

Supporting Information

Engaging Vinylene Carbonate in Ruthenium-Catalyzed Regioselective C-4 Methylenation and C-8 Formylmethylation of Isoquinolinones.

Dolly David Thalakkottukara^a and Thirumanavelan Gandhi*^a

^aDepartment of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore, Tamil Nadu-632014, India. E-mail: velan.g@vit.ac.in

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1. General experimental methods and materials.

Unless otherwise mentioned all the reactions were carried out in Schlenk tube (15 mL). Chemicals were purchased from Sigma-Aldrich, Alfa Aesar, TCI, AVRA and Carbanio and used without further purification. Vinylene carbonate was purchased from TCI chemicals and used as such for the transformations. Anhydrous DCE, MeOH, TFE and HFIP were purchased from commercial sources and used without further purification. Thin layer chromatography was carried out on 250 mm diameter aluminium supported silica gel TLC plates (MERCK TLC Plates) and with narrow tip capillary. The products were purified by column chromatography using 100-200 mesh silica gel. ^1H NMR spectra were recorded on Bruker spectrometer (400 MHz) and reported in units *ppm* (parts per million) relative to the signals for residual chloroform (7.26 *ppm*) in the deuterated solvent. $^{13}\text{C}\{^1\text{H}\}$ NMR spectra were recorded on Bruker spectrometer (100 MHz) and are reported in *ppm* relative to deuterated chloroform (77.23 *ppm*) with tetramethyl silane as an internal standard. ^{19}F NMR spectra were recorded on Bruker spectrometer (376 MHz) and are reported in *ppm*. Peaks at $\delta = 1.56\text{--}1.61$ ppm in ^1H NMR spectra of compounds recorded in CDCl_3 correspond to water present, if any. Additional peaks at $\delta = 0.86\text{--}0.88$ ppm and $\delta = 1.25\text{--}1.28$ ppm in ^1H NMR spectra and $\delta = 29.7\text{--}29.8$ ppm in $^{13}\text{C}\{^1\text{H}\}$ -NMR spectra of compounds recorded in CDCl_3 correspond to grease present, if any. Coupling constants (*J*) are reported in Hz; splitting patterns are assigned *s* = singlet, *d* = doublet, *t* = triplet, *q* = quartet, *dd* = doublet of doublet, *td* = triplet of doublet, *br* = broad signal. High-resolution mass spectra (HRMS) were performed on TOF-Q analyser.

1. 1 X-ray crystallography of compounds **3c** and **3n**.

Single crystal X-ray structural data of the compounds **3c** and **3n** were collected on a CMOS based Bruker D8 Venture PHOTON 100 diffractometer equipped with a INCOATEC microfocus source with graphite monochromated Mo $K\alpha$ radiation ($\lambda = 0.71073$ Å) operating at 50 kV and 30mA. The SAINT¹ program was used for the integration of diffraction profiles and absorption correction was applied with the SADABS² program. Both the structures were initially solved by SIR 92³ and refined by the full matrix least squares method using SHELXL-2013⁴ WinGX system, Ver2013.3.⁵ The non-hydrogen atoms in all the structures were located using the difference Fourier map and refined anisotropically. The hydrogen atoms were fixed by HFIX and placed in ideal positions and

included in the refinement process using a riding model with isotropic thermal parameters. All the crystallographic and structure refinement data of the compounds are summarized in section 5.

2. Experimental procedure

2. 1. Synthesis of *N*-substituted Isoquinolones.

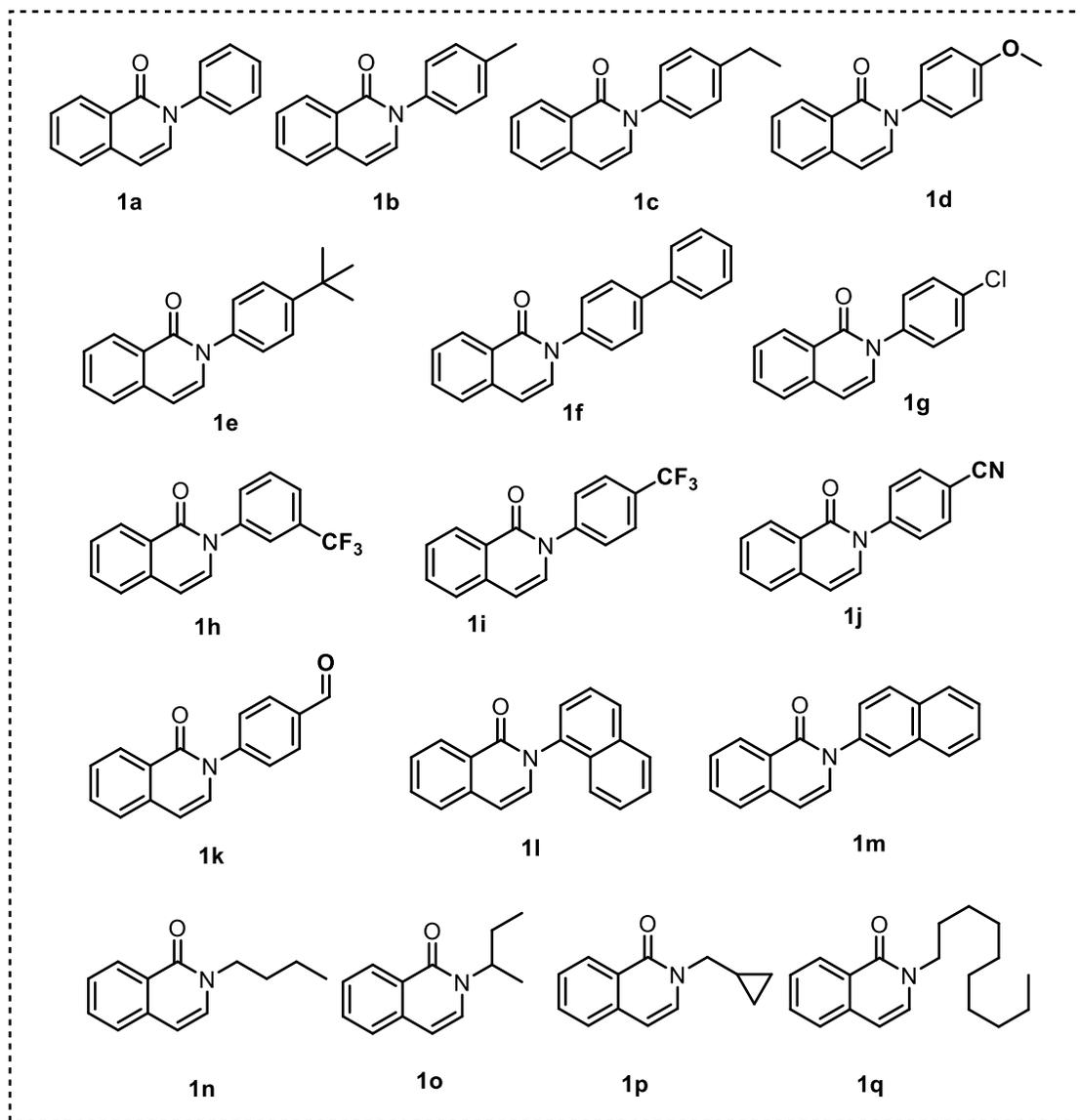
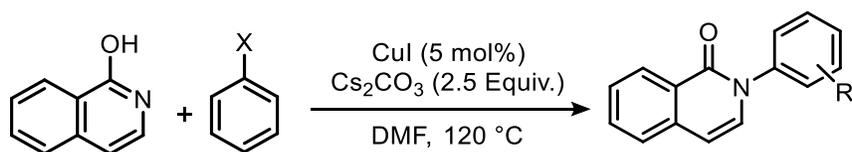


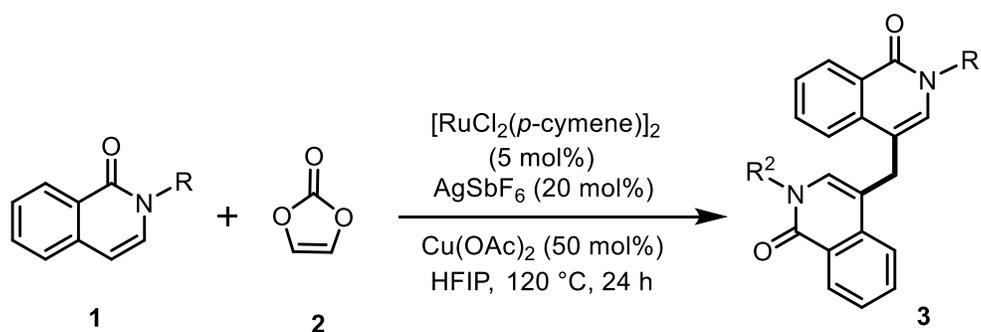
Table 1. *N*-substituted Isoquinolones



Scheme S1. Synthesis of *N*-substituted Isoquinolones

N-substituted isoquinolinones were synthesized using reported procedure.⁶ Derivatives of isoquinolinones were synthesised by charging 1-Hydroxy isoquinoline (1 equiv) in an oven dried tube followed by aryl or alkyl halides (1.2 equiv). To this copper iodide (5 mol%) and cesium carbonate (2.5 Equiv.) added along with 1 mL of DMF as solvent. The reaction is allowed to stir for 24 h at 120 °C. After completion of the reaction, the mixture was cooled to room temperature and diluted with DCM. This was extracted with water and dried over Na₂SO₄, filtered, and concentrated under reduced pressure. The residue was purified by column chromatography on 100-200 mesh silica gel using hexane and ethyl acetate to afford the desired products of *N*-substituted isoquinolinone derivatives (Scheme S1).

2. 2. Regioselective C4-methylenation of isoquinolinones



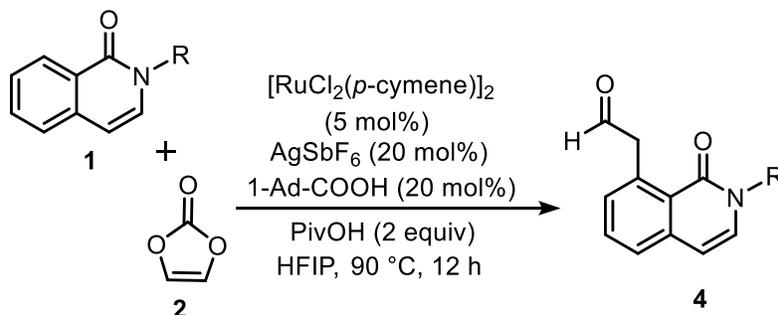
Scheme S2. Regioselective C4-methylenation of isoquinolinones

To an oven-dried Schlenk tube (15 mL) equipped with a stir bar was charged with 1mL of HFIP and isoquinolinone **1a** (2 equiv) and vinylene carbonate **2** (0.58 mmol, 1 equiv). To this reaction mixture, [Ru(*p*-cymene)Cl₂]₂ (5 mol%), AgSbF₆ (20 mol%) and Cu(OAc)₂ (50 mol%). The tube was flushed with nitrogen and screw capped under nitrogen flow and placed in a preheated oil bath at 120 °C for 24 h. After the indicated time, the reaction mixture was cooled and concentrated. The crude material was purified by column chromatography on silica gel (100-200 mesh) using *n*-hexane – ethyl acetate as eluent, to yield the title compound (Scheme S2).

2.3. Regioselective C8-formylmethylation of isoquinolinones.

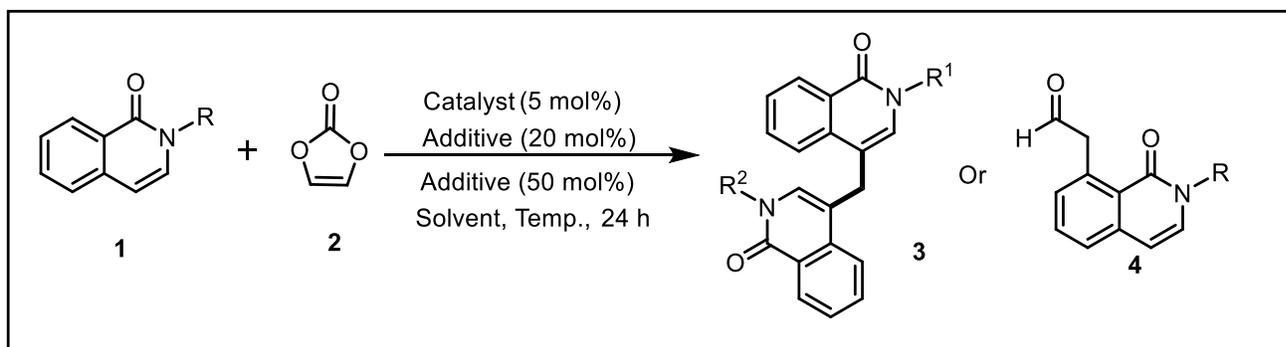
To an oven-dried Schlenk tube (15 mL) equipped with a stir bar was charged with 1mL of HFIP isoquinolinone **1a** (0.22 mmol, 1 equiv) and vinylene carbonate **2** (2 equiv) added. To this reaction mixture, [Ru(*p*-cymene)Cl₂]₂ (5 mol%), AgSbF₆ (20 mol%), 1-Ad-COOH (20 mol%) and PivOH (0.44 mmol, 2 equiv). The tube was flushed with nitrogen and screw capped under nitrogen flow and placed in a preheated oil bath at 90 °C for 12 h. After the indicated time, the reaction mixture

was cooled and concentrated. The crude material was purified by column chromatography on silica gel (100-200 mesh) using *n*-hexane – ethyl acetate as eluent, to yield the title compound (Scheme S3).



Scheme S3. Regioselective C8-formylmethylation of isoquinolinones

3. Optimization table



Sl. No	Catalyst	Additive	Solvent	Additive	Temperature	Yield of 3 (%)	Yield of 4 (%)
1	$[Ru(p\text{-cymene})Cl_2]_2$	PivOH/1-Ad-COOH	HFIP	$AgSbF_6$	120 °C	ND	34
2	$[Ru(p\text{-cymene})Cl_2]_2$	PivOH/1-Ad-COOH	HFIP	$AgOTf$	120 °C	ND	ND
3	$[Ru(p\text{-cymene})Cl_2]_2$	PivOH/1-Ad-COOH	HFIP	$AgOAc$	120 °C	ND	ND
4	$[Ru(p\text{-cymene})Cl_2]_2$	PivOH/1-Ad-COOH	DCE	$AgSbF_6$	90 °C	ND	ND
5	$[Ru(p\text{-cymene})Cl_2]_2$	PivOH/1-Ad-COOH	Isopropanol	$AgSbF_6$	90 °C	ND	ND
6	$[Ru(p\text{-cymene})Cl_2]_2$	PivOH/1-Ad-COOH	HFIP	$AgSbF_6$	90 °C	ND	43
7	$[Ru(p\text{-cymene})Cl_2]_2$	PivOH/1-Ad-COOH	HFIP	$AgSbF_6$	90 °C	ND	61
8	$[Ru(p\text{-cymene})Cl_2]_2$	$Cu(OAc)_2/1\text{-Ad-COOH}$	HFIP	$AgSbF_6$	120 °C	81	ND

9	[Ru(<i>p</i> -cymene)Cl ₂] ₂	Cu(OAc) ₂ (2 Equiv.)	HFIP	AgSbF ₆	120 °C	81	ND
10	[Ru(<i>p</i> -cymene)Cl ₂] ₂	CuI	HFIP	AgSbF ₆	120 °C	ND	ND
11	[Ru(<i>p</i> -cymene)Cl ₂] ₂	NaOAc	HFIP	AgSbF ₆	120 °C	ND	ND
12	[Ru(<i>p</i> -cymene)Cl ₂] ₂	K ₂ CO ₃	HFIP	AgSbF ₆	120 °C	ND	ND
13	[Ru(<i>p</i> -cymene)Cl ₂] ₂	Cu(OAc) ₂ (1 Equiv.)	HFIP	AgSbF ₆	120 °C	79	ND
14	[Ru(<i>p</i> -cymene)Cl ₂] ₂	Cu(OAc) ₂ (0.5 Equiv.)	HFIP	AgSbF ₆	120 °C	78	ND
15	[Ru(<i>p</i> -cymene)Cl ₂] ₂	Cu(OAc) ₂ (0.5 Equiv.)	DCE	AgSbF ₆	120 °C	ND	ND
16	[Ru(<i>p</i> -cymene)Cl ₂] ₂	Cu(OAc) ₂ (0.5 Equiv.)	Isopropanol	AgSbF ₆	120 °C	ND	ND
17	[Ru(<i>p</i> -cymene)Cl ₂] ₂	Cu(OAc) ₂ (0.5 Equiv.)	HFIP	AgSbF ₆	140 °C	56	ND
18	[Ru(<i>p</i> -cymene)Cl ₂] ₂	-	HFIP		120 °C	ND	ND
19	-	Cu(OAc) ₂ (0.2 Equiv.)	HFIP	AgSbF ₆	120 °C	ND	ND
20		Cu(OAc) ₂ / Bipyridyl	HFIP	AgSbF ₆	120 °C	ND	ND

4. Reluctant substrates

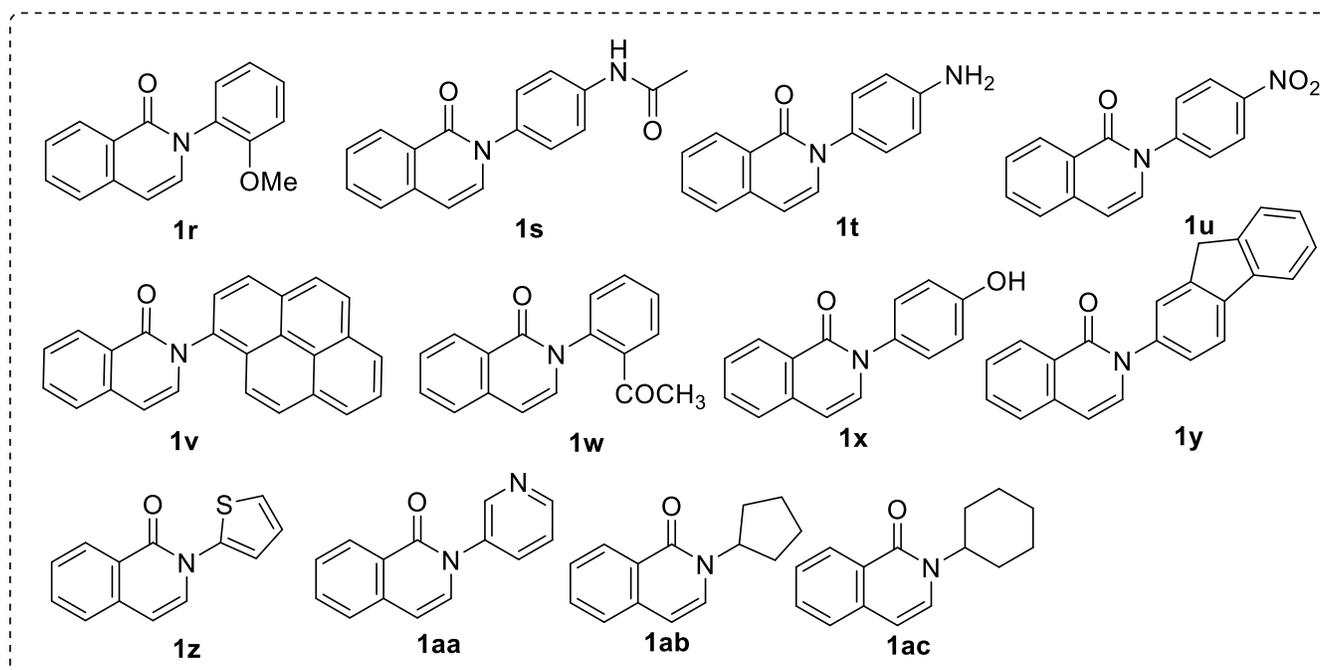


Table 2. Reluctant substrates

5. Crystallographic data

5.1. Crystallographic data for 3c

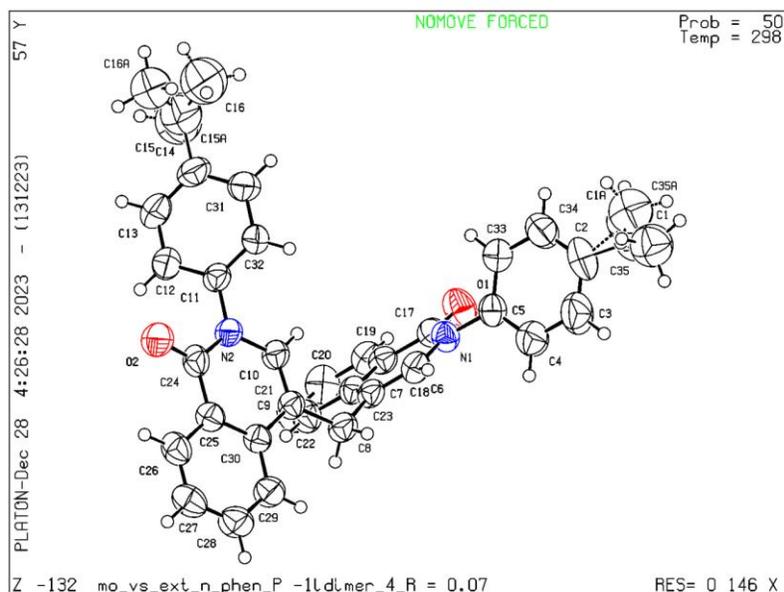


Fig 1. Perspective view of the X-ray structure of **3c**. Hydrogen atoms are omitted for clarity.

Compound	3c
CCDC No.	2351517
Formula	$C_{35}H_{30}N_2O_2$
<i>D</i> calc./ g cm ⁻³	1.237
μ /mm ⁻¹	0.077
Formula Weight	510.61
Colour	metallic light colourless
Shape	block-shaped
Size/mm ³	0.14×0.08×0.02
<i>T</i> /K	298
Crystal System	triclinic
Space Group	<i>P</i> -1
<i>a</i> /Å	10.4851(5)
<i>b</i> /Å	11.5807(5)
<i>c</i> /Å	13.2811(7)
α /°	66.245(2)
β /°	74.285(2)
γ /°	70.005(2)
<i>V</i> /Å ³	1370.34(12)
<i>Z</i>	2
<i>Z</i> '	1
Wavelength/Å	0.71073

Radiation type	MoK α
$\Theta_{min}/^\circ$	1.992
$\Theta_{max}/^\circ$	26.730
Measured Refl's.	42356
Indep't Refl's	5817
Refl's $I \geq 2 \sigma(I)$	2495
R_{int}	0.1295
Parameters	395
Restraints	78
Largest Peak	0.347
Deepest Hole	-0.285
GooF	1.019
$wR2$ (all data)	0.2278
$wR2$	0.1716
RI (all data)	0.1771
RI	0.0691

5.1.1. Bond distances of 3c

Atom	Atom	Distance Å	Atom	Atom	Distance Å
O1	C17	1.225(3)	C2	C3	1.376(6)
O2	C24	1.228(4)	C2	C34	1.369(5)
N1	C5	1.439(4)	C2	C1A	1.556(11)
N1	C6	1.394(4)	C3	C4	1.376(6)
N1	C17	1.380(4)	C4	C5	1.362(5)
N2	C10	1.397(4)	C5	C33	1.380(5)
N2	C11	1.444(4)	C6	C7	1.335(4)
N2	C24	1.386(4)	C7	C8	1.500(4)
C1	C2	1.525(10)	C7	C23	1.449(4)
C1	C35	1.377(11)	C8	C9	1.513(4)
C9	C10	1.342(4)	C13	C14	1.370(5)
C9	C30	1.442(4)	C14	C15	1.547(18)

C11	C12	1.385(4)	C14	C31	1.375(5)
C11	C32	1.365(4)	C14	C15A	1.515(6)
C12	C13	1.371(4)	C15	C16	1.42(2)
C9	C10	1.342(4)	C17	C18	1.461(4)
C9	C30	1.442(4)			
C11	C12	1.385(4)			

5.1.2. Bond angles of 3c

Atom	Atom	Atom	Angle [°]	Atom	Atom	Atom	Angle [°]
C14	N1	C4	119.19(17)	C27	C8		122.56(18)
C14	N1	C4	118.16(17)	C8	C9		123.47(19)
C9	N1	C5	122.61(18)	N2	C10		111.92(18)
C21	N2	C10	118.21(17)	C12	C11		112.3(2)
C21	N2	C9	122.63(17)	C13	C12		112.8(2)
C1	N2	C10	119.06(17)	O2	C14		120.9(2)
C2	C2	C3	117.7(4)	O2	C14		123.4(2)
N1	C3	C4	113.8(3)	N1	C14		115.67(18)
C6	C4	C3	112.0(2)	C16	C15		120.97(18)
C5	C5	N1	123.34(18)	C20	C15		119.0(2)
C5	C6	C7	122.82(17)	C20	C15		120.0(2)
C16	C6	C16	118.06(17)	C15	C16		119.16(19)
C8	C6	C7	119.10(17)	C15	C16		117.57(18)
C9	C7	C6	117.08(17)	C17	C16		123.25(19)

C9	C8	C7	119.21(18)		C18	C17		121.2(2)
C20	C8	C27	118.17(18)		C17	C18		120.5(2)
C19	C19	C18	119.9(2)		C24	C22	C21	121.08(18)
O1	C20	C15	120.7(2)		C23	C23	C22	120.3(2)
O1	C21	N2	121.19(19)		C26	C24	C25	119.6(2)
N1	C21	C22	123.3(2)		C25	C25	C24	121.2(2)
C23	C21	C22	115.53(17)		C22	C26	C27	120.5(2)
C23	C22	C21	118.49(18)		C22	C27	C8	119.09(17)
C27	C22	C27	120.41(19)		C26	C27	C26	117.96(19)
						C27	C8	122.95(18)

5.2. Crystallographic data for **3m**

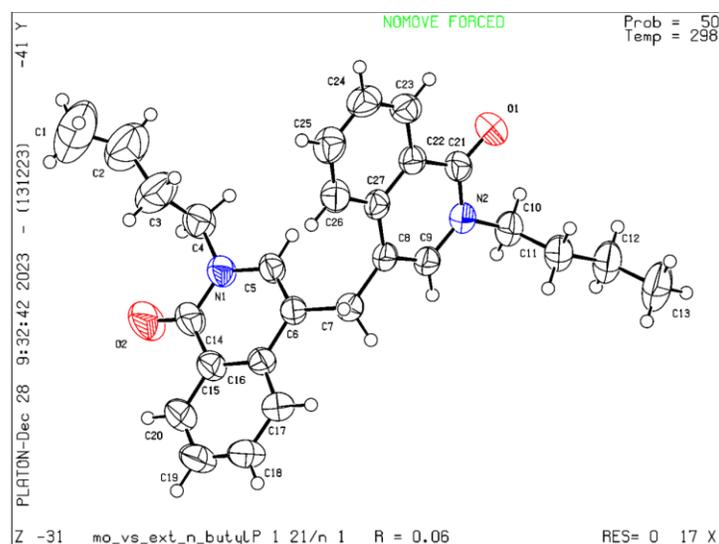


Fig 2. Perspective view of the X-ray structure of **3m**. Hydrogen atoms are omitted for clarity.

