

Electronic supplementary information for

I₂-TBHP-catalyzed one-pot highly efficient synthesis of 4,3-fused 1,2,4-triazoles from *N*-tosylhydrazones and aromatic *N*-heterocycles via intermolecular formal 1,3-dipolar cycloaddition

Surendra Babu Inturi,^{a,b} Biswajit Kalita^{*a} and A. Jafar Ahamed^{*b}

^a*Medicinal Chemistry Division, Jubilant Biosys Ltd, #96, Industrial Suburb, 2nd Stage, Yeshwanthpur, Bangalore 560022, Karnataka, India.*

^b*Post Graduate and Research Department of Chemistry, Jamal Mohamed College (Autonomous), affiliated to Bharathidasan University, Tiruchirappalli - 620020, Tamil Nadu, India.*

**Corresponding authors. Tel.: +91-80-6662-8645.
E-mail address: biswajit_kalita@jubilantbiosys.com
E-mail address: agjafar@yahoo.co.in*

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¹H and ¹³C NMR Spectra of compounds 3a-l, 3o-q, 5a-j:

NUCLEUS : H1
FREQ (MHz) : 399.63
AT (sec) : 2.27
SW (ppm) : 18.08
RD (sec) : 1.00
DW (usec) : 6.60
Scans : 64
Solvent : cdcl3
Data Points : 32768
LB (Hz) : 1.00
TEMP (K) : 303.15
EXP : s2pul
DATE : Nov 4 2015
System : VNMR5_400

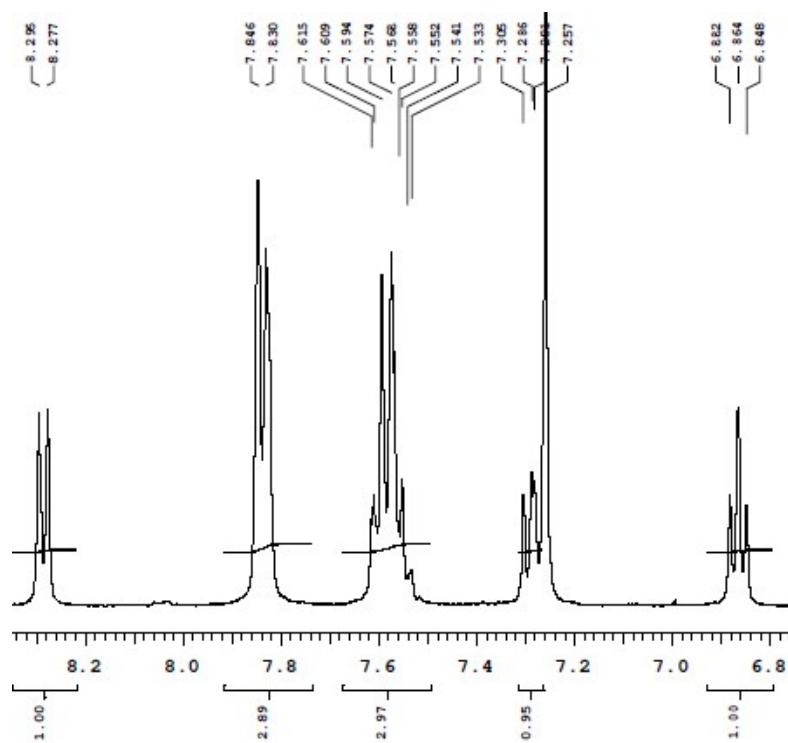
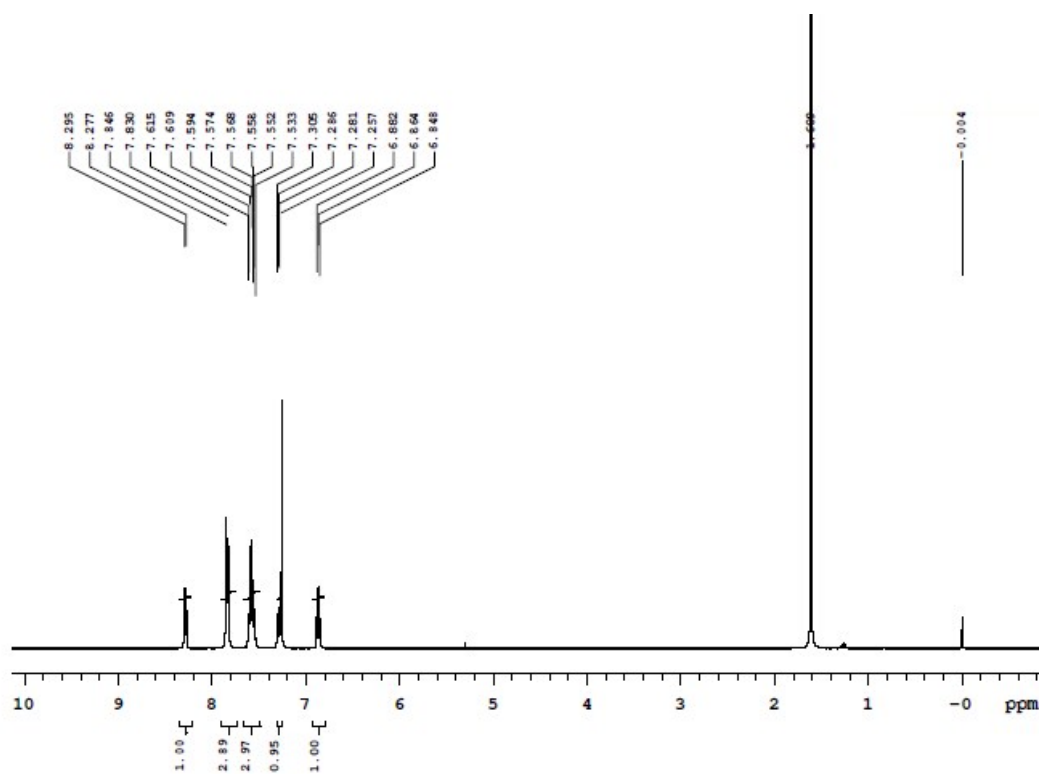
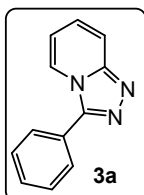


Figure S3. ¹H NMR Spectra & its expansion for compound 3a in CDCl₃

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AT (sec) : 1.28
SW (ppm) : 253.84
RE (sec) : 1.00
DW (usec) : 5.05
Scans : 1500
Solvent : cdcl3
Data Points : 65536
LB (Hz) : 4.00
TEMP (K) : 303.15
EXP : s2pul
DATE : Nov 20 2015
System : VNMRB_400

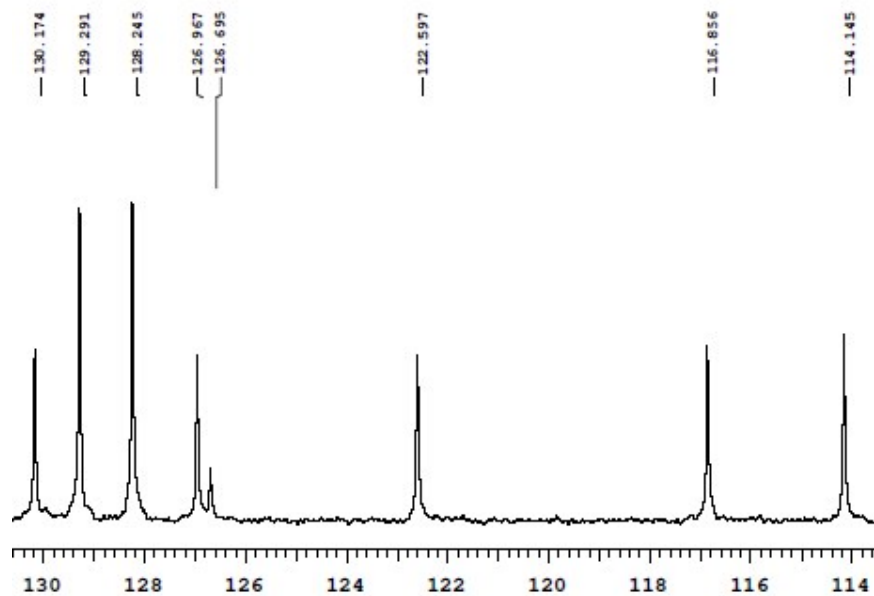
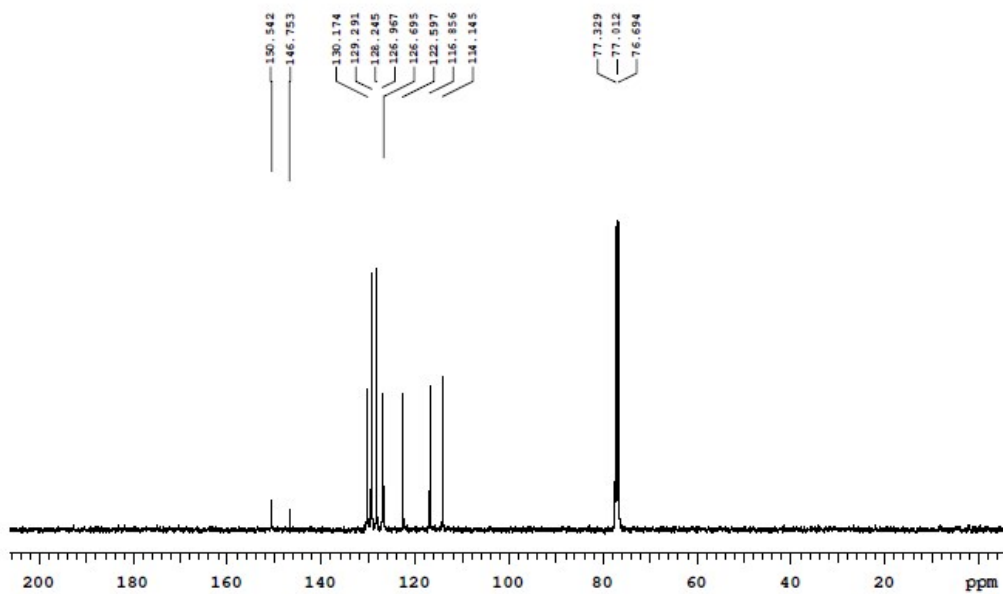
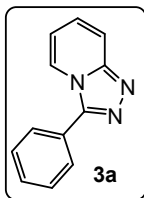


Figure S4. ^{13}C NMR Spectra & its expansion for compound **3a** in CDCl_3

NUCLEUS : H1
 FRQ (MHz) : 399.63
 AT (sec) : 2.27
 SW (ppm) : 18.08
 RD (sec) : 1.00
 PW (usec) : 6.60
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 System : VNMR5_400

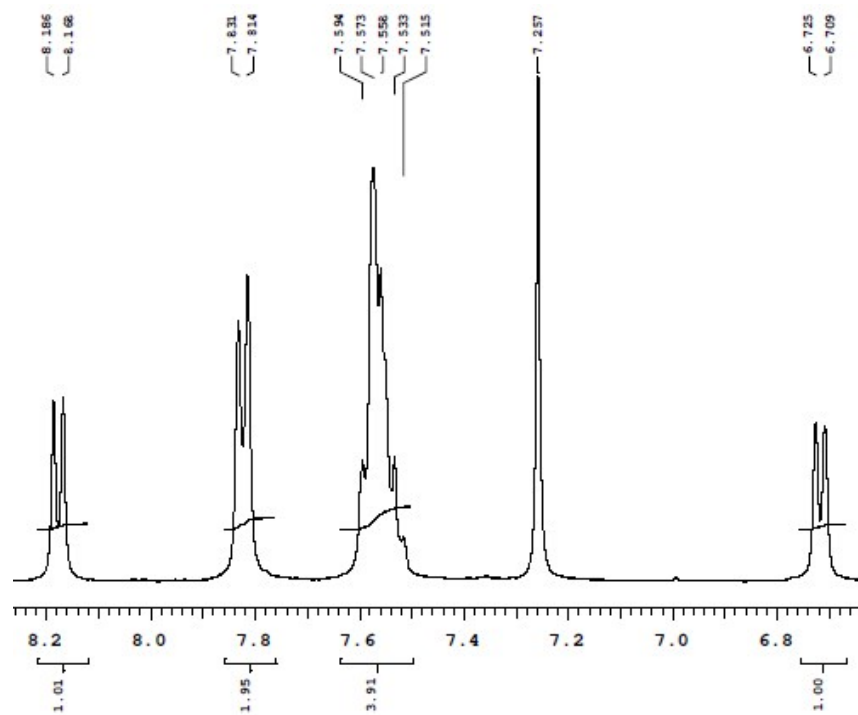
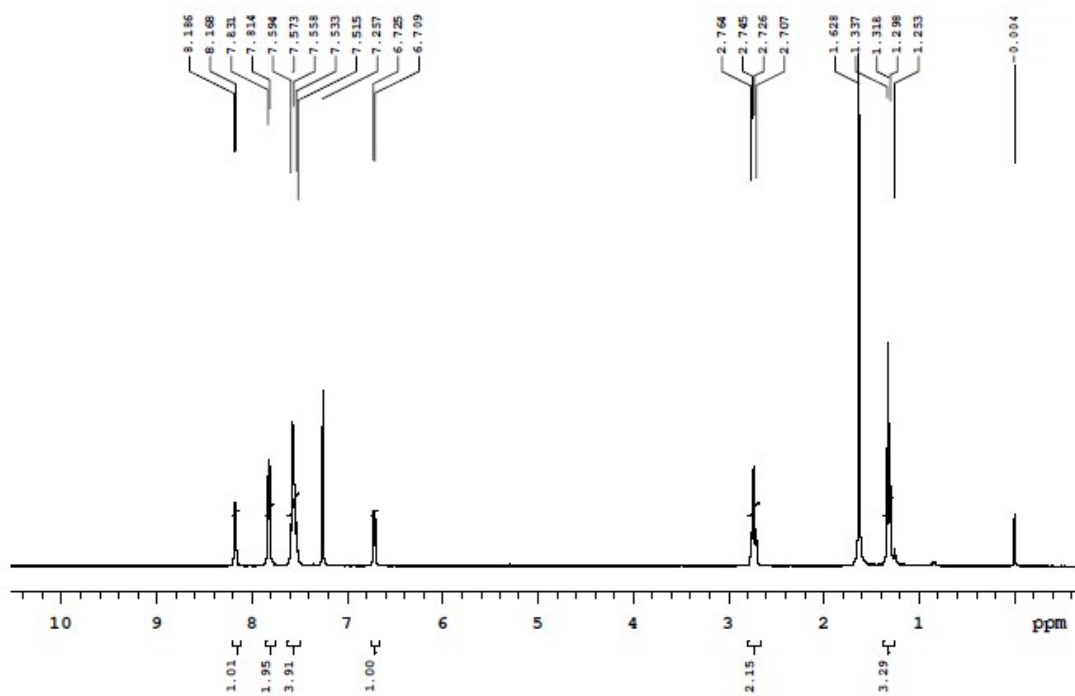
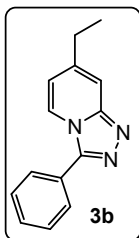


Figure S5. ^1H NMR Spectra & its expansion for compound **3b** in CDCl_3

NUCLEUS : C13
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AT (sec) : 1.28
SW (ppm) : 253.84
RD (sec) : 1.00
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System : VNMR_400

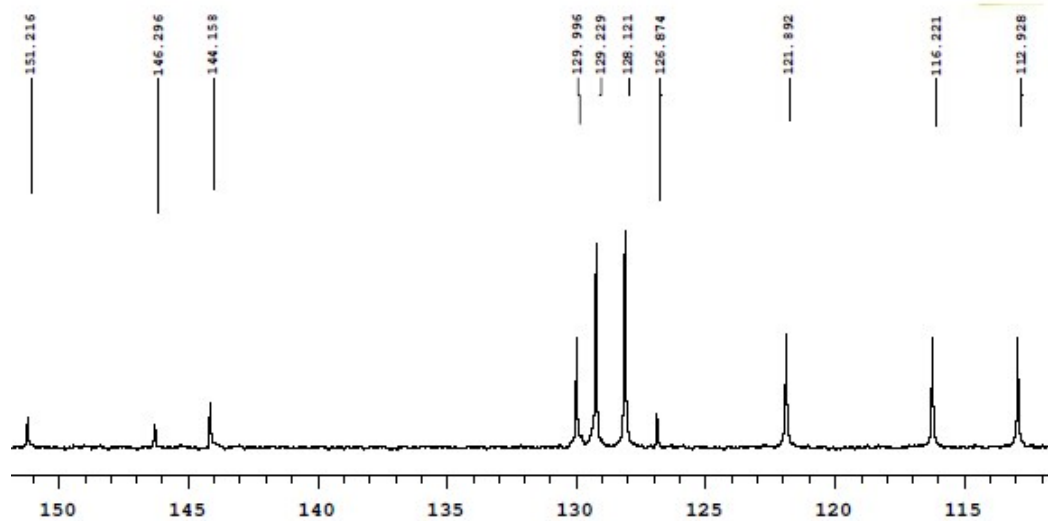
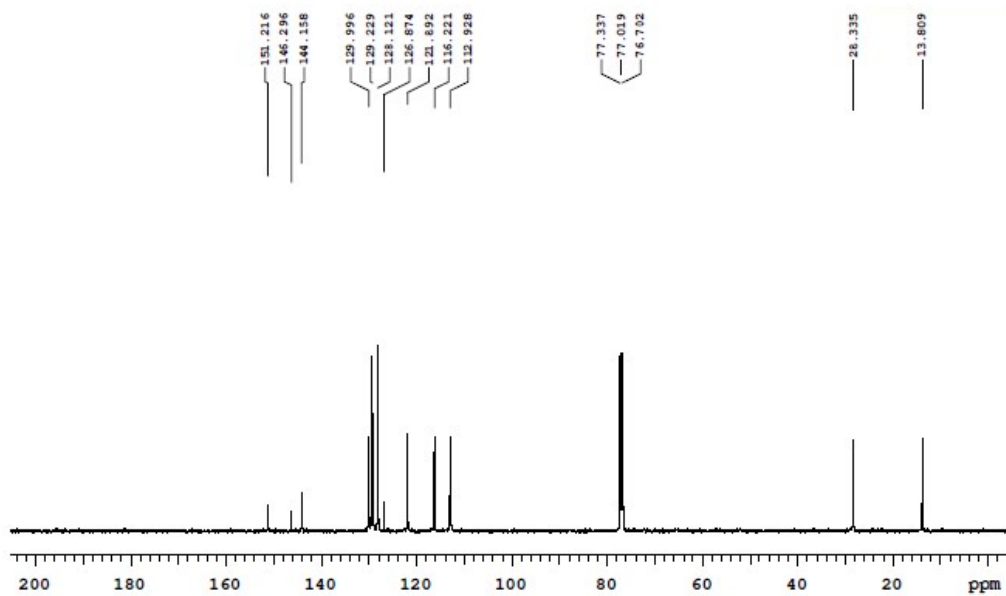
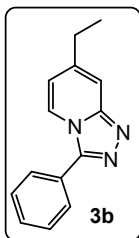


Figure S6. ^{13}C NMR Spectra & its expansion for compound **3b** in CDCl_3

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 SW (ppm) : 18.08
 RD (sec) : 1.00
 PW (usec) : 6.40
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 DATE : Dec 29 2015
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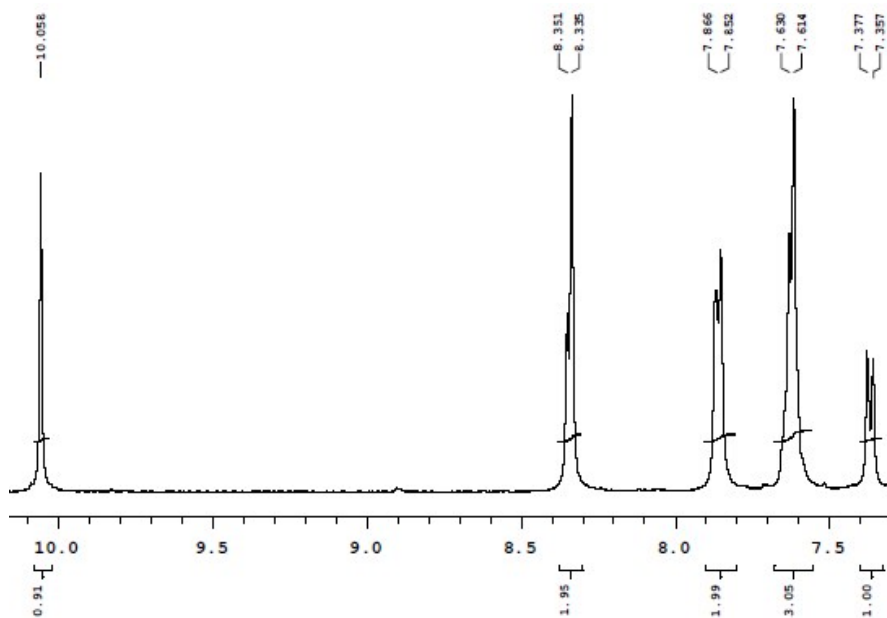
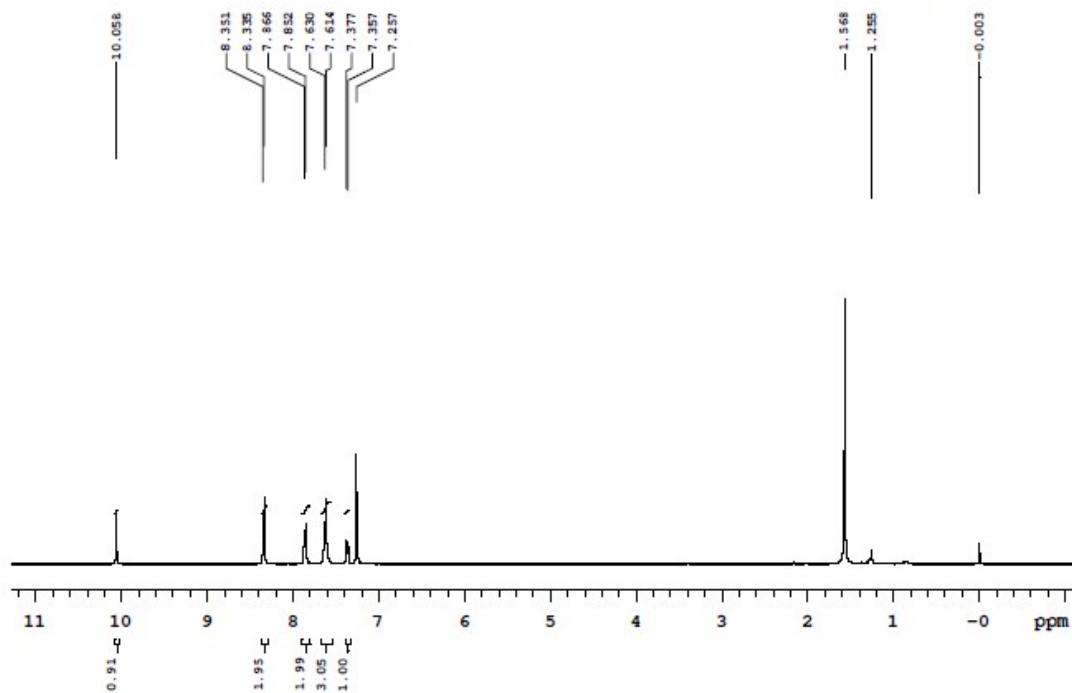
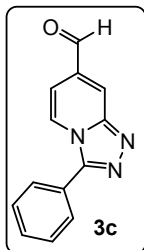


Figure S7. ^1H NMR Spectra & its expansion for compound **3c** in CDCl_3

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 RD (sec) : 1.00
 DW (usec) : 5.05
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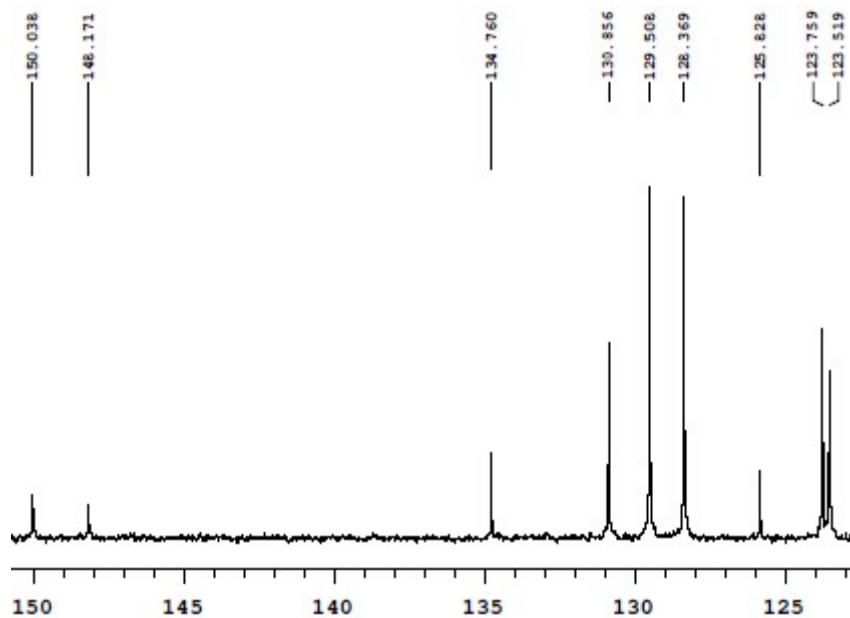
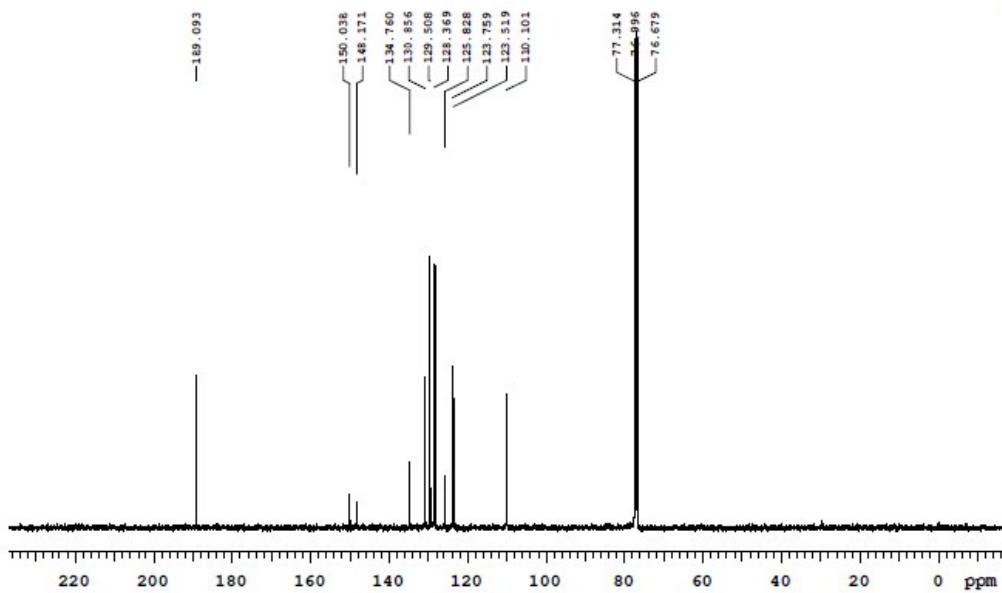
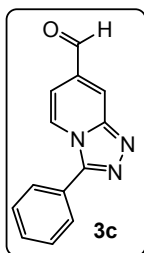


Figure S8. ^{13}C NMR Spectra & its expansion for compound **3c** in CDCl_3

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 FREQ (MHz) : 399.64
 AT (sec) : 2.27
 SW (ppm) : 18.08
 RD (sec) : 1.00
 PW (usec) : 6.60
 Scans : 64
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 LB (Hz) : 1.00
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 DATE : Nov 20 2015
 System : VNMR_400

