

Electronic Supplementary Information (ESI) of the manuscript:

Planar chiral asymmetric naphthalenediimide cyclophanes: Synthesis, characterization and tunable FRET properties

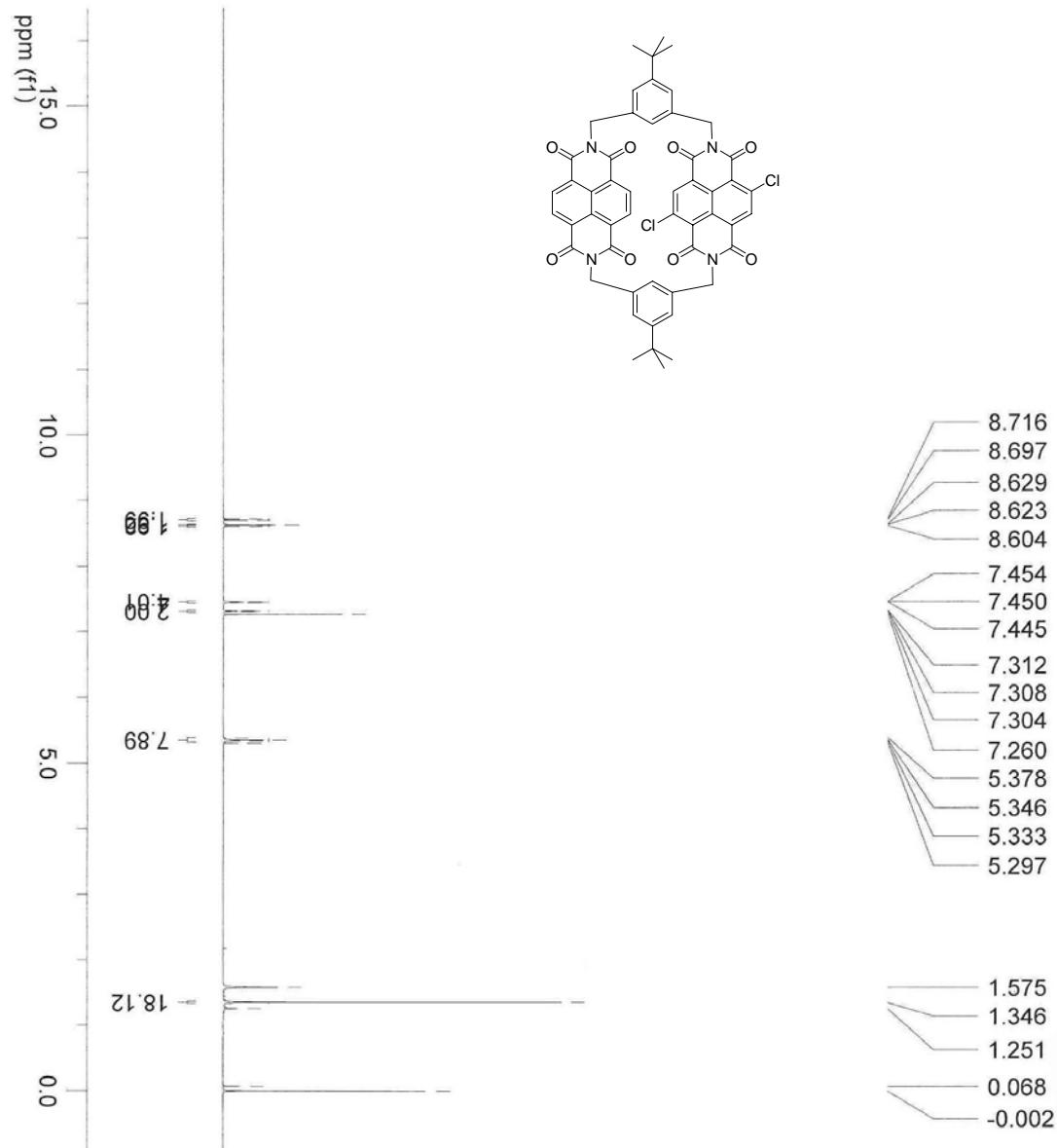
Sandro Gabutti,^a Silvia Schaffner,^a Markus Neuburger,^a Matthias Fischer,^b Gabriel Schäfer^a and Marcel Mayor^{*a,b}

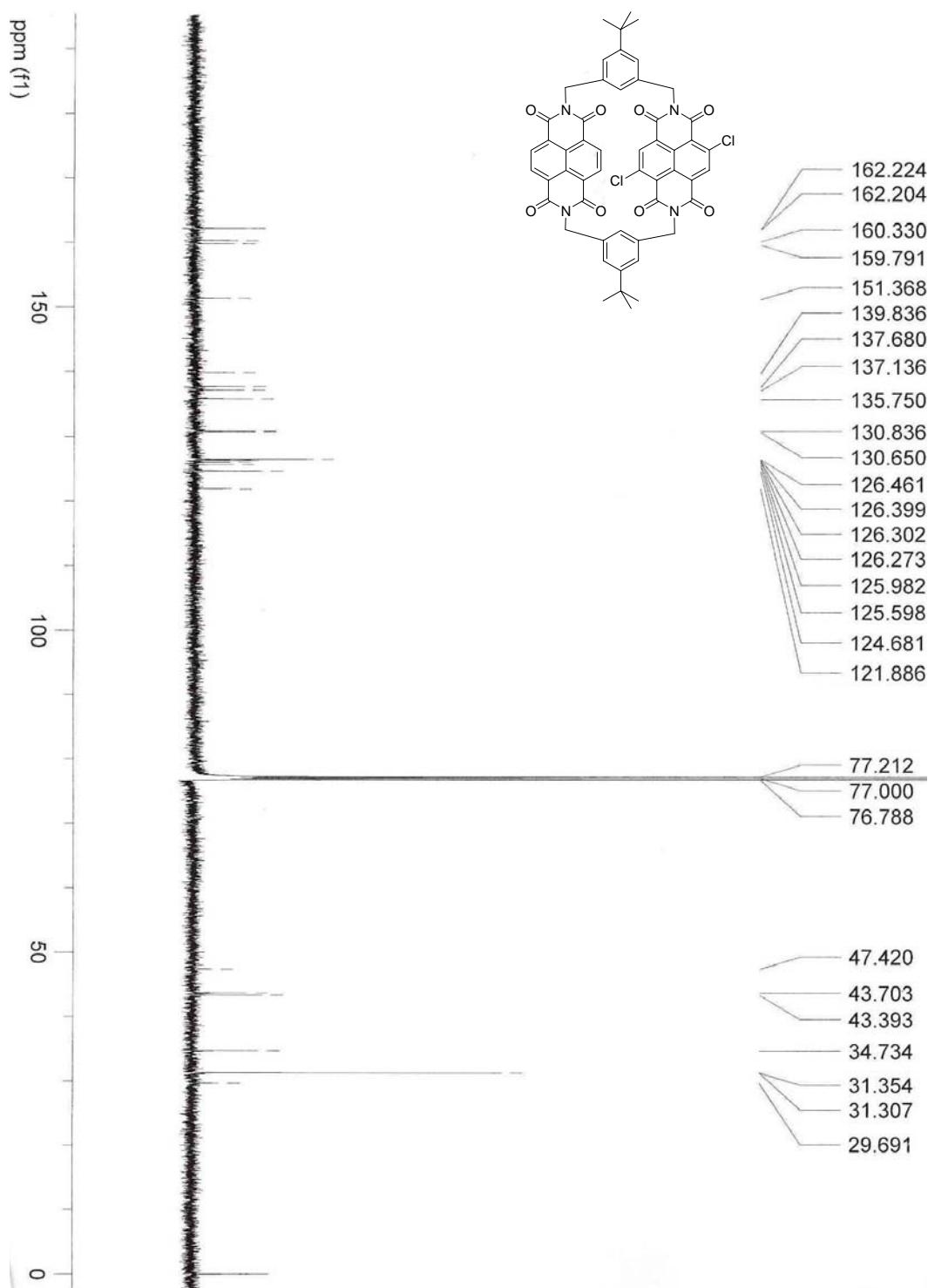
^a University of Basel, Department of Chemistry, St. Johannsring 19, CH-4056 Basel, Switzerland, Fax: +41 61 267 1016; Tel: +41 61 267 1006; E-mail: marcel.mayor@unibas.ch

