Supporting information for

Simple Approach to Pyrrolylimidazole Derivatives by Azirine Ring Expansion with Imidazolium Ylides

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Table of contents

X-ray diffraction experiments 2

Experimental (X-ray) and calculated bond lengths of molecules **6b**, **7a** 4

Computational Details 5

^{1}H (400 MHz) and ^{13}C (100 MHz) NMR spectra 19

X-ray diffraction experiments

For single crystal X-ray diffraction experiment, crystal of **4a**, **4n** or **6b** was fixed on a micro mount and placed on a Agilent Technologies Excalibur Eos diffractometer and measured at a temperature of 100K using monochromated Mo$K\alpha$ radiation.

The unit cell parameters of **4b** were refined by least square techniques using 11961 reflections in the 2θ range of 5.34–55.00°. The structure have been solved with the ShelXS structure solution program[1] using Direct Methods and refined with the ShelXL refinement package[4] using Least Squares minimization incorporated in the *OLEX2* program package[2] to R_1 = 0.035 (wR_2 = 0.074) for 4613 unique reflections with I≥2σ (I).

The unit cell parameters of **4n** were refined by least square techniques using 22772 reflections in the 2θ range of 7.36–141.98°. The structure have been solved by the direct methods and refined R_1 = 0.059 (wR_2 = 0.143) for 4507 unique reflections with $|F_o| \geq 4\sigma_F$ by means of the ShelXL–97 program[4] incorporated in the *OLEX2* program package[5].

The unit cell parameters of **6b** were refined by least square techniques using 7769 reflections in the 2θ range of 5.40–50.00°. The structure have been solved by the direct methods and refined R_1 = 0.044 (wR_2 = 0.091) for 2331 unique reflections with $|F_o| \geq 4\sigma_F$ by means of the ShelXL–97 program[4] incorporated in the *OLEX2* program package[5].

The carbon-bound H atoms were placed in calculated positions and were included in the refinement in the 'riding' model approximation, with U_{iso}(H) set to 1.5U_{eq}(C) and C–H 0.96 Å for CH_3 group, U_{iso}(H) set to 1.2U_{eq}(C) and C–H 0.97 Å for the CH_2 group, U_{iso}(H) set to 1.2U_{eq}(C) and C–H 0.93 Å for the CH groups and U_{iso}(H) set to 1.2U_{eq}(N) and N–H 0.86 Å for the NH group. Empirical absorption correction was applied in CrysAlisPro [3] program complex using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm. Supplementary crystallographic data for this paper have been deposited at Cambridge Crystallographic Data Centre (CCDC **4b** 992831, **4n** 992996, **6b** 991739) and can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif.

Table 1. Crystallographic data for **4b**, **4n** and **6b**.

Compound	**4b**	**4n**	**6b**
Formula	$C_{41}H_{36}N_8O_4Br_2Cl_2$	$C_{28}H_{24}BrN_4$	$C_{20}H_{16}N_4O_2$
Crystal System	Monoclinic	Triclinic	Monoclinic
a (Å)	19.6382(7)	9.1221(2)	11.4914(4)
b (Å)	10.7068(3)	10.9612(3)	11.8011(3)
c (Å)	21.8503(9)	12.8679(3)	13.0430(6)
α (°)	90.00	71.798(2)	90
β (°)	119.245(5)	79.244(2)	107.162(5)
γ (°)	90.00	88.953(2)	90
V (Å^3)	4008.7(2)	1199.69(5)	1690.02(11)
Molecular weight	935.50	496.42	344.37
Space group	*C*2/*c*	*P*-1	$P2_1/c$
μ (mm^{-1})	2.209	2.505	0.091
Temperature (K)	100(2)	100(2)	100(2)
Z	4	2	4
D_{calc} (g/cm^3)	1.550	1.374	1.353
Crystal size (mm^3)	0.22 × 0.16 × 0.08	0.18×0.12×0.09	0.16×0.12×0.09
Total reflections	11961	22772	7769

[1] Sheldrick, G. M. *Acta Cryst.* **2008**, A64, 112

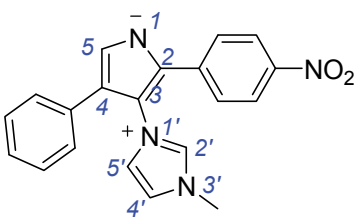
[2] Dolomanov, O.V.; Bourhis, L.J.; Gildea, R.J.; Howard, J.A.K.; Puschmann, H. *J. Appl. Cryst.* **2009**, *42*, 339. OLEX2: A complete structure solution, refinement and analysis program

[3] CrysAlisPro, Agilent Technologies, Version 1.171.36.32 (release 02-08-2013)

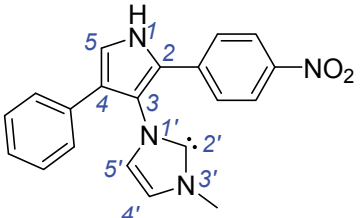
Unique reflections	4613	4636	2827
Angle range 2θ (°)	5.34 to 55	7.36–141.98	5.40–50.00
R_{int}	0.0350	0.0415	0.0325
R_1 ($\|F_o\| \geq 4\sigma_F$)	0.0347	0.0593	0.0436
wR_2 ($\|F_o\| \geq 4\sigma_F$)	0.0735	0.1439	0.0907
R_1 (all data)	0.0469	0.0607	0.0638
wR_2 (all data)	0.0784	0.1449	0.1171
S	1.019	1.081	1.124
ρ_{min}, ρ_{max}, e/Å^3	0.48, –0.44	–1.022, 1.823	–0.311, 0.333

$R_1=\Sigma||F_o|-|F_c||/\Sigma|F_o|$; $wR_2=\{\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$; $w=1/[\sigma^2(F_o^2)+(aP)^2+bP]$, where $P=(F_o^2+2F_c^2)/3$; $s=\{\Sigma[w(F_o^2-F_c^2)]/(n-p)\}^{1/2}$ where n is the number of reflections and p is the number of refinement parameters.

Experimental (X-ray) and calculated bond lengths of molecules 6b, 7a



6b



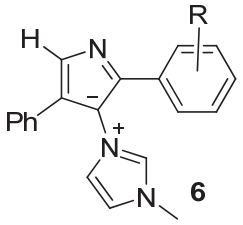
7a

Table 2. Experimental (X-ray) and calculated [DFT B3LYP/6-31G(d) and 6-311G++(dp)] bond lengths of molecules **6b**, **7a**.

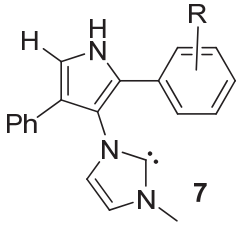
bond	X-ray (±0.003)	ylide, (Δ) [6-31G(d)]	ylide, (Δ) [6-311G++(dp)]	carbene, (Δ) [6-31G(d)]	carbene, (Δ) [6-311G++(dp)]
N-C^2	1.377	1.363 (−0.014)	1.361 (−0.016)	1.383 (+0.006)	1.380 (+0.003)
C^2-C^3	1.397	1.420 (+0.023)	1.418 (+0.021)	1.395 (−0.002)	1.392 (−0.005)
C^3-C^4	1.416	1.416 (0.000)	1.413 (−0.003)	1.433 (+0.017)	1.430 (+0.014)
C^4-C^5	1.406	1.413 (+0.008)	1.412 (+0.007)	1.385 (−0.021)	1.383 (−0.023)
C^5-N	1.342	1.343 (+0.001)	1.342 (+0.000)	1.366 (+0.024)	1.367 (+0.025)
C^3-$N^{3'}$	1.441	1.426 (−0.015)	1.428 (−0.013)	1.419 (−0.022)	1.420 (−0.021)
$N^{3'}$-$C^{2'}$	1.336	1.338 (+0.002)	1.336 (0.000)	1.380 (+0.044)	1.376 (+0.040)
$C^{2'}$-$N^{1'}$	1.327	1.345 (+0.018)	1.343 (+0.016)	1.366 (+0.039)	1.362 (+0.035)
$N^{1'}$-$C^{4'}$	1.381	1.384 (+0.003)	1.384 (+0.003)	1.394 (+0.013)	1.393 (+0.012)
$C^{4'}$-$C^{5'}$	1.343	1.364 (+0.021)	1.361 (+0.018)	1.354 (+0.011)	1.352 (+0.009)
$C^{5'}$-$N^{3'}$	1.378	1.387 (+0.009)	1.385 (+0.007)	1.397 (+0.019)	1.396 (+0.018)
∑|Δ| ([∑|Δ|]/11)		0.114 (0.010)	0.104 (0.009)	0.218 (0.020)	0.205 (0.019)

Computational Details

All calculations were performed with the B3LYP density functional method[4] by using the Gaussian 09 suite of quantum chemical programs[5] at Resource center "Computer center of Saint Petersburg State University". Geometry optimizations of molecules were performed at the B3LYP/6-31G(d) or 6-311++G(dp) level in the gas phase or with pcm solvent model for CH_2Cl_2 and MeOH.



6



7

Table 3. B3LYP/6-31G(d) Absolute Energies (au), Cartesian Coordinates of stationary points

Compound **6b, R = *p*-NO_2**				Compound **7a, R = *p*-NO_2**			
E = -1141.07525493, **H (0K)** = -1140.748539, **H (298K)** = -1140.726253, **G (298K)** = -1140.802016 au.				**E** = -1141.07065935, **H (0K)** = -1140.743677, **H (298K)** = -1140.721454, **G (298K)** = -1140.796395 au.			
Imaginary frequency = 0.				Imaginary frequency = 0.			
C	1.2302700	3.0212730	0.8457270	C	1.4025480	2.7471090	1.3652450
C	1.5516980	1.7183220	1.0872450	C	1.4374280	1.3963550	1.4483830
N	0.9324270	0.9483240	0.1140440	N	0.9336270	0.9209690	0.2347390
C	0.2643080	1.7720490	-0.7008900	C	0.5880610	1.9364960	-0.6329900
C	0.9463510	-0.4738150	0.0106650	C	0.8622850	-0.4598090	-0.0844930
C	-0.1909320	-1.3196030	-0.0830090	C	-0.3011360	-1.2184200	-0.2121820
N	0.2275550	-2.6075330	-0.2348470	C	1.4817240	-2.5982220	-0.4035550
C	1.5700420	-2.5843670	-0.2027580	C	1.9955940	-1.3285360	-0.1992640
C	2.1054160	-1.2850400	-0.0594720	C	-1.7249330	-0.8955390	-0.1357430
C	-1.6121090	-1.0126410	0.0032800	C	-2.6344820	-1.8394540	0.3885860
C	-2.5457750	-1.9099420	-0.5689450	C	-3.9958000	-1.5728390	0.4427790
C	-3.9069500	-1.6588980	-0.5299880	C	-4.4572640	-0.3414080	-0.0216590
C	-4.3725940	-0.4947270	0.0930210	C	-3.5848910	0.6171520	-0.5377230
C	-3.4859310	0.3961640	0.7018180	C	-2.2254540	0.3373670	-0.6021600
C	-2.1247120	0.1324130	0.6599700	C	3.4270480	-0.9799840	-0.1427710
C	3.5248610	-0.9122960	-0.0439100	C	4.3456430	-1.8436230	0.4783310
C	4.4634300	-1.7358250	0.6104480	C	5.7070030	-1.5441720	0.5012940
C	5.8196400	-1.4180570	0.6222650	C	6.1763260	-0.3682840	-0.0867690
C	6.2809430	-0.2594990	-0.0078600	C	5.2727430	0.5018940	-0.7005470
C	5.3673190	0.5694490	-0.6613660	C	3.9120510	0.2009020	-0.7321600
C	4.0111750	0.2454310	-0.6841000	H	1.6928270	3.5049870	2.0779100
H	1.5052370	3.9267170	1.3638760	H	1.7672650	0.7387490	2.2376100
H	2.1581800	1.2609140	1.8514720	H	1.9924980	-3.5286150	-0.6041210
H	-0.3222520	1.4541500	-1.5474860	H	-4.6997300	-2.2885260	0.8491510
H	2.1442230	-3.4976080	-0.3231890	H	-3.9821190	1.5588920	-0.8964380
H	-2.1610440	-2.8066160	-1.0416530	H	-1.5324380	1.0632670	-1.0202060
H	-4.6201840	-2.3399770	-0.9785120	H	3.9824220	-2.7480160	0.9598960

[4] (a) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648. (b) Becke, A. D. *Phys. Rev. A* **1998**, *38*, 3098. (c) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1998**, *37*, 785.

[5] 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	-3.8800900	1.2657910	1.2138510	H	6.4002110	-2.2258840	0.9874040
H	-1.4515350	0.7978580	1.1916740	H	7.2366340	-0.1310900	-0.0653410
H	4.1104470	-2.6258710	1.1236460	H	5.6295830	1.4173320	-1.1654510
H	6.5194410	-2.0738370	1.1344450	H	3.2178110	0.8727050	-1.2277000
H	7.3383080	-0.0093140	0.0059290	N	0.8857870	3.0455590	0.1059220
H	5.7141510	1.4652760	-1.1714560	C	0.6780940	4.3963090	-0.3902370
H	3.3228570	0.8781290	-1.2384380	H	-0.0334460	4.9388920	0.2421000
N	0.4136480	3.0383730	-0.2716300	H	1.6226950	4.9506870	-0.4168750
N	-5.7980520	-0.2095710	0.1197300	H	0.2767520	4.3154900	-1.4006520
O	-6.1707660	0.8392200	0.6604290	N	0.1173720	-2.5237010	-0.3926170
O	-6.5643910	-1.0249840	-0.4032360	H	-0.5004600	-3.2742570	-0.6635020
C	-0.2039590	4.2202420	-0.8691280	H	-2.2665220	-2.7789620	0.7916200
H	-0.9208660	4.6615640	-0.1718290	N	-5.8924900	-0.0505800	0.0370090
H	0.5664580	4.9535420	-1.1191610	O	-6.2734910	1.0488790	-0.3682620
H	-0.7260800	3.9244360	-1.7798840	O	-6.6377070	-0.9227730	0.4888920

Compound **6b, R = *p*-NO_2**
B3LYP/ 6-311++G(dp)
E = -1141.37358561, **H (0K)** = -1141.049382,
H (298K) = -1141.027969, **G (298K)** = -1141.102802 au.
Imaginary frequency = 0.

C	1.1851520	3.0033740	0.8806390	C	1.2637210	2.7192140	1.4116360
C	1.4955480	1.7018890	1.1307830	C	1.2763130	1.3697440	1.4894200
N	0.9270630	0.9384630	0.1243630	N	0.9144380	0.9053120	0.2233420
C	0.2982440	1.7635440	-0.7174510	C	0.6795200	1.9298170	-0.6650320
C	0.9444850	-0.4854210	0.0152950	C	0.8601300	-0.4739510	-0.1091960
C	-0.1903650	-1.3305280	-0.0815800	C	-0.2951160	-1.2378140	-0.2467440
N	0.2327240	-2.6146480	-0.2376770	C	1.4948720	-2.6040170	-0.4374070
C	1.5737690	-2.5938800	-0.2029300	C	1.9976310	-1.3340530	-0.2212320
C	2.1024240	-1.2925150	-0.0567600	C	-1.7169170	-0.9123640	-0.1651240
C	-1.6096520	-1.0204970	0.0001460	C	-2.6249840	-1.8391540	0.3846140
C	-2.5447600	-1.8972340	-0.5956970	C	-3.9815070	-1.5601010	0.4527570
C	-3.9026320	-1.6380040	-0.5573460	C	-4.4385180	-0.3343670	-0.0234900
C	-4.3634900	-0.4871660	0.0888770	C	-3.5677240	0.6063980	-0.5675790
C	-3.4754330	0.3815510	0.7222600	C	-2.2135280	0.3141870	-0.6434950
C	-2.1173390	0.1110060	0.6791470	C	3.4254730	-0.9752250	-0.1431490
C	3.5195840	-0.9109770	-0.0418010	C	4.3282560	-1.7928800	0.5536170
C	4.4584880	-1.7029670	0.6452520	C	5.6848960	-1.4817400	0.6000030
C	5.8108410	-1.3754100	0.6529860	C	6.1638430	-0.3401300	-0.0403390
C	6.2671390	-0.2386710	-0.0147820	C	5.2751190	0.4844250	-0.7294210
C	5.3525900	0.5592490	-0.7007200	C	3.9195960	0.1714710	-0.7837000
C	4.0005760	0.2249010	-0.7186920	H	1.4765450	3.4656440	2.1588710
H	1.4333380	3.9029780	1.4171030	H	1.5057490	0.7094910	2.3081370
H	2.0619650	1.2453430	1.9228500	H	2.0119060	-3.5277670	-0.6398660
H	-0.2416190	1.4498990	-1.5939030	H	-4.6827900	-2.2634340	0.8800010
H	2.1474630	-3.5044700	-0.3208790	H	-3.9594680	1.5437270	-0.9381500
H	-2.1674950	-2.7842950	-1.0874190	H	-1.5277170	1.0257560	-1.0883670
H	-4.6151110	-2.3048380	-1.0237330	H	3.9590110	-2.6697100	1.0745110
H	-3.8638890	1.2386490	1.2555230	H	6.3661400	-2.1265240	1.1442690
H	-1.4460630	0.7583410	1.2302590	H	7.2191640	-0.0946540	-0.0019230
H	4.1120140	-2.5766170	1.1854840	H	5.6399070	1.3714650	-1.2355770
H	6.5112340	-2.0063420	1.1896090	H	3.2393250	0.8074040	-1.3376340
H	7.3204340	0.0175450	-0.0060360	N	0.9006740	3.0316830	0.1038790
H	5.6963730	1.4353460	-1.2407800	C	0.7678220	4.3910810	-0.4005090
H	3.3135750	0.8317500	-1.2984560	H	-0.0119040	4.9307170	0.1431730
N	0.4262020	3.0250700	-0.2759490	H	1.7122550	4.9319590	-0.3009750
N	-5.7925570	-0.1944010	0.1186500	H	0.4974700	4.3285250	-1.4523230
O	-6.1598790	0.8415610	0.6759400	N	0.1293040	-2.5376630	-0.4350000
O	-6.5588690	-0.9918940	-0.4187500	H	-0.4802970	-3.2939270	-0.7016980
C	-0.1614380	4.2118970	-0.8975870	H	-2.2623450	-2.7741800	0.7960900

Compound **7a, R = *p*-NO_2**
B3LYP/ 6-311++G(dp)
E = -1141.37162018, **H (0K)** = -1141.047213,
H (298K) = -1141.025744, **G (298K)** = -1141.100580 au.
Imaginary frequency = 0.

H	-0.9093240	4.6482730	-0.2345020
H	0.6195180	4.9431220	-1.1069230
H	-0.6388340	3.9217310	-1.8316560

Compound **6b, R = *p*-NO_2**
pcm CH_2Cl_2
E = -1141.10565263, **H (0K)** = -1140.778472, **H (298K)** = -1140.756305, **G (298K)** = -1140.831614 au.
Imaginary frequency = 0.

C	1.1759060	2.9687890	1.0314270
C	1.3154740	1.6398390	1.2994530
N	0.9279670	0.9468840	0.1624320
C	0.5695170	1.8415280	-0.7692160
C	0.9006120	-0.4761950	-0.0018370
C	-0.2543640	-1.2959190	-0.1051440
N	0.1408820	-2.5982420	-0.2811430
C	1.4811710	-2.5985370	-0.2545290
C	2.0396270	-1.3066600	-0.0905560
C	-1.6663470	-0.9666000	-0.0332880
C	-2.6213300	-1.9205780	-0.4737450
C	-3.9785800	-1.6648100	-0.4298880
C	-4.4310740	-0.4327640	0.0659220
C	-3.5220470	0.5260470	0.5289950
C	-2.1642160	0.2578790	0.4819770
C	3.4697130	-0.9730980	-0.0473240
C	4.3860110	-1.8837800	0.5188270
C	5.7517660	-1.6088010	0.5545230
C	6.2450510	-0.4083040	0.0357810
C	5.3531840	0.5072280	-0.5275130
C	3.9872470	0.2277110	-0.5736520
H	1.3667180	3.8394350	1.6388060
H	1.6473400	1.1218640	2.1843270
H	0.2217650	1.5989210	-1.7606870
H	2.0409700	-3.5199280	-0.3868910
H	-2.2569610	-2.8676950	-0.8538140
H	-4.6972850	-2.3970840	-0.7772900
H	-3.8917490	1.4608530	0.9321910
H	-1.4833410	0.9973270	0.8861750
H	4.0126990	-2.8090700	0.9487600
H	6.4325840	-2.3308380	0.9984450
H	7.3090700	-0.1905890	0.0687400
H	5.7227590	1.4406010	-0.9450960
H	3.3194830	0.9388820	-1.0504000
N	0.7040620	3.0739070	-0.2654670
N	-5.8446080	-0.1529920	0.1089580
O	-6.2197550	0.9470320	0.5456660
O	-6.6341250	-1.0215780	-0.2935610
C	0.3989870	4.3240570	-0.9679030
H	-0.3967170	4.8524710	-0.4395720
H	1.2955180	4.9451750	-1.0078620
H	0.0722200	4.0869680	-1.9799980

Compound **6b, R = *p*-NO_2**
pcm MeOH
E = -1141.11023928, **H (0K)** = -1140.783179, **H (298K)** = -1140.760952, **G (298K)** = -1140.836713 au.
Imaginary frequency = 0.

C	1.1769260	2.9634140	1.0462560
C	1.2943640	1.6324860	1.3141210
N	0.9276090	0.9472270	0.1651670
N	-5.8768330	-0.0286090	0.0512700
O	-6.2517250	1.0633090	-0.3619760
O	-6.6194530	-0.8836590	0.5236320

Compound **7a, R = *p*-NO_2**
pcm CH_2Cl_2
E = -1141.08612017, **H (0K)** = -1140.759091, **H (298K)** = -1140.736866, **G (298K)** = -1140.811892 au.
Imaginary frequency = 0.

C	1.1899110	2.7410080	1.3941670
C	1.1892090	1.3898910	1.4941250
N	0.9011770	0.9087370	0.2146650
C	0.7287240	1.9196670	-0.7073490
C	0.8596730	-0.4749100	-0.1049210
C	-0.2959330	-1.2488550	-0.2361210
C	1.4989220	-2.6075240	-0.4139040
C	2.0017980	-1.3300210	-0.2085920
C	-1.7163720	-0.9232480	-0.1577310
C	-2.6413410	-1.8789040	0.3182230
C	-3.9976160	-1.5946740	0.3830510
C	-4.4430870	-0.3343980	-0.0215290
C	-3.5550330	0.6357100	-0.4926600
C	-2.2016900	0.3378810	-0.5661730
C	3.4298720	-0.9720450	-0.1300920
C	4.3504930	-1.8538630	0.4646340
C	5.7095660	-1.5452490	0.5134730
C	6.1767810	-0.3420560	-0.0210580
C	5.2720640	0.5456170	-0.6087730
C	3.9134370	0.2350420	-0.6672230
H	1.3595480	3.5044550	2.1388310
H	1.3586690	0.7367220	2.3362890
H	2.0161100	-3.5367000	-0.6028220
H	-4.7062370	-2.3248220	0.7531940
H	-3.9317980	1.6001330	-0.8099530
H	-1.5054070	1.0729580	-0.9576700
H	3.9920840	-2.7808440	0.9044590
H	6.4026430	-2.2416400	0.9782500
H	7.2348140	-0.0981260	0.0214480
H	5.6258280	1.4820960	-1.0322290
H	3.2203380	0.9226070	-1.1423500
N	0.9088120	3.0331500	0.0616050
C	0.8179520	4.3874620	-0.4671820
H	0.0210040	4.9453340	0.0348280
H	1.7645230	4.9196050	-0.3289160
H	0.5948000	4.3149570	-1.5316890
N	0.1371330	-2.5479470	-0.4128790
H	-0.4655240	-3.3202260	-0.6601890
H	-2.2930320	-2.8449430	0.6704100
N	-5.8655450	-0.0263360	0.0495040
O	-6.2386750	1.0976690	-0.3020990
O	-6.6342460	-0.9031670	0.4585540

Compound **7a, R = *p*-NO_2**
pcm MeOH
E = -1141.08872995, **H (0K)** = -1140.761656, **H (298K)** = -1140.739437, **G (298K)** = -1140.814454 au.
Imaginary frequency = 0.

C	1.1653220	2.7409030	1.3953140
C	1.1596090	1.3897330	1.4966770
N	0.8981610	0.9078600	0.2118560

C	0.6029930	1.8491130	-0.7728450	C	0.7474000	1.9183290	-0.7142090
C	0.8950660	-0.4751840	-0.0050380	C	0.8592540	-0.4762710	-0.1072800
C	-0.2622030	-1.2918470	-0.1094020	C	-0.2957900	-1.2522590	-0.2370040
N	0.1297110	-2.5962510	-0.2859540	C	1.5002970	-2.6087120	-0.4130620
C	1.4701070	-2.5996870	-0.2592210	C	2.0022550	-1.3299750	-0.2096360
C	2.0313260	-1.3088970	-0.0940080	C	-1.7159340	-0.9263420	-0.1584210
C	-1.6732260	-0.9599430	-0.0391710	C	-2.6434940	-1.8840620	0.3087370
C	-2.6305370	-1.9200130	-0.4626200	C	-3.9991640	-1.5976350	0.3738050
C	-3.9873560	-1.6639160	-0.4176310	C	-4.4422600	-0.3333360	-0.0216460
C	-4.4382780	-0.4246630	0.0623730	C	-3.5516220	0.6389050	-0.4841380
C	-3.5267590	0.5415320	0.5063650	C	-2.1990160	0.3389340	-0.5575560
C	-2.1693010	0.2729810	0.4581000	C	3.4301900	-0.9715240	-0.1293490
C	3.4630120	-0.9807620	-0.0474780	C	4.3504070	-1.8544750	0.4648810
C	4.3748260	-1.8977240	0.5159730	C	5.7093750	-1.5454160	0.5165620
C	5.7418210	-1.6284370	0.5545260	C	6.1773710	-0.3407710	-0.0144490
C	6.2403560	-0.4276860	0.0411600	C	5.2733130	0.5479110	-0.6018980
C	5.3527630	0.4939230	-0.5193420	C	3.9147590	0.2367590	-0.6633640
C	3.9856370	0.2201950	-0.5683930	H	1.3202180	3.5050910	2.1423510
H	1.3619390	3.8300180	1.6610480	H	1.3088910	0.7370820	2.3430620
H	1.5981370	1.1090710	2.2058360	H	2.0177090	-3.5384160	-0.5985110
H	0.2788040	1.6141740	-1.7740350	H	-4.7086840	-2.3303040	0.7370810
H	2.0280500	-3.5224110	-0.3911570	H	-3.9252840	1.6066620	-0.7947330
H	-2.2686210	-2.8726440	-0.8310170	H	-1.5020890	1.0763330	-0.9428470
H	-4.7066180	-2.4016770	-0.7519610	H	3.9920810	-2.7827140	0.9019310
H	-3.8931680	1.4836490	0.8951730	H	6.4017630	-2.2427060	0.9809220
H	-1.4876080	1.0205600	0.8446880	H	7.2352070	-0.0965850	0.0305680
H	3.9978200	-2.8234610	0.9418120	H	5.6274510	1.4854970	-1.0225750
H	6.4191840	-2.3548920	0.9964710	H	3.2225090	0.9255230	-1.1380970
H	7.3051270	-0.2141720	0.0765670	N	0.9132960	3.0323470	0.0569530
H	5.7261150	1.4279340	-0.9318430	C	0.8364940	4.3873470	-0.4734280
H	3.3217670	0.9367680	-1.0420010	H	0.0304540	4.9462990	0.0122260
N	0.7402340	3.0773350	-0.2620070	H	1.7809290	4.9171660	-0.3144000
N	-5.8503350	-0.1460840	0.1082270	H	0.6357790	4.3165750	-1.5425220
O	-6.2266050	0.9588700	0.5326980	N	0.1391480	-2.5505640	-0.4127940
O	-6.6422480	-1.0206190	-0.2791460	H	-0.4617120	-3.3269670	-0.6521560
C	0.4655510	4.3334630	-0.9671560	H	-2.2988180	-2.8540930	0.6528840
H	-0.3685840	4.8459360	-0.4844530	N	-5.8630450	-0.0233840	0.0491720
H	1.3559230	4.9635060	-0.9395700	O	-6.2349730	1.1035640	-0.2960850
H	0.2094790	4.1059680	-2.0014220	O	-6.6352650	-0.9006280	0.4517450

Compound **6h, R = *p*-F**

E = -1035.79991198, **H (0K)** = -1035.484283, **H (298K)** = -1035.463645, **G (298K)** = -1035.535121 au.

Imaginary frequency = 0.

C	0.6748300	3.0251880	0.8306090
C	1.0536670	1.7308250	1.0319970
N	0.3685930	0.9451410	0.1150800
C	-0.3939430	1.7540960	-0.6293930
C	0.4121260	-0.4729180	0.0071650
C	-0.7059250	-1.3384190	-0.0717790
N	-0.2723070	-2.6167750	-0.2097460
C	1.0776630	-2.5720980	-0.1881380
C	1.5913970	-1.2703590	-0.0577620
C	-2.1440550	-1.0434530	0.0145630
C	-3.0568140	-1.8708740	-0.6708150
C	-4.4286340	-1.6415690	-0.6180890
C	-4.9045140	-0.5678860	0.1275360
C	-4.0451880	0.2617270	0.8358430
C	-2.6726110	0.0124290	0.7828960

Compound **7b, R = *p*-F**

E = -1035.80060575, **H (0K)** = -1035.484541, **H (298K)** = -1035.463970, **G (298K)** = -1035.534682 au.

Imaginary frequency = 0.

C	0.7621850	2.7630060	1.3753540
C	0.7880900	1.4129400	1.4766490
N	0.3703440	0.9224310	0.2378270
C	0.0855890	1.9255730	-0.6640920
C	0.3078350	-0.4641870	-0.0648580
C	-0.8529990	-1.2213530	-0.1785640
C	0.9298890	-2.6042750	-0.3699750
C	1.4437210	-1.3336540	-0.1820070
C	-2.2799240	-0.8877910	-0.1073700
C	-3.1872070	-1.7823590	0.4913770
C	-4.5515720	-1.5042750	0.5381000
C	-5.0062740	-0.3103380	-0.0088560
C	-4.1396200	0.6026040	-0.5989430
C	-2.7792210	0.3088150	-0.6556900
C	2.8740970	-0.9814220	-0.1385860

C	3.0036920	-0.8756680	-0.0592150	C	3.8032500	-1.8459130	0.4661730
C	3.9648370	-1.6800740	0.5881740	C	5.1638300	-1.5426180	0.4763840
C	5.3161160	-1.3425030	0.5810570	C	5.6235850	-0.3606090	-0.1072030
C	5.7532630	-0.1794320	-0.0586350	C	4.7100290	0.5109830	-0.7038990
C	4.8183730	0.6320100	-0.7040540	C	3.3499910	0.2055740	-0.7238860
C	3.4672310	0.2864880	-0.7102970	H	1.0051010	3.5296800	2.0963900
H	0.9723500	3.9355910	1.3271210	H	1.0595420	0.7642110	2.2950780
H	1.7415150	1.2875390	1.7326540	H	1.4376730	-3.5381810	-0.5613020
H	-1.0477170	1.4242010	-1.4197080	H	-5.2562660	-2.1864770	1.0023640
H	-2.6596710	-2.7071030	-1.2363710	H	-4.5360390	1.5212320	-1.0196060
H	-5.1308530	-2.2789160	-1.1467290	H	-2.0865490	1.0030580	-1.1243580
H	-4.4541100	1.0671600	1.4385410	H	3.4478450	-2.7546430	0.9454090
H	-2.0085030	0.6249450	1.3870270	H	5.8643410	-2.2260600	0.9497990
H	3.6309180	-2.5719720	1.1108850	H	6.6833880	-0.1199990	-0.0951900
H	6.0317200	-1.9855230	1.0880770	H	5.0586310	1.4315470	-1.1652910
H	6.8067890	0.0873320	-0.0578150	H	2.6480650	0.8785310	-1.2068900
H	5.1447360	1.5313930	-1.2218580	N	0.3342580	3.0453220	0.0796030
H	2.7628760	0.9056530	-1.2597870	C	0.1660850	4.3884920	-0.4483680
N	-0.2438380	3.0241370	-0.2035100	H	-0.5867690	4.9425900	0.1237960
C	-0.9369190	4.1901980	-0.7418500	H	1.1115670	4.9415580	-0.4164220
H	-1.5405190	4.6608930	0.0387940	H	-0.1630360	4.2934190	-1.4834520
H	-0.2125530	4.9110240	-1.1299390	N	-0.4375280	-2.5263070	-0.3537690
H	-1.5920290	3.8689300	-1.5526770	H	-1.0613510	-3.2783510	-0.6053230
H	1.6627770	-3.4782040	-0.3109440	H	-2.8195660	-2.6950450	0.9535470
F	-6.2380470	-0.3307470	0.1734530	F	-6.3271380	-0.0302610	0.0372660

Compound **6h, R = *p*-F**

pcm CH_2Cl_2

E = -1035.82640276, **H (0K)** = -1035.510157, **H (298K)** = -1035.489677, **G (298K)** = -1035.560386 au.

Imaginary frequency = 0.

C	0.5422690	2.9824250	1.0051580
C	0.7978920	1.6688750	1.2649100
N	0.3501120	0.9360910	0.1758560
C	-0.1590660	1.7929740	-0.7188560
C	0.3809840	-0.4880190	0.0291360
C	-0.7414640	-1.3393150	-0.0561000
N	-0.3184860	-2.6275040	-0.2199410
C	1.0322320	-2.5904430	-0.2089200
C	1.5532790	-1.2904920	-0.0625850
C	-2.1765650	-1.0246650	0.0112850
C	-3.1022440	-1.8763350	-0.6273250
C	-4.4723670	-1.6311900	-0.5854990
C	-4.9320420	-0.5126060	0.1011150
C	-4.0618680	0.3493170	0.7551880
C	-2.6921420	0.0838990	0.7131840
C	2.9700230	-0.9085610	-0.0541930
C	3.9391340	-1.7910680	0.4699330
C	5.2949440	-1.4693560	0.4622870
C	5.7301590	-0.2454180	-0.0548680
C	4.7870520	0.6447070	-0.5737990
C	3.4309920	0.3168740	-0.5797900
H	0.7317990	3.8710280	1.5863480
H	1.2481750	1.1854850	2.1162580
H	-0.5834500	1.5141530	-1.6696360
H	-2.7228410	-2.7431190	-1.1576010
H	-5.1806060	-2.2884210	-1.0807430
H	-4.4551620	1.2006730	1.3020770
H	-2.0239620	0.7360530	1.2666820
H	3.6130620	-2.7338990	0.9005090

Compound **7b, R = *p*-F**

pcm CH_2Cl_2

E = -1035.81265916, **H (0K)** = -1035.496428, **H (298K)** = -1035.475904, **G (298K)** = -1035.546323 au.

Imaginary frequency = 0.

C	0.5888310	2.7607910	1.3964640
C	0.5856120	1.4102310	1.5071330
N	0.3475630	0.9165890	0.2229270
C	0.2069950	1.9183350	-0.7131340
C	0.3074010	-0.4718990	-0.0826890
C	-0.8478370	-1.2398490	-0.1992180
C	0.9428870	-2.6085660	-0.3820960
C	1.4501940	-1.3331710	-0.1928140
C	-2.2741440	-0.9028320	-0.1242020
C	-3.1910640	-1.8062010	0.4469940
C	-4.5523920	-1.5137550	0.5034100
C	-4.9933930	-0.2980250	-0.0052050
C	-4.1196680	0.6244910	-0.5690310
C	-2.7626200	0.3151540	-0.6345390
C	2.8793060	-0.9775720	-0.1314190
C	3.8071160	-1.8596250	0.4527530
C	5.1672360	-1.5534330	0.4848500
C	5.6304260	-0.3508830	-0.0549220
C	4.7193850	0.5376850	-0.6314150
C	3.3596530	0.2287180	-0.6741820
H	0.7301980	3.5311410	2.1400360
H	0.7242530	0.7643840	2.3605790
H	1.4533080	-3.5429610	-0.5633470
H	-5.2623900	-2.2051420	0.9452560
H	-4.5042110	1.5602370	-0.9618900
H	-2.0683490	1.0163040	-1.0881610
H	3.4523890	-2.7856200	0.8977010
H	5.8646810	-2.2510400	0.9415230
H	6.6892800	-0.1083480	-0.0248160

H	6.0147690	-2.1732250	0.8733610	H	5.0691700	1.4739720	-1.0589560
H	6.7865510	0.0093060	-0.0537440	H	2.6617530	0.9169610	-1.1413670
H	5.1088590	1.5966780	-0.9896930	N	0.3568700	3.0403540	0.0518440
H	2.7229440	1.0098410	-1.0245790	C	0.2832490	4.3890370	-0.4922220
N	-0.0629490	3.0395660	-0.2377080	H	-0.5355470	4.9492360	-0.0290720
C	-0.5162320	4.2563510	-0.9159680	H	1.2213070	4.9268120	-0.3205150
H	-1.2719090	4.7538070	-0.3052030	H	0.1043120	4.3061880	-1.5644040
H	0.3331020	4.9239010	-1.0726810	N	-0.4228450	-2.5397980	-0.3743960
H	-0.9478570	3.9820050	-1.8782650	H	-1.0356150	-3.3103490	-0.6005020
H	1.6123280	-3.4991620	-0.3436100	H	-2.8373980	-2.7399960	0.8750380
F	-6.2662620	-0.2611000	0.1397010	F	-6.3134780	-0.0037320	0.0514640
Compound **6h, R = *p*-F** pcm MeOH **E** = -1035.83065033, **H (0K)** = -1035.514345, **H (298K)** = -1035.493871, **G (298K)** = -1035.564515 au. Imaginary frequency = 0.				Compound **7b, R = *p*-F** pcm MeOH **E** = -1035.81483010, **H (0K)** = -1035.498608, **H (298K)** = -1035.478069, **G (298K)** = -1035.548618 au. Imaginary frequency = 0.			
C	0.5341660	2.9805250	1.0131590	C	0.5670700	2.7615500	1.3968360
C	0.7809020	1.6659260	1.2752460	C	0.5594280	1.4108870	1.5084120
N	0.3482000	0.9365040	0.1775490	N	0.3453980	0.9166900	0.2201940
C	-0.1442050	1.7970560	-0.7239310	C	0.2245460	1.9183830	-0.7185450
C	0.3785340	-0.4878310	0.0292670	C	0.3071980	-0.4720910	-0.0856070
C	-0.7438000	-1.3387540	-0.0553810	C	-0.8477200	-1.2413410	-0.2019260
N	-0.3213960	-2.6282980	-0.2182510	C	0.9436870	-2.6088290	-0.3830550
C	1.0299310	-2.5911940	-0.2078140	C	1.4506320	-1.3328000	-0.1943030
C	1.5505520	-1.2909660	-0.0626870	C	-2.2740810	-0.9040970	-0.1263320
C	-2.1791780	-1.0232110	0.0097780	C	-3.1925350	-1.8103980	0.4379220
C	-3.1053610	-1.8753810	-0.6274680	C	-4.5535450	-1.5164680	0.4956380
C	-4.4756520	-1.6299480	-0.5856950	C	-4.9927510	-0.2965820	-0.0045010
C	-4.9342120	-0.5099370	0.0992470	C	-4.1178640	0.6289610	-0.5616040
C	-4.0635150	0.3535800	0.7506910	C	-2.7612180	0.3180100	-0.6283340
C	-2.6939570	0.0876470	0.7088470	C	2.8798630	-0.9776370	-0.1305110
C	2.9682200	-0.9105060	-0.0532880	C	3.8064640	-1.8617100	0.4531060
C	3.9365820	-1.7976490	0.4646280	C	5.1667520	-1.5561520	0.4884190
C	5.2931230	-1.4781580	0.4569810	C	5.6317990	-0.3523420	-0.0473730
C	5.7294120	-0.2520290	-0.0542650	C	4.7222350	0.5381500	-0.6234800
C	4.7868810	0.6426620	-0.5667940	C	3.3623040	0.2296810	-0.6696240
C	3.4301220	0.3171730	-0.5728240	H	0.6950280	3.5324530	2.1421790
H	0.7169400	3.8676780	1.5986200	H	0.6798080	0.7655020	2.3649960
H	1.2152880	1.1804950	2.1336500	H	1.4538950	-3.5438360	-0.5615470
H	-0.5541300	1.5221810	-1.6822010	H	-5.2642130	-2.2107270	0.9317750
H	-2.7276560	-2.7424740	-1.1585540	H	-4.5008300	1.5680090	-0.9480500
H	-5.1839520	-2.2874100	-1.0804960	H	-2.0668600	1.0217910	-1.0774060
H	-4.4552440	1.2077600	1.2941120	H	3.4509820	-2.7888490	0.8949000
H	-2.0256960	0.7429270	1.2581930	H	5.8628640	-2.2553340	0.9445980
H	3.6101800	-2.7425000	0.8906620	H	6.6906540	-0.1103810	-0.0144620
H	6.0123290	-2.1853050	0.8634220	H	5.0732650	1.4754080	-1.0478380
H	6.7861350	0.0011840	-0.0529980	H	2.6658810	0.9199190	-1.1362020
H	5.1092110	1.5967850	-0.9770220	N	0.3615920	3.0407530	0.0479860
H	2.7230510	1.0147810	-1.0113980	C	0.3008110	4.3903390	-0.4968360
N	-0.0503490	3.0415040	-0.2392800	H	-0.5247400	4.9516520	-0.0477230
C	-0.4888970	4.2618870	-0.9219760	H	1.2367110	4.9255700	-0.3074390
H	-1.2488240	4.7614800	-0.3186000	H	0.1409420	4.3094210	-1.5721850
H	0.3662440	4.9244620	-1.0662380	N	-0.4215810	-2.5405700	-0.3771180
H	-0.9096530	3.9907630	-1.8897750	H	-1.0331920	-3.3146600	-0.5949440
H	1.6101050	-3.5002790	-0.3405620	H	-2.8412870	-2.7483280	0.8585100
F	-6.2686010	-0.2584270	0.1383020	F	-6.3128030	-0.0009780	0.0537310
Compound **6a, R = H** **E** = -936.56618208, **H (0K)** = -936.242318,				Compound **7c, R = H** **E** = -936.56703379, **H (0K)** = -936.242662,			

H (298K) = -936.222555, **G (298K)** = -936.291814 au.			
Imaginary frequency = 0.			
C	-0.2836940	3.0167020	0.8317490
C	-0.7011290	1.7343370	1.0330940
N	-0.0320760	0.9271330	0.1231850
C	0.7593920	1.7115910	-0.6169050
C	-0.1096730	-0.4898730	0.0205880
C	0.9893410	-1.3805200	-0.0509350
N	0.5263730	-2.6491210	-0.1902050
C	-0.8216500	-2.5731610	-0.1765060
C	-1.3066010	-1.2591460	-0.0518100
C	2.4325630	-1.1155940	0.0430350
C	3.3326250	-1.9610760	-0.6358290
C	4.7068540	-1.7481020	-0.5726910
C	5.2289180	-0.6829220	0.1680450
C	4.3535890	0.1521830	0.8644120
C	2.9761590	-0.0650980	0.8097500
C	-2.7092150	-0.8325720	-0.0656730
C	-3.1392810	0.3448460	-0.7126860
C	-4.4820750	0.7213690	-0.7180600
C	-5.4424160	-0.0730500	-0.0890810
C	-5.0388450	-1.2507360	0.5460720
C	-3.6958880	-1.6193680	0.5650650
H	-0.5588500	3.9366090	1.3235930
H	-1.4060850	1.3126880	1.7300580
H	1.4123560	1.3598670	-1.3983690
H	-1.4268500	-3.4657900	-0.3012990
H	2.9217740	-2.7909480	-1.2015660
H	5.3777010	-2.4169050	-1.1070990
H	6.3021010	-0.5169540	0.2142050
H	4.7453090	0.9637640	1.4742550
H	2.3177770	0.5599360	1.4083600
H	-2.4150050	0.9521180	-1.2492750
H	-4.7819740	1.6320510	-1.2321700
H	-6.4894910	0.2179500	-0.0972580
H	-5.7744120	-1.8809330	1.0405360
H	-3.3884120	-2.5224400	1.0847840
N	0.6426800	2.9864520	-0.1952340
C	1.3720410	4.1305890	-0.7318340
H	0.6725360	4.8638910	-1.1418690
H	1.9707600	4.5956500	0.0558880
H	2.0358310	3.7858120	-1.5257940

H (298K) = -936.222969, **G (298K)** = -936.291430 au.			
Imaginary frequency = 0.			
C	-0.3832600	2.7575290	1.3988170
C	-0.3873630	1.4073510	1.5025430
N	-0.0454590	0.9198540	0.2396910
C	0.1695210	1.9239550	-0.6797270
C	0.0158840	-0.4668990	-0.0646630
C	1.1775530	-1.2234130	-0.1752520
C	-0.6039520	-2.6076270	-0.3667560
C	-1.1191870	-1.3368580	-0.1812930
C	2.6036510	-0.8863010	-0.1051790
C	3.5155170	-1.7853760	0.4795880
C	4.8777530	-1.4946510	0.5213470
C	5.3546050	-0.2943230	-0.0086270
C	4.4567140	0.6086710	-0.5825970
C	3.0947790	0.3183260	-0.6409510
C	-2.5497030	-0.9855600	-0.1381030
C	-3.0265600	0.1999530	-0.7257090
C	-4.3868490	0.5044420	-0.7049510
C	-5.2995290	-0.3664670	-0.1059170
C	-4.8386480	-1.5470720	0.4796600
C	-3.4778920	-1.8494940	0.4689780
H	-0.5870220	3.5226800	2.1334970
H	-0.5963660	0.7567590	2.3377210
H	-1.1108060	-3.5421870	-0.5575720
H	3.1500960	-2.7043430	0.9322290
H	5.5649710	-2.2009790	0.9800960
H	6.4162280	-0.0645680	0.0270870
H	4.8206430	1.5431450	-1.0021710
H	2.3981700	1.0116560	-1.1044060
H	-2.3249170	0.8723380	-1.2100710
H	-4.7364000	1.4239020	-1.1679140
H	-6.3595080	-0.1264720	-0.0936080
H	-5.5384080	-2.2300000	0.9549990
H	-3.1214710	-2.7569890	0.9498410
N	-0.0437480	3.0422180	0.0775510
C	0.0736880	4.3858820	-0.4621570
H	-0.8746650	4.9275360	-0.3712140
H	0.8544470	4.9508160	0.0599340
H	0.3376170	4.2919790	-1.5158640
N	0.7631960	-2.5286870	-0.3479250
H	1.3891410	-3.2813670	-0.5920950

Compound **6a, R = H**
pcm CH_2Cl_2
E = -936.59280208, **H (0K)** = -936.268250,
H (298K) = -936.248649, **G (298K)** = -936.317320 au.
Imaginary frequency = 0.

C	-0.1834120	2.9762230	0.9951340
C	-0.4789360	1.6705650	1.2522160
N	-0.0177110	0.9220380	0.1795600
C	0.5392880	1.7618750	-0.7025230
C	-0.0763160	-0.5014310	0.0384190
C	1.0302980	-1.3745400	-0.0404730
N	0.5820850	-2.6547370	-0.2045240
C	-0.7673310	-2.5908980	-0.1993820
C	-1.2635950	-1.2802890	-0.0584120
C	2.4704050	-1.0857870	0.0347470
C	3.3850510	-1.9466610	-0.6069900
C	4.7573570	-1.7148500	-0.5538590
C	5.2645320	-0.6109620	0.1396760

Compound **7c, R = H**
pcm CH_2Cl_2
E = -936.57927230, **H (0K)** = -936.254725,
H (298K) = -936.235055, **G (298K)** = -936.303443 au.
Imaginary frequency = 0.

C	-0.2510480	2.7615900	1.4017390
C	-0.2322640	1.4111040	1.5122580
N	-0.0298370	0.9191450	0.2214300
C	0.0729920	1.9215110	-0.7186510
C	0.0157700	-0.4694040	-0.0843570
C	1.1741290	-1.2340930	-0.1963840
C	-0.6124860	-2.6084160	-0.3817370
C	-1.1241260	-1.3341670	-0.1949650
C	2.5999760	-0.8949640	-0.1177680
C	3.5182000	-1.8061180	0.4389110
C	4.8782170	-1.5046480	0.4951470
C	5.3484160	-0.2823060	0.0092490
C	4.4450600	0.6327250	-0.5379580

C	4.3752910	0.2461000	0.7918000	C	3.0857220	0.3311110	-0.6099040
C	3.0003450	0.0099580	0.7468380	C	-2.5546190	-0.9841340	-0.1334710
C	-2.6727420	-0.8709890	-0.0606970	C	-3.0412540	0.2174880	-0.6809590
C	-3.1069090	0.3599210	-0.5963530	C	-4.4022400	0.5208500	-0.6364350
C	-4.4563450	0.7141220	-0.6000960	C	-5.3083010	-0.3688110	-0.0538010
C	-5.4195830	-0.1543260	-0.0814360	C	-4.8388510	-1.5669080	0.4904600
C	-5.0112180	-1.3834960	0.4451430	C	-3.4775020	-1.8674100	0.4567610
C	-3.6619660	-1.7314420	0.4625770	H	-0.3761190	3.5309400	2.1492530
H	-0.3692180	3.8720110	1.5665200	H	-0.3382970	0.7642440	2.3696140
H	-0.9662460	1.2024870	2.0916100	H	-1.1198870	-3.5444650	-0.5631450
H	0.9865070	1.4677810	-1.6380260	H	3.1629900	-2.7461710	0.8533110
H	-1.3650510	-3.4881700	-0.3346170	H	5.5691750	-2.2218870	0.9301090
H	2.9923790	-2.8026290	-1.1462370	H	6.4077170	-0.0453570	0.0572280
H	5.4362640	-2.3964740	-1.0611740	H	4.8020600	1.5838790	-0.9243530
H	6.3350080	-0.4274860	0.1777750	H	2.3893990	1.0353630	-1.0554520
H	4.7529490	1.0971470	1.3538840	H	-2.3469520	0.9065550	-1.1523530
H	2.3370580	0.6664760	1.3024360	H	-4.7569580	1.4537000	-1.0674670
H	-2.3830430	1.0362400	-1.0412690	H	-6.3681030	-0.1305550	-0.0223820
H	-4.7571240	1.6697060	-1.0234040	H	-5.5323130	-2.2653270	0.9519630
H	-6.4707960	0.1209370	-0.0878540	H	-3.1177750	-2.7897230	0.9053460
H	-5.7469540	-2.0708730	0.8559770	N	-0.0636170	3.0425490	0.0504790
H	-3.3568240	-2.6780320	0.9002020	C	-0.0189310	4.3915450	-0.4957290
N	0.4601080	3.0127200	-0.2291330	H	-0.9562240	4.9209840	-0.2960230
C	0.9647540	4.2146330	-0.8971490	H	0.8082830	4.9595230	-0.0576590
H	0.1386310	4.9051500	-1.0771690	H	0.1284210	4.3099620	-1.5728210
H	1.7176760	4.6925790	-0.2675410	N	0.7526520	-2.5354350	-0.3703490
H	1.4136060	3.9266390	-1.8475140	H	1.3690470	-3.3047620	-0.5905240

Compound **6a, R = H**
pcm MeOH
E = -936.59713921, **H (0K)** = -936.272499,
H (298K) = -936.252916, **G (298K)** = -936.321332 au.
Imaginary frequency = 0.

