Simultaneous enhancement of fluorescence and solubility by *N*-alkylation and functionalization of 2-(2-thienyl)imidazo[4,5-*f*][1,10]-phenanthroline with heterocyclic bridges

Yu-Xin Peng, Na Wang, Yuan Dai, Bin Hu, Bin-Bin Ma and Wei Huang*

State Key Laboratory of Coordination Chemistry, Nanjing National Laboratory of Microstructures, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210093, P. R. China

E-mail: whuang@nju.edu.cn

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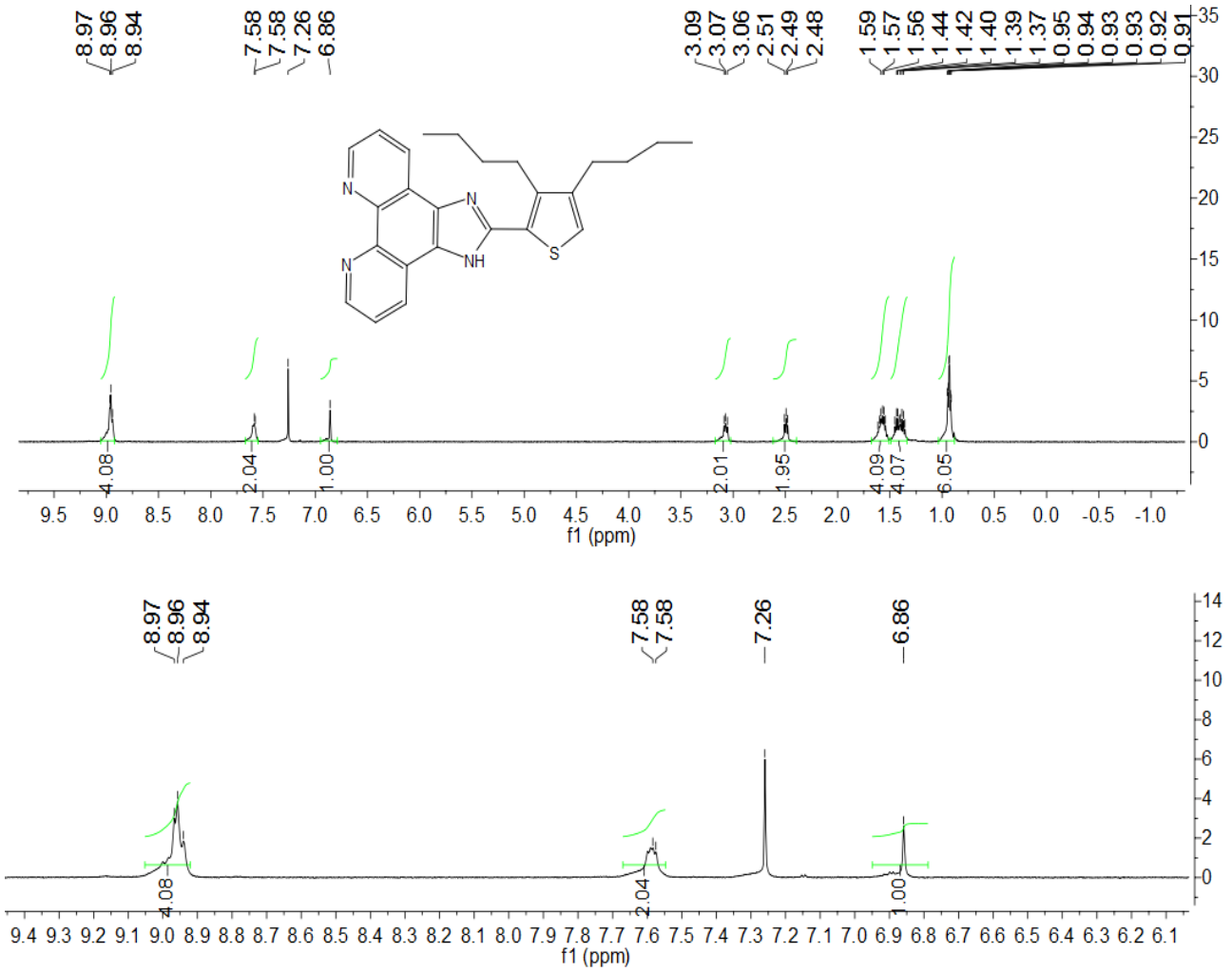
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8.94
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3.07
3.06
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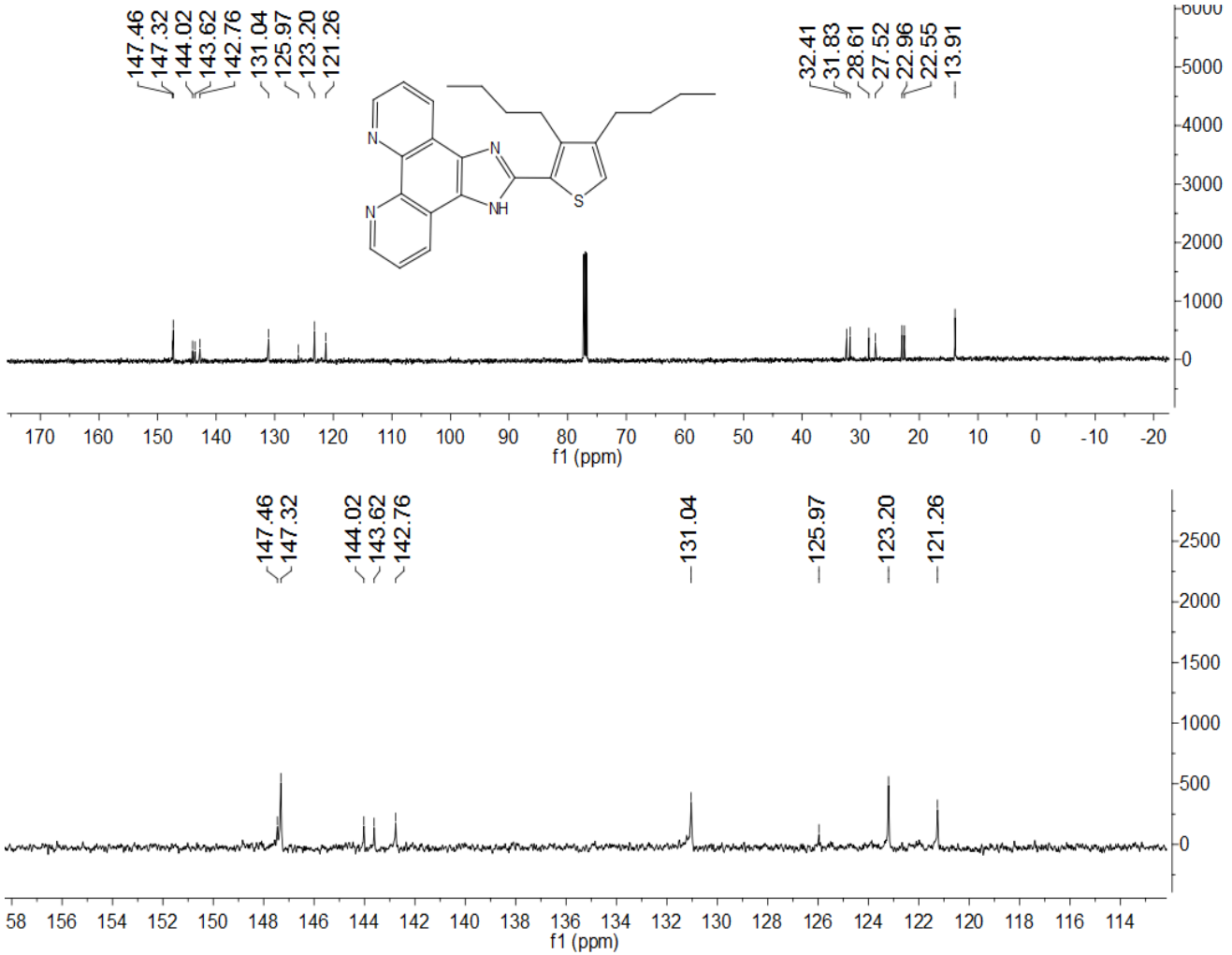
2.49
2.48
1.59
1.57
1.56
1.44
1.42
1.40
1.39
1.37
0.95
0.94
0.93
0.93
0.92
0.91
N
N
NH
S
4.08
2.04
1.00
2.01
1.95
4.09
4.07
6.05
f1 (ppm)
8.97
8.96
8.94
7.58
7.58
7.26
6.86
4.08
2.04
1.00
f1 (ppm)

a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123.20
121.26
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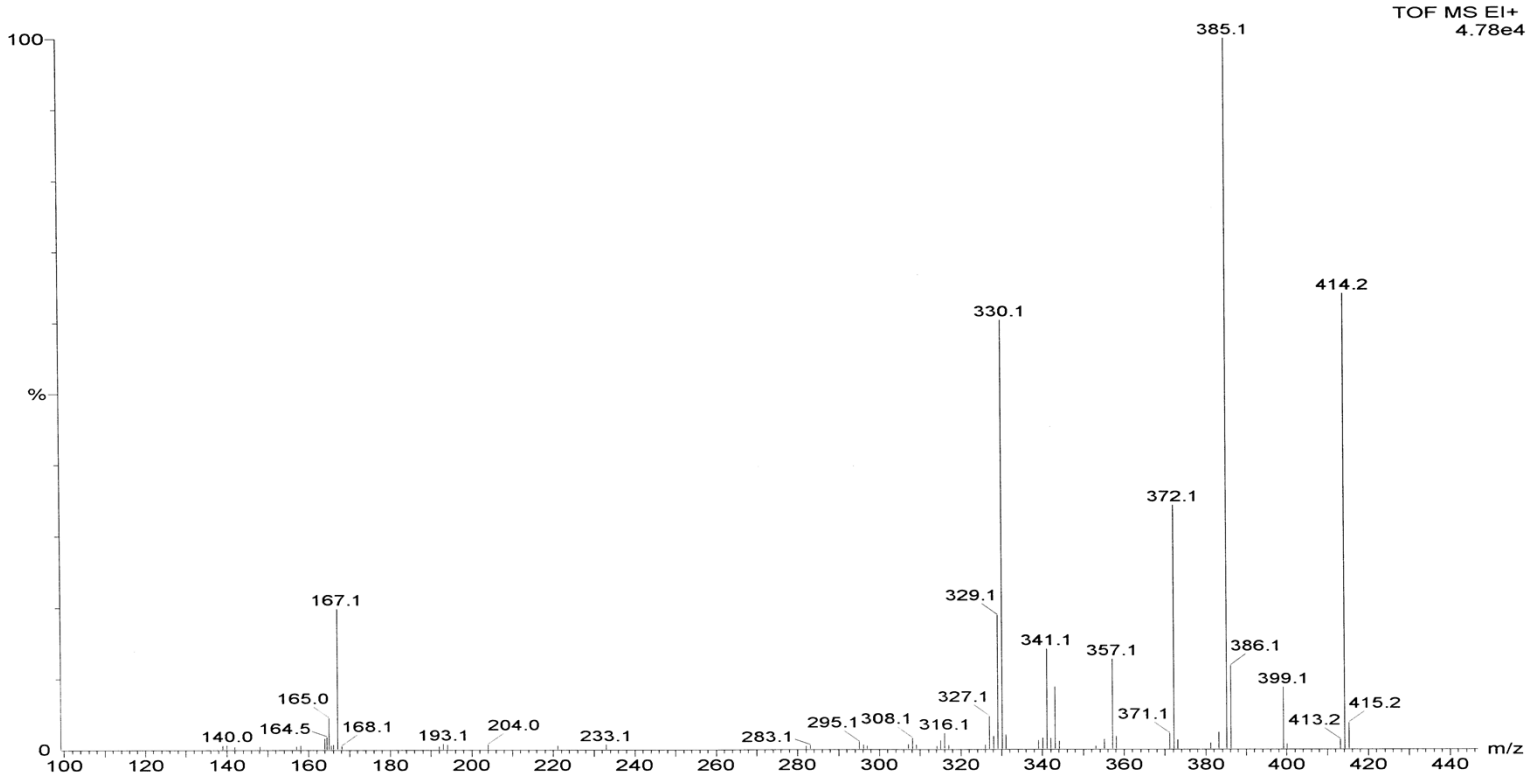
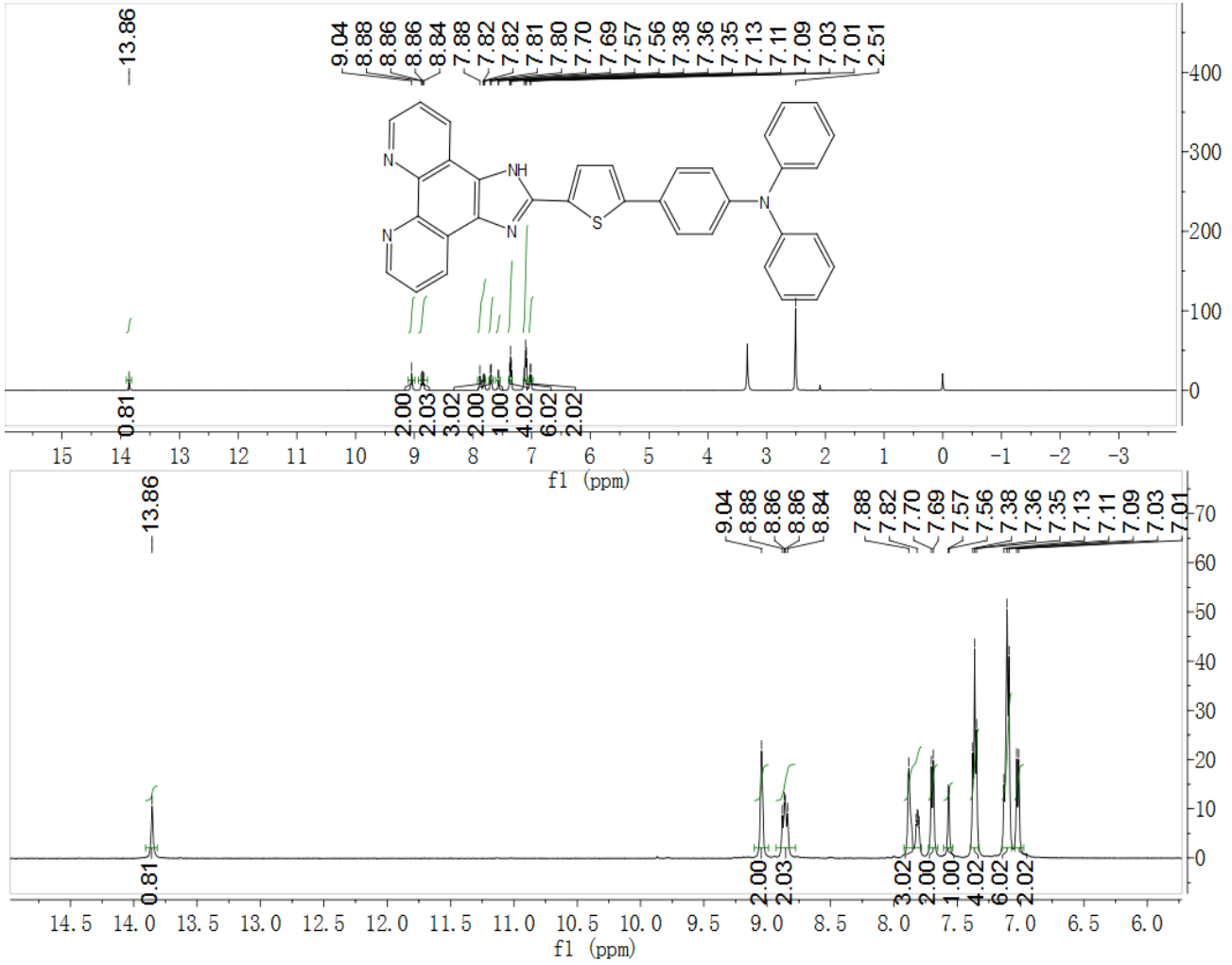
31.83
28.61
27.52
22.96
22.55
13.91
N
N
NH
S
f1 (ppm)

b



c

Fig. SI1. ^{1}H (**a**), ^{13}C NMR (**b**) and EI-TOF-MS (**c**) spectra of compound **1**.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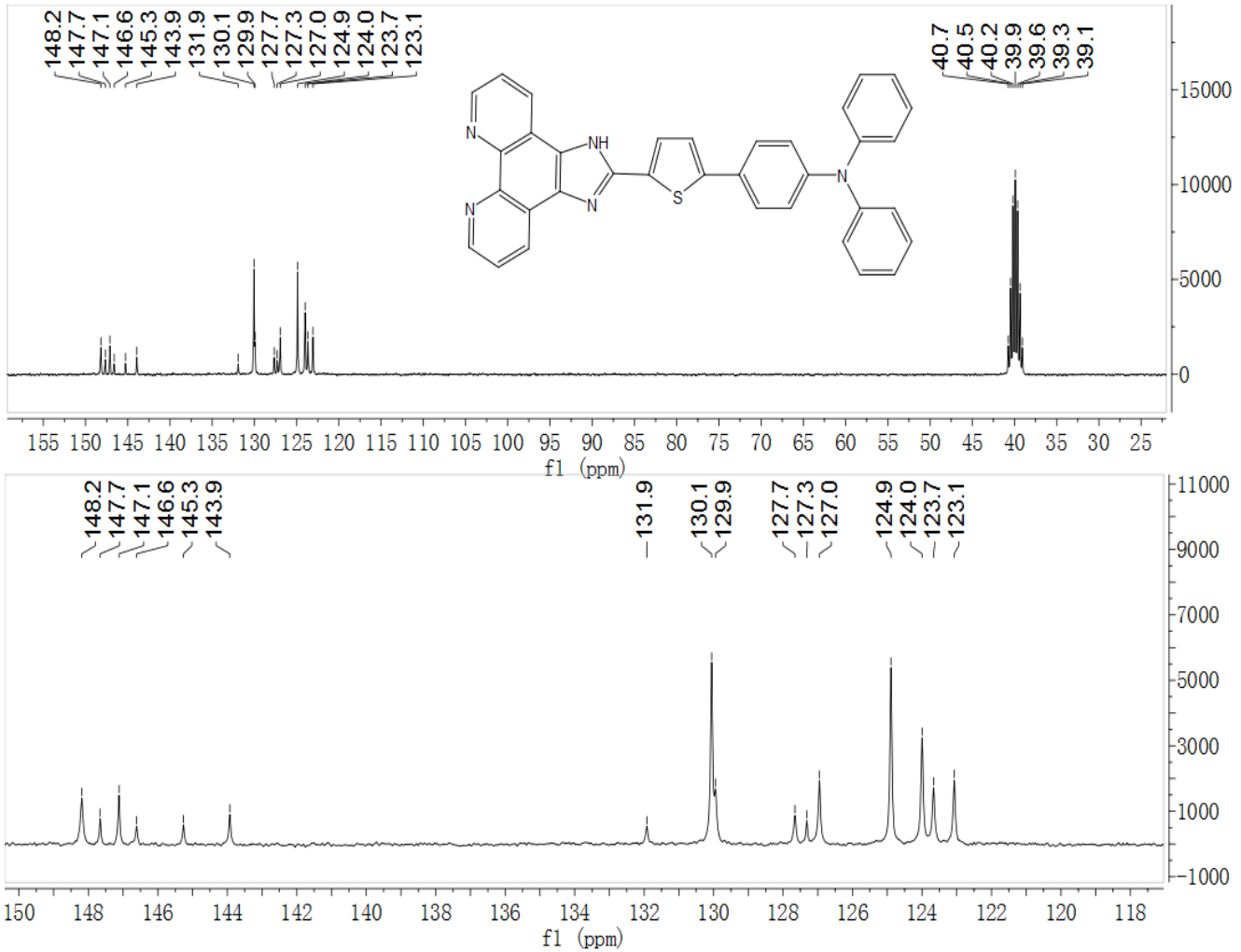
8.88
8.86
8.86
8.84
7.88
7.82
7.82
7.81
7.80
7.70
7.69
7.57
7.56
7.38
7.36
7.35
7.13
7.11
7.09
7.03
7.01
2.51
N
NH
N
N
S
N
0.81
2.00
2.03
3.02
2.00
1.00
4.02
6.02
2.02
f1 (ppm)
13.86
9.04
8.88
8.86
8.86
8.84
7.88
7.82
7.70
7.69
7.57
7.56
7.38
7.36
7.35
7.13
7.11
7.09
7.03
7.01
0.81
2.00
2.03
3.02
2.00
1.00
4.02
6.02
2.02
f1 (ppm)

a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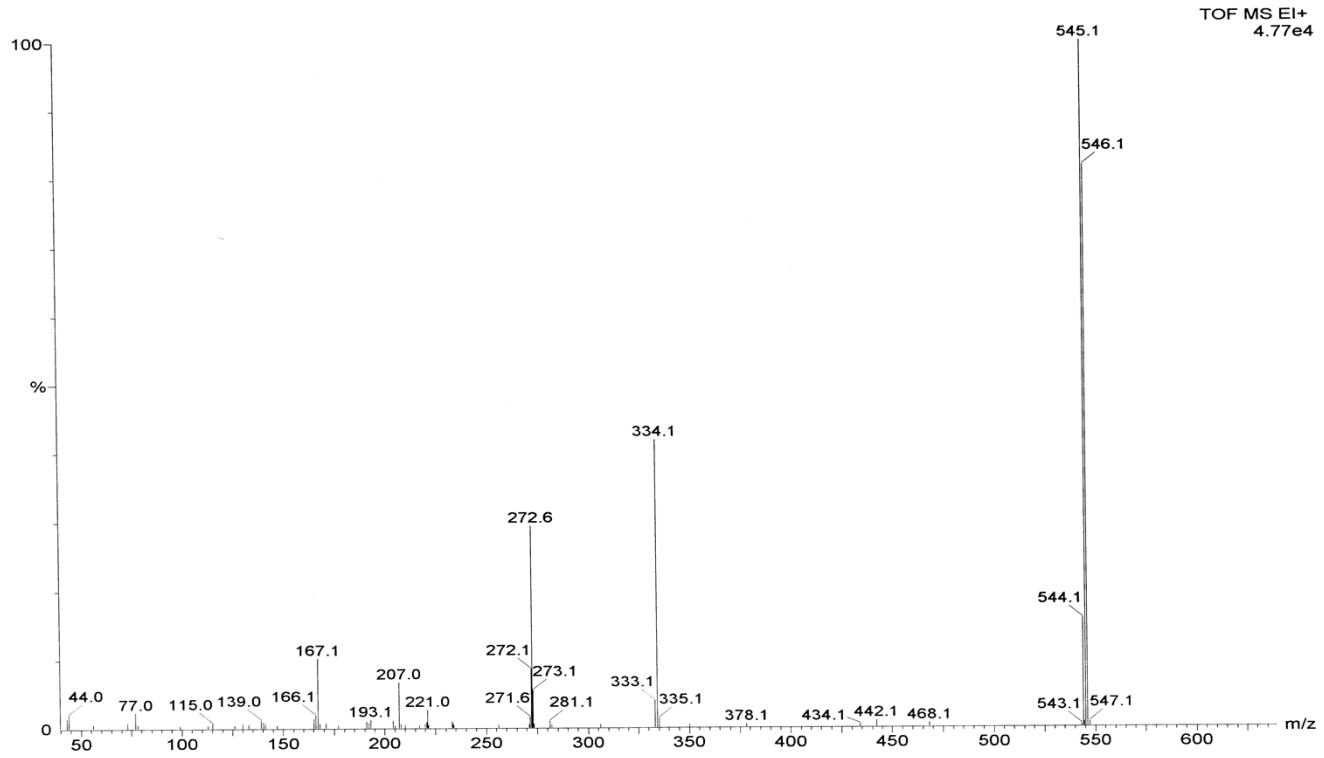
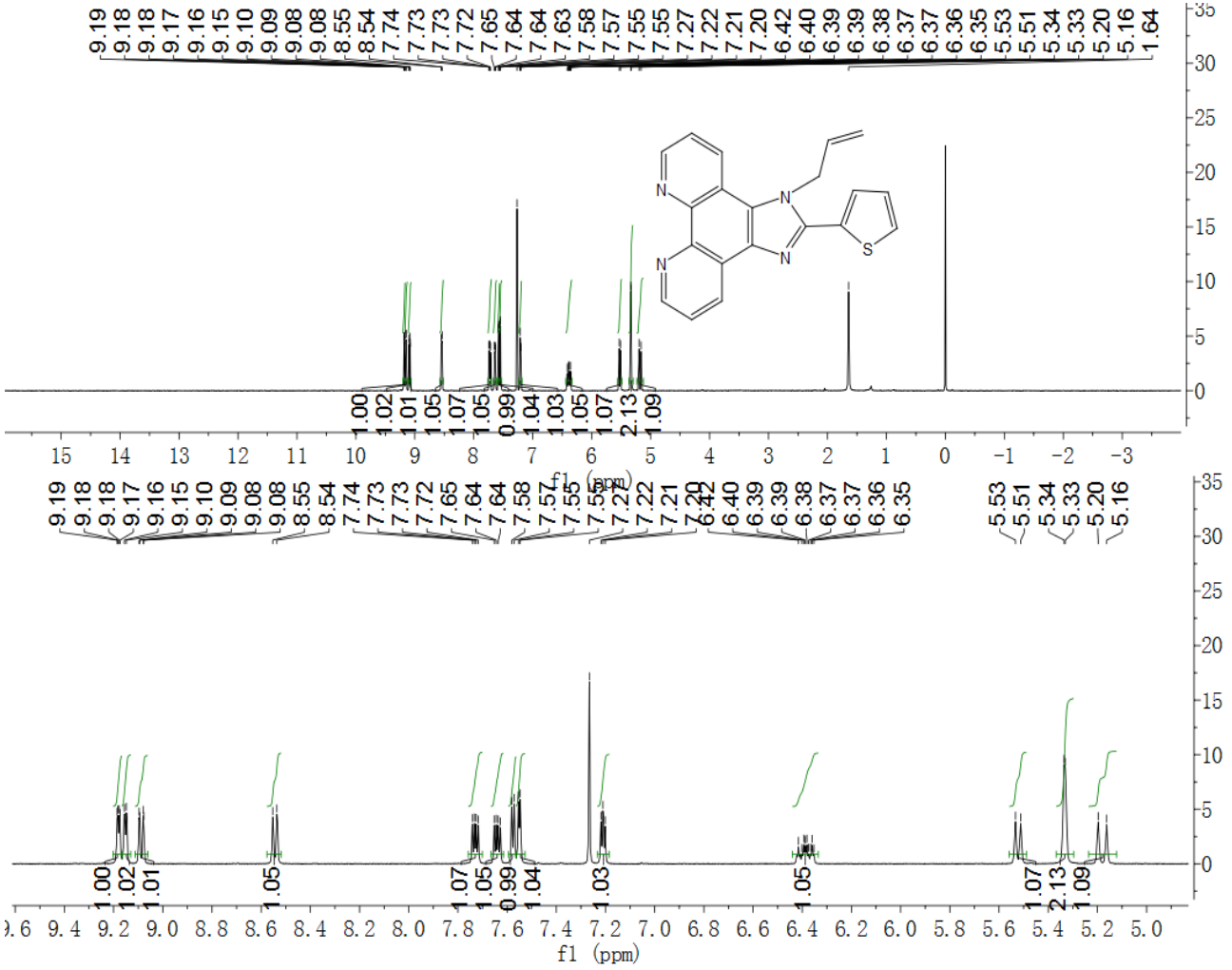
147.7
147.1
146.6
145.3
143.9
131.9
130.1
129.9
127.7
127.3
127.0
124.9
124.0
123.7
123.1
40.7
40.5
40.2
39.9
39.6
39.3
39.1
N
NH
N
N
S
N
15000
10000
5000
0
155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25
f1 (ppm)
148.2
147.7
147.1
146.6
145.3
143.9
131.9
130.1
129.9
127.7
127.3
127.0
124.9
124.0
123.7
123.1
11000
9000
7000
5000
3000
1000
-1000
150 148 146 144 142 140 138 136 134 132 130 128 126 124 122 120 118
f1 (ppm)

