

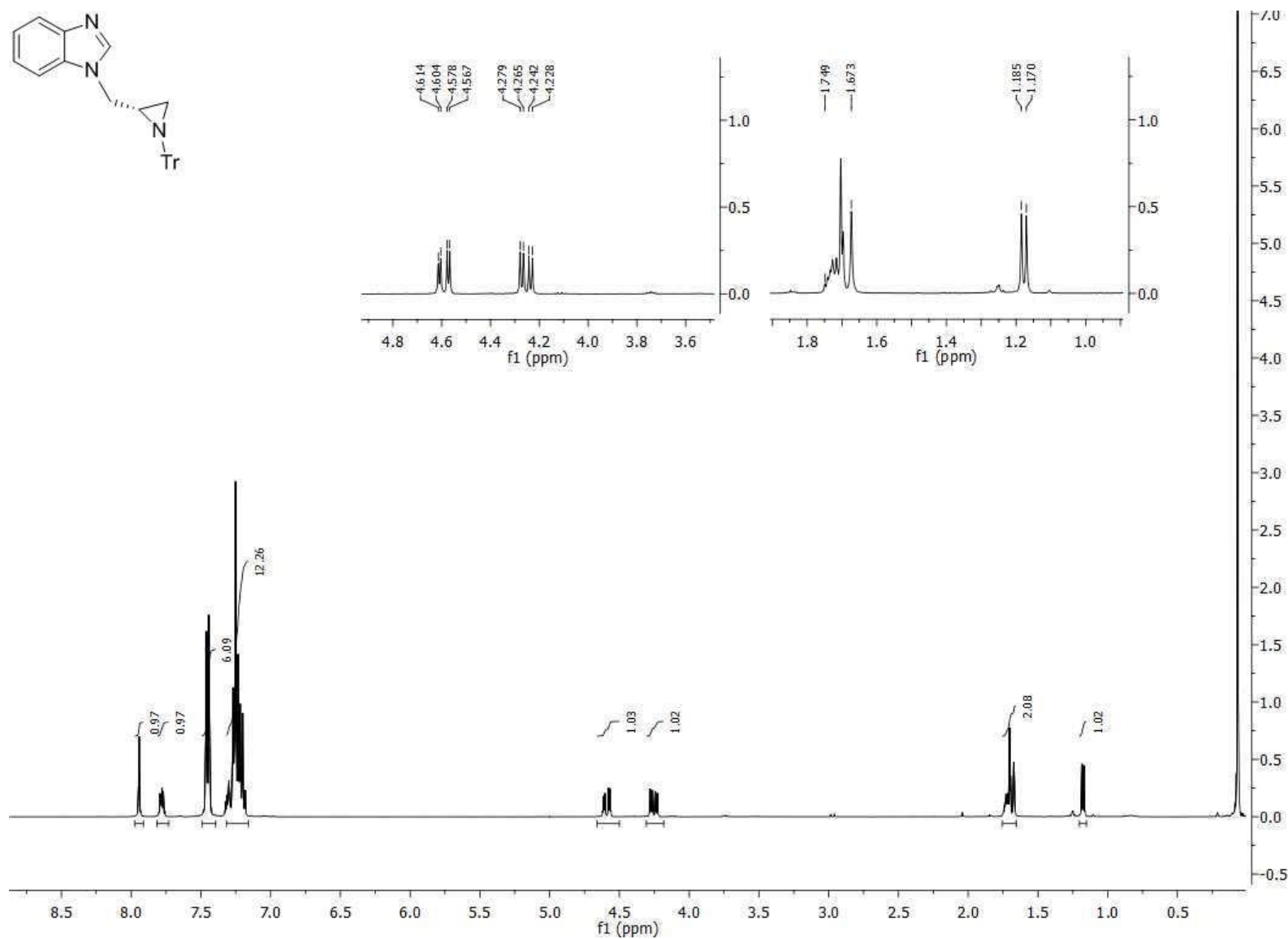
Electronic Supplementary Information (ESI)
for
First synthesis of an aziridinyf fused pyrrolo[1,2-*a*]benzimidazole
and toxicity evaluation towards normal and breast cancer cell lines

Sarah Bonham,^a Liz O'Donovan,^a Michael P. Carty^b and Fawaz Aldabbagh*^a

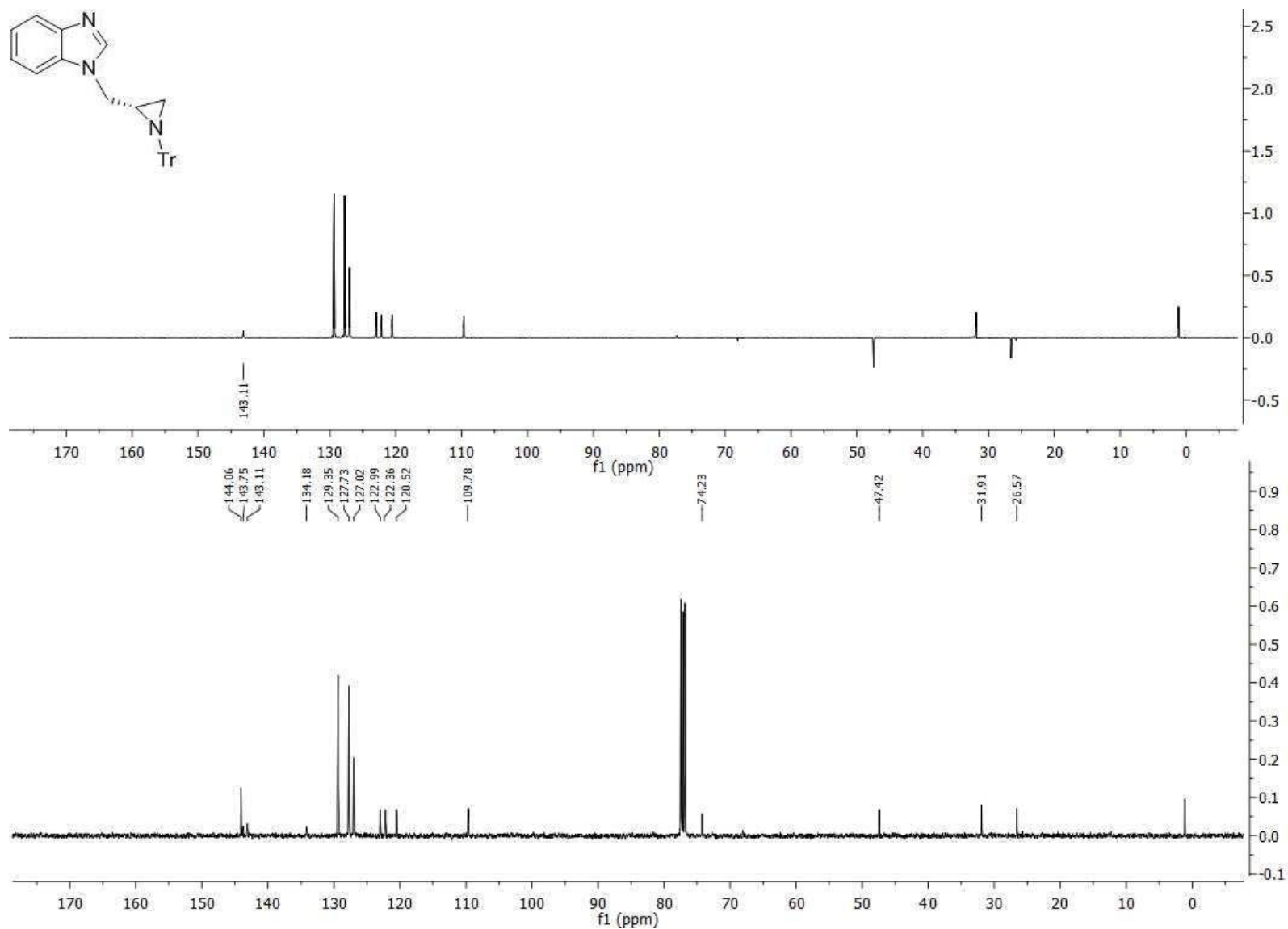
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Galway, Ireland.*

