

Supplementary information for

Fe(II)-Catalyzed isomerization of 5-chloroisoxazoles to 2*H*-azirine-2-carbonylchlorides as a key stage in the synthesis of pyrazole-nitrogen heterocycle dyads

*Kirill I. Mikhailov, Ekaterina E. Galenko, Alexey V. Galenko, Mikhail S. Novikov, Alexander Yu. Ivanov, Galina L. Starova and Alexander F. Khlebnikov**

Saint Petersburg State University, Institute of Chemistry, 7/9 Universitetskaya nab., St. Petersburg 199034, Russia

*Corresponding author e-mail: a.khlebnikov@spbu.ru

Table of contents

UV-Vis absorption spectra of oxazoles 7a-h	S2
Crystallographic data of compounds 3a, 5e, 6e, 7e	S3
NMR spectra.....	S7
Computational Details.....	S120

Figure S1. Absorption spectra of **7a-d** in MeCN.

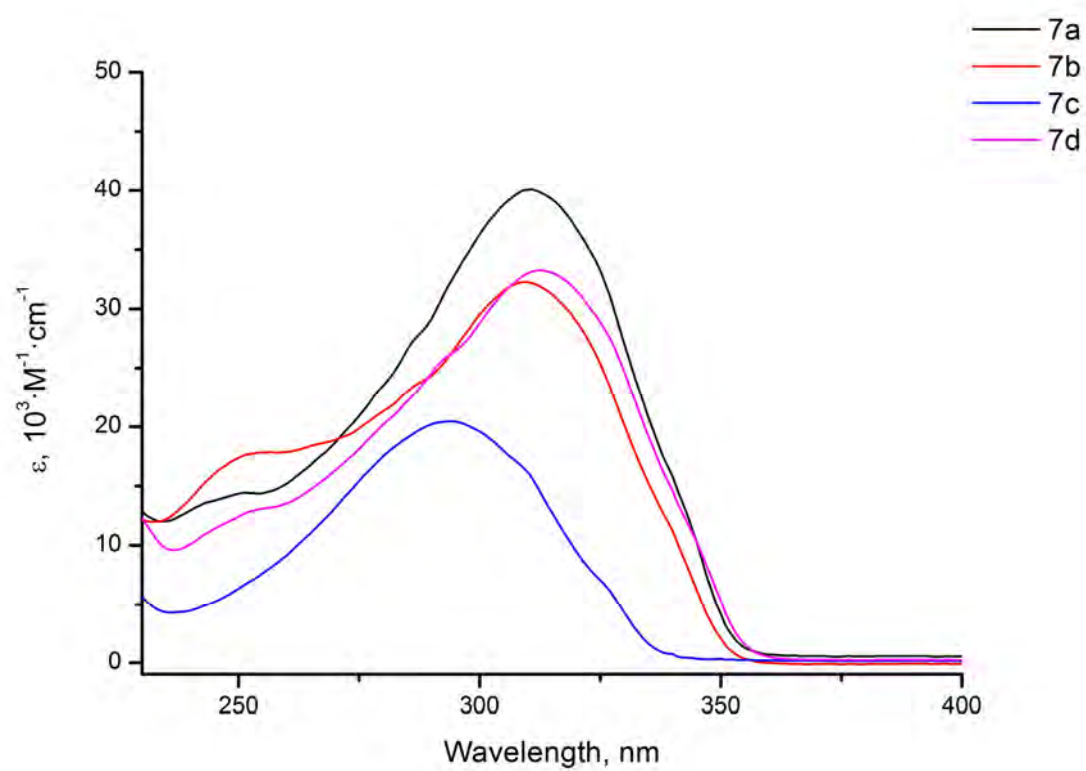
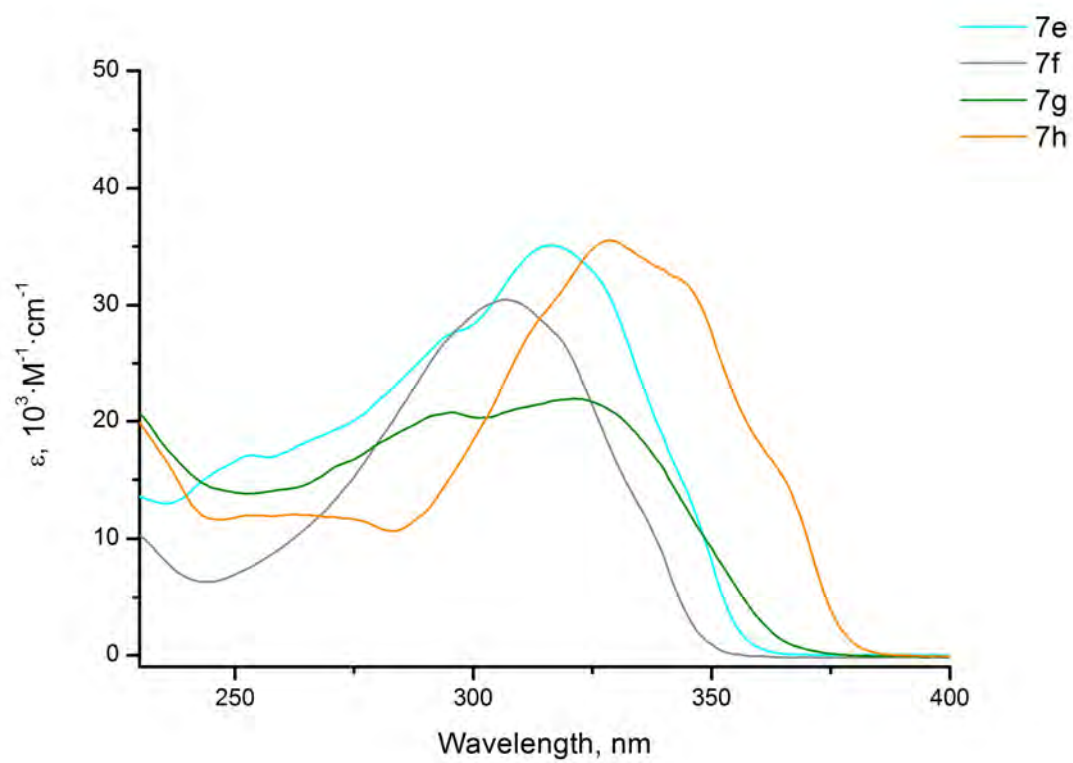


Figure S2. Absorption spectra of **7e-h** in MeCN.



Crystallographic data of compounds 3a, 5e, 6e, 7e.

Single crystals of compounds **3a**, **5e**, **6e**, **7e** were grown by slow evaporation of CH₂Cl₂/petrol ether solution at 4°C. A suitable crystal was selected and studied on a diffractometer. The crystal was kept at 100(2) K during data collection. Using Olex2 [1], the structure was solved with the ShelXS [2] structure solution program using Direct Methods and refined with the ShelXL [3] refinement package using Least Squares minimization.

1. Dolomanov, O.V.; Bourhis, L.J.; Gildea, R.J.; Howard, J.A.K.; Puschmann, H. *J. Appl. Cryst.* **2009**, 42, 339-341.
2. Sheldrick, G.M. *Acta Cryst.* **2008**; A64, 112-122.
3. Sheldrick, G.M. *Acta Cryst.* **2015**, C71, 3-8.

Table S1 Crystal data and structure refinement for compounds **3a**, **5e**.

Identification code	3a	5e
Empirical formula	C ₁₂ H ₉ N ₃ O	C ₁₆ H ₁₅ N ₃ O
Formula weight	211.22	265.31
Temperature/K	100(2)	100(2)
Crystal system	monoclinic	monoclinic
Space group	P2 ₁ /c	P2 ₁ /c
a/Å	6.6661(3)	14.8678(6)
b/Å	14.0379(6)	8.0055(3)
c/Å	10.8986(5)	11.3689(5)
α/°	90	90
β/°	98.965(4)	100.528(4)
γ/°	90	90
Volume/Å ³	1007.40(8)	1330.39(9)
Z	4	4
ρ _{calc} /g/cm ³	1.393	1.325
μ/mm ⁻¹	0.757	0.086
F(000)	440.0	560.0
Crystal size/mm ³	0.30 × 0.22 × 0.10	0.32 × 0.18 × 0.12
Radiation	CuKα (λ = 1.54184)	MoKα (λ = 0.71073)
2θ range for data collection/°	10.356 to 139.91	5.802 to 54.992
Index ranges	-8 ≤ h ≤ 5, -16 ≤ k ≤ 17, -13 ≤ l ≤ 13	-19 ≤ h ≤ 19, -10 ≤ k ≤ 10, -14 ≤ l ≤ 12
Reflections collected	4378	10687
Independent reflections	1904 [R _{int} = 0.0311, R _{sigma} = 0.0384]	3051 [R _{int} = 0.0285, R _{sigma} = 0.0307]
Data/restraints/parameters	1904/0/145	3051/0/181
Goodness-of-fit on F ²	1.068	1.036
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0394, wR ₂ = 0.0984	R ₁ = 0.0432, wR ₂ = 0.0894
Final R indexes [all data]	R ₁ = 0.0477, wR ₂ = 0.1054	R ₁ = 0.0571, wR ₂ = 0.0958
Largest diff. peak/hole / e Å ⁻³	0.23/-0.24	0.29/-0.22

Table S2 Crystal data and structure refinement for compounds 6e, 7e.

Identification code	6e	7e
Empirical formula	C ₁₈ H ₁₇ N ₃ O ₃	C ₁₉ H ₁₅ N ₃ O ₂
Formula weight	323.34	317.34
Temperature/K	100(2)	100(2)
Crystal system	triclinic	monoclinic
Space group	P-1	P2 ₁ /n
a/Å	7.4133(3)	12.8169(5)
b/Å	11.6571(6)	7.2190(3)
c/Å	18.6337(9)	16.4865(6)
α /°	88.156(4)	90
β /°	87.588(4)	99.444(4)
γ /°	77.800(4)	90
Volume/Å ³	1572.07(14)	1504.75(10)
Z	4	4
ρ_{calc} /g/cm ³	1.366	1.401
μ /mm ⁻¹	0.779	0.093
F(000)	680.0	664.0
Crystal size/mm ³	0.32 × 0.24 × 0.12	0.34 × 0.22 × 0.16
Radiation	CuK α (λ = 1.54184)	MoK α (λ = 0.71073)
2 Θ range for data collection/°	7.762 to 139.984	6.174 to 54.992
Index ranges	-5 ≤ h ≤ 9, -12 ≤ k ≤ 14, -22 ≤ l ≤ 22	-14 ≤ h ≤ 16, -9 ≤ k ≤ 8, -21 ≤ l ≤ 21
Reflections collected	11776	10110
Independent reflections	5935 [R_{int} = 0.0428, R_{sigma} = 0.0529]	3463 [R_{int} = 0.0265, R_{sigma} = 0.0314]
Data/restraints/parameters	5935/0/437	3463/0/218
Goodness-of-fit on F ²	1.026	1.046
Final R indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0439, wR_2 = 0.1102	R_1 = 0.0408, wR_2 = 0.0951
Final R indexes [all data]	R_1 = 0.0599, wR_2 = 0.1222	R_1 = 0.0515, wR_2 = 0.1028
Largest diff. peak/hole / e Å ⁻³	0.31/-0.25	0.29/-0.27

Figure S3. Molecular structure of compound **3a**, displacement parameters are drawn at 50% probability level.

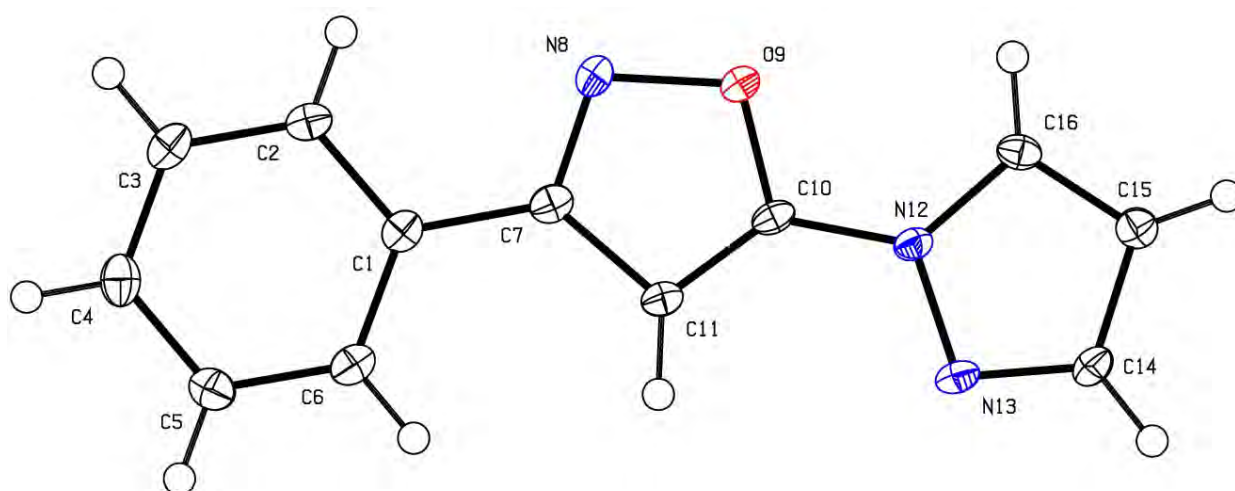


Figure S4. Molecular structure of compound **5l**, displacement parameters are drawn at 50% probability level.

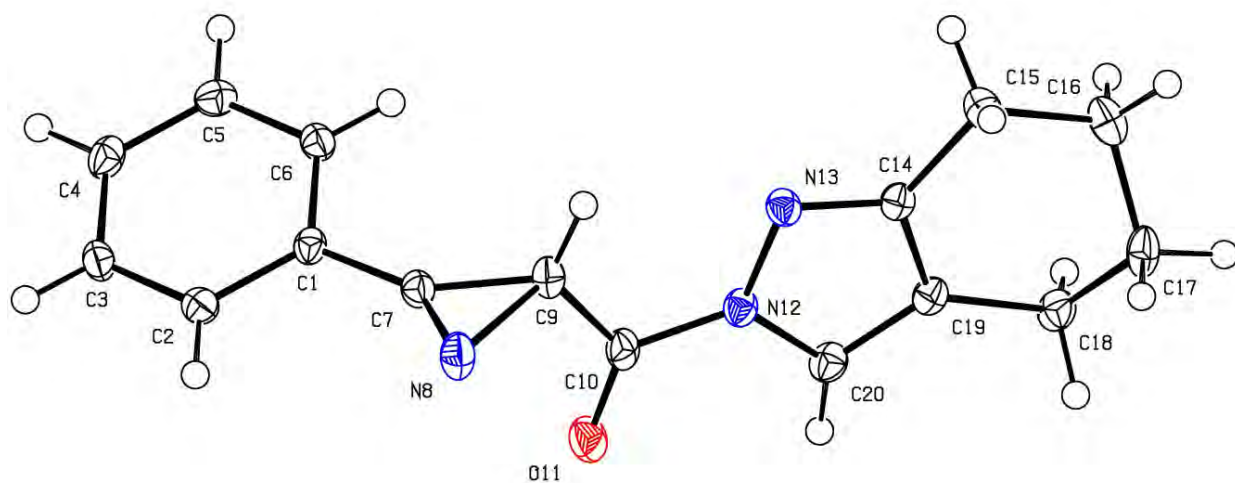


Figure S5. Molecular structure of compound **6e**, displacement parameters are drawn at 50% probability level.

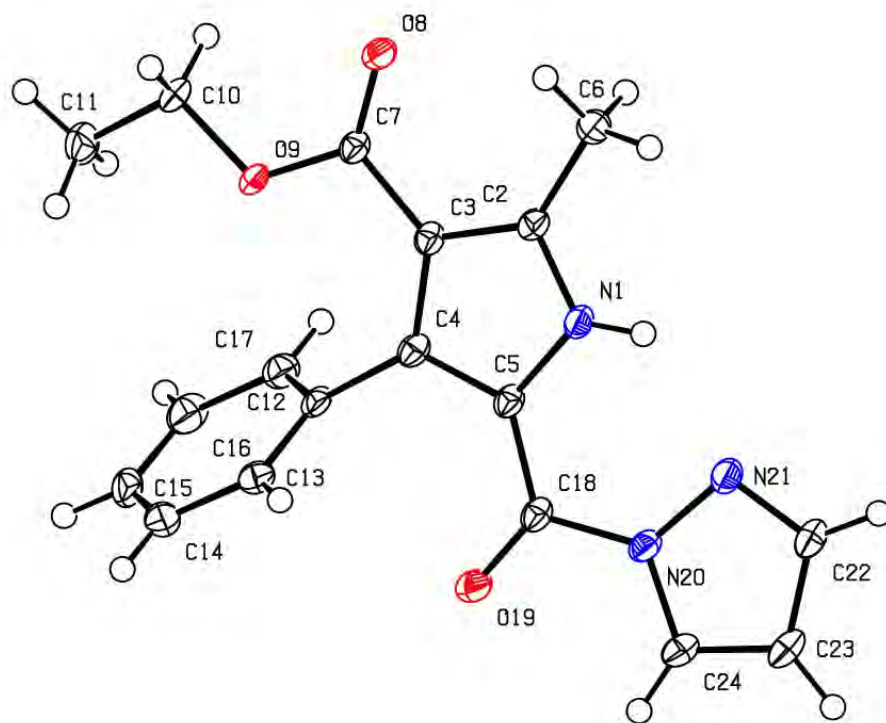
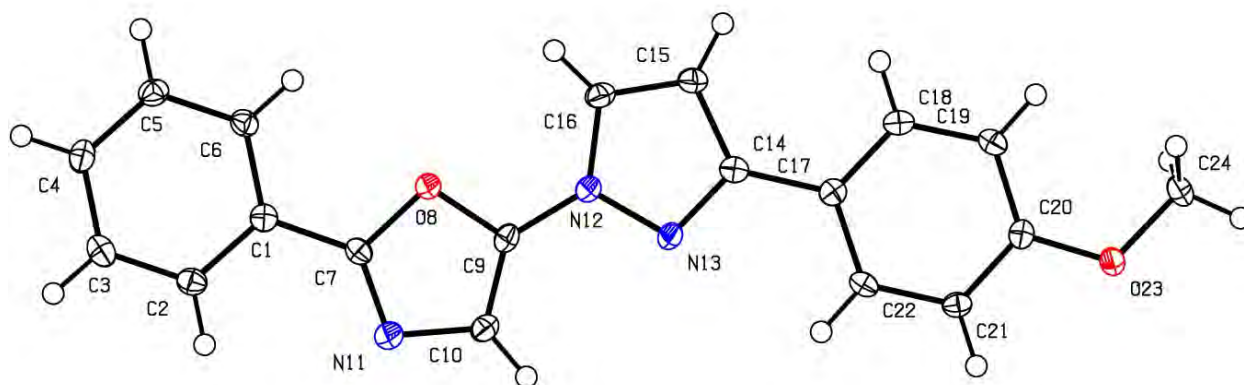


Figure S6. Molecular structure of compound **7e**, displacement parameters are drawn at 50% probability level.



NMR Spectra

HMBC ^1H - ^{15}N NMR spectroscopy (Fig. S7) was used to establish the structure of compound **5k**. Additionally two N-H spin-spin coupling constants (8.5 and 13.7 Hz) were defined using a selective HSQMBC IPAP ^1H - ^{15}N experiment.¹ The azirine nitrogen, which has the most intensive cross-peak with the azirine proton at 4.40 ppm has a chemical shift of 263 ppm. The nitrogen with chemical shift of 220 ppm has a weaker cross-peak with the azirine proton at 4.40 ppm, but shows an intensive cross-peak with indazole proton H^3 at 8.30 ppm. Consequently this nitrogen is connected to the carbonyl group. Typically the pyrrole nitrogen atom in indazole has a chemical shift of about 200 ppm, pyridine nitrogen – about 300 ppm.² Analysis of the spin-spin coupling constants permit the assignment of the nitrogen with chemical shift of 311 ppm to a pyridine type N since it is known that $J_{\text{N-H}}^2$ for a pyridine type nitrogen is extraordinary high (13-14 Hz) and $J_{\text{N-H}}^3$ is extraordinary small (1-2 Hz), compared with typical N-H constants, whereas for a pyrrole type nitrogen both constants are about equal 6-8 Hz. For example, 1-phenylpyrazole has $J_{\text{H}(3)\text{-N}(1)}^3 = 7.4$ Hz, $J_{\text{H}(3)\text{-N}(2)}^2 = 14.2$ Hz, $J_{\text{H}(4)\text{-N}(2)}^3 = 1.0$ Hz.³ Since in compound **5k** the nitrogen at 220 ppm has $J = 8.5$ Hz and nitrogen at 311 ppm $J = 13.7$ Hz it was concluded that the pyridine nitrogen (311 ppm) is in a vicinal position to H^3 of the indazole and this is N^2 , and consequently the carbonyl group is bound to the N^1 atom of indazole.

(1) Gil, S.; Espinosa, J. F.; Parella, T. *J. Magn. Reson.* **2010** 207, 312;

(2) Witanowski, M.; Stefaniak, L.; Webb, G. A. *In Annual Reports on NMR Spectroscopy. Nitrogen NMR Spectroscopy*, Webb, G. A., Ed.; Academic Press: London, UK, 1981, vol. 11B, pp. 1-502.

(3) Hawkes, G. E. *J. Chem. Soc., Perkin Trans.* **1977**, 2, 1024.

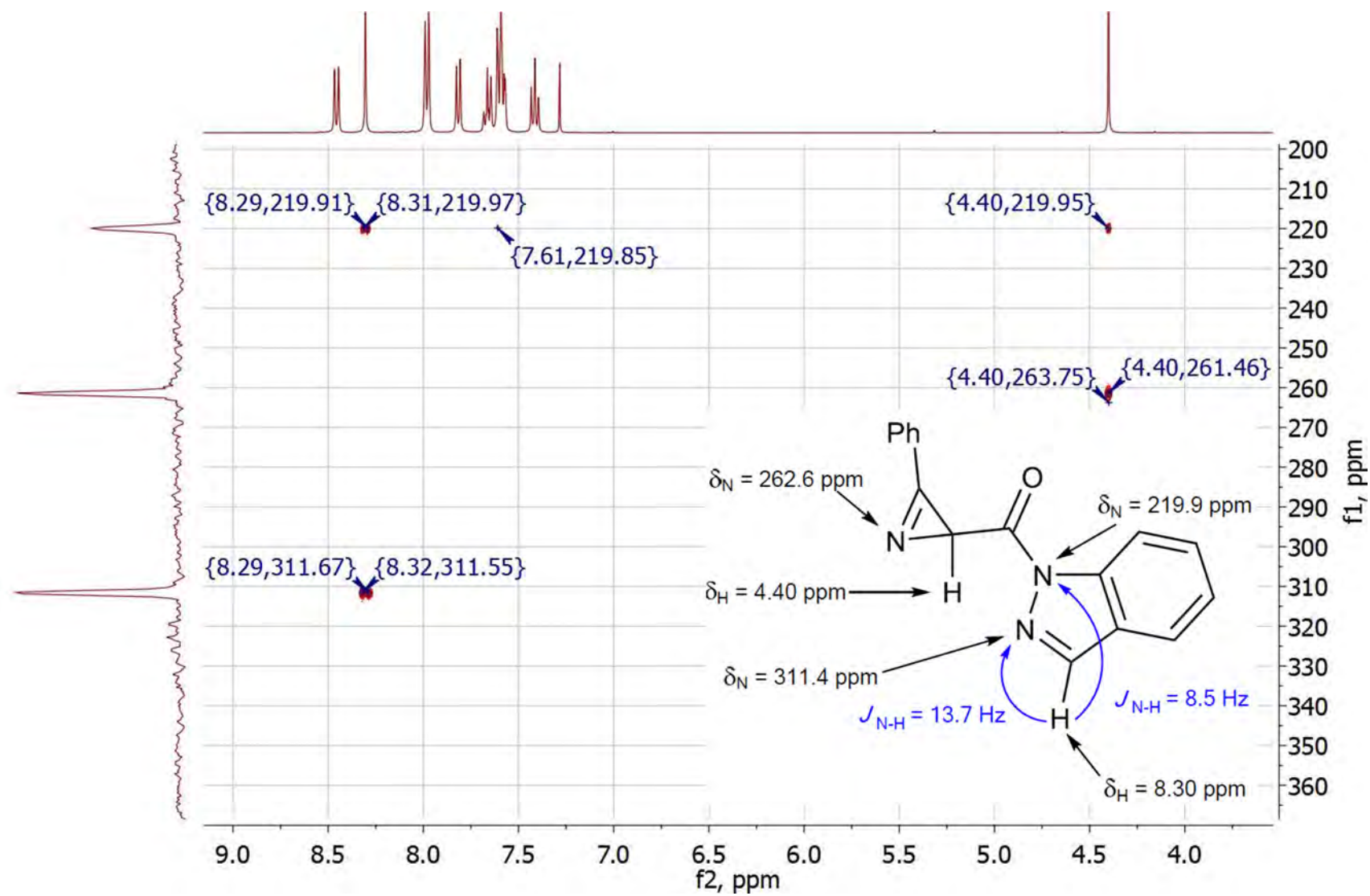
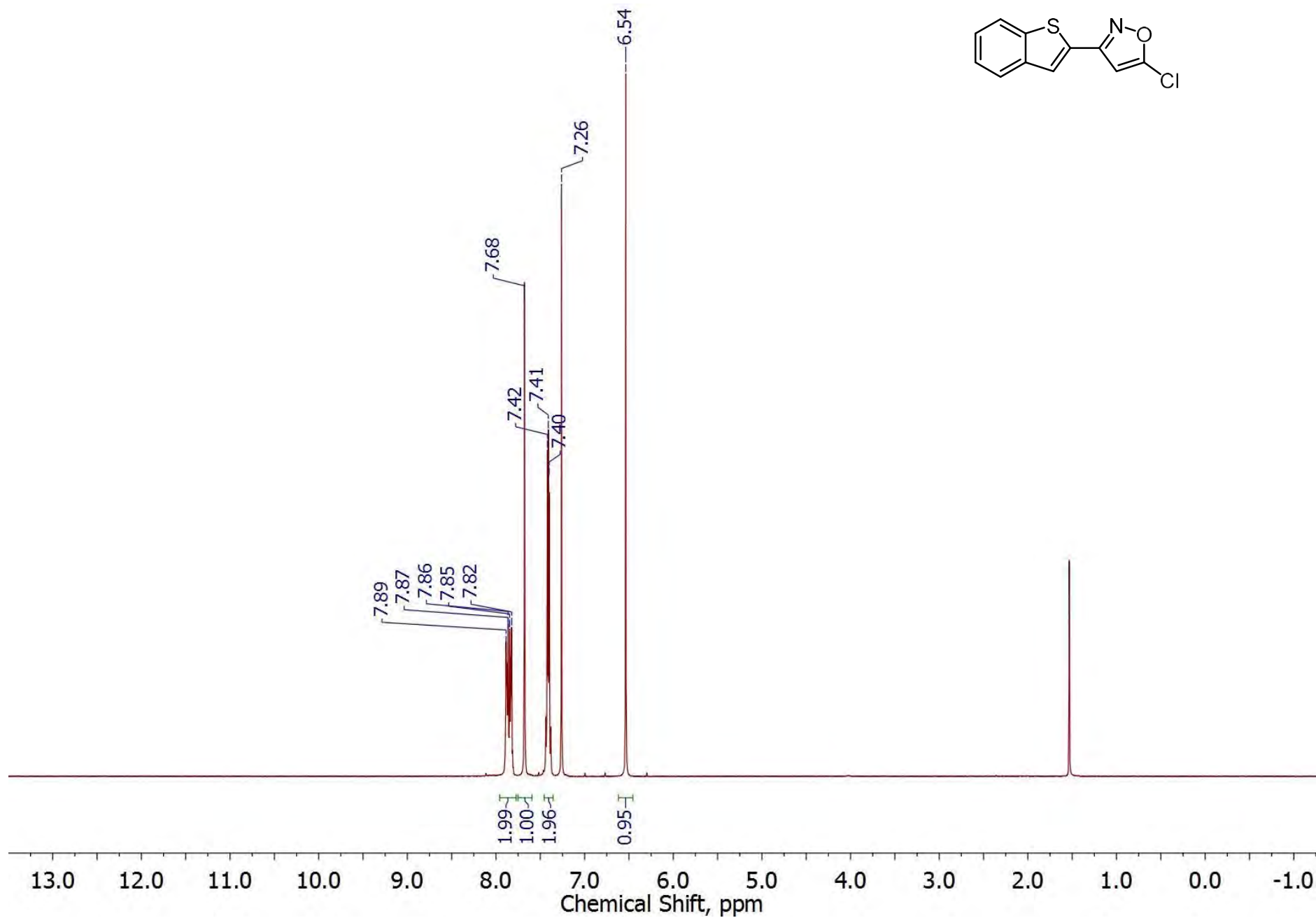
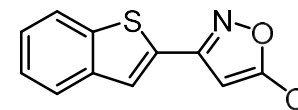
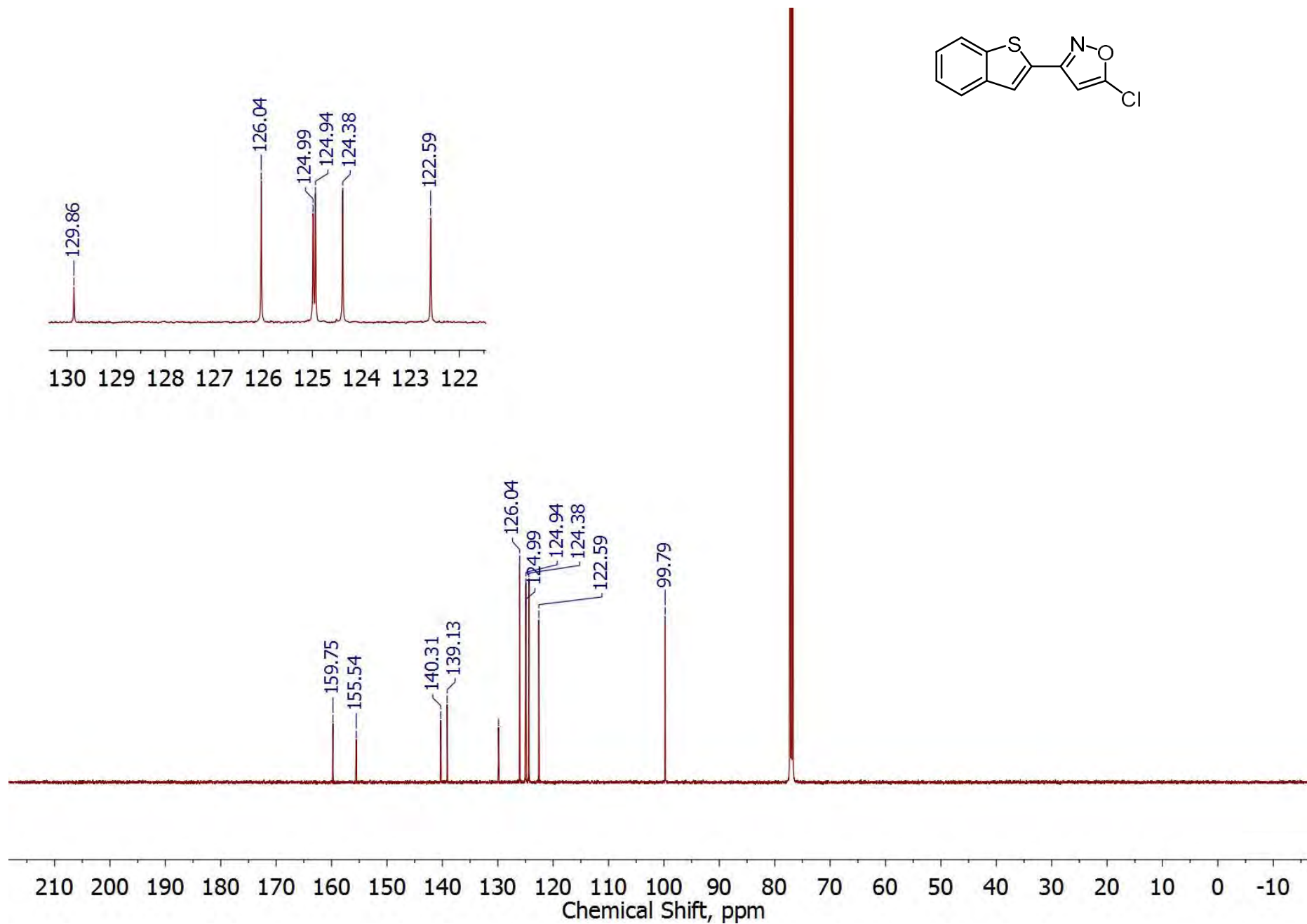
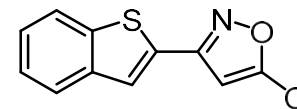


Figure S7. Correlation spectrum HMBC ^1H - ^{15}N of compound **5k**.

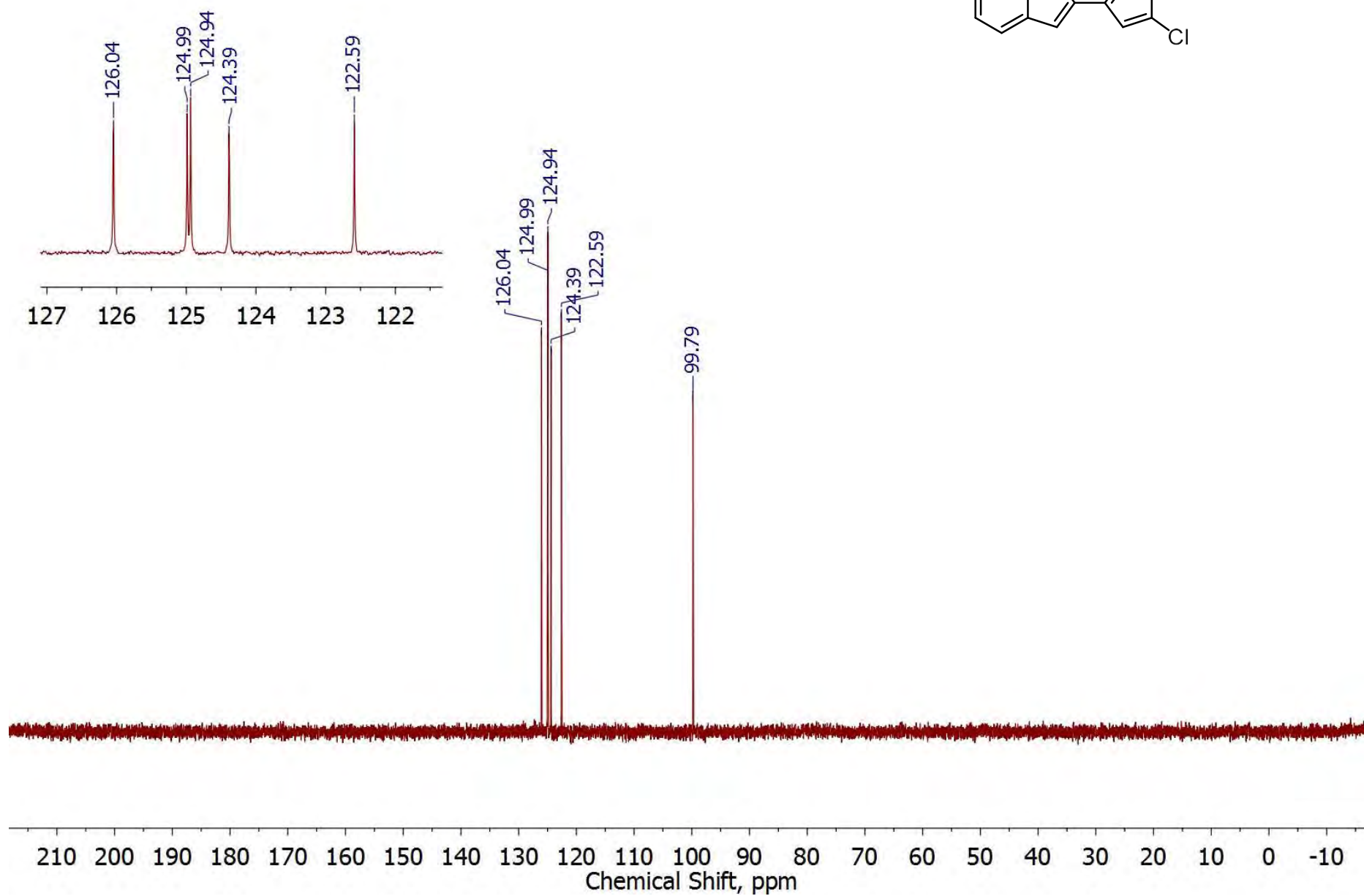
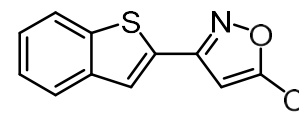
3-(Benzo[*b*]thiophen-2-yl)-5-chloroisoxazole (1e), 400 (^1H) MHz, CDCl_3



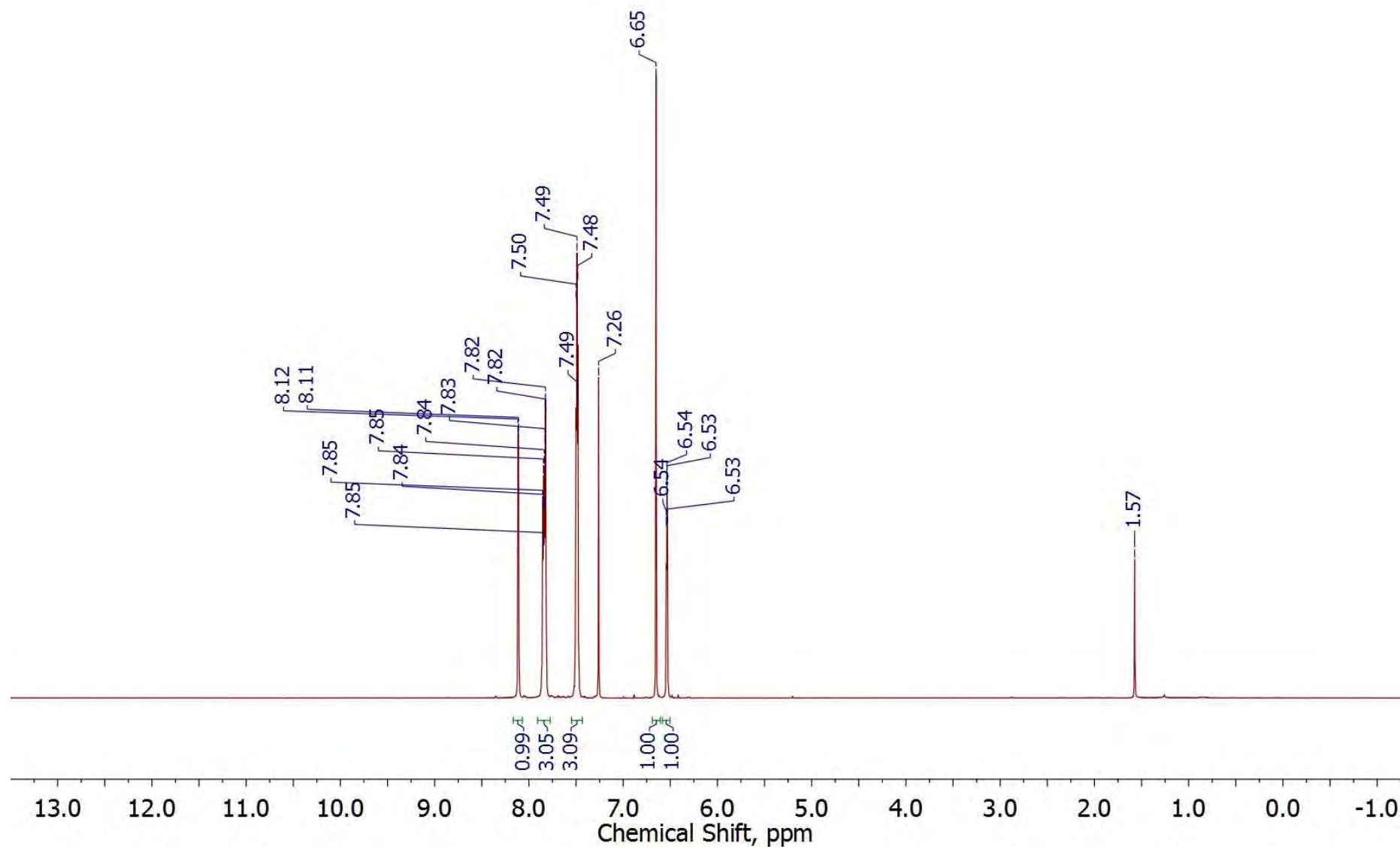
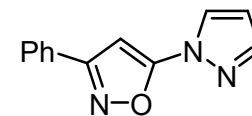
3-(Benzo[*b*]thiophen-2-yl)-5-chloroisoxazole (1e), 100 (^{13}C) MHz, CDCl_3



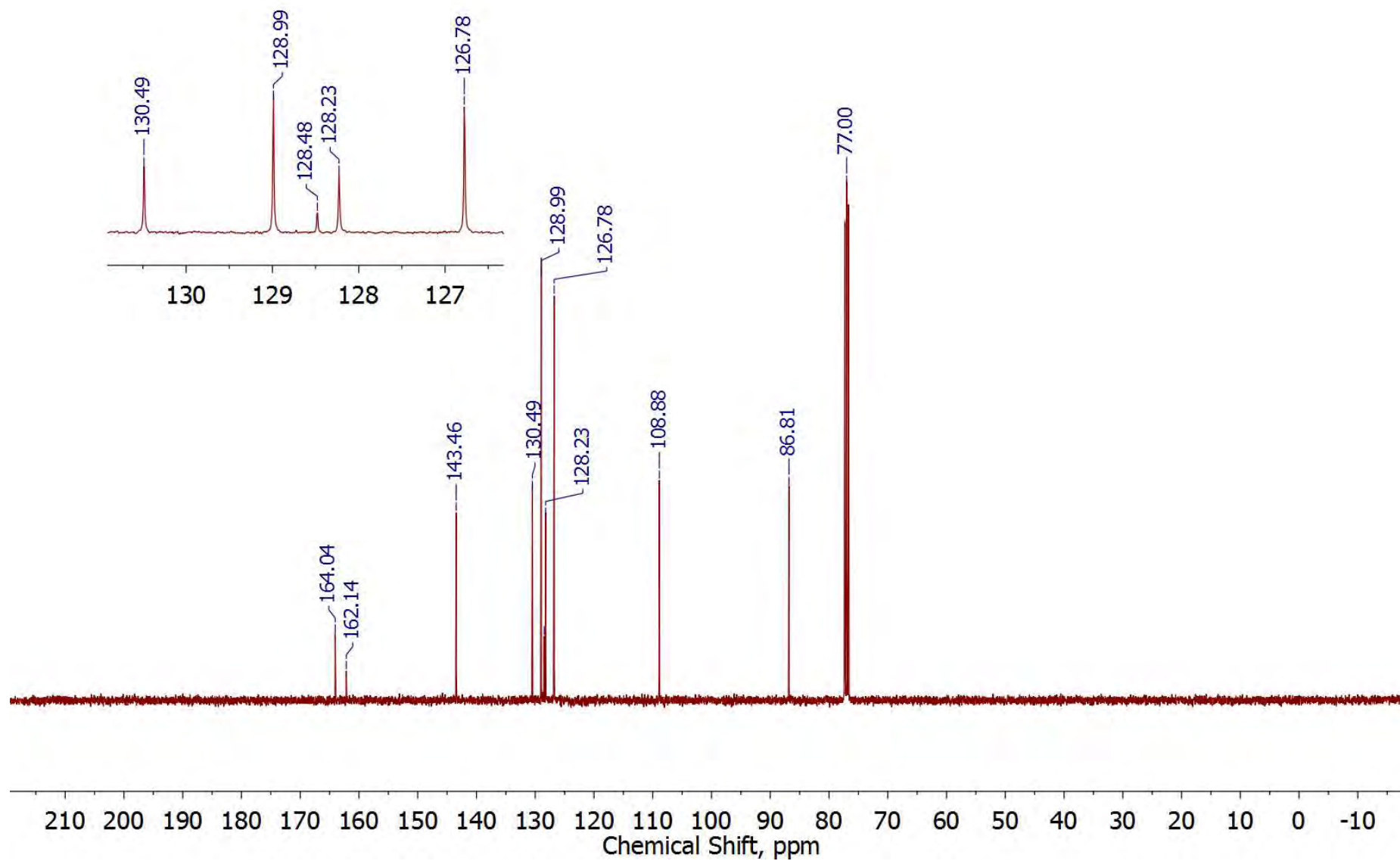
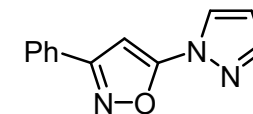
3-(Benzo[*b*]thiophen-2-yl)-5-chloroisoxazole (1e), 100 (DEPT) MHz, CDCl₃



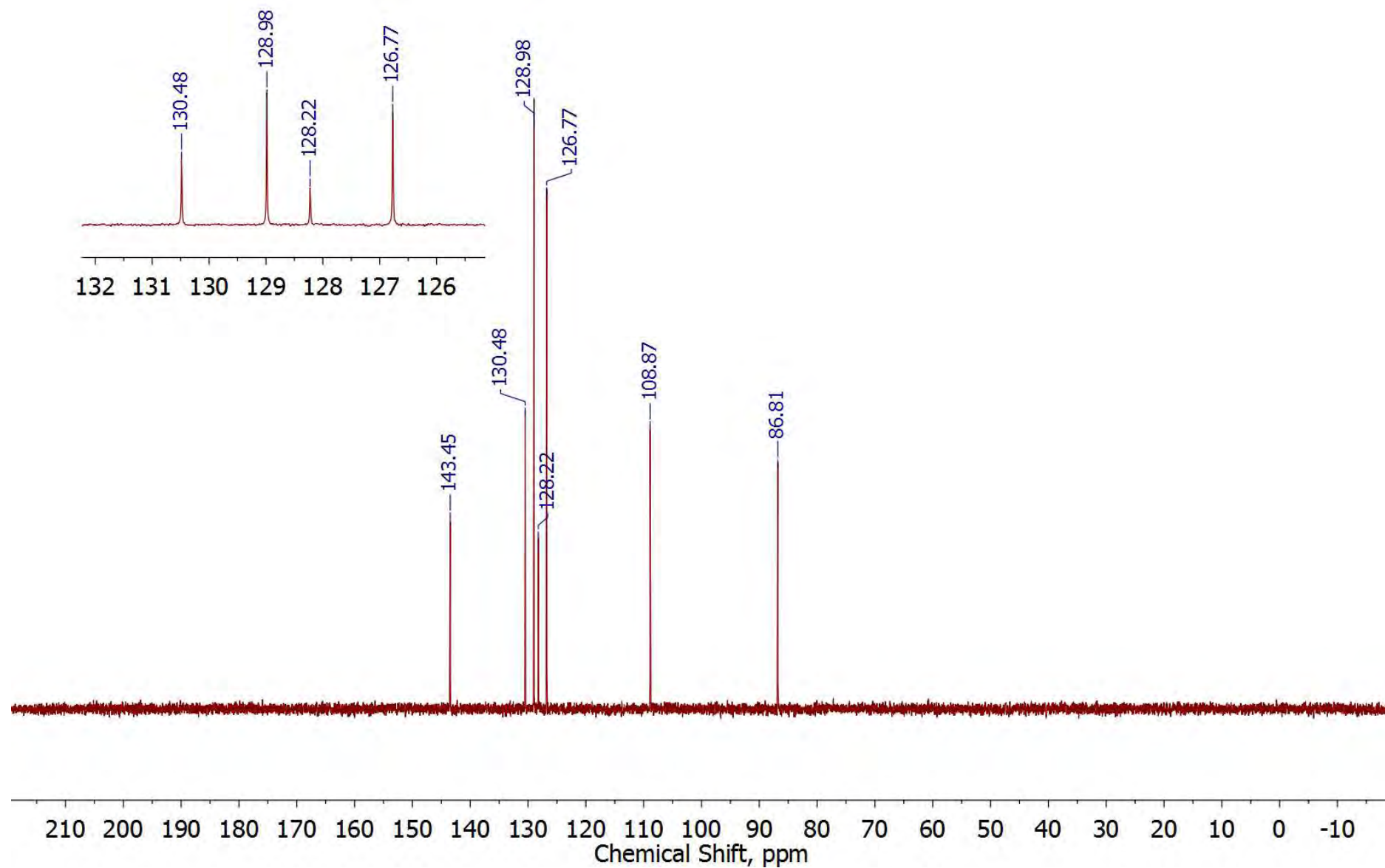
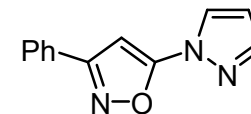
3-Phenyl-5-(1*H*-pyrazol-1-yl)isoxazole (3a), 400 (¹H) MHz, CDCl₃



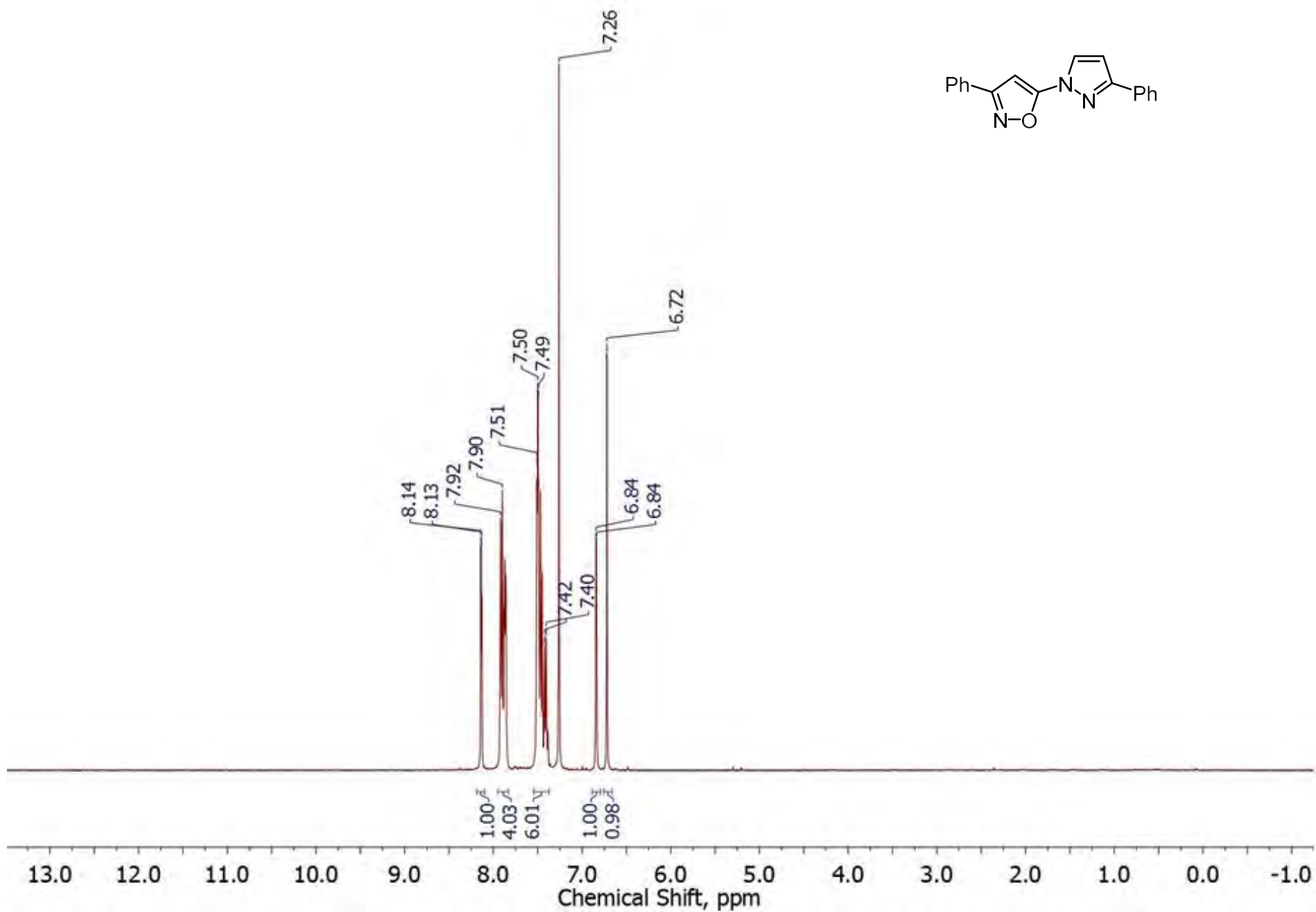
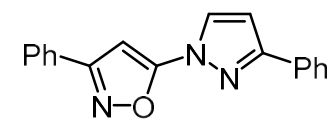
3-Phenyl-5-(1*H*-pyrazol-1-yl)isoxazole (3a), 100 (^{13}C) MHz, CDCl_3



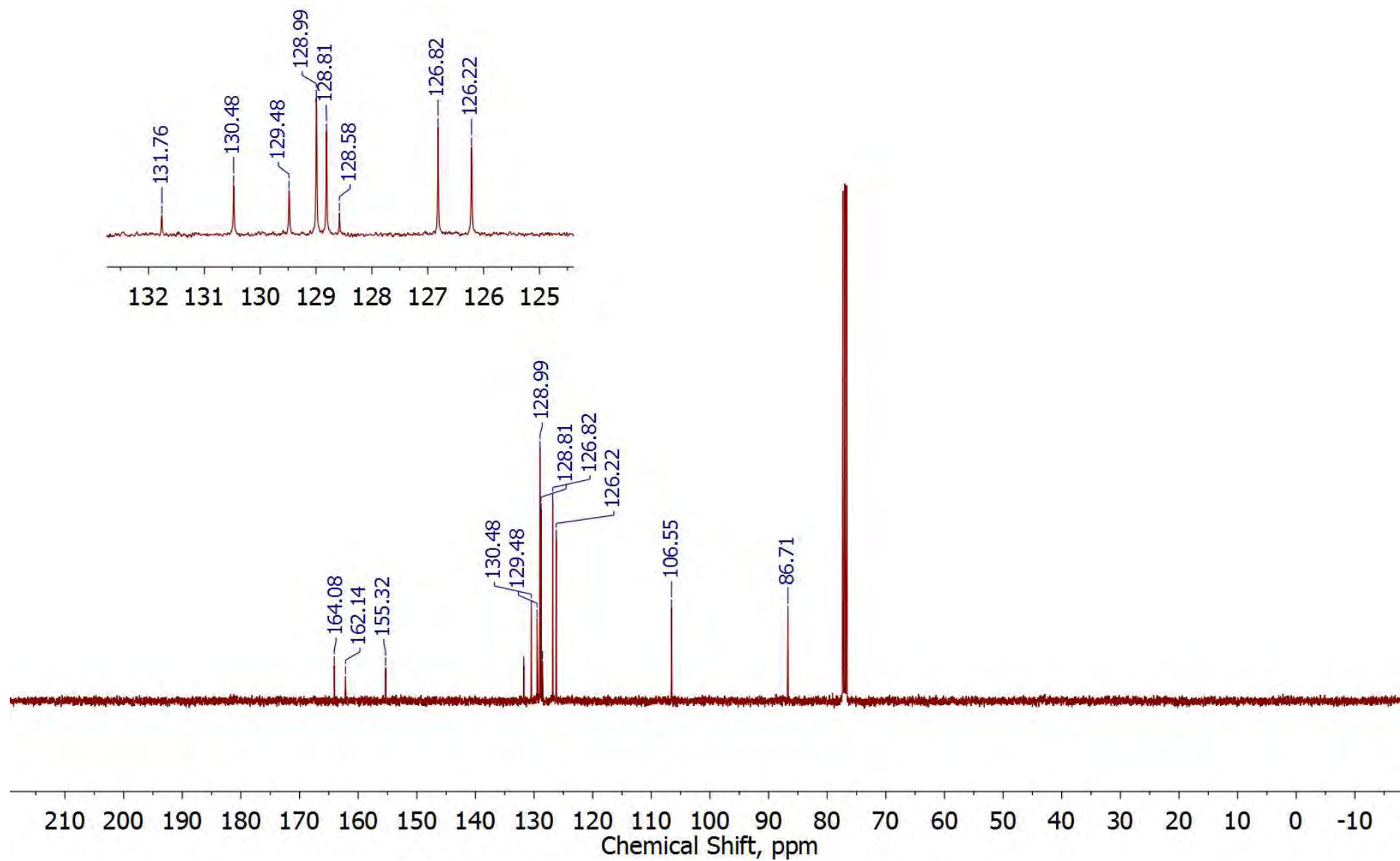
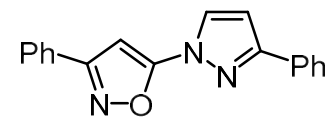
3-Phenyl-5-(1*H*-pyrazol-1-yl)isoxazole (3a), 100 (DEPT) MHz, CDCl₃



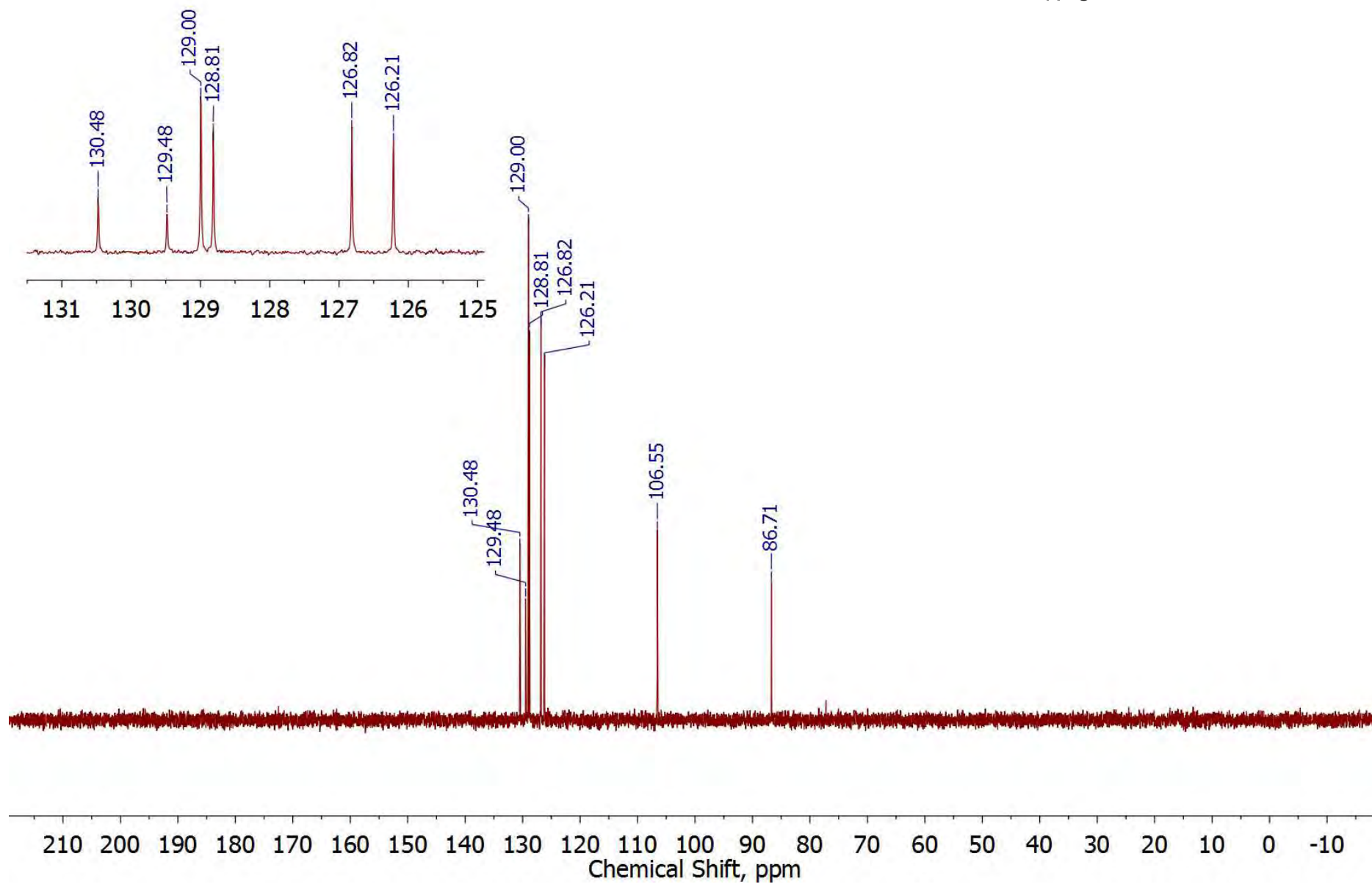
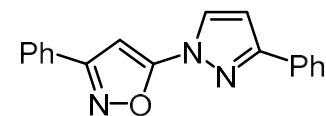
3-Phenyl-5-(3-phenyl-1*H*-pyrazol-1-yl)isoxazole (3b), 400 (¹H) MHz, CDCl₃



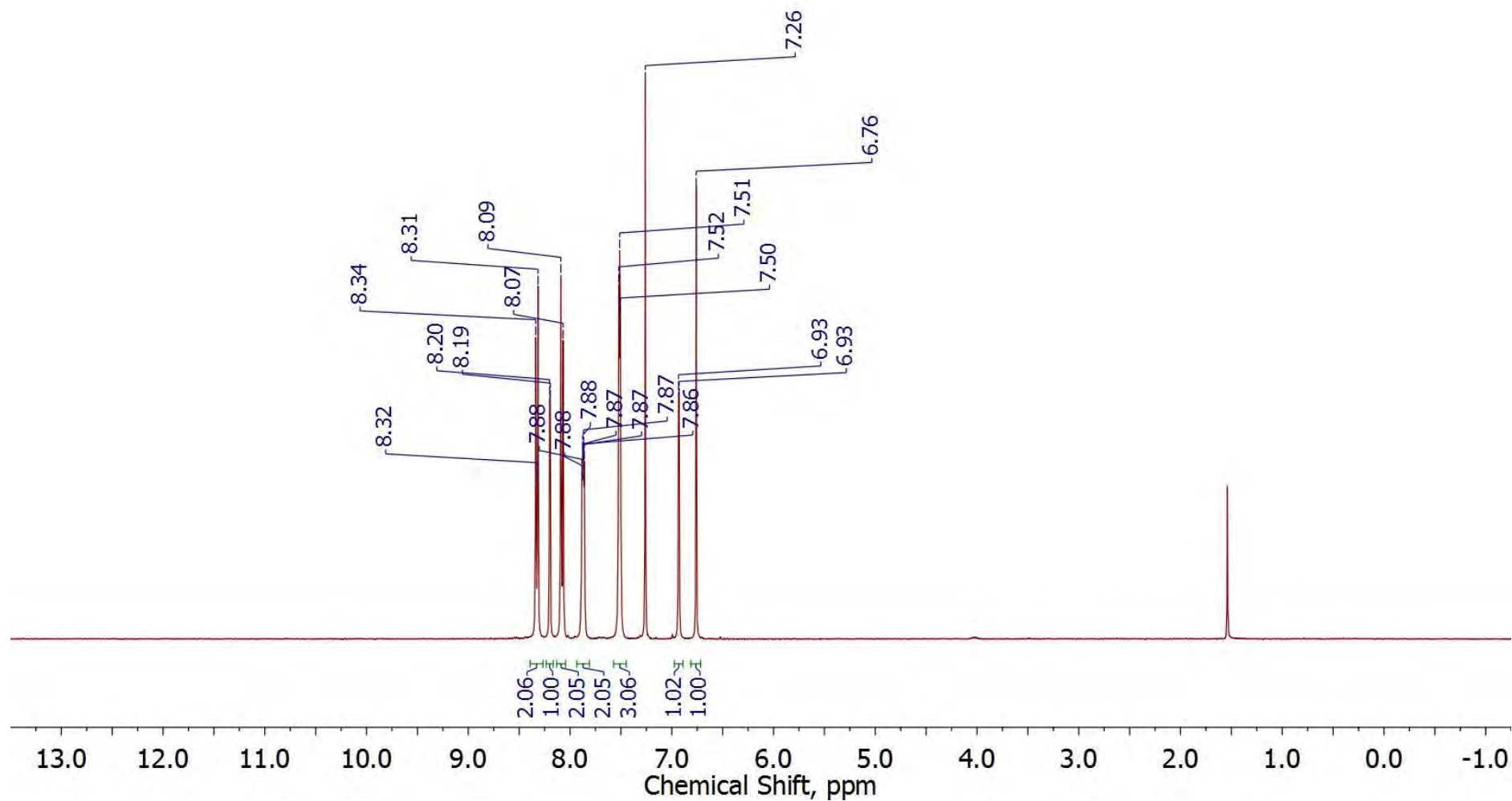
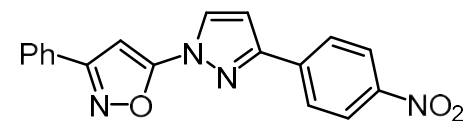
3-Phenyl-5-(3-phenyl-1*H*-pyrazol-1-yl)isoxazole (3b), 100 (^{13}C) MHz, CDCl_3



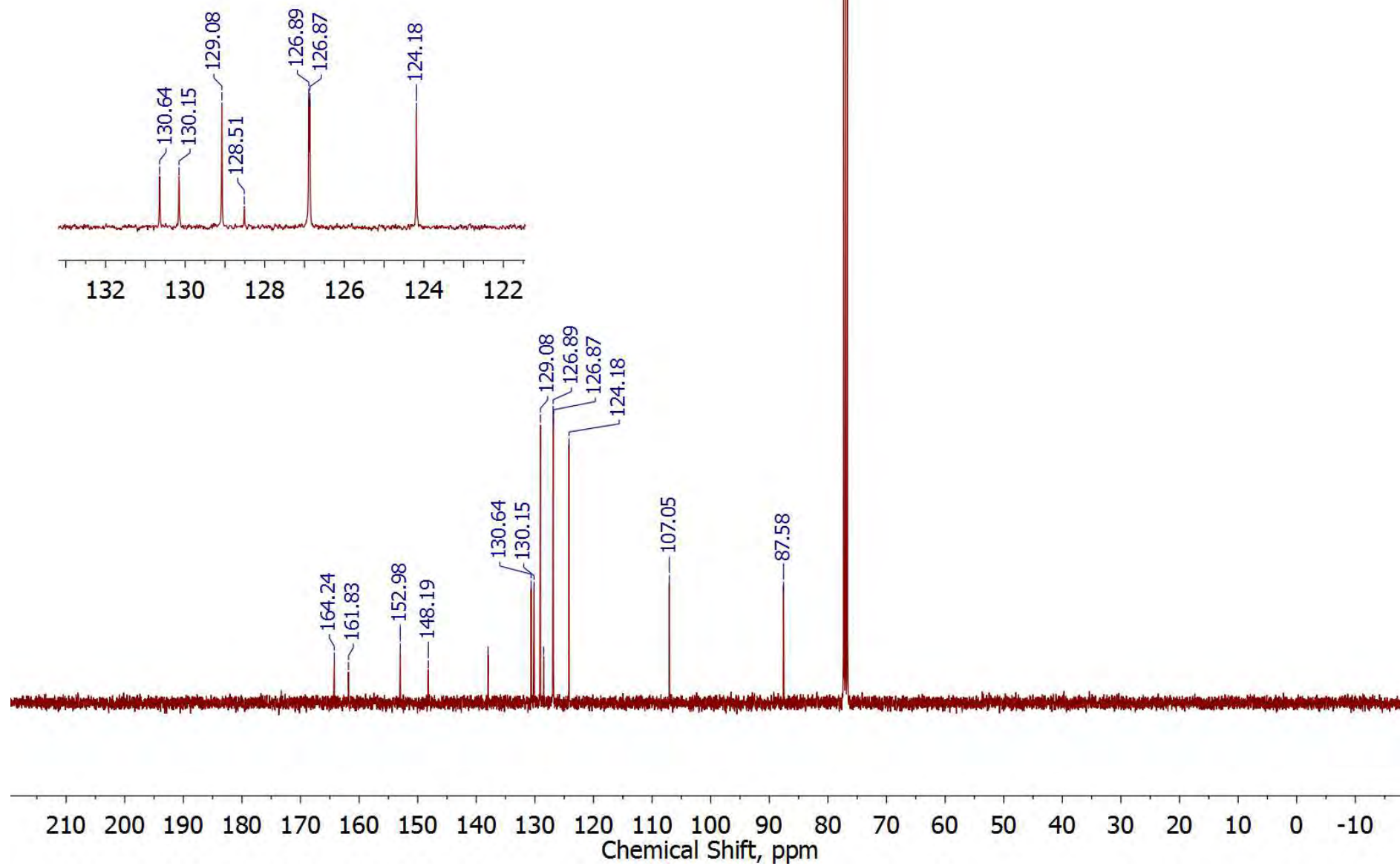
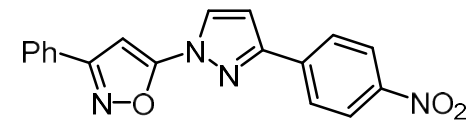
3-Phenyl-5-(3-phenyl-1*H*-pyrazol-1-yl)isoxazole (3b), 100 (DEPT) MHz, CDCl₃



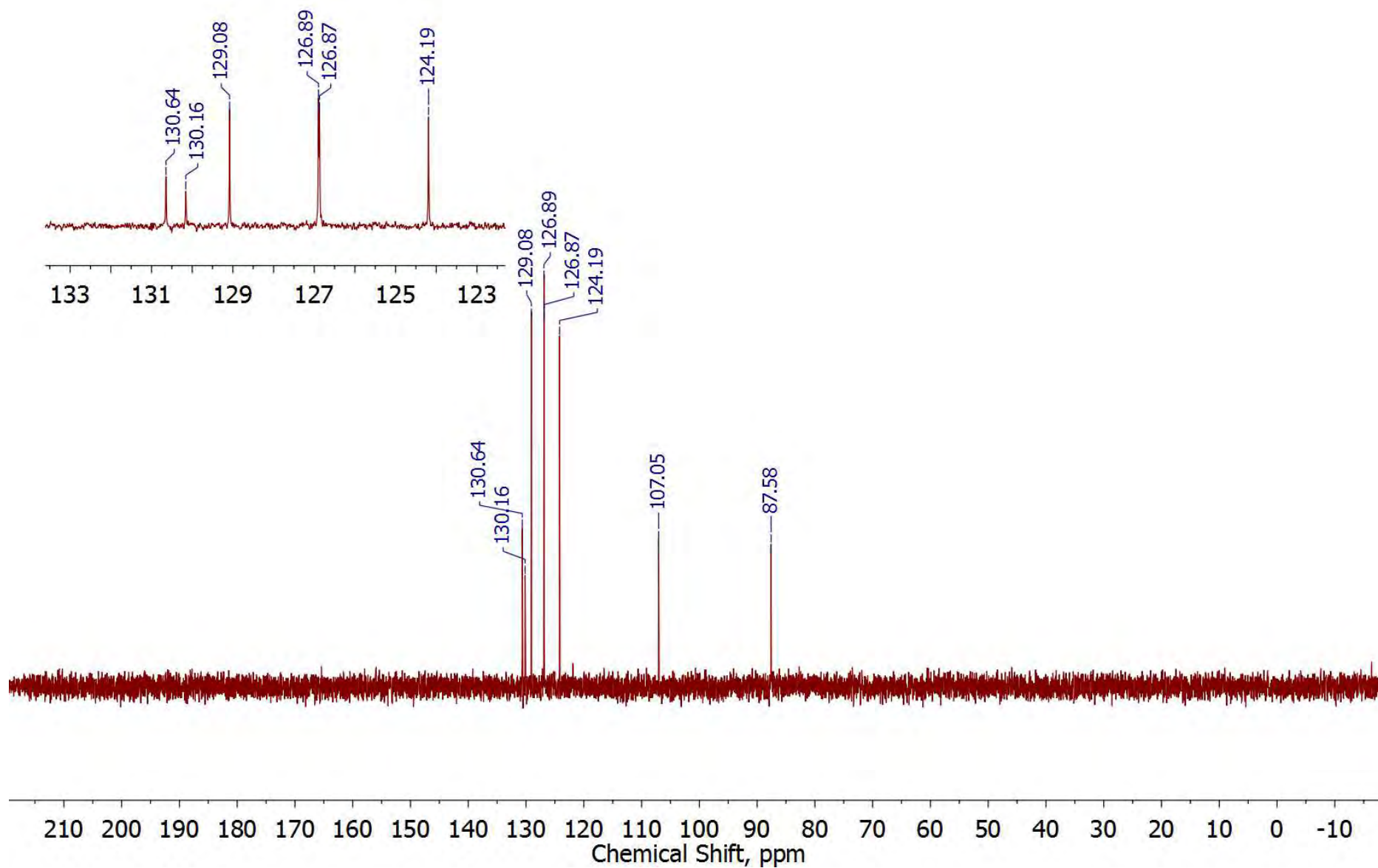
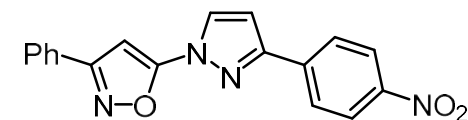
5-(3-(4-Nitrophenyl)-1*H*-pyrazol-1-yl)-3-phenyloxazole (3c), 400 (¹H) MHz, CDCl₃



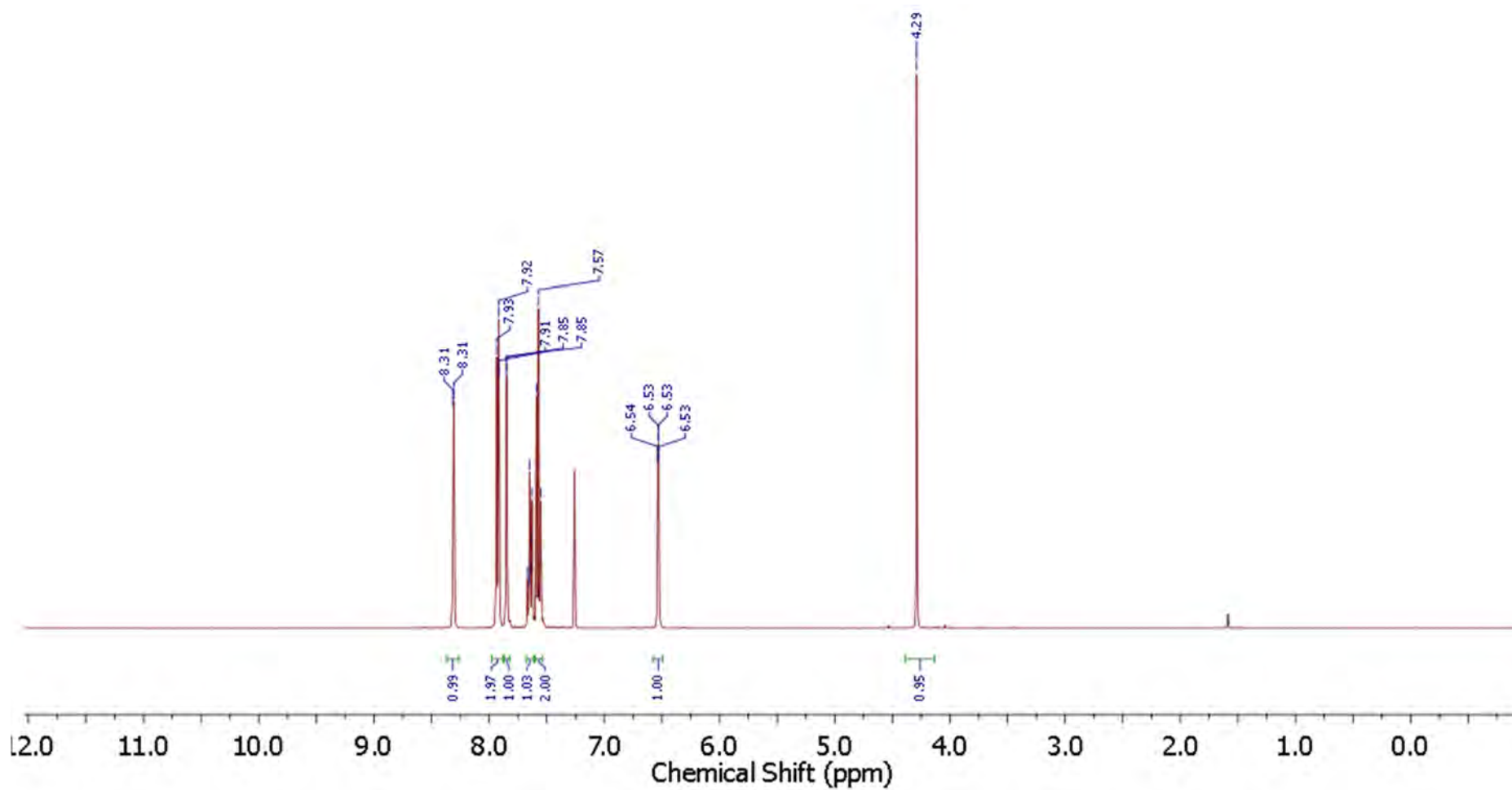
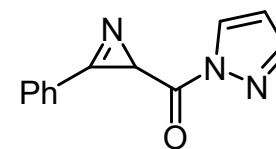
5-(3-(4-Nitrophenyl)-1*H*-pyrazol-1-yl)-3-phenyloxazole (3c), 100 (^{13}C) MHz, CDCl_3