C	-0.1745600	2.9698080	1.0166250
C	-0.4460050	1.6599390	1.2777860
N	-0.0167340	0.9221140	0.1844570
C	0.4980380	1.7729720	-0.7134520
C	-0.0690290	-0.5017180	0.0379030
C	1.0402860	-1.3709010	-0.0412090
N	0.5962470	-2.6536710	-0.2049990
C	-0.7538640	-2.5940970	-0.2001410
C	-1.2536260	-1.2848220	-0.0591480
C	2.4799370	-1.0775290	0.0309020
C	3.3974050	-1.9424470	-0.6017720
C	4.7694210	-1.7074940	-0.5495460
C	5.2733200	-0.5958080	0.1338890
C	4.3812110	0.2664950	0.7754730
C	3.0067650	0.0271720	0.7315520
C	-2.6647360	-0.8807060	-0.0591380
C	-3.1028290	0.3536030	-0.5837140
C	-4.4539110	0.7019220	-0.5867150
C	-5.4146050	-0.1758080	-0.0786020
C	-5.0021610	-1.4082130	0.4373480
C	-3.6512510	-1.7504850	0.4540380
H	-0.3474830	3.8606110	1.5995540
H	-0.8959890	1.1829210	2.1328470
H	0.9123050	1.4898210	-1.6673750
H	-1.3488680	-3.4935080	-0.3343470
H	3.0080780	-2.8038570	-1.1348910
H	5.4502090	-2.3922380	-1.0500560
H	6.3432460	-0.4092520	0.1709850

Compound **7c, R = H**
pcm MeOH
E = -936.58152148, **H (0K)** = -936.256965,
H (298K) = -936.237281, **G (298K)** = -936.305811 au.
Imaginary frequency = 0.

C	-0.2272830	2.7633150	1.4013520
C	-0.2052890	1.4127920	1.5130770
N	-0.0276520	0.9195160	0.2190690
C	0.0564350	1.9212850	-0.7233630
C	0.0153760	-0.4694150	-0.0866030
C	1.1732590	-1.2356570	-0.1982070
C	-0.6143640	-2.6083050	-0.3822120
C	-1.1254120	-1.3333080	-0.1961010
C	2.5992820	-0.8965700	-0.1192230
C	3.5190360	-1.8106940	0.4302920
C	4.8788410	-1.5079760	0.4874210
C	5.3477220	-0.2817090	0.0098110
C	4.4430510	0.6362600	-0.5304820
C	3.0839330	0.3333740	-0.6031890
C	-2.5560230	-0.9835770	-0.1324780
C	-3.0444830	0.2195490	-0.6755120
C	-4.4056730	0.5224470	-0.6279780
C	-5.3105350	-0.3695900	-0.0468860
C	-4.8395040	-1.5694240	0.4926110
C	-3.4780010	-1.8693310	0.4560610
H	-0.3383350	3.5336430	2.1499960
H	-0.2937840	0.7669120	2.3731820
H	-1.1217620	-3.5448920	-0.5606410
H	3.1660450	-2.7546000	0.8374250
H	5.5707420	-2.2277830	0.9164250
H	6.4067720	-0.0440770	0.0586980
H	4.7987030	1.5904620	-0.9104800
H	2.3874410	1.0404860	-1.0437160

H	4.7558600	1.1253650	1.3273170	H	-2.3514360	0.9110080	-1.1453700
H	2.3420600	0.6904740	1.2768220	H	-4.7614020	1.4566460	-1.0552050
H	-2.3814830	1.0383580	-1.0192610	H	-6.3703380	-0.1319160	-0.0129600
H	-4.7575020	1.6606070	-1.0006010	H	-5.5318570	-2.2697760	0.9527170
H	-6.4668930	0.0951870	-0.0843580	H	-3.1178050	-2.7932000	0.9008900
H	-5.7356860	-2.1025000	0.8403720	N	-0.0662310	3.0431170	0.0466130
H	-3.3435810	-2.7000790	0.8834810	C	-0.0326700	4.3927430	-0.5003240
N	0.4212060	3.0194750	-0.2309840	H	-0.9660620	4.9212730	-0.2819000
C	0.8842840	4.2317510	-0.9116650	H	0.8023560	4.9605230	-0.0776050
H	0.0414710	4.9092190	-1.0595540	H	0.0940380	4.3124520	-1.5801460
H	1.6501910	4.7181780	-0.3050580	N	0.7503390	-2.5362480	-0.3721190
H	1.3044990	3.9534580	-1.8776820	H	1.3653030	-3.3091120	-0.5846460
Compound **6g, R = *p*-MeO**				Compound **7d, R = *p*-MeO**			
E = -1051.08732112, **H (0K)** = -1050.730858, **H (298K)** = -1050.708411, **G (298K)** = -1050.784367 au.				**E** = -1051.08994597, **H (0K)** = -1050.732860, **H (298K)** = -1050.710520, **G (298K)** = -1050.785175 au.			
Imaginary frequency = 0.				Imaginary frequency = 0.			
C	0.9042070	3.0252360	0.7701240	C	0.9494640	2.7348480	1.4208500
C	1.3217250	1.7453670	0.9869280	C	1.0248230	1.3858560	1.5129850
N	0.6691660	0.9293520	0.0723000	N	0.6613070	0.8893270	0.2599680
C	-0.1123830	1.7069190	-0.6858490	C	0.3618500	1.8870760	-0.6424770
C	0.7546890	-0.4871670	-0.0189970	C	0.6585090	-0.4972600	-0.0520870
C	-0.3381250	-1.3820640	-0.1171370	C	-0.4697740	-1.3030590	-0.1549210
N	0.1316790	-2.6499310	-0.2271690	C	1.3698340	-2.6065960	-0.3764520
C	1.4798960	-2.5699560	-0.1696980	C	1.8302500	-1.3156580	-0.1892920
C	1.9567710	-1.2547810	-0.0410100	C	-1.9079350	-1.0297530	-0.0677270
C	-1.7859620	-1.1212060	-0.0711360	C	-2.7776580	-1.9593420	0.5384580
C	-2.6632400	-1.9605770	-0.7909910	C	-4.1451420	-1.7336980	0.5997310
C	-4.0354130	-1.7640020	-0.7709450	C	-4.6884570	-0.5568030	0.0641120
C	-4.5923110	-0.7128650	-0.0265450	C	-3.8395530	0.3822550	-0.5334530
C	-3.7489800	0.1238230	0.7098580	C	-2.4670160	0.1401840	-0.6039140
C	-2.3662510	-0.0927870	0.6879010	C	3.2440890	-0.9016280	-0.1622010
C	3.3580000	-0.8253160	-0.0117500	C	4.2204420	-1.7332520	0.4140390
C	4.3233700	-1.6006380	0.6649240	C	5.5663340	-1.3703240	0.4086730
C	5.6656720	-1.2299370	0.6875610	C	5.9645740	-0.1597470	-0.1616110
C	6.0899130	-0.0609200	0.0497810	C	5.0039040	0.6796830	-0.7295940
C	5.1510490	0.7222190	-0.6242340	C	3.6585230	0.3144510	-0.7348480
C	3.8093910	0.3432170	-0.6606410	H	1.1426990	3.5046140	2.1535810
H	1.1696090	3.9492040	1.2597420	H	1.2974680	0.7412130	2.3342850
H	2.0157520	1.3306250	1.6987580	H	1.9148380	-3.5171890	-0.5775350
H	-0.7515530	1.3481330	-1.4753890	H	-4.8135330	-2.4471670	1.0717920
H	2.0908240	-3.4619940	-0.2679580	H	-4.2336550	1.2974490	-0.9608680
H	-4.7042470	-2.4148880	-1.3266610	H	-1.8137770	0.8652470	-1.0821500
H	-4.1513870	0.9225740	1.3239980	H	3.9131230	-2.6642070	0.8837820
H	-1.7367210	0.5337770	1.3153410	H	6.3035710	-2.0296990	0.8600960
H	3.9988590	-2.4965680	1.1866710	H	7.0128250	0.1274840	-0.1612470
H	6.3842200	-1.8515440	1.2167780	H	5.3041030	1.6222710	-1.1806080
H	7.1362400	0.2319200	0.0740980	H	2.9202650	0.9631720	-1.1963700
H	5.4675270	1.6257580	-1.1410860	N	0.5465720	3.0103310	0.1155690
H	3.1038670	0.9408080	-1.2320070	C	0.3420910	4.3494120	-0.4085550
N	-0.0067480	2.9853530	-0.2699080	H	-0.4464950	4.8712780	0.1458400
C	-0.7189330	4.1258170	-0.8355730	H	1.2645230	4.9380760	-0.3477450
H	-1.2794590	4.6409260	-0.0510520	H	0.0450430	4.2488830	-1.4528480
H	-0.0135280	4.8215230	-1.2983080	O	-6.0432620	-0.4241880	0.1775200
H	-1.4172910	3.7666630	-1.5927230	C	-6.6464160	0.7525500	-0.3353380
O	-5.9580900	-0.5981580	-0.0819840	H	-7.7147670	0.6539090	-0.1336510
C	-6.5720790	0.4074020	0.7003030	H	-6.2647970	1.6531010	0.1639820
H	-7.6458670	0.3153580	0.5236350	H	-6.4896800	0.8489180	-1.4179660
H	-6.3692680	0.2705070	1.7715990	N	-0.0000100	-2.5873810	-0.3427990

H	-6.2436970	1.4137590	0.4027620	H	-0.5953470	-3.3653300	-0.5840450
H	-2.2338640	-2.7813920	-1.3561250	H	-2.3718380	-2.8596290	0.9940860
Compound **6g, R = *p*-MeO** pcm CH_2Cl_2 **E** = -1051.11578780, **H (0K)** = -1050.758599, **H (298K)** = -1050.736340, **G (298K)** = -1050.811243 au. Imaginary frequency = 0.				Compound **7d, R = *p*-MeO** pcm CH_2Cl_2 **E** = -1051.10351762, **H (0K)** = -1050.746259, **H (298K)** = -1050.723959, **G (298K)** = -1050.798421 au. Imaginary frequency = 0.			
C	0.7509930	2.9748330	0.9428900	C	0.7824630	2.7283810	1.4322240
C	1.0603150	1.6759660	1.2175170	C	0.8332380	1.3779380	1.5334930
N	0.6426600	0.9126250	0.1375070	N	0.6389160	0.8840060	0.2423510
C	0.0976090	1.7371990	-0.7660710	C	0.4727840	1.8856010	-0.6893400
C	0.7291290	-0.5106600	0.0089180	C	0.6585150	-0.5035770	-0.0716700
C	-0.3606790	-1.4010380	-0.0884900	C	-0.4632630	-1.3208420	-0.1779220
N	0.1101210	-2.6758070	-0.2237580	C	1.3854610	-2.6086690	-0.3892510
C	1.4593390	-2.5914610	-0.1835580	C	1.8377850	-1.3130170	-0.2003600
C	1.9319080	-1.2730670	-0.0442240	C	-1.9019240	-1.0478160	-0.0876220
C	-1.8073980	-1.1308010	-0.0567840	C	-2.7789410	-1.9901030	0.4886150
C	-2.6952120	-1.9971630	-0.7313120	C	-4.1449450	-1.7545460	0.5577150
C	-4.0669590	-1.7893770	-0.7207050	C	-4.6820030	-0.5564320	0.0613300
C	-4.6145550	-0.6945240	-0.0334560	C	-3.8260770	0.3952890	-0.5075490
C	-3.7600460	0.1742240	0.6528020	C	-2.4556150	0.1426350	-0.5847110
C	-2.3797440	-0.0539960	0.6412070	C	3.2503740	-0.8952840	-0.1532900
C	3.3335110	-0.8414570	-0.0128270	C	4.2242400	-1.7408360	0.4100080
C	4.3239000	-1.6828000	0.5392740	C	5.5697950	-1.3749540	0.4287730
C	5.6672300	-1.3126950	0.5538100	C	5.9726750	-0.1474750	-0.1033480
C	6.0688260	-0.0791410	0.0320400	C	5.0157050	0.7053220	-0.6589630
C	5.1045460	0.7708750	-0.5144850	C	3.6705850	0.3365130	-0.6890350
C	3.7614900	0.3942970	-0.5429910	H	0.8786780	3.4985320	2.1832200
H	0.9053290	3.8773710	1.5129780	H	0.9832100	0.7319180	2.3849060
H	1.5310910	1.2212830	2.0735160	H	1.9342760	-3.5190440	-0.5801850
H	-0.3177060	1.4291870	-1.7117580	H	-4.8153630	-2.4817390	1.0057750
H	2.0731480	-3.4812300	-0.2942590	H	-4.2132350	1.3262580	-0.9054790
H	-4.7382720	-2.4630570	-1.2461580	H	-1.8022590	0.8785960	-1.0441740
H	-4.1516000	1.0165210	1.2125320	H	3.9167630	-2.6861610	0.8495150
H	-1.7482470	0.6130220	1.2211290	H	6.3030570	-2.0456360	0.8695110
H	4.0236270	-2.6323060	0.9739870	H	7.0200210	0.1416930	-0.0832060
H	6.4035340	-1.9861440	0.9862410	H	5.3180980	1.6607290	-1.0804440
H	7.1152160	0.2134430	0.0507260	H	2.9371240	0.9978490	-1.1403770
H	5.3999140	1.7296600	-0.9344810	N	0.5629500	3.0077280	0.0854250
H	3.0381810	1.0567210	-1.0091260	C	0.4447040	4.3559060	-0.4513780
N	0.1425080	2.9926350	-0.2994880	H	-0.4056500	4.8790650	-0.0017730
C	-0.3580630	4.1828780	-0.9908770	H	1.3561050	4.9307430	-0.2573560
H	-1.1330640	4.6569960	-0.3856180	H	0.2910890	4.2733280	-1.5275210
H	0.4643950	4.8819130	-1.1541260	O	-6.0339760	-0.4162340	0.1799810
H	-0.7775810	3.8824110	-1.9507430	C	-6.6321690	0.7840550	-0.3009240
O	-5.9776920	-0.5701860	-0.0913150	H	-7.7000680	0.6862250	-0.0999920
C	-6.5783090	0.5162730	0.6016970	H	-6.2418460	1.6643210	0.2243430
H	-7.6515920	0.4310740	0.4228750	H	-6.4746020	0.9059360	-1.3795660
H	-6.3850910	0.4621090	1.6807000	N	0.0173990	-2.5995060	-0.3656370
H	-6.2227310	1.4825470	0.2212160	H	-0.5647900	-3.3957980	-0.5825780
H	-2.2810200	-2.8464050	-1.2651820	H	-2.3839630	-2.9110710	0.9097830
Compound **6g, R = *p*-MeO** pcm MeOH **E** = -1051.12048922, **H (0K)** = -1050.763201, **H (298K)** = -1050.740960, **G (298K)** = -1050.815573 au. Imaginary frequency = 0.				Compound **7d, R = *p*-MeO** pcm MeOH **E** = -1051.10595734, **H (0K)** = -1050.748695, **H (298K)** = -1050.726386, **G (298K)** = -1050.800945 au. Imaginary frequency = 0.			
C	-1.1987330	3.2636940	-0.1311790	C	0.7542680	2.7290840	1.4320610
C	-1.6629580	2.0562650	-0.5621850	C	0.8030330	1.3785020	1.5348640

N	-0.8941270	1.0679140	0.0418480	N	0.6358610	0.8841820	0.2400090
C	0.0062250	1.6747370	0.8267530	C	0.4888350	1.8858920	-0.6946050
C	-0.9796970	-0.3293010	-0.1820030	C	0.6592590	-0.5036090	-0.0739620
C	0.1272790	-1.1956260	-0.3426040	C	-0.4614710	-1.3229570	-0.1805950
N	-0.3064270	-2.4517710	-0.5893080	C	1.3889300	-2.6081270	-0.3896650
C	-1.6605070	-2.3879600	-0.6047160	C	1.8398900	-1.3115530	-0.2010920
C	-2.1673460	-1.1018610	-0.3601600	C	-1.9004700	-1.0506030	-0.0905040
C	1.5621510	-0.8231490	-0.3707560	C	-2.7782530	-1.9952820	0.4809120
C	2.4915060	-1.3397140	0.5710080	C	-4.1441350	-1.7589000	0.5508100
C	3.8407800	-0.9903170	0.5102320	C	-4.6808110	-0.5579830	0.0602640
C	4.3004750	-0.1089610	-0.4801280	C	-3.8242730	0.3960130	-0.5042060
C	3.4090840	0.4279950	-1.4087310	C	-2.4539530	0.1424300	-0.5820480
C	2.0613940	0.0513530	-1.3381110	C	3.2524300	-0.8934930	-0.1515360
C	-3.5773520	-0.7226230	-0.2348250	C	4.2259310	-1.7417680	0.4089510
C	-4.5500230	-1.3117180	-1.0704110	C	5.5715830	-1.3760770	0.4306790
C	-5.9001490	-0.9910710	-0.9507650	C	5.9754690	-0.1461270	-0.0954130
C	-6.3265360	-0.0548320	-0.0046550	C	5.0191650	0.7093250	-0.6483130
C	-5.3805700	0.5429660	0.8303390	C	3.6738980	0.3405600	-0.6815740
C	-4.0306810	0.2095130	0.7227450	H	0.8345020	3.4997240	2.1843550
H	-1.5211570	4.2672030	-0.3611610	H	0.9348320	0.7328730	2.3896020
H	-2.4633780	1.7987350	-1.2351060	H	1.9382720	-3.5187660	-0.5777020
H	0.7467100	1.1650400	1.4198080	H	-4.8145160	-2.4885580	0.9949360
H	-2.2516240	-3.2883100	-0.7423580	H	-4.2107300	1.3291270	-0.8976670
H	4.5666700	-1.3791380	1.2138960	H	-1.8011100	0.8806660	-1.0384040
H	3.7403380	1.0988330	-2.1929170	H	3.9184330	-2.6892050	0.8437050
H	1.3692380	0.4362280	-2.0828760	H	6.3041290	-2.0489690	0.8691030
H	-4.2253810	-2.0202110	-1.8273920	H	7.0227800	0.1427800	-0.0727080
H	-6.6237890	-1.4662060	-1.6092510	H	5.3221200	1.6666210	-1.0650360
H	-7.3792330	0.2009420	0.0827630	H	2.9413700	1.0044840	-1.1307750
H	-5.6971660	1.2607580	1.5842140	N	0.5628070	3.0082590	0.0811170
H	-3.3167820	0.6494430	1.4144800	C	0.4549320	4.3574680	-0.4568540
N	-0.1452440	3.0134310	0.7268760	H	-0.4049280	4.8789860	-0.0242830
C	0.6780620	4.0115700	1.3982220	H	1.3615200	4.9322880	-0.2423730
H	1.2486340	4.5889860	0.6650810	H	0.3240440	4.2769570	-1.5361580
H	0.0464840	4.6856240	1.9828840	O	-6.0323880	-0.4174550	0.1795220
H	1.3725410	3.5036010	2.0688350	C	-6.6304730	0.7861760	-0.2960330
O	1.9760710	-2.1546470	1.5326180	H	-7.6982770	0.6876870	-0.0954170
O	5.6434190	0.1597130	-0.4374940	H	-6.2394560	1.6633110	0.2335220
C	2.8669010	-2.8081740	2.4177350	H	-6.4726680	0.9125600	-1.3739290
H	3.5931420	-3.4265050	1.8741800	N	0.0212740	-2.6005850	-0.3679990
H	3.4104050	-2.0952760	3.0544850	H	-0.5587360	-3.4005100	-0.5782710
H	2.2449190	-3.4489570	3.0455550	H	-2.3847880	-2.9192430	0.8965910
C	6.1850090	0.9928850	-1.4465900				
H	7.2561680	1.0550540	-1.2436210				
H	6.0294010	0.5698060	-2.4479640				
H	5.7526530	2.0027980	-1.4157250				

Compound **6o, R = *o,p*-(MeO)$_2$**

E = -1165.60345766, **H (0K)** = -1165.214446, **H (298K)** = -1165.189326, **G (298K)** = -1165.271132 au.

Imaginary frequency = 0.

C	-1.1987330	3.2636940	-0.1311790
C	-1.6629580	2.0562650	-0.5621850
N	-0.8941270	1.0679140	0.0418480
C	0.0062250	1.6747370	0.8267530
C	-0.9796970	-0.3293010	-0.1820030
C	0.1272790	-1.1956260	-0.3426040
N	-0.3064270	-2.4517710	-0.5893080
C	-1.6605070	-2.3879600	-0.6047160

Compound **7e, R = *o,p*-(MeO)$_2$**

E = -1165.61313335, **H (0K)** = -1165.222972, **H (298K)** = -1165.198098, **G (298K)** = -1165.278165 au.

Imaginary frequency = 0.

C	1.3741400	2.7485110	1.6334330
C	1.2725760	1.3980220	1.6138030
N	0.9911860	1.0468950	0.2927410
C	0.9182160	2.1387010	-0.5435260
C	0.8629620	-0.3056370	-0.1319660
C	-0.3316690	-1.0041630	-0.3119590
C	1.3943580	-2.4382900	-0.6024070
C	1.9614810	-1.2072590	-0.3185720

C	-2.1673460	-1.1018610	-0.3601600	C	-1.7355830	-0.5756130	-0.2648980
C	1.5621510	-0.8231490	-0.3707560	C	-2.7924440	-1.4462650	0.1167470
C	2.4915060	-1.3397140	0.5710080	C	-4.1084650	-1.0003560	0.1691890
C	3.8407800	-0.9903170	0.5102320	C	-4.4198340	0.3263520	-0.1635000
C	4.3004750	-0.1089610	-0.4801280	C	-3.4063310	1.1978210	-0.5626640
C	3.4090840	0.4279950	-1.4087310	C	-2.0909020	0.7332390	-0.6169470
C	2.0613940	0.0513530	-1.3381110	C	3.4054000	-0.9219380	-0.2473180
C	-3.5773520	-0.7226230	-0.2348250	C	4.2920290	-1.8699270	0.2939290
C	-4.5500230	-1.3117180	-1.0704110	C	5.6646140	-1.6302100	0.3326230
C	-5.9001490	-0.9910710	-0.9507650	C	6.1813860	-0.4293440	-0.1575300
C	-6.3265360	-0.0548320	-0.0046550	C	5.3113680	0.5240430	-0.6907260
C	-5.3805700	0.5429660	0.8303390	C	3.9391460	0.2823400	-0.7407180
C	-4.0306810	0.2095130	0.7227450	H	1.5792810	3.4301260	2.4458970
H	-1.5211570	4.2672030	-0.3611610	H	1.3732450	0.6633160	2.3977150
H	-2.4633780	1.7987350	-1.2351060	H	1.8637160	-3.3811660	-0.8422920
H	0.7467100	1.1650400	1.4198080	H	-4.9233490	-1.6511610	0.4595180
H	-2.2516240	-3.2883100	-0.7423580	H	-3.6184700	2.2217410	-0.8465670
H	4.5666700	-1.3791380	1.2138960	H	-1.3072640	1.4058900	-0.9530530
H	3.7403380	1.0988330	-2.1929170	H	3.8932630	-2.7951840	0.7022580
H	1.3692380	0.4362280	-2.0828760	H	6.3302100	-2.3785570	0.7559990
H	-4.2253810	-2.0202110	-1.8273920	H	7.2508040	-0.2380050	-0.1226580
H	-6.6237890	-1.4662060	-1.6092510	H	5.7039250	1.4601680	-1.0803710
H	-7.3792330	0.2009420	0.0827630	H	3.2710610	1.0204520	-1.1743370
H	-5.6971660	1.2607580	1.5842140	N	1.1540530	3.1696570	0.3232740
H	-3.3167820	0.6494430	1.4144800	C	1.1753780	4.5584650	-0.1008550
N	-0.1452440	3.0134310	0.7268760	H	0.4029640	5.1386260	0.4172860
C	0.6780620	4.0115700	1.3982220	H	2.1519720	5.0137250	0.0996900
H	1.2486340	4.5889860	0.6650810	H	0.9821210	4.5746550	-1.1738610
H	0.0464840	4.6856240	1.9828840	O	-2.4423140	-2.7420590	0.4189380
H	1.3725410	3.5036010	2.0688350	O	-5.7439880	0.6489100	-0.0729620
O	1.9760710	-2.1546470	1.5326180	C	-3.4470350	-3.6255740	0.8953990
O	5.6434190	0.1597130	-0.4374940	H	-3.9149190	-3.2403060	1.8096260
C	2.8669010	-2.8081740	2.4177350	H	-4.2222040	-3.8016330	0.1386030
H	3.5931420	-3.4265050	1.8741800	H	-2.9376640	-4.5653790	1.1174010
H	3.4104050	-2.0952760	3.0544850	C	-6.1308500	1.9726420	-0.4059360
H	2.2449190	-3.4489570	3.0455550	H	-7.2121110	2.0140380	-0.2610340
C	6.1850090	0.9928850	-1.4465900	H	-5.6483450	2.7107530	0.2481720
H	7.2561680	1.0550540	-1.2436210	H	-5.8954500	2.2112250	-1.4514780
H	6.0294010	0.5698060	-2.4479640	N	0.0359610	-2.2996700	-0.6042450
H	5.7526530	2.0027980	-1.4157250	H	-0.6404160	-3.0396620	-0.7103050

Compound **6o, R = *o,p*-(MeO)$_2$**

pcm CH_2Cl_2

E = -1165.63369080, **H (0K)** = -1165.244134, **H (298K)** = -1165.219152, **G (298K)** = -1165.299952 au.

Imaginary frequency = 0.

C	-1.0985510	3.2510610	-0.2899100
C	-1.4772220	2.0404300	-0.7882250
N	-0.8860140	1.0626150	-0.0005870
C	-0.1680010	1.6763190	0.9491580
C	-0.9619630	-0.3501430	-0.1947990
C	0.1444940	-1.2099350	-0.3370070
N	-0.2889190	-2.4850870	-0.5455240
C	-1.6432290	-2.4237080	-0.5534960
C	-2.1482790	-1.1286290	-0.3381200
C	1.5764640	-0.8277240	-0.3665780
C	2.5313160	-1.3763170	0.5318760
C	3.8745770	-1.0068890	0.4607030
C	4.3046370	-0.0687340	-0.4915060
C	3.3873380	0.5031510	-1.3736420

Compound **7e, R = *o,p*-(MeO)$_2$**

pcm CH_2Cl_2

E = -1165.62739039, **H (0K)** = -1165.237321, **H (298K)** = -1165.212406, **G (298K)** = -1165.292908 au.

Imaginary frequency = 0.

C	1.2176180	2.7866890	1.6128660
C	1.0993770	1.4365570	1.6104540
N	0.9775610	1.0588190	0.2723410
C	1.0216440	2.1341290	-0.5873010
C	0.8666700	-0.2991140	-0.1421370
C	-0.3260180	-1.0048930	-0.3160590
C	1.4044550	-2.4333130	-0.6023230
C	1.9695710	-1.1986720	-0.3222500
C	-1.7307880	-0.5771150	-0.2627660
C	-2.7859460	-1.4550580	0.1130250
C	-4.1031630	-1.0094740	0.1680990
C	-4.4174440	0.3206130	-0.1516040
C	-3.4047030	1.2001270	-0.5401910
C	-2.0891920	0.7359500	-0.5970510

C	2.0469190	0.1055220	-1.2949950	C	3.4144640	-0.9205930	-0.2334590
C	-3.5586620	-0.7418110	-0.2300210	C	4.2916030	-1.8897700	0.2892390
C	-4.5438680	-1.4216860	-0.9788410	C	5.6656640	-1.6598680	0.3486880
C	-5.8944900	-1.0964570	-0.8690590	C	6.1962050	-0.4479110	-0.1007170
C	-6.3094260	-0.0665500	-0.0191030	C	5.3370310	0.5262270	-0.6151190
C	-5.3505530	0.6225990	0.7273930	C	3.9631300	0.2937850	-0.6865630
C	-3.9999460	0.2869520	0.6296010	H	1.3306620	3.4858880	2.4281670
H	-1.3363630	4.2541590	-0.6069630	H	1.0883160	0.7203110	2.4176770
H	-2.1051590	1.7794340	-1.6237470	H	1.8726990	-3.3795180	-0.8306440
H	0.4029060	1.1753440	1.7133660	H	-4.9136180	-1.6677280	0.4543110
H	-2.2362820	-3.3269330	-0.6705320	H	-3.6189900	2.2267600	-0.8113550
H	4.6161810	-1.4188080	1.1340900	H	-1.3089280	1.4153760	-0.9242920
H	3.6916490	1.2256660	-2.1214770	H	3.8856660	-2.8250490	0.6658430
H	1.3362800	0.5302090	-1.9993720	H	6.3214660	-2.4248610	0.7568090
H	-4.2334210	-2.2059610	-1.6640540	H	7.2661060	-0.2644900	-0.0487300
H	-6.6264600	-1.6420930	-1.4600770	H	5.7388830	1.4711120	-0.9726440
H	-7.3616420	0.1932450	0.0602010	H	3.3053840	1.0501850	-1.1042870
H	-5.6559520	1.4192750	1.4019860	N	1.1661610	3.1817020	0.2781480
H	-3.2785310	0.8117300	1.2494960	C	1.2579300	4.5675100	-0.1584620
N	-0.2731020	3.0047370	0.7915320	H	0.4371270	5.1600760	0.2586730
C	0.3828450	4.0193630	1.6178830	H	2.2087720	5.0099230	0.1559760
H	1.1203380	4.5606190	1.0212690	H	1.1958520	4.5786730	-1.2468150
H	-0.3662580	4.7151510	2.0000370	O	-2.4309500	-2.7449090	0.4081700
H	0.8794330	3.5262670	2.4533070	O	-5.7397870	0.6419200	-0.0592370
O	2.0517250	-2.2500310	1.4635280	C	-3.4422280	-3.6603210	0.8250000
O	5.6430170	0.2140030	-0.4630610	H	-3.9341180	-3.3151620	1.7414740
C	2.9678590	-2.8439130	2.3742360	H	-4.1927680	-3.8096650	0.0401090
H	3.7301640	-3.4341920	1.8507130	H	-2.9264430	-4.6014180	1.0200500
H	3.4631900	-2.0903580	3.0001170	C	-6.1302750	1.9748560	-0.3775740
H	2.3720770	-3.5037780	3.0071550	H	-7.2110020	2.0113700	-0.2325140
C	6.1491140	1.1415820	-1.4161810	H	-5.6484280	2.7021910	0.2869250
H	7.2204220	1.2163530	-1.2221430	H	-5.8938590	2.2229090	-1.4194170
H	5.9889790	0.7895960	-2.4428500	N	0.0465840	-2.3002420	-0.6008730
H	5.6885290	2.1305390	-1.2983960	H	-0.6226560	-3.0469770	-0.7168670

Compound **6o, R = *o,p*-(MeO)$_2$**
pcm MeOH
E = -1165.63891303, **H (0K)** = -1165.249283, **H (298K)** = -1165.224295, **G (298K)** = -1165.305301 au.
Imaginary frequency = 0.

C	-1.0985510	3.2510610	-0.2899100
C	-1.4772220	2.0404300	-0.7882250
N	-0.8860140	1.0626150	-0.0005870
C	-0.1680010	1.6763190	0.9491580
C	-0.9619630	-0.3501430	-0.1947990
C	0.1444940	-1.2099350	-0.3370070
N	-0.2889190	-2.4850870	-0.5455240
C	-1.6432290	-2.4237080	-0.5534960
C	-2.1482790	-1.1286290	-0.3381200
C	1.5764640	-0.8277240	-0.3665780
C	2.5313160	-1.3763170	0.5318760
C	3.8745770	-1.0068890	0.4607030
C	4.3046370	-0.0687340	-0.4915060
C	3.3873380	0.5031510	-1.3736420
C	2.0469190	0.1055220	-1.2949950
C	-3.5586620	-0.7418110	-0.2300210
C	-4.5438680	-1.4216860	-0.9788410
C	-5.8944900	-1.0964570	-0.8690590
C	-6.3094260	-0.0665500	-0.0191030
C	-5.3505530	0.6225990	0.7273930

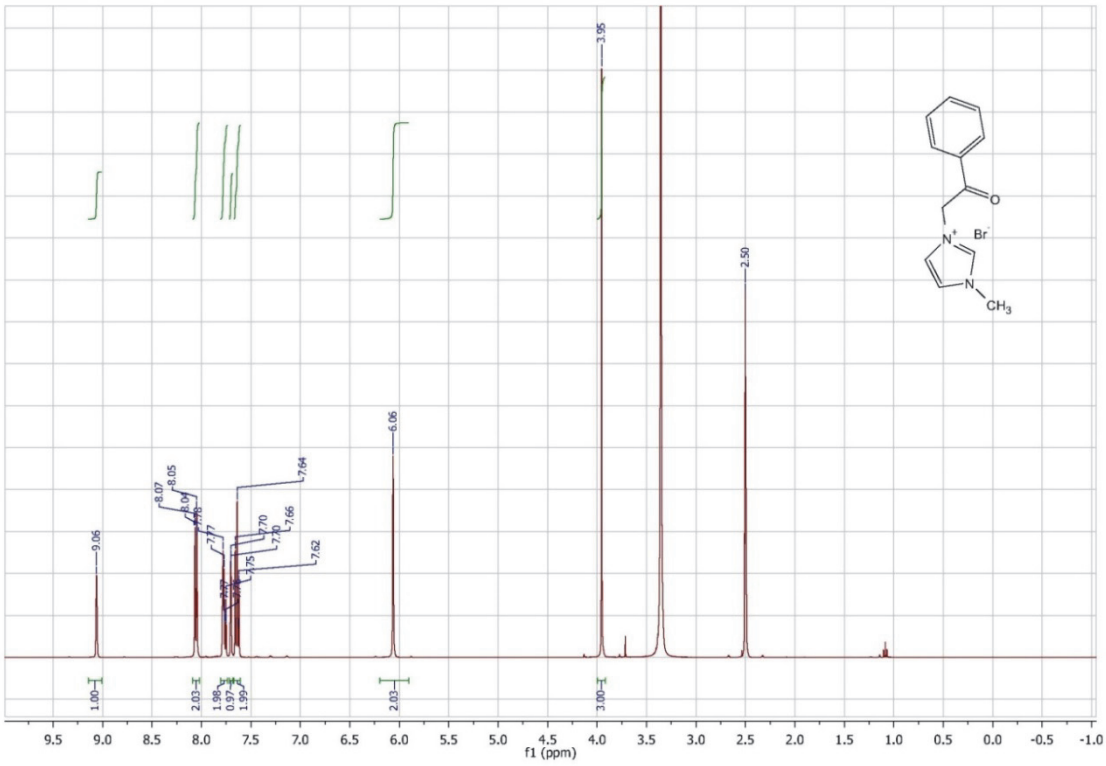
Compound **6e, R = *o,p*-(MeO)$_2$**
pcm MeOH
E = -1165.62994871, **H (0K)** = -1165.239930, **H (298K)** = -1165.214984, **G (298K)** = -1165.295749 au.
Imaginary frequency = 0.

C	1.1978220	2.7997600	1.6005070
C	1.0809270	1.4493420	1.6053860
N	0.9776630	1.0628120	0.2681330
C	1.0316520	2.1331180	-0.5972310
C	0.8685380	-0.2972010	-0.1404840
C	-0.3242800	-1.0042990	-0.3119630
C	1.4068190	-2.4328780	-0.5942030
C	1.9719340	-1.1971200	-0.3176320
C	-1.7295150	-0.5771840	-0.2581870
C	-2.7853560	-1.4584950	0.1093180
C	-4.1029160	-1.0134170	0.1646190
C	-4.4173580	0.3189170	-0.1458510
C	-3.4040330	1.2020030	-0.5256630
C	-2.0883430	0.7384370	-0.5827890
C	3.4172290	-0.9205800	-0.2276160
C	4.2926080	-1.8919100	0.2947320
C	5.6670520	-1.6641710	0.3558230
C	6.2002600	-0.4524150	-0.0915180
C	5.3431670	0.5237940	-0.6056810
C	3.9688100	0.2933810	-0.6788220

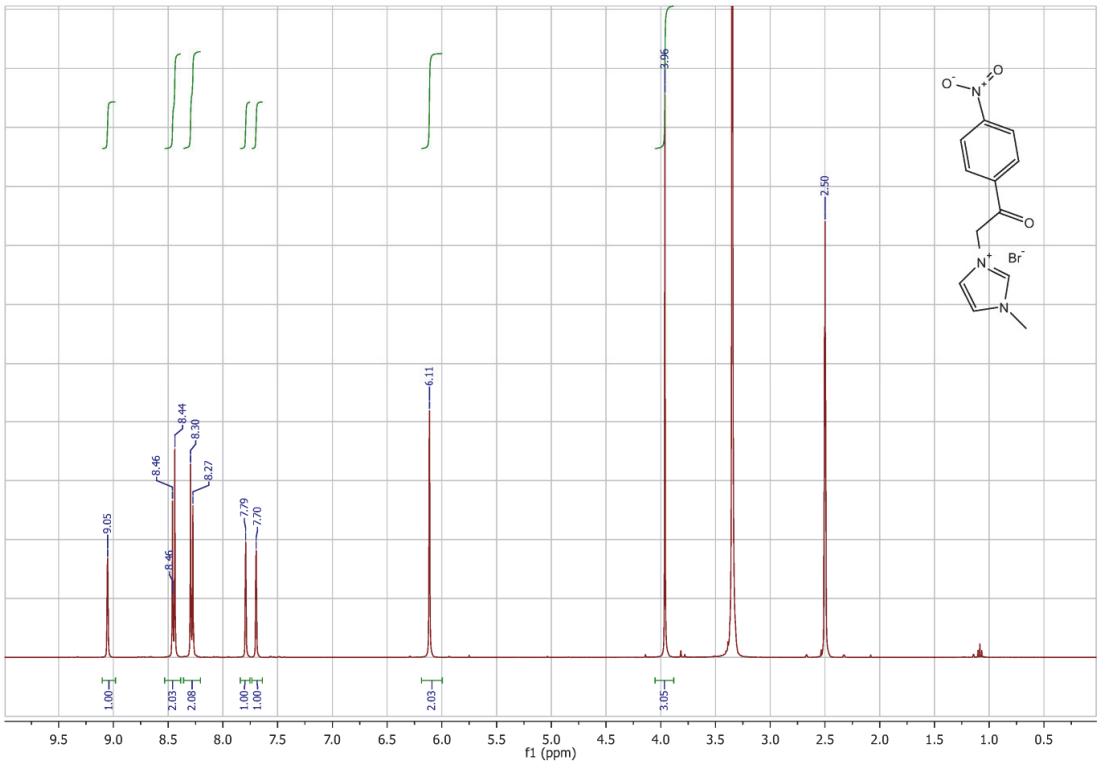
C	-3.9999460	0.2869520	0.6296010	H	1.2987220	3.5047340	2.4123550
H	-1.3363630	4.2541590	-0.6069630	H	1.0591010	0.7385920	2.4172740
H	-2.1051590	1.7794340	-1.6237470	H	1.8746940	-3.3803980	-0.8176720
H	0.4029060	1.1753440	1.7133660	H	-4.9131470	-1.6745660	0.4447620
H	-2.2362820	-3.3269330	-0.6705320	H	-3.6180800	2.2306470	-0.7892060
H	4.6161810	-1.4188080	1.1340900	H	-1.3083270	1.4212150	-0.9032580
H	3.6916490	1.2256660	-2.1214770	H	3.8853070	-2.8272720	0.6694520
H	1.3362800	0.5302090	-1.9993720	H	6.3210610	-2.4307750	0.7636180
H	-4.2334210	-2.2059610	-1.6640540	H	7.2703310	-0.2707880	-0.0380540
H	-6.6264600	-1.6420930	-1.4600770	H	5.7468850	1.4685300	-0.9614190
H	-7.3616420	0.1932450	0.0602010	H	3.3131350	1.0519230	-1.0959800
H	-5.6559520	1.4192750	1.4019860	N	1.1638980	3.1863180	0.2629650
H	-3.2785310	0.8117300	1.2494960	C	1.2596190	4.5705680	-0.1796190
N	-0.2731020	3.0047370	0.7915320	H	0.4361270	5.1646430	0.2293400
C	0.3828450	4.0193630	1.6178830	H	2.2081280	5.0136940	0.1401610
H	1.1203380	4.5606190	1.0212690	H	1.2053670	4.5777320	-1.2684130
H	-0.3662580	4.7151510	2.0000370	O	-2.4306840	-2.7492030	0.3968490
H	0.8794330	3.5262670	2.4533070	O	-5.7395680	0.6390720	-0.0539150
O	2.0517250	-2.2500310	1.4635280	C	-3.4441960	-3.6730540	0.7923560
O	5.6430170	0.2140030	-0.4630610	H	-3.9437590	-3.3419500	1.7096860
C	2.9678590	-2.8439130	2.3742360	H	-4.1874670	-3.8116430	-0.0010710
H	3.7301640	-3.4341920	1.8507130	H	-2.9277240	-4.6156000	0.9774090
H	3.4631900	-2.0903580	3.0001170	C	-6.1305640	1.9752310	-0.3622560
H	2.3720770	-3.5037780	3.0071550	H	-7.2114520	2.0096700	-0.2186600
C	6.1491140	1.1415820	-1.4161810	H	-5.6500870	2.6968990	0.3090530
H	7.2204220	1.2163530	-1.2221430	H	-5.8924150	2.2313410	-1.4015590
H	5.9889790	0.7895960	-2.4428500	N	0.0492250	-2.3003070	-0.5928930
H	5.6885290	2.1305390	-1.2983960	H	-0.6191420	-3.0483120	-0.7080810

^{1}H (400 MHz) and ^{13}C (100 MHz) NMR spectra

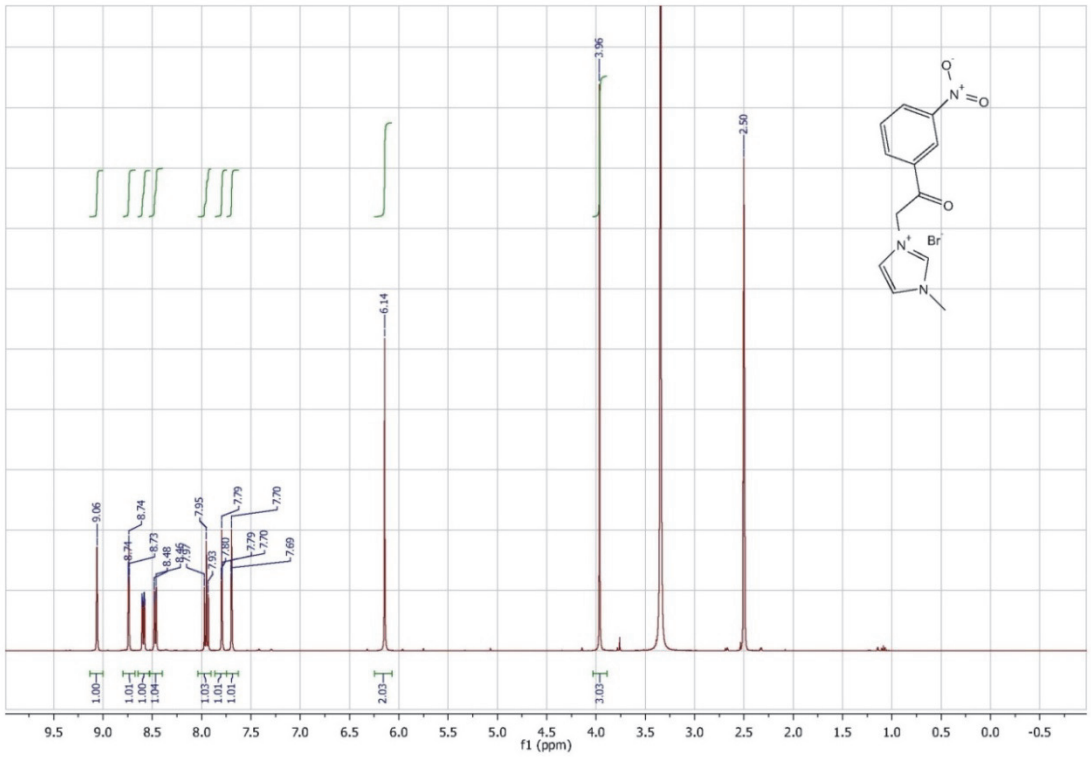
^{1}H NMR spectrum of 1-methyl-3-(2-oxo-2-phenylethyl)-1*H*-imidazol-3-ium bromide (1a), DMSO-d_6



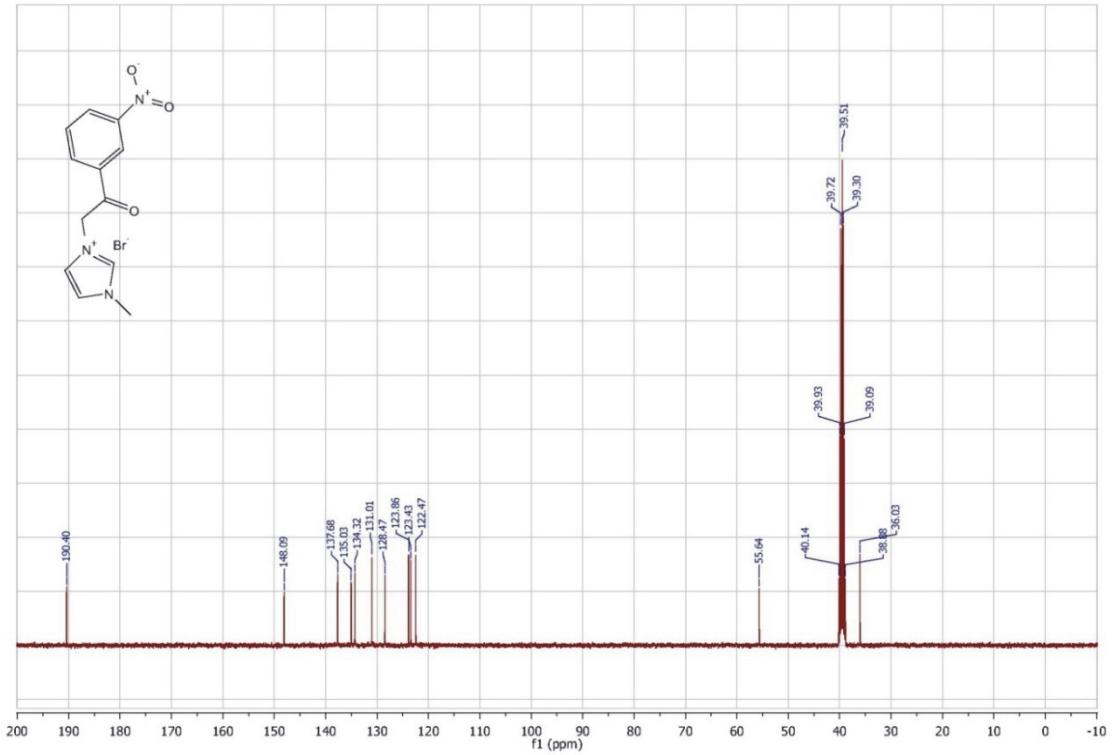
^{1}H NMR spectrum of 1-methyl-3-(2-(4-nitrophenyl)-2-oxoethyl)-1*H*-imidazol-3-ium bromide (1b), DMSO-d_6



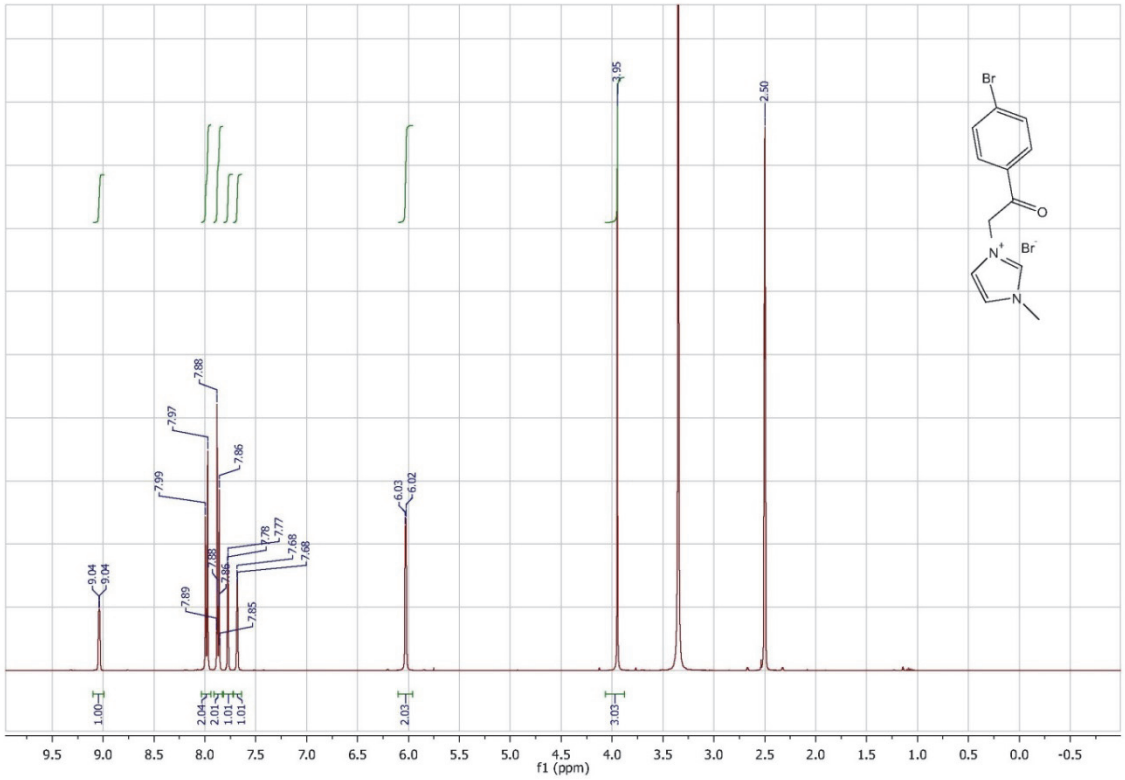
^{1}H NMR spectrum of 1-methyl-3-(2-(3-nitrophenyl)-2-oxoethyl)-1*H*-imidazol-3-ium bromide (1c), DMSO-d_6



