Electronic Supplementary Material (ESI) for RSC Advances.

Amidic C-N bond cleavage of isatin: Chemoselective synthesis of pyrrolo[2,3,4-*kl*]acridin-1-ones using Ag NPs decorated rGO composite as an efficient and recoverable catalyst under microwave irradiation

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Supporting Information

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1. Calculation of green metrics:

1.1. *E-factor calculations:*

$$\text{E-factor} = \frac{\text{Total waste (g)}}{\text{Product (g)}} = \frac{\text{Total input (g) - Total output (g)}}{\text{Total ouput (g)}}$$

S. No.	Input (quantity in g)*				Output (quantity in g)*	Total (quantity in g)		E-factor = (x - y)/ y
	Reactant 1	Reactant 2	Reactant 3	Solvent	Product	Input (x)	Ouput (y)	
a.	0.294	0.186	0.280	2.367	0.580	3.127	0.580	4.39
b.	0.294	0.214	0.280	2.367	0.632	3.155	0.632	3.99
c.	0.294	0.256	0.280	2.367	0.650	3.197	0.650	3.92
d.	0.294	0.222	0.280	2.367	0.640	3.163	0.640	3.94
e.	0.294	0.344	0.280	2.367	0.737	3.285	0.737	3.46
f.	0.452	0.214	0.280	2.367	0.754	3.313	0.754	3.39
g.	0.452	0.256	0.280	2.367	0.801	3.355	0.801	3.19
h.	0.452	0.344	0.280	2.367	0.871	3.443	0.871	2.95
i.	0.330	0.186	0.280	2.367	0.640	3.163	0.640	3.94
j.	0.330	0.214	0.280	2.367	0.652	3.191	0.652	3.89
k.	0.330	0.256	0.280	2.367	0.697	3.233	0.697	3.64
l.	0.330	0.344	0.280	2.367	0.770	3.321	0.770	3.31
m.	0.384	0.214	0.280	2.367	0.685	3.245	0.685	3.74
n.	0.384	0.256	0.280	2.367	0.731	3.287	0.731	3.50
o.	0.322	0.344	0.280	2.367	0.771	3.313	0.771	3.30
p.	0.322	0.186	0.280	2.367	0.605	3.155	0.605	4.21

*** Since the catalyst was recovered during the reaction, therefore it's used amount is not included in the calculations.**

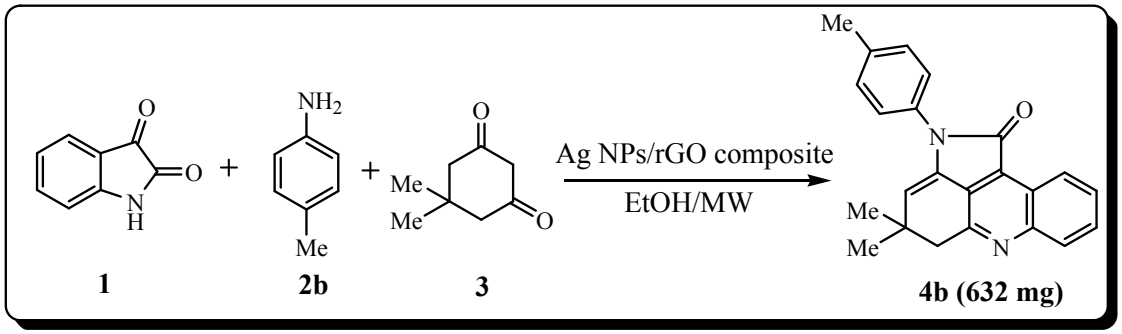
1.2. *Calculation of Atom Economy:*

$$\text{Atom Economy} = \frac{\text{Molecular weight of the product}}{\text{Sum of the molecular weights of reactants}} \text{ X } 100$$

$$\text{e.g. For the product } \mathbf{4b};\ \text{Atom Economy} = \frac{340}{147 + 107 + 140} \text{ X } 100$$

$$\text{Atom Economy} = 86.29\ \%$$

2. Calculation of percentage yield and turn over frequency (TOF):



2.1. ***Calculation of %ge yield:***

$$\%\text{ge yield} = \frac{\text{Experimental yield}}{\text{Theoritical yield}} \text{ X } 100$$

$$\text{e.g. For the product } \mathbf{4b};\ \%\text{ge yield} = \frac{632 \text{ mg}}{680 \text{ mg}} \text{ X } 100$$

$$\%\text{ge yield} = 92.94\ \%$$

2.2. ***Calculation of TOF value:***

$$\text{TOF (Turn Over Frequency)} = \frac{\text{No. of moles of final product produced}}{\text{Amount of loaded catalyst X Time}}$$

$$\text{wt\% of loaded catalyst} = \frac{\text{Amount of loaded catalyst}}{\text{Total amount}} \text{ X } 100$$

e.g. For the product **4b**; Assunming amount of loaded catalyst = x gm

$$\frac{4}{100} = \frac{x}{0.294 + 0.280 + 0.214 + x} = \frac{x}{0.788 + x}$$

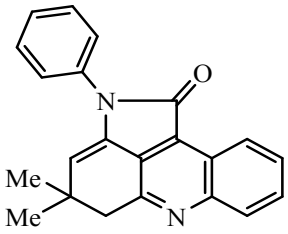
$$x = \frac{3.152}{96} = 0.033 \text{ g}$$

$$\text{TOF} = \frac{0.632}{340 \text{ X } 0.033 \text{ X } 2} = 0.02816 \text{ mol g}^{-1} \text{ min}^{-1}$$

$$\text{TOF} = 28.16 \text{ X } 10^{-3} \text{ mol g}^{-1} \text{ min}^{-1}$$

3. Characterizations of the compounds:

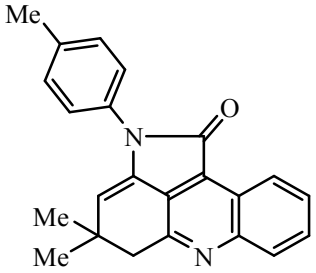
4,4-Dimethyl-2-phenyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4a: 89 %, 0.580 g)



Yellow solid, m.p. 191-193 °C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm): 8.60 (d, J = 8.0 Hz, 1H, ArH), 8.12 (d, J = 8.4 Hz, 1H, ArH), 7.85-7.75 (m, 2H, ArH), 7.65-7.49 (m, 5H, ArH), 5.66 (s, 1H, =C-H), 3.15 (s, 2H, CH_2), 1.25 (s, 6H, 2xCH_3); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm): 165.8 (>C=O), 154.2, 150.2 (Ar-C), 136.9 (=CH-C-N), 133.7, 132.4, 131.8, 129.5, 128.1, 127.6, 126.5, 126.2,

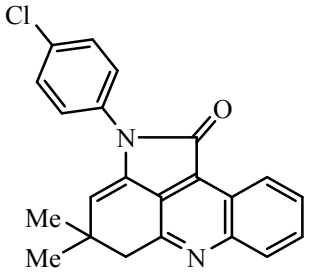
124.2, 123.5, 122.2 (Ar-C), 119.8 (=C-H), 44.1 (CH_2), 36.8 (CH_3-C-CH_3), 30.4 (CH_3-C-CH_3); IR (KBr, *v*, cm^{-1}): 3035, 2940, 1695, 1650, 1530, 1460, 1342, 1097, 774; MS (ESI) m/z: 326 $[M]^+$.

4,4-Dimethyl-2-*p*-tolyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4b: 93 %, 0.632 g)



Yellow solid, m.p. 218-220 °C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm): 8.64 (d, *J* = 8.0 Hz, 1H, ArH), 8.08 (d, *J* = 8.4 Hz, 1H, ArH), 7.67-7.57 (m, 2H, ArH), 7.31-7.25 (m, 4H, ArH), 5.51 (s, 1H, =C-H), 3.13 (s, 2H, CH_2), 2.35 (s, 3H, CH_3), 1.24 (s, 6H, 2xCH_3); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm): 166.8 (>C=O), 154.6, 149.6 (Ar-C), 137.5 (=CH-C-N), 133.5, 132.0, 130.0, 129.5, 129.4, 127.7, 126.4, 126.3, 125.1, 124.3, 122.6 (Ar-C), 118.2 (=C-H), 44.2 (CH_2), 37.1 (CH_3-C-CH_3), 30.9 (CH_3-C-CH_3), 21.1 (Ar-CH_3); IR (KBr, *v*, cm^{-1}): 3040, 2960, 1700, 1655, 1520, 1465, 1350, 1120, 775; MS (ESI) m/z: 340 $[M]^+$.

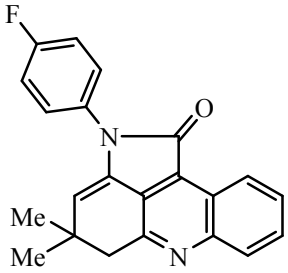
2-(4-Chlorophenyl)-4,4-dimethyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4c: 90 %, 0.650 g)



Yellow solid, m.p. 189-190 °C; ^{1}H NMR (400 MHz, DMSO-d_6) (δ, ppm): 8.56 (d, *J* = 7.2 Hz, 1H, ArH), 8.16 (d, *J* = 8.0 Hz, 1H, ArH), 7.86-7.84 (m, 1H, ArH), 7.72-7.56 (m, 1H, ArH), 7.67-7.57 (m, 4H, ArH), 5.81 (s, 1H, =C-H), 3.18 (s, 2H, CH_2), 1.29 (s, 6H, 2xCH_3); ^{13}C NMR (100 MHz, DMSO-d_6) (δ, ppm): 165.7 (>C=O), 154.7, 148.8 (Ar-C), 133.2 (=CH-C-N), 132.0, 131.7, 129.5, 129.3,

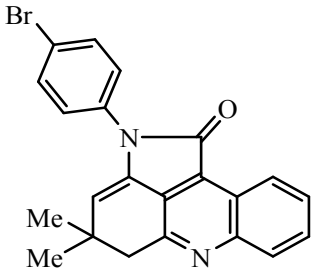
128.1, 127.9, 126.1, 125.4, 123.6, 123.2, 121.6 (Ar-C), 119.2 (=C-H), 43.1 (CH_2), 36.8 (CH_3-C-CH_3), 30.1 (CH_3-C-CH_3); IR (KBr, *v*, cm^{-1}): 3033, 2950, 1700, 1645, 1530, 1450, 1345, 1110, 820; MS (ESI) m/z: 361 $[M]^+$.

2-(4-Fluorophenyl)-4,4-dimethyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4d: 93 %, 0.640 g)



Yellow solid, m.p. 186-187 °C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm): 8.58 (d, *J* = 7.8 Hz, 1H, ArH), 8.14 (d, *J* = 8.2 Hz, 1H, ArH), 7.90-7.80 (m, 2H, ArH), 7.70-7.62 (m, 4H, ArH), 5.60 (s, 1H, =C-H), 3.16 (s, 2H, CH_2), 1.25 (s, 6H, 2xCH_3); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm): 166.2 (>C=O), 153.4, 149.2 (Ar-C), 136.8 (=CH-C-N), 132.8, 132.2, 130.4, 129.2, 128.8, 127.9, 126.6, 126.3, 125.4, 124.5, 122.8 (Ar-C), 118.4 (=C-H), 44.6 (CH_2), 37.4 (CH_3-C-CH_3), 31.2 (CH_3-C-CH_3); IR (KBr, *v*, cm^{-1}): 3036, 2960, 1705, 1650, 1525, 1460, 1335, 1115, 790; MS (ESI) m/z: 344 $[M]^+$.

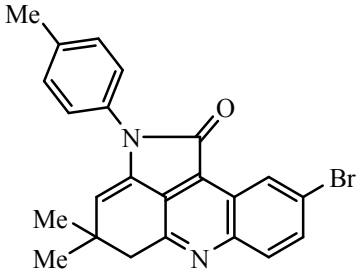
2-(4-Bromophenyl)-4,4-dimethyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4e: 91 %, 0.737 g)



Yellow solid, m.p. 189-191 °C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm): 8.58 (d, *J* = 7.6 Hz, 1H, ArH), 8.22 (d, *J* = 8.2 Hz, 1H, ArH), 7.97-7.85 (m, 2H, ArH), 7.76-7.64 (m, 4H, ArH), 5.85 (s, 1H, =C-H), 3.21 (s, 2H, CH_2), 1.29 (s, 6H, 2xCH_3); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm): 165.9 (>C=O), 155.1, 150.3 (Ar-C), 134.1 (=CH-C-N), 133.1, 132.1, 131.9, 129.5, 129.1, 127.6, 126.6, 124.1,

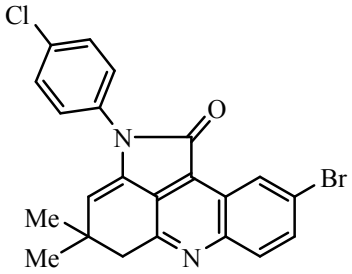
123.6, 122.2, 121.3 (Ar-C), 118.9 (=C-H), 43.9 (CH_2), 36.8 (CH_3-C-CH_3), 30.6 (CH_3-C-CH_3); IR (KBr, *v*, cm^{-1}): 3030, 2950, 1700, 1650, 1500, 1540, 1450, 1350, 1120, 820; MS (ESI) m/z: 405 $[M]^+$.

9-Bromo-4,4-dimethyl-2-*p*-tolyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4f: 90 %, 0.754 g)



Yellow solid, m.p. 204-206 °C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm): 8.85 (s, 1H, ArH), 7.99 (d, *J* = 8.8 Hz, 1H, ArH), 7.79 (d, *J* = 8.4 Hz, 1H, ArH), 7.35 (d, *J* = 3.2 Hz, 4H, ArH), 5.64 (s, 1H, =C-H), 3.18 (s, 2H, CH_2), 2.44 (s, 3H, CH_3), 1.32 (s, 6H, 2xCH_3); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm): 166.2 (>C=O), 155.0, 148.2 (Ar-C), 137.5 (=CH-C-N), 133.2, 132.7, 131.8, 130.9, 130.0, 127.8, 126.7, 126.3, 124.0, 123.6, 122.0 (Ar-C), 119.1 (=C-H), 44.1 (CH_2), 37.1 (CH_3-C-CH_3), 30.9 (CH_3-C-CH_3), 21.2 (Ar-CH_3); IR (KBr, *v*, cm^{-1}): 3030, 2950, 1705, 1650, 1510, 1455, 1350, 1120, 810; MS (ESI) m/z: 420 $[M+H]^+$.

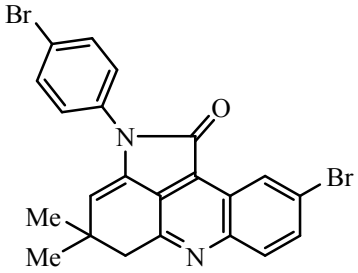
9-Bromo-2-(4-chlorophenyl)-4,4-dimethyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4g: 91 %, 0.801 g)



Yellow solid, m.p. 219-221 °C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm): 8.81 (d, *J* = 2.0 Hz, 1H, ArH), 7.99 (d, *J* = 9.2 Hz, 1H, ArH), 7.80 (dd, J_1 = 2.4 Hz, J_2 = 2.0 Hz, 1H, ArH), 7.52- 7.43 (m, 4H, ArH), 5.66 (s, 1H, =C-H), 3.19 (s, 2H, CH_2), 1.34 (s, 6H, 2xCH_3); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm): 166.0 (>C=O), 155.0, 148.2 (Ar-C), 133.2 (=CH-C-N), 133.0, 132.8, 131.0, 129.6, 127.5, 126.9,

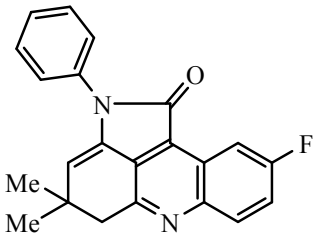
126.4, 123.7, 123.4, 122.2, (Ar-C), 119.3 (=C-H), 44.0 (CH_2), 37.2 (CH_3-C-CH_3), 30.8 (CH_3-C-CH_3); IR (KBr, *v*, cm^{-1}): 3035, 2950, 1700, 1655, 1500, 1450, 1350, 1120, 820; MS (ESI) m/z: 440 $[M]^+$.

9-Bromo-2-(4-bromophenyl)-4,4-dimethyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4h: 90 %, 0.871 g)



Yellow solid, m.p. 185-187 °C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm): 8.72 (d, *J* = 2.0 Hz, 1H, ArH), 7.96-7.82 (m, 2H, ArH), 7.62-7.51 (m, 4H, ArH), 5.72 (s, 1H, =C-H), 3.19 (s, 2H, CH_2), 1.33 (s, 6H, 2xCH_3); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm): 166.4 (>C=O), 155.2, 149.0 (Ar-C), 134.2 (=CH-C-N), 133.3, 132.2, 131.7, 130.8, 127.4, 126.6, 126.1, 124.1, 123.6, 122.1, 121.4 (Ar-C), 119.1 (=C-H), 44.2 (CH_2), 37.1 (CH_3-C-CH_3), 30.6 (CH_3-C-CH_3); IR (KBr, *v*, cm^{-1}): 3030, 2940, 1705, 1650, 1490, 1450, 1345, 1125, 815; MS (ESI) m/z: 484 $[M]^+$.

