

Supporting Information

for

Design and synthesis of C_3 -symmetric molecules bearing propellane moieties via cyclotrimerization and a ring-closing metathesis sequence

Sambasivarao Kotha*, Saidulu Todeti, and Vikas R. Aswar

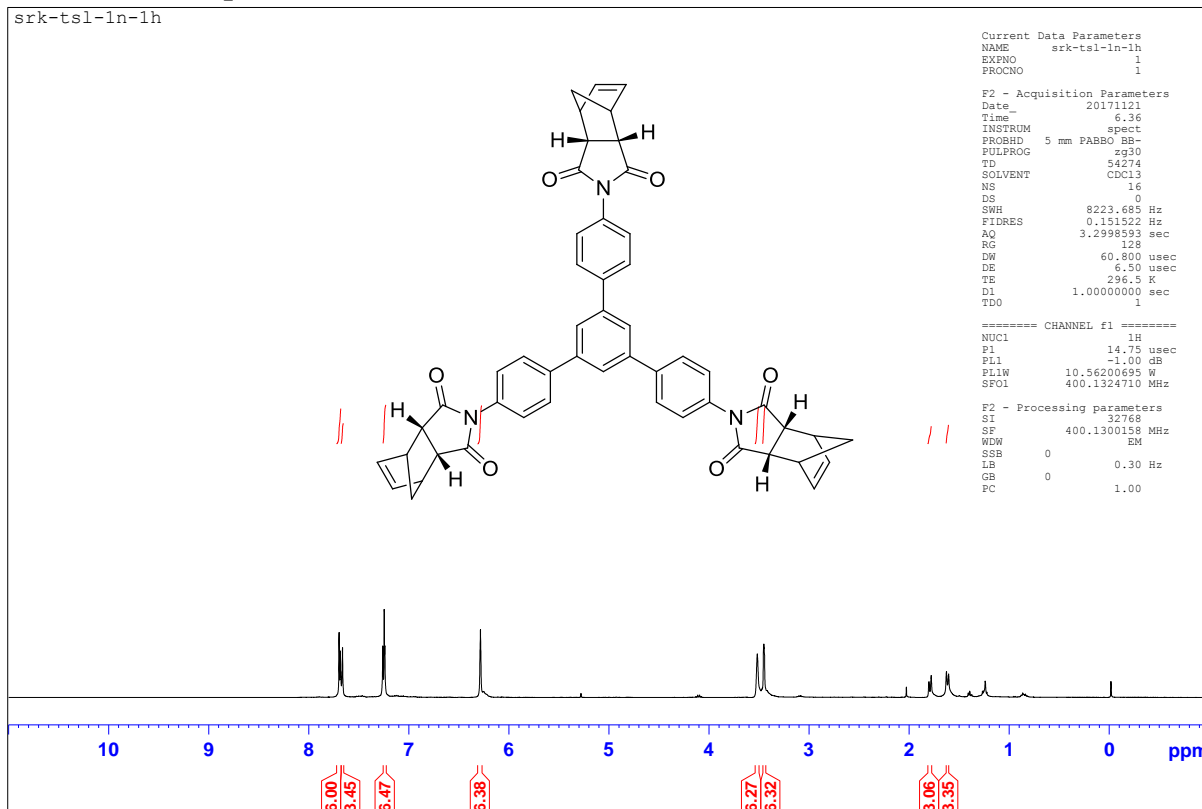
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Email: Sambasivarao Kotha - srk@chem.iitb.ac.in

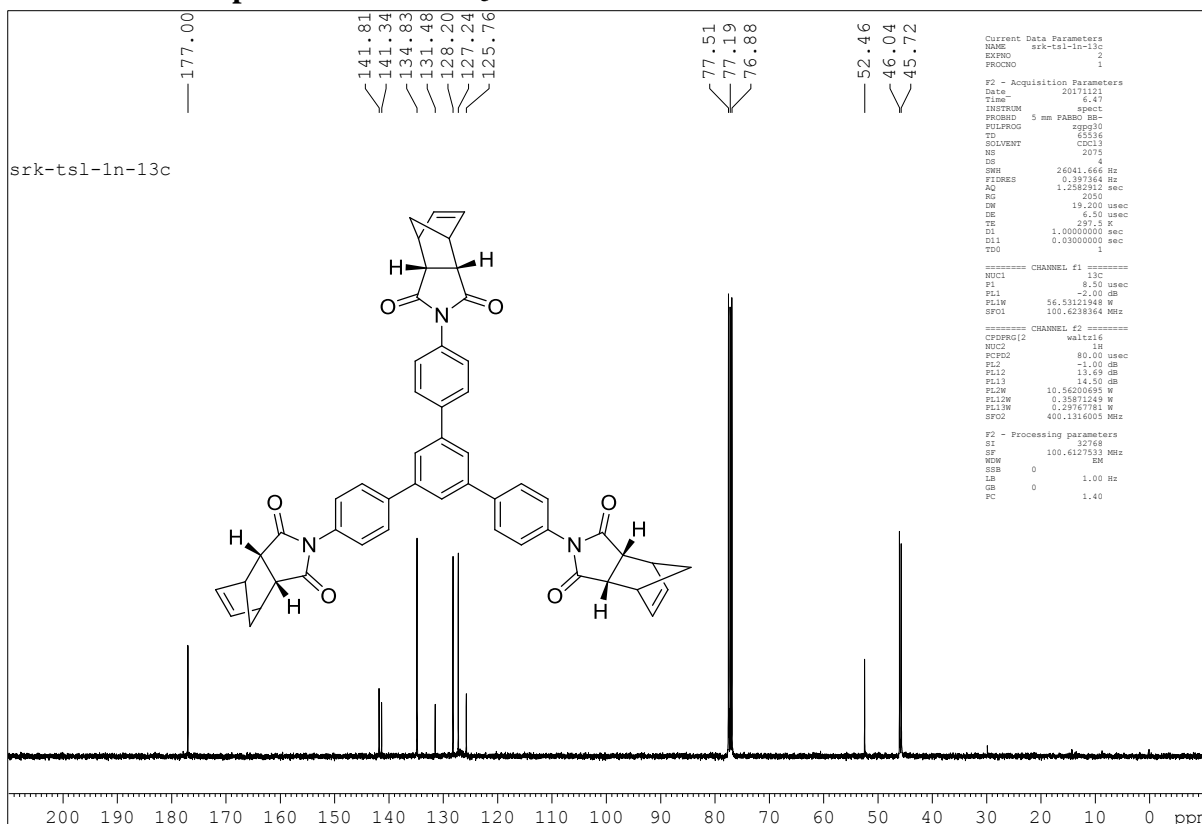
*Corresponding author

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

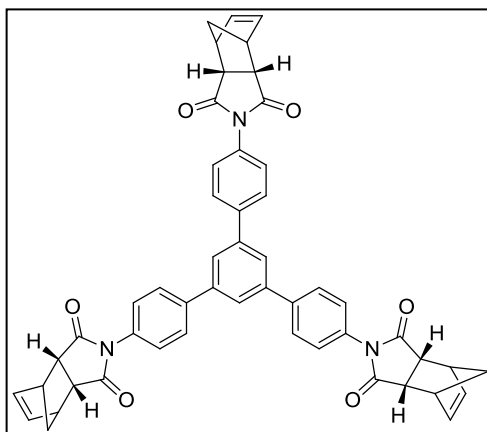
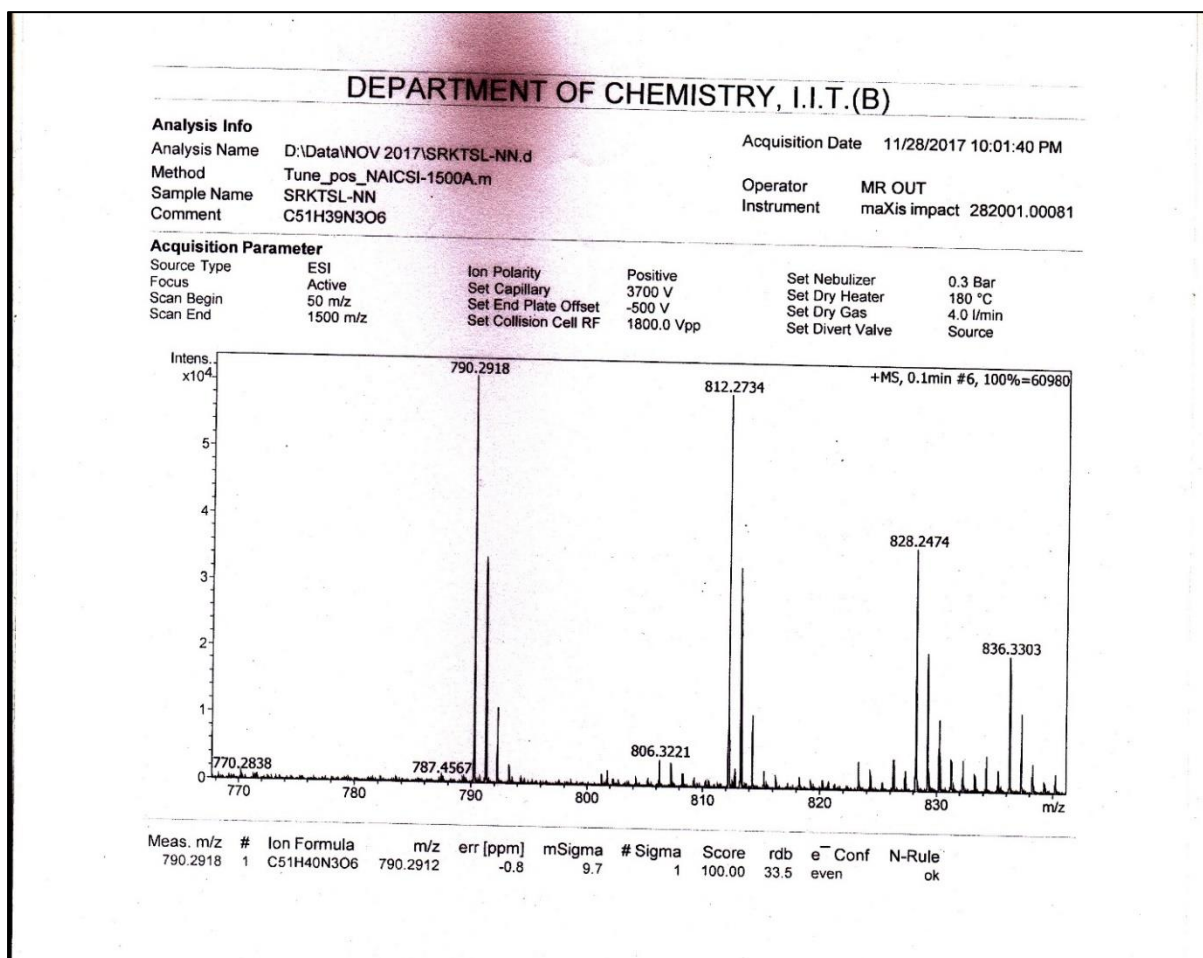
¹H NMR of compound 11 in CDCl₃



