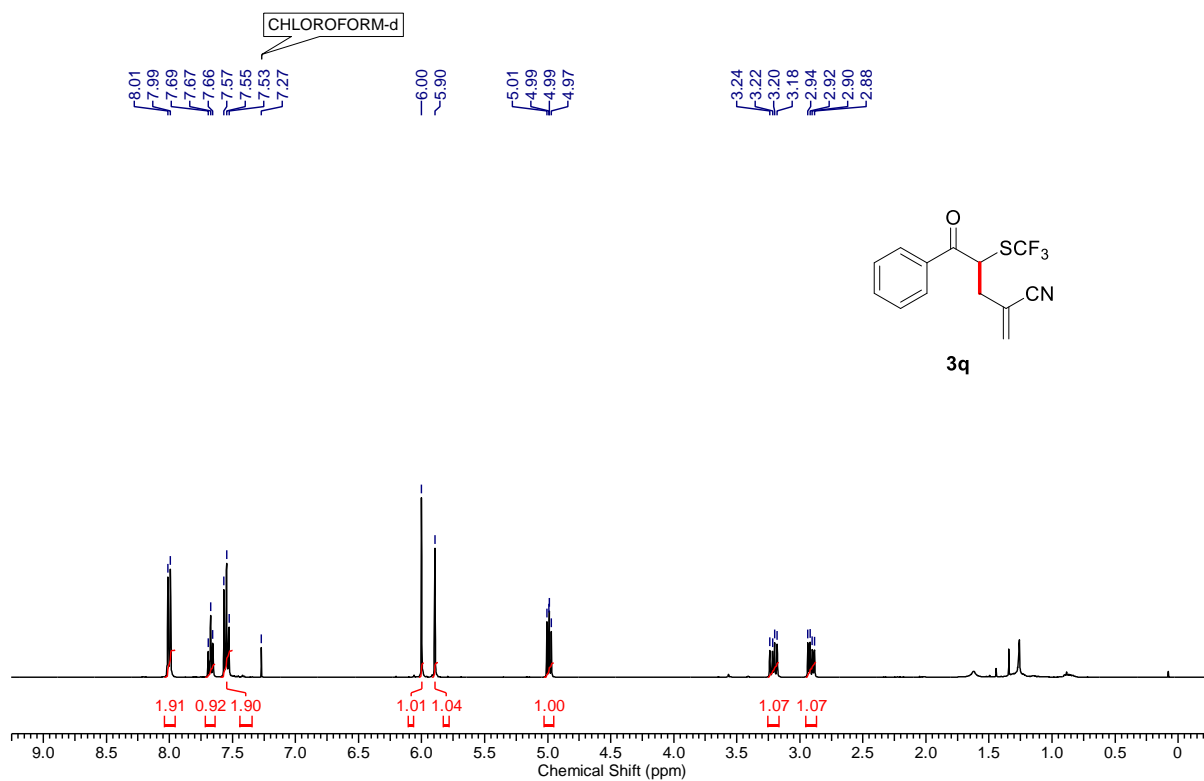


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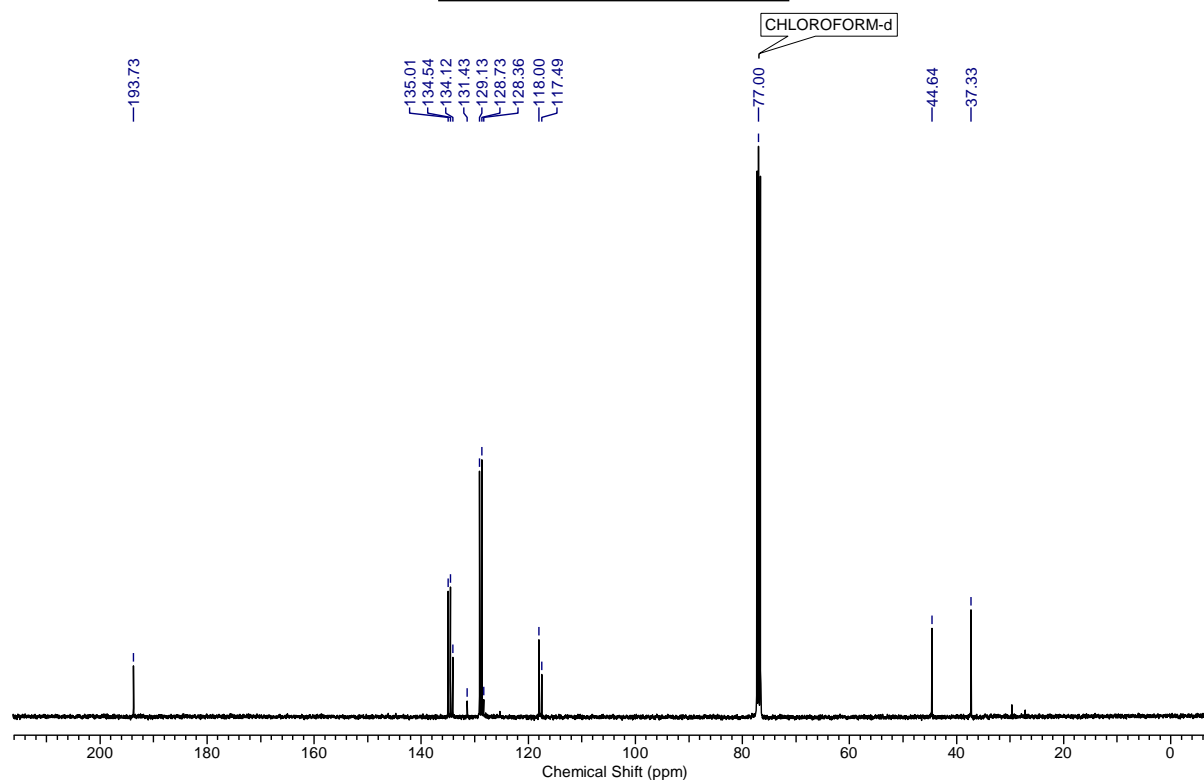
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¹H NMR, 400 MHz

