Supporting Information

Catalytic formal [4+1] isocyanide-based cycloaddition: an efficient strategy for the synthesis of 1H-cyclopenta[*b*]quinolin-1-one derivatives

Milad Motaghi,[a] Hormoz Khosravi,[a] Saeed Balalaie,[*,a,b] Frank Rominger[c]

[a] Peptide Chemistry Research Center, K. N. Toosi University of Technology, P. O. Box 15875-4416, Tehran, Iran

[b] Medical Biology Research Center, Kermanshah University of Medical Sciences, Kermanshah, Iran

[c] Organisch-Chemisches Institut der Universität Heidelberg, Im Neuenheimer Feld 270, D-69120 Heidelberg, Germany

Table of Contents

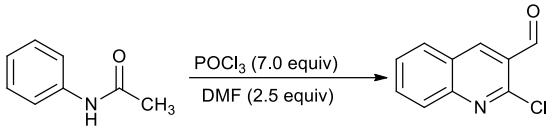
A. General information

All reagents were commercial and used without further purification, unless otherwise indicated. Flash column chromatography was carried out using 63-200 mesh silica gel. All reactions were monitored by TLC, which was performed on precoated aluminum sheets of silica gel 60 (F254) and visualized by exposure to UV light (254 nm). Melting points were measured using a melting point instrument and were uncorrected. ^{1}H NMR spectra were recorded on Bruker spectrometers (at 300 or 400 MHz) and reported relative to tetramethylsilane as internal standard. Data for ^{1}H NMR spectra were reported as follows: chemical shift (δ/ppm), multiplicity (*s* = singlet, *d* = doublet, *t* = triplet, *q* = quartet, *m* = multiplet), coupling constant (*J*/Hz) and integration. ^{13}C NMR spectra were recorded on Bruker Spectrometers (75 or 100 MHz). Data for ^{13}C NMR spectra were reported in terms of chemical shift. High-resolution mass spectra (HRMS) and LC-MS (ESI) were obtained using a Bruker APEX-II Quazar area detector and Agillent 6410 QQQQ spectrometer. Mass spectra are reported as m/z (% of relative intensity). Elemental analyses for C, H and N were performed using a Heraeus CHN-O-Rapid analyzer.

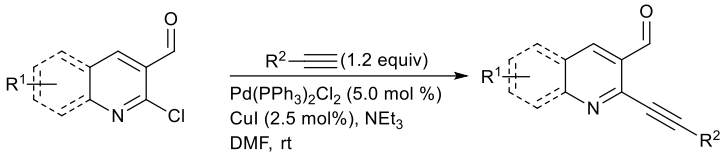
B. Experimental procedures

B1. Typical Procedure for the Synthesis of quinoline-based starting materials

2-chloroquinoline-3-carbaldehydes: They were prepared by the reported procedure.[1]

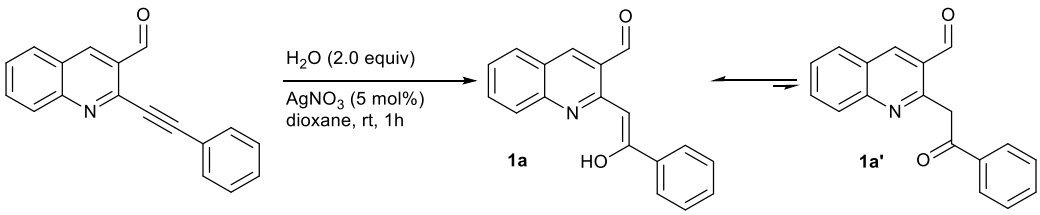


2-(alkylethynyl)quinoline-3-carbaldehydes and 2-(alkylethynyl)nicotinaldehyde: They were prepared by the Sonogashira coupling reaction of 2-chloroquinoline-3-carbaldehydes and 2-Chloro-3-pyridinecarboxaldehyde with terminal alkynes.[2] All commercially available compounds were used as received.



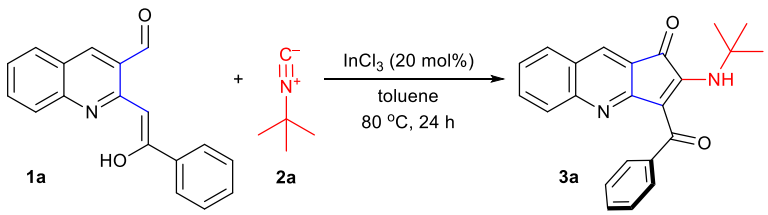
Typical Procedure for the Preparation of 1 Using 1a as the Example

They were prepared by slight modification of a literature procedure.[3] Unless otherwise specified, (Z)-2-(2-hydroxy-2-phenylvinyl)quinoline-3-carbaldehyde **1a** (as an example) derivatives were synthesized *via* the following step:



To a stirred solution of 2-(phenylethynyl)quinoline-3-carbaldehyde (640 mg, 2.50 mmol), $AgNO_3$ (5 mol%) in dioxane (8 mL) was added H_2O (2.0 equiv). The solution was stirred for 1 h at rt. Upon completion of the reaction indicated by TLC, The reaction mixture was washed with H_2O and extracted with CH_2Cl_2 (20 mL) for three times. The combined organic phases were washed with brine, dried over with anhydrous Na_2SO_4, filtered and concentrated under reduced pressure. The residue was purified by column chromatography (*n*-hexane/EtOAc = 4:1 to 1:2) as eluent to afford the tautomeric mixture of **1a** and **1a'** (610 mg, 95 %).

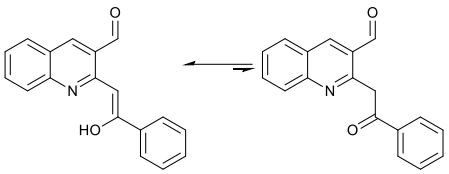
B2. General Procedure for the Synthesis of 3 Using 3a as the Examples



(Z)-2-(2-hydroxy-2-phenylvinyl)quinoline-3-carbaldehyde (**1a**, 82.5 mg, 0.3 mmol), $InCl_3$ (13.3 mg, 20 mol%) were added to a tube equipped with magnetic stirrer bar in 3 mL toluene, then *tert*-butyl isocyanide (**2a**, 3.0 equiv) was added finally. The reaction was stirred at 80 ˚C for 24 h. After the reaction finished (monitored by TLC), the solvent was evaporated under vacuum and the product was purified with flash chromatography (*n*-hexane/EtOAc = 15:1) as eluent to afford the desired product **3a**, 84%.

C. Characterization Data

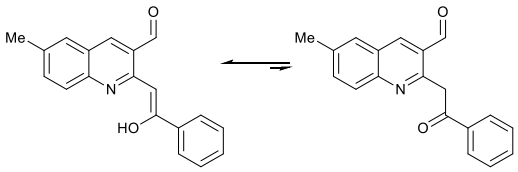
(Z)-2-(2-hydroxy-2-phenylvinyl)quinoline-3-carbaldehyde (1a)



Red crystalline solid, m.p. 155-157 ˚C, Yield 95%; **^{1}H NMR** (300 MHz, $CDCl_3$): δ (ppm) = 16.28 (*s*, 1H, OH), 10.03 (*s*, 1H, CHO), 8.15 (*s*, 1H, H-Ar), 8.05 – 7.97 (*m*, 2H, H-Ar), 7.67 – 7.57 (*m*, 2H, H-Ar), 7.53 – 7.39 (*m*, 5H, H-Ar), 7.33 – 7.20 (*m*, 1H, H-Ar); **^{13}C NMR** (75 MHz, $CDCl_3$): δ (ppm) = 189.5, 150.7, 147.9, 140.1, 139.2, 134.7, 130.9, 129.5, 128.4, 128.2, 127.0, 126.0, 124.1, 121.4, 118.4, 88.5; **IR (KBr): *ν*max** = 3476 (OH); 1698 (C=O) cm^{-1} ; **HRMS-ESI** (m/z): calc. for $C_{18}H_{14}NO_2$ $[M+H]^+$ 276.1019, found 276.1020.

This compound was detected as a tautomeric mixture of enol (90%) and keto form (10%) in chloroform solution. The characterization data are listed only for enol form.

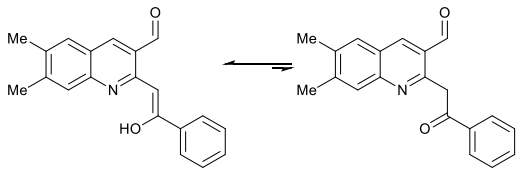
(Z)-2-(2-hydroxy-2-phenylvinyl)-6-methylquinoline-3-carbaldehyde (1b)



Red solid, m.p. 163-165 ˚C, Yield 90%; **^{1}H NMR** (300 MHz, $CDCl_3$): δ (ppm) = 16.35 (*s*, 1H, OH), 9.97 (*s*, 1H, CHO), 8.03 (*s*, 1H, H-Ar), 8.02 – 7.95 (*m*, 2H, H-Ar), 7.49 – 7.41 (*m*, 4H, H-Ar), 7.32 (*d*, *J* = 8.6 Hz, 3H, H-Ar), 2.38 (*s*, 3H, CH_3); **^{13}C NMR** (75 MHz, $CDCl_3$): δ (ppm) = 189.6, 150.9, 147.5, 139.0, 138.5, 136.4, 134.2, 130.7, 128.7, 128.6, 128.3, 128.2, 126.9, 125.7, 121.7, 118.6, 88.2, 21.0; **IR (KBr): *ν*max** = 3419 (OH); 1691 (C=O) cm^{-1} ; **HRMS-ESI** (m/z): calc. for $C_{19}H_{16}NO_2$ $[M+H]^+$ 290.1176, found 290.1177.

This compound was detected as a tautomeric mixture of enol (90%) and keto form (10%) in chloroform solution. The characterization data are listed only for enol form.

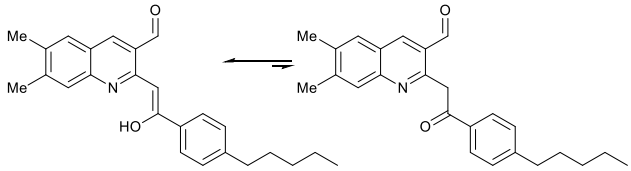
(Z)-2-(2-hydroxy-2-phenylvinyl)-6,7-dimethylquinoline-3-carbaldehyde (1c)



Red solid, m.p. 172-174 ˚C, Yield 87%; **^{1}H NMR** (300 MHz, $CDCl_3$): δ (ppm) = 16.34 (*s*, 1H, OH), 9.93 (*s*, 1H, CHO), 8.00 (*d*, *J* = 4.4 Hz, 3H, H-Ar), 7.46 (*d*, *J* = 4.0 Hz, 3H, H-Ar), 7.34 (*s*, 1H, H-Ar), 7.28 (*s*, 1H, H-Ar), 7.18 (*s*, 1H, H-Ar), 2.34 (*s*, 3H, CH_3), 2.27 (*s*, 3H, CH_3); **^{13}C NMR** (75 MHz, $CDCl_3$): δ (ppm) = 189.5, 150.8, 147.3, 145.9, 139.3, 138.7, 133.9, 130.6, 129.0, 128.6, 128.3, 128.2, 126.9, 124.8, 120.0, 118.7, 87.9, 20.8, 19.4; **IR (KBr): *ν*max** = 3392 (OH); 1690 (C=O) cm^{-1}; **HRMS-ESI** (m/z): calc. for $C_{20}H_{18}NO_2$ $[M+H]^+$ 304.1332, found 304.1336.

This compound was detected as a tautomeric mixture of enol (92%) and keto form (8%) in chloroform solution. The characterization data are listed only for enol form.

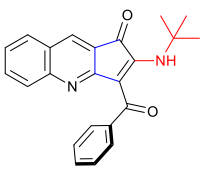
(Z)-2-(2-hydroxy-2-(4-pentylphenyl)vinyl)-6,7-dimethylquinoline-3-carbaldehyde (1d)



Red solid; m.p. 175-177 ˚C, Yield 86%; **^{1}H NMR** (300 MHz, $CDCl_3$): δ (ppm) = 16.34 (*s*, 1H, OH), 9.96 (*s*, 1H, CHO), 8.02 (*s*, 1H, H-Ar), 7.93 (*d*, *J* = 8.2 Hz, 2H, H-Ar), 7.34 (*s*, 1H, H-Ar), 7.33 – 7.24 (*m*, 3H, H-Ar), 7.21 (*s*, 1H, H-Ar), 2.73 – 2.63 (*m*, 2H, H-*n*-pentyl), 2.36 (*s*, 3H, CH_3), 2.29 (*s*, 3H, CH_3), 1.42 – 1.29 (*m*, 5H, H-*n*-pentyl), 0.95–0.88 (*m*, 4H, H-*n*-pentyl); **^{13}C NMR** (100 MHz, $CDCl_3$): δ (ppm) = 189.6, 169.8, 154.3, 150.5, 147.4, 146.1, 145.9, 138.6, 136.9, 133.7, 129.1, 127.0, 124.8, 119.9, 118.5, 87.7, 35.9, 31.5, 31.0, 22.6, 20.9, 19.4, 14.1; **IR (KBr): *ν*max** = 3392 (OH); 1690 (C=O) cm^{-1}; **HRMS-ESI** (m/z): calc. for $C_{25}H_{28}NO_2$ $[M+H]^+$ 374.2115, found 374.2119.

This compound was detected as a tautomeric mixture of enol (86%) and keto form (14%) in chloroform solution. The characterization data are listed only for enol form.

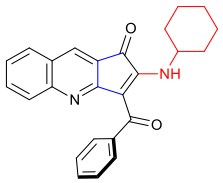
3-benzoyl-2-(*tert*-butylamino)-1H-cyclopenta[*b*]quinolin-1-one (3a)



Navy blue solid, m.p. 163-165 ˚C, R_f = 0.3 (*n*-hexane/EtOAc = 15:1), Yield 84%; **^{1}H NMR** (300 MHz, $CDCl_3$): δ (ppm) = 11.03 (*s*, 1H, NH), 7.92 (*s*, 1H, H-Ar), 7.89 – 7.80 (*m*, 2H, H-Ar), 7.60 (*d*, *J* = 7.9 Hz, 1H, H-Ar), 7.57 – 7.38 (*m*, 5H, H-Ar), 7.26 (*ddd*, *J* = 8.1, 6.9, 1.4 Hz, 1H), 1.61 (*s*, 9H, *t*-Bu); **^{13}C NMR** (75 MHz, $CDCl_3$):

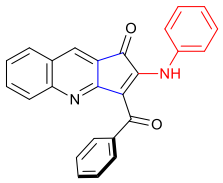
δ (ppm) = 193.1, 188.4, 163.3, 157.5, 150.4, 139.8, 132.1, 132.0, 131.3, 130.3, 129.1, 127.2, 125.6, 125.4, 122.2, 112.7, 54.7, 29.8; **IR (KBr):** ***ν*max** = 3419 (NH), 1721 (C=O), 1635 (C=O) cm^{-1}; **HRMS-ESI** (m/z): calcd for $C_{23}H_{21}N_2O_2$ $[M+H]^+$ 357.1598, found 357.1598.

3-benzoyl-2-(cyclohexylamino)-1H-cyclopenta[*b*]quinolin-1-one (3b)



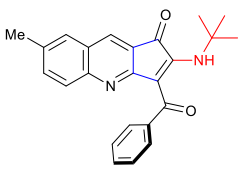
Navy blue solid, m.p. 165-167 °C, R_f = 0.3 (*n*-hexane/EtOAc = 15:1), Yield 78%; **^{1}H NMR** (300 MHz, $CDCl_3$): **(mixture of two rotamer)** δ (ppm) = 10.99 (*s*, 0H, NH (minor rotamer)), 10.41 (*s*, 1H, NH, (major rotamer)), 7.96 (*s*, 1H, H-Ar), 7.88 (*d*, *J* = 7.4 Hz, 2H, H-Ar), 7.62 (*d*, *J* = 7.7 Hz, 1H, H-Ar), 7.58 – 7.39 (*m*, 5H, H-Ar), 7.33 – 7.21 (*m*, 1H, H-Ar), 4.68 (*s*, 1H, CH-cyclohexyl (major rotamer)), 4.40 (*s*, 0H, CH-cyclohexyl (minor rotamer)), 2.17 – 1.94 (*m*, 2H, H-cyclohexyl), 1.92 – 1.59 (*m*, 3H, H-cyclohexyl), 1.58 – 1.17 (*m*, 5H, H-cyclohexyl); **^{13}C NMR** (75 MHz, $CDCl_3$): **(major rotamer)** δ (ppm) = 192.8, 189.4, 163.2, 155.5, 150.5, 139.7, 132.1, 132.0, 131.4, 130.3, 129.1, 129.1, 127.2, 125.5, 125.4, 122.3, 111.2, 51.8, 34.0, 33.4, 25.3, 24.3; **IR (KBr)** ***ν*max** = 3432 (NH), 1725 (C=O), 1632 (C=O) cm^{-1}; **HRMS-ESI** (m/z): calc. for $C_{25}H_{23}N_2O_2$ $[M+H]^+$ 383.1754, found 383.1755.

3-benzoyl-2-(phenylamino)-1H-cyclopenta[*b*]quinolin-1-one (3c)



Navy blue solid, m.p. 174-176 °C, R_f = 0.3 (*n*-hexane/EtOAc = 15:1), Yield 82%; **^{1}H NMR** (300 MHz, $CDCl_3$): δ (ppm) = 10.02 (*s*, 1H, NH), 8.01 (*s*, 1H, H-Ar), 7.96 – 7.87 (*m*, 2H, H-Ar), 7.68 (*d*, *J* = 8.0 Hz, 1H, H-Ar), 7.62 – 7.51 (*m*, 3H, H-Ar), 7.48 – 7.40 (*m*, 2H, H-Ar), 7.39 – 7.26 (*m*, 3H, H-Ar), 7.25 – 7.15 (*m*, 3H, H-Ar); **^{13}C NMR** (75 MHz, $CDCl_3$): δ (ppm) = 193.1, 188.2, 163.6, 150.3, 149.8, 138.6, 137.2, 132.4, 132.2, 132.0, 130.4, 129.4, 128.9, 127.6, 126.3, 126.0, 125.8, 123.8, 122.1, 116.1; **IR (KBr)** ***ν*max** = 3440 (NH), 1731 (C=O), 1637 (C=O) cm^{-1}; **HRMS-ESI** (m/z): calc. for $C_{25}H_{17}N_2O_2$ $[M+H]^+$ 377.1285, found 377.1285.

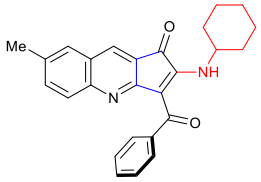
3-benzoyl-2-(*tert*-butylamino)-7-methyl-1H-cyclopenta[*b*]quinolin-1-one (3d)



Navy blue solid, m.p. 158-160 °C, R_f = 0.3 (*n*-hexane/EtOAc = 15:1), Yield 80%; **^{1}H NMR** (300 MHz, $CDCl_3$): **(mixture of two rotamers)** δ (ppm) = 10.99 (*s*, 1H, NH), 7.99 – 7.92 (*m*, 0H, H-Ar (minor rotamer)), 7.87 (*s*, 1H, H-Ar (major rotamer)), 7.85 – 7.81 (*m*, 2H, H-Ar), 7.57–7.48 (*m*, 1H, H-Ar), 7.45 – 7.35 (*m*, 3H, H-Ar),

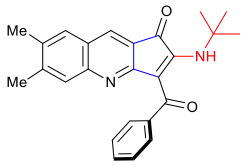
7.33 (*s*, 2H, H-Ar), 2.40 (*s*, 3H, -CH_3), 1.64 (*s*, 0H, *t*-Bu), 1.60 (*s*, 9H, *t*-Bu); **^{13}C NMR** (75 MHz, $CDCl_3$): **(major rotamer)** δ (ppm) = 192.7, 189.5, 148.9, 139.7, 135.1, 134.0, 133.9, 131.5, 131.3, 129.6, 129.2, 128.8, 127.2, 125.4, 125.0, 122.2, 119.3, 111.2, 51.8, 34.0, 33.4, 25.3, 24.4, 21.1; **IR (KBr) *ν*max** = 3420 (NH), 1720 (C=O), 1637 (C=O) cm^{-1}; **HRMS-ESI** (m/z): calcd for $C_{24}H_{23}N_2O_2$ $[M+H]^+$ 371.1754, found 371.1754.

3-benzoyl-2-(cyclohexylamino)-7-methyl-1H-cyclopenta[*b*]quinolin-1-one (3e)



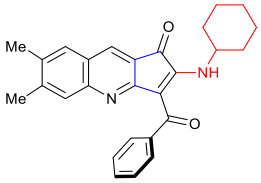
Navy blue solid, m.p. 181-183 ˚C, R_f = 0.3 (*n*-hexane/EtOAc = 15:1), Yield 75%; **^{1}H NMR** (300 MHz, $CDCl_3$): **(mixture of two rotamer)** δ (ppm) = 10.98 (*s*, 0H, NH (minor rotamer)), 10.39 (*s*, 1H, NH (major rotamer)), 7.88 (*s*, 1H, H-Ar), 7.85 (*s*, 2H, H-Ar), 7.56 – 7.48 (*m*, 1H, H-Ar), 7.46 – 7.27 (*m*, 5H, H-Ar), 4.64 (*s*, 1H, CH-cyclohexyl (major rotamer)), 4.36 (*s*, 0H, CH-cyclohexyl (minor rotamer)), 2.41 (*s*, 0H, -CH_3 (minor rotamer)), 2.40 (*s*, 3H, -CH_3 (major rotamer)), 2.14 – 1.94 (*m*, 2H, H-cyclohexyl), 1.89 – 1.59 (*m*, 3H, H-cyclohexyl), 1.53 – 1.24 (*m*, 5H, H-cyclohexyl); **^{13}C NMR** (75 MHz, $CDCl_3$): **(major rotamer)** δ (ppm) = 192.7, 189.5, 162.6, 155.4, 148.9, 139.8, 135.1, 134.0, 131.5, 129.6, 129.2, 128.8, 127.2, 125.4, 125.0, 122.2, 111.2, 51.8, 34.0, 33.4, 25.3, 24.4, 21.1; **IR (KBr): *ν*max** = 3425 (NH), 1727 (C=O), 1609 (C=O) cm^{-1}; **HRMS-ESI** (m/z): calc. for $C_{26}H_{24}N_2O_2$ $[M+H]^+$ 397.1911, found 397.1911.

3-benzoyl-2-(tert-butylamino)-6,7-dimethyl-1H-cyclopenta[*b*]quinolin-1-one (3f)



Navy blue solid, m.p. 163-165 ˚C, R_f = 0.3 (*n*-hexane/EtOAc = 15:1), Yield 82%; **^{1}H NMR** (300 MHz, $CDCl_3$): **(mixture of two rotamer)** δ (ppm) = 11.02 (*s*, 1H, NH), 7.97 – 7.91 (*m*, 0H, H-Ar (minor rotamer)), 7.87 (*s*, 1H, H-Ar (major rotamer)), 7.85 – 7.78 (*m*, 2H, H-Ar (major rotamer)), 7.58 – 7.49 (*m*, 1H, H-Ar), 7.47 – 7.38 (*m*, 2H, H-Ar), 7.35 (*s*, 1H, H-Ar), 7.21 (*s*, 1H, H-Ar), 2.31 (*s*, 6H, -2CH_3), 1.62 (*s*, 0H, *t*-Bu (minor rotamer)), 1.60 (*s*, 9H, *t*-Bu (major rotamer)); **^{13}C NMR** (75 MHz, $CDCl_3$): (**major rotamer**) δ (ppm) = 192.9, 188.6, 162.9, 157.5, 149.3, 142.8, 139.9, 134.9, 131.5, 131.2, 129.9, 129.1, 127.2, 123.9, 121.4, 112.5, 54.6, 29.8, 20.4, 19.5; **IR (KBr): *ν*max** = 3405 (NH), 1715 (C=O), 1621 (C=O) cm^{-1}; **HRMS-ESI** (m/z): calc. for $C_{25}H_{25}N_2O_2$ $[M+H]^+$ 358.1911, found 385.1913.

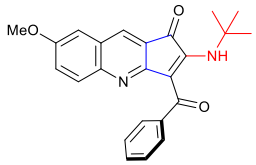
3-benzoyl-2-(cyclohexylamino)-6,7-dimethyl-1H-cyclopenta[*b*]quinolin-1-one (3g)



Navy blue solid, m.p. 181-183 ˚C, R_f = 0.3 (*n*-hexane/EtOAc = 15:1), Yield 76%; **^{1}H NMR** (300 MHz, $CDCl_3$): **(mixture of two rotamer)** δ (ppm) = 11.01 (*s*, 0H, NH (minor rotamer)), 10.43 (*s*, 1H, NH (major rotamer)),

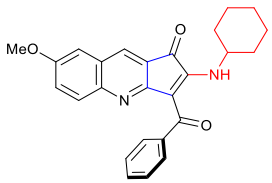
7.88 (*d*, *J* = 7.1 Hz, 2H, H-Ar), 7.84 (*s*, 1H, H-Ar), 7.55 (*t*, *J* = 7.3 Hz, 1H, H-Ar), 7.49 – 7.39 (*m*, 2H, H-Ar), 7.33 (*s*, 1H, H-Ar), 7.24 (*s*, 1H, H-Ar), 4.67 (*s*, 1H, CH-cyclohexyl (major rotamer)), 4.36 (*s*, 0H, CH-cyclohexyl (minor rotamer)), 2.32 (*s*, 6H, -2CH_3), 2.05 (*d*, *J* = 9.4 Hz, 2H, H-cyclohexyl), 1.90 – 1.59 (*m*, 3H, H-cyclohexyl), 1.55 – 1.16 (*m*, 5H, H-cyclohexyl); **^{13}C NMR** (75 MHz, $CDCl_3$): **(major rotamer)** δ (ppm) = 192.6, 189.5, 162.8, 155.5, 149.3, 142.8, 139.8, 134.9, 131.3, 130.0, 129.9, 129.2, 129.1, 127.2, 123.8, 121.4, 111.0, 51.7, 34.0, 33.4, 25.3, 24.4, 20.4, 19.5; **IR (KBr) *ν*max** = 3423 (NH), 1718 (C=O), 1630 (C=O) cm^{-1}; **HRMS-ESI** (m/z): calc. for $C_{27}H_{27}N_2O_2$ $[M+H]^+$ 411.2067, found 411.2068.

3-benzoyl-2-(tert-butylamino)-7-methoxy-1H-cyclopenta[*b*]quinolin-1-one (3h)



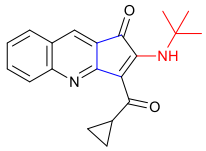
Navy blue solid, m.p. 148-150 ˚C, R_f = 0.3 (*n*-hexane/EtOAc = 15:1), Yield 67%; **^{1}H NMR** (300 MHz, $CDCl_3$): δ (ppm) = 10.98 (*s*, 1H, NH), 7.87 (*s*, 1H, H-Ar), 7.86 – 7.80 (*m*, 2H, H-Ar), 7.57 – 7.48 (*m*, 1H, H-Ar), 7.46 – 7.32 (*m*, 3H, H-Ar), 7.15 (*dd*, *J* = 9.1, 2.9 Hz, 1H, H-Ar), 6.96 (*d*, *J* = 2.8 Hz, 1H, H-Ar), 3.87 (*s*, 3H, CH_3-OMe), 1.61 (*s*, 9H, *t*-Bu); **^{13}C NMR** (75 MHz, $CDCl_3$): δ (ppm) = 192.9, 188.8, 161.5, 157.0, 156.9, 146.0, 139.9, 131.2, 131.1, 130.3, 129.0, 127.1, 126.3, 123.0, 122.4, 112.8, 109.2, 55.5, 54.5, 29.8; **IR (KBr): *ν*max** = 3392 (NH), 1725 (C=O), 1628 (C=O) cm^{-1}; **HRMS-ESI** (m/z): calc. for $C_{24}H_{23}N_2O_3$ $[M+H]^+$ 387.1703, found 387.1704.

3-benzoyl-2-(cyclohexylamino)-7-methoxy-1H-cyclopenta[*b*]quinolin-1-one (3i)



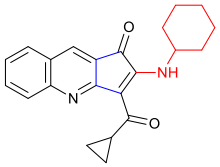
Navy blue solid, m.p. 146-148 ˚C, R_f = 0.3 (*n*-hexane/EtOAc = 15:1), Yield 73%; **^{1}H NMR** (300 MHz, $CDCl_3$): **(mixture of two rotamer)** δ (ppm) = 10.99 (*s*, 0H, NH (minor rotamer)), 10.38 (*s*, 1H, NH (major rotamer)), 7.91 – 7.84 (*m*, 2H, H-Ar), 7.82 (*s*, 1H, H-Ar), 7.57 – 7.49 (*m*, 1H, H-Ar), 7.46 – 7.31 (*m*, 3H, H-Ar), 7.13 (*ddd*, *J* = 9.2, 6.4, 2.8 Hz, 1H, H-Ar), 6.92 (*t*, *J* = 2.6 Hz, 1H, H-Ar), 4.62 (*s*, 1H, CH-cyclohexyl (major rotamer)), 4.37 (*s*, 0H, CH-cyclohexyl (minor rotamer)), 3.86 (*s*, 0H, CH_3-OMe (minor rotamer)), 3.84 (*s*, 3H, CH_3-OMe (major rotamer)), 2.12 – 1.90 (*m*, 2H, H-cyclohexyl), 1.90 – 1.60 (*m*, 3H, H-cyclohexyl), 1.53 – 1.22 (*m*, 5H, H-cyclohexyl); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 192.6, 189.8, 161.5, 157.0, 156.3, 146.1, 139.8, 131.1, 130.3, 129.2, 127.2, 126.2, 123.1, 122.4, 119.5, 111.2, 109.2, 55.6, 51.8, 34.0, 33.4, 25.3, 24.4; **IR (KBr) *ν*max** = 3416 (NH), 1726 (C=O), 1616 (C=O) cm^{-1}; **HRMS-ESI** (m/z): calc. for $C_{26}H_{25}N_2O_3$ $[M+H]^+$ 413.1860, found 413.1862.

2-(tert-butylamino)-3-(cyclopropanecarbonyl)-1H-cyclopenta[*b*]quinolin-1-one (3j)



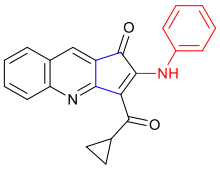
Navy blue solid, m.p. 232-234 ˚C, R_f = 0.3 (*n*-hexane/EtOAc = 15:1), Yield 79%; **^{1}H NMR** (300 MHz, $CDCl_3$): δ (ppm) = 11.15 (*s*, 1H, NH), 7.94 (*d*, *J* = 2.8 Hz, 1H, H-Ar), 7.81 (*d*, *J* = 8.3 Hz, 1H, H-Ar), 7.70 – 7.55 (*m*, 2H, H-Ar), 7.36 – 7.26 (*m*, 1H, H-Ar), 4.23 – 4.10 (*m*, 1H, CH-cyclopropyl), 1.55 (*s*, 9H, *t*-Bu), 1.28 – 1.18 (*m*, 2H, H-cyclopropyl), 1.13 – 1.02 (*m*, 2H, H-cyclopropyl); **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 199.7, 188.9, 164.3, 155.7, 150.6, 132.1, 131.8, 130.4, 128.9, 125.5, 125.3, 123.0, 113.0, 54.4, 29.8, 18.7, 12.0; **IR (KBr): *ν*max** = 3416 (NH), 1729 (C=O), 1632 (C=O) cm^{-1}; **HRMS-ESI** (m/z): calcd for $C_{20}H_{21}N_2O_2$ $[M+H]^+$ 321.1598, found 321.1598.

2-(cyclohexylamino)-3-(cyclopropanecarbonyl)-1H-cyclopenta[*b*]quinolin-1-one (3k)



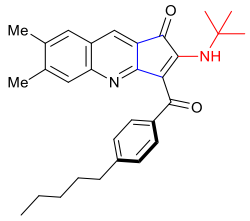
Navy blue solid, m.p. 227-229 ˚C, R_f = 0.3 (*n*-hexane/EtOAc = 15:1), Yield 65%; **^{1}H NMR** (300 MHz, $CDCl_3$): δ (ppm) = 10.28 (*d*, *J* = 8.6 Hz, 1H, NH), 7.90 (*s*, 1H, H-Ar), 7.78 (*d*, *J* = 8.2 Hz, 1H, H-Ar), 7.66 – 7.53 (*m*, 2H, H-Ar), 7.35 – 7.23 (*m*, 1H, H-Ar), 4.63 – 4.48 (*m*, 1H, CH-cyclohexyl), 4.07 (*tt*, *J* = 7.9, 4.7 Hz, 1H, CH-cyclopropyl), 2.05 – 1.92 (*m*, 2H, H-cyclohexyl), 1.88 – 1.73 (*m*, 2H, H-cyclohexyl), 1.71 – 1.57 (*m*, 1H, H-cyclohexyl), 1.55 – 1.24 (*m*, 5H, H-cyclohexyl), 1.25 – 1.18 (*m*, 1H, H-cyclopropyl), 1.08 (*dt*, *J* = 8.3, 3.3 Hz, 1H, H-cyclopropyl); **^{13}C NMR** (75 MHz, $CDCl_3$): δ (ppm) = 199.5, 189.9, 164.3, 153.2, 150.6, 132.1, 131.8, 130.4, 128.9, 125.4, 125.3, 123.0, 111.6, 51.6, 34.1, 25.2, 24.4, 18.7, 11.8; **IR (KBr): *ν*max** = 3405 (NH), 1718 (C=O), 1609 (C=O) cm^{-1}; **HRMS-ESI** (m/z): calc. for $C_{22}H_{23}N_2O_2$ $[M+H]^+$ 347.1754, found 347.1757.

3-(cyclopropanecarbonyl)-2-(phenylamino)-1H-cyclopenta[*b*]quinolin-1-one (3l)



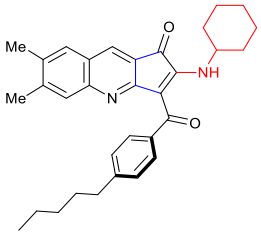
Navy blue solid, m.p. 234-236 ˚C, R_f = 0.3 (*n*-hexane/EtOAc = 15:1), Yield 72%; **^{1}H NMR** (300 MHz, $CDCl_3$): δ (ppm) = 11.64 (*s*, 1H, NH), 7.95 (*s*, 1H, H-Ar), 7.91 – 7.85 (*m*, 1H, H-Ar), 7.71 – 7.61 (*m*, 2H, H-Ar), 7.44 – 7.33 (*m*, 3H, H-Ar), 7.33 – 7.23 (*m*, 3H, H-Ar), 4.18 (*tt*, *J* = 7.9, 4.7 Hz, 1H, CH-cyclopropyl), 1.34 – 1.26 (*m*, 2H, H-cyclopropyl), 1.22 – 1.13 (*m*, 2H, H-cyclopropyl); **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 200.7, 187.8, 163.4, 151.1, 150.3, 137.0, 132.2, 132.0, 130.5, 129.3, 129.2, 128.9, 126.6, 125.9, 125.8, 124.2, 123.1, 119.8, 115.5, 19.41, 12.8; **IR (KBr): *ν*max** = 3414 (NH), 1717 (C=O), 1621 (C=O) cm^{-1}; **HRMS-ESI** (m/z): calc. for $C_{22}H_{17}N_2O_2$ $[M+H]^+$ 341.1285, found 341.1285.

2-(tert-butylamino)-6,7-dimethyl-3-(4-pentylbenzoyl)-1H-cyclopenta[*b*]quinolin-1-one (3m)



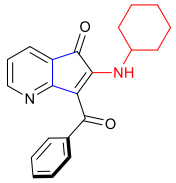
Navy blue solid, m.p. 156-158 °C, R_f = 0.3 (*n*-hexane/EtOAc = 15:1), Yield 80%; **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 10.88 (*s*, 1H, NH), 7.85 (*s*, 1H, H-Ar), 7.77 (*d*, *J* = 8.1 Hz, 2H, H-Ar), 7.34 (*s*, 1H, H-Ar), 7.22 (*d*, *J* = 7.5 Hz, 3H, H-Ar), 2.70 (*t*, *J* = 7.6 Hz, 2H, H-*n*-pentyl), 2.31 (*s*, 6H, -2CH_3), 1.76 – 1.63 (*m*, 2H, H-*n*-pentyl), 1.58 (*s*, 9H, *t*-Bu), 1.44 – 1.29 (*m*, 4H, H-*n*-pentyl), 0.92 (*t*, *J* = 6.8 Hz, 3H, H-*n*-pentyl); **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 192.8, 188.7, 163.1, 157.1, 149.3, 146.8, 142.6, 137.2, 134.9, 131.3, 129.9, 129.3, 129.1, 127.3, 123.9, 121.5, 112.9, 54.4, 36.0, 31.3, 30.9, 29.8, 22.6, 20.4, 19.6, 14.1; **IR (KBr): *ν*max** = 3416 (NH), 1729 (C=O), 1632 (C=O) cm^{-1}; **HRMS-ESI** (m/z): calc. for $C_{30}H_{35}N_2O_2$ $[M+H]^+$ 455.2693, found 4552695.

2-(cyclohexylamino)-6,7-dimethyl-3-(4-pentylbenzoyl)-1H-cyclopenta[*b*]quinolin-1-one (3n)



Navy blue solid, m.p. 163-165 °C, R_f = 0.3 (*n*-hexane/EtOAc = 15:1), Yield 82%; **^{1}H NMR** (300 MHz, $CDCl_3$): (**mixture of two rotamer**) δ (ppm) = 10.34 (*s*, 1H, NH), 7.86 (*s*, 2H, H-Ar), 7.82 (*s*, 1H, H-Ar), 4.63 (*s*, 1H, CH-cyclohexyl (major rotamer)), 4.36 (*s*, 0H, CH-cyclohexyl (minor rotamer)), 2.73 (*t*, *J* = 7.5 Hz, 2H, H-*n*-pentyl), 2.33 (*s*, 6H, -2CH_3), 2.09 – 1.95 (*m*, 2H, H-cyclohexyl), 1.88 – 1.59 (*m*, 6H, H-cyclohexyl), 1.57 – 1.34 (*m*, 9H, H-*n*-pentyl), 1.33 – 1.24 (*m*, 2H, H-cyclohexyl); **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 192.5, 189.7, 163.0, 155.4, 149.4, 146.8, 142.7, 137.2, 134.9, 131.3, 130.0, 129.4, 129.1, 127.3, 123.8, 121.6, 111.3, 51.7, 36.1, 34.0, 33.4, 31.4, 30.9, 25.3, 24.4, 22.6, 20.4, 19.6, 14.1; **IR (KBr): *ν*max** = 3415 (NH), 1713 (C=O), 1607 (C=O) cm^{-1}; **HRMS-ESI** (m/z): calc. for $C_{32}H_{37}N_2O_2$ $[M+H]^+$ 481.2850, found 481.2852.

7-benzoyl-6-(cyclohexylamino)-5H-cyclopenta[*b*]pyridin-5-one (3p)

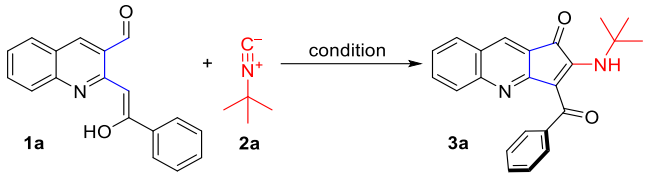


Navy blue solid, m.p. 53-56 °C, R_f = 0.3 (*n*-hexane/EtOAc = 10:1), Yield 35%; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 10.61 (*s*, 1H, NH), 8.04 (*dd*, *J* = 5.2, 1.8 Hz, 1H, H-Ar), 7.67 (*d*, *J* = 7.4 Hz, 2H, H-Ar), 7.45 (*dd*, *J* = 7.3, 1.8 Hz, 1H, H-Ar), 7.41 (*t*, *J* = 7.4 Hz, 1H, H-Ar), 7.33 (*t*, *J* = 7.4 Hz, 2H, H-Ar), 6.65 (*dd*, *J* = 7.3, 5.2 Hz, 1H, H-Ar), 4.52 (*m*, 1H, CH-Cyclohexyl), 1.98 – 1.87 (*m*, 3H), 1.79 – 1.66 (*m*, 2H), 1.6 (dq, *J* = 13.2, 4.5 Hz, 1H),

1.46-1.26 (*m*, 4H), 1.26 – 1.14 (*m*, 1H);**^{13}C NMR** (100 MHz, $CDCl_3$): δ 191.4, 190.4, 168.8, 154.4, 154.2, 139.9, 131.2, 130.9, 128.6, 127.5, 120.4, 118.3, 108.5, 52.0, 33.8, 29.7, 25.2, 24.3; **IR (KBr): *ν*max** = 3432 (NH), 1725 (C=O), 1606 (C=O) cm^{-1}; **LC-MS (ESI)** (m/z): calc. for $C_{21}H_{20}N_2O_2$ $[M+H]^+$ 233.2, found 233.2. **Anal. Calcd** for $C_{21}H_{20}N_2O_2$: C, 79.29; H, 4.32; N, 8.85; O, 9.81. Found: C, 79.08; H, 4.21; N, 8.67; O, 9.76.

D. Optimization of reaction conditions for synthesis of 3a

Table S1. Optimization of reaction conditions[a]



entry	Catalyst[b]	solvent	temp (°C)	time (h)	yield(%)[c]
1	$PdCl_2$	toluene	80	24	n.d
2	CuI	toluene	80	24	8
3	$InCl_3$	toluene	80	24	70
4	$InCl_3$	toluene	100	24	85
5[d]	$InCl_3$	toluene	80	24	47
6[e]	$InCl_3$	toluene	80	24	87
7[f]	$InCl_3$	toluene	80	24	63
8	$InCl_3$	dioxane	80	24	68
9	$InCl_3$	MeOH	reflux	24	55

[a] Until otherwise noted, all reactions were carried out with (Z)-2-(2-hydroxyphenylvinyl)quinoline-3carbaldehyde **1a** (0.3 mmol), *tert*-butyl isocyanide **2a** (3.0 equiv), solvent (3 ml), air atmosphere. [b] catalyst (20 mol%). [c] Isolated yields. [d] The amount of $InCl_3$ was 10 mol%. [e] The amount of $InCl_3$ was 30 mol%. [f] The reaction was under dry condition.