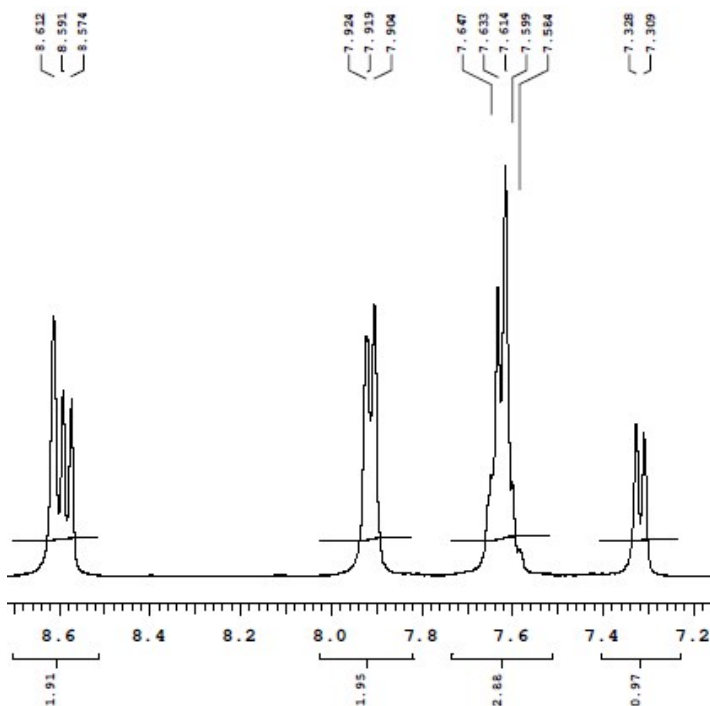
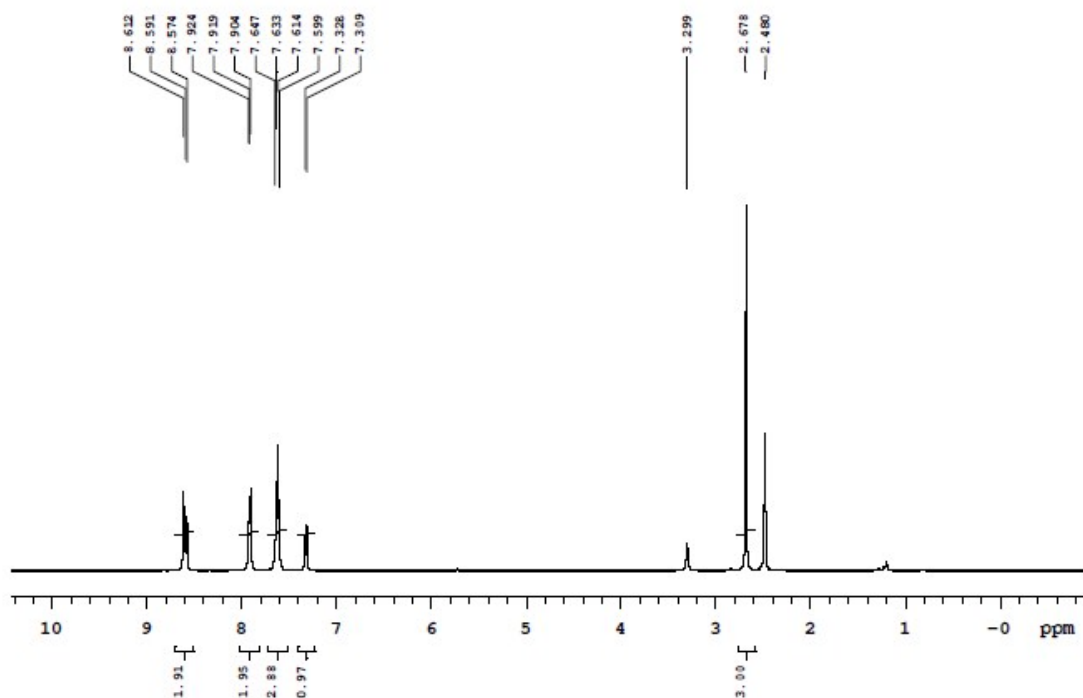
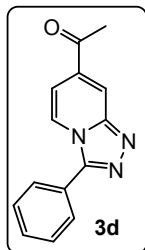


Figure S9. ^1H NMR Spectra & its expansion for compound **3d** in $\text{DMSO-}d_6$

NUCLEUS : C13
PQ (MHz) : 100.50
AT (sec) : 1.28
SW (ppm) : 253.84
RD (sec) : 1.00
DW (usec) : 5.05
Scans : 2000
Solvent : dms0
Data Points : 65536
LB (Hz) : 5.00
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DATE : Nov 21 2015
System : VNMR5_400

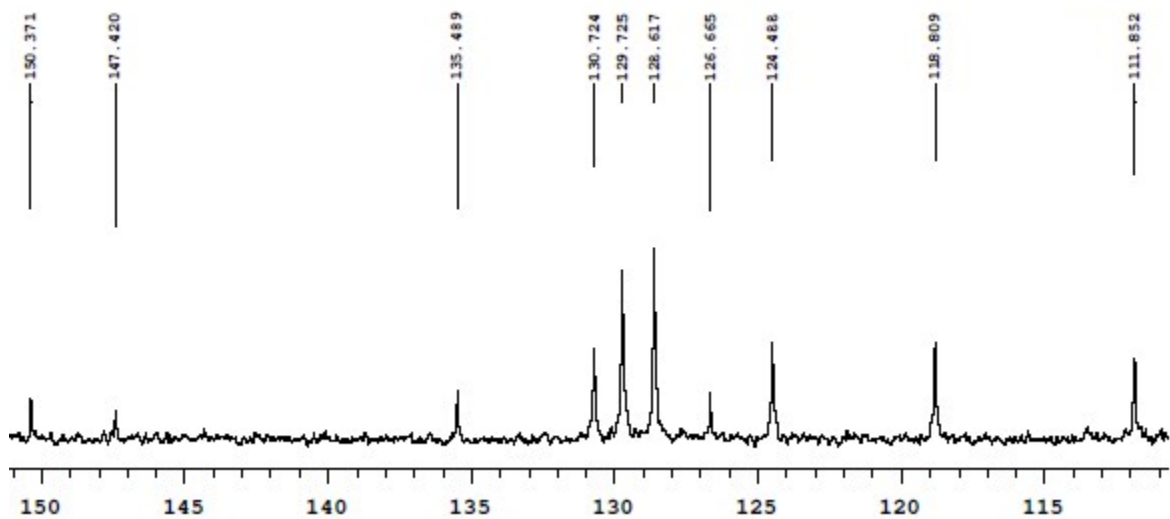
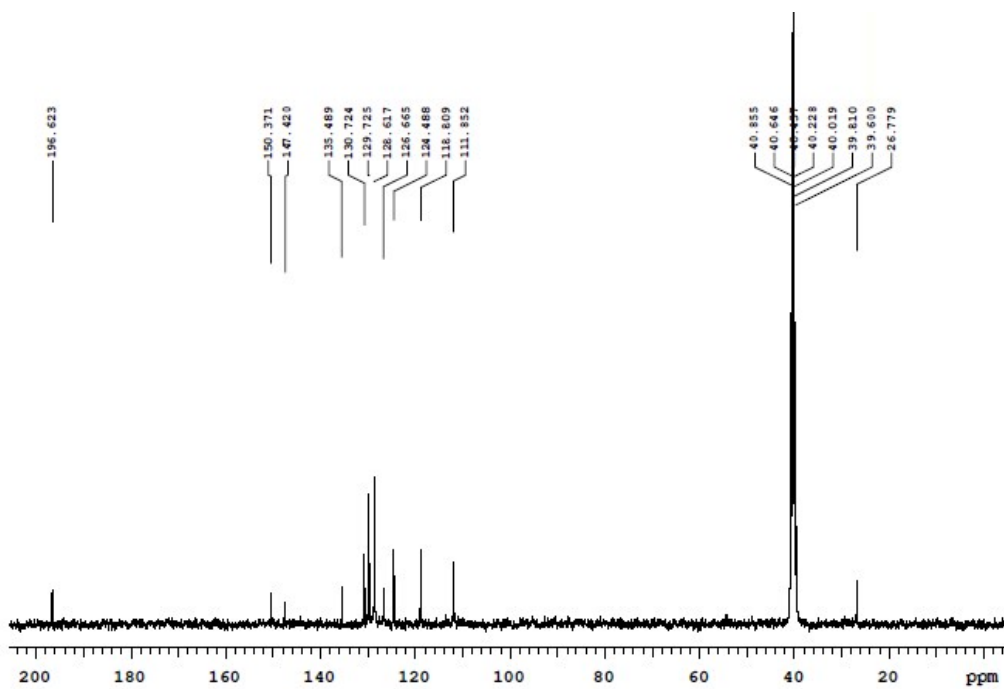
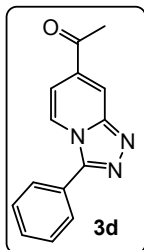


Figure S10. ^{13}C NMR Spectra & its expansion for compound **3d** in $\text{DMSO-}d_6$

NUCLEUS : H1
 FREQ (MHz) : 399.63
 AT (sec) : 2.27
 SW (ppm) : 18.08
 RD (sec) : 1.00
 DW (usec) : 6.60
 Scans : 64
 Solvent : cdcl3
 Data Points : 32768
 LB (Hz) : 2.00
 TEMP (K) : 303.15
 EXP : s2pul
 DATE : Nov 26 2015
 System : VNMR5_400

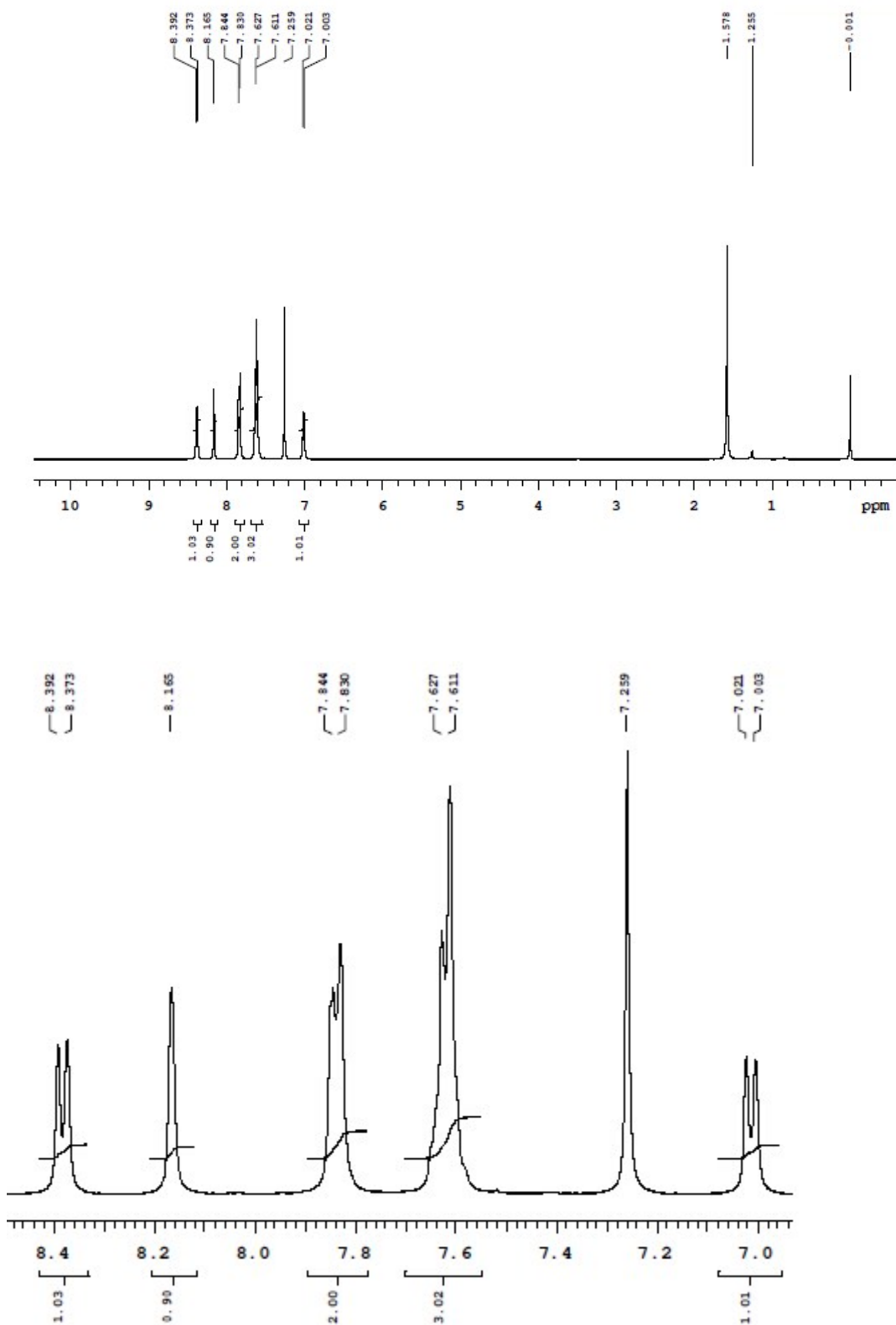
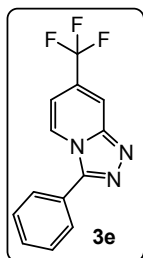


Figure S11. ^1H NMR Spectra & its expansion for compound **3e** in CDCl_3

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 SW (ppm) : 253.84
 FD (sec) : 1.00
 DW (usec) : 5.05
 Scans : 3000
 Solvent : cdcl3
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 LB (Hz) : 2.00
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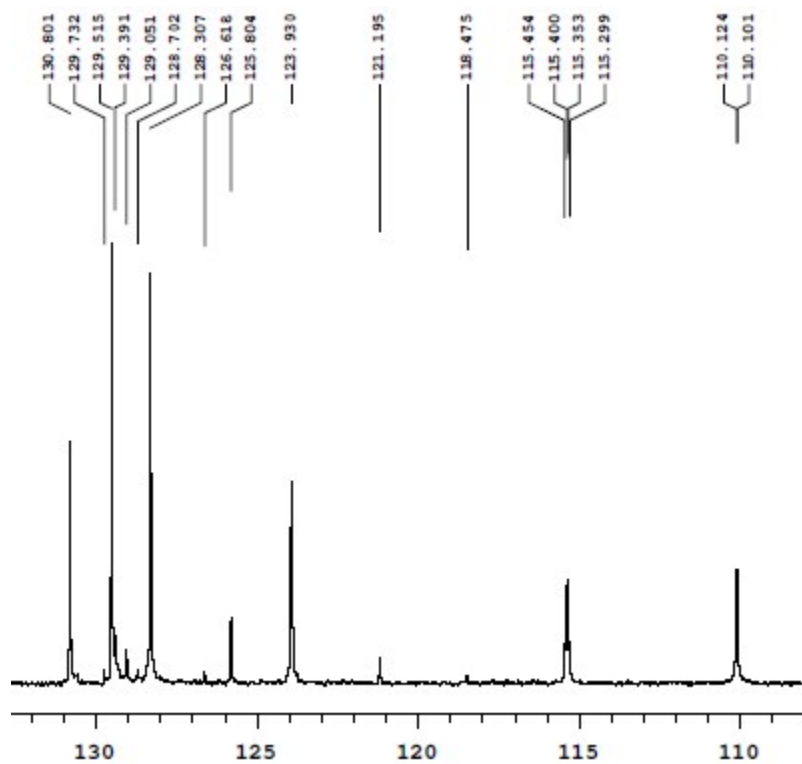
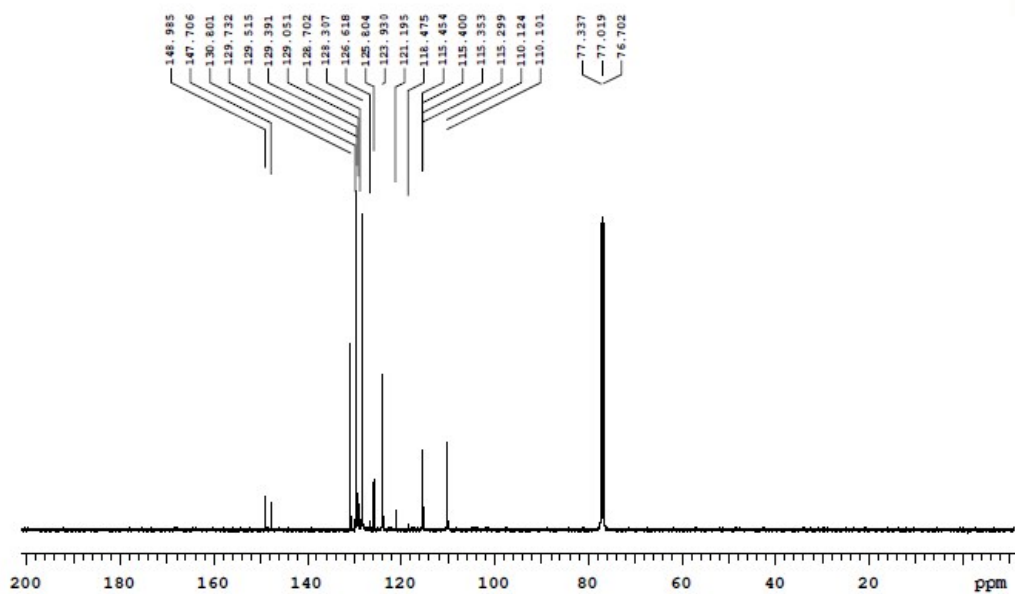
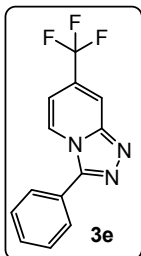


Figure S12. ^{13}C NMR Spectra & its expansion for compound **3e** in CDCl_3

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 FRQ (MHz) : 399.63
 AT (sec) : 2.27
 SW (ppm) : 18.08
 RD (sec) : 1.00
 FWH (usec) : 6.60
 Scans : 64
 Solvent : cdcl3
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 LB (Hz) : 2.00
 TEMP (K) : 303.15
 EXP : s2pul
 DATE : Nov 20 2015
 System : VNMR5_400

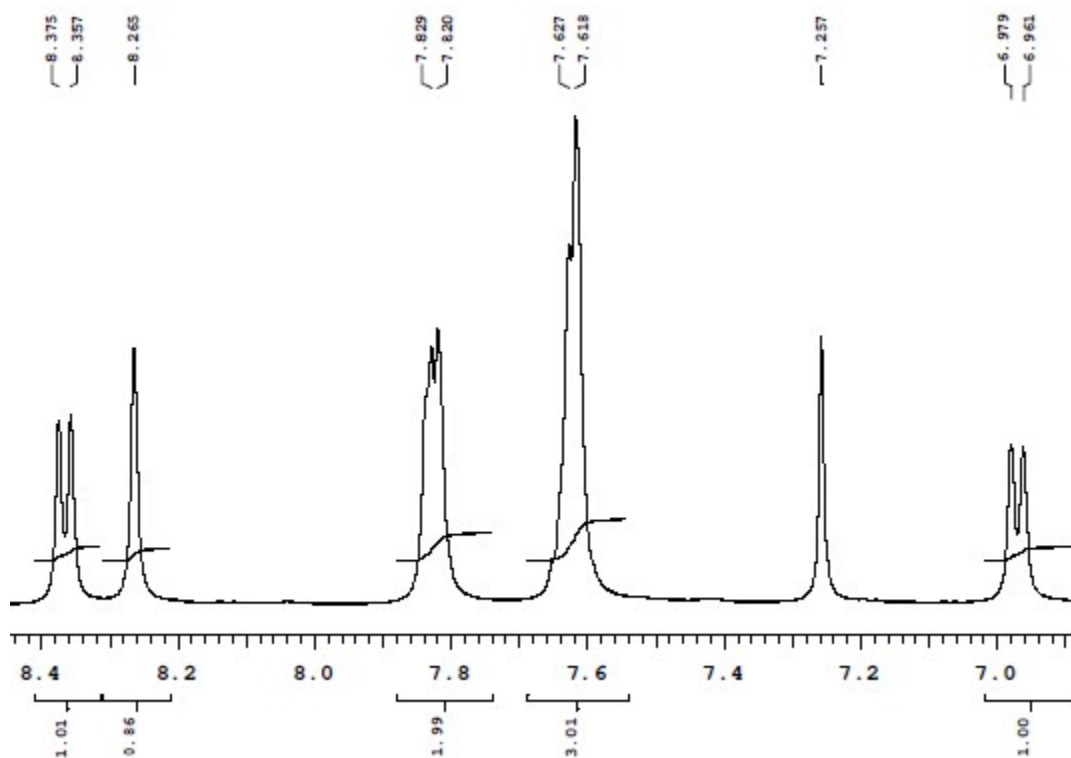
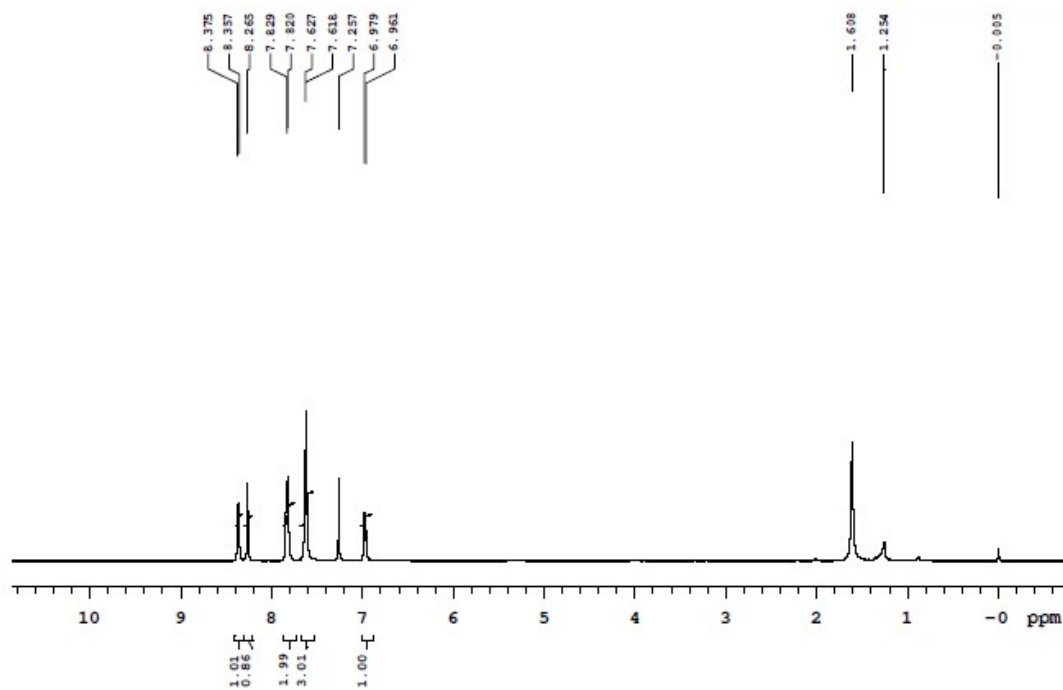
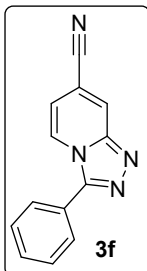


Figure S13. ^1H NMR Spectra & its expansion for compound **3f** in CDCl_3

NUCLEUS : C13
FRQ (MHz) : 100.50
AT (sec) : 1.28
SW (ppm) : 253.84
RE (sec) : 1.00
PW (usec) : 5.05
Scans : 1500
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LB (Hz) : 4.00
TEMP (K) : 303.15
EXP : #2pul
DATE : Nov 24 2015
System : VNMRB_400

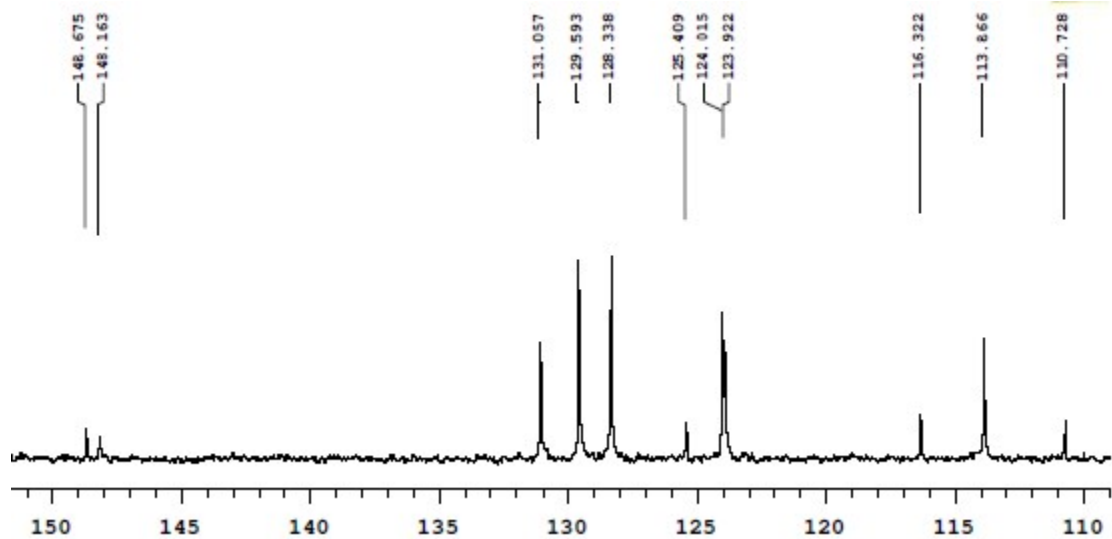
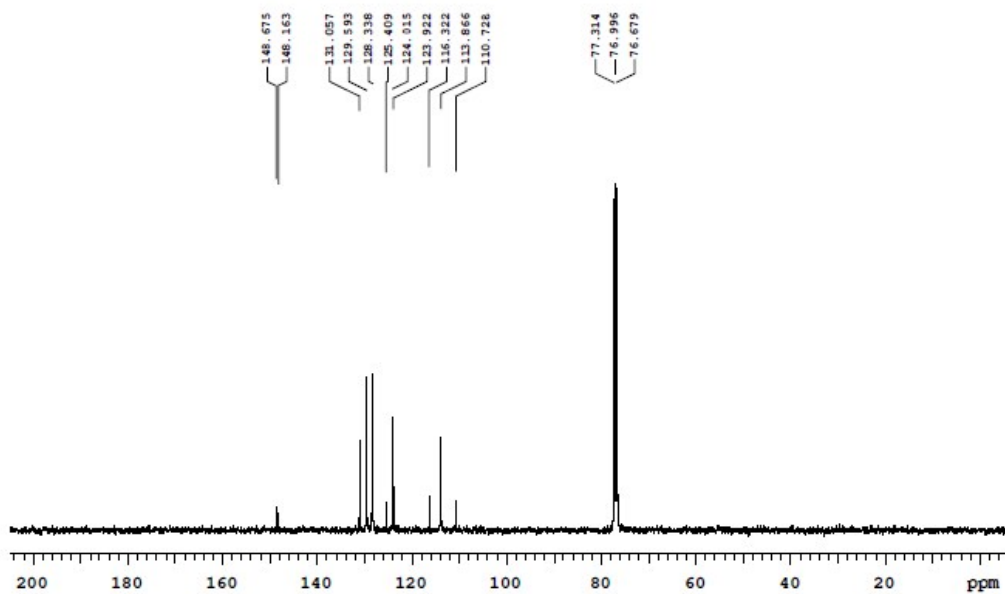
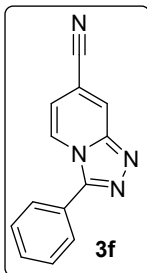


Figure S14. ^{13}C NMR Spectra & its expansion for compound **3f** in CDCl_3

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 RD (sec) : 1.00
 PW (usec) : 6.60
 Scans : 64
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 END : s2pul
 DATE : Nov 9 2015
 System : VNMR_400

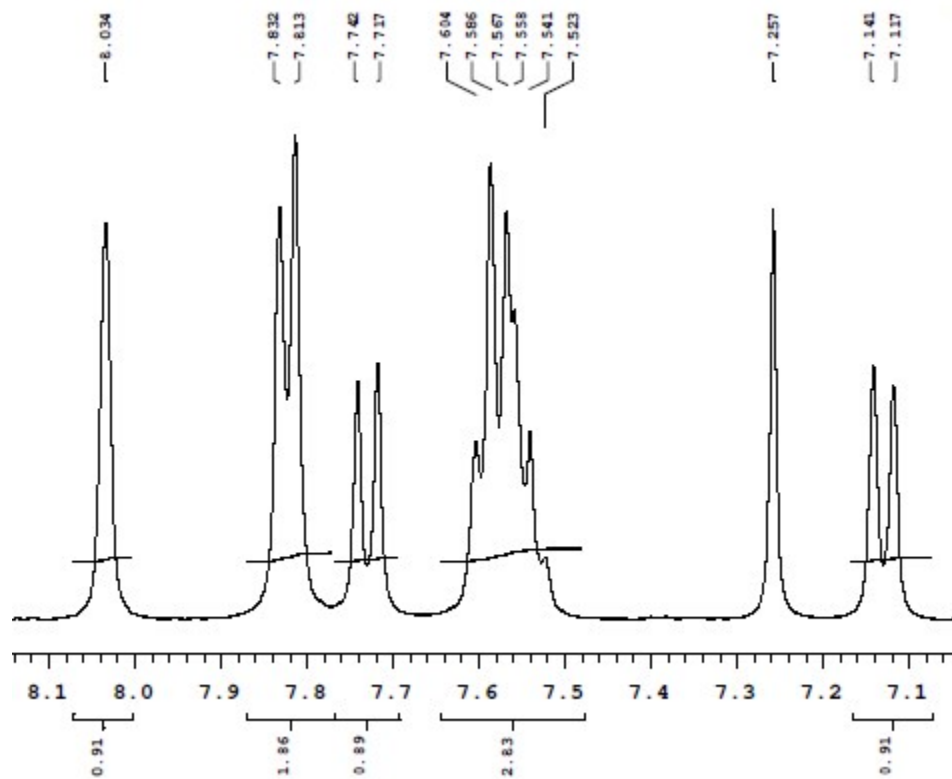
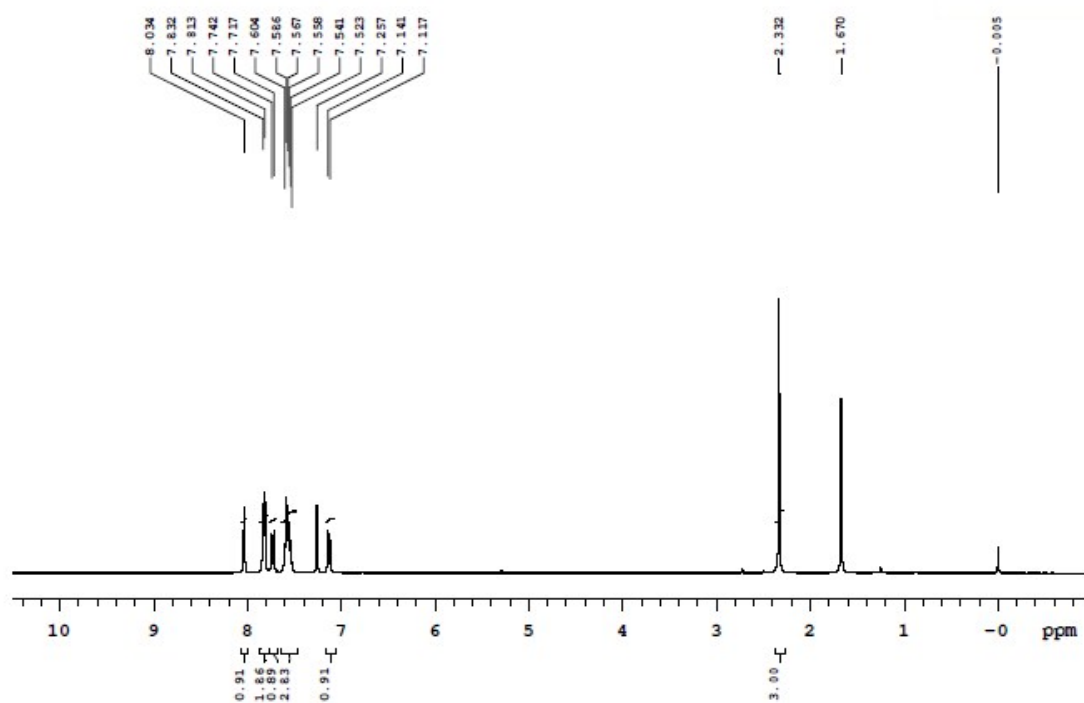
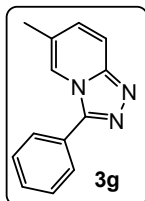