Compound	3m
CCDC No.	2351516
Empirical formula	C ₂₇ H ₃₀ N ₂ O ₂
Formula weight	414.53
Temperature/K	298
Crystal system	Monoclinic
Wavelength	0.71073 Å
Space group	P 21/n
a/Å	10.0243(4)
b/Å	12.5308(5)
c/Å	18.4588(8)
α/°	90
β/°	97.5810(10)
γ/°	90
Volume	2318.54(16)
Z	4
Calculated density g/cm ³	1.188
Absorption coefficient (μ/mm ⁻¹)	0.83
F(000)	888
	-16<h<17
Index ranges	-18<k<18
	-11<l<11
Reflections collected	32117
Independent reflections	5118
Data/restraint/parameters	3969/0/210
Goodness of fit on F ²	1.032
Final R indices[I>2σ(I)]	R ₁ =0.0590
	wR ₂ =0.1564
Final R indices [all data]	R ₁ =0.0947
	wR ₂ =0.1808

5.2.1. Bond distances of 3n

Atom	Atom	Distance Å	Atom	Atom	Distance Å
O(1)	C(21)	1.233(2)	C(11)	C(12)	1.507(3)
O(2)	C(14)	1.226(3)	C(12)	C(13)	1.505(4)
N(1)	C(4)	1.470(3)	C(14)	C(15)	1.464(3)
N(1)	C(5)	1.382(2)	C(15)	C(16)	1.406(3)
N(1)	C(14)	1.375(3)	C(15)	C(20)	1.401(3)
N(2)	C(9)	1.380(2)	C(16)	C(17)	1.407(3)
N(2)	C(10)	1.468(3)	C(17)	C(18)	1.370(3)
N(2)	C(21)	1.373(3)	C(18)	C(19)	1.385(4)
C(1)	C(2)	1.375(5)	C(19)	C(20)	1.360(4)
C(2)	C(3)	1.476(4)	C(21)	C(22)	1.464(3)
C(3)	C(4)	1.507(3)	C(22)	C(23)	1.397(3)
C(5)	C(6)	1.342(3)	C(22)	C(27)	1.404(3)
C(6)	C(7)	1.513(3)	C(23)	C(24)	1.369(3)
C(6)	C(16)	1.442(3)	C(24)	C(25)	1.386(3)
C(7)	C(8)	1.509(3)	C(25)	C(26)	1.367(3)
C(8)	C(9)	1.339(3)	C(26)	C(27)	1.405(3)
C(8)	C(9)	1.438(3)			
C(10)	C(11)	1.509(3)			

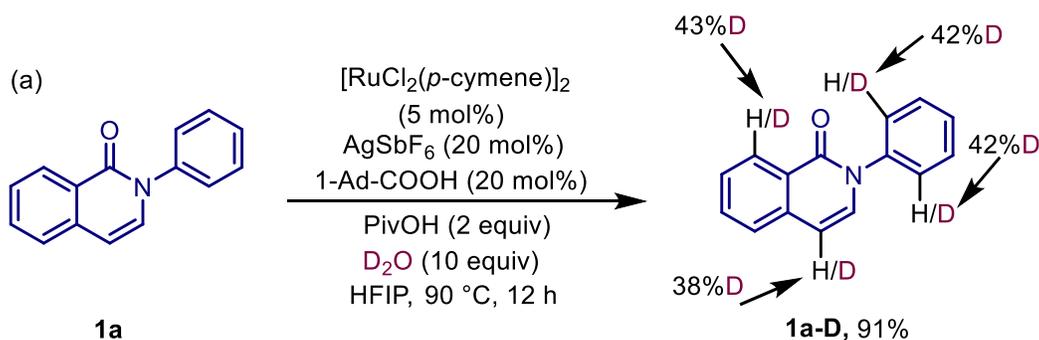
5.2.2. Bond angles of 3n

Atom	Atom	Atom	Angle [°]		Atom	Atom	Atom	Angle [°]
C5	N1	C4	119.19(17)		C24	C23	C22	120.3(2)
C14	N1	C4	118.16(17)		C23	C24	C25	119.6(2)
C14	N1	C5	122.61(18)		C26	C25	C24	121.2(2)
C9	N2	C10	118.21(17)		C25	C26	C27	120.5(2)
C21	N2	C9	122.63(17)		C22	C27	C8	119.09(17)
C21	N2	C10	119.06(17)		C22	C27	C26	117.96(19)
C1	C2	C3	117.7(4)		C26	C27	C8	122.95(18)
C2	C3	C4	113.8(3)		C27	C8		122.56(18)
N1	C4	C3	112.0(2)		C8	C9		123.47(19)
C6	C5	N1	123.34(18)		N2	C10		111.92(18)
C5	C6	C7	122.82(17)		C12	C11		112.3(2)
C5	C6	C16	118.06(17)		C13	C12		112.8(2)
C16	C6	C7	119.10(17)		O2	C14		120.9(2)
C8	C7	C6	117.08(17)		O2	C14		123.4(2)
C9	C8	C7	119.21(18)		N1	C14		115.67(18)
C9	C8	C27	118.17(18)		C16	C15		120.97(18)
C20	C19	C18	119.9(2)		C20	C15		119.0(2)
C19	C20	C15	120.7(2)		C20	C15		120.0(2)
O1	C21	N2	121.19(19)		C15	C16		119.16(19)
O1	C21	C22	123.3(2)		C15	C16		117.57(18)
N1	C21	C22	115.53(17)		C17	C16		123.25(19)

C23	C22	C21	118.49(18)		C18	C17		121.2(2)
C23	C22	C27	120.41(19)		C17	C18		120.5(2)
C27	C22	C21	121.08(18)					

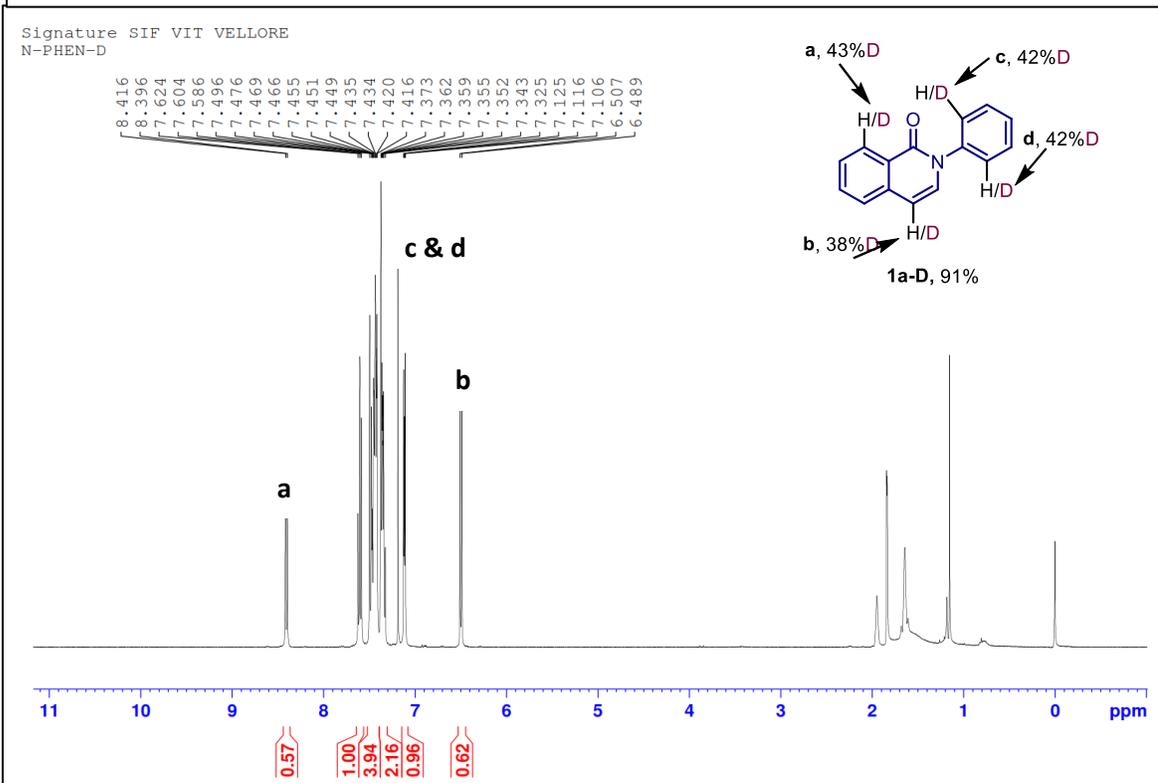
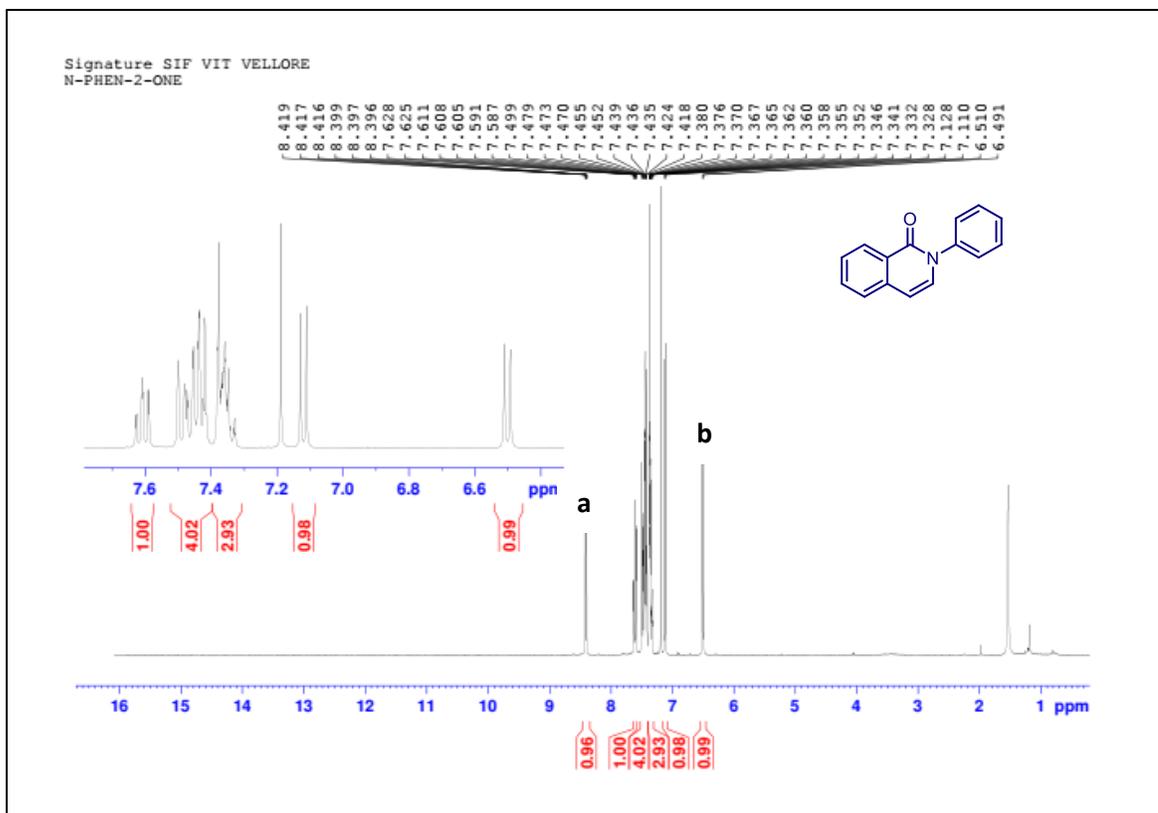
6. Mechanistic studies

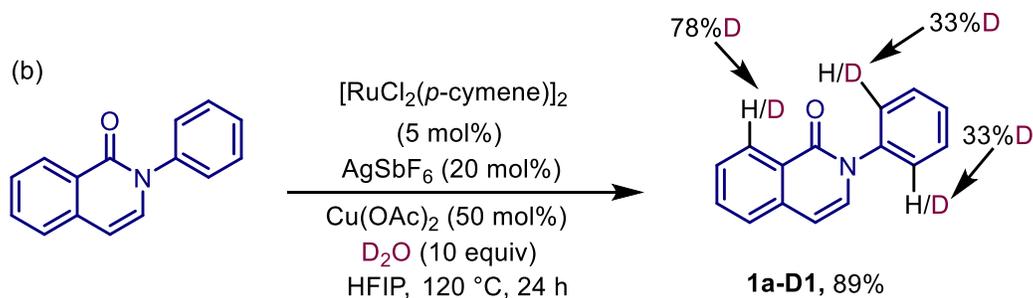
6. 1. H/D exchange experiment without vinylene carbonate:



Scheme S4. H/D exchange experiment without vinylene carbonate

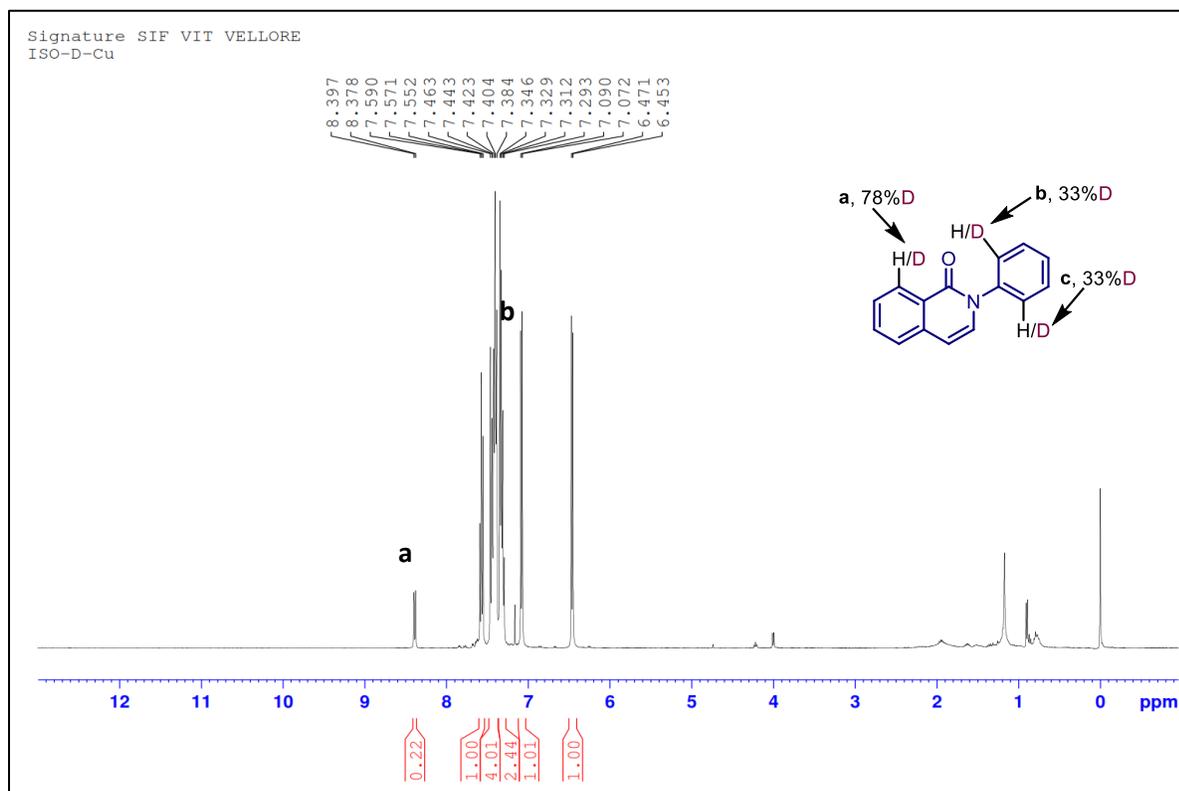
To an oven-dried Schlenk tube (15 mL) equipped with a stir bar, 1 mL of HFIP and isoquinolinone **1a** (0.22 mmol, 1 equiv) were added. To this reaction mixture, $[\text{Ru}(p\text{-cymene})\text{Cl}_2]_2$ (5 mol%), AgSbF_6 (20 mol%), 1-Ad-COOH (20 mol%), PivOH (0.44 mmol, 2 equiv) and D_2O (10 equiv). The tube was flushed with nitrogen and screw capped under nitrogen flow and placed in a preheated oil bath at 90 °C for 12 h. After the indicated time, the reaction mixture was cooled and concentrated. The crude material was purified by column chromatography on silica gel (100-200 mesh) using *n*-hexane – ethyl acetate as eluent, to yield the title compound (Scheme S4).



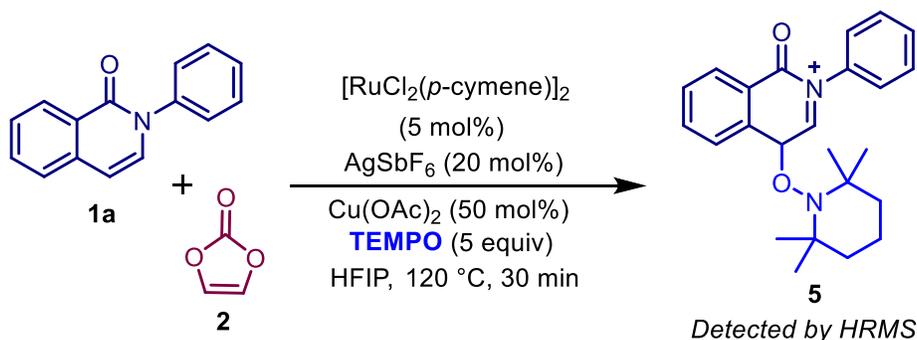


Scheme S5. H/D exchange experiment without vinylene carbonate

To an oven-dried Schlenk tube (15 mL) equipped with a stir bar, 1 mL of HFIP and isoquinolinone **1a** (0.22 mmol, 1 equiv) were added. To this reaction mixture, $[Ru(p\text{-cymene})Cl_2]_2$ (5 mol%), $AgSbF_6$ (20 mol%), $Cu(OAc)_2$ (50 mol%) and D_2O (10 equiv). The tube was flushed with nitrogen and screw capped under nitrogen flow and placed in a preheated oil bath at 120 °C for 24 h. After the indicated time, the reaction mixture was cooled and concentrated. The crude material was purified by column chromatography on silica gel (100-200 mesh) using *n*-hexane – ethyl acetate as eluent, to yield the title compound (Scheme S5).

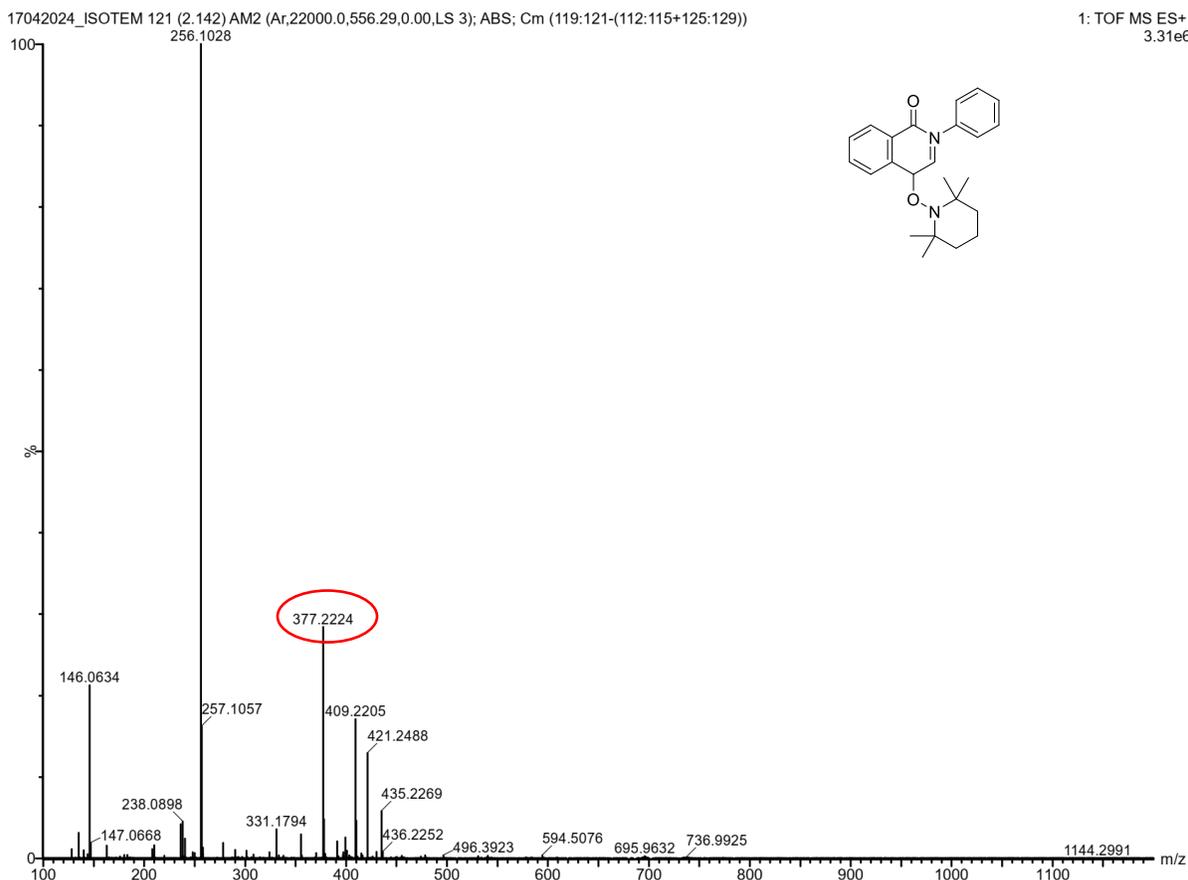


6.2 Radical inhibition experiment

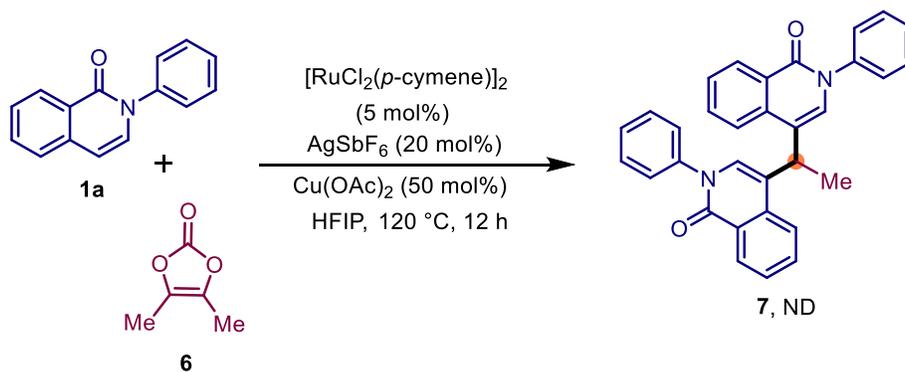


Scheme S6. Radical inhibition experiment

To an oven-dried Schlenk tube (15 mL) equipped with a stir bar, 1 mL of HFIP and isoquinolinone **1a** (2 equiv) were added. To this reaction mixture, vinylene carbonate **2** (0.58 mmol, 1 equiv.), [Ru(*p*-cymene)Cl₂]₂ (5 mol%), AgSbF₆ (20 mol%), Cu(OAc)₂ (50 mol%) and TEMPO (5 equiv) were added. The tube was flushed with nitrogen and screw capped under nitrogen flow and placed in a preheated oil bath at 120 °C for 30 min. This reaction mixture was subjected to mass spectrometry analysis (ESI-HRMS) (Scheme S6).



6.3 Reaction with 4,5-Dimethyl-1,3-dioxol-2-one.

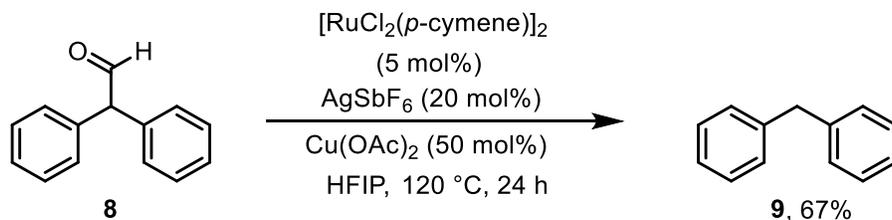


Scheme S7. Reaction of isoquinolinone with derivative of vinylene carbonate.

To an oven-dried Schlenk tube (15 mL) equipped with a stir bar, 1 mL of HFIP, **1a** (0.25 mmol, 1 equiv) and 4,5-Dimethyl-1,3-dioxol-2-one **6** (0.58 mmol, 1 equiv.) were added. To this reaction mixture, $[\text{Ru}(p\text{-cymene})\text{Cl}_2]_2$ (5 mol%), AgSbF_6 (20 mol%) and $\text{Cu}(\text{OAc})_2$ (50 mol%) were added. The tube was flushed with nitrogen and screw capped under nitrogen flow and placed in a preheated oil bath at 120 °C for 24 h. After the indicated time, the reaction mixture was cooled and concentrated. (Scheme S7).

