

Supporting Information

## Enantioselective Synthesis of $\alpha$ -Halo- $\alpha$ -alkylmalonates via Phase-Transfer Catalytic $\alpha$ -Alkylation

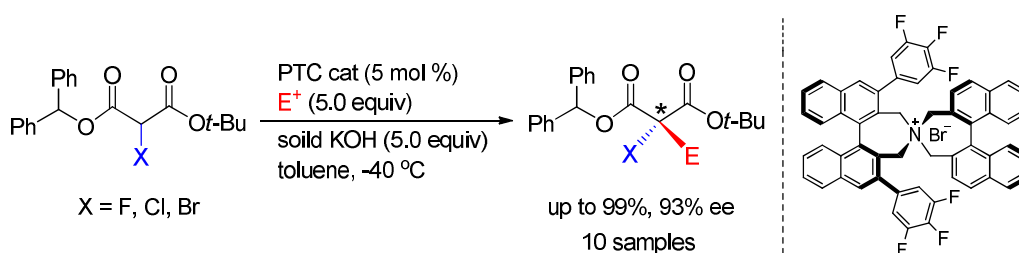
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<sup>[c]</sup> *College of Pharmacy, Gachon University, Incheon 406-799, Korea*

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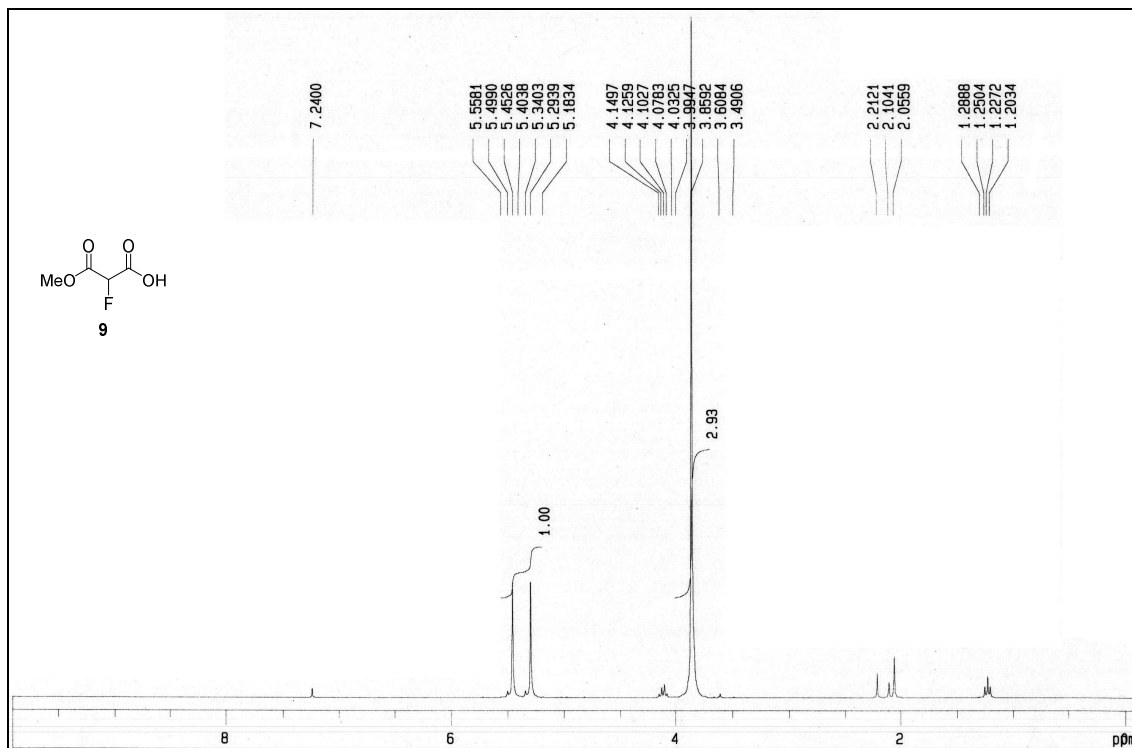


### Contents

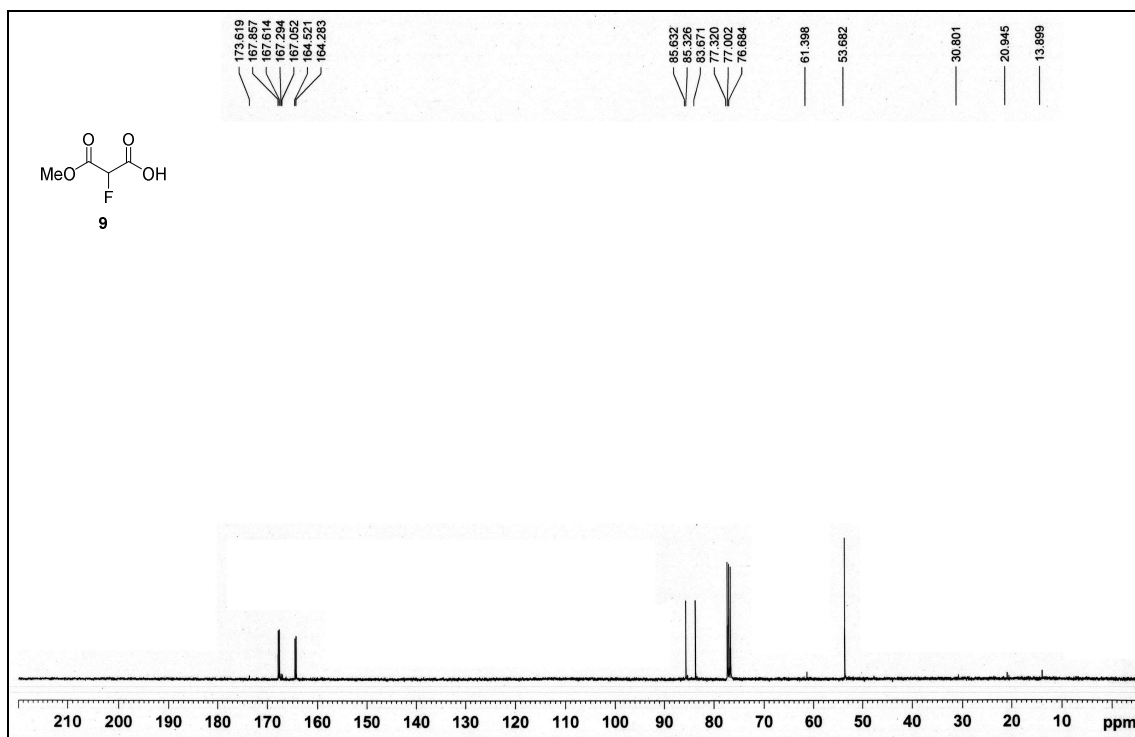
$^1\text{H}$ & $^{13}\text{C}$ NMR Spectra	S-02
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# $^1\text{H}$ & $^{13}\text{C}$ NMR Spectra

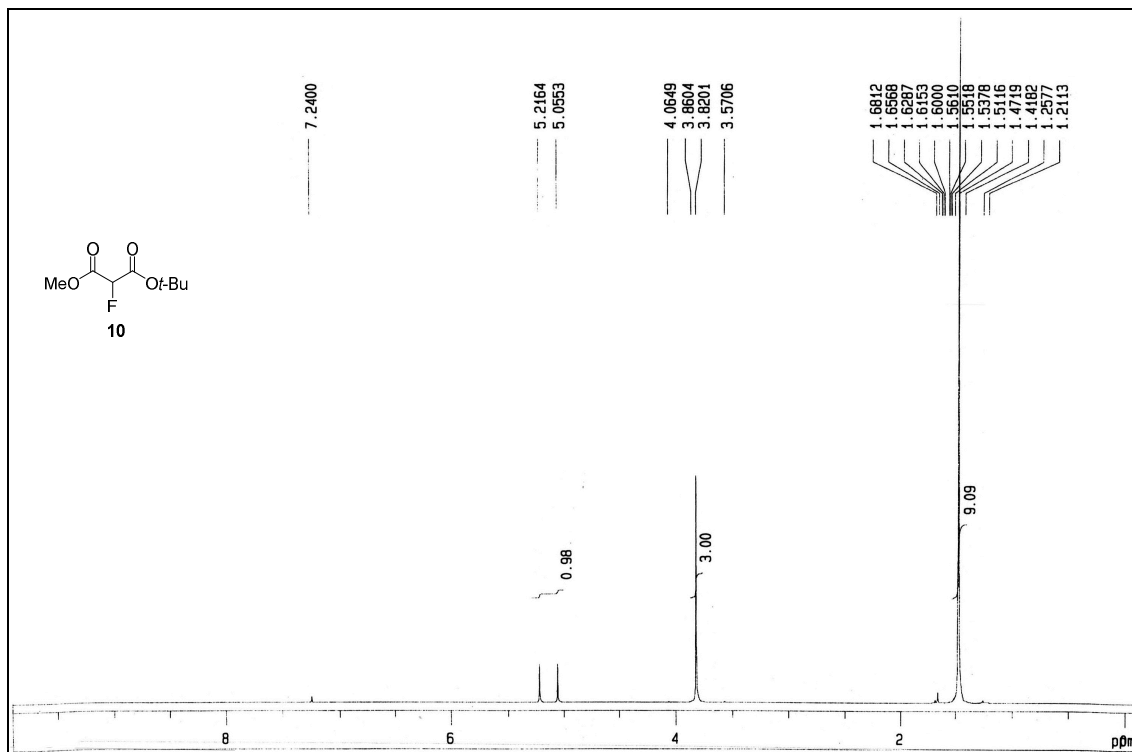
$^1\text{H}$ -NMR of compound **9** (300 MHz)



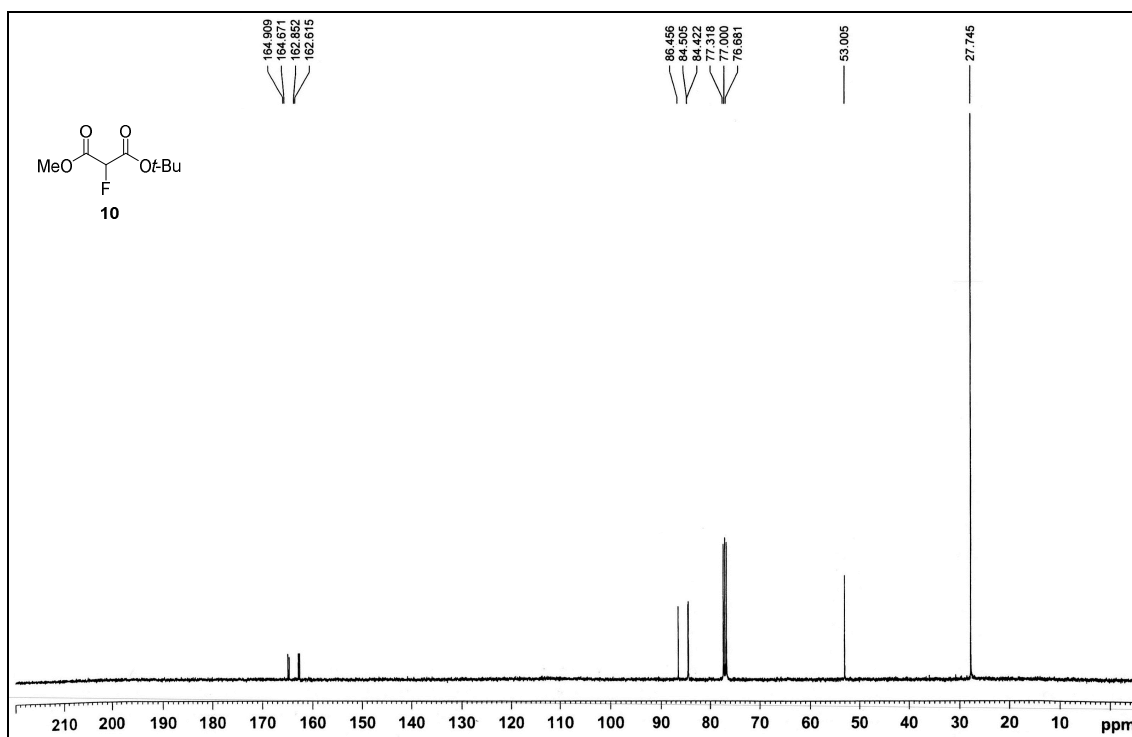
$^{13}\text{C}$ -NMR of compound **9** (100 MHz)



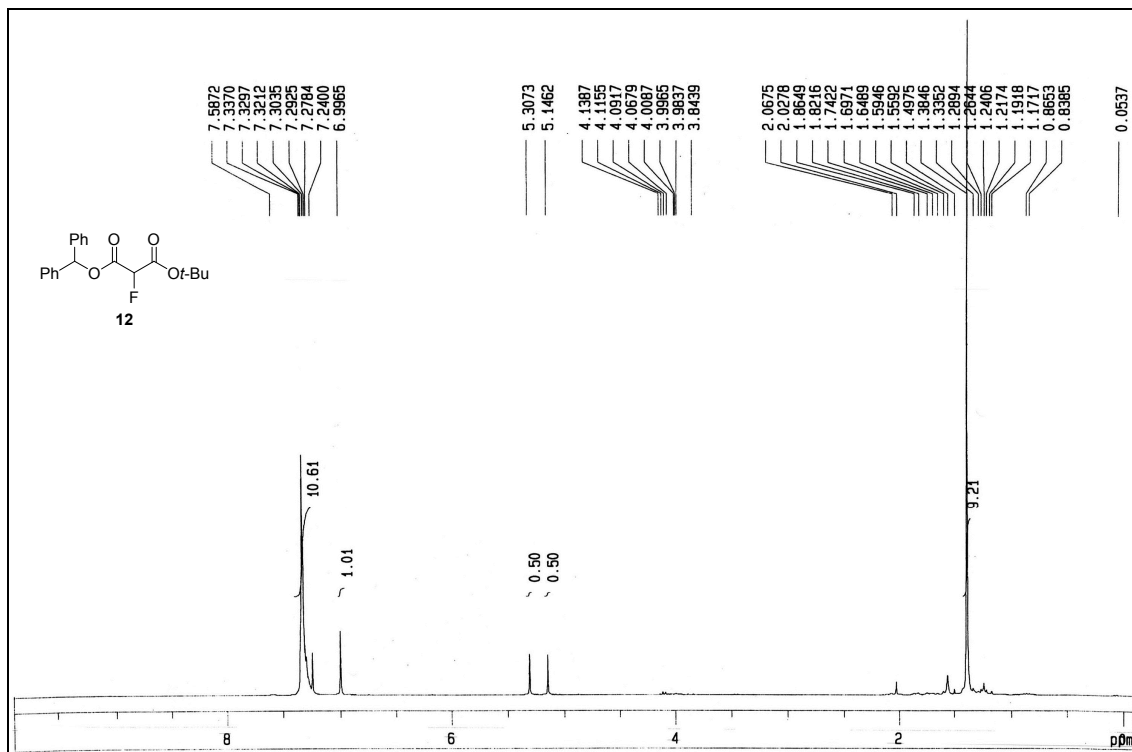
$^1\text{H}$ -NMR of compound **10** (300 MHz)



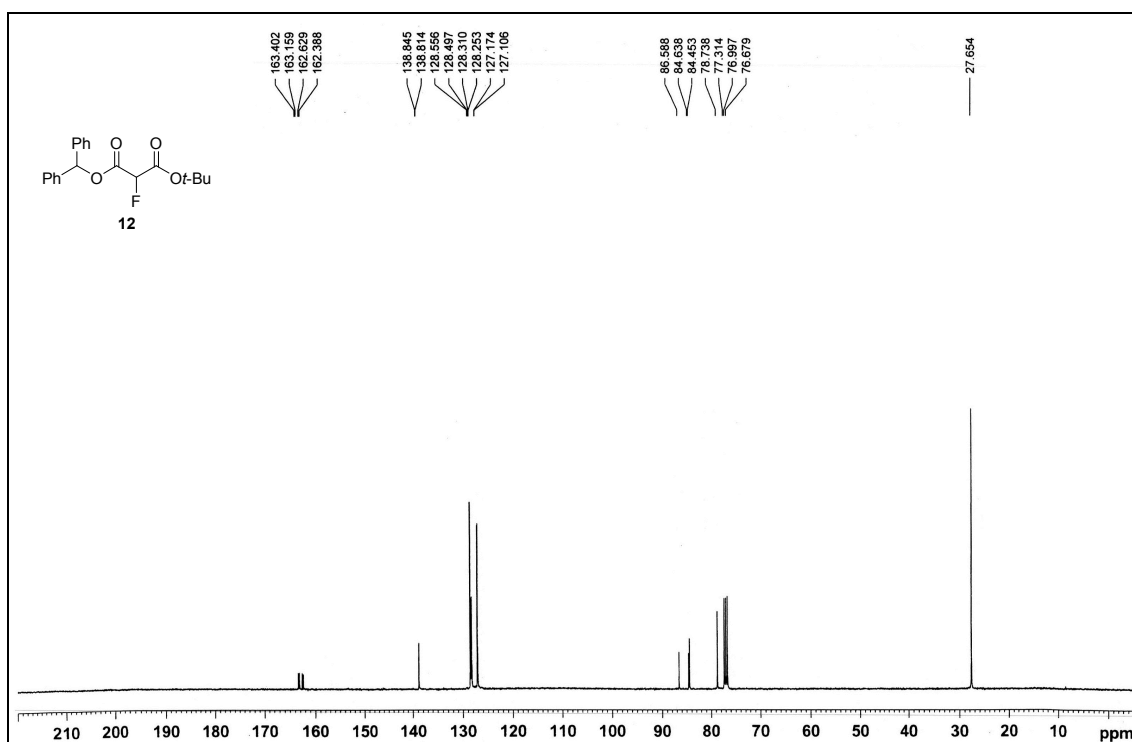
$^{13}\text{C}$ -NMR of compound **10** (100 MHz)



