

SUPPLEMENTARY MATERIAL

Regioselective synthesis, characterization and antimicrobial evaluation of amide-ether linked 1,4-disubstituted 1,2,3-triazoles

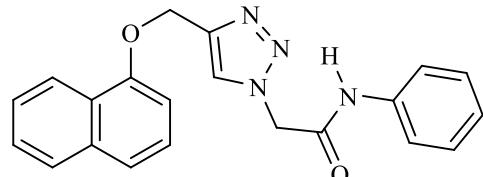
CHANDER PRAKASH KAUSHIK¹ *, KRISHAN KUMAR¹, DEVINDER KUMAR¹,
SATBIR MOR¹, ASHWANI KUMAR² and DEEPAK KUMAR JINDAL²

¹Department of Chemistry, Guru Jambheshwar University of Science & Technology, Hisar, Haryana, India

²Department of Pharmaceutical Sciences, Guru Jambheshwar University of Science & Technology, Hisar, Haryana, India

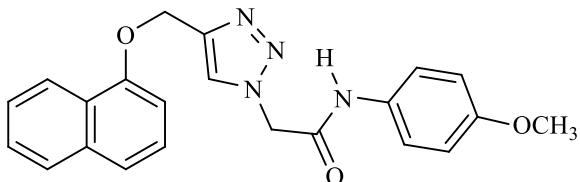
* Corresponding Author: E-mail: kaushikcp@gmail.com

PHYSICAL & SPECTRAL DATA OF THE SYNTHESIZED COMPOUNDS



*2-(4-((naphthalen-1-yloxy)methyl)-1*H*-1,2,3-triazol-1-yl)-N-phenylacetamide (7a):*

19 White solid; Yield: 68%; m.p. 242-244 °C; FTIR (KBr): 3296 (N-H str., amide), 3138 (C-H
 20 str., triazole ring), 3055 (C-H str., aromatic ring), 2929, 1664 (C=O str., amide), 1583, 1508,
 21 1465 (C=C str., aromatic ring), 1267 (C-O asym. str., ether), 1101 (C-O sym. str., ether) cm⁻¹;
 22 ¹H NMR (400 MHz, DMSO-*d*₆, δ / ppm): 5.42 (s, 2H, OCH₂), 5.58 (s, 2H, NCH₂), 7.05-7.11
 23 (m, 1H, Ar-H), 7.22-7.55 (m, 7H, Ar-H), 7.58-7.89 (m, 3H, Ar-H), 8.14 (d, 1H, *J* = 8.0 Hz,
 24 Ar-H), 8.43 (s, 1H, C-H triazole), 11.14 (s, 1H, N-H amide); ¹³C NMR (100 MHz, DMSO-*d*₆,
 25 δ / ppm): 52.7, 62.1, 106.2, 119.7, 120.8, 122.0, 124.3, 125.4, 125.8, 126.6, 126.7 (C-5
 26 triazole), 126.9, 128.0, 134.5, 138.9, 143.2 (C-4 triazole), 145.0, 154.0, 165.7 (C=O amide);
 27 ESI-HRMS (*m/z*) calculated for [C₂₁H₁₈N₄O₂+H]⁺: 359.1430 Observed: 359.2213.

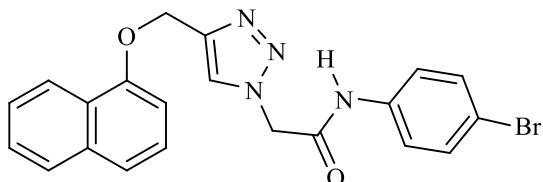


29

30 *N*-(4-methoxyphenyl)-2-(4-((naphthalen-1-yloxy)methyl)-1*H*-1,2,3-triazol-1-yl)acetamide31 (**7b**):

32 Dark brown solid; Yield: 75%; m.p. 210-212 °C; FTIR (KBr): 3269 (N-H str., amide), 3143
 33 (C-H str., triazole ring), 3093 (C-H str., aromatic ring), 2945, 1662 (C=O str., amide), 1606,
 34 1558, 1474 (C=C str., aromatic ring), 1242 (C-O asym. str., ether), 1103 (C-O sym. str., ether)
 35 cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆, δ / ppm): 3.73 (s, 3H, OCH₃), 5.35 (s, 2H, OCH₂), 5.39
 36 (s, 2H, NCH₂), 6.91 (d, 2H, *J* = 8.0 Hz, Ar-H), 7.22 (d, 1H, *J* = 8.0 Hz, Ar-H), 7.44-7.55 (m,
 37 6H, Ar-H), 7.88 (d, 1H, *J* = 8.0 Hz, Ar-H), 8.13 (d, 1H, *J* = 8.0 Hz, Ar-H), 8.38 (s, 1H, C-H
 38 triazole), 10.38 (s, 1H, N-H amide); ¹³C NMR (100 MHz, DMSO-*d*₆, δ / ppm): 52.6, 55.6,
 39 62.1, 106.2, 114.5, 120.8, 122.0, 125.4, 125.6, 125.8, 126.6, 126.8 (C-5 triazole), 126.9,
 40 128.0, 132.0, 134.5, 143.2 (C-4 triazole), 154.0, 156.0, 165.8 (C=O amide); ESI-HRMS (*m/z*)
 41 calculated for [C₂₂H₂₀N₄O₃+H]⁺: 389.1535 Observed: 389.0061.

42

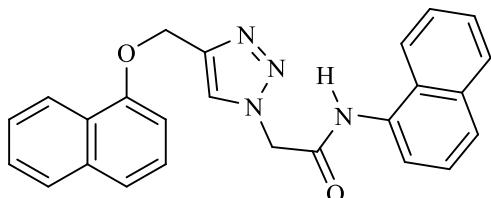
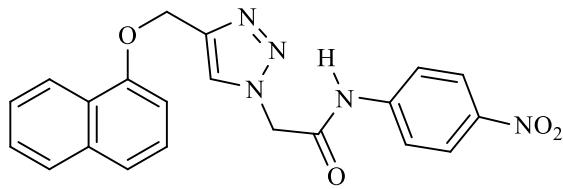


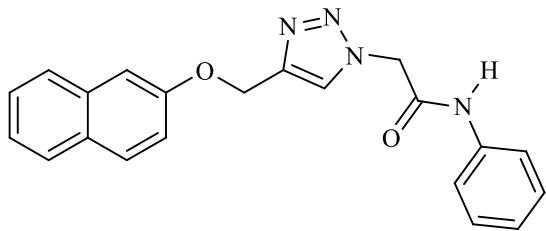
43

44 *N*-(4-bromophenyl)-2-(4-((naphthalen-1-yloxy)methyl)-1*H*-1,2,3-triazol-1-yl)acetamide (**7c**):

45 Dark brown solid; Yield: 65%; m.p. 186-188 °C; FTIR (KBr): 3261 (N-H str., amide), 3126
 46 (C-H str., triazole ring), 3059 (C-H str., aromatic ring), 2943, 1668 (C=O str., amide), 1585,
 47 1550, 1489 (C=C str., aromatic ring), 1269 (C-O asym. str., ether), 1101 (C-O sym. str., ether)
 48 cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆, δ / ppm): 5.39 (s, 2H, OCH₂), 5.39 (s, 2H, NCH₂), 7.23
 49 (d, 1H, *J* = 8.0 Hz, Ar-H), 7.44-7.55 (m, 8H, Ar-H), 7.87 (d, 1H, *J* = 8.0 Hz, Ar-H), 8.13 (d,
 50 1H, *J* = 8.0 Hz, Ar-H), 8.38 (s, 1H, C-H triazole), 10.65 (s, 1H, N-H amide); ¹³C NMR (100
 51 MHz, DMSO-*d*₆, δ / ppm): 52.7, 62.1, 106.2, 115.9, 120.8, 122.0, 125.4, 125.8, 126.6, 126.7
 52 (C-5 triazole), 126.9, 128.0, 132.2, 134.5, 143.2 (C-4 triazole), 154.0, 165.8 (C=O amide);
 53 ESI-HRMS (*m/z*) calculated for [C₂₁H₁₇BrN₄O₂+H]⁺: 437.0535 Observed: 436.8784.

54



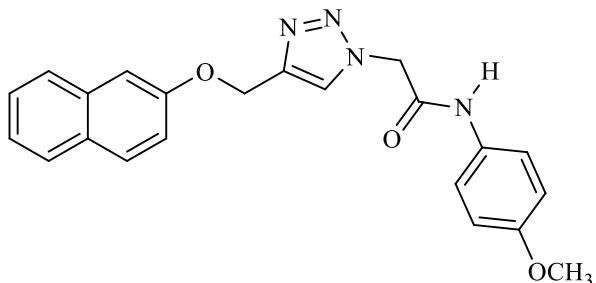


83

84 2-((naphthalen-2-yloxy)methyl)-1H-1,2,3-triazol-1-yl-N-phenylacetamide (10a):

85 White solid; Yield: 67%; m.p. 202-204 °C; FTIR (KBr): 3267 (N-H str., amide), 3136 (C-H
86 str., triazole ring), 3084 (C-H str., aromatic ring), 2927, 1668 (C=O str., amide), 1608, 1554,
87 1504 (C=C str., aromatic ring), 1261 (C-O asym. str., ether), 1178 (C-O sym. str., ether) cm⁻¹;
88 ¹H NMR (400 MHz, DMSO-d₆, δ / ppm): 5.31 (s, 2H, OCH₂), 5.38 (s, 2H, NCH₂), 7.10 (t,
89 1H, J = 8.0 Hz, Ar-H), 7.22 (d, 1H, J = 8.0 Hz, Ar-H), 7.33-7.39 (m, 3H, Ar-H), 7.55-7.59
90 (m, 2H, Ar-H), 7.60 (d, 2H, J = 8.0 Hz, Ar-H), 7.85 (d, 3H, J = 8.0 Hz, Ar-H), 8.34 (s, 1H, C-
91 H triazole), 10.51 (s, 1H, N-H amide); ¹³C NMR (100 MHz, DMSO-d₆, δ / ppm): 52.7, 61.5,
92 107.6, 119.2, 119.7, 124.2, 124.3, 126.9 (C-5 triazole), 127.2, 128.0, 129.1, 129.4, 129.8,
93 134.7, 138.9, 142.9 (C-4 triazole), 156.4, 164.7 (C=O amide); ESI-HRMS (m/z) calculated for
94 [C₂₁H₁₈N₄O₂+H]⁺: 359.1430 Observed: 358.9767.

95

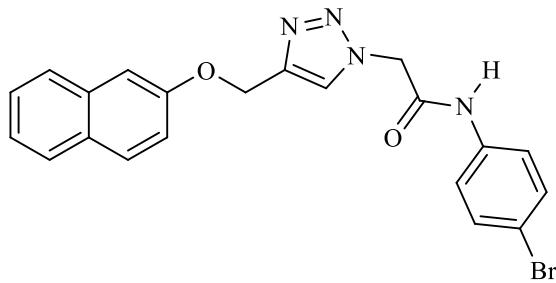


96

97 N-(4-methoxyphenyl)-2-((naphthalen-2-yloxy)methyl)-1H-1,2,3-triazol-1-ylacetamide

98 (10b):

99 White solid; Yield: 62%; m.p. 198-200 °C; FTIR (KBr): 3282 (N-H str., amide), 3138 (C-H
100 str., triazole ring), 3059 (C-H str., aromatic ring), 2947, 1678 (C=O str., amide), 1600, 1546,
101 1514 (C=C str., aromatic ring), 1240 (C-O asym. str., ether), 1178 (C-O sym. str., ether) cm⁻¹;
102 ¹H NMR (400 MHz, DMSO-d₆, δ / ppm): 3.73 (s, 3H, OCH₃), 5.30 (s, 2H, OCH₂), 5.33 (s,
103 2H, NCH₂), 6.91 (d, 2H, J = 12.0 Hz, Ar-H), 7.22 (d, 1H, J = 8.0 Hz, Ar-H), 7.37 (d, 1H, J =
104 8.0 Hz, Ar-H), 7.48-7.55 (m, 4H, Ar-H), 7.85 (d, 3H, J = 8.0 Hz, Ar-H), 8.32 (s, 1H, C-H
105 triazole), 10.36 (s, 1H, N-H amide); ¹³C NMR (100 MHz, DMSO-d₆, δ / ppm): 52.6, 55.6,
106 61.5, 107.6, 114.5, 119.2, 121.2, 124.2, 126.9 (C-5 triazole), 127.2, 128.0, 129.1, 129.8,
107 132.0, 134.7, 142.8 (C-4 triazole), 156.4, 164.1 (C=O amide); ESI-HRMS (m/z) calculated for
108 [C₂₂H₂₀N₄O₃+H]⁺: 389.1535 Observed: 388.9711.

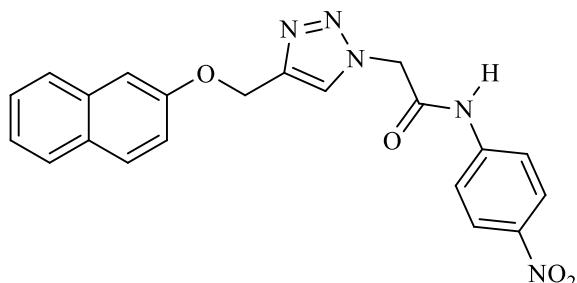


109

110 *N*-(4-bromophenyl)-2-((naphthalen-2-yloxy)methyl)-1*H*-1,2,3-triazol-1-yl)acetamide (10c**):**

111 Light brown solid; Yield: 87%; m.p. 226-228 °C; FTIR (KBr): 3258 (N-H str., amide), 3126
 112 (C-H str., triazole ring), 3045 (C-H str., aromatic ring), 2918, 1664 (C=O str., amide), 1595,
 113 1550, 1475 (C=C str., aromatic ring), 1267 (C-O asym. str., ether), 1182 (C-O sym. str., ether)
 114 cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆, δ / ppm): 5.31 (s, 2H, OCH₂), 5.38 (s, 2H, NCH₂), 7.21
 115 (d, 1H, *J* = 8.0 Hz, Ar-H), 7.38 (d, 1H, *J* = 8.0 Hz, Ar-H), 7.46-7.58 (m, 6H, Ar-H), 7.84 (d,
 116 3H, *J* = 8.0 Hz, Ar-H), 8.33 (s, 1H, C-H triazole), 10.66 (s, 1H, N-H amide); ¹³C NMR (100
 117 MHz, DMSO-*d*₆, δ / ppm): 52.7, 61.5, 107.6, 115.9, 119.2, 121.6, 124.2, 126.9 (C-5 triazole),
 118 127.2, 128.0, 129.1, 129.8, 132.2, 134.7, 138.3, 142.9 (C-4 triazole), 156.4, 164.9 (C=O
 119 amide); ESI-HRMS (*m/z*) calculated for [C₂₁H₁₇BrN₄O₂+H]⁺: 437.0535 Observed: 436.9047.

120

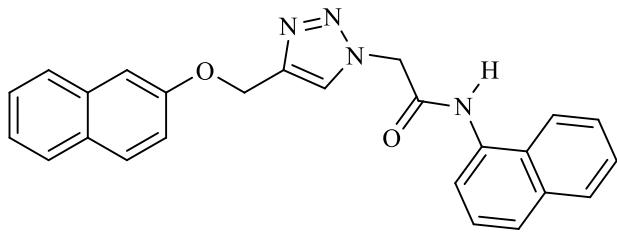


121

122 2-((naphthalen-2-yloxy)methyl)-1*H*-1,2,3-triazol-1-yl)-*N*-(4-nitrophenyl) acetamide (10d**):**

123 Brown solid; Yield: 78%; m.p. 218-220 °C; FTIR (KBr): 3317 (N-H str., amide), 3153 (C-H
 124 str., triazole ring), 3061 (C-H str., aromatic ring), 2945, 1699 (C=O str., amide), 1610, 1583,
 125 1478 (C=C str., aromatic ring), 1504 (N-O str., asym., NO₂), 1340 (N-O str., sym., NO₂),
 126 1257 (C-O asym. str., ether), 1180 (C-O sym. str., ether) cm⁻¹; ¹H NMR (400 MHz, DMSO-
 127 *d*₆, δ / ppm): 5.32 (s, 2H, OCH₂), 5.48 (s, 2H, NCH₂), 7.22 (d, 1H, *J* = 8.0 Hz, Ar-H), 7.37 (d,
 128 1H, *J* = 8.0 Hz, Ar-H), 7.48-7.54 (m, 2H, Ar-H), 7.84-7.85 (m, 5H, Ar-H), 8.26 (d, 2H, *J* =
 129 8.0 Hz, Ar-H), 8.35 (s, 1H, C-H triazole), 11.14 (s, 1H, N-H amide); ¹³C NMR (100 MHz,
 130 DMSO-*d*₆, δ / ppm): 52.8, 61.5, 107.6, 119.2, 119.5, 124.2, 125.6, 126.9 (C-5 triazole), 127.2,
 131 128.0, 129.1, 129.9, 134.7, 143.0 (C-4 triazole), 143.1, 145.0, 156.4, 165.8 (C=O amide);
 132 ESI-HRMS (*m/z*) calculated for [C₂₁H₁₇N₅O₄+H]⁺: 404.1281 Observed: 403.8690.

133

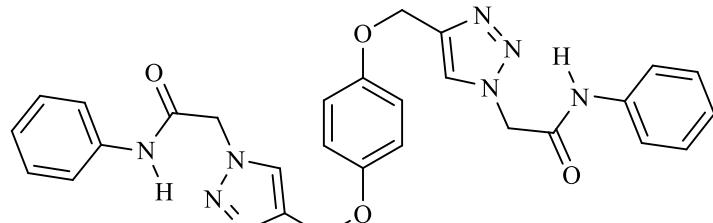


134

135 *N*-(naphthalen-1-yl)-2-(4-((naphthalen-2-yloxy)methyl)-1*H*-1,2,3-triazol-1-yl)acetamide136 (**10e**):

137 White solid; Yield: 92%; m.p. 220-222 °C; FTIR (KBr): 3259 (N-H str., amide), 3165 (C-H
138 str., triazole ring), 3055 (C-H str., aromatic ring), 2916, 1678 (C=O str., amide), 1601, 1544,
139 1462 (C=C str., aromatic ring), 1263 (C-O asym. str., ether), 1178 (C-O sym. str., ether) cm⁻¹;
140 ¹H NMR (400 MHz, DMSO-*d*₆, δ / ppm): 5.38 (s, 2H, OCH₂), 5.59 (s, 2H, NCH₂), 7.22 (d,
141 1H, *J* = 8.0 Hz, Ar-H), 7.37 (d, 1H, *J* = 8.0 Hz, Ar-H), 7.48-7.59 (m, 5H, Ar-H), 7.73-7.98
142 (m, 6H, Ar-H), 8.18 (d, 1H, *J* = 8.0 Hz, Ar-H), 8.39 (s, 1H, C-H triazole), 10.47 (s, 1H, N-H
143 amide); ¹³C NMR (100 MHz, DMSO-*d*₆, δ / ppm): 52.5, 61.6, 107.6, 119.2, 122.0, 123.1,
144 124.2, 126.1, 126.2, 126.5, 126.7, 126.9 (C-5 triazole), 127.2, 128.0, 128.7, 129.1, 129.8,
145 133.2, 134.2, 134.7, 143.0 (C-4 triazole), 156.4, 165.6 (C=O amide); ESI-HRMS (*m/z*)
146 calculated for [C₂₅H₂₀N₄O₂+H]⁺: 409.1586 Observed: 408.9673.

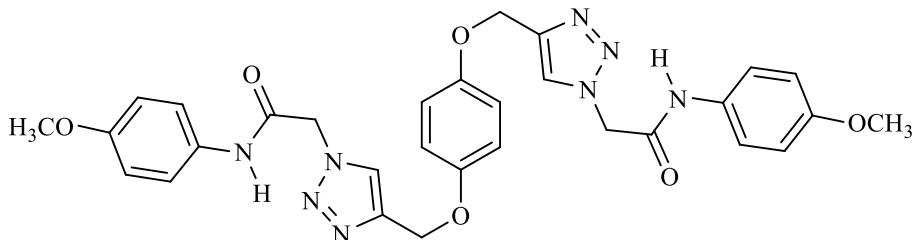
147



148

149 2,2'-(4,4'-(1,4-phenylenebis(oxy))bis(methylene)bis(1*H*-1,2,3-triazole-4,1-diyl))bis(*N*-phenylacetamide) (**13a**):

150 Dark brown solid; Yield: 83%; m.p. >250 °C; FTIR (KBr): 3278 (N-H str., amide), 3142 (C-H
151 str., triazole ring), 3095 (C-H str., aromatic ring), 2947, 1680 (C=O str., amide), 1604, 1556,
152 1508 (C=C str., aromatic ring), 1236 (C-O str., asym., ether), 1056 (C-O str., sym., ether) cm⁻¹;
153 ¹H NMR (400 MHz, DMSO-*d*₆, δ / ppm): 5.08 (s, 4H, OCH₂), 5.36 (s, 4H, NCH₂), 7.01 (s,
154 4H, Ar-H), 7.09 (t, 2H, *J* = 8.0 Hz, Ar-H), 7.34 (t, 2H, *J* = 8.0 Hz, Ar-H), 7.59 (d, 4H, *J* = 8.0
155 Hz, Ar-H), 8.24 (s, 2H, C-H triazole), 10.49 (s, 2H, N-H amide); ¹³C NMR (100 MHz,
156 DMSO-*d*₆, δ / ppm): 52.7, 62.1, 116.0, 119.7, 124.2, 126.6 (C-5 triazole), 129.4, 138.9, 143.2
157 (C-4 triazole), 152.8, 164.7 (C=O amide); ESI-HRMS (*m/z*) calculated for [C₂₈H₂₆N₈O₄+H]⁺:
158 539.2077 Observed: 539.2239.



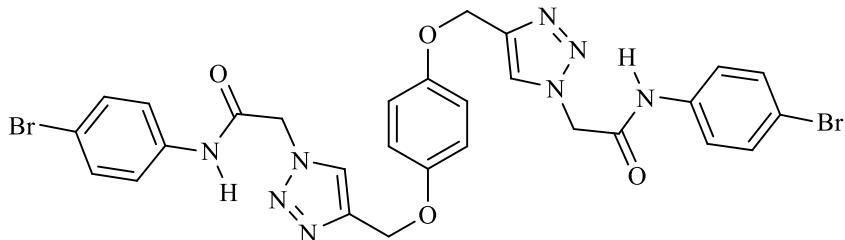
160

161 *2,2'-(4,4'-(1,4-phenylenebis(oxy))bis(methylene)bis(1H-1,2,3-triazole-4,1-diyl))bis (N-(4-*

162 *methoxyphenyl)acetamide) (13b):*

163 Dark brown solid; Yield: 88%; m.p. >250 °C; FTIR (KBr): 3275 (N-H str., amide), 3140 (C-H
164 str., triazole ring), 3089 (C-H str., aromatic ring), 2951, 1674 (C=O str., amide), 1606, 1552,
165 1510 (C=C str., aromatic ring), 1238 (C-O str., asym., ether), 1053 (C-O str., sym., ether) cm⁻¹
166 ; ¹H NMR (400 MHz, DMSO-d₆, δ / ppm): 3.72 (s, 6H, OCH₃), 5.11 (s, 4H, OCH₂), 5.31 (s,
167 4H, NCH₂), 6.92 (s, 4H, Ar-H), 7.00 (d, 4H, J = 8.0 Hz, Ar-H), 7.49 (d, 4H, J = 8.0 Hz, Ar-
168 H), 8.24 (s, 2H, C-H triazole), 10.36 (s, 2H, N-H amide); ¹³C NMR (100 MHz, DMSO-d₆, δ /
169 ppm): 52.6, 55.6, 61.9, 114.5, 116.2, 121.2, 126.6 (C-5 triazole), 132.0, 143.2 (C-4 triazole),
170 152.8, 156.0, 164.1 (C=O amide); ESI-HRMS (m/z) calculated for [C₃₀H₃₀N₈O₆+H]⁺:
171 599.2425 Observed: 599.2288.

