

Supporting Information

Synthetic studies towards (+)-allokainic acid via diphenylprolinol-catalyzed direct cross-aldol reaction

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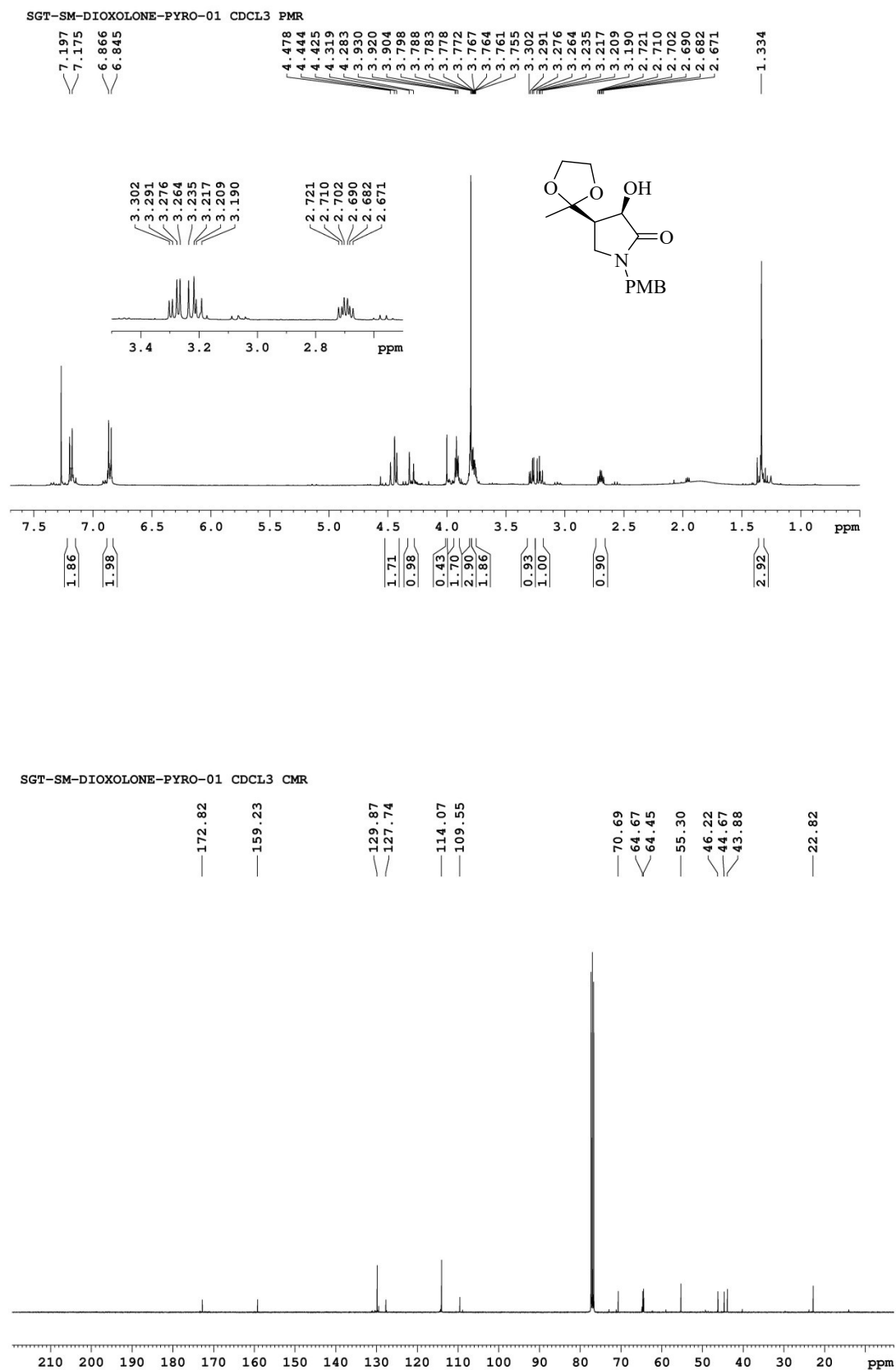
^[b] Department of Chemistry, Dhemphe College of Arts & Science, Miramar, Goa, 403001 (India)

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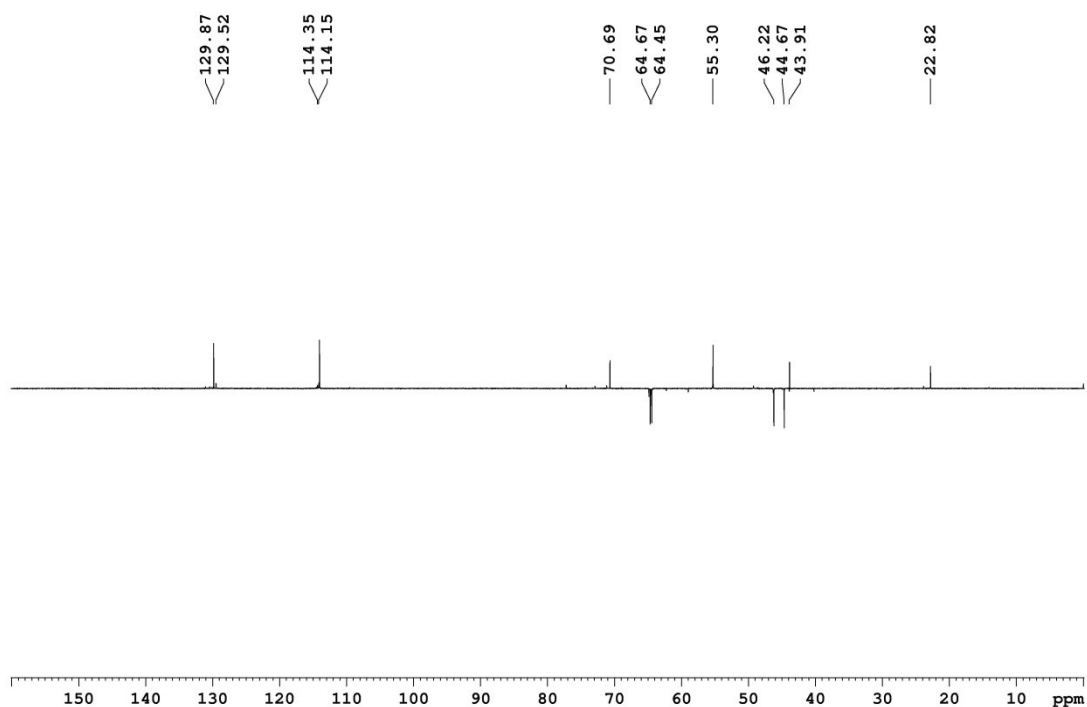
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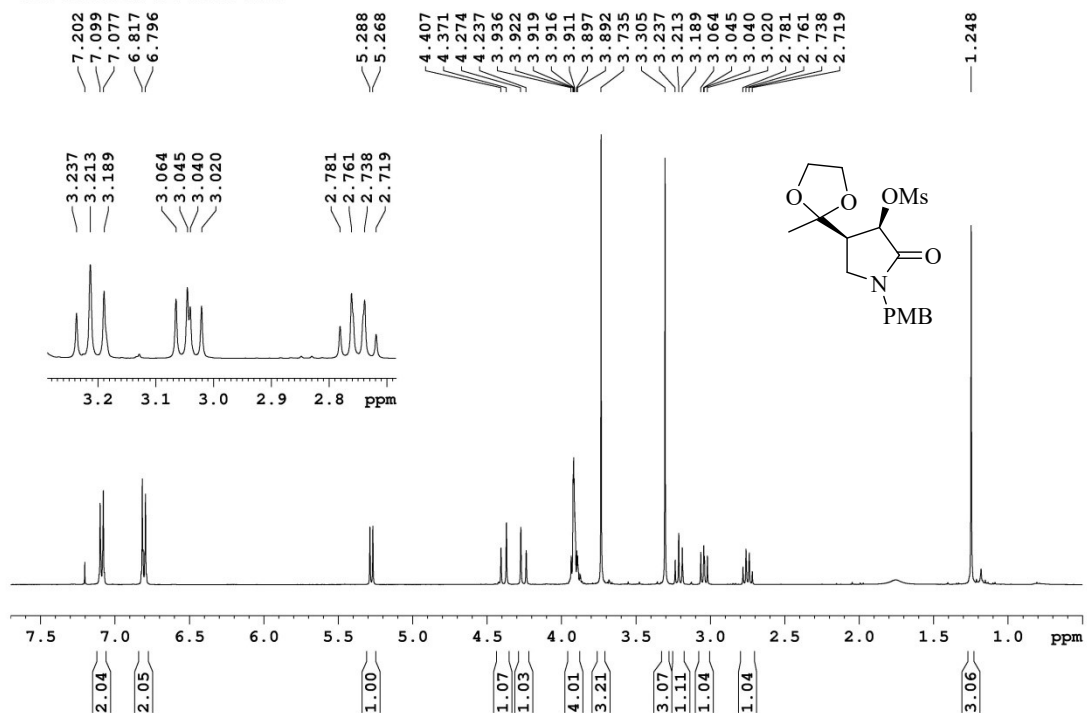
Spectral data



