Solvent-Free Synthesis of 1,2-Dihydro-1-arylnaphtho[1,2-e] [1,3] oxazine-3-ones Using Magnetic Nickel -Zinc Ferrite Nanocatalyst

Sreelakshmi Sreekandan[1], Anjitha Thadathil,[2] Bindu Mavila,[3] Kannan Vellayan[1*], Pradeepan Periyat[3*]

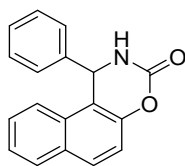[1]Department of Chemistry, Government College, Kattappana

[2]Department of Chemistry, University of Calicut

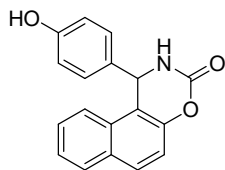[3]Department of Environmental Studies, Kannur University

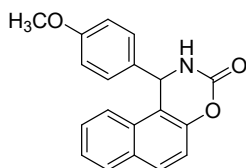*Correspondence: Email: kannanpvl@gmail.com, pperiyat@kannuruniv.ac.in

Reaction No.1   Product Code: NU1
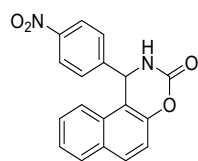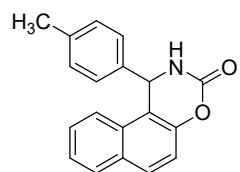

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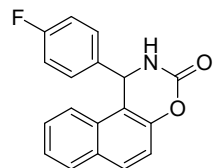

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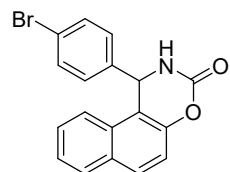
Reaction No. 5 Product Code: NU5

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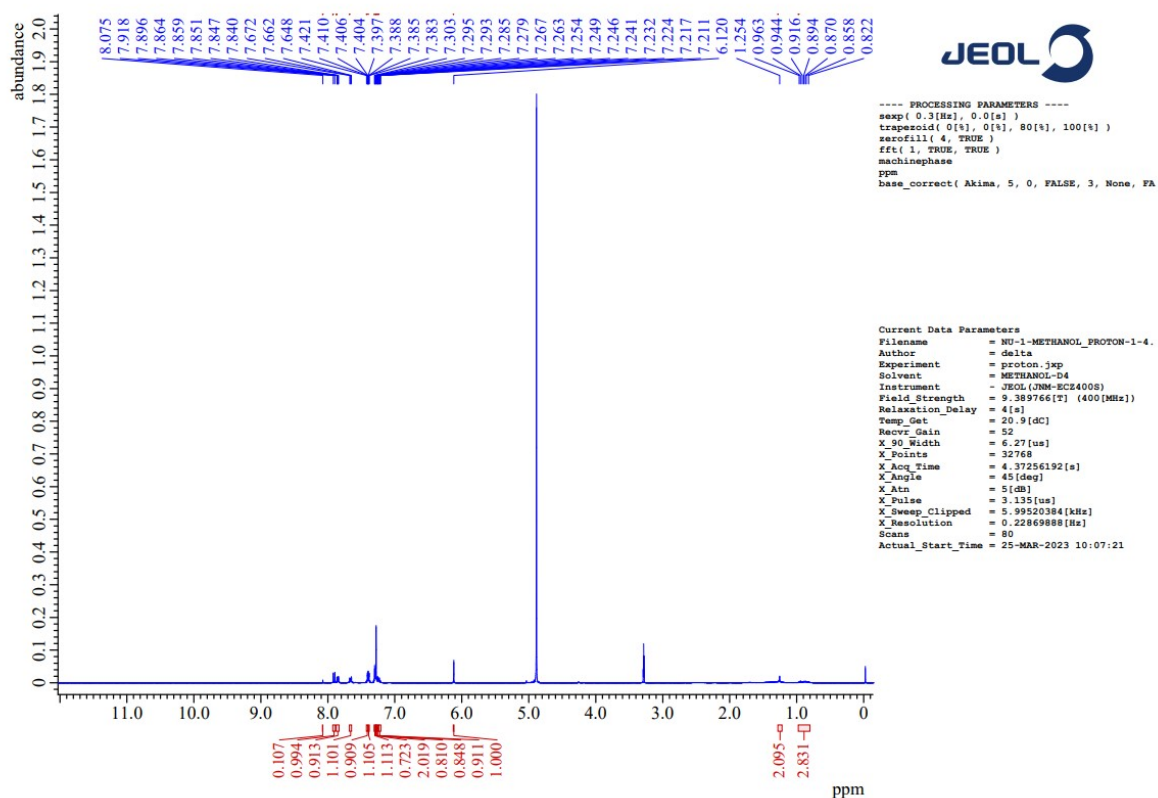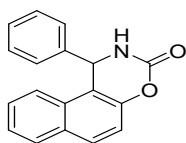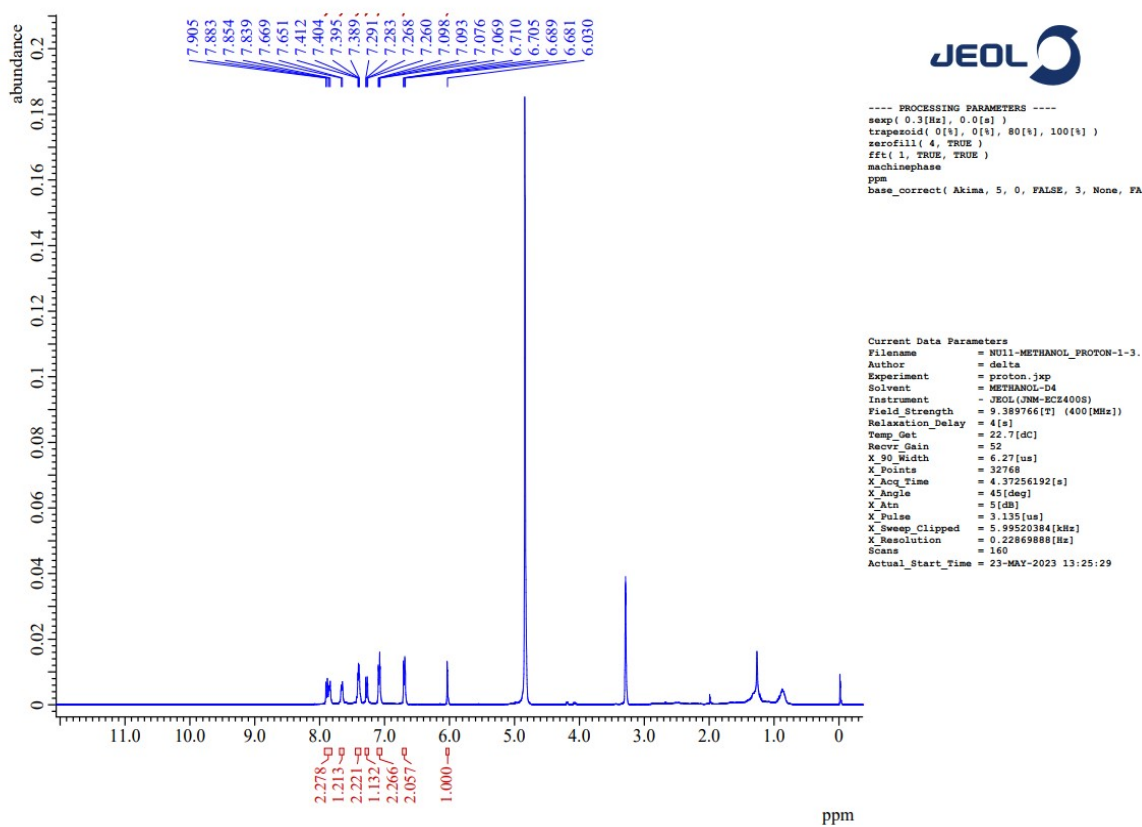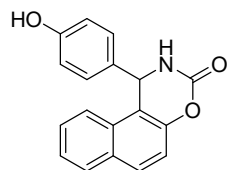