172

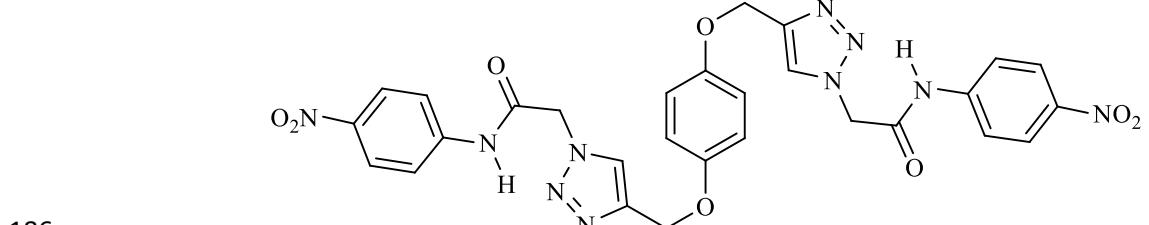


173

174 *2,2'-(4,4'-(1,4-phenylenebis(oxy))bis(methylene)bis(1H-1,2,3-triazole-4,1-diyl))bis (N-(4-*

175 *bromophenyl)acetamide) (13c):*

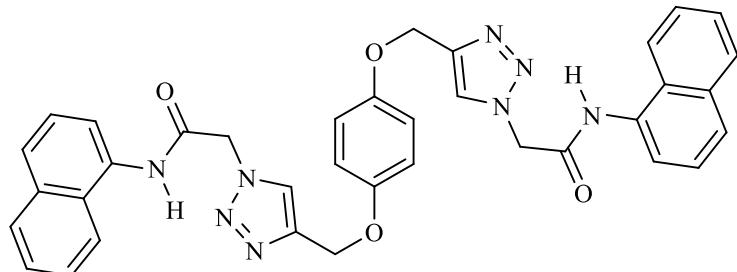
176 Dark brown solid; Yield: 86%; m.p. >250 °C; FTIR (KBr): 3273 (N-H str., amide), 3124 (C-H
177 str., triazole ring), 3070 (C-H str., aromatic ring), 2947, 1680 (C=O str., amide), 1604, 1544,
178 1508 (C=C str., aromatic ring), 1236 (C-O str., asym., ether), 1074, 1055 (C-O str., sym.,
179 ether) cm⁻¹; ¹H NMR (400 MHz, DMSO-d₆, δ / ppm): 5.12 (s, 4H, OCH₂), 5.36 (s, 4H,
180 NCH₂), 6.99 (s, 4H, Ar-H), 7.52 (d, 4H, J = 12.0 Hz, Ar-H), 7.56 (d, 4H, J = 12.0 Hz, Ar-H),
181 8.24 (s, 2H, C-H triazole), 10.64 (s, 2H, N-H amide); ¹³C NMR (100 MHz, DMSO-d₆, δ /
182 ppm): 52.7, 61.9, 115.9, 116.0, 121.6, 126.6 (C-5 triazole), 132.2, 138.3, 143.2 (C-4 triazole),
183 152.8, 164.9 (C=O amide); ESI-HRMS (m/z) calculated for [C₂₈H₂₄Br₂N₈O₄+H]⁺: 697.3494
184 Observed: 697.3443 and (m/z) calculated for [C₂₈H₂₄Br₂N₈O₄+2]⁺: 698.3494 Observed:
185 698.3538.



187 *2,2'-(4,4'-(1,4-phenylenebis(oxy))bis(methylene)bis(1H-1,2,3-triazole-4,1-diyl))bis(N-(4-nitrophenyl)acetamide) (13d):*

189 Dark brown solid; Yield: 82%; m.p. >250 °C; FTIR (KBr): 3253 (N-H str., amide), 3155 (C-H
190 str., triazole ring), 3089 (C-H str., aromatic ring), 2954, 1705 (C=O str., amide), 1597, 1552,
191 1510 (C=C str., aromatic ring), 1506 (N-O str., asym., NO₂), 1342 (N-O str., sym., NO₂),
192 1261 (C-O str., asym., ether), 1060 (C-O str., sym., ether) cm⁻¹; ¹H NMR (400 MHz, DMSO-
193 *d*₆, δ / ppm): 5.13 (s, 4H, OCH₂), 5.45 (s, 4H, NCH₂), 7.00 (s, 4H, Ar-H), 7.84 (d, 4H, J = 8.0
194 Hz, Ar-H), 8.25 (s, 2H, C-H triazole), 8.26 (d, 4H, J = 8.0 Hz, Ar-H), 11.12 (s, 2H, N-H
195 amide); ¹³C NMR (100 MHz, DMSO-*d*₆, δ / ppm): 52.7, 61.9, 116.1, 119.5, 125.6, 126.6 (C-5
196 triazole), 143.2 (C-4 triazole), 145.0, 152.8, 164.8 (C=O amide); ESI-HRMS (*m/z*) calculated
197 for [C₂₈H₂₄N₁₀O₈+H]⁺: 629.1779 Observed: 629.4429.

198



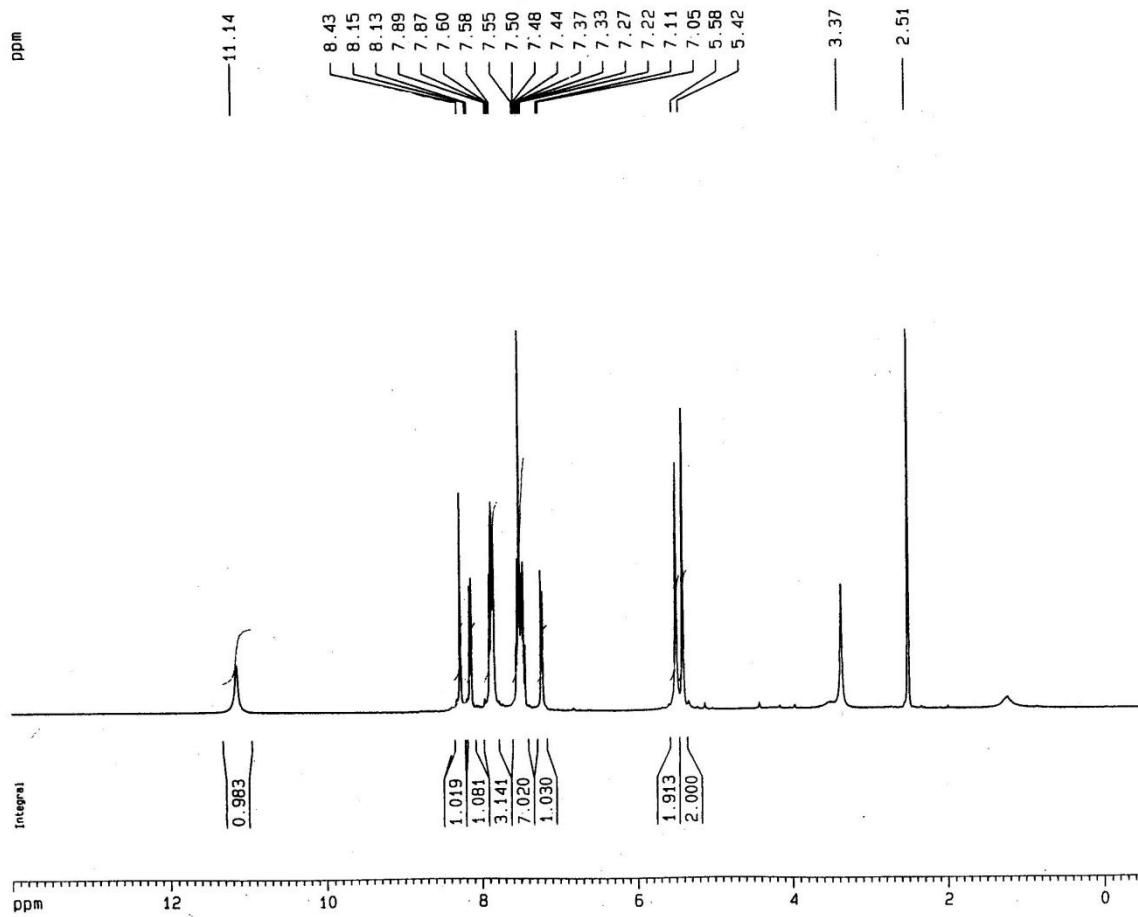
200 *2,2'-(4,4'-(1,4-phenylenebis(oxy))bis(methylene)bis(1H-1,2,3-triazole-4,1-diyl))bis(N-(naphthalen-1-yl)acetamide) (13e):*

202 Dark brown solid; Yield: 85%; m.p. >250 °C; FTIR (KBr): 3261 (N-H str., amide), 3138 (C-H
203 str., triazole ring), 3088 (C-H str., aromatic ring), 2947, 1678 (C=O str., amide), 1597, 1543,
204 1508 (C=C str., aromatic ring), 1236 (C-O str., asym., ether), 1055 (C-O str., sym., ether) cm⁻¹
205 ; ¹H NMR (400 MHz, DMSO-*d*₆, δ / ppm): 5.13 (s, 4H, OCH₂), 5.56 (s, 4H, NCH₂), 7.00 (s,
206 4H, Ar-H), 7.49-7.82 (m, 10H, Ar-H), 7.97 (d, 2H, J = 8.0 Hz, Ar-H), 8.17 (d, 2H, J = 8.0 Hz,
207 Ar-H), 8.27 (s, 2H, C-H triazole), 10.46 (s, 2H, N-H amide); ¹³C NMR (100 MHz, DMSO-*d*₆,
208 δ / ppm): 52.7, 62.1, 116.0, 122.0, 123.1, 126.1, 126.2, 126.5, 126.6 (C-5 triazole), 126.8,
209 128.0, 128.7, 133.2, 134.2, 143.2 (C-4 triazole), 152.8, 164.7 (C=O amide); ESI-HRMS (*m/z*)
210 calculated for [C₃₆H₃₀N₈O₄+H]⁺: 639.2390 Observed: 639.2136.

211

¹H NMR, ¹³C NMR and HRMS of Compounds

212



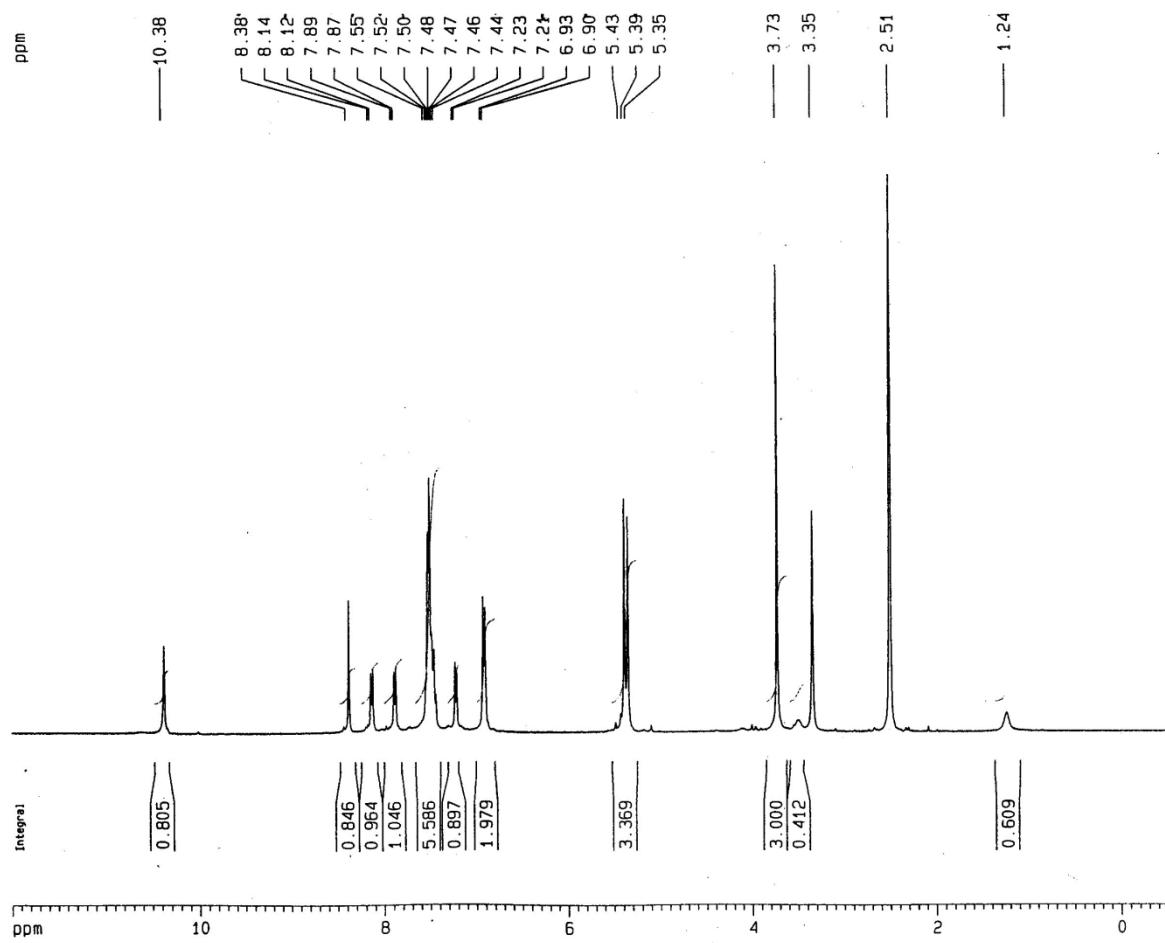
213

Figure S1. ¹H NMR spectrum (DMSO-*d*₆, 400 MHz) of compound 7a

214

215

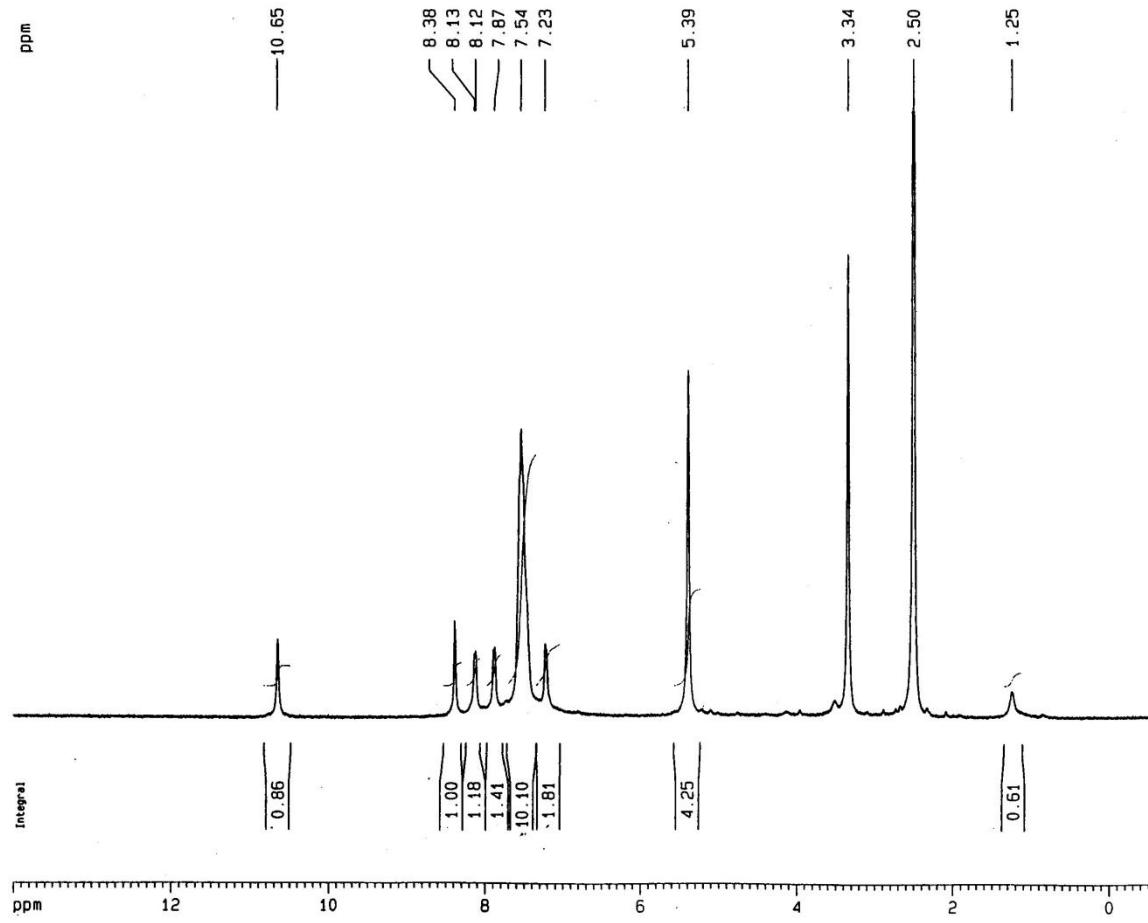
216



217

218

Figure S2. ^1H NMR spectrum ($\text{DMSO}-d_6$, 400 MHz) of compound **7b**

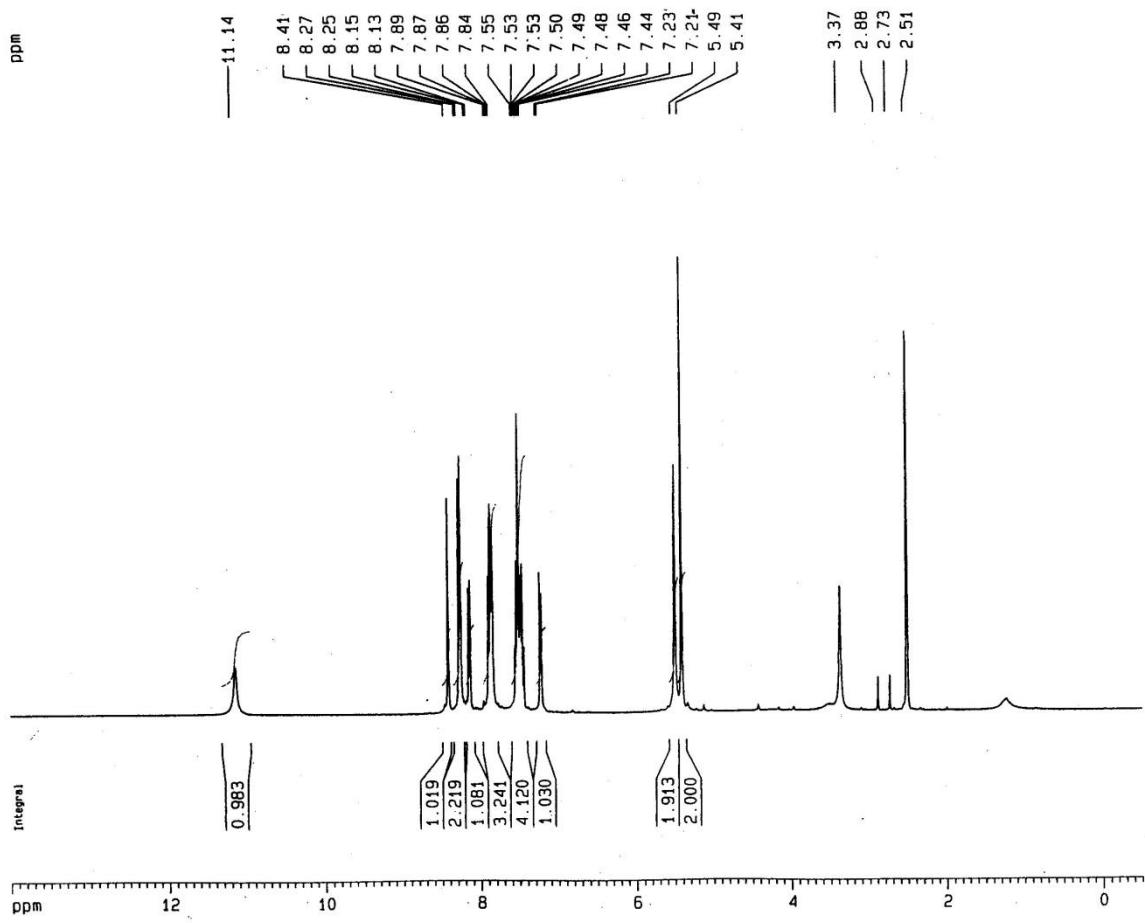


219

220

Figure S3. ^1H NMR spectrum ($\text{DMSO}-d_6$, 400 MHz) of compound **7c**

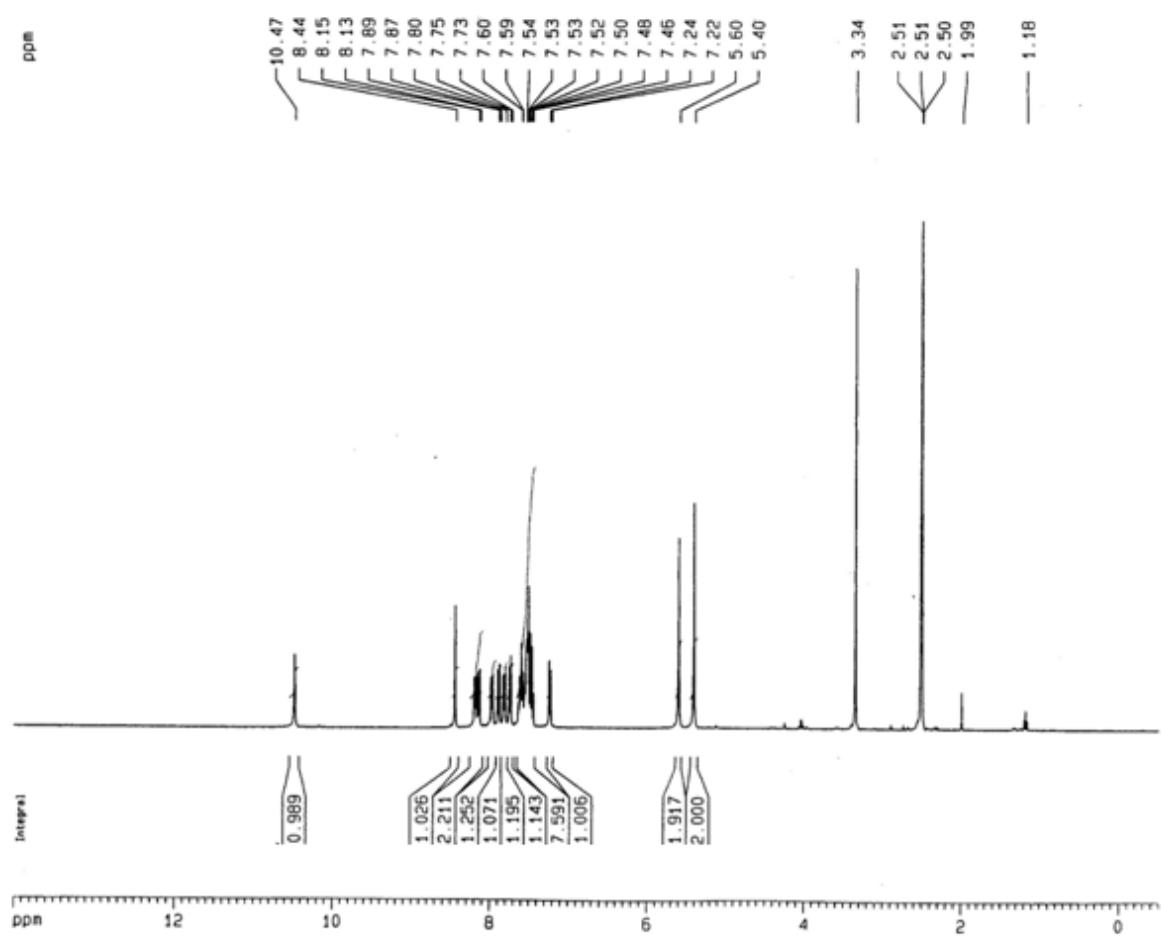
221



222

223

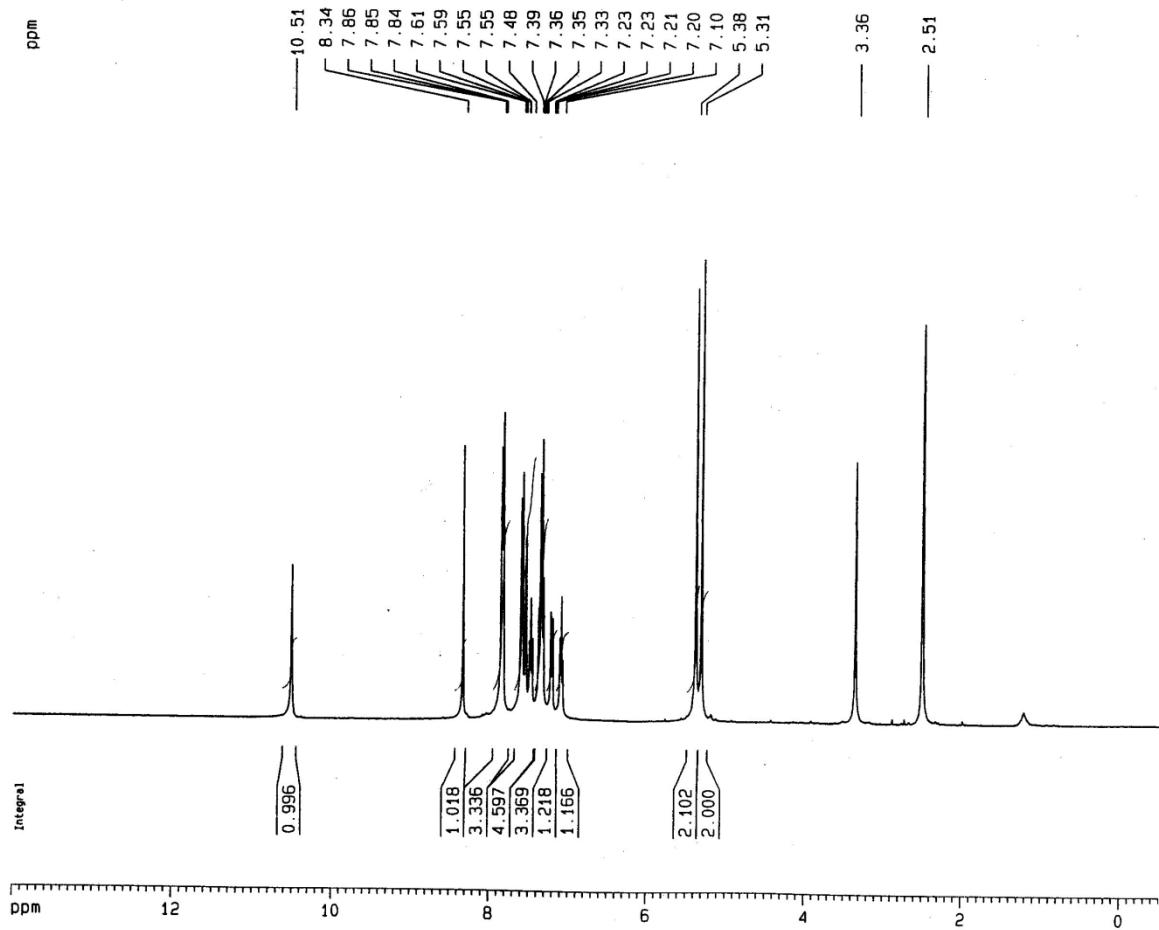
Figure S4. ^1H NMR spectrum (DMSO- d_6 , 400 MHz) of compound **7d**