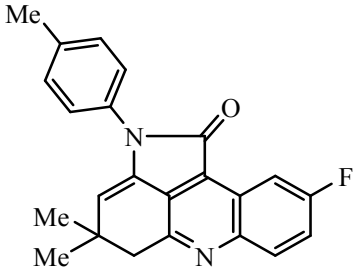
9-Fluoro-4,4-dimethyl-2-phenyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4i: 93 %, 0.640 g)



Yellow solid, m.p. 160-162 °C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm): 8.20 (d, *J* = 3.6 Hz, 1H, ArH), 7.92-7.88 (m, 1H, ArH), 7.65-7.48 (m, 6H, ArH), 5.67 (s, 1H, =C-H), 3.18 (s, 2H, CH_2), 1.29 (s, 6H, 2xCH_3); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm): 166.2 (>C=O), 162.6, 159.9, 153.6, 146.4 (Ar-C), 137.6 (=CH-C-N), 133.6, 131.7, 131.1, 129.2, 126.9, 126.4, 124.6 (Ar-C), 119.4 (=C-H), 119.1,

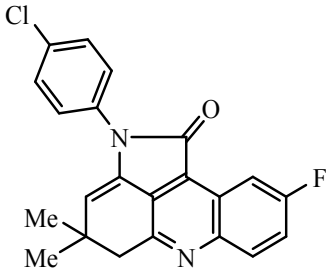
108.0 (Ar-C), 43.5 (CH_2), 37.2 (CH_3-C-CH_3), 30.9 (CH_3-C-CH_3); IR (KBr, *v*, cm^{-1}): 3030, 2950, 1700, 1640, 1495, 1450, 1380, 1125, 820; MS (ESI) m/z: 344 $[M]^+$.

9-Fluoro-4,4-dimethyl-2-*p*-tolyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4j: 91%, 0.652 g)



Yellow solid, m.p. 181-183 °C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm): 8.33 (d, *J* = 2.8 Hz, 1H, ArH), 8.32- 8.12 (m, 1H, ArH), 7.51-7.33 (m, 5H, ArH), 5.63 (s, 1H, =C-H), 3.19 (s, 2H, CH_2), 2.44 (s, 3H, CH_3), 1.32 (s, 6H, 2xCH_3); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm): 166.4 (>C=O), 162.5, 160.1, 153.8, 146.7 (Ar-C), 137.5 (=CH-C-N), 133.3, 131.7, 130.0, 126.9, 126.2, 124.7, 123.3 (Ar-C), 119.3 (=C-H), 119.0, 108.3 (Ar-C), 43.9 (CH_2), 37.1 (CH_3-C-CH_3), 30.8 (CH_3-C-CH_3), 21.2 (Ar-CH_3); IR (KBr, *v*, cm^{-1}): 3035, 2955, 1705, 1650, 1505, 1455, 1330, 1125, 825; MS (ESI) m/z: 358 $[M]^+$.

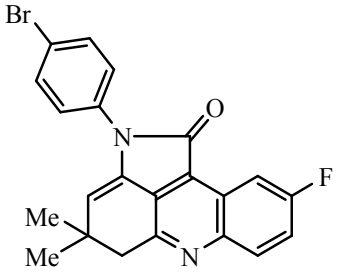
2-(4-Chlorophenyl)-9-fluoro-4,4-dimethyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4k: 92 %, 0.697 g)



Yellow solid, m.p. 183-185 °C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm): 8.28 (d, *J* = 6.4 Hz, 1H, ArH), 8.27- 8.12 (m, 1H, ArH), 7.52-7.44 (m, 5H, ArH), 5.65 (s, 1H, =C-H), 3.20 (s, 2H, CH_2), 1.34 (s, 6H, 2xCH_3); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm): 166.2 (>C=O), 162.6, 160.1, 153.7, 146.7 (Ar-C), 133.2 (=CH-C-N), 133.0, 131.7, 129.6, 127.5, 126.9, 124.5, 123.2 (Ar-C), 119.5 (=C-H), 119.1,

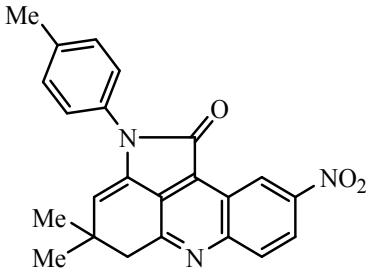
108.2 (Ar-C), 43.9 (CH_2), 37.2 (CH_3-C-CH_3), 30.8 (CH_3-C-CH_3); IR (KBr, *v*, cm^{-1}): 3030, 2960, 1700, 1640, 1500, 1450, 1320, 1120, 815; MS (ESI) m/z: 379 $[M]^+$.

2-(4-Bromophenyl)-9-fluoro-4,4-dimethyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4l: 91 %, 0.770 g)



Yellow solid, m.p. 173-175 °C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm): 8.34 (d, *J* = 7.2 Hz, 1H, ArH), 7.99-7.89 (m, 1H, ArH), 7.56-7.42 (m, 5H, ArH), 5.71 (s, 1H, =C-H), 3.16 (s, 2H, CH_2), 1.31 (s, 6H, 2×CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm): 166.5 (>C=O), 162.9, 159.2, 155.4, 145.4 (Ar-C), 133.8 (=CH-C-N), 132.9, 132.2, 131.7, 130.8, 127.6, 126.8, 124.5 (Ar-C), 119.5 (=C-H), 118.9, 108.2 (Ar-C), 44.1 (CH_2), 37.1 (CH_3-C-CH_3), 30.7 (CH_3-C-CH_3); IR (KBr, *v*, cm^{-1}): 3035, 2955, 1705, 1650, 1500, 1455, 1370, 1110, 815; MS (ESI) m/z: 423 $[M]^+$.

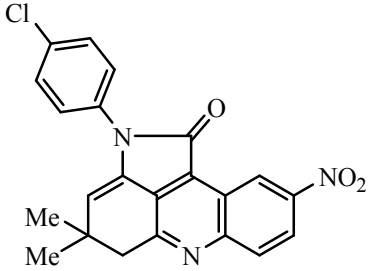
4,4-Dimethyl-9-nitro-2-*p*-tolyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4m: 89 %, 0.685 g)



Yellow solid, m.p. 270-272 °C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm): 8.58 (d, *J* = 5.6 Hz, 1H, ArH), 8.35- 8.10 (m, 2H, ArH), 7.68-7.43 (m, 4H, ArH), 5.82 (s, 1H, =C-H), 3.22 (s, 2H, CH_2), 2.51 (s, 3H, CH_3), 1.31 (s, 6H, 2xCH_3); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm): 166.5 (>C=O), 155.8, 148.9 (Ar-C), 134.6 (=CH-C-N), 133.6, 132.9, 131.2, 130.8, 130.1, 127.9, 127.1, 126.8, 124.1, 123.6,

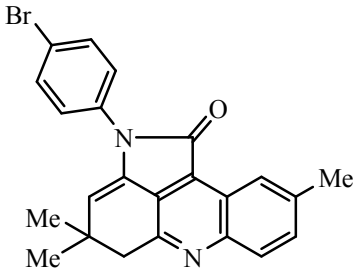
122.8 (Ar-C), 119.8 (=C-H), 44.6 (CH_2), 37.4 (CH_3-C-CH_3), 31.1 (CH_3-C-CH_3) 21.2 (Ar-CH_3); IR (KBr, *v*, cm^{-1}): 3035, 2955, 1710, 1650, 1500, 1555, 1455, 1365, 1115, 815; MS (ESI) m/z: 403 $[M+H_2O]^+$.

2-(4-Chlorophenyl)-4,4-dimethyl-9-nitro-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4n: 90 %, 0.731 g)



Yellow solid, m.p. 274-276 °C; ^{1}H NMR (400 MHz, $CDCl_3$) (*δ*, ppm): 8.83 (d, *J* = 2.0 Hz, 1H, ArH), 8.00 (d, *J* = 8.8 Hz, 1H, ArH), 7.82 (dd, J_1 = 2.4 Hz, J_2 = 2.0 Hz, 1H, ArH), 7.53- 7.44 (m, 4H, ArH), 5.66 (s, 1H, =C-H), 3.19 (s, 2H, CH_2), 1.34 (s, 6H, 2xCH_3); ^{13}C NMR (100 MHz, $CDCl_3$) (*δ*, ppm): 166.0 (>C=O), 154.9, 148.2 (Ar-C), 133.2 (=CH-C-N), 133.0, 132.8, 131.0, 129.6, 127.5, 126.9, 126.4, 123.8, 123.4, 122.2, (Ar-C), 119.2 (=C-H), 44.0 (CH_2), 37.2 (CH_3-C-CH_3), 30.8 (CH_3-C-CH_3); IR (KBr, *v*, cm^{-1}): 3030, 2940, 1700, 1645, 1510, 1550, 1450, 1360, 1110, 820; MS (ESI) m/z: 406 $[M]^+$.

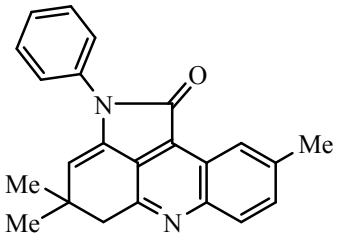
2-(4-Bromophenyl)-4,4,9-trimethyl-4,5-dihydro-2H-pyrrolo[2,3,4-kl]acridin-1-one (4o: 92 %, 0.771 g)



Yellow solid, m.p. 164-165 °C; ^{1}H NMR (400 MHz, $CDCl_3$) (*δ*, ppm): 8.22 (d, *J* = 8.4 Hz, 1H, ArH), 7.84 (d, *J* = 8.2 Hz, 1H, ArH), 7.72-7.68 (m, 1H, ArH), 7.58-7.42 (m, 4H, ArH), 5.65 (s, 1H, =C-H), 3.10 (s, 2H, CH_2), 2.49 (s, 3H, CH_3), 1.24 (s, 6H, 2xCH_3); ^{13}C NMR (100 MHz, $CDCl_3$) (*δ*, ppm): 166.7 (>C=O), 154.2, 148.6 (Ar-C), 137.4 (=CH-C-N), 134.8, 133.1, 132.6, 131.8, 129.7, 128.4,

126.5, 123.6, 122.2, 121.4, 120.6 (Ar-C), 119.4 (=C-H), 44.3 (CH_2), 37.6 (CH_3-C-CH_3), 30.2 (CH_3-C-CH_3), 21.5 (Ar-CH_3); IR (KBr, *v*, cm^{-1}): 3040, 2940, 1705, 1645, 1550, 1510, 1450, 1350, 1115, 820; MS (ESI) m/z: 419 $[M]^+$.

4,4,9-Trimethyl-2-phenyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4p: 89 %, 0.605 g)



Yellow solid, m.p. 200-202 °C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm): 8.86 (d, *J* = 8.6 Hz, 1H, ArH), 8.08 (d, *J* = 8.2 Hz, 1H, ArH), 7.68-7.64 (m, 1H, ArH), 7.58-7.24 (m, 5H, ArH), 5.51 (s, 1H, =C-H), 3.12 (s, 2H, CH_2), 2.35 (s, 3H, CH_3), 1.23 (s, 6H, 2xCH_3); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm): 166.8(>C=O), 154.6, 149.7 (Ar-C), 137.5 (=CH-C-N), 133.5, 132.1, 130.0, 129.5, 129.4, 127.7, 126.4, 126.3, 125.0, 124.3, 122.6 (Ar-C), 118.2 (=C-H), 44.2 (CH_2), 37.2 (CH_3-C-CH_3), 30.9 (CH_3-C-CH_3), 21.2 (Ar-CH_3); IR (KBr, *v*, cm^{-1}): 3035, 2945, 1700, 1650, 1505, 1445, 1370, 1120, 825; MS (ESI) m/z: 340 $[M]^+$.

4. Crystal structural data of compound 4b-

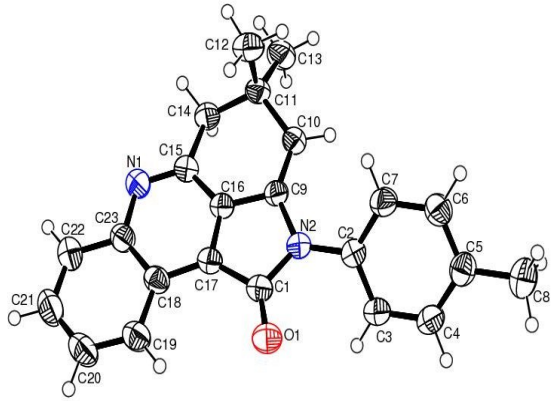
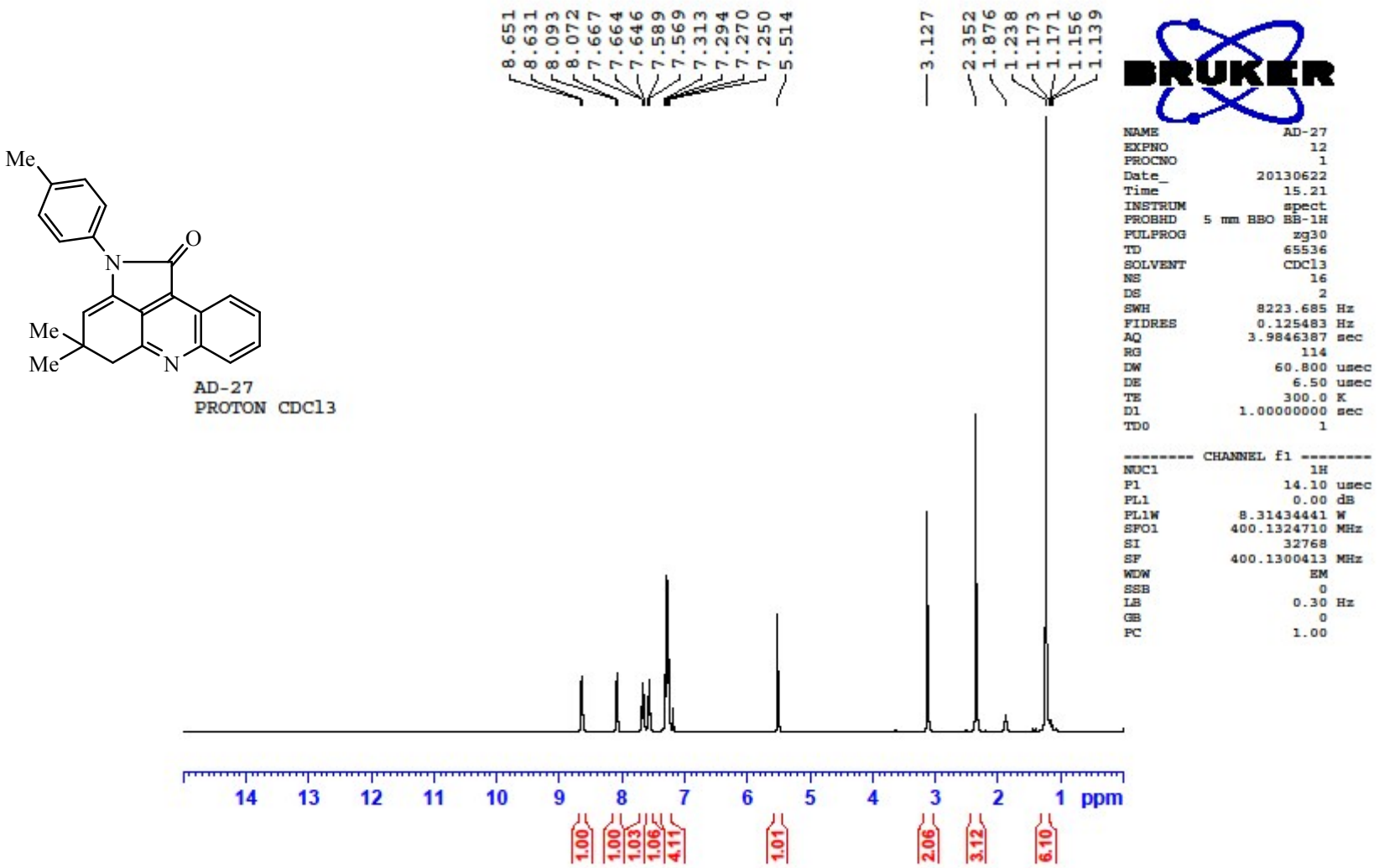


Table 1. Crystal data and structure refinement for uor005.