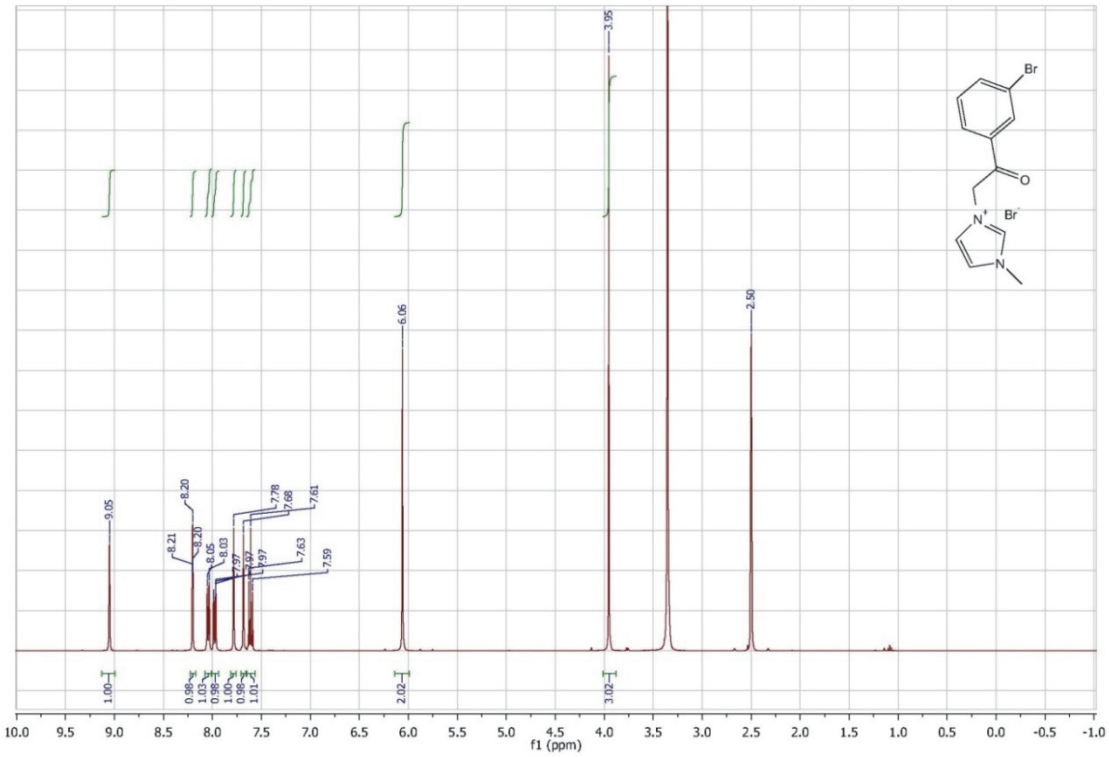
^{13}C NMR spectrum of 1-methyl-3-(2-(3-nitrophenyl)-2-oxoethyl)-1*H*-imidazol-3-ium bromide (1c), DMSO-d_6



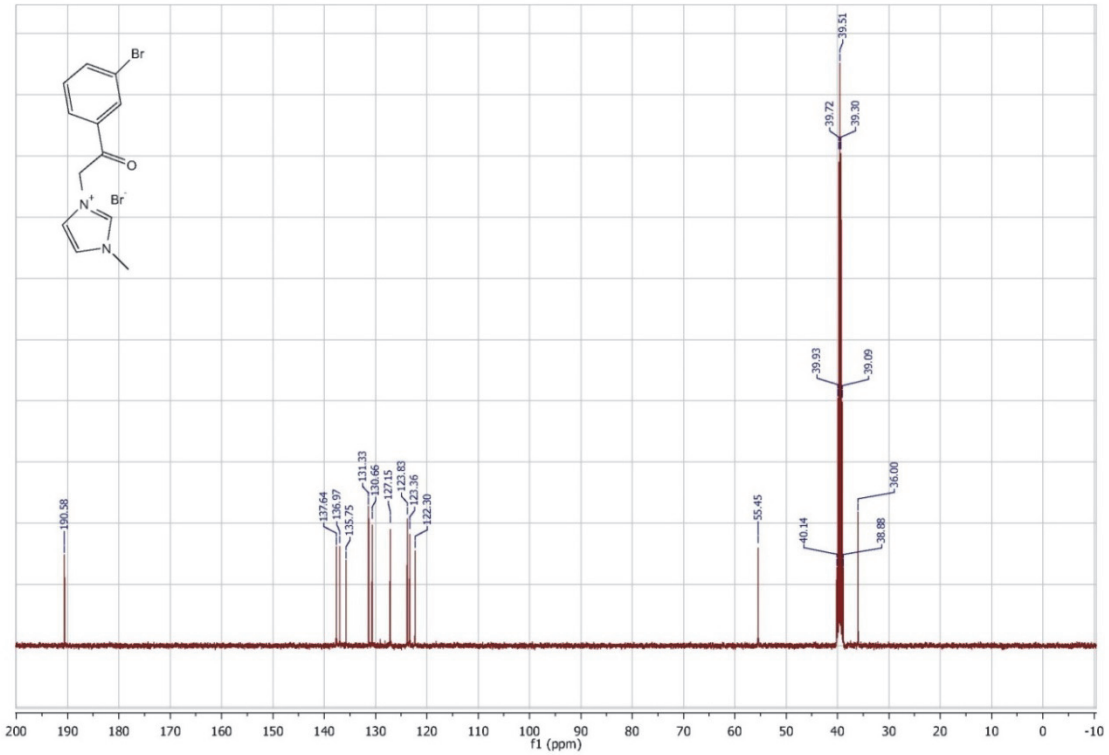
^{1}H NMR spectrum of 3-(2-(4-bromophenyl)-2-oxoethyl)-1-methyl-1*H*-imidazol-3-ium bromide (1d), DMSO-d_6



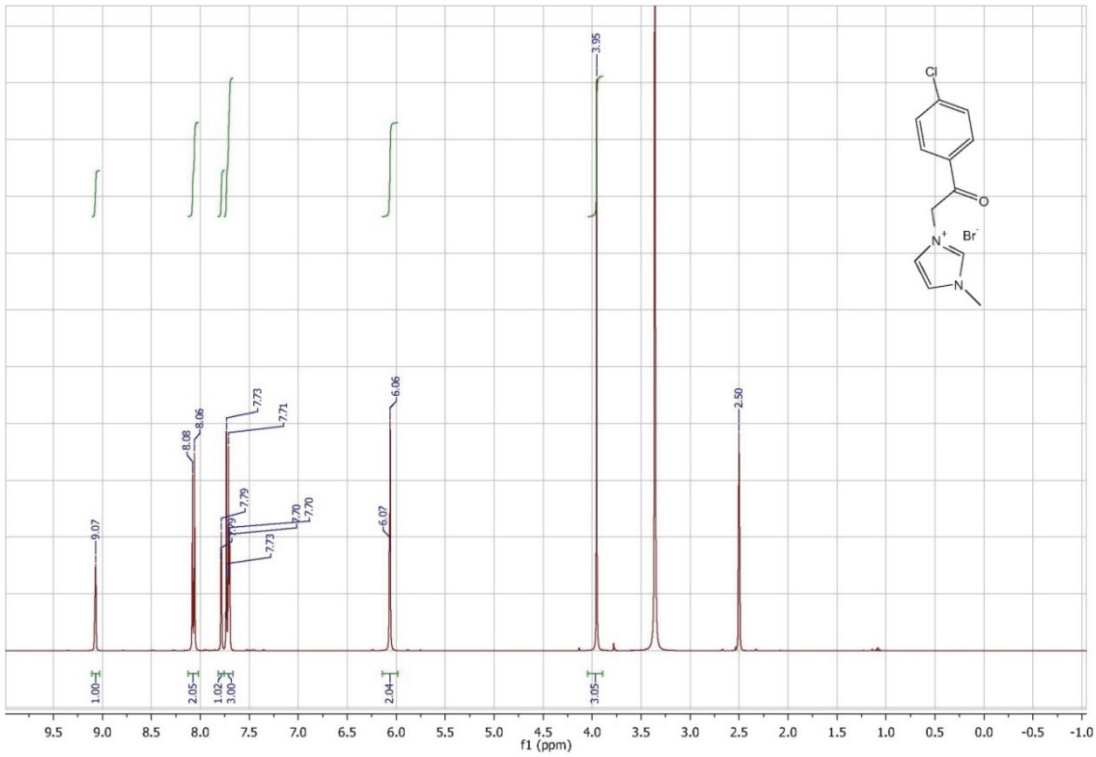
^{1}H NMR spectrum of 3-(2-(3-bromophenyl)-2-oxoethyl)-1-methyl-1*H*-imidazol-3-ium bromide (1e), DMSO-d_6



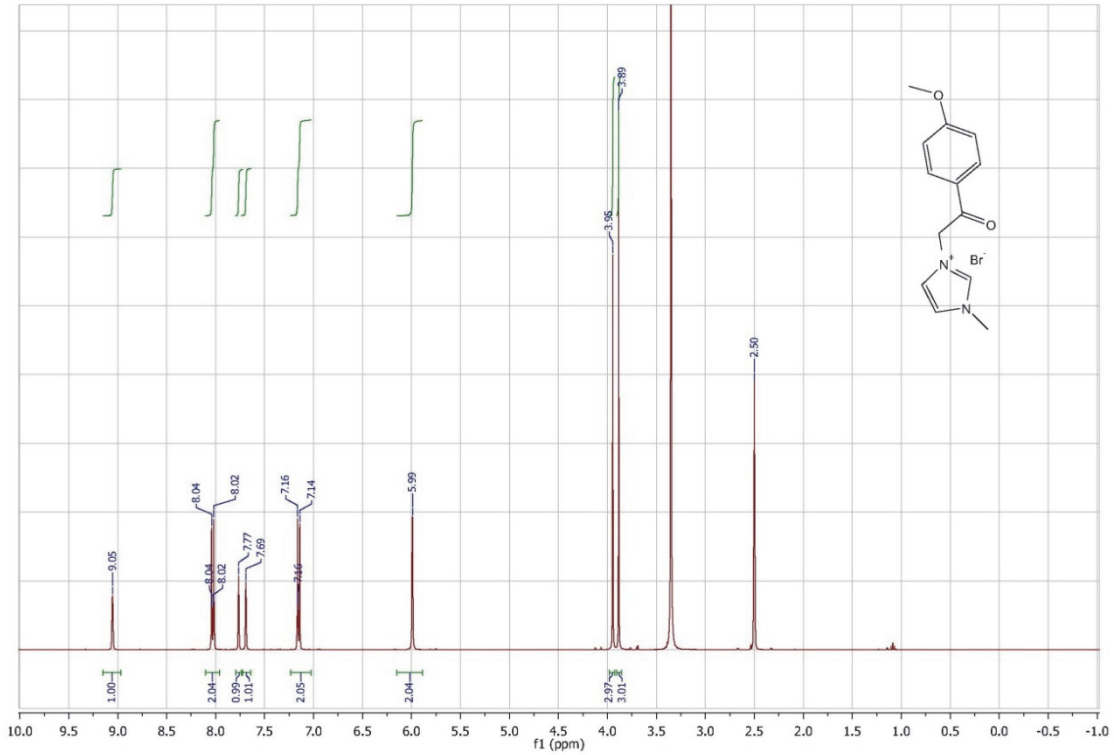
^{13}C NMR spectrum of 3-(2-(3-bromophenyl)-2-oxoethyl)-1-methyl-1*H*-imidazol-3-ium bromide (1e), DMSO-d_6



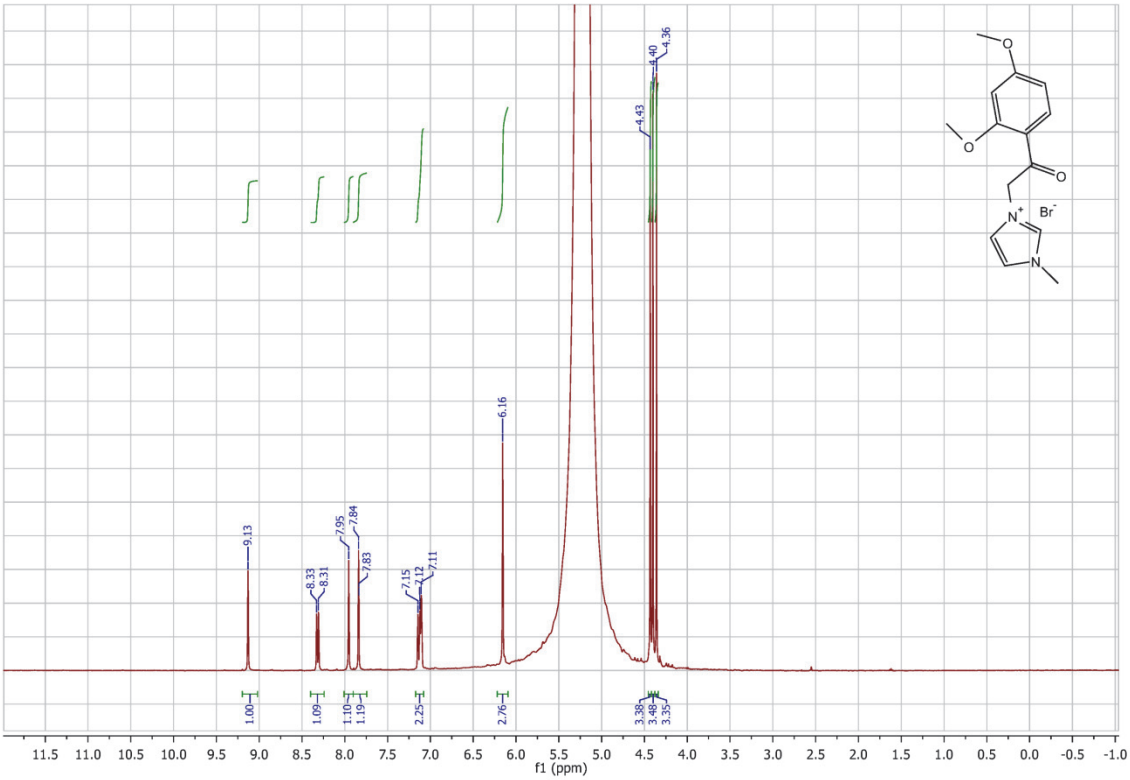
^{1}H NMR spectrum of 3-(2-(4-chlorophenyl)-2-oxoethyl)-1-methyl-1*H*-imidazol-3-ium bromide (1f), DMSO-d_6



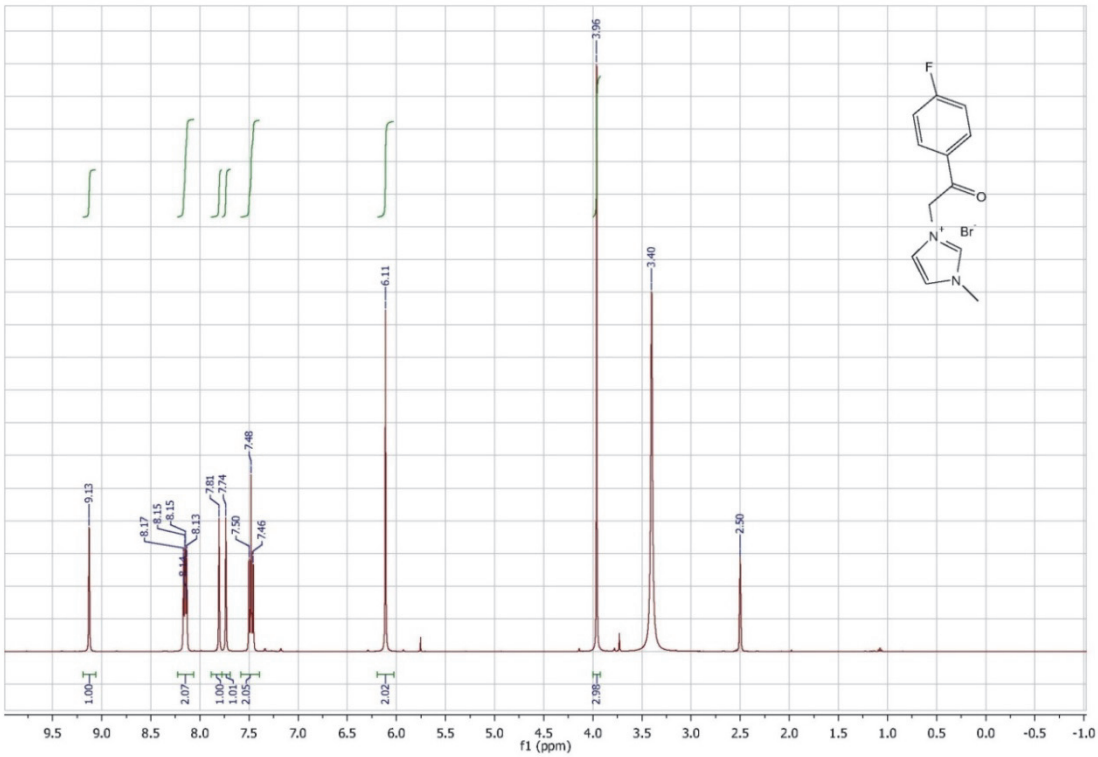
^{1}H NMR spectrum of 3-(2-(4-methoxyphenyl)-2-oxoethyl)-1-methyl-1*H*-imidazol-3-ium bromide (1g), DMSO-d_6



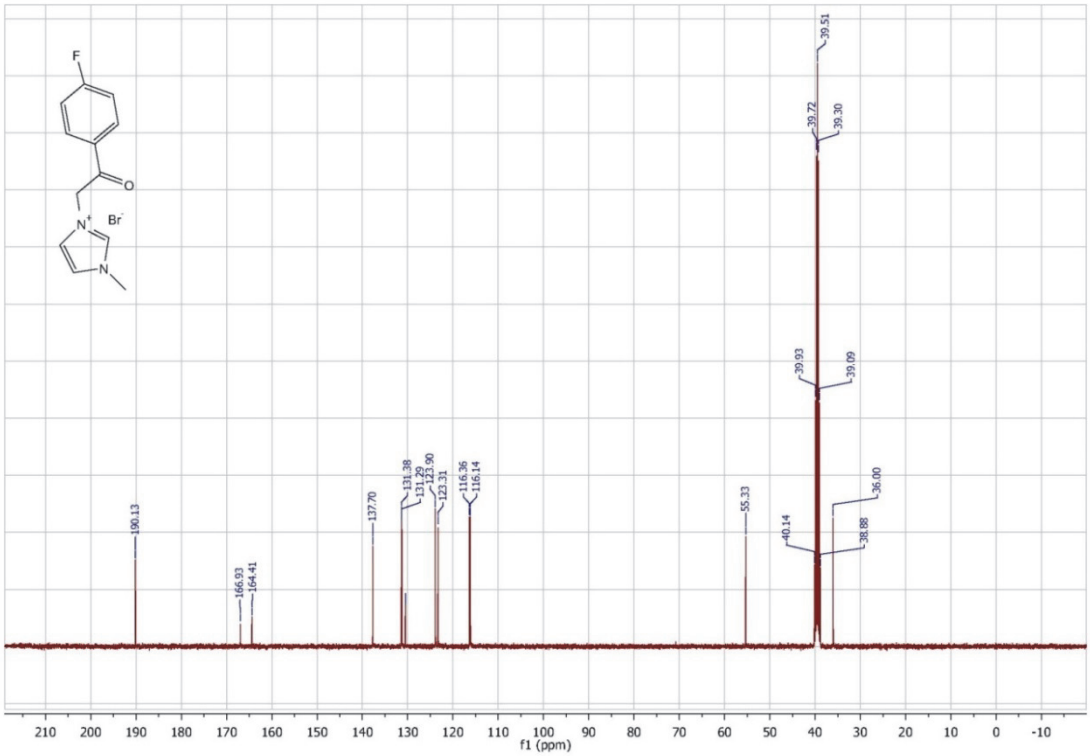
^{1}H NMR spectrum of 3-(2-(2,4-dimethoxyphenyl)-2-oxoethyl)-1-methyl-1*H*-imidazol-3-ium bromide (1h), D_2O



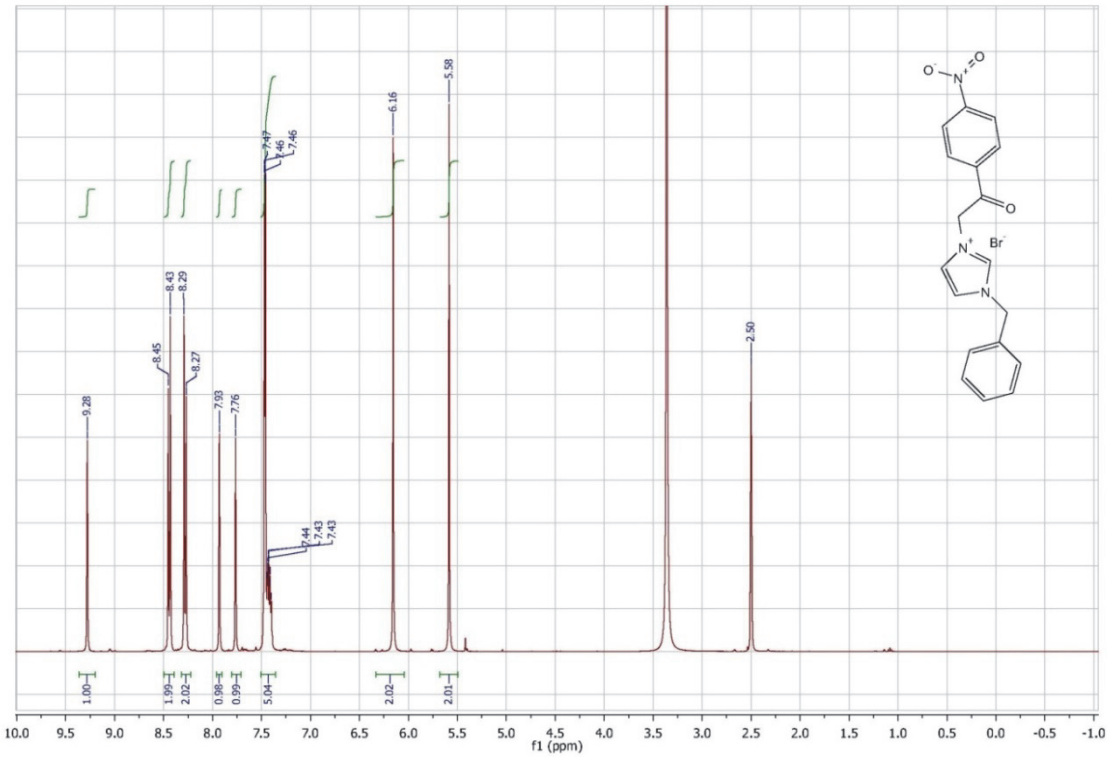
^{1}H NMR spectrum of 3-(2-(4-fluorophenyl)-2-oxoethyl)-1-methyl-1*H*-imidazol-3-ium bromide (1i), DMSO-d_6



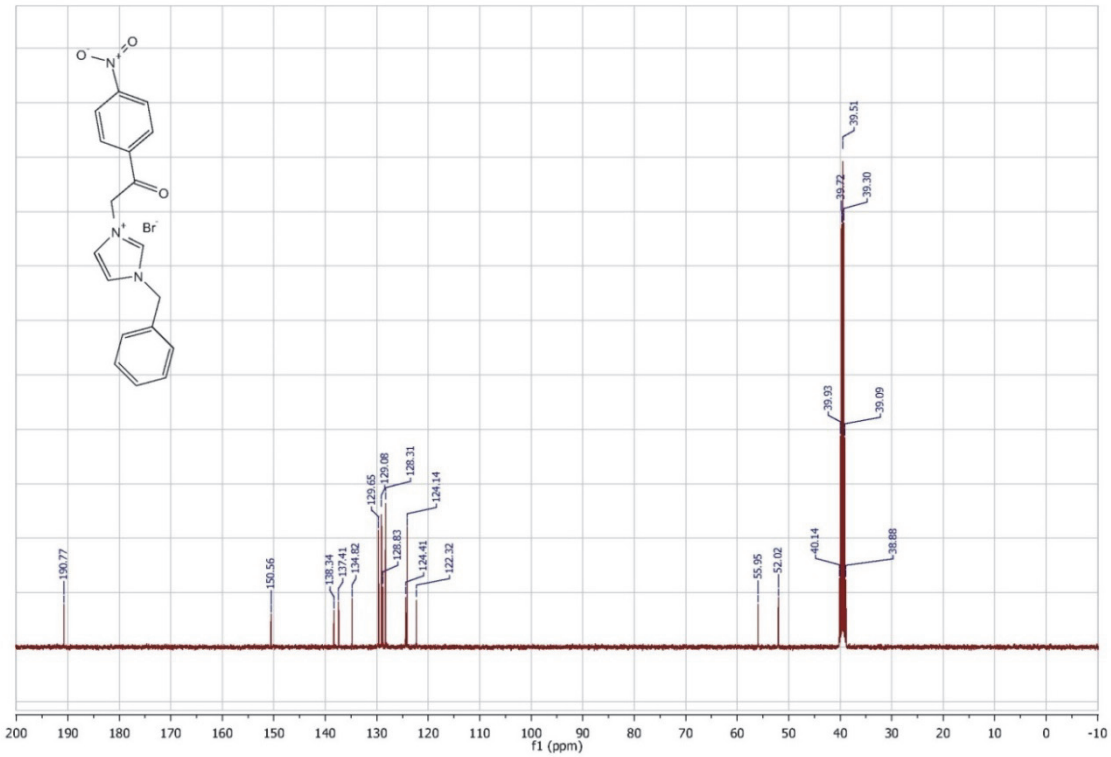
^{13}C NMR spectrum of 3-(2-(4-fluorophenyl)-2-oxoethyl)-1-methyl-1*H*-imidazol-3-ium bromide (1i), DMSO-d_6



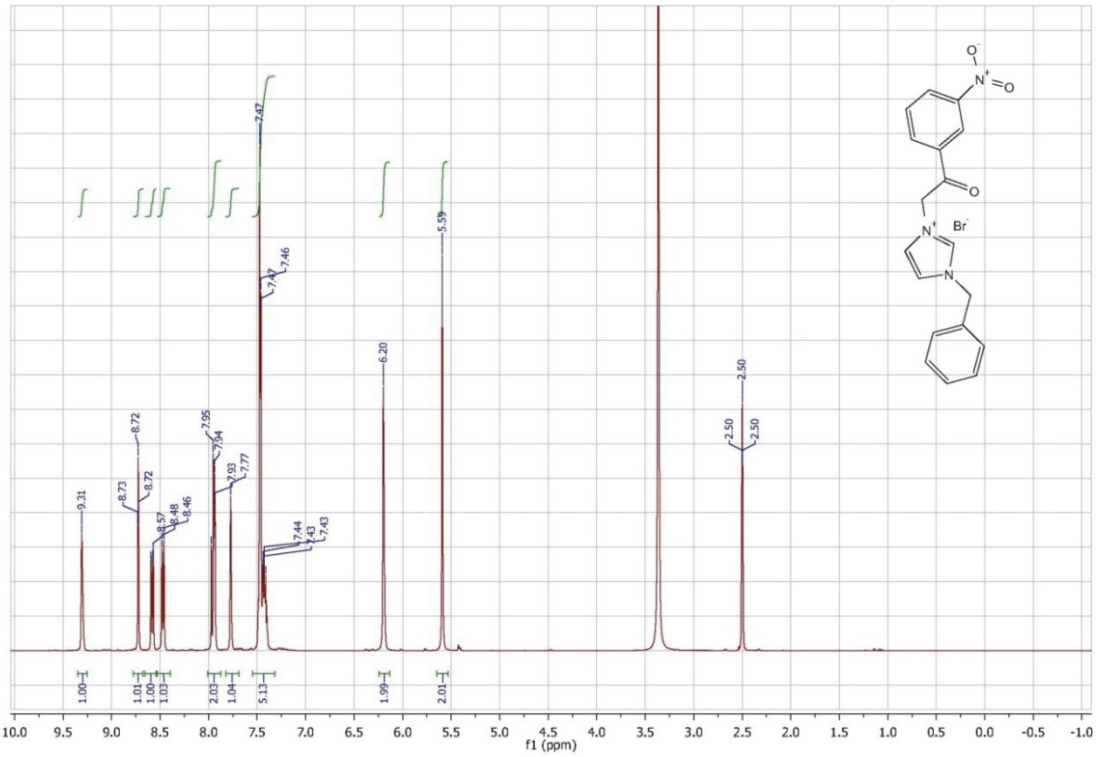
^{1}H NMR spectrum of 1-benzyl-3-(2-(4-nitrophenyl)-2-oxoethyl)-1*H*-imidazol-3-ium bromide (1k), DMSO-d_6



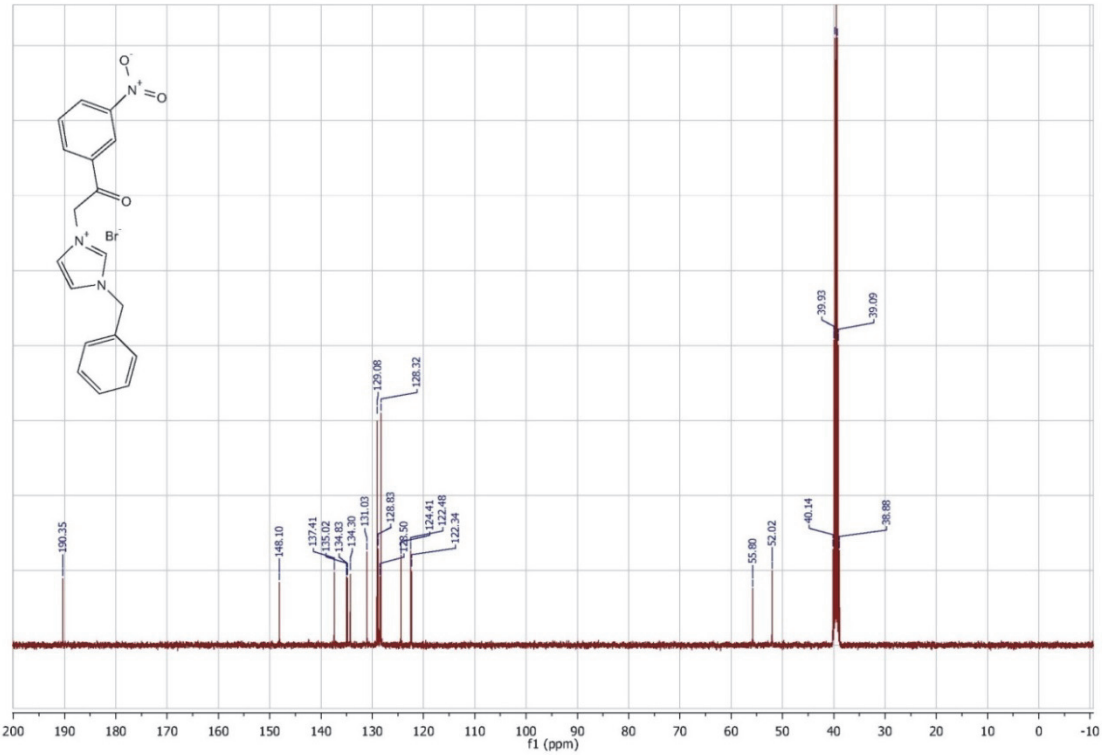
^{13}C NMR spectrum of 1-benzyl-3-(2-(4-nitrophenyl)-2-oxoethyl)-1*H*-imidazol-3-ium bromide (1k), DMSO-d_6



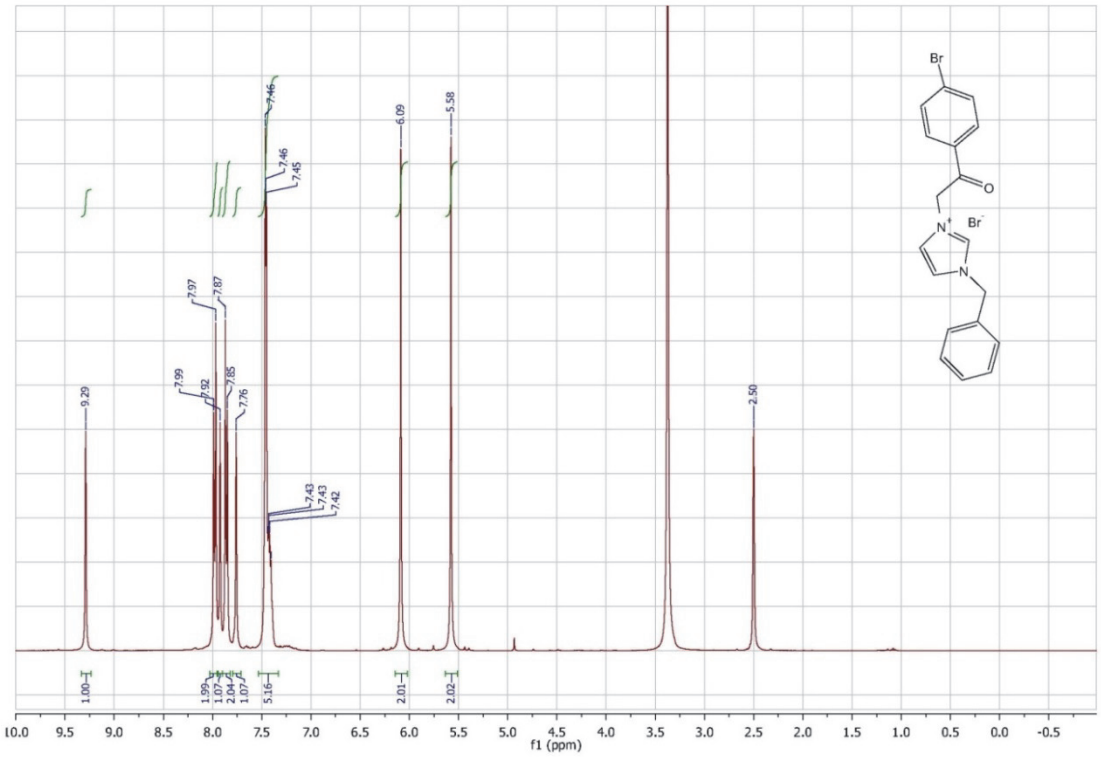
^{1}H NMR spectrum of 1-benzyl-3-(2-(3-nitrophenyl)-2-oxoethyl)-1*H*-imidazol-3-ium bromide (1l), DMSO-d_6



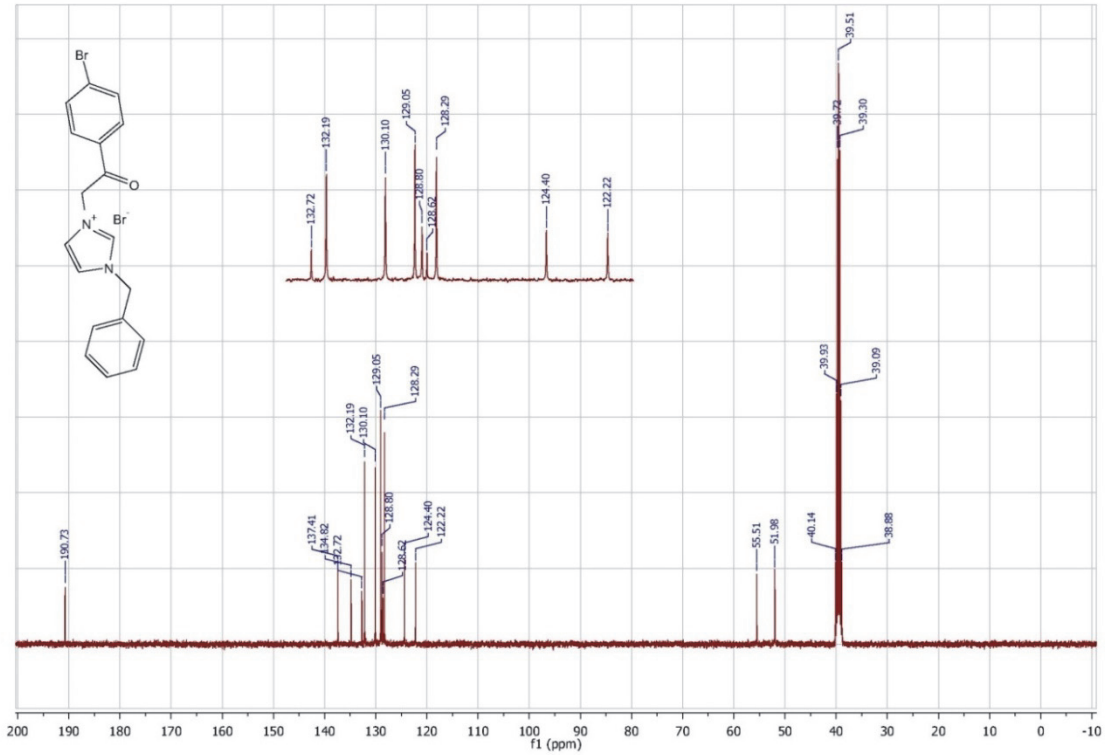
^{13}C NMR spectrum of 1-benzyl-3-(2-(3-nitrophenyl)-2-oxoethyl)-1*H*-imidazol-3-ium bromide (1l), DMSO-d_6



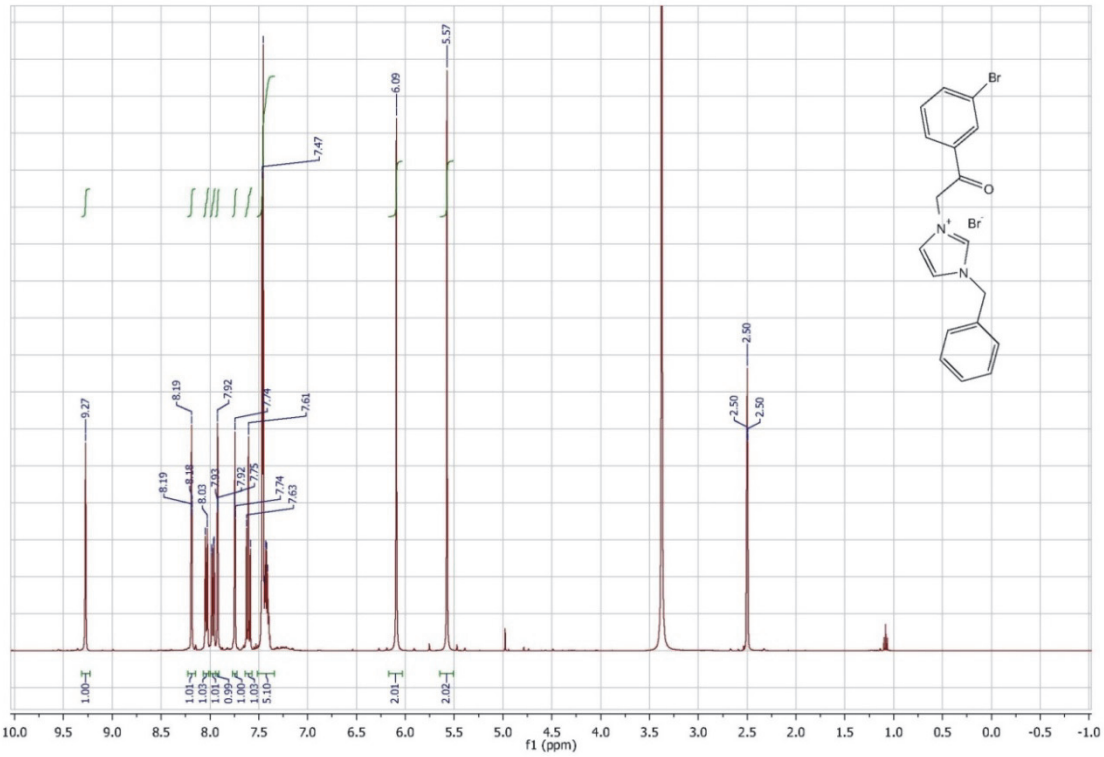
^{1}H NMR spectrum of 1-benzyl-3-(2-(4-bromophenyl)-2-oxoethyl)-1*H*-imidazol-3-ium bromide (1m), DMSO-d_6



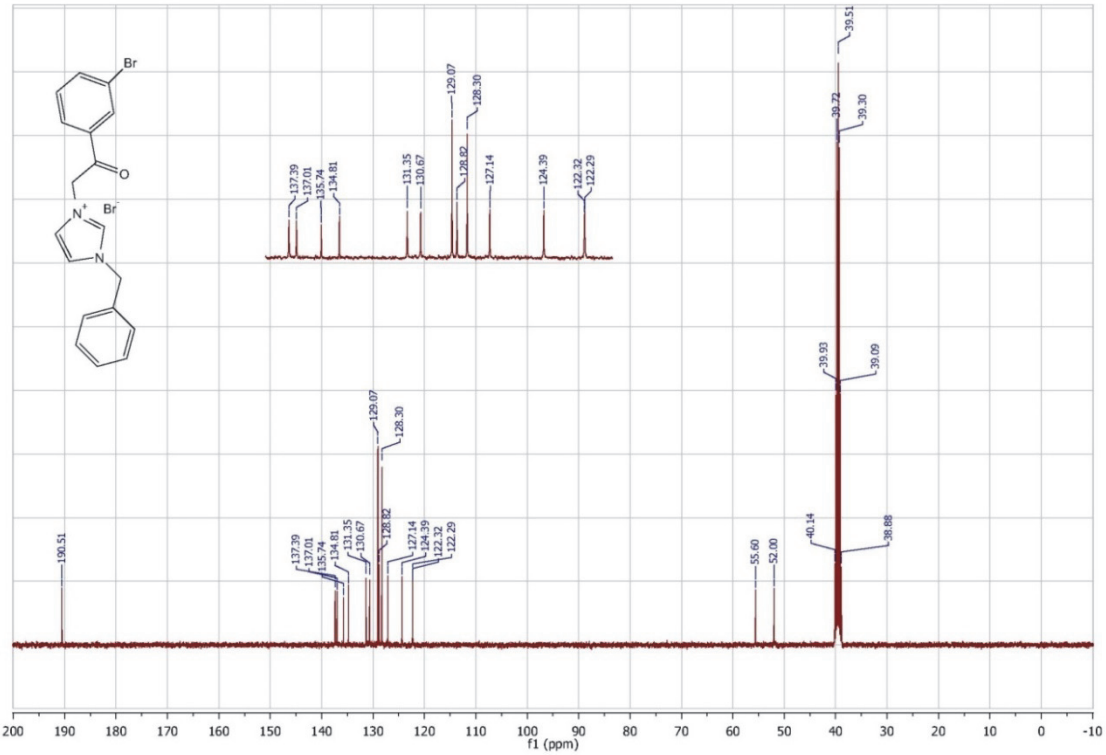
^{13}C NMR spectrum of 1-benzyl-3-(2-(4-bromophenyl)-2-oxoethyl)-1*H*-imidazol-3-ium bromide (1m), DMSO-d_6



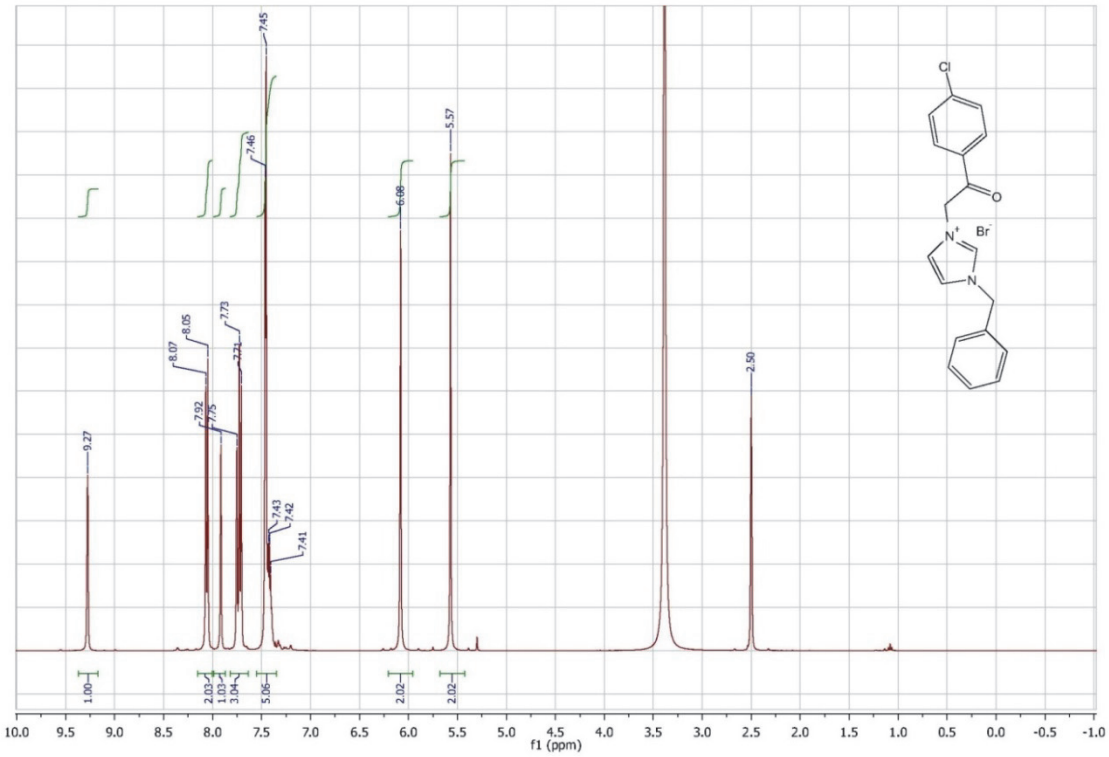
^{1}H NMR spectrum of 1-benzyl-3-(2-(3-bromophenyl)-2-oxoethyl)-1*H*-imidazol-3-ium bromide (1n), DMSO-d_6



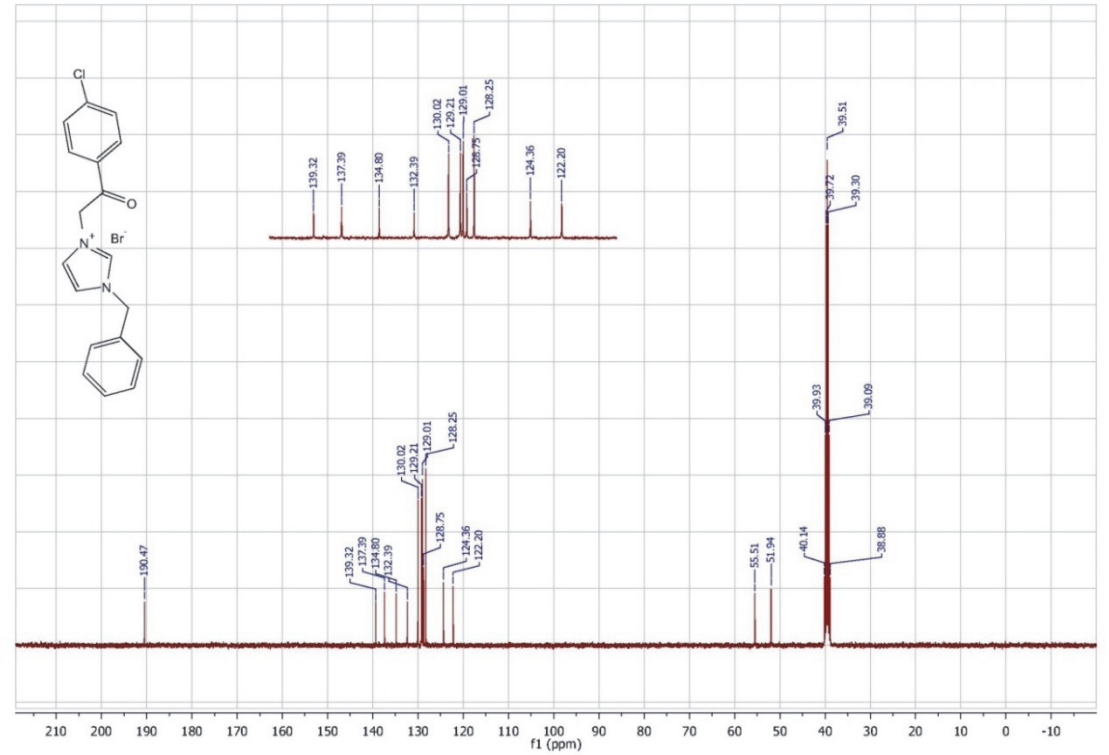
^{13}C NMR spectrum of 1-benzyl-3-(2-(3-bromophenyl)-2-oxoethyl)-1*H*-imidazol-3-ium bromide (1n), DMSO-d_6