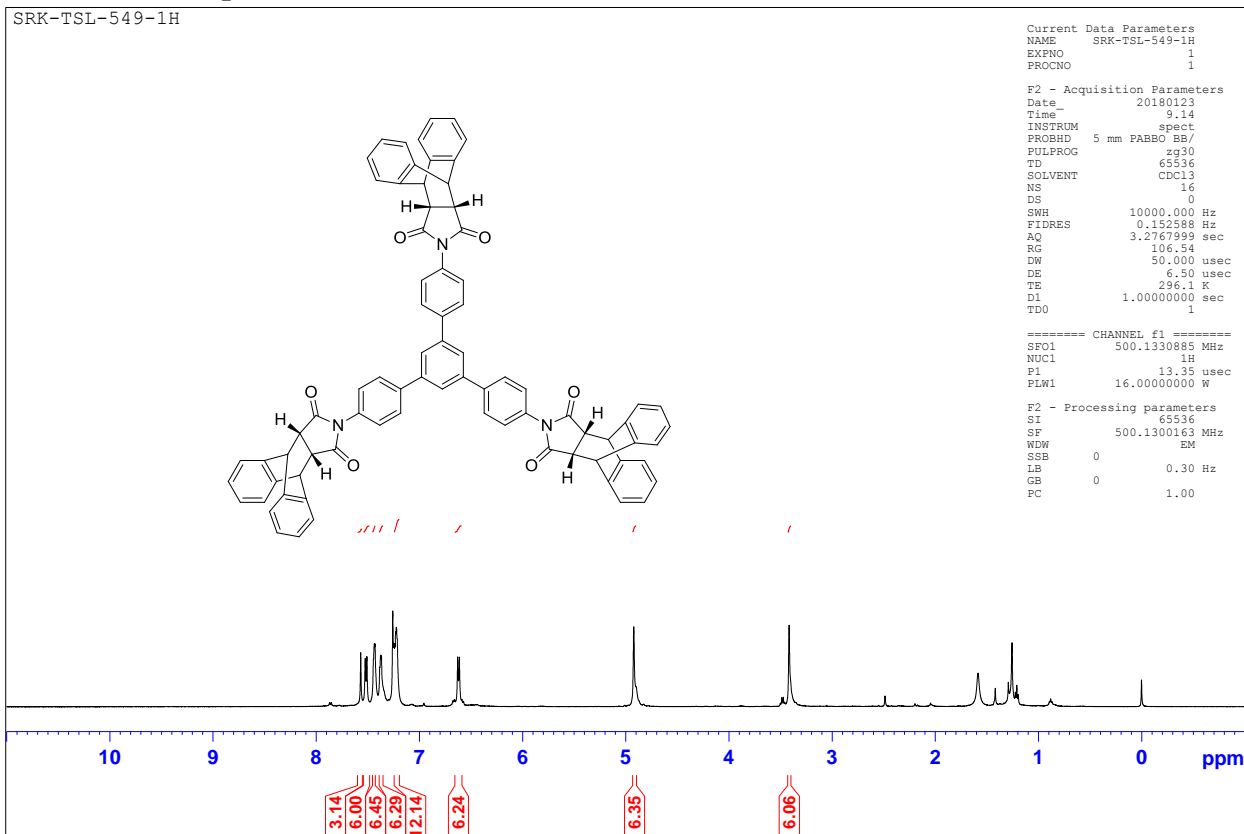
¹³C NMR of compound 11 in CDCl₃



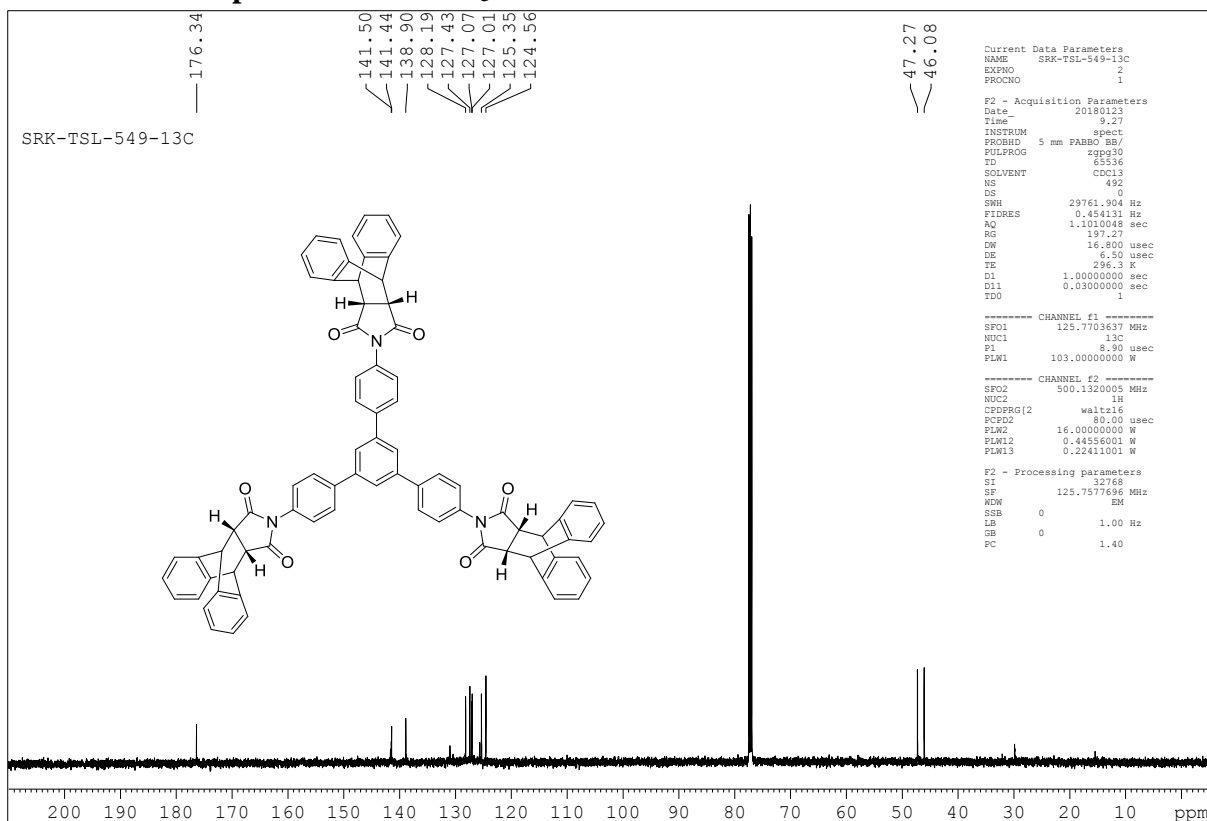
HRMS of Compound 11



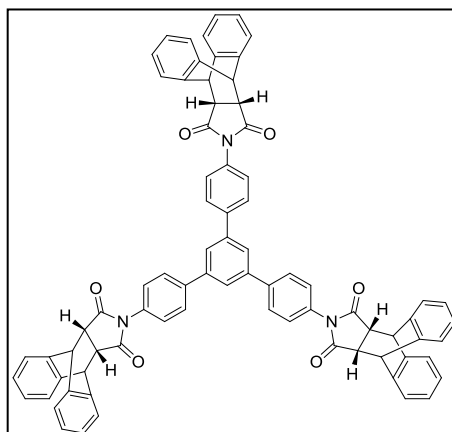
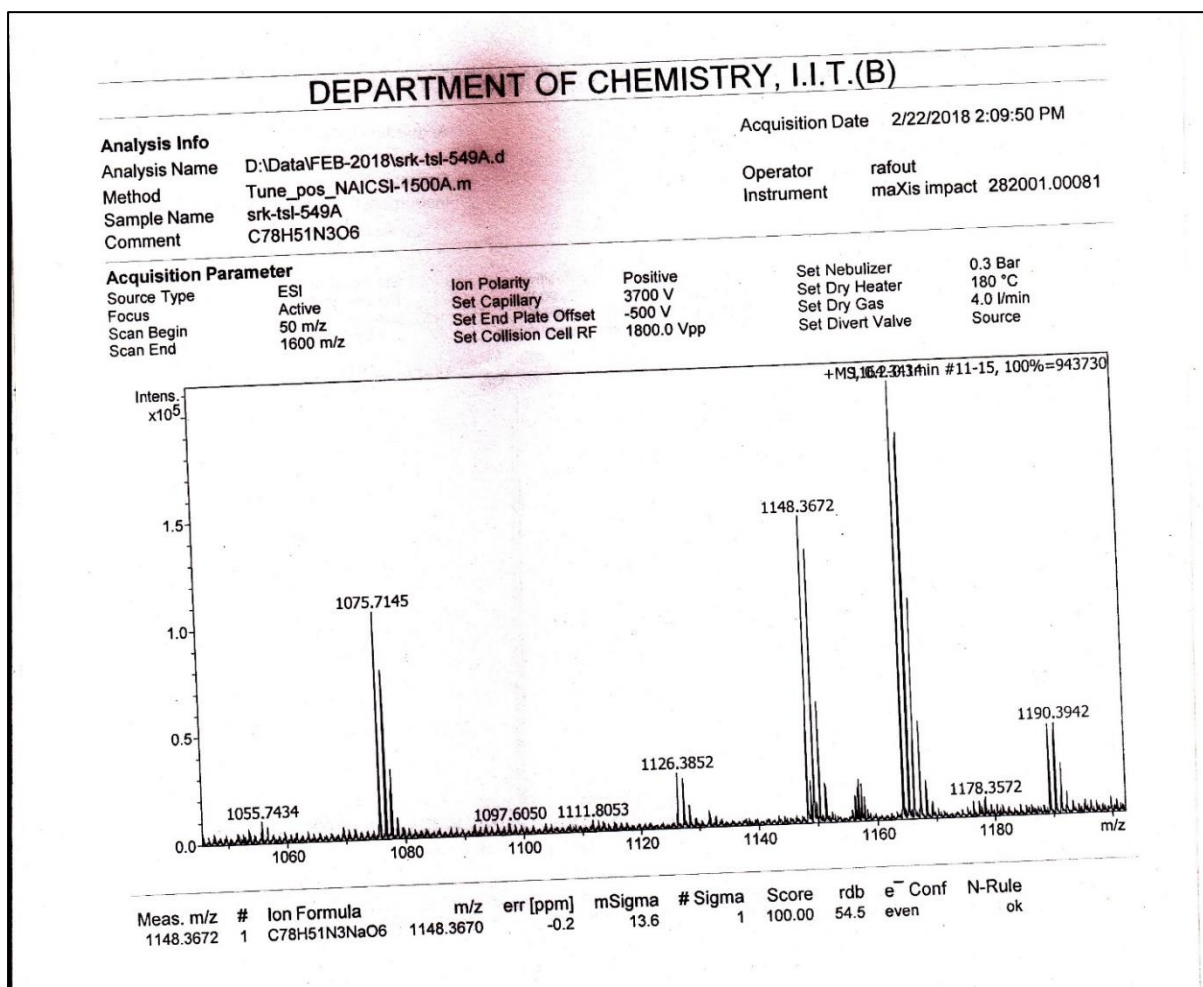
¹H NMR of compound 19 in CDCl₃



