Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Cu-Catalyzed C-H Amination/Ullmann *N*-Arylation Domino Reaction: Straightforward Synthesis of 9,14-Diaryl-9,14-dihydrodibenzo[a,c]phenazine

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I. General Information

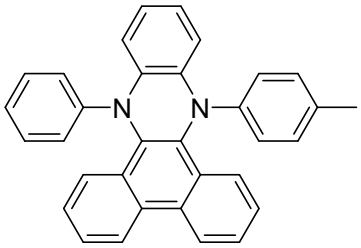
Unless otherwise noted, all reagents were obtained commercially available and used without further purification.

NMR spectrum: ^{1}H and ^{13}C NMR spectra were collected on 400 MHz and 300 MHz NMR spectrometers (Bruker AVANCE) using $CDCl_3$ or DMSO-d_6. Chemical shifts are reported in parts per million (ppm). Chemical shifts for protons are reported in parts per million downfield and are referenced to residual protium in the NMR solvent ($CHCl_3$ = δ 7.26). Chemical shifts for carbon are reported in parts per million downfield and are referenced to the carbon resonances of the solvent ($CDCl_3$ =δ 77.0). Data are represented as follows: chemical shift, multiplicity (br. s = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants in Hertz (Hz), integration.

Mass spectroscopy: Mass spectra were in general recorded on an AMD 402/3 or a HP 5989A mass selective detector.

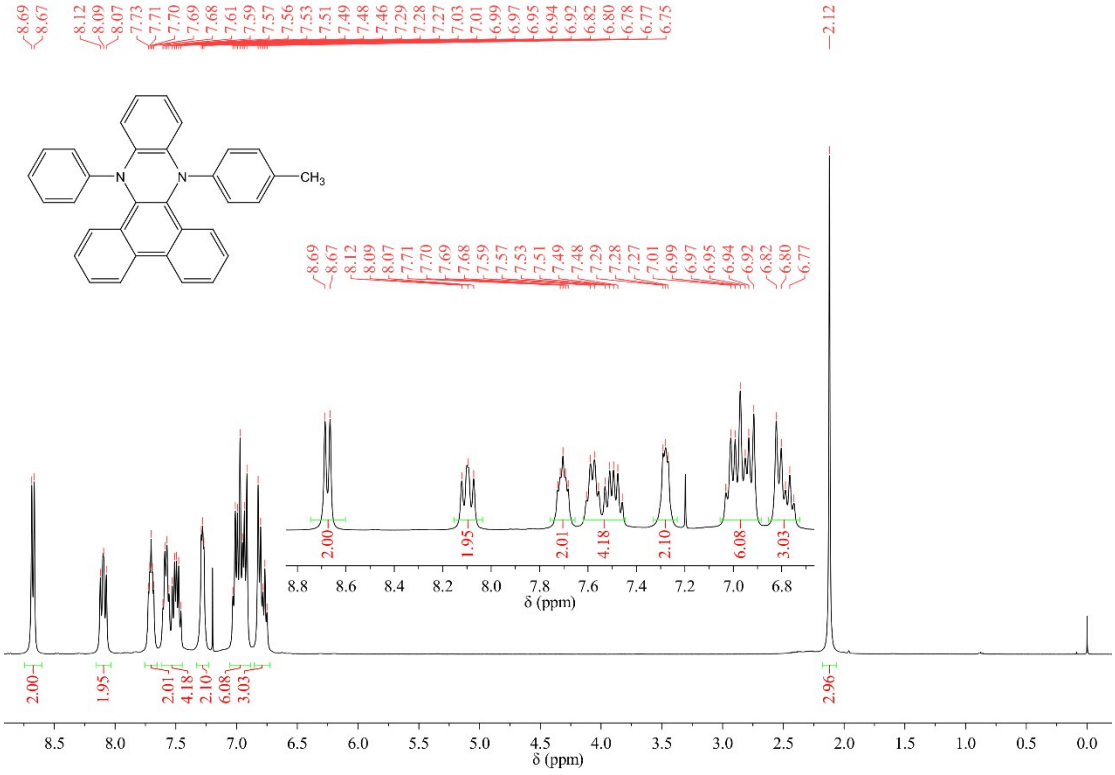
Column Chromatography: Column chromatography was performed with silica gel (200-300 mesh ASTM).

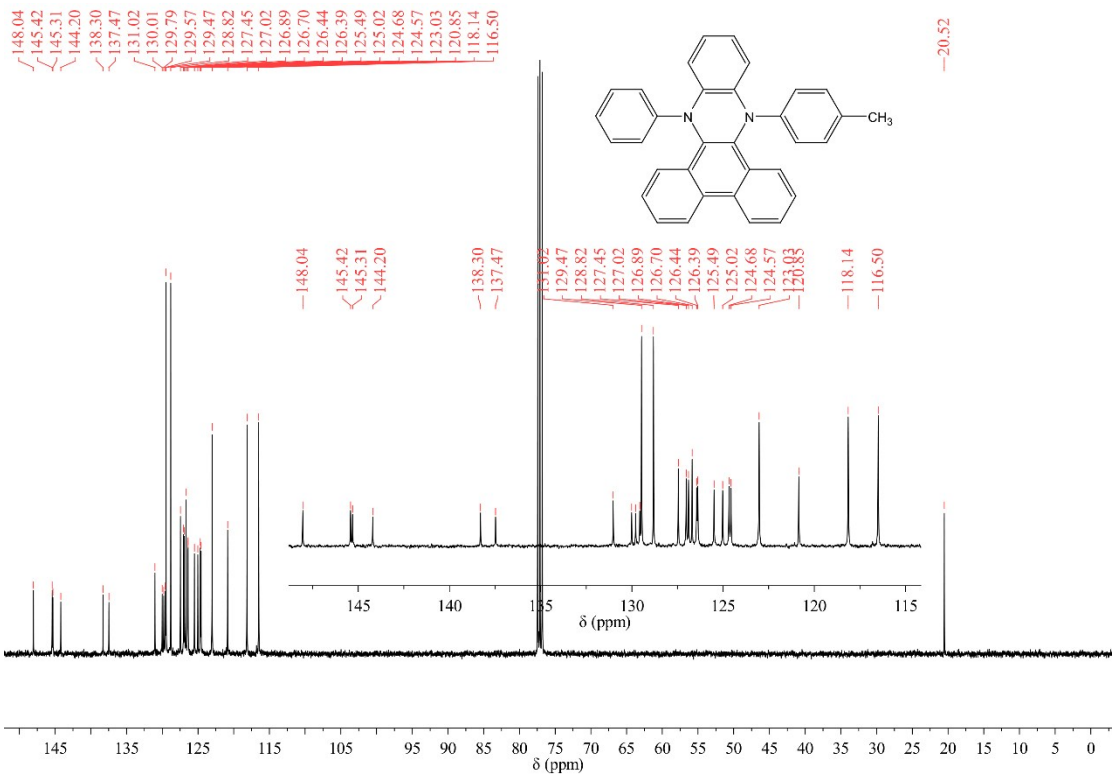
II. The Data and NMR Spectra of Products

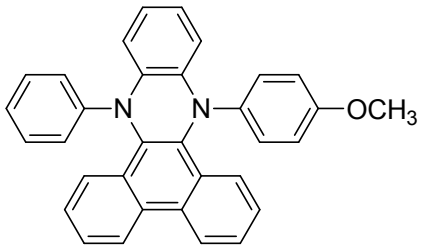


11-methyl-9,14-diphenyl-9,14-dihydrodibenzo[a,c]phenazine (1aa)

m.p. 183-185 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.68 (d, J = 8.0 Hz, 2H), 8.07-8.12 (m, 2H), 7.68-7.73 (m, 2H), 7.46-7.61 (m, 4H), 7.21-7.29 (m, 2H), 6.92-7.03 (m, 6H), 6.75-6.82 (m, 3H), 2.12 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 148.04, 145.42, 145.31, 144.20, 138.30, 137.47, 131.02, 130.01, 129.79, 129.57, 129.47, 128.82, 127.45, 127.02, 126.89, 126.70, 126.44, 126.39, 125.49, 125.02, 124.68, 124.57, 123.03, 120.85, 118.14, 116.50, 20.52; HRMS ESI (m/z) $[M]^+$: calcd. for $C_{33}H_{24}N_2$ 448.1939, found 448.1938.

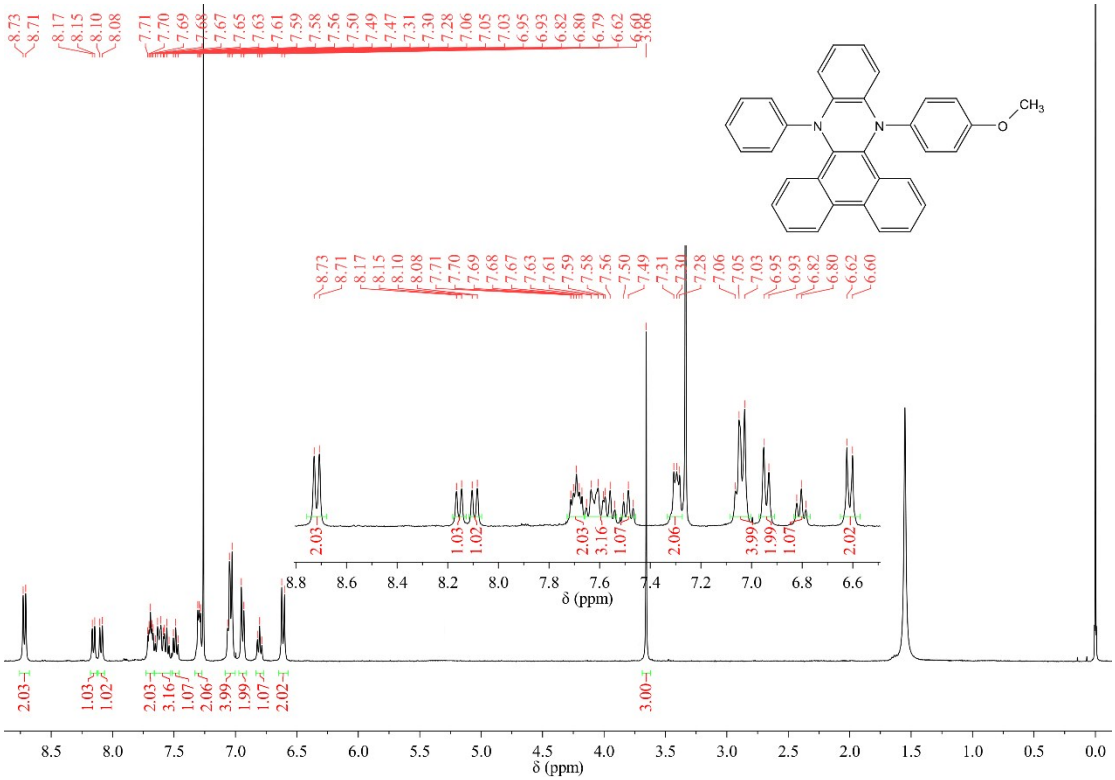






11-methoxy-9,14-diphenyl-9,14-dihydrodibenzo[a,c]phenazine (1ab)

m.p. 138-140 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.71 (d, J = 8.4 Hz, 2H), 8.15 (d, J = 8.0 Hz, 1H), 8.09 (d, J = 8.4 Hz, 1H), 7.67-7.71 (m, 2H), 7.54-7.65 (m, 3H), 7.47-7.52 (m, 1H), 7.28-7.31 (m, 2H), 7.03-7.06 (m, 4H), 6.94 (d, J = 8.0 Hz, 2H), 6.79-6.82 (m, 1H), 6.60-6.62 (m, 2H), 3.66 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 155.18, 148.44, 145.78, 143.38, 141.53, 138.44, 136.62, 130.07, 129.58, 129.55, 129.28, 128.74, 127.53, 127.00, 126.72, 126.29, 126.18, 125.62, 125.56, 124.62, 124.51, 124.39, 122.95, 122.89, 121.39, 120.62, 116.08, 114.16, 55.36; HRMS ESI (m/z) $[M]^+$: calcd. for $C_{33}H_{24}N_2O$ 464.1889, found 464.1890.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8.17
8.15
8.10
8.08
7.71
7.70
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7.68
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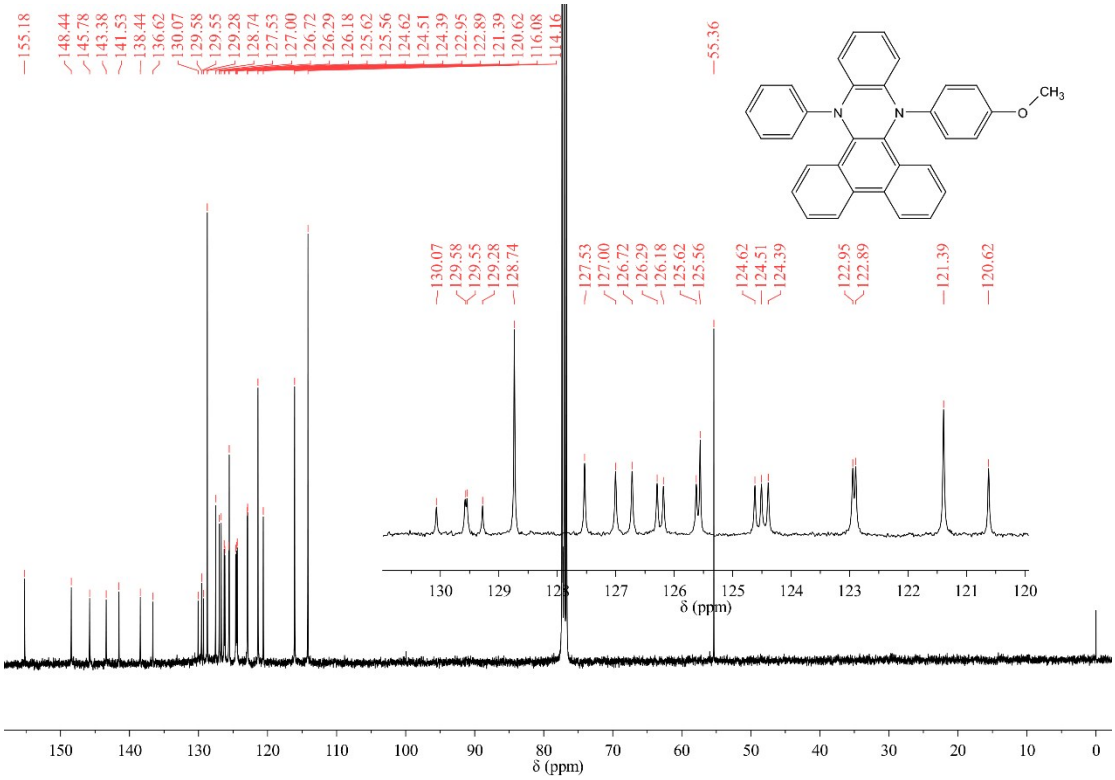
7.61
7.59
7.58
7.56
7.50
7.49
7.47
7.31
7.30
7.28
7.06
7.05
7.03
6.95
6.93
6.82
6.80
6.79
6.62
6.60
3.88
CH3
O
N
N
2.03
3.16
1.07
2.06
3.99
1.99
1.07
2.02
δ (ppm)
1.03
1.02
3.00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130.07
129.58
129.55
129.28
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127.00
126.72
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125.62
125.56
124.62
124.51
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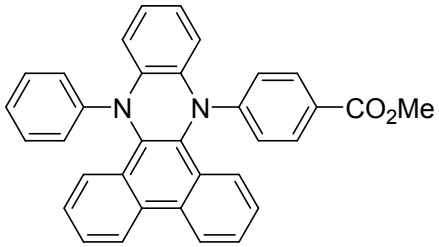
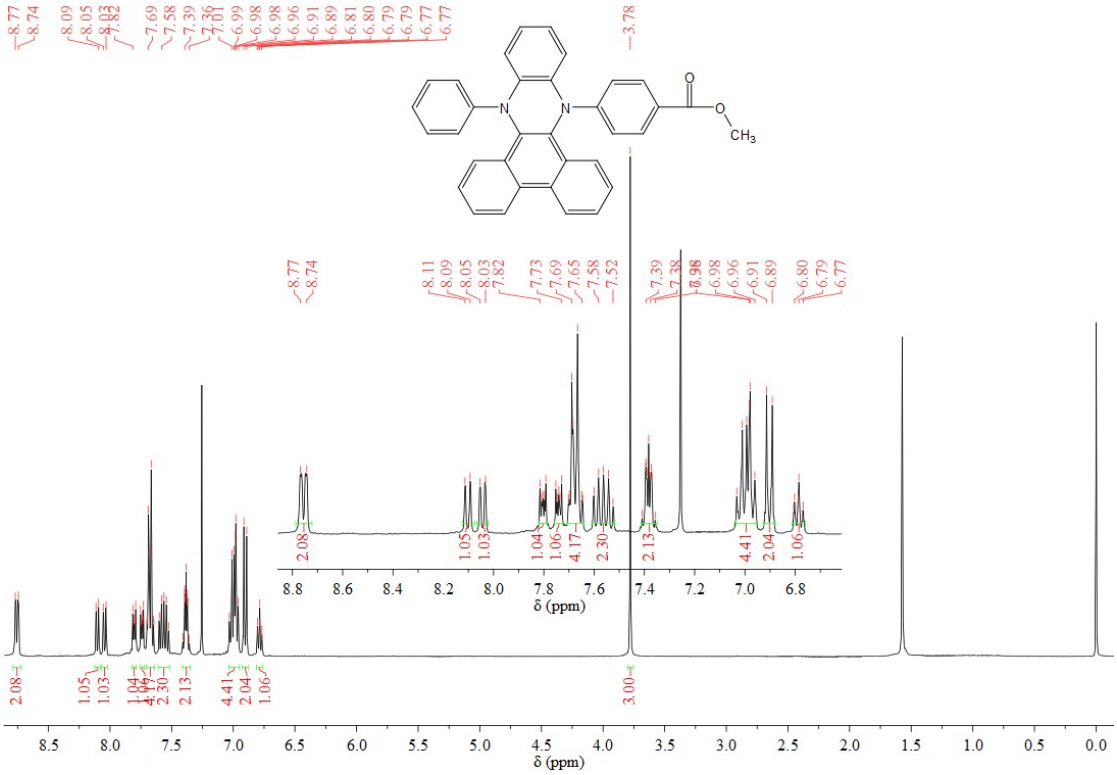
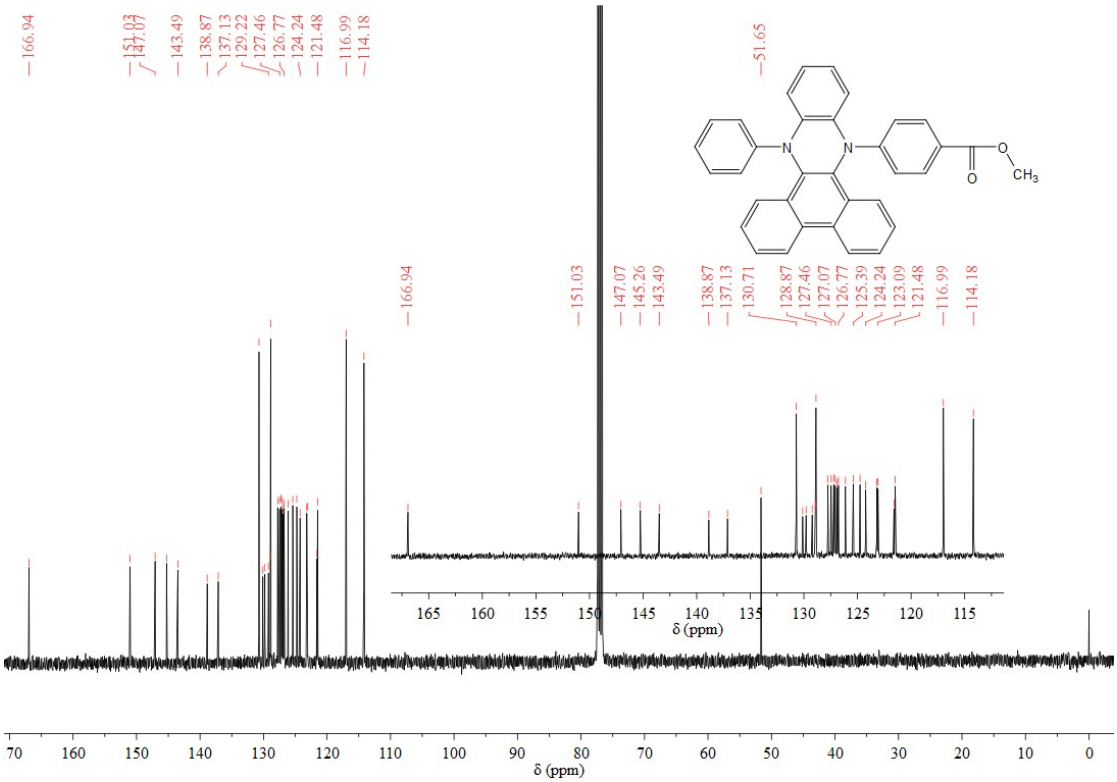
114.16
55.36
CH3
O
N
N
δ (ppm)