Reaction No. 7 Product Code: NU7
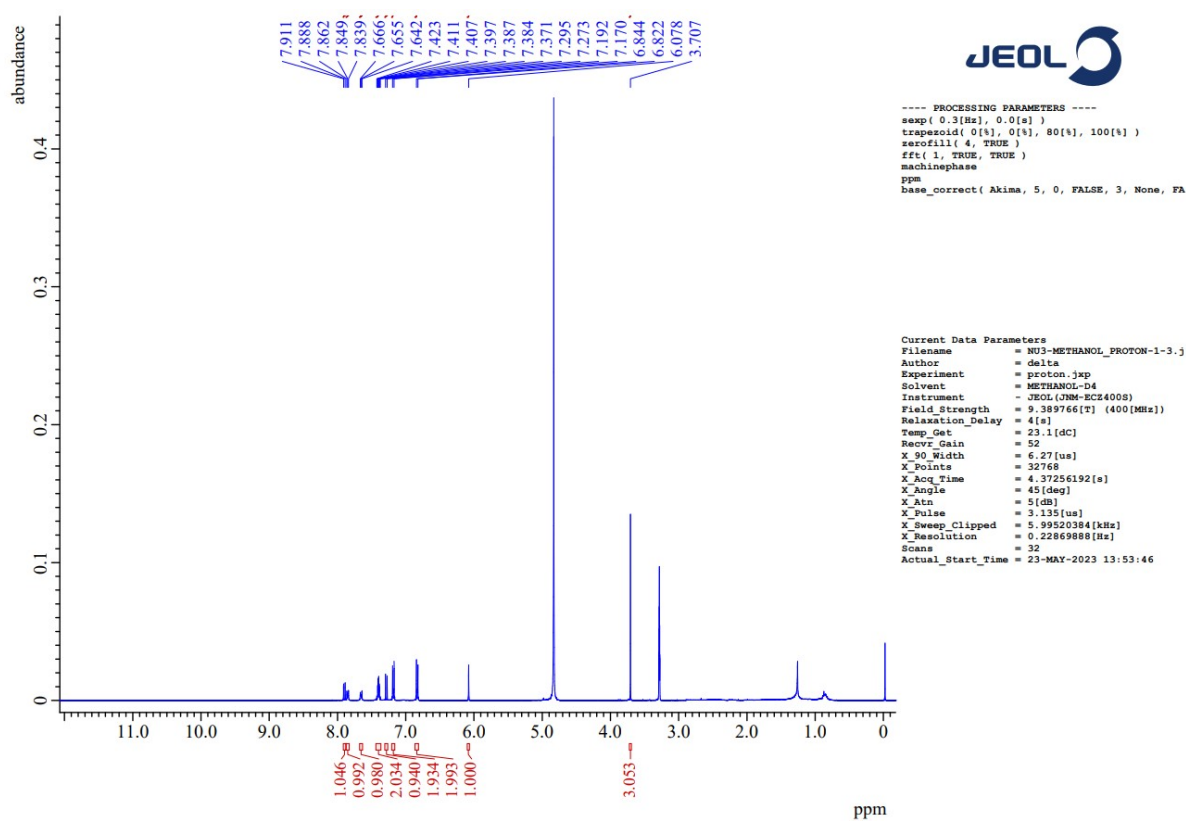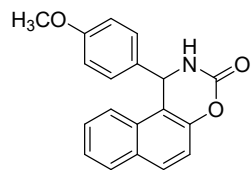