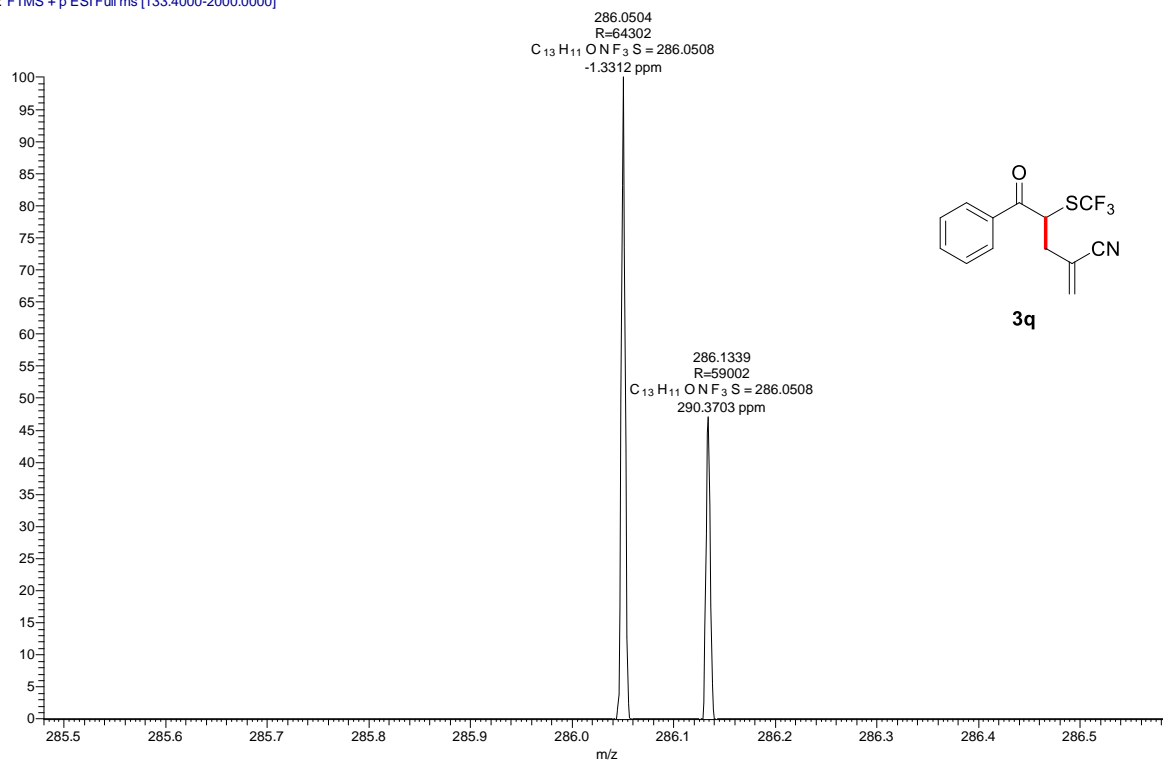


¹³C NMR, 100 MHz

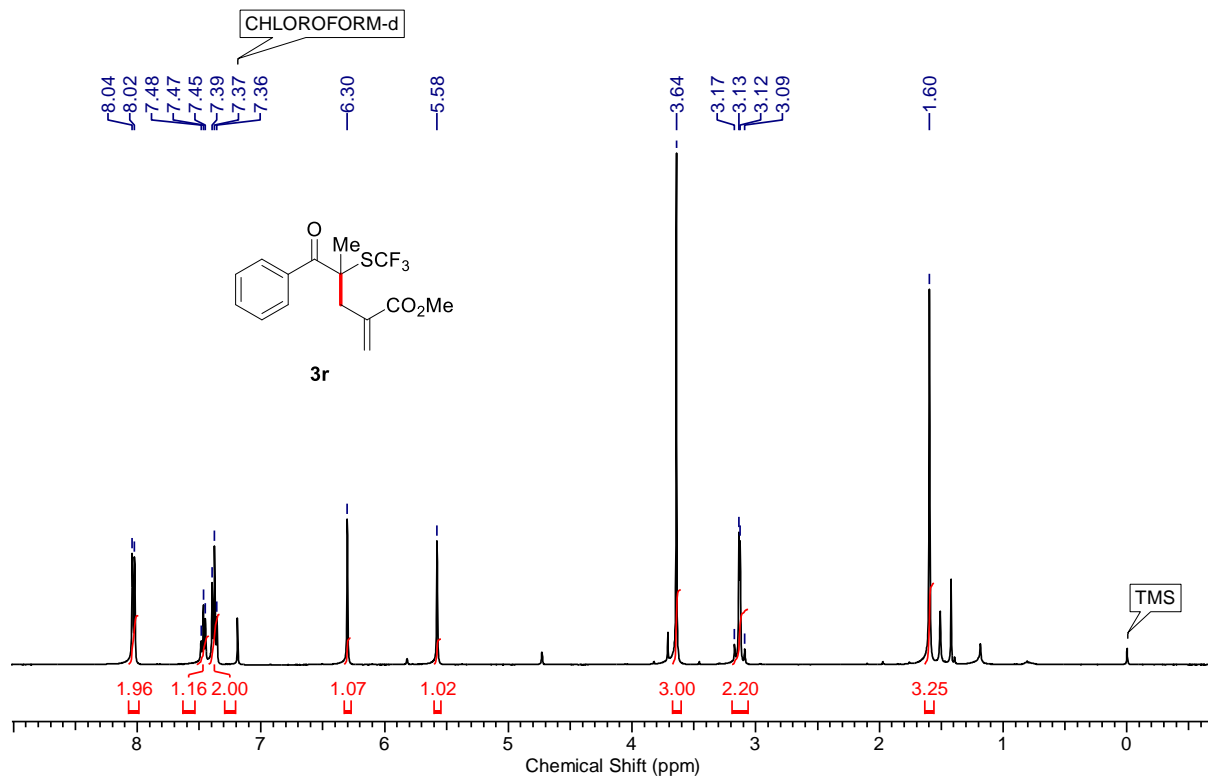


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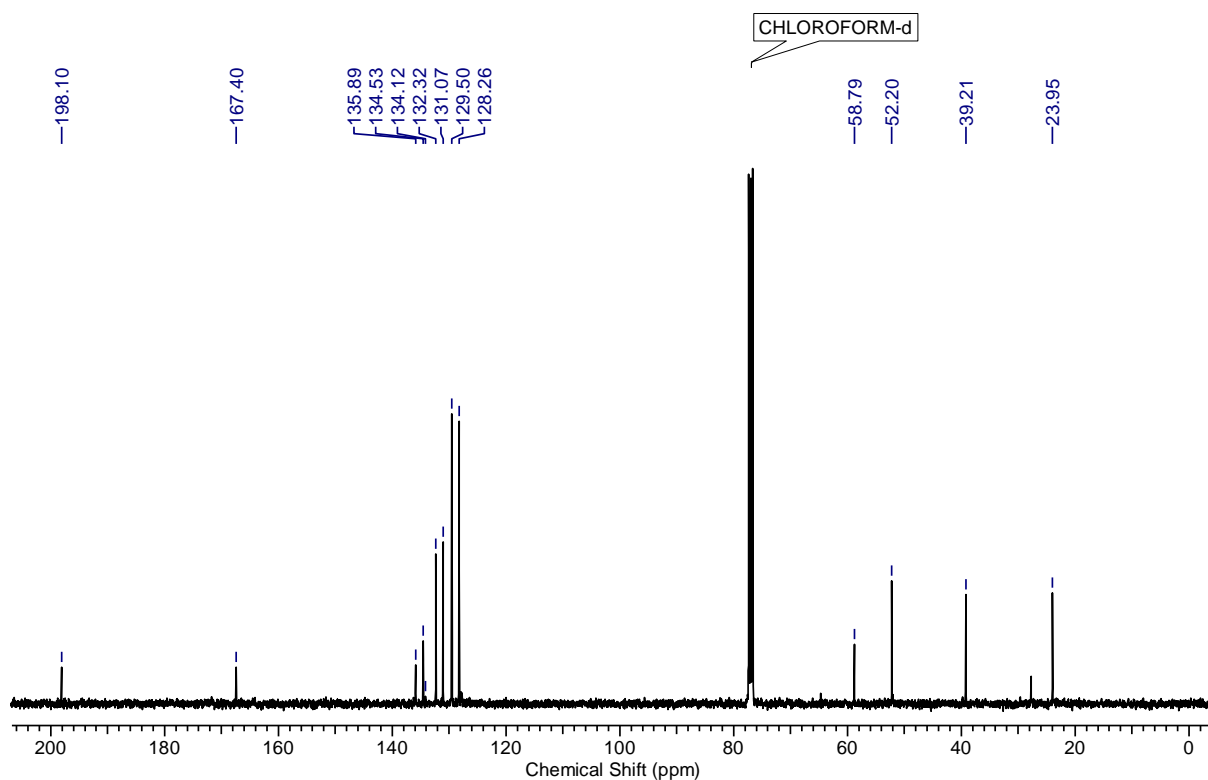
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¹H NMR, 400 MHz

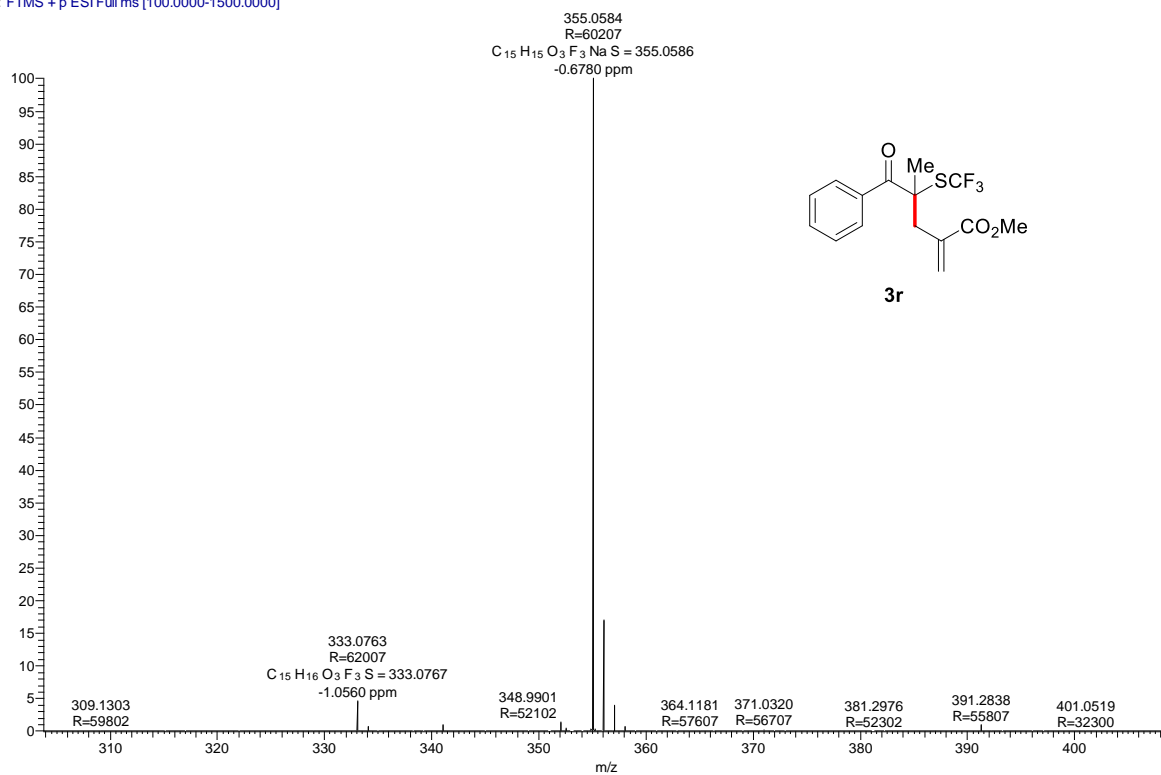


¹³C NMR, 100 MHz

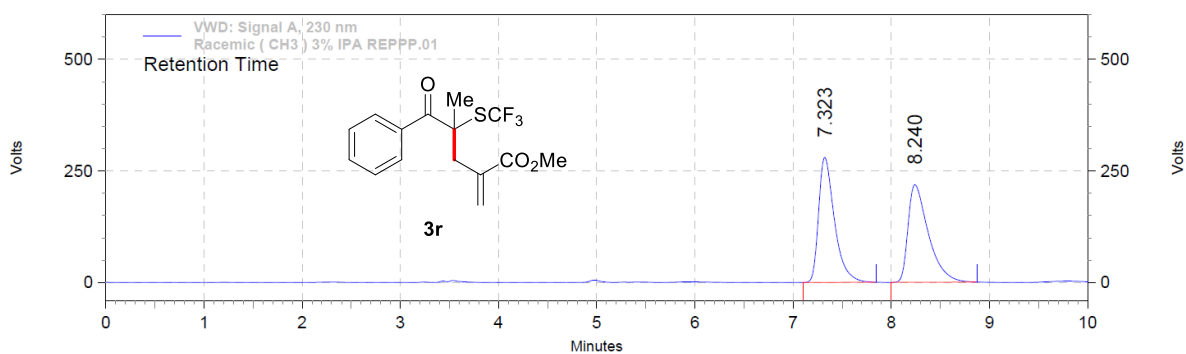


ESI-HRMS

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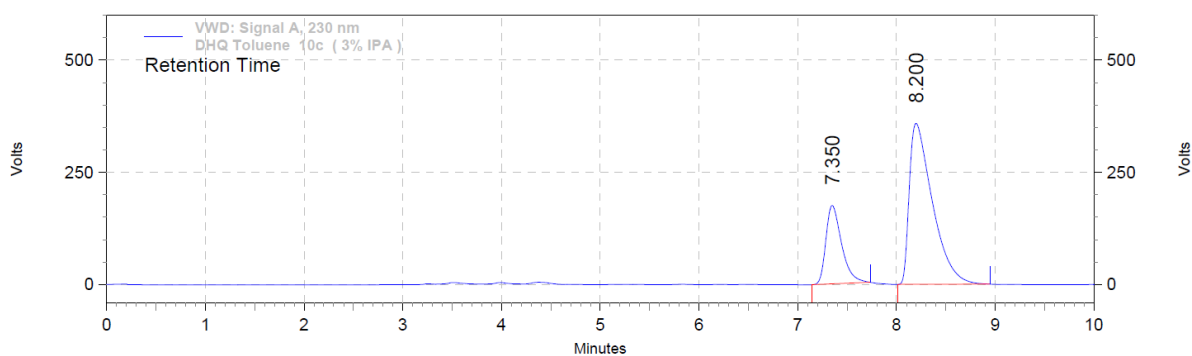
HPLC