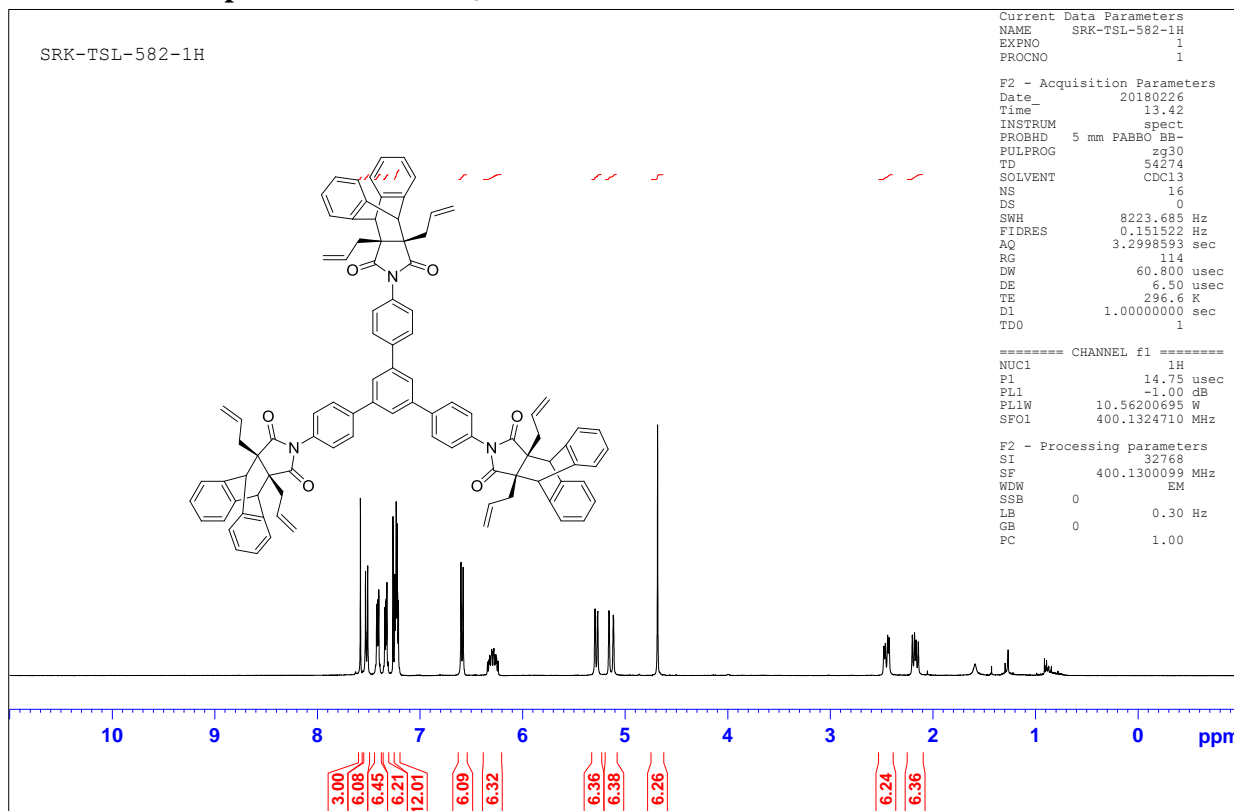
¹³C NMR of compound 19 in CDCl₃



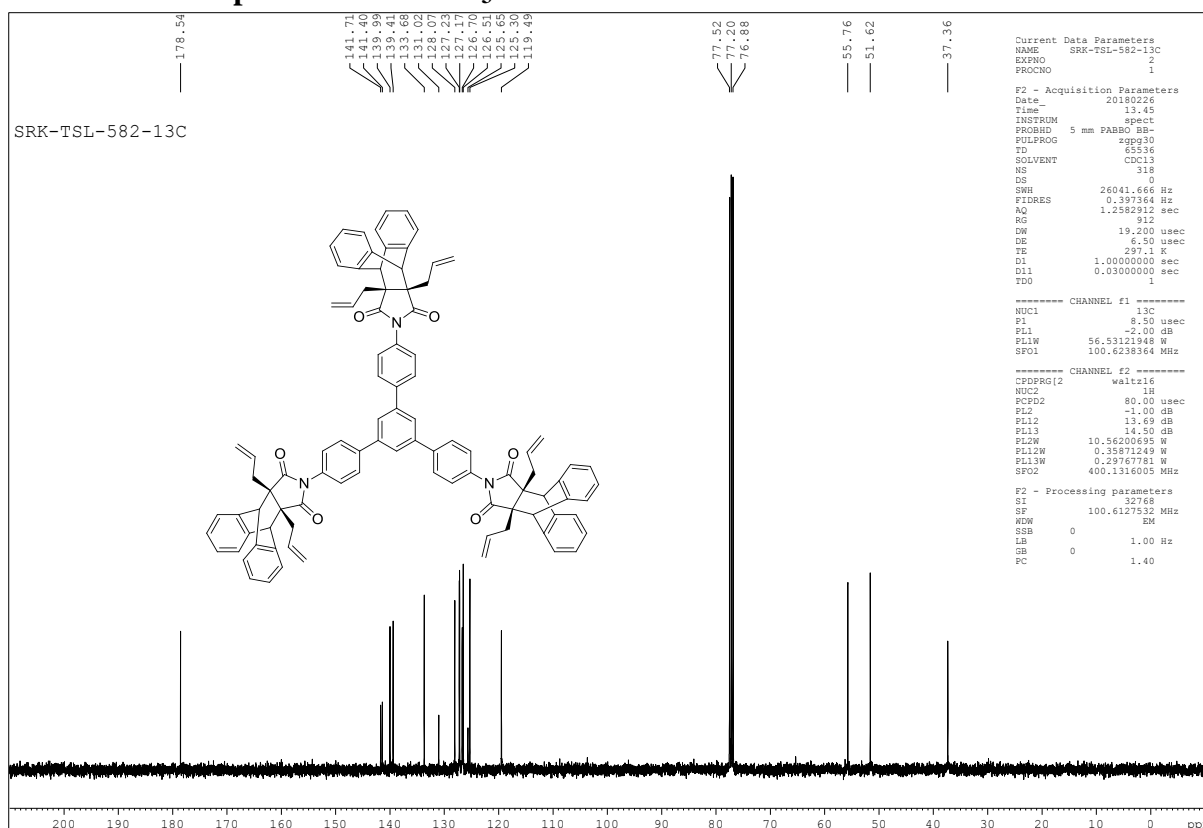
HRMS of Compound 19



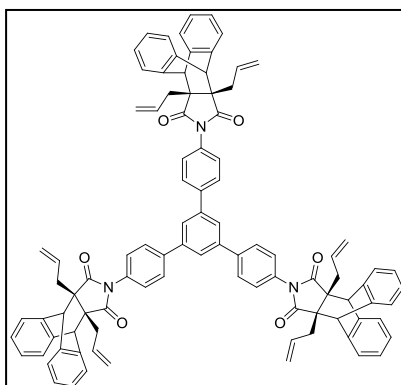
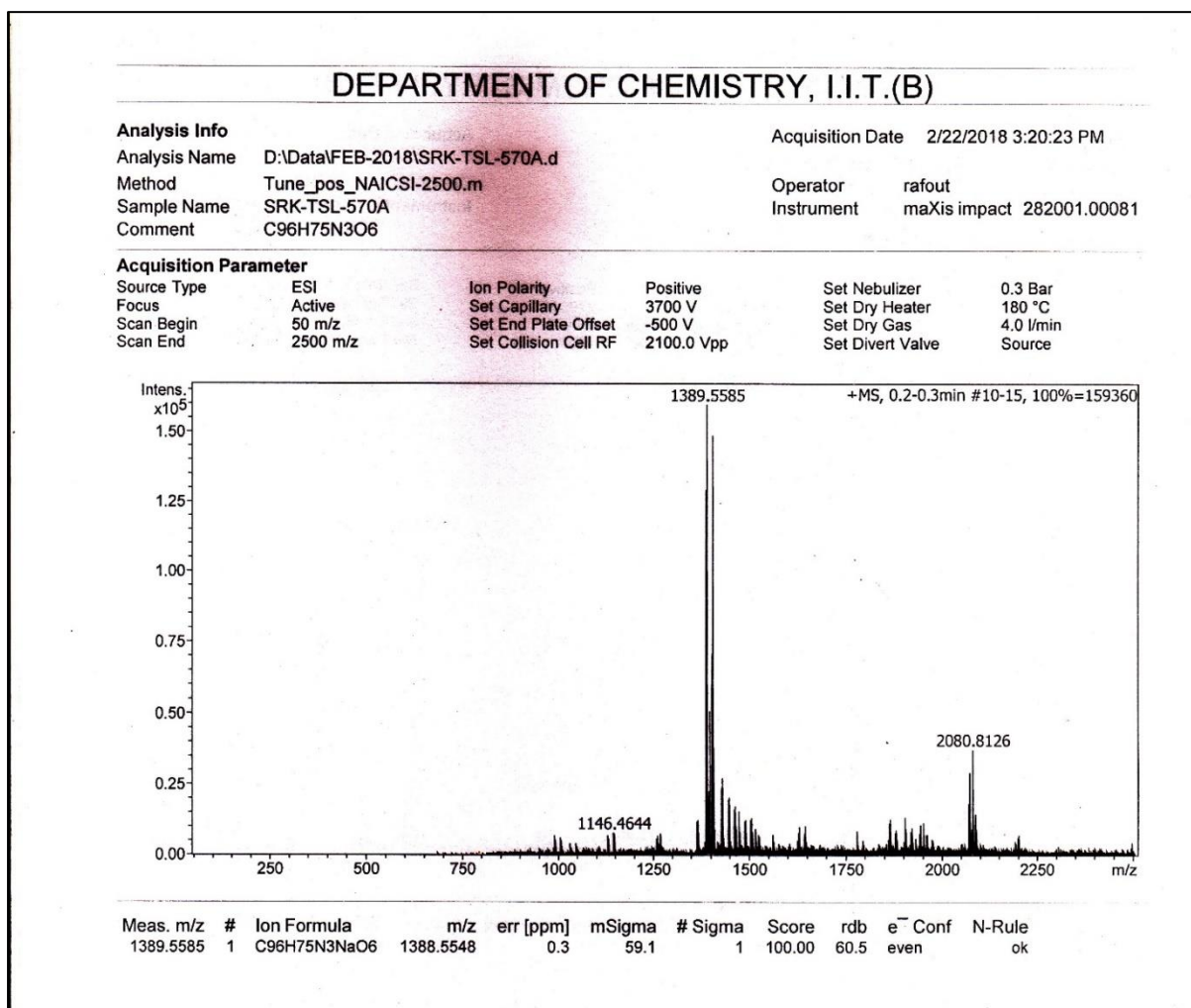
¹H NMR of compound 20 in CDCl₃



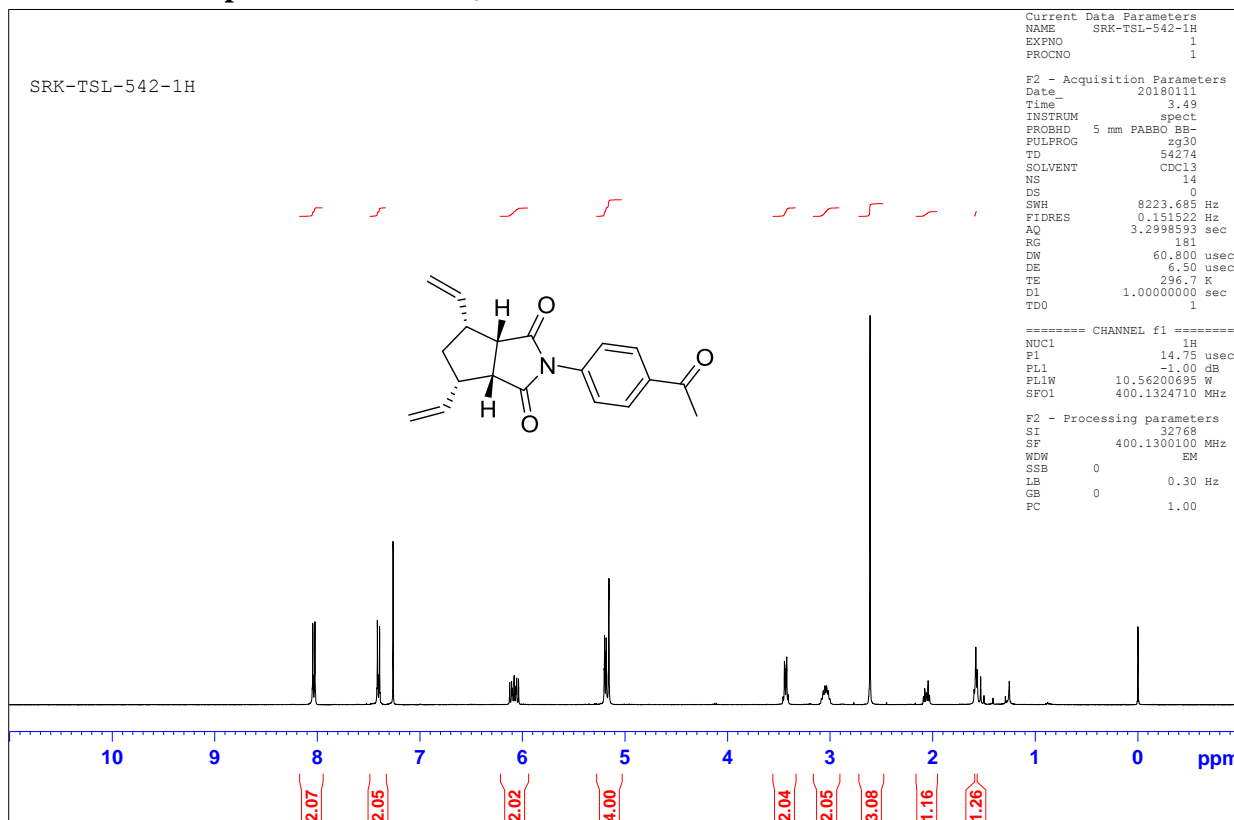
¹³C NMR of compound 20 in CDCl₃



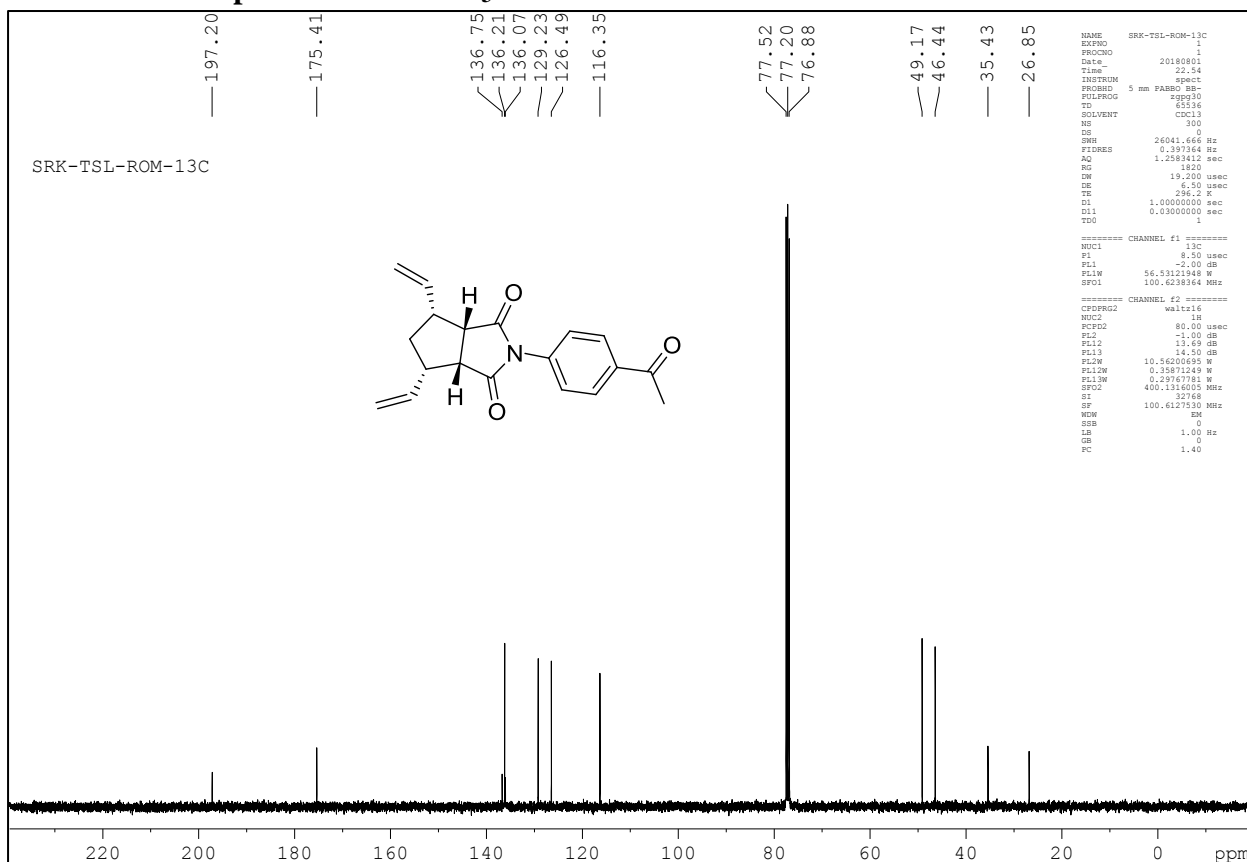
