Supporting Information

Synthesis of Stable [28π] *m*-Benzihexaphyrins (1.0.0.1.1.1)

Sunit Kumar and Mangalampalli Ravikanth*

Indian Institute of Technology, Powai, Mumbai, 400076, India, Fax: 91-22-5723480;

Tel: 91-22-5767176; E-mail: ravikanth@chem.iitb.ac.in

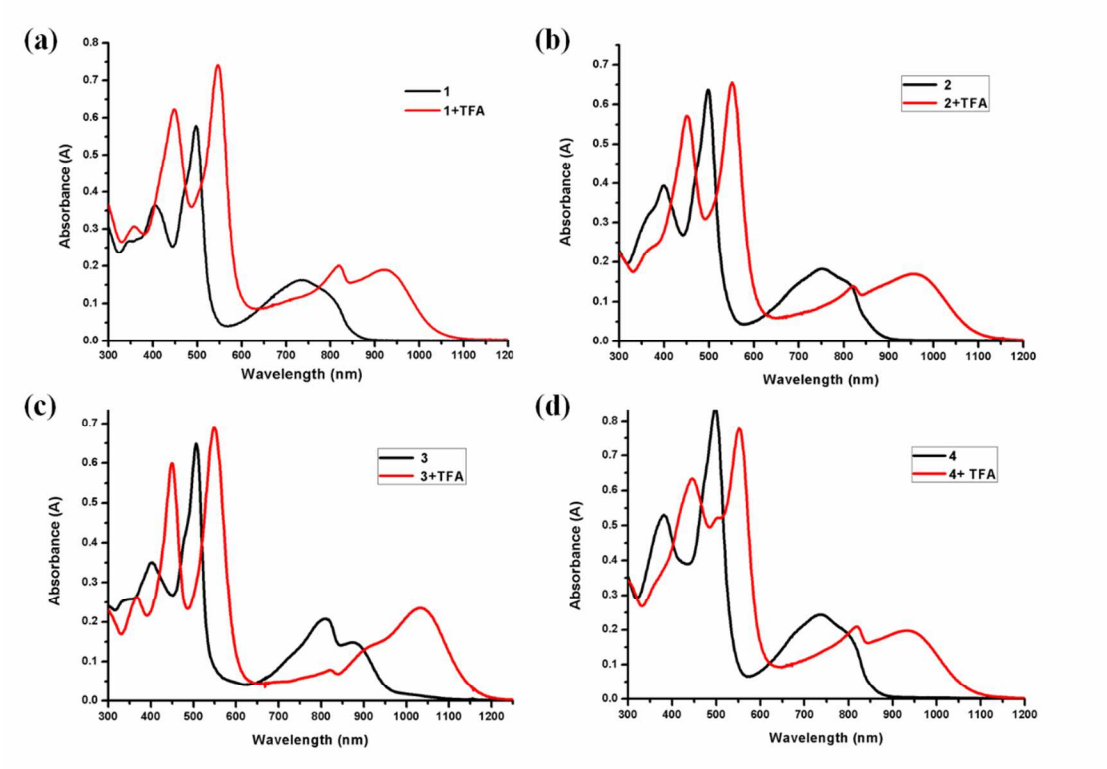


Figure S1a: Comparison of absorption spectra of compounds **1-4** (1×10^{-5} M) free base and in presence of TFA (excess of equivalents) recorded in $CHCl_3$ solution at room temperature.

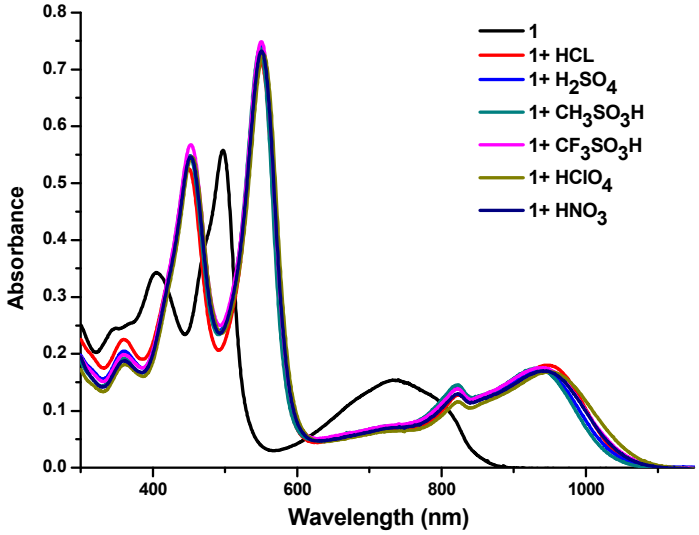


Figure S1b: Absorption spectra of compounds **1** (1×10^{-5} M) in presence of various acids (excess of equivalents) recorded in $CHCl_3$ solution at room temperature.

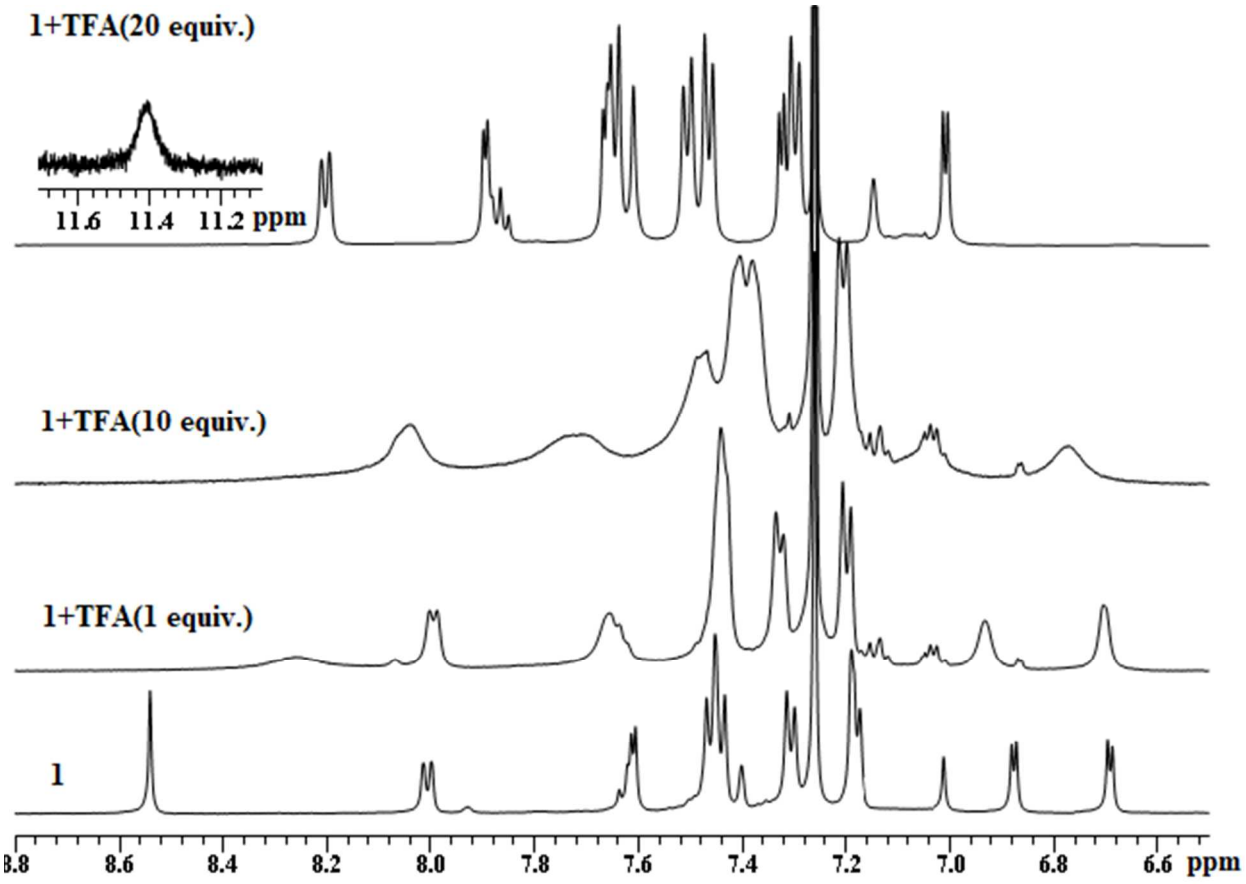


Figure S2a. Partial ^{1}H NMR spectra of compound **1** (3×10^{-3} M) in the presence of different concentrations of TFA in $CDCl_3$ at 233 K. Concentration of TFA was varied from 0-20 equiv.