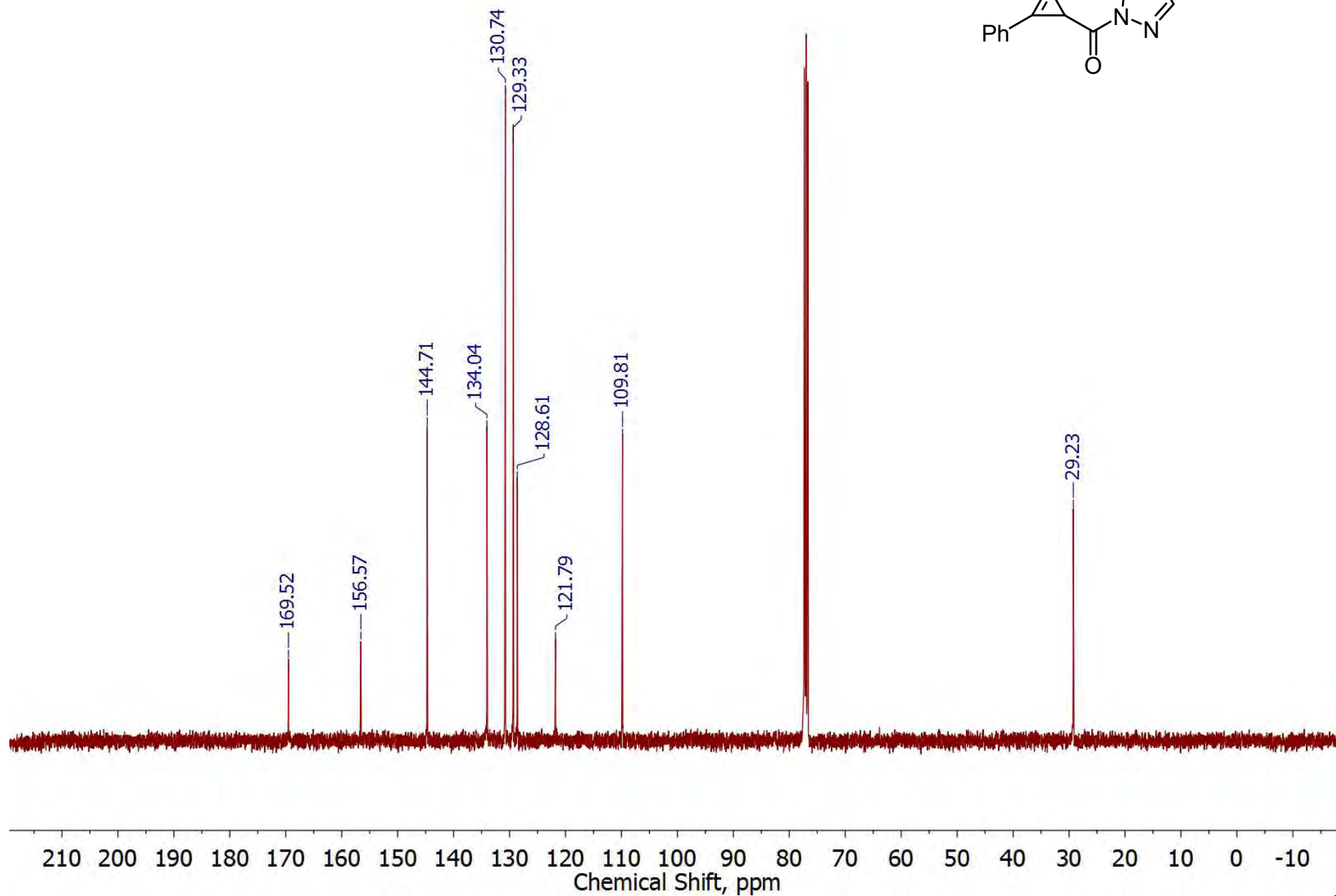
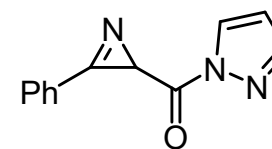
5-(3-(4-Nitrophenyl)-1*H*-pyrazol-1-yl)-3-phenyloxazole (3c), 100 (DEPT) MHz, CDCl₃



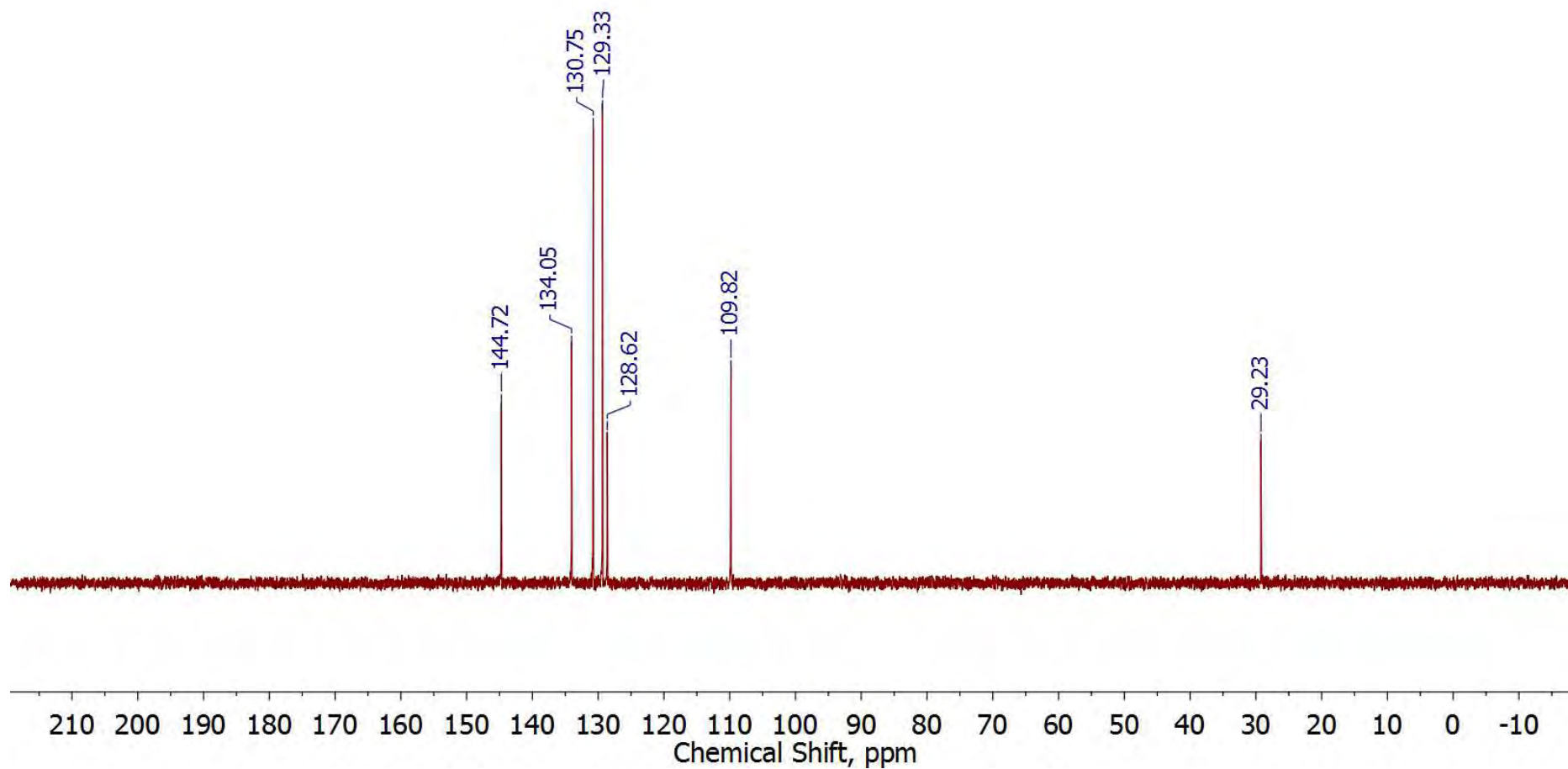
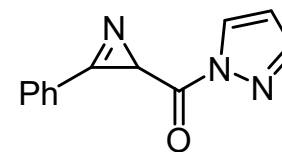
(3-Phenyl-2*H*-azirin-2-yl)(1*H*-pyrazol-1-yl)methanone (5a), 400 (¹H) MHz, CDCl₃



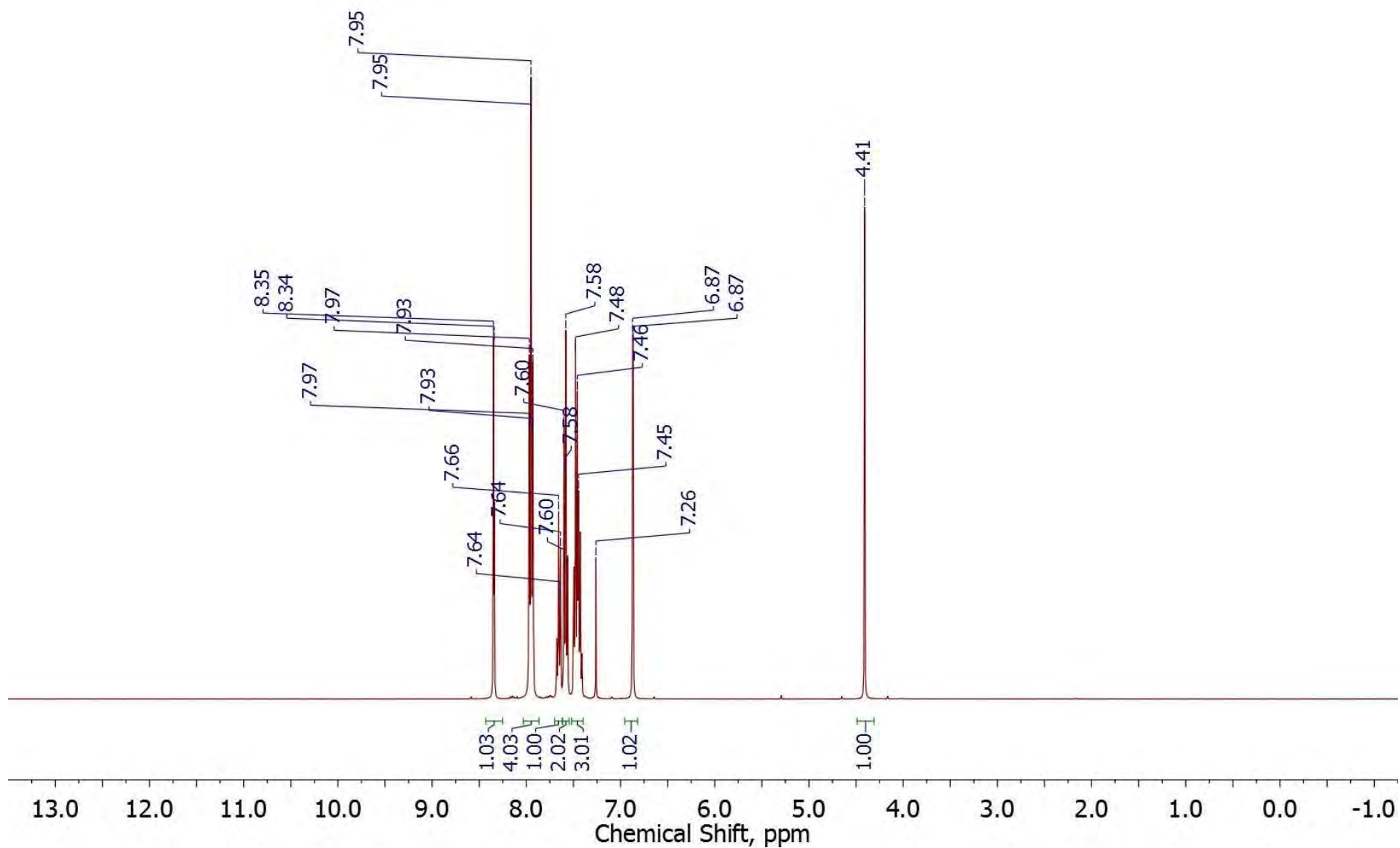
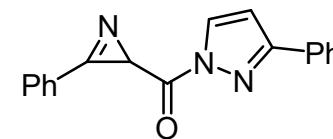
(3-Phenyl-2*H*-azirin-2-yl)(1*H*-pyrazol-1-yl)methanone (5a), 100 (¹³C) MHz, CDCl₃



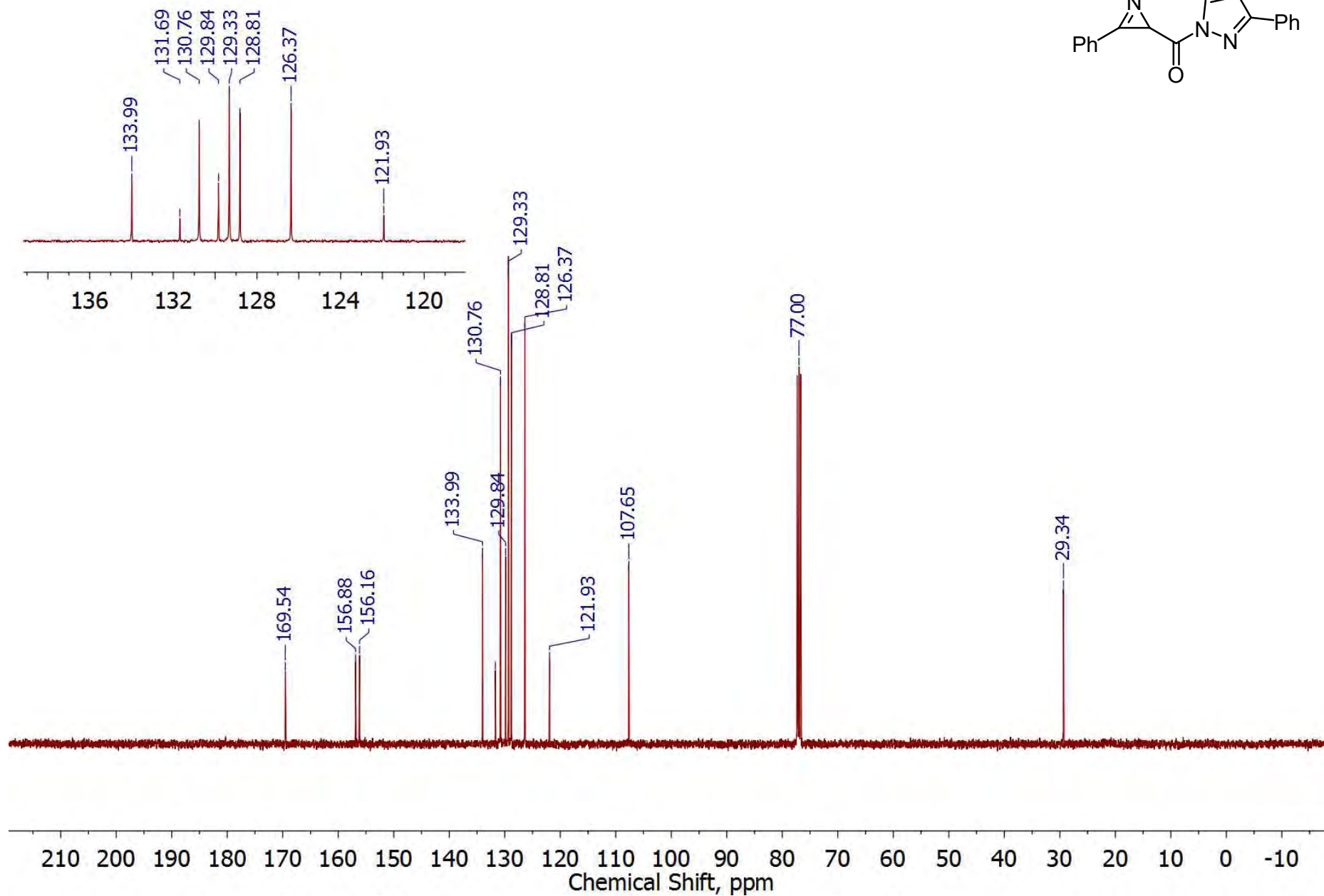
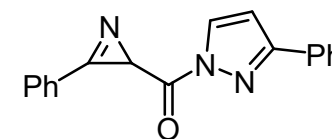
(3-Phenyl-2*H*-azirin-2-yl)(1*H*-pyrazol-1-yl)methanone (5a), 100 (DEPT) MHz, CDCl₃



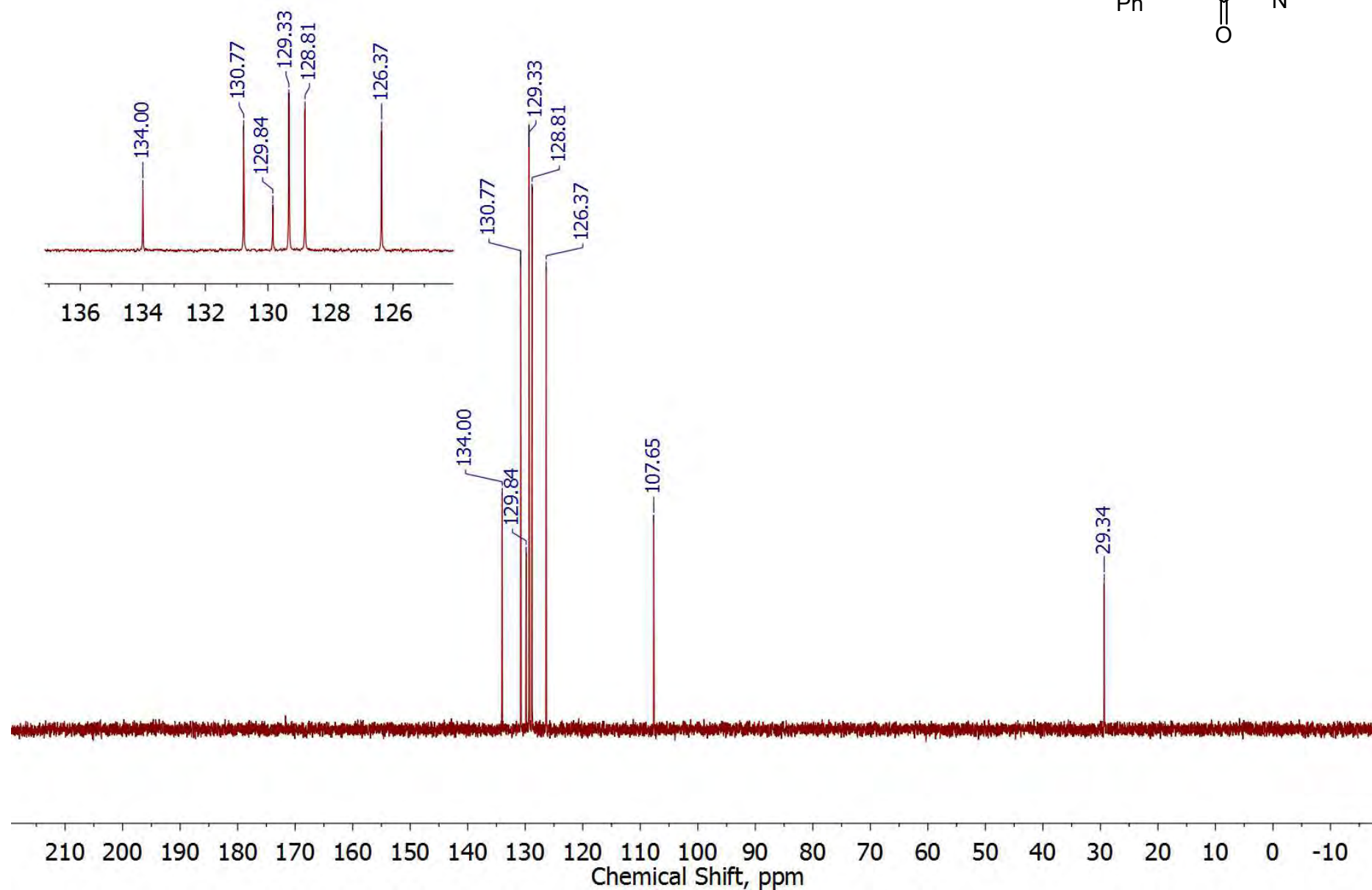
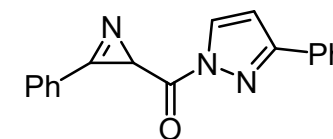
(3-Phenyl-1*H*-pyrazol-1-yl)(3-phenyl-2*H*-azirin-2-yl)methanone (5b), 400 (¹H) MHz, CDCl₃



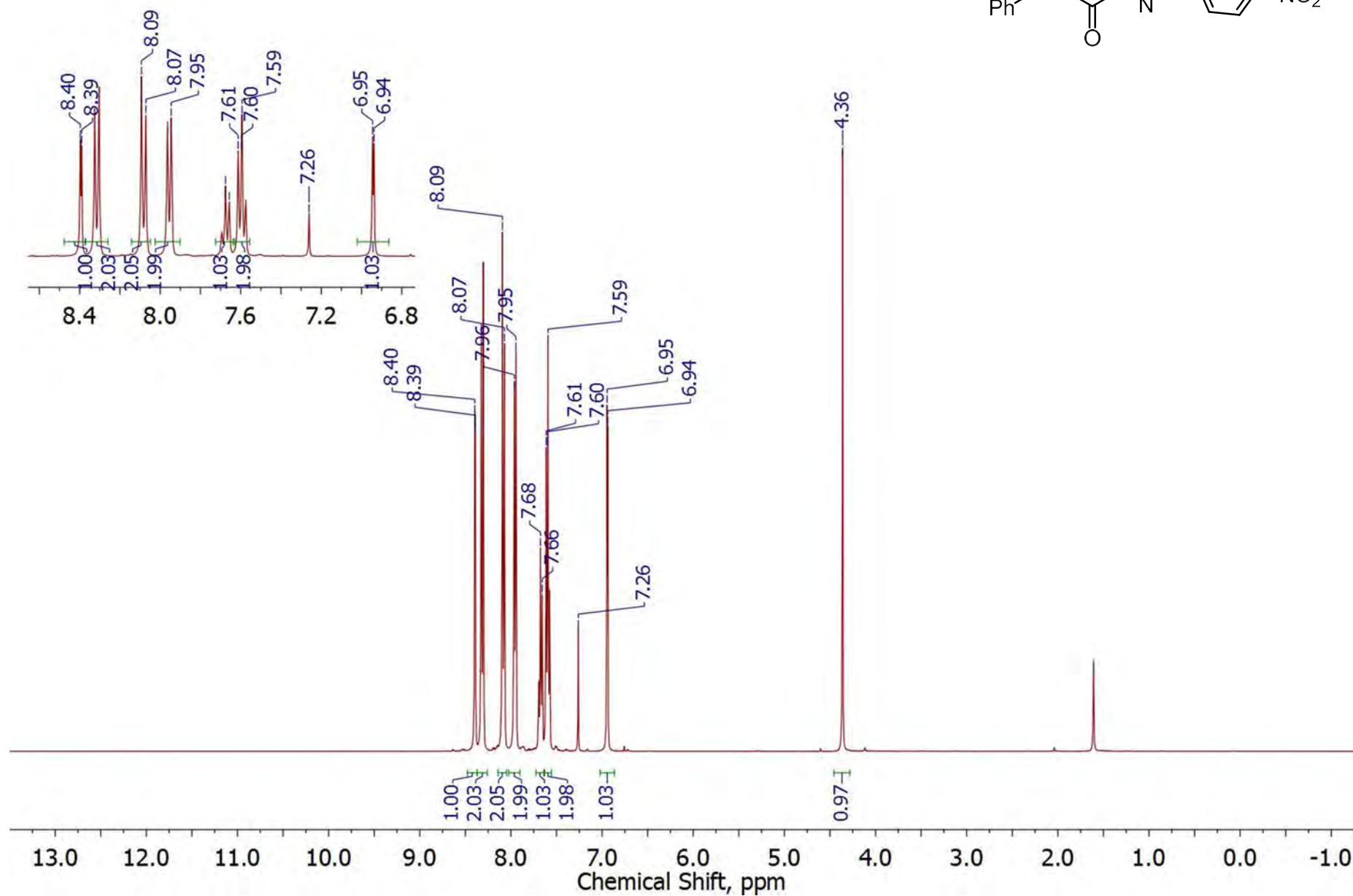
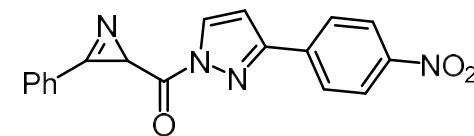
(3-Phenyl-1*H*-pyrazol-1-yl)(3-phenyl-2*H*-azirin-2-yl)methanone (5b), 100 (¹³C) MHz, CDCl₃



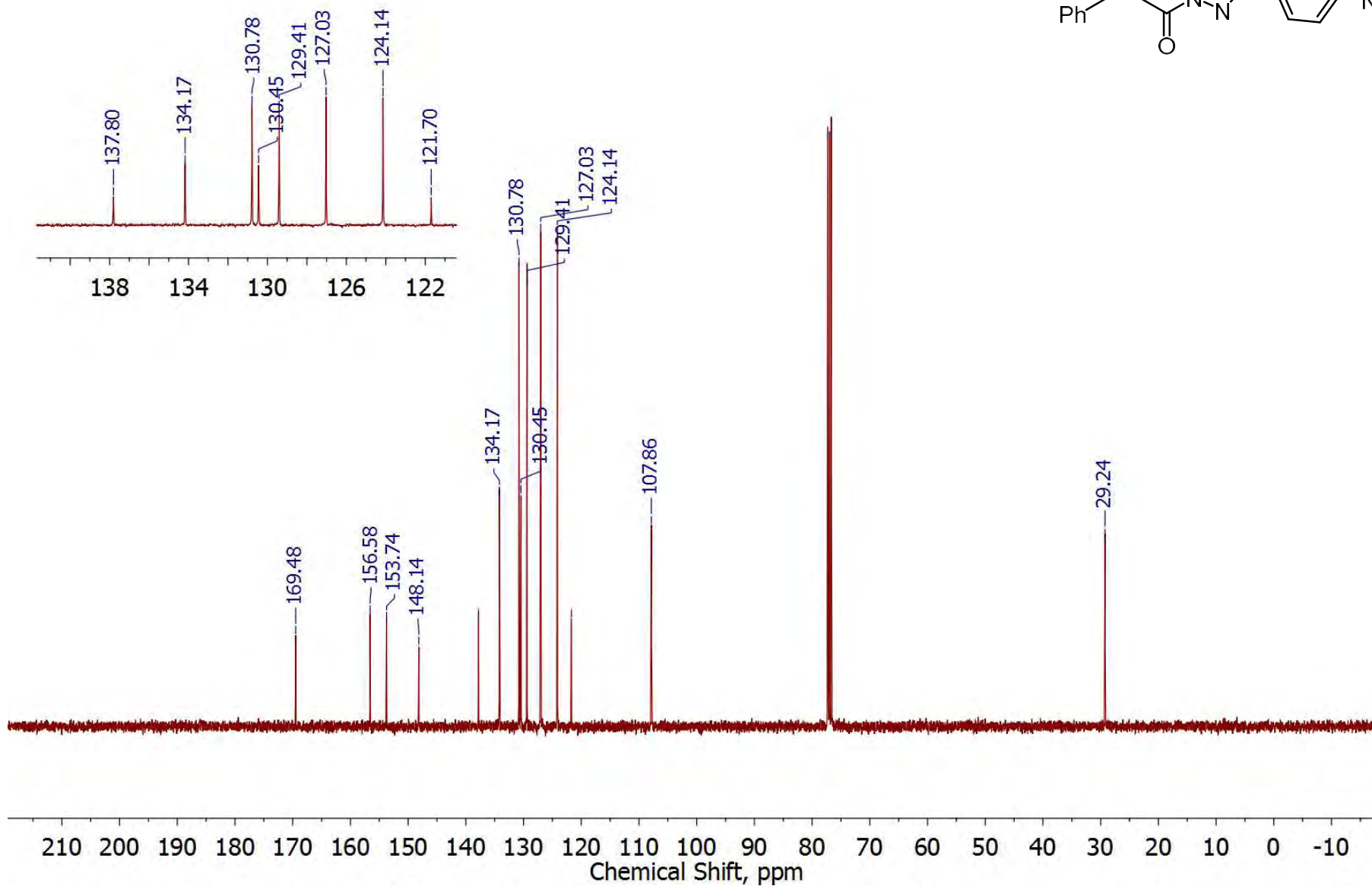
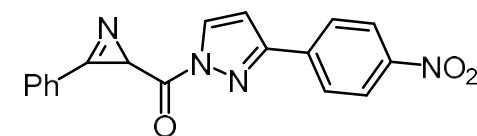
(3-Phenyl-1*H*-pyrazol-1-yl)(3-phenyl-2*H*-azirin-2-yl)methanone (5b), 100 (DEPT) MHz, CDCl₃



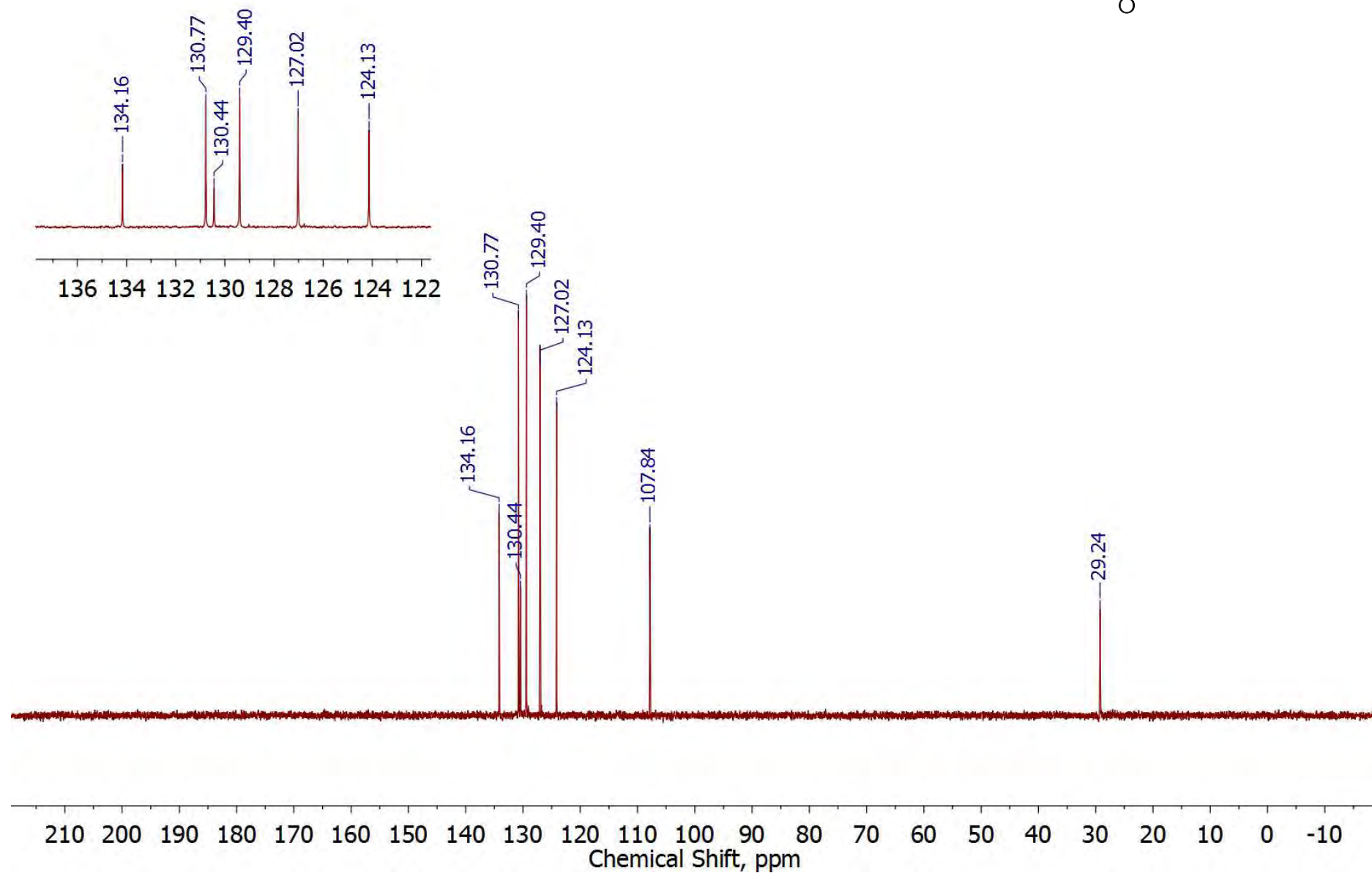
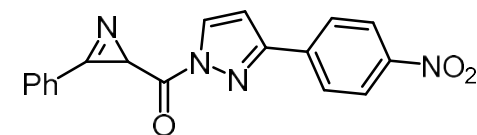
(3-(4-Nitrophenyl)-1*H*-pyrazol-1-yl)(3-phenyl-2*H*-azirin-2-yl)methanone (5c), 400 (¹H) MHz, CDCl₃



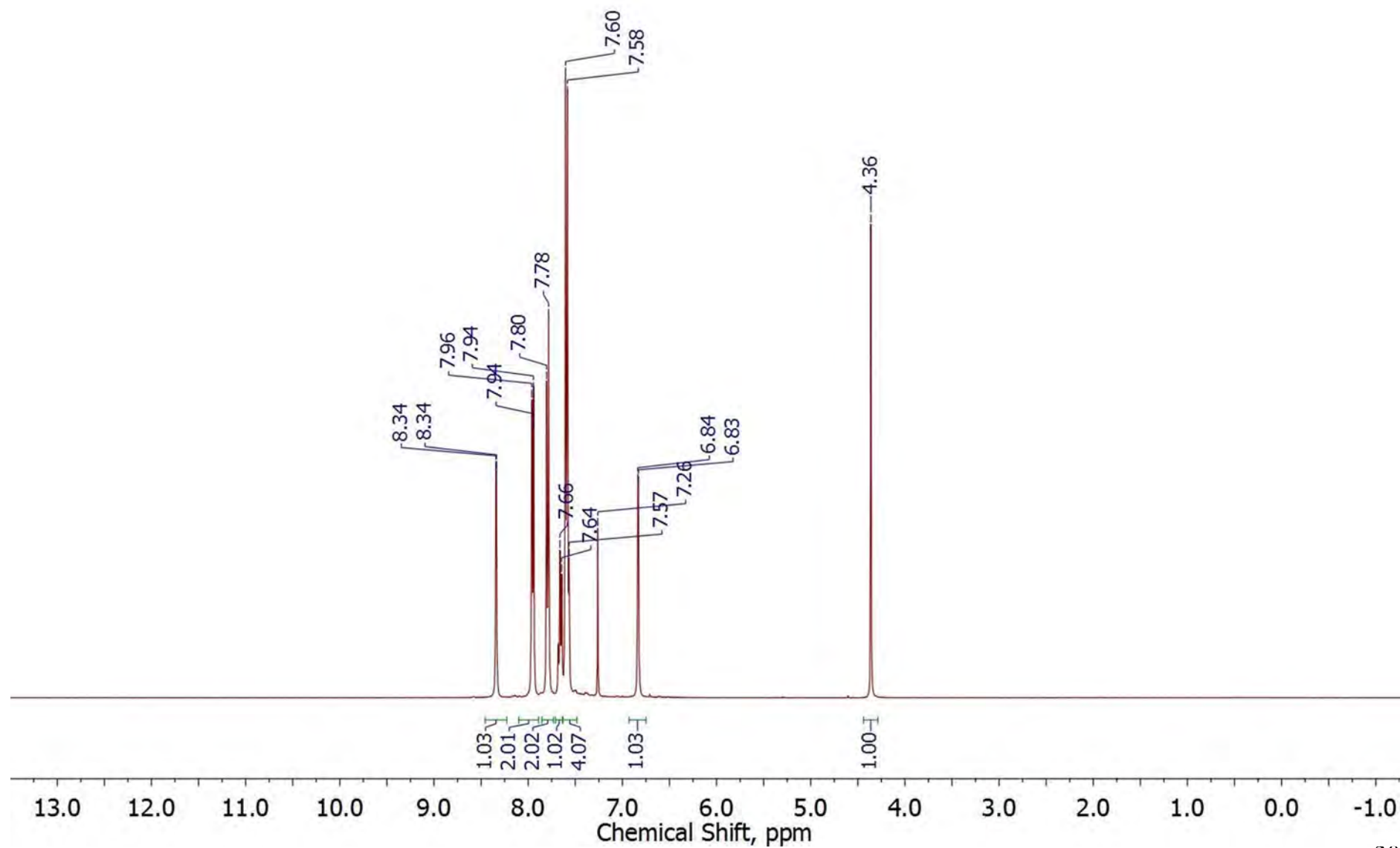
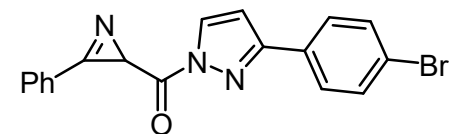
(3-(4-Nitrophenyl)-1*H*-pyrazol-1-yl)(3-phenyl-2*H*-azirin-2-yl)methanone (5c), 100 (^{13}C) MHz, CDCl_3



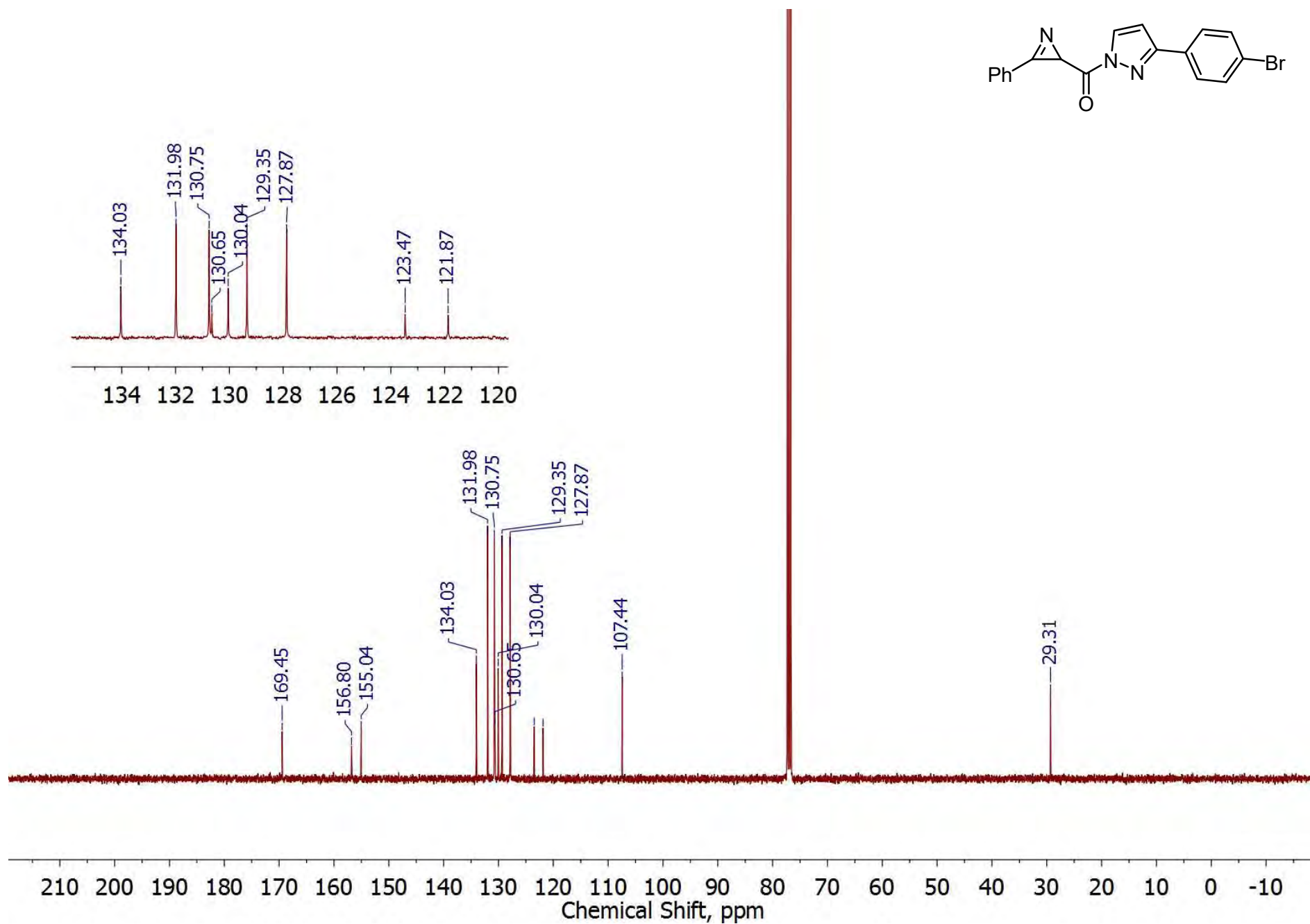
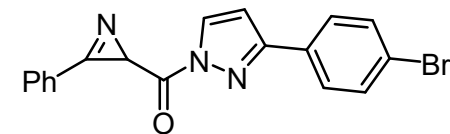
(3-(4-Nitrophenyl)-1*H*-pyrazol-1-yl)(3-phenyl-2*H*-azirin-2-yl)methanone (5c), 100 (DEPT) MHz, CDCl₃



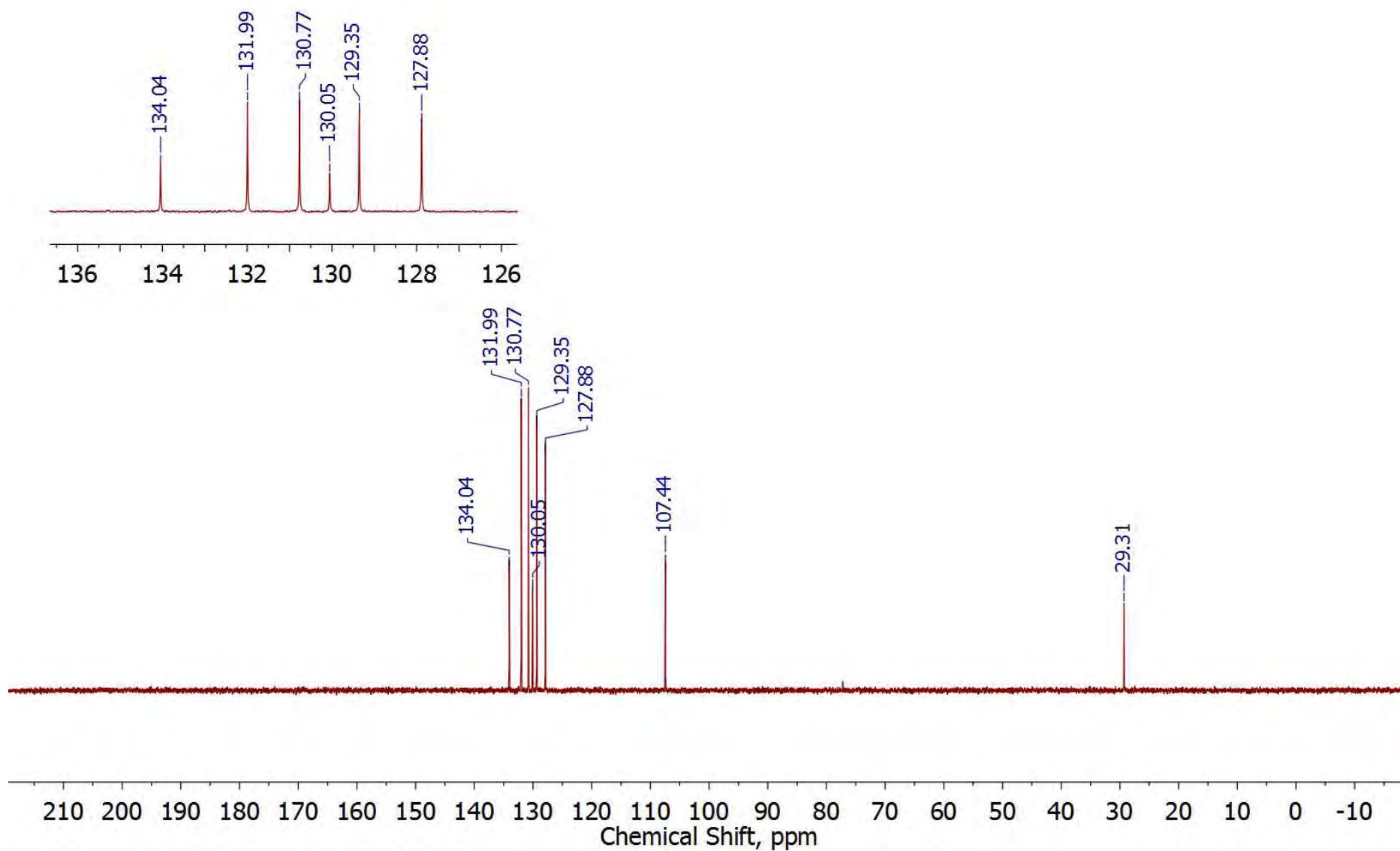
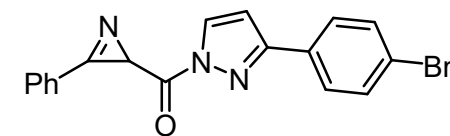
(3-(4-Bromophenyl)-1*H*-pyrazol-1-yl)(3-phenyl-2*H*-azirin-2-yl)methanone (5d), 400 (¹H) MHz, CDCl₃



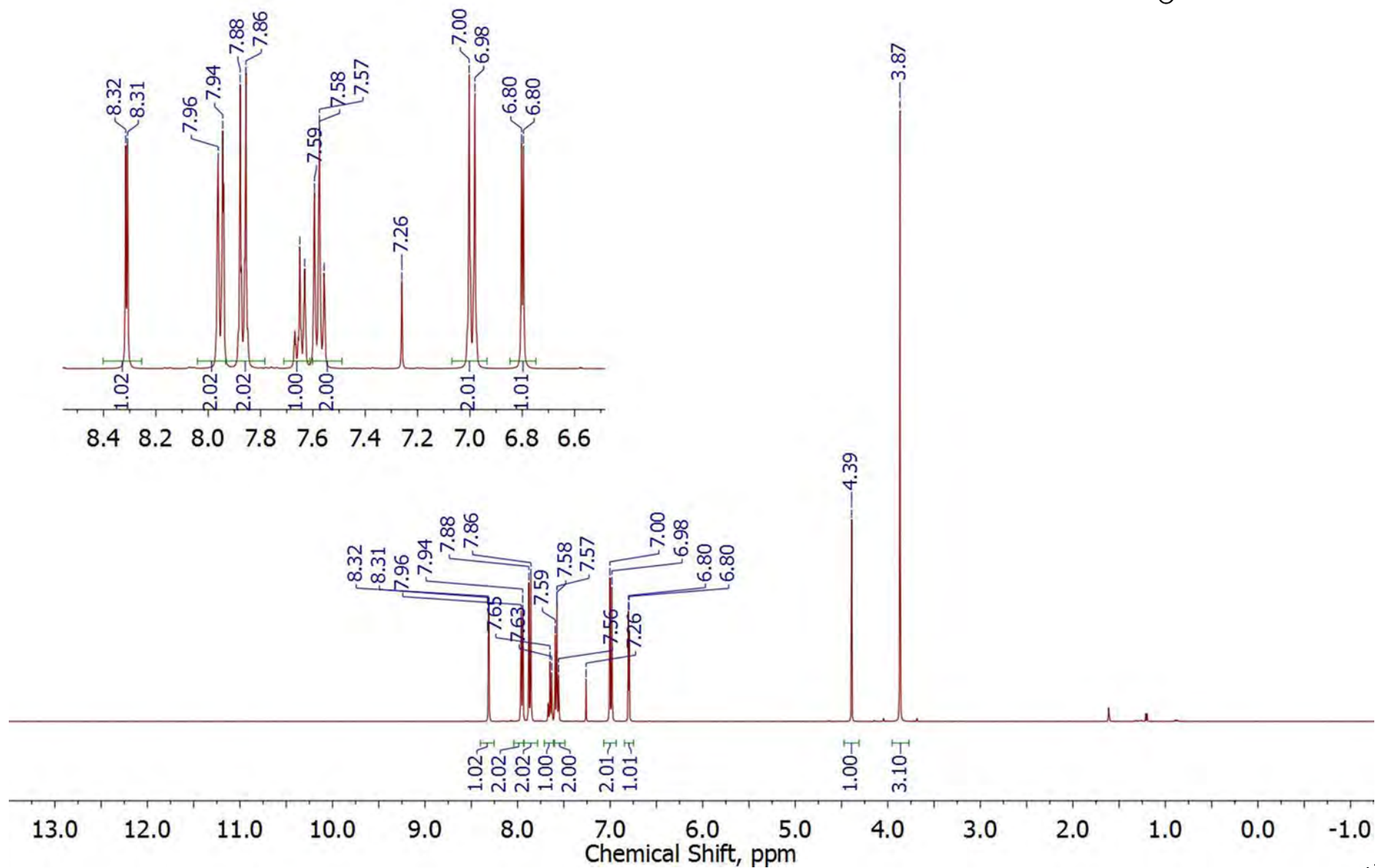
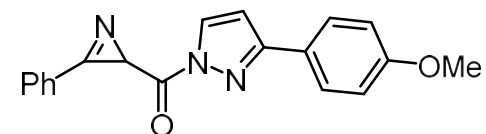
(3-(4-Bromophenyl)-1*H*-pyrazol-1-yl)(3-phenyl-2*H*-azirin-2-yl)methanone (5d), 100 (^{13}C) MHz, CDCl_3



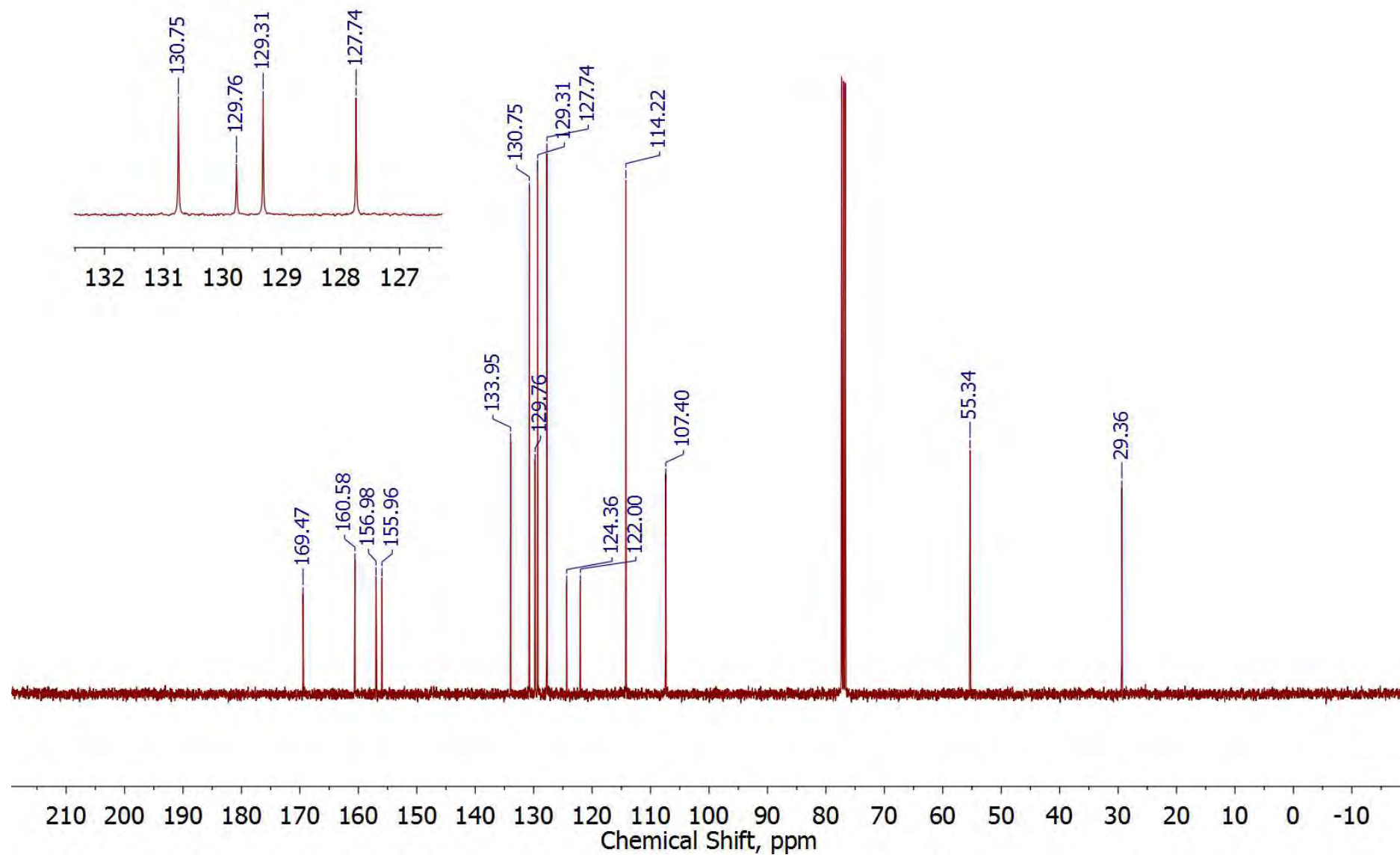
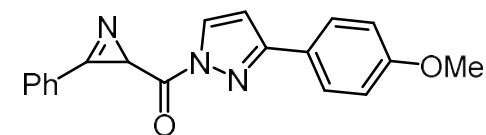
(3-(4-Bromophenyl)-1*H*-pyrazol-1-yl)(3-phenyl-2*H*-azirin-2-yl)methanone (5d), 100 (DEPT) MHz, CDCl₃



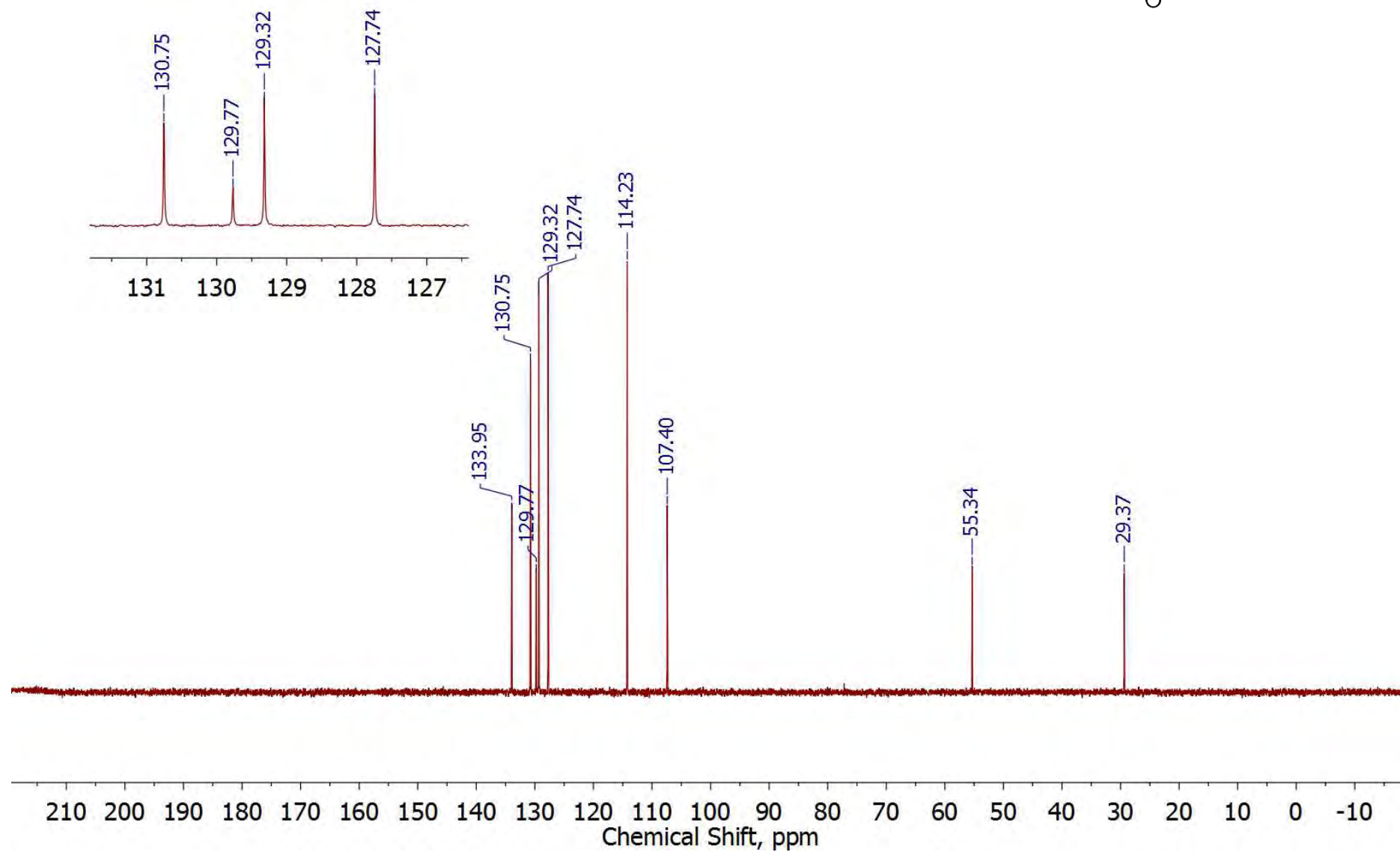
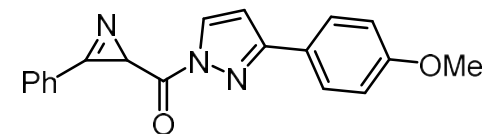
(3-(4-Methoxyphenyl)-1*H*-pyrazol-1-yl)(3-phenyl-2*H*-azirin-2-yl)methanone (5e), 400 (¹H) MHz, CDCl₃



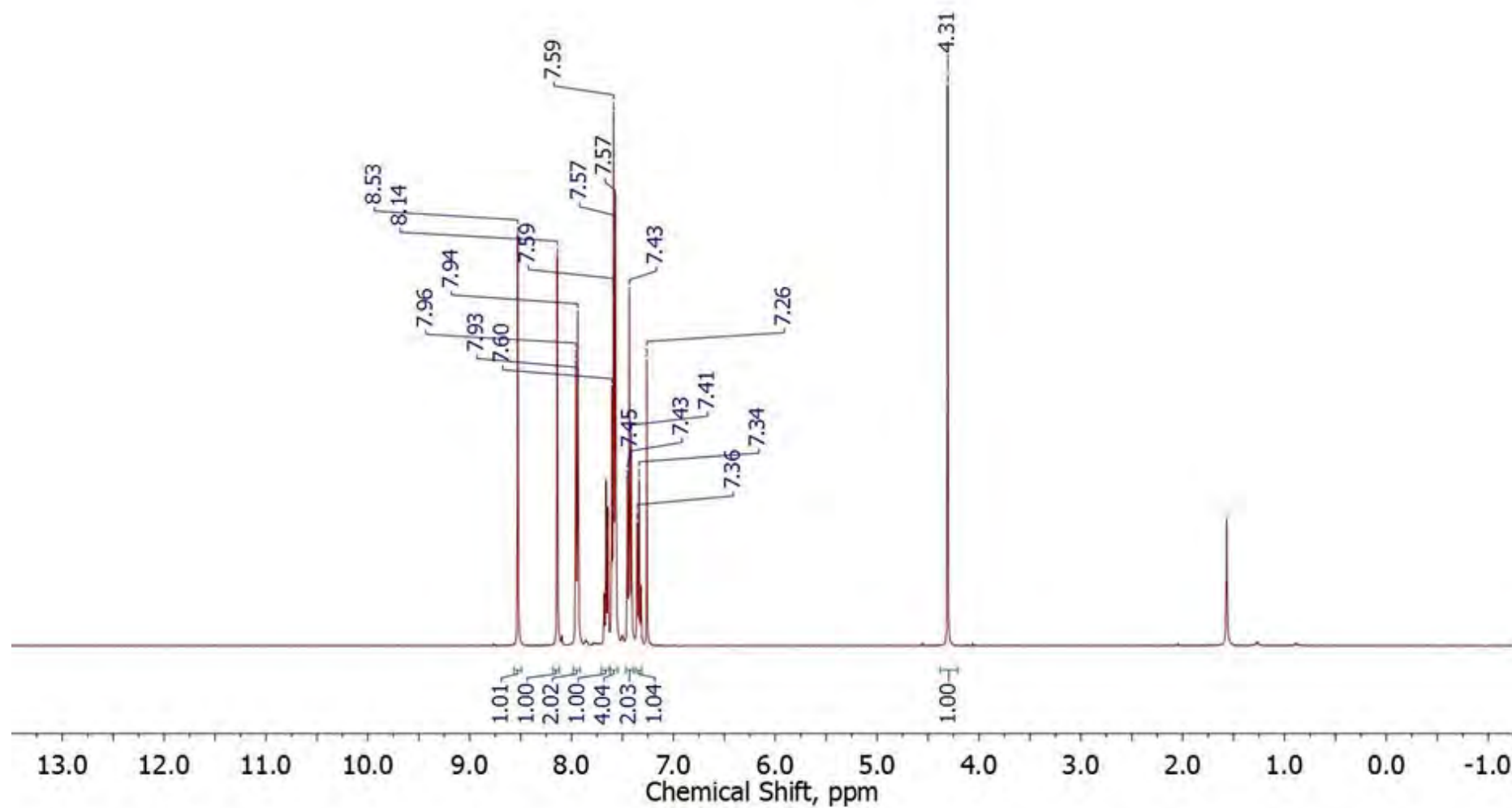
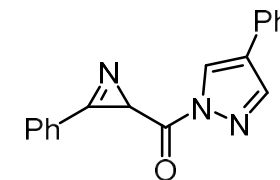
(3-(4-Methoxyphenyl)-1*H*-pyrazol-1-yl)(3-phenyl-2*H*-azirin-2-yl)methanone (5e), 100 (¹³C) MHz, CDCl₃



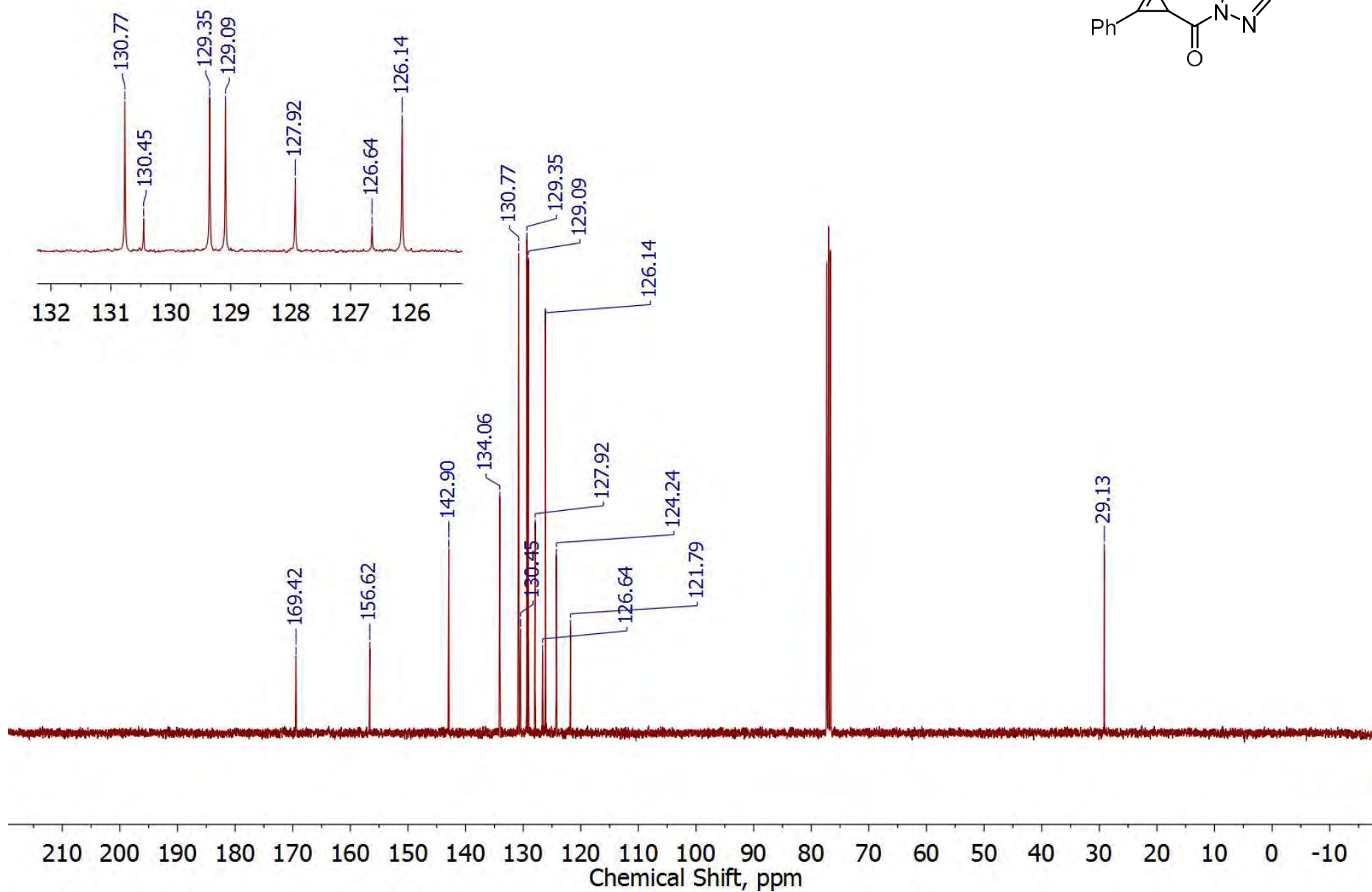
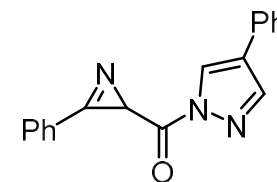
(3-(4-Methoxyphenyl)-1*H*-pyrazol-1-yl)(3-phenyl-2*H*-azirin-2-yl)methanone (5e), 100 (DEPT) MHz, CDCl₃



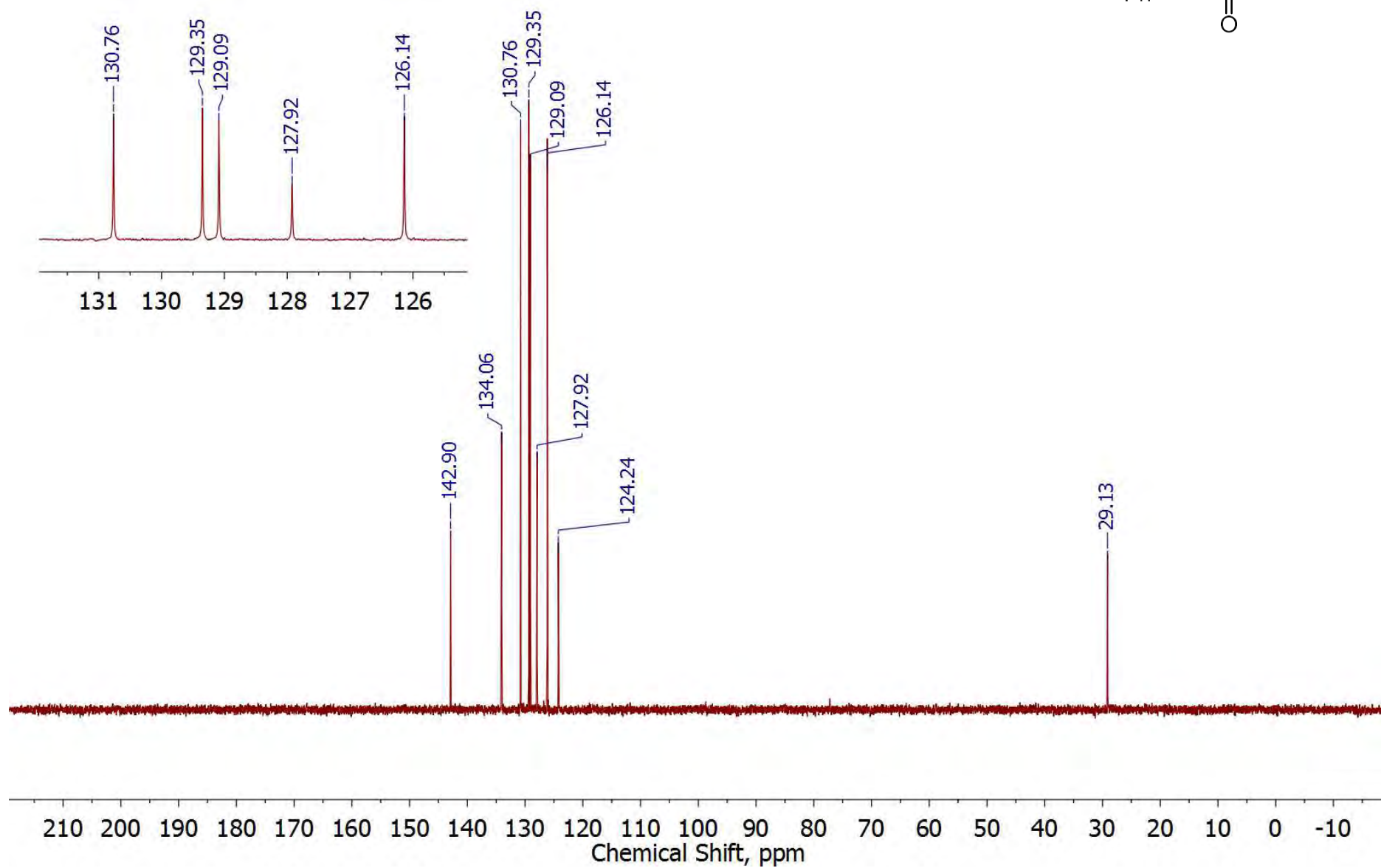
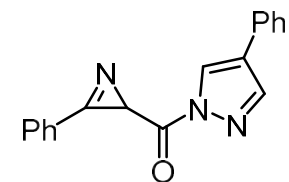
(4-Phenyl-1*H*-pyrazol-1-yl)(3-phenyl-2*H*-azirin-2-yl)methanone (5f), 400 (¹H) MHz, CDCl₃



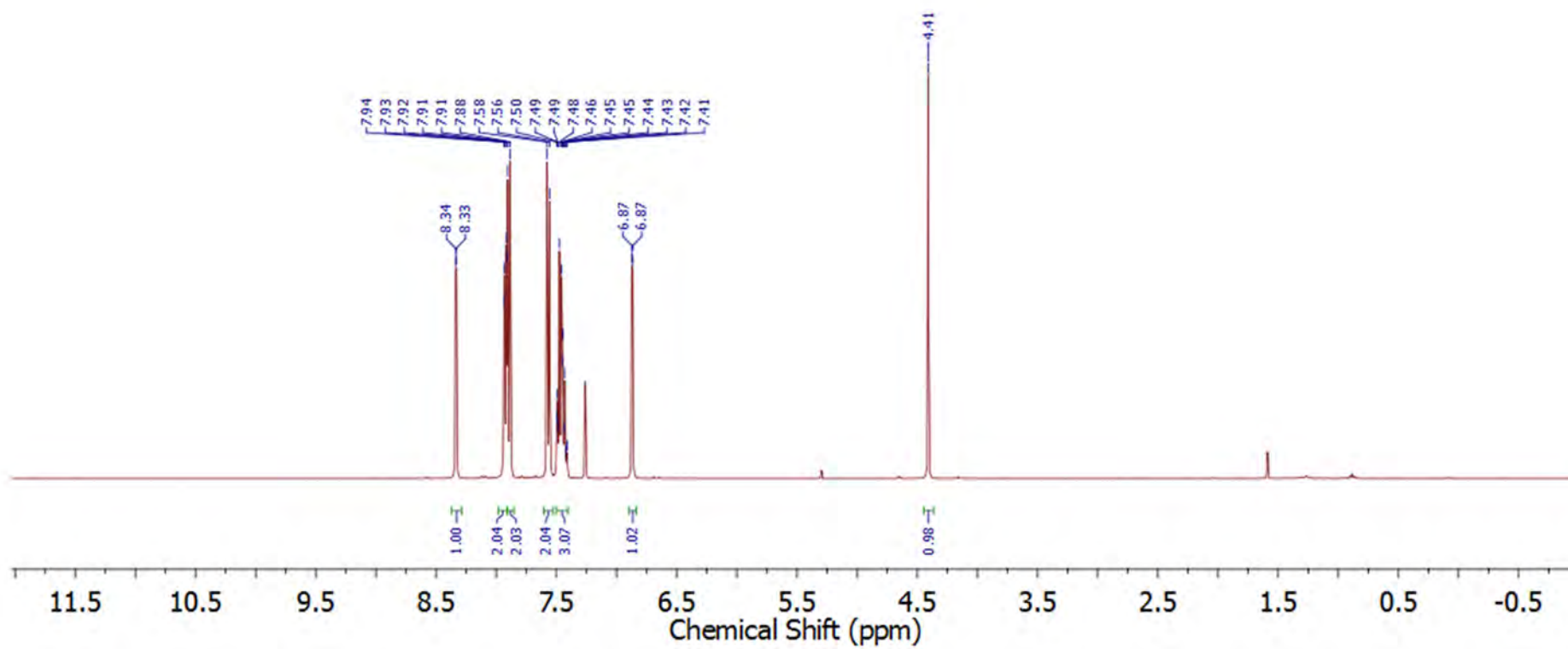
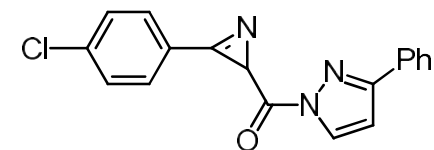
(4-Phenyl-1*H*-pyrazol-1-yl)(3-phenyl-2*H*-azirin-2-yl)methanone (5f), 100 (^{13}C) MHz, CDCl_3



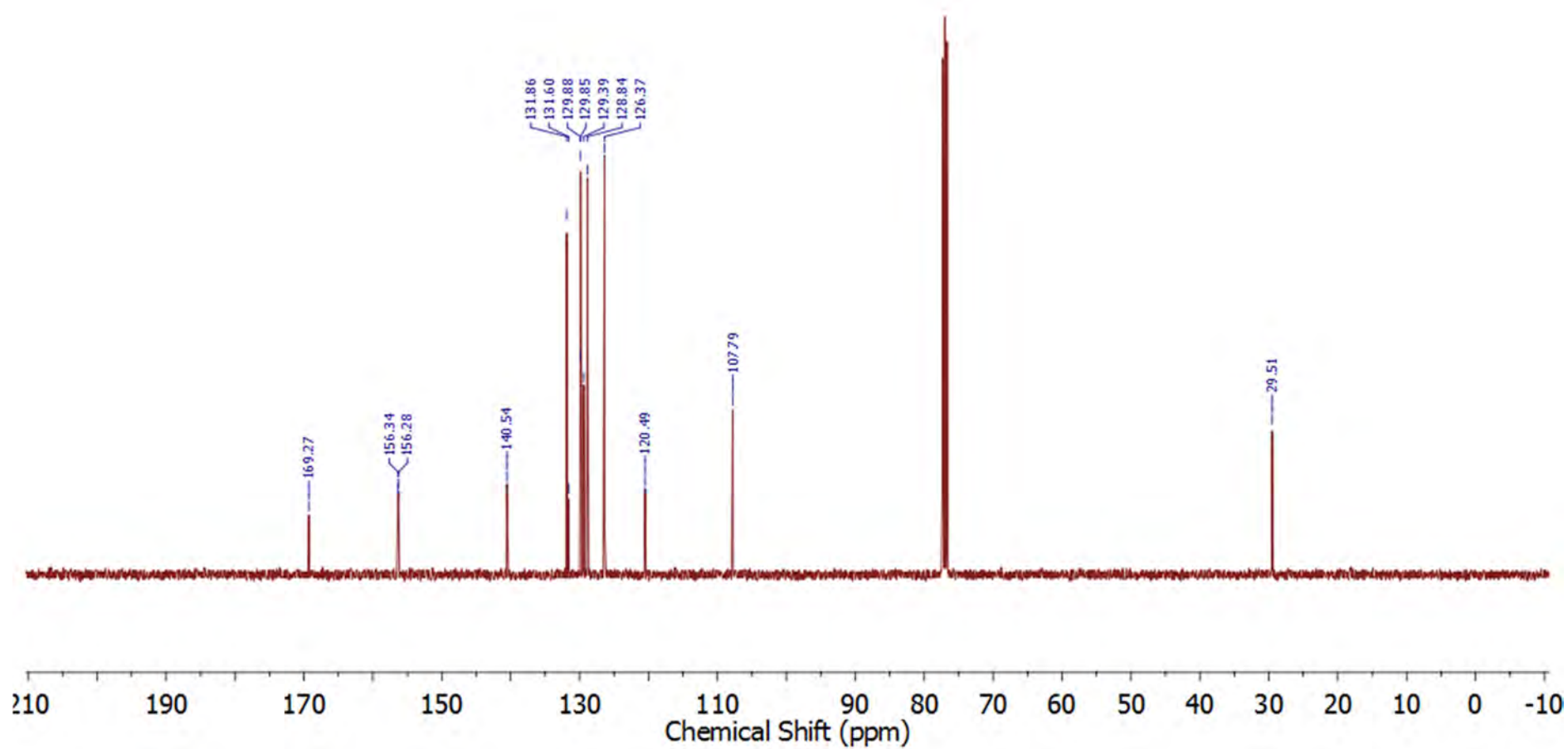
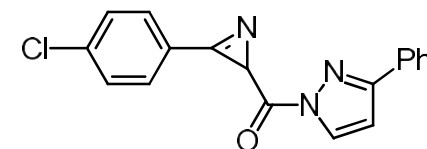
(4-Phenyl-1*H*-pyrazol-1-yl)(3-phenyl-2*H*-azirin-2-yl)methanone (5f), 100 (DEPT) MHz, CDCl₃