$^1\text{H}$ -NMR of compound **12** (300 MHz)

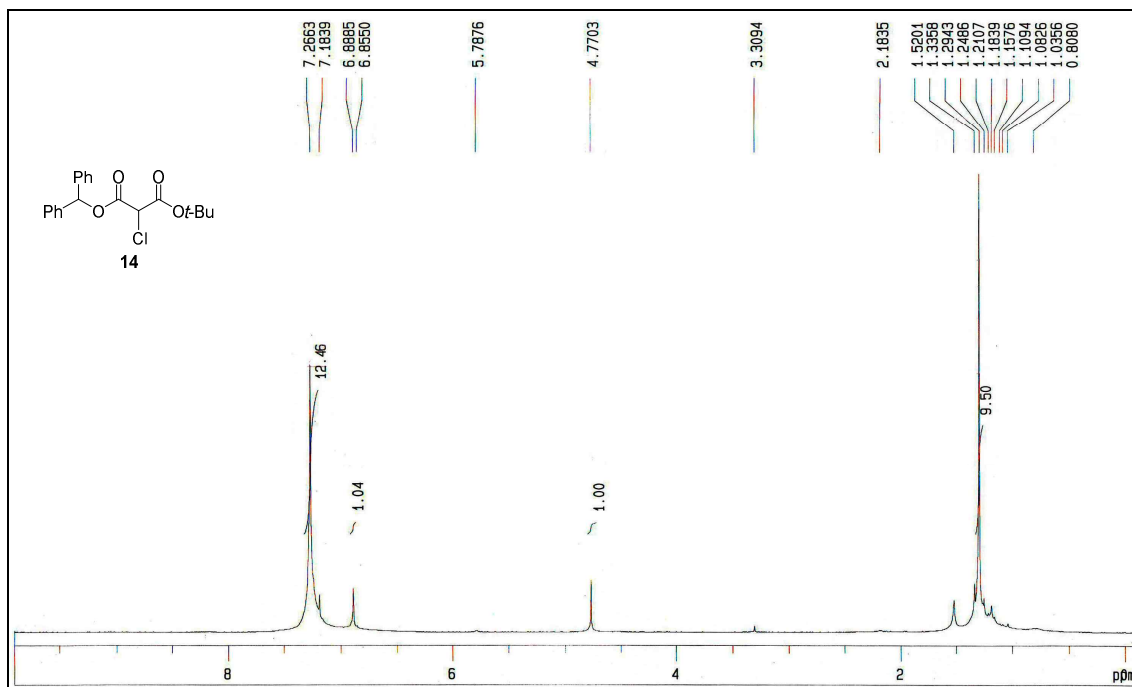


$^{13}\text{C}$ -NMR of compound **12** (100 MHz)

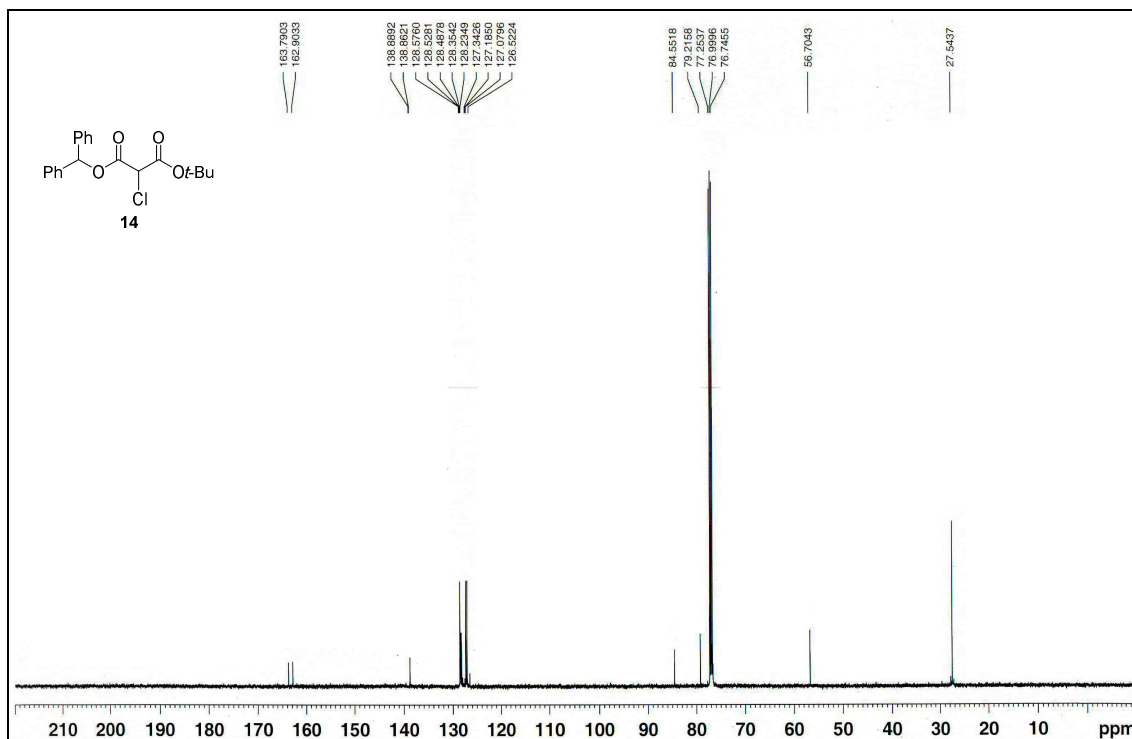




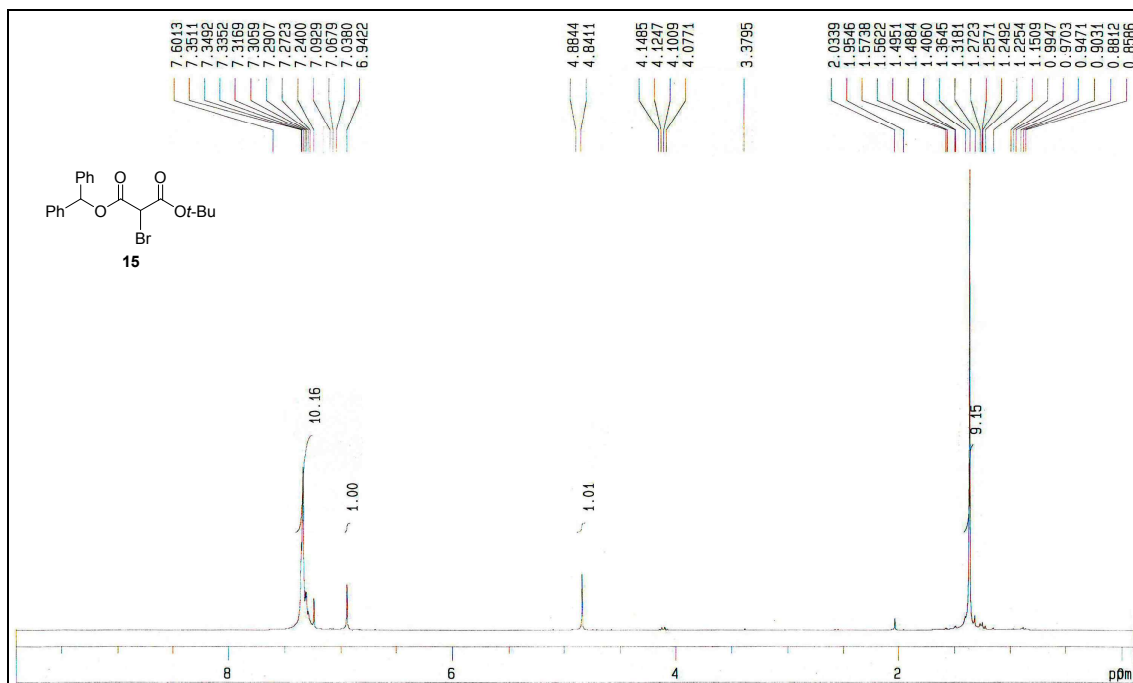
<sup>1</sup>H-NMR of compound **14** (300 MHz)



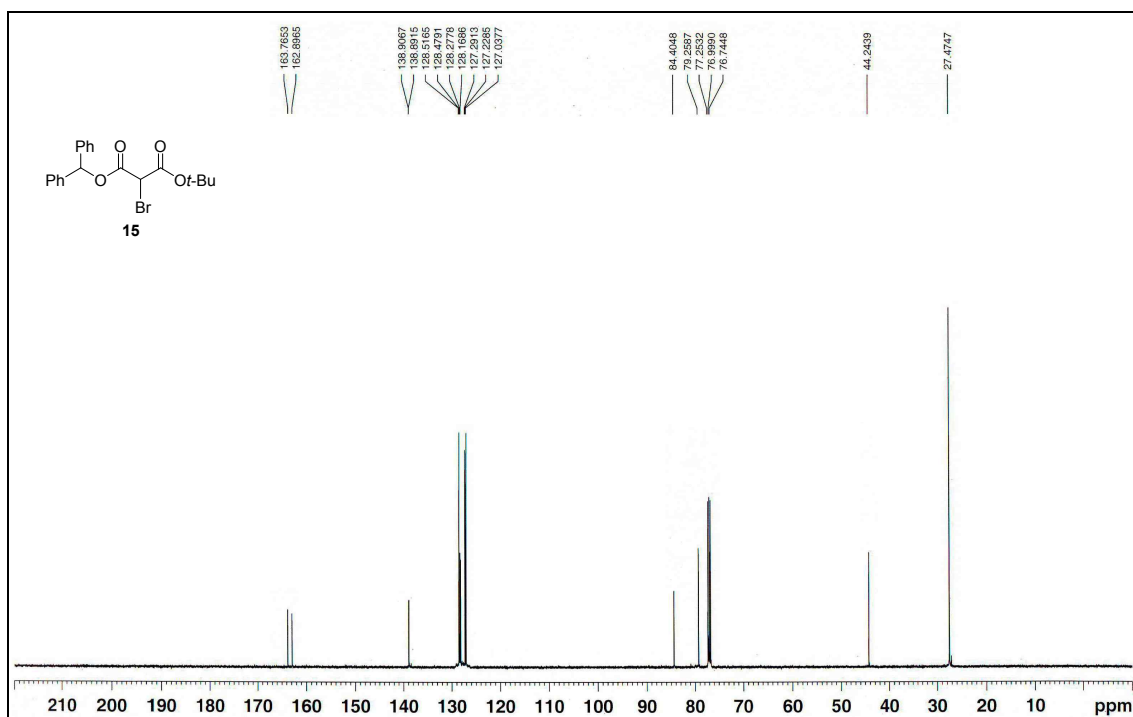
<sup>13</sup>C-NMR of compound **14** (125 MHz)



<sup>1</sup>H-NMR of compound **15** (300 MHz)



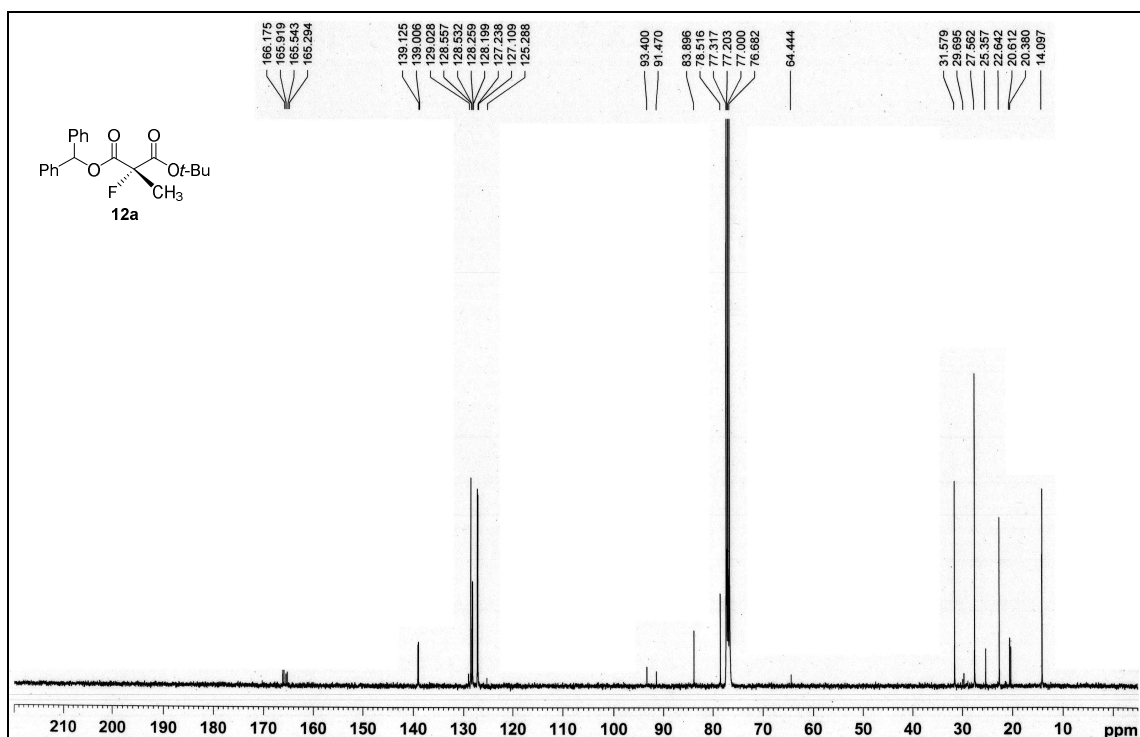
<sup>13</sup>C-NMR of compound **15** (125 MHz)



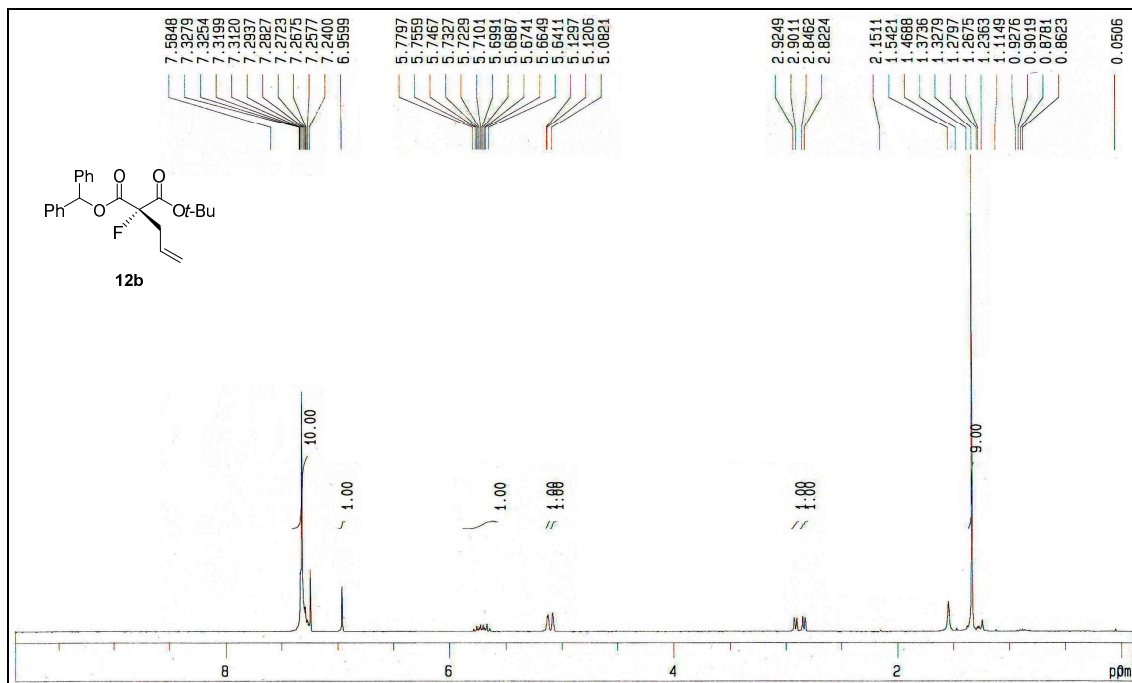
<sup>1</sup>H-NMR of compound **12a** (300 MHz)