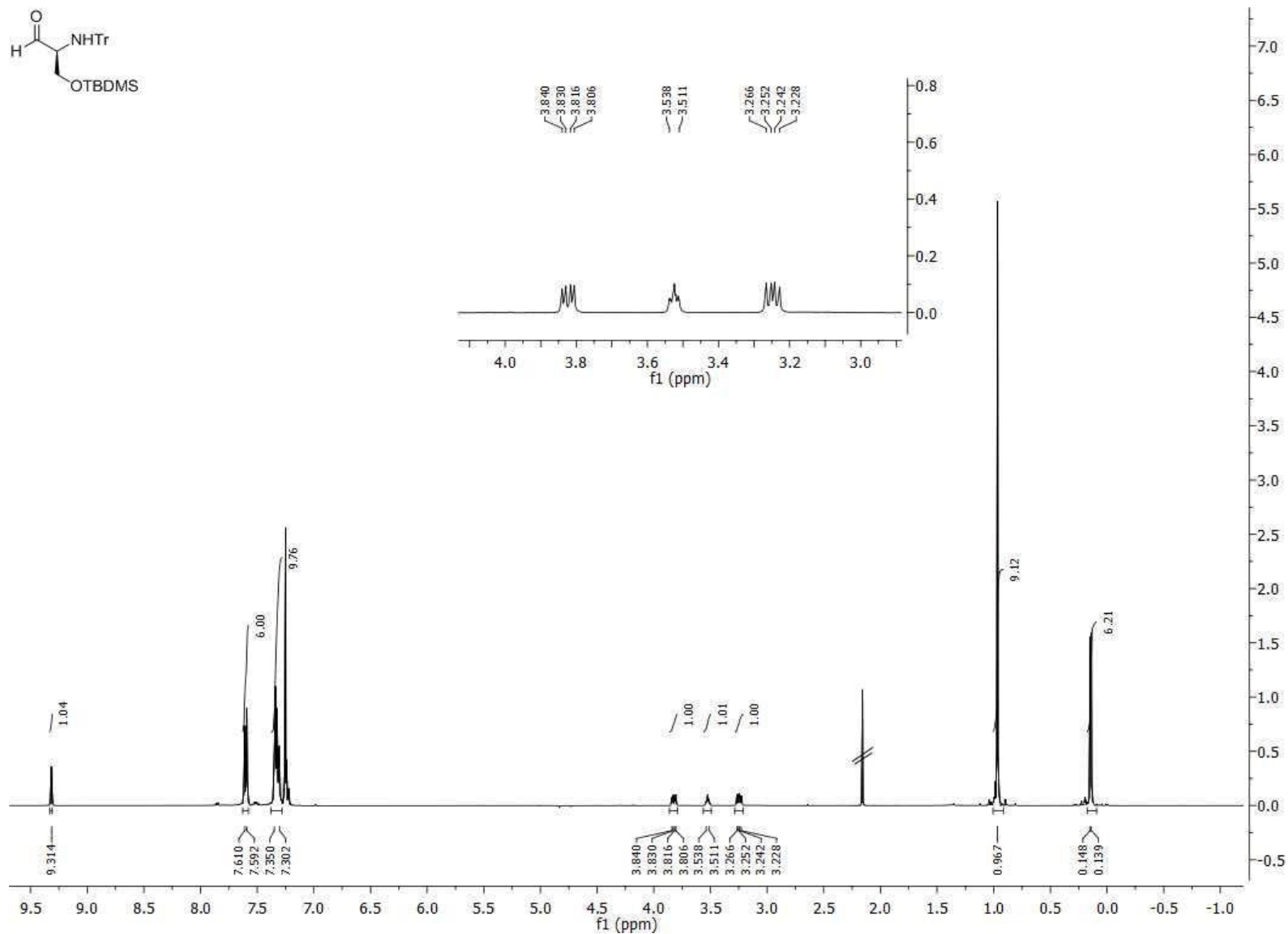
¹H NMR, 400 MHz, CDCl₃: *N*-[(1-*tritylaziridin*-(2*S*)-yl)methyl]-1*H*-benzimidazole (2)



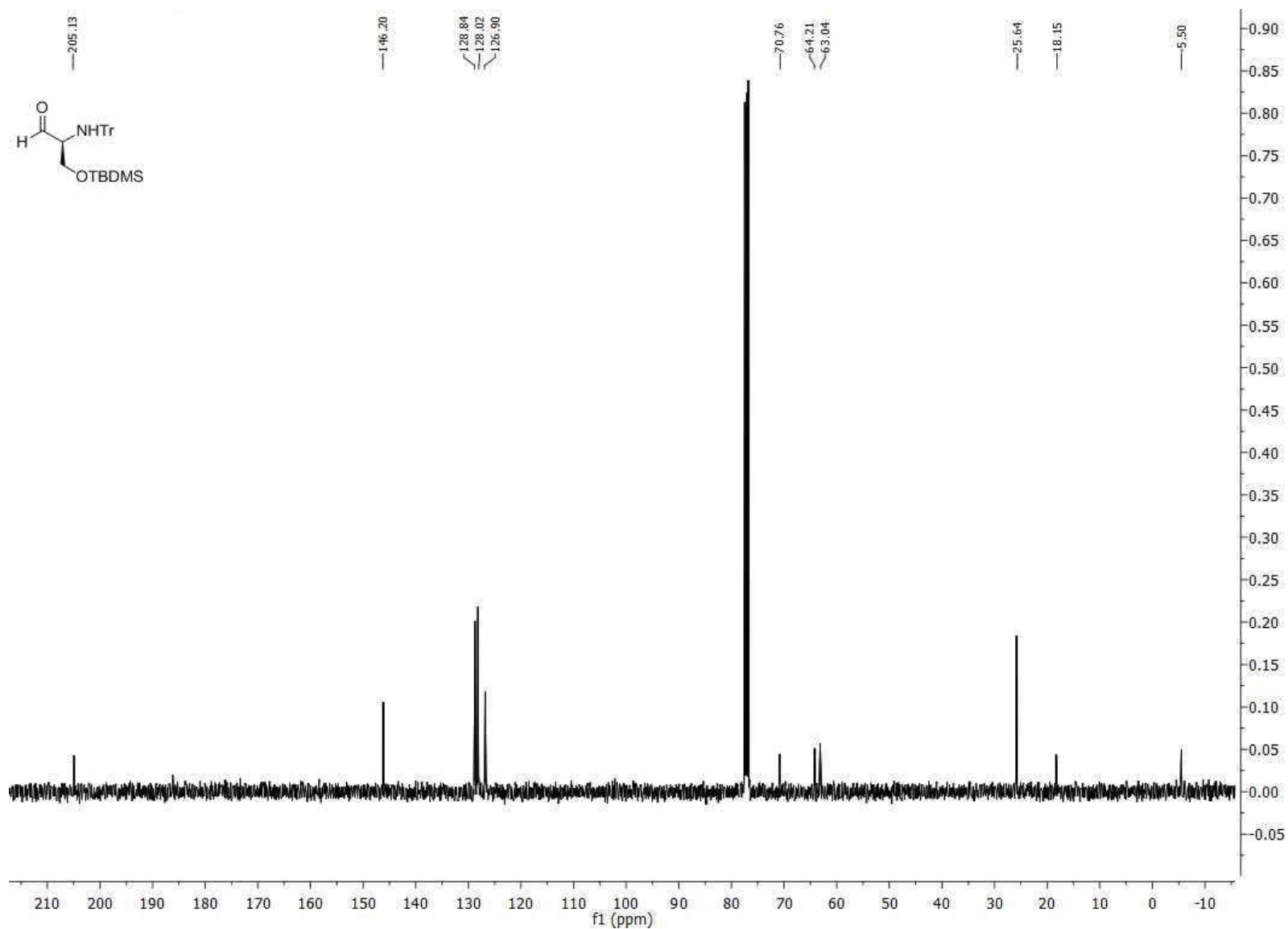
¹³C NMR AND DEPT, 100 MHz, CDCl₃: N-[(1-tritylaziridin-(2S)-yl)methyl]-1H-benzimidazole (2)