b

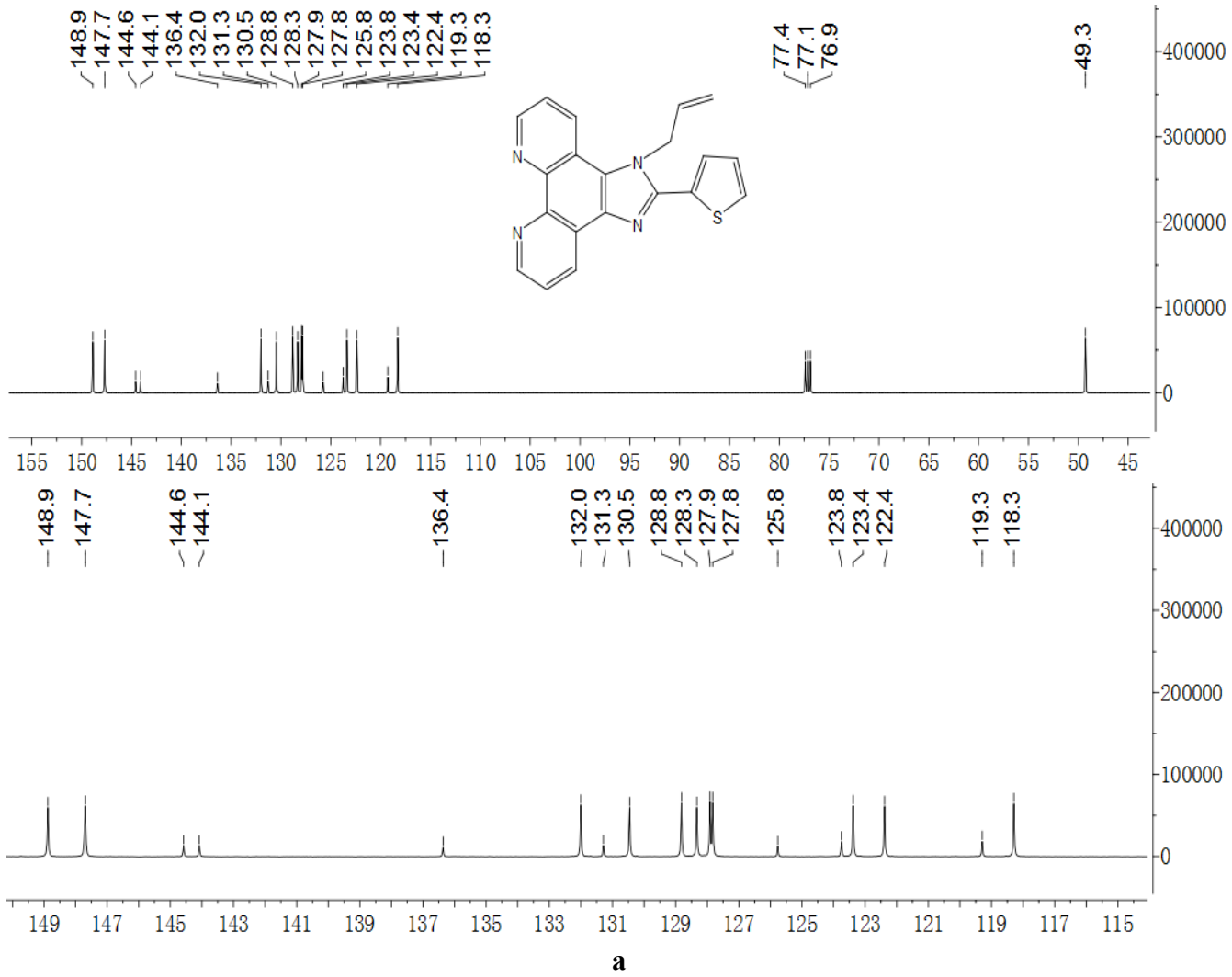


c

Fig. SI2. ^{1}H (**a**), ^{13}C NMR (**b**) and EI-TOF-MS (**c**) spectra of compound **2**.



a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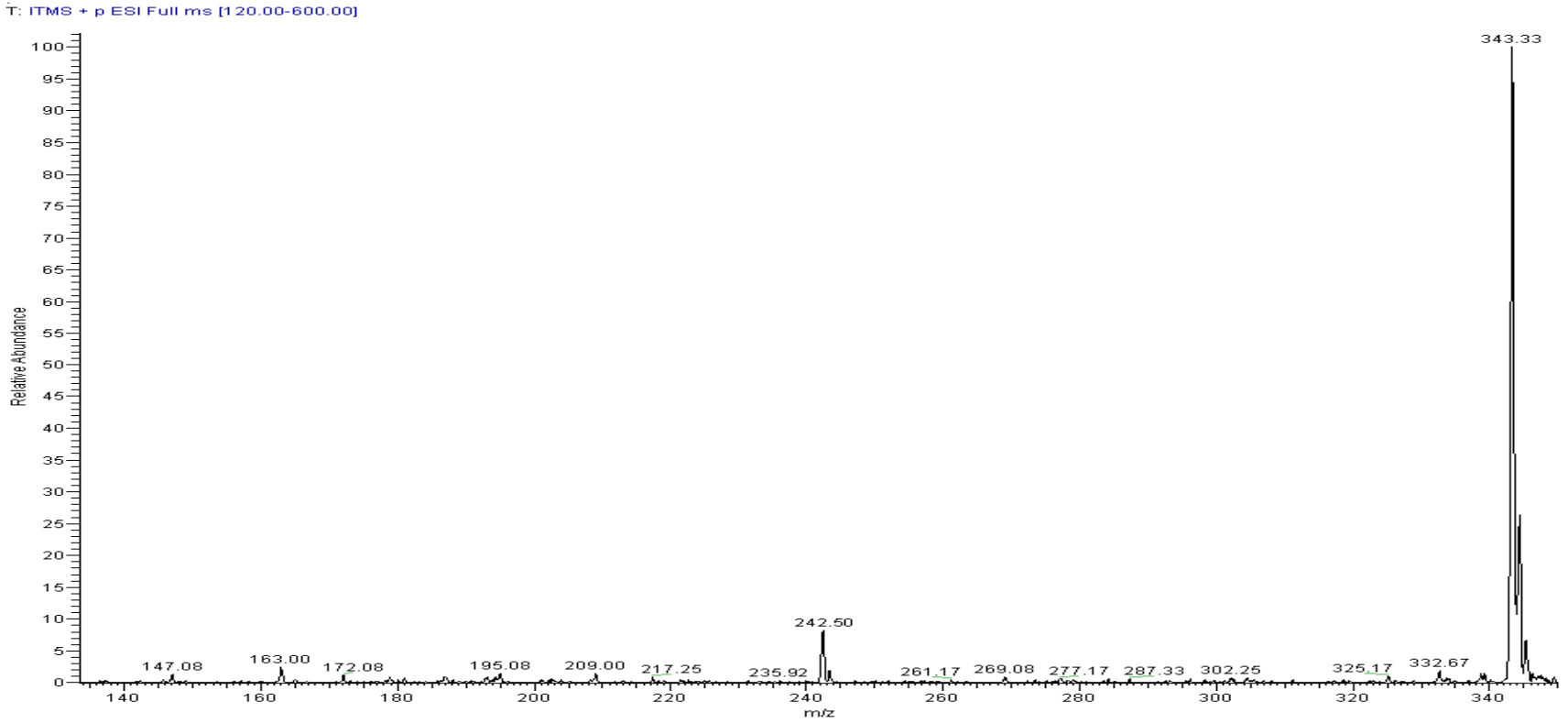
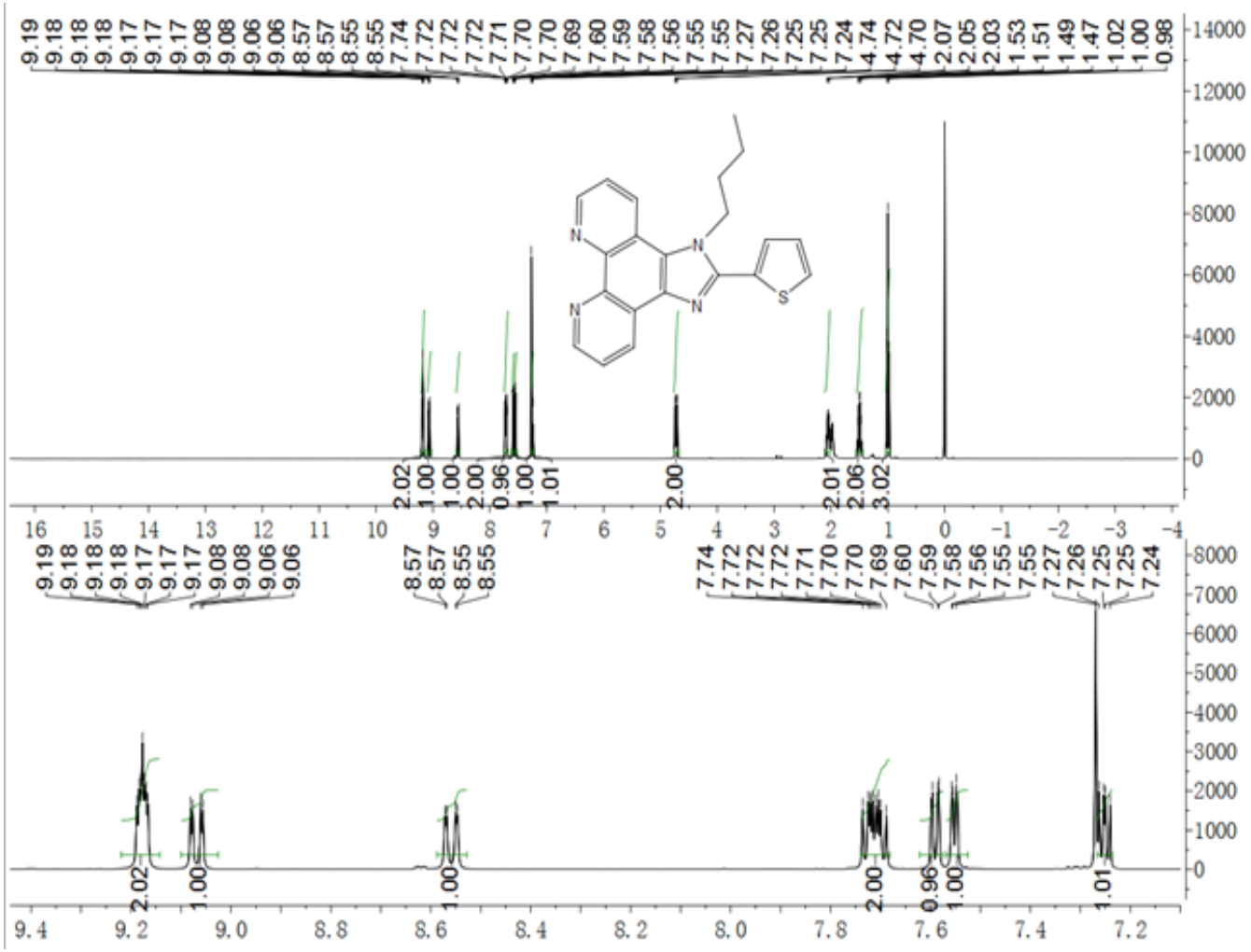
147.7
144.6
144.1
136.4
132.0
131.3
130.5
128.8
128.3
127.9
127.8
125.8
123.8
123.4
122.4
119.3
118.3
77.4
77.1
76.9
49.3
N
N
N
S
400000
300000
200000
100000
0
155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45
148.9
147.7
144.6
144.1
136.4
132.0
131.3
130.5
128.8
128.3
127.9
127.8
125.8
123.8
123.4
122.4
119.3
118.3
400000
300000
200000
100000
0
149 147 145 143 141 139 137 135 133 131 129 127 125 123 121 119 117 115

a

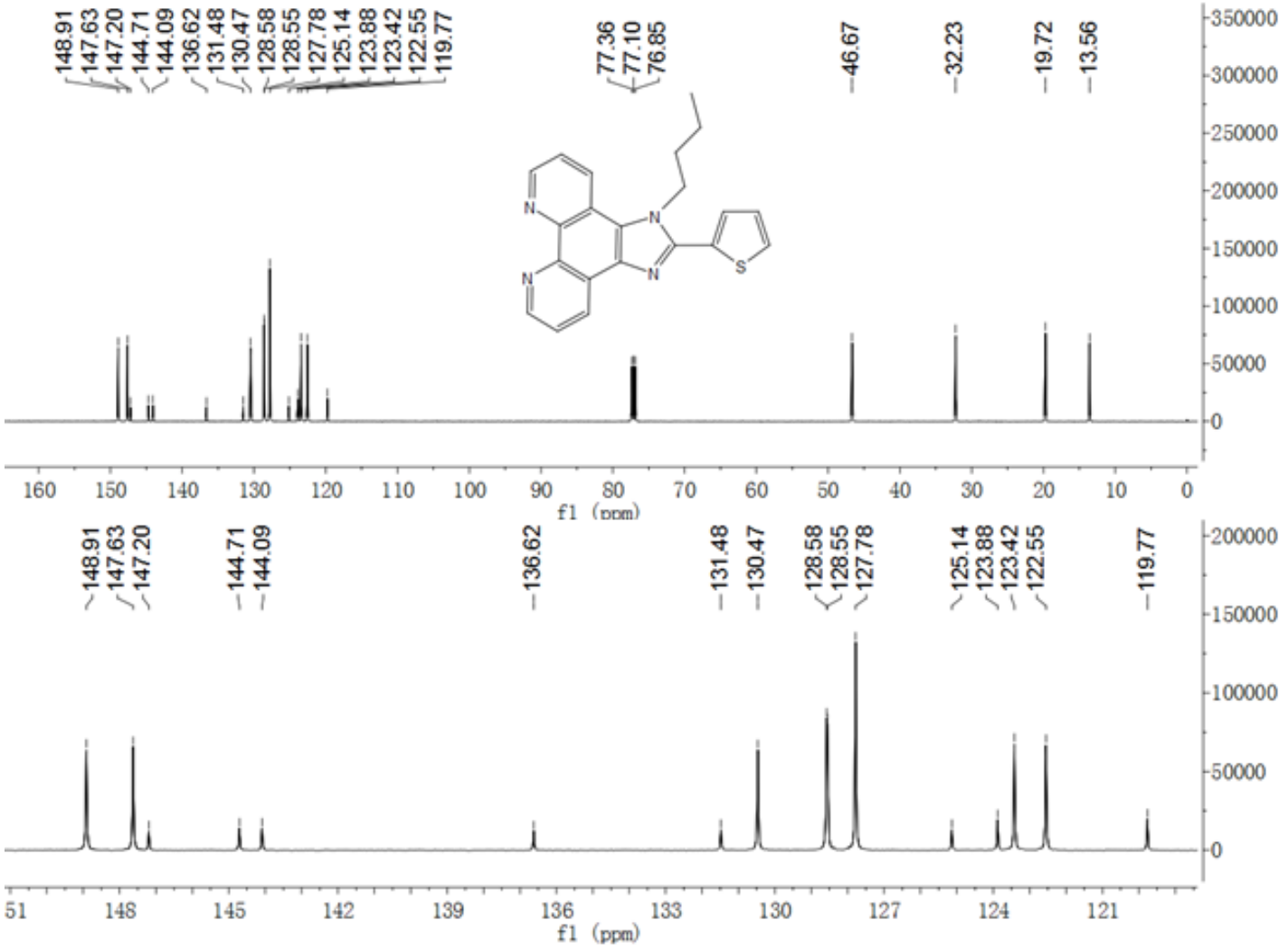


c

Fig. SI3. ^{1}H (**a**), ^{13}C NMR (**b**) and EI-TOF-MS (**c**) spectra of compound **3**.



a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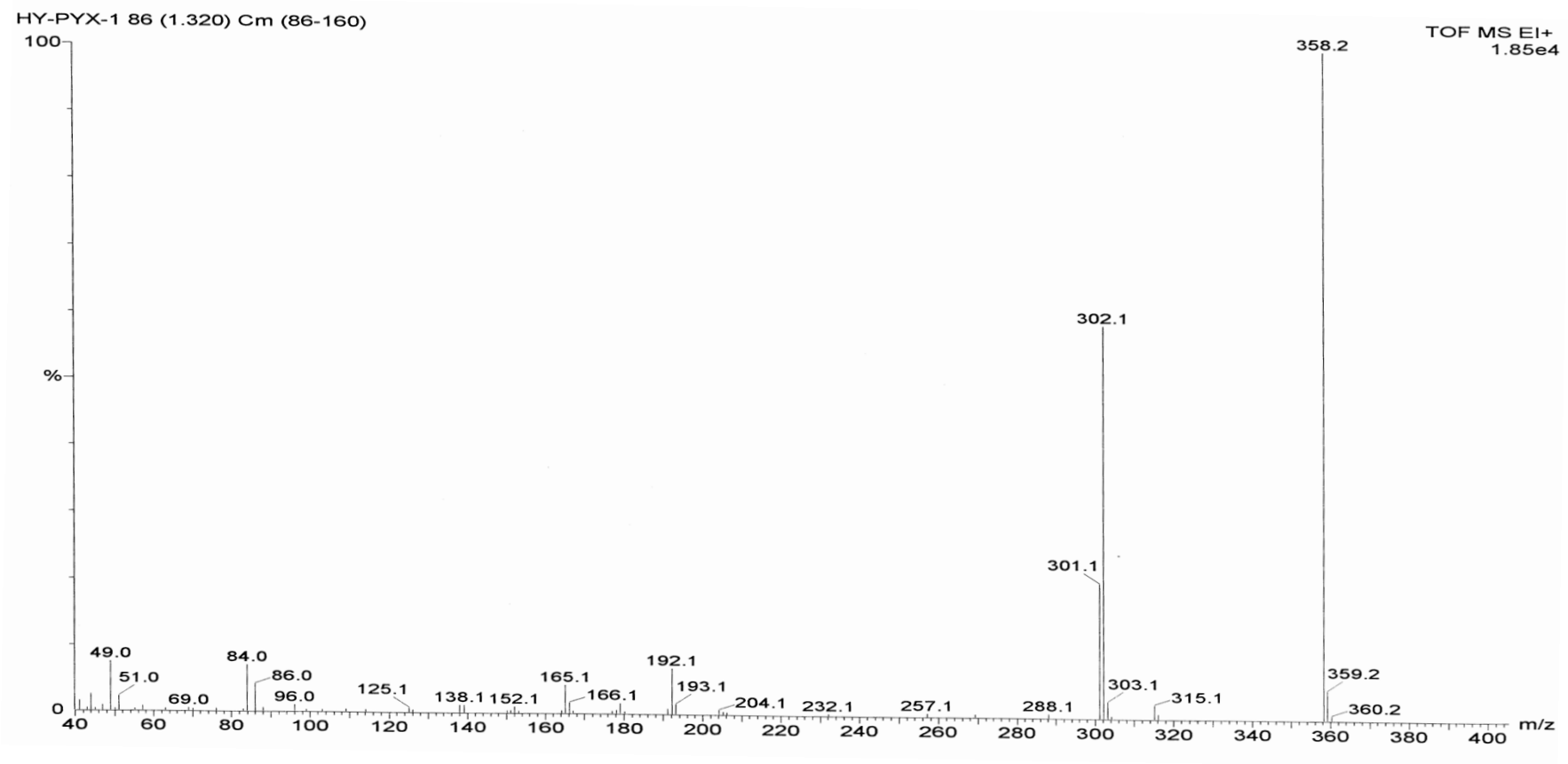
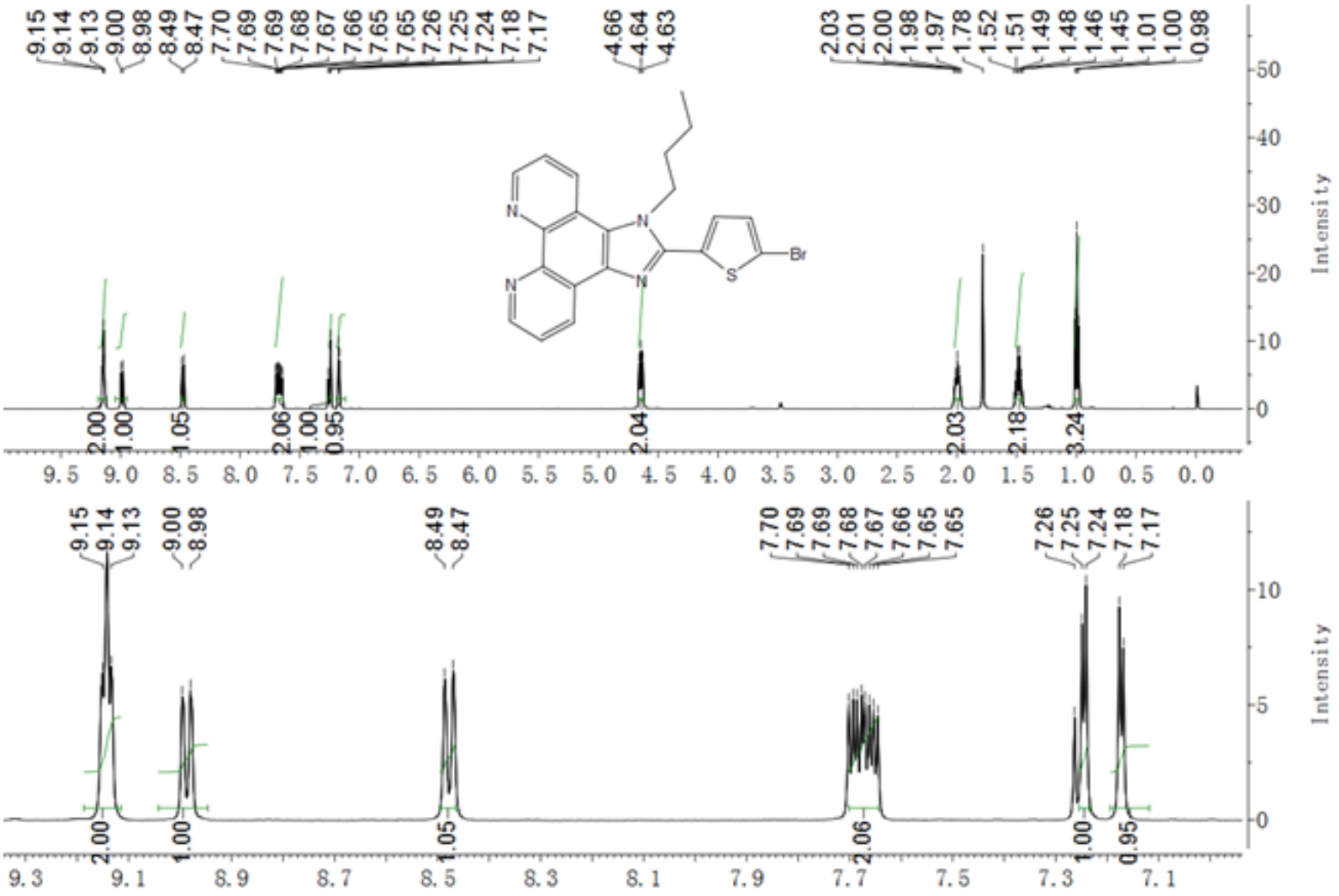
147.63
147.20
144.71
144.09
136.62
131.48
130.47
128.58
128.55
127.78
125.14
123.88
123.42
122.55
119.77
77.36
77.10
76.85
46.67
32.23
19.72
13.56
N
N
N
S
f1 (ppm)
f1 (ppm)