6.4. Experimental proof for conversion of formyl group to methylene group

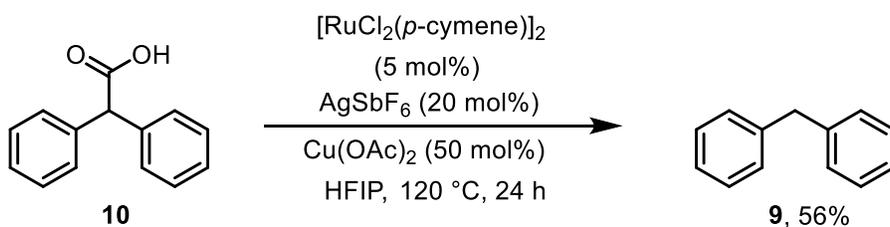
To an oven-dried Schlenk tube (15 mL) equipped with a stir bar, 1 mL of HFIP and diphenyl acetaldehyde **8** (0.25 mmol, 1 equiv) were added. To this reaction mixture, $[\text{Ru}(p\text{-cymene})\text{Cl}_2]_2$ (5 mol%), AgSbF_6 (20 mol%) and $\text{Cu}(\text{OAc})_2$ (50 mol%) were added. The tube was flushed with nitrogen and screw capped under nitrogen flow and placed in a preheated oil bath at 120 °C for 24 h. After the indicated time, the reaction mixture was cooled and concentrated. The crude material was purified by column chromatography on silica gel (100-200 mesh) using *n*-hexane – ethyl acetate as eluent, to yield the title compound (Scheme S8).



Scheme S8. Conversion of formyl group to methylene group

6.5. Experimental proof for conversion of carboxylic acid to methylene group

To an oven-dried Schlenk tube (15 mL) equipped with a stir bar, 1 mL of HFIP and diphenyl acetic acid **10** (0.23 mmol, 1 equiv) were added. To this reaction mixture, $[\text{Ru}(p\text{-cymene})\text{Cl}_2]_2$ (5 mol%), AgSbF_6 (20 mol%) and $\text{Cu}(\text{OAc})_2$ (50 mol%) were added. The tube was flushed with nitrogen and screw capped under nitrogen flow and placed in a preheated oil bath at 120 °C for 24 h. After the indicated time, the reaction mixture was cooled and concentrated. The crude material was purified by column chromatography on silica gel (100-200 mesh) using *n*-hexane – ethyl acetate as eluent, to yield the title compound (Scheme S9).



Scheme S9. Conversion of acid group to methylene group

7. Detection of CO₂ by GC-MS

To an oven-dried Schlenk tube (15 mL) equipped with a stir bar, 1 mL of HFIP, **1a** (0.25 mmol, 1 equiv) and vinylene carbonate **2** (0.58 mmol, 1 equiv.) were added. To this reaction mixture, $[\text{Ru}(p\text{-cymene})\text{Cl}_2]_2$ (5 mol%), AgSbF_6 (20 mol%) and $\text{Cu}(\text{OAc})_2$ (50 mol%) were added. The tube was flushed with nitrogen and closed with septum, then placed in a preheated oil bath at 120 °C for 4 h. After the indicated time, the reaction mixture was cooled and gas inside the reaction tube was monitored with GC-MS.

At the first the air blank was loaded with atmospheric air to monitor the presence of carbon dioxide and then the sample air was loaded in which shown much higher peak of CO₂ as compared to the blank one. Hereby, in the attached chromatogram peak in orange colour shows airblank and other one in blue colour shows the sample peak.

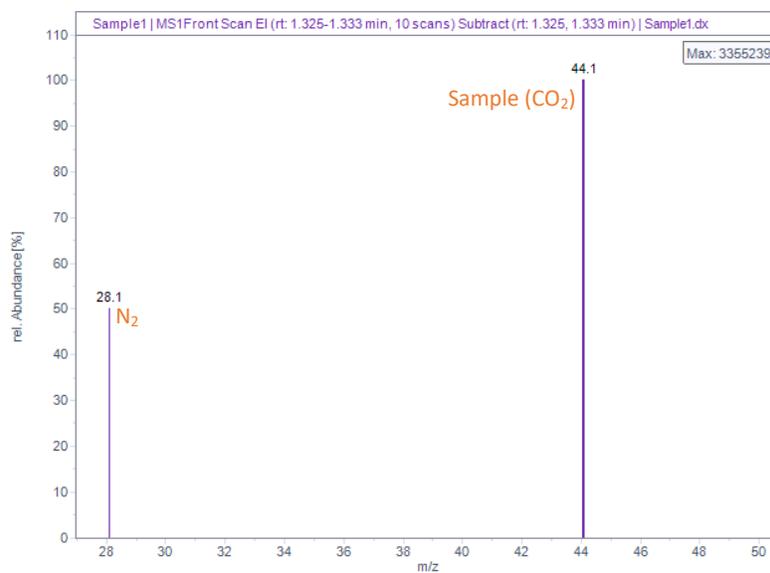


Fig 3. Mass spectrum for sample

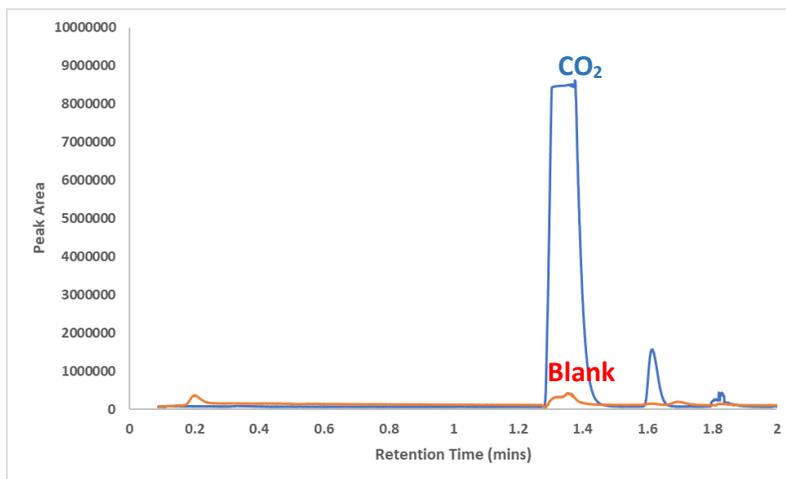
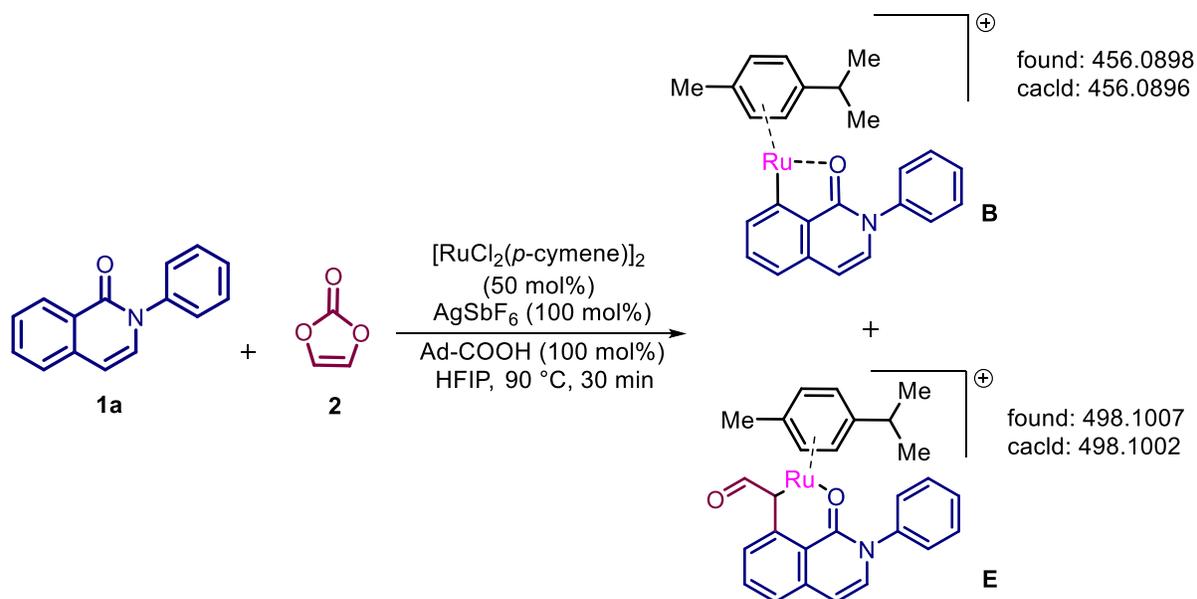


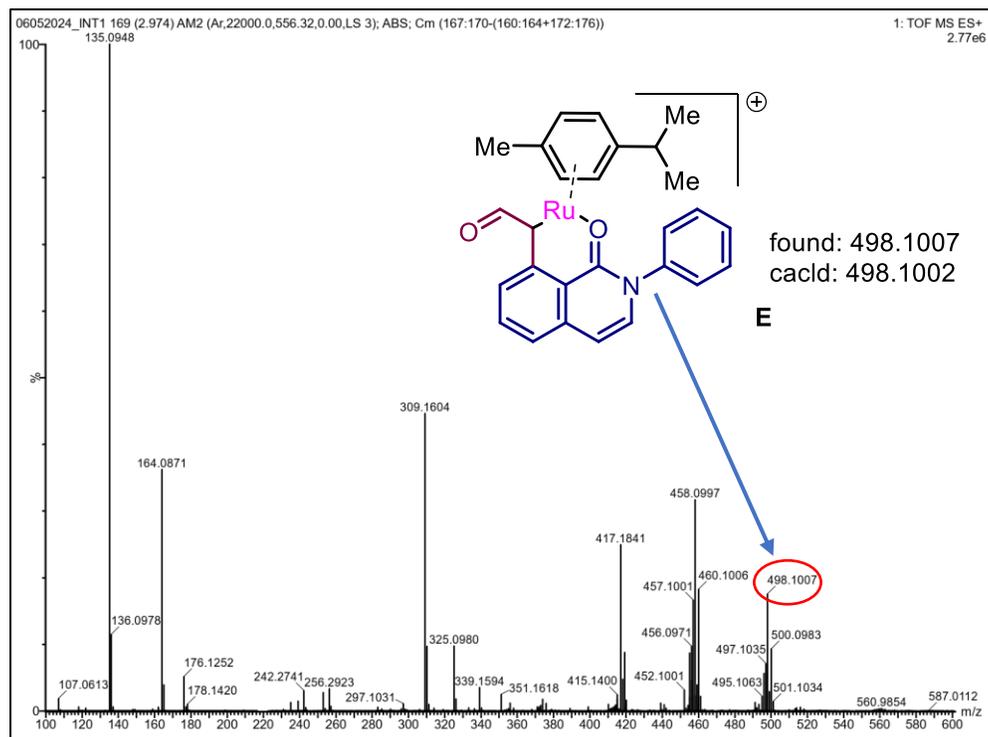
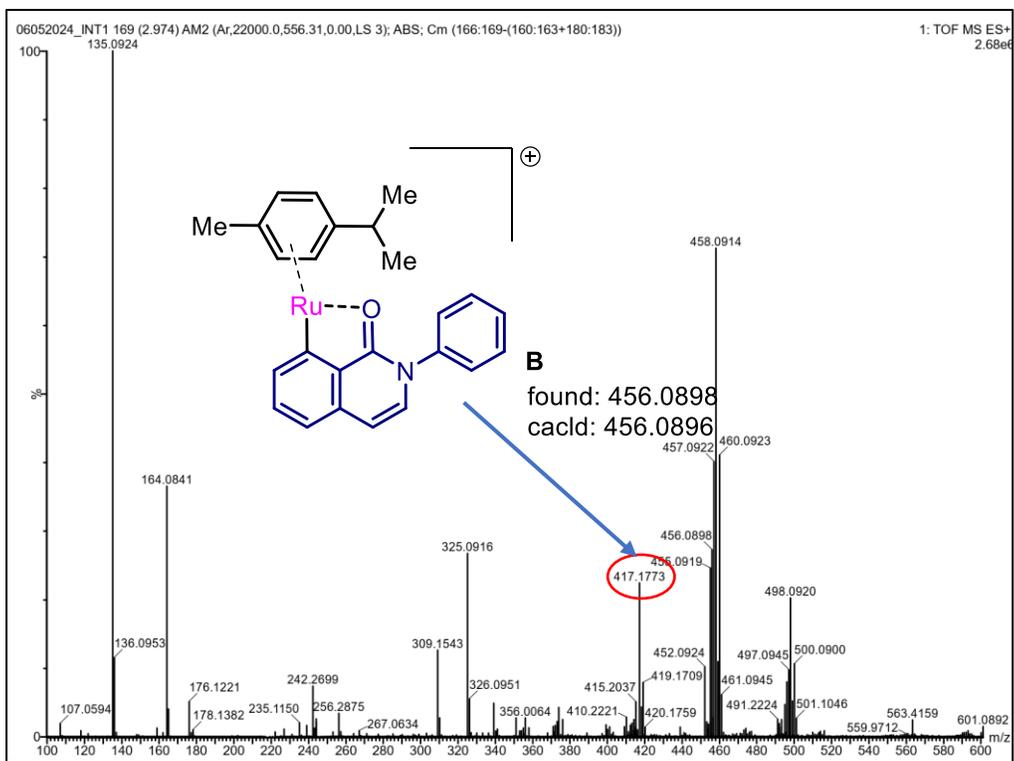
Fig 4. Chromatogram with mass filter from 42-47

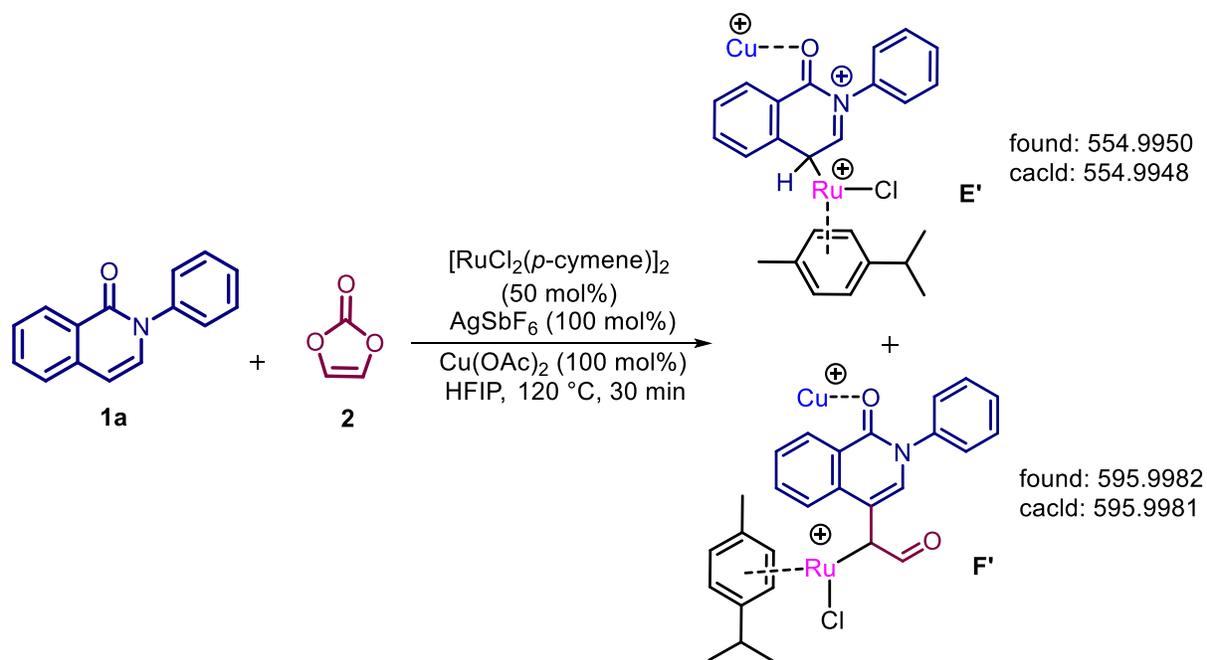
8. Mass spectrometry studies for determining intermediates



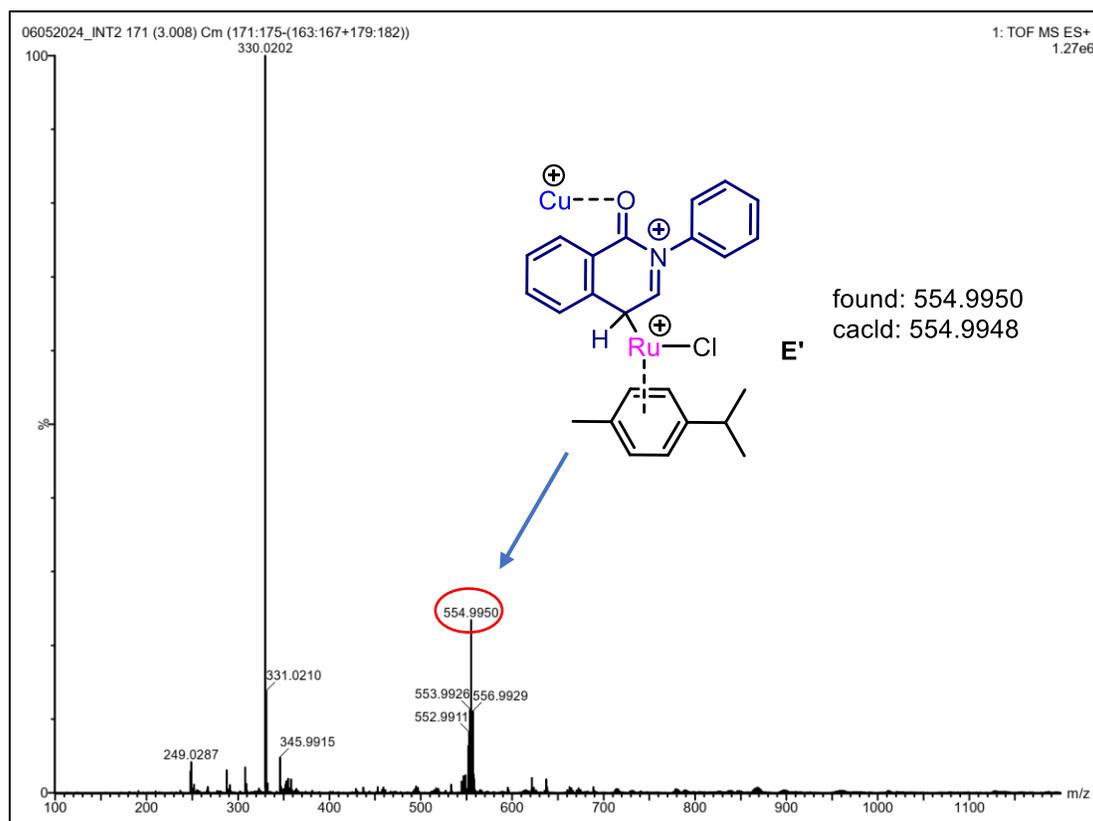
Scheme S10. Formyl methylation of isoquinolones

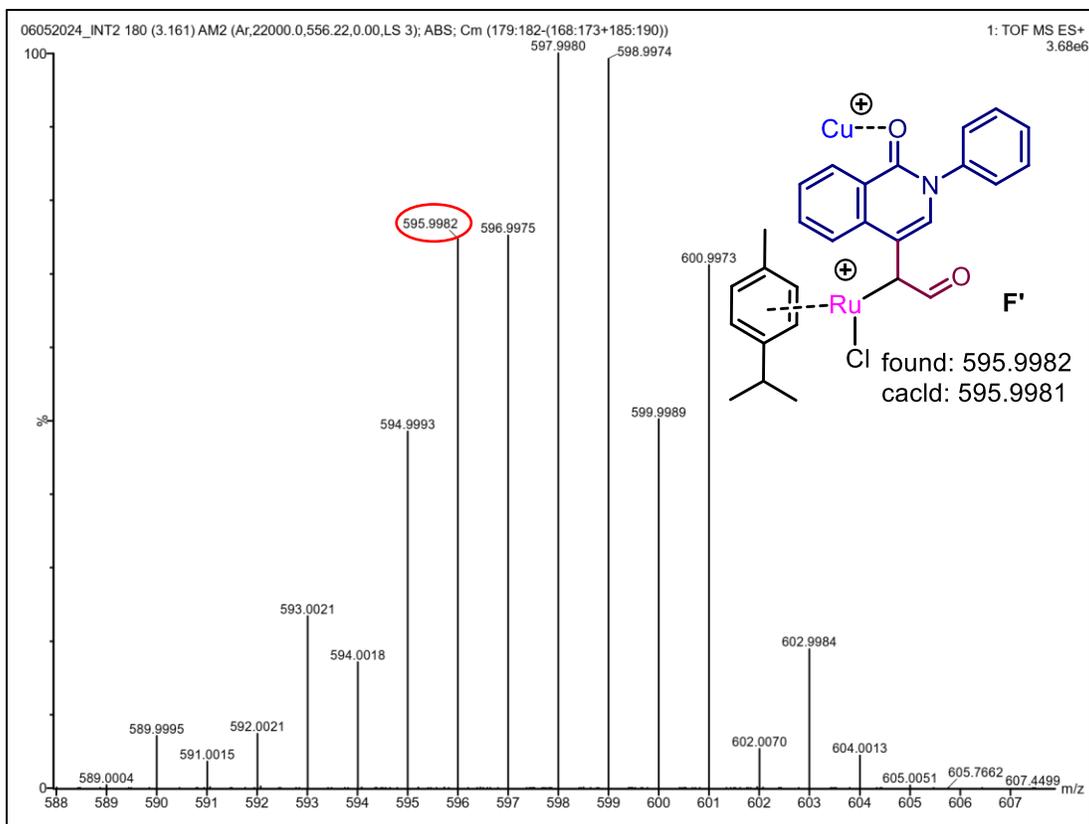
To an oven-dried Schlenk tube (15 mL) equipped with a stir bar was charged with 1 mL of HFIP and isoquinolinone **1a** (0.22 mmol, 2 equiv) and Vinylene carbonate **2** (1 equiv.) To this reaction mixture, $[\text{Ru}(p\text{-cymene})\text{Cl}_2]_2$ (5 mol%), AgSbF_6 (20 mol%) and $\text{Cu}(\text{OAc})_2$ (50 mol%) .The tube was flushed with nitrogen and screw capped under nitrogen flow and placed in a preheated oil bath at 120 °C for 30 min. This reaction mixture was subjected to mass spectrometry analysis (ESI-HRMS) (Scheme S10).





Scheme S11. Methylenation of isoquinolones





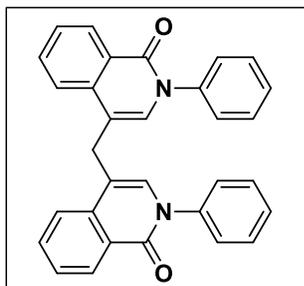
9. Characterization Data:

4,4'-methylenebis(2-phenylisoquinolin-1(2*H*)-one) (3a)

Purified by column chromatography on silica gel using (hexane/ethyl acetate = 80/20)

Yield: 38 mg, 78%, off-white coloured solid

Gram scale: 141 mg, 67%

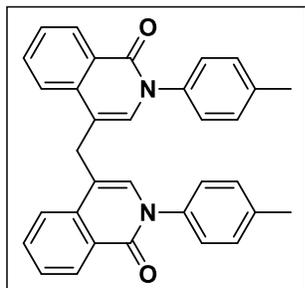


¹H NMR (400 MHz, CDCl₃) δ : 8.46 (d, J = 8.04 Hz, 2H), 7.64 (dt, J = 7.96 Hz, 2H), 7.60 (d, J = 7.88 Hz, 2H), 7.48 (t, J = 7.2 Hz, 2H), 7.33 (t, J = 7.6 Hz, 4H), 7.26 (t, J = 7.08 Hz, 2H), 7.2 (d, J = 7.9 Hz, 4H), 6.84 (s, 2H), 4.05 (s, 2H).

¹³C{¹H} NMR (100 MHz, CDCl₃) δ : 161.6, 141.1, 136.4, 132.7, 131.5, 129.2, 129.0, 128.0, 127.4, 126.7, 126.6, 122.8, 112.6, 29.3.

HR-MS: [M+H]⁺ calculated for C₃₁H₂₂N₂O₂, 477.1573 found, 477.1563.

4,4'-methylenebis(2-(p-tolyl)isoquinolin-1(2H)-one) (3b)



Purified by column chromatography on silica gel using (hexane/ethyl acetate = 84/16)

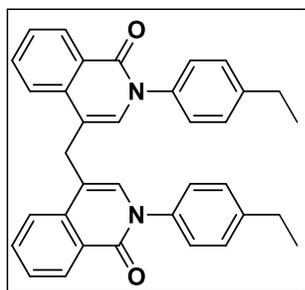
Yield: 27 mg, 54%, off-white coloured solid

¹H NMR (400 MHz, CDCl₃) δ: 8.47 (d, *J* = 8.04 Hz, 2H), 7.67 (dt, *J* = 8.0 Hz, 2H), 7.61 (d, *J* = 7.48 Hz, 2H), 7.50 (t, *J* = 7.0 Hz, 2H), 7.15 (d, *J* = 8.32 Hz, 4H), 7.09 (d, *J* = 8.32 Hz, 4H), 6.83 (s, 2H), 4.06 (s, 2H), 2.29 (s, 6H).

¹³C{¹H} NMR (100 MHz, CDCl₃) δ: 161.7, 138.5, 138.0, 136.4, 132.6, 131.7, 129.8, 129.0, 127.3, 126.6, 126.4, 122.84, 112.5, 29.3, 21.1.

HR-MS: [M+H]⁺ calculated for C₃₃H₂₆N₂NaO₂⁺, 505.1886; found, 505.1886.

4,4'-methylenebis(2-(4-ethylphenyl)isoquinolin-1(2H)-one) (3c)



Purified by column chromatography on silica gel using (hexane/ethyl acetate = 80/20)

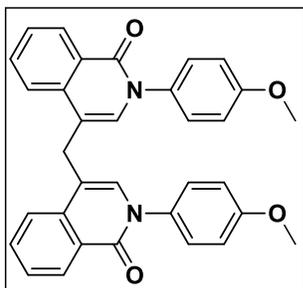
Yield: 36 mg, 71%, off-white coloured solid

¹H NMR (400 MHz, CDCl₃) δ: 8.46 (d, *J* = 8.0 Hz, 2H), 7.65 (t, *J* = 7.2 Hz, 2H), 7.60 (t, *J* = 5.64, 2H), 7.47 (t, *J* = 6.8 Hz, 2H), 7.16 (d, *J* = 8.32 Hz, 4H), 7.11 (d, *J* = 8.36 Hz, 4H), 6.83 (s, 2H), 4.04 (s, 2H), 2.61-2.55 (m, 4H), 1.15 (t, *J* = 7.52 Hz, 6H).