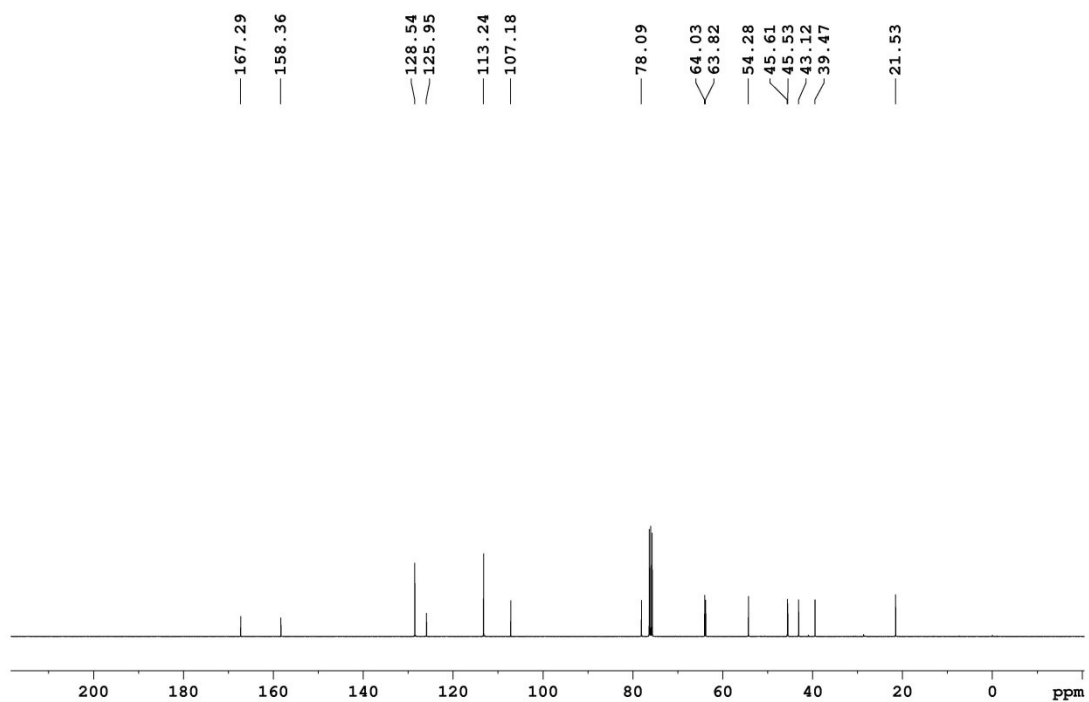
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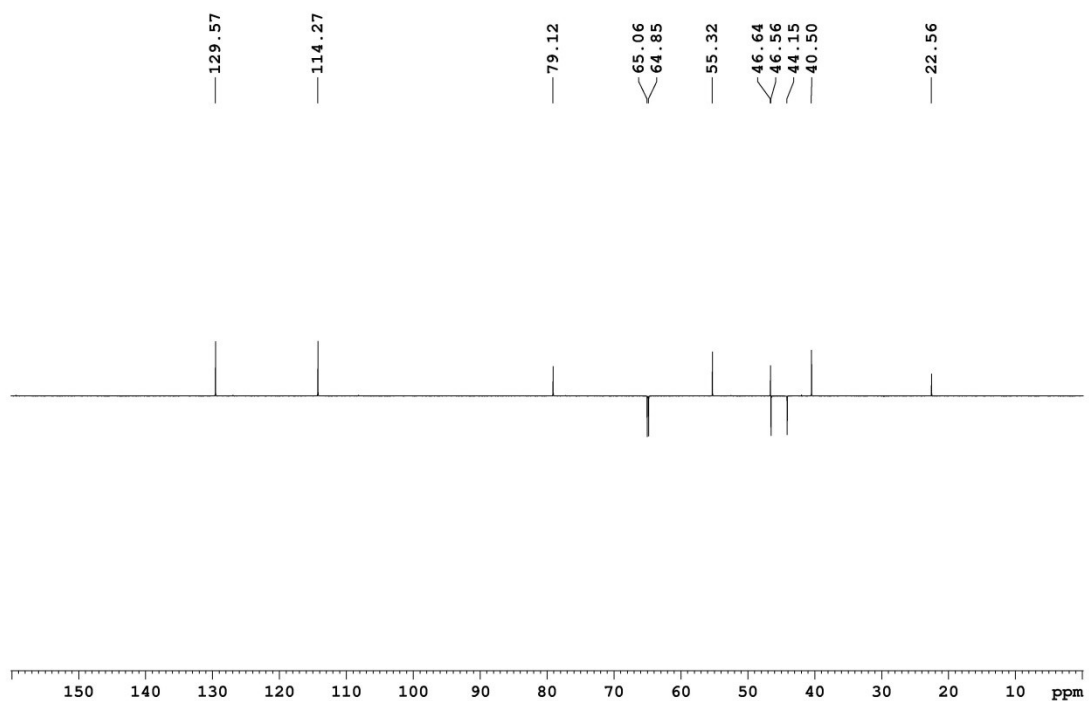
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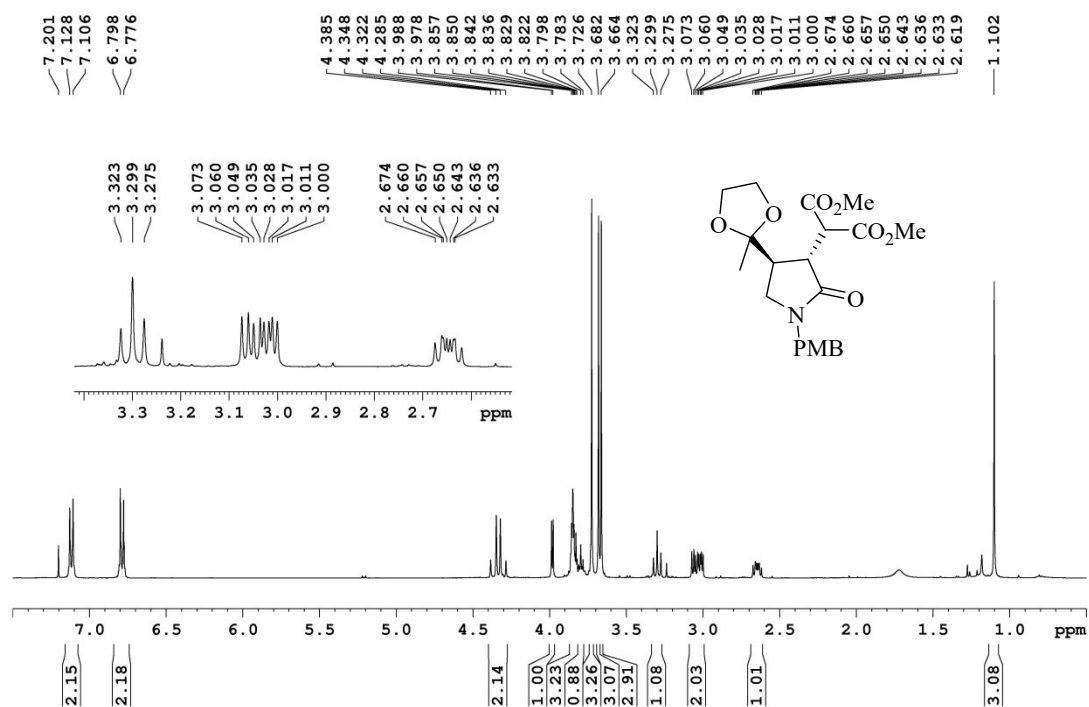
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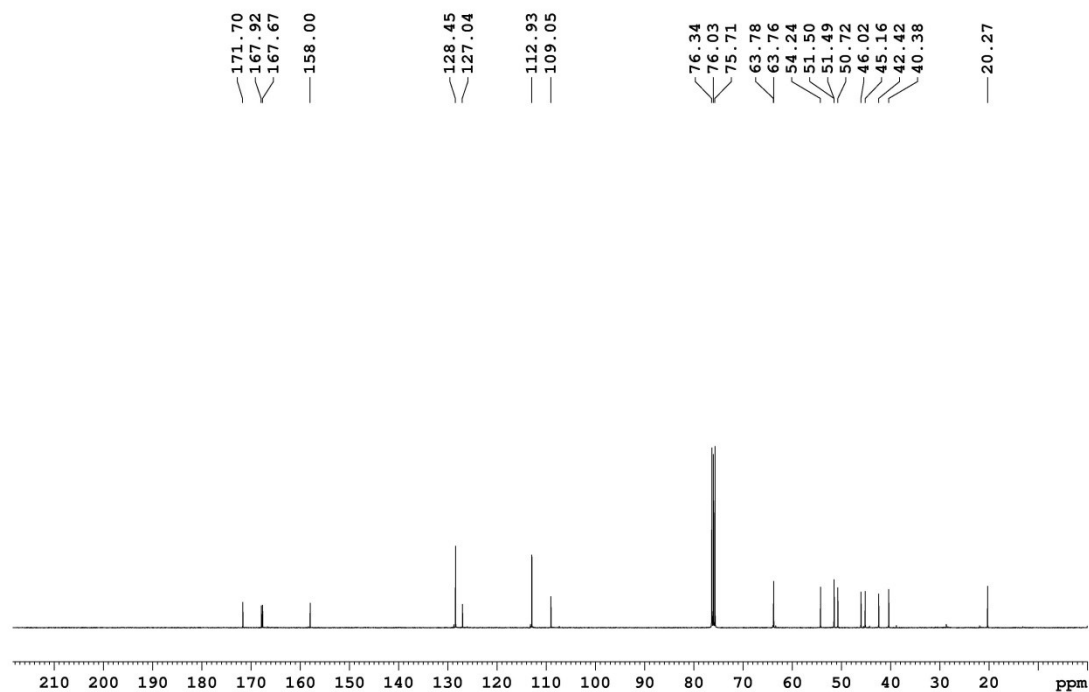