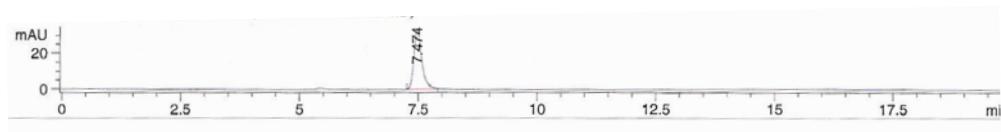
^b Forschungszentrum Karlsruhe GmbH, Institute for Nanotechnology, P. O. Box 3640, D-76021 Karlsruhe, Germany.

Table of Contents

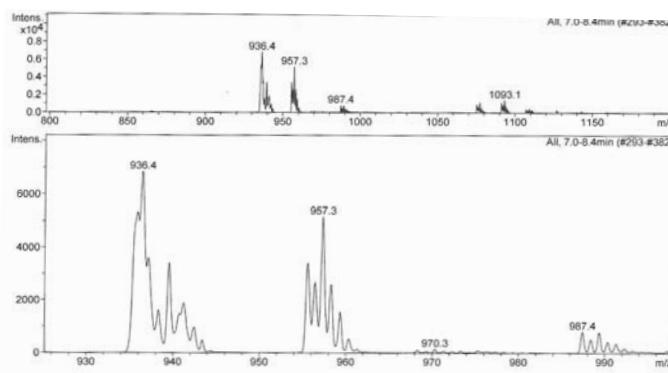
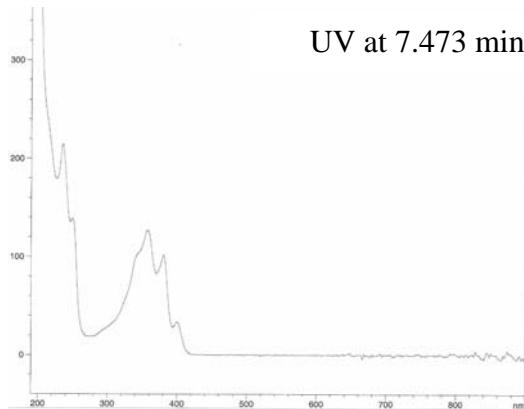
1. Characterisation of asymmetric Cl₂-NDI cyclophane (1)	
¹ H-NMR, ¹³ C-NMR spectra and HPLC-MS traces	ESI-2
2. Characterisation of asymmetric ('BuS)₂-NDI cyclophane (2)	
¹ H-NMR, ¹³ C-NMR spectra, chiral HPLC and HPLC-MS traces	ESI-5
3. Characterisation of asymmetric Cl-MeO-NDI cyclophane	
¹ H-NMR, ¹³ C-NMR spectra and HPLC-MS traces	ESI-9
4. Characterisation of asymmetric (MeO)₂-NDI cyclophane (3)	
¹ H-NMR, ¹³ C-NMR spectra, chiral HPLC and HPLC-MS traces	ESI-11
5. Characterisation of asymmetric asymmetric ((CH₂)₅N)₂-NDI cyclophane (4)	
¹ H-NMR, ¹³ C-NMR spectra, chiral HPLC and HPLC-MS traces	ESI-15

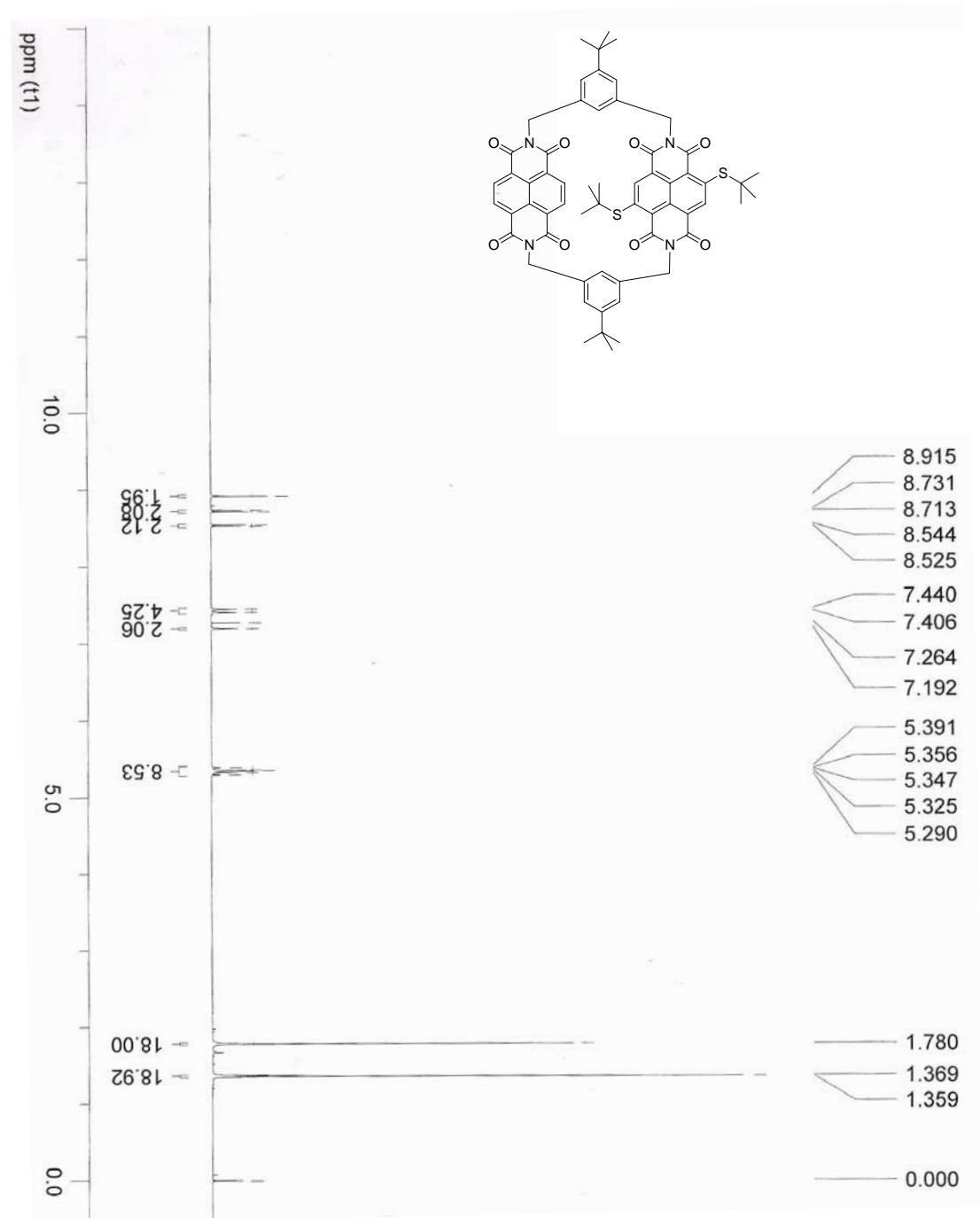
1. Characterisation of asymmetric $\text{Cl}_2\text{-NDI}$ cyclophane (1**)** **$^1\text{H-NMR}$ spectra**