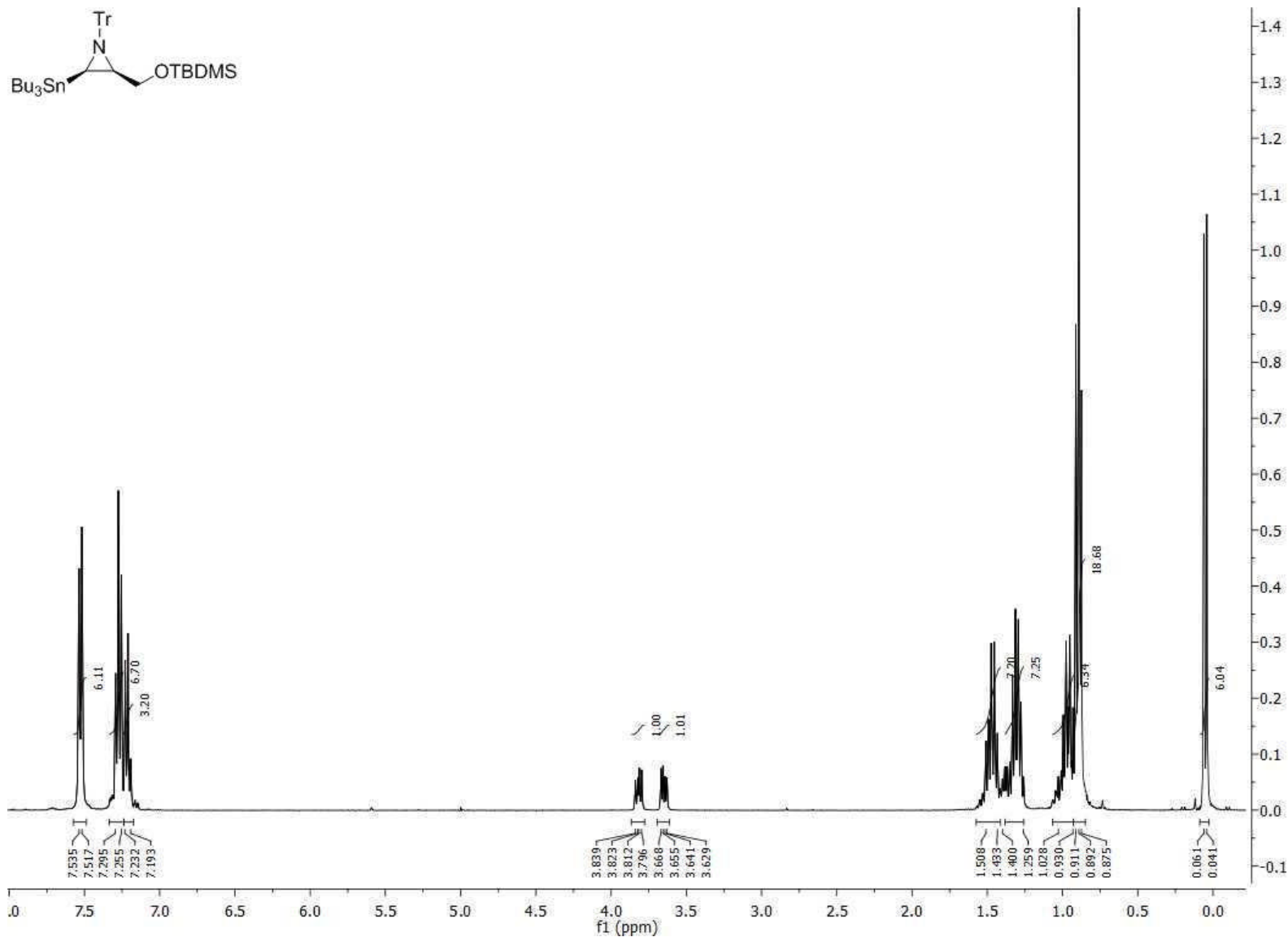
¹H NMR, 400 MHz, CDCl₃: *N*-trityl-*O*-(*tert*-butyldimethylsiloxy)-*S*-serinal (4)



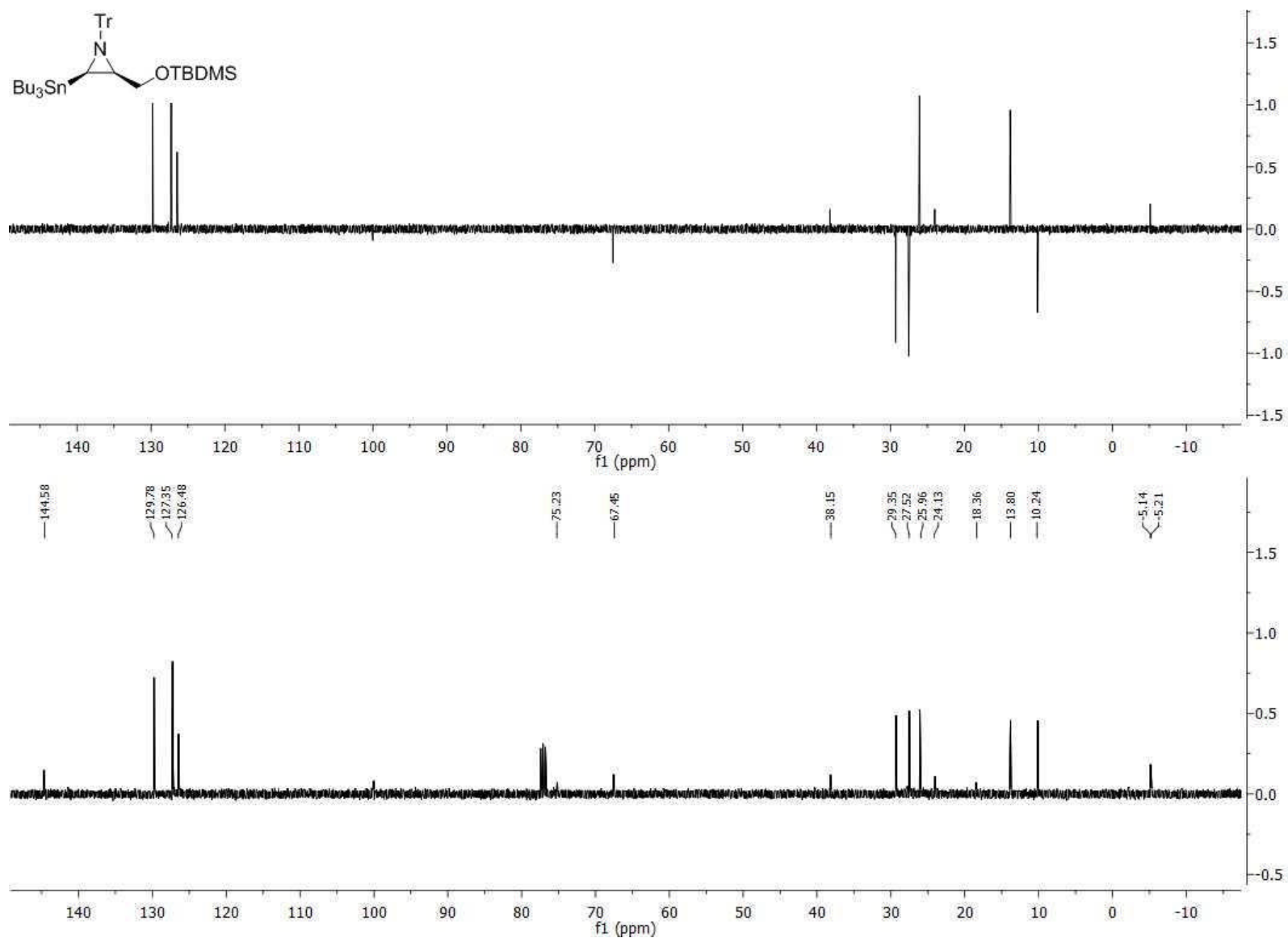
¹³C NMR, 100 MHz, CDCl₃: *N*-trityl-*O*-(*tert*-butyldimethylsiloxy)-*S*-serinal (4)



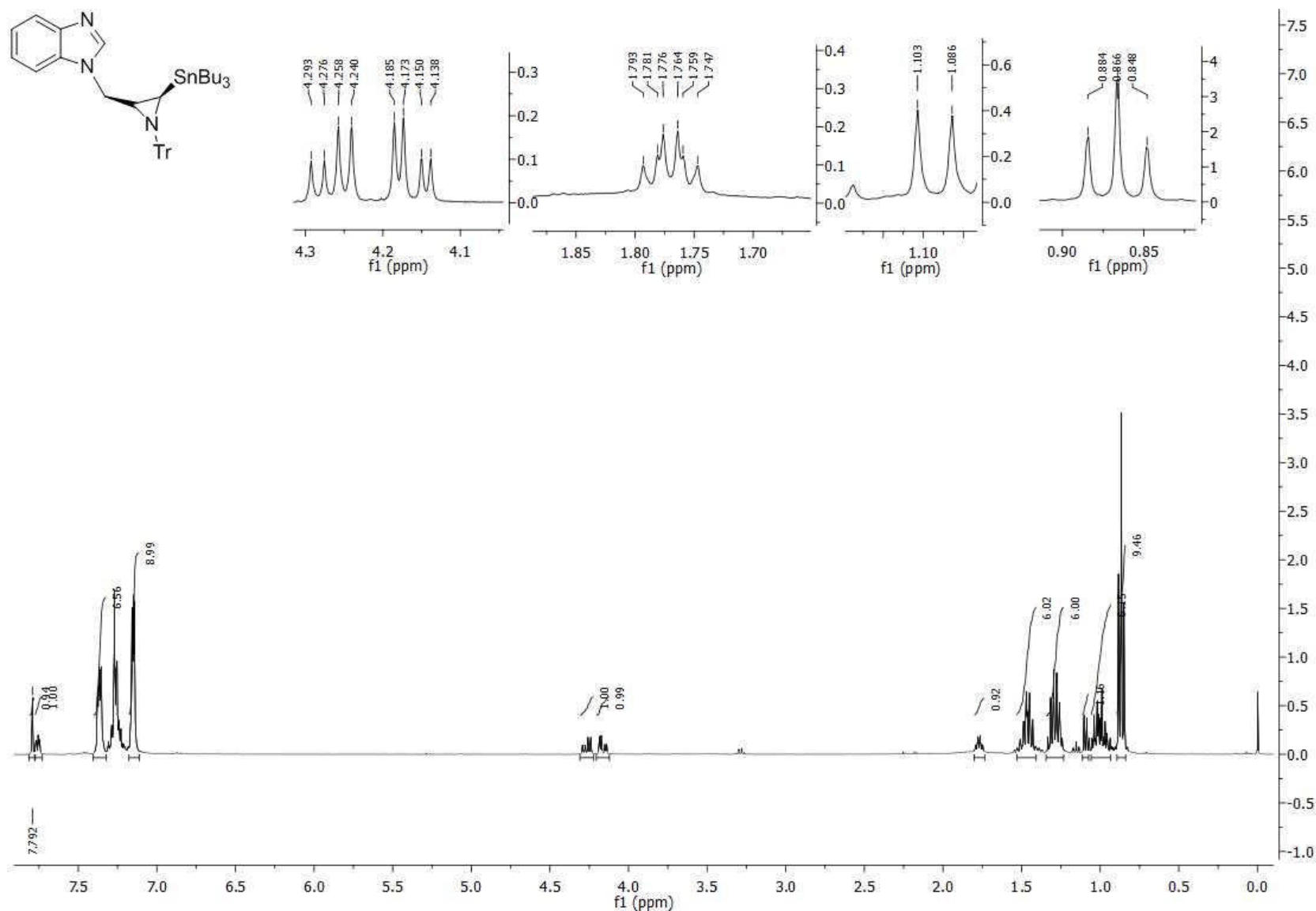
¹H NMR, 400 MHz, CDCl₃: (2*S*,3*R*)-2-({*tert*-butyl(dimethyl)silyl}oxy)methyl)-3-(tributylstannyl)-1-tritylaziridine (5)