224

225

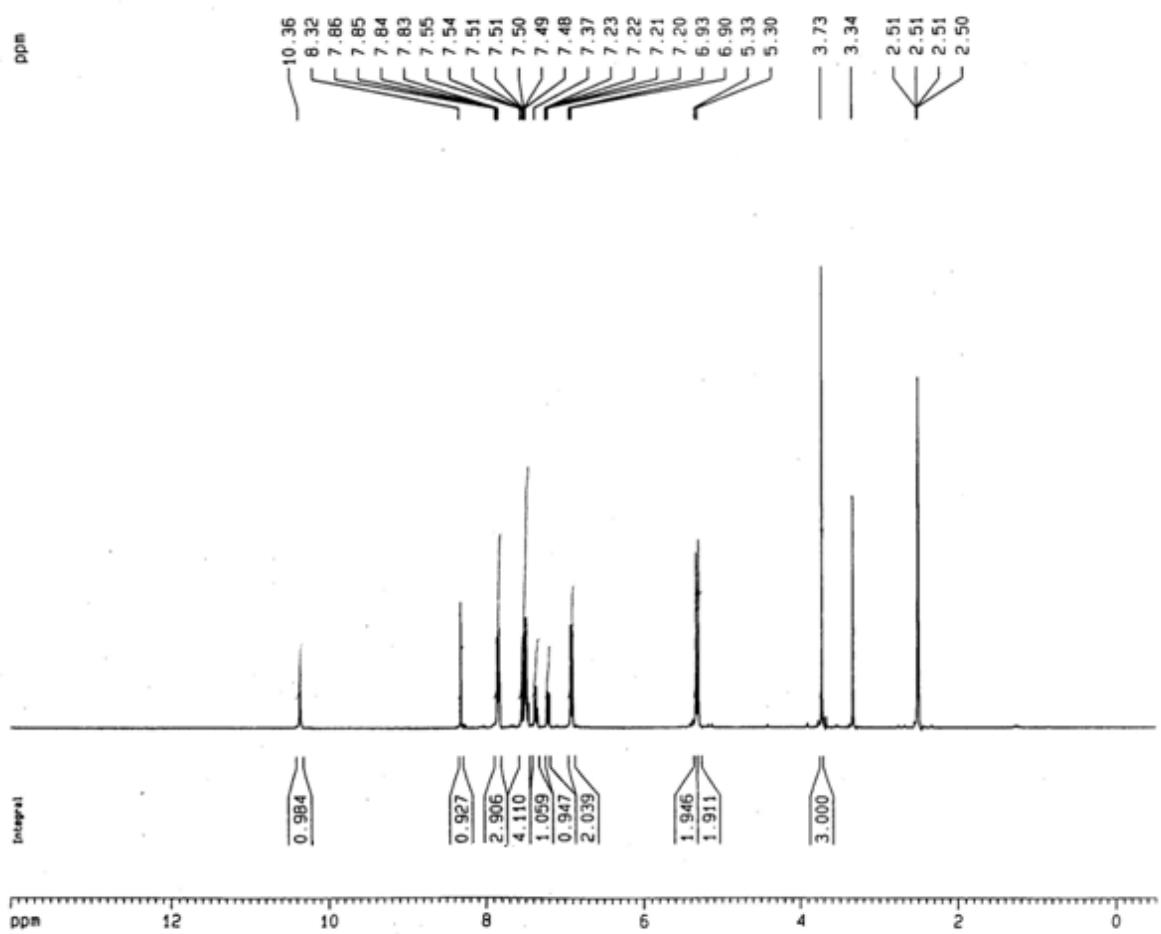
Figure S5. ^1H NMR spectrum (DMSO- d_6 , 400 MHz) of compound **7e**



226

227

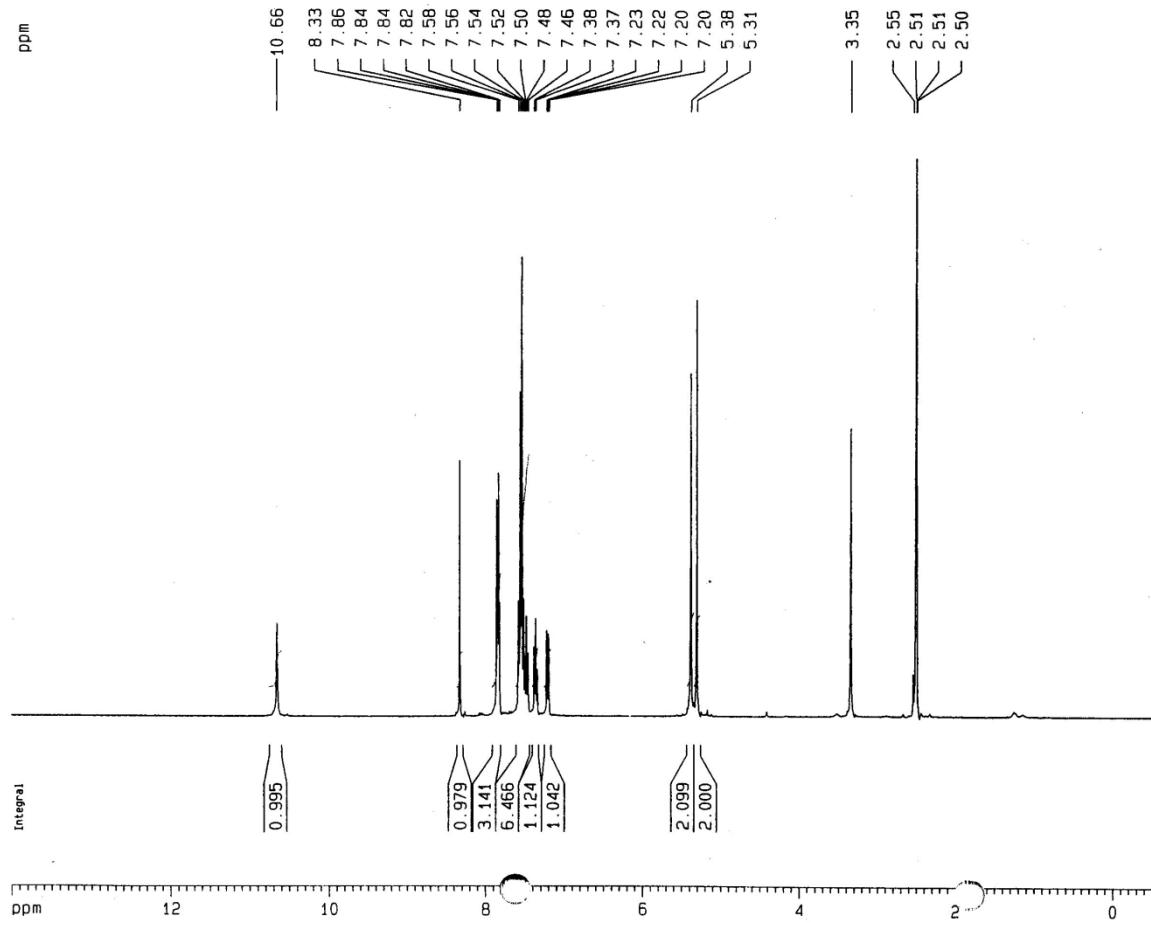
Figure S6. ^1H NMR spectrum (DMSO- d_6 , 400 MHz) of compound **10a**



228

229

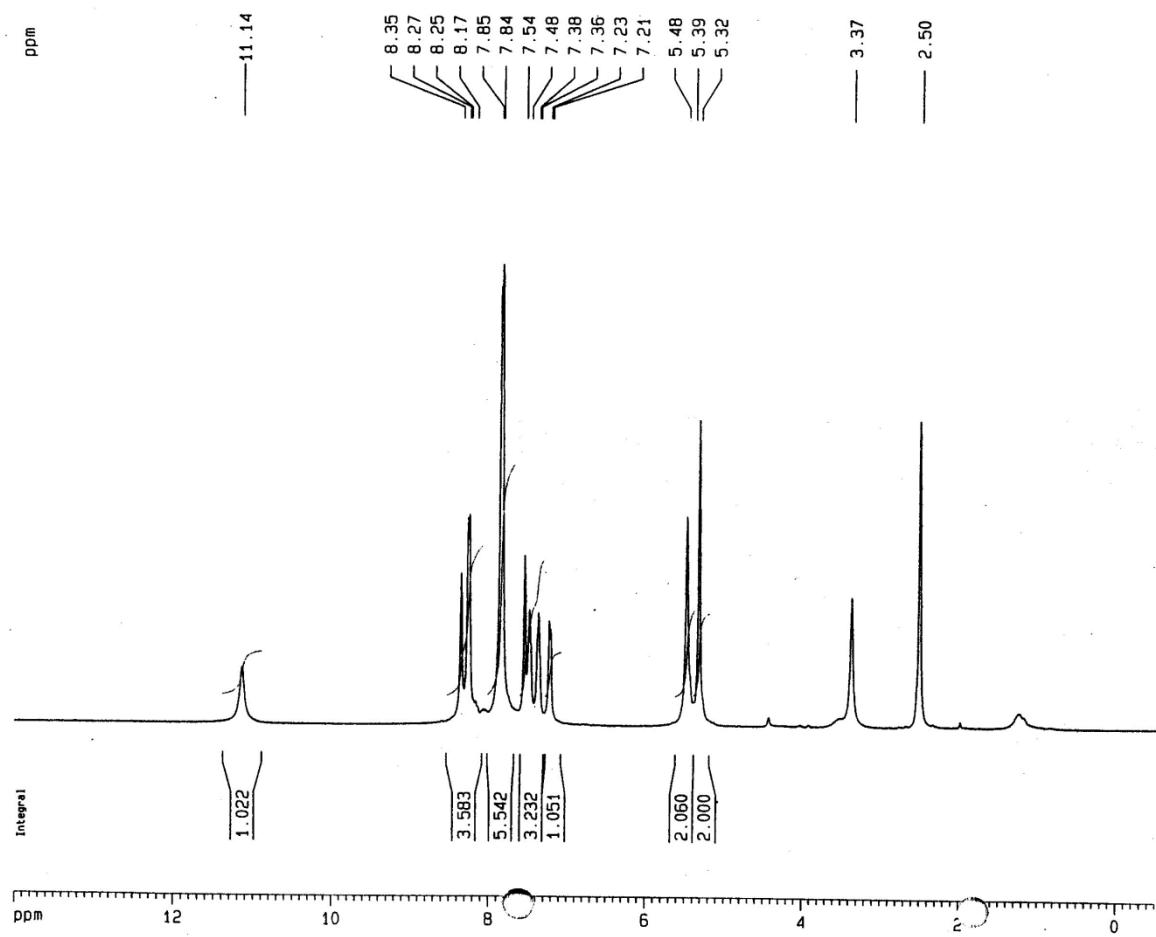
Figure S7. ^1H NMR spectrum (DMSO- d_6 , 400 MHz) of compound **10b**



230

231

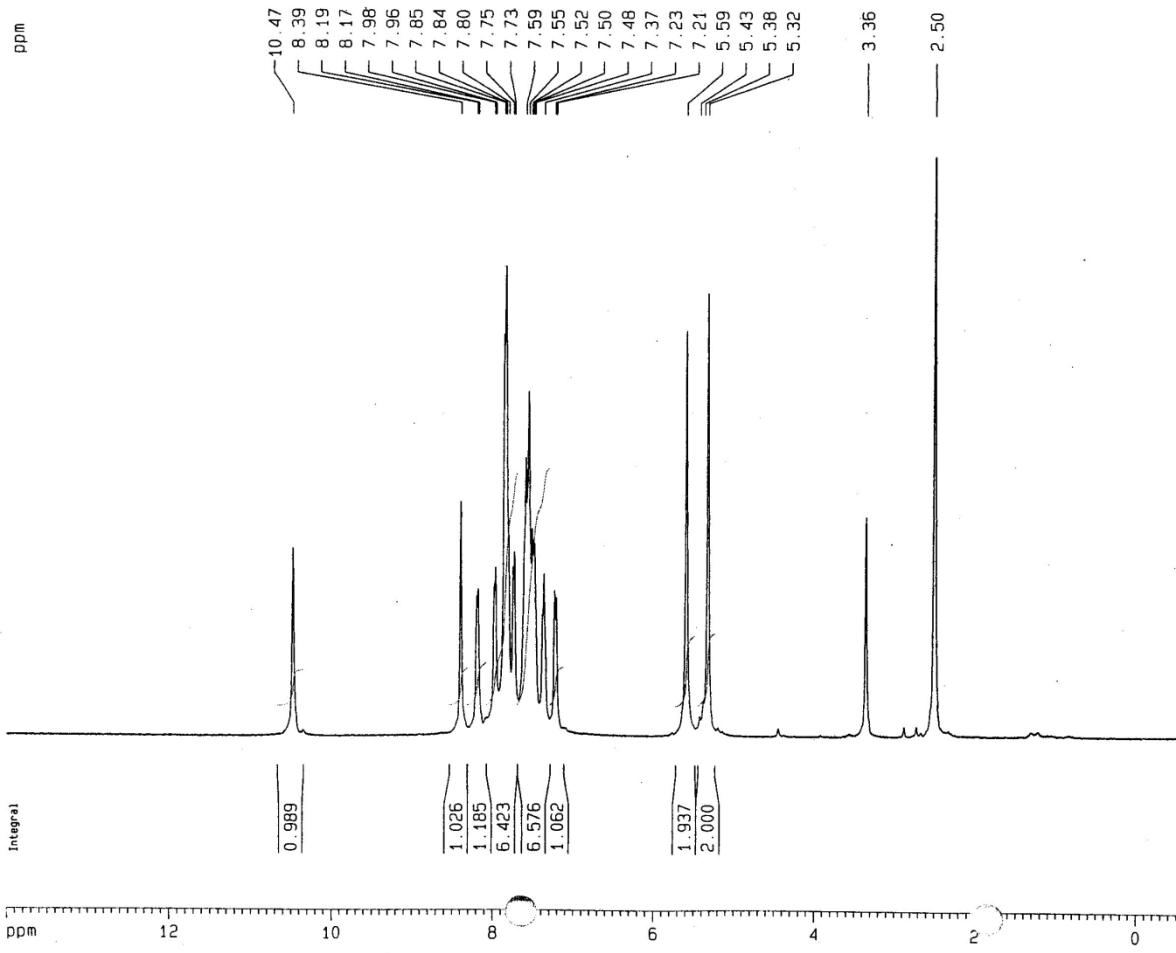
Figure S8. ^1H NMR spectrum ($\text{DMSO}-d_6$, 400 MHz) of compound **10c**



232

233

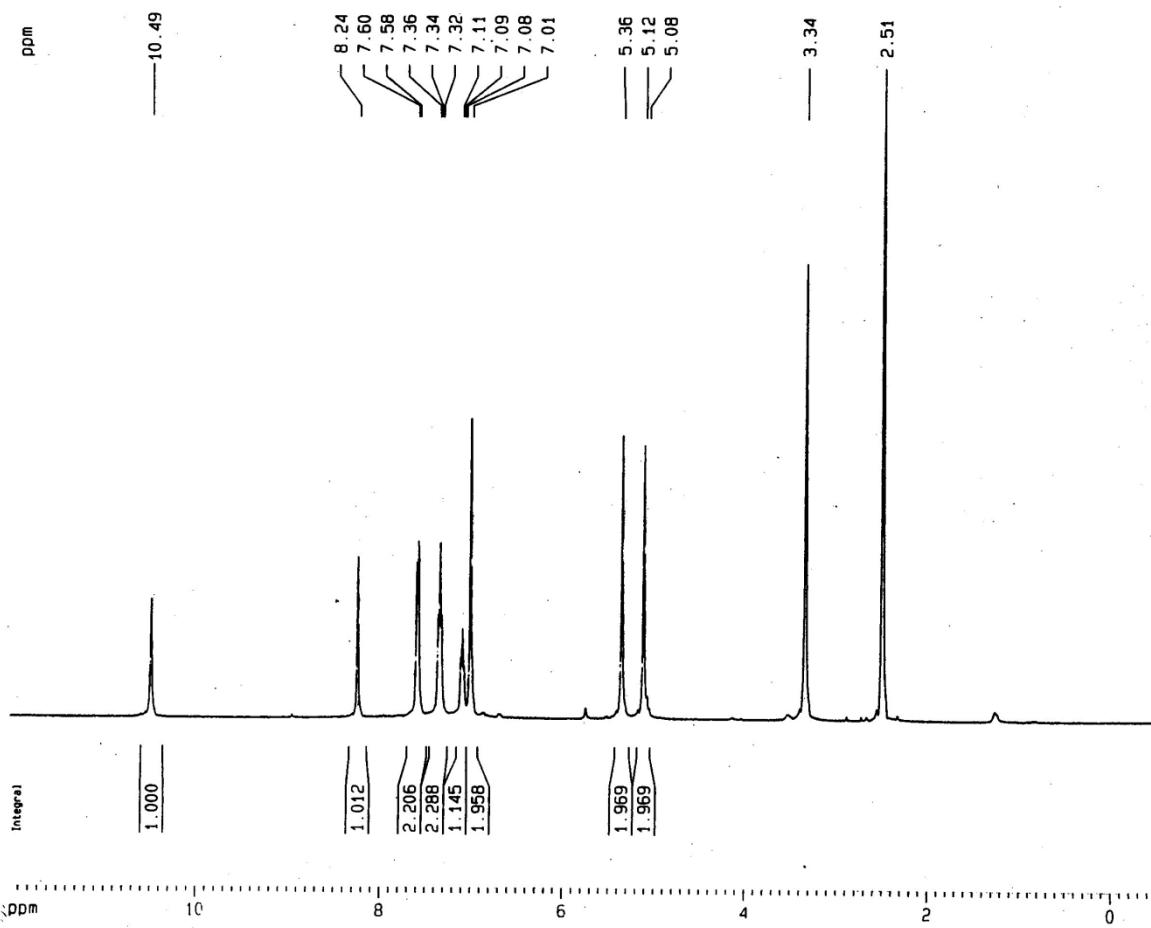
Figure S9. ^1H NMR spectrum ($\text{DMSO}-d_6$, 400 MHz) of compound **10d**



