Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information for

Azirine-triazole hybrids: selective synthesis of 5-(2*H*-azirin-2-yl)-, 5-(1*H*-pyrrol-2-yl)-1*H*-1,2,3-triazoles and 2-(5-(2*H*-azirin-2-yl)-1*H*-1,2,3-triazol-1-yl)pyridines

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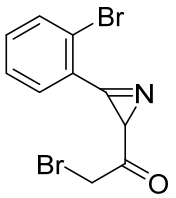
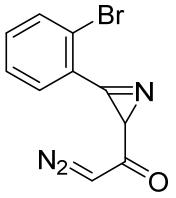
Table of contents

Synthesis of starting materials

2-Bromo-1-(3-(4-fluorophenyl)-2H-azirin-2-yl)ethan-1-one (1.18 g, 90%) was obtained according to the reported procedure[1]. Colorless solid, mp 79–80 °C (hexane/EtOAc). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.98–7.92 (m, 2H), 7.33–7.27 (m, 2H), 3.91 (d, J = 11.5 Hz, 1H), 3.82 (d, J = 11.5 Hz, 1H), 3.15 (s, 1H). ^{13}C{1H} NMR (101 MHz, $CDCl_3$): δ 199.9 (C), 166.4 (d, J = 258.2 Hz, C), 157.3 (C), 133.4 (d, J = 9.9 Hz, CH), 118.3 (d, J = 3.1 Hz, C), 117.2 (d, J = 22.9 Hz, CH), 35.8 (CH), 30.8 (CH_2). HRMS (ESI) m/z: $[M + Na]^+$ 277.9587 Calcd for $C_{10}H_7{}^{79}BrFNNaO^+$; Found 277.9588.



2-Bromo-1-(3-(2-bromophenyl)-2H-azirin-2-yl)ethan-1-one (0.91 g, 81%) was obtained according to the reported procedure[1] from 1-(3-(2-bromophenyl)-2*H*-azirin-2-yl)-2-diazoethan-1-one. Colorless solid, mp 102–104 °C (hexane/EtOAc). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.90–7.83 (m, 1H), 7.79–7.74 (m, 1H), 7.56–7.47 (m, 2H), 3.92 (d, J = 12.1 Hz, 1H), 3.87 (d, J = 12.1 Hz, 1H), 3.22 (s, 1H). ^{13}C{1H} NMR (101 MHz, $CDCl_3$): δ 199.5 (C), 158.6 (C), 135.1 (CH), 134.4 (CH), 133.9 (CH), 128.2 (CH), 126.0 (C), 122.5 (C), 36.5 (CH), 31.2 (CH_2).). HRMS (ESI) m/z: $[M + Na]^+$ 337.8787 Calcd for $C_{10}H_7{}^{79}Br_2NNaO^+$; Found 337.8788.

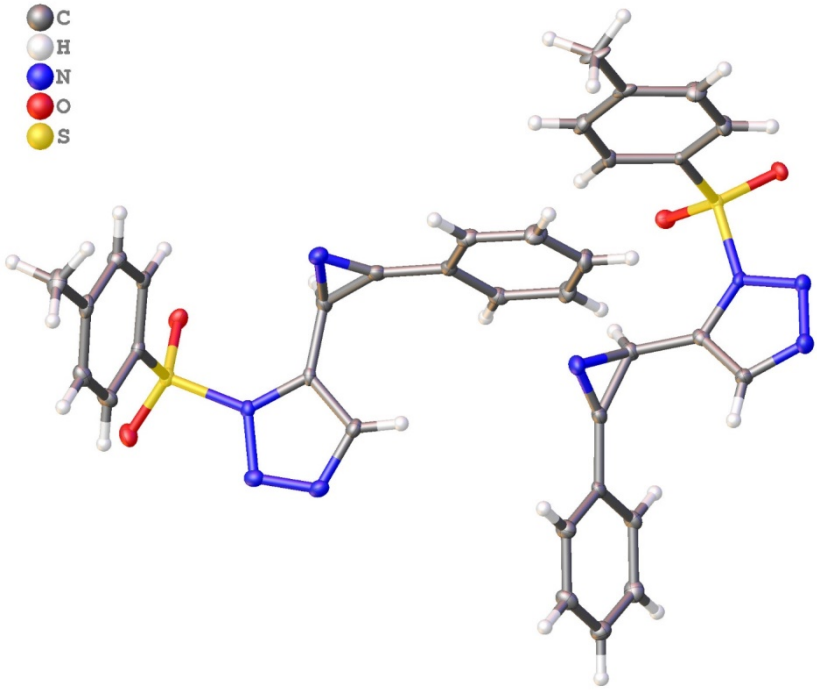


1-(3-(2-Bromophenyl)-2*H*-azirin-2-yl)-2-diazoethan-1-one (1.18 g, 42%) was obtained according to the reported procedure[2]. Orange oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.88–7.82 (m, 1H), 7.79–7.74 (m, 1H), 7.55–7.46 (m, 2H), 5.18 (s, 1H), 2.94 (s, 1H). ^{13}C{1H} NMR (101 MHz, $CDCl_3$): δ 192.0 (C), 160.6 (C), 135.0 (CH), 134.4 (CH), 133.6 (CH), 128.1 (CH), 125.9 (C), 123.0 (C), 53.4 (CH), 37.1 (CH). HRMS (ESI) m/z: $[M + Na]^+$ 285.9586 Calcd for $C_{10}H_6{}^{79}BrN_3NaO^+$; Found 285.9594.

X-ray diffraction experiments

Single crystals of **4a** and **24** were obtained by slow evaporation of DCM/hexane solution at 5 C°. X-ray diffraction studies of **4a** and **24** were performed at 100(2) K on Rigaku Oxford Diffraction «XtaLAB Supernova» diffractometer (HyPix-3000 type detector) using Cu$K\alpha$ (λ = 1.54184 Å) radiation in case of **24** and on Agilent Technologies (Oxford Diffraction) «Xcalibur» (Eos CCD type detector) using Mo$K\alpha$ (λ = 0.71073) in case of **4a**. The structures were solved with the ShelXT[3] structure solution program using Intrinsic Phasing and refined with the ShelXL[4] refinement package incorporated in the OLEX2 program package[5] using Least Squares minimization. The hydrogen atom positions were fixed geometrically at calculated distances and allowed to ride on the parent atoms. Crystallographic data for the structures **4a** and **24** have been deposited with the Cambridge Crystallographic Data Centre (CCDC **2167839** and **2167840**, respectively).

Figure S1. Molecular structure of compound **4a**, displacement parameters are drawn at 50% probability level.



Crystal Data for $C_{17}H_{14}N_4O_2S$ (M = 338.38 g/mol): monoclinic, space group $P2_1/c$ (no. 14), a = 7.6565(4) Å, b = 44.4687(14) Å, c = 9.8470(4) Å, V = 3132.8(2) Å^3, Z = 8, T = 100 (2) K, μ(Cu$K\alpha$) = 0.225 mm^{-1}, D_{calc} =1.435 g/cm^3, 34619 reflections measured (5.21° ≤ 2Θ ≤ 59.992°), 9126 unique (R_{int} = 0.0567, R_{sigma} = 0.0575) which were used in all calculations. The final R_1 was 0.1175 ($I \geq 2\sigma(I)$) and wR_2 was 0.2181 ($I \geq 2\sigma(I)$).

Table S1. Crystal data and structure refinement for 4a.

Identification code	4a
Empirical formula	$C_{17}H_{14}N_4O_2S$
Formula weight	338.38

Temperature/K	100(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	7.6565(4)
b/Å	44.4687(14)
c/Å	9.8470(4)
α/°	90
β/°	110.866(5)
γ/°	90
Volume/Å^3	3132.8(2)
Z	8
ρ_{calc}g/cm^3	1.435
μ/mm^{-1}	0.225
F(000)	1408.0
Crystal size/mm^3	0.4 × 0.2 × 0.14
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	5.21 to 59.992
Index ranges	$-9 \le h \le 10$, $-62 \le k \le 62$, $-13 \le l \le 13$
Reflections collected	34619
Independent reflections	9126 [R_{int} = 0.0567, R_{sigma} = 0.0575]
Data/restraints/parameters	9126/0/435
Goodness-of-fit on F^2	1.299
Final R indexes [I>=2σ (I)]	R_1 = 0.1175, wR_2 = 0.2181
Final R indexes [all data]	R_1 = 0.1257, wR_2 = 0.2212
Largest diff. peak/hole / e Å^{-3}	0.45/-0.90

Table S2. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 4a. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
S1	-3084.8(14)	3152.7(2)	-2572.1(11)	12.15(19)
O1	-3892(4)	3432.1(7)	-3206(3)	16.2(6)
O2	-3793(5)	2871.6(7)	-3224(4)	19.1(6)
N1	-849(5)	3165.9(8)	-2584(4)	12.1(6)
N2	9(5)	2899.1(8)	-2667(4)	15.2(7)
N3	1666(5)	2969.1(8)	-2638(4)	15.6(7)
N4	372(6)	3849.8(9)	-766(4)	18.3(7)
C1	1898(6)	3273.1(10)	-2529(5)	14.4(8)
C2	307(5)	3405.6(9)	-2482(4)	10.8(7)
C3	-67(6)	3727.0(10)	-2352(5)	15.4(8)
C4	1471(6)	3907.8(9)	-1429(5)	14.2(8)
C5	3278(6)	4045.4(9)	-1179(5)	12.9(7)
C6	3975(6)	4060.8(9)	-2308(5)	14.9(8)
C7	5717(7)	4190.2(10)	-2052(5)	18.1(8)
C8	6750(6)	4298.3(11)	-679(5)	19.9(9)
C9	6072(7)	4277.6(11)	453(5)	20.0(9)
C10	4338(6)	4152.4(10)	198(5)	16.3(8)
C11	-2798(6)	3146.4(10)	-730(5)	13.4(7)
C12	-2966(6)	3413.5(9)	-46(5)	12.7(7)

Table S2. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 4a. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C13	-2828(6)	3400.7(10)	1398(5)	15.9(8)
C14	-2506(6)	3126.5(10)	2153(5)	15.8(8)
C15	-2323(6)	2864.0(10)	1440(5)	17.1(8)
C16	-2487(7)	2869.4(10)	-6(5)	16.9(8)
C17	-2385(7)	3115.8(12)	3718(5)	21.6(9)
S1'	11861.5(14)	4627.8(2)	3244.0(10)	10.09(18)
O1'	10177(4)	4503.2(7)	2253(3)	14.3(6)
O2'	12739(4)	4878.8(6)	2857(3)	13.8(6)
N1'	13469(5)	4340.9(8)	3541(4)	11.4(6)
N2'	15322(5)	4418.0(8)	4013(4)	14.6(7)
N3'	16261(5)	4166.0(8)	4347(4)	17.1(7)
N4'	11243(6)	3669.9(8)	4474(4)	17.7(7)
C1'	15046(6)	3931.0(9)	4116(5)	14.6(8)
C2'	13254(6)	4035.5(9)	3614(4)	12.5(7)
C3'	11486(6)	3867.4(9)	3220(5)	13.8(8)
C4'	11631(6)	3542.8(9)	3473(5)	14.1(8)
C5'	12110(6)	3256.6(9)	2987(5)	13.2(7)
C6'	12318(6)	3240.3(9)	1643(5)	14.8(8)
C7'	12814(7)	2969.6(10)	1180(5)	18.3(8)
C8'	13076(6)	2716.9(10)	2058(5)	17.6(8)
C9'	12863(7)	2733.9(10)	3399(5)	17.7(8)
C10'	12389(6)	3002.7(10)	3879(5)	16.1(8)
C11'	11711(5)	4678.8(8)	4958(4)	9.8(7)
C12'	10271(6)	4541.3(9)	5272(5)	13.3(7)
C13'	10211(6)	4584.6(10)	6661(5)	17.2(8)
C14'	11554(6)	4756.3(10)	7703(5)	15.7(8)
C15'	12968(7)	4891.7(10)	7331(5)	18.6(8)
C16'	13076(6)	4853.7(10)	5967(5)	15.3(8)
C17'	11485(8)	4796.6(11)	9204(5)	23.7(10)

Table S3. Anisotropic Displacement Parameters (Å^2×10^3) for 4a. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S1	10.5(4)	15.2(4)	11.1(4)	0.1(3)	4.3(3)	-1.4(4)
O1	14.7(14)	18.5(15)	16.1(15)	6.1(12)	6.3(12)	4.0(12)
O2	18.9(16)	20.9(16)	18.5(15)	-4.8(12)	7.8(13)	-7.6(13)
N1	12.5(16)	13.0(15)	12.3(15)	-0.1(12)	6.4(13)	-1.7(13)
N2	18.8(18)	13.5(16)	15.2(17)	-0.1(13)	8.2(14)	1.1(14)
N3	17.4(18)	14.4(16)	16.8(17)	1.1(13)	8.4(14)	3.3(14)
N4	19.0(18)	15.5(17)	23.9(19)	-1.5(14)	11.8(16)	1.3(14)
C1	12.5(18)	18.2(19)	14.6(18)	-1.3(15)	7.3(15)	-0.6(16)
C2	8.9(17)	14.6(18)	9.1(16)	1.0(13)	3.4(14)	-2.4(14)
C3	13.4(19)	14.5(18)	18(2)	0.3(15)	5.8(16)	-2.5(15)

Table S3. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 4a. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C4	14.5(19)	11.1(17)	16.6(19)	-0.4(14)	5.0(15)	2.1(14)
C5	14.5(18)	9.2(16)	16.4(19)	2.0(14)	7.2(15)	1.4(14)
C6	17(2)	13.3(18)	12.0(18)	-0.6(14)	2.6(15)	0.5(15)
C7	20(2)	21(2)	17(2)	2.5(16)	11.3(17)	0.2(17)
C8	14(2)	23(2)	23(2)	-1.2(18)	7.6(17)	-4.2(17)
C9	18(2)	23(2)	16(2)	-8.0(17)	3.5(17)	-1.2(17)
C10	20(2)	17.3(19)	12.3(18)	0.5(15)	7.1(16)	4.3(16)
C11	9.5(17)	17.7(19)	13.6(18)	0.7(15)	4.9(14)	-1.7(15)
C12	10.2(17)	14.1(18)	14.9(19)	2.1(14)	6.0(15)	-0.1(14)
C13	16(2)	17.5(19)	14.8(19)	-1.3(15)	6.3(16)	0.0(16)
C14	12.3(18)	23(2)	13.7(19)	2.4(16)	6.1(15)	-2.9(16)
C15	16(2)	15.8(19)	17(2)	2.8(15)	2.9(16)	-1.9(15)
C16	21(2)	12.3(18)	17(2)	2.3(15)	7.5(17)	-0.5(16)
C17	21(2)	33(3)	13(2)	-0.9(18)	8.4(17)	-4.4(19)
S1'	10.8(4)	10.2(4)	9.5(4)	-0.6(3)	3.9(3)	-1.1(3)
O1'	12.6(14)	15.9(14)	11.2(13)	-2.0(11)	0.5(11)	-0.1(11)
O2'	17.9(15)	11.5(13)	14.0(14)	1.3(11)	7.9(12)	-2.3(11)
N1'	9.3(15)	13.5(15)	12.6(15)	-3.3(12)	5.4(13)	-2.1(12)
N2'	11.9(16)	14.9(16)	17.5(17)	-0.9(13)	5.7(14)	-1.5(13)
N3'	14.4(17)	16.0(17)	21.5(19)	0.0(14)	7.5(15)	-1.1(14)
N4'	19.8(19)	15.5(17)	22.0(19)	-2.2(14)	12.6(16)	-4.3(14)
C1'	13.5(19)	12.7(18)	19(2)	-0.1(15)	6.7(16)	0.9(15)
C2'	15.5(19)	12.1(17)	10.1(17)	-2.0(13)	4.9(15)	-2.0(14)
C3'	14.0(19)	12.3(17)	15.1(19)	0.5(14)	5.3(15)	-1.3(14)
C4'	12.6(19)	12.6(17)	17.4(19)	-0.3(14)	5.7(15)	-2.8(14)
C5'	11.0(18)	10.7(17)	17.4(19)	-1.3(14)	4.5(15)	-2.7(14)
C6'	17(2)	12.3(17)	14.3(19)	2.6(14)	5.2(16)	-1.3(15)
C7'	20(2)	22(2)	13.8(19)	-0.7(16)	6.6(17)	-3.0(17)
C8'	19(2)	18(2)	17(2)	-1.6(16)	7.4(17)	0.7(16)
C9'	22(2)	13.3(18)	16(2)	2.8(15)	3.6(17)	-0.1(16)
C10'	20(2)	14.8(19)	14.6(19)	0.2(15)	7.0(16)	-0.2(16)
C11'	10.1(17)	7.8(16)	12.3(17)	1.0(13)	5.2(14)	1.8(13)
C12'	10.4(18)	13.1(17)	16.4(19)	0.1(14)	4.8(15)	-1.1(14)
C13'	18(2)	20(2)	18(2)	3.0(16)	10.9(17)	3.2(16)
C14'	22(2)	14.3(18)	13.7(18)	2.9(15)	9.7(16)	9.9(16)
C15'	22(2)	20(2)	14(2)	-5.3(16)	6.5(17)	-2.0(17)
C16'	14.0(19)	17.0(19)	14.7(19)	-2.2(15)	4.7(16)	-4.0(15)
C17'	35(3)	27(2)	15(2)	2.5(17)	16(2)	17(2)

Table S4. Bond Lengths for 4a.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S1	O1	1.428(3)	S1'	O1'	1.424(3)
S1	O2	1.422(3)	S1'	O2'	1.422(3)