E. DFT study of mechanism and its datas

All the DFT calculations have been carried out with the Gaussian 09 package of program.[4] Full geometry optimization was performed with the hybrid B3LYP[5,6,7] functional, the basis set was the Stuttgart-Dresden[8] (SDD) double-*zeta* valence with effective core potential (ECP) for In and the 6-31G(d) for all other atoms . All reported structures fully optimized in gas phase (T=298 K, P=1 bar), and the zero-point and Gibbs free energy corrections were obtained from the analytical frequency calculations. The correctness of the optimized structures has been verified by harmonic vibrational frequency calculations. In addition, the transition state (TS) structures were further confirmed whit the intrinsic reaction coordinate (IRC) calculation which authenticated the corresponding reactant and product of each TS. Chemical hardness[9] (η), electronic chemical potential (μ) and global electrophilicity (ω)[10] were calculated by the reported equations.

Dimeric In_2Cl_6 was assumed as a precursor for generating the $InCl_3$, so the reaction energies were obtained from Eq. 1:

$$\text{Substrate} + 1/2\ In_2Cl_6 \longrightarrow \text{Substrate-}InCl_3 \qquad \text{Eq. 1}$$

Furthermore, the reaction between **INT1** and methyl isocyanide was used as a reaction model to investigation the mechanism of reaction.

Figure S1. Gibbs free energy profile for the [4+1] cycloaddition mechanism of **INT1** and methyl isocyanide (Electronic energies are given in Parentheses).

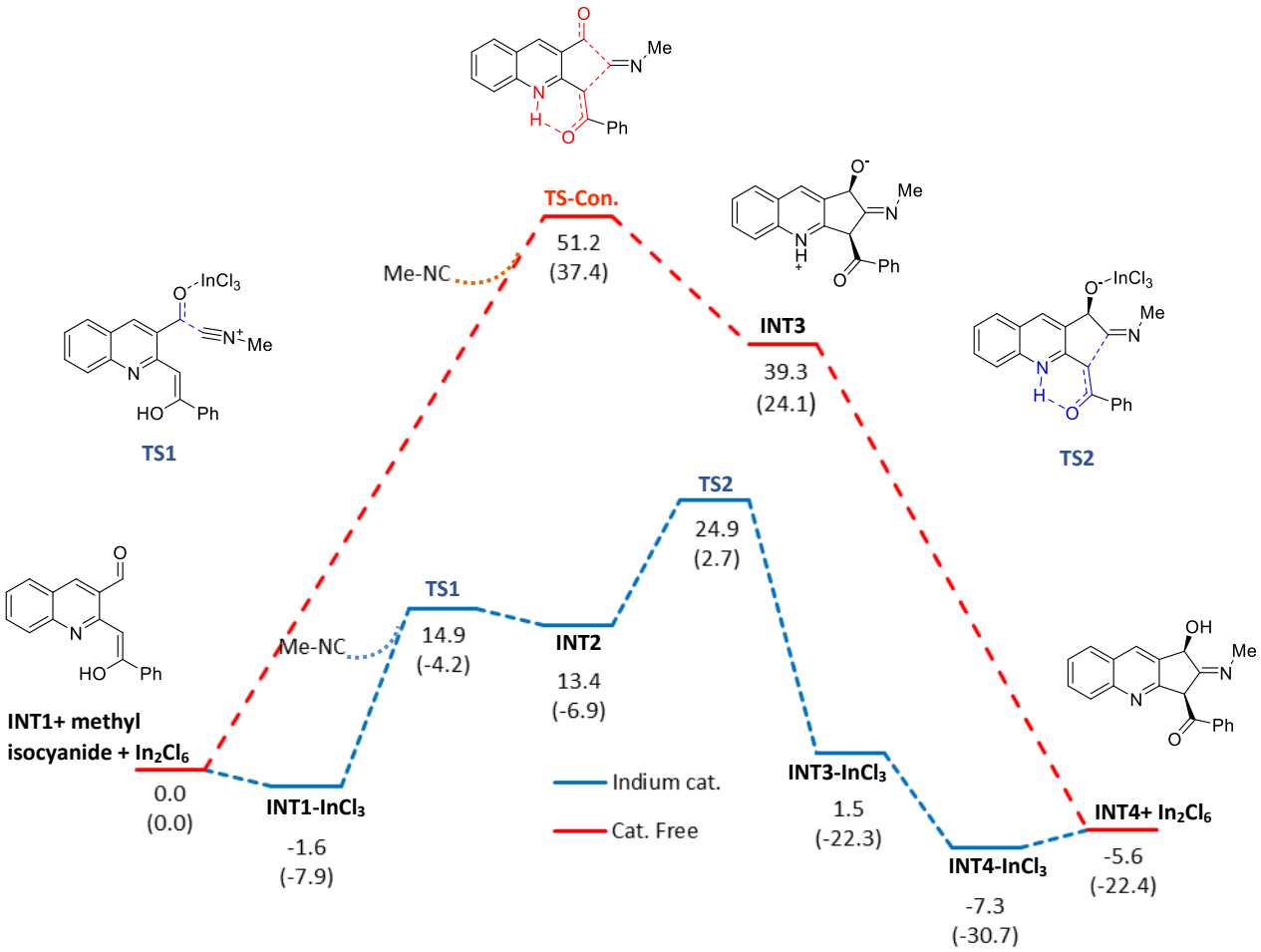


Figure S2. Gibbs free energy surface for the imine−enamine tautomerization of **INT4** (Electronic energies are given in Parentheses).

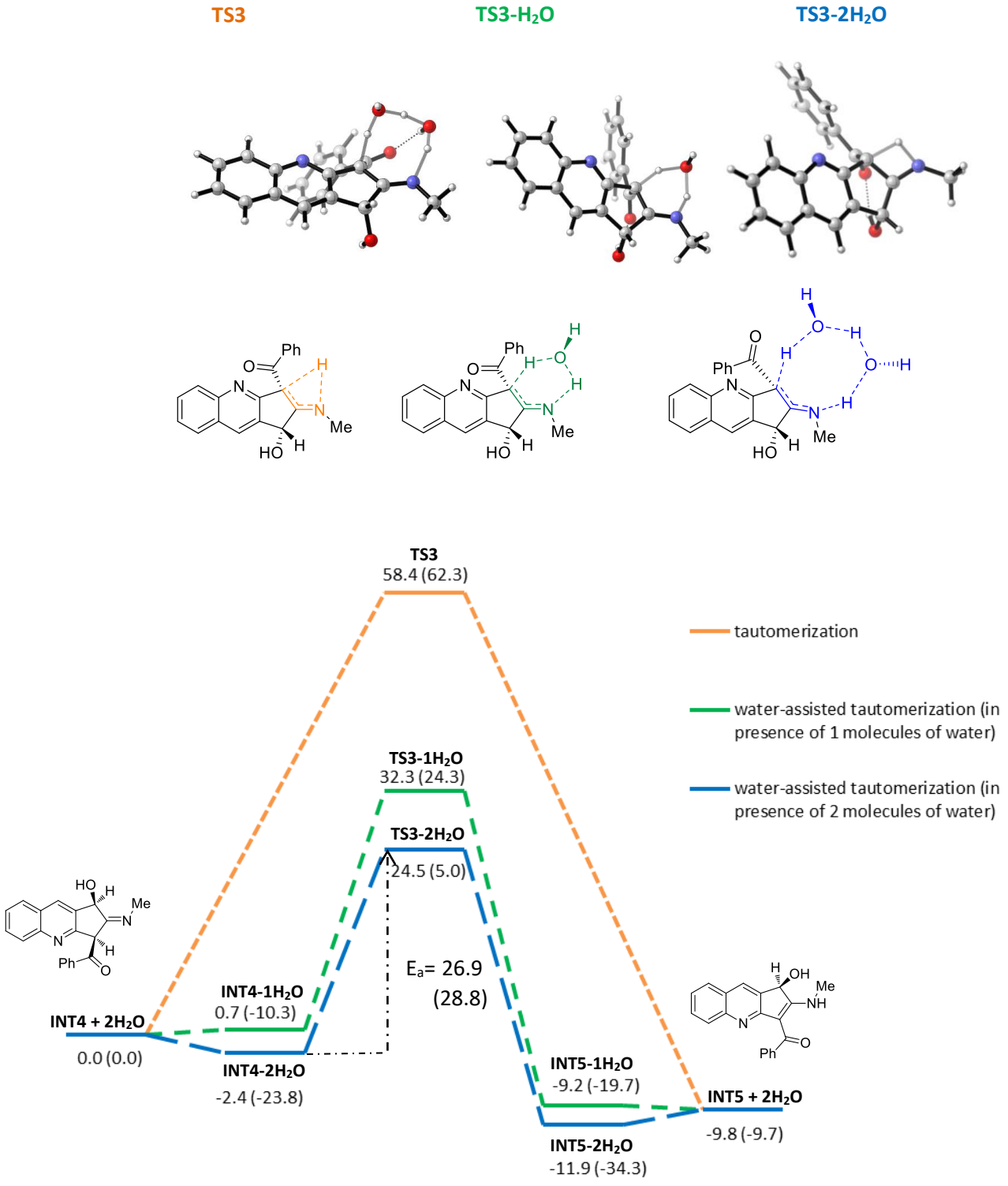
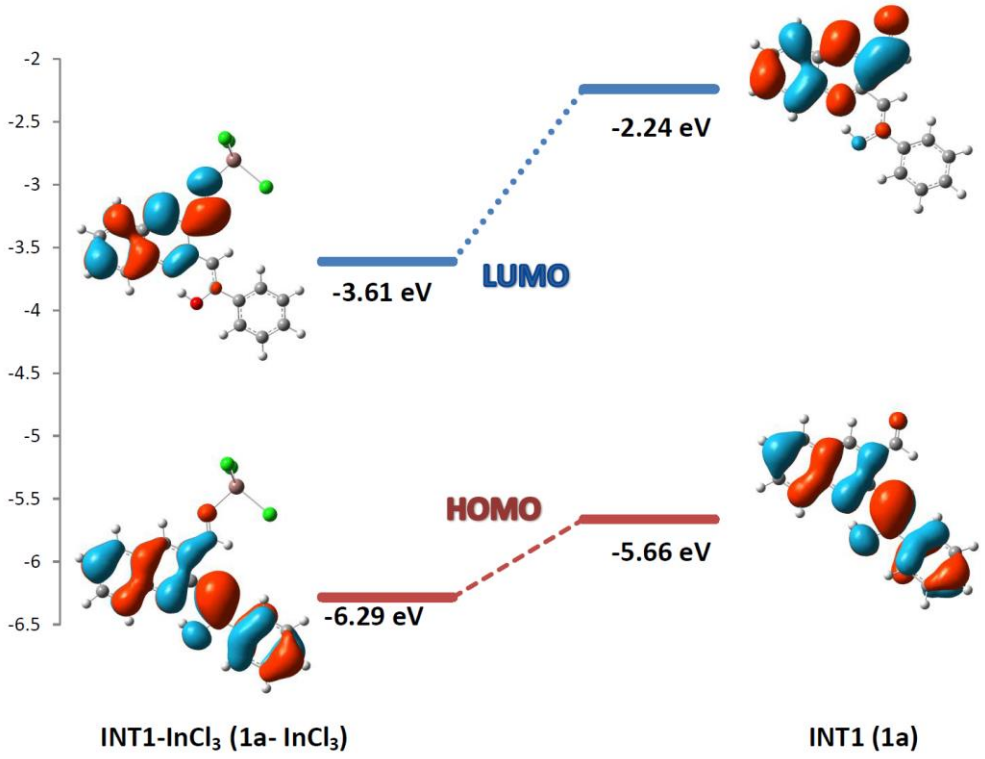


Figure S3. The HOMO-LUMO energy value of **1a** and **1a-InCl$_3$** (in eV).



Z-matrix data

Methyl isocyanide

C	0.00000000	0.00000000	1.48827100
C	0.00000000	0.00000000	-1.10940500
N	0.00000000	0.00000000	0.31106900
H	0.00000000	1.02848500	-1.48356000
H	0.89069400	-0.51424300	-1.48356000
H	-0.89069400	-0.51424300	-1.48356000

Energy= -132.71657278 (Hartree/Particle)

Zero-point correction= 0.045463

Thermal correction to Energy= 0.049285

Thermal correction to Enthalpy= 0.050230

Thermal correction to Gibbs Free Energy= 0.022317

In_2Cl_6

In	1.83684500	-0.00011900	0.00007400
Cl	0.00005200	-0.00106300	1.71816300
Cl	2.88277600	2.03123100	0.00157900
Cl	2.88544000	-2.03001100	-0.00193800
In	-1.83684200	-0.00016600	0.00001500
Cl	-2.88463600	-2.03063300	0.00104900
Cl	-0.00013000	0.00044400	-1.71792000
Cl	-2.88351200	2.03085400	-0.00119300

Energy= -2765.29349444 (Hartree/Particle)

Zero-point correction= 0.007471

Thermal correction to Energy= 0.021383

Thermal correction to Enthalpy= 0.022328

Thermal correction to Gibbs Free Energy= -0.039615

INT1

C	4.34403700	-2.44240000	0.08921300
C	2.98152200	-2.23311400	0.09024200
C	2.46227900	-0.91408800	0.03617200
C	3.37698900	0.18475100	-0.01833900
C	4.77348400	-0.06416700	-0.01796200
C	5.25071100	-1.35492000	0.03474100
H	-0.24268200	-1.66889400	0.07311000

H	4.73140100	-3.45683800	0.13078100
H	2.28225200	-3.06262400	0.13186400
C	2.81585700	1.47871800	-0.06790800
H	5.45594400	0.78114400	-0.05957400
H	6.31994600	-1.54458900	0.03499400
C	1.44889800	1.66723000	-0.06396500
C	0.58395700	0.50732800	-0.01358700
H	3.45453400	2.35768900	-0.10673300
N	1.11635500	-0.72581600	0.03528200
C	-0.85572500	0.60817800	-0.01841800
C	-1.70051100	-0.47613900	0.04413500
H	-1.30632900	1.58438600	-0.11276500
O	-1.25308300	-1.73237700	0.09615000
C	-3.17552900	-0.36387100	0.03353400
C	-3.94602700	-1.48232100	-0.32717700
C	-3.83648400	0.82684500	0.38023700
C	-5.33646100	-1.40349000	-0.36110500
H	-3.44083400	-2.40638300	-0.58439800
C	-5.22639700	0.90192800	0.34760800
H	-3.26551400	1.69096600	0.70492400
C	-5.98219300	-0.21167900	-0.02699100
H	-5.91725900	-2.27563200	-0.64905300
H	-5.72104300	1.82871000	0.62516400
H	-7.06693000	-0.15188500	-0.05063000
C	0.95309100	3.06451700	-0.10350200
O	1.68514400	4.03712300	-0.16307900
H	-0.14344000	3.20687200	-0.07080100

Energy= -898.95161899 (Hartree/Particle)

Zero-point correction=	0.264752
Thermal correction to Energy=	0.281094
Thermal correction to Enthalpy=	0.282038
Thermal correction to Gibbs Free Energy=	0.219447

INT1-$InCl_3$

C	3.14224400	5.53486200	-0.03919400
C	3.47122000	4.19642800	-0.05035900
C	2.44995300	3.21190400	-0.02111000
C	1.08101100	3.64524600	0.01852200
C	0.77701100	5.03518500	0.02901400
C	1.78926800	5.96442300	0.00101300
H	3.93319300	6.27943600	-0.06160200
H	4.50551600	3.86897800	-0.08100000
C	0.09975100	2.64494600	0.03846200
H	-0.26487300	5.34311900	0.05882000
H	1.56203400	7.02576100	0.00882900
C	0.44823700	1.29614800	0.02177500
C	1.85803600	0.92829600	-0.00359900
H	-0.95361200	2.91044900	0.05916600
N	2.79010400	1.89931900	-0.02839200
C	2.30883800	-0.43180200	0.00366100
C	3.64088200	-0.80112600	-0.03989000
H	1.58170700	-1.22552200	0.08281700
O	4.62363800	0.09378500	-0.07347200
C	4.09801900	-2.20514800	-0.02975600
C	5.43733700	-2.48494400	0.29515200
C	3.23756200	-3.27381900	-0.33907200
C	5.89647900	-3.79937000	0.32819400

H	6.10560800	-1.66348500	0.52660400
C	3.70139300	-4.58610000	-0.30775000
H	2.20962200	-3.08511500	-0.63123700
C	5.03080800	-4.85391600	0.02952800
H	6.93190100	-4.00091900	0.58807300
H	3.02555200	-5.39981000	-0.55429300
H	5.39024600	-5.87892800	0.05358800
C	-0.60595100	0.31795200	0.01105500
O	-1.81947200	0.63512300	0.05410400
H	-0.35486500	-0.74601800	-0.04586300
In	-3.51633800	-0.70630900	0.01337000
Cl	-2.32324800	-2.70443500	-0.23312600
Cl	-4.46783600	-0.33683500	2.09149600
Cl	-4.66128300	0.04220900	-1.85402300
H	4.18212000	1.00373300	-0.05313200

Energy= -2281.61096607 (Hartree/Particle)

Zero-point correction= 0.270100

Thermal correction to Energy= 0.294225

Thermal correction to Enthalpy= 0.295169

Thermal correction to Gibbs Free Energy= 0.209756

INT2

C	3.06241600	5.67181600	0.12178700
C	3.44264800	4.34685000	0.07774800
C	2.46132600	3.32608200	-0.00266800
C	1.08094600	3.69342600	-0.03261300
C	0.72166000	5.06291400	0.01365700
C	1.69492400	6.03685600	0.08931500
H	4.25461600	1.15544800	-0.00921300

H	3.82077700	6.44770500	0.18050500
H	4.48903100	4.05774200	0.09898200
C	0.12977800	2.64155500	-0.09295500
H	-0.33175800	5.33025900	-0.01191000
H	1.41645400	7.08595900	0.12349900
C	0.54367900	1.33684300	-0.14564200
C	1.95246300	1.03406300	-0.13880800
H	-0.93390400	2.85807900	-0.10274400
N	2.85419600	2.02262100	-0.05397400
C	2.43657300	-0.32671600	-0.21013000
C	3.77049600	-0.66542000	-0.14435500
H	1.72695500	-1.12080800	-0.39665800
O	4.72402900	0.25554100	-0.00656800
C	4.27810500	-2.05191700	-0.23535200
C	5.65072100	-2.26273900	-0.45420900
C	3.43659200	-3.17166200	-0.11158300
C	6.16186300	-3.55460100	-0.56040700
H	6.30507400	-1.40365000	-0.54573000
C	3.94993000	-4.46134000	-0.21849200
H	2.37701700	-3.04227600	0.08531500
C	5.31478300	-4.65841200	-0.44558100
H	7.22442000	-3.69900300	-0.73548300
H	3.28421600	-5.31427400	-0.12036200
H	5.71375900	-5.66557300	-0.52888700
C	-0.50582600	0.22828200	-0.19732700
O	-1.78442300	0.68733800	-0.26364800
H	-0.25006000	-0.51695500	-0.96911200
In	-3.44254700	-0.53113700	-0.35699700

Cl	-4.17095900	-0.58798000	1.89193300
Cl	-4.95922400	0.29110700	-1.89397900
Cl	-2.37866900	-2.59677100	-0.81743200
C	-0.41429700	-0.54516200	1.12387900
N	-0.59564800	-1.04212600	2.14870700
C	-0.97844200	-1.66600800	3.37351800
H	-2.06696400	-1.57983100	3.45127400
H	-0.67778400	-2.71566500	3.34155900
H	-0.48525300	-1.15426500	4.20283700

Energy= -2414.32594148 (Hartree/Particle)

Zero-point correction= 0.318823

Thermal correction to Energy= 0.346982

Thermal correction to Enthalpy= 0.347926

Thermal correction to Gibbs Free Energy= 0.254241

INT3

C	4.97891800	-2.27480200	0.26468700
C	3.60419900	-2.29576500	0.13391200
C	2.91457900	-1.08932600	-0.09270800
C	3.61082200	0.15607000	-0.17282100
C	5.02236000	0.13009800	-0.02945600
C	5.69132100	-1.05699100	0.18042500
H	0.97303700	-1.89574200	0.04109000
H	5.51622800	-3.20289300	0.43480800
H	3.04950100	-3.22810900	0.19762300
C	2.85696000	1.35285600	-0.32793200
H	5.56417300	1.06992200	-0.08488200
H	6.77180900	-1.06001500	0.28814100
C	1.49839700	1.27889600	-0.52148900

C	0.85290400	0.03964800	-0.46242900
H	3.31865600	2.33509400	-0.25618800
N	1.53920600	-1.08222400	-0.21977600
C	-0.64502900	0.17619000	-0.52831700
C	-1.43826000	-0.95893900	0.10281200
H	-0.94657300	0.23734000	-1.58637300
O	-0.84328200	-1.88368600	0.66970100
C	-2.91540700	-0.99230800	-0.03350500
C	-3.59656200	-2.10629700	0.48989400
C	-3.64636400	0.01346800	-0.68654900
C	-4.97636700	-2.21309700	0.36181600
H	-3.01962300	-2.87520700	0.99238000
C	-5.02914800	-0.09989400	-0.81845000
H	-3.14449600	0.89373200	-1.06784300
C	-5.69543100	-1.20974700	-0.29604000
H	-5.49431100	-3.07590000	0.77138200
H	-5.58741000	0.68353900	-1.32290900
H	-6.77427000	-1.29285700	-0.39846000
C	0.50530800	2.44966400	-0.52705100
O	0.91968700	3.54594700	0.03398100
H	0.19017900	2.52886700	-1.62523700
C	-0.77133500	1.65680700	0.03306900
N	-1.73927000	2.00209400	0.75849900
C	-1.82163000	3.37838600	1.26282600
H	-0.95806900	3.98697700	0.98207600
H	-2.75235400	3.81902800	0.88359000
H	-1.91867700	3.32954700	2.35411700

Energy= -1031.62976805 (Hartree/Particle)

Zero-point correction= 0.314229

Thermal correction to Energy= 0.333494

Thermal correction to Enthalpy= 0.334438

Thermal correction to Gibbs Free Energy= 0.266047

INT3-$InCl_3$

C	-0.75137200	6.06321800	-0.14876100
C	-1.61542200	4.99432800	-0.01703700
C	-1.08223400	3.69425500	0.07806400
C	0.32624100	3.46870400	0.02705900
C	1.17837400	4.59589700	-0.11079400
C	0.64923200	5.86545100	-0.19330500
H	-2.92395200	2.67962400	0.07758500
H	-1.15292300	7.06950600	-0.21913700
H	-2.69111600	5.14239200	0.01858900
C	0.81752900	2.13556700	0.06935600
H	2.25085600	4.43115700	-0.15176900
H	1.30707700	6.72245700	-0.29768700
C	-0.06727800	1.09141200	0.22724000
C	-1.44117800	1.35472900	0.30120100
H	1.88356200	1.94708600	-0.04586200
N	-1.91158200	2.59971400	0.20835500
C	-2.24654200	0.09135900	0.41034800
C	-3.68857000	0.18127700	-0.10862100
H	-2.30965100	-0.17532300	1.47960700
O	-4.08208800	1.25189200	-0.57746800
C	-4.61044000	-0.96580300	0.04562800
C	-5.91143200	-0.83336200	-0.47481300
C	-4.25683100	-2.14466800	0.72334800

C	-6.83551500	-1.86095500	-0.32626600
H	-6.17279900	0.08325300	-0.99243100
C	-5.18977900	-3.16681400	0.88199900
H	-3.25542500	-2.27505700	1.11489500
C	-6.47626000	-3.02852800	0.35565300
H	-7.83534000	-1.75514800	-0.73717000
H	-4.91055600	-4.07401400	1.40939200
H	-7.19920600	-3.83084100	0.47543600
C	0.18965800	-0.41137900	0.18227900
O	1.22432300	-0.76263900	-0.64368500
H	0.33207300	-0.76006900	1.22769500
In	3.10439700	-1.15306600	0.02023900
Cl	3.99802700	-2.86804900	-1.27729600
Cl	4.28219600	0.89674600	-0.18273800
Cl	2.76781400	-1.67365700	2.30307800
C	-1.22884900	-0.92714500	-0.22501100
N	-1.63590300	-1.89717300	-0.91255200
C	-0.74340000	-2.88186600	-1.51740800
H	0.31857600	-2.67698800	-1.37994500
H	-0.99941900	-3.86179600	-1.09757500
H	-0.97493900	-2.92757300	-2.58742300

Energy=	-2414.35040940	(Hartree/Particle)
Zero-point correction=	0.321834	
Thermal correction to Energy=	0.348775	
Thermal correction to Enthalpy=	0.349719	
Thermal correction to Gibbs Free Energy=	0.259833	

INT4

C	-4.15747900	-2.79056400	-0.23982300

C	-2.85625400	-2.47756200	-0.56510500
C	-2.35123600	-1.17152200	-0.33891300
C	-3.21791300	-0.17943800	0.23274000
C	-4.55327100	-0.53670000	0.55653000
C	-5.01356200	-1.81365700	0.32576100
H	-4.53439900	-3.79440900	-0.41563500
H	-2.18226700	-3.21074500	-0.99704000
C	-2.69664300	1.12577000	0.44074700
H	-5.20600100	0.21710800	0.99058500
H	-6.03691700	-2.07728200	0.57788400
C	-1.39421100	1.37661500	0.09056700
C	-0.62247900	0.31259400	-0.45463500
H	-3.33071600	1.90009200	0.86783000
N	-1.04873300	-0.90900200	-0.67176200
C	0.79837800	0.78123400	-0.72906500
C	1.71724900	0.28967200	0.40893300
O	1.74688400	0.90614700	1.47097600
C	2.54567600	-0.92942200	0.21120500
C	3.60540400	-1.16049700	1.10518000
C	2.28989200	-1.85616200	-0.81203500
C	4.40986300	-2.28570800	0.96351300
H	3.78162500	-0.44103600	1.89797400
C	3.08811800	-2.99240400	-0.93870600
H	1.44153000	-1.71733600	-1.47350600
C	4.15230800	-3.20344200	-0.06012200
H	5.23608500	-2.45196800	1.64917300
H	2.87803800	-3.71360300	-1.72351600
H	4.77919900	-4.08455000	-0.16924900

C	-0.58762800	2.65591500	0.18229400
O	-0.24289600	3.03264000	1.50990900
C	0.66316500	2.30593600	-0.65656400
N	1.50890800	3.06189400	-1.21978000
C	1.39028100	4.50766700	-1.11589400
H	1.32854900	4.92741200	-2.12710900
H	0.54618400	4.87286200	-0.51766300
H	2.31562700	4.89095600	-0.66993700
H	-1.13454000	3.50613400	-0.23704000
H	0.43199900	2.38592700	1.80292000
H	1.17491700	0.45994200	-1.70161400

Energy= -1031.70386845 (Hartree/Particle)

Zero-point correction= 0.317023

Thermal correction to Energy= 0.336233

Thermal correction to Enthalpy= 0.337177

Thermal correction to Gibbs Free Energy= 0.268474

INT4-$InCl_3$

C	-3.43296000	4.89433500	-0.48488500
C	-3.65090600	3.58785800	-0.10606100
C	-2.55995400	2.74712800	0.23122800
C	-1.22625400	3.28000400	0.17525000
C	-1.03788900	4.63059800	-0.22138300
C	-2.11824400	5.42045000	-0.54453100
H	-4.27463800	5.53066100	-0.74373500
H	-4.64924200	3.16494700	-0.05717000
C	-0.14518500	2.42907600	0.52512000
H	-0.02659900	5.02611800	-0.26840000
H	-1.96622700	6.45180800	-0.84912900

C	-0.43004800	1.13600700	0.89384800
C	-1.78857300	0.70959000	0.90385600
H	0.87439800	2.80454900	0.48581600
N	-2.82213200	1.45190200	0.59386600
C	-1.87801300	-0.75505600	1.31310000
C	-2.03513300	-1.62235700	0.05004500
H	-2.67809900	-0.95248900	2.02712800
O	-1.03876700	-1.88999300	-0.63138600
C	-3.36998000	-2.11552400	-0.34956500
C	-3.43964800	-3.13732700	-1.31517500
C	-4.55635000	-1.58003400	0.18147600
C	-4.67364900	-3.62978600	-1.72366400
H	-2.51594500	-3.53274300	-1.72392600
C	-5.79075500	-2.06584900	-0.24587600
H	-4.51846400	-0.75568100	0.88533000
C	-5.85070400	-3.09477100	-1.18858800
H	-4.72240200	-4.42745600	-2.45916400
H	-6.70571600	-1.64091700	0.15626300
H	-6.81502600	-3.47845200	-1.51054600
C	0.48156000	0.02183400	1.32884200
O	1.14327300	-0.62771200	0.18981000
H	1.28864800	0.32693400	1.99506600
In	3.14816100	-0.29148800	-0.52514500
Cl	3.47613000	-2.19964600	-1.78902400
Cl	3.00276600	1.74163700	-1.64713300
Cl	4.19185500	-0.11999200	1.55389700
C	-0.50215500	-0.99308800	1.94586900
N	-0.32260700	-1.87906900	2.82934600

C	0.97921300	-2.10944500	3.43252000
H	1.79476400	-1.46743600	3.07702000
H	0.87900700	-1.99863100	4.51823000
H	1.25438700	-3.15393300	3.24608700
H	0.44942400	-1.17837000	-0.28678100

Energy= -2414.36379083 (Hartree/Particle)

Zero-point correction= 0.321593

Thermal correction to Energy= 0.348428

Thermal correction to Enthalpy= 0.349372

Thermal correction to Gibbs Free Energy= 0.259170

INT4-1H_2O

C	-4.54501300	2.56472700	0.77494800
C	-3.19991700	2.32266300	0.94486700
C	-2.63116400	1.09079300	0.53008900
C	-3.48116900	0.09927000	-0.06774600
C	-4.86313800	0.38208400	-0.22814700
C	-5.38421200	1.58809400	0.18360400
H	-4.97052400	3.51202700	1.09477100
H	-2.53780900	3.05646100	1.39364000
C	-2.89489100	-1.13150900	-0.46593500
H	-5.50242200	-0.37134300	-0.68246000
H	-6.44294700	1.79576600	0.05593200
C	-1.55016100	-1.31135600	-0.26276000
C	-0.80226200	-0.25394700	0.32690900
H	-3.51181000	-1.90456400	-0.91966000
N	-1.28776800	0.90033900	0.71548400
C	0.66874700	-0.63462600	0.41932200
C	1.40683900	0.04941200	-0.75525200

H	2.70305400	-2.01331200	1.90662600
O	1.13951300	-0.29974700	-1.90392800
C	2.36616100	1.15304100	-0.49946600
C	3.02884900	1.31944300	0.72830300
C	2.63454800	2.03882800	-1.55983700
C	3.93973200	2.36472400	0.88530400
H	2.89077300	0.61064400	1.53997200
C	3.52698000	3.08977600	-1.38763900
H	2.12470700	1.88703100	-2.50540100
C	4.18142100	3.25447900	-0.16192800
H	4.46377500	2.47906500	1.82994300
H	3.71767900	3.77960700	-2.20516500
H	4.88370200	4.07330800	-0.02814800
C	-0.67146800	-2.50383100	-0.57672800
O	-0.43296800	-2.70690000	-1.96227600
H	0.05112100	-1.90915300	-2.26360800
C	0.62423100	-2.14542100	0.18719800
N	1.55354000	-2.90470000	0.60513200
C	1.52337600	-4.33777000	0.34151800
H	0.70936400	-4.66663800	-0.31292100
H	2.47467600	-4.61488800	-0.12604900
H	1.46742800	-4.87502900	1.29598400
H	-1.10848200	-3.43777300	-0.20975400
O	3.01929400	-1.40339900	2.61229600
H	1.11594800	-0.38898000	1.38153300
H	2.53970700	-1.69458800	3.40196300

Energy= -1108.12919108 (Hartree/Particle)

Zero-point correction= 0.341895

Thermal correction to Energy= 0.364145

Thermal correction to Enthalpy= 0.365089

Thermal correction to Gibbs Free Energy= 0.289516

INT4-2H_2O

C	4.71584100	-2.32506700	0.76873500
C	3.35511200	-2.15085600	0.89047700
C	2.74502100	-0.93632400	0.48353200
C	3.56925900	0.10927900	-0.05529900
C	4.96828700	-0.10434000	-0.16744500
C	5.52982100	-1.29518500	0.23529100
H	5.17342600	-3.25941200	1.08232400
H	2.71164600	-2.92609200	1.29436900
C	2.93995900	1.32038500	-0.44825900
H	5.58803000	0.68969700	-0.57750600
H	6.60137900	-1.44992400	0.14488400
C	1.58121600	1.43127900	-0.29521200
C	0.86243200	0.32587100	0.24035200
H	3.53558800	2.13246700	-0.86034800
N	1.38797800	-0.81417900	0.61824500
C	-0.62982300	0.62978000	0.27717100
C	-1.27709000	-0.07462000	-0.93622000
O	-1.14058100	0.43121000	-2.05063700
C	-2.00386500	-1.35785300	-0.76644400
C	-2.20708500	-1.96495600	0.48479500
C	-2.50342800	-1.97915700	-1.92776100
C	-2.90020900	-3.17392000	0.56239100
H	-1.85289200	-1.50523600	1.40145900
C	-3.19105400	-3.18268700	-1.84143300

H	-2.33593600	-1.49669500	-2.88479800
C	-3.39028400	-3.78327500	-0.59276600
H	-3.05769400	-3.63533900	1.53301600
H	-3.57231100	-3.65634200	-2.74195100
H	-3.92909600	-4.72489100	-0.52382700
C	0.65962000	2.58685500	-0.61992600
O	0.48153600	2.82654700	-2.00975200
H	-0.01480100	2.05133700	-2.34709500
C	-0.65993900	2.14000100	0.04726100
N	-1.66884000	2.84511200	0.36429800
C	-1.69709000	4.27825600	0.09418700
H	-0.85335100	4.64601000	-0.49756100
H	-2.62197100	4.50263500	-0.44855100
H	-1.74535400	4.81753200	1.04756900
H	1.02668800	3.52831800	-0.19880100
H	-1.09256200	0.34913100	1.22755400
O	-2.17038400	-0.17220300	3.17081400
H	-2.80761500	0.50602500	2.83613800
O	-3.74014400	1.73357000	1.95173300
H	-4.32849000	1.25068300	1.35174400
H	-1.63961800	0.30013800	3.82888800
H	-3.06264600	2.14965900	1.35686900

Energy= -1184.55964538 (Hartree/Particle)

Zero-point correction= 0.366853

Thermal correction to Energy= 0.391957

Thermal correction to Enthalpy= 0.392902

Thermal correction to Gibbs Free Energy= 0.309531

INT5

C	-3.91589400	2.79246900	-0.31521800
C	-2.57518700	2.46522300	-0.29606300
C	-2.16057600	1.12194200	-0.11682400
C	-3.16395500	0.11054800	0.04280700
C	-4.53063800	0.47633500	0.01666600
C	-4.90354300	1.79378300	-0.15791400
H	-4.21791900	3.82736200	-0.45340100
H	-1.80165100	3.21723900	-0.41706400
C	-2.72176600	-1.23435200	0.22386300
H	-5.28374500	-0.29943900	0.13848300
H	-5.95527800	2.06568200	-0.17529100
C	-1.38111100	-1.47645600	0.23337100
C	-0.44701600	-0.39688300	0.05754000
H	-3.44776700	-2.03660000	0.34216300
N	-0.81499300	0.85557600	-0.10942200
C	0.91972500	-0.94755500	0.04759100
C	2.22481800	-0.31850800	-0.13842500
O	3.22018500	-1.03286800	-0.38980600
C	2.45633800	1.15587900	-0.01768500
C	3.49033500	1.71567500	-0.78494400
C	1.77327600	1.96530900	0.89974200
C	3.81055300	3.06506900	-0.66489400
H	4.03551200	1.07348600	-1.46889300
C	2.11380400	3.31036900	1.03958100
H	0.98397200	1.54429600	1.50949600
C	3.12332700	3.86570000	0.25152100
H	4.60095000	3.49136400	-1.27710300
H	1.58724400	3.92596800	1.76409200

H	3.37785000	4.91762700	0.35423200
C	-0.63999100	-2.78127100	0.36703700
O	-1.07151500	-3.81416500	-0.51475600
C	0.81033500	-2.34194500	0.15537200
N	1.81279900	-3.21578200	0.08876100
C	1.72067800	-4.66042500	0.22677100
H	2.68203900	-5.03276700	0.59029000
H	0.94482900	-4.93722900	0.94391700
H	1.48803100	-5.14815200	-0.72668200
H	-0.75151500	-3.20940000	1.37212100
H	-1.14393000	-3.42004500	-1.40011800
H	2.70630100	-2.76712600	-0.13449100

Energy= -1031.71934363 (Hartree/Particle)

Zero-point correction= 0.317165

Thermal correction to Energy= 0.336653

Thermal correction to Enthalpy= 0.337597

Thermal correction to Gibbs Free Energy= 0.268399

INT5-1H_2O

C	-4.98586200	1.06345700	-0.41168900
C	-3.62495200	1.29218000	-0.39281700
C	-2.71524200	0.22762000	-0.17435200
C	-3.23931500	-1.09194000	0.02566200
C	-4.63949300	-1.29543000	-0.00077000
C	-5.50055500	-0.23808400	-0.21438200
H	-5.67086500	1.89031600	-0.58026300
H	-3.20965100	2.28388700	-0.54314600
C	-2.30356900	-2.14743400	0.24223400
H	-5.02637500	-2.30089600	0.15139200

H	-6.57419000	-0.40349200	-0.23207900
C	-0.97617500	-1.83978800	0.25162100
C	-0.54432700	-0.48739000	0.03642100
H	-2.65425400	-3.16757100	0.38653100
N	-1.37388000	0.51333500	-0.17030400
C	0.92877900	-0.44998100	0.03642200
C	1.84124200	0.66561900	-0.16251000
H	3.37440400	-1.51247300	-0.01525800
O	3.03529200	0.44654900	-0.46279200
C	1.43462500	2.09618800	0.01225300
C	0.51861300	2.51347500	0.98727100
C	2.09660600	3.06328200	-0.76010400
C	0.26761500	3.87103600	1.18132600
H	0.01159300	1.77929700	1.60149000
C	1.82402100	4.41751200	-0.58613700
H	2.82512200	2.73395400	-1.49388500
C	0.91001600	4.82466900	0.38924400
H	-0.43372700	4.18408300	1.95018600
H	2.32927100	5.15593500	-1.20310000
H	0.70271700	5.88191000	0.53419600
C	0.21920600	-2.74143500	0.40811300
O	0.21943400	-3.86991200	-0.46445600
H	0.04146700	-3.53847700	-1.36052900
C	1.38971100	-1.77006300	0.19077300
N	2.64644700	-2.20090900	0.17633300
C	3.10308700	-3.54962100	0.49138400
H	3.12947000	-3.72031200	1.57669900
H	2.45390500	-4.29486300	0.03105000

H	4.11776700	-3.64646300	0.10114700
H	0.28172000	-3.17166900	1.41591800
O	5.35272000	-1.05755100	-0.47589400
H	4.75929900	-0.34024300	-0.76791800
H	5.75059000	-0.69581400	0.33070800

Energy= -1108.14421452 (Hartree/Particle)

Zero-point correction= 0.341795

Thermal correction to Energy= 0.364566

Thermal correction to Enthalpy= 0.365511

Thermal correction to Gibbs Free Energy= 0.288658

INT5-2H_2O

C	-5.23548900	1.30665800	-0.35958700
C	-3.86463800	1.46498400	-0.35707400
C	-3.00793900	0.35393800	-0.15484100
C	-3.59687600	-0.93808300	0.04625500
C	-5.00608700	-1.06892800	0.03691300
C	-5.81407500	0.03221500	-0.16121800
H	-5.87909500	2.16842300	-0.51601400
H	-3.40102900	2.43480200	-0.50903600
C	-2.71493100	-2.04137900	0.24803400
H	-5.44227400	-2.05382700	0.19016700
H	-6.89494300	-0.07757900	-0.16576900
C	-1.37292900	-1.80367300	0.23961800
C	-0.87510400	-0.47454300	0.02234700
H	-3.11649000	-3.04202700	0.39630500
N	-1.65393100	0.56996000	-0.16730600
C	0.59645200	-0.51349600	-0.00054600
C	1.56151300	0.54483300	-0.19787000

H	3.00403600	-1.74081100	-0.09763900
O	2.74226400	0.23955900	-0.49724100
C	1.24356500	1.99656900	-0.02786200
C	0.37596400	2.46947200	0.96636000
C	1.93396200	2.92088600	-0.82781500
C	0.20523400	3.83971300	1.15639100
H	-0.15563400	1.76690200	1.59678900
C	1.74102900	4.28952000	-0.65607000
H	2.61658300	2.55116800	-1.58659800
C	0.87863500	4.75187100	0.34103500
H	-0.45819000	4.19575700	1.93999200
H	2.26756000	4.99484600	-1.29341400
H	0.73393200	5.81970800	0.48376500
C	-0.22330400	-2.76441000	0.38827200
O	-0.28368900	-3.90215000	-0.46655900
H	-0.47794700	-3.57573500	-1.36102600
C	0.99381200	-1.85906800	0.14705200
N	2.21846500	-2.36447000	0.11900400
C	2.57370300	-3.75140600	0.40325000
H	2.06240000	-4.11555900	1.30028200
H	2.31011600	-4.41302500	-0.42694600
H	3.65137300	-3.76979300	0.56626000
H	-0.17064000	-3.18186900	1.40242000
O	5.06802400	-1.86258400	-0.17564400
H	5.29726800	-1.96856300	-1.11096800
H	5.27644900	-0.91209300	-0.00170900
O	5.31875100	0.88201900	0.04476900
H	4.36231000	0.91003200	-0.19308100

H	5.34471600	1.18202500	0.96587800

Energy= -1184.57642700 (Hartree/Particle)

Zero-point correction= 0.367300

Thermal correction to Energy= 0.392500

Thermal correction to Enthalpy= 0.393444

Thermal correction to Gibbs Free Energy= 0.311199

TS1

C	3.11828100	5.65001400	0.12799400
C	3.48278000	4.32143300	0.06759300
C	2.48856300	3.31184100	0.00089600
C	1.11203000	3.69668200	0.00094700
C	0.76906500	5.07064000	0.06259100
C	1.75448700	6.03228400	0.12535100
H	4.25820000	1.13131900	-0.05332600
H	3.88671700	6.41664100	0.17687200
H	4.52606300	4.02076400	0.06643600
C	0.15077800	2.65782600	-0.05290800
H	-0.28157900	5.34999000	0.05928100
H	1.48983400	7.08440600	0.17206900
C	0.54332700	1.34298300	-0.12435700
C	1.95186300	1.02426300	-0.13847100
H	-0.90932300	2.89287900	-0.04590200
N	2.86439900	2.00542200	-0.06494000
C	2.42381200	-0.33706800	-0.21108200
C	3.75742900	-0.68500000	-0.16600800
H	1.70409400	-1.12831500	-0.35965600
O	4.72164500	0.22825300	-0.06060200
C	4.24947400	-2.07716700	-0.24809000

C	5.61115800	-2.30536800	-0.51324100
C	3.40255600	-3.18534000	-0.06929100
C	6.10614900	-3.60394700	-0.61229200
H	6.26944200	-1.45465900	-0.64617700
C	3.90023600	-4.48180000	-0.16878700
H	2.35342200	-3.04016100	0.16786600
C	5.25363300	-4.69668000	-0.44323200
H	7.16002300	-3.76251400	-0.82386900
H	3.23144200	-5.32608700	-0.02676100
H	5.64011800	-5.70921400	-0.52044800
C	-0.50675300	0.27879900	-0.19315100
O	-1.74525100	0.67038600	-0.16827400
H	-0.26673700	-0.57860300	-0.83168800
In	-3.43139000	-0.54002000	-0.39515100
Cl	-4.25300600	-0.64616800	1.80567200
Cl	-4.81503500	0.48274200	-1.93953000
Cl	-2.39593900	-2.56089800	-1.00547000
C	-0.28753800	-0.64890300	1.41051200
N	-0.64962800	-1.08241900	2.42408400
C	-1.18175900	-1.61901200	3.63329100
H	-2.27252400	-1.56694500	3.56937800
H	-0.85590400	-2.65671600	3.73701300
H	-0.81948200	-1.02732200	4.47731800

Energy=	-2414.32157292 (Hartree/Particle)
Zero-point correction=	0.317653
Thermal correction to Energy=	0.345791
Thermal correction to Enthalpy=	0.346735
Thermal correction to Gibbs Free Energy=	0.252342

Imaginary Frequency= 269.98i

TS2

C	3.62938600	5.48151900	0.31293500
C	3.85122400	4.13213400	0.14046000
C	2.75985700	3.25108300	-0.05953100
C	1.42529000	3.77509400	-0.06630100
C	1.23433000	5.16882400	0.11778200
C	2.31368600	6.00540000	0.30058300
H	4.06002800	0.75557500	0.29022900
H	4.47087900	6.15273400	0.45927000
H	4.85498300	3.71814200	0.14225100
C	0.34598500	2.85949600	-0.19680700
H	0.22118500	5.56203500	0.11422000
H	2.15887000	7.07133500	0.43912100
C	0.62230600	1.53237800	-0.39368300
C	1.97458500	1.10694000	-0.45371400
H	-0.68309000	3.19451700	-0.10072900
N	3.00418900	1.91578900	-0.23948600
C	2.16827300	-0.34994800	-0.59921100
C	3.35285000	-0.95506100	-0.12277900
H	1.72337200	-0.82310300	-1.47197600
O	4.28148900	-0.22746000	0.46371500
C	3.62229800	-2.38953100	-0.19731700
C	4.88997400	-2.87600100	0.18361300
C	2.63994300	-3.30188800	-0.63244800
C	5.16629700	-4.23669600	0.12202700
H	5.64556500	-2.17452800	0.51810100
C	2.92520500	-4.66286100	-0.69374200

H	1.65249400	-2.95554900	-0.91389000
C	4.18623600	-5.13280600	-0.31782500
H	6.14681200	-4.60177600	0.41312000
H	2.16162500	-5.35696700	-1.03155500
H	4.40541300	-6.19571800	-0.36703500
C	-0.38797000	0.40883500	-0.36702200
O	-1.54261600	0.71248200	0.26859800
H	-0.52264500	-0.01266700	-1.38361300
In	-3.32676000	-0.23351000	-0.07150100
Cl	-4.12809600	-0.81975400	2.05105100
Cl	-4.70217600	1.17651300	-1.31134900
Cl	-2.57994600	-2.15493500	-1.25776000
C	0.36841700	-0.76344200	0.36312400
N	0.23879900	-1.66301600	1.12668000
C	-0.64086900	-2.41289500	1.98755300
H	-1.34073300	-1.73759800	2.48913800
H	-1.21083500	-3.10480800	1.36027900
H	-0.05466800	-2.97368600	2.71857000

Energy= -2414.31058496 (Hartree/Particle)

Zero-point correction= 0.318727

Thermal correction to Energy= 0.345635

Thermal correction to Enthalpy= 0.346579

Thermal correction to Gibbs Free Energy= 0.257271

Imaginary Frequency= 209.01i

TS-Con.