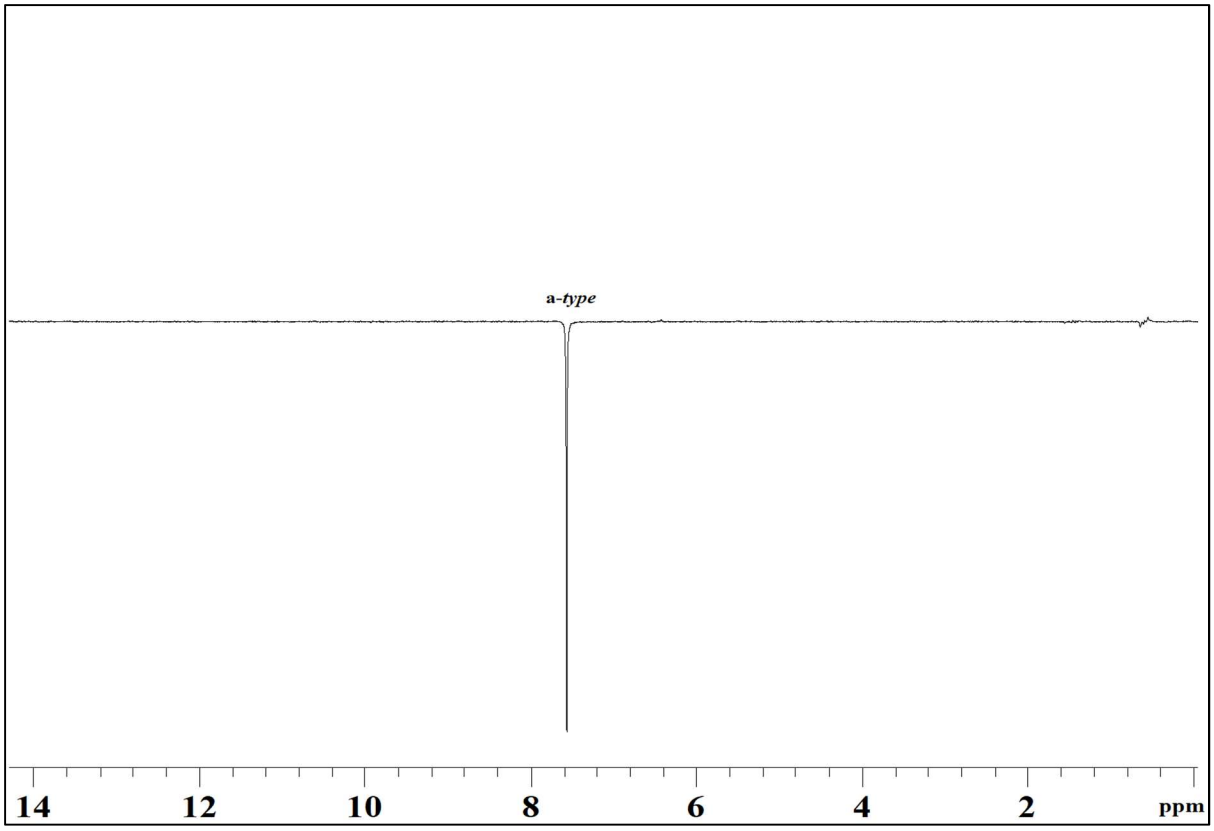


Figure S2b. NOE spectrum of compound **1H**$^{2+}$ recorded in $CDCl_3$ at 233 K.

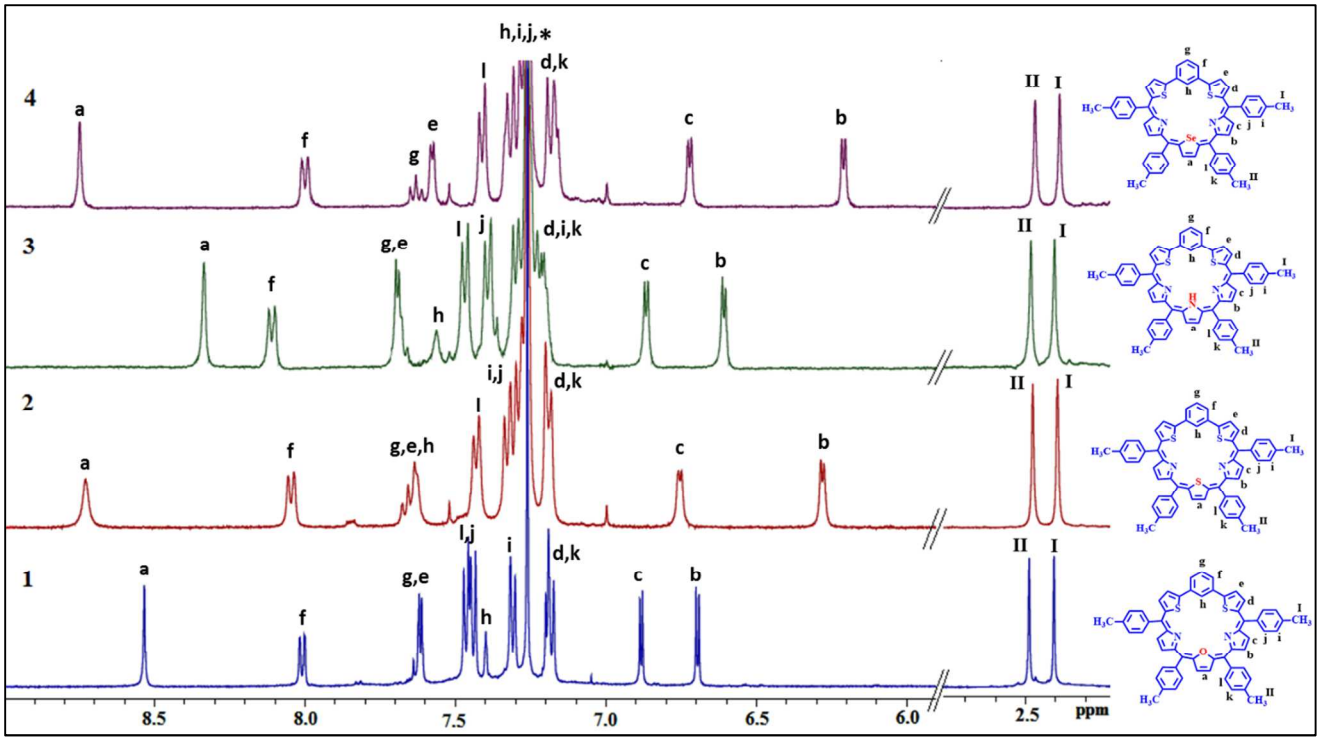
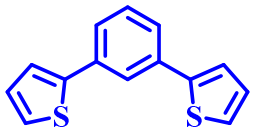


Figure S2c. Comparison of ^{1}H NMR spectra of compound **1**-**4** recorded in $CDCl_3$.



5

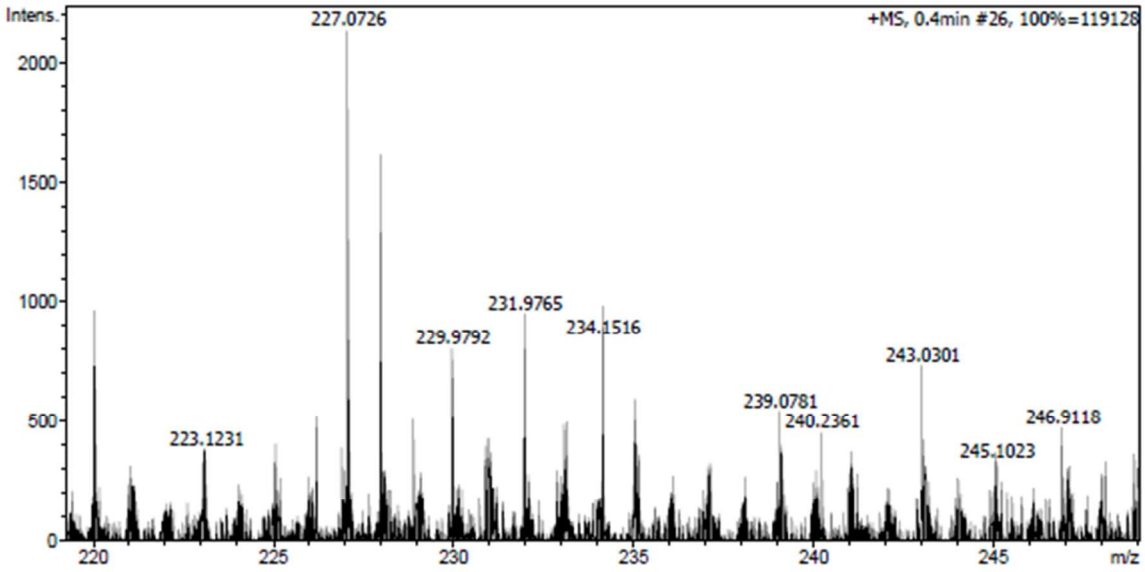
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

Analysis Name	D:\Data\OCT 2017\MR-SK-BITHIA.d	Acquisition Date	10/5/2017 4:07:08 PM
Method	Tune_pos_NAF-500.m	Operator	iitb
Sample Name	MR-SK-BITHIA	Instrument	maXis impact 282001.00081
Comment	C14H10S2		

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	700 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
243.0301	1	C14H11S2	243.0297	-1.7	107.0	1	100.00	9.5	even	ok