VWD: Signal A, 230 nm Results

Retention Time	Area	Area %	Height	Height %
7.323	52743143	49.99	4696233	56.15
8.240	52770429	50.01	3667304	43.85

Totals	105513572	100.00	8363537	100.00
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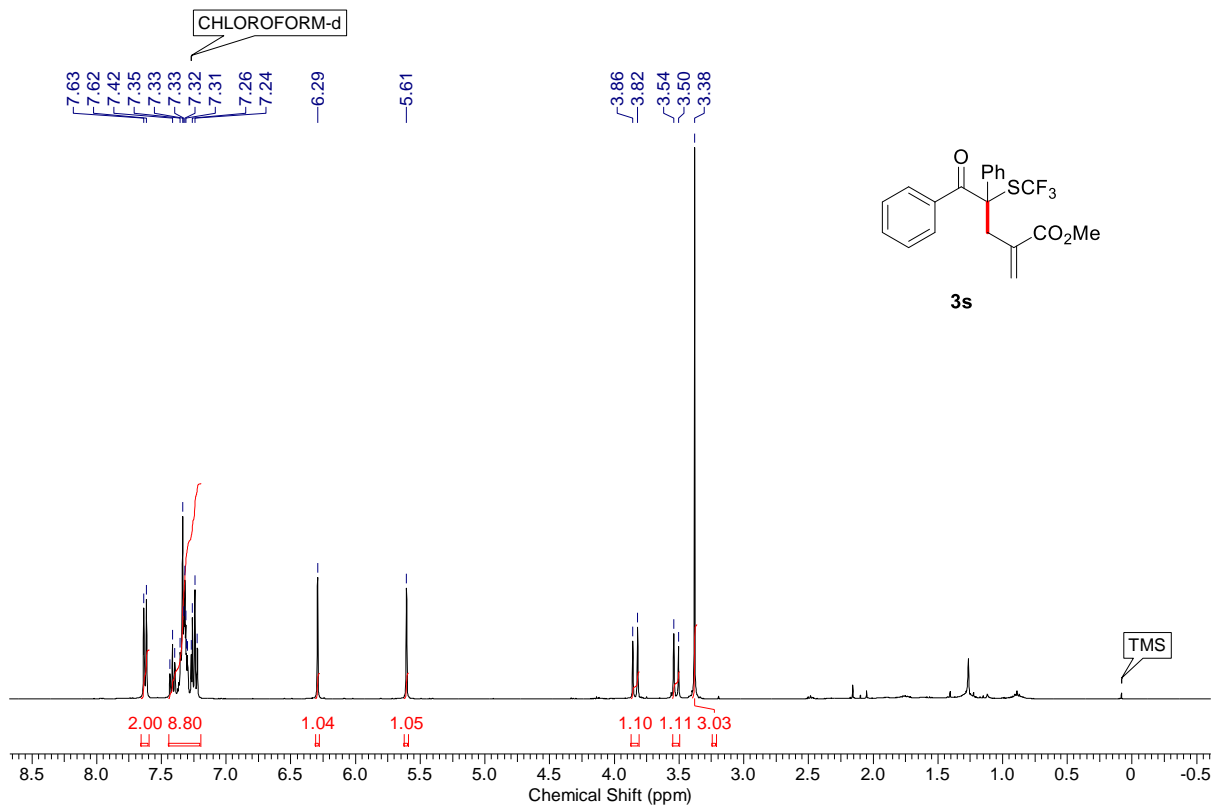


VWD: Signal A, 230 nm Results

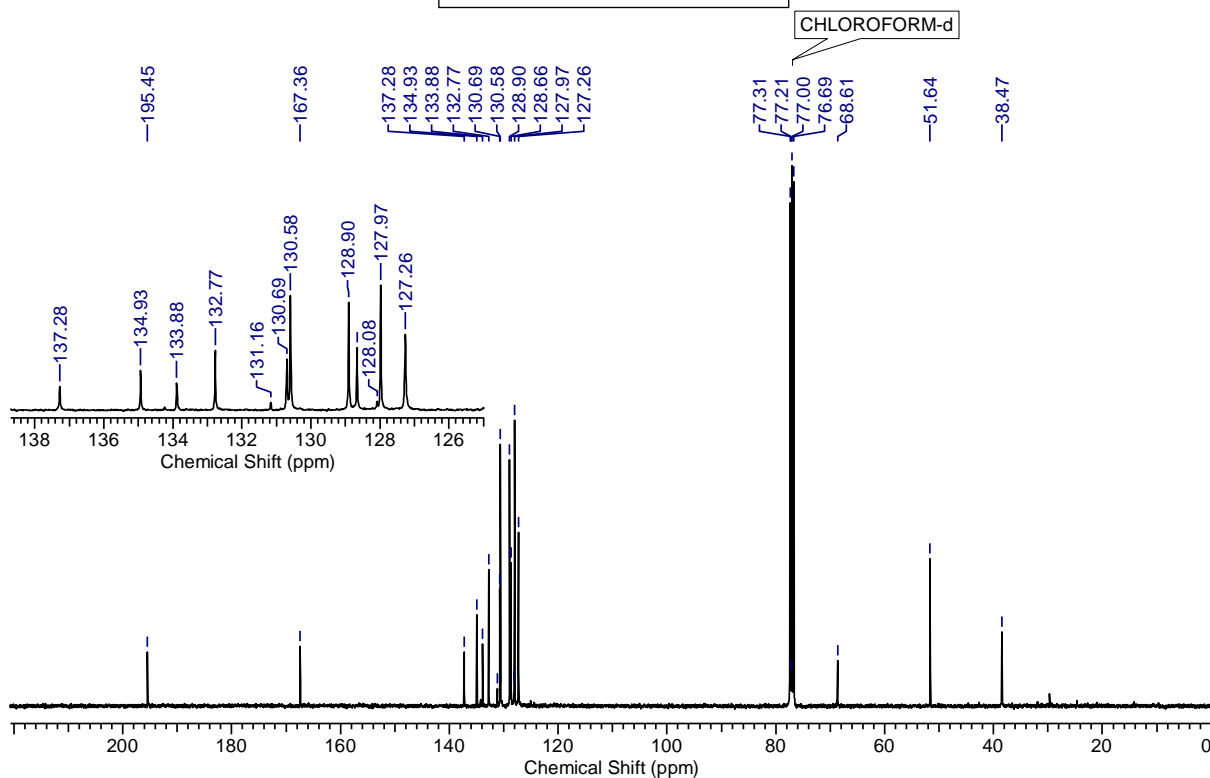
Retention Time	Area	Area %	Height	Height %
7.350	32428607	24.93	2931492	32.76
8.200	97657369	75.07	6017369	67.24

Totals	130085976	100.00	8948861	100.00
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¹H NMR, 400 MHz