H^1-NMR

Reaction No.1   Product Code: NU1

H¹-NMR

Reaction No.2.   Product Code: NU2

H¹-NMR

Reaction No.3. Product Code: NU3

H^1-NMR

Reaction No. 4. Product Code: NU4

Peak labels: 10.008, 9.940, 8.948, 8.272, 8.250, 8.064, 8.046, 7.911, 7.867, 7.820, 7.675, 7.648, 7.585, 7.571, 7.527, 7.506, 7.458, 7.436, 7.330, 7.264, 7.222, 7.192, 7.166, 5.989

Integration values: 0.226, 0.134, 0.148, 1.200, 1.012, 1.035, 1.126, 1.273, 0.270

---- PROCESSING PARAMETERS ----
sexp(0.3[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(4, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
base_correct(Akima, 5, 0, FALSE, 3, None, FA

Current Data Parameters
Filename   = NU4-DMSO_PROTON-2-4.jdf
Author   = delta
Experiment   = proton.jxp
Solvent   = DMSO-D6
Instrument   - JEOL(JNM-ECZ400S)
Field_Strength   = 9.389766[T] (400[MHz])
Relaxation_Delay = 4[s]
Temp_Get   = 23.3[dC]
Recvr_Gain   = 62
X_90_Width   = 6.27[us]
X_Points   = 32768
X_Acq_Time   = 4.37256192[s]
X_Angle   = 45[deg]
X_Atn   = 5[dB]
X_Pulse   = 3.135[us]
X_Sweep_Clipped   = 5.99520384[kHz]
X_Resolution   = 0.22869888[Hz]
Scans   = 160
Actual_Start_Time = 23-JAN-2024 13:59:13

C¹³-NMR

Reaction No. 4. Product Code: NU4

Peaks: 166.753, 149.600, 140.521, 131.182, 129.443, 123.995, 118.686, 40.659, 40.448, 40.242, 40.031, 39.825, 39.614, 39.404

JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 3.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 2, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
thresh( 5[%], 1 )
peak_pick( 0[Hz], 0.1[ppm], Peaks, 0[Hz] )
```

```
Current Data Parameters
Filename            = NU4-DMSO_CARBON-1-3.jdf
Author              = delta
Experiment          = carbon.jxp
Solvent             = DMSO-D6
Instrument          - JEOL(JNM-ECZ400S)
Field_Strength      = 9.389766[T] (400[MHz])
Relaxation_Delay    = 2[s]
Temp_Get            = 22.6[dC]
Recvr_Gain          = 52
X_90_Width          = 11.1[us]
X_Points            = 32768
X_Acq_Time          = 1.03809024[s]
X_Angle             = 30[deg]
X_Atn               = 8.1[dB]
X_Pulse             = 3.7[us]
X_Sweep_Clipped     = 25.25252525[kHz]
X_Resolution        = 0.96330739[Hz]
Scans               = 5000
Actual_Start_Time   = 29-JAN-2024 16:35:01
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H¹-NMR

Reaction No. 5. Product Code: NU5

C[13]-NMR

Reaction No. 5. Product Code: NU5
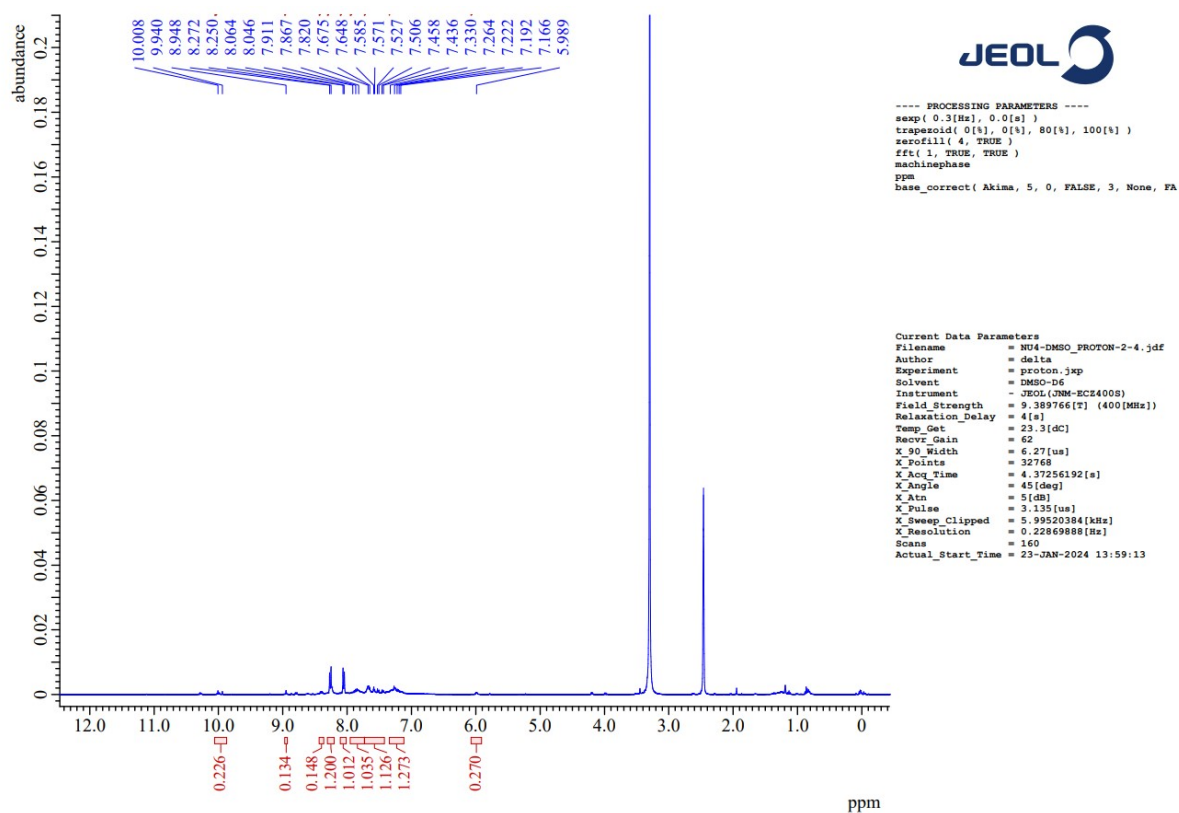
H¹-NMR