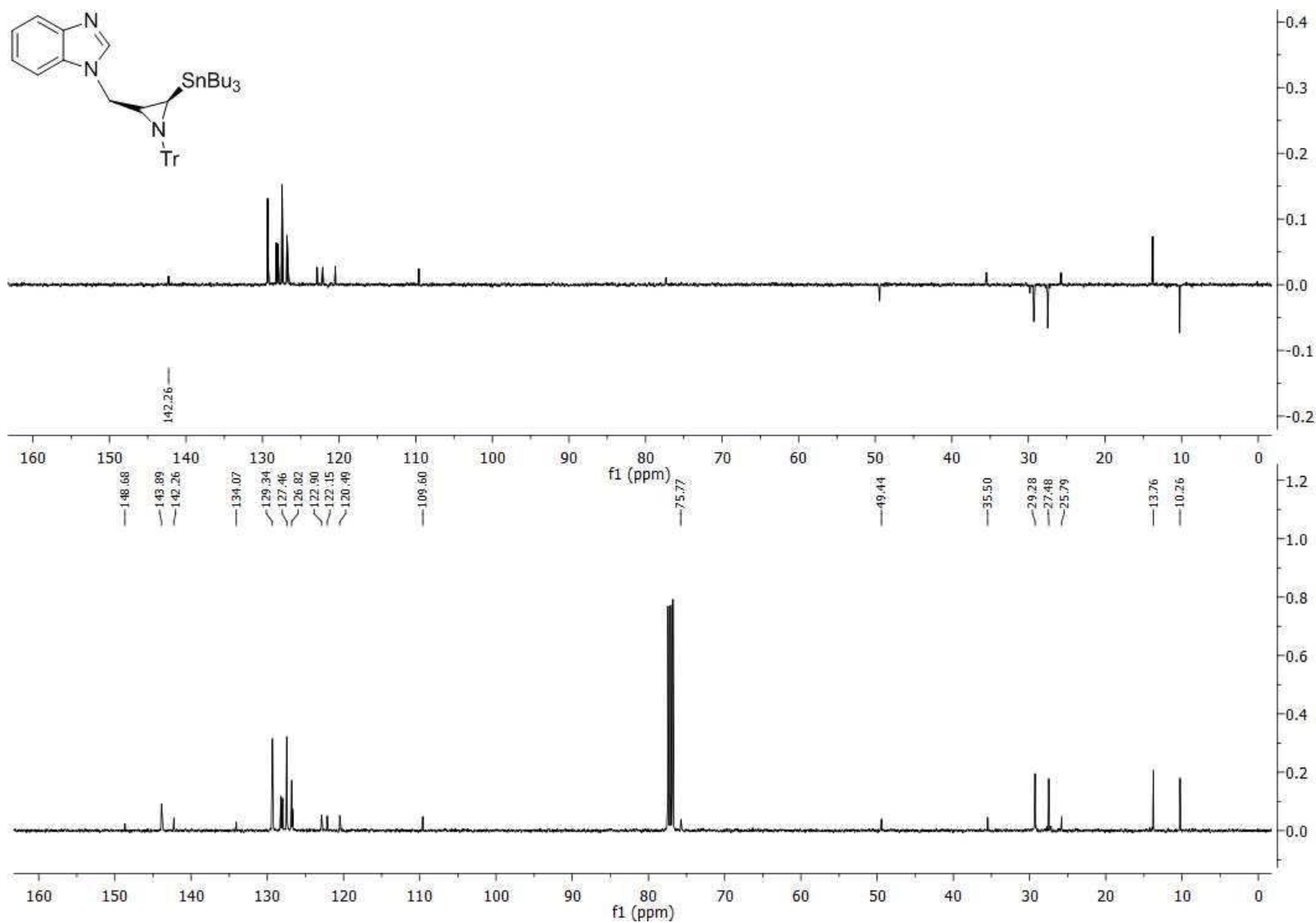
¹³C NMR AND DEPT, 100 MHz, CDCl₃: (2*S*,3*R*)-2-({*tert*-butyl(dimethyl)silyl}oxy)methyl)-3-(tributylstannyl)-1-tritylaziridine (5)



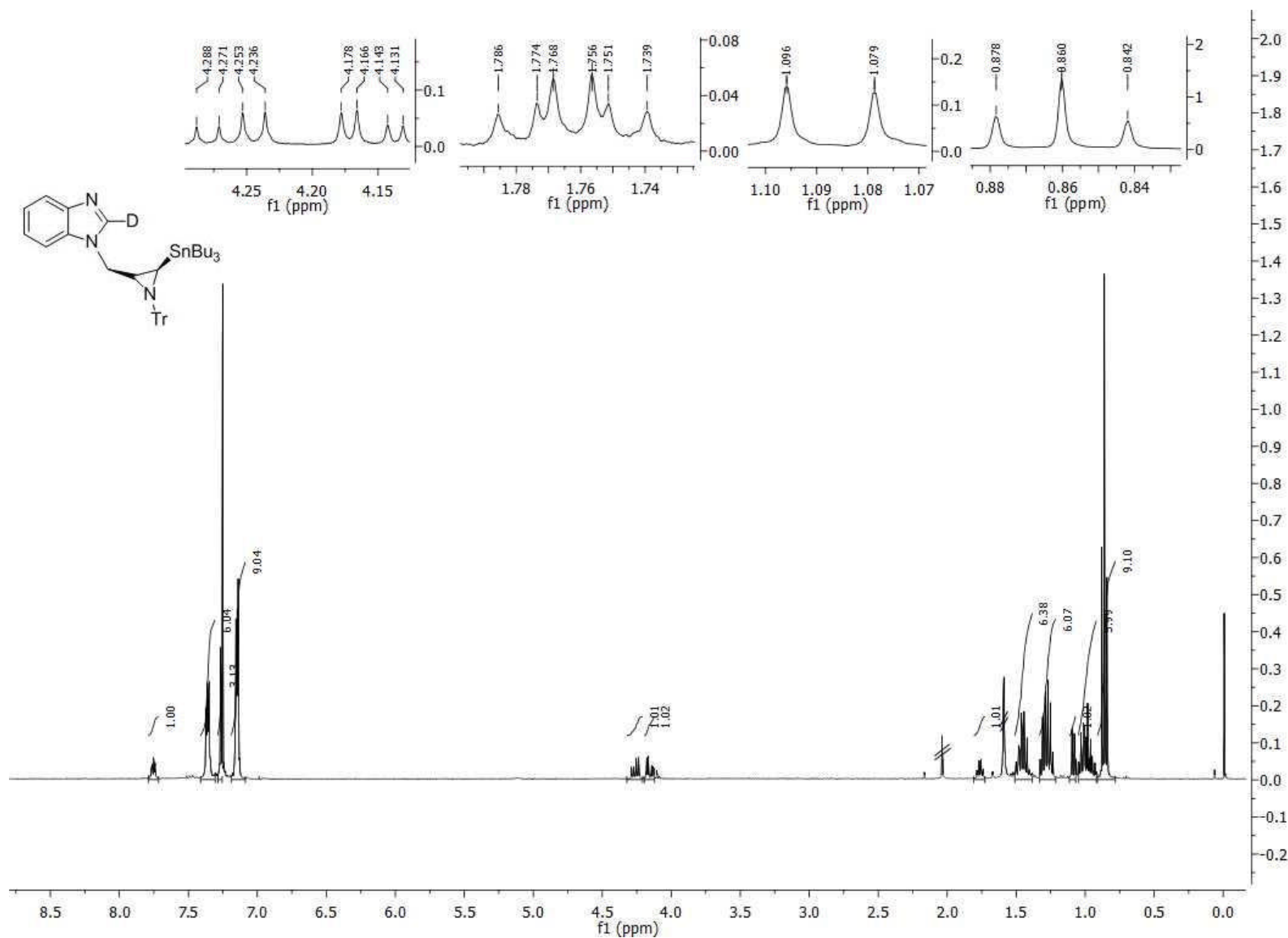
¹H NMR, 400 MHz, CDCl₃: 1-[(2*S*,3*R*)-3-(tributylstannyl)-1-tritylaziridin-2-yl]methyl}-1*H*-benzimidazole (9)