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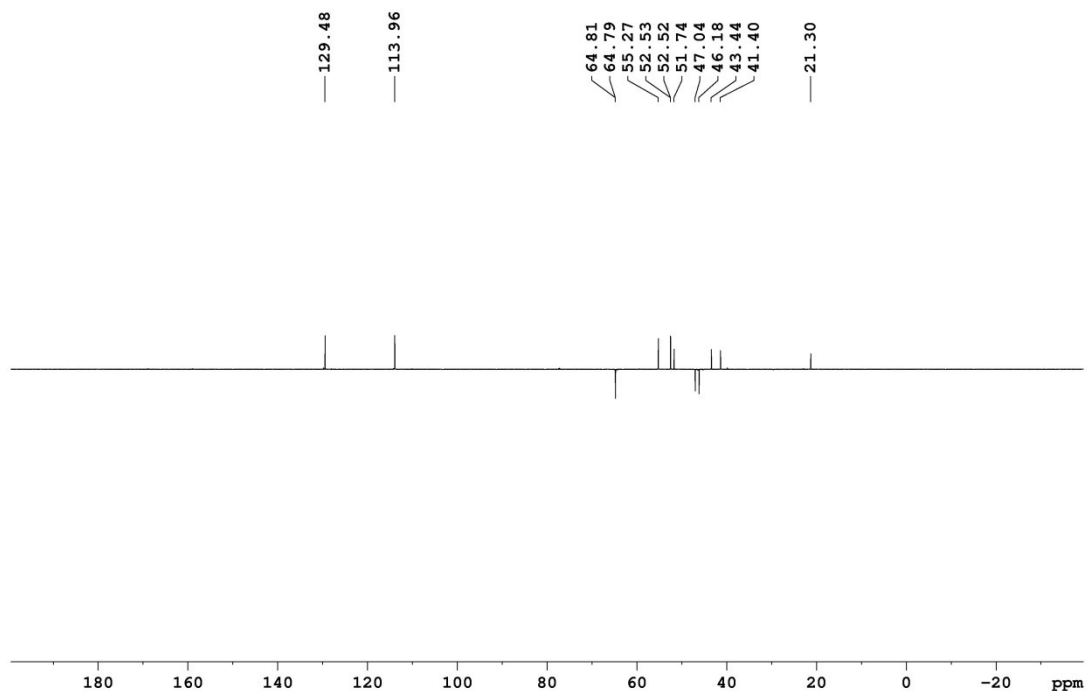
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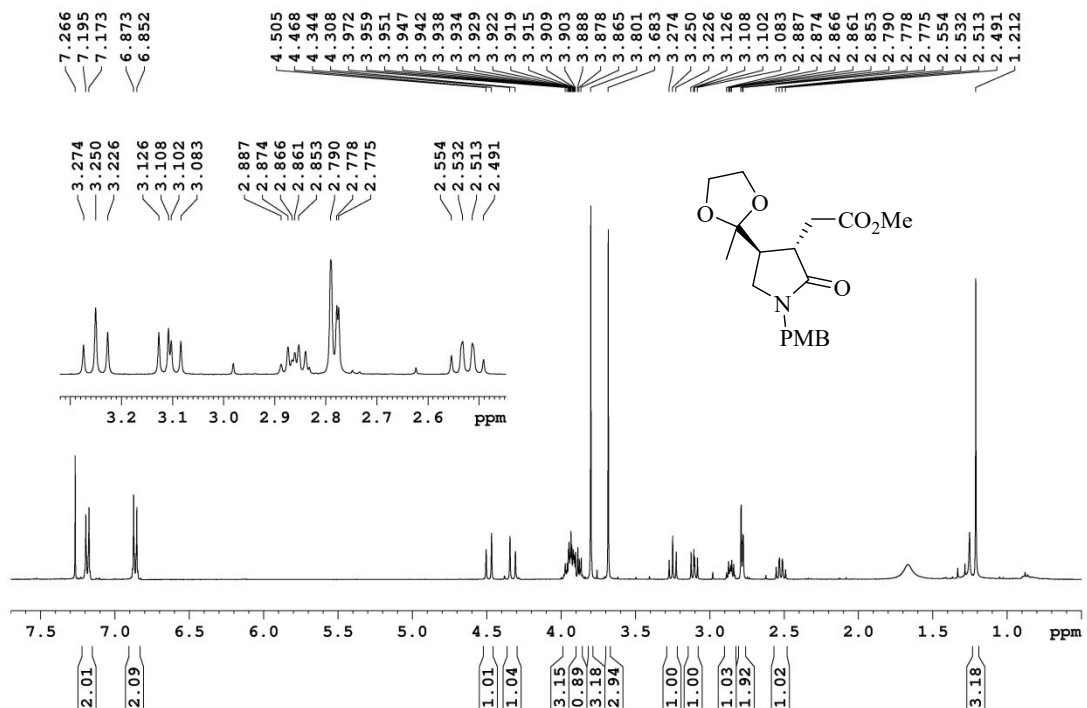
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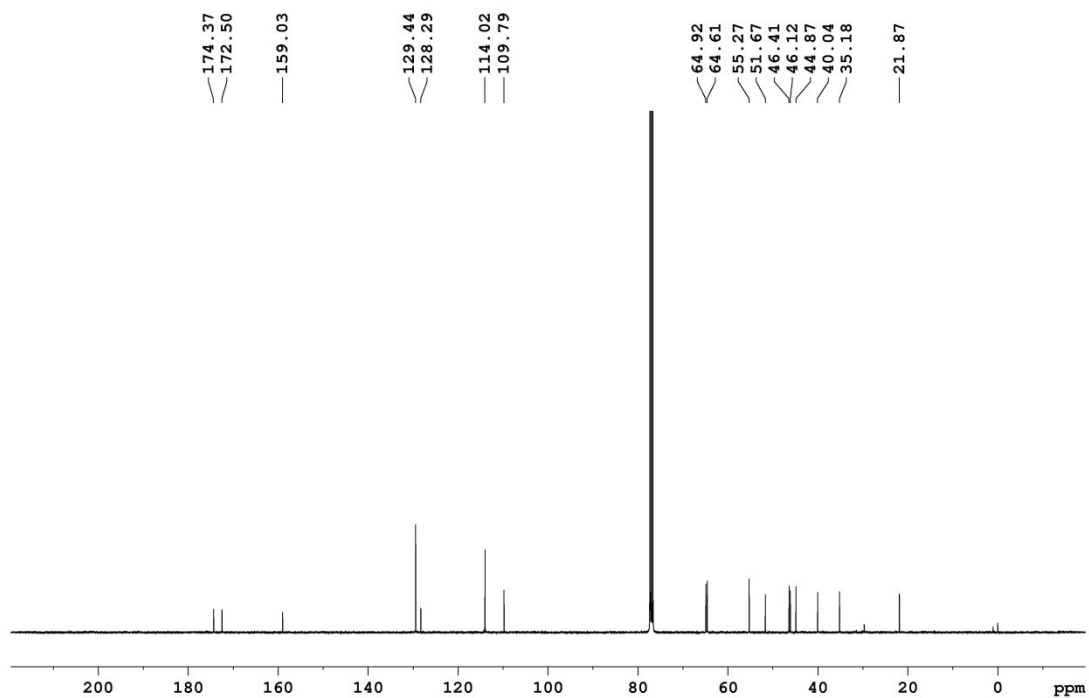