Reaction No.6   Product Code: NU6
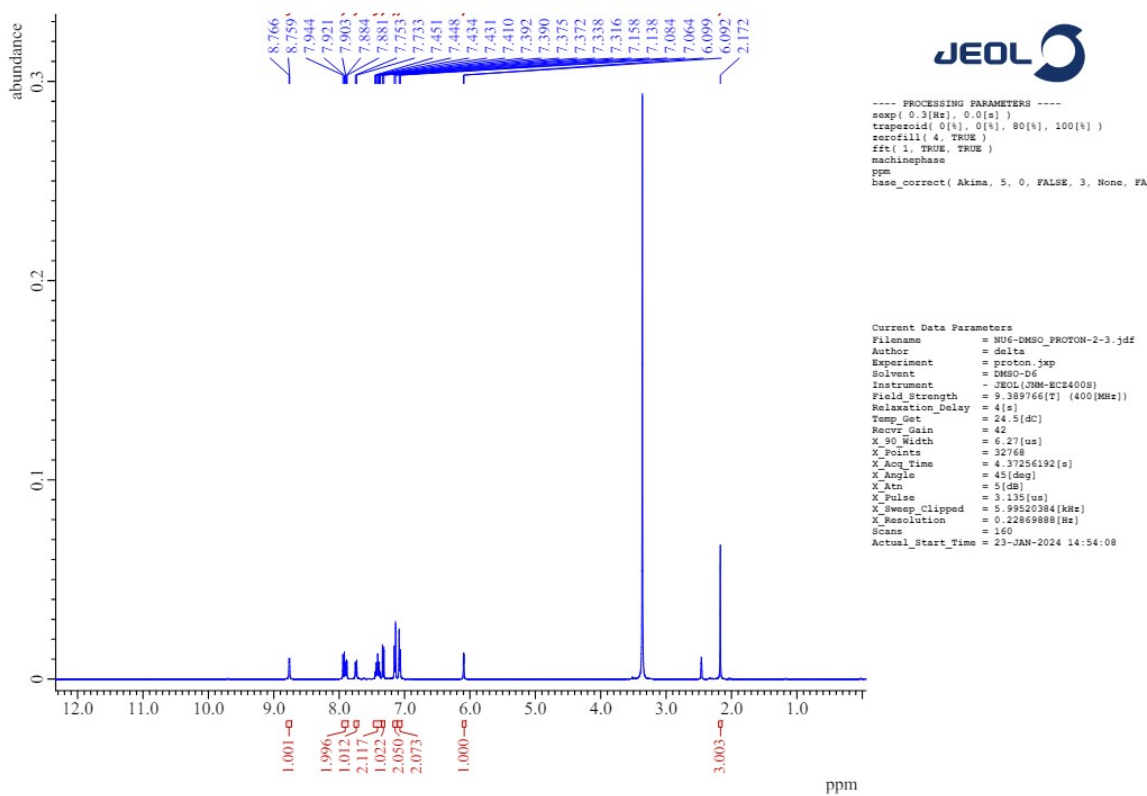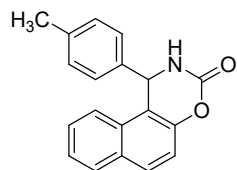
C^{13}-NMR