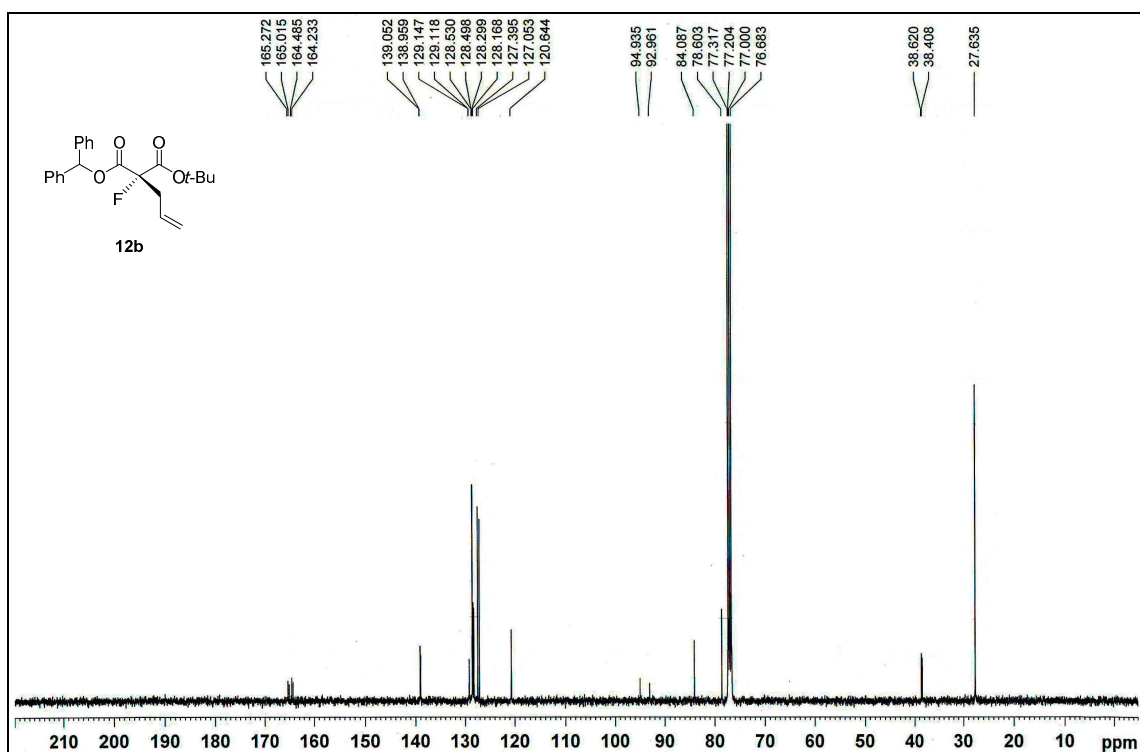
<sup>13</sup>C-NMR of compound **12a** (100 MHz)



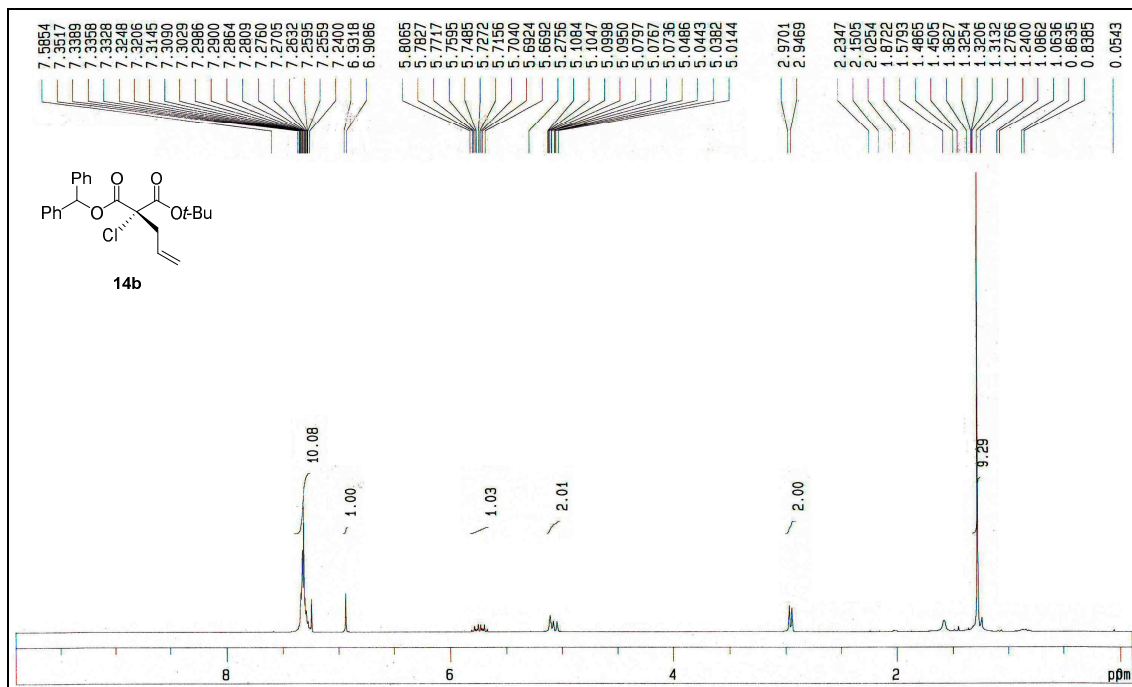
<sup>1</sup>H-NMR of compound **12b** (300 MHz)



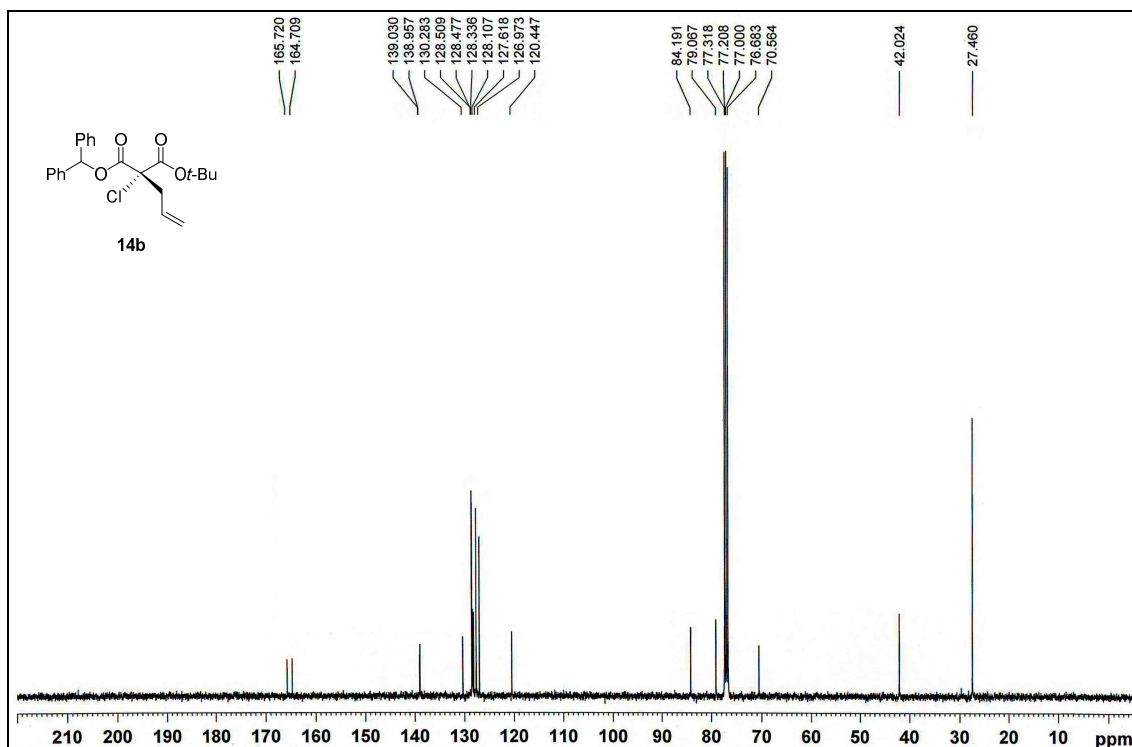
<sup>13</sup>C-NMR of compound **12b** (100 MHz)



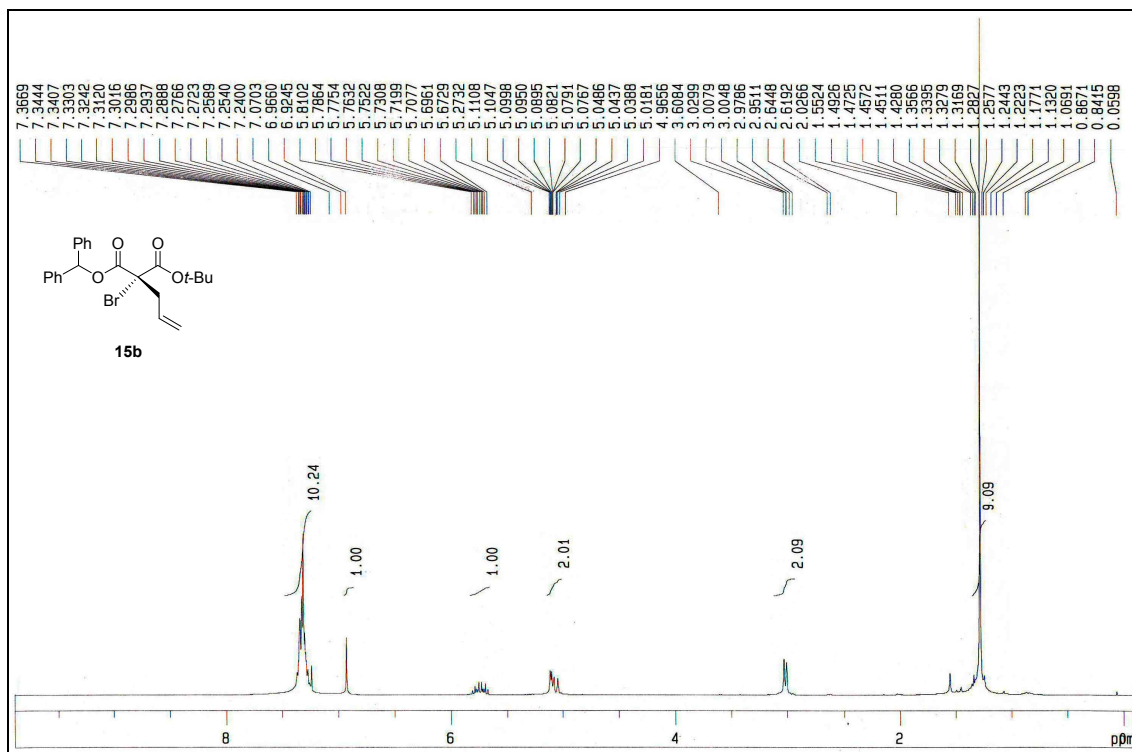
<sup>1</sup>H-NMR of compound **14b** (300 MHz)



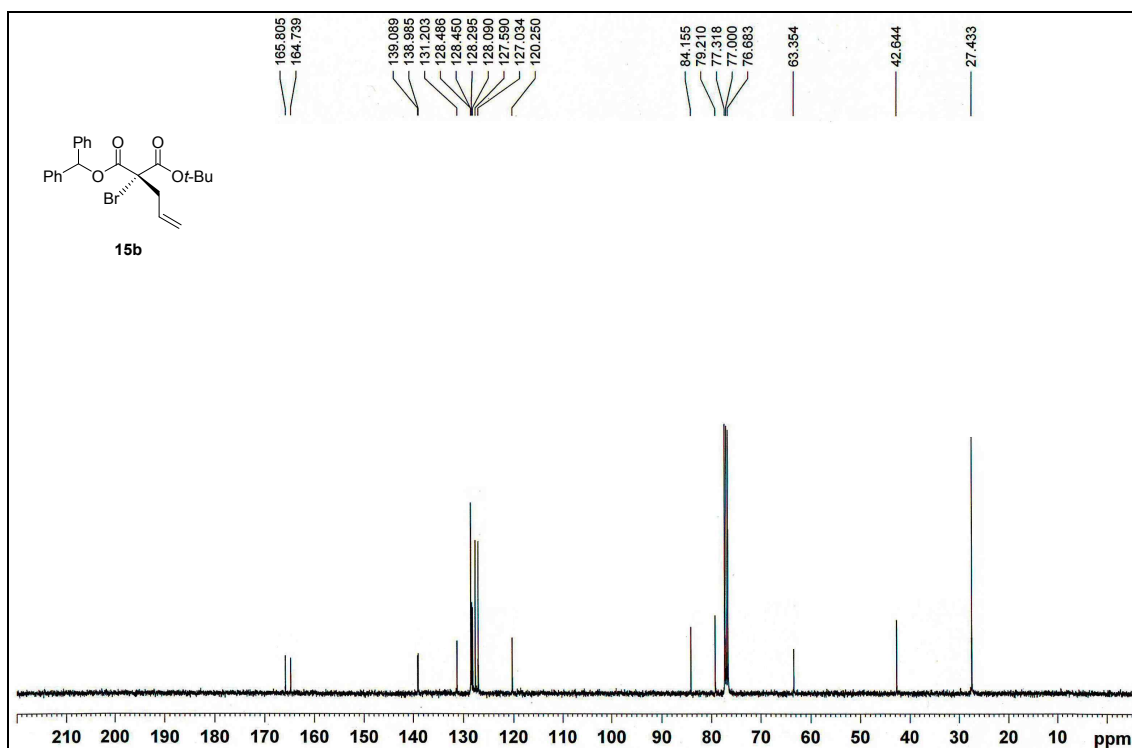
<sup>13</sup>C-NMR of compound **14b** (100 MHz)



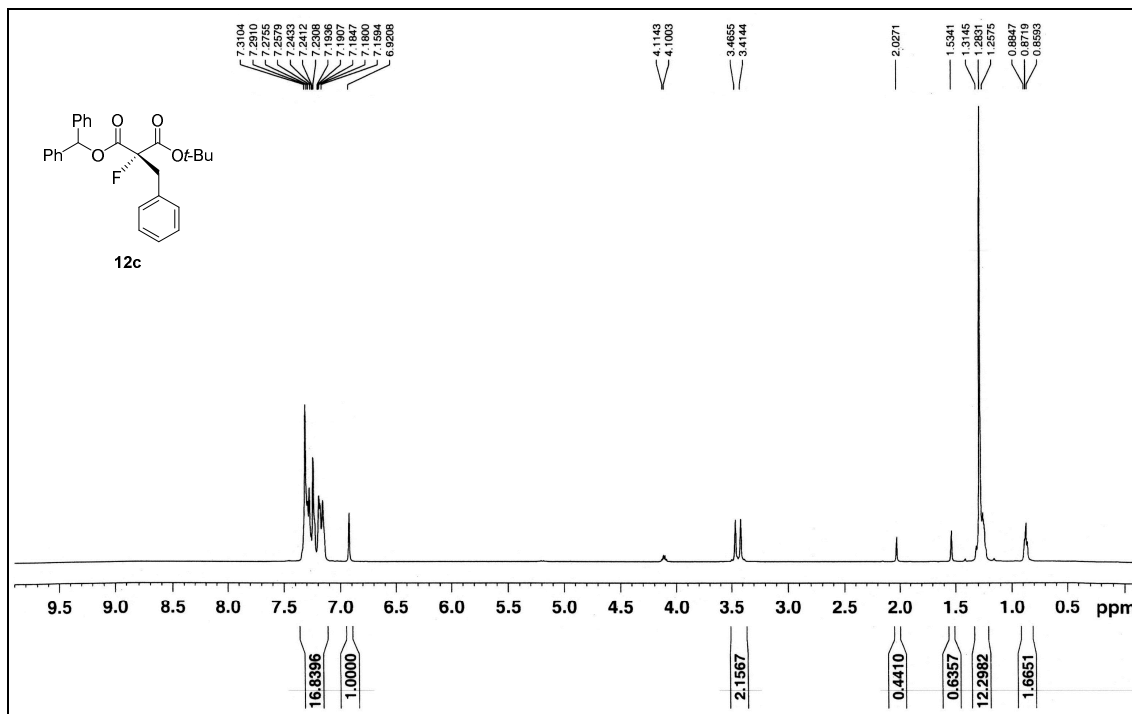
$^1\text{H}$ -NMR of compound **15b** (300 MHz)



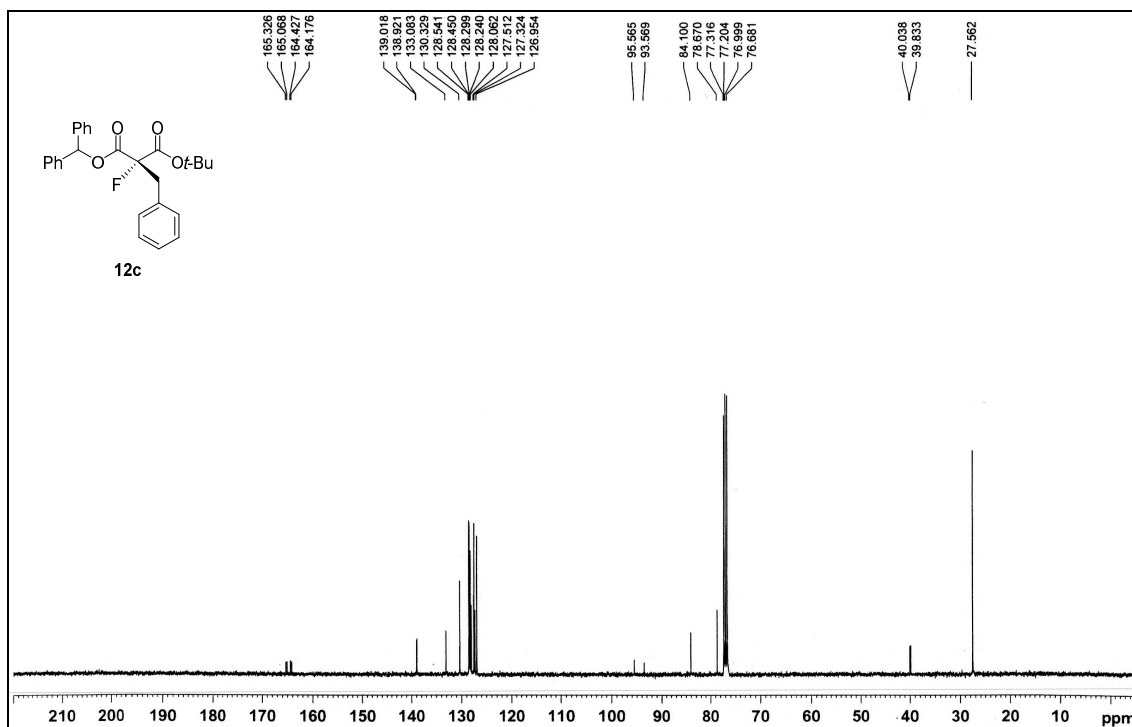
$^{13}\text{C}$ -NMR of compound **15b** (100 MHz)