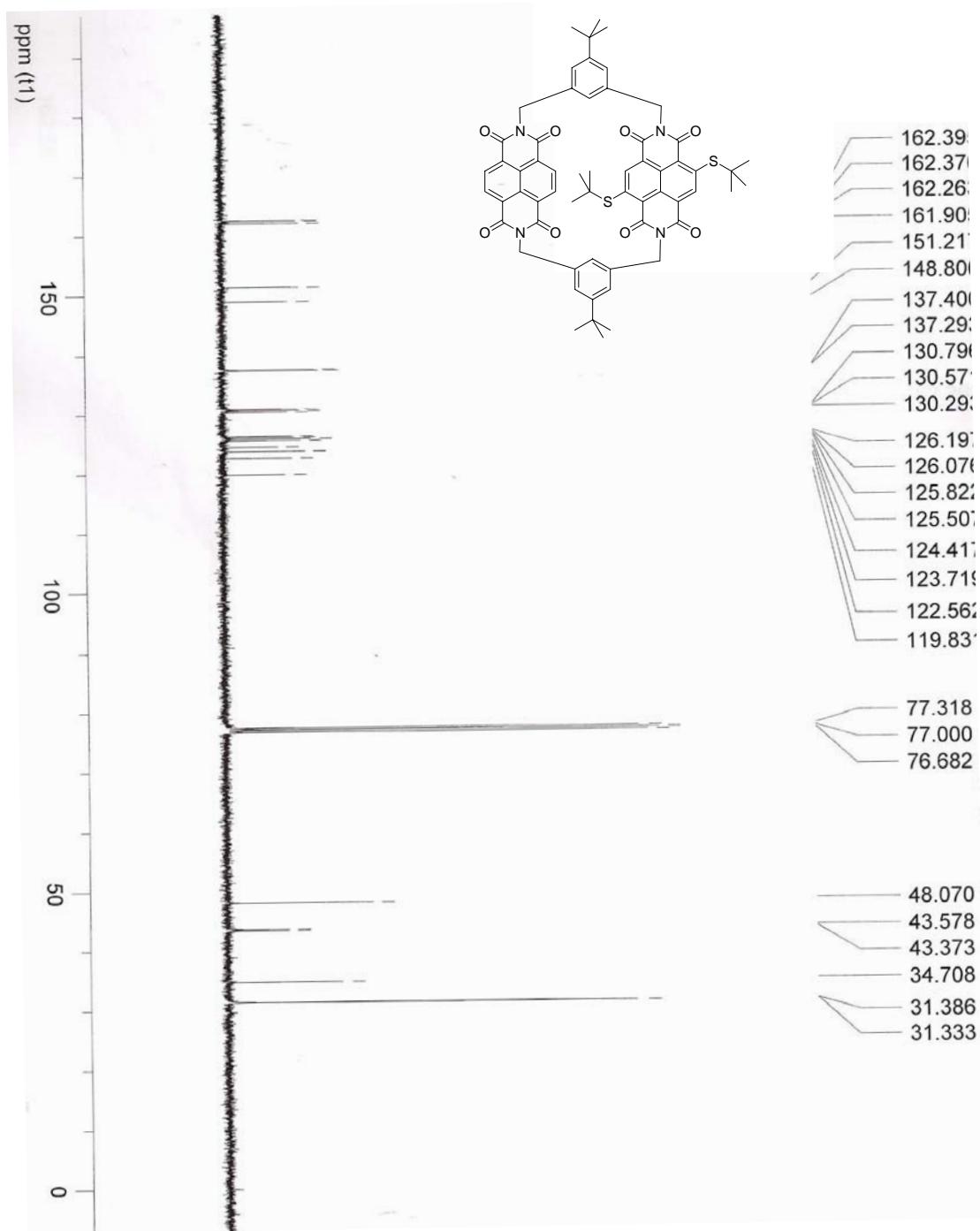
¹³C-NMR spectra

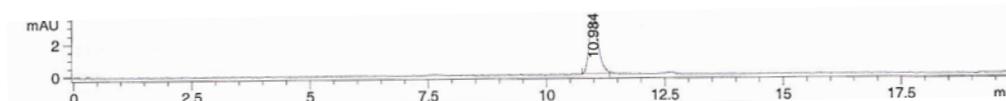
HPLC-ESI-MS

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.425	BB	0.1748	42.74128	3.64438	2.7895
2	7.473	VB	0.1828	1489.47290	123.39246	97.2105
Totals :				1532.21418	127.03685	