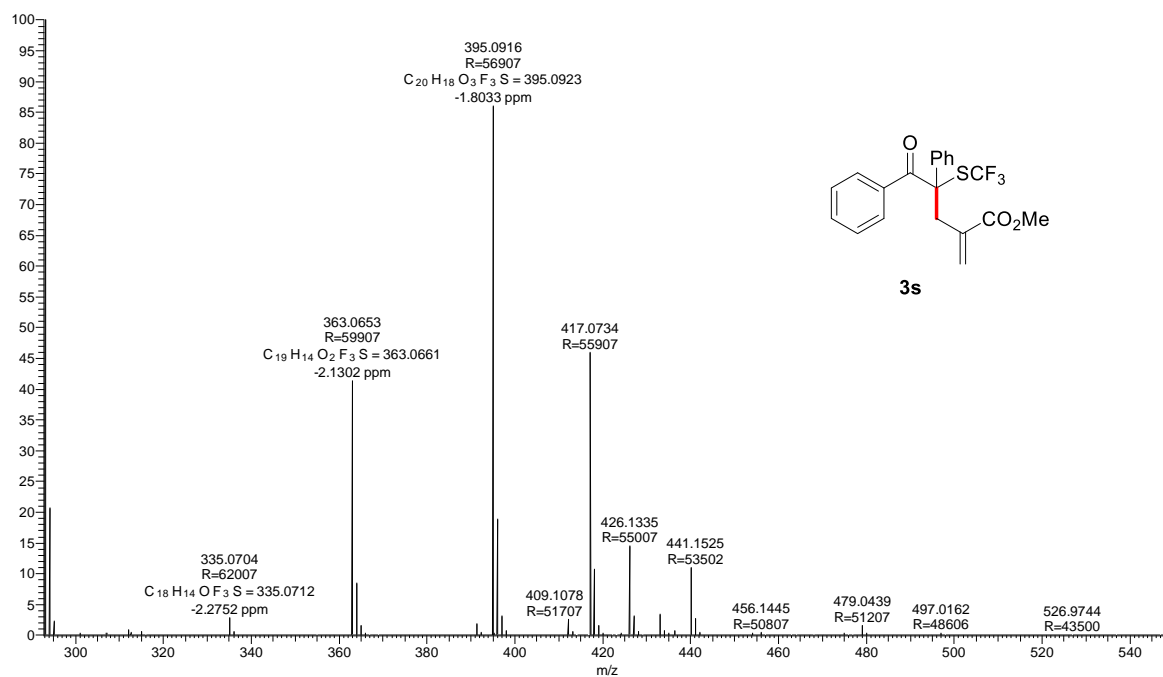


¹³C NMR, 100 MHz

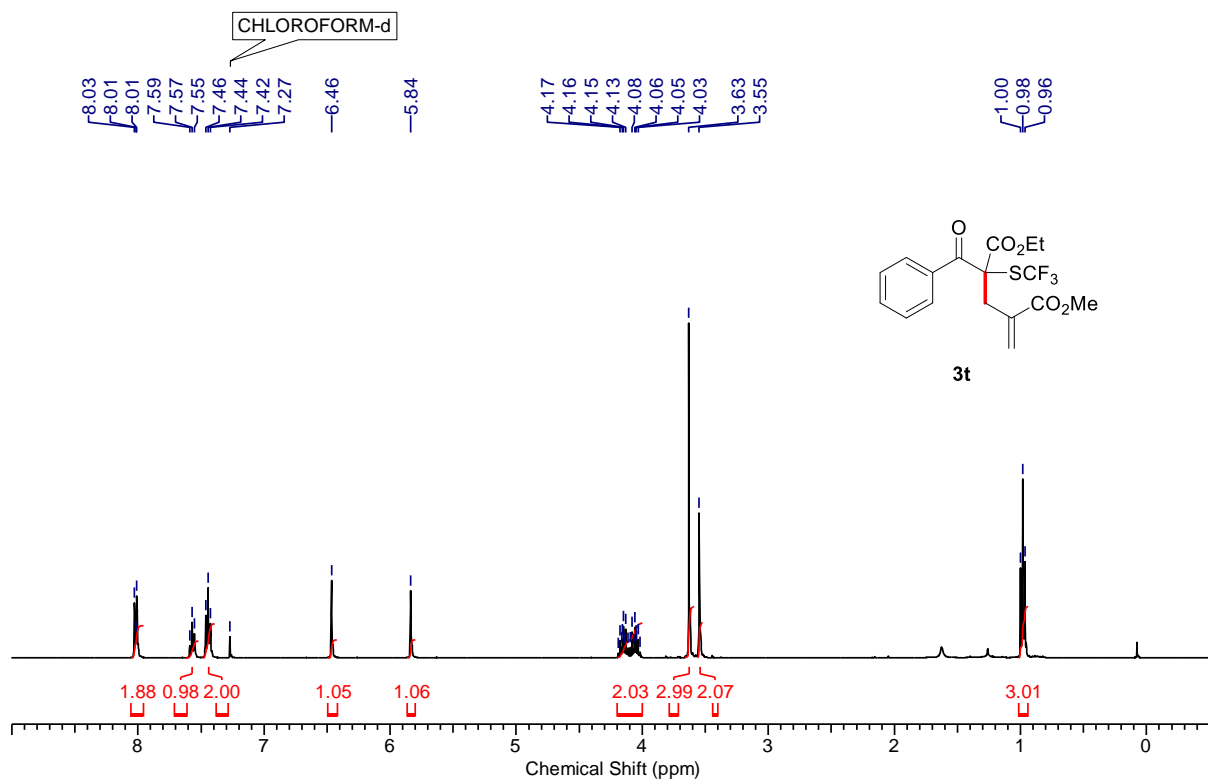


ESI-HRMS

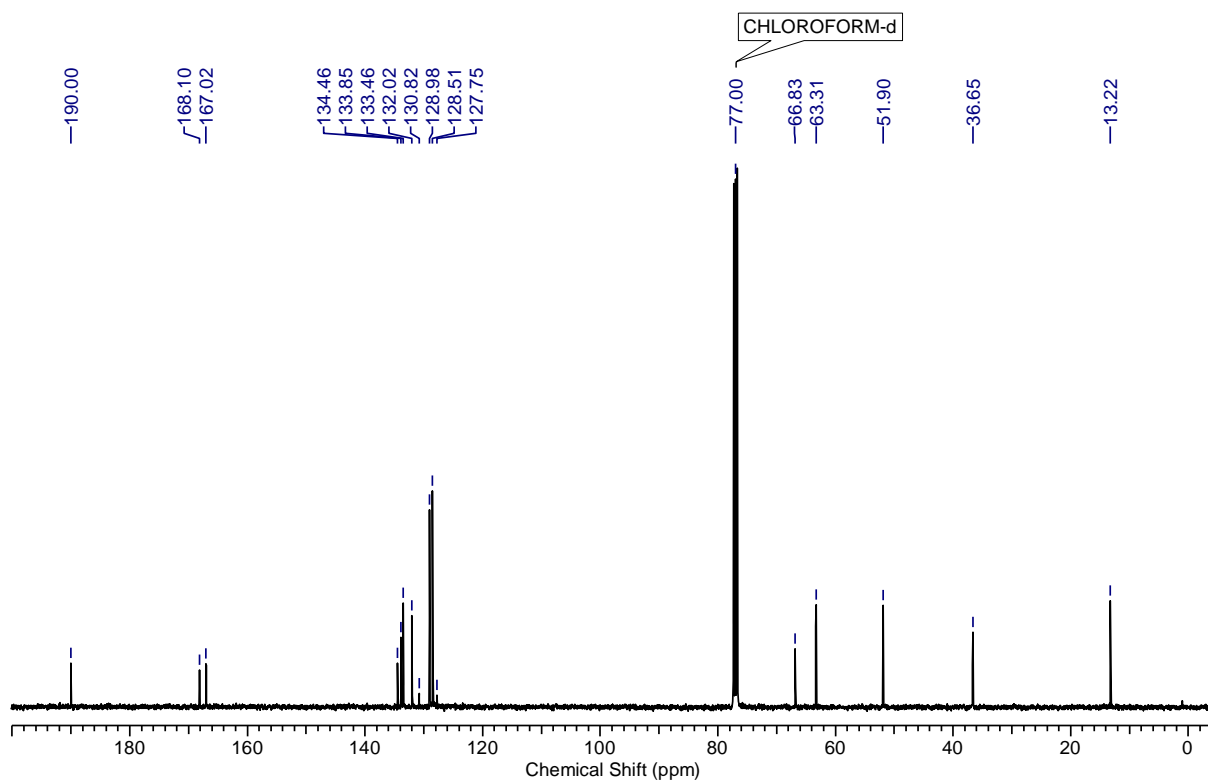
SeF3-3 #310 RT: 1.84 AV: 1 NL: 4.95E8
 T: FTMS + p ESI Full ms [100.0000-1500.0000]



¹H NMR, 400 MHz

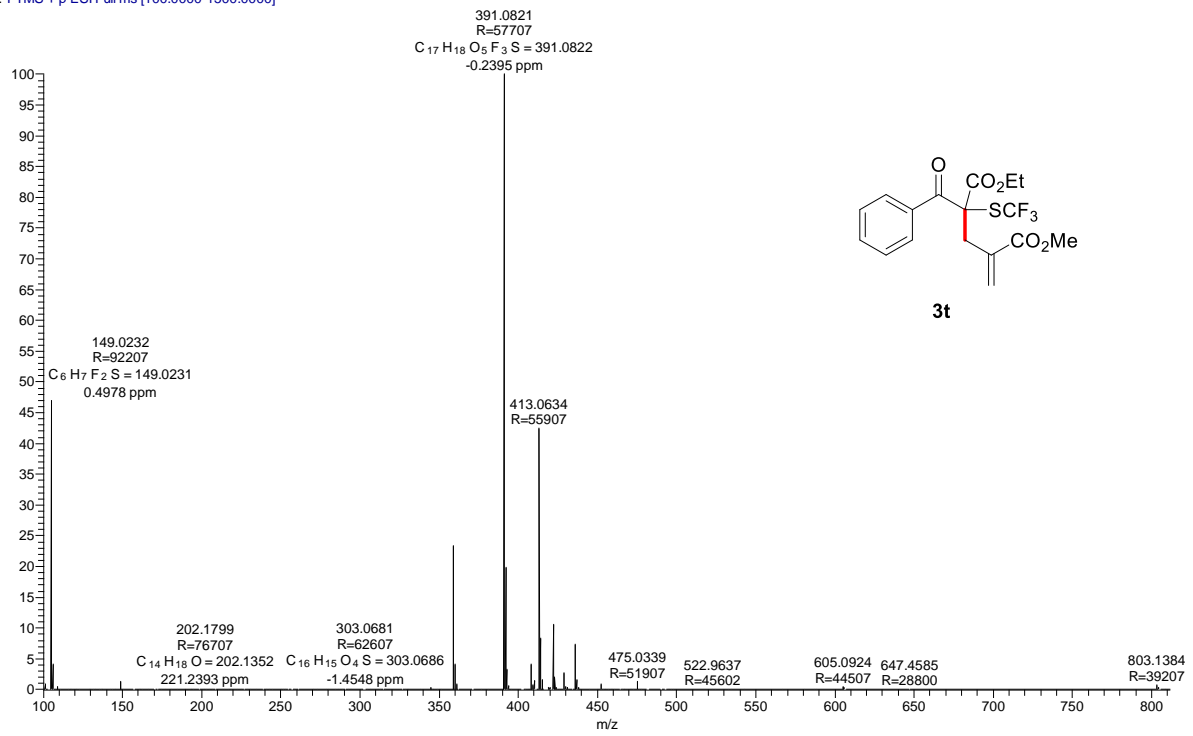


¹³C NMR, 100 MHz

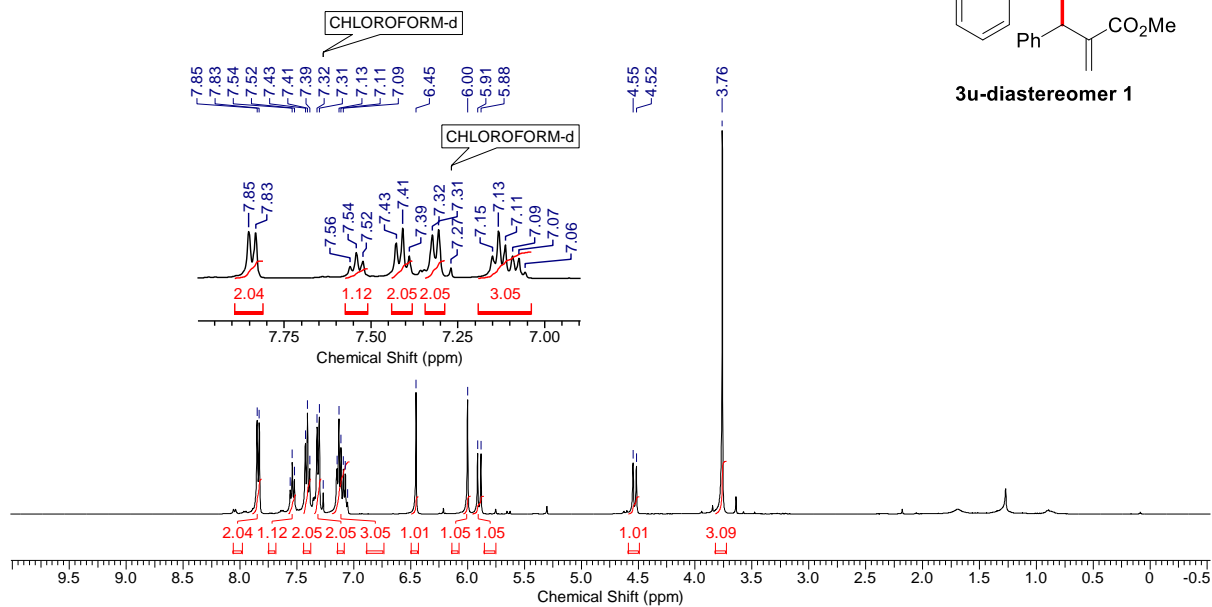
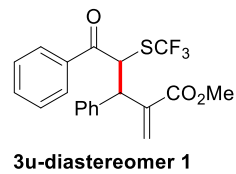