Table S4. Bond Lengths for 4a.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S1	N1	1.717(4)	S1'	N1'	1.724(4)
S1	C11	1.748(4)	S1'	C11'	1.747(4)
N1	N2	1.373(5)	N1'	N2'	1.369(5)
N1	C2	1.366(5)	N1'	C2'	1.373(5)
N2	N3	1.296(5)	N2'	N3'	1.309(5)
N3	C1	1.363(5)	N3'	C1'	1.363(5)
N4	C3	1.573(6)	N4'	C3'	1.580(6)
N4	C4	1.262(6)	N4'	C4'	1.260(6)
C1	C2	1.368(6)	C1'	C2'	1.364(6)
C2	C3	1.472(6)	C2'	C3'	1.472(6)
C3	C4	1.448(6)	C3'	C4'	1.462(6)
C4	C5	1.451(6)	C4'	C5'	1.452(6)
C5	C6	1.395(6)	C5'	C6'	1.390(6)
C5	C10	1.393(6)	C5'	C10'	1.400(6)
C6	C7	1.391(6)	C6'	C7'	1.387(6)
C7	C8	1.386(6)	C7'	C8'	1.388(6)
C8	C9	1.391(7)	C8'	C9'	1.389(6)
C9	C10	1.378(6)	C9'	C10'	1.381(6)
C11	C12	1.394(6)	C11'	C12'	1.389(5)
C11	C16	1.401(6)	C11'	C16'	1.394(6)
C12	C13	1.389(6)	C12'	C13'	1.398(6)
C13	C14	1.404(6)	C13'	C14'	1.393(7)
C14	C15	1.395(6)	C14'	C15'	1.396(6)
C14	C17	1.511(6)	C14'	C17'	1.509(6)
C15	C16	1.384(6)	C15'	C16'	1.385(6)

Table S5. Bond Angles for 4a.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	S1	N1	104.15(18)	O1'	S1'	N1'	104.24(18)
O1	S1	C11	110.0(2)	O1'	S1'	C11'	110.96(19)
O2	S1	O1	122.1(2)	O2'	S1'	O1'	121.38(19)
O2	S1	N1	104.34(19)	O2'	S1'	N1'	104.43(18)
O2	S1	C11	110.0(2)	O2'	S1'	C11'	110.90(18)
N1	S1	C11	104.51(18)	N1'	S1'	C11'	102.76(18)
N2	N1	S1	118.1(3)	N2'	N1'	S1'	117.6(3)
C2	N1	S1	130.4(3)	N2'	N1'	C2'	111.0(3)
C2	N1	N2	111.6(3)	C2'	N1'	S1'	130.5(3)
N3	N2	N1	106.0(3)	N3'	N2'	N1'	106.3(3)
N2	N3	C1	109.8(4)	N2'	N3'	C1'	109.4(4)
C4	N4	C3	60.2(3)	C4'	N4'	C3'	60.8(3)
N3	C1	C2	109.7(4)	N3'	C1'	C2'	109.8(4)
N1	C2	C1	102.9(4)	N1'	C2'	C3'	127.2(4)
N1	C2	C3	128.5(4)	C1'	C2'	N1'	103.4(4)
C1	C2	C3	128.6(4)	C1'	C2'	C3'	129.4(4)

Table S5. Bond Angles for 4a.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C2	C3	N4	116.3(4)	C2'	C3'	N4'	115.4(3)
C4	C3	N4	49.2(3)	C4'	C3'	N4'	48.8(2)
C4	C3	C2	117.0(4)	C4'	C3'	C2'	116.7(4)
N4	C4	C3	70.6(3)	N4'	C4'	C3'	70.5(3)
N4	C4	C5	140.3(4)	N4'	C4'	C5'	144.0(4)
C3	C4	C5	148.6(4)	C5'	C4'	C3'	145.2(4)
C6	C5	C4	119.8(4)	C6'	C5'	C4'	119.2(4)
C10	C5	C4	119.9(4)	C6'	C5'	C10'	120.8(4)
C10	C5	C6	120.3(4)	C10'	C5'	C4'	120.0(4)
C7	C6	C5	119.3(4)	C7'	C6'	C5'	119.7(4)
C8	C7	C6	119.8(4)	C6'	C7'	C8'	119.6(4)
C7	C8	C9	120.8(4)	C7'	C8'	C9'	120.5(4)
C10	C9	C8	119.4(4)	C10'	C9'	C8'	120.5(4)
C9	C10	C5	120.3(4)	C9'	C10'	C5'	118.9(4)
C12	C11	S1	119.3(3)	C12'	C11'	S1'	119.3(3)
C12	C11	C16	122.1(4)	C12'	C11'	C16'	122.6(4)
C16	C11	S1	118.6(3)	C16'	C11'	S1'	118.1(3)
C13	C12	C11	118.2(4)	C11'	C12'	C13'	117.6(4)
C12	C13	C14	120.9(4)	C14'	C13'	C12'	121.5(4)
C13	C14	C17	120.2(4)	C13'	C14'	C15'	118.8(4)
C15	C14	C13	119.4(4)	C13'	C14'	C17'	120.8(4)
C15	C14	C17	120.4(4)	C15'	C14'	C17'	120.4(4)
C16	C15	C14	121.0(4)	C16'	C15'	C14'	121.4(4)
C15	C16	C11	118.4(4)	C15'	C16'	C11'	118.1(4)

Table S6. Torsion Angles for 4a.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
S1	N1	N2	N3	-179.1(3)	S1'	N1'	N2'	N3'	171.6(3)
S1	N1	C2	C1	178.9(3)	S1'	N1'	C2'	C1'	-169.9(3)
S1	N1	C2	C3	-1.1(6)	S1'	N1'	C2'	C3'	10.7(6)
S1	C11	C12	C13	176.8(3)	S1'	C11'	C12'	C13'	179.3(3)
S1	C11	C16	C15	-177.9(3)	S1'	C11'	C16'	C15'	-179.4(3)
O1	S1	N1	N2	-151.6(3)	O1'	S1'	N1'	N2'	157.2(3)
O1	S1	N1	C2	30.5(4)	O1'	S1'	N1'	C2'	-34.8(4)
O1	S1	C11	C12	-13.4(4)	O1'	S1'	C11'	C12'	13.9(4)
O1	S1	C11	C16	163.8(3)	O1'	S1'	C11'	C16'	-167.2(3)
O2	S1	N1	N2	-22.5(3)	O2'	S1'	N1'	N2'	28.9(3)
O2	S1	N1	C2	159.6(4)	O2'	S1'	N1'	C2'	-163.1(4)
O2	S1	C11	C12	-150.6(3)	O2'	S1'	C11'	C12'	151.9(3)
O2	S1	C11	C16	26.6(4)	O2'	S1'	C11'	C16'	-29.1(4)
N1	S1	C11	C12	97.9(3)	N1'	S1'	C11'	C12'	-97.0(3)
N1	S1	C11	C16	-84.9(4)	N1'	S1'	C11'	C16'	81.9(3)
N1	N2	N3	C1	0.4(5)	N1'	N2'	N3'	C1'	-0.8(5)
N1	C2	C3	N4	87.7(5)	N1'	C2'	C3'	N4'	-122.0(4)

Table S6. Torsion Angles for 4a.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
N1	C2	C3	C4	143.2(4)	N1'	C2'	C3'	C4'	-176.7(4)
N2	N1	C2	C1	0.9(4)	N2'	N1'	C2'	C1'	-1.4(5)
N2	N1	C2	C3	-179.0(4)	N2'	N1'	C2'	C3'	179.3(4)
N2	N3	C1	C2	0.2(5)	N2'	N3'	C1'	C2'	-0.1(5)
N3	C1	C2	N1	-0.7(5)	N3'	C1'	C2'	N1'	0.9(5)
N3	C1	C2	C3	179.3(4)	N3'	C1'	C2'	C3'	-179.8(4)
N4	C3	C4	C5	171.6(8)	N4'	C3'	C4'	C5'	-173.9(8)
N4	C4	C5	C6	-179.8(5)	N4'	C4'	C5'	C6'	176.5(6)
N4	C4	C5	C10	2.3(8)	N4'	C4'	C5'	C10'	-4.6(9)
C1	C2	C3	N4	-92.3(5)	C1'	C2'	C3'	N4'	58.8(6)
C1	C2	C3	C4	-36.8(6)	C1'	C2'	C3'	C4'	4.1(7)
C2	N1	N2	N3	-0.8(5)	C2'	N1'	N2'	N3'	1.4(5)
C2	C3	C4	N4	-102.6(4)	C2'	C3'	C4'	N4'	101.4(4)
C2	C3	C4	C5	69.0(9)	C2'	C3'	C4'	C5'	-72.5(8)
C3	N4	C4	C5	-173.2(7)	C3'	N4'	C4'	C5'	174.1(8)
C3	C4	C5	C6	12.6(10)	C3'	C4'	C5'	C6'	-13.3(9)
C3	C4	C5	C10	-165.2(6)	C3'	C4'	C5'	C10'	165.5(6)
C4	N4	C3	C2	103.9(4)	C4'	N4'	C3'	C2'	-104.2(4)
C4	C5	C6	C7	-179.3(4)	C4'	C5'	C6'	C7'	178.6(4)
C4	C5	C10	C9	178.6(4)	C4'	C5'	C10'	C9'	-179.3(4)
C5	C6	C7	C8	0.9(7)	C5'	C6'	C7'	C8'	0.7(7)
C6	C5	C10	C9	0.8(6)	C6'	C5'	C10'	C9'	-0.4(7)
C6	C7	C8	C9	0.4(7)	C6'	C7'	C8'	C9'	-0.6(7)
C7	C8	C9	C10	-1.0(7)	C7'	C8'	C9'	C10'	0.0(7)
C8	C9	C10	C5	0.5(7)	C8'	C9'	C10'	C5'	0.6(7)
C10	C5	C6	C7	-1.5(6)	C10'	C5'	C6'	C7'	-0.2(7)
C11	S1	N1	N2	92.9(3)	C11'	S1'	N1'	N2'	-87.0(3)
C11	S1	N1	C2	-84.9(4)	C11'	S1'	N1'	C2'	81.0(4)
C11	C12	C13	C14	0.7(6)	C11'	C12'	C13'	C14'	-0.7(6)
C12	C11	C16	C15	-0.8(7)	C12'	C11'	C16'	C15'	-0.4(6)
C12	C13	C14	C15	0.0(7)	C12'	C13'	C14'	C15'	1.2(7)
C12	C13	C14	C17	-179.2(4)	C12'	C13'	C14'	C17'	-179.0(4)
C13	C14	C15	C16	-1.1(7)	C13'	C14'	C15'	C16'	-1.2(7)
C14	C15	C16	C11	1.5(7)	C14'	C15'	C16'	C11'	0.9(7)
C16	C11	C12	C13	-0.3(6)	C16'	C11'	C12'	C13'	0.3(6)
C17	C14	C15	C16	178.0(4)	C17'	C14'	C15'	C16'	178.9(4)

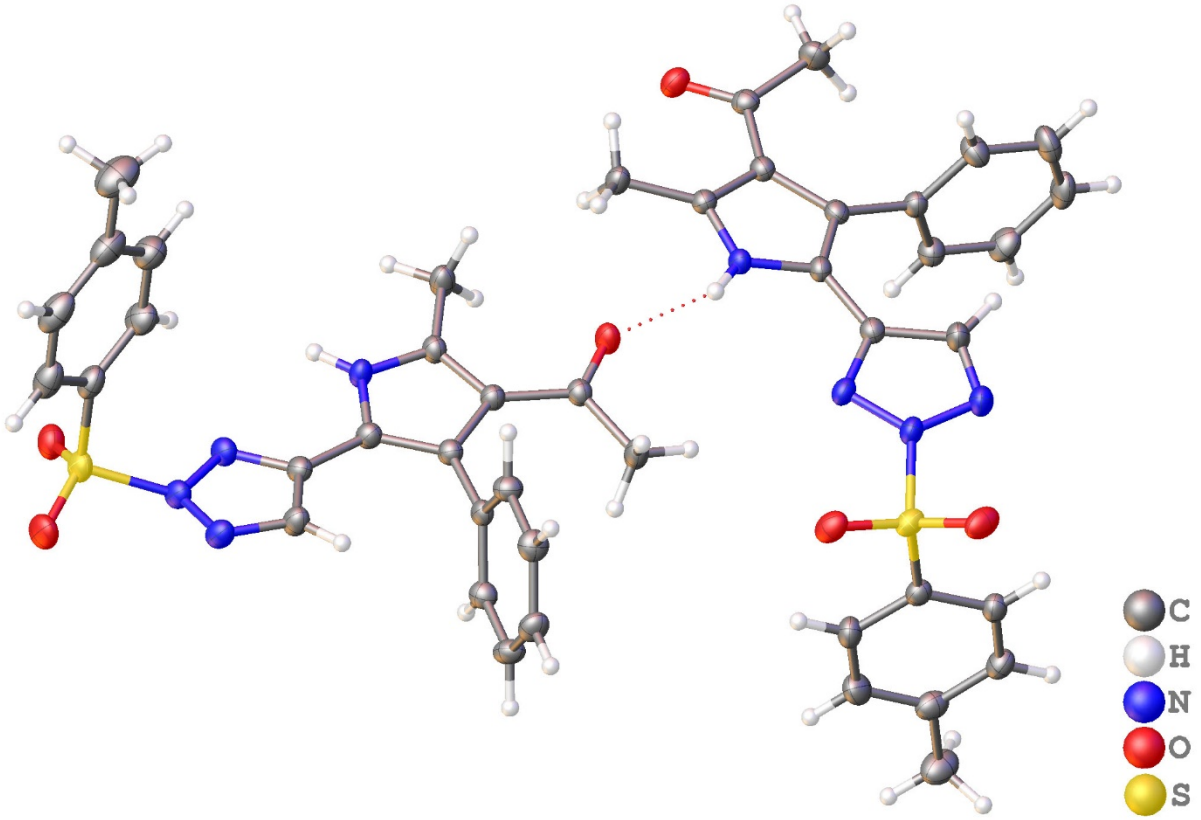
Table S7. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 4a.

Atom	*x*	*y*	*z*	U(eq)
H1	2973.84	3375.11	-2492.48	17
H3	-1050.91	3825.14	-3156.9	18
H6	3281.38	3985.21	-3222.38	18
H7	6188.19	4204.26	-2799.88	22

Table S7. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 4a.

Atom	*x*	*y*	*z*	U(eq)
H8	7911.3	4385.77	-513.77	24
H9	6782.63	4347.76	1374.78	24
H10	3872.25	4139.19	949.42	20
H12	-3166.59	3595.54	-543.26	15
H13	-2950.61	3576.1	1870.5	19
H15	-2087.44	2682.58	1942.94	20
H16	-2392.96	2693.34	-485.35	20
H17A	-1697.56	3286.99	4229.35	32
H17B	-1758.16	2934.75	4164.78	32
H17C	-3621.67	3118.77	3752.68	32
H1'	15387.13	3729.73	4275.43	18
H3'	10370.11	3948.29	2463.73	17
H6'	12126	3410.19	1057.35	18
H7'	12970.1	2957.57	287.29	22
H8'	13396.36	2534.74	1745.47	21
H9'	13041.82	2563.09	3977.2	21
H10'	12256.7	3014.74	4780.47	19
H12'	9379.1	4424.66	4584.06	16
H13'	9252.2	4496.77	6895.26	21
H15'	13855.52	5009.88	8014.41	22
H16'	14030.75	4942.28	5731.29	18
H17D	12216.06	4642.4	9834.87	36
H17E	10212.93	4782.64	9156.14	36
H17F	11981.16	4990.28	9576.39	36

Figure S2. Molecular structure of compound **24**, displacement parameters are drawn at 50% probability level.



Crystal Data for $C_{22}H_{20}N_4O_3S$ (M = 420.48 g/mol): triclinic, space group P-1 (no. 2), a = 6.89270(10) Å, b = 17.0842(2) Å, c = 19.2068(2) Å, V = 2069.21(5) Å^3, Z = 4, T = 100(2) K, μ(Cu$K\alpha$) = 1.656 mm^{-1}, D_{calc} = 1.350 g/cm^3, 22886 reflections measured (4.96° ≤ 2Θ ≤ 139.99°), 7834 unique (R_{int} = 0.0294, R_{sigma} = 0.0314) which were used in all calculations. The final R_1 was 0.0373 ($I \geq 2\sigma(I)$) and wR_2 was 0.0937 ($I \geq 2\sigma(I)$).

Table S8. Crystal data and structure refinement for 24.

Identification code	24
Empirical formula	$C_{22}H_{20}N_4O_3S$
Formula weight	420.48
Temperature/K	100(2)
Crystal system	triclinic
Space group	P-1
a/Å	6.89270(10)
b/Å	17.0842(2)
c/Å	19.2068(2)
α/°	111.2290(10)
β/°	91.7750(10)
γ/°	99.4960(10)
Volume/Å^3	2069.21(5)
Z	4
ρ_{calc}g/cm^3	1.350
μ/mm^{-1}	1.656

$F(000)$	880.0
Crystal size/mm^3	0.14 × 0.1 × 0.08
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	4.96 to 139.99
Index ranges	$-8 \le h \le 8$, $-20 \le k \le 17$, $-20 \le l \le 23$
Reflections collected	22886
Independent reflections	7834 [R_{int} = 0.0294, R_{sigma} = 0.0314]
Data/restraints/parameters	7834/0/547
Goodness-of-fit on F^2	1.042
Final R indexes [I>=2σ (I)]	R_1 = 0.0373, wR_2 = 0.0937
Final R indexes [all data]	R_1 = 0.0422, wR_2 = 0.0967
Largest diff. peak/hole / e Å^{-3}	0.46/-0.39

Table S9. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 24. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
S1	4084.0(6)	5935.6(2)	8246.5(2)	23.86(10)
O1	5393.7(19)	5478.3(8)	8450.2(7)	30.8(3)
O2	2924(2)	6436.8(8)	8761.8(7)	32.7(3)
O3	-202.6(18)	590.9(7)	4141.6(7)	27.9(3)
N1	2381(2)	5159.3(8)	7575.2(8)	24.0(3)
N2	2740(2)	4377.6(8)	7165.3(7)	22.1(3)
N3	738(2)	5353.0(9)	7341.7(9)	30.5(3)
N4	2008.4(19)	2590.7(8)	6169.9(7)	20.2(3)
C1	-57(3)	4649.1(11)	6768.2(10)	29.0(4)
C2	1173(2)	4034.8(10)	6658.4(9)	21.2(3)
C3	5274(2)	6524.7(10)	7752.3(9)	22.4(3)
C4	4368(2)	7128.9(10)	7610.6(9)	24.5(3)
C5	5344(3)	7593.2(11)	7224.7(10)	27.3(3)
C6	7209(3)	7469.1(11)	6991.7(10)	29.5(4)
C7	8079(3)	6865.6(12)	7148.9(11)	32.1(4)
C8	7120(3)	6386.7(11)	7528.7(10)	28.2(4)
C9	8256(3)	7988.1(13)	6580.9(12)	40.4(5)
C10	881(2)	3167.2(10)	6113.8(9)	20.3(3)
C11	-405(2)	2769.3(10)	5469.4(9)	20.3(3)
C12	-24(2)	1917.1(10)	5123.2(9)	20.8(3)
C13	1488(2)	1839.4(10)	5580.4(9)	20.5(3)
C14	-965(2)	1220.5(10)	4429.0(9)	22.2(3)
C15	-2891(3)	1267.2(12)	4073.5(10)	30.6(4)
C16	-1778(2)	3197.4(10)	5186.5(9)	21.7(3)
C17	-3723(3)	3161.1(12)	5370.1(10)	29.4(4)
C18	-4990(3)	3560.7(13)	5100.3(11)	34.3(4)
C19	-4341(3)	3995.8(12)	4641.2(10)	33.6(4)
C20	-2403(3)	4047.3(11)	4466.0(10)	33.1(4)
C21	-1126(3)	3651.1(11)	4736.7(10)	26.7(3)
C22	2461(2)	1102.9(10)	5512.8(9)	24.9(3)
S1'	16148.4(6)	126.9(3)	8188.3(2)	27.93(10)