b



c

Fig. SI4. ^{1}H (**a**), ^{13}C NMR (**b**) and EI-TOF-MS (**c**) spectra of compound **4**.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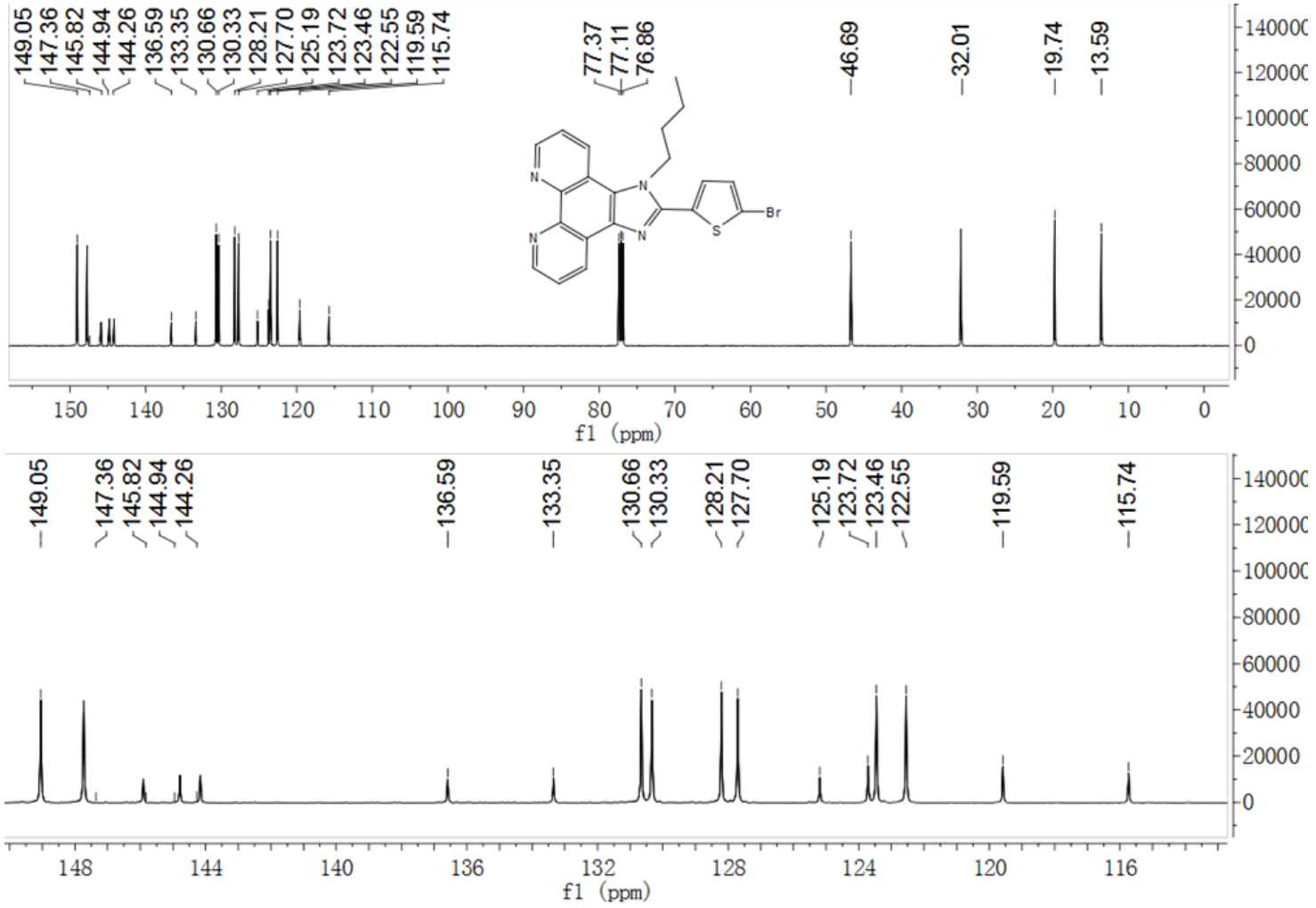
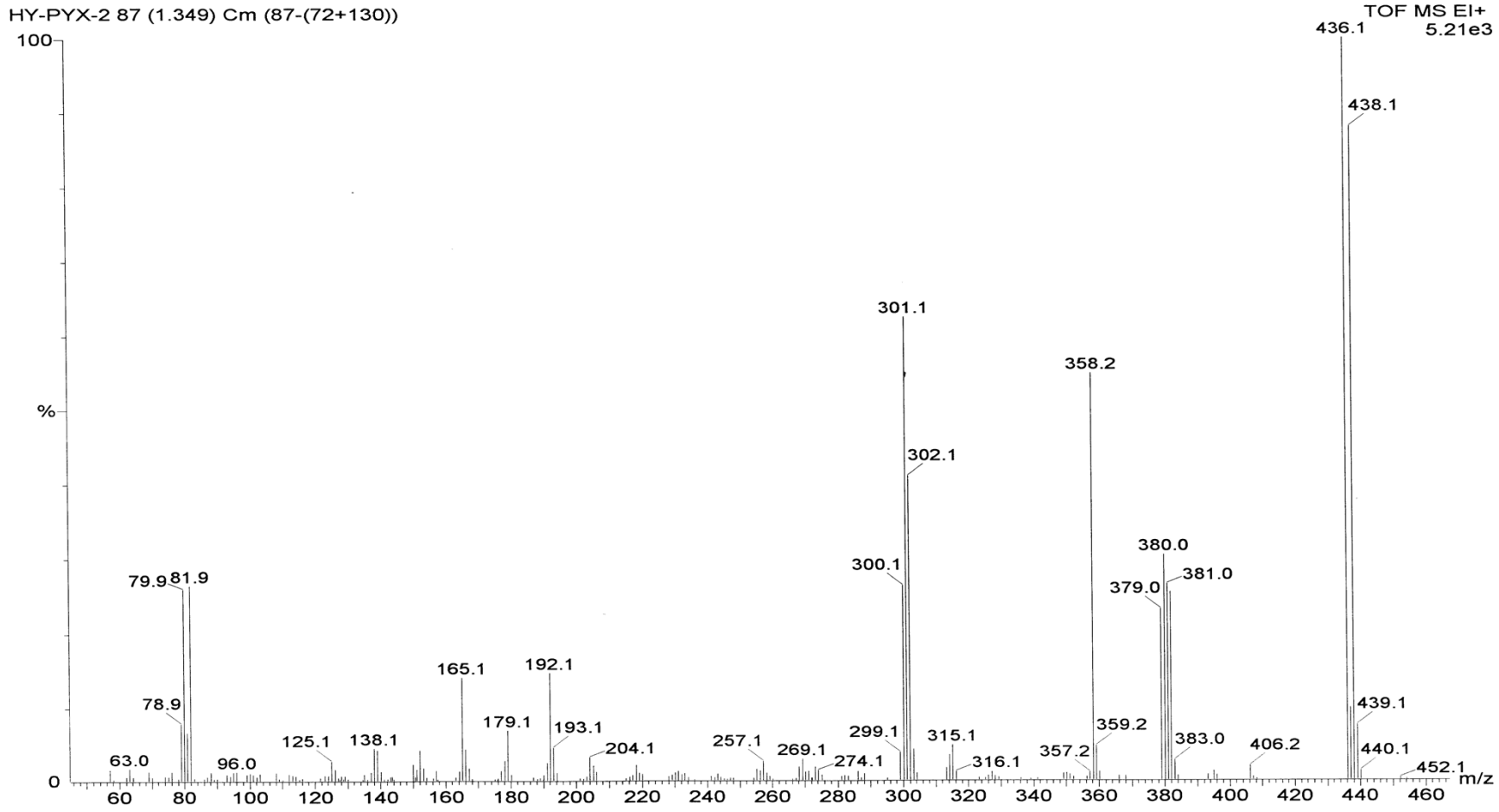
9.14
9.13
9.00
8.98
8.49
8.47
7.70
7.69
7.69
7.68
7.67
7.66
7.65
7.65
7.26
7.25
7.24
7.18
7.17
4.66
4.64
4.63
2.03
2.01
2.00
1.98
1.97
1.78
1.52
1.51
1.49
1.48
1.46
1.45
1.01
1.00
0.98
N
N
N
S
Br
Intensity
2.00
1.00
1.05
2.06
1.00
0.95
2.04
2.03
2.18
3.24
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
9.3
9.1
8.9
8.7
8.5
8.3
8.1
7.9
7.7
7.5
7.3
7.1

a

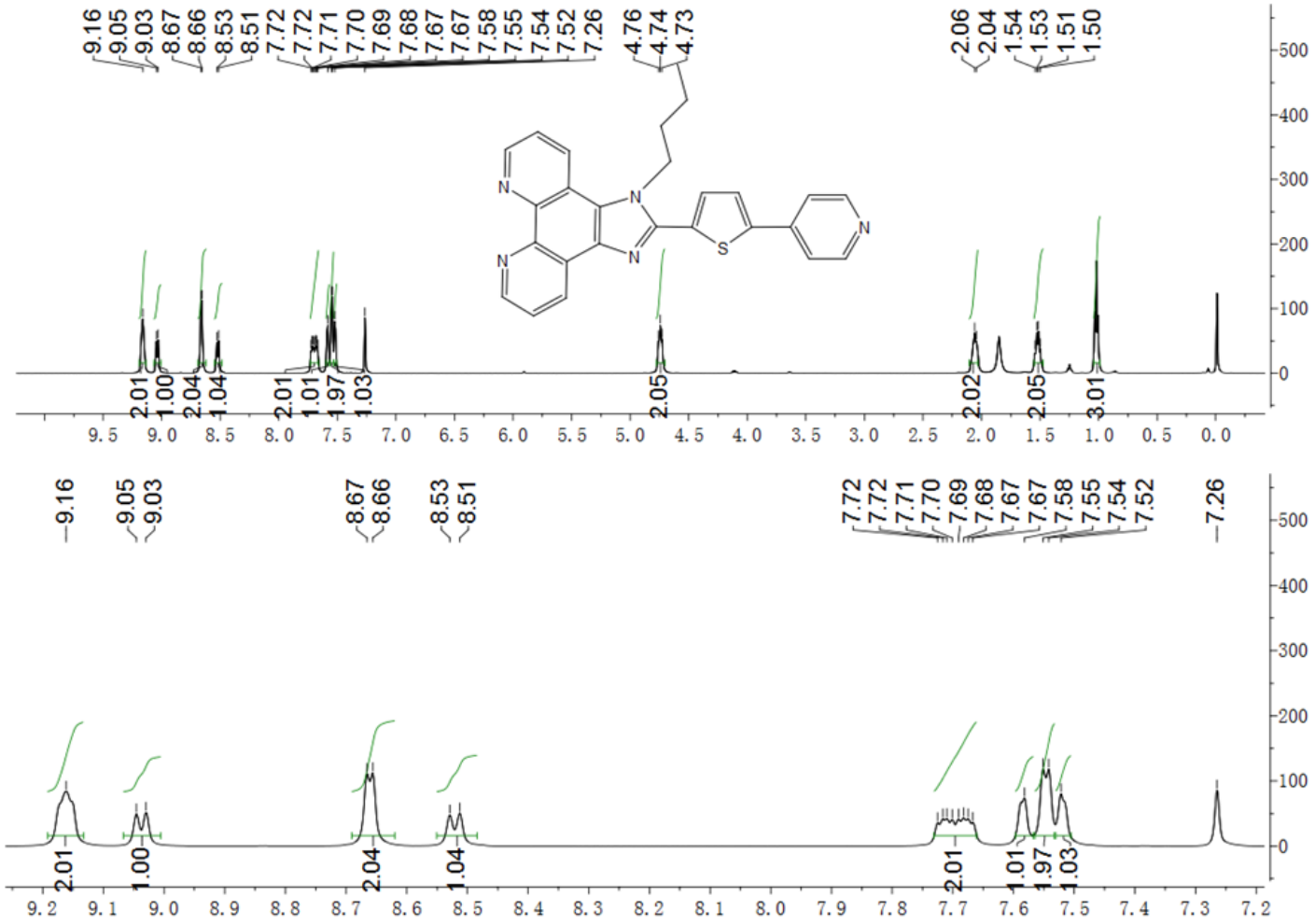

149.05
147.36
145.82
144.94
144.26
136.59
133.35
130.66
130.33
128.21
127.70
125.19
123.72
123.46
122.55
119.59
115.74
77.37
77.11
76.86
46.69
32.01
19.74
13.59
Br
f1 (ppm)
f1 (ppm)

b

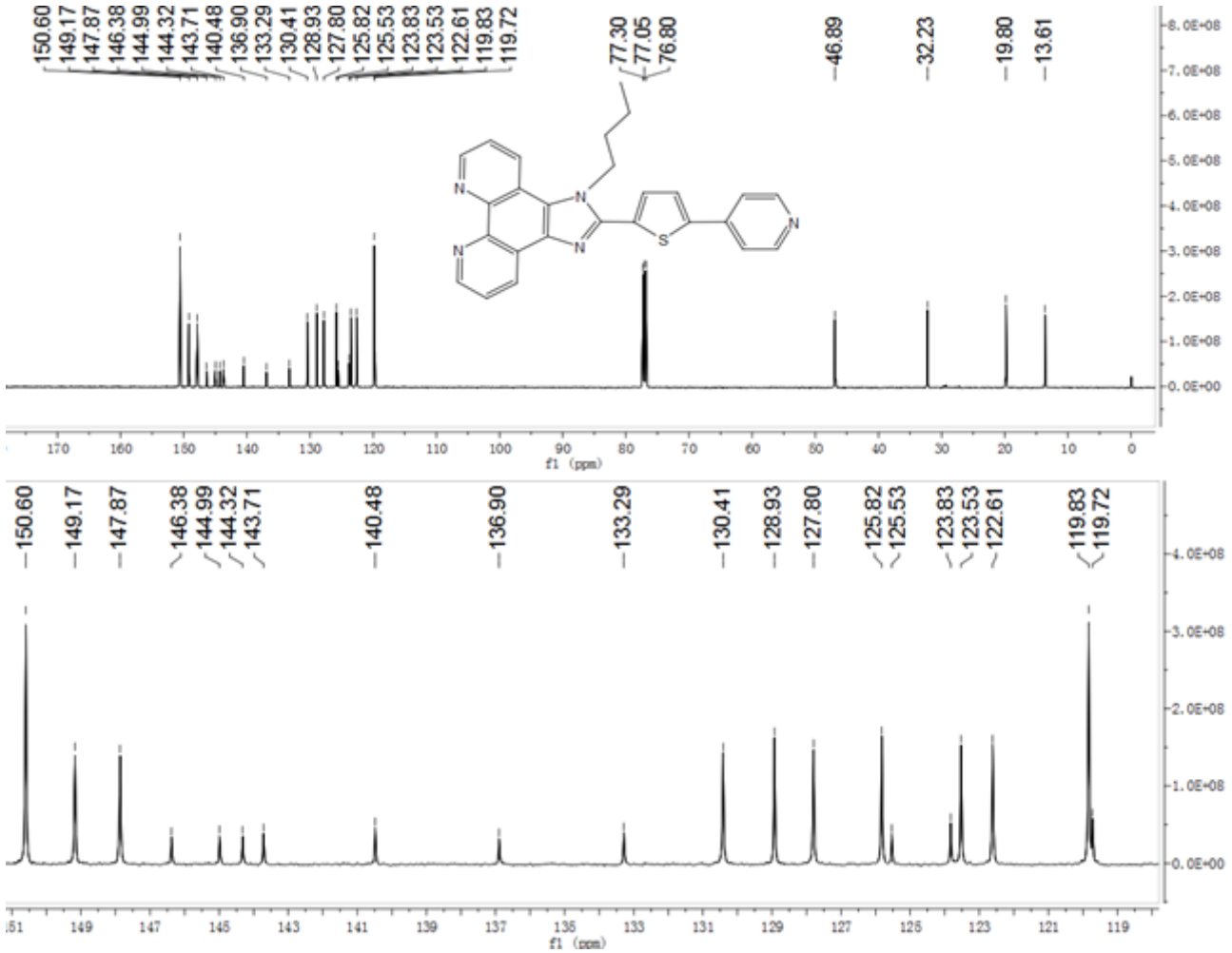


c

Fig. SI5. ^{1}H (**a**), ^{13}C NMR (**b**) and EI-TOF-MS (**c**) spectra of compound **5**.



a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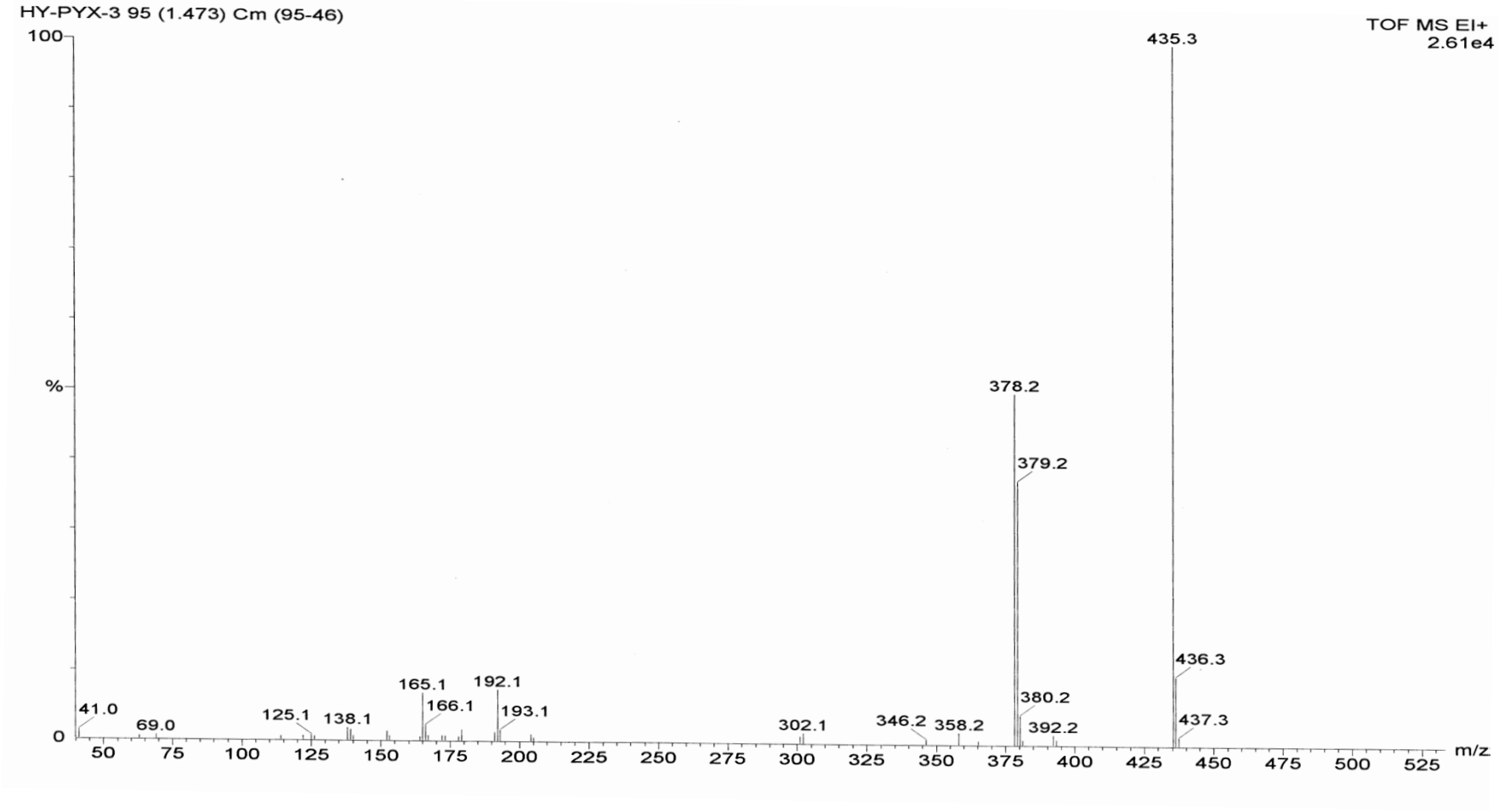
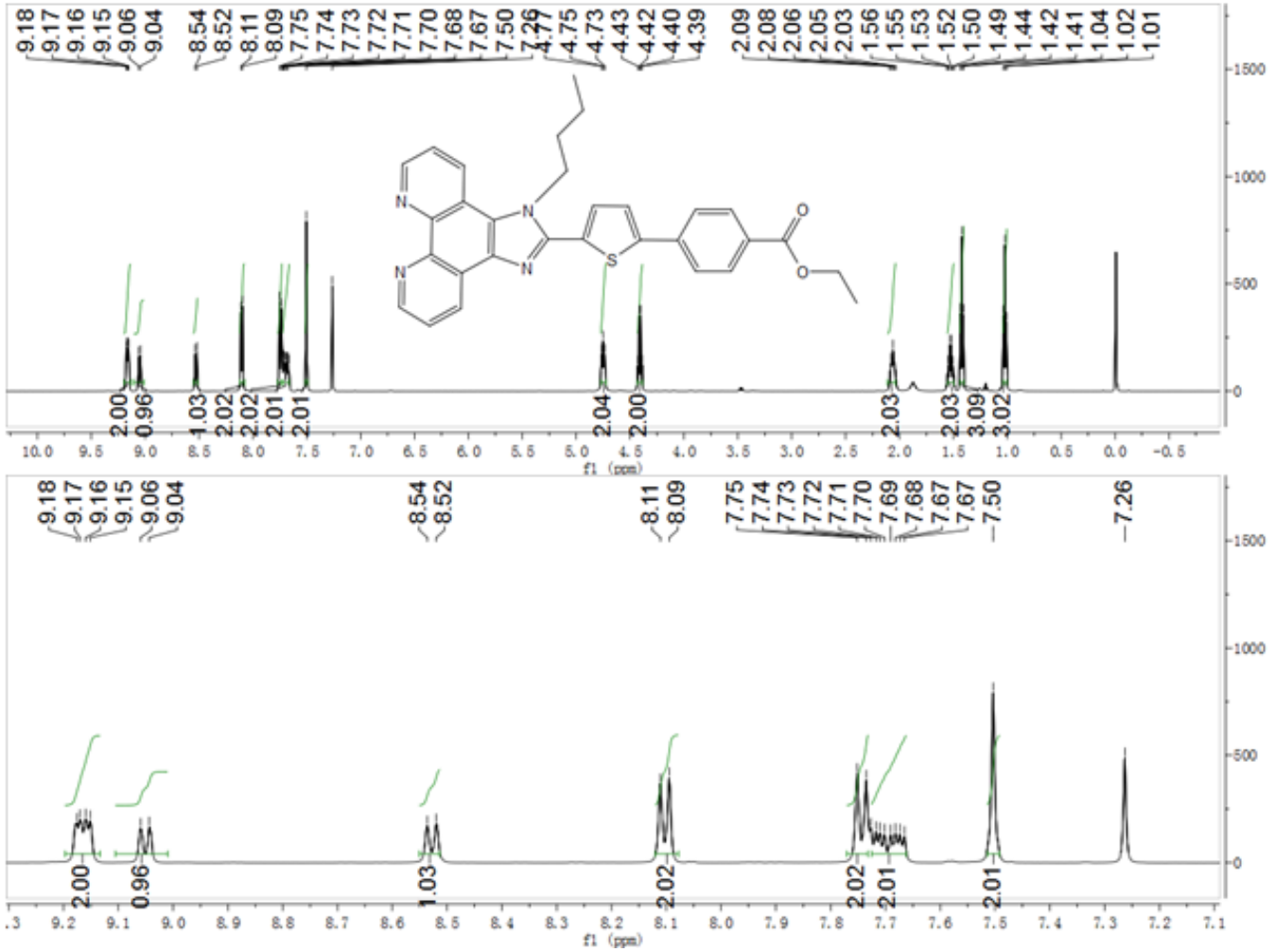
149.17
147.87
146.38
144.99
144.32
143.71
140.48
136.90
133.29
130.41
128.93
127.80
125.82
125.53
123.83
123.53
122.61
119.83
119.72
77.30
77.05
76.80
46.89
32.23
19.80
13.61
f1 (ppm)

b



c

Fig. SI6. ^{1}H (**a**), ^{13}C NMR (**b**) and EI-TOF-MS (**c**) spectra of compound **6**.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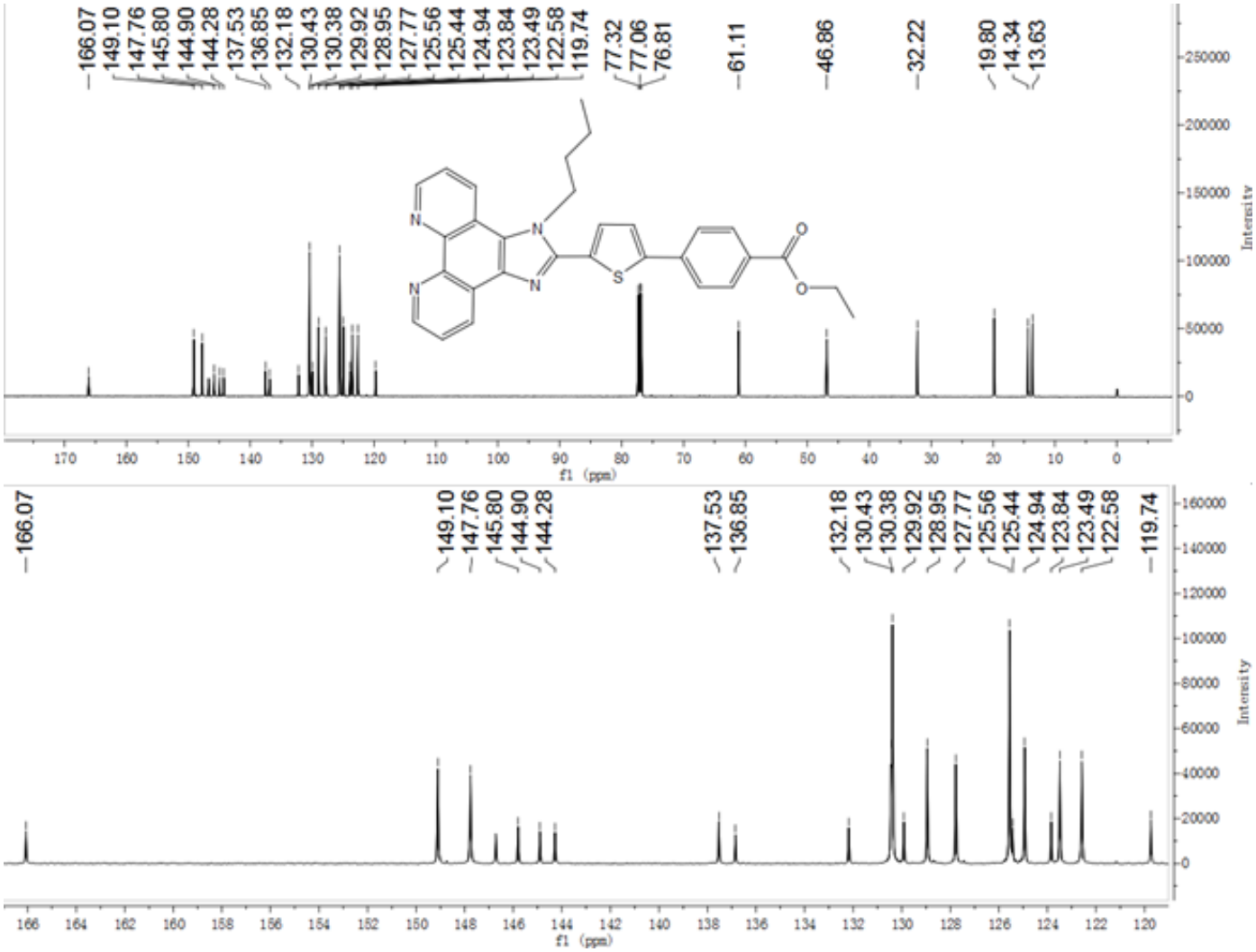
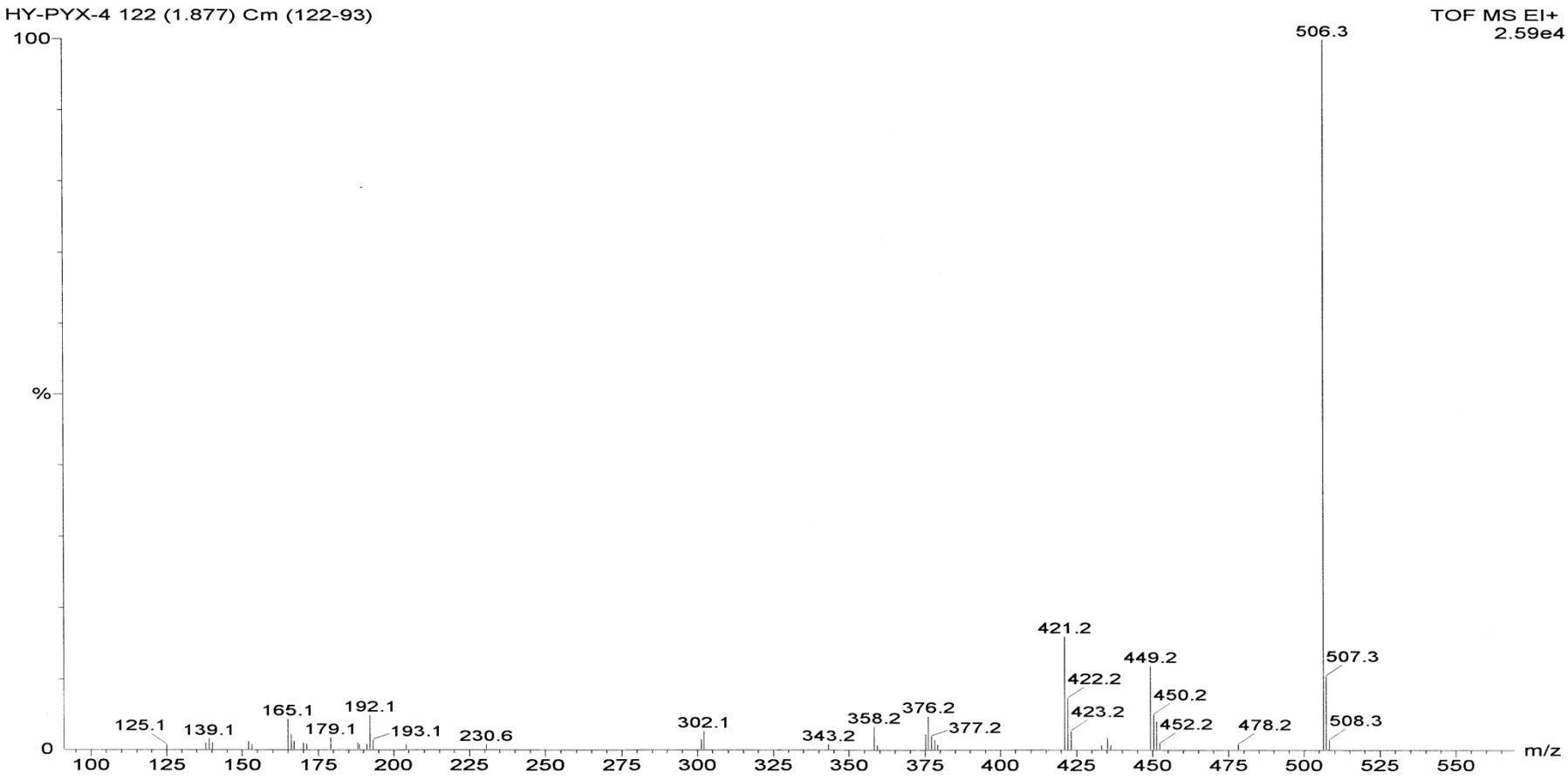
9.17
9.16
9.15
9.06
9.04
8.54
8.52
8.11
8.09
7.75
7.74
7.73
7.72
7.71
7.70
7.68
7.67
7.50
7.26
4.77
4.75
4.73
4.43
4.42
4.40
4.39
2.09
2.08
2.06
2.05
2.03
1.56
1.55
1.53
1.52
1.50
1.49
1.44
1.42
1.41
1.04
1.02
1.01
2.00
0.96
1.03
2.02
2.02
2.01
2.01
2.04
2.00
2.03
2.03
3.09
3.02
f1 (ppm)
2.00
0.96
1.03
2.02
2.02
2.01
2.01
f1 (ppm)