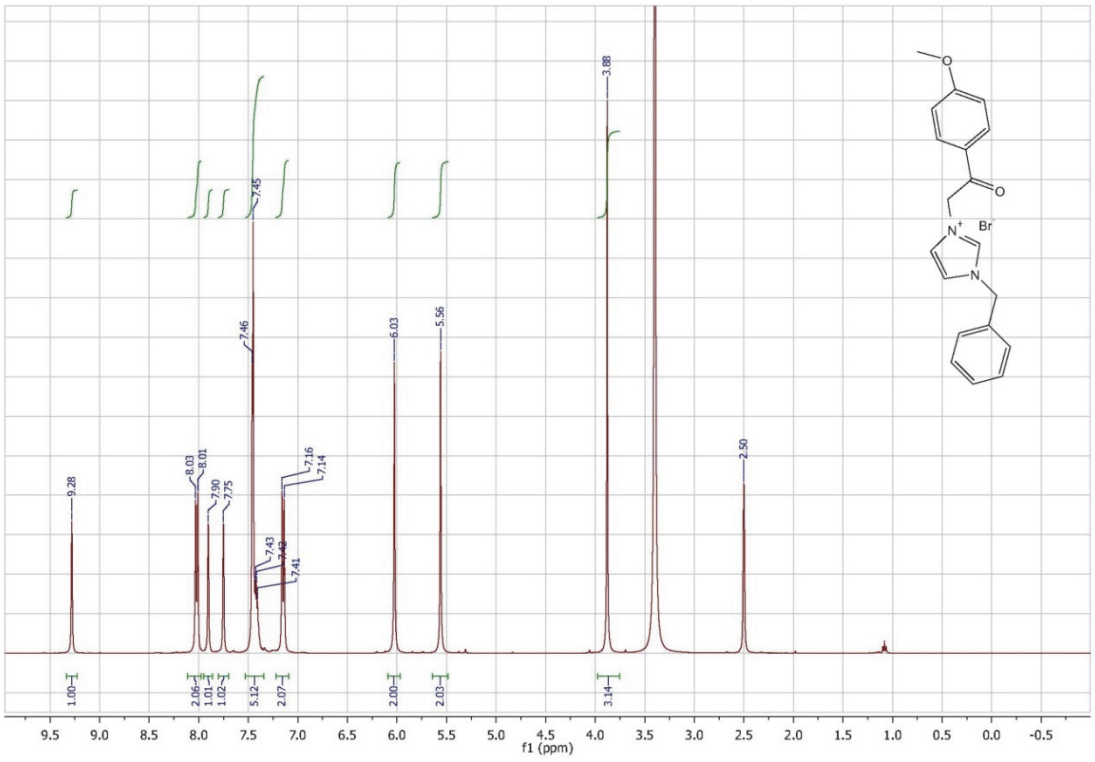
^{1}H NMR spectrum of 1-benzyl-3-(2-(4-chlorophenyl)-2-oxoethyl)-1*H*-imidazol-3-ium bromide (1o), DMSO-d_6



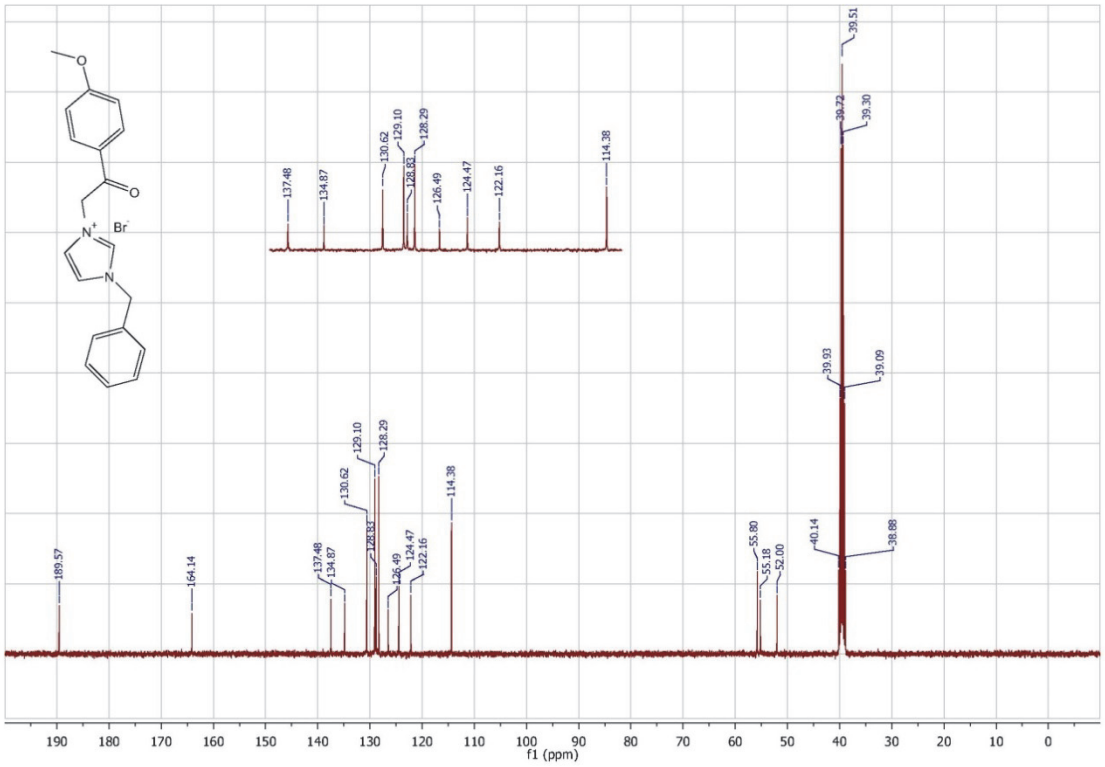
^{13}C NMR spectrum of 1-benzyl-3-(2-(4-chlorophenyl)-2-oxoethyl)-1*H*-imidazol-3-ium bromide (1o), DMSO-d_6



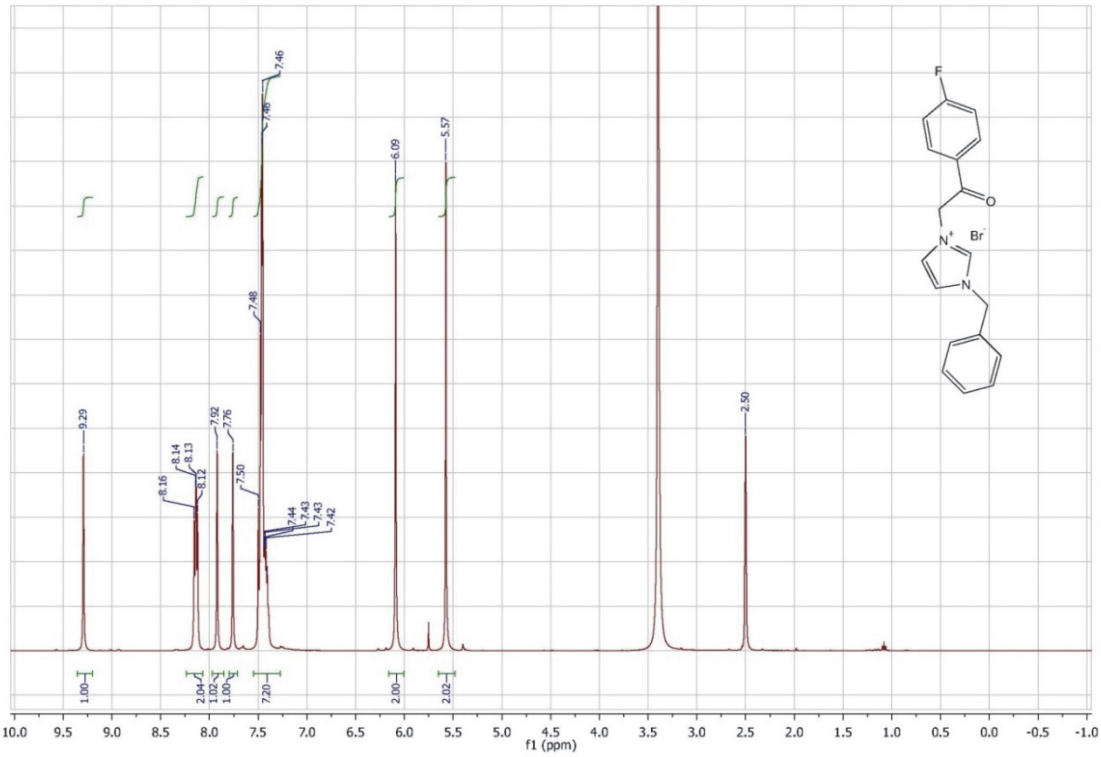
^{1}H NMR spectrum of 1-benzyl-3-(2-(4-methoxyphenyl)-2-oxoethyl)-1*H*-imidazol-3-ium bromide (1p), DMSO-d_6



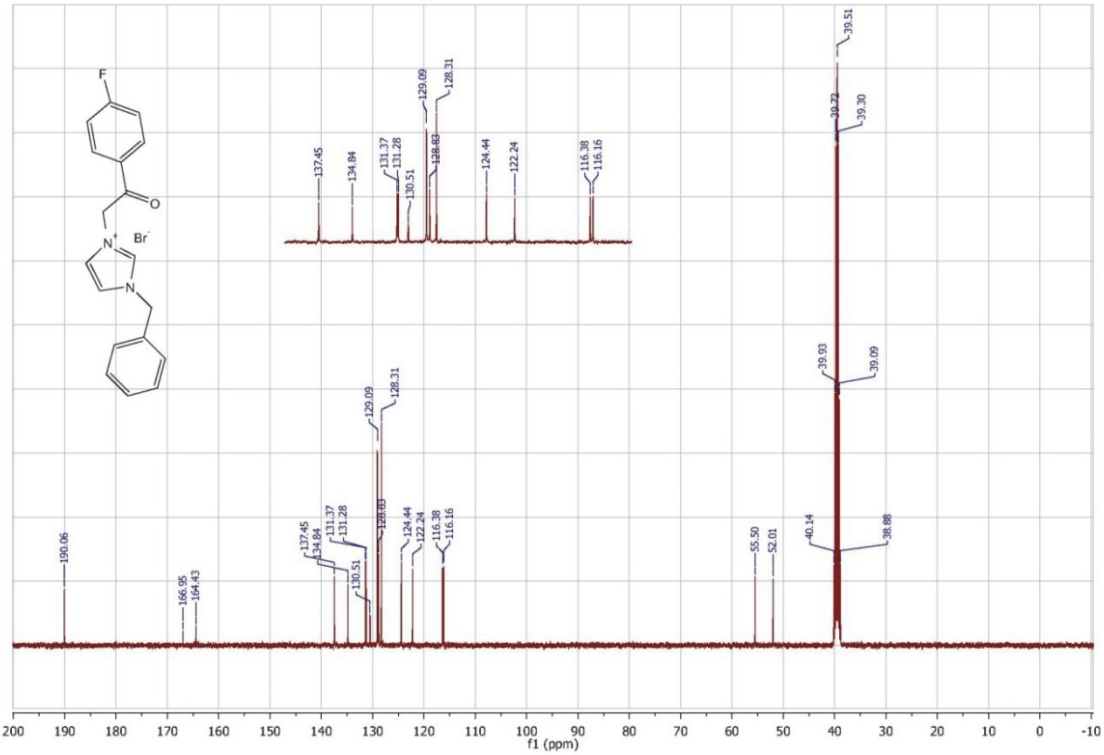
^{13}C NMR spectrum of 1-benzyl-3-(2-(4-methoxyphenyl)-2-oxoethyl)-1*H*-imidazol-3-ium bromide (1p), DMSO-d_6



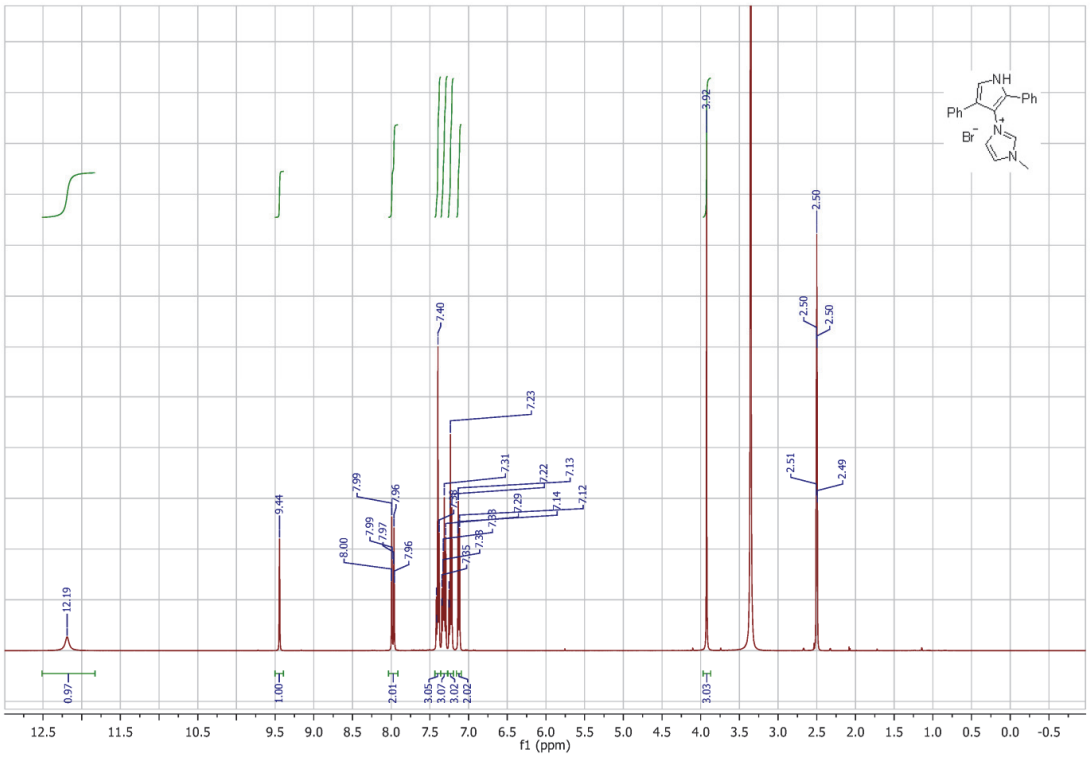
^{1}H NMR spectrum of 1-benzyl-3-(2-(4-fluorophenyl)-2-oxoethyl)-1*H*-imidazol-3-ium bromide (1q), DMSO-d_6



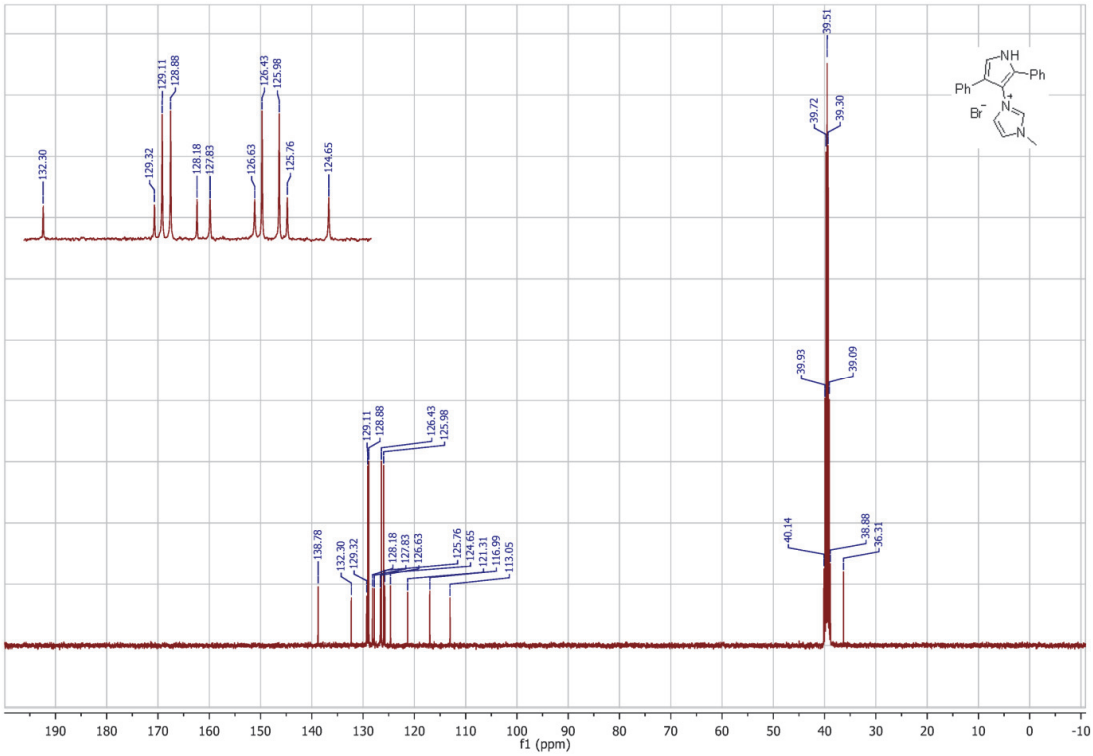
^{13}C NMR spectrum of 1-benzyl-3-(2-(4-fluorophenyl)-2-oxoethyl)-1*H*-imidazol-3-ium bromide (1q), DMSO-d_6



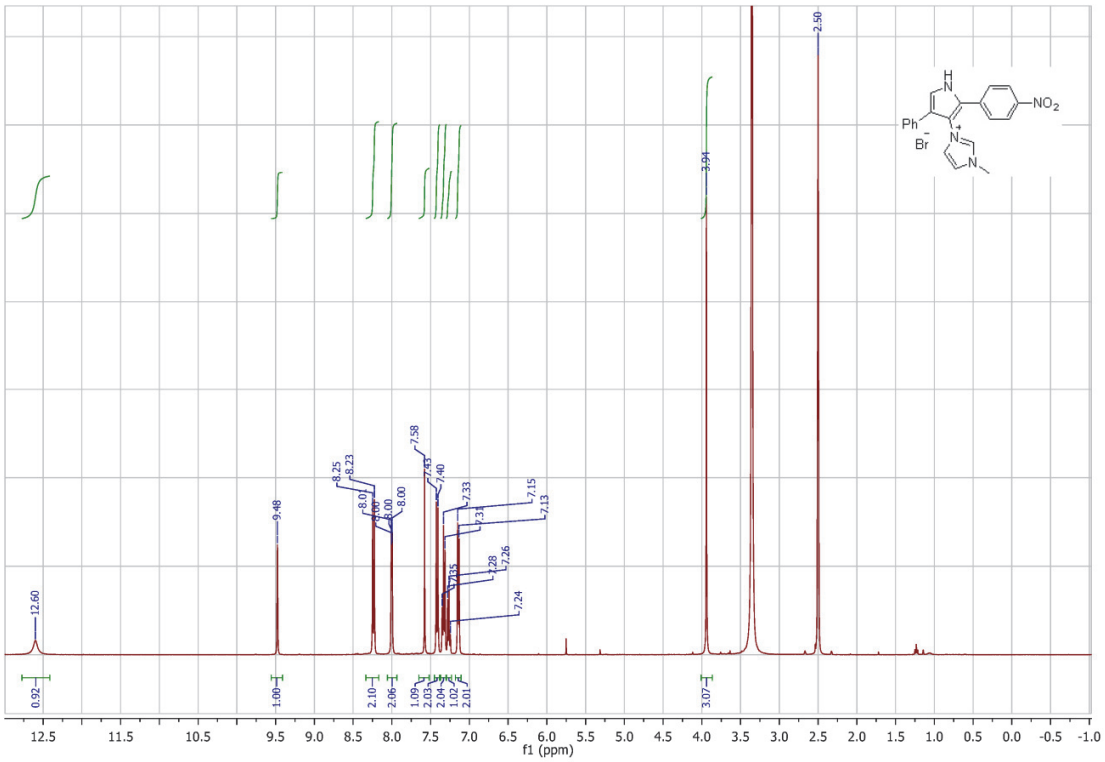
^{1}H NMR spectrum of 3-(2,4-diphenyl-1*H*-pyrrol-3-yl)-1-methyl-1*H*-imidazol-3-ium bromide (4a), DMSO-d_6



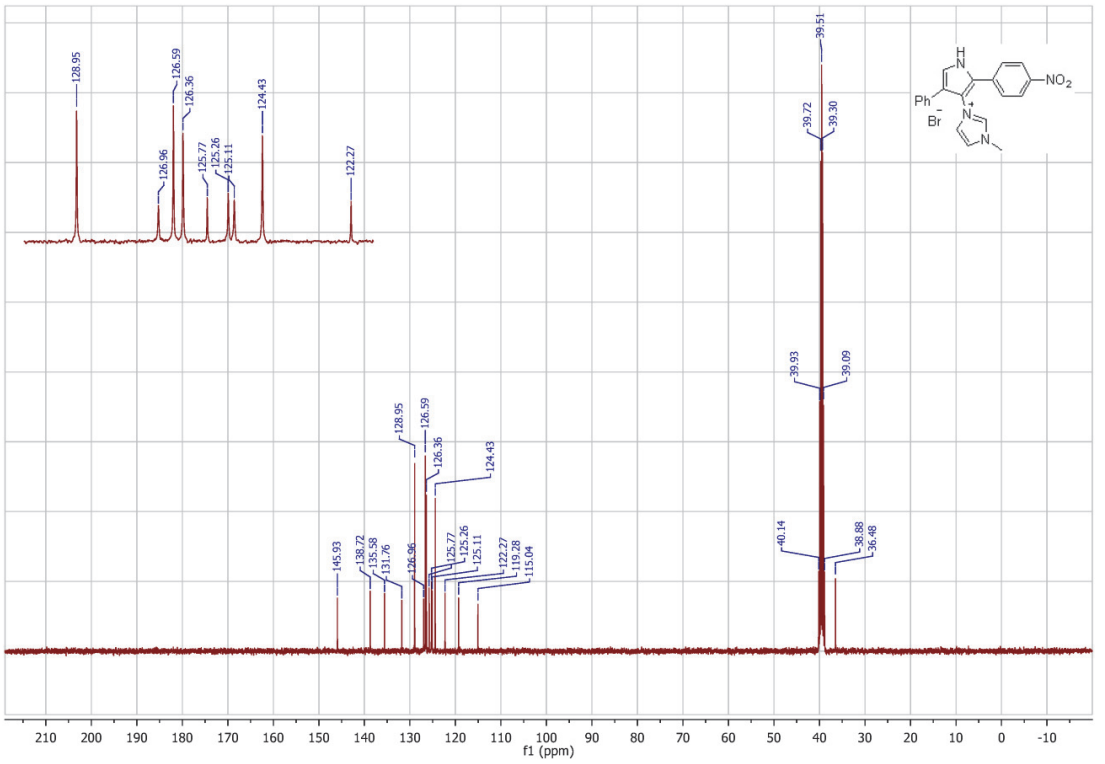
^{13}C NMR spectrum of 3-(2,4-diphenyl-1*H*-pyrrol-3-yl)-1-methyl-1*H*-imidazol-3-ium bromide (4a), DMSO-d_6



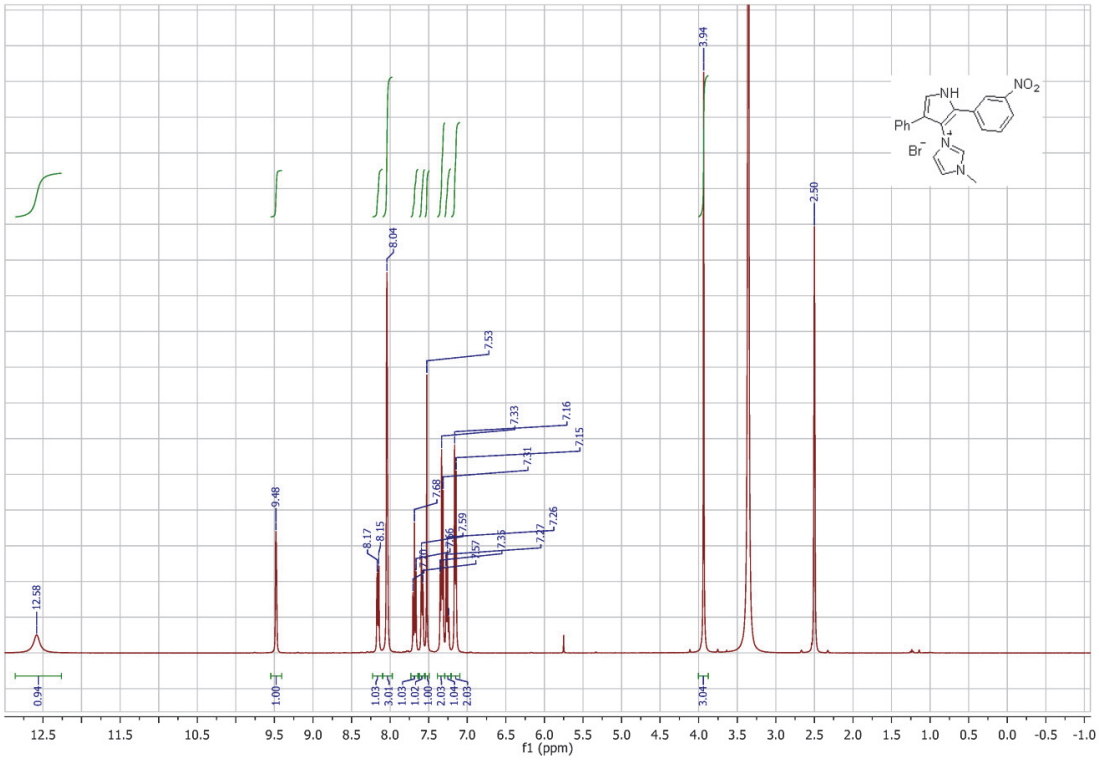
^{1}H NMR spectrum of 1-methyl-3-(2-(4-nitrophenyl)-4-phenyl-1*H*-pyrrol-3-yl)-1*H*-imidazol-3-ium bromide (4b), DMSO-d_6



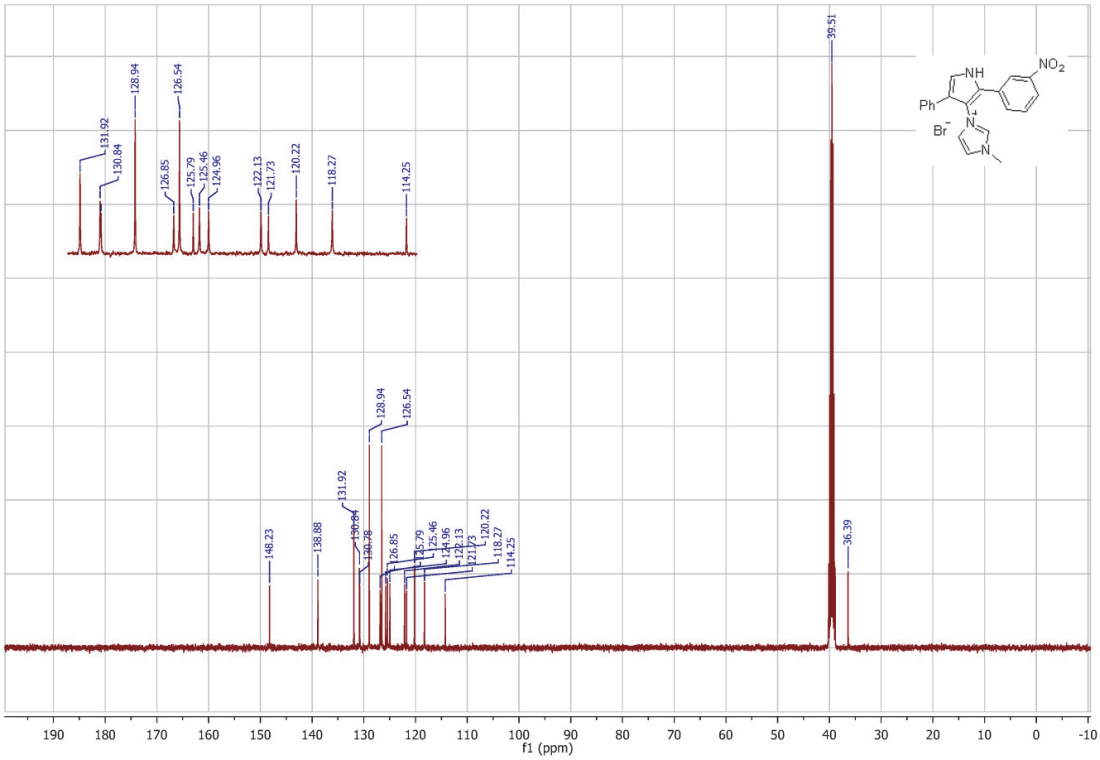
^{13}C NMR spectrum of 1-methyl-3-(2-(4-nitrophenyl)-4-phenyl-1*H*-pyrrol-3-yl)-1*H*-imidazol-3-ium bromide (4b), DMSO-d_6



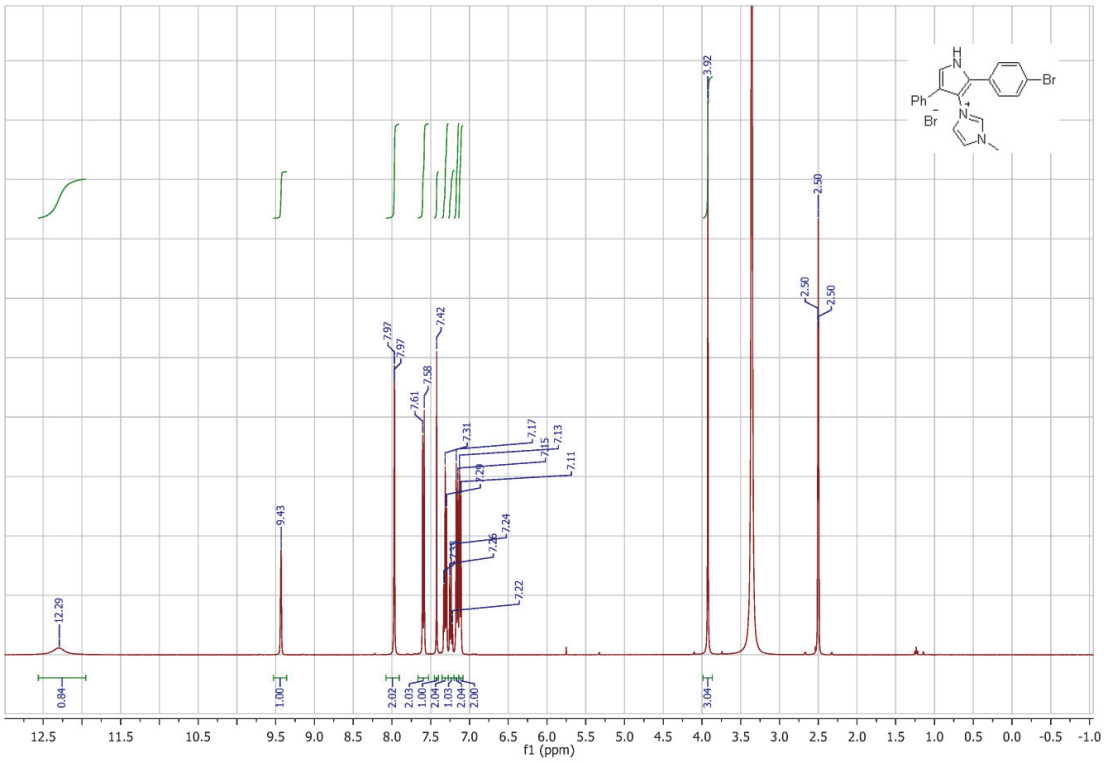
^{1}H NMR spectrum of 1-methyl-3-(2-(3-nitrophenyl)-4-phenyl-1*H*-pyrrol-3-yl)-1*H*-imidazol-3-ium bromide (4c), DMSO-d_6



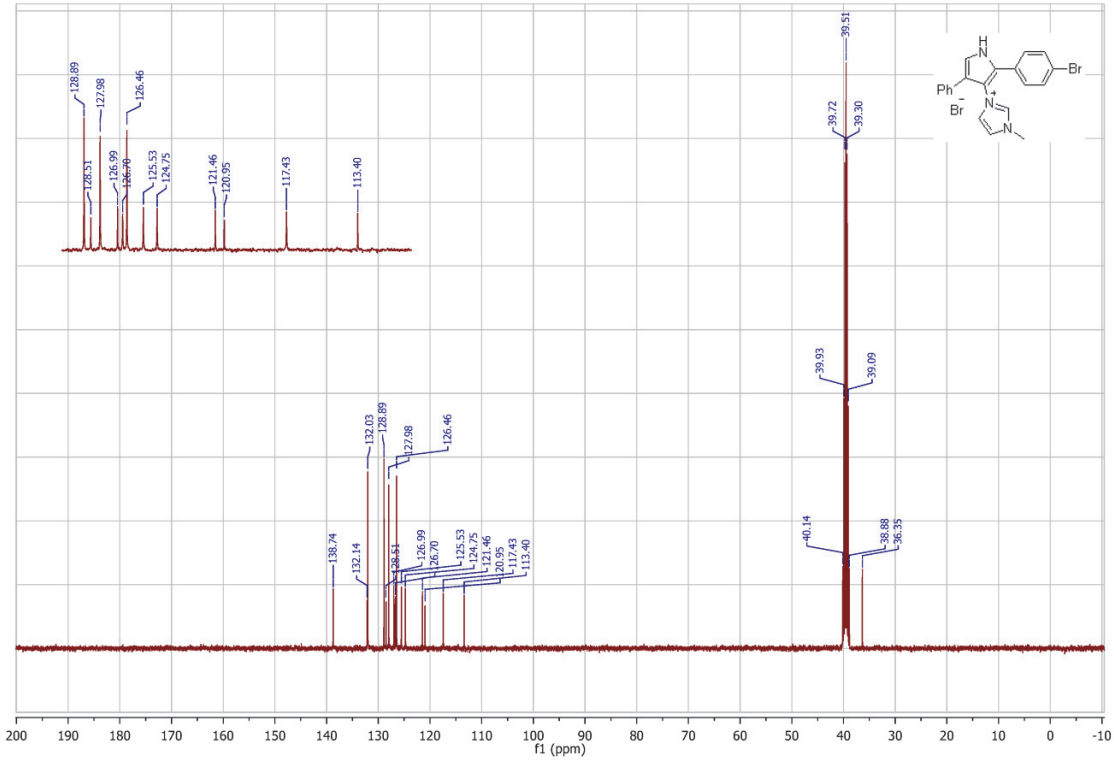
^{13}C NMR spectrum of 1-methyl-3-(2-(3-nitrophenyl)-4-phenyl-1*H*-pyrrol-3-yl)-1*H*-imidazol-3-ium bromide (4c), DMSO-d_6



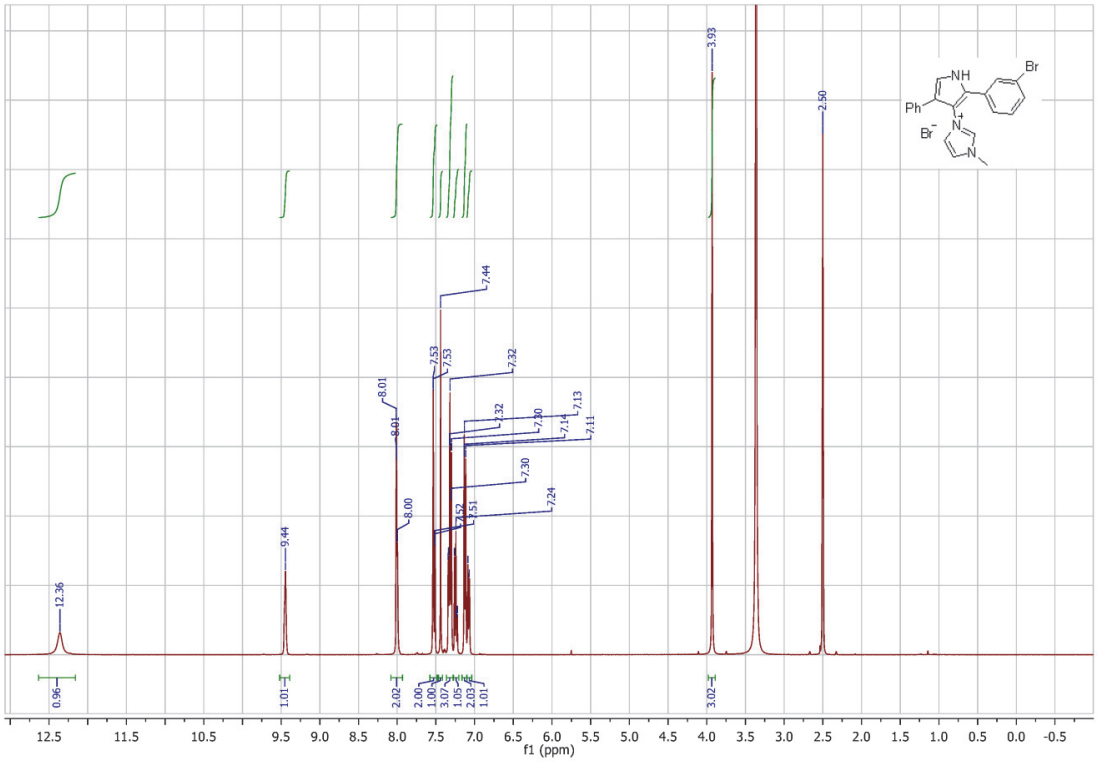
^{1}H NMR spectrum of 3-(2-(4-bromophenyl)-4-phenyl-1*H*-pyrrol-3-yl)-1-methyl-1*H*-imidazol-3-ium bromide (4d), DMSO-d_6



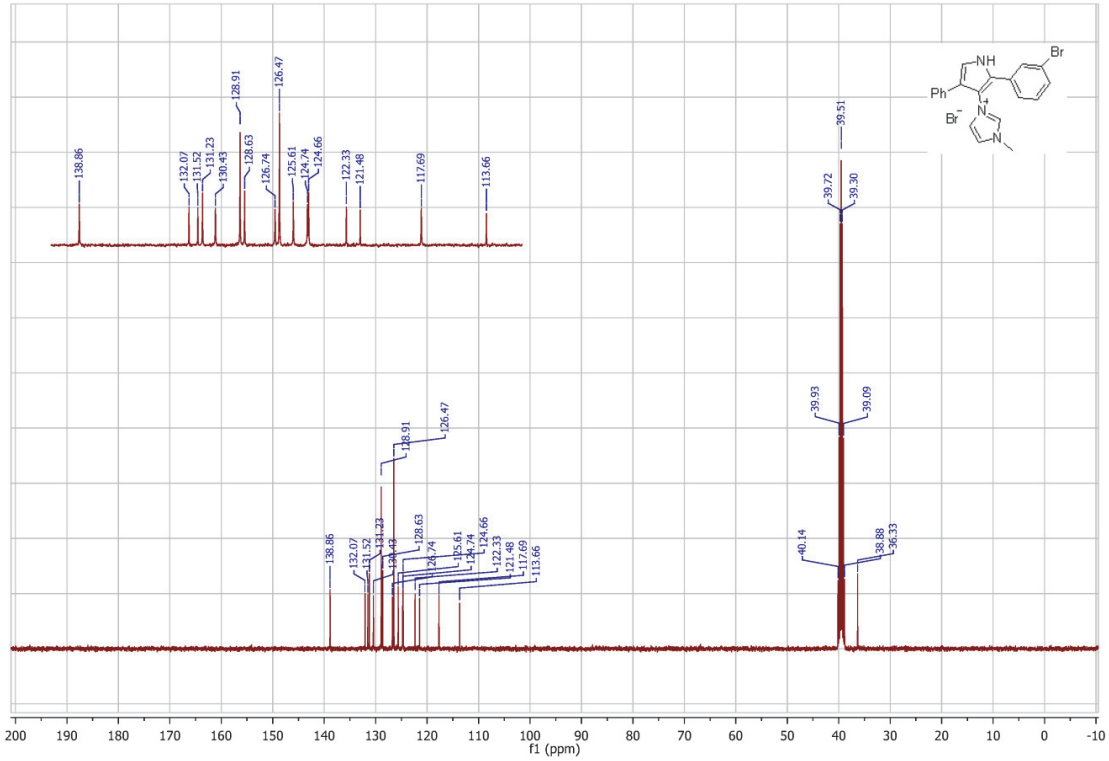
^{13}C NMR spectrum of 3-(2-(4-bromophenyl)-4-phenyl-1*H*-pyrrol-3-yl)-1-methyl-1*H*-imidazol-3-ium bromide (4d), DMSO-d_6



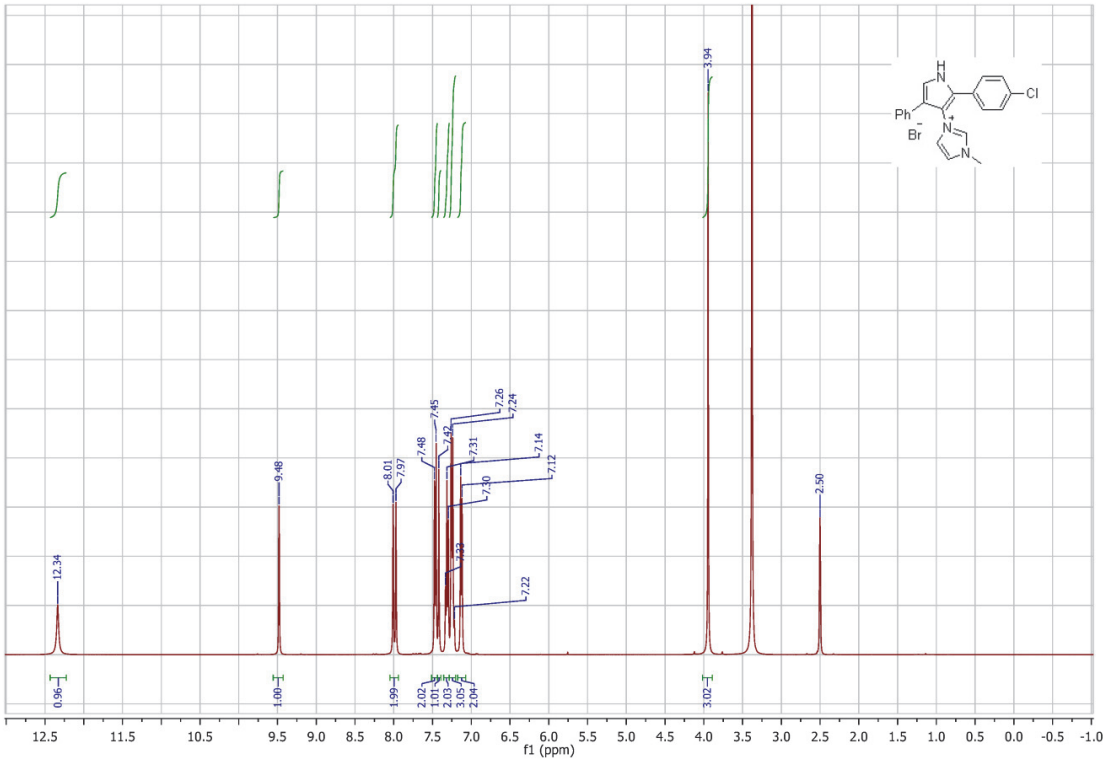
^{1}H NMR spectrum of 3-(2-(3-bromophenyl)-4-phenyl-1*H*-pyrrol-3-yl)-1-methyl-1*H*-imidazol-3-ium bromide (4e), DMSO-d_6



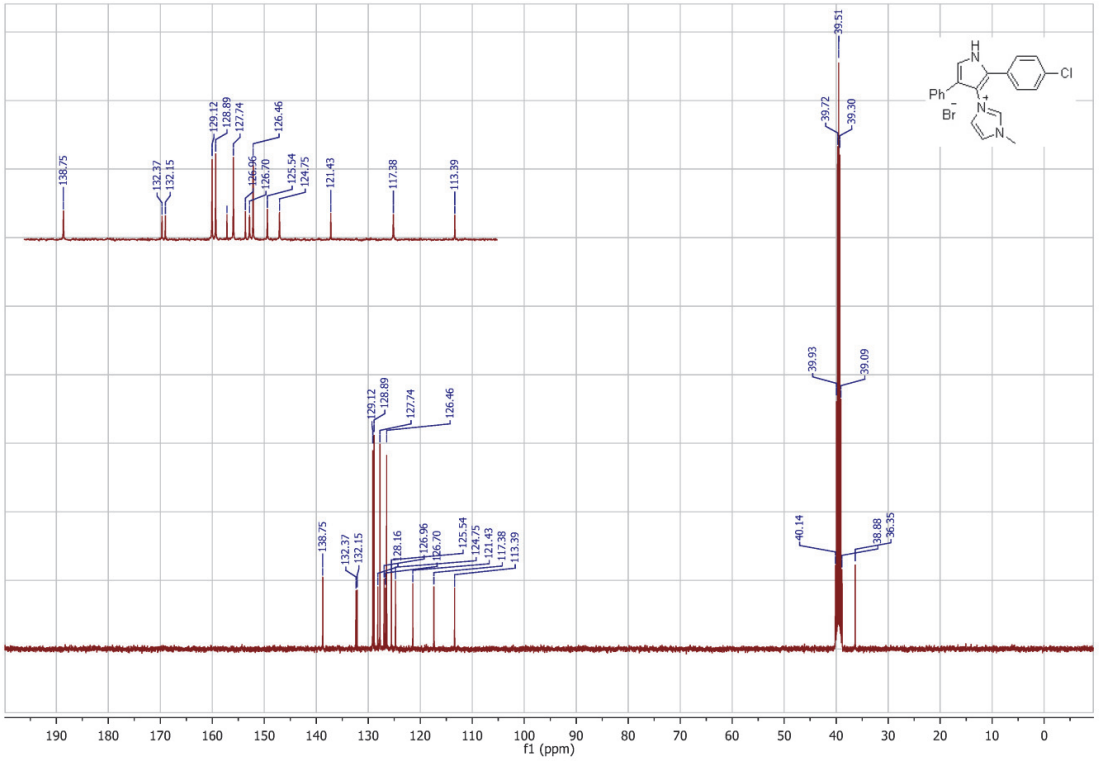
^{13}C NMR spectrum of 3-(2-(3-bromophenyl)-4-phenyl-1*H*-pyrrol-3-yl)-1-methyl-1*H*-imidazol-3-ium bromide (4e), DMSO-d_6



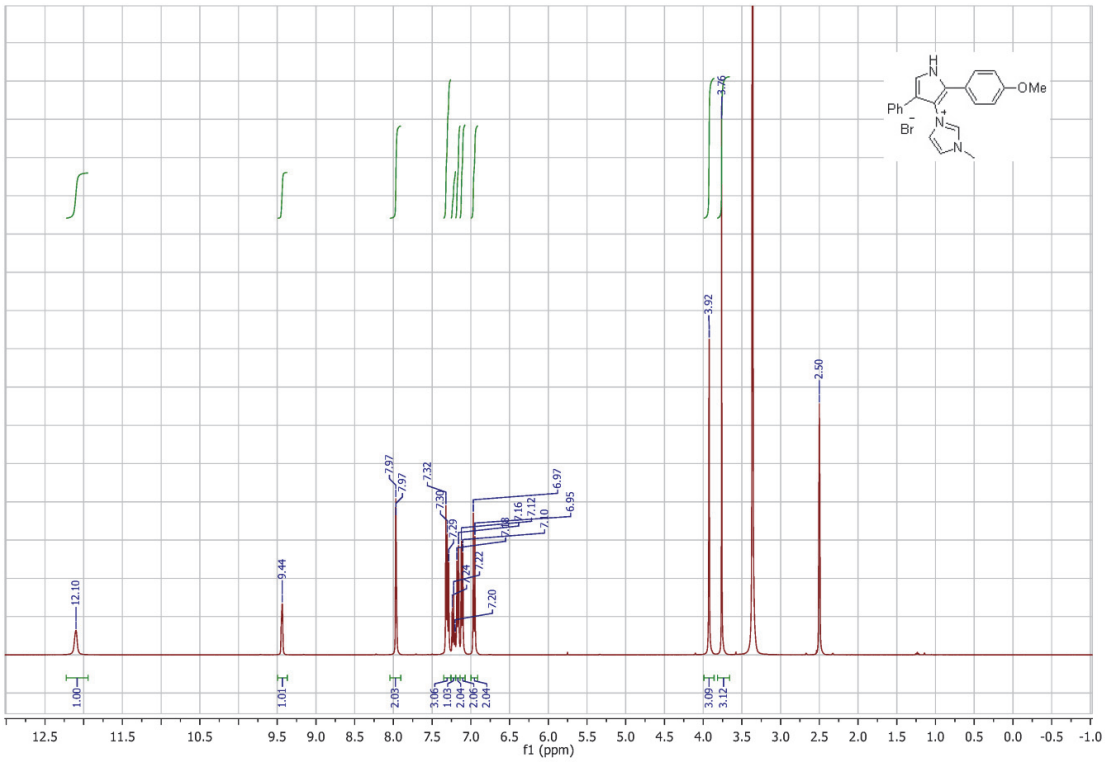
^{1}H NMR spectrum of 3-(2-(4-chlorophenyl)-4-phenyl-1*H*-pyrrol-3-yl)-1-methyl-1*H*-imidazol-3-ium bromide (4f), DMSO-d$_6$



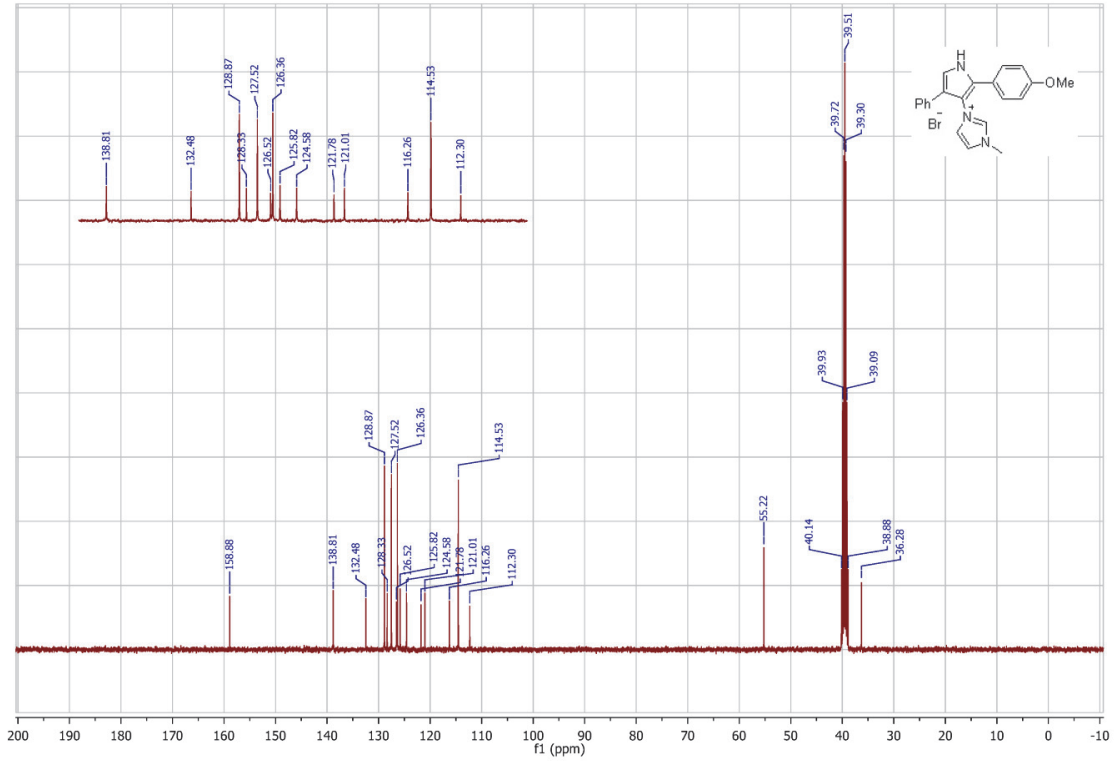
^{13}C NMR spectrum of 3-(2-(4-chlorophenyl)-4-phenyl-1*H*-pyrrol-3-yl)-1-methyl-1*H*-imidazol-3-ium bromide (4f), DMSO-d$_6$