Figure S3. HR mass spectrum of compound **5**

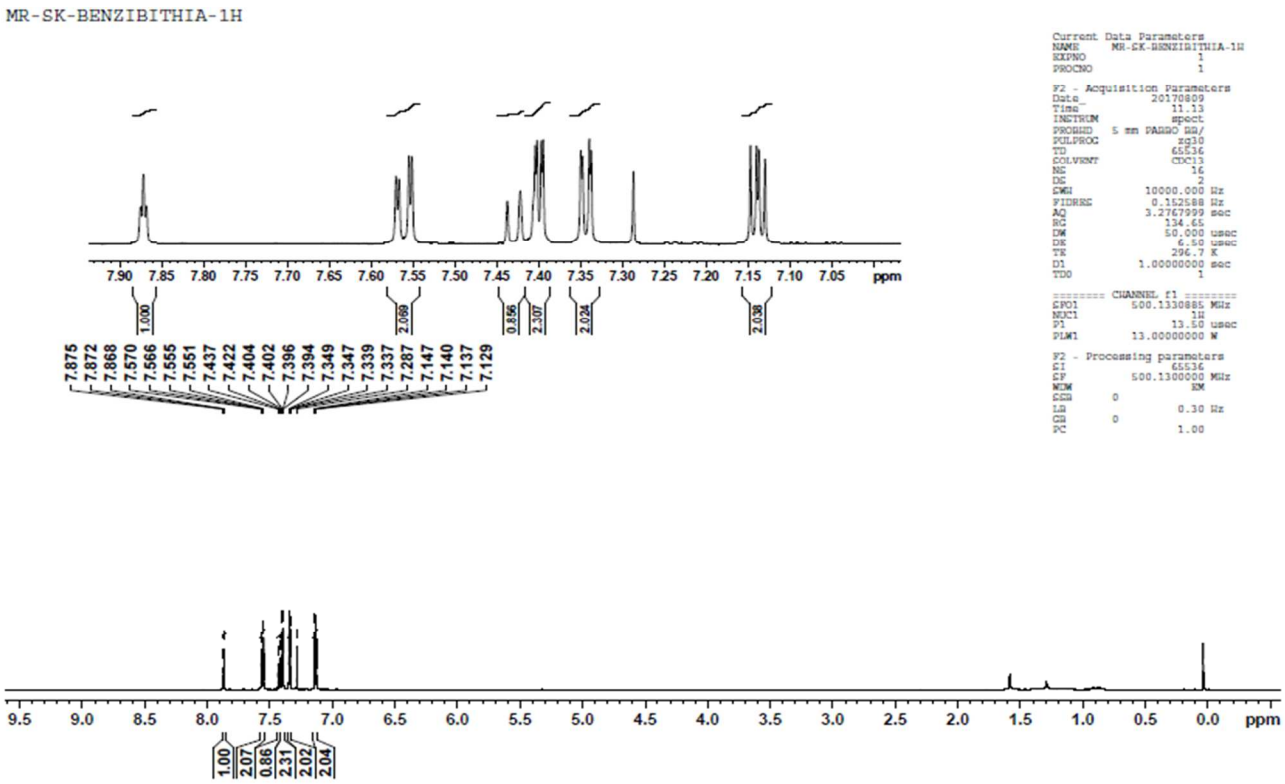


Figure S4. ^{1}H NMR spectrum of compound **5** recorded in $CDCl_3$

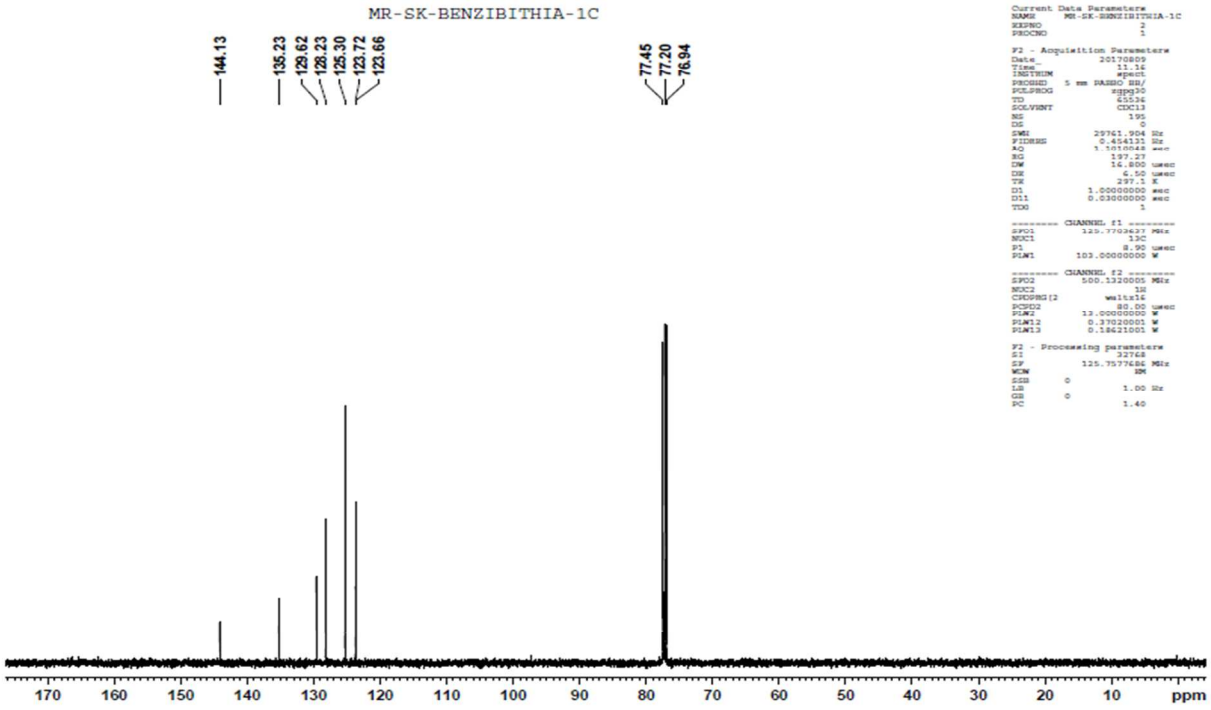
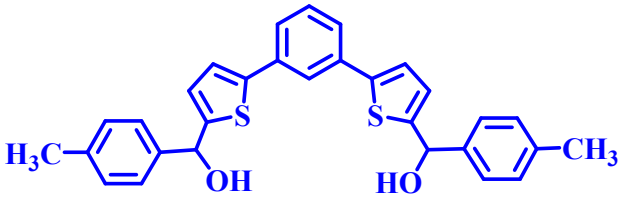