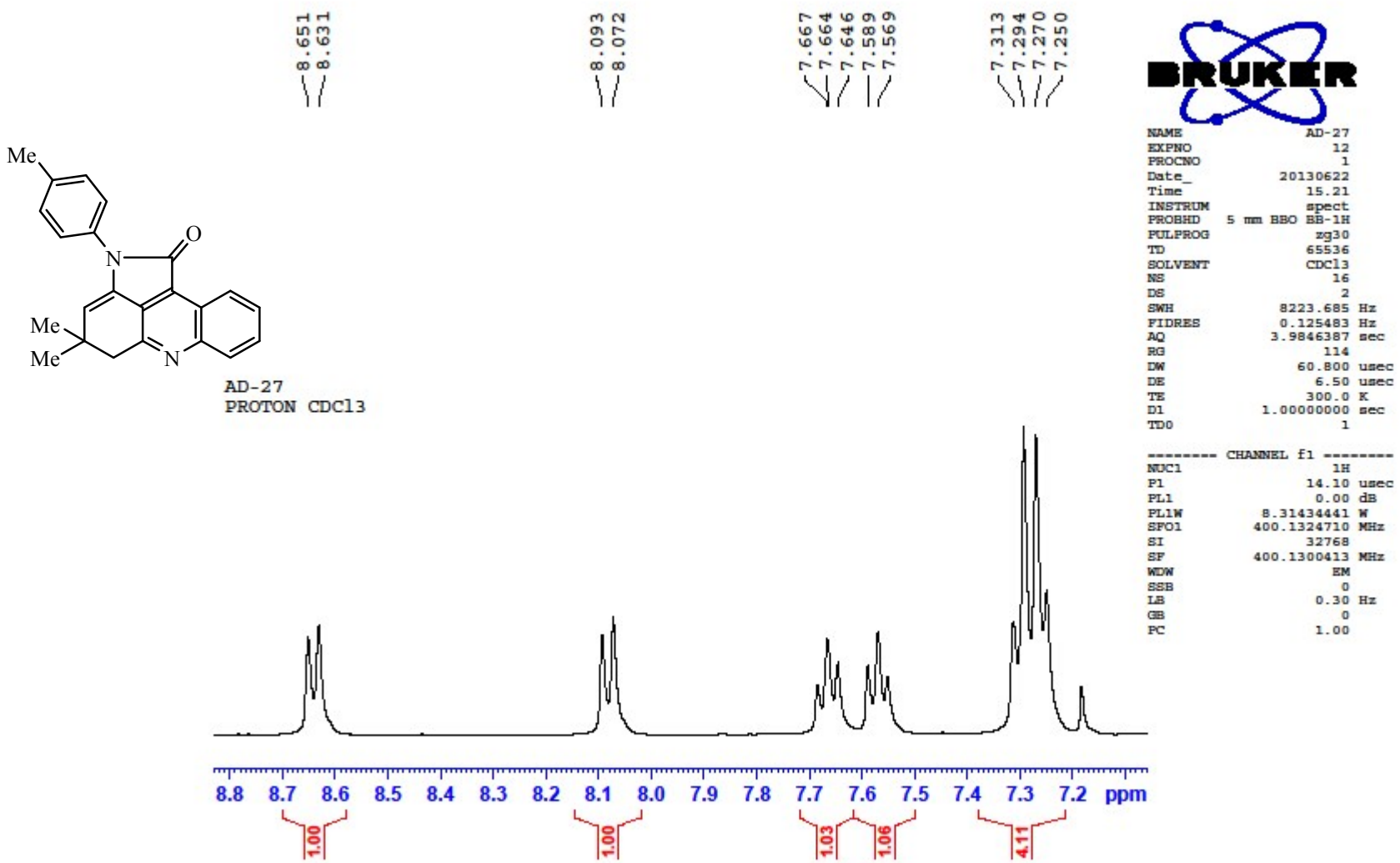
Identification code	uor005
Empirical formula	C23 H20 N2 O
Formula weight	340.41
Temperature	150(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 9.7936(7) A alpha = 110.403(5) deg. b = 10.0349(4) A beta = 101.163(6) deg. c = 10.3079(6) A gamma = 102.888(5) deg.

Volume	883.80(9) A^3
Z, Calculated density	2, 1.279 Mg/m^3
Absorption coefficient	0.079 mm^-1
F(000)	360
Crystal size	0.23 x 0.18 x 0.13 mm
Theta range for data collection	3.26 to 25.00 deg.
Limiting indices	-8<=h<=11, -11<=k<=11, -12<=l<=12
Reflections collected / unique	6407 / 3110 [R(int) = 0.0165]
Completeness to theta = 25.00	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9898 and 0.9821
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3110 / 0 / 239
Goodness-of-fit on F^2	1.081
Final R indices [I>2sigma(I)]	R1 = 0.0425, wR2 = 0.1143
R indices (all data)	R1 = 0.0494, wR2 = 0.1195
Extinction coefficient	0.016(3)
Largest diff. peak and hole	0.173 and -0.142 e.A^-3

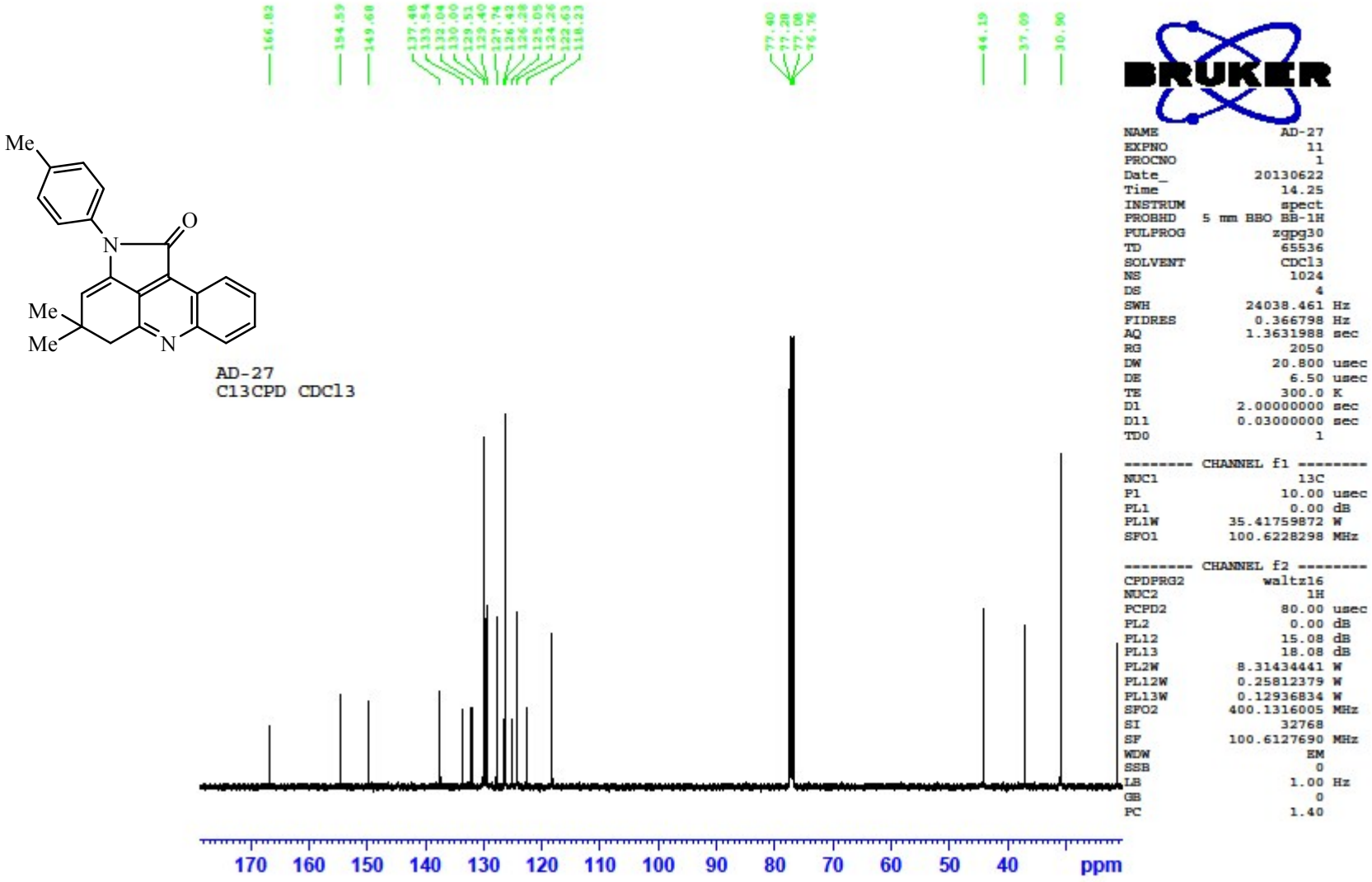
5. ^{1}H and ^{13}C-NMR spectra of the compounds



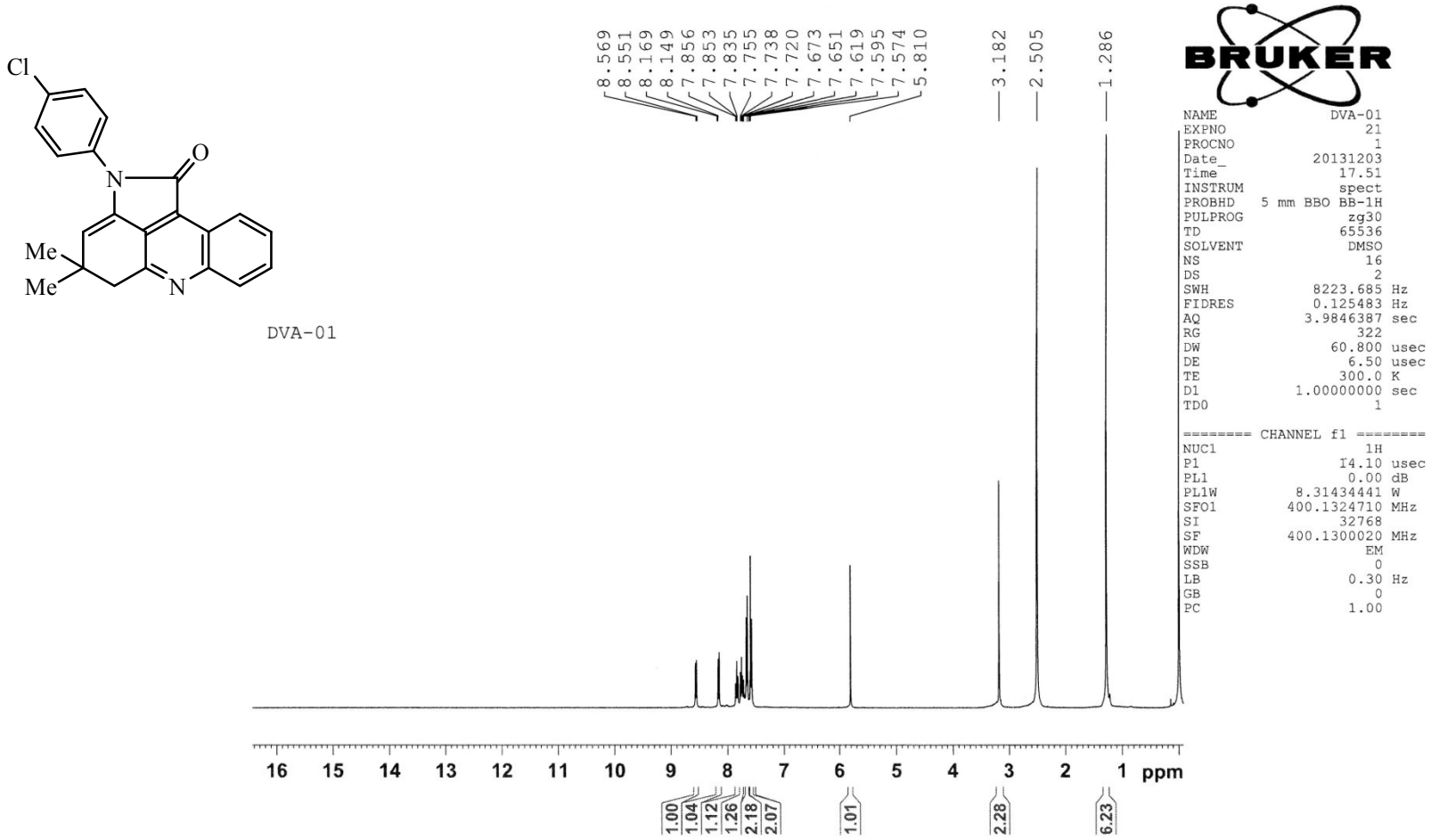
^{1}H-NMR of 4,4-Dimethyl-2-*p*-tolyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4b)



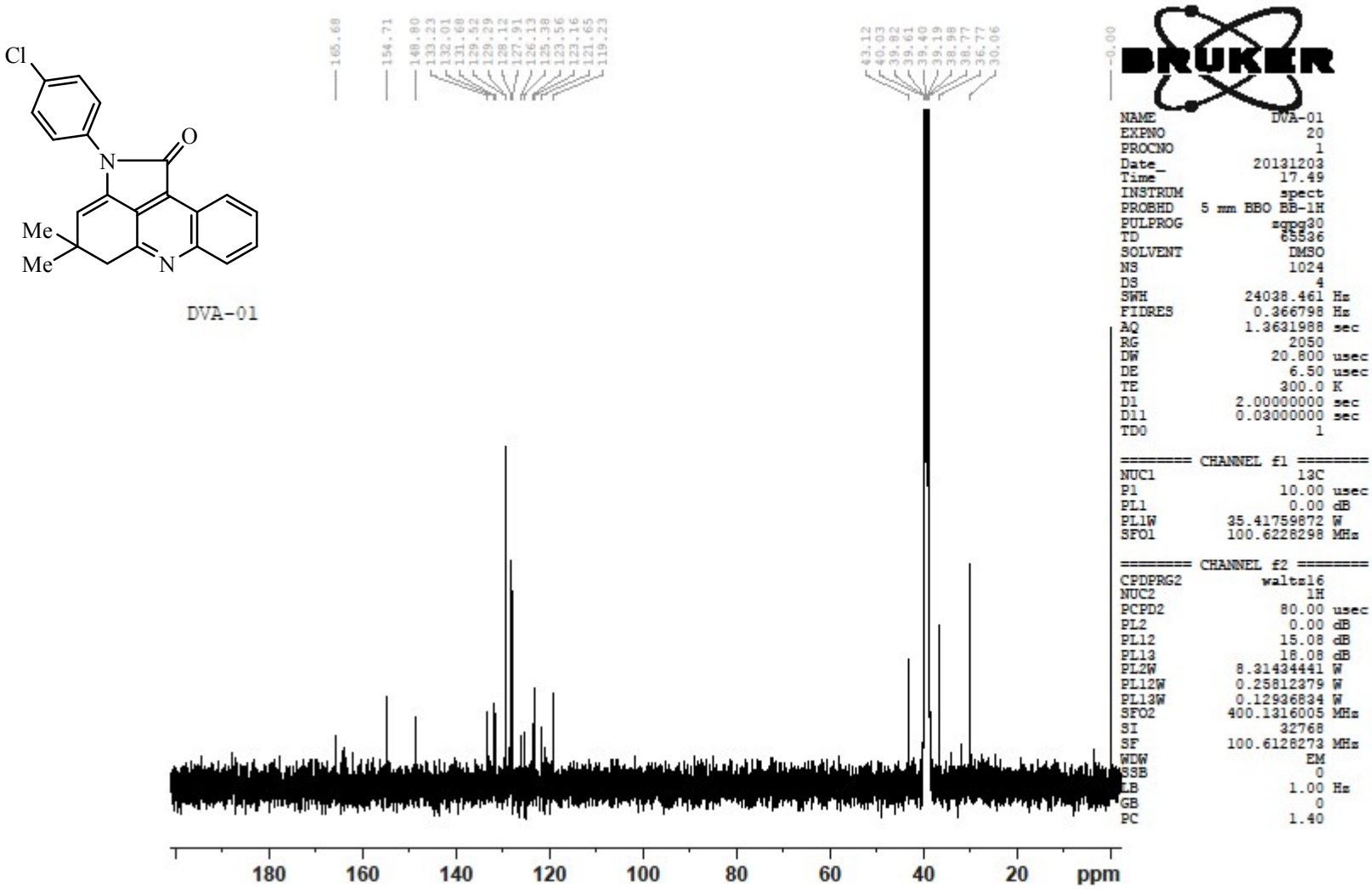
^{1}H-NMR of 4,4-Dimethyl-2-*p*-tolyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4b)



