



Supporting Information

for

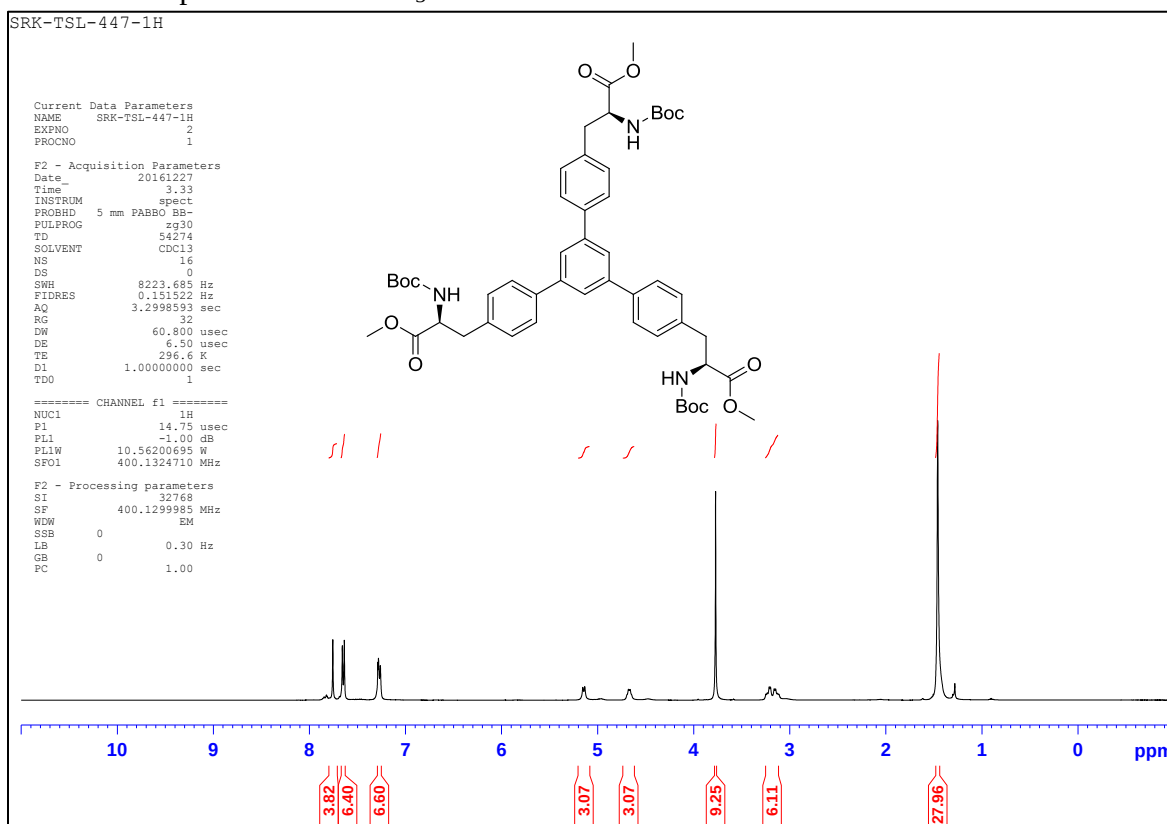
Synthesis of C_3 -symmetric star-shaped molecules containing α -amino acids and dipeptides via Negishi coupling as a key step

Sambasivarao Kotha and Saidulu Todeti

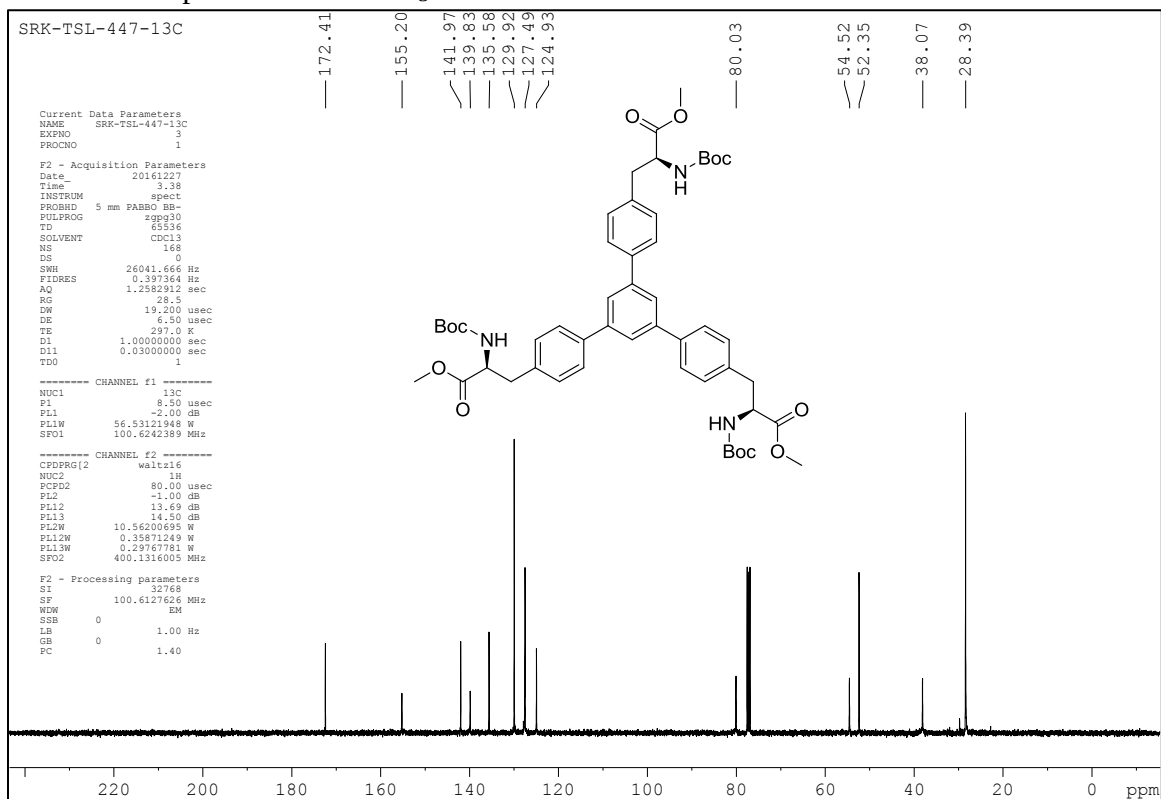
Beilstein J. Org. Chem. **2019**, *15*, 371–377. [doi:10.3762/bjoc.15.33](https://doi.org/10.3762/bjoc.15.33)