Figure S5. ^{13}C NMR spectrum of compound **5** recorded in $CDCl_3$



6

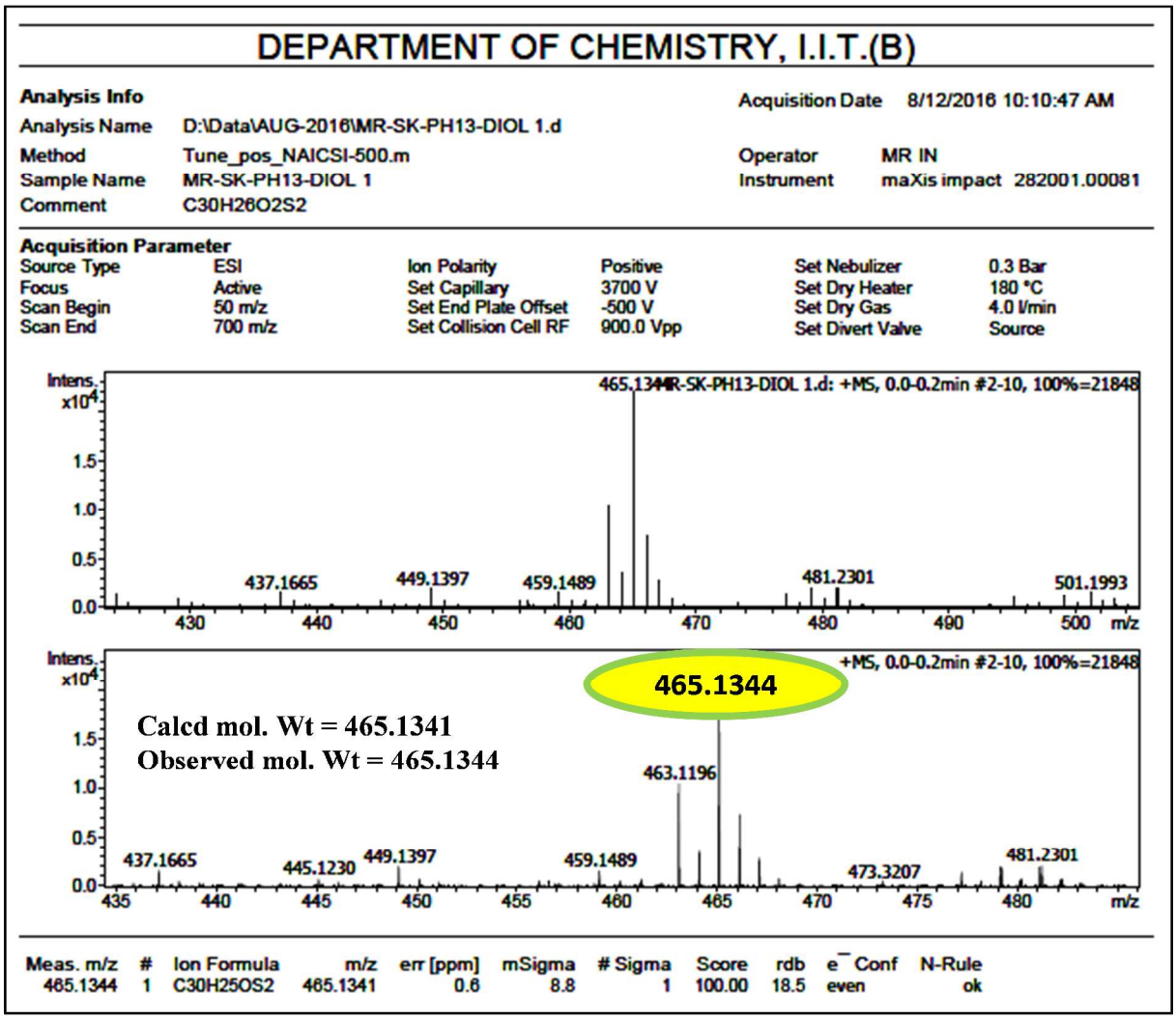


Figure S6. HR mass spectrum of compound **6**

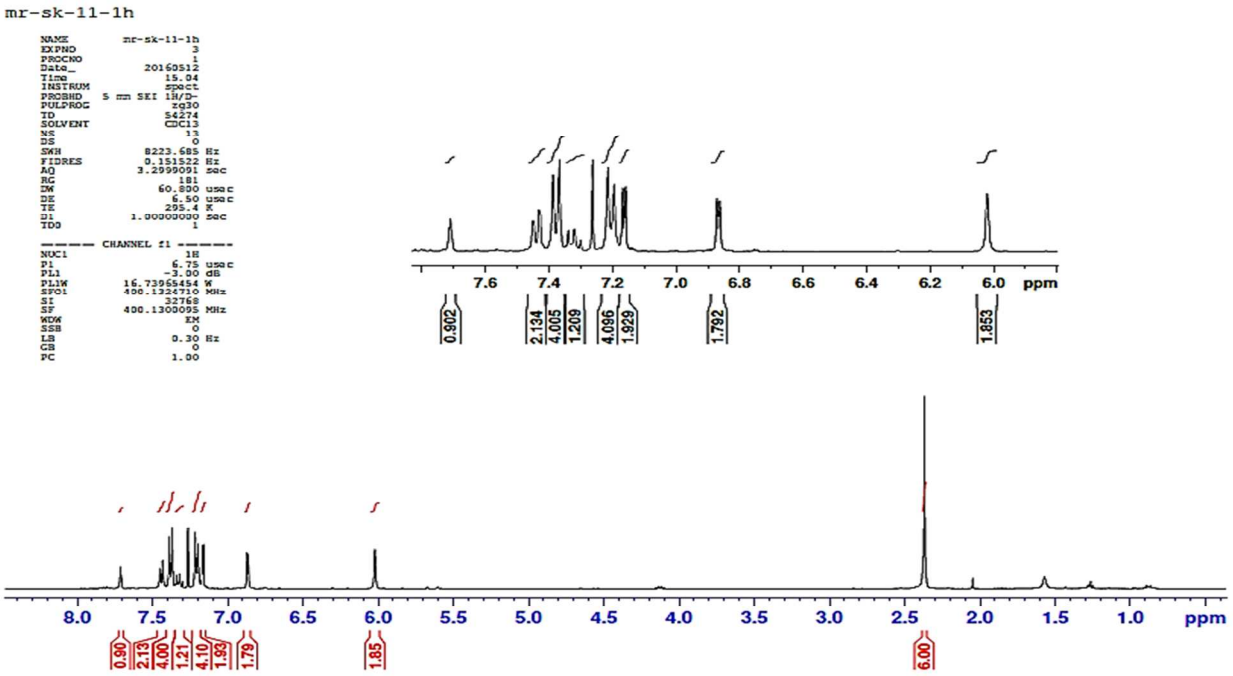


Figure S7. ^{1}H NMR spectrum of compound **6** recorded in $CDCl_3$

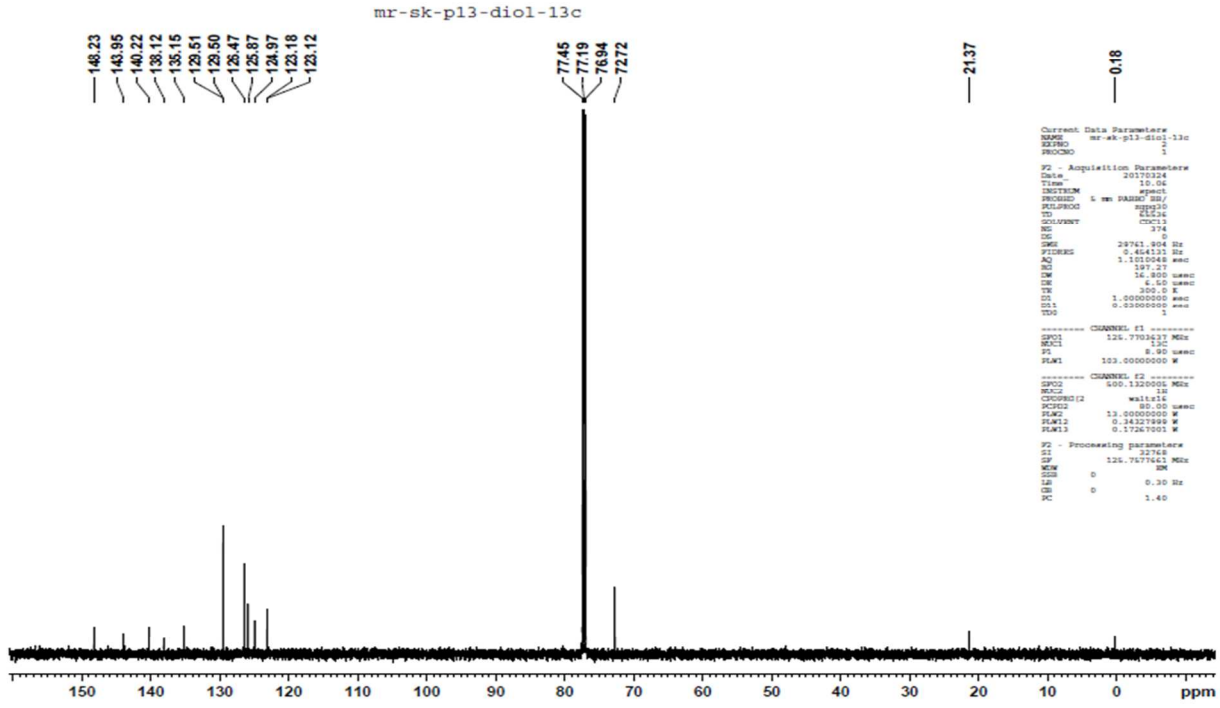
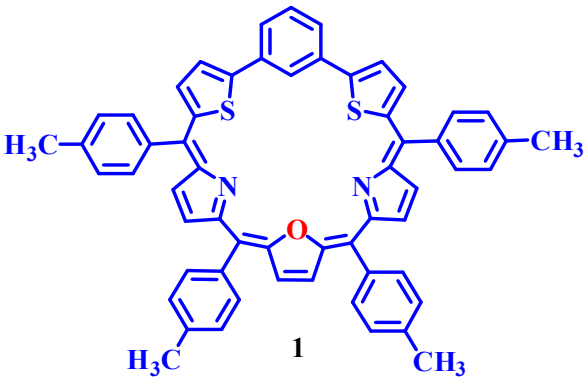