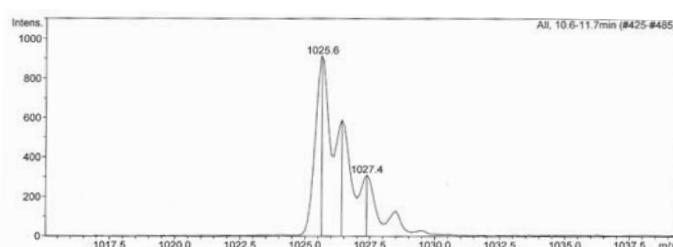
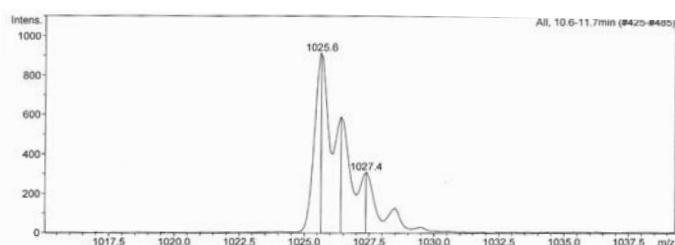
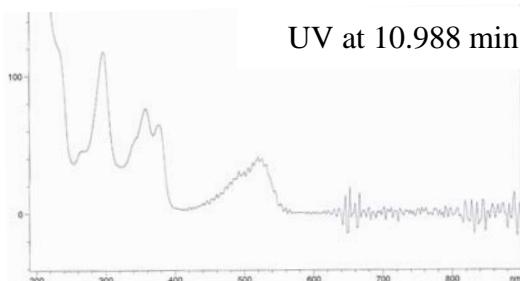


2. Characterisation of asymmetric (^tBuS)₂-NDI cyclophane (2)**¹H-NMR spectra**

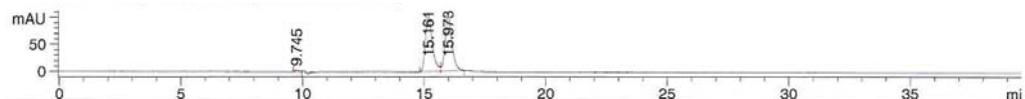
¹³C-NMR spectra

HPLC-ESI-MS

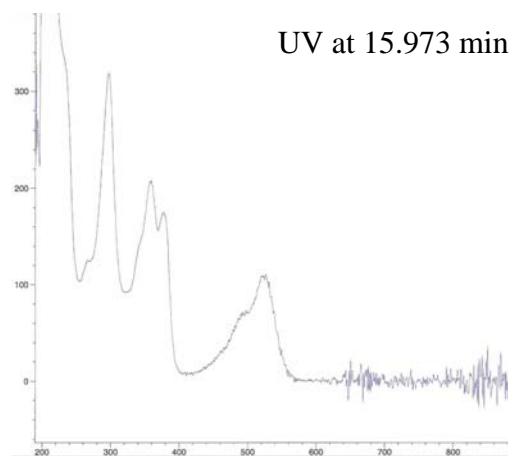
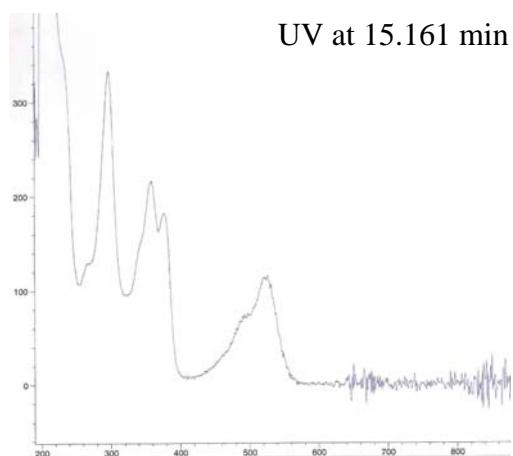
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.609	BB	0.2119	18.02073	1.13119	1.7649
2	10.988	BB	0.2062	1003.02545	73.97566	98.2351
Totals :					1021.04618	75.10685



Chiral HPLC

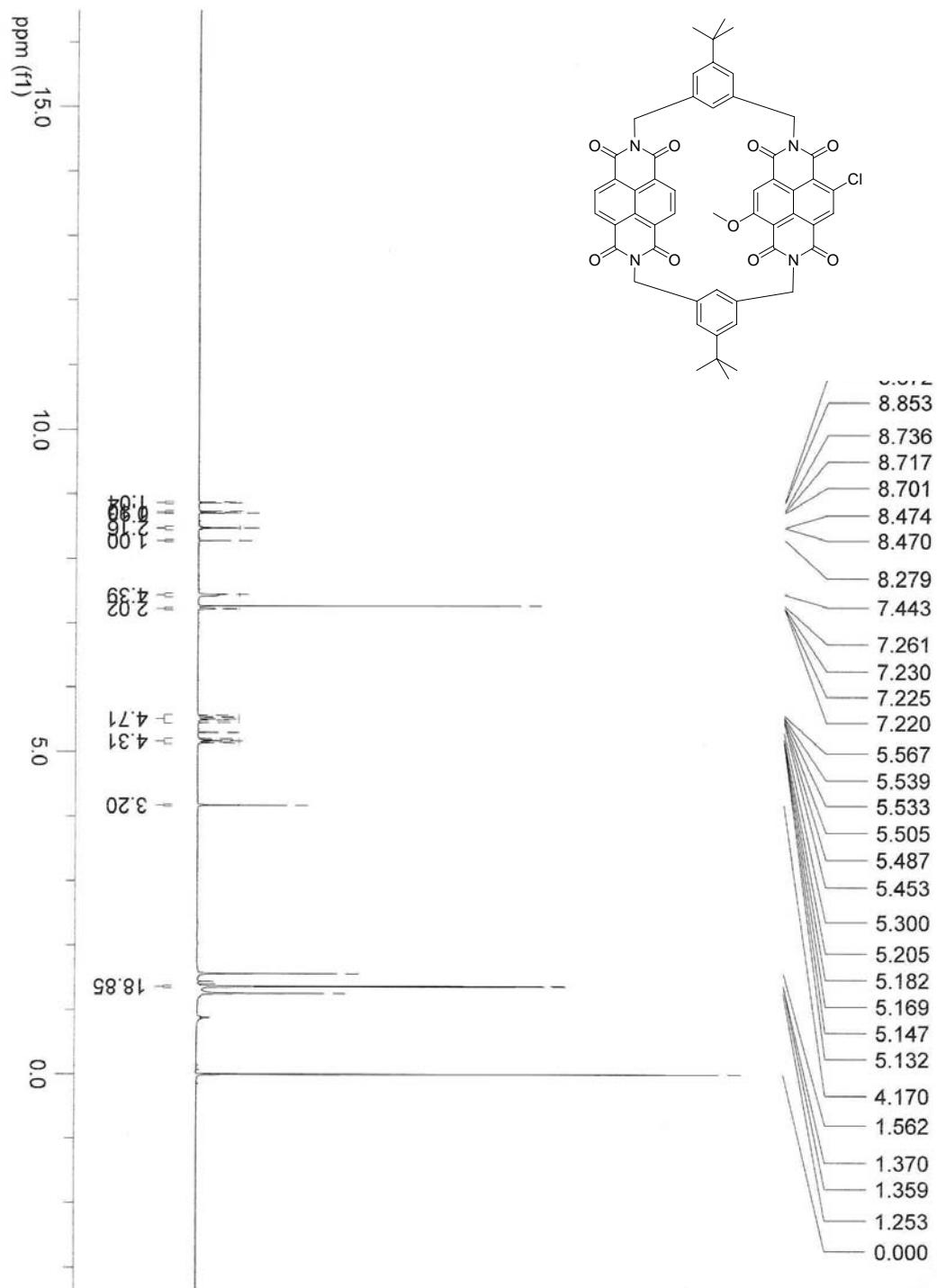


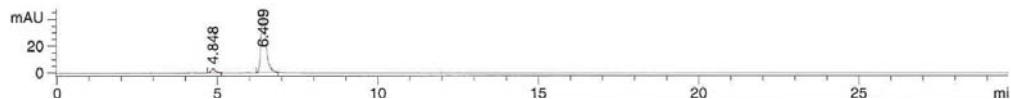
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.745	BB	0.1724	40.31122	3.12643	0.9699
2	15.161	PV	0.2861	2066.74365	107.57854	49.7270
3	15.973	VB	0.3029	2049.12524	101.76608	49.3031