$^1\text{H}$ -NMR of compound **12c** (400 MHz)

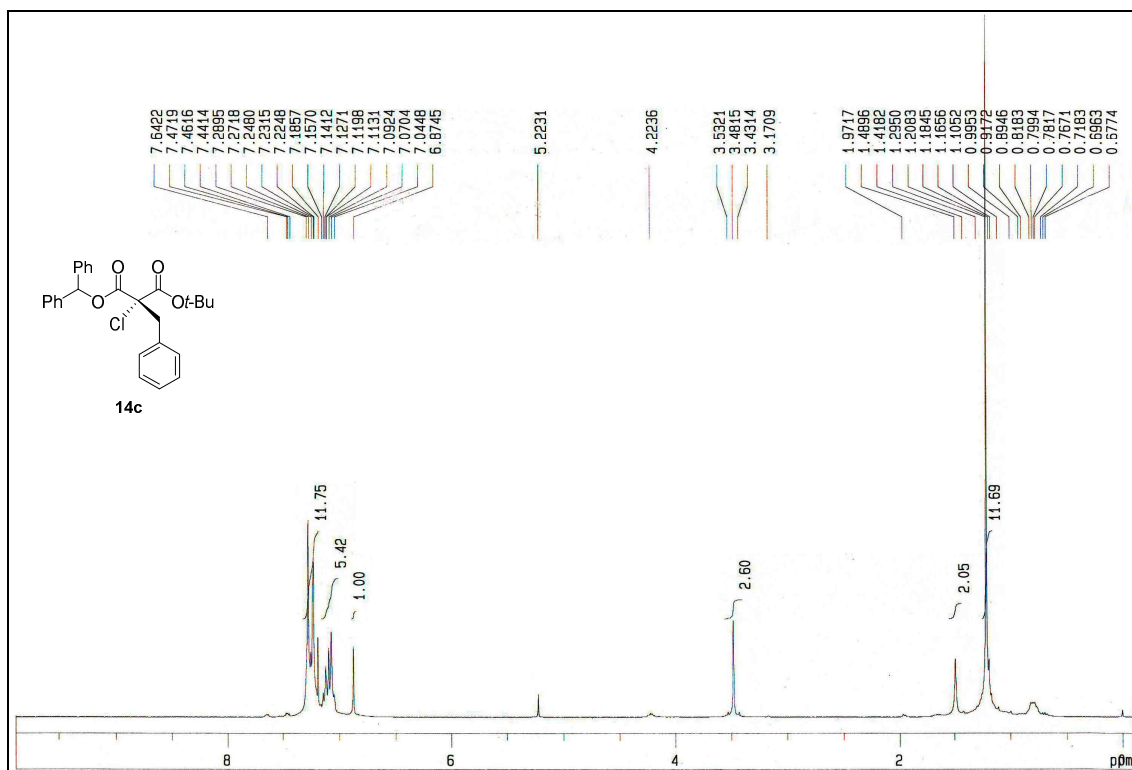


$^{13}\text{C}$ -NMR of compound **12c** (100 MHz)

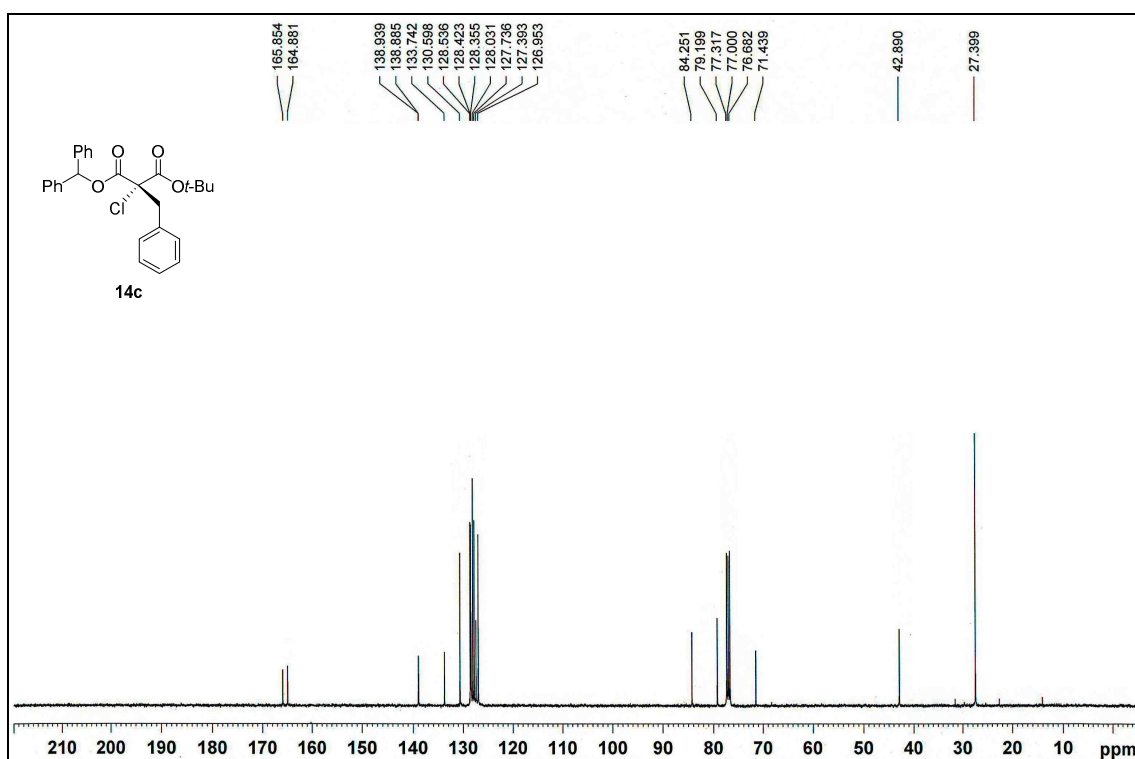




$^1\text{H}$ -NMR of compound **14c** (300 MHz)

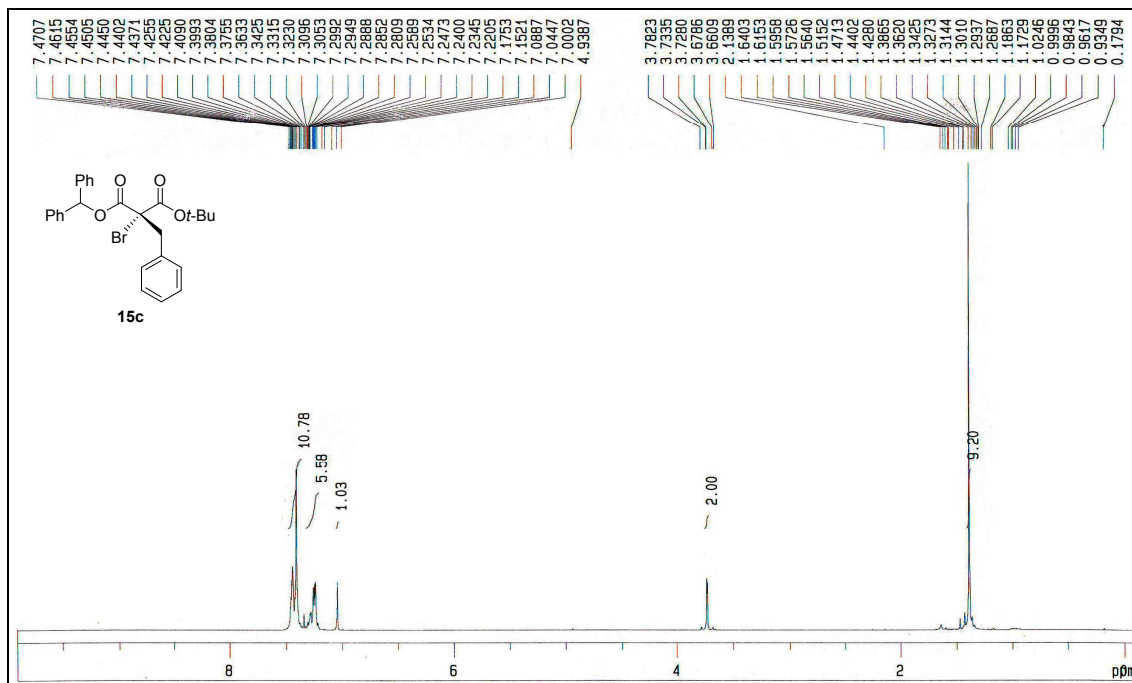


$^{13}\text{C}$ -NMR of compound **14c** (100 MHz)

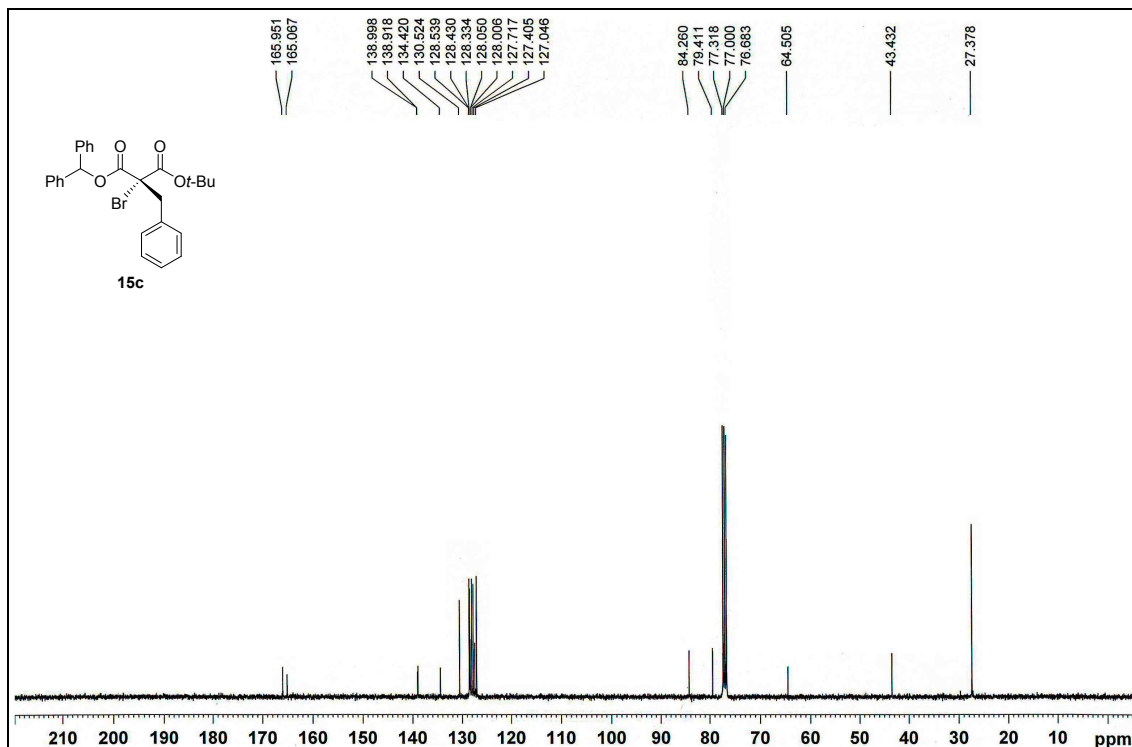




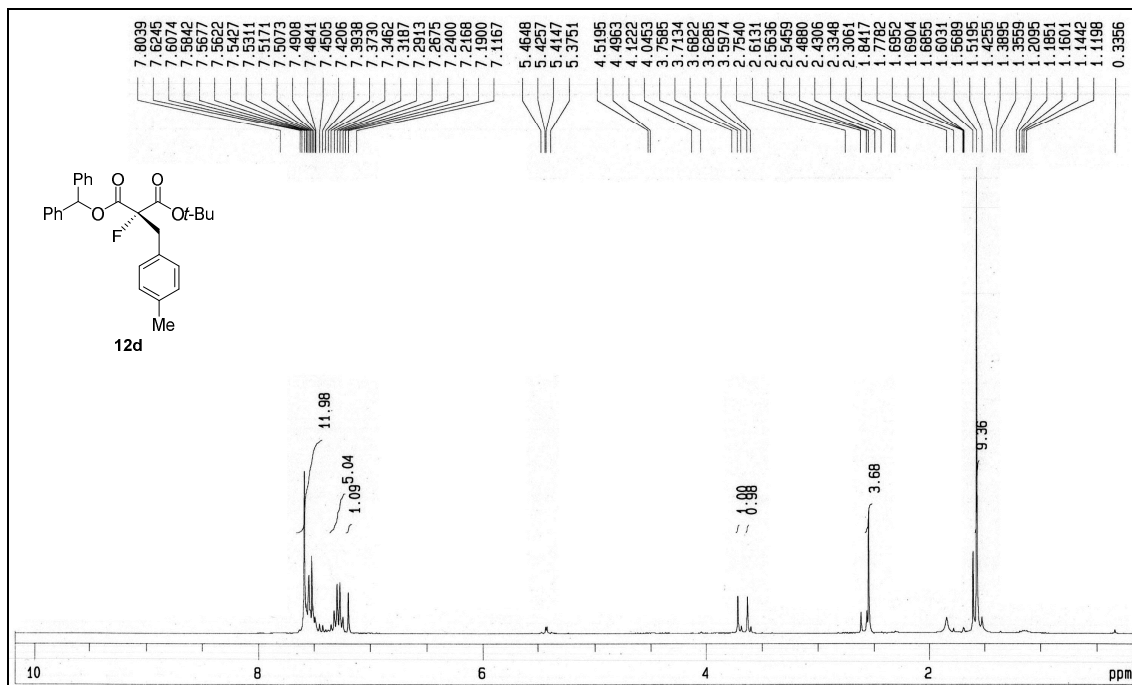
<sup>1</sup>H-NMR of compound **15c** (300 MHz)



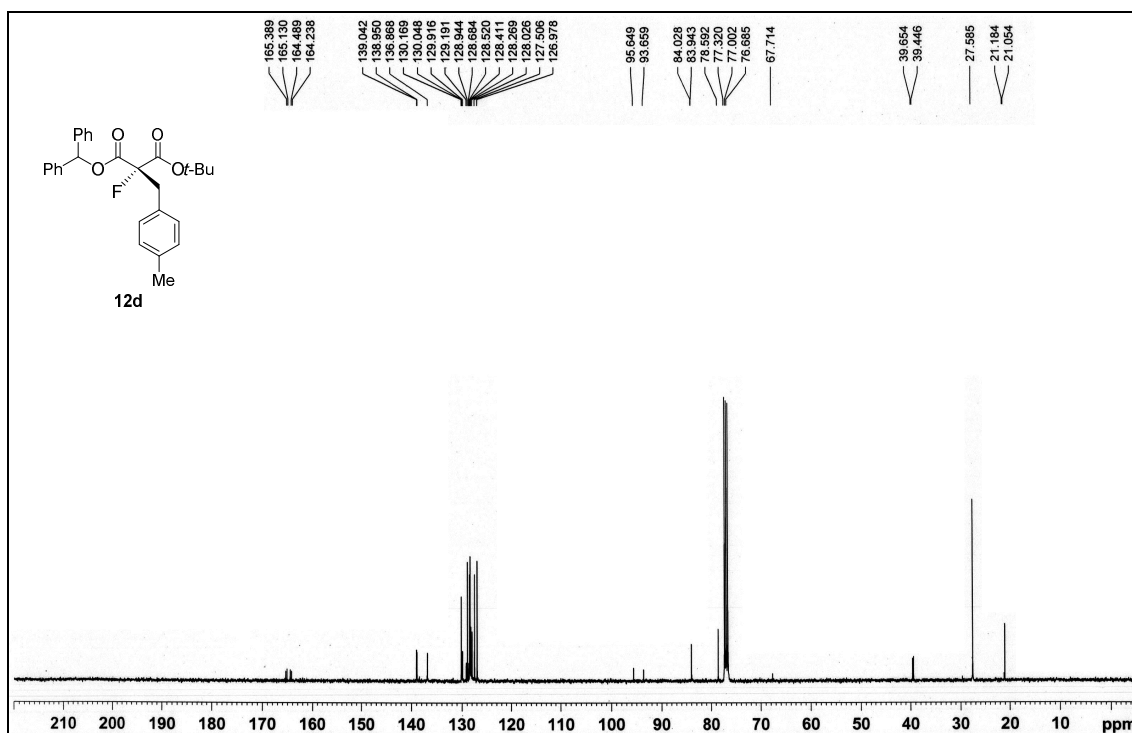
<sup>13</sup>C-NMR of compound **15c** (100 MHz)