Figure S15. ^1H NMR Spectra & its expansion for compound **3g** in CDCl_3

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 PW (usec) : 5.05
 Scans : 1500
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 LB (Hz) : 3.00
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 System : VNMR5_400

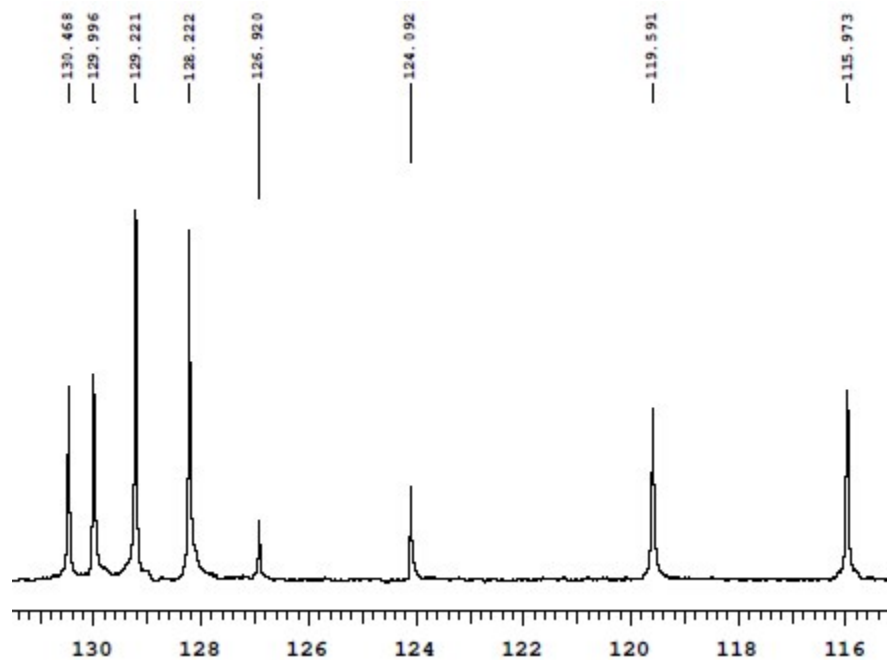
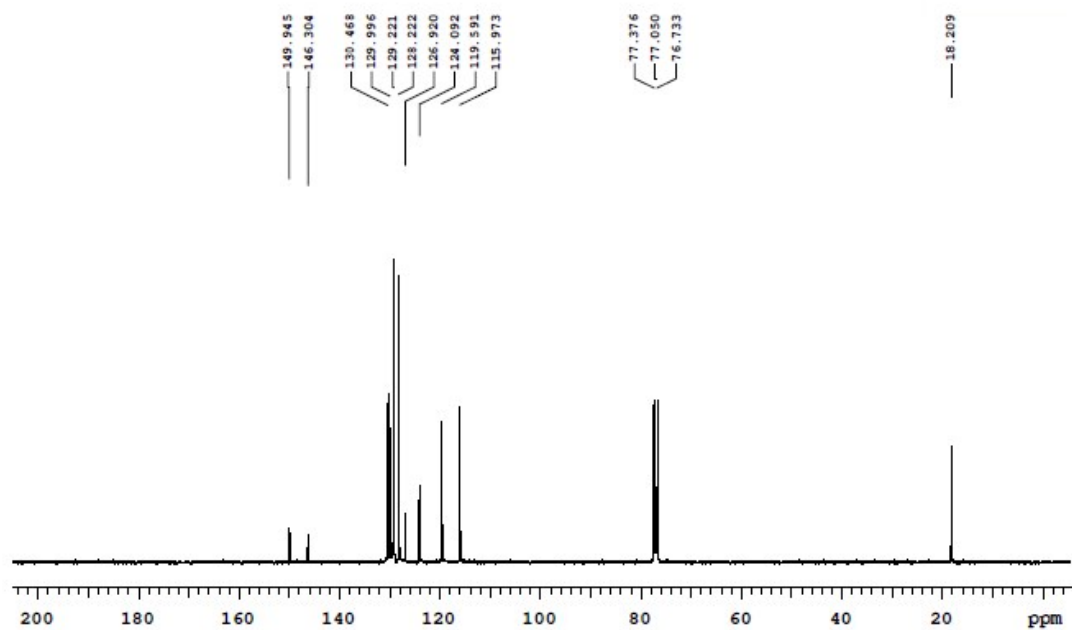
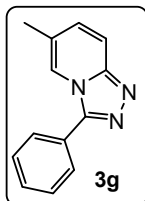


Figure S16. ^{13}C NMR Spectra & its expansion for compound **3g** in CDCl_3

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 RD (sec) : 1.00
 FWH (usec) : 6.60
 Scans : 64
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 LB (Hz) : 2.00
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 DATE : Nov 20 2015
 System : VNMR5_400

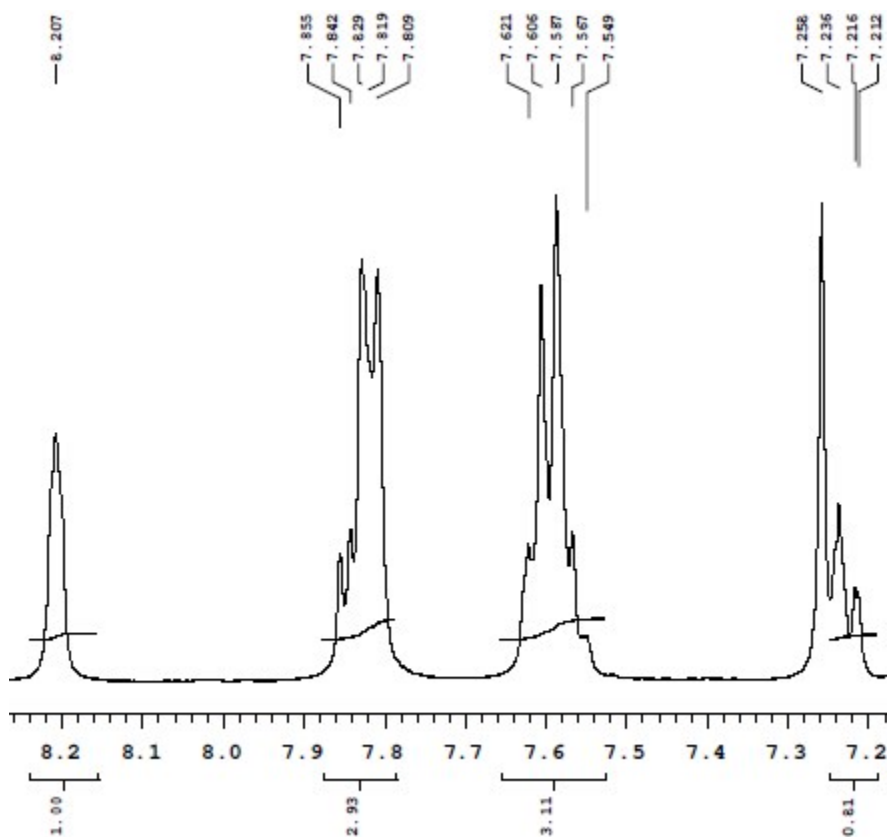
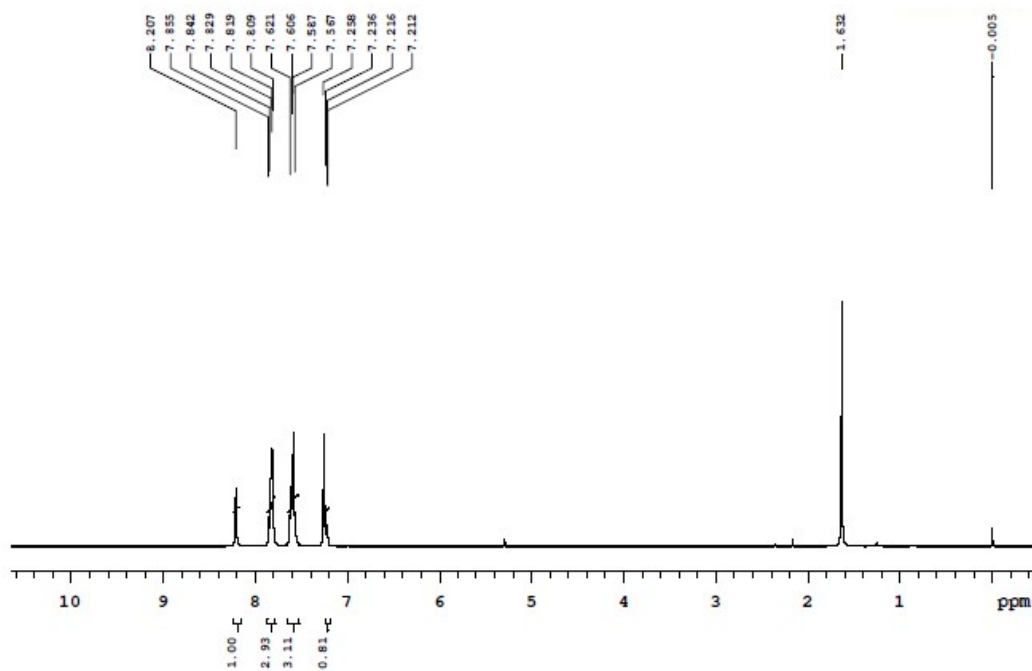
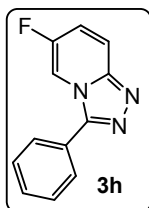


Figure S17. ¹H NMR Spectra & its expansion for compound **3h** in CDCl₃

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 AT (sec) : 1.28
 SW (ppm) : 253.84
 RD (sec) : 1.00
 FWH (usec) : 5.05
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 System : VNMR5_400

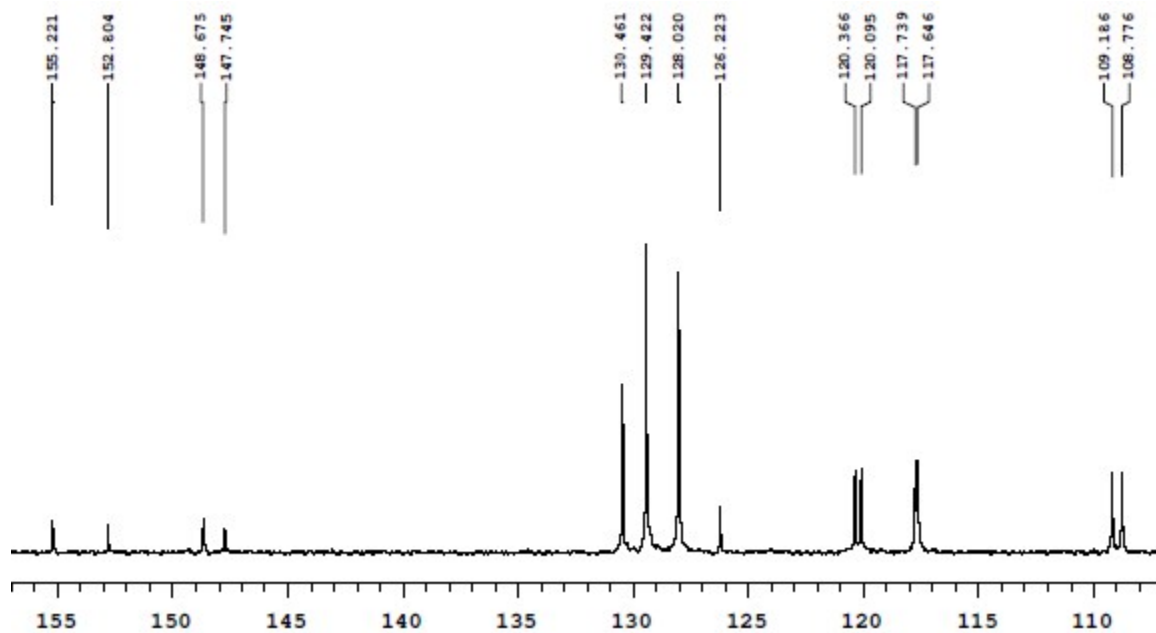
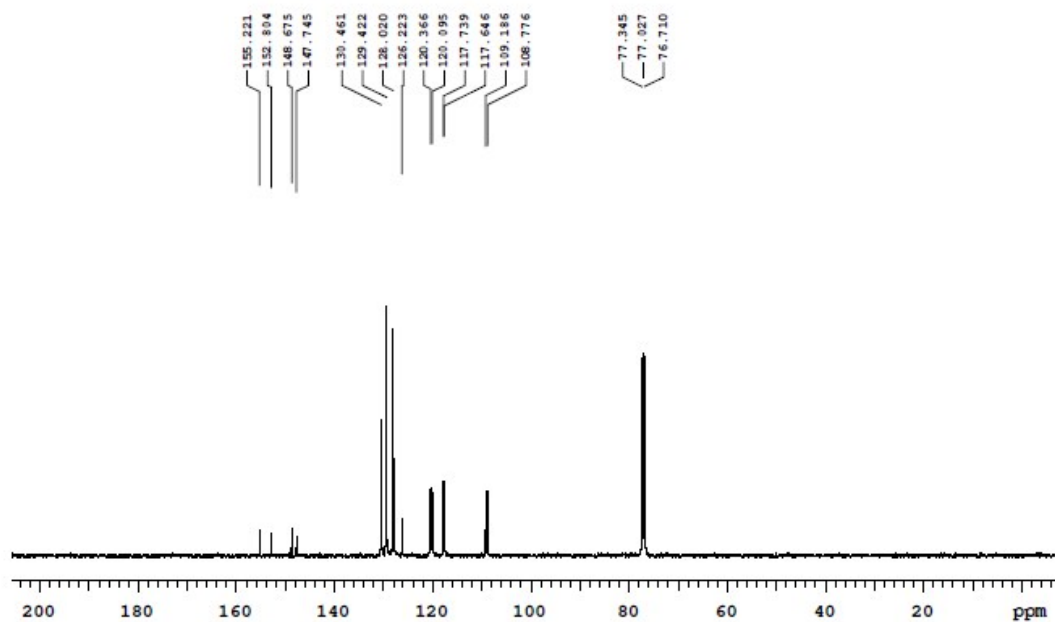
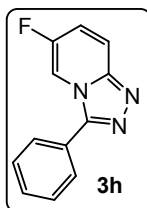


Figure S18. ^{13}C NMR Spectra & its expansion for compound **3h** in CDCl_3

NUCLEUS : H1
FRQ (MHz) : 399.64
AT (sec) : 2.27
SW (ppm) : 18.08
RD (sec) : 1.00
FID (usec) : 6.40
Scans : 32
Solvent : dms0
Data Points : 32768
LB (Hz) : 2.00
TEMP (K) : 303.15
EXP : s2pul
DATE : Dec 2 2015
System : VNMR5_400

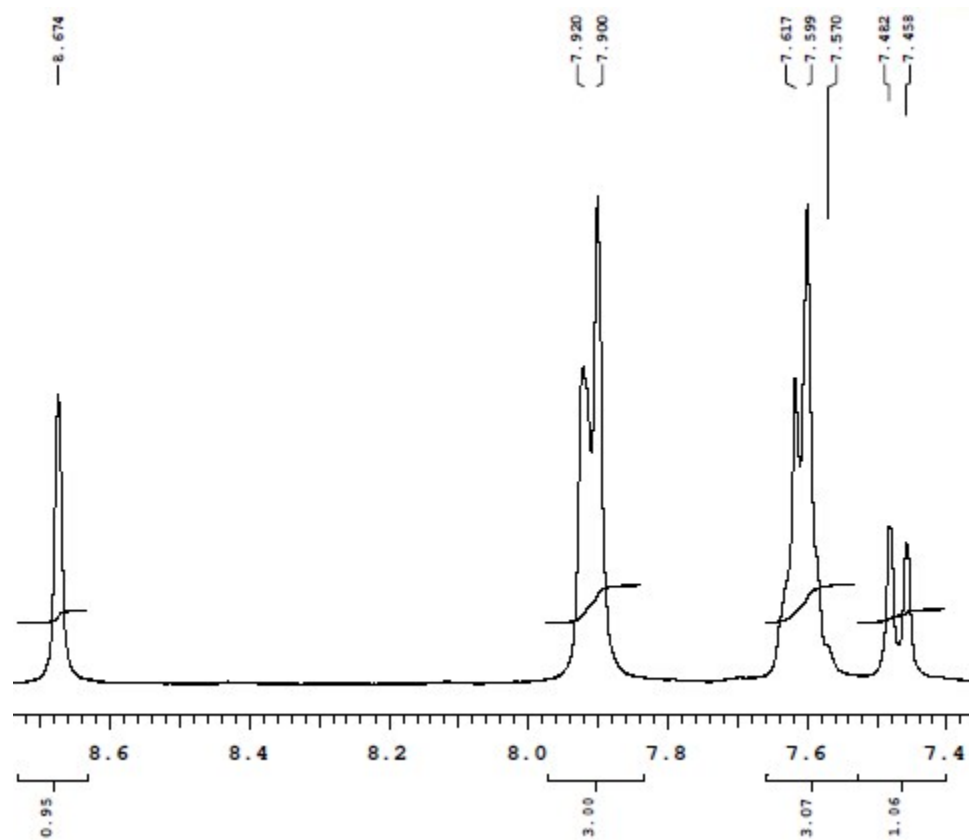
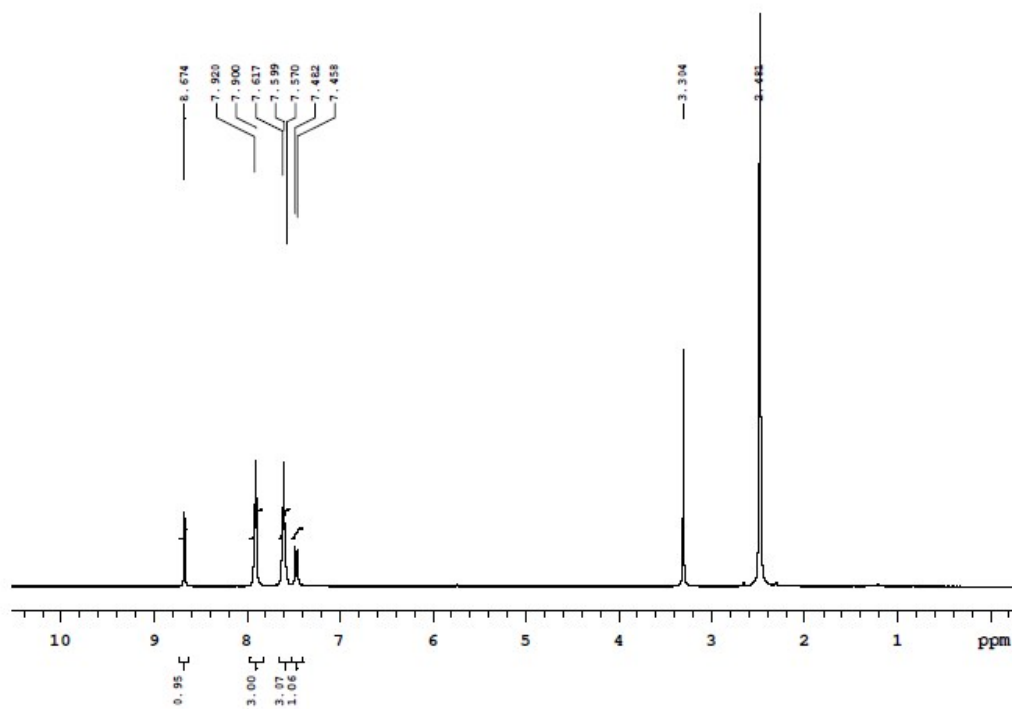
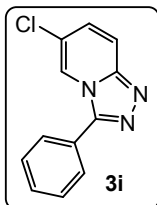


Figure S19. ^1H NMR Spectra & its expansion for compound **3i** in $\text{DMSO-}d_6$

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 FRQ (MHz) : 100.50
 AT (sec) : 1.28
 SW (ppm) : 253.84
 RD (sec) : 1.00
 PW (usec) : 5.05
 Scans : 3000
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 Data Points : 65536
 LB (Hz) : 2.00
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 DATE : Dec 5 2015
 System : VNMR_400

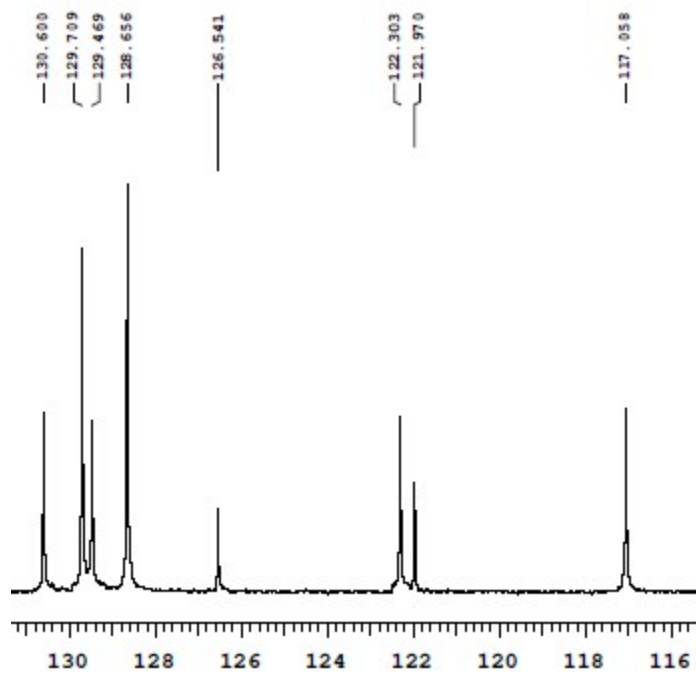
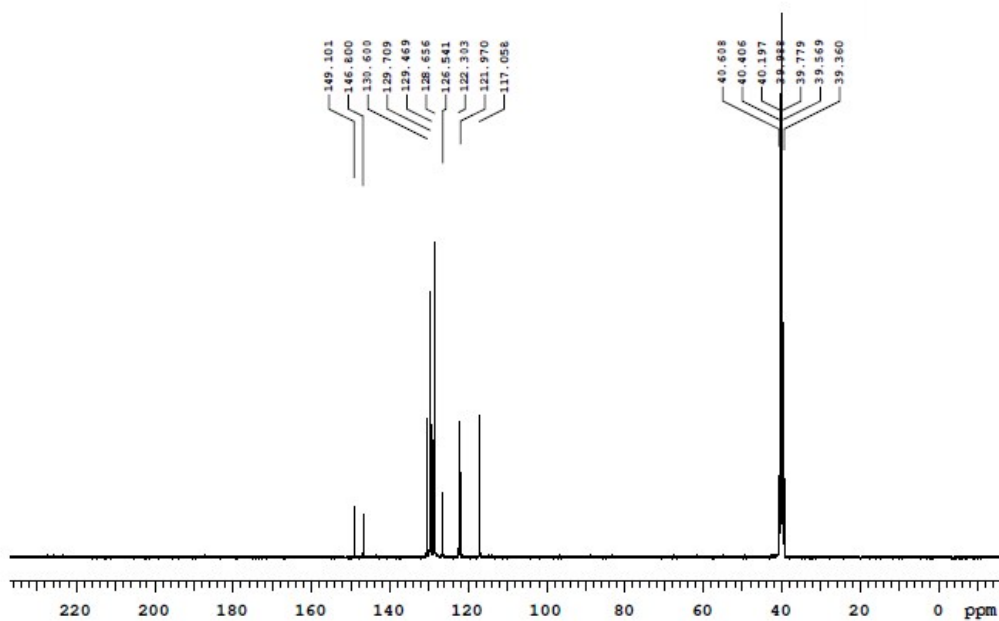
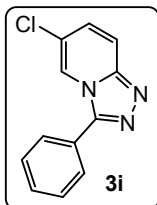


Figure S20. ^{13}C NMR Spectra & its expansion for compound **3i** in $\text{DMSO-}d_6$

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 FREQ (MHz) : 399.63
 AT (sec) : 2.27
 SW (ppm) : 18.08
 RD (sec) : 1.00
 DW (usec) : 6.60
 Scans : 64
 Solvent : cdcl3
 Data Points : 32768
 LB (Hz) : 1.00
 TEMP (K) : 303.15
 END : s2pul
 DATE : Nov 4 2015
 System : VNMR5_400

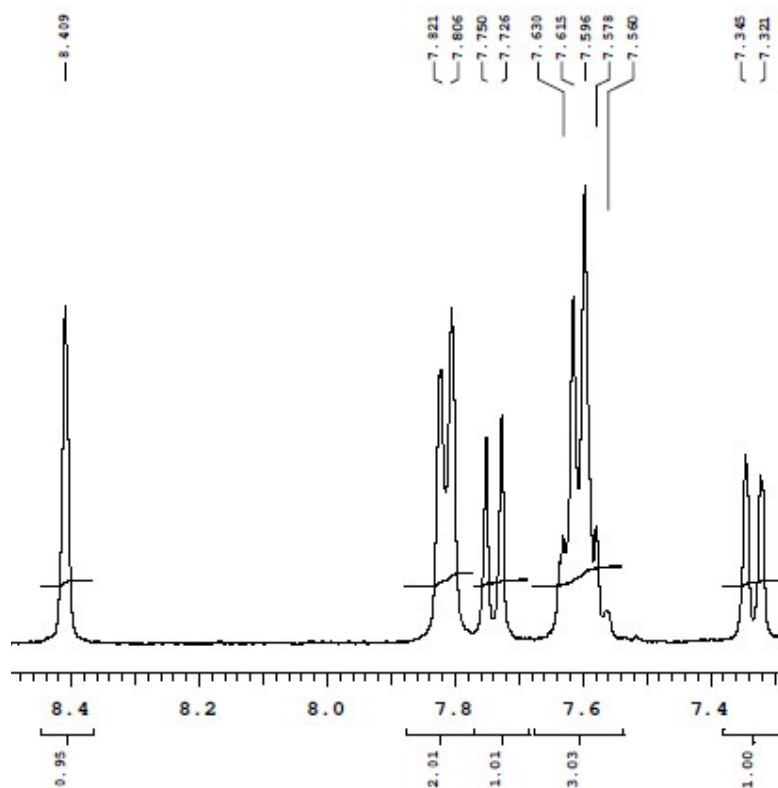
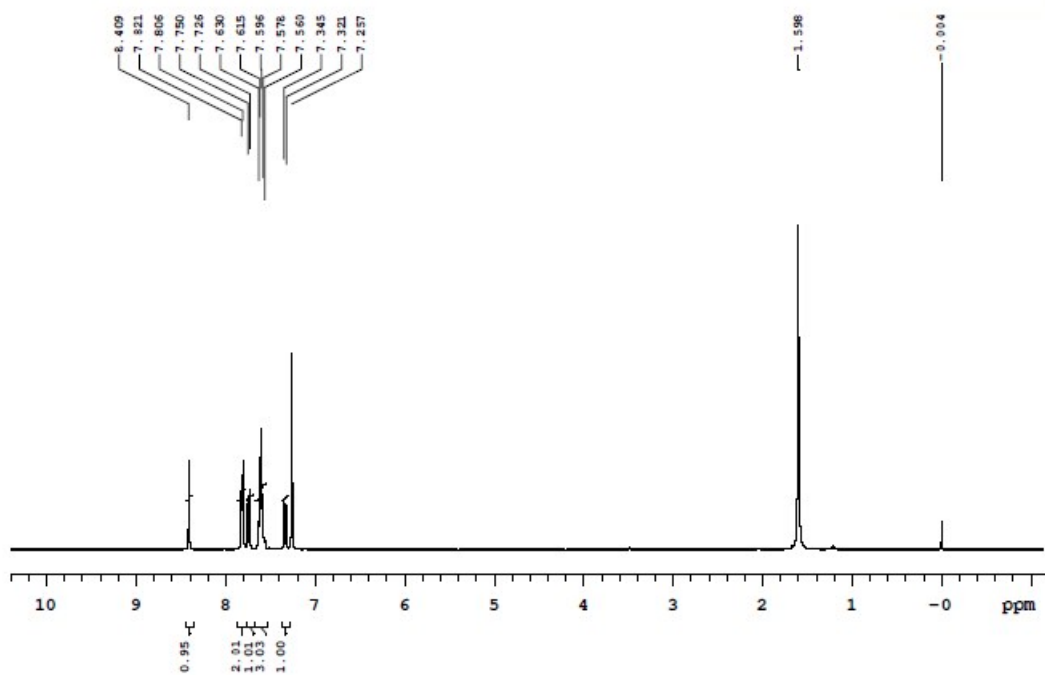
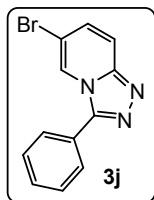