¹³C{¹H} NMR (100 MHz, CDCl₃) δ: 161.7, 144.2, 138.7, 136.4, 132.6, 131.7, 129.0, 128.7, 127.3, 126.6, 126.4, 122.8, 112.5, 29.3, 28.5, 15.4.

HR-MS: [M+Na]⁺ calculated for C₃₅H₃₀N₂O₂Na, 534.2272; found, 534.2233.

4,4'-methylenebis(2-(4-methoxyphenyl)isoquinolin-1(2H)-one) (3d)



Purified by column chromatography on silica gel using (hexane/ethyl acetate = 84/16)

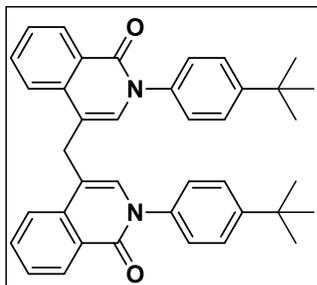
Yield: 28 mg, 56%, off-white coloured solid

¹H NMR (400 MHz, CDCl₃) δ: 8.44 (d, *J* = 7.64 Hz, 2H), 7.65 (td, *J* = 8.08 Hz, 2H), 7.61 (d, *J* = 7.2, 2H), 7.46 (td, *J* = 7.96 Hz, 2H), 7.11 (d, *J* = 8.8 Hz, 4H), 6.83 (s, 2H), 6.81 (d, *J* = 2.88, 4H), 4.03 (s, 2H), 3.70 (s, 6H)

¹³C{¹H} NMR (100 MHz, CDCl₃) δ: 161.9, 159.1, 136.4, 133.9, 132.6, 131.9, 128.9, 127.7, 127.3, 126.5, 122.8, 114.4, 112.5, 55.5, 29.3

HR-MS: $[M+H]^+$ calculated for $C_{33}H_{26}N_2O_4Na$, 537.1785; found, 537.1772.

4,4'-methylenebis(2-(4-(tert-butyl)phenyl)isoquinolin-1(2H)-one) (3e)



Purified by column chromatography on silica gel using (hexane/ethyl acetate = 84/16)

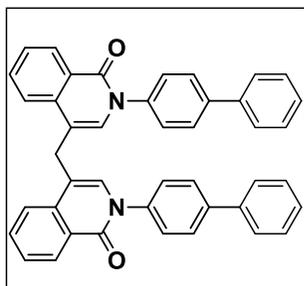
Yield: 24 mg, 48%, off-white coloured solid

1H NMR (400 MHz, $CDCl_3$) δ : 8.49 (d, $J = 7.88$ Hz, 2H), 7.66 (td, $J = 8.08$ Hz, 2H), 7.61 (d, $J = 7.24$, 2H), 7.50 (td, $J = 8.04$ Hz, 2H), 7.37 (d, $J = 8.56$ Hz, 2H), 7.15 (d, $J = 8.56$ Hz, 2H), 6.86 (s, 2H), 4.06 (s, 2H), 1.25 (s, 18H)

$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ : 161.6, 141.0, 136.4, 132.7, 131.5, 129.2, 129.0, 128.1, 126.6, 126.6, 122.8, 112.6, 30.0, 29.7, 29.3.

HR-MS: $[M+H]^+$ calculated for $C_{39}H_{39}N_2O_2$, 567.3006; found, 567.3007.

4,4'-methylenebis(2-([1,1'-biphenyl]-4-yl)isoquinolin-1(2H)-one) (3f)



Purified by column chromatography on silica gel using (hexane/ethyl acetate = 84/16)

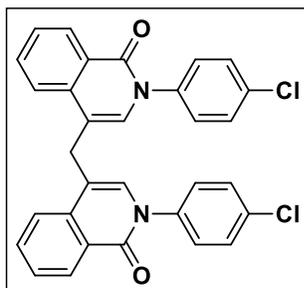
Yield: 12 mg, 36%, off-white coloured solid

1H NMR (400 MHz, $CDCl_3$) δ : 8.52 (d, $J = 7.92$ Hz, 2H), 7.69 (td, $J = 6.84$ Hz, 2H), 7.65 (d, $J = 7.2$, 2H), 7.56 (d, $J = 8.52$ Hz, 4H), 7.51 (d, $J = 7.12$ Hz, 6H), 7.37 (t, $J = 7.24$, 4H), 7.31 (d, $J = 8.44$, 6H), 6.9 (s, 2H), 4.11 (s, 2H)

$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ : 161.7, 141.1, 140.1, 140.1, 136.4, 132.8, 131.4, 129.0, 128.8, 128.0, 127.7, 127.5, 127.2, 126.9, 126.5, 122.9, 112.8, 29.4

HR-MS: $[M+H]^+$ calculated for $C_{43}H_{31}N_2O_2$, 607.2380; found, 607.2374.

4,4'-methylenebis(2-(4-chlorophenyl)isoquinolin-1(2H)-one) (3g)



Purified by column chromatography on silica gel using (hexane/ethyl acetate = 80/20)

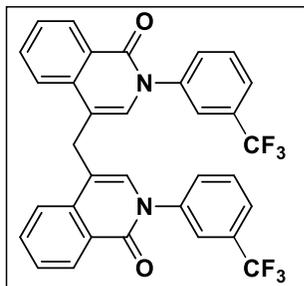
Yield: 37 mg, 73%, off-white coloured solid

1H NMR (400 MHz, $CDCl_3$) δ : 8.45 (d, $J = 7.96$ Hz, 2H), 7.67 (dt, $J = 8.12$ Hz, 2H), 7.60 (d, $J = 7.68$, 2H), 7.50 (td, $J = 7.12$ Hz, 2H), 7.30 (d, $J = 4.68$ Hz, 2H), 7.15 (d, $J = 8.68$ Hz, 2H), 6.7 (s, 2H), 4.03 (s, 2H).

$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ : 161.5, 139.4, 133.9, 132.9, 131.0, 129.0, 129.0, 128.0, 127.6, 122.9, 112.9, 29.3.

HR-MS: $[M+Na]^+$ calculated for $C_{31}H_{21}Cl_2N_2O_2$, 523.0975; found, 523.0975.

4,4'-methylenebis(2-(3-(trifluoromethyl)phenyl)isoquinolin-1(2H)-one) (3h)



Purified by column chromatography on silica gel using (hexane/ethyl acetate = 84/16)

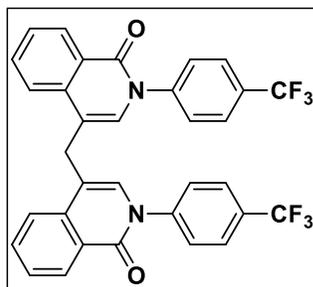
Yield: 30 mg, 60%, off-white coloured solid

1H NMR (400 MHz, $CDCl_3$) δ : 8.44 (d, $J = 7.52$ Hz, 2H), 7.70 (td, $J = 8.16$ Hz, 2H), 7.62 (d, $J = 7.64$ Hz, 2H), 7.52 (d, $J = 7.08$ Hz, 4H), 7.52 (t, $J = 6.84$ Hz, 4H), 7.43 (d, $J = 7.88$ Hz, 2H), 6.81 (s, 2H), 4.09 (s, 2H).

$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ : 161.5, 141.3, 136.3, 133.1, 132.2, 131.9, 131.6, 131.3, 130.8, 130.2, 129.9, 129.0, 127.8, 126.4, 124.9, 124.8, 124.8, 124.8, 123.8, 123.8, 123.7, 123.0, 122.1, 113.2, 29.3.

HR-MS: $[M+H]^+$ calculated for $C_{33}H_{21}F_6N_2O_2$, 591.1502; found, 591.1506.

4,4'-methylenebis(2-(4-(trifluoromethyl)phenyl)isoquinolin-1(2H)-one) (3i)



Purified by column chromatography on silica gel using (hexane/ethyl acetate = 84/16)

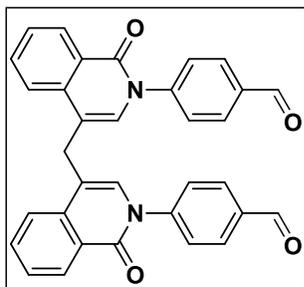
Yield: 32 mg, 64%, off-white coloured solid

1H NMR (400 MHz, $CDCl_3$) δ : 8.45 (d, $J = 8.0$ Hz, 2H), 7.70 (td, $J = 8.16$ Hz, 2H), 7.62 (d, $J = 7.84$ Hz, 2H), 7.58 (d, $J = 8.44$ Hz, 4H), 7.52 (td, $J = 7.08$ Hz, 2H), 7.34 (d, $J = 8.28$ Hz, 4H), 6.81 (s, 2H), 4.08 (s, 2H).

$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ : 161.4, 143.8, 136.2, 133.1, 130.6, 130.3, 129.9, 129.6, 127.8, 127.7, 126.5, 126.4, 126.4, 126.4, 125.0, 123.0, 122.3, 113.2, 29.4.

HR-MS: $[M+H]^+$ calculated for $C_{33}H_{21}F_6N_2O_2$, 591.1502; found, 591.1506.

4,4'-(methylenebis(1-oxoisoquinoline-4,2(1H)-diyl)dibenzaldehyde) (3j)



Purified by column chromatography on silica gel using (hexane/ethyl acetate = 84/16)

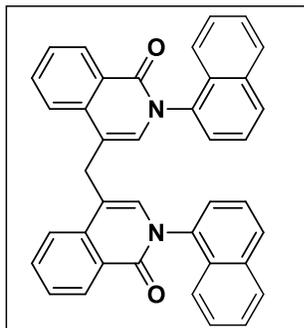
Yield: 17 mg, 36%, off-white coloured solid

1H NMR (400 MHz, $CDCl_3$) δ : 9.96 (s, 2H), 8.48 (d, $J = 8.0$ Hz, 2H), 7.89 (d, $J = 8.48$ Hz, 4H), 7.74 (td, $J = 6.92$ Hz, 2H), 7.65 (d, $J = 7.52$ Hz, 2H), 7.55 (td, $J = 7.0$ Hz, 2H), 7.43 (d, $J = 8.36$ Hz, 4H), 6.85 (s, 2H), 4.1 (s, 2H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) δ : 199.09, 162.4, 141.4, 139.1, 136.4, 132.3, 132.2, 131.5, 129.4, 128.2, 126.9, 126.3, 124.3, 106.7, 50.4.

HR-MS: $[\text{M}+\text{H}]^+$ calculated for $\text{C}_{33}\text{H}_{23}\text{N}_2\text{O}_4$, 511.1652; found, 511.1654.

4,4'-methylenebis(2-(naphthalen-1-yl)isoquinolin-1(2H)-one) (3k)



Purified by column chromatography on silica gel using (hexane/ethyl acetate = 84/16)

Yield: 27 mg, 54%, off-white coloured solid

^1H NMR (400 MHz, CDCl_3) δ : 8.45 (d, $J = 7.92$ Hz, 2H), 7.83 (d, $J = 8.0$, 2H), 7.81 (d, $J = 7.28$ Hz, 2H), 7.70 (s, 2H), 7.53 – 7.48 (m, 3H), 7.44 (d, $J = 8.12$, 2H), 7.40 – 7.37 (m, 2H), 7.34 (t, $J = 6.44$ Hz, 2H), 7.26 (t, $J = 7.12$ Hz, 1H), 7.21 (d, $J = 4.92$ Hz, 2H), 7.18 (s, 1H), 7.05 (td, $J = 7.28$ Hz, 1H), 6.8 (s, 2H), 4.1 (s, 2H).

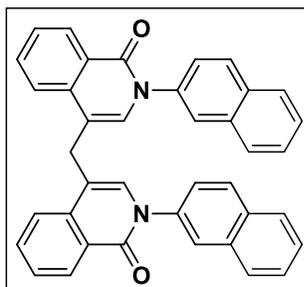
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) δ : 162.0, 162.0, 137.7, 137.5, 136.6, 134.4, 134.4, 132.8, 132.8, 132.5, 132.4, 129.5, 129.5, 129.3, 129.1, 128.5, 128.4, 127.4, 127.2, 127.2, 126.6, 126.6, 126.5, 126.5, 125.5, 125.4, 125.4, 122.9, 122.9, 122.2, 122.1, 112.6, 112.5, 29.3.

HR-MS: $[\text{M}+\text{H}]^+$ calculated for $\text{C}_{39}\text{H}_{27}\text{N}_2\text{O}_2$, 555.2067; found, 555.2066.

4,4'-methylenebis(2-(naphthalen-2-yl)isoquinolin-1(2H)-one) (3l)

Purified by column chromatography on silica gel using (hexane/ethyl acetate = 84/16)

Yield: 24mg, 48%, off-white coloured solid

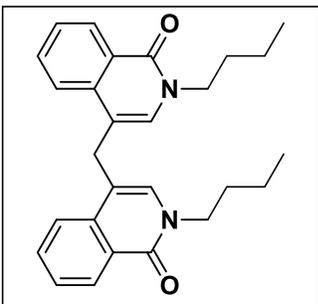


^1H NMR (400 MHz, CDCl_3) δ : 8.45 (d, $J = 7.84$ Hz, 2H), 7.80 (d, $J = 8.8$, 2H), 7.77 (d, $J = 3.56$ Hz, 2H), 7.70 (d, $J = 1.08$, 2H), 7.68 – 7.66 (m, 4H), 7.61 (s, 2H), 7.55 (t, $J = 1.2$ Hz, 3H), 7.44 – 7.40 (m, 3H), 7.39 (d, $J = 2$ Hz, 1H), 7.37 (d, $J = 2$ Hz, 1H), 6.9 (s, 2H), 4.1 (s, 2H)

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) δ : 161.8, 138.7, 136.5, 133.3, 132.8, 132.5, 131.8, 129.0, 128.0, 127.7, 127.4, 126.7, 126.7, 126.6, 125.0, 124.7, 122.9, 112.8, 29.4.

HR-MS: $[\text{M}+\text{H}]^+$ calculated for $\text{C}_{39}\text{H}_{27}\text{N}_2\text{O}_2$, 555.2067; found, 555.2066.

4,4'-methylenebis(2-butylisoquinolin-1(2H)-one) (3m)



Purified by column chromatography on silica gel using (hexane/ethyl acetate = 85/15)

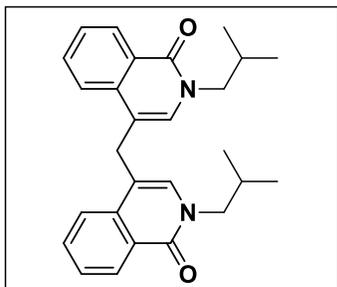
Yield: 42 mg, 82%, off-white coloured solid

¹H NMR (400 MHz, CDCl₃) δ: 8.46 (d, *J* = 8.0 Hz, 2H), 7.59 (t, *J* = 7.0 Hz, 2H), 7.53 (d, *J* = 7.76 Hz, 2H), 7.44 (t, *J* = 7.0 Hz, 2H), 6.62 (s, 2H), 3.99 (s, 2H), 3.81 (t, *J* = 7.2 Hz, 4H), 1.15 (m, 4H), 1.17 (m, 4H), 0.76 (t, *J* = 7.36, 6H).

¹³C{¹H} NMR (100 MHz, CDCl₃) δ: 160.7, 135.2, 131.1, 130.2, 127.4, 125.8, 125.2, 121.6, 111.4, 47.9, 30.1, 28.2, 18.7, 12.6.

HR-MS: [M+H]⁺ calculated for C₂₇H₃₁N₂O₂, 415.2380; found, 415.2389.

4,4'-methylenebis(2-isobutylisoquinolin-1(2H)-one) (3n)



Purified by column chromatography on silica gel using (hexane/ethyl acetate = 84/16)

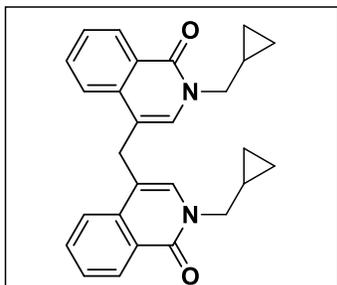
Yield: 35 mg, 68%, off-white coloured solid

¹H NMR (400 MHz, CDCl₃) δ: 8.44 (d, *J* = 7.96 Hz, 2H), 7.58 (td, *J* = 8.0 Hz, 2H), 7.51 (d, *J* = 7.36 Hz, 2H), 7.43 (td, *J* = 6.8 Hz, 2H), 6.5 (s, 2H), 3.9 (s, 2H), 3.5 (d, *J* = 7.4 Hz, 4H), 2.05-1.9 (m, 2H), 0.7 (d, *J* = 6.7 Hz, 12H).

¹³C{¹H} NMR (100 MHz, CDCl₃) δ: 161.9, 136.2, 132.2, 131.8, 128.5, 126.9, 126.2, 122.7, 112.1, 56.1, 29.1, 28.0, 19.8.

HR-MS: [M+H]⁺ calculated for C₂₇H₃₁N₂O₂, 415.2380; found, 415.2385.

4,4'-methylenebis(2-(cyclopropylmethyl)isoquinolin-1(2H)-one) (3o)



Purified by column chromatography on silica gel using (hexane/ethyl acetate = 84/16)

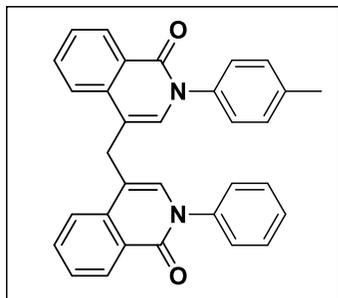
Yield: 34 mg, 67%, off-white coloured solid

¹H NMR (400 MHz, CDCl₃) δ: 8.45 (d, *J* = 8.08 Hz, 2H), 7.58 (td, *J* = 7.92 Hz, 2H), 7.56 (d, *J* = 7.32 Hz, 2H), 7.47 (td, *J* = 6.8 Hz, 2H), 6.75 (s, 2H), 4.04 (s, 2H), 3.7 (d, *J* = 7.08 Hz, 4H), 1.18 (s, 2H), 0.36-0.34 (m, 4H), 0.15-0.11 (m, 4H).

¹³C{¹H} NMR (100 MHz, CDCl₃) δ: 161.9, 136.3, 132.2, 130.9, 128.5, 126.9, 126.2, 122.7, 112.4, 53.0, 29.4, 10.6, 3.6.

HR-MS: $[M+H]^+$ calculated for $C_{27}H_{26}N_2O_2$, 411.2067; found, 411.2069.

4-((1-oxo-2-(p-tolyl)-1,2-dihydroisoquinolin-4-yl)methyl)-2-phenylisoquinolin-1(2H)-one (3p)



Purified by column chromatography on silica gel using (hexane/ethyl acetate = 84/16)

Yield: 12 mg, 23%, off-white coloured solid

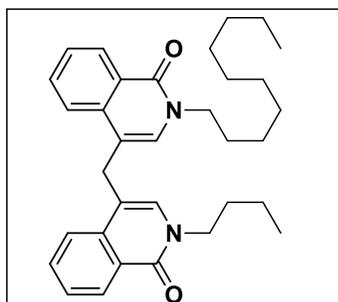
1H NMR (400 MHz, $CDCl_3$) δ : 8.48 (d, $J = 7.76$ Hz, 2H), 7.66 (dt, $J = 6.92$ Hz, 2H), 7.62 (d, $J = 8.16$ Hz, 2H), 7.50 (td, $J = 6.88$ Hz, 2H), 7.37 (t, $J = 7.04$ Hz, 2H), 7.29 (t, $J = 7.56$ Hz, 1H), 7.15 (d, $J = 7.44$ Hz, 2H), 7.15 (d, $J = 8.28$ Hz, 2H), 7.09 (d, $J = 8.32$ Hz, 2H),

6.86 (s, 1H), 6.83 (s, 1H), 4.07 (s, 2H), 2.29 (s, 3H).

$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ : 16179, 136.3, 136.3, 132.1, 132.1, 131.2, 131.2, 128.5, 1226.9, 126.3, 122.7, 122.6, 112.5, 112.4, 49.3, 49.0, 31.9, 31.2, 29.6, 29.5, 29.4, 29.3, 29.2, 29.2, 26.6, 22.6, 19.8, 19.1, 14.1, 13.6.

HR-MS: $[M+H]^+$ calculated for $C_{32}H_{25}N_2O_2$, 469.1911; found, 469.1911.

2-butyl-4-((2-decyl-1-oxo-1,2-dihydroisoquinolin-4-yl)methyl)isoquinolin-1(2H)-one (3q)



Purified by column chromatography on silica gel using (hexane/ethyl acetate = 84/16)

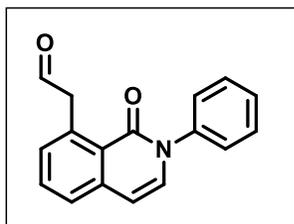
Yield: 13 mg, 23%, off-white coloured solid

1H NMR (400 MHz, $CDCl_3$) δ : 8.45 (d, $J = 7.88$ Hz, 2H), 7.58 (td, $J = 6.96$ Hz, 2H), 7.54 (d, $J = 4.8$ Hz, 2H), 7.47 (td, $J = 7.92$ Hz, 2H), 6.62 (d, $J = 8.4$, 2H), 4.0 (s, 2H), 3.8-3.7 (m, 4H), 1.56-1.53 (m, 4H), 1.15 (d, $J = 8.04$, 16H), 0.81-0.75 (m, 6H).

$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ : 16179, 136.3, 136.3, 132.1, 132.1, 131.2, 131.2, 128.5, 1226.9, 126.3, 122.7, 122.6, 112.5, 112.4, 49.3, 49.0, 31.9, 31.2, 29.6, 29.5, 29.4, 29.3, 29.2, 29.2, 26.6, 22.6, 19.8, 19.1, 14.1, 13.6.

HR-MS: $[M+H]^+$ calculated for $C_{17}H_{15}N_2O_2$, 279.1128; found, 279.1129.

2-(1-oxo-2-phenyl-1,2-dihydroisoquinolin-8-yl)acetaldehyde (4a)



Purified by column chromatography on silica gel using (hexane/ethyl acetate = 84/16)

Yield: 36 mg, 61%, off-white coloured solid

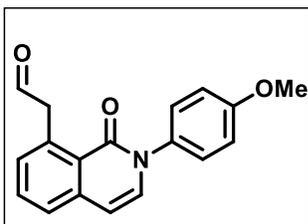
¹H NMR (400 MHz, CDCl₃) δ: 9.80 (br, 1H), 7.53 (t, *J* = 7.84 Hz, 1H), 7.44 (td, *J* = 8.16 Hz, 2H), 7.41 (d, *J* = 1.52 Hz, 1H), 7.35 (td, *J* = 7.48 Hz, 1H), 7.32-7.30 (m, 1H), 7.22-7.29 (m, 1H), 7.16 (d, *J* = 7.16 Hz, 1H), 7.10 (d, *J* = 7.32 Hz, 1H), 6.49 (d, *J* = 7.76 Hz, 1H), 4.25 (s, 2H).s

¹³C{¹H} NMR (100 MHz, CDCl₃) δ: 199.0, 162.4, 141.4, 139.1, 136.4, 132.3 (d, *J* = 21.2 Hz), 131.5, 129.4, 128.2, 126.9, 126.3, 124.3, 106.7, 50.4.

HR-MS: [M+H]⁺ calculated for C₁₇H₁₄NO₂, 264.1019; found, 264.1060

2-(2-(4-methoxyphenyl)-1-oxo-1,2-dihydroisoquinolin-8-yl)acetaldehyde (4b)

Purified by column chromatography on silica gel using (hexane/ethyl acetate = 84/16)



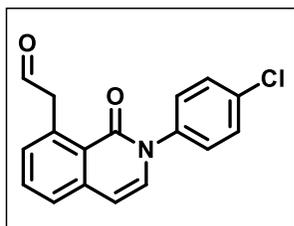
Yield: 36 mg, 63%, off-white coloured solid

¹H NMR (400 MHz, CDCl₃) δ: 9.79 (br, 1H), 7.53 (t, *J* = 7.52 Hz, 1H), 7.42 (dd, *J* = 6.92 Hz, 1H), 7.20 (d, *J* = 8.96 Hz, 2H), 7.15 (d, *J* = 7.04 Hz, 1H), 7.07 (d, *J* = 7.32 Hz, 1H), 6.92-6.90 (m, 2H), 6.46 (d, *J* = 7.36 Hz, 1H), 4.23 (s, 2H), 3.76 (s, 3H).

¹³C{¹H} NMR (100 MHz, CDCl₃) δ: 199.1, 162.6, 159.2, 139.1, 136.4, 134.2, 132.6, 132.1, 131.4, 128.0, 126.2, 124.3, 114., 106.5, 55.5, 50.4.

HR-MS: [M+H]⁺ calculated for C₁₈H₁₆NO₃, 294.1125; found, 294.1149.

2-(2-(4-chlorophenyl)-1-oxo-1,2-dihydroisoquinolin-8-yl)acetaldehyde (4c)



Purified by column chromatography on silica gel using (hexane/ethyl acetate = 84/16)

Yield: 32 mg, 54%, off-white coloured solid

¹H NMR (400 MHz, CDCl₃) δ: 9.80 (br, 1H), 7.56 (t, *J* = 8.12 Hz, 1H), 7.53 (d, *J* = 7.72 Hz, 1H), 7.44 (d, *J* = 7.92 Hz, 1H), 7.39 (d, *J* = 8.48 Hz, 2H), 7.25 (d, *J* = 8.44 Hz, 2H), 7.05 (d, *J* = 7.36 Hz, 1H), 6.50 (d, *J* = 7.4 Hz, 1H), 4.24 (s, 2H).