Figure S8. ^{13}C NMR spectrum of compound **6** recorded in $CDCl_3$



1

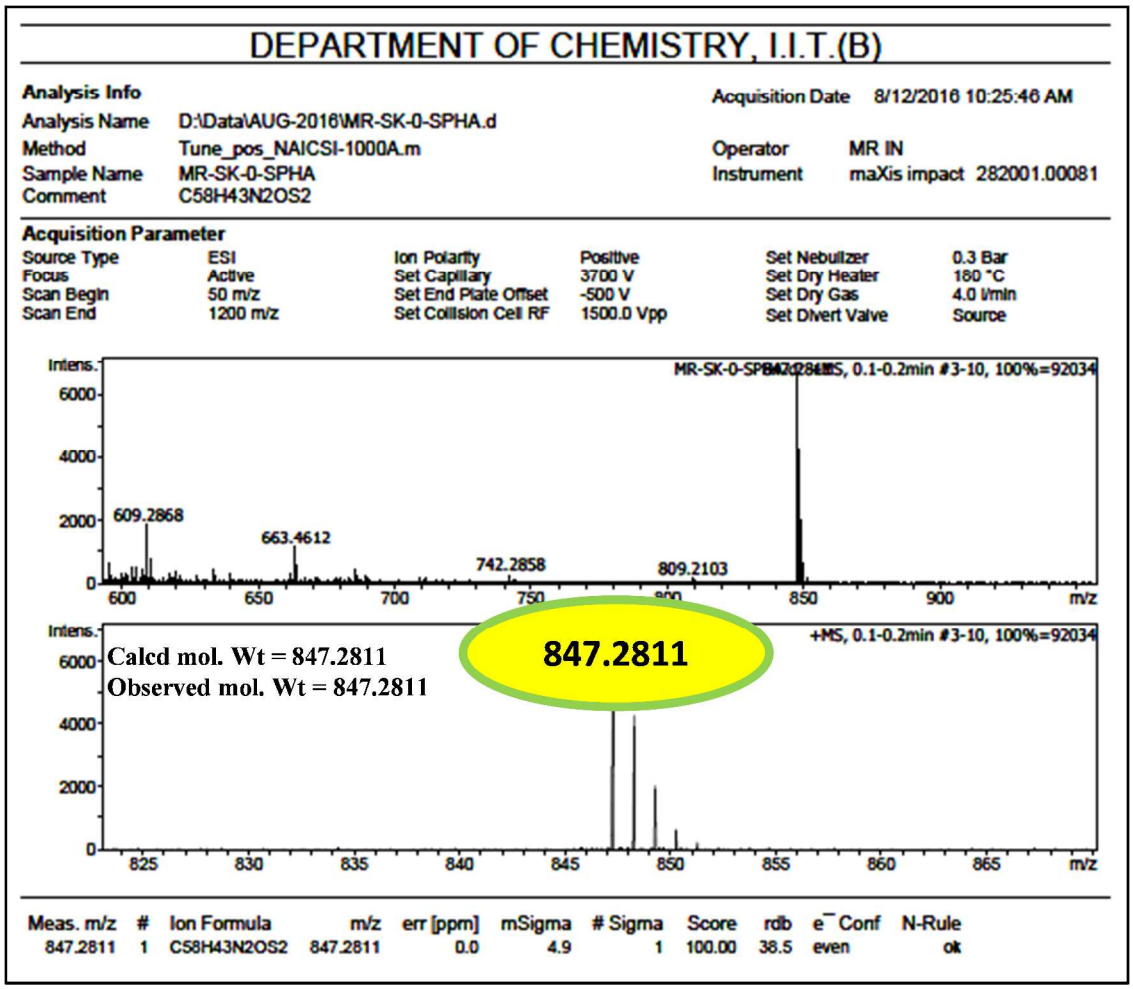


Figure S9. HR mass spectrum of compound **1**

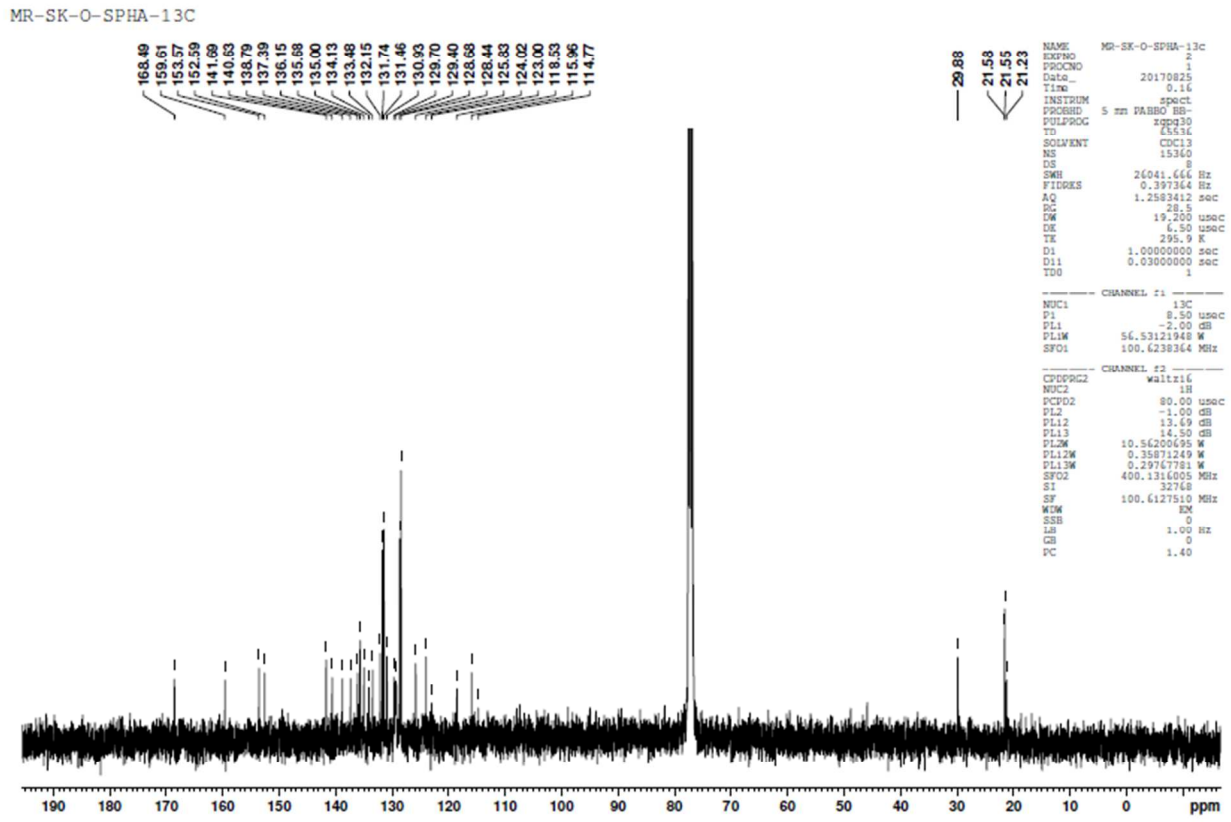
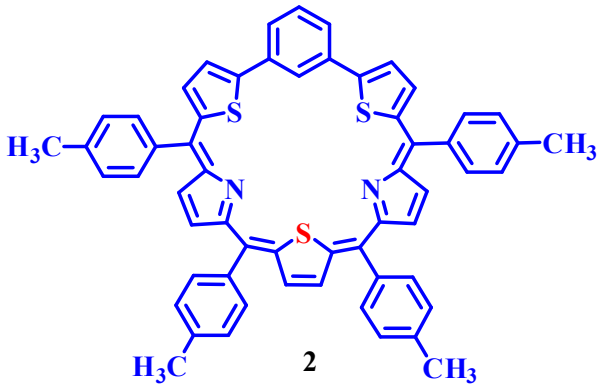


Figure S10. ^{13}C NMR spectrum of compound **1** recorded in $CDCl_3$



2

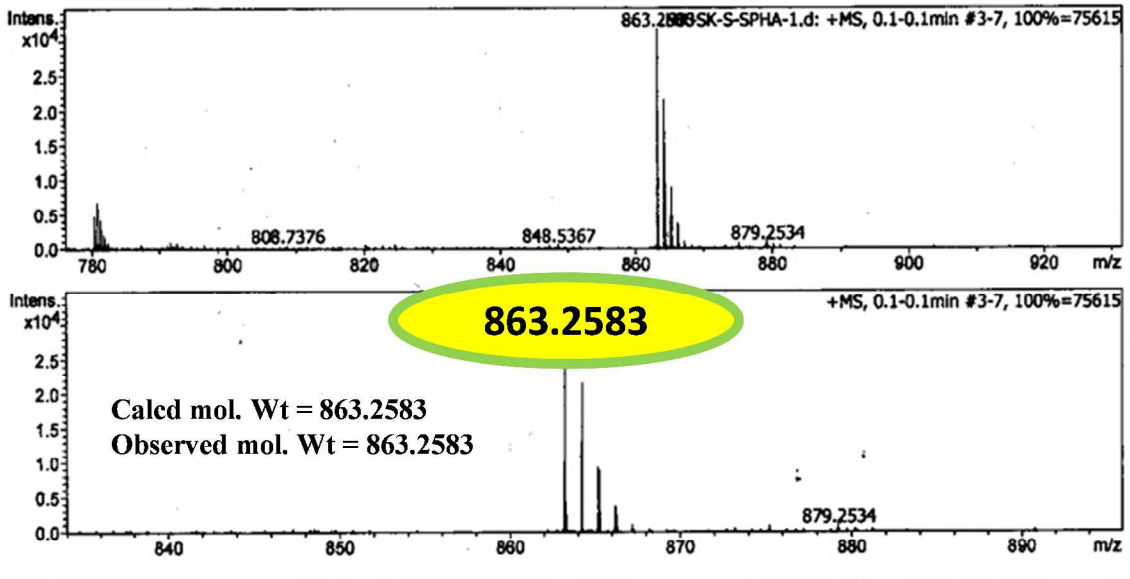
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

Analysis Name	D:\Data\AUG-2016\MR-SK-S-SPHA-1.d	Acquisition Date	8/15/2016 5:52:09 PM
Method	Tune_pos_NAICSI-2500.m	Operator	MR IN
Sample Name	MR-SK-S-SPHA-1	Instrument	maXis impact 282001.00081
Comment	C58H43N2S3		

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	2500 m/z	Set Collision Cell RF	2100.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
863.2583	1	C58H43N2S3	863.2583	0.0	28.0	1	100.00	38.5	even	ok

Figure S11. HR mass spectrum of compound **2**

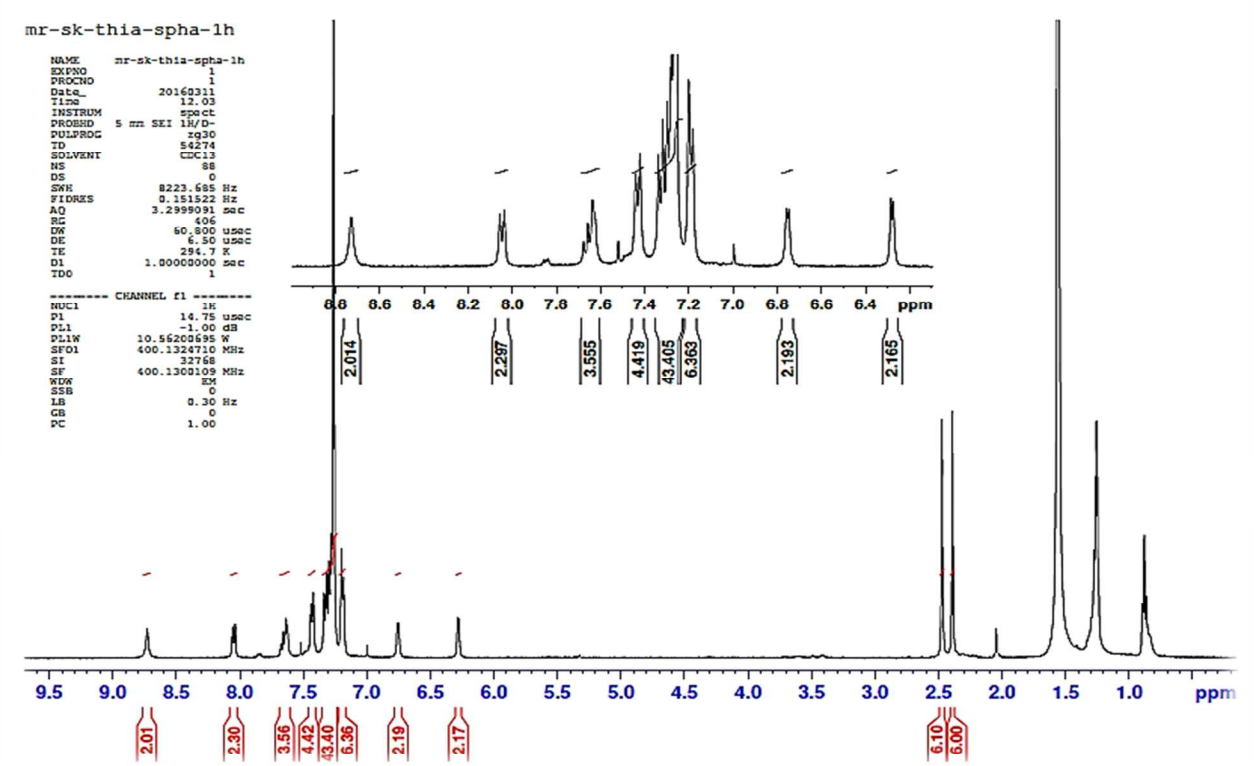


Figure S12. ^{1}H NMR spectrum of compound **2** recorded in $CDCl_3$.