Figure S21. ^1H NMR Spectra & its expansion for compound **3j** in CDCl_3

NUCLEUS : C13
FRQ (MHz) : 100.50
AT (sec) : 1.28
SW (ppm) : 253.84
RD (sec) : 1.00
PW (usec) : 5.05
Scans : 1500
Solvent : cdcl3
Data Points : 65536
LS (Hz) : 2.00
TEMP (K) : 303.15
EXP : s2p01
DATE : Dec 15 2015
System : VNMR5_400

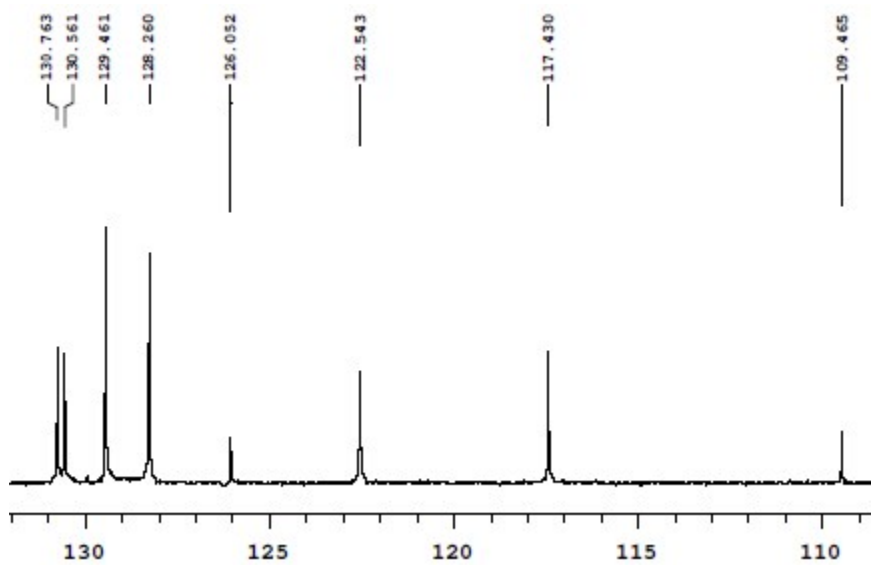
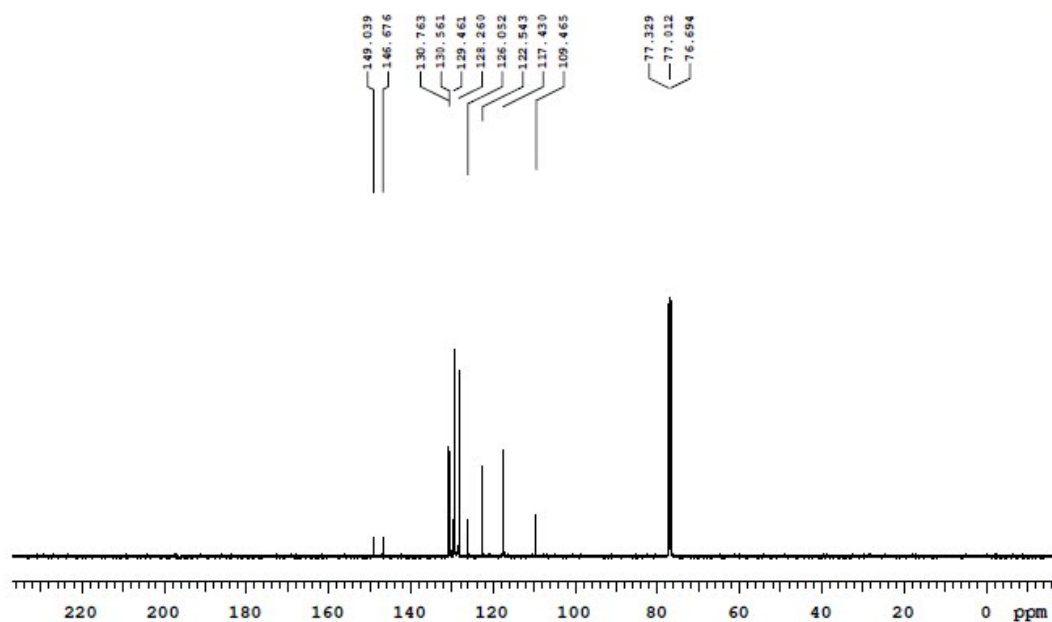
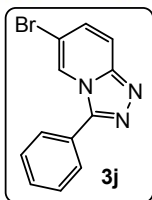


Figure S22. ^{13}C NMR Spectra & its expansion for compound **3j** in CDCl_3

NUCLEUS : H1
 FREQ (MHz) : 399.63
 AT (sec) : 2.27
 SW (ppm) : 18.08
 RD (sec) : 1.00
 PW (usec) : 6.60
 Scans : 64
 Solvent : cdcl3
 Data Points : 32768
 LB (Hz) : 1.00
 TEMP (K) : 303.15
 EXP : s2pu1
 DATE : Nov 5 2015
 System : VNMR5_400

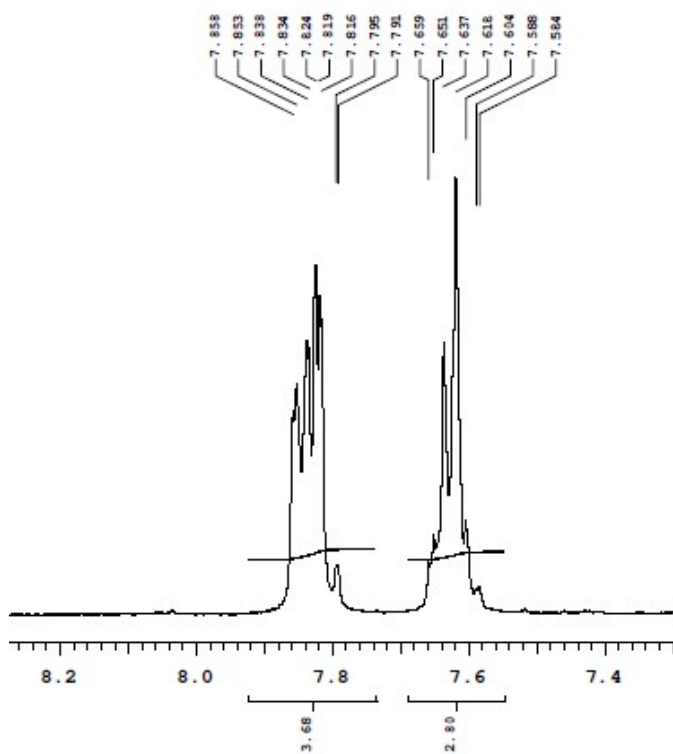
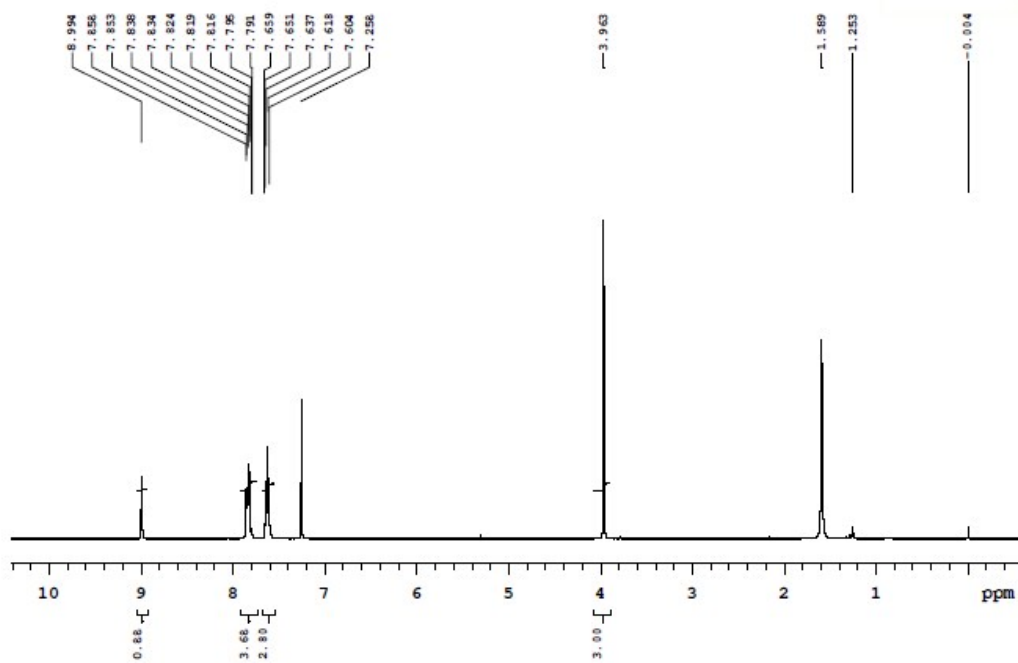
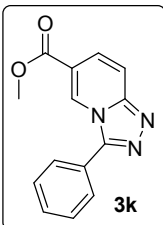


Figure S23. ^1H NMR Spectra & its expansion for compound **3k** in CDCl_3

NUCLEUS : C13
FRQ (MHz) : 100.50
AT (sec) : 1.28
SW (ppm) : 253.84
RD (sec) : 1.00
PW (usec) : 5.05
Scans : 1500
Solvent : cdcl3
Data Points : 65536
LB (Hz) : 8.00
TEMP (K) : 303.15
END : s2pul
DATE : Nov 21 2015
System : VNMR5_400

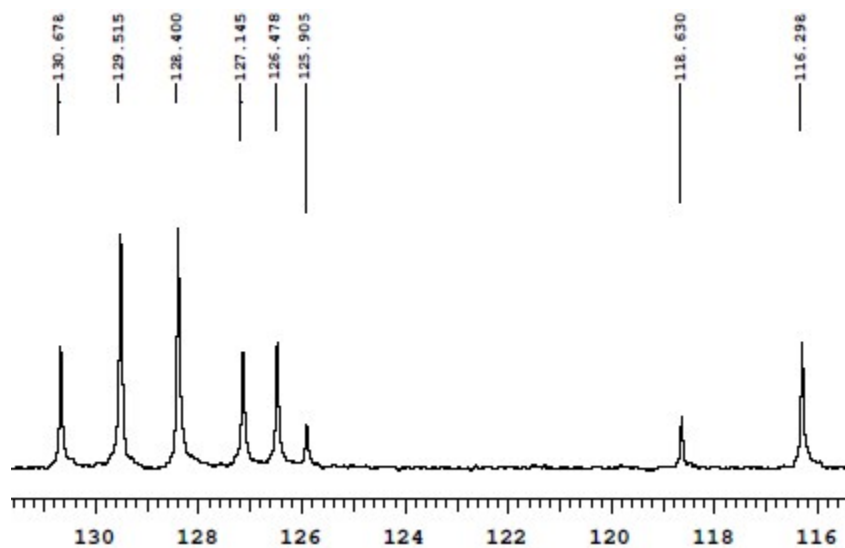
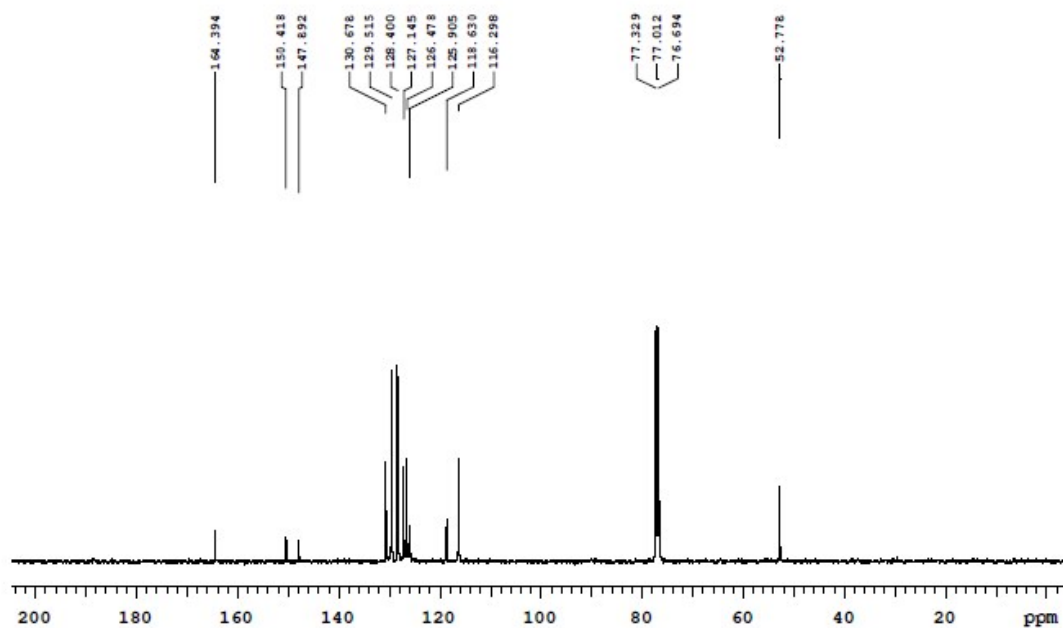
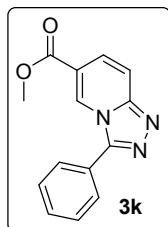


Figure S24. ¹³C NMR Spectra & its expansion for compound **3k** in CDCl₃

NUCLEUS : H1
 FREQ (MHz) : 399.63
 AT (sec) : 2.27
 SW (ppm) : 18.08
 RD (sec) : 1.00
 PW (usec) : 6.40
 Scans : 64
 Solvent : cdcl3
 Data Points : 32768
 LB (Hz) : 2.00
 TEMP (K) : 303.15
 EXP : s2pu1
 DATE : May 17 2016
 System : VNMR5_400

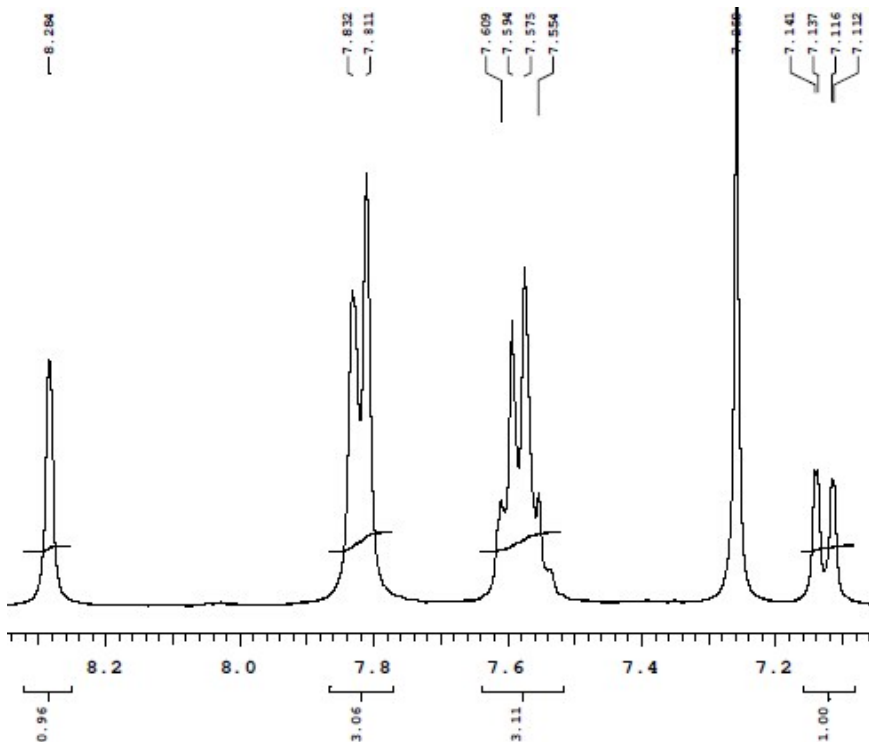
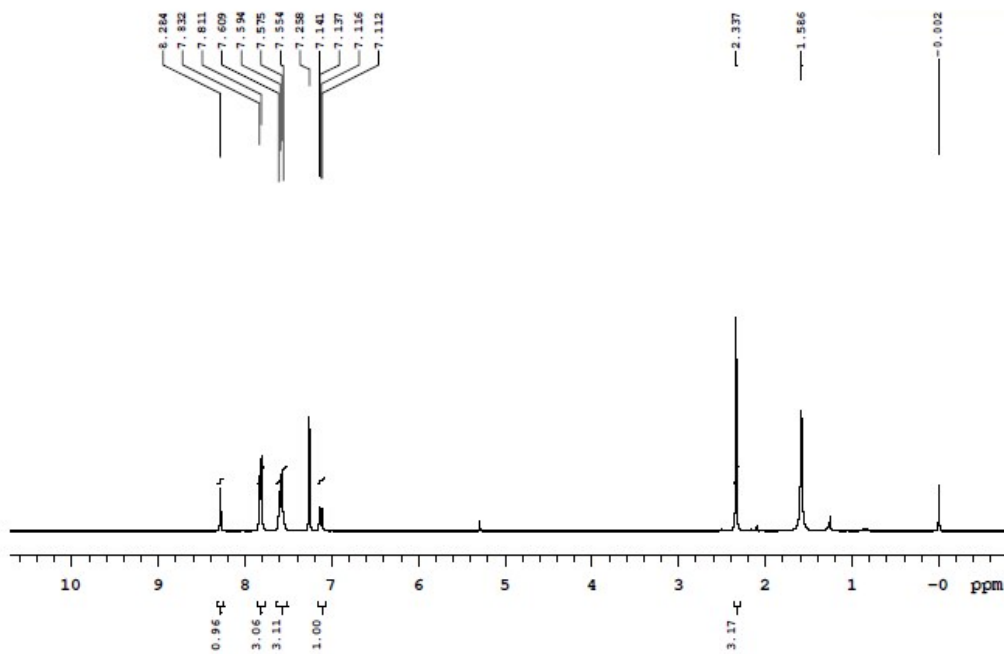
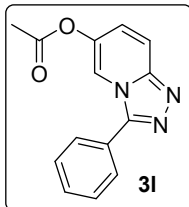


Figure S25. ^1H NMR Spectra & its expansion for compound **31** in CDCl_3

NUCLEUS : C13
 FREQ (MHz) : 100.50
 AT (sec) : 1.28
 SW (ppm) : 253.84
 FD (Hz) : 1.00
 DW (usec) : 5.05
 Scans : 4000
 Solvent : cdcl3
 Data Points : 65536
 LB (Hz) : 6.00
 TEMP (K) : 303.15
 EXP : s2pul
 DATE : May 18 2016
 System : VNMR5_400

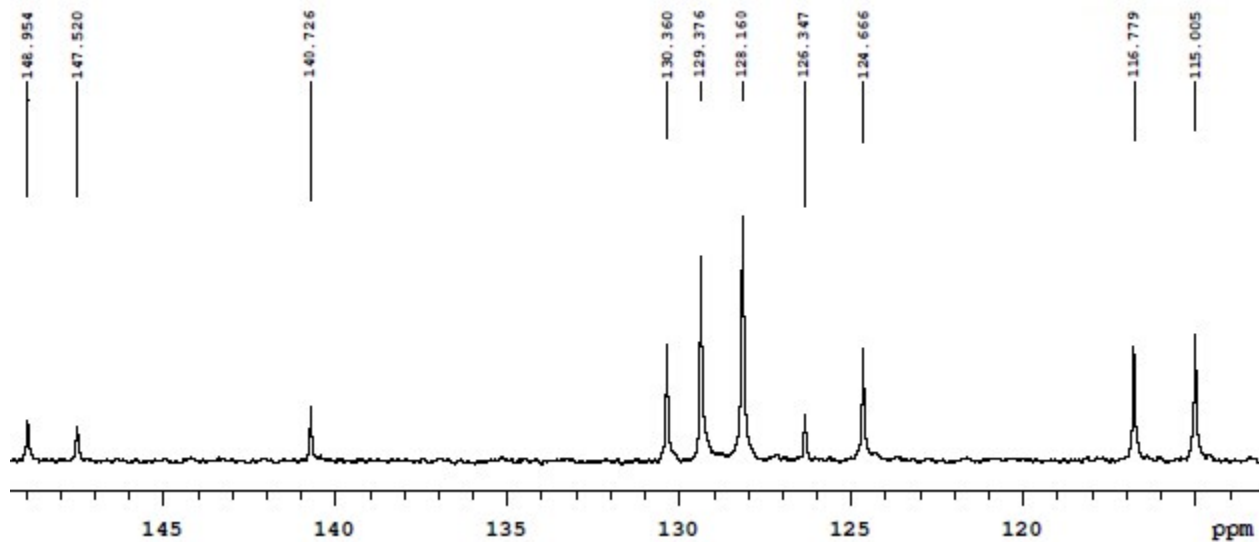
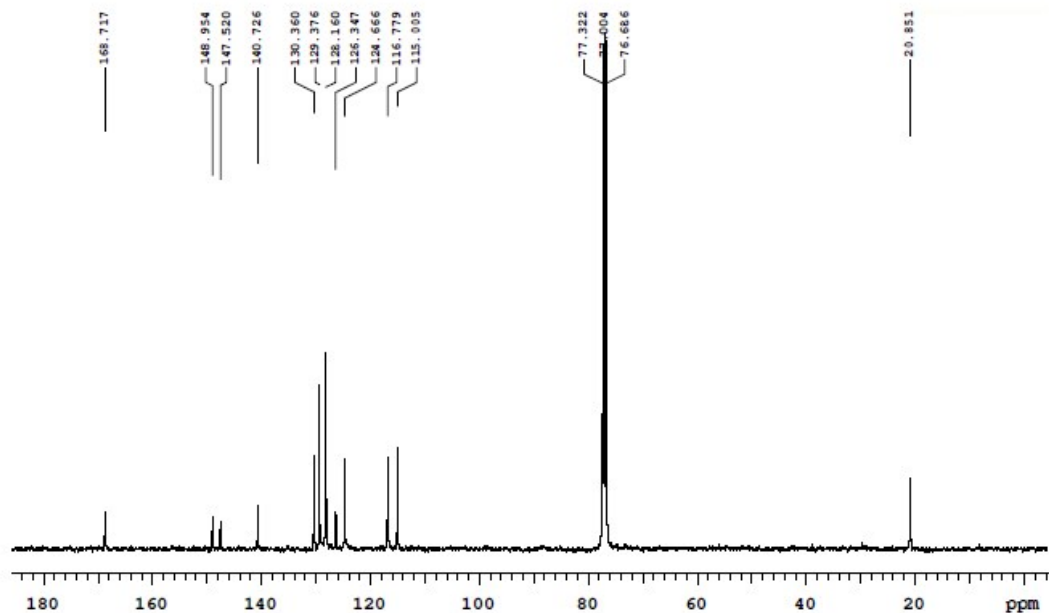
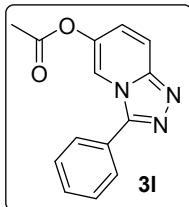


Figure S26. ^{13}C NMR Spectra & its expansion for compound **3I** in CDCl_3

NUCLEUS : H1
 FREQ (MHz) : 399.63
 AT (sec) : 2.27
 SW (ppm) : 18.08
 RD (sec) : 1.00
 PW (usec) : 6.60
 Scans : 64
 Solvent : cdcl3
 Data Points : 32768
 LB (Hz) : 1.00
 TEMP (K) : 303.15
 EXP : s2pul
 DATE : Nov 4 2015
 System : VNMR5_400

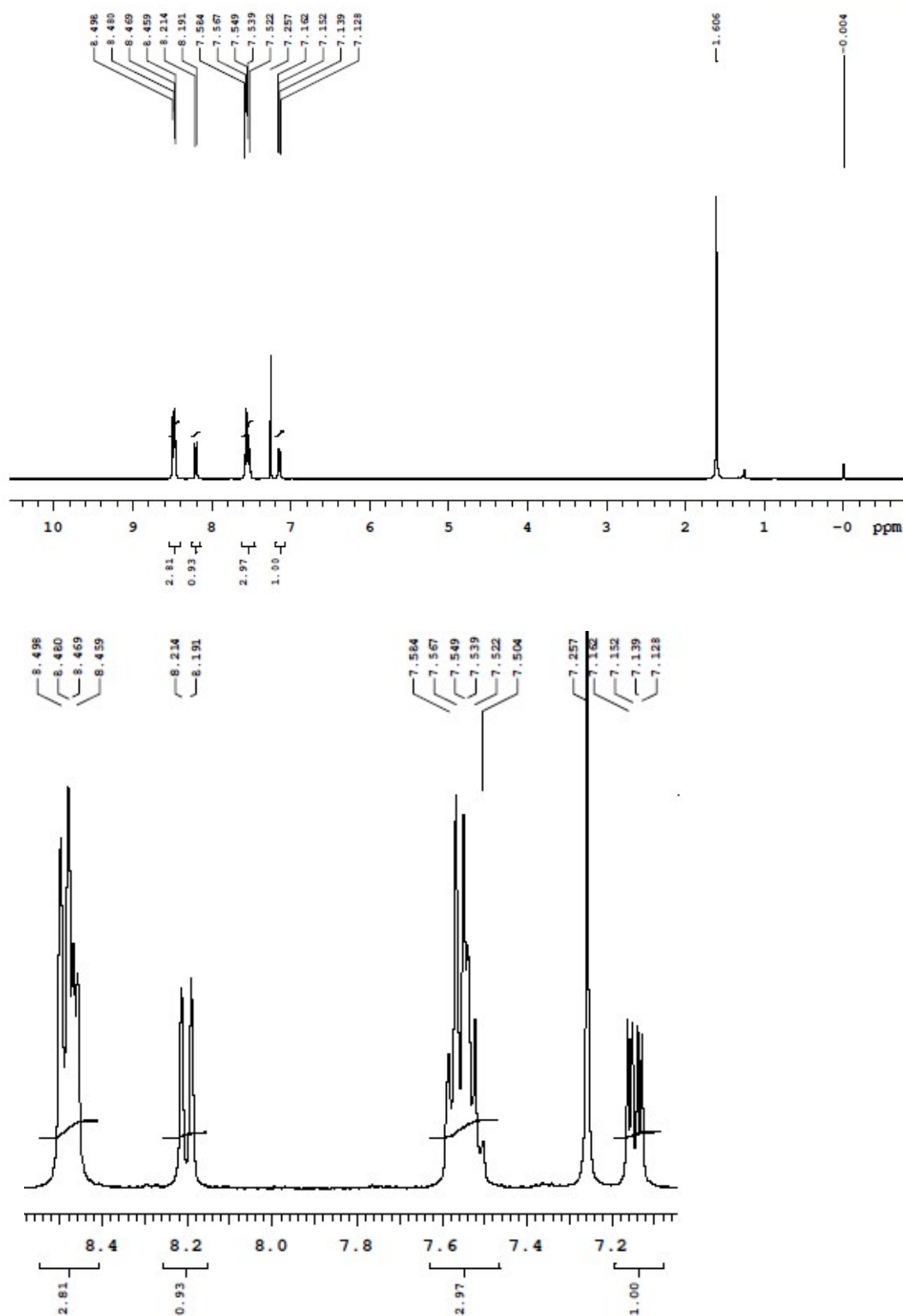
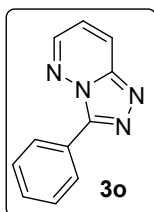


Figure S27. ¹H NMR Spectra & its expansion for compound **30** in CDCl₃

NUCLEUS : C13
FREQ (MHz) : 100.50
AQ (sec) : 1.28
SW (ppm) : 253.84
RD (sec) : 1.00
PW (usec) : 5.05
Scans : 1500
Solvent : cdc13
Data Points : 65536
LB (Hz) : 3.00
TEMP (K) : 303.15
EXP : s2pul
DATE : Nov 20 2015
System : VNMR-400