Reaction No.6   Product Code: NU6
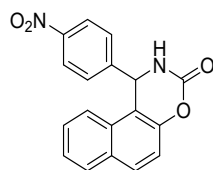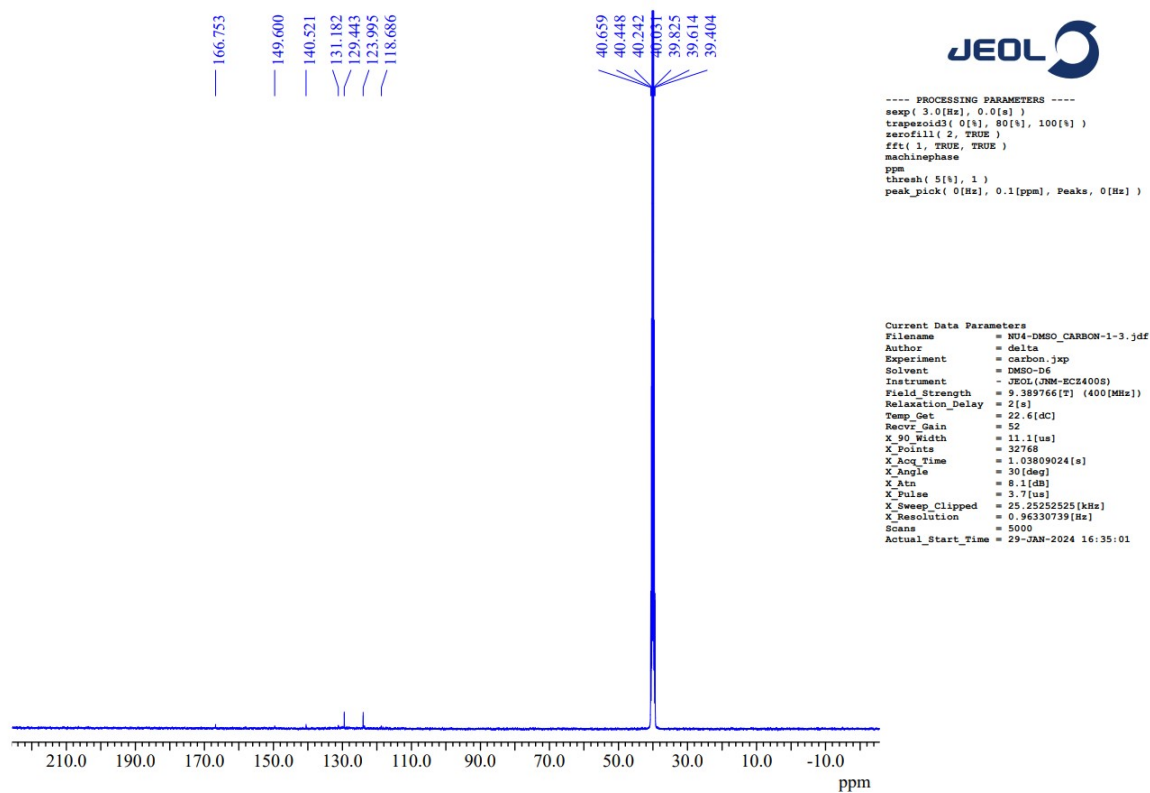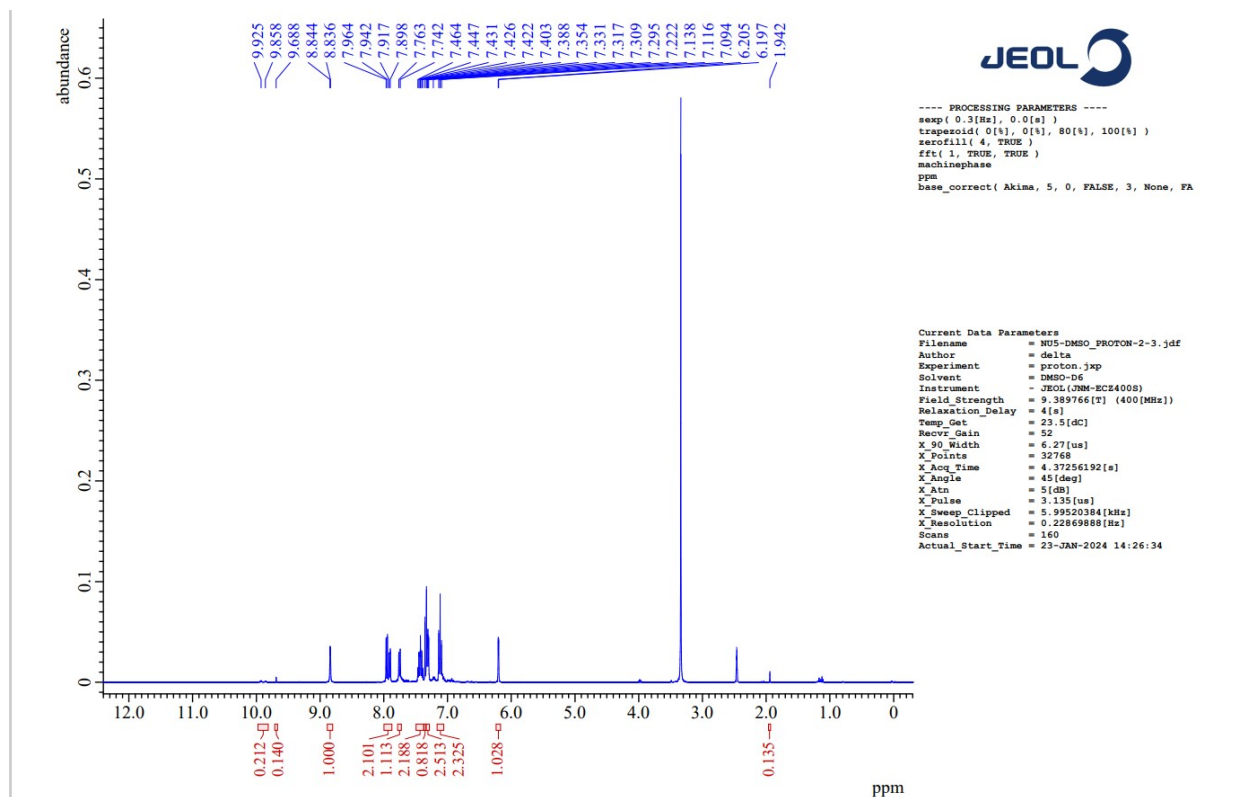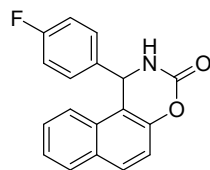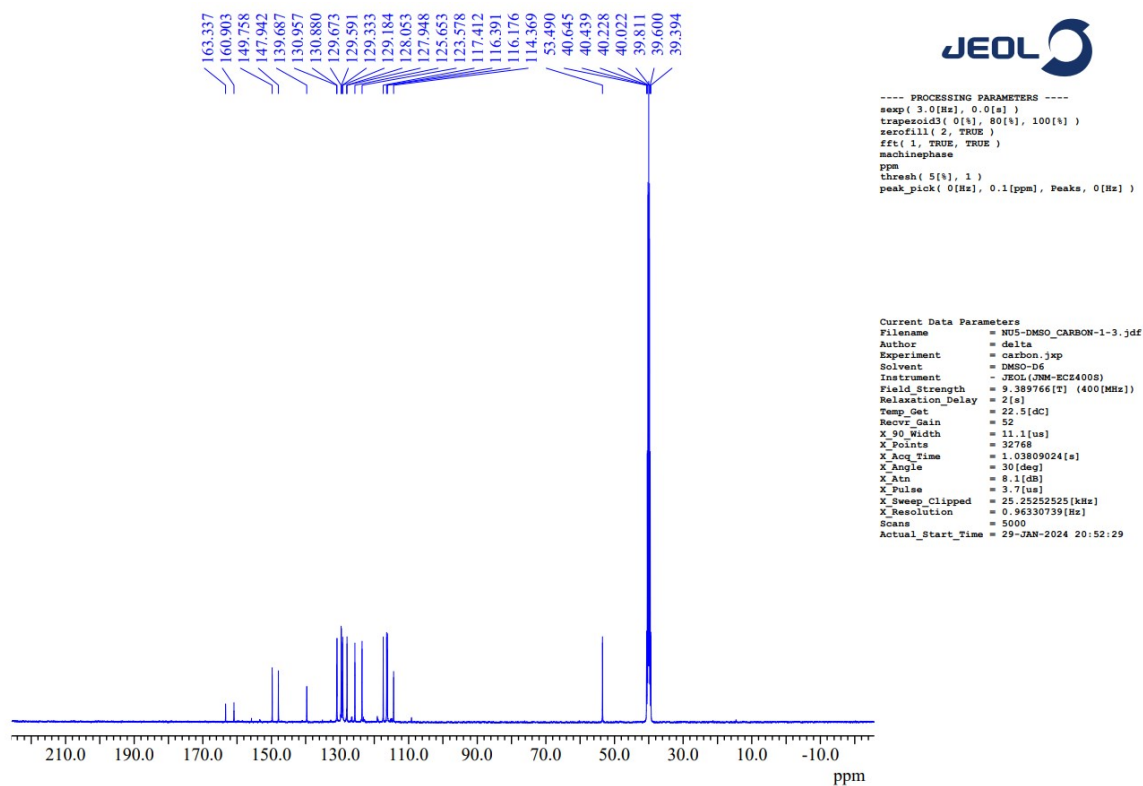
H¹-NMR