C	4.86454500	-2.33840300	0.39584100
C	3.49375000	-2.32796900	0.25484400
C	2.81643100	-1.12302600	-0.05700900

C	3.56876200	0.08661800	-0.21099000
C	4.97790100	0.03935000	-0.05417400
C	5.61353700	-1.14720700	0.23955600
H	0.13148600	-1.90339600	0.52455400
H	5.37761500	-3.26742600	0.62871800
H	2.90539000	-3.23381400	0.36768700
C	2.85224500	1.28856300	-0.45876500
H	5.54612600	0.95914200	-0.16830700
H	6.69336600	-1.17243000	0.35584100
C	1.49524300	1.23863200	-0.63167200
C	0.83627600	-0.01496200	-0.52163800
H	3.35780000	2.25138400	-0.47085700
N	1.45430300	-1.14222600	-0.19569100
C	-0.64800100	0.02919500	-0.62395400
C	-1.42725800	-0.97468400	-0.01161600
H	-1.05235100	0.41785700	-1.55776400
O	-0.86115800	-1.91992300	0.72872300
C	-2.88511800	-1.03829300	-0.09562000
C	-3.55599800	-2.19334400	0.35504100
C	-3.64343600	0.02960800	-0.61440700
C	-4.94109500	-2.28064200	0.27296800
H	-2.97489700	-3.01455700	0.75860800
C	-5.02951700	-0.06616100	-0.69577200
H	-3.15259800	0.94261300	-0.92971500
C	-5.68265800	-1.21958600	-0.25497200
H	-5.44554100	-3.17868700	0.61843900
H	-5.60264000	0.76556600	-1.09554100
H	-6.76510600	-1.28994600	-0.31844000

C	0.59425400	2.46882500	-0.72159600
O	0.99260700	3.58077600	-0.21574200
H	0.12849100	2.49908400	-1.74970600
C	-0.72316600	1.89367500	0.11381300
N	-1.54508000	2.31223500	0.89298800
C	-1.65567200	3.63287900	1.50031600
H	-0.81587300	4.25694500	1.17800500
H	-2.61156000	4.07578800	1.20432000
H	-1.66200700	3.51656200	2.58807500

Energy= -1031.60854590 (Hartree/Particle)

Zero-point correction= 0.312105

Thermal correction to Energy= 0.331444

Thermal correction to Enthalpy= 0.332388

Thermal correction to Gibbs Free Energy= 0.263730

Imaginary Frequency= 234.68i

TS3

C	-4.16291000	-2.60403600	-0.37887400
C	-2.84691700	-2.30623800	-0.66374900
C	-2.30762600	-1.03472900	-0.34474700
C	-3.15825500	-0.06338800	0.28022000
C	-4.50596900	-0.40031800	0.56055100
C	-5.00121900	-1.64581900	0.23796800
H	-4.56264100	-3.58343400	-0.62806000
H	-2.18684900	-3.02801700	-1.13464600
C	-2.59948300	1.20890200	0.59320200
H	-5.14313100	0.34155500	1.03702100
H	-6.03549300	-1.89537700	0.45782100
C	-1.28757500	1.43946300	0.28867600

C	-0.51434600	0.39217100	-0.34750500
H	-3.21554800	1.96391000	1.07826400
N	-0.99384000	-0.79071000	-0.65411200
C	0.88377100	0.89501000	-0.54770400
C	1.94506700	0.38694100	0.36052800
H	1.60420600	1.68471500	-1.68963400
O	2.39900800	1.12339600	1.25410600
C	2.47764900	-0.99064400	0.17714400
C	3.40021800	-1.48163600	1.11572900
C	2.09099500	-1.80228900	-0.89993400
C	3.92867700	-2.76108700	0.97875700
H	3.68695100	-0.83927100	1.94186900
C	2.61896100	-3.08614800	-1.03147000
H	1.37054700	-1.43157600	-1.61977200
C	3.53832500	-3.56590900	-0.09655600
H	4.64312400	-3.13450900	1.70759900
H	2.31444900	-3.71161700	-1.86627000
H	3.95069700	-4.56604800	-0.20395200
C	-0.43939300	2.69098500	0.55653400
O	0.07045400	2.79161100	1.87817900
H	0.87426200	2.22676100	1.92473000
C	0.66458400	2.35658100	-0.41302000
N	1.31756700	2.93149600	-1.35929200
C	1.46268400	4.35476800	-1.62703000
H	1.20569900	4.55514200	-2.67158500
H	0.82220000	4.95080200	-0.96815200
H	2.50555100	4.64595800	-1.46593100
H	-0.97923800	3.61996700	0.34392200

Energy=	-1031.60461649 (Hartree/Particle)
Zero-point correction=	0.310769
Thermal correction to Energy=	0.329954
Thermal correction to Enthalpy=	0.330898
Thermal correction to Gibbs Free Energy=	0.262321
Imaginary Frequency=	1864.80i

TS3-1H_2O

C	-4.56887800	2.07713700	0.52104500
C	-3.21618400	1.95135900	0.75762500
C	-2.52738800	0.76521100	0.40041700
C	-3.26456500	-0.30226100	-0.21184700
C	-4.65380700	-0.14154100	-0.44254900
C	-5.29553700	1.02461600	-0.08382100
H	-5.08440500	2.99253000	0.79916400
H	-2.64018000	2.74789500	1.21815500
C	-2.55494600	-1.48698700	-0.55945400
H	-5.20487400	-0.95496400	-0.90943600
H	-6.36039600	1.13948200	-0.26602800
C	-1.21663600	-1.54765700	-0.28768000
C	-0.56967500	-0.41868800	0.32333300
H	-3.08085200	-2.31141200	-1.03748200
N	-1.18207500	0.69207900	0.65906100
C	0.90361600	-0.69646800	0.47754500
C	1.72747200	0.02179000	-0.57894400
H	2.48895300	-2.20832300	1.54056100
O	2.09785600	-0.58426900	-1.59183500
C	2.06062000	1.45789200	-0.39426000
C	1.74440400	2.15858500	0.77915900

C	2.72233700	2.12519900	-1.44003700
C	2.08463700	3.50505800	0.90138200
H	1.22762200	1.65415000	1.58569600
C	3.06319100	3.46689900	-1.31327900
H	2.95949100	1.56780000	-2.34006800
C	2.74418900	4.15935500	-0.14029300
H	1.83732600	4.04269900	1.81250500
H	3.57625600	3.97610500	-2.12466600
H	3.01090200	5.20845300	-0.04000500
C	-0.22269500	-2.66269600	-0.55303600
O	0.18953800	-2.80884100	-1.90892300
H	0.79767600	-2.06135600	-2.10144500
C	0.95900500	-2.16538900	0.26860900
N	1.90585800	-2.85873700	0.80592800
C	2.09664200	-4.29446400	0.66216600
H	1.44447400	-4.70479700	-0.11067100
H	3.13679800	-4.48183500	0.37957200
H	1.90537700	-4.79469400	1.61808500
H	-0.59940200	-3.64168500	-0.23913400
O	2.64544400	-1.00693600	2.32733500
H	1.64560400	-0.60933400	1.60510500
H	2.31563500	-1.17543400	3.22606200

Energy=	-1108.07404032 (Hartree/Particle)
Zero-point correction=	0.335542
Thermal correction to Energy=	0.356653
Thermal correction to Enthalpy=	0.357597
Thermal correction to Gibbs Free Energy=	0.284614
Imaginary Frequency=	1462.24i

TS3-2H_2O

C	-0.53750000	-1.80491000	-0.45947000
C	-0.31705400	-0.57995000	0.24750700
C	1.13206500	-0.26557200	0.30893600
C	1.66717400	1.11078600	0.15264800
O	2.85374400	1.39029300	0.38656000
C	0.76687400	-2.37544200	-0.94539500
O	0.86843800	-2.49873500	-2.36597600
H	0.66857500	-1.62783700	-2.74721300
C	1.82617900	-1.41729000	-0.33117400
N	3.09538100	-1.62846100	-0.32839800
C	3.68293000	-2.76050900	-1.03478300
H	4.38574100	-3.26947000	-0.36421800
H	2.96287800	-3.48655300	-1.42394800
H	4.26646300	-2.38406600	-1.88410200
H	0.92710100	-3.39463600	-0.57604600
O	2.09881100	-0.54618600	2.75882200
H	3.19421400	-0.52944100	2.39401300
O	4.29473300	-0.40722000	1.71606700
H	4.12512400	0.49863500	1.36026300
H	1.88527300	-1.42588700	3.11353200
H	4.01505800	-0.92684100	0.87667000
H	1.54418100	-0.43344700	1.73961300
N	-1.27488300	0.11814200	0.82493700
C	-1.81055200	-2.28129700	-0.61236100
H	-2.01455600	-3.19726700	-1.16403200
C	-2.88252200	-1.54449800	-0.03462100
C	-2.55482600	-0.34626700	0.68554200

C	-3.60695400	0.39380000	1.28439800
C	-4.91523300	-0.02656900	1.17378300
C	-5.23669300	-1.20656200	0.46122800
C	-4.23753000	-1.94937000	-0.13043400
H	-3.34001000	1.29715400	1.82392300
H	-5.71053400	0.55214100	1.63627500
H	-6.27275600	-1.52397000	0.38218500
H	-4.47510000	-2.85823300	-0.67928300
C	0.79224900	2.24645700	-0.30261700
C	-0.16647600	2.11034600	-1.31532500
C	1.04582100	3.52094400	0.22564400
C	-0.86200700	3.22312800	-1.78534100
H	-0.36149800	1.13550500	-1.75037700
C	0.33129400	4.62893600	-0.22277300
H	1.81058900	3.62594800	0.98822100
C	-0.62324200	4.48270300	-1.23228500
H	-1.59360600	3.10610200	-2.58029500
H	0.52493200	5.60819200	0.20694400
H	-1.17534500	5.34779800	-1.59033900

Energy= -1184.51379372 (Hartree/Particle)

Zero-point correction= 0.360283

Thermal correction to Energy= 0.383602

Thermal correction to Enthalpy= 0.384546

Thermal correction to Gibbs Free Energy= 0.306563

Imaginary Frequency= 1232.76i

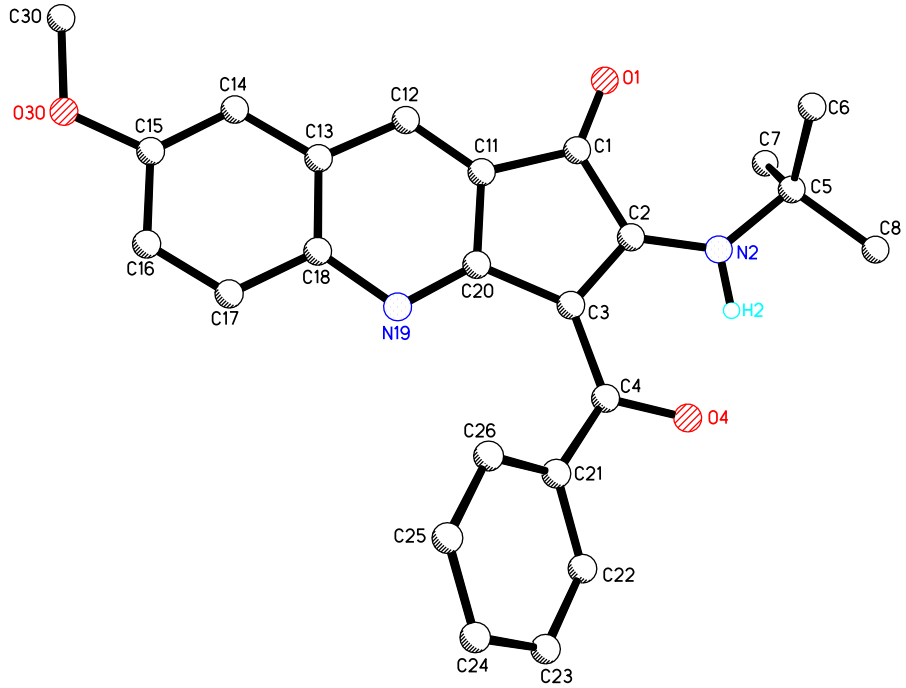
F. X-ray crystallographic analysis for product 3h

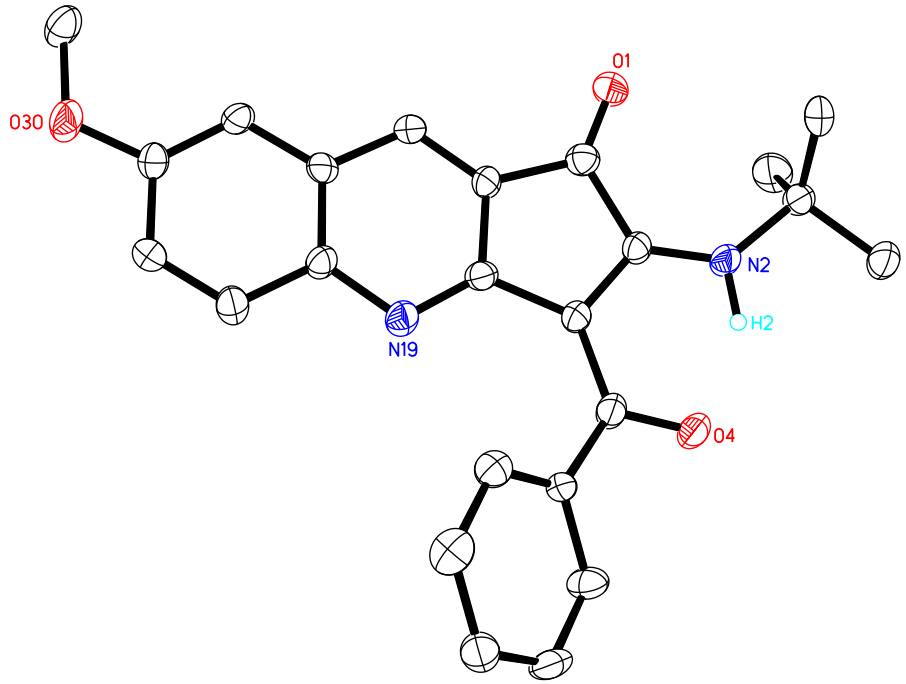
CCDC: 1861937

Crystal data and structure refinement for sba158. Table 1:

Identification code	sba158
Empirical formula	$C_{24}H_{22}N_2O_3$
Formula weight	386.43

Temperature	200(2) K
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	$P2_1$
Z	2
Unit cell dimensions	a = 11.6212(12) Å α = 90 ° b = 6.9157(8) Å β = 109.534(3) ° c = 12.8041(14) Å γ = 90 °
Volume	969.82(18) $Å^3$
Density (calculated)	1.32 g/cm^3
Absorption coefficient	0.09 mm^{-1}
Crystal shape	plank
Crystal size	0.318 x 0.148 x 0.042 mm^3
Crystal colour	red
Theta range for data collection	1.7 to 25.1 deg.
Index ranges	$-13 \leq h \leq 13$, $-8 \leq k \leq 8$, $-15 \leq l \leq 15$
Reflections collected	6224
Independent reflections	3417 (R(int) = 0.0437)
Observed reflections	2017 ($I > 2\sigma(I)$)
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.96 and 0.86
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	3417 / 438 / 314
Goodness-of-fit on F^2	1.01
Final R indices (I>2sigma(I))	R1 = 0.055, wR2 = 0.107
Absolute structure parameter	-2(5)
Largest diff. peak and hole	0.19 and -0.22 $eÅ^{-3}$


C30
O30
C14
C15
C12
C13
C11
O1
C1
C6
C7
C5
C2
C8
N2
C16
C18
C20
C3
H2
C17
N19
C4
O4
C26
C21
C25
C22
C24
C23


O1
O30
N2
H2
N19
O4

suggestion for a short experimental part:

sba158: red crystal (plank), dimensions 0.318 x 0.148 x 0.042 mm^3, crystal system monoclinic, space group $P2_1$, Z=2, a=11.6212(12) Å, b=6.9157(8) Å, c=12.8041(14) Å, alpha=90 deg, beta=109.534(3) deg, gamma=90 deg, V=969.82(18) $Å^3$, rho=1.323 g/cm^3, T=200(2) K, $Theta_{max}$= 25.086 deg, radiation MoKα, lambda=0.71073 Å, 0.5 deg omega-scans with CCD area detector, covering the asymmetric unit in reciprocal space with a mean redundancy of 5.46and a completeness of 99.9% to a resolution of 0.84 Å, 6224 reflections measured, 3417 unique (R(int)=0.0437), 2017 observed ($I > 2\sigma(I)$), intensities were corrected for Lorentz and polarization effects, an empirical scaling and absorption correction was applied using SADABS[1] based on the Laue symmetry of the reciprocal space, mu=0.09mm^{-1}, T_{min}=0.86, T_{max}=0.96, structure solved with SHELXT-2014 (Sheldrick 2014)[2] and refined against F^2 with a Full-matrix least-squares algorithm using the SHELXL-2018/3 (Sheldrick, 2018) software[3], 314 parameters refined, hydrogen atoms were treated using appropriate riding models, Flack absolute structure parameter -2(5), goodness of fit 1.01 for observed reflections, final residual values R1(F)=0.055, $wR(F^2)$=0.107 for observed reflections, residual electron density -0.22 to 0.19 $eÅ^{-3}$. CCDC 1861937 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via https://www.ccdc.cam.ac.uk/structures/.

Lit. 1: (SADABS-2016/2 - Bruker AXS area detector scaling and absorption correction)

Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10.

Lit. 2: (SHELXT - Integrated space-group and crystal structure determination)

Sheldrick G. M., Acta Cryst. A71 (2015) 3-8.

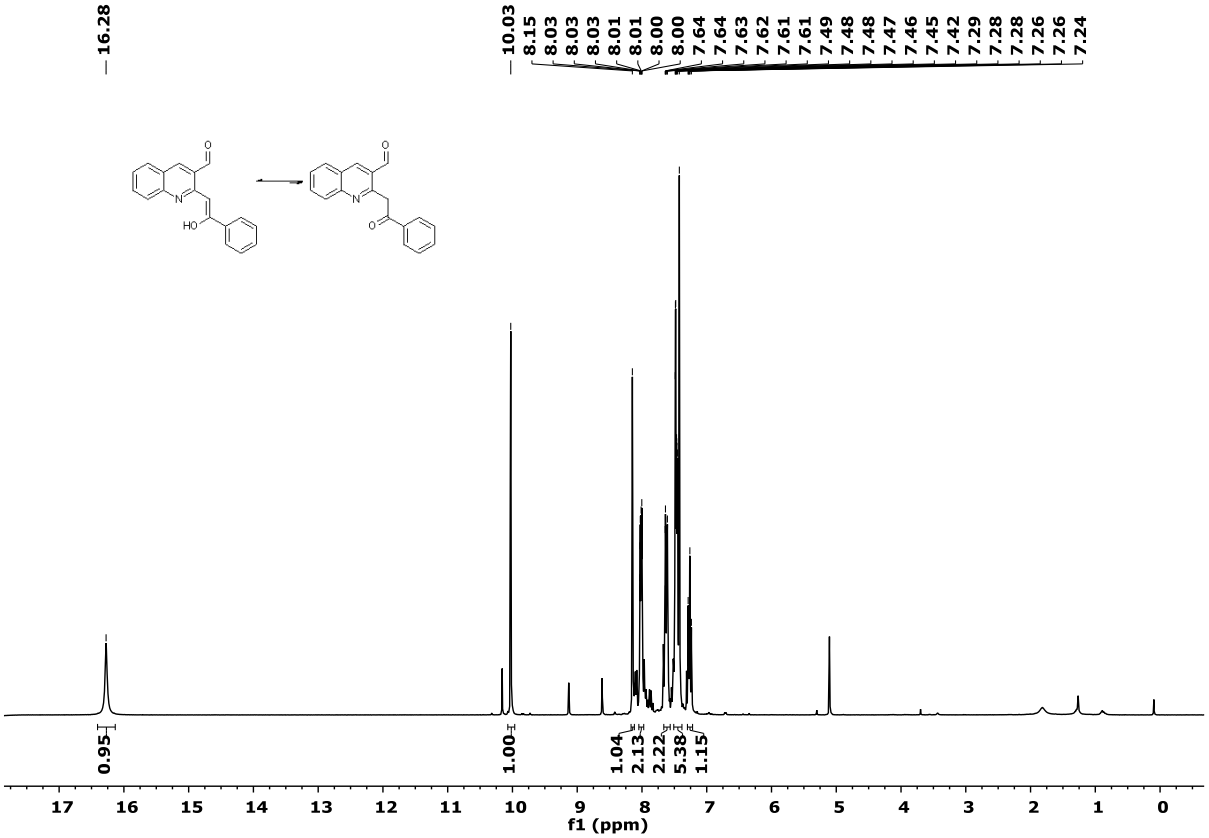
Lit. 3: (program SHELXL-2018/3 (Sheldrick, 2018) for structure refinement)

Sheldrick G. M., Acta Cryst. (2015). C71, 3-8

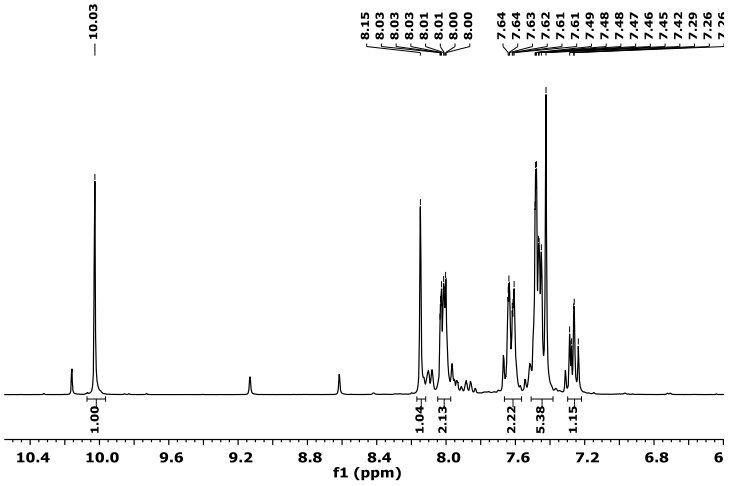
Lit. APEX, APEX2, SMART, SAINT, SAINT-Plus:

Bruker (2007). "Program name(s)". Bruker AXS Inc., Madison, Wisconsin, USA.

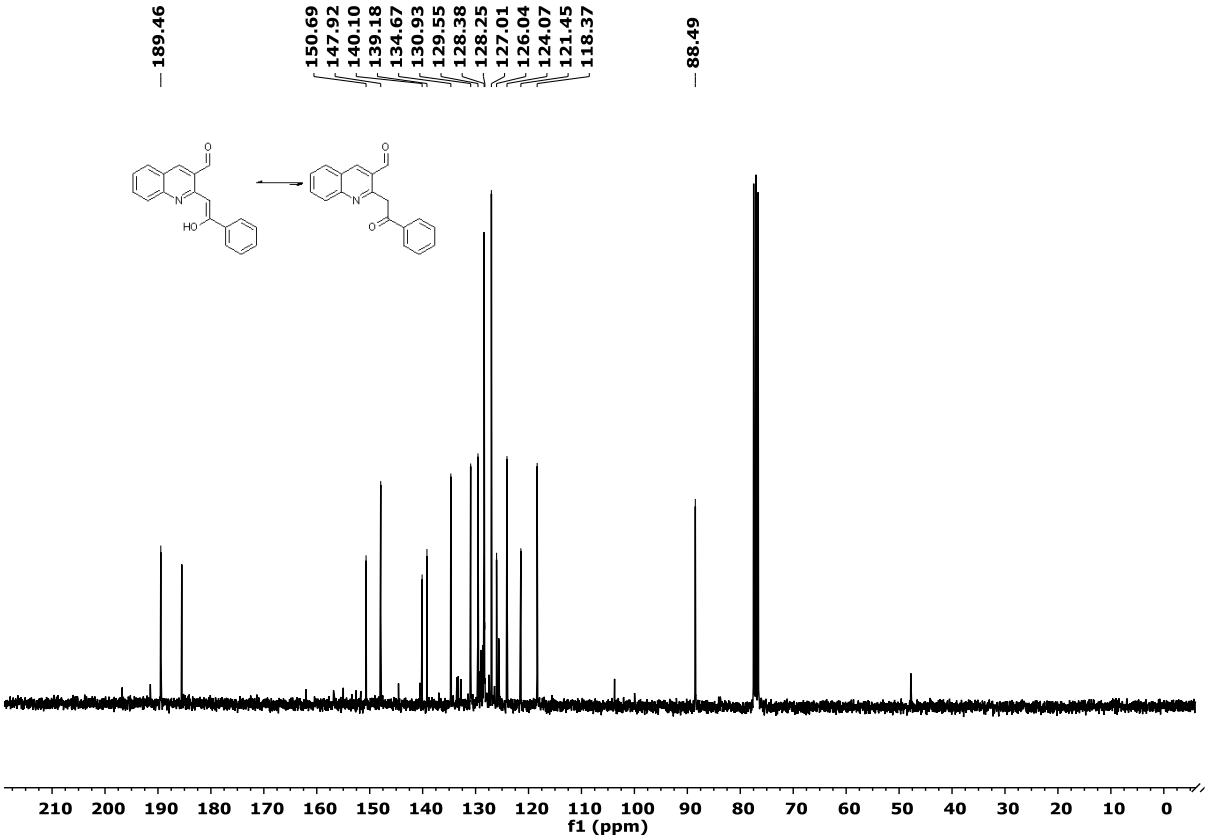
G. ^{1}H, ^{13}C NMR and HRMS spectra



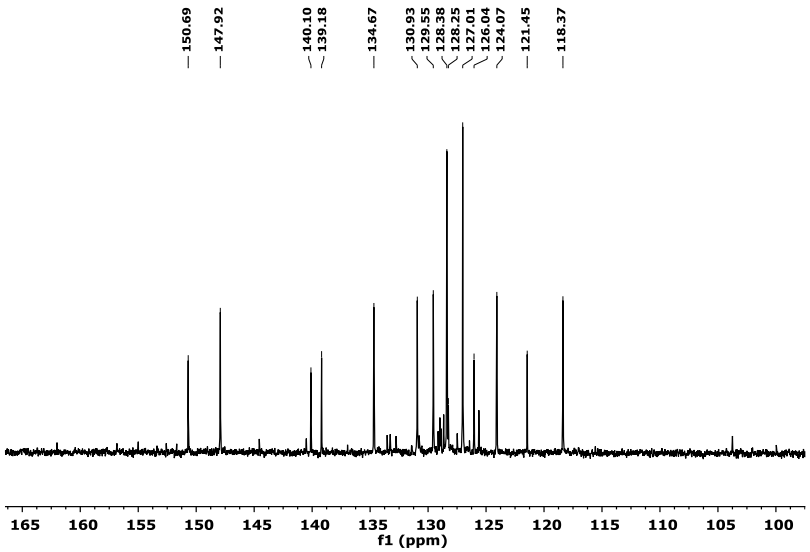
^{1}H-NMR of compound **(1a)** (300 MHz, $CDCl_3$)



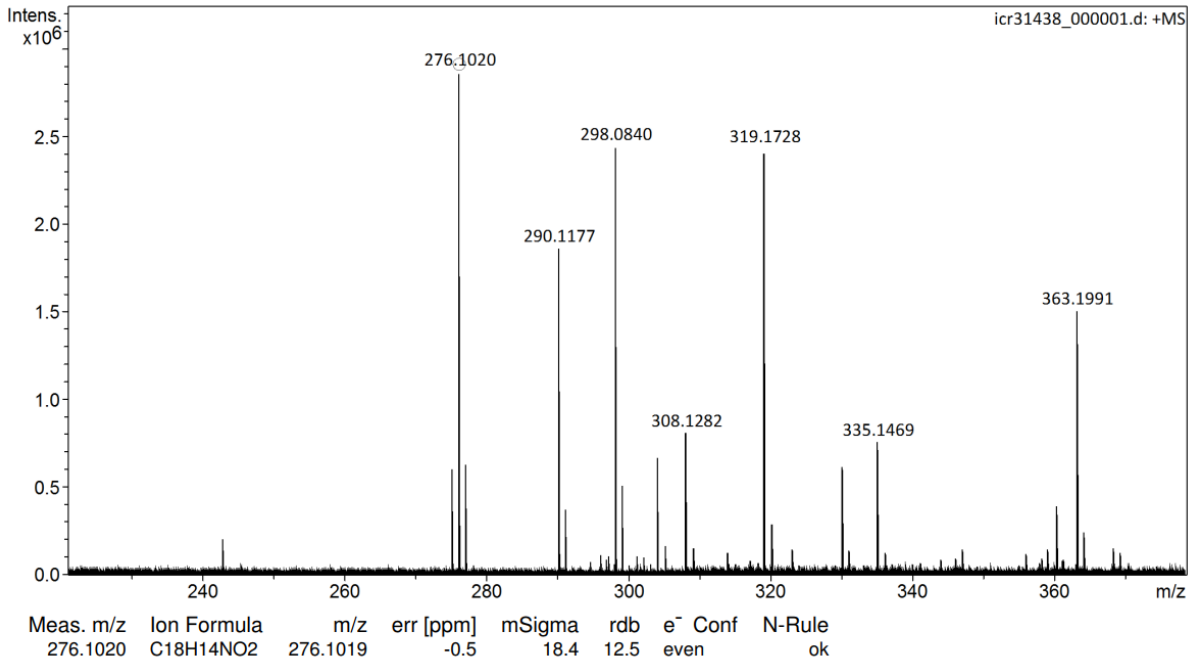
^{1}H-NMR of compound **(1a)** (300 MHz, $CDCl_3$)



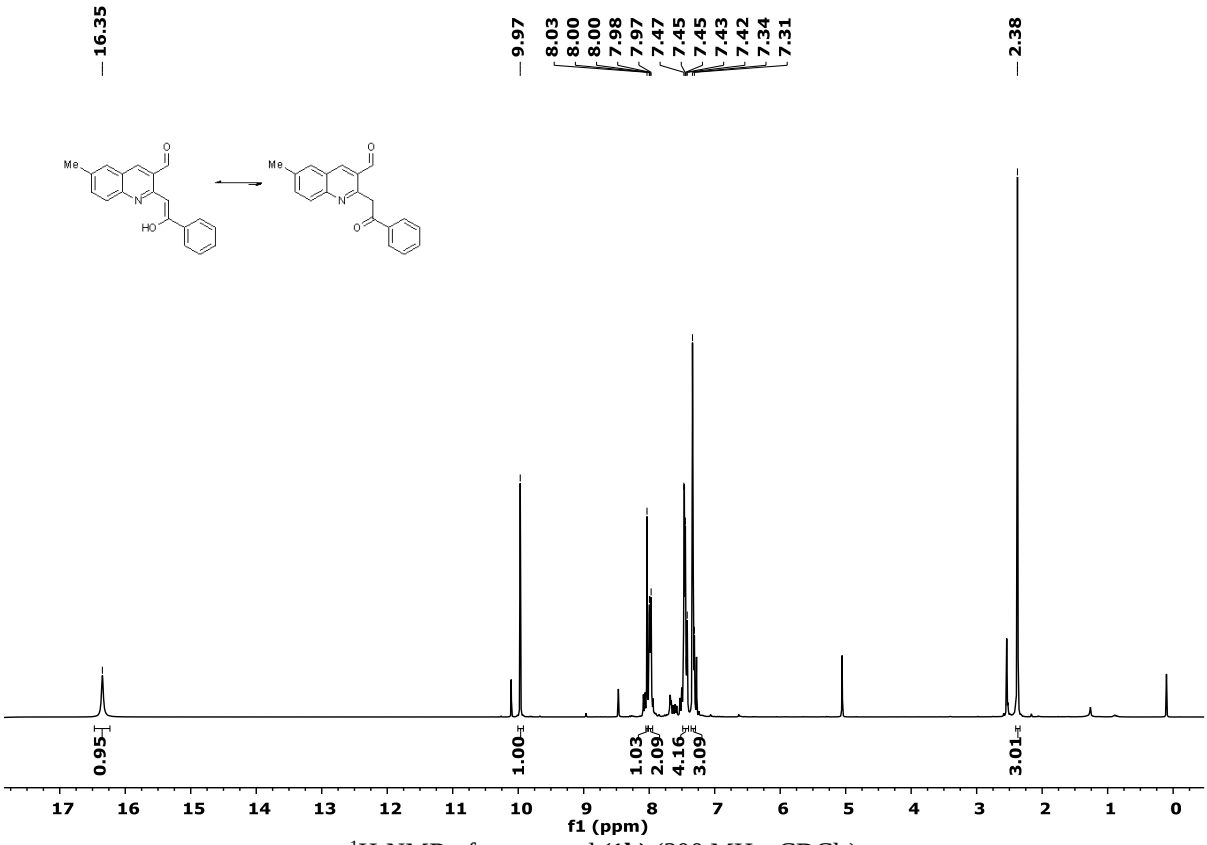
^{13}C-NMR of compound **(1a)** (75 MHz, $CDCl_3$)



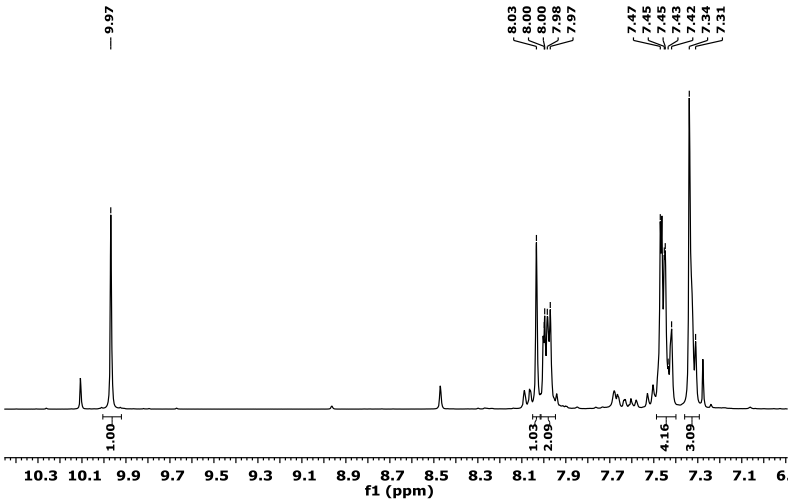
^{13}C-NMR of compound **(1a)** (75 MHz, $CDCl_3$)



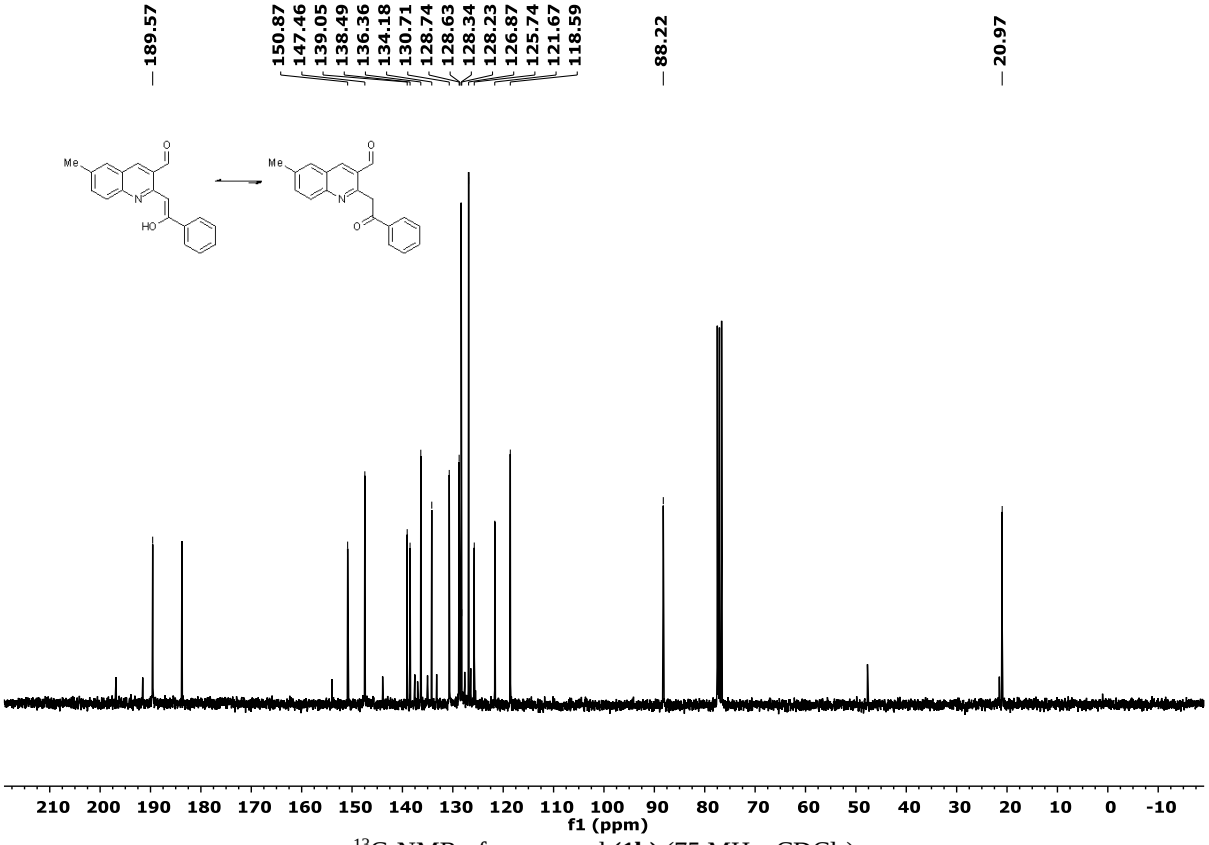
HRMS-ESI (m/z) of (**1a**)