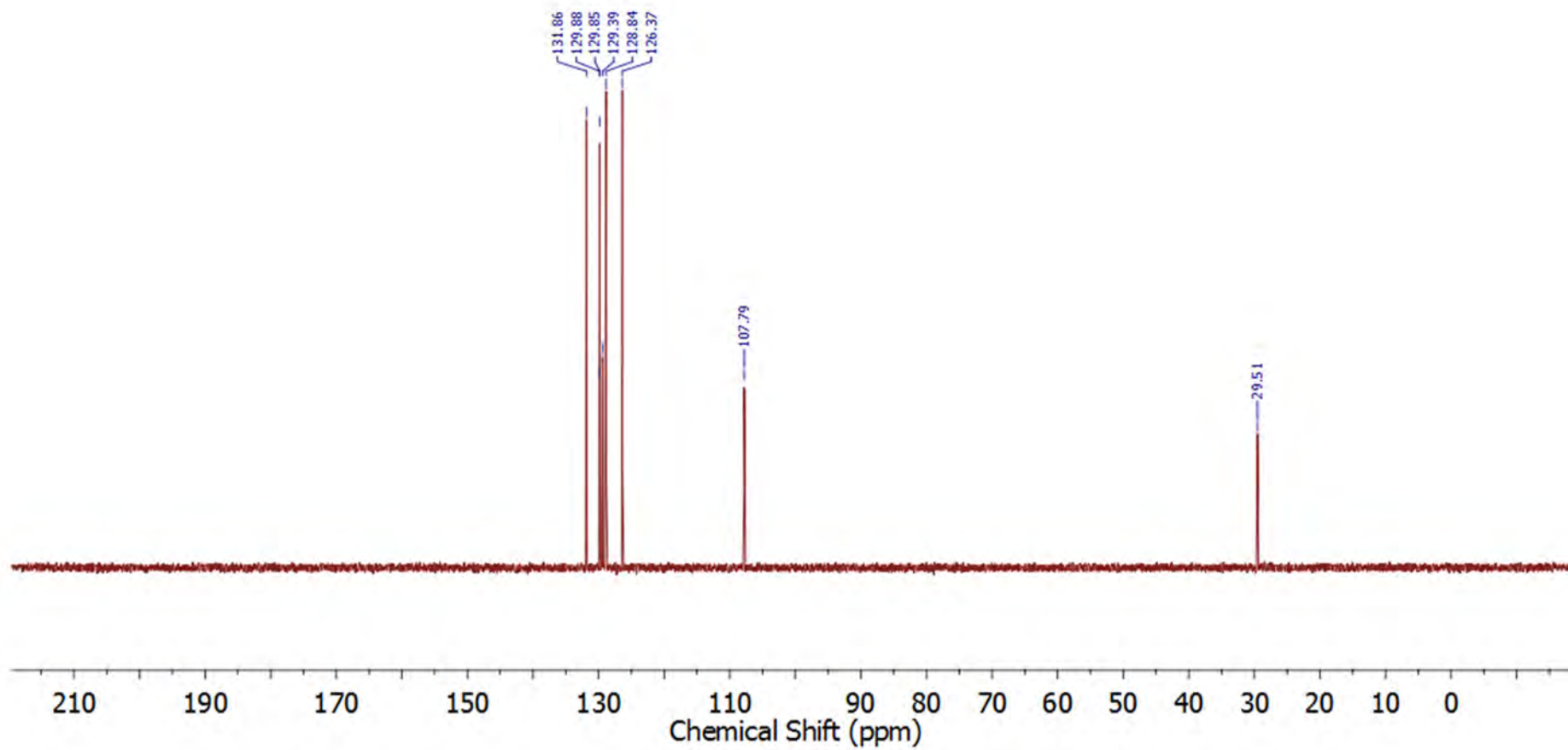
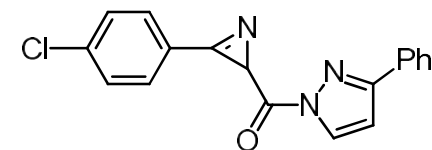
(3-(4-Chlorophenyl)-2*H*-azirin-2-yl)(3-phenyl-1*H*-pyrazol-1-yl)methanone (5g), 400 (¹H) MHz, CDCl₃



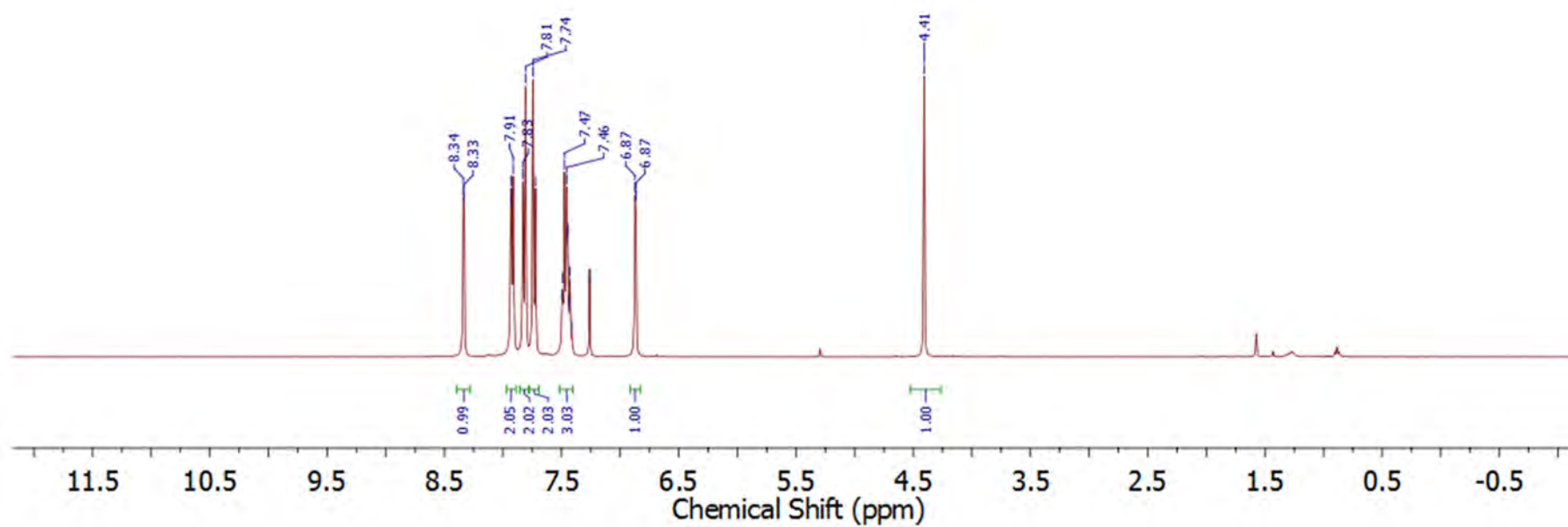
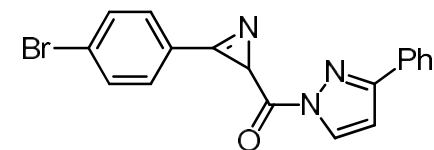
(3-(4-Chlorophenyl)-2*H*-azirin-2-yl)(3-phenyl-1*H*-pyrazol-1-yl)methanone (5g), 100 (^{13}C) MHz, CDCl_3



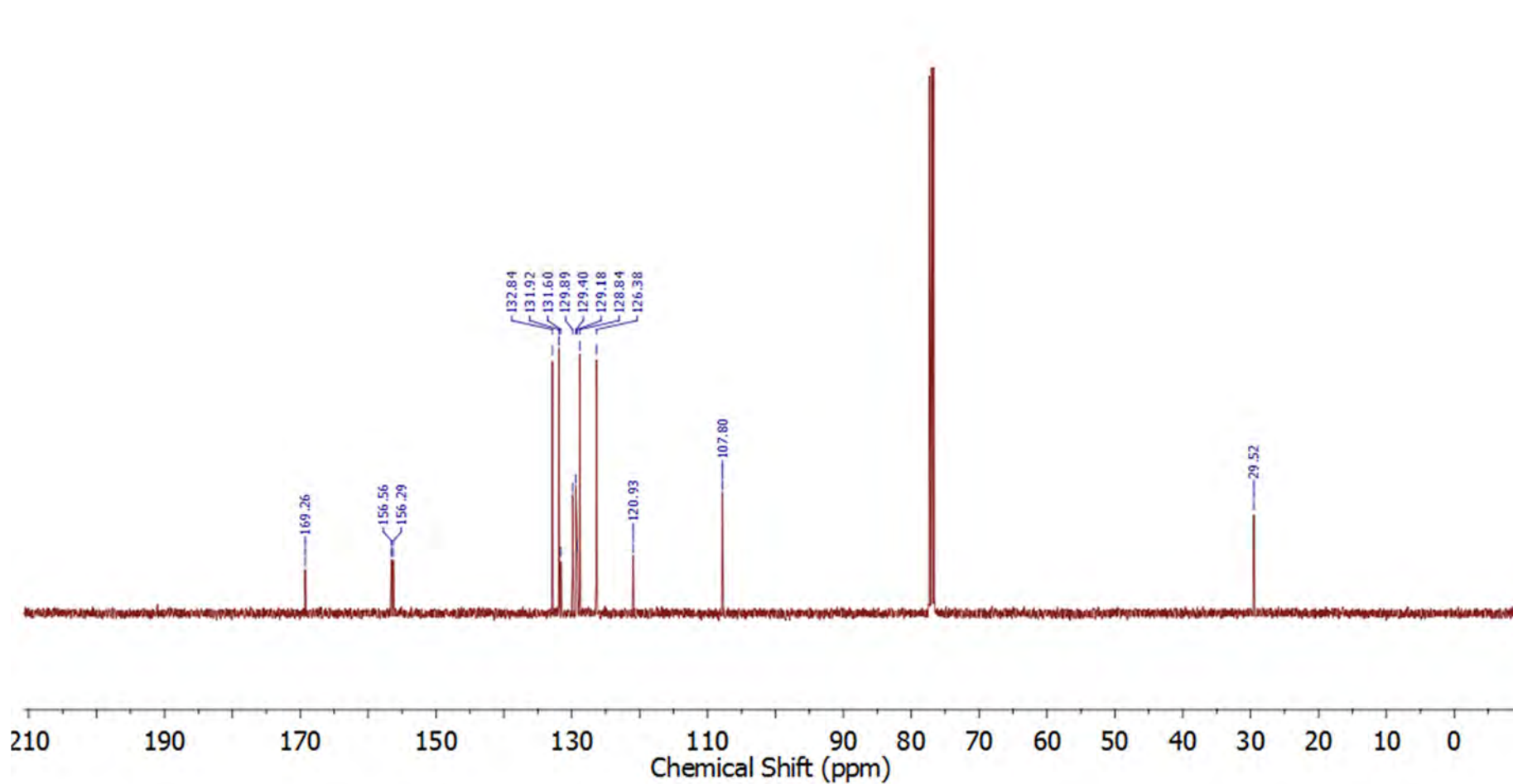
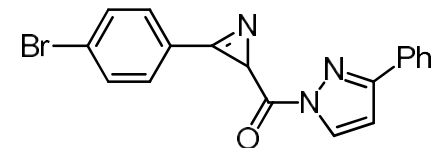
(3-(4-Chlorophenyl)-2*H*-azirin-2-yl)(3-phenyl-1*H*-pyrazol-1-yl)methanone (5g), 100 (DEPT) MHz, CDCl₃



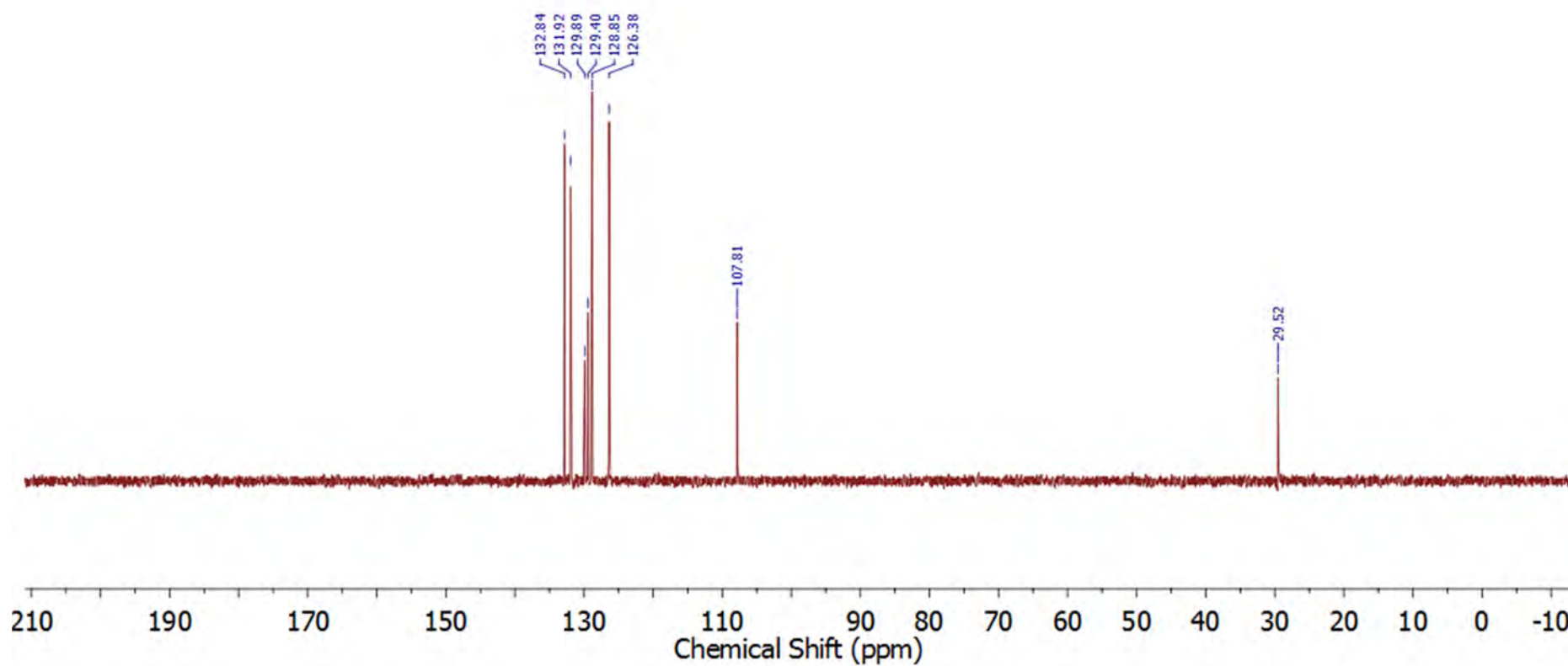
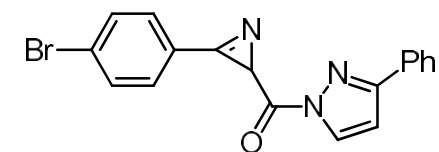
(3-(4-Bromophenyl)-2*H*-azirin-2-yl)(3-phenyl-1*H*-pyrazol-1-yl)methanone (5h), 400 (¹H) MHz, CDCl₃



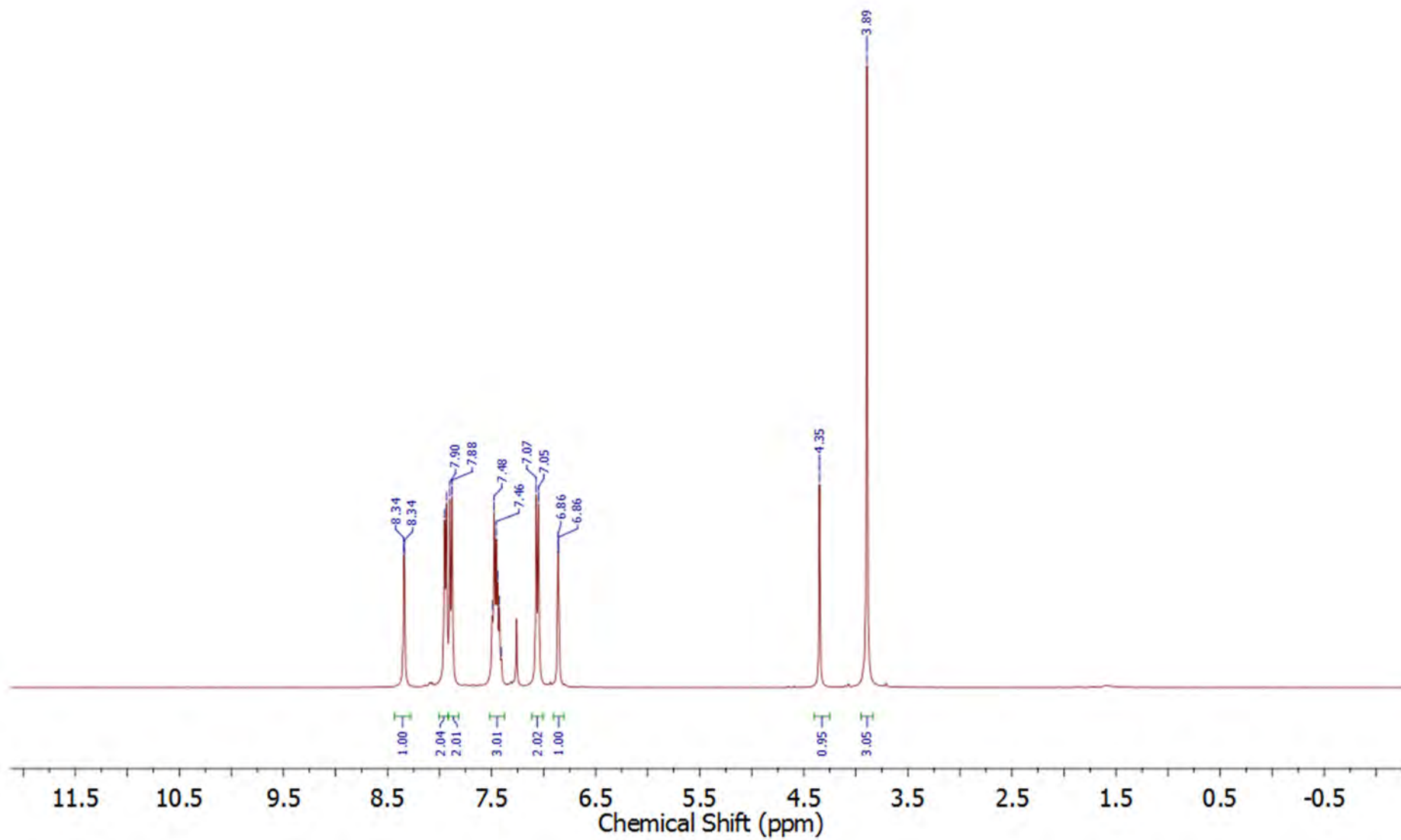
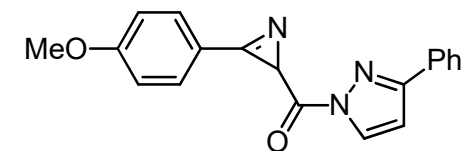
(3-(4-Bromophenyl)-2*H*-azirin-2-yl)(3-phenyl-1*H*-pyrazol-1-yl)methanone (5h), 100 (¹³C) MHz, CDCl₃



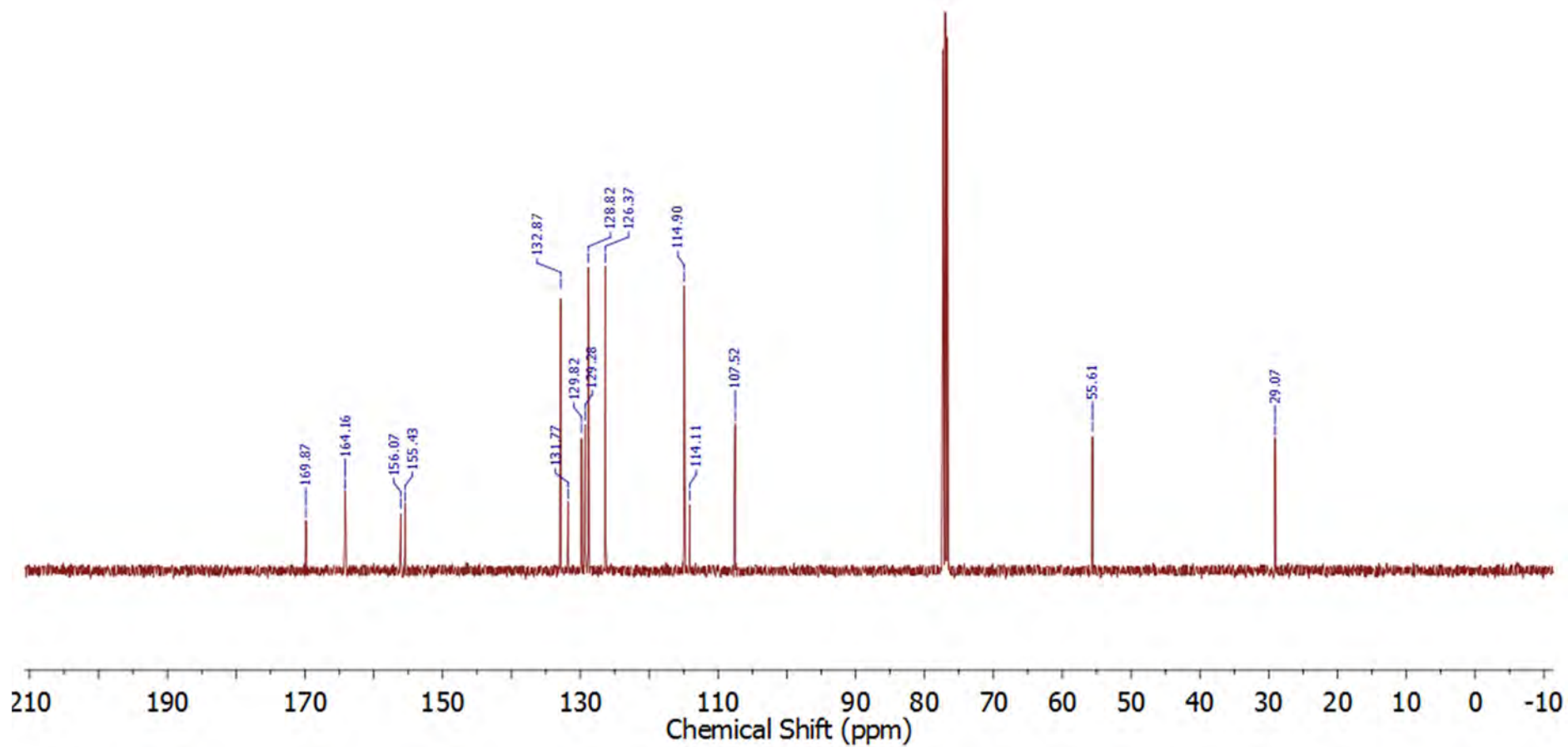
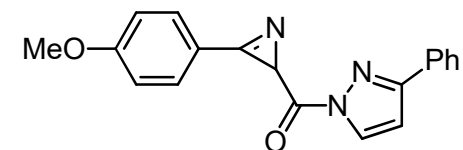
(3-(4-Bromophenyl)-2*H*-azirin-2-yl)(3-phenyl-1*H*-pyrazol-1-yl)methanone (5h), 100 (DEPT) MHz, CDCl₃



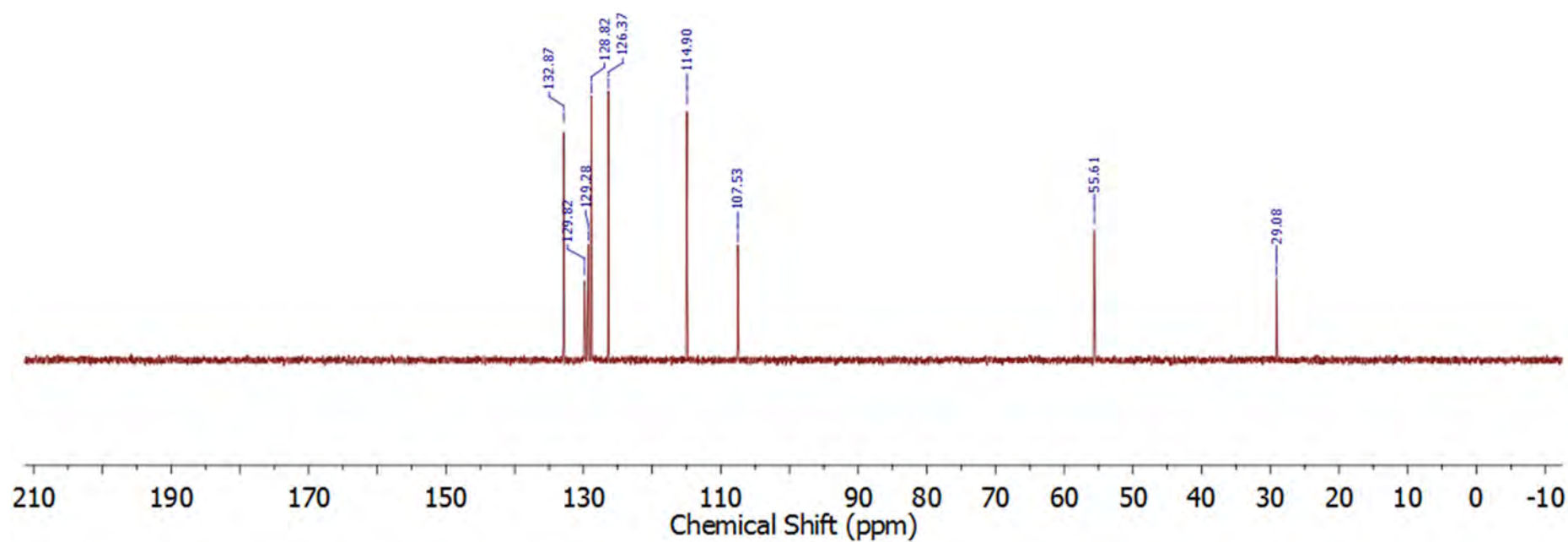
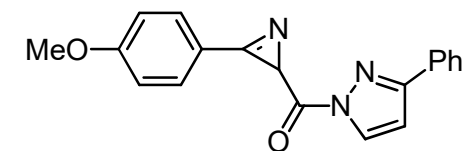
(3-(4-Methoxyphenyl)-2*H*-azirin-2-yl)(3-phenyl-1*H*-pyrazol-1-yl)methanone (5i), 400 (¹H) MHz, CDCl₃



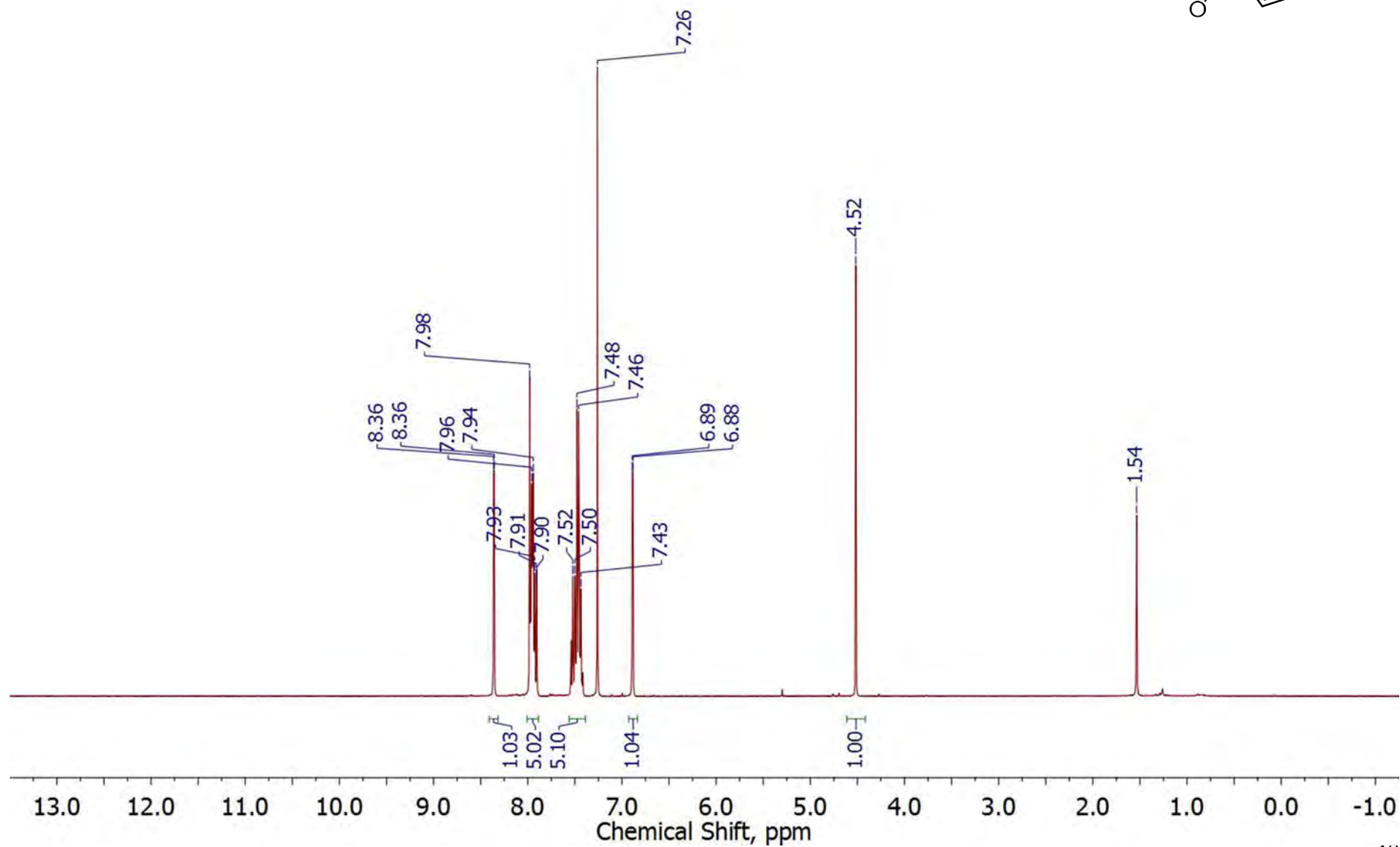
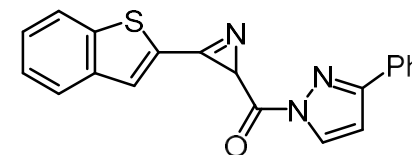
(3-(4-Methoxyphenyl)-2*H*-azirin-2-yl)(3-phenyl-1*H*-pyrazol-1-yl)methanone (5i), 100 (^{13}C) MHz, CDCl_3



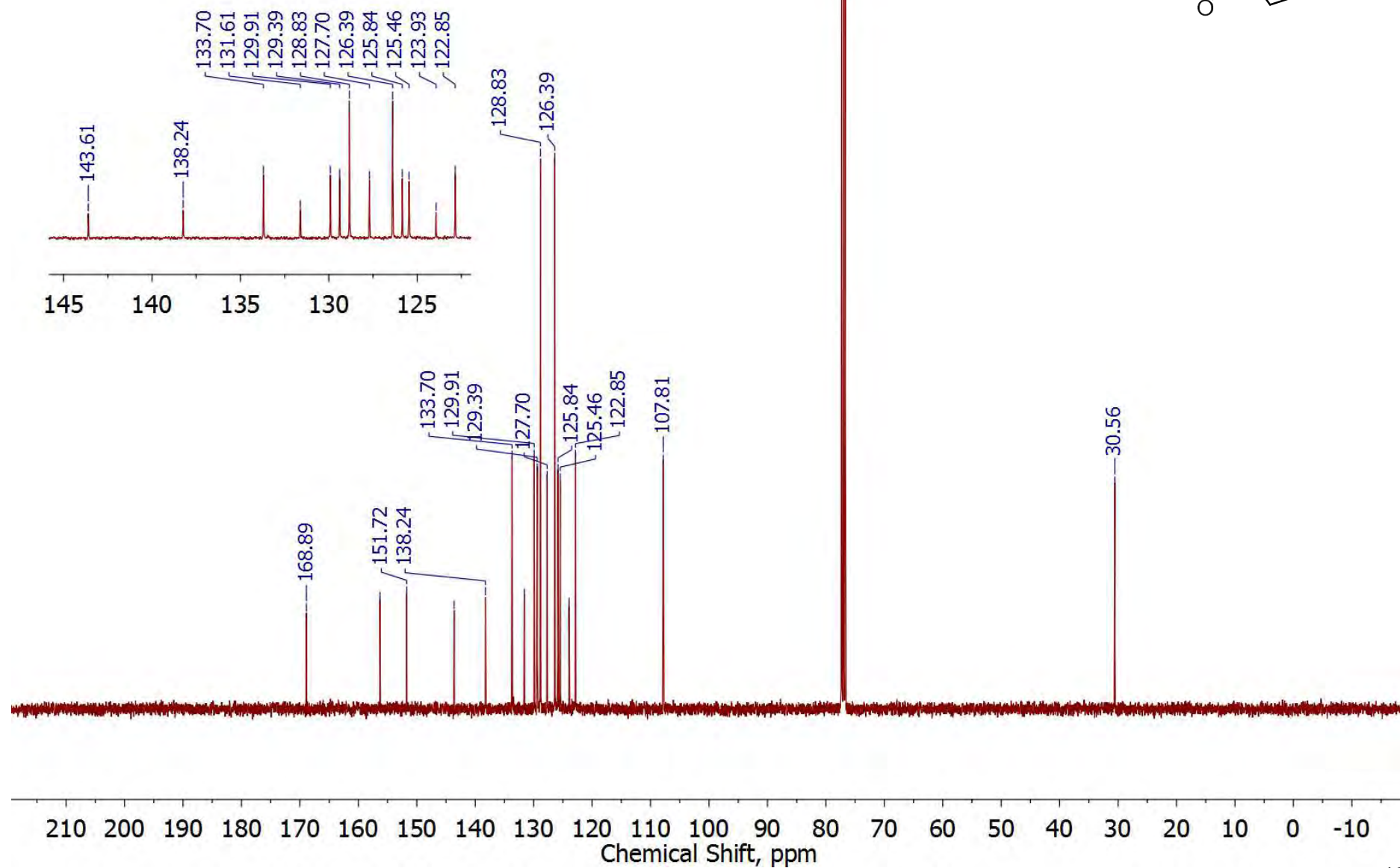
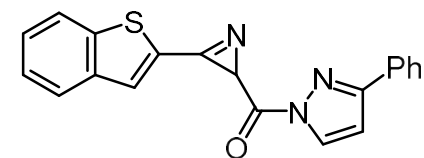
(3-(4-Methoxyphenyl)-2*H*-azirin-2-yl)(3-phenyl-1*H*-pyrazol-1-yl)methanone (5i), 100 (DEPT) MHz, CDCl₃



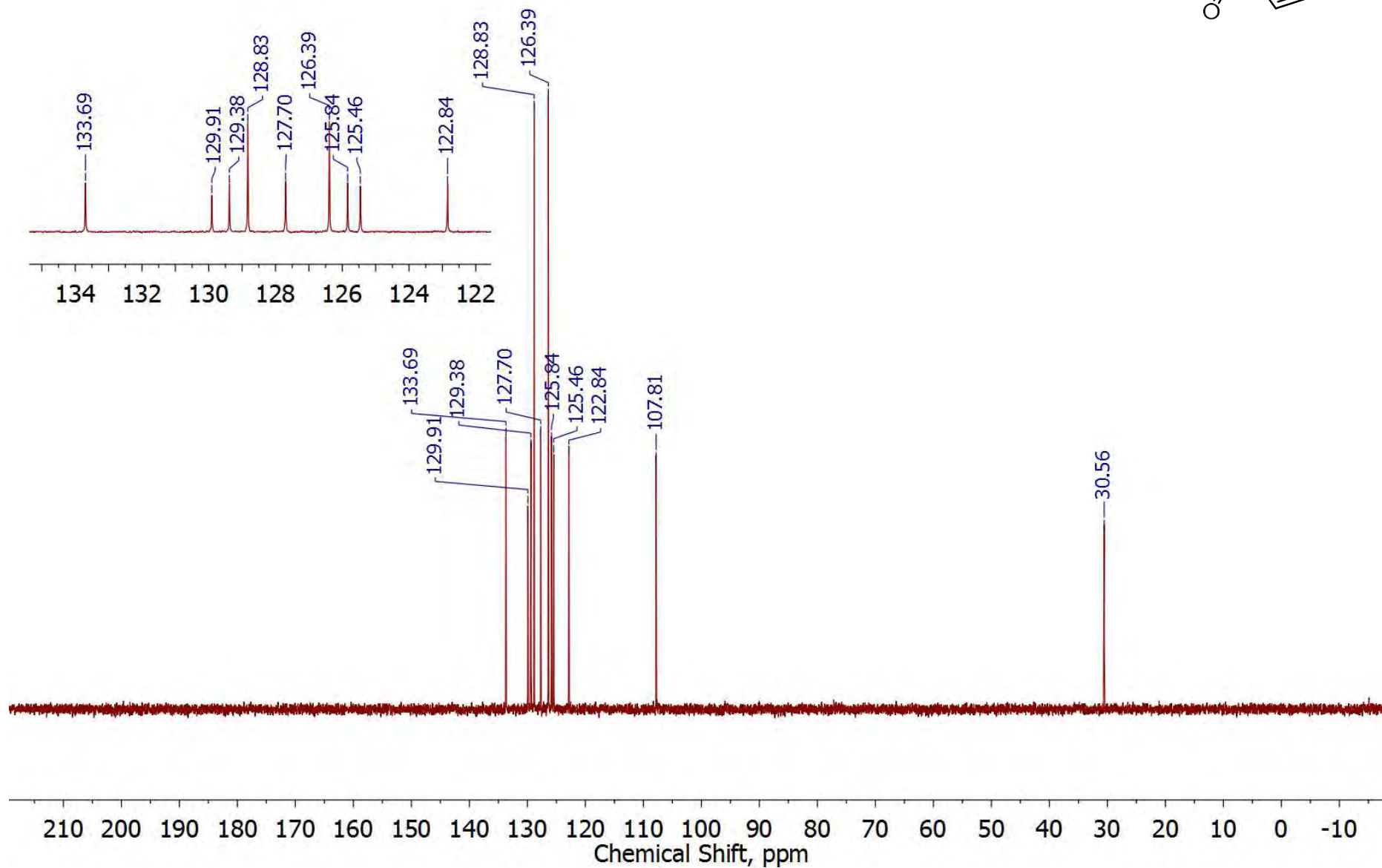
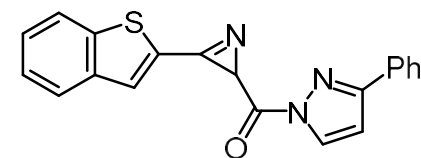
(3-(Benzo[*b*]thiophen-2-yl)-2*H*-azirin-2-yl)(3-phenyl-1*H*-pyrazol-1-yl)methanone (5j), 400 (¹H) MHz, CDCl₃



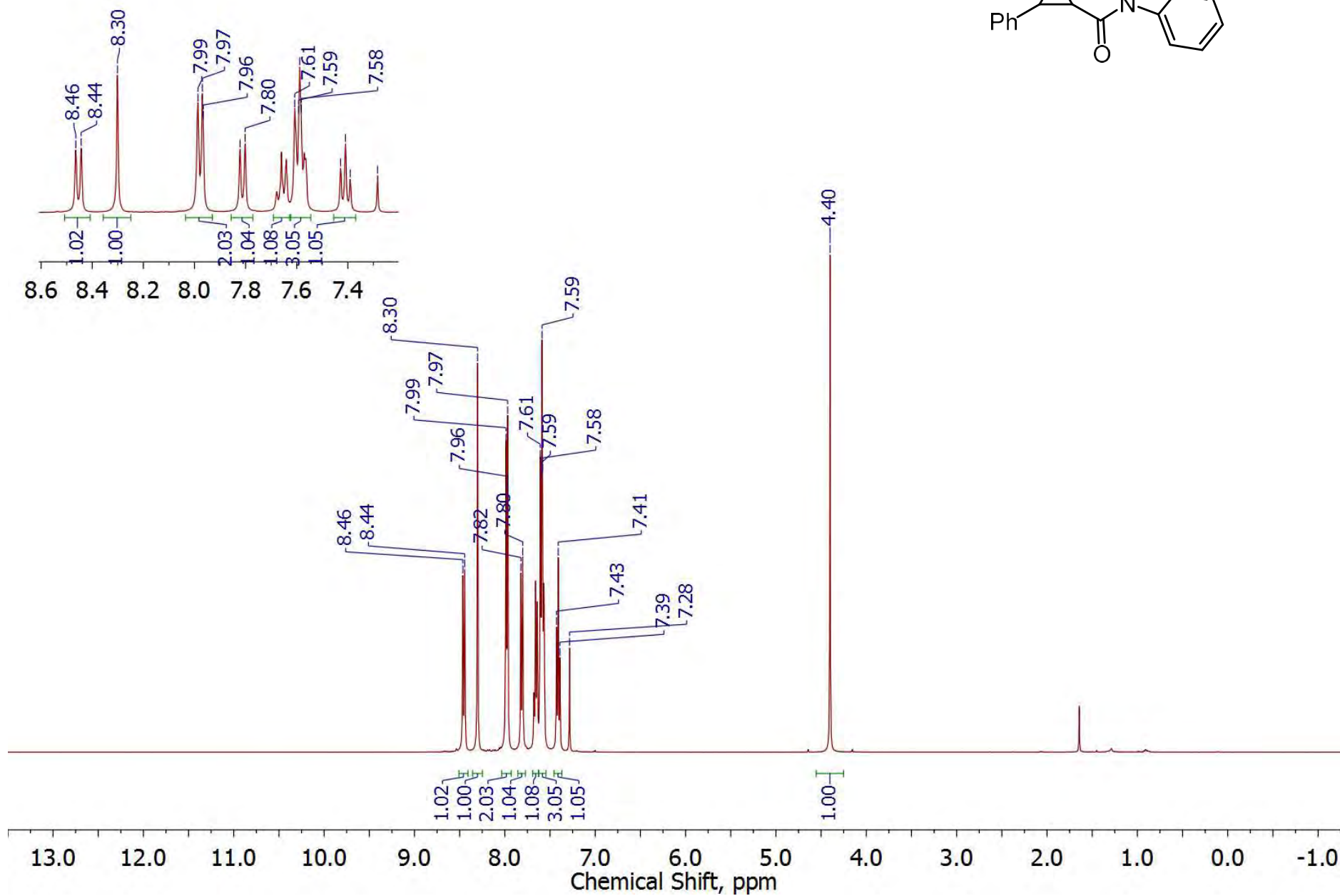
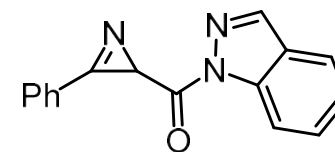
(3-(Benzo[*b*]thiophen-2-yl)-2*H*-azirin-2-yl)(3-phenyl-1*H*-pyrazol-1-yl)methanone (5j), 100 (¹³C) MHz, CDCl₃



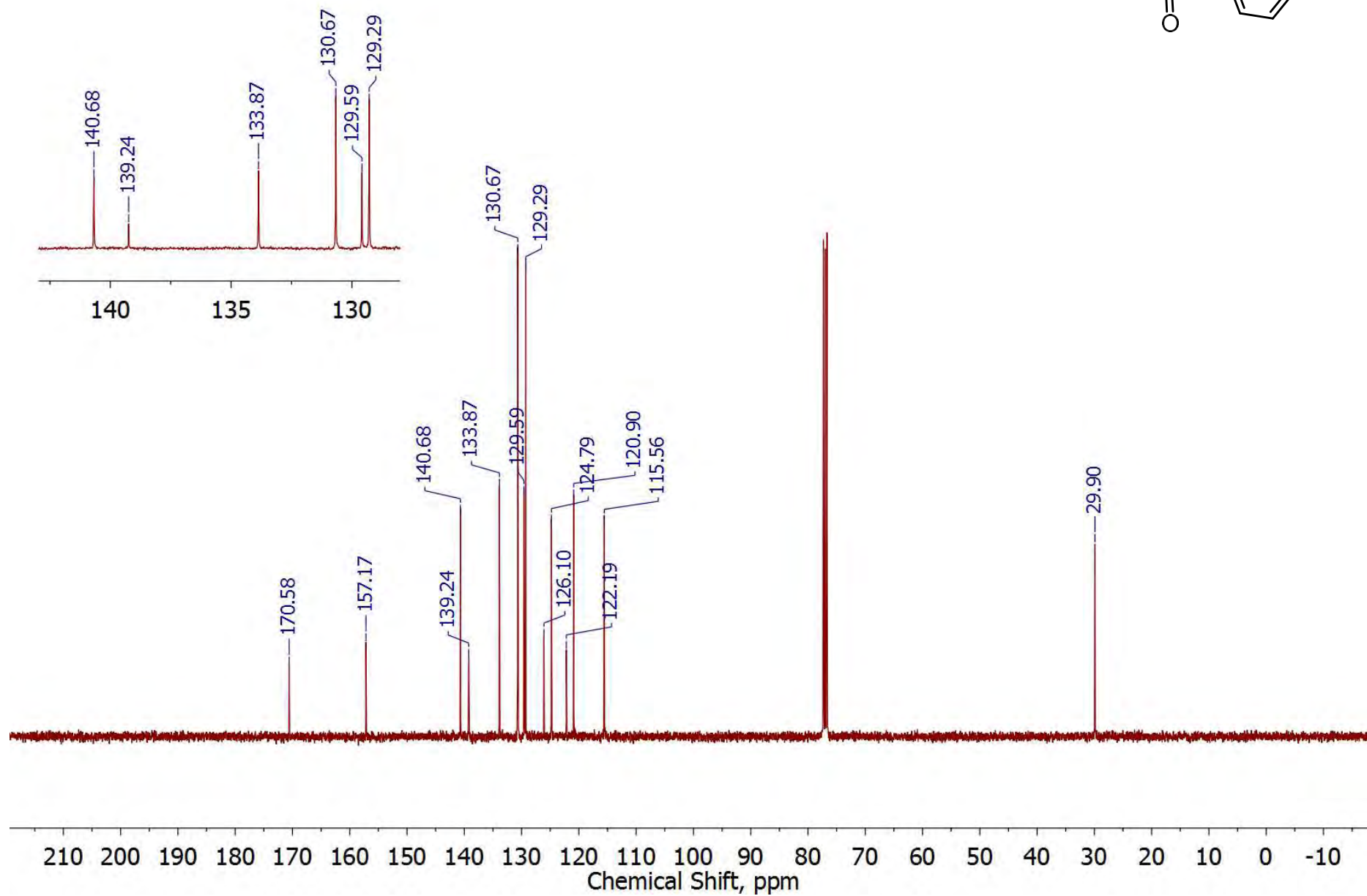
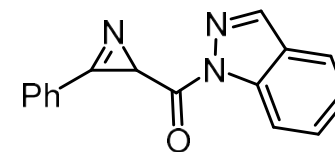
(3-(Benzo[*b*]thiophen-2-yl)-2*H*-azirin-2-yl)(3-phenyl-1*H*-pyrazol-1-yl)methanone (5j), 100 (DEPT) MHz, CDCl₃



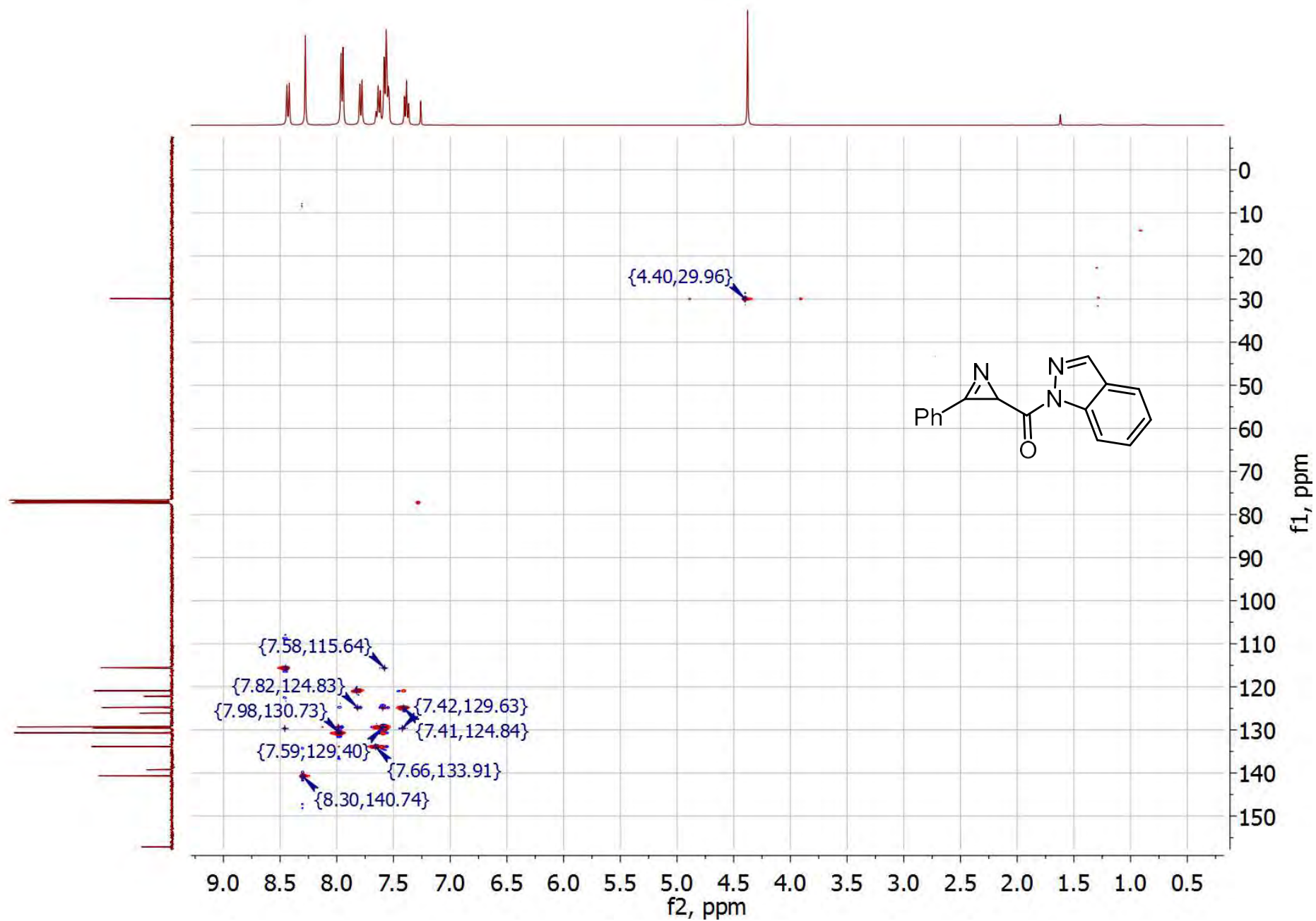
(1*H*-Indazol-1-yl)(3-phenyl-2*H*-azirin-2-yl)methanone (5k), 400 (¹H) MHz, CDCl₃



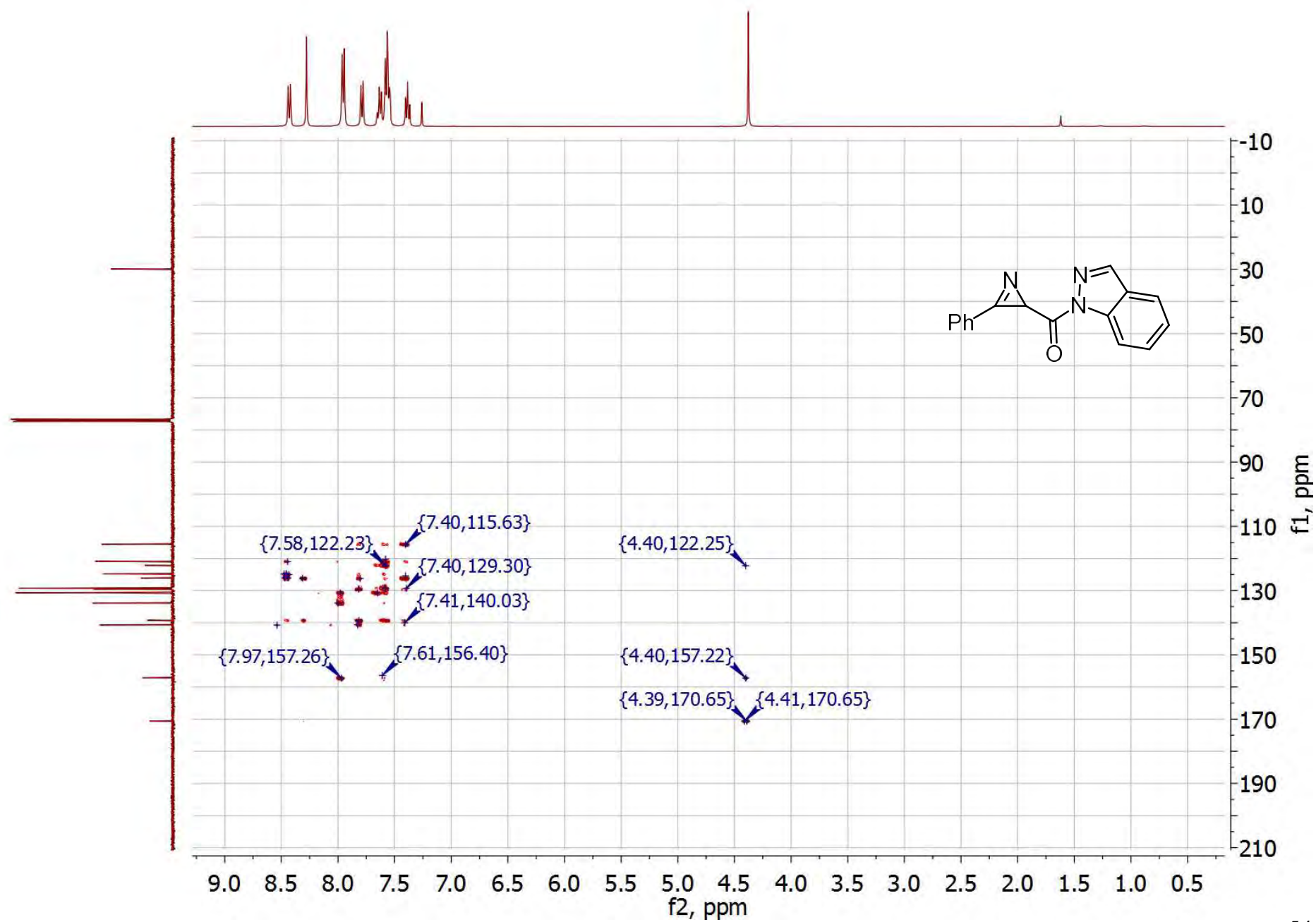
(1*H*-Indazol-1-yl)(3-phenyl-2*H*-azirin-2-yl)methanone (5k), 100 (¹³C) MHz, CDCl₃



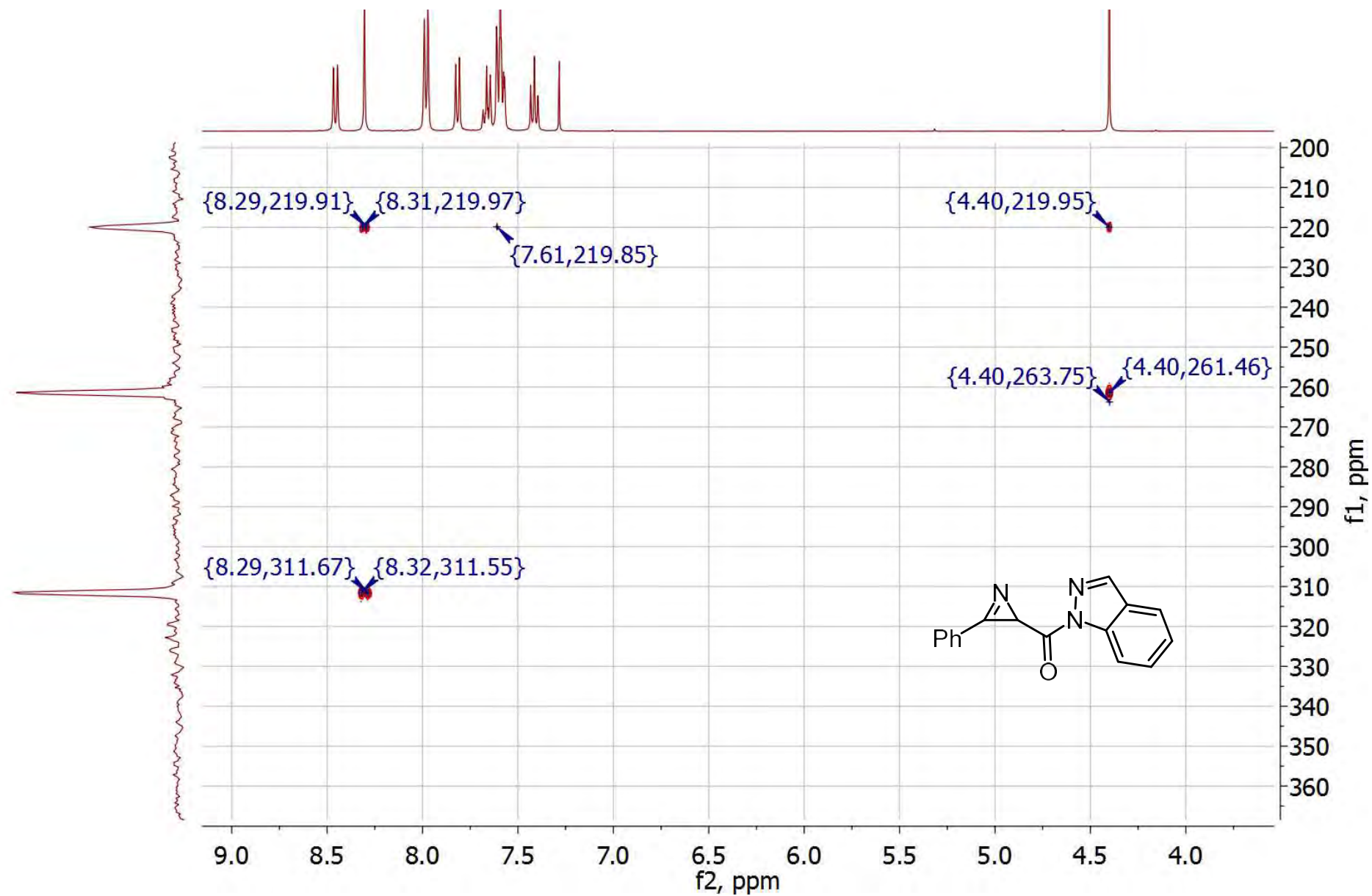
(1*H*-Indazol-1-yl)(3-phenyl-2*H*-azirin-2-yl)methanone (5k), 2D HSQC ^1H - ^{13}C , CDCl_3



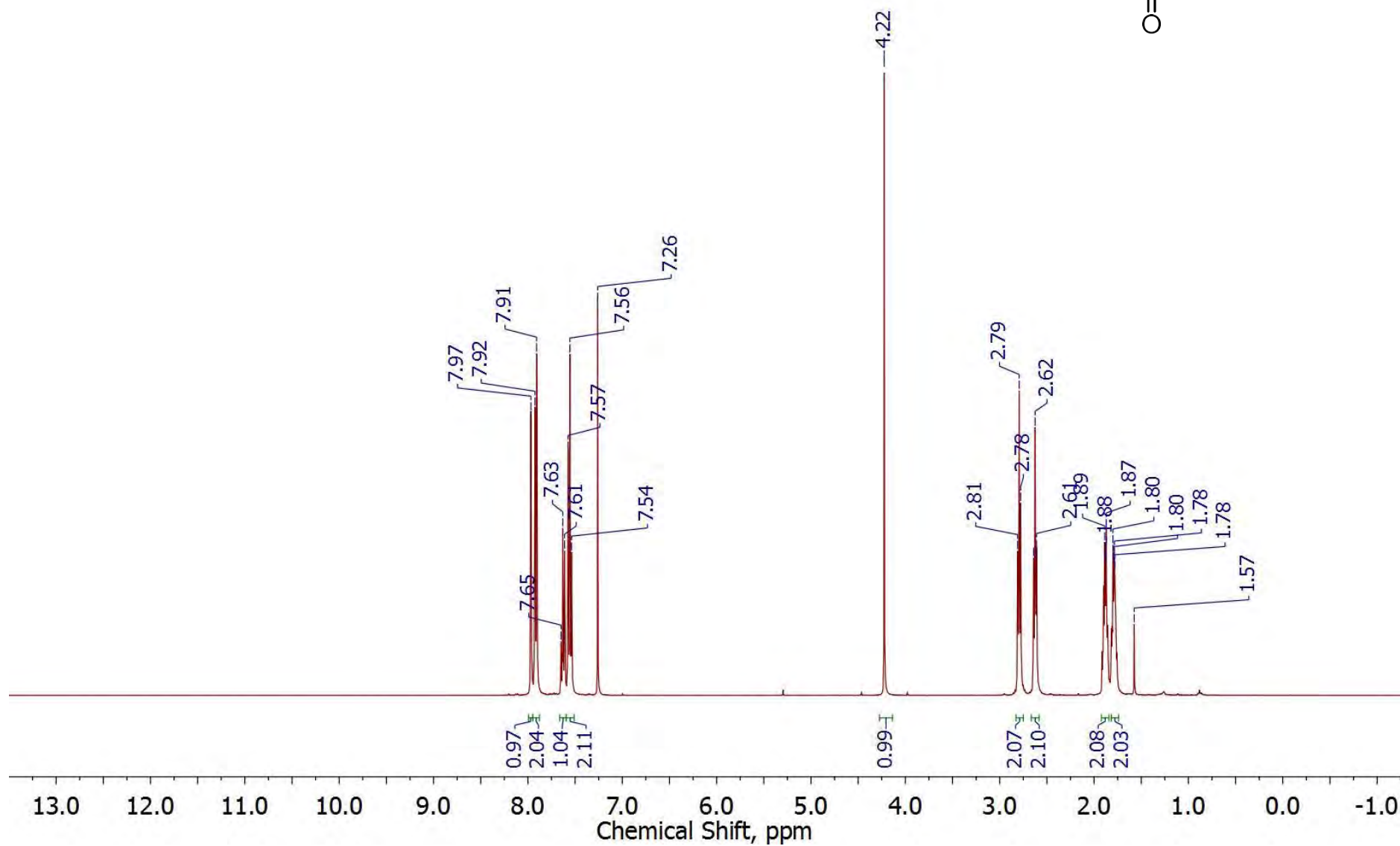
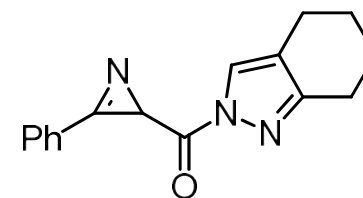
(1*H*-Indazol-1-yl)(3-phenyl-2*H*-azirin-2-yl)methanone (5k), 2D HMBC ^1H - ^{13}C , CDCl_3



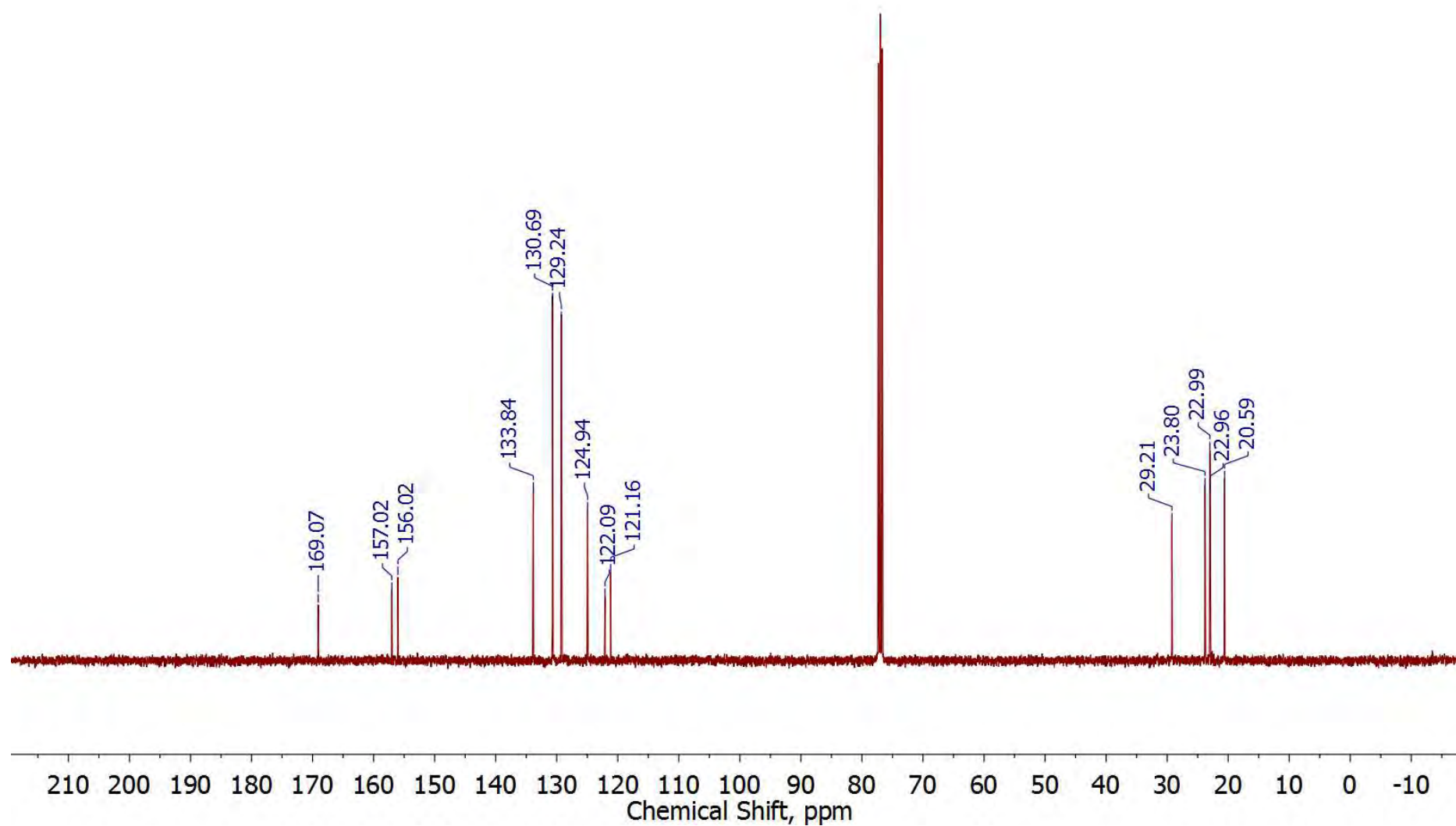
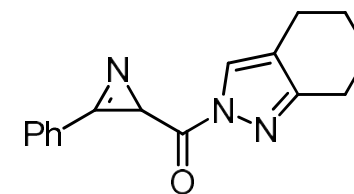
(1*H*-Indazol-1-yl)(3-phenyl-2*H*-azirin-2-yl)methanone (5k), 2D HMBC ^1H - ^{15}N , CDCl_3



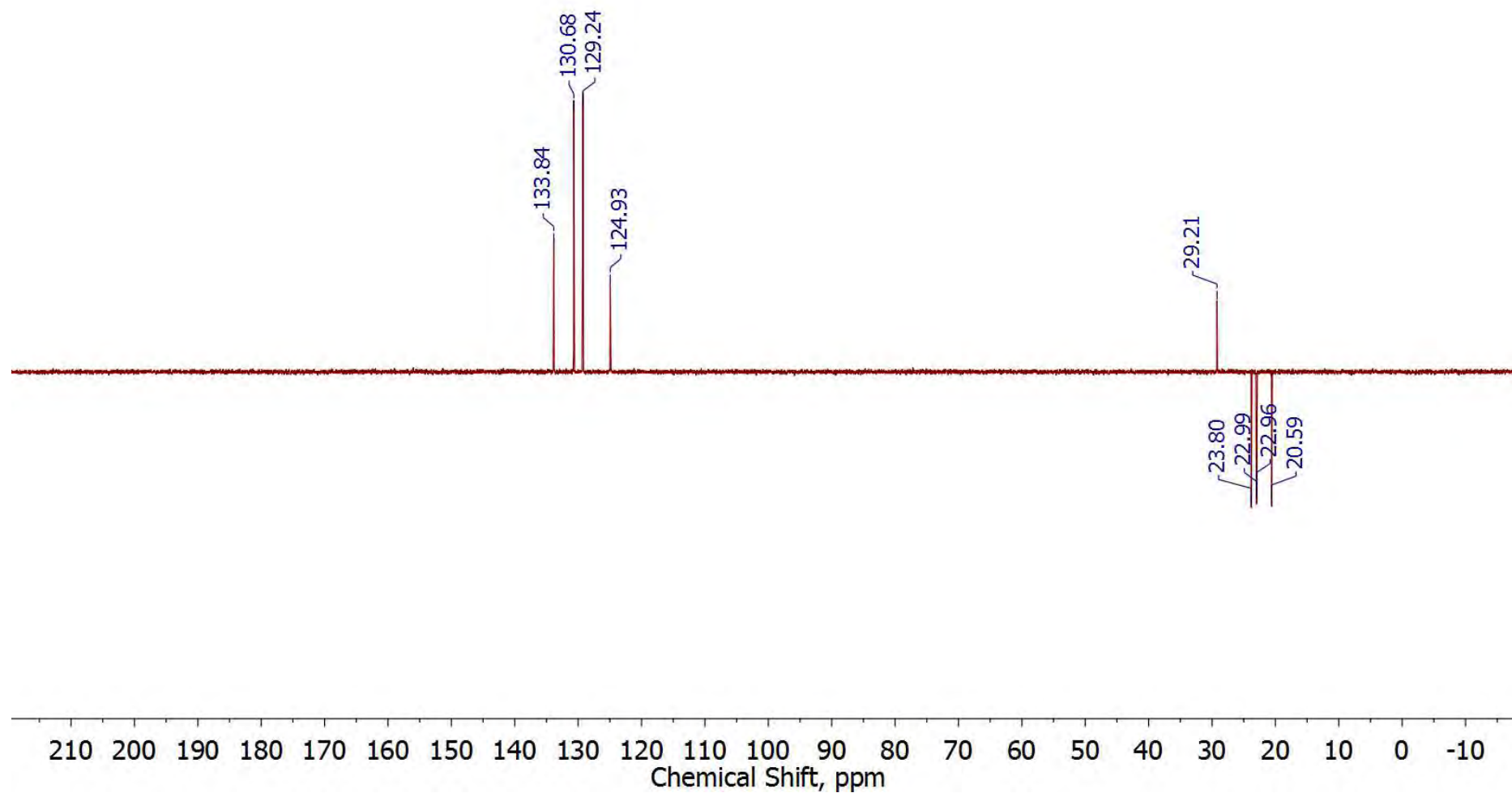
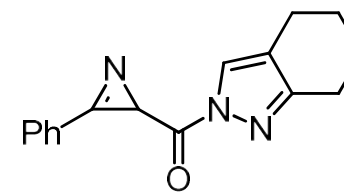
(3-Phenyl-2*H*-azirin-2-yl)(4,5,6,7-tetrahydro-2*H*-indazol-2-yl)methanone (5l), 400 (¹H) MHz, CDCl₃



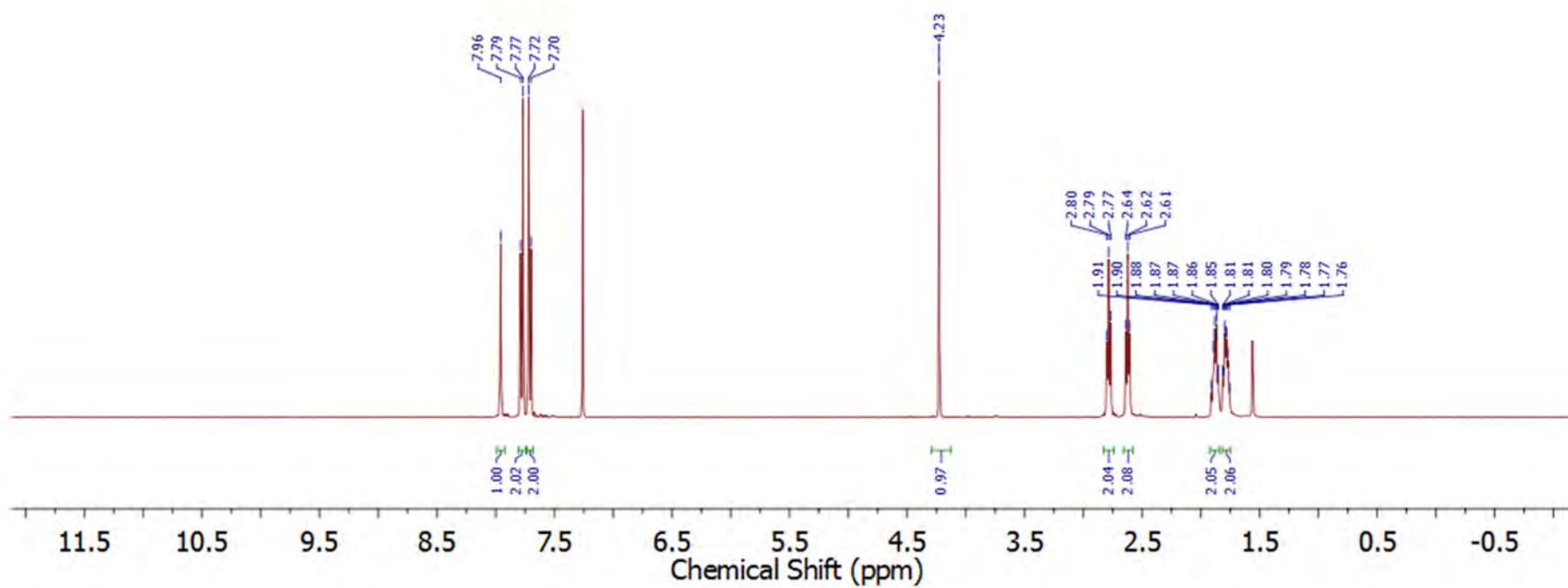
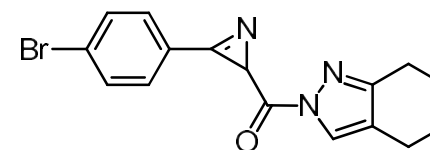
(3-Phenyl-2*H*-azirin-2-yl)(4,5,6,7-tetrahydro-2*H*-indazol-2-yl)methanone (5l), 100 (¹³C) MHz, CDCl₃



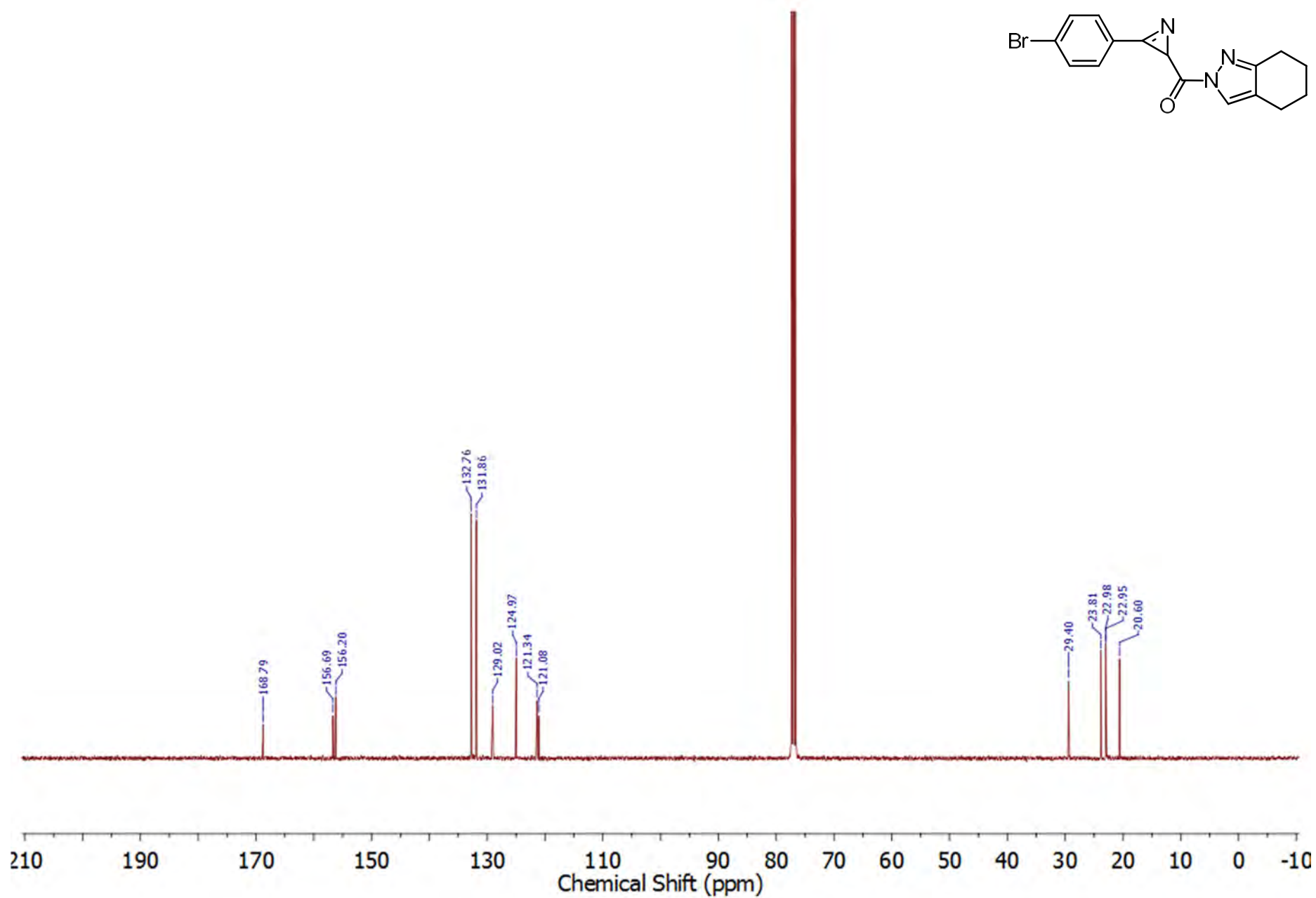
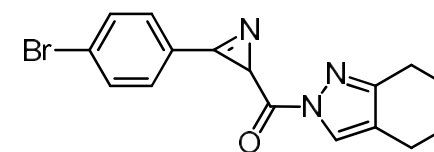
(3-Phenyl-2*H*-azirin-2-yl)(4,5,6,7-tetrahydro-2*H*-indazol-2-yl)methanone (5l), 100 (DEPT) MHz, CDCl₃.