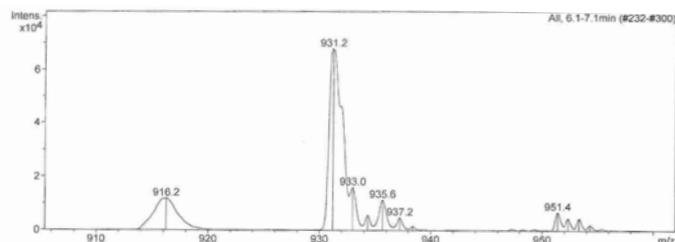
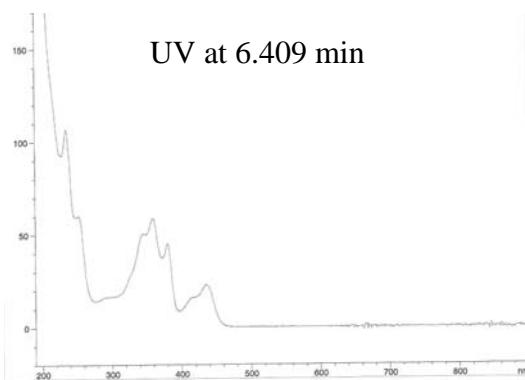
3. Characterisation of asymmetric Cl-MeO-NDI cyclophane