HRMS of compound 20



¹H NMR of compound 13 in CDCl₃



¹³C NMR of compound 13 in CDCl₃



HRMS of Compound 13

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Analysis Info

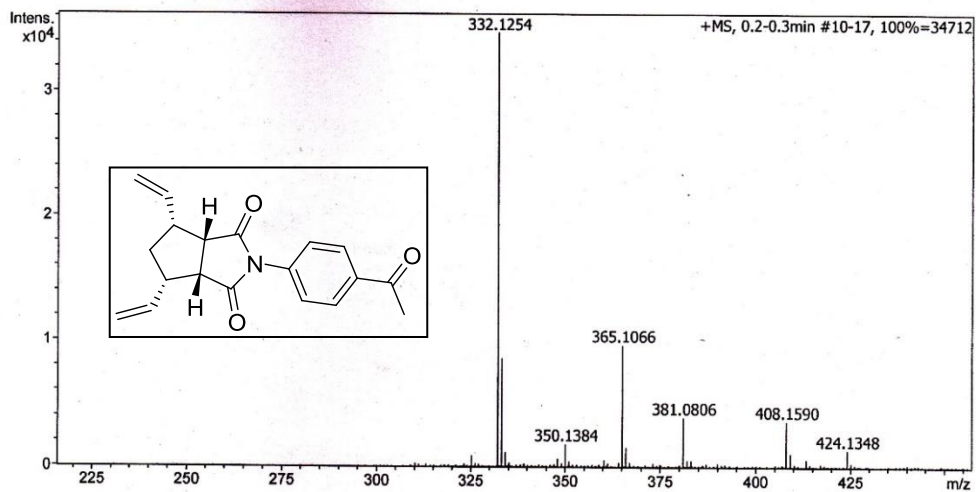
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 Method Tune_pos_NAICSI-500a.m
 Sample Name SRK-TSL-562
 Comment C19H19NO3