a

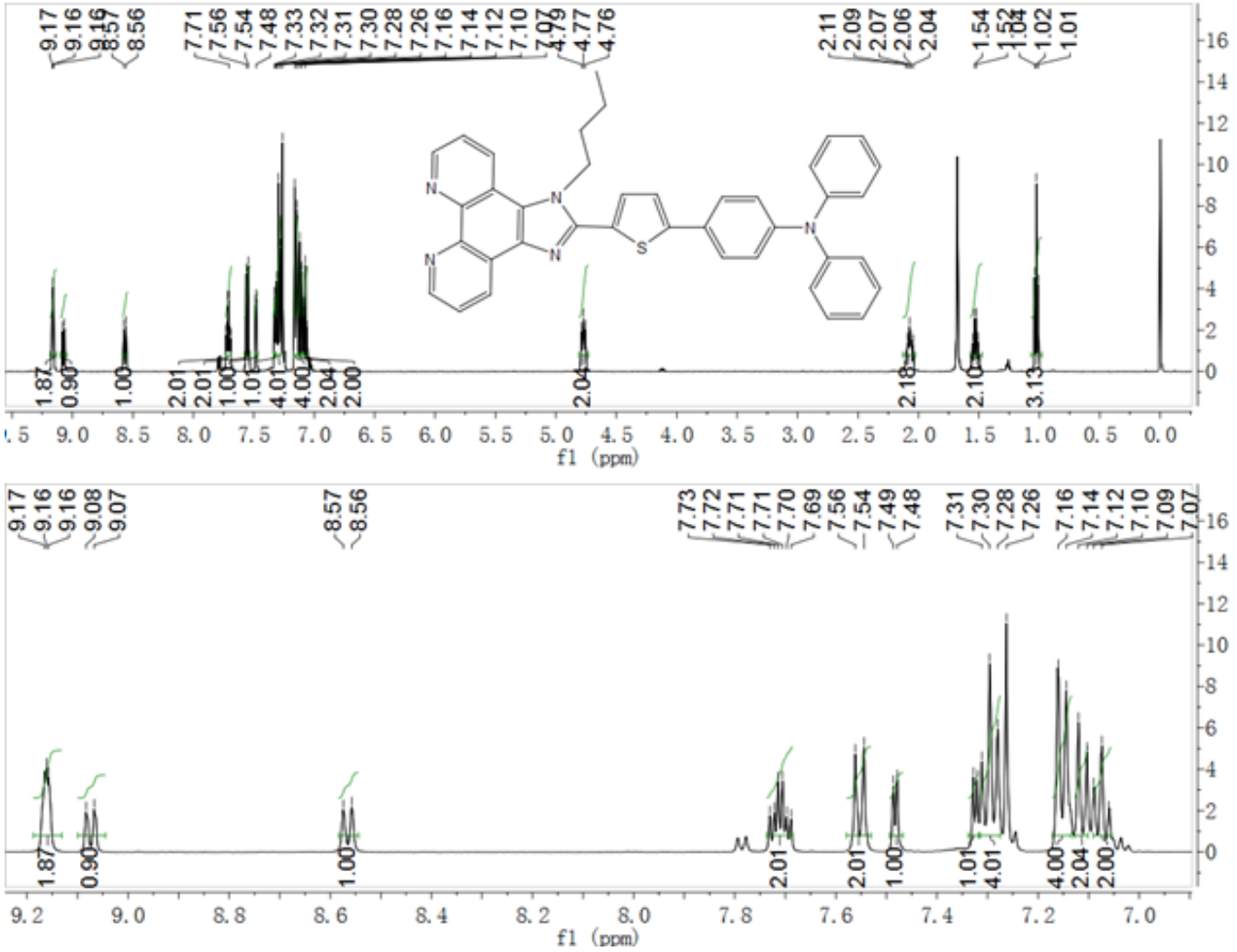

166.07
149.10
147.76
145.80
144.90
144.28
137.53
136.85
132.18
130.43
130.38
129.92
128.95
127.77
125.56
125.44
124.94
123.84
123.49
122.58
119.74
77.32
77.06
76.81
61.11
46.86
32.22
19.80
14.34
13.63
Intensity
f1 (ppm)

b



c

Fig. SI7. ^{1}H (**a**), ^{13}C NMR (**b**) and EI-TOF-MS (**c**) spectra of compound **7**.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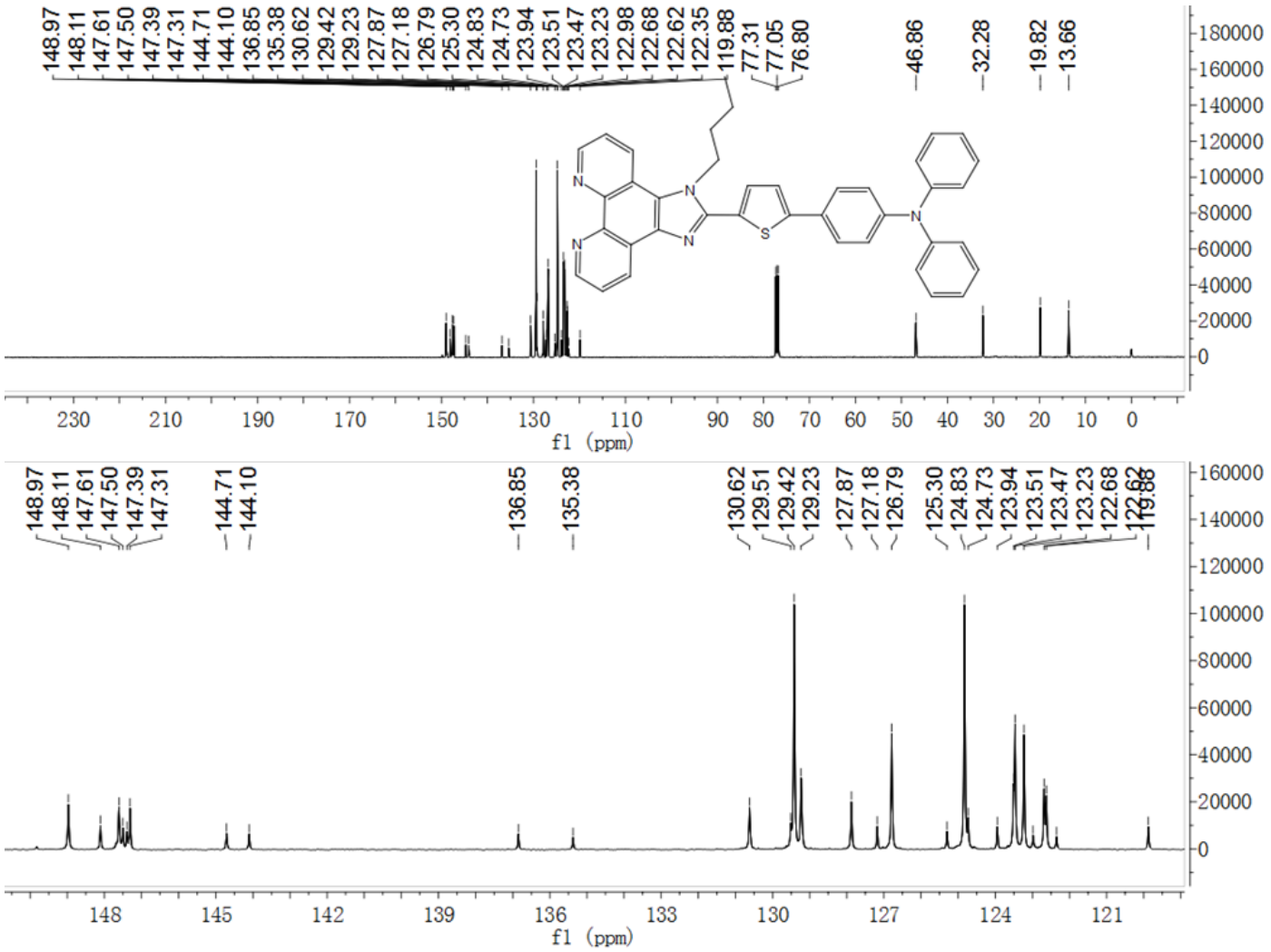
9.16
9.16
8.57
8.56
7.71
7.56
7.54
7.48
7.33
7.32
7.31
7.30
7.28
7.26
7.16
7.14
7.12
7.10
4.77
4.76
2.11
2.09
2.07
2.06
2.04
1.54
1.02
1.01
1.87
0.90
1.00
2.01
2.01
1.00
1.01
4.01
4.00
2.04
2.00
2.04
2.18
2.10
3.13
f1 (ppm)
9.17
9.16
9.16
9.08
9.07
8.57
8.56
7.73
7.72
7.71
7.71
7.70
7.69
7.56
7.54
7.49
7.48
7.31
7.30
7.28
7.26
7.16
7.14
7.12
7.10
7.09
7.07
1.87
0.90
1.00
2.01
2.01
1.00
1.01
4.01
4.00
2.04
2.00
f1 (ppm)

a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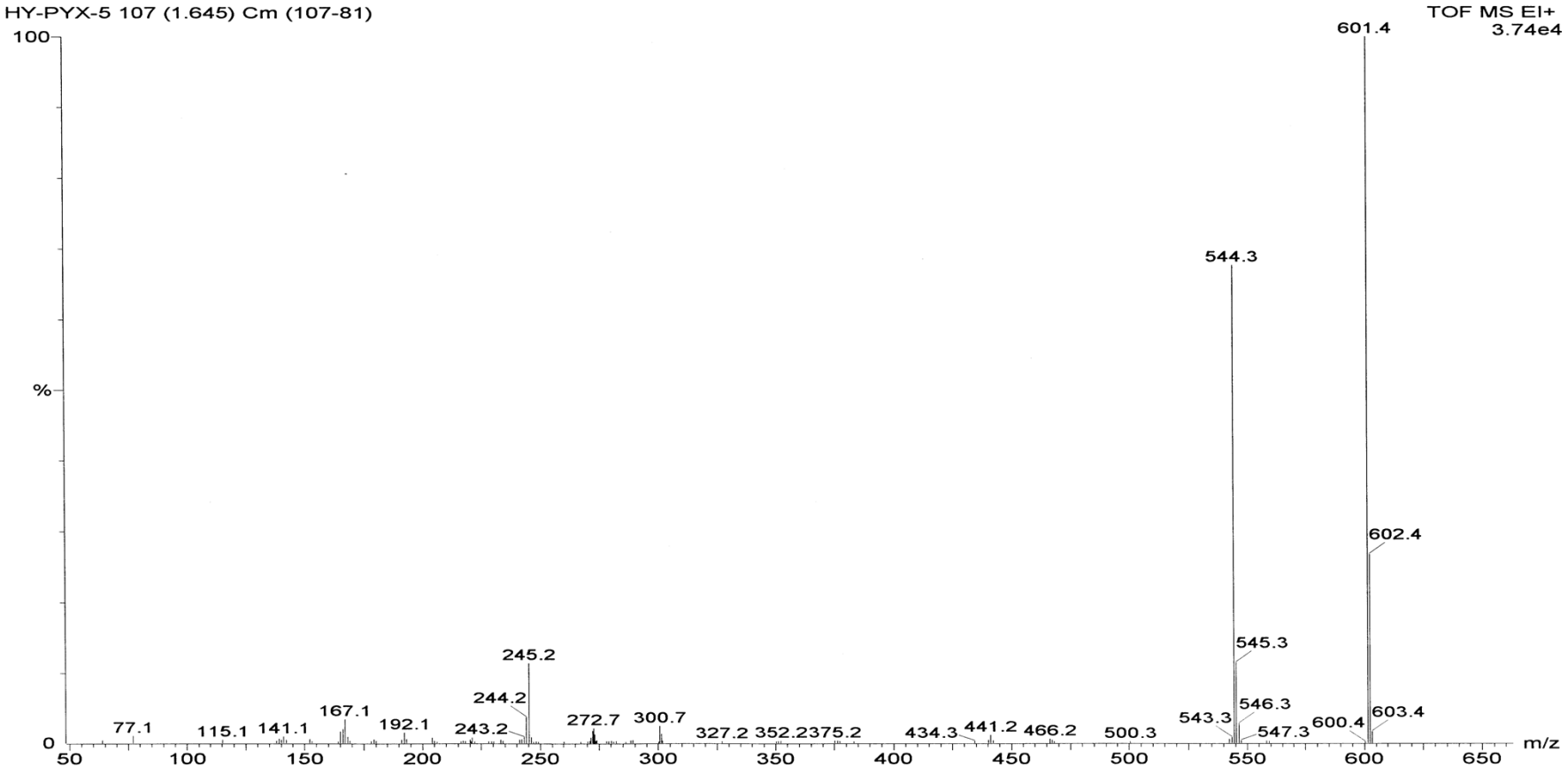
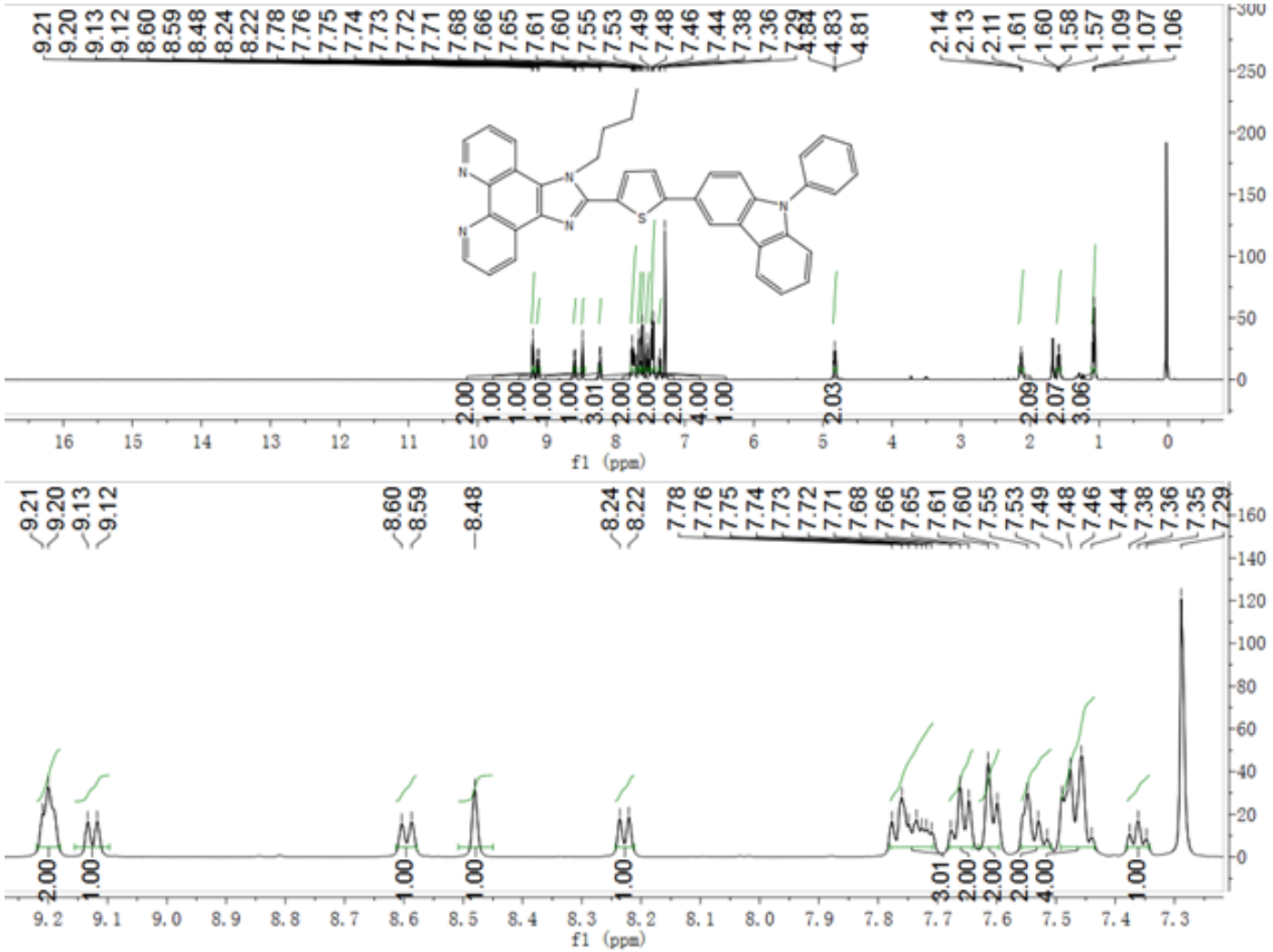
147.39
147.31
144.71
144.10
136.85
135.38
130.62
129.42
129.23
127.87
127.18
126.79
125.30
124.83
124.73
123.94
123.51
123.47
123.23
122.98
122.68
122.62
122.35
119.88
77.31
77.05
76.80
46.86
32.28
19.82
13.66
f1 (ppm)

b

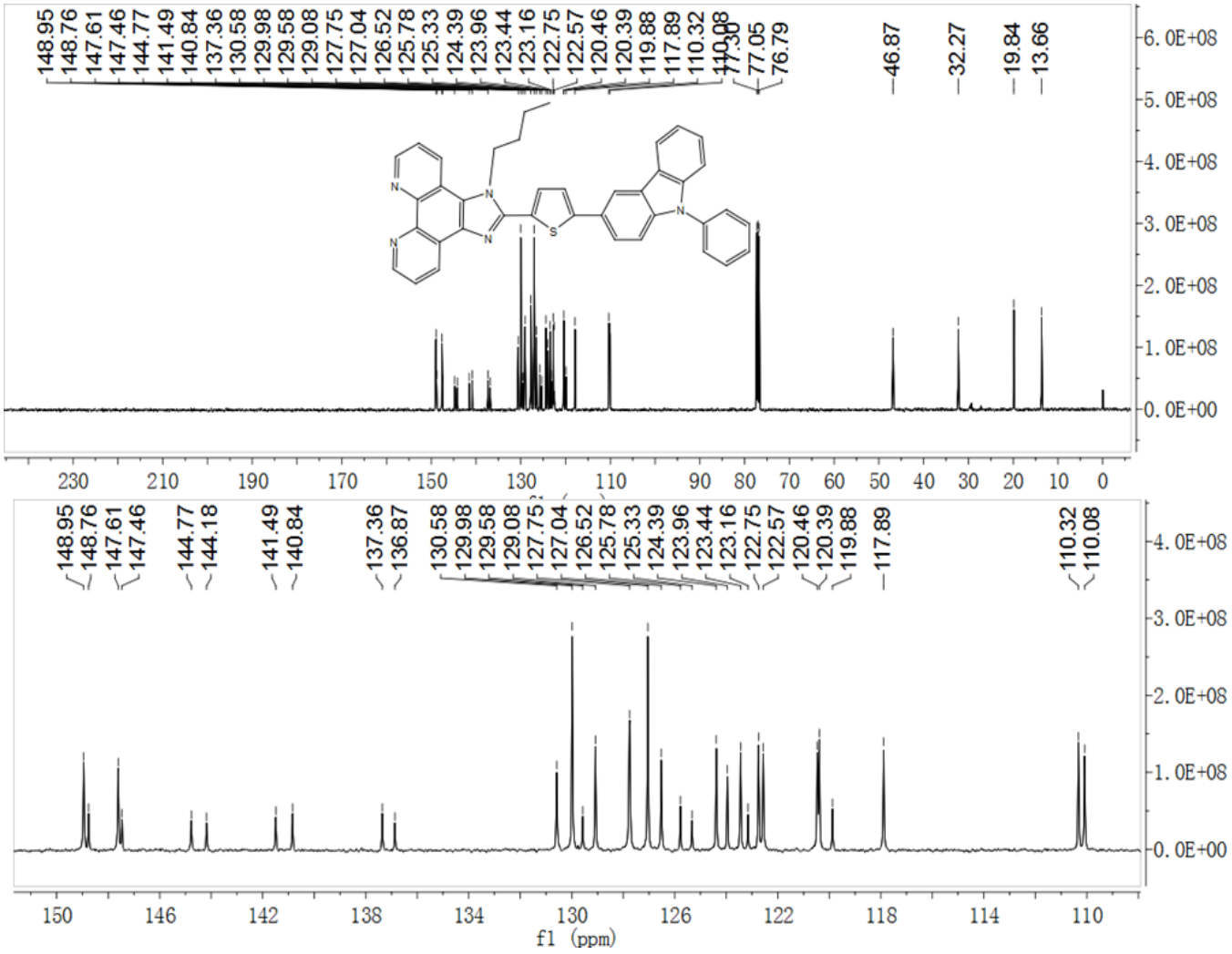


c

Fig. SI8. ^{1}H (**a**), ^{13}C NMR (**b**) and EI-TOF-MS (**c**) spectra of compound **8**.


9.21 9.20 9.13 9.12 8.60 8.59 8.48 8.24 8.22 7.78 7.76 7.75 7.74 7.73 7.72 7.71 7.68 7.66 7.65 7.61 7.60 7.55 7.53 7.49 7.48 7.46 7.44 7.38 7.36 7.29 4.84 4.83 4.81 2.14 2.13 2.11 1.61 1.60 1.58 1.57 1.09 1.07 1.06
2.00 1.00 1.00 1.00 1.00 3.01 2.00 2.00 2.00 4.00 1.00 2.03 2.09 2.07 3.06
f1 (ppm)
9.21 9.20 9.13 9.12 8.60 8.59 8.48 8.24 8.22 7.78 7.76 7.75 7.74 7.73 7.72 7.71 7.68 7.66 7.65 7.61 7.60 7.55 7.53 7.49 7.48 7.46 7.44 7.38 7.36 7.35 7.29
2.00 1.00 1.00 1.00 1.00 3.01 2.00 2.00 2.00 4.00 1.00
f1 (ppm)

a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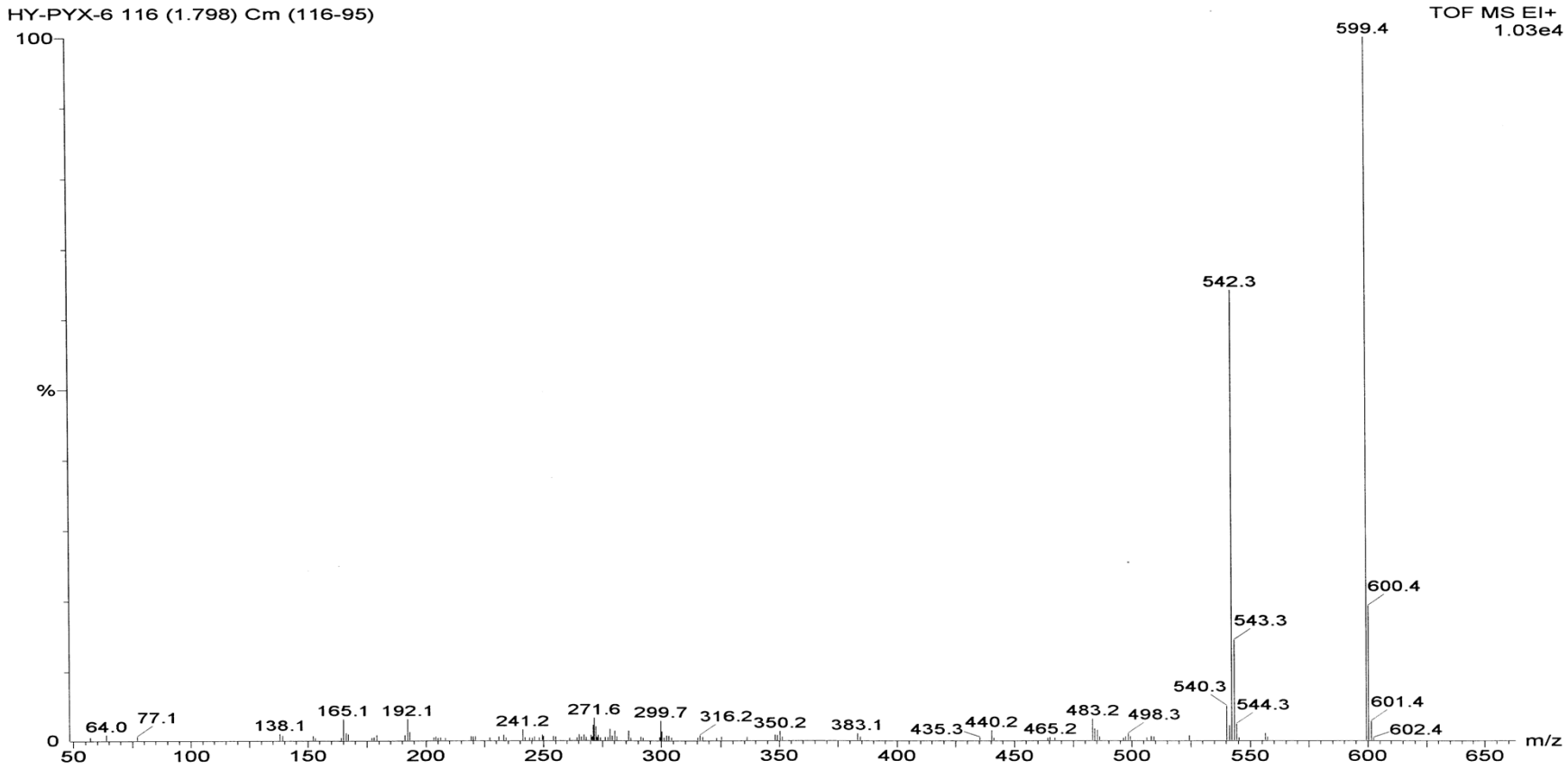
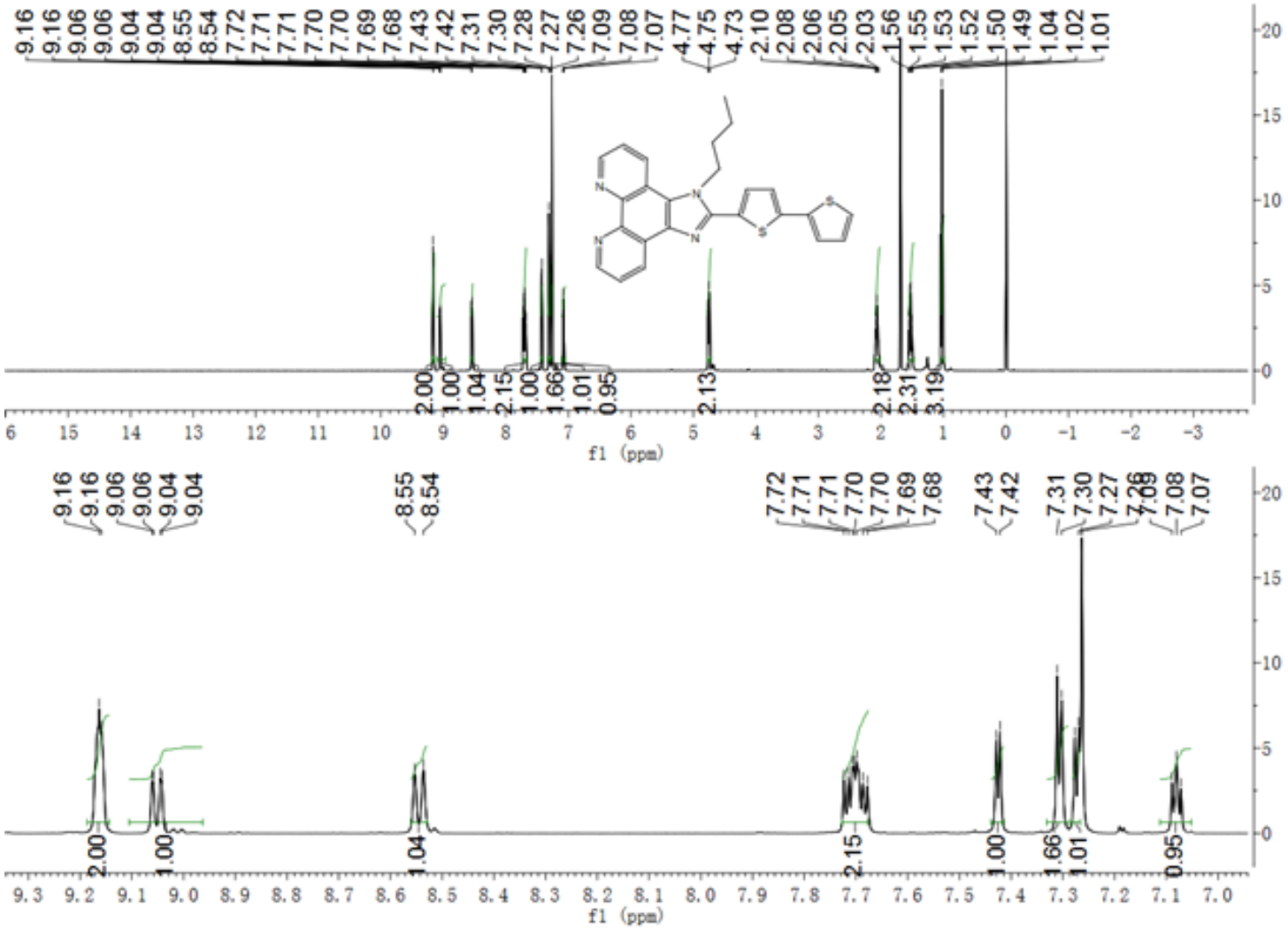
141.49
140.84
137.36
130.58
129.98
129.58
129.08
127.75
127.04
126.52
125.78
125.33
124.39
123.96
123.44
123.16
122.75
122.57
120.46
120.39
119.88
117.89
110.32
110.08
77.30
77.05
76.79
46.87
32.27
19.84
13.66
6.0E+08
5.0E+08
4.0E+08
3.0E+08
2.0E+08
1.0E+08
0.0E+00
230
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
148.95
148.76
147.61
147.46
144.77
144.18
141.49
140.84
137.36
136.87
130.58
129.98
129.58
129.08
127.75
127.04
126.52
125.78
125.33
124.39
123.96
123.44
123.16
122.75
122.57
120.46
120.39
119.88
117.89
110.32
110.08
4.0E+08
3.0E+08
2.0E+08
1.0E+08
0.0E+00
150
146
142
138
134
130
126
122
118
114
110
f1 (ppm)