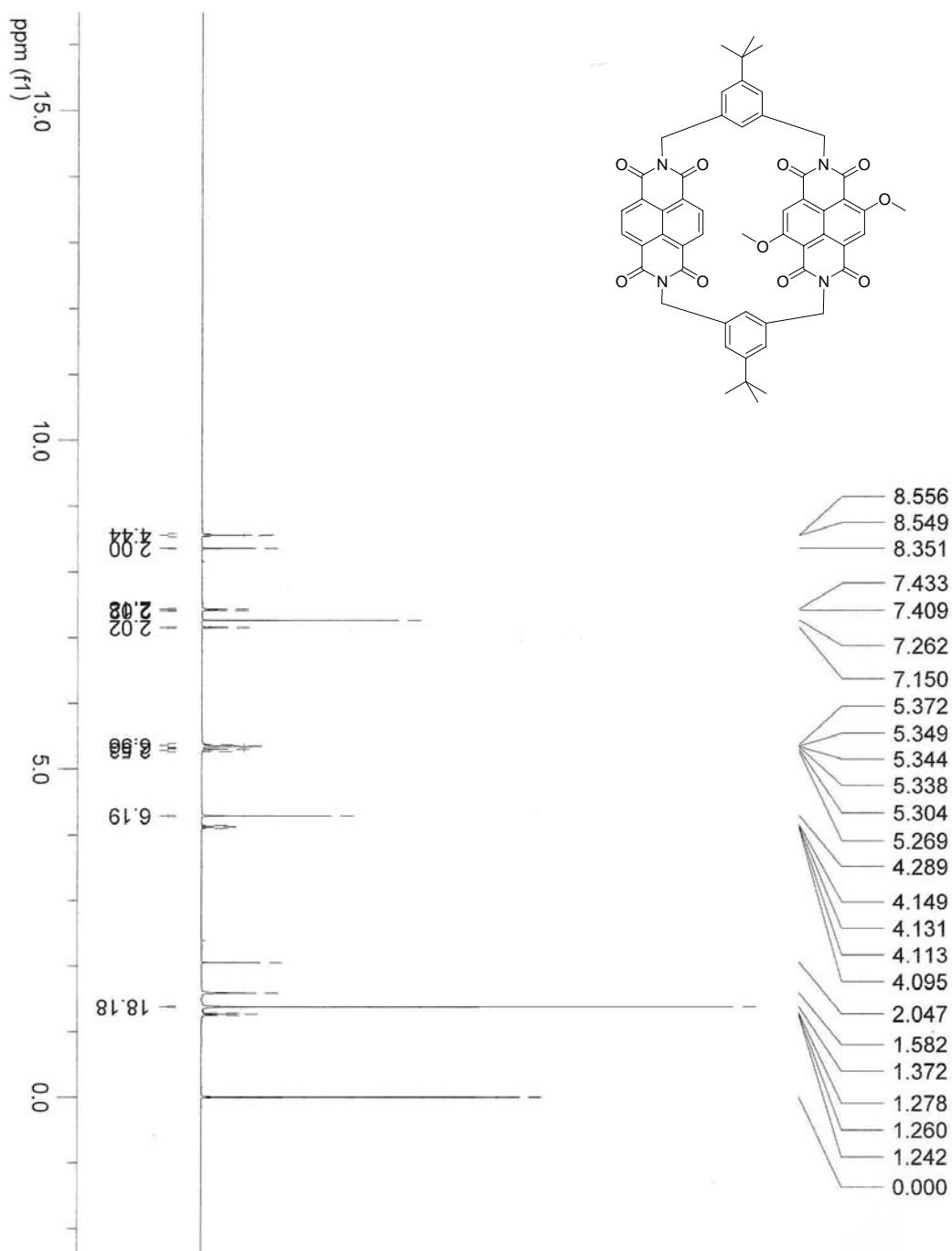
¹H-NMR spectra

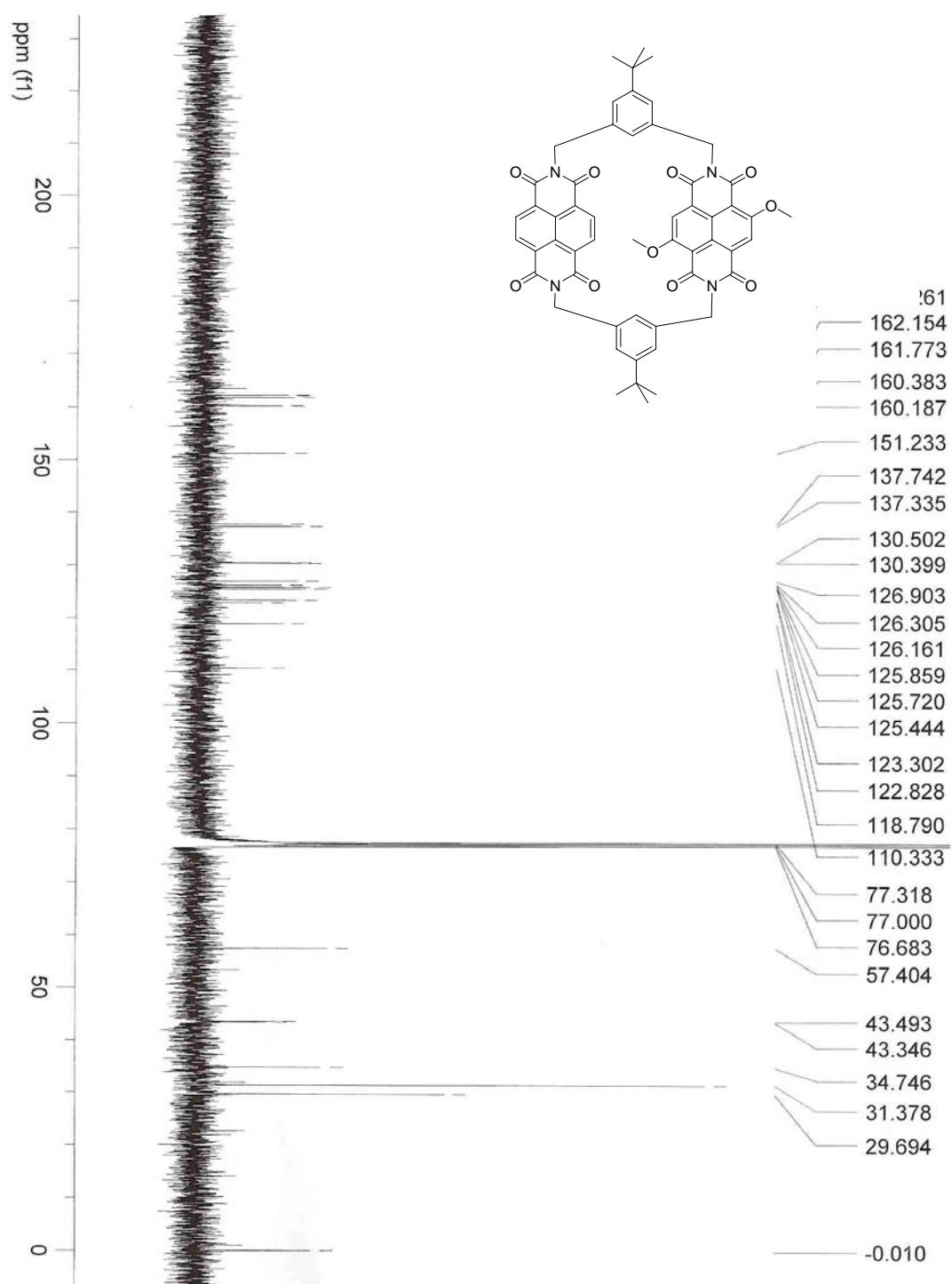


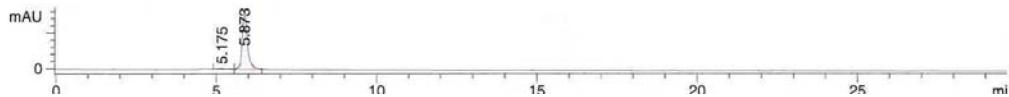
HPLC-ESI-MS

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.848	PB	0.1523	32.33945	3.18963	6.0800
2	6.409	PB	0.1642	499.56085	45.44943	93.9200
Totals :				531.90030	48.63906	

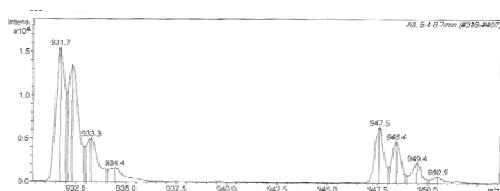
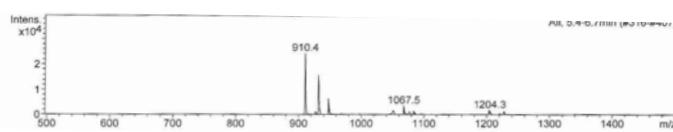