Copies of ^1H , ^{13}C NMR and HRMS spectra of new compounds

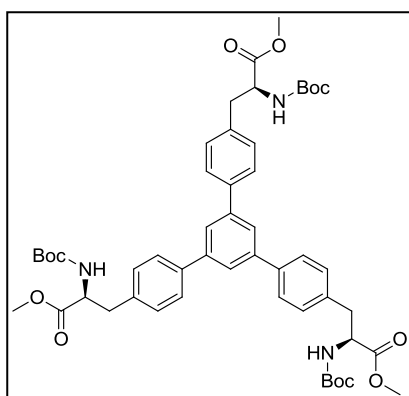
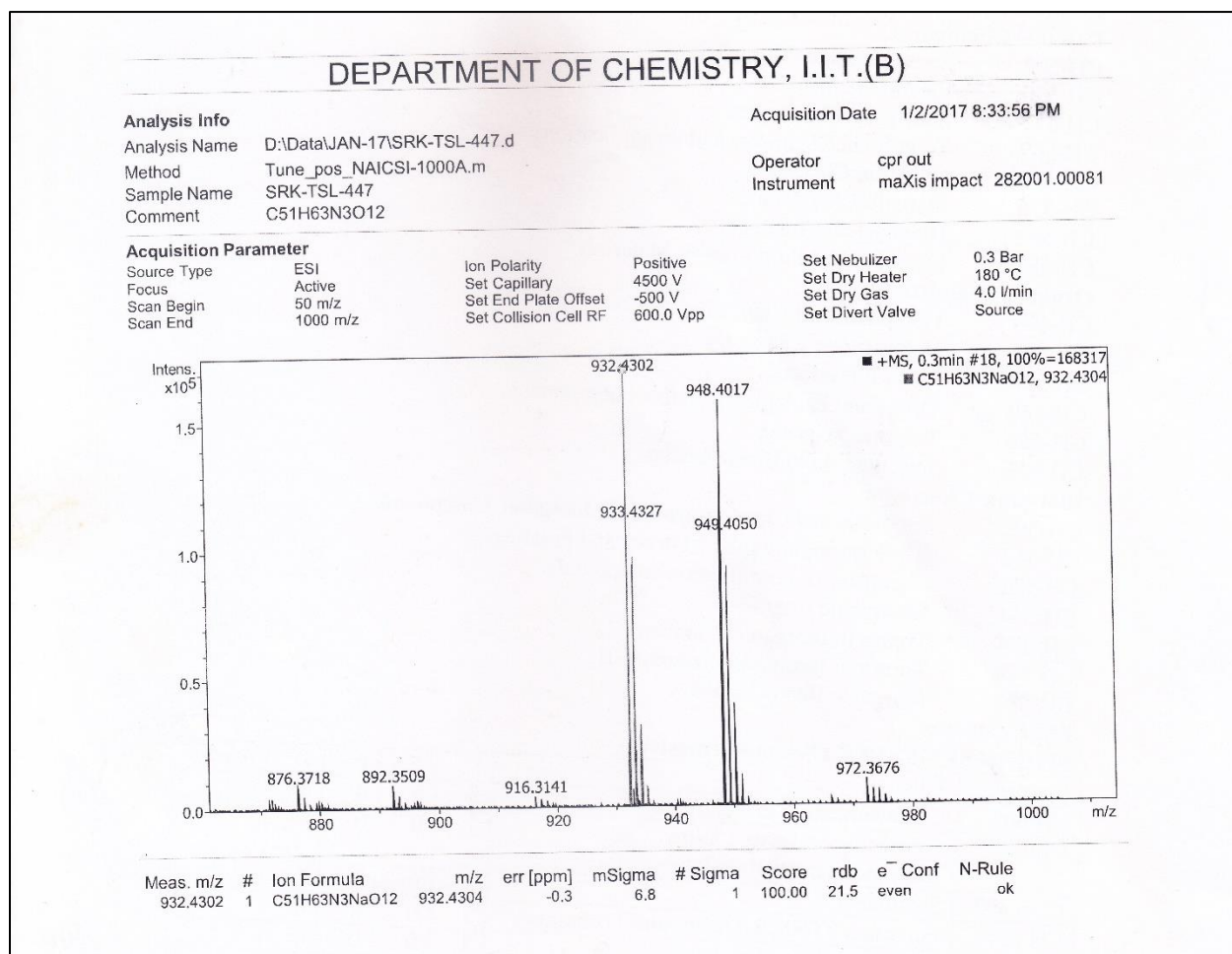
¹H NMR of compound **10** in CDCl₃