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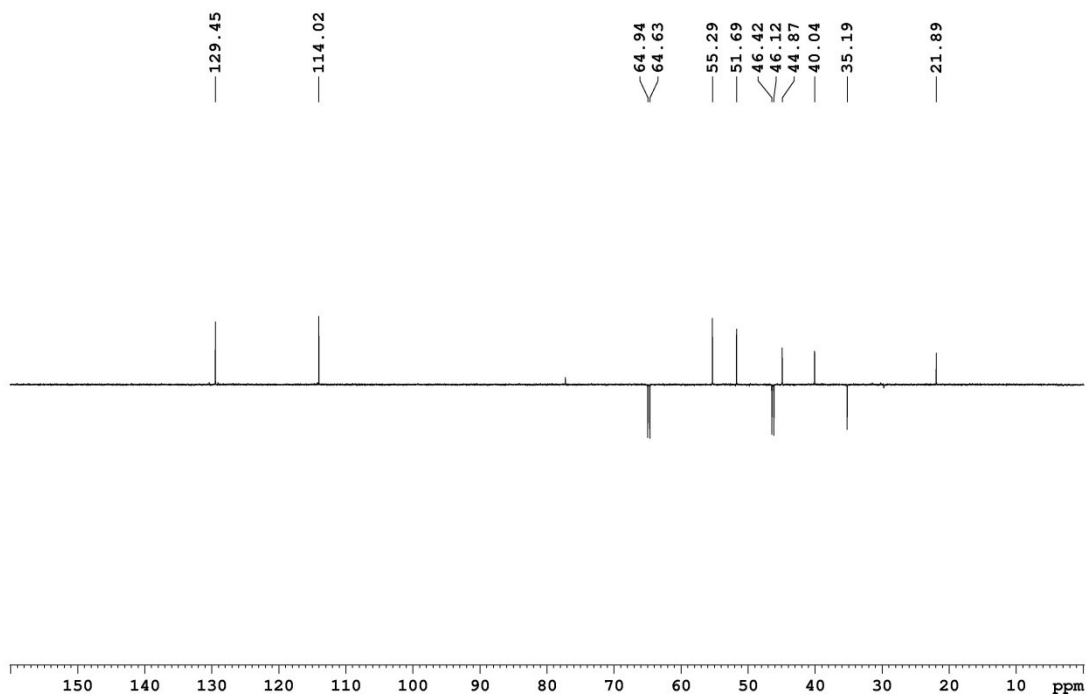
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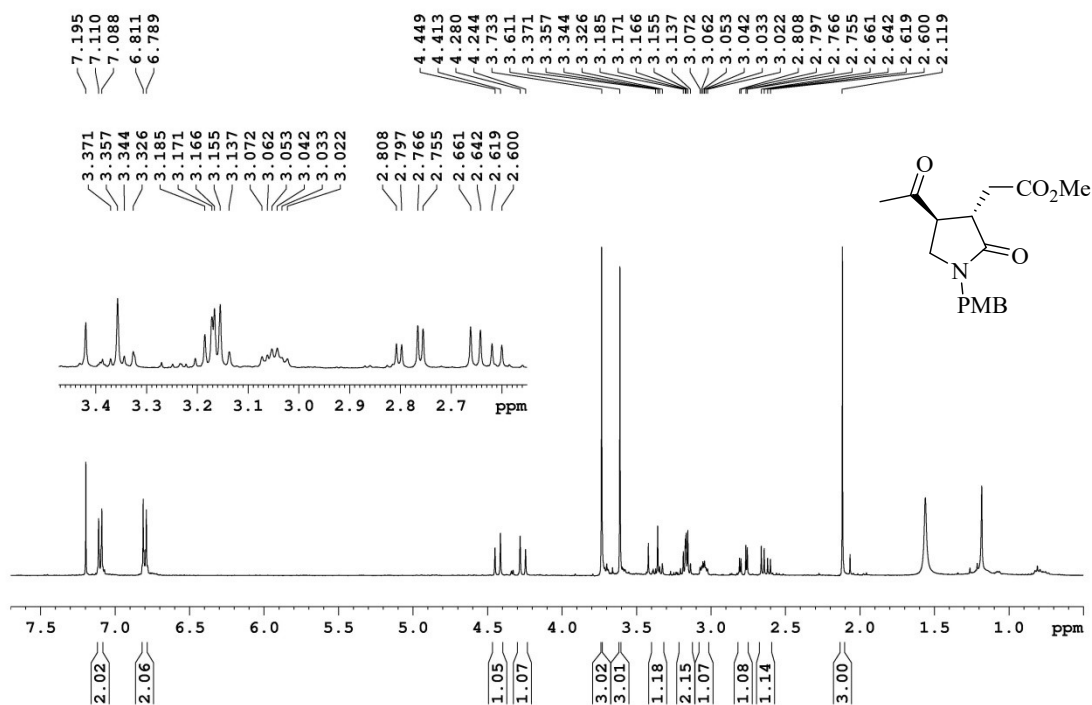
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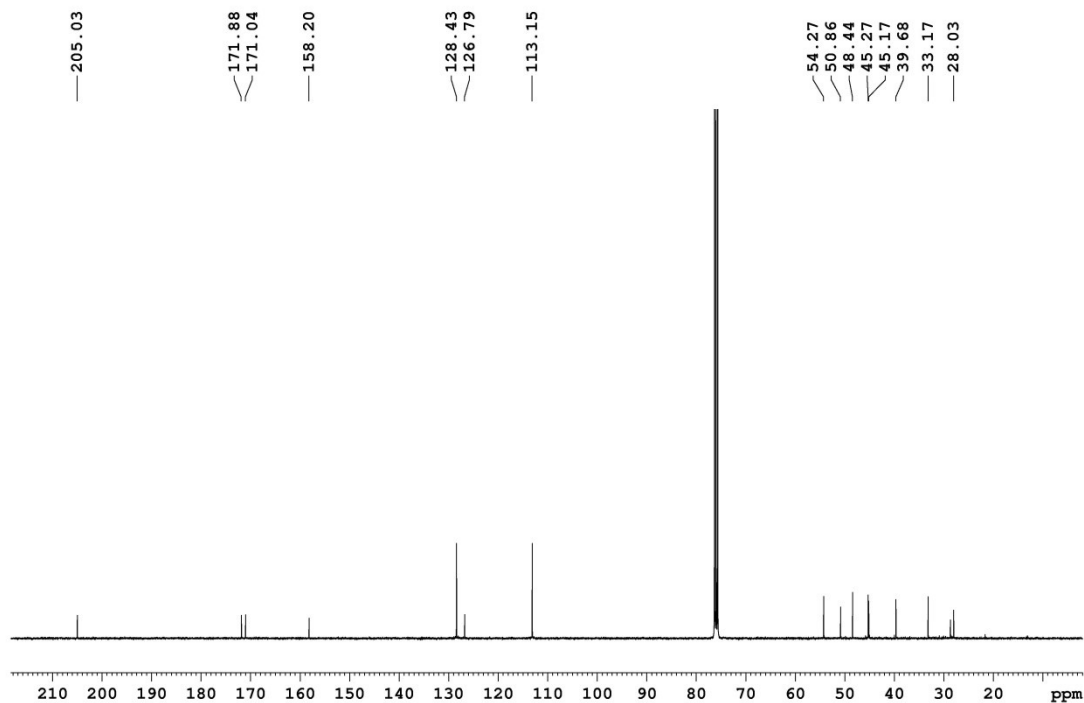
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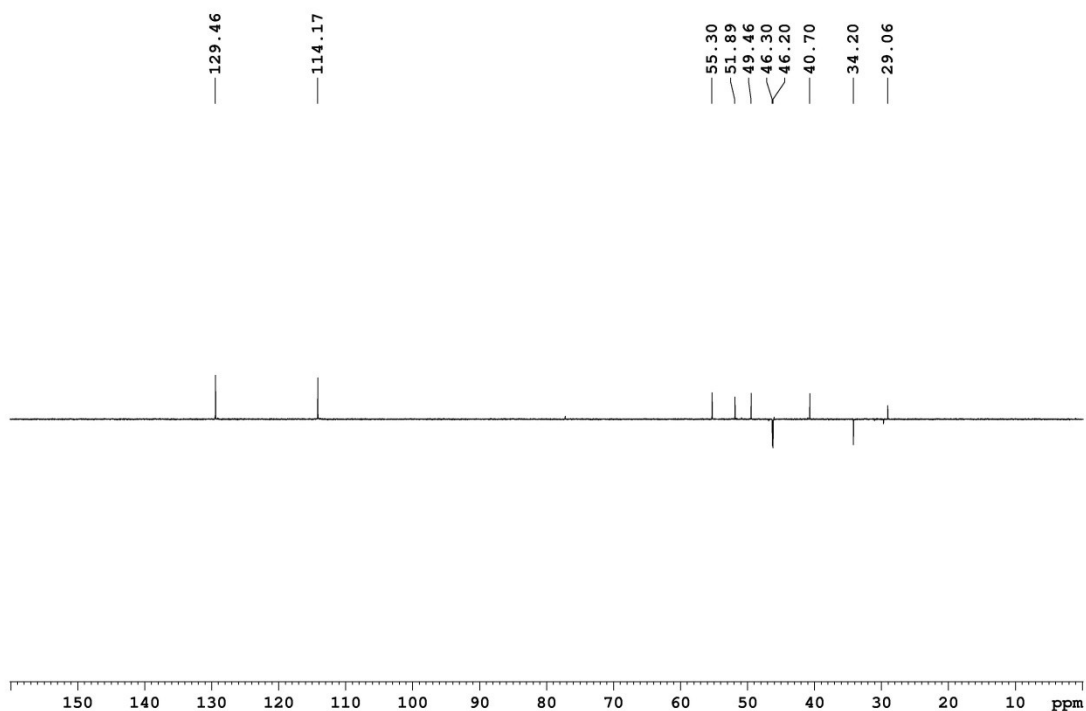