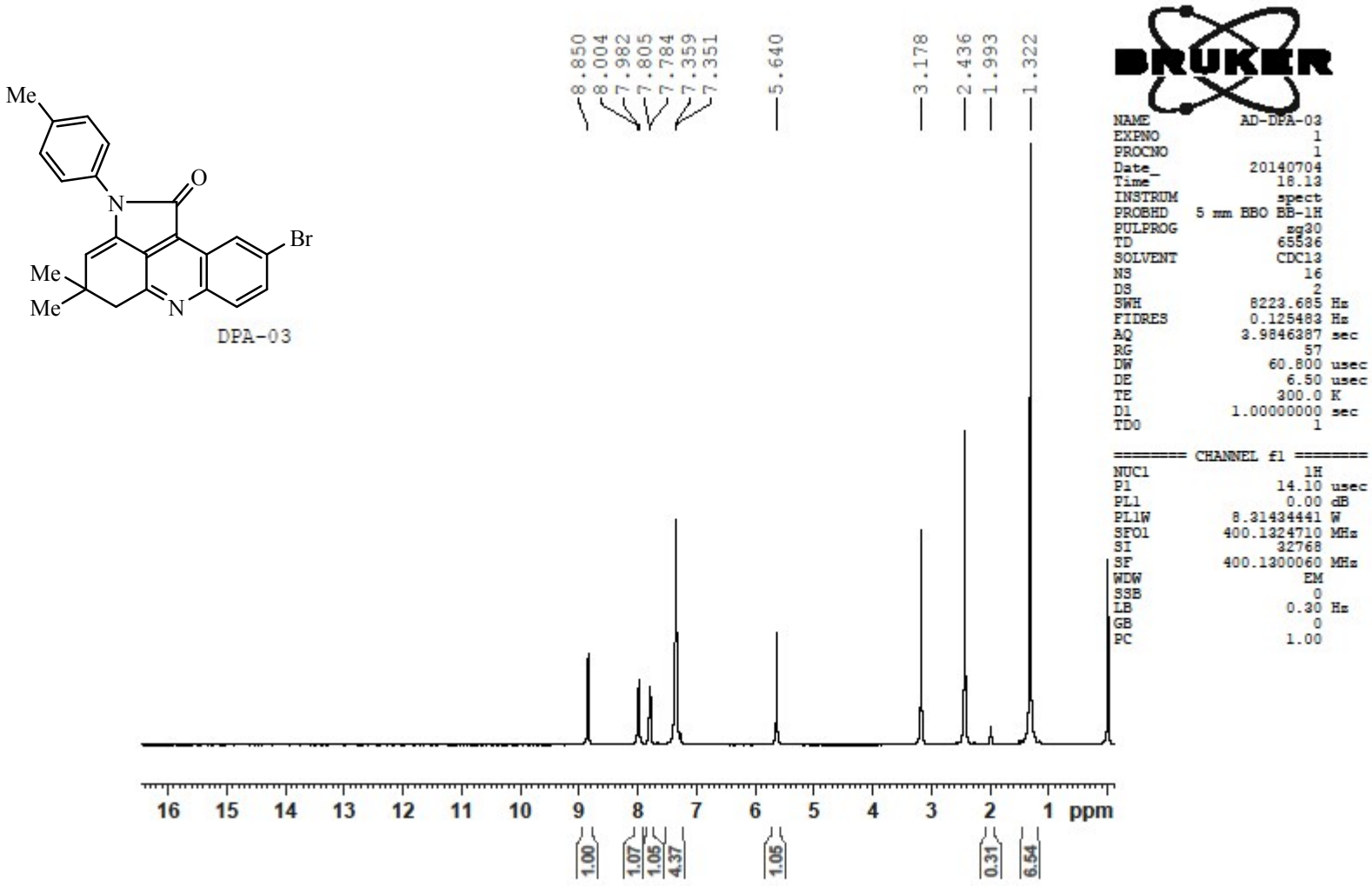
^{13}C-NMR of 4,4-Dimethyl-2-*p*-tolyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4b)



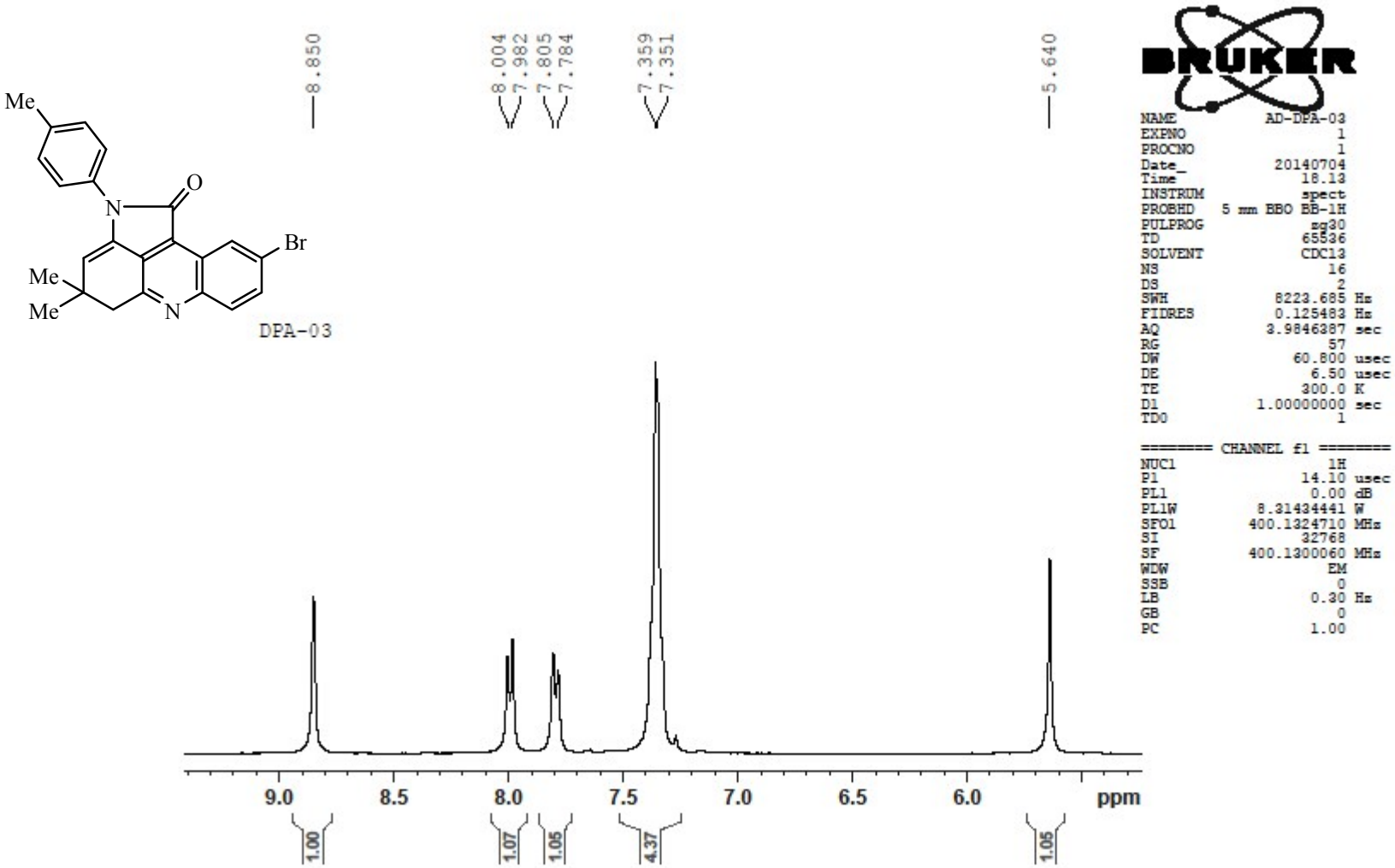
^{1}H-NMR of 2-(4-Chlorophenyl)-4,4-dimethyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4c)



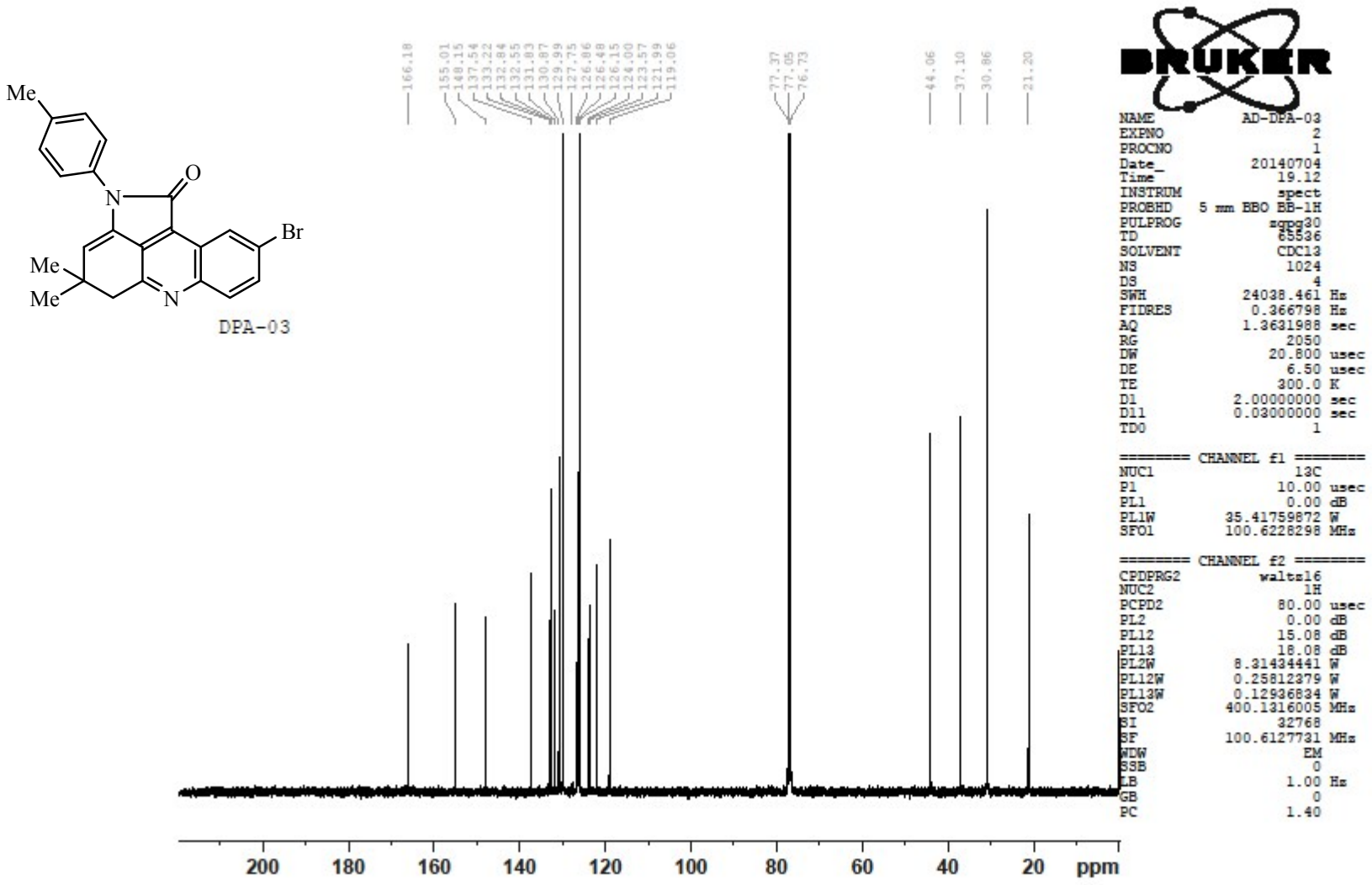
^{13}C-NMR of 2-(4-Chlorophenyl)-4,4-dimethyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4c)



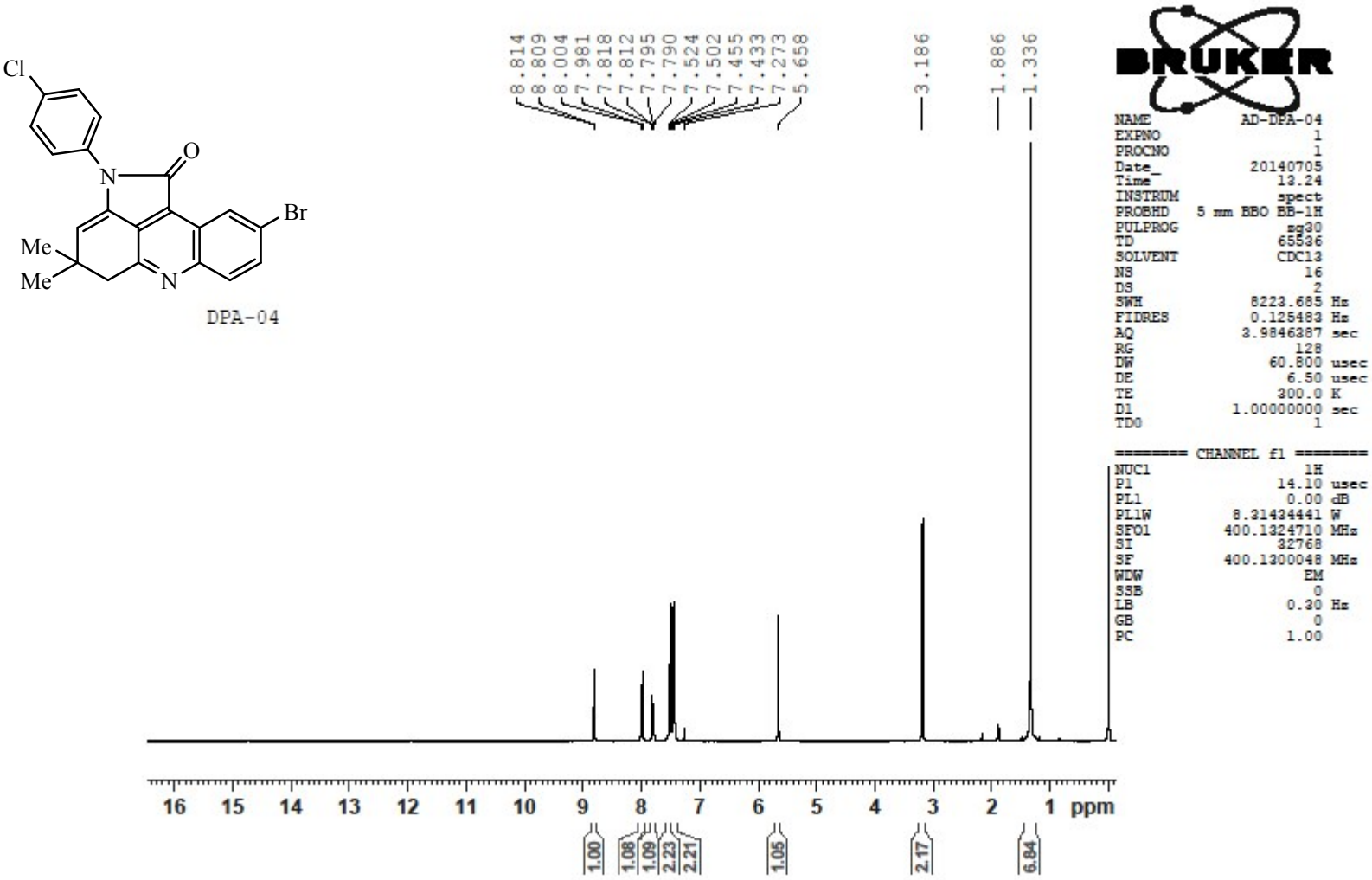
[1]H-NMR of 9-Bromo-4,4-dimethyl-2-*p*-tolyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4f)



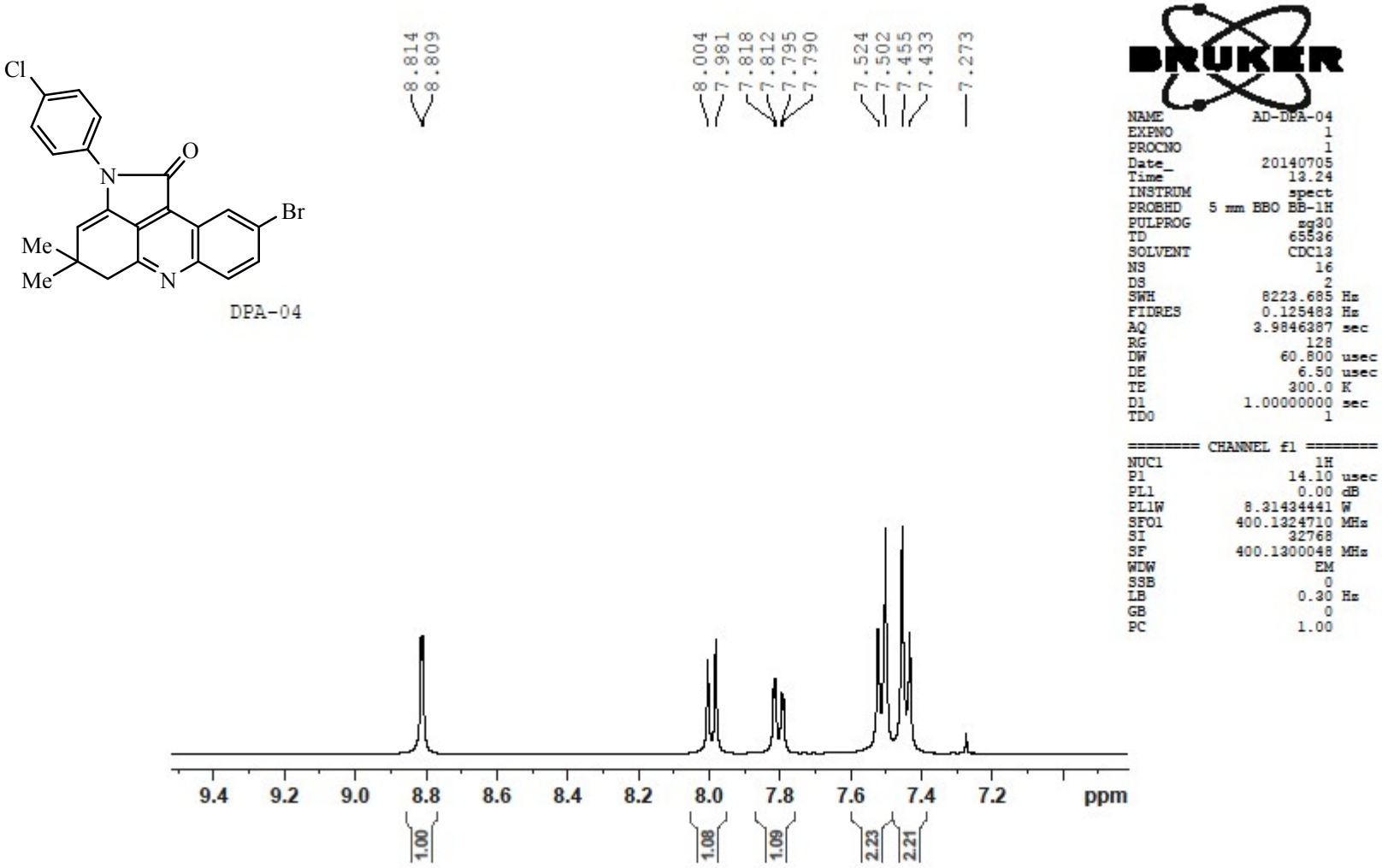
^{1}H-NMR of 9-Bromo-4,4-dimethyl-2-*p*-tolyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4f)