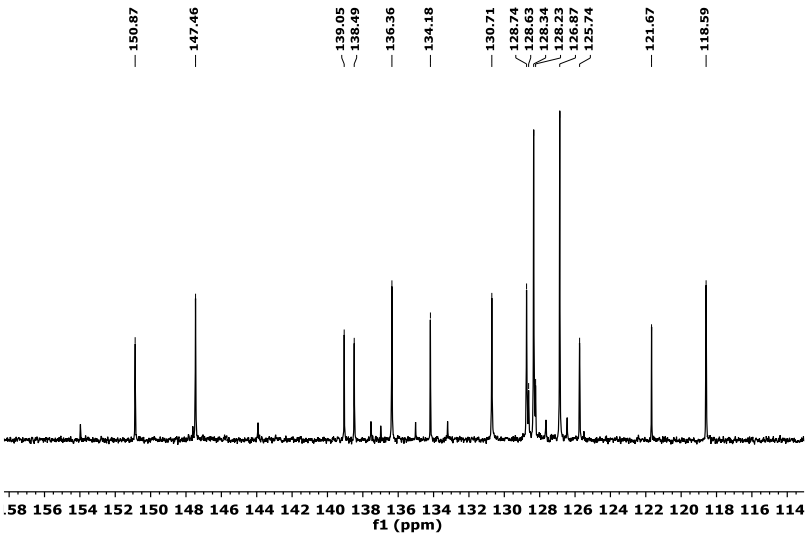
^{1}H-NMR of compound **(1b)** (300 MHz, $CDCl_3$)



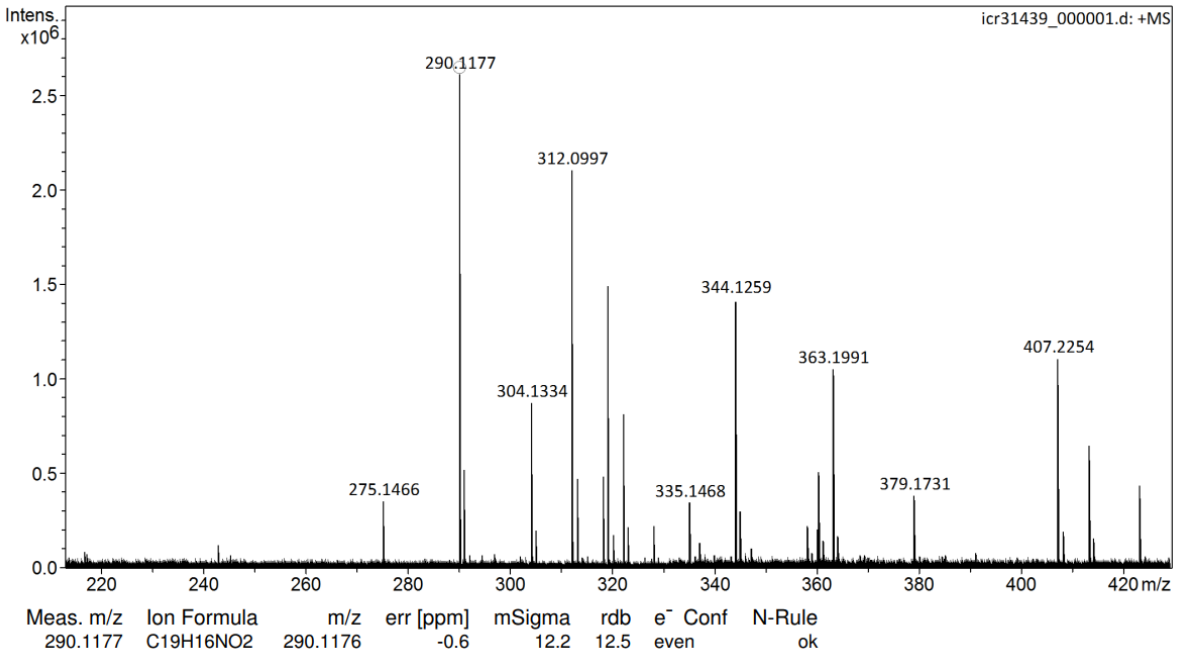
^{1}H-NMR of compound **(1b)** (300 MHz, $CDCl_3$)



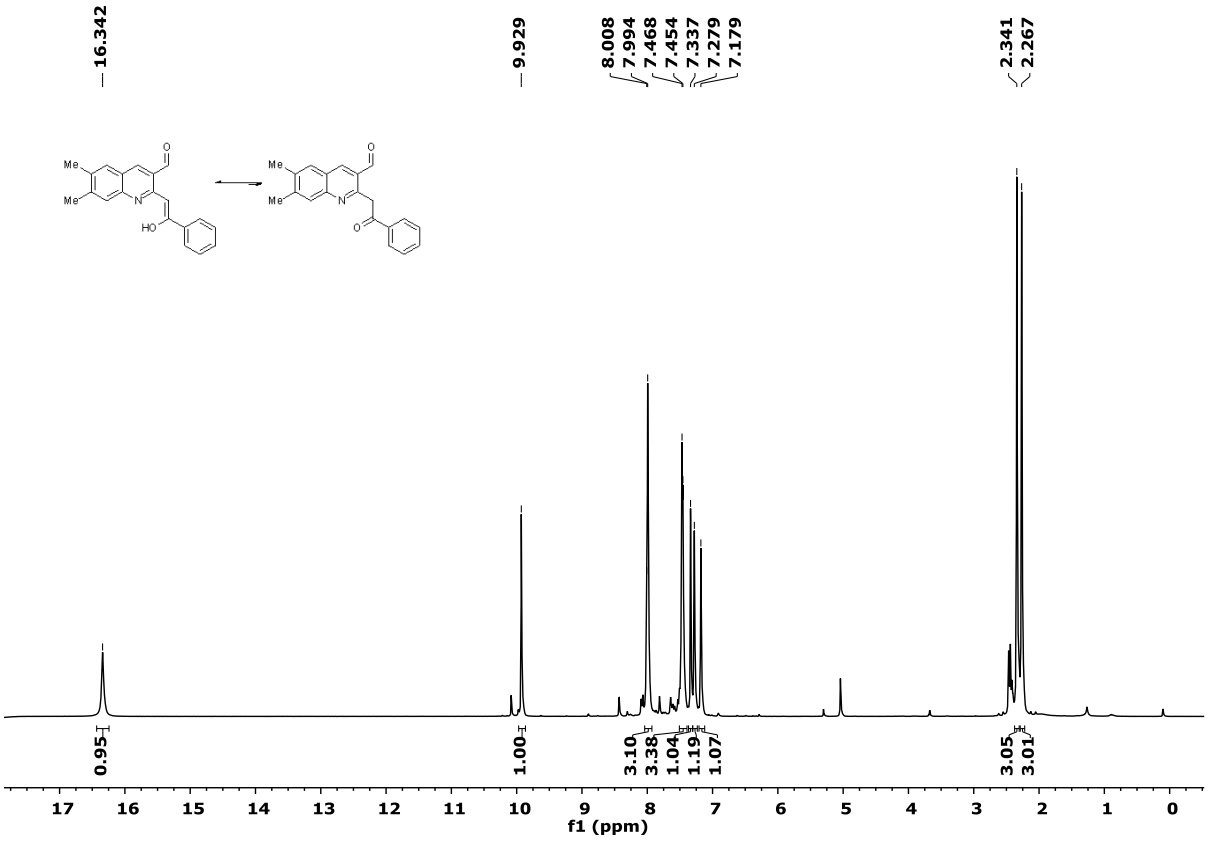
^{13}C-NMR of compound **(1b)** (75 MHz, $CDCl_3$)



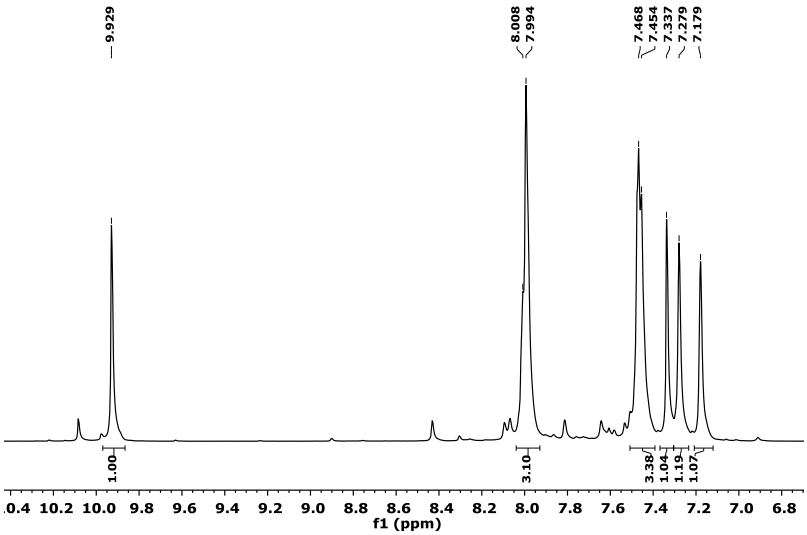
^{13}C-NMR of compound **(1b)** (75 MHz, $CDCl_3$)



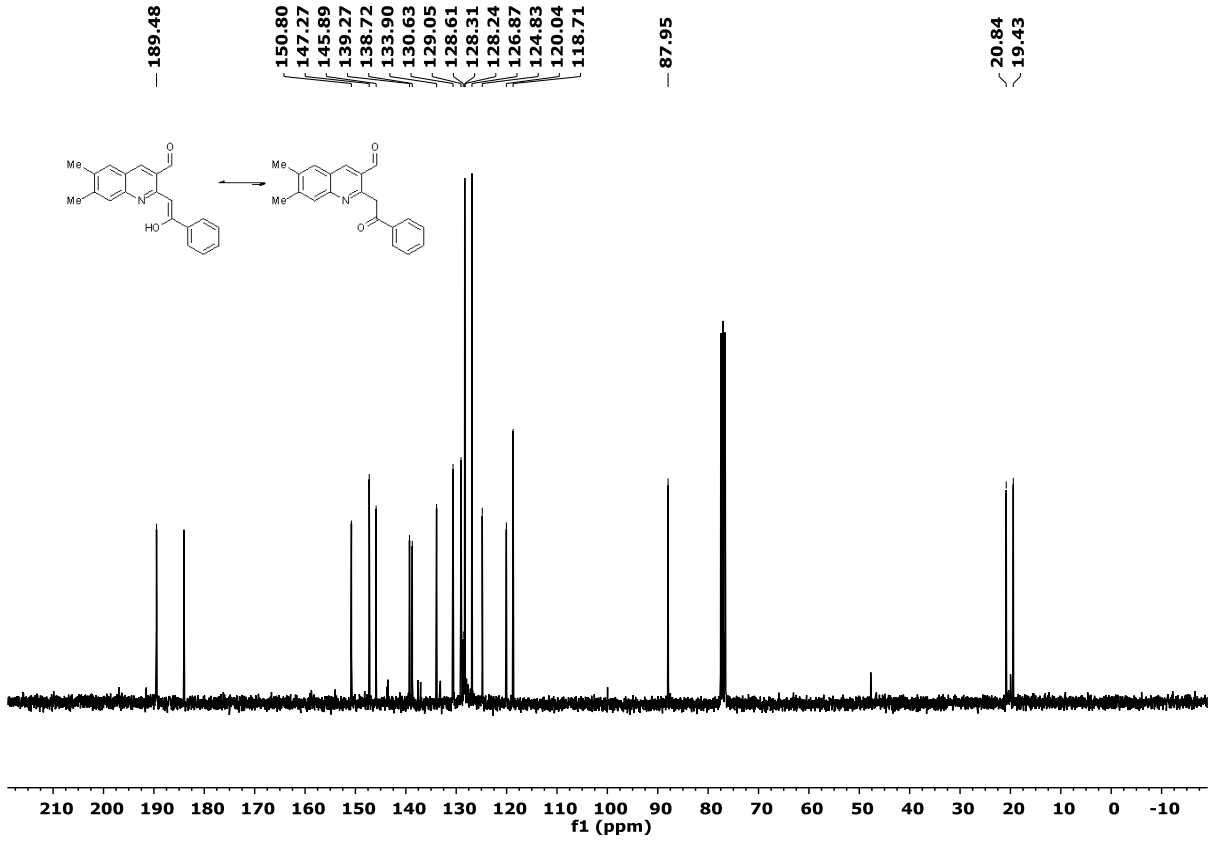
HRMS-ESI (m/z) of (**1b**)



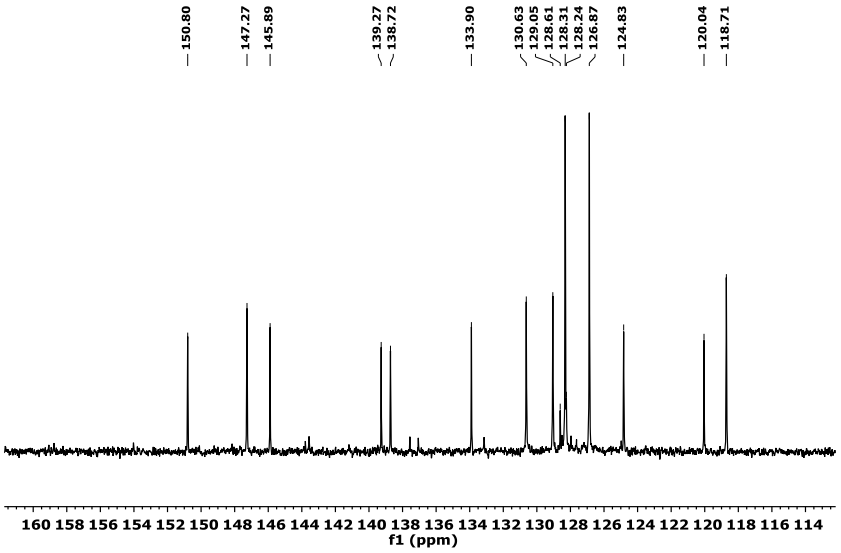
^{1}H-NMR of compound **(1c)** (300 MHz, $CDCl_3$)



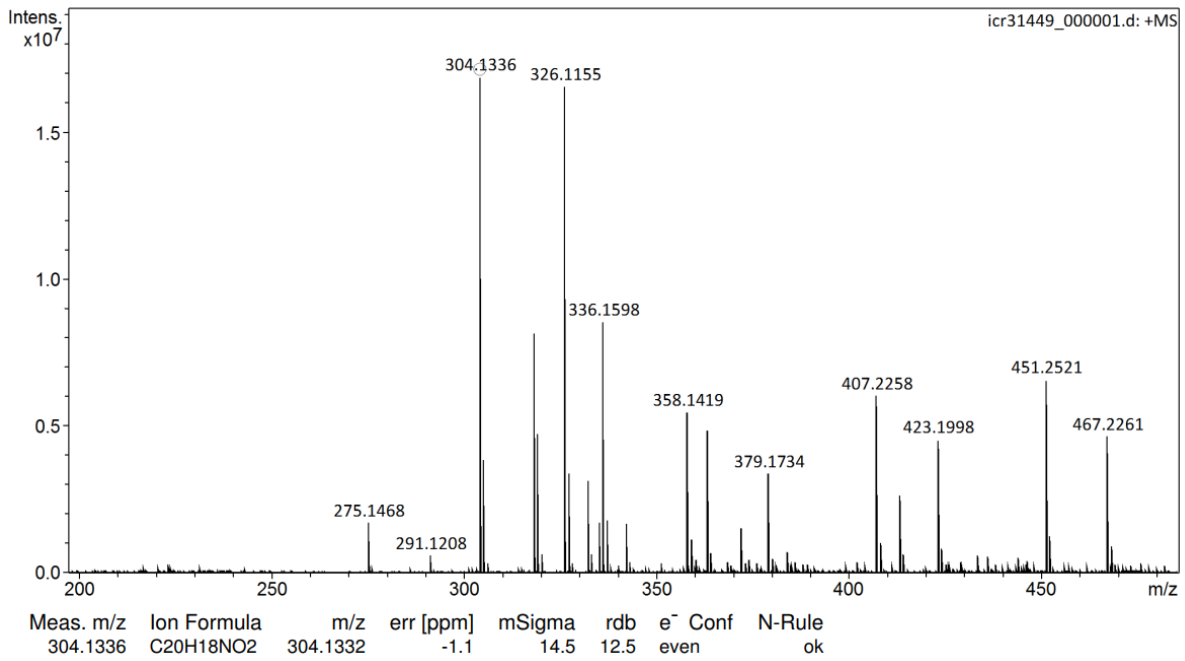
^{1}H-NMR of compound **(1c)** (300 MHz, $CDCl_3$)



^{13}C-NMR of compound **(1c)** (75 MHz, $CDCl_3$)

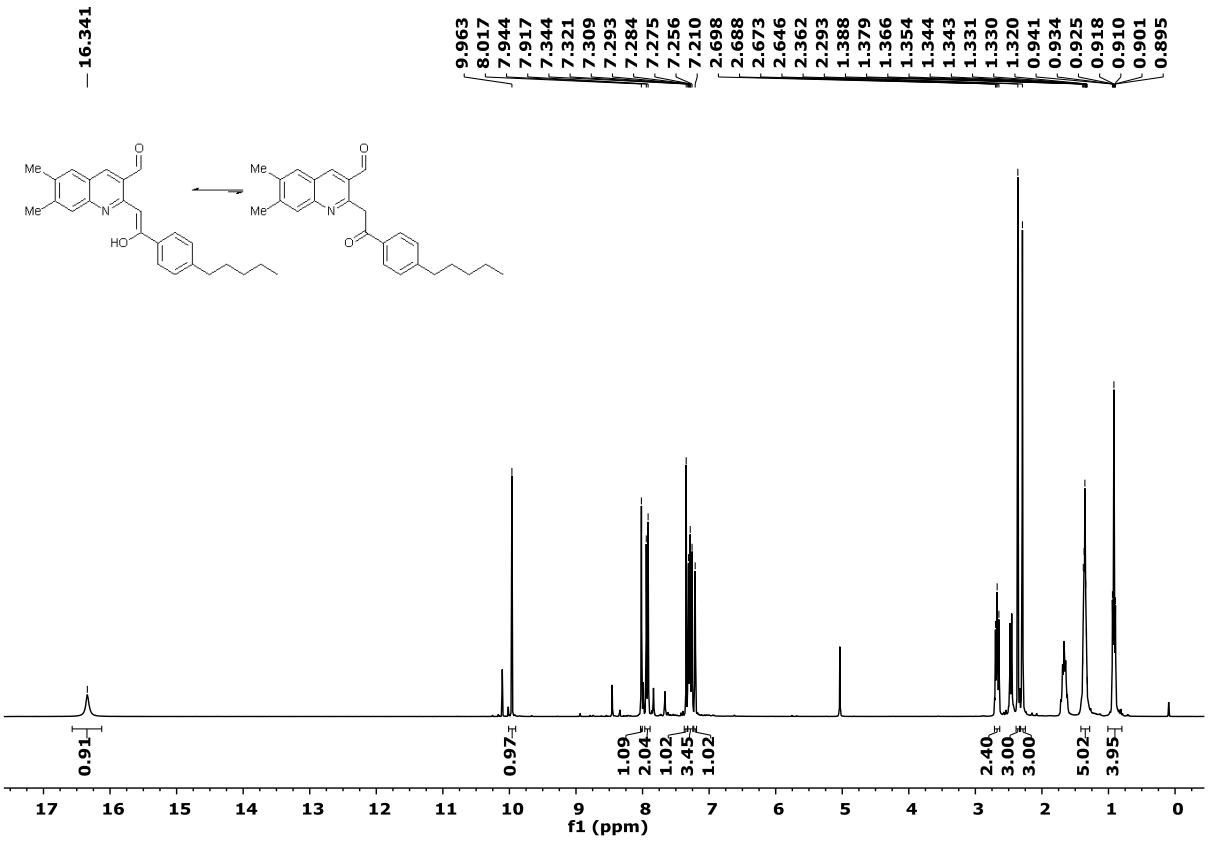


^{13}C-NMR of compound **(1c)** (75 MHz, $CDCl_3$)

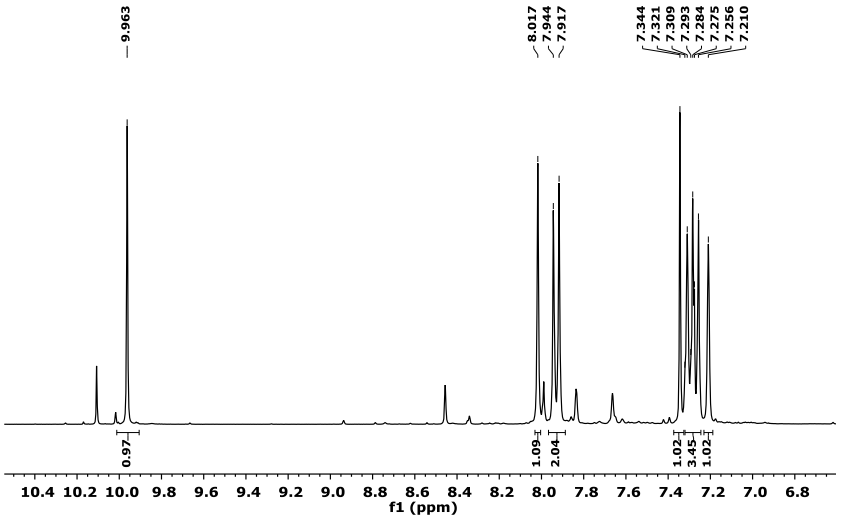


Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
304.1336	C20H18NO2	304.1332	-1.1	14.5	12.5	even	ok

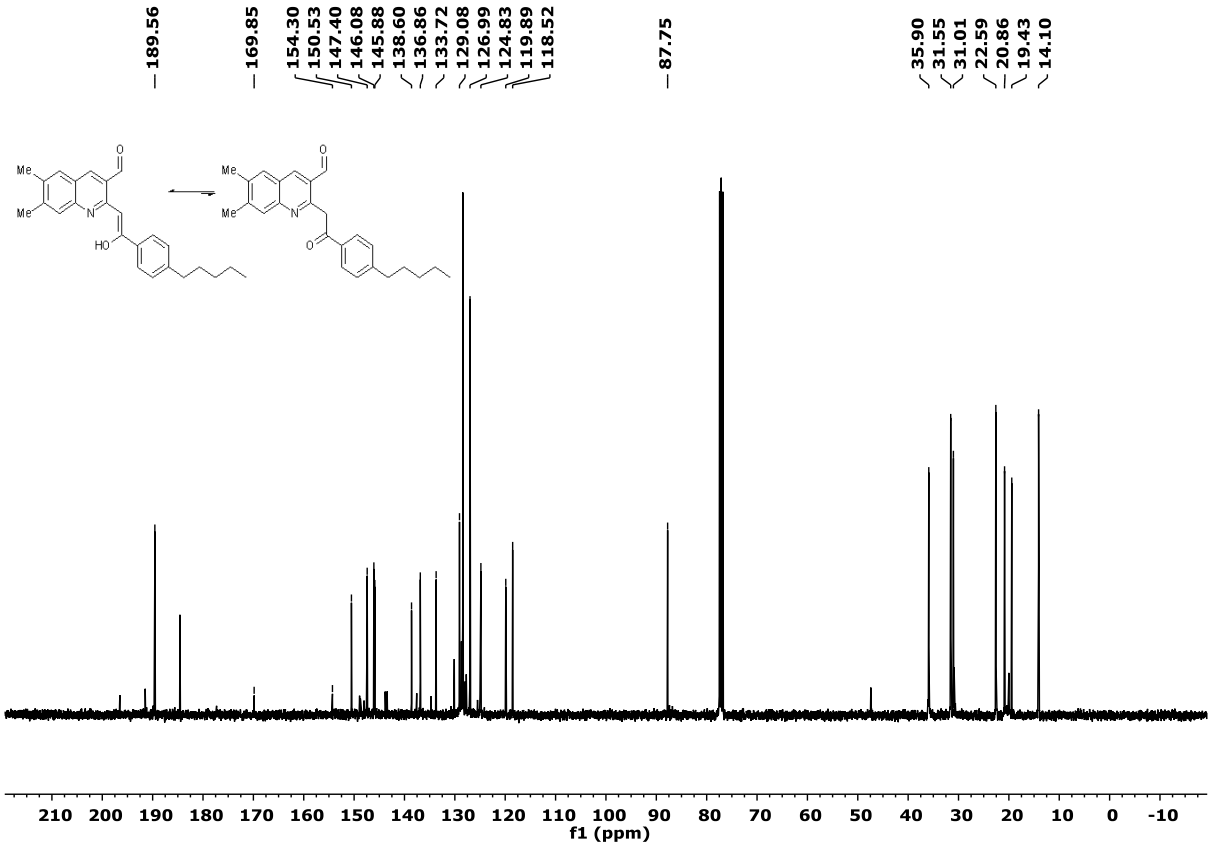
HRMS-ESI (m/z) of (**1c**)



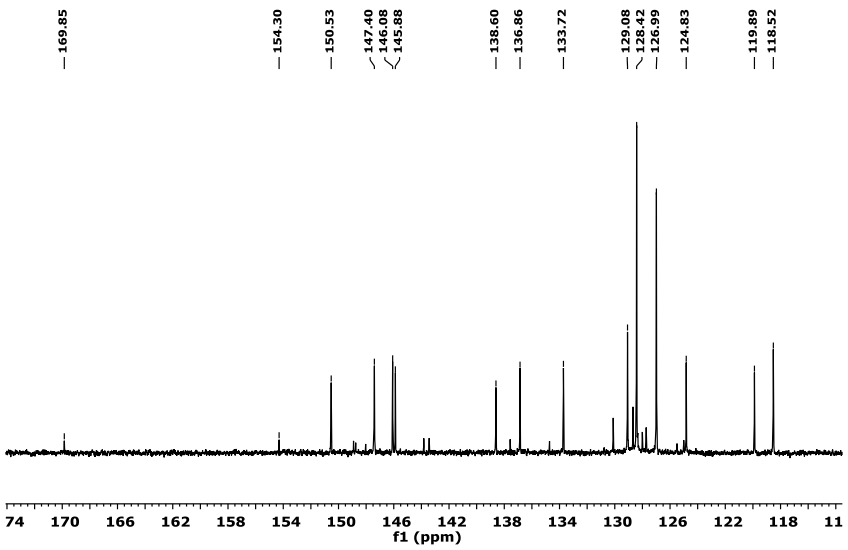
^{1}H-NMR of compound **(1d)** (300 MHz, $CDCl_3$)



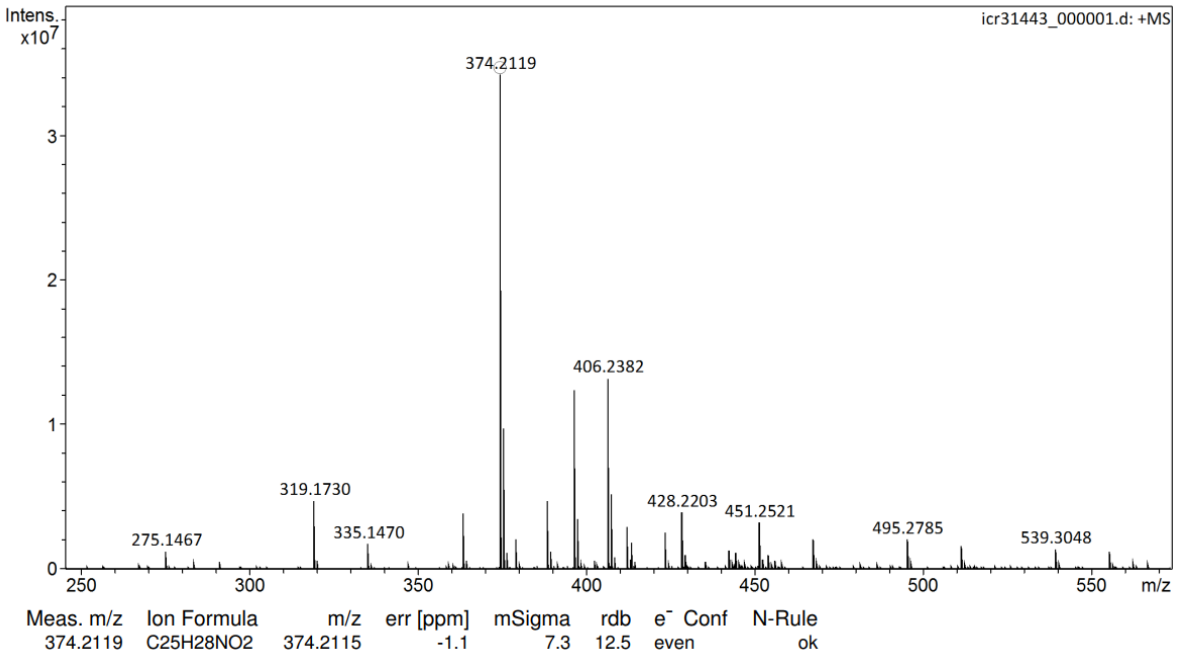
^{1}H-NMR of compound **(1d)** (300 MHz, $CDCl_3$)



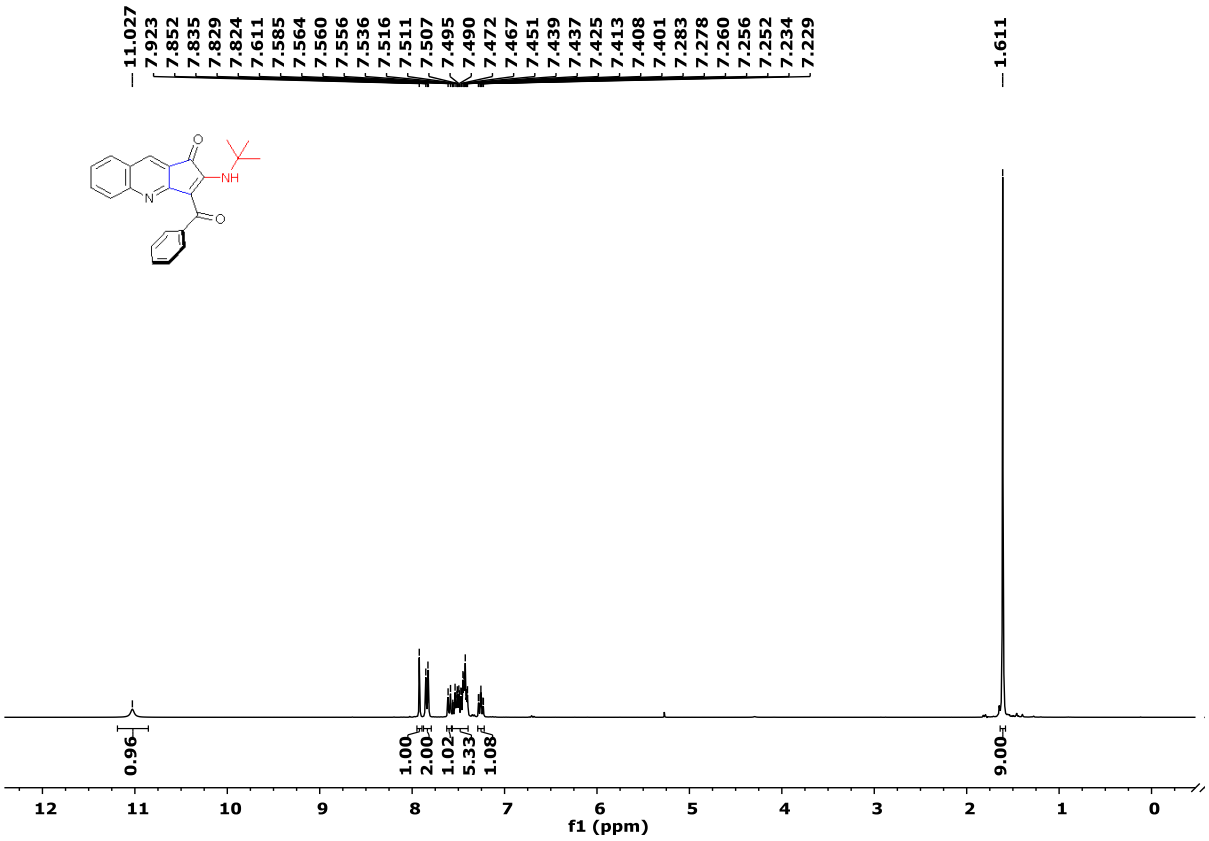
^{13}C-NMR of compound **(1d)** (100 MHz, $CDCl_3$)



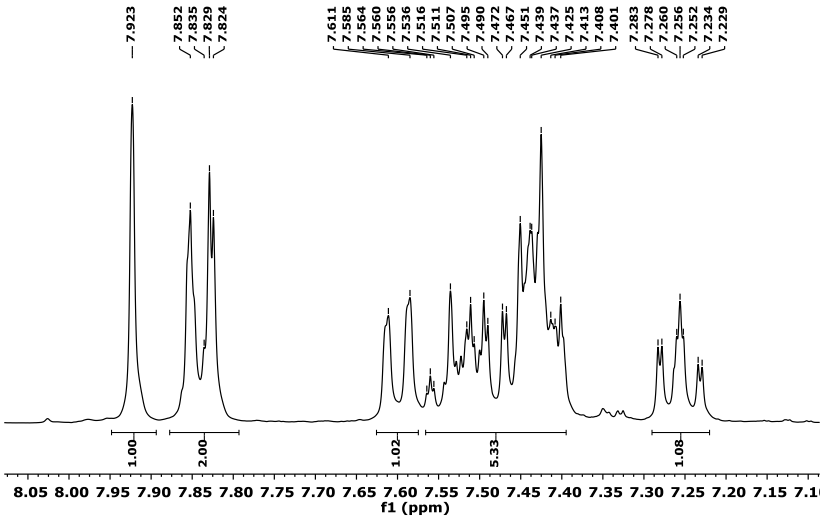
^{13}C-NMR of compound **(1d)** (100 MHz, $CDCl_3$)



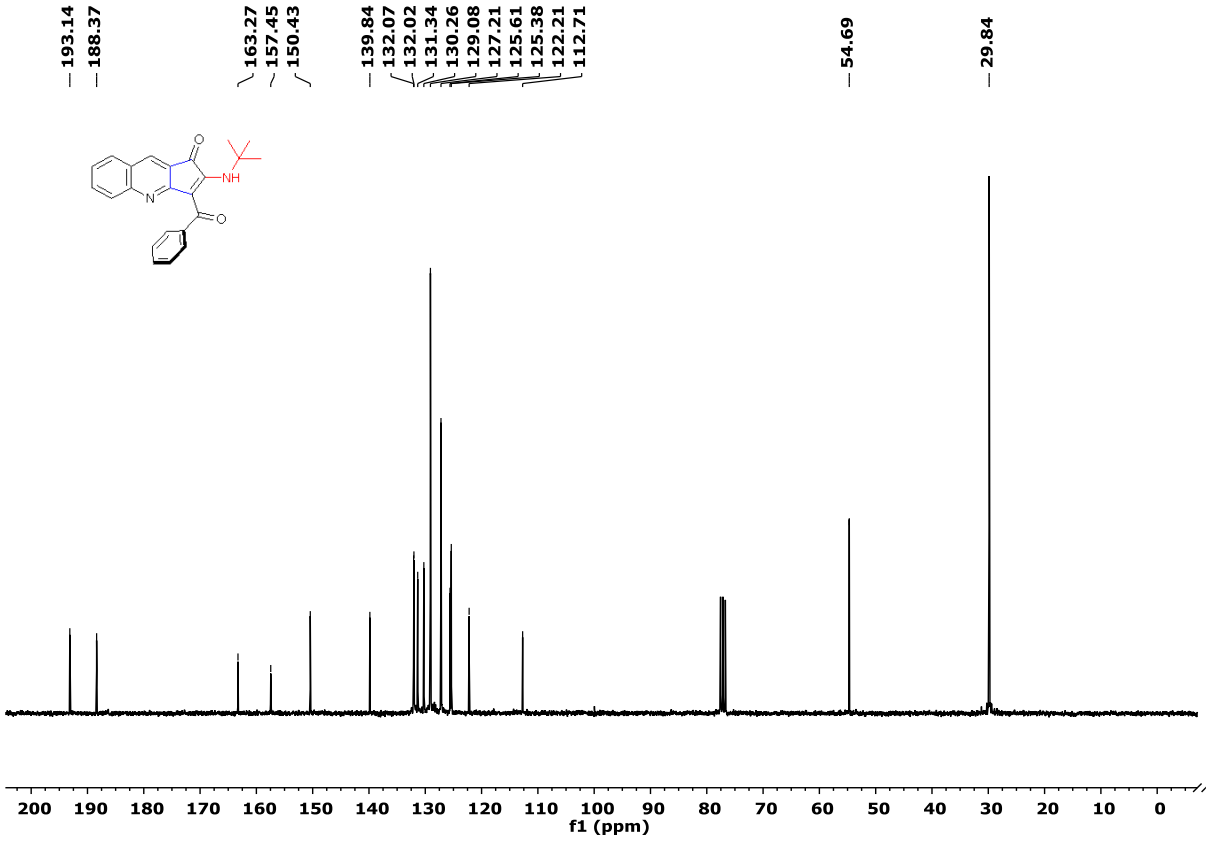
HRMS-ESI (m/z) of (**1d**)



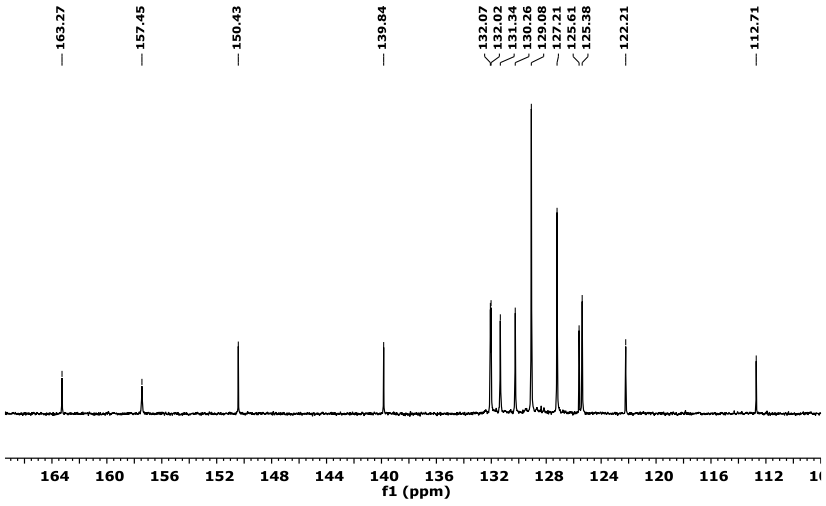
^{1}H-NMR of compound **(3a)** (300 MHz, $CDCl_3$)



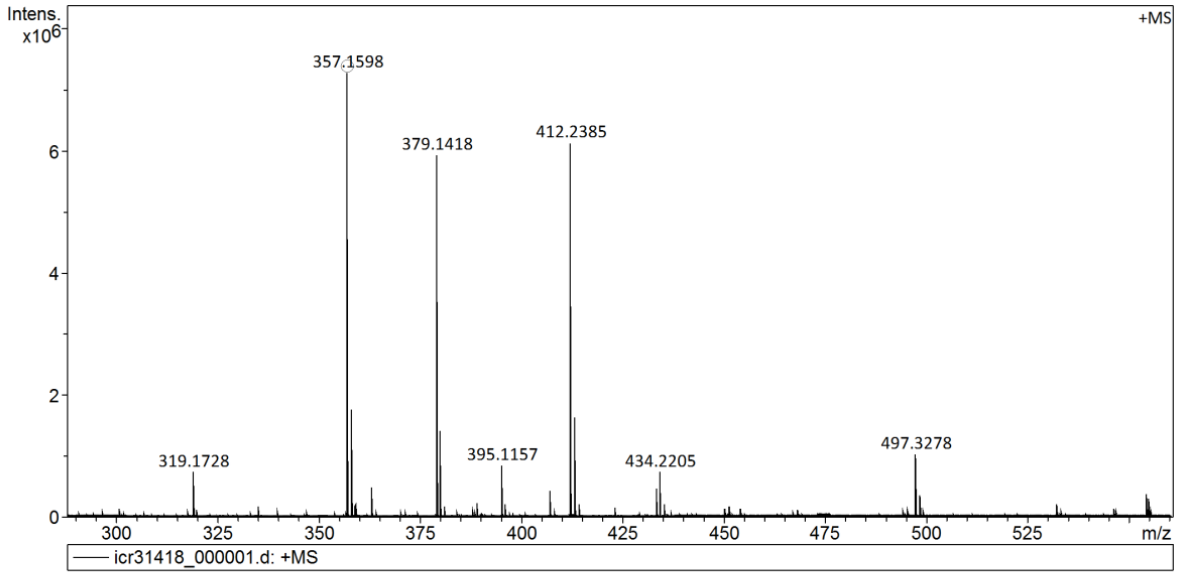
^{1}H-NMR of compound **(3a)** (300 MHz, $CDCl_3$)



^{13}C-NMR of compound **(3a)** (75 MHz, $CDCl_3$)