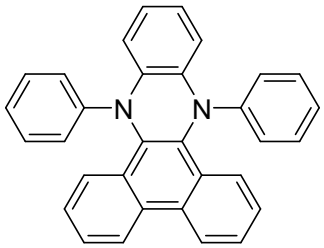


methyl 4-(14-phenyldibenzo[a,c]phenazin-9(14H)-yl)benzoate (1ac)

m.p. 182-185 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.74-8.77 (m, 2H), 8.09-8.11 (m, 1H), 8.03-8.06 (m, 1H), 7.79-7.82 (m, 1H), 7.73-7.75 (m, 1H), 7.65-7.70 (m, 4H), 7.52-7.60 (m, 2H), 7.37-7.40 (m, 2H), 6.96-7.03 (m, 4H), 6.89-6.91 (m, 2H), 6.77-6.81 (m, 1H), 3.78 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 166.94, 151.03, 147.07, 145.26, 143.49, 138.87, 137.13, 130.71, 130.11, 129.79, 129.22, 128.94, 128.87, 127.77, 127.46, 127.21, 127.07, 126.90, 126.77, 126.12, 125.39, 124.76, 124.24, 123.19, 123.09, 121.59, 121.48, 116.99, 114.18, 51.65; HRMS ESI (*m/z*) $[M]^+$: calcd. for $C_{34}H_{24}N_2O_2$ 492.1838, found 492.1836.

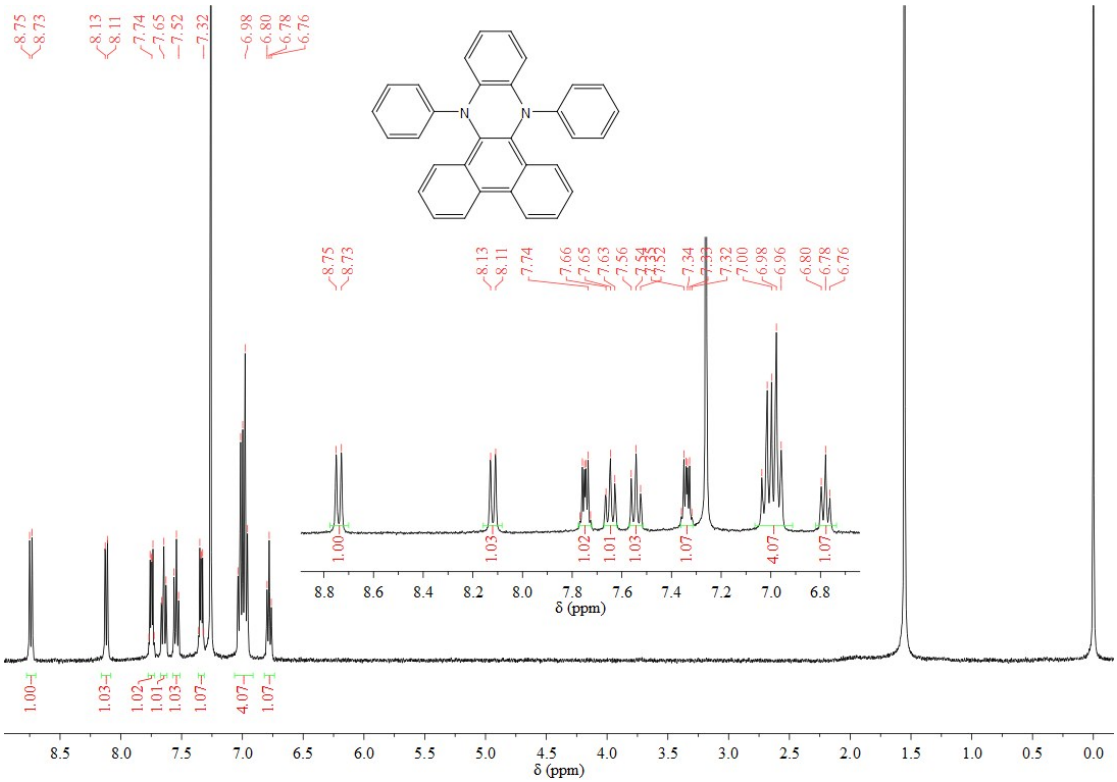






9,14-diphenyl-9,14-dihydrodibenzo[a,c]phenazine (1ad)

m.p. 241-243 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.74 (d, J = 8.0 Hz, 2H), 8.12 (d, J = 8.0 Hz, 2H), 7.74-7.76 (m, 2H), 7.63-7.67 (m, 2H), 7.52-7.56 (m, 2H), 7.33-7.35 (m, 2H), 6.96-7.04 (m, 8H), 6.76-6.80 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 147.69, 144.83, 138.13, 129.88, 129.48, 128.76, 127.39, 126.98, 126.51, 125.37, 124.61, 123.02, 121.02, 116.76; HRMS ESI (m/z) $[M+H]^+$: calcd. for $C_{32}H_{23}N_2$ 435.1861, found 435.1851.


8.75
8.73
8.13
8.11
7.74
7.65
7.52
7.32
6.98
6.80
6.78
6.76
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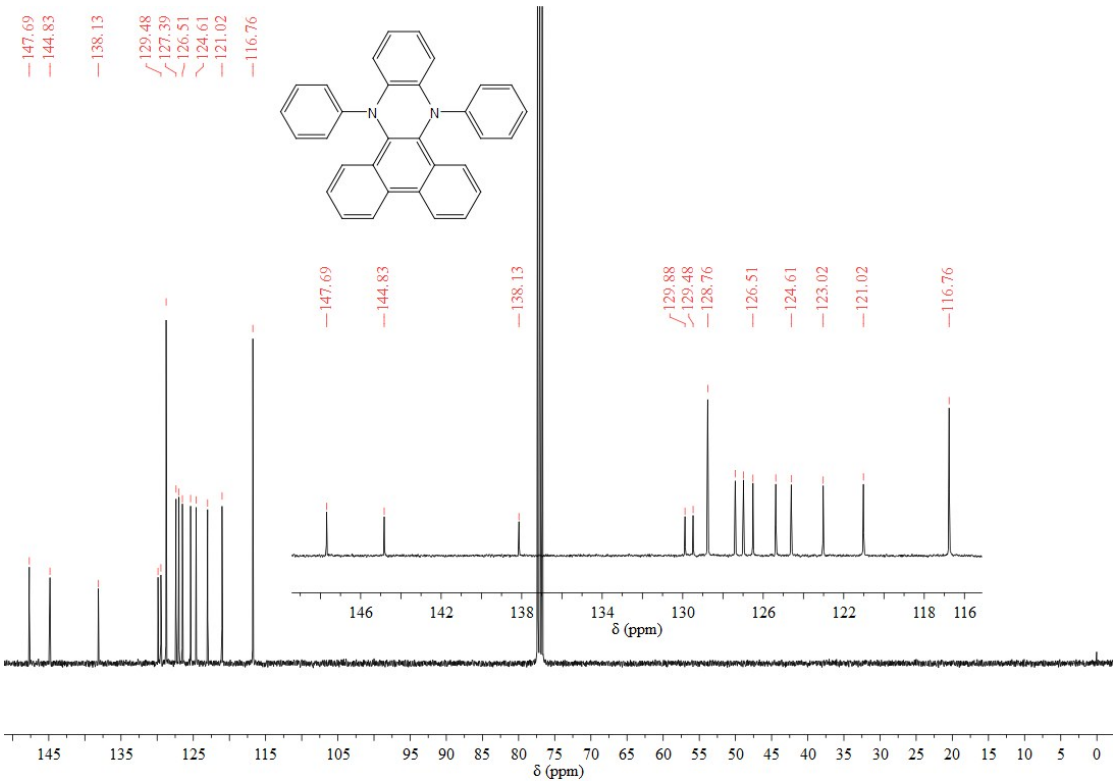
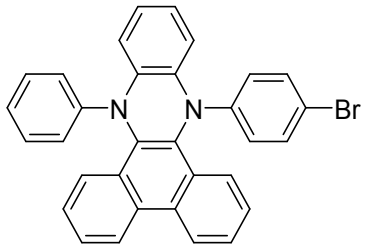
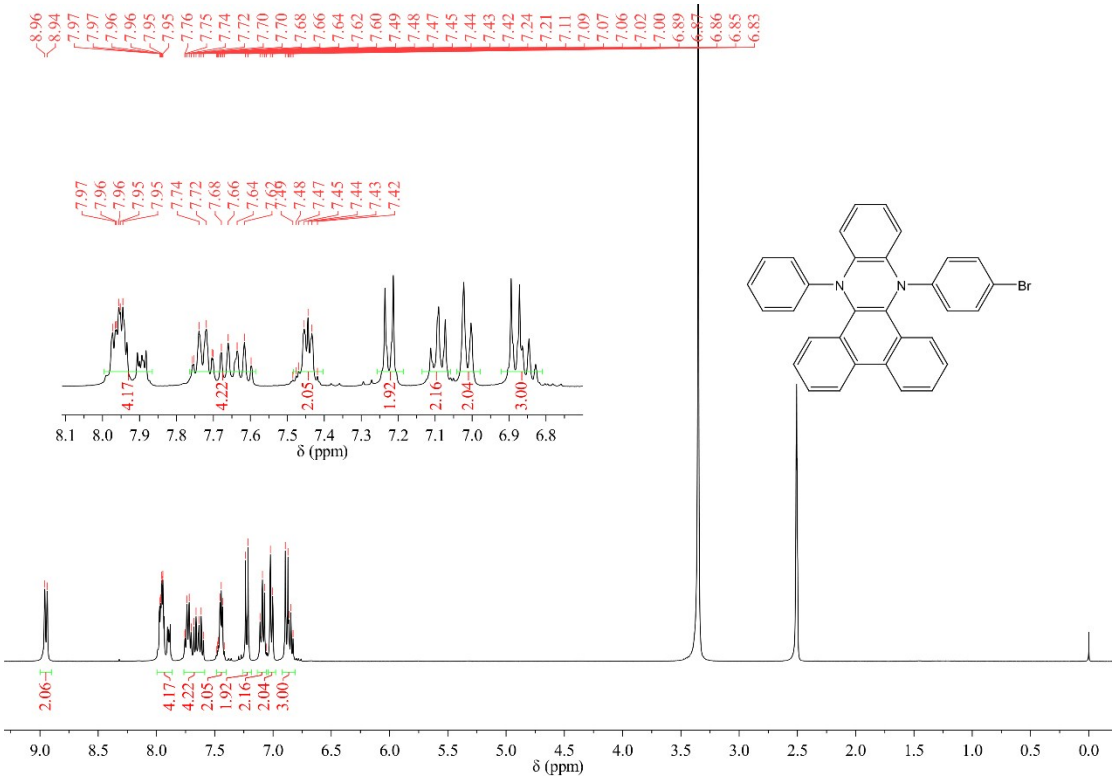
1.01
1.03
1.07
4.07
1.07
δ (ppm)

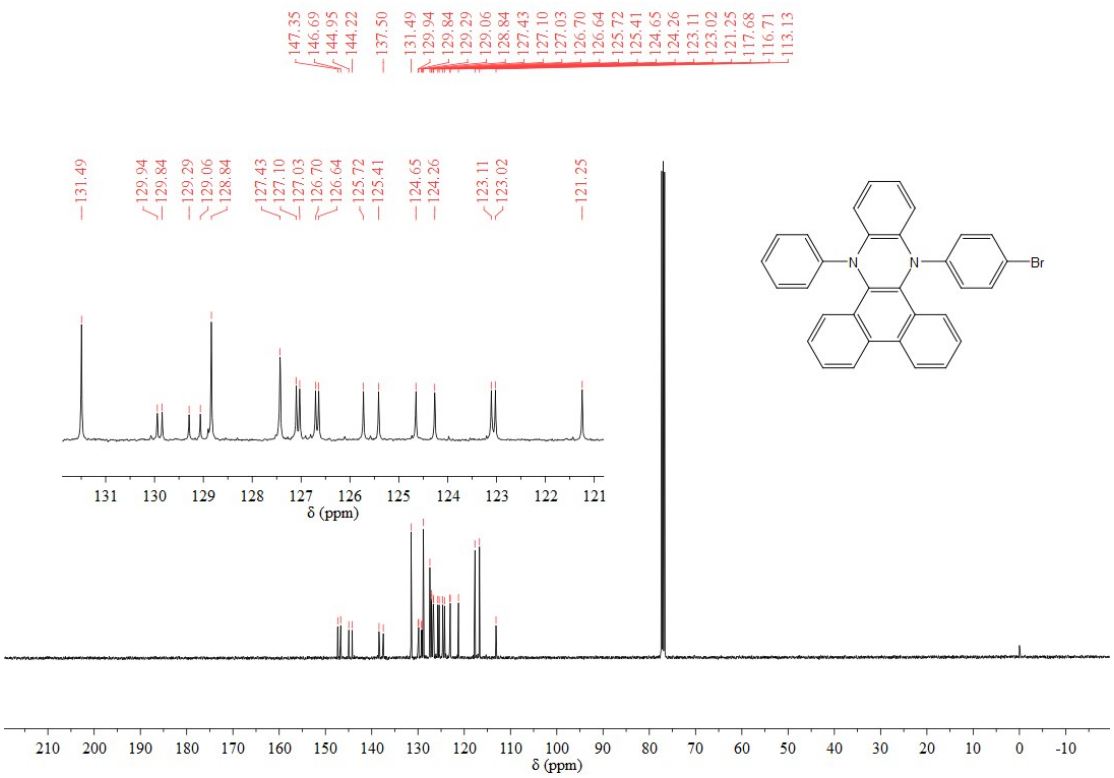

147.69
144.83
138.13
129.48
127.39
126.51
124.61
121.02
116.76
δ (ppm)