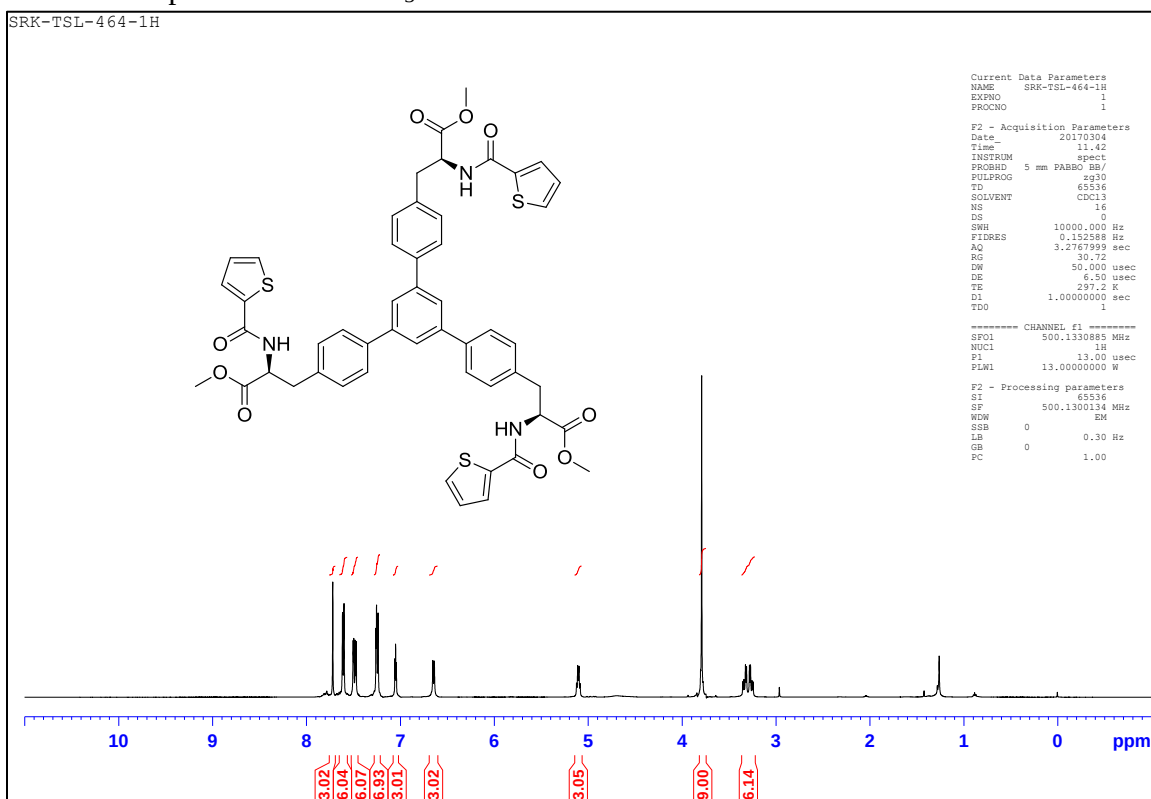
¹³C NMR of compound **10** in CDCl₃



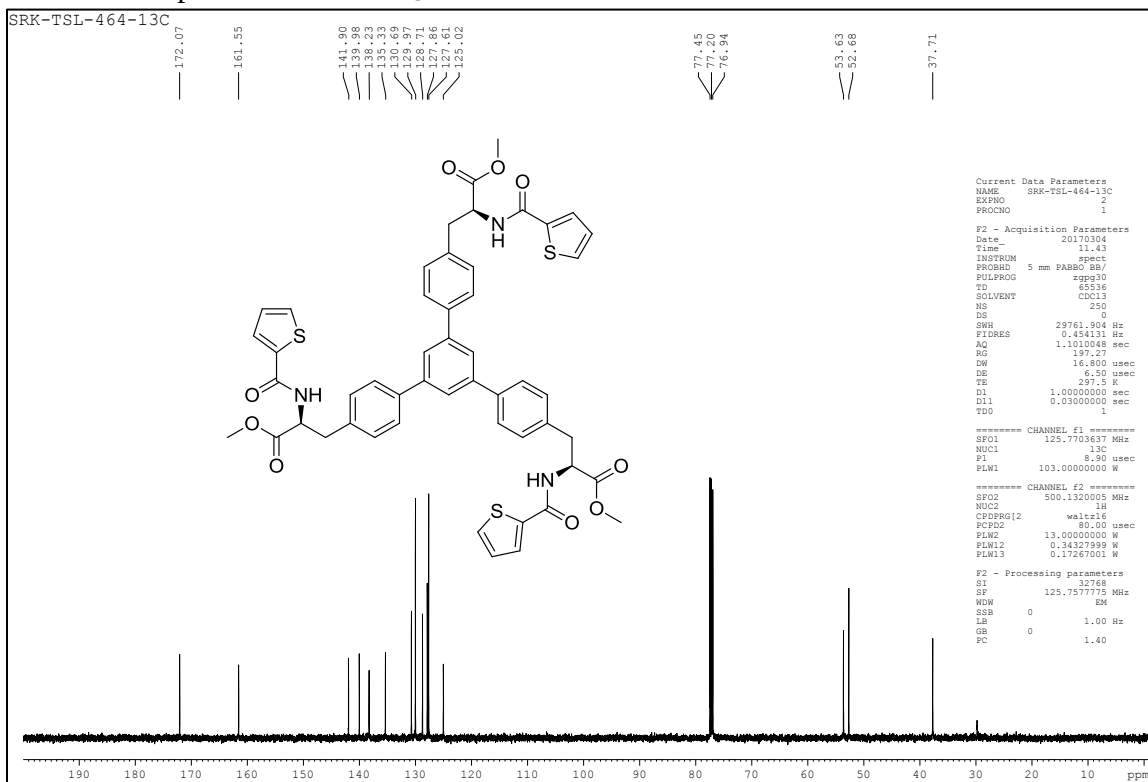
HRMS of Compound 10



¹H NMR of compound **11** in CDCl₃



¹³C NMR of compound **11** in CDCl₃



HRMS of Compound 11

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Analysis Info

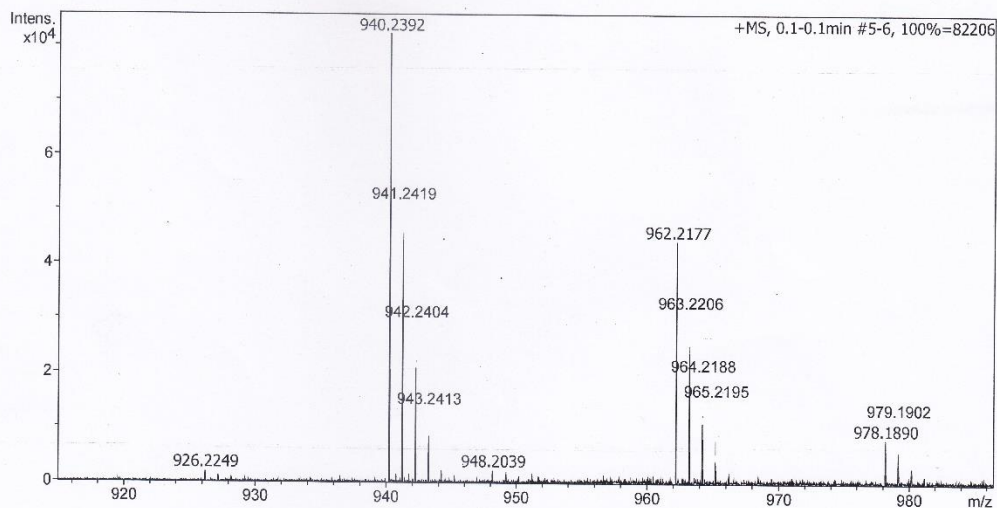