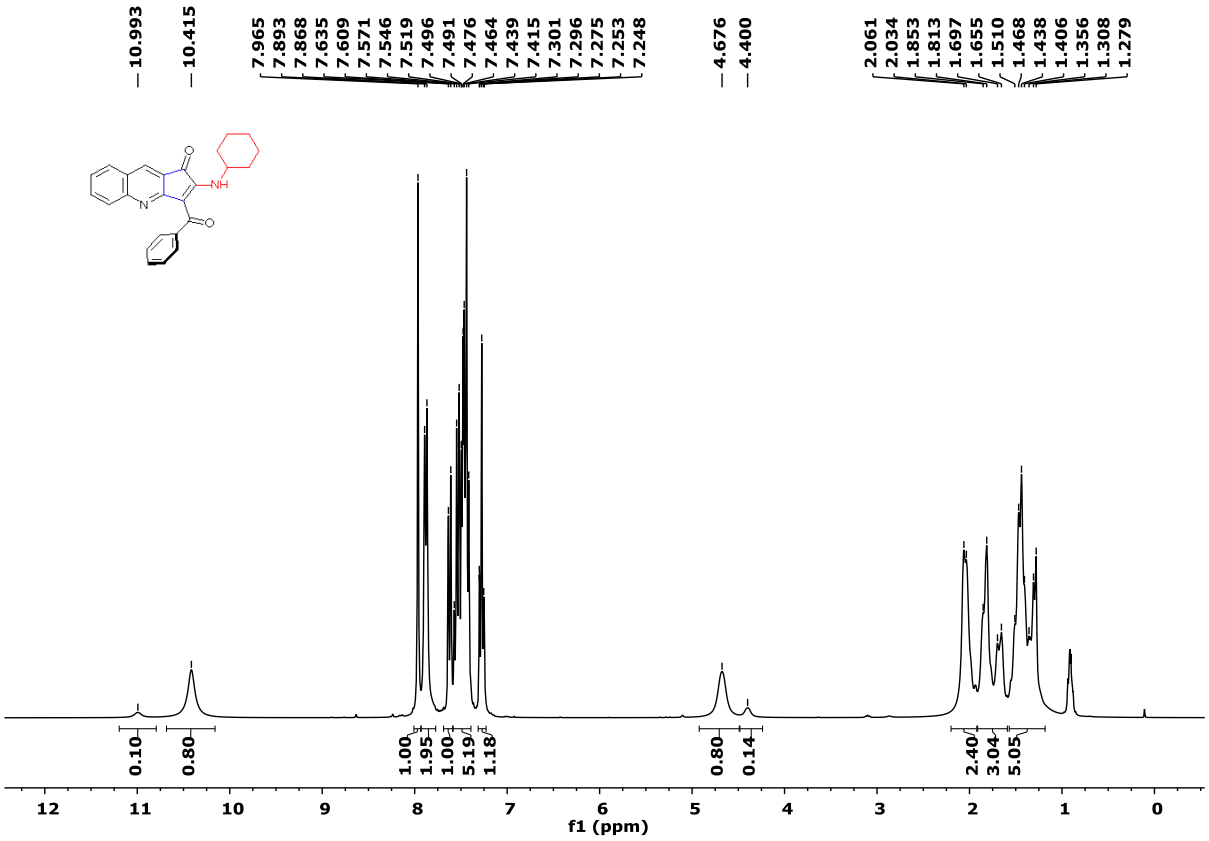


^{13}C-NMR of compound **(3a)** (75 MHz, $CDCl_3$)

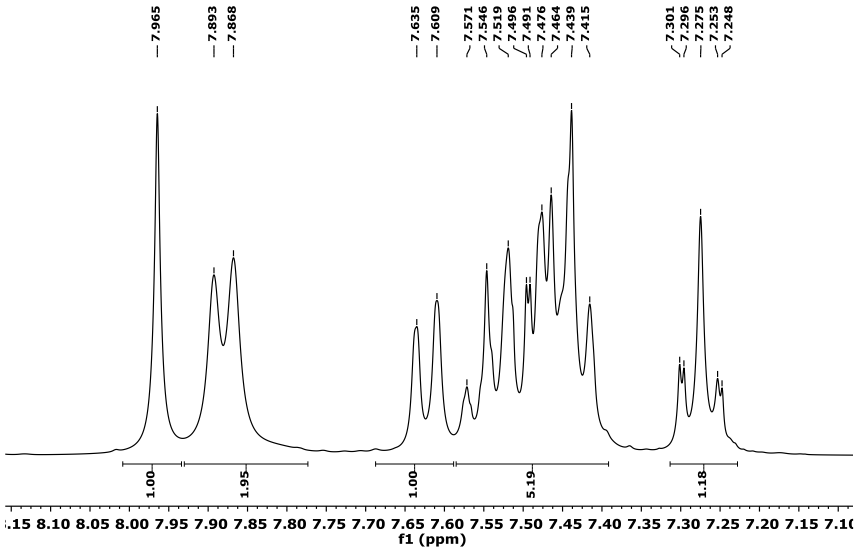


Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
357.1598	C23H21N2O2	357.1598	-0.3	15.6	14.5	even	ok
	C21H19N5O	357.1584	-4.0	17.5	15.0	odd	ok

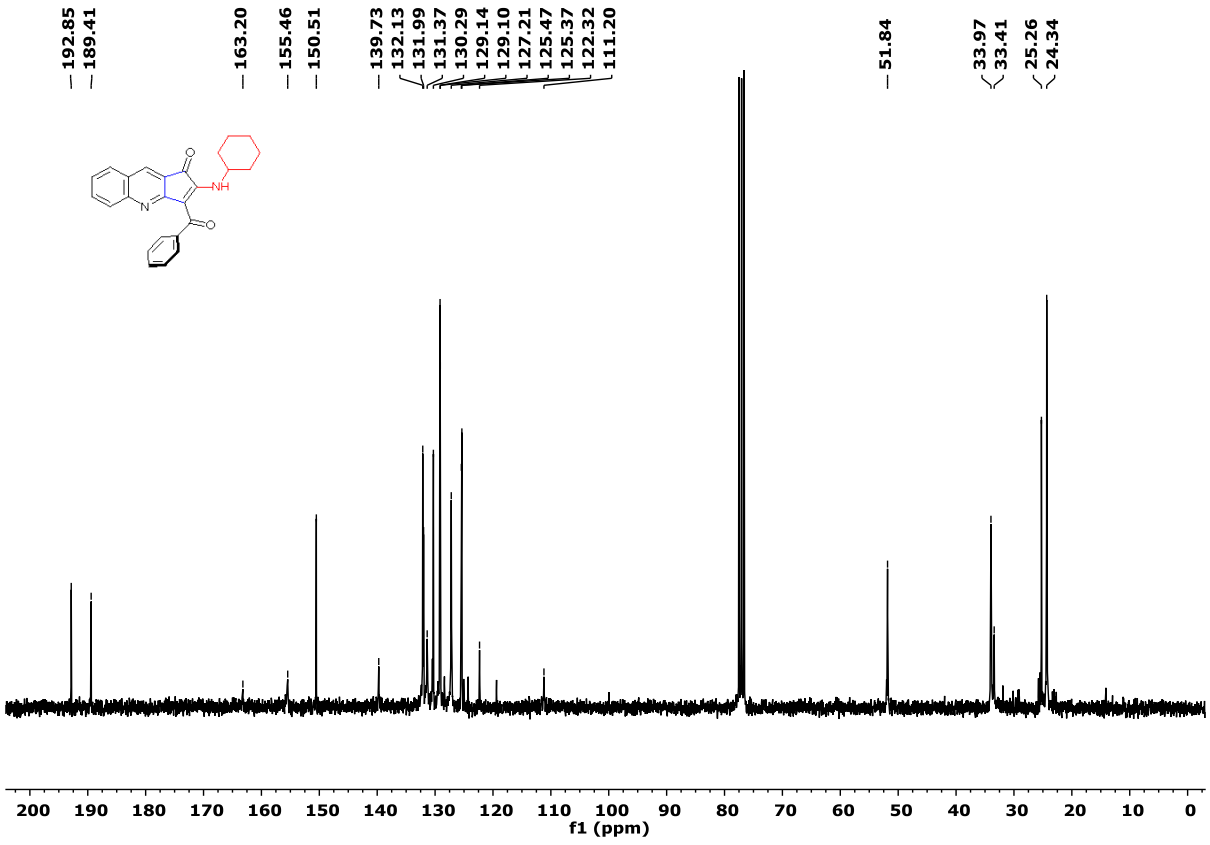
HRMS-ESI (m/z) of (**3a**)



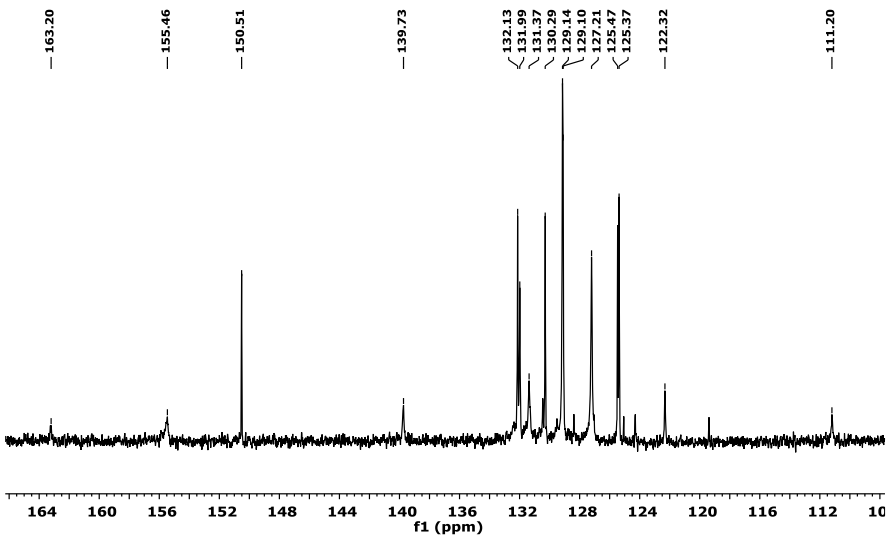
^{1}H-NMR of compound **(3b)** (300 MHz, $CDCl_3$)



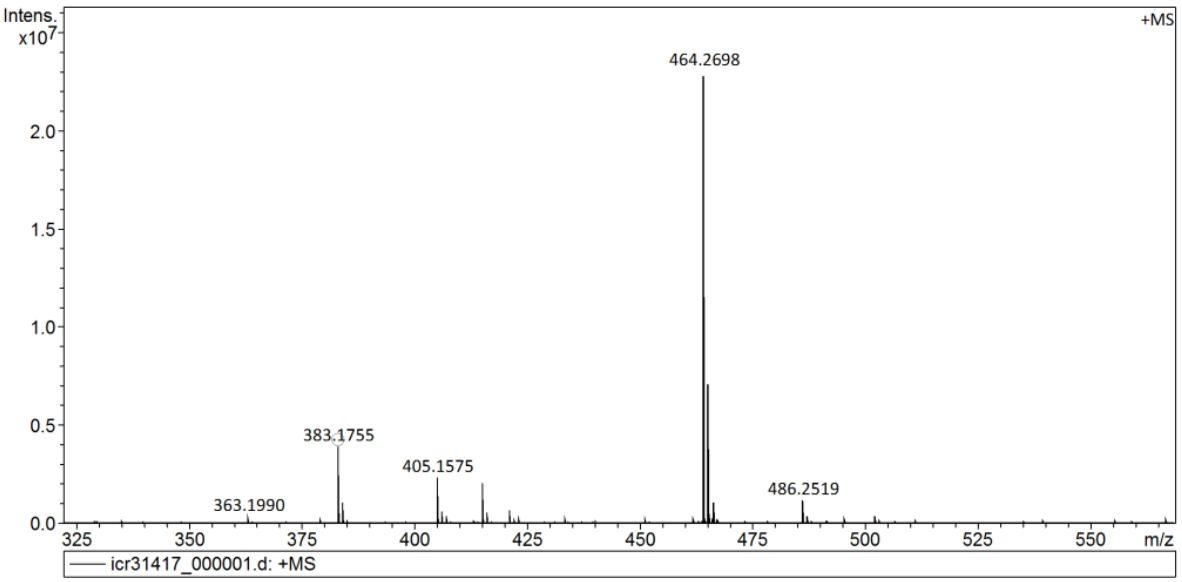
^{1}H-NMR of compound **(3b)** (300 MHz, $CDCl_3$)



^{13}C-NMR of compound **(3b)** (75 MHz, $CDCl_3$)

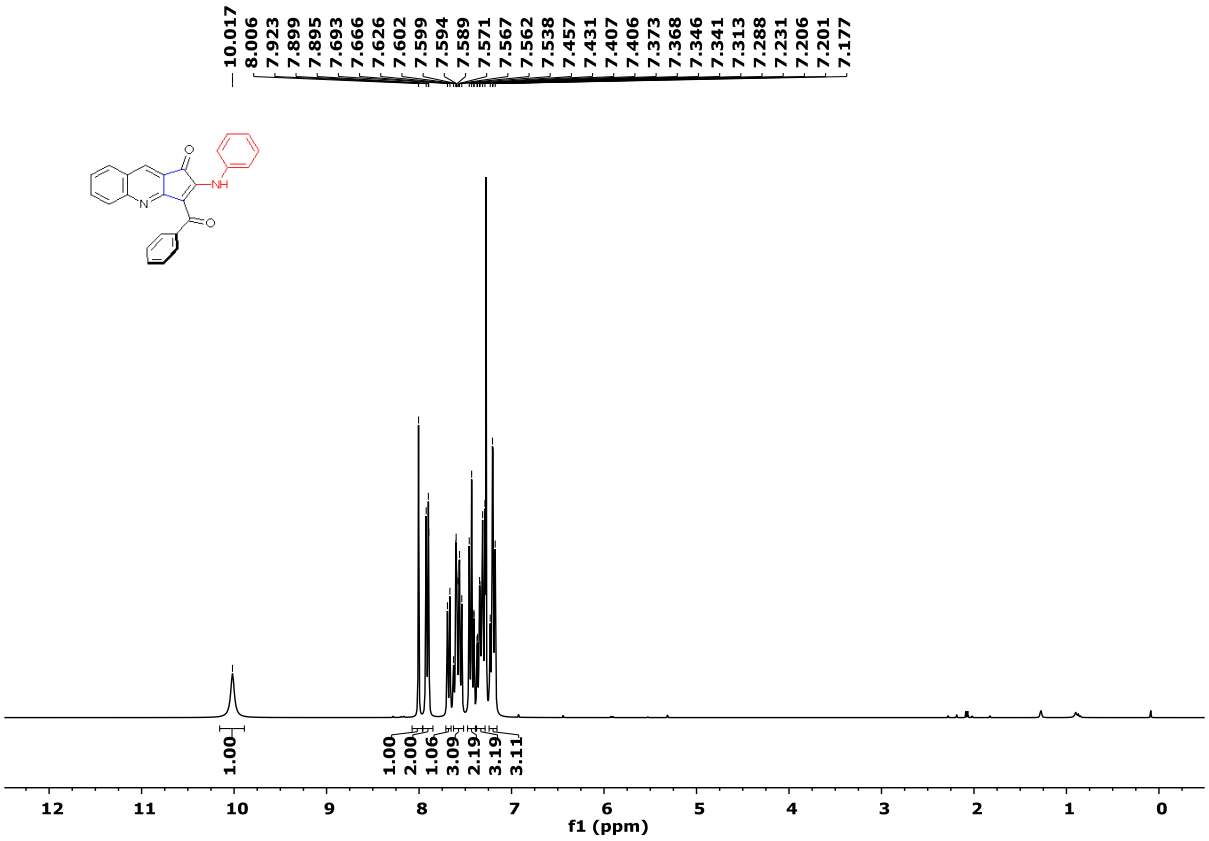


^{13}C-NMR of compound **(3b)** (75 MHz, $CDCl_3$)

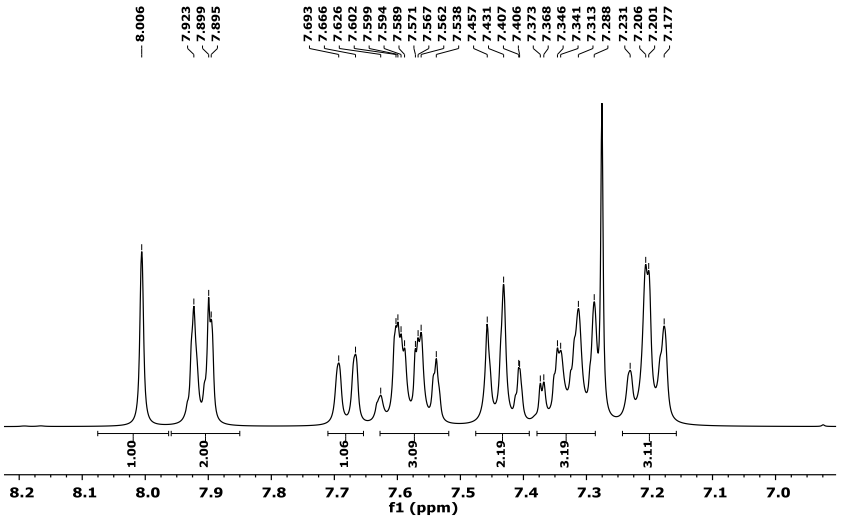


Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
383.1755	C25H23N2O2	383.1754	-0.3	18.0	15.5	even	ok
	C23H21N5O	383.1741	-3.8	20.4	16.0	odd	ok

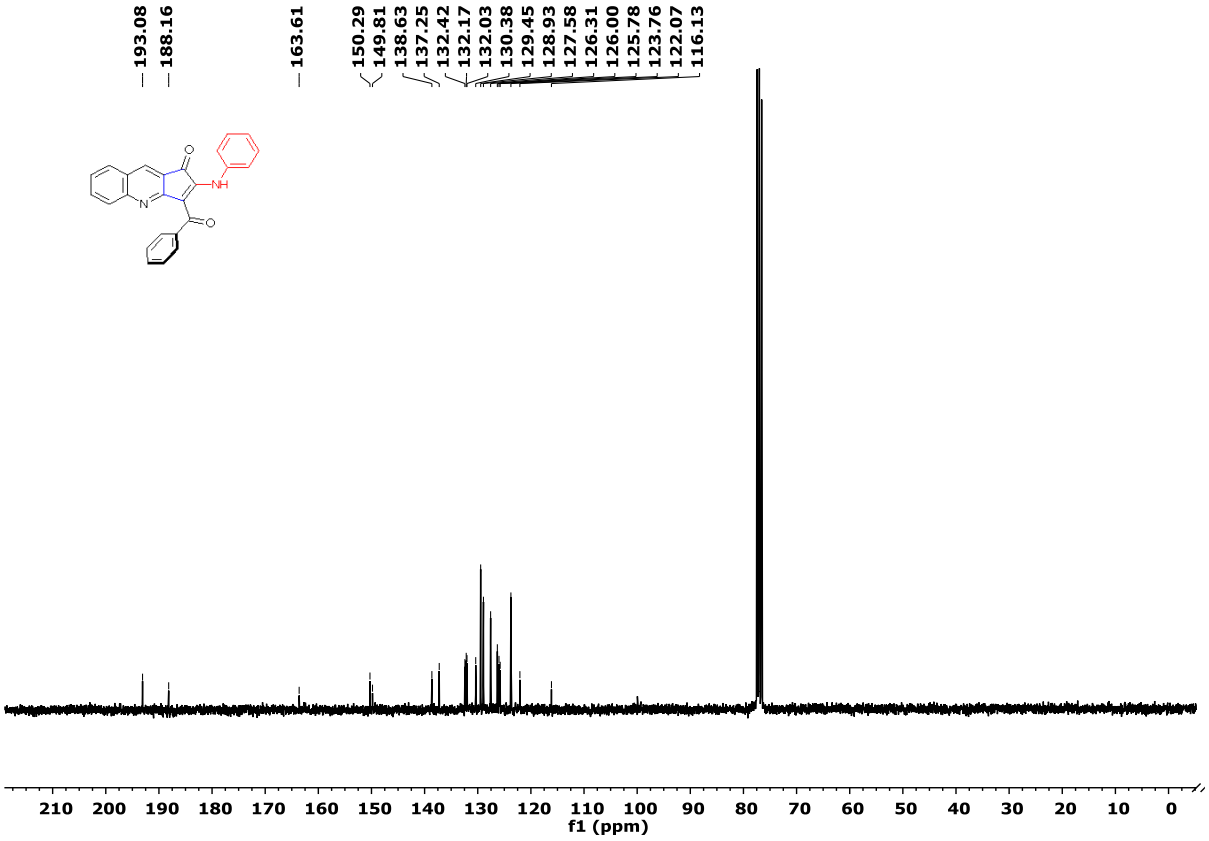
HRMS-ESI (m/z) of (**3b**)



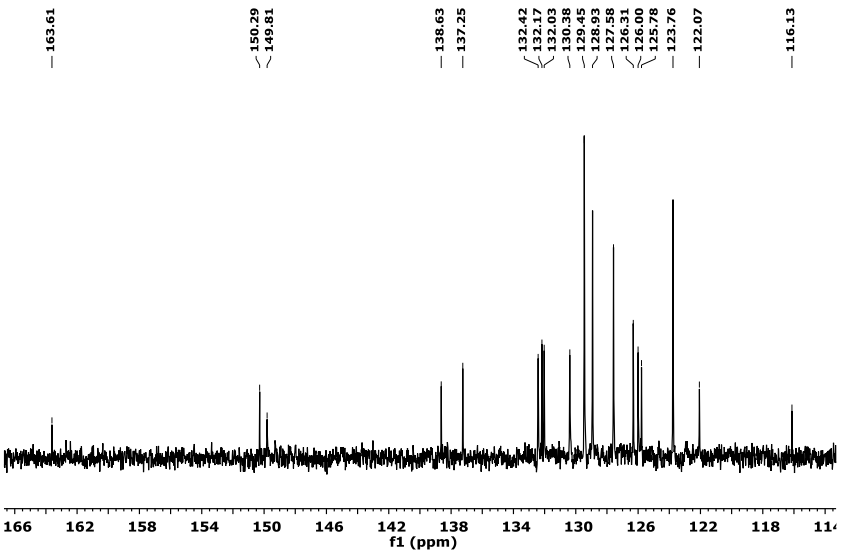
^{1}H-NMR of compound **(3c)** (300 MHz, $CDCl_3$)



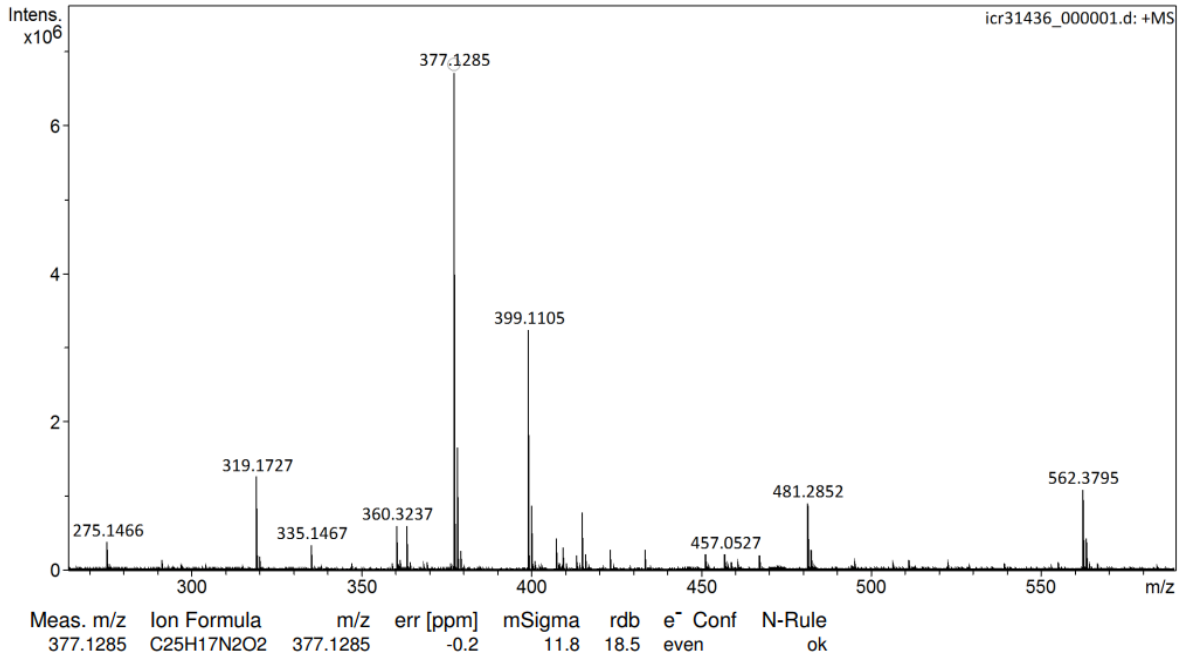
^{1}H-NMR of compound **(3c)** (300 MHz, $CDCl_3$)



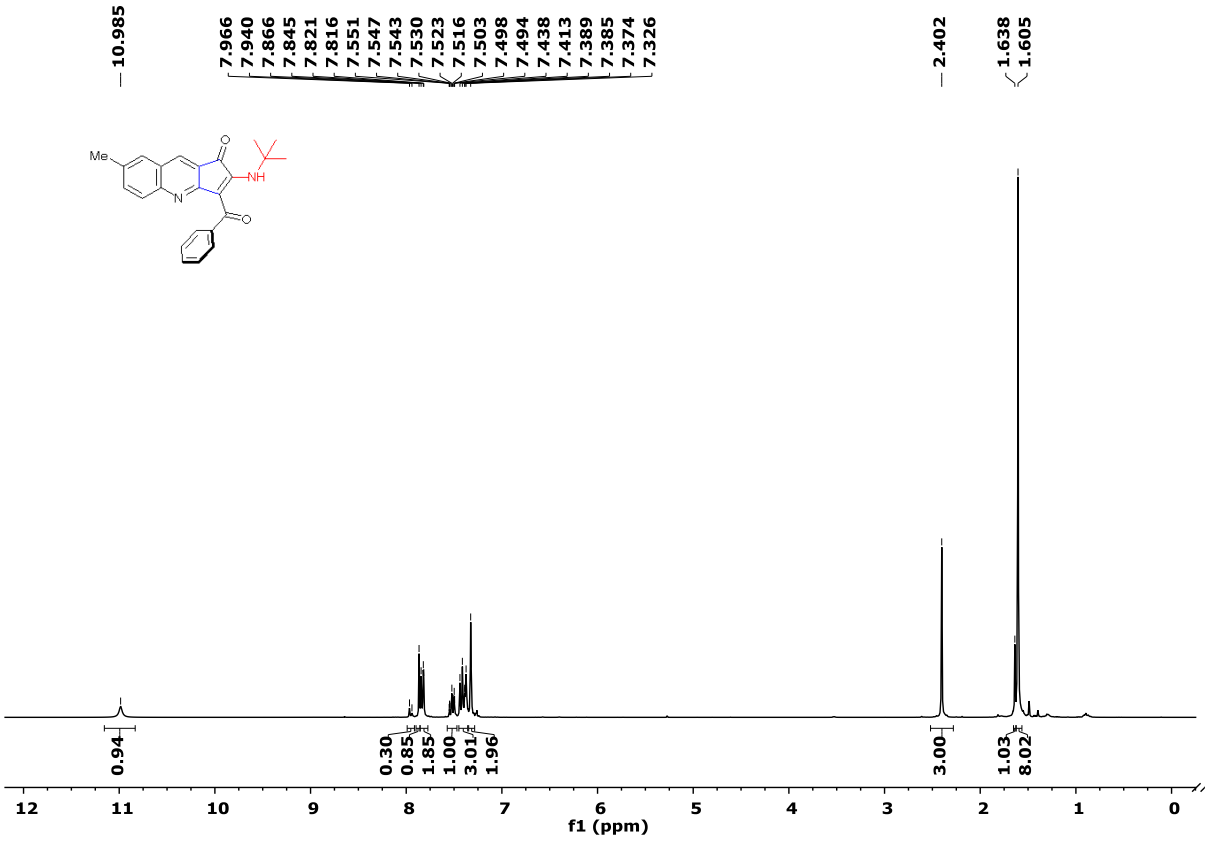
^{13}C-NMR of compound **(3c)** (75 MHz, $CDCl_3$)



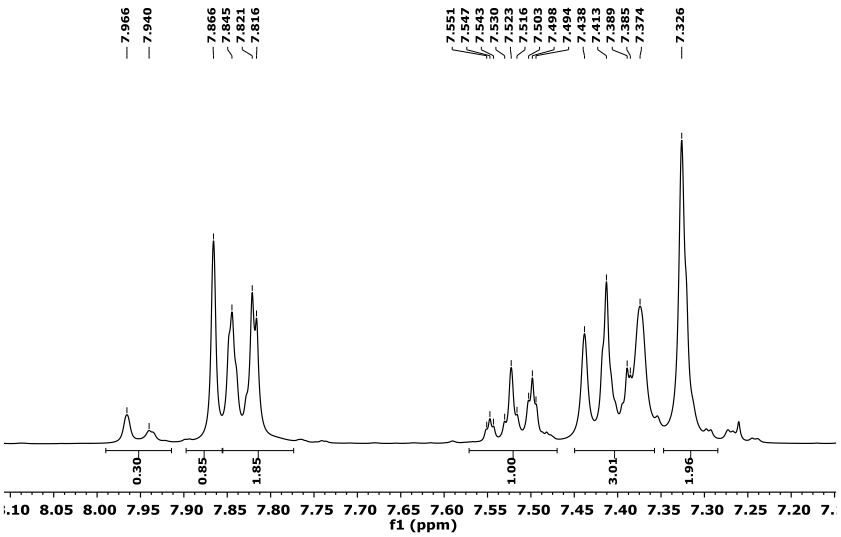
^{13}C-NMR of compound **(3c)** (75 MHz, $CDCl_3$)



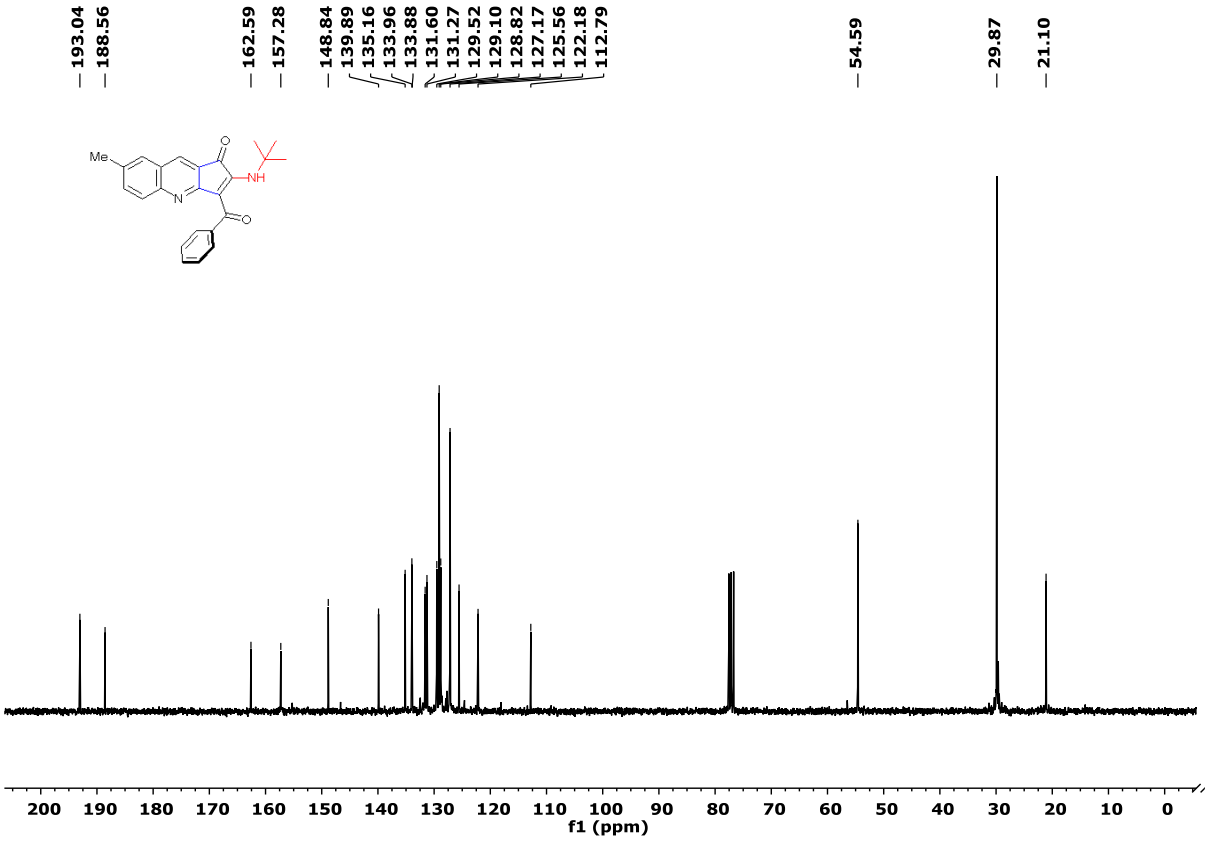
HRMS-ESI (m/z) of (**3c**)



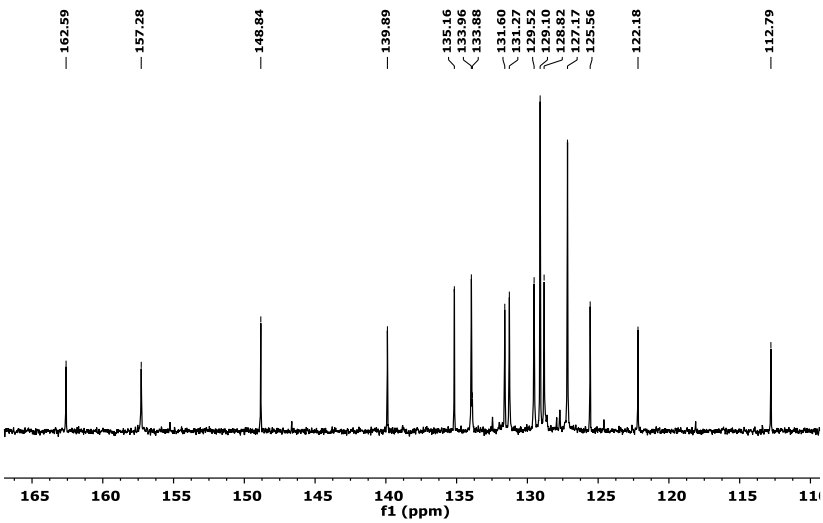
^{1}H-NMR of compound **(3d)** (300 MHz, $CDCl_3$)



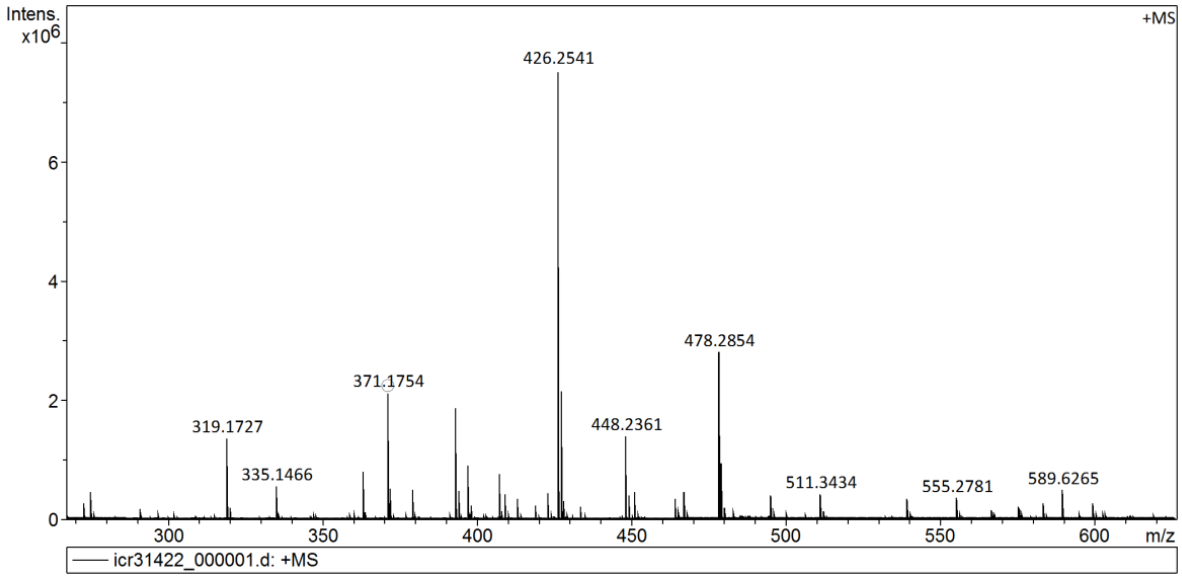
^{1}H-NMR of compound **(3d)** (300 MHz, $CDCl_3$)



^{13}C-NMR of compound **(3d)** (75 MHz, $CDCl_3$)

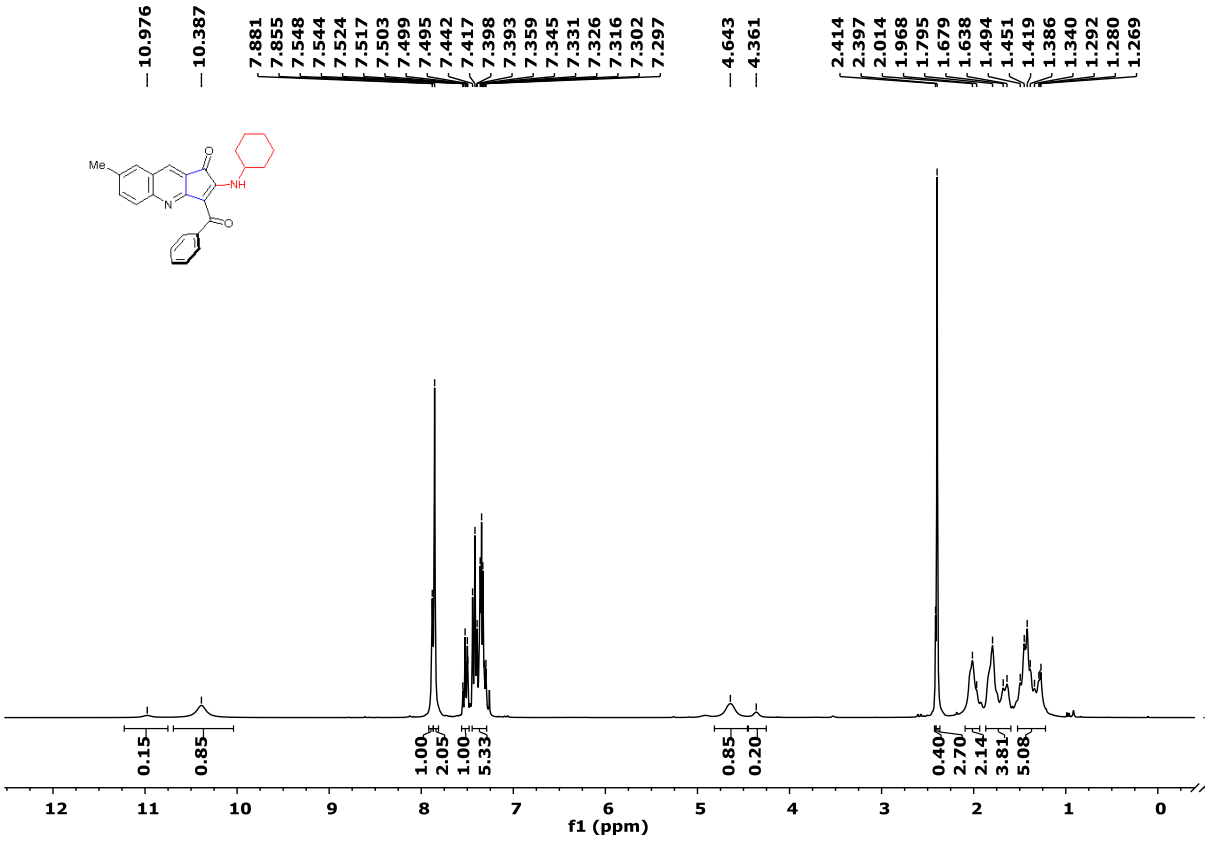


^{13}C-NMR of compound **(3d)** (75 MHz, $CDCl_3$)

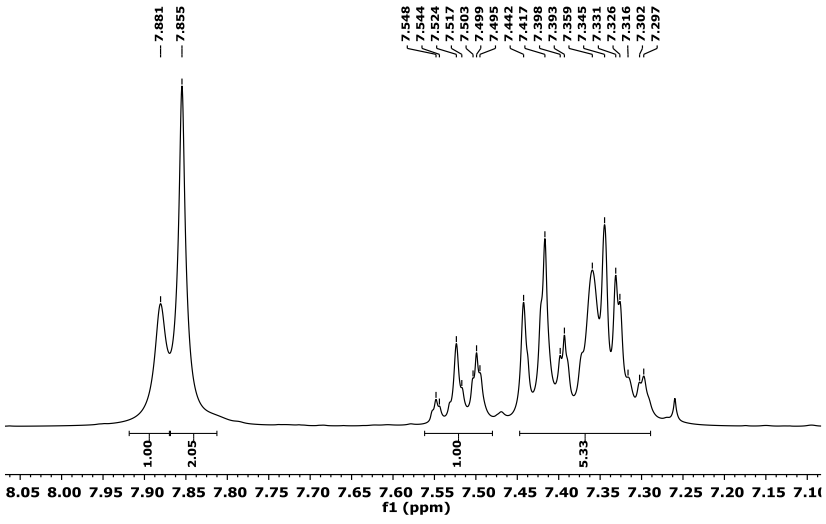


Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
371.1754	C24H23N2O2	371.1754	-0.1	18.7	14.5	even	ok