b

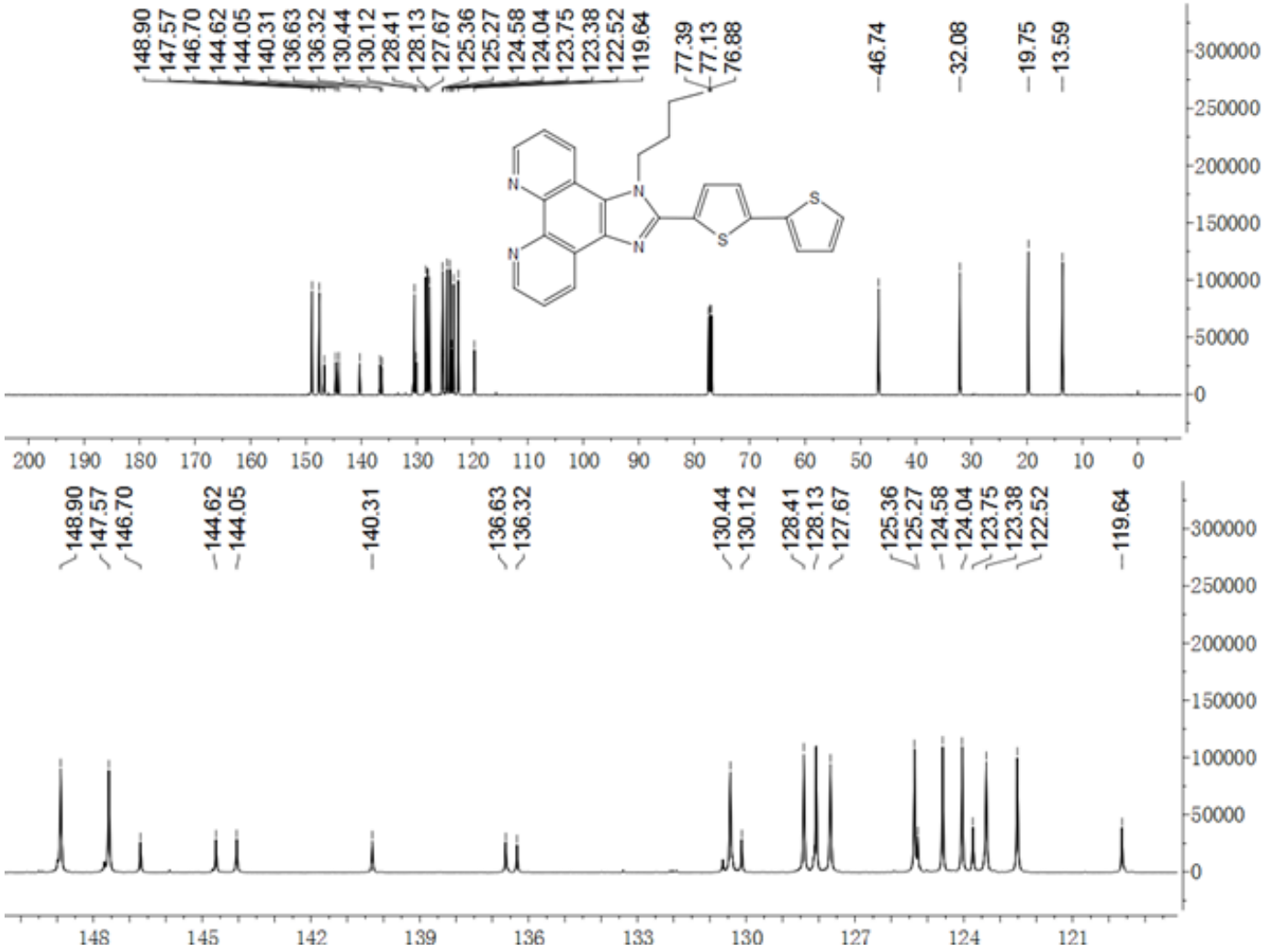


c

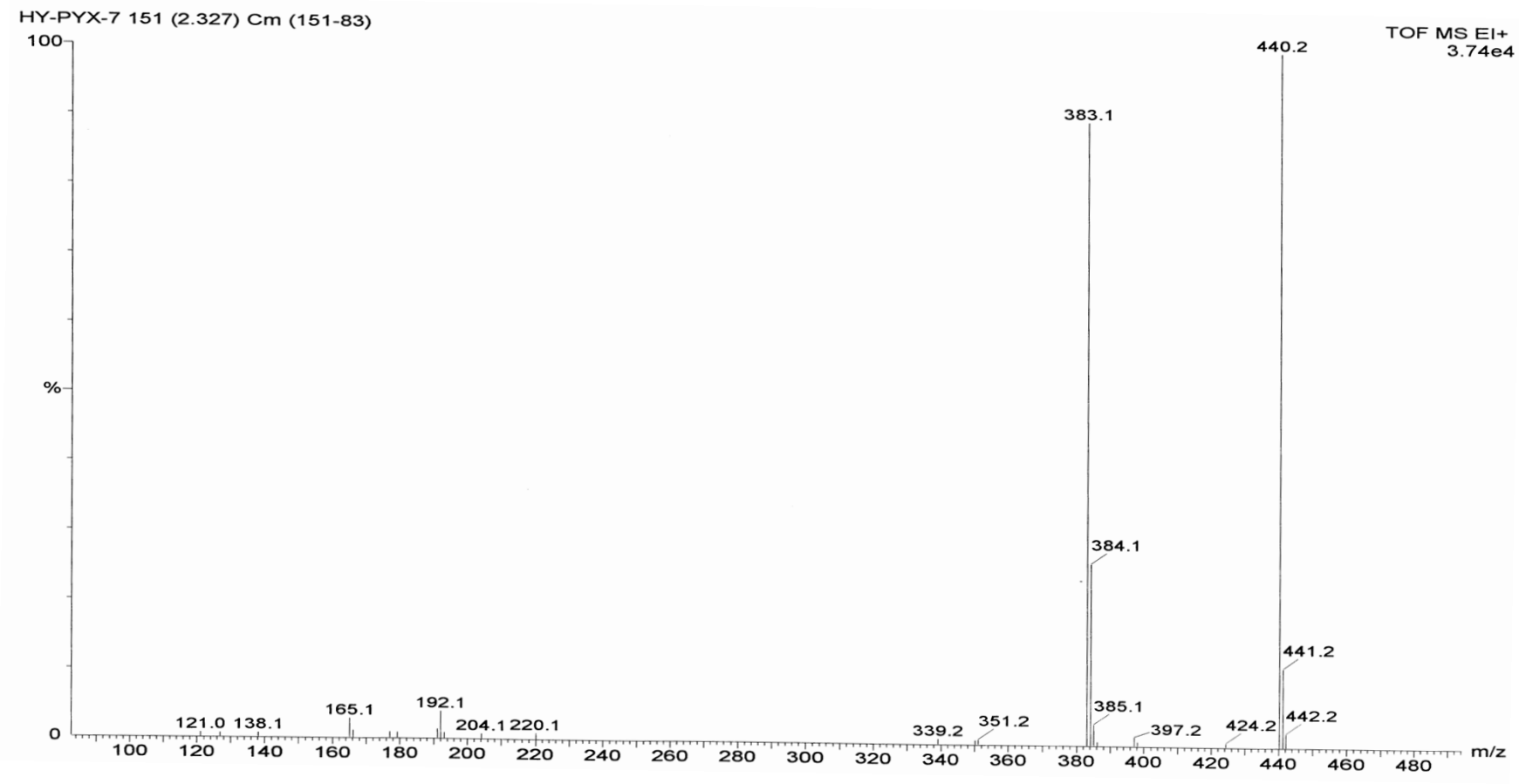
Fig. SI9. ^{1}H (**a**), ^{13}C NMR (**b**) and EI-TOF-MS (**c**) spectra of compound **9**.



a

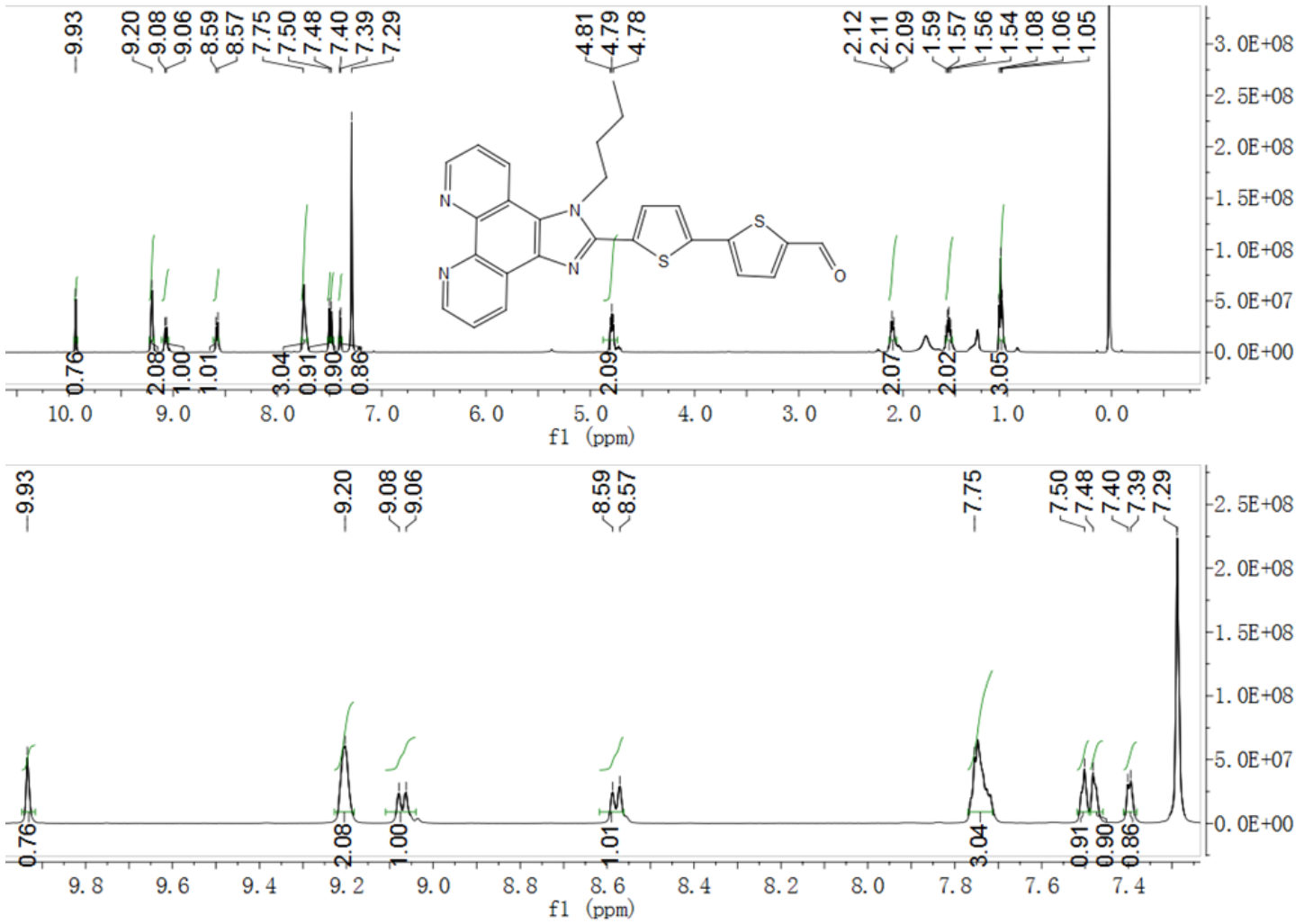

148.90
147.57
146.70
144.62
144.05
140.31
136.63
136.32
130.44
130.12
128.41
128.13
127.67
125.36
125.27
124.58
124.04
123.75
123.38
122.52
119.64
77.39
77.13
76.88
46.74
32.08
19.75
13.59
N
N
N
S
S
300000
250000
200000
150000
100000
50000
0
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
148 145 142 139 136 133 130 127 124 121

b

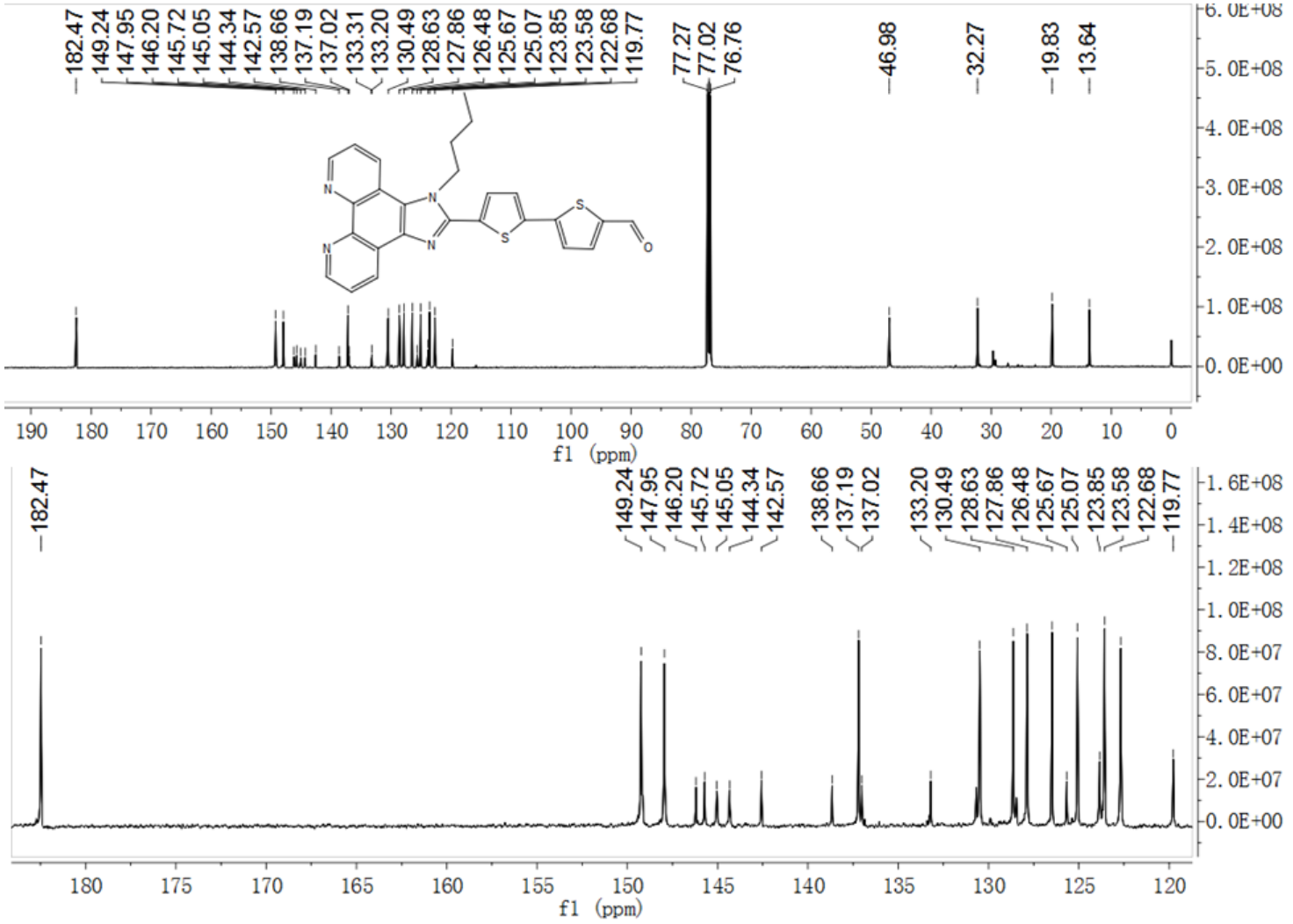


c

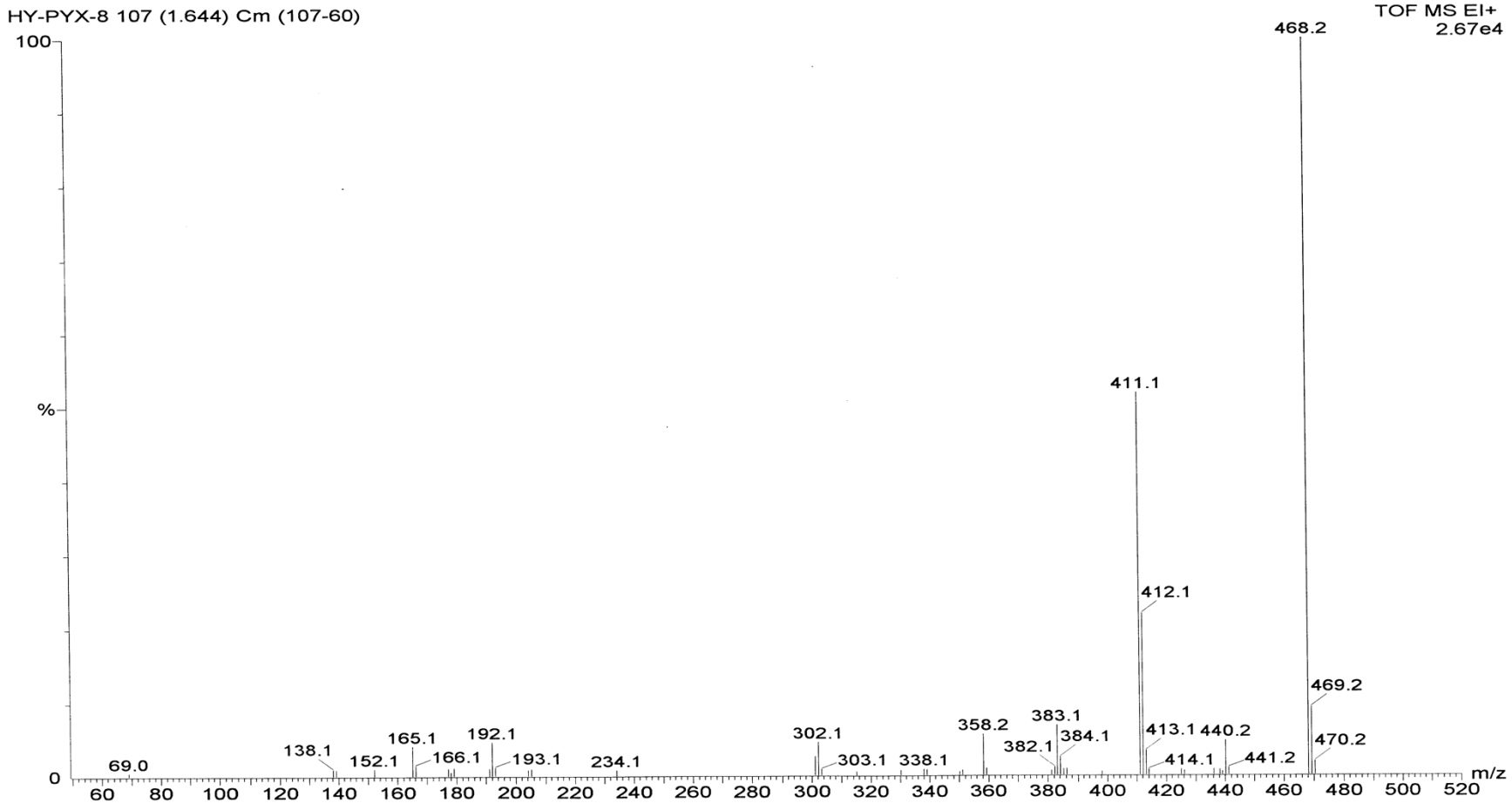
Fig. SI10. ^{1}H (**a**), ^{13}C NMR (**b**) and EI-TOF-MS (**c**) spectra of compound **10**.


9.93
9.20
9.08
9.06
8.59
8.57
7.75
7.50
7.48
7.40
7.39
7.29
4.81
4.79
4.78
2.12
2.11
2.09
1.59
1.57
1.56
1.54
1.08
1.06
1.05
0.76
2.08
1.00
1.01
3.04
0.91
0.90
0.86
2.09
2.07
2.02
3.05
f1 (ppm)
9.93
9.20
9.08
9.06
8.59
8.57
7.75
7.50
7.48
7.40
7.39
7.29
0.76
2.08
1.00
1.01
3.04
0.91
0.90
0.86
f1 (ppm)

a

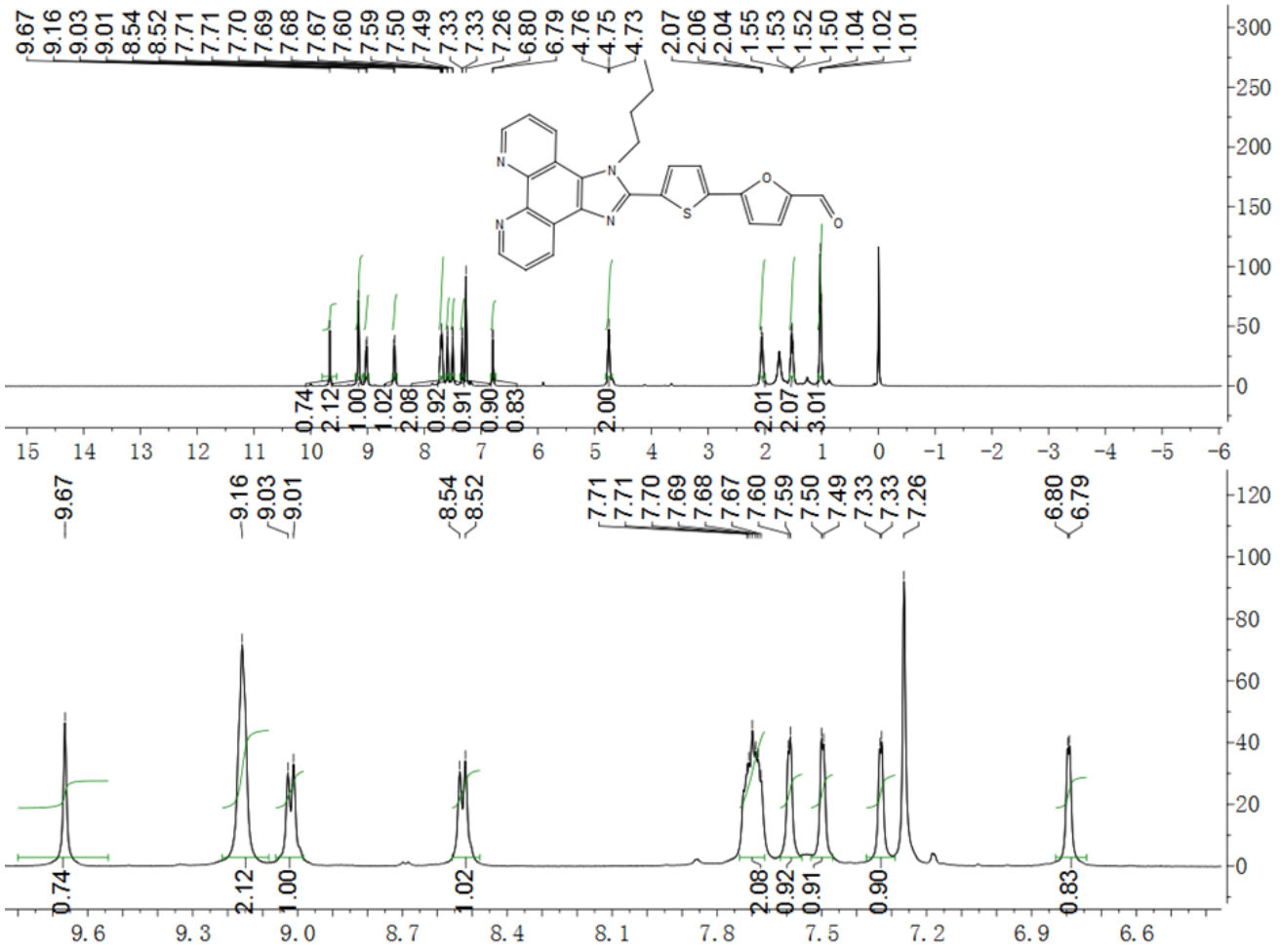

182.47
149.24
147.95
146.20
145.72
145.05
144.34
142.57
138.66
137.19
137.02
133.31
133.20
130.49
128.63
127.86
126.48
125.67
125.07
123.85
123.58
122.68
119.77
77.27
77.02
76.76
46.98
32.27
19.83
13.64
f1 (ppm)