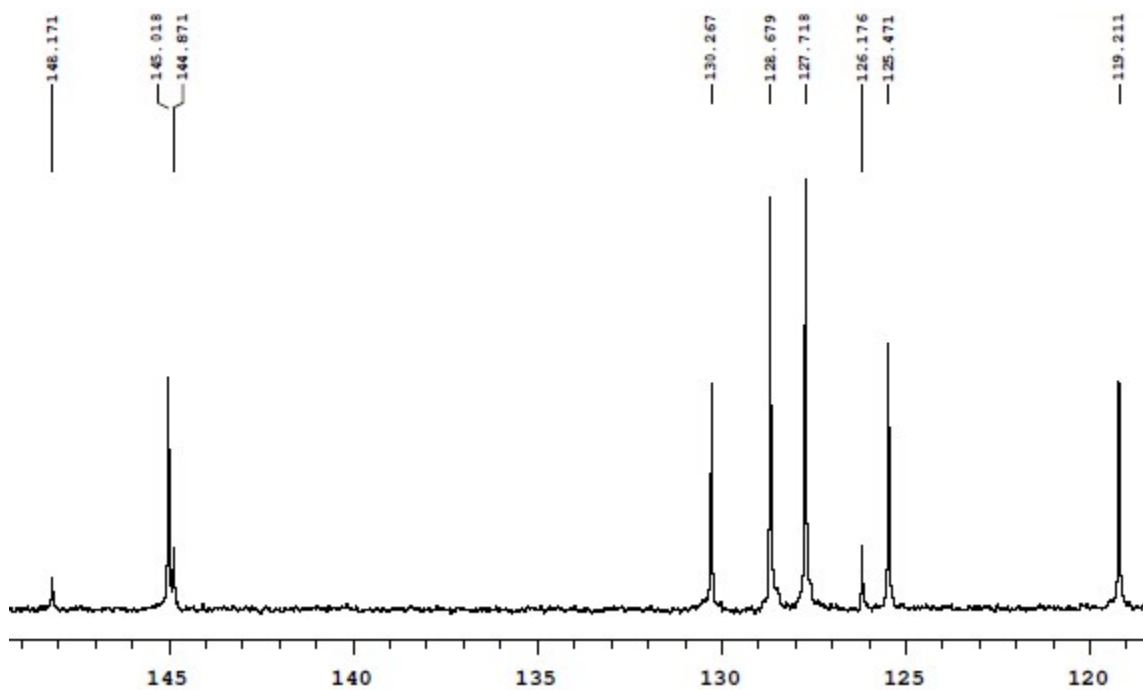
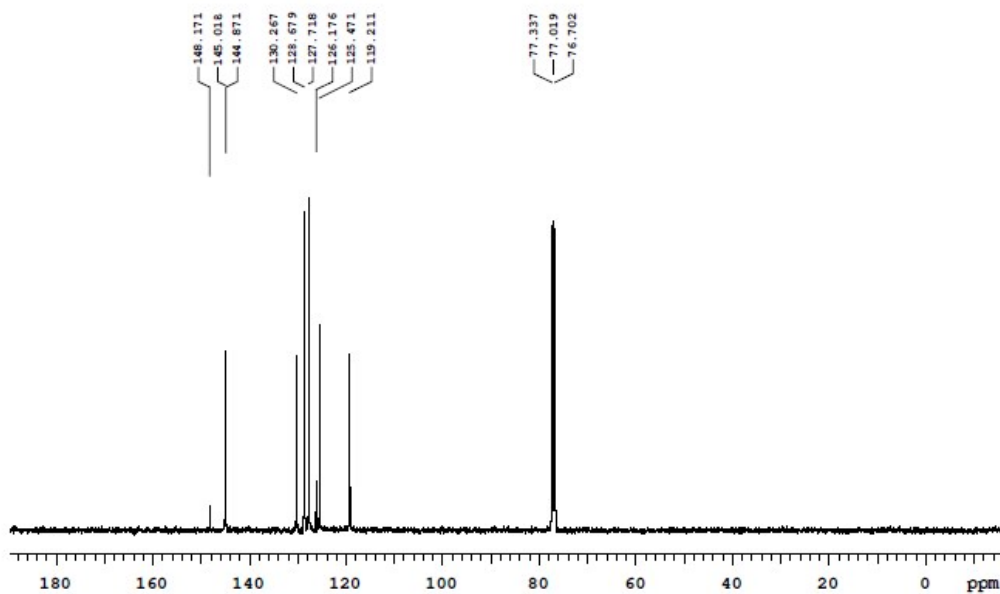
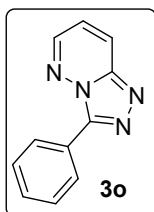


Figure S28. ^{13}C NMR Spectra & its expansion for compound **3o** in CDCl_3

NUCLEUS : H1
 FREQ (MHz) : 399.63
 AT (sec) : 2.27
 SW (ppm) : 18.08
 HD (sec) : 1.00
 DW (usec) : 6.60
 Scans : 64
 Solvent : cdcl3
 Data Points : 32768
 LB (Hz) : 1.00
 TEMP (K) : 303.15
 EXP : s2pul
 DATE : Nov 3 2015
 System : VNMRS_400

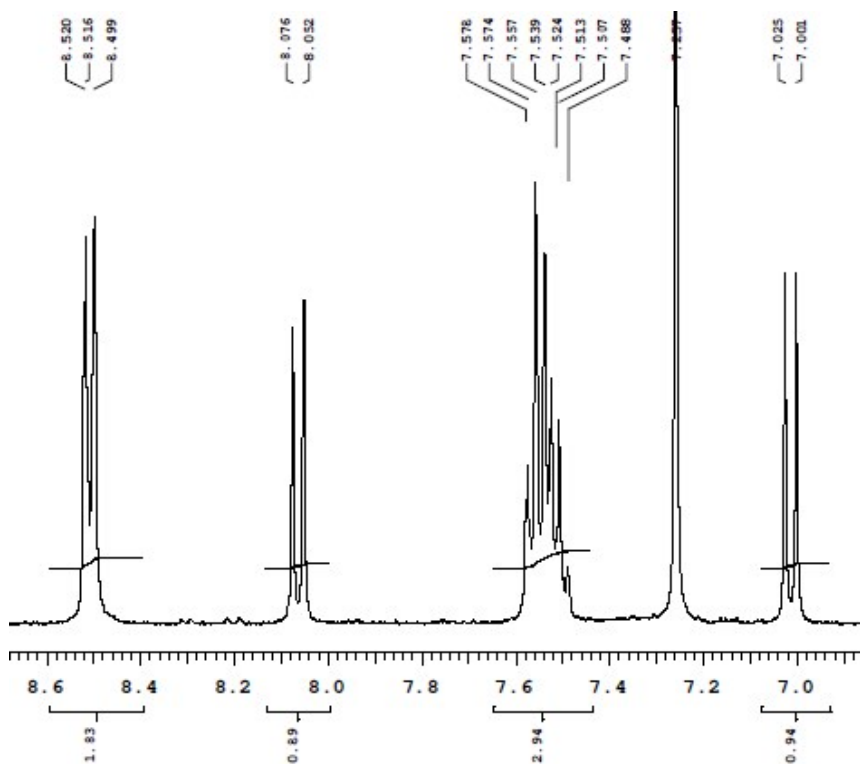
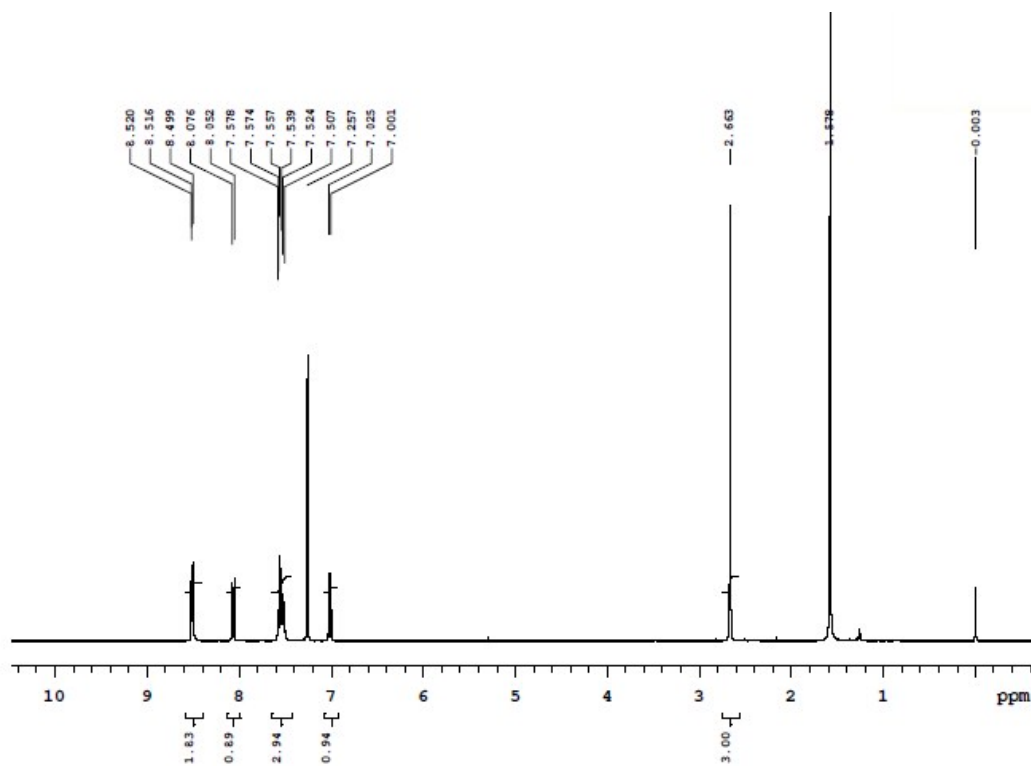
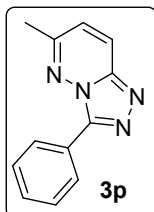


Figure S29. ^1H NMR Spectra & its expansion for compound **3p** in CDCl_3

NUCLEUS : C13
 FRQ (MHz) : 100.50
 AT (sec) : 1.28
 SW (ppm) : 253.84
 RD (sec) : 1.00
 PW (usec) : 5.05
 Scans : 1500
 Solvent : cdcl3
 Data Points : 65536
 LB (Hz) : 4.00
 TEMP (K) : 303.15
 EXP : s2pul
 DATE : Nov 21 2015
 System : VNMR5_400

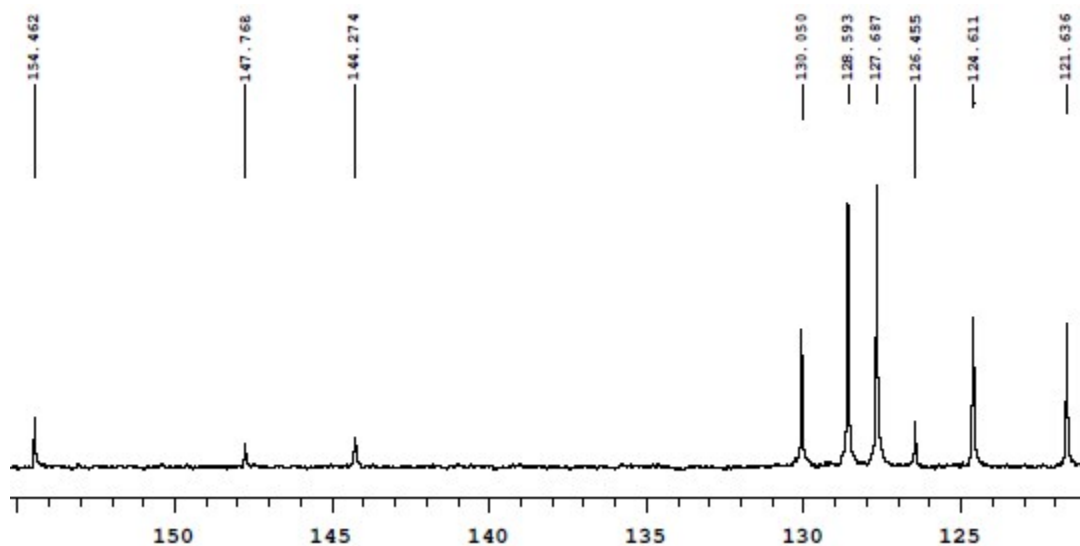
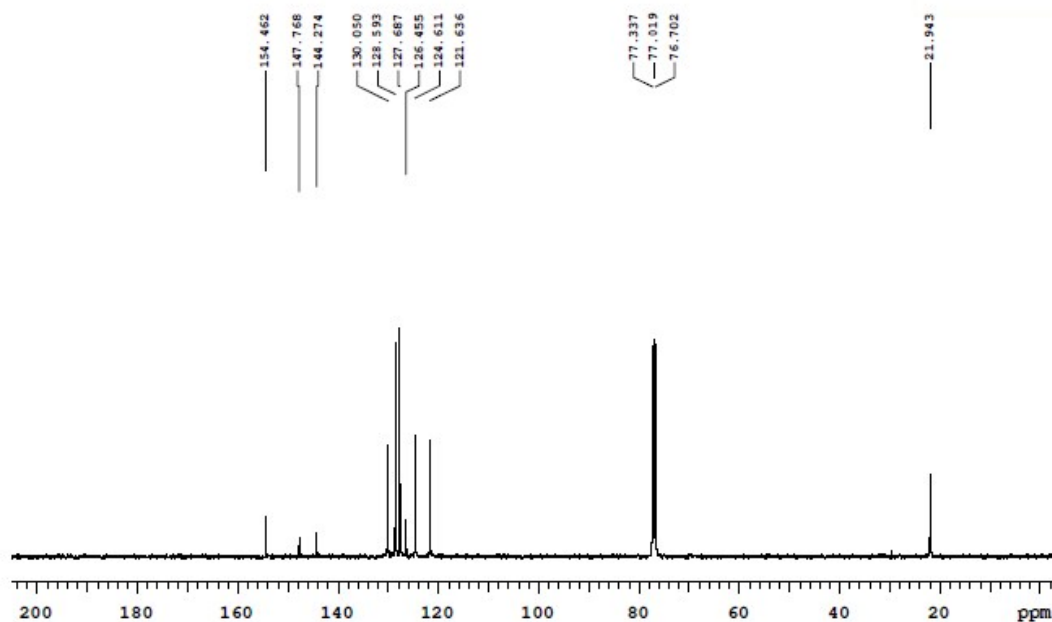
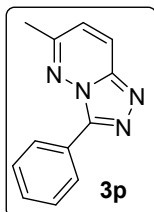


Figure S30. ^{13}C NMR Spectra & its expansion for compound **3p** in CDCl_3

NUCLEUS : H1
 FREQ (MHz) : 399.64
 AT (sec) : 2.27
 SW (ppm) : 18.08
 RD (sec) : 1.00
 DW (usec) : 6.60
 Scans : 64
 Solvent : dms0
 Data Points : 32768
 LB (Hz) : 1.00
 TEMP (K) : 303.15
 EXP : s2pu1
 DATE : Feb 18 2016
 System : VNMR5_400

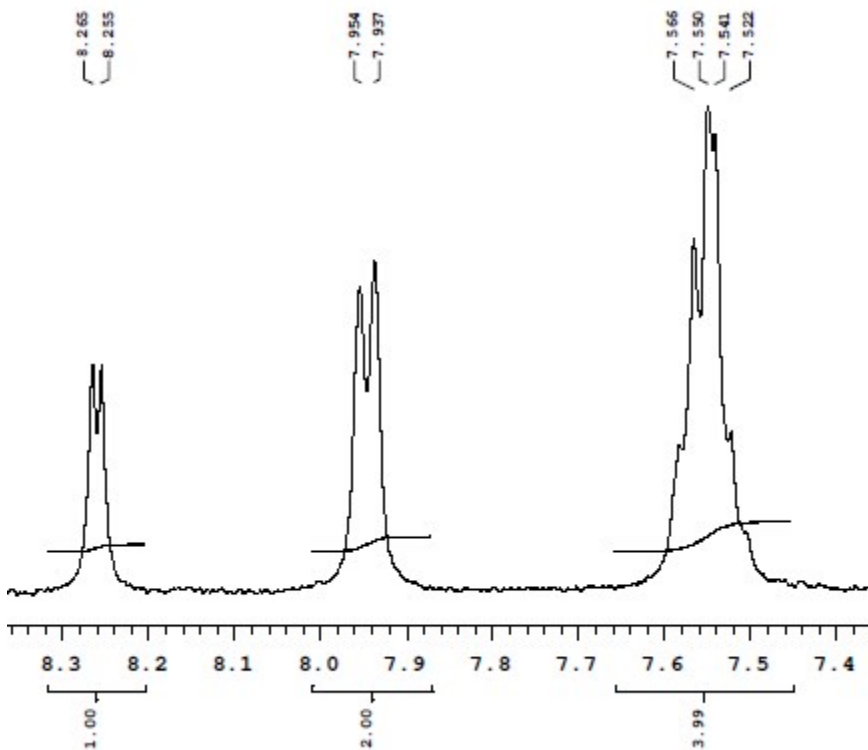
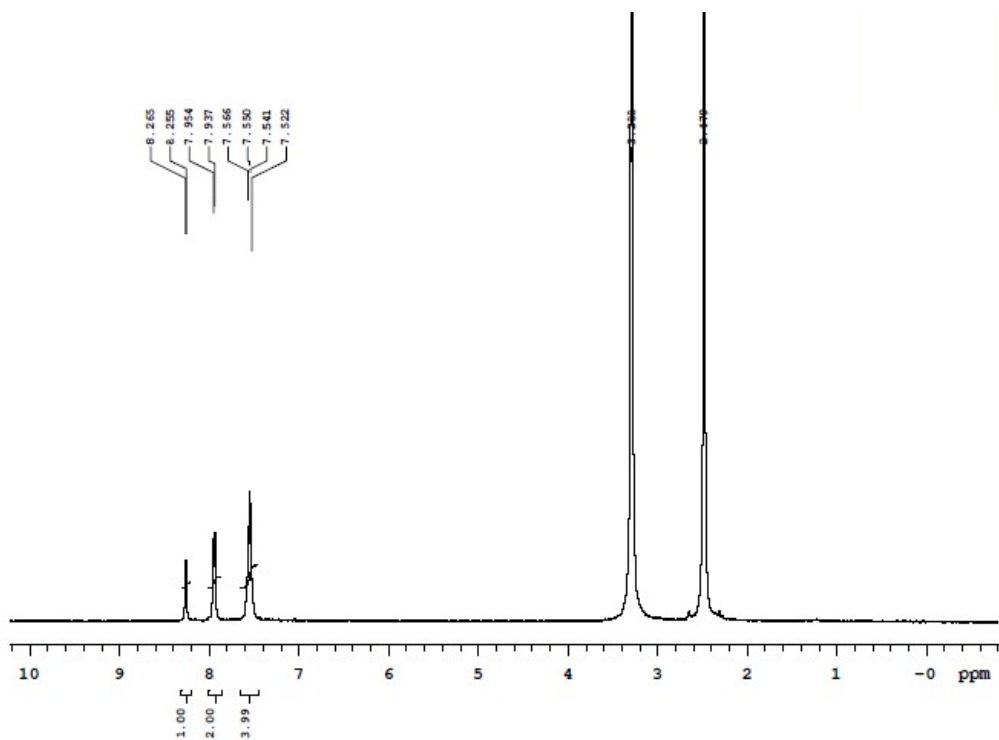
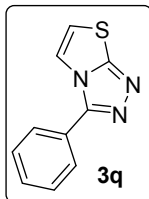


Figure S31. ^1H NMR Spectra & its expansion for compound **3q** in $\text{DMSO-}d_6$

NUCLEUS : C13
 FRQ (MHz) : 100.50
 AT (sec) : 1.28
 SW (ppm) : 253.84
 RD (sec) : 1.00
 FWH (usec) : 5.05
 Scans : 6000
 Solvent : dmsc
 Data Points : 65536
 LB (Hz) : 8.00
 TEMP (K) : 303.15
 EXP : s2pul
 DATE : Feb 19 2016
 System : VNMR5_400

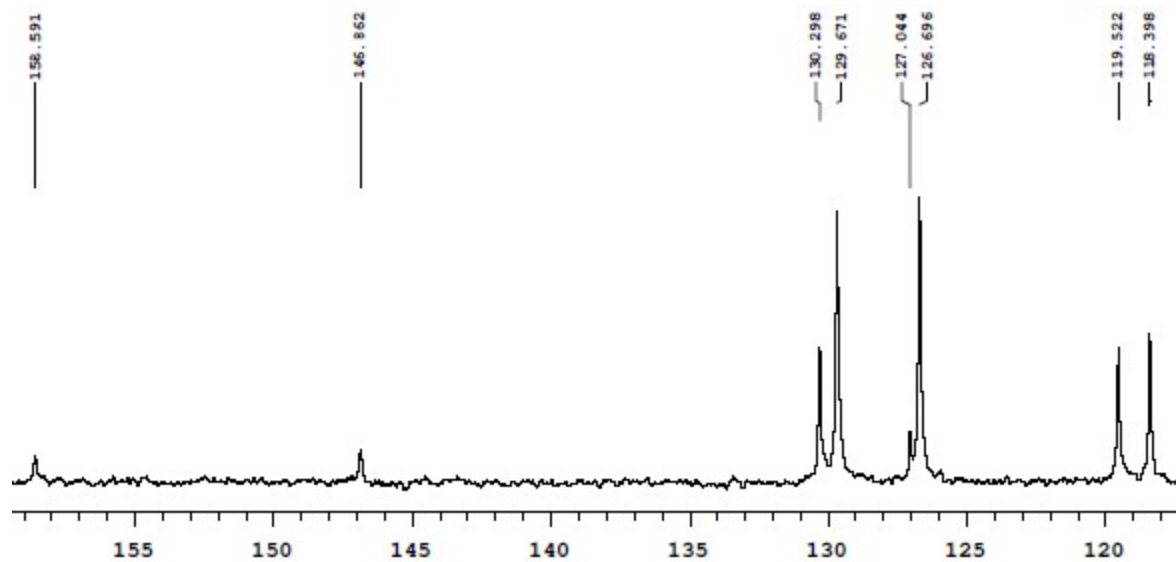
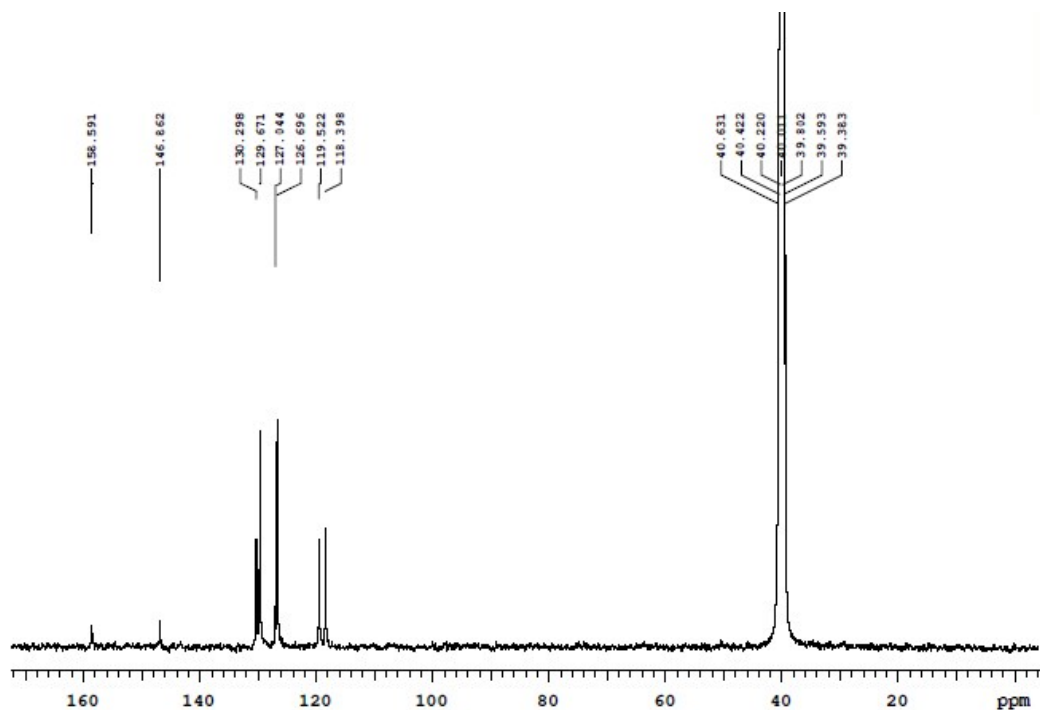
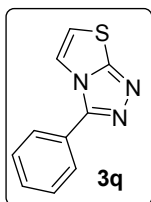


Figure S32. ^{13}C NMR Spectra & its expansion for compound **3q** in $\text{DMSO-}d_6$

NUCLEUS : H1
 FREQ (MHz) : 399.64
 AT (sec) : 2.27
 SW (ppm) : 18.08
 RD (sec) : 1.00
 FWH (usec) : 6.60
 Scans : 64
 Solvent : dms0
 Data Points : 32768
 LB (Hz) : 1.00
 TEMP (K) : 303.15
 EXP : s2pa1
 DATE : Sep 23 2015
 System : VNMR5_400

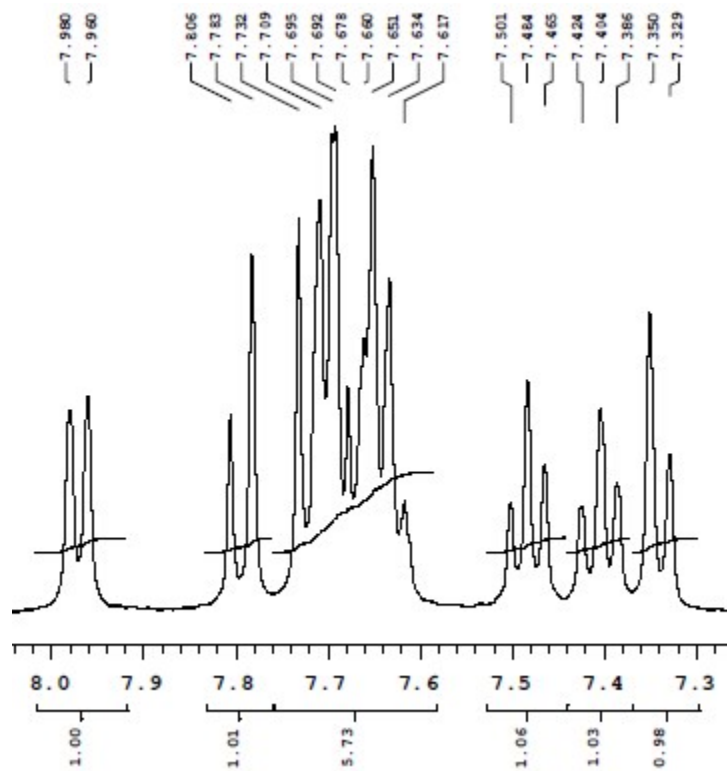
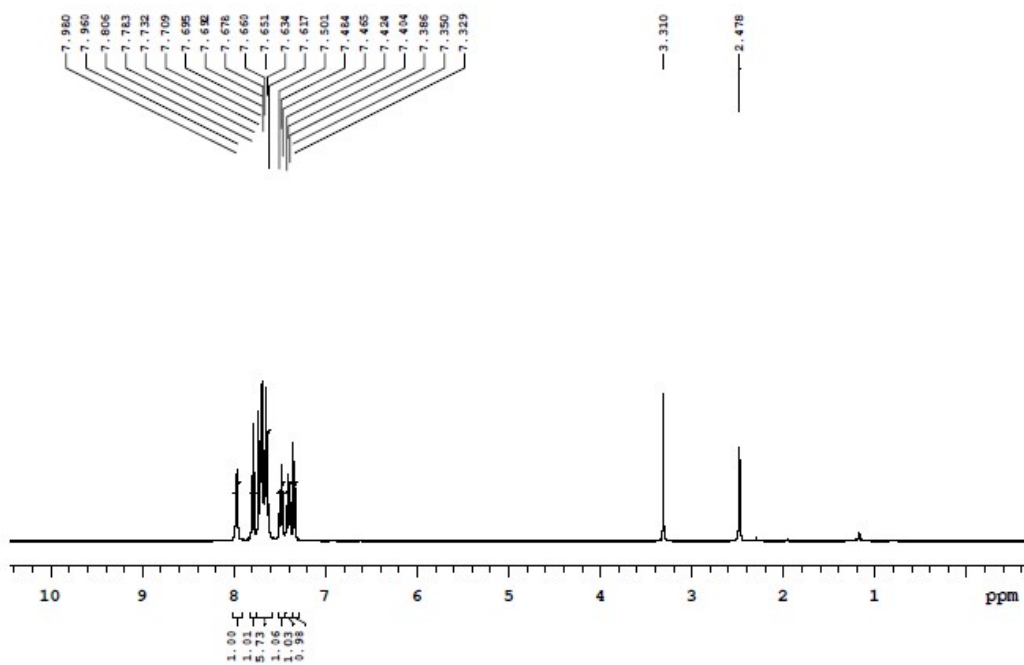
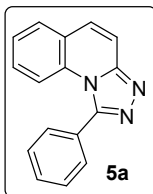


Figure S33. ^1H NMR Spectra & its expansion for compound **5a** in $\text{DMSO-}d_6$

NUCLEUS : C13
 FREQ (MHz) : 100.50
 AT (sec) : 1.28
 SW (ppm) : 253.84
 FD (sec) : 1.00
 PW (usec) : 5.05
 Scans : 1600
 Solvent : dmsd
 Data Points : 65536
 LB (Hz) : 2.00
 TEMP (K) : 303.15
 EXP : s2pul
 DATE : Sep 26 2015
 System : VNMR5_400

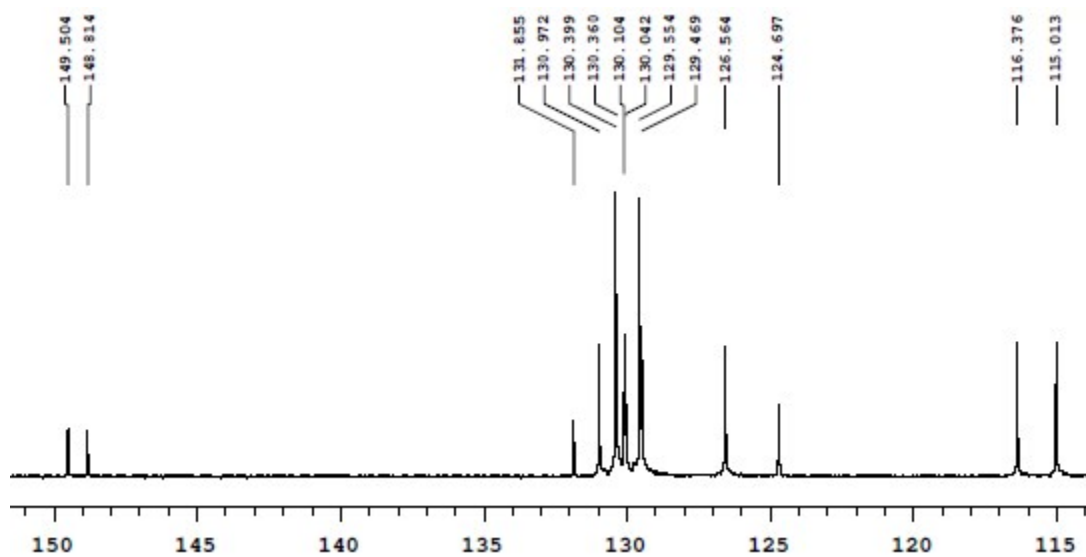
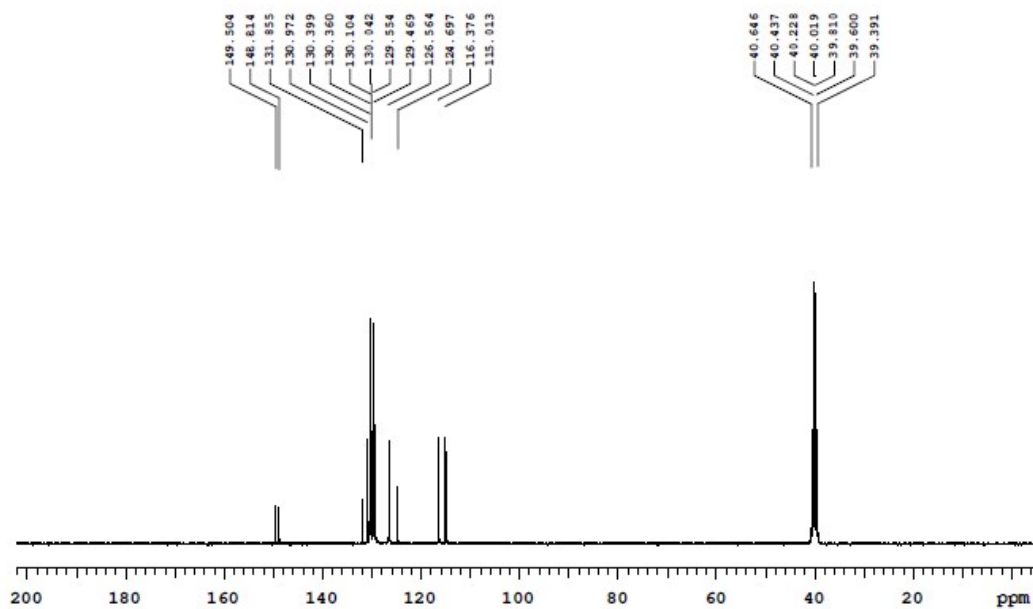
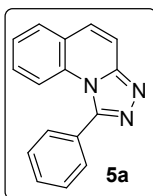