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 Comment C51H45N3O9S3

Acquisition Date 3/20/2017 12:29:39 PM

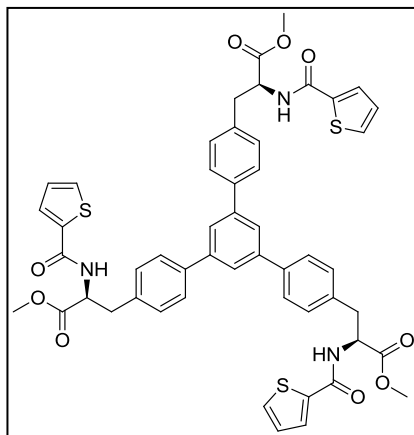
Operator SSKOUT
 Instrument maXis impact 282001.00081

Acquisition Parameter

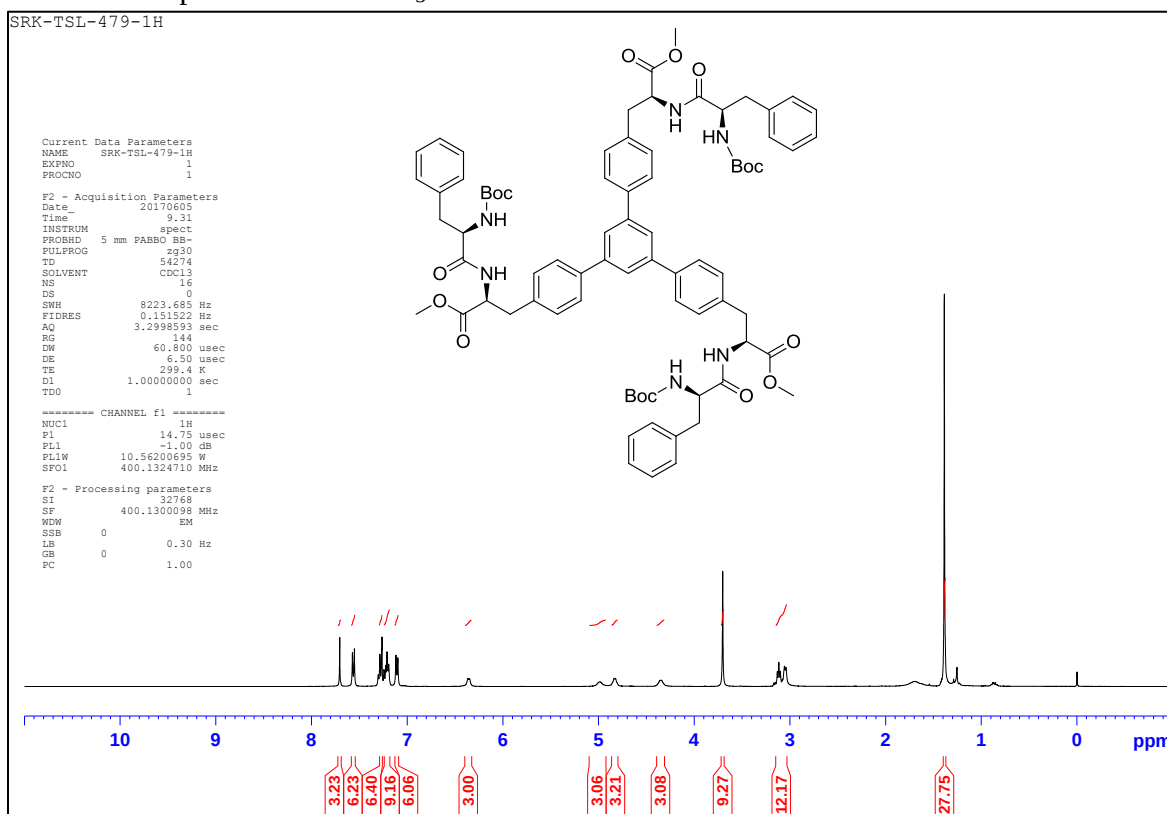
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Scan End	1500 m/z	Set Collision Cell RF	1800.0 Vpp	Set Divert Valve	Source