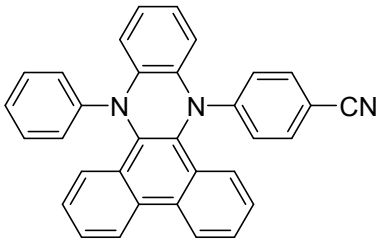

N
N
Br

9-(4-bromophenyl)-14-phenyl-9,14-dihydrodibenzo[a,c]phenazine (1ae)

m.p. 188-189 °C; ^{1}H NMR (400 MHz, DMSO) δ: 8.95 (d, *J* = 8.4 Hz, 2H), 8.02-7.86 (m, 4H), 7.78-7.58 (m,4H), 7.50-7.39 (m, 2H), 7.22 (d, *J* = 9.1 Hz,2H), 7.14-7.05 (m, 2H), 7.01 (d, *J* = 7.8 Hz, 2H), 6.91-6.81 (m, 3H); 13C NMR (100 MHz, CDCl3) δ 147.35, 146.69, 144.95, 144.22, 138.43, 137.50, 131.49, 129.94, 129.84, 129.29, 129.06, 128.84, 127.43, 127.10, 127.03, 126.70, 126.64, 125.72, 125.41, 124.65, 124.26, 123.11, 123.02, 121.25, 117.68, 116.71, 113.13; HRMS ESI (m/z) $[M+H]^+$: calcd. for $C_{32}H_{22}N_2Br$ 513.0966, found 513.0968.

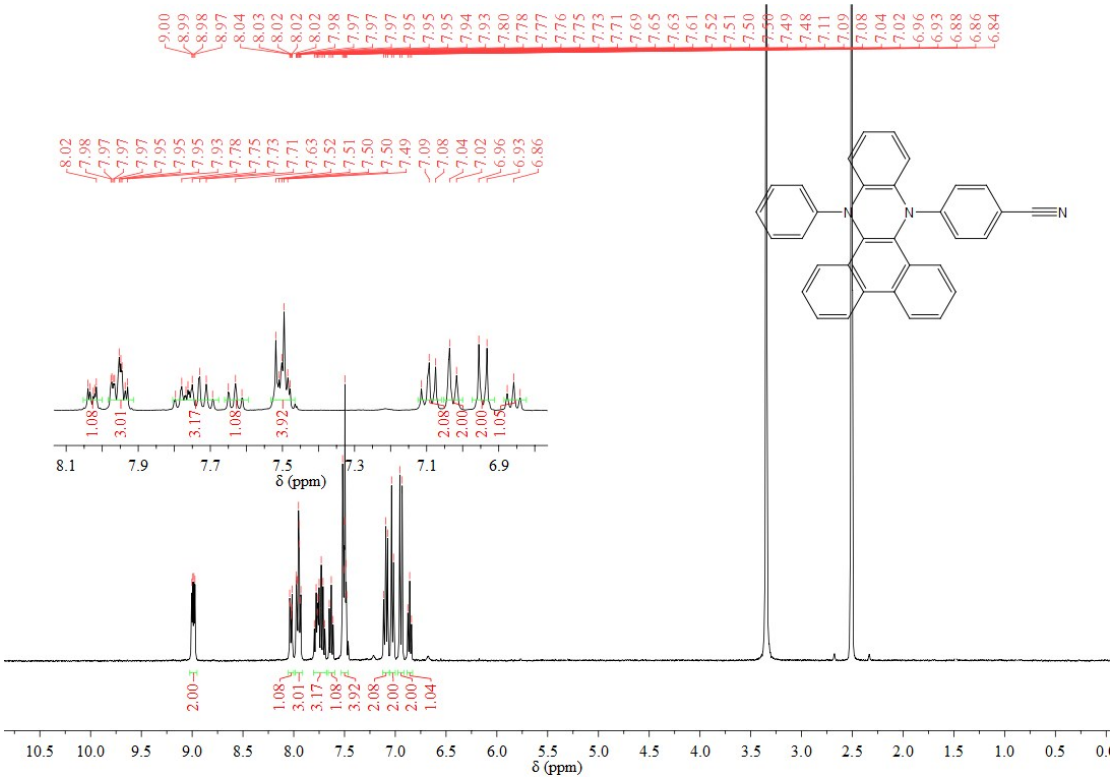






4-(14-phenyldibenzo[a,c]phenazin-9(14H)-yl)benzonitrile (1ae)

m.p. 231-231 ^{o}C; ^{1}H NMR (400 MHz, DMSO-d_6) δ: 8.97-9.00 (m, 2H), 8.02-8.04 (m, 1H), 7.93-7.97 (m, 3H), 7.69-7.80 (m, 3H), 7.61-7.65 (m, 1H), 7.48-7.52 (m, 4H), 7.08-7.11 (m, 2H), 7.02-7.04 (m, 2H), 6.93-6.96 (m, 2H), 6.84-6.88 (m, 1H); ^{13}C NMR (100 MHz, CDCl3) δ: 150.76, 146.89, 145.35, 142.97, 139.15, 136.64, 133.09, 130.19, 129.81, 129.11, 128.95, 128.68, 127.74, 127.64, 127.44, 127.22, 127.17, 126.97, 126.56, 125.56, 124.85, 123.91, 123.36, 123.16, 121.73, 119.72, 117.00, 114.73, 102.52.; HRMS ESI (*m/z*) $[M+H]^+$: calcd. for $C_{33}H_{22}N_3$ 460.1814, found 460.1813.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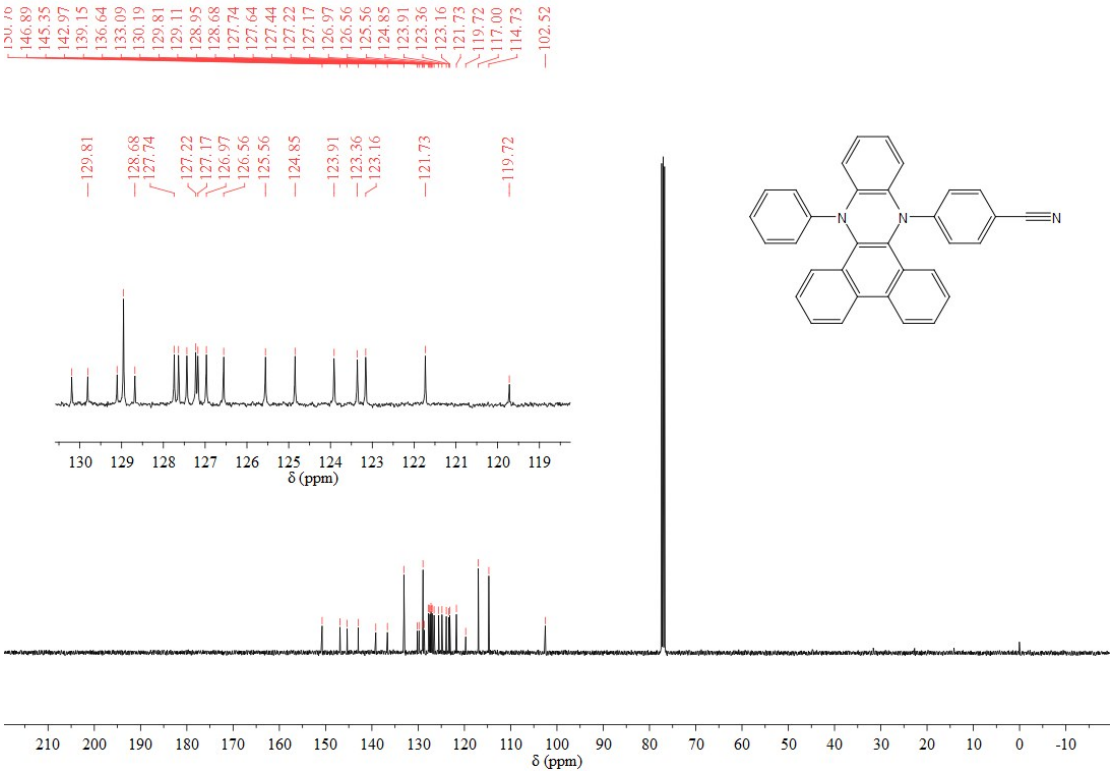
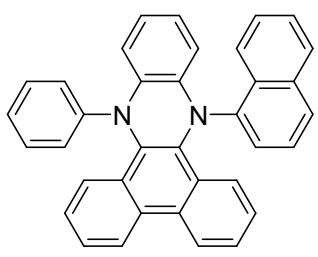
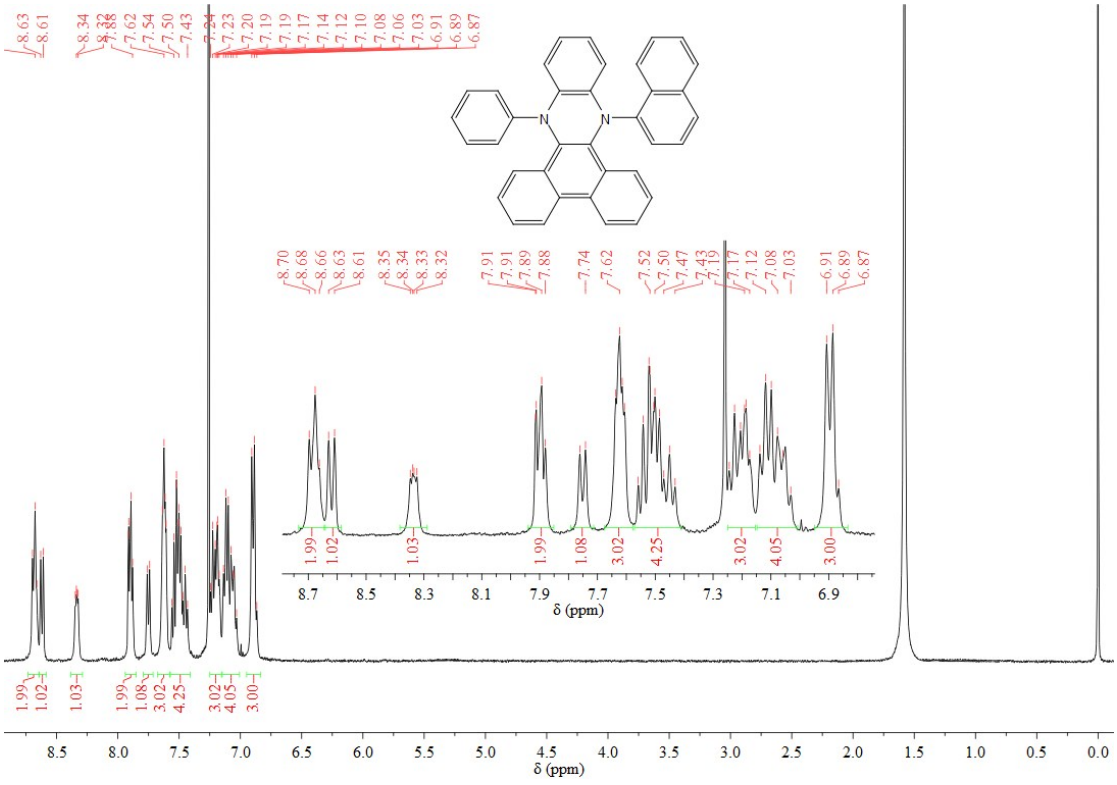
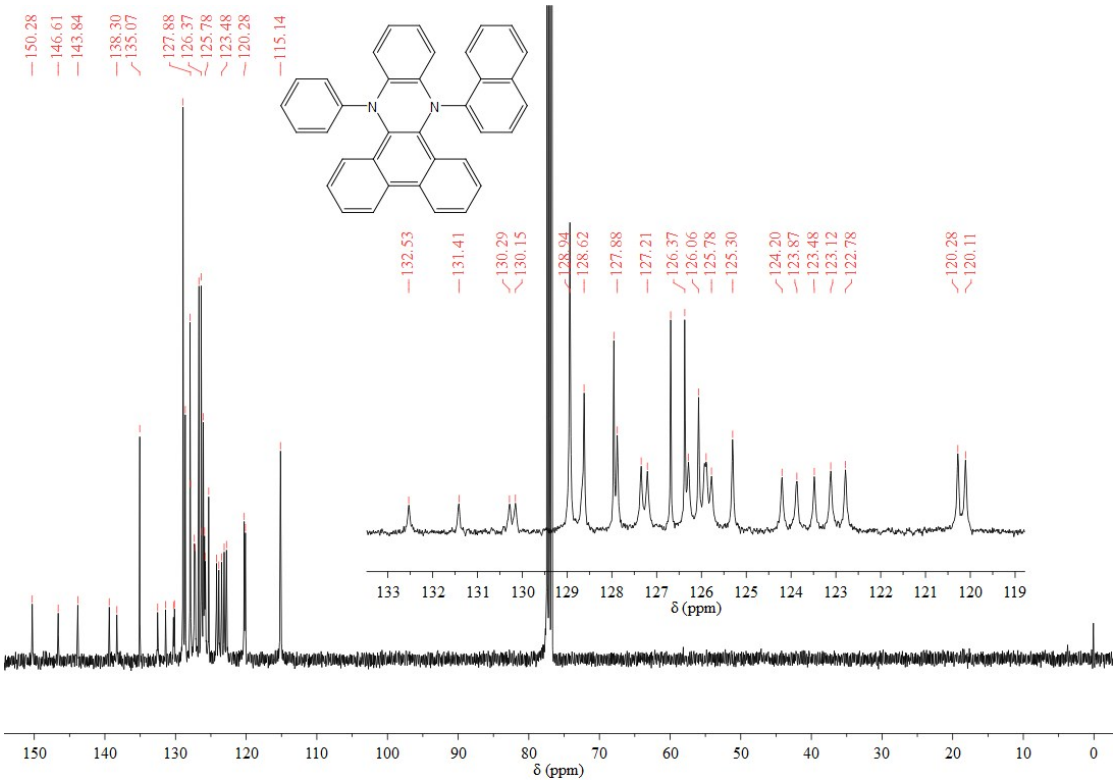

δ (ppm)

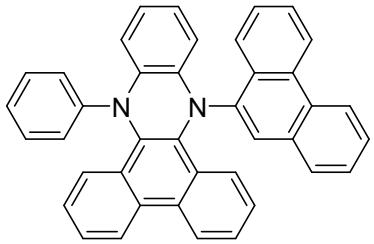


9-(naphthalen-1-yl)-14-phenyl-9,14-dihydrodibenzo[a,c]phenazine (1ag)

m.p. 215-218 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.66-8.70 (m, 2H), 8.61-8.63 (d, J = 8.4 Hz, 1H), 8.32-8.35 (m, 1H), 7.88-7.91 (m, 2H), 7.74-7.76 (d, J = 8.0 Hz, 1H), 7.61-7.64 (m, 3H), 7.43-7.56 (m, 4H), 7.17-7.26 (m, 3H), 7.03-7.14 (m, 4H), 6.87-6.91 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 150.28, 146.61, 143.84, 139.38, 138.30, 135.07, 132.53, 131.41, 130.29, 130.15, 128.94, 128.62, 127.96, 127.88, 127.35, 127.21, 126.69, 126.29, 126.06, 125.90, 125.78, 125.30, 124.20, 123.87, 123.48, 123.12, 122.78, 120.28, 120.11, 115.14; HRMS ESI (m/z) $[M+H]^+$: calcd. for $C_{36}H_{25}N_2$ 485.2018, found 485.2011.