Table S9. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 24. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1'	16187.4(19)	-312.6(8)	7402.8(7)	32.3(3)
O2'	17915.0(19)	451.3(9)	8684.2(8)	37.2(3)
O3'	5498.0(17)	2409.2(7)	6901.5(7)	27.2(3)
N1'	15120(2)	987.2(9)	8251.5(8)	25.4(3)
N2'	13624(2)	904.5(9)	7735.5(8)	24.6(3)
N3'	15161(2)	1623.6(9)	8923.2(8)	27.7(3)
N4'	10036(2)	1108.1(8)	7064.4(7)	22.0(3)
C1'	13722(3)	2003.8(11)	8822.8(10)	26.5(3)
C2'	12741(2)	1556.6(10)	8083.9(9)	22.3(3)
C3'	14386(3)	-459.5(11)	8543.9(10)	29.5(4)
C4'	14985(3)	-718.7(12)	9111.0(10)	35.0(4)
C5'	13589(3)	-1191.3(12)	9378.6(11)	39.7(5)
C6'	11597(3)	-1394.3(12)	9103.7(11)	37.8(4)
C7'	11045(3)	-1127.3(12)	8533.6(12)	37.7(4)
C8'	12421(3)	-670.2(12)	8245.8(11)	33.8(4)
C9'	10093(4)	-1892.1(15)	9411.5(13)	51.7(6)
C10'	11035(2)	1709.3(10)	7729.1(9)	21.6(3)
C11'	10048(2)	2382.5(10)	7966.4(9)	20.6(3)
C12'	8386(2)	2179.5(10)	7420.4(9)	20.5(3)
C13'	8438(2)	1377.5(10)	6874.5(9)	21.5(3)
C14'	6917(2)	2696.5(10)	7388.2(9)	21.1(3)
C15'	7136(3)	3596.7(10)	7951.4(10)	27.9(4)
C16'	10634(2)	3127.4(10)	8682.1(9)	20.0(3)
C17'	12149(2)	3801.0(10)	8731.5(9)	23.4(3)
C18'	12762(3)	4471.8(11)	9413.6(10)	27.4(4)
C19'	11880(3)	4472.9(11)	10052.6(9)	27.9(4)
C20'	10368(3)	3810.0(11)	10008.5(9)	28.0(4)
C21'	9740(2)	3140.1(11)	9327.9(9)	24.9(3)
C22'	7073(3)	832.0(11)	6193.9(9)	27.1(3)

Table S10. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 24. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S1	29.5(2)	17.88(18)	22.93(19)	6.27(15)	2.24(15)	4.17(15)
O1	39.0(7)	23.8(6)	29.4(6)	10.7(5)	-5.7(5)	4.9(5)
O2	41.3(7)	23.4(6)	29.8(6)	5.4(5)	12.5(5)	5.2(5)
O3	32.0(6)	20.6(6)	28.1(6)	5.9(5)	-2.5(5)	5.5(5)
N1	23.9(7)	18.0(6)	29.4(7)	6.5(5)	1.4(6)	7.6(5)
N2	25.1(7)	16.7(6)	24.8(7)	6.9(5)	3.0(5)	6.8(5)
N3	24.7(7)	23.2(7)	41.9(8)	8.1(6)	1.7(6)	9.7(6)
N4	18.1(6)	18.6(6)	23.7(6)	7.4(5)	-1.4(5)	5.1(5)
C1	22.5(8)	23.2(8)	38.5(9)	6.5(7)	-0.5(7)	8.8(7)
C2	19.4(7)	21.0(7)	24.8(8)	10.0(6)	3.1(6)	4.6(6)

Table S10. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 24. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C3	23.9(8)	18.4(7)	23.0(7)	5.6(6)	0.7(6)	4.3(6)
C4	23.6(8)	21.8(8)	26.8(8)	6.2(6)	1.7(6)	7.4(6)
C5	32.1(9)	21.5(8)	29.2(8)	10.1(7)	1.3(7)	6.8(7)
C6	34.3(9)	23.7(8)	27.1(8)	6.7(7)	5.3(7)	2.4(7)
C7	26.2(9)	30.8(9)	37.5(10)	8.8(8)	8.6(7)	8.3(7)
C8	26.1(8)	25.2(8)	34.2(9)	9.4(7)	3.5(7)	10.9(7)
C9	48.0(12)	33.0(10)	42.2(11)	15.9(9)	17.1(9)	6.3(9)
C10	17.9(7)	19.2(7)	25.4(8)	9.3(6)	2.9(6)	5.9(6)
C11	16.2(7)	21.4(7)	24.7(8)	10.4(6)	2.8(6)	3.3(6)
C12	18.5(7)	20.4(7)	24.7(8)	9.9(6)	1.6(6)	3.7(6)
C13	18.9(7)	18.6(7)	23.9(7)	7.9(6)	1.5(6)	3.3(6)
C14	22.0(8)	20.9(8)	24.7(8)	11.0(6)	0.7(6)	1.5(6)
C15	25.5(8)	29.0(9)	32.4(9)	7.4(7)	-6.4(7)	2.9(7)
C16	20.2(7)	19.0(7)	24.7(8)	6.6(6)	-0.9(6)	4.6(6)
C17	22.2(8)	36.9(9)	32.9(9)	16.3(8)	3.8(7)	8.1(7)
C18	24.1(9)	43.9(11)	36.9(10)	13.6(8)	0.3(7)	15.7(8)
C19	35.9(10)	31.5(9)	34.6(9)	9.9(8)	-5.4(8)	16.9(8)
C20	42.3(10)	27.4(9)	33.8(9)	16.1(8)	-1.4(8)	8.3(8)
C21	24.7(8)	25.7(8)	31.6(9)	12.0(7)	3.4(7)	6.8(6)
C22	25.1(8)	19.4(7)	28.2(8)	5.9(6)	-2.7(6)	6.7(6)
S1'	25.7(2)	25.3(2)	33.9(2)	10.87(17)	-4.35(16)	9.55(16)
O1'	31.5(6)	30.9(6)	37.0(7)	12.7(5)	1.8(5)	13.1(5)
O2'	28.9(7)	36.4(7)	46.5(8)	15.1(6)	-10.4(6)	10.4(5)
O3'	25.2(6)	25.0(6)	29.1(6)	6.0(5)	-5.5(5)	9.3(5)
N1'	23.8(7)	23.5(7)	29.1(7)	10.3(6)	-6.1(6)	5.5(5)
N2'	22.6(7)	24.5(7)	28.1(7)	11.5(6)	-3.3(5)	5.8(5)
N3'	27.7(7)	22.7(7)	30.9(7)	8.9(6)	-7.0(6)	4.0(6)
N4'	23.0(7)	18.8(6)	22.6(6)	4.5(5)	-2.2(5)	7.6(5)
C1'	27.3(8)	22.2(8)	28.6(8)	7.4(7)	-4.7(7)	6.5(6)
C2'	21.2(7)	20.1(7)	26.8(8)	10.4(6)	-0.5(6)	3.9(6)
C3'	36.6(10)	22.8(8)	30.6(9)	9.7(7)	-1.3(7)	10.8(7)
C4'	46.8(11)	27.7(9)	30.2(9)	8.4(7)	-5.3(8)	13.8(8)
C5'	65.5(14)	27.9(9)	28.4(9)	12.2(8)	-0.9(9)	13.6(9)
C6'	55.9(12)	24.2(9)	33.3(10)	9.5(7)	7.2(9)	9.7(8)
C7'	39.5(11)	30.5(9)	44.8(11)	16.3(8)	0.7(8)	6.8(8)
C8'	37.2(10)	30.1(9)	38.2(10)	17.7(8)	-3.4(8)	7.4(8)
C9'	72.7(16)	38.6(11)	48.7(12)	22.4(10)	13.4(11)	8.3(11)
C10'	21.9(8)	20.1(7)	22.0(7)	7.4(6)	-1.9(6)	3.8(6)
C11'	20.4(7)	20.1(7)	22.0(7)	8.9(6)	-0.3(6)	3.8(6)
C12'	20.3(7)	19.5(7)	21.5(7)	7.0(6)	0.1(6)	4.6(6)
C13'	20.6(7)	21.9(8)	22.8(7)	8.5(6)	-0.2(6)	6.4(6)
C14'	20.2(7)	22.0(8)	22.1(7)	9.0(6)	1.5(6)	5.4(6)
C15'	27.0(8)	22.4(8)	32.3(9)	6.3(7)	-3.2(7)	9.4(6)
C16'	18.6(7)	19.4(7)	22.8(7)	8.1(6)	-2.0(6)	5.8(6)
C17'	22.6(8)	25.4(8)	23.5(8)	11.3(6)	0.2(6)	3.9(6)

Table S10. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 24. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C18'	25.7(8)	23.3(8)	31.1(9)	11.1(7)	-5.8(7)	-1.9(6)
C19'	32.5(9)	22.2(8)	23.9(8)	3.8(6)	-4.6(7)	4.1(7)
C20'	31.0(9)	30.1(9)	23.1(8)	9.4(7)	3.6(7)	7.5(7)
C21'	23.6(8)	23.9(8)	26.8(8)	10.3(7)	0.9(6)	1.5(6)
C22'	27.8(8)	24.3(8)	24.7(8)	2.5(7)	-4.0(7)	9.8(7)

Table S11. Bond Lengths for 24.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S1	O1	1.4179(13)	S1'	O1'	1.4245(14)
S1	O2	1.4188(13)	S1'	O2'	1.4214(13)
S1	N1	1.7185(14)	S1'	N1'	1.7021(14)
S1	C3	1.7477(16)	S1'	C3'	1.7582(19)
O3	C14	1.230(2)	O3'	C14'	1.235(2)
N1	N2	1.3507(19)	N1'	N2'	1.3613(19)
N1	N3	1.339(2)	N1'	N3'	1.349(2)
N2	C2	1.331(2)	N2'	C2'	1.330(2)
N3	C1	1.321(2)	N3'	C1'	1.317(2)
N4	C10	1.3820(19)	N4'	C10'	1.386(2)
N4	C13	1.352(2)	N4'	C13'	1.350(2)
C1	C2	1.417(2)	C1'	C2'	1.428(2)
C2	C10	1.448(2)	C2'	C10'	1.447(2)
C3	C4	1.391(2)	C3'	C4'	1.391(3)
C3	C8	1.385(2)	C3'	C8'	1.390(3)
C4	C5	1.383(2)	C4'	C5'	1.384(3)
C5	C6	1.399(3)	C5'	C6'	1.397(3)
C6	C7	1.390(3)	C6'	C7'	1.395(3)
C6	C9	1.503(3)	C6'	C9'	1.503(3)
C7	C8	1.386(3)	C7'	C8'	1.384(3)
C10	C11	1.380(2)	C10'	C11'	1.375(2)
C11	C12	1.438(2)	C11'	C12'	1.437(2)
C11	C16	1.486(2)	C11'	C16'	1.484(2)
C12	C13	1.396(2)	C12'	C13'	1.399(2)
C12	C14	1.469(2)	C12'	C14'	1.462(2)
C13	C22	1.488(2)	C13'	C22'	1.488(2)
C14	C15	1.501(2)	C14'	C15'	1.505(2)
C16	C17	1.394(2)	C16'	C17'	1.393(2)
C16	C21	1.394(2)	C16'	C21'	1.397(2)
C17	C18	1.386(2)	C17'	C18'	1.388(2)
C18	C19	1.386(3)	C18'	C19'	1.386(3)
C19	C20	1.384(3)	C19'	C20'	1.383(3)
C20	C21	1.388(2)	C20'	C21'	1.387(2)

Table S12. Bond Angles for 24.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	S1	O2	122.92(8)	O1'	S1'	N1'	104.26(7)
O1	S1	N1	104.45(7)	O1'	S1'	C3'	110.47(8)
O1	S1	C3	110.20(8)	O2'	S1'	O1'	121.37(8)
O2	S1	N1	104.33(8)	O2'	S1'	N1'	106.28(7)
O2	S1	C3	109.60(8)	O2'	S1'	C3'	109.96(9)
N1	S1	C3	103.22(7)	N1'	S1'	C3'	102.56(8)
N2	N1	S1	123.21(11)	N2'	N1'	S1'	119.83(11)
N3	N1	S1	120.35(11)	N3'	N1'	S1'	120.03(11)
N3	N1	N2	115.51(13)	N3'	N1'	N2'	115.04(13)
C2	N2	N1	103.20(13)	C2'	N2'	N1'	103.39(13)
C1	N3	N1	103.47(13)	C1'	N3'	N1'	103.57(13)
C13	N4	C10	110.18(13)	C13'	N4'	C10'	110.10(13)
N3	C1	C2	109.28(15)	N3'	C1'	C2'	109.52(15)
N2	C2	C1	108.46(14)	N2'	C2'	C1'	108.31(14)
N2	C2	C10	122.47(14)	N2'	C2'	C10'	121.85(14)
C1	C2	C10	129.06(15)	C1'	C2'	C10'	129.80(15)
C4	C3	S1	119.33(13)	C4'	C3'	S1'	119.44(15)
C8	C3	S1	118.60(13)	C8'	C3'	S1'	119.59(14)
C8	C3	C4	122.05(16)	C8'	C3'	C4'	120.96(18)
C5	C4	C3	118.36(15)	C5'	C4'	C3'	118.93(19)
C4	C5	C6	120.94(16)	C4'	C5'	C6'	121.43(17)
C5	C6	C9	120.10(17)	C5'	C6'	C9'	120.79(19)
C7	C6	C5	119.15(16)	C7'	C6'	C5'	118.21(19)
C7	C6	C9	120.75(17)	C7'	C6'	C9'	121.0(2)
C8	C7	C6	120.93(16)	C8'	C7'	C6'	121.4(2)
C3	C8	C7	118.56(16)	C7'	C8'	C3'	119.06(17)
N4	C10	C2	121.93(14)	N4'	C10'	C2'	121.50(14)
C11	C10	N4	108.08(13)	C11'	C10'	N4'	108.18(13)
C11	C10	C2	129.95(14)	C11'	C10'	C2'	130.20(15)
C10	C11	C12	106.74(13)	C10'	C11'	C12'	106.75(14)
C10	C11	C16	124.37(14)	C10'	C11'	C16'	123.35(14)
C12	C11	C16	128.72(14)	C12'	C11'	C16'	129.81(14)
C11	C12	C14	129.82(14)	C11'	C12'	C14'	128.91(14)
C13	C12	C11	106.95(14)	C13'	C12'	C11'	107.03(13)
C13	C12	C14	123.23(14)	C13'	C12'	C14'	124.01(14)
N4	C13	C12	108.04(13)	N4'	C13'	C12'	107.93(14)
N4	C13	C22	120.96(14)	N4'	C13'	C22'	120.71(14)
C12	C13	C22	130.99(14)	C12'	C13'	C22'	131.34(14)
O3	C14	C12	120.50(14)	O3'	C14'	C12'	121.06(14)
O3	C14	C15	119.56(15)	O3'	C14'	C15'	119.08(14)
C12	C14	C15	119.94(14)	C12'	C14'	C15'	119.85(14)
C17	C16	C11	120.95(14)	C17'	C16'	C11'	120.81(14)
C21	C16	C11	120.18(14)	C17'	C16'	C21'	119.00(15)
C21	C16	C17	118.86(15)	C21'	C16'	C11'	120.10(14)
C18	C17	C16	120.37(16)	C18'	C17'	C16'	120.35(15)
C19	C18	C17	120.37(17)	C19'	C18'	C17'	120.18(15)

Table S12. Bond Angles for 24.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C20	C19	C18	119.66(16)	C20'	C19'	C18'	119.91(16)
C19	C20	C21	120.21(17)	C19'	C20'	C21'	120.24(16)
C20	C21	C16	120.50(16)	C20'	C21'	C16'	120.32(15)