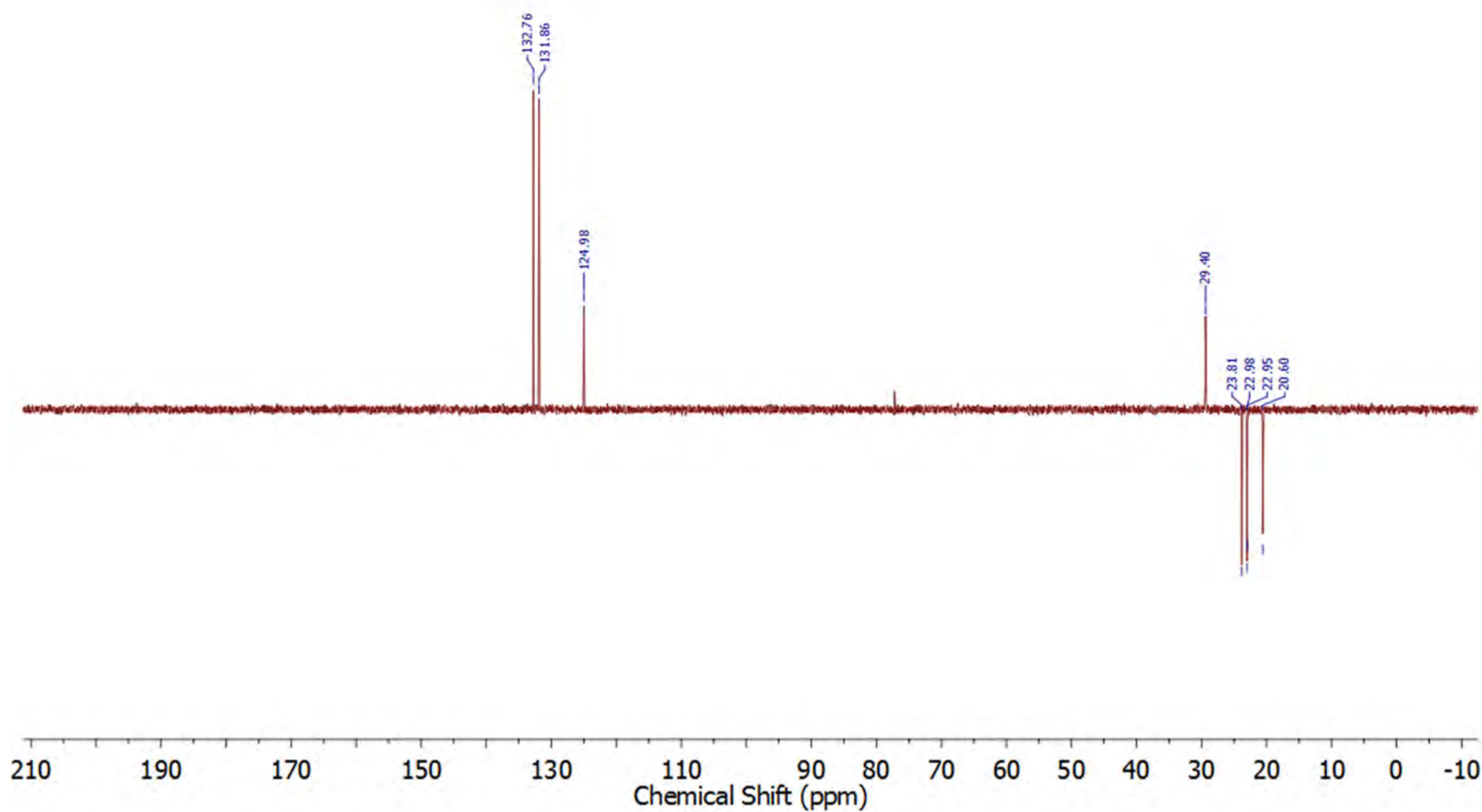
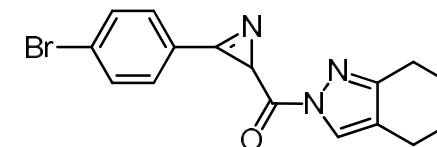
(3-(4-Bromophenyl)-2H-azirin-2-yl)(4,5,6,7-tetrahydro-2H-indazol-2-yl)methanone (5m), 400 (^1H) MHz, CDCl_3



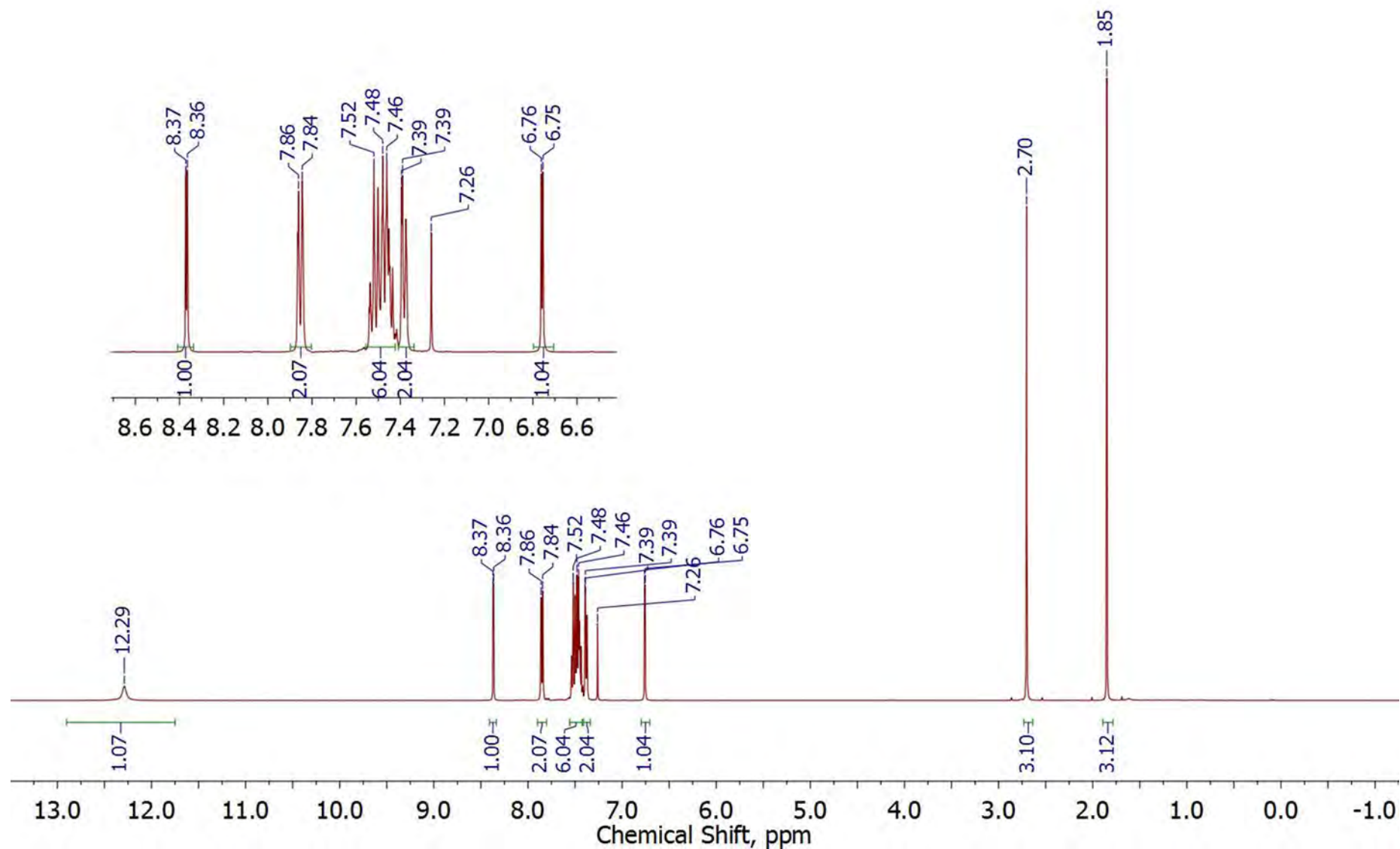
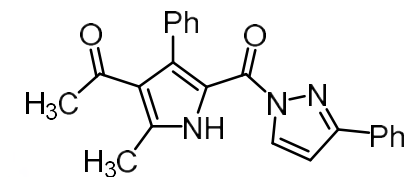
(3-(4-Bromophenyl)-2*H*-azirin-2-yl)(4,5,6,7-tetrahydro-2*H*-indazol-2-yl)methanone (5m), 100 (^{13}C) MHz, CDCl_3



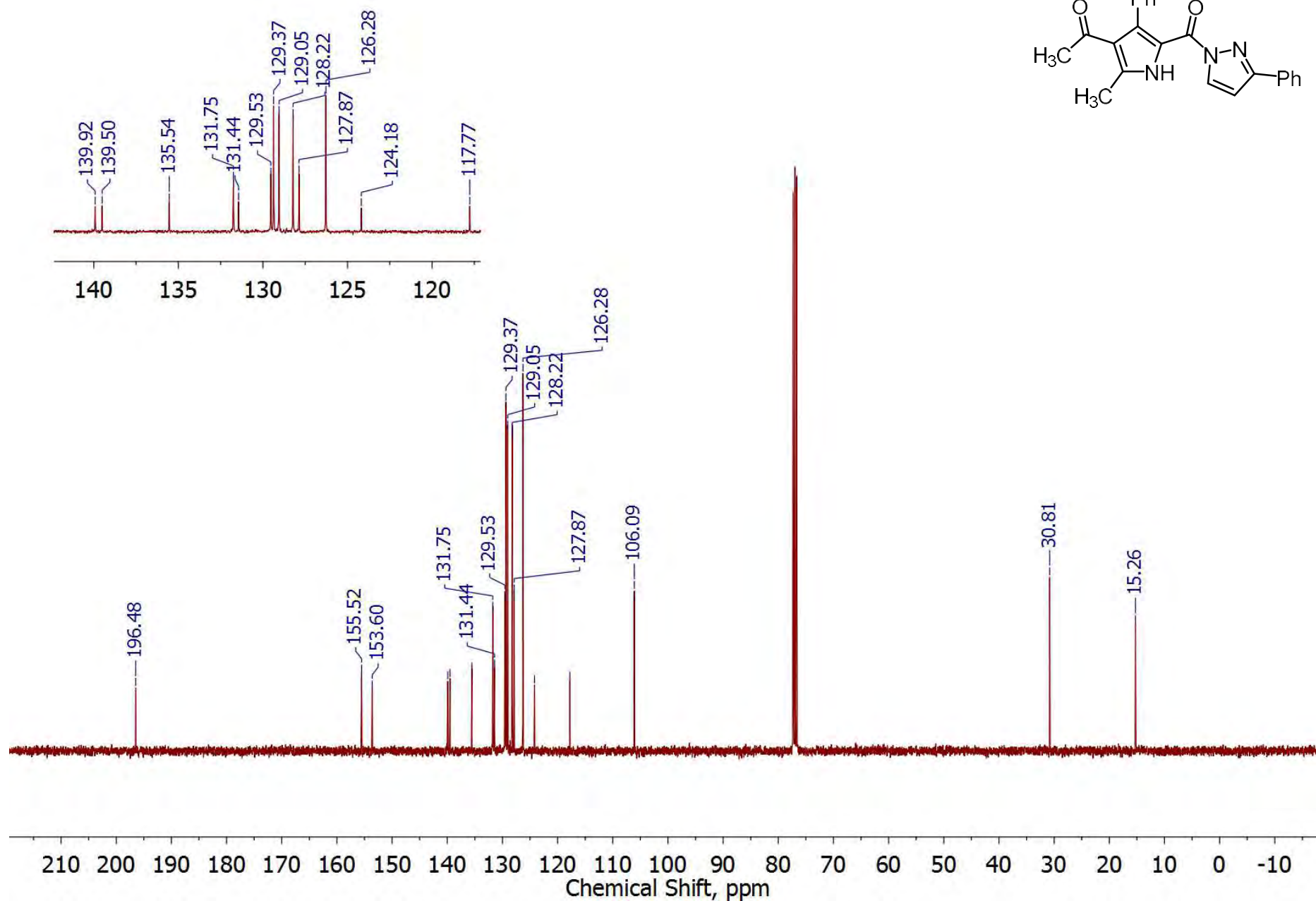
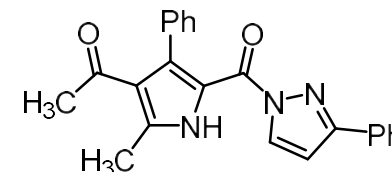
(3-(4-Bromophenyl)-2H-azirin-2-yl)(4,5,6,7-tetrahydro-1H-indazol-2-yl)methanone (5m), 100 (DEPT) MHz, CDCl₃



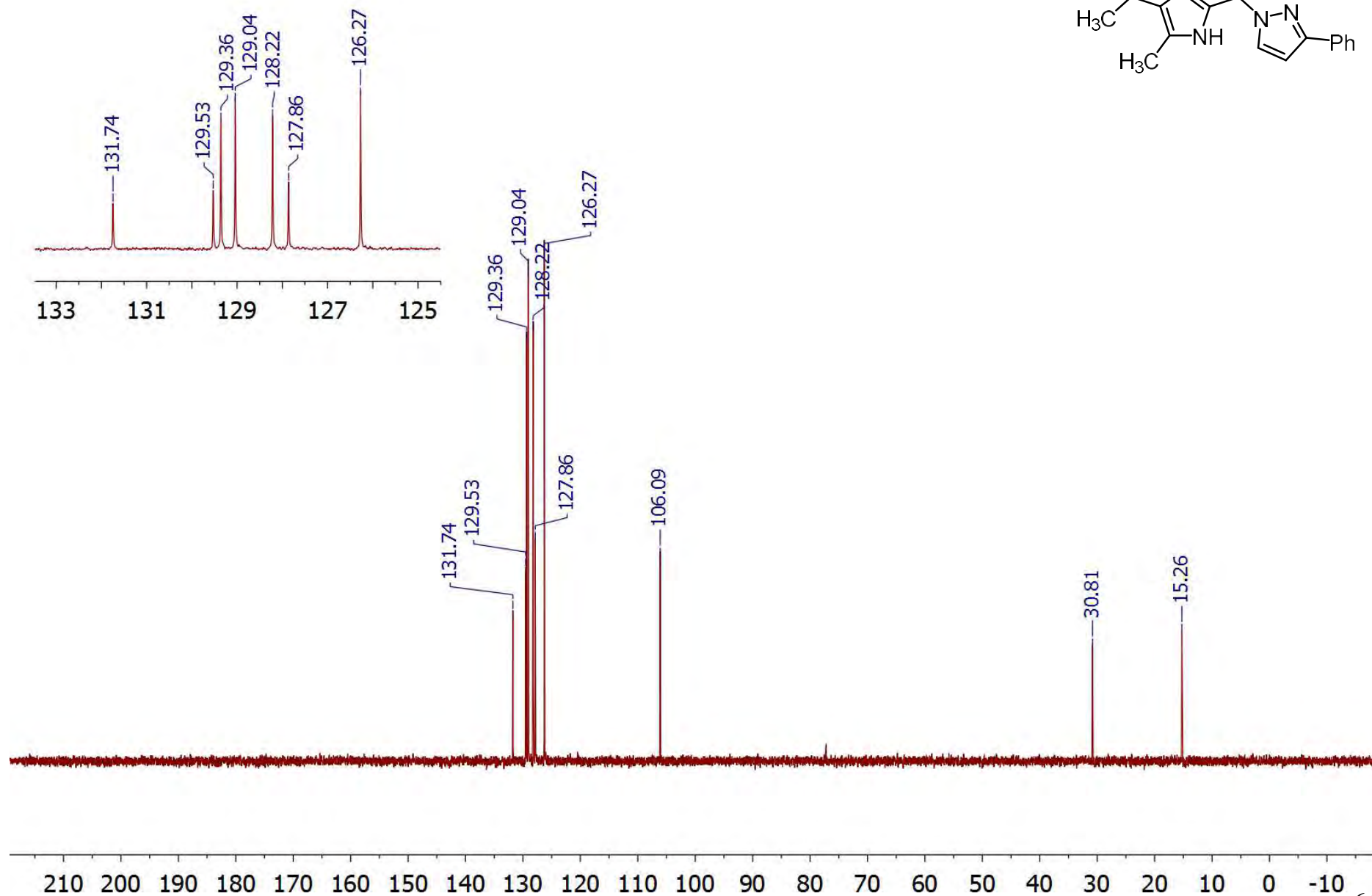
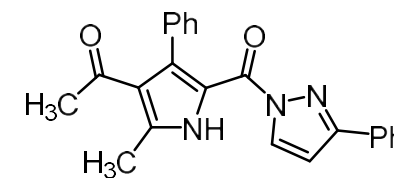
1-(2-Methyl-4-phenyl-5-(3-phenyl-1*H*-pyrazole-1-carbonyl)-1*H*-pyrrol-3-yl)ethanone (6a), 400 (¹H) MHz, CDCl₃



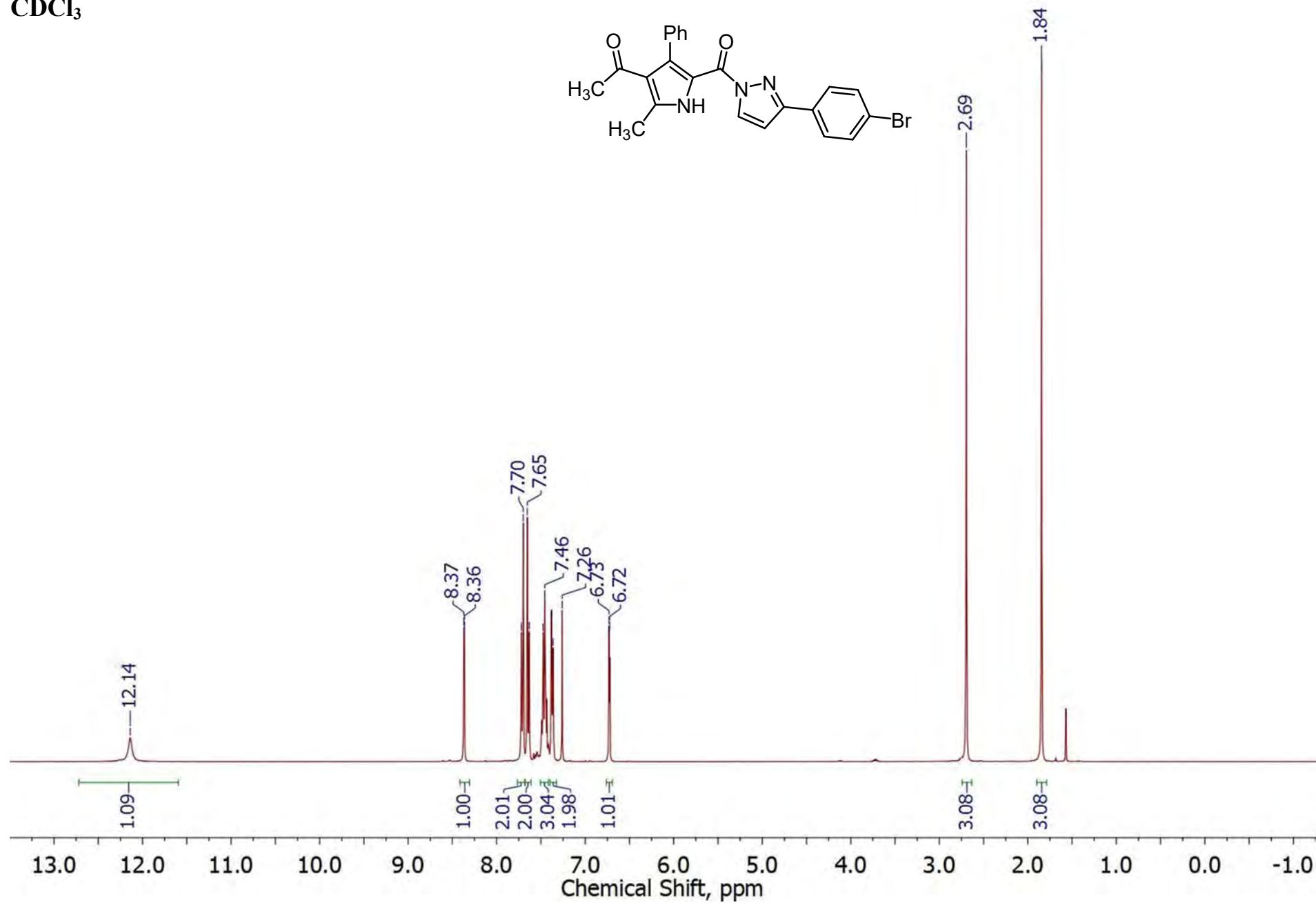
1-(2-Methyl-4-phenyl-5-(3-phenyl-1*H*-pyrazole-1-carbonyl)-1*H*-pyrrol-3-yl)ethanone (6a), 100 (^{13}C) MHz, CDCl_3



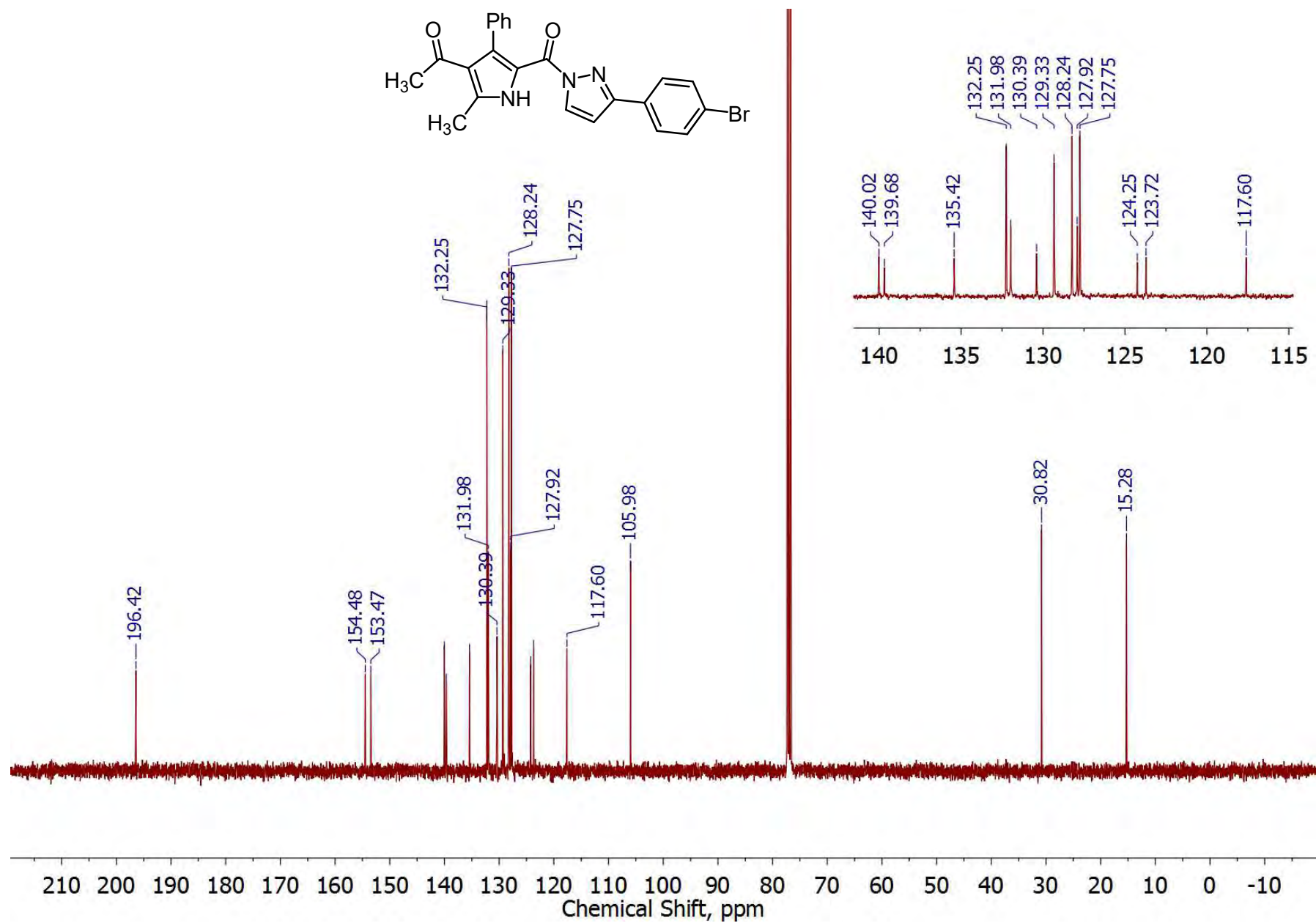
1-(2-Methyl-4-phenyl-5-(3-phenyl-1*H*-pyrazole-1-carbonyl)-1*H*-pyrrol-3-yl)ethanone (6a), 100 (DEPT) MHz, CDCl₃



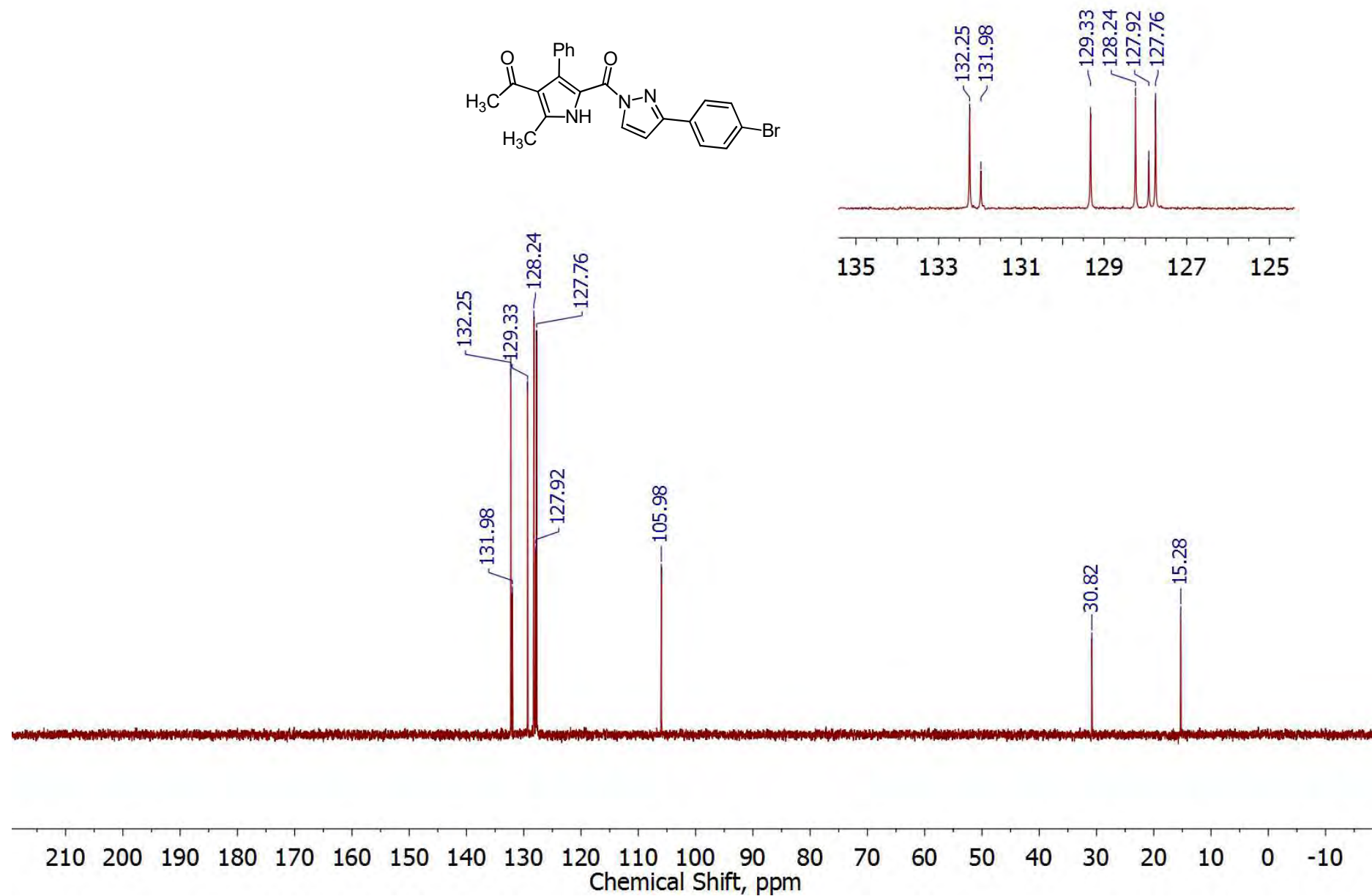
1-(5-(3-(4-Bromophenyl)-1*H*-pyrazole-1-carbonyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone (6b), 400 (¹H) MHz, CDCl₃



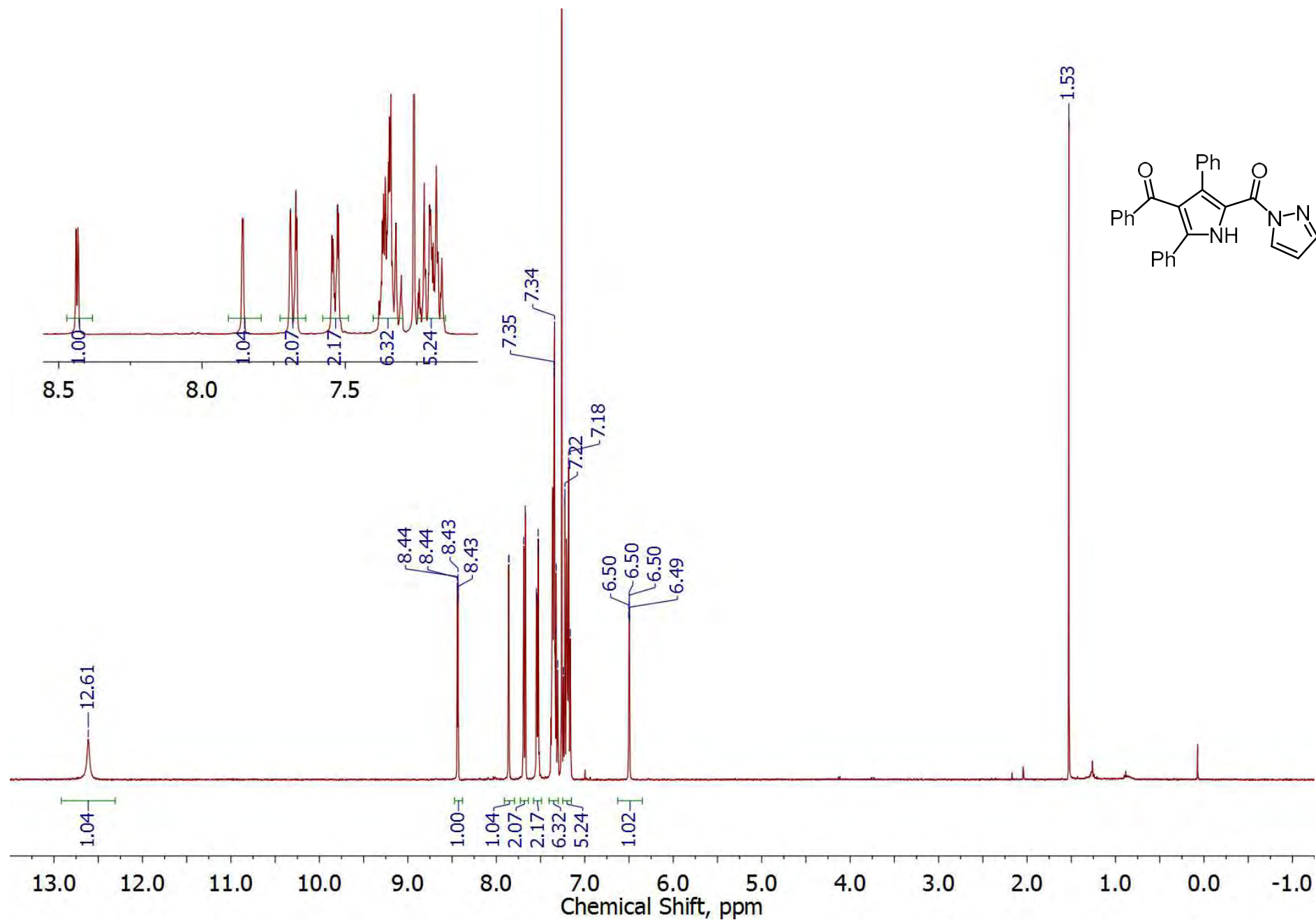
1-(5-(3-(4-Bromophenyl)-1*H*-pyrazole-1-carbonyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone (6b), 100 (^{13}C) MHz, CDCl_3



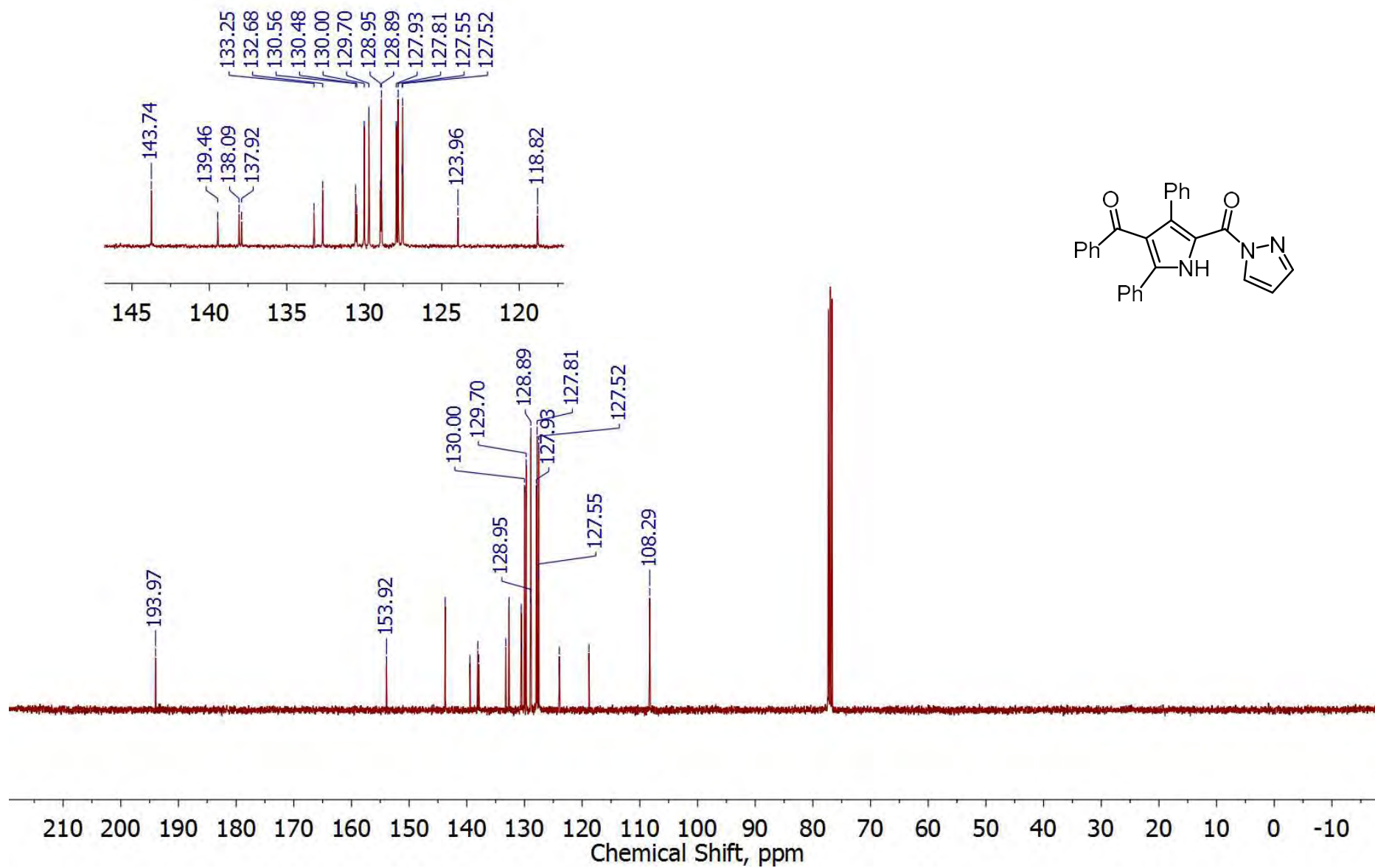
1-(5-(3-(4-Bromophenyl)-1*H*-pyrazole-1-carbonyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)ethanone (6b), 100 (DEPT) MHz, CDCl₃



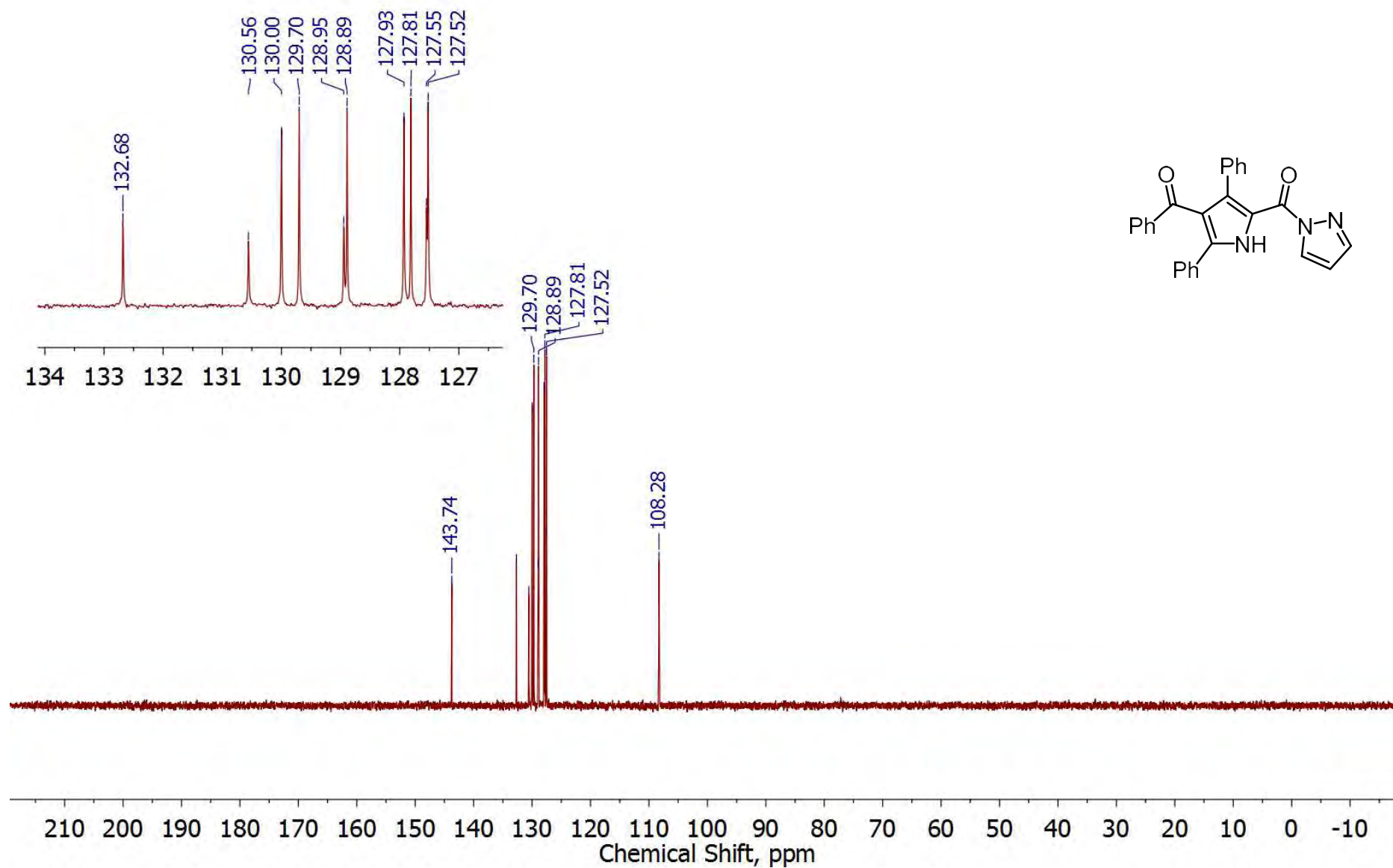
(4-Benzoyl-3,5-diphenyl-1*H*-pyrrol-2-yl)(1*H*-pyrazol-1-yl)methanone (6c), 400 (¹H) MHz, CDCl₃



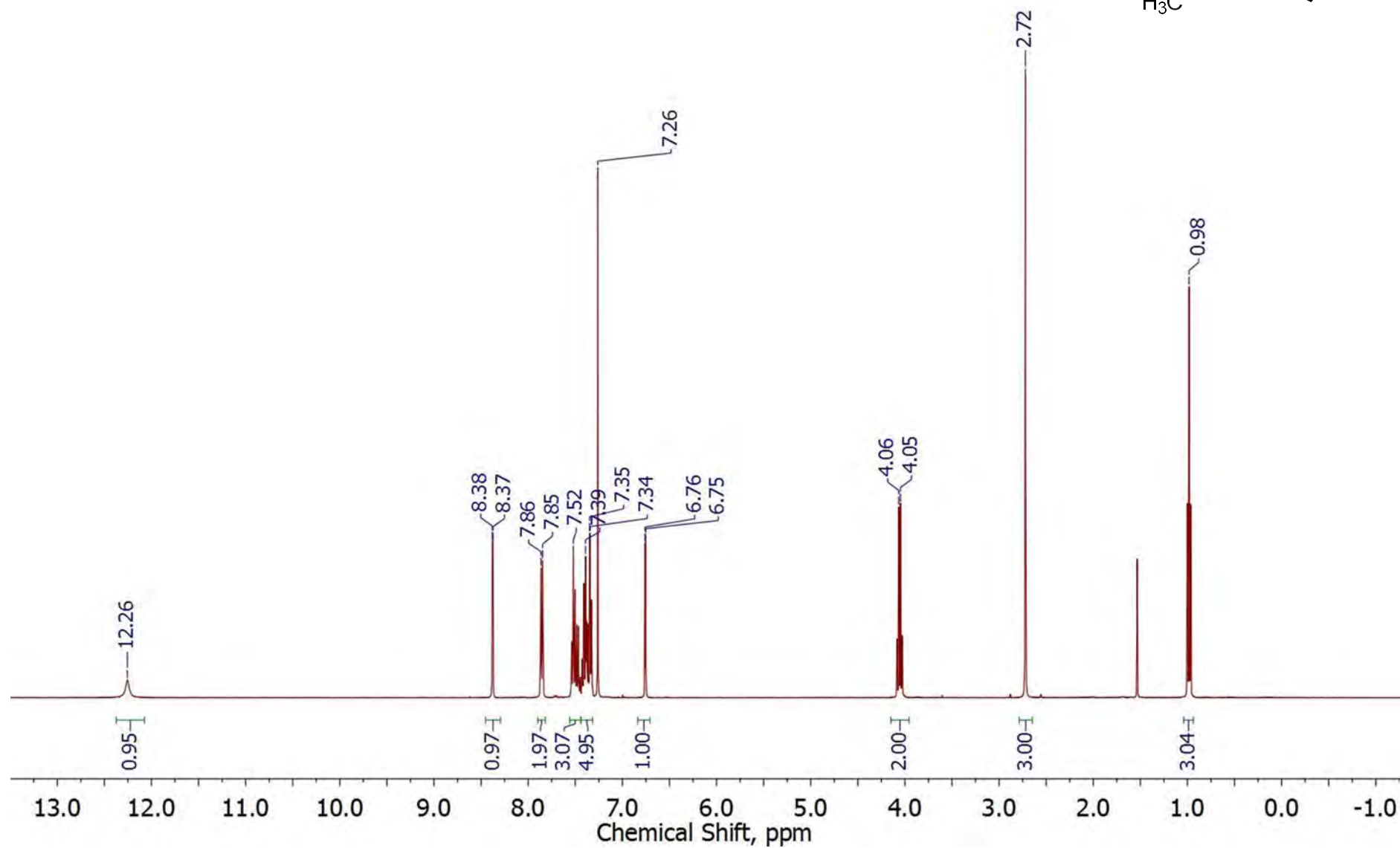
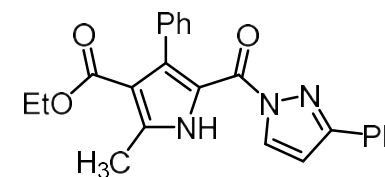
(4-Benzoyl-3,5-diphenyl-1*H*-pyrrol-2-yl)(1*H*-pyrazol-1-yl)methanone (6c), 100 (¹³C) MHz, CDCl₃



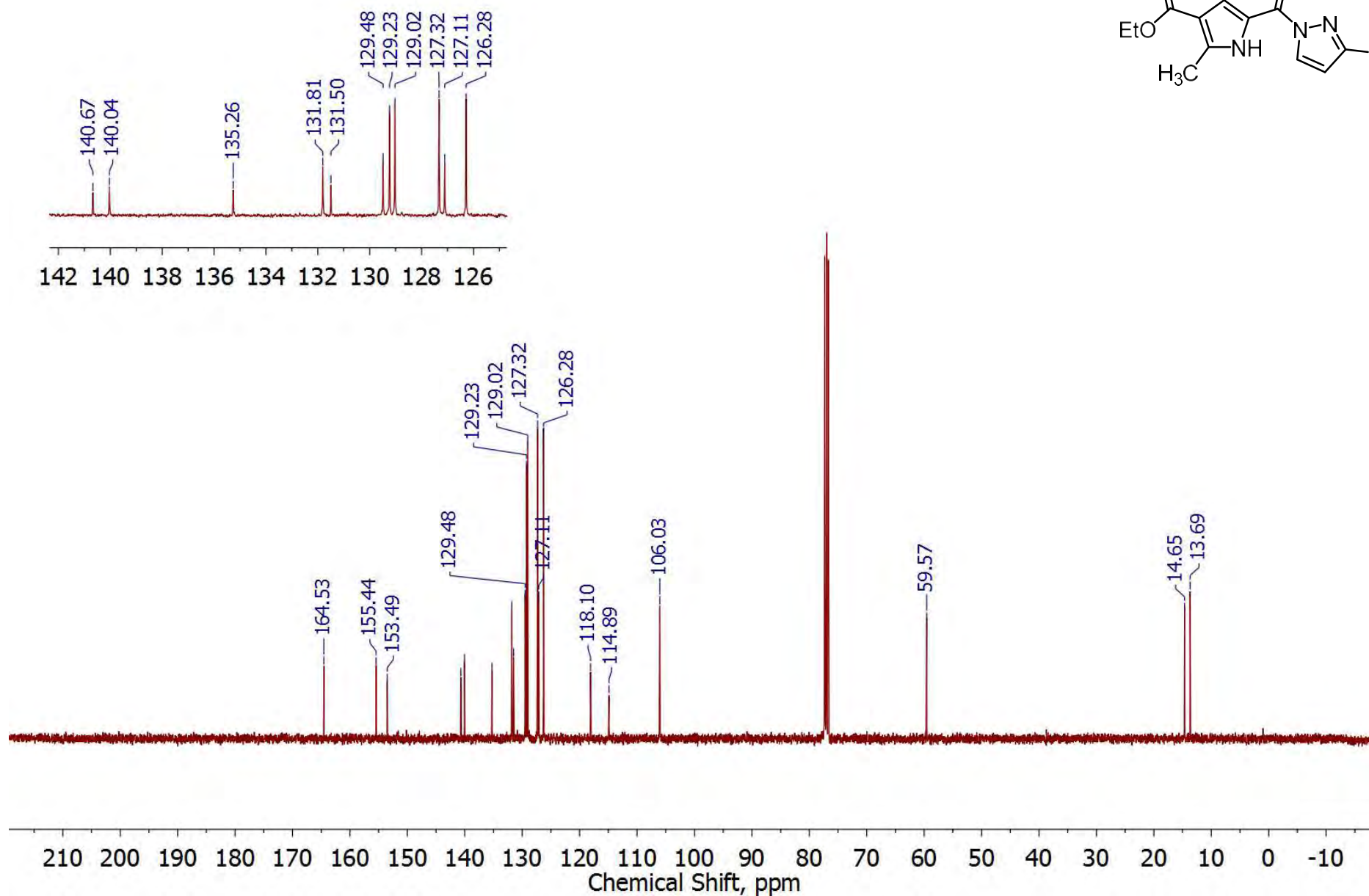
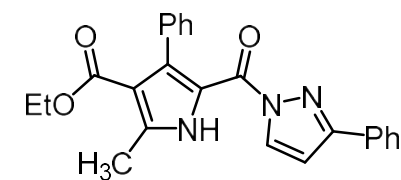
(4-Benzoyl-3,5-diphenyl-1*H*-pyrrol-2-yl)(1*H*-pyrazol-1-yl)methanone (6c), 100 (DEPT) MHz, CDCl₃



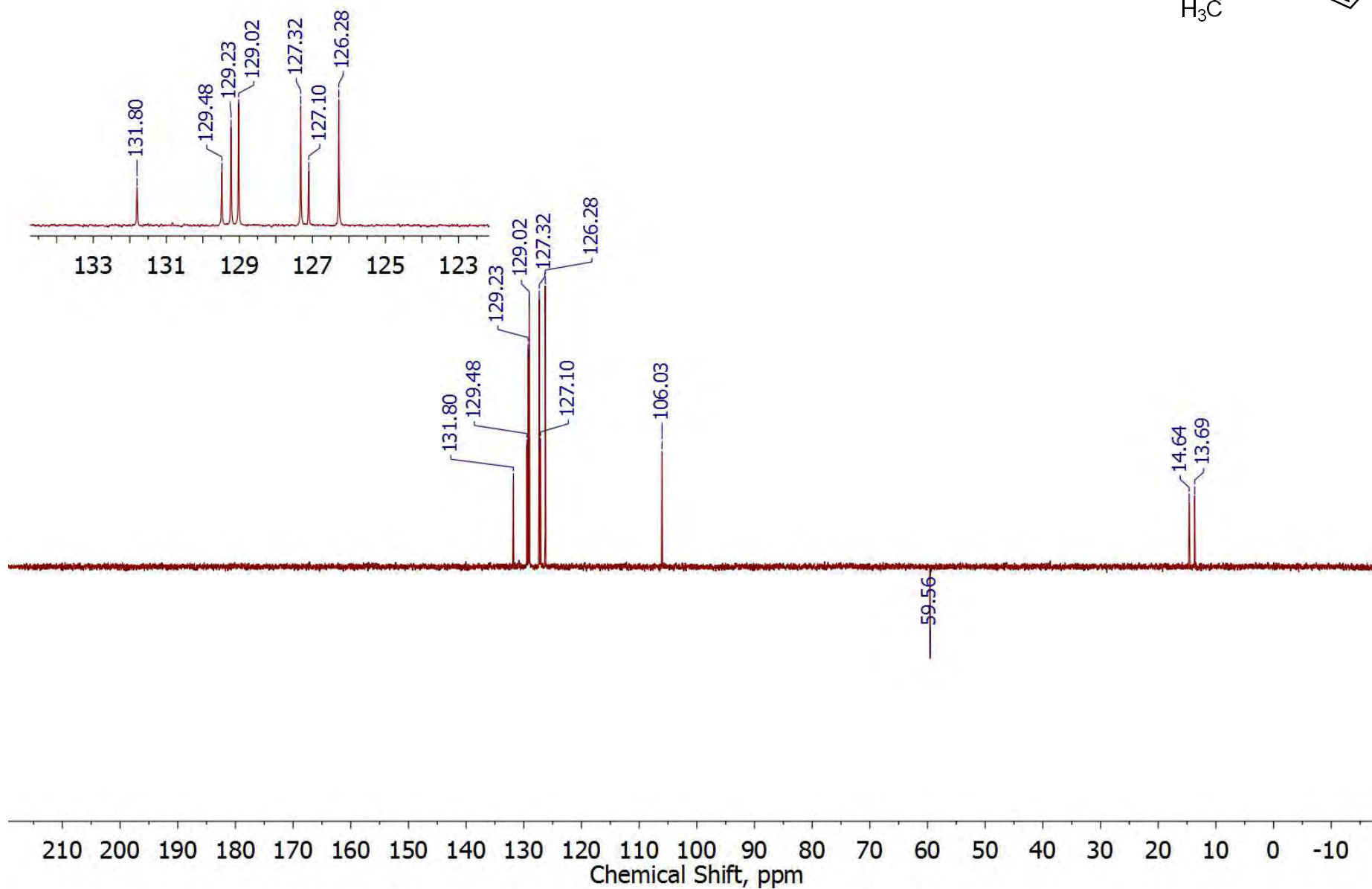
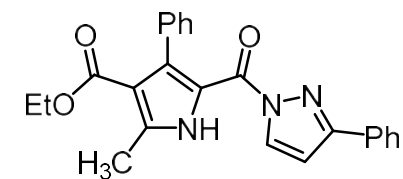
Ethyl 2-methyl-4-phenyl-5-(3-phenyl-1*H*-pyrazole-1-carbonyl)-1*H*-pyrrole-3-carboxylate (6d), 400 (¹H) MHz, CDCl₃



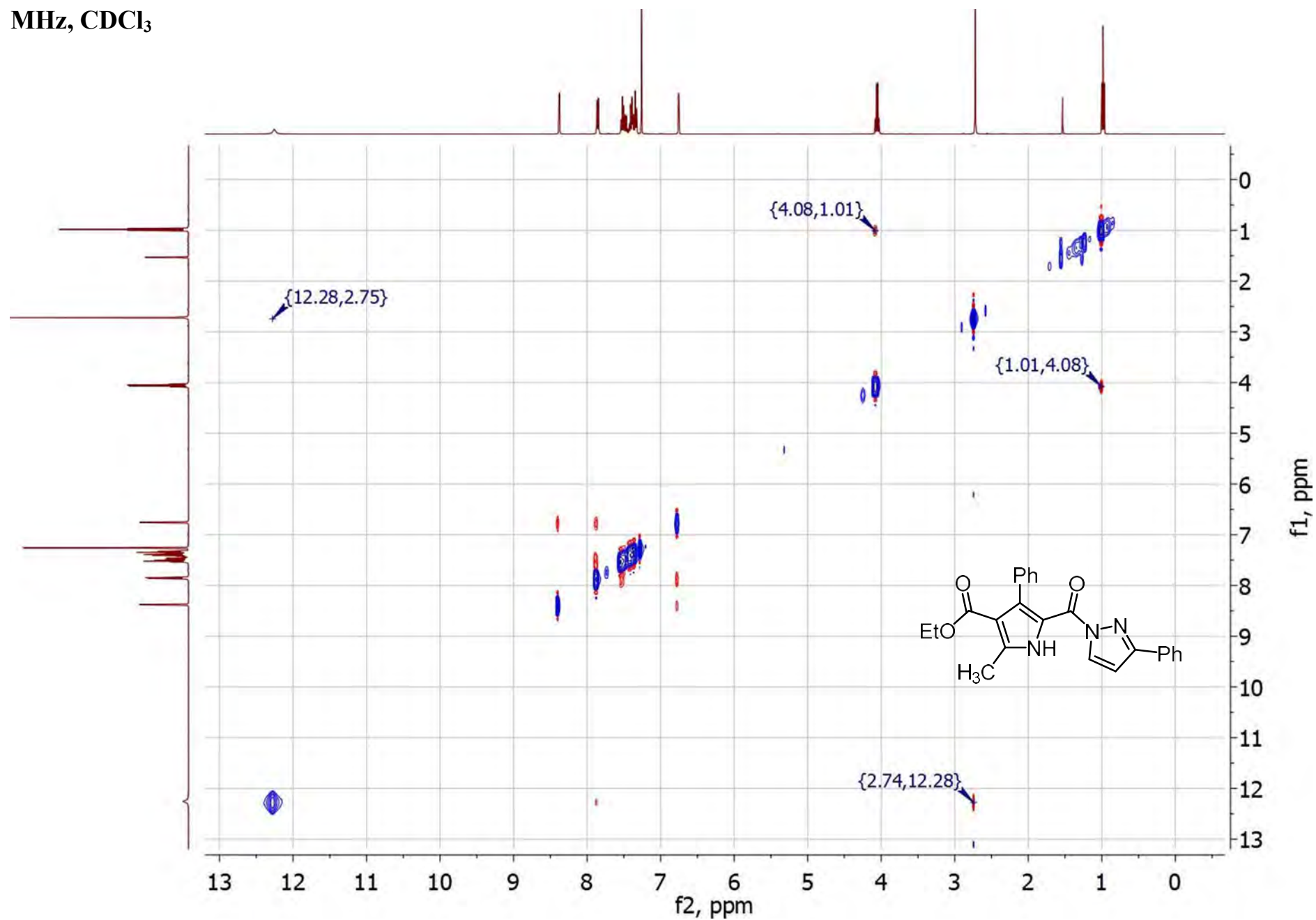
Ethyl 2-methyl-4-phenyl-5-(3-phenyl-1*H*-pyrazole-1-carbonyl)-1*H*-pyrrole-3-carboxylate (6d), 100 (¹³C) MHz, CDCl₃



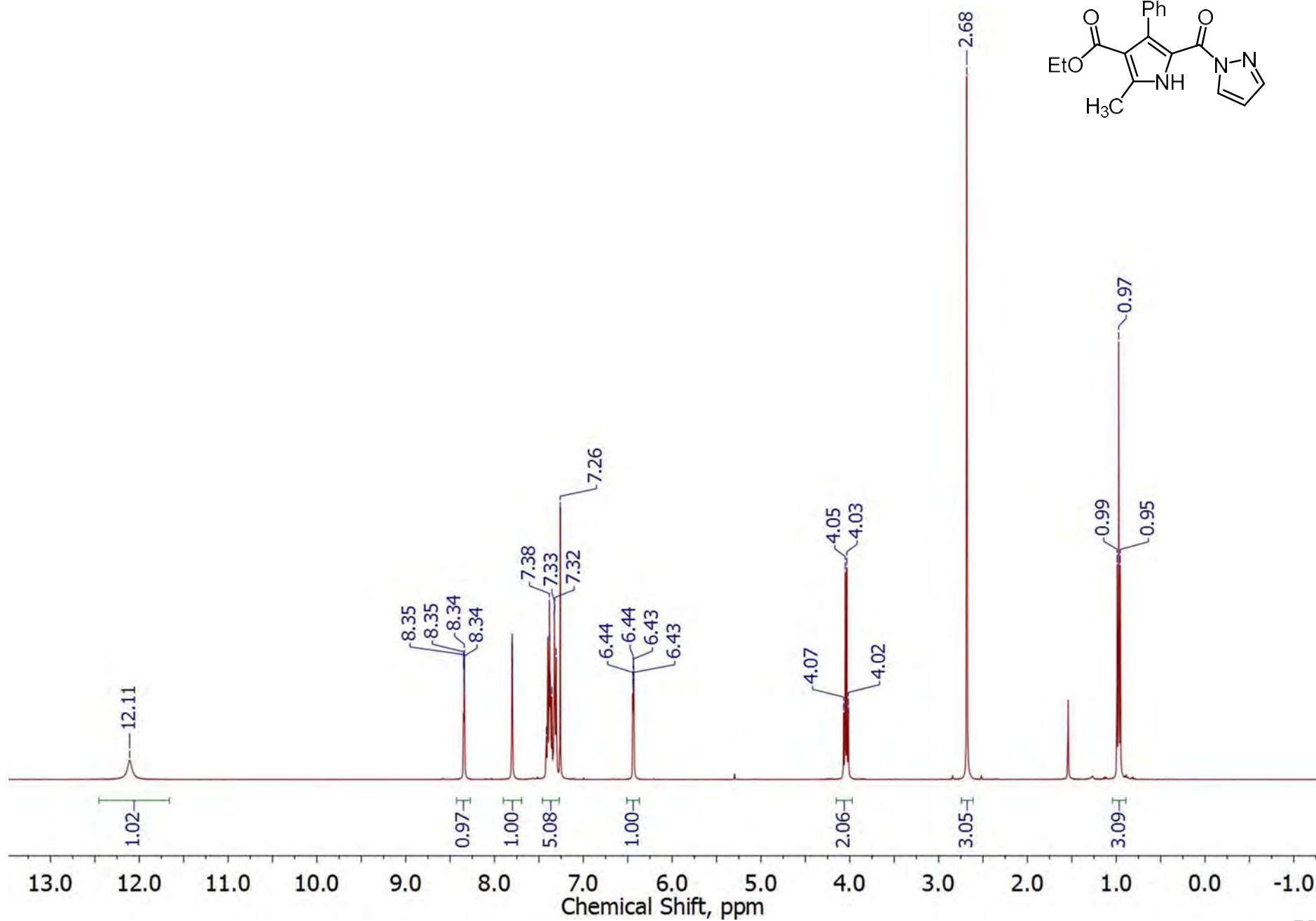
Ethyl 2-methyl-4-phenyl-5-(3-phenyl-1*H*-pyrazole-1-carbonyl)-1*H*-pyrrole-3-carboxylate (6d), 100 (DEPT) MHz, CDCl₃



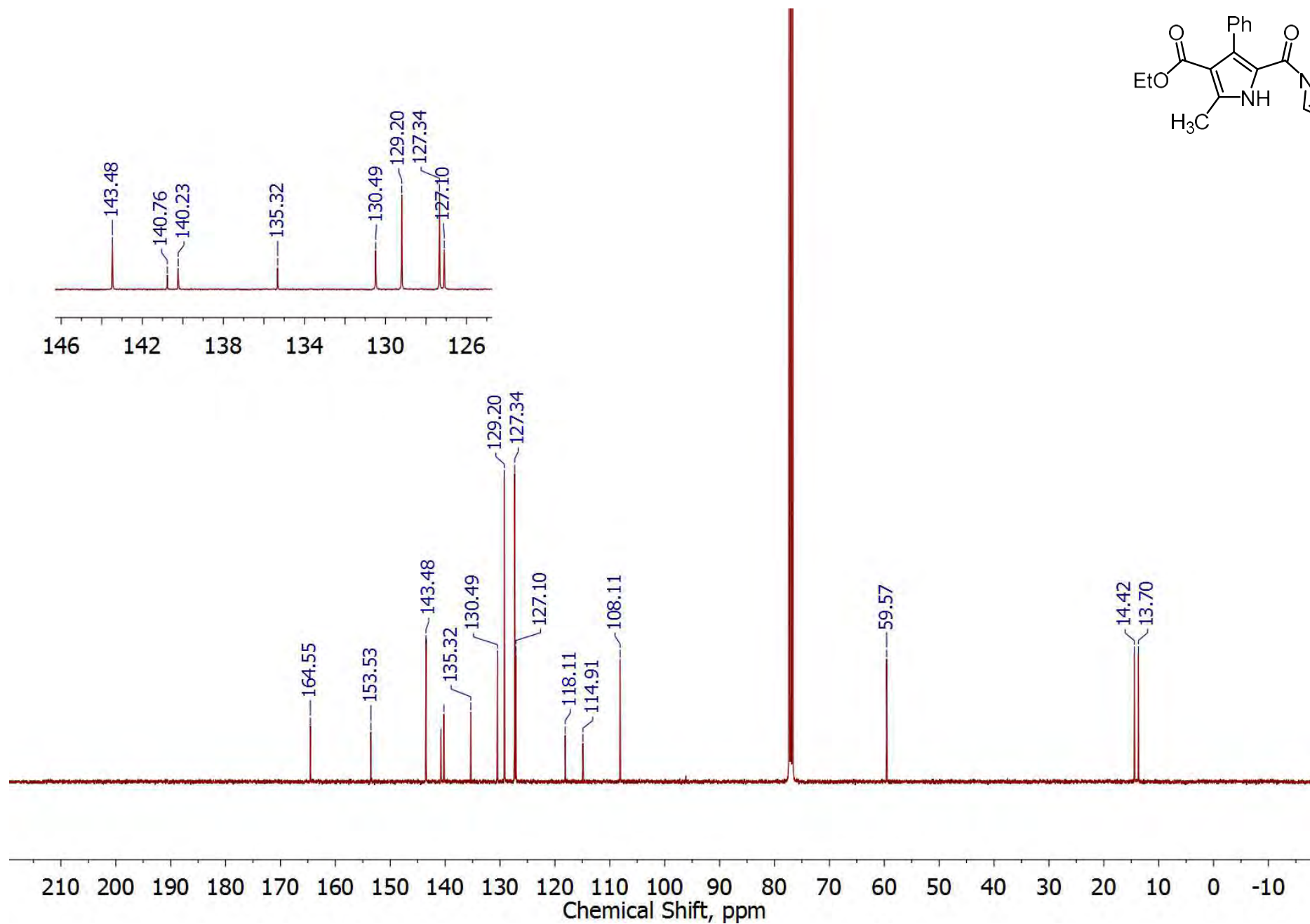
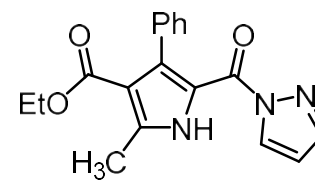
Ethyl 2-methyl-4-phenyl-5-(3-phenyl-1*H*-pyrazole-1-carbonyl)-1*H*-pyrrole-3-carboxylate (6d), 400 (2D ¹H NOESY)
MHz, CDCl₃



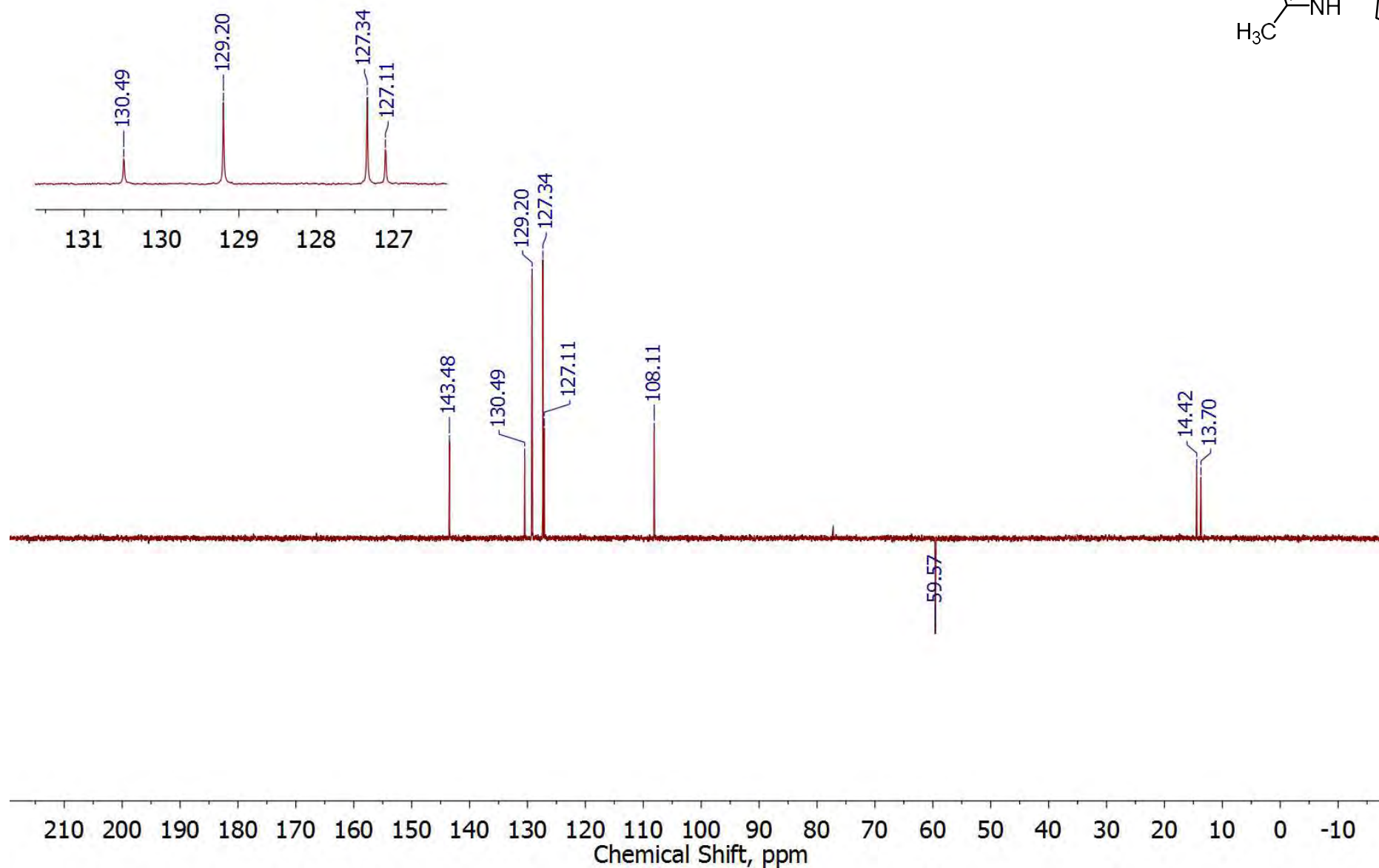
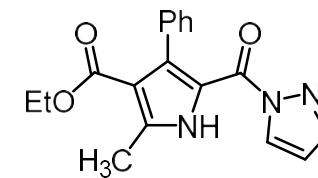
Ethyl 2-methyl-4-phenyl-5-(1*H*-pyrazole-1-carbonyl)-1*H*-pyrrole-3-carboxylate (6e), 400 (¹H) MHz, CDCl₃



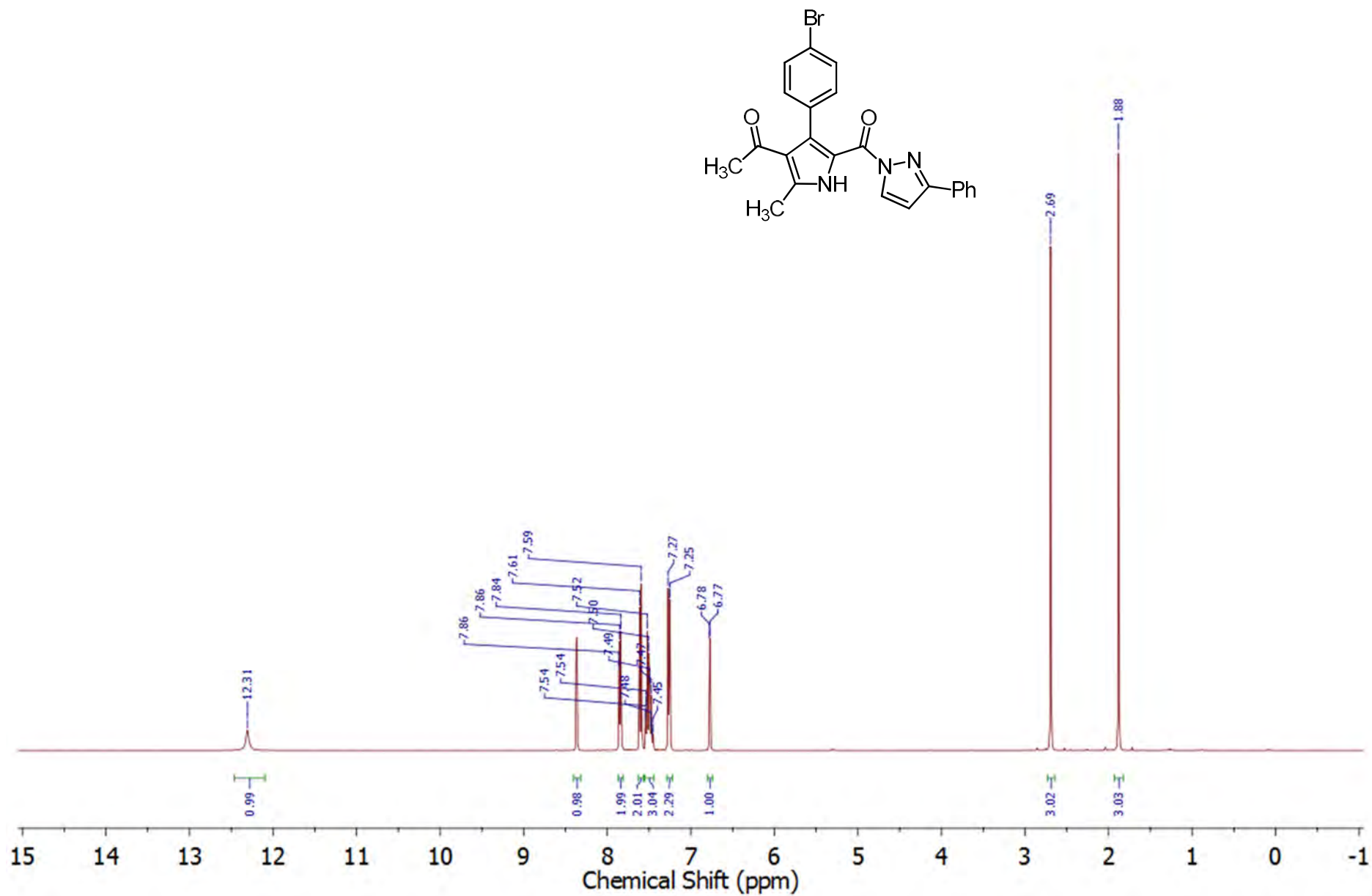
Ethyl 2-methyl-4-phenyl-5-(1*H*-pyrazole-1-carbonyl)-1*H*-pyrrole-3-carboxylate (6e), 100 (¹³C) MHz, CDCl₃