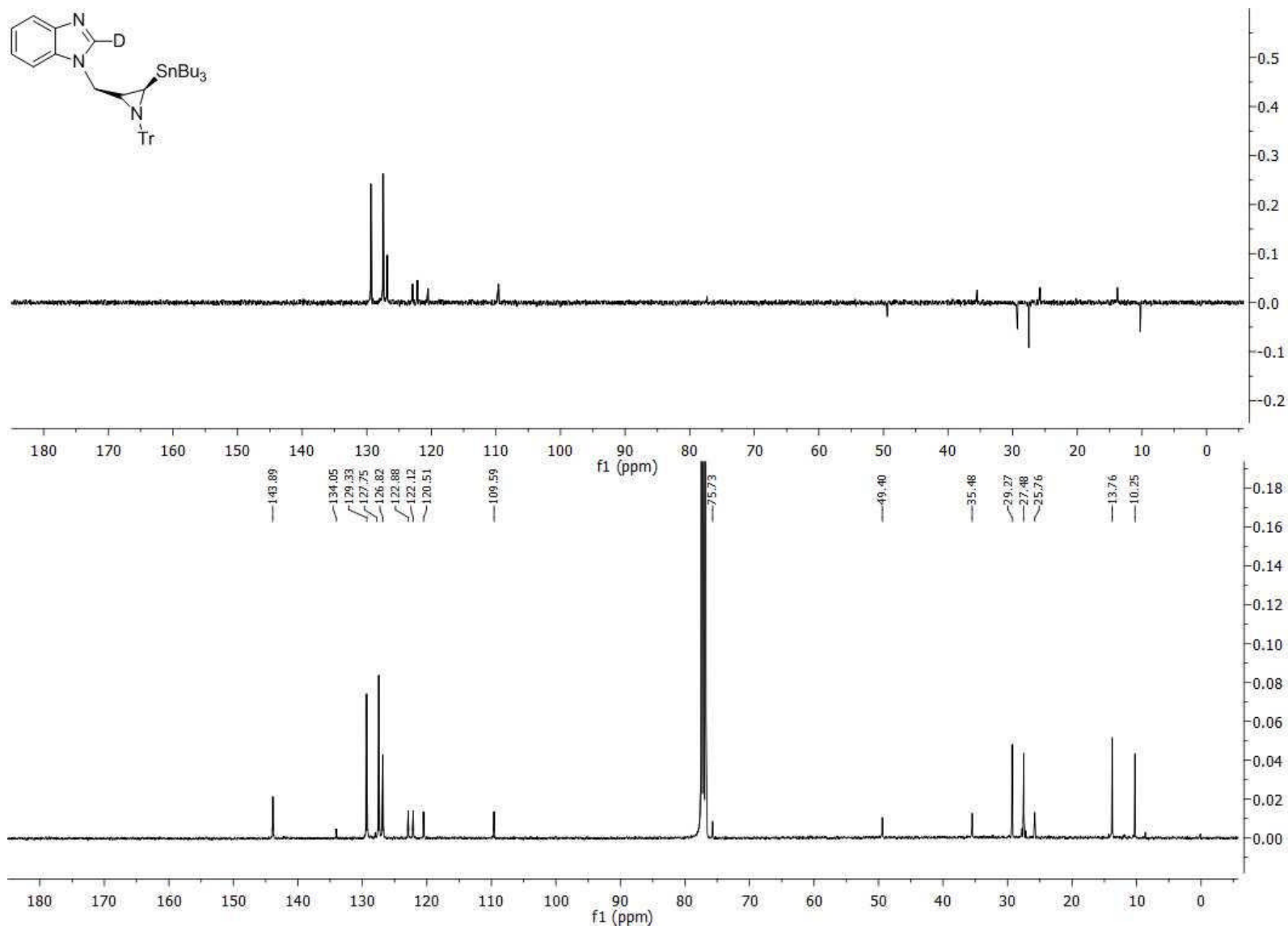
¹³C NMR AND DEPT, 100 MHz, CDCl₃: 1-{[(2*S*,3*R*)-3-(tributylstannyl)-1-tritylaziridin-2-yl]methyl}-1*H*-benzimidazole (9)



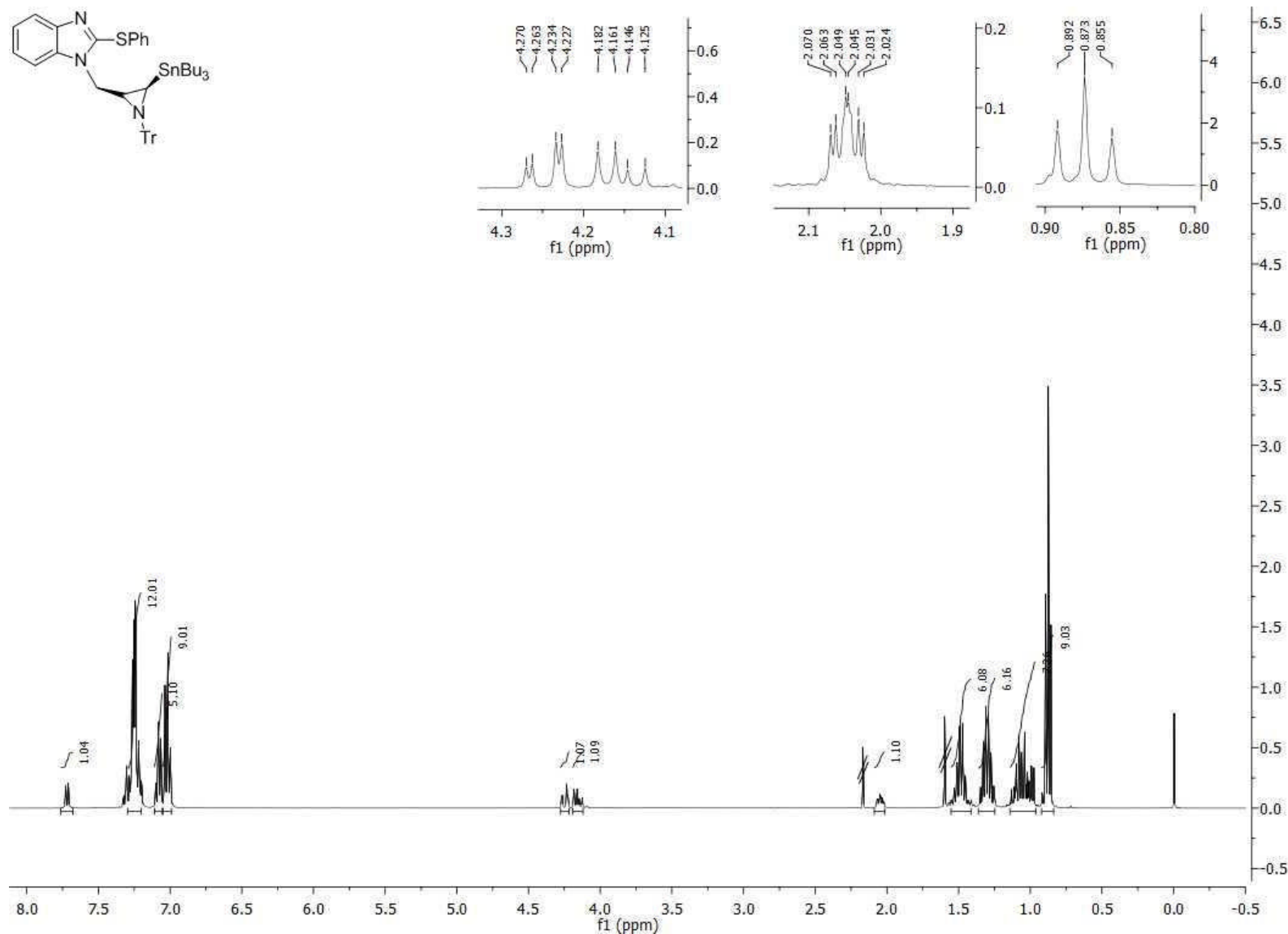
¹H NMR, 400MHz, CDCl₃: 2-Deutero-1-[(2*S*,3*R*)-3-(tributylstannyl)-1-tritylaziridin-2-yl]methyl}-1*H*-benzimidazole (11)