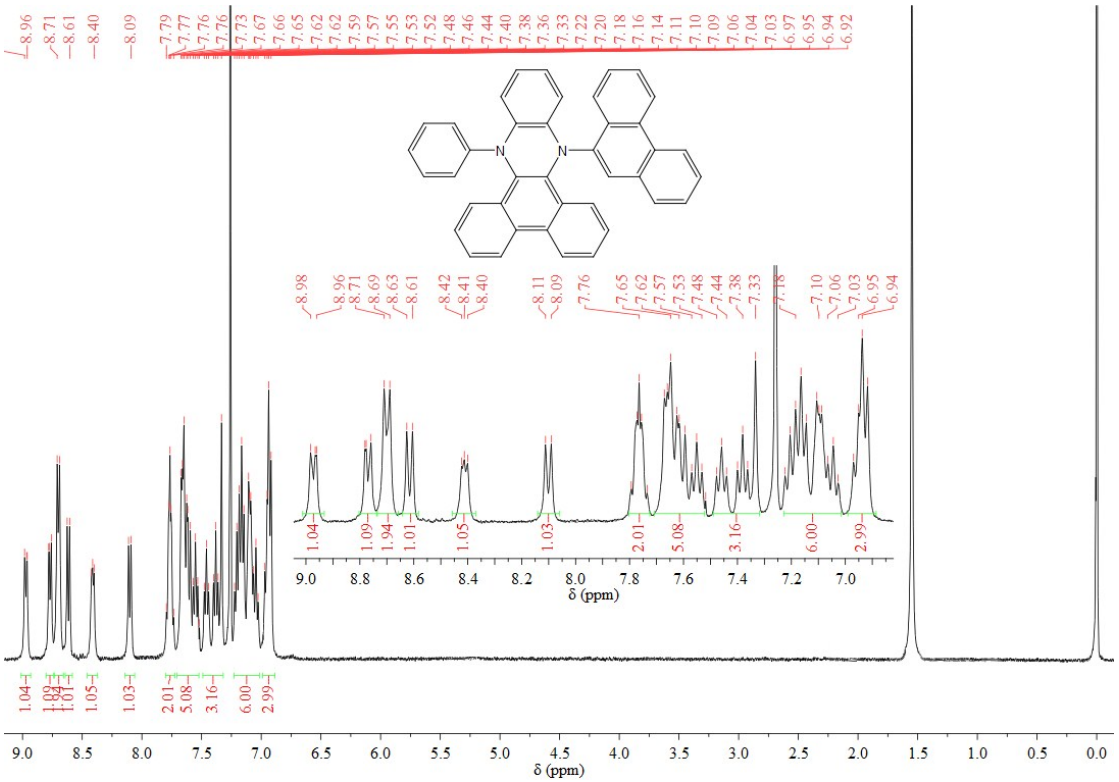


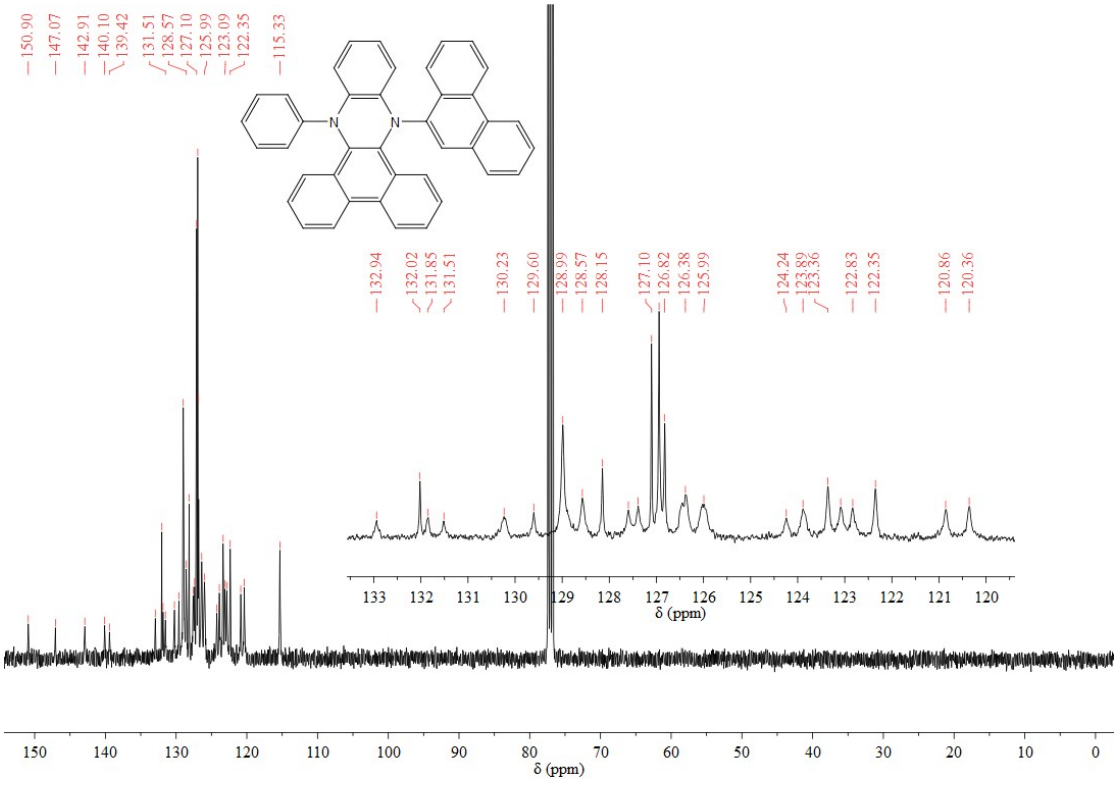


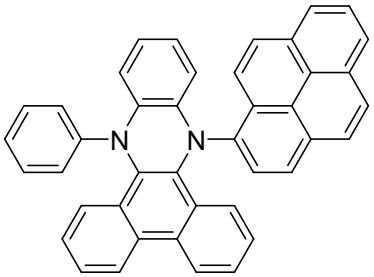


9-(phenanthren-9-yl)-14-phenyl-9,14-dihydrodibenzo[a,c]phenazine (1ah)

m.p. 282-285 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.96-8.98 (m, 1H), 8.76-8.78 (m, 1H), 8.69-8.71 (d, J =8.4 Hz, 2H), 8.61-8.63 (d, J =8.4 Hz, 1H), 8.40-8.42(m, 1H), 8.09-8.11 (d, J =8.4 Hz, 1H), 7.74-7.79 (m, 2H), 7.52-7.67 (m, 5H), 7.33-7.48 (m, 3H), 7.03-7.22 (m, 6H), 6.92-7.00 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 150.90, 147.07, 142.91, 140.10, 139.42, 132.94, 132.02, 131.85, 131.51, 130.23, 129.60, 128.99, 128.57, 128.15, 127.59, 127.39, 127.10, 126.94, 126.82, 126.38, 125.99, 124.24, 123.89, 123.36, 123.09, 122.83, 122.35, 120.86, 120.36, 115.33; HRMS ESI (m/z) $[M+H]^+$: calcd. for $C_{40}H_{27}N_2$ 535.2174, found 535.2175.

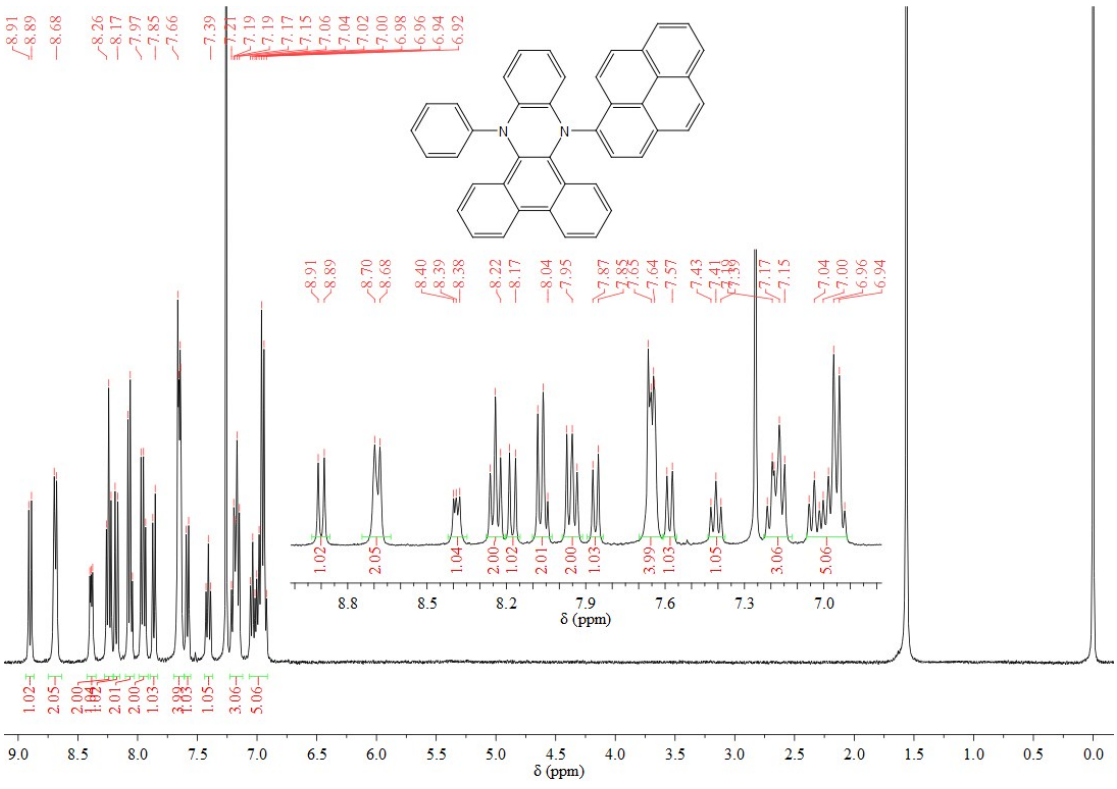

δ (ppm)

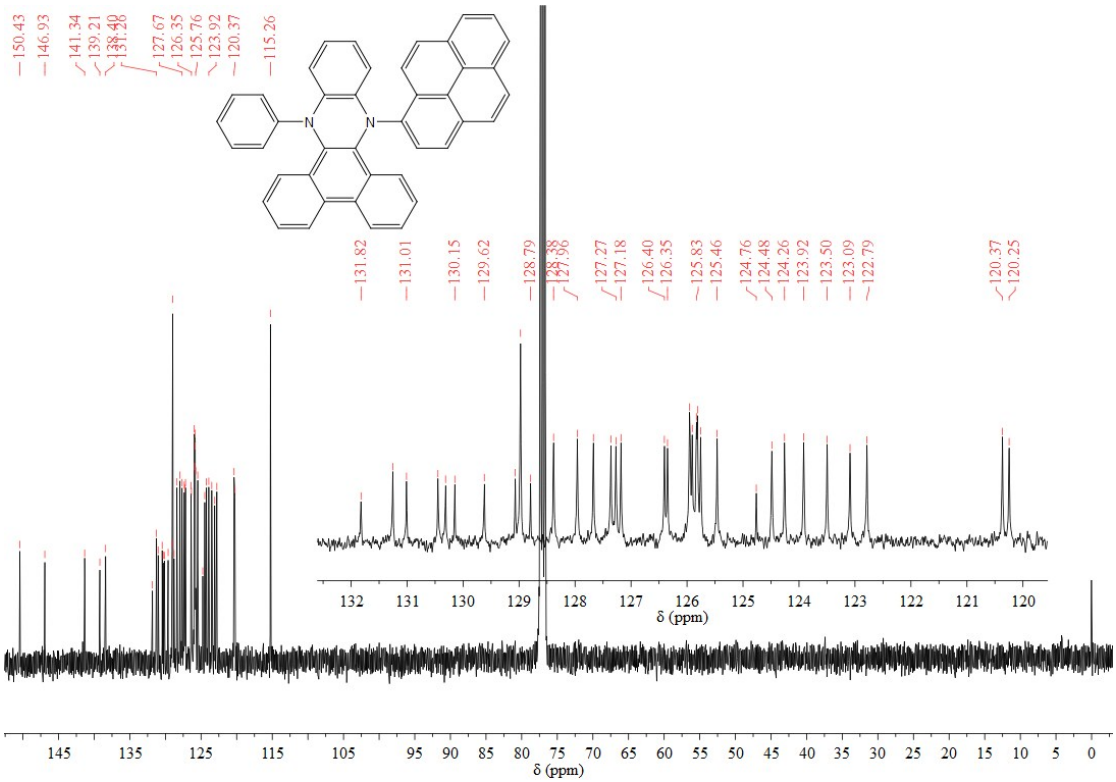

δ (ppm)

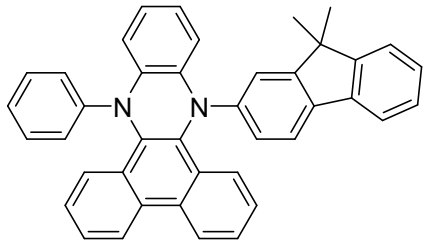


9-phenyl-14-(pyren-1-yl)-9,14-dihydrodibenzo[a,c]phenazine (1ai)

m.p. 324-326 °C; ^{1}H NMR (400 MHZ, $CDCl_3$) δ: 8.89-8.91 (d, J =9.2 Hz, 1H), 8.68-8.70 (d, J =8.0 Hz, 2H), 8.38-8.40 (m, 1H), 8.22-8.26 (t, J =8.0 Hz, 2H), 8.17-8.19 (d, J =8.4 Hz, 1H), 8.04-8.08 (m, 2H), 7.93-7.97 (m, 2H), 7.85-7.87 (d, J =8.0 Hz, 1H), 7.64-7.66 (m, 4H), 7.57-7.59 (d, J =8.0 Hz, 1H), 7.39-7.43 (t, J =7.6 Hz, 1H), 7.15-7.21 (m, 3H), 6.92-7.01 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 150.43, 146.93, 141.34, 139.21, 138.40, 131.82, 131.26, 131.01, 130.45, 130.31, 130.15, 129.62, 129.07, 128.97, 128.79, 128.38, 127.96, 127.67, 127.36, 127.27, 127.18, 126.40, 126.35, 125.95, 125.91, 125.83, 125.81, 125.76, 125.46, 124.76, 124.48, 124.26, 123.92, 123.50, 123.09, 122.79, 120.37, 120.25, 115.26; HRMS ESI (m/z) $[M]^+$: calcd. for $C_{42}H_{26}N_2$ 558.2096, found 558.2095.