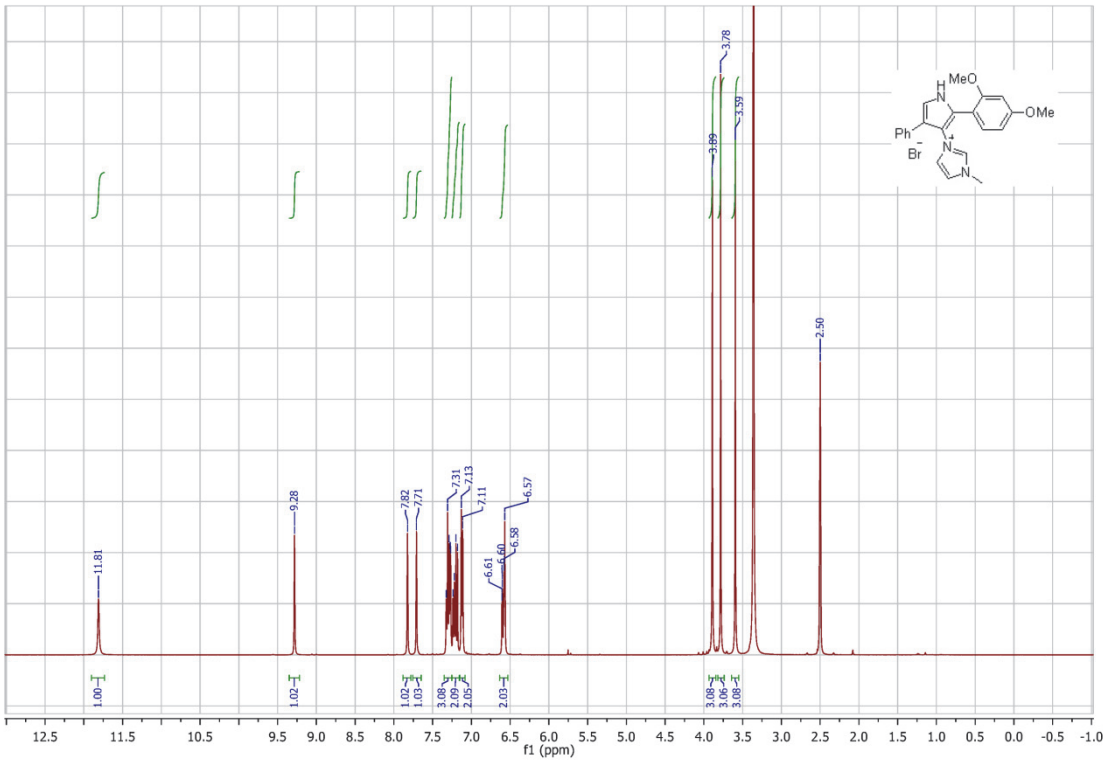
^{1}H NMR spectrum of 3-(2-(4-methoxyphenyl)-4-phenyl-1*H*-pyrrol-3-yl)-1-methyl-1*H*-imidazol-3-ium bromide (4g), DMSO-d_6



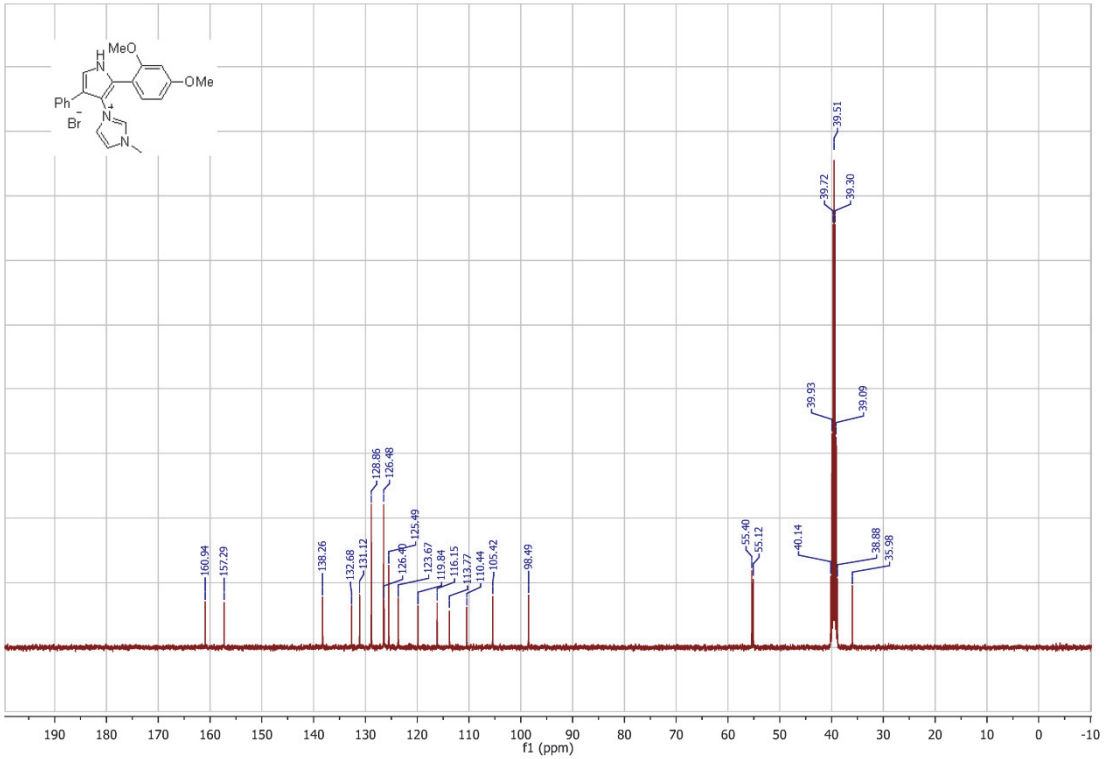
^{13}C NMR spectrum of 3-(2-(4-methoxyphenyl)-4-phenyl-1*H*-pyrrol-3-yl)-1-methyl-1*H*-imidazol-3-ium bromide (4g), DMSO-d_6



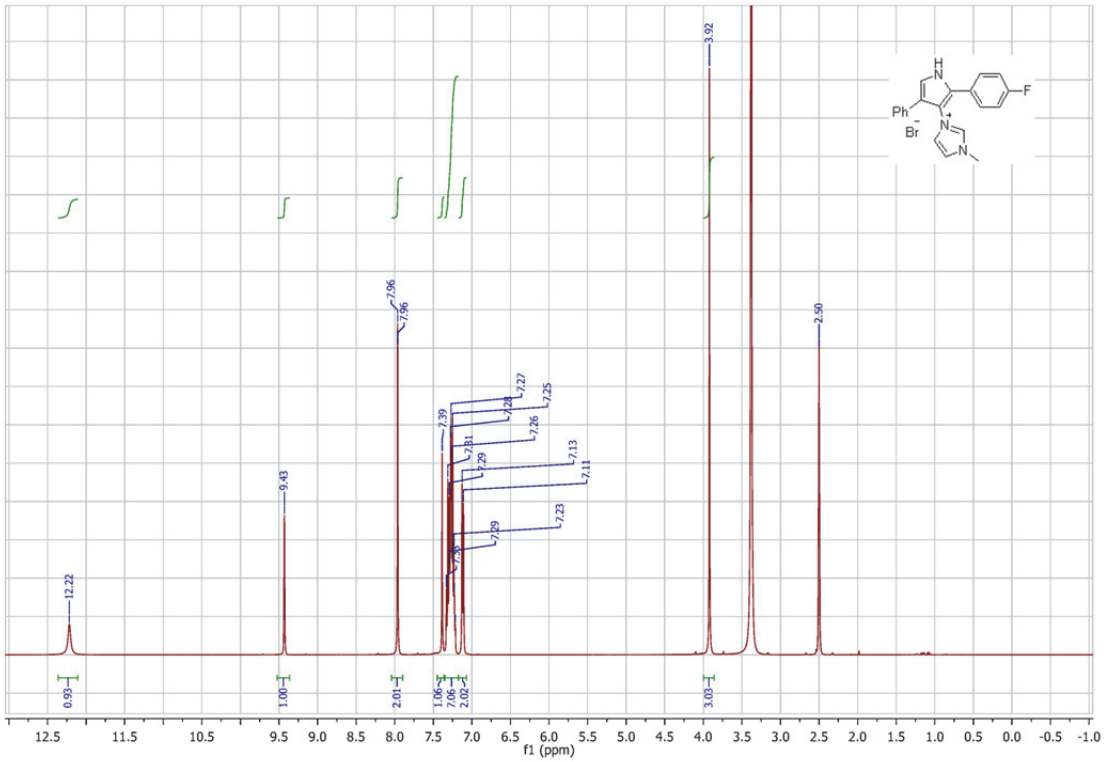
^{1}H NMR spectrum of 3-(2-(3,4-dimethoxyphenyl)-4-phenyl-1*H*-pyrrol-3-yl)-1-methyl-1*H*-imidazol-3-ium bromide (4h), DMSO-d_6



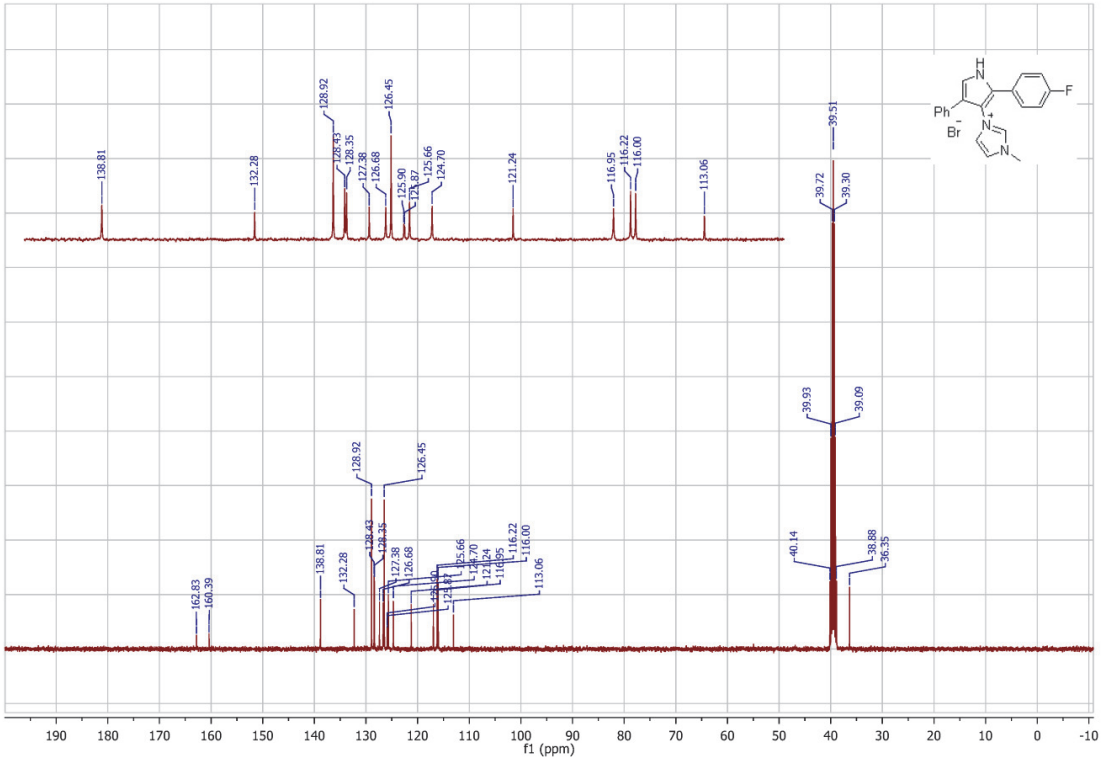
^{13}C NMR spectrum of 3-(2-(3,4-dimethoxyphenyl)-4-phenyl-1*H*-pyrrol-3-yl)-1-methyl-1*H*-imidazol-3-ium bromide (4h), DMSO-d_6



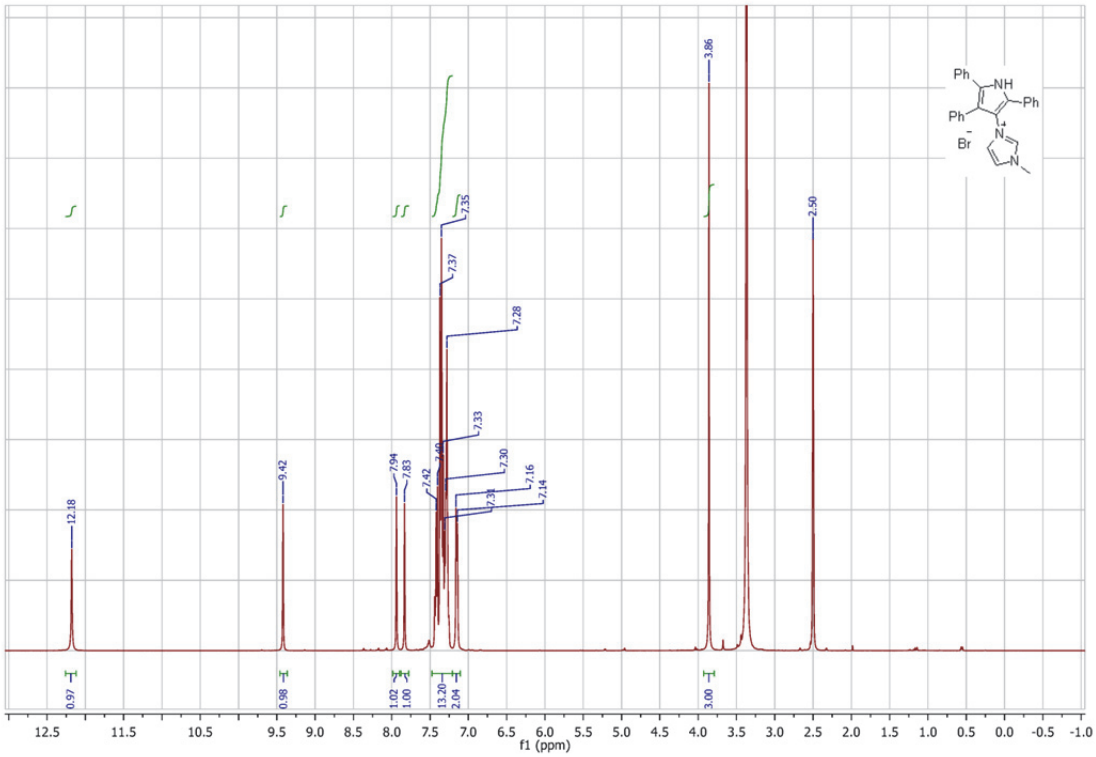
^{1}H NMR spectrum of 3-(2-(4-fluorophenyl)-4-phenyl-1*H*-pyrrol-3-yl)-1-methyl-1*H*-imidazol-3-ium bromide (4i), DMSO-d_6



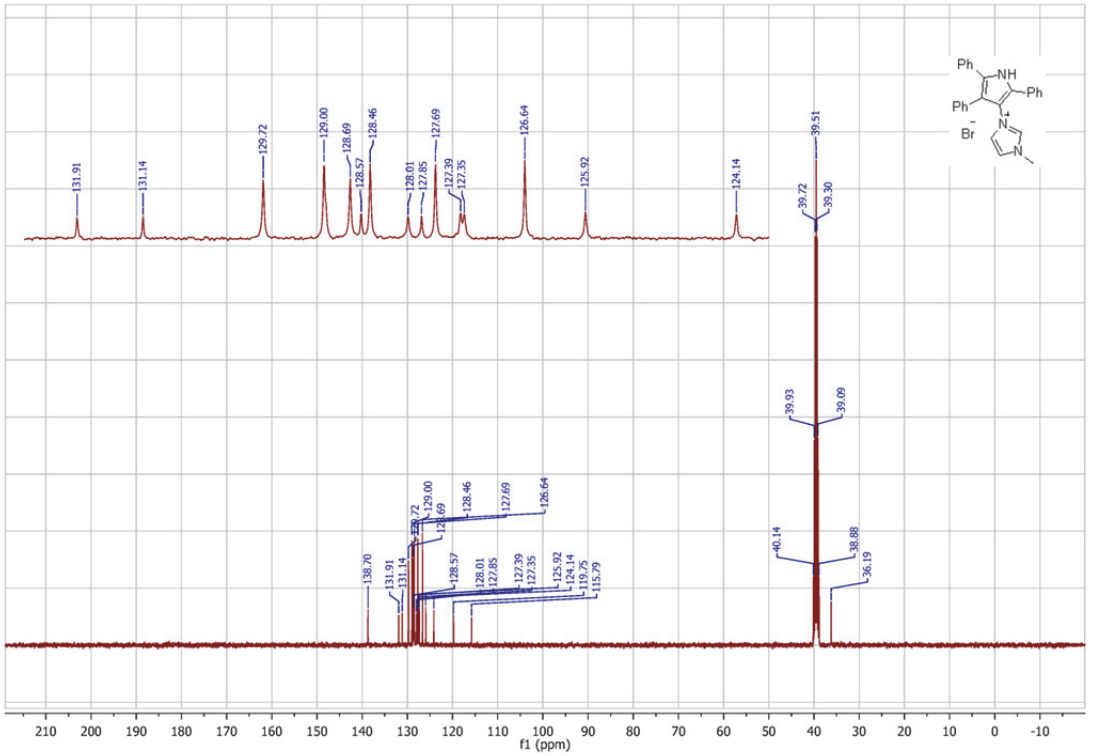
^{13}C NMR spectrum of 3-(2-(4-fluorophenyl)-4-phenyl-1*H*-pyrrol-3-yl)-1-methyl-1*H*-imidazol-3-ium bromide (4i), DMSO-d_6



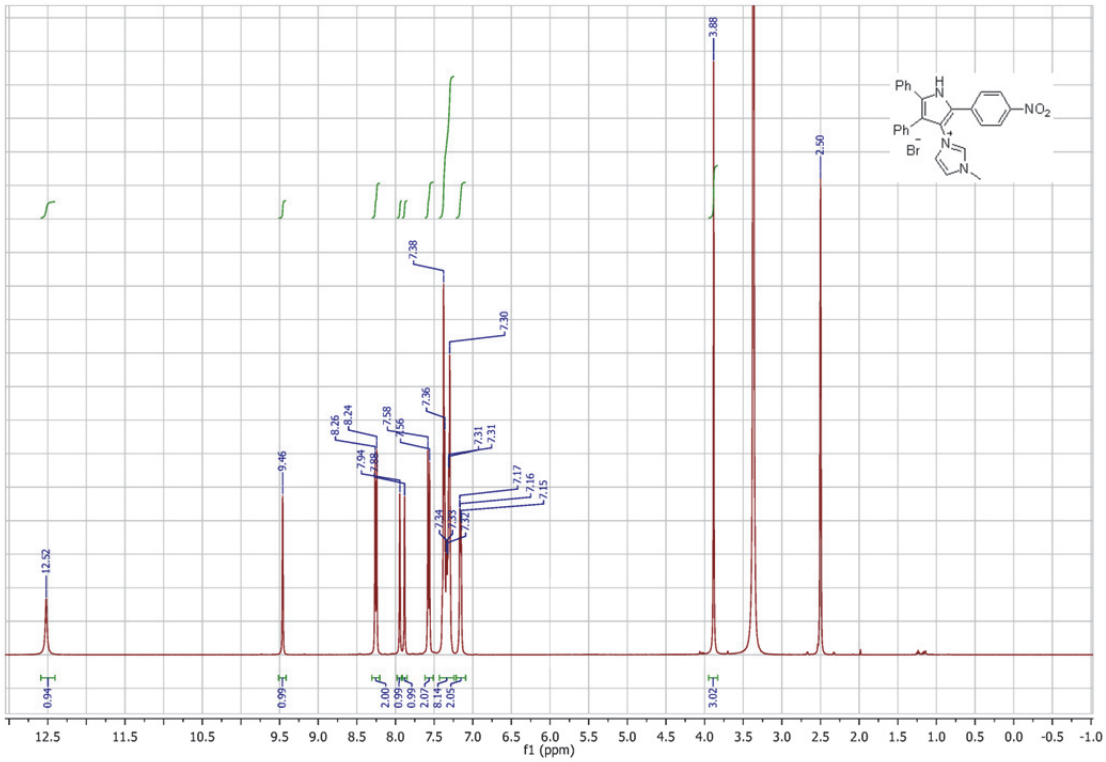
^{1}H NMR spectrum of 1-methyl-3-(2,4,5-triphenyl-1*H*-pyrrol-3-yl)-1*H*-imidazol-3-ium bromide (4j), DMSO-d_6



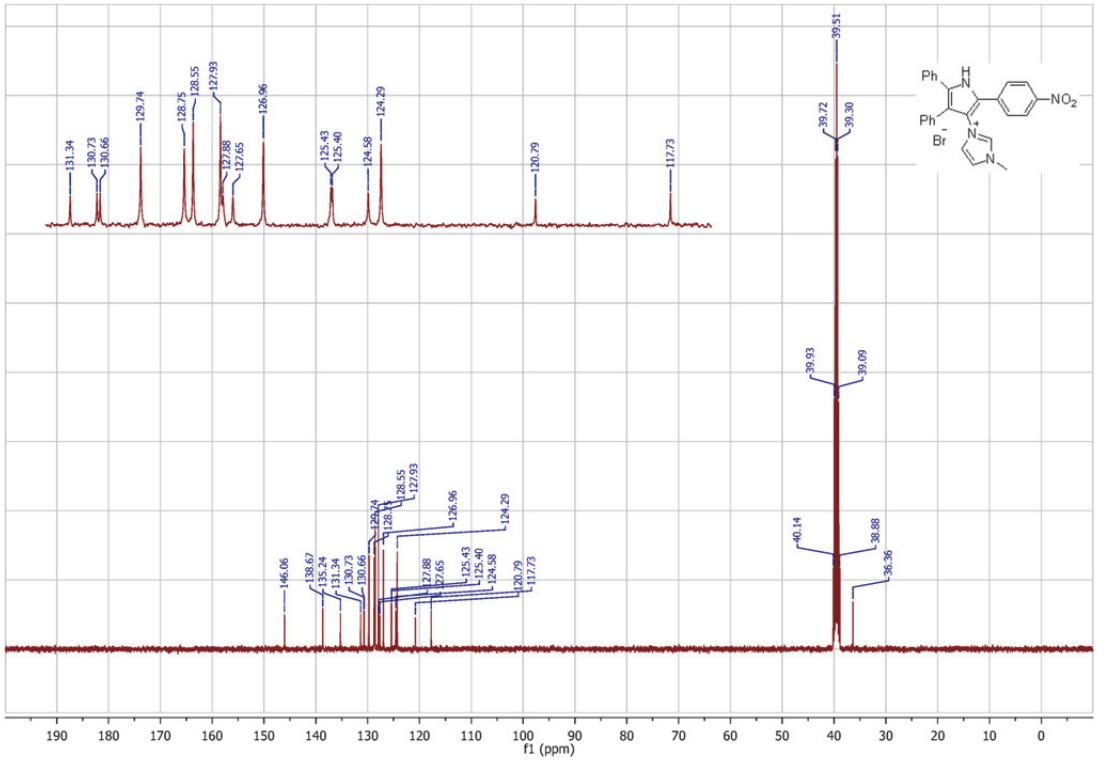
^{13}C NMR spectrum of 1-methyl-3-(2,4,5-triphenyl-1*H*-pyrrol-3-yl)-1*H*-imidazol-3-ium bromide (4j), DMSO-d_6



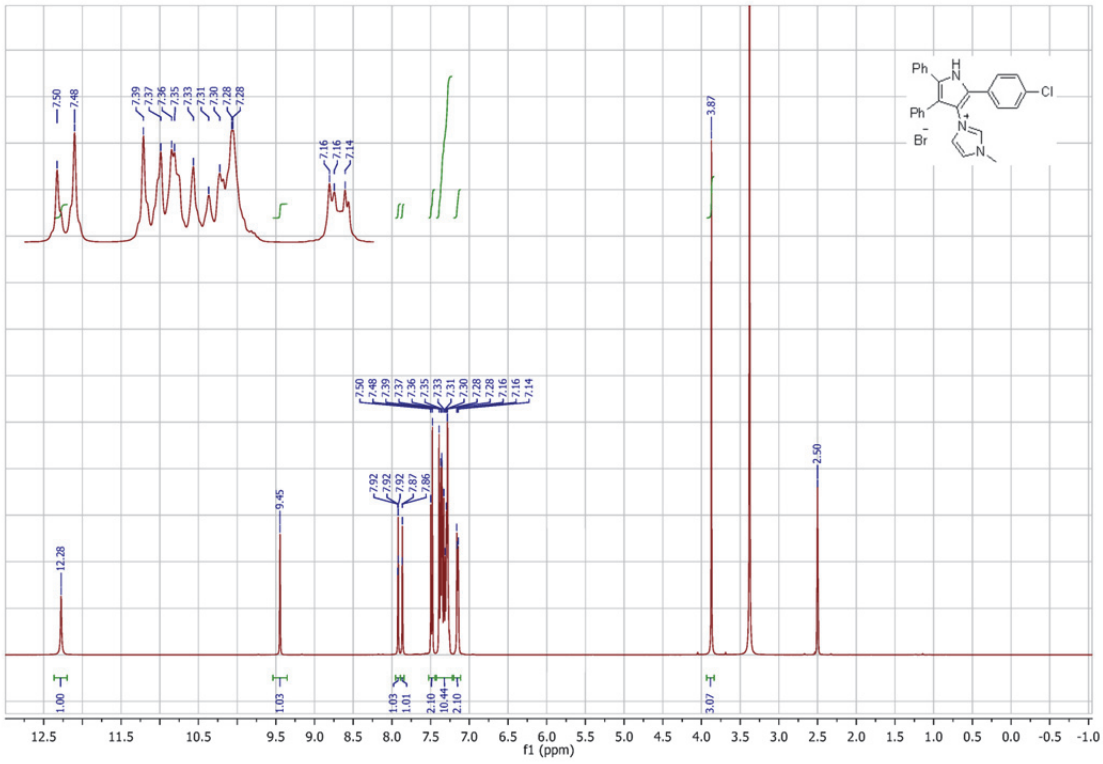
^{1}H NMR spectrum of 1-methyl-3-(2-(4-nitrophenyl)-4,5-diphenyl-1*H*-pyrrol-3-yl)-1*H*-imidazol-3-ium bromide (4k), DMSO-d_6



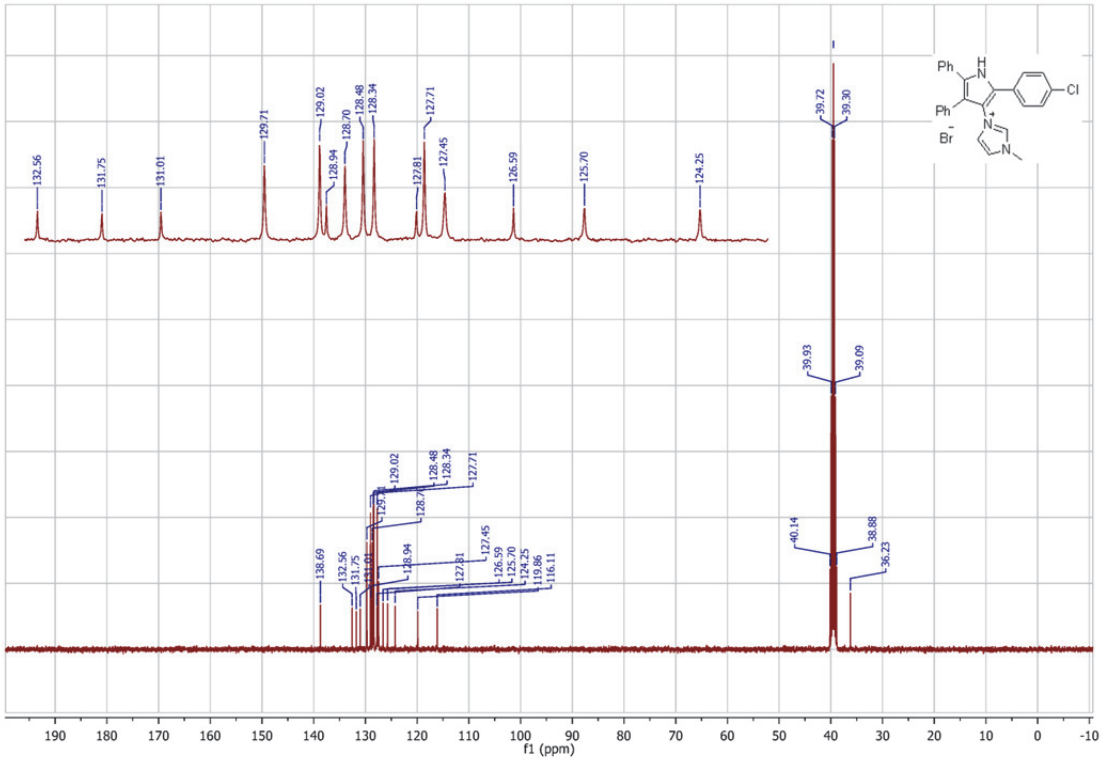
^{13}C NMR spectrum of 1-methyl-3-(2-(4-nitrophenyl)-4,5-diphenyl-1*H*-pyrrol-3-yl)-1*H*-imidazol-3-ium bromide (4k), DMSO-d_6



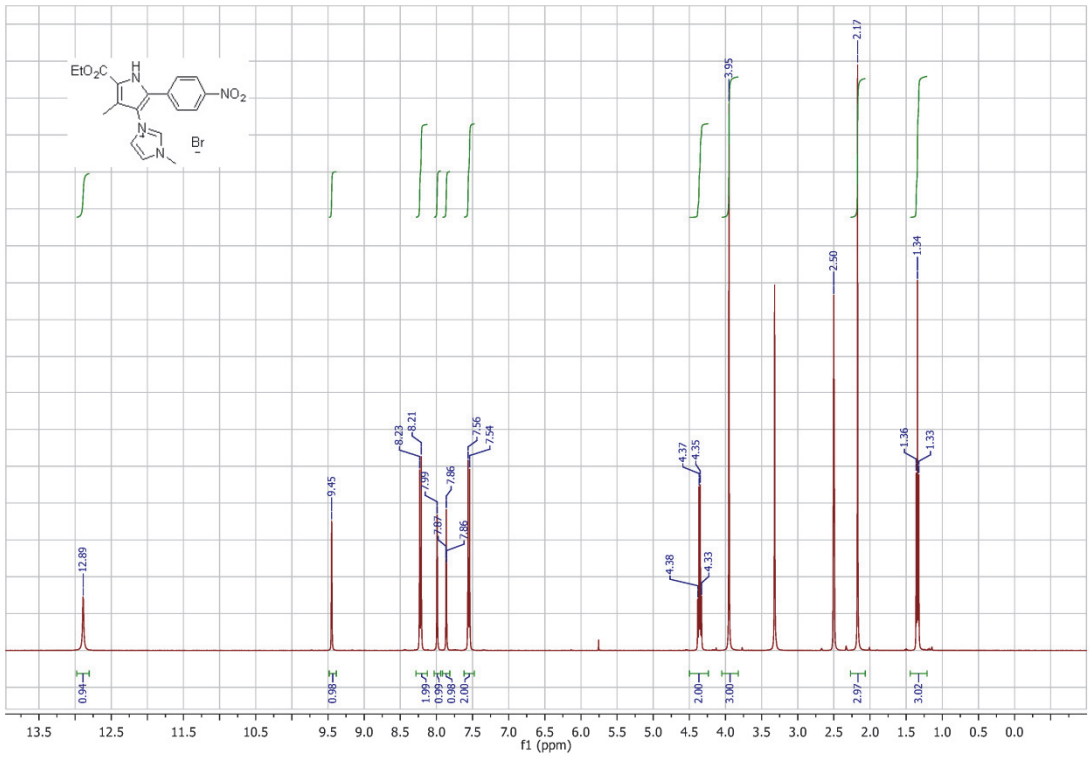
^{1}H NMR spectrum of 3-(2-(4-chlorophenyl)-4,5-diphenyl-1*H*-pyrrol-3-yl)-1-methyl-1*H*-imidazol-3-ium bromide (4l), DMSO-d_6



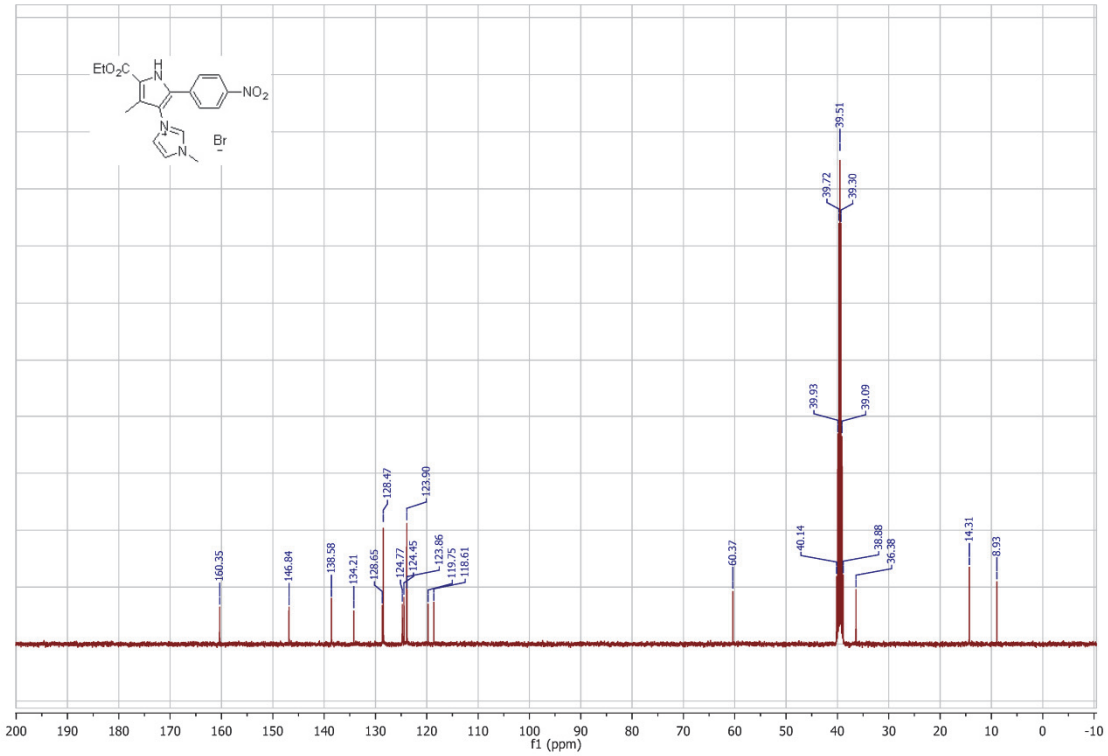
^{13}C NMR spectrum of 3-(2-(4-chlorophenyl)-4,5-diphenyl-1*H*-pyrrol-3-yl)-1-methyl-1*H*-imidazol-3-ium bromide (4l), DMSO-d_6



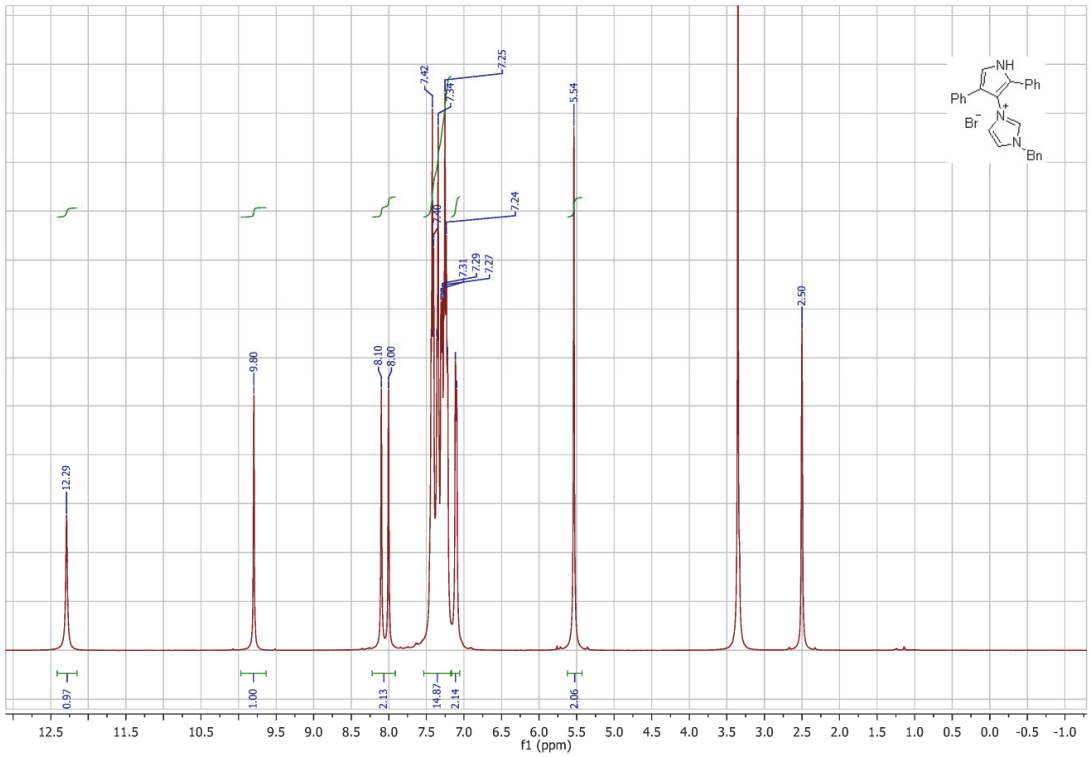
^{1}H NMR spectrum of 3-(5-ethoxycarbonyl-4-methyl-2-(4-nitrophenyl)-1*H*-pyrrol-3-yl)-1-methyl-1*H*-imidazol-3-ium bromide (4m), DMSO-d_6



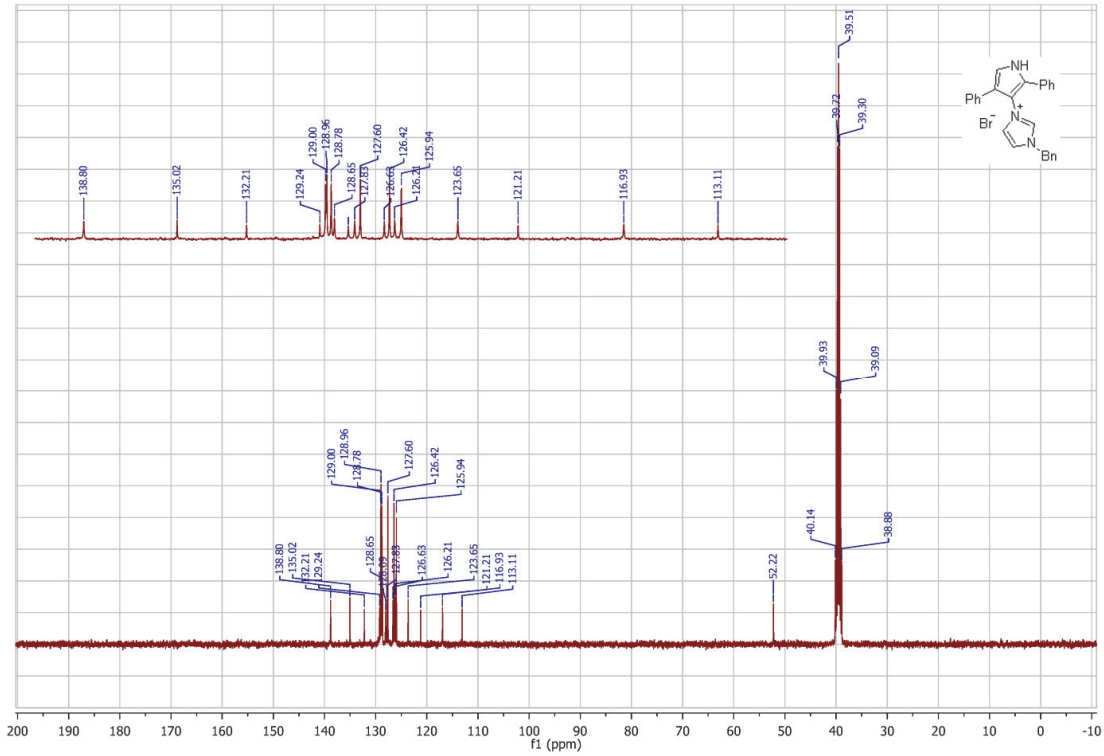
^{13}C NMR spectrum of 3-(5-ethoxycarbonyl-4-methyl-2-(4-nitrophenyl)-1*H*-pyrrol-3-yl)-1-methyl-1*H*-imidazol-3-ium bromide (4m), DMSO-d_6



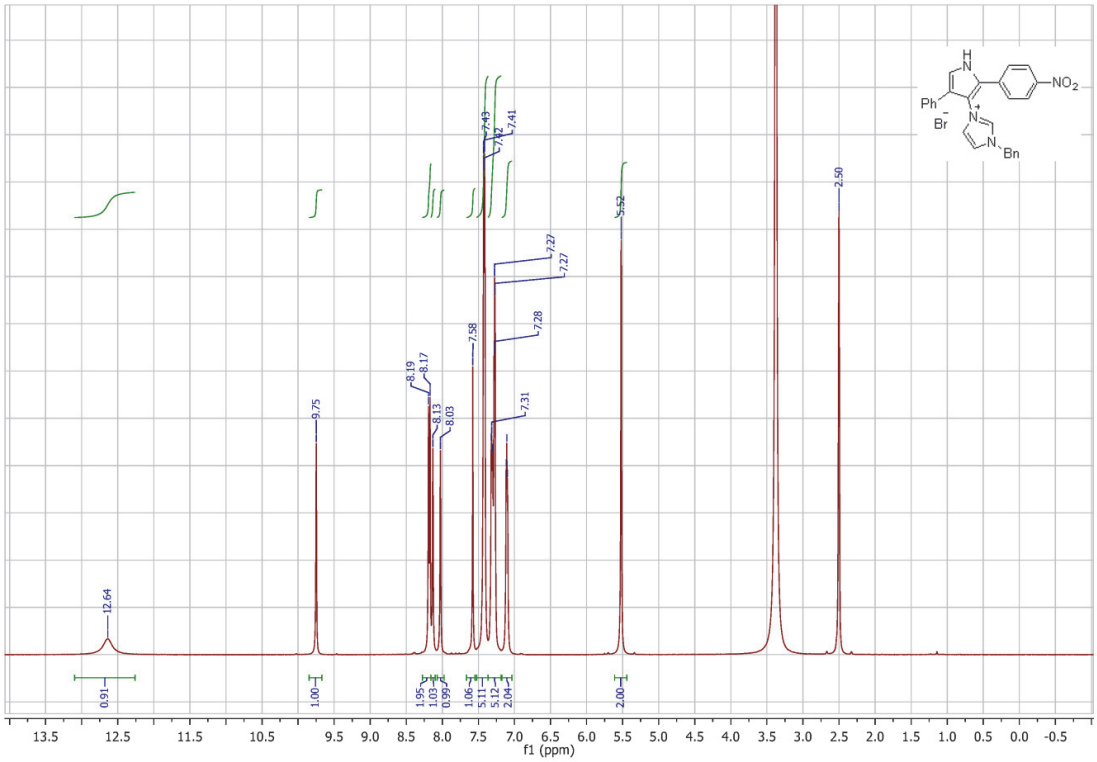
^{1}H NMR spectrum of 1-benzyl-3-(2,4-diphenyl-1*H*-pyrrol-3-yl)- 1*H*-imidazol-3-ium bromide (4n), DMSO-d_6



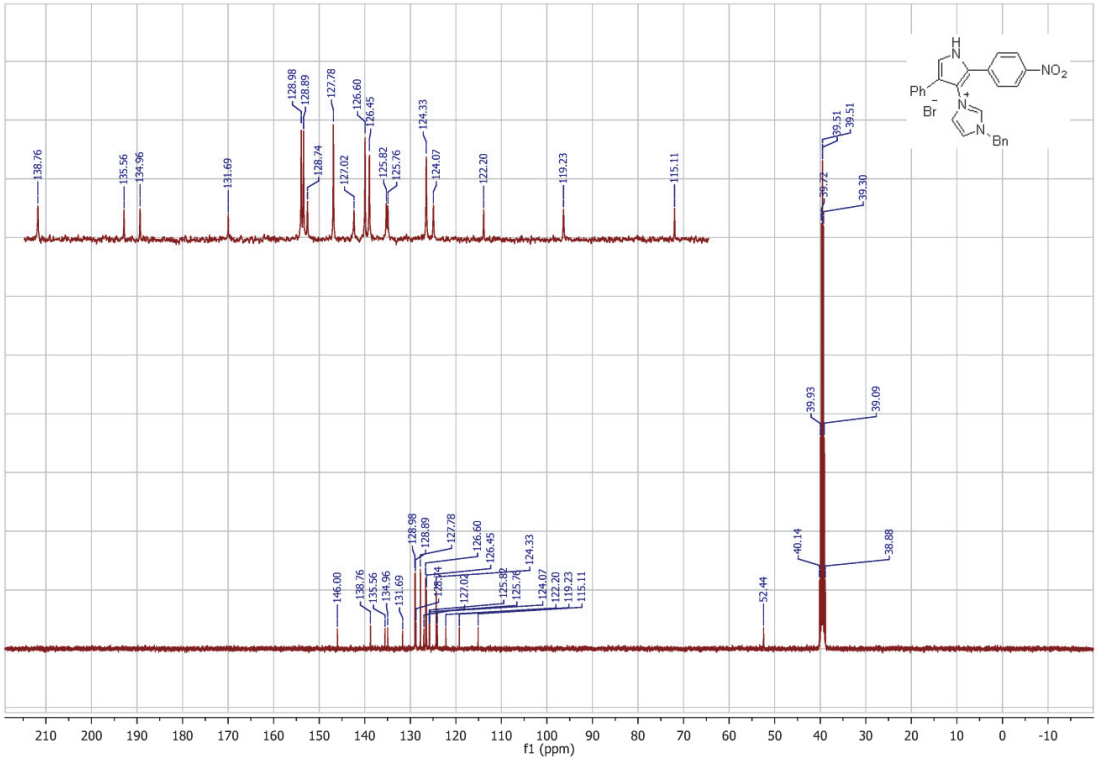
^{13}C NMR spectrum of 1-benzyl-3-(2,4-diphenyl-1*H*-pyrrol-3-yl)- 1*H*-imidazol-3-ium bromide (4n), DMSO-d_6



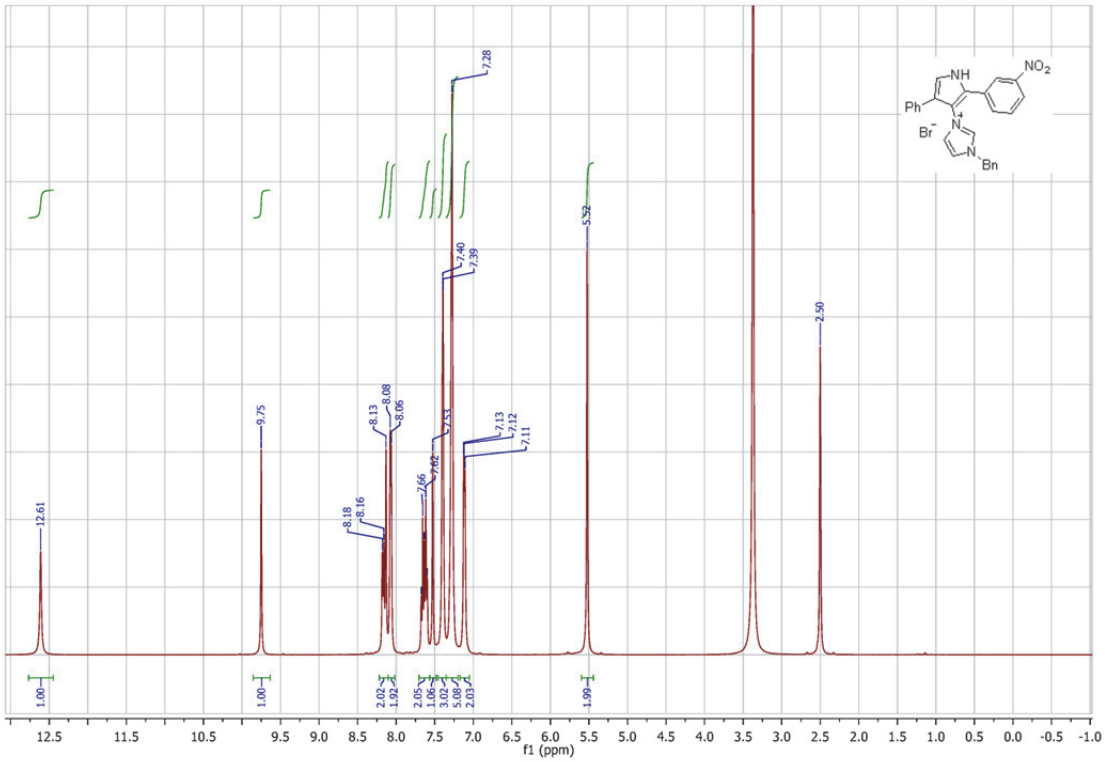
^{1}H NMR spectrum of 1-benzyl-3-(2-(4-nitrophenyl)-4-phenyl-1*H*-pyrrol-3-yl)-1*H*-imidazol-3-ium bromide (4o), DMSO-d_6