ESI-HRMS

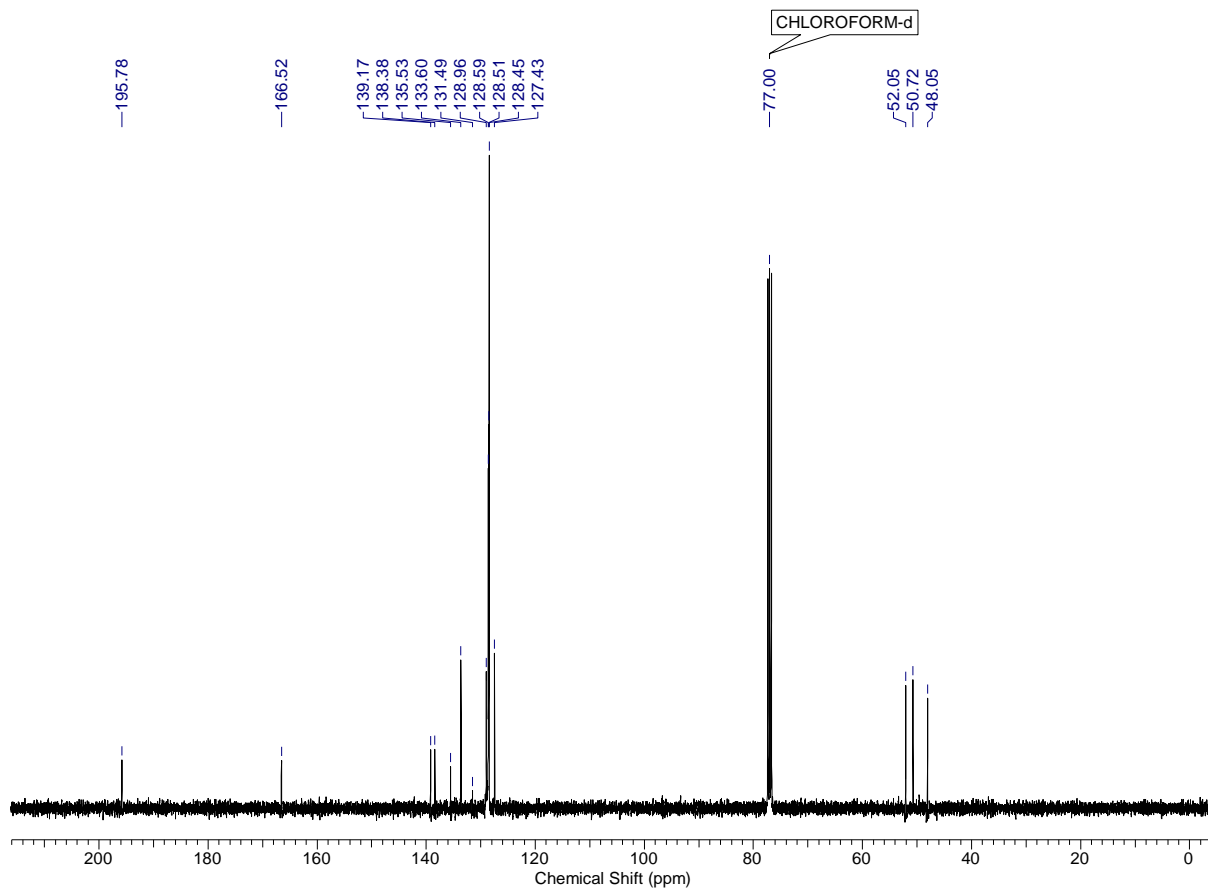
SeF3-4 #285 RT: 1.72 AV: 1 NL: 8.15E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



¹H NMR, 400 MHz

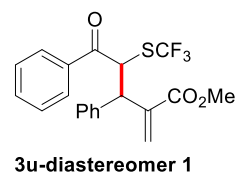
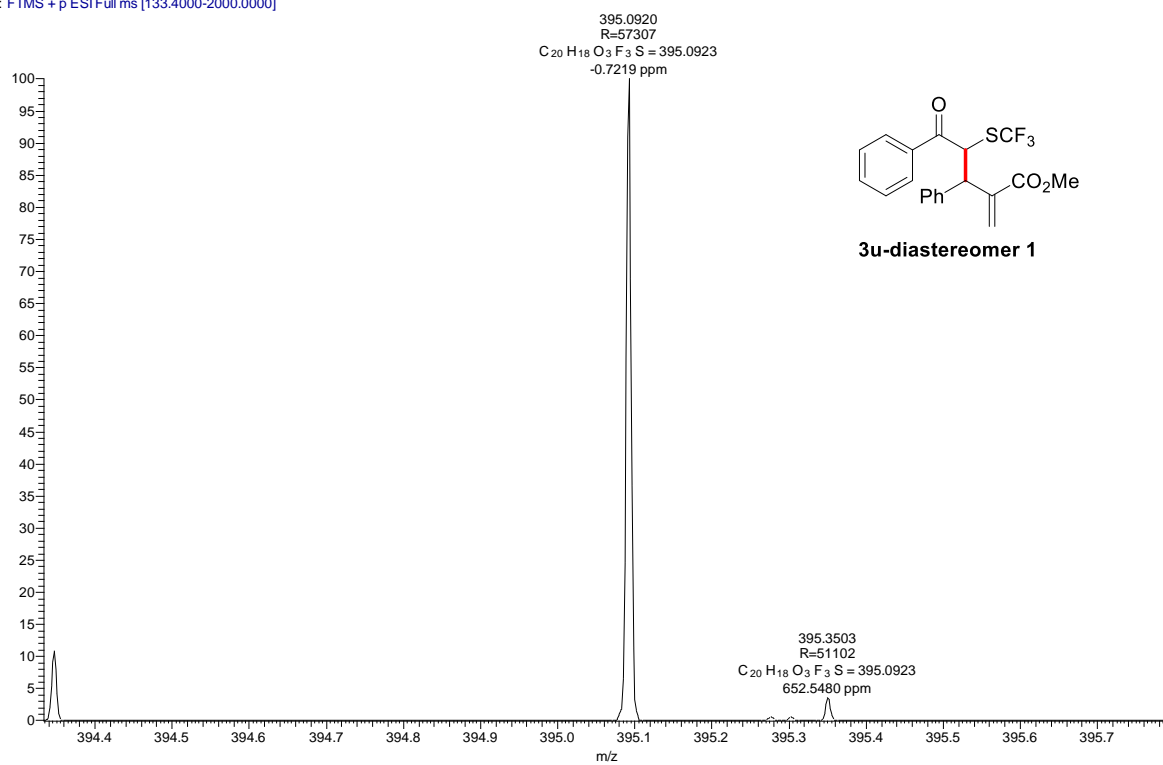