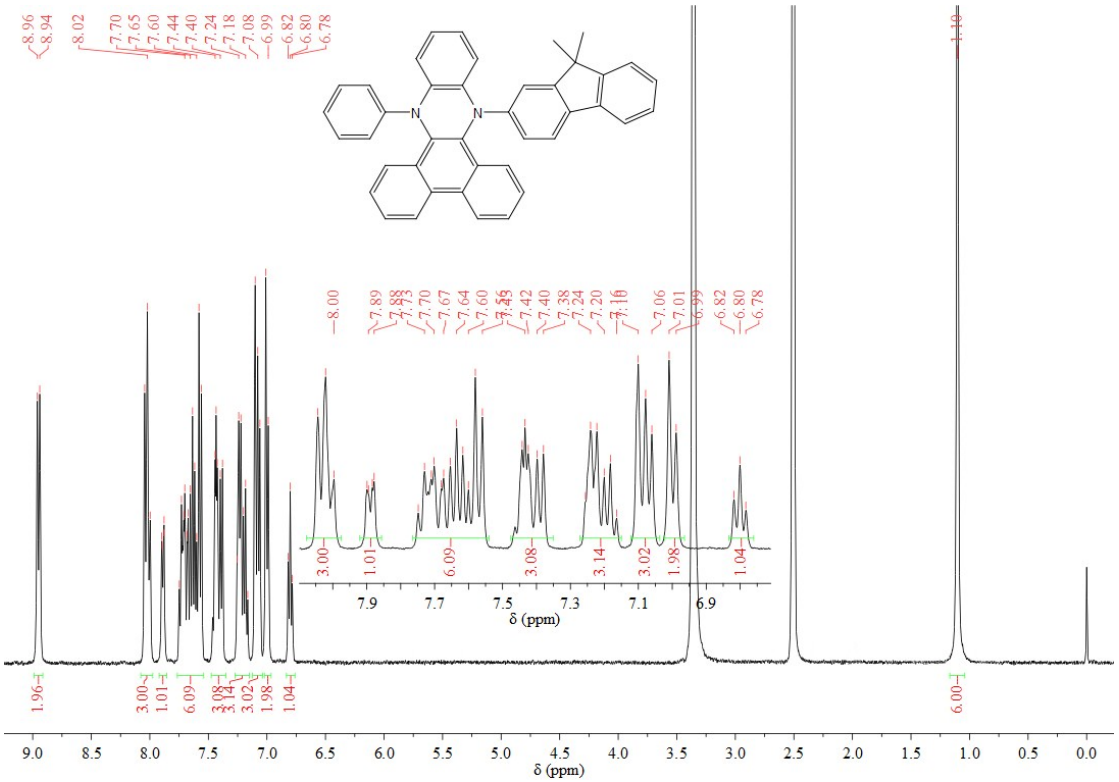


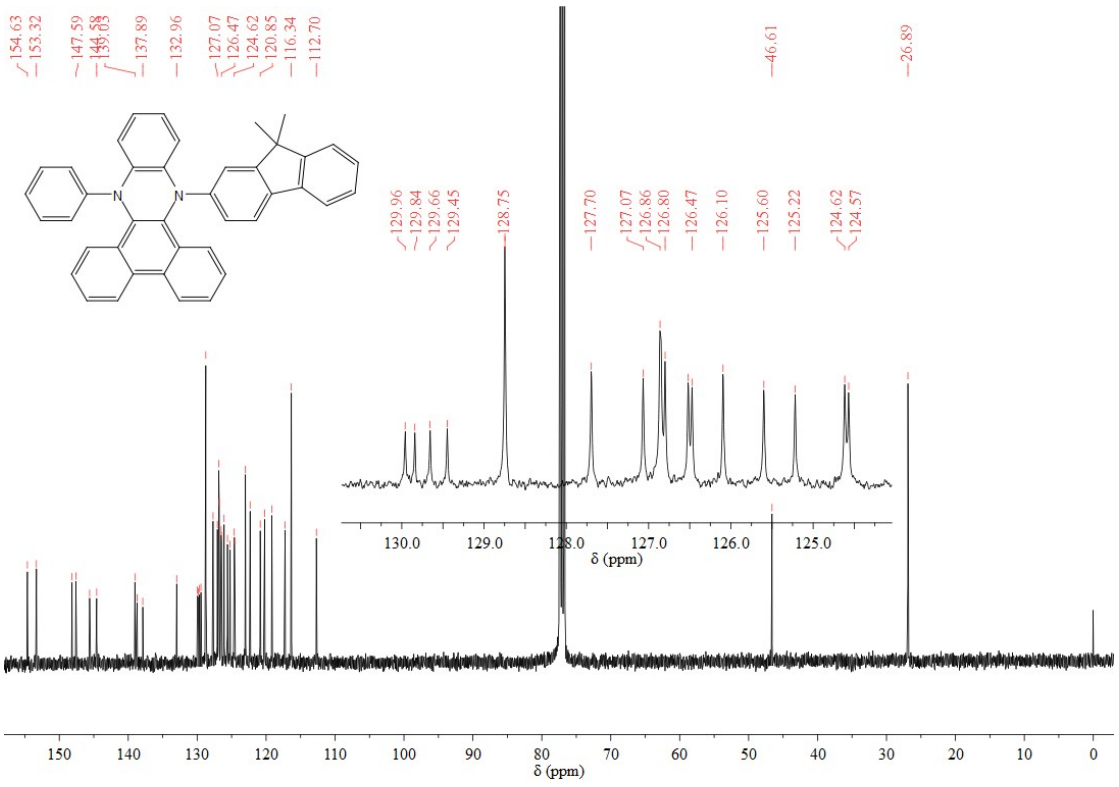


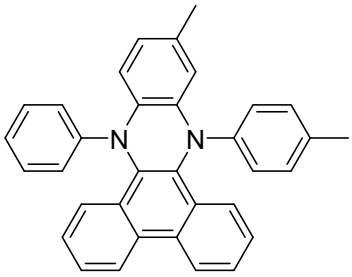


9-(9,9-dimethyl-9H-fluoren-2-yl)-14-phenyl-9,14-dihydrodibenzo[a,c]phenazine (1aj)

m.p. 226-228 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ: 8.95 (d, J = 8.0 Hz, 2H), 7.99-8.05 (m, 3H), 7.87-7.90 (m, 1H), 7.55-7.75 (m, 6H), 7.37-7.45 (m, 3H), 7.16-7.26 (m, 3H), 7.06-7.10 (m, 3H), 6.98-7.01 (d, J = 8.0 Hz, 2H), 6.80 (t, J = 7.2 Hz, 1H), 1.10 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 154.63, 153.32, 148.16, 147.59, 145.60, 144.58, 139.03, 138.71, 137.89, 132.96, 129.96, 129.84, 129.66, 129.45, 128.75, 127.70, 127.07, 126.86, 126.80, 126.52, 126.47, 126.10, 125.60, 125.22, 124.62, 124.57, 123.00, 122.31, 120.85, 120.20, 119.17, 117.24, 116.34, 112.70, 46.61, 26.89; HRMS ESI (m/z) $[M]^+$: calcd. for $C_{41}H_{30}N_2$ 550.2409, found 550.2407.

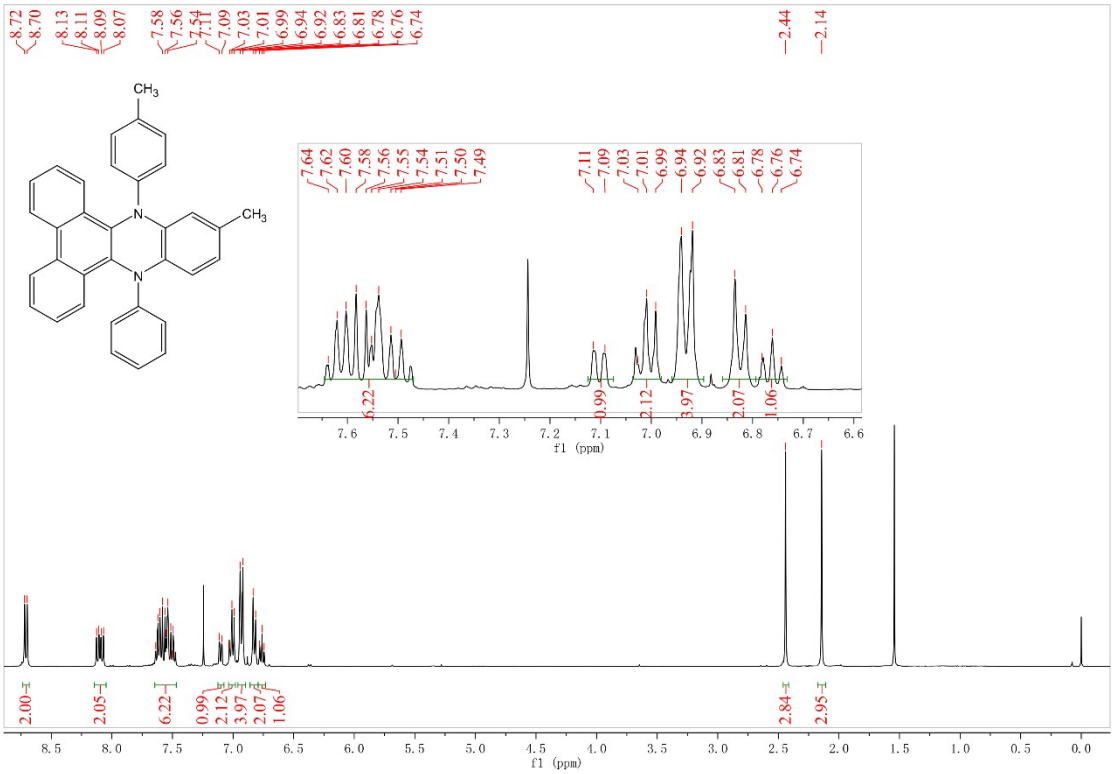

8.96
8.94
8.02
7.70
7.65
7.60
7.44
7.40
7.24
7.18
7.08
6.99
6.82
6.80
6.78
1.10
8.00
7.89
7.88
7.73
7.70
7.67
7.64
7.60
7.45
7.42
7.40
7.38
7.24
7.20
7.16
7.06
7.01
6.99
6.82
6.80
6.78
3.00
1.01
6.09
3.08
3.14
3.02
1.98
1.04
δ (ppm)
1.96
3.00
1.01
6.09
3.08
3.14
3.02
1.98
1.04
6.00
δ (ppm)

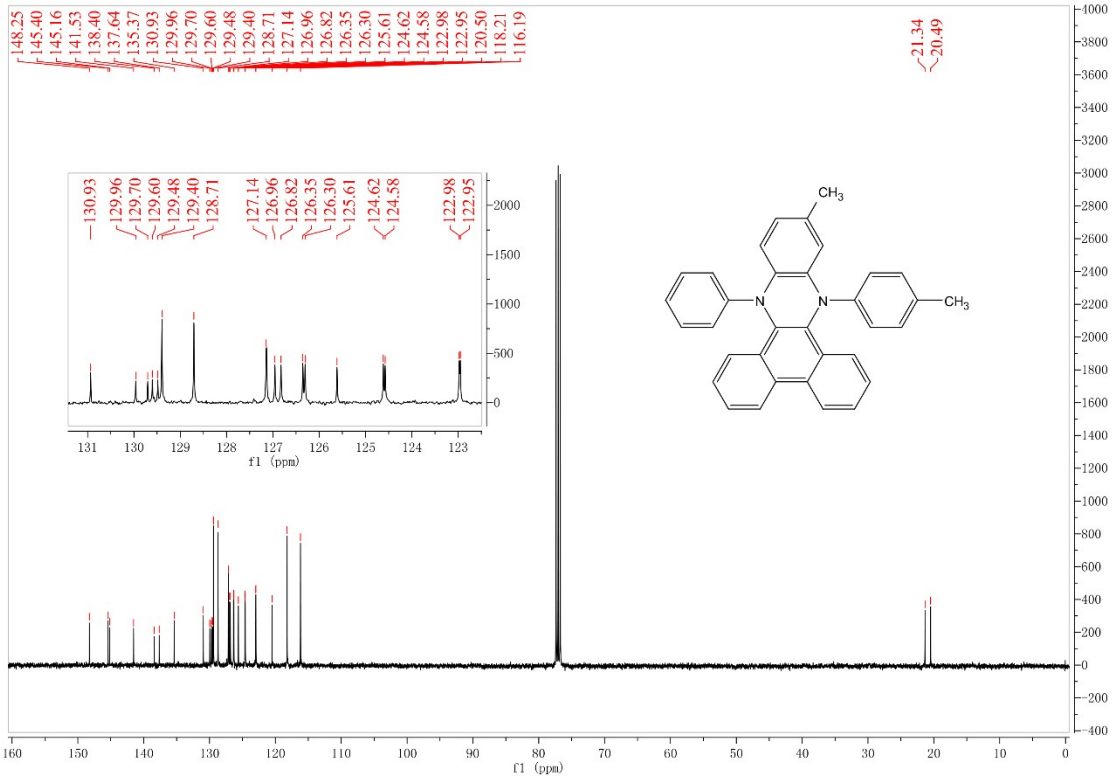

154.63
153.32
147.59
144.58
139.03
137.89
132.96
127.07
126.47
124.62
120.85
116.34
112.70
46.61
26.89
129.96
129.84
129.66
129.45
128.75
127.70
127.07
126.86
126.80
126.47
126.10
125.60
125.22
124.62
124.57
δ (ppm)
δ (ppm)

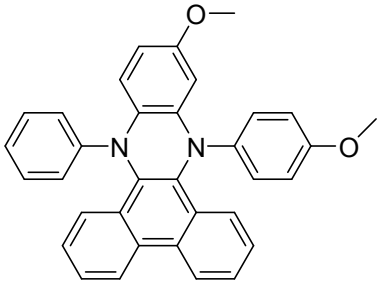


11-methyl-14-phenyl-9-(p-tolyl)-9,14-dihydrodibenzo[a,c]phenazine (1dd)

m.p. 254-255 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.71 (d, *J* = 8.3 Hz, 2H), 8.06-8.15 (m, 2H), 7.47-7.64 (m, 6H), 7.10 (dd, *J* = 8.0, 1.1 Hz, 1H), 7.01 (dd, J = 11.3, 4.6 Hz, 2H), 6.89-6.96 (m, 4H), 6.82 (d, *J* = 8.4 Hz, 2H), 6.77 (dd, *J* = 12.2, 5.0 Hz, 1H), 2.44 (s, 3H), 2.14 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 148.25, 145.40, 145.16, 141.53, 138.40, 137.64, 135.37, 130.93, 129.96, 129.70, 129.60, 129.48, 129.40, 128.71, 127.14, 126.96, 126.82, 126.35, 126.30, 125.61, 124.62, 124.58, 122.98, 122.95, 120.50, 118.21, 116.19, 21.34, 20.49; HRMS ESI (m/z) $[M]^+$: calcd. for $C_{34}H_{26}N_2$ 462.2096, found 462.2090.

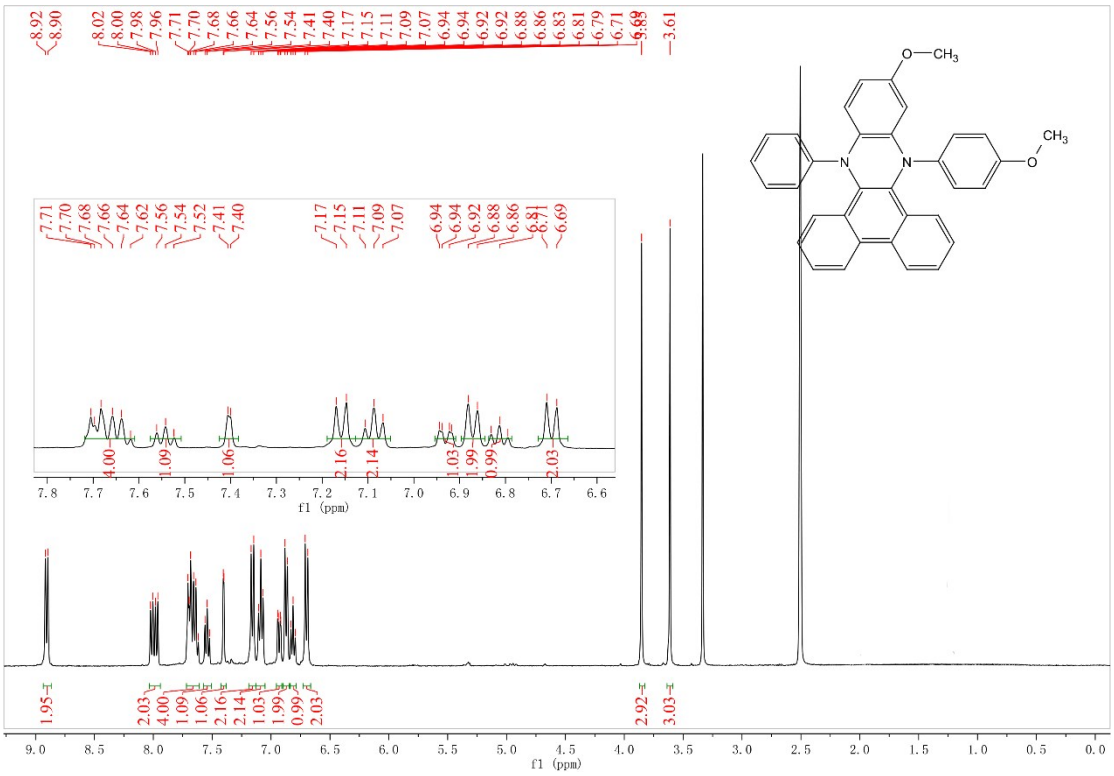


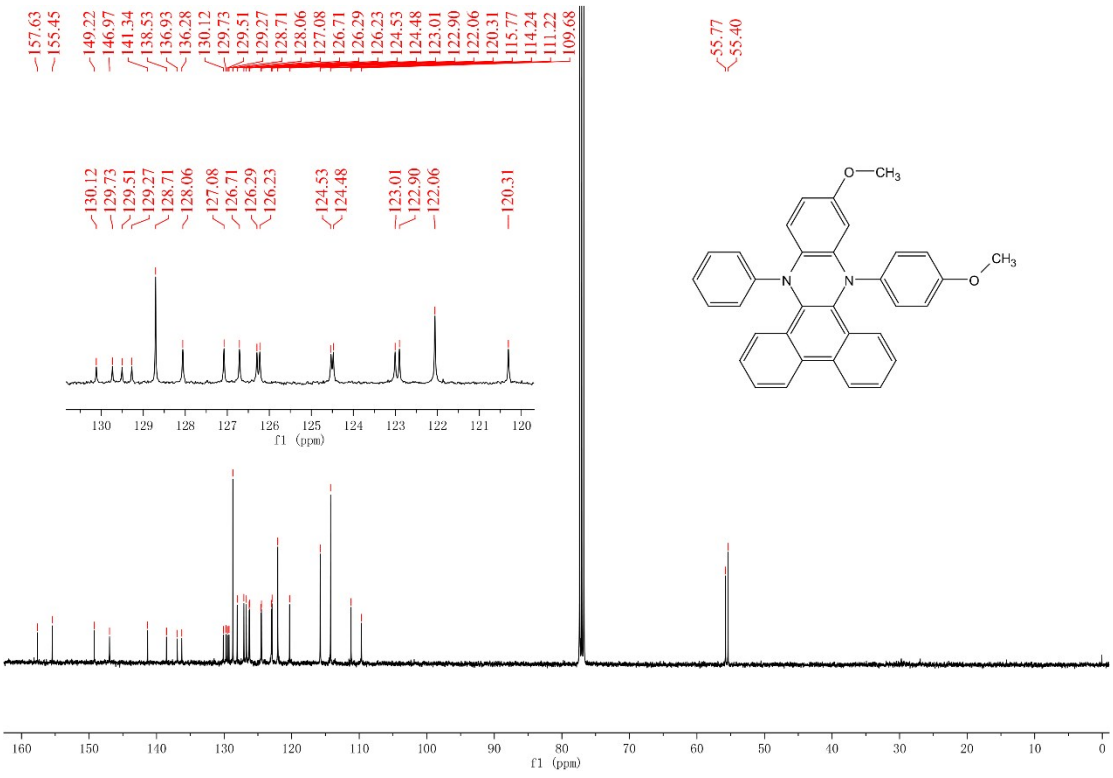


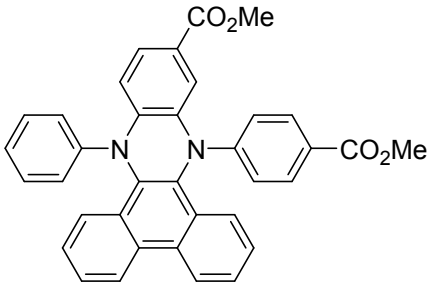


11-methoxy-9-(4-methoxyphenyl)-14-phenyl-9,14-dihydrodibenzo[a,c]phenazine (1ed)