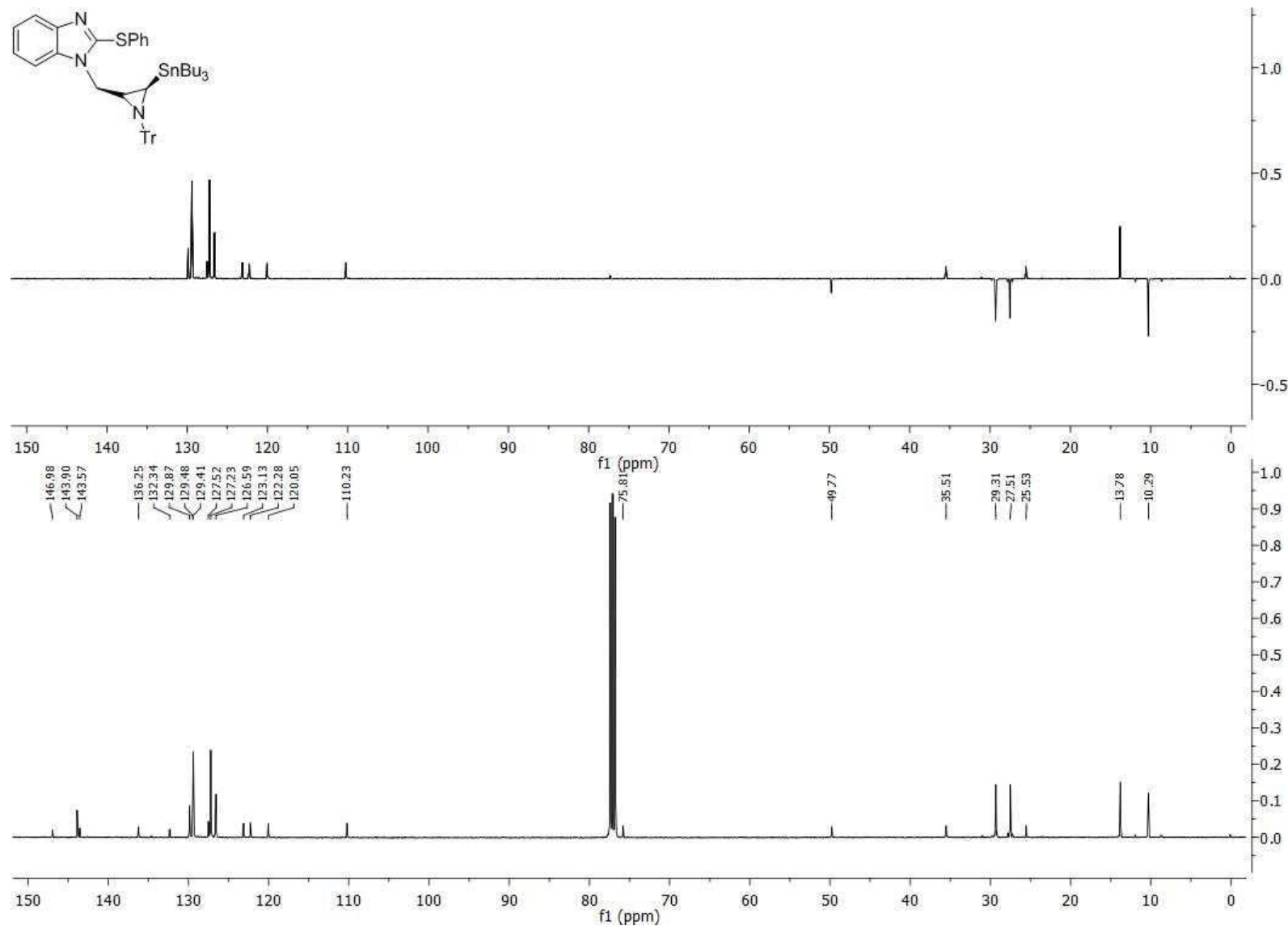
¹³C NMR AND DEPT, 100 MHz, CDCl₃: 2-Deutero-1-{[(2*S*,3*R*)-3-(tributylstannyl)-1-tritylaziridin-2-yl]methyl}-1*H*-benzimidazole (11)



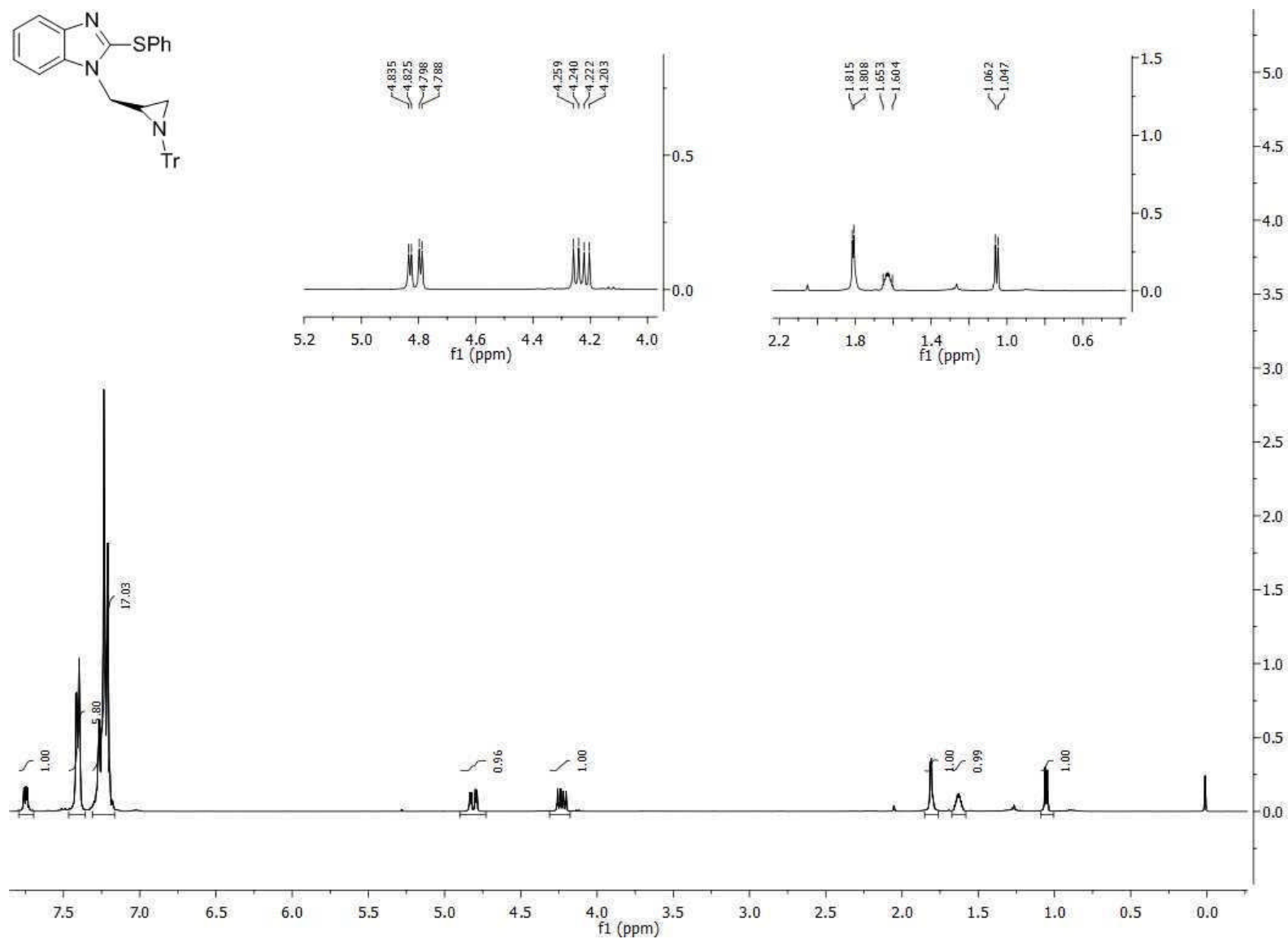
¹H NMR, 400MHz, CDCl₃: 2-(Phenylsulfanyl)-1-{[(2*S*,3*R*)-3-(tributylstannyl)-1-tritylaziridin-2-yl]methyl}-1*H*-benzimidazole (10)