234

235

Figure S10. ^1H NMR spectrum ($\text{DMSO}-d_6$, 400 MHz) of compound **10e**

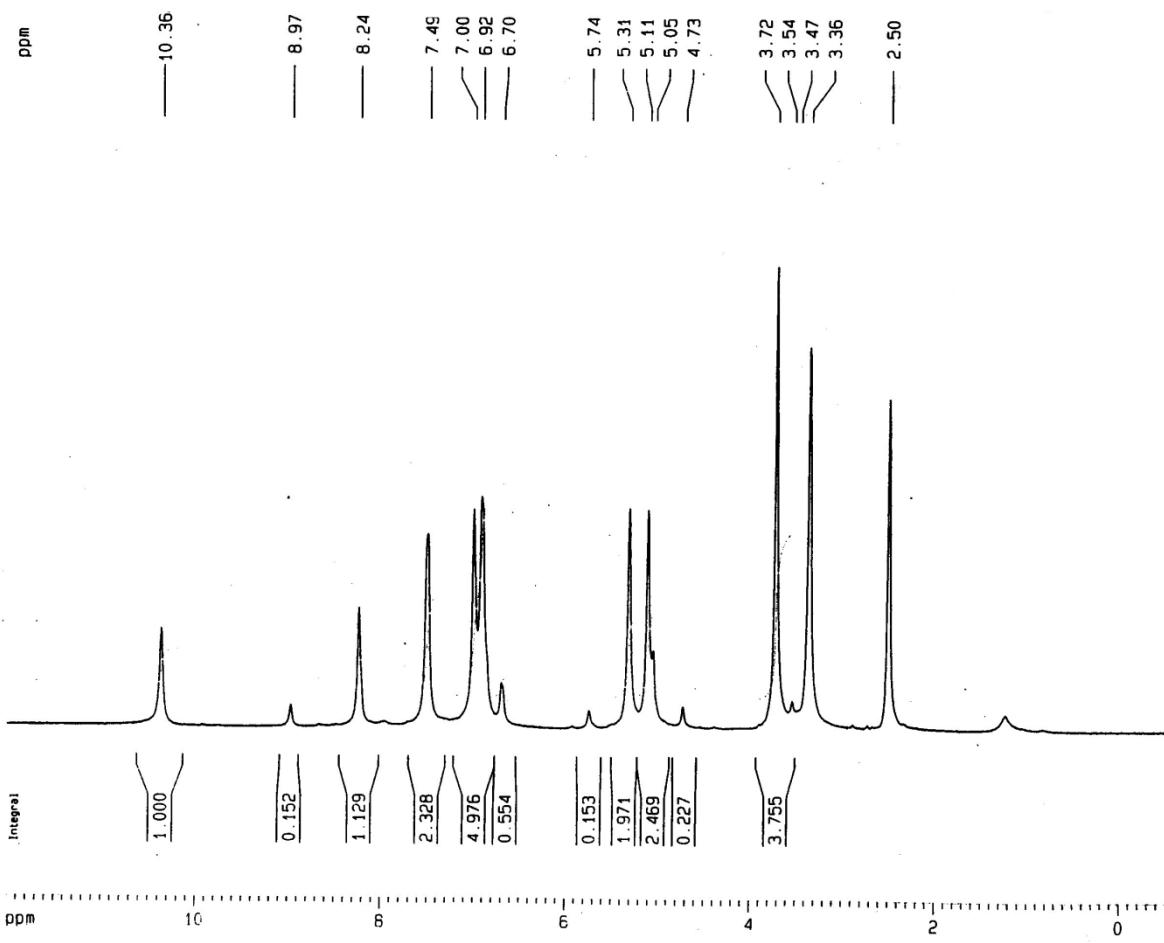


236

237

Figure S11. ^1H NMR spectrum ($\text{DMSO}-d_6$, 400 MHz) of compound **13a**

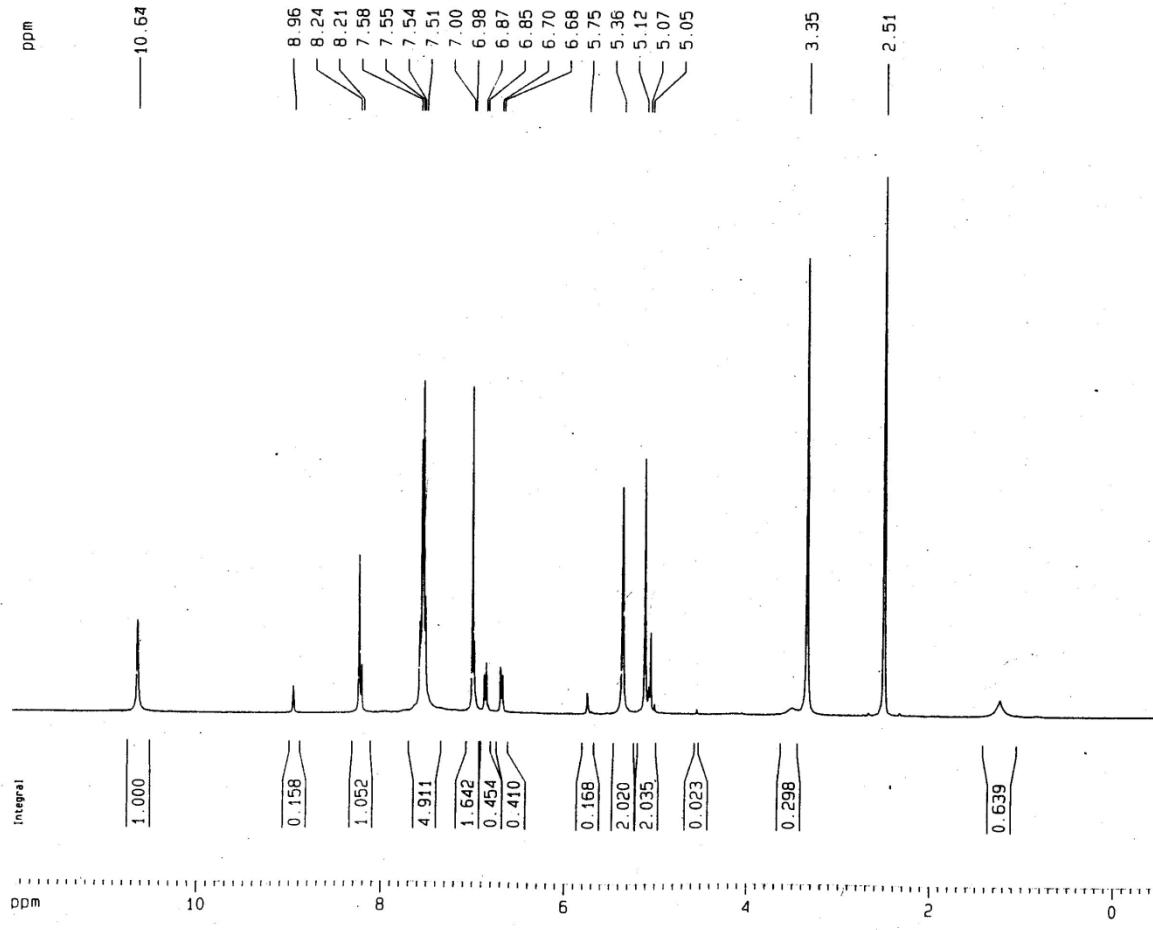
238



239

240

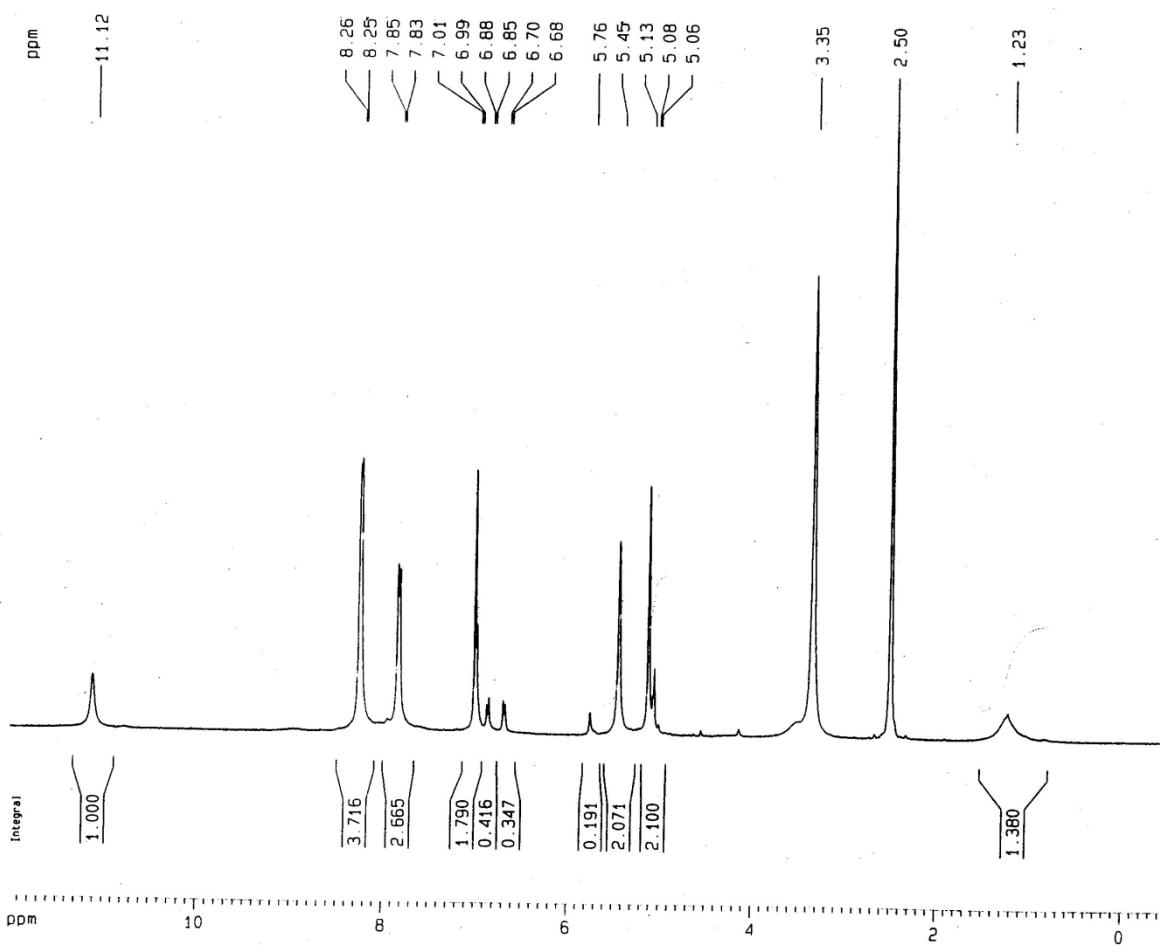
Figure S12. ^1H NMR spectrum (DMSO- d_6 , 400 MHz) of compound **13b**



241

242

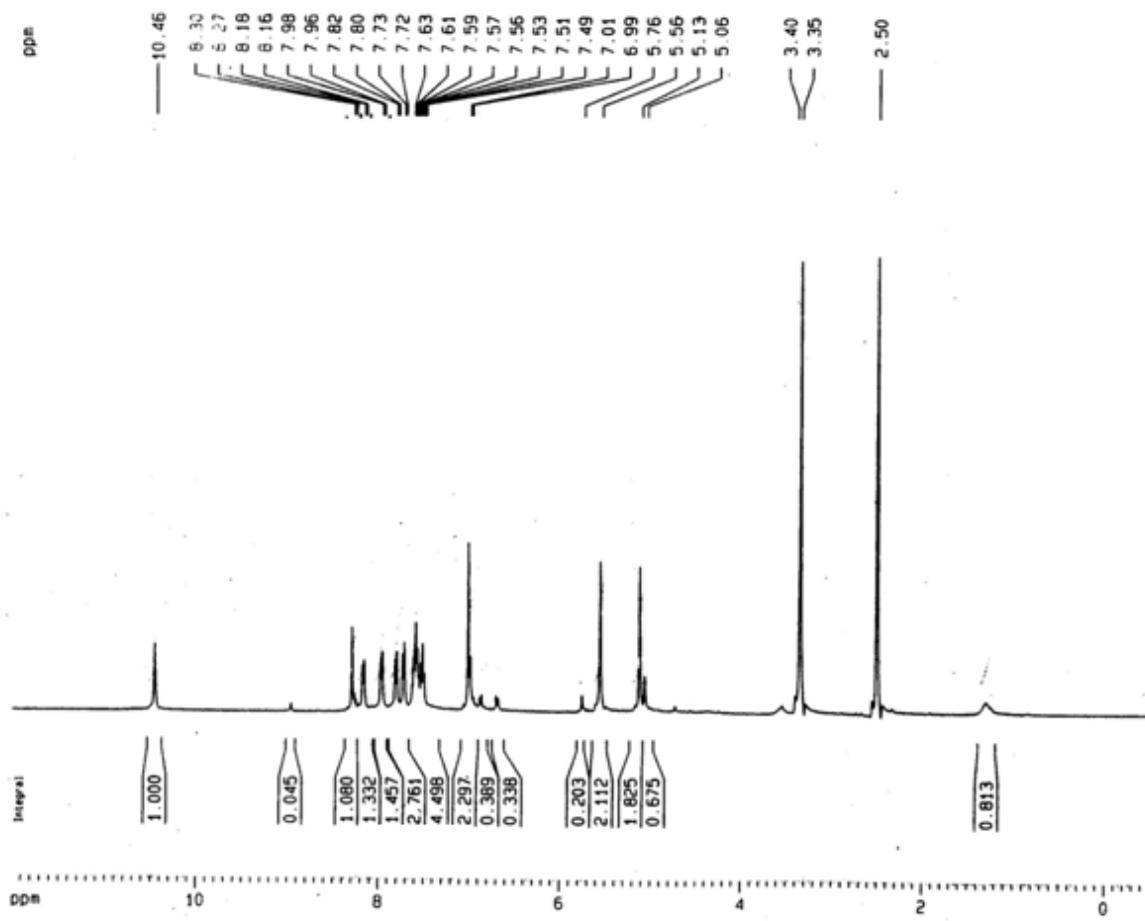
Figure S13. ^1H NMR spectrum ($\text{DMSO}-d_6$, 400 MHz) of compound **13c**



243

244

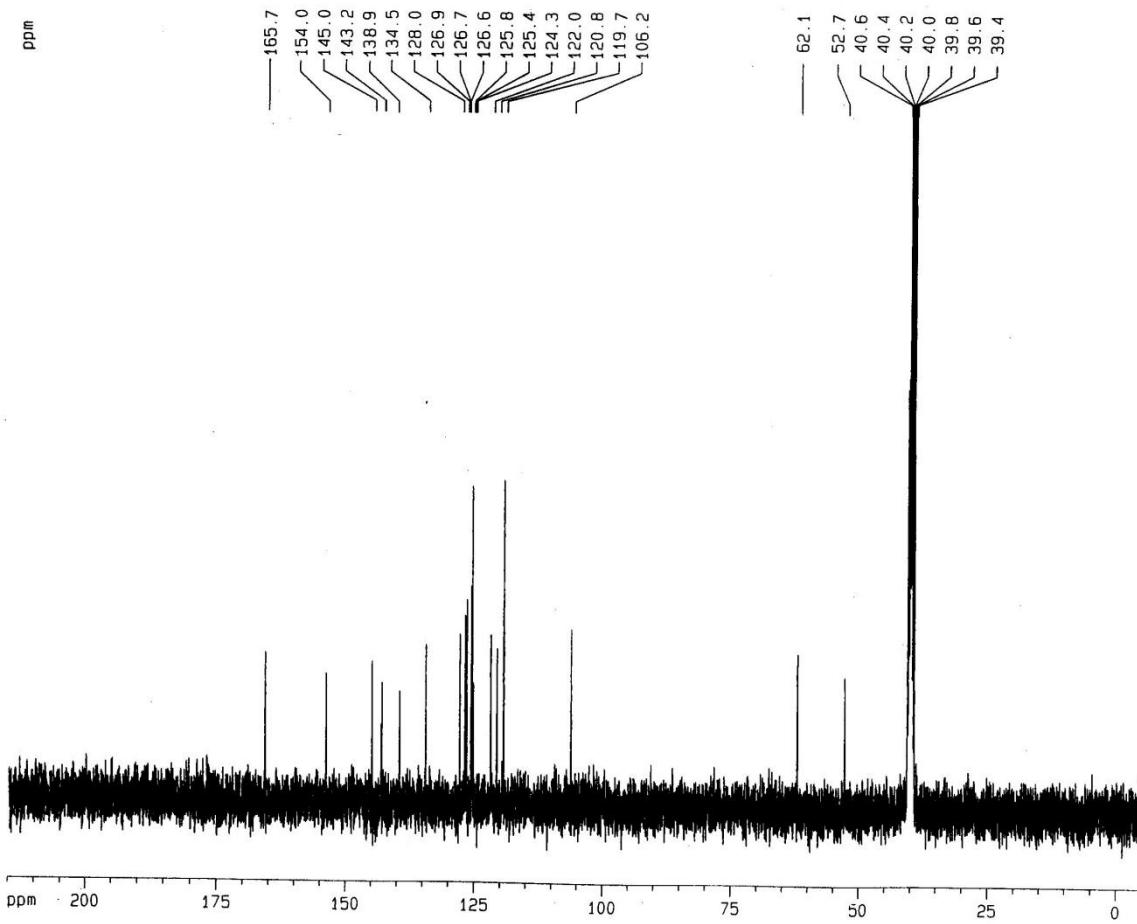
Figure S14. ^1H NMR spectrum (DMSO- d_6 , 400 MHz) of compound **13d**



245

246

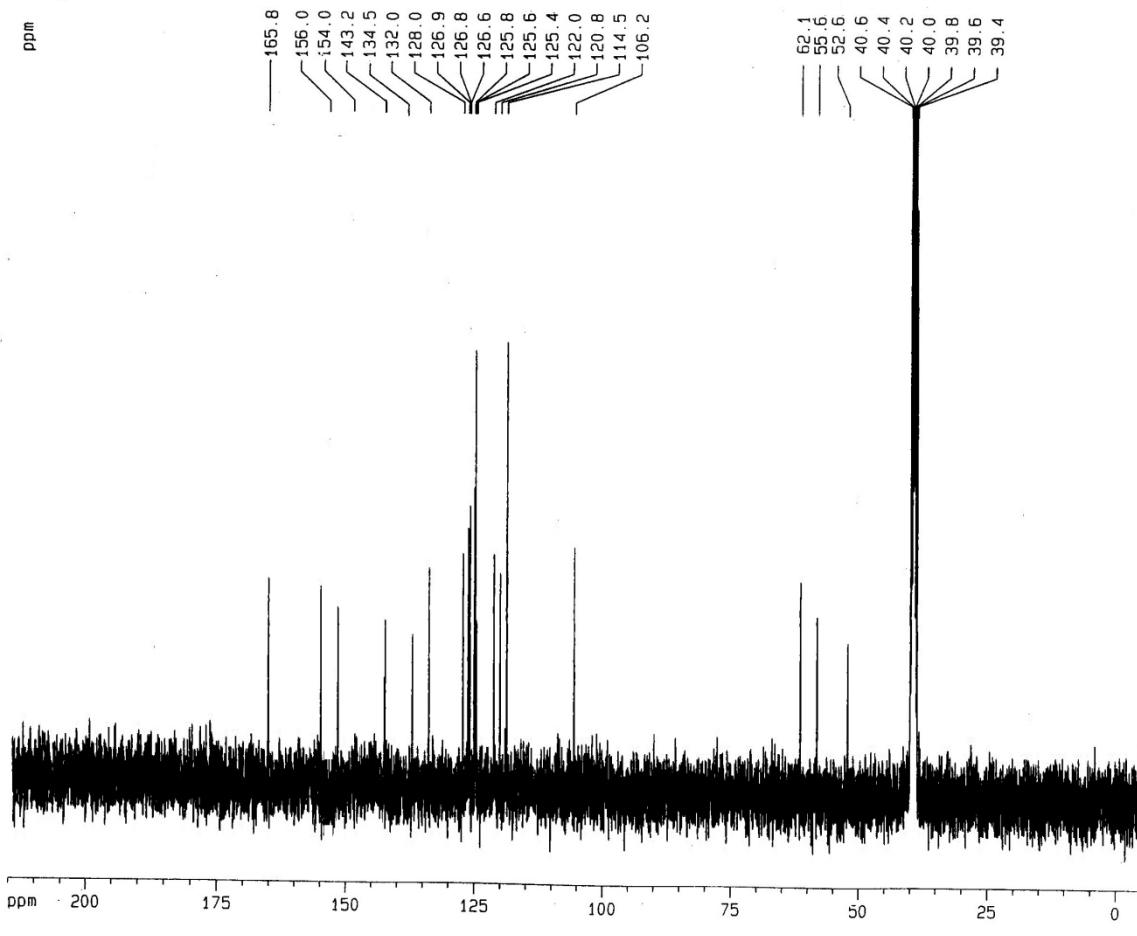
Figure S15. ^1H NMR spectrum (DMSO- d_6 , 400 MHz) of compound **13e**



247

248

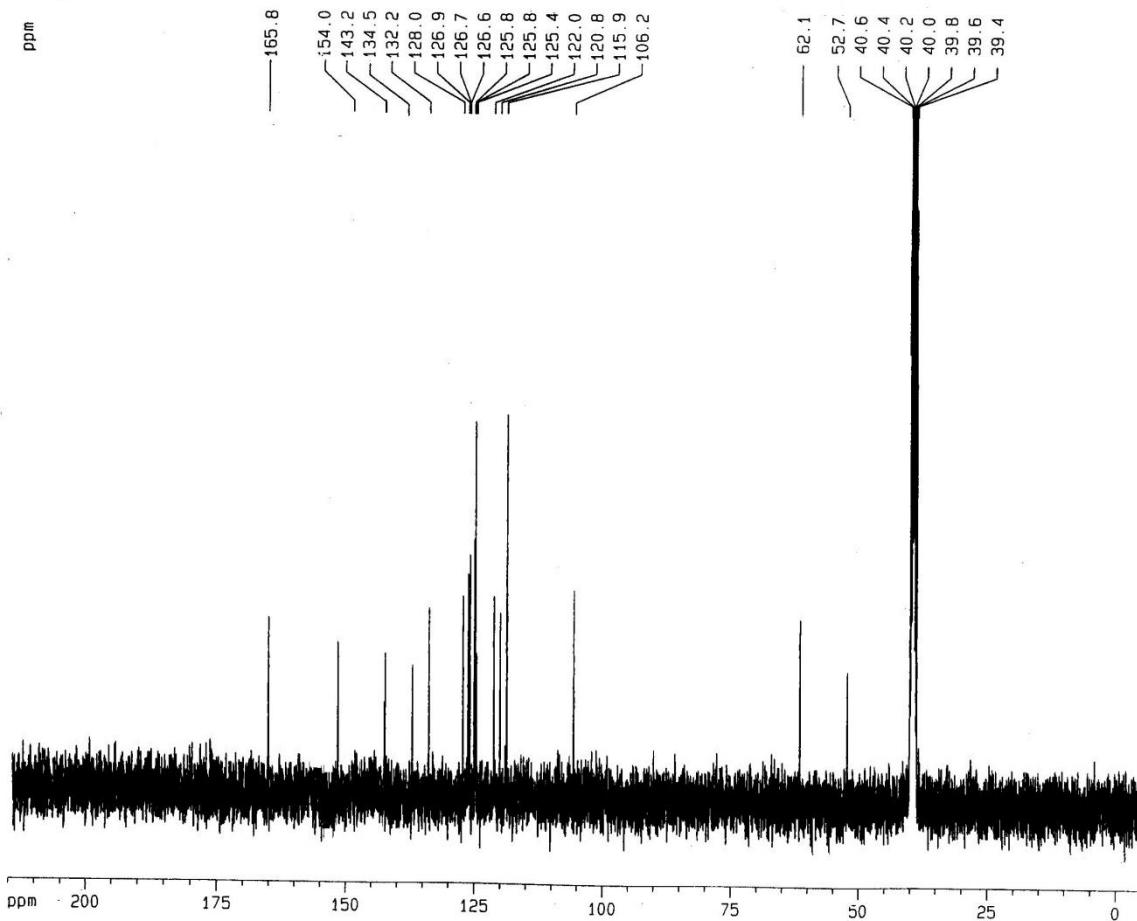
Figure S16. ¹³C NMR spectrum (DMSO-*d*₆, 100 MHz) of compound 7a