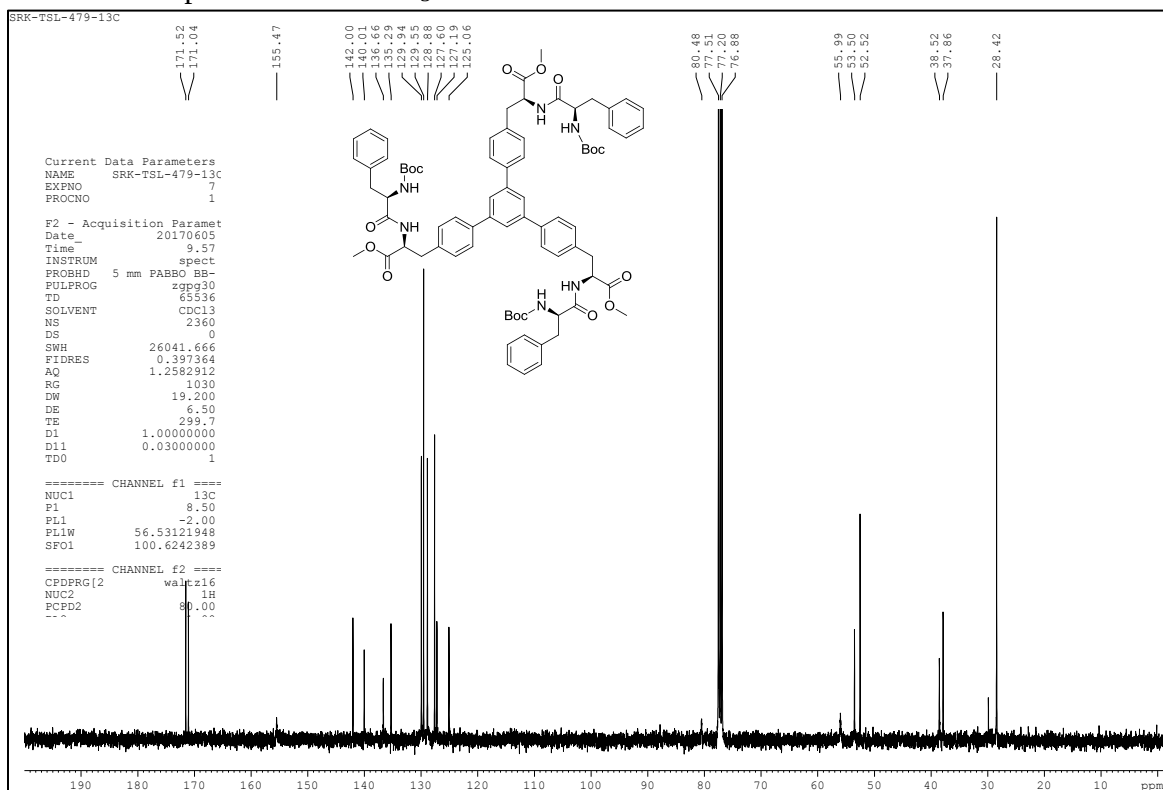
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940.2392	1	C51H46N3O9S3	940.2391	-0.1	40.7	1	100.00	30.5	even	ok