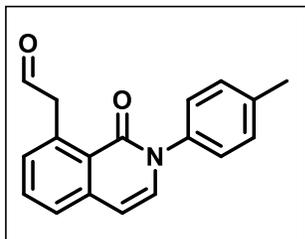
¹³C{¹H} NMR (100 MHz, CDCl₃) δ: 198.9, 162.3, 139.0, 136.4, 134.1, 132.4, 131.7, 131.7, 129.6, 128.3, 126.3, 107.1, 50.4.

HR-MS: [M+H]⁺ calculated for C₁₇H₁₃ClNO₂, 298.0629; found, 298.0623.

2-(1-oxo-2-(p-tolyl)-1,2-dihydroisoquinolin-8-yl)acetaldehyde (4d)

Purified by column chromatography on silica gel using (hexane/ethyl acetate = 84/16)

Yield: 30 mg, 51%, off-white coloured solid



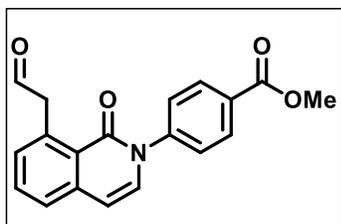
^1H NMR (400 MHz, CDCl_3) δ : 9.68 (br, 1H), 7.54 (t, $J = 7.76$ Hz, 1H), 7.44 (d, $J = 7.24$ Hz, 1H), 7.23 (d, $J = 8.32$ Hz, 3H), 7.18 (d, $J = 3.0$ Hz, 2H), 7.10 (d, $J = 7.32$ Hz, 1H), 6.51 (d, $J = 7.32$ Hz, 1H), 4.22 (s, 2H), 2.3 (s, 3H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) δ : 198.1, 161.4, 137.9, 137.2, 135.3, 131.4, 131.1, 130.4, 128.9, 127.9, 125.6, 125.2, 105.5, 49.4,

20.1.

HR-MS: $[\text{M}+\text{H}]^+$ calculated for $\text{C}_{17}\text{H}_{14}\text{NO}_2$, 264.1019; found, 264.1060

2-(1-oxo-2-phenyl-1,2-dihydroisoquinolin-8-yl)acetaldehyde (4e)



Purified by column chromatography on silica gel using (hexane/ethyl acetate = 84/16)

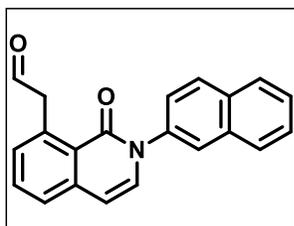
Yield: 17 mg, 34%, off-white coloured solid

^1H NMR (400 MHz, CDCl_3) δ : 9.81 (br, 1H), 7.74 (t, $J = 7.8$ Hz, 1H), 7.63 (d, $J = 4.24$ Hz, 1H), (t, $J = 7.6$ Hz, 2H), 7.39 (d, $J = 7.92$ Hz, 2H), 7.13 (d, $J = 7.32$ Hz, 1H), 7.0 (d, $J = 7.2$ Hz, 1H), 4.2 (s, 3H), 3.4 (s, 2H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) δ : 193.7, 172.3, 146.5, 139.4, 135.5, 132.6, 132.5, 132.0, 131.8, 131.6, 131.4, 131.1, 129.9, 126.5, 126.1, 109.8, 108.69, 106.2, 86.51, 39.01, 37.3.

HR-MS: $[\text{M}+\text{H}]^+$ calculated for $\text{C}_{18}\text{H}_{16}\text{NNaO}_3^{2+}$, 317.1017; found, 317.1086.

2-(2-(naphthalen-2-yl)-1-oxo-1,2-dihydroisoquinolin-8-yl)acetaldehyde (4f)



Purified by column chromatography on silica gel using (hexane/ethyl acetate = 84/16)

Yield: 30 mg, 53%, off-white coloured solid

^1H NMR (400 MHz, CDCl_3) δ : 9.80 (br, 1H), 7.87 (d, $J = 8.64$ Hz, 1H), 7.81-7.76 (m, 3H), 7.73 (br, 1H), 7.53 (t, $J = 7.72$ Hz, 1H), 7.46 (s, 1H),

7.44-7.42 (m, 2H), 7.40 (d, $J = 1.92$ Hz, 1H), 7.17 (d, $J = 6.8$ Hz, 1H), 6.53 (d, $J = 7.32$ Hz, 1H), 4.25 (s, 2H).

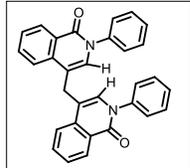
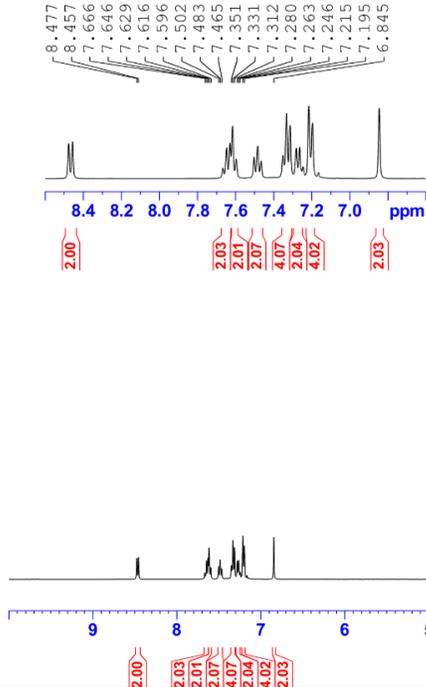
$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) δ : 199.1, 162.6, 139.2, 139.0, 136.4, 133.5, 132.7, 132.4, 132.3, 131.5, 129.2, 128.0, 127.8, 126.8, 126.7, 126.3, 125.2, 125.0, 124.3, 106.9, 50.4.

HR-MS: $[\text{M}+\text{H}]^+$ calculated for $\text{C}_{21}\text{H}_{16}\text{NO}_2$, 314.1176; found, 314.1205.

9.1. NMR data

¹H NMR of 3a

Signature SIF VIT VELLORE
N-PHT-DUMER



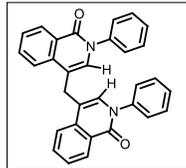
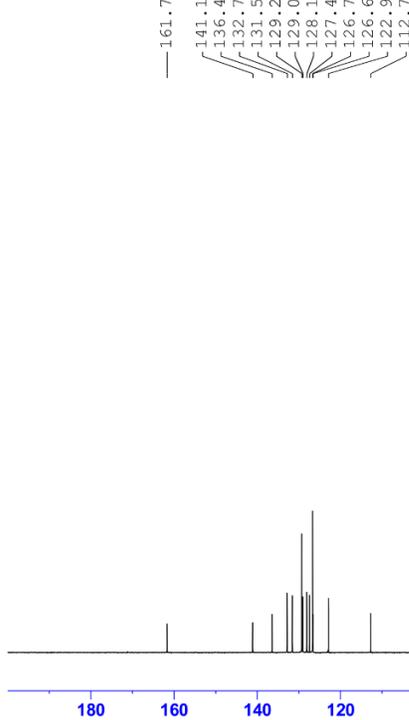
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TD 65536
SOLVENT CDCl3
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DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 71.13
DW 62.400 usec
DE 6.50 usec
TE 305.8 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 14.95499992 W

F2 - Processing parameters
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SF 400.2580479 MHz
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LB 0.30 Hz
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PC 1.00

¹³C NMR of 3a

Signature SIF VIT VELLORE
N-PHE-DUMON



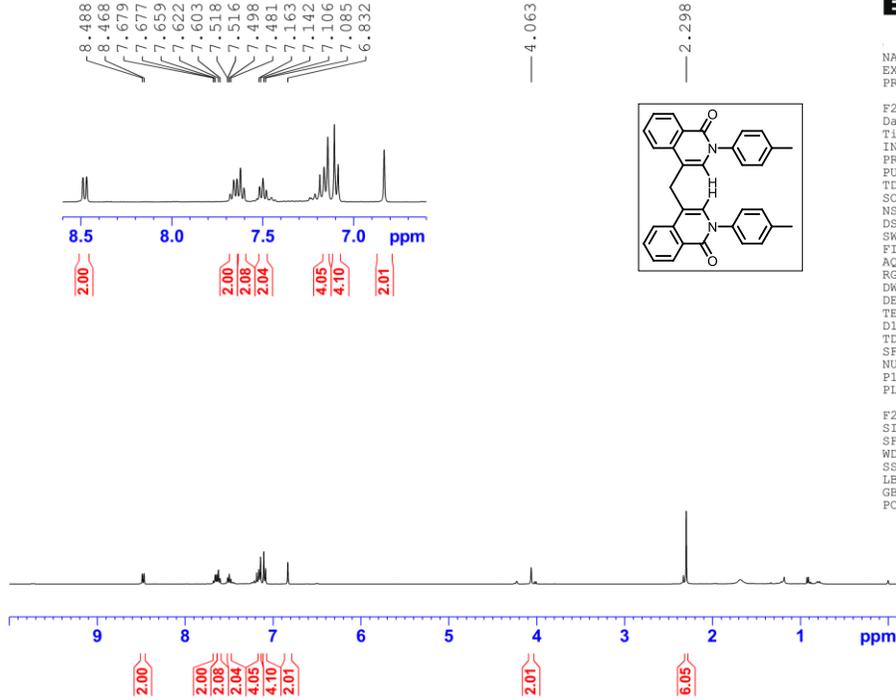
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TD 65536
SOLVENT CDCl3
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DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 304.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 58.22499847 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG(2) waltz16
PCPD2 90.00 usec
PLM2 14.95499992 W
PLM12 0.41542000 W
PLM13 0.20895000 W

F2 - Processing parameters
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WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

¹H NMR of 3b

Signature SIF VIT VELLORE
4MEDIM



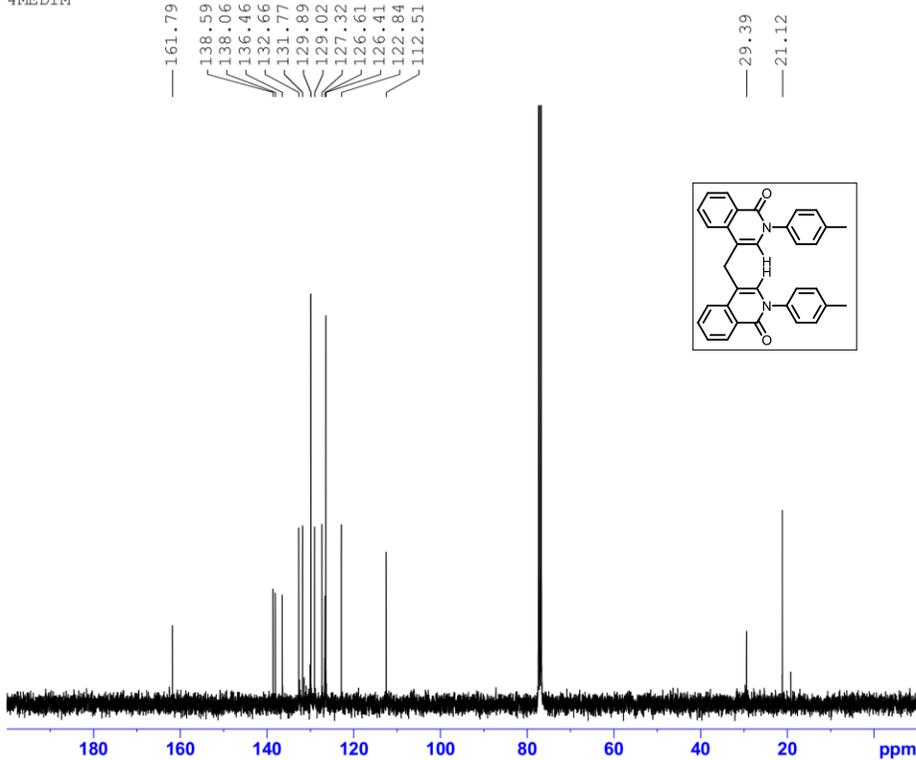
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EXPNO 106
PROCNO 1

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PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 156.91
DW 62.400 usec
DE 6.50 usec
TE 303.8 K
D1 1.00000000 sec
TDO 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
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SSB 0
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PC 1.00

¹³C NMR of 3b

Signature SIF VIT VELLORE
4MEDIM



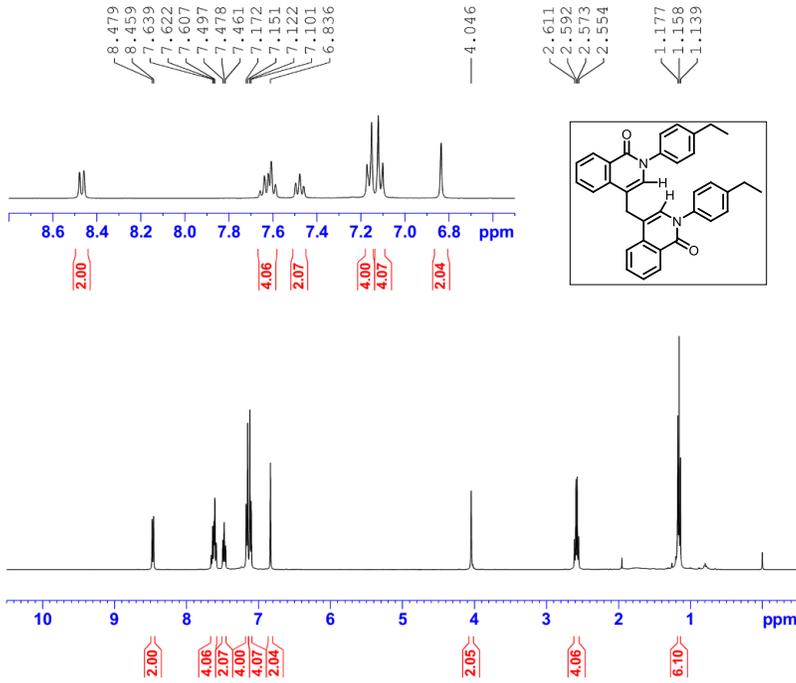
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EXPNO 107
PROCNO 1

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DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 304.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.21399975 W
PLW12 0.42261001 W
PLW13 0.21257000 W

F2 - Processing parameters
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SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

¹H NMR of 3c

Signature SIF VIT VELLORE
4-ETHYL-DIMER



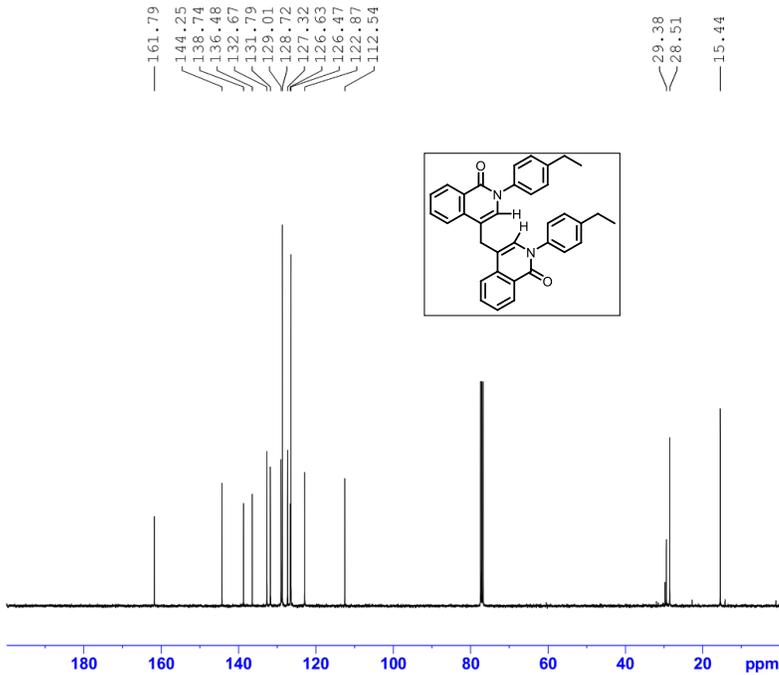
Current Data Parameters
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EXPNO 41
PROCNO 1

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PULPROG 65536
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SOLVENT CDCl3
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DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 63.11
DW 62.400 usec
DE 6.50 usec
TE 306.5 K
D1 1.00000000 sec
TDO 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 14.95499992 W

F2 - Processing parameters
SI 65536
SF 400.2580476 MHz
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LB 0.30 Hz
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PC 1.00

¹³C NMR of 3c

Signature SIF VIT VELLORE
4-ETHYL DIMER



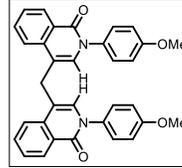
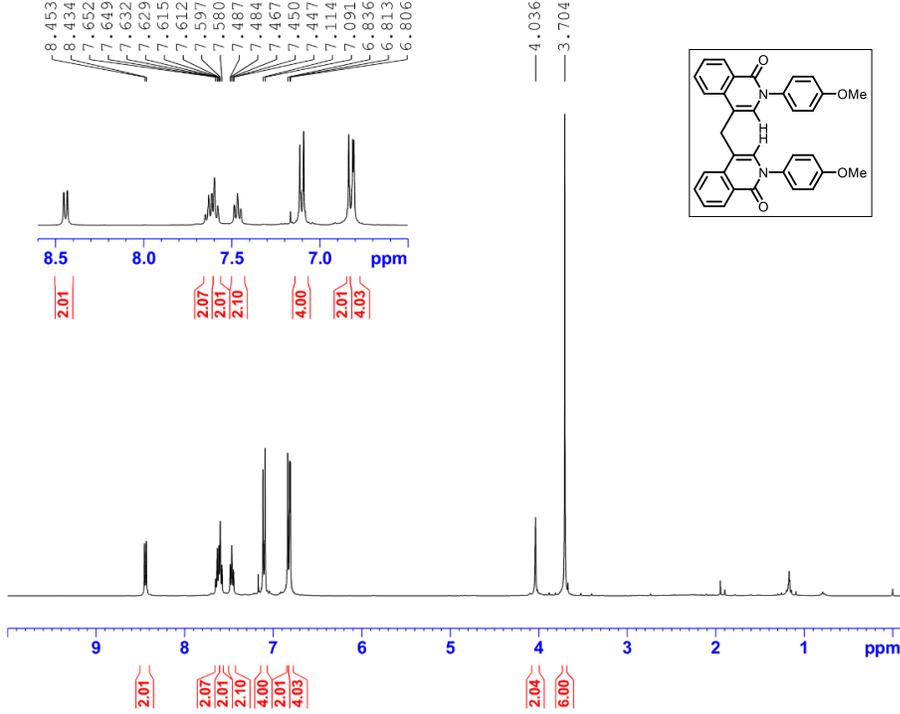
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EXPNO 56
PROCNO 1

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TD 65536
SOLVENT CDCl3
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DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3531488 sec
RG 112.69
DW 20.800 usec
DE 6.50 usec
TE 305.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLM1 58.22499847 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLM2 14.95499992 W
PLM12 0.41542000 W
PLM13 0.20895000 W

F2 - Processing parameters
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SF 100.6449542 MHz
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LB 1.00 Hz
GB 0
PC 1.40

¹H NMR of 3d

Signature SIF VIT VELLORE
4-M2O-PHE-DEMEN



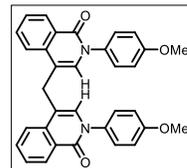
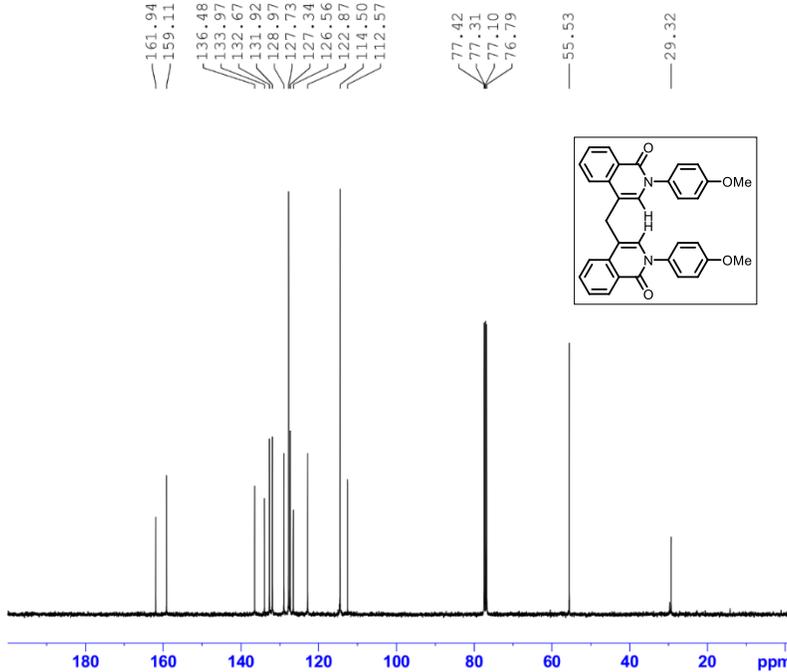
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EXPNO 54
PROCNO 1

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DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 58.47
DW 62.400 usec
DE 6.50 usec
TE 303.3 K
D1 1.0000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 14.95499992 W

F2 - Processing parameters
SI 65536
SF 400.2580471 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C NMR of 3d

Signature SIF VIT VELLORE
4-MEO-N-PHE-DUMN



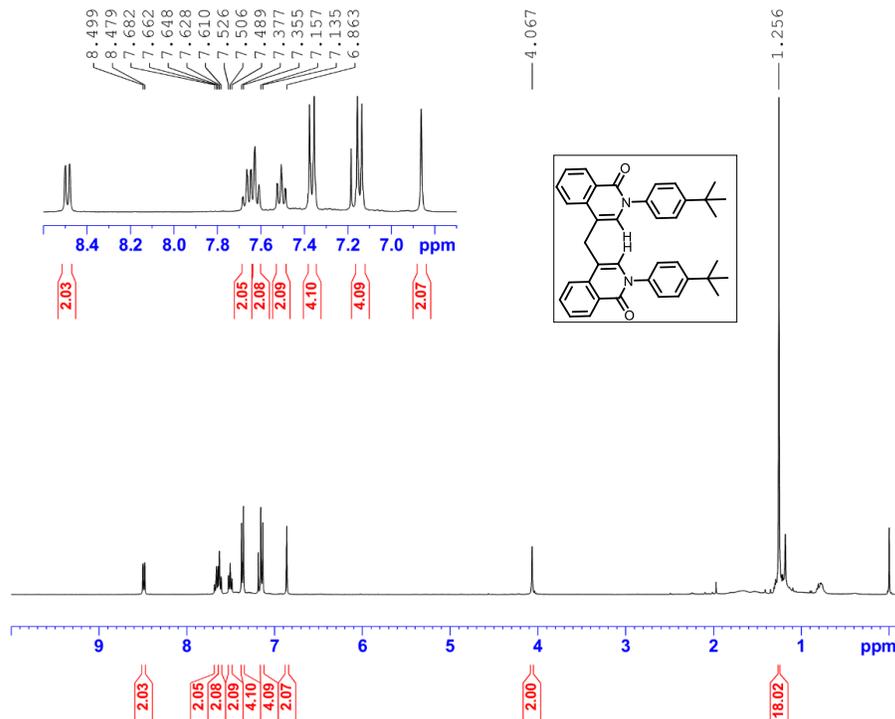
Current Data Parameters
NAME Dr.GTV300323
EXPNO 92
PROCNO 1

F2 - Acquisition Parameters
Date 20230330
Time 15.25 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 305.7 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 58.22499847 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W
PLW13 0.20895000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

¹H NMR of 3e

Signature SIF VIT VELLORE
NP-4-TBU-DIMER



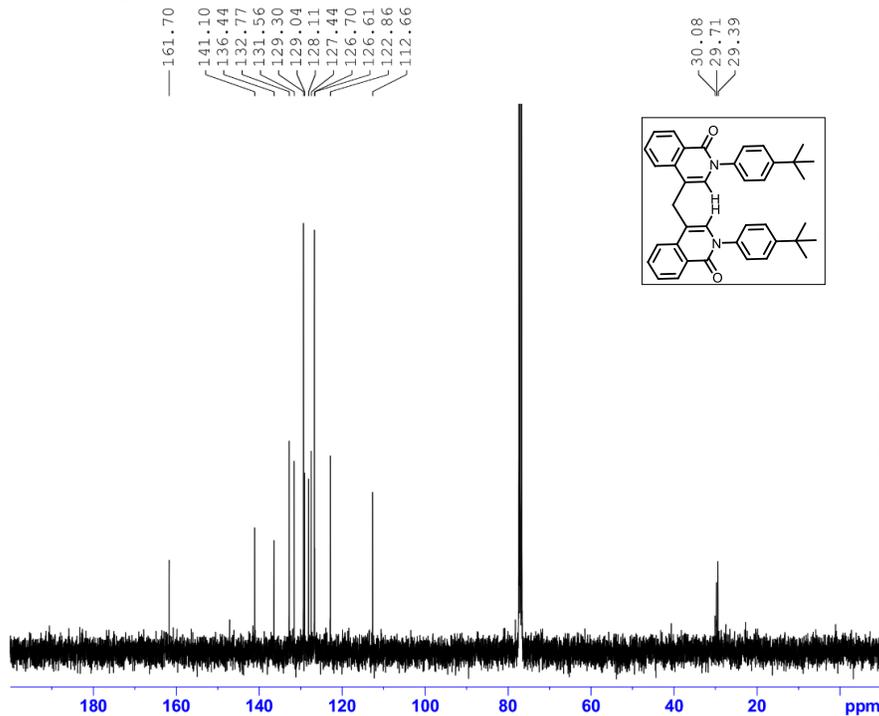
Current Data Parameters
NAME Dr.NAP21023
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231020
Time_ 14.00 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 127.79
DW 62.400 usec
DE 6.50 usec
TE 305.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 14.95499992 W

F2 - Processing parameters
SI 65536
SF 400.2580396 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C NMR of 3e