m.p. 226-228 ^{o}C; ^{1}H NMR (400 MHz, DMSO) δ: 8.91 (d, *J* = 8.3 Hz, 2H), 7.99 (dd, *J* = 16.5, 8.0 Hz, 2H), 7.61-7.72 (m, 4H), 7.54 (t, *J* = 7.6 Hz, 1H), 7.41 (s, 1H), 7.16 (d, *J* = 8.9 Hz, 2H), 7.09 (t, *J* = 7.8 Hz, 2H), 6.93 (d, *J* = 8.8 Hz, 1H), 6.87 (d, *J* = 8.1 Hz, 2H), 6.81 (t, *J* = 7.3 Hz, 1H), 6.70 (d, *J* = 8.9 Hz, 2H), 3.85 (s, 3H), 3.61 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 157.63, 155.45, 149.22, 146.97, 141.34, 138.53, 136.93, 136.28, 130.12, 129.73, 129.51, 129.27, 128.71, 128.06, 127.08, 126.71, 126.29, 126.23, 124.53, 124.48, 123.01, 122.90, 122.06, 120.31, 115.77, 114.24, 111.22, 109.68, 55.77, 55.40; HRMS ESI (m/z) [M+H]+: calcd. for $C_{34}H_{27}N_2O_2$ 495.2073, found 495.2075.

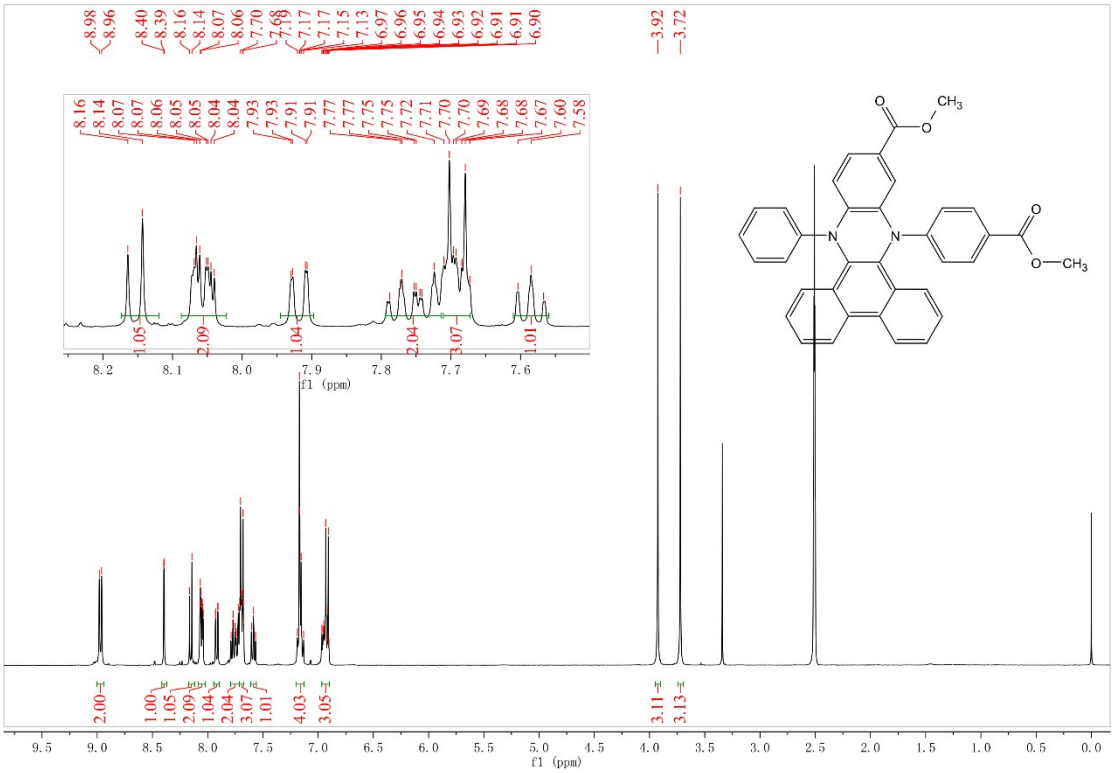

8.92
8.90
8.02
8.00
7.98
7.96
7.71
7.70
7.68
7.66
7.64
7.56
7.54
7.41
7.40
7.17
7.15
7.11
7.09
7.07
6.94
6.94
6.92
6.92
6.88
6.86
6.83
6.81
6.79
6.71
3.61
O—CH3
CH3
O
N
N
1.95
2.03
4.00
1.09
1.06
2.16
2.14
1.03
1.99
0.99
2.03
2.92
3.03
f1 (ppm)

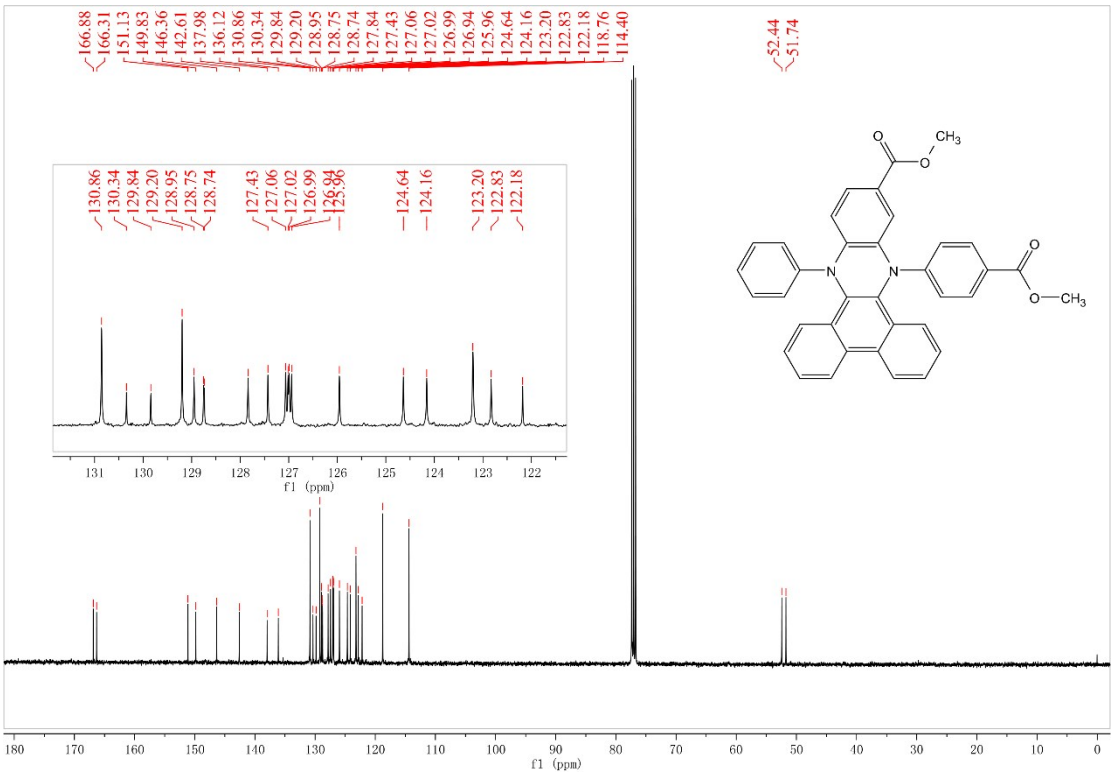

157.63
155.45
149.22
146.97
141.34
138.53
136.93
136.28
130.12
129.73
129.51
129.27
128.71
128.06
127.08
126.71
126.29
126.23
124.53
124.48
123.01
122.90
122.06
120.31
115.77
114.24
111.22
109.68
55.77
55.40
O—CH3
CH3
O
N
N
f1 (ppm)

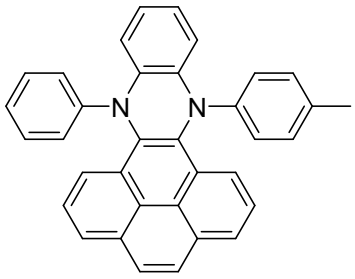


methyl 9-(4-(methoxycarbonyl)phenyl)-14-phenyl-9,14-dihydrodibenzo[a,c]phenazine-11-carboxylate (1fd)

m.p. 271-272 °C; ^{1}H NMR (400 MHz, DMSO) δ: 8.97 (d, J = 8.3 Hz, 2H), 8.40 (d, J = 1.9 Hz, 1H), 8.15 (d, J = 8.4 Hz, 1H), 8.03-8.08 (m, 2H), 7.89-7.94 (m, 1H), 7.72-7.76 (m, 2H), 7.67-7.71 (m, 3H), 7.57-7.60 (t, J = 7.6 Hz, 1H), 7.13-7.20 (m, 4H), 6.89-6.97 (m, 3H), 3.92 (s, 3H), 3.72 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 166.88, 166.31, 151.13, 149.83, 146.36, 142.61, 137.98, 136.12, 130.86, 130.34, 129.84, 129.20, 128.95, 128.75, 128.74, 127.84, 127.43, 127.06, 127.02, 126.99, 126.94, 125.96, 124.64, 124.16, 123.20, 122.83, 122.18, 118.76, 114.40, 52.44, 51.74; HRMS ESI (m/z) $[M+H]^+$: calcd. for $C_{36}H_{27}N_2O_4$ 551.1971, found 551.1970.

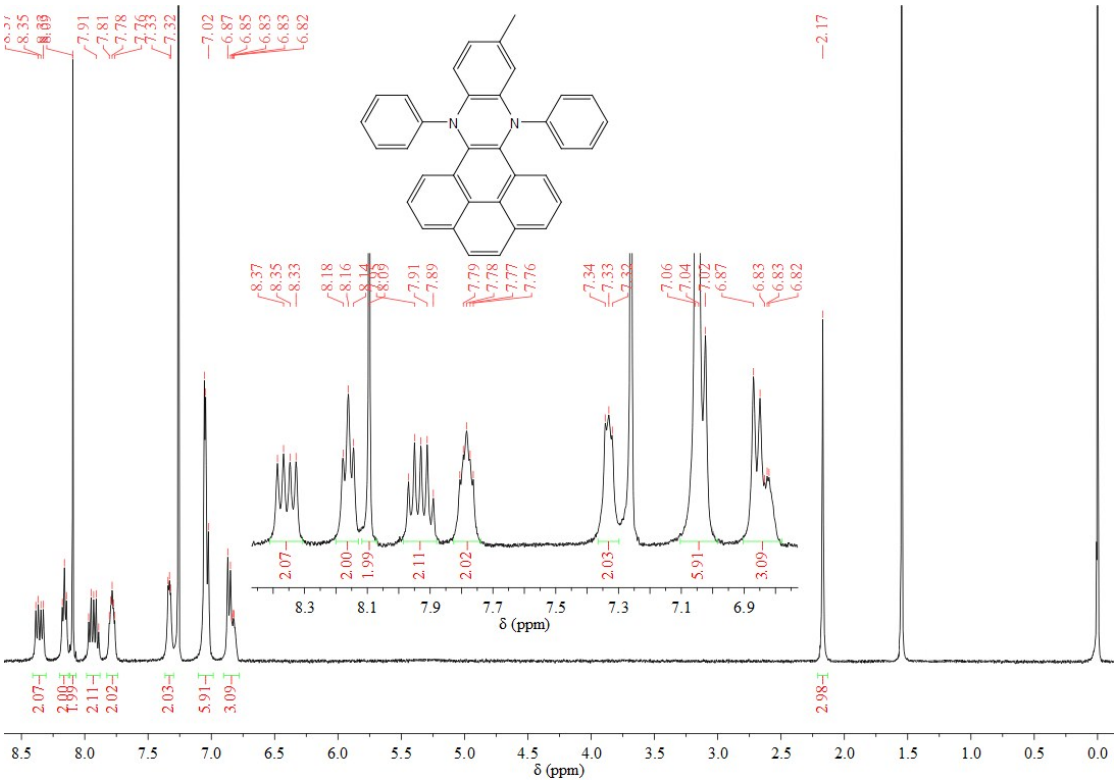


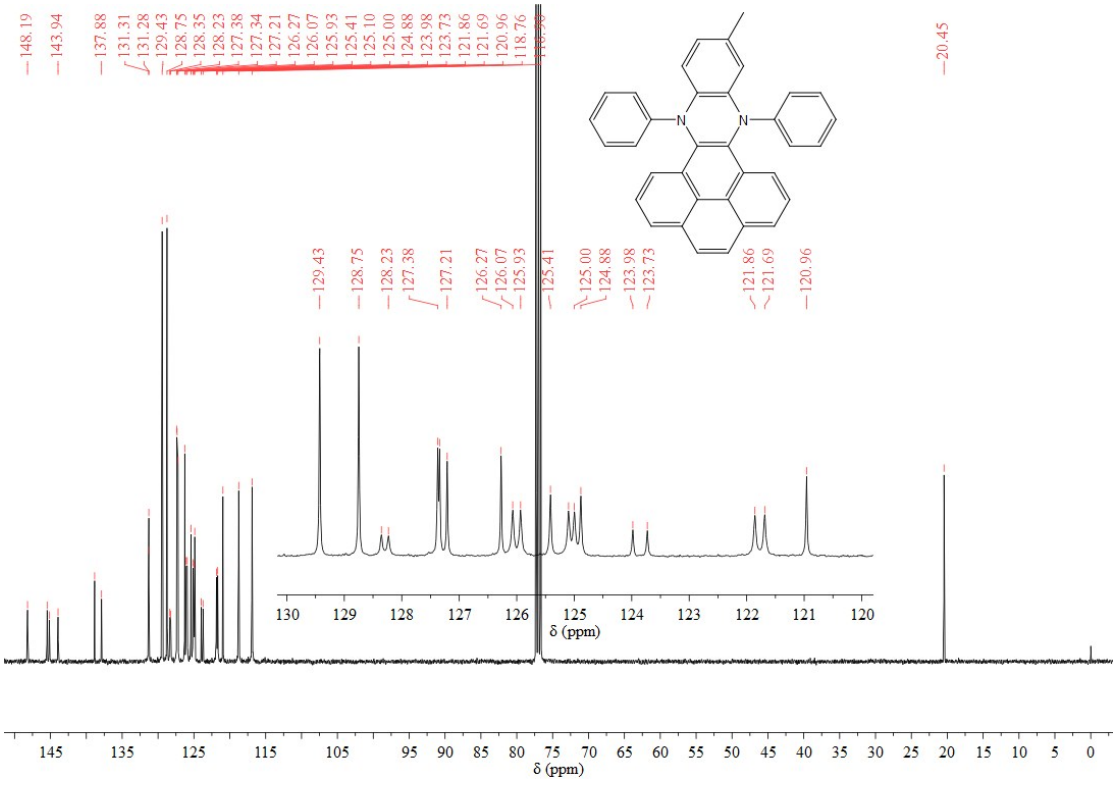


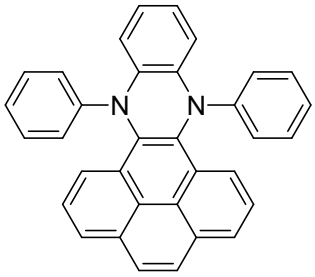


11-methyl-9,14-diphenyl-9,14-dihydrophenanthro[4,5-abc]phenazine (1ca)

m.p. 221-224 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.36 (dd, *J* = 15.9, 7.7 Hz, 2H), 8.16 (t, *J* = 6.8 Hz, 2H), 8.09 (s, 2H), 8.01-7.86 (m, 2H), 7.85-7.67 (m, 2H), 7.39-7.28 (m, 2H), 7.13-6.96 (m, 6H), 6.92-6.75 (m, 3H), 2.17 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 148.19, 145.46, 145.16, 143.94, 138.84, 137.88, 131.31, 131.28, 129.43, 128.75, 128.35, 128.23, 127.38, 127.34, 127.21, 126.27, 126.07, 125.93, 125.41, 125.10, 125.00, 124.88, 123.98, 123.73, 121.86, 121.69, 120.96, 118.76, 116.90, 20.45; HRMS ESI (*m/z*) $[M+H]^+$: calcd. for $C_{35}H_{25}N_2$ 473.2018, found 473.2021.