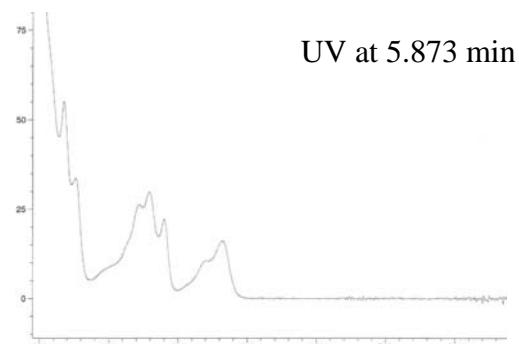


4. Characterisation of asymmetric (MeO)₂-NDI cyclophane (3)**¹H-NMR spectra**

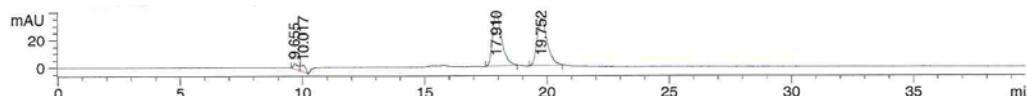
¹³C-NMR spectra

HPLC-ESI-MS

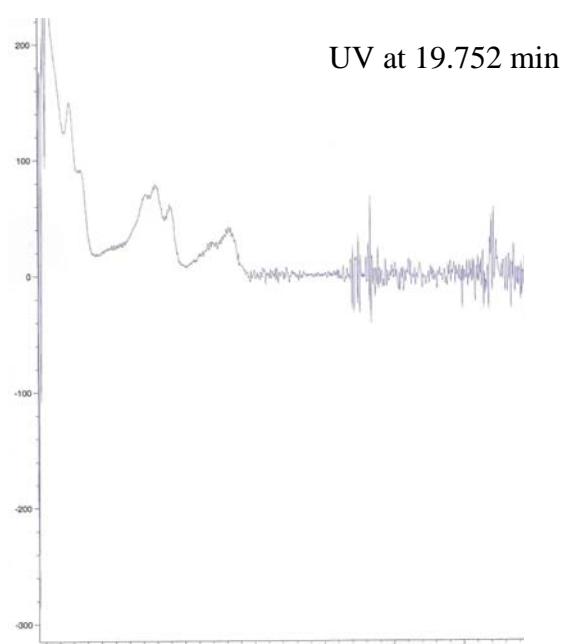
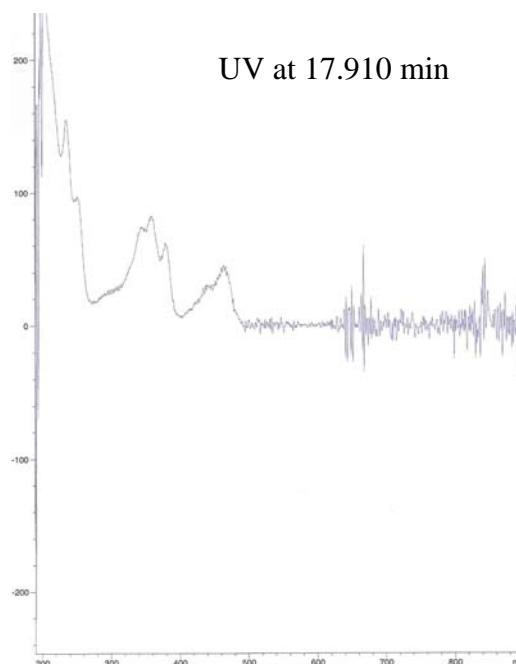
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.175	BV	0.2569	23.60901	1.24671	2.5109
2	5.873	VB	0.1674	916.65375	81.37714	97.4891
Totals :				940.26275	82.62386	