¹H NMR of compound **13** in CDCl₃



¹³C NMR of compound **13** in CDCl₃



HRMS of Compound 13

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Analysis Info

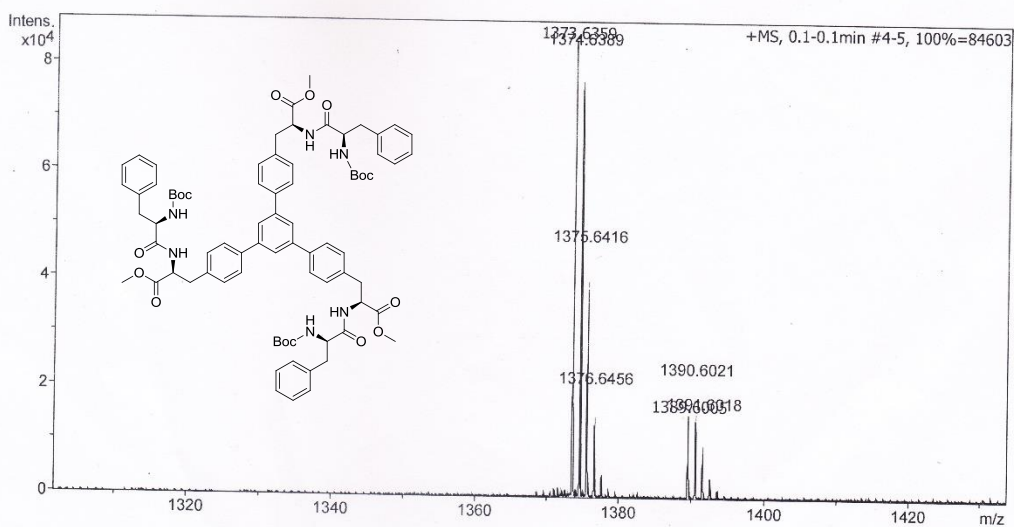
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Acquisition Date 5/2/2017 6:14:47 PM

Operator SRK-IN
 Instrument maXis impact 282001.00081

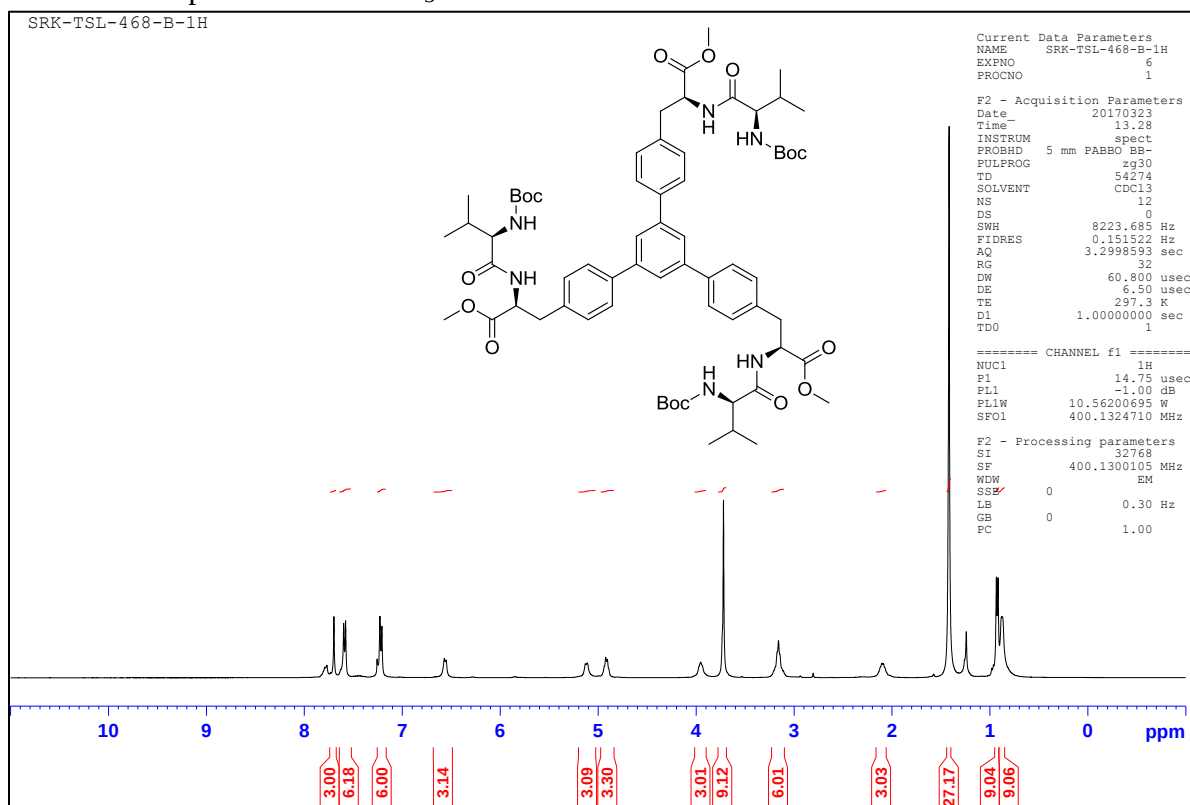
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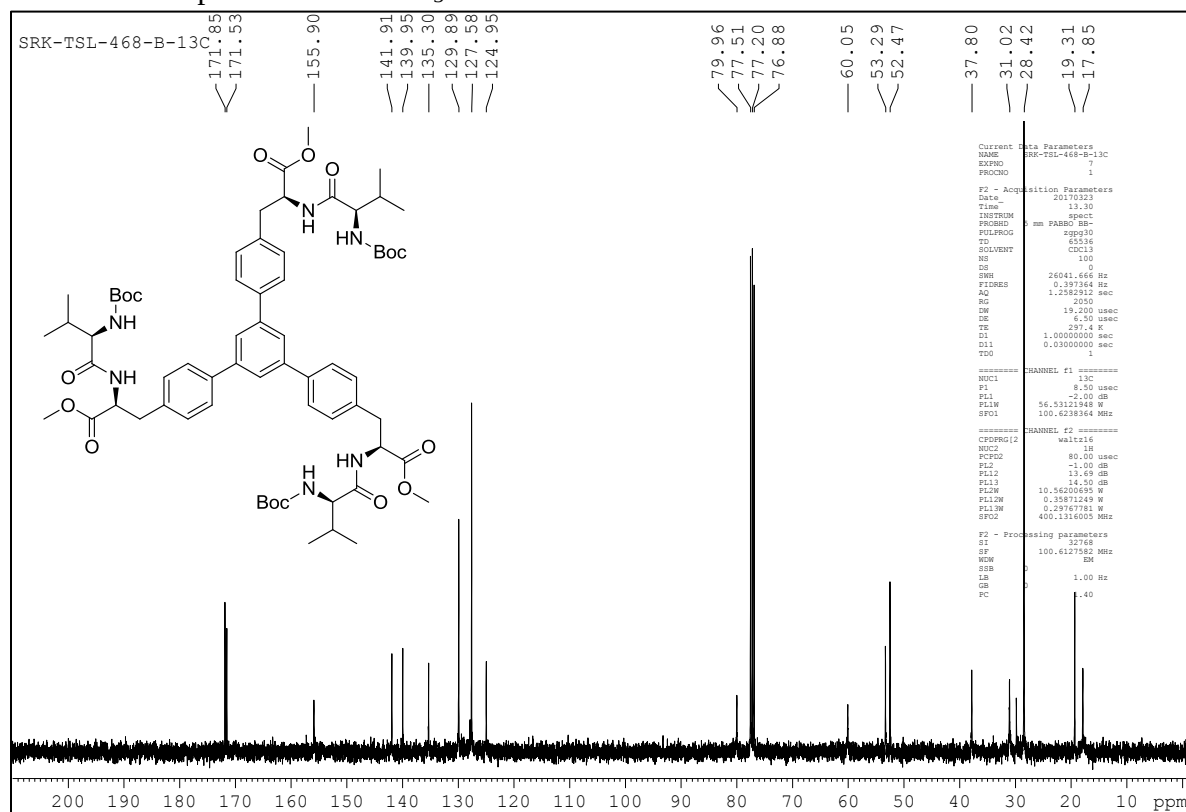