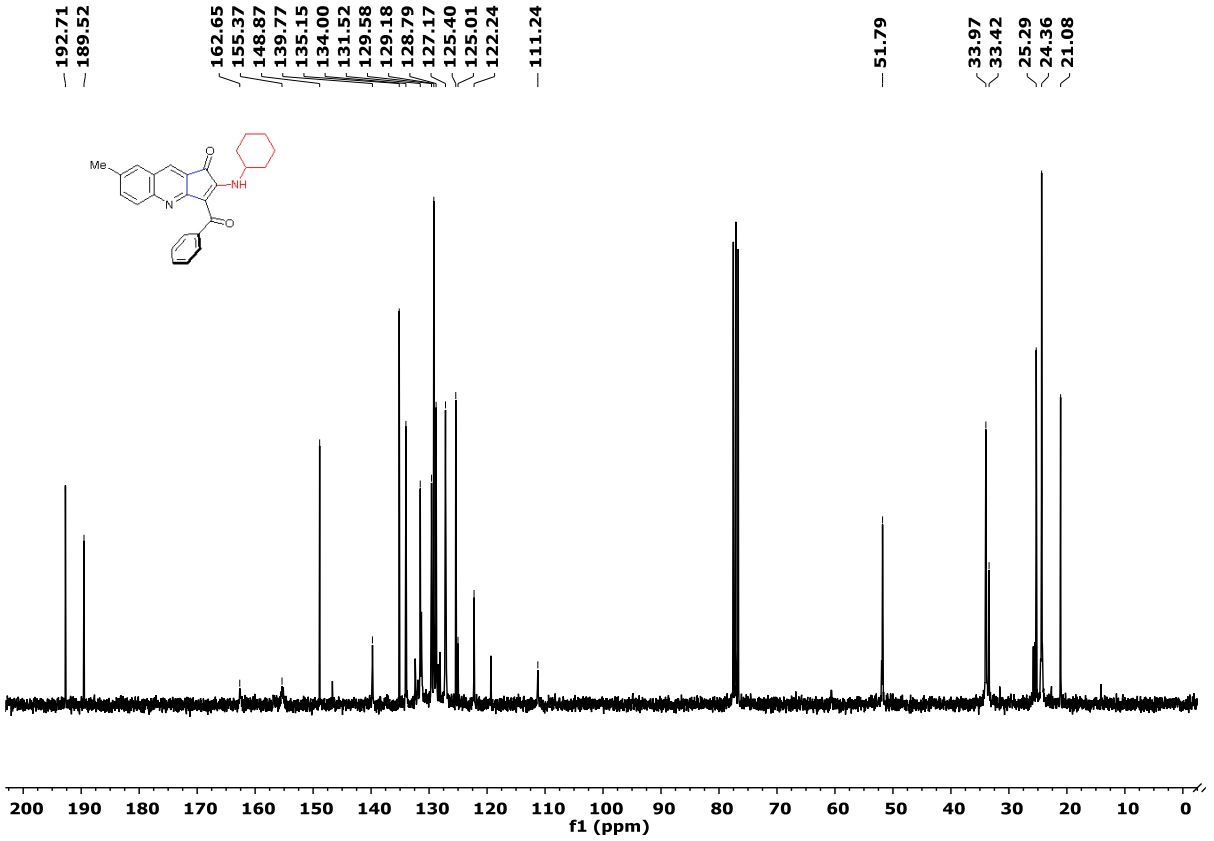
HRMS-ESI (m/z) of (**3d**)



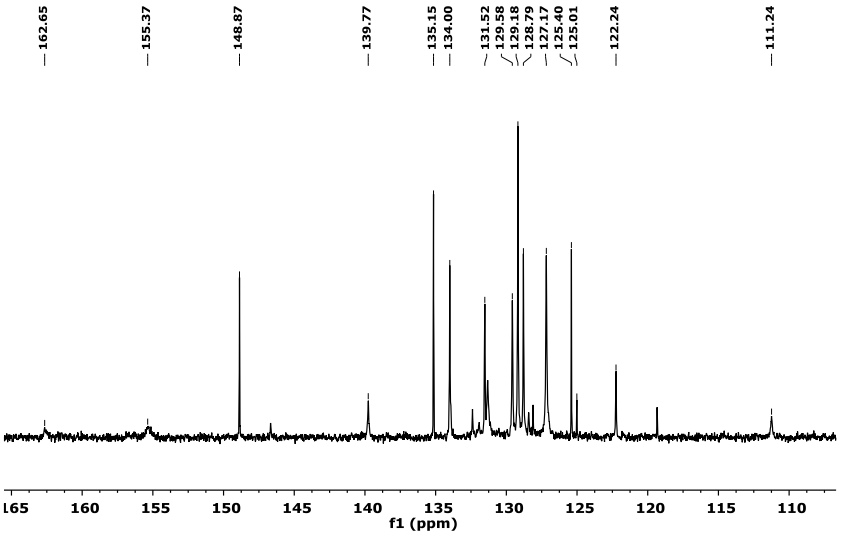
^{1}H-NMR of compound **(3e)** (300 MHz, $CDCl_3$)



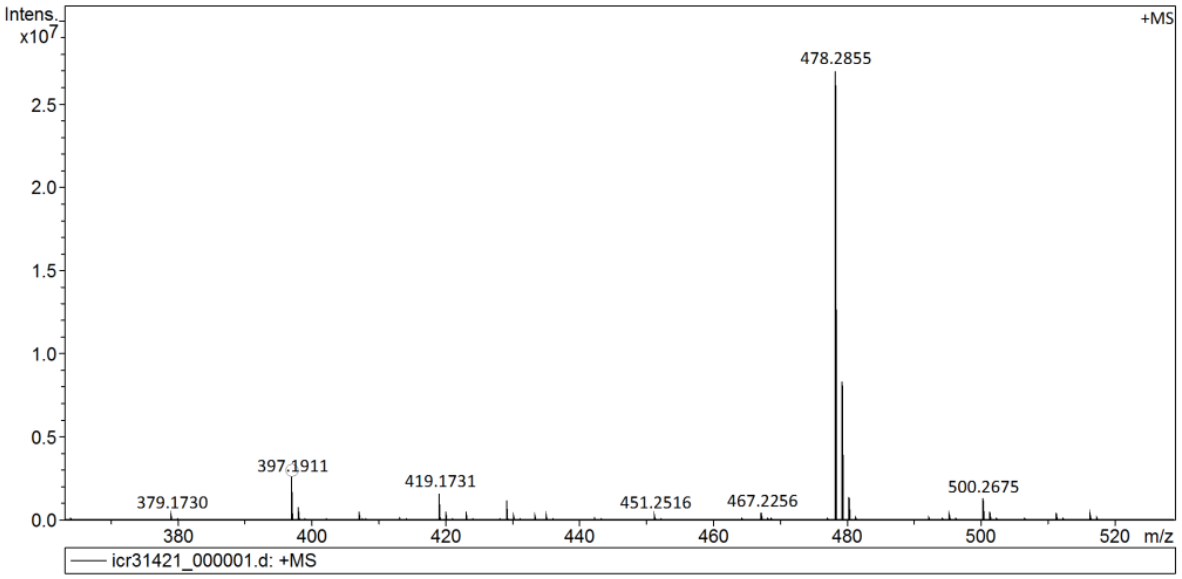
^{1}H-NMR of compound **(3e)** (300 MHz, $CDCl_3$)



^{13}C-NMR of compound **(3e)** (75 MHz, $CDCl_3$)

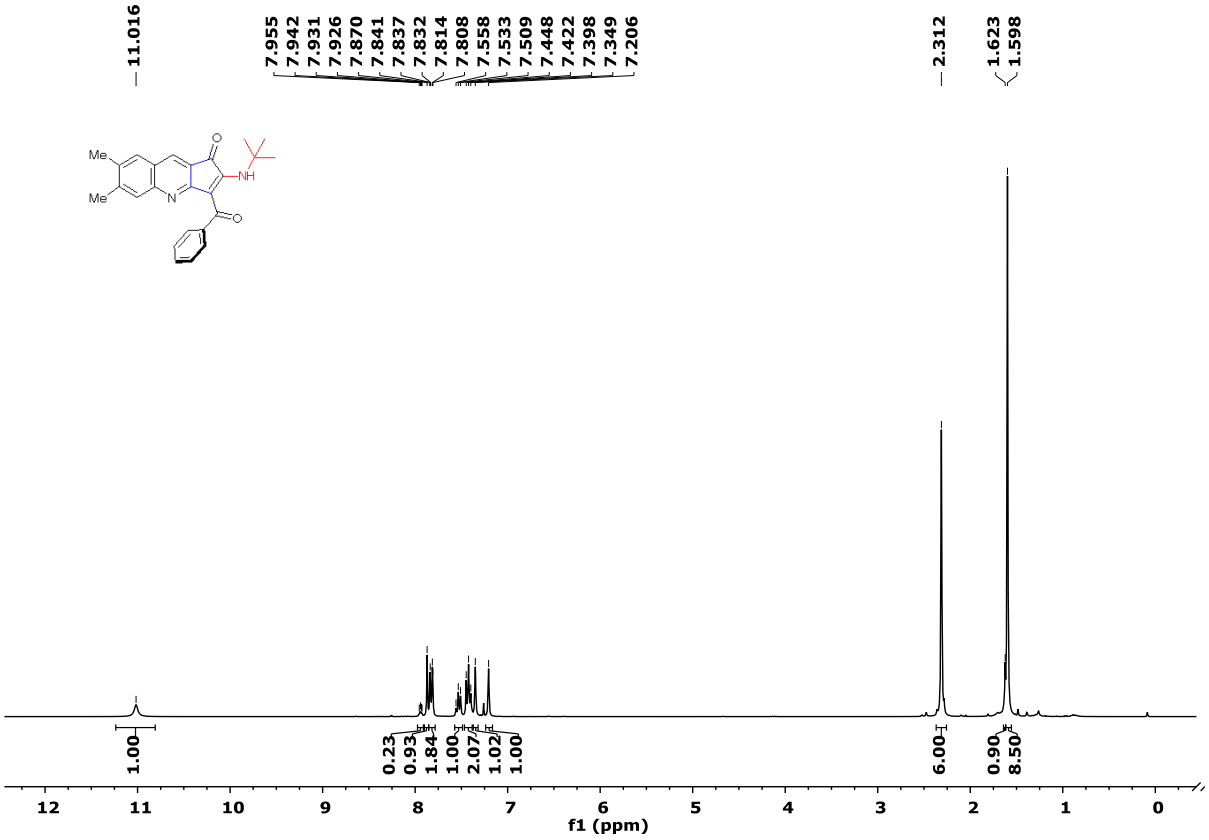


^{13}C-NMR of compound **(3e)** (75 MHz, $CDCl_3$)

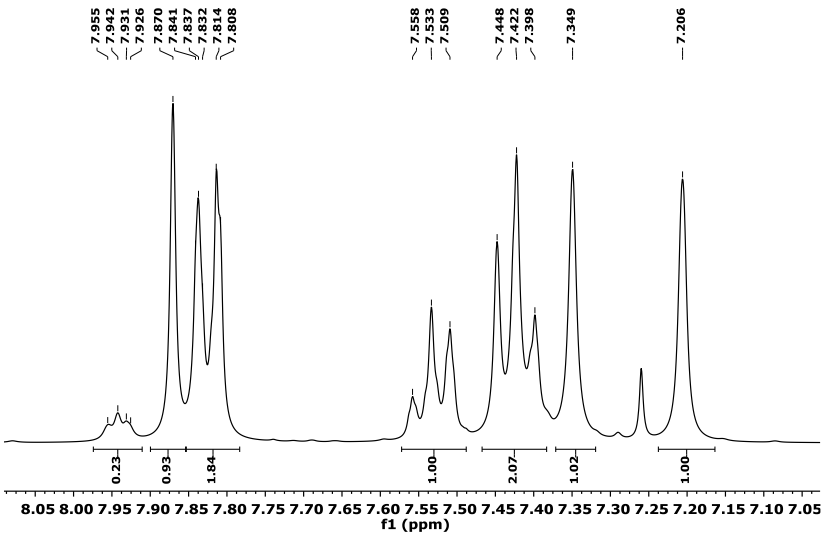


Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
397.1911	C26H25N2O2	397.1911	-0.2	17.8	15.5	even	ok

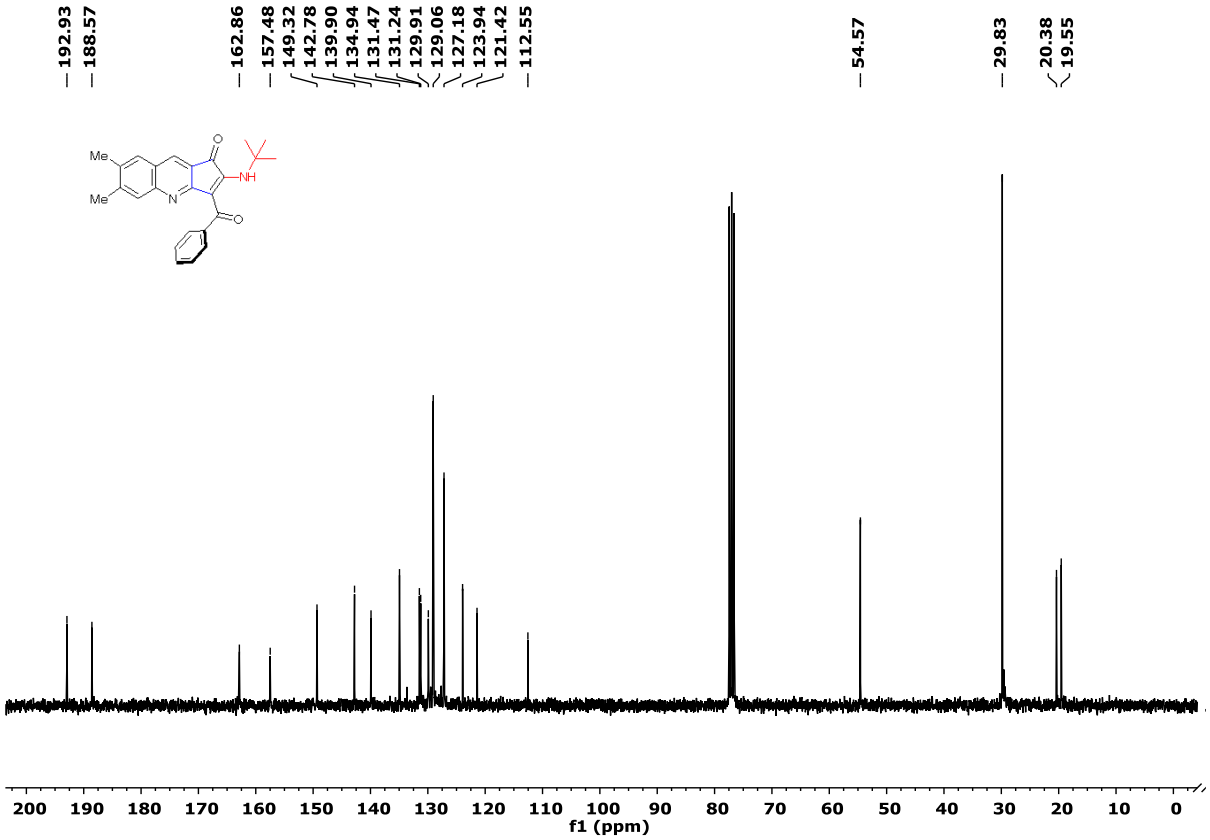
HRMS-ESI (m/z) of (**3e**)



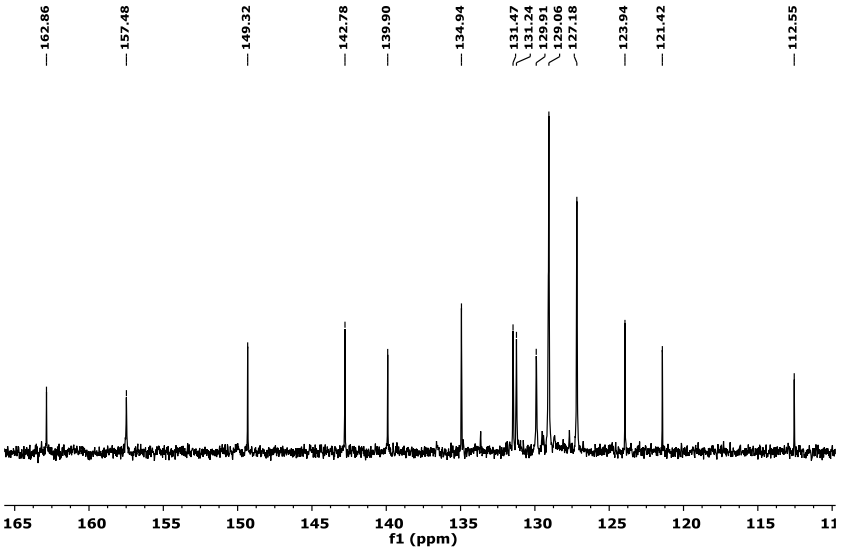
^{1}H-NMR of compound **(3f)** (300 MHz, $CDCl_3$)



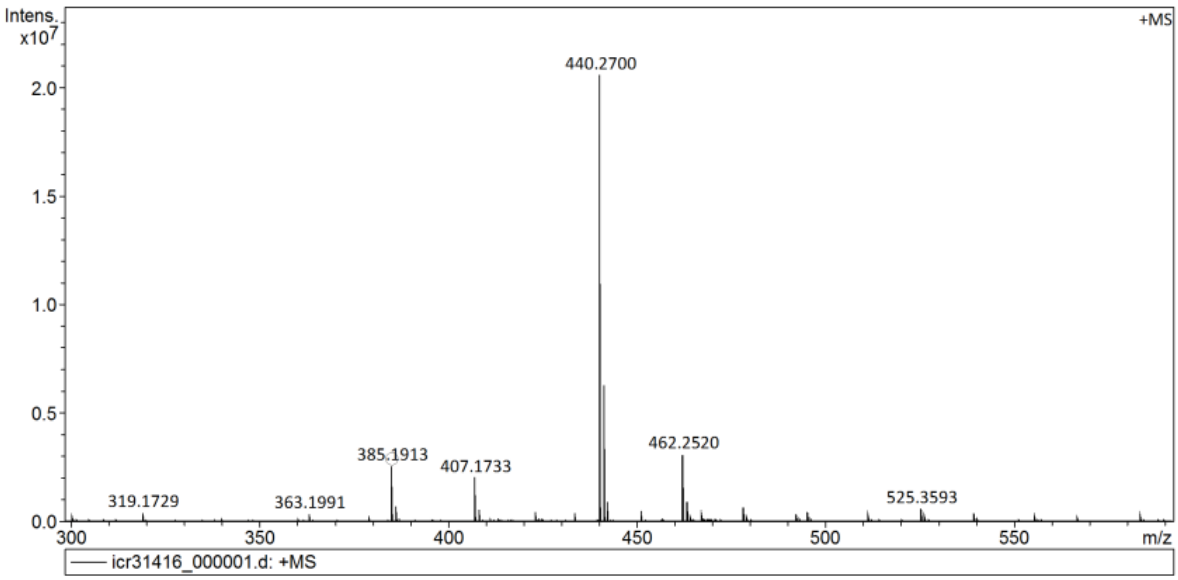
^{1}H-NMR of compound **(3f)** (300 MHz, $CDCl_3$)



^{13}C-NMR of compound **(3f)** (75 MHz, $CDCl_3$)

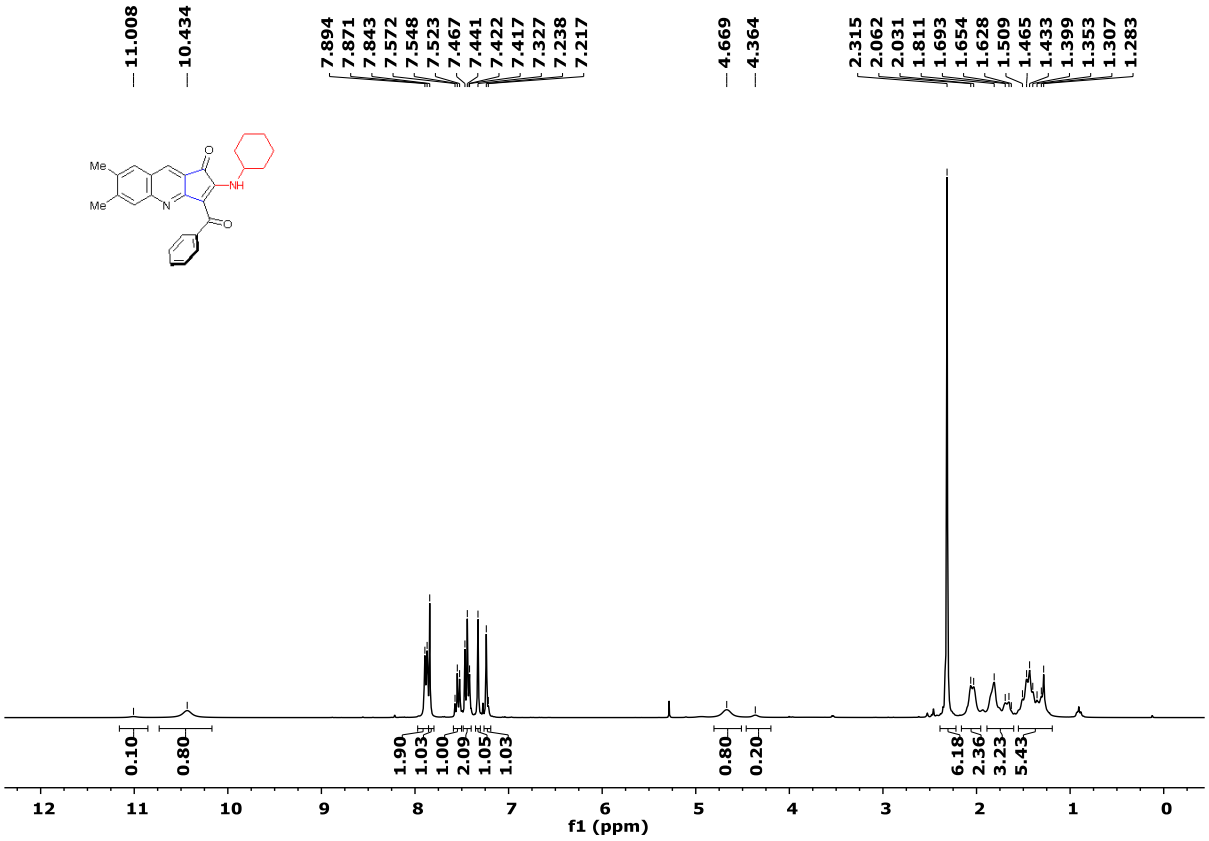


^{13}C-NMR of compound **(3f)** (75 MHz, $CDCl_3$)

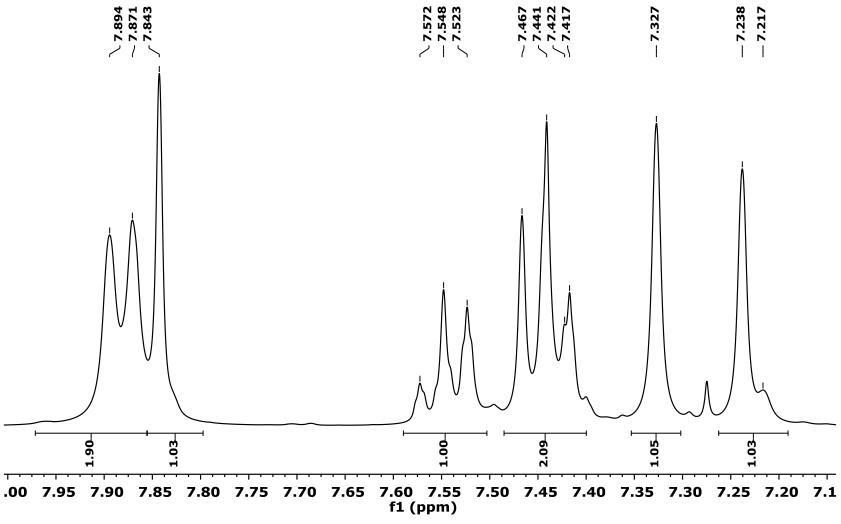


Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
385.1913	C23H23N5O	385.1897	-4.0	18.1	15.0	odd	ok
	C25H25N2O2	385.1911	-0.5	19.0	14.5	even	ok

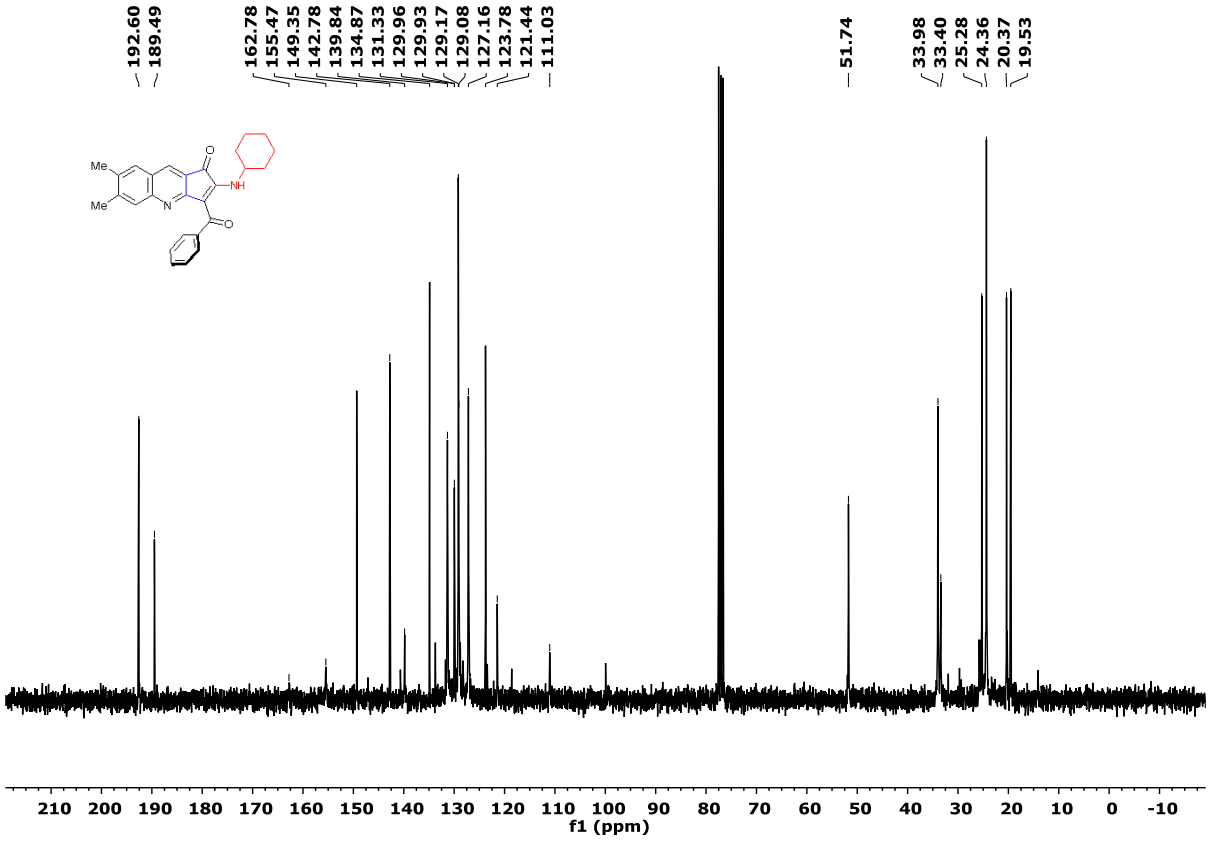
HRMS-ESI (m/z) of (**3f**)



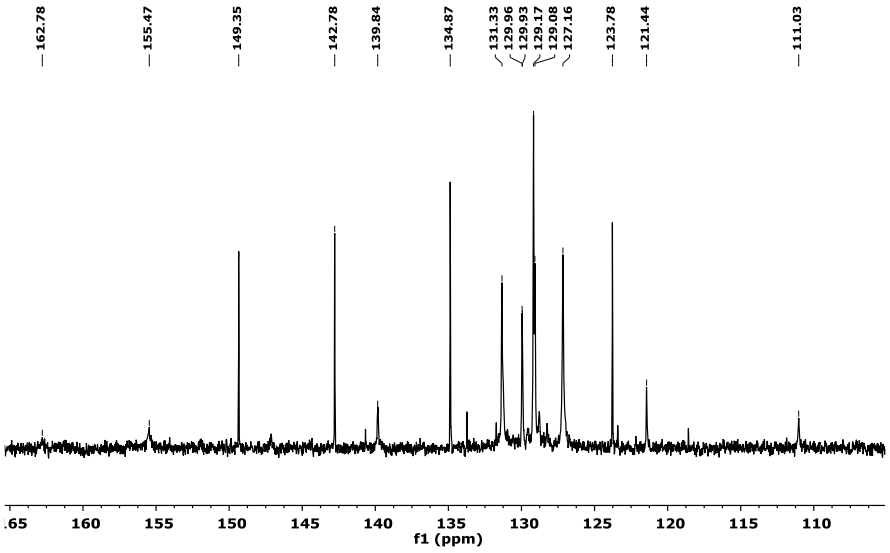
^{1}H-NMR of compound **(3g)** (300 MHz, $CDCl_3$)



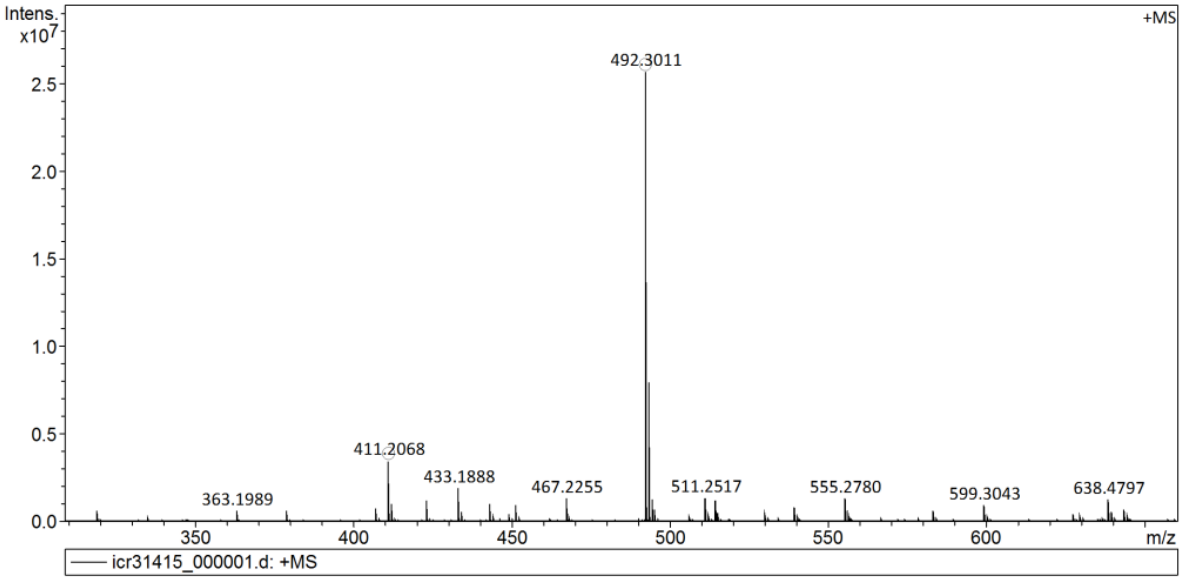
^{1}H-NMR of compound **(3g)** (300 MHz, $CDCl_3$)



^{13}C-NMR of compound **(3g)** (75 MHz, $CDCl_3$)

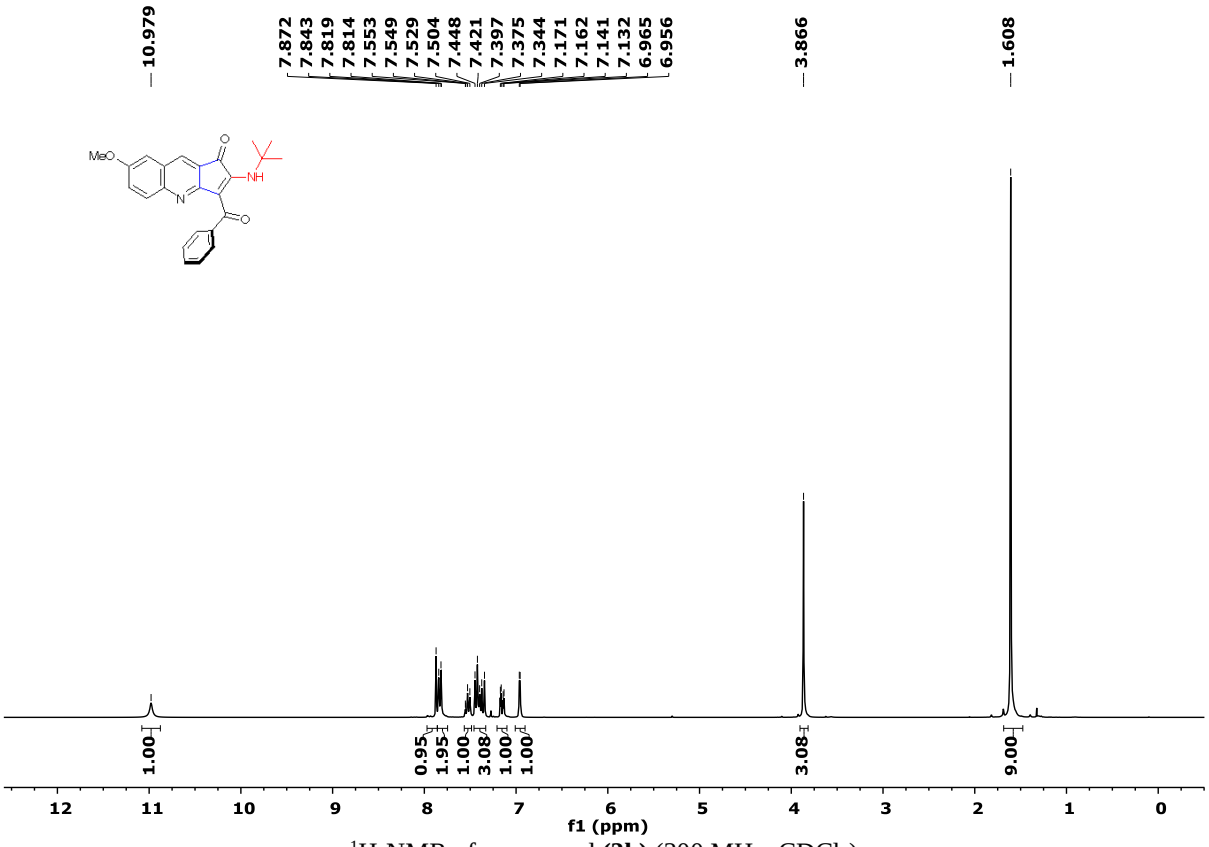


^{13}C-NMR of compound **(3g)** (75 MHz, $CDCl_3$)

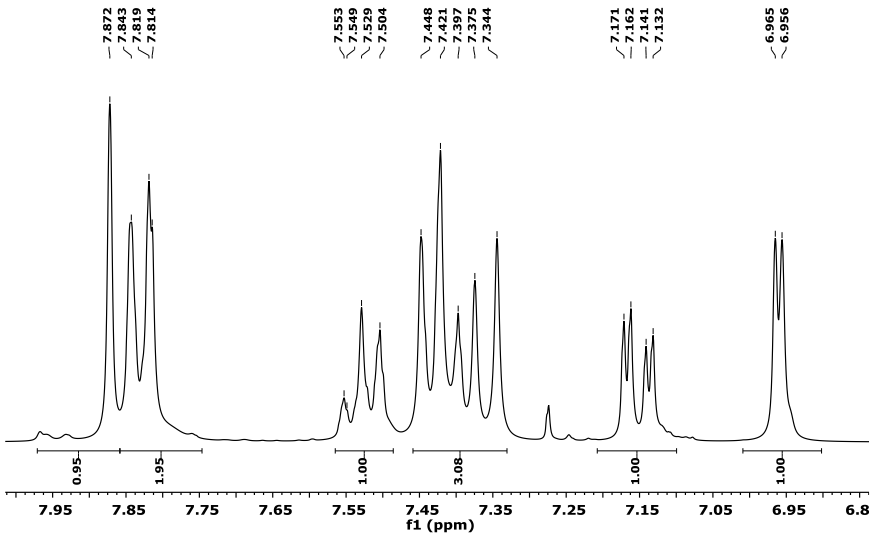


Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
411.2068	C27H27N2O2	411.2067	-0.3	18.9	15.5	even	ok
	C25H25N5O	411.2054	-3.6	21.8	16.0	odd	ok
492.3011	C31H36N6	492.2996	-3.0	14.9	17.0	odd	ok
	C33H38N3O	492.3009	-0.3	21.9	16.5	even	ok
	C21H42N5O8	492.3028	3.5	36.2	3.5	even	ok
	C35H40O2	492.3023	2.5	36.3	16.0	odd	ok

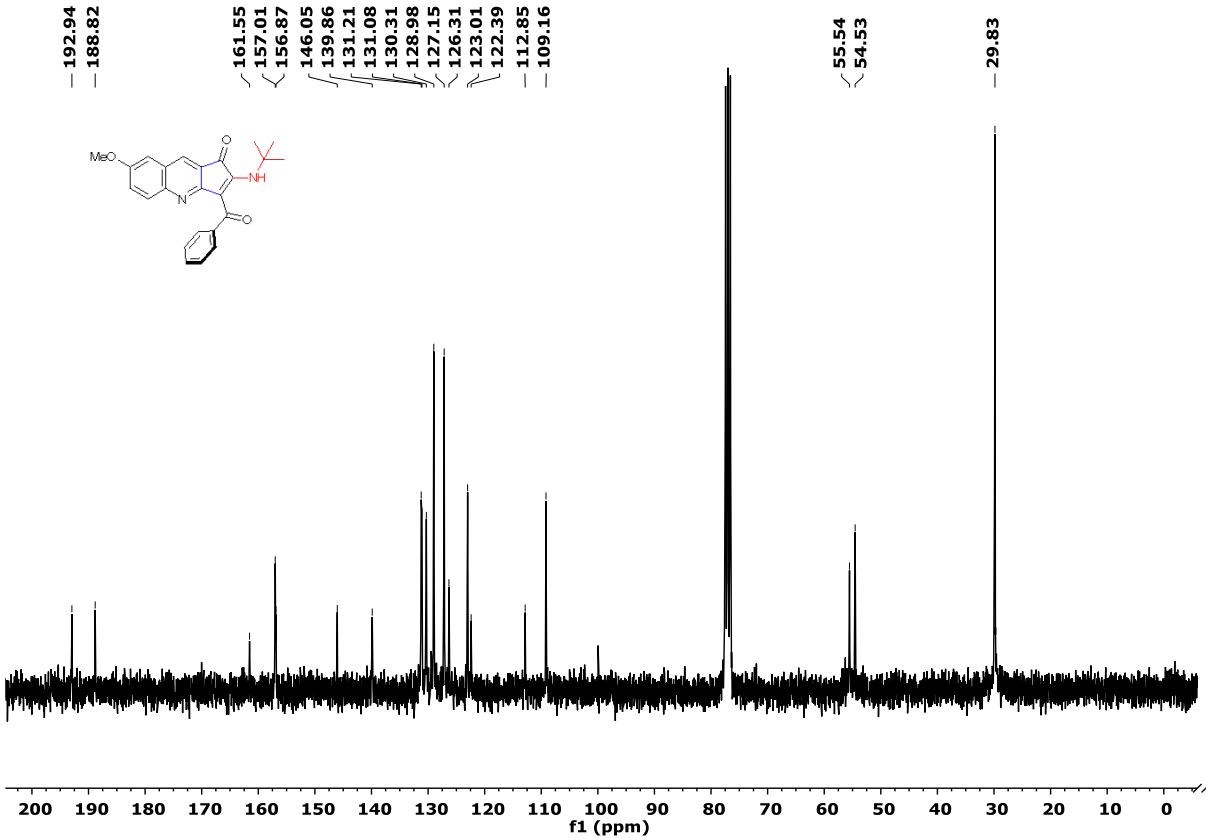
HRMS-ESI (m/z) of (**3g**)



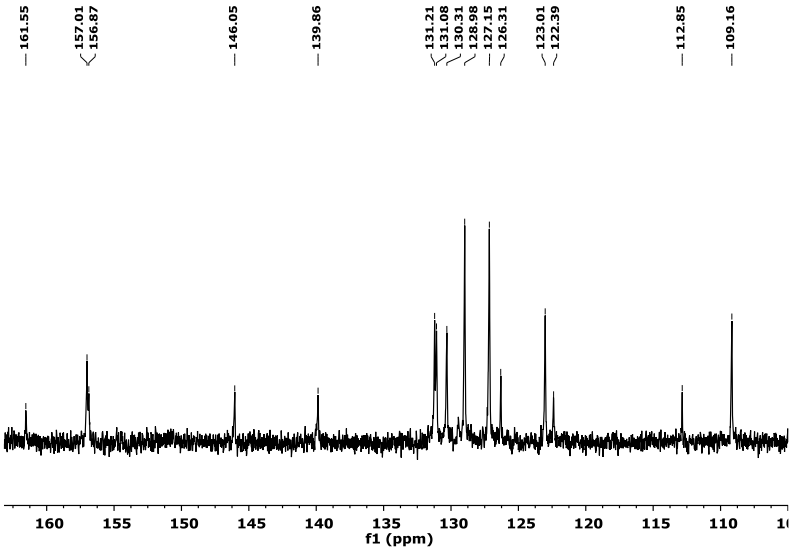
^{1}H-NMR of compound **(3h)** (300 MHz, $CDCl_3$)