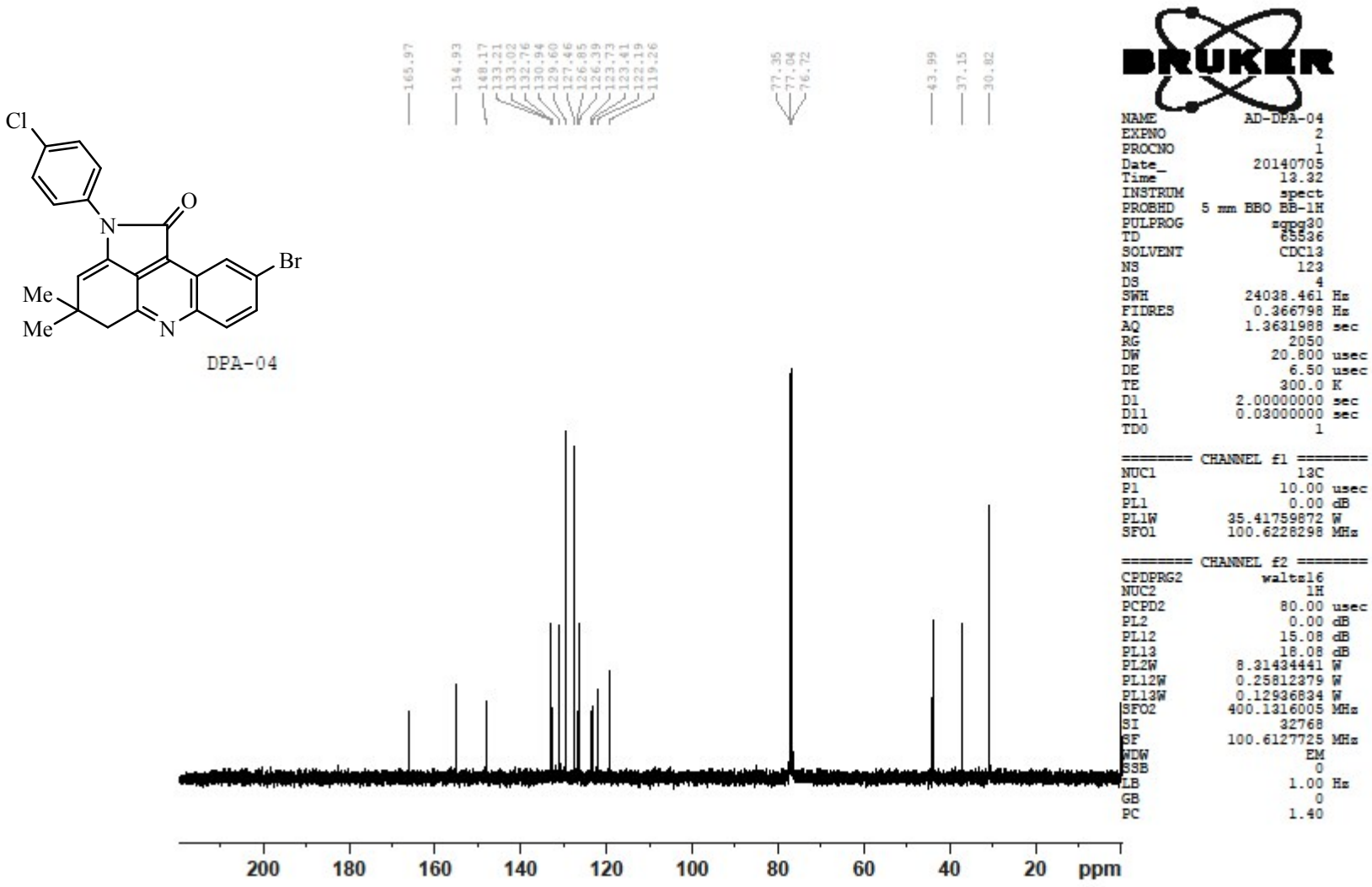
^{13}C-NMR of 9-Bromo-4,4-dimethyl-2-*p*-tolyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4f)



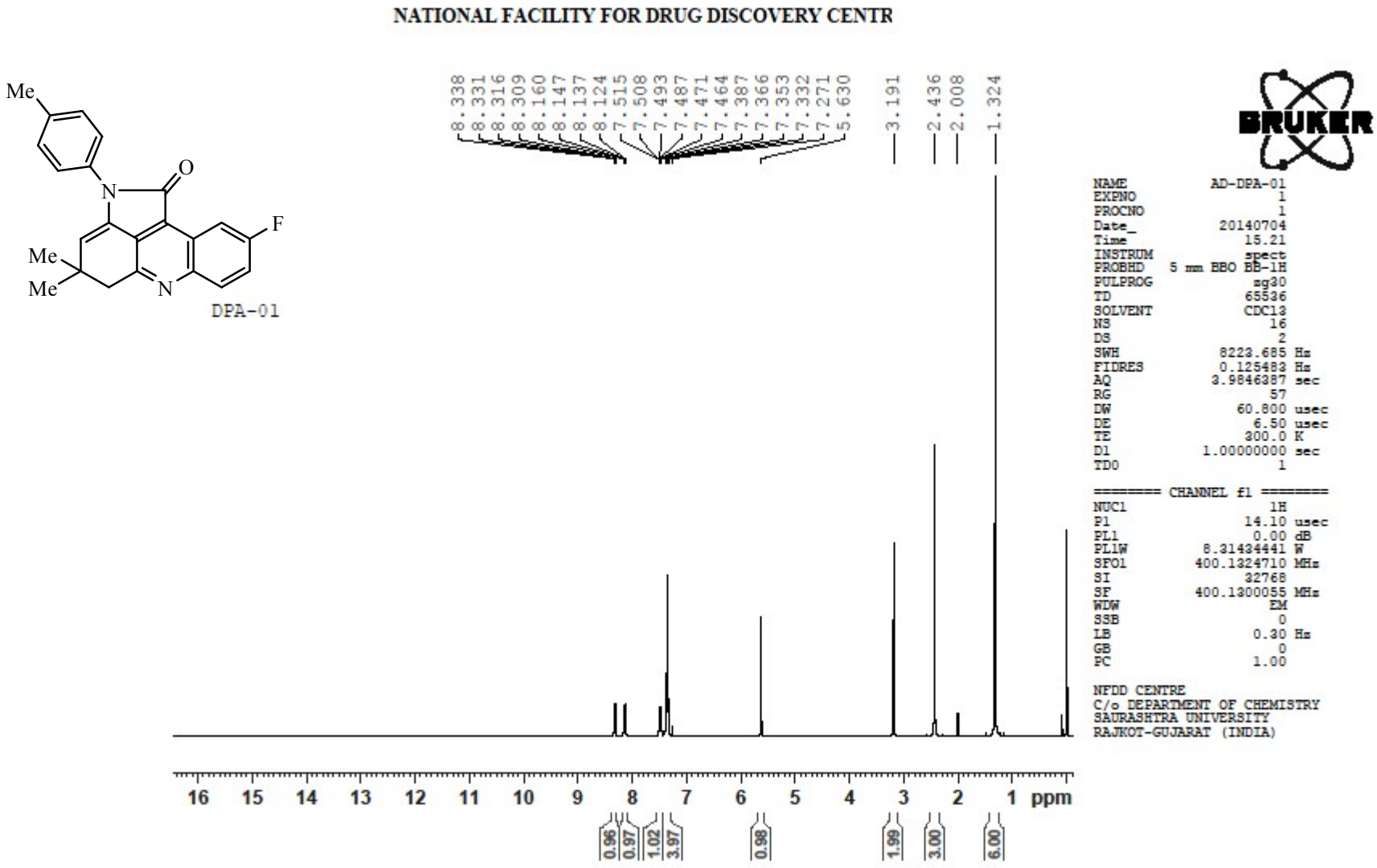
^{1}H-NMR of 9-Bromo-2-(4-chlorophenyl)-4,4-dimethyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4g)



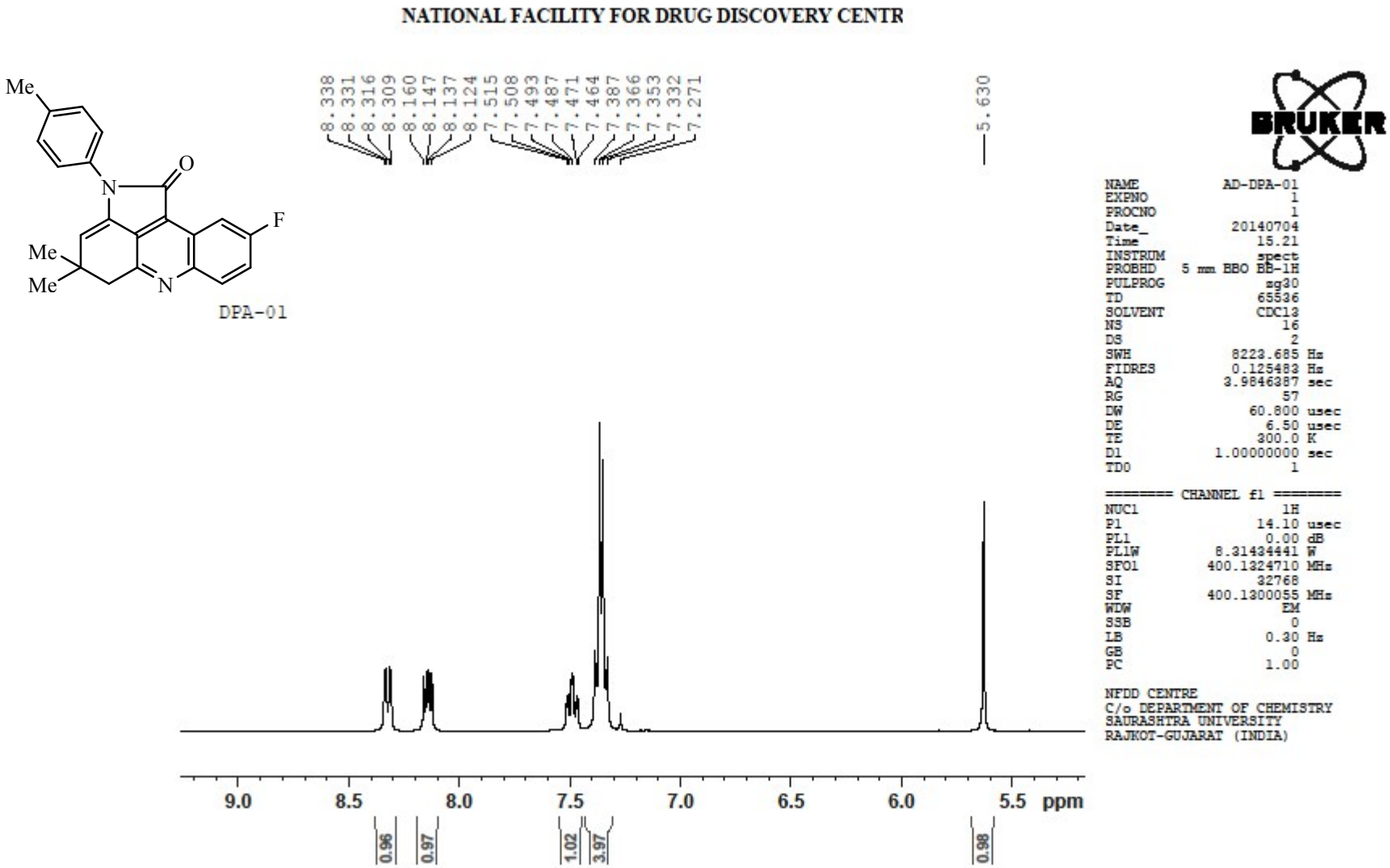
^{1}H-NMR of 9-Bromo-2-(4-chlorophenyl)-4,4-dimethyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4g)



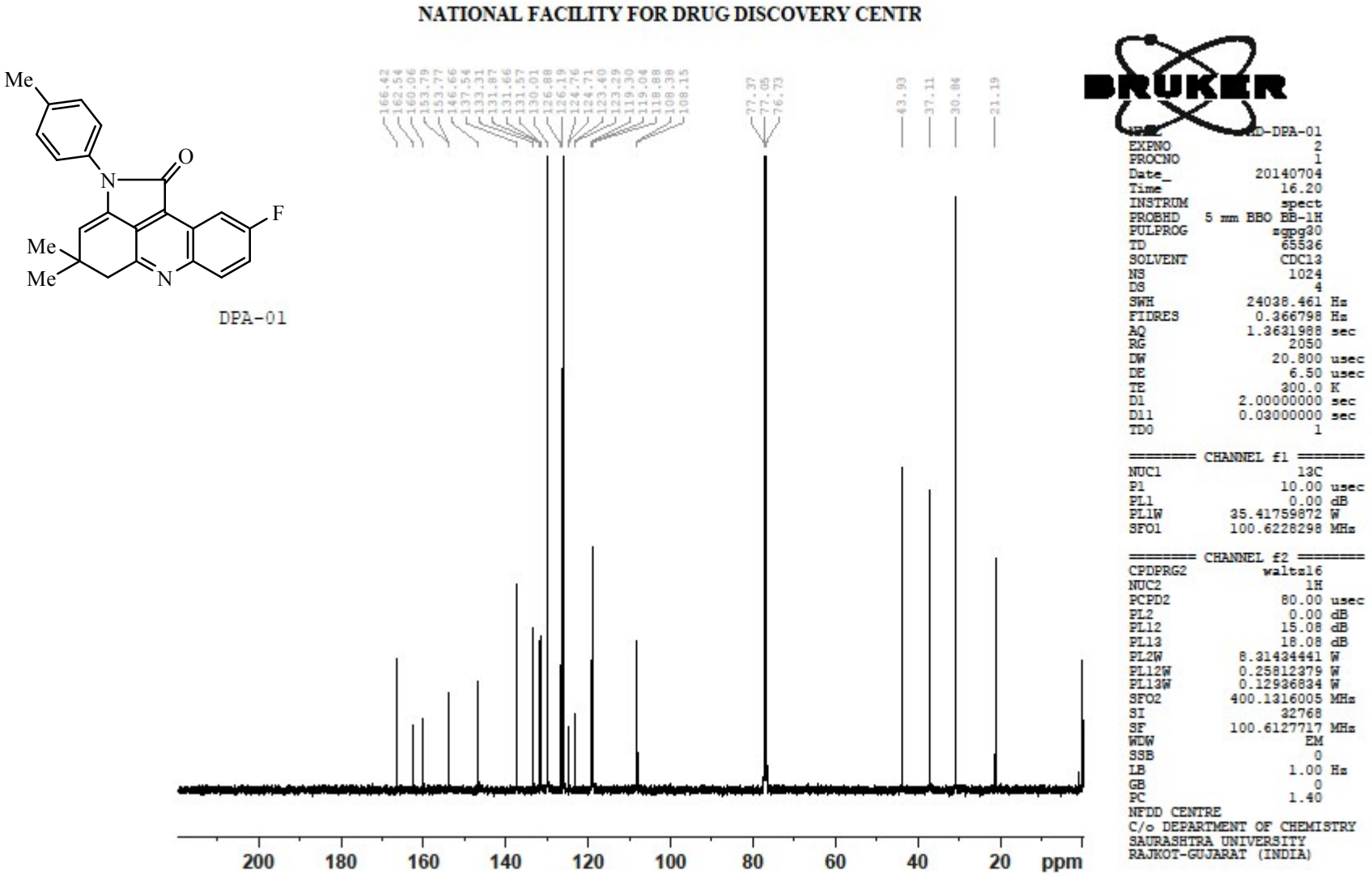
^{13}C-NMR of 9-Bromo-2-(4-chlorophenyl)-4,4-dimethyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4g)