Signature SIF VIT VELLORE
N-7-TBU-DIMER



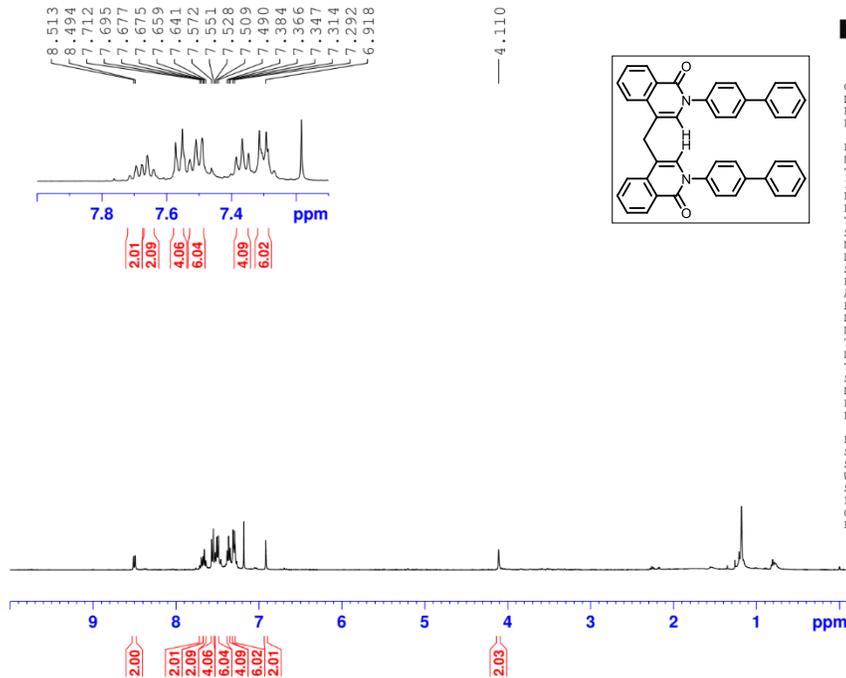
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NAME Dr.GTV90124
EXPNO 29
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240110
Time_ 0.22 h
INSTRUM spect
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 303.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.21399975 W
PLW12 0.42261001 W
PLW13 0.21257000 W

F2 - Processing parameters
SI 32768
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WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

¹H NMR of 3f

Signature SIF VIT VELLORE
NBIPED



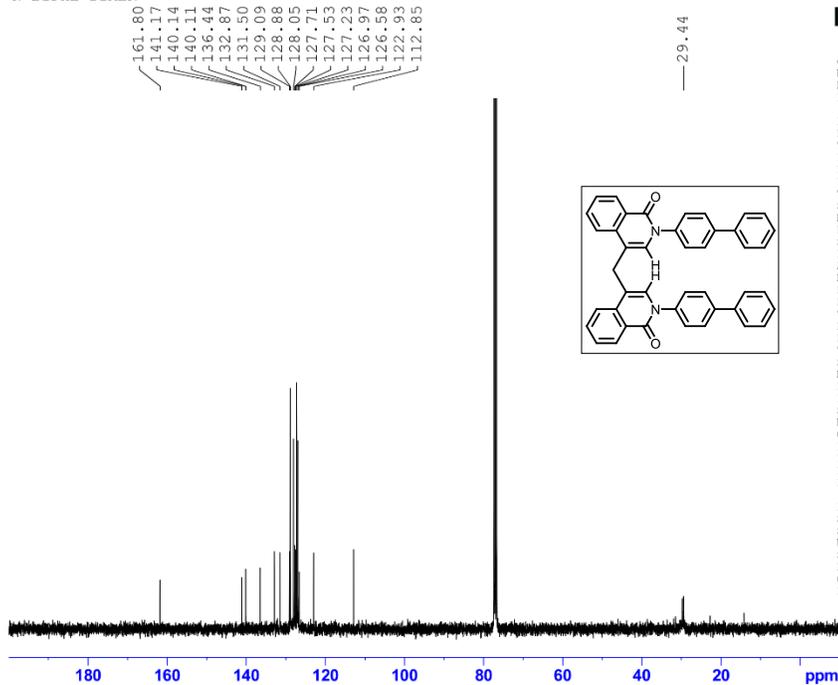
Current Data Parameters
NAME Dr.GTV290724
EXPNO 64
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240729
Time 15.29 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 143.73
DM 62.400 usec
DE 6.50 usec
TE 303.7 K
D1 1.00000000 sec
TDO 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580404 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C NMR of 3f

Signature SIF VIT VELLORE
N-BIPHE-DIMER



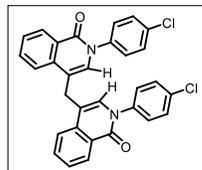
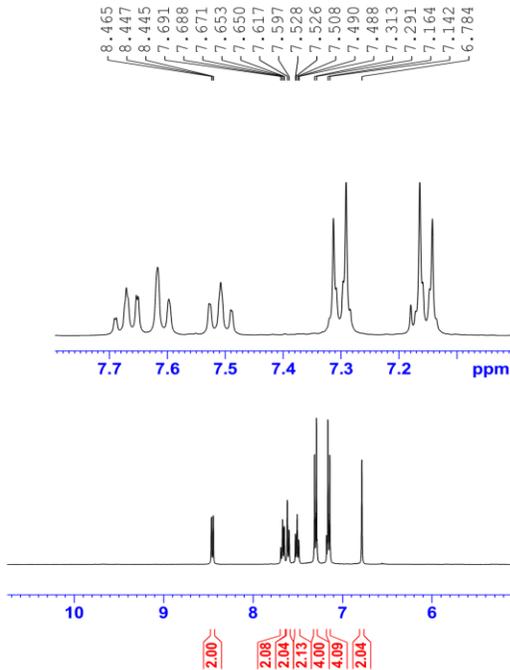
Current Data Parameters
NAME Dr.GTV040124
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240104
Time 20.34 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 156.91
DM 20.800 usec
DE 6.50 usec
TE 301.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLM2 15.21399975 W
PLM12 0.42261001 W
PLM13 0.21257000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

¹H NMR of 3g

Signature SIF VIT VELLORE
N-4-CL-ALD



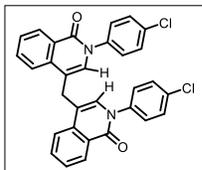
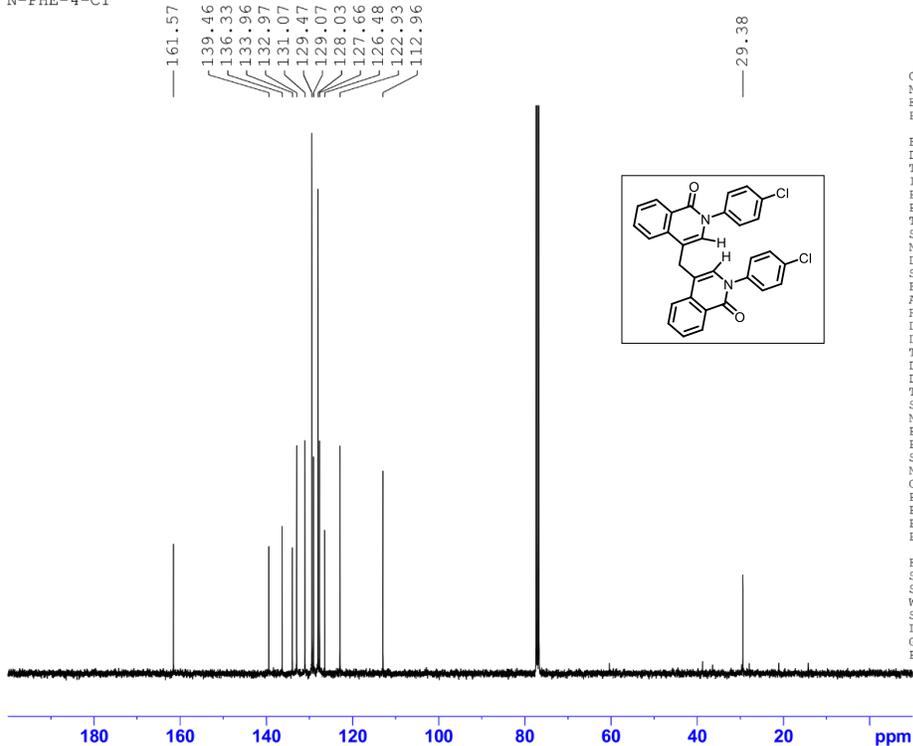
Current Data Parameters
NAME Dr.LKA180323
EXPNO 83
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230318
Time 13:48 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 88.69
DW 62.400 usec
DE 6.50 usec
TE 303.9 K
D1 1.0000000 sec
TDO 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 14.95499992 W

F2 - Processing parameters
SI 65536
SF 400.2580418 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C NMR of 3g

Signature SIF VIT VELLORE
N-PHE-4-CT



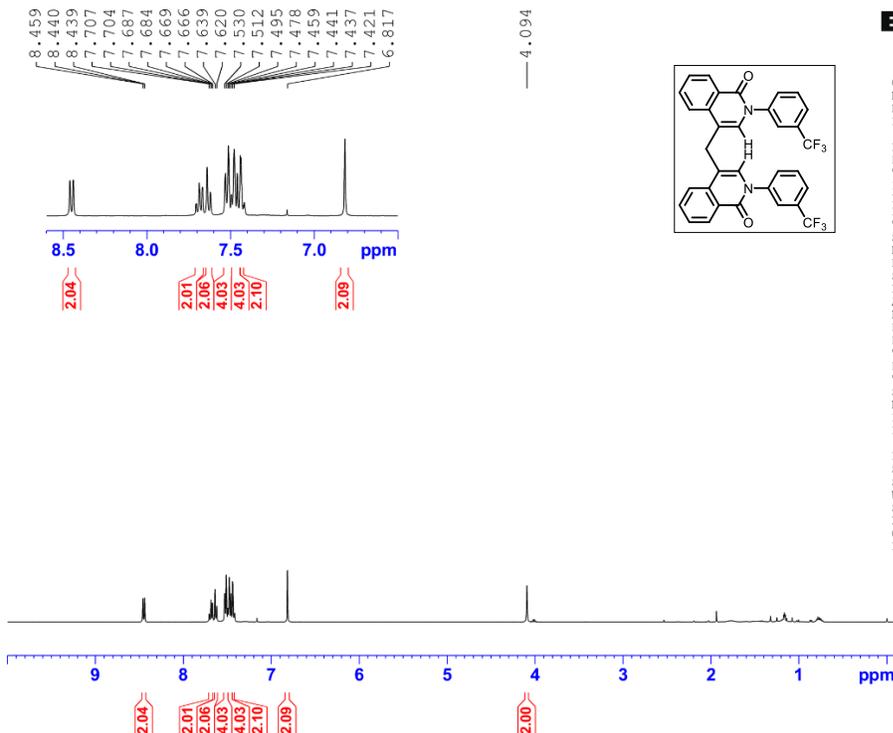
Current Data Parameters
NAME C13
EXPNO 58
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230320
Time 19:12 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 304.9 K
D1 2.0000000 sec
D11 0.0300000 sec
TDO 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 58.22499847 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W
PLW13 0.20895000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

¹H NMR of 3h

Signature SIF VIT VELLORE
N-3-CF₃-DIMER



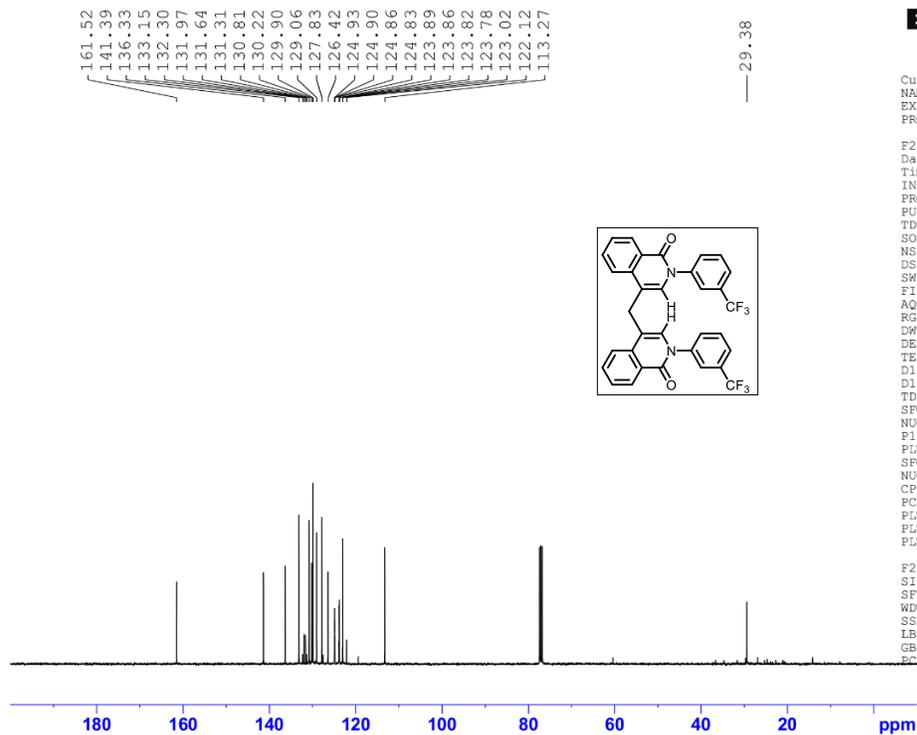
Current Data Parameters
NAME Dr.RGL131023
EXPNO 24
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231013
Time 16.22 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 58.47
DW 62.400 usec
DE 6.50 usec
TE 305.1 K
D1 1.0000000 sec
TDO 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 14.95499992 W

F2 - Processing parameters
SI 65536
SF 400.2580488 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C NMR of 3h

Signature SIF VIT VELLORE
3-CF₃-DIMER



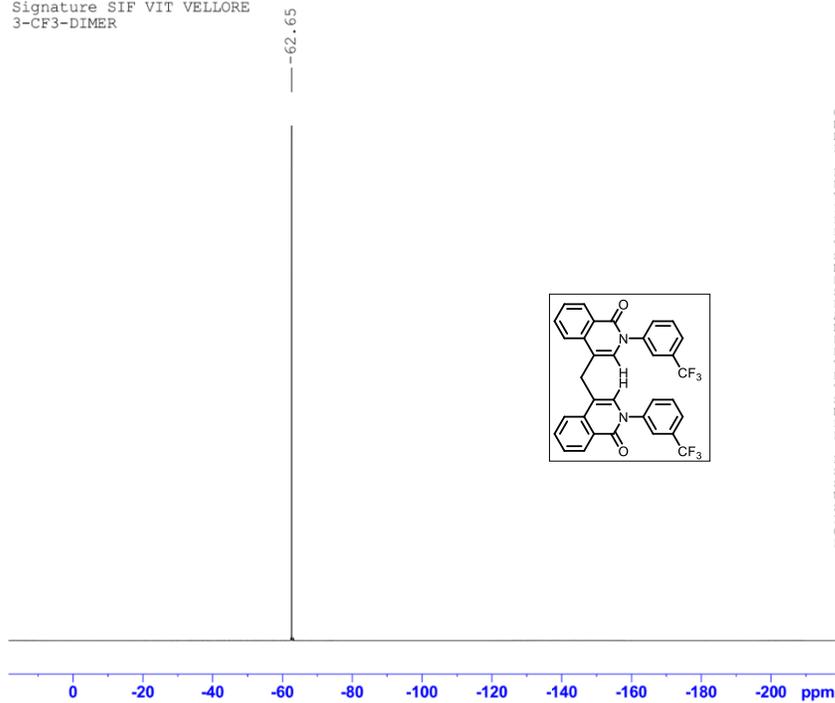
Current Data Parameters
NAME Dr.GTV161023
EXPNO 45
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231017
Time 11.32 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 306.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TDO 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 58.22499847 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W
PLW13 0.20895000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

¹⁹F NMR of 3h

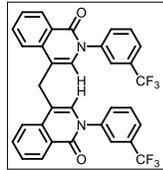
Signature SIF VIT VELLORE
3-CF₃-DIMER



Current Data Parameters
NAME Dr.GTV161023
EXPNO 44
PROCNO 1

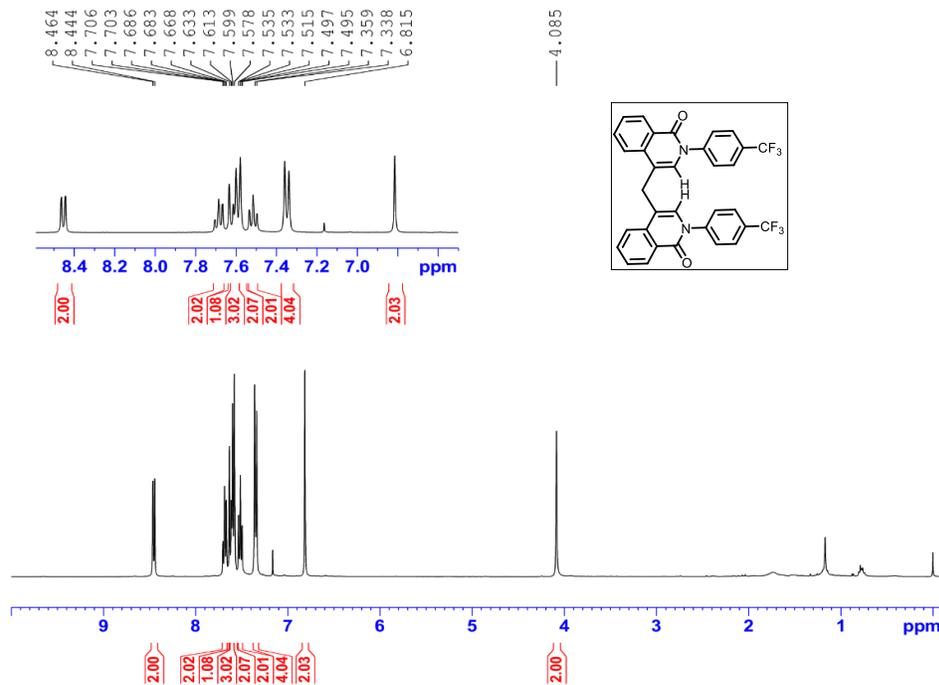
F2 - Acquisition Parameters
Date_ 20231017
Time 11.00 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgpg30
TD 131072
SOLVENT CDCl₃
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 1.362392 Hz
AQ 0.7340032 sec
RG 199.6
DW 5.600 usec
DE 6.50 usec
TE 305.7 K
D1 1.00000000 sec
TDO 1
SFO1 376.5811447 MHz
NUC1 19F
P1 15.00 usec
PLW1 20.11800003 W

F2 - Processing parameters
SI 65536
SF 376.6188065 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹H NMR of 3i

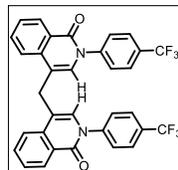
Signature SIF VIT VELLORE
N-4-CF₃-DIMER



Current Data Parameters
NAME Dr.GTV171023
EXPNO 47
PROCNO 1

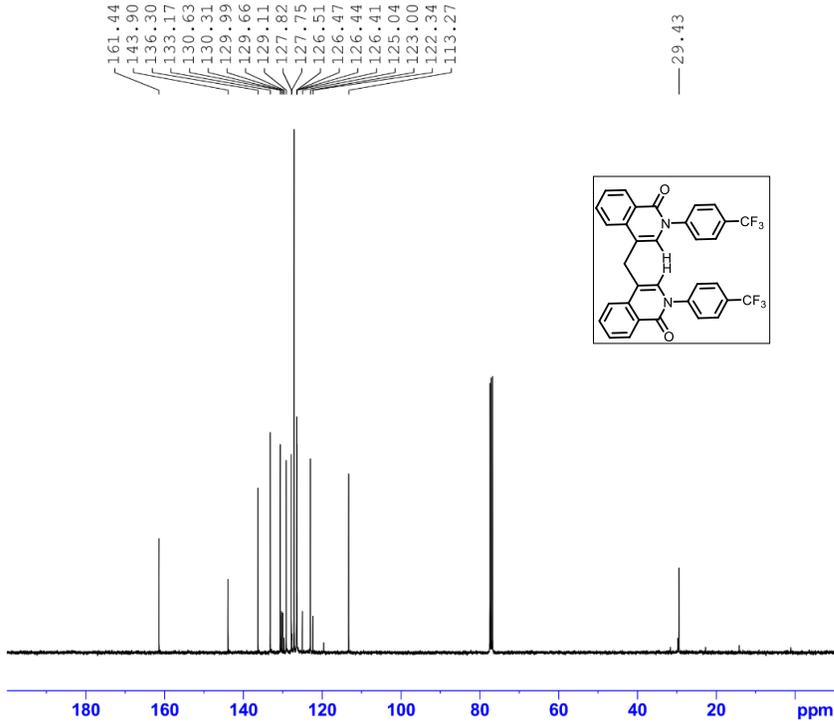
F2 - Acquisition Parameters
Date_ 20231017
Time 18.02 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 71.13
DW 62.400 usec
DE 6.50 usec
TE 305.2 K
D1 1.00000000 sec
TDO 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 14.95499992 W

F2 - Processing parameters
SI 65536
SF 400.2580482 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C NMR of 3i

Signature SIF VIT VELLORE
N-4-CF₃-DIMER



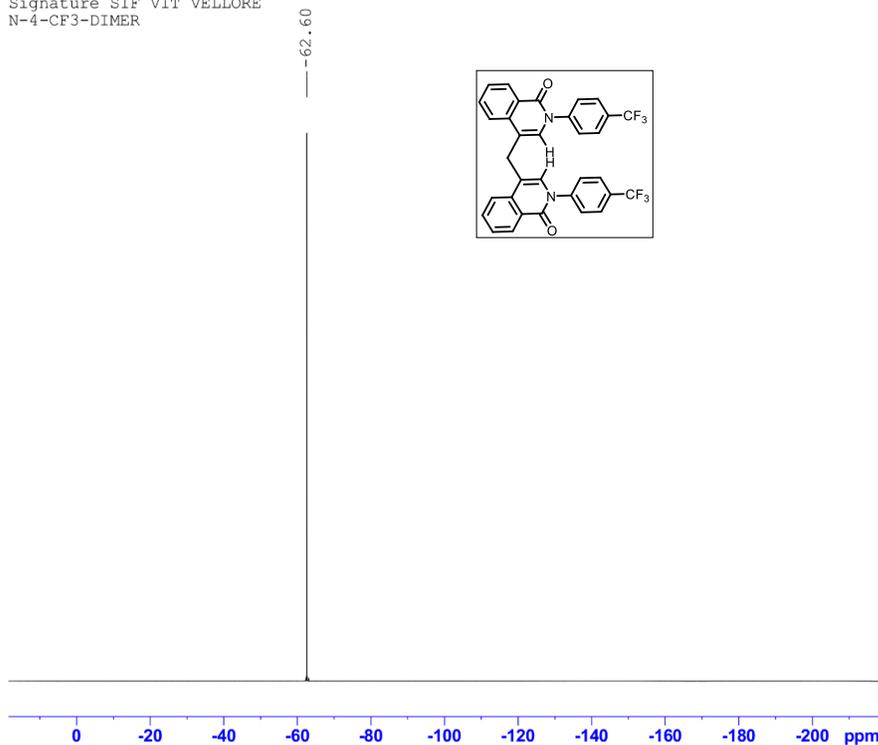
Current Data Parameters
NAME Dr.GTV191023
EXPNO 61
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231020
Time 5.13 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 306.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
F1 10.00 usec
PLW1 58.22499847 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W
PLW13 0.20895000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
FC 1.40

¹⁹F NMR of 3i

Signature SIF VIT VELLORE
N-4-CF₃-DIMER



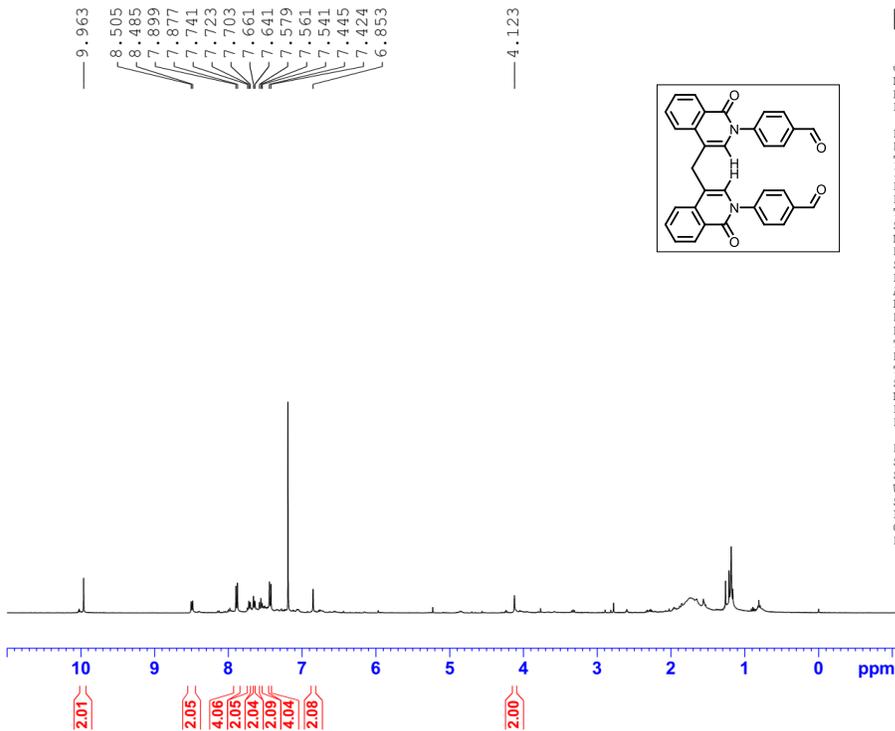
Current Data Parameters
NAME Dr.GTV171023
EXPNO 48
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231017
Time 18.04 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zgflgn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 1.362392 Hz
AQ 0.7340032 sec
RG 199.6
DW 5.600 usec
DE 6.50 usec
TE 305.3 K
D1 1.00000000 sec
TD0 1
SFO1 376.5811447 MHz
NUC1 19F
F1 15.00 usec
PLW1 20.11800003 W

F2 - Processing parameters
SI 65536
SF 376.6188065 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
FC 1.00

¹H NMR of 3j

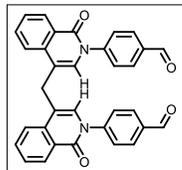
Signature SIF VIT VELLORE
N-BENZ-OLD-DIMER