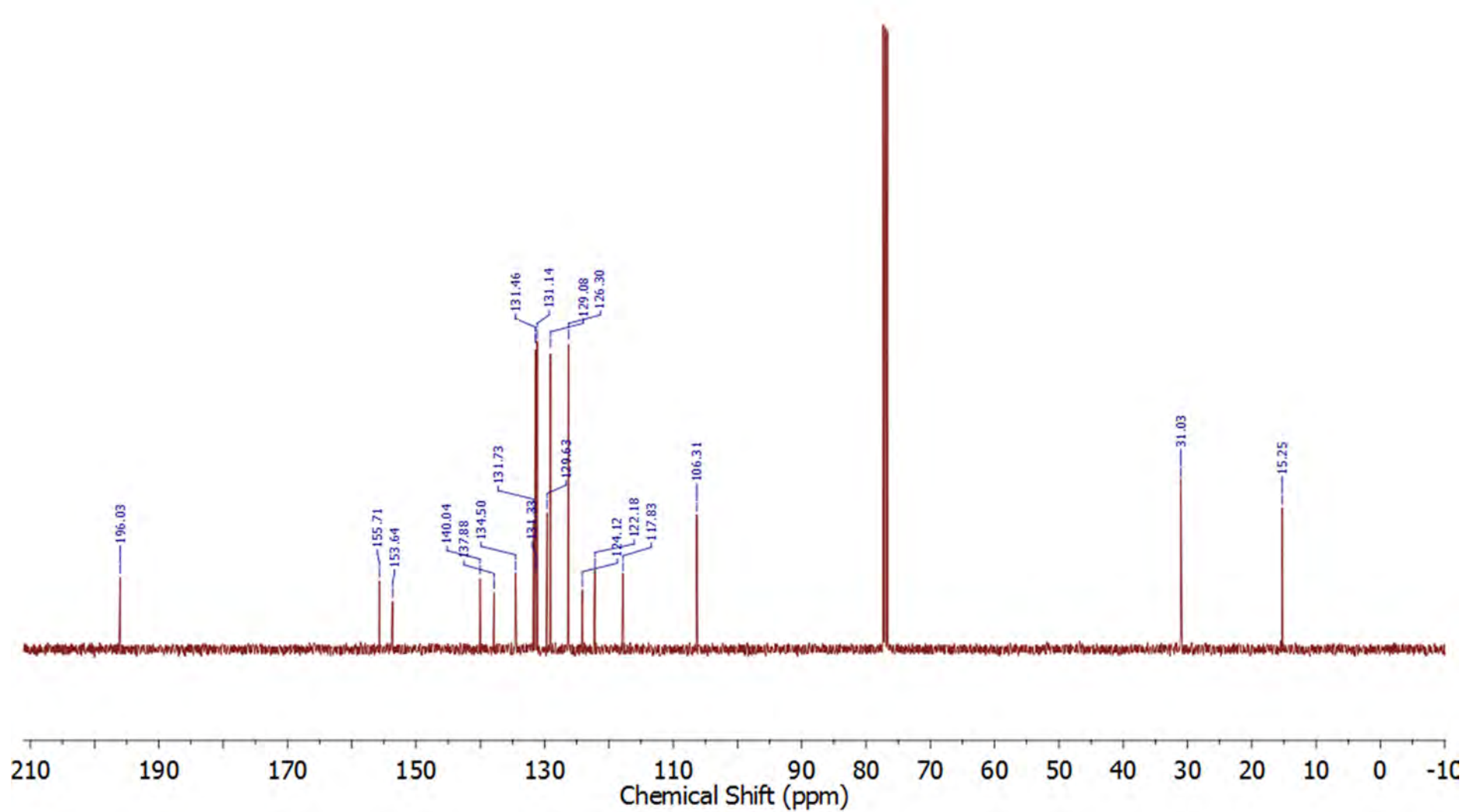
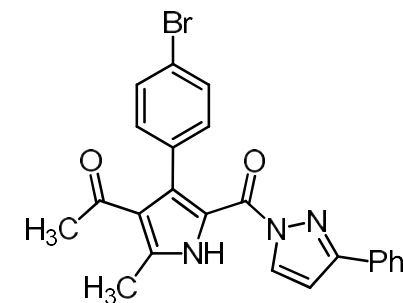
Ethyl 2-methyl-4-phenyl-5-(1*H*-pyrazole-1-carbonyl)-1*H*-pyrrole-3-carboxylate (6e), 100 (DEPT) MHz, CDCl₃



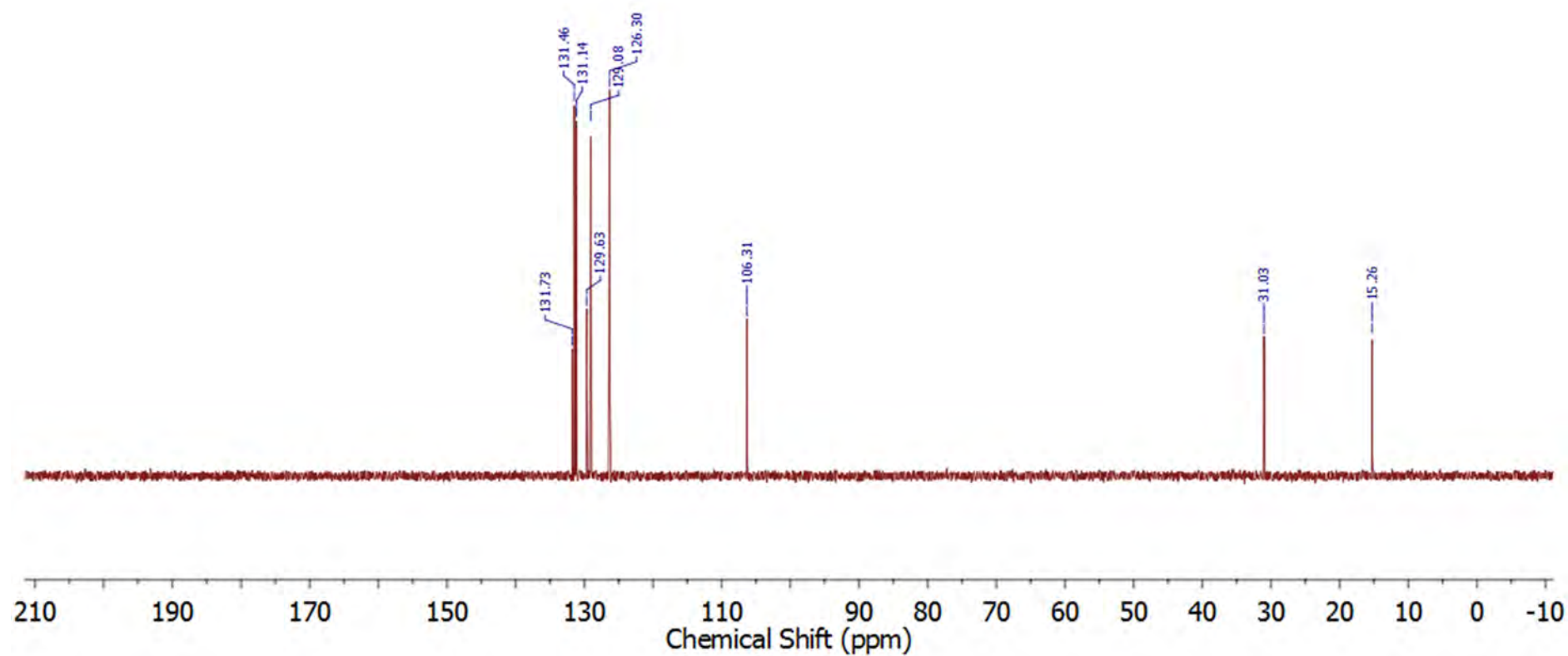
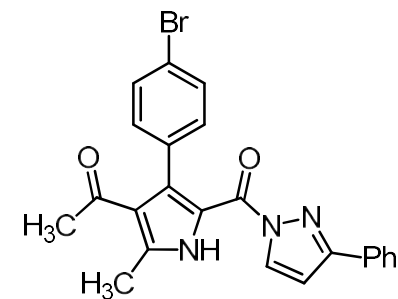
1-(4-(4-Bromophenyl)-2-methyl-5-(3-phenyl-1*H*-pyrazole-1-carbonyl)-1*H*-pyrrol-3-yl)ethanone (6f), 400 (¹H) MHz, CDCl₃



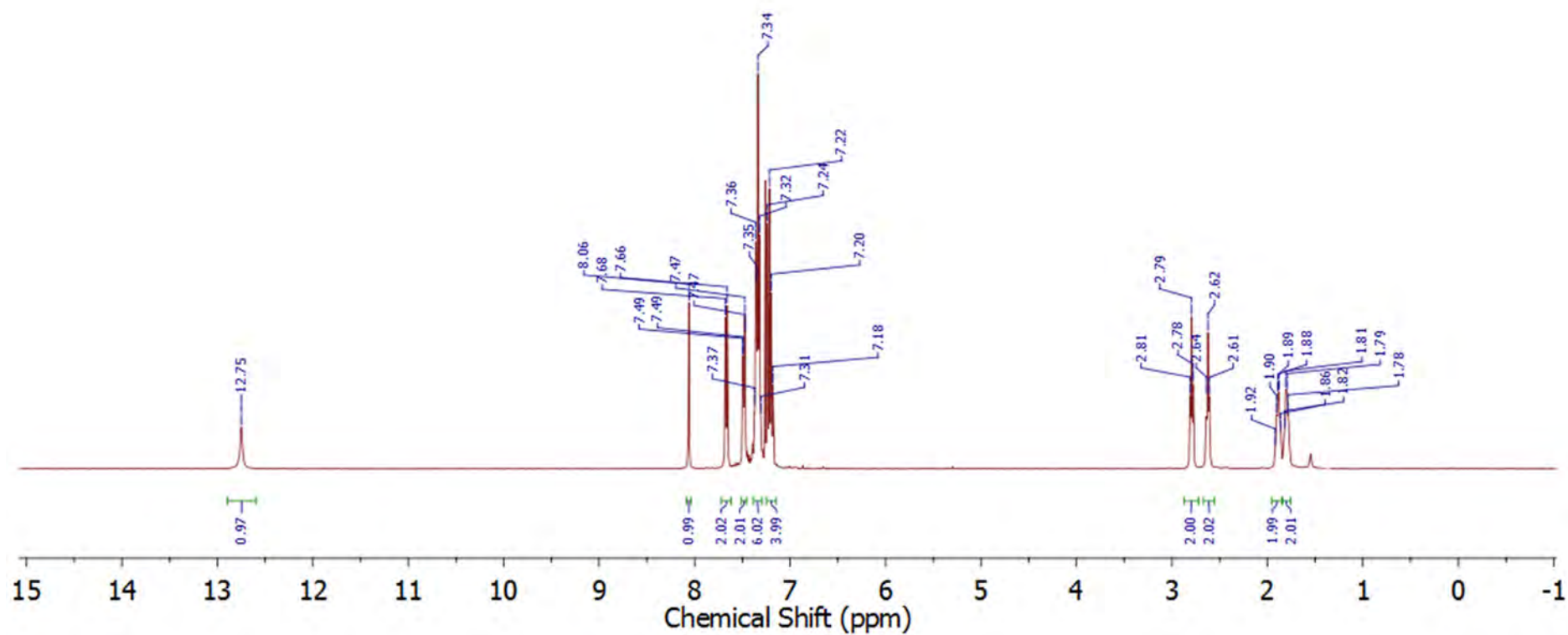
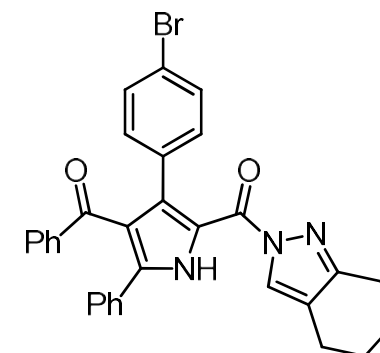
1-(4-(4-Bromophenyl)-2-methyl-5-(3-phenyl-1*H*-pyrazole-1-carbonyl)-1*H*-pyrrol-3-yl)ethanone (6f), 100 (¹³C) MHz, CDCl₃



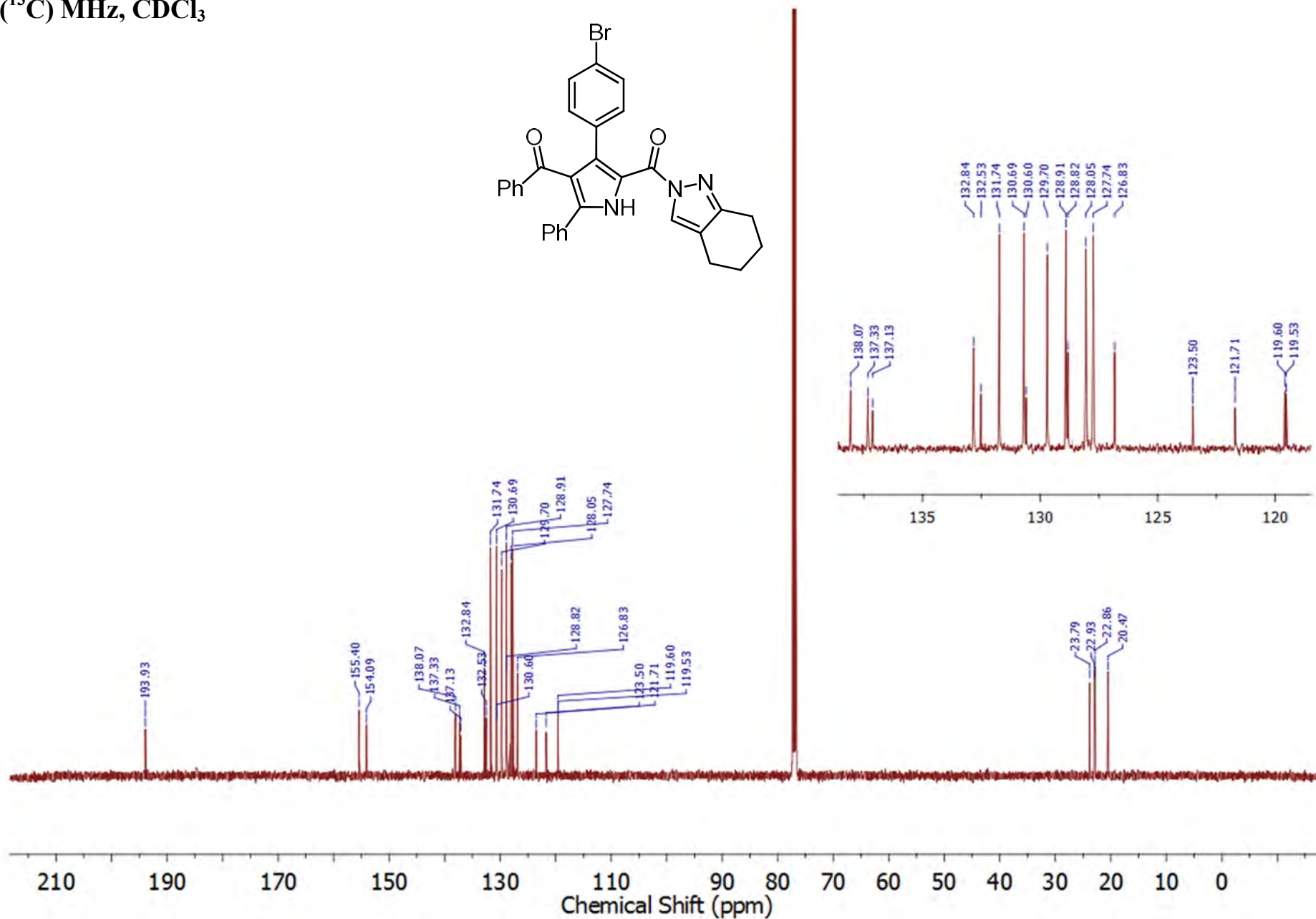
1-(4-(4-Bromophenyl)-2-methyl-5-(3-phenyl-1*H*-pyrazole-1-carbonyl)-1*H*-pyrrol-3-yl)ethanone (6f), 100 (DEPT)
MHz, CDCl₃



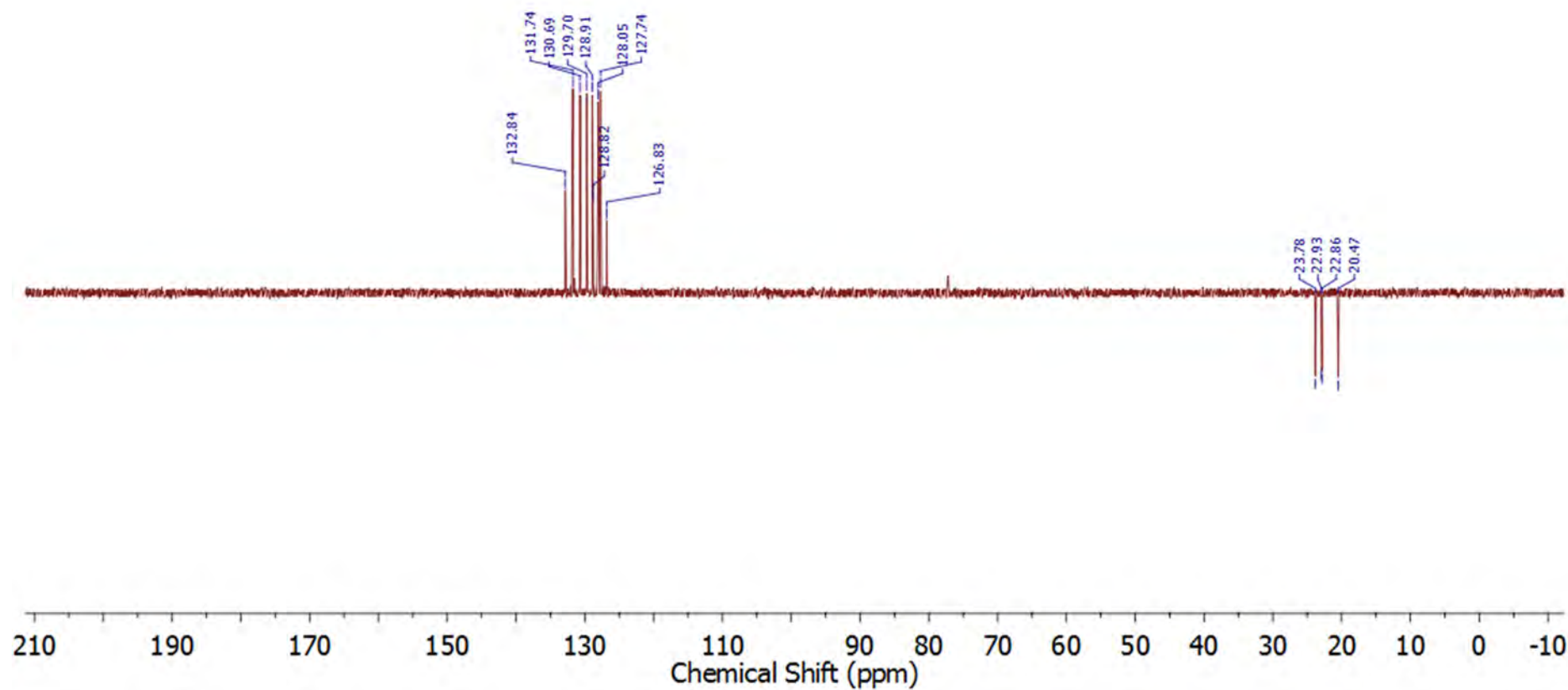
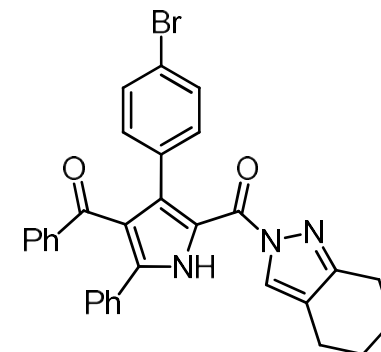
(4-Benzoyl-3-(4-bromophenyl)-5-phenyl-1*H*-pyrrol-2-yl)(4,5,6,7-tetrahydro-2*H*-indazol-2-yl)methanone (6g), 400 (¹H) MHz, CDCl₃



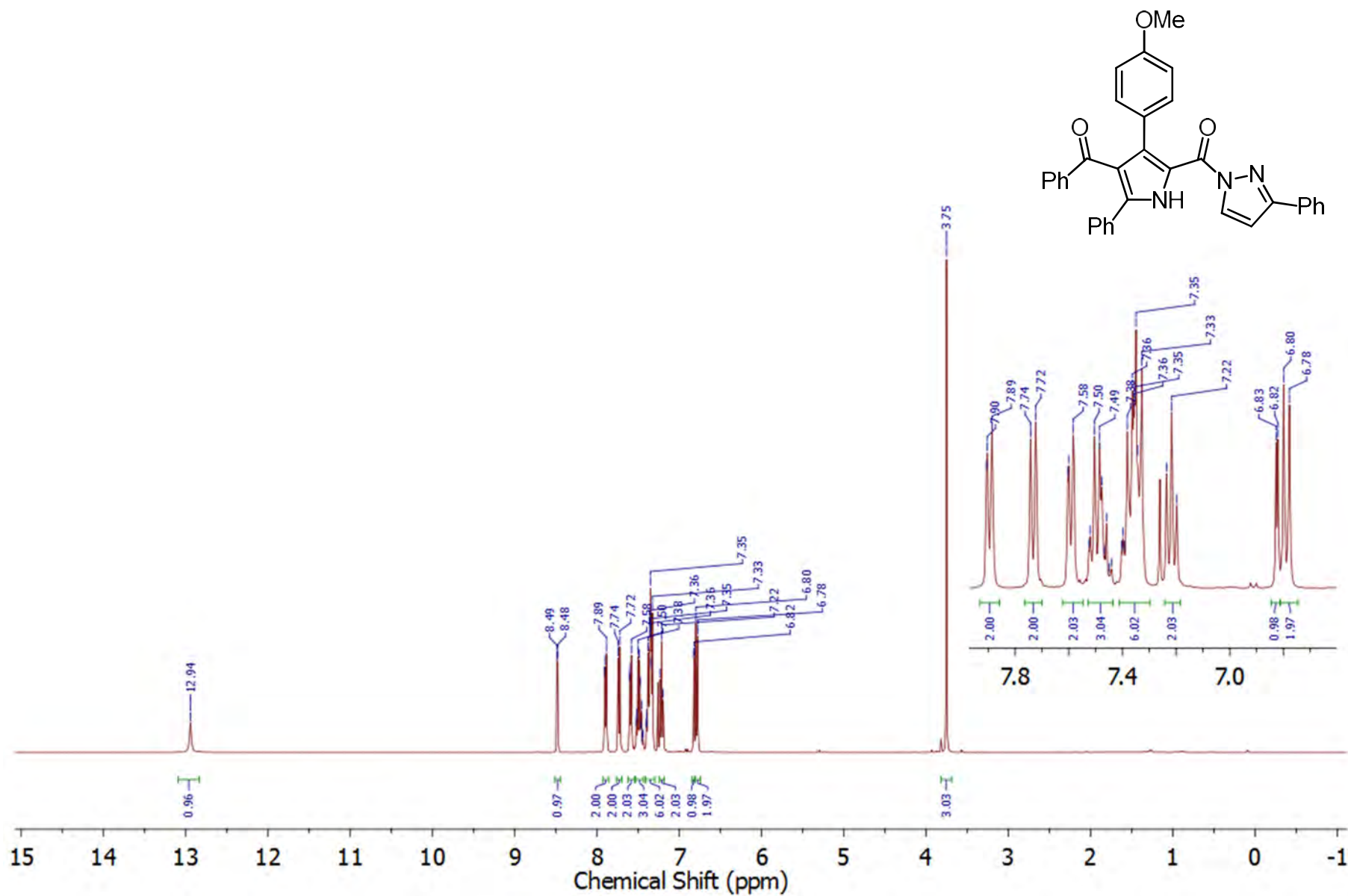
(4-Benzoyl-3-(4-bromophenyl)-5-phenyl-1*H*-pyrrol-2-yl)(4,5,6,7-tetrahydro-2*H*-indazol-2-yl)methanone (6g), 100
¹³C) MHz, CDCl₃



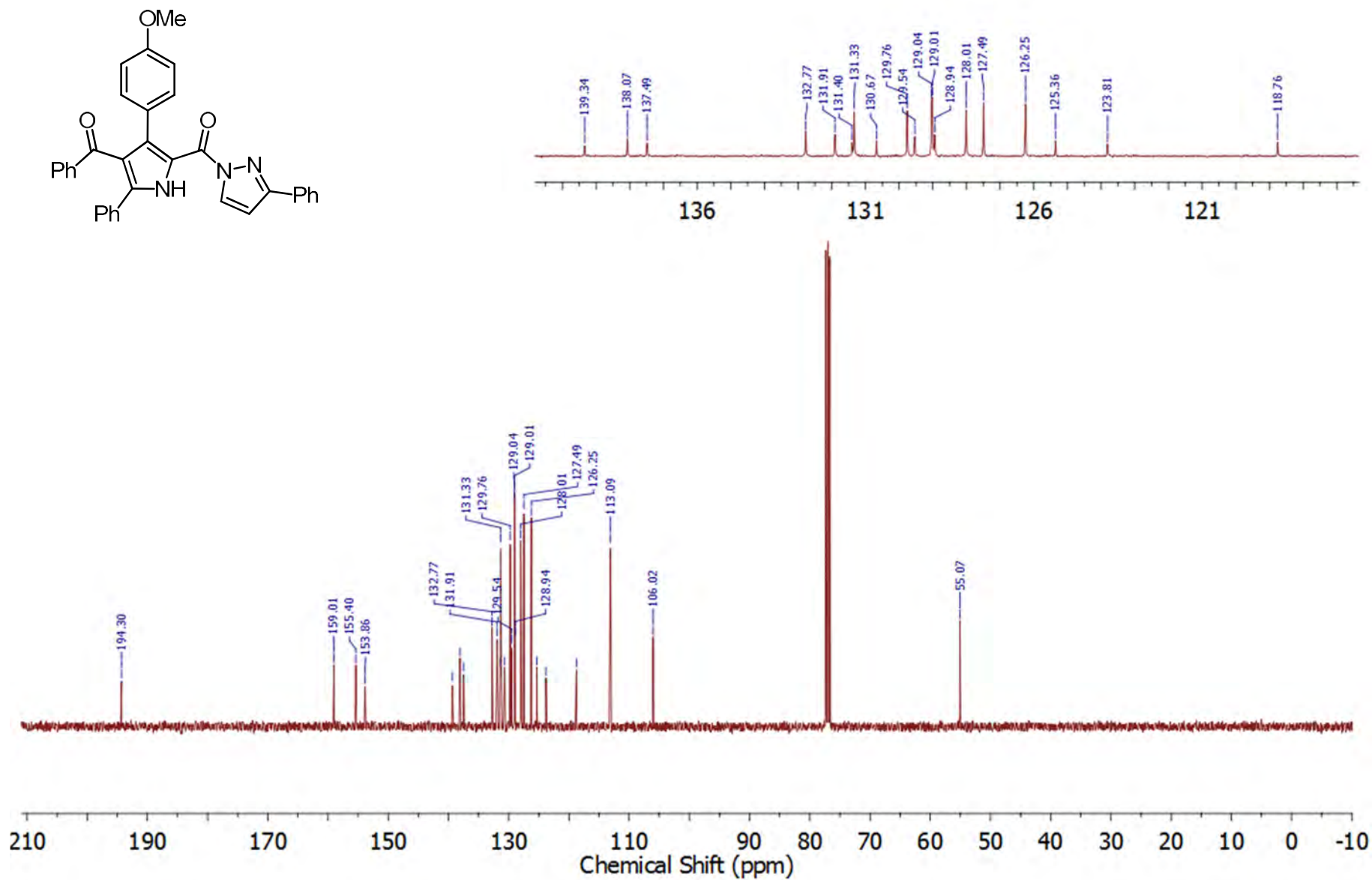
(4-Benzoyl-3-(4-bromophenyl)-5-phenyl-1*H*-pyrrol-2-yl)(4,5,6,7-tetrahydro-2*H*-indazol-2-yl)methanone (6g), 100 (DEPT) MHz, CDCl₃



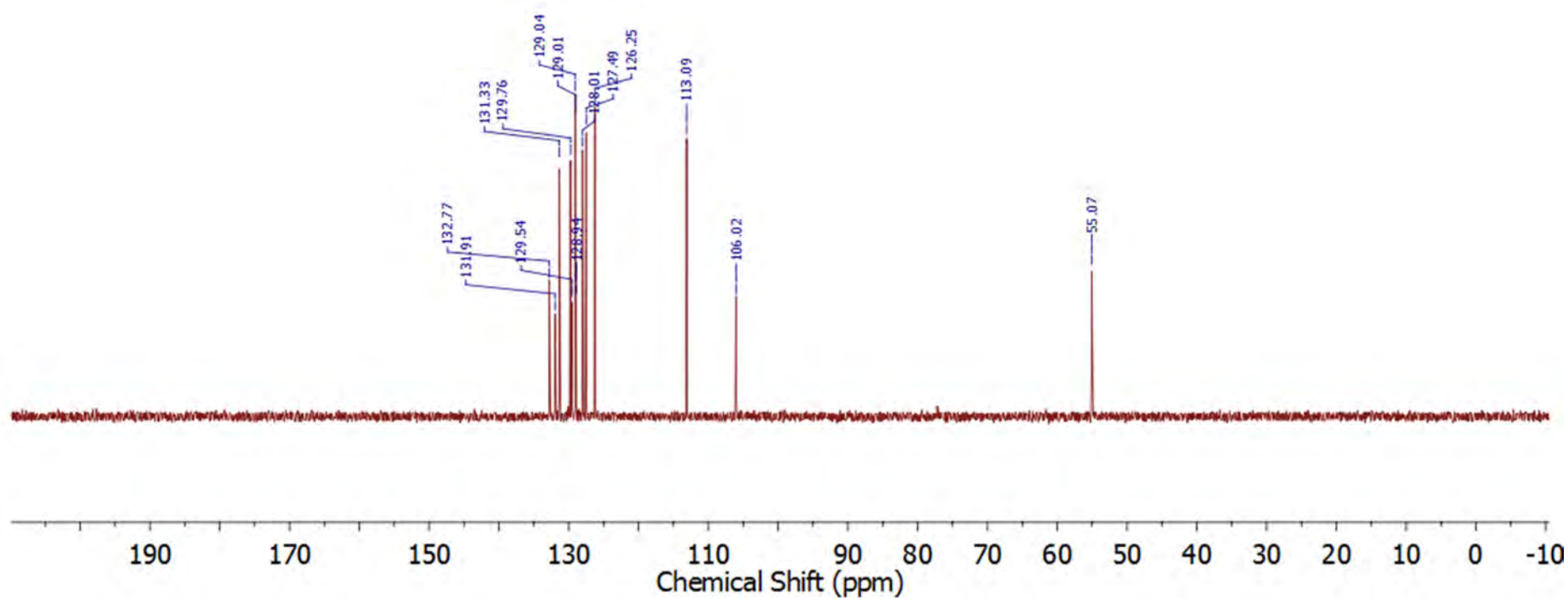
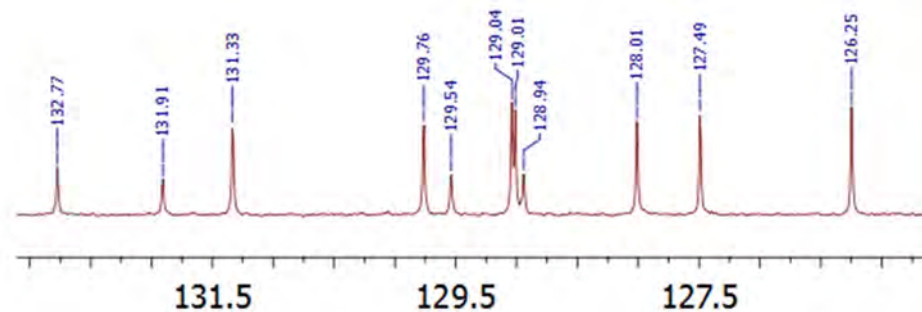
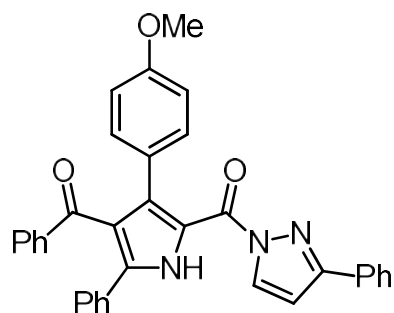
(4-Benzoyl-3-(4-methoxyphenyl)-5-phenyl-1*H*-pyrrol-2-yl)(3-phenyl-1*H*-pyrazol-1-yl)methanone (6h), 400 (¹H) MHz, CDCl₃



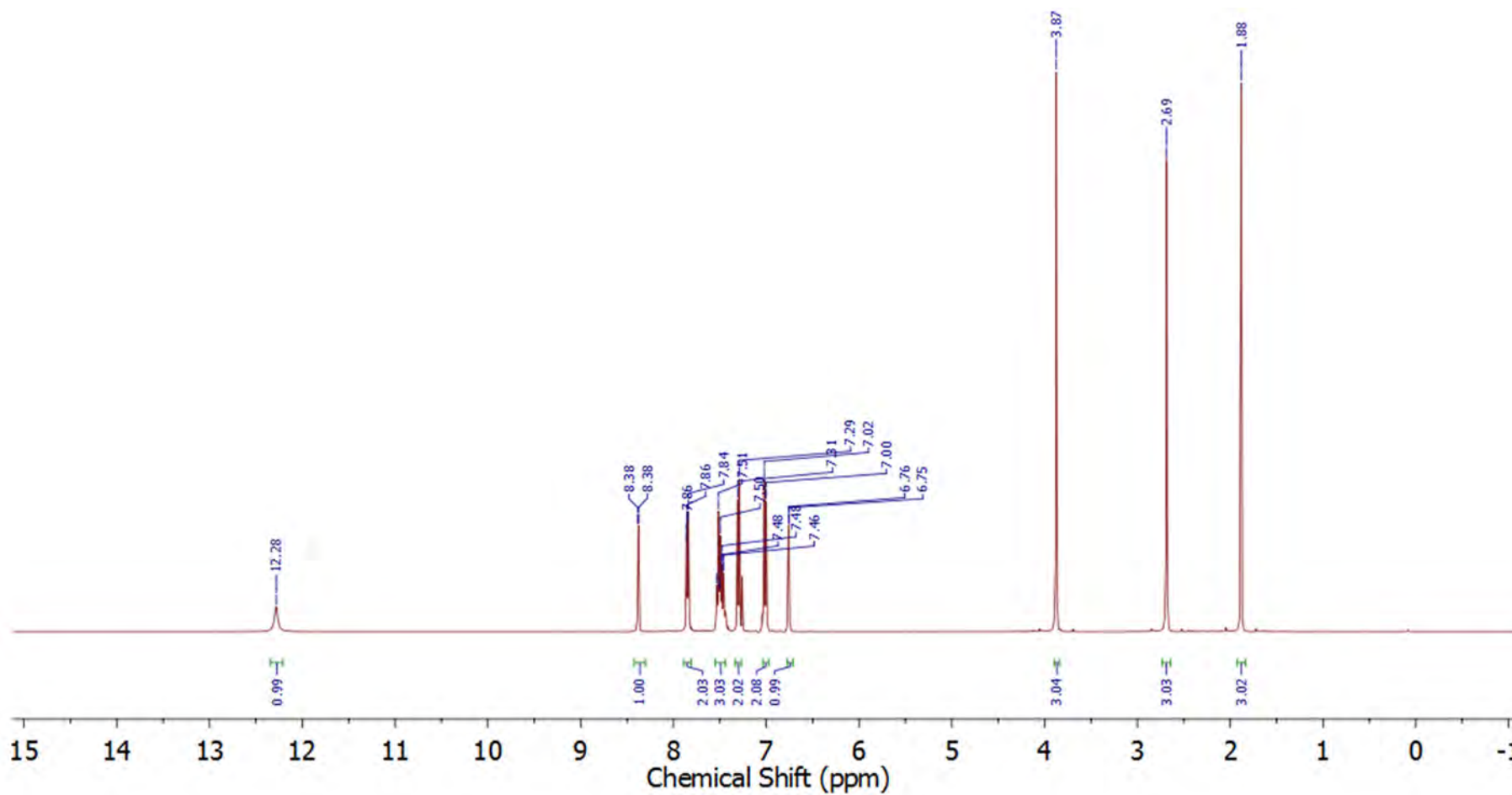
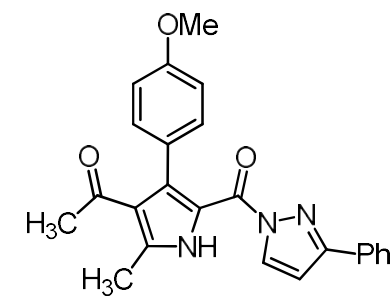
(4-Benzoyl-3-(4-methoxyphenyl)-5-phenyl-1*H*-pyrrol-2-yl)(3-phenyl-1*H*-pyrazol-1-yl)methanone (6h), 100 (^{13}C) MHz, CDCl_3



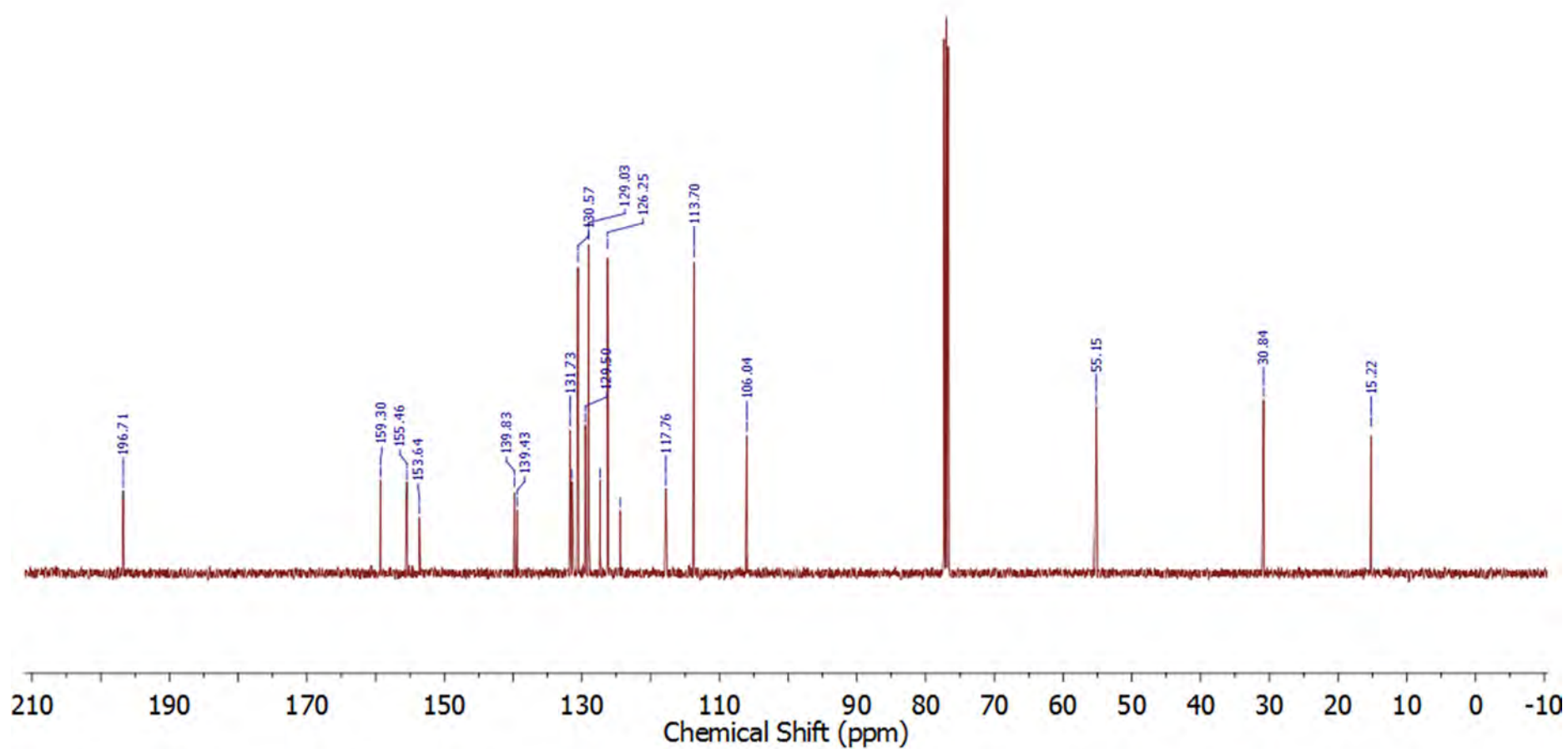
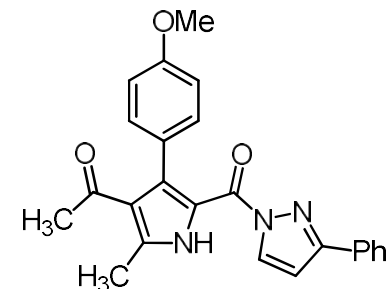
(4-Benzoyl-3-(4-methoxyphenyl)-5-phenyl-1*H*-pyrrol-2-yl)(3-phenyl-1*H*-pyrazol-1-yl)methanone (6h), 100 (DEPT) MHz, CDCl₃



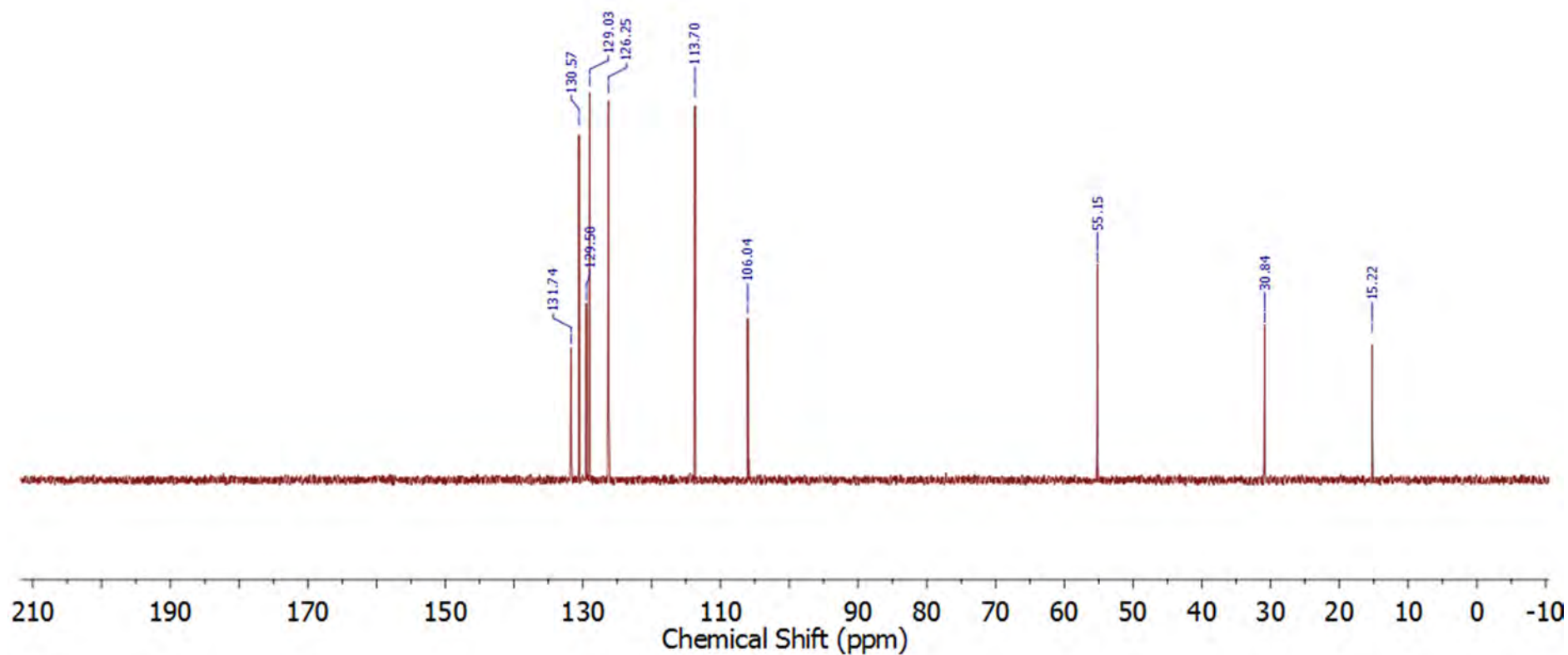
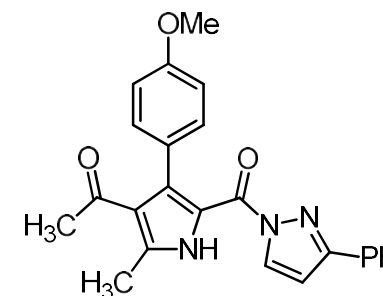
1-(4-(4-Methoxyphenyl)-2-methyl-5-(3-phenyl-1*H*-pyrazole-1-carbonyl)-1*H*-pyrrol-3-yl)ethanone (6i), 400 (¹H) MHz, CDCl₃



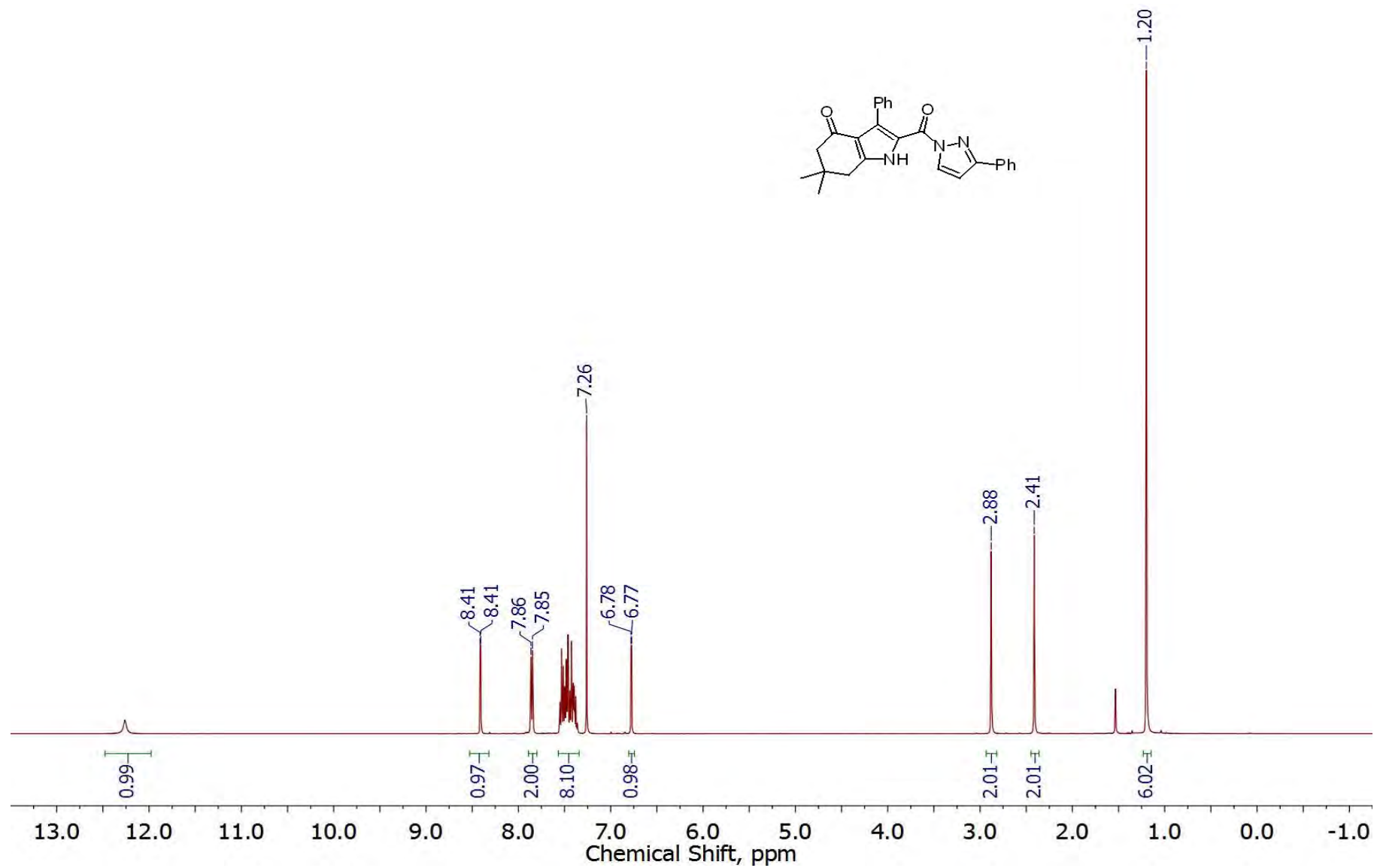
1-(4-(4-Methoxyphenyl)-2-methyl-5-(3-phenyl-1*H*-pyrazole-1-carbonyl)-1*H*-pyrrol-3-yl)ethanone (6i), 100 (¹³C) MHz, CDCl₃



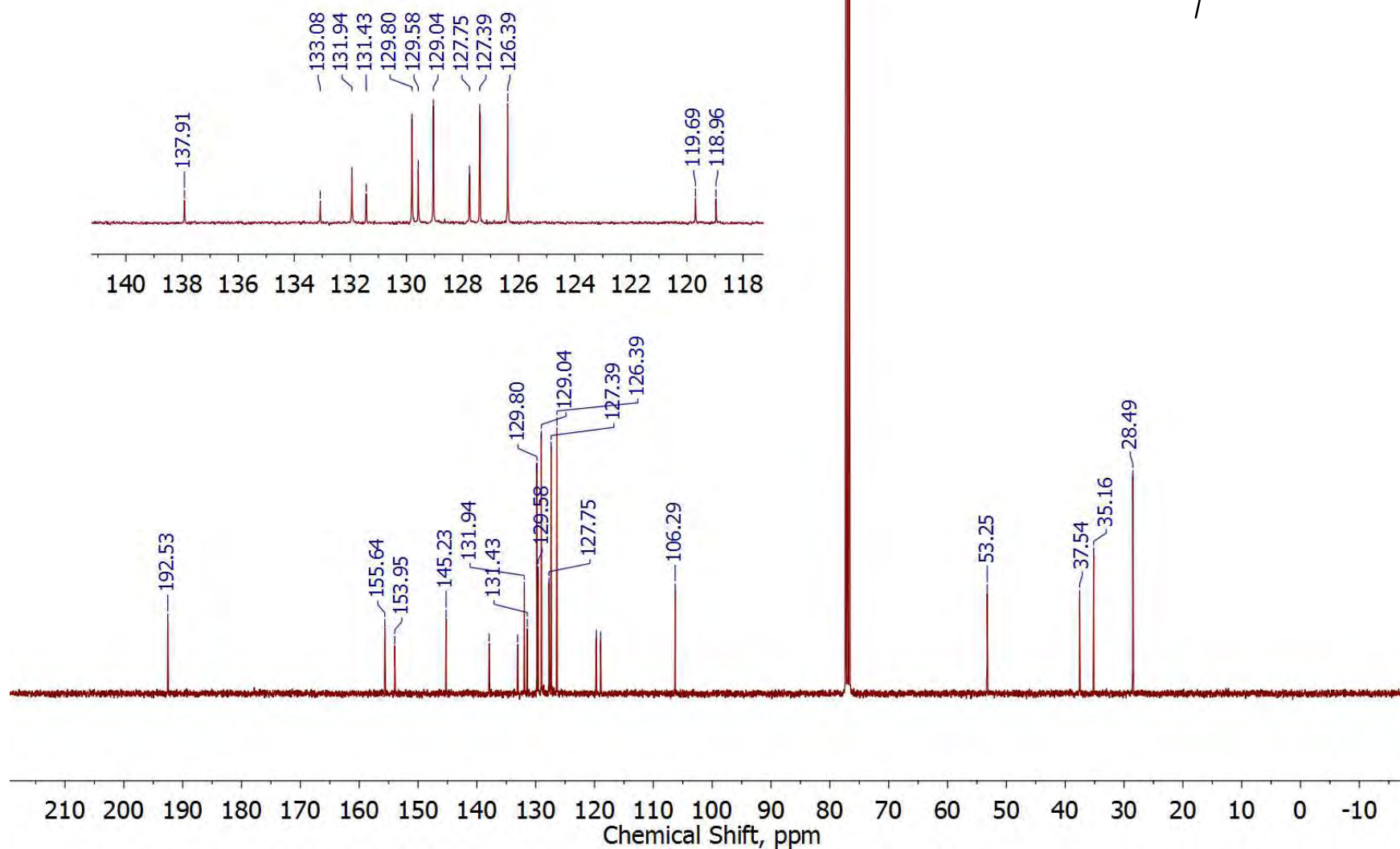
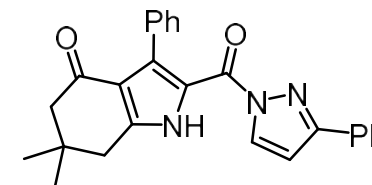
1-(4-(4-Methoxyphenyl)-2-methyl-5-(3-phenyl-1*H*-pyrazole-1-carbonyl)-1*H*-pyrrol-3-yl)ethanone (6i), 100 (DEPT) MHz, CDCl₃



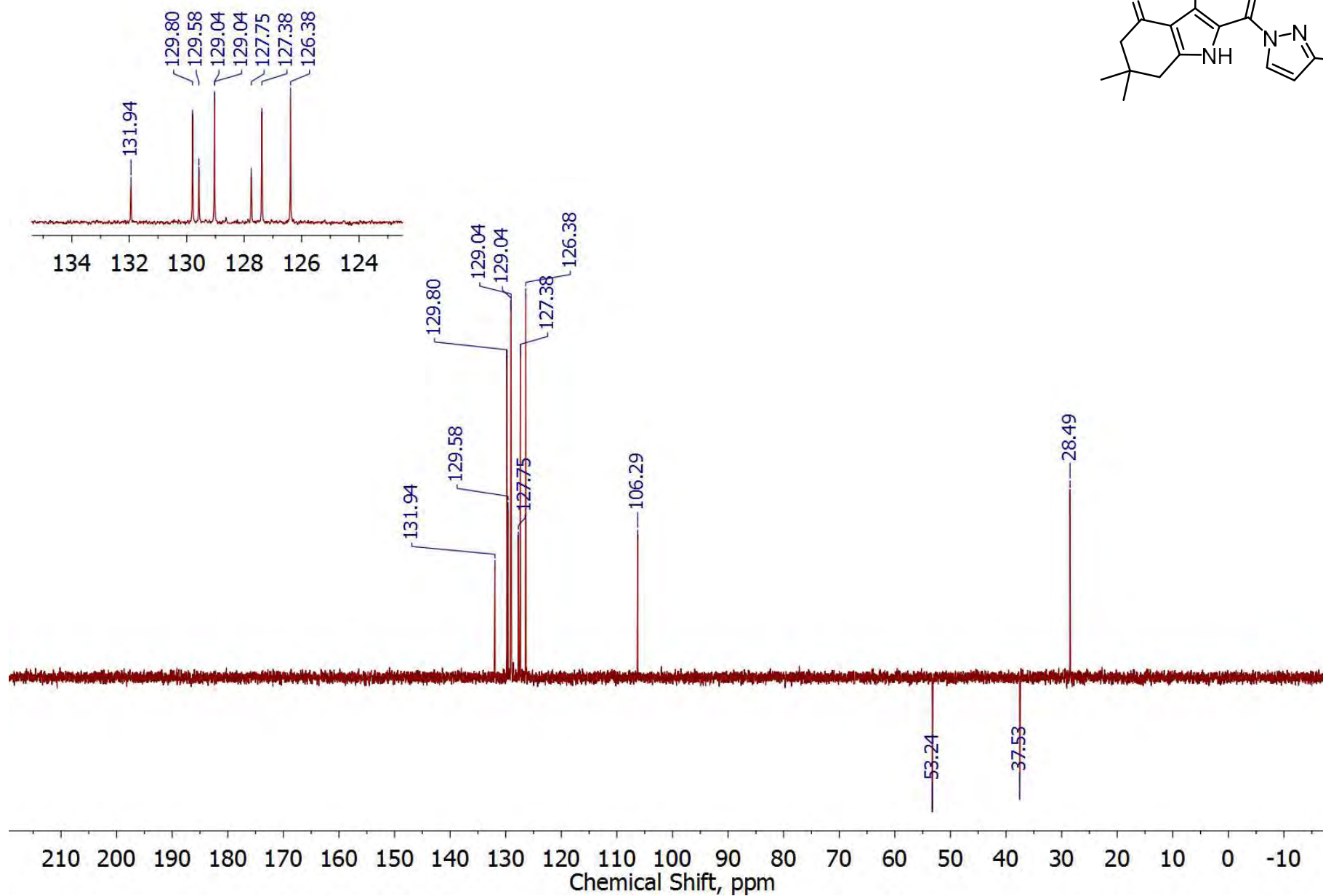
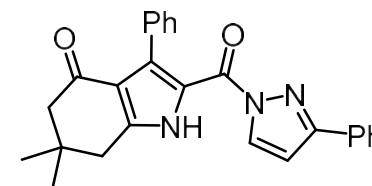
6,6-Dimethyl-3-phenyl-2-(3-phenyl-1*H*-pyrazole-1-carbonyl)-6,7-dihydro-1*H*-indol-4(5*H*)-one (6j), 400 (¹H) MHz, CDCl₃



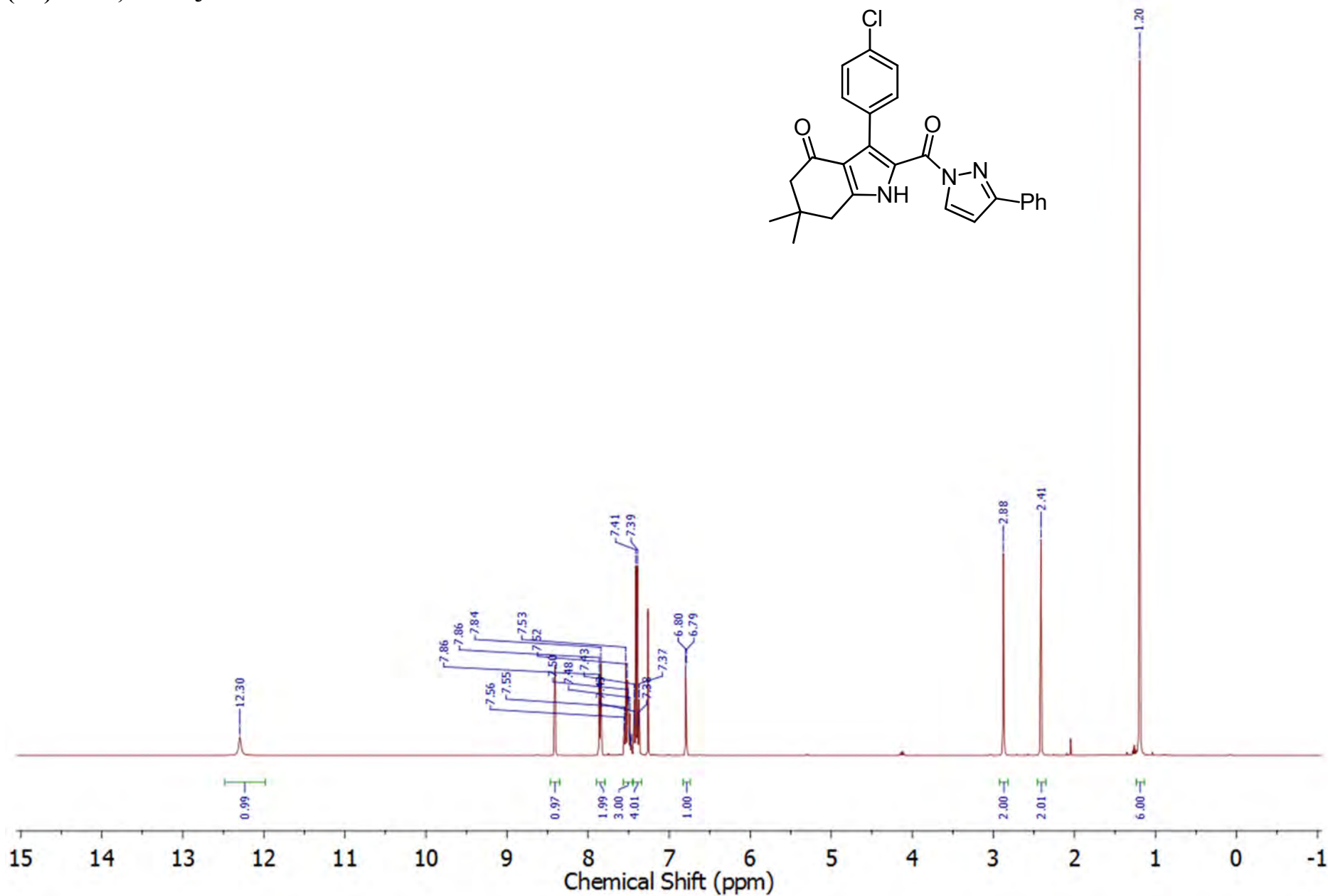
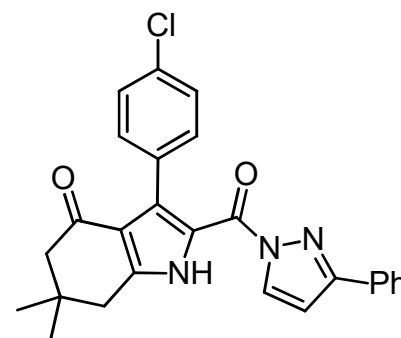
6,6-Dimethyl-3-phenyl-2-(3-phenyl-1*H*-pyrazole-1-carbonyl)-6,7-dihydro-1*H*-indol-4(5*H*)-one (6j), 100 (¹³C) MHz, CDCl₃



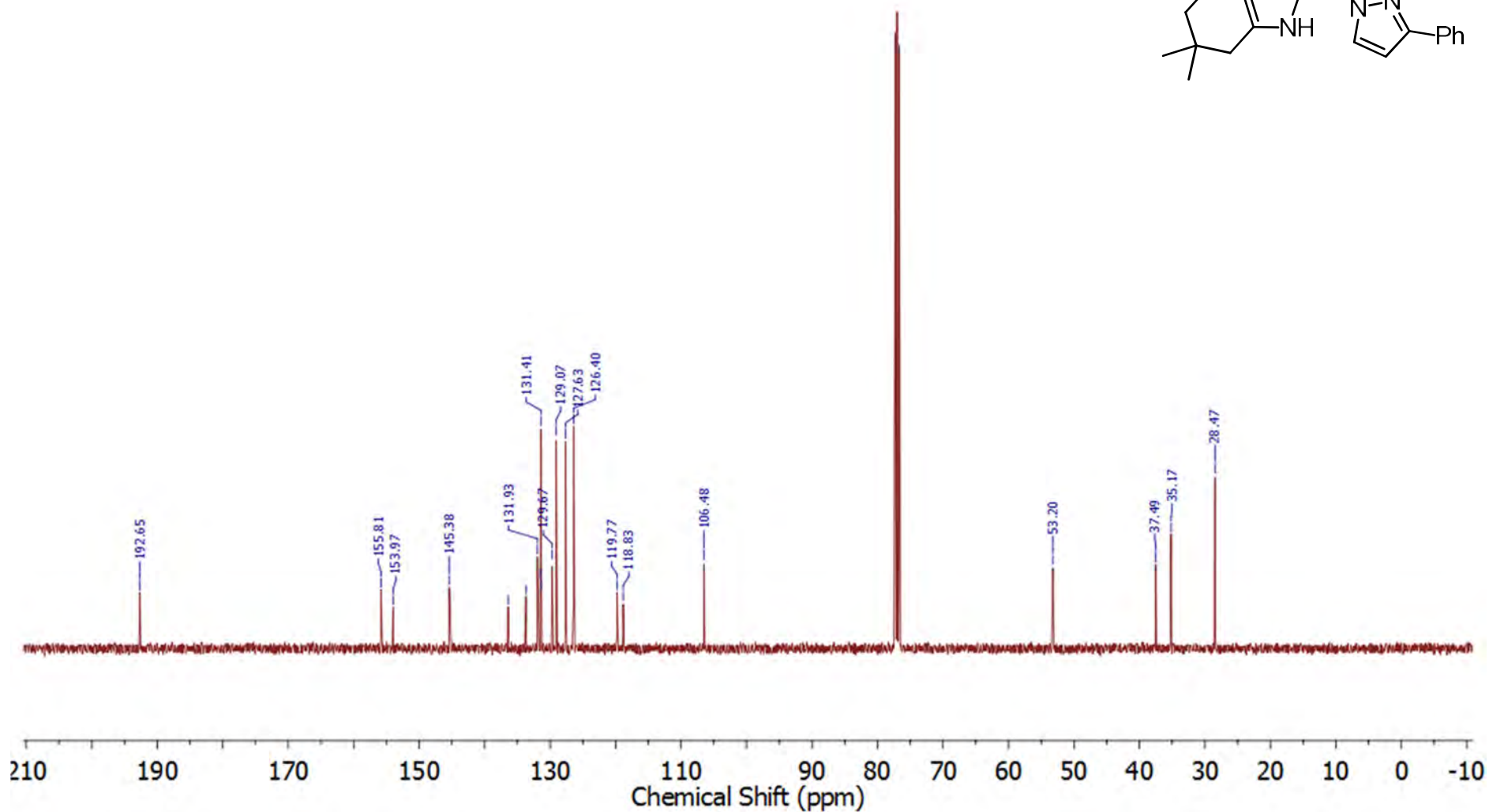
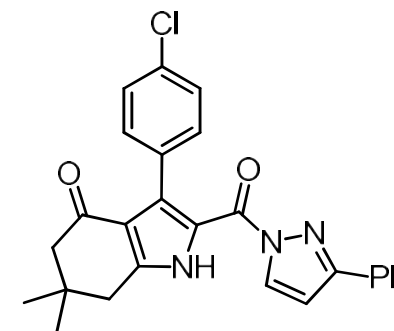
6,6-Dimethyl-3-phenyl-2-(3-phenyl-1*H*-pyrazole-1-carbonyl)-6,7-dihydro-1*H*-indol-4(5*H*)-one (6j), 100 (DEPT) MHz, CDCl₃



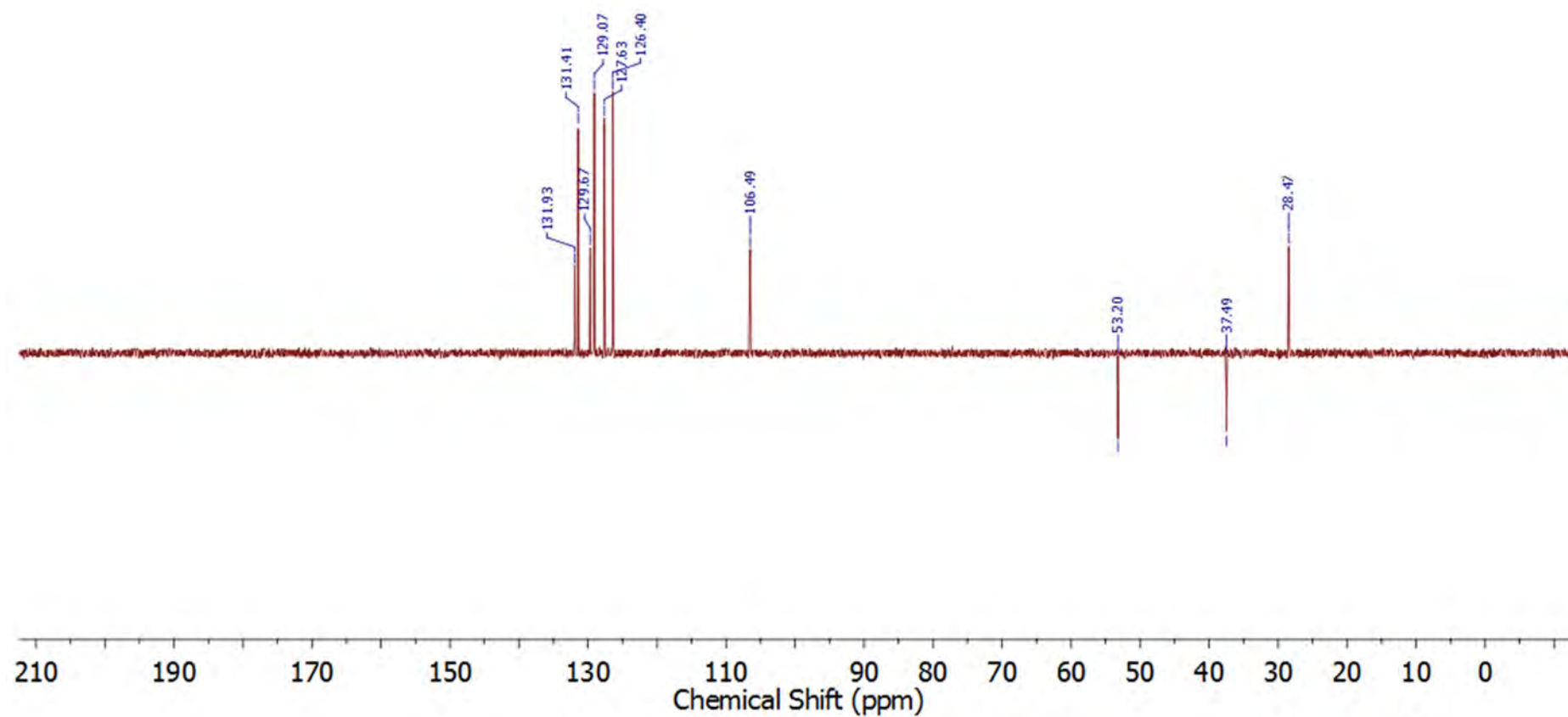
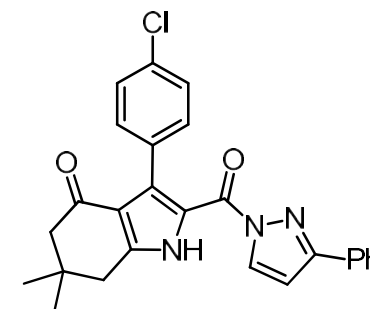
3-(4-Chlorophenyl)-6,6-dimethyl-2-(3-phenyl-1*H*-pyrazole-1-carbonyl)-6,7-dihydro-1*H*-indol-4(5*H*)-one (6k), 400 (¹H) MHz, CDCl₃



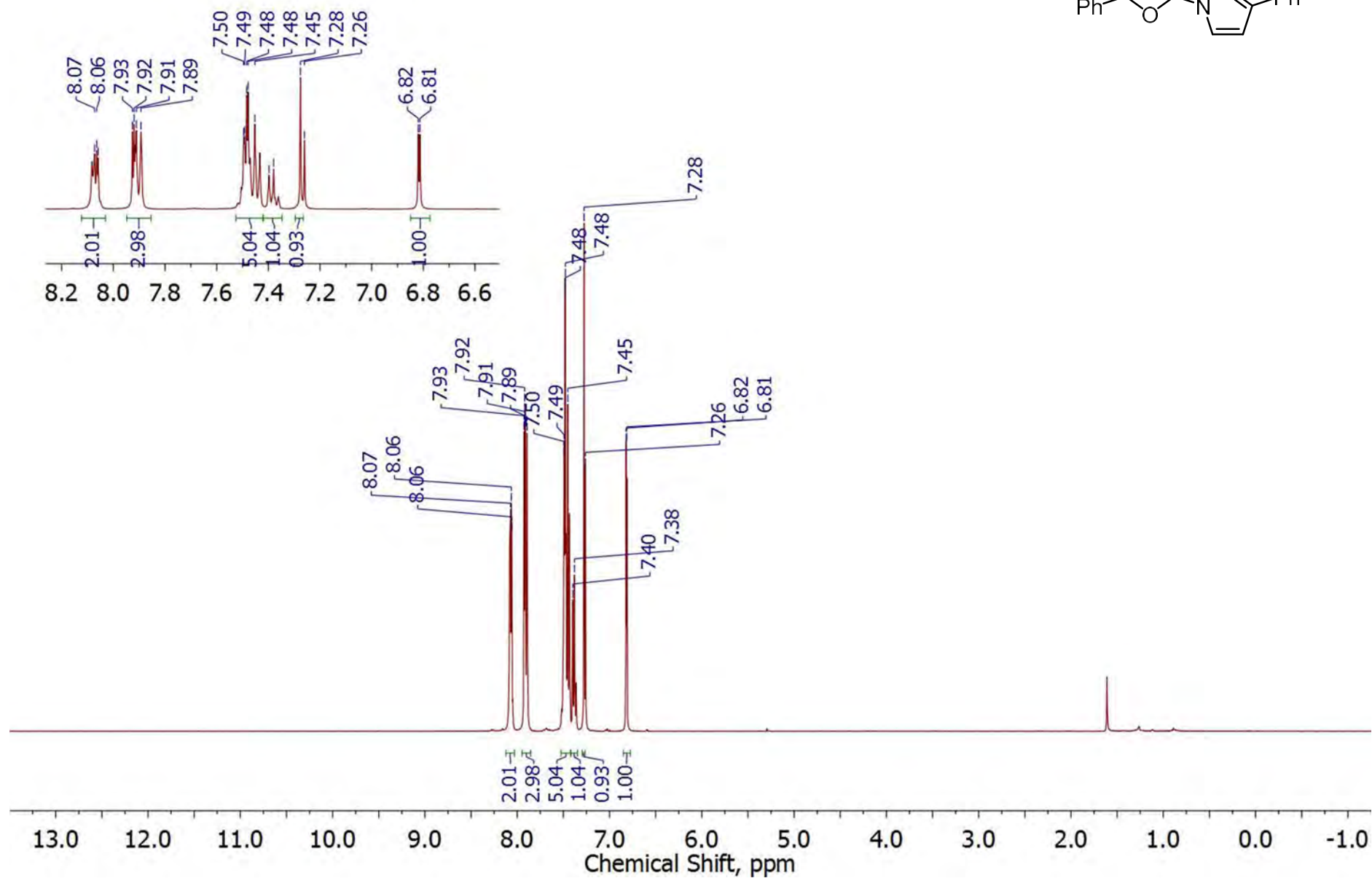
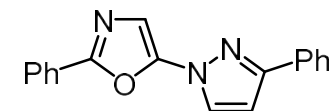
3-(4-Chlorophenyl)-6,6-dimethyl-2-(3-phenyl-1*H*-pyrazole-1-carbonyl)-6,7-dihydro-1*H*-indol-4(5*H*)-one (6k), 100 (¹³C) MHz, CDCl₃