Figure S34. ^{13}C NMR Spectra & its expansion for compound **5a** in $\text{DMSO-}d_6$

NUCLEUS : H1
 FREQ (MHz) : 399.64
 AT (sec) : 2.27
 SW (ppm) : 18.08
 RD (sec) : 1.00
 PW (usec) : 6.60
 Scans : 64
 Solvent : dmsc
 Data Points : 32768
 LB (Hz) : 2.00
 TEMP (K) : 303.15
 EXP : s2pul
 DATE : Feb 12 2016
 System : VNMR5_400

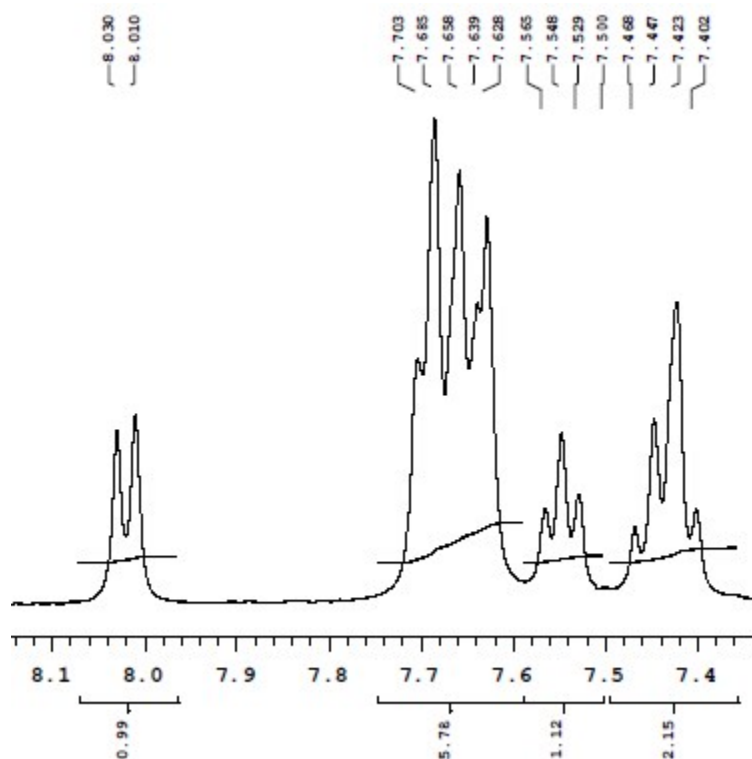
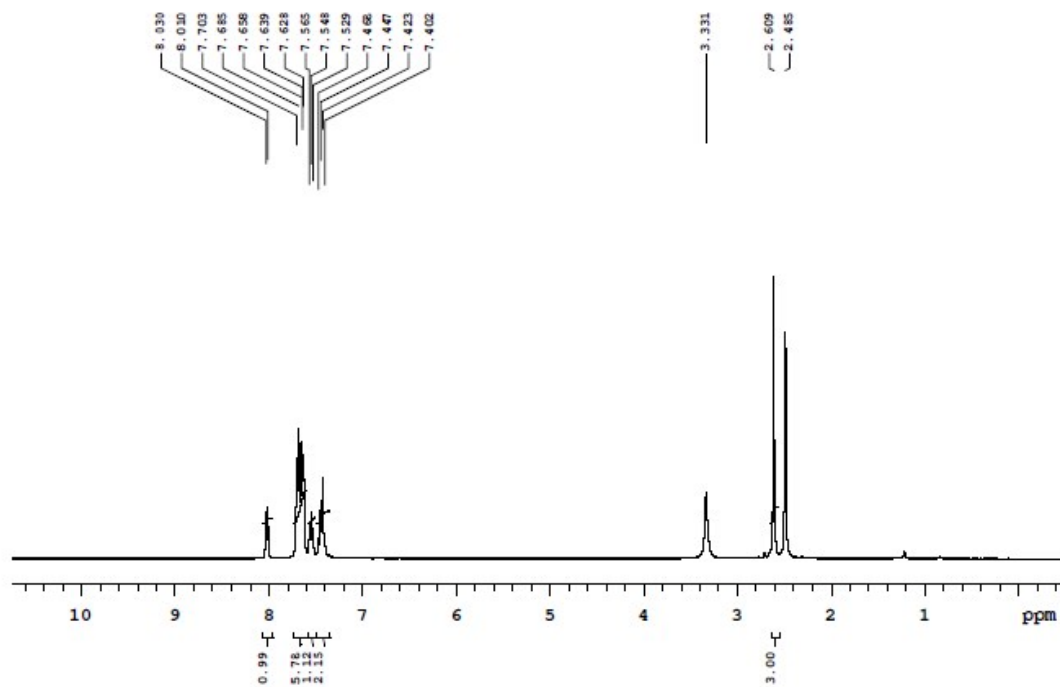
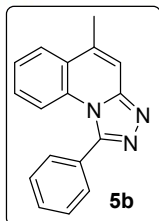


Figure S35. ^1H NMR Spectra & its expansion for compound **5b** in $\text{DMSO-}d_6$

NUCLEUS : C13
 FREQ (MHz) : 100.50
 AT (sec) : 1.28
 SW (ppm) : 253.84
 RD (sec) : 1.00
 PW (usec) : 5.05
 Scans : 2000
 Solvent : dmsc
 Data Points : 65536
 LB (Hz) : 2.00
 TEMP (K) : 303.15
 EXP : s2pu1
 DATE : Feb 13 2016
 System : VNM6S_400

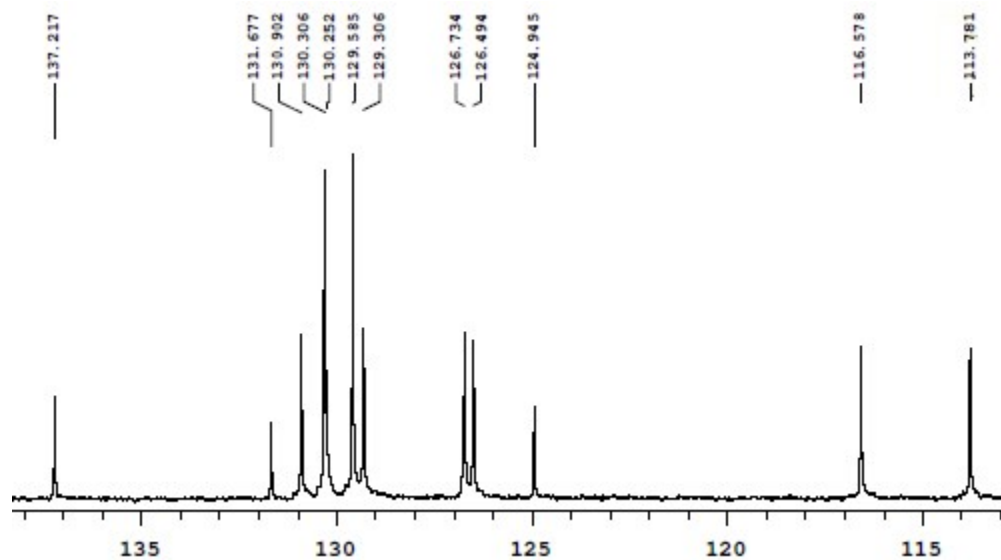
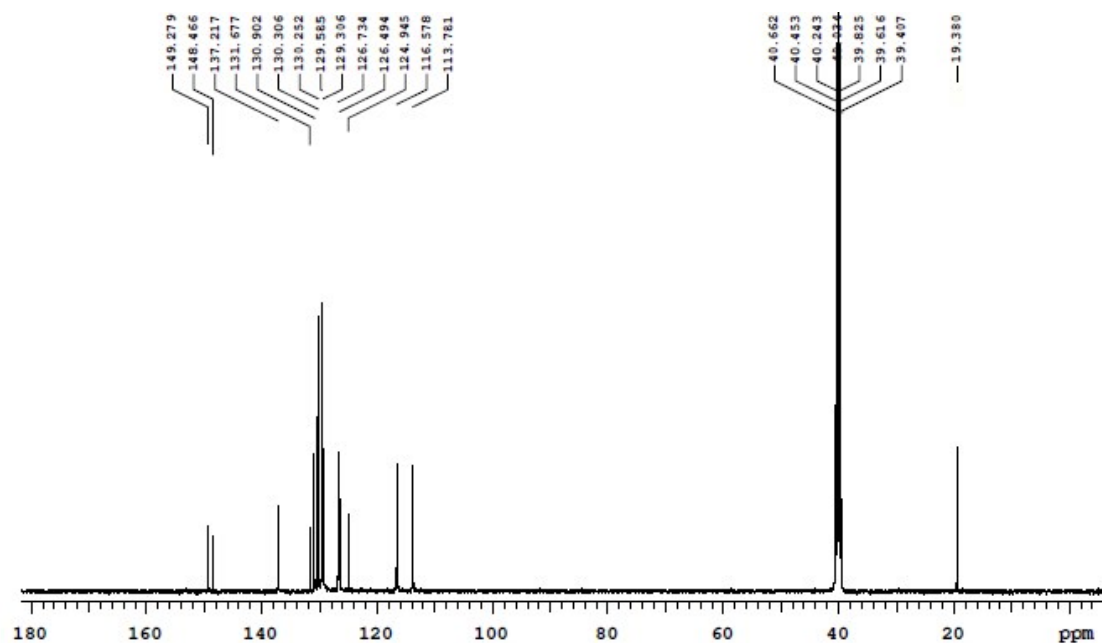
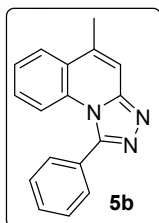


Figure S36. ^{13}C NMR Spectra & its expansion for compound **5b** in $\text{DMSO-}d_6$

NUCLEUS : H1
 FREQ (MHz) : 399.63
 AT (sec) : 2.27
 SW (ppm) : 18.08
 RD (sec) : 1.00
 DW (usec) : 6.40
 Scans : 32
 Solvent : cdcl3
 Data Points : 32768
 LB (Hz) : 1.00
 TEMP (K) : 303.15
 EXP : s2pul
 DATE : Nov 30 2015
 System : VNMRS_400

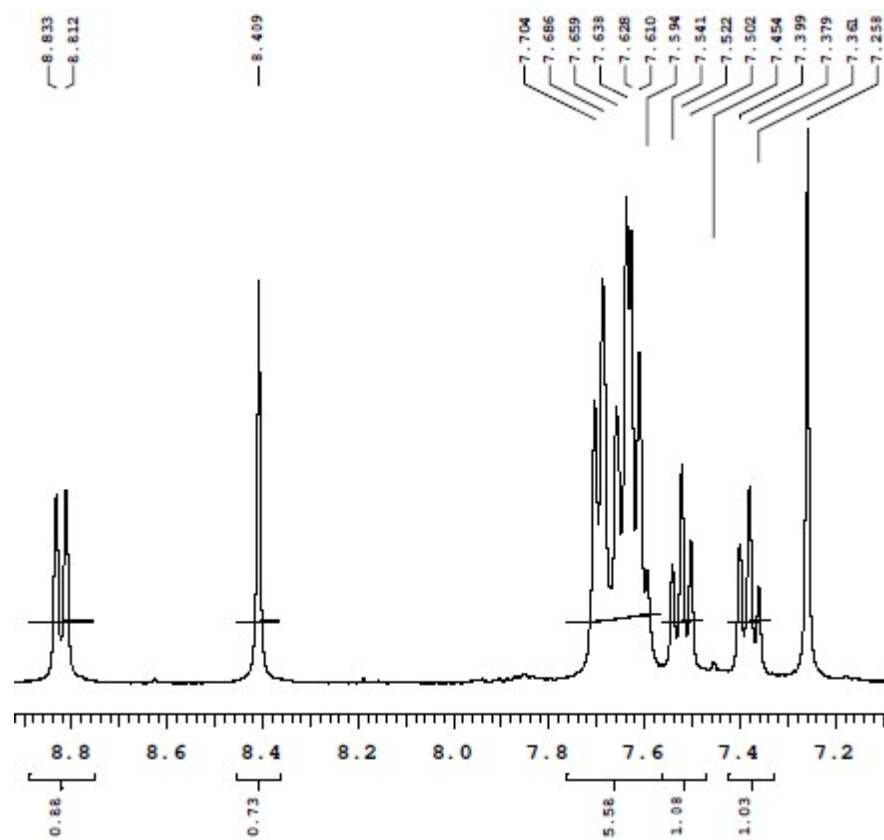
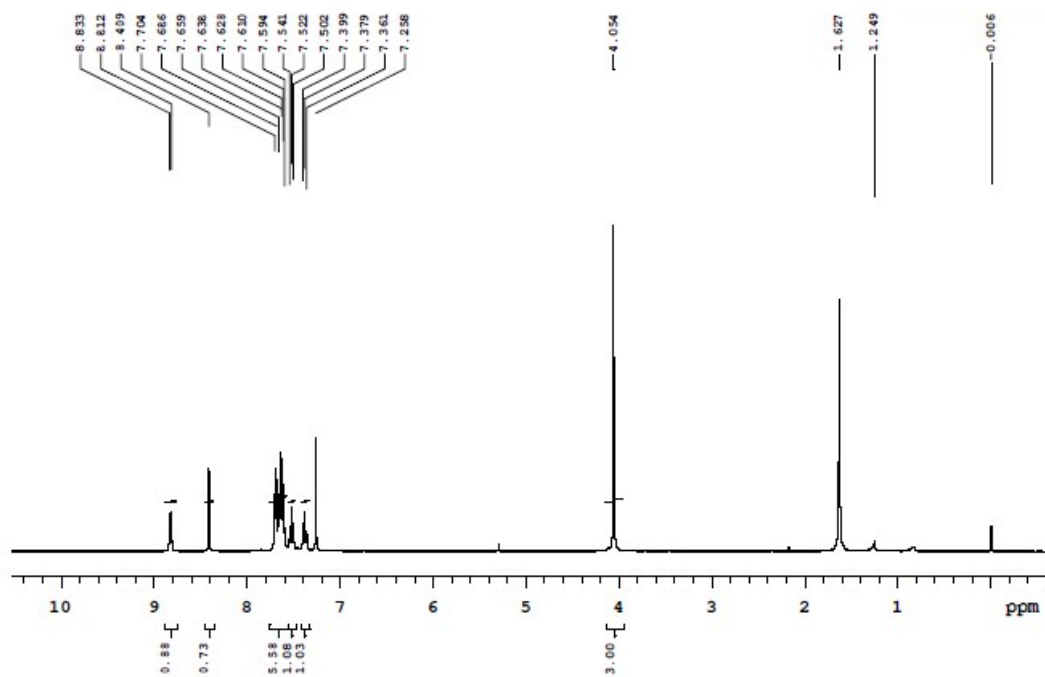
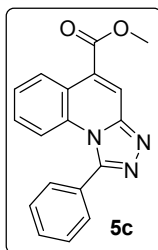


Figure S37. ^1H NMR Spectra & its expansion for compound **5c** in CDCl_3

NUCLEUS : C13
 FREQ (MHz) : 100.50
 AT (sec) : 1.28
 SW (ppm) : 253.84
 RD (sec) : 1.00
 PW (usec) : 5.05
 Scans : 6000
 Solvent : cdcl3
 Data Points : 65536
 LB (Hz) : 2.00
 TEMP (K) : 303.15
 EXP : s2pul
 DATE : Dec 5 2015
 System : VNMR5_400

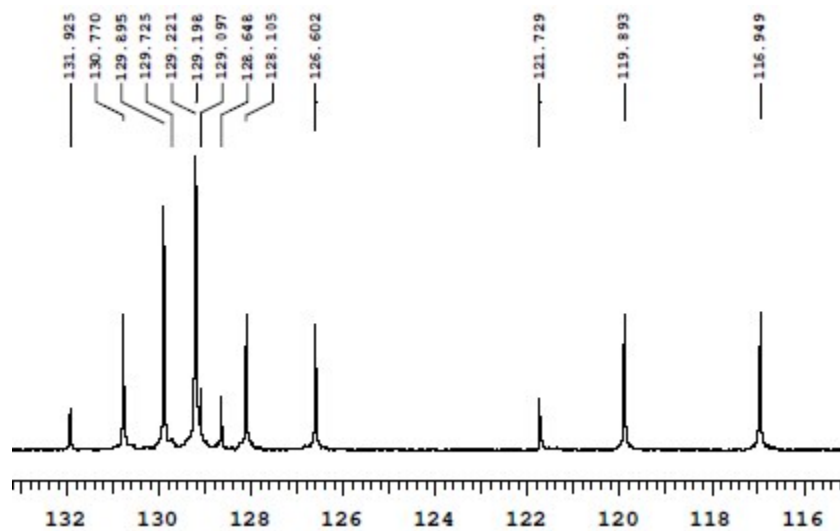
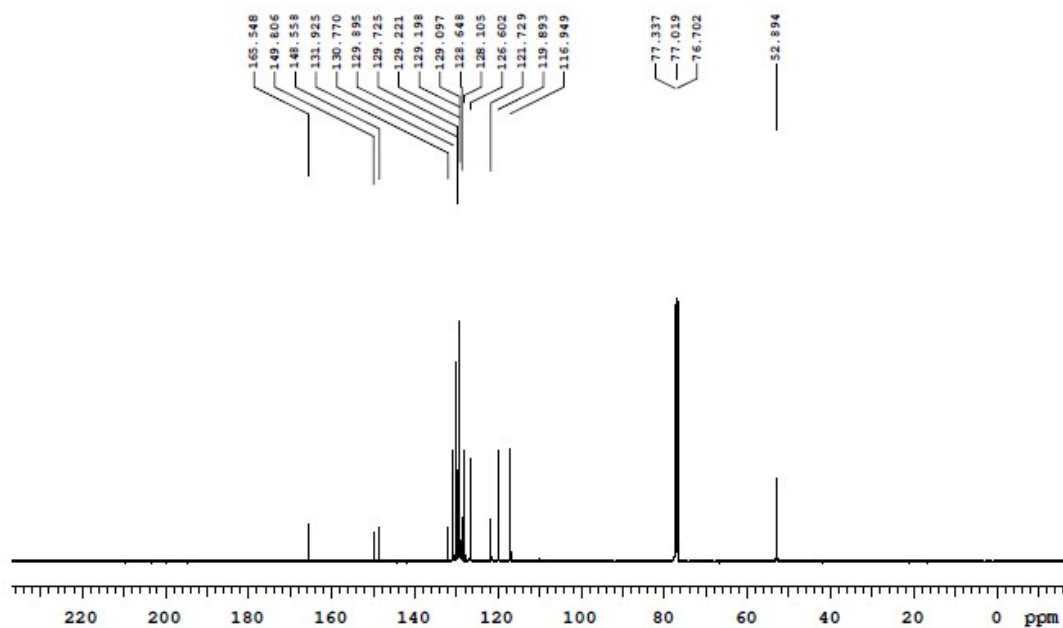
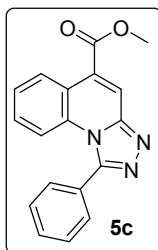


Figure S38. ^{13}C NMR Spectra & its expansion for compound **5c** in CDCl_3

NUCLEUS : H1
 FRQ (MHz) : 399.64
 AT (sec) : 2.27
 SW (ppm) : 18.08
 RD (sec) : 1.00
 DW (usec) : 6.60
 Scans : 64
 Solvent : dmsc
 Data Points : 32768
 LB (Hz) : 2.00
 TEMP (K) : 303.15
 EXP : s2pul
 DATE : Feb 12 2016
 System : VNMR_400

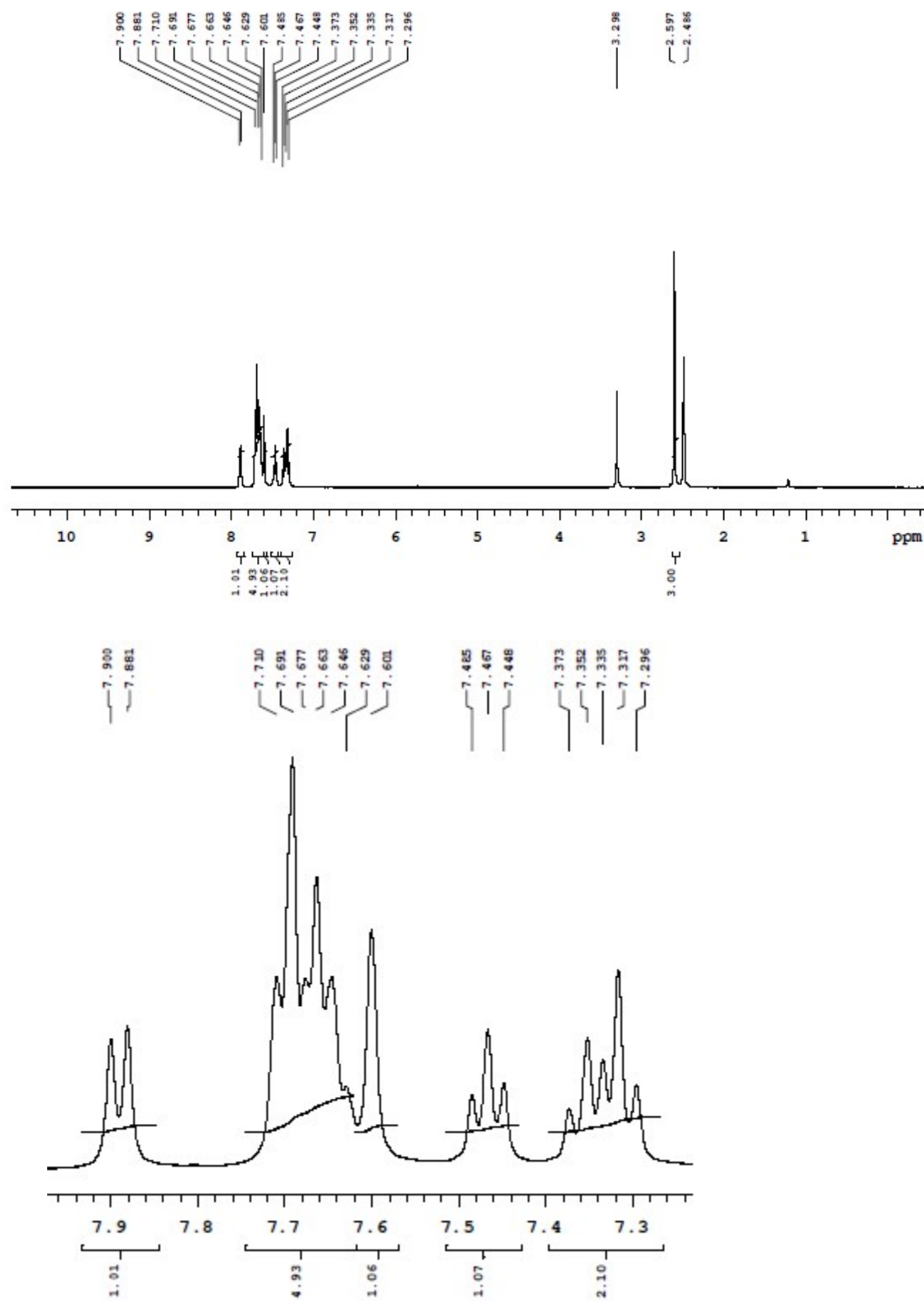
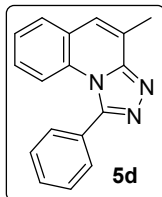


Figure S39. ^1H NMR Spectra & its expansion for compound **5d** in $\text{DMSO-}d_6$

NUCLEUS : C13
 FREQ (MHz) : 100.50
 AT (sec) : 1.28
 SW (ppm) : 253.84
 RD (sec) : 1.00
 FWH (usec) : 5.05
 Scans : 2000
 Solvent : DMSO
 Data Points : 65536
 LB (Hz) : 2.00
 TEMP (K) : 303.15
 EXP : s2pul
 DATE : Feb 13 2016
 System : VNMR_400

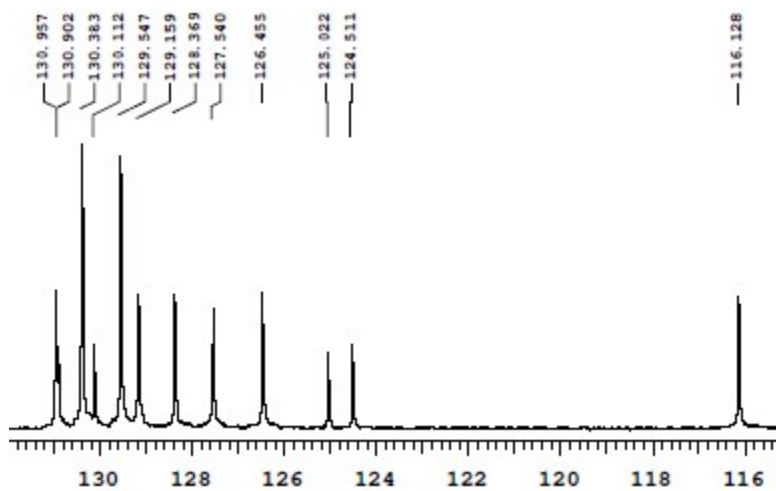
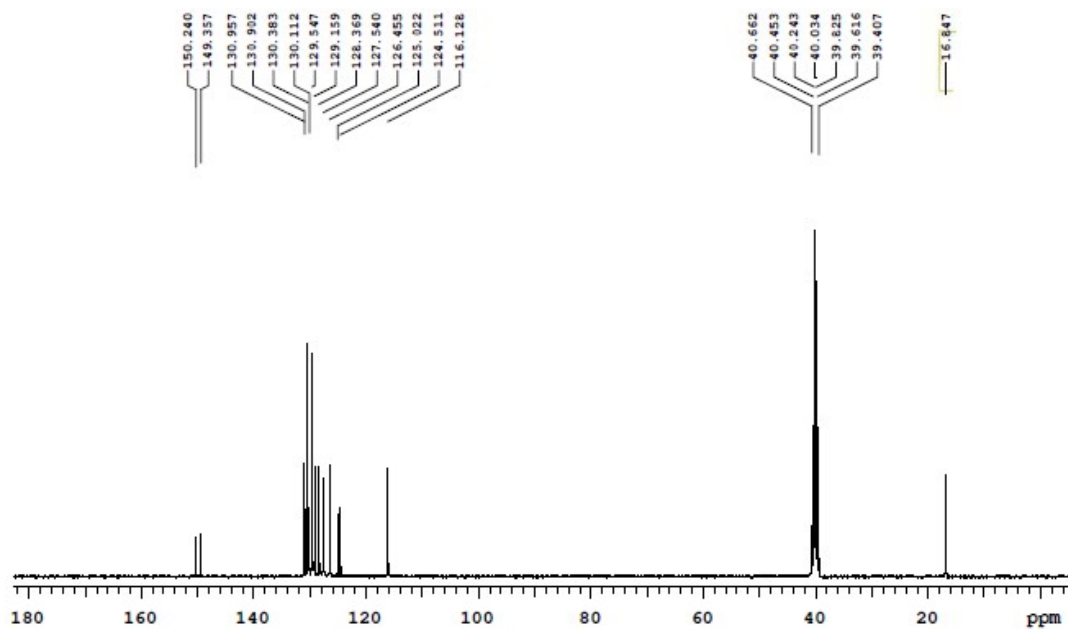
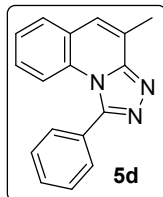


Figure S40. ^{13}C NMR Spectra & its expansion for compound **5d** in $\text{DMSO-}d_6$

NUCLEUS : H1
 FREQ (MHz) : 399.63
 AT (sec) : 2.27
 SW (ppm) : 18.08
 RD (sec) : 1.00
 FWH (sec) : 6.60
 Scans : 64
 Solvent : cdcl3
 Data Points : 32768
 LB (Hz) : 1.00
 TEMP (K) : 303.15
 EXP : s2pul
 DATE : Nov 4 2015
 System : VNMR5_400