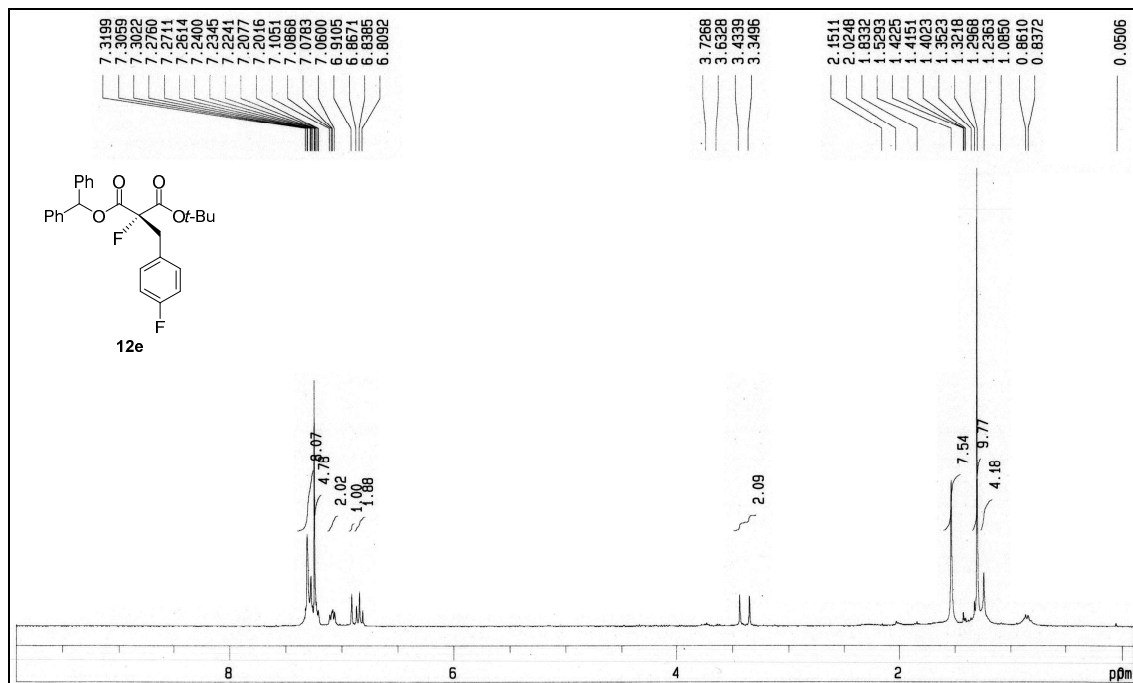
<sup>1</sup>H-NMR of compound **12d** (300 MHz)



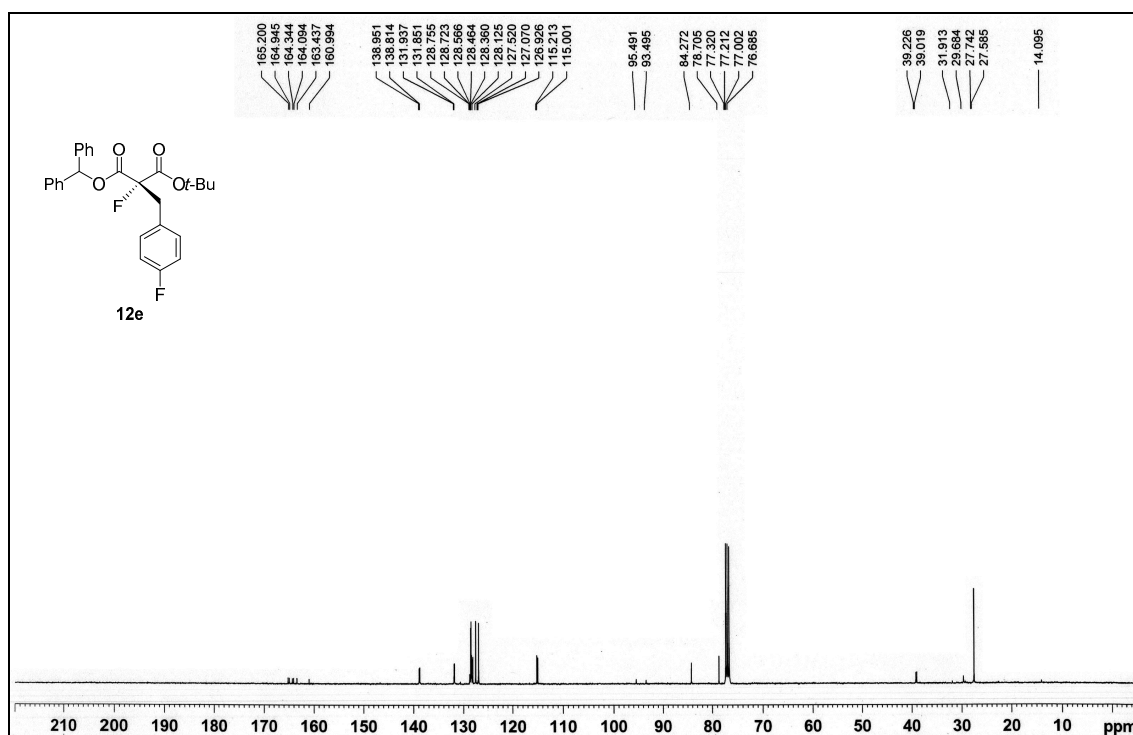
<sup>13</sup>C-NMR of compound **12d** (100 MHz)



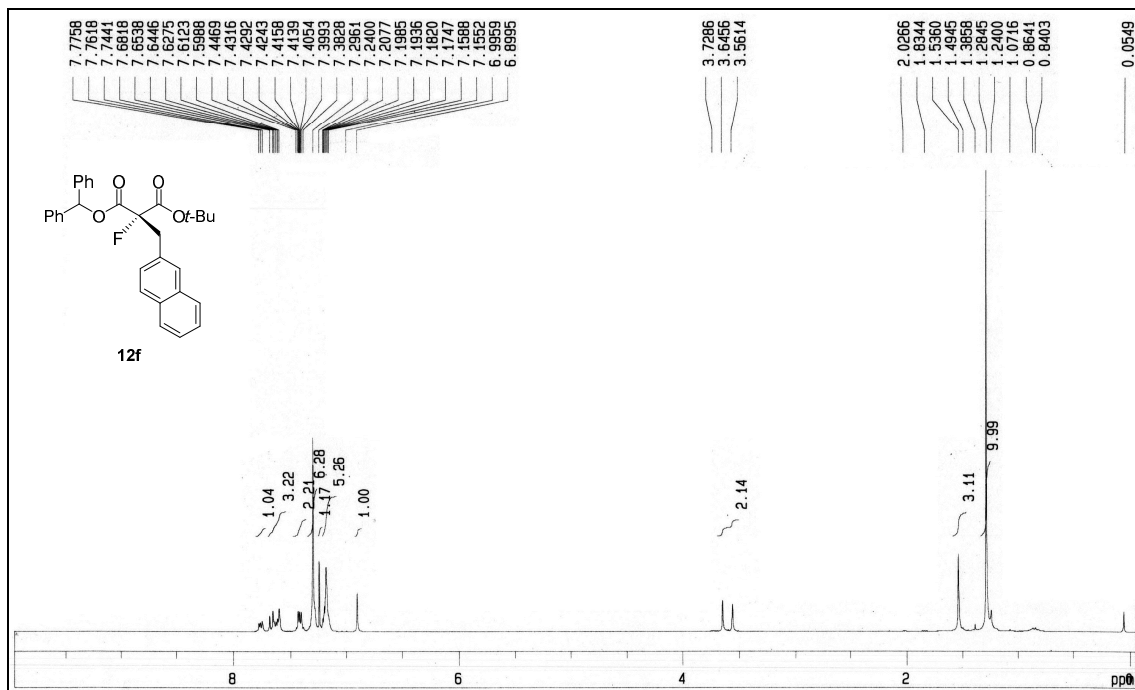
<sup>1</sup>H-NMR of compound **12e** (300 MHz)



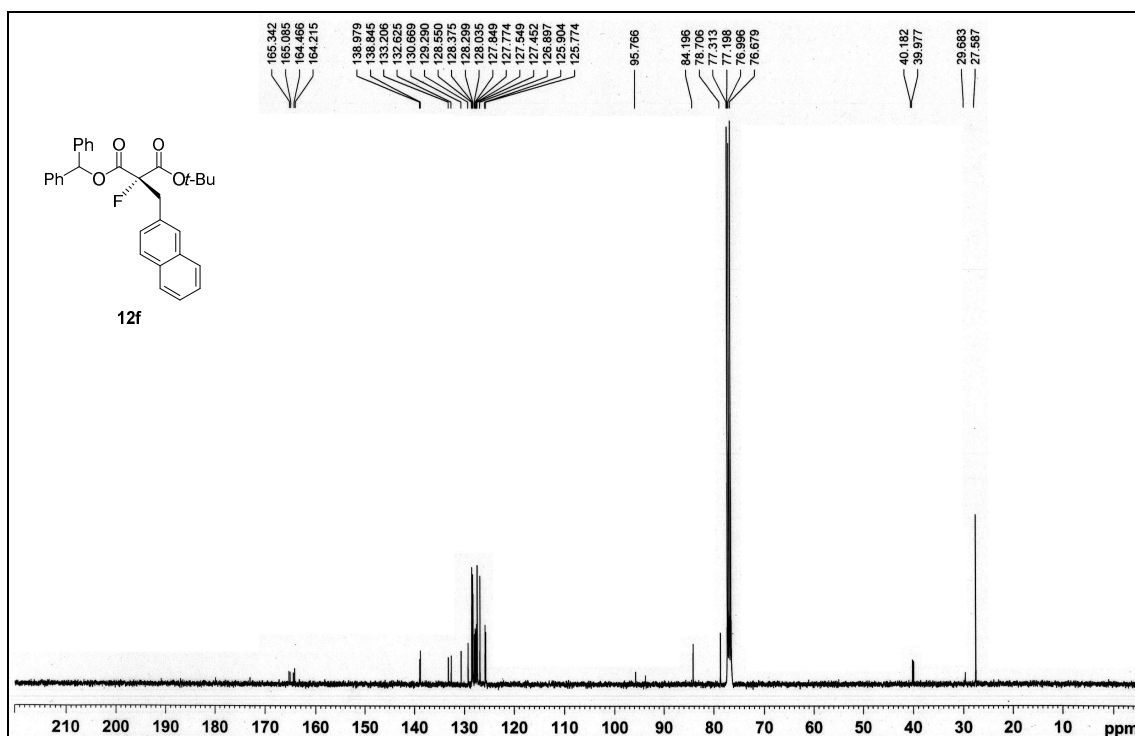
<sup>13</sup>C-NMR of compound **12e** (100 MHz)



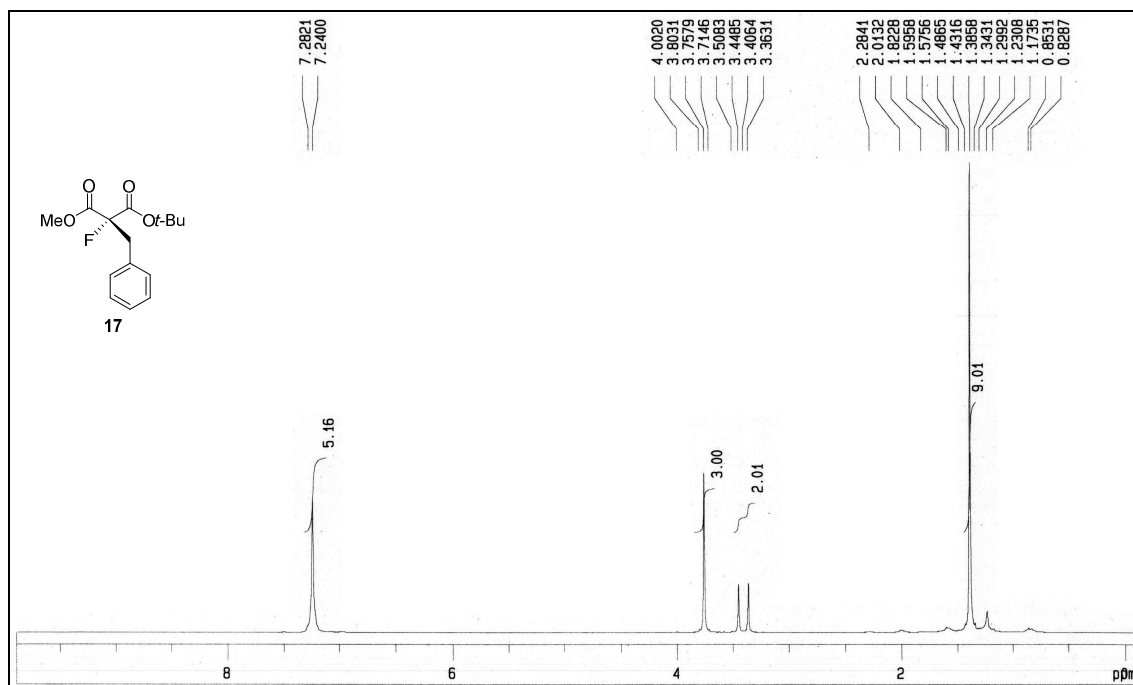
$^1\text{H}$ -NMR of compound **12f** (300 MHz)



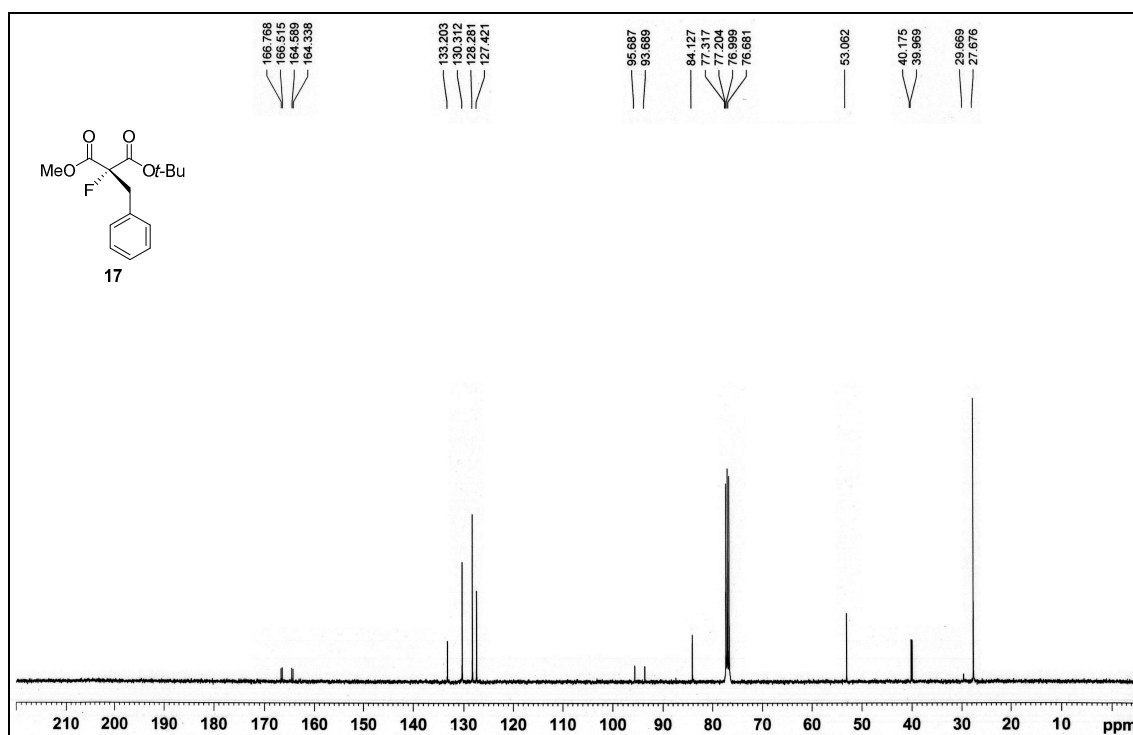
$^{13}\text{C}$ -NMR of compound **12f** (100 MHz)



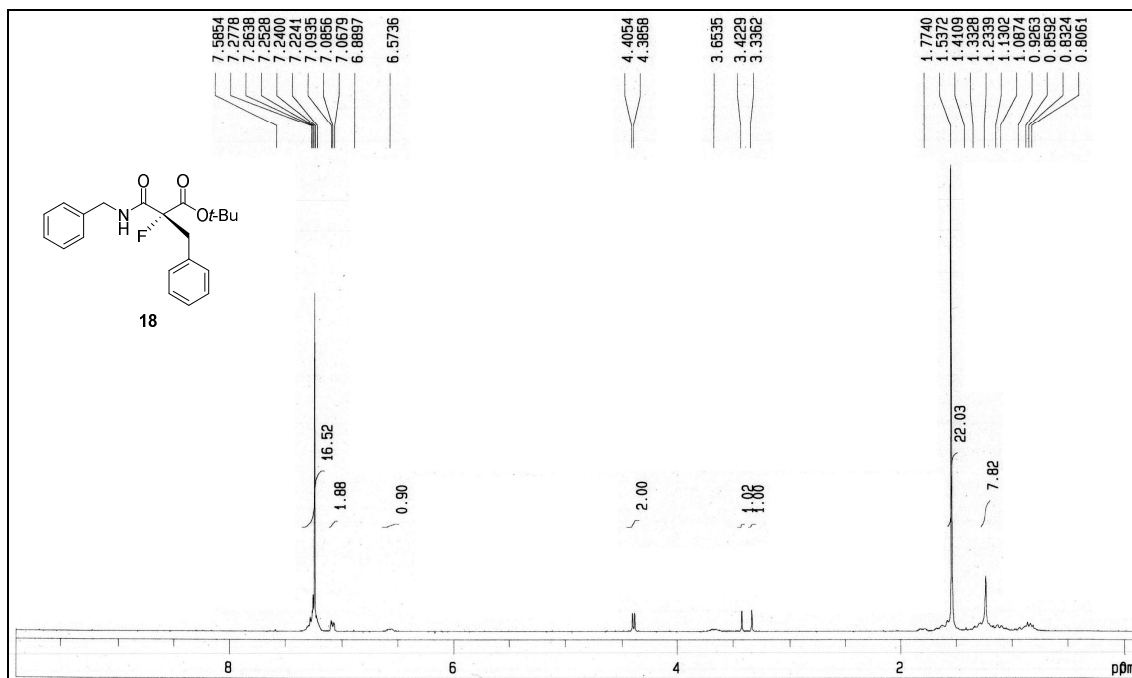
$^1\text{H}$ -NMR of compound **17** (300 MHz)