b

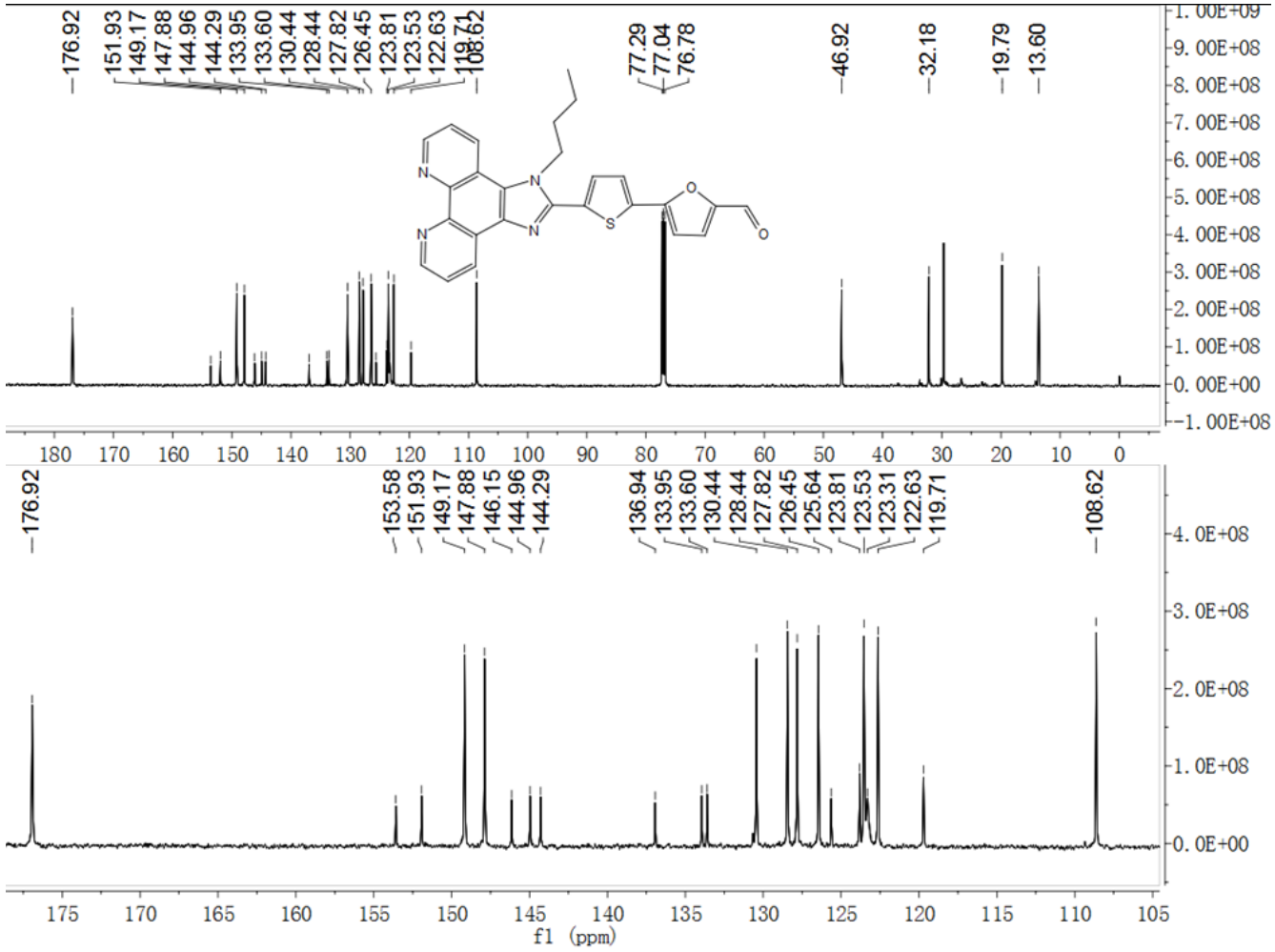


c

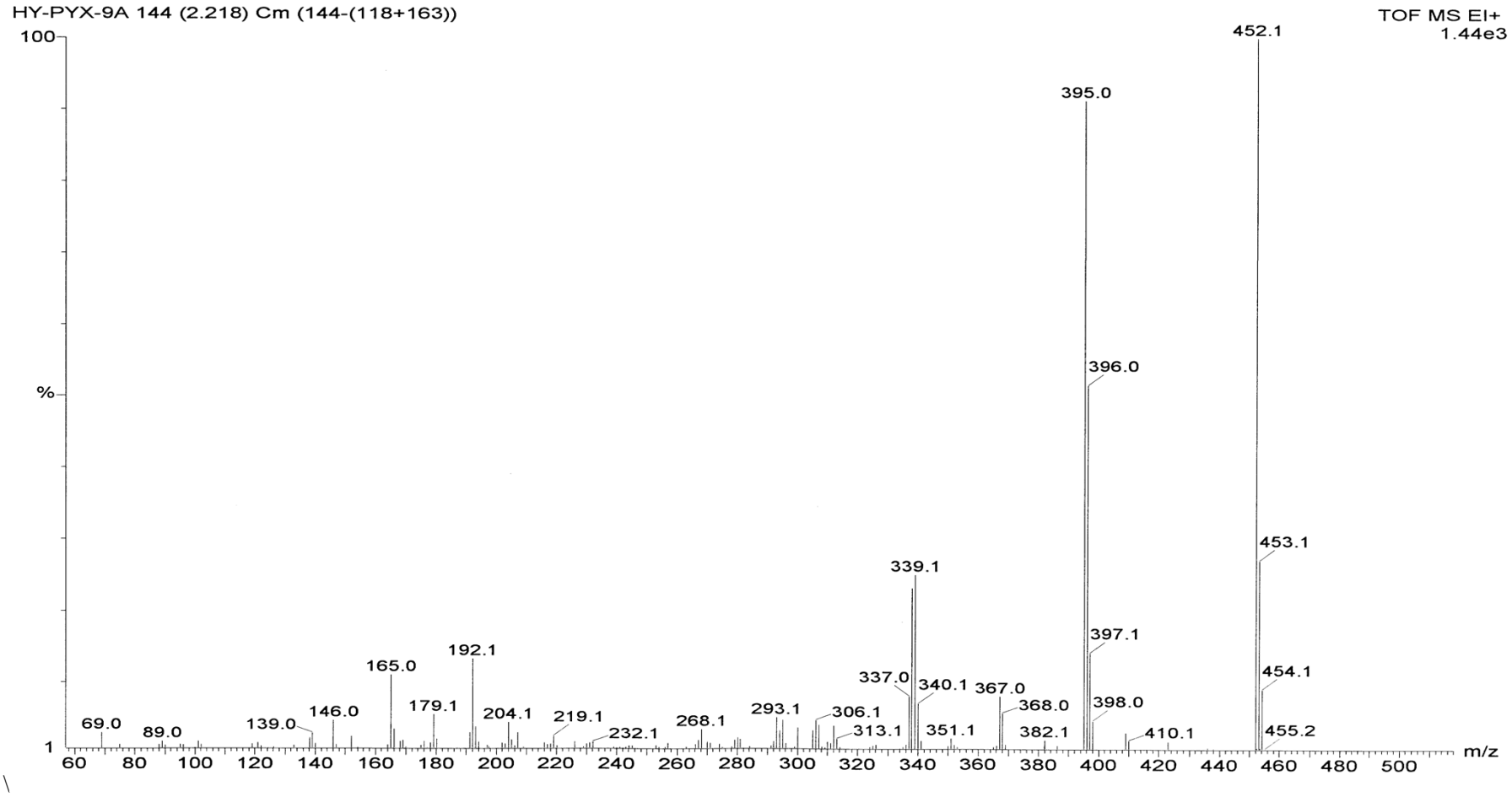
Fig. SI11. ^{1}H (**a**), ^{13}C NMR (**b**) and EI-TOF-MS (**c**) spectra of compound **11**.


9.67
9.16
9.03
9.01
8.54
8.52
7.71
7.71
7.70
7.69
7.68
7.67
7.60
7.59
7.50
7.49
7.33
7.33
7.26
6.80
6.79
4.76
4.75
4.73
2.07
2.06
2.04
1.55
1.53
1.52
1.50
1.04
1.02
1.01
0.74
2.12
1.00
1.02
2.08
0.92
0.91
0.90
0.83
2.00
2.01
2.07
3.01
N
N
N
S
O
O

a

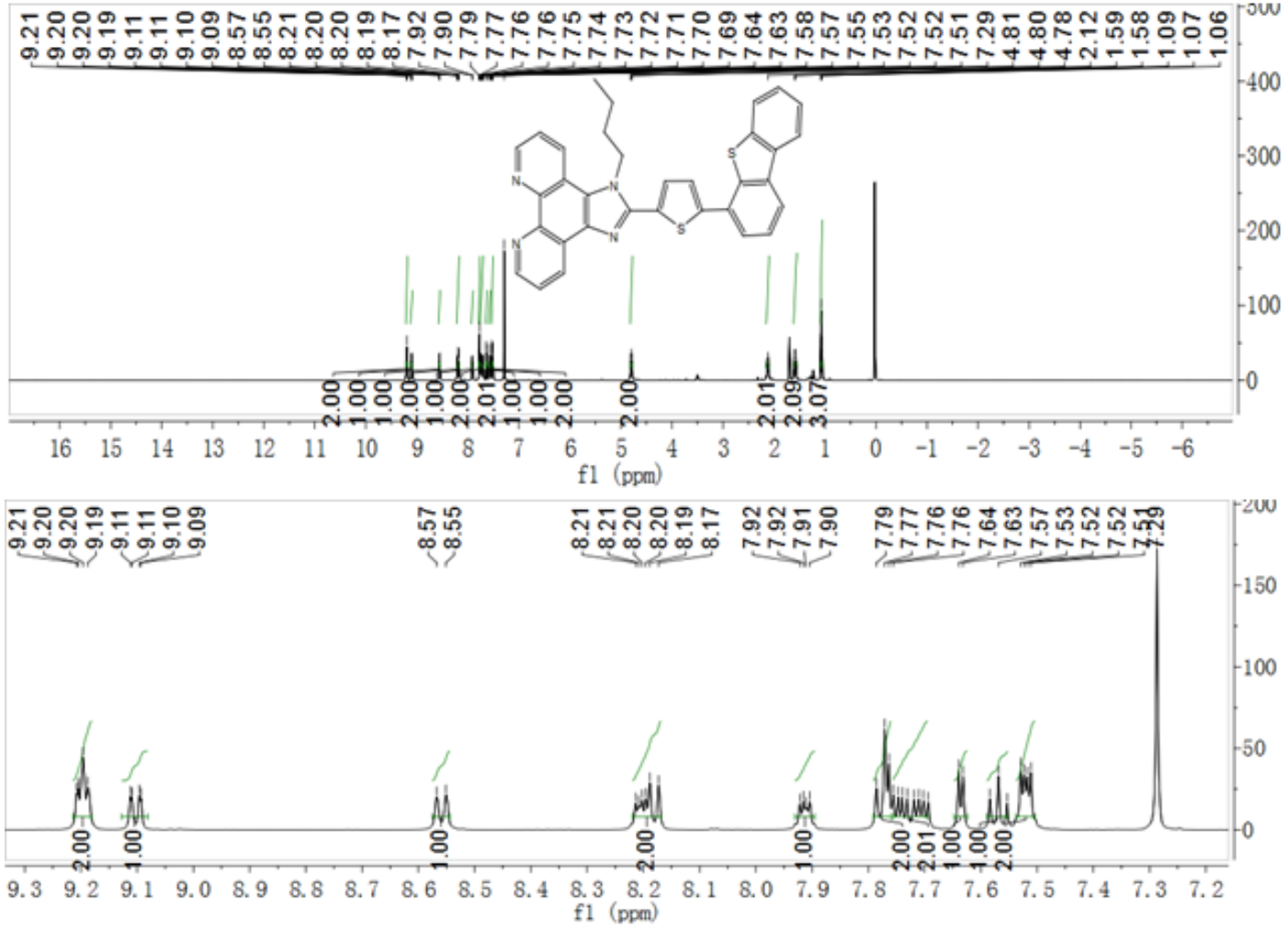

176.92
151.93
149.17
147.88
144.96
144.29
133.95
133.60
130.44
128.44
127.82
126.45
123.81
123.53
122.63
119.71
108.62
77.29
77.04
76.78
46.92
32.18
19.79
13.60
153.58
151.93
149.17
147.88
146.15
144.96
144.29
136.94
133.95
133.60
130.44
128.44
127.82
126.45
125.64
123.81
123.53
123.31
122.63
119.71
108.62
f1 (ppm)

b

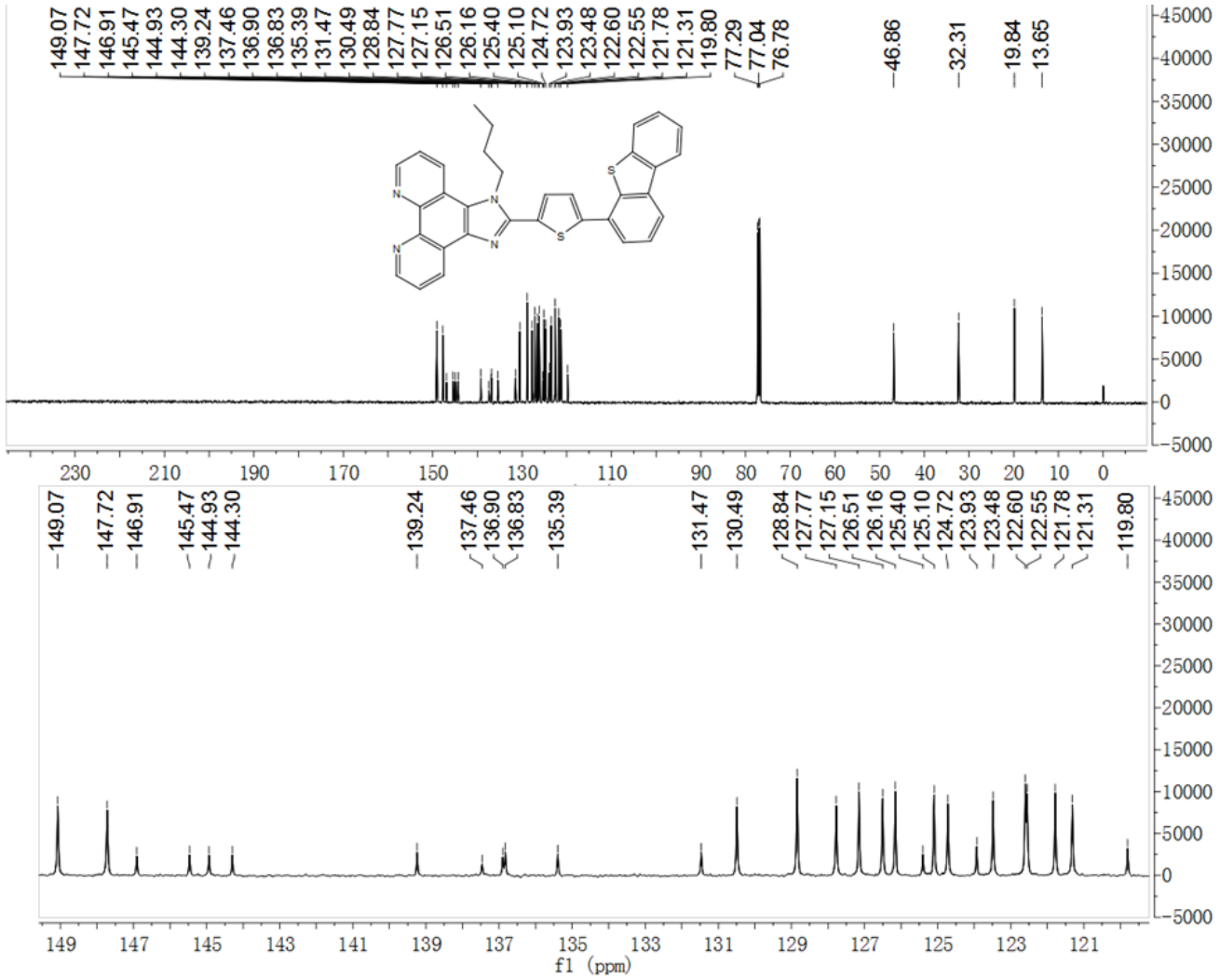


c

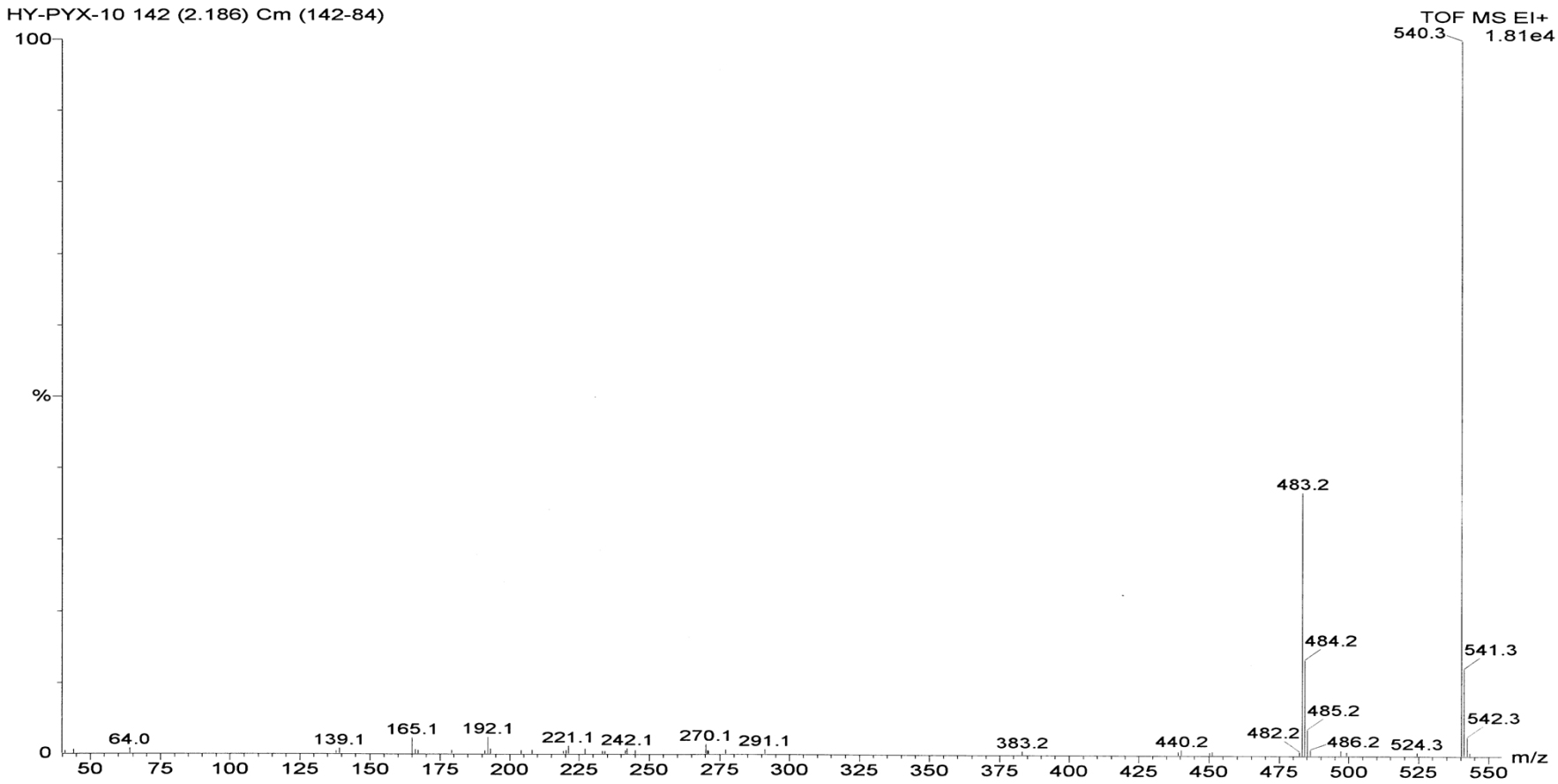
Fig. SI12. ^{1}H (**a**), ^{13}C NMR (**b**) and EI-TOF-MS (**c**) spectra of compound **12**.



a


149.07
147.72
146.91
145.47
144.93
144.30
139.24
137.46
136.90
136.83
135.39
131.47
130.49
128.84
127.77
127.15
126.51
126.16
125.40
125.10
124.72
123.93
123.48
122.60
122.55
121.78
121.31
119.80
77.29
77.04
76.78
46.86
32.31
19.84
13.65
f1 (ppm)

b



c

Fig. SI13. ^{1}H (**a**), ^{13}C NMR (**b**) and EI-TOF-MS (**c**) spectra of compound **13**.

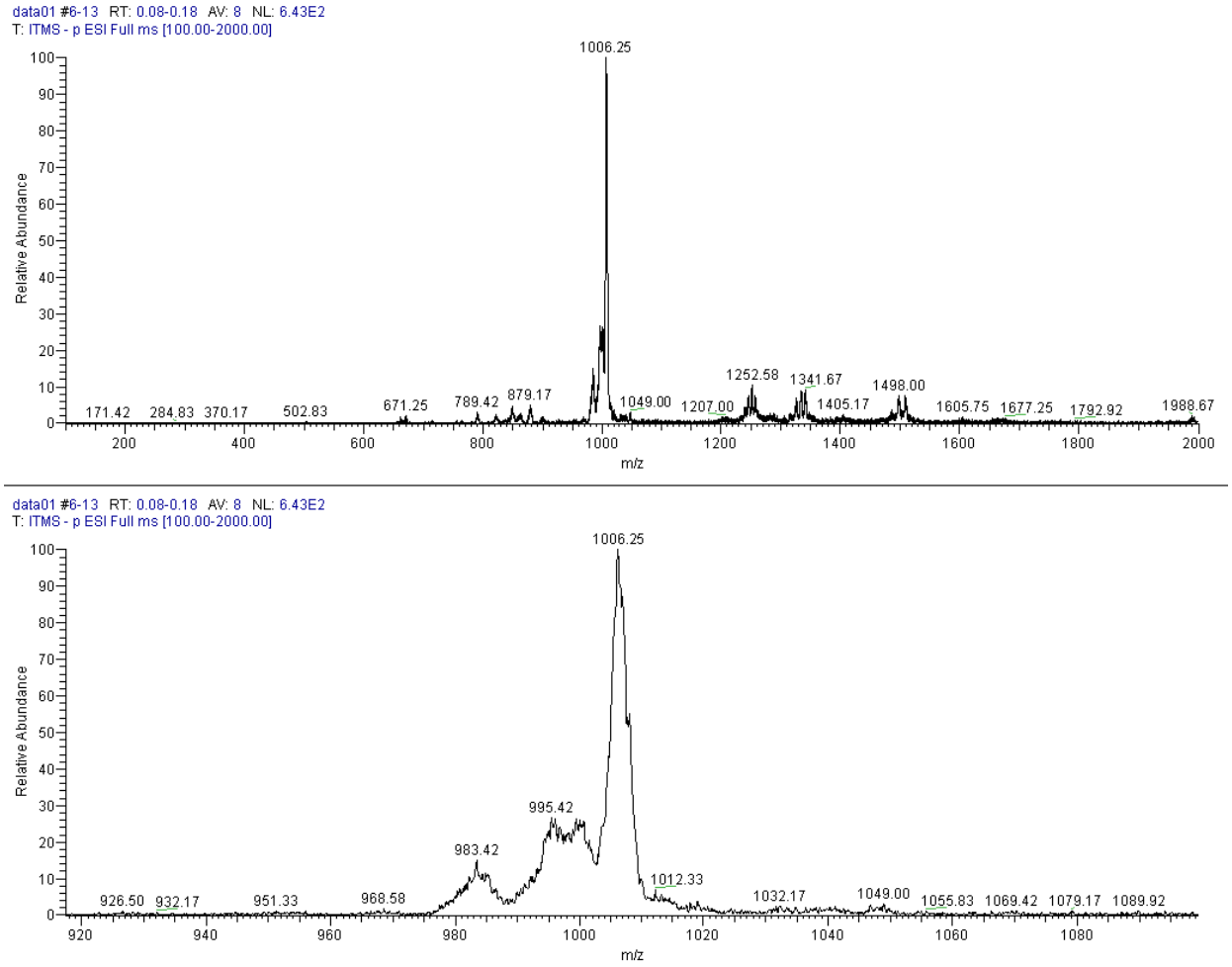


Fig. SI14. ESI-MS spectrum of compound **BM3**.

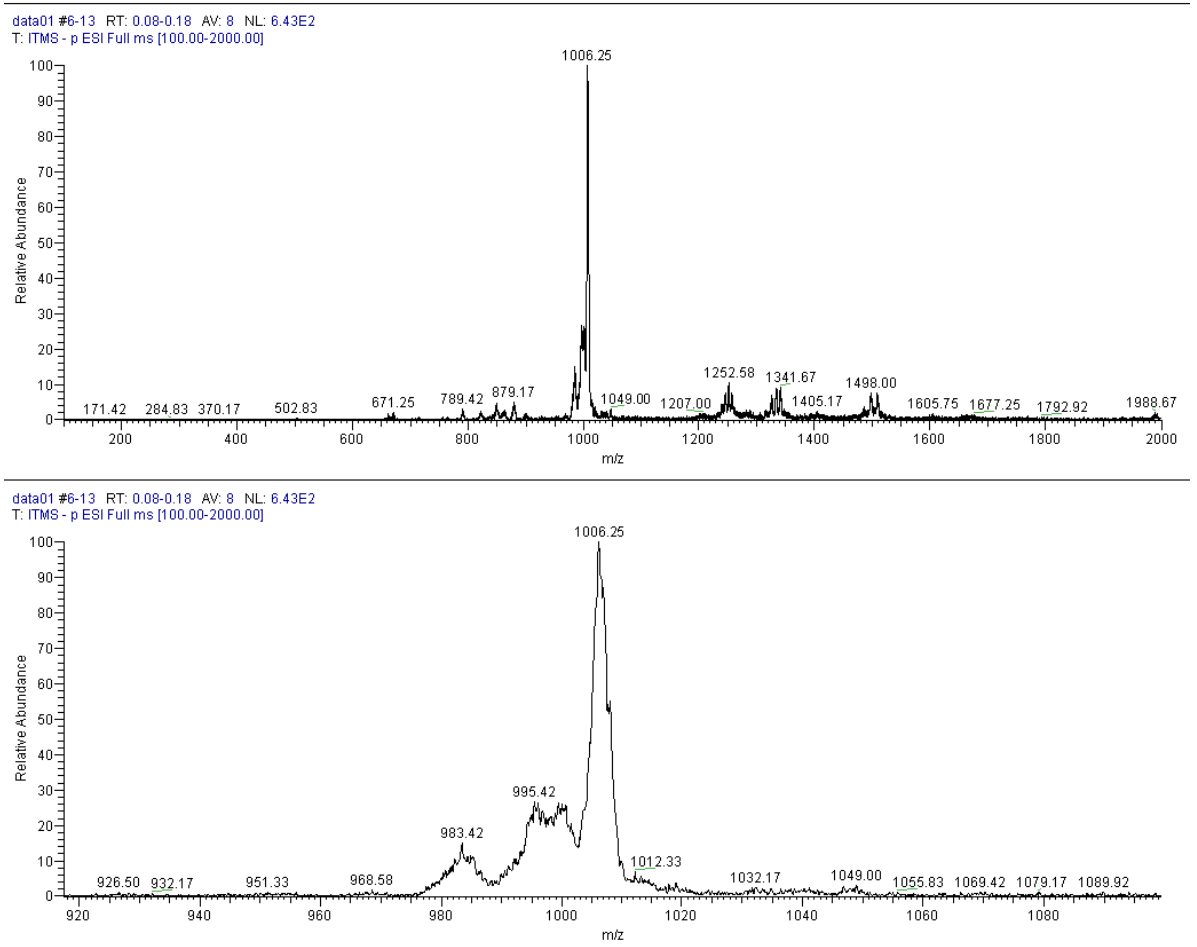


Fig. SI15. ESI-MS spectrum of compound **BM4**.