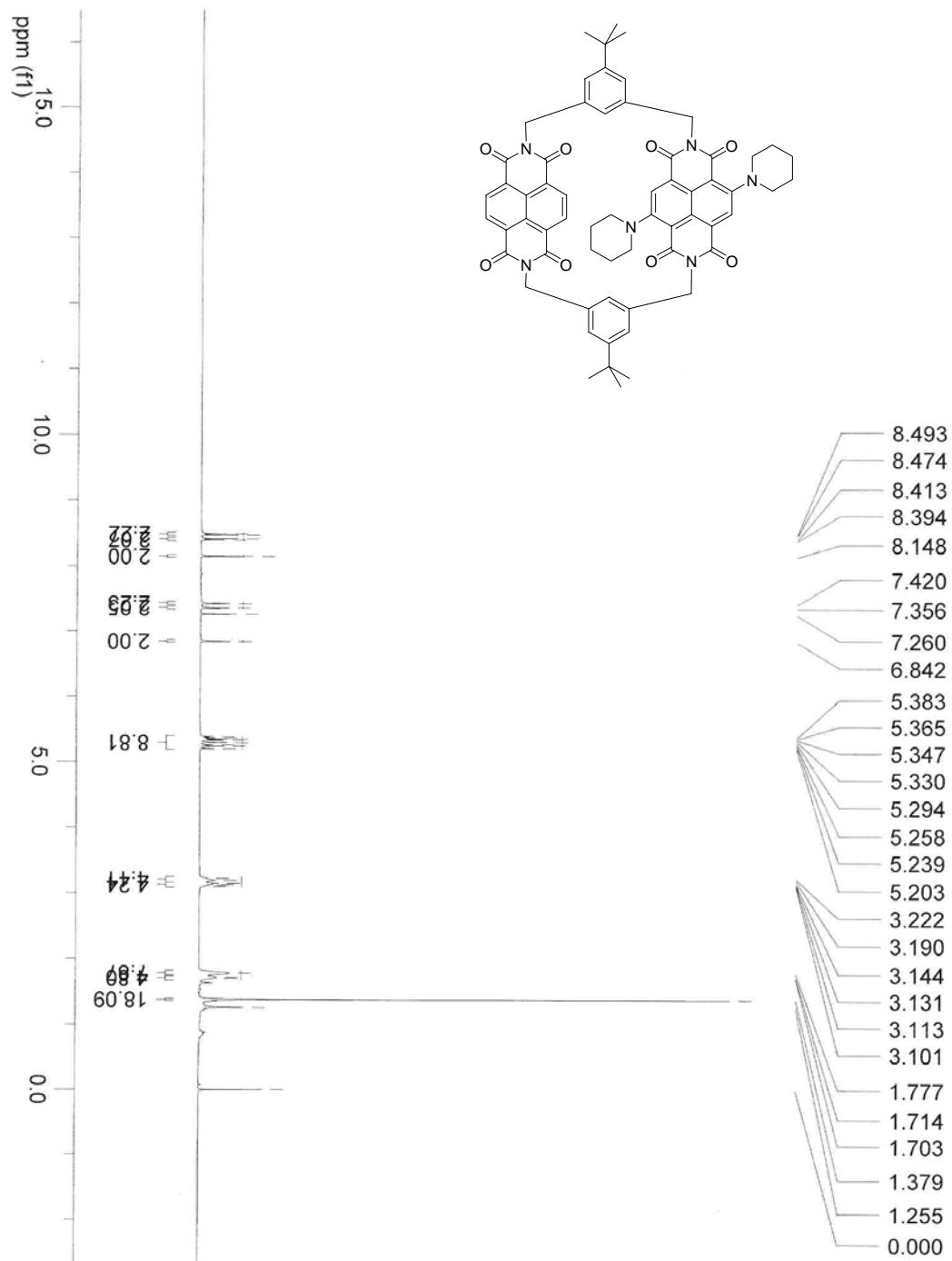


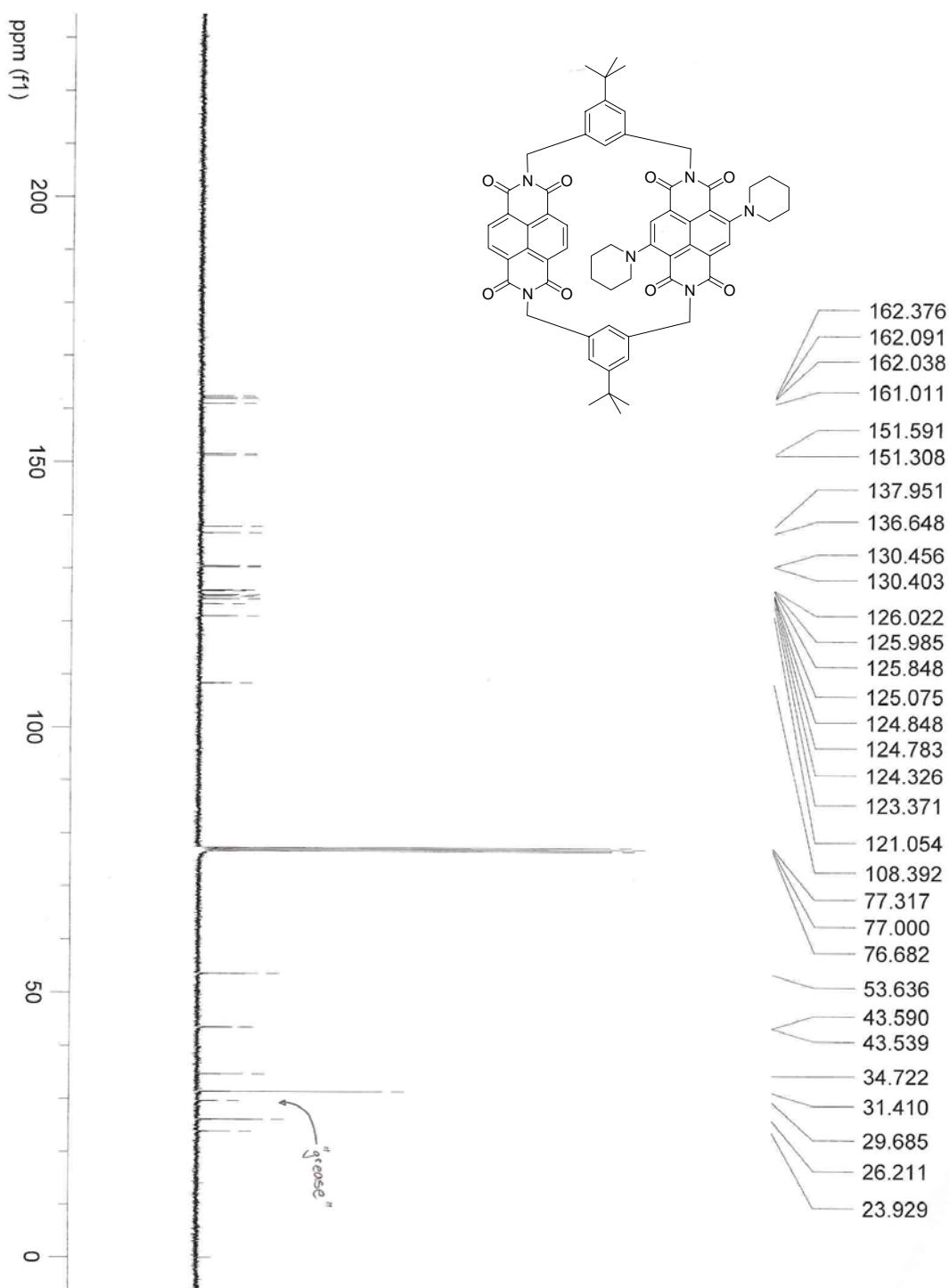
Chiral HPLC

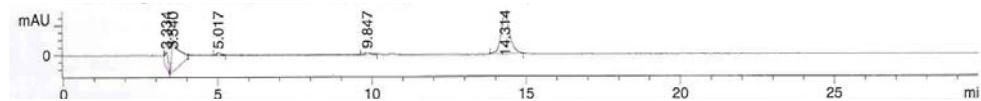


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.655	BB	0.1892	61.15757	4.26846	2.9033
2	10.017	BP	0.1938	59.48710	4.63175	2.8240
3	17.910	BB	0.3897	995.01764	38.22557	47.2353
4	19.752	BB	0.4388	990.85254	34.31944	47.0375
Totals :				2106.51485	81.44523	

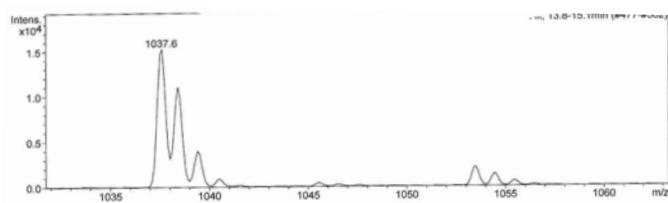
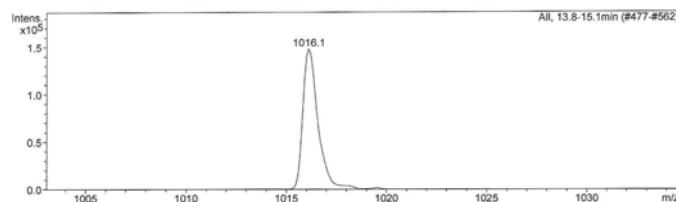
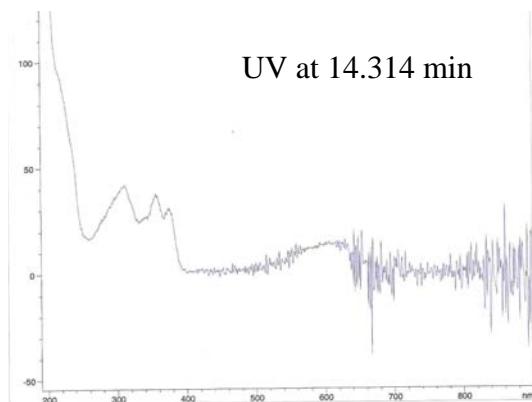


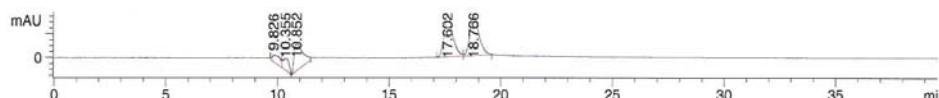
5. Characterisation of asymmetric asymmetric $((\text{CH}_2)_5\text{N})_2\text{-NDI}$ cyclophane (4) **$^1\text{H-NMR}$ spectra**

¹³C-NMR spectra

HPLC-ESI-MS

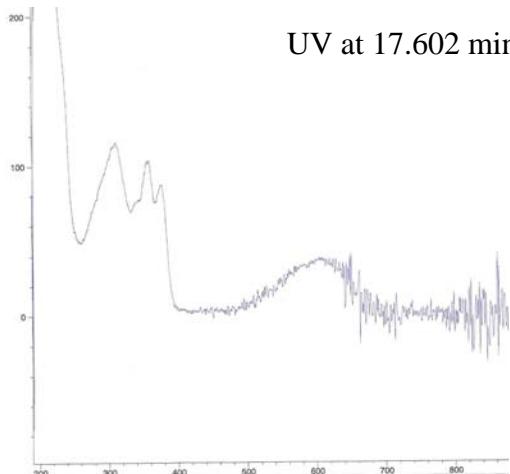
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.334	BP	0.1104	72.40755	10.24580	7.1509
2	3.540	VB	0.2194	357.85532	21.58412	35.3417
3	5.017	PB	0.1429	15.41575	1.65210	1.5225
4	9.847	PB	0.2097	17.29118	1.20293	1.7077
5	14.314	BB	0.2946	549.58966	27.56345	54.2773
Totals :				1012.55946	62.24840	



Chiral HPLC

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.826	BV	0.3604	164.53619	5.74107	5.6566
2	10.355	VP	0.3140	192.15764	10.00996	6.6062
3	10.852	BV	0.3926	603.66461	22.67355	20.7535
4	17.602	BV	0.4169	971.71588	35.11010	33.4068
5	18.766	VB	0.4300	976.66461	33.91465	33.5769
Totals :				2908.73894	107.44932	

UV at 17.602 min



UV at 18.766 min