Reaction No.7   Product Code: NU7

C[13]-NMR
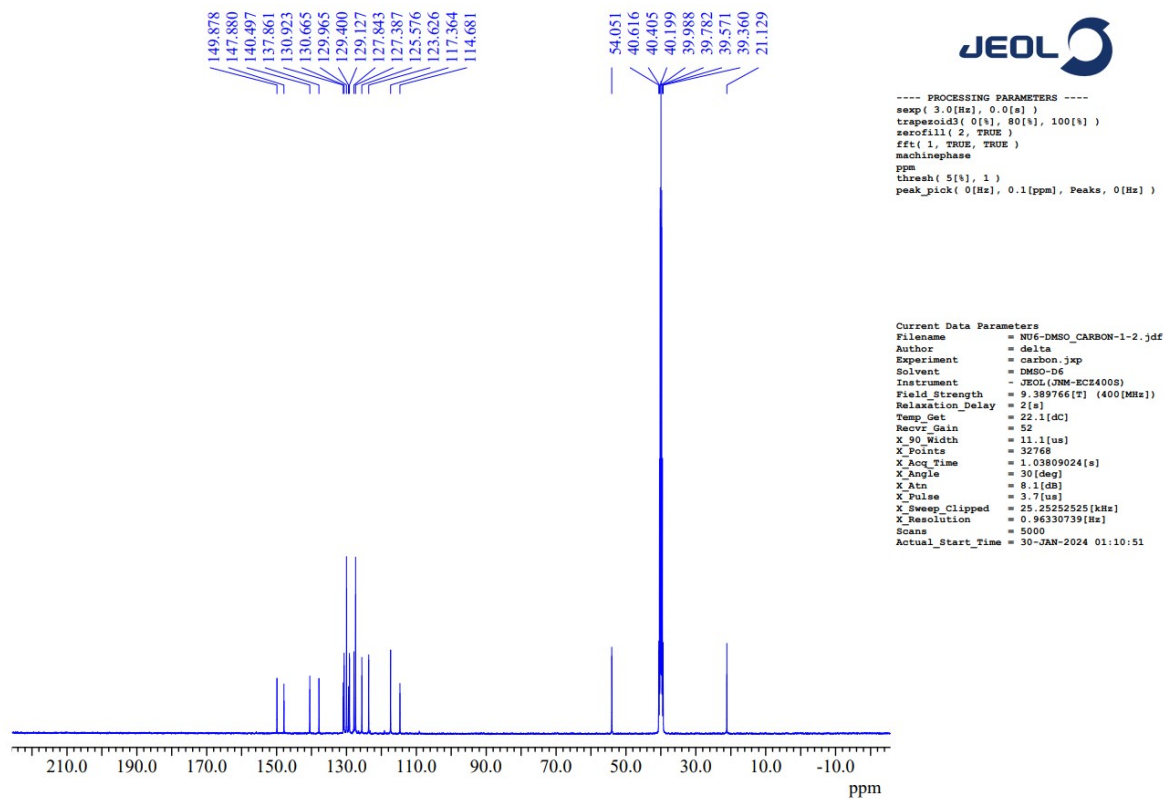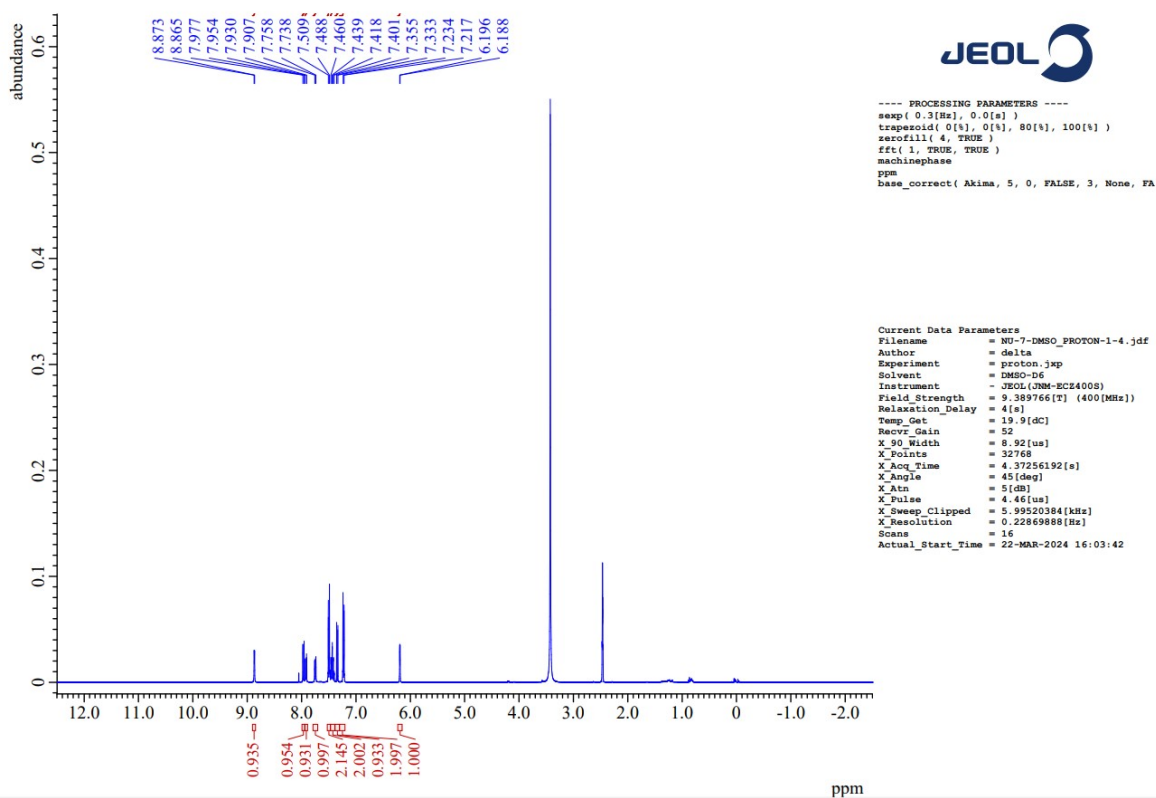