249

250

Figure S17. ^{13}C NMR spectrum ($\text{DMSO}-d_6$, 100 MHz) of compound **7b**



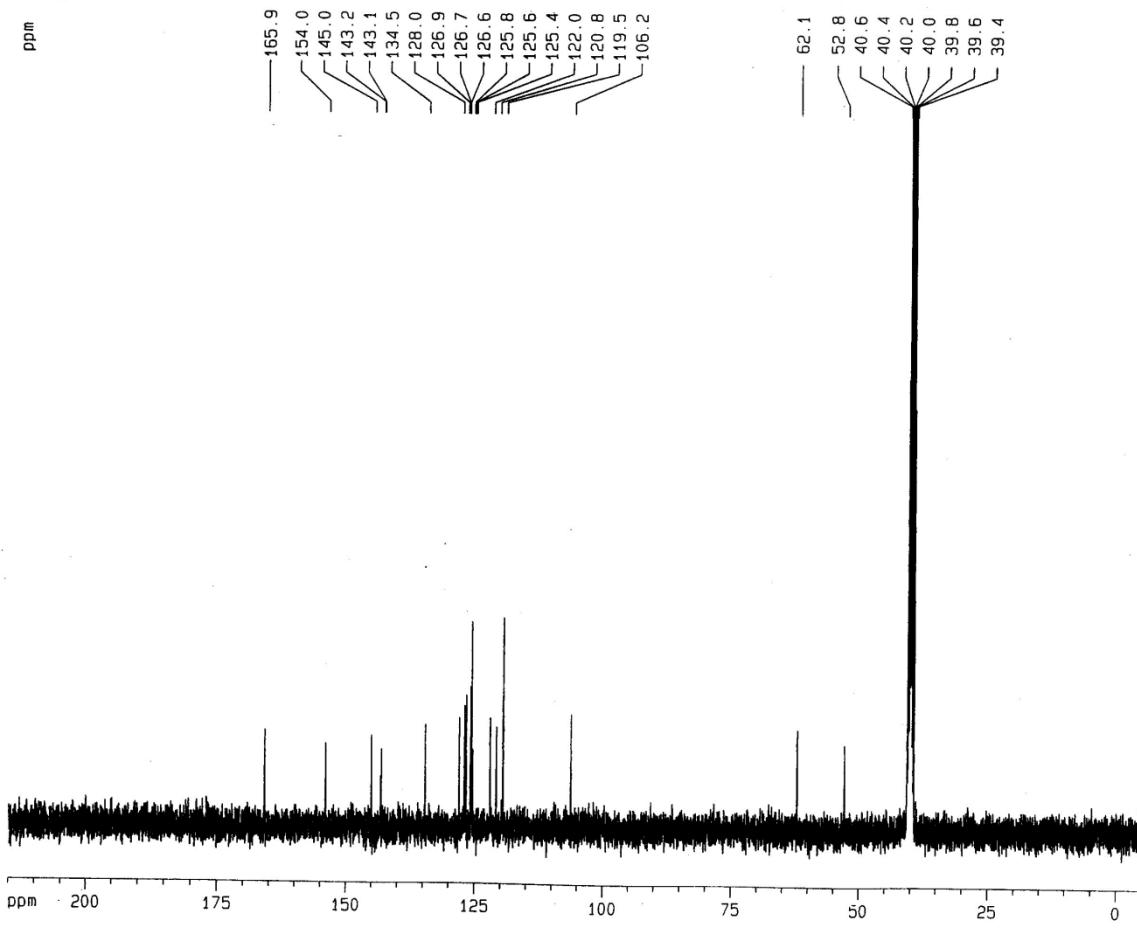
251

252

Figure S18. ^{13}C NMR spectrum ($\text{DMSO}-d_6$, 100 MHz) of compound **7c**

253

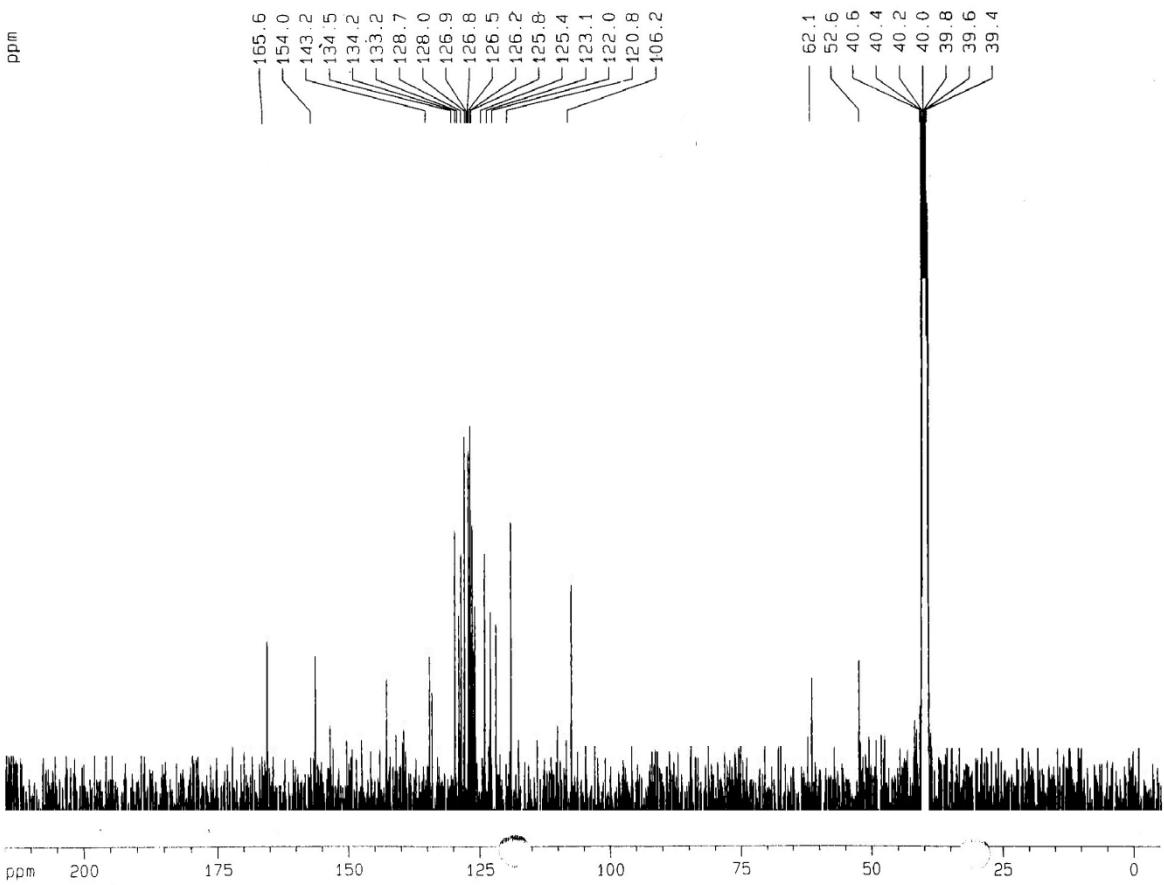
254



255

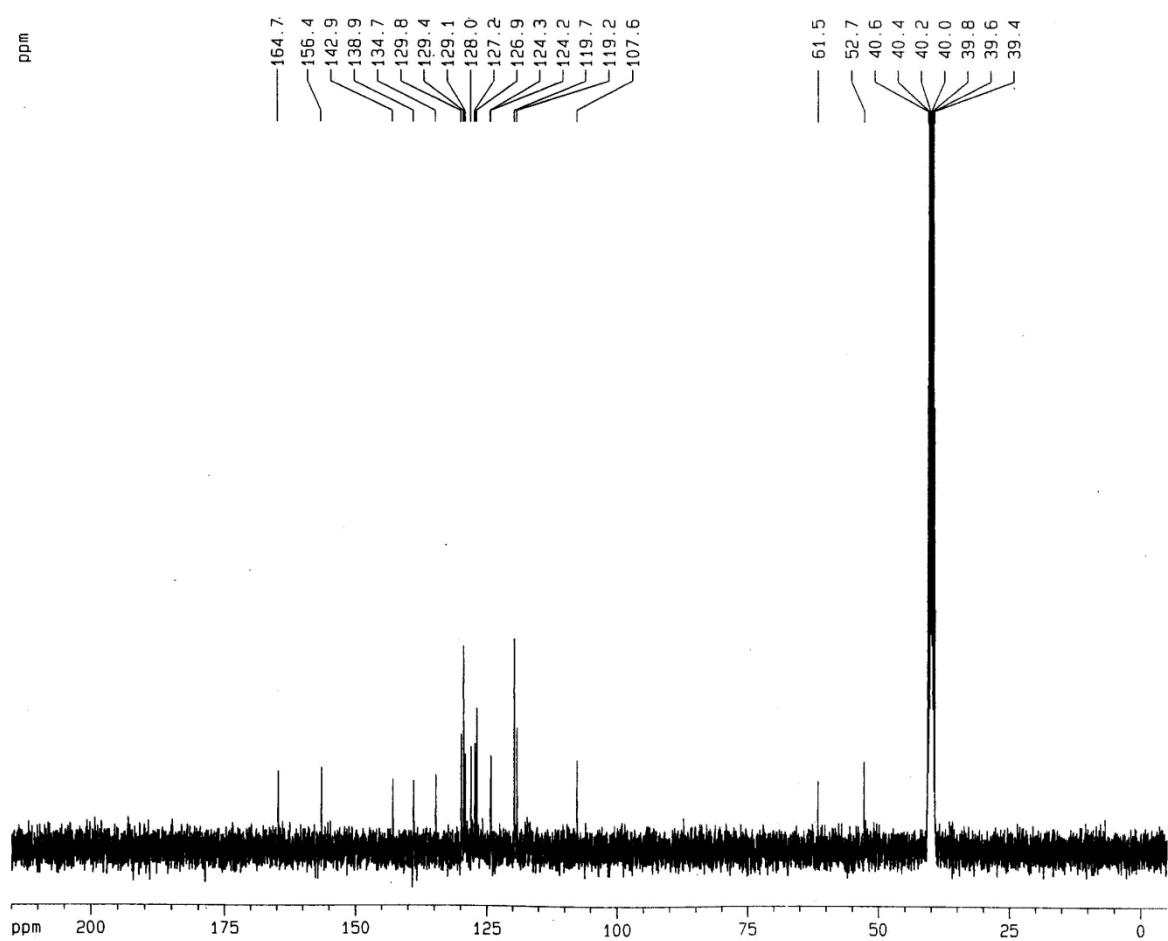
256

Figure S19. ^{13}C NMR spectrum ($\text{DMSO}-d_6$, 100 MHz) of compound **7d**



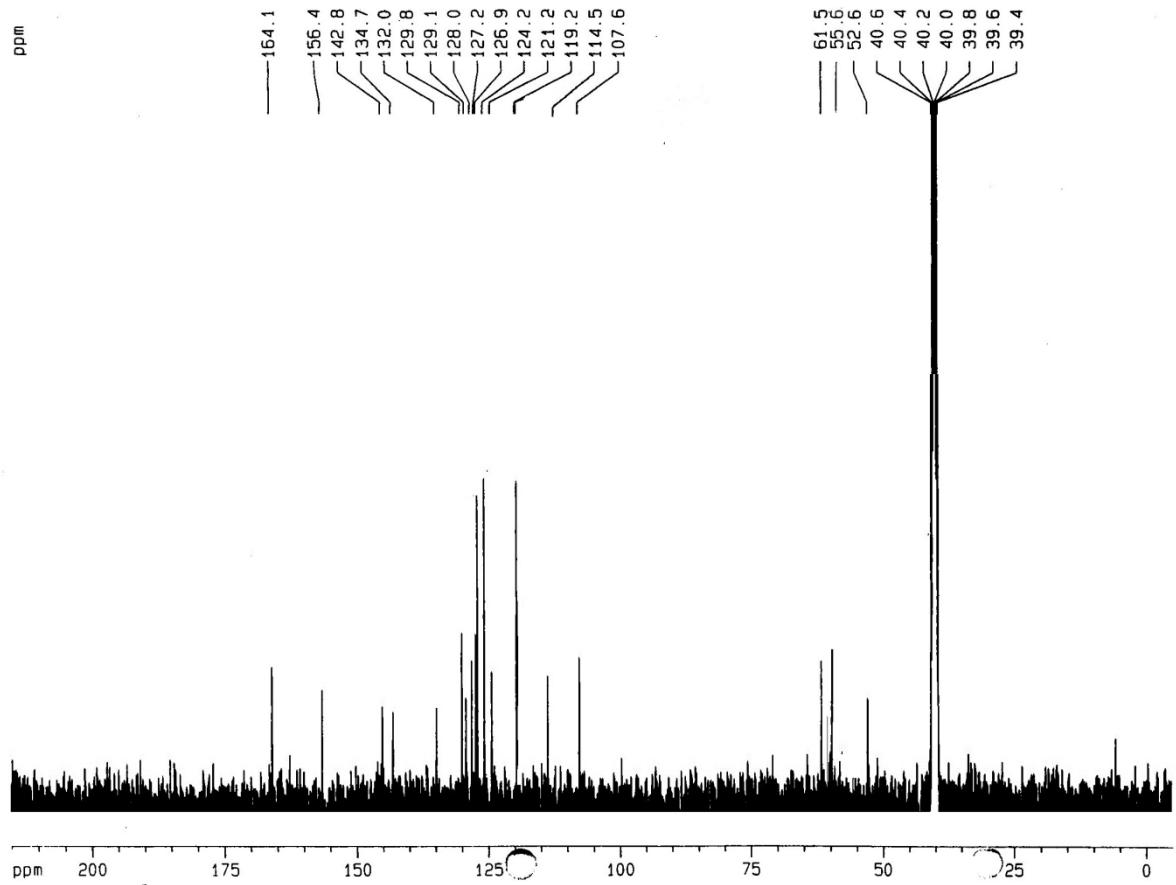
257
258
259

Figure S20. ^{13}C NMR spectrum ($\text{DMSO}-d_6$, 100 MHz) of compound **7e**



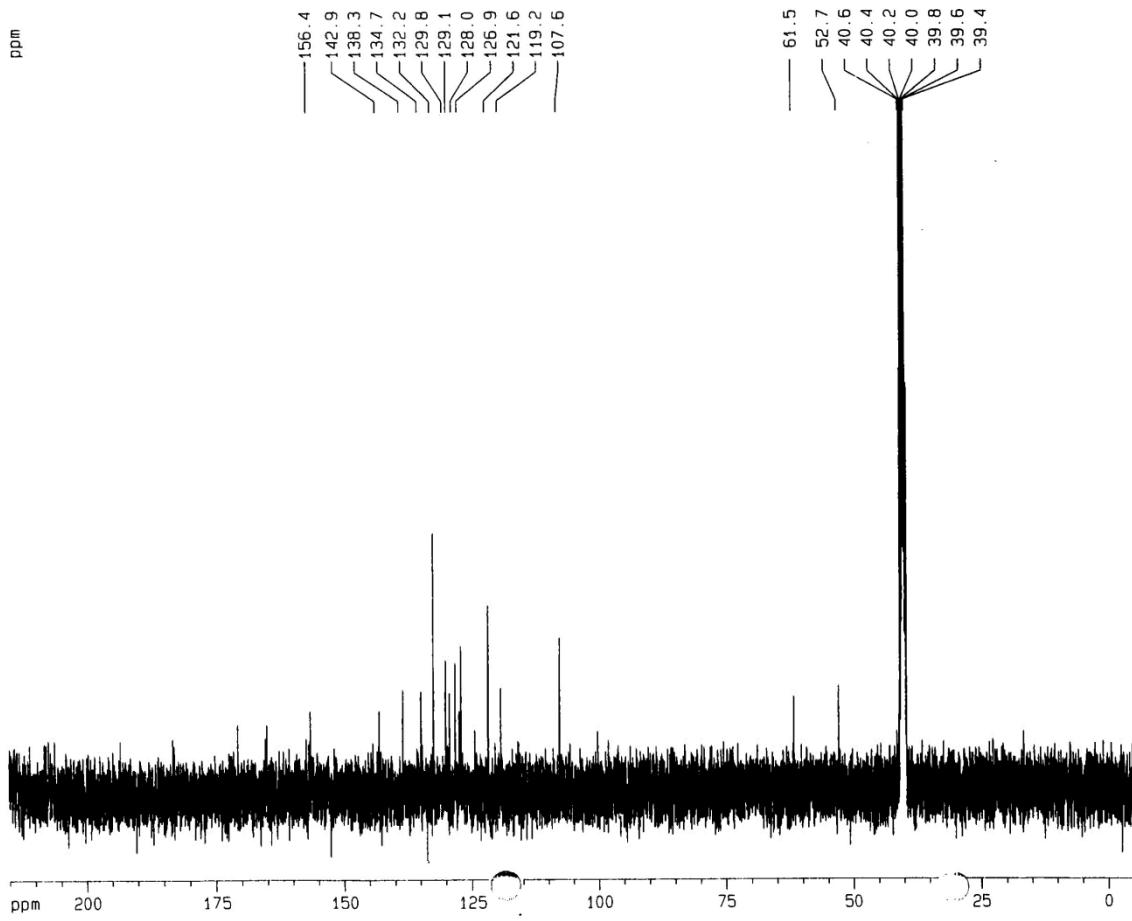
260
261

Figure S21. ^{13}C NMR spectrum (DMSO- d_6 , 100 MHz) of compound 10a



262
263
264

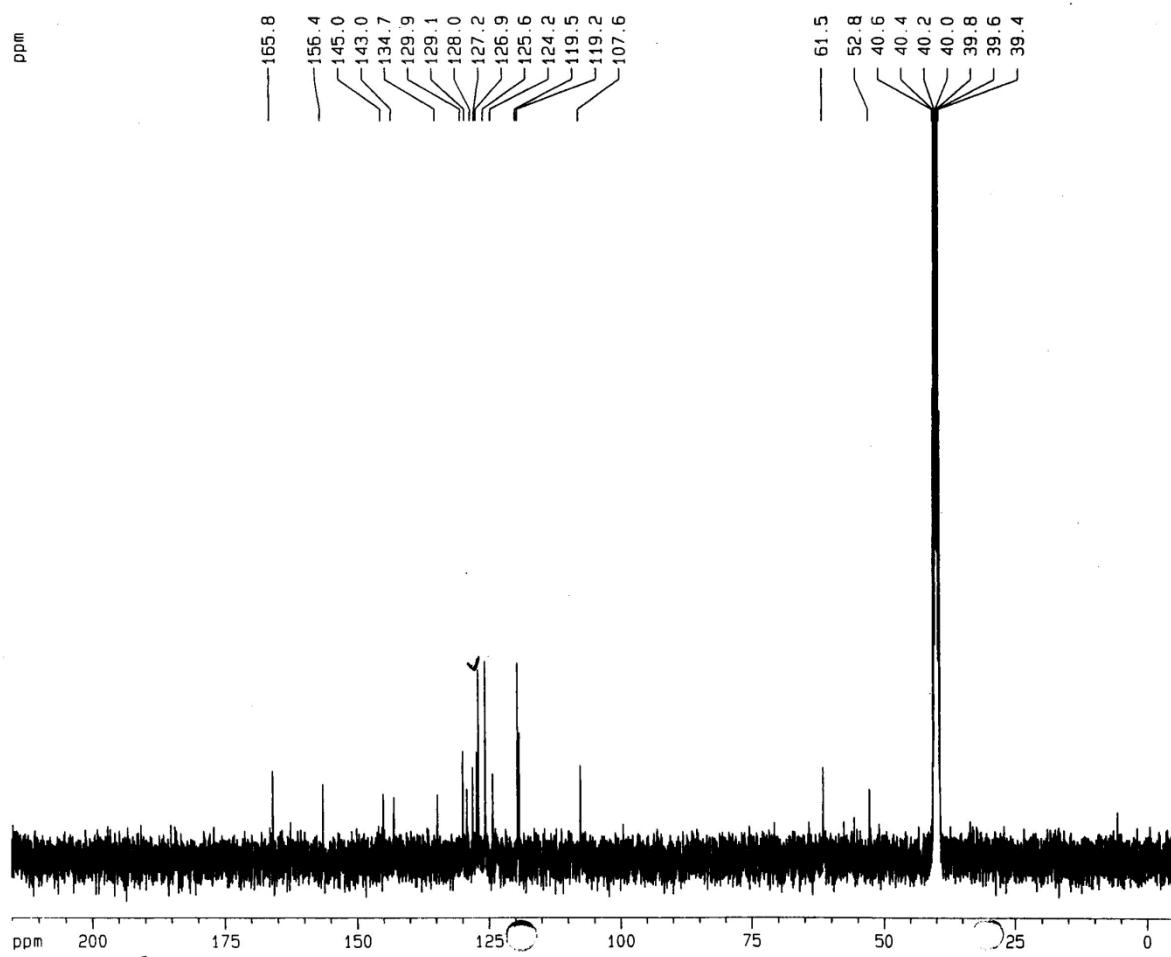
Figure S22. ^{13}C NMR spectrum ($\text{DMSO}-d_6$, 100 MHz) of compound **10b**



265

266

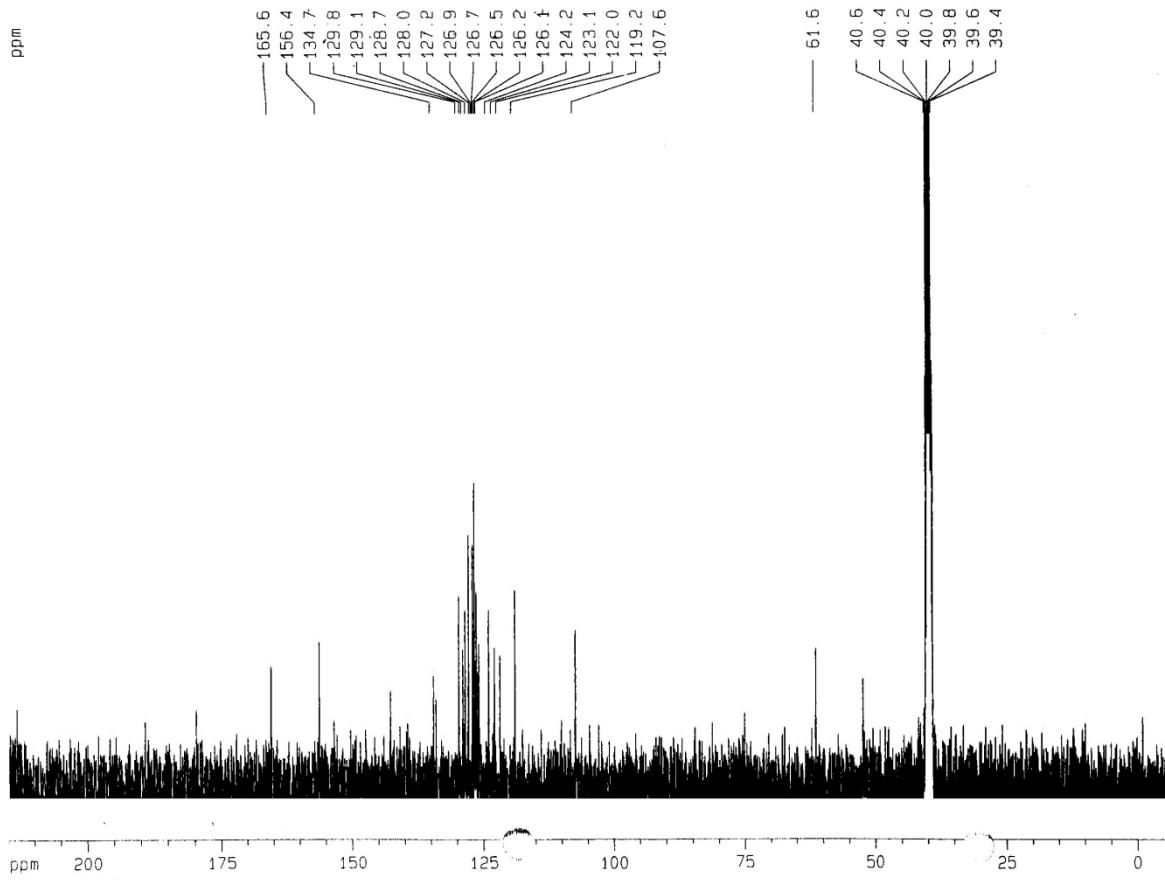
Figure S23. ^{13}C NMR spectrum ($\text{DMSO}-d_6$, 100 MHz) of compound **10c**