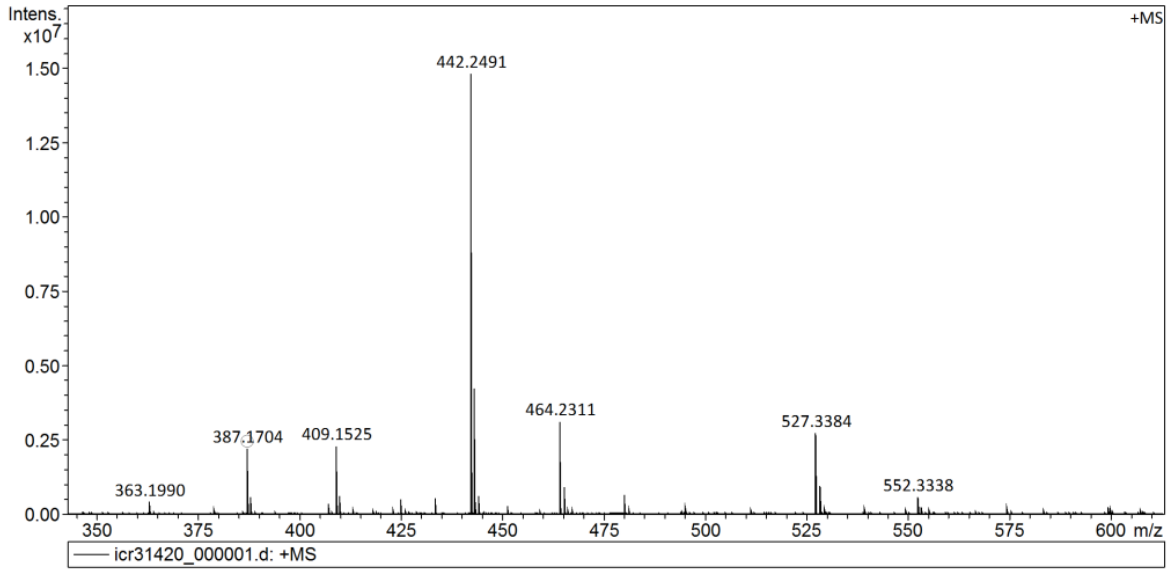
^{1}H-NMR of compound **(3h)** (300 MHz, $CDCl_3$)



^{13}C-NMR of compound **(3h)** (75 MHz, $CDCl_3$)

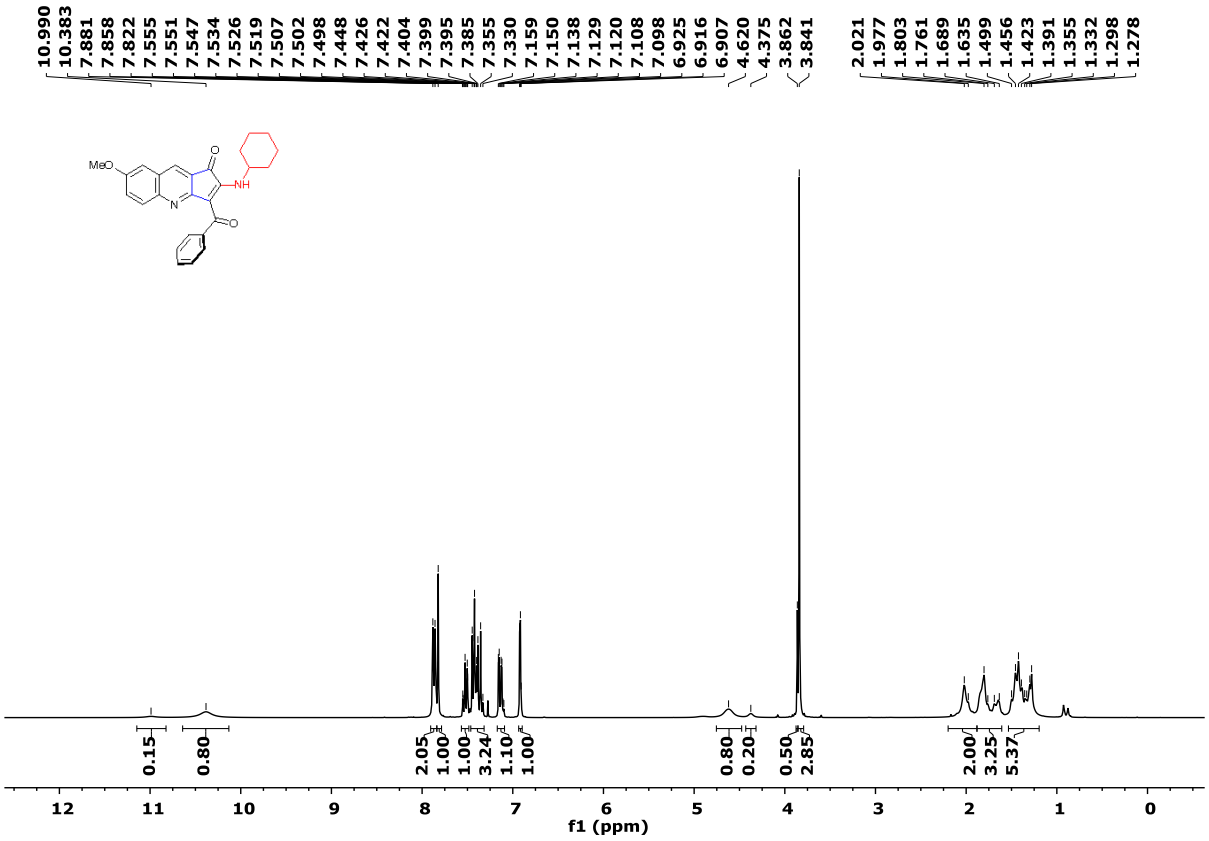


^{13}C-NMR of compound **(3h)** (75 MHz, $CDCl_3$)

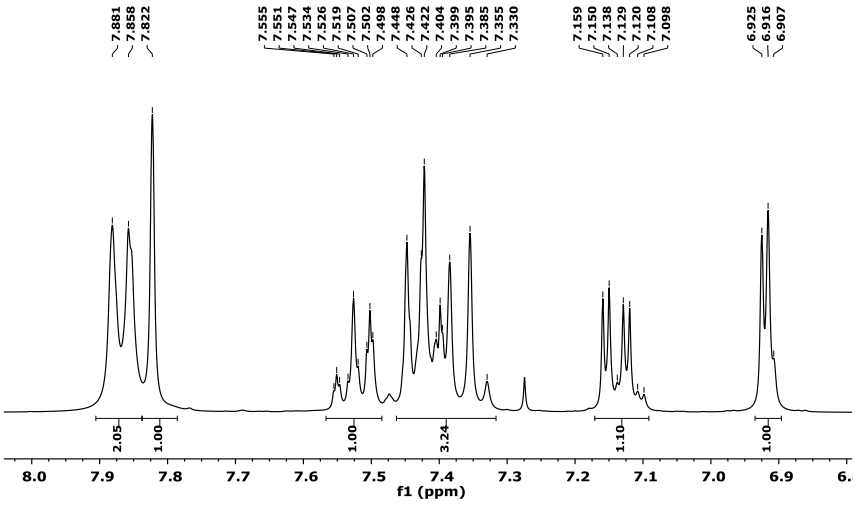


Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
387.1704	C24H23N2O3	387.1703	-0.3	15.4	14.5	even	ok

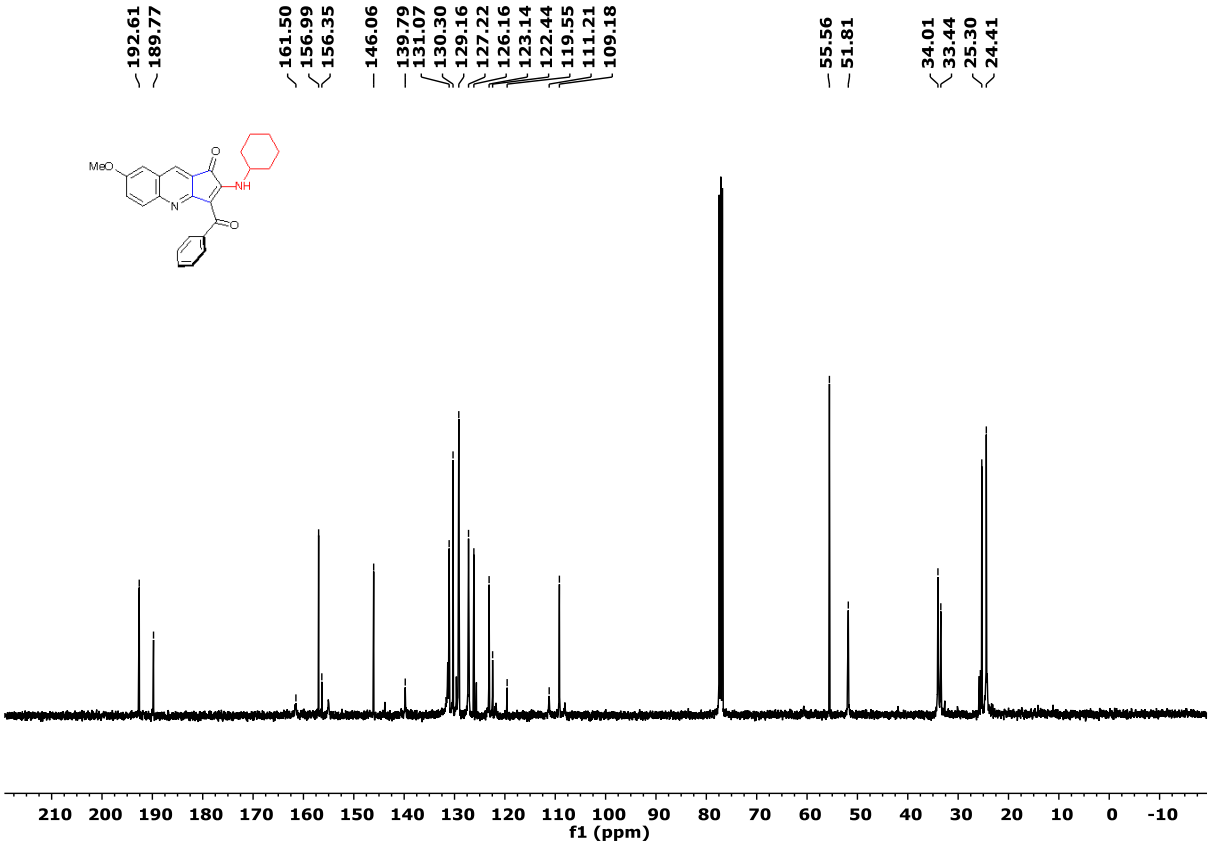
HRMS-ESI (m/z) of (**3h**)



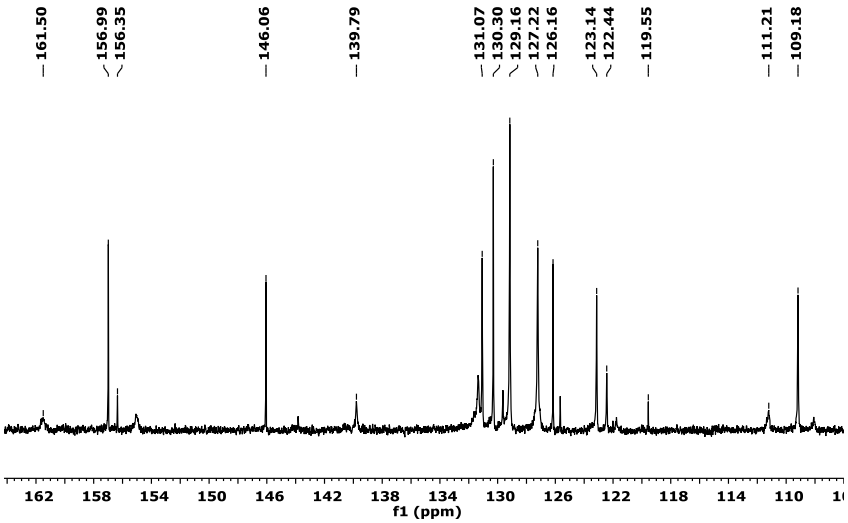
^{1}H-NMR of compound **(3i)** (300 MHz, $CDCl_3$)



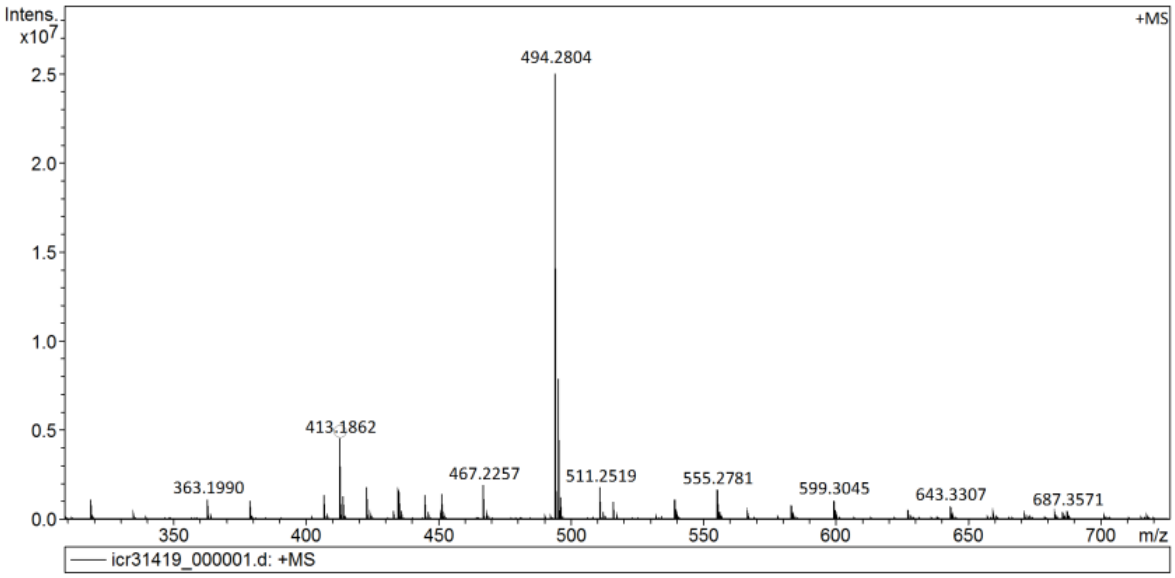
^{1}H-NMR of compound **(3i)** (300 MHz, $CDCl_3$)



^{13}C-NMR of compound **(3i)** (100 MHz, $CDCl_3$)

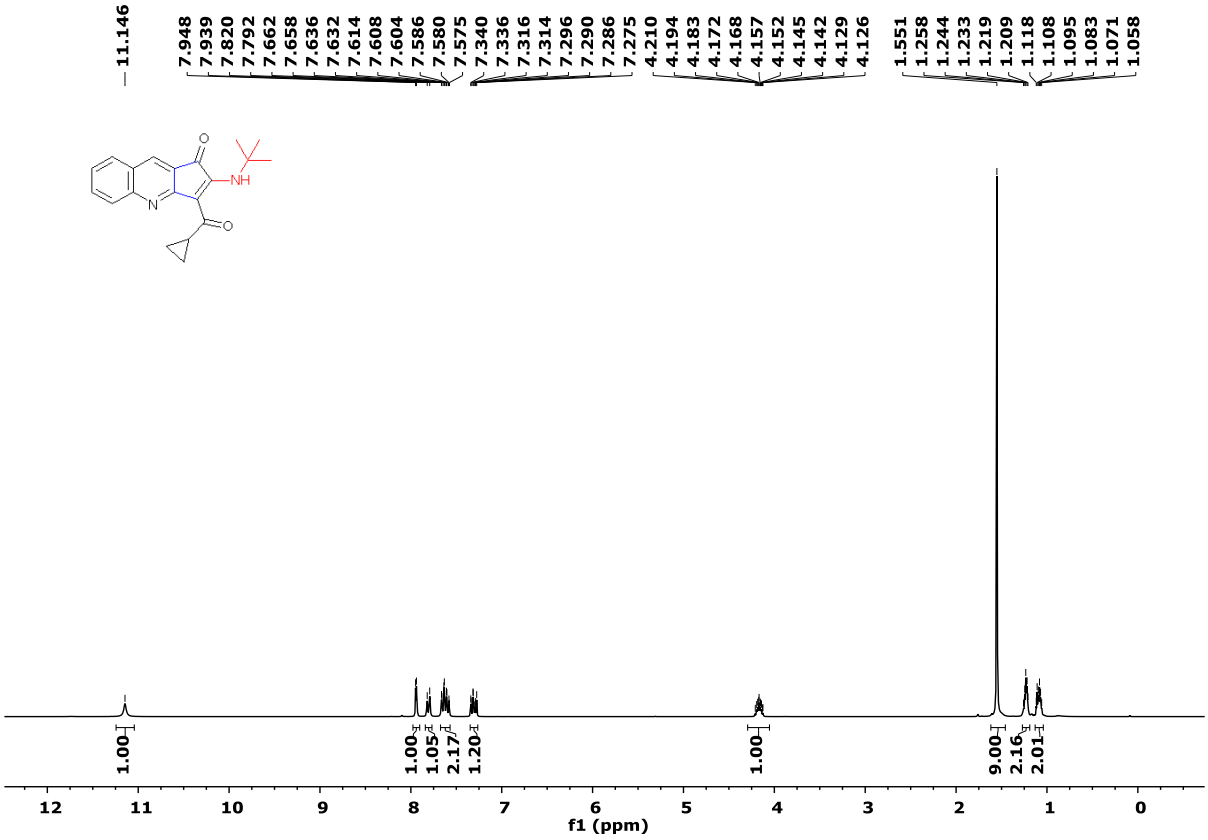


^{13}C-NMR of compound **(3i)** (100 MHz, $CDCl_3$)

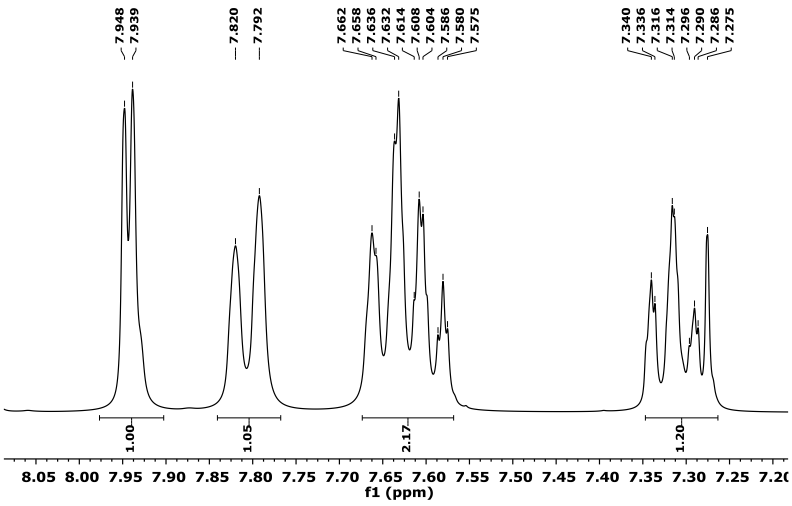


Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
413.1862	C26H25N2O3	413.1860	-0.5	17.8	15.5	even	ok

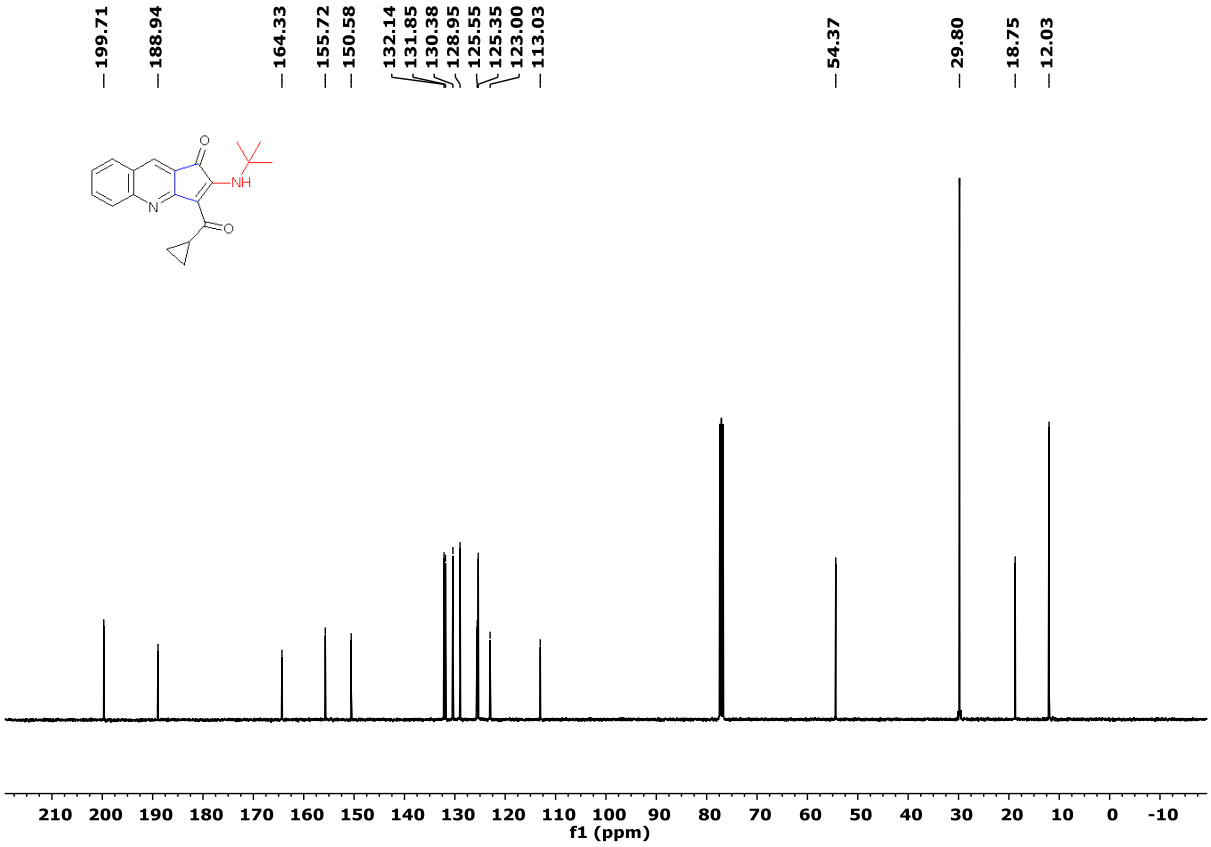
HRMS-ESI (m/z) of (**3i**)



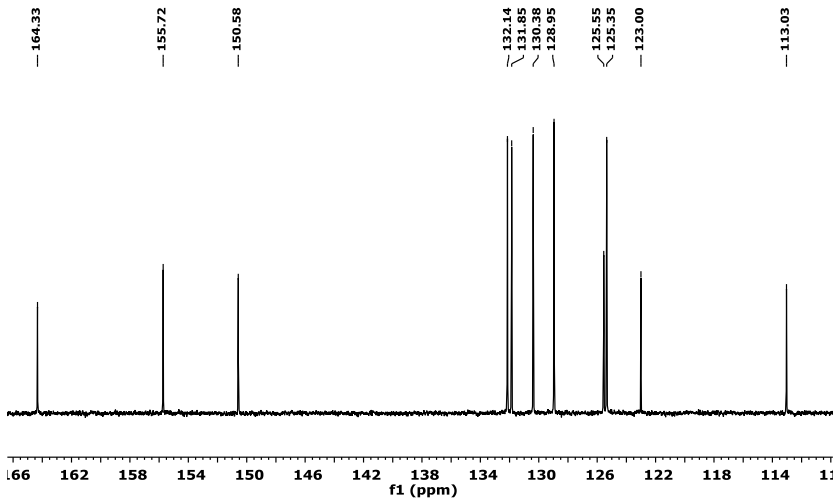
^{1}H-NMR of compound **(3j)** (300 MHz, $CDCl_3$)



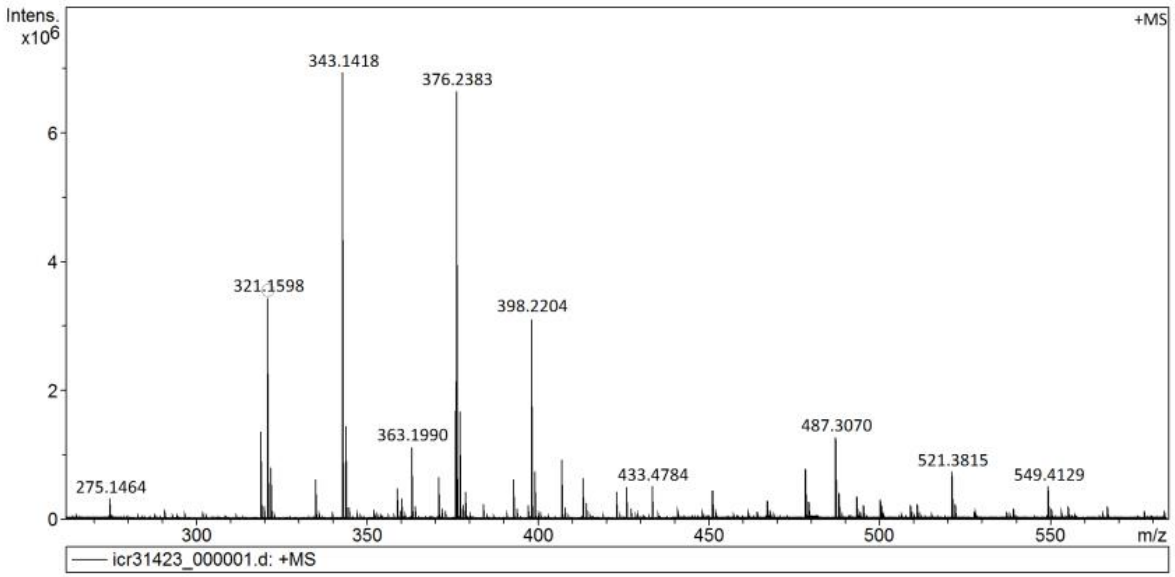
^{1}H-NMR of compound **(3j)** (300 MHz, $CDCl_3$)



^{13}C-NMR of compound **(3j)** (100 MHz, $CDCl_3$)

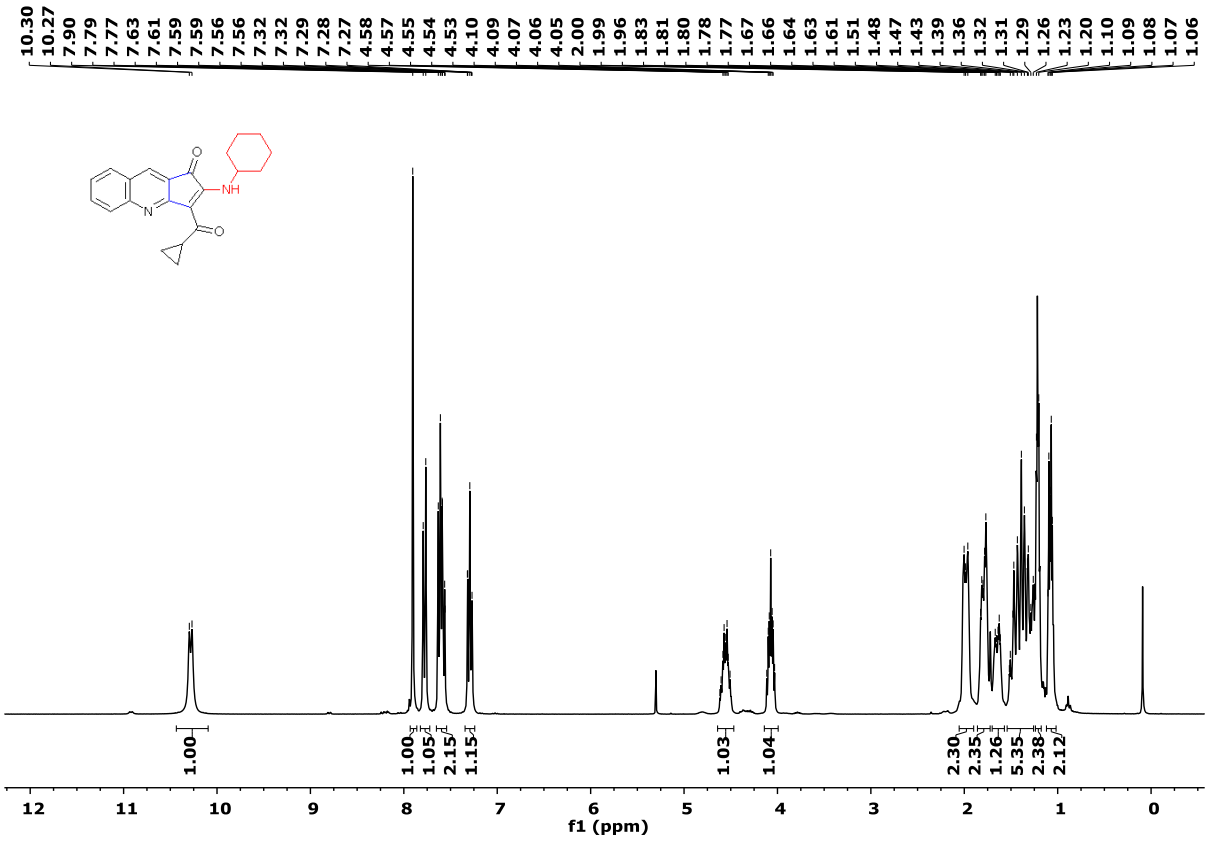


^{13}C-NMR of compound **(3j)** (100 MHz, $CDCl_3$)

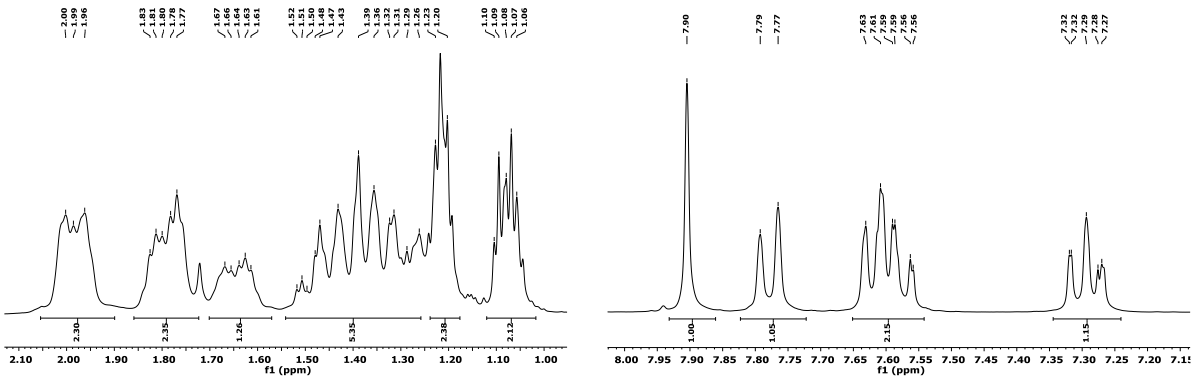


Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
321.1598	C20H21N2O2	321.1598	-0.1	15.0	11.5	even	ok

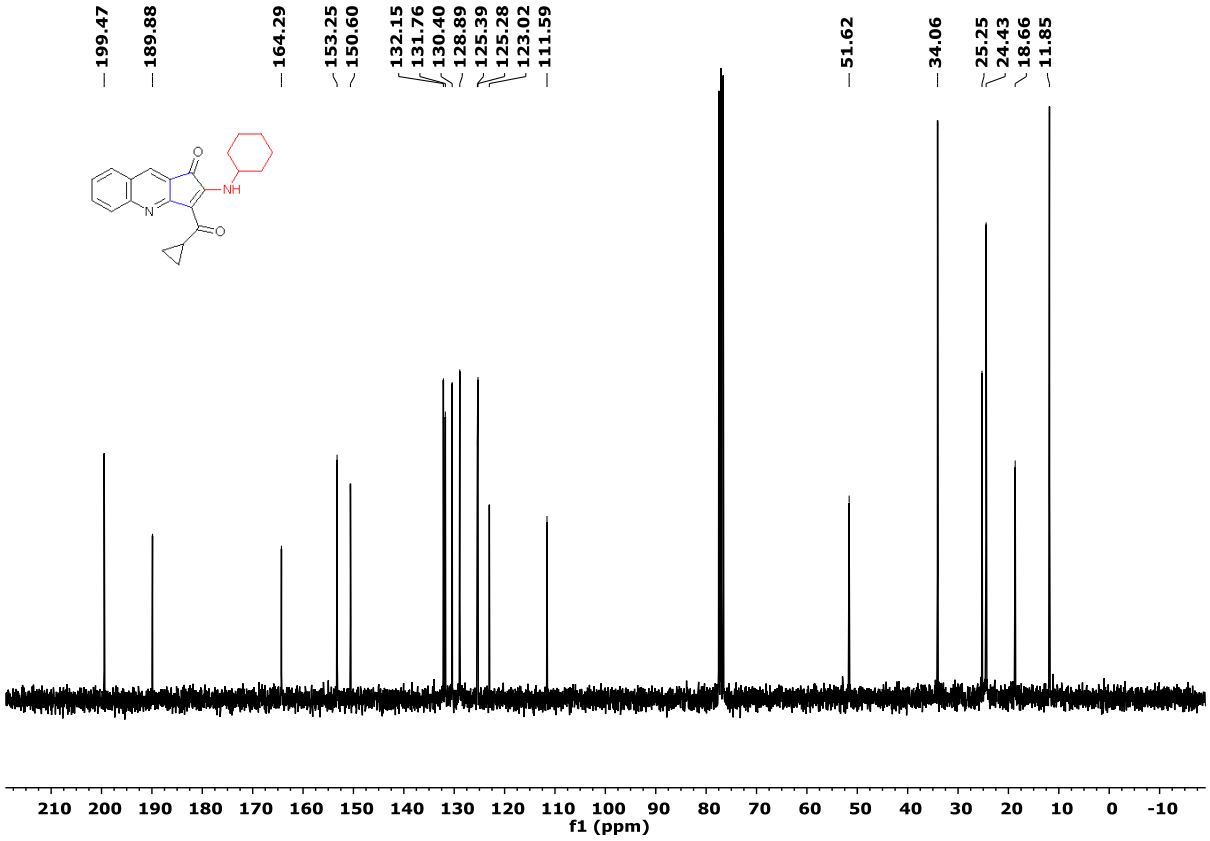
HRMS-ESI (m/z) of (**3j**)



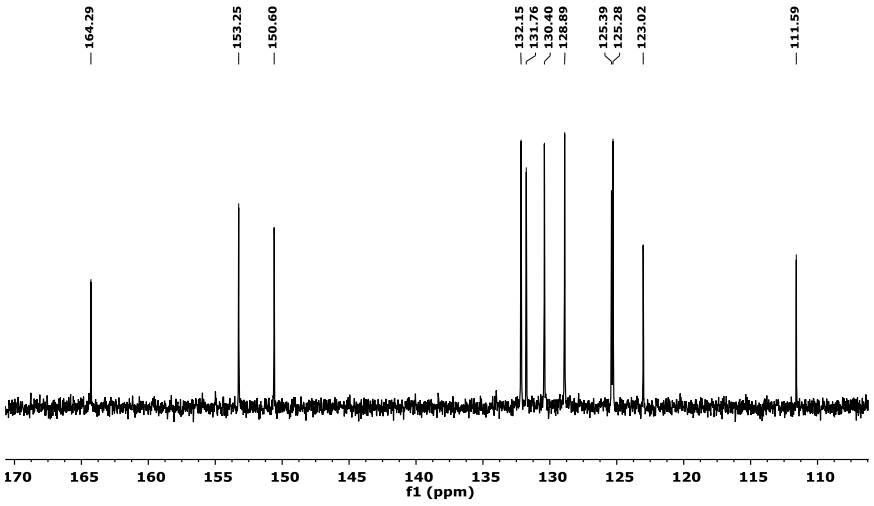
^{1}H-NMR of compound **(3k)** (300 MHz, $CDCl_3$)



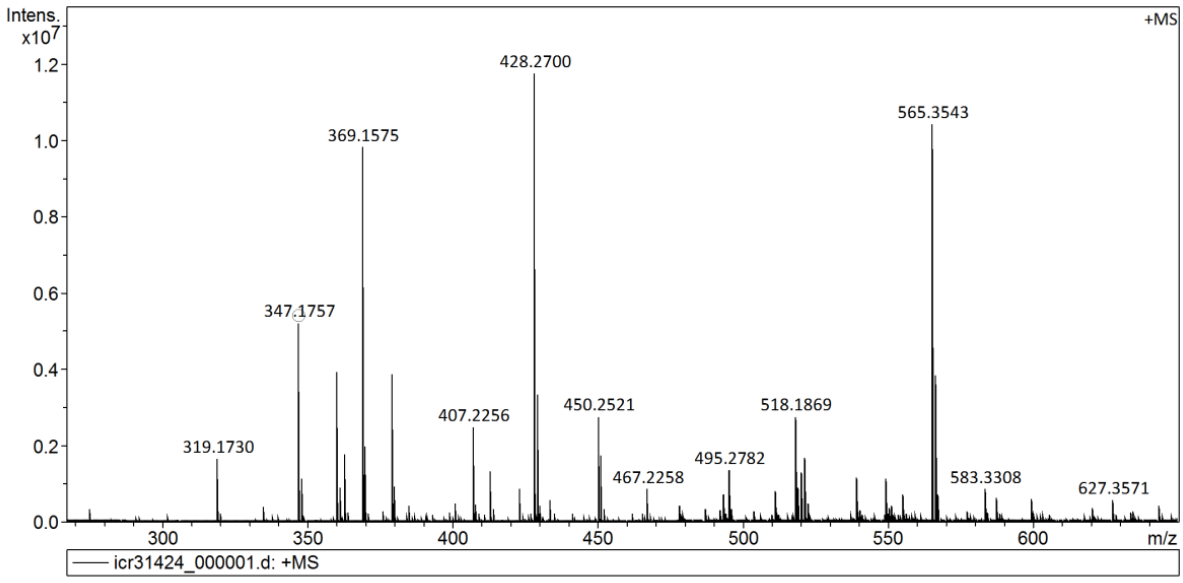
^{1}H-NMR of compound **(3k)** (300 MHz, $CDCl_3$)



^{13}C-NMR of compound **(3k)** (75 MHz, $CDCl_3$)

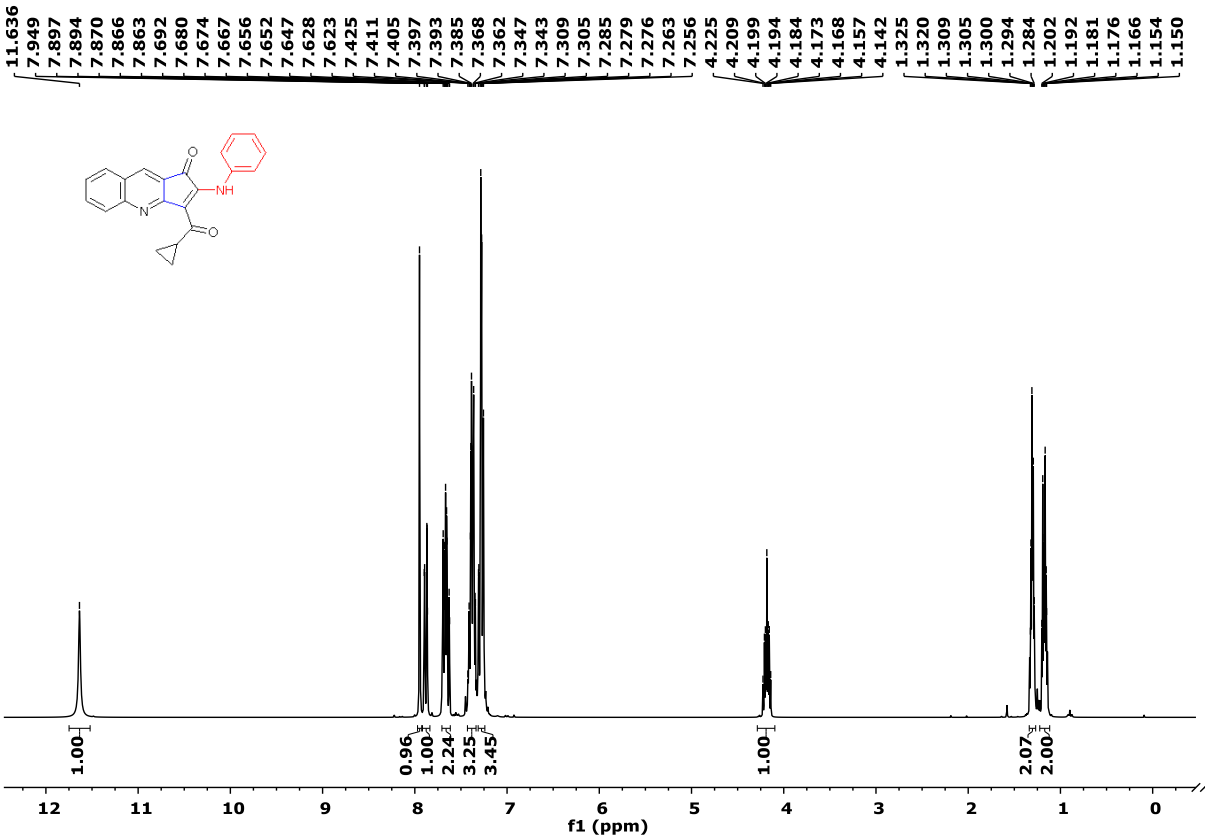


^{13}C-NMR of compound **(3k)** (75 MHz, $CDCl_3$)

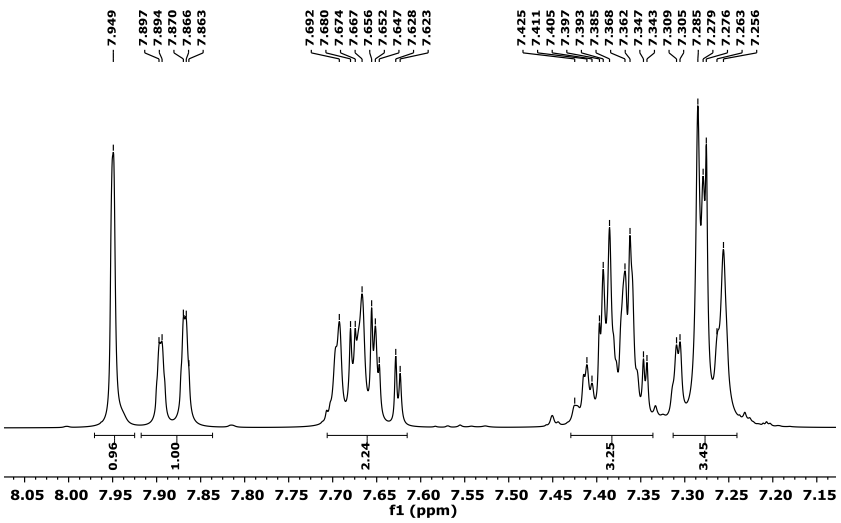


Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
347.1757	C22H23N2O2	347.1754	-0.7	18.4	12.5	even	ok