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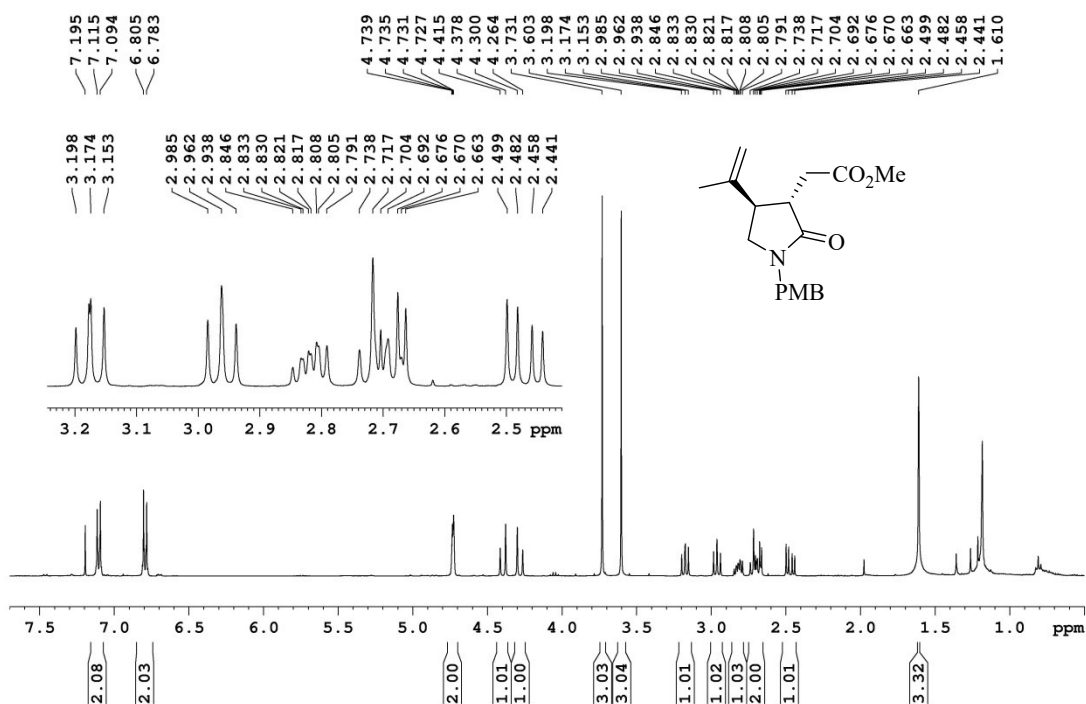
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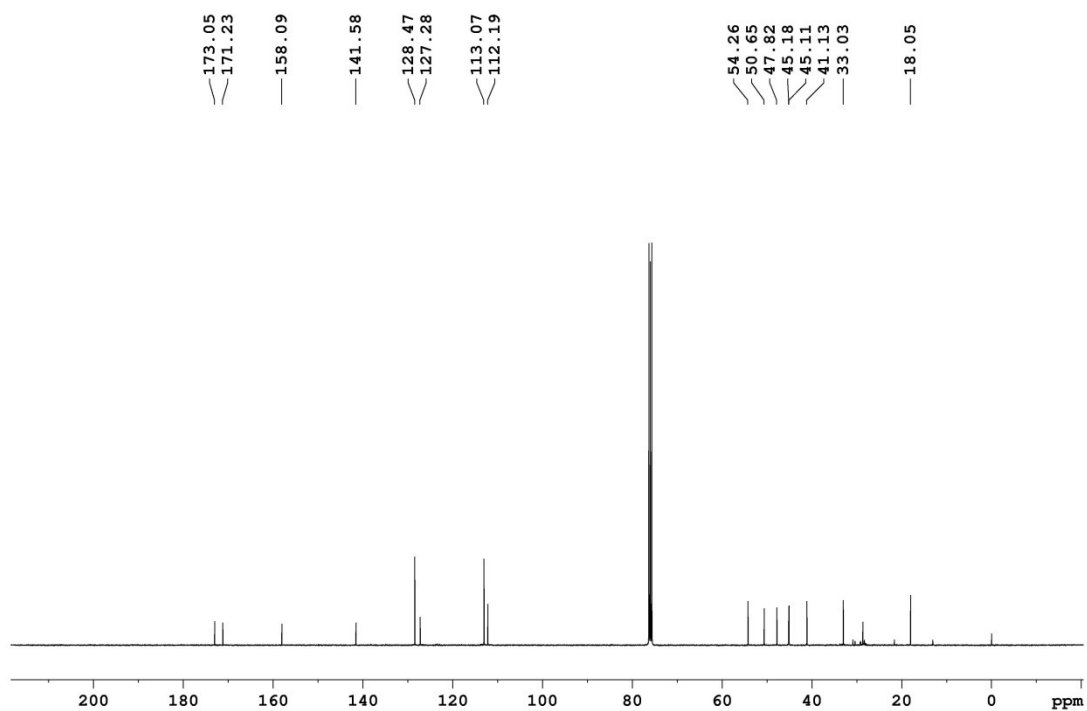
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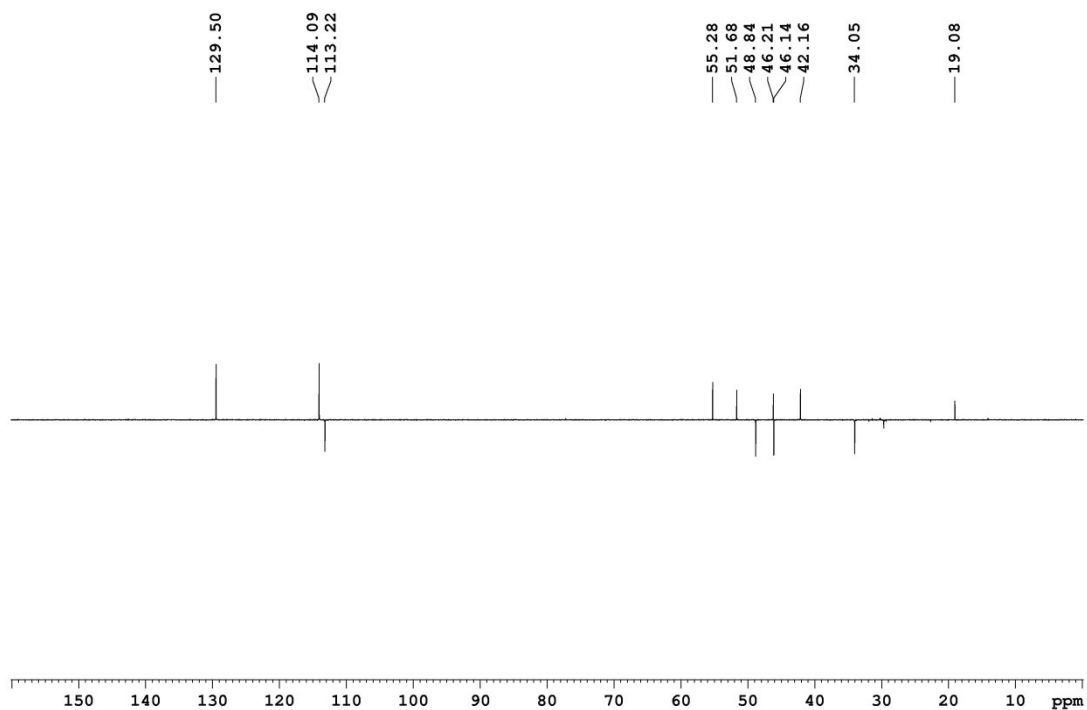