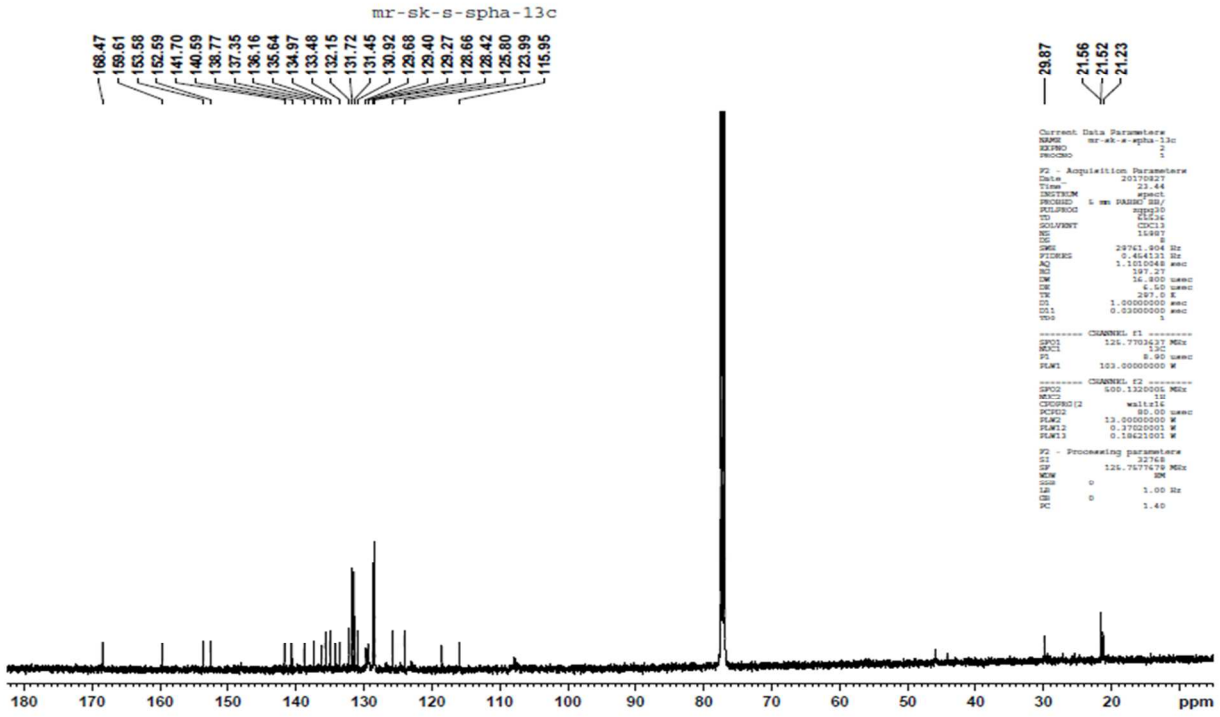
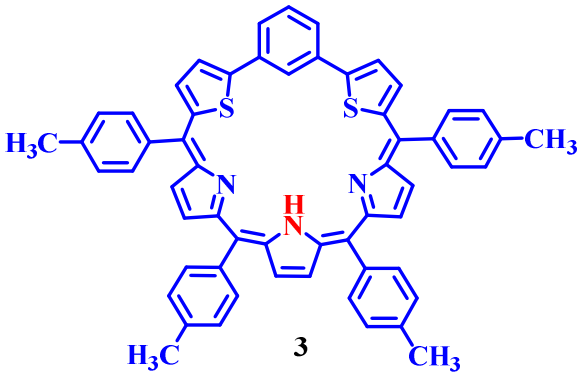


Figure S13. ^{13}C NMR spectrum of compound **2** recorded in $CDCl_3$



3

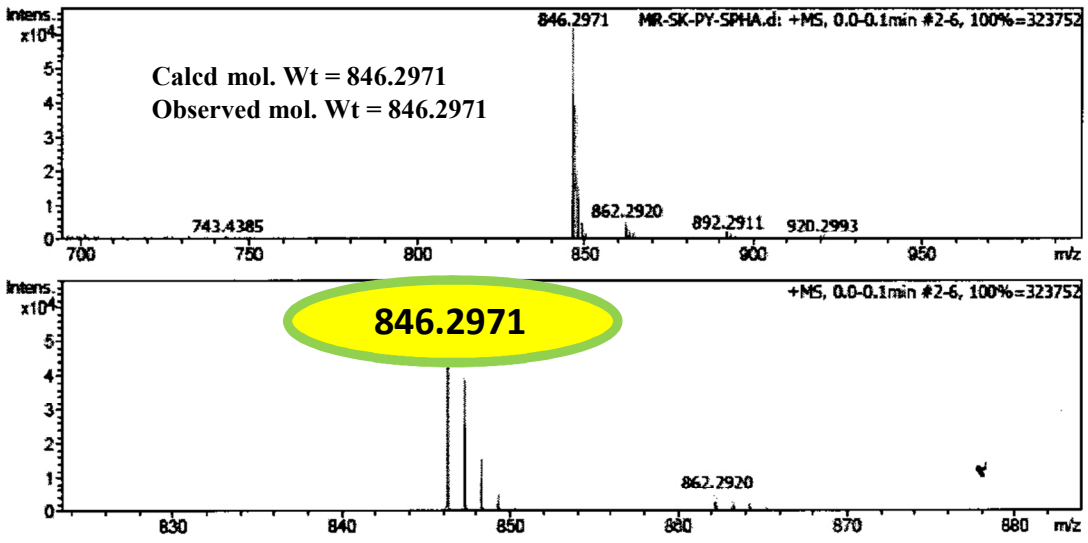
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

Analysis Name	D:\Data\APRIL-2016\MR-SK-PY-SPHA.d	Acquisition Date	4/22/2016 5:48:15 PM
Method	Tune_pos_NAF-1000.m	Operator	MR-IN
Sample Name	MR-SK-PY-SPHA	Instrument	maXis impact 282001.00081
Comment	C58H43N3S2		

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	1000 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
846.2971	1	C58H44N3S2	846.2971	-0.1	27.2	1	100.00	38.5	even	ok

Figure S14. HR mass spectrum of compound **3**

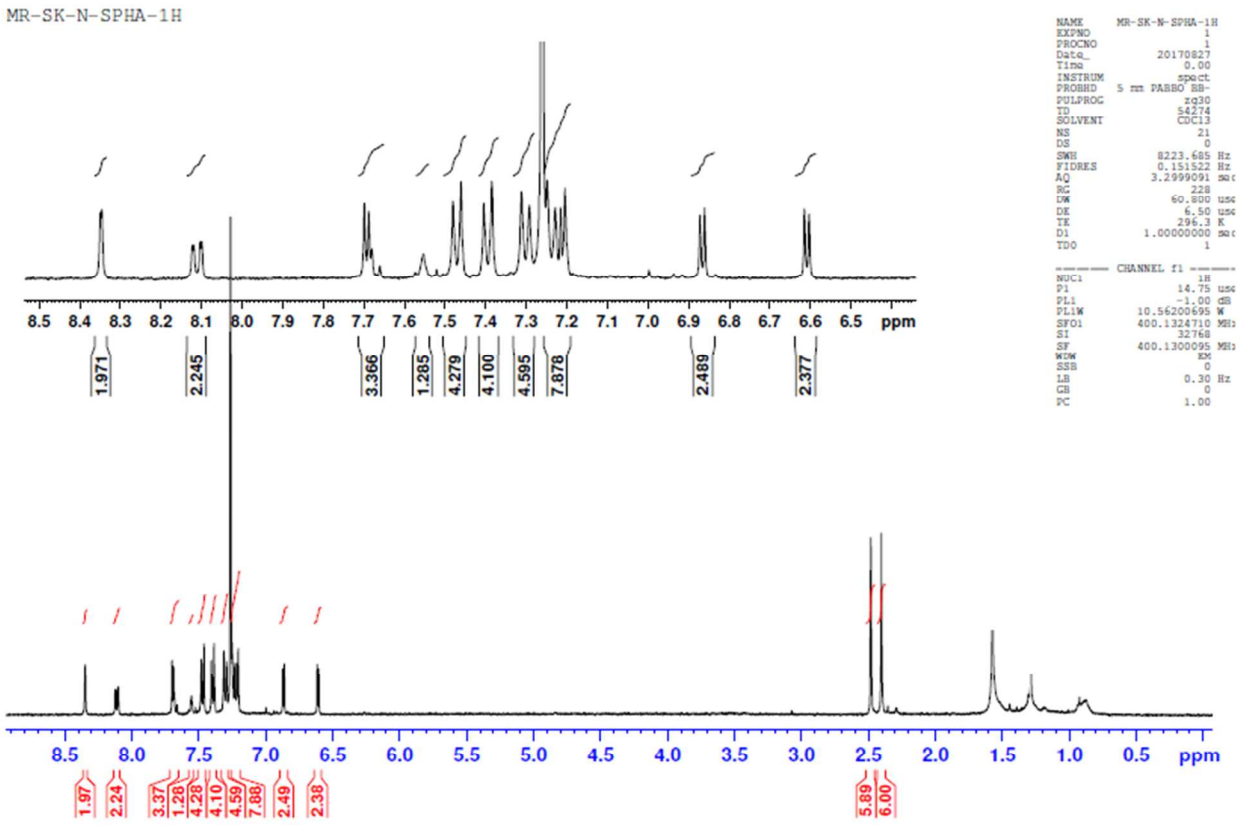


Figure S15. ^{1}H NMR spectrum of compound **3** recorded in $CDCl_3$.