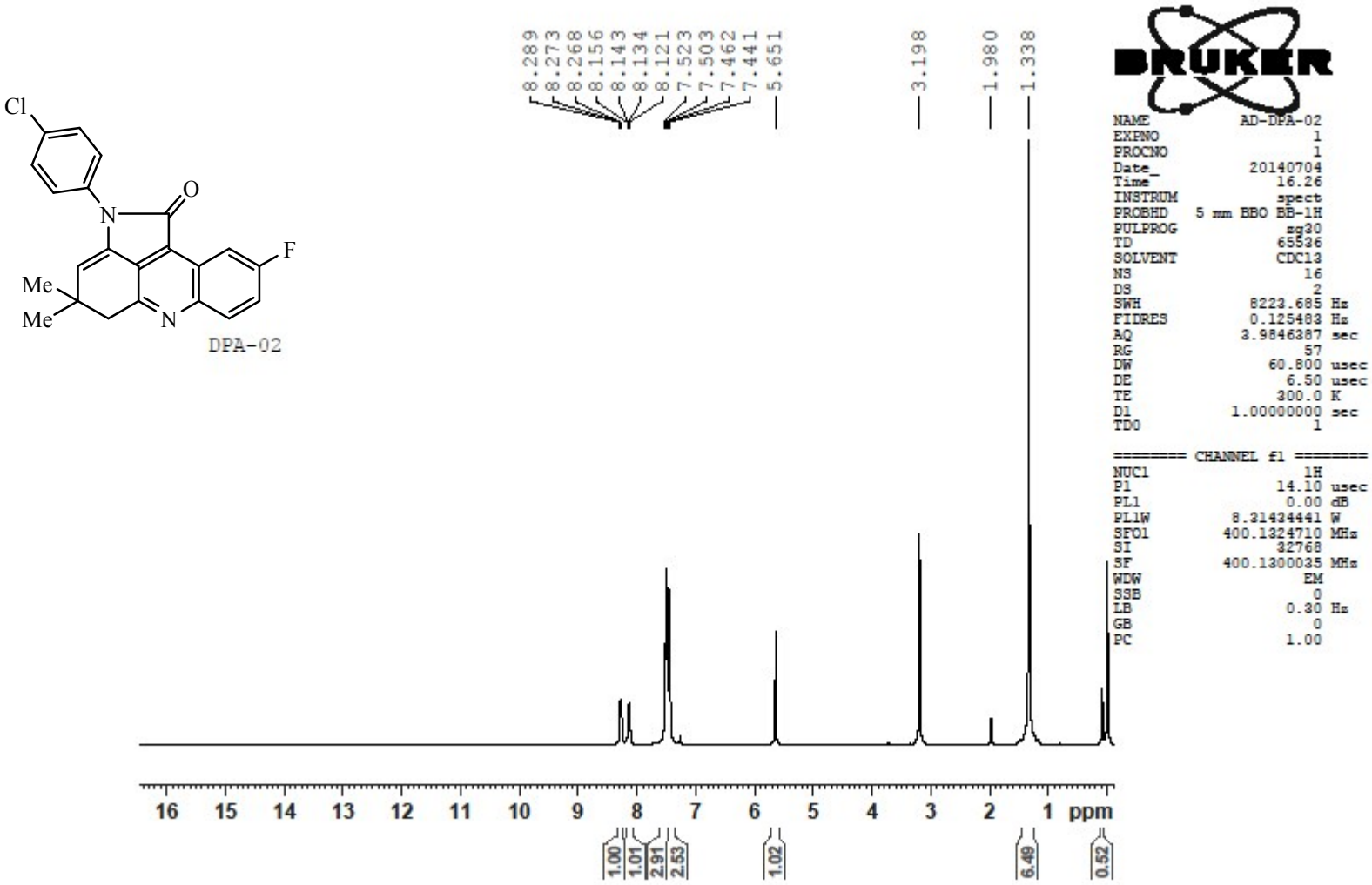
^{1}H-NMR of 9-Fluoro-4,4-dimethyl-2-*p*-tolyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4j)



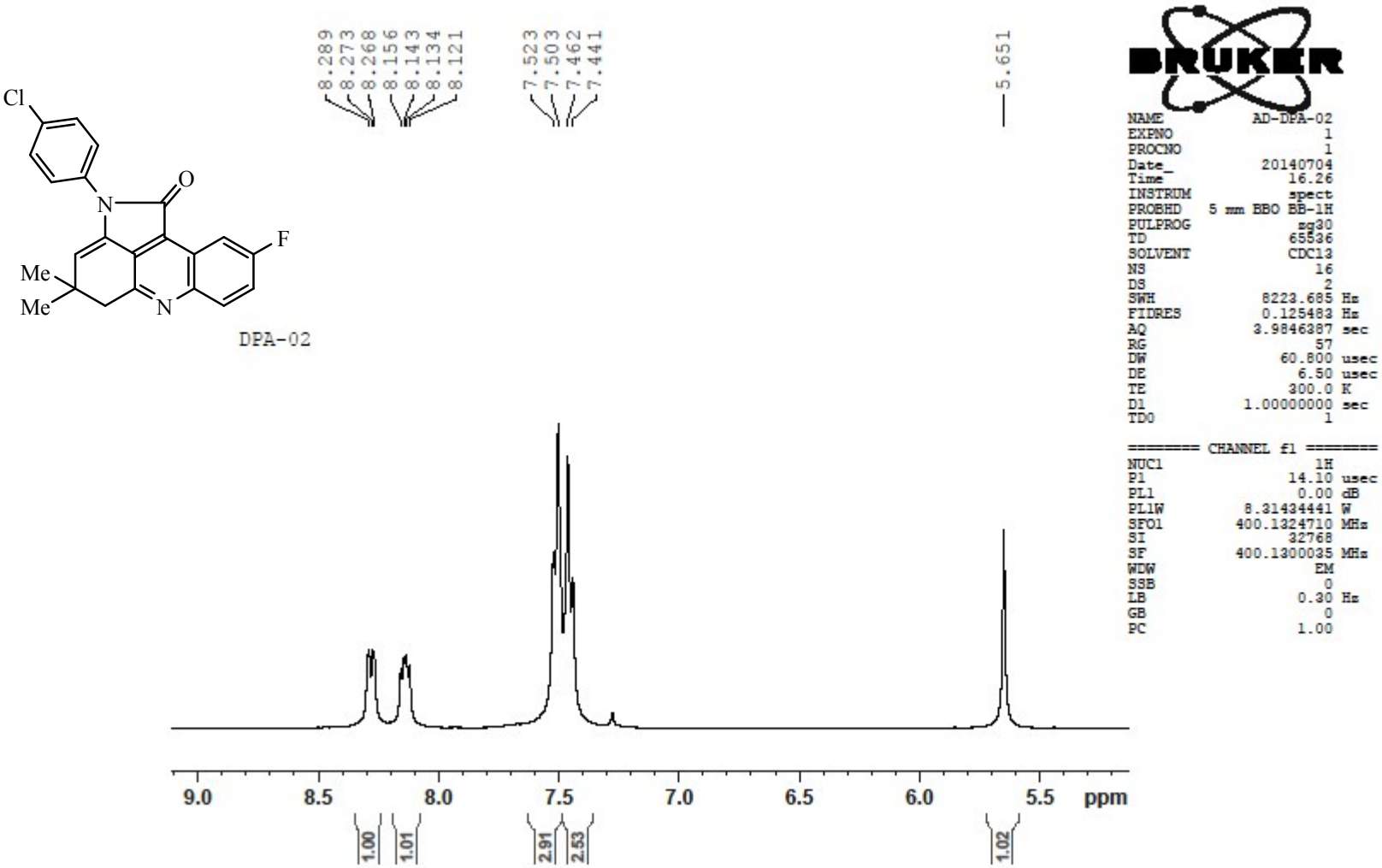
^{1}H-NMR of 9-Fluoro-4,4-dimethyl-2-*p*-tolyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4j)



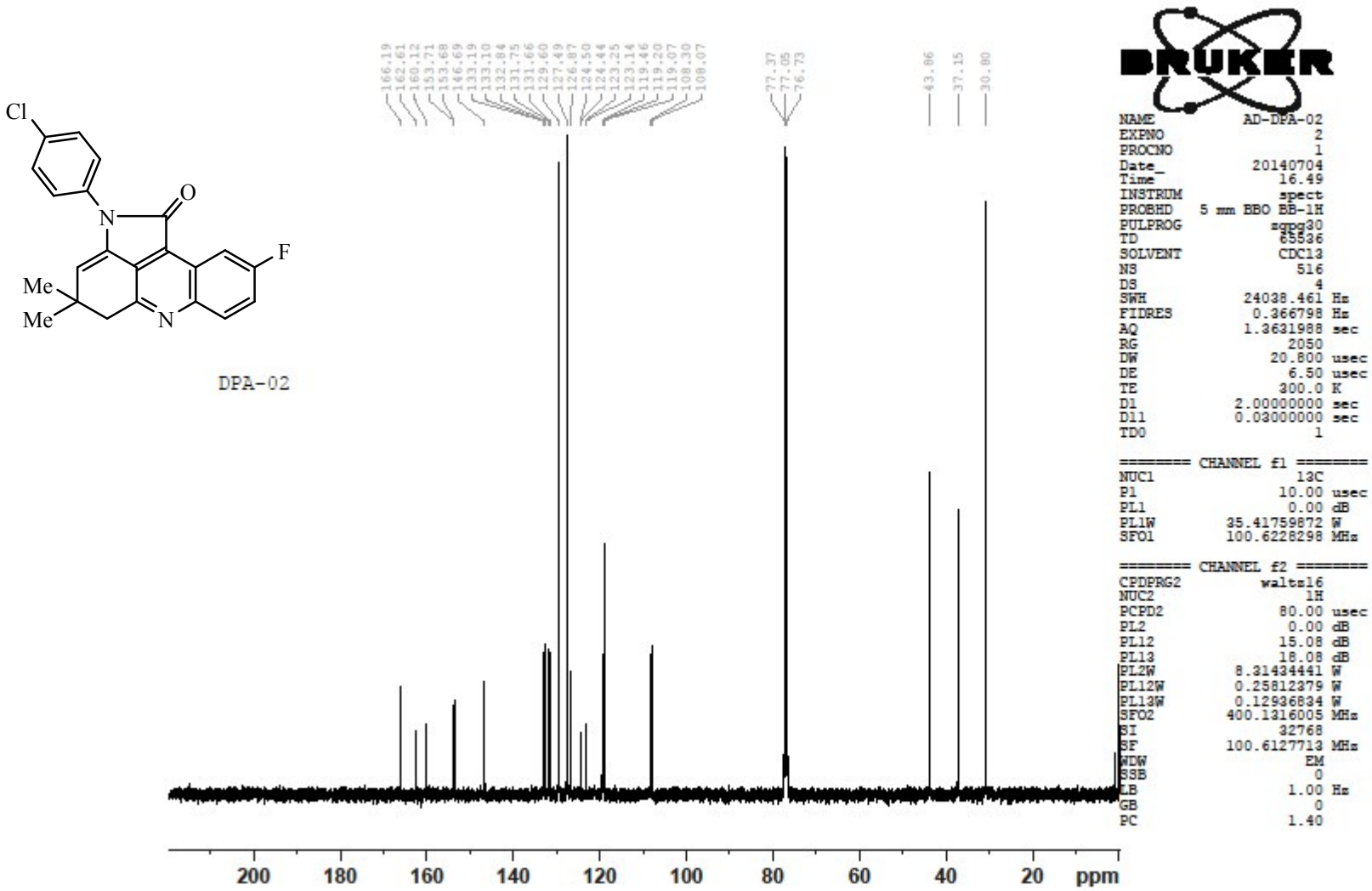
^{13}C-NMR of 9-Fluoro-4,4-dimethyl-2-*p*-tolyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4j)



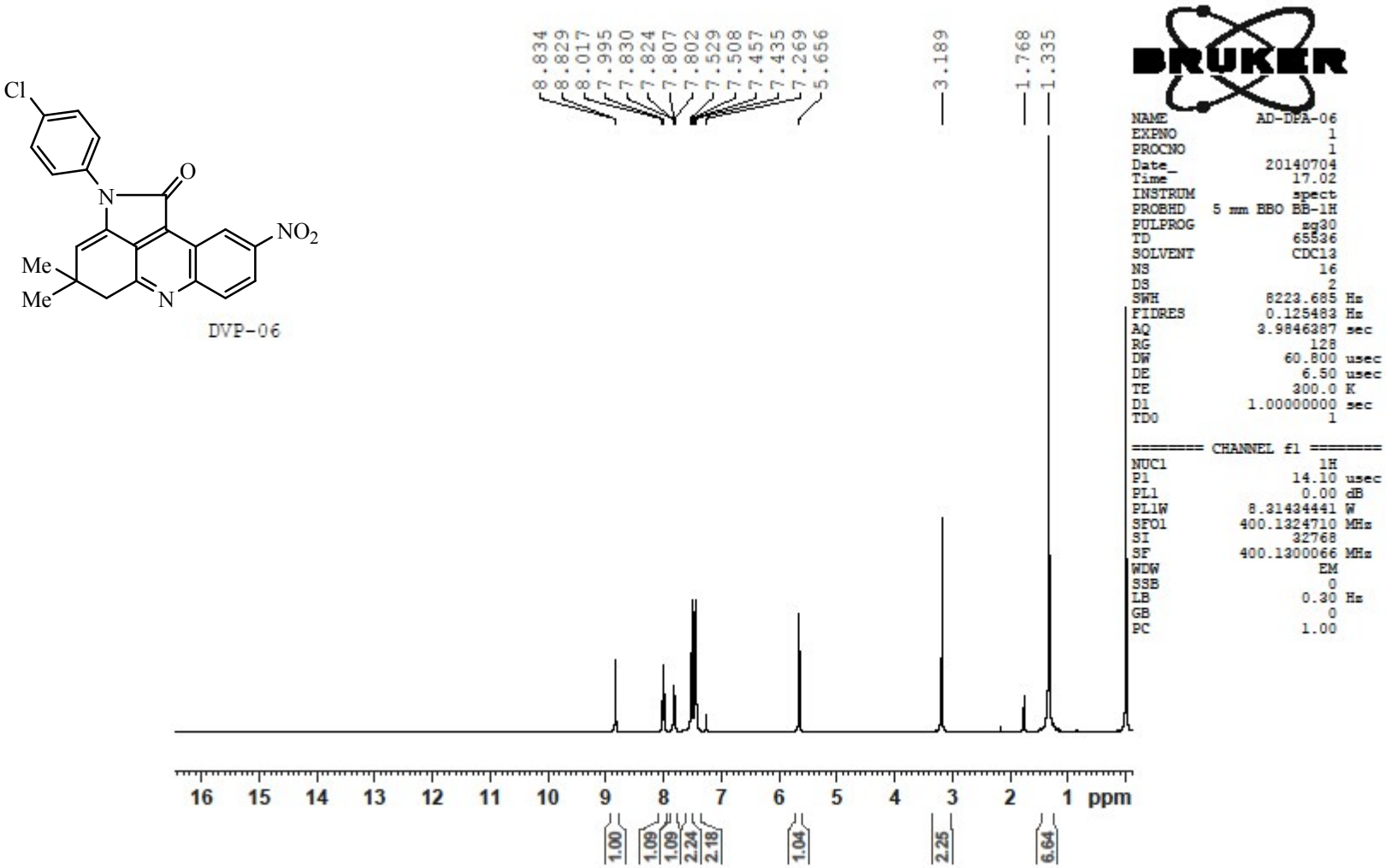
^{1}H-NMR of 2-(4-Chlorophenyl)-9-fluoro-4,4-dimethyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4k)