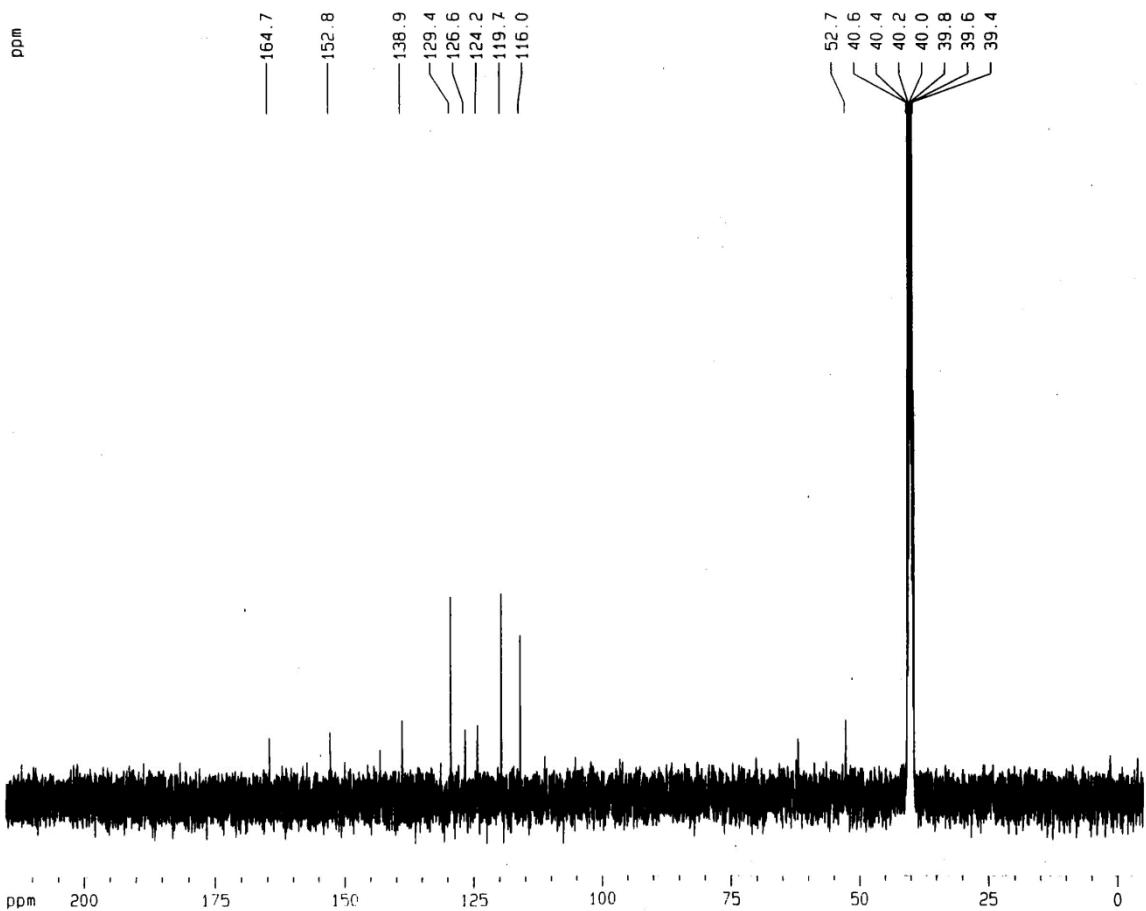


267

268

Figure S24. ^{13}C NMR spectrum ($\text{DMSO}-d_6$, 100 MHz) of compound **10d**

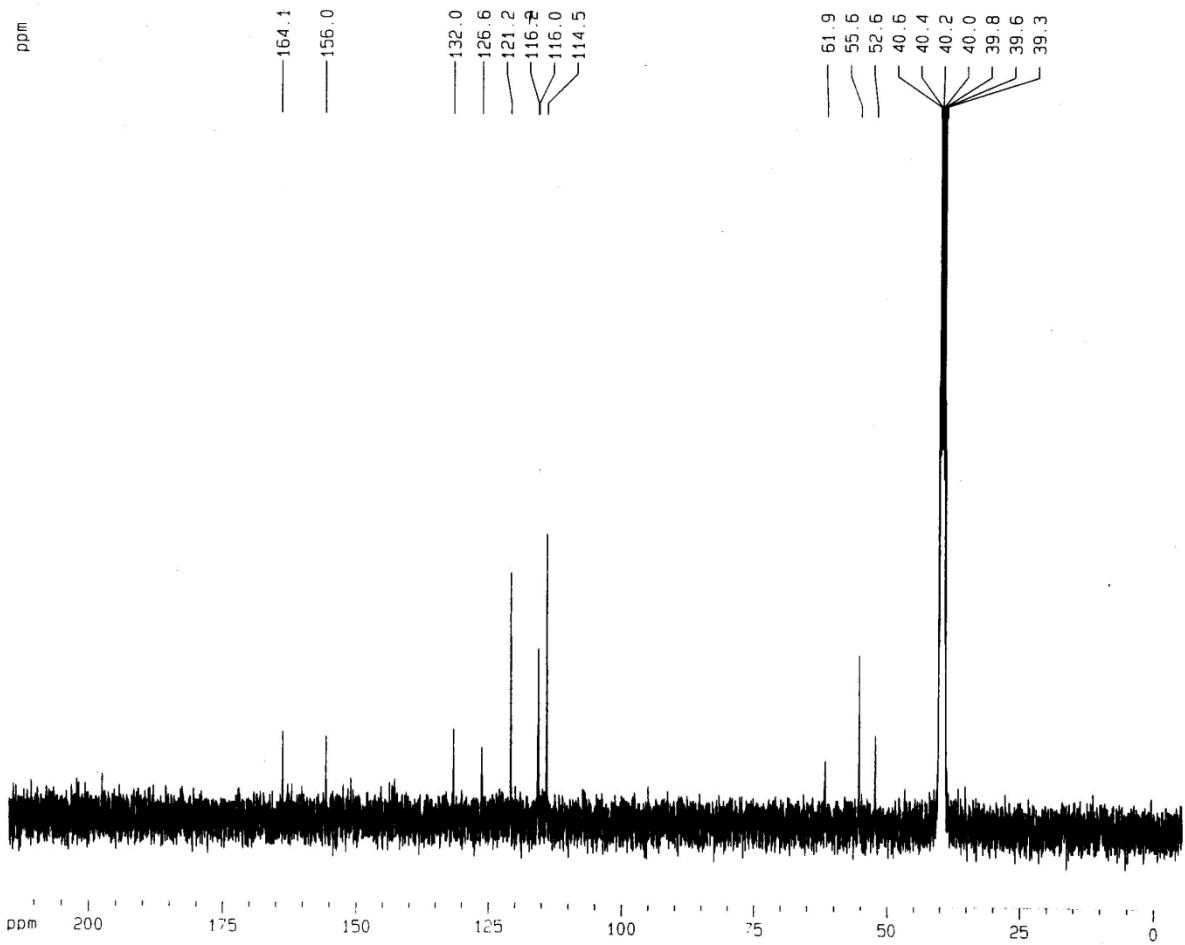




271

272

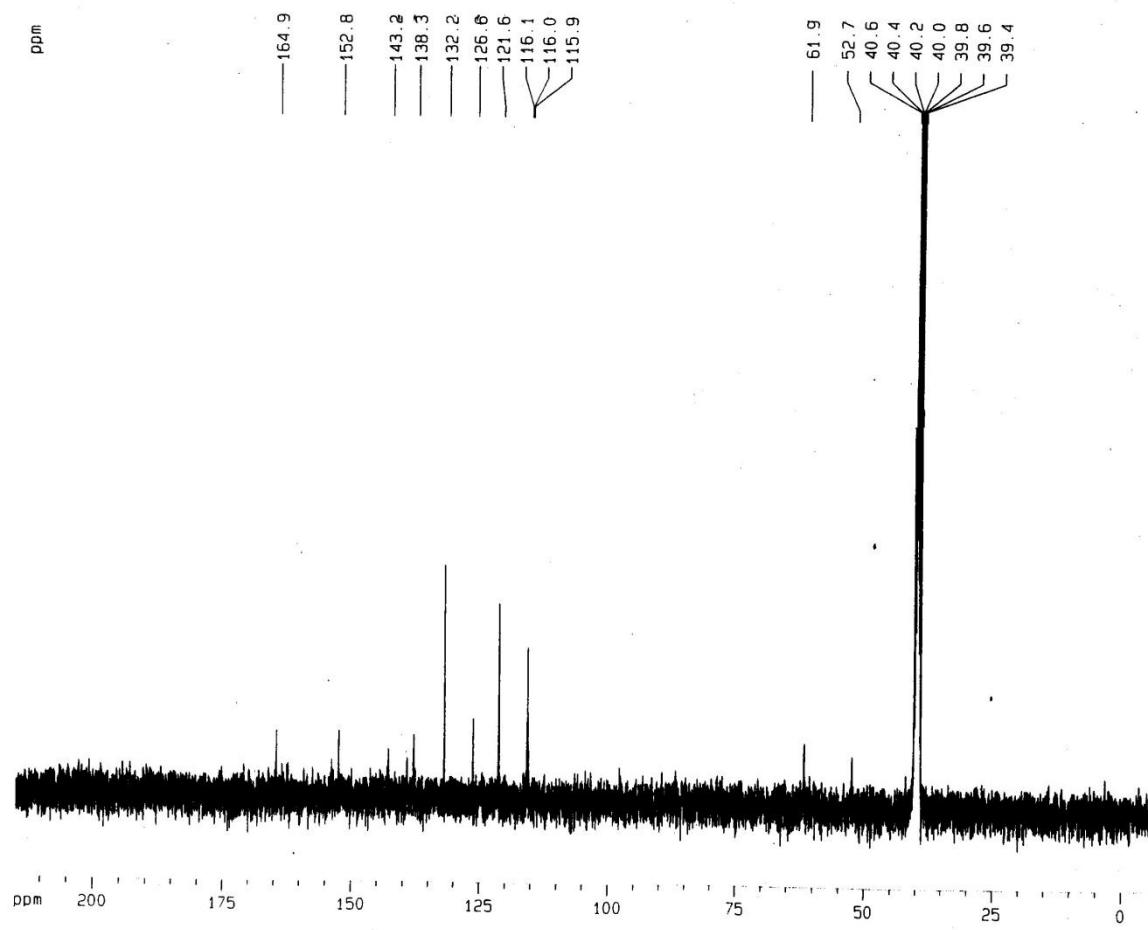
Figure S26. ^{13}C NMR spectrum ($\text{DMSO}-d_6$, 100 MHz) of compound **13a**



273

274

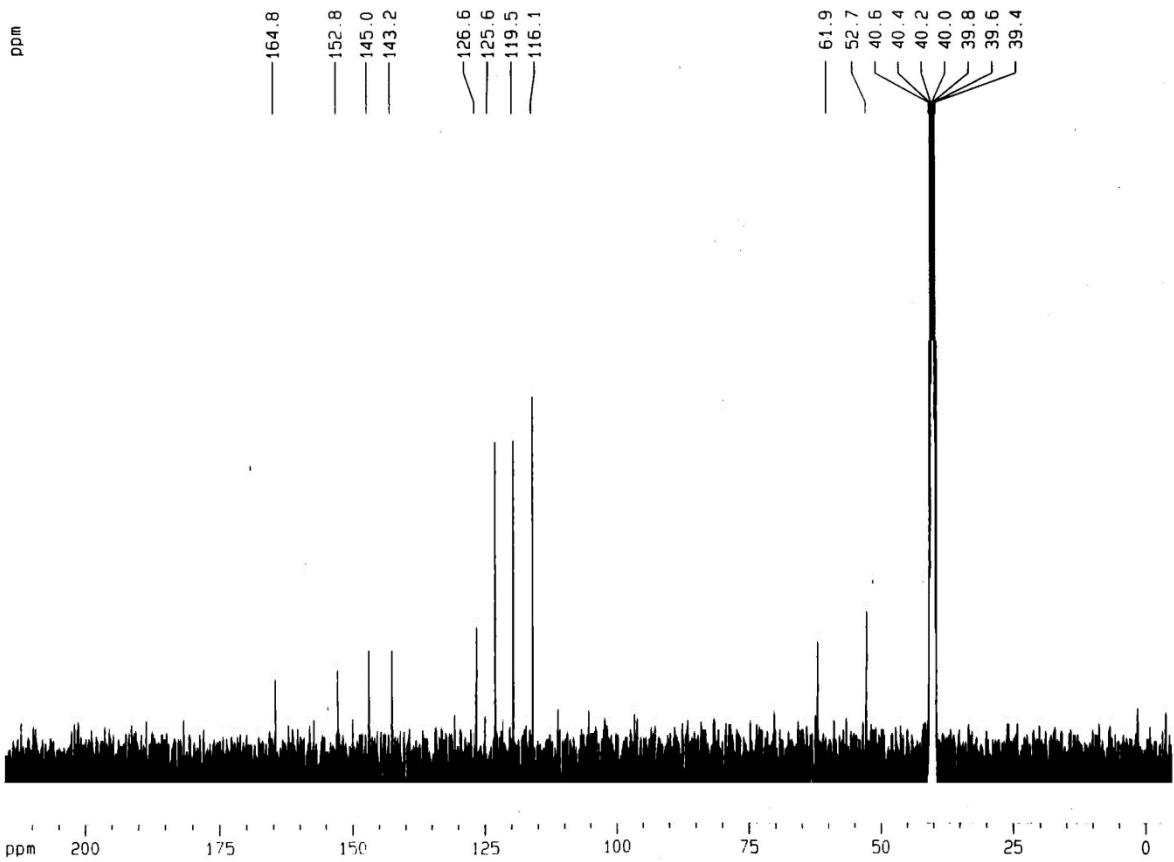
Figure S27. ^{13}C NMR spectrum ($\text{DMSO}-d_6$, 100 MHz) of compound **13b**



275

276

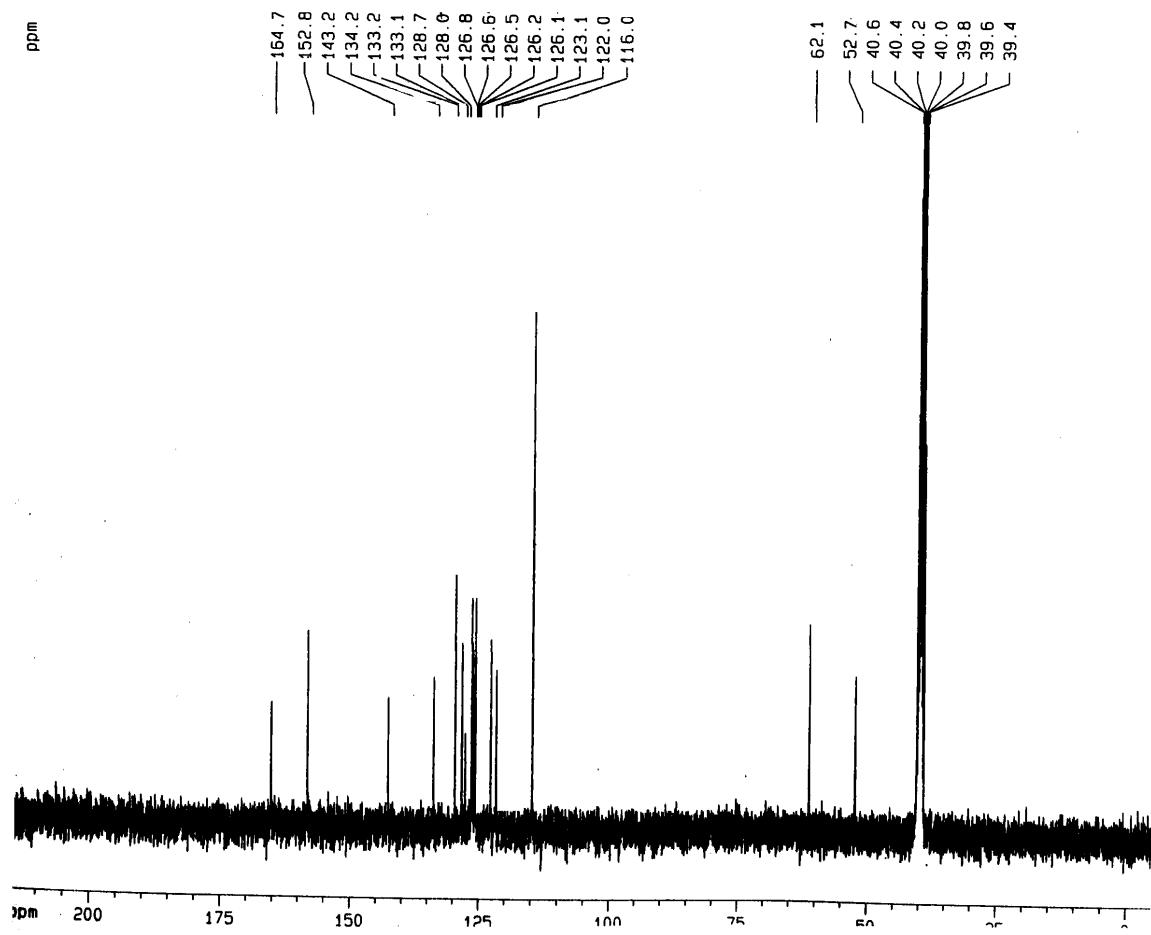
Figure S28. ^{13}C NMR spectrum ($\text{DMSO}-d_6$, 100 MHz) of compound **13c**



277

278

Figure S29. ^{13}C NMR spectrum (DMSO- d_6 , 100 MHz) of compound **13d**



279
280 **Figure S30.** ^{13}C NMR spectrum (DMSO- d_6 , 100 MHz) of compound 13e
281
282

301213_30 #9 RT: 0.34 AV: 1 SB: 45 0.00-0.26 , 0.43-1.99 NL: 7.01E5
T: + c ESI Full ms [50.00-2000.00]

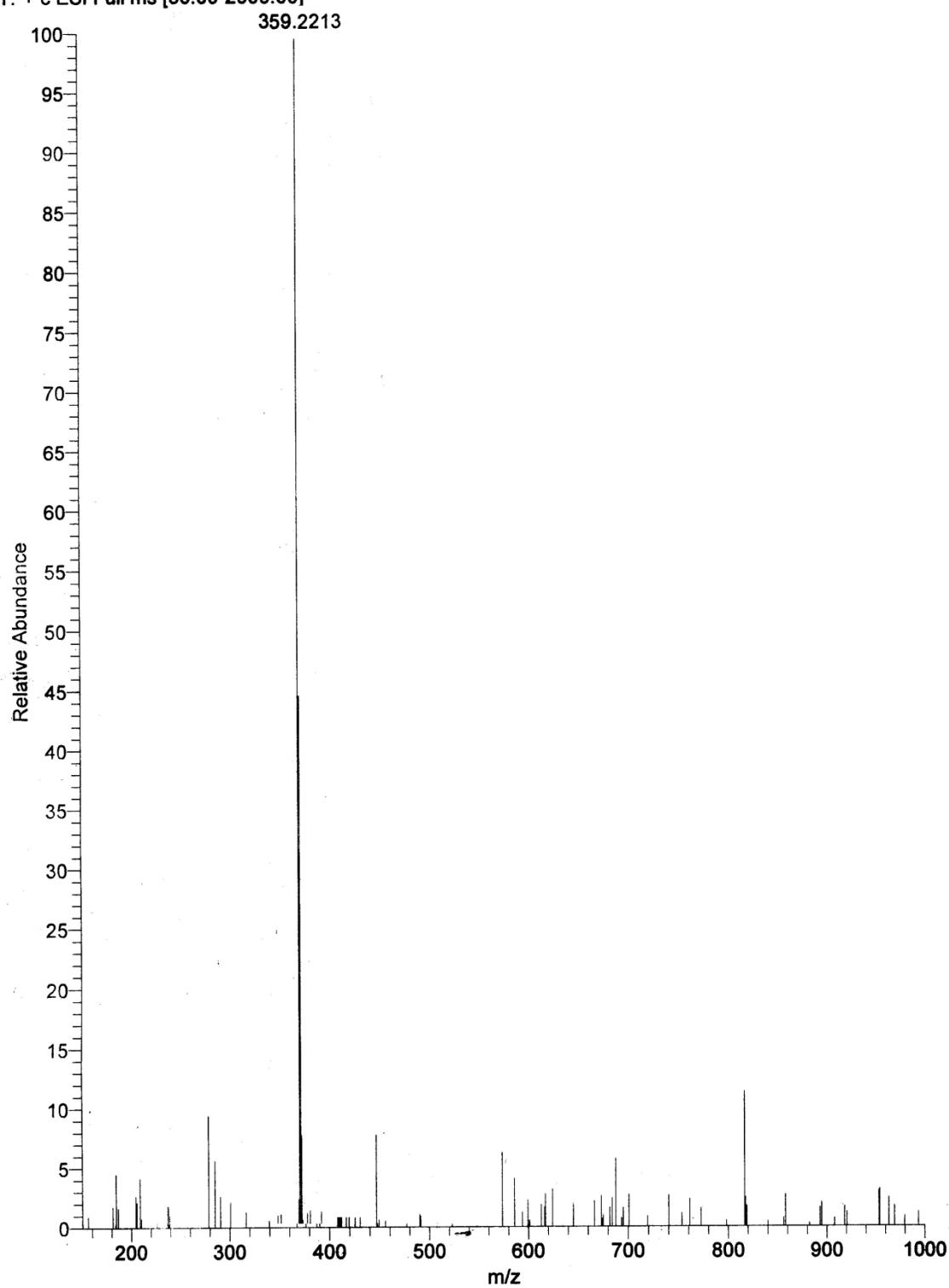
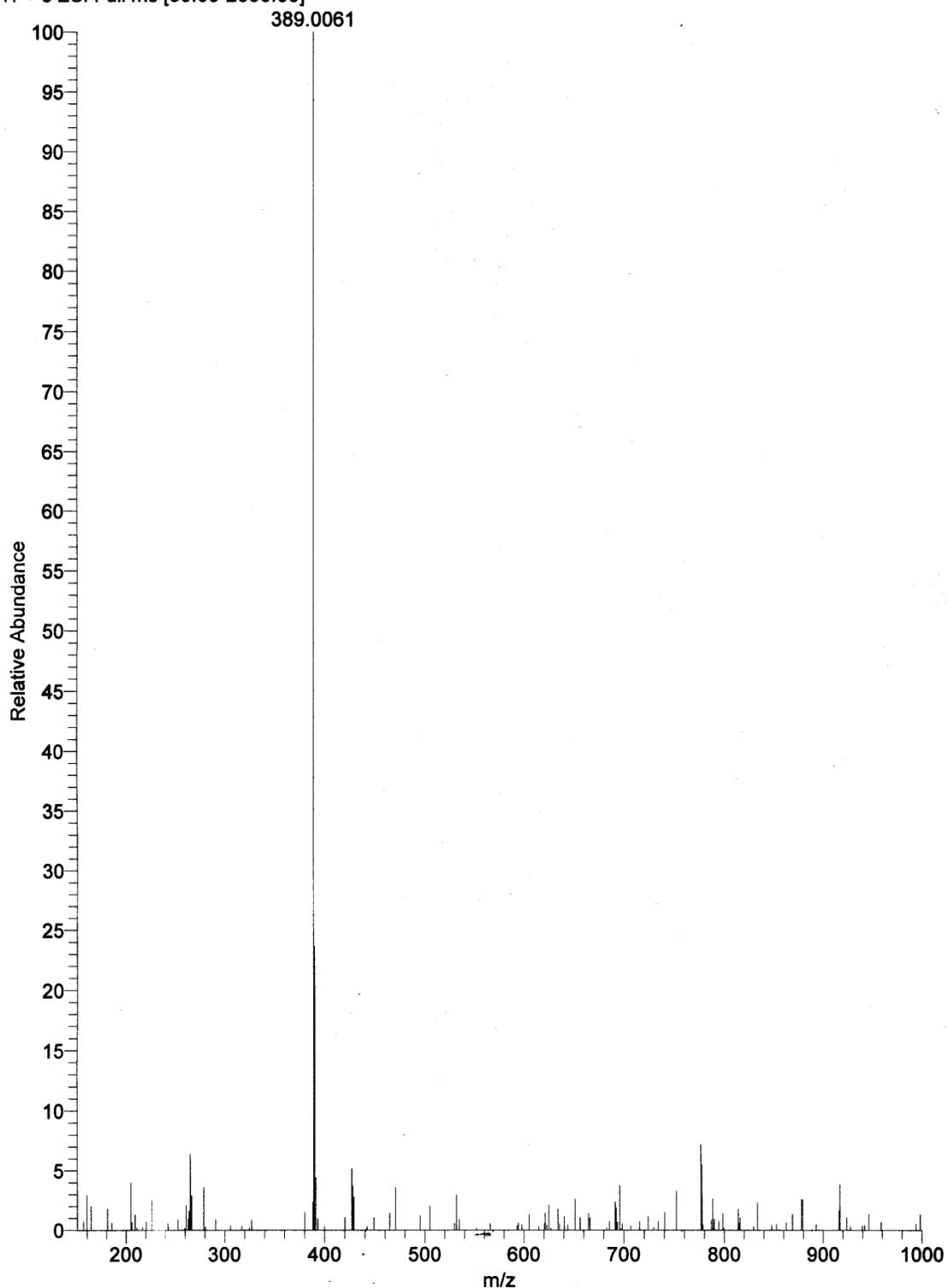


Figure S31. HRMS of compound 7a

301213_23 #7 RT: 0.26 AV: 1 SB: 45 0.01-0.26 , 0.43-2.00 NL: 1.39E6
T: + c ESI Full ms [50.00-2000.00]

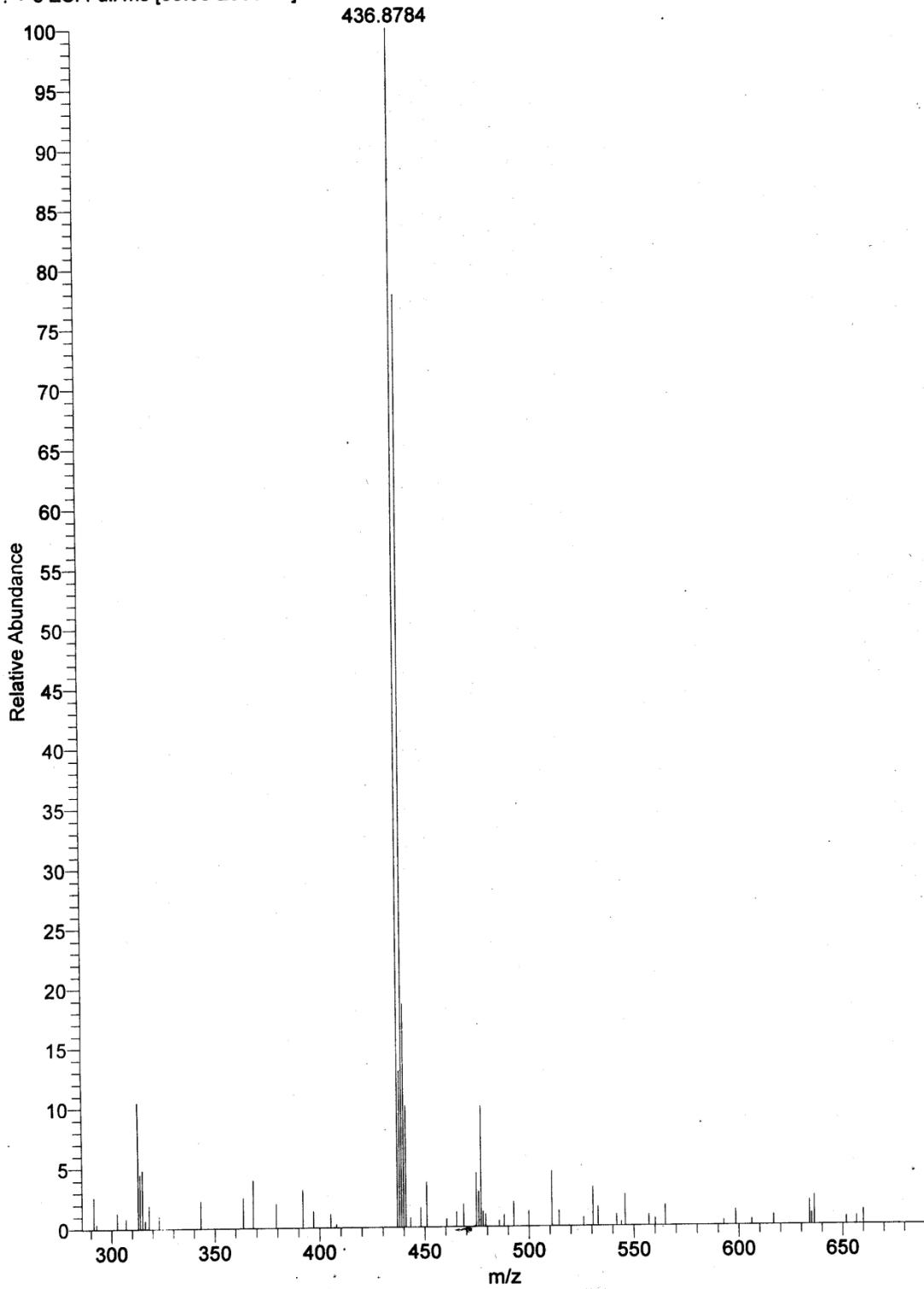


286

287

Figure S32. HRMS of compound 7b

301213_26 #7 RT: 0.26 AV: 1 SB: 36 0.01-0.22 , 0.56-1.79 NL: 6.44E5
T: + c ESI Full ms [50.00-2000.00]