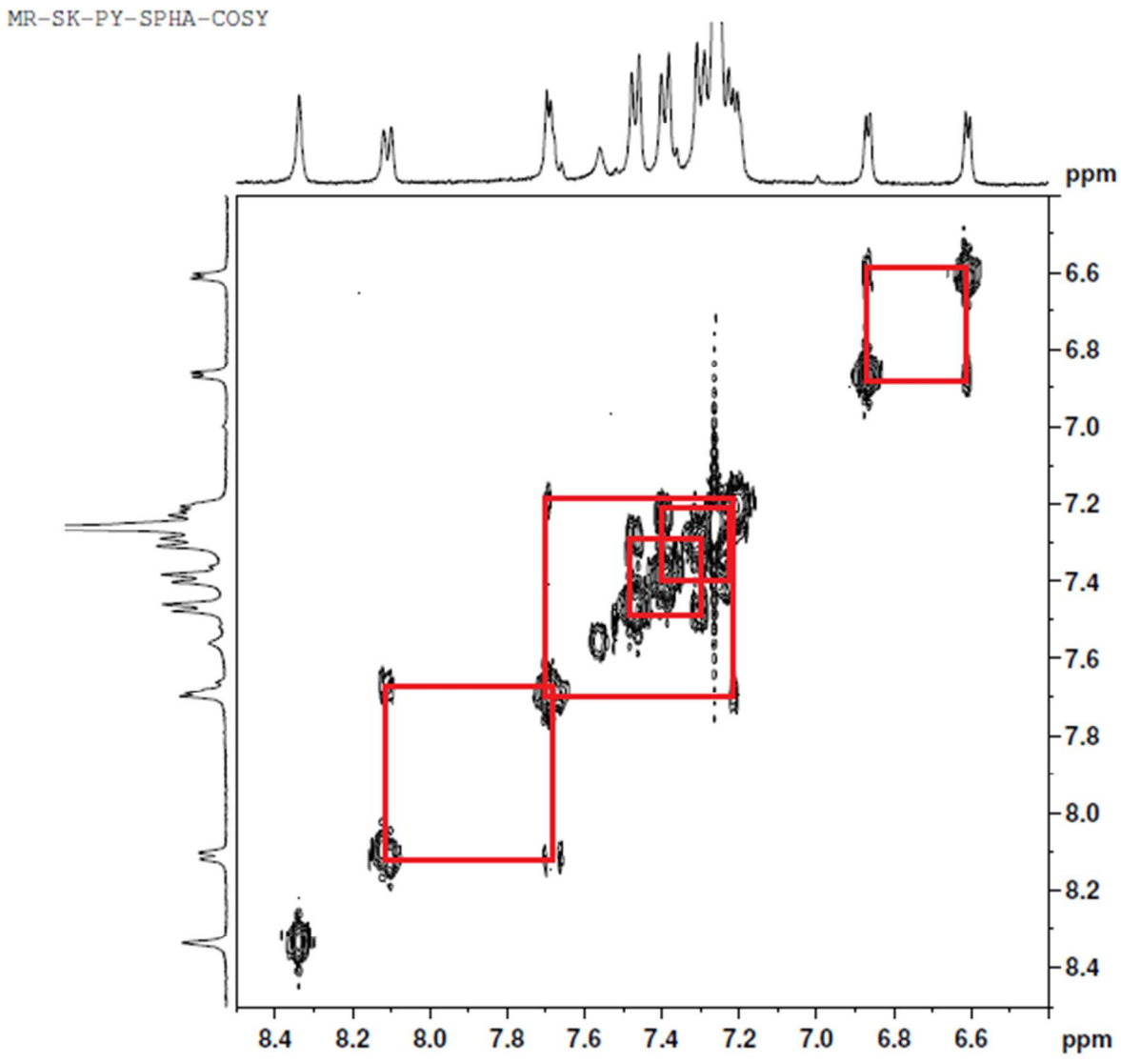


Figure S16. ^{1}H-^{1}H COSY spectrum of compound **3** recorded in $CDCl_3$.

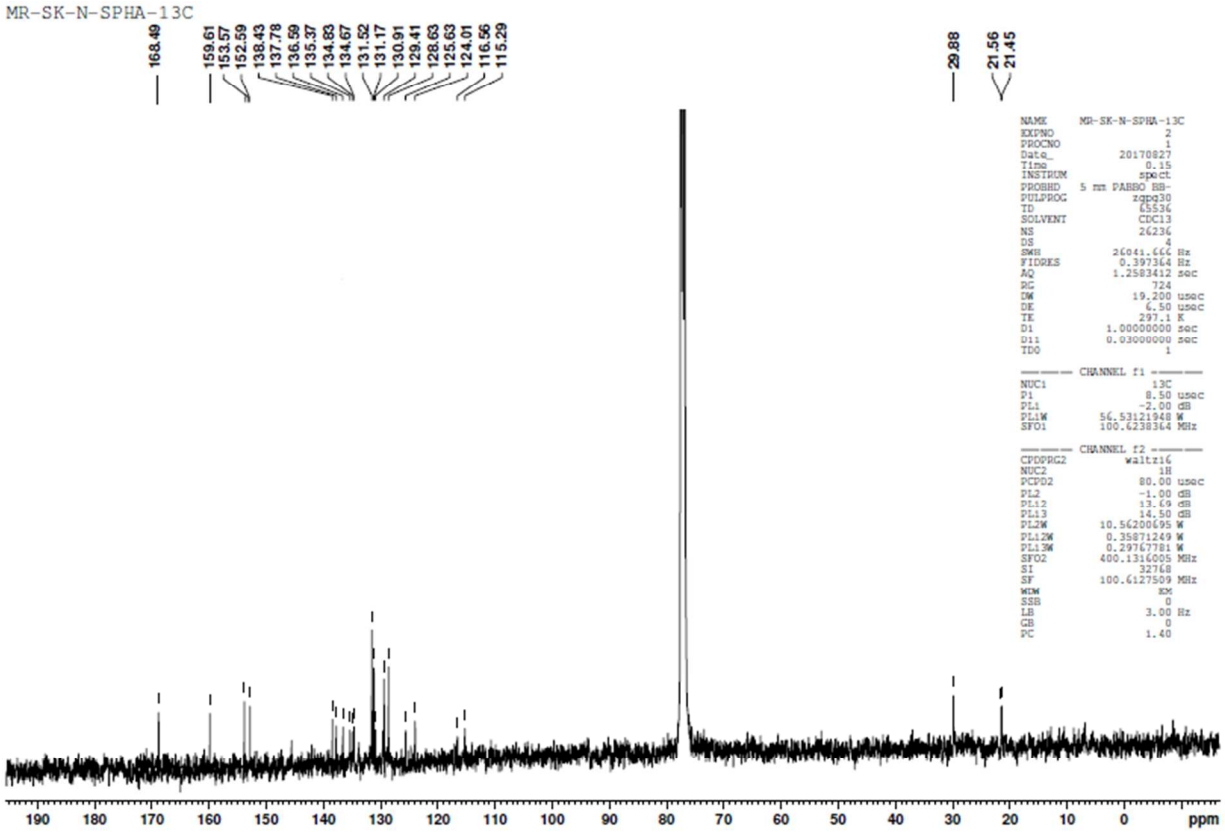
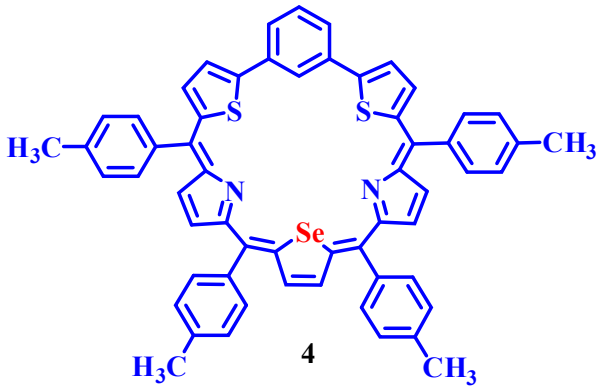


Figure S17. ^{13}C NMR spectrum of compound **3** recorded in $CDCl_3$



4

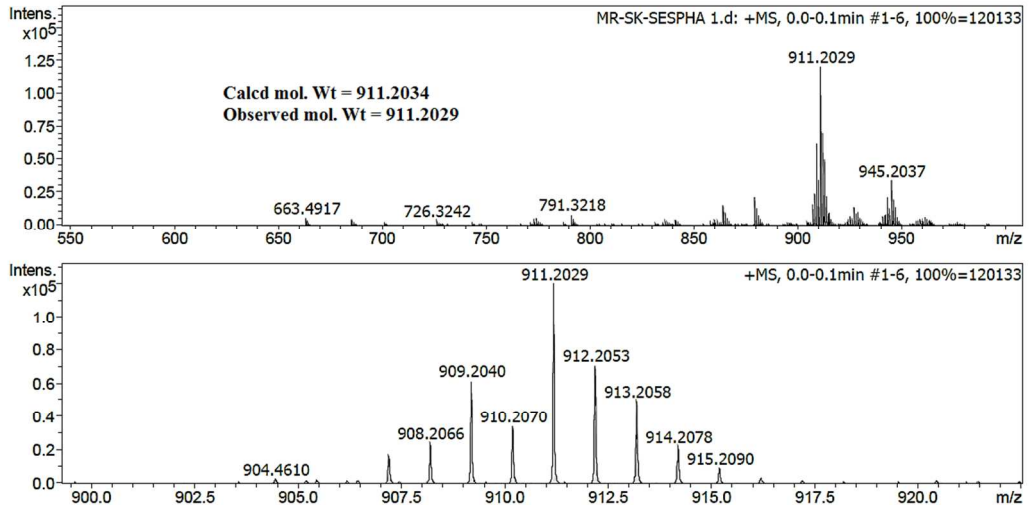
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

Analysis Name	D:\Data\MAR-2017\MR-SK-SESPHA 1.d	Acquisition Date	3/29/2017 3:37:11 PM
Method	Tune_pos_NAICSI-1500A.m	Operator	MR IN
Sample Name	MR-SK-SESPHA 1	Instrument	maXis impact 282001.00081
Comment	C58H42N2S2SE		

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



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
911.2029	1	C58H43N2S2Se	911.2034	-0.5	23.6	1	100.00	38.5	even	ok