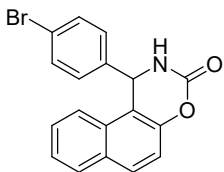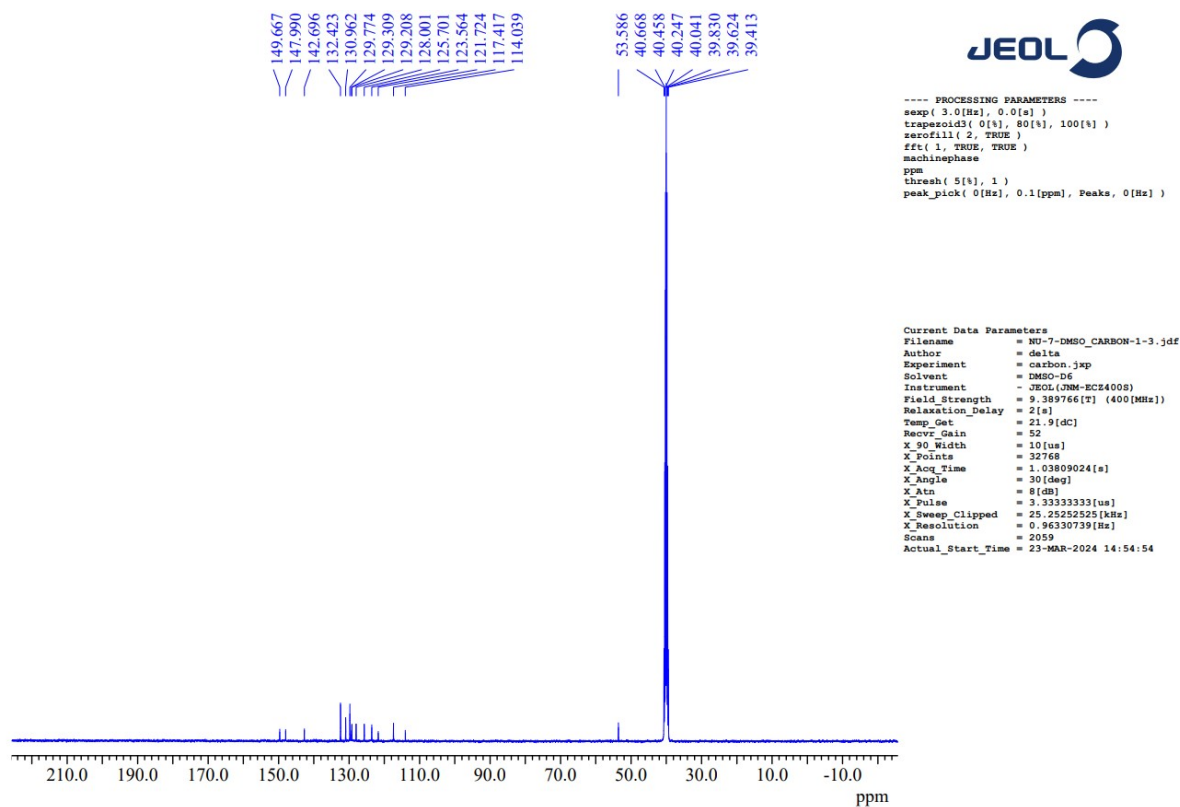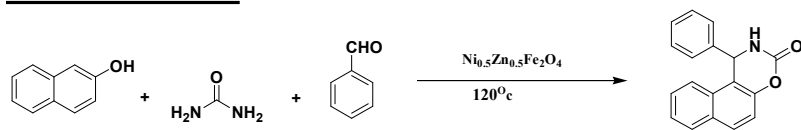
Reaction No.7   Product Code: NU7