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
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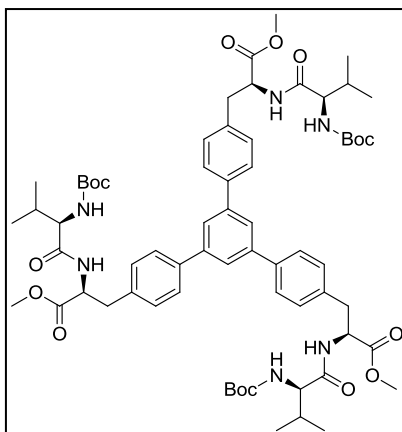
¹H NMR of compound **12** in CDCl₃



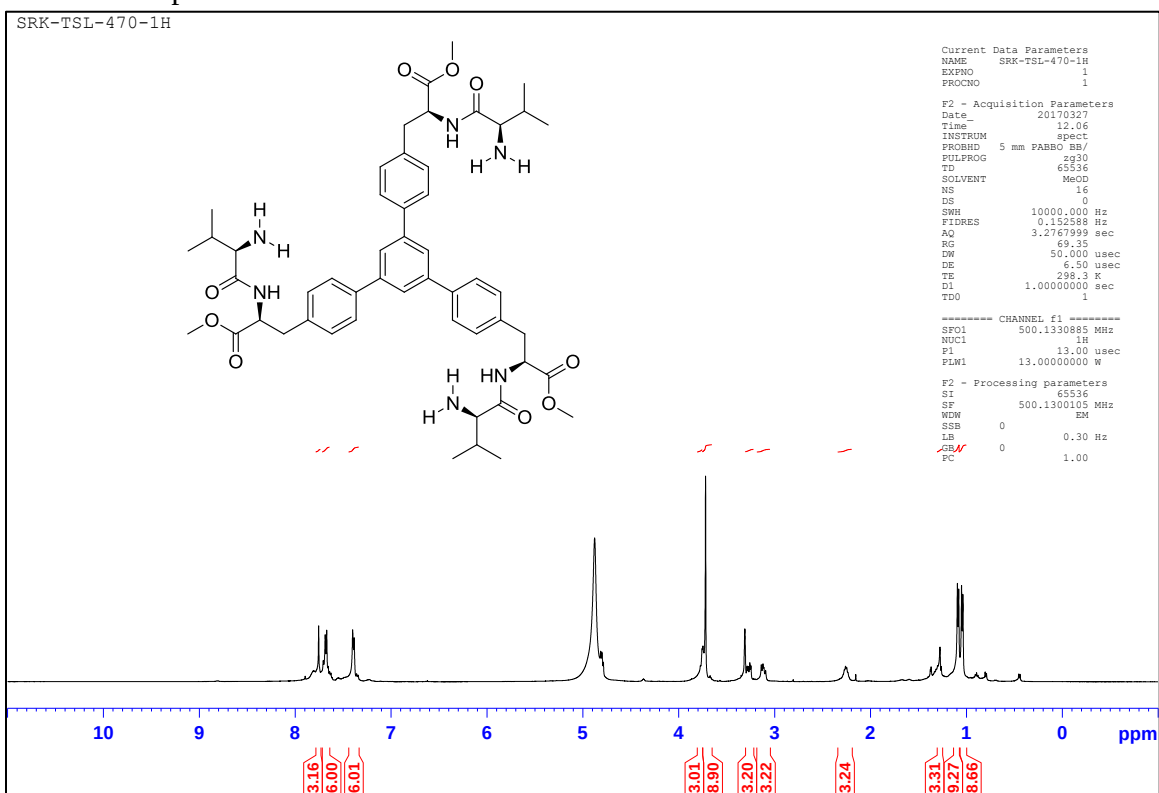
¹³C NMR of compound **12** in CDCl₃



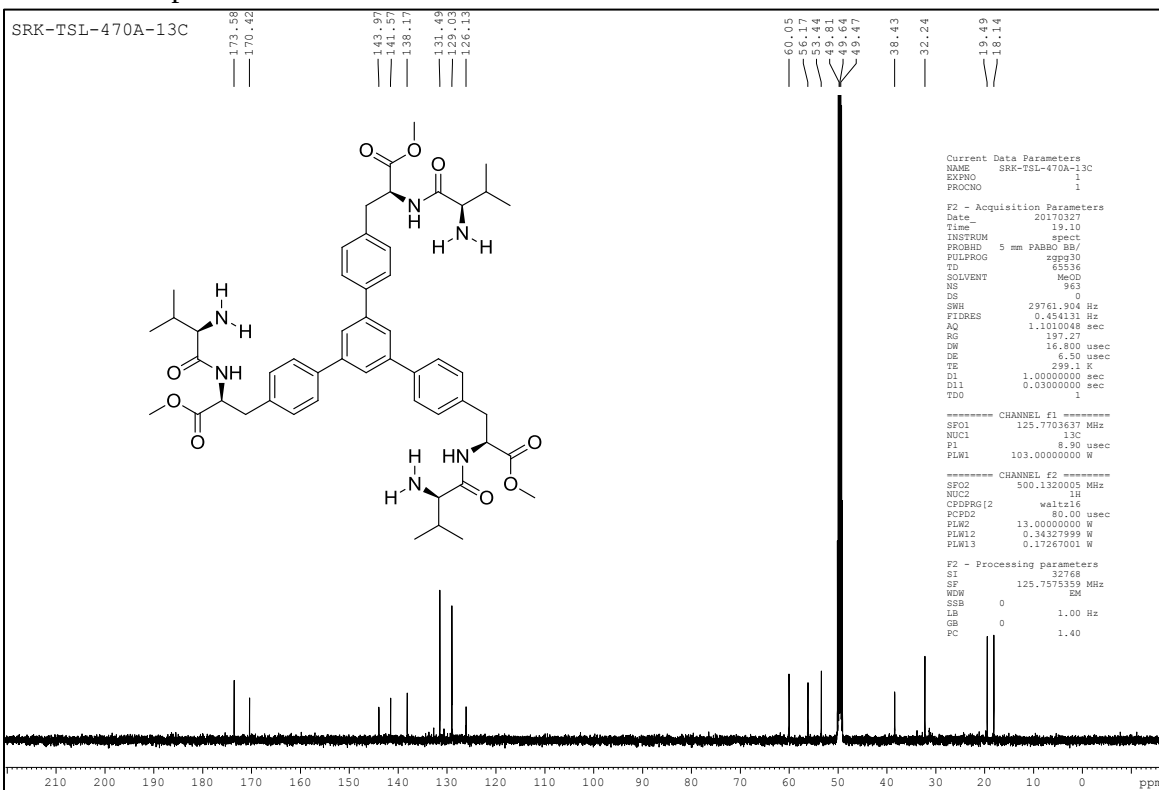
DEPARTMENT OF CHEMISTRY, I.I.T.(B)																															
Analysis Info					Acquisition Date 3/23/2017 9:01:06 AM																										
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Method Tune_pos_NAICSI-1500A.m					Operator srk-in																										
Sample Name SRK-TSL-468					Instrument maXis impact 282001.00081																										
Comment C66H90N6O15																															
Acquisition Parameter																															
Source Type ESI		Ion Polarity Positive		Set Nebulizer 0.3 Bar																											
Focus Active		Set Capillary 3700 V		Set Dry Heater 180 °C																											
Scan Begin 50 m/z		Set End Plate Offset -500 V		Set Dry Gas 4.0 l/min																											
Scan End 1500 m/z		Set Collision Cell RF 1800.0 Vpp		Set Divert Valve Source																											
Intens. +MS, 0.4-0.5min #23-24, 100%=674																															
<table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th>Meas. m/z</th> <th>#</th> <th>Ion Formula</th> <th>m/z</th> <th>err [ppm]</th> <th>mSigma</th> <th># Sigma</th> <th>Score</th> <th>rdb</th> <th>e⁻ Conf</th> <th>N-Rule</th> </tr> </thead> <tbody> <tr> <td>1229.6359</td> <td>1</td> <td>C66H90N6NaO15</td> <td>1229.6356</td> <td>-0.3</td> <td>28.2</td> <td>1</td> <td>100.00</td> <td>24.5</td> <td>even</td> <td>ok</td> </tr> </tbody> </table>										Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule	1229.6359	1	C66H90N6NaO15	1229.6356	-0.3	28.2	1	100.00	24.5	even	ok
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule																					
1229.6359	1	C66H90N6NaO15	1229.6356	-0.3	28.2	1	100.00	24.5	even	ok																					



¹H NMR of compound **14** in MeOD



¹H NMR of compound **14** in MeOD



HRMS of Compound 14