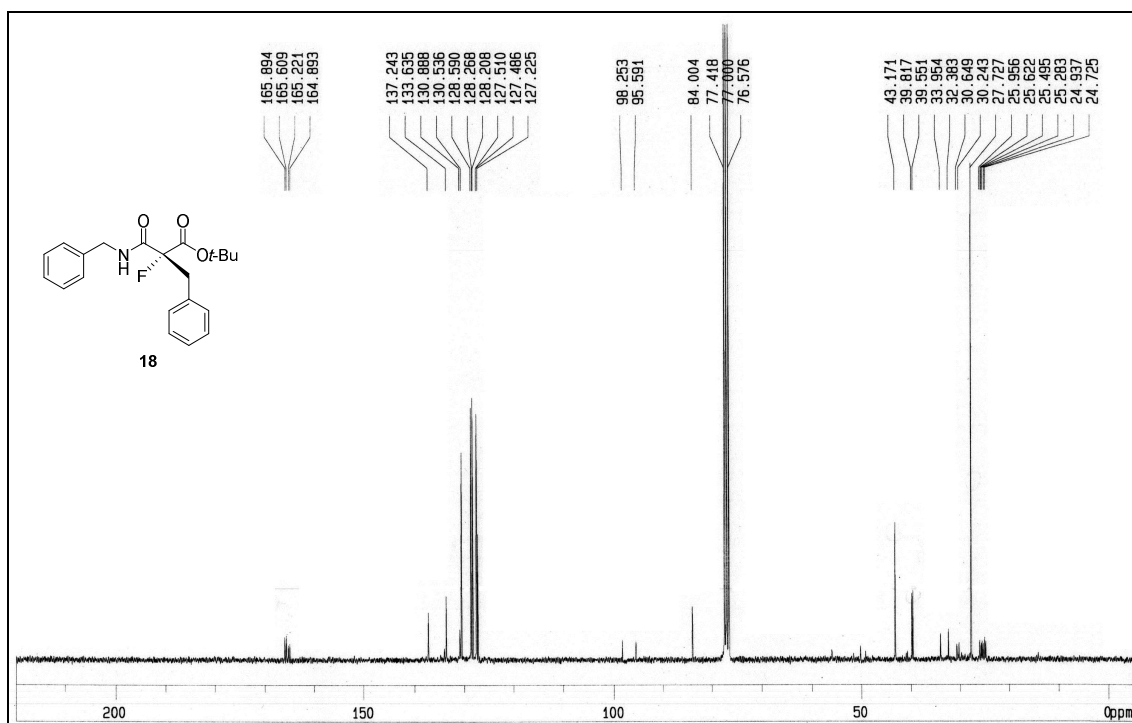
$^{13}\text{C}$ -NMR of compound **17** (100 MHz)



<sup>1</sup>H-NMR of compound **18** (300 MHz)

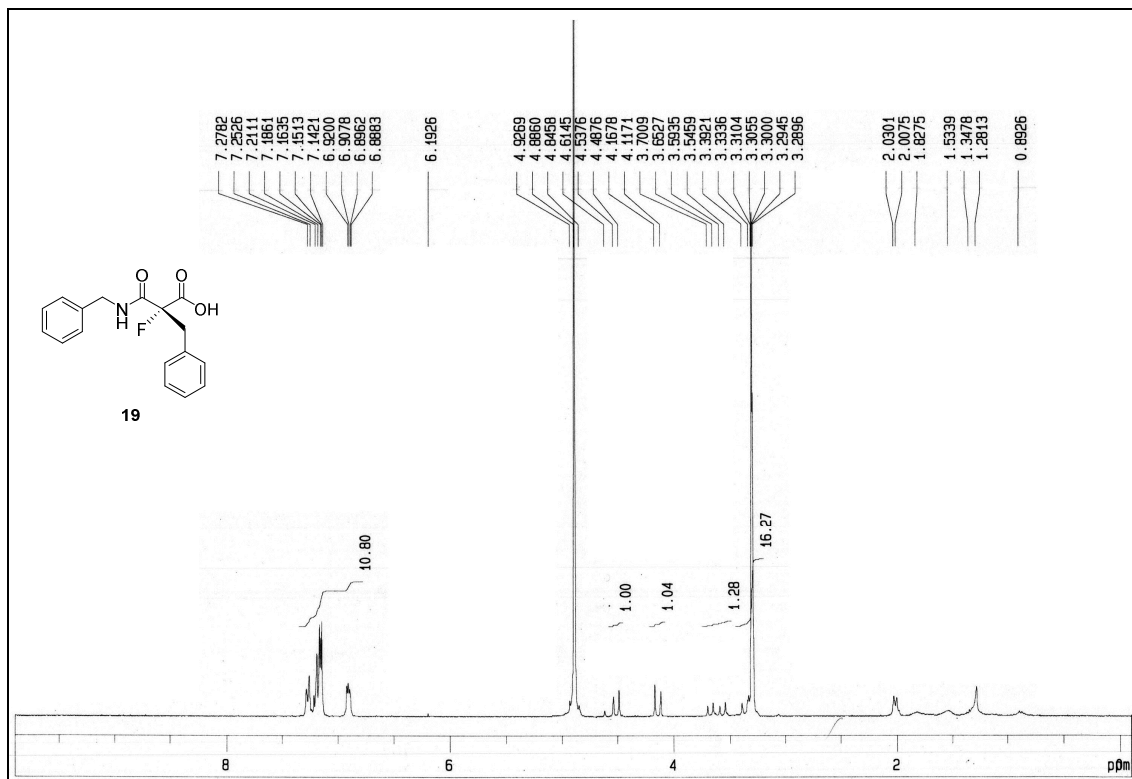


<sup>13</sup>C-NMR of compound **18** (75 MHz)

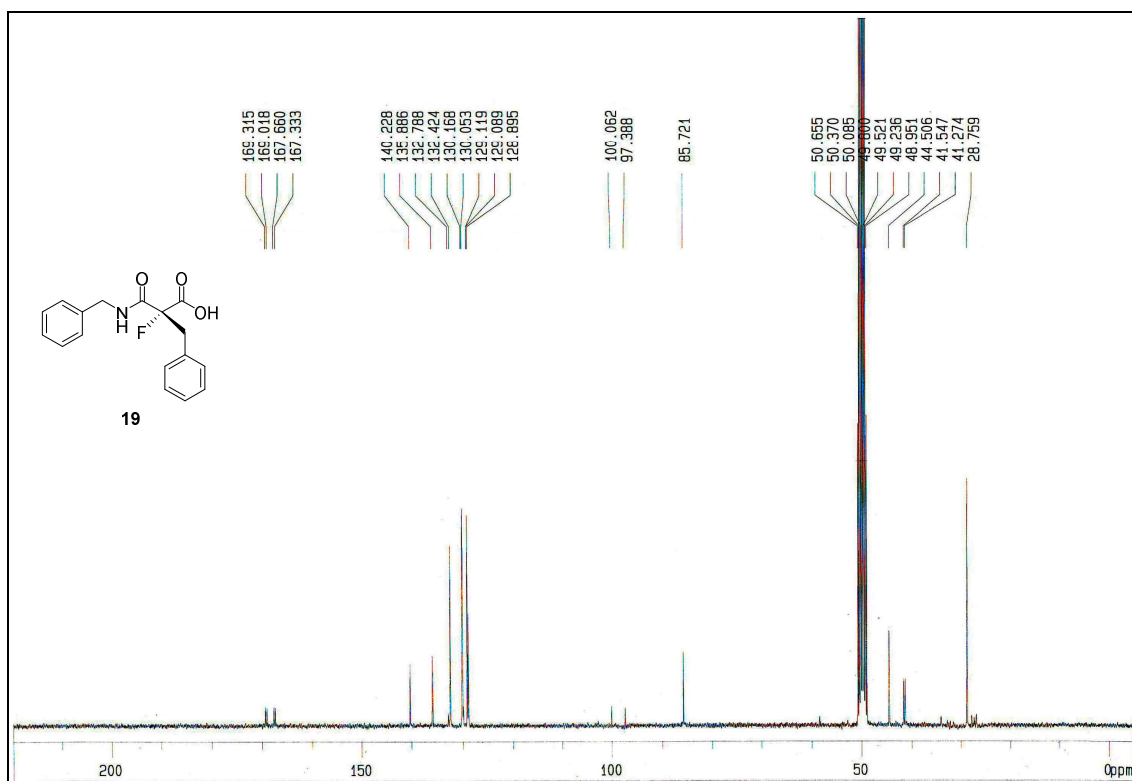




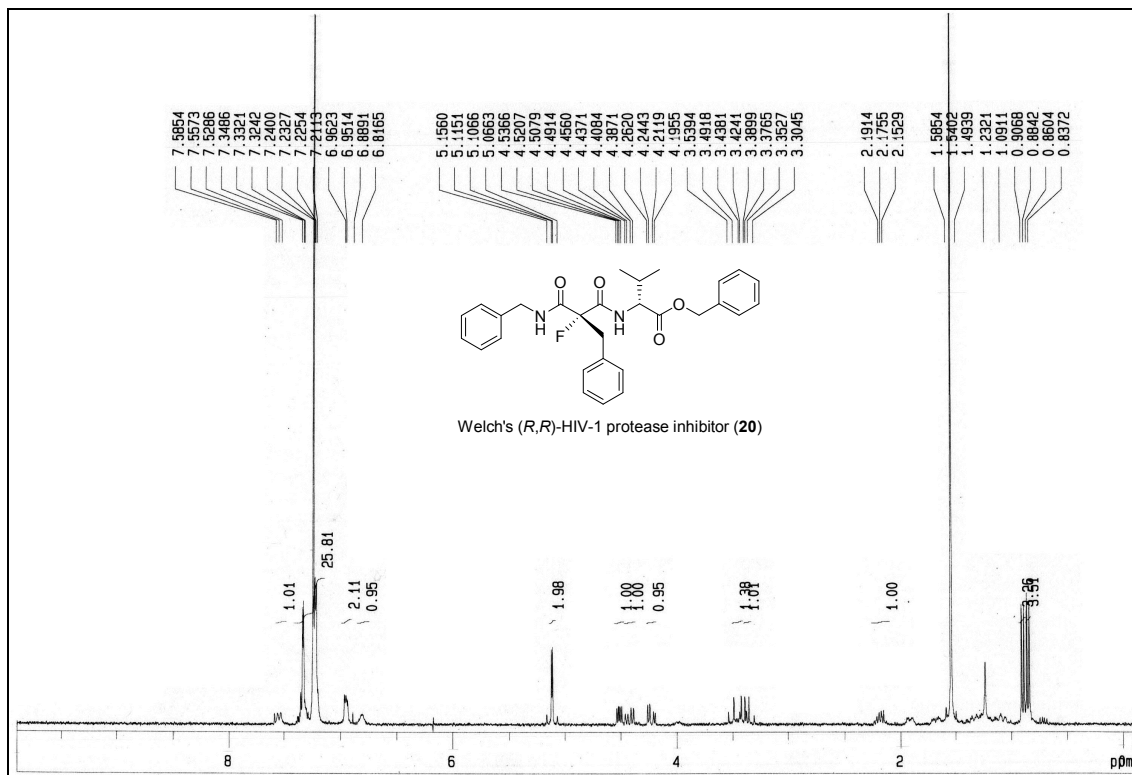
<sup>1</sup>H-NMR of compound **19** (300 MHz)



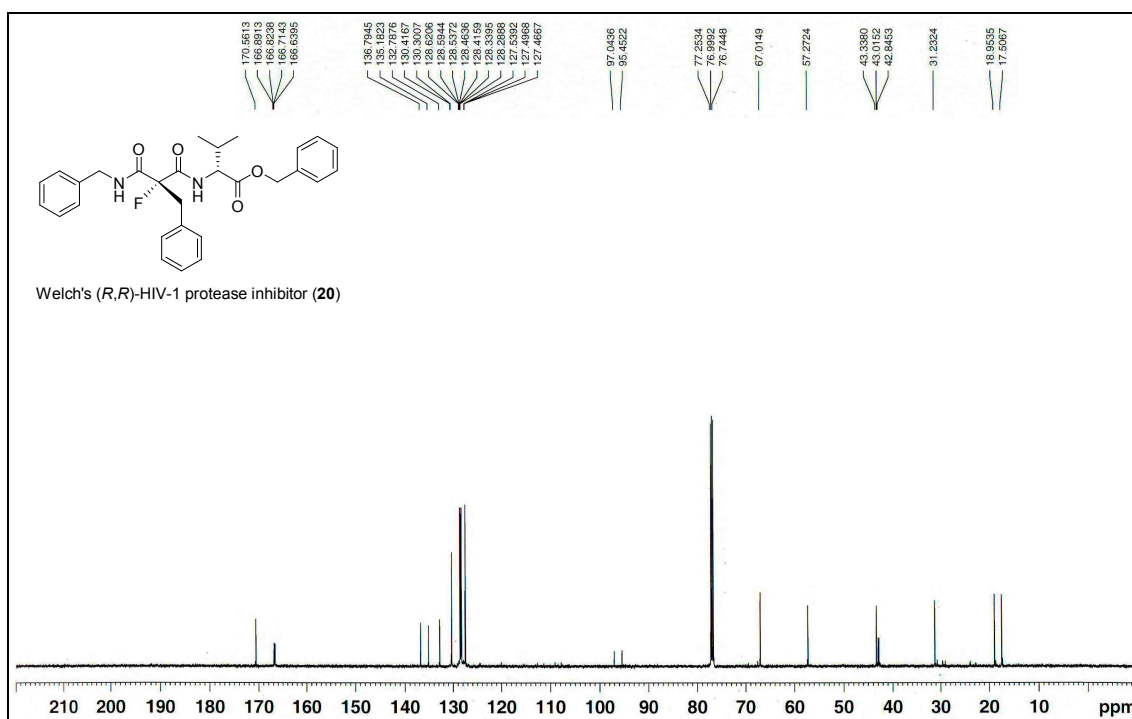
<sup>13</sup>C-NMR of compound **19** (75 MHz)



$^1\text{H}$ -NMR of Welch's (*R,R*)-HIV-1 protease inhibitor(**20**) (300 MHz)



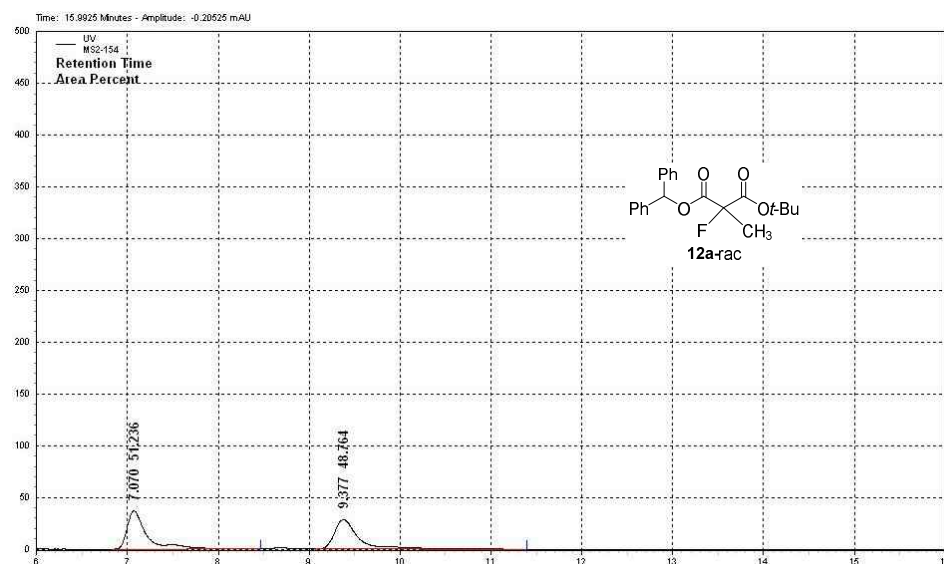
$^{13}\text{C}$ -NMR of Welch's (*R,R*)-HIV-1 protease inhibitor(**20**) (125 MHz)