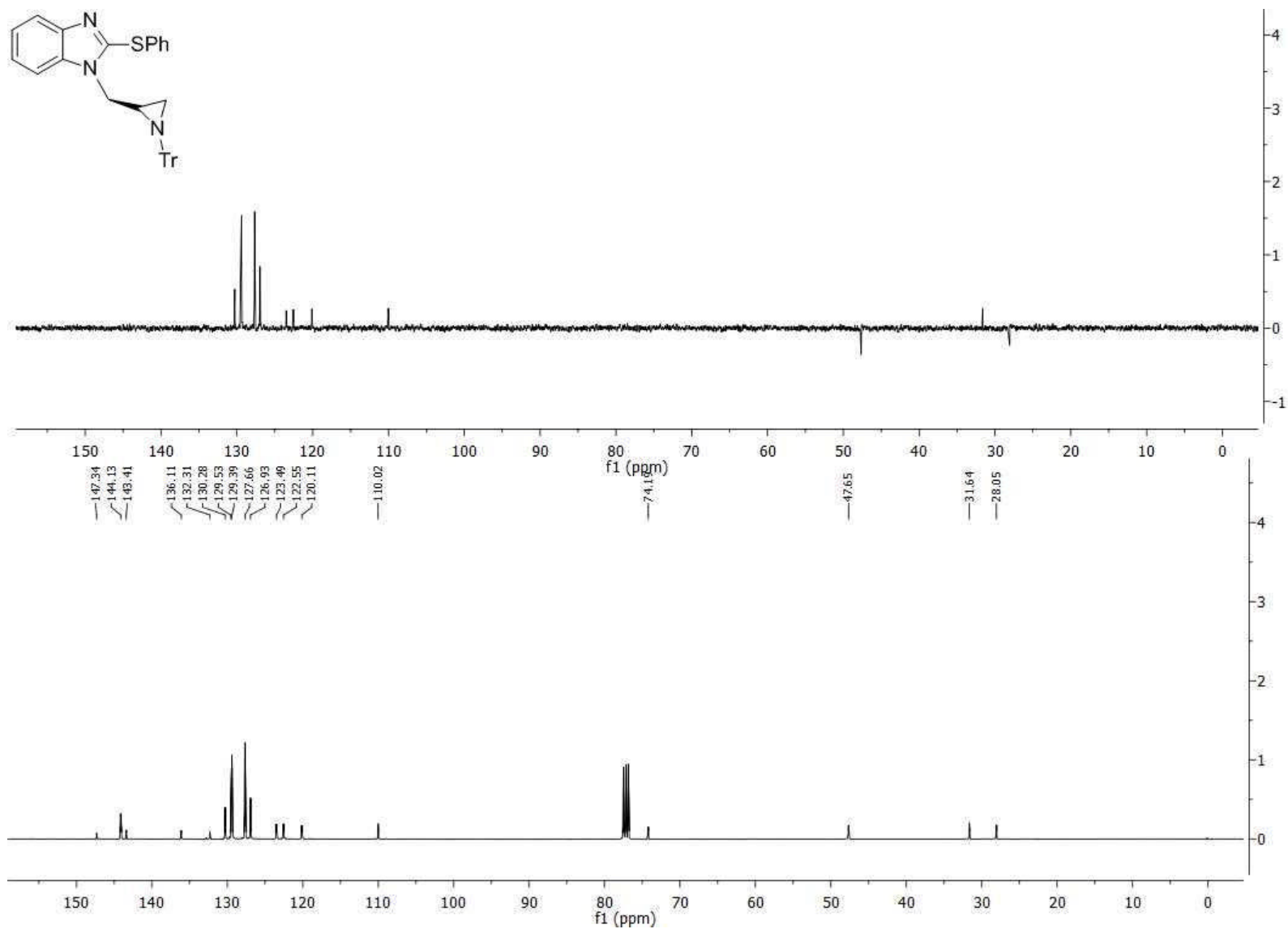
¹³C NMR AND DEPT, 100 MHz, CDCl₃: 2-(Phenylsulfanyl)-1-[(2*S*,3*R*)-3-(tributylstannyl)-1-tritylaziridin-2-yl]methyl}-1*H*-benzimidazole (10)



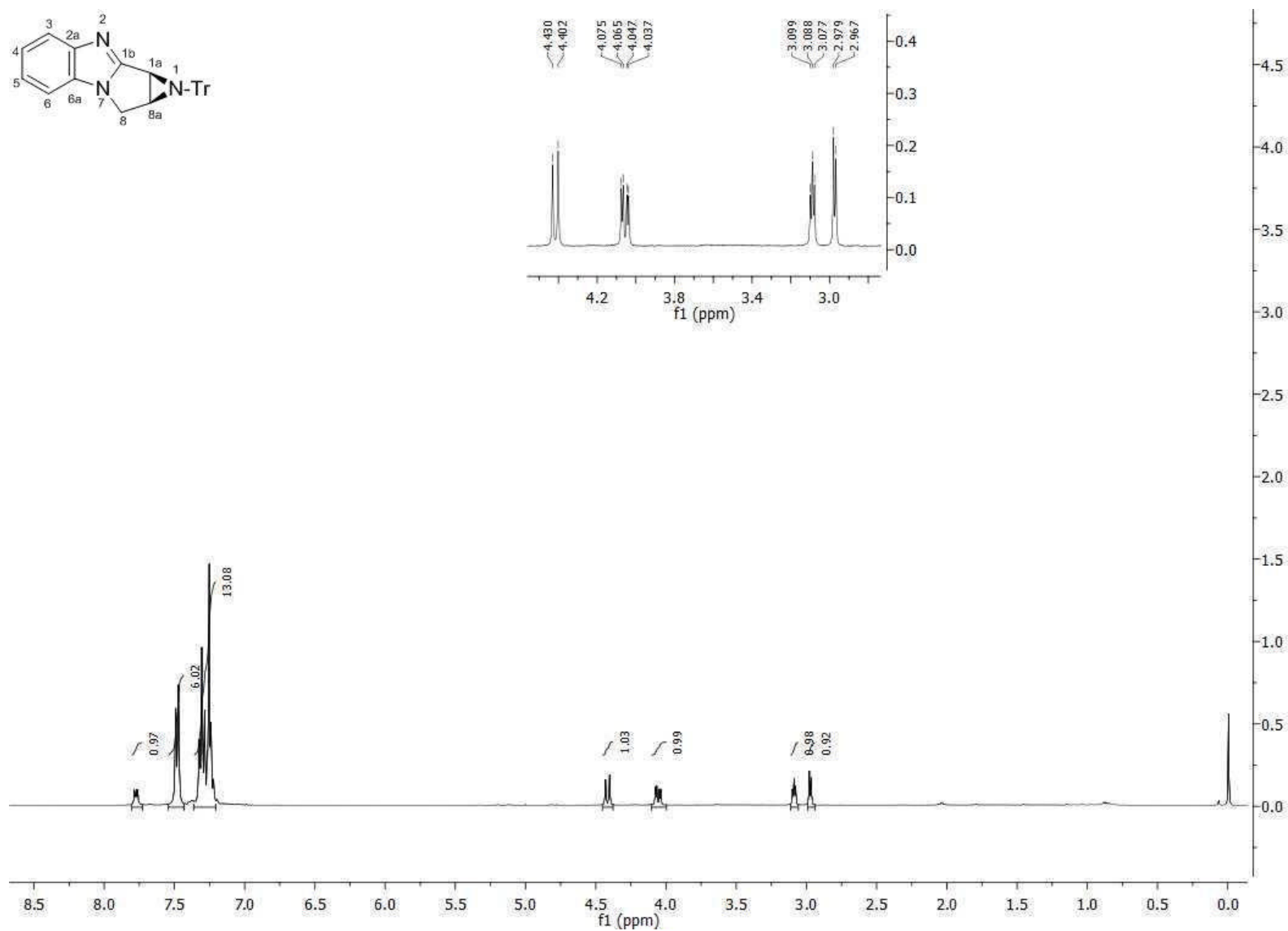
¹H NMR, 400MHz, CDCl₃: 2-(Phenylsulfanyl)-1-{[(2*R*)-1-tritylaziridin-2-yl]methyl}-1*H*-benzimidazole (8b)