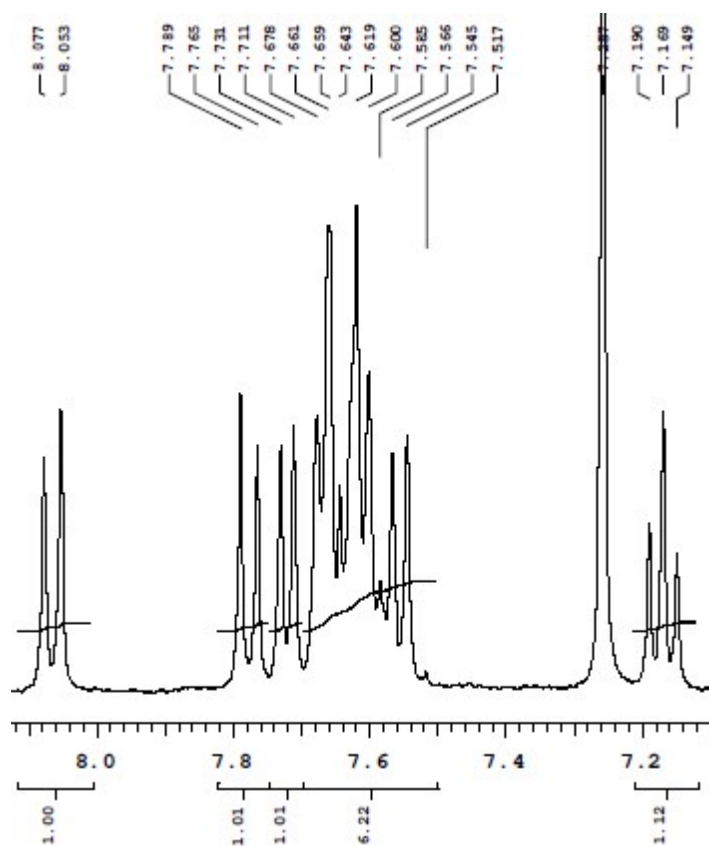
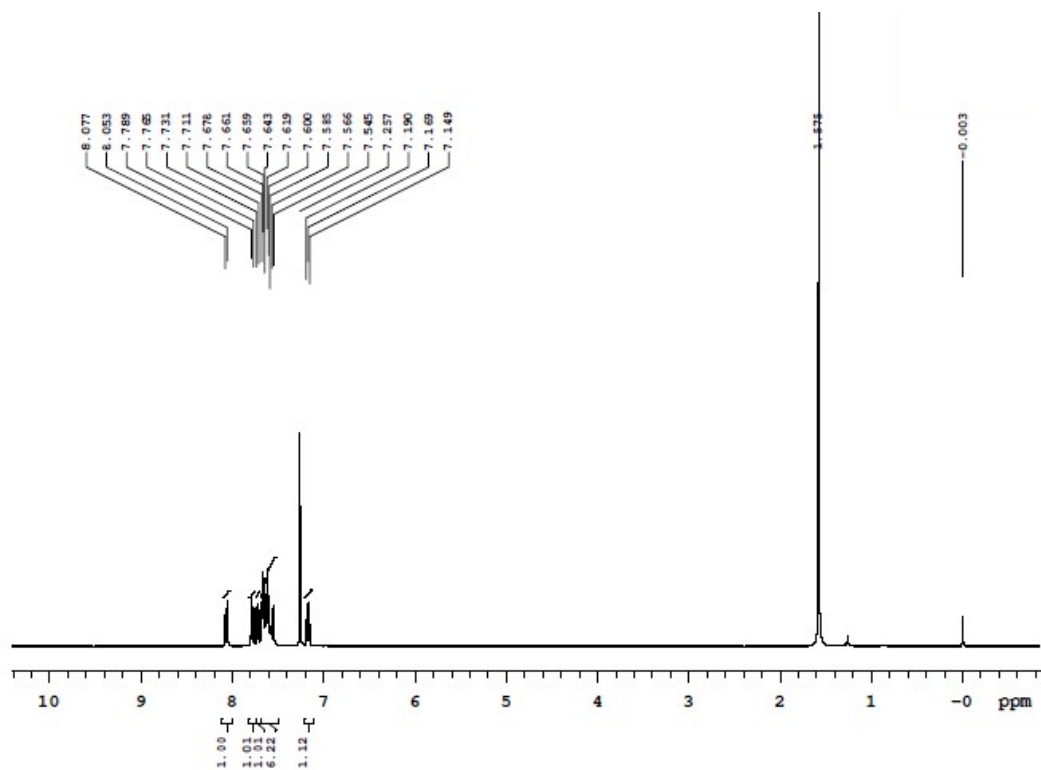
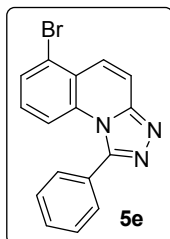


Figure S41. ^1H NMR Spectra & its expansion for compound **5e** in CDCl_3

NUCLEUS : C13
 FRQ (MHz) : 100.50
 AT (sec) : 1.28
 SW (ppm) : 253.84
 RD (sec) : 1.00
 DW (usec) : 5.05
 Scans : 2000
 Solvent : cdcl3
 Data Points : 65536
 LB (Hz) : 5.00
 TEMP (K) : 303.15
 EXP : s2p01
 DATE : Nov 21 2015
 System : VNMR5_400

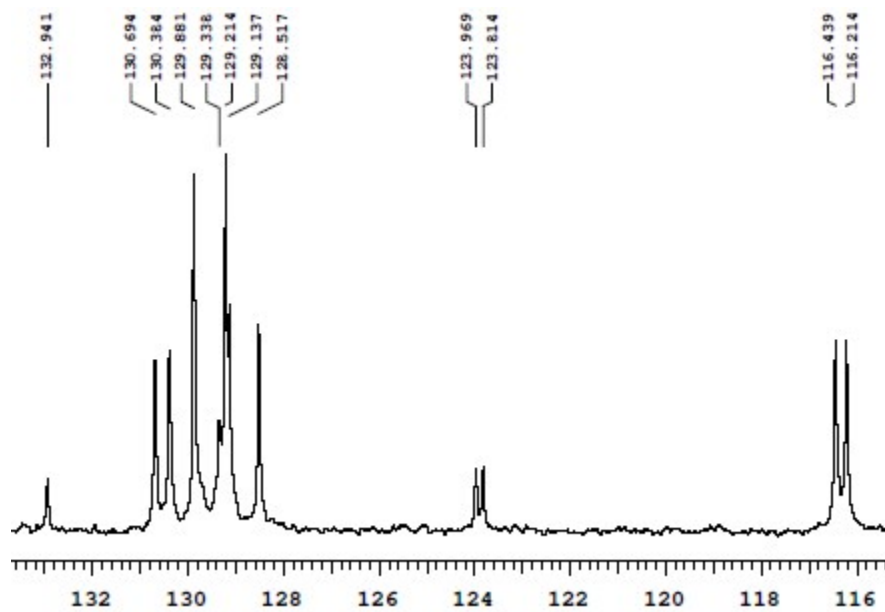
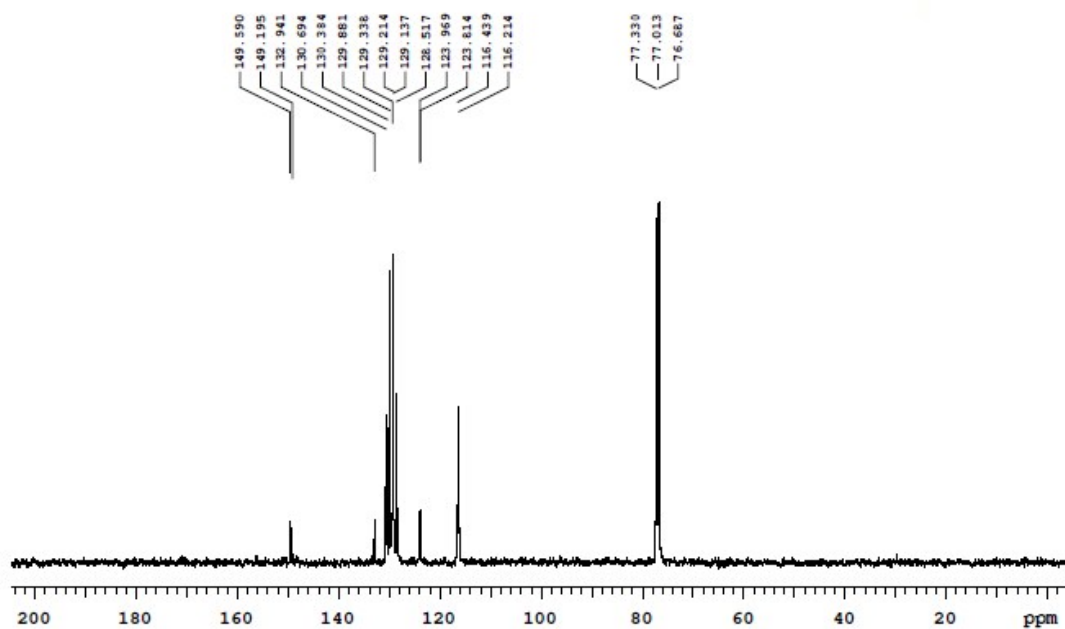
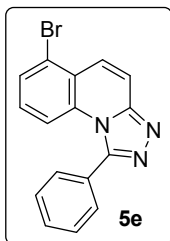


Figure S42. ^{13}C NMR Spectra & its expansion for compound **5e** in CDCl_3

NUCLEUS : H1
 FREQ (MHz) : 399.63
 AT (sec) : 2.27
 SW (ppm) : 18.08
 RD (sec) : 1.00
 FWH (usec) : 6.60
 Scans : 64
 Solvent : cdcl3
 Data Points : 32768
 LB (Hz) : 2.00
 TEMP (K) : 303.15
 EXP : s2pul
 DATE : Nov 17 2015
 System : VNMR5_400

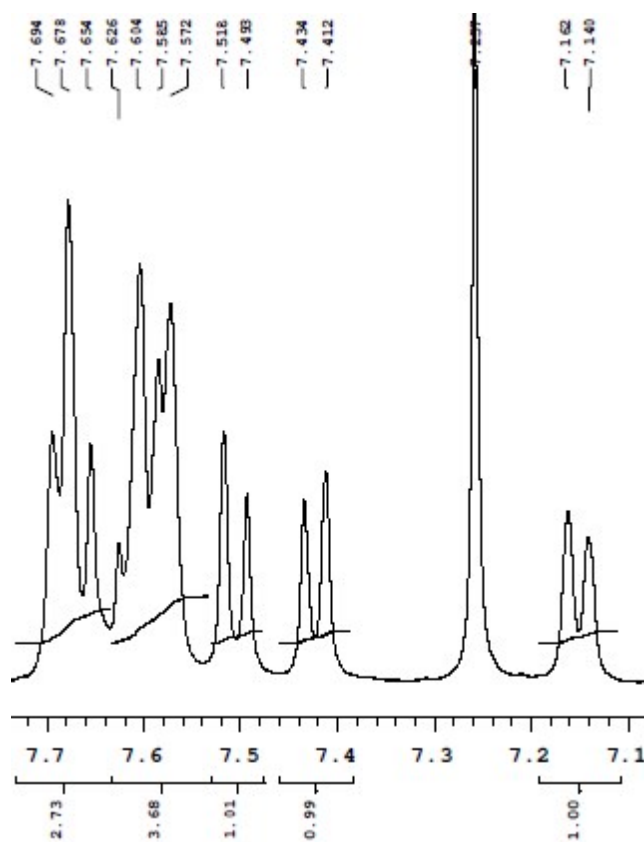
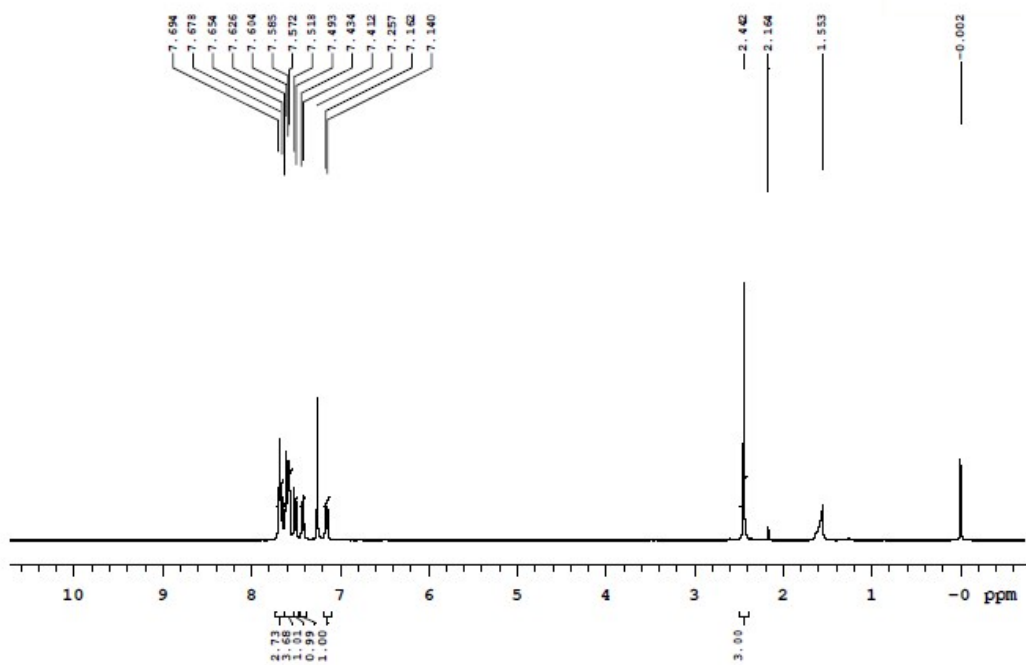
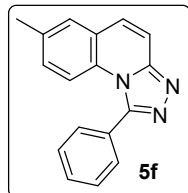


Figure S43. ^1H NMR Spectra & its expansion for compound **5f** in CDCl_3

NUCLEUS : C13
FRQ (MHz) : 100.50
AT (sec) : 1.28
SW (ppm) : 253.84
RD (sec) : 1.00
FID (usec) : 5.05
Scans : 2400
Solvent : cdcl3
Data Points : 65536
LB (Hz) : 4.00
TEMP (K) : 303.15
EXP : s2pul
DATE : Nov 20 2015
System : VNMR5_400

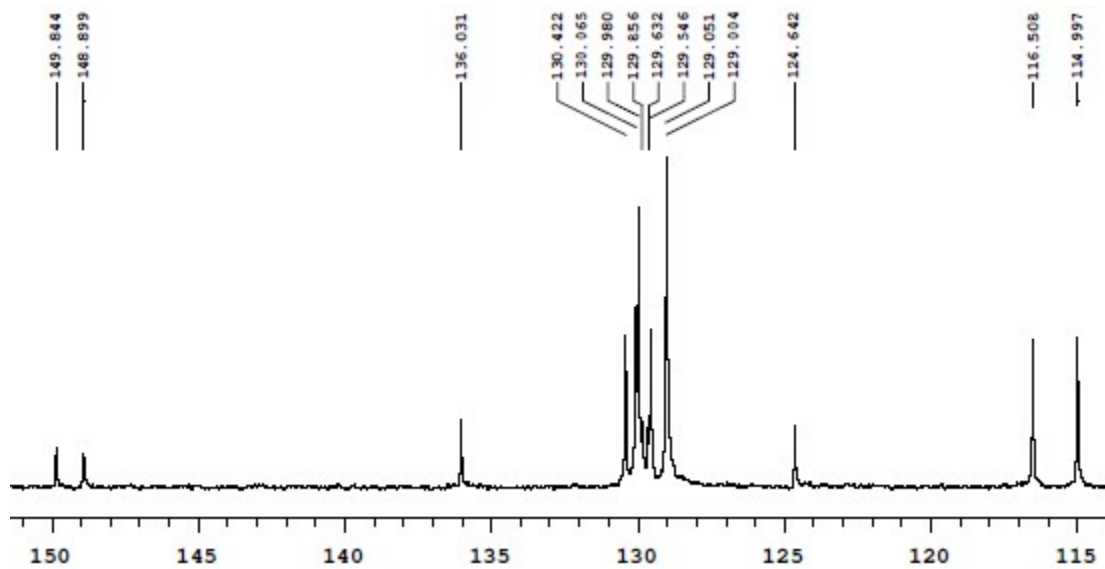
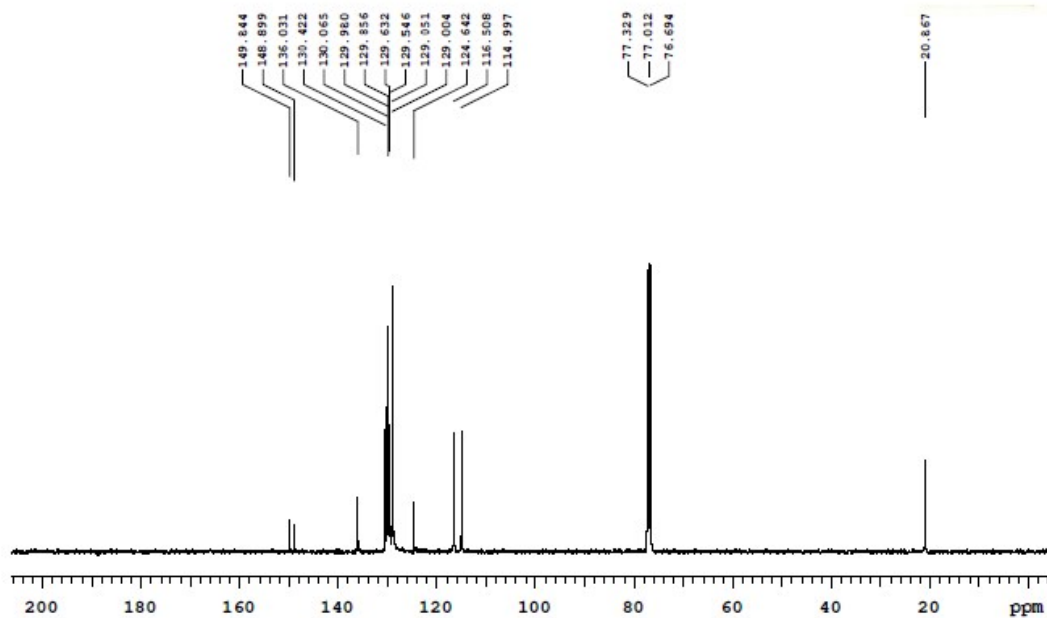
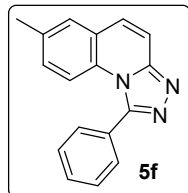


Figure S44. ^{13}C NMR Spectra & its expansion for compound **5f** in CDCl_3

NUCLEUS : H1
 FREQ (MHz) : 399.63
 AT (sec) : 2.27
 SW (ppm) : 18.08
 RD (sec) : 1.00
 FWH (usec) : 6.60
 Scans : 64
 Solvent : cdcl3
 Data Points : 32768
 LB (Hz) : 2.00
 TEMP (K) : 303.15
 EXP : e2pul
 DATE : Nov 4 2015
 System : VNMR5_400

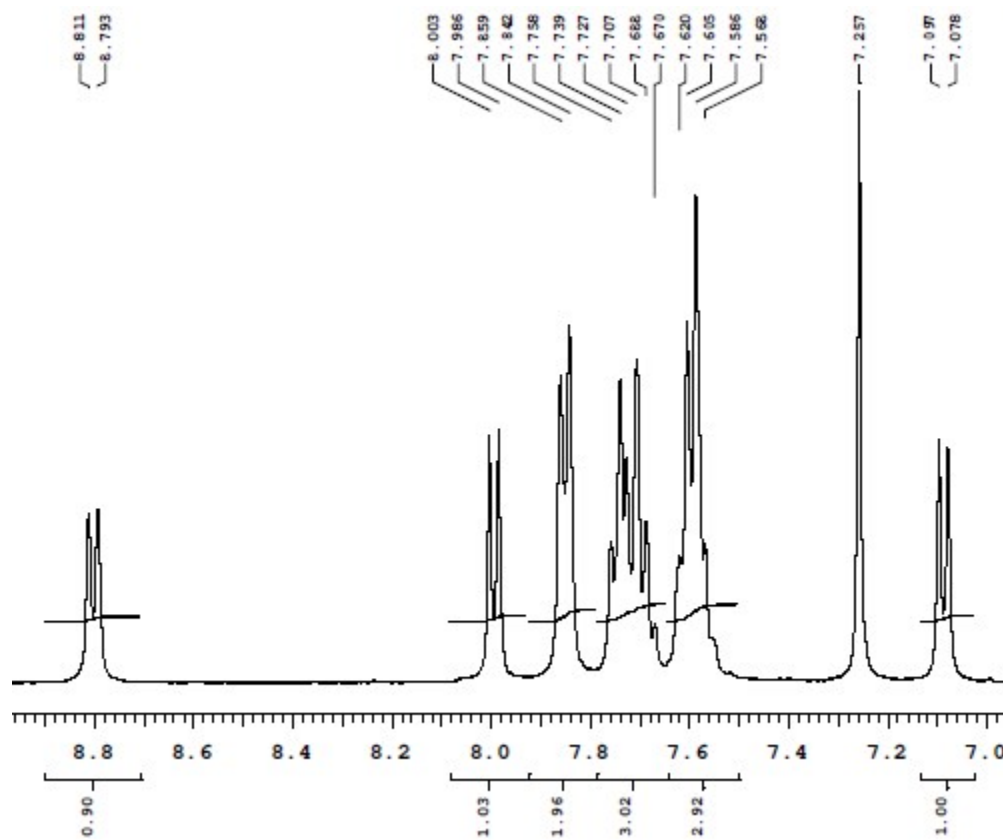
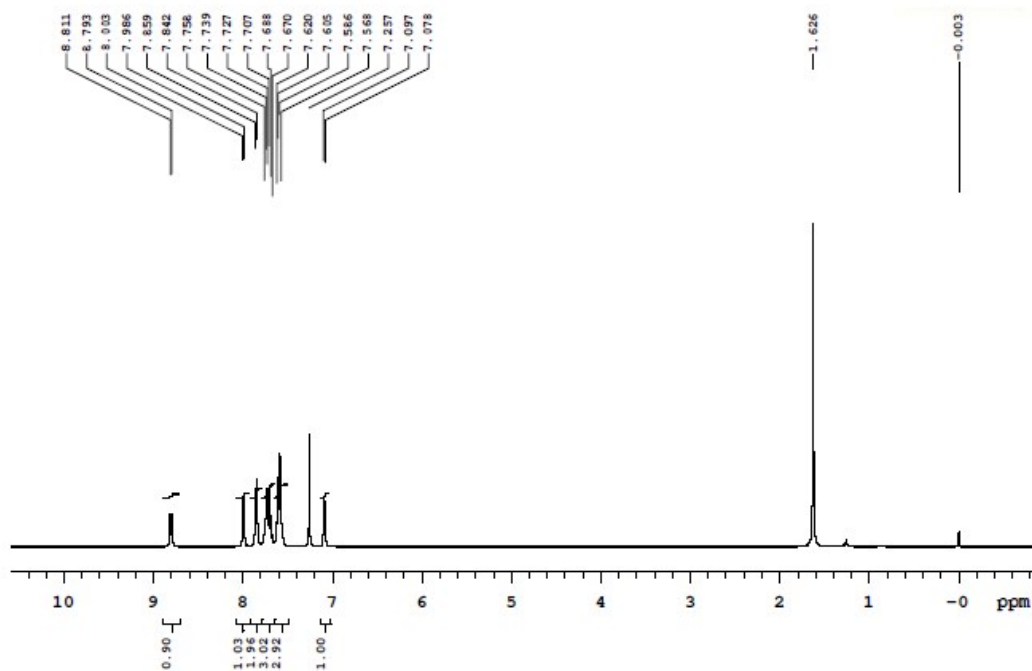
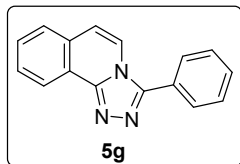


Figure S45. ^1H NMR Spectra & its expansion for compound **5g** in CDCl_3

NUCLEUS : C13
 FREQ (MHz) : 100.50
 AT (sec) : 1.28
 SW (ppm) : 253.84
 RD (sec) : 1.00
 PW (usec) : 5.05
 Scans : 1500
 Solvent : cdcl3
 Data Points : 65536
 LB (Hz) : 3.00
 TEMP (K) : 303.15
 EXP : s2pul
 DATE : Nov 20 2015
 System : VNMR5_400

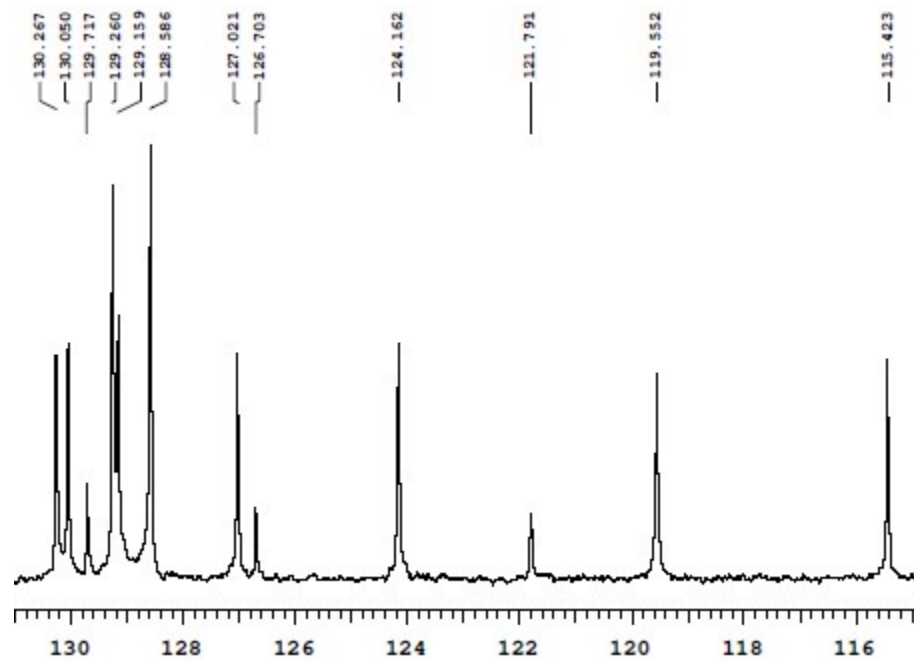
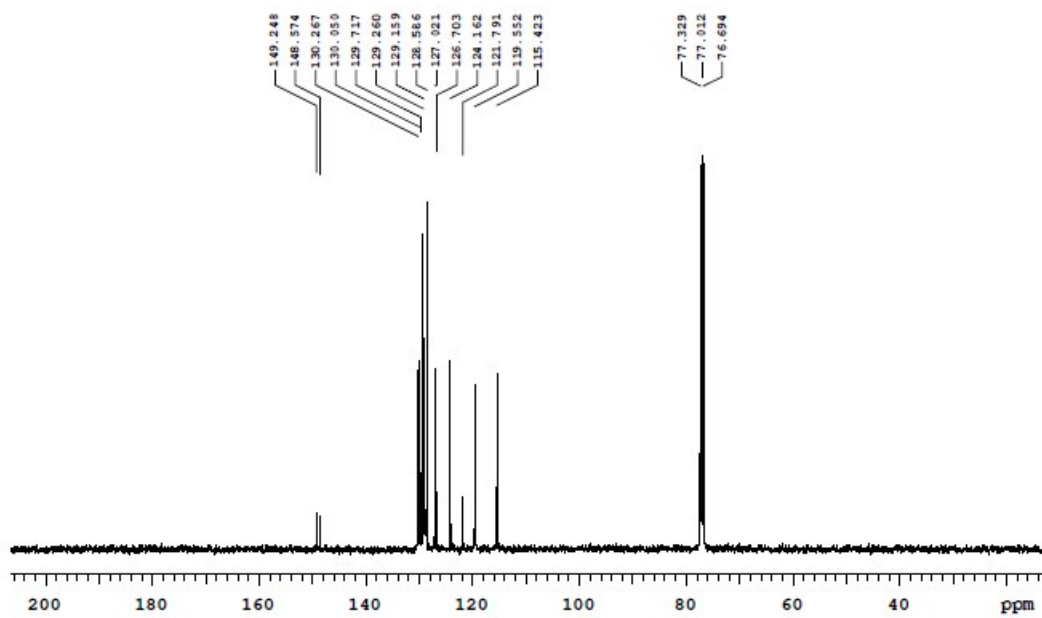
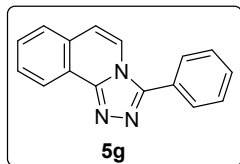


Figure S46. ^{13}C NMR Spectra & its expansion for compound **5g** in CDCl_3

NUCLEUS : H1
 FRQ (MHz) : 399.64
 AT (sec) : 2.27
 SW (ppm) : 18.08
 RD (sec) : 1.00
 FWH (usec) : 6.60
 Scans : 64
 Solvent : dmsc
 Data Points : 32768
 LB (Hz) : 1.00
 TEMP (K) : 303.15
 EXP : s2pul
 DATE : Feb 12 2016
 System : VNMR5_400