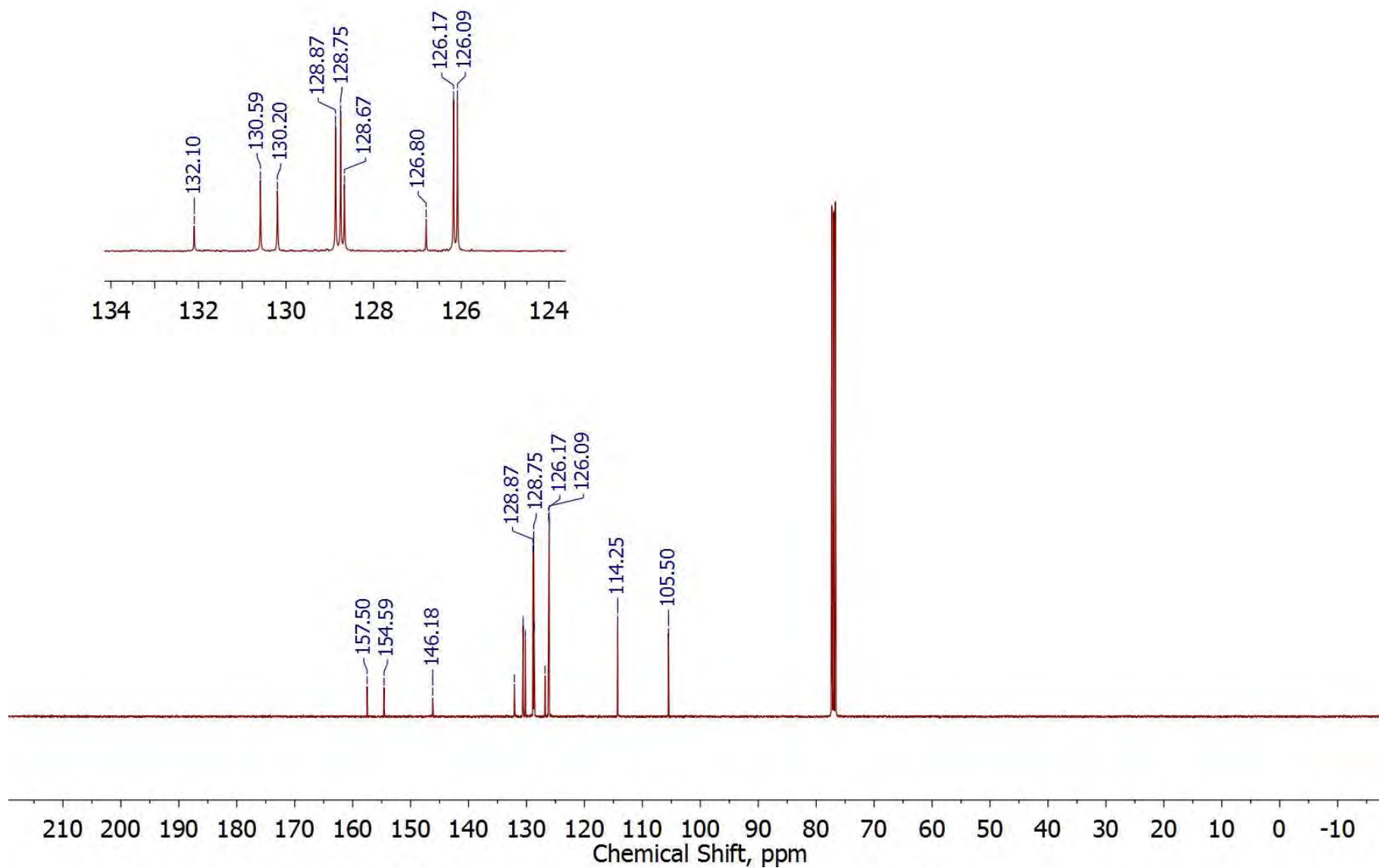
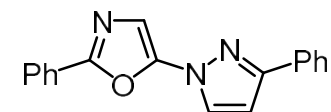
3-(4-Chlorophenyl)-6,6-dimethyl-2-(3-phenyl-1*H*-pyrazole-1-carbonyl)-6,7-dihydro-1*H*-indol-4(5*H*)-one (6k), 100 (DEPT) MHz, CDCl₃



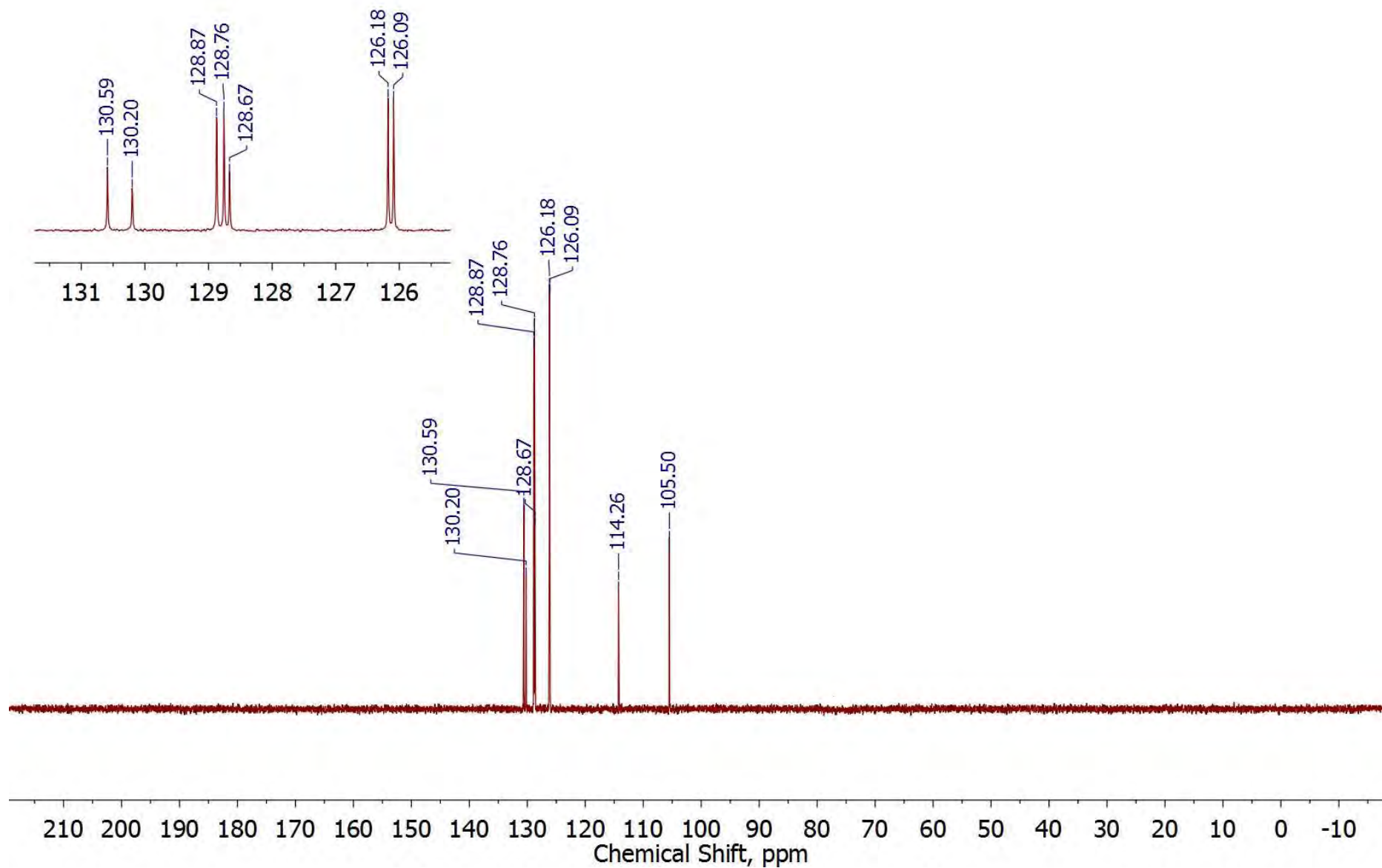
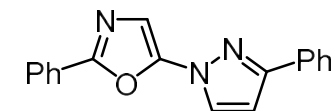
2-Phenyl-5-(3-phenyl-1*H*-pyrazol-1-yl)oxazole (7a), 400 (¹H) MHz, CDCl₃



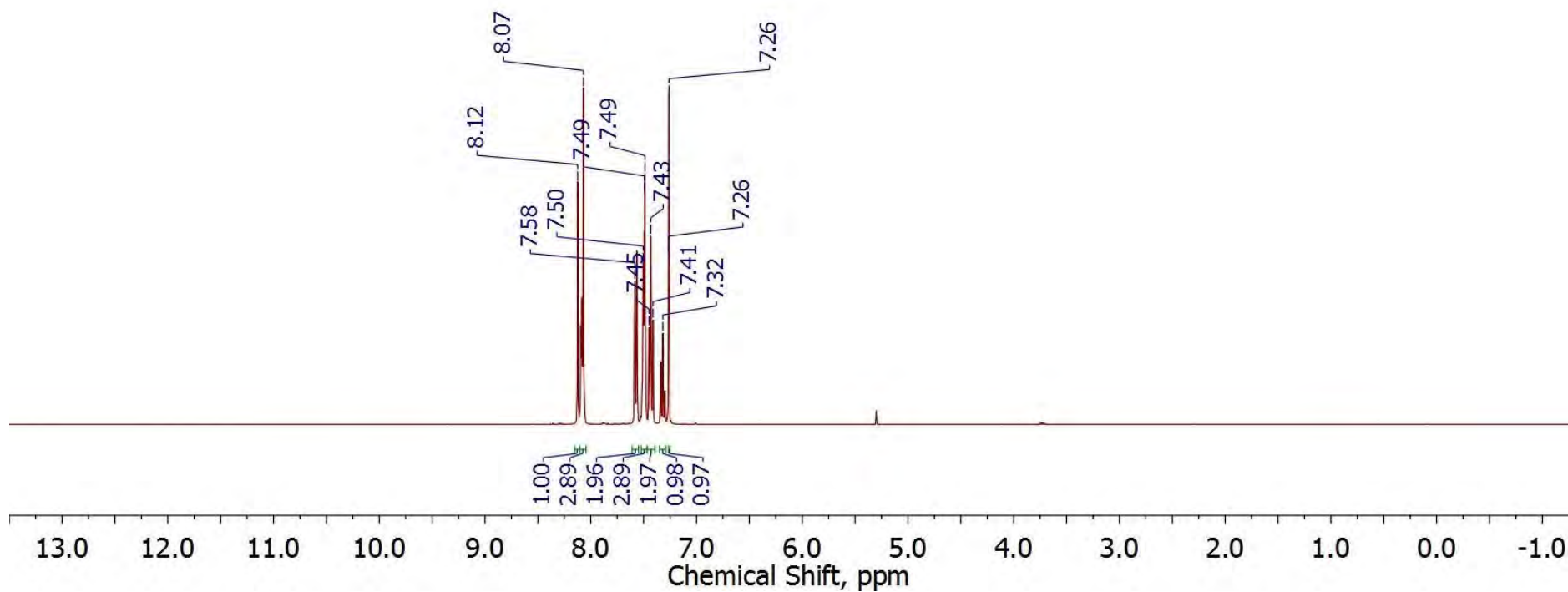
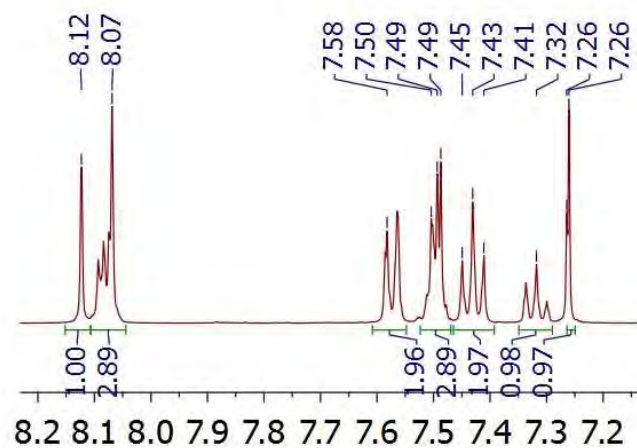
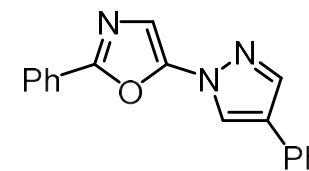
2-Phenyl-5-(3-phenyl-1*H*-pyrazol-1-yl)oxazole (7a), 100 (¹³C) MHz, CDCl₃



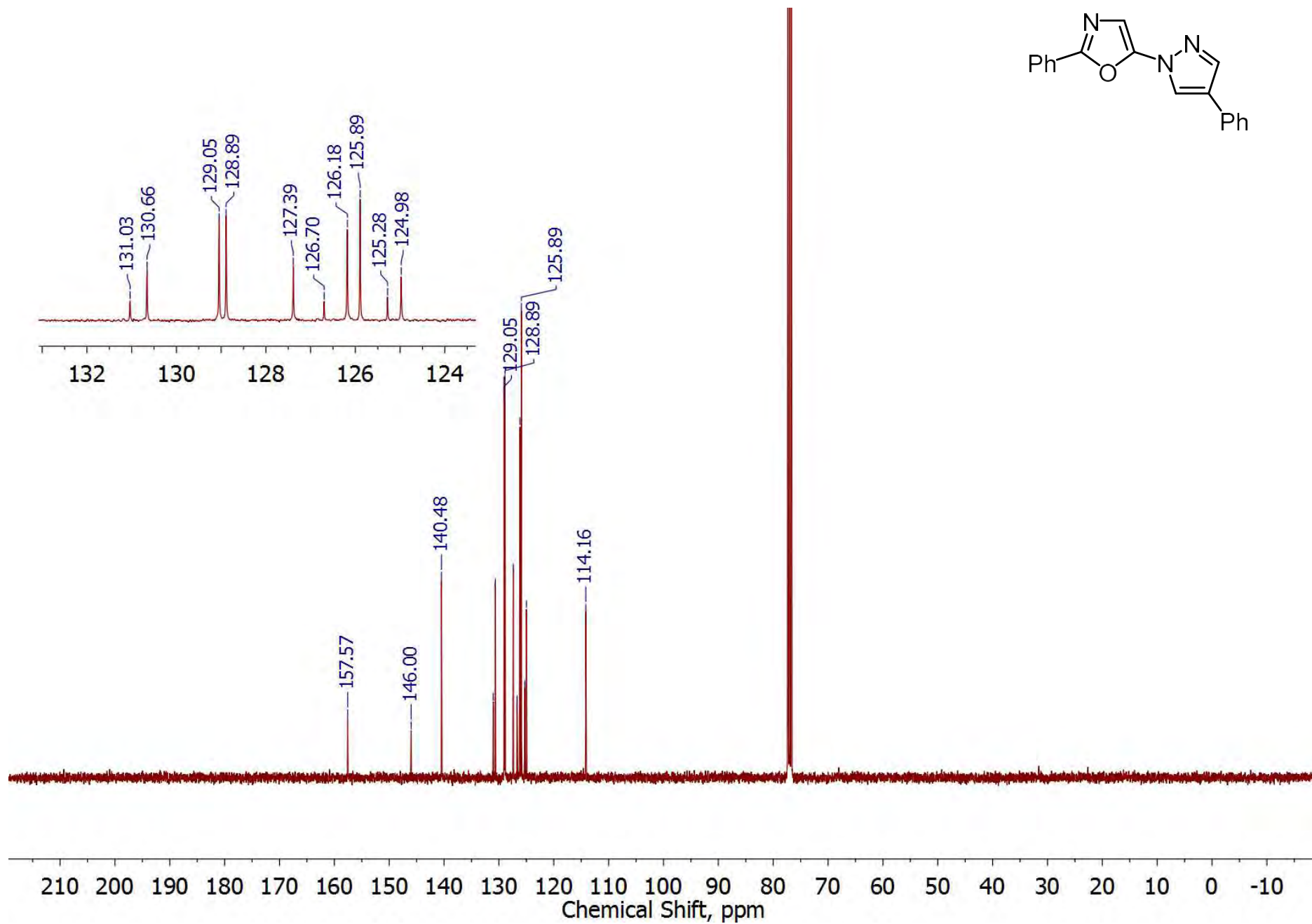
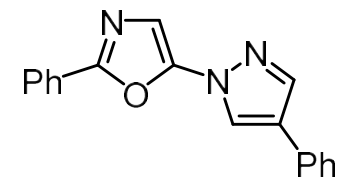
2-Phenyl-5-(3-phenyl-1*H*-pyrazol-1-yl)oxazole (7a), 100 (DEPT) MHz, CDCl₃



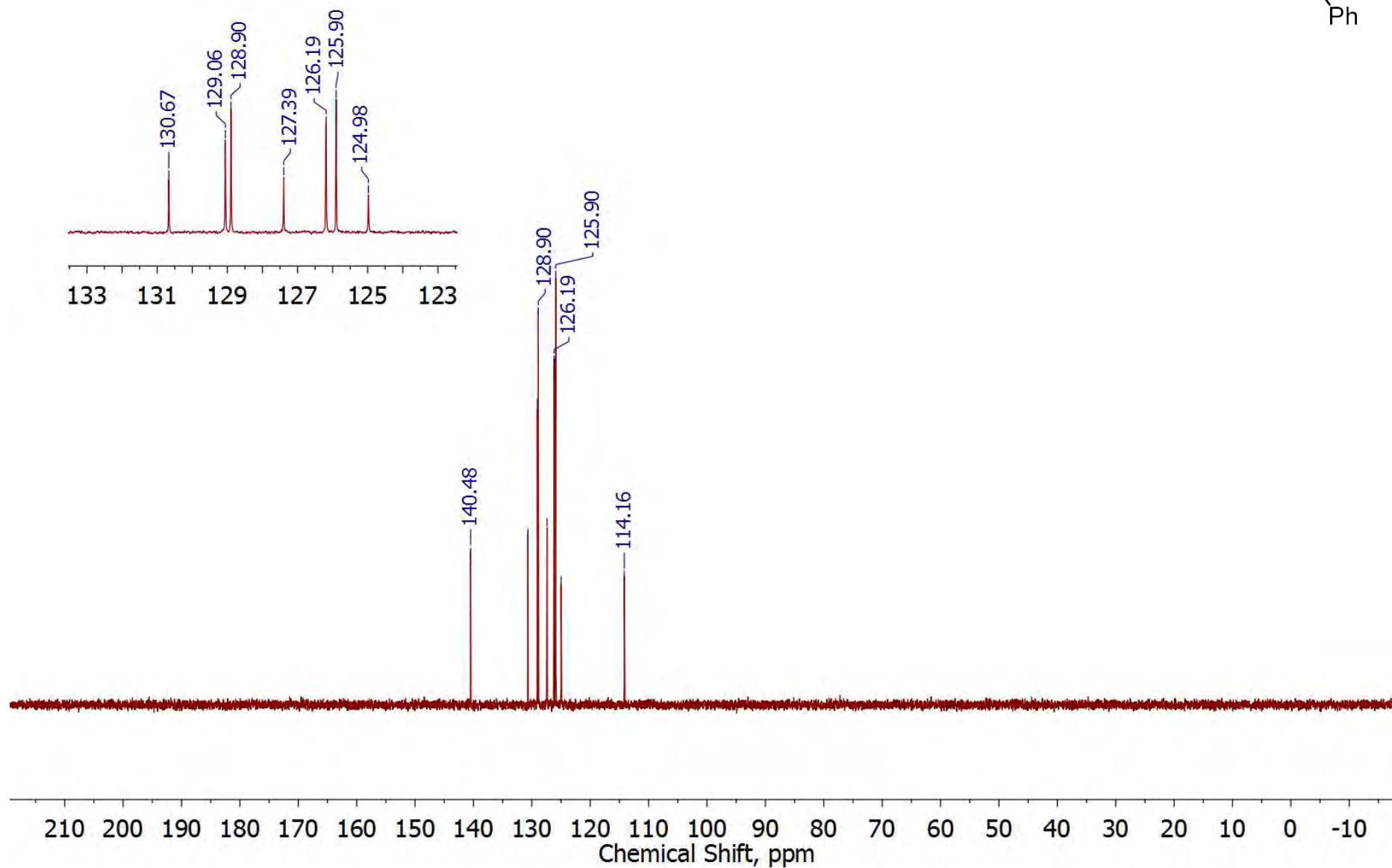
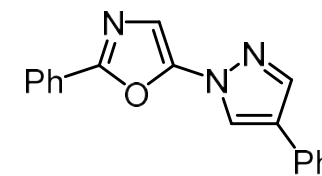
2-Phenyl-5-(4-phenyl-1*H*-pyrazol-1-yl)oxazole (7b), 400 (¹H) MHz, CDCl₃



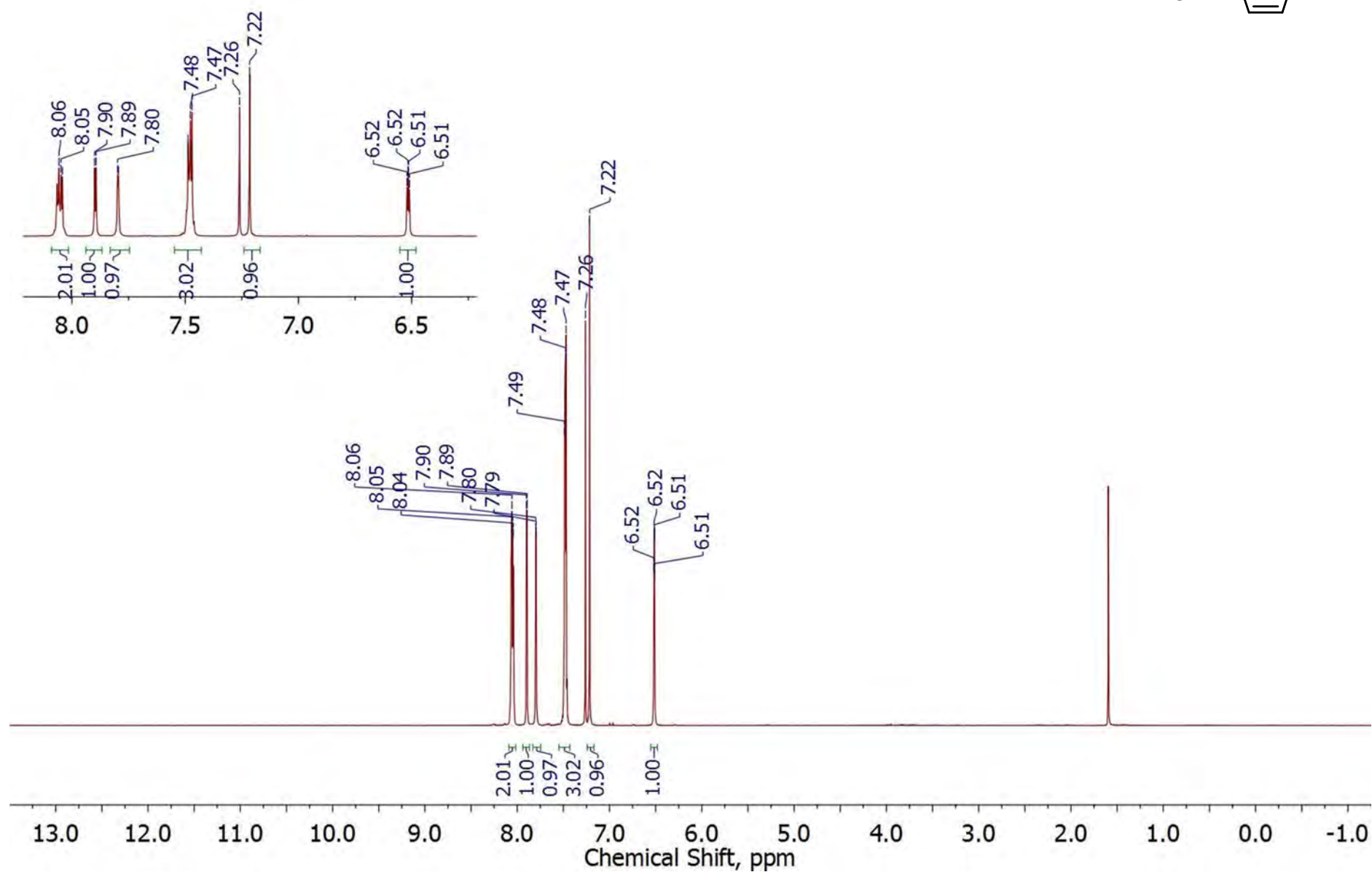
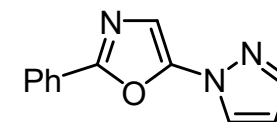
2-Phenyl-5-(4-phenyl-1*H*-pyrazol-1-yl)oxazole (7b), 100 (^{13}C) MHz, CDCl_3



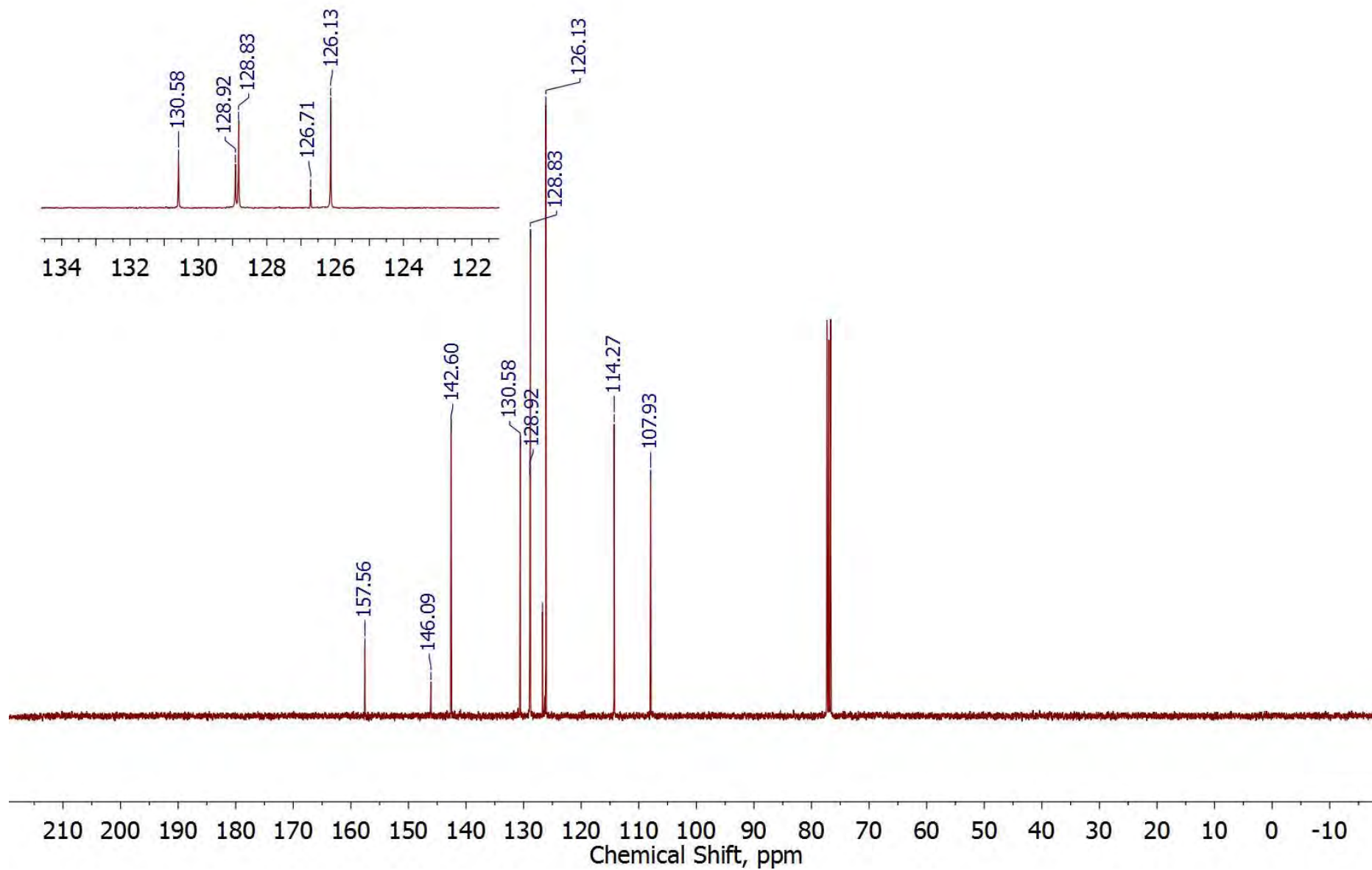
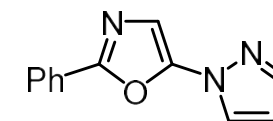
2-Phenyl-5-(4-phenyl-1*H*-pyrazol-1-yl)oxazole (7b), 100 (DEPT) MHz, CDCl₃



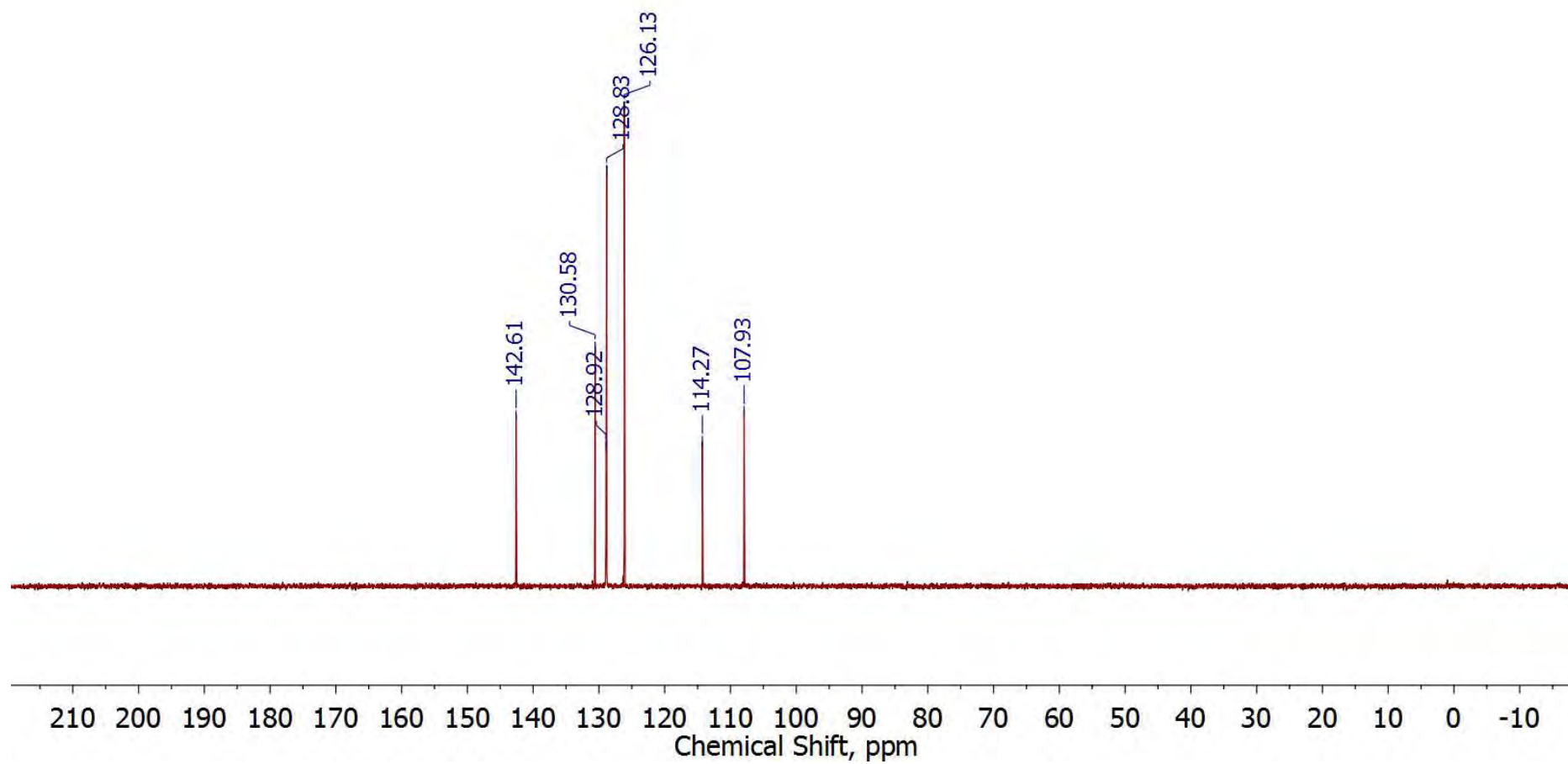
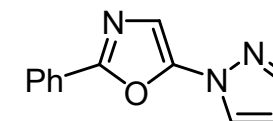
2-Phenyl-5-(1*H*-pyrazol-1-yl)oxazole (7c), 400 (¹H) MHz, CDCl₃



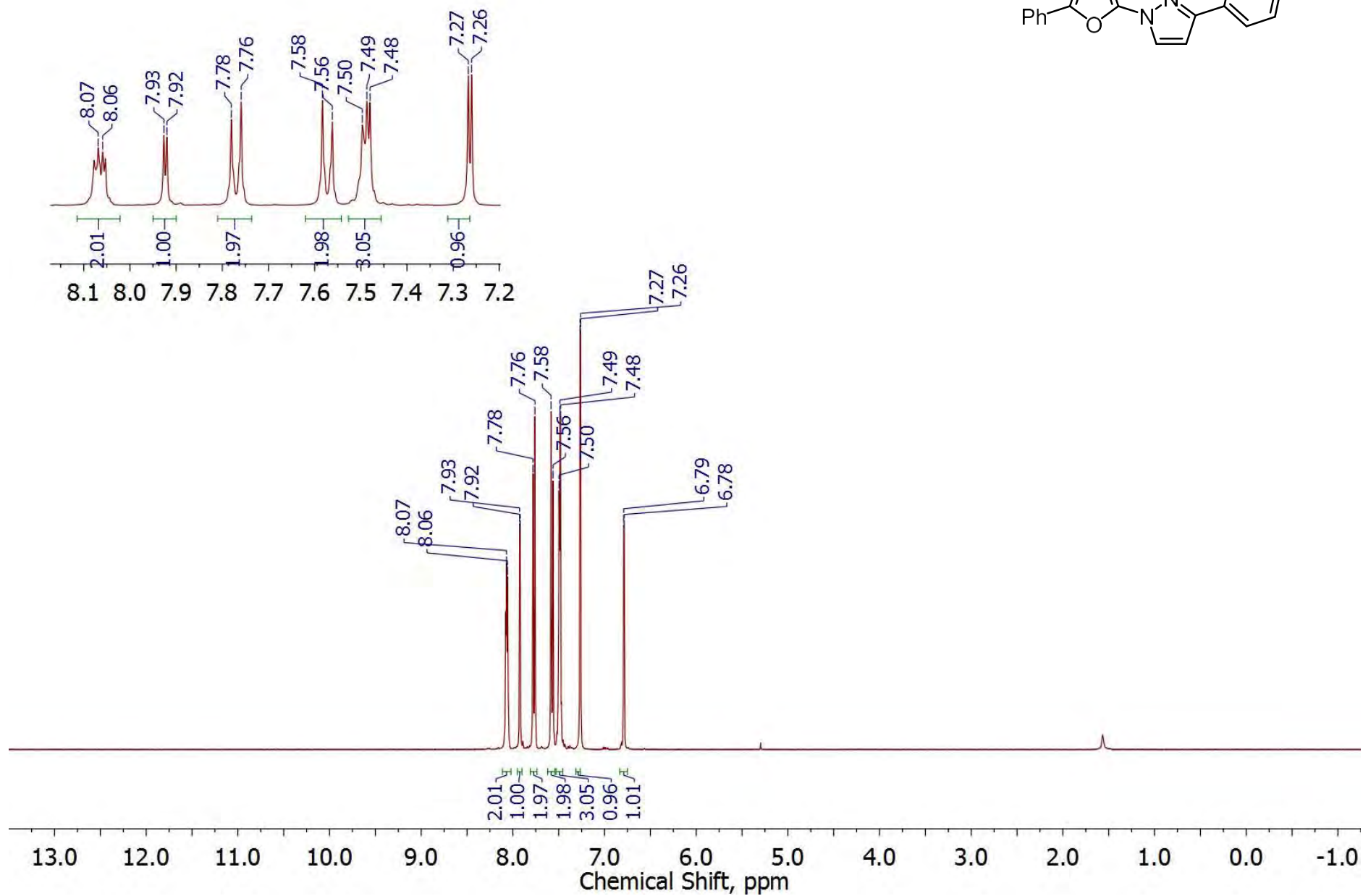
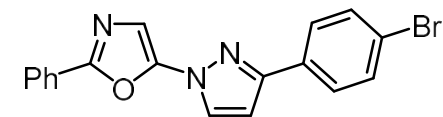
2-Phenyl-5-(1*H*-pyrazol-1-yl)oxazole (7c), 100 (¹³C) MHz, CDCl₃



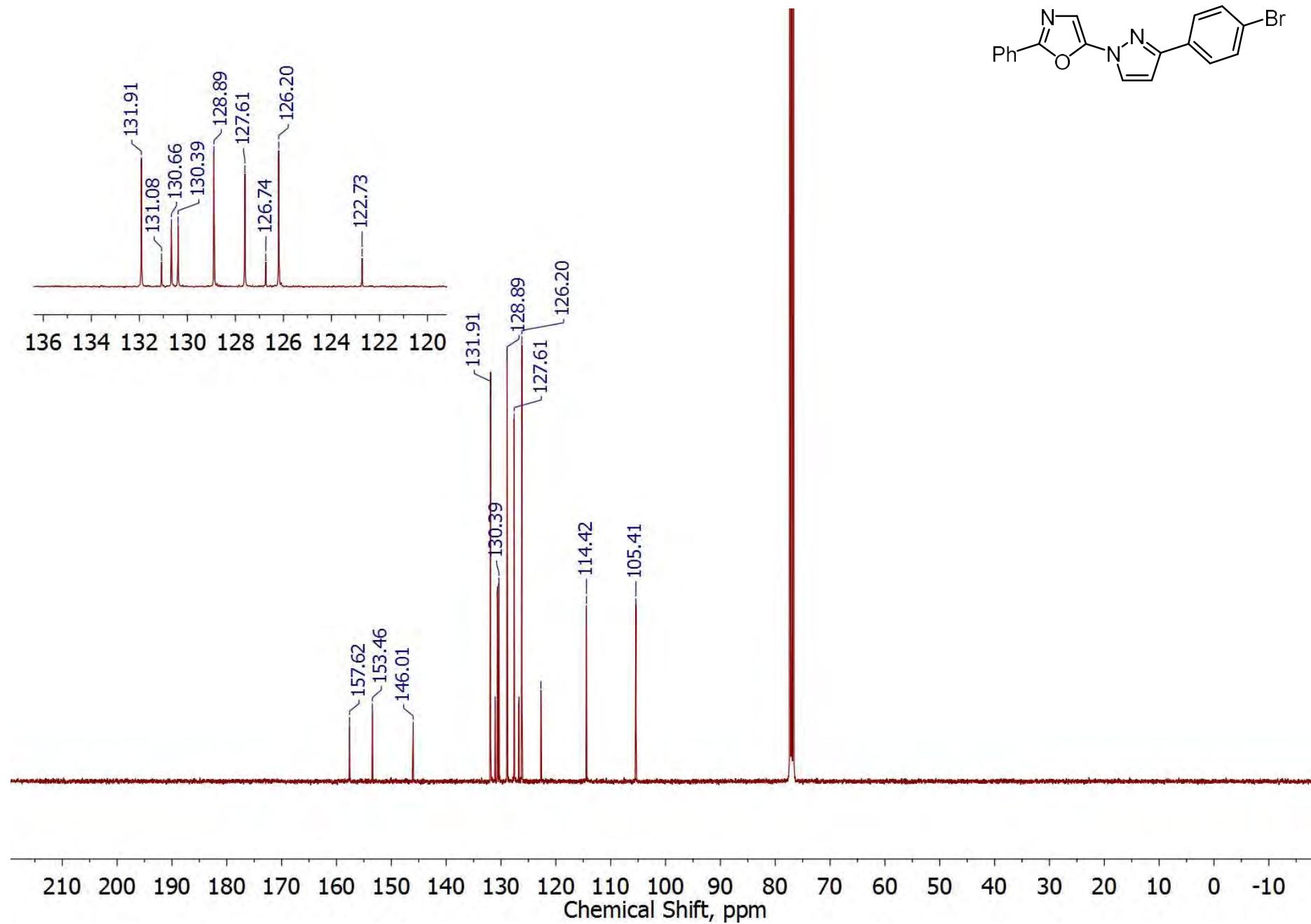
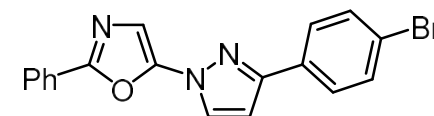
2-Phenyl-5-(1*H*-pyrazol-1-yl)oxazole (7c), 100 (DEPT) MHz, CDCl₃



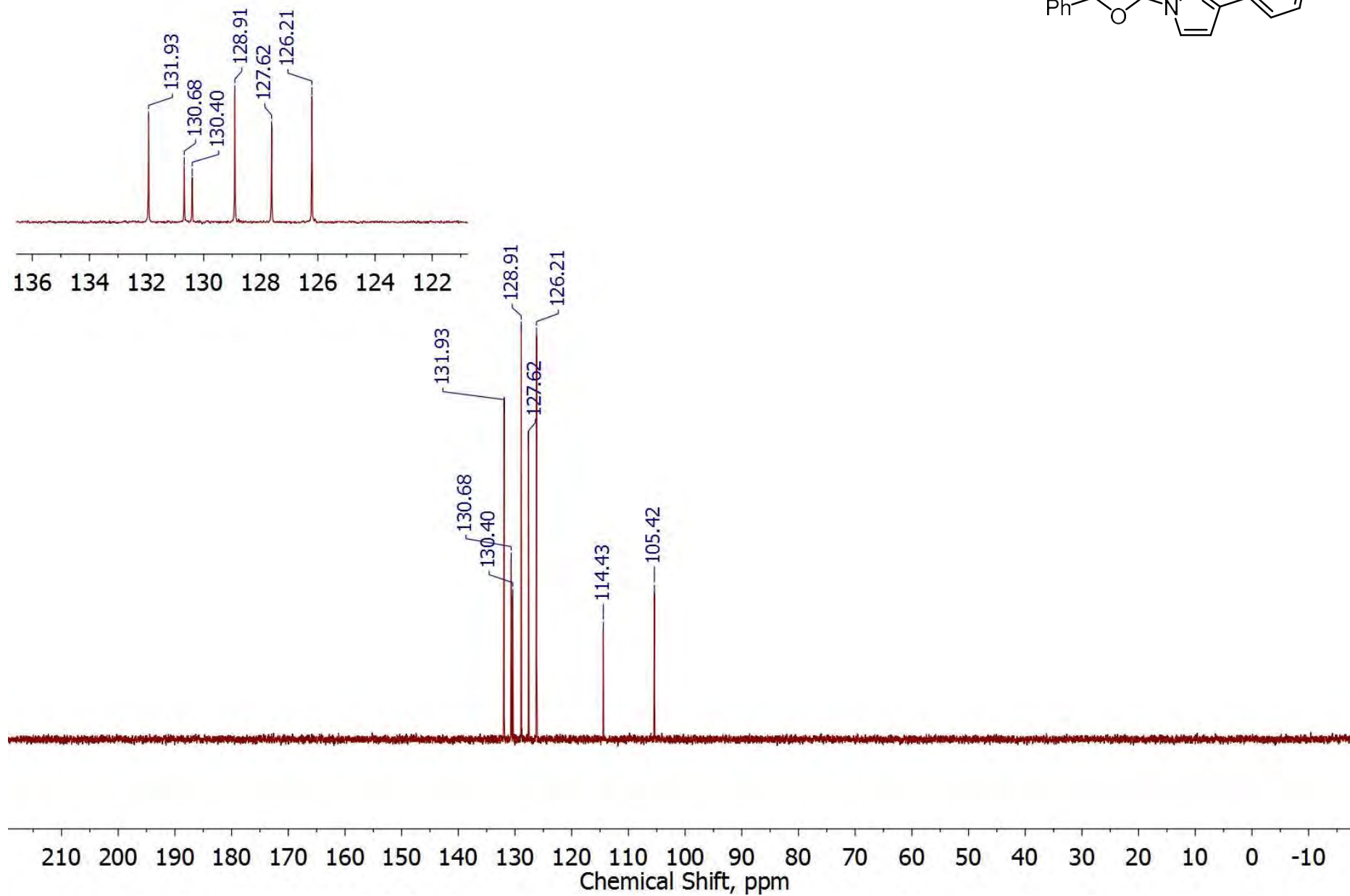
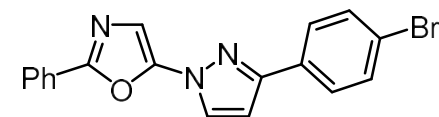
5-(3-(4-Bromophenyl)-1*H*-pyrazol-1-yl)-2-phenyloxazole (7d), 400 (¹H) MHz, CDCl₃



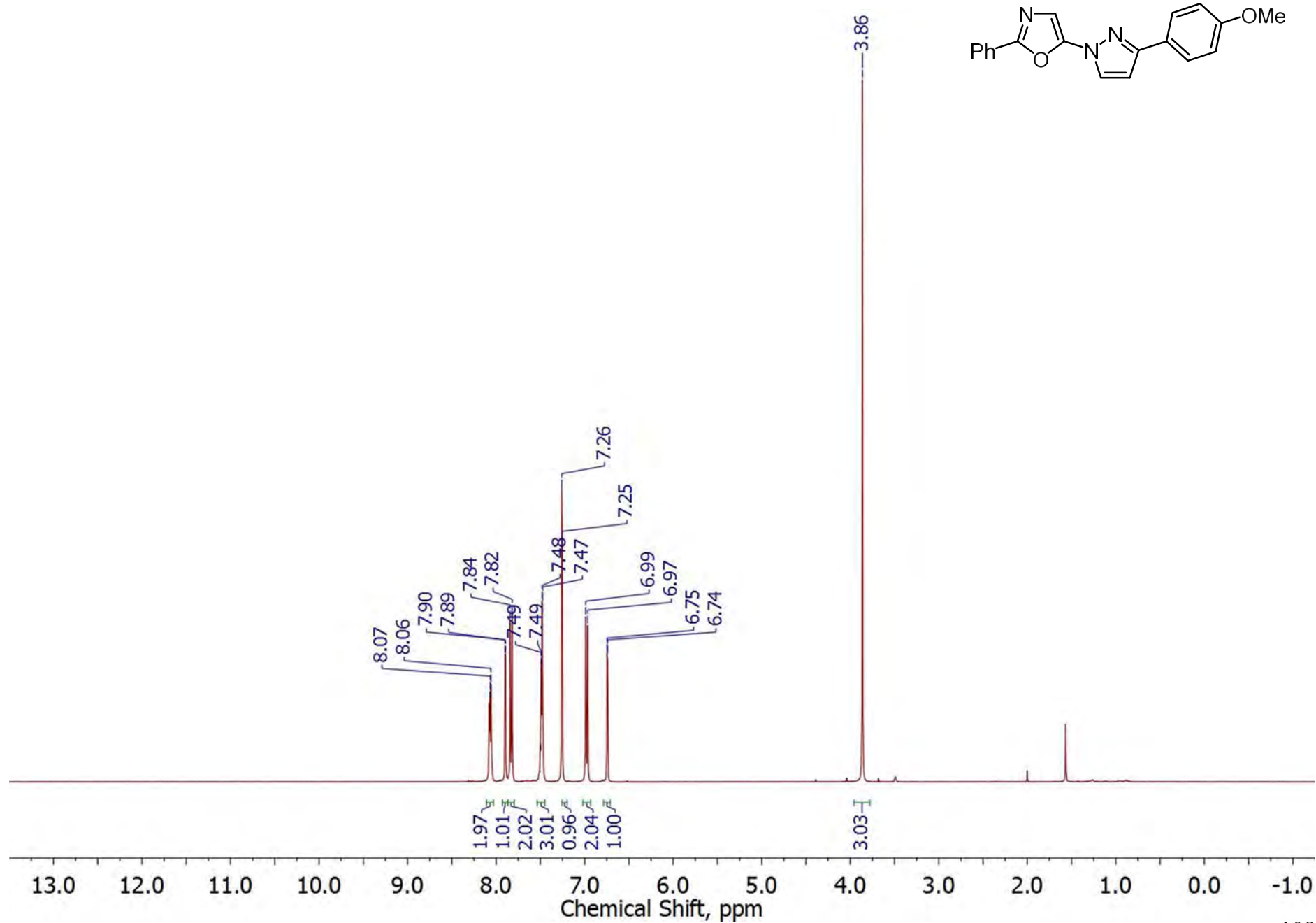
5-(3-(4-Bromophenyl)-1*H*-pyrazol-1-yl)-2-phenyloxazole (7d), 100 (¹³C) MHz, CDCl₃



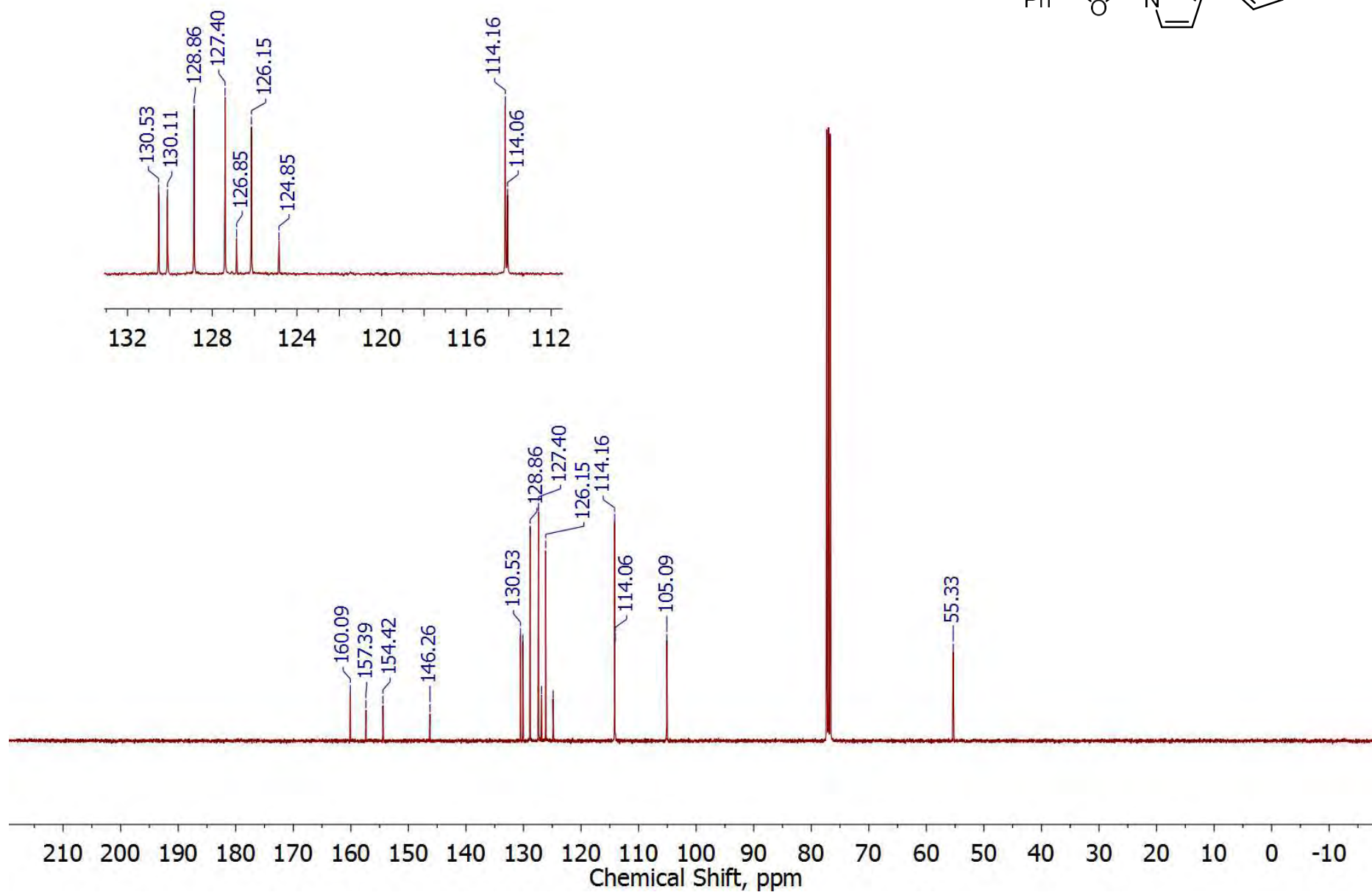
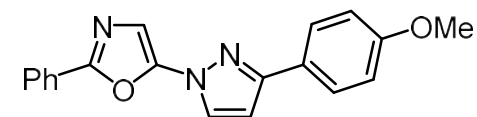
5-(3-(4-Bromophenyl)-1*H*-pyrazol-1-yl)-2-phenyloxazole (7d), 100 (DEPT) MHz, CDCl₃



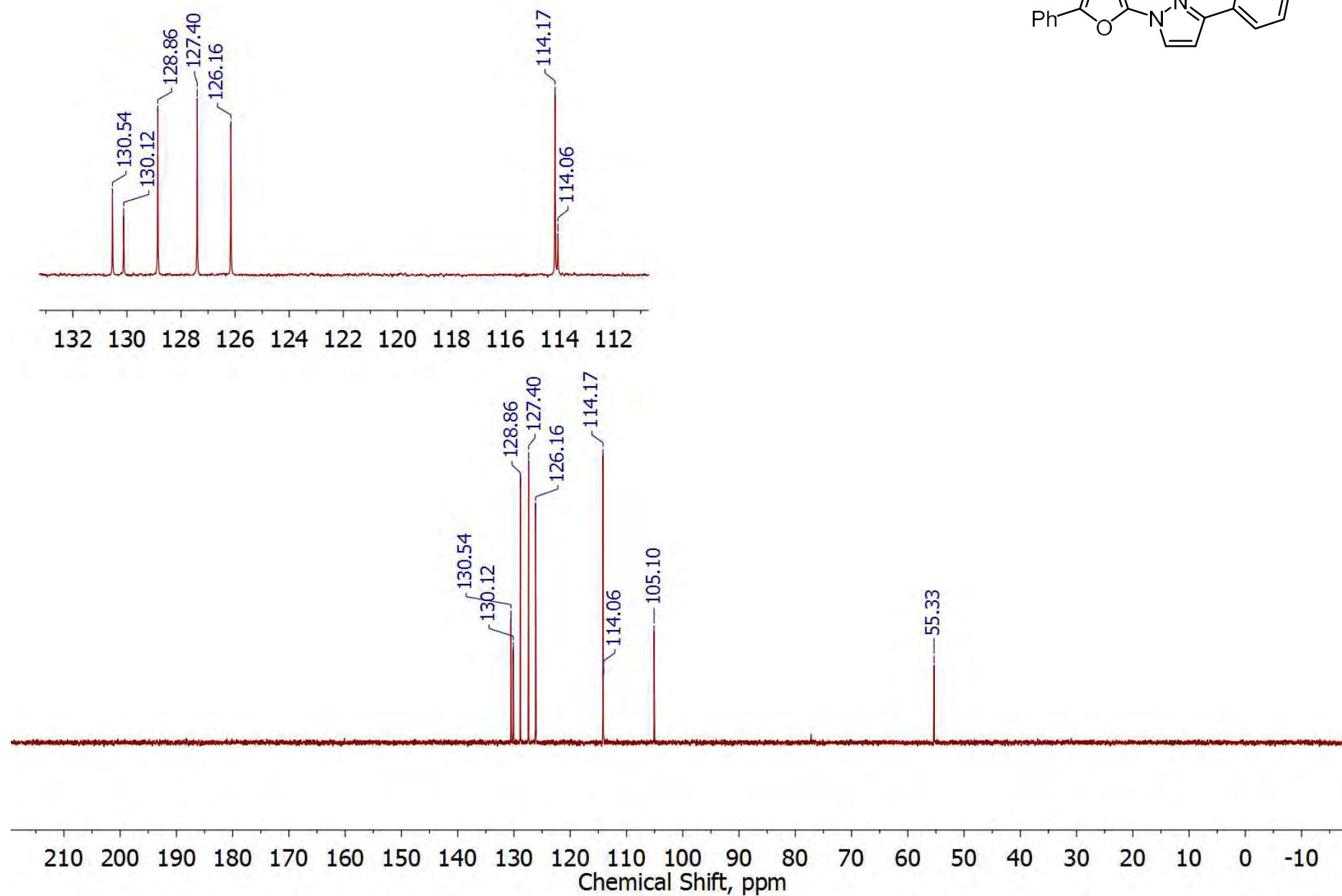
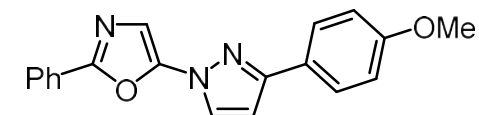
5-(3-(4-Methoxyphenyl)-1H-pyrazol-1-yl)-2-phenyloxazole (7e), 400 (¹H) MHz, CDCl₃



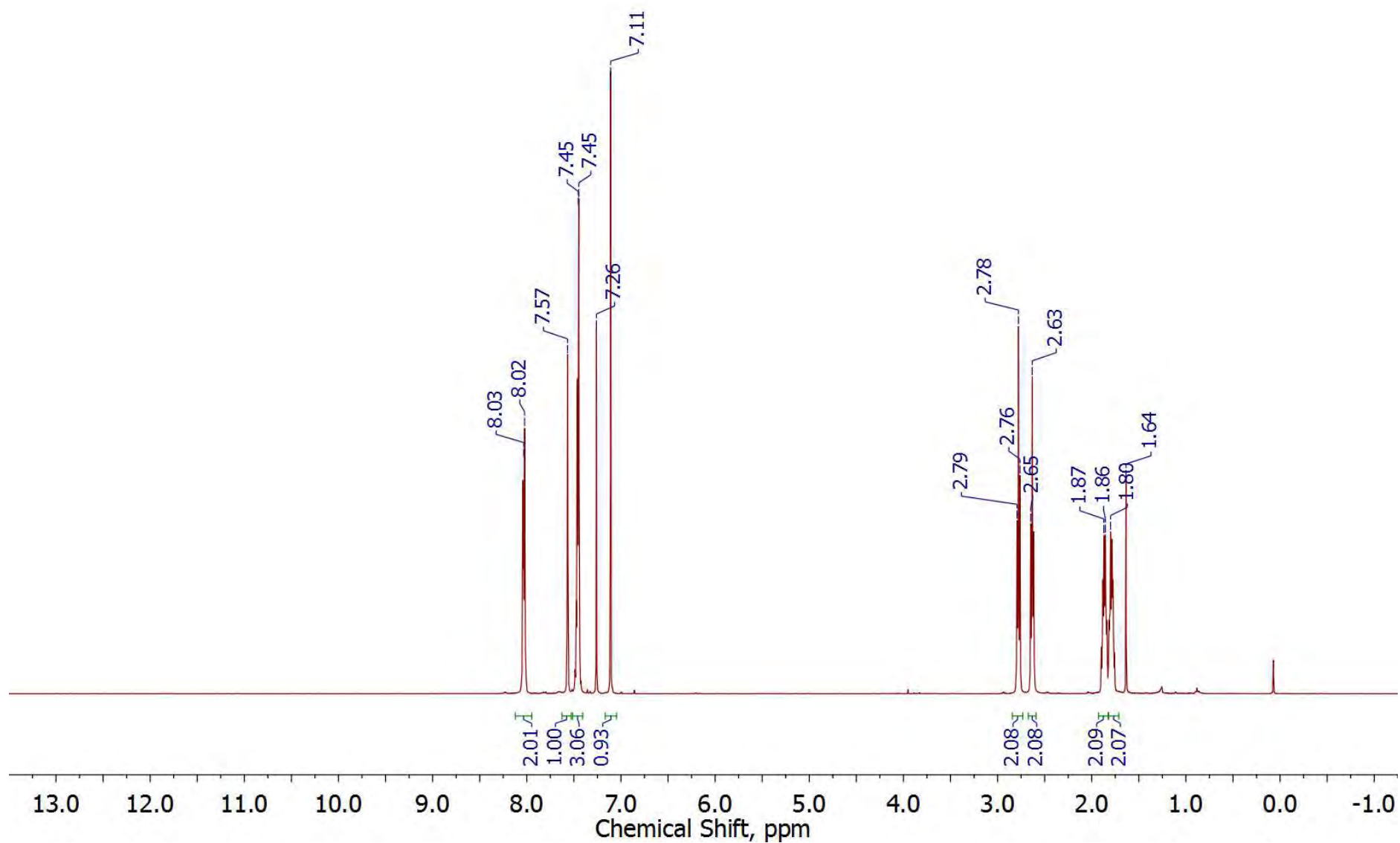
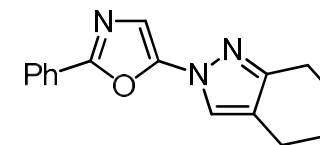
5-(3-(4-Methoxyphenyl)-1*H*-pyrazol-1-yl)-2-phenyloxazole (7e), 100 (¹³C) MHz, CDCl₃



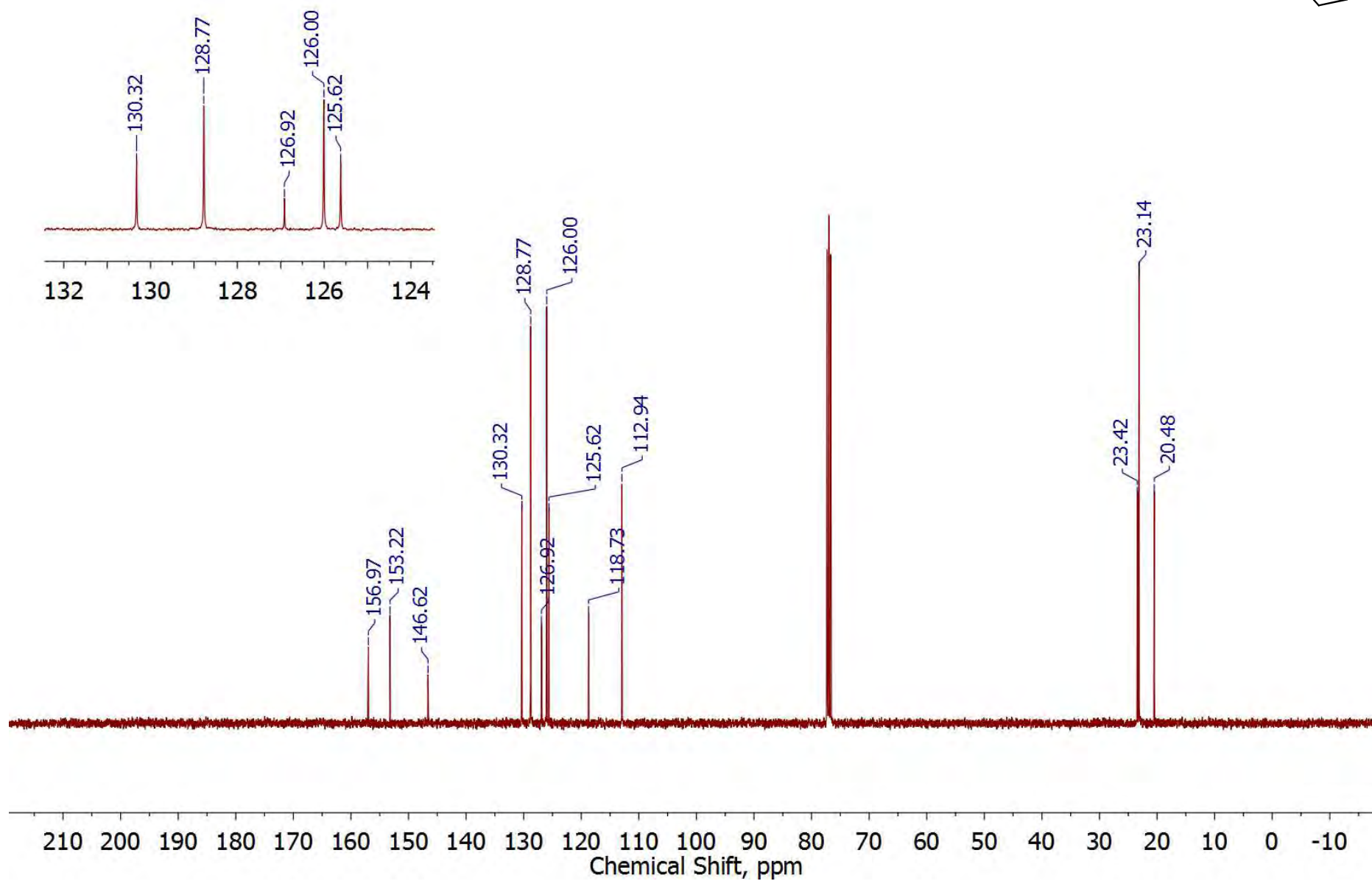
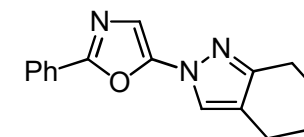
5-(3-(4-Methoxyphenyl)-1*H*-pyrazol-1-yl)-2-phenyloxazole (7e), 100 (DEPT) MHz, CDCl₃



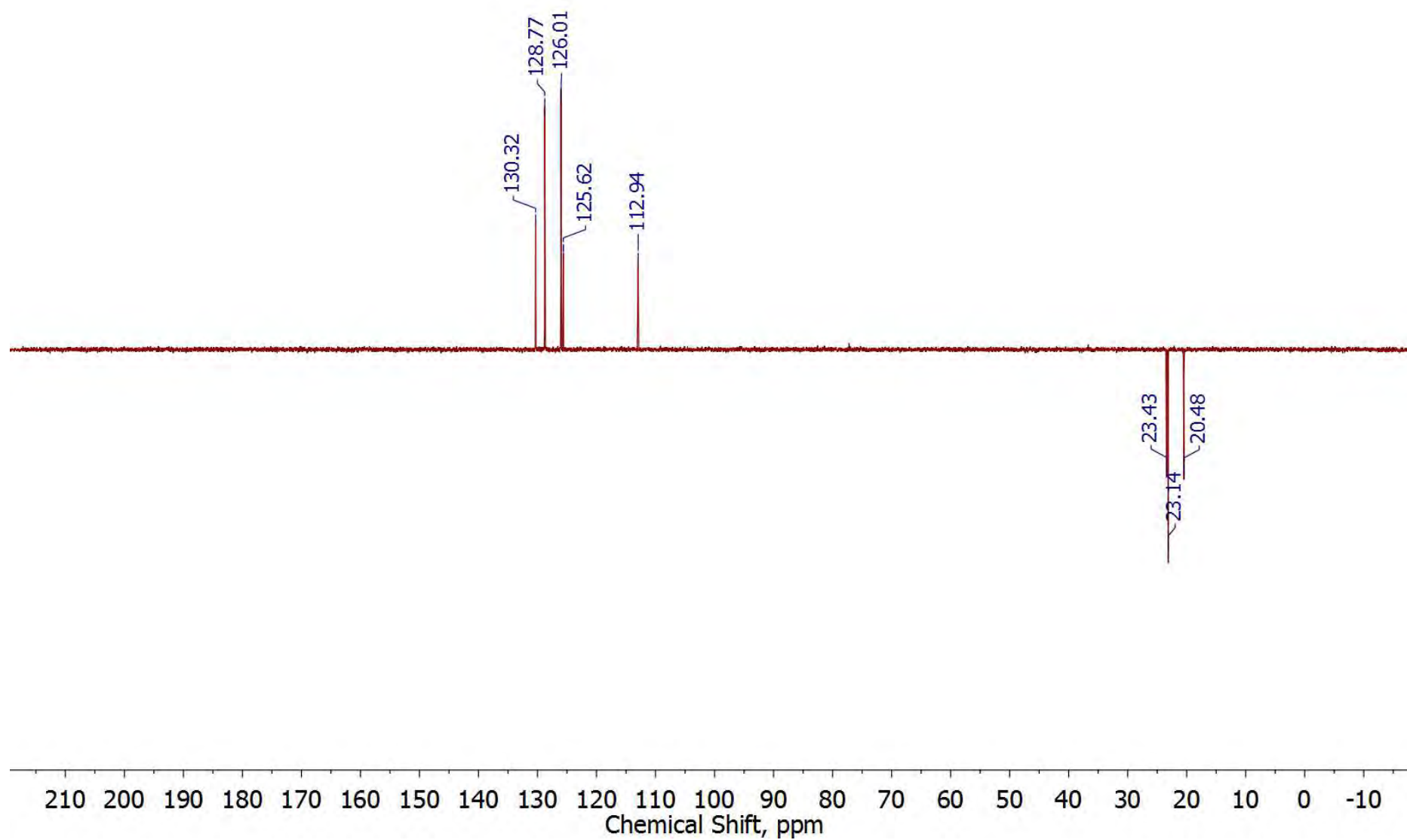
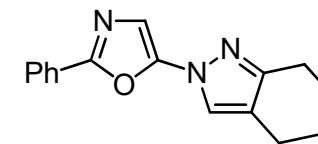
2-Phenyl-5-(4,5,6,7-tetrahydro-2*H*-indazol-2-yl)oxazole (7f), 400 (¹H) MHz, CDCl₃



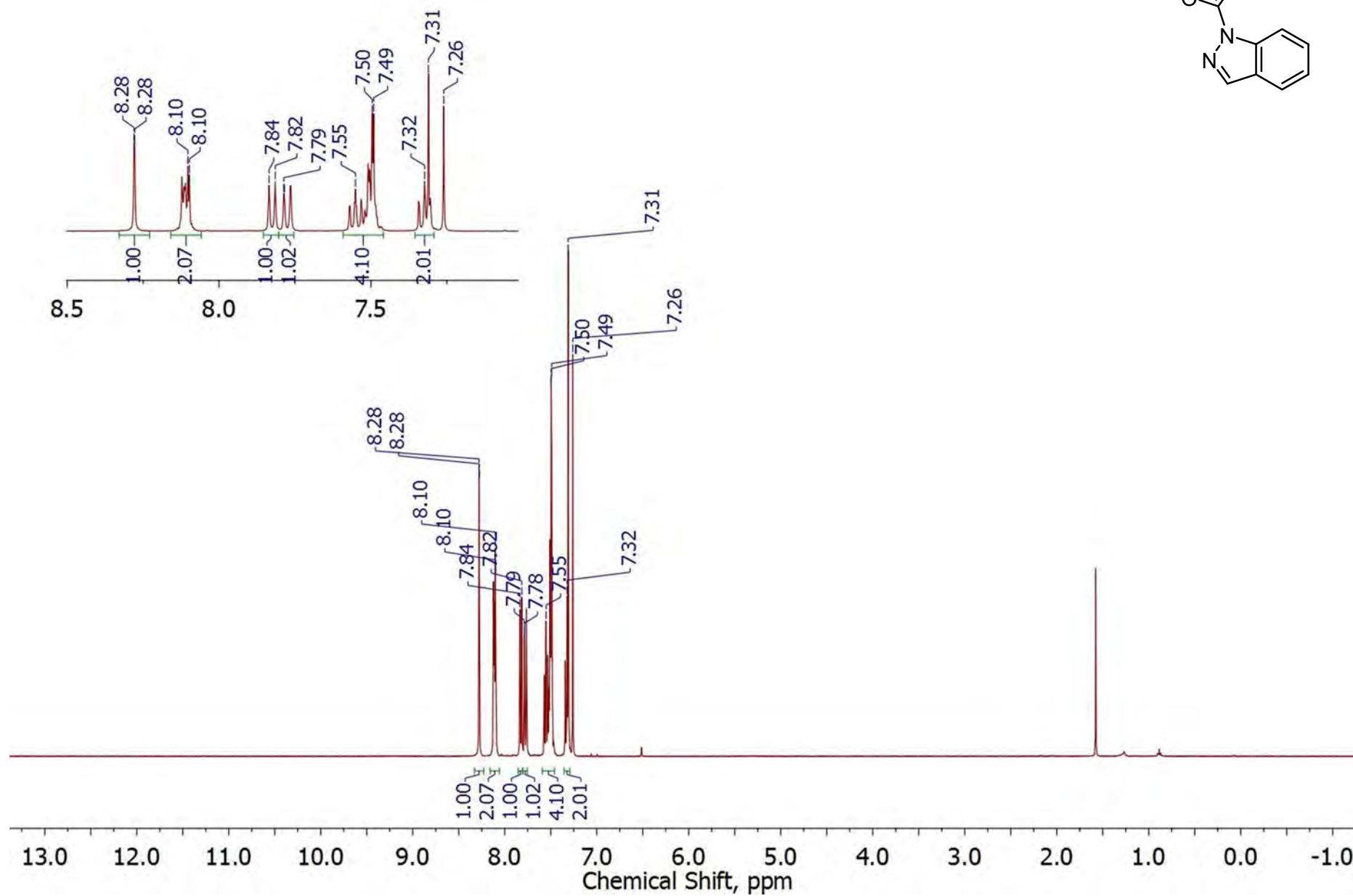
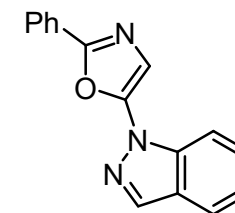
2-Phenyl-5-(4,5,6,7-tetrahydro-2*H*-indazol-2-yl)oxazole (7f), 100 (^{13}C) MHz, CDCl_3



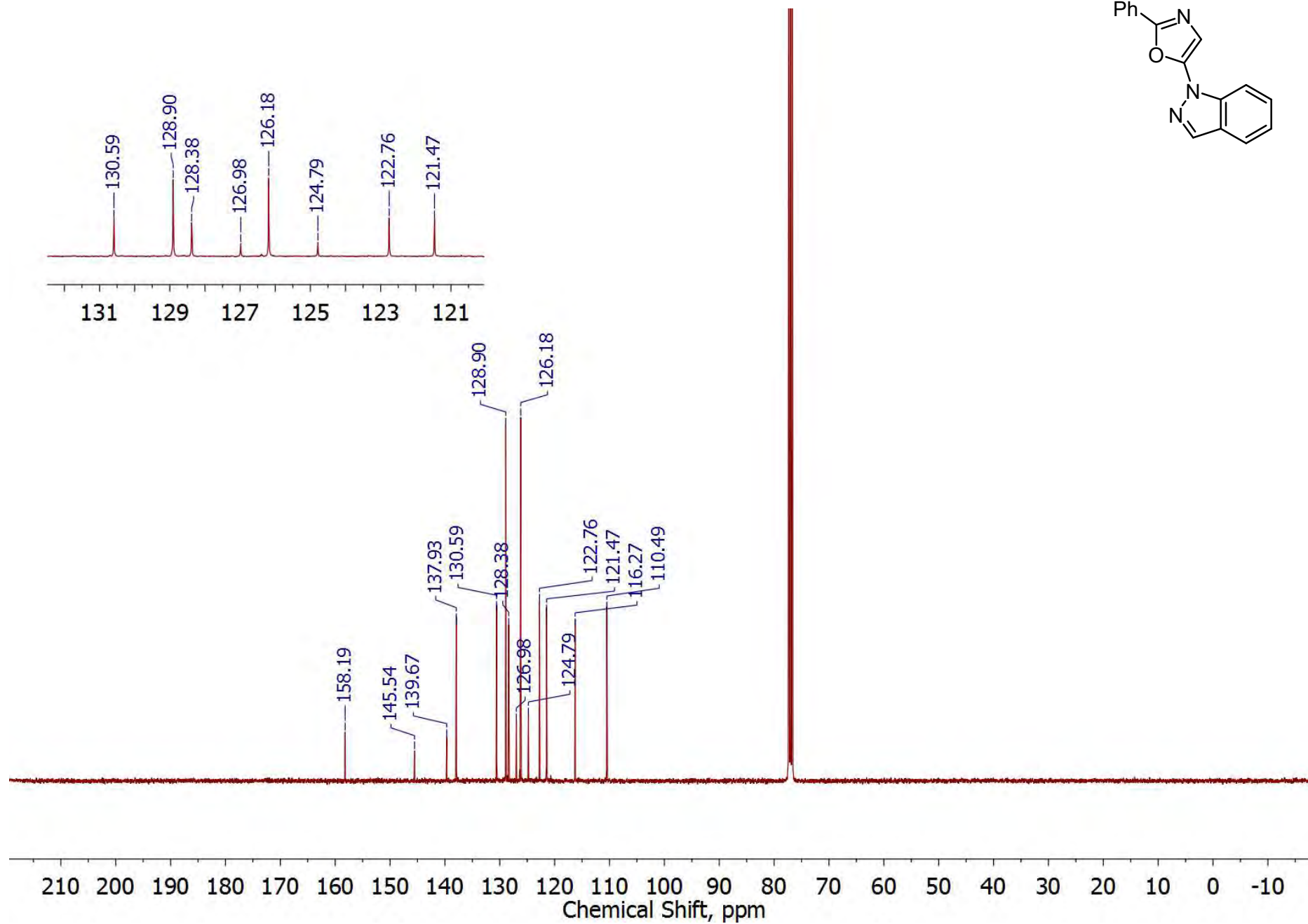
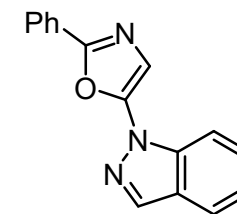
2-Phenyl-5-(4,5,6,7-tetrahydro-2*H*-indazol-2-yl)oxazole (7f), 100 (DEPT) MHz, CDCl₃