Table S13. Torsion Angles for 24.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
S1	N1	N2	C2	-171.95(11)	S1'	N1'	N2'	C2'	158.64(12)
S1	N1	N3	C1	171.76(12)	S1'	N1'	N3'	C1'	-158.99(12)
S1	C3	C4	C5	179.42(12)	S1'	C3'	C4'	C5'	-179.02(14)
S1	C3	C8	C7	-178.82(13)	S1'	C3'	C8'	C7'	-179.59(15)
O1	S1	N1	N2	-22.18(14)	O1'	S1'	N1'	N2'	37.71(14)
O1	S1	N1	N3	169.41(13)	O1'	S1'	N1'	N3'	-168.79(13)
O1	S1	C3	C4	-169.22(13)	O1'	S1'	C3'	C4'	121.03(15)
O1	S1	C3	C8	9.31(16)	O1'	S1'	C3'	C8'	-57.85(17)
O2	S1	N1	N2	-152.35(13)	O2'	S1'	N1'	N2'	167.05(12)
O2	S1	N1	N3	39.24(15)	O2'	S1'	N1'	N3'	-39.46(15)
O2	S1	C3	C4	-31.00(16)	O2'	S1'	C3'	C4'	-15.59(17)
O2	S1	C3	C8	147.53(13)	O2'	S1'	C3'	C8'	165.53(14)
N1	S1	C3	C4	79.71(14)	N1'	S1'	C3'	C4'	-128.33(15)
N1	S1	C3	C8	-101.76(14)	N1'	S1'	C3'	C8'	52.79(16)
N1	N2	C2	C1	2.21(17)	N1'	N2'	C2'	C1'	-1.80(17)
N1	N2	C2	C10	-176.92(14)	N1'	N2'	C2'	C10'	-179.81(14)
N1	N3	C1	C2	-0.89(19)	N1'	N3'	C1'	C2'	2.84(18)
N2	N1	N3	C1	2.49(19)	N2'	N1'	N3'	C1'	-4.29(19)
N2	C2	C10	N4	12.0(2)	N2'	C2'	C10'	N4'	11.1(2)
N2	C2	C10	C11	-165.69(16)	N2'	C2'	C10'	C11'	-173.21(16)
N3	N1	N2	C2	-3.03(18)	N3'	N1'	N2'	C2'	3.88(18)
N3	C1	C2	N2	-0.9(2)	N3'	C1'	C2'	N2'	-0.7(2)
N3	C1	C2	C10	178.17(16)	N3'	C1'	C2'	C10'	177.12(16)
N4	C10	C11	C12	-0.22(17)	N4'	C10'	C11'	C12'	-0.16(17)
N4	C10	C11	C16	-175.93(14)	N4'	C10'	C11'	C16'	176.73(14)
C1	C2	C10	N4	-166.91(16)	C1'	C2'	C10'	N4'	-166.42(16)
C1	C2	C10	C11	15.4(3)	C1'	C2'	C10'	C11'	9.2(3)
C2	C10	C11	C12	177.74(15)	C2'	C10'	C11'	C12'	-176.27(16)
C2	C10	C11	C16	2.0(3)	C2'	C10'	C11'	C16'	0.6(3)
C3	S1	N1	N2	93.08(13)	C3'	S1'	N1'	N2'	-77.52(14)
C3	S1	N1	N3	-75.33(14)	C3'	S1'	N1'	N3'	75.97(14)
C3	C4	C5	C6	-1.0(2)	C3'	C4'	C5'	C6'	-1.5(3)
C4	C3	C8	C7	-0.3(3)	C4'	C3'	C8'	C7'	1.5(3)
C4	C5	C6	C7	0.4(3)	C4'	C5'	C6'	C7'	1.7(3)
C4	C5	C6	C9	-179.26(17)	C4'	C5'	C6'	C9'	-178.70(19)
C5	C6	C7	C8	0.3(3)	C5'	C6'	C7'	C8'	-0.2(3)
C6	C7	C8	C3	-0.3(3)	C6'	C7'	C8'	C3'	-1.3(3)
C8	C3	C4	C5	0.9(2)	C8'	C3'	C4'	C5'	-0.2(3)

Table S13. Torsion Angles for 24.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C9	C6	C7	C8	179.89(17)	C9'	C6'	C7'	C8'	-179.86(19)
C10	N4	C13	C12	-0.20(17)	C10'	N4'	C13'	C12'	0.67(18)
C10	N4	C13	C22	-179.00(14)	C10'	N4'	C13'	C22'	-177.94(14)
C10	C11	C12	C13	0.10(17)	C10'	C11'	C12'	C13'	0.55(18)
C10	C11	C12	C14	179.87(15)	C10'	C11'	C12'	C14'	-176.91(15)
C10	C11	C16	C17	-94.0(2)	C10'	C11'	C16'	C17'	81.9(2)
C10	C11	C16	C21	85.4(2)	C10'	C11'	C16'	C21'	-94.70(19)
C11	C12	C13	N4	0.06(17)	C11'	C12'	C13'	N4'	-0.75(18)
C11	C12	C13	C22	178.69(16)	C11'	C12'	C13'	C22'	177.65(17)
C11	C12	C14	O3	165.91(16)	C11'	C12'	C14'	O3'	-175.77(15)
C11	C12	C14	C15	-15.2(2)	C11'	C12'	C14'	C15'	4.7(2)
C11	C16	C17	C18	-179.77(16)	C11'	C16'	C17'	C18'	-176.36(15)
C11	C16	C21	C20	179.53(15)	C11'	C16'	C21'	C20'	176.00(15)
C12	C11	C16	C17	91.3(2)	C12'	C11'	C16'	C17'	-102.0(2)
C12	C11	C16	C21	-89.3(2)	C12'	C11'	C16'	C21'	81.4(2)
C13	N4	C10	C2	-177.89(14)	C13'	N4'	C10'	C2'	176.20(15)
C13	N4	C10	C11	0.27(17)	C13'	N4'	C10'	C11'	-0.31(18)
C13	C12	C14	O3	-14.3(2)	C13'	C12'	C14'	O3'	7.2(2)
C13	C12	C14	C15	164.51(15)	C13'	C12'	C14'	C15'	-172.36(15)
C14	C12	C13	N4	-179.73(14)	C14'	C12'	C13'	N4'	176.87(14)
C14	C12	C13	C22	-1.1(3)	C14'	C12'	C13'	C22'	-4.7(3)
C16	C11	C12	C13	175.56(15)	C16'	C11'	C12'	C13'	-176.06(15)
C16	C11	C12	C14	-4.7(3)	C16'	C11'	C12'	C14'	6.5(3)
C16	C17	C18	C19	0.4(3)	C16'	C17'	C18'	C19'	0.5(2)
C17	C16	C21	C20	-1.1(3)	C17'	C16'	C21'	C20'	-0.6(2)
C17	C18	C19	C20	-1.5(3)	C17'	C18'	C19'	C20'	-0.9(3)
C18	C19	C20	C21	1.3(3)	C18'	C19'	C20'	C21'	0.5(3)
C19	C20	C21	C16	0.0(3)	C19'	C20'	C21'	C16'	0.3(3)
C21	C16	C17	C18	0.9(3)	C21'	C16'	C17'	C18'	0.2(2)

Table S14. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 24.

Atom	*x*	*y*	*z*	U(eq)
H4	2931.31	2697.17	6536.28	24
H1	-1262.55	4567.57	6475.41	35
H4A	3109.06	7220.22	7774.93	29
H5	4738.34	8002.4	7116.2	33
H7	9348.79	6780.1	6993.97	39
H8	7716.14	5972.92	7633.31	34
H9A	7565.81	7813.31	6079.26	61
H9B	9618.47	7893.32	6535.53	61
H9C	8266.97	8596.11	6860.2	61
H15A	-2721.32	1774.89	3940.33	46
H15B	-3895.77	1303.41	4428.3	46

Table S14. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 24.

Atom	*x*	*y*	*z*	U(eq)
H15C	-3314.57	753.7	3619.66	46
H17	-4182.94	2860.85	5681.81	35
H18	-6310.74	3536.06	5230.98	41
H19	-5221.57	4257.52	4447.56	40
H20	-1945.9	4354.79	4159.61	40
H21	202.33	3689.4	4614.41	32
H22A	3372.03	1031.49	5122.07	37
H22B	1453.68	581.54	5378.53	37
H22C	3198	1210.59	5993.17	37
H4'	10391.36	621.75	6804.13	26
H1'	13387.65	2499.21	9185.85	32
H4'A	16330.46	-573.74	9311.4	42
H5'	13995.61	-1381.64	9757.43	48
H7'	9696.74	-1261.93	8338.71	45
H8'	12029.11	-502.84	7850.09	41
H9'A	10284.7	-2485.59	9247.2	78
H9'B	8760.82	-1879.86	9226.87	78
H9'C	10251.58	-1635.36	9961.1	78
H15D	6216.06	3892.38	7790.24	42
H15E	8494.28	3901.08	7987.56	42
H15F	6841.77	3582.45	8443.04	42
H17'	12765.71	3801.17	8295.95	28
H18'	13787.95	4931.23	9442.45	33
H19'	12314.48	4928.62	10520.26	33
H20'	9757.52	3813.32	10445.99	34
H21'	8696.99	2687.62	9300.9	30
H22D	7627.56	330.11	5910.78	41
H22E	6905.55	1160.8	5878.18	41
H22F	5786.7	645.83	6344.61	41

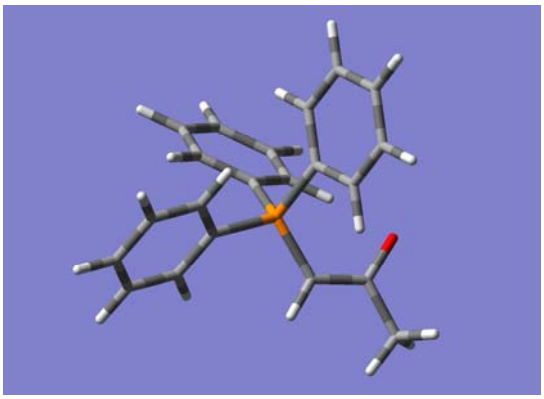
Computational Details

All calculations were performed by using the Gaussian 16 suite of quantum chemical programs[6] at Resource center "Computer center of Saint Petersburg State University". Geometry optimizations of molecules were performed with the B3LYP[7]-D3[8] density functional method and 6-311+G(d,p) basis set using SMD[9] solvent model. Stationary points on the respective potential-energy surfaces were characterized at the same level of theory by evaluating the corresponding Hessian indices. Careful verification of the unique imaginary frequency for the transition state was carried out to check whether the frequency indeed pertains to the desired reaction coordinate.

Table S15. B3LYP-D3/6-311+G(d,p), SMD solvent model for DCM.

Absolute Energies (au), Cartesian Coordinates of stationary points

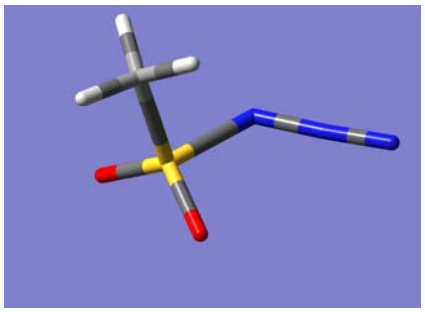
Molecule **6**



E = --1228.563172, H (0K) = -1228.226966,
H (298K) = -1228.204937,
G (298K) = -1228.279408 au.
Imaginary frequency = 0.

C	0.5263620	0.0634750	2.0958230
C	1.8660800	-0.1775450	2.4534100
O	2.7651470	-0.5257410	1.6459860
C	2.2503500	0.0114240	3.9155180
P	0.0012480	0.0107720	0.4398440
C	-1.6998450	0.6669930	0.3951780
C	-2.0567420	1.7152220	-0.4587380
C	-3.3693860	2.1876050	-0.4692050
C	-4.3265350	1.6160610	0.3672110
C	-3.9728630	0.5668510	1.2180460
C	-2.6651860	0.0896600	1.2327120
C	1.0214800	1.0401620	-0.6729870
C	1.5974200	2.2076420	-0.1601950
C	2.3336500	3.0442840	-0.9950660
C	2.4988300	2.7190480	-2.3424800
C	1.9284210	1.5536420	-2.8538920
C	1.1899780	0.7125840	-2.0224150
C	-0.0751720	-1.6508650	-0.3287530
C	-1.1346090	-2.0083850	-1.1718140
C	-1.1655230	-3.2759610	-1.7527350
C	-0.1428290	-4.1882620	-1.4958060
C	0.9143800	-3.8323040	-0.6564620
C	0.9535400	-2.5683600	-0.0721160
H	-0.2181970	0.3694340	2.8179180

Molecule **2d**

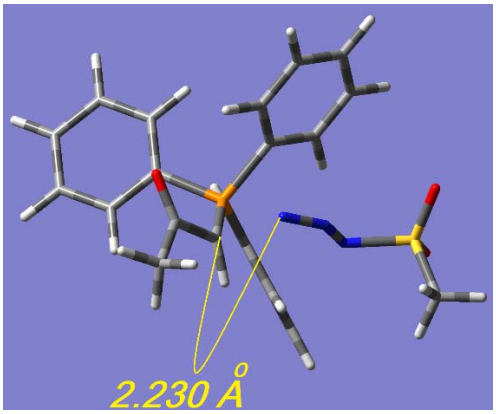


E = -752.813028, H (0K) = -752.753356,
H (298K) = -752.744992,
G (298K) = -752.785989 au.
Imaginary frequency = 0.

N	2.8127790	0.1379110	0.2018140
N	1.8097420	-0.0110990	-0.2890270
N	0.7613440	-0.1979910	-0.9236740
S	-0.6952960	-0.1629390	0.0787330
O	-0.3179360	-0.4480390	1.4617670
C	-1.1898800	1.5503490	-0.0828010
O	-1.6271170	-1.0247070	-0.6325340
H	-2.1253610	1.6556220	0.4696410
H	-1.3310850	1.7592460	-1.1425350
H	-0.4061770	2.1702880	0.3523220

H	3.0096270	0.7972190	3.9827440
H	2.7036240	-0.9123410	4.2879190
H	1.4064340	0.2784130	4.5551960
H	-1.3196490	2.1650910	-1.1125960
H	-3.6402020	3.0021480	-1.1314880
H	-5.3461310	1.9849700	0.3568510
H	-4.7155380	0.1183370	1.8682190
H	-2.3987560	-0.7313120	1.8888150
H	1.4763270	2.4510240	0.8893350
H	2.7835960	3.9450800	-0.5929090
H	3.0762370	3.3694330	-2.9902770
H	2.0605500	1.2950840	-3.8985710
H	0.7558610	-0.1941320	-2.4261790
H	-1.9355580	-1.3076550	-1.3756290
H	-1.9896280	-3.5483670	-2.4027110
H	-0.1693880	-5.1740890	-1.9469960
H	1.7115040	-4.5396470	-0.4560490
H	1.7785920	-2.2821720	0.5694530

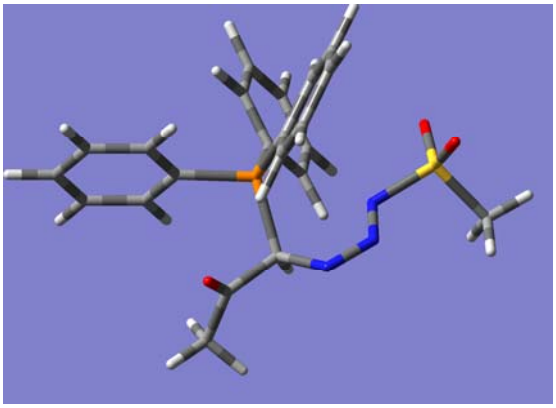
TS6/2d-7



E = -1981.377234, H (0K) = -1980.980593,
H (298K) = -1980.950336,
G (298K) = -1981.045001 au.
Imaginary frequency = 1 (-196.58 cm^{-1}).

C	-0.5611760	-0.6865510	-1.7446980
C	-1.3295370	-1.8200000	-2.2031390
O	-1.9959070	-2.5351780	-1.4439620
C	-1.1991710	-2.1698130	-3.6718510
P	-0.9687750	0.0511840	-0.1819430
C	-0.5519950	1.8270120	-0.1821650
C	-1.1954420	2.6523820	0.7511660
C	-0.9018590	4.0126690	0.8000390
C	0.0255470	4.5596360	-0.0861990
C	0.6614630	3.7418300	-1.0194750
C	0.3804280	2.3783960	-1.0681330
C	-2.7673490	-0.0195010	0.1310210
C	-3.6315330	0.3592360	-0.9033430
C	-5.0057600	0.3735790	-0.6884260
C	-5.5229600	0.0132910	0.5580800
C	-4.6623430	-0.3599520	1.5885460
C	-3.2830010	-0.3760180	1.3794500

Molecule **7**



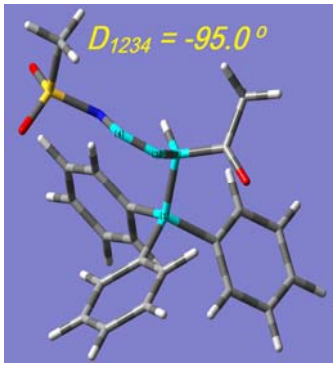
E = -1981.400133, H (0K) = -1980.999998,
H (298K) = -1980.970595,
G (298K) = -1981.060242 au.
Imaginary frequency = 0.

C	0.7901879	-0.3002980	1.1137481
C	2.0827059	-0.8897070	1.7062501
O	2.5402149	-1.9214480	1.2636551
C	2.6784669	-0.1437630	2.8618331
P	1.0160969	0.1505360	-0.7071689
C	0.5276789	1.8506380	-1.1368939
C	0.9446059	2.3272850	-2.3881729
C	0.6459959	3.6322960	-2.7698819
C	-0.0388211	4.4756320	-1.8953749
C	-0.4341161	4.0071650	-0.6432059
C	-0.1659081	2.6943180	-0.2650799
C	2.8212619	0.1655770	-1.0225739
C	3.5831699	1.1646650	-0.3990989
C	4.9603279	1.2116920	-0.5900229
C	5.5843919	0.2704930	-1.4109149
C	4.8269679	-0.7153490	-2.0403849
C	3.4468679	-0.7725280	-1.8477909

C	-0.1398460	-0.7570980	1.2236730
C	0.6370020	-0.0272260	2.1290000
C	1.2827800	-0.6871510	3.1719260
C	1.1571770	-2.0687670	3.3111790
C	0.3821470	-2.7960770	2.4067140
C	-0.2678460	-2.1462010	1.3609460
H	-0.1537740	-0.0042330	-2.4800070
H	-1.1902340	-1.2810790	-4.3074260
H	-2.0136320	-2.8326920	-3.9669610
H	-0.2497330	-2.6966340	-3.8210570
H	-1.9260420	2.2412390	1.4374950
H	-1.4012950	4.6426010	1.5272520
H	0.2518370	5.6194400	-0.0495150
H	1.3860060	4.1615190	-1.7079890
H	0.9055790	1.7546850	-1.7764940
H	-3.2329480	0.6346040	-1.8737850
H	-5.6730650	0.6620290	-1.4927240
H	-6.5946450	0.0221700	0.7229950
H	-5.0603580	-0.6416280	2.5568720
H	-2.6214030	-0.6690770	2.1851650
H	0.7588190	1.0424460	2.0149570
H	1.8951050	-0.1217750	3.8649950
H	1.6687240	-2.5798390	4.1192660
H	0.2877900	-3.8711570	2.5101880
H	-0.8648620	-2.7068150	0.6511040
N	1.2303060	-1.9914310	-1.5024660
N	2.1096670	-1.3491450	-1.0885130
N	2.3443620	-0.1316630	-0.7298570
S	3.9131100	0.0689370	-0.0903690
O	4.2828280	-1.0486950	0.7902710
C	4.9876710	0.0321210	-1.5317960
O	3.8902600	1.4299390	0.4560110
H	6.0064990	0.1972800	-1.1782860
H	4.6742320	0.8265930	-2.2084210
H	4.8950910	-0.9480790	-2.0003770

C	0.2816729	-1.1133920	-1.7741359
C	-0.5082861	-0.7623890	-2.8734529
C	-1.0554421	-1.7634930	-3.6699029
C	-0.8265821	-3.1061400	-3.3674229
C	-0.0436961	-3.4523170	-2.2669099
C	0.5163839	-2.4596560	-1.4659219
H	0.5379349	0.6484730	1.5973071
H	2.9105619	0.8811410	2.5553051
H	3.5791329	-0.6421480	3.2188401
H	1.9385689	-0.0771420	3.6674091
H	1.5029659	1.6902630	-3.0639289
H	0.9577049	3.9894090	-3.7446659
H	-0.2633411	5.4949060	-2.1893139
H	-0.9695271	4.6585730	0.0380081
H	-0.5156791	2.3331670	0.6902411
H	3.1041249	1.9101050	0.2260681
H	5.5439999	1.9853080	-0.1042309
H	6.6572669	0.3099380	-1.5623779
H	5.3067899	-1.4442720	-2.6835359
H	2.8710889	-1.5447300	-2.3408529
H	-0.7181391	0.2756570	-3.0960529
H	-1.6761511	-1.4927800	-4.5161739
H	-1.2652181	-3.8819220	-3.9850879
H	0.1292909	-4.4946110	-2.0247169
H	1.1226709	-2.7286170	-0.6091299
N	-0.2574821	-1.3148830	1.3982501
N	-1.4215271	-1.0531800	0.9649031
N	-1.5551951	0.0526510	0.2601931
S	-3.1108401	0.2059610	-0.3715779
O	-3.5928401	-1.0327070	-1.0107439
C	-4.1559631	0.5196170	1.0619701
O	-3.0659891	1.4274760	-1.1933379
H	-5.1733891	0.6606470	0.6944701
H	-3.7933301	1.4183840	1.5599311
H	-4.0983161	-0.3470550	1.7202821

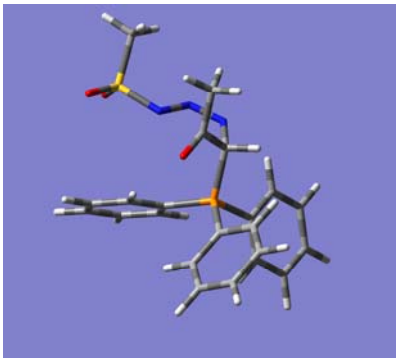
TS7-8



E = -1981.395931, H (0K) = -1980.996422,
H (298K) = -1980.967525,
G (298K) = -1981.056958 au.
Imaginary frequency = 1 (-23.81 cm^{-1}).