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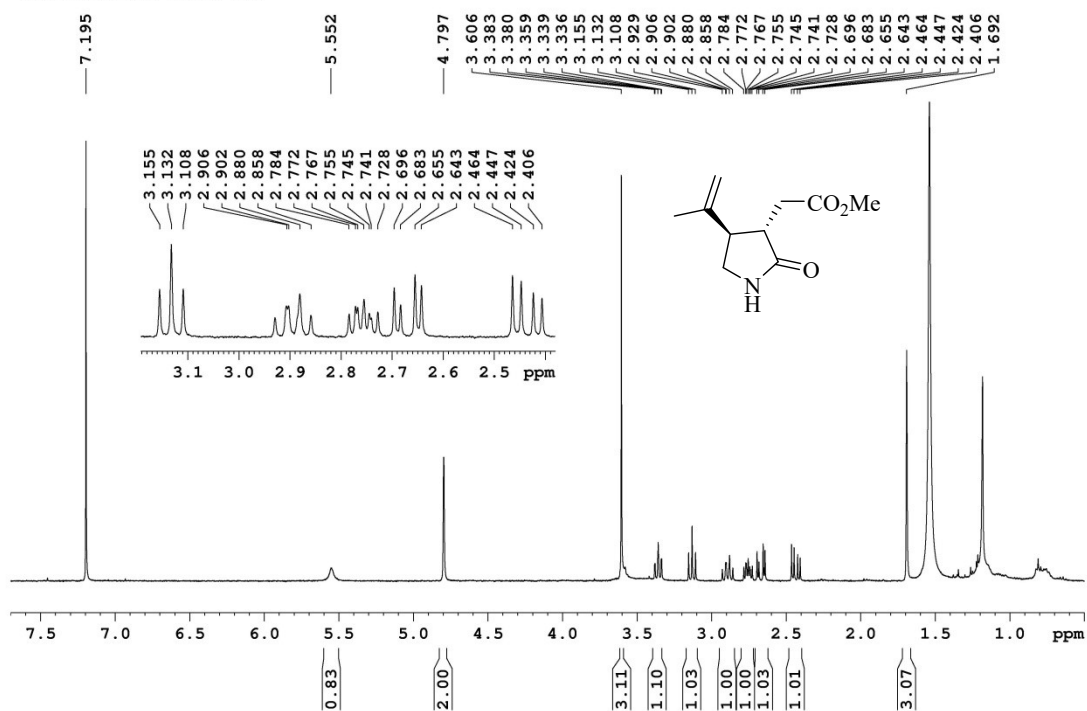
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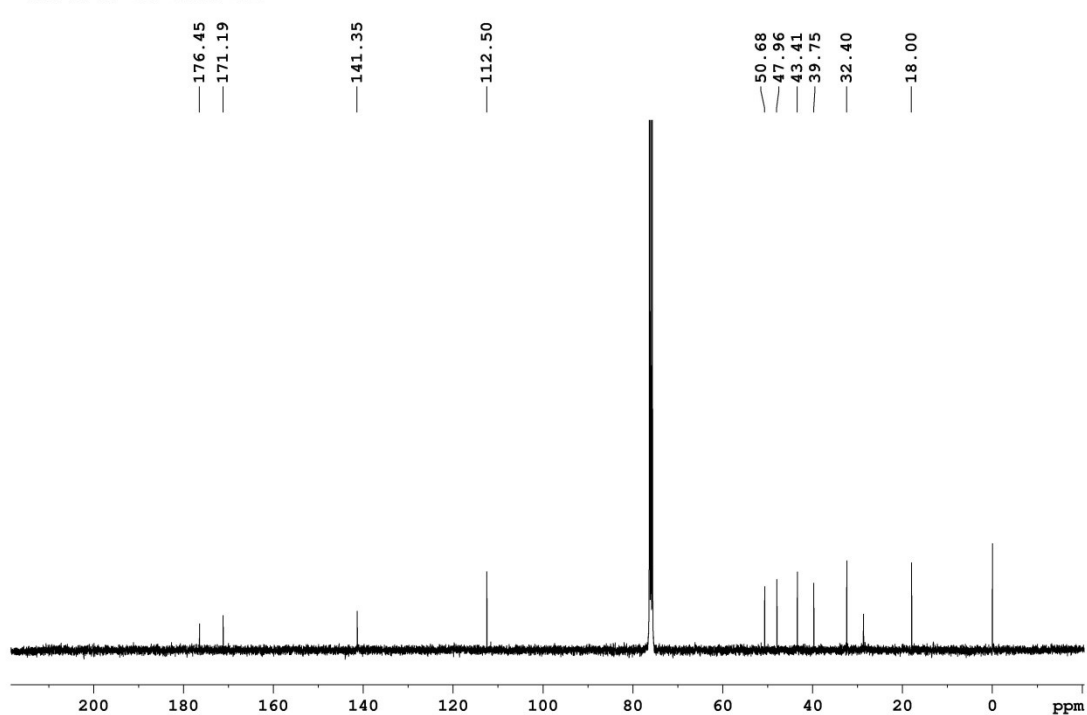
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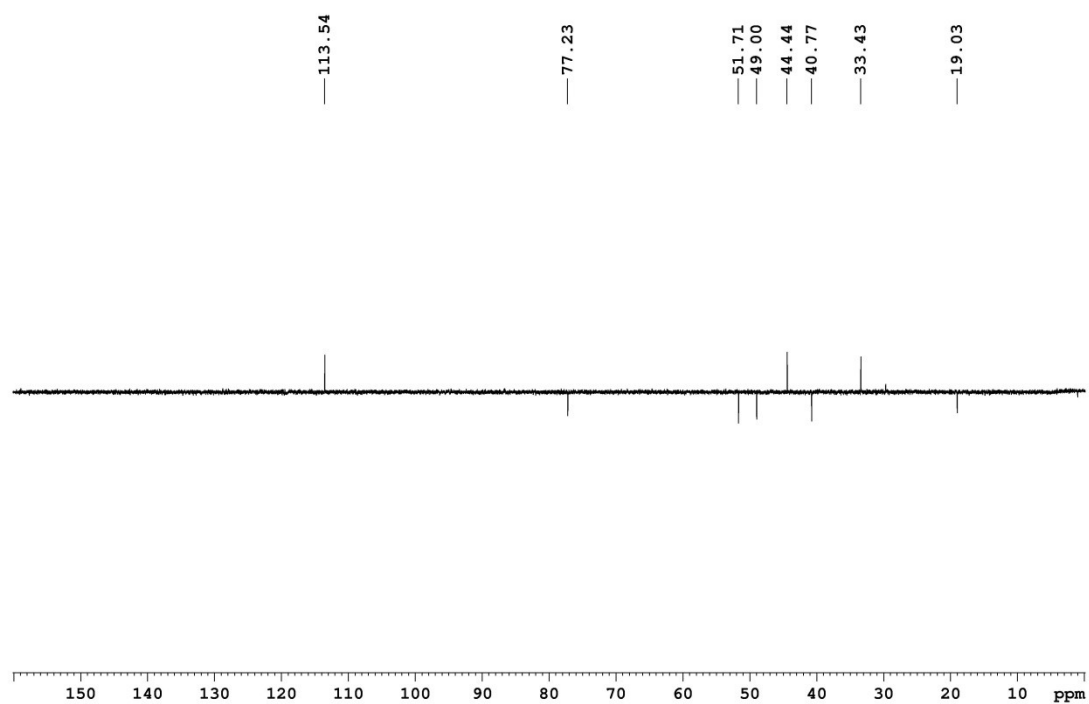
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SGT-SM-20-144 CDCL3 CMR