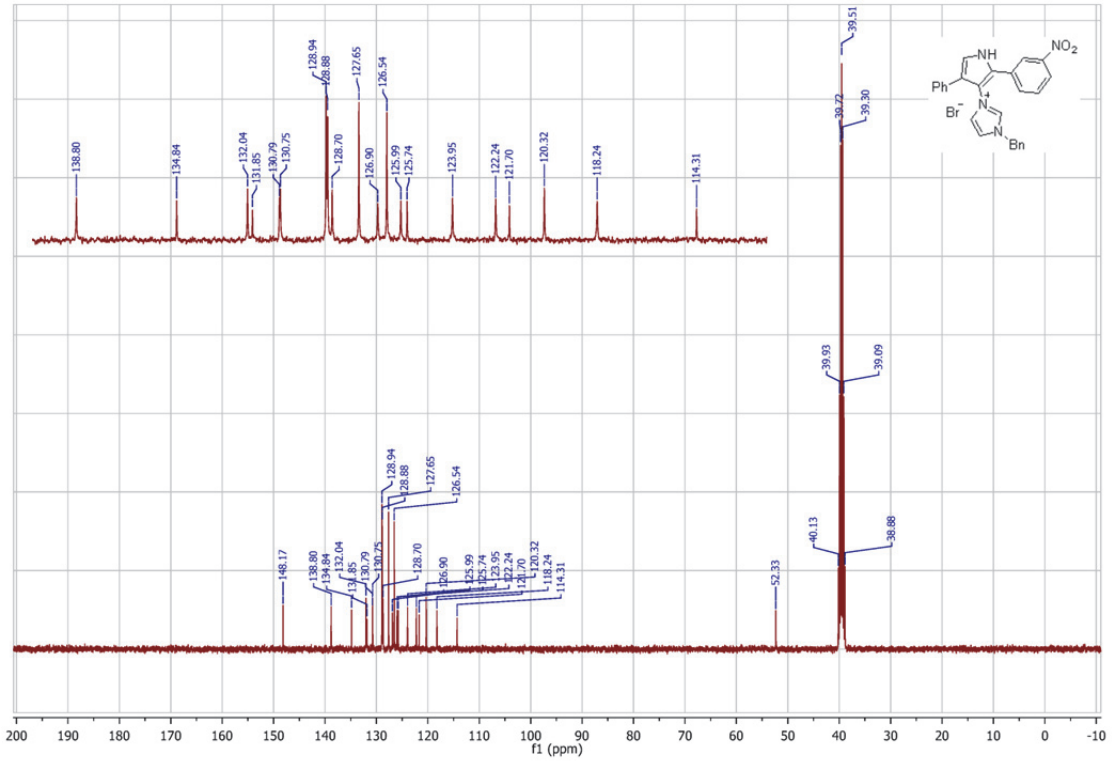
^{13}C NMR spectrum of 1-benzyl-3-(2-(4-nitrophenyl)-4-phenyl-1*H*-pyrrol-3-yl)-1*H*-imidazol-3-ium bromide (4o), DMSO-d_6



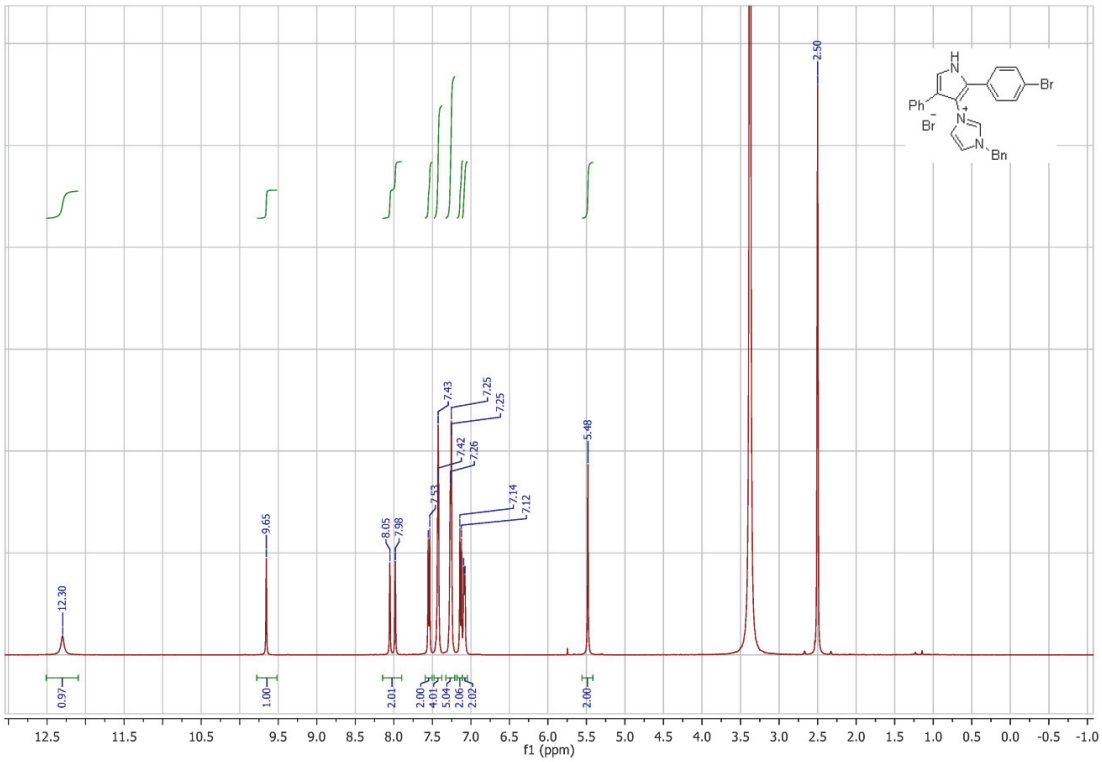
^{1}H NMR spectrum of 1-benzyl-3-(2-(3-nitrophenyl)-4-phenyl-1*H*-pyrrol-3-yl)-1*H*-imidazol-3-ium bromide (4p), DMSO-d_6



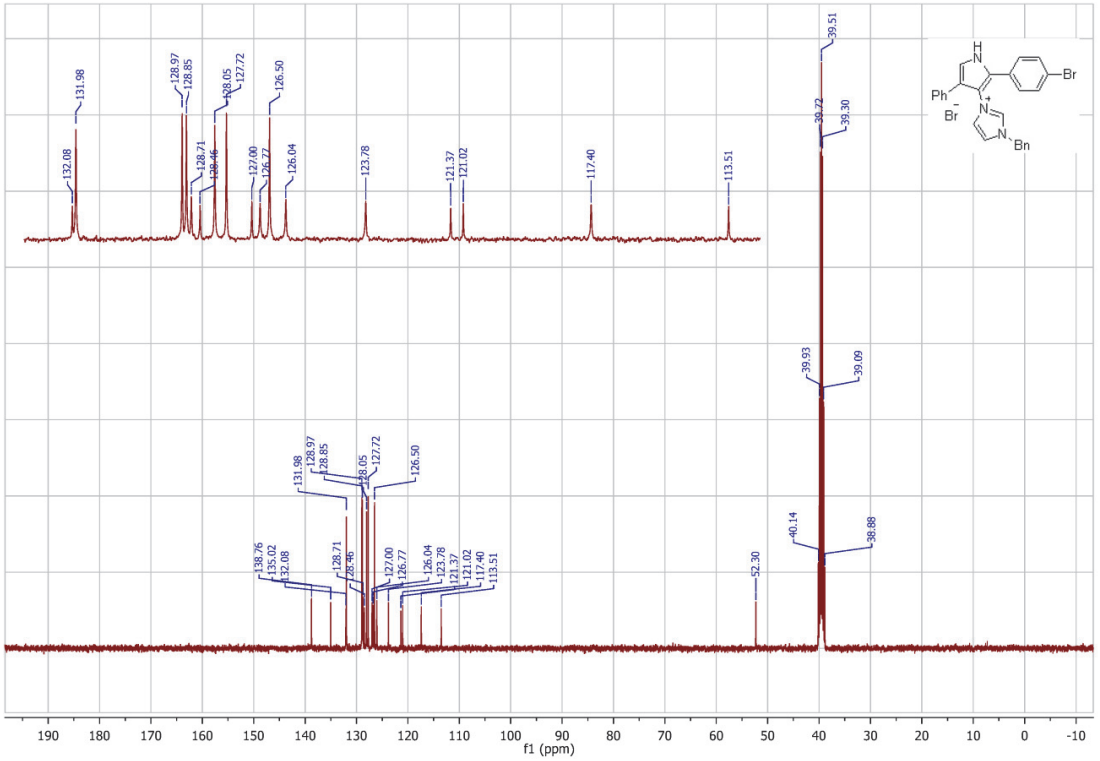
^{13}C NMR spectrum of 1-benzyl-3-(2-(3-nitrophenyl)-4-phenyl-1*H*-pyrrol-3-yl)-1*H*-imidazol-3-ium bromide (4p), DMSO-d_6



^{1}H NMR spectrum of 1-benzyl-3-(2-(4-bromophenyl)-4-phenyl-1*H*-pyrrol-3-yl)-1*H*-imidazol-3-ium bromide (4q), DMSO-d_6



^{13}C NMR spectrum of 1-benzyl-3-(2-(4-bromophenyl)-4-phenyl-1*H*-pyrrol-3-yl)-1*H*-imidazol-3-ium bromide (4q), DMSO-d_6



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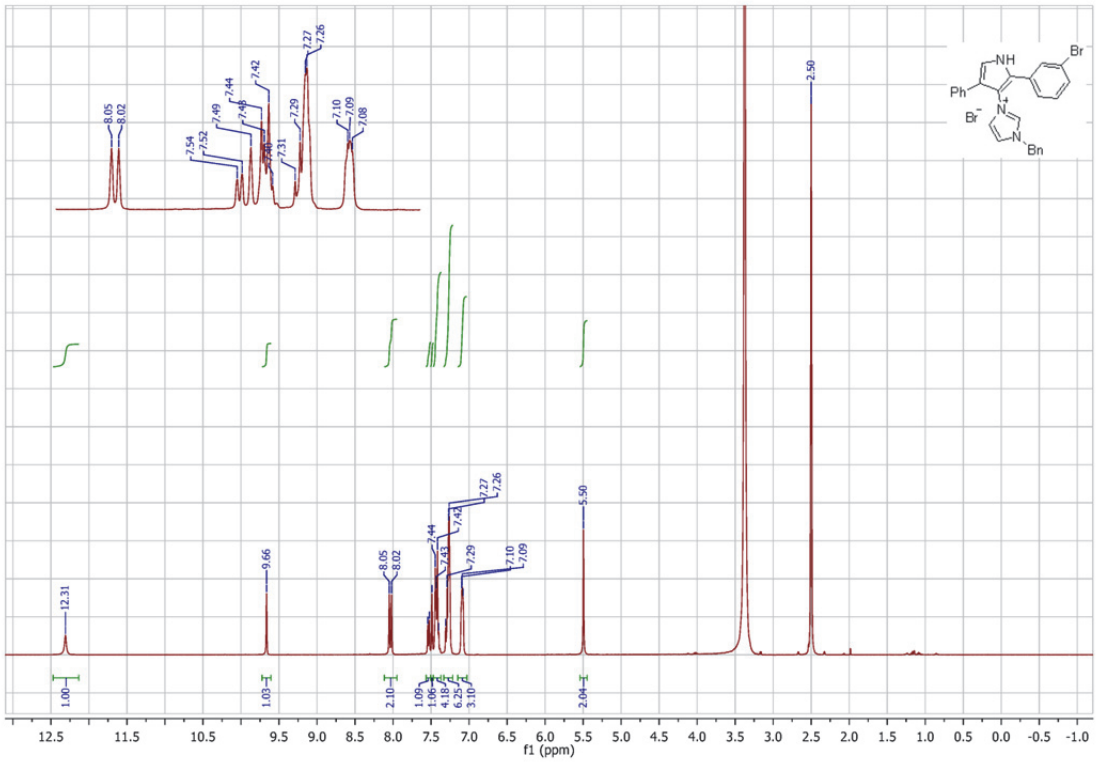
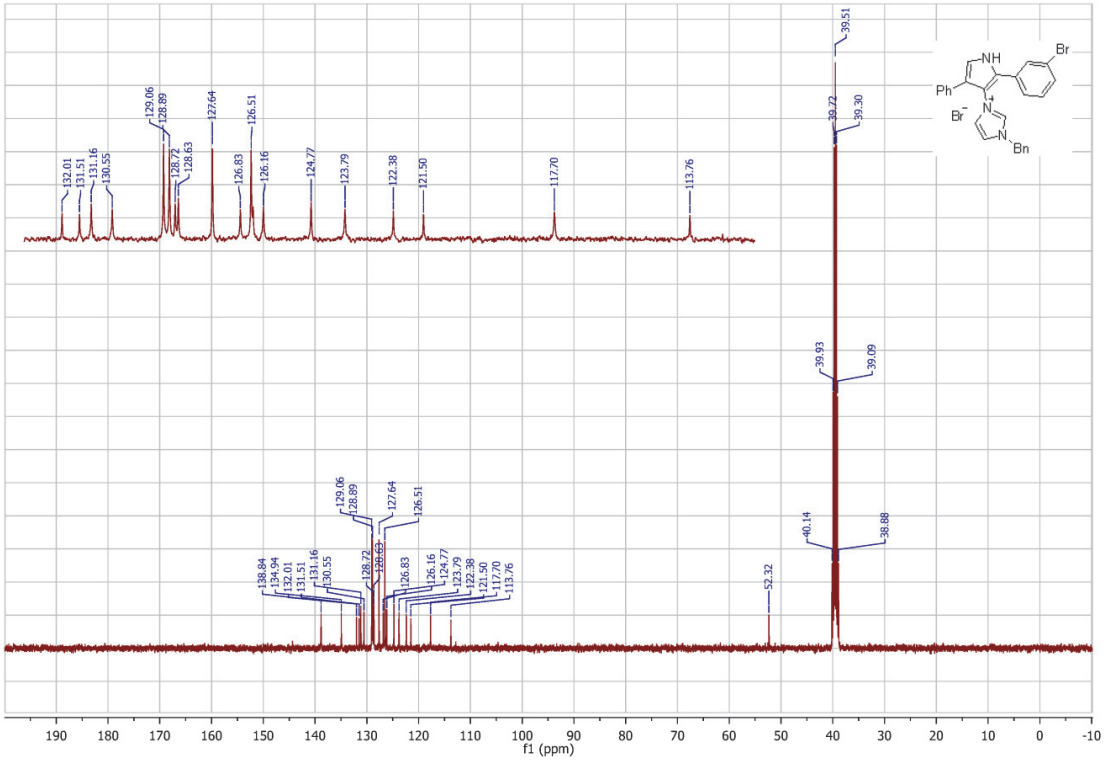
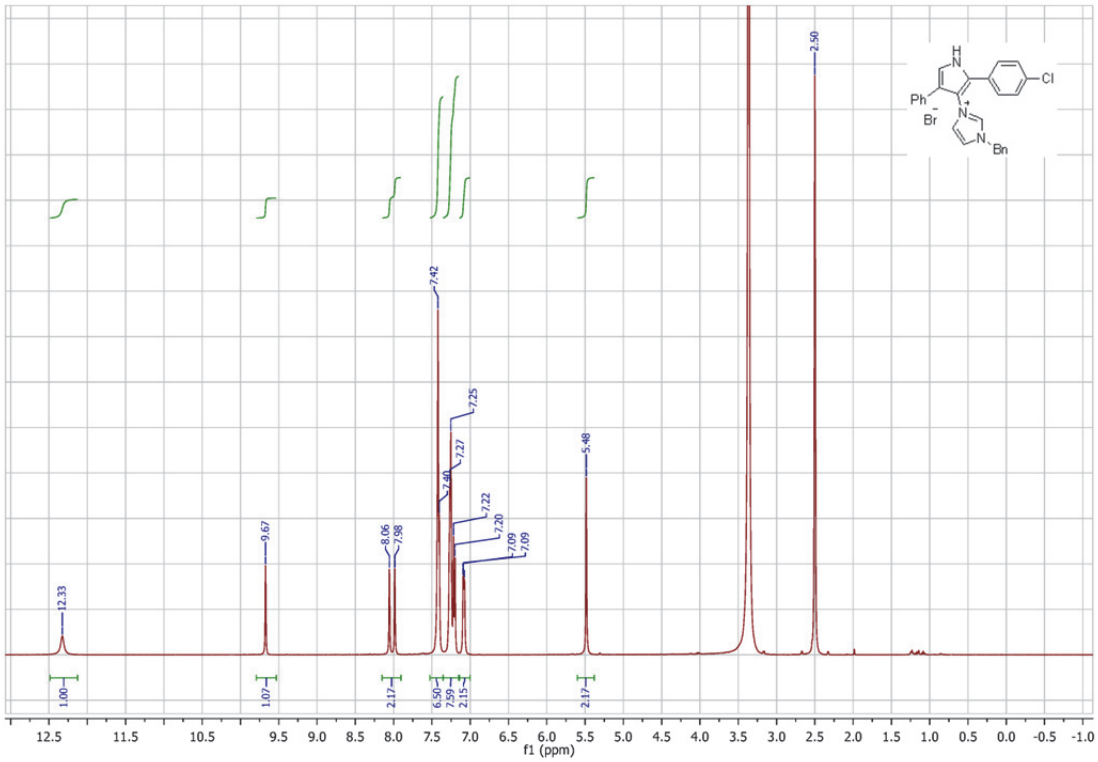


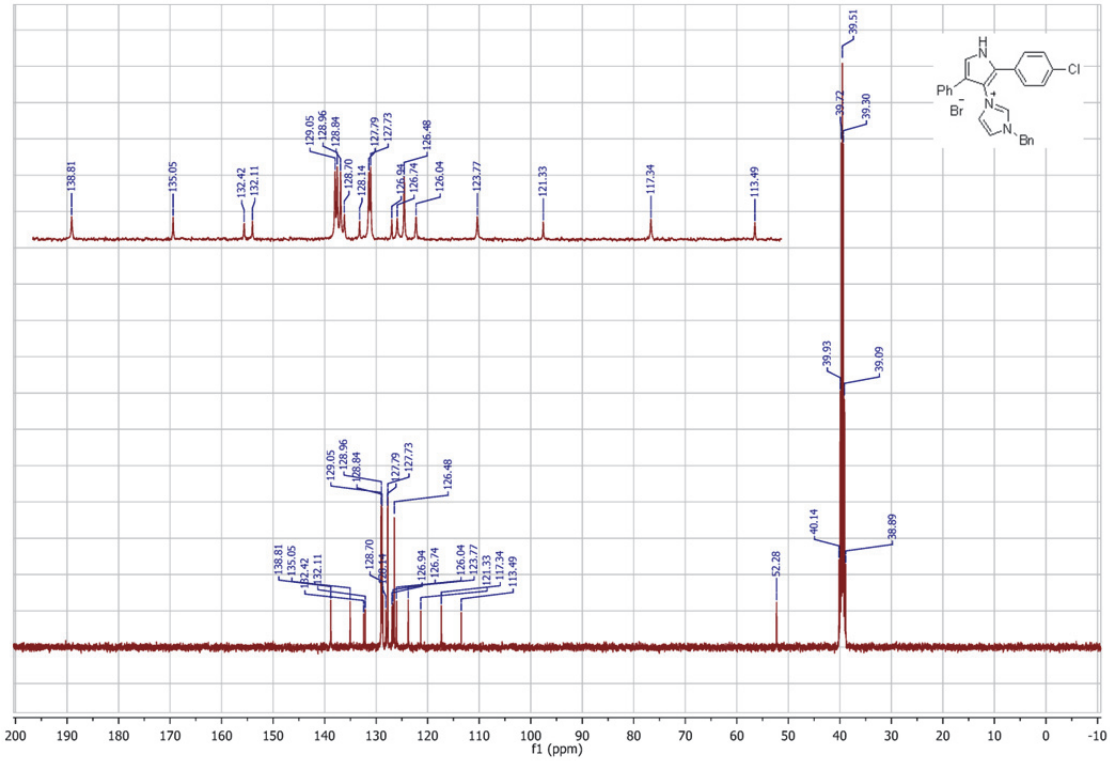
^{13}C NMR spectrum of 1-benzyl-3-(2-(3-bromophenyl)-4-phenyl-1*H*-pyrrol-3-yl)-1*H*-imidazol-3-ium bromide (4r), DMSO-d_6



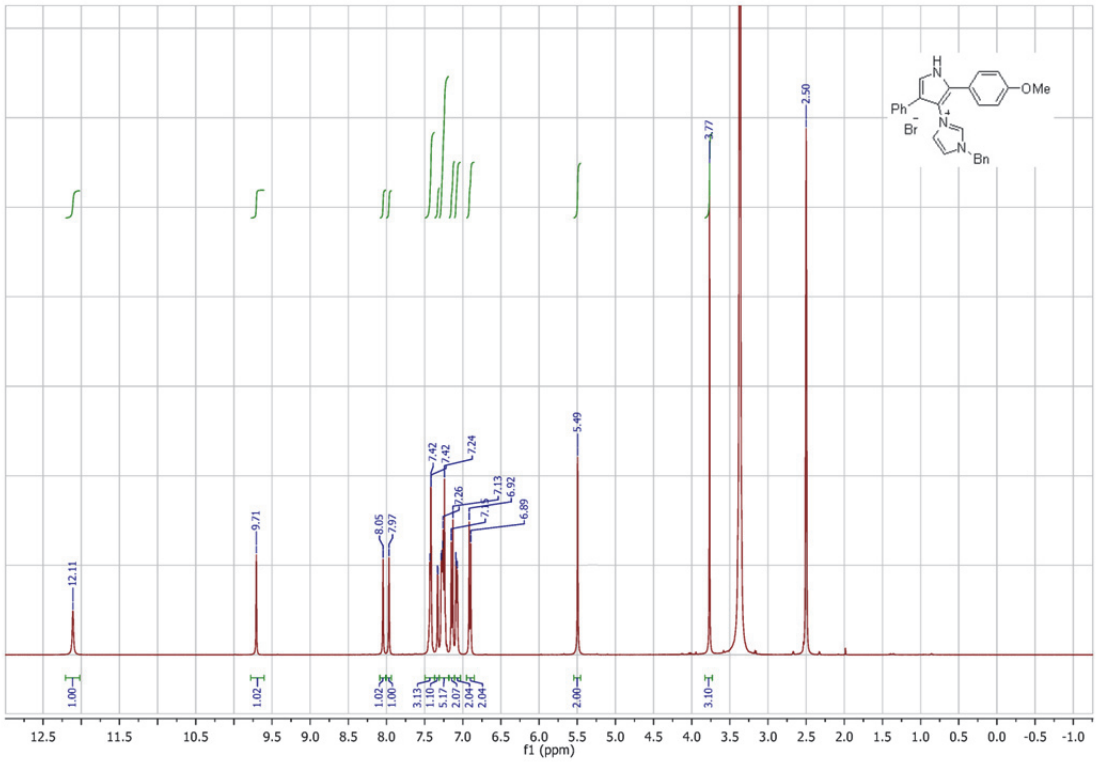
^{1}H NMR spectrum of 1-benzyl-3-(2-(4-chlorophenyl)-4-phenyl-1*H*-pyrrol-3-yl)-1*H*-imidazol-3-ium bromide (4s), DMSO-d_6



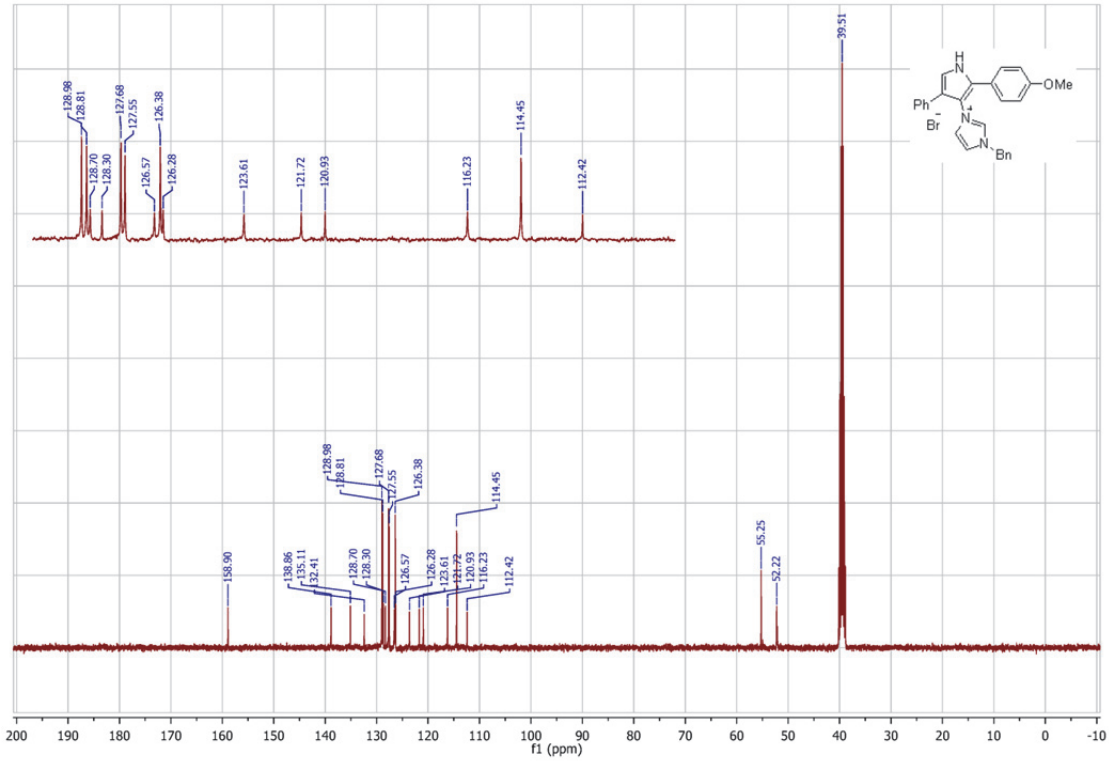
^{13}C NMR spectrum of 1-benzyl-3-(2-(4-chlorophenyl)-4-phenyl-1*H*-pyrrol-3-yl)-1*H*-imidazol-3-ium bromide (4s), DMSO-d_6



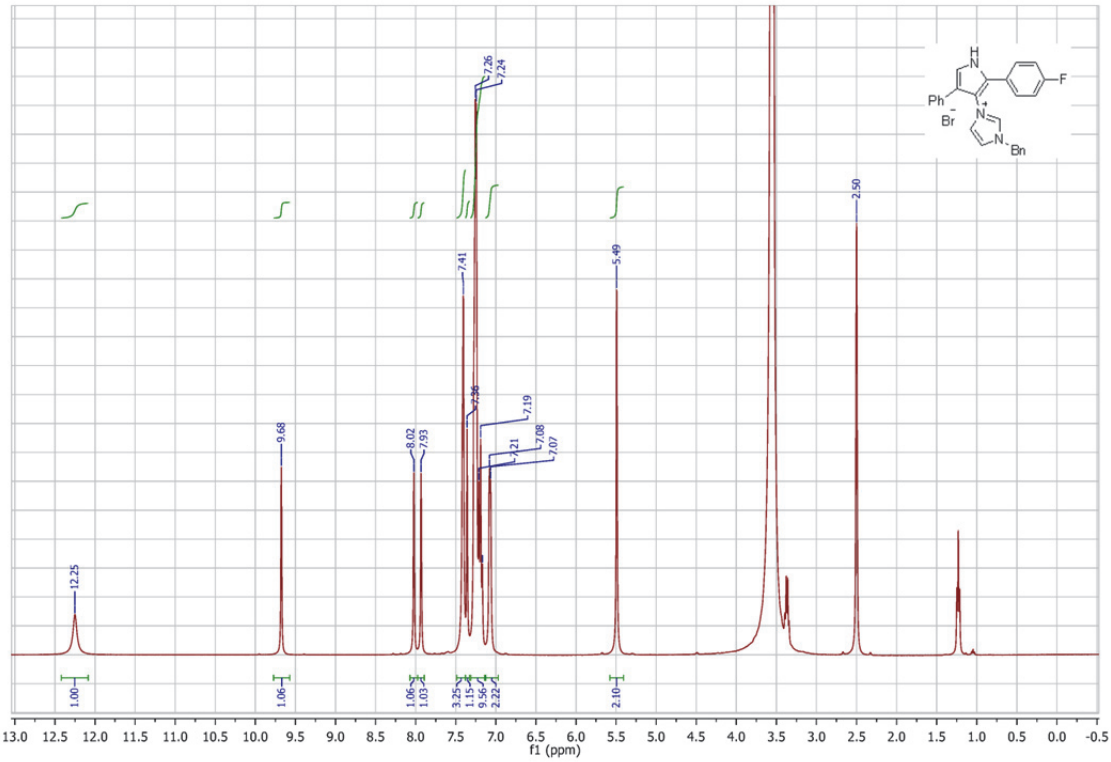
^{1}H NMR spectrum of 1-benzyl-3-(2-(4-methoxyphenyl)-4-phenyl-1*H*-pyrrol-3-yl)-1*H*-imidazol-3-ium bromide (4t), DMSO-d_6



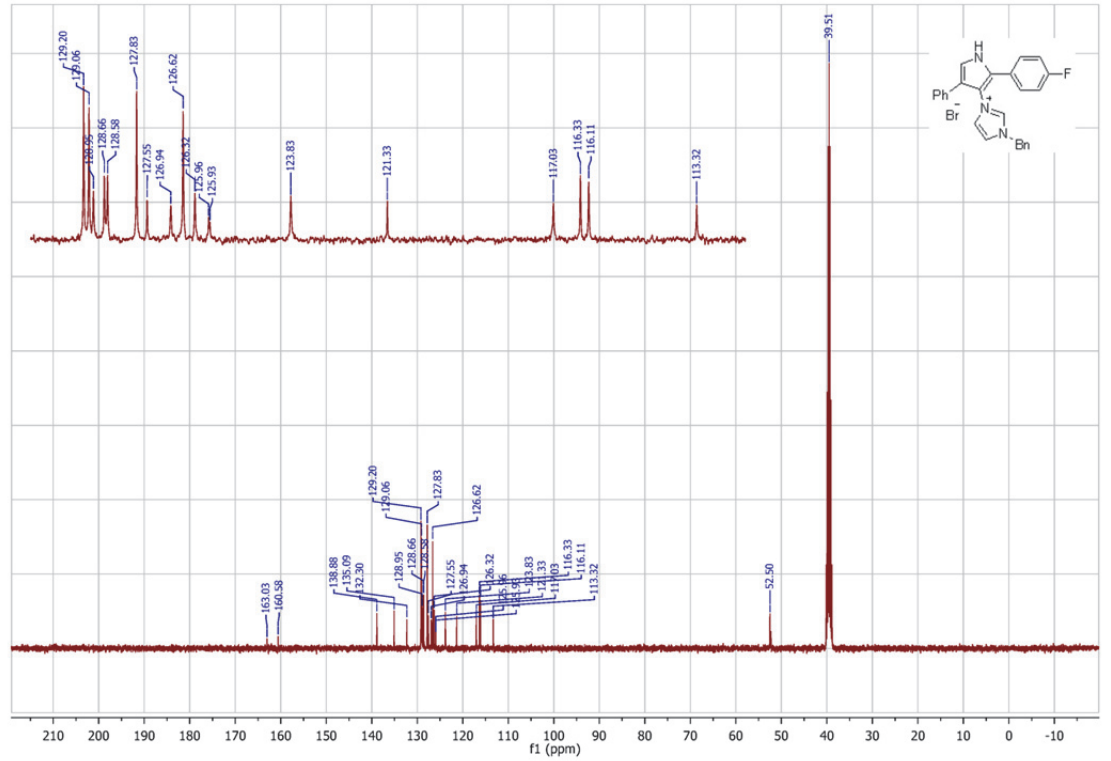
^{13}C NMR spectrum of 1-benzyl-3-(2-(4-methoxyphenyl)-4-phenyl-1*H*-pyrrol-3-yl)-1*H*-imidazol-3-ium bromide (4t), DMSO-d_6



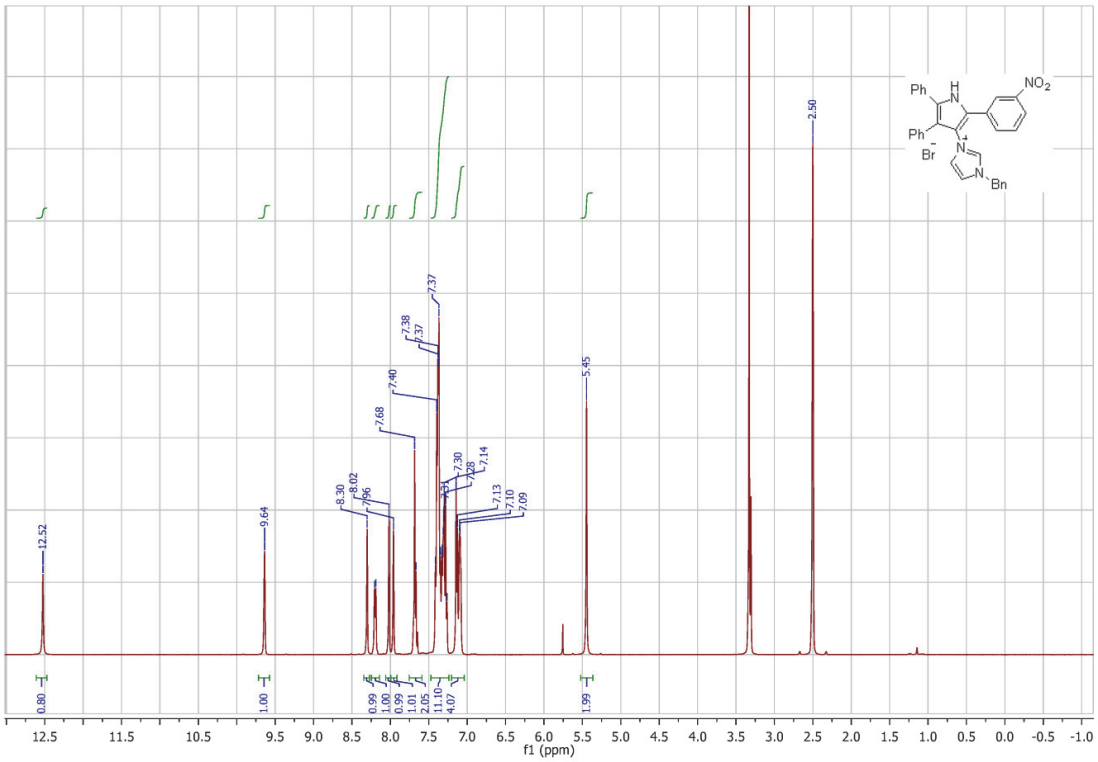
^{1}H NMR spectrum of 1-benzyl-3-(2-(4-fluorophenyl)-4-phenyl-1*H*-pyrrol-3-yl)-1*H*-imidazol-3-ium bromide (4u), DMSO-d_6



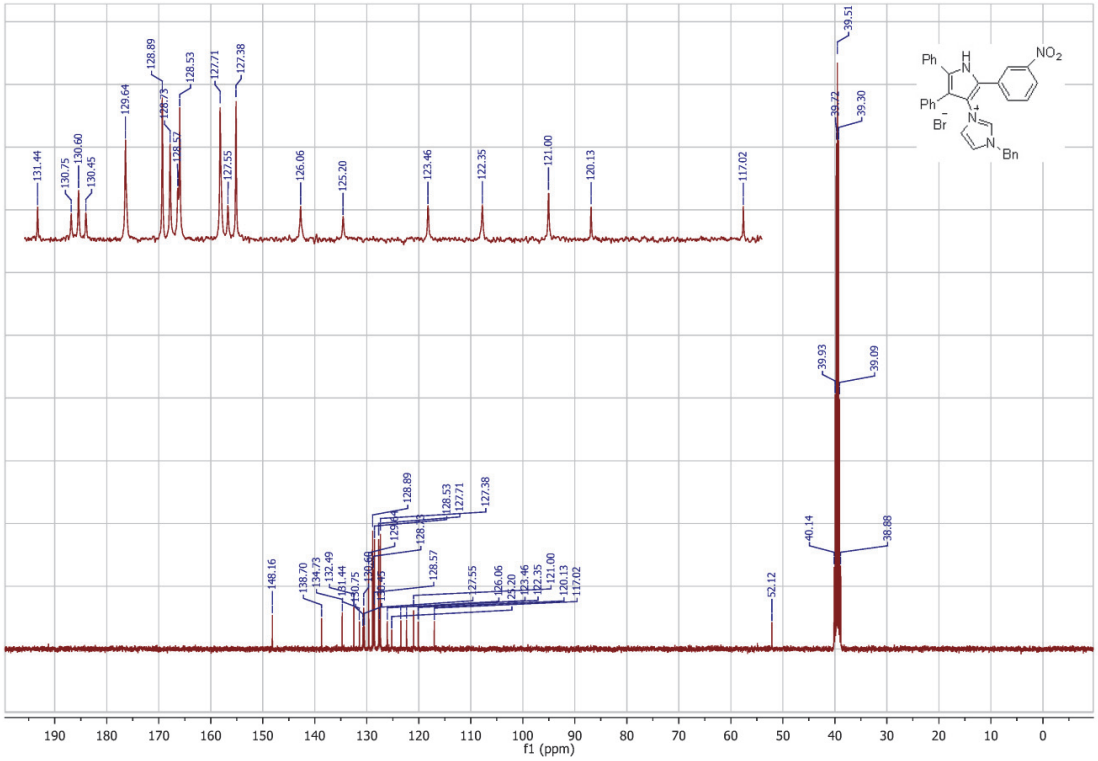
^{13}C NMR spectrum of 1-benzyl-3-(2-(4-fluorophenyl)-4-phenyl-1*H*-pyrrol-3-yl)-1*H*-imidazol-3-ium bromide (4u), DMSO-d_6



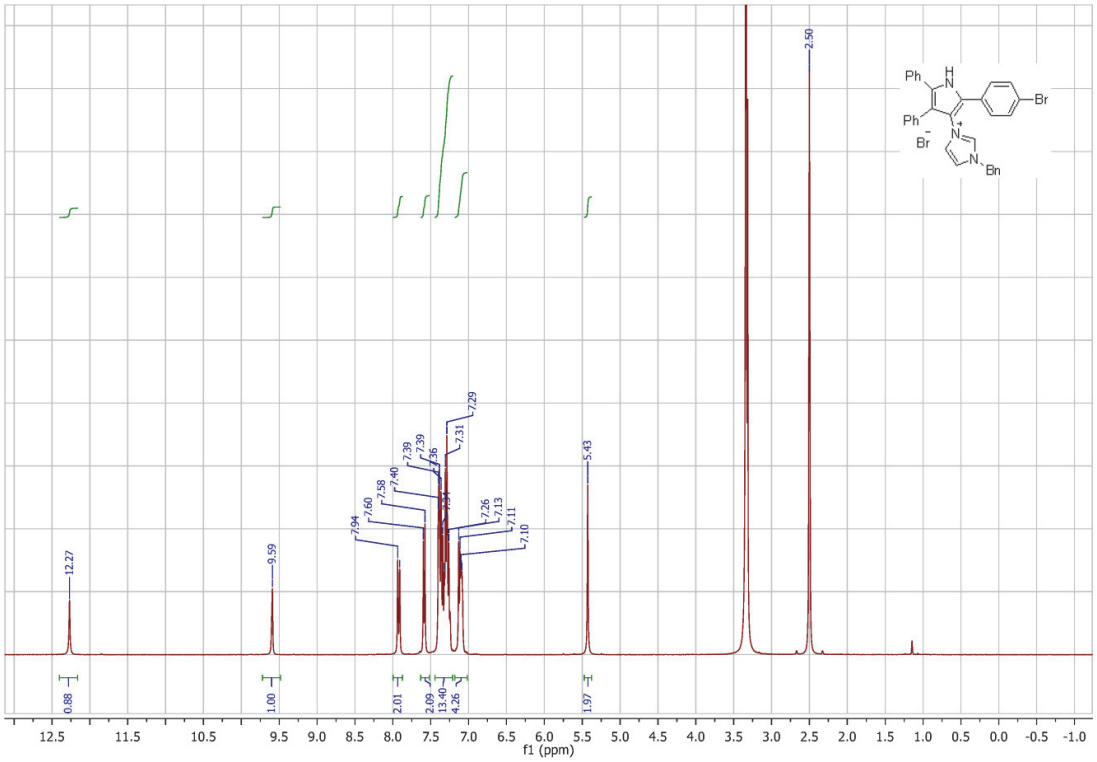
^{1}H NMR spectrum of 1-benzyl-3-(2-(3-nitrophenyl)-4,5-diphenyl-1*H*-pyrrol-3-yl)-1*H*-imidazol-3-ium bromide (4v), DMSO-d_6



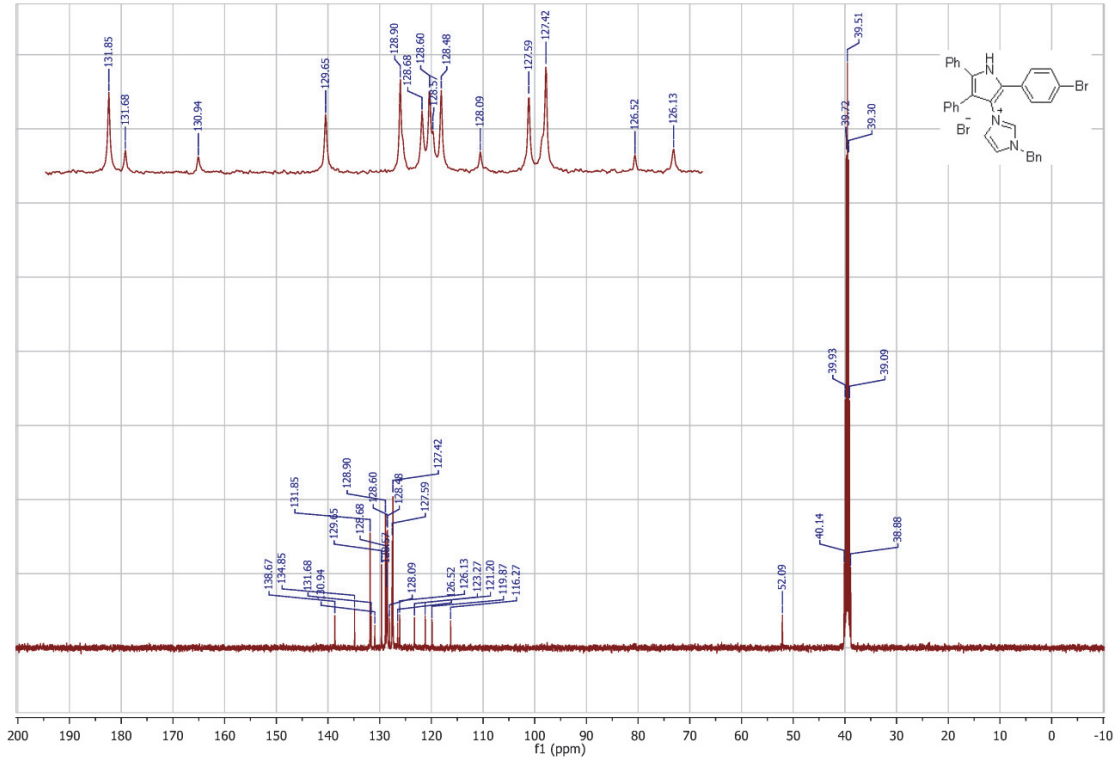
^{13}C NMR spectrum of 1-benzyl-3-(2-(3-nitrophenyl)-4,5-diphenyl-1*H*-pyrrol-3-yl)-1*H*-imidazol-3-ium bromide (4v), DMSO-d_6



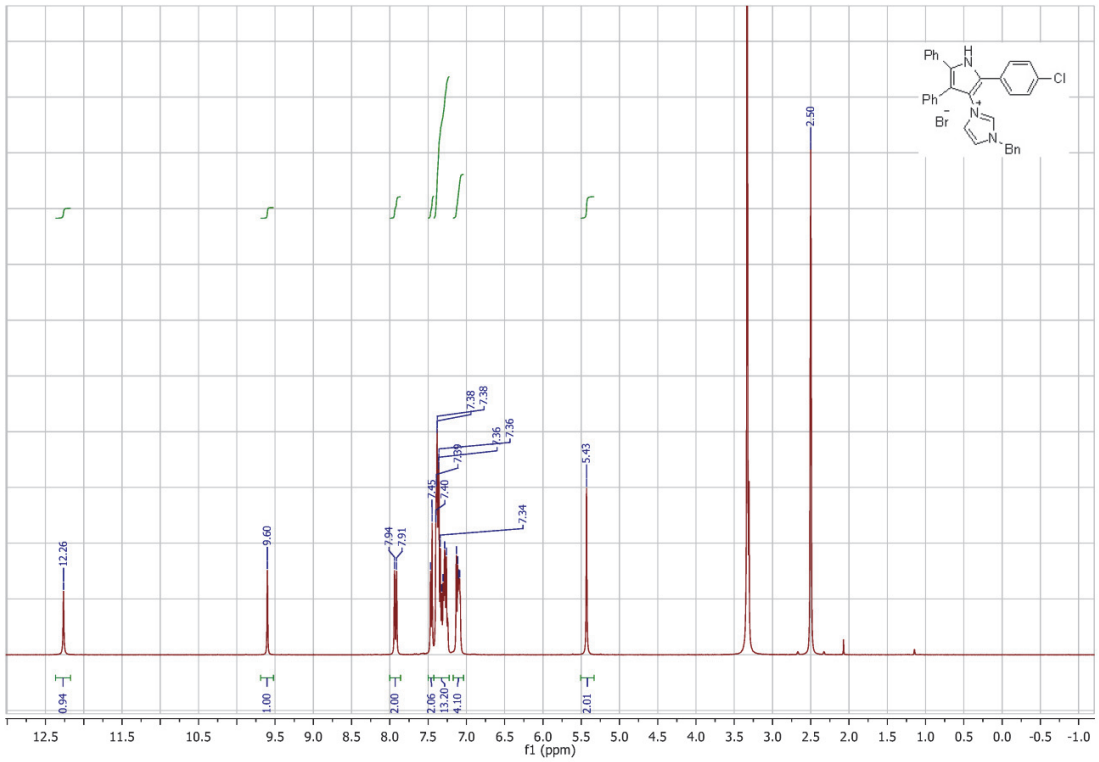
^{1}H NMR spectrum of 1-benzyl-3-(2-(4-bromophenyl)-4,5-diphenyl-1*H*-pyrrol-3-yl)-1*H*-imidazol-3-ium bromide (4w), DMSO-d_6



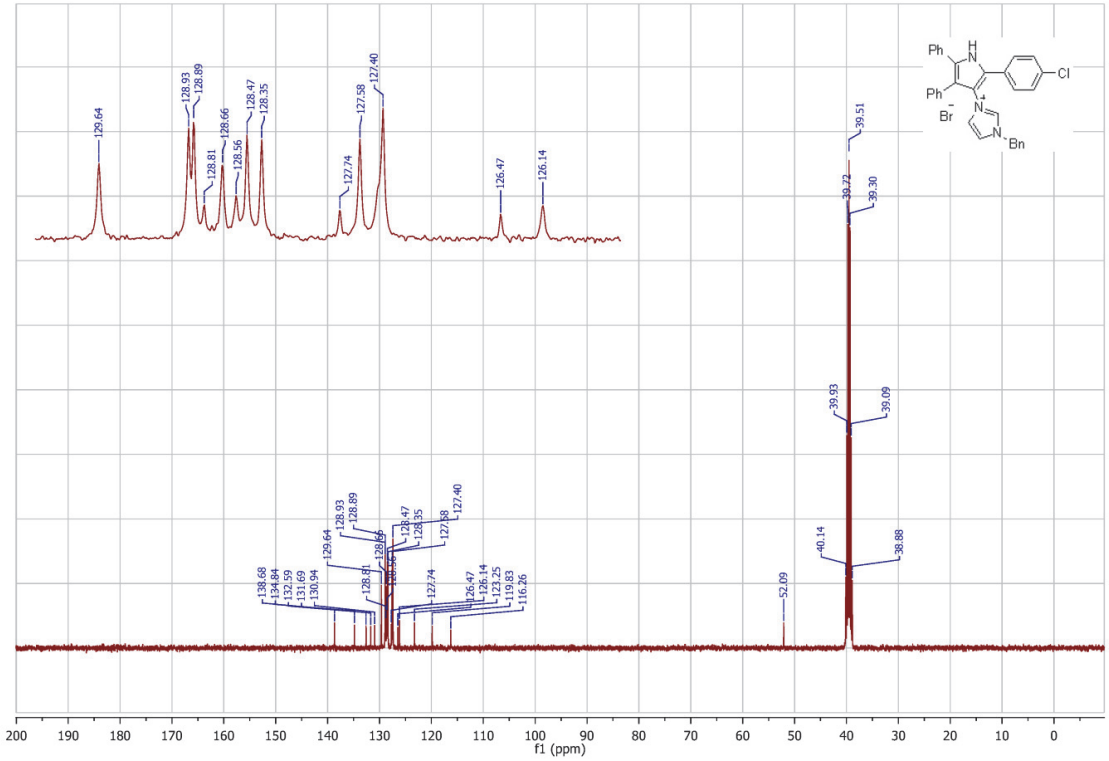
^{13}C NMR spectrum of 1-benzyl-3-(2-(4-bromophenyl)-4,5-diphenyl-1*H*-pyrrol-3-yl)-1*H*-imidazol-3-ium bromide (4w), DMSO-d_6