Acquisition Date 2/6/2018 9:40:42 PM

Operator ssk out
 Instrument maXis impact 282001.00081

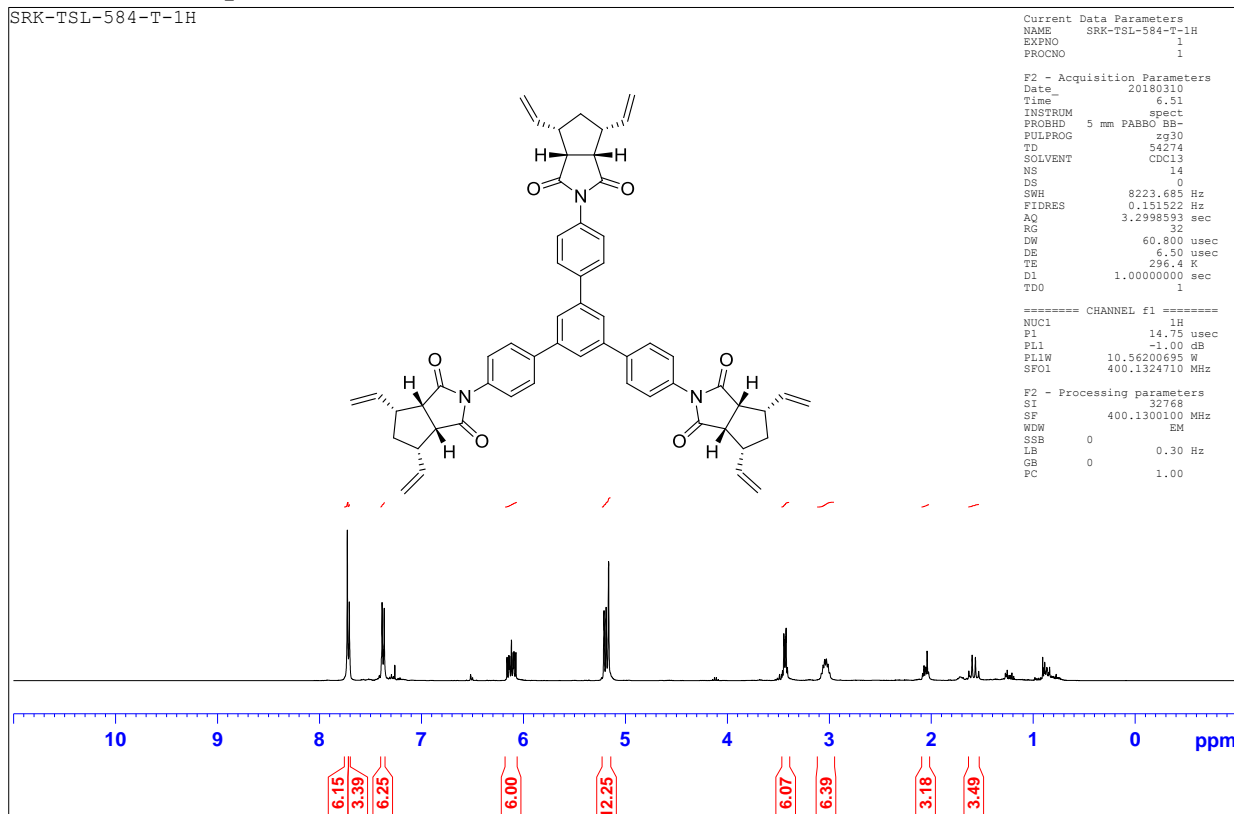
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 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	1000 m/z	Set Collision Cell RF	950.0 Vpp	Set Divert Valve	Source

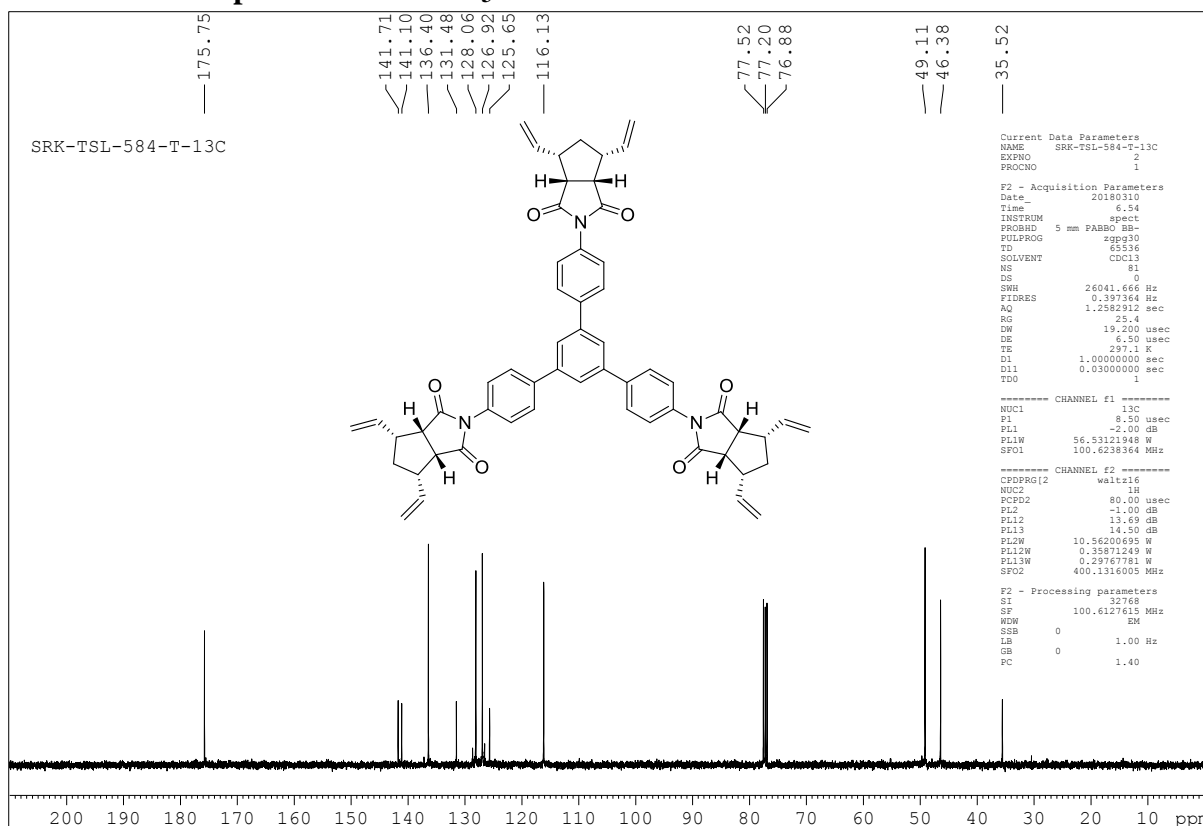


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
332.1254	1	C19H19NNaO3	332.1257	-0.8	20.8	1	100.00	10.5	even	ok

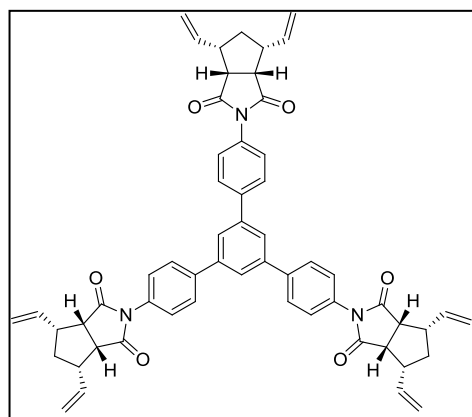
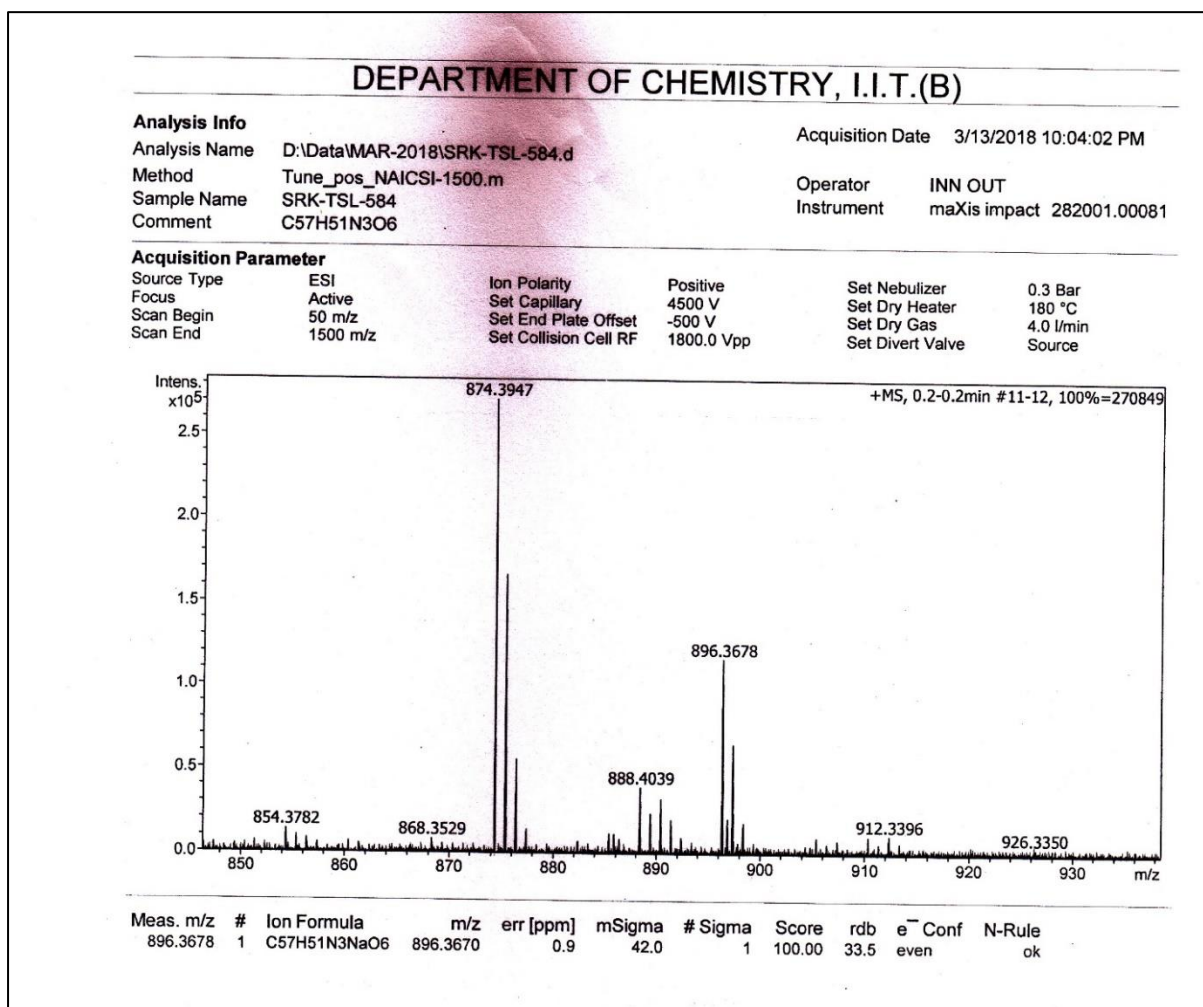
¹H NMR of compound 12 in CDCl₃