C	-0.0607070	-0.7933430	1.3233320
C	0.8528210	-1.6326880	2.2296210

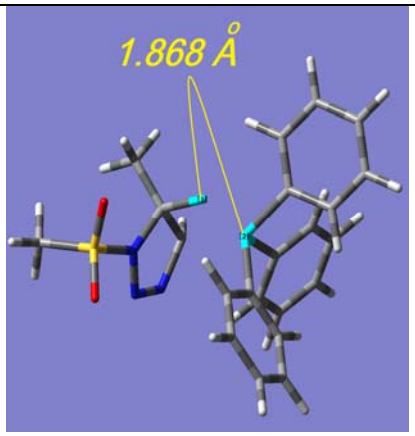
Molecule **8**



E = -1981.400387, H (0K) = -1980.999874,
H (298K) = -1980.970527,
G (298K) = -1981.060828 au.
Imaginary frequency = 0.

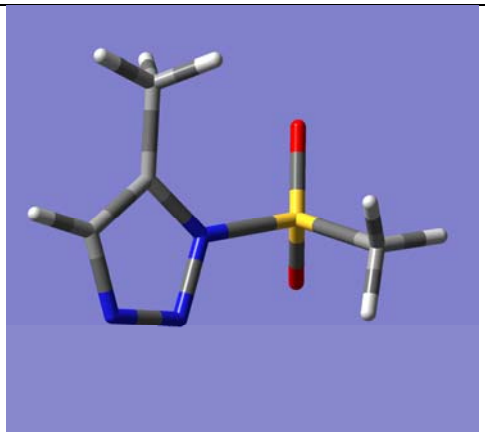
C	-0.5049167	1.1498810	-1.1433865
C	0.1761303	-0.2298910	-1.0468985

O	1.6322180	-2.4309680	1.7545820	O	-0.0939097	-1.0176320	-0.1599055
C	0.6453590	-1.4409180	3.7028120	C	1.0108693	-0.6172930	-2.2409405
P	0.9138680	0.0632260	-0.0464950	P	-1.5695187	1.5248610	0.3465955
C	0.4801280	1.8202090	-0.2169470	C	-2.6282957	2.9515820	-0.0555015
C	1.4726680	2.7081350	-0.6628860	C	-3.7928217	3.1302020	0.7069165
C	1.1549020	4.0462750	-0.8760880	C	-4.6214077	4.2208710	0.4621955
C	-0.1426660	4.5053240	-0.6448420	C	-4.2993457	5.1330600	-0.5438205
C	-1.1264070	3.6222030	-0.2029390	C	-3.1437347	4.9548560	-1.3021385
C	-0.8226790	2.2789450	0.0084890	C	-2.3015547	3.8702790	-1.0605775
C	2.6867100	0.0275320	0.3542330	C	-2.7013047	0.1441710	0.6826075
C	3.0975170	0.5957530	1.5682390	C	-3.3607507	-0.4589600	-0.3966555
C	4.4481280	0.6189270	1.8973230	C	-4.2741967	-1.4813490	-0.1619285
C	5.3911560	0.0838120	1.0170150	C	-4.5386327	-1.8997800	1.1437185
C	4.9816270	-0.4726420	-0.1929880	C	-3.8894107	-1.2915490	2.2161995
C	3.6287360	-0.5026100	-0.5302360	C	-2.9695667	-0.2682400	1.9909185
C	0.6154720	-0.8035690	-1.6039700	C	-0.5733787	1.9233950	1.8018955
C	0.1463560	-0.1120280	-2.7256000	C	-0.4889687	3.2496880	2.2400565
C	-0.0755080	-0.8050870	-3.9143030	C	0.3253383	3.5642010	3.3265175
C	0.1714460	-2.1752470	-3.9815440	C	1.0412203	2.5612630	3.9762745
C	0.6384610	-2.8627620	-2.8592920	C	0.9509743	1.2380490	3.5399955
C	0.8568950	-2.1839950	-1.6654420	C	0.1533503	0.9139190	2.4497675
H	-0.5584330	0.0003000	1.8840540	H	-1.2280237	1.0904180	-1.9653365
H	0.8991540	-0.4102060	3.9728220	H	0.3463623	-1.1123810	-2.9595465
H	1.2595930	-2.1386800	4.2713390	H	1.7766353	-1.3283660	-1.9304355
H	-0.4133140	-1.5819440	3.9452110	H	1.4643273	0.2425340	-2.7337755
H	2.4843270	2.3662230	-0.8423830	H	-4.0566667	2.4246630	1.4859115
H	1.9227370	4.7290900	-1.2213330	H	-5.5193967	4.3548740	1.0543015
H	-0.3845050	5.5494310	-0.8097730	H	-4.9488617	5.9799180	-0.7352895
H	-2.1367820	3.9715100	-0.0235820	H	-2.8892747	5.6621590	-2.0832055
H	-1.5904930	1.5895120	0.3377060	H	-1.3928157	3.7479630	-1.6357845
H	2.3696240	1.0176590	2.2527700	H	-3.1656277	-0.1407740	-1.4145945
H	4.7647920	1.0543920	2.8379840	H	-4.7788287	-1.9519240	-0.9978865
H	6.4438850	0.1029380	1.2754840	H	-5.2507447	-2.6975190	1.3225175
H	5.7122770	-0.8853400	-0.8790720	H	-4.0948127	-1.6107040	3.2315735
H	3.3194530	-0.9363190	-1.4726210	H	-2.4721267	0.1990880	2.8311325
H	-0.0514900	0.9515700	-2.6762620	H	-1.0412657	4.0340990	1.7380135
H	-0.4450200	-0.2729760	-4.7832110	H	0.4010783	4.5932580	3.6581655
H	-0.0058560	-2.7110530	-4.9074400	H	1.6787293	2.8101480	4.8172735
H	0.8225170	-3.9296410	-2.9102990	H	1.5200933	0.4602600	4.0352565
H	1.2041710	-2.7164180	-0.7881400	H	0.1119883	-0.1050540	2.0885735
N	-1.0118060	-1.8132770	0.7797940	N	0.3529863	2.3213300	-1.4840125
N	-2.2145740	-1.4556520	0.5786790	N	1.5117713	2.3588060	-0.9509405
N	-2.5835240	-0.2173250	0.8316340	N	1.8611863	1.3664390	-0.1711535
S	-4.2038830	0.0144880	0.4305690	S	3.4384893	1.5386200	0.3898485
O	-4.4859820	-0.3226390	-0.9795300	O	3.7071383	0.3032130	1.1457975
C	-5.1432050	-1.1268080	1.4615760	C	4.4740333	1.5365770	-1.0859575
O	-4.4971630	1.3924170	0.8687130	O	3.6497313	2.8251260	1.0819575
H	-6.1987880	-0.9617590	1.2416750	H	5.5091983	1.6206850	-0.7524785
H	-4.9237810	-0.9048490	2.5056130	H	4.1935613	2.3904470	-1.7019535
H	-4.8464890	-2.1428580	1.2035230	H	4.3113633	0.5977230	-1.6145685
TS8-9				Molecule **9**			



E = -1981.374202, H (0K) = -1980.972057,
H (298K) = -1980.944703,
G (298K) = -1981.029436 au.
Imaginary frequency = 1 (-31.15 cm^{-1}).

C	-0.4831050	-0.4731550	-1.6009560
C	-1.4009900	0.6888470	-1.2378280
O	-0.6249820	1.3213090	-0.2702070
C	-1.8661450	1.6289950	-2.3322900
P	0.7890340	0.1034400	-0.1854890
C	2.2047500	-0.9533780	-0.8849090
C	3.4584540	-0.4193980	-1.2063340
C	4.4439190	-1.2093870	-1.8049830
C	4.1947730	-2.5493230	-2.0874760
C	2.9462880	-3.0940550	-1.7796010
C	1.9604010	-2.3015800	-1.1982530
C	1.8391140	1.5614600	0.3067460
C	1.8404360	2.7410700	-0.4441750
C	2.6777220	3.7986970	-0.0903750
C	3.5062530	3.6942350	1.0270230
C	3.4999460	2.5234650	1.7849370
C	2.6793790	1.4562200	1.4202880
C	0.3254020	-0.7589650	1.3740190
C	1.0890110	-1.8147590	1.8910350
C	0.7322550	-2.4191710	3.0951470
C	-0.3882970	-1.9791820	3.7980250
C	-1.1448150	-0.9215700	3.2961110
C	-0.7892170	-0.3102810	2.0962400
H	-0.0177520	-0.4891580	-2.5838930
H	-0.9876480	2.0599420	-2.8164460
H	-2.4646180	2.4370670	-1.9116720
H	-2.4522730	1.0917580	-3.0813850
H	3.6844960	0.6179380	-0.9988730
H	5.4057250	-0.7699710	-2.0469140
H	4.9608120	-3.1639750	-2.5475290
H	2.7377880	-4.1365110	-1.9950500
H	0.9973410	-2.7465570	-0.9788550
H	1.1837350	2.8393730	-1.2989880
H	2.6746350	4.7070190	-0.6830820
H	4.1488000	4.5214480	1.3080240
H	4.1348670	2.4365650	2.6598950
H	2.6978150	0.5479780	2.0110890

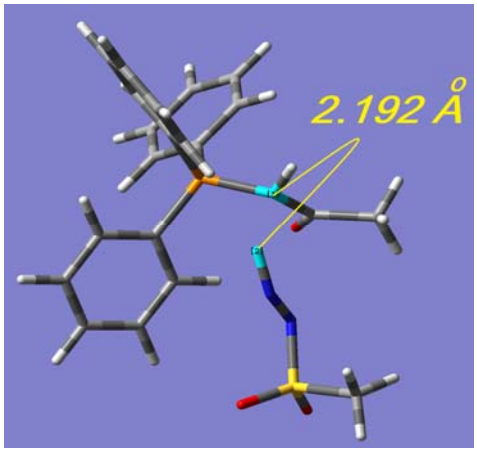


E = -869.610526, H (0K) = -869.487146,
H (298K) = -869.476317,
G (298K) = -869.522873 au.
Imaginary frequency = 0.

C	-2.5525020	-0.2362630	0.0812200
C	-1.4726670	0.6131140	0.0142360
C	-1.3969830	2.0982550	0.0545410
N	-2.1252070	-1.5299540	0.0054100
N	-0.8370680	-1.5559890	-0.1105030
N	-0.4158870	-0.2569110	-0.1182120
S	1.3166660	0.0381390	-0.1547880
O	1.8700140	-0.8972300	-1.1188580
C	1.7769760	-0.4323010	1.5072090
O	1.4527840	1.4751400	-0.3432690
H	-3.5965450	0.0172430	0.1733460
H	-2.4031880	2.4976290	0.1849350
H	-0.7705170	2.4432450	0.8798010
H	-0.9734310	2.4972240	-0.8689150
H	1.5263450	-1.4843760	1.6398860
H	1.2327700	0.2077680	2.2012940
H	2.8537170	-0.2690870	1.5831790

H	1.9671450	-2.1690960	1.3695010
H	1.3336210	-3.2349220	3.4808370
H	-0.6677950	-2.4554680	4.7314080
H	-2.0167240	-0.5681390	3.8349750
H	-1.3739040	0.5172020	1.7219050
N	-1.1733640	-1.7097640	-1.3047430
N	-2.2796550	-1.4810560	-0.7613450
N	-2.5172200	-0.1303010	-0.6509410
S	-4.0620960	0.3532720	-0.1397610
O	-3.9656640	1.7982720	0.0550810
C	-5.1113210	-0.0004030	-1.5487810
O	-4.4530140	-0.5115100	0.9693400
H	-6.1296990	0.2648160	-1.2606010
H	-5.0326550	-1.0656710	-1.7660020
H	-4.7700140	0.6073910	-2.3859950

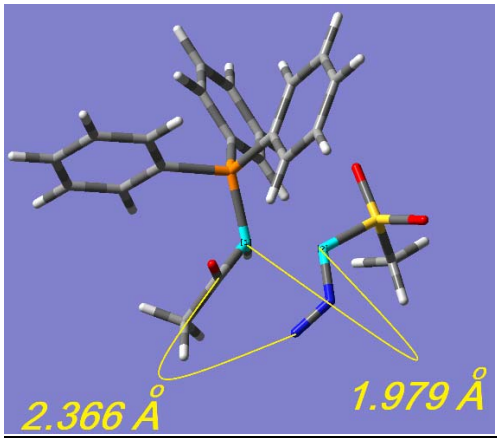
TS6/2d-8



E = -1981.375728, H (0K) = -1980.978865,
H (298K) = -1980.948709,
G (298K) = -1981.042574 au.
Imaginary frequency = 1 (-208.81 cm^{-1}).

C	-0.1355570	-0.3365600	-1.5475870
C	0.4607080	-1.6540130	-1.6214960
O	0.3929010	-2.4796260	-0.7003470
C	1.1569840	-2.0116020	-2.9209580
P	-1.2330750	0.0081320	-0.1931260
C	-2.2610310	1.4402940	-0.6462590
C	-3.6091730	1.4830300	-0.2693170
C	-4.3825610	2.5997110	-0.5811790
C	-3.8165830	3.6746160	-1.2653690
C	-2.4723890	3.6348800	-1.6376530
C	-1.6911170	2.5240680	-1.3290860
C	-2.3639700	-1.3701180	0.1767120
C	-2.9823960	-2.0294330	-0.8924520
C	-3.8848620	-3.0580510	-0.6410850
C	-4.1714070	-3.4315450	0.6738730
C	-3.5541820	-2.7750120	1.7373960
C	-2.6493940	-1.7421210	1.4929260
C	-0.3267750	0.4276100	1.3306990
C	-0.6838470	1.5551390	2.0796800

TS6/2d-10



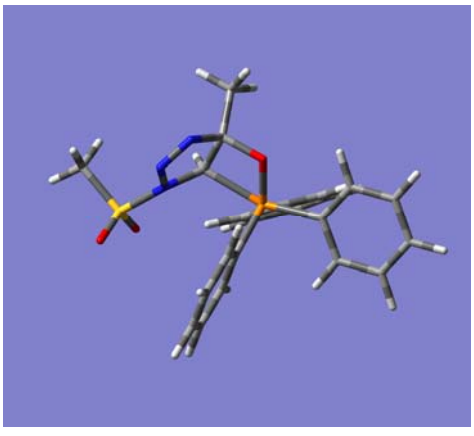
E = -1981.338664, H (0K) = -1980.941515,
H (298K) = -1980.912087,
G (298K) = -1981.001264 au.
Imaginary frequency = 1 (-365.36 cm^{-1}).