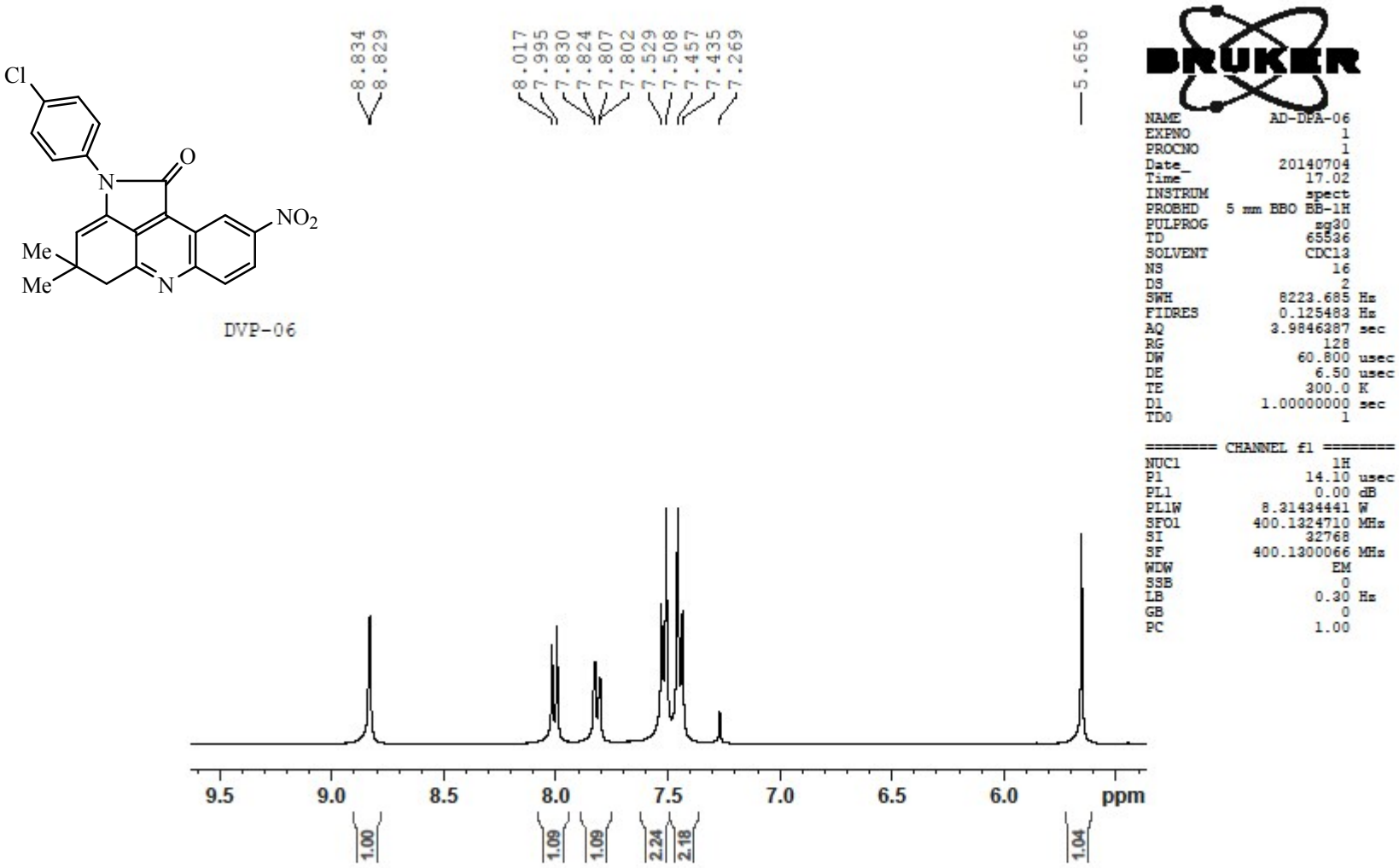
^{1}H-NMR of 2-(4-Chlorophenyl)-9-fluoro-4,4-dimethyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4k)



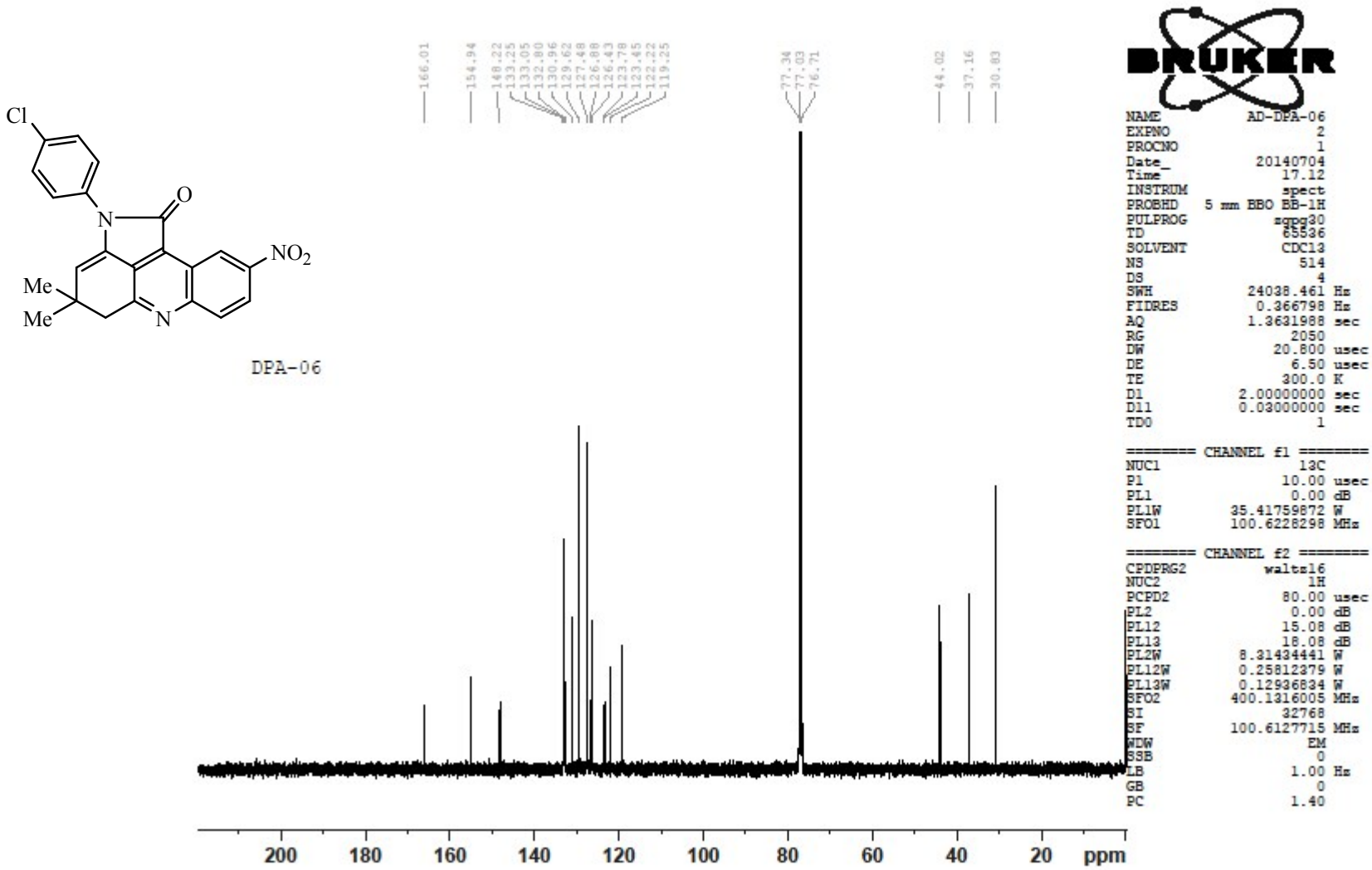
^{13}C-NMR of 2-(4-Chlorophenyl)-9-fluoro-4,4-dimethyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4k)



^{1}H-NMR of 2-(4-Chlorophenyl)-4,4-dimethyl-9-nitro-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4n)



^{1}H-NMR of 2-(4-Chlorophenyl)-4,4-dimethyl-9-nitro-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4n)



^{13}C-NMR of 2-(4-Chlorophenyl)-4,4-dimethyl-9-nitro-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4n)

6. Mass spectra of the compounds

NATIONAL FACILITY FOR DRUG DISCOVERY
SAURASHTRA UNIVERSITY RAJKOT

Sample Information

Analyzed by : Admin
Analyzed : 6/12/2013 4:24:17 PM
Sample Name : AD-27
Data File : E:\MS DATA\YEAR 2013\JUNE\120613\AD-27.qgd
Method File : E:\Method\DI NFDD 300113 N.qgm
Tuning File : E:\TUNING FILES\TUNE030613.qgt
SEndIfSModified by : Admin
Modified : 6/13/2013 4:26:15 PM

Spectrum

Line#:1 R.Time:6.120(Scan#:1225)
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RawMode:Averaged 1.480-7.025(297-1406) BasePeak:325(34150)
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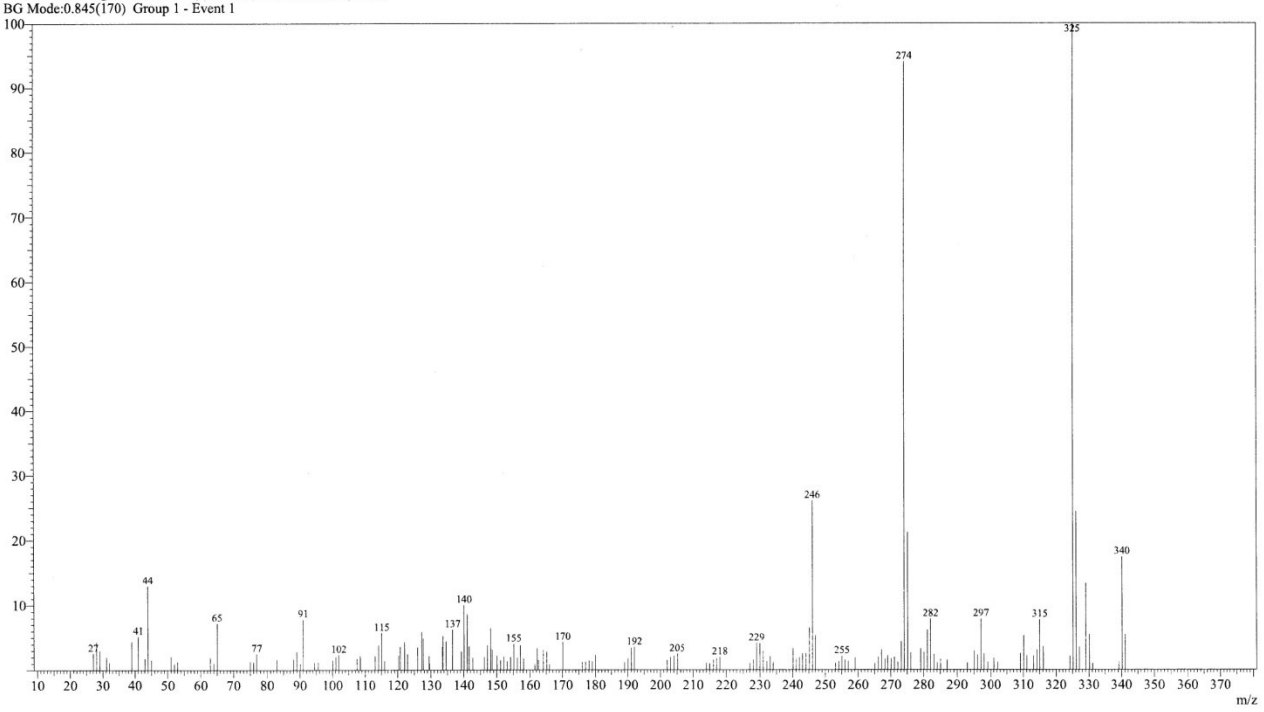

Mass spectrum of 4,4-Dimethyl-2-*p*-tolyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4b)

1 / 1

NATIONAL FACILITY FOR DRUG DISCOVERY
SAURASHTRA UNIVERSITY RAJKOT

12/08/2014

Sample Information

Analyzed by	: PINAKIN
Analyzed	: 7/16/2014 12:44:41 PM
Sample Name	: DPA 03
Data File	: E:\MS DATA\YEAR 2014\JULY\150714\DPA03.qgd
Method File	: E:\DI NFDD 300113 P.qgm
Tuning File	: E:\TUNING FILES\TUNE 150714.qgt
$EndIf$Modified by	: PINAKIN
Modified	: 8/12/2014 3:29:53 PM

Spectrum

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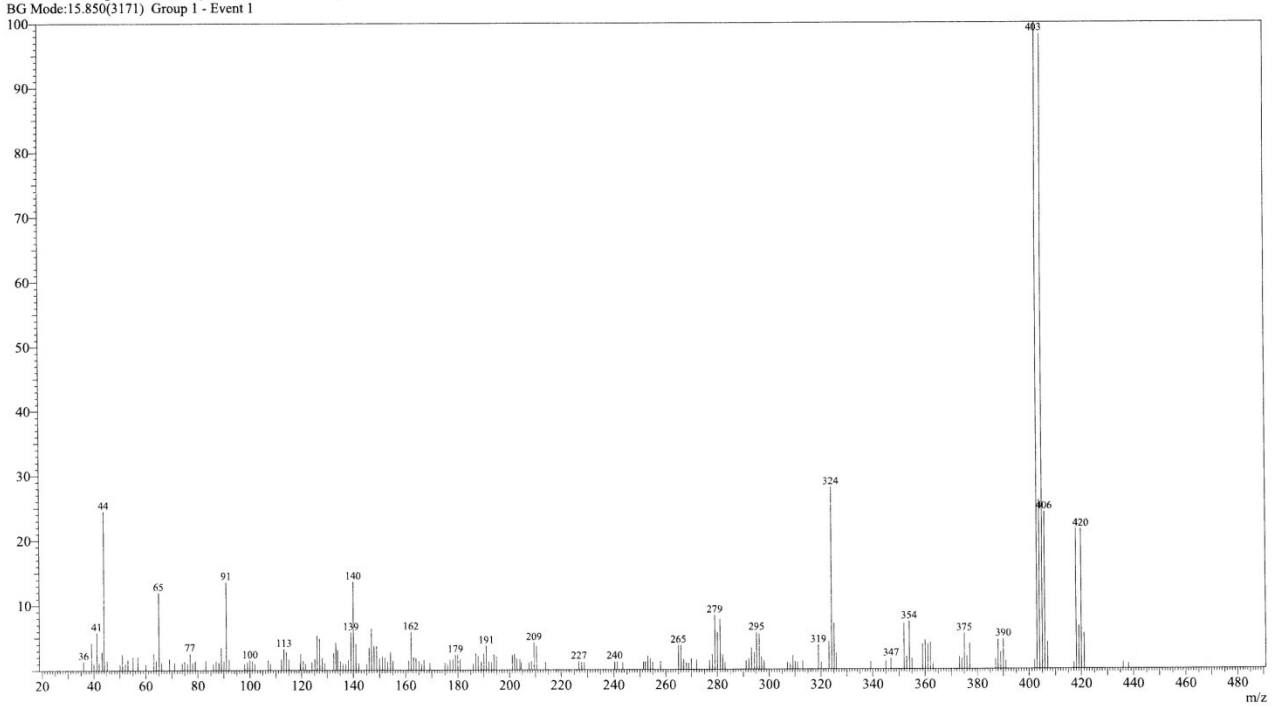


Mass spectrum of 9-Bromo-4,4-dimethyl-2-*p*-tolyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4f)

1 / 1

NATIONAL FACILITY FOR DRUG DISCOVERY
SAURASHTRA UNIVERSITY RAJKOT

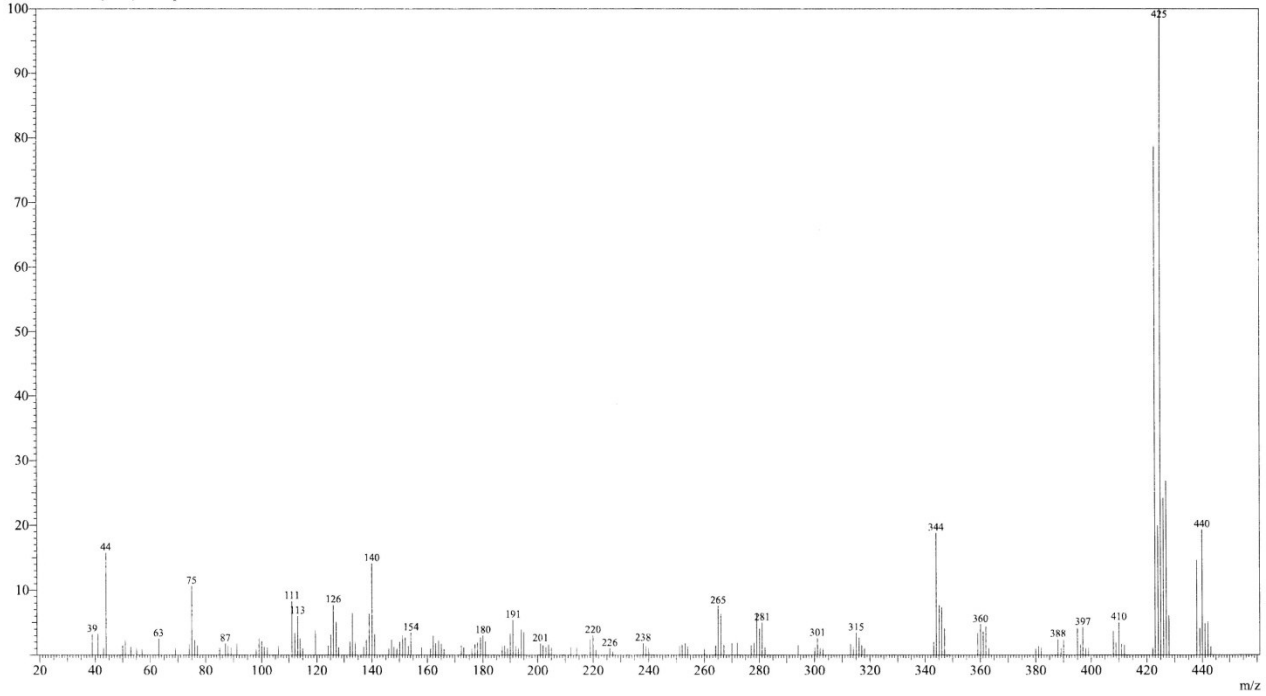
12/08/2014

Sample Information

Analyzed by	: PINAKIN
Analyzed	: 7/15/2014 3:37:40 PM
Sample Name	: DPA 04
Data File	: E:\MS DATA\YEAR 2014\JULY\150714\DPA04.qgd
Method File	: E:\DI NFDD 300113 P.qgm
Tuning File	: E:\TUNING FILES\TUNE 150714.qgt
SEndIf$Modified by	: PINAKIN
Modified	: 8/12/2014 3:29:57 PM