---- PROCESSING PARAMETERS ----
sexp(3.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(2, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
thresh(5[%], 1)
peak_pick(0[Hz], 0.1[ppm], Peaks, 0[Hz])

Current Data Parameters
Filename   = NU-7-DMSO_CARBON-1-3.jdf
Author   = delta
Experiment   = carbon.jxp
Solvent   = DMSO-D6
Instrument   - JEOL(JNM-ECZ400S)
Field_Strength   = 9.389766[T] (400[MHz])
Relaxation_Delay = 2[s]
Temp_Get   = 21.9[dC]
Recvr_Gain   = 52
X_90_Width   = 10[us]
X_Points   = 32768
X_Acq_Time   = 1.03809024[s]
X_Angle   = 30[deg]
X_Atn   = 8[dB]
X_Pulse   = 3.33333333[us]
X_Sweep_Clipped   = 25.25252525[kHz]
X_Resolution   = 0.96330739[Hz]
Scans   = 2059
Actual_Start_Time = 23-MAR-2024 14:54:54

Reaction Scheme

Optimized transition state 1

**Figure S1: Optimized transition state 1**   **E(RPM6) = -0.04357821 a.u.**

Optimized transition state 2
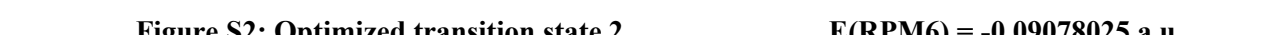
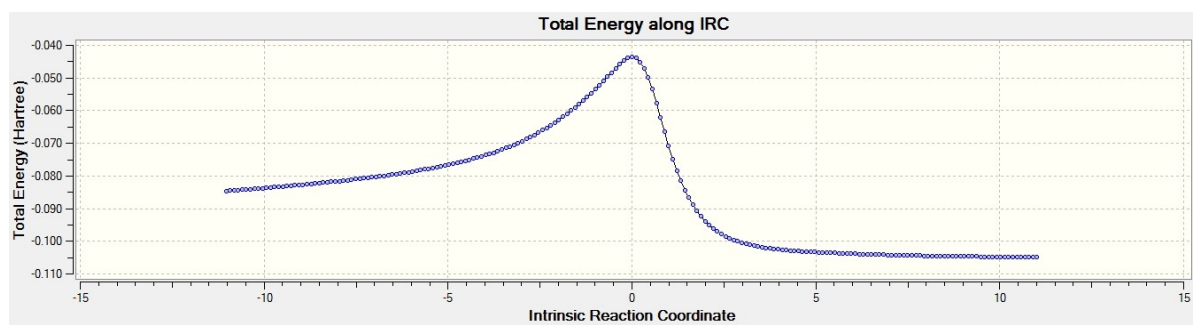**Figure S2: Optimized transition state 2**   **E(RPM6) = -0.09078025 a.u.**

Predicted transition state structures have been shown as Figure S1 and Figure S2. The proposed mechanism is in agreement with computational studies. The predicted energy of transition state 1 is E(RPM6) = -0.04357821 a.u., transition state 2 is E(RPM6) = -0.09078025 a.u. Reaction pathways are supported by a number of energy states. IRC calculations were done and the results are shown in graphs.
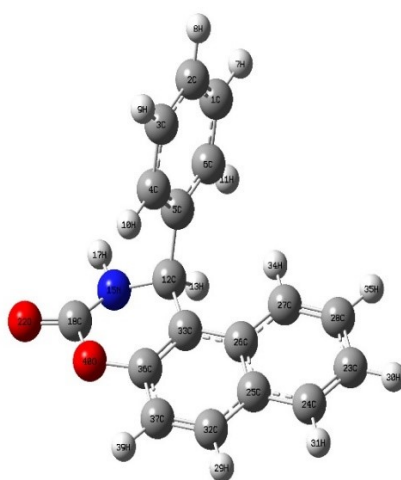
Figure S3: Optimized Product

IRC -TS1

IRC -TS 2