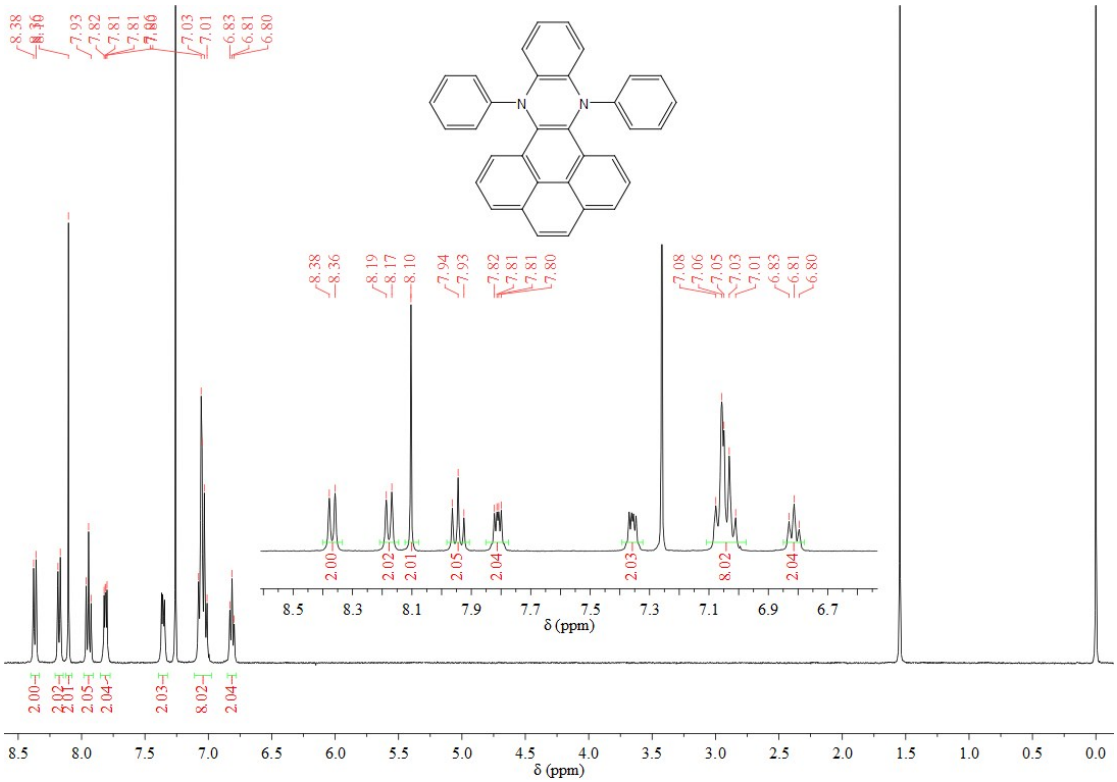

8.37
8.35
8.33
8.18
8.16
8.14
8.09
7.91
7.89
7.79
7.78
7.77
7.76
7.34
7.33
7.32
7.06
7.04
7.02
6.87
6.83
6.82
2.07
2.00
1.99
2.11
2.02
2.03
5.91
3.09
δ (ppm)
2.17
2.98
δ (ppm)

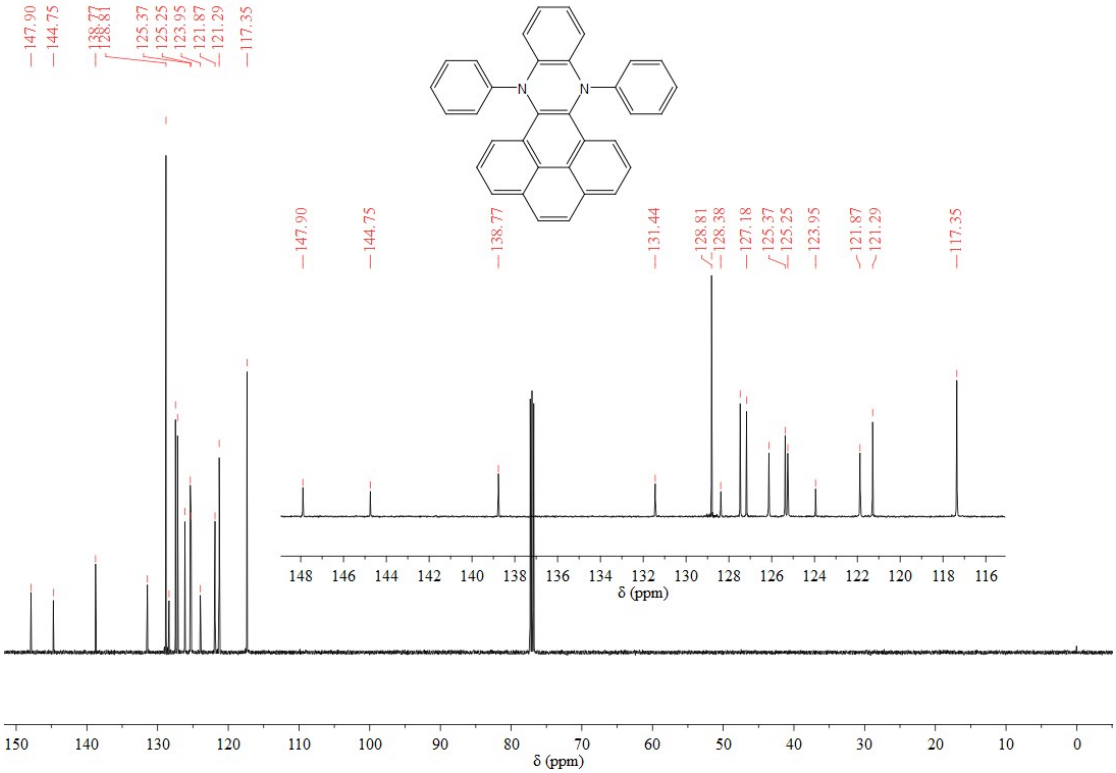

148.19
143.94
137.88
131.31
131.28
129.43
128.75
128.35
128.23
127.38
127.34
127.21
126.27
126.07
125.93
125.41
125.10
125.00
124.88
123.98
123.73
121.86
121.69
121.69
120.96
118.76
118.66
20.45
δ (ppm)
δ (ppm)

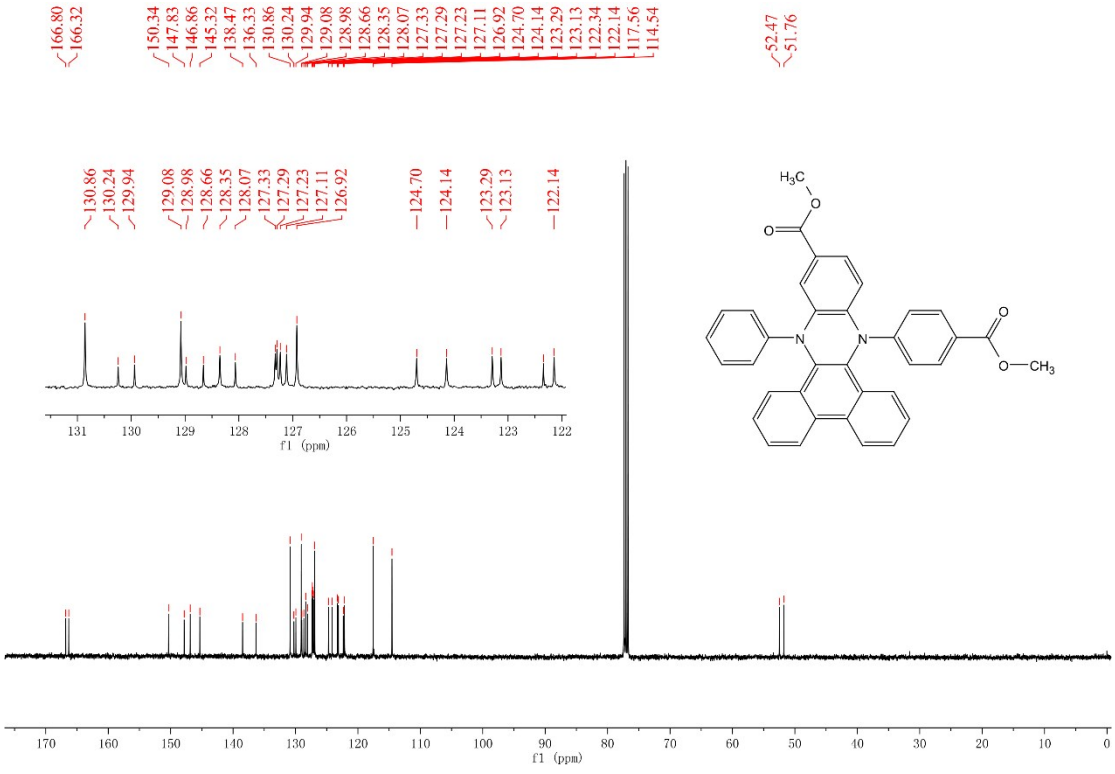


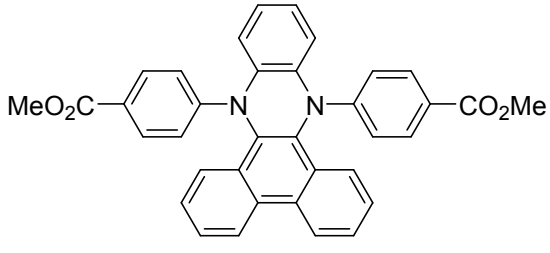
9,14-diphenyl-9,14-dihydrophenanthro[4,5-abc]phenazine (1cc)

m.p. 240-241 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.37 (d, *J* = 7.8 Hz, 2H), 8.18 (d, *J* = 7.5 Hz, 2H), 8.10 (s, 2H), 7.94 (t, *J* = 7.8 Hz, 2H), 7.86-7.74 (m, 2H), 7.36 (dd, *J* = 5.9, 3.4 Hz, 2H), 7.12-6.98 (m, 8H), 6.81 (t, *J* = 6.8 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 147.90, 144.75, 138.77, 131.44, 128.81, 128.38, 127.47, 127.18, 126.13, 125.37, 125,25, 123.95, 121.87, 121.29, 117.35; HRMS ESI (*m/z*) $[M+H]^+$: calcd. for $C_{34}H_{23}N_2$ 459.1861, found 459.1861.



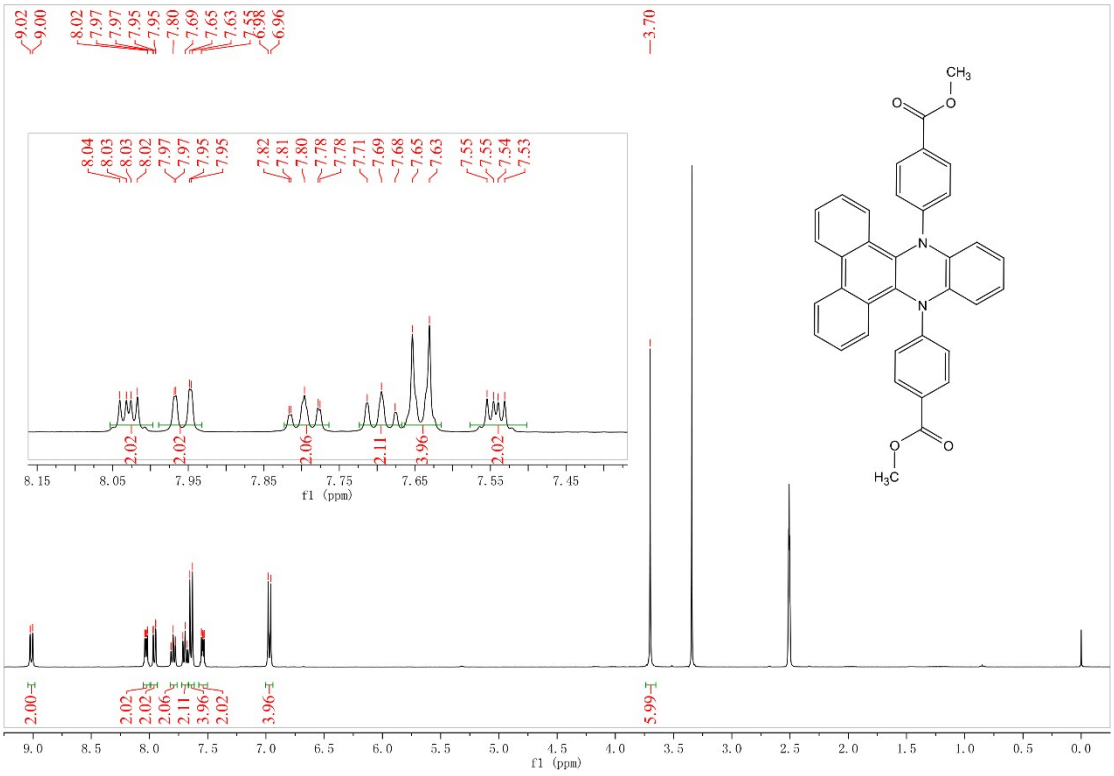

147.90
144.75
138.77
131.44
128.81
128.38
127.18
125.37
125.25
123.95
121.87
121.29
117.35
δ (ppm)

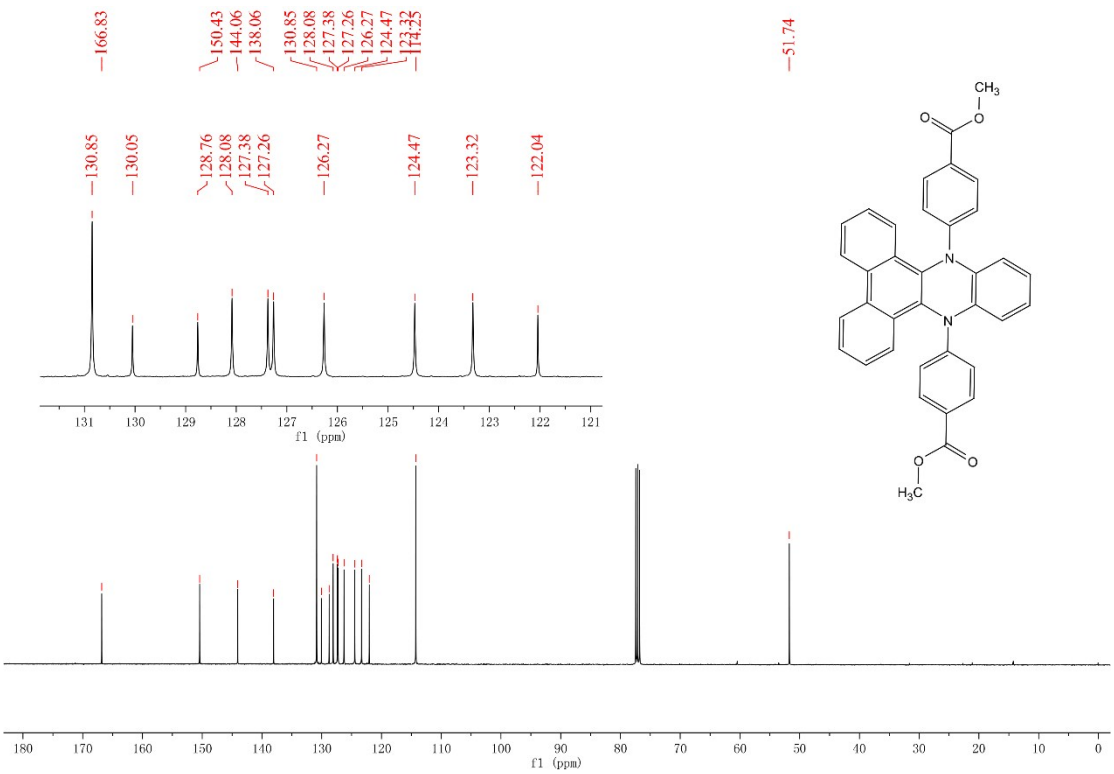

166.80
166.32
150.34
147.83
146.86
145.32
138.47
136.33
130.86
130.24
129.94
129.08
128.98
128.66
128.35
128.07
127.33
127.29
127.23
127.11
126.92
124.70
124.14
123.29
123.13
122.34
122.14
117.56
114.54
52.47
51.76
f1 (ppm)

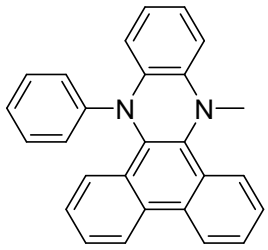

MeO2C
N
N
CO2Me

dimethyl 4,4'-(dibenzo[a,c]phenazine-9,14-diyl)dibenzoate (1cc-2)

^{1}H NMR (400 MHz, DMSO) δ: 9.01 (d, *J* = 8.3 Hz, 2H), 8.02 (dt, *J* = 7.3, 3.7 Hz, 2H), 7.94-7.98 (m, 2H), 7.77-7.82 (m, 2H), 7.69 (t, *J* = 7.4 Hz, 2H), 7.64 (d, *J* = 9.0 Hz, 4H), 7.54 (dd, *J* = 5.9, 3.4 Hz, 2H), 6.97 (d, *J* = 9.0 Hz, 4H), 3.70 (s, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.83, 150.43, 144.06, 138.06, 130.85, 130.05, 128.76, 128.08, 127.38, 127.26, 126.27, 124.47, 123.32, 122.04, 114.25, 51.74; HRMS ESI (m/z) $[M+H]^+$: calcd. for $C_{36}H_{27}N_2O_4$ 551.1971, found 551.1840.