C	0.2280480	-0.8133730	-1.2798880
C	-0.2599000	-2.1916910	-1.4797690
O	-0.5677040	-2.9074200	-0.5065920
C	-0.7167500	-2.5659560	-2.8801340
P	-0.6421450	0.1126860	0.0075510
C	-0.7444220	1.8655600	-0.4732980
C	-1.7782820	2.6401290	0.0741810
C	-1.8940110	3.9860260	-0.2621410
C	-0.9916480	4.5632960	-1.1553340
C	0.0305060	3.7928360	-1.7082840
C	0.1610920	2.4490860	-1.3663040
C	-2.3732120	-0.4648040	0.0452610
C	-3.1236560	-0.3602330	-1.1336990
C	-4.4498910	-0.7798090	-1.1501440
C	-5.0332870	-1.2973650	0.0081360
C	-4.2880920	-1.3945850	1.1818120
C	-2.9566410	-0.9800490	1.2046890
C	0.0475140	-0.0644290	1.6784570
C	0.1642000	1.0450130	2.5214040

C	0.0274130	1.8707600	3.2361370
C	1.0920970	1.0678030	3.6440000
C	1.4442220	-0.0577940	2.8985190
C	0.7375070	-0.3853950	1.7449870
H	-0.4150130	0.1464390	-2.4761140
H	0.4447460	-2.5414650	-3.5640370
H	1.9922540	-2.6817030	-2.7127530
H	1.5133220	-1.1307820	-3.4588630
H	-4.0582000	0.6524070	0.2613080
H	-5.4263140	2.6265190	-0.2897300
H	-4.4206880	4.5416900	-1.5082590
H	-2.0283810	4.4699450	-2.1675120
H	-0.6469380	2.5090450	-1.6124490
H	-2.7540290	-1.7453200	-1.9141130
H	-4.3603660	-3.5713450	-1.4691620
H	-4.8720880	-4.2362100	0.8670800
H	-3.7720180	-3.0661690	2.7587020
H	-2.1689230	-1.2381580	2.3227970
H	-1.5027170	2.1901090	1.7637560
H	-0.2469420	2.7478960	3.8113020
H	1.6501720	1.3212080	4.5385790
H	2.2775040	-0.6787920	3.2068930
H	1.0146550	-1.2568490	1.1663440
N	1.3691900	1.2341470	-1.2748430
N	2.3991630	0.8211270	-0.9107140
N	2.9690820	-0.2901480	-0.5992530
S	4.5741020	-0.0525580	-0.0573840
O	4.9514200	-1.3576310	0.4948630
C	5.5091570	0.2393860	-1.5652020
O	4.6819650	1.1406880	0.7962600
H	6.5558590	0.3517170	-1.2790330
H	5.1334140	1.1527660	-2.0268000
H	5.3717990	-0.6212660	-2.2191550

C	0.6699830	0.8797990	3.8084650
C	1.0594380	-0.3840780	4.2514220
C	0.9427830	-1.4882210	3.4064340
C	0.4381420	-1.3356310	2.1177960
H	0.3950080	-0.2287050	-2.1767400
H	-1.7948000	-2.3772010	-2.9426380
H	-0.5500980	-3.6318050	-3.0440390
H	-0.2110380	-1.9959340	-3.6610040
H	-2.4946790	2.1978220	0.7565130
H	-2.6926370	4.5787880	0.1686940
H	-1.0865750	5.6100290	-1.4217410
H	0.7330560	4.2370290	-2.4040690
H	0.9722800	1.8756690	-1.7897870
H	-2.6764480	0.0479410	-2.0332540
H	-5.0273310	-0.7018230	-2.0642450
H	-6.0671390	-1.6237870	-0.0061360
H	-4.7385660	-1.7967130	2.0820780
H	-2.3830600	-1.0649020	2.1188520
H	-0.1150260	2.0336170	2.1802920
H	0.7679650	1.7408780	4.4597580
H	1.4591720	-0.5073420	5.2519450
H	1.2509180	-2.4704530	3.7463420
H	0.3453100	-2.1856810	1.4525330
N	1.9686460	-2.7869240	-2.0045270
N	2.5941630	-2.0828440	-1.2892980
N	2.0729670	-1.0400380	-0.6007610
S	3.2199840	0.1811660	-0.2351100
O	2.3945740	1.2890010	0.2593560
C	3.9389690	0.6510090	-1.8151540
O	4.2881920	-0.3452510	0.6204150
H	3.1317130	0.9667480	-2.4757590
H	4.4741910	-0.2066200	-2.2212280
H	4.6239780	1.4763270	-1.6146650

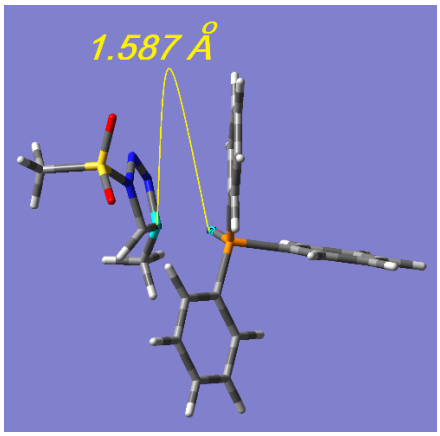
Molecule **10**



E = -1981.372916, H (0K) = -1980.970566,
H (298K) = -1980.942498,
G (298K) = -1981.028205 au.
Imaginary frequency = 0.

C	-1.0566090	0.7847150	1.0285250
C	-0.6388430	0.2612460	2.3898990

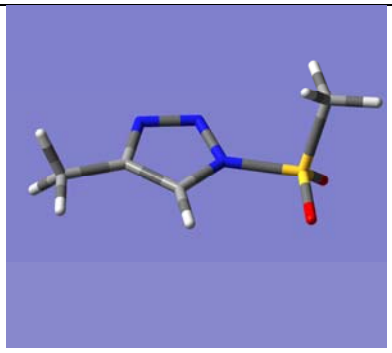
TS10-11



E = -1981.363754, H (0K) = -1980.963570,
H (298K) = -1980.935492,
G (298K) = -1981.021761 au.
Imaginary frequency = 1 (-351.23 cm^{-1}).

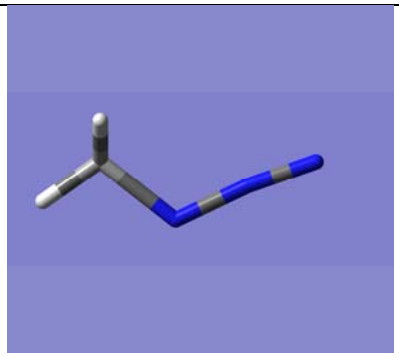
C	-1.2910680	1.0069010	0.9479470
C	-0.7038290	0.6425420	2.2417200

O	0.6013380	-0.3676630	2.0276460	O	0.6710470	-0.0675570	1.8885010
C	-0.4483570	1.2048450	3.5538590	C	-0.2968560	1.6854870	3.2566490
N	-1.6379760	-0.7984480	2.7182960	N	-1.5628450	-0.4122500	2.7777190
N	-2.4783880	-0.9115380	1.8021000	N	-2.4786690	-0.7044310	1.9328440
N	-2.2192070	-0.0431200	0.7666120	N	-2.3694340	0.0852650	0.8492040
S	-3.4871150	0.2925540	-0.3205450	S	-3.6083190	0.1104900	-0.3260470
O	-2.8990430	1.2013850	-1.3038100	O	-3.0423540	0.8667040	-1.4418800
C	-4.6769960	1.1852320	0.6804860	C	-4.8879570	1.0801380	0.4703230
O	-4.0651680	-0.9794930	-0.7346140	O	-4.0896300	-1.2520000	-0.5142750
P	0.7530610	0.0285980	0.3586490	P	0.9685980	-0.0029130	0.3042480
C	1.2376830	1.6264680	-0.4593600	C	1.2703600	1.5925000	-0.5335020
C	2.5130570	2.1770030	-0.2773280	C	2.4610060	2.2762400	-0.2530040
C	2.8454470	3.3999900	-0.8606550	C	2.7213040	3.5057970	-0.8583350
C	1.9193760	4.0732140	-1.6548970	C	1.8134420	4.0436800	-1.7676950
C	0.6467020	3.5312410	-1.8422330	C	0.6285820	3.3601910	-2.0546270
C	0.2985540	2.3303630	-1.2293080	C	0.3445630	2.1523130	-1.4269600
C	2.4968340	-0.7266750	0.3847790	C	2.6578020	-0.7451600	0.3550160
C	3.2726150	-0.8700130	1.5426950	C	3.3153500	-1.0461250	1.5528320
C	4.5743710	-1.3726520	1.4748720	C	4.5952710	-1.6029990	1.5288650
C	5.1248710	-1.7394160	0.2486130	C	5.2267080	-1.8622580	0.3140750
C	4.3643870	-1.5984100	-0.9131700	C	4.5750170	-1.5635000	-0.8841760
C	3.0670040	-1.0958360	-0.8423350	C	3.2986870	-1.0088050	-0.8638090
C	-0.0042870	-1.1870500	-0.7933630	C	0.0343200	-1.2015150	-0.6797770
C	-0.3158910	-0.9056990	-2.1257970	C	-0.1221940	-1.1082610	-2.0686270
C	-0.9182330	-1.8807640	-2.9204190	C	-0.7955940	-2.1138290	-2.7570420
C	-1.2231960	-3.1326700	-2.3887780	C	-1.3107280	-3.2152630	-2.0722980
C	-0.9160140	-3.4132810	-1.0573990	C	-1.1476540	-3.3121290	-0.6917300
C	-0.3048740	-2.4469030	-0.2621570	C	-0.4771560	-2.3114580	0.0070150
H	-1.2571080	1.8472520	0.9195210	H	-1.4983080	2.0293100	0.6624760
H	-1.3974790	1.6746940	3.8211450	H	-1.1849900	2.2059340	3.6217810
H	-0.0655460	0.6584960	4.4189410	H	0.2121630	1.2167980	4.1017090
H	0.2686430	1.9821140	3.2793510	H	0.3764360	2.4132930	2.7986310
H	-4.1845530	2.0713970	1.0808270	H	-4.4686000	2.0531250	0.7258860
H	-5.0159010	0.5191840	1.4736660	H	-5.2145750	0.5376360	1.3572780
H	-5.5022820	1.4612880	0.0223560	H	-5.7015870	1.1811970	-0.2498540
H	3.2543580	1.6586220	0.3166750	H	3.1876660	1.8558660	0.4319830
H	3.8329460	3.8182330	-0.6996510	H	3.6387790	4.0338530	-0.6239600
H	2.1833970	5.0166070	-2.1201050	H	2.0222780	4.9932780	-2.2478610
H	-0.0823750	4.0491300	-2.4557550	H	-0.0846900	3.7774710	-2.7566330
H	-0.7058700	1.9474450	-1.3573910	H	-0.6011900	1.6592870	-1.6130790
H	2.8640290	-0.5881710	2.5032410	H	2.8291130	-0.8466200	2.4981770
H	5.1554400	-1.4767400	2.3852220	H	5.0959320	-1.8332300	2.4629540
H	6.1348450	-2.1315360	0.1967530	H	6.2209230	-2.2951290	0.2985370
H	4.7801620	-1.8799980	-1.8747680	H	5.0599290	-1.7629960	-1.8333260
H	2.4990820	-0.9903480	-1.7599550	H	2.8055120	-0.7798750	-1.8023330
H	-0.0863120	0.0596230	-2.5567710	H	0.2799830	-0.2671960	-2.6175330
H	-1.1521170	-1.6564770	-3.9553060	H	-0.9179860	-2.0341990	-3.8314580
H	-1.7003710	-3.8848840	-3.0071270	H	-1.8405400	-3.9916040	-2.6128340
H	-1.1535950	-4.3831940	-0.6347620	H	-1.5513890	-4.1610150	-0.1518610
H	-0.0651080	-2.6743380	0.7708670	H	-0.3528430	-2.3935140	1.0800670
Molecule **11**				Molecule **2e**			



E = -869.610196, H (0K) = -869.487385,
H (298K) = -869.476230,
G (298K) = -869.524128 au.
Imaginary frequency = 0.

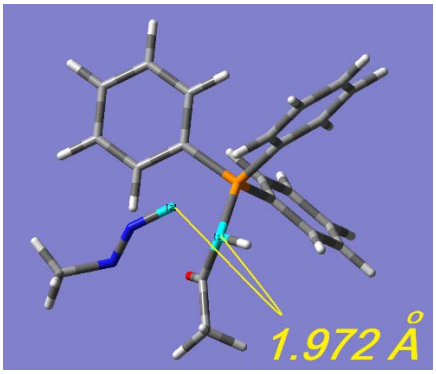
C	-0.3913689	-0.4452362	0.4323753
C	-1.5447729	0.3009878	0.4200743
C	-2.9677569	-0.1333722	0.5154753
N	-1.1911489	1.6218058	0.2970173
N	0.0999471	1.7344398	0.2267123
N	0.6038971	0.4806558	0.3046873
S	2.3405411	0.2183678	0.2685233
O	2.4819591	-1.2287762	0.3575923
C	2.8364671	1.0108418	1.7905023
O	2.8534821	0.9518198	-0.8766747
H	-0.1956089	-1.5007742	0.5099063
H	-3.4494979	0.3095058	1.3916353
H	-3.5274769	0.1828598	-0.3690237
H	-3.0342739	-1.2194022	0.5965193
H	2.3210381	0.5140918	2.6117863
H	2.5730231	2.0658038	1.7212613
H	3.9173731	0.8779298	1.8642283



E = -204.157276, H (0K) = -204.107129,
H (298K) = -204.101763,
G (298K) = -204.133569 au.
Imaginary frequency = 0.

N	1.7895970	0.2757350	0.0000120
N	0.7176870	-0.1017620	-0.0000210
N	-0.3863600	-0.6300020	0.0000090
C	-1.5507620	0.2843970	0.0000000
H	-2.4392310	-0.3428220	-0.0004070
H	-1.5515390	0.9140330	0.8944720
H	-1.5511230	0.9146080	-0.8940600

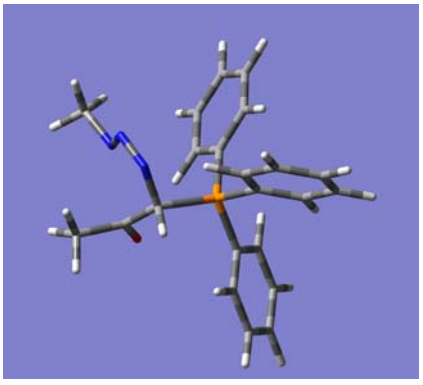
TS6/2e-7



E = -1432.699208, H (0K) = -1432.311983,
H (298K) = -1432.285213,
G (298K) = -1432.370321 au.
Imaginary frequency = 1 (-355.62 cm^{-1}).

C	0.8226390	-0.3290460	-1.4453560
C	1.4543290	-1.6497460	-1.3621250
O	1.4229120	-2.3356990	-0.3324410
C	2.0317690	-2.2075990	-2.6470590
P	-0.3696320	0.0231090	-0.1551230

Molecule **12**



E = -1432.718375, H (0K) = -1432.328376,
H (298K) = -1432.302081,
G (298K) = -1432.385309 au.
Imaginary frequency = 0.

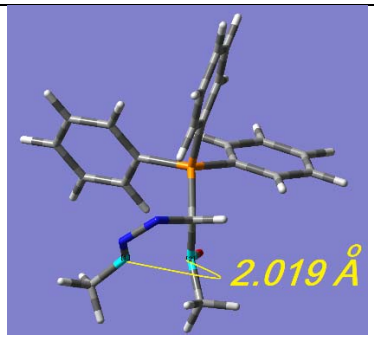
C	-0.6488120	0.2690070	-1.7229340
C	-1.4853430	1.5547060	-1.6137940
O	-1.3144460	2.3642670	-0.7085530
C	-2.2503020	1.9234480	-2.8648850

C	-1.4917040	1.3347610	-0.7399590
C	-2.8586830	1.2761190	-0.4384370
C	-3.7066680	2.3011540	-0.8539610
C	-3.1976830	3.3842840	-1.5691870
C	-1.8359410	3.4447180	-1.8676340
C	-0.9793580	2.4272160	-1.4542460
C	-1.4169500	-1.4169100	0.2340450
C	-2.0063030	-2.1132820	-0.8287500
C	-2.8338150	-3.2013900	-0.5690600
C	-3.0765320	-3.5971460	0.7480280
C	-2.4889480	-2.9036620	1.8048150
C	-1.6582950	-1.8121970	1.5519020
C	0.4182920	0.5967260	1.3803220
C	-0.2545190	1.5047050	2.2073360
C	0.3324630	1.9196040	3.4010990
C	1.5875260	1.4343600	3.7680070
C	2.2577900	0.5329270	2.9400490
C	1.6783640	0.1084960	1.7469730
H	0.4391450	-0.0535800	-2.4227760
H	1.2531030	-2.8035820	-3.1394030
H	2.8719490	-2.8640510	-2.4184200
H	2.3530380	-1.4233480	-3.3336420
H	-3.2654780	0.4379600	0.1134990
H	-4.7638470	2.2495040	-0.6194580
H	-3.8599170	4.1792760	-1.8936730
H	-1.4366640	4.2859730	-2.4228660
H	0.0779820	2.4835360	-1.6793430
H	-1.8179770	-1.8101020	-1.8531520
H	-3.2868820	-3.7413170	-1.3927750
H	-3.7196780	-4.4468660	0.9482610
H	-2.6716200	-3.2118470	2.8280610
H	-1.1988990	-1.2825240	2.3773980
H	-1.2247950	1.8944640	1.9228250
H	-0.1883170	2.6253570	4.0383210
H	2.0448750	1.7620420	4.6950970
H	3.2367680	0.1601850	3.2196380
H	2.2031180	-0.5877590	1.1058770
N	2.0003740	1.2491930	-1.3361480
N	3.1586940	0.9525160	-1.1474510
N	3.7636720	-0.1549870	-0.9975490
C	5.2046460	-0.0104840	-0.7714500
H	5.6239430	-1.0154060	-0.6934790
H	5.7089410	0.5070760	-1.5981330
H	5.4287060	0.5252690	0.1604390

TS12-13

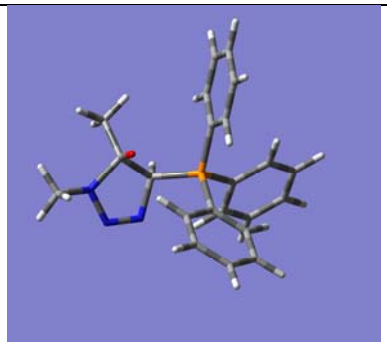
P	0.3271790	-0.0163100	-0.1401260
C	1.5534170	-1.3285930	-0.4617750
C	2.6686200	-1.4063750	0.3864970
C	3.6228770	-2.4005710	0.1921030
C	3.4762650	-3.3167580	-0.8505520
C	2.3699060	-3.2389940	-1.6947910
C	1.4029280	-2.2525130	-1.5031910
C	1.3192390	1.4387470	0.3210390
C	2.0915260	2.0423040	-0.6805450
C	2.8893050	3.1398440	-0.3728260
C	2.9277770	3.6337930	0.9325620
C	2.1691510	3.0243230	1.9305170
C	1.3638680	1.9262560	1.6299100
C	-0.7255450	-0.5400010	1.2408500
C	-0.6465430	-1.8508260	1.7224780
C	-1.4825130	-2.2565090	2.7633410
C	-2.3825240	-1.3564330	3.3285210
C	-2.4587600	-0.0467310	2.8473880
C	-1.6418560	0.3635450	1.8002860
H	0.1367070	0.4431020	-2.4677060
H	-1.5882370	2.5389290	-3.4865590
H	-3.1215360	2.5219430	-2.5960170
H	-2.5532260	1.0502850	-3.4426590
H	2.7977580	-0.6941540	1.1929770
H	4.4815770	-2.4554760	0.8515520
H	4.2231260	-4.0880850	-1.0029770
H	2.2516460	-3.9499260	-2.5048000
H	0.5285500	-2.2059660	-2.1406480
H	2.0756170	1.6582360	-1.6945630
H	3.4810910	3.6083170	-1.1510150
H	3.5499030	4.4894410	1.1701590
H	2.2017190	3.4007100	2.9467150
H	0.7802600	1.4602290	2.4136140
H	0.0527840	-2.5560760	1.2913490
H	-1.4253720	-3.2755060	3.1286270
H	-3.0286930	-1.6735100	4.1396430
H	-3.1646960	0.6527870	3.2804010
H	-1.7195170	1.3674620	1.4042330
N	-1.3472430	-0.9582570	-2.1301820
N	-2.5709430	-1.0541920	-1.6606920
N	-3.0145540	-0.0899130	-0.9571580
C	-4.3916690	-0.2336590	-0.5198560
H	-4.9847960	0.6200800	-0.8694740
H	-4.8471550	-1.1586250	-0.8944240
H	-4.4365200	-0.2351990	0.5760400

Molecule **13**



E = -1432.717887, H (0K) = -1432.327991,
H (298K) = -1432.302493,
G (298K) = -1432.384119 au.
Imaginary frequency = 1 (-113.47 cm^{-1}).