¹³C NMR, 100 MHz

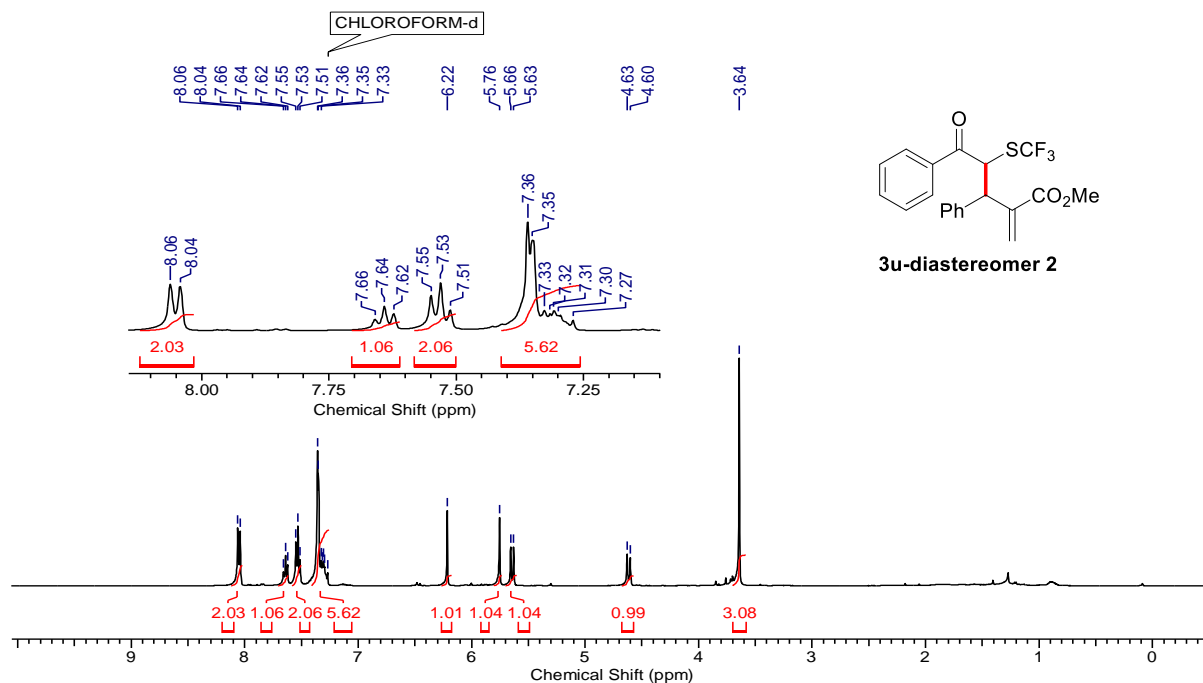


ESI-HRMS

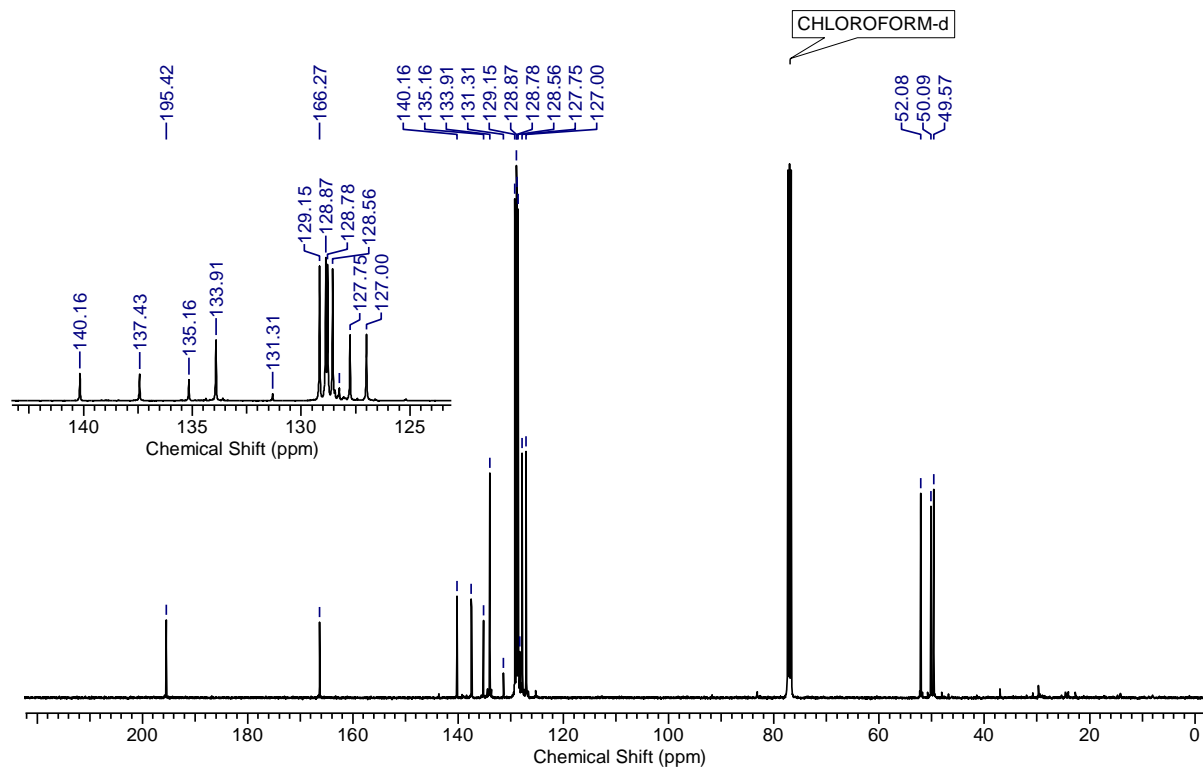
SEF3-19 #268 RT: 1.19 AV: 1 NL: 1.38E7
T: FTMS + p ESI Full ms [133.4000-2000.0000]