Current Data Parameters
NAME Dr.GTV120923
EXPNO 46
PROCNO 1

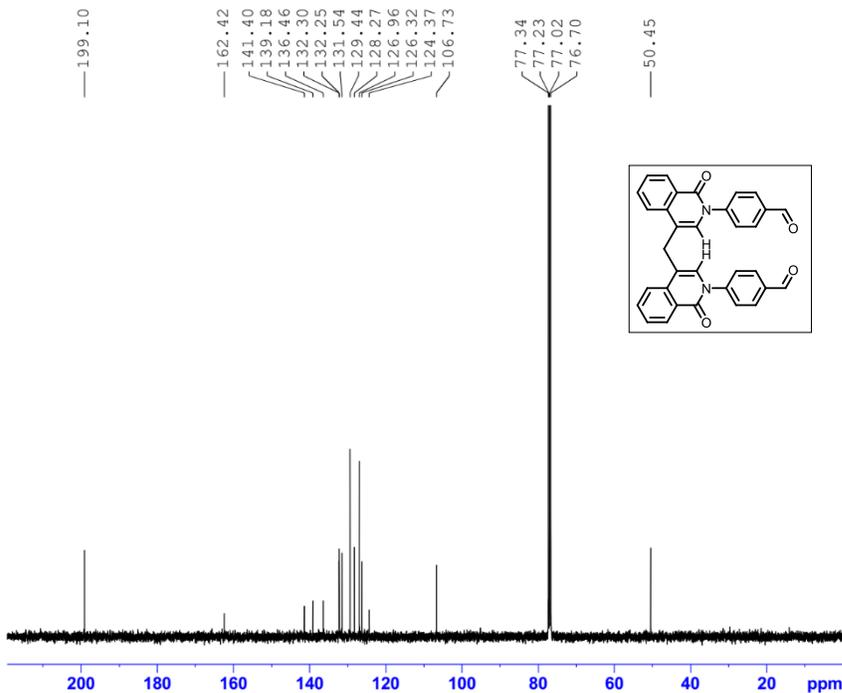
F2 - Acquisition Parameters
Date_ 20230912
Time 15.08 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 199.6
DW 62.400 usec
DE 6.50 usec
TE 305.8 K
D1 1.00000000 sec
*TDO 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 14.95499992 W

F2 - Processing parameters
SI 65536
SF 400.2580367 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹H NMR of 3j

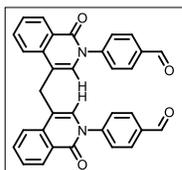
Signature SIF VIT VELLORE
N-BEN-ALD



Current Data Parameters
NAME Dr.GTV151222
EXPNO 38
PROCNO 1

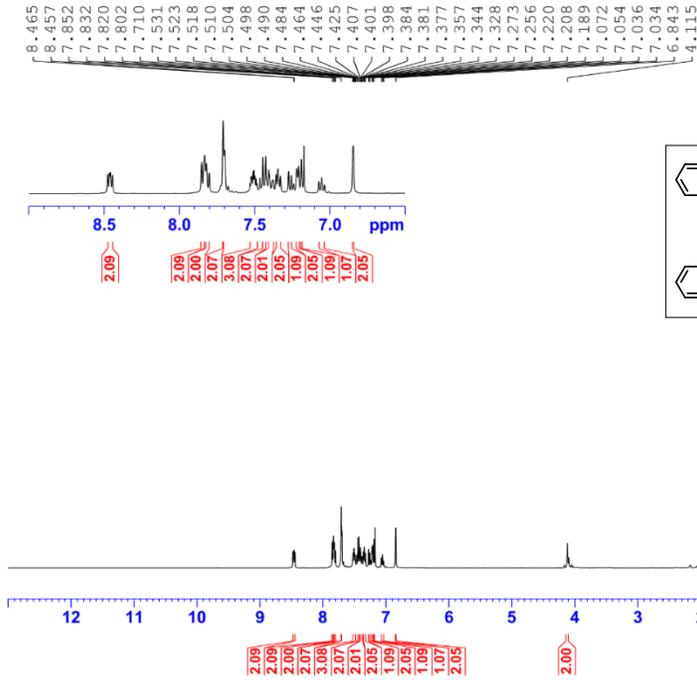
F2 - Acquisition Parameters
Date_ 20221215
Time 0.57 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 304.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 58.22499847 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCFD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W
PLW13 0.20895000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



¹H NMR of 3k

Signature SIF VIT VELLORE
N-1-NAPH-DIMER



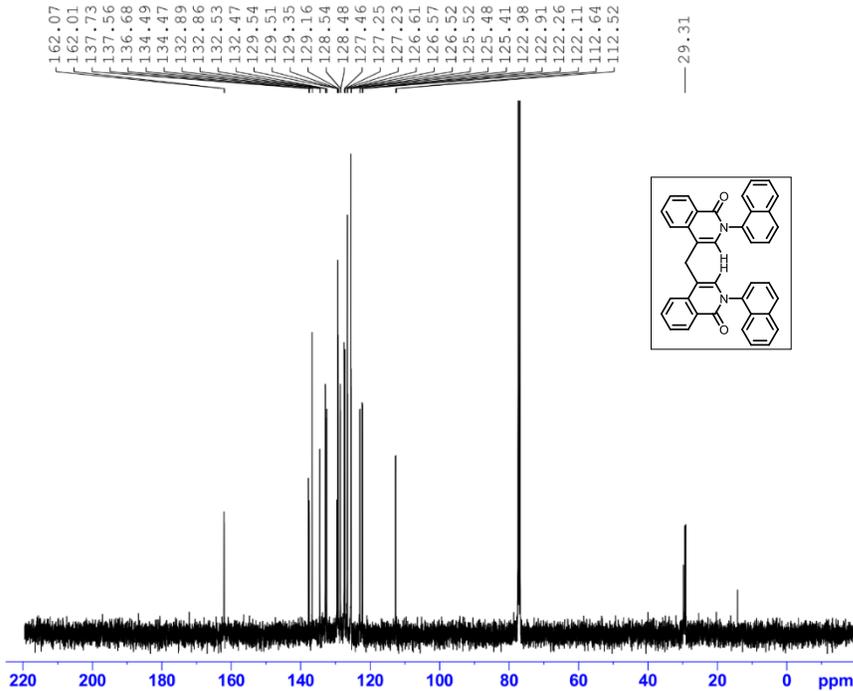
Current Data Parameters
NAME Dr.RGL131023
EXPNO 25
PROCNO 1

F2 - Acquisition Parameters
Date 20231013
Time 20.22 h
INSTRUM spect
PROBHD z108618_0505 (1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 112.69
DW 62.400 usec
DE 6.50 usec
TE 305.5 K
D1 1.0000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 14.95499992 W

F2 - Processing parameters
SI 65536
SF 400.2580448 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C NMR of 3k

Signature SIF VIT VELLORE
N-1-NAPH-DIMER



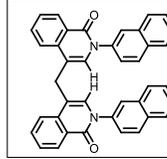
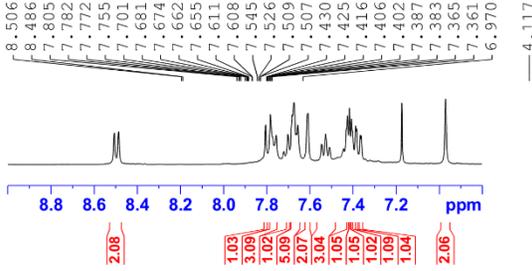
Current Data Parameters
NAME Dr.RGL131023
EXPNO 26
PROCNO 1

F2 - Acquisition Parameters
Date 20231013
Time 20.53 h
INSTRUM spect
PROBHD z108618_0505 (1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 306.1 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 58.22459847 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 30.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W
PLW13 0.20895000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

¹H NMR of 3I

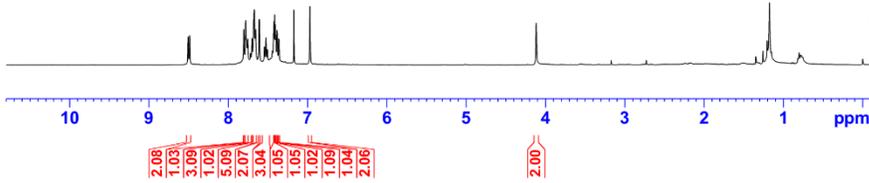
Signature SIF VIT VELLORE
N2NAPH



Current Data Parameters
NAME Dr.GTV290724
EXPNO 62
PROCNO 1

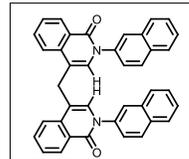
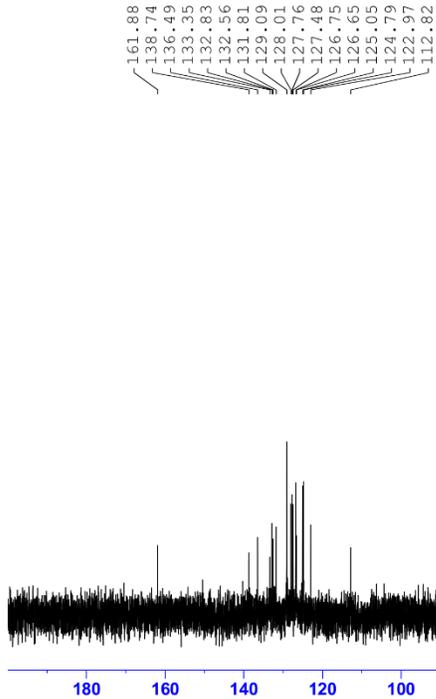
F2 - Acquisition Parameters
Date_ 20240729
Time 15.18 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 98.85
DW 62.400 usec
DE 6.50 usec
TE 303.6 K
D1 1.00000000 sec
TDD 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580447 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C NMR of 3I

Signature SIF VIT VELLORE
N2-N



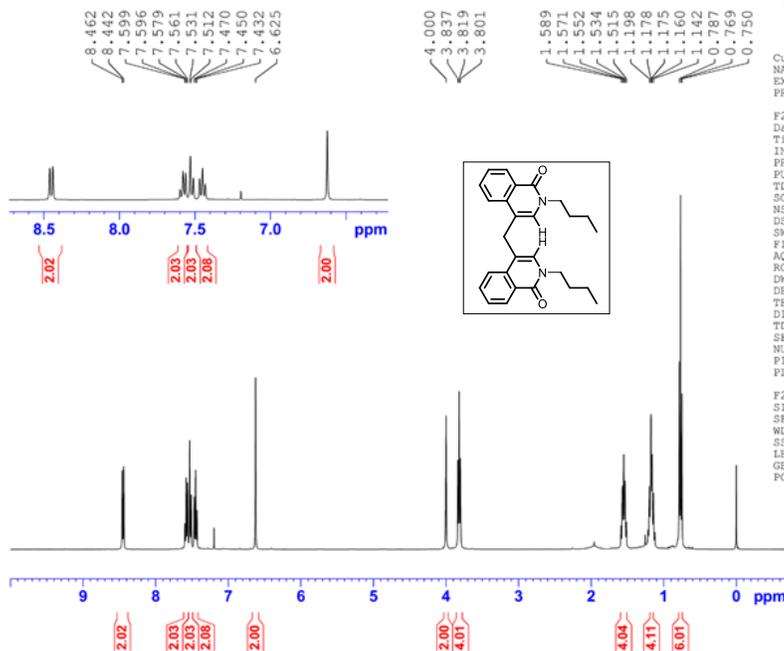
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NAME Dr.REI100824
EXPNO 16
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240811
Time 18.50 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2000
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 303.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TDD 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.21399975 W
PLW12 0.42261001 W
PLW13 0.21257000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
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SSB 0
LB 1.00 Hz
GB 0
PC 1.40

¹H NMR of 3m

Signature SIF VIT VELLORE
N-B-DIMER



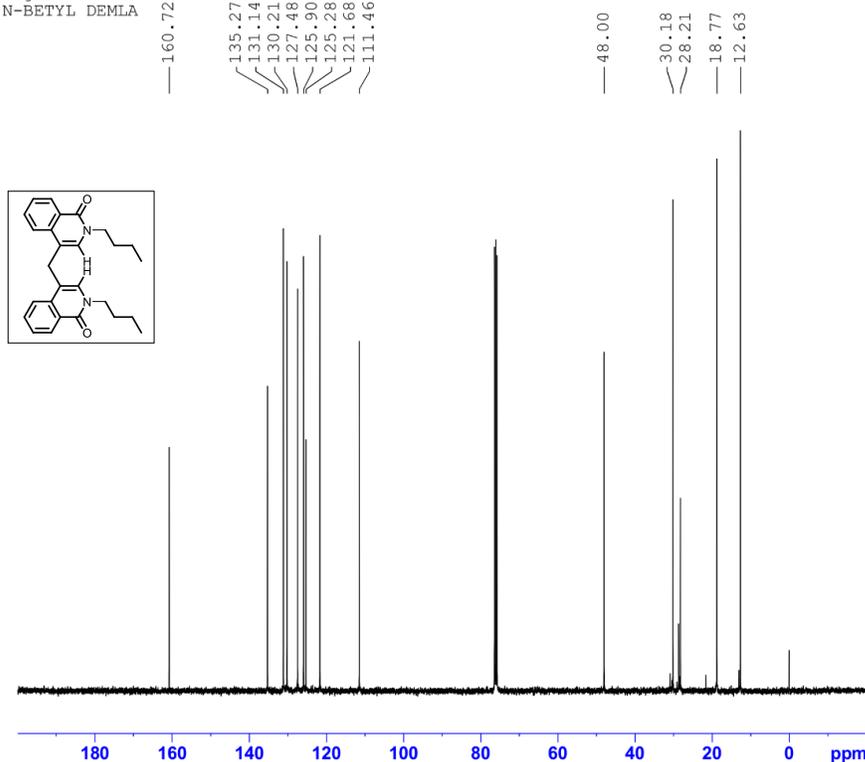
Current Data Parameters
NAME Dr.GTV240823
EXPNO 65
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230824
Time 14.35 h
INSTRUM spect
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PULPROG zq30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 58.47
DW 62.400 usec
DE 6.50 usec
TE 305.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 14.95499992 W

F2 - Processing parameters
SI 65536
SF 400.2580353 MHz
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SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C NMR of 3m

Signature SIF VIT VELLORE
N-BEYTL DEMLA



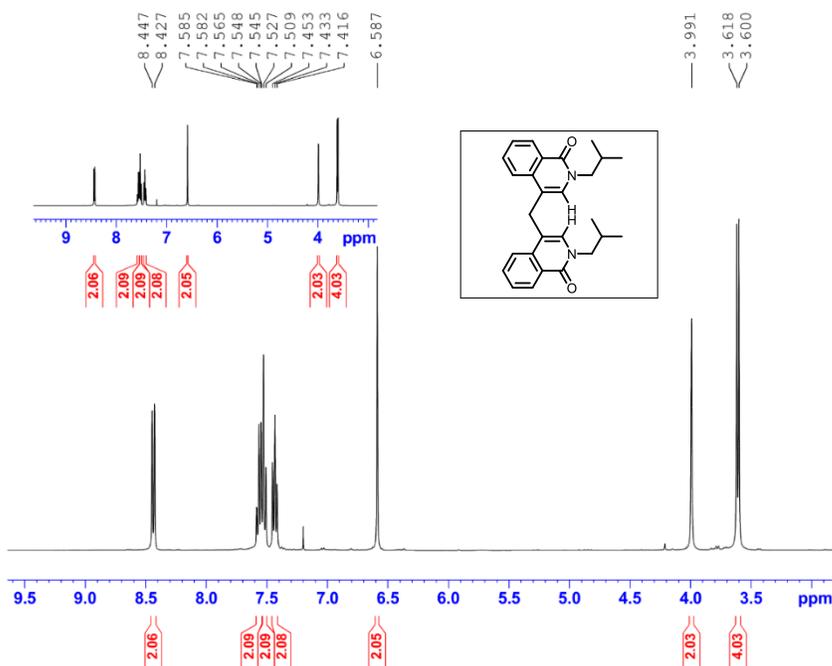
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NAME Dr.NAP250823
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters
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Time 20.44 h
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PULPROG zppq30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 305.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 58.22499847 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W
PLW13 0.20895000 W

F2 - Processing parameters
SI 32768
SF 100.6450580 MHz
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¹H NMR of 3n

Signature SIF VIT VELLORE
i-2-Me-PROP DIMER



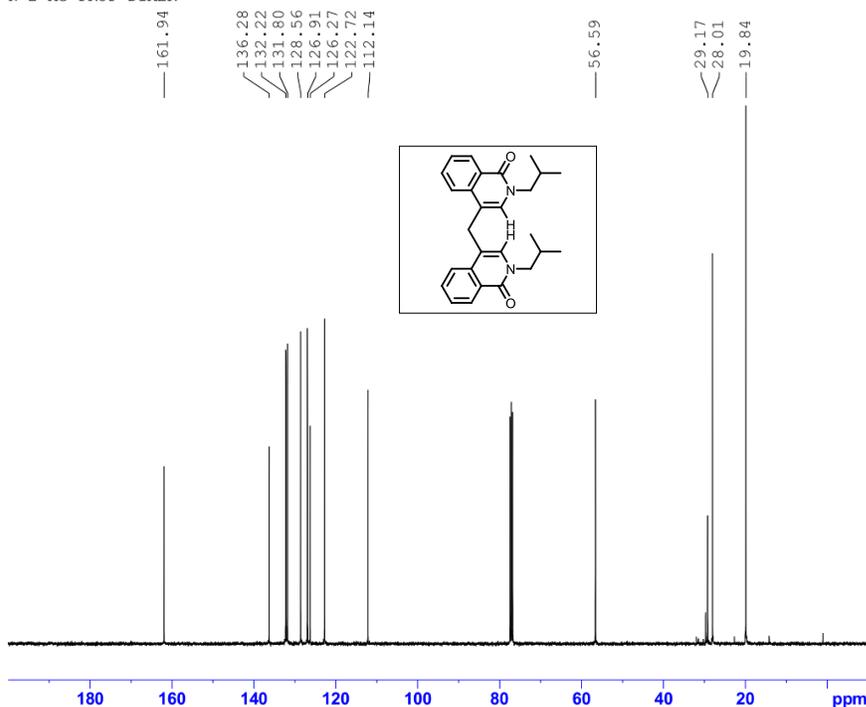
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NAME Dr.GTV040923
EXPNO 15
PROCNO 1

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Date 20230904
Time 19.32 h
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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 35.49
DW 62.400 usec
DE 6.50 usec
TE 305.4 K
D1 1.00000000 sec
TDO 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 14.95499992 W

F2 - Processing parameters
SI 65536
SF 400.2580337 MHz
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LB 0.30 Hz
GB 0
FC 1.00

¹³C NMR of 3n

Signature SIF VIT VELLORE
N-2-Me-PROP DIMER



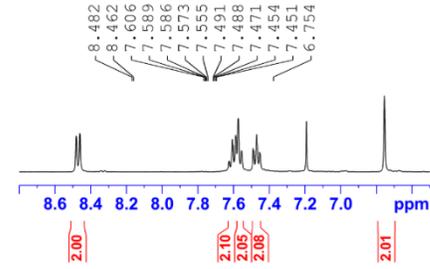
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NAME Dr.GTV040923
EXPNO 16
PROCNO 1

F2 - Acquisition Parameters
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Time 20.04 h
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 305.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 58.22499847 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W
PLW13 0.20895000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

¹H NMR of 30

Signature SIF VIT VELLORE
N-CP-DIMER



4.043
3.724
3.706

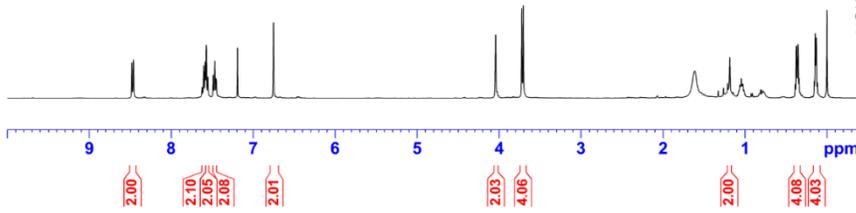
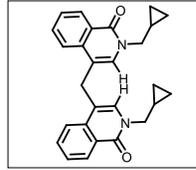
1.185
0.387
0.372
0.354
0.340
0.156
0.143



Current Data Parameters
NAME Dr.GTV090124
EXPNO 22
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240108
Time_ 18.01 h
INSTRUM spect
PROBHD z108618_0505 ()
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 156.91
DW 62.400 usec
DE 6.50 usec
TE 305.9 K
D1 1.00000000 sec
TDO 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580367 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C NMR of 30

Signature SIF VIT VELLORE
N-CP-DIMER

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136.40
132.23
130.92
128.60
126.93
126.29
122.79
112.51

53.04

29.44

10.66

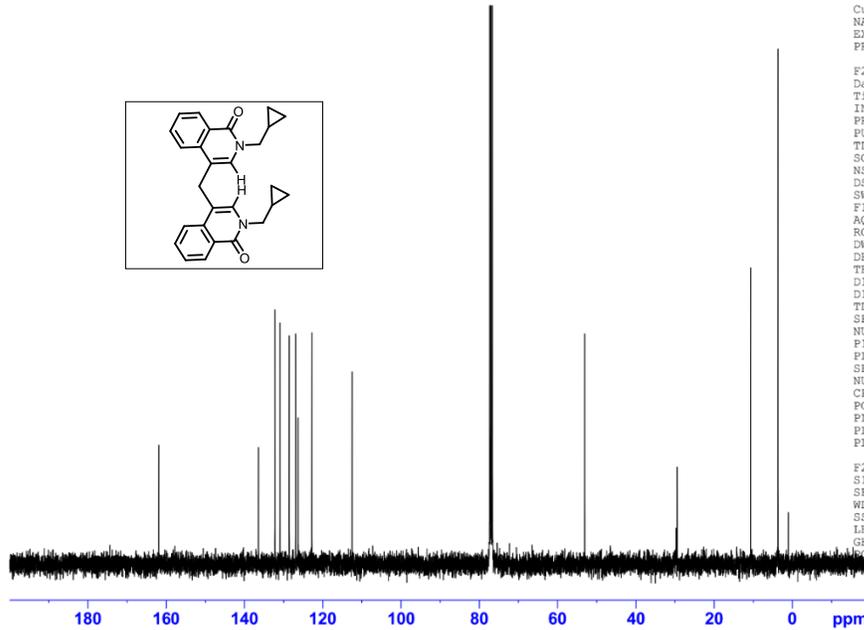
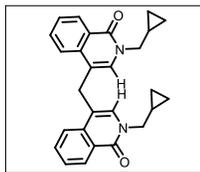
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Current Data Parameters
NAME Dr.GTV090124
EXPNO 23
PROCNO 1

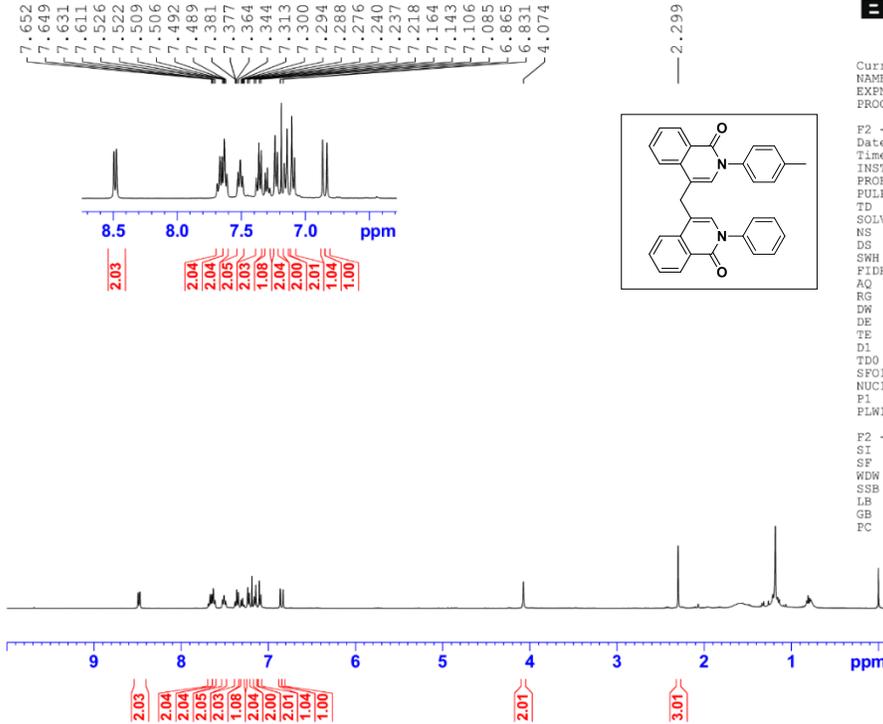
F2 - Acquisition Parameters
Date_ 20240108
Time_ 18.33 h
INSTRUM spect
PROBHD z108618_0505 ()
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 305.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLN1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLN2 15.21399975 W
PLN12 0.42261001 W
PLN13 0.21257000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



¹H NMR of 3p

Signature SIF VIT VELLORE
UNSYMMETRICAL-S2



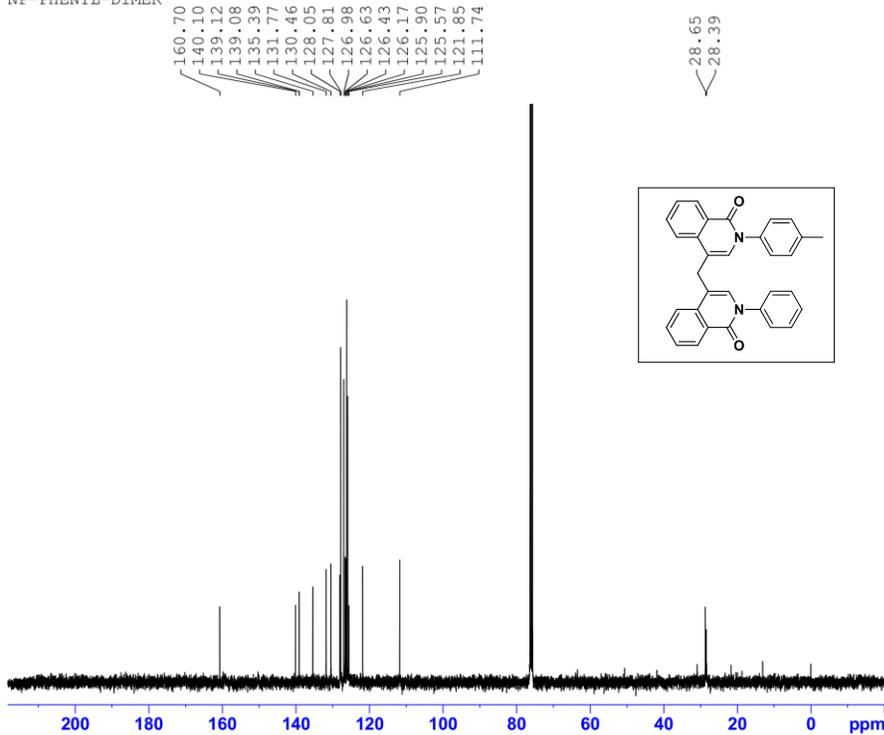
Current Data Parameters
NAME Dr.GTV161023
EXPNO 42
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231017
Time 9.28 h
INSTRUM spect
PROBHD z108618_0505 ()
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 143.73
DW 62.400 usec
DE 6.50 usec
TE 305.9 K
D1 1.00000000 sec
TDO 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 14.95499992 W