Table SI1. Selected bond lengths [Å] and bond angles [°] for compounds **3-13**.

Bond distances		Bond angles	
3·$CHCl_3$			
N1–C1	1.323(5)	C1–N1–C12	117.8(2)
N1–C12	1.354(4)	C10–N2–C11	117.3(3)
N2–C10	1.322(6)	C5–N3–C13	105.9(2)
N2–C11	1.349(4)	C6–N4–C13	104.3(3)
N3–C18	1.458(4)	S1–C17–C16	113.0(4)
N3–C5	1.385(3)	S1–C14–C15	110.8(3)
N3–C13	1.378(4)		
N4–C6	1.381(4)		
N4–C13	1.322(4)		
N4–C13	1.322(4)		
S1–C17	1.708(5)		
S1–C14	1.716(4)		
4			
N1–C1	1.321(3)	C1–N1–C12	118.1(2)
N1–C12	1.356(2)	C10–N2–C11	118.3(2)
N2–C10	1.320(3)	C13–N3–C5	105.9(2)
N2–C11	1.351(2)	C5–N3–C18	127.93(2)

N3–C5	1.387(2)	C5–N3–C18	127.93(2)
N3–C13	1.375(2)	C13–N4–C6	104.56(2)
N3–C18	1.460(2)	C17–S1–C14	91.7(1)
N4–C6	1.372(2)		
N4–C13	1.319(2)		
S1–C14	1.710(2)		
S1–C17	1.702(3)		
5·$CHCl_3$			
Br1–C17	1.864(5)	C1–N1–C12	117.1(4)
N1–C1	1.326(6)	C10–N2–C11	118.4(4)
N1–C12	1.373(5)	C13–N3–C6	106.2(3)
N2–C10	1.318(6)	C13–N3–C18	126.2(3)
N2–C11	1.340(6)	C6–N3–C18	127.4(4)
N3–C6	1.393(5)	C13–N4–C5	104.9(4)
N3–C13	1.362(6)	C14–S1–C17	91.1(2)
N3–C18	1.467(5)	C16–C17–Br1	127.7(3)
N4–C5	1.361(5)	S1–C17–Br1	119.7(3)
N4–C13	1.325(5)		
S1–C14	1.722(5)		
S1–C17	1.722(4)		

6·H_2O			
N1–C1	1.323(4)	C1–N1–C12	117.5(3)
N1–C12	1.357(3)	C10–N2–C11	117.5(3)
N2–C10	1.323(4)	C13–N3–C5	106.8(2)
N2–C11	1.357(3)	C13–N3–C14	126.0(2)
N3–C5	1.386(3)	C5–N3–C14	127.1(2)
N3–C13	1.374(3)	C13–N4–C6	105.0(2)
N3–C14	1.476(3)	C24–N5–C25	115.1(3)
N4–C6	1.371(3)	C18–S1–C21	92.6(1)
N4–C13	1.327(3)		
N5–C24	1.322(4)		
N5–C25	1.335(4)		
S1–C18	1.725(3)		
S1–C21	1.727(3)		
(**7**)$_2$·C_2H_5OH·$(CHCl_3)_2$			
N1–C1	1.307(6)	C1–N1–C12	118.9(4)
N1–C12	1.342(6)	C10–N2–C11	117.3(4)
N2–C10	1.324(6)	C5–N3–C13	106.4(4)
N2–C11	1.354(5)	C5–N3–C14	128.2(4)
N3–C5	1.376(5)	C13–N3–C14	124.7(4)

N3–C13	1.386(6)	C13–N4–C6	118.3(2)104.4(4)
N3–C14	1.484(6)	C28–O2–C29	118.2(5)
N4–C6	1.372(5)	C21–S1–C18	92.9(2)
N4–C13	1.330(5)		
O1–C28	1.193(6)		
O2–C28	1.341(6)		
O2–C29	1.448(6)		
S1–C18	1.718(5)		
S1–C21	1.708(4)		
8·$CHCl_3$			
N1–C1	1.316(6)	C1–N1–C12	118.0(4)
N1–C12	1.344(5)	C10–N2–C11	117.0(4)
N2–C10	1.327(6)	C13–N3–C5	106.5(3)
N2–C11	1.349(5)	C13–N3–C14	125.0(4)
N3–C5	1.393(5)	C5–N3–C14	127.1(3)
N3–C13	1.369(5)	C13–N4–C6	104.8(3)
N3–C14	1.507(5)	C34–N5–C25	117.9(3)
N4–C6	1.374(5)	C34–N5–C28	119.0(3)
N4–C13	1.324(5)	C25–N5–C28	120.0(3)
N5–C25	1.419(5)	C18–S1–C21	93.3(2)

N5–C28	1.420(5)		
N5–C34	1.418(5)		
S1–C18	1.719(4)		
S1– C21	1.728(4)		
9·$CHCl_3$			
N1–C1	1.310(3)	C1–N1–C12	117.4(2)
N1–C12	1.356(3)	C10–N2–C11	118.1(2)
N2–C10	1.310(3)	C13–N3–C6	105.9(2)
N2–C11	1.351(3)	C13–N3–C36	126.4(2)
N3–C6	1.392(3)	C6–N3–C36	127.5(2)
N3–C13	1.376(3)	C13–N4–C5	104.6(2)
N3–C36	1.456(3)	C21–N5–C25	108.2(2)
N4–C5	1.366(3)	C21–N5–C30	126.3(2)
N4–C13	1.310(3)	C25–N5–C30	125.4(2)
N5–C21	1.393(3)	C14–S1–C17	92.9(1)
N5–C25	1.399(3)		
N5–C30	1.422(3)		
S1–C14	1.715(2)		
S1–C17	1.716(3)		
10			

N1–C1	1.312(5)	C1–N1–C12	117.2(3)
N1–C12	1.361(4)	C10–N2–C11	118.0(3)
N2–C10	1.314(5)	C13–N3–C5	106.3(3)
N2–C11	1.341(5)	C13–N3–C22	125.3(3)
N3–C5	1.374(4)	C5–N3–C22	128.1(3)
N3–C13	1.371(4)	C13–N4–C6	104.9(3)
N3–C22	1.481(4)	C17–S1–C14	92.7(2)
N4–C6	1.353(4)	C18–S2–C21	93.2(2)
N4–C13	1.320(4)		
S1–C14	1.729(4)		
S1–C17	1.710(4)		
S2–C18	1.682(4)		
S2–C21	1.687(4)		
10·$CHCl_3$			
S1–C17	1.716(5)	C14–S1–C17	92.8(2)
S1–C14	1.726(5)	C18–S1'–C20	94.4(8)
S1'–C18	1.685(18)	C18–S2–C21	94.0(4)
S1'–C20	1.582(18)	C1–N1–C12	118.0(4)
S2–C18	1.684(8)	C10–N2–C11	117.0(4)
S2–C21	1.624(9)	C5–N3–C22	126.3(4)

N1–C12	1.360(6)	C13–N3–C22	126.6(4)
N1–C1	1.318(6)	C5–N3–C13	106.3(3)
N2–C11	1.355(5)	C6–N4–C13	104.7(4)
N2–C10	1.310(7)		
N3–C22	1.522(6)		
N3–C5	1.384(5)		
N3–C13	1.367(6)		
N4–C6	1.372(6)		
N4–C13	1.319(5)		
11·$CHCl_3$			
N1–C1	1.319(5)	C10–N2–C11	117.1(4)
N1–C12	1.360(5)	C13–N3–C5	106.3(3)
N2–C10	1.310(5)	C13–N3–C22	126.6(3)
N2–C11	1.355(5)	C5–N3–C22	126.4(4)
N3–C5	1.384(5)	C13–N4–C6	104.7(3)
N3–C13	1.367(5)	C17–S1–C14	92.8(2)
N3–C22	1.522(5)	C21–S2–C18	94.0(4)
N4–C6	1.372(5)	C20–S1'–C18	94.4(6)
N4–C13	1.319(5)		
S1–C14	1.726(4)		

S1–C17	1.716(4)		
S1'–C18	1.685(2)		
S1'–C20	1.582(1)		
S2–C18	1.684(7)		
S2–C21	1.624(9)		
12			
N1–C1	1.321(6)	C1–N1–C12	118.5(5)
N1–C12	1.343(6)	C10–N2–C1	1117.5(5)
N2–C10	1.319(7)	C5–N3–C13	105.6(4)
N2–C11	1.365(6)	C5–N3–C23	126.5(4)
N3–C5	1.379(6)	C1–N3–C23	126.9(4)
N3–C13	1.384(6)	C1–N4–C6	104.7(4)
N3–C23	1.480(6)	C21–O1–C18	91.6(4)
N4– C6	1.371(6)	C14–S1–C17	92.3(3)
N4–C13	1.310(6)		
O1–C18	1.495(7)		
O1–C21	1.451(7)		
O2–C22	1.268(11)		
13·$CHCl_3$			
N1–C1	1.325(4)	C1–N1–C12	117.2(2)

N1– C12	1.352(3)	C10–N2–C11	118.0(2)
N2 –C10	1.318(4)	C1–N3–C5	104.9(2)
N2–C11	1.356(3)	C13–N4–C6	105.8(2)
N –C5	1.360(3)	C13–N4–C30	125.5(2)
N3–C13	1.315(3)	C6–N4–C30	128.3(2)
N4–C6	1.384(3)	C14–S1–C17	92.6(1)
N4–C13	1.377(3)	C28–S2–C29	91.6(1)
N4 –C30	1.467(3)		
S1–C14	1.725(2)		
S1– C17	1.731(3)		
S2–C28	1.744(3)		
S2–C29	1.749(3)		

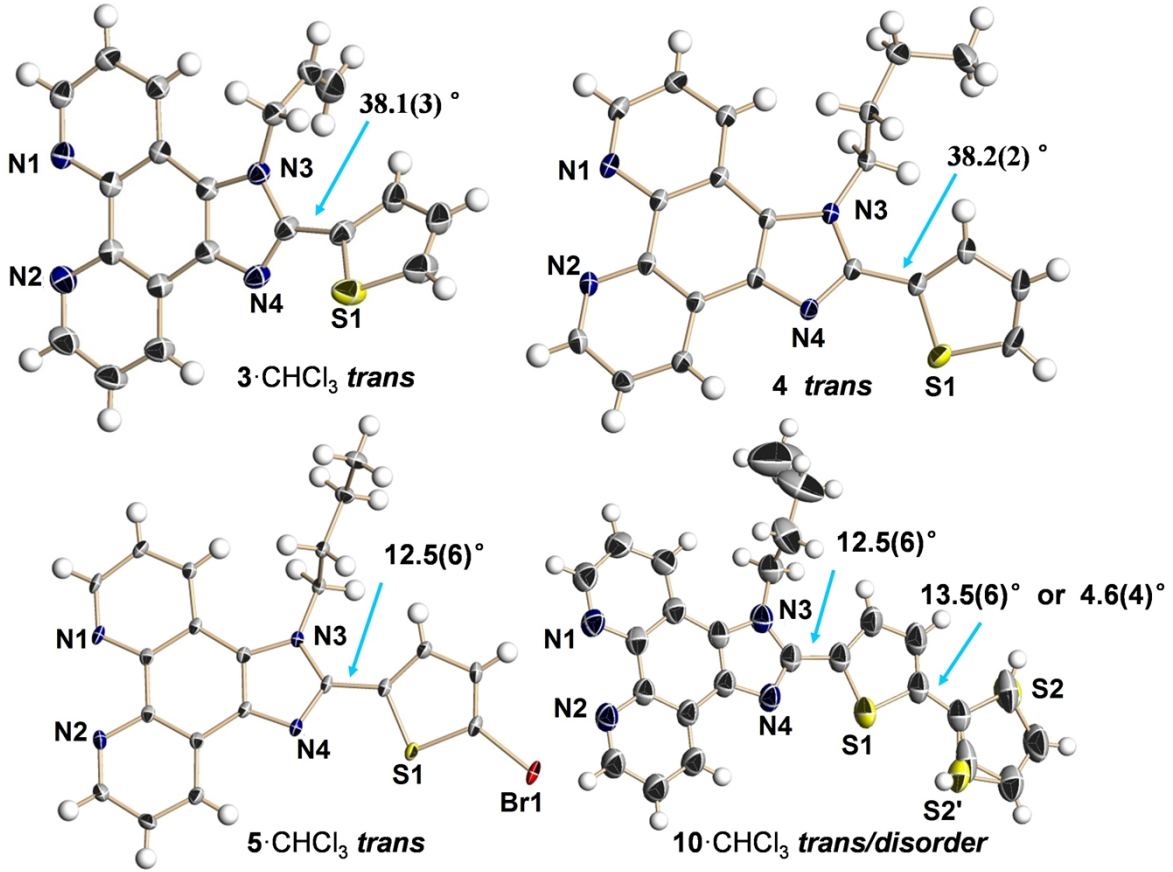
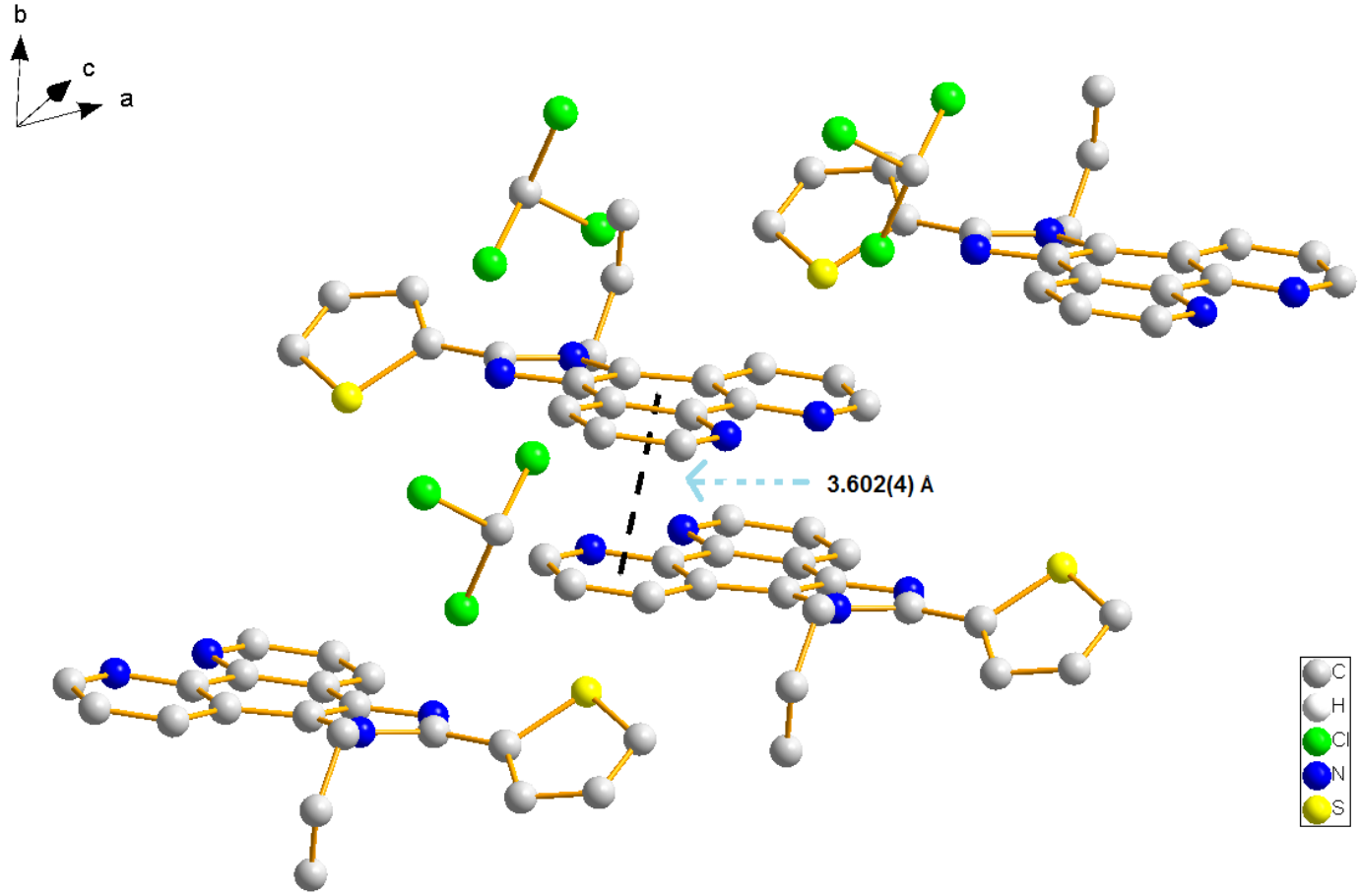
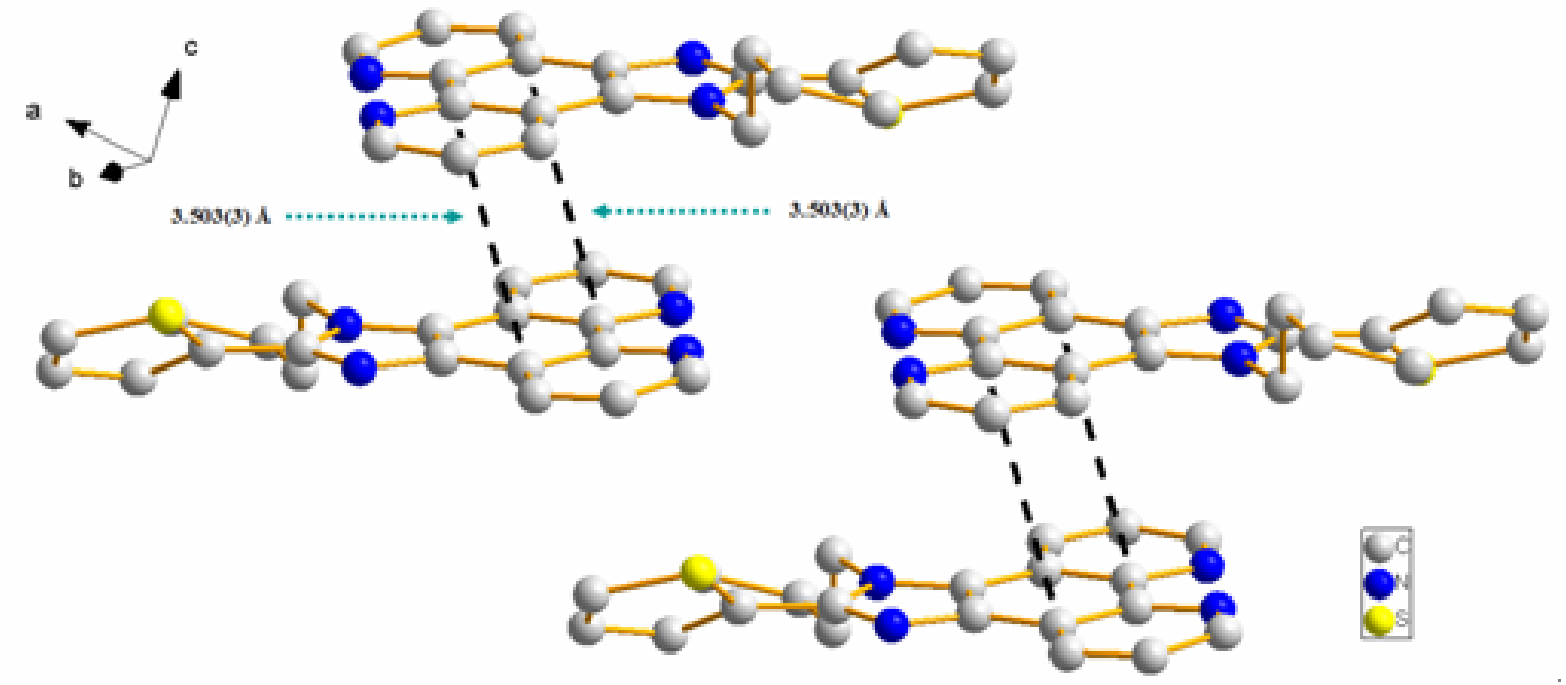


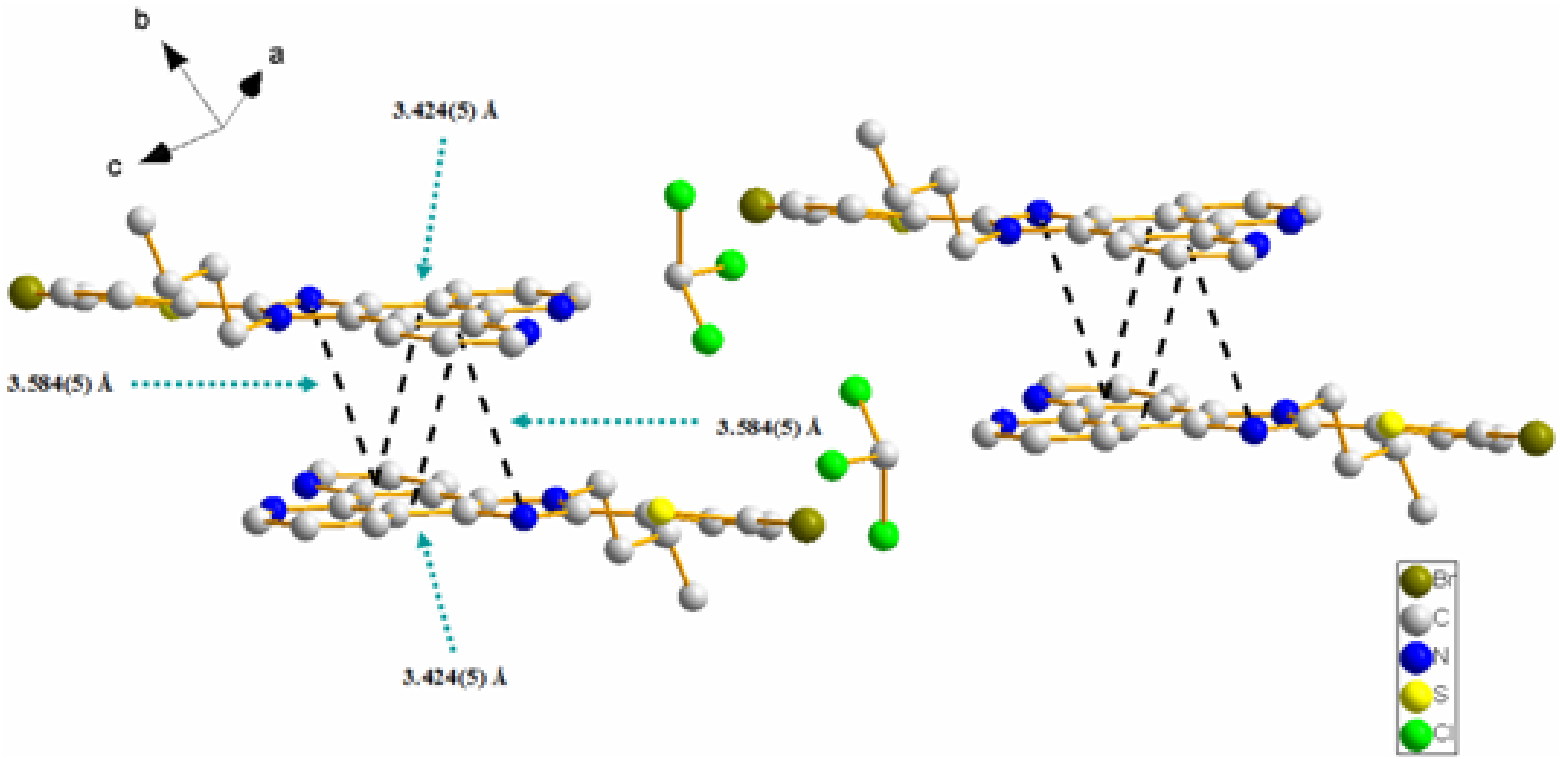
Fig. SI16. ORTEP diagrams (30 % thermal probability ellipsoids) of the molecular structures of **3**·$CHCl_3$, **4**, **5**·$CHCl_3$ and **10**·$CHCl_3$ showing the dihedral angles and relative configurations between adjacent aromatic heterocycles. All the solvent molecules are omitted for clarity.