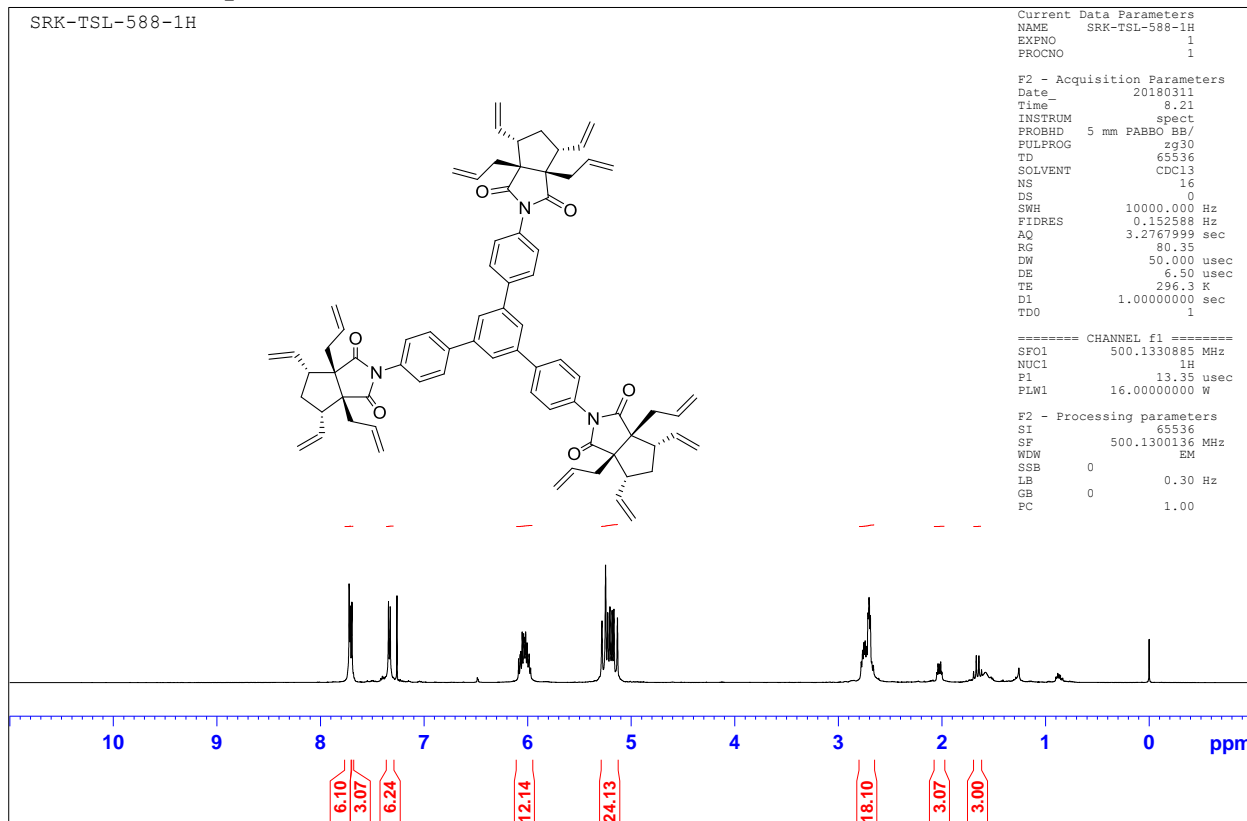
¹³C NMR of compound 12 in CDCl₃



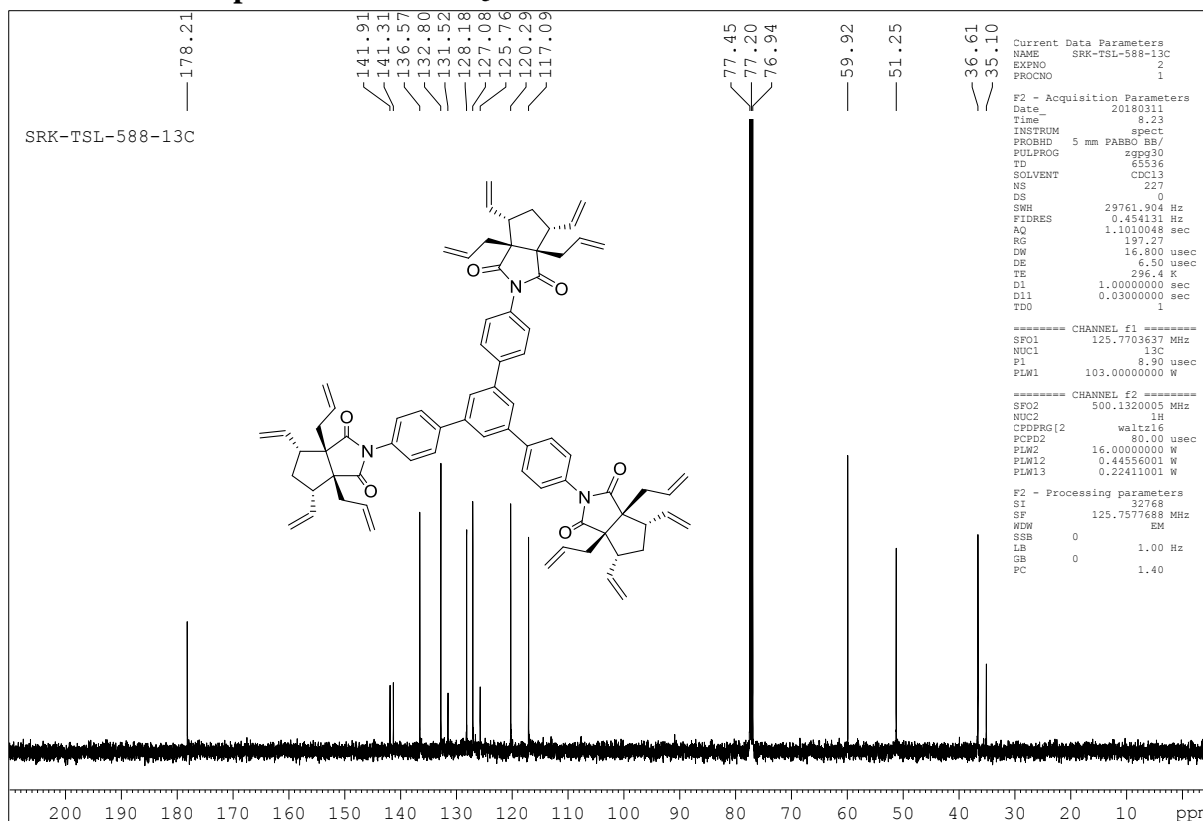
HRMS of Compound 12



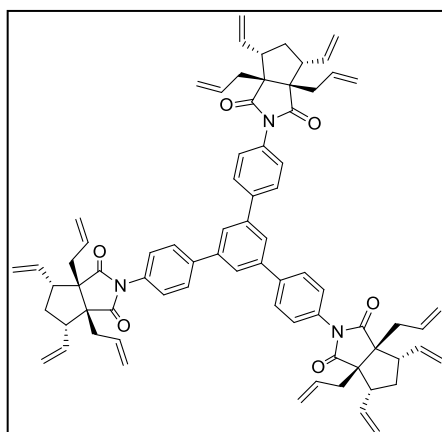
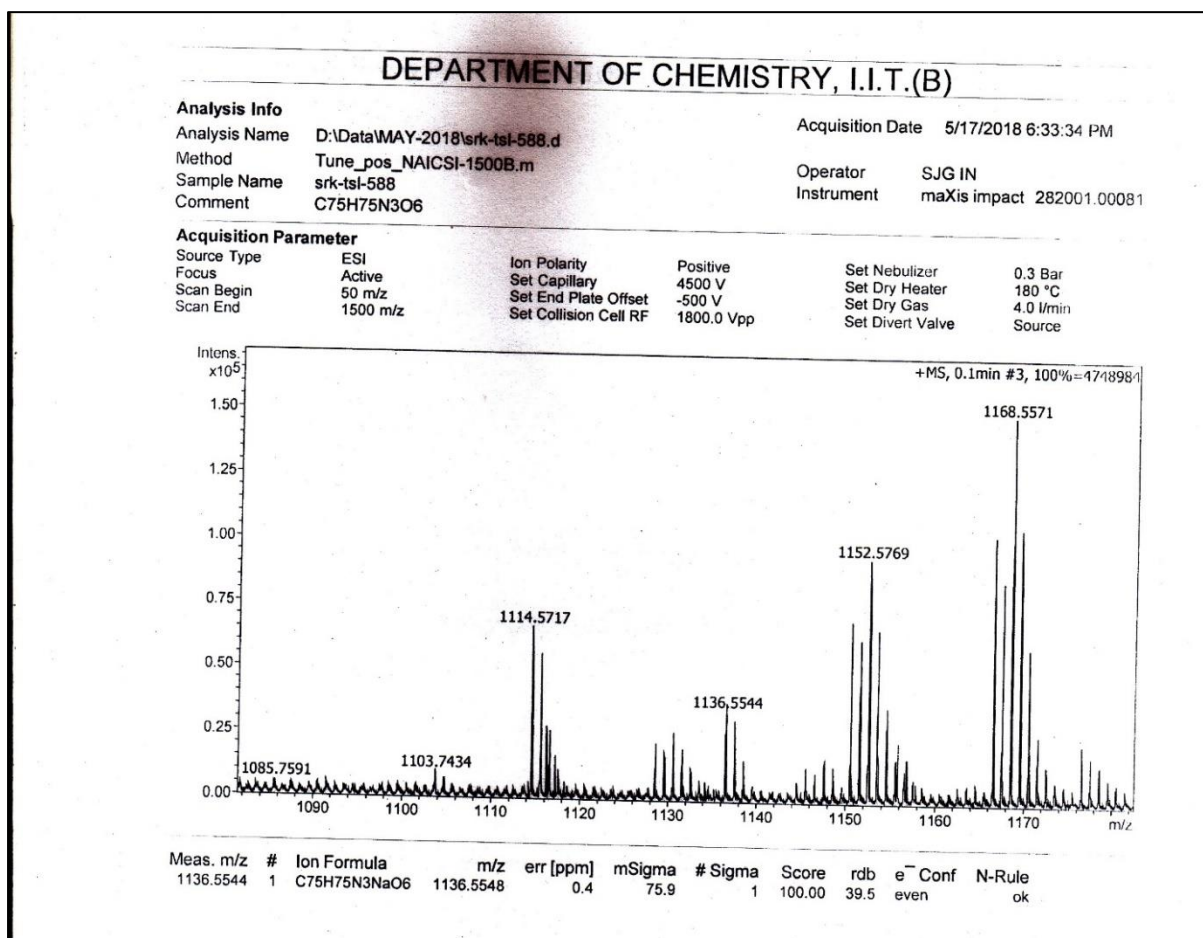
¹H NMR of compound 14 in CDCl₃