F2 - Processing parameters
SI 65536
SF 400.2580389 MHz
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SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C NMR of 3p

Signature SIF VIT VELLORE
NP-PHENYL-DIMER



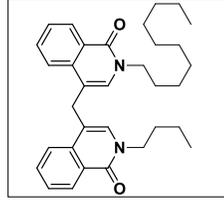
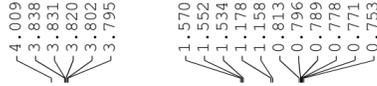
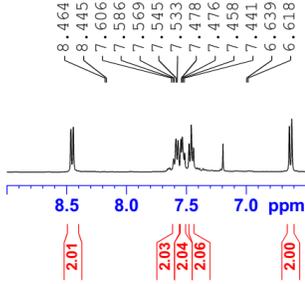
Current Data Parameters
NAME Dr.MAP201023
EXPNO 32
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231020
Time 22.32 h
INSTRUM spect
PROBHD z108618_0505 ()
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 306.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 58.22499847 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W
PLW13 0.20895000 W

F2 - Processing parameters
SI 32768
SF 100.6450606 MHz
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SSB 0
LB 1.00 Hz
GB 0
PC 1.40

¹H NMR of 3q

Signature SIF VIT VELLORE
N-BUDO-3



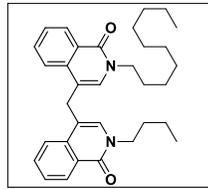
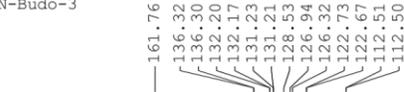
Current Data Parameters
NAME Dr.GTV070324
EXPNO 16
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240307
Time 12.59 h
INSTRUM spect
PROBHD Z108618_0505 (1
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 58.47
DW 62.400 usec
DE 6.50 usec
TE 302.4 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
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SF 400.2580360 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C NMR of 3q

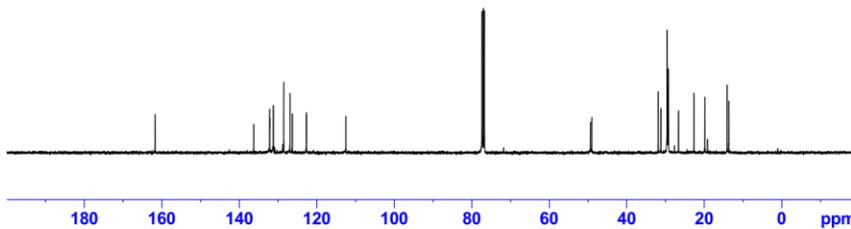
Signature SIF VIT VELLORE
N-Budo-3



Current Data Parameters
NAME Dr.GTV040324
EXPNO 2
PROCNO 1

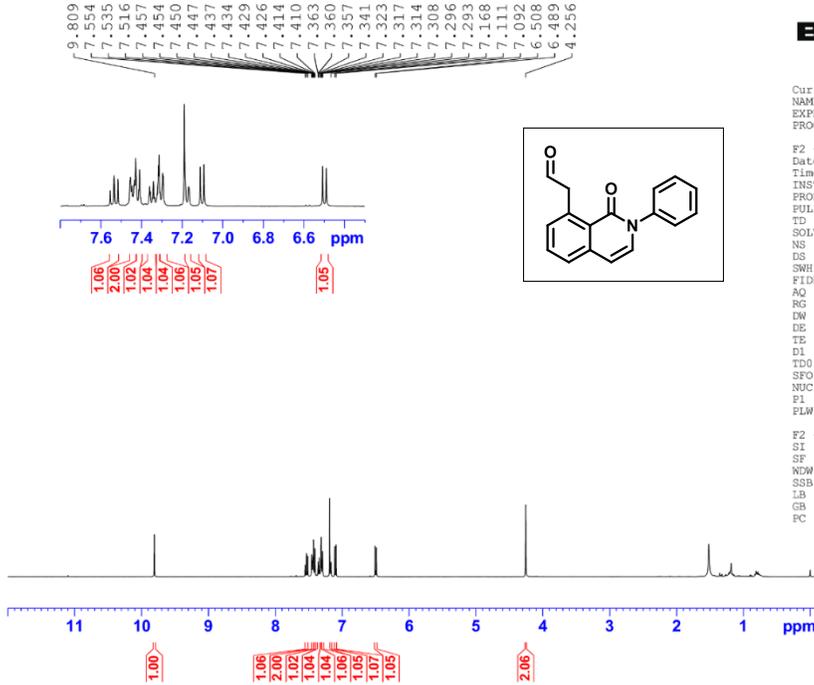
F2 - Acquisition Parameters
Date_ 20240304
Time 23.26 h
INSTRUM spect
PROBHD Z108618_0505 (1
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 304.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 15.21399975 W
PLW12 0.42261001 W
PLW13 0.21257000 W

F2 - Processing parameters
SI 32768
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SSB 0
LB 1.00 Hz
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PC 1.40



¹H NMR of 4a

Signature SIF VIT VELLORE
N-PHEN-ALD



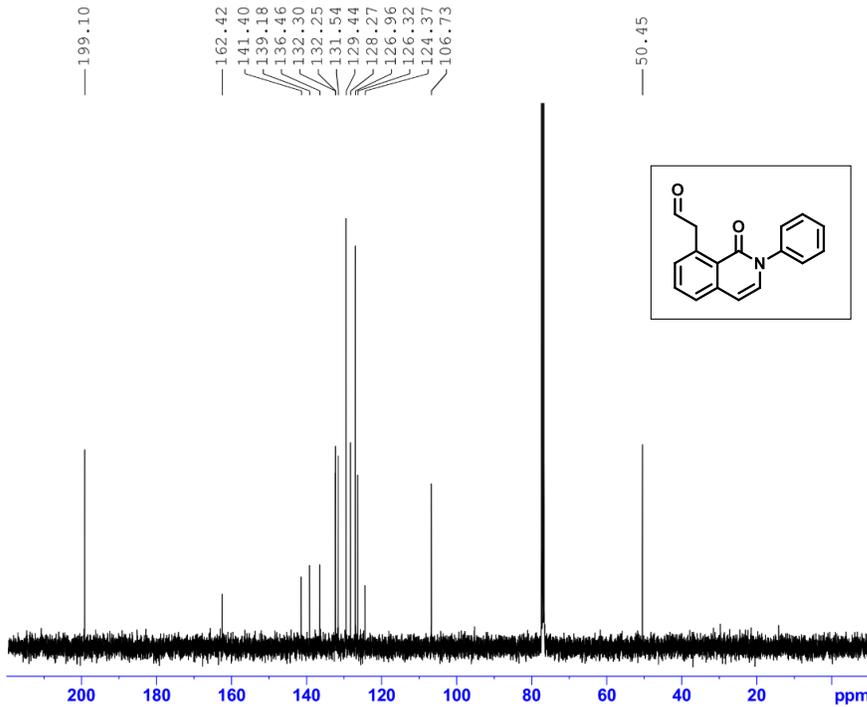
Current Data Parameters
NAME Dr.GTV131222
EXPNO 39
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221213
Time 15.28 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 175.97
DW 62.400 usec
DE 6.50 usec
TE 303.1 K
D1 1.00000000 sec
TDO 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 14.95499992 W

F2 - Processing parameters
SI 65536
SF 400.2580381 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C NMR of 4a

Signature SIF VIT VELLORE
N-BEN-ALD



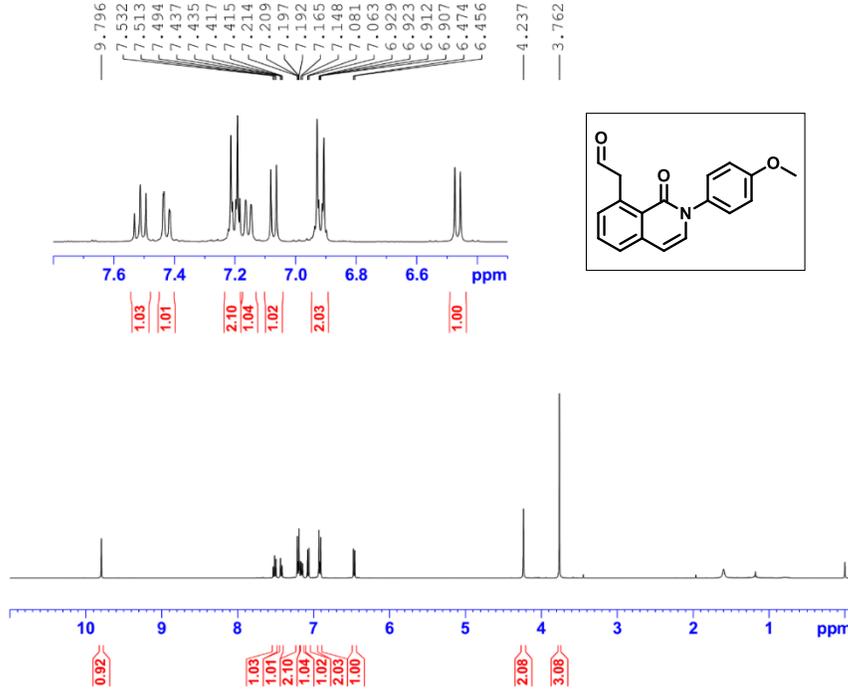
Current Data Parameters
NAME Dr.GTV141222
EXPNO 38
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221215
Time 0.57 h
INSTRUM spect
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 304.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 58.22499847 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
FCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W
PLW13 0.20895000 W

F2 - Processing parameters
SI 32768
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PC 1.40

¹H NMR of 4b

Signature SIF VIT VELLORE
N-NAPH-ALD



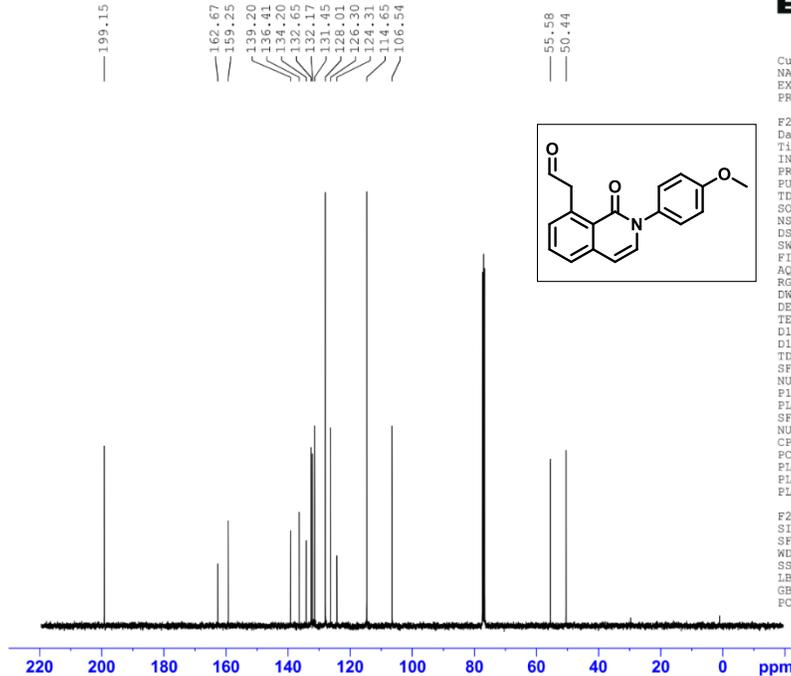
Current Data Parameters
NAME H1
EXPNO 67
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221223
Time_ 9.54 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 98.85
DW 62.400 usec
DE 6.50 usec
TE 304.7 K
D1 1.00000000 sec
TDO 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 14.95499992 W

F2 - Processing parameters
SI 65536
SF 400.2580399 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C NMR of 4b

Signature SIF VIT VELLORE
N-NAPH-ALD



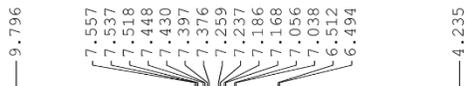
Current Data Parameters
NAME C13
EXPNO 74
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221224
Time_ 0.11 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 304.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 58.22499847 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
F1W2 14.95499992 W
F1W12 0.41542000 W
F1W13 0.20895000 W

F2 - Processing parameters
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SF 100.6449542 MHz
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LB 1.00 Hz
GB 0
PC 1.40

¹H NMR of 4c

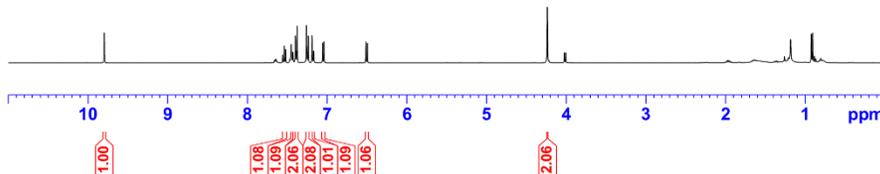
Signature SIF VIT VELLORE
JCL1



Current Data Parameters
NAME Dr.GTV090824
EXPNO 24
PROCNO 1

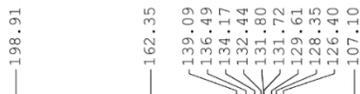
F2 - Acquisition Parameters
Date 20240809
Time 13.30 h
INSTRUM spect
PROBHD z108618_0505 ()
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 98.85
DW 62.400 usec
DE 6.50 usec
TE 303.3 K
D1 1.00000000 sec
TDO 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580391 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C NMR of 4c

Signature SIF VIT VELLORE
4-CL-PHE-ALD



Current Data Parameters
NAME Dr.GSK10423
EXPNO 1
PROCNO 1

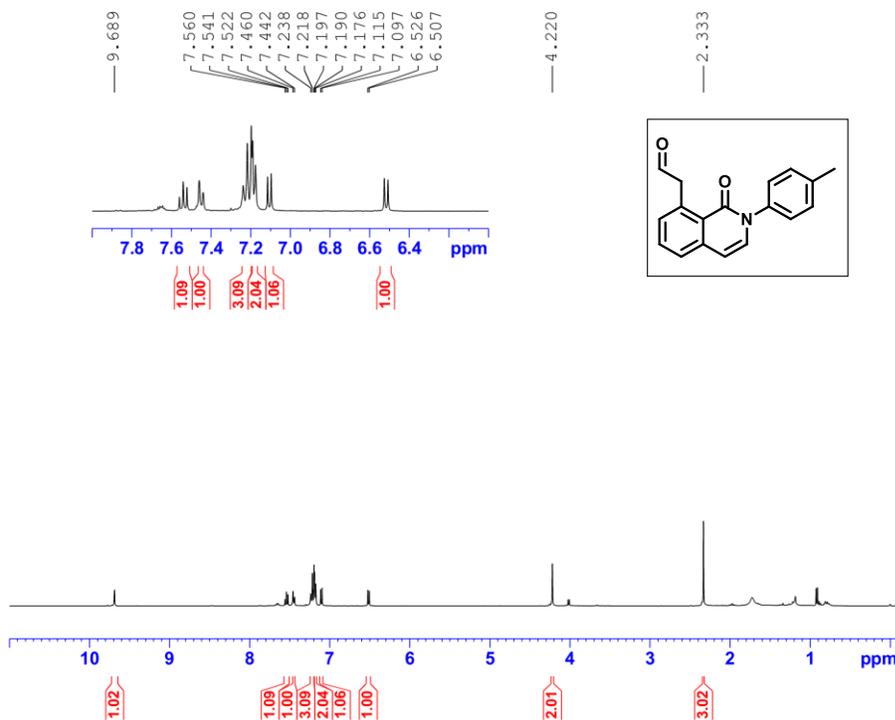
F2 - Acquisition Parameters
Date 20230402
Time 18.33 h
INSTRUM spect
PROBHD z108618_0505 ()
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2000
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 112.69
DW 20.800 usec
DE 6.50 usec
TE 304.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 58.22499847 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W
PLW13 0.20895000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



¹H NMR of 4d

Signature SIF VIT VELLORE
4MEALD



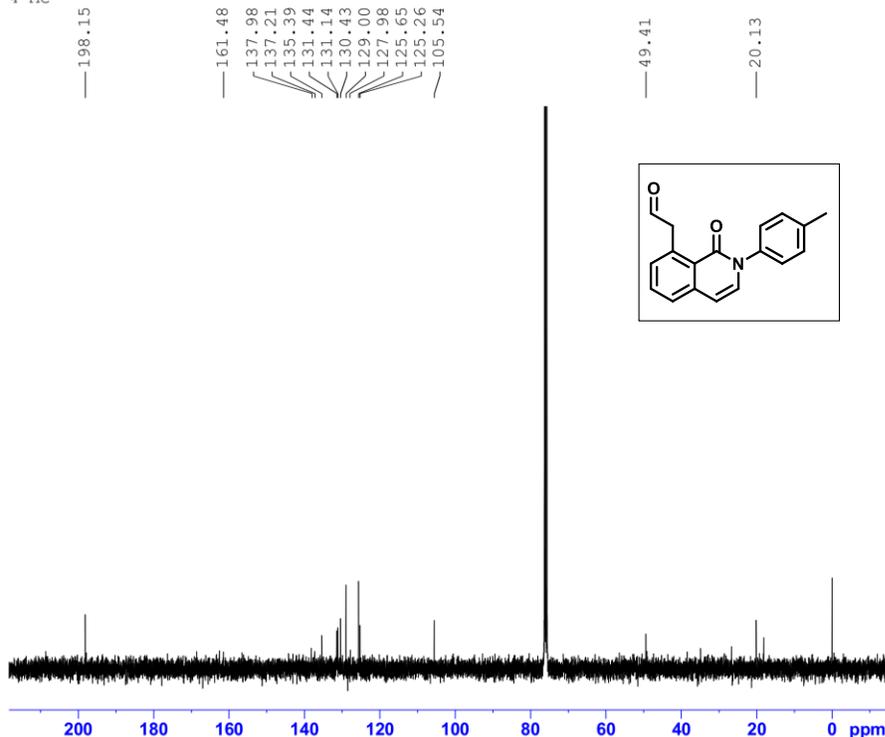
Current Data Parameters
NAME Dr.GTV250624
EXPNO 99
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240625
Time_ 16.02 h
INSTRUM spect
PROBHD Z108618_0505 (zg30)
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 156.91
RW 62.400 usec
DE 6.50 usec
TE 303.8 K
D1 1.00000000 sec
TD0
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580378 MHz
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SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C NMR of 4d

Signature SIF VIT VELLORE
4-Me



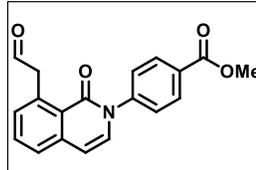
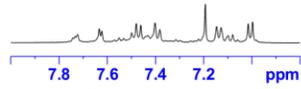
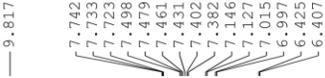
Current Data Parameters
NAME Dr.GTV120624
EXPNO 50
PROCNO 1

F2 - Acquisition Parameters
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Time_ 4.25 h
INSTRUM spect
PROBHD Z108618_0505 (zgpg30)
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 175.97
RW 20.800 usec
DE 6.50 usec
TE 303.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.21399975 W
PLW12 0.42261001 W
PLW13 0.21257000 W

F2 - Processing parameters
SI 32768
SF 100.6450580 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

¹H NMR of 4e

Signature SIF VIT VELLORE
N-PHE-ESTER-ALD



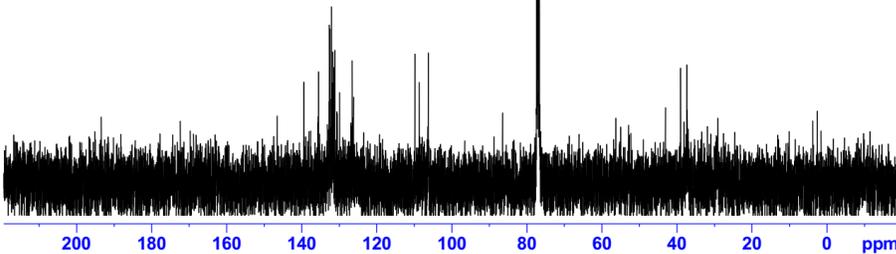
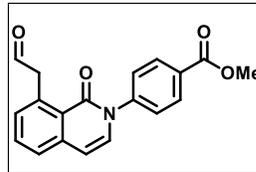
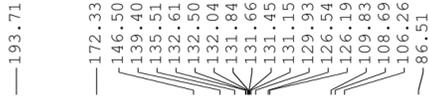
NAME Dr.GTV180123
EXPNO 45
PROCNO 1

F2 - Acquisition Parameters
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Time 15:38 h
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PROBHD Z108618_0505 ()
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 156.91
DW 62.400 usec
DE 6.50 usec
TE 305.6 K
D1 1.00000000 sec
TDO 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PL1 14.95499992 W

F2 - Processing parameters
SI 65536
SF 400.2580365 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C NMR of 4e

Signature SIF VIT VELLORE
N-PHE-EST-ALD



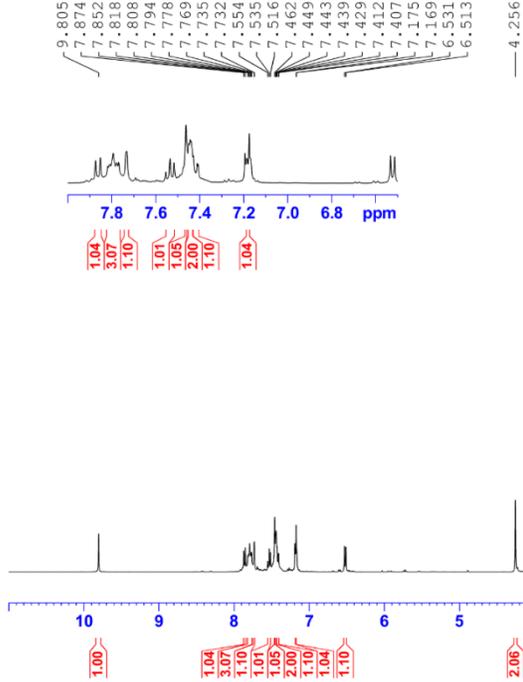
Current Data Parameters
NAME Dr.GTV190324
EXPNO 65
PROCNO 1

F2 - Acquisition Parameters
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 306.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PL1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.21399975 W
PLW12 0.42261001 W
PLW13 0.21257000 W

F2 - Processing parameters
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SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

¹H NMR of 4f

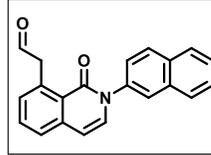
Signature SIF VIT VELLORE
NAPH-ACD



Current Data Parameters
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EXPNO 23
PROCNO 1

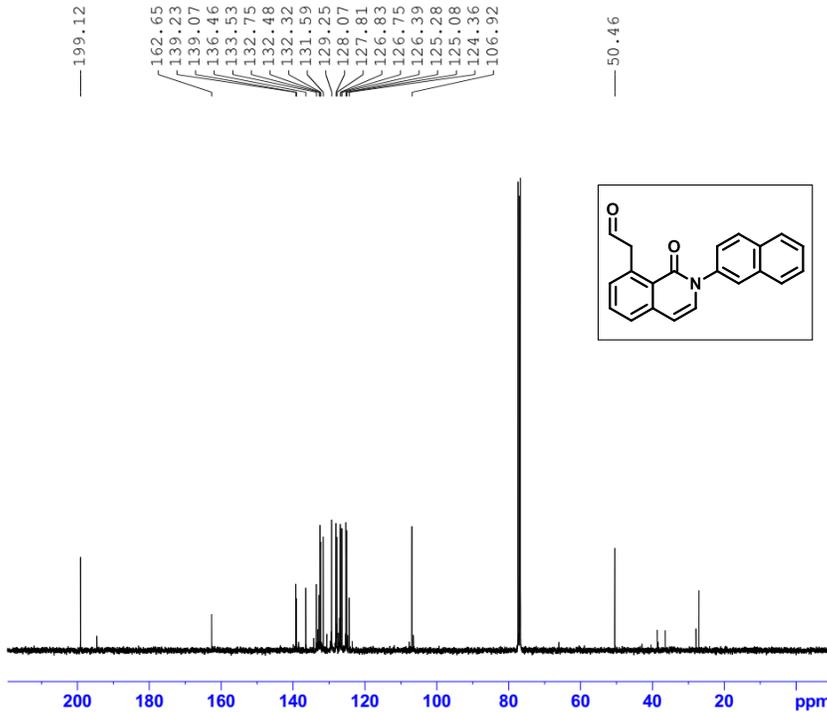
F2 - Acquisition Parameters
Date_ 20221223
Time 11:54 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 98.85
DW 62.400 usec
DE 6.50 usec
TE 304.6 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 14.95499992 W

F2 - Processing parameters
SI 65536
SF 400.2580438 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C NMR of 4f

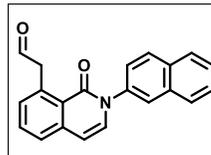
Signature SIF VIT VELLORE
N-NAPH-ALD



Current Data Parameters
NAME Dr.GTV040123
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230105
Time 7:45 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 305.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 58.22499847 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W
PLW13 0.20895000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



10. References

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