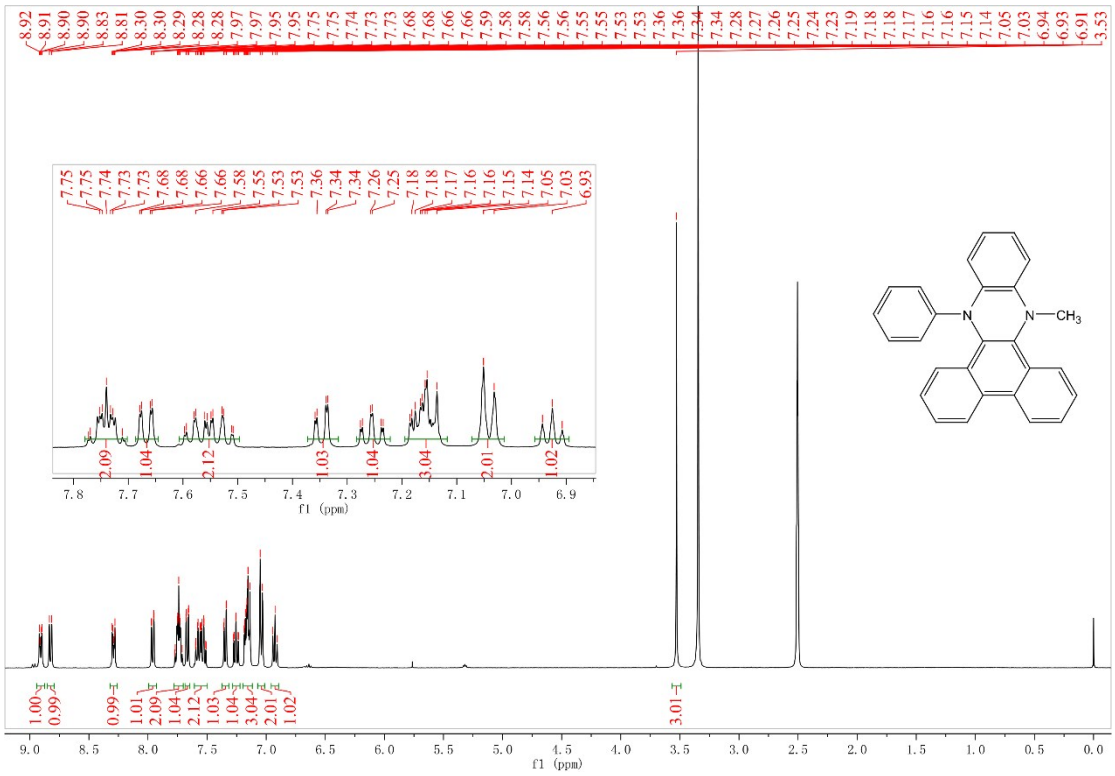


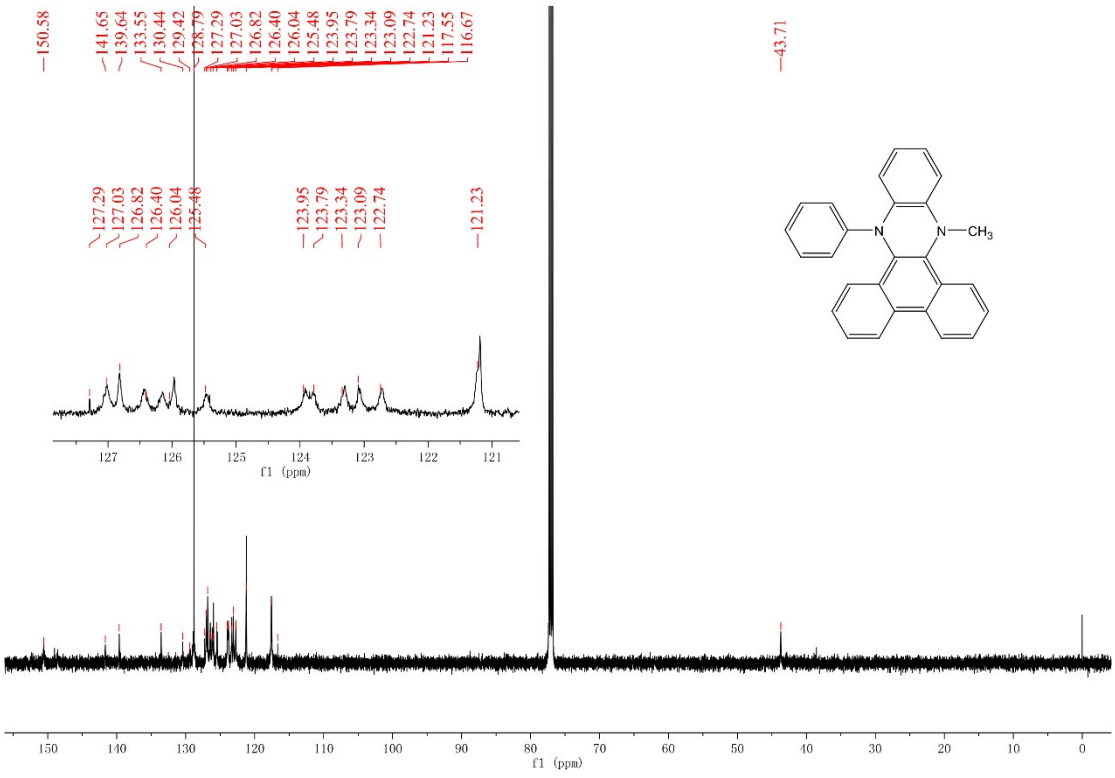




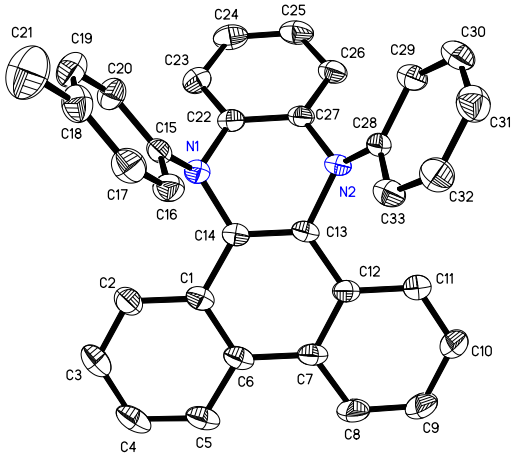
9-methyl-14-phenyl-9,14-dihydrodibenzo[a,c]phenazine (4)

m.p. 212-213 ^{o}C; ^{1}H NMR (400 MHz, DMSO) δ: 8.91 (dd, *J* = 6.8, 2.7 Hz, 1H), 8.82 (d, *J* = 7.7 Hz, 1H), 8.26-8.31 (m, 1H), 7.96 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.74 (m, 2H), 7.67 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.50-7.60 (m, 2H), 7.35 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.26 (m, 1H), 7.13- 7.19 (m, 3H), 7.04 (d, *J* = 7.8 Hz, 2H), 6.93 (t, *J* = 7.2 Hz, 1H), 3.53 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 150.58, 141.65, 139.64, 133.55, 130.44, 129.42, 128.79, 127.29, 127.03, 126.82, 126.40, 126.04, 125.48, 123.95, 123.79, 123.34, 123.09, 122.74, 121.23, 117.55, 116.67, 43.71; HRMS ESI (m/z) $[M+H]^+$: calcd. for $C_{37}H_{20}N_2$ 373.1705, found 373.1691.


8.92 8.91 8.90 8.90 8.83 8.81 8.30 8.30 8.29 8.28 8.28 7.97 7.97 7.95 7.95 7.75 7.75 7.74 7.73 7.73 7.68 7.68 7.66 7.66 7.59 7.58 7.58 7.56 7.56 7.55 7.55 7.53 7.53 7.36 7.36 7.34 7.34 7.28 7.27 7.26 7.25 7.24 7.23 7.19 7.18 7.18 7.17 7.17 7.16 7.16 7.15 7.14 7.05 7.03 6.94 6.93 6.91 3.53
1.00 0.99 0.99 1.01 2.09 1.04 2.12 1.03 1.04 3.04 2.01 1.02 3.01
f1 (ppm)
N
N—CH3


150.58 141.65 139.64 133.55 130.44 129.42 128.79 127.29 127.03 126.82 126.40 126.04 125.48 123.95 123.79 123.34 123.09 122.74 121.23 117.55 116.67 43.71
f1 (ppm)
N
N—CH3

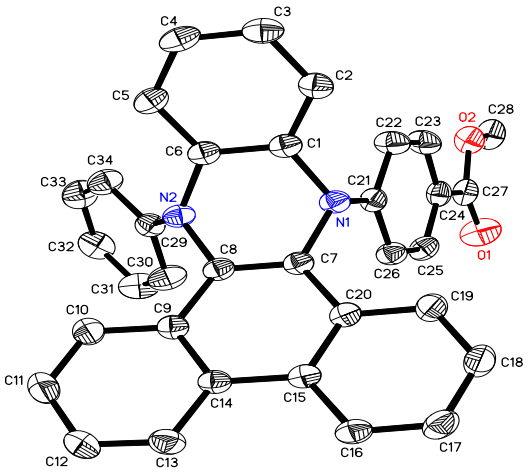
III. The X-ray Analysis



1aa

Identification code	cd15118	
Empirical formula	C33 H24 N2	
Formula weight	448.54	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 13.670(2) Å	α= 90°.
	b = 10.7087(18) Å	β= 98.766(4)°.
	c = 16.477(3) Å	γ = 90°.
Volume	2384.0(7) $Å^3$	
Z	4	
Density (calculated)	1.250 Mg/m^3	
Absorption coefficient	0.073 mm^{-1}	
F(000)	944	
Crystal size	0.220 x 0.170 x 0.130 mm^3	
Theta range for data collection	1.806 to 25.500°.	
Index ranges	-15<=h<=16, -11<=k<=12, -19<=l<=19	
Reflections collected	13421	
Independent reflections	4424 [R(int) = 0.0480]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6237	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4424 / 0 / 317	

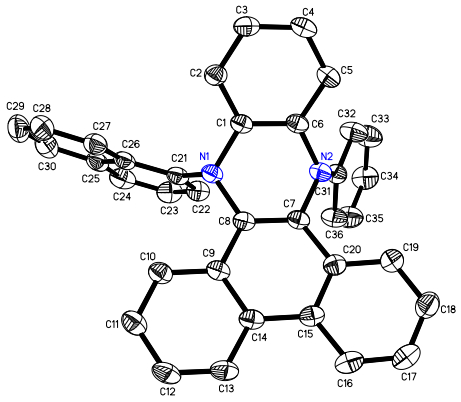
Goodness-of-fit on F^2	1.095
Final R indices [I>2sigma(I)]	R1 = 0.0653, wR2 = 0.1363
R indices (all data)	R1 = 0.1028, wR2 = 0.1521
Extinction coefficient	n/a
Largest diff. peak and hole	0.264 and -0.160 e.$Å^{-3}$



1ac

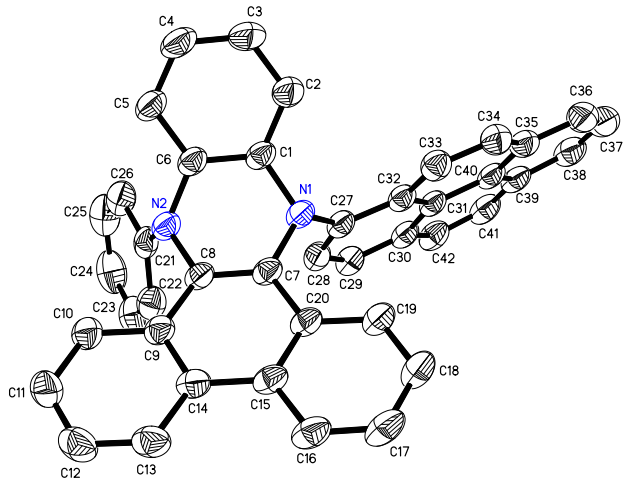
Identification code	cd21251
Empirical formula	C34.50 H25 Cl N2 O2
Formula weight	535.02
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, C2/c
Unit cell dimensions	a = 15.3088(9) A alpha = 90 deg. b = 17.9930(11) A beta = 92.570(2) deg. c = 19.4932(12) A gamma = 90 deg.
Volume	5364.0(6) A^3
Z, Calculated density	8, 1.325 Mg/m^3
Absorption coefficient	0.178 mm^{-1}
F(000)	2232
Crystal size	0.311 x 0.257 x 0.205 mm
Theta range for data collection	1.75 to 25.50 deg.
Limiting indices	-18<=h<=18, -20<=k<=21, -23<=l<=23
Reflections collected / unique	15604 / 5002 [R(int) = 0.0233]
Completeness to theta = 25.50	99.9 %
Absorption correction	Empirical
Max. and min. transmission	1.00000 and 0.77314
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5002 / 0 / 358

Goodness-of-fit on F^2	1.019
Final R indices [I>2sigma(I)]	R1 = 0.0581, wR2 = 0.1653
R indices (all data)	R1 = 0.0710, wR2 = 0.1780
Largest diff. peak and hole	0.491 and -0.650 e.A^{-3}



1ag

Identification code	cd211425
Empirical formula	C36 H24 N2
Formula weight	484.57
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, C2/c
Unit cell dimensions	a = 14.0547(18) A alpha = 90 deg. b = 19.251(3) A beta = 90.832(3) deg. c = 18.410(2) A gamma = 90 deg.
Volume	4980.7(11) A_3
Z, Calculated density	8, 1.292 Mg/m^3
Absorption	0.075 mm^{-1}
F(000)	2032
Crystal size	0.309 x 0.238 x 0.197 mm
Theta range for data collection	2.10 to 26.00 deg.
Limiting indices	-17<=h<=16, -23<=k<=23, -22<=l<=12
Reflections collected / unique	13435 / 4891 [R(int) = 0.0210]
Completeness to theta = 26.00	99.8 %
Absorption correction	Empirical
Max. and min.	1.00000 and 0.84202
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4891 / 0 / 343
Final R indices [I>2sigma(I)]	R1 = 0.0398, wR2 = 0.1038
R indices (all data)	R1 = 0.0549, wR2 = 0.1145
Largest diff. peak and hole	0.181 and -0.145 e.A^{-3}



1ai

Identification code	cd21252
Empirical formula	C42 H26 N2
Formula weight	558.65
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 11.4684(6) A alpha = 90 deg. b = 18.0050(9) A beta = 92.9890(10) deg. c = 13.8450(7) A gamma = 90 deg.
Volume	2854.9(3) A^3
Z, Calculated density	4, 1.300 Mg/m^3
Absorption coefficient	0.075 mm^{-1}
F(000)	1168
Crystal size	0.321 x 0.212 x 0.156 mm
Theta range for data collection	1.86 to 26.00 deg.
Limiting indices	-14<=h<=13, -22<=k<=16, -17<=l<=17
Reflections collected / unique	17144 / 5607 [R(int) = 0.0235]
Completeness to theta = 26.00	99.9 %
Absorption correction	Empirical
Max. and min. transmission	1.00000 and 0.58903
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5607 / 6 / 397
Goodness-of-fit on F^2	1.023
Final R indices [I>2sigma(I)]	R1 = 0.0486, wR2 = 0.1257
R indices (all data)	R1 = 0.0703, wR2 = 0.1407
Largest diff. peak and hole	0.163 and -0.122 $e.A^{-3}$