C	-0.7102680	0.1837700	-1.6870940
C	-1.7325680	1.3285930	-1.4795130
O	-1.5750480	2.1607660	-0.5642650
C	-2.4435560	1.7435800	-2.7598420
P	0.3406110	-0.0099710	-0.1501580
C	1.6927040	-1.1757640	-0.5261870
C	2.8528250	-1.1220270	0.2607180
C	3.8949680	-2.0143950	0.0255880
C	3.7907640	-2.9585130	-0.9967690
C	2.6397850	-3.0105000	-1.7815440
C	1.5865190	-2.1270270	-1.5487460
C	1.1662790	1.5363030	0.3297580
C	1.7705890	2.3027630	-0.6750800
C	2.4517890	3.4684640	-0.3394280
C	2.5388090	3.8703980	0.9949800
C	1.9445580	3.1016560	1.9943100
C	1.2579650	1.9329450	1.6666190
C	-0.6260250	-0.6829220	1.2308560
C	-0.4020340	-1.9923210	1.6693310
C	-1.1737370	-2.5151910	2.7071020
C	-2.1552010	-1.7324740	3.3111490
C	-2.3748090	-0.4237420	2.8744260
C	-1.6211920	0.1028990	1.8313340
H	0.0030590	0.4434870	-2.4749440
H	-1.7953820	2.4530160	-3.2874510
H	-3.3755870	2.2527190	-2.5086930
H	-2.6489240	0.8998620	-3.4218200
H	2.9493600	-0.3865760	1.0504640
H	4.7885050	-1.9685310	0.6377430
H	4.6053800	-3.6502520	-1.1806850
H	2.5547280	-3.7428140	-2.5765390
H	0.6824740	-2.1830440	-2.1418090
H	1.7094210	1.9978650	-1.7135360
H	2.9130850	4.0637270	-1.1192800
H	3.0696780	4.7798910	1.2532570
H	2.0129980	3.4085490	3.0318860
H	0.7996320	1.3425980	2.4501150
H	0.3610510	-2.6057480	1.2068550
H	-1.0046330	-3.5331450	3.0391600

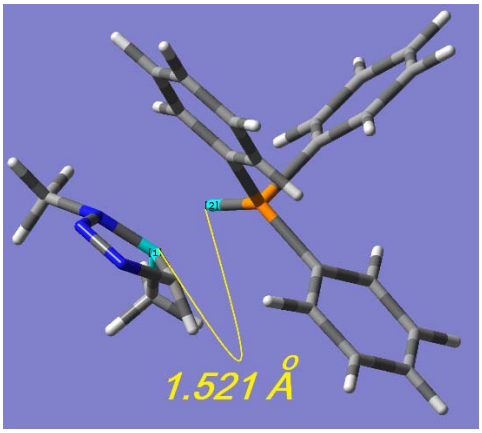


E = -1432.725175, H (0K) = -1432.333616,
H (298K) = -1432.308109,
G (298K) = -1432.389440 au.
Imaginary frequency = 0.

C	-0.9848120	-0.0006080	-1.4070270
C	-2.3116460	0.7062680	-0.9410040
O	-2.4709400	0.7475350	0.3647760
C	-2.5487260	2.0421140	-1.6641340
P	0.3076660	-0.0062980	-0.0829310
C	1.8977740	-0.3151990	-0.9216330
C	3.0720440	0.2911680	-0.4577970
C	4.2897030	0.0089130	-1.0738410
C	4.3412230	-0.8764290	-2.1499570
C	3.1727090	-1.4838230	-2.6108600
C	1.9514070	-1.2098620	-1.9999000
C	0.4499800	1.6156360	0.7119940
C	0.6931350	2.7354530	-0.0931520
C	0.8287800	3.9904920	0.4938810
C	0.7357550	4.1279410	1.8793990
C	0.5071160	3.0083270	2.6794730
C	0.3633170	1.7497100	2.1001180
C	0.0801090	-1.3353050	1.1384110
C	1.1777780	-2.1307300	1.4959050
C	1.0205880	-3.1367700	2.4469150
C	-0.2243640	-3.3554340	3.0359980
C	-1.3156870	-2.5643430	2.6752280
C	-1.1719390	-1.5514550	1.7302430
H	-0.5229940	0.4730270	-2.2787670
H	-1.8411690	2.7812970	-1.2813630
H	-3.5577170	2.3944620	-1.4337890
H	-2.4380130	1.9668530	-2.7500780
H	3.0420480	0.9807040	0.3770920
H	5.1953210	0.4824320	-0.7121820
H	5.2896500	-1.0925360	-2.6291390
H	3.2095840	-2.1733440	-3.4465920
H	1.0499000	-1.6944120	-2.3552420
H	0.7789340	2.6318530	-1.1688050
H	1.0094740	4.8583410	-0.1300440
H	0.8434470	5.1061480	2.3345580
H	0.4361690	3.1132860	3.7560870
H	0.1742330	0.8850920	2.7242260
H	2.1475040	-1.9778340	1.0395390
H	1.8711000	-3.7503210	2.7216300

H	-2.7519610	-2.1408650	4.1193380
H	-3.1425650	0.1841890	3.3395380
H	-1.8053110	1.1043210	1.4638650
N	-1.3206220	-1.1158730	-2.0274350
N	-2.5425650	-1.1969680	-1.5789560
N	-2.9863270	-0.1677490	-0.9632420
C	-4.3855390	-0.1581690	-0.5923430
H	-4.9547750	0.5154730	-1.2454840
H	-4.8183870	-1.1617970	-0.6607790
H	-4.4898050	0.2046910	0.4349690

TS13-14



E = -1432.715855, H (0K) = -1432.324257,
H (298K) = -1432.299666,
G (298K) = -1432.378238 au.
Imaginary frequency = 1 (-183.97 cm^{-1}).

C	-1.5935440	-1.6925480	0.0642620
C	-1.8099700	-1.2201890	-1.3402700
O	-0.6633310	-0.2451690	-1.5614030
C	-1.7434810	-2.1817340	-2.5109410
N	-2.7100050	-1.3251170	0.8138030
N	-3.5150110	-0.6251370	0.1220920
N	-3.0285790	-0.4915570	-1.1743600
P	0.1691990	-0.0926210	-0.1591450
C	1.3366260	-1.3680040	0.4603940
C	2.4935260	-1.6425240	-0.2808010
C	3.3795040	-2.6334630	0.1422230
C	3.1348820	-3.3349620	1.3207990
C	1.9849690	-3.0611940	2.0653870
C	1.0783220	-2.1016540	1.6270500
C	1.3931790	1.1305660	-0.8610220
C	1.4759180	1.4454610	-2.2224810
C	2.4273390	2.3591430	-2.6816000
C	3.3066450	2.9679560	-1.7887610
C	3.2321930	2.6595670	-0.4290560
C	2.2835850	1.7493200	0.0288150
C	-0.5931350	0.9385420	1.1321240
C	-0.1729210	0.9314720	2.4681680
C	-0.7775550	1.7829260	3.3900110
C	-1.7998310	2.6448910	2.9904130
C	-2.2140520	2.6555780	1.6596610
H	-0.3437740	-4.1426050	3.7725120
H	-2.2850570	-2.7348620	3.1303780
H	-1.9986160	-0.9108160	1.4348780
N	-1.3315050	-1.4001250	-1.7442470
N	-2.5960460	-1.4981860	-1.8163080
N	-3.2435770	-0.3583480	-1.6256460
C	-4.6421980	-0.4581420	-1.2391200
H	-5.1360100	0.4906770	-1.4535620
H	-5.1183190	-1.2460550	-1.8244800
H	-4.7475520	-0.6781120	-0.1725360

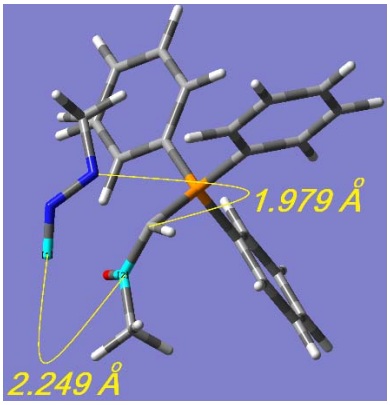
Molecule **14**

E = -320.970182, H (0K) = -320.856087,
H (298K) = -320.848280,
G (298K) = -320.887192 au.
Imaginary frequency = 0.

C	-1.0576490	-1.1466880	0.0000020
C	0.2522320	-0.7072020	0.0000040
C	1.5573420	-1.4225460	-0.0000020
N	-1.8836960	-0.0685030	-0.0000090
N	-1.1602060	1.0210230	0.0000010
N	0.1352940	0.6448190	0.0000160
H	-1.4319220	-2.1582310	0.0000120
H	1.3899530	-2.5000750	-0.0000720
H	2.1492220	-1.1649990	-0.8836040
H	2.1491820	-1.1650970	0.8836540
C	1.2017480	1.6350450	-0.0000050
H	1.8195810	1.5167100	-0.8915900
H	0.7427530	2.6217400	-0.0001460
H	1.8194450	1.5169170	0.8917020

C	-1.6157260	1.8069230	0.7302840
H	-1.1719700	-2.6661920	0.2810140
H	-0.7964100	-2.7239470	-2.4807940
H	-2.5633230	-2.9006720	-2.4433610
H	-1.8111920	-1.6548690	-3.4656400
H	2.7113990	-1.0861360	-1.1842720
H	4.2645350	-2.8464840	-0.4468750
H	3.8307650	-4.0959180	1.6562000
H	1.7847310	-3.6077490	2.9801850
H	0.1663150	-1.9345640	2.1858450
H	0.7995910	0.9775230	-2.9246350
H	2.4776710	2.5925740	-3.7397380
H	4.0441800	3.6778440	-2.1470270
H	3.9115760	3.1281390	0.2745650
H	2.2429630	1.5221790	1.0886290
H	0.6288410	0.2821650	2.7947370
H	-0.4440320	1.7745420	4.4218510
H	-2.2690370	3.3038420	3.7124830
H	-3.0090260	3.3204490	1.3407850
H	-1.9454730	1.8181570	-0.3014070
C	-3.9782190	-0.1927290	-2.2263770
H	-4.4991420	-1.0881350	-2.5883590
H	-4.7161060	0.5080040	-1.8336190
H	-3.4625480	0.2825480	-3.0626090

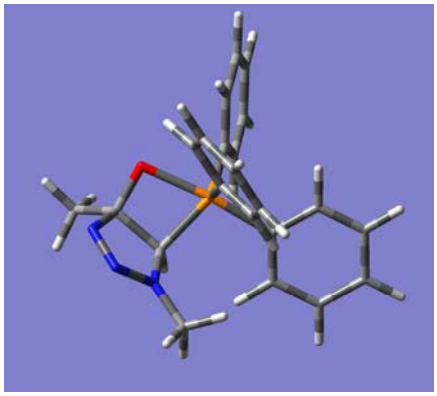
TS6/2e-15



E = -1432.670588, H (0K) = -1432.281737,
H (298K) = -1432.256066,
G (298K) = -1432.336182 au.
Imaginary frequency = 1 (-441.69 cm^{-1}).

C	-0.6844900	0.8054380	-1.3797300
C	-0.7548680	2.2633440	-1.2117030
O	-0.9054100	2.7825760	-0.0723600
C	-0.1696040	3.1123460	-2.3329680
P	0.1697340	-0.0803630	-0.0744530
C	0.7383610	-1.6666650	-0.7635210
C	1.8985590	-2.2638550	-0.2520900
C	2.3222910	-3.4947330	-0.7469500
C	1.5962490	-4.1318950	-1.7534380
C	0.4441380	-3.5367640	-2.2668840
C	0.0107410	-2.3071300	-1.7754520

Molecule **15**

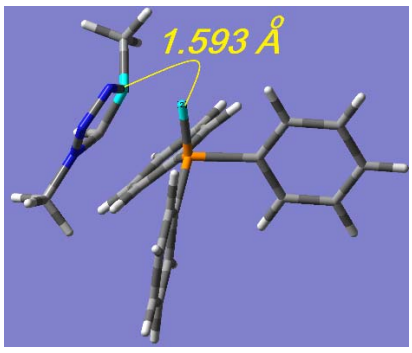


E = -1432.717410, H (0K) = -1432.324797,
H (298K) = -1432.299672,
G (298K) = -1432.379578 au.
Imaginary frequency = 0.

C	-0.8813600	0.4370850	-1.7777880
C	-1.2352060	1.9042210	-1.4643880
O	-0.5739280	2.1131300	-0.2698750
C	-0.9200600	2.9453730	-2.5246920
P	0.0883270	0.2311490	-0.1312830
C	0.8539460	-1.4886430	-0.3562530
C	1.5603710	-2.0455080	0.7239630
C	2.1927040	-3.2790300	0.6132440
C	2.1483460	-3.9822420	-0.5939320
C	1.4692840	-3.4371640	-1.6791580
C	0.8277870	-2.1998590	-1.5591740
C	1.7036000	1.0264800	0.2756440

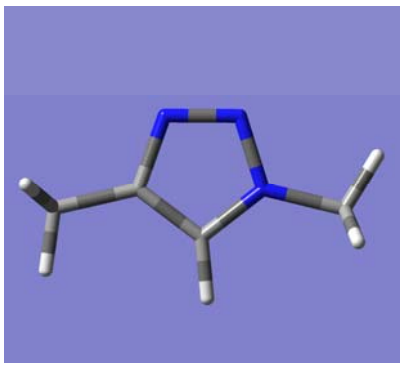
C	1.6670870	0.8444030	0.4047120	C	2.7586760	0.9211980	-0.6369780
C	2.5221930	1.2823060	-0.6156410	C	3.9789300	1.5415320	-0.3716450
C	3.6871710	1.9714490	-0.2939890	C	4.1641410	2.2428070	0.8194800
C	4.0038070	2.2244290	1.0423650	C	3.1173650	2.3334050	1.7377450
C	3.1542900	1.7863270	2.0566370	C	1.8853200	1.7418370	1.4630660
C	1.9845530	1.0947170	1.7422350	C	-1.0509910	-0.1223780	1.2744430
C	-0.7886090	-0.4156600	1.4384910	C	-1.5083540	-1.4277930	1.5031770
C	-0.7940930	-1.6982600	2.0002630	C	-2.4182170	-1.6906550	2.5258710
C	-1.5253350	-1.9402700	3.1615960	C	-2.8648180	-0.6588590	3.3490950
C	-2.2461790	-0.9091840	3.7634890	C	-2.4144200	0.6426330	3.1288370
C	-2.2372230	0.3685290	3.2025420	C	-1.5299400	0.9148550	2.0880190
C	-1.5130040	0.6222340	2.0404280	H	-0.2880360	0.2288410	-2.6671840
H	-0.3301070	0.4643970	-2.3466120	H	0.1584140	2.9685310	-2.7011590
H	0.8829940	3.3122810	-2.0989660	H	-1.2386440	3.9296380	-2.1726480
H	-0.6933050	4.0695510	-2.3730880	H	-1.4330750	2.7238810	-3.4649120
H	-0.2303130	2.6324920	-3.3120020	H	1.6131400	-1.5089360	1.6656800
H	2.4712500	-1.7722280	0.5253930	H	2.7235020	-3.6914720	1.4645710
H	3.2207820	-3.9521280	-0.3488310	H	2.6443490	-4.9423710	-0.6851400
H	1.9302770	-5.0884050	-2.1396450	H	1.4349700	-3.9688020	-2.6240600
H	-0.1191480	-4.0267020	-3.0528400	H	0.3166330	-1.8069680	-2.4277750
H	-0.8844110	-1.8547150	-2.1837910	H	2.6391710	0.3501370	-1.5509950
H	2.2791050	1.0897410	-1.6544040	H	4.7871030	1.4639960	-1.0907280
H	4.3455320	2.3127470	-1.0847010	H	5.1178670	2.7127640	1.0326870
H	4.9107790	2.7644160	1.2905570	H	3.2559980	2.8704760	2.6697910
H	3.3966120	1.9840530	3.0946150	H	1.0798650	1.8353260	2.1798980
H	1.3275310	0.7610620	2.5356540	H	-1.1674360	-2.2471490	0.8856380
H	-0.2439280	-2.5086220	1.5387550	H	-2.7734090	-2.7039730	2.6767760
H	-1.5320020	-2.9352600	3.5920350	H	-3.5664450	-0.8650660	4.1499720
H	-2.8159030	-1.1022280	4.6658280	H	-2.7662330	1.4546780	3.7554510
H	-2.8004280	1.1707320	3.6660020	H	-1.2347400	1.9332020	1.8830630
H	-1.5077000	1.6047720	1.5803330	N	-2.7335830	1.8456140	-1.2645630
N	-2.7832760	2.2326410	-2.1814250	N	-3.1481190	0.6759290	-1.4308760
N	-3.1980490	1.1441370	-1.9291270	N	-2.1701520	-0.1956970	-1.7902300
N	-2.5149370	0.0787360	-1.5753800	C	-2.4900020	-1.5832010	-2.0522040
C	-3.2032530	-0.8311700	-0.6477660	H	-2.1413460	-1.8732580	-3.0476740
H	-2.5252920	-1.6508240	-0.4176520	H	-2.0406260	-2.2466520	-1.3100890
H	-3.5048320	-0.3436310	0.2839810	H	-3.5741380	-1.6865720	-2.0114610
H	-4.0830740	-1.2548810	-1.1391760				

TS15-16



E = -1432.710492, H (0K) = -1432.319053,
H (298K) = -1432.294493,
G (298K) = -1432.372209 au.