SGT-SM-20-144 CDCL3 DEPT



HPLC data

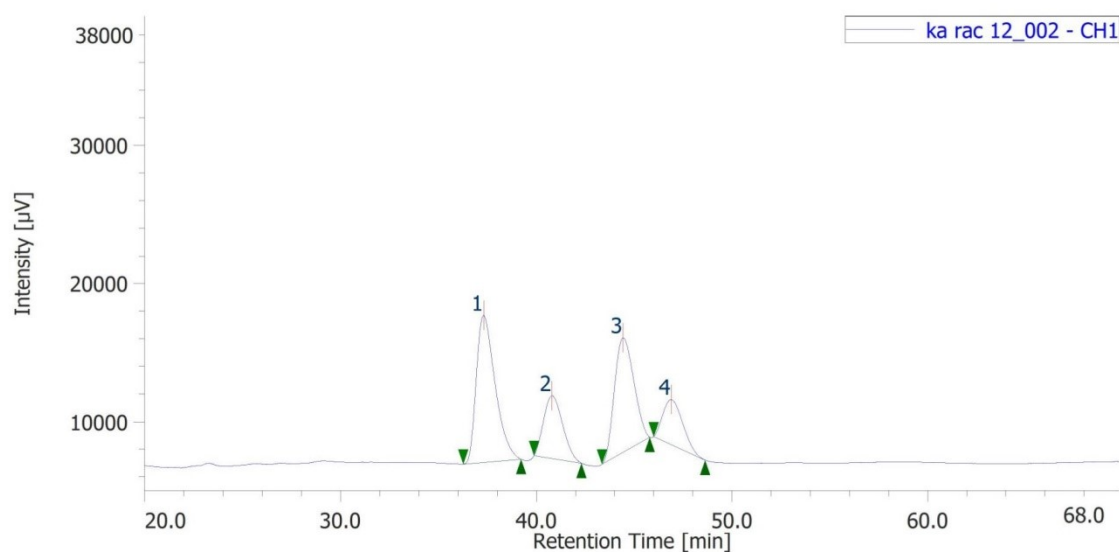
1. 3-hydroxy-1-(4-methoxybenzyl)-4-(2-methyl-1,3-dioxolan-2-yl)pyrrolidin-2-one (Racemic) **13**.