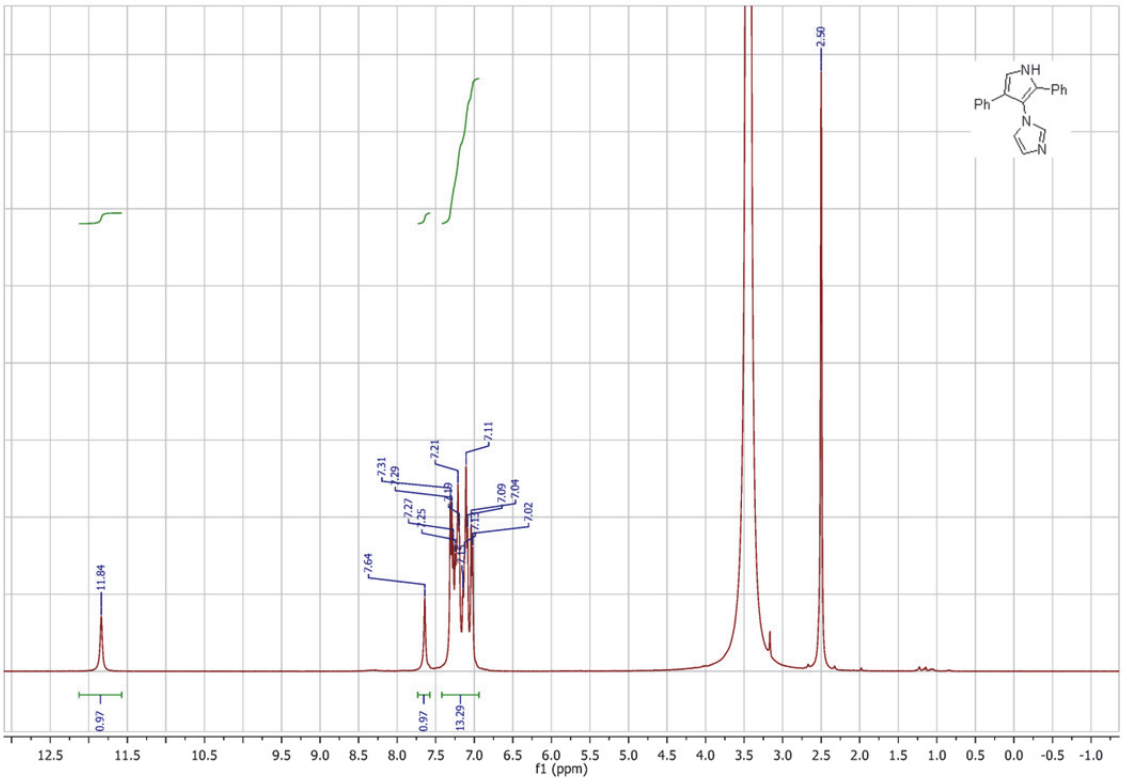
^{1}H NMR spectrum of 1-benzyl-3-(2-(4-chlorophenyl)-4,5-diphenyl-1*H*-pyrrol-3-yl)-1*H*-imidazol-3-ium bromide (4x), DMSO-d_6



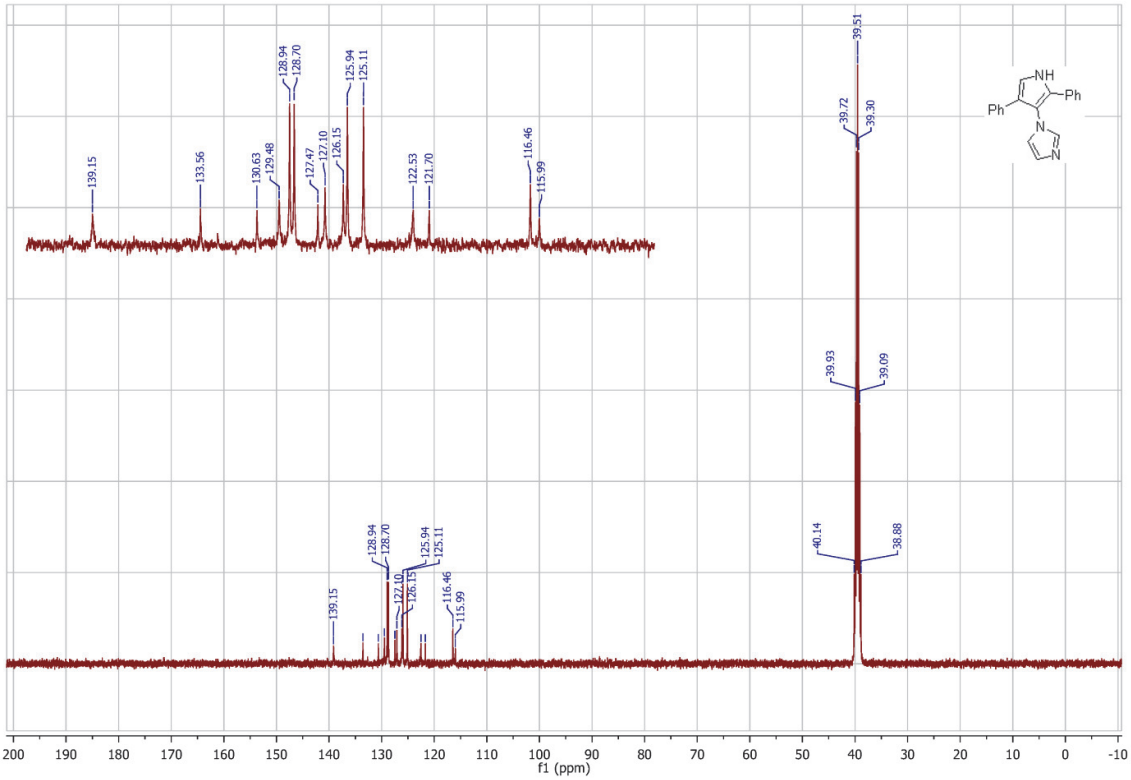
^{13}C NMR spectrum of 1-benzyl-3-(2-(4-chlorophenyl)-4,5-diphenyl-1*H*-pyrrol-3-yl)-1*H*-imidazol-3-ium bromide (4x), DMSO-d_6



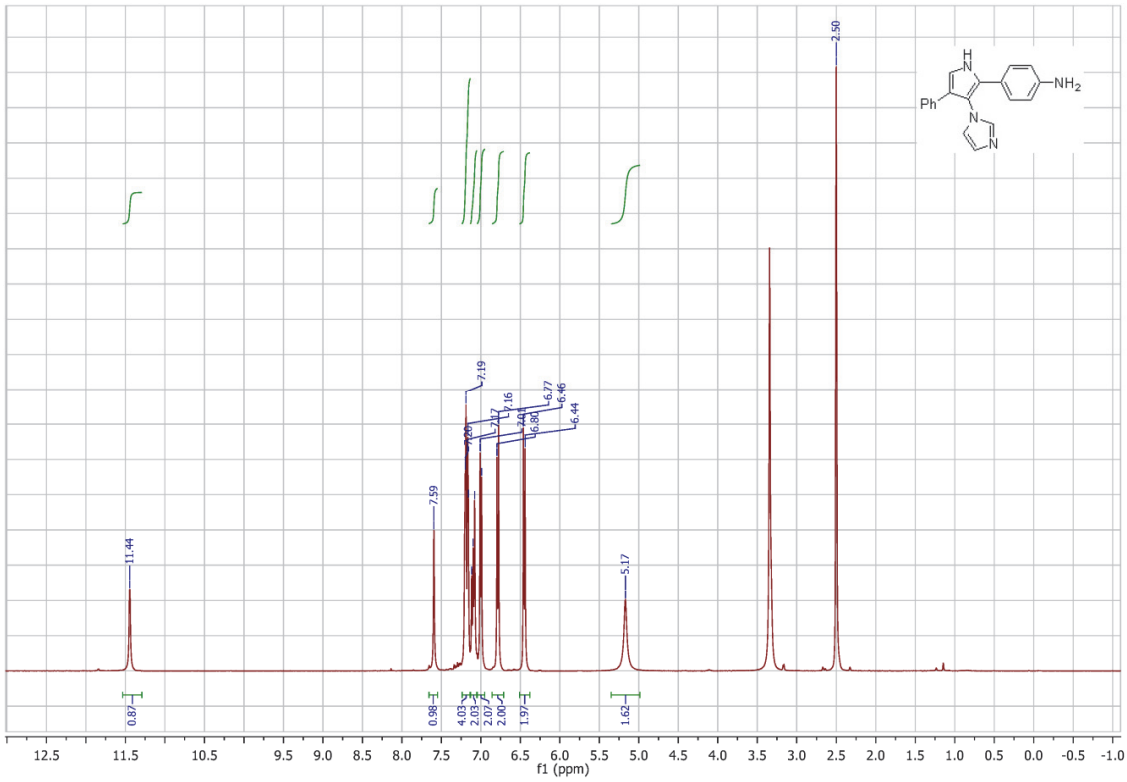
^{1}H NMR spectrum of 1-(2,4-diphenyl-1*H*-pyrrol-3-yl)-1*H*-imidazole (5a), DMSO-d_6



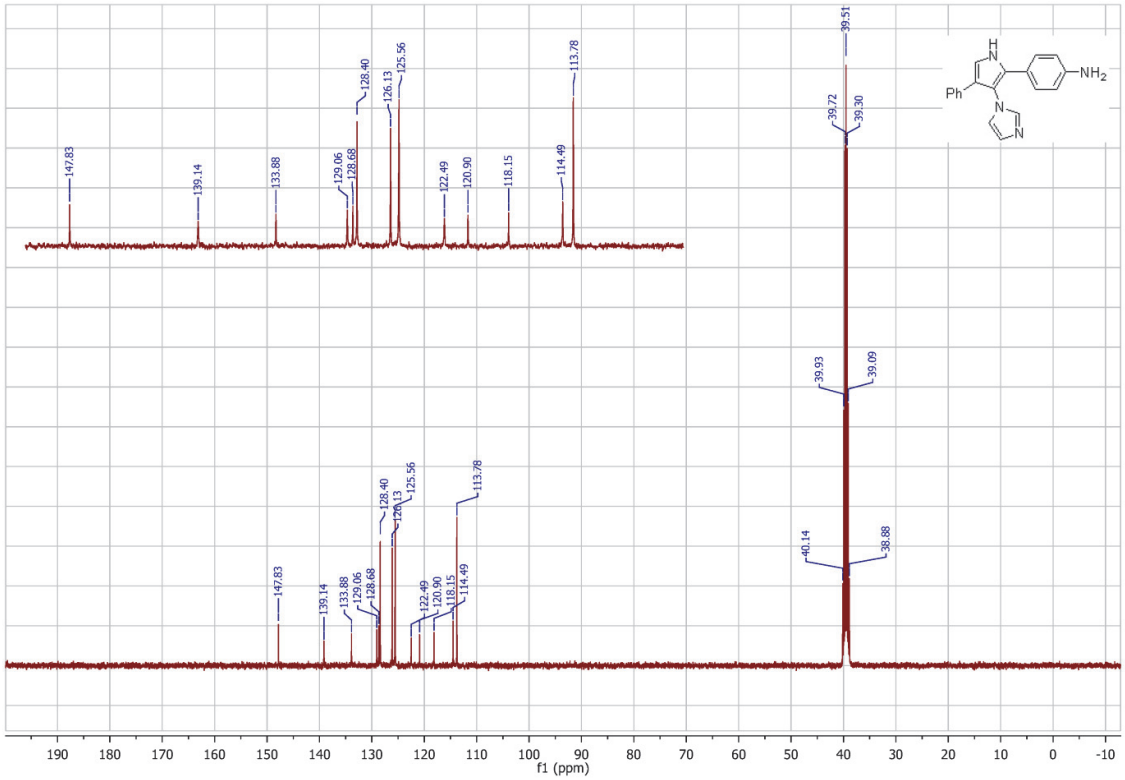
^{13}C NMR spectrum of 1-(2,4-diphenyl-1*H*-pyrrol-3-yl)-1*H*-imidazole (5a), DMSO-d_6



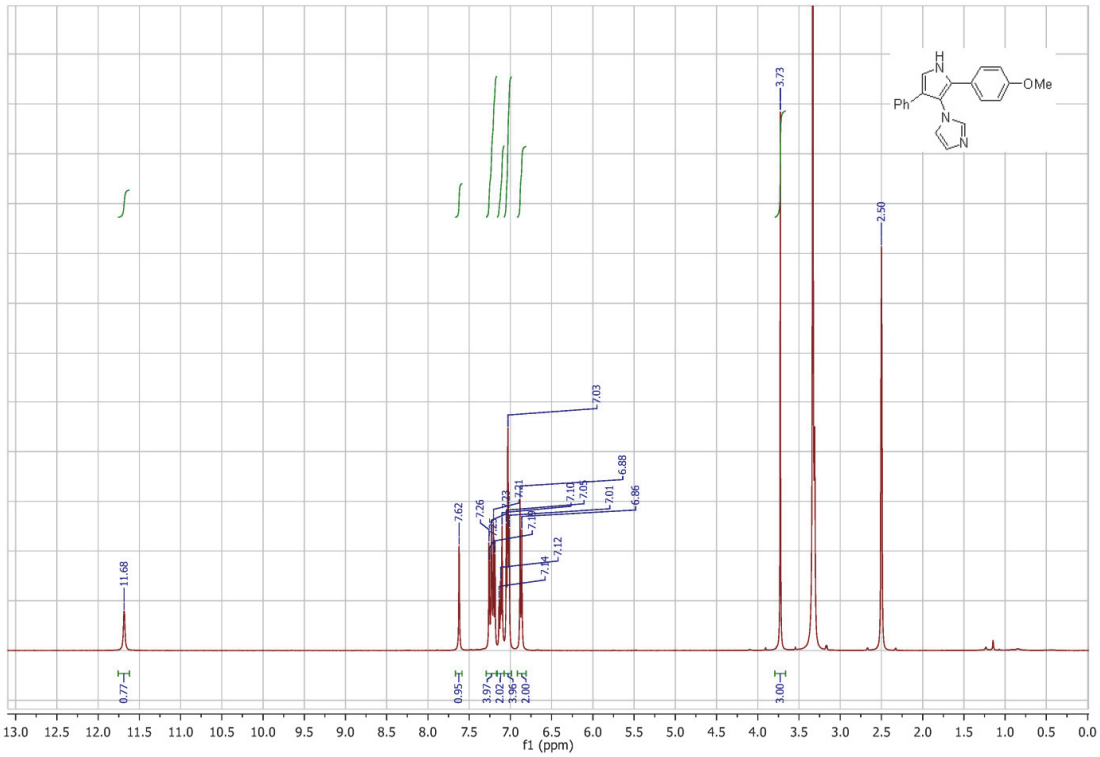
^{1}H NMR spectrum of 4-(3-(1*H*-imidazol-1-yl)-4-phenyl-1*H*-pyrrol-2-yl)aniline (5b), DMSO-d_6



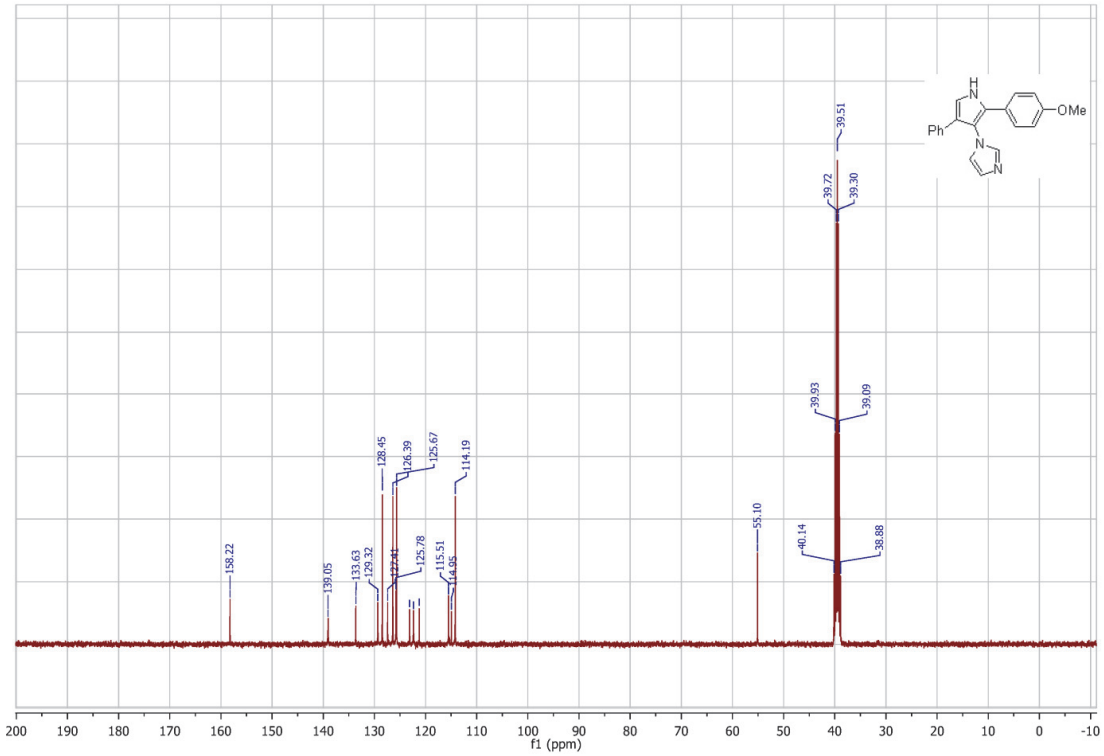
^{13}C NMR spectrum of 4-(3-(1*H*-imidazol-1-yl)-4-phenyl-1*H*-pyrrol-2-yl)aniline (5b), DMSO-d_6



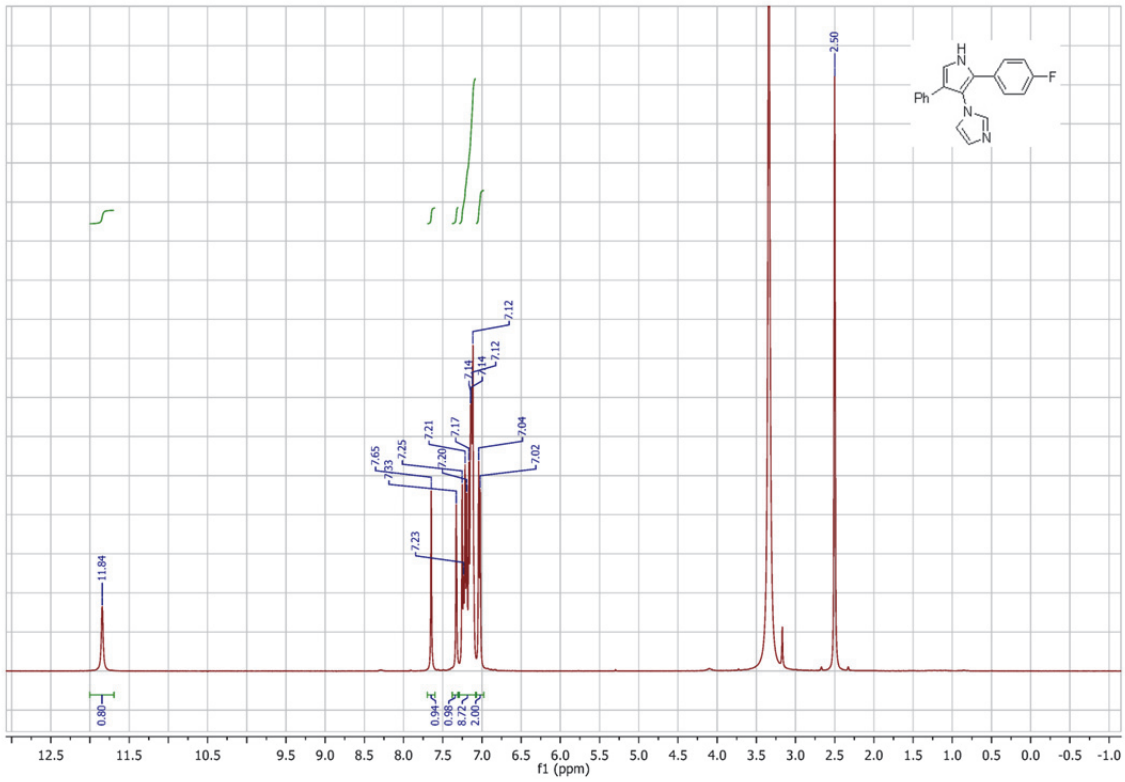
^{1}H NMR spectrum of 1-(2-(4-methoxyphenyl)-4-phenyl-1*H*-pyrrol-3-yl)-1*H*-imidazole (5c), DMSO-d_6



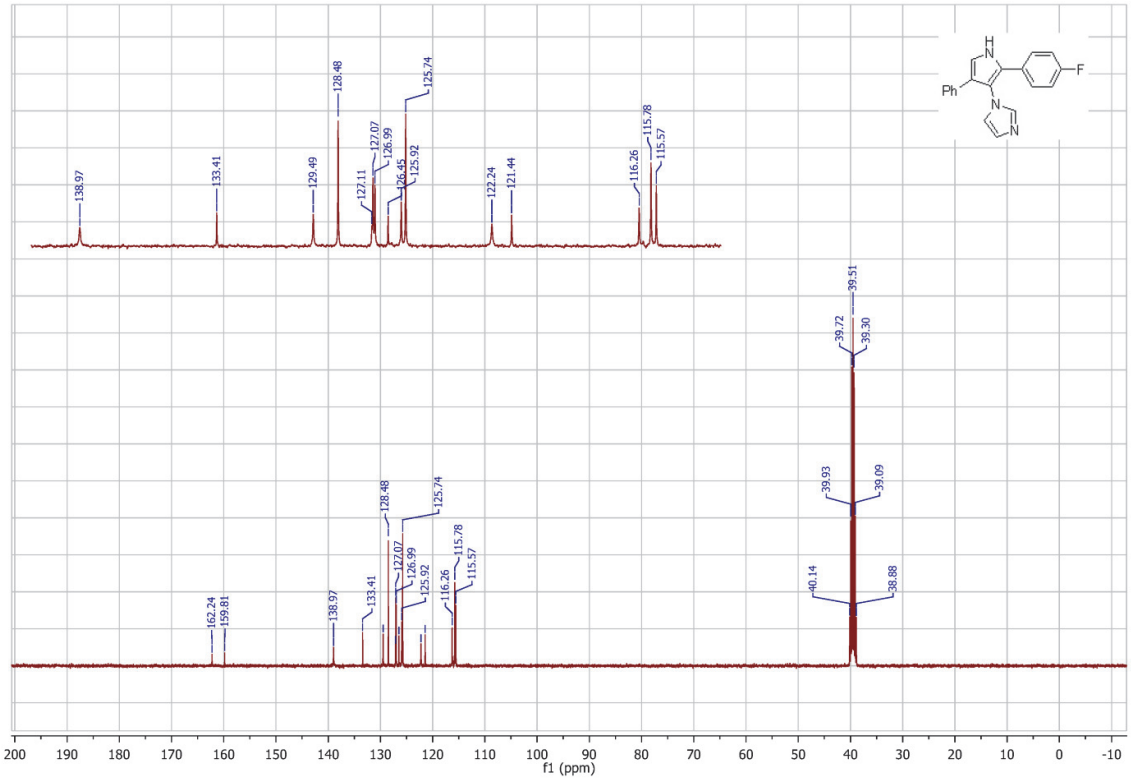
^{13}C NMR spectrum of 1-(2-(4-methoxyphenyl)-4-phenyl-1*H*-pyrrol-3-yl)-1*H*-imidazole (5c), DMSO-d_6



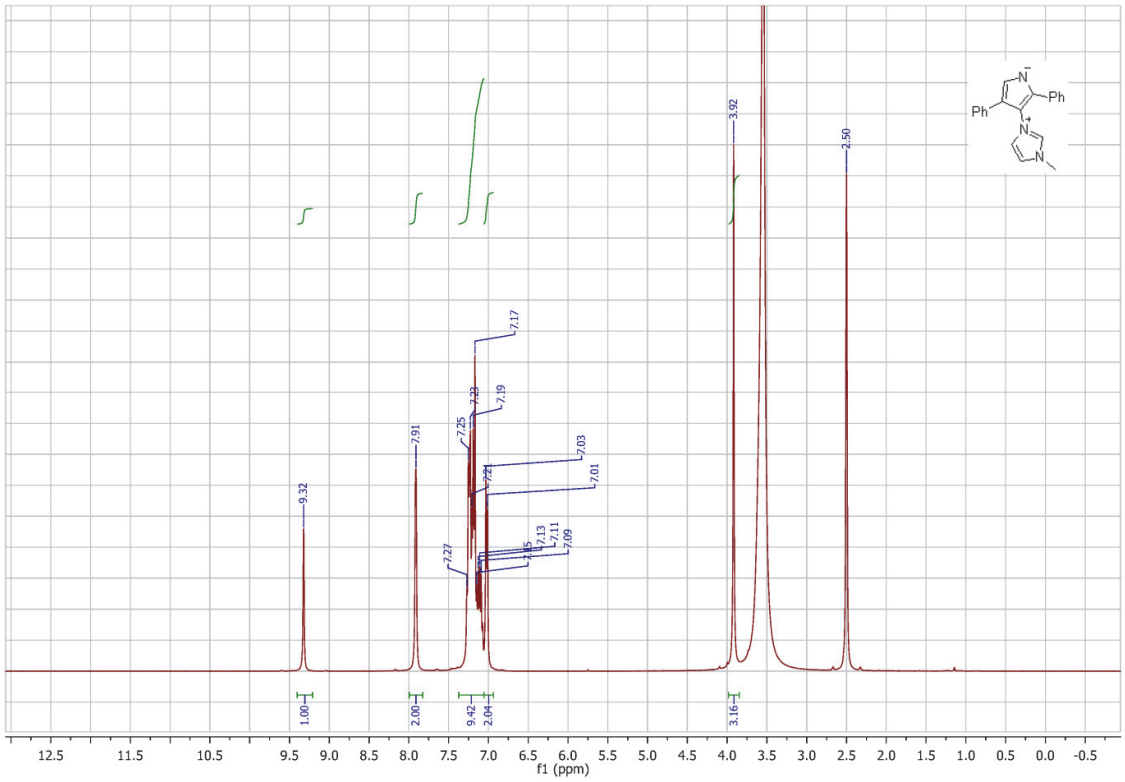
^{1}H NMR spectrum of 1-(2-(4-fluorophenyl)-4-phenyl-1*H*-pyrrol-3-yl)-1*H*-imidazole (5d), DMSO-d_6



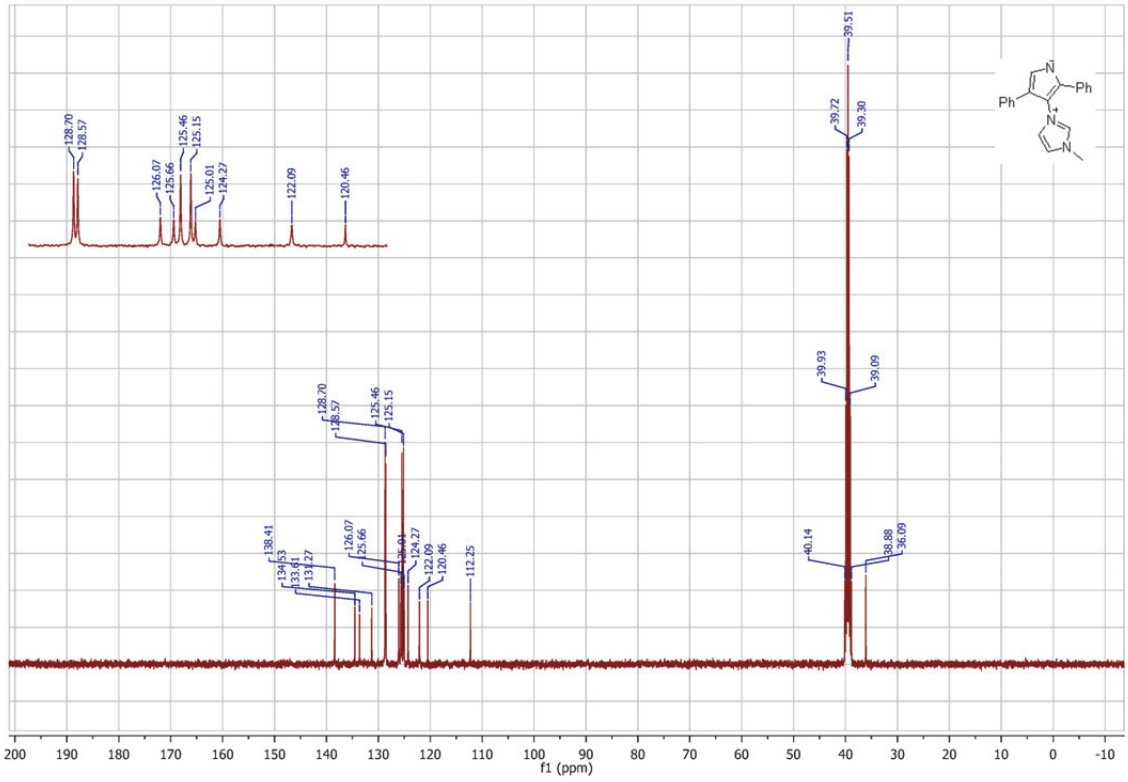
^{13}C NMR spectrum of 1-(2-(4-fluorophenyl)-4-phenyl-1*H*-pyrrol-3-yl)-1*H*-imidazole (5d), DMSO-d_6



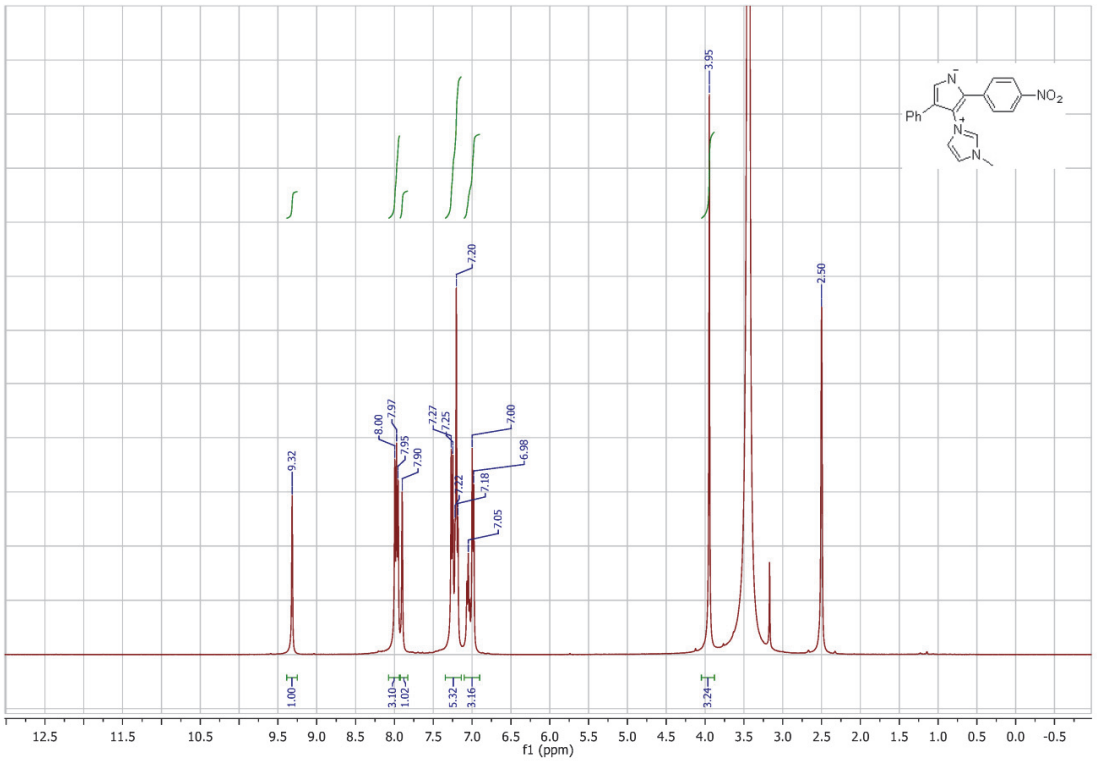
^{1}H NMR spectrum of 3-(1-methyl-1*H*-imidazol-3-ium-3-yl)-2,4-diphenylpyrrol-1-ide (6a), DMSO-d_6



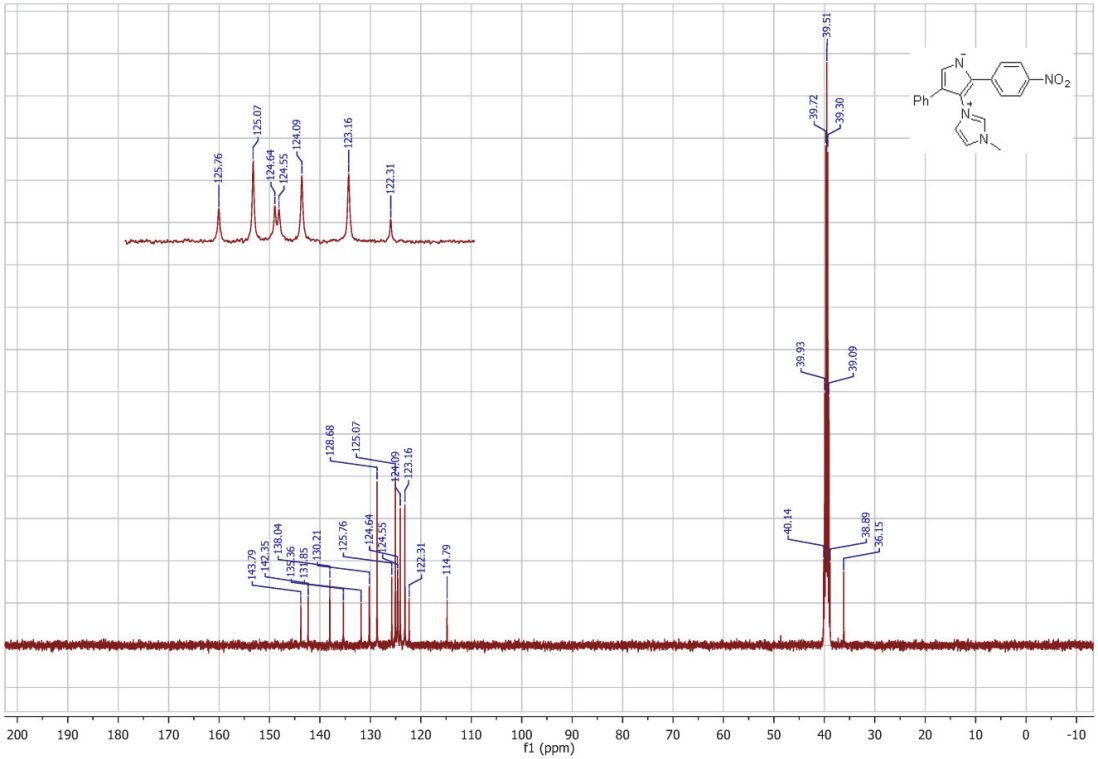
^{13}C NMR spectrum of 3-(1-methyl-1*H*-imidazol-3-ium-3-yl)-2,4-diphenylpyrrol-1-ide (6a), DMSO-d_6



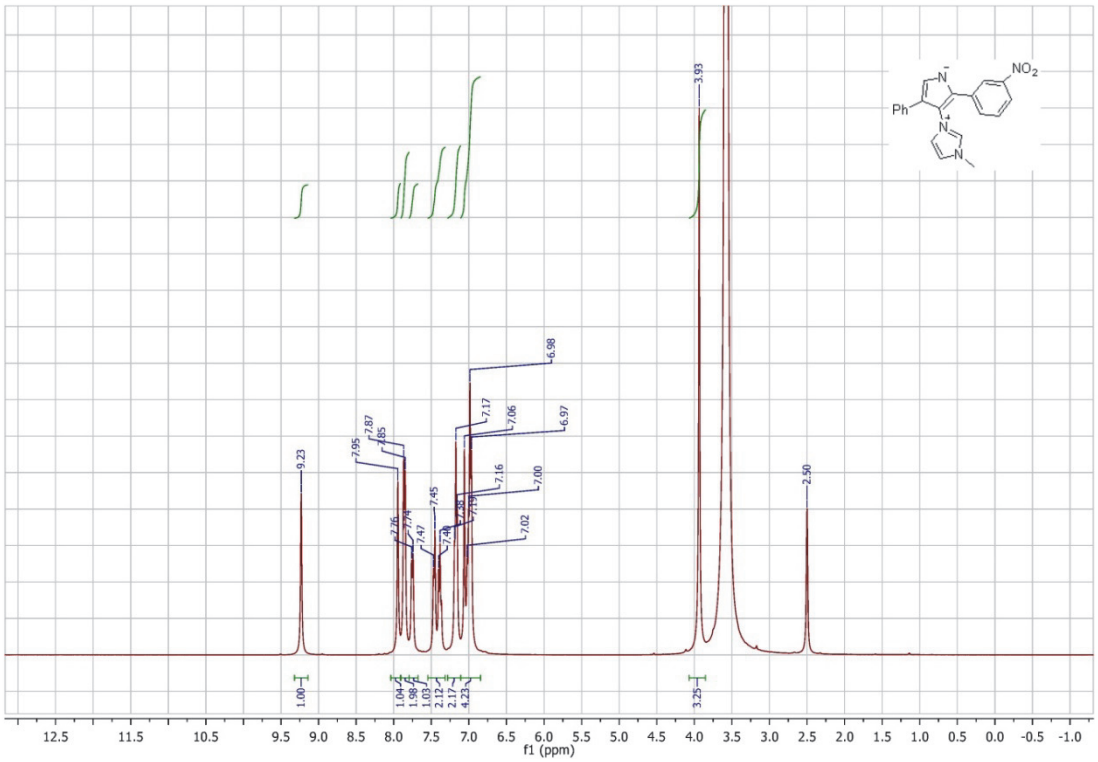
^{1}H NMR spectrum of 3-(1-methyl-1*H*-imidazol-3-ium-3-yl)-2-(4-nitrophenyl)-4-phenylpyrrol-1-ide (6b), DMSO-d_6



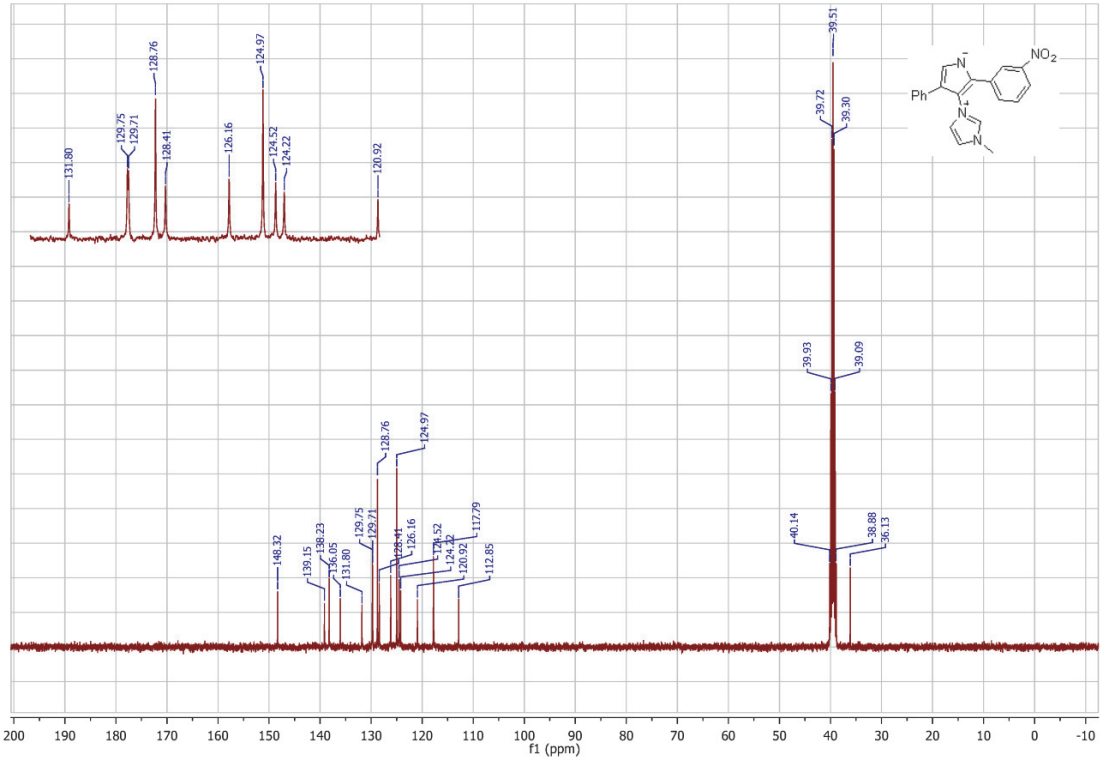
^{13}C NMR spectrum of 3-(1-methyl-1*H*-imidazol-3-ium-3-yl)-2-(4-nitrophenyl)-4-phenylpyrrol-1-ide (6b), DMSO-d_6



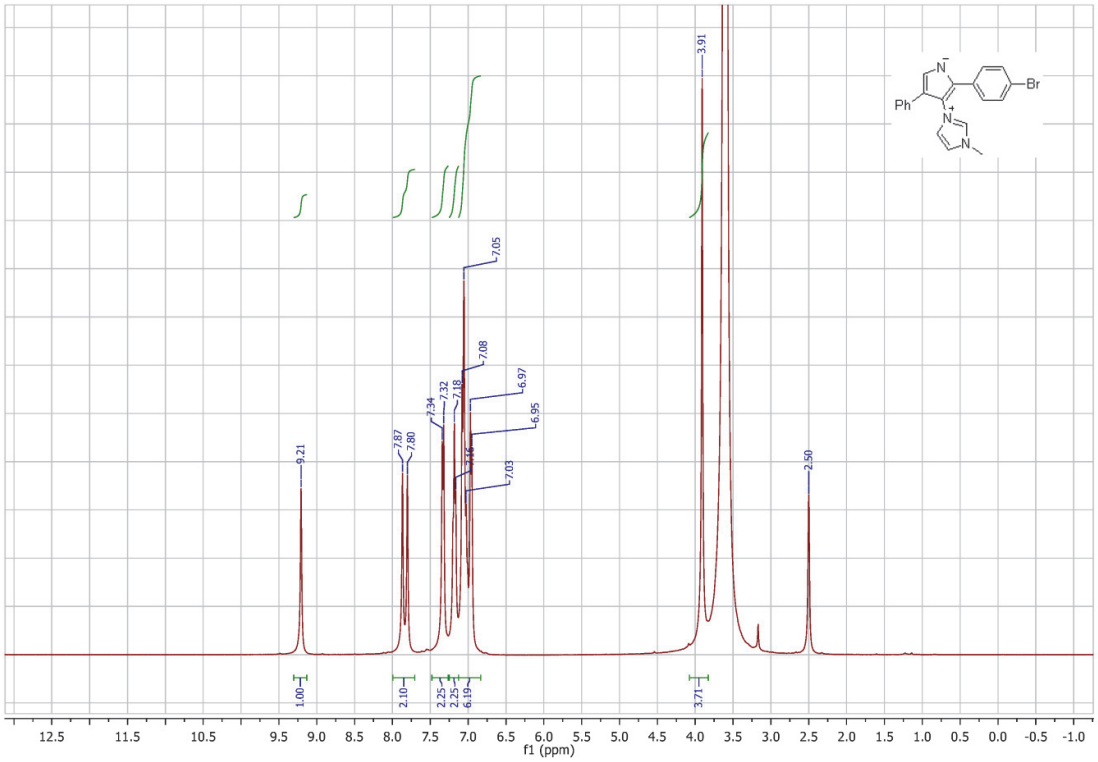
^{1}H NMR spectrum of 3-(1-methyl-1*H*-imidazol-3-ium-3-yl)-2-(3-nitrophenyl)-4-phenylpyrrol-1-ide (6c), DMSO-d_6



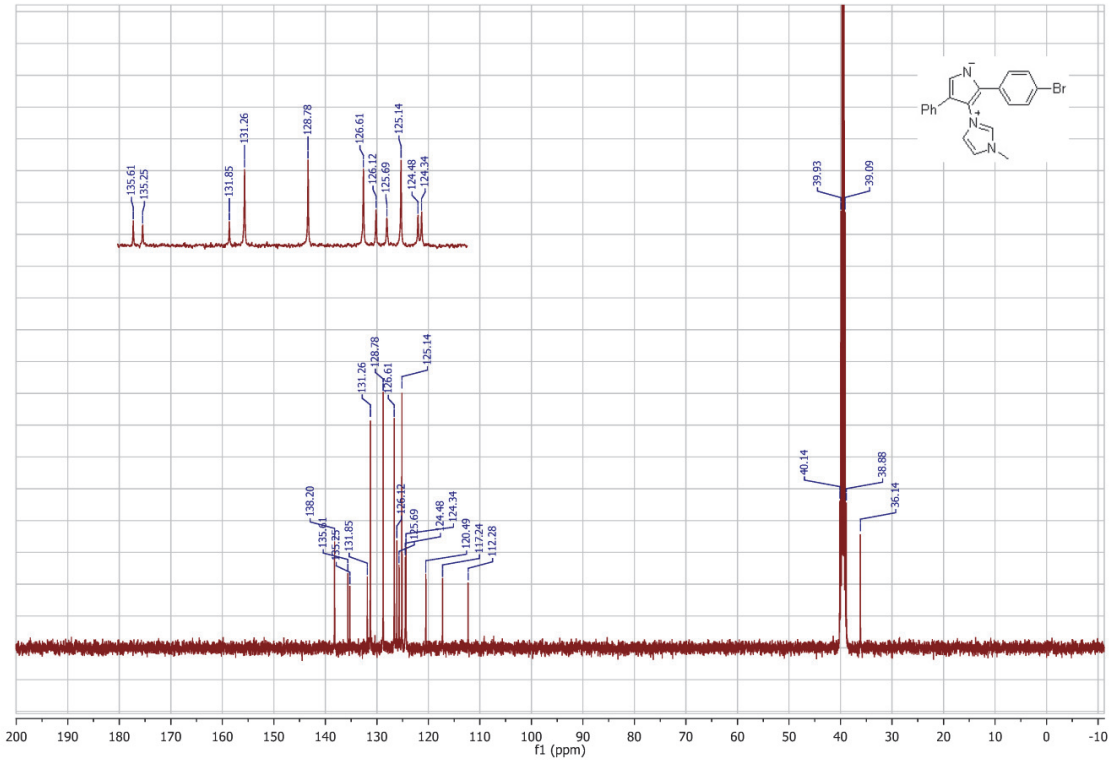
^{13}C NMR spectrum of 3-(1-methyl-1*H*-imidazol-3-ium-3-yl)-2-(3-nitrophenyl)-4-phenylpyrrol-1-ide (6c), DMSO-d_6



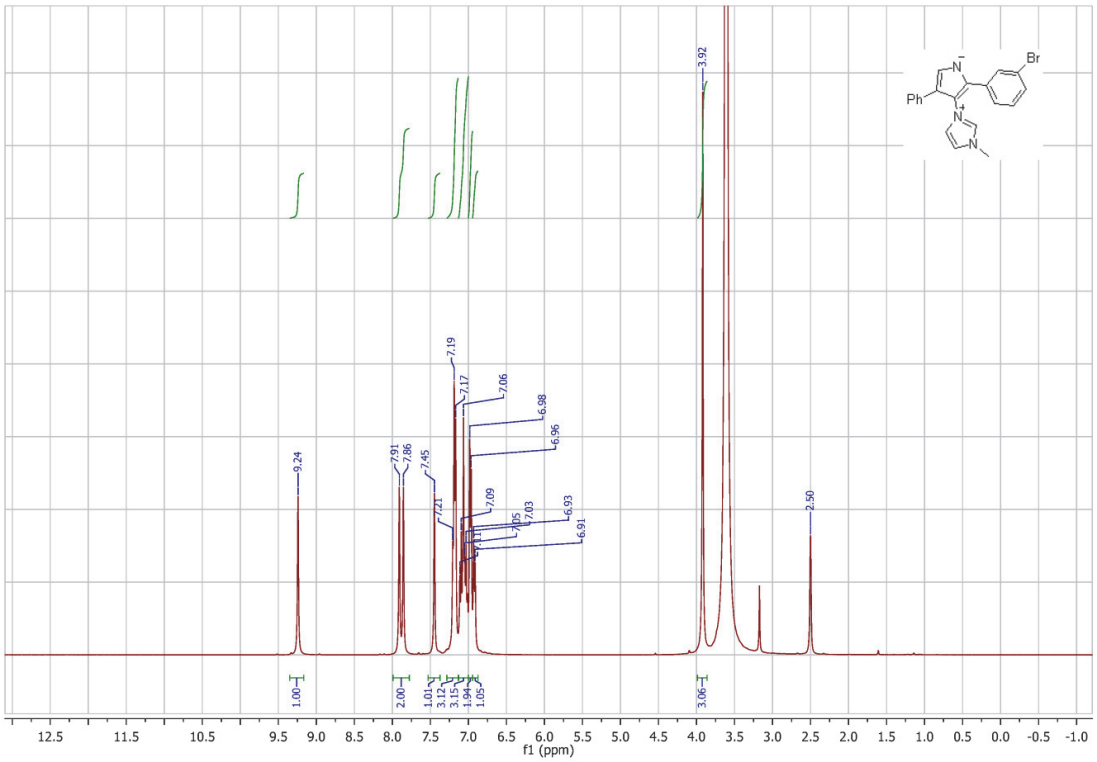
^{1}H NMR spectrum of 2-(4-bromophenyl)-3-(1-methyl-1*H*-imidazol-3-ium-3-yl)-4-phenylpyrrol-1-ide (6d), DMSO-d_6



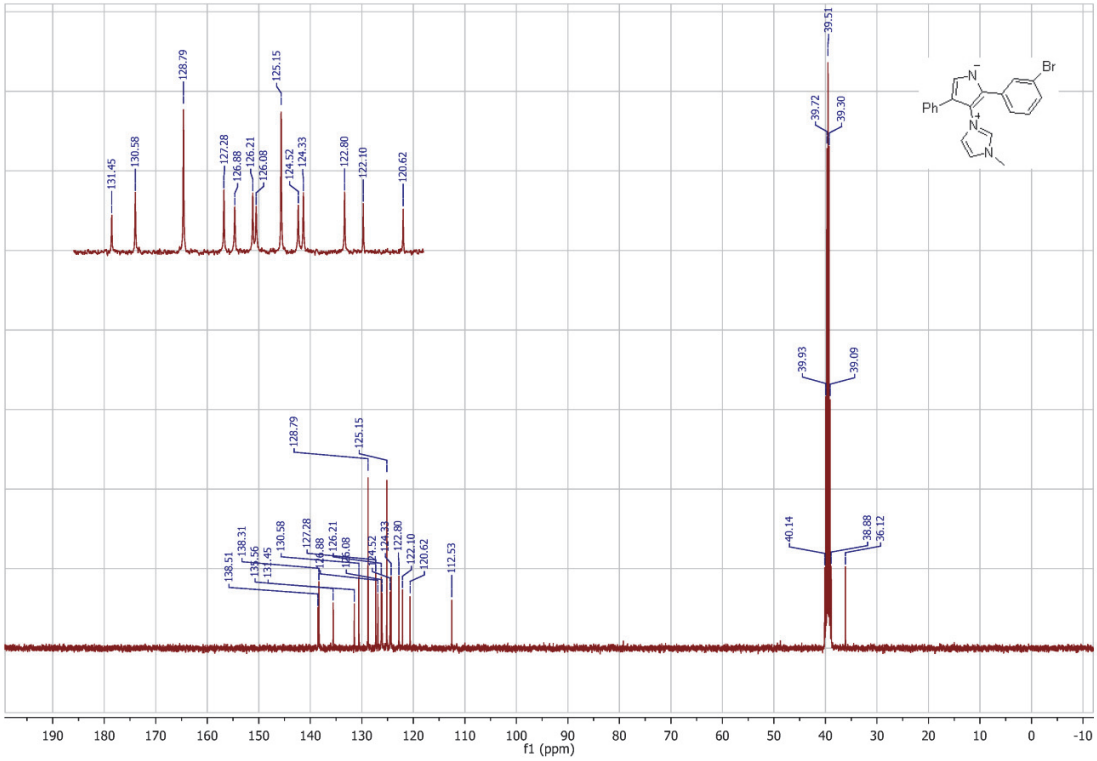
^{13}C NMR spectrum of 2-(4-bromophenyl)-3-(1-methyl-1*H*-imidazol-3-ium-3-yl)-4-phenylpyrrol-1-ide (6d), DMSO-d_6