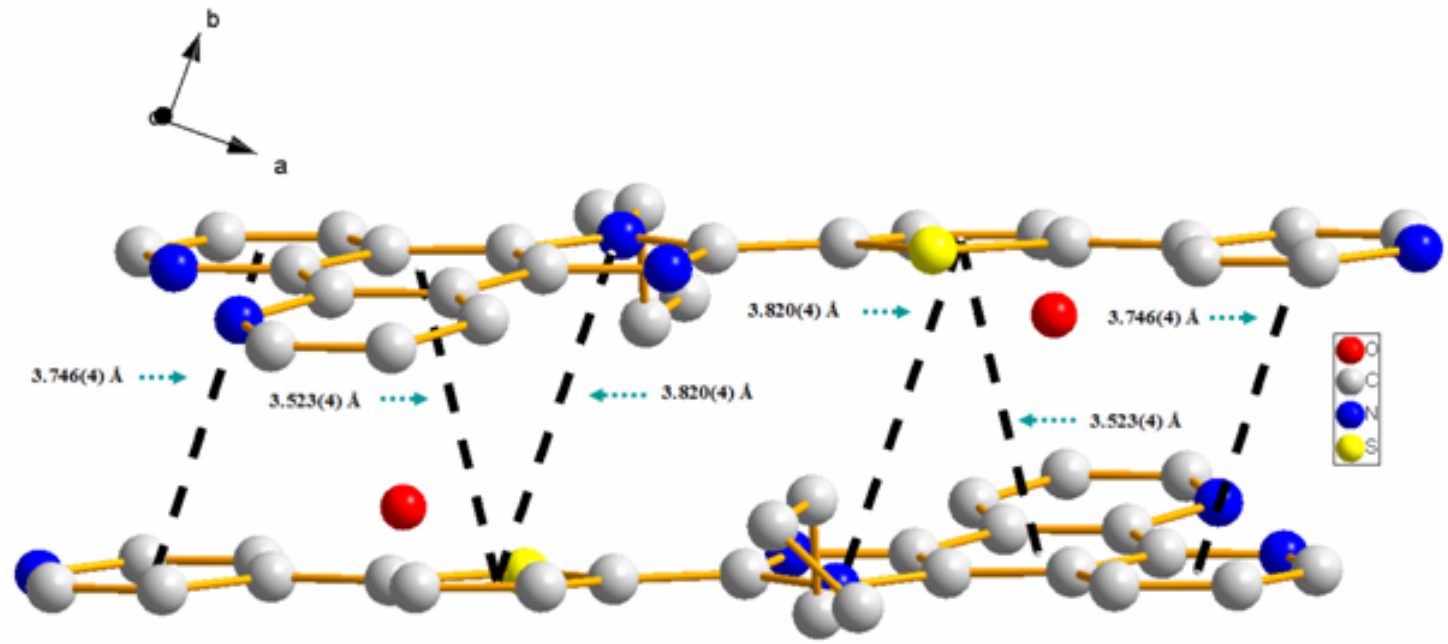
a



b



c



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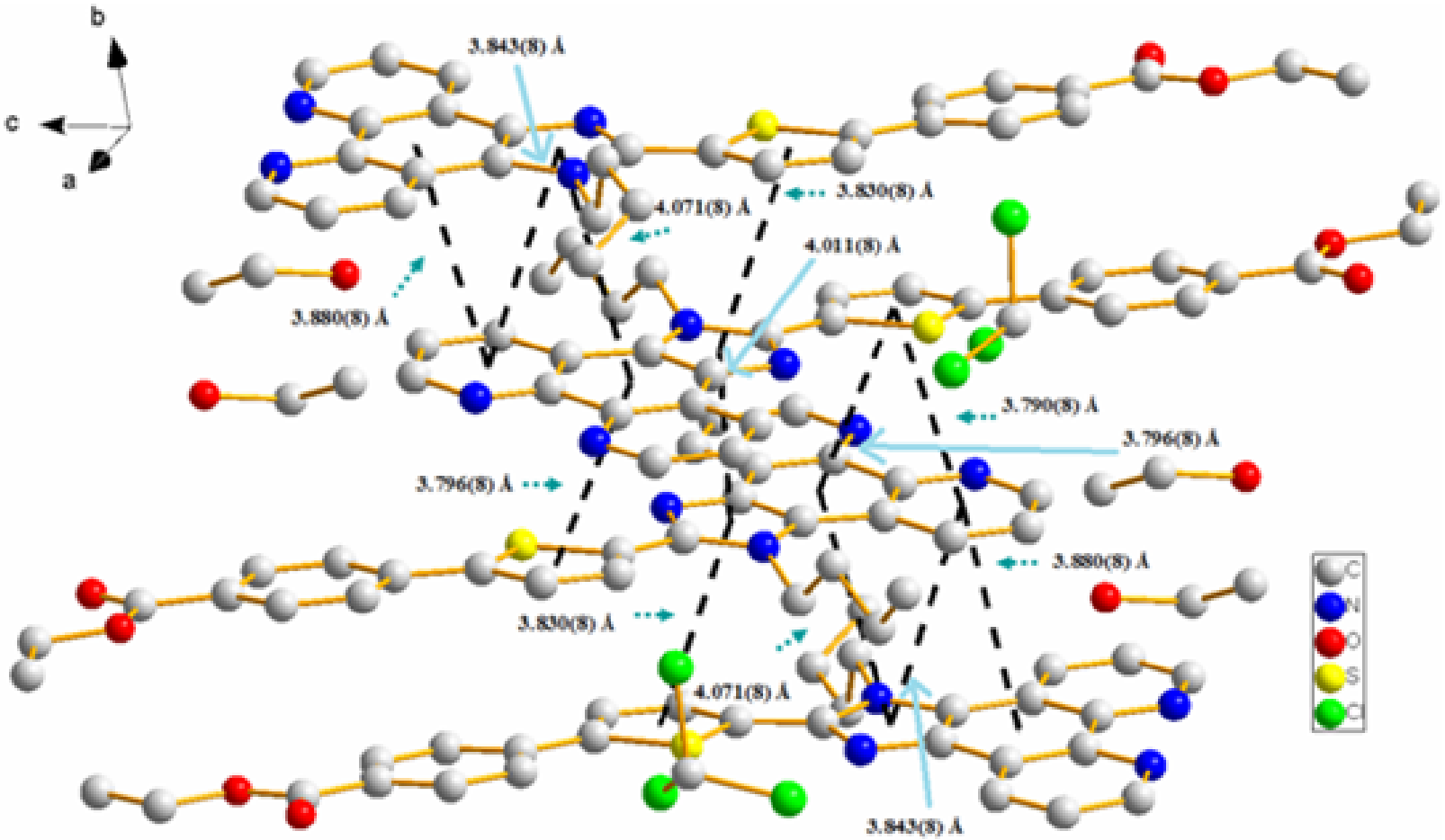
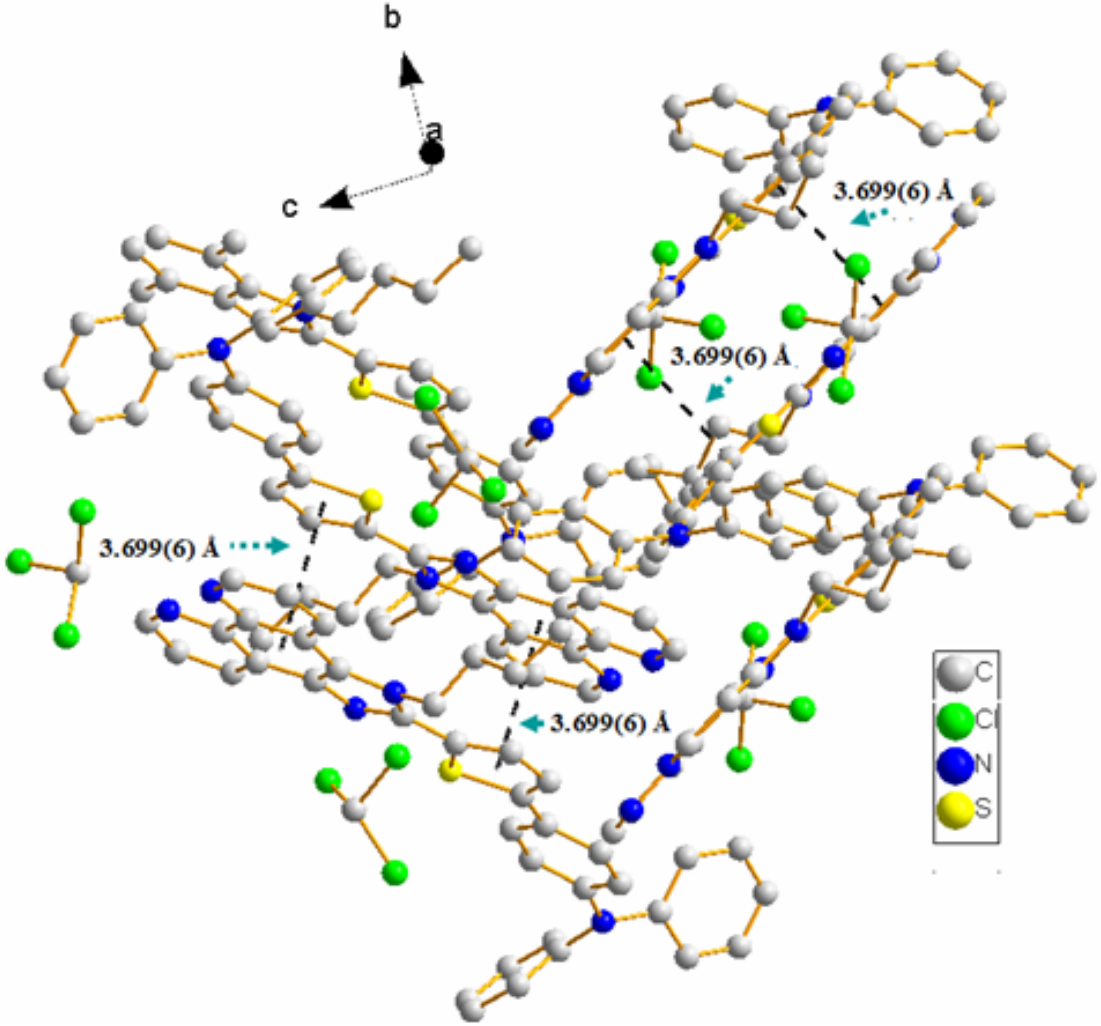
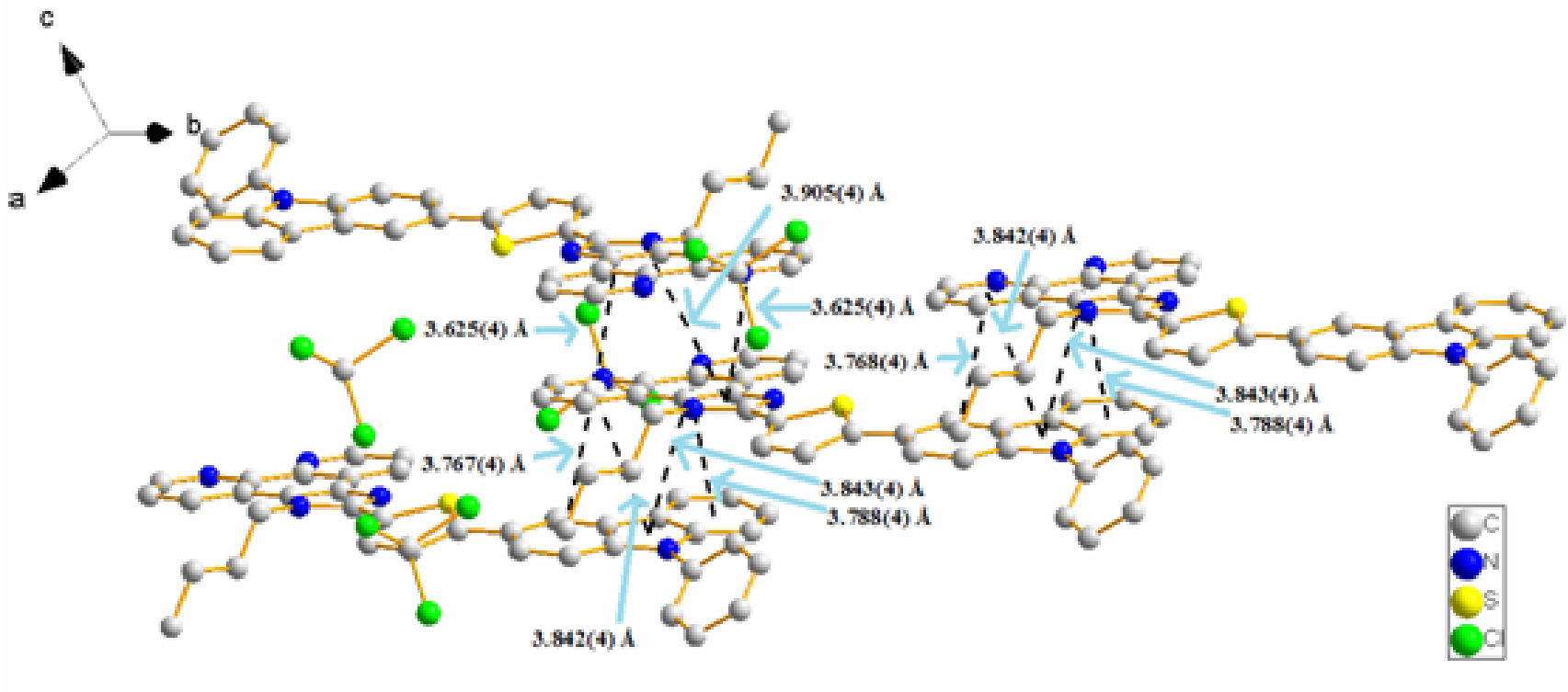

b
c
a
3.843(8) Å
3.830(8) Å
4.071(8) Å
4.011(8) Å
3.880(8) Å
3.790(8) Å
3.796(8) Å
3.796(8) Å
3.880(8) Å
3.830(8) Å
4.071(8) Å
3.843(8) Å
C
N
O
S
Cl

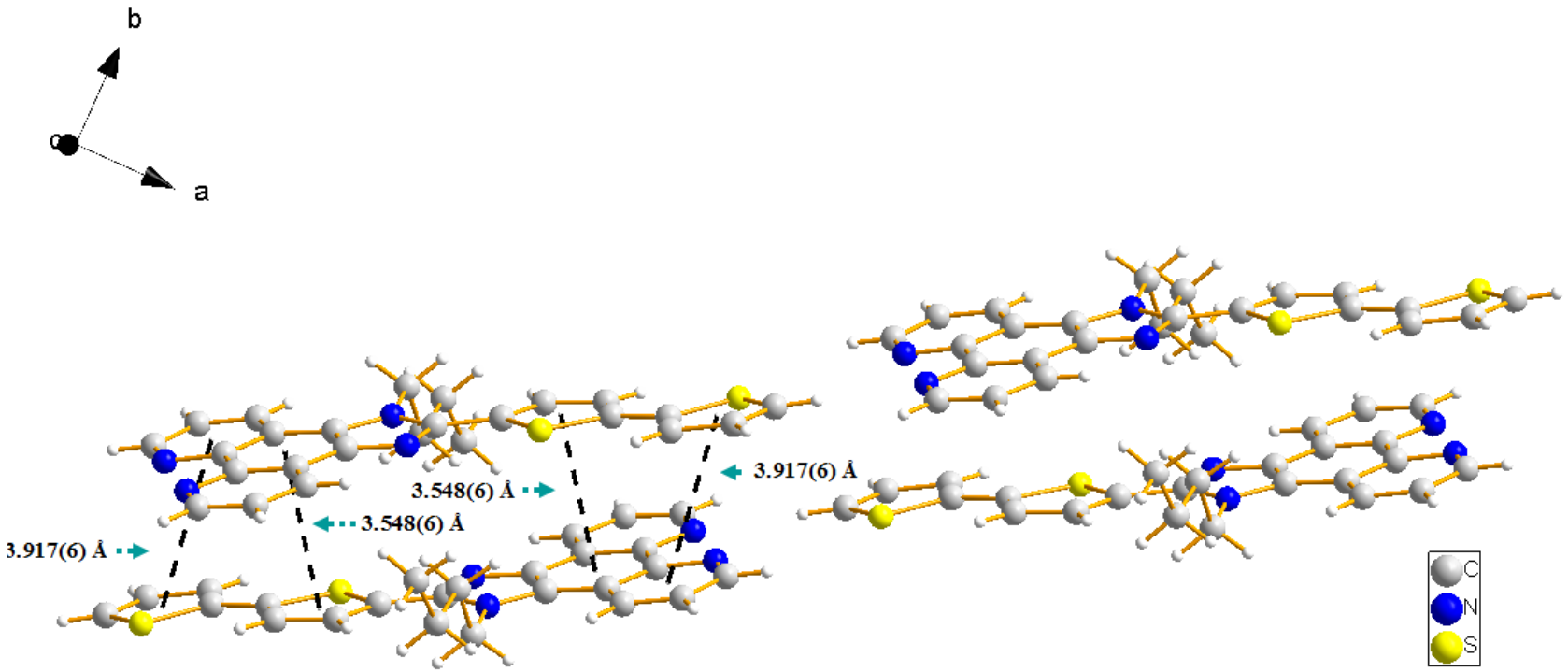
e



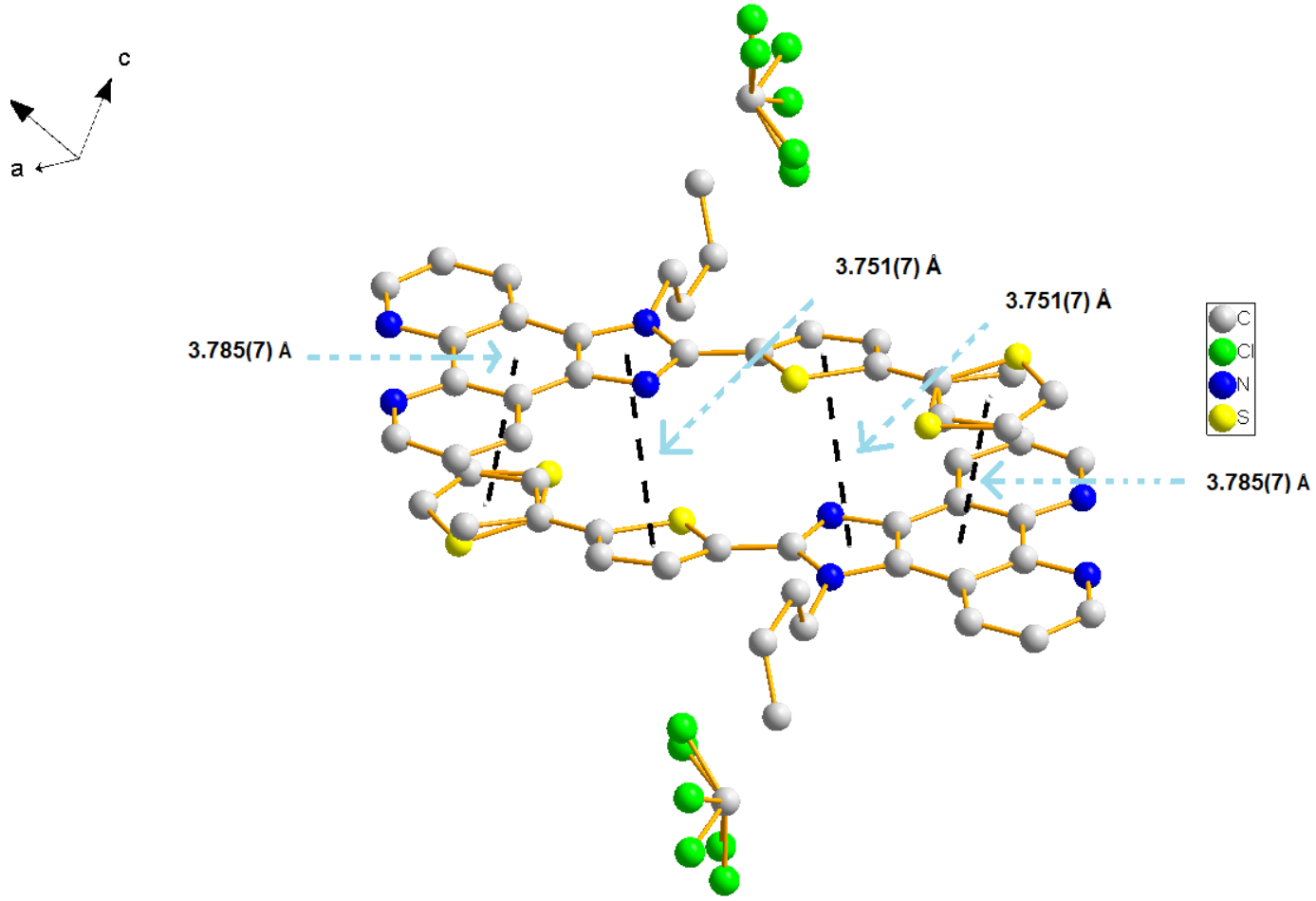
f


c
b
a
3.905(4) Å
3.625(4) Å
3.625(4) Å
3.842(4) Å
3.768(4) Å
3.843(4) Å
3.788(4) Å
3.767(4) Å
3.843(4) Å
3.788(4) Å
3.842(4) Å
C
N
S
Cl

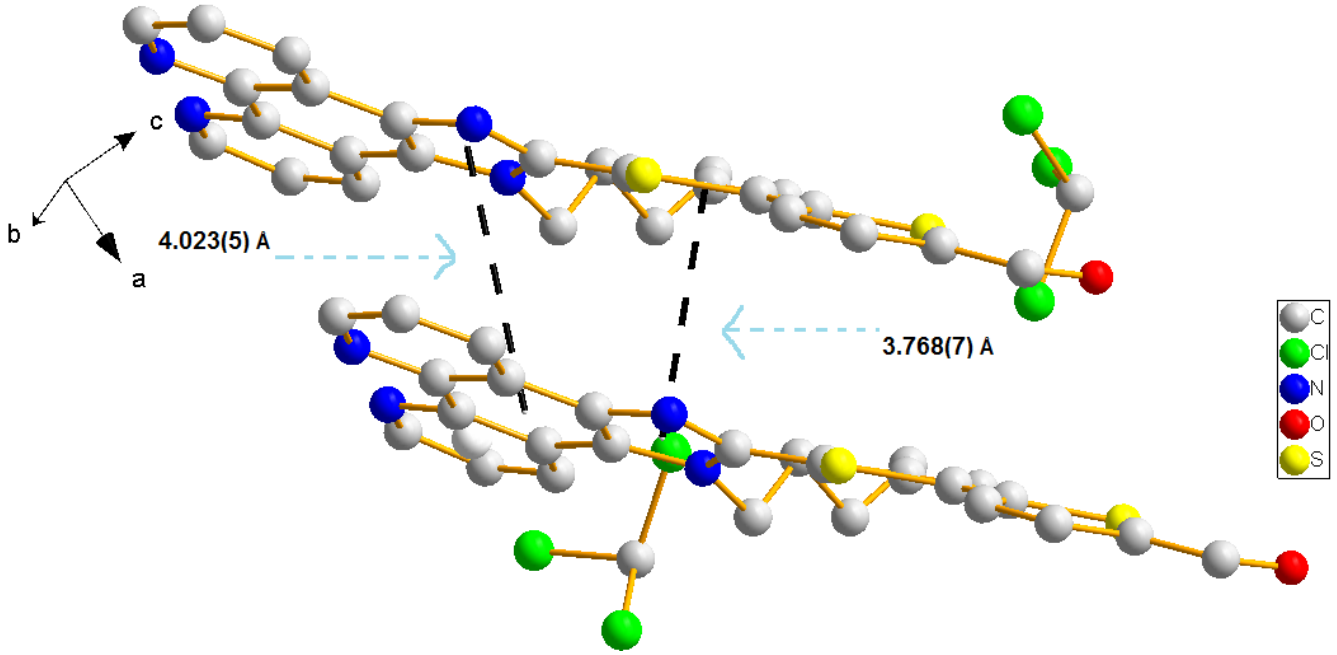
g



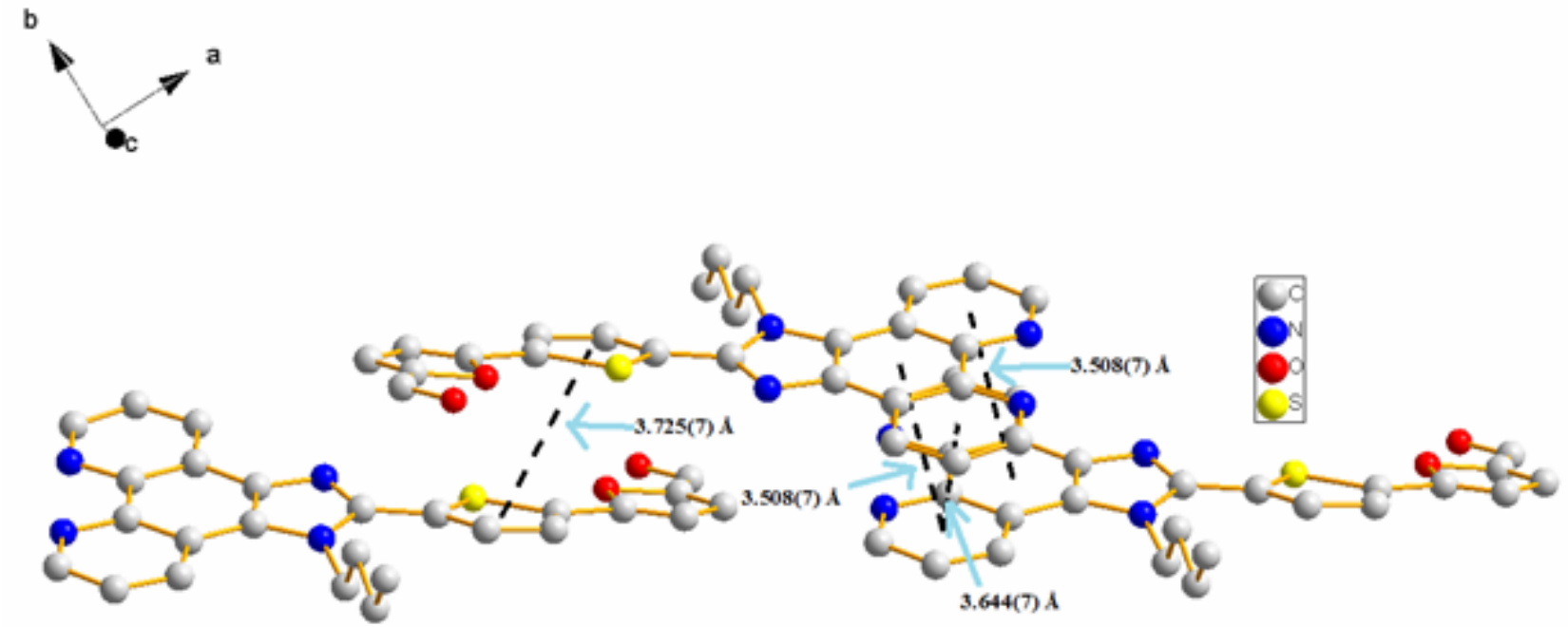
h



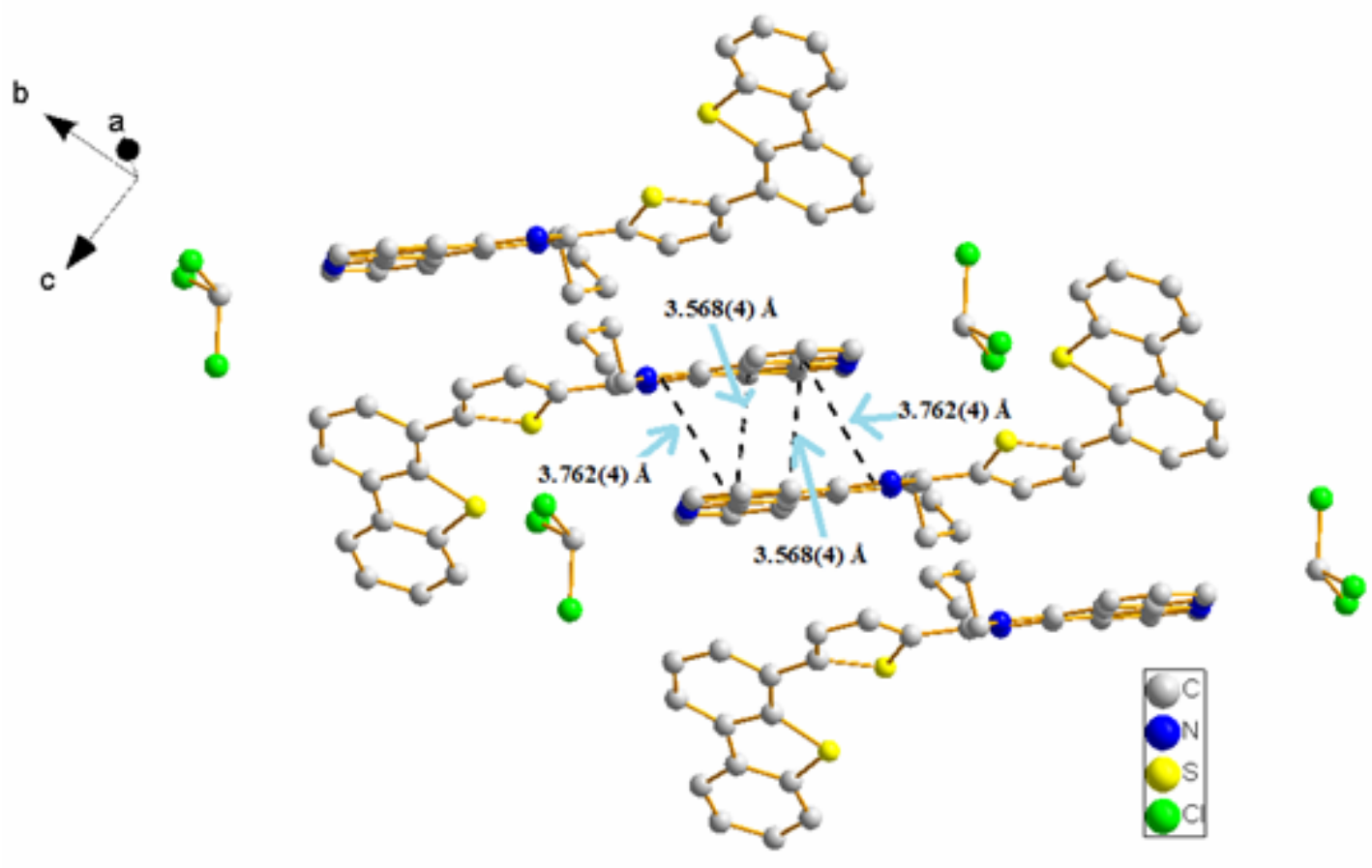
i



j



k



1

Fig. SI17. Perspective view of the packing structure in compounds **3**·$CHCl_3$, **4**, **5**·$CHCl_3$, **6**·H_2O, (**7**)$_2$·C_2H_5OH·$(CHCl_3)_2$, **8**·$CHCl_3$, **9**·$CHCl_3$, **10**·$CHCl_3$, **11**·$CHCl_3$, **12**, **13**·$CHCl_3$.