¹H NMR, 400 MHz

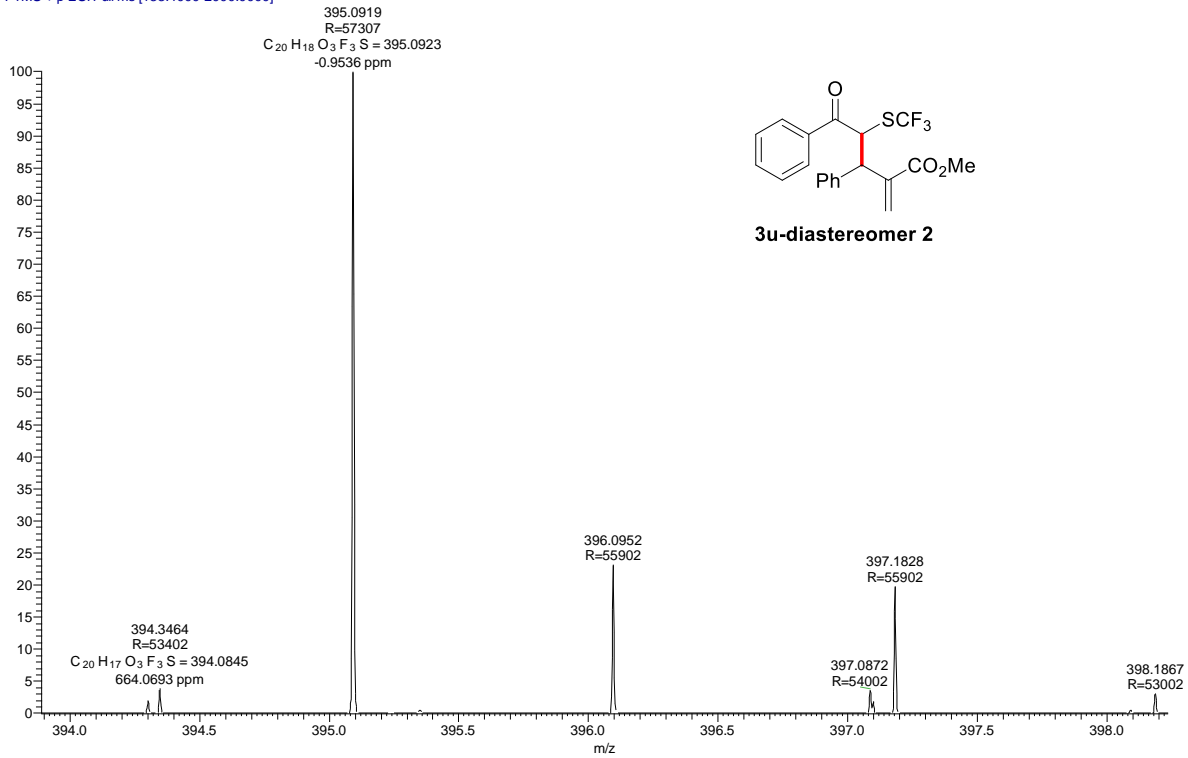


¹³C NMR, 100 MHz

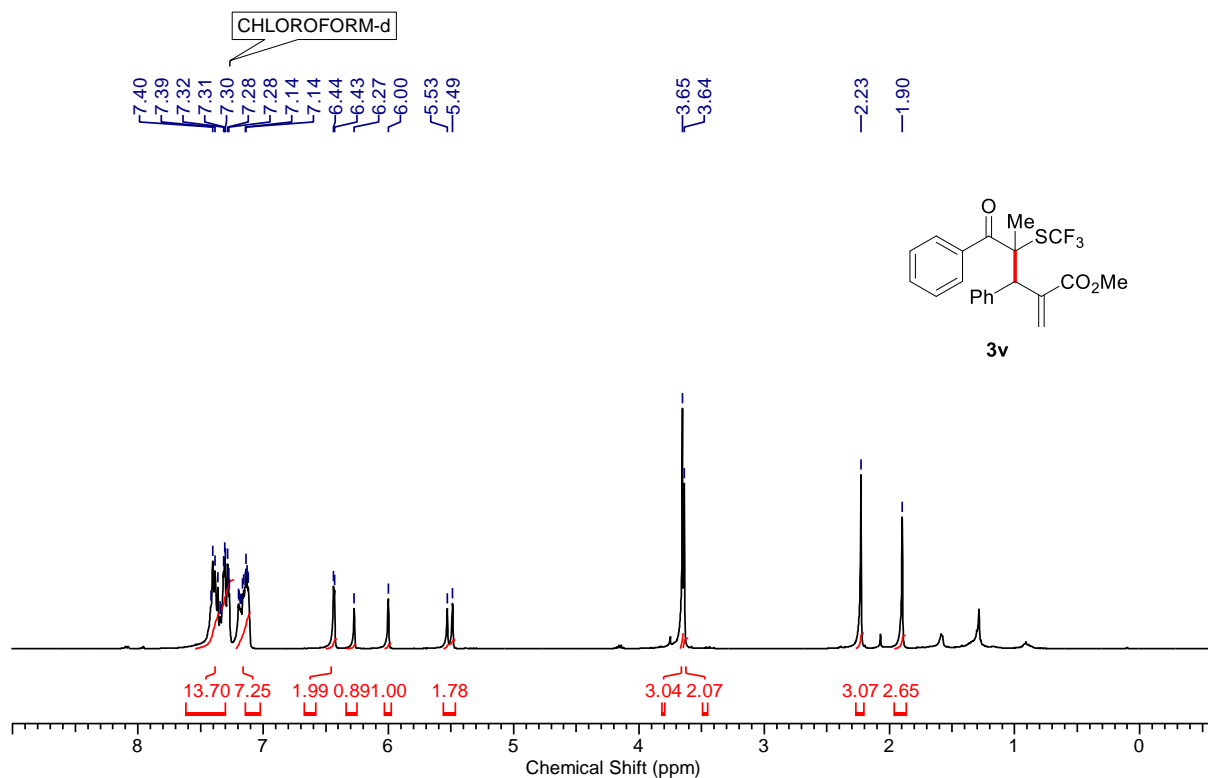


ESI-HRMS

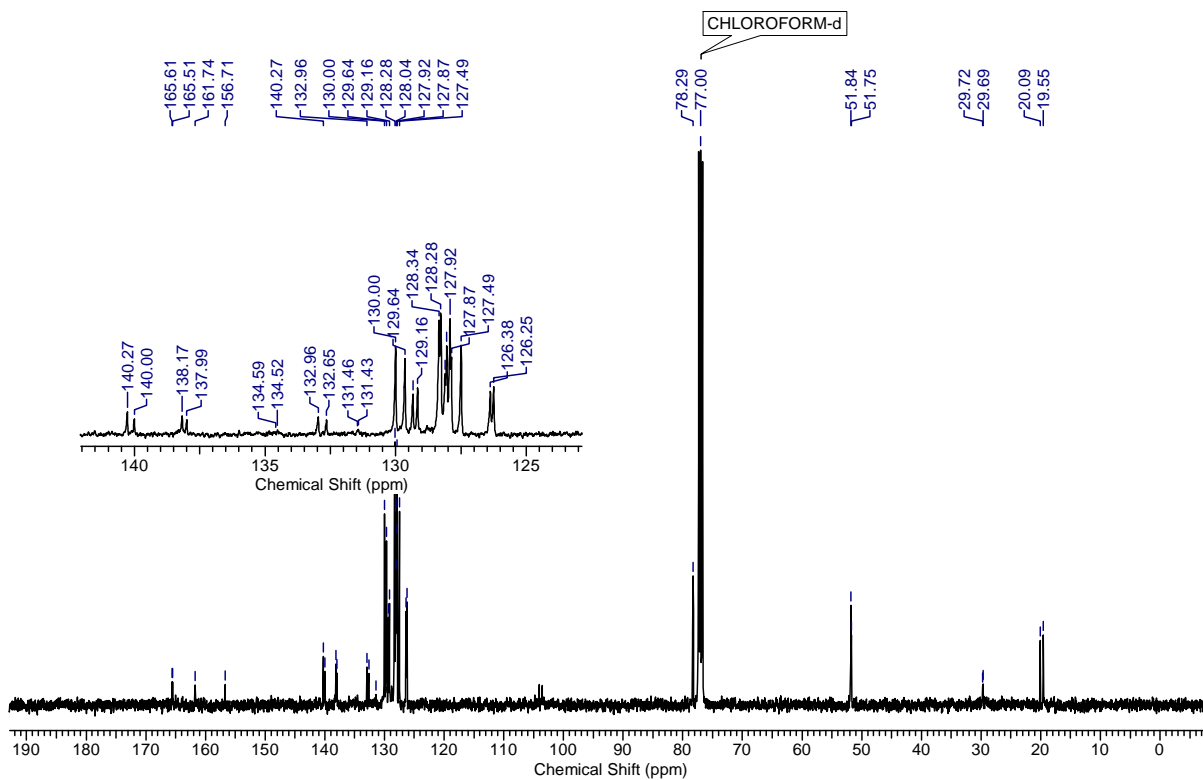
SEF3-19II #278 RT: 1.24 AV: 1 NL: 3.09E7
T: FTMS + p ESI Full ms [133.4000-2000.0000]



¹H NMR, 400 MHz

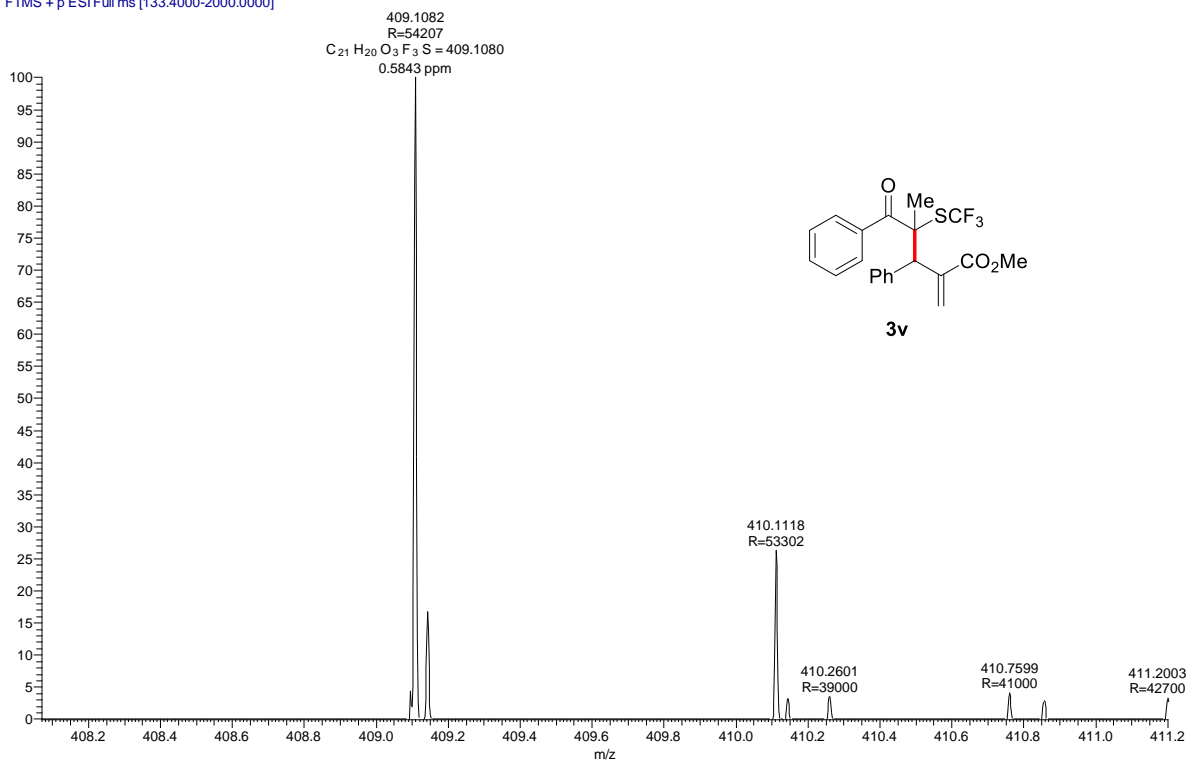


¹³C NMR, 100 MHz

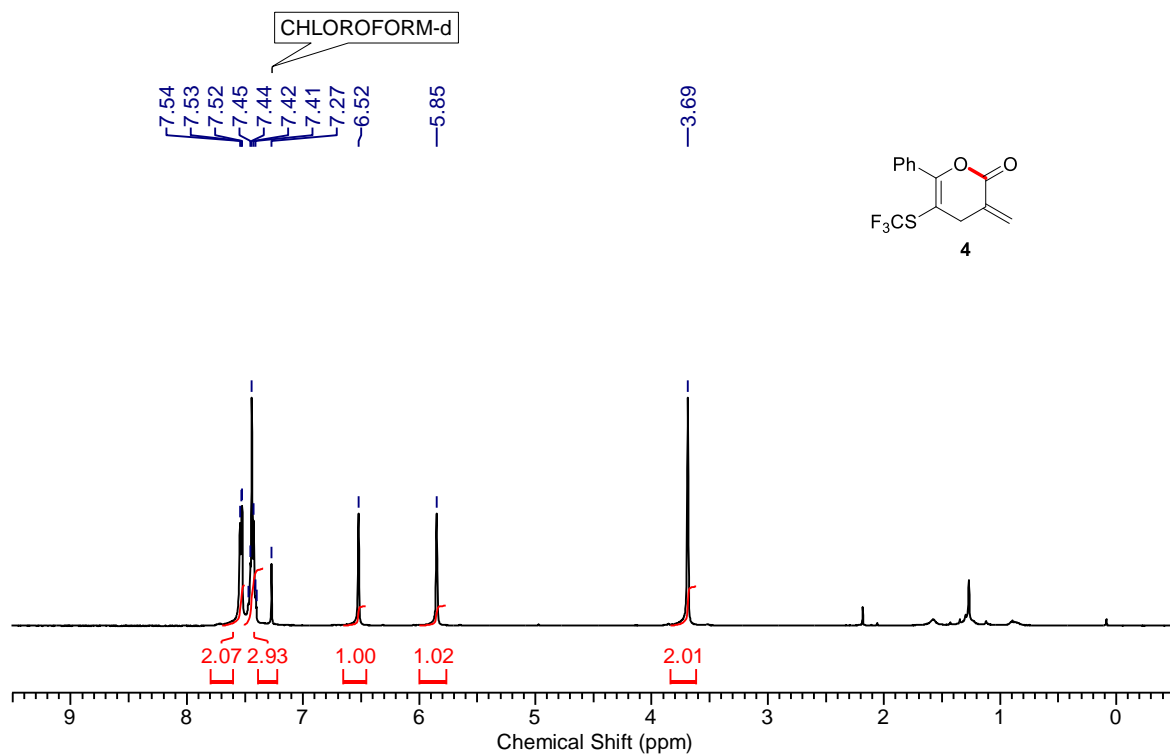


ESI-HRMS

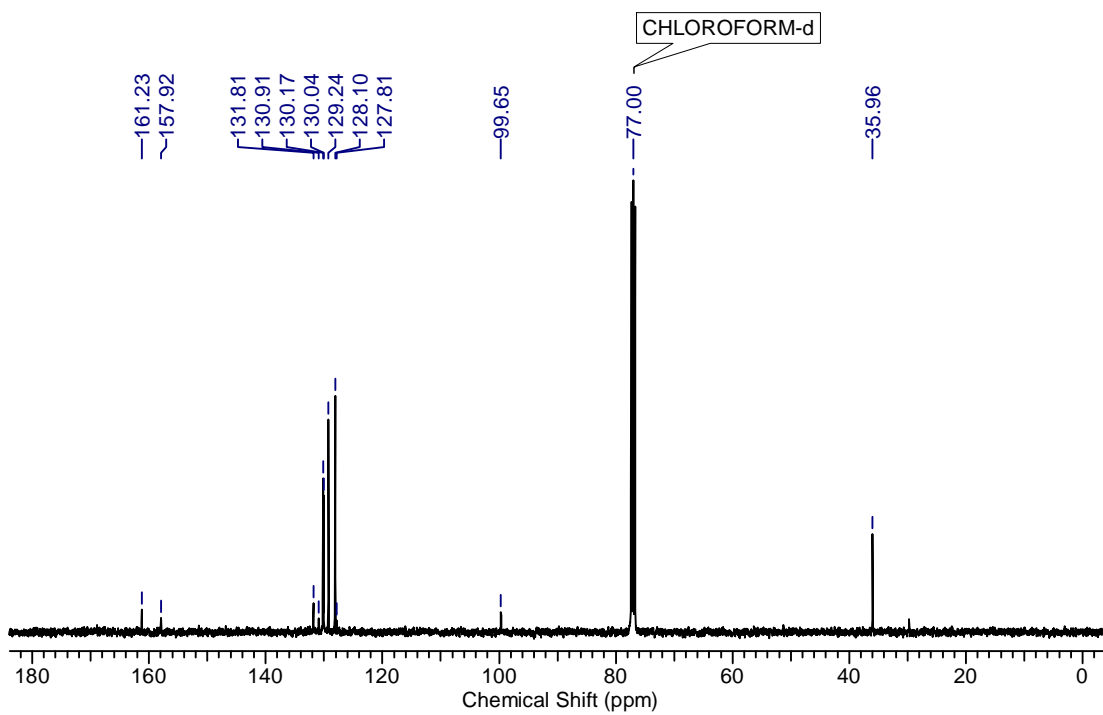
SEF3-20 #313 RT: 1.39 AV: 1 NL: 2.60E6
T: FTMS + p ESI Full ms [133.4000-2000.0000]