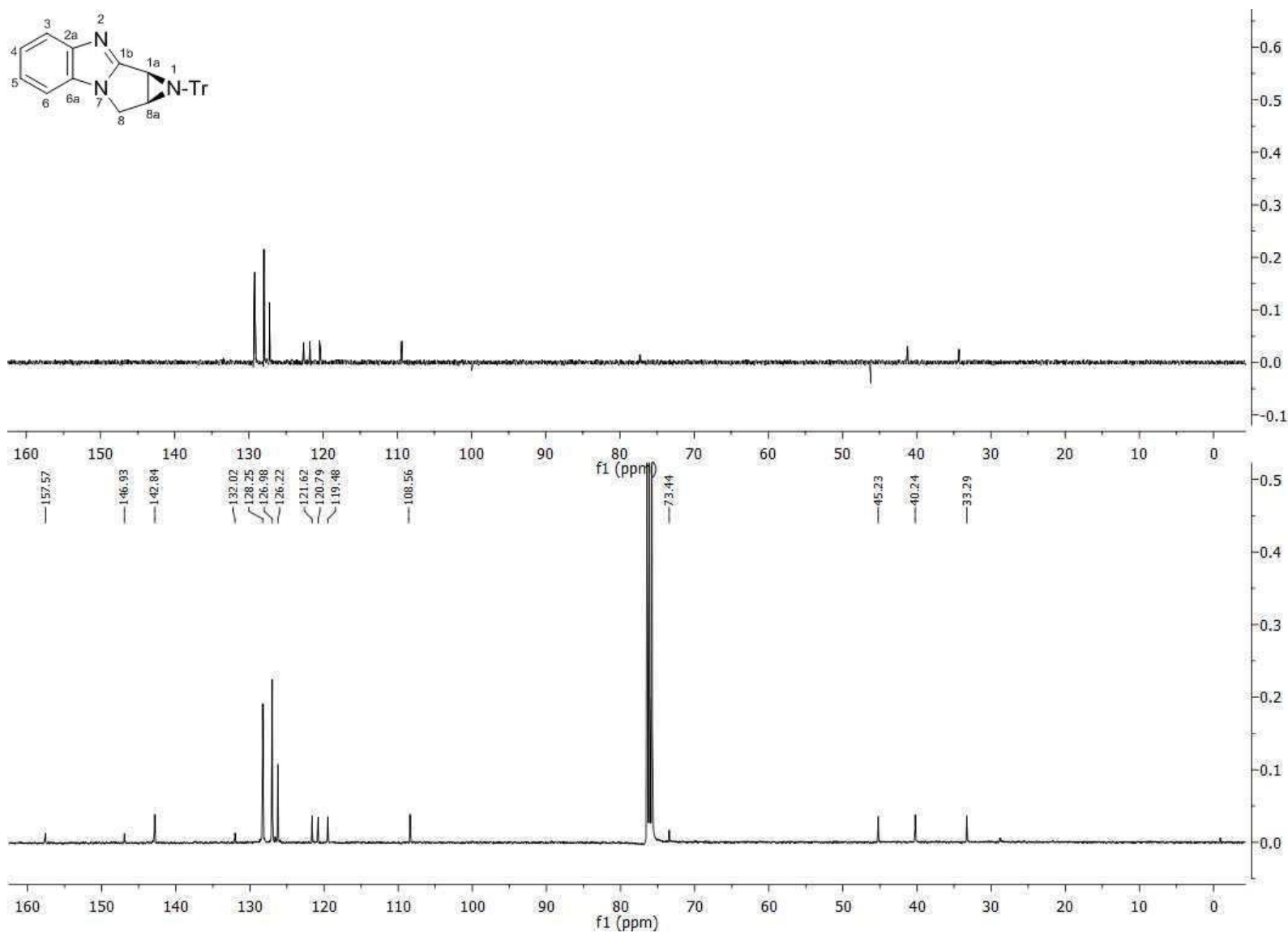
¹³C NMR AND DEPT, 100 MHz, CDCl₃: 2-(Phenylsulfanyl)-1-[(2*R*)-1-tritylaziridin-2-yl]methyl)-1*H*-benzimidazole (8b)



¹H NMR, 400MHz, CDCl₃: (1a*S*,8a*S*)-1-trityl-1,1a,8,8a-tetrahydroazireno[2',3':3,4]pyrrolo[1,2-*a*]benzimidazole (1)



¹³C NMR AND DEPT, 100 MHz, CDCl₃: (1a*S*,8a*S*)-1-trityl-1,1a,8,8a-tetrahydroazireno[2',3':3,4]pyrrolo[1,2-*a*]benzimidazole (1)

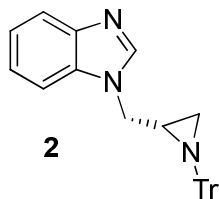


HPLC: Column: Hyperclone 5u ODS (C18) 120A, 250 x 4.6 mm

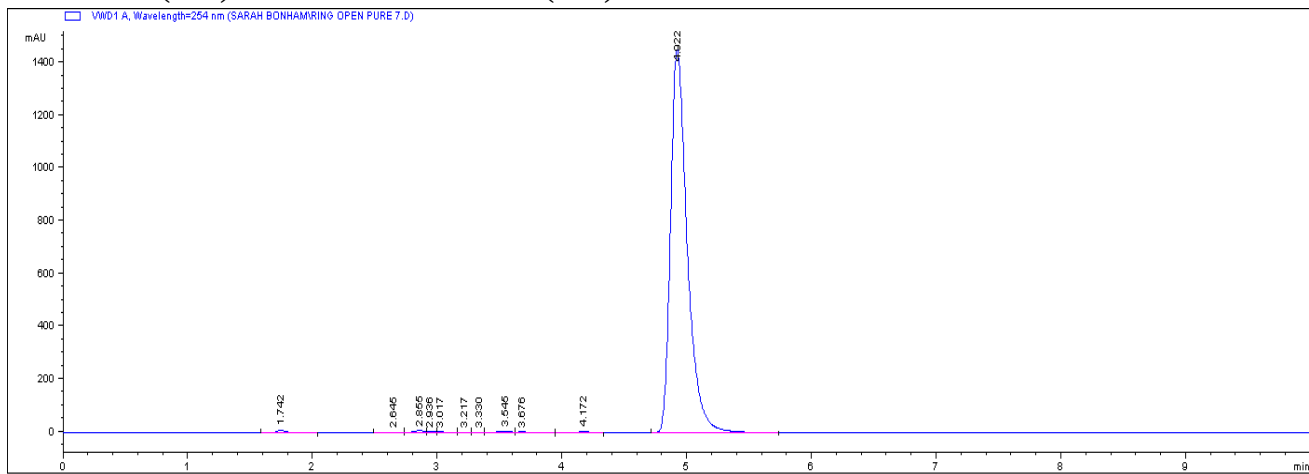
Eluent: 75:25 Methanol/water and 1% triethylamine

Flow rate: 1 mLmin⁻¹

UV: 254 nm



Peak	Ret Time (min)	Type	Width (min)	Area	Height	Area
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(mAu)	(%)					(mAu)
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1	1.742	VB	0.0840	57.78114	9.71114	0.4159
2	2.645	VV	0.1380	20.71963	2.25039	0.1491
3	2.855	VV	0.0864	55.50575	9.20216	0.3995
4	2.936	VV	0.0621	20.95259	4.84045	0.1508
5	3.017	VV	0.1023	25.83384	3.32420	0.1859
6	3.217	VV	0.0866	14.07858	2.32790	0.1013
7	3.330	VV	0.0853	11.97441	2.01627	0.0862
8	3.545	VV	0.1126	55.50553	7.02441	0.3995
9	3.676	VV	0.1435	38.94022	3.60615	0.2803
10	4.172	VV	0.1103	41.86848	5.43302	0.3013
11	4.922	VV	0.1394	1.35513 ⁴	1453.20178	97.5302

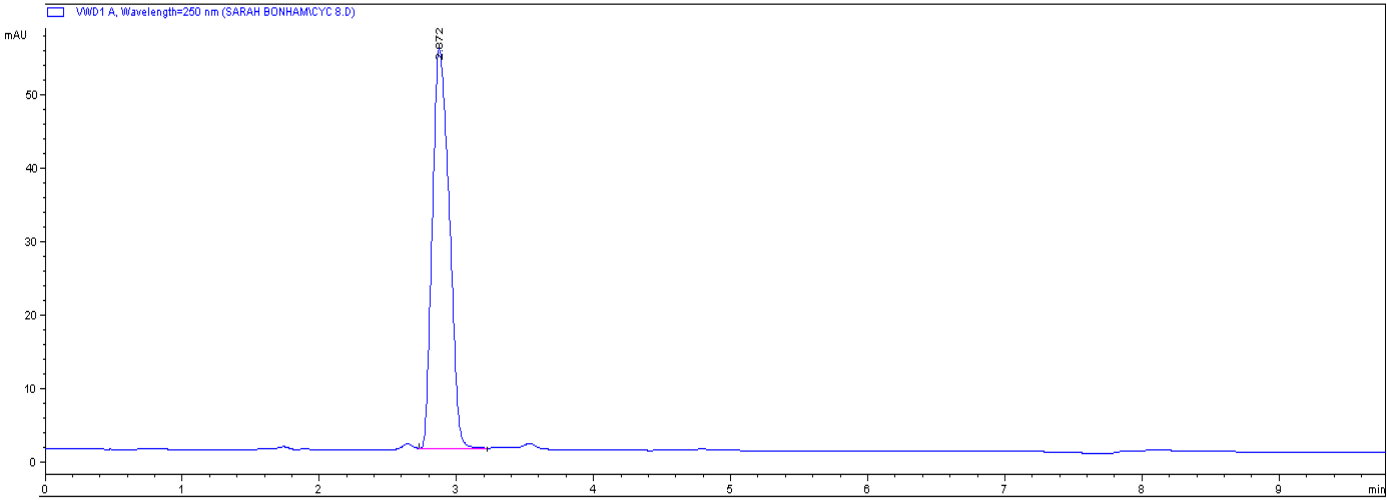
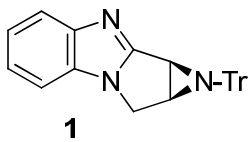
Totals	1.38944 ⁴	1502.93787
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Column: Hyperclone 5u ODS (C18) 120A, 250 x 4.6 mm

Eluent: 90:10 Methanol/water and 1% triethylamine

Flow rate: 1 mLmin⁻¹

UV: 250 nm



Peak	Ret Time (min)	Type	Width (min)	Area (mAu)	Height (mAu)	Area (%)
1	2.872	VB	0.1422	4.68.98206	54.74240	100.0000
Totals				4.68.98206	54.74240	