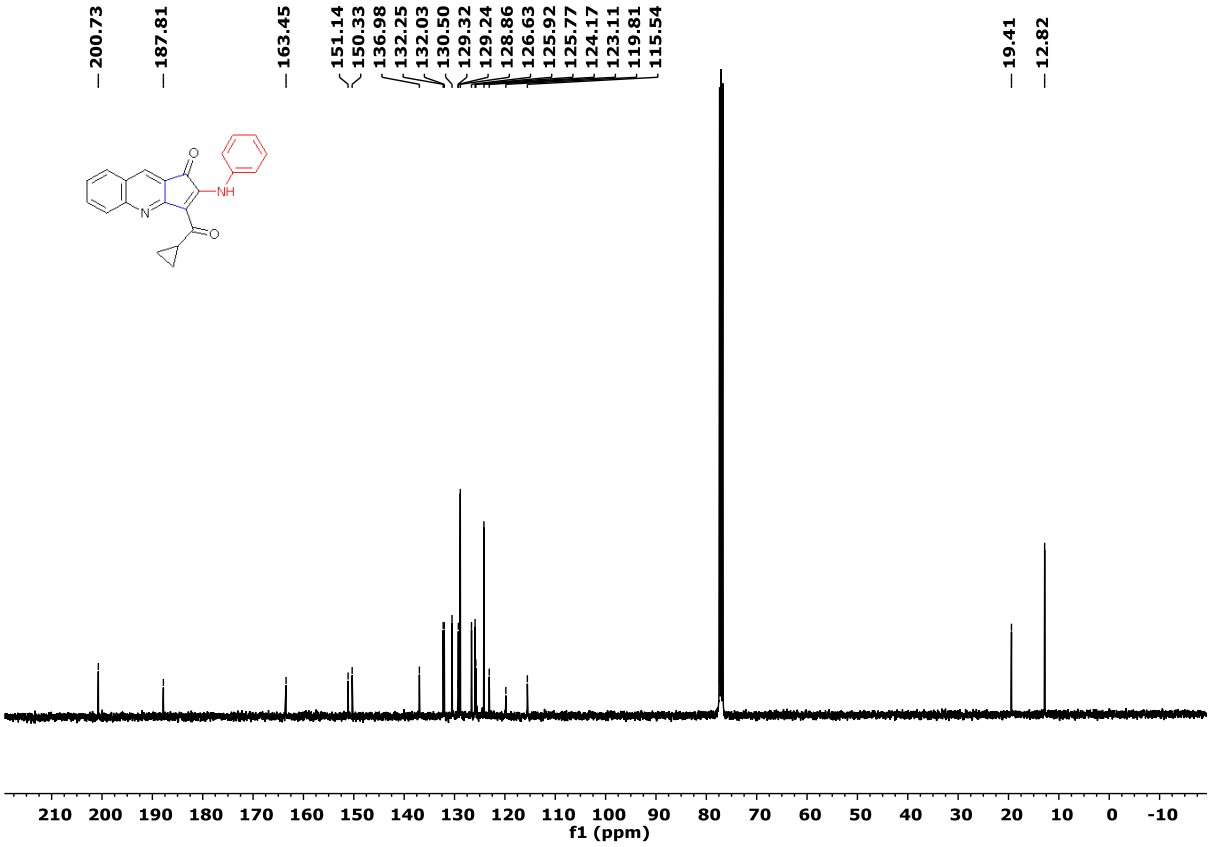
HRMS-ESI (m/z) of (**3k**)



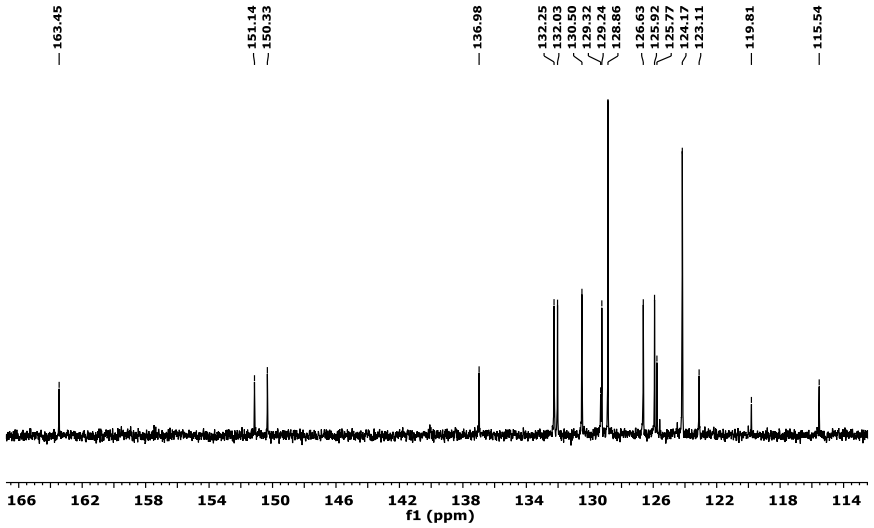
^{1}H-NMR of compound **(3l)** (300 MHz, $CDCl_3$)



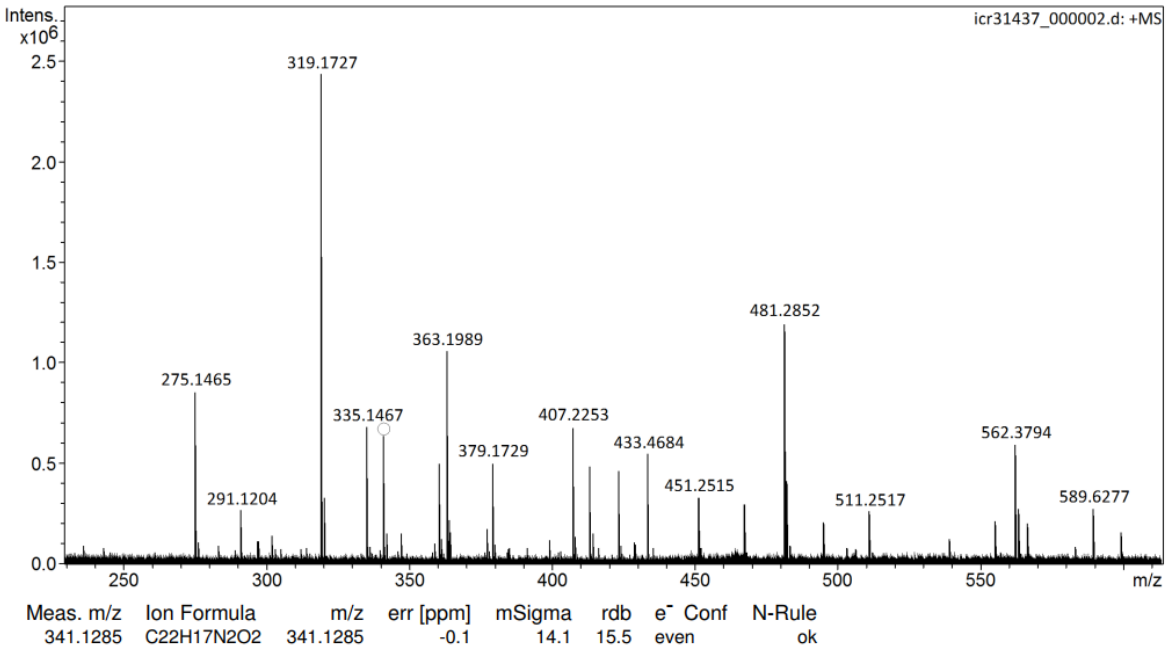
^{1}H-NMR of compound **(3l)** (300 MHz, $CDCl_3$)



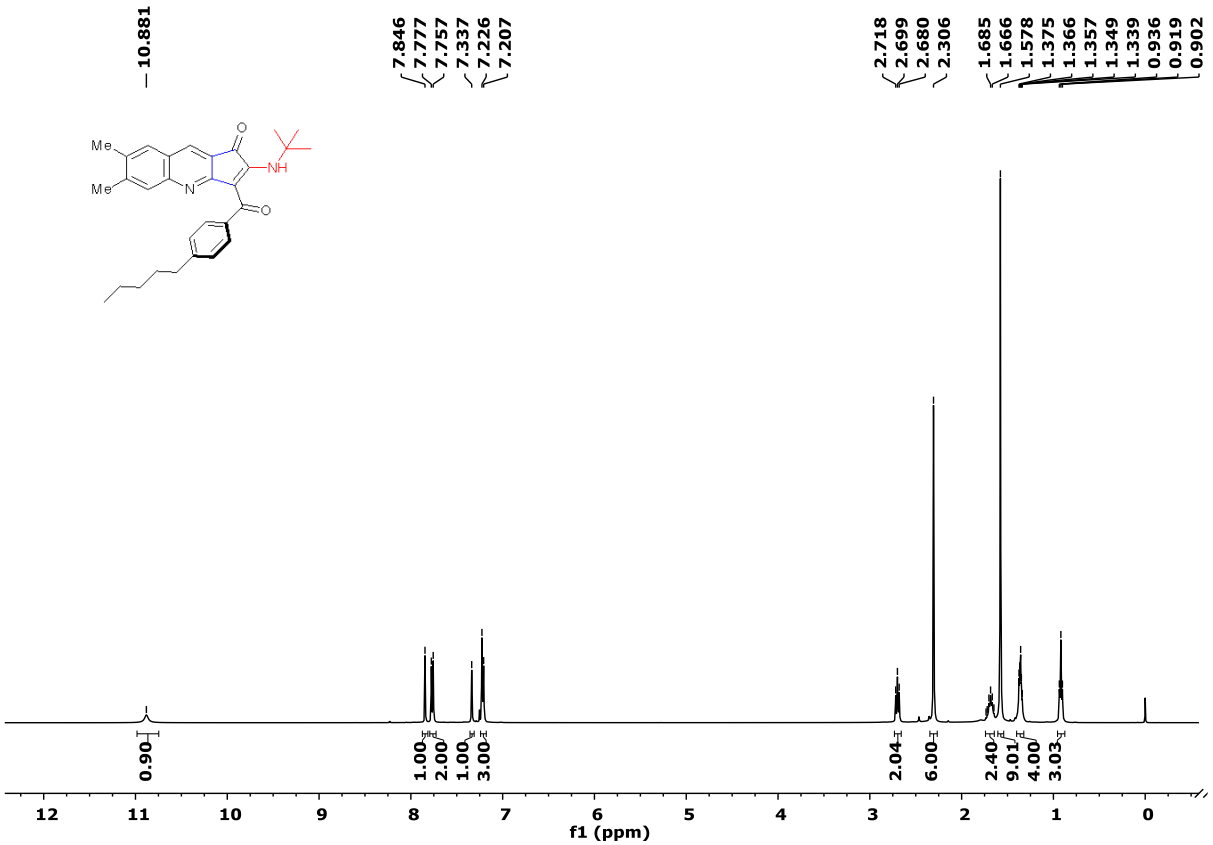
^{13}C-NMR of compound **(3l)** (100 MHz, $CDCl_3$)



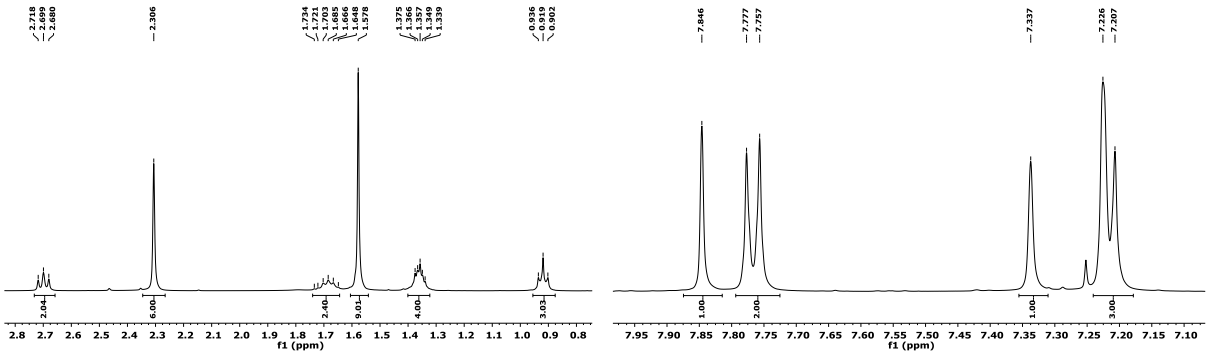
^{13}C-NMR of compound **(3l)** (100 MHz, $CDCl_3$)



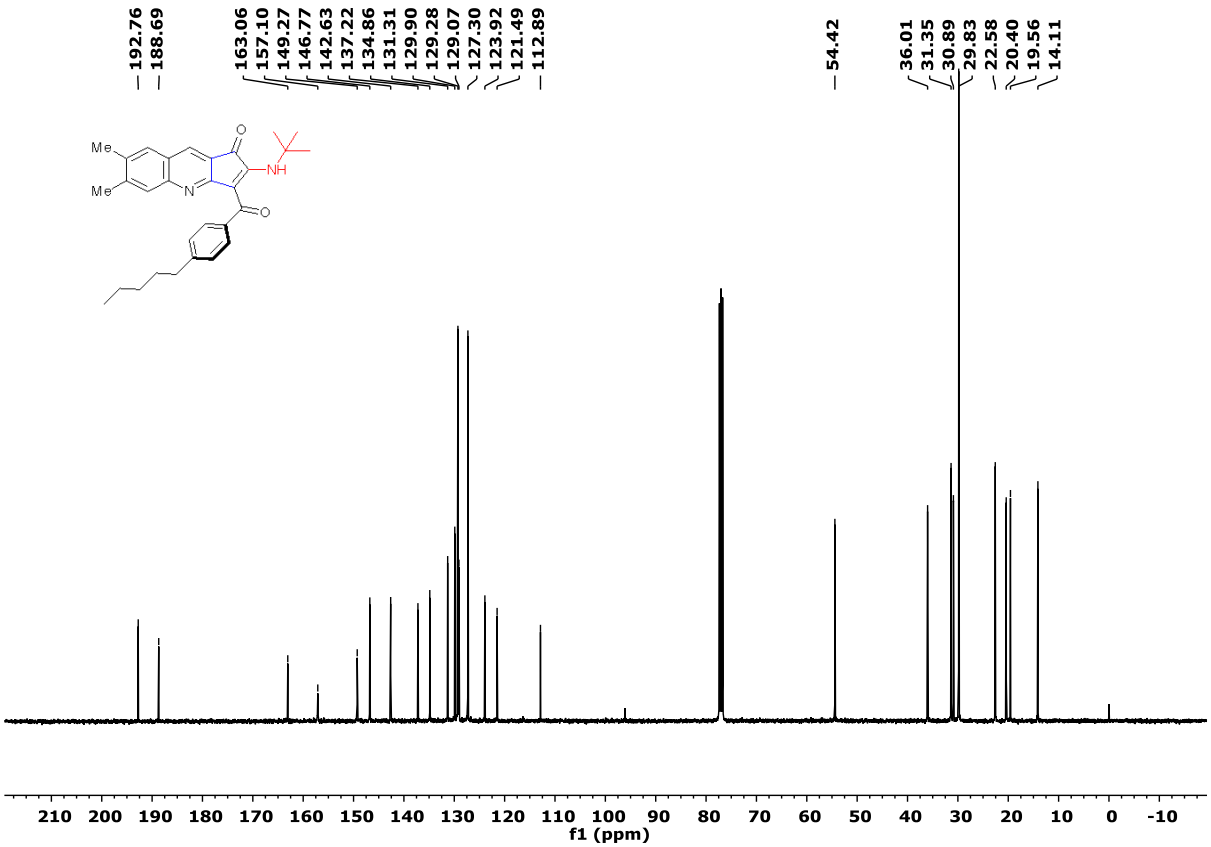
HRMS-ESI (m/z) of (**3l**)



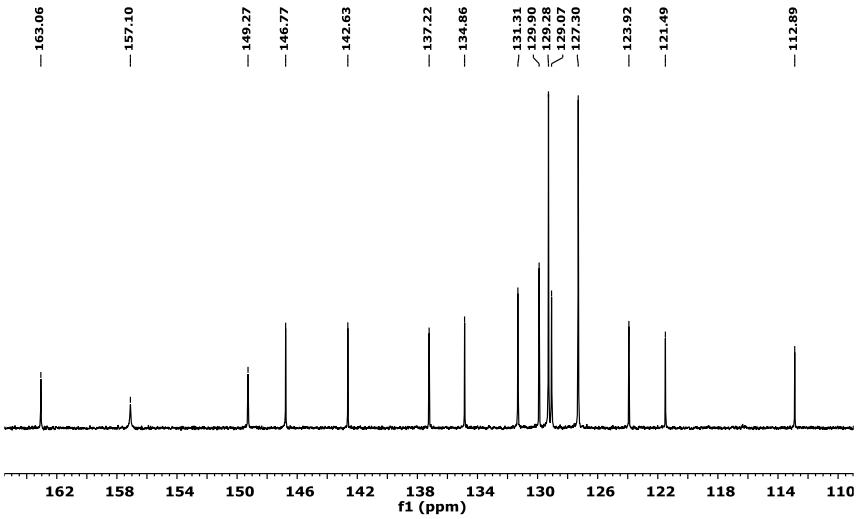
^{1}H-NMR of compound **(3m)** (400 MHz, $CDCl_3$)



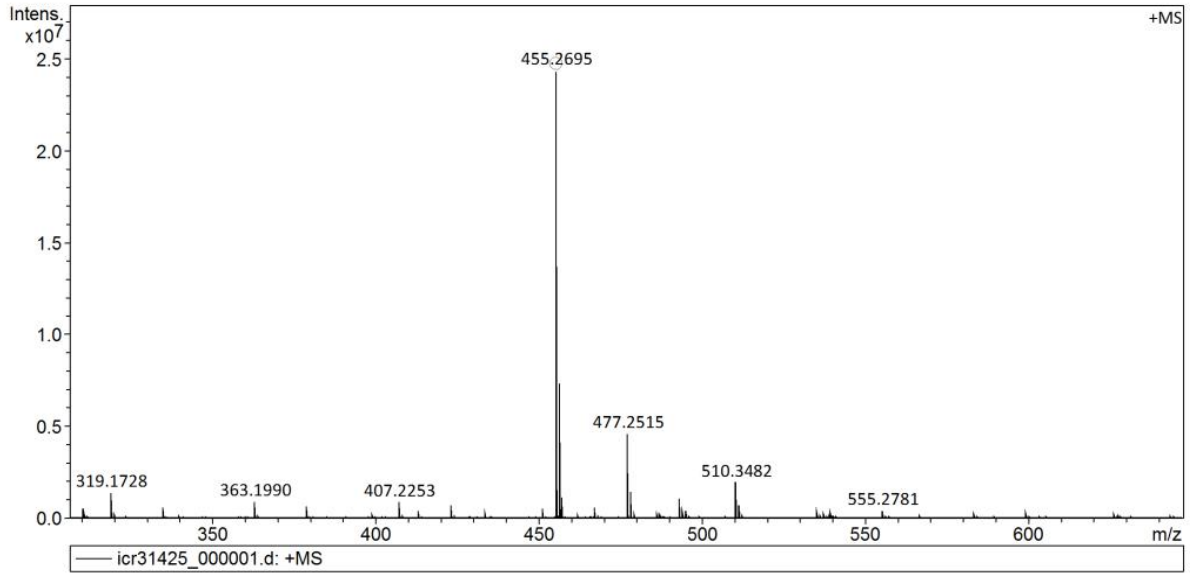
^{1}H-NMR of compound **(3m)** (400 MHz, $CDCl_3$)



^{13}C-NMR of compound **(3m)** (100 MHz, $CDCl_3$)

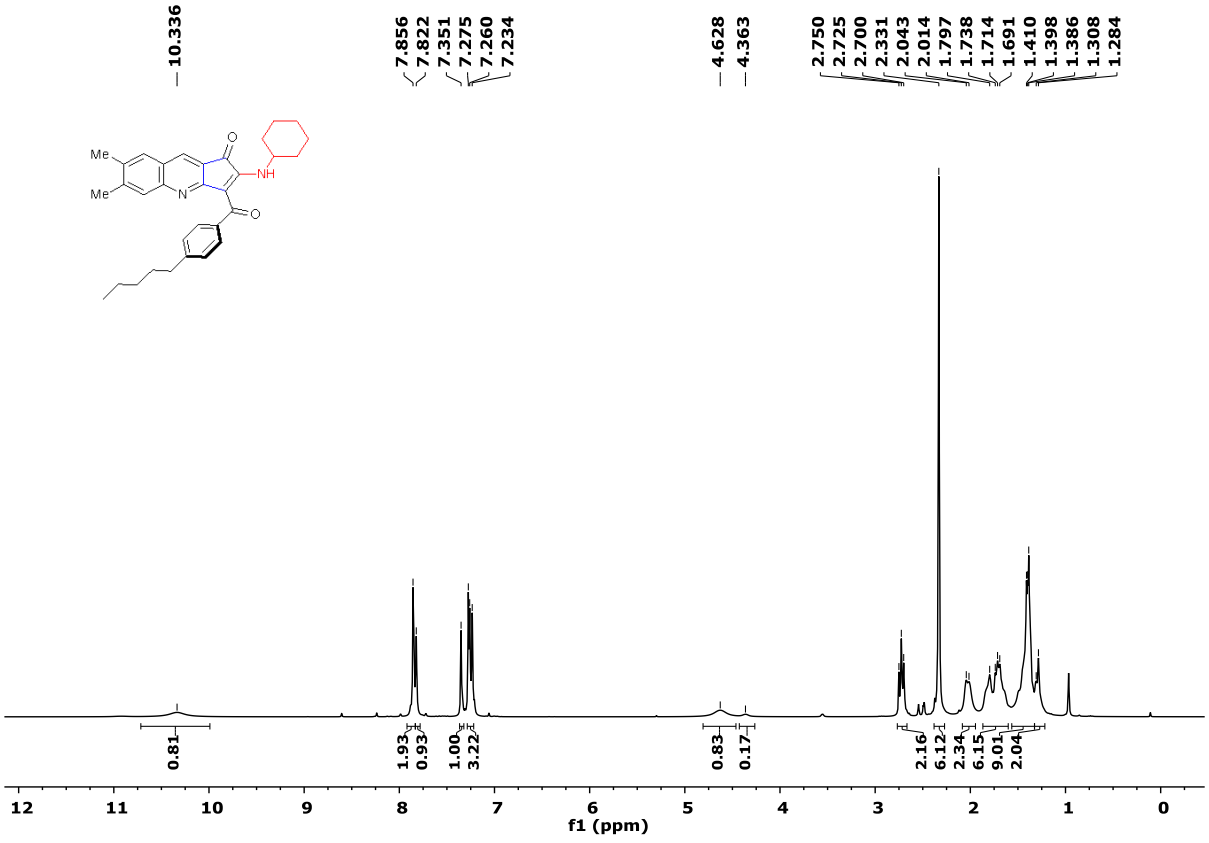


^{13}C-NMR of compound **(3m)** (100 MHz, $CDCl_3$)

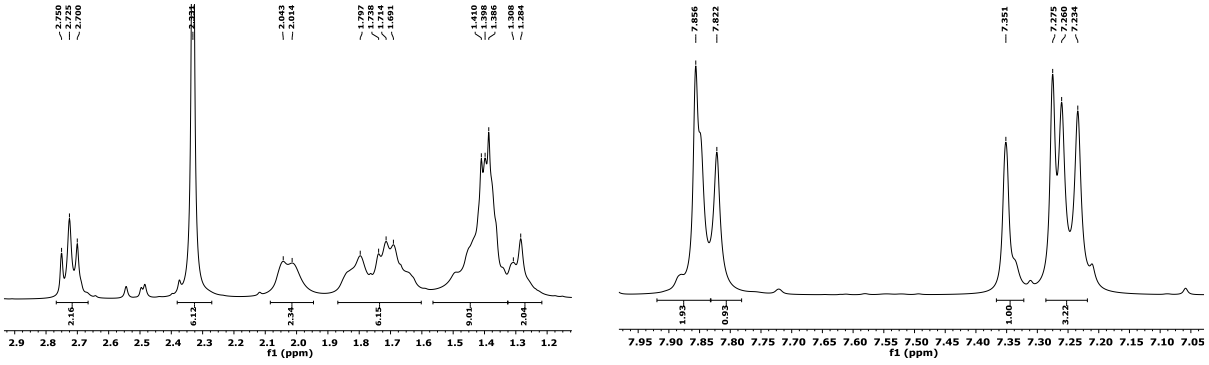


Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
455.2695	C30H35N2O2	455.2693	-0.5	10.5	14.5	even	ok

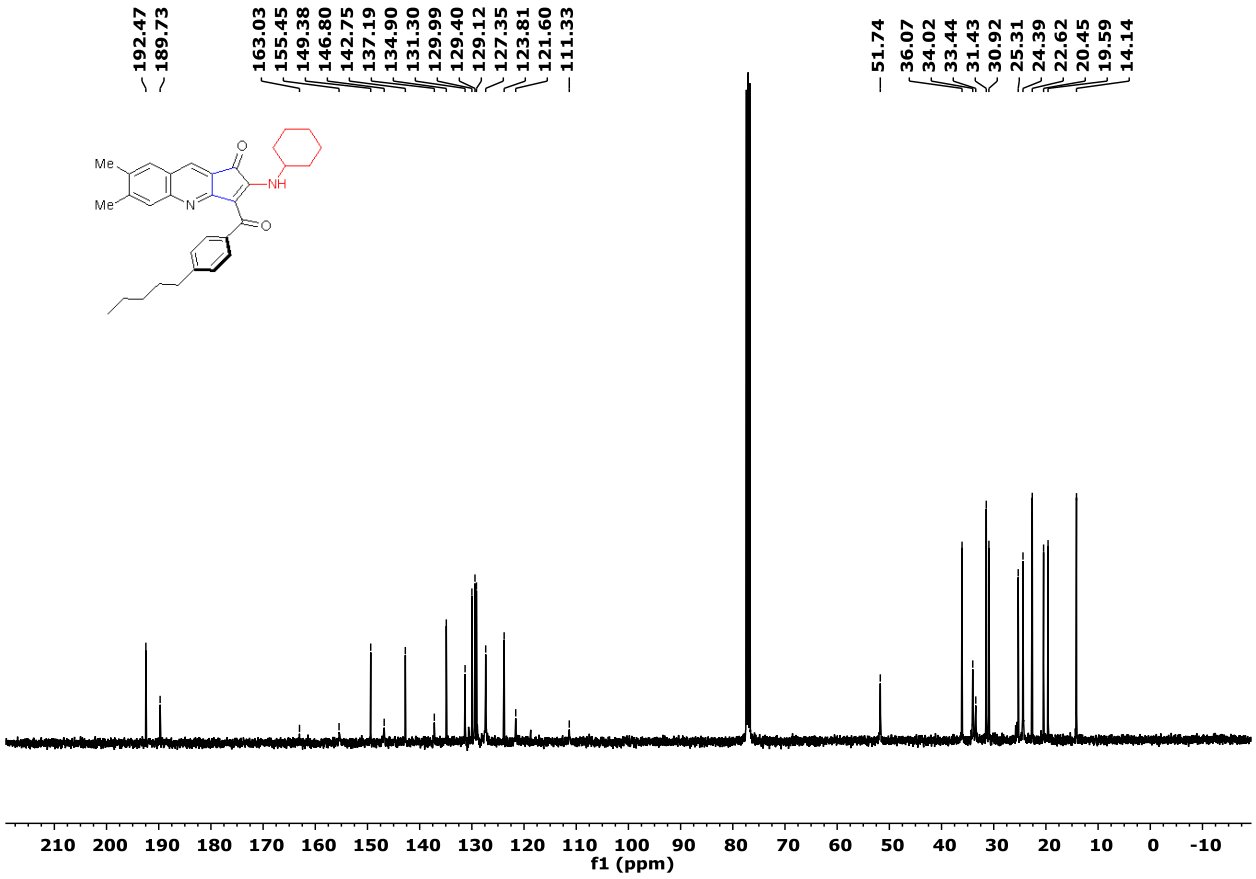
HRMS-ESI (m/z) of (**3m**)



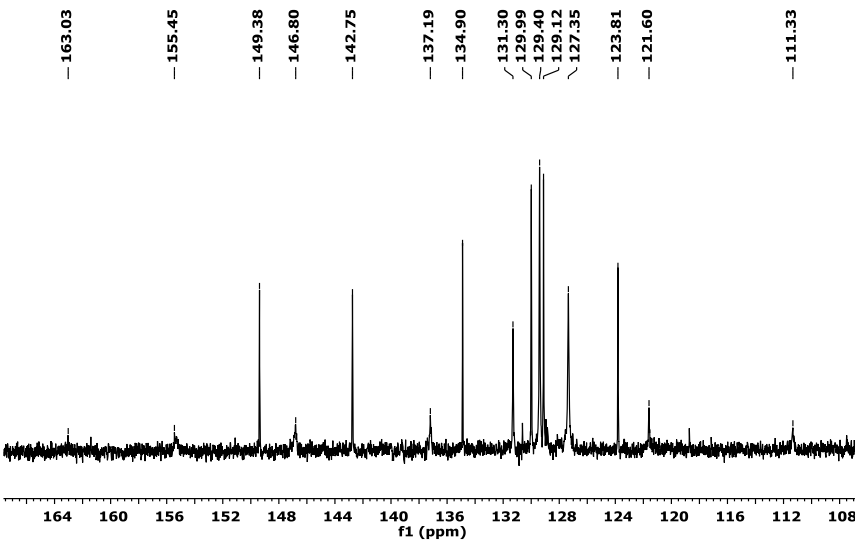
^{1}H-NMR of compound **(3n)** (300 MHz, $CDCl_3$)



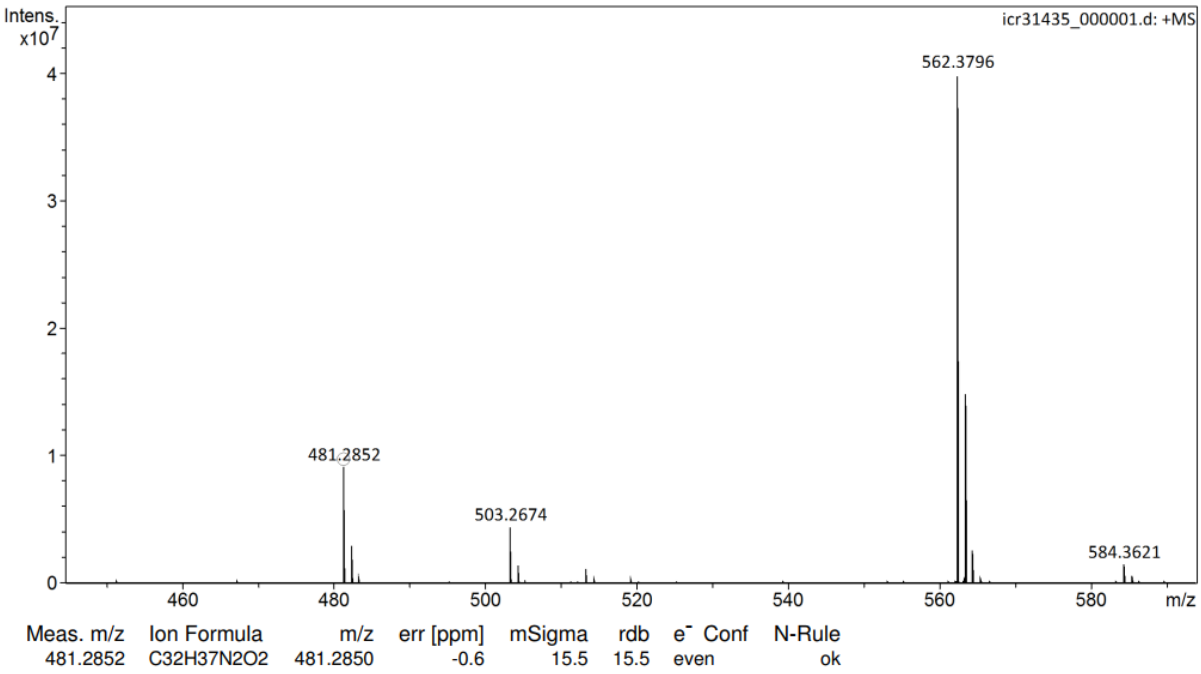
^{1}H-NMR of compound **(3n)** (300 MHz, $CDCl_3$)



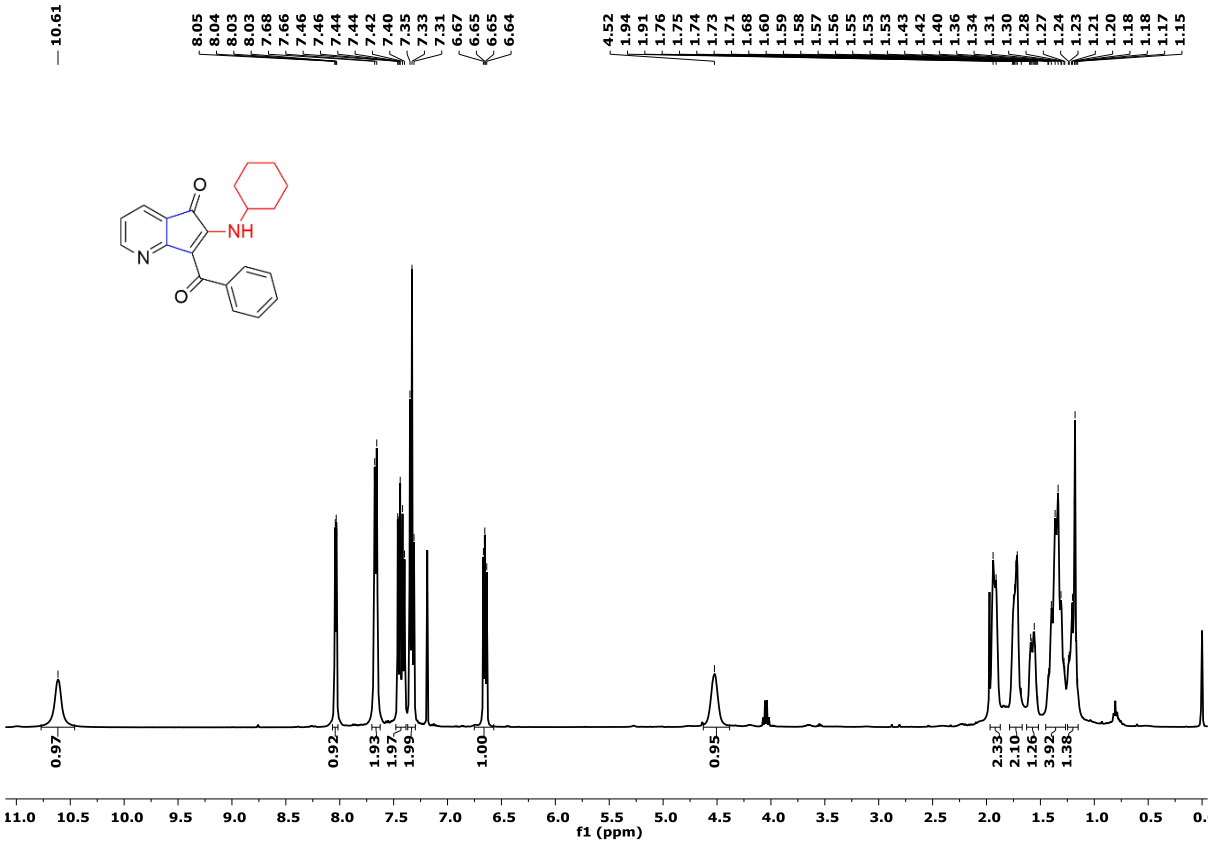
^{13}C-NMR of compound **(3n)** (100 MHz, $CDCl_3$)



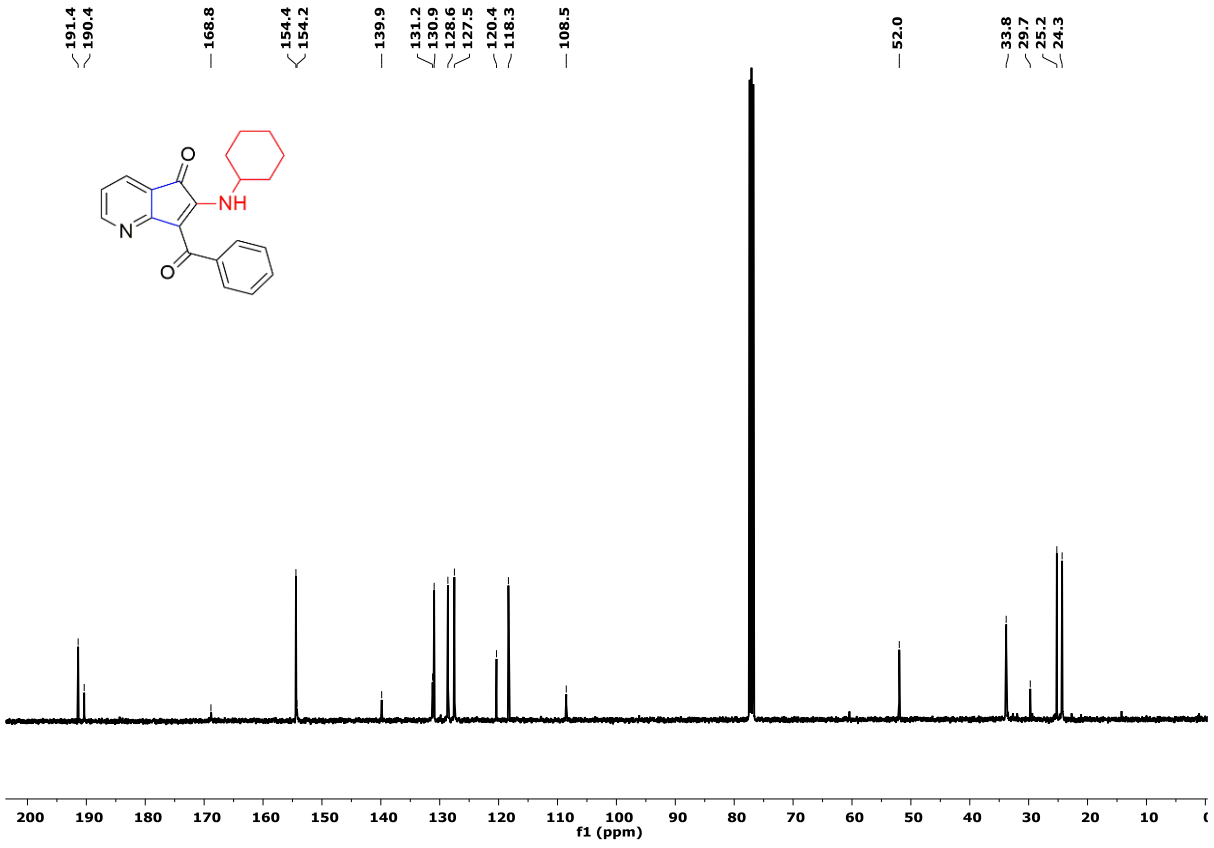
^{13}C-NMR of compound **(3n)** (100 MHz, $CDCl_3$)



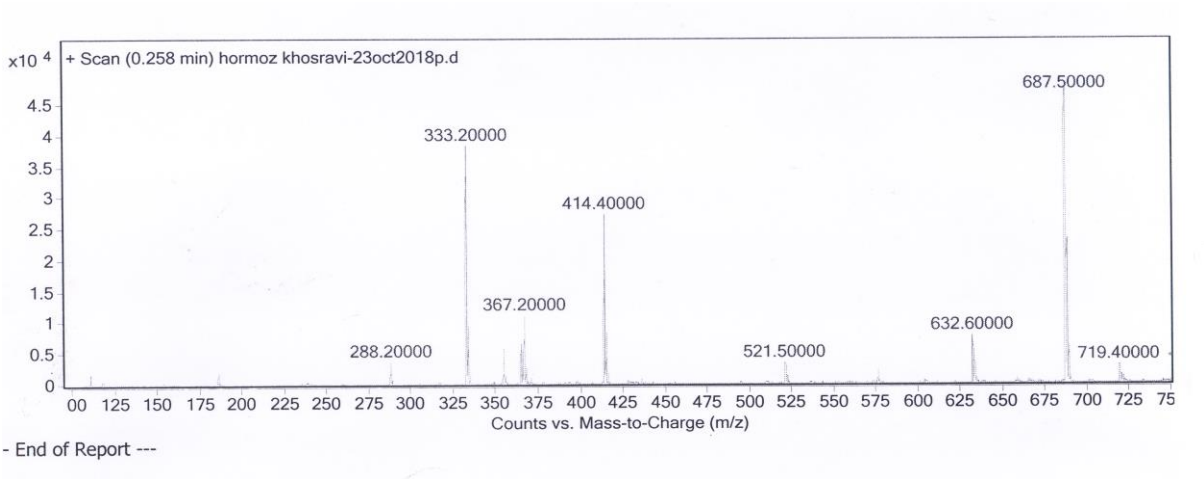
HRMS-ESI (m/z) of (**3n**)



^{1}H-NMR of compound **(3p)** (300 MHz, $CDCl_3$)



^{13}C-NMR of compound **(3p)** (100 MHz, $CDCl_3$)



LC-MS (ESI) (m/z) of (**3p**)

H. References

1. O. Meth-Cohn, B. Narine and B. Tarnowski, *J. Chem. Soc., Perkin Trans. 1*, 1981, **0**, 1520.

2. T. Godet, C. Vaxelaire, C. Michel, A. Milet and P. Belmont, *Chem. Eur. J.*, 2007, **13**, 5632.

3. R. Buksnaitiene and I. Cikotiene, *Synlett*, 2011, 2529.

4. Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

5. A. D. Becke, *Phys. Rev. A*, 1988, **38**, 3098.

6. A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648.

7. C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785.

8. D. Andrae, U. Häussermann, M. Dolg, H. Stoll and H. Preuss, *Theor. Chim. Acta.*, 1990, **77**, 123.

9. Y. Xia, D. Yin, C. Rong, Q. Xu, D. Yin and S. Liu, *J. Phys. Chem. A*. 2008, **112**, 9970.

10. R. G. Parr, L. V. Szentpaly and S. J. Liu, *Am. Chem. Soc.*1999, **121**, 1922.