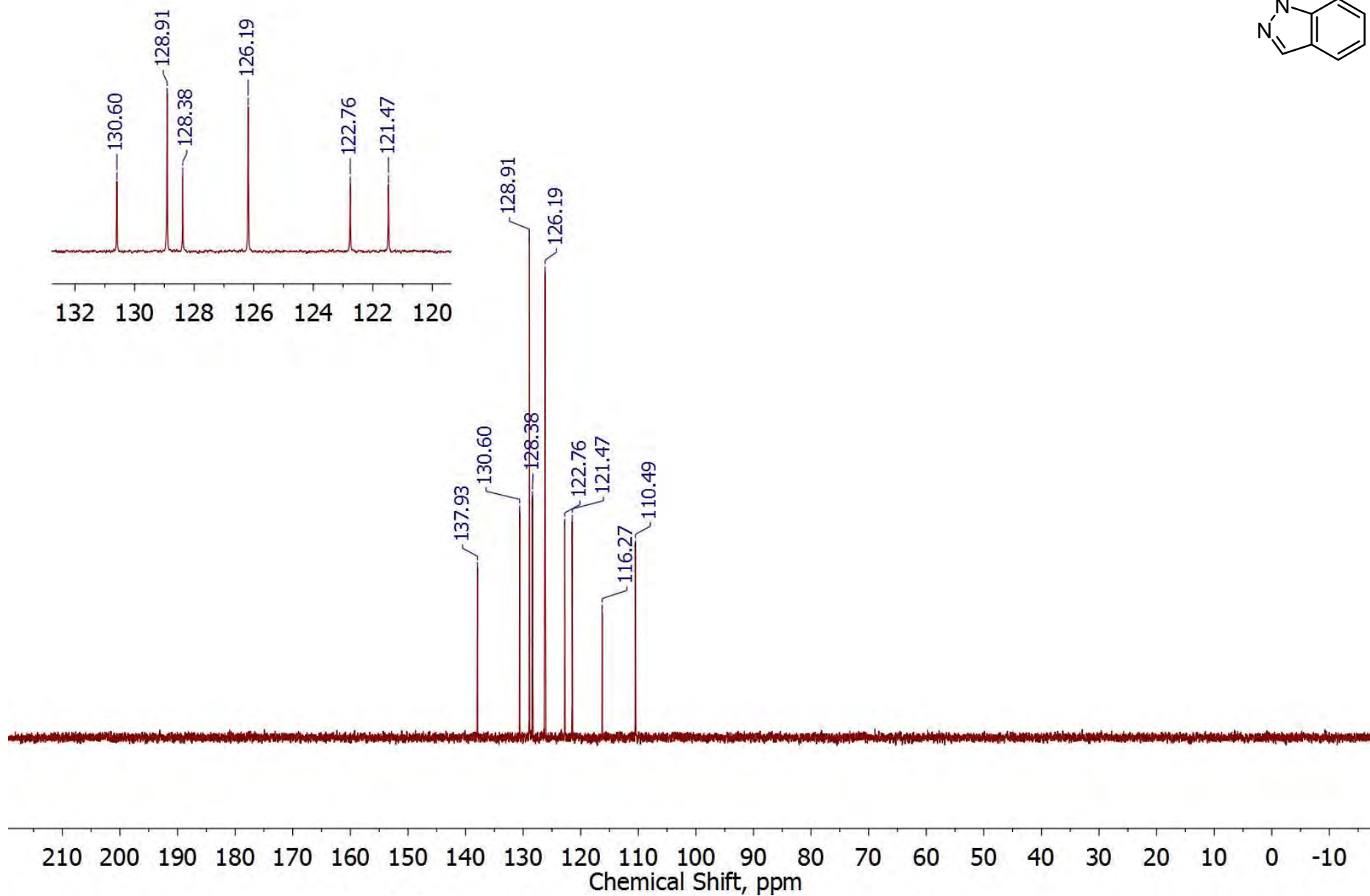
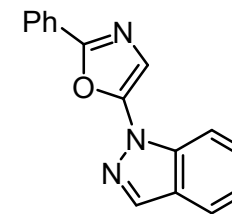
5-(1*H*-Indazol-1-yl)-2-phenyloxazole (7g), 400 (¹H) MHz, CDCl₃



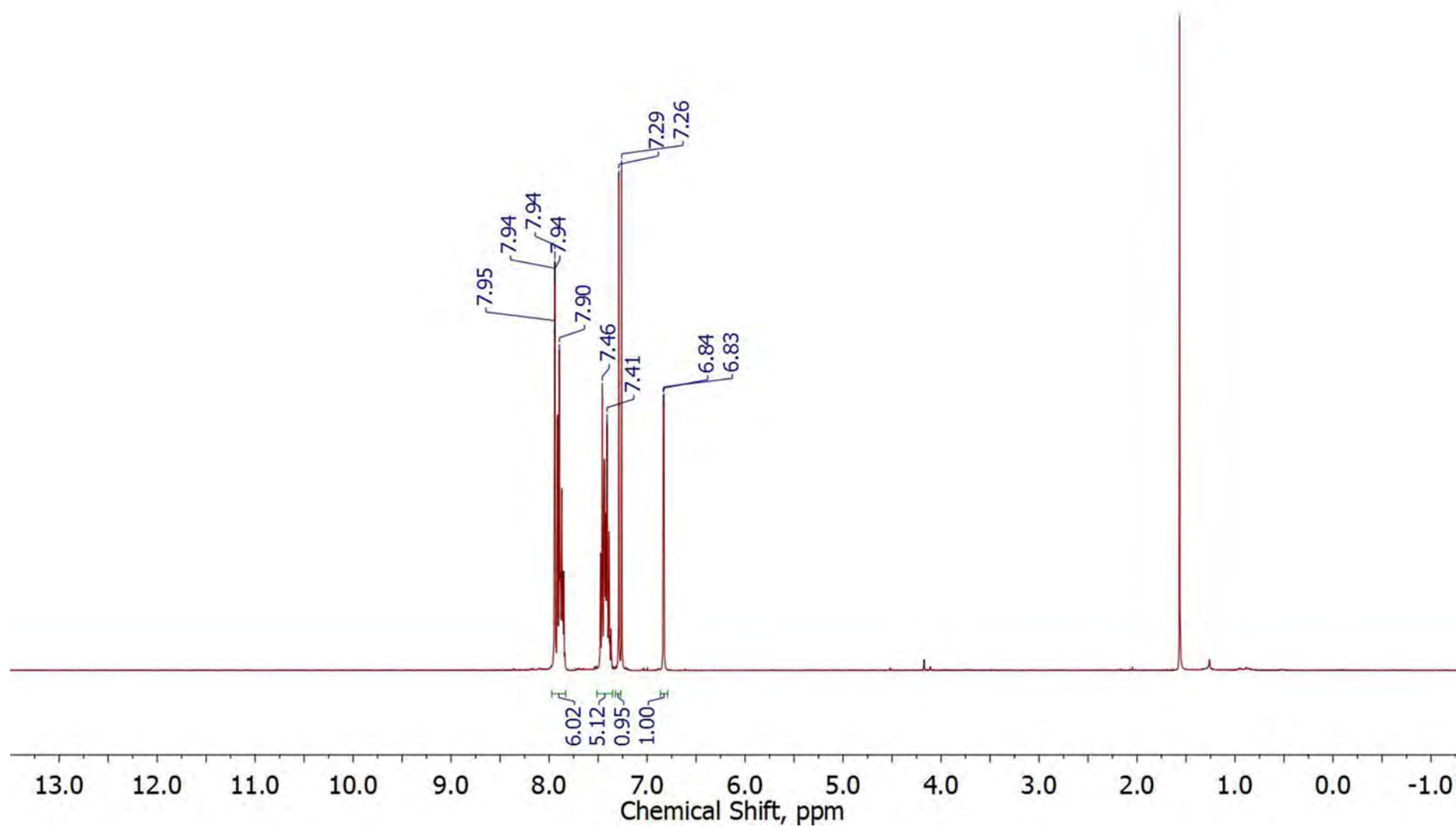
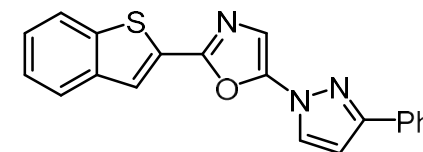
5-(1*H*-Indazol-1-yl)-2-phenyloxazole (7g), 100 (¹³C) MHz, CDCl₃



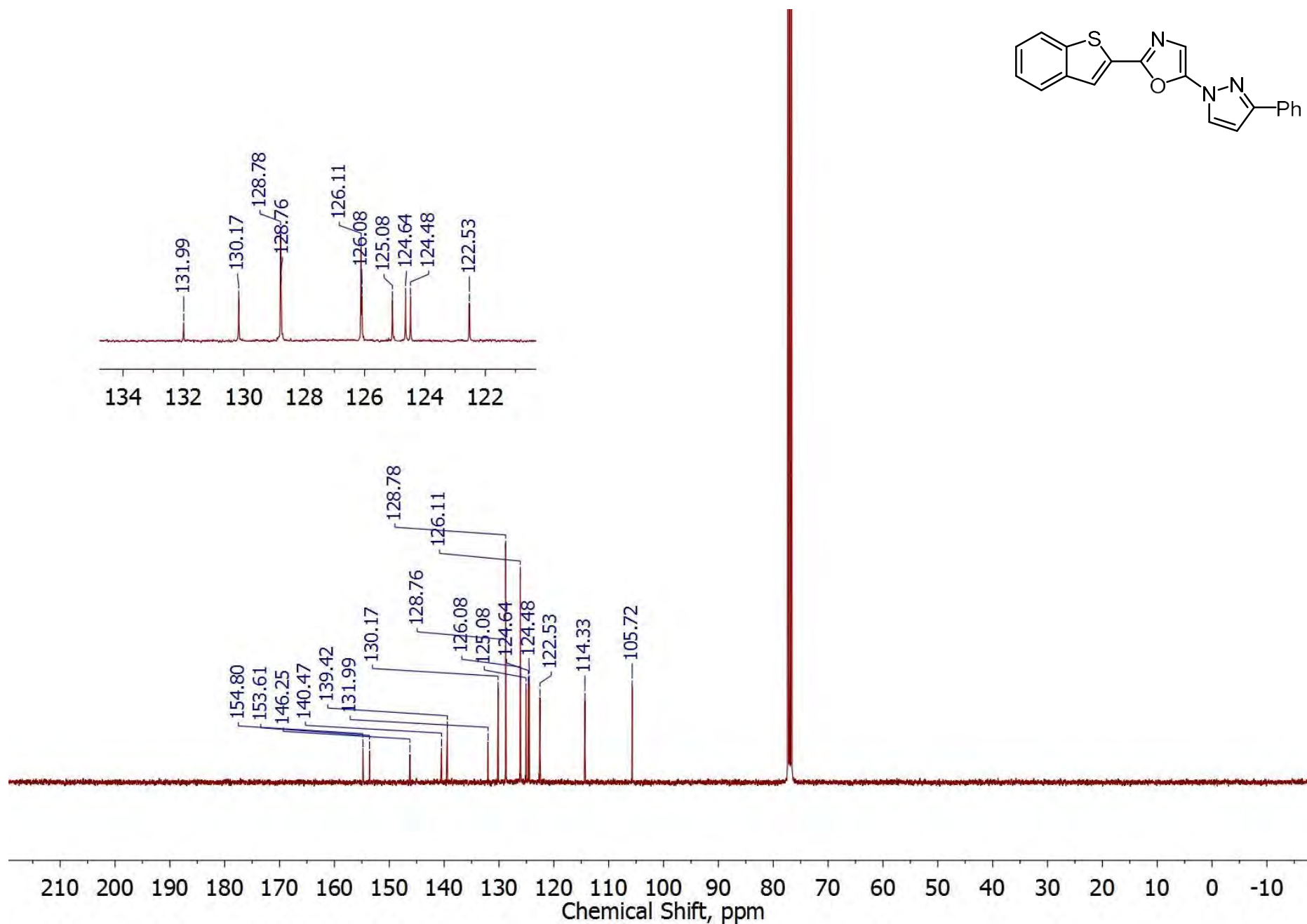
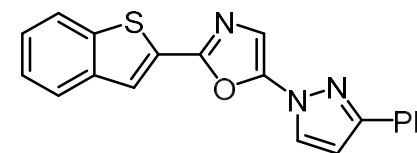
5-(1*H*-Indazol-1-yl)-2-phenyloxazole (7g), 100 (DEPT) MHz, CDCl₃



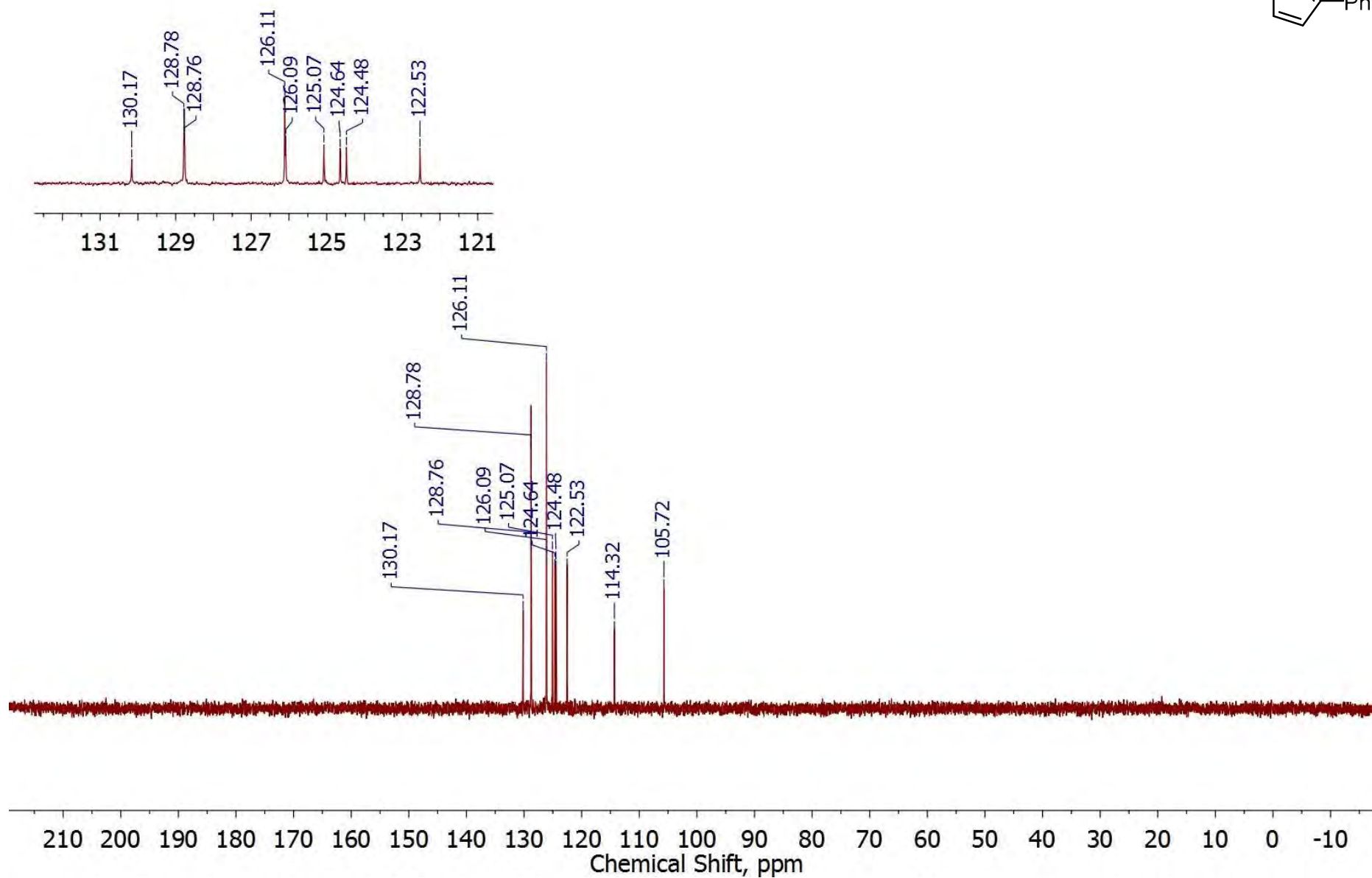
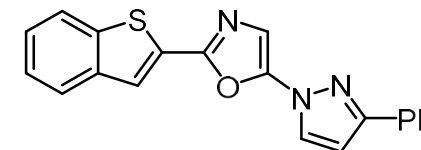
2-(Benzo[*b*]thiophen-2-yl)-5-(3-phenyl-1*H*-pyrazol-1-yl)oxazole (7h), 400 (¹H) MHz, CDCl₃



2-(Benzo[*b*]thiophen-2-yl)-5-(3-phenyl-1*H*-pyrazol-1-yl)oxazole (7h), 100 (¹³C) MHz, CDCl₃

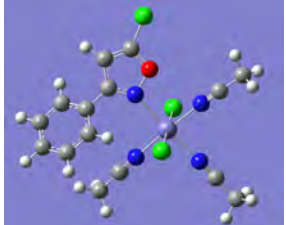
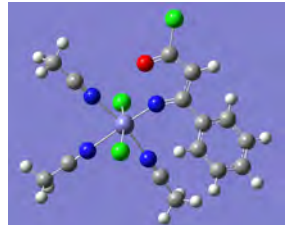


2-(Benzo[*b*]thiophen-2-yl)-5-(3-phenyl-1*H*-pyrazol-1-yl)oxazole (7h), 100 (DEPT) MHz, CDCl₃



Computational Details

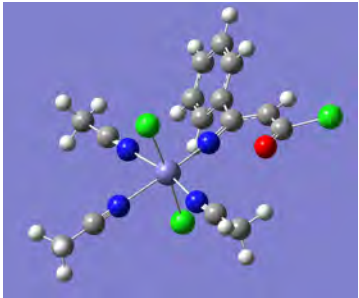
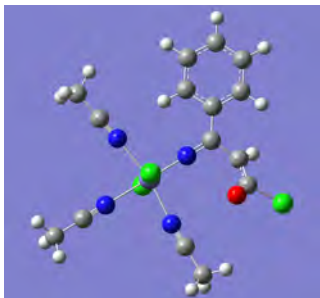
All calculations were performed with the B3LYP density functional method¹ by using the Gaussian 09 suite of quantum chemical programs² at Resource center "Computer center of Saint Petersburg State University". Geometry optimizations of Fe(II)-complexes of intermediates, transition states, reactants, and products (**8-10a-d**) for quintet state were performed at the B3LYP/6-31G(d){CHNOCl}/SDD{Fe} level using PCM solvent model for MeCN. Geometry optimizations of molecules **2b,g,h**, **2'b,g,h**; **4a**, **5b,k,l**, **5'b,k,l**; **7a** and the corresponding transition states were performed at the B3LYP/6-31+G(d,p) level using PCM solvent model for MeCN. Stationary points on the respective potential-energy surfaces were characterized at the same level of theory by evaluating the corresponding Hessian indices. Careful verification of the unique imaginary frequencies for transition states was carried out to check whether the frequency indeed pertains to the desired reaction coordinate.

Table S3. B3LYP/6-31G(d){CHNOCl}/SDD{Fe}, PCM solvent model for MeCN. Absolute Energies (au), Cartesian Coordinates of stationary points												
Molecule 8a						TS ^{8a-9a}						
												
E = -2379.47649854, H (0K) = -2379.202836, H (298K) = -2379.170698, G (298K) = -2379.276164 au.						E = -2379.43736487, H (0K) = -2379.166595, H (298K) = -2379.134750, G (298K) = -2379.238268 au.						
Imaginary frequency = 0.						Imaginary frequency = 1.						
C	-4.0883290	0.0123940	-0.4634360			C	2.5708880	-1.1585330	1.2634290			
C	-2.8987720	0.0713500	0.2823060			C	2.7692680	-0.2304650	0.2315580			
C	-2.6401990	-0.9100960	1.2520710			C	3.8600790	-0.3701780	-0.6406060			
C	-3.5599040	-1.9379520	1.4641300			C	4.7455220	-1.4355650	-0.4791190			
C	-4.7384560	-1.9976390	0.7143180			C	4.5543240	-2.3568540	0.5550880			
C	-4.9995610	-1.0211170	-0.2514410			C	3.4697810	-2.2143070	1.4253840			
C	-1.9700630	1.1954150	0.0676550			C	1.8586180	0.9463480	0.0707690			
O	-0.1290110	2.3654300	-0.0587440			O	0.1265790	2.7629620	-0.1091250			
C	-1.1568800	3.1977850	-0.2750790			C	1.3138500	3.1467750	-0.1732820			
C	-2.3447250	2.5426010	-0.2167480			C	2.3717370	2.2520390	-0.0907610			
H	-4.2923540	0.7659140	-1.2185750			H	1.7239280	-1.0470230	1.9326480			
H	-1.7263650	-0.8612680	1.8356140			H	4.0078660	0.3462160	-1.4427910			

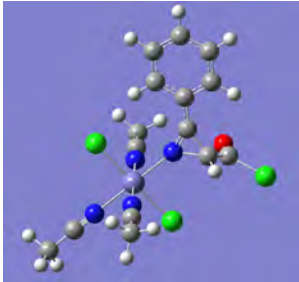
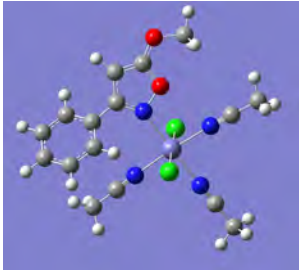
¹ (a) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648–5652. (b) Becke, A. D. *Phys. Rev. A* **1988**, *38*, 3098–3100. (c) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785–789.

² Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, **2013**.

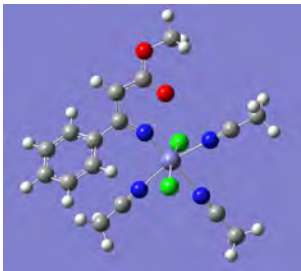
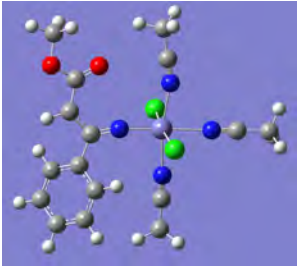
H	-3.3581870	-2.6896160	2.2220680	H	5.5862920	-1.5424140	-1.1581910
H	-5.4532080	-2.7975770	0.8858750	H	5.2502310	-3.1809380	0.6836940
H	-5.9127840	-1.0622140	-0.8377710	H	3.3224250	-2.9245350	2.2339140
N	-0.6494000	1.0782240	0.1495360	N	0.5646990	0.7540380	0.0918260
Cl	0.9490770	-1.0148770	2.3529190	Cl	-1.3494890	0.0053360	-2.3924000
Cl	1.3360030	0.1035720	-2.3692230	Cl	-1.0761070	-0.8029910	2.3398350
C	3.3448920	1.9705620	0.7905260	C	-3.2478210	2.1796250	0.5651720
Fe	1.1371030	-0.4560620	-0.0098050	Fe	-1.0521680	-0.2800440	-0.0183440
N	2.5570710	1.1682740	0.5181080	N	-2.4839800	1.3349540	0.3679700
C	4.3360300	2.9822900	1.1325100	C	-4.2051710	3.2481190	0.8115990
H	5.0534950	3.0891350	0.3138030	H	-3.6871700	4.2115250	0.8185520
H	3.8421630	3.9430780	1.3038190	H	-4.9640340	3.2533170	0.0238830
H	4.8697260	2.6865380	2.0403380	H	-4.6912310	3.0937820	1.7792120
C	3.8038340	-2.5636790	-0.2834020	C	-3.8625790	-2.2187220	-0.1871760
N	2.9025950	-1.8434450	-0.1908800	N	-2.9055570	-1.5718330	-0.1287370
C	-0.8166210	-3.0583060	-0.8782620	C	0.4613820	-3.1961690	-0.6888280
N	-0.1664710	-2.1529940	-0.5683550	N	-0.0462530	-2.1862830	-0.4465750
C	4.9376380	-3.4717800	-0.3995360	C	-5.0679080	-3.0335150	-0.2611790
H	4.5919960	-4.5071840	-0.3294760	H	-5.1826890	-3.6111150	0.6604990
H	5.4338870	-3.3240540	-1.3630630	H	-5.9418310	-2.3888800	-0.3921890
H	5.6525080	-3.2773970	0.4050980	H	-4.9987790	-3.7201620	-1.1097900
C	-1.6528830	-4.1881390	-1.2594270	C	1.1170290	-4.4607990	-0.9862420
H	-2.6370550	-4.0843400	-0.7928650	H	2.1191430	-4.4605120	-0.5472880
H	-1.7704190	-4.2138490	-2.3465770	H	0.5376550	-5.2873300	-0.5650740
H	-1.1924840	-5.1225320	-0.9259080	H	1.1966840	-4.5913160	-2.0692520
H	-3.3368080	2.9515500	-0.3211350	H	3.4210340	2.5017860	-0.0934390
Cl	-0.7638600	4.8375080	-0.5461870	Cl	1.6307630	4.8930740	-0.3645340

Molecule 9a				TS ^{9a-10a}			
							
E = -2379.44350988, H (0K) = -2379.173695, H (298K) = -2379.140638, G (298K) = -2379.248225 au.				E = -2379.44255634, H (0K) = -2379.172914, H (298K) = -2379.140606, G (298K) = -2379.245560 au.			
Imaginary frequency = 0.				Imaginary frequency = 1.			
C	-2.0913090	-2.1832990	-0.9483860	C	2.3912930	-2.3712050	0.2906540
C	-2.5986020	-1.1730160	-0.1174120	C	2.8578120	-1.0685500	0.0488590
C	-3.7401860	-1.4202420	0.6598750	C	4.2140390	-0.8597040	-0.2456710
C	-4.3640700	-2.6677340	0.6087920	C	5.0941940	-1.9407510	-0.2961340
C	-3.8612150	-3.6690620	-0.2258270	C	4.6261560	-3.2339620	-0.0506450
C	-2.7270650	-3.4234220	-1.0061700	C	3.2741400	-3.4467890	0.2420070
C	-1.9091960	0.1613520	-0.0603710	C	1.9270610	0.0893080	0.0889500
O	-1.1685910	3.0900470	0.3483280	O	1.2367970	2.7558190	-1.2126790
C	-2.2767130	2.6871060	0.1352160	C	2.0013200	2.6229310	-0.2958760
C	-2.7555250	1.3317590	-0.0531720	C	2.4557420	1.4329970	0.3751180
H	-1.2133160	-1.9833800	-1.5540450	H	1.3436860	-2.5268890	0.5247100
H	-4.1302110	-0.6492960	1.3187850	H	4.5774980	0.1434200	-0.4514610
H	-5.2412700	-2.8556800	1.2209620	H	6.1413620	-1.7732120	-0.5296090
H	-4.3521870	-4.6370470	-0.2695790	H	5.3121470	-4.0753670	-0.0878120
H	-2.3403970	-4.1964390	-1.6642380	H	2.9113740	-4.4518130	0.4368010
N	-0.6244430	0.2318520	-0.0627980	N	0.6589010	0.0080460	0.0285650

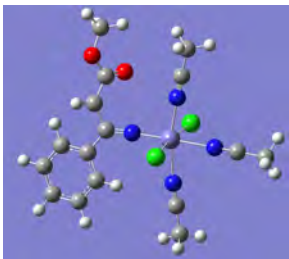
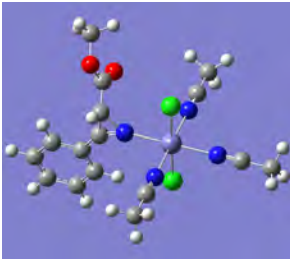
Cl	1.3269460	0.1862960	2.4030500	Cl	-1.3784140	-0.1549290	-2.3797830
Cl	1.4313680	-0.2740290	-2.4004630	Cl	-1.3648200	-0.2333060	2.4260600
C	1.9422630	3.2583800	-0.2772730	C	-1.7718940	3.1728060	0.0396170
Fe	1.2701200	-0.0168680	-0.0007650	Fe	-1.2491310	-0.1526740	0.0197260
N	1.8221960	2.1114360	-0.1976060	N	-1.6602540	2.0223070	0.0632130
C	2.0651370	4.7055120	-0.3731550	C	-1.8928090	4.6230400	0.0035620
H	1.0804740	5.1584630	-0.2242300	H	-0.9826720	5.0504190	-0.4274170
H	2.7521410	5.0738790	0.3939870	H	-2.7519260	4.9100550	-0.6093630
H	2.4455240	4.9833370	-1.3602440	H	-2.0282690	5.0100880	1.0174830
C	4.6352620	-0.5368620	0.0997460	C	-4.6457860	-0.4295290	0.0267640
N	3.4910050	-0.3702270	0.0734180	N	-3.4928300	-0.3378650	0.0264270
C	1.1154780	-3.3846650	0.3622950	C	-1.4539580	-3.5342120	-0.0624310
N	1.1887140	-2.2376390	0.2343090	N	-1.3382130	-2.3840240	-0.0206100
C	6.0763470	-0.7466050	0.1314220	C	-6.0977360	-0.5462500	0.0267160
H	6.4736320	-0.7412160	-0.8876110	H	-6.4626310	-0.6331090	1.0540910
H	6.5537610	0.0511930	0.7075800	H	-6.5398580	0.3397660	-0.4379400
H	6.2996800	-1.7098150	0.5990440	H	-6.3971010	-1.4341240	-0.5375940
C	-0.108380	-4.8287010	0.5182080	C	-1.5956950	-4.9825760	-0.1164210
H	-0.0153290	-5.1449280	0.3088060	H	-0.6069440	-5.4502800	-0.1277070
H	1.6908200	-5.3274280	-0.1783870	H	-2.1494400	-5.3330730	0.7592850
H	1.2729650	-5.1118130	1.5416770	H	-2.1379370	-5.2667990	-1.0228300
H	-3.8165730	1.2001100	-0.2214170	H	3.1641160	1.5410820	1.1890380
Cl	-3.6644950	3.8993390	0.0237760	Cl	2.8440060	4.1263660	0.3834460

Molecule 10a				Molecule 8b			
							
E = -2379.48493907, H (0K) = -2379.213451, H (298K) = -2379.180078, G (298K) = -2379.292688 au. Imaginary frequency = 0.				E = -2034.41769294, H (0K) = -2034.101742, H (298K) = -2034.068027, G (298K) = -2034.175767 au. Imaginary frequency = 0.			
C	-4.3849720	-0.6015870	0.3208160	C	-4.0294970	0.7835950	-0.4956350
C	-3.0607760	-0.9618110	0.0126820	C	-2.8607480	0.6371330	0.2705350
C	-2.7751840	-2.2042010	-0.5876680	C	-2.8069720	-0.3542500	1.2626660
C	-3.8212090	-3.0747090	-0.8756690	C	-3.9058840	-1.1875550	1.4770450
C	-5.1400370	-2.7153200	-0.5707440	C	-5.0638570	-1.0426400	0.7072120
C	-5.4220360	-1.4822510	0.0265080	C	-5.1221310	-0.0557170	-0.2812910
C	-1.9965850	-0.0454620	0.3188820	C	-1.7347210	1.5654020	0.0526870
O	-1.7038140	2.5861120	-1.1049030	O	0.2964530	2.3689690	-0.0643420
C	-1.7922740	2.4796230	0.0789900	C	-0.5522750	3.3779210	-0.3079010
C	-1.6205560	1.2538410	0.9023650	C	-1.8504500	2.9435750	-0.2546630
H	-4.5870880	0.3587180	0.7851980	H	-4.0763930	1.5458190	-1.2679360
H	-1.7446360	-2.4669670	-0.8094050	H	-1.9079340	-0.4672990	1.8600790
H	-3.6126520	-4.0349850	-1.3372850	H	-3.8590060	-1.9476680	2.2519740
H	-5.9511640	-3.4005590	-0.7992860	H	-5.9182750	-1.6910700	0.8802410
H	-6.4464310	-1.2106910	0.2610150	H	-6.0180420	0.0620840	-0.8840130
N	-0.7541530	0.1699040	0.2806150	C	1.3638770	4.7589870	-0.5426020
Cl	0.9923630	-2.4977280	-0.5956170	H	1.5192080	5.8173120	-0.7447950
Cl	1.8563680	2.1401810	0.5677910	H	1.7838010	4.4914130	0.4300990
C	1.6609090	-1.0232030	3.2639960	H	1.8154180	4.1501000	-1.3294870
Fe	1.4517410	-0.1797820	-0.0151570	O	-0.0722810	4.5860240	-0.5358690
				N	-0.4596360	1.1919850	0.1584380

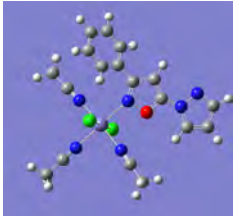
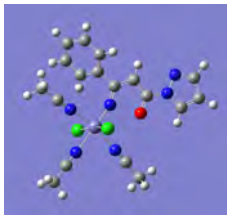
N	1.5921180	-0.7467910	2.1422470	Cl	0.6796630	-1.1743150	2.3672260
C	1.7482030	-1.3688140	4.6767810	Cl	1.3096740	-0.1377930	-2.3687200
H	2.6755860	-0.9708160	5.0986230	C	3.6299650	1.2846790	0.8090610
H	0.8973500	-0.9425590	5.2159940	Fe	0.9507940	-0.6209320	0.0006550
H	1.7385080	-2.4562220	4.7937310	N	2.6918120	0.6664270	0.5327420
C	4.7736410	-0.7287000	-0.3625310	C	4.8093730	2.0673970	1.1555480
N	3.6374350	-0.5420770	-0.2468660	H	4.6026280	3.1321420	1.0140650
C	1.2252280	0.6785540	-3.2823750	H	5.0778330	1.8907530	2.2010750
N	1.3088600	0.3795810	-2.1675530	H	5.6483910	1.7773470	0.5165170
C	6.2041570	-0.9636210	-0.5081060	C	3.1548010	-3.2231510	-0.2730900
H	6.7049060	-0.0338650	-0.7930580	N	2.4063140	-2.3457040	-0.1751340
H	6.6200060	-1.3192850	0.4389900	C	-1.4582120	-2.8044490	-0.8900830
H	6.3789630	-1.7167170	-1.2818700	N	-0.6509150	-2.0386200	-0.5737000
C	1.1192190	1.0562590	-4.6855450	C	4.0979170	-4.3274510	-0.3976220
H	1.9764110	1.6737490	-4.9688540	H	3.5621570	-5.2467660	-0.6510190
H	1.1015570	0.1589050	-5.3106070	H	4.8241890	-4.1076970	-1.1854030
H	0.1988190	1.6245370	-4.8477490	H	4.6281370	-4.4713540	0.5481940
H	-1.5626830	1.3900640	1.9774580	C	-2.4908900	-3.7550570	-1.2791370
Cl	-2.2192250	3.9290890	1.1090620	H	-3.4422890	-3.4626680	-0.8248060
				H	-2.5985920	-3.7629040	-2.3675780
				H	-2.2218400	-4.7588800	-0.9380070
				H	-2.7469440	3.5303310	-0.3719500

TS^{8b-9b}  E = -2034.37840726, H (0K) = -2034.065079, H (298K) = -2034.031756, G (298K) = -2034.137705 au. Imaginary frequency = 1.				Molecule 9b  E = -2034.38913991, H (0K) = -2034.076422, H (298K) = -2034.042064, G (298K) = -2034.151042 au. Imaginary frequency = 0.			
C	-3.8582130	0.6207220	-0.6507140	C	-3.4947350	-1.9596560	-0.6415950
C	-2.7770290	0.5043490	0.2362170	C	-2.4111740	-1.5331480	0.1409650
C	-2.8331930	-0.4202140	1.2885020	C	-1.7718550	-2.4445930	0.9944640
C	-3.9710370	-1.2117080	1.4567490	C	-2.2197300	-3.7639070	1.0698750
C	-5.0481540	-1.0959510	0.5731210	C	-3.2964900	-4.1870780	0.2844790
C	-4.9879700	-0.1804630	-0.4817370	C	-3.9303030	-3.2841030	-0.5729290
C	-1.5940870	1.4102740	0.0661100	C	-1.9241440	-0.1099070	0.0647560
O	0.5586500	2.7498000	-0.1286990	O	-1.6157100	2.8956830	-0.4035650
C	-0.4979810	3.4314720	-0.1901800	C	-2.6807370	2.3580880	-0.1443550
C	-1.7523850	2.7830410	-0.0939330	C	-2.9235080	0.9218950	0.0475410
H	-3.8093990	1.3314040	-1.4700310	H	-3.9869000	-1.2647960	-1.3165170
H	-1.9920700	-0.5135550	1.9679730	H	-0.9380330	-2.1084640	1.6025810
H	-4.0156450	-1.9182360	2.2808240	H	-1.7313700	-4.4604570	1.7456810
H	-5.9311900	-1.7144770	0.7068800	H	-3.6411200	-5.2156830	0.3420360
H	-5.8209100	-0.0870330	-1.1726650	H	-4.7638150	-3.6086020	-1.1891860
C	0.8199270	5.3852370	-0.4168110	C	-3.7669910	4.4588550	-0.1808220
H	0.6221250	6.4513300	-0.5237910	H	-4.7862080	4.8221650	-0.0549180
H	1.3932010	5.1943560	0.4939440	H	-3.1074410	4.9008550	0.5705680
H	1.3716430	5.0121690	-1.2832910	H	-3.3933440	4.6996710	-1.1792280
O	-0.4778090	4.7636180	-0.3370130	O	-3.8429930	3.0325420	-0.0040480
N	-0.3914280	0.8626240	0.0805990	N	-0.6571620	0.1264360	0.0528960
Cl	0.7669910	-1.1039940	2.3401770	Cl	1.4516480	-0.1937450	2.4093770

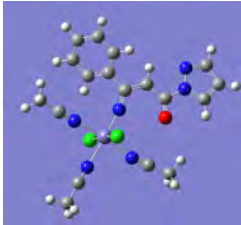
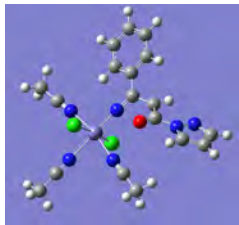
Cl	1.3229270	-0.3438540	-2.4024380	Cl	1.3498680	0.3876200	-2.4033500
C	3.6614600	1.2302940	0.6251430	C	1.3229850	3.4372880	0.3739530
Fe	0.8784320	-0.5220100	-0.0199640	Fe	1.2555460	0.1150200	0.0052150
N	2.6975100	0.6323830	0.4034790	N	1.5035770	2.2990210	0.2807610
C	4.8738420	1.9866970	0.9042500	C	1.0529940	4.8630760	0.4809720
H	5.6787470	1.3036770	1.1904410	H	1.2964360	5.2181720	1.4863310
H	5.1750870	2.5439280	0.0125430	H	1.6503940	5.4152060	-0.2500280
H	4.6906220	2.6891500	1.7223910	H	-0.0101810	5.0275840	0.2822720
C	3.0903480	-3.1539120	-0.1817250	C	4.6661570	0.0116270	-0.0735930
N	2.3425690	-2.2730830	-0.1257760	N	3.5101380	0.0407200	-0.0454590
C	-1.3520660	-2.9250510	-0.7391630	C	1.4681670	-3.2418870	-0.4724320
N	-0.5801540	-2.1029730	-0.4850420	N	1.4324710	-2.0989420	-0.2989420
C	4.0321070	-4.2636360	-0.2518770	C	6.1221140	-0.0265570	-0.1095320
H	3.8018650	-4.9957860	0.5273250	H	6.5011550	-0.5515860	0.7719490
H	3.9641470	-4.7470010	-1.2306750	H	6.4567400	-0.5488720	-1.0103960
H	5.0509670	-3.8934770	-0.1056450	H	6.5188940	0.9926500	-0.1179830
C	-2.3386270	-3.9483530	-1.0521500	C	1.4971090	-4.6818130	-0.6887140
H	-2.4410930	-4.0453330	-2.1367920	H	1.7582510	-4.8959000	-1.7290820
H	-2.0245300	-4.9083080	-0.6325040	H	2.2385990	-5.1425640	-0.0298180
H	-3.3031700	-3.6633490	-0.6215910	H	0.5109360	-5.1026160	-0.4712020
H	-2.7061020	3.2894170	-0.0857620	H	-3.9556490	0.6313070	0.2067950

TS^{9b-10b} 				Molecule 10b 			
E = -2034.38628075, H (0K) = -2034.074183, H (298K) = -2034.041223, G (298K) = -2034.146628 au. Imaginary frequency = 1.				E = -2034.43187369, H (0K) = -2034.117131, H (298K) = -2034.082605, G (298K) = -2034.193788 au. Imaginary frequency = 0.			
C	-4.3255090	-0.5844010	0.0190020	C	-4.3691760	-0.7862590	0.1778270
C	-2.9634820	-0.8825280	0.1790440	C	-3.0415580	-0.9897080	-0.2385810
C	-2.5615710	-2.2177140	0.3484760	C	-2.7371790	-1.9752500	-1.1976520
C	-3.5114730	-3.2359230	0.3597400	C	-3.7648650	-2.7471480	-1.7309250
C	-4.8686430	-2.9333730	0.2003590	C	-5.0866950	-2.5434670	-1.3159370
C	-5.2738470	-1.6075230	0.0286380	C	-5.3888450	-1.5652060	-0.3631020
C	-1.9628450	0.2176700	0.1606920	C	-2.0000490	-0.1747930	0.3319990
O	-1.3908510	2.7454580	-1.3919600	O	-1.8408600	2.7344650	-0.2747220
C	-1.9753790	2.7606130	-0.3184180	C	-1.8544080	2.3234840	0.8707110
C	-2.3804540	1.5944020	0.4637880	C	-1.6450300	0.8957150	1.2684690
H	-4.6414680	0.4450720	-0.1258460	H	-4.5878660	-0.0233640	0.9188760
H	-1.5088820	-2.4441270	0.4790380	H	-1.7054230	-2.1205300	-1.5053660
H	-3.1965980	-4.2662760	0.4977480	H	-3.5393230	-3.5093210	-2.4707550
H	-5.6072680	-3.7298700	0.2102320	H	-5.8834000	-3.1499400	-1.7371120
H	-6.3256130	-1.3694550	-0.0998790	H	-6.4152540	-1.4118380	-0.0445800
C	-2.1256070	5.1173930	-0.4211440	N	-0.7603260	0.0674410	0.3472350
H	-2.5348080	5.9121430	0.2016910	Cl	0.9899740	-1.9937670	-1.6018280
H	-1.0492670	5.2521880	-0.5561130	Cl	1.9004670	1.6198570	1.5335580
H	-2.6134370	5.1068710	-1.3993320	C	1.5213140	-2.4112380	2.5323560
O	-2.3940990	3.8951570	0.2884820	Fe	1.4294900	-0.1814020	-0.0292860
N	-0.7103280	0.0538950	0.0110720	N	1.4992120	-1.6597030	1.6524240
Cl	1.2504900	-0.6012940	2.3996460	C	1.5481860	-3.3557200	3.6416630
Cl	1.4587810	0.0284370	-2.3835940	H	2.4455420	-3.1930370	4.2455060

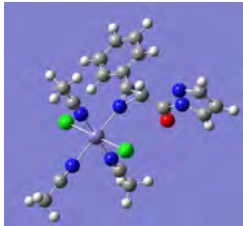
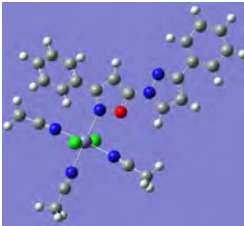
C	2.1388300	2.9712900	0.4781670	H	0.6634970	-3.2153010	4.2693250
Fe	1.2005460	-0.2439080	-0.0000080	H	1.5557600	-4.3795030	3.2567190
N	1.7927440	1.8791490	0.3196080	C	4.7650200	-0.5995870	-0.5014100
C	2.5786410	4.3453090	0.6783670	N	3.6259250	-0.4639730	-0.3484500
H	2.5289060	4.5987080	1.7412270	C	1.3648710	2.0199520	-2.6018100
H	3.6095530	4.4573890	0.3305260	N	1.3941350	1.2697960	-1.7211370
H	1.9342970	5.0268550	0.1157250	C	6.1995630	-0.7689600	-0.6931440
C	4.5732030	-0.8233930	0.0812050	H	6.7027550	0.1974190	-0.5958310
N	3.4336480	-0.6260140	0.0548750	H	6.5957680	-1.4566860	0.0594660
C	1.1132240	-3.6088690	-0.4798790	H	6.3949850	-1.1762080	-1.6892900
N	1.0969850	-2.4655950	-0.3031670	C	1.3260820	2.9631940	-3.7116040
C	6.0084600	-1.0722050	0.1138440	H	2.2080260	3.6093870	-3.6804810
H	6.3449710	-1.1690730	1.1500120	H	1.3138760	2.4186670	-4.6601310
H	6.2361480	-1.9962430	-0.4253180	H	0.4263080	3.5810740	-3.6410310
H	6.5391350	-0.2412770	-0.3597710	H	-1.5667760	0.6972170	2.3343150
C	1.1297270	-5.0481220	-0.7030600	O	-2.0720600	3.0882700	1.9509780
H	0.1636790	-5.3717410	-1.1011670	C	-2.3077940	4.4880960	1.6968580
H	1.9161800	-5.3021490	-1.4194950	H	-2.4733570	4.9376450	2.6751260
H	1.3218480	-5.5670080	0.2404420	H	-1.4378390	4.9360290	1.2109450
H	-2.9605780	1.7674330	1.3657830	H	-3.1874040	4.6157600	1.0615070

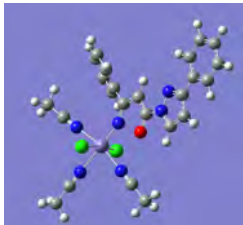
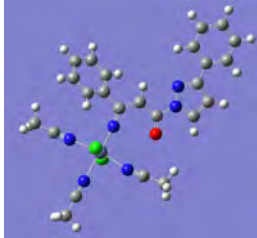
Molecule 8c				TS ^{8c-9c}			
							
E = -2144.89228867, H (0K) = -2144.557678, H (298K) = -2144.522929, G (298K) = -2144.633397 au.				E = -2144.85030077, H (0K) = -2144.518479, H (298K) = -2144.484091, G (298K) = -2144.593401 au.			
Imaginary frequency = 0.				Imaginary frequency = 1.			
C	0.1774190	4.0611300	-0.3814100	C	0.5178320	2.8921270	1.2963110
C	0.0134370	2.8812510	0.3639350	C	-0.4329200	2.6691780	0.2904870
C	-1.0445880	2.7850030	1.2814770	C	-0.7847510	3.7085890	-0.5841400
C	-1.9264000	3.8544900	1.4426190	C	-0.1891920	4.9629750	-0.4493050
C	-1.7637980	5.0238270	0.6936160	C	0.7517790	5.1889300	0.5597380
C	-0.7107720	5.1236680	-0.2204960	C	1.1008430	4.1534870	1.4316650
C	0.9898660	1.7880770	0.2045870	C	-1.1154380	1.3396590	0.1578070
O	1.8698770	-0.2114980	0.1451920	O	-2.1151810	-1.0235730	0.0209990
C	2.8568340	0.6728080	-0.0477580	C	-2.9422180	-0.0745590	-0.0303390
C	2.3845420	1.9509010	-0.0267630	C	-2.5082740	1.2602850	0.0364440
H	0.9910400	4.1408430	-1.0964020	H	0.7910290	2.0839310	1.9671720
H	-1.1702070	1.8778640	1.8639310	H	-1.5147610	3.5315270	-1.3679160
H	-2.7381320	3.7761410	2.1604030	H	-0.4629290	5.7633690	-1.1306110
H	-2.4503130	5.8554110	0.8257420	H	1.2088030	6.1685460	0.6673390
H	-0.5791680	6.0286630	-0.8063720	H	1.8270930	4.3266600	2.2207540
N	0.6627390	0.5027160	0.2945250	N	-0.3679570	0.2601170	0.1694730
Cl	-1.8458790	-0.7333590	2.2954230	Cl	0.9881830	-1.2065350	-2.3758350
Cl	-0.3792050	-1.3044290	-2.3163460	Cl	1.8604760	-0.5620840	2.3115720
C	0.8185020	-3.5968090	0.9944570	C	-0.0817500	-3.7723650	0.6932390
Fe	-1.1021100	-1.0007420	-0.0101540	Fe	1.2031190	-0.7678110	-0.0087960
N	0.2084310	-2.6767700	0.6477360	N	0.3671110	-2.7365960	0.4459540
C	1.5898070	-4.7534730	1.4313670	C	-0.6524890	-5.0740450	1.0069110
H	1.2091650	-5.6575670	0.9475250	H	-0.5857400	-5.7277770	0.1326180
H	2.6422830	-4.6205600	1.1647860	H	-0.1051090	-5.5272970	1.8383650
H	1.5066070	-4.8657120	2.5162080	H	-1.7027810	-4.9565040	1.2890650
C	-3.5850630	-3.2974210	-0.4825650	C	4.1344430	-2.5246250	-0.3198140

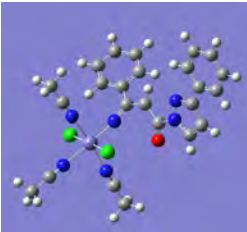
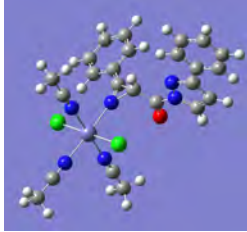
N	-2.7384140	-2.5226420	-0.3325090	N	3.1484340	-1.9292060	-0.2144810
C	-3.2845460	1.3464890	-1.0543490	C	3.1691140	1.8286270	-0.7981410
N	-2.5205590	0.5559350	-0.6942080	N	2.5012280	0.9273540	-0.5194030
C	-4.6522760	-4.2721310	-0.6698720	C	5.3765530	-3.2740560	-0.4545060
H	-5.6236350	-3.7906860	-0.5246570	H	6.0210310	-3.0835840	0.4083970
H	-4.6047300	-4.6847790	-1.6817000	H	5.1581060	-4.3443980	-0.5094350
H	-4.5437280	-5.0849390	0.0540280	H	5.8966980	-2.9676000	-1.3665870
C	-4.2354690	2.3573540	-1.4961950	C	3.9954360	2.9760210	-1.1422640
H	-4.0131500	3.3059960	-0.9984690	H	3.5491430	3.8811250	-0.7196490
H	-4.1596890	2.4920470	-2.5789670	H	5.0018250	2.8447990	-0.7346530
H	-5.2535730	2.0474260	-1.2435710	H	4.0566640	3.0761950	-2.2296840
H	2.9454560	2.8655450	-0.1218800	H	-3.1599370	2.1191300	0.0463870
N	4.1257410	0.1542630	-0.2125900	N	-4.3095320	-0.3902980	-0.1483750
C	4.5137300	-1.1649470	-0.2313110	C	-4.8531810	-1.6495560	-0.2125920
C	6.2256070	0.2101270	-0.5227320	C	-6.4046080	-0.0754080	-0.3230950
C	5.8719230	-1.1629580	-0.4306400	C	-6.2110420	-1.4843270	-0.3262820
H	3.7982270	-1.9627670	-0.1046160	H	-4.2256620	-2.5260320	-0.1718200
H	7.2065690	0.6395940	-0.6793540	H	-7.3360590	0.4719380	-0.3949160
H	6.5212800	-2.0227790	-0.5013040	H	-6.9610930	-2.2578580	-0.4011890
N	5.1771280	1.0107270	-0.3922350	N	-5.2627110	0.5881140	-0.2164820

Molecule 9c				TS ^{9c-10c}			
							
E = -2144.85544428, H (0K) = -2144.524413, H (298K) = -2144.488890, G (298K) = -2144.601721 au.				E = -2144.85424056, H (0K) = -2144.523324, H (298K) = -2144.488631, G (298K) = -2144.598597 au.			
Imaginary frequency = 0.				Imaginary frequency = 1.			
C	0.1955340	3.0253350	0.9810270	C	0.3921700	3.5090320	0.2835020
C	-0.8082800	2.5594300	0.1188970	C	-0.8474850	2.9148320	-0.0046760
C	-1.5296420	3.4732360	-0.6640710	C	-1.9567740	3.7282400	-0.2830540
C	-1.2458880	4.8377910	-0.5875070	C	-1.8291040	5.1174970	-0.2715090
C	-0.2514750	5.2995950	0.2787130	C	-0.5947070	5.7029710	0.0199170
C	0.4651440	4.3918390	1.0646640	C	0.5148350	4.8961560	0.2965990
C	-1.0978440	1.0835600	0.0373300	C	-0.9919430	1.4328600	-0.0300570
O	-2.3035170	-1.6614830	-0.3758430	O	-2.2943400	-0.7758570	-1.5886090
C	-2.9799570	-0.6631960	-0.1632950	C	-2.8089490	-0.3009910	-0.5816440
C	-2.4856940	0.6972810	0.0188770	C	-2.3172640	0.8353510	0.1751170
H	0.7457910	2.3146390	1.5896210	H	1.2465590	2.8779860	0.5038880
H	-2.2993400	3.1201460	-1.3448910	H	-2.9152080	3.2758660	-0.5225640
H	-1.8022120	5.5381060	-1.2038060	H	-2.6911650	5.7400030	-0.4922230
H	-0.0373620	6.3626620	0.3429990	H	-0.4959060	6.7846980	0.0313840
H	1.2309210	4.7485700	1.7478190	H	1.4739880	5.3507910	0.5271790
N	-0.1209210	0.2459390	0.0214990	N	-0.0116740	0.6227180	-0.0974330
Cl	1.5177310	-0.9862330	-2.4060570	Cl	1.6864270	-0.8017940	-2.4055010
Cl	1.8285420	-0.4828010	2.4046710	Cl	1.4809930	-0.5782590	2.4115850
C	0.0168120	-3.6384600	0.3499850	C	-0.5050830	-3.3678760	0.0365280
Fe	1.5556850	-0.6876600	-0.0014010	Fe	1.4580850	-0.6168000	-0.0120100
N	0.7026300	-2.7110770	0.2701560	N	0.1982480	-2.4499450	0.0328200
C	-0.8781910	-4.7824520	0.4392980	C	-1.3991560	-4.5175910	0.0411370
H	-0.5956140	-5.5386760	-0.2984920	H	-1.1923550	-5.1514310	-0.8259140
H	-0.8302480	-5.2207120	1.4401420	H	-1.2512390	-5.0996320	0.9552370
H	-1.8988620	-4.4429700	0.2394190	H	-2.4372550	-4.1754140	-0.0034690

C	4.5717810	-2.2818930	-0.0179650	C	4.0566070	-2.8248600	0.2127490
N	3.5547340	-1.7308790	-0.0136850	N	3.1783730	-2.0758700	0.1365520
C	3.3890040	2.1301500	-0.4811740	C	3.9894300	1.6446730	-0.0276980
N	2.8011540	1.1493300	-0.3077270	N	3.0956420	0.9102060	-0.0170080
C	5.8525990	-2.9762590	-0.0223870	C	5.1630280	-3.7678060	0.3095550
H	6.6677910	-2.2493890	0.0359710	H	6.0840660	-3.2329710	0.5586330
H	5.9111050	-3.6503770	0.8370420	H	4.9542380	-4.5047570	1.0903010
H	5.9557610	-3.5580160	-0.9428500	H	5.2951900	-4.2840140	-0.6456540
C	4.1135910	3.3746730	-0.6979350	C	5.1134710	2.5707700	-0.0405520
H	3.4681460	4.2201820	-0.4420090	H	4.7444100	3.6003120	-0.0555160
H	5.0074910	3.4002120	-0.0683440	H	5.7256560	2.4214440	0.8534590
H	4.4106850	3.4534760	-1.7476020	H	5.7263640	2.3961220	-0.9294670
H	-3.2302270	1.4685110	0.1661370	H	-2.9334930	1.2145190	0.9828070
N	-4.3927400	-0.7923840	-0.0890440	N	-4.0327190	-0.8517990	-0.1107440
C	-5.0927070	-1.9643080	-0.2496590	C	-4.7245780	-1.8772220	-0.7079940
C	-6.4371880	-0.2503030	0.1507410	C	-5.7278010	-1.1705660	1.1357500
C	-6.4192550	-1.6525660	-0.1011260	C	-5.8286680	-2.1116940	0.0720490
H	-4.5801140	-2.8911520	-0.4527630	H	-4.3660170	-2.3276680	-1.6201270
H	-7.2950750	0.3869070	0.3243760	H	-6.4049970	-1.0265770	1.9680940
H	-7.2617950	-2.3254610	-0.1633760	H	-6.6023150	-2.8474660	-0.0913640
N	-5.2224620	0.2715330	0.1589230	N	-4.6493440	-0.4110140	1.0299160

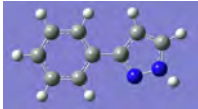
Molecule 10c				Molecule 8d			
							
E = -2144.89732065, H (0K) = -2144.564274, H (298K) = -2144.528615, G (298K) = -2144.644229 au.				E = -2375.95044591, H (0K) = -2375.534786, H (298K) = -2375.495326, G (298K) = -2375.617112 au.			
Imaginary frequency = 0.				Imaginary frequency = 0.			
C	-3.6228920	2.3316670	-0.4340730	C	0.5761240	3.9720910	0.3136090
C	-2.2329140	2.2605410	-0.2336900	C	0.9380420	2.8250530	-0.4129350
C	-1.4891610	3.4255060	0.0376730	C	2.0462700	2.8727390	-1.2729540
C	-2.1447320	4.6508310	0.1075550	C	2.7821340	4.0521330	-1.3960840
C	-3.5293420	4.7206390	-0.0899620	C	2.4232890	5.1887740	-0.6653920
C	-4.2673470	3.5638330	-0.3608250	C	1.3195950	5.1451870	0.1915940
C	-1.5806440	0.9791030	-0.3089810	C	0.1093340	1.6105090	-0.2984150
O	-2.0865320	-1.0487840	1.7518450	O	-0.4975330	-0.4888390	-0.2538380
C	-2.2261560	-1.3193100	0.5719560	C	-1.6059770	0.2573640	-0.1555370
C	-1.7228030	-0.4639820	-0.5452850	C	-1.3076080	1.5873280	-0.1723130
H	-4.1824340	1.4251520	-0.6441480	H	-0.2781190	3.9406300	0.9836130
H	-0.4146370	3.3523670	0.1794540	H	2.3235510	1.9907880	-1.8414190
H	-1.5793770	5.5543490	0.3150430	H	3.6336200	4.0845580	-2.0700440
H	-4.0339940	5.6808480	-0.0332700	H	2.9969180	6.1057250	-0.7675510
H	-5.3403150	3.6240900	-0.5141380	H	1.0358400	6.0242440	0.7628350
N	-0.4835860	0.3630200	-0.2162280	N	0.6111110	0.3800470	-0.3338970
Cl	2.1321820	2.4037080	-0.1288520	Cl	3.3036020	-0.5197300	-2.2509040
Cl	1.3129230	-2.3942690	0.0673740	Cl	1.8134970	-1.2560410	2.3366830
C	1.9047260	-0.1671860	-3.4121200	C	1.0319190	-3.7148790	-0.9788030
Fe	1.7161970	0.0007760	-0.0259820	Fe	2.5454110	-0.8683740	0.0422460
N	1.8444530	-0.1092170	-2.2577770	N	1.4971790	-2.7153940	-0.6274670
C	1.9810530	-0.2405740	-4.8654130	C	0.4442520	-4.9722290	-1.4230410
H	2.9034750	-0.7473950	-5.1631600	H	0.6083350	-5.7457080	-0.6671960
H	1.1241130	-0.7983370	-5.2539070	H	-0.6310570	-4.8455760	-1.5783670

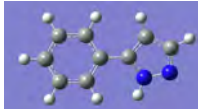
H	1.9737000	0.7682530	-5.2879930	H	0.9075710	-5.2856590	-2.3630510
C	5.0566680	-0.5504600	0.1862860	C	5.3134190	-2.7813640	0.6223480
N	3.9175260	-0.3607790	0.1110950	N	4.3693100	-2.1424860	0.4221090
C	1.5380390	0.1685940	3.3527750	C	4.3671400	1.7464480	1.1330490
N	1.6101150	0.1191920	2.1988270	N	3.7213120	0.8661770	0.7505100
C	6.4909660	-0.7888280	0.2816760	C	6.5036830	-3.5835860	0.8746420
H	6.6980490	-1.4783490	1.1051570	H	7.3456580	-2.9303130	1.1211690
H	6.8576810	-1.2250830	-0.6519250	H	6.3218390	-4.2646700	1.7109420
H	7.0119000	0.1552890	0.4651700	H	6.7526370	-4.1681080	-0.0157350
C	1.4454120	0.2291180	4.8055920	C	5.1670220	2.8694350	1.6022690
H	2.2988680	-0.2876740	5.2538200	H	4.8316280	3.7852240	1.1064120
H	1.4452780	1.2723830	5.1340030	H	5.0518080	2.9823950	2.6840610
H	0.5205540	-0.2512080	5.1376890	H	6.2220880	2.6992150	1.3695930
H	-1.8007330	-0.8561330	-1.5523100	H	-1.9900990	2.4200680	-0.1406940
N	-2.9104550	-2.4901490	0.1918580	N	-2.8023990	-0.4243400	-0.0749000
C	-3.4721510	-3.4063940	1.0535770	C	-3.0114840	-1.7837330	-0.0586720
C	-4.0391570	-4.3790390	0.2746870	C	-4.9241810	-0.6441760	0.0674850
H	-3.4083590	-3.2692850	2.1215080	C	-4.3655330	-1.9615040	0.0323550
C	-3.7745290	-3.9730080	-1.0660340	H	-2.1895620	-2.4809790	-0.1121420
H	-4.5684490	-5.2597720	0.6073770	H	-4.8840450	-2.9074930	0.0676540
H	-4.0571980	-4.4739150	-1.9833420	N	-3.9662060	0.2812470	0.0020410
N	-3.0971960	-2.8395320	-1.1222750	C	-6.3420190	-0.2573900	0.1592770
				C	-7.3488040	-1.2328410	0.2488280
				C	-6.7136180	1.0991510	0.1579730
				C	-8.6911840	-0.8622050	0.3341860
				H	-7.0873760	-2.2866110	0.2530560
				C	-8.0546080	1.4664840	0.2433940
				H	-5.9419640	1.8587750	0.0888320
				C	-9.0499420	0.4877280	0.3317600
				H	-9.4563320	-1.6303990	0.4028160
				H	-8.3244010	2.5190080	0.2407230
				H	-10.0953940	0.7755760	0.3980390
TS^{8d-9d}  E = -2375.90844489, H (0K) = -2375.495552, H (298K) = -2375.456498, G (298K) = -2375.576347 au. Imaginary frequency = 1.				Molecule 9d  E = -2375.91381770, H (0K) = -2375.501714, H (298K) = -2375.461469, G (298K) = -2375.586090 au. Imaginary frequency = 0.			
C	-1.5238920	2.8992450	-1.3331690	C	-1.0978980	3.0182120	0.8605350
C	-0.5600890	2.5579710	-0.3738740	C	-0.1812710	2.4258480	-0.0212570
C	-0.0316880	3.5466120	0.4703510	C	0.6277100	3.2385550	-0.8297740
C	-0.4642530	4.8675890	0.3511480	C	0.5176080	4.6281840	-0.7585790
C	-1.4179150	5.2103560	-0.6119900	C	-0.3902070	5.2150090	0.1268100
C	-1.9434370	4.2253820	-1.4533180	C	-1.1942170	4.4079520	0.9376520
C	-0.0508150	1.1513580	-0.2611080	C	-0.0802270	0.9255890	-0.0978920
O	0.6409910	-1.3223820	-0.1603200	O	0.7418840	-1.9397850	-0.6096430
C	1.5846650	-0.4874070	-0.1396510	C	1.5499460	-1.0435740	-0.3968380
C	1.3237860	0.8925720	-0.1939460	C	1.2453520	0.3661700	-0.1800230
H	-1.9345490	2.1310830	-1.9804380	H	-1.7160110	2.3850870	1.4893320
H	0.7076300	3.2794630	1.2190950	H	1.3297440	2.7886410	-1.5263540
H	-0.0537980	5.6282740	1.0088920	H	1.1409450	5.2502010	-1.3944420

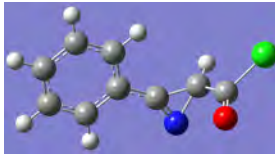
H	-1.7479970	6.2408850	-0.7076990	H	-0.4694980	6.2967950	0.1864220
H	-2.6804190	4.4883400	-2.2068580	H	-1.8934090	4.8611510	1.6348660
N	-0.9307860	0.1763240	-0.2389420	N	-1.1516520	0.2143210	-0.0516710
Cl	-2.2962830	-1.1357130	2.3805240	Cl	-3.0400700	-0.2323740	2.4526050
Cl	-3.3740570	-0.3294740	-2.2425720	Cl	-3.0458040	-0.9057750	-2.3518060
C	-1.7975580	-3.7854510	-0.7553800	C	-1.6886310	-3.6299310	0.4413960
Fe	-2.6079860	-0.6395000	0.0341150	Fe	-2.9136880	-0.5369430	0.0419750
N	-2.0822370	-2.6992540	-0.4821030	N	-2.2568710	-2.6270340	0.3530490
C	-1.4336780	-5.1517210	-1.1011040	C	-0.9436000	-4.8761090	0.5411030
H	-0.3566270	-5.2899960	-0.9695100	H	0.0952810	-4.6879780	0.2543260
H	-1.9680480	-5.8522550	-0.4530570	H	-0.9748420	-5.2512010	1.5679980
H	-1.6977870	-5.3519100	-2.1435220	H	-1.3746710	-5.6255110	-0.1287570
C	-5.7227160	-1.9930120	0.5267250	C	-6.0663710	-1.8267060	0.2217020
N	-4.6772550	-1.5263610	0.3621770	N	-5.0026010	-1.3760220	0.1641080
C	-4.1788590	2.1866770	0.9123200	C	-4.4808180	2.4379000	-0.4337370
N	-3.6346850	1.2091330	0.6219050	N	-3.9792950	1.4098740	-0.2625130
C	-7.0390600	-2.5819820	0.7339020	C	-7.4055270	-2.3961070	0.2929780
H	-7.0555390	-3.5992480	0.3321250	H	-7.3518300	-3.4824320	0.1769340
H	-7.2669770	-2.6147610	1.8031320	H	-7.8578960	-2.1604980	1.2605040
H	-7.7978480	-1.9828050	0.2224470	H	-8.0275110	-1.9808190	-0.5051570
C	-4.8534290	3.4270380	1.2645670	C	-5.0990510	3.7389630	-0.6484780
H	-4.3007180	4.2710660	0.8414520	H	-4.3673620	4.5275610	-0.4495670
H	-5.8703690	3.4224940	0.8617700	H	-5.4430640	3.8200910	-1.6835540
H	-4.8967260	3.5311380	2.3524120	H	-5.9523890	3.8614490	0.0246020
H	2.0797540	1.6603330	-0.2321780	H	2.0884410	1.0335950	-0.0592230
N	2.9019280	-0.9773300	-0.0665840	N	2.9335840	-1.3601730	-0.3640240
C	3.2776870	-2.2974880	-0.0217170	C	3.4629300	-2.6125060	-0.5701930
C	5.0378910	-0.9345250	0.0547670	C	5.0515010	-1.1008130	-0.1663810
C	4.6440390	-2.3116550	0.0562400	C	4.8185990	-2.4884750	-0.4519640
H	2.5414130	-3.0853990	-0.0495070	H	2.8248390	-3.4561420	-0.7801300
H	5.2750400	-3.1862150	0.1064360	H	5.5470330	-3.2786110	-0.5550320
N	3.9731200	-0.1364120	-0.0198190	N	3.9037770	-0.4302850	-0.1162180
C	6.3994890	-0.3762930	0.1246260	C	6.3393700	-0.4226260	0.0546580
C	7.5182620	-1.2197810	0.2261430	C	7.5476660	-1.1354070	-0.0205000
C	6.6047520	1.0148830	0.0929040	C	6.3829730	0.9531110	0.3449870
C	8.8063990	-0.6877550	0.2942240	C	8.7669140	-0.4904340	0.1891160
H	7.3864740	-2.2971590	0.2535960	H	7.5402980	-2.1977080	-0.2441820
C	7.8917290	1.5438370	0.1612140	C	7.6015360	1.5945710	0.5536930
H	5.7462120	1.6736800	0.0141680	H	5.4543210	1.5109640	0.4054200
C	8.9990990	0.6952950	0.2623240	C	8.7992980	0.8759690	0.4768160
H	9.6593570	-1.3561200	0.3728920	H	9.6914530	-1.0574880	0.1268520
H	8.0317640	2.6210900	0.1354490	H	7.6177370	2.6577090	0.7772570
H	10.0022020	1.1090900	0.3156450	H	9.7489760	1.3776470	0.6399830
TS^{9d-10d}  E = -2375.90398437, H (0K) = -2375.493295, H (298K) = -2375.453172, G (298K) = -2375.578280 au. Imaginary frequency = 1.				Molecule 10d  E = -2375.95546552, H (0K) = -2375.541285, H (298K) = -2375.501005, G (298K) = -2375.626997 au. Imaginary frequency = 0.			
C	-1.5470400	3.5526850	-0.3951780	C	-0.1459450	4.2631610	-0.6639270
C	-0.3722880	2.9109290	-0.8223810	C	0.8652780	3.2872670	-0.6166980

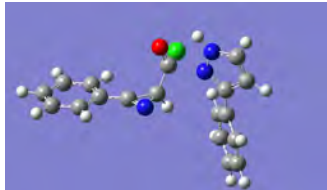
C	0.6846110	3.6692250	-1.3503380	C	2.2072480	3.6356970	-0.8652280
C	0.5731010	5.0565630	-1.4389000	C	2.5240390	4.9588090	-1.1570770
C	-0.5931010	5.6929080	-1.0066130	C	1.5166840	5.9305520	-1.2019320
C	-1.6516110	4.9384840	-0.4890930	C	0.1841130	5.5839200	-0.9564540
C	-0.2326370	1.4337810	-0.7296470	C	0.5087720	1.9262090	-0.3102700
O	0.6370400	-0.9664250	-2.2790230	O	-0.4356790	1.2262010	2.3760630
C	1.3827580	-0.4061310	-1.4813390	C	-1.0885250	0.9163370	1.3939580
C	1.0892170	0.8106570	-0.7456750	C	-0.5658440	0.9721470	-0.0045890
H	-2.3696050	2.9636300	-0.0020610	H	-1.1759760	3.9786010	-0.4716400
H	1.5863790	3.1765060	-1.7021030	H	2.9738770	2.8665520	-0.8336020
H	1.3940230	5.6374040	-1.8486060	H	3.5556650	5.2366060	-1.3510650
H	-0.6791890	6.7735380	-1.0758260	H	1.7720390	6.9614500	-1.4298880
H	-2.5597120	5.4323660	-0.1556780	H	-0.5928110	6.3411810	-0.9935510
N	-1.1994760	0.6264090	-0.5244350	N	0.9383500	0.7527950	-0.1362580
Cl	-1.1494600	-2.3146020	0.9055740	Cl	4.1175590	0.3914710	-1.0035420
Cl	-4.3843990	1.1322510	-0.2982260	Cl	0.5486490	-2.3914660	0.7851640
C	-3.3182890	-2.1479860	-2.6707950	C	1.3212780	-1.7356880	-3.2655010
Fe	-2.6999000	-0.5552480	0.2517140	Fe	2.3270170	-0.9994510	-0.1064160
N	-3.1064120	-1.5974950	-1.6754800	N	1.6672620	-1.4826720	-2.1904150
C	-3.5851330	-2.8421580	-3.9234050	C	0.8860620	-2.0560090	-4.6187210
H	-3.8088780	-2.1151440	-4.7093110	H	1.2889900	-3.0281370	-4.9172450
H	-2.7087220	-3.4278090	-4.2154480	H	-0.2063720	-2.0935150	-4.6574520
H	-4.4403830	-3.5128260	-3.8005010	H	1.2435470	-1.2909350	-5.3138760
C	-5.1935710	-2.4104970	1.6182680	C	4.4227070	-3.6657950	-0.1463500
N	-4.3487180	-1.7716900	1.1525740	N	3.7012070	-2.7610060	-0.1372050
C	-2.2877040	0.8711760	3.3137150	C	3.3719110	-0.2900550	3.0374710
N	-2.4347530	0.4012540	2.2665550	N	3.0150990	-0.5336840	1.9638840
C	-6.2561230	-3.2159690	2.2056340	C	5.3332710	-4.8032550	-0.1565590
H	-7.1257880	-3.2236030	1.5424120	H	5.1687300	-5.4177300	0.7332140
H	-5.9058650	-4.2420580	2.3502780	H	5.1588190	-5.4108430	-1.0491440
H	-6.5467450	-2.7965810	3.1731840	H	6.3679790	-4.4484870	-0.1609350
C	-2.1015230	1.4595880	4.6335290	C	3.8217810	0.0171510	4.3887950
H	-1.1329330	1.9655350	4.6803350	H	3.8916640	-0.9038990	4.9745600
H	-2.8955870	2.1853350	4.8312120	H	4.8053510	0.4942270	4.3520600
H	-2.1338550	0.6756360	5.3956970	H	3.1119390	0.6956370	4.8705880
H	1.8770260	1.2576270	-0.1504280	H	-1.1926130	0.5707730	-0.7919960
N	2.6877970	-0.9232180	-1.2765670	N	-2.4208300	0.4879510	1.5394190
C	3.2142310	-2.0214760	-1.9129990	C	-3.0989950	0.3755880	2.7334720
C	4.6662450	-1.1219200	-0.4797190	C	-4.3541590	-0.0658960	2.4287530
C	4.4826270	-2.1824240	-1.4290400	H	-2.6172670	0.6188940	3.6673340
H	2.6351050	-2.5715230	-2.6376570	C	-4.3748190	-0.2047420	0.9994150
H	5.1843370	-2.9527910	-1.7110850	H	-5.1510560	-0.2678690	3.1285220
N	3.5728400	-0.3677390	-0.3974080	N	-3.2012920	0.1334150	0.4736950
C	5.8565080	-0.8280370	0.3356700	C	-5.4890520	-0.6532250	0.1468410
C	7.0150500	-1.6148530	0.2243140	C	-6.7354210	-0.9786550	0.7069670
C	5.8551330	0.2479370	1.2417750	C	-5.3243740	-0.7641720	-1.2456230
C	8.1417800	-1.3336980	0.9976590	C	-7.7890110	-1.4039940	-0.1029250
H	7.0416840	-2.4502820	-0.4685390	H	-6.8880350	-0.8999550	1.7789390
C	6.9813690	0.5266520	2.0124830	C	-6.3778050	-1.1887010	-2.0520280
H	4.9641610	0.8600910	1.3348310	H	-4.3645030	-0.5156610	-1.6862340
C	8.1301090	-0.2627760	1.8942660	C	-7.6151590	-1.5108270	-1.4846120
H	9.0288940	-1.9528520	0.8980810	H	-8.7459710	-1.6515630	0.3478370
H	6.9633850	1.3613790	2.7078170	H	-6.2335860	-1.2694560	-3.1259240
H	9.0076770	-0.0443840	2.4962540	H	-8.4357410	-1.8423570	-2.1146620

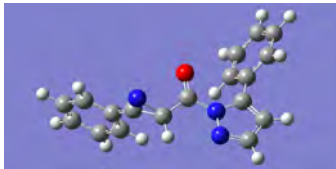
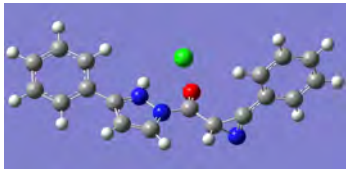
Table S4. B3LYP/6-31+G(d,p), PCM solvent model for MeCN.
Absolute Energies (au), Cartesian Coordinates of stationary points

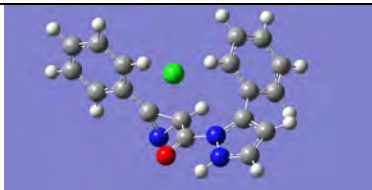
Molecule 2b			
			
E = -457.302825, H (0K) = -457.150560, H (298K) = -457.141394, G (298K) = -457.184958 au. Imaginary frequency = 0.			
C	1.0206400	0.0374460	0.0001510
C	1.8907010	1.1612360	0.0685970
C	3.1666500	0.6315960	0.0385190
N	3.0193040	-0.7141530	-0.0419500
N	1.7284890	-1.1031160	-0.0675870
H	4.1409590	1.0967060	0.0696630
H	1.6327660	2.2070610	0.1370220
C	-0.4549670	0.0154170	-0.0002780
C	-1.1599200	-1.2020550	0.0416490
C	-1.1913520	1.2128540	-0.0418600
C	-2.5552980	-1.2188870	0.0412600
H	-0.6057740	-2.1339230	0.0767250
C	-2.5880940	1.1946350	-0.0407660
H	-0.6747290	2.1667670	-0.0795880
C	-3.2779020	-0.0209090	0.0005350
H	-3.0798510	-2.1696510	0.0748840
H	-3.1362070	2.1318550	-0.0740650
H	-4.3638170	-0.0351590	0.0012350
H	3.7493520	-1.4107720	-0.0859620

Molecule 2'b			
			
E = -457.301856, H (0K) = -457.149596, H (298K) = -457.140412, G (298K) = -457.183669 au. Imaginary frequency = 0.			
C	1.0234340	0.0824680	0.0189160
C	1.9096970	1.1162930	0.3165030
C	3.1944730	0.5576300	0.1591410
N	3.1344200	-0.7255420	-0.2132290
H	4.1565710	1.0303850	0.3048320
H	1.6585230	2.1191800	0.6278630
C	-0.4449170	0.0337900	0.0117170
C	-1.1409480	-1.1740690	0.2039400
C	-1.1850680	1.2145200	-0.1847470
C	-2.5369570	-1.2000470	0.1897920
H	-0.5970730	-2.0957210	0.3890090
C	-2.5800260	1.1868050	-0.1884110
H	-0.6649730	2.1533110	-0.3479720
C	-3.2625930	-0.0208210	-0.0051780
H	-3.0563680	-2.1415010	0.3418850
H	-3.1341360	2.1078690	-0.3432340
H	-4.3481570	-0.0418940	-0.0123890
N	1.8103140	-0.9900850	-0.2853680
H	1.5099100	-1.9016430	-0.5998510

Molecule 4a			
			
E = -936.72646798, H (0K) = -936.599191, H (298K) = -936.587974, G (298K) = -936.637234 au. Imaginary frequency = 0.			
C	-1.4850720	1.1160000	-0.2396980
C	-1.3207760	-0.2792030	-0.2042870
C	-2.4230380	-1.1216760	0.0390390
C	-3.6805820	-0.5618840	0.2467640
C	-3.8436680	0.8297770	0.2123210
C	-2.7491150	1.6665420	-0.0305060
C	-0.0146650	-0.8529640	-0.4226650
N	0.6430480	-1.9237910	-0.5010560
O	2.2308350	-0.4897330	1.5466210
C	2.2999600	-0.1906720	0.3905010
H	-0.6285190	1.7548650	-0.4299420
H	-2.2851470	-2.1979530	0.0636820
H	-4.5339750	-1.2052690	0.4352750
H	-4.8267050	1.2610400	0.3748310
H	-2.8808670	2.7433070	-0.0565450
C	1.4033750	-0.5943820	-0.7155830
H	1.7334300	-0.3610410	-1.7221730
Cl	3.6444260	0.9011890	-0.1874130

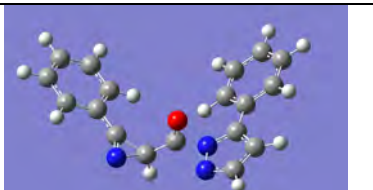
TS ^{2b}			
			
E = -1394.009084, H (0K) = -1393.728507, H (298K) = -1393.708132, G (298K) = -1393.779839 au. Imaginary frequency = 1.			
C	-3.8078650	0.4100670	0.8460310
C	-3.3131060	0.3692070	-0.4686580
C	-4.1903040	0.5072400	-1.5614390
C	-5.5522500	0.6854730	-1.3327790
C	-6.0438510	0.7265590	-0.0207510
C	-5.1737160	0.5892580	1.0659910
C	-1.8973260	0.1889250	-0.6954480
N	-1.0191680	0.1021100	-1.6046310
O	-0.6264950	-2.4015960	0.0172810
C	-0.1401190	-1.3398860	0.3293150
H	-3.1218010	0.3000490	1.6799920
H	-3.7988100	0.4739960	-2.5733980
H	-6.2323340	0.7923560	-2.1719350
H	-7.1066870	0.8655020	0.1525910
H	-5.5588560	0.6209690	2.0801480
C	-0.5623930	0.0194840	-0.1417800
H	0.0000910	0.8568730	0.2555830
Cl	0.1082620	-1.1303900	2.3633400
N	1.6612000	-1.4446600	-0.1296550

C	-6.5204090	-1.1009320	0.5601350	H	5.1745540	0.9765480	-1.1319510
C	-6.6506570	-1.5748440	-0.7495620	C	5.8642130	-2.0385370	0.2793930
H	-5.6956590	-1.7585870	-2.6769870	H	4.4331870	-3.2685650	1.3293480
H	-7.3295770	-1.2346100	1.2716050	H	7.0410720	-0.5960430	-0.8129330
H	-7.5632350	-2.0737430	-1.0611350	H	6.6888370	-2.7310080	0.4197890
H	-3.5760340	1.7226520	2.2085130				
C	-5.3471400	-0.4628940	0.9632260				
H	-5.2476060	-0.1161840	1.9868730				
Molecule 5^b				Molecule 5bH⁺-Cl⁻			
							
E = -933.217275, H (0K) = -932.948503, H (298K) = -932.930002, G (298K) = -932.997854 au. Imaginary frequency = 0.				E = -1394.038981, H (0K) = -1393.756780, H (298K) = -1393.735455, G (298K) = -1393.812278 au. Imaginary frequency = 0.			
C	2.8826623	-0.1497362	1.8503755	C	3.9659140	0.9642230	0.2959170
C	2.9919963	-0.6073112	0.5266035	C	4.1742450	-0.3515630	-0.1525020
C	4.0842213	-0.2169672	-0.2716065	C	5.4160260	-0.7386760	-0.6942020
C	5.0566183	0.6270798	0.2586315	C	6.4447490	0.1946240	-0.7812690
C	4.9460113	1.0829338	1.5793955	C	6.2398890	1.5074460	-0.3336210
C	3.8616503	0.6951838	2.3735435	C	5.0052340	1.8903130	0.2007520
C	1.9800203	-1.4871202	-0.0135545	C	3.1071950	-1.3174480	-0.0517630
N	1.6332433	-2.1368082	-1.0354175	N	2.7600980	-2.5009620	-0.3064550
O	-0.6725307	-0.4308922	-0.5394795	O	0.6192720	-0.8801250	-1.5605960
C	-0.5513837	-1.4495802	0.1205325	C	0.6032670	-1.1410560	-0.3735770
H	2.0367533	-0.4580582	2.4568245	H	2.9977860	1.2547560	0.6980150
H	4.1602553	-0.5754522	-1.2933655	H	5.5630930	-1.7583580	-1.0359160
H	5.9002513	0.9311628	-0.3528225	H	7.4049830	-0.0958680	-1.1953440
H	5.7068353	1.7409588	1.9881355	H	7.0460630	2.2315210	-0.4036390
H	3.7798233	1.0501518	3.3958445	H	4.8518650	2.9090630	0.5421620
C	0.7270513	-2.2111282	0.2213725	C	1.7489750	-1.5932970	0.4377130
H	0.7196693	-3.1484282	0.7620365	H	1.5874270	-1.8149340	1.4866390
C	-2.8993817	-1.4104762	1.0763745	Cl	0.4693890	2.2446940	1.1760210
C	-3.6566077	-2.4059662	1.6555775	C	-1.0752070	-1.2760760	1.5809670
C	-2.8010187	-3.5334372	1.7584945	C	-2.4134620	-0.9685580	1.6652280
N	-1.5940737	-3.2834612	1.2843135	C	-2.8093740	-0.5015660	0.3884410
N	-1.6438467	-1.9749062	0.8553085	H	-0.3987830	-1.6421520	2.3357710
H	-3.0260937	-4.5109362	2.1647965	N	-1.7180980	-0.5558660	-0.3935020
H	-4.6772487	-2.3156432	1.9967255	H	-1.5839210	-0.3583990	-1.3808960
C	-3.2916177	-0.0092642	0.8230705	N	-0.6557370	-1.0259260	0.3089350
C	-2.5544217	1.0677588	1.3445045	C	-4.1103410	-0.0276250	-0.0772060
C	-4.4809767	0.2527848	0.1240355	C	-4.2217080	0.8355150	-1.1834760
C	-2.9941207	2.3781578	1.1587995	C	-5.4766130	1.2682350	-1.6067940
H	-1.6415827	0.8789488	1.9003855	H	-3.3361860	1.1961750	-1.6967920
C	-4.9180557	1.5673978	-0.0626655	C	-6.5241530	-0.0038310	0.1703140
H	-5.0557487	-0.5734812	-0.2832175	C	-6.6291530	0.8489340	-0.9333850
C	-4.1759547	2.6332398	0.4526645	H	-5.5538460	1.9398740	-2.4555250
H	-2.4166467	3.2012128	1.5692385	H	-7.4161250	-0.3319320	0.6939700
H	-5.8358407	1.7554068	-0.6118515	H	-7.6049370	1.1894840	-1.2654010
H	-4.5149447	3.6548118	0.3085955	H	-3.0309820	-1.0397710	2.5460300
Molecule 5^bbH⁺-Cl⁻				C	-5.2726550	-0.4403800	0.6005980
				H	-5.2010350	-1.1142540	1.4476800
				TS ^{5b-5^b}			



E = -1394.030142, **H (0K)** = -1393.747873,
H (298K) = -1393.727692, **G (298K)** = -1393.801170 au.
Imaginary frequency = 0.