Figure S18. HR mass spectrum of compound **4**

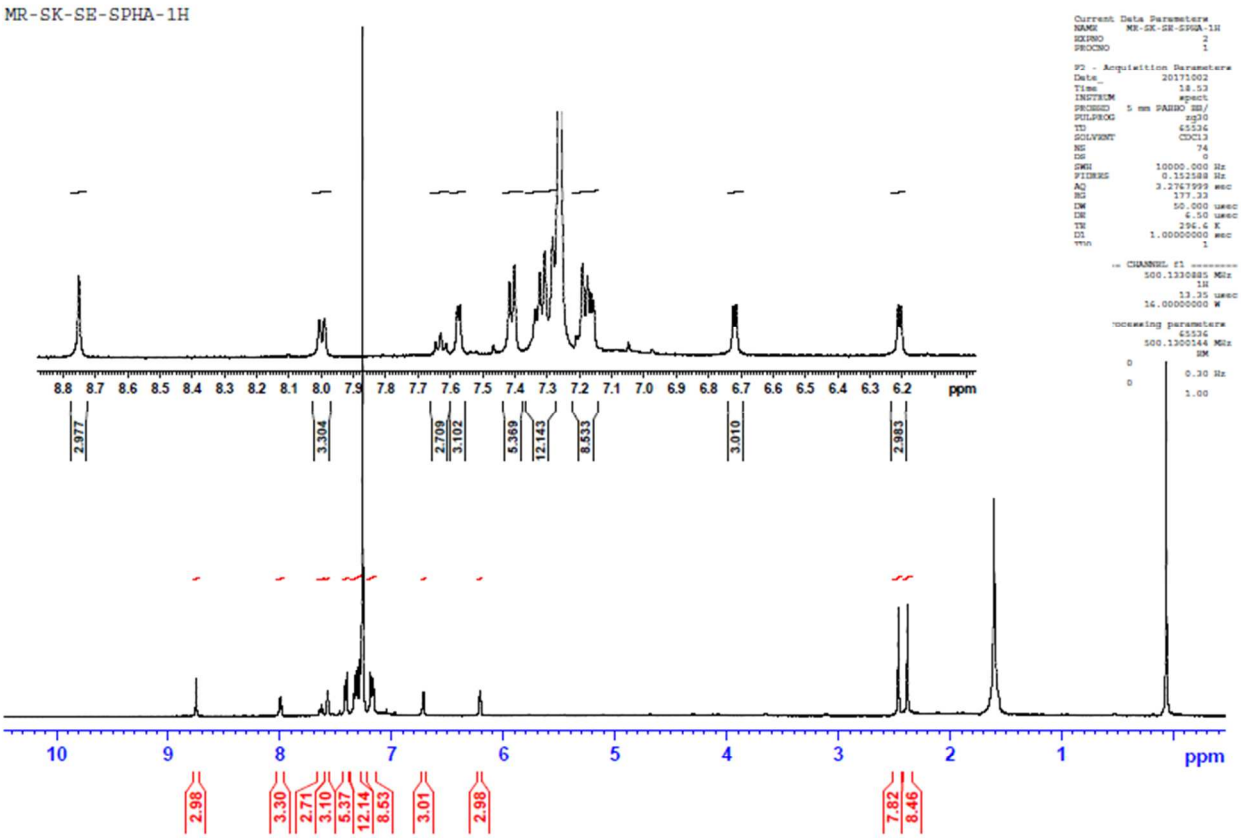


Figure S19. ^{1}H NMR spectrum of compound **4** recorded in $CDCl_3$.

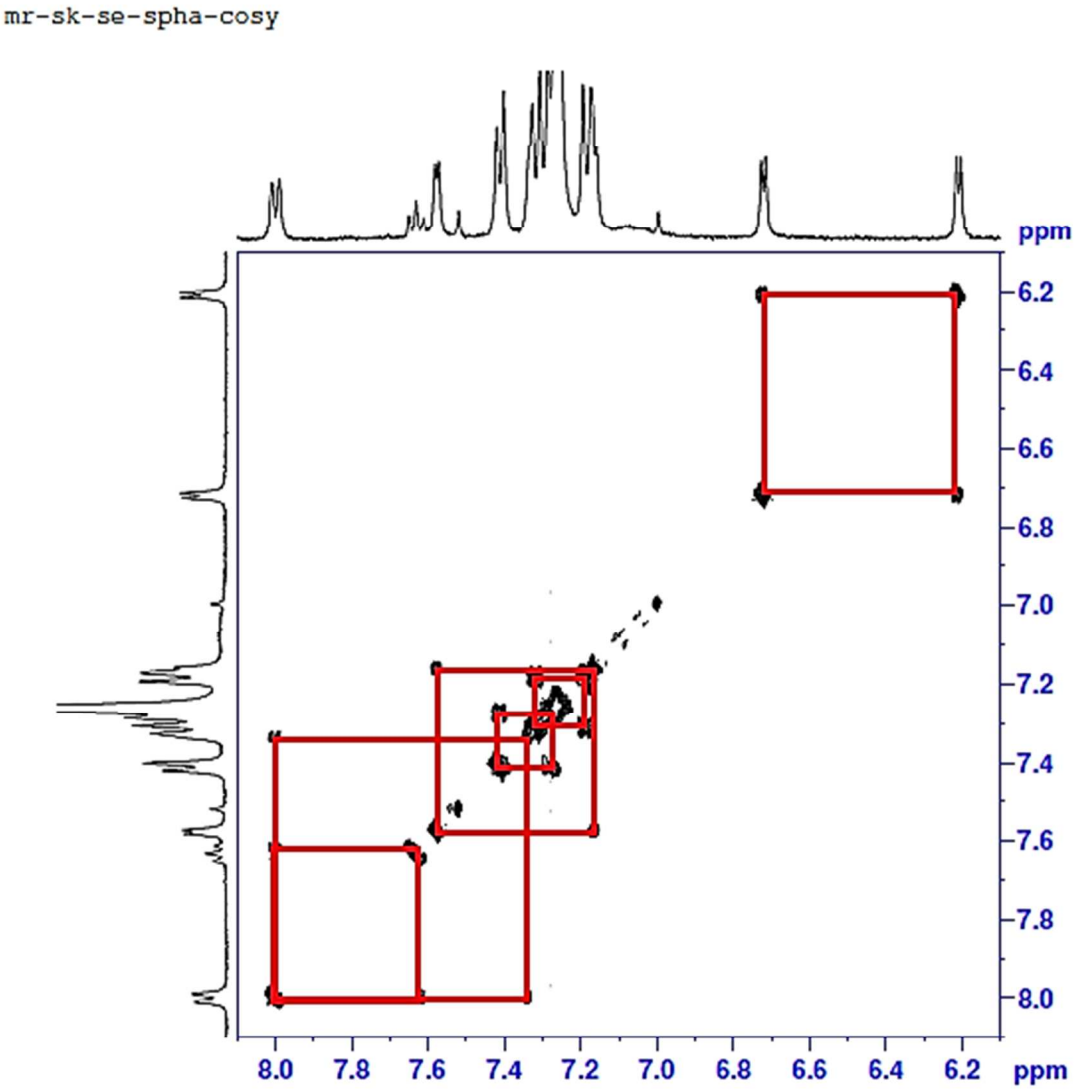


Figure S20. ^{1}H-^{1}H COSY NMR spectrum of compound **4** recorded in $CDCl_3$.

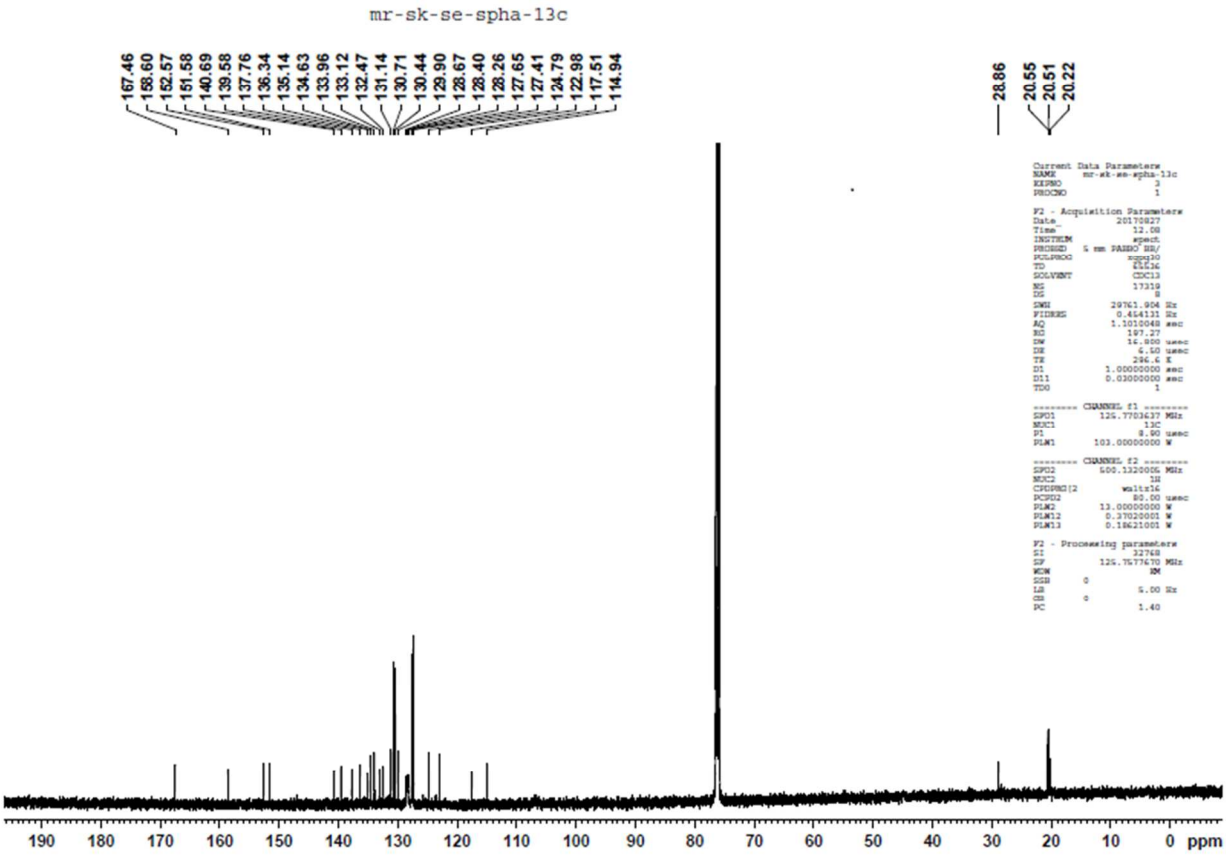


Figure S21. ^{13}C NMR spectrum of compound **4** recorded in $CDCl_3$