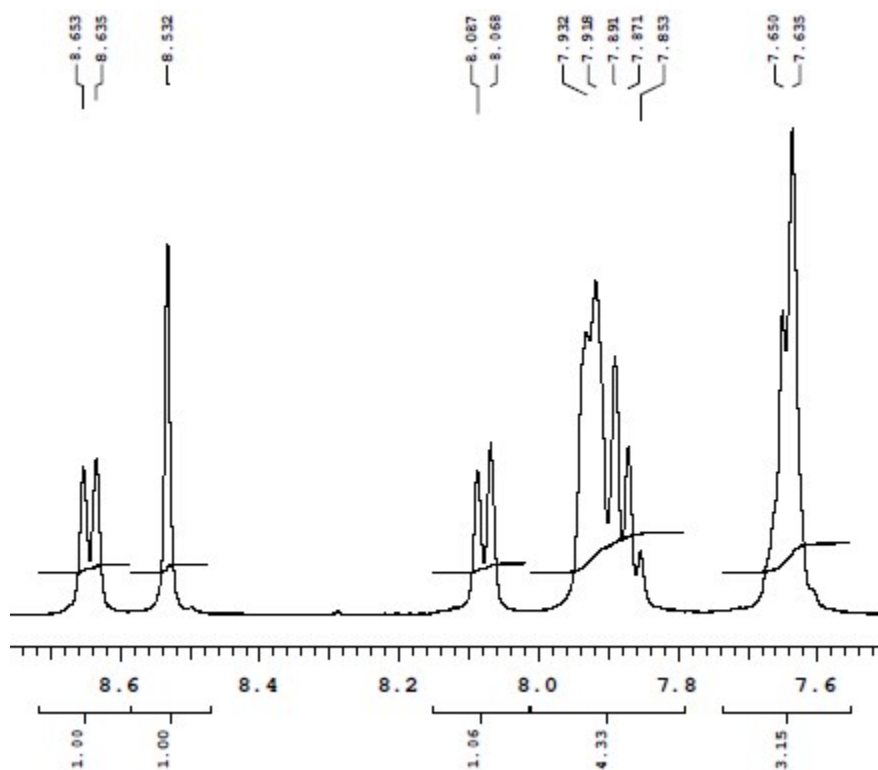
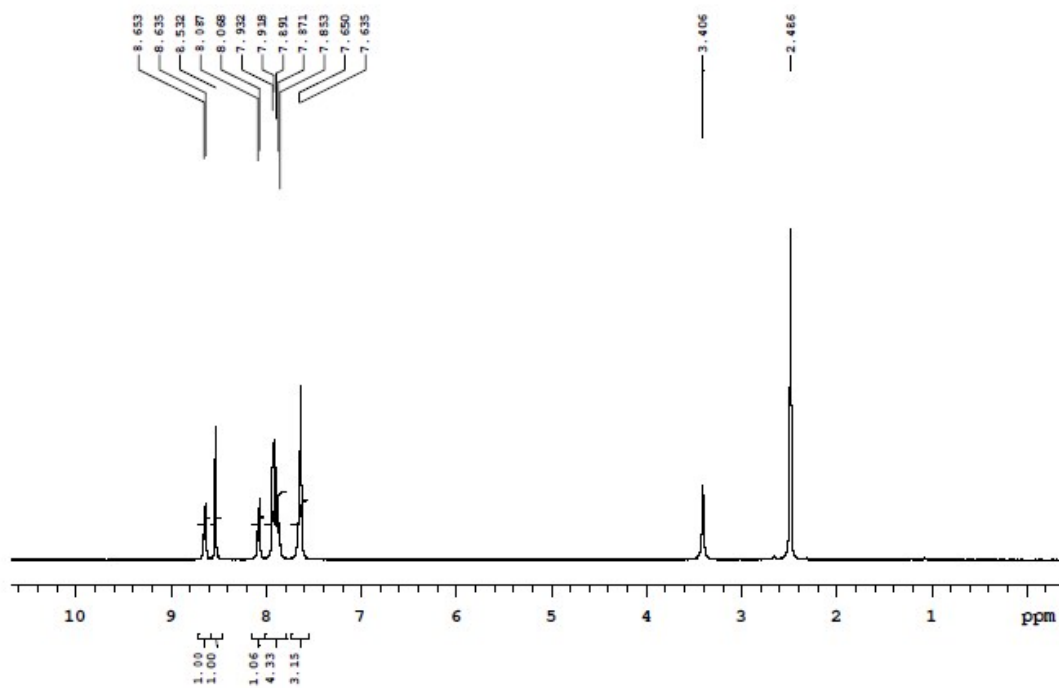
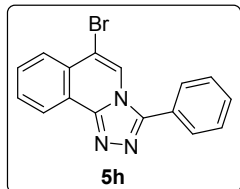


Figure S47. ^1H NMR Spectra & its expansion for compound **5h** in $\text{DMSO-}d_6$

NUCLEUS : C13
 FRQ (MHz) : 100.50
 AT (sec) : 1.28
 SW (ppm) : 253.84
 RD (sec) : 1.00
 PW (usec) : 5.05
 Scans : 3000
 Solvent : dmsd
 Data Points : 65536
 LS (Hz) : 4.00
 TEMP (K) : 303.15
 EXP : s2p1
 DATE : Feb 15 2016
 System : VNMR5_400

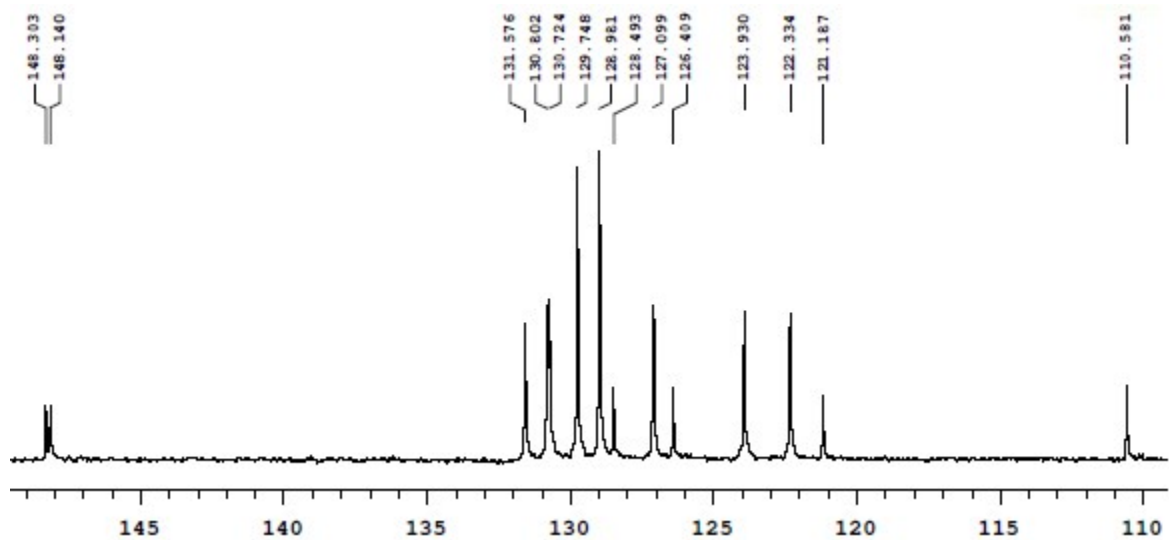
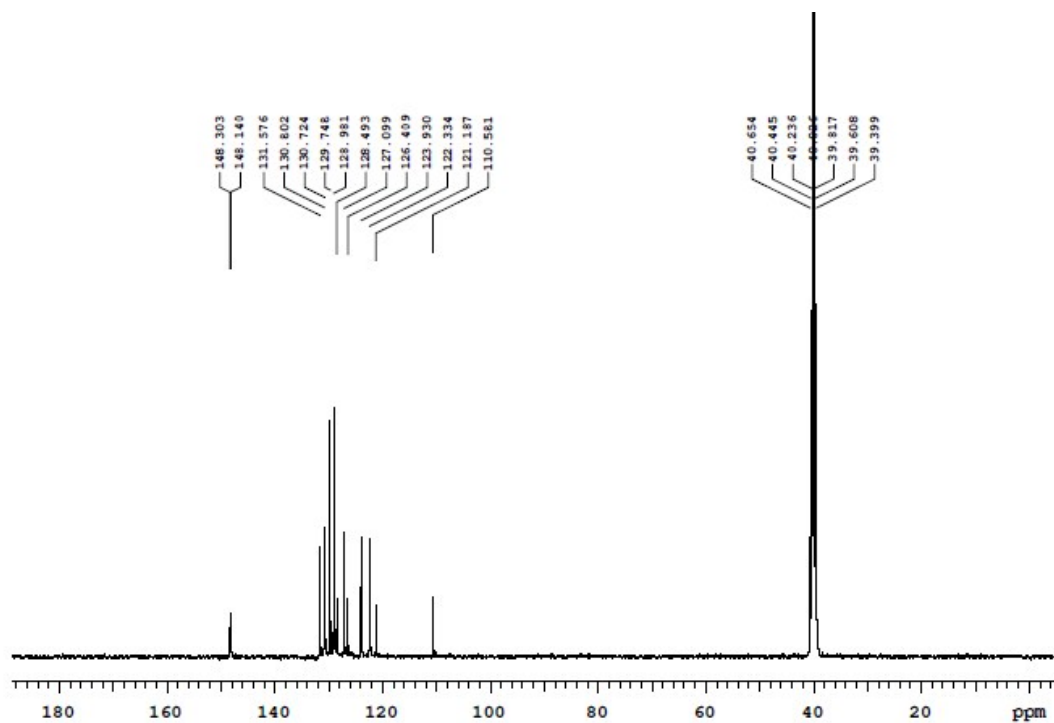
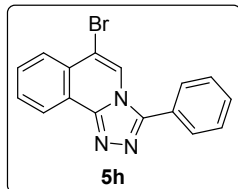


Figure S48. ^{13}C NMR Spectra & its expansion for compound **5h** in $\text{DMSO-}d_6$

NUCLEUS : H1
FREQ (MHz) : 399.63
AT (sec) : 2.27
SW (ppm) : 18.08
RD (sec) : 1.00
DW (usec) : 6.60
SCANS : 64
Solvent : cdcl3
Data Points : 32768
LB (Hz) : 1.00
TEMP (K) : 303.15
EXP : s2pul
DATE : Nov 16 2015
System : VNMR5_400

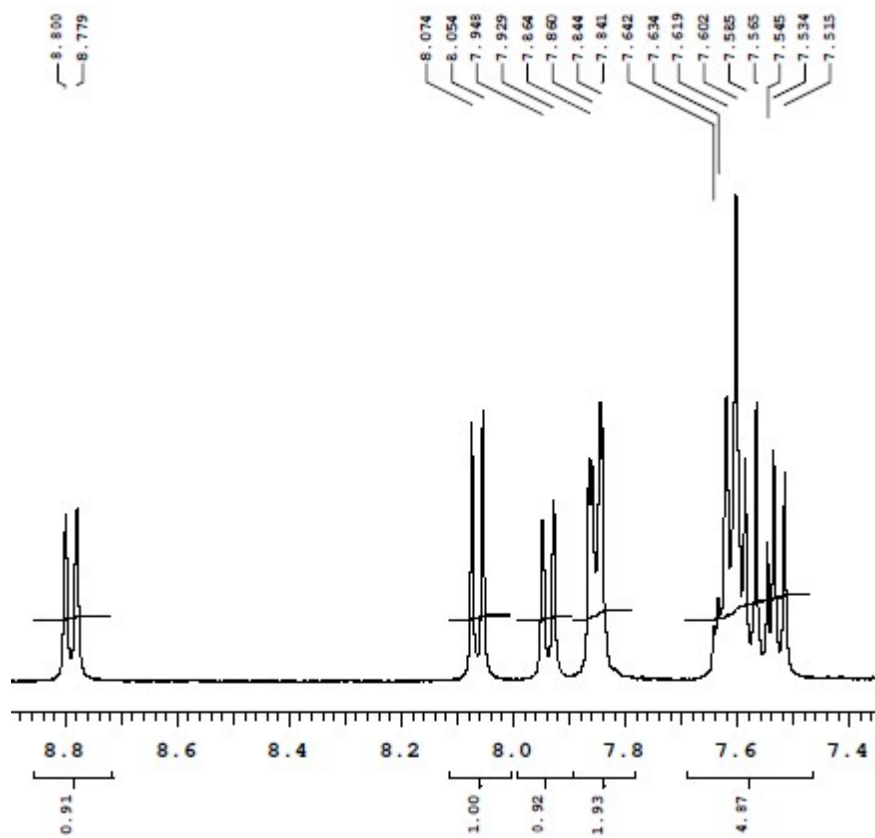
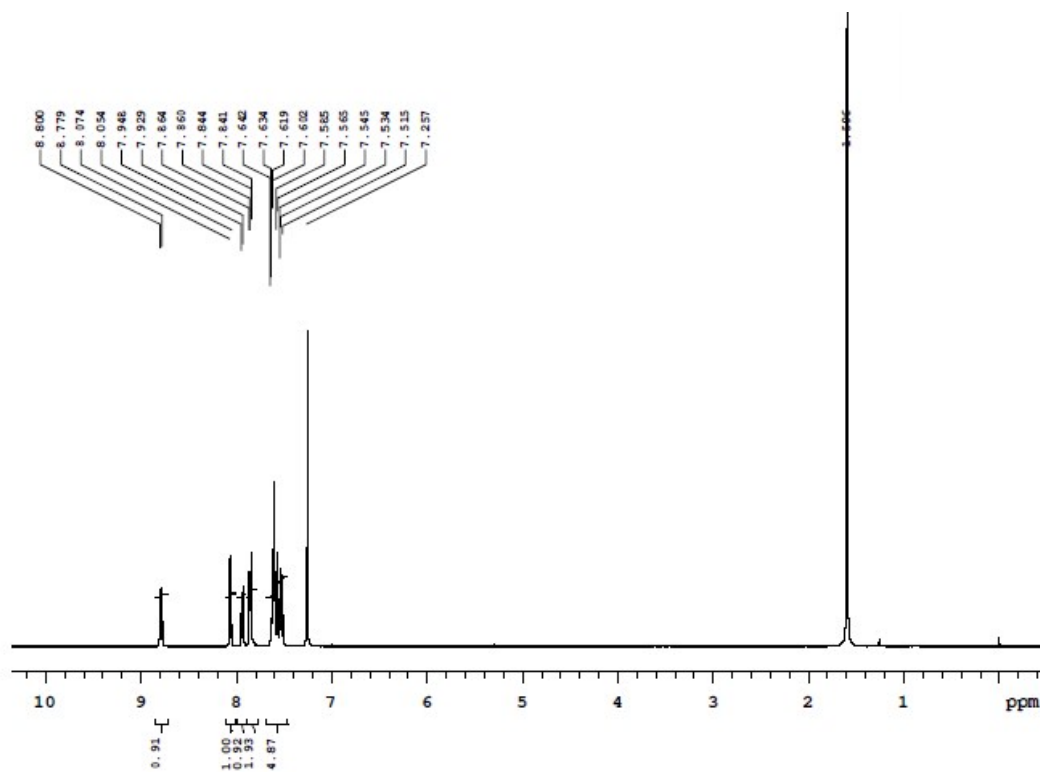
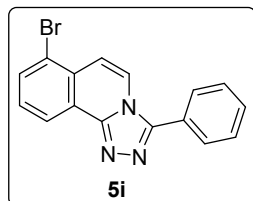


Figure S49. ^1H NMR Spectra & its expansion for compound **5i** in CDCl_3

NUCLEUS : C13
 FREQ (MHz) : 100.50
 AT (sec) : 1.28
 SW (ppm) : 253.84
 RD (sec) : 1.00
 PW (usec) : 5.05
 Scans : 1500
 Solvent : cdcl3
 Data Points : 65536
 LB (Hz) : 4.00
 TEMP (K) : 303.15
 EXP : s2pul
 DATE : Nov 24 2015
 System : VNMR5_400

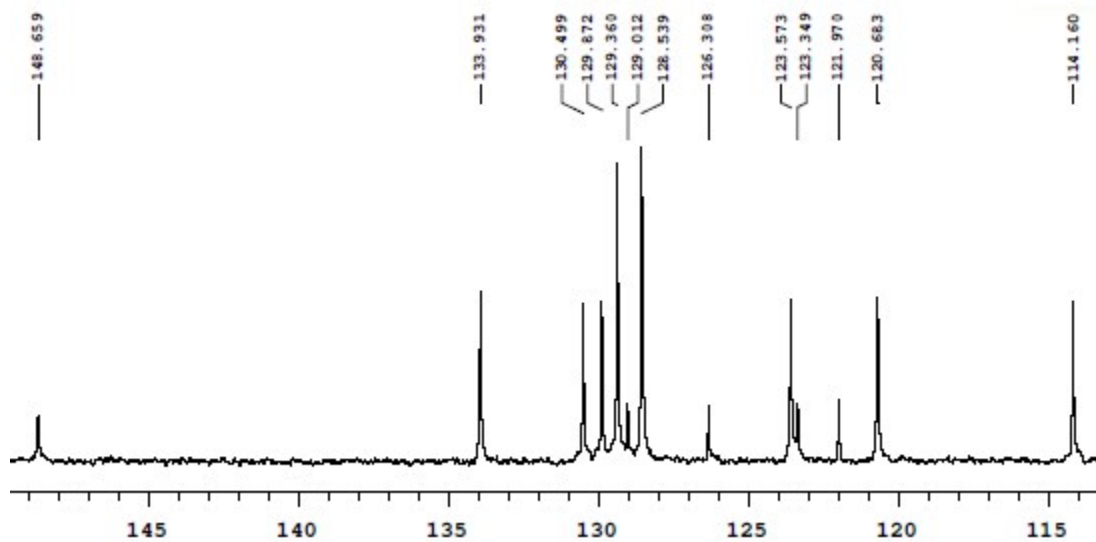
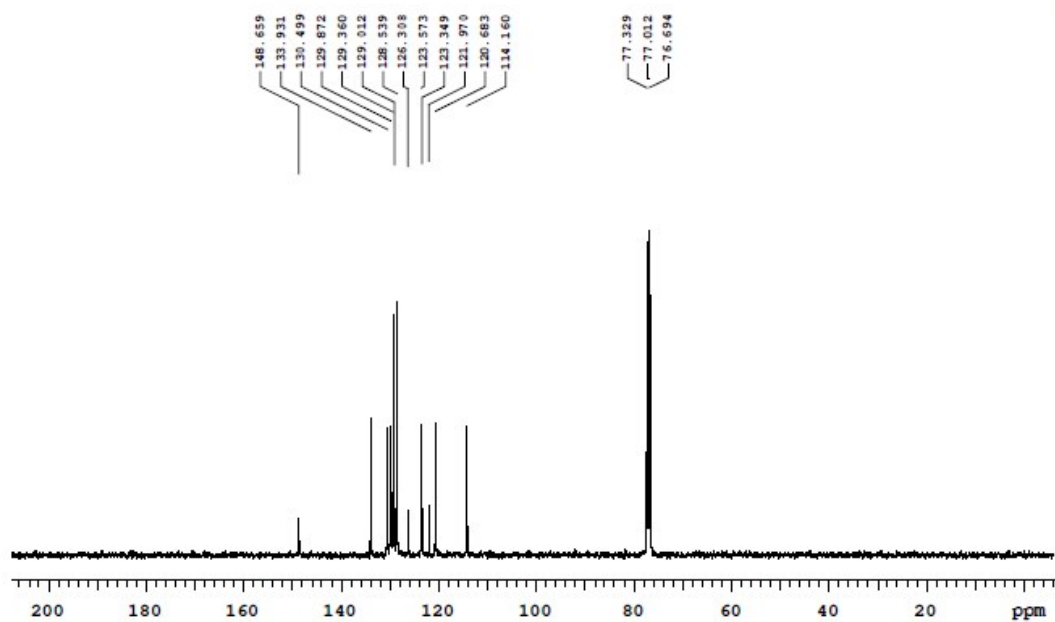
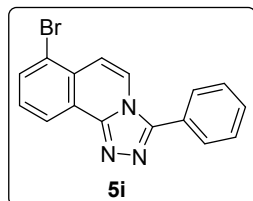


Figure S50. ^{13}C NMR Spectra & its expansion for compound **5i** in CDCl_3

NUCLEUS : H1
 FREQ (MHz) : 399.63
 AT (sec) : 2.27
 SW (ppm) : 18.08
 RD (sec) : 1.00
 PW (usec) : 6.60
 Scans : 64
 Solvent : cdcl3
 Data Points : 32768
 LB (Hz) : 1.00
 TEMP (K) : 303.15
 EXP : s2p1
 DATE : Nov 16 2015
 System : VNMRS_400

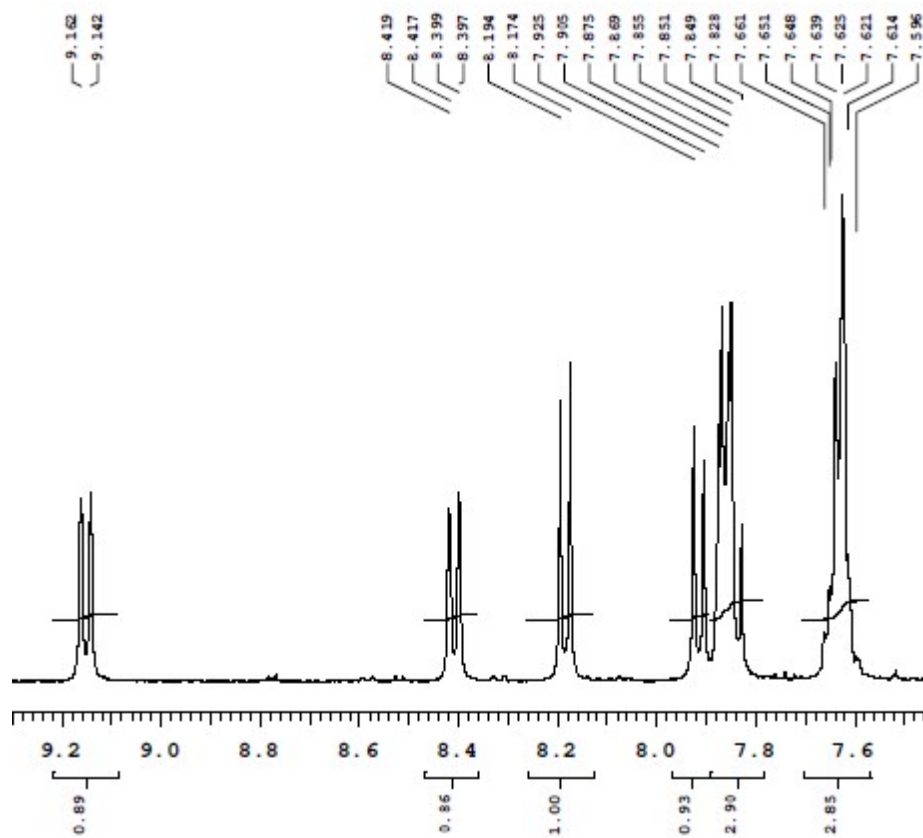
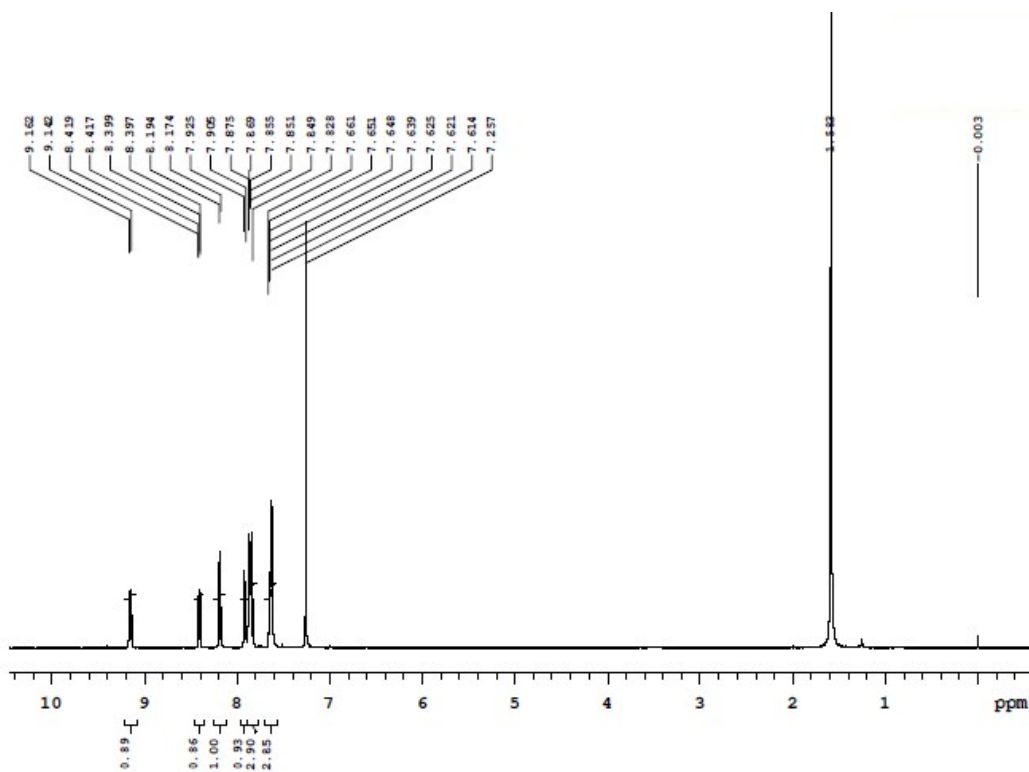
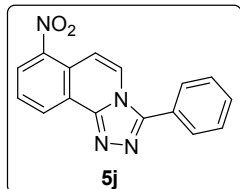


Figure S51. ^1H NMR Spectra & its expansion for compound **5j** in CDCl_3

NUCLEUS : C13
 FREQ (MHz) : 100.50
 AT (sec) : 1.28
 SW (ppm) : 253.84
 RD (sec) : 1.00
 FW (usec) : 5.05
 Scans : 1500
 Solvent : cdcl3
 Data Points : 65536
 LB (Hz) : 3.00
 TEMP (K) : 303.15
 EXP : s2pul
 DATE : Nov 24 2015
 System : VNMR5_400

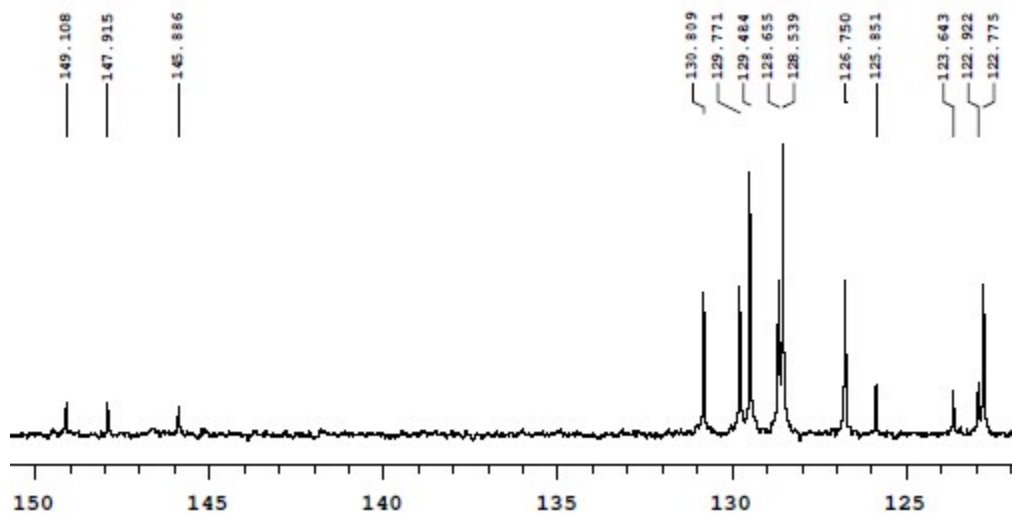
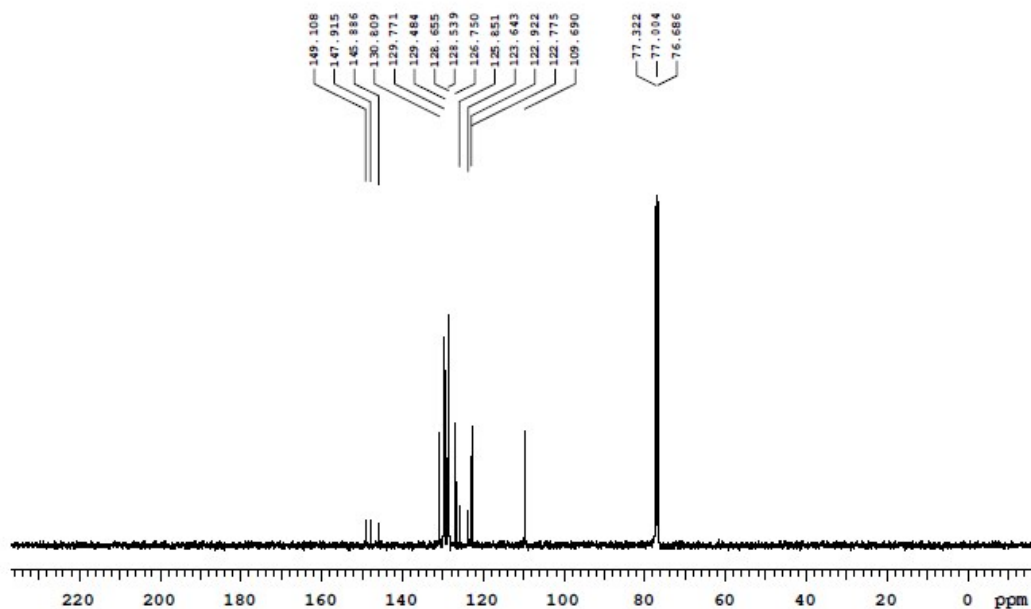
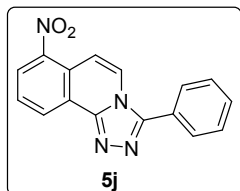


Figure S52. ^{13}C NMR Spectra & its expansion for compound **5j** in CDCl_3