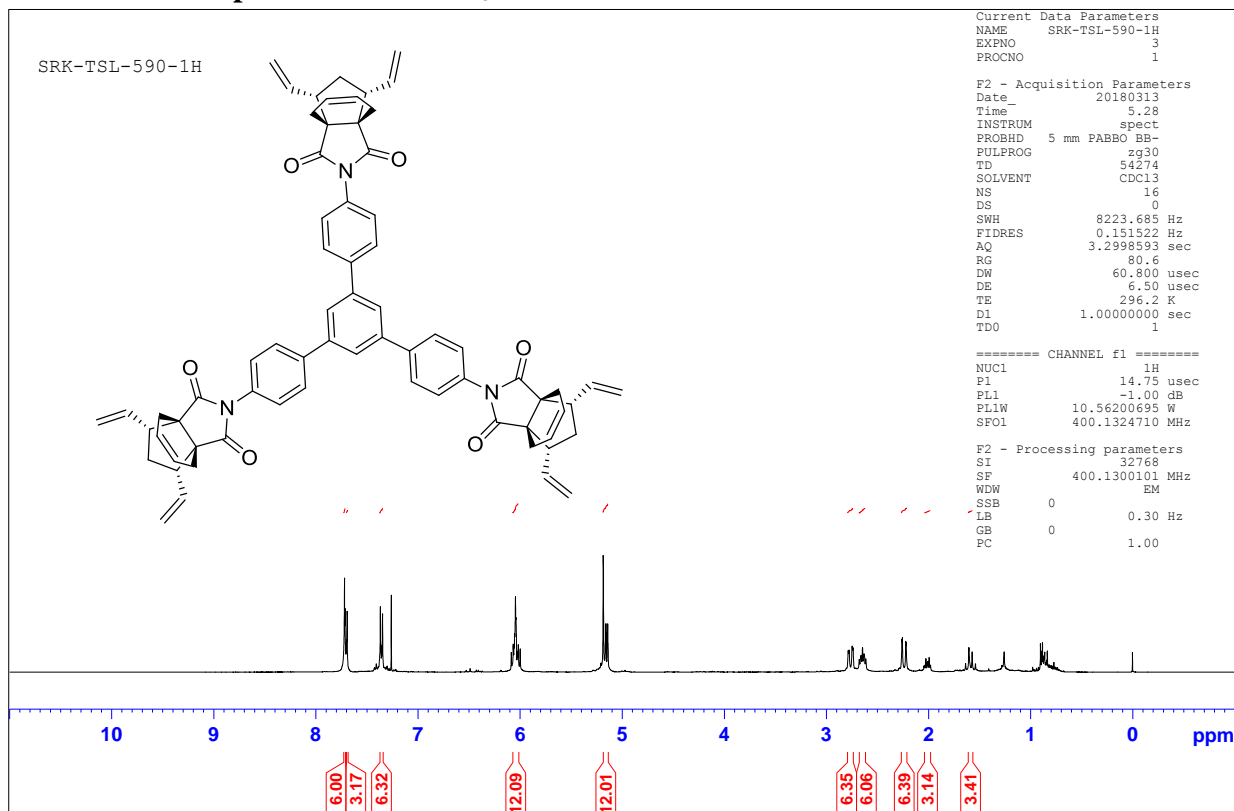
¹³C NMR of compound 14 in CDCl₃



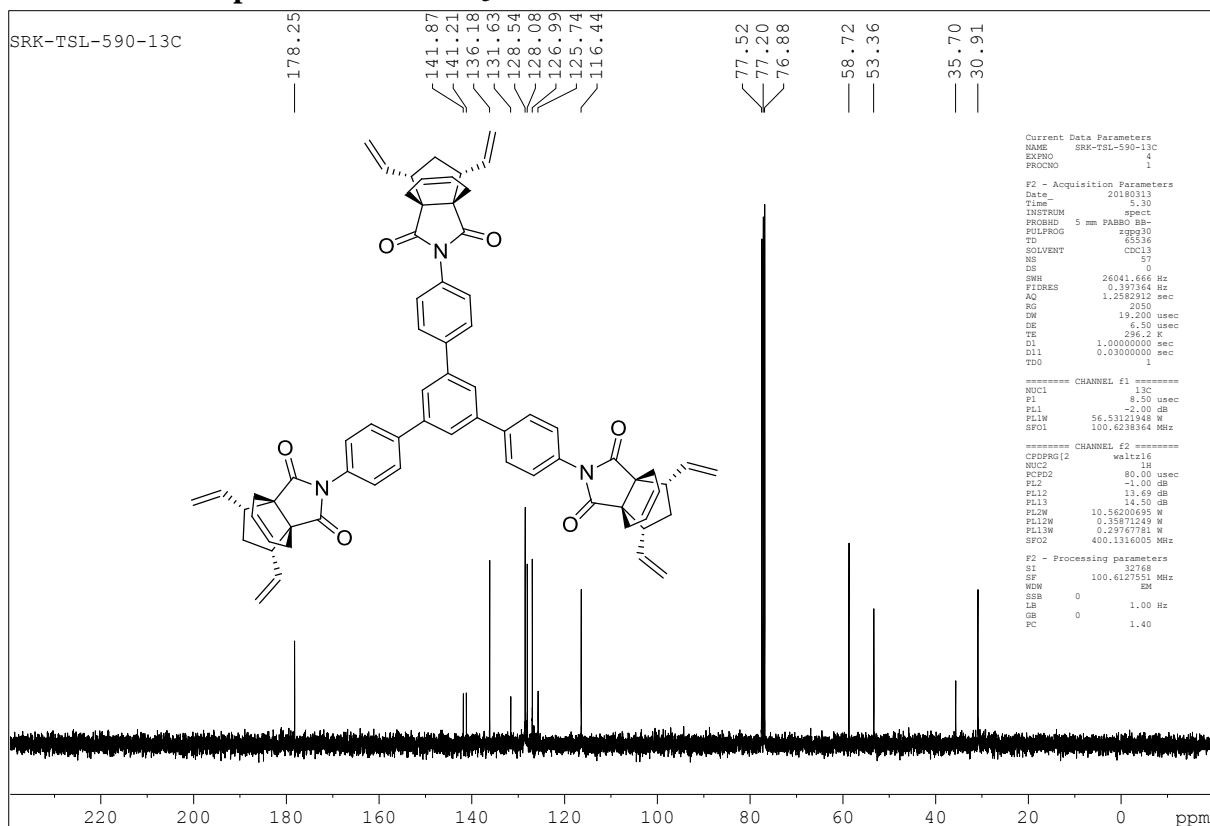
HRMS of Compound 14



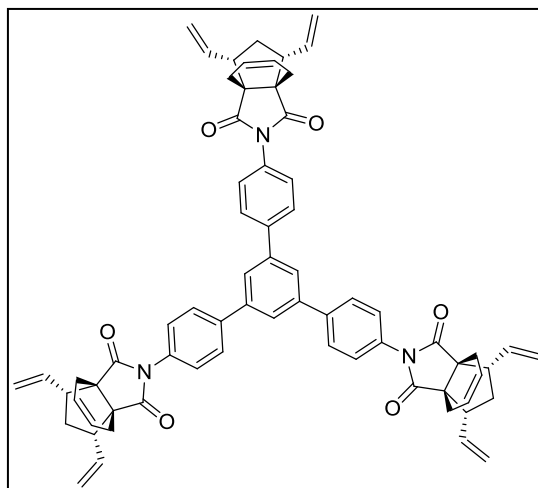
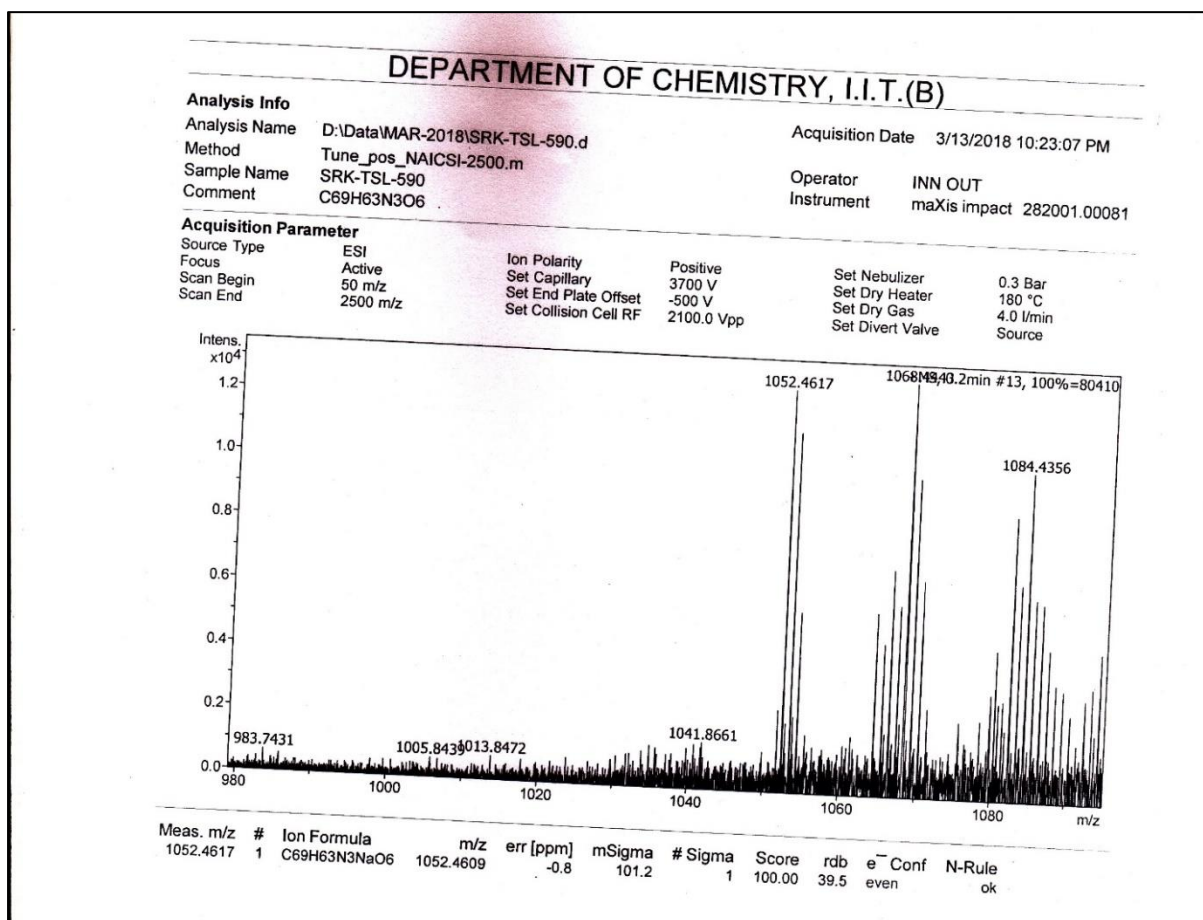
¹³C NMR of compound 15 in CDCl₃