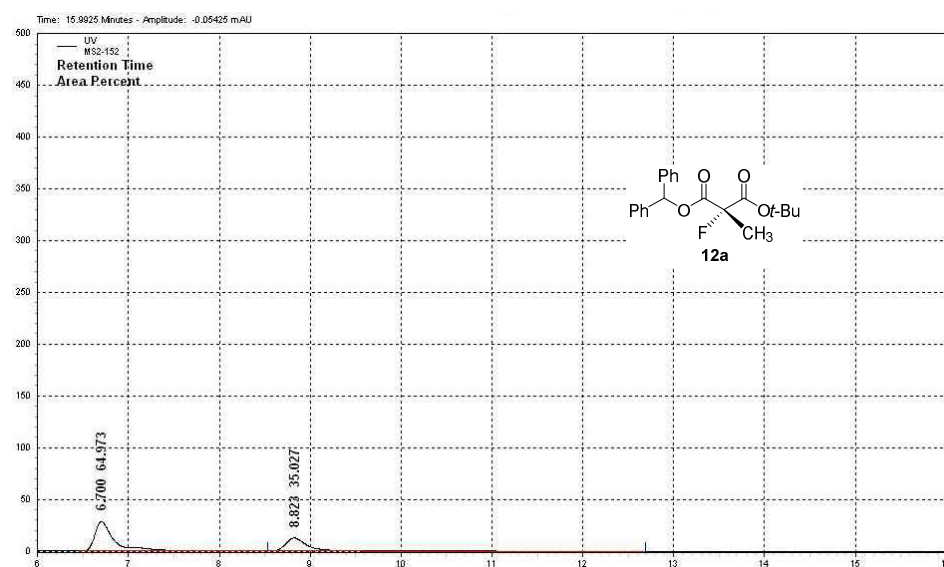


## Chiral HPLC analysis

### HPLC chart of compound **12a**

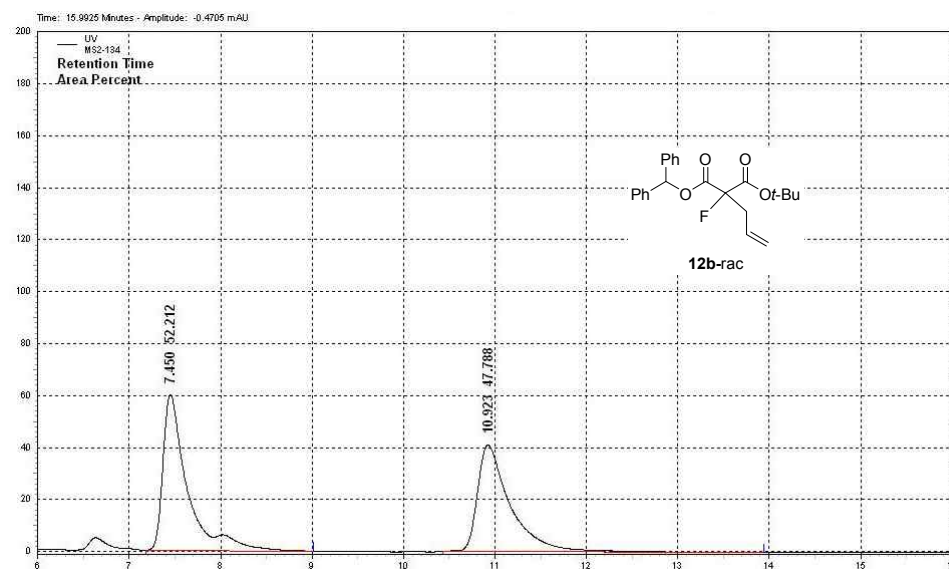


UV Results				
Name	Retention Time	Area	Area Percent	Integration Codes
	7.070	2242448	51.236	IB
	9.377	2134278	48.764	BI



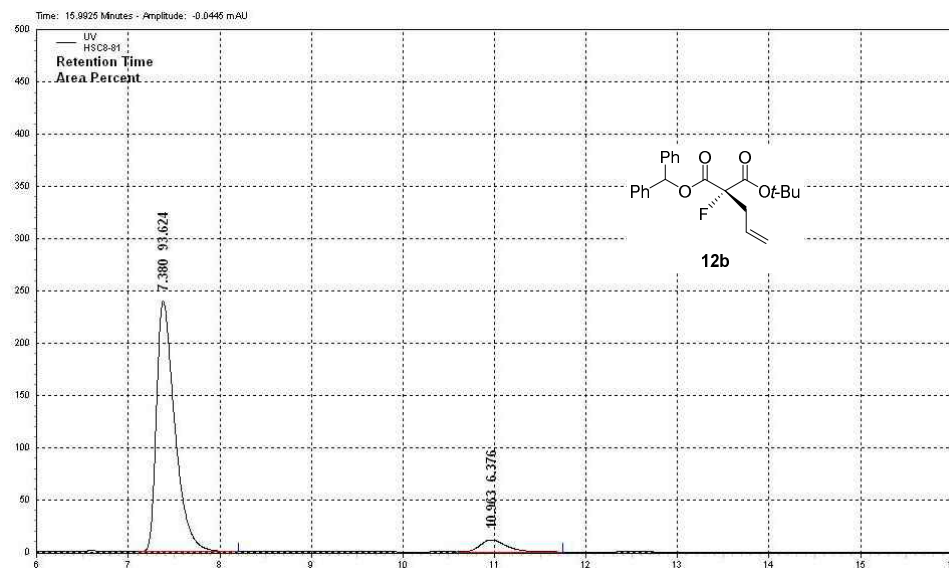
UV Results				
Name	Retention Time	Area	Area Percent	Integration Codes
	6.700	1790266	64.973	BV
	8.823	965117	35.027	VI

# HPLC chart of compound **12b**



## UV Results

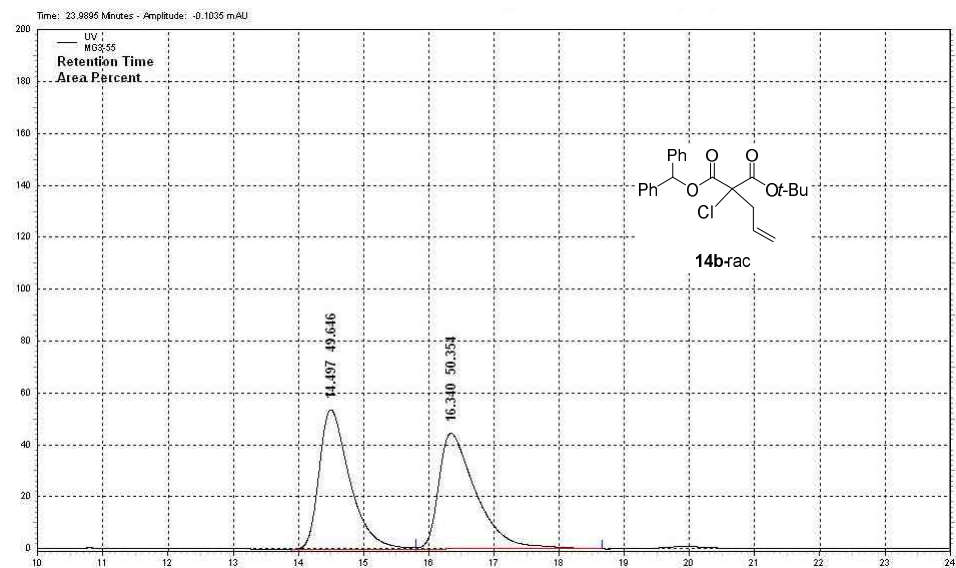
Name	Retention Time	Area	Area Percent	Integration Codes
	7.450	4452217	52.212	II
	10.923	4074953	47.788	II



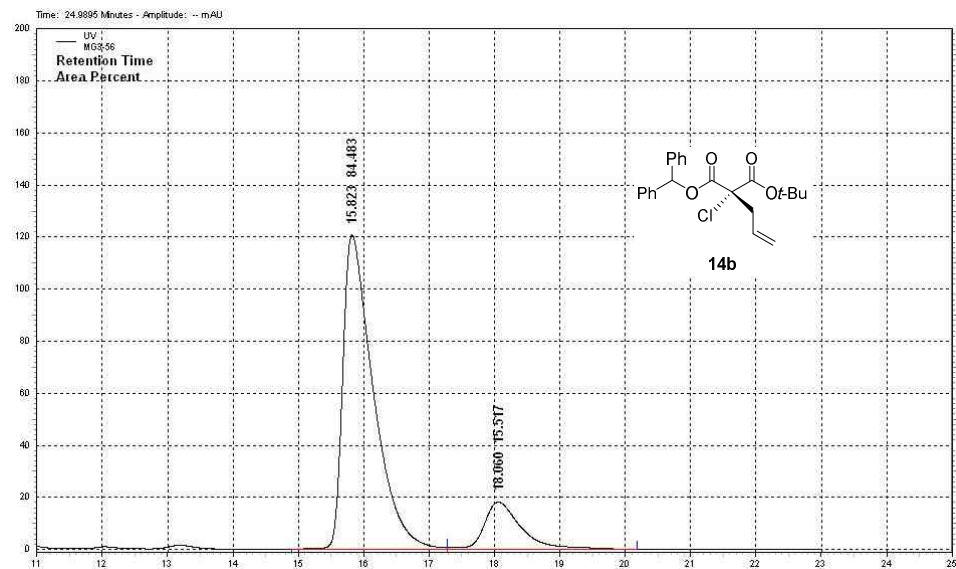
## UV Results

Name	Retention Time	Area	Area Percent	Integration Codes
	7.380	13360006	93.624	BB
	10.963	909885	6.376	BI

HPLC chart of compound **14b**

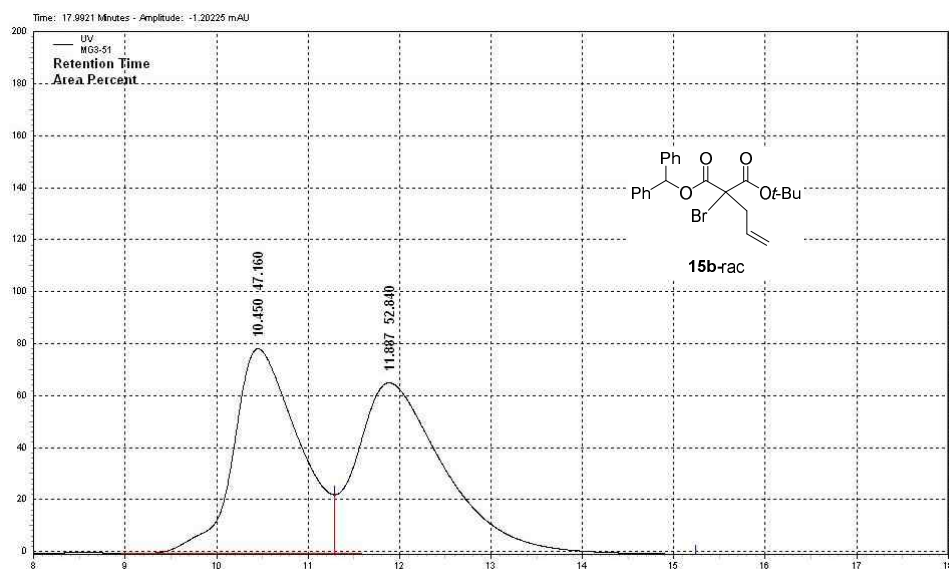


UV Results				
Name	Retention Time	Area	Area Percent	Integration Codes
	14.497	6995194	49.646	BV
	16.340	7094845	50.354	VI



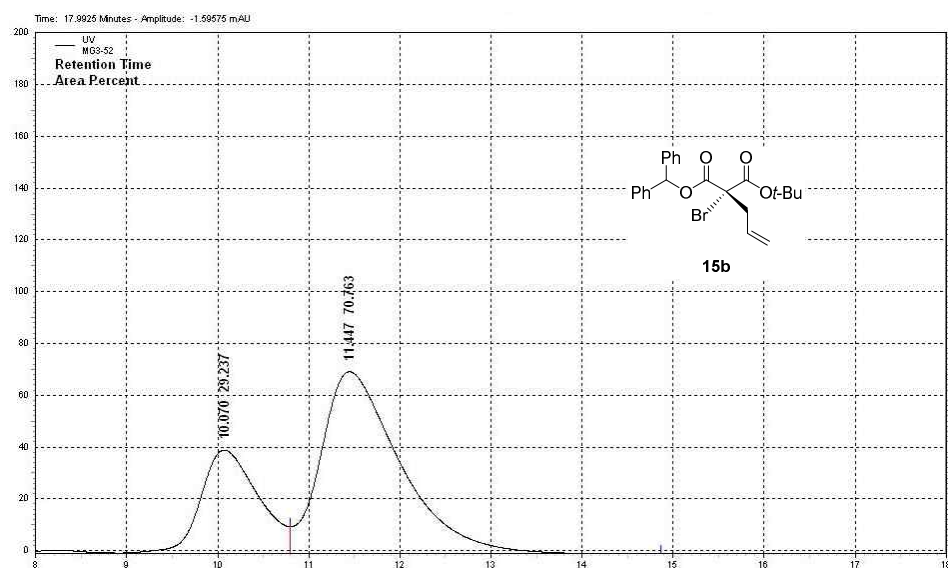
UV Results				
Name	Retention Time	Area	Area Percent	Integration Codes
	15.823	15665459	84.483	BV
	18.060	2877231	15.517	VI

# HPLC chart of compound **15b**



## UV Results

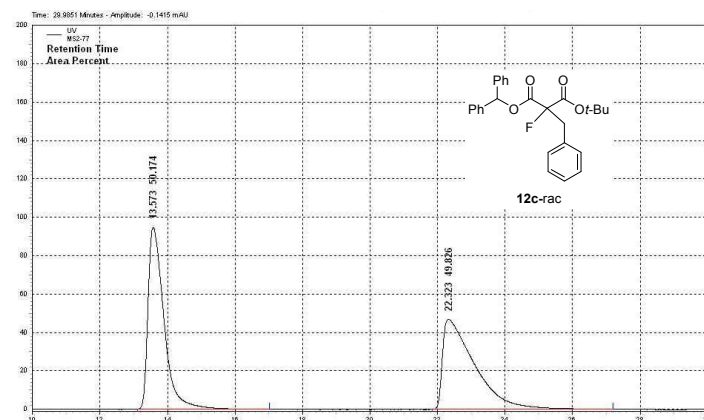
Name	Retention Time	Area	Area Percent	Integration Codes
	10.450	15673974	47.160	BV
	11.887	17561576	52.840	VI



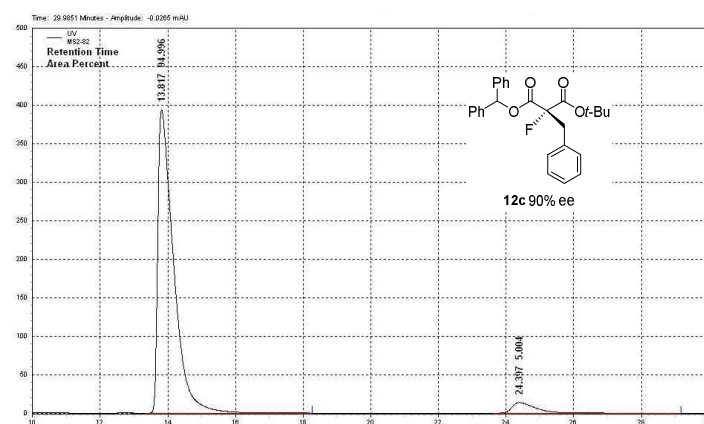
## UV Results

Name	Retention Time	Area	Area Percent	Integration Codes
	10.070	6999001	29.237	BV
	11.447	16939541	70.763	VB

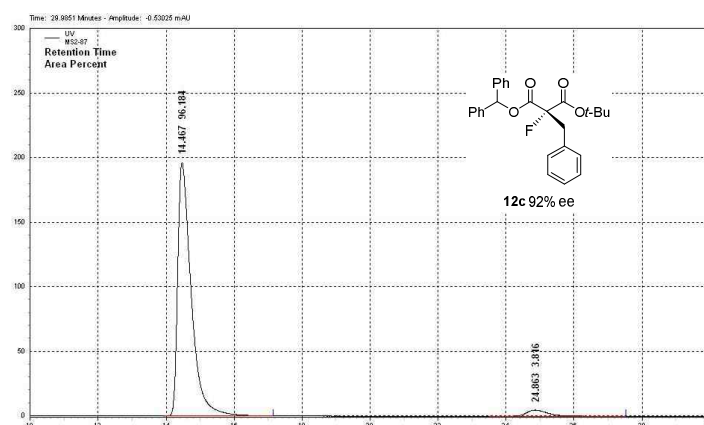
# HPLC chart of compound **12c**



UV Results Name	Retention Time	Area	Area Percent	Integration Codes
	13.573	12464418	50.174	II
	22.323	12378134	49.826	II

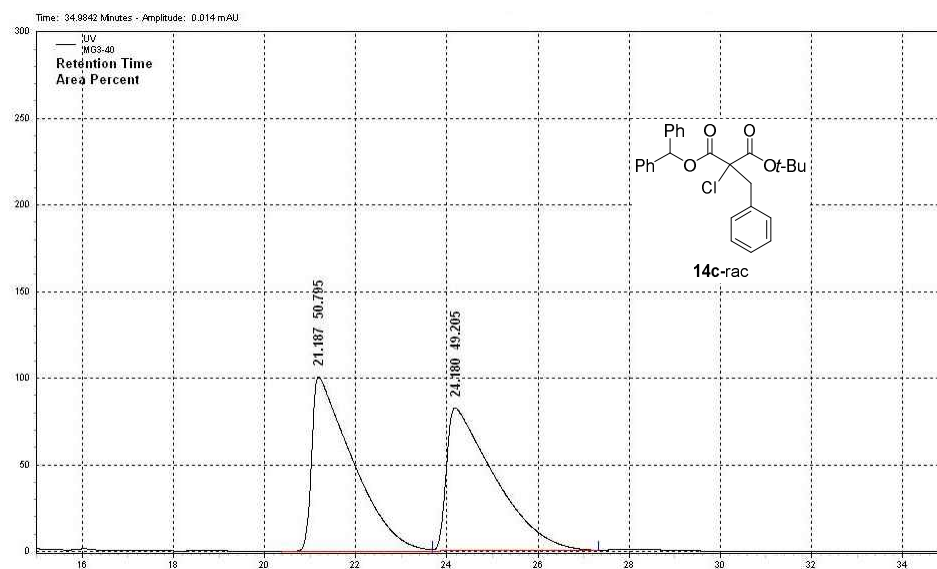


UV Results Name	Retention Time	Area	Area Percent	Integration Codes
	13.817	50827775	94.996	BI
	24.397	2677273	5.004	BB