¹H NMR, 400 MHz

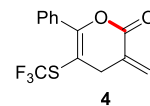
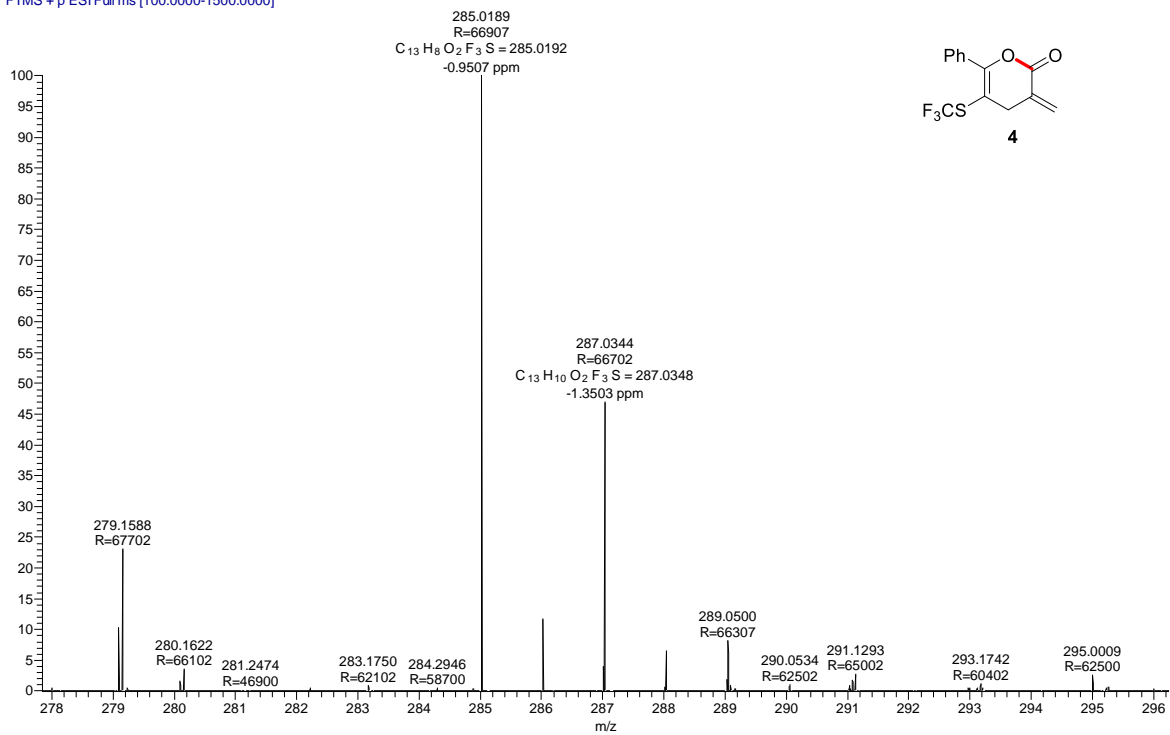


¹³C NMR, 100 MHz

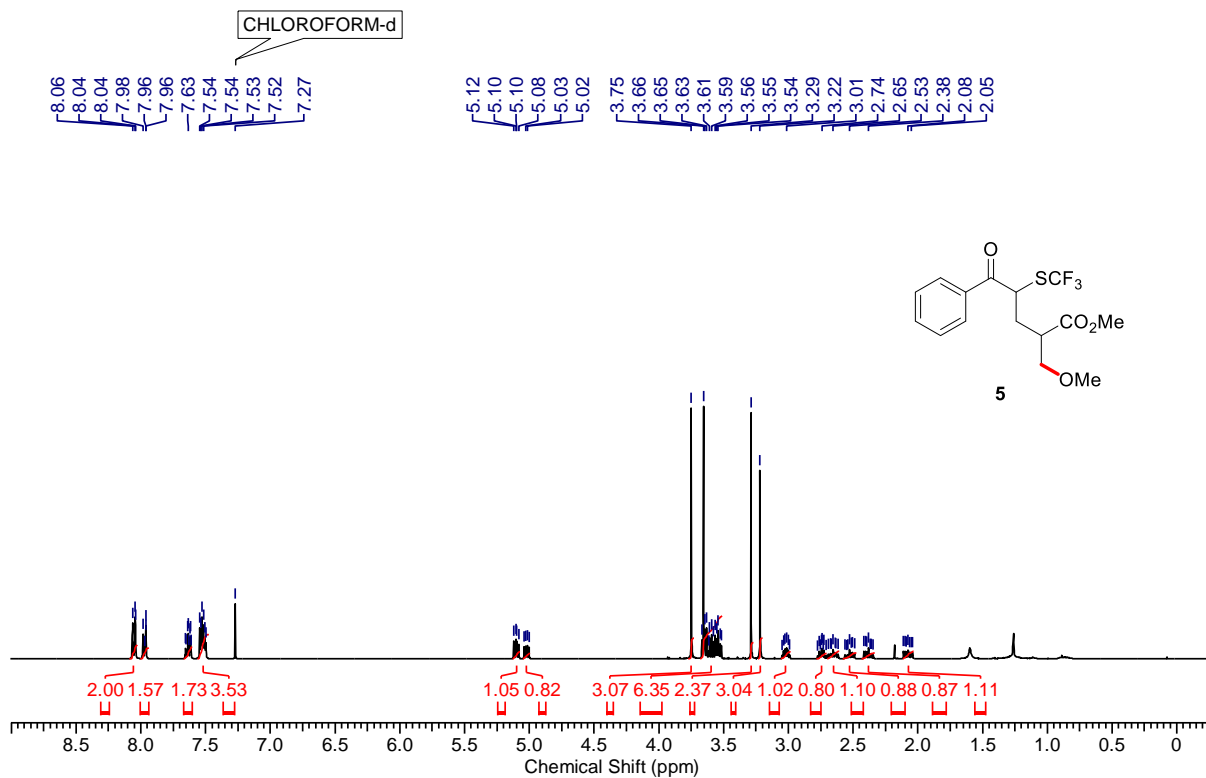


ESI-HRMS

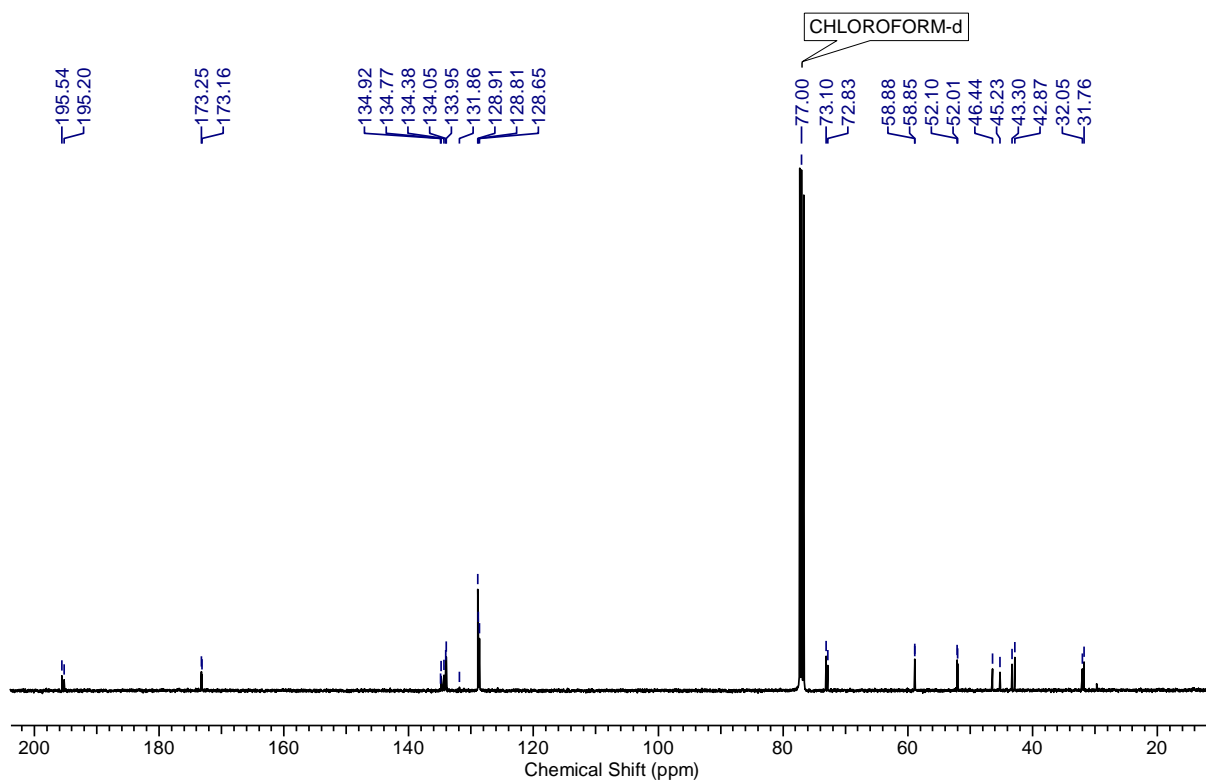
SeF3-6 #262 RT: 1.59 AV: 1 NL: 8.47E6
T: FTMS + p ESI Full ms [100.0000-1500.0000]



¹H NMR, 500 MHz



¹³C NMR, 125 MHz



ESI-HRMS

SeF3-5 #266 RT: 1.60 AV: 1 NL: 6.95E8
T: FTMS +p ESI Full ms [100.0000-1500.0000]