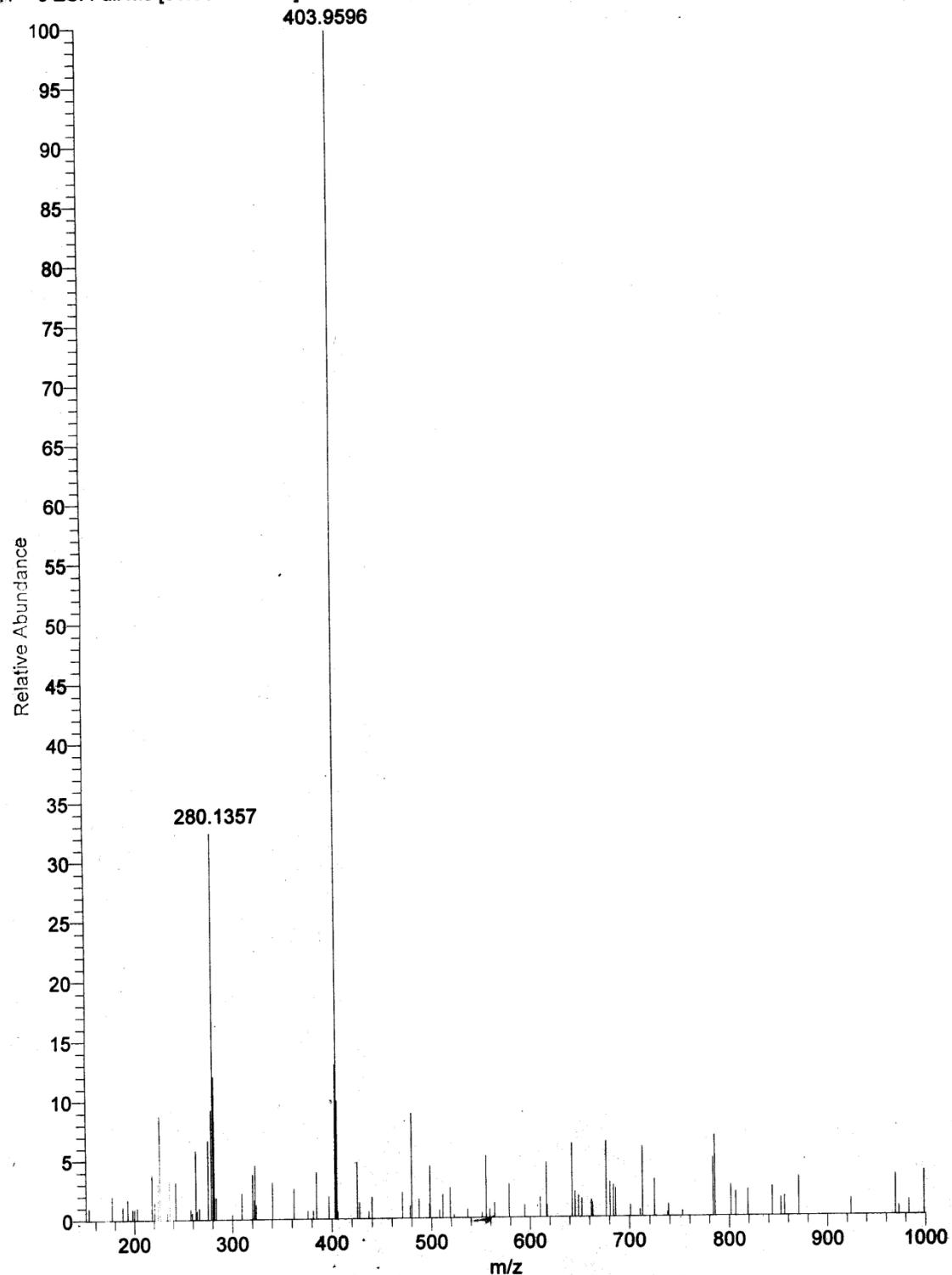


288

289

Figure S33. HRMS of compound 7c

311213_07 #7 RT: 0.26 AV: 1 SB: 45 0.00-0.26 , 0.43-2.00 NL: 4.82E5
T: + c ESI Full ms [50.00-2000.00]

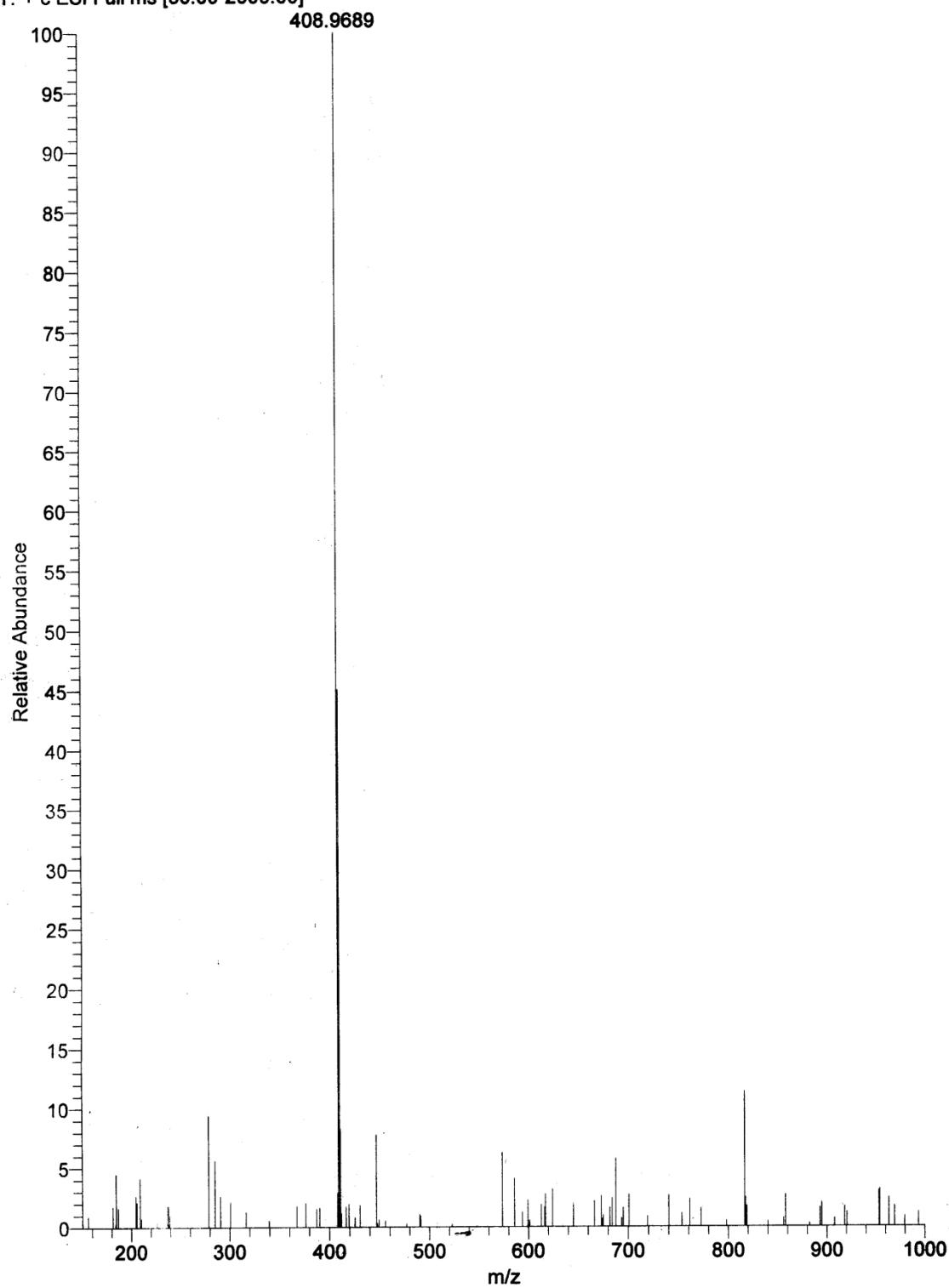


290

291

Figure S34. HRMS of compound 7d

301213_30 #9 RT: 0.34 AV: 1 SB: 45 0.00-0.26 , 0.43-1.99 NL: 7.01E5
T: + c ESI Full ms [50.00-2000.00]

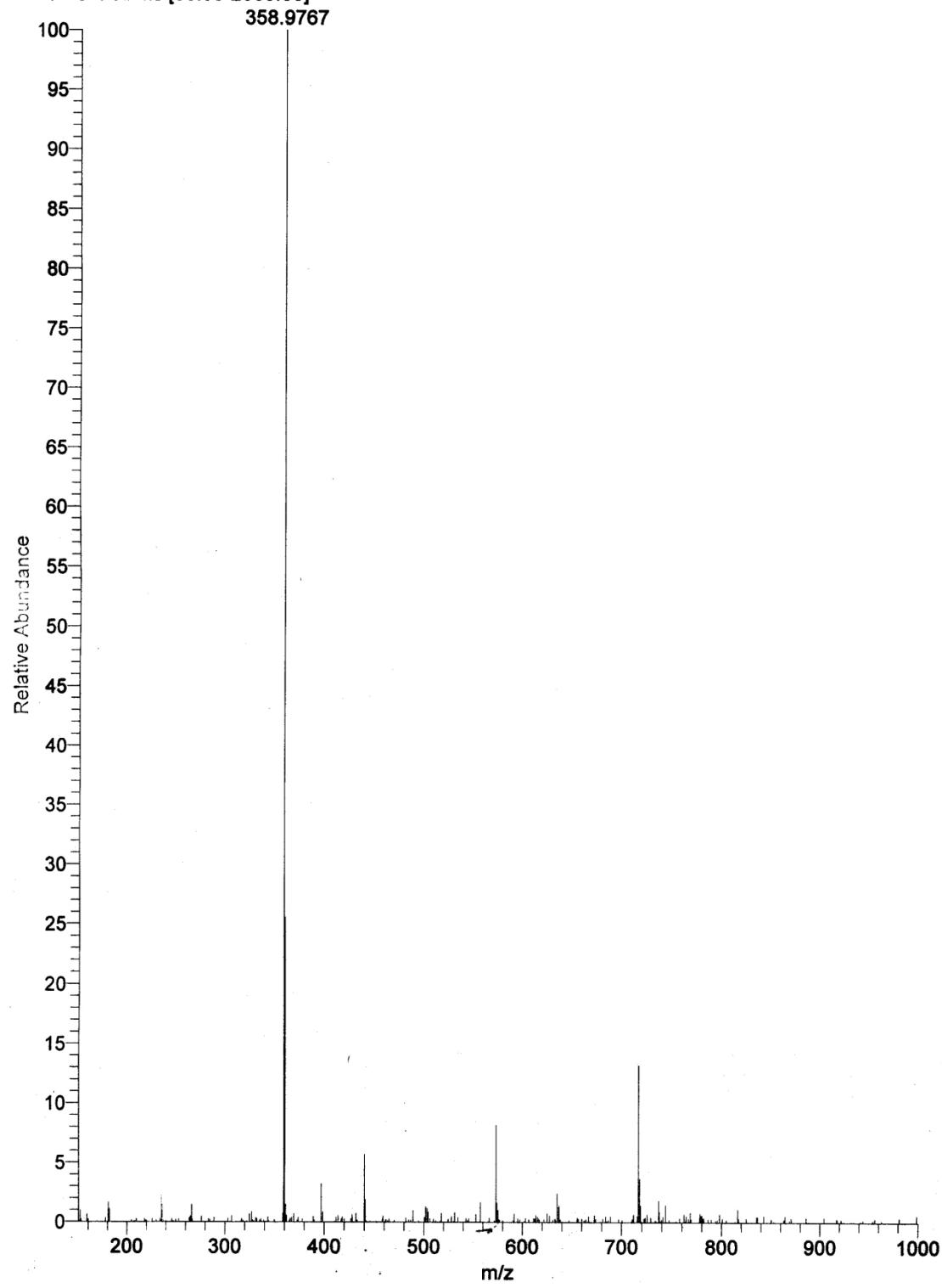


292

293

Figure S35. HRMS of compound 7e

311213_14 #7 RT: 0.26 AV: 1 SB: 45 0.01-0.26 , 0.44-2.01 NL: 5.15E6
T: + c ESI Full ms [50.00-2000.00]

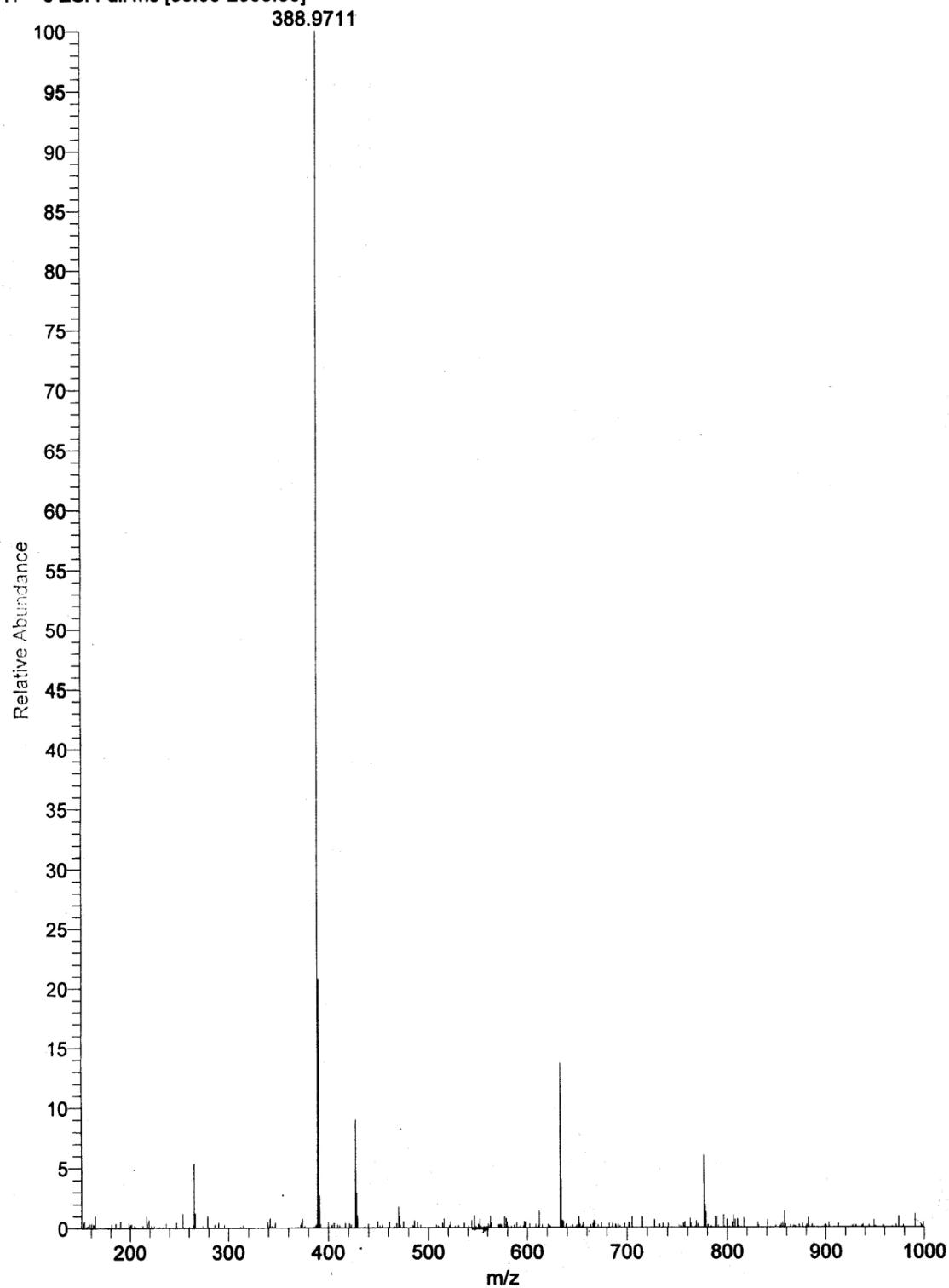


294

295

Figure S36. HRMS of compound 10a

311213_12 #7 RT: 0.26 AV: 1 SB: 45 0.01-0.26 , 0.43-2.01 NL: 4.50E6
T: + c ESI Full ms [50.00-2000.00]

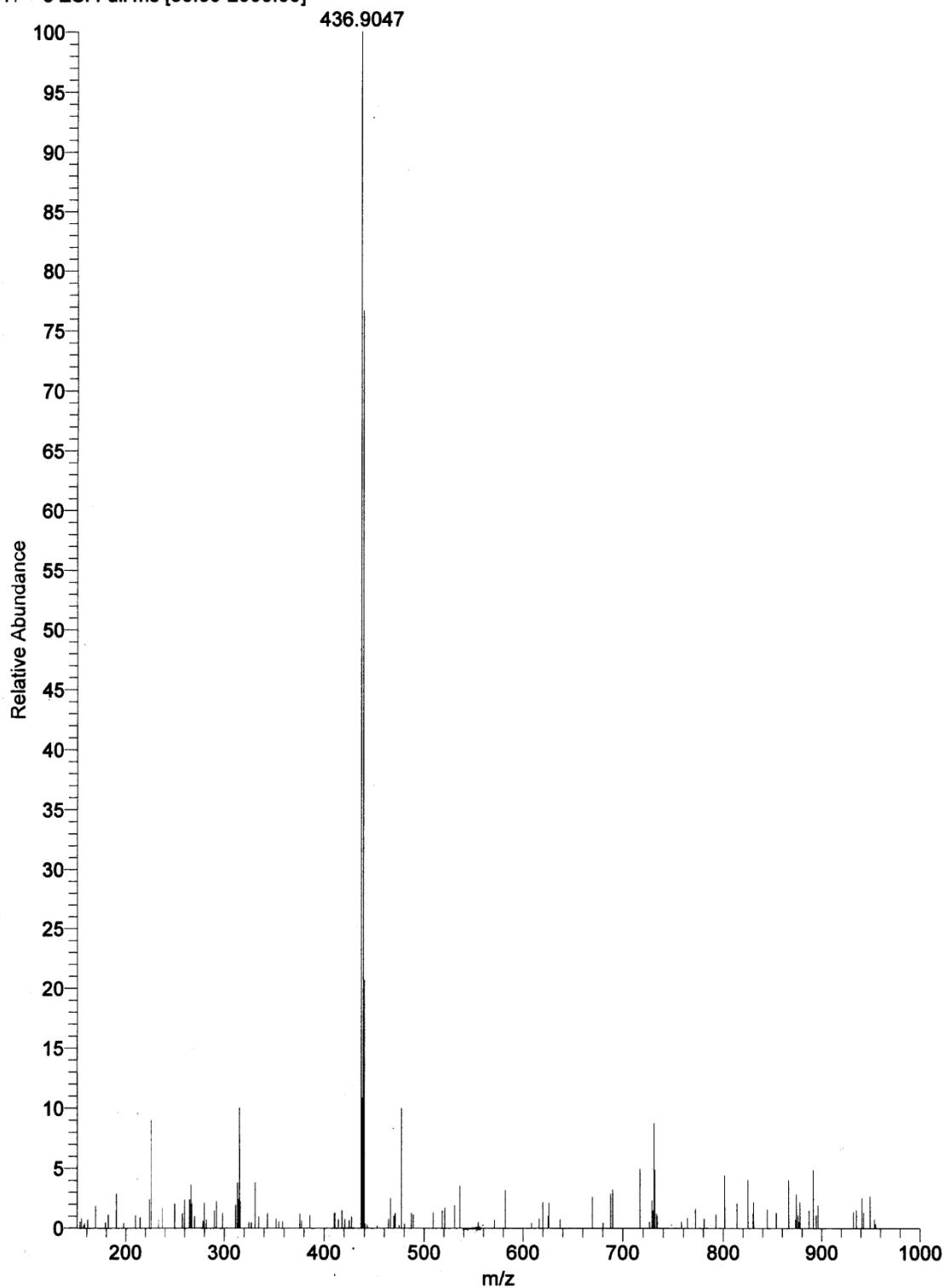


296

297

Figure S37. HRMS of compound **10b**

3:1213_16 #9 RT: 0.35 AV: 1 SB: 45 0.01-0.26 , 0.43-2.00 NL: 8.38E5
T: + c ESI Full ms [50.00-2000.00]