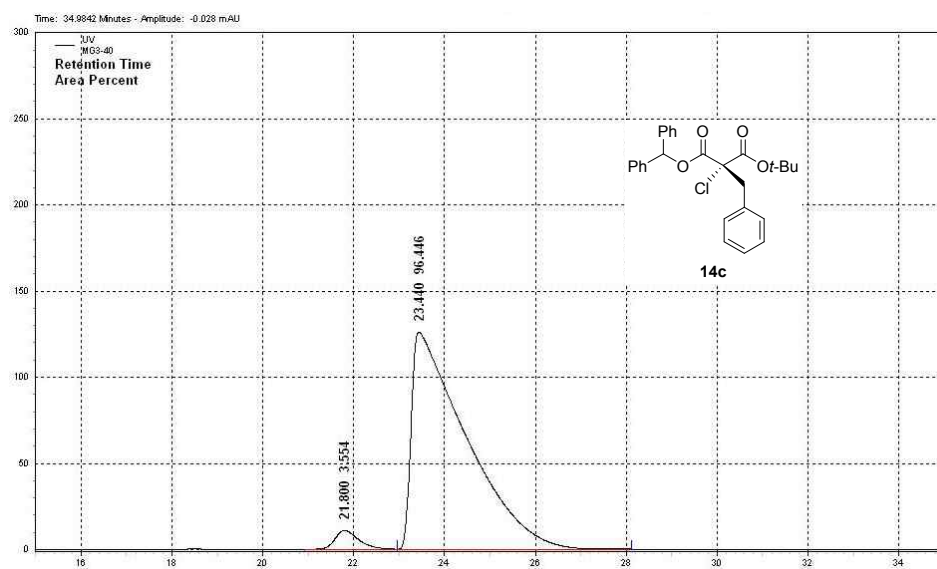
UV Results Name	Retention Time	Area	Area Percent	Integration Codes
	14.467	21659572	96.184	BI
	24.863	859233	3.816	BB

# HPLC chart of compound **14c**



## UV Results

Name	Retention Time	Area	Area Percent	Integration Codes
	21.187	24877957	50.795	IV
	24.180	24099305	49.205	VI

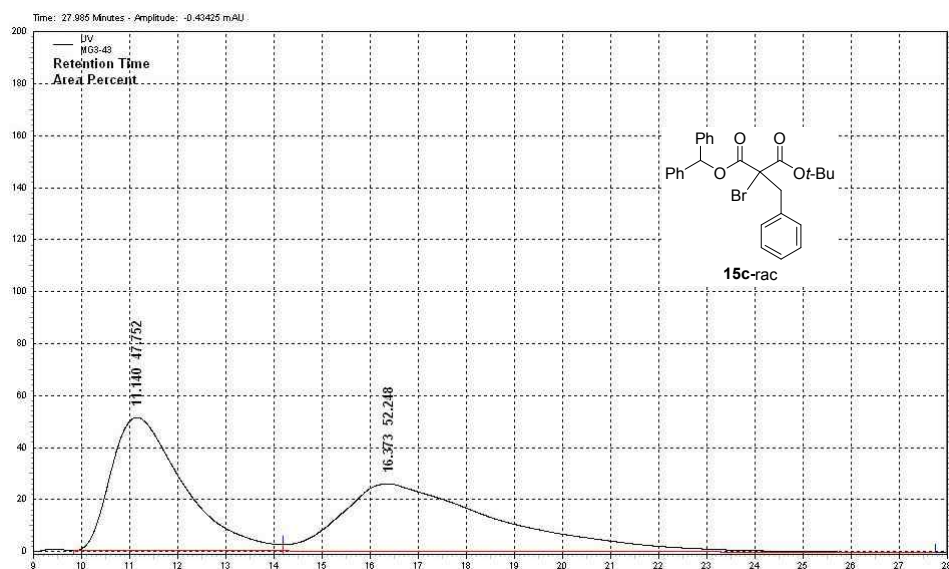


## UV Results

Name	Retention Time	Area	Area Percent	Integration Codes
	21.800	1555175	3.554	BB
	23.440	42198622	96.446	BI

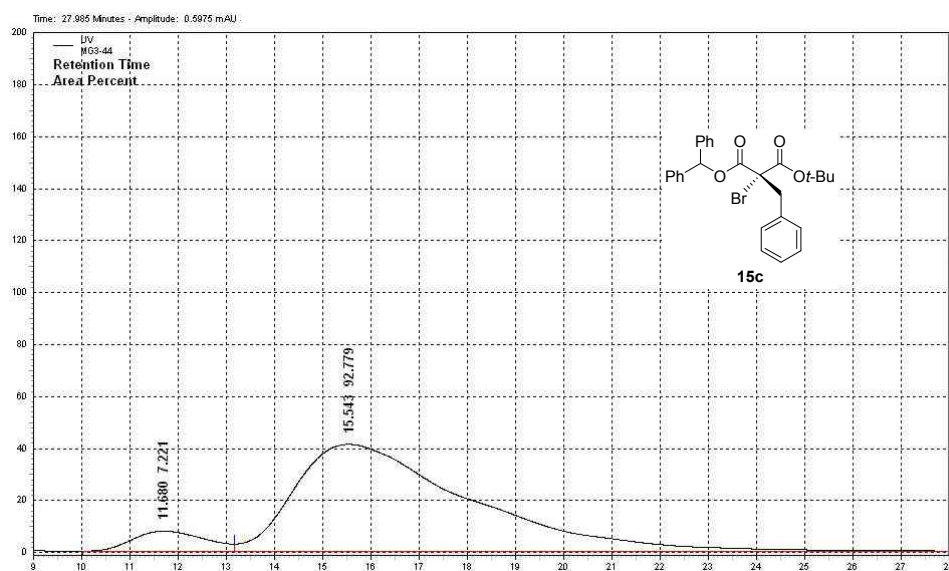


# HPLC chart of compound **15c**



## UV Results

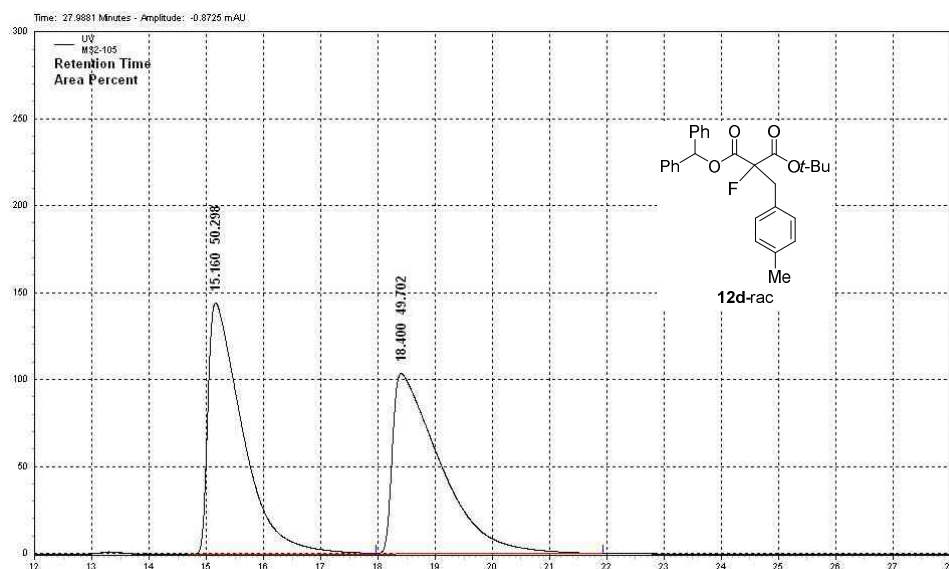
Name	Retention Time	Area	Area Percent	Integration Codes
	11.140	21549447	47.752	IV
	16.373	23578299	52.248	VE



## UV Results

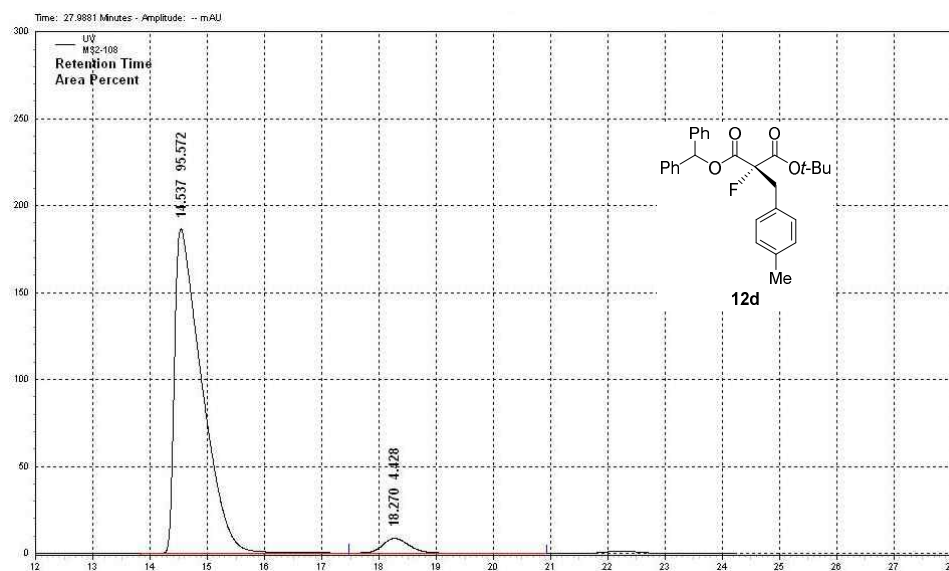
Name	Retention Time	Area	Area Percent	Integration Codes
	11.680	3190661	7.221	BV
	15.543	40992902	92.779	VB

# HPLC chart of compound **12d**



## UV Results

Name	Retention Time	Area	Area Percent	Integration Codes
	15.160	24231212	50.298	BV
	18.400	23944374	49.702	VI

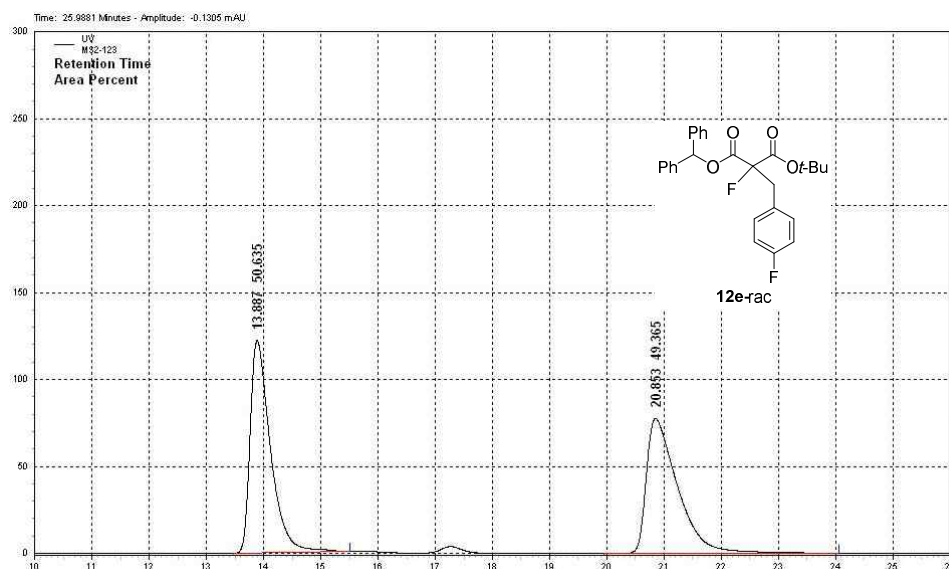


## UV Results

Name	Retention Time	Area	Area Percent	Integration Codes
	14.537	24732111	95.572	BV
	18.270	1145757	4.428	VB

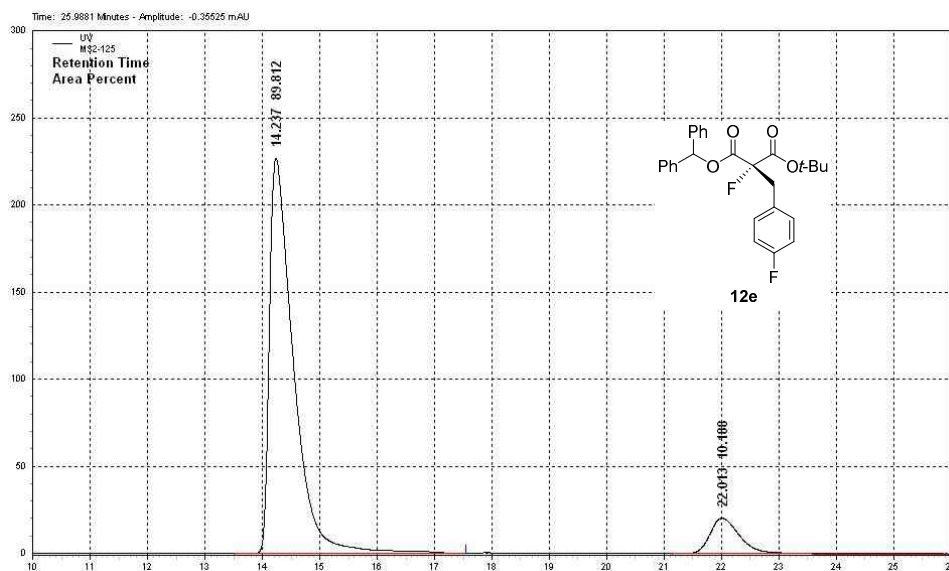


# HPLC chart of compound **12e**



## UV Results

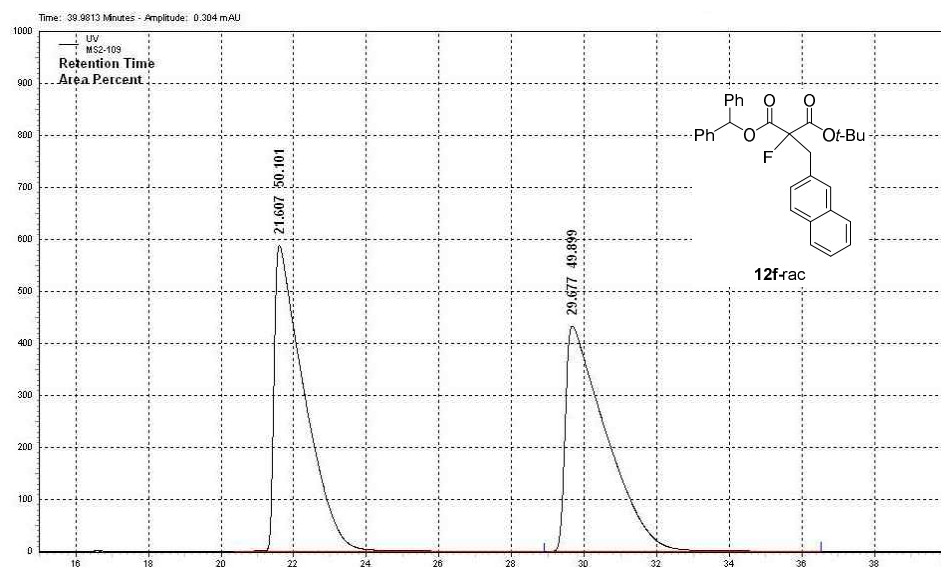
Name	Retention Time	Area	Area Percent	Integration Codes
	13.887	12059886	50.635	BB
	20.853	11757402	49.365	BB



## UV Results

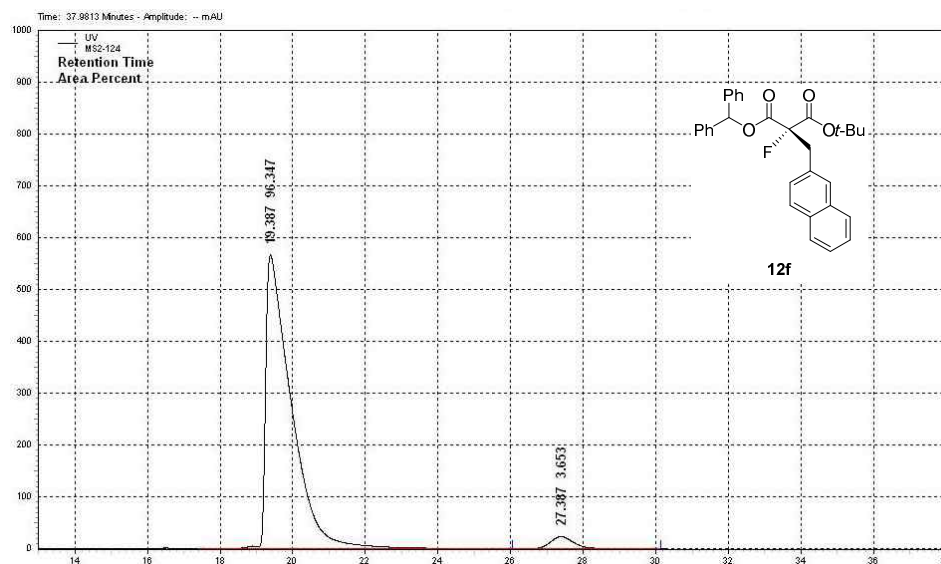
Name	Retention Time	Area	Area Percent	Integration Codes
	14.237	26301089	89.812	BB
	22.013	2983537	10.188	BB

# HPLC chart of compound **12f**



## UV Results

Name	Retention Time	Area	Area Percent	Integration Codes
	21.607	135200285	50.101	BB
	29.677	134655599	49.899	BB



## UV Results

Name	Retention Time	Area	Area Percent	Integration Codes
	19.387	110548264	96.347	BV
	27.387	4191319	3.653	VE