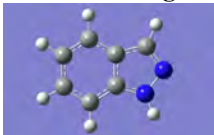
C	-2.8840460	0.1890530	0.7439070
C	-2.9453180	0.0807400	-0.6559720
C	-4.1778240	0.1858020	-1.3305770
C	-5.3417120	0.4054950	-0.5996520
C	-5.2822290	0.5155840	0.7966060
C	-4.0586640	0.4043590	1.4652110
C	-1.7381270	-0.1418880	-1.4151970
N	-1.2736320	-0.3839260	-2.5591530
O	-0.0844810	-2.5653420	-1.0722430
C	0.3864620	-1.4519610	-0.9671780
H	-1.9325120	0.0792660	1.2570450
H	-4.2113790	0.1002740	-2.4120800
H	-6.2942530	0.4912180	-1.1126620
H	-6.1931160	0.6864870	1.3623550
H	-4.0196490	0.4831900	2.5468770
C	-0.2669290	-0.2020750	-1.3945800
H	0.3169390	0.7083470	-1.4024210
Cl	0.0254890	-1.3899970	2.7804250
N	1.7478460	-1.3759710	-0.4543190
N	2.3802160	-2.5745130	-0.3436290
C	3.6531480	-2.3916520	-0.0033330
C	3.8697220	-1.0200140	0.1275870
C	2.6572980	-0.3876100	-0.1419560
H	1.8454150	-3.4184190	-0.5309370
H	4.3152290	-3.2336810	0.1350670
C	2.3682360	1.0533810	-0.0378670
C	3.1463690	1.9611920	-0.7756180
C	1.3943300	1.5245000	0.8601270
C	2.9307400	3.3330610	-0.6354280
H	3.9017520	1.5939350	-1.4631330
C	1.1938750	2.8985190	0.9982510
H	0.8238110	0.8157710	1.4562160
C	1.9551070	3.8027240	0.2498420
H	3.5244260	4.0321870	-1.2157600
H	0.4461970	3.2624740	1.6960850
H	1.7922700	4.8705230	0.3598780
H	4.7837590	-0.5332700	0.4288620



E = -933.159824, **H (0K)** = -932.893474,
H (298K) = -932.875326, **G (298K)** = -932.941624 au.
Imaginary frequency = 1.

C	-2.7167690	1.2520440	-0.3826040
C	-3.2609310	-0.0117360	-0.0980100
C	-4.5812200	-0.1245420	0.3782860
C	-5.3454620	1.0240830	0.5669740
C	-4.8008130	2.2839190	0.2825950
C	-3.4894810	2.3975710	-0.1911260
C	-2.4615130	-1.1989780	-0.3001120
N	-2.4809220	-2.4605670	-0.2116420
O	-0.0627300	-1.7022440	1.4167570
C	-0.0428370	-1.7988120	0.2164810
H	-1.6979150	1.3271280	-0.7492330
H	-4.9933280	-1.1050730	0.5953350
H	-6.3635030	0.9421860	0.9343380
H	-5.4006110	3.1766830	0.4314260
H	-3.0714100	3.3749490	-0.4097280
C	-1.1964800	-1.7867900	-0.7266670
H	-0.9513190	-1.9151800	-1.7758580
C	2.5259540	-0.8499990	-0.1500520
C	3.2407250	-1.9926150	0.2611200
C	2.3849520	-3.0694280	0.0520860
N	1.2518850	-2.6434600	-0.5508710
N	1.3408920	-1.2517310	-0.6785690
H	2.5286390	-4.1170050	0.2798410
H	4.2508630	-2.0351130	0.6432250
C	2.8979320	0.5688260	-0.0873720
C	2.1509660	1.5370560	-0.7843960
C	4.0030060	0.9856620	0.6773440
C	2.4985470	2.8860890	-0.7124970
H	1.3064350	1.2251360	-1.3898360
C	4.3499920	2.3355840	0.7436740
H	4.5864180	0.2575460	1.2317970
C	3.5993860	3.2910180	0.0504210
H	1.9138910	3.6209590	-1.2578330
H	5.2041130	2.6412510	1.3403980
H	3.8708500	4.3410810	0.1027750

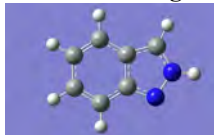
Molecule 2g



E = 379.87860765, **H (0K)** = -379.760401,
H (298K) = -379.753348, **G (298K)** = -379.790641 au.
Imaginary frequency = 0.

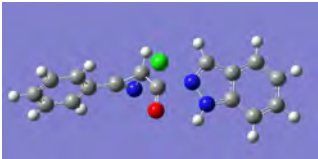
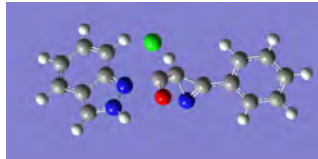
C	1.6405740	1.1049840	0.0002570
C	0.2575140	0.7460080	0.0000380

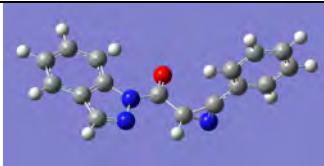
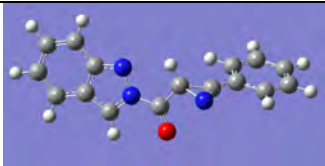
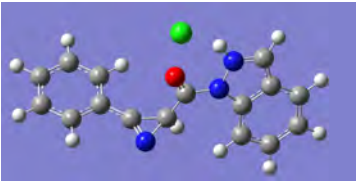
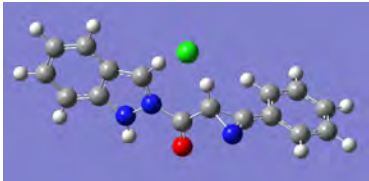
Molecule 2'g

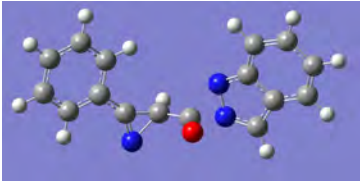
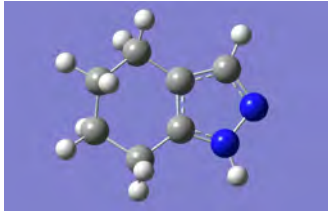


E = -379.87256475, **H (0K)** = -379.754090,
H (298K) = -379.747180, **G (298K)** = -379.784224 au.
Imaginary frequency = 0.

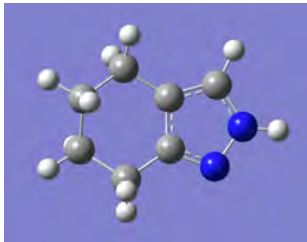
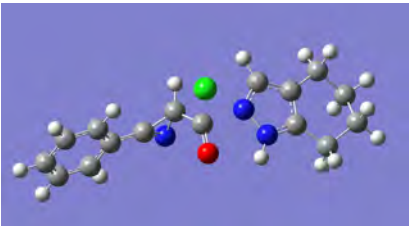
N	-1.5357330	-1.1849120	-0.0000680
N	-2.2986810	-0.0710840	-0.0000220

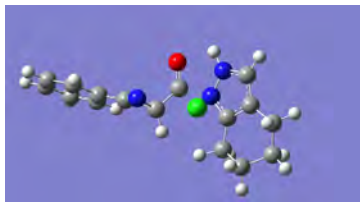
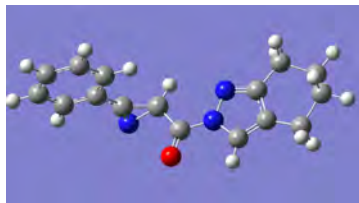
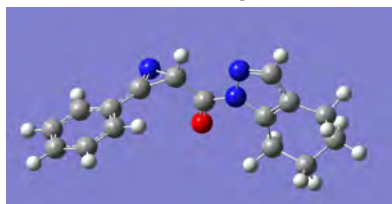
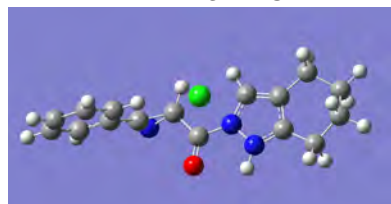
C	0.2631610	-0.6737890	-0.0000350	C	-1.6166940	1.0930650	0.0000970
H	2.0830170	2.0922220	0.0008730	C	-0.2613370	0.7383680	-0.0000070
N	1.5800910	-1.0418170	-0.0002200	C	-0.2719770	-0.7003060	-0.0000450
H	1.9682670	-1.9733160	-0.0004370	H	-3.3054660	-0.1708810	0.0000500
N	2.4171390	0.0307180	-0.0000790	H	-2.1209090	2.0478510	0.0001370
C	-0.9710330	1.4395860	-0.0001510	C	0.9690800	1.4473640	-0.0000310
C	-2.1441140	0.6993340	-0.0000910	C	2.1385590	0.7169580	-0.0000360
C	-2.1169830	-0.7198450	0.0001480	C	2.1245370	-0.7135510	0.0000250
C	-0.9239100	-1.4289800	0.0001540	C	0.9466480	-1.4301740	0.0000490
H	-0.9955860	2.5252750	-0.0003300	H	0.9855250	2.5332020	-0.0000760
H	-3.0567470	-1.2642980	0.0002140	H	3.0952580	1.2308050	-0.0000310
H	-0.9074600	-2.5140610	0.0003620	H	3.0728070	-1.2434460	0.0001080
H	-3.1033540	1.2080830	-0.0005200	H	0.9407900	-2.5159020	0.0001270
TS^{2g}				TS^{2g}			
							
E = -1316.58822640, H (0K) = -1316.341857, H (298K) = -1316.323475, G (298K) = -1316.390900 au.				E = -1316.583696, H (0K) = -1316.337135, H (298K) = -1316.318866, G (298K) = -1316.386032 au.			
Imaginary frequency = 1.				Imaginary frequency = 1.			
C	-4.2505220	0.7078120	-0.1902680	C	3.9191940	0.9087850	0.2425190
C	-3.6364700	-0.5546690	-0.2534720	C	3.4096660	-0.3875910	0.4288290
C	-4.4027330	-1.7251510	-0.0934980	C	4.2862080	-1.4804090	0.5709110
C	-5.7739130	-1.6254400	0.1274440	C	5.6619860	-1.2700140	0.5264700
C	-6.3847310	-0.3653810	0.1898520	C	6.1682310	0.0238200	0.3409010
C	-5.6248160	0.7984390	0.0314020	C	5.2988480	1.1106100	0.1993820
C	-2.2137150	-0.6485750	-0.4881930	C	1.9802900	-0.5951840	0.4784340
N	-1.2616840	-1.4722050	-0.6318460	N	1.0887310	-1.4836150	0.6254240
O	-0.2931210	0.3186720	1.5900760	O	0.3192770	-0.1957930	-1.9722340
C	-0.1943700	0.6144100	0.4231540	C	0.0282330	0.2915610	-0.9043830
H	-3.6488690	1.6028670	-0.3133140	H	3.2336020	1.7431310	0.1326760
H	-3.9196830	-2.6960020	-0.1436560	H	3.8835210	-2.4782840	0.7141110
H	-6.3687950	-2.5248040	0.2513710	H	6.3414620	-2.1093790	0.6354800
H	-7.4542530	-0.2927750	0.3625710	H	7.2417700	0.1829130	0.3067100
H	-6.1016820	1.7720780	0.0811480	H	5.6951560	2.1106450	0.0554100
C	-0.9465540	0.0239280	-0.7337110	C	0.6382350	-0.0340410	0.4288860
H	-0.6934470	0.4201810	-1.7125950	H	0.2045960	0.4776620	1.2826390
Cl	-0.1438330	2.6047300	0.0441840	Cl	-0.2466490	2.2666200	-0.9018970
C	2.3734970	0.3068350	-1.1257600	N	-1.8039630	-0.1934360	-0.6168880
C	3.6901370	-0.0875730	-0.7584820	N	-2.2521260	-0.9506470	-1.6306230
C	3.6173490	-0.3599140	0.6356700	C	-3.5404960	-1.2967790	-1.5109680
H	1.9817090	0.6097340	-2.0857300	C	-3.9950580	-0.7200940	-0.3121950
N	2.3256670	-0.1259870	1.0064660	C	-2.8580690	-0.0242420	0.2189260
H	1.8615620	-0.2049380	1.9045200	H	-1.5942740	-1.1705280	-2.3747150
N	1.5955980	0.2705190	-0.0538590	H	-4.0320180	-1.9067290	-2.2537930
C	4.9170070	-0.2415940	-1.4416680	C	-5.2317990	-0.7032650	0.3808450
C	6.0172360	-0.6586960	-0.7132690	C	-5.2997340	0.0003790	1.5645960
C	5.9232930	-0.9261060	0.6797780	C	-4.1648690	0.6949460	2.0816900
C	4.7348640	-0.7845410	1.3777240	C	-2.9464840	0.6979120	1.4337450
H	4.9894260	-0.0376800	-2.5050360	H	-6.0947720	-1.2297620	-0.0140190
H	6.8120180	-1.2513560	1.2118300	H	-6.2316220	0.0339420	2.1200220
H	4.6673630	-0.9897430	2.4403970	H	-4.2686530	1.2396110	3.0152600
H	6.9743480	-0.7863220	-1.2087750	H	-2.0947340	1.2361070	1.8334200
Molecule 5k				Molecule 5k			

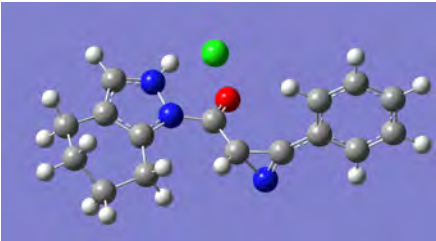
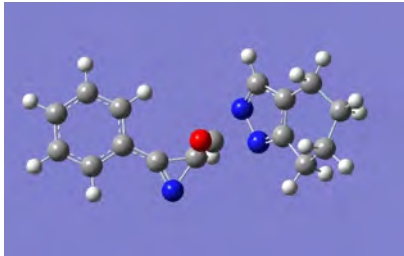
 E = -855.805544, H (0K) = -855.570222, H (298K) = -855.553973, G (298K) = -855.615520 au. Imaginary frequency = 0. <table> <tr><td>C</td><td>-3.1441100</td><td>0.4857520</td><td>-1.1513850</td></tr> <tr><td>C</td><td>-3.2603910</td><td>-0.1961110</td><td>0.0714490</td></tr> <tr><td>C</td><td>-4.4666030</td><td>-0.1524500</td><td>0.7964240</td></tr> <tr><td>C</td><td>-5.5449670</td><td>0.5718930</td><td>0.2948120</td></tr> <tr><td>C</td><td>-5.4271540</td><td>1.2519830</td><td>-0.9250650</td></tr> <tr><td>C</td><td>-4.2294480</td><td>1.2089880</td><td>-1.6464800</td></tr> <tr><td>C</td><td>-2.1363740</td><td>-0.9486160</td><td>0.5823490</td></tr> <tr><td>N</td><td>-1.7452720</td><td>-1.6747220</td><td>1.5350870</td></tr> <tr><td>O</td><td>0.2440290</td><td>0.4375990</td><td>1.5747840</td></tr> <tr><td>C</td><td>0.3506910</td><td>-0.4397960</td><td>0.7245810</td></tr> <tr><td>H</td><td>-2.2095460</td><td>0.4444740</td><td>-1.7021550</td></tr> <tr><td>H</td><td>-4.5473420</td><td>-0.6825360</td><td>1.7402790</td></tr> <tr><td>H</td><td>-6.4767720</td><td>0.6087330</td><td>0.8502330</td></tr> <tr><td>H</td><td>-6.2708500</td><td>1.8154310</td><td>-1.3118990</td></tr> <tr><td>H</td><td>-4.1422590</td><td>1.7369110</td><td>-2.5906860</td></tr> <tr><td>C</td><td>-0.7526150</td><td>-1.3838370</td><td>0.3797770</td></tr> <tr><td>H</td><td>-0.5245920</td><td>-2.2065210</td><td>-0.2861570</td></tr> <tr><td>C</td><td>2.9098160</td><td>-1.4567960</td><td>-1.4191730</td></tr> <tr><td>C</td><td>3.6303940</td><td>-0.3887420</td><td>-0.7833560</td></tr> <tr><td>C</td><td>2.7213170</td><td>0.1539920</td><td>0.1513950</td></tr> <tr><td>H</td><td>3.2545430</td><td>-2.1251750</td><td>-2.1978360</td></tr> <tr><td>N</td><td>1.5497480</td><td>-0.5977950</td><td>0.0235470</td></tr> <tr><td>N</td><td>1.6930410</td><td>-1.5786620</td><td>-0.9474270</td></tr> <tr><td>C</td><td>4.9230550</td><td>0.1443010</td><td>-0.9125960</td></tr> <tr><td>C</td><td>5.2718620</td><td>1.2144590</td><td>-0.0964980</td></tr> <tr><td>C</td><td>4.3518410</td><td>1.7465020</td><td>0.8336490</td></tr> <tr><td>C</td><td>3.0649540</td><td>1.2319950</td><td>0.9788750</td></tr> <tr><td>H</td><td>5.6256430</td><td>-0.2692040</td><td>-1.6291610</td></tr> <tr><td>H</td><td>4.6552940</td><td>2.5823560</td><td>1.4567700</td></tr> <tr><td>H</td><td>2.3642220</td><td>1.6417920</td><td>1.6927990</td></tr> <tr><td>H</td><td>6.2632120</td><td>1.6500900</td><td>-0.1714570</td></tr> </table>				C	-3.1441100	0.4857520	-1.1513850	C	-3.2603910	-0.1961110	0.0714490	C	-4.4666030	-0.1524500	0.7964240	C	-5.5449670	0.5718930	0.2948120	C	-5.4271540	1.2519830	-0.9250650	C	-4.2294480	1.2089880	-1.6464800	C	-2.1363740	-0.9486160	0.5823490	N	-1.7452720	-1.6747220	1.5350870	O	0.2440290	0.4375990	1.5747840	C	0.3506910	-0.4397960	0.7245810	H	-2.2095460	0.4444740	-1.7021550	H	-4.5473420	-0.6825360	1.7402790	H	-6.4767720	0.6087330	0.8502330	H	-6.2708500	1.8154310	-1.3118990	H	-4.1422590	1.7369110	-2.5906860	C	-0.7526150	-1.3838370	0.3797770	H	-0.5245920	-2.2065210	-0.2861570	C	2.9098160	-1.4567960	-1.4191730	C	3.6303940	-0.3887420	-0.7833560	C	2.7213170	0.1539920	0.1513950	H	3.2545430	-2.1251750	-2.1978360	N	1.5497480	-0.5977950	0.0235470	N	1.6930410	-1.5786620	-0.9474270	C	4.9230550	0.1443010	-0.9125960	C	5.2718620	1.2144590	-0.0964980	C	4.3518410	1.7465020	0.8336490	C	3.0649540	1.2319950	0.9788750	H	5.6256430	-0.2692040	-1.6291610	H	4.6552940	2.5823560	1.4567700	H	2.3642220	1.6417920	1.6927990	H	6.2632120	1.6500900	-0.1714570
C	-3.1441100	0.4857520	-1.1513850																																																																																																																												
C	-3.2603910	-0.1961110	0.0714490																																																																																																																												
C	-4.4666030	-0.1524500	0.7964240																																																																																																																												
C	-5.5449670	0.5718930	0.2948120																																																																																																																												
C	-5.4271540	1.2519830	-0.9250650																																																																																																																												
C	-4.2294480	1.2089880	-1.6464800																																																																																																																												
C	-2.1363740	-0.9486160	0.5823490																																																																																																																												
N	-1.7452720	-1.6747220	1.5350870																																																																																																																												
O	0.2440290	0.4375990	1.5747840																																																																																																																												
C	0.3506910	-0.4397960	0.7245810																																																																																																																												
H	-2.2095460	0.4444740	-1.7021550																																																																																																																												
H	-4.5473420	-0.6825360	1.7402790																																																																																																																												
H	-6.4767720	0.6087330	0.8502330																																																																																																																												
H	-6.2708500	1.8154310	-1.3118990																																																																																																																												
H	-4.1422590	1.7369110	-2.5906860																																																																																																																												
C	-0.7526150	-1.3838370	0.3797770																																																																																																																												
H	-0.5245920	-2.2065210	-0.2861570																																																																																																																												
C	2.9098160	-1.4567960	-1.4191730																																																																																																																												
C	3.6303940	-0.3887420	-0.7833560																																																																																																																												
C	2.7213170	0.1539920	0.1513950																																																																																																																												
H	3.2545430	-2.1251750	-2.1978360																																																																																																																												
N	1.5497480	-0.5977950	0.0235470																																																																																																																												
N	1.6930410	-1.5786620	-0.9474270																																																																																																																												
C	4.9230550	0.1443010	-0.9125960																																																																																																																												
C	5.2718620	1.2144590	-0.0964980																																																																																																																												
C	4.3518410	1.7465020	0.8336490																																																																																																																												
C	3.0649540	1.2319950	0.9788750																																																																																																																												
H	5.6256430	-0.2692040	-1.6291610																																																																																																																												
H	4.6552940	2.5823560	1.4567700																																																																																																																												
H	2.3642220	1.6417920	1.6927990																																																																																																																												
H	6.2632120	1.6500900	-0.1714570																																																																																																																												
 E = -855.793258, H (0K) = -855.558430, H (298K) = -855.543072, G (298K) = -855.603841au. Imaginary frequency = 0. <table> <tr><td>C</td><td>-3.1510530</td><td>1.2822970</td><td>0.2592990</td></tr> <tr><td>C</td><td>-3.3731610</td><td>-0.0005250</td><td>-0.2687050</td></tr> <tr><td>C</td><td>-4.6782540</td><td>-0.5245200</td><td>-0.3391770</td></tr> <tr><td>C</td><td>-5.7499010</td><td>0.2370240</td><td>0.1194870</td></tr> <tr><td>C</td><td>-5.5270120</td><td>1.5164520</td><td>0.6466570</td></tr> <tr><td>C</td><td>-4.2308250</td><td>2.0379160</td><td>0.7163270</td></tr> <tr><td>C</td><td>-2.2554860</td><td>-0.7826560</td><td>-0.7455700</td></tr> <tr><td>N</td><td>-1.9218800</td><td>-1.8797040</td><td>-1.2653050</td></tr> <tr><td>O</td><td>-0.2787470</td><td>-1.8851930</td><td>1.1369330</td></tr> <tr><td>C</td><td>0.0679340</td><td>-1.1973370</td><td>0.1910220</td></tr> <tr><td>H</td><td>-2.1405720</td><td>1.6759290</td><td>0.3072900</td></tr> <tr><td>H</td><td>-4.8395070</td><td>-1.5165680</td><td>-0.7491300</td></tr> <tr><td>H</td><td>-6.7579220</td><td>-0.1619820</td><td>0.0679340</td></tr> <tr><td>H</td><td>-6.3661490</td><td>2.1061440</td><td>1.0030110</td></tr> <tr><td>H</td><td>-4.0628680</td><td>3.0290770</td><td>1.1251000</td></tr> <tr><td>C</td><td>-0.8047470</td><td>-0.8470900</td><td>-0.9583280</td></tr> <tr><td>H</td><td>-0.3462410</td><td>-0.3505520</td><td>-1.8040870</td></tr> <tr><td>C</td><td>2.3410220</td><td>-0.9003170</td><td>1.1169550</td></tr> <tr><td>C</td><td>3.4769100</td><td>-0.2216200</td><td>0.7010110</td></tr> <tr><td>C</td><td>3.0984190</td><td>0.3859190</td><td>-0.5539960</td></tr> <tr><td>H</td><td>2.1228770</td><td>-1.5014120</td><td>1.9852410</td></tr> <tr><td>N</td><td>1.8300510</td><td>0.1010850</td><td>-0.8818740</td></tr> <tr><td>N</td><td>1.3943800</td><td>-0.6828230</td><td>0.1525590</td></tr> <tr><td>C</td><td>4.7902110</td><td>-0.0391090</td><td>1.2230440</td></tr> <tr><td>C</td><td>5.6690330</td><td>0.7271350</td><td>0.4965680</td></tr> <tr><td>C</td><td>5.2890300</td><td>1.3304080</td><td>-0.7509380</td></tr> <tr><td>C</td><td>4.0324540</td><td>1.1757500</td><td>-1.2850010</td></tr> <tr><td>H</td><td>5.0812960</td><td>-0.4932850</td><td>2.1648720</td></tr> <tr><td>H</td><td>6.0256880</td><td>1.9259470</td><td>-1.2820630</td></tr> <tr><td>H</td><td>3.7503050</td><td>1.6329470</td><td>-2.2278440</td></tr> <tr><td>H</td><td>6.6777820</td><td>0.8870200</td><td>0.8646190</td></tr> </table>				C	-3.1510530	1.2822970	0.2592990	C	-3.3731610	-0.0005250	-0.2687050	C	-4.6782540	-0.5245200	-0.3391770	C	-5.7499010	0.2370240	0.1194870	C	-5.5270120	1.5164520	0.6466570	C	-4.2308250	2.0379160	0.7163270	C	-2.2554860	-0.7826560	-0.7455700	N	-1.9218800	-1.8797040	-1.2653050	O	-0.2787470	-1.8851930	1.1369330	C	0.0679340	-1.1973370	0.1910220	H	-2.1405720	1.6759290	0.3072900	H	-4.8395070	-1.5165680	-0.7491300	H	-6.7579220	-0.1619820	0.0679340	H	-6.3661490	2.1061440	1.0030110	H	-4.0628680	3.0290770	1.1251000	C	-0.8047470	-0.8470900	-0.9583280	H	-0.3462410	-0.3505520	-1.8040870	C	2.3410220	-0.9003170	1.1169550	C	3.4769100	-0.2216200	0.7010110	C	3.0984190	0.3859190	-0.5539960	H	2.1228770	-1.5014120	1.9852410	N	1.8300510	0.1010850	-0.8818740	N	1.3943800	-0.6828230	0.1525590	C	4.7902110	-0.0391090	1.2230440	C	5.6690330	0.7271350	0.4965680	C	5.2890300	1.3304080	-0.7509380	C	4.0324540	1.1757500	-1.2850010	H	5.0812960	-0.4932850	2.1648720	H	6.0256880	1.9259470	-1.2820630	H	3.7503050	1.6329470	-2.2278440	H	6.6777820	0.8870200	0.8646190
C	-3.1510530	1.2822970	0.2592990																																																																																																																												
C	-3.3731610	-0.0005250	-0.2687050																																																																																																																												
C	-4.6782540	-0.5245200	-0.3391770																																																																																																																												
C	-5.7499010	0.2370240	0.1194870																																																																																																																												
C	-5.5270120	1.5164520	0.6466570																																																																																																																												
C	-4.2308250	2.0379160	0.7163270																																																																																																																												
C	-2.2554860	-0.7826560	-0.7455700																																																																																																																												
N	-1.9218800	-1.8797040	-1.2653050																																																																																																																												
O	-0.2787470	-1.8851930	1.1369330																																																																																																																												
C	0.0679340	-1.1973370	0.1910220																																																																																																																												
H	-2.1405720	1.6759290	0.3072900																																																																																																																												
H	-4.8395070	-1.5165680	-0.7491300																																																																																																																												
H	-6.7579220	-0.1619820	0.0679340																																																																																																																												
H	-6.3661490	2.1061440	1.0030110																																																																																																																												
H	-4.0628680	3.0290770	1.1251000																																																																																																																												
C	-0.8047470	-0.8470900	-0.9583280																																																																																																																												
H	-0.3462410	-0.3505520	-1.8040870																																																																																																																												
C	2.3410220	-0.9003170	1.1169550																																																																																																																												
C	3.4769100	-0.2216200	0.7010110																																																																																																																												
C	3.0984190	0.3859190	-0.5539960																																																																																																																												
H	2.1228770	-1.5014120	1.9852410																																																																																																																												
N	1.8300510	0.1010850	-0.8818740																																																																																																																												
N	1.3943800	-0.6828230	0.1525590																																																																																																																												
C	4.7902110	-0.0391090	1.2230440																																																																																																																												
C	5.6690330	0.7271350	0.4965680																																																																																																																												
C	5.2890300	1.3304080	-0.7509380																																																																																																																												
C	4.0324540	1.1757500	-1.2850010																																																																																																																												
H	5.0812960	-0.4932850	2.1648720																																																																																																																												
H	6.0256880	1.9259470	-1.2820630																																																																																																																												
H	3.7503050	1.6329470	-2.2278440																																																																																																																												
H	6.6777820	0.8870200	0.8646190																																																																																																																												
Molecule 5kH⁺-Cl⁻  E = -1316.610275, H (0K) = -1316.361586, H (298K) = -1316.342573, G (298K) = -1316.412224 au. Imaginary frequency = 0. <table> <tr><td>C</td><td>-3.2534590</td><td>0.6417980</td><td>-0.6169130</td></tr> <tr><td>C</td><td>-3.2016290</td><td>-0.6497080</td><td>-0.0641210</td></tr> <tr><td>C</td><td>-4.3858810</td><td>-1.3555180</td><td>0.2251050</td></tr> <tr><td>C</td><td>-5.6172730</td><td>-0.7641500</td><td>-0.0422090</td></tr> <tr><td>C</td><td>-5.6713480</td><td>0.5235120</td><td>-0.5940660</td></tr> <tr><td>C</td><td>-4.4941740</td><td>1.2234880</td><td>-0.8792350</td></tr> <tr><td>C</td><td>-1.9200030</td><td>-1.2567980</td><td>0.2014940</td></tr> </table>				C	-3.2534590	0.6417980	-0.6169130	C	-3.2016290	-0.6497080	-0.0641210	C	-4.3858810	-1.3555180	0.2251050	C	-5.6172730	-0.7641500	-0.0422090	C	-5.6713480	0.5235120	-0.5940660	C	-4.4941740	1.2234880	-0.8792350	C	-1.9200030	-1.2567980	0.2014940																																																																																																
C	-3.2534590	0.6417980	-0.6169130																																																																																																																												
C	-3.2016290	-0.6497080	-0.0641210																																																																																																																												
C	-4.3858810	-1.3555180	0.2251050																																																																																																																												
C	-5.6172730	-0.7641500	-0.0422090																																																																																																																												
C	-5.6713480	0.5235120	-0.5940660																																																																																																																												
C	-4.4941740	1.2234880	-0.8792350																																																																																																																												
C	-1.9200030	-1.2567980	0.2014940																																																																																																																												
Molecule 5*kH⁺-Cl⁻  E = -1316.609323, H (0K) = -1316.361093, H (298K) = -1316.341957, G (298K) = -1316.411567 au. Imaginary frequency = 0. <table> <tr><td>C</td><td>-3.4097620</td><td>0.9789880</td><td>-0.0966320</td></tr> <tr><td>C</td><td>-3.5313870</td><td>-0.4144310</td><td>-0.2368510</td></tr> <tr><td>C</td><td>-4.7876480</td><td>-1.0424270</td><td>-0.1246550</td></tr> <tr><td>C</td><td>-5.9176240</td><td>-0.2699900</td><td>0.1271550</td></tr> <tr><td>C</td><td>-5.7994310</td><td>1.1201050</td><td>0.2668840</td></tr> <tr><td>C</td><td>-4.5508660</td><td>1.7410900</td><td>0.1562550</td></tr> <tr><td>C</td><td>-2.3568710</td><td>-1.2086430</td><td>-0.5025730</td></tr> </table>				C	-3.4097620	0.9789880	-0.0966320	C	-3.5313870	-0.4144310	-0.2368510	C	-4.7876480	-1.0424270	-0.1246550	C	-5.9176240	-0.2699900	0.1271550	C	-5.7994310	1.1201050	0.2668840	C	-4.5508660	1.7410900	0.1562550	C	-2.3568710	-1.2086430	-0.5025730																																																																																																
C	-3.4097620	0.9789880	-0.0966320																																																																																																																												
C	-3.5313870	-0.4144310	-0.2368510																																																																																																																												
C	-4.7876480	-1.0424270	-0.1246550																																																																																																																												
C	-5.9176240	-0.2699900	0.1271550																																																																																																																												
C	-5.7994310	1.1201050	0.2668840																																																																																																																												
C	-4.5508660	1.7410900	0.1562550																																																																																																																												
C	-2.3568710	-1.2086430	-0.5025730																																																																																																																												

N	-1.3367210	-2.2788130	0.6530110	N	-1.9212000	-2.3760120	-0.6861080
O	-0.2744220	0.1586720	2.1048180	O	-0.2644070	-1.3259720	1.5430040
C	0.2318890	-0.2984630	1.0959020	C	0.0067820	-1.1038090	0.3818960
H	-2.3300170	1.1777110	-0.8245910	H	-2.4308370	1.4471020	-0.1763420
H	-4.3313050	-2.3524480	0.6510650	H	-4.8666760	-2.1193100	-0.2354260
H	-6.5343860	-1.3016130	0.1768080	H	-6.8893380	-0.7453650	0.2146960
H	-6.6345940	0.9801930	-0.8007140	H	-6.6843460	1.7179770	0.4632490
H	-4.5432790	2.2209500	-1.3042110	H	-4.4664720	2.8173850	0.2677780
C	-0.4631190	-1.1264840	0.0911160	C	-0.9113910	-1.2015670	-0.7666100
H	0.0245100	-1.3002130	-0.8598940	H	-0.5415890	-0.9511270	-1.7540010
Cl	0.0770040	2.6477300	-0.8991600	Cl	0.0887550	2.4923790	-0.0463350
N	1.6100070	0.0056110	0.8574010	C	2.0343790	-0.4798320	-1.0607890
N	2.1330050	1.0235060	1.6023760	C	3.3580440	-0.1654030	-0.7420300
C	3.3891900	1.2677760	1.2848110	C	3.4514460	-0.2545160	0.6821610
C	3.7676520	0.3513490	0.2778860	H	1.5402750	-0.5274310	-2.0174900
C	2.6223370	-0.4545870	0.0224310	N	2.2298930	-0.6108270	1.1415200
H	1.5186940	1.4830160	2.2707030	H	1.8707650	-0.7659190	2.0776590
H	3.9431920	2.0572980	1.7720970	N	1.3801950	-0.7476540	0.0884880
C	4.9796490	0.1307070	-0.4082270	C	4.4976300	0.1900120	-1.5099200
C	5.0185930	-0.9020490	-1.3254300	C	5.6684470	0.4396380	-0.8314930
C	3.8812800	-1.7159020	-1.5493400	C	5.7388730	0.3447750	0.5918530
C	2.6759430	-1.5196440	-0.8880110	C	4.6516500	0.0003050	1.3715570
H	5.8456090	0.7521920	-0.2096270	H	4.4356560	0.2604960	-2.5898750
H	5.9312050	-1.1062200	-1.8743900	H	6.6867300	0.5525120	1.0778590
H	3.9530110	-2.5325780	-2.2602340	H	4.7139910	-0.0688250	2.4510510
H	1.8417410	-2.1831670	-1.0665200	H	6.5624140	0.7155200	-1.3800390
TS^{5k-5k}  E = -855.731671, H (0K) = -855.499344, H (298K) = -855.483331, G (298K) = -855.543975 au. Imaginary frequency = 1.				Molecule 2h  E = -382.29587080, H (0K) = -382.131201, H (298K) = -382.123131, G (298K) = -382.162629 au. Imaginary frequency = 0.			
C	-2.9706330	1.1621950	-0.4672420	C	1.7473830	1.0981320	-0.0528350
C	-3.1960810	-0.1750140	-0.0990640	C	0.3782060	0.7402820	-0.0401650
C	-4.4413540	-0.5651490	0.4298270	C	-0.8914130	1.5471560	-0.0935490
C	-5.4495260	0.3823860	0.5870080	C	-2.0900700	0.6747170	0.3378170
C	-5.2228710	1.7158080	0.2191740	C	-2.0664380	-0.7141300	-0.3279480
C	-3.9863610	2.1047900	-0.3068790	C	-0.8231130	-1.5336750	0.0826590
C	-2.1445300	-1.1514970	-0.2709250	C	0.3820010	-0.6456430	0.0277480
N	-1.8614880	-2.3753560	-0.1224630	H	2.1874300	2.0865560	-0.0996370
O	0.3559990	-1.0049850	1.3813840	H	-0.8196100	2.4332180	0.5484790
C	0.3576300	-1.1313190	0.1849520	H	-1.0602970	1.9205470	-1.1138120
H	-2.0068130	1.4511540	-0.8744860	H	-3.0266040	1.1886430	0.0940420
H	-4.6064030	-1.6005190	0.7111630	H	-2.0721210	0.5488500	1.4292610
H	-6.4110270	0.0866290	0.9945910	H	-2.0718220	-0.5903560	-1.4192040
H	-6.0121960	2.4509560	0.3436010	H	-2.9714030	-1.2734340	-0.0673610
H	-3.8151030	3.1383140	-0.5903220	H	-0.7023350	-2.4048090	-0.5722270
C	-0.7869830	-1.4447380	-0.7149170	H	-0.9533080	-1.9238500	1.1017610
H	-0.5435240	-1.5654850	-1.7652710	N	1.6862650	-1.0269350	0.0520740
C	3.0152470	-1.7168200	-0.0430130	H	2.0550640	-1.9657570	0.1017270
C	3.6119850	-0.4425320	0.0640610	N	2.5445460	0.0239860	0.0042990
C	2.6014960	0.4668980	-0.3763160				
H	3.3909030	-2.6872790	0.2517740				
N	1.5163160	-0.2326170	-0.8233660				

N	1.8001360	-1.5878330	-0.5962150	
C	4.8711480	0.0443190	0.4956250	
C	5.0622390	1.4117240	0.5062050	
C	4.0391780	2.3125950	0.0855480	
C	2.8110220	1.8638960	-0.3617770	
H	5.6537450	-0.6365190	0.8144040	
H	4.2393470	3.3793010	0.1161660	
H	2.0379280	2.5489310	-0.6933470	
H	6.0107770	1.8197820	0.8413570	

Molecule 2 ^h				TS ^{2h}			
							
E = -382.29541556, H (0K) = -382.130962, H (298K) = -382.122889, G (298K) = -382.162375 au. Imaginary frequency = 0.				E = -1319.009545, H (0K) = -1318.716778, H (298K) = -1318.697352, G (298K) = -1318.767052 au. Imaginary frequency = 1.			
N	1.6400430	-1.1724230	0.0532030	C	-4.4362950	0.6682980	-0.1960180
N	2.4292670	-0.0711180	0.0040540	C	-3.7822290	-0.5737280	-0.2627140
C	1.7209280	1.0874670	-0.0489720	C	-4.5116600	-1.7683890	-0.1094990
C	0.3815080	0.7310060	-0.0334110	C	-5.8859260	-1.7129830	0.1081300
C	-0.8821350	1.5476550	-0.0943280	C	-6.5365180	-0.4731850	0.1741010
C	-2.0895920	0.6879400	0.3346210	C	-5.8133430	0.7146460	0.0223610
C	-2.0740930	-0.6980950	-0.3361810	C	-2.3562330	-0.6210670	-0.4932530
C	-0.8485590	-1.5305200	0.0945890	N	-1.3775450	-1.4129600	-0.6362020
C	0.3931290	-0.6860060	0.0307540	O	-0.4434810	0.3662130	1.5945340
H	3.4332380	-0.1761070	0.0085970	C	-0.3843230	0.7023570	0.4368940
H	2.2139010	2.0483190	-0.0944980	H	-3.8630970	1.5825560	-0.3138620
H	-0.8065080	2.4399440	0.5382880	H	-3.9980600	-2.7233090	-0.1621350
H	-1.0453040	1.9096280	-1.1195160	H	-6.4523870	-2.6312110	0.2269210
H	-3.0193230	1.2141560	0.0905080	H	-7.6082240	-0.4350880	0.3443320
H	-2.0755590	0.5581130	1.4258510	H	-6.3207790	1.6725810	0.0747930
H	-2.0620180	-0.5687440	-1.4273900	C	-1.1076880	0.0910170	-0.7269540
H	-2.9917460	-1.2453060	-0.0931470	H	-0.8592640	0.5007800	-1.7014040
H	-0.7425080	-2.4217050	-0.5346680	Cl	-0.3670000	2.6582670	0.1020790
H	-0.9964450	-1.8901920	1.1227470	C	2.3118060	0.4736800	-1.1240400
				C	3.5951580	0.0264060	-0.7505680
				C	4.8950690	-0.0654690	-1.5032170
				C	5.8805450	-0.9779200	-0.7418300
				C	5.9199040	-0.6614560	0.7648510
				C	4.5577570	-0.9157190	1.4470770
				C	3.4718020	-0.3528330	0.5840890
				H	1.9633630	0.8626320	-2.0707100
				H	4.7308900	-0.4461080	-2.5175980
				H	5.3328590	0.9360350	-1.6149820
				H	6.8827350	-0.8715580	-1.1705610
				H	5.5848620	-2.0266570	-0.8810700
				H	6.2034260	0.3897690	0.9064460
				H	6.6871430	-1.2670650	1.2579600
				H	4.5334220	-0.4697890	2.4477260
				H	4.3994040	-1.9946670	1.5785520
				N	2.1839090	-0.1322100	0.9385830
				H	1.7117490	-0.2769740	1.8244910

TS^{2h}  E = -1319.00851304, H (0K) = -1318.715841, H (298K) = -1318.696432, G (298K) = -1318.765858 au. Imaginary frequency = 1. <table><tr><td>C</td><td>4.0452200</td><td>0.3122590</td><td>0.8911200</td></tr><tr><td>C</td><td>3.5321550</td><td>-0.5712400</td><td>-0.0737870</td></tr><tr><td>C</td><td>4.4056860</td><td>-1.3102460</td><td>-0.8945000</td></tr><tr><td>C</td><td>5.7820770</td><td>-1.1611830</td><td>-0.7448770</td></tr><tr><td>C</td><td>6.2918550</td><td>-0.2794750</td><td>0.2181760</td></tr><tr><td>C</td><td>5.4254420</td><td>0.4554250</td><td>1.0343850</td></tr><tr><td>C</td><td>2.1021140</td><td>-0.7216380</td><td>-0.2181980</td></tr><tr><td>N</td><td>1.2069760</td><td>-1.3385590</td><td>-0.8688790</td></tr><tr><td>O</td><td>0.4779380</td><td>1.5534480</td><td>-1.2580820</td></tr><tr><td>C</td><td>0.1656150</td><td>0.9354570</td><td>-0.2683730</td></tr><tr><td>H</td><td>3.3617750</td><td>0.8774970</td><td>1.5169550</td></tr><tr><td>H</td><td>4.0003040</td><td>-1.9902860</td><td>-1.6372180</td></tr><tr><td>H</td><td>6.4595100</td><td>-1.7284400</td><td>-1.3753020</td></tr><tr><td>H</td><td>7.3658880</td><td>-0.1664350</td><td>0.3306850</td></tr><tr><td>H</td><td>5.8243230</td><td>1.1373660</td><td>1.7785010</td></tr><tr><td>C</td><td>0.7614830</td><td>-0.3541470</td><td>0.2153300</td></tr><tr><td>H</td><td>0.3243950</td><td>-0.7645750</td><td>1.1199860</td></tr><tr><td>Cl</td><td>-0.1598410</td><td>2.0291230</td><td>1.3637630</td></tr><tr><td>N</td><td>-1.6879770</td><td>0.4237510</td><td>-0.5675630</td></tr><tr><td>N</td><td>-2.1163840</td><td>0.9413360</td><td>-1.7318420</td></tr><tr><td>C</td><td>-3.4291670</td><td>0.6890260</td><td>-1.9321940</td></tr><tr><td>C</td><td>-3.8773120</td><td>-0.0343850</td><td>-0.8338370</td></tr><tr><td>C</td><td>-5.2282770</td><td>-0.6010720</td><td>-0.4897080</td></tr><tr><td>C</td><td>-5.2935150</td><td>-0.9298750</td><td>1.0156650</td></tr><tr><td>C</td><td>-4.0449610</td><td>-1.6968230</td><td>1.4853900</td></tr><tr><td>C</td><td>-2.7567150</td><td>-0.8598220</td><td>1.3362620</td></tr><tr><td>C</td><td>-2.7450200</td><td>-0.1750920</td><td>0.0014440</td></tr><tr><td>H</td><td>-1.4530500</td><td>1.4554420</td><td>-2.3012380</td></tr><tr><td>H</td><td>-3.9339460</td><td>1.0348650</td><td>-2.8225120</td></tr><tr><td>H</td><td>-6.0240580</td><td>0.1000400</td><td>-0.7647020</td></tr><tr><td>H</td><td>-5.4061510</td><td>-1.5171420</td><td>-1.0696070</td></tr><tr><td>H</td><td>-6.1940900</td><td>-1.5177940</td><td>1.2226760</td></tr><tr><td>H</td><td>-5.3826690</td><td>0.0026220</td><td>1.5895220</td></tr><tr><td>H</td><td>-3.9478530</td><td>-2.6198170</td><td>0.8981830</td></tr><tr><td>H</td><td>-4.1568640</td><td>-1.9980220</td><td>2.5321300</td></tr><tr><td>H</td><td>-1.8736360</td><td>-1.4953250</td><td>1.4579450</td></tr><tr><td>H</td><td>-2.7084640</td><td>-0.1013800</td><td>2.1288730</td></tr></table>	C	4.0452200	0.3122590	0.8911200	C	3.5321550	-0.5712400	-0.0737870	C	4.4056860	-1.3102460	-0.8945000	C	5.7820770	-1.1611830	-0.7448770	C	6.2918550	-0.2794750	0.2181760	C	5.4254420	0.4554250	1.0343850	C	2.1021140	-0.7216380	-0.2181980	N	1.2069760	-1.3385590	-0.8688790	O	0.4779380	1.5534480	-1.2580820	C	0.1656150	0.9354570	-0.2683730	H	3.3617750	0.8774970	1.5169550	H	4.0003040	-1.9902860	-1.6372180	H	6.4595100	-1.7284400	-1.3753020	H	7.3658880	-0.1664350	0.3306850	H	5.8243230	1.1373660	1.7785010	C	0.7614830	-0.3541470	0.2153300	H	0.3243950	-0.7645750	1.1199860	Cl	-0.1598410	2.0291230	1.3637630	N	-1.6879770	0.4237510	-0.5675630	N	-2.1163840	0.9413360	-1.7318420	C	-3.4291670	0.6890260	-1.9321940	C	-3.8773120	-0.0343850	-0.8338370	C	-5.2282770	-0.6010720	-0.4897080	C	-5.2935150	-0.9298750	1.0156650	C	-4.0449610	-1.6968230	1.4853900	C	-2.7567150	-0.8598220	1.3362620	C	-2.7450200	-0.1750920	0.0014440	H	-1.4530500	1.4554420	-2.3012380	H	-3.9339460	1.0348650	-2.8225120	H	-6.0240580	0.1000400	-0.7647020	H	-5.4061510	-1.5171420	-1.0696070	H	-6.1940900	-1.5177940	1.2226760	H	-5.3826690	0.0026220	1.5895220	H	-3.9478530	-2.6198170	0.8981830	H	-4.1568640	-1.9980220	2.5321300	H	-1.8736360	-1.4953250	1.4579450	H	-2.7084640	-0.1013800	2.1288730	N1.47247100.3674420-0.0876610 Molecule 5I  E = -858.222702, H (0K) = -857.941499, H (298K) = -857.924133, G (298K) = -857.988020 au. Imaginary frequency = 0. <table><tr><td>C</td><td>-3.3139800</td><td>1.2913830</td><td>0.2482060</td></tr><tr><td>C</td><td>-3.5301050</td><td>0.0048350</td><td>-0.2730230</td></tr><tr><td>C</td><td>-4.8342040</td><td>-0.5204440</td><td>-0.3491910</td></tr><tr><td>C</td><td>-5.9102950</td><td>0.2425980</td><td>0.0968410</td></tr><tr><td>C</td><td>-5.6929740</td><td>1.5257120</td><td>0.6173040</td></tr><tr><td>C</td><td>-4.3978220</td><td>2.0489230</td><td>0.6927090</td></tr><tr><td>C</td><td>-2.4069670</td><td>-0.7787740</td><td>-0.7367010</td></tr><tr><td>N</td><td>-2.0763320</td><td>-1.8821610</td><td>-1.2471090</td></tr><tr><td>O</td><td>-0.4663110</td><td>-1.8621700</td><td>1.1776290</td></tr><tr><td>C</td><td>-0.0884890</td><td>-1.1954390</td><td>0.2209840</td></tr><tr><td>H</td><td>-2.3041970</td><td>1.6863430</td><td>0.3010450</td></tr><tr><td>H</td><td>-4.9913970</td><td>-1.5153930</td><td>-0.7538030</td></tr><tr><td>H</td><td>-6.9174530</td><td>-0.1580790</td><td>0.0406120</td></tr><tr><td>H</td><td>-6.5353330</td><td>2.1166760</td><td>0.9638870</td></tr><tr><td>H</td><td>-4.2338050</td><td>3.0429300</td><td>1.0962750</td></tr><tr><td>C</td><td>-0.9578180</td><td>-0.8519990</td><td>-0.9393710</td></tr><tr><td>H</td><td>-0.4925100</td><td>-0.3664620</td><td>-1.7882220</td></tr><tr><td>C</td><td>2.1943310</td><td>-0.9142010</td><td>1.1449350</td></tr><tr><td>C</td><td>3.3250950</td><td>-0.2711060</td><td>0.7159940</td></tr><tr><td>C</td><td>2.9578940</td><td>0.3119120</td><td>-0.5429580</td></tr><tr><td>H</td><td>1.9756220</td><td>-1.4933440</td><td>2.0286450</td></tr><tr><td>N</td><td>1.7037950</td><td>0.0468150</td><td>-0.8694920</td></tr><tr><td>N</td><td>1.2274960</td><td>-0.7139480</td><td>0.1774580</td></tr><tr><td>C</td><td>3.8893970</td><td>1.1503040</td><td>-1.3693670</td></tr><tr><td>H</td><td>3.7652410</td><td>0.9241870</td><td>-2.4338640</td></tr><tr><td>H</td><td>3.6230350</td><td>2.2085300</td><td>-1.2401700</td></tr><tr><td>C</td><td>5.3476340</td><td>0.9309250</td><td>-0.9163200</td></tr><tr><td>H</td><td>5.9884530</td><td>1.6876330</td><td>-1.3809730</td></tr><tr><td>H</td><td>5.6995700</td><td>-0.0461380</td><td>-1.2744310</td></tr><tr><td>C</td><td>5.4835920</td><td>0.9878280</td><td>0.6159030</td></tr><tr><td>H</td><td>5.1086730</td><td>1.9559850</td><td>0.9752320</td></tr><tr><td>H</td><td>6.5390190</td><td>0.9306820</td><td>0.9028170</td></tr><tr><td>C</td><td>4.7046430</td><td>-0.1528090</td><td>1.3032680</td></tr><tr><td>H</td><td>4.6560190</td><td>0.0088740</td><td>2.3857570</td></tr><tr><td>H</td><td>5.2452440</td><td>-1.0978760</td><td>1.1548780</td></tr></table>	C	-3.3139800	1.2913830	0.2482060	C	-3.5301050	0.0048350	-0.2730230	C	-4.8342040	-0.5204440	-0.3491910	C	-5.9102950	0.2425980	0.0968410	C	-5.6929740	1.5257120	0.6173040	C	-4.3978220	2.0489230	0.6927090	C	-2.4069670	-0.7787740	-0.7367010	N	-2.0763320	-1.8821610	-1.2471090	O	-0.4663110	-1.8621700	1.1776290	C	-0.0884890	-1.1954390	0.2209840	H	-2.3041970	1.6863430	0.3010450	H	-4.9913970	-1.5153930	-0.7538030	H	-6.9174530	-0.1580790	0.0406120	H	-6.5353330	2.1166760	0.9638870	H	-4.2338050	3.0429300	1.0962750	C	-0.9578180	-0.8519990	-0.9393710	H	-0.4925100	-0.3664620	-1.7882220	C	2.1943310	-0.9142010	1.1449350	C	3.3250950	-0.2711060	0.7159940	C	2.9578940	0.3119120	-0.5429580	H	1.9756220	-1.4933440	2.0286450	N	1.7037950	0.0468150	-0.8694920	N	1.2274960	-0.7139480	0.1774580	C	3.8893970	1.1503040	-1.3693670	H	3.7652410	0.9241870	-2.4338640	H	3.6230350	2.2085300	-1.2401700	C	5.3476340	0.9309250	-0.9163200	H	5.9884530	1.6876330	-1.3809730	H	5.6995700	-0.0461380	-1.2744310	C	5.4835920	0.9878280	0.6159030	H	5.1086730	1.9559850	0.9752320	H	6.5390190	0.9306820	0.9028170	C	4.7046430	-0.1528090	1.3032680	H	4.6560190	0.0088740	2.3857570	H	5.2452440	-1.0978760	1.1548780
C	4.0452200	0.3122590	0.8911200																																																																																																																																																																																																																																																																																														
C	3.5321550	-0.5712400	-0.0737870																																																																																																																																																																																																																																																																																														
C	4.4056860	-1.3102460	-0.8945000																																																																																																																																																																																																																																																																																														
C	5.7820770	-1.1611830	-0.7448770																																																																																																																																																																																																																																																																																														
C	6.2918550	-0.2794750	0.2181760																																																																																																																																																																																																																																																																																														
C	5.4254420	0.4554250	1.0343850																																																																																																																																																																																																																																																																																														
C	2.1021140	-0.7216380	-0.2181980																																																																																																																																																																																																																																																																																														
N	1.2069760	-1.3385590	-0.8688790																																																																																																																																																																																																																																																																																														
O	0.4779380	1.5534480	-1.2580820																																																																																																																																																																																																																																																																																														
C	0.1656150	0.9354570	-0.2683730																																																																																																																																																																																																																																																																																														
H	3.3617750	0.8774970	1.5169550																																																																																																																																																																																																																																																																																														
H	4.0003040	-1.9902860	-1.6372180																																																																																																																																																																																																																																																																																														
H	6.4595100	-1.7284400	-1.3753020																																																																																																																																																																																																																																																																																														
H	7.3658880	-0.1664350	0.3306850																																																																																																																																																																																																																																																																																														
H	5.8243230	1.1373660	1.7785010																																																																																																																																																																																																																																																																																														
C	0.7614830	-0.3541470	0.2153300																																																																																																																																																																																																																																																																																														
H	0.3243950	-0.7645750	1.1199860																																																																																																																																																																																																																																																																																														
Cl	-0.1598410	2.0291230	1.3637630																																																																																																																																																																																																																																																																																														
N	-1.6879770	0.4237510	-0.5675630																																																																																																																																																																																																																																																																																														
N	-2.1163840	0.9413360	-1.7318420																																																																																																																																																																																																																																																																																														
C	-3.4291670	0.6890260	-1.9321940																																																																																																																																																																																																																																																																																														
C	-3.8773120	-0.0343850	-0.8338370																																																																																																																																																																																																																																																																																														
C	-5.2282770	-0.6010720	-0.4897080																																																																																																																																																																																																																																																																																														
C	-5.2935150	-0.9298750	1.0156650																																																																																																																																																																																																																																																																																														
C	-4.0449610	-1.6968230	1.4853900																																																																																																																																																																																																																																																																																														
C	-2.7567150	-0.8598220	1.3362620																																																																																																																																																																																																																																																																																														
C	-2.7450200	-0.1750920	0.0014440																																																																																																																																																																																																																																																																																														
H	-1.4530500	1.4554420	-2.3012380																																																																																																																																																																																																																																																																																														
H	-3.9339460	1.0348650	-2.8225120																																																																																																																																																																																																																																																																																														
H	-6.0240580	0.1000400	-0.7647020																																																																																																																																																																																																																																																																																														
H	-5.4061510	-1.5171420	-1.0696070																																																																																																																																																																																																																																																																																														
H	-6.1940900	-1.5177940	1.2226760																																																																																																																																																																																																																																																																																														
H	-5.3826690	0.0026220	1.5895220																																																																																																																																																																																																																																																																																														
H	-3.9478530	-2.6198170	0.8981830																																																																																																																																																																																																																																																																																														
H	-4.1568640	-1.9980220	2.5321300																																																																																																																																																																																																																																																																																														
H	-1.8736360	-1.4953250	1.4579450																																																																																																																																																																																																																																																																																														
H	-2.7084640	-0.1013800	2.1288730																																																																																																																																																																																																																																																																																														
C	-3.3139800	1.2913830	0.2482060																																																																																																																																																																																																																																																																																														
C	-3.5301050	0.0048350	-0.2730230																																																																																																																																																																																																																																																																																														
C	-4.8342040	-0.5204440	-0.3491910																																																																																																																																																																																																																																																																																														
C	-5.9102950	0.2425980	0.0968410																																																																																																																																																																																																																																																																																														
C	-5.6929740	1.5257120	0.6173040																																																																																																																																																																																																																																																																																														
C	-4.3978220	2.0489230	0.6927090																																																																																																																																																																																																																																																																																														
C	-2.4069670	-0.7787740	-0.7367010																																																																																																																																																																																																																																																																																														
N	-2.0763320	-1.8821610	-1.2471090																																																																																																																																																																																																																																																																																														
O	-0.4663110	-1.8621700	1.1776290																																																																																																																																																																																																																																																																																														
C	-0.0884890	-1.1954390	0.2209840																																																																																																																																																																																																																																																																																														
H	-2.3041970	1.6863430	0.3010450																																																																																																																																																																																																																																																																																														
H	-4.9913970	-1.5153930	-0.7538030																																																																																																																																																																																																																																																																																														
H	-6.9174530	-0.1580790	0.0406120																																																																																																																																																																																																																																																																																														
H	-6.5353330	2.1166760	0.9638870																																																																																																																																																																																																																																																																																														
H	-4.2338050	3.0429300	1.0962750																																																																																																																																																																																																																																																																																														
C	-0.9578180	-0.8519990	-0.9393710																																																																																																																																																																																																																																																																																														
H	-0.4925100	-0.3664620	-1.7882220																																																																																																																																																																																																																																																																																														
C	2.1943310	-0.9142010	1.1449350																																																																																																																																																																																																																																																																																														
C	3.3250950	-0.2711060	0.7159940																																																																																																																																																																																																																																																																																														
C	2.9578940	0.3119120	-0.5429580																																																																																																																																																																																																																																																																																														
H	1.9756220	-1.4933440	2.0286450																																																																																																																																																																																																																																																																																														
N	1.7037950	0.0468150	-0.8694920																																																																																																																																																																																																																																																																																														
N	1.2274960	-0.7139480	0.1774580																																																																																																																																																																																																																																																																																														
C	3.8893970	1.1503040	-1.3693670																																																																																																																																																																																																																																																																																														
H	3.7652410	0.9241870	-2.4338640																																																																																																																																																																																																																																																																																														
H	3.6230350	2.2085300	-1.2401700																																																																																																																																																																																																																																																																																														
C	5.3476340	0.9309250	-0.9163200																																																																																																																																																																																																																																																																																														
H	5.9884530	1.6876330	-1.3809730																																																																																																																																																																																																																																																																																														
H	5.6995700	-0.0461380	-1.2744310																																																																																																																																																																																																																																																																																														
C	5.4835920	0.9878280	0.6159030																																																																																																																																																																																																																																																																																														
H	5.1086730	1.9559850	0.9752320																																																																																																																																																																																																																																																																																														
H	6.5390190	0.9306820	0.9028170																																																																																																																																																																																																																																																																																														
C	4.7046430	-0.1528090	1.3032680																																																																																																																																																																																																																																																																																														
H	4.6560190	0.0088740	2.3857570																																																																																																																																																																																																																																																																																														
H	5.2452440	-1.0978760	1.1548780																																																																																																																																																																																																																																																																																														
Molecule 5I 	Molecule 5IH⁺-Cl⁻ 																																																																																																																																																																																																																																																																																																

E = -858.220154, H (0K) = -857.938709, H (298K) = -857.921371, G (298K) = -857.985283 au. Imaginary frequency = 0.				E = -1319.039507, H (0K) = -1318.744749, H (298K) = -1318.724536, G (298K) = -1318.797451 au. Imaginary frequency = 0.			
C	-3.2611130	-0.5176110	1.1406980	C	-3.5286490	0.9524960	-0.2073590
C	-3.3865600	0.1990990	-0.0610530	C	-3.6641700	-0.4465920	-0.2175130
C	-4.5907240	0.1578530	-0.7895340	C	-4.9290990	-1.0473010	-0.0617460
C	-5.6578660	-0.5989780	-0.3124200	C	-6.0531930	-0.2430780	0.1016190
C	-5.5310020	-1.3136270	0.8866150	C	-5.9207740	1.1526280	0.1109950
C	-4.3353390	-1.2729570	1.6115500	C	-4.6637210	1.7469740	-0.0414390
C	-2.2742900	0.9857930	-0.5456000	C	-2.4976720	-1.2776810	-0.3935080
N	-1.8948370	1.7510110	-1.4717290	N	-2.0799240	-2.4647720	-0.4482080
O	0.1151710	-0.3358660	-1.5783860	O	-0.4040960	-1.2081110	1.6540820
C	0.2178490	0.5150660	-0.7040520	C	-0.1271410	-1.1090040	0.4740450
H	-2.3282010	-0.4775290	1.6943680	H	-2.5448480	1.4040610	-0.3151200
H	-4.6786160	0.7149640	-1.7170460	H	-5.0191910	-2.1289830	-0.0717980
H	-6.5880070	-0.6342490	-0.8707330	H	-7.0312180	-0.6981780	0.2210100
H	-6.3660590	-1.9021270	1.2544320	H	-6.8009120	1.7756460	0.2385370
H	-4.2411090	-1.8275920	2.5396350	H	-4.5676850	2.8279890	-0.0300910
C	-0.8966470	1.4336970	-0.3272940	C	-1.0531030	-1.3233010	-0.6557230
H	-0.6788750	2.2347880	0.3671010	H	-0.6805390	-1.1904600	-1.6651740
C	2.7970640	1.5495990	1.3876160	Cl	-0.0527810	2.5986860	-0.0862820
C	3.4868690	0.4629300	0.7762600	C	1.9107510	-0.6454220	-1.0371820
C	2.5823010	-0.0876130	-0.1016100	C	3.2129420	-0.2856130	-0.7493540
H	3.1659890	2.2389270	2.1374590	C	4.3909700	0.0065050	-1.6361120
N	1.4202980	0.6705470	0.0049570	C	5.6956820	-0.0271340	-0.8130180
N	1.5624850	1.6817350	0.9354850	C	5.5681390	0.7564200	0.5054020
C	2.8355430	-1.2726650	-0.9831360	C	4.5098070	0.1390510	1.4451080
H	1.9931020	-1.9689560	-0.9490920	C	3.2885440	-0.2014690	0.6592000
H	2.9117440	-0.9437680	-2.0280030	H	1.4269120	-0.8173980	-1.9852690
C	4.1394470	-1.9711200	-0.5396260	H	4.4325630	-0.7104460	-2.4617530
H	4.4577510	-2.6631990	-1.3263690	H	4.2610530	0.9992180	-2.0852610
H	3.9358230	-2.5779640	0.3528000	H	6.5092350	0.3887800	-1.4148420
C	5.2649220	-0.9726530	-0.2204770	H	5.9621150	-1.0691050	-0.5928670
H	5.4679090	-0.3596000	-1.1090710	H	5.2976100	1.7973010	0.2895570
H	6.1900120	-1.5105950	0.0129970	H	6.5289490	0.7777620	1.0273960
C	4.8871210	-0.0521960	0.9571140	H	4.2581070	0.8135130	2.2697360
H	5.5945040	0.7816600	1.0353070	H	4.8951730	-0.7846770	1.8968150
H	4.9615960	-0.6085700	1.9020230	N	2.0859490	-0.5027440	1.1538270
				H	1.7391430	-0.5496890	2.1077770
				N	1.2265030	-0.7800520	0.1379530
Molecule 5⁺·IH⁺-Cl⁻ 				TS^{5I-5I} 			
E = -1319.034765, H (0K) = -1318.739722, H (298K) = -1318.719653, G (298K) = -1318.791483 au. Imaginary frequency = 0.				E = -858.155522, H (0K) = -857.876912, H (298K) = -857.859851, G (298K) = -857.922653 au. Imaginary frequency = 1.			
C	3.3326220	0.6914890	0.6014900	C	-3.6143980	1.0805510	-0.3361920
C	3.2976680	-0.6186460	0.0931600	C	-3.4913820	-0.2997540	-0.1037180
C	4.4905750	-1.3260140	-0.1542430	C	-4.5780440	-1.0310910	0.4127810
C	5.7140230	-0.7172210	0.1101000	C	-5.7761380	-0.3788620	0.6928640

C	5.7516210	0.5891080	0.6178440	C	-5.8967370	0.9981220	0.4603970
C	4.5658630	1.2901200	0.8615740	C	-4.8182520	1.7261970	-0.0531280
C	2.0247980	-1.2450090	-0.1706570	C	-2.2441050	-0.9672610	-0.4022690
N	1.4579970	-2.2885910	-0.5910810	N	-1.6676930	-2.0931540	-0.3844250
O	0.3959440	0.0047890	-2.1957260	O	0.2055810	-0.3633750	1.1972900
C	-0.1179970	-0.3594190	-1.1559630	C	0.2013380	-0.3716730	-0.0107400
H	2.4023340	1.2272440	0.7779650	H	-2.7701160	1.6343790	-0.7348580
H	4.4487700	-2.3373320	-0.5463850	H	-4.4742810	-2.0972100	0.5890240
H	6.6377180	-1.2554710	-0.0770140	H	-6.6164670	-0.9386120	1.0911730
H	6.7087760	1.0593320	0.8224860	H	-6.8329710	1.5021410	0.6804120
H	4.6023040	2.3018870	1.2527490	H	-4.9155890	2.7922880	-0.2316170
C	0.5639300	-1.1202050	-0.0924920	C	-0.8792790	-0.8779690	-0.9066060
H	0.0588380	-1.2662880	0.8521770	H	-0.6681620	-0.8412880	-1.9705440
Cl	0.0214700	2.6039170	0.8458570	C	1.9626890	1.6852180	-0.3768710
N	-1.5099860	-0.0232440	-0.9661130	C	3.1622650	1.0368450	-0.0703150
N	-2.0257230	0.8605050	-1.8614440	C	2.9161310	-0.3204680	-0.3319070
C	-3.3020700	1.1050210	-1.5756270	H	1.6938340	2.7277380	-0.2650000
C	-3.6560730	0.3446160	-0.4542860	N	1.6858320	-0.4683080	-0.8731770
C	-4.9708090	0.2369740	0.2662400	N	1.0801440	0.8041520	-0.9010530
C	-4.7718180	-0.4376870	1.6360030	C	3.8909960	-1.4304790	-0.0861630
C	-3.8757340	-1.6800010	1.5230400	H	3.3857370	-2.2848360	0.3793630
C	-2.4468220	-1.3304040	1.0532650	H	4.2816830	-1.7872770	-1.0488970
C	-2.5123850	-0.3627830	-0.0878690	C	5.0508460	-0.9204490	0.7953220
H	-1.4174510	1.2218920	-2.5898540	H	5.8660360	-1.6511060	0.7797510
H	-3.8771670	1.7956740	-2.1753640	H	4.7103990	-0.8462250	1.8366470
H	-5.4159940	1.2303300	0.3817580	C	5.5613780	0.4552670	0.3297920
H	-5.6678420	-0.3515660	-0.3438470	H	5.8862400	0.3831210	-0.7170060
H	-5.7463500	-0.7149080	2.0489700	H	6.4398890	0.7477960	0.9143360
H	-4.3192410	0.2774300	2.3347840	C	4.4766110	1.5460450	0.4536030
H	-4.3223300	-2.3918120	0.8177610	H	4.7800360	2.4541100	-0.0792060
H	-3.8044020	-2.1891640	2.4884710	H	4.3575950	1.8317250	1.5075920
H	-1.9140690	-2.2405960	0.7640120				
H	-1.8867900	-0.8718780	1.8785660				