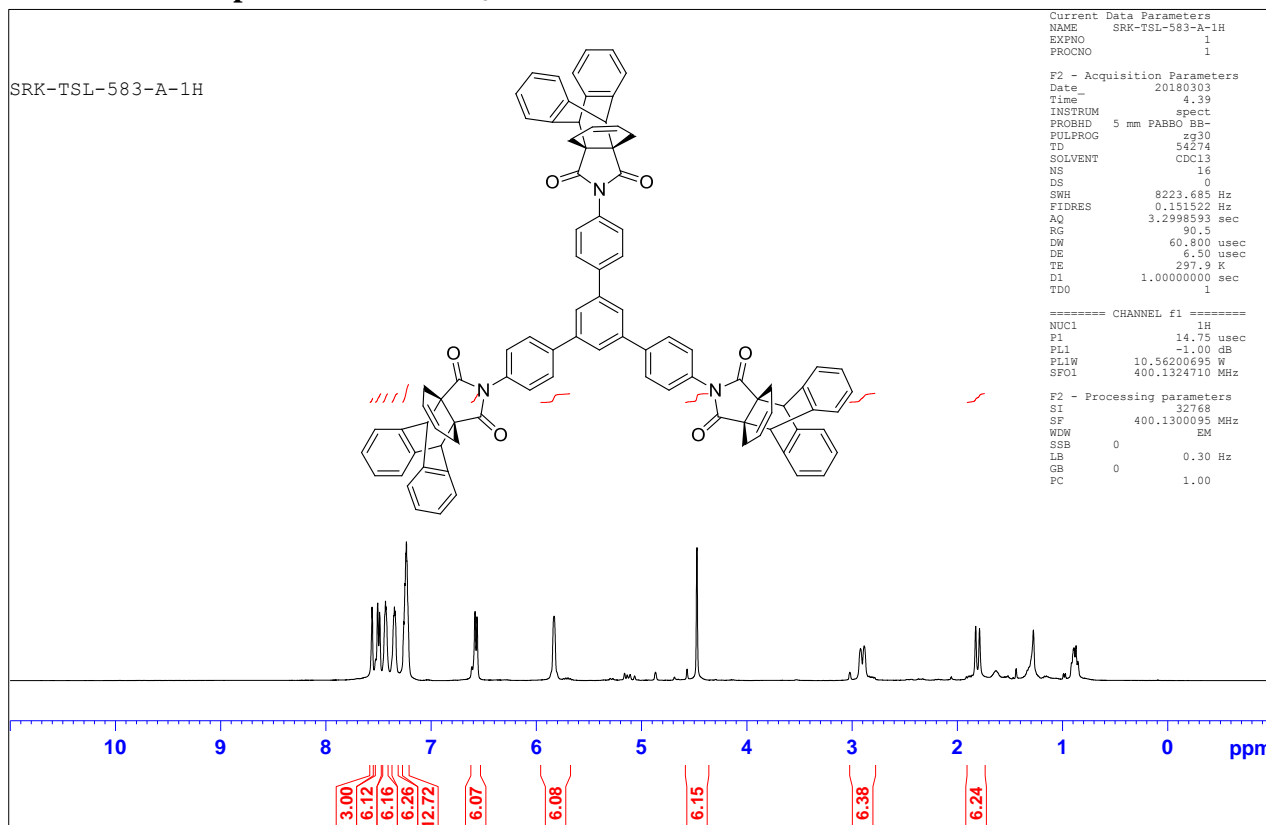
¹³C NMR of compound 15 in CDCl₃



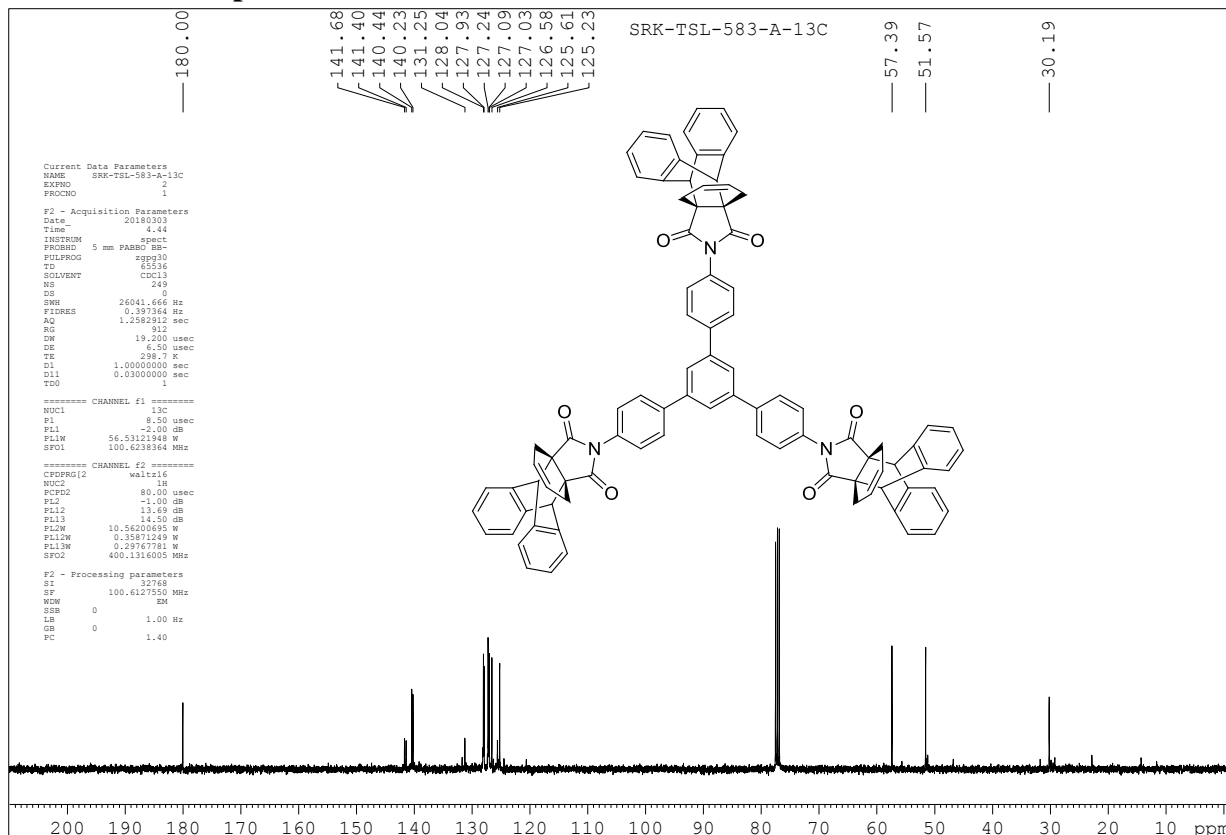
HRMS of Compound 15



¹³C NMR of compound 21 in CDCl₃



¹³C NMR of compound 21 in CDCl₃



HRMS of Compound 21