Spectrum

Line#:1 R.Time:3.515(Scan#:704)
MassPeaks:161
RawMode:Averaged 1.165-4.400(234-881) BasePeak:425(27962)
BG Mode:6.480(1297) Group 1 - Event 1



Mass spectrum of 9-Bromo-2-(4-chlorophenyl)-4,4-dimethyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4g)

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NATIONAL FACILITY FOR DRUG DISCOVERY
SAURASHTRA UNIVERSITY RAJKOT

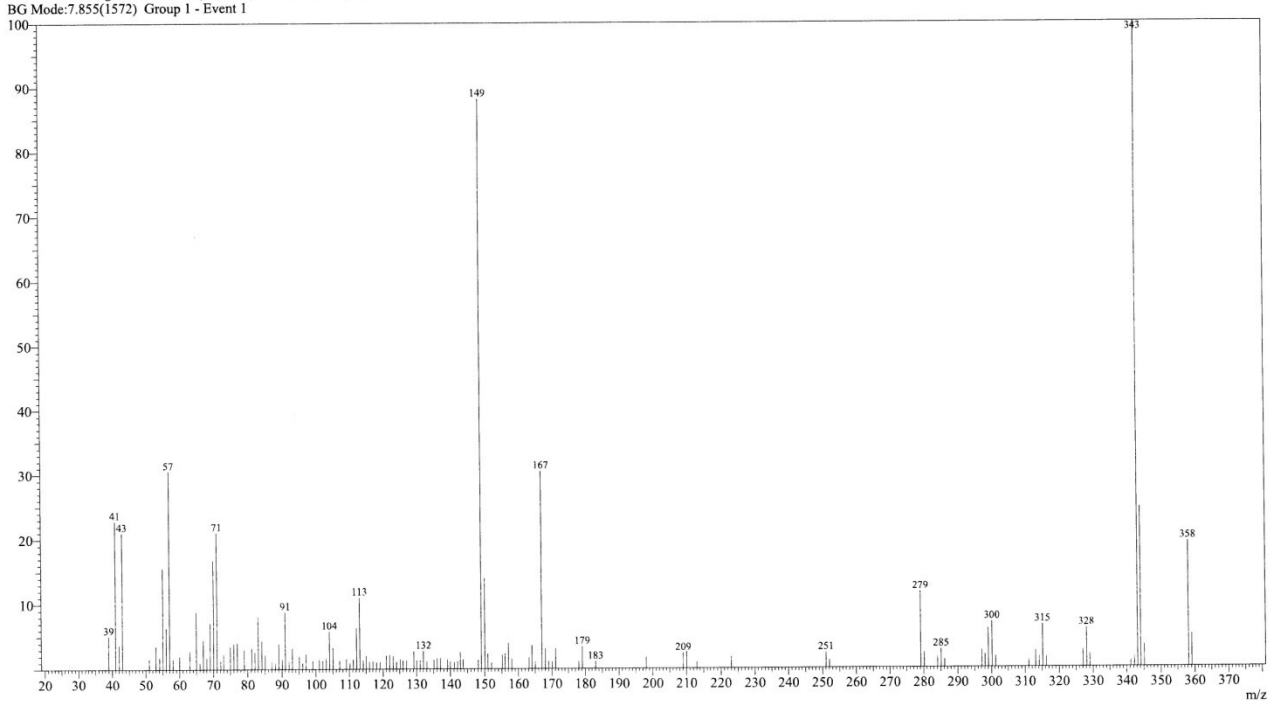
12/08/2014

Sample Information

Analyzed by	: PINAKIN
Analyzed	: 7/15/2014 4:33:20 PM
Sample Name	: DPA 01
Data File	: E:\MS DATA\YEAR 2014\JULY\150714\DPA01.qgd
Method File	: E:\DI NFDD 300113 P.qgm
Tuning File	: E:\TUNING FILES\TUNE 150714.qgt
SEndIf$Modified by	: PINAKIN
Modified	: 8/12/2014 3:29:46 PM

Spectrum

Line#:1 R.Time:1.750(Scan#:351)
MassPeaks:132
RawMode:Averaged 0.165-6.680(34-1337) BasePeak:343(17967)
BG Mode:7.855(1572) Group 1 - Event 1



Mass spectrum of 9-Fluoro-4,4-dimethyl-2-*p*-tolyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4j)

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NATIONAL FACILITY FOR DRUG DISCOVERY
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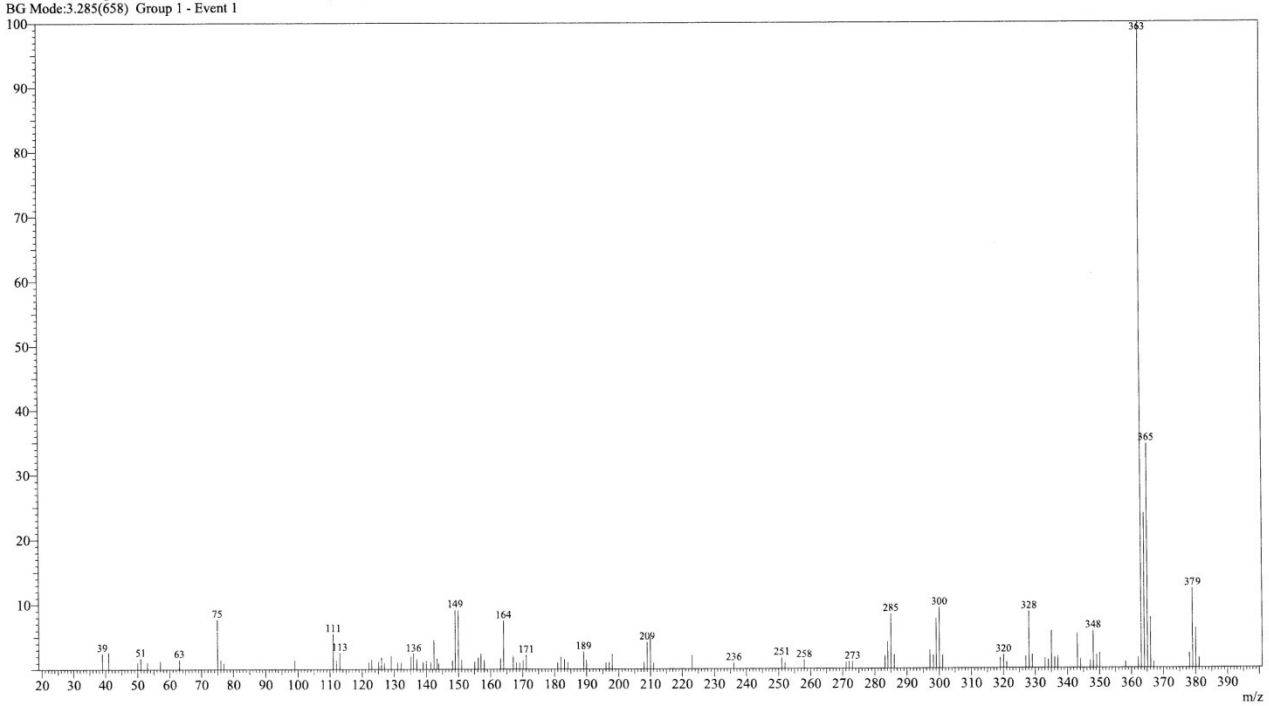
12/08/2014

Sample Information

Analyzed by	: PINAKIN
Analyzed	: 7/15/2014 5:29:14 PM
Sample Name	: DPA 02
Data File	: E:\MS DATA\YEAR 2014\JULY\150714\DPA02.qgd
Method File	: E:\DI NFDD 300113 P.qgm
Tuning File	: E:\TUNING FILES\TUNE 150714.qgt
SEndIf$Modified by	: PINAKIN
Modified	: 8/12/2014 3:29:51 PM

Spectrum

Line#:1 R.Time:2.045(Scan#:410)
MassPeaks:104
RawMode:Averaged 0.030-2.955(7-592) BasePeak:363(68673)
BG Mode:3.285(658) Group 1 - Event 1



Mass spectrum of 2-(4-Chlorophenyl)-9-fluoro-4,4-dimethyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4k)

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NATIONAL FACILITY FOR DRUG DISCOVERY
SAURASHTRA UNIVERSITY RAJKOT

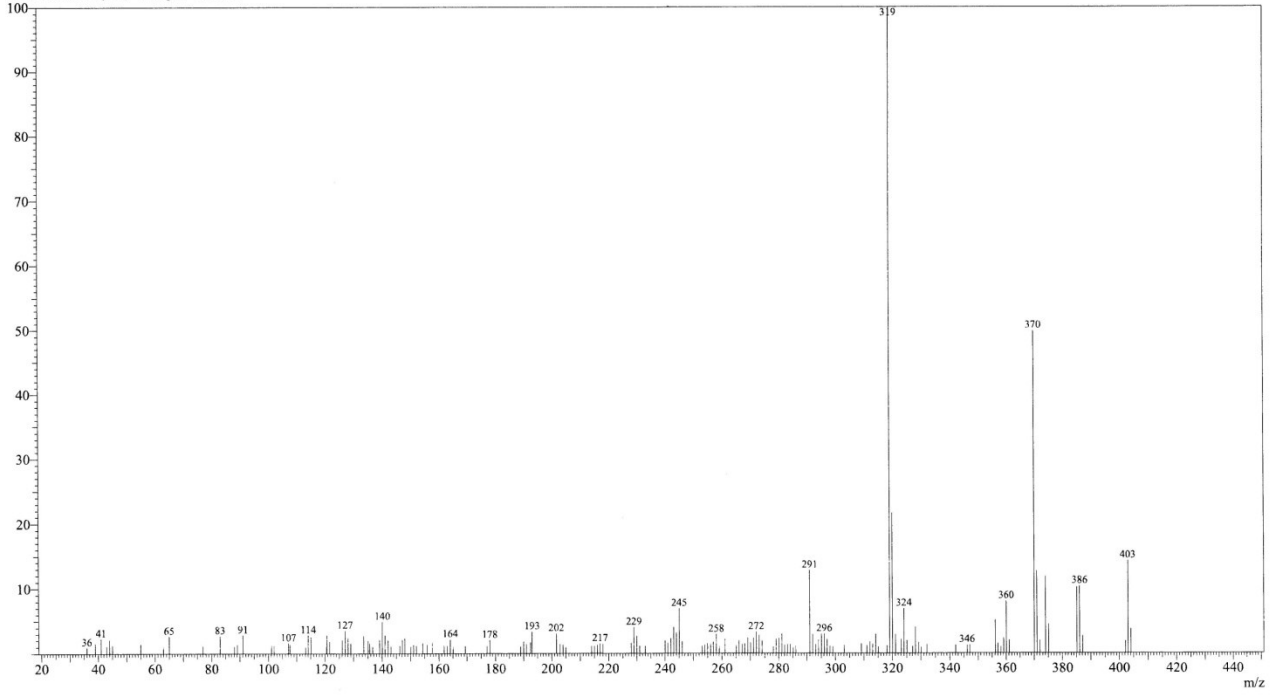
12/08/2014

Sample Information

Analyzed by	: PINAKIN
Analyzed	: 7/16/2014 11:32:52 AM
Sample Name	: DPA 05
Data File	: E:\MS DATA\YEAR 2014\JULY\150714\DPA05.qgd
Method File	: E:\DI NFDD 300113 P.qgm
Tuning File	: E:\TUNING FILES\TUNE 150714.qgt
SEndIf$Modified by	: PINAKIN
Modified	: 8/12/2014 3:30:02 PM

Spectrum

Line#:1 R.Time:2.820(Scan#:565)
MassPeaks:157
RawMode:Averaged 1.545-8.090(310-1619) BasePeak:319(12927)
BG Mode:0.565(114) Group 1 - Event 1



Mass spectrum of 4,4-Dimethyl-9-nitro-2-*p*-tolyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4m)

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SAURASHTRA UNIVERSITY RAJKOT

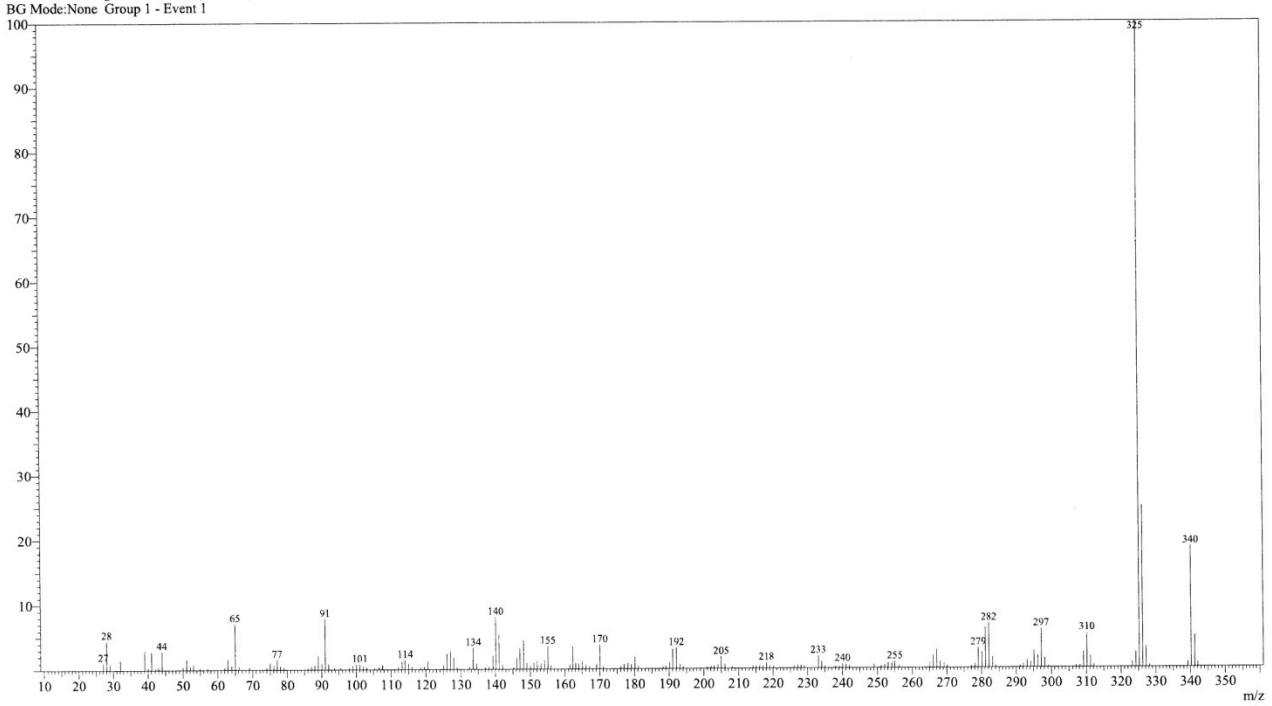
21/06/2013

Sample Information

Analyzed by	: Admin
Analyzed	: 6/12/2013 3:28:39 PM
Sample Name	: AD-26
Data File	: E:\MS DATA\YEAR 2013\JUNE\120613\AD-26.qgd
Method File	: E:\Method\DI NFDD 300113 N.qgm
Tuning File	: E:\TUNING FILES\TUNE030613.qgt
SEndIf$Modified by	: Admin
Modified	: 6/13/2013 4:25:20 PM

Spectrum

Line#:1 R.Time:3.040(Scan#:609)
MassPeaks:178
RawMode:Averaged 1.760-3.795(353-760) BasePeak:325(214081)
BG Mode:None Group 1 - Event 1



Mass spectrum of 4,4,9-Trimethyl-2-phenyl-4,5-dihydro-2*H*-pyrrolo[2,3,4-*kl*]acridin-1-one (4p)