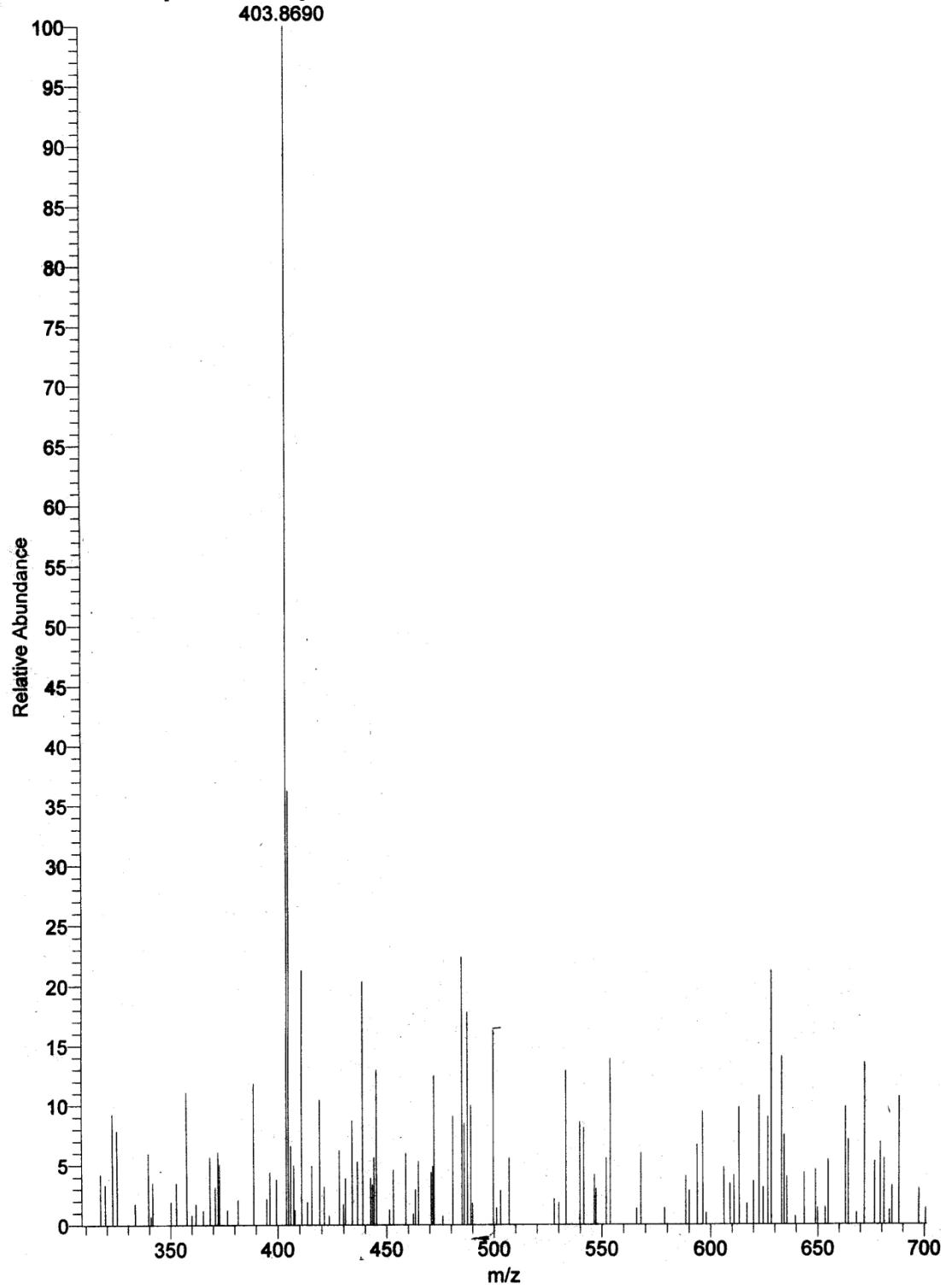


298

299

Figure S38. HRMS of compound **10c**

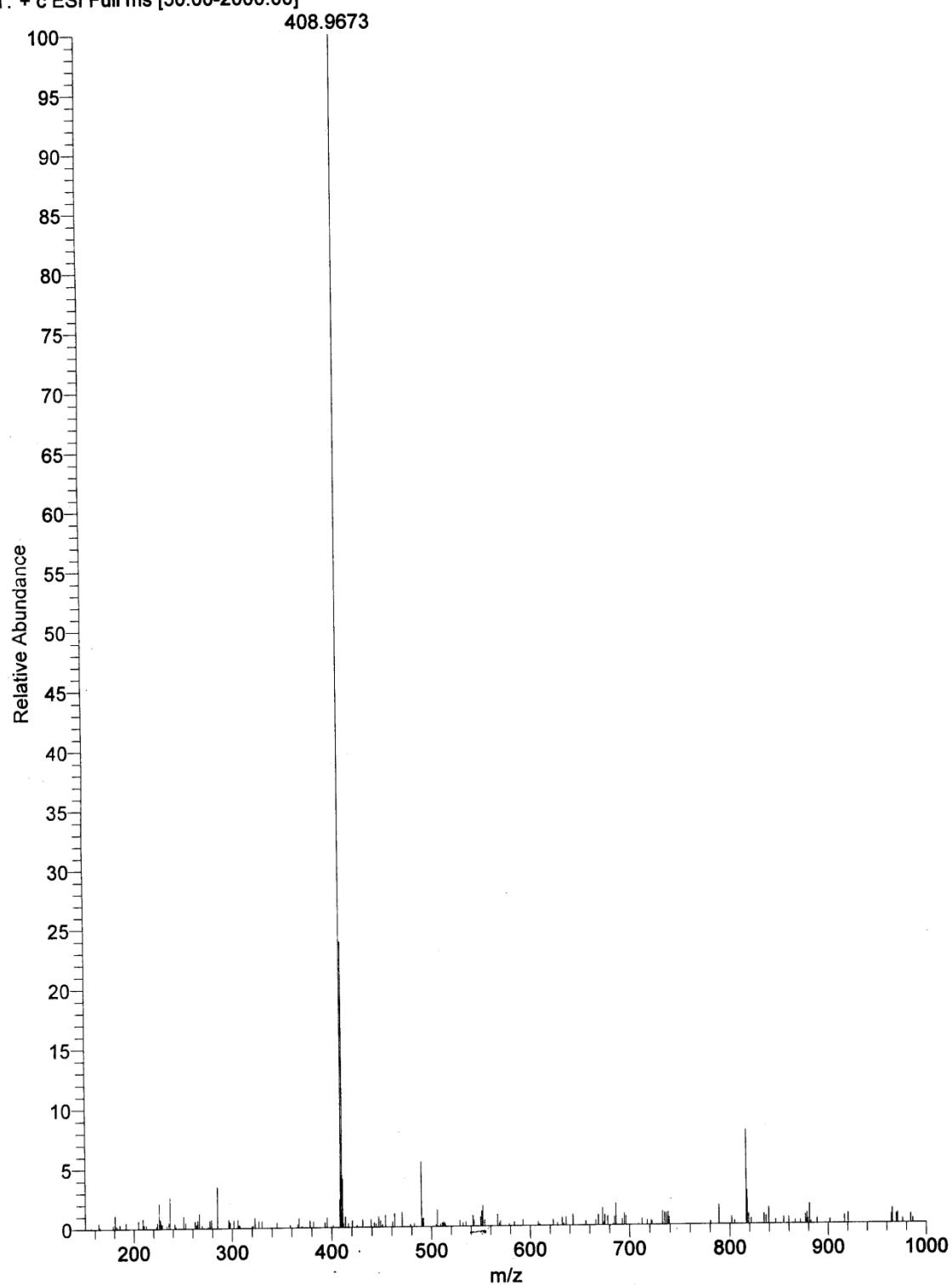
311213_18 #7 RT: 0.26 AV: 1 SB: 40 0.00-0.22 , 0.52-1.92 NL: 2.79E5
T: + c ESI Full ms [50.00-2000.00]



300
301

Figure S39. HRMS of compound **10d**

311213_21 #7 RT: 0.26 AV: 1 SB: 45 0.00-0.26 , 0.43-2.00 NL: 2.89E6
T: + c ESI Full ms [50.00-2000.00]

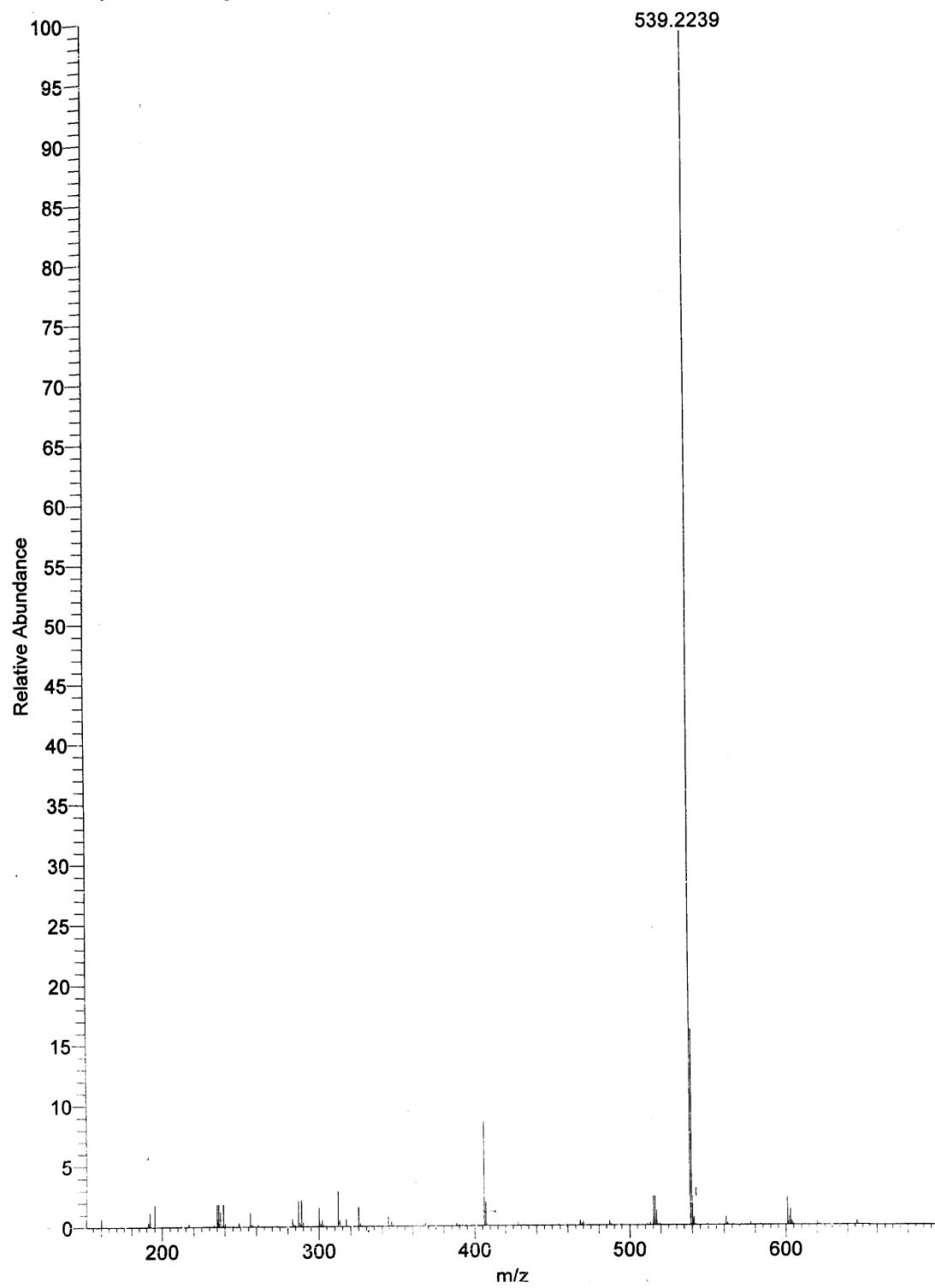


302

303

Figure S40. HRMS of compound 10e

060614_15 #41 RT: 0.33 AV: 1 SB: 155 0.00-0.32 , 0.44-1.37 NL: 6.27E8
T: FTMS + p ESI Full ms [66.70-1000.00]

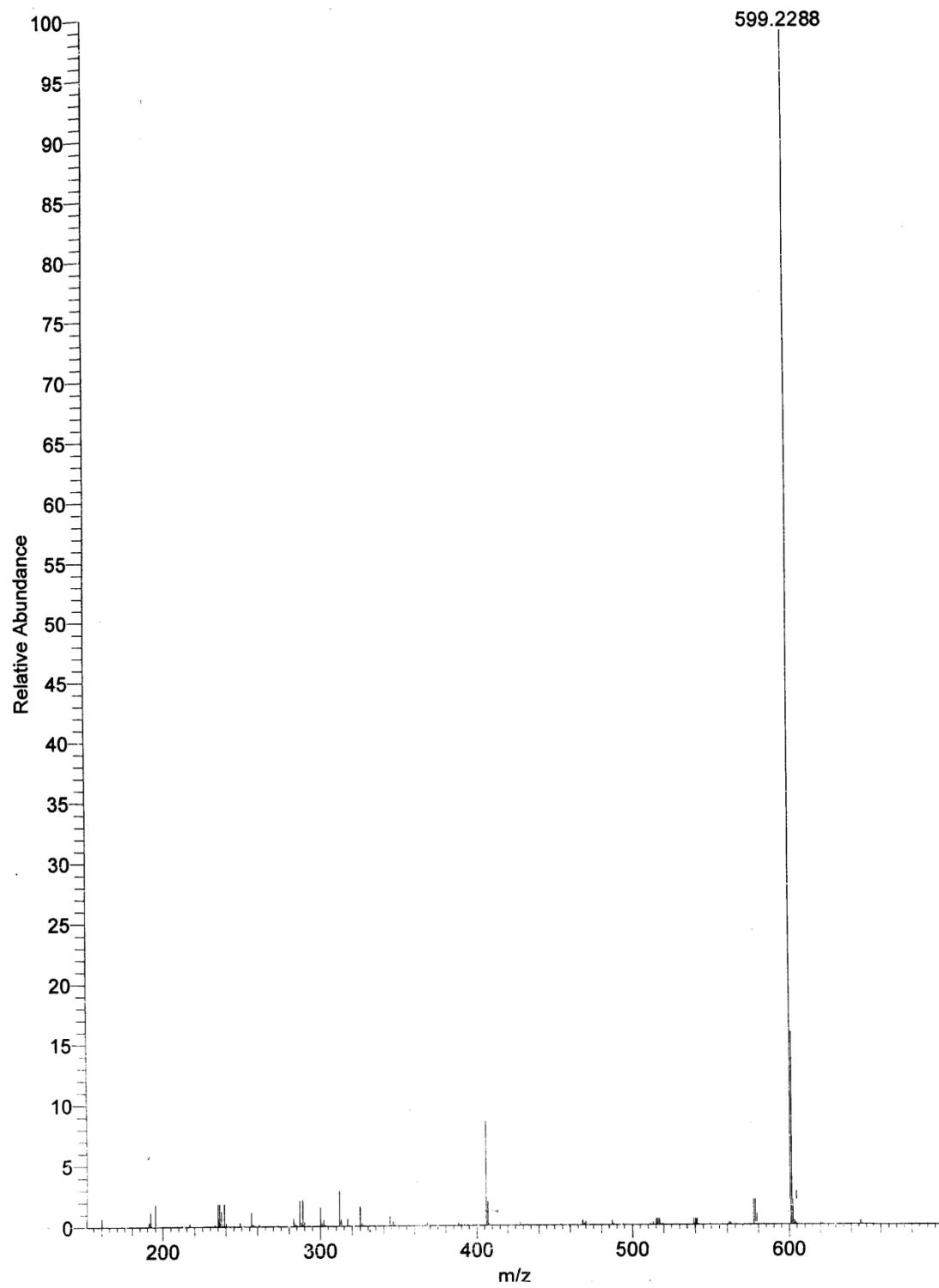


304

305

Figure S41. HRMS of compound 13a

060614_15 #41 RT: 0.33 AV: 1 SB: 155 0.00-0.32 , 0.44-1.37 NL: 6.27E8
T: FTMS + p ESI Full ms [66.70-1000.00]

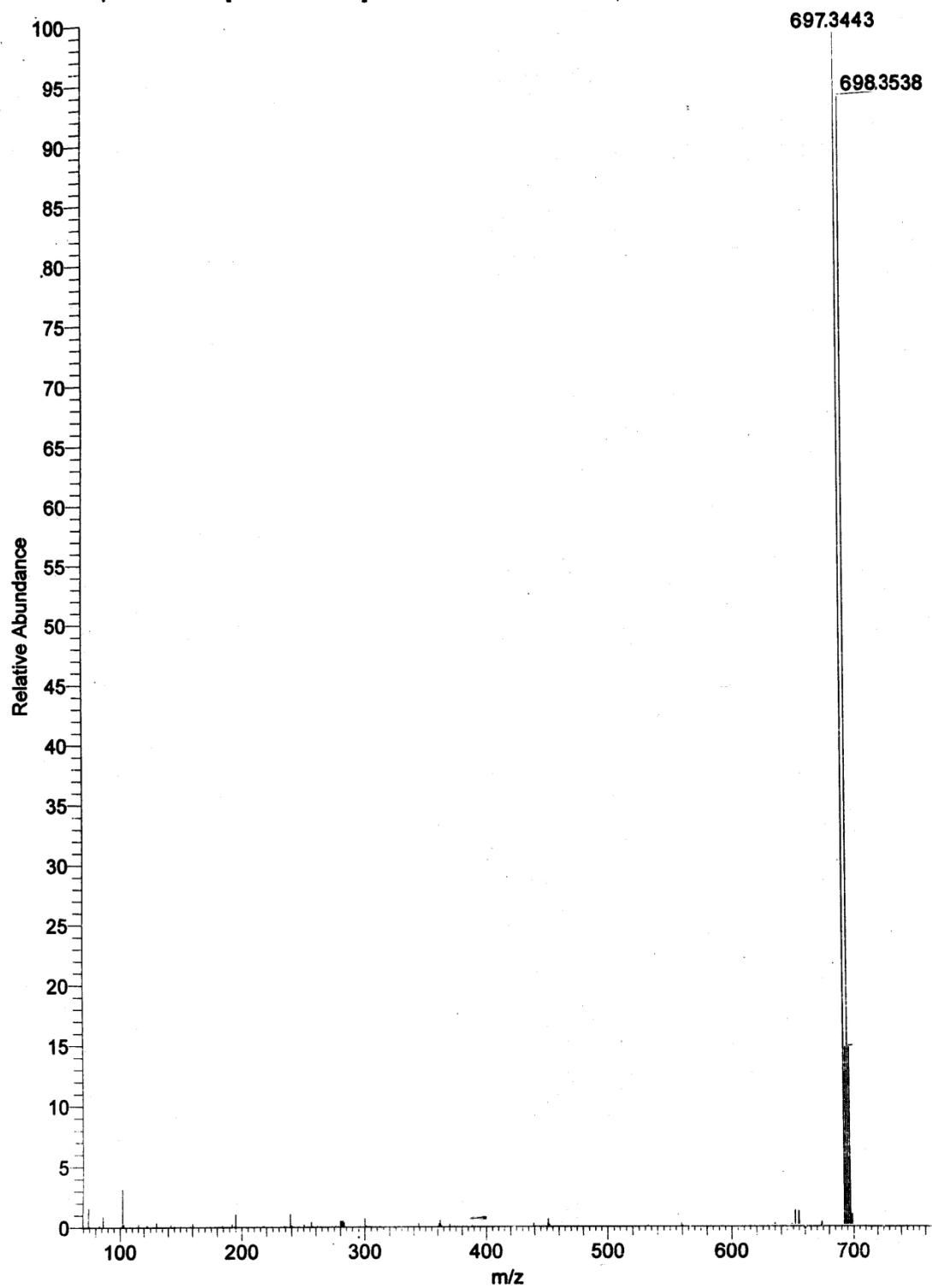


306

307

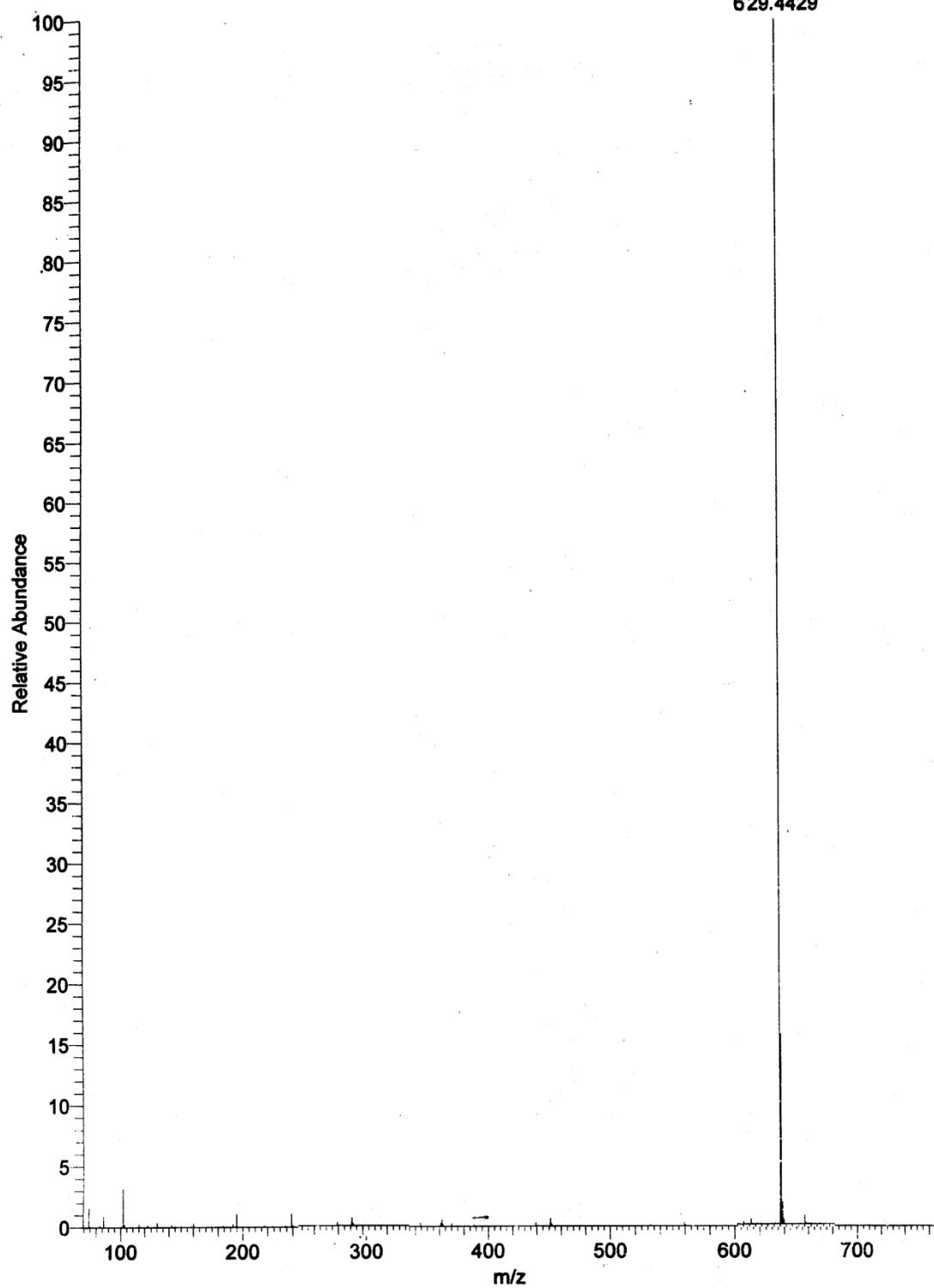
Figure S42. HRMS of compound **13b**

060614_17#39 RT: 0.31 AV: 1 NL: 3.85E9
T: FTMS + pESI Full ms [66.70-1000.00]



060614_17#39 RT: 0.31 AV: 1 NL: 3.85E9
T: FTMS + pESI Full ms [66.70-1000.001]

629.4429



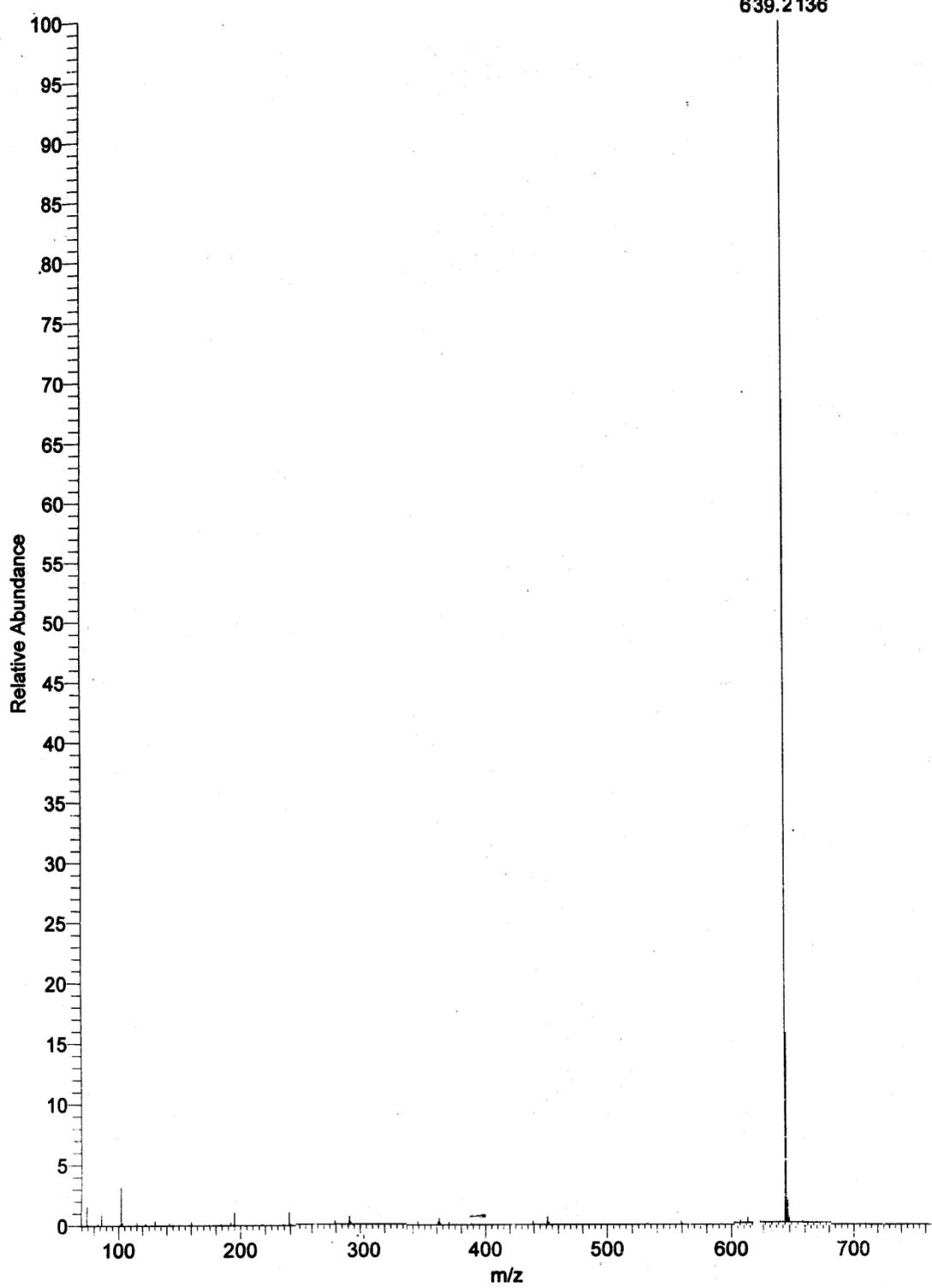
310

311

Figure S44. HRMS of compound 13d

060614_17#39 RT: 0.31 AV: 1 NL: 3.85E9
T: FTMS + pESI Full ms [66.70-1000.001]

639.2136



312

313

314

Figure S45. HRMS of compound 13e