Flow rate: 0.7 mL/min

Solvent: IPA: Hexane, 50:50

Column: CHIRALPAK IC

Chromatogram



Chromatogram Information

User Name	Administrator
Date Modified	14-01-2021 16:08:53
Description	
HPLC System Name	JASCO HPLC 4000
Injection Date	14-01-2021 14:22:43
Volume	10.00 [μL]
Sample #	2
Project Name	INSTALLATION
Acquisition Time	69.8 [min]
Acquisition Sequence	
Control Method	ka rac 12
Peak ID Table	
Calibration Method	
Additional Information	

Channel & Peak Information Table

Chromatogram Name	ka rac 12_002-CH1
Sample Name	
Channel Name	CH1
Sampling Interval	500 [msec]
Peak Method	(Manual)

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	1	37.300	711610	10620	38.960	39.726	N/A	7194	1.937	1.51	
2	Unknown	1	40.792	309386	4555	16.939	17.040	N/A	7737	1.938	1.23	
3	Unknown	1	44.425	572099	8291	31.322	31.014	N/A	8711	1.267	1.18	
4	Unknown	1	46.875	233410	3267	12.779	12.219	N/A	9024	N/A	1.30	

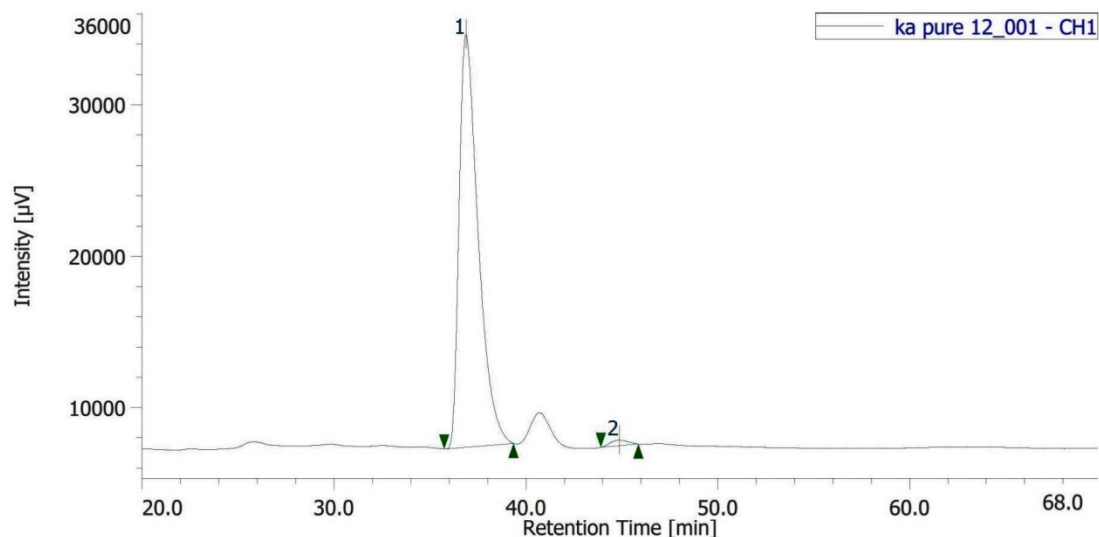
2. (3*R*,4*R*)-3-hydroxy-1-(4-methoxybenzyl)-4-(2-methyl-1,3-dioxolan-2-yl)pyrrolidin-2-one (Enantiopure) **13**. (Using (*S*)-*a,a*-diphenyl-2-pyrrolidinemethanol)

Flow rate: 0.7 mL/min

Solvent: IPA: Hexane, 50:50

Column: CHIRALPAK IC

Chromatogram



Chromatogram Information

User Name	Administrator
Date Modified	14-01-2021 16:08:52
Description	
HPLC System Name	JASCO HPLC 4000
Injection Date	14-01-2021 12:41:55
Volume	10.00 [μL]
Sample #	1
Project Name	INSTALLATION
Acquisition Time	69.8 [min]
Acquisition Sequence	
Control Method	ka pure 12
Peak ID Table	
Calibration Method	
Additional Information	

Channel & Peak Information Table

Chromatogram Name	ka pure 12_001-CH1
Sample Name	
Channel Name	CH1
Sampling Interval	500 [msec]
Peak Method	(Manual)

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	1	36.858	1884655	27243	98.751	98.662	N/A	6848	4.448	1.72	
2	Unknown	1	44.867	23846	370	1.249	1.338	N/A	9626	N/A	1.00	

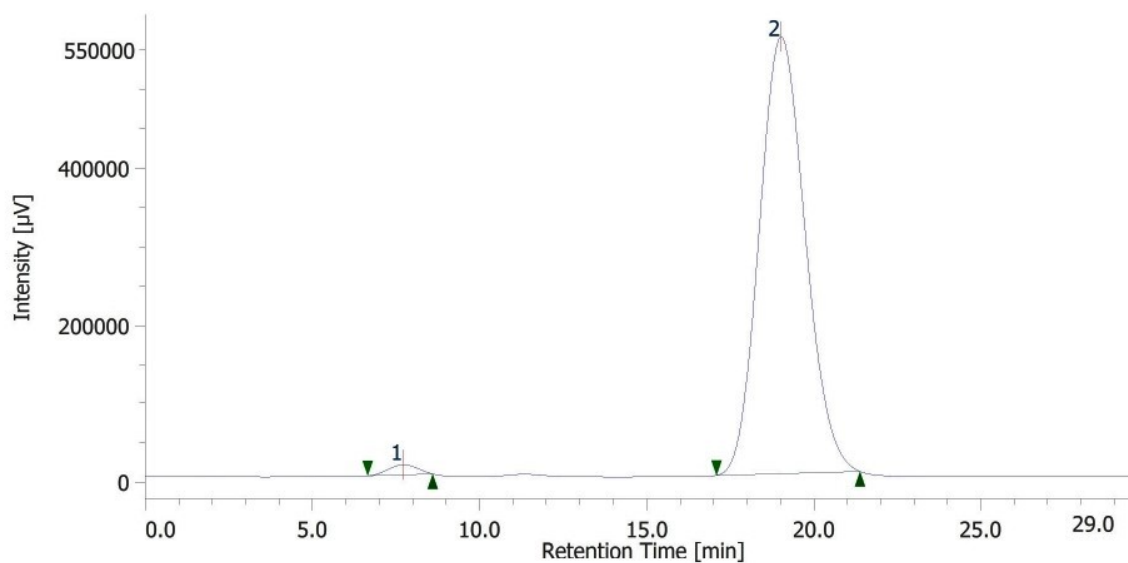
3. methyl 2-((3S,4R)-1-(4-methoxybenzyl)-2-oxo-4-(prop-1-en-2-yl)pyrrolidin-3-yl)acetate (Enantiopure) **26**

Flow rate: 0.5 mL/min

Solvent: IPA: Hexane, 50:50

Column: CHIRALPAK IC

Chromatogram



Chromatogram Information

User Name	Administrator
Date Modified	10-12-2019 13:03:02
Description	
HPLC System Name	JASCO HPLC 4000
Injection Date	10-12-2019 12:33:14
Volume	10.00 [μL]
Sample #	5
Project Name	INSTALLATION
Acquisition Time	29.8 [min]
Acquisition Sequence	
Control Method	kainic ester 01
Peak ID Table	
Calibration Method	
Additional Information	

Channel & Peak Information Table

Chromatogram Name	kainic ester 01_001-CH1
Sample Name	
Channel Name	CH1
Sampling Interval	500 [msec]
Peak Method	(Manual)

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
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2	Unknown	1	19.008	53210236	555694	98.579	97.763	N/A	890	N/A	1.13	