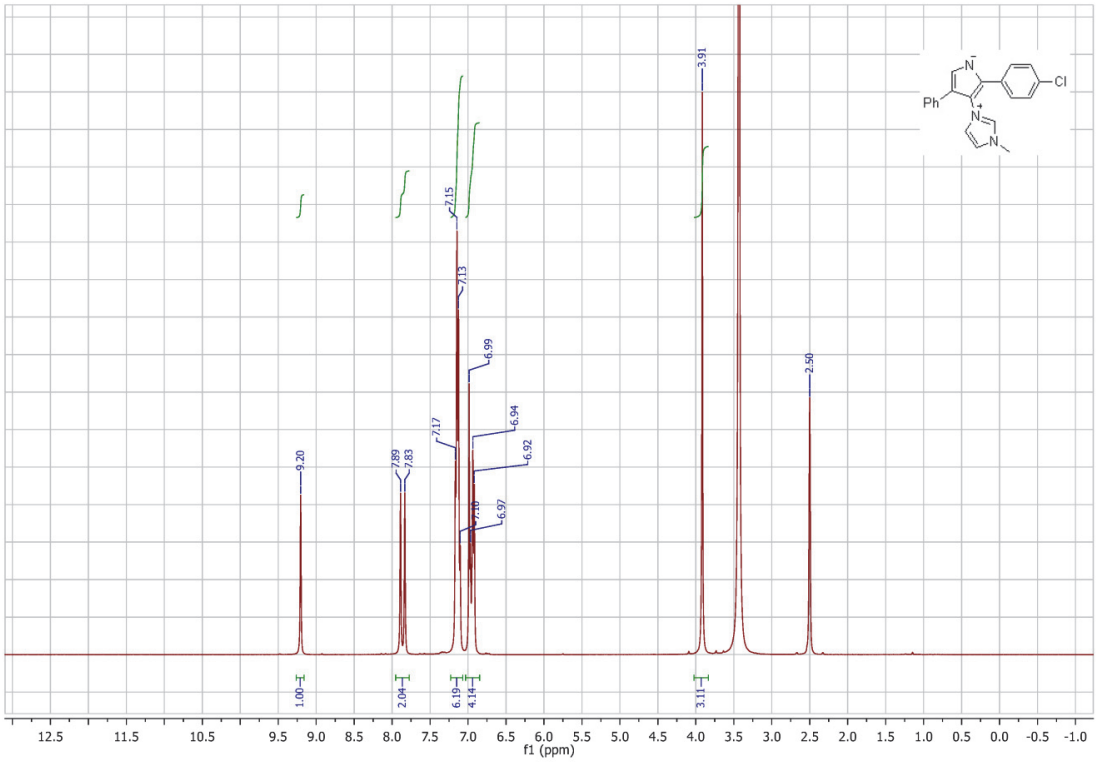
^{1}H NMR spectrum of 2-(3-bromophenyl)-3-(1-methyl-1*H*-imidazol-3-ium-3-yl)-4-phenylpyrrol-1-ide (6e), DMSO-d_6



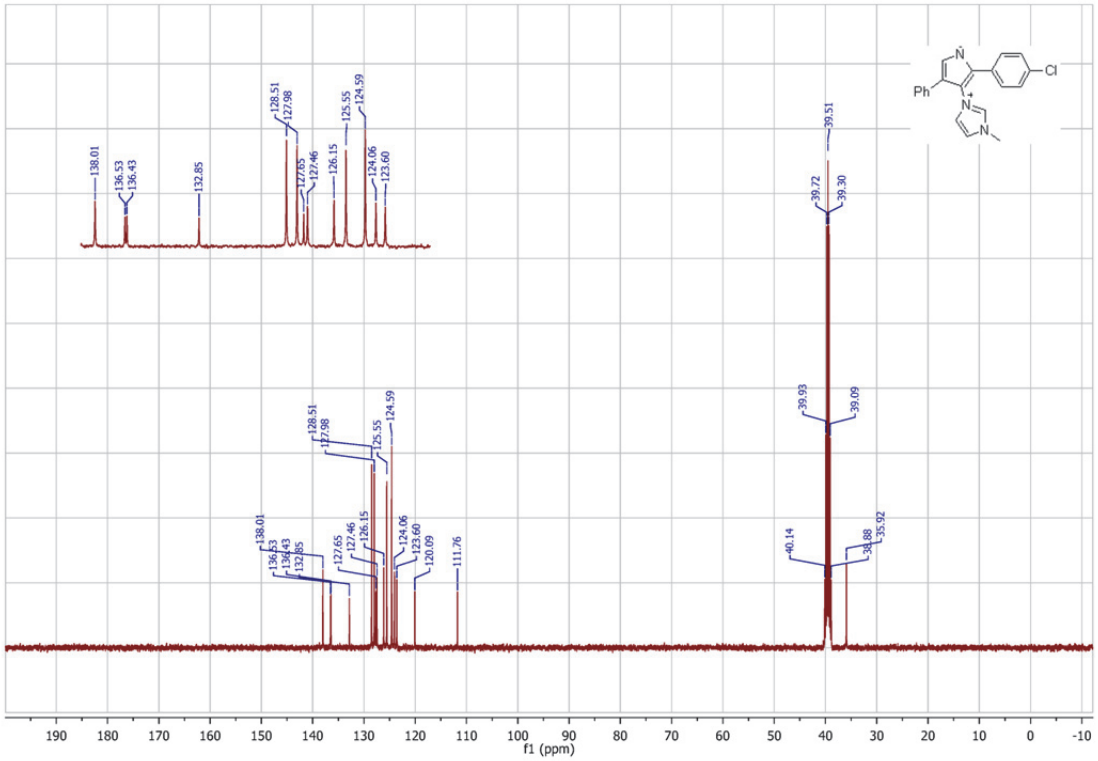
^{13}C NMR spectrum of 2-(3-bromophenyl)-3-(1-methyl-1*H*-imidazol-3-ium-3-yl)-4-phenylpyrrol-1-ide (6e), DMSO-d_6



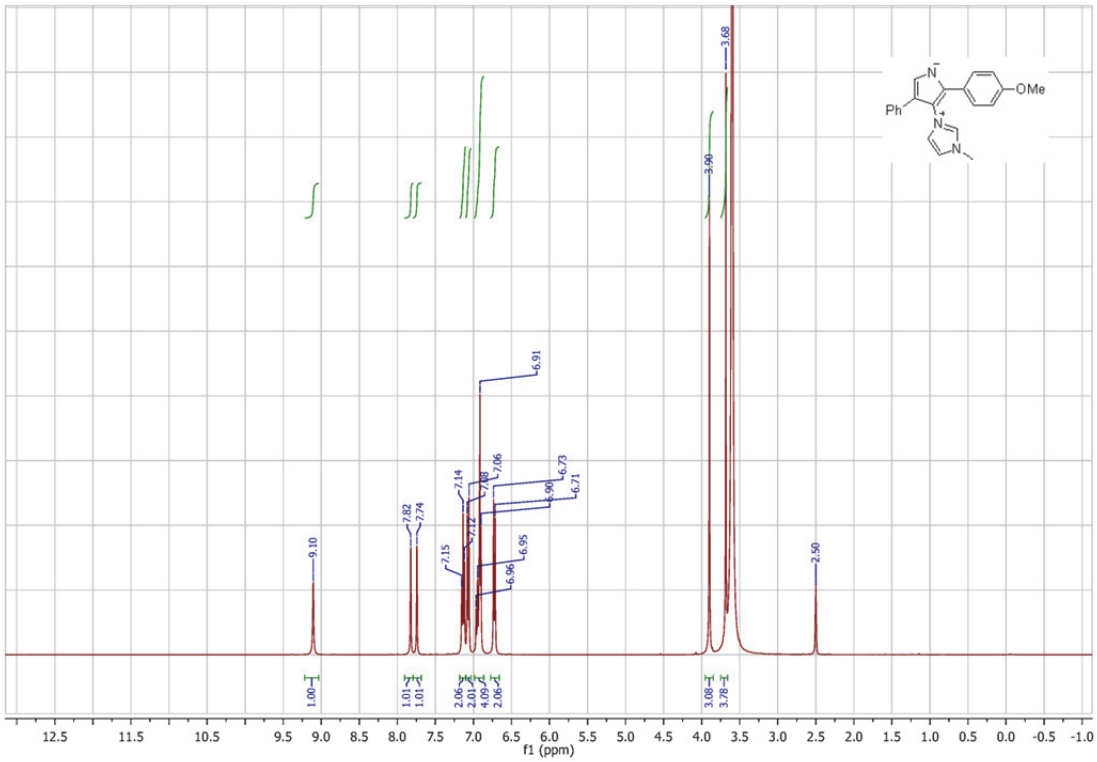
^{1}H NMR spectrum of 2-(4-chlorophenyl)-3-(1-methyl-1*H*-imidazol-3-ium-3-yl)-4-phenylpyrrol-1-ide (6f), DMSO-d_6



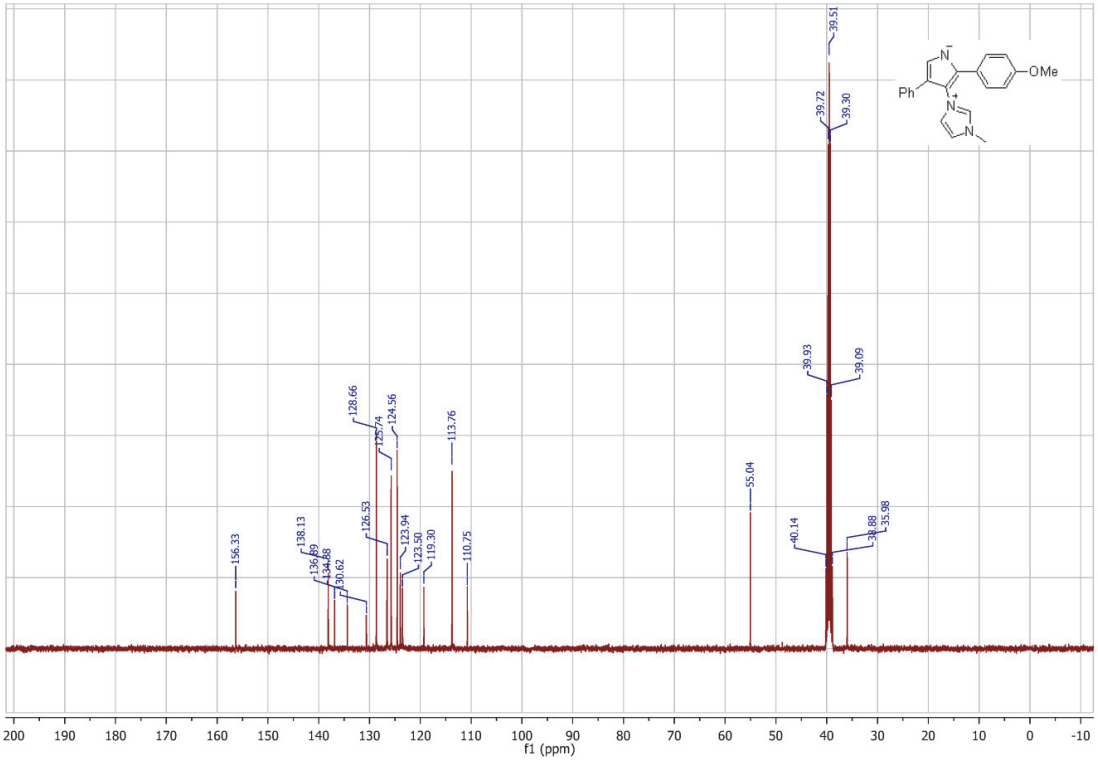
^{13}C NMR spectrum of 2-(4-chlorophenyl)-3-(1-methyl-1*H*-imidazol-3-ium-3-yl)-4-phenylpyrrol-1-ide (6f), DMSO-d_6



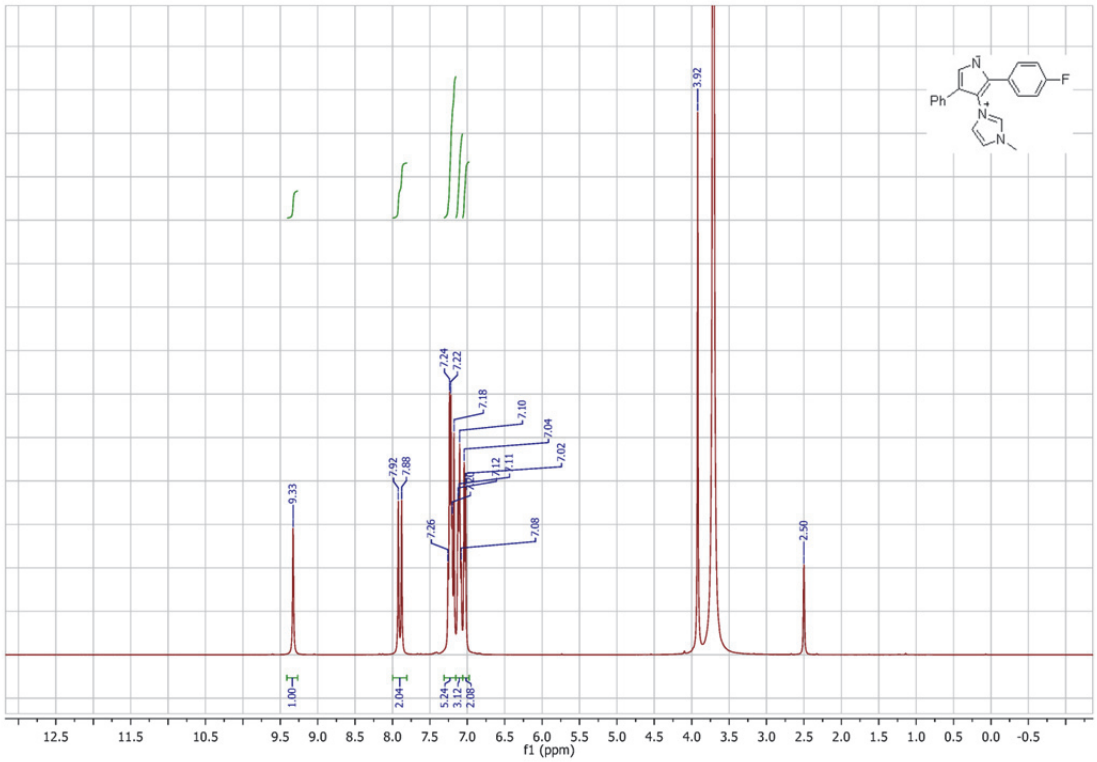
^{1}H NMR spectrum of 2-(4-methoxyphenyl)-3-(1-methyl-1*H*-imidazol-3-ium-3-yl)-4-phenylpyrrol-1-ide (6g), DMSO-d_6



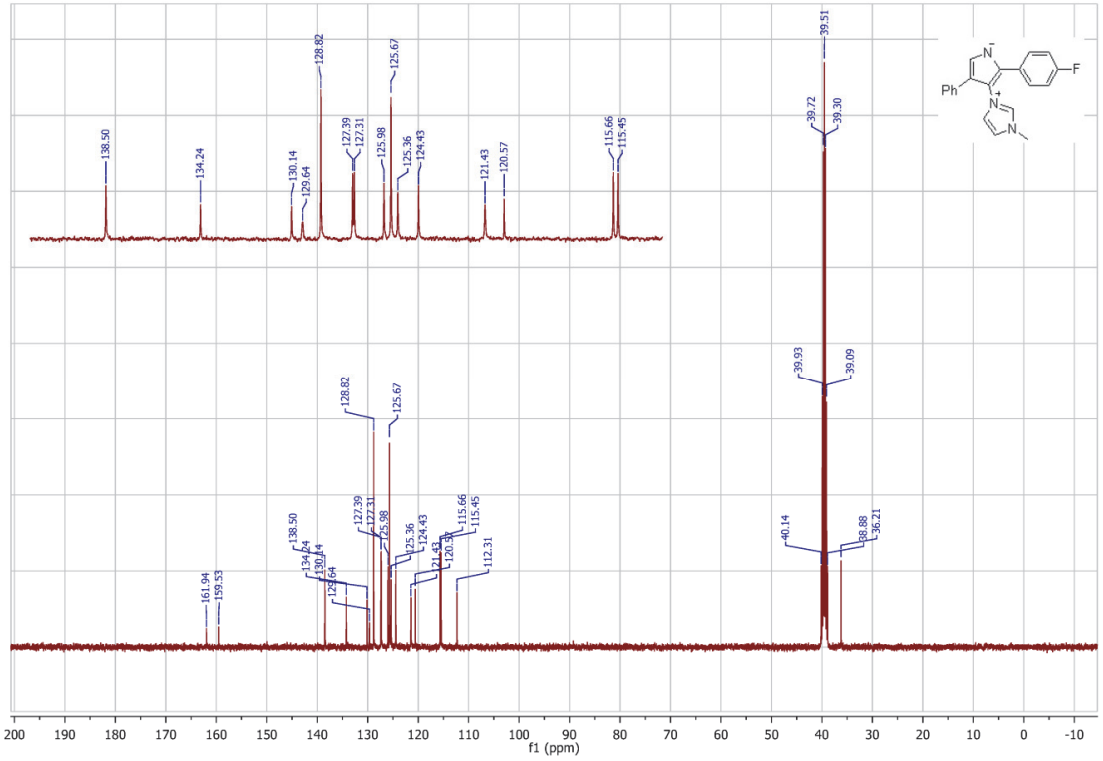
^{13}C NMR spectrum of 2-(4-methoxyphenyl)-3-(1-methyl-1*H*-imidazol-3-ium-3-yl)-4-phenylpyrrol-1-ide (6g), DMSO-d_6



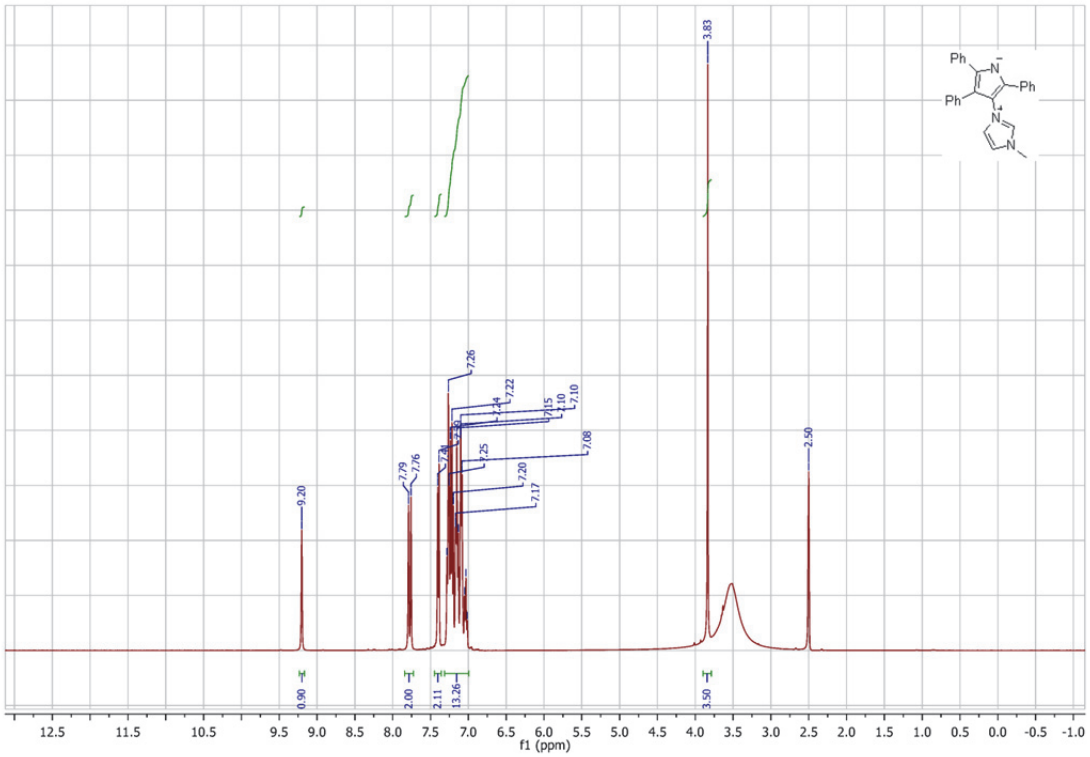
^{1}H NMR spectrum of 2-(4-fluorophenyl)-3-(1-methyl-1*H*-imidazol-3-ium-3-yl)-4-phenylpyrrol-1-ide (6h), DMSO-d_6



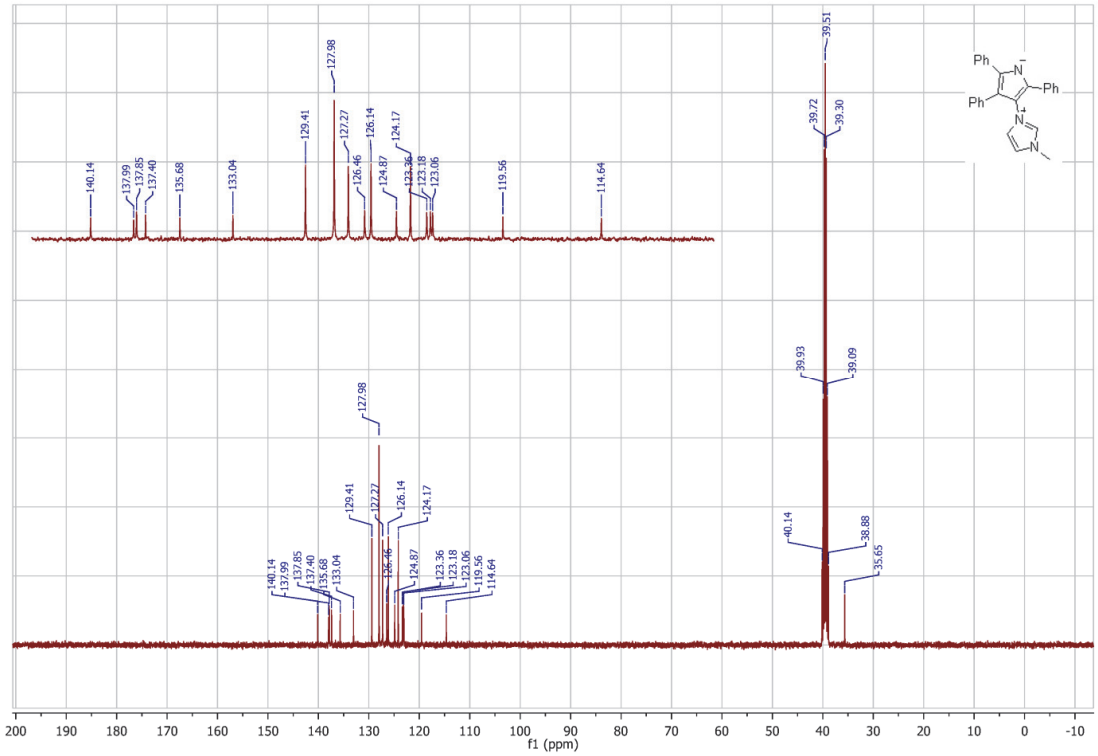
^{13}C NMR spectrum of 2-(4-fluorophenyl)-3-(1-methyl-1*H*-imidazol-3-ium-3-yl)-4-phenylpyrrol-1-ide (6h), DMSO-d_6



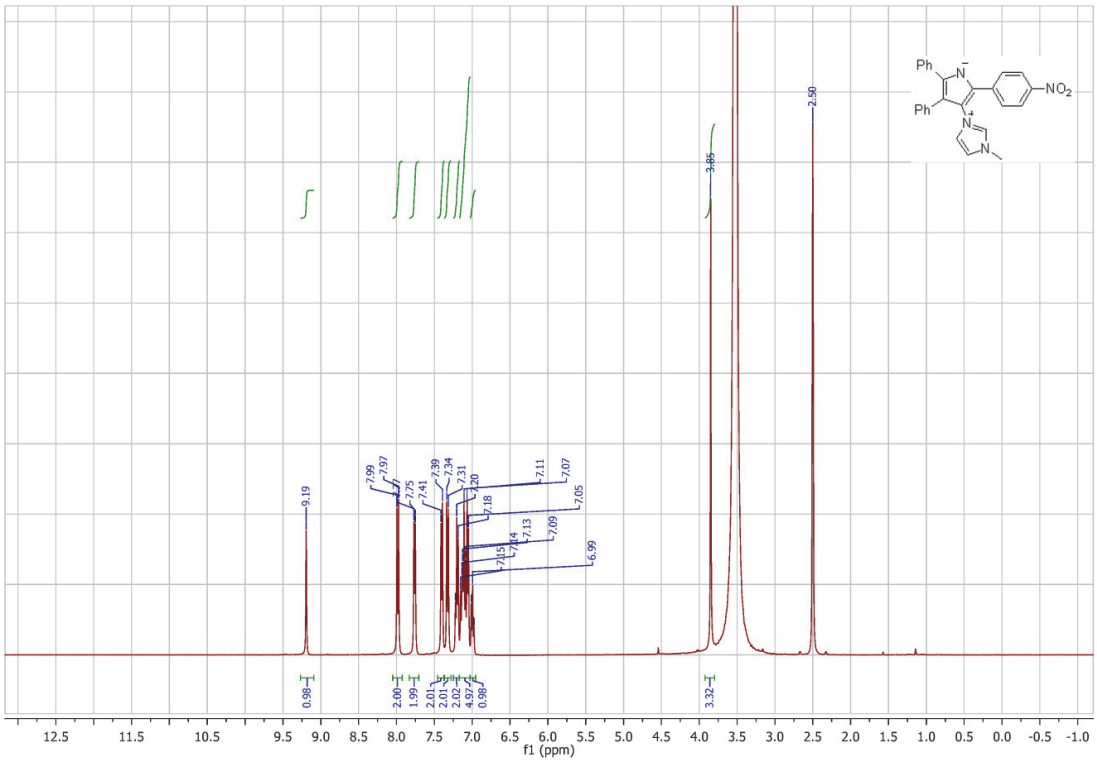
^{1}H NMR spectrum of 3-(1-methyl-1*H*-imidazol-3-ium-3-yl)-2,4,5-triphenylpyrrol-1-ide (6i), DMSO-d_6



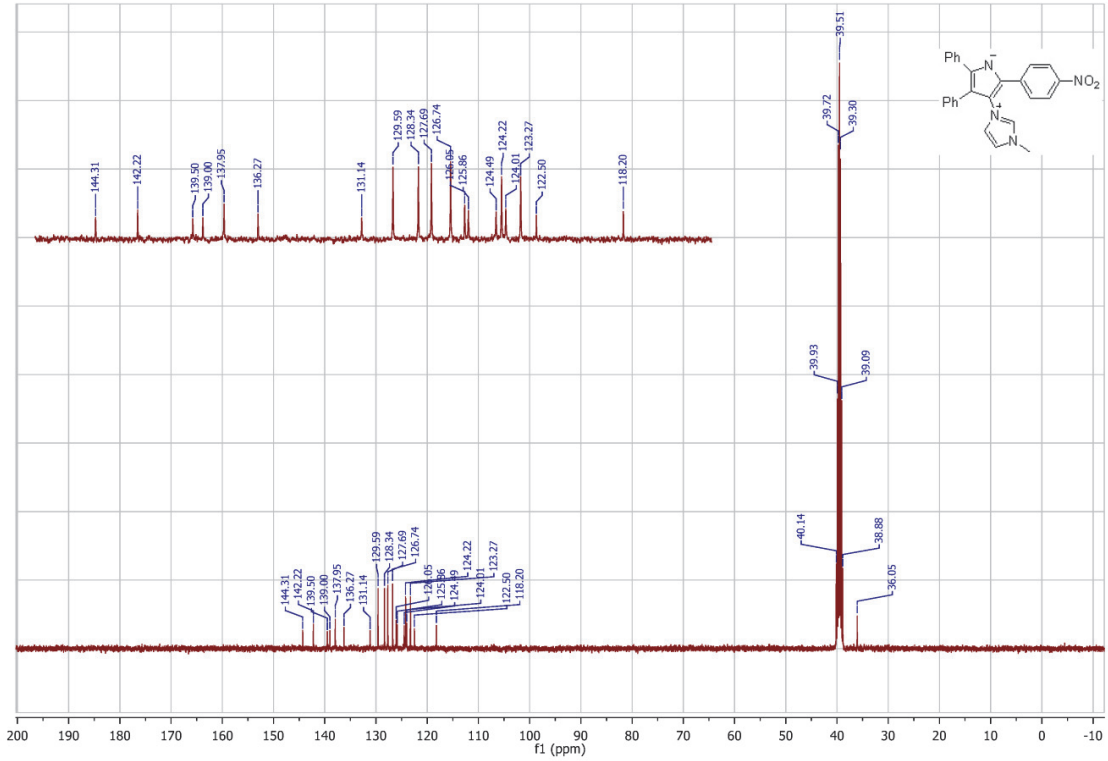
^{13}C NMR spectrum of 3-(1-methyl-1*H*-imidazol-3-ium-3-yl)-2,4,5-triphenylpyrrol-1-ide (6i), DMSO-d_6



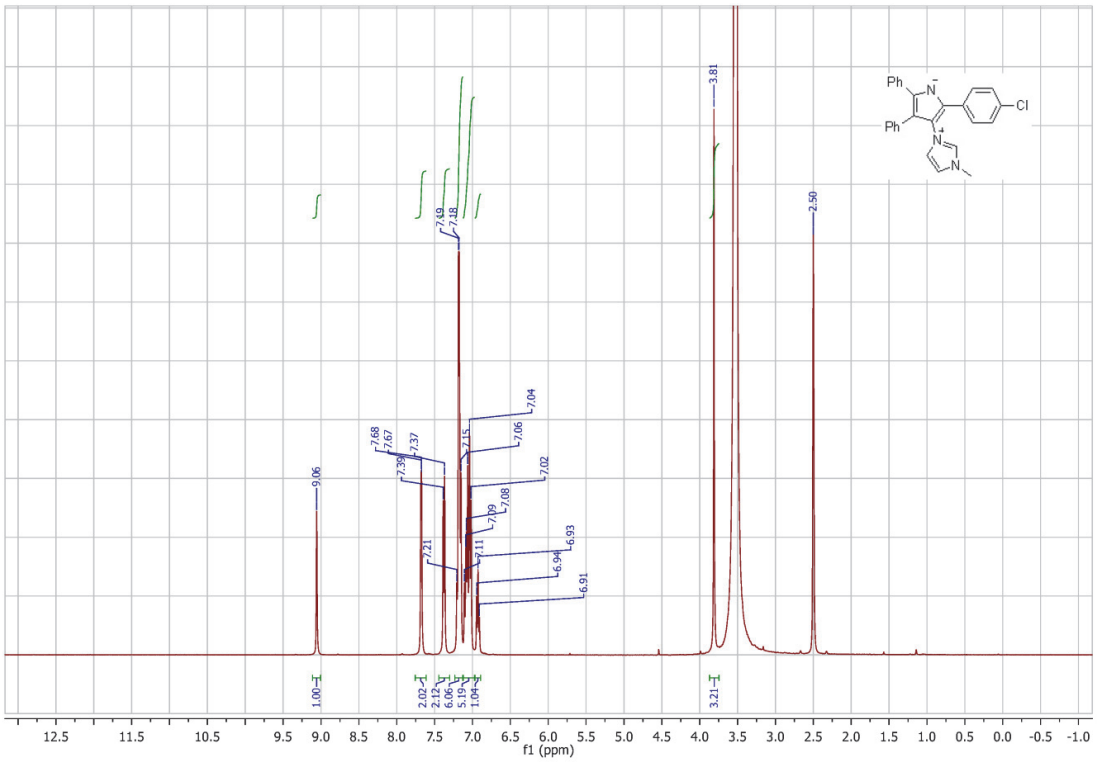
^{1}H NMR spectrum of 3-(1-methyl-1*H*-imidazol-3-ium-3-yl)-2-(4-nitrophenyl)-4,5-diphenylpyrrol-1-ide (6j), DMSO-d_6



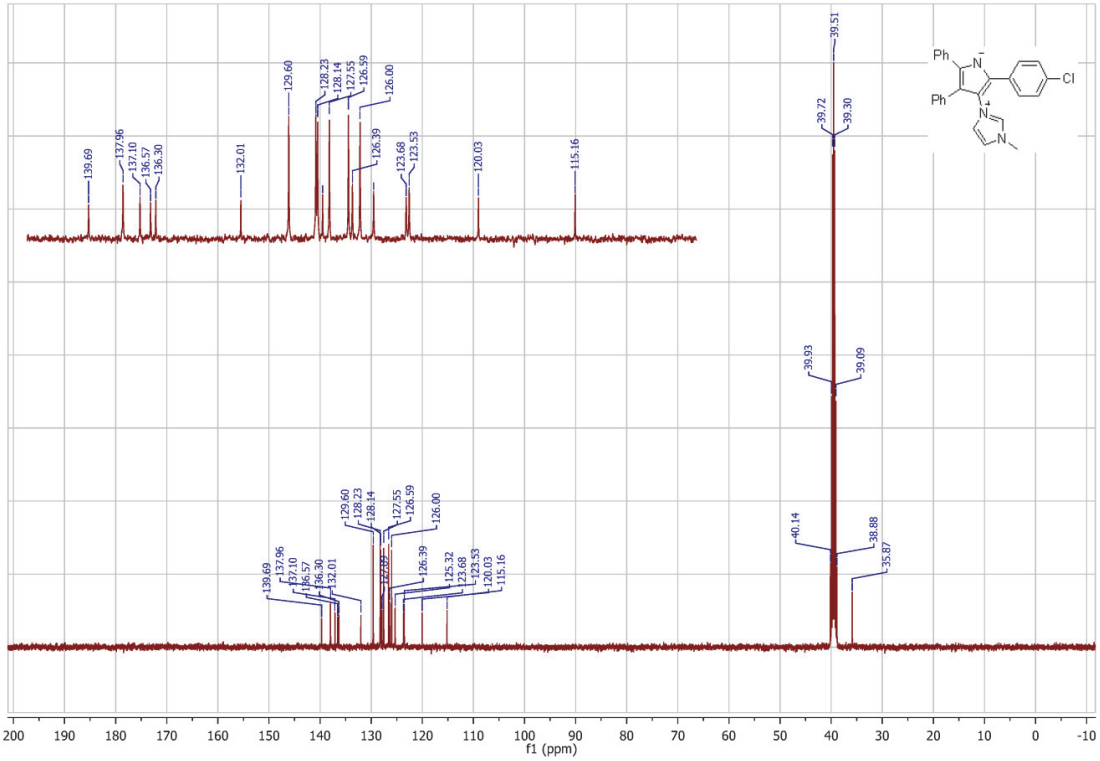
^{13}C NMR spectrum of 3-(1-methyl-1*H*-imidazol-3-ium-3-yl)-2-(4-nitrophenyl)-4,5-diphenylpyrrol-1-ide (6j), DMSO-d_6



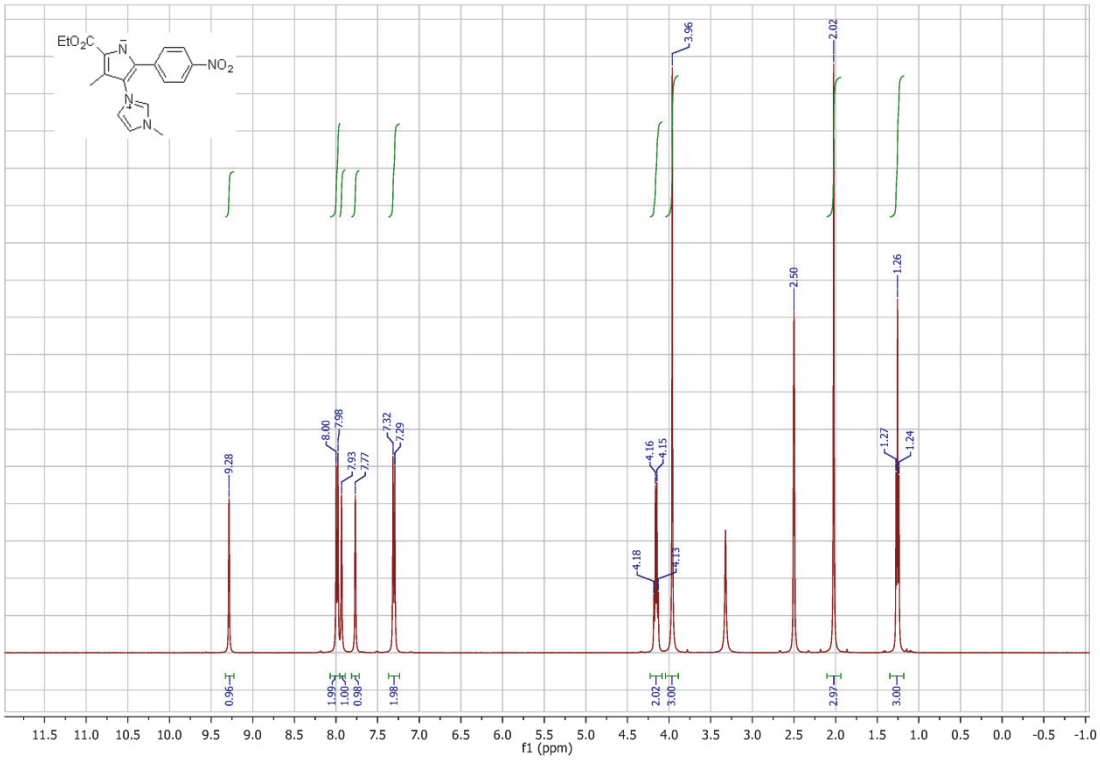
^{1}H NMR spectrum of 2-(4-chlorophenyl)-3-(1-methyl-1*H*-imidazol-3-ium-3-yl)-4,5-diphenylpyrrol-1-ide (6k), DMSO-d_6



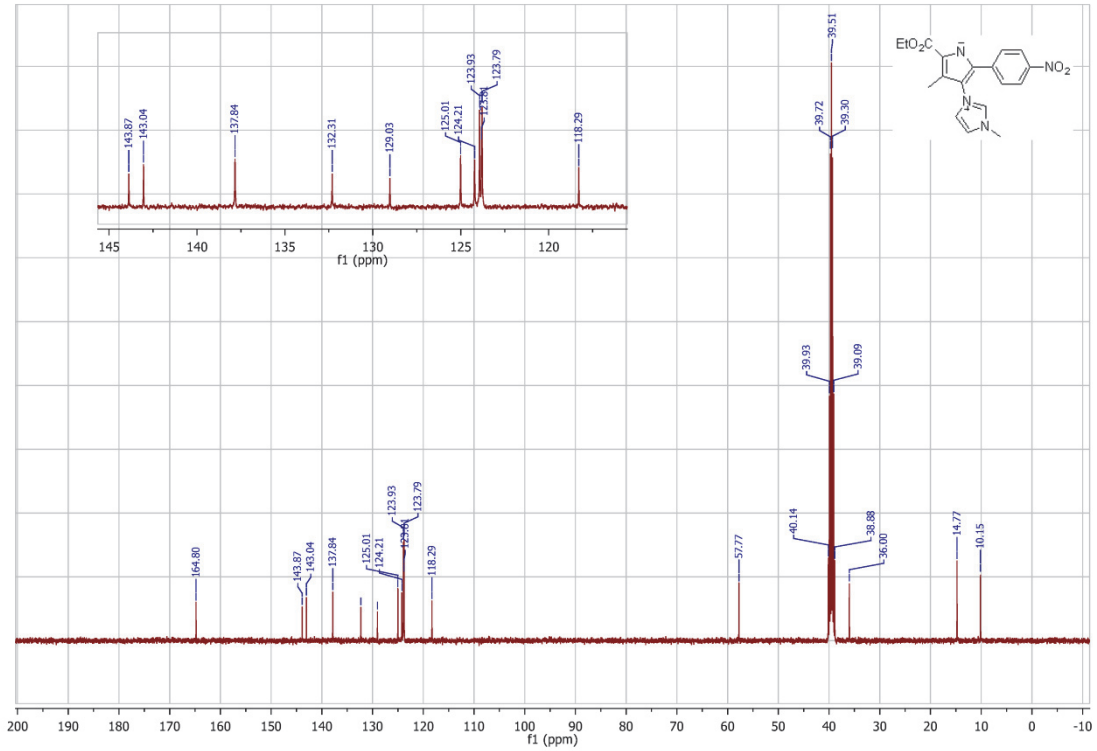
^{13}C NMR spectrum of 2-(4-chlorophenyl)-3-(1-methyl-1*H*-imidazol-3-ium-3-yl)-4,5-diphenylpyrrol-1-ide (6k), DMSO-d_6



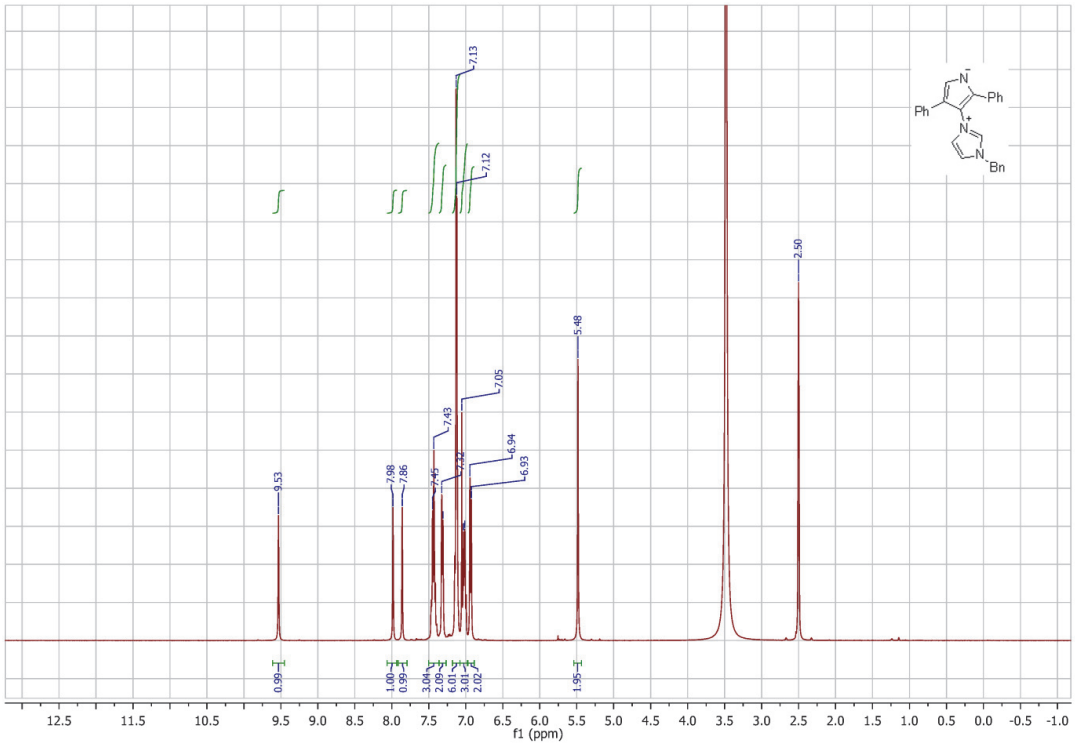
^{1}H NMR spectrum of 2-(ethoxycarbonyl)-3-methyl-4-(1-methyl-1*H*-imidazol-3-ium-3-yl)-5-(4-nitrophenyl)pyrrol-1-ide (6l), DMSO-d_6



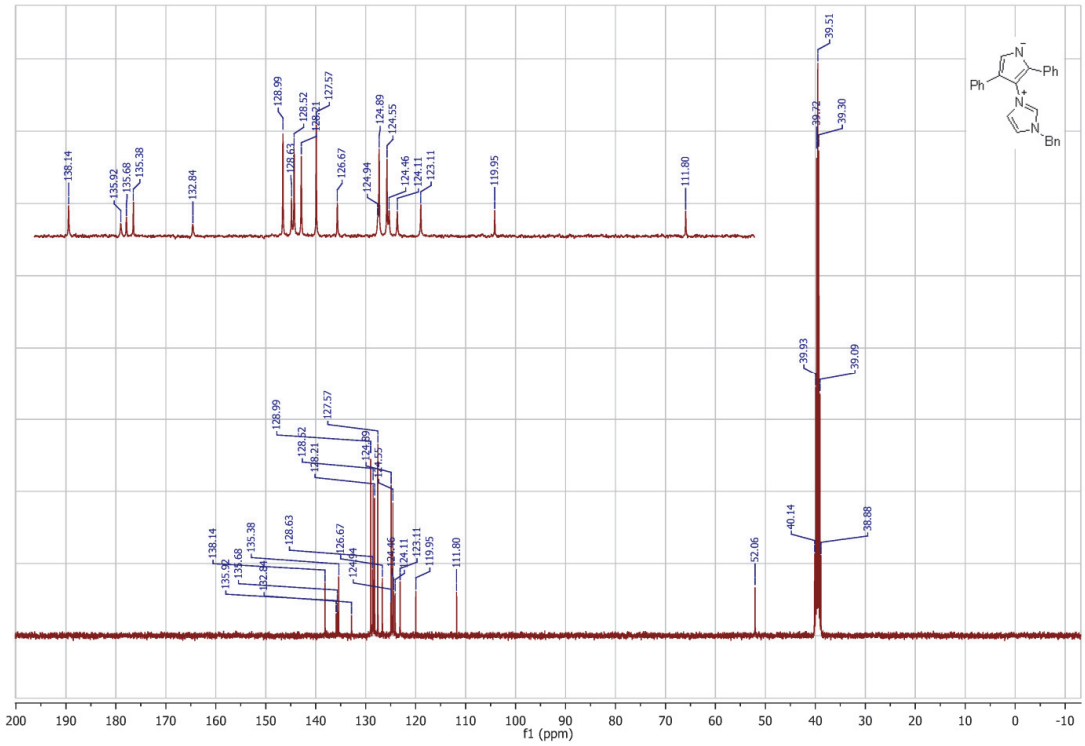
^{13}C NMR spectrum of 2-(ethoxycarbonyl)-3-methyl-4-(1-methyl-1*H*-imidazol-3-ium-3-yl)-5-(4-nitrophenyl)pyrrol-1-ide (6l), DMSO-d_6



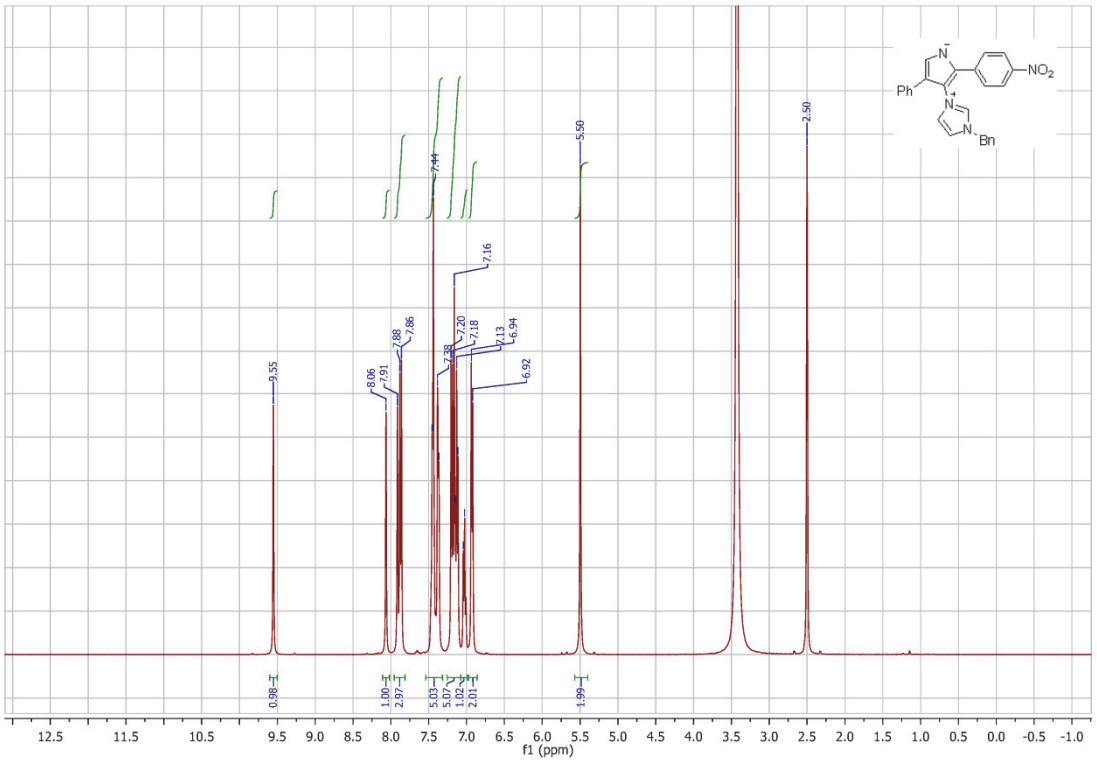
^{1}H NMR spectrum of 3-(1-benzyl-1*H*-imidazol-3-ium-3-yl)-2,4-diphenylpyrrol-1-ide (6m), DMSO-d_6



^{13}C NMR spectrum of 3-(1-benzyl-1*H*-imidazol-3-ium-3-yl)-2,4-diphenylpyrrol-1-ide (6m), DMSO-d_6



^{1}H NMR spectrum of 3-(1-benzyl-1*H*-imidazol-3-ium-3-yl)-2-(4-nitrophenyl)-4-phenylpyrrol-1-ide (6n), DMSO-d_6



^{13}C NMR spectrum of 3-(1-benzyl-1*H*-imidazol-3-ium-3-yl)-2-(4-nitrophenyl)-4-phenylpyrrol-1-ide (6n), DMSO-d_6