Molecule **16**



E = -320.968487, H (0K) = -320.854627,
H (298K) = -320.846631,

Imaginary frequency = 1 (-342.11 cm^{-1}).

C	-1.7842860	1.3850040	0.5413190
C	-1.3953560	1.1548740	1.9488170
O	-0.1535360	0.1651250	1.8261900
C	-0.8671040	2.2664800	2.8254470
P	0.2604090	0.0280740	0.2721110
C	0.9763670	1.4533930	-0.6195530
C	2.1906510	1.9771400	-0.1550230
C	2.7567880	3.0907870	-0.7748110
C	2.1321670	3.6718950	-1.8766220
C	0.9228740	3.1509120	-2.3439580
C	0.3357560	2.0624530	-1.7070450
C	1.7701040	-1.0158890	0.5543530
C	2.1574990	-1.4693520	1.8203850
C	3.2833410	-2.2830540	1.9635790
C	4.0322920	-2.6507620	0.8476500
C	3.6517220	-2.2026770	-0.4189850
C	2.5284410	-1.3932720	-0.5634810
C	-0.7381380	-1.0934340	-0.7459940
C	-0.6683310	-1.1340960	-2.1458570
C	-1.4459950	-2.0481390	-2.8520500
C	-2.2934660	-2.9270760	-2.1740910
C	-2.3494370	-2.8984870	-0.7814930
C	-1.5728200	-1.9900900	-0.0644090
H	-1.7579230	2.3642230	0.0758890
H	-0.0208460	2.7626970	2.3446850
H	-0.5420970	1.8688900	3.7897840
H	-1.6563120	3.0023740	2.9958480
H	2.6981720	1.5190790	0.6858560
H	3.6902900	3.4949860	-0.3996270
H	2.5791890	4.5301750	-2.3657580
H	0.4283290	3.6035050	-3.1962040
H	-0.6251790	1.6981880	-2.0464300
H	1.5817880	-1.1854890	2.6908290
H	3.5726020	-2.6267080	2.9508660
H	4.9066790	-3.2822300	0.9613310
H	4.2288820	-2.4836360	-1.2931110
H	2.2475940	-1.0522450	-1.5542000
H	-0.0078650	-0.4687640	-2.6866610
H	-1.3862820	-2.0754060	-3.9345440
H	-2.9000480	-3.6341340	-2.7288990
H	-2.9998610	-3.5817430	-0.2469520
H	-1.6182390	-1.9775930	1.0179260
N	-2.4748900	0.3843700	2.5256310
N	-3.3396240	0.1161900	1.5937340
N	-3.0128610	0.6990940	0.4578880
C	-3.8239380	0.5399840	-0.7300090
H	-4.0716700	1.5233880	-1.1397950
H	-3.2872960	-0.0385660	-1.4852890
H	-4.7409190	0.0197840	-0.4565180

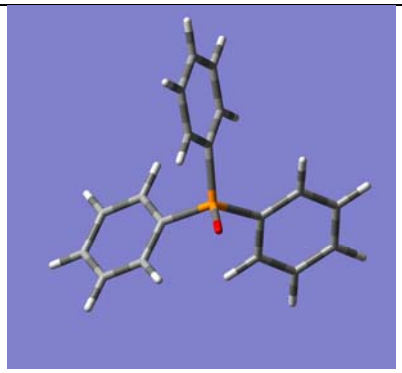
Molecule **Ph_3PO**

G (298K) = -320.886512 au.

Imaginary frequency = 0.

C	-0.0083020	-0.9184000	-0.0000030
C	-1.1084540	-0.0854020	0.0000090
C	-2.5635850	-0.4183670	0.0000020
N	-0.6504440	1.1987950	0.0000040
N	0.6603830	1.1933270	-0.0000080
N	1.0599180	-0.0865920	-0.0000200
H	0.0932380	-1.9908990	-0.0000260
H	-3.0588790	-0.0040150	0.8829270
H	-3.0589500	-0.0035990	-0.8826860
H	-2.7129540	-1.4996970	-0.0002430
C	2.4756860	-0.4307620	0.0000100
H	3.0450350	0.4968500	0.0001290
H	2.7156760	-1.0099560	0.8926590
H	2.7157640	-1.0098070	-0.8927110

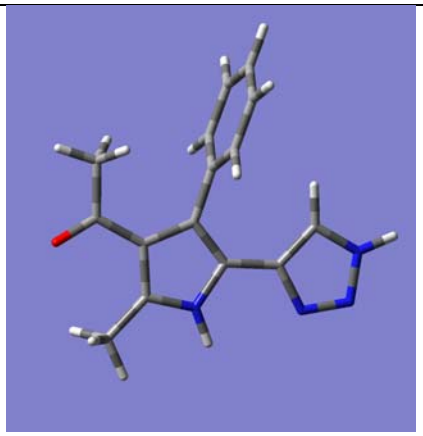
Molecule **23a(1,4)**



E = -1111.838808, H (0K) = -1111.561743,
H (298K) = -1111.543951,
G (298K) = -1111.608854 au.
Imaginary frequency = 0.

O	-0.0429640	0.1143250	2.4289710
P	-0.0089360	0.0246280	0.9209160
C	0.3602520	-1.6500700	0.2885200
C	-0.6444400	-2.4844630	-0.2156380
C	-0.3410290	-3.7889660	-0.6052920
C	0.9634880	-4.2678990	-0.4917380
C	1.9683590	-3.4421340	0.0162580
C	1.6695010	-2.1393460	0.4060770
C	-1.6067800	0.5223460	0.1823490
C	-2.6721500	0.7825820	1.0498670
C	-3.9124590	1.1659320	0.5385590
C	-4.0914730	1.2905880	-0.8384280
C	-3.0285190	1.0330080	-1.7074330
C	-1.7890030	0.6511320	-1.2005610
C	1.2585240	1.1255070	0.1958190
C	1.7877970	0.9320160	-1.0864260
C	2.7208080	1.8313440	-1.5990660
C	3.1324170	2.9246420	-0.8351420
C	2.6119630	3.1170560	0.4448990
C	1.6777220	2.2201520	0.9609220
H	-1.6615600	-2.1223580	-0.3083090
H	-1.1240290	-4.4286580	-0.9971170
H	1.1976950	-5.2820210	-0.7963890
H	2.9834730	-3.8122550	0.1074460
H	2.4560740	-1.5031990	0.7973330
H	-2.5236310	0.6851580	2.1190970
H	-4.7353000	1.3670620	1.2155980
H	-5.0553450	1.5892920	-1.2357920
H	-3.1656970	1.1311240	-2.7786090
H	-0.9709330	0.4529530	-1.8837380
H	1.4842000	0.0784550	-1.6813800
H	3.1303800	1.6754790	-2.5909620
H	3.8604870	3.6217240	-1.2353160
H	2.9349470	3.9620670	1.0428550
H	1.2771280	2.3606000	1.9584940

Molecule **23a(2,4)**



E = -874.531142, H (0K) = -874.263717,
H (298K) = -874.245397,
G (298K) = -874.310826 au.
Imaginary frequency = 0.

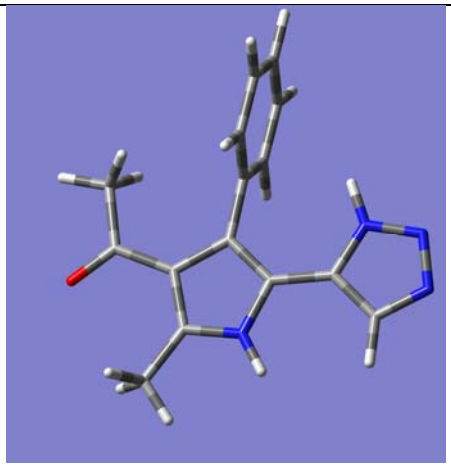
C	0.3948560	-1.1926020	-0.0001140
C	-0.4498860	-0.1019580	0.0000050
C	-1.8019400	-0.6171230	-0.0000400
C	-1.7073670	-2.0209040	-0.0003110
N	-0.3919690	-2.3335640	-0.0001810
C	-3.0708520	0.1023500	0.0003660
O	-4.1492710	-0.5079150	0.0001340
C	-3.0755230	1.6124780	0.0011160
C	-2.7533150	-3.0814670	-0.0004870
C	0.0245110	1.3035860	0.0000120
C	1.8396360	-1.2916960	-0.0000800
N	2.4716590	-2.5069190	0.0008530
N	3.7668480	-2.3235300	0.0005800
N	3.9741940	-1.0015590	-0.0005230
C	2.8163910	-0.3088490	-0.0009340
C	0.2745930	1.9697250	1.2057860
C	0.7567420	3.2781210	1.2065890
C	0.9977590	3.9363440	-0.0001250
C	0.7549610	3.2786590	-1.2067750
C	0.2728090	1.9702640	-1.2058380
H	-0.0262720	-3.2774790	-0.0004030
H	-2.5542730	2.0011210	-0.8774750
H	-4.1065060	1.9673970	0.0020800
H	-2.5527940	2.0003980	0.8791270
H	-3.3988460	-2.9917330	-0.8777980
H	-3.3975190	-2.9933370	0.8780030
H	-2.2931950	-4.0725630	-0.0016740
H	2.7800910	0.7662620	-0.0018050
H	0.0904560	1.4581920	2.1443840
H	0.9451170	3.7823560	2.1484570
H	1.3730120	4.9540340	-0.0001720
H	0.9419550	3.7833020	-2.1487000
H	0.0872910	1.4591500	-2.1443910
H	4.9202680	-0.6363640	-0.0008170

Molecule **23a(1,5)**

E = -874.532494, H (0K) = -874.264918,
H (298K) = -874.246524,
G (298K) = -874.312076 au.
Imaginary frequency = 0.

C	0.4329610	-1.1846290	-0.0001110
C	-0.4405940	-0.1157720	-0.0001040
C	-1.7781970	-0.6659460	-0.0002030
C	-1.6470860	-2.0671210	-0.0002460
N	-0.3248270	-2.3455520	-0.0001340
C	-3.0669080	0.0192120	0.0001990
O	-4.1272220	-0.6215190	0.0002480
C	-3.1147960	1.5284070	0.0006190
C	-2.6637330	-3.1554070	-0.0002420
C	-0.0104160	1.3040310	-0.0000140
C	1.8796340	-1.2428890	-0.0000630
N	2.5329390	-2.4167070	0.0006910
N	3.8139170	-2.0701690	0.0003180
N	4.0588930	-0.7683120	-0.0005390
C	2.8478840	-0.2123550	-0.0008170
C	0.2159560	1.9778160	1.2059540
C	0.6546090	3.3013460	1.2067210
C	0.8742320	3.9669950	0.0000580
C	0.6532950	3.3018550	-1.2066490
C	0.2146290	1.9783340	-1.2059530
H	0.0633850	-3.2805020	-0.0003420
H	-2.6042830	1.9320080	-0.8774570
H	-4.1556270	1.8532620	0.0008120
H	-2.6041980	1.9313230	0.8789940
H	-2.1765700	-4.1334490	-0.0005180
H	-3.3105110	-3.0835850	0.8777910
H	-3.3109310	-3.0832600	-0.8779230
H	2.7213820	0.8568130	-0.0015520
H	0.0490410	1.4603000	2.1444440
H	0.8268330	3.8112430	2.1486010
H	1.2168640	4.9960990	0.0000920
H	0.8245080	3.8121330	-2.1485070
H	0.0467040	1.4612020	-2.1444750
H	4.5559050	-2.7595120	0.0007990

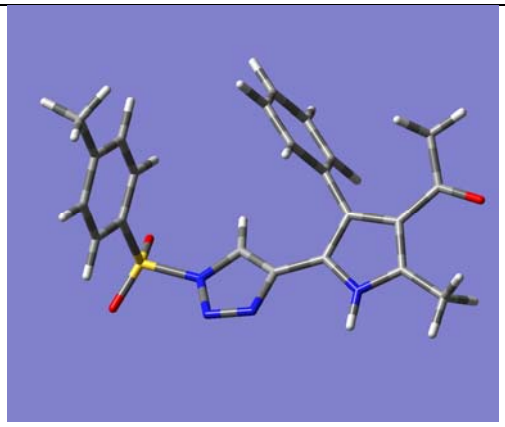
Molecule **24(1,4)**



E = -874.530912, H (0K) = -874.263621,
H (298K) = -874.245206,
G (298K) = -874.311173 au.
Imaginary frequency = 0.

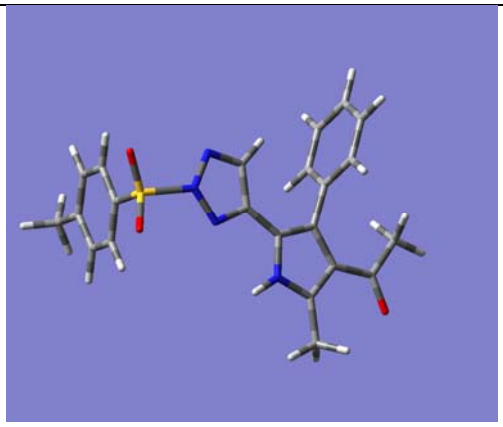
C	-0.2701270	-1.2714720	0.0004660
C	0.4547250	-0.0942230	-0.0015230
C	1.8506790	-0.4597820	-0.0035950
C	1.9092840	-1.8659110	0.0017820
N	0.6374400	-2.3211260	0.0045700
C	3.0366000	0.3942250	-0.0074680
O	4.1706700	-0.0991980	-0.0508220
C	2.8809030	1.8946170	0.0433560
C	3.0641270	-2.8059140	0.0093870
C	-0.1615500	1.2554270	0.0019630
C	-1.6899230	-1.5253920	-0.0016160
N	-2.6609010	-0.5766470	-0.0589080
N	-3.8911880	-1.1209330	-0.0480210
N	-3.7370480	-2.4174260	0.0159460
C	-2.4125660	-2.7106670	0.0462400
C	-0.4591830	1.9056790	-1.2024840
C	-1.0720820	3.1582340	-1.1971140
C	-1.3953570	3.7745960	0.0121500
C	-1.1061460	3.1318690	1.2164050
C	-0.4939480	1.8793360	1.2114900
H	0.3900450	-3.3030950	0.0087710
H	2.3220940	2.1968890	0.9326010
H	3.8686710	2.3559350	0.0553740
H	2.3199660	2.2533120	-0.8235190
H	2.7155930	-3.8389650	0.0804170
H	3.6600430	-2.6968750	-0.9005770
H	3.7276180	-2.5968860	0.8515260
H	-2.0512950	-3.7250440	0.1000510
H	-0.2108830	1.4253010	-2.1425790
H	-1.2976300	3.6511980	-2.1365580
H	-1.8724620	4.7485750	0.0161010
H	-1.3578270	3.6043220	2.1597580
H	-0.2721240	1.3782360	2.1473790
H	-2.5579160	0.4298640	-0.1139110

Molecule **24**



E = -1693.618712, H (0K) = -1693.235171,
H (298K) = -1693.206684,
G (298K) = -1693.297856 au.
Imaginary frequency = 0.

C	1.9672040	-1.2405890	0.2185210
C	2.6228110	-0.0430920	0.0140710
C	3.9803650	-0.2267640	0.4715280
C	4.0810940	-1.5493330	0.9434400
N	2.8680280	-2.1260890	0.7855340
C	5.0788200	0.7335660	0.5264830
O	6.2131710	0.3833680	0.8780460
C	4.8294510	2.1761190	0.1565070
C	5.2204940	-2.3000110	1.5406020
C	1.9559940	1.1481000	-0.5653670
C	0.5984790	-1.6150470	-0.0600650
N	-0.0152530	-2.6801050	0.5603420
N	-1.2465520	-2.7754370	0.1614650
N	-1.4385710	-1.7906360	-0.7489570
C	-0.3190940	-1.0310240	-0.9065670
C	2.1472330	1.4996280	-1.9069670
C	1.4507050	2.5711570	-2.4642720
C	0.5521250	3.3041980	-1.6874610
C	0.3566520	2.9619040	-0.3490480
C	1.0544340	1.8911140	0.2076240
C	-3.5848860	-0.2105970	-0.0706080
C	-3.2324830	1.1320270	-0.2215670
C	-3.6022800	2.0239070	0.7759030
C	-4.3091030	1.5943770	1.9091290
C	-4.6389590	0.2368260	2.0262150
C	-4.2795820	-0.6784640	1.0444120
C	-4.7302480	2.5802880	2.9632950
S	-3.0578270	-1.3689420	-1.2993010
O	-2.8198040	-0.6965510	-2.5699880
O	-3.8181650	-2.6057570	-1.2182610
H	2.6531590	-3.0830100	1.0374860
H	3.9491940	2.5739670	0.6662360
H	5.7087570	2.7679890	0.4125480
H	4.6419400	2.2583160	-0.9179090
H	5.6299760	-1.7637440	2.4000160
H	6.0337250	-2.4133280	0.8188300
H	4.8981440	-3.2927720	1.8640730



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H (298K) = -1693.209872,
G (298K) = -1693.301355 au.
Imaginary frequency = 0.

C	-1.3949560	0.6739990	0.6011570
C	-2.6067300	0.2454420	0.0904590
C	-3.4268690	1.4189500	-0.0801440
C	-2.6612940	2.5234630	0.3439530
N	-1.4607490	2.0517470	0.7405920
C	-4.7928730	1.5343360	-0.5874630
O	-5.3508710	2.6367700	-0.6536330
C	-5.5337430	0.2985850	-1.0366880
C	-2.9741330	3.9774830	0.4034000
C	-2.9259790	-1.1729800	-0.2019370
C	-0.2047480	-0.0539770	0.9655380
N	0.8715960	0.5580730	1.4539560
N	1.7266870	-0.4494420	1.7245870
N	1.2989430	-1.6687920	1.3409090
C	0.0762280	-1.4558560	0.9018250
C	-2.6167910	-1.7258950	-1.4500610
C	-2.8810360	-3.0694270	-1.7128240
C	-3.4561780	-3.8753240	-0.7294600
C	-3.7647540	-3.3313730	0.5179990
C	-3.5004880	-1.9878160	0.7803470
C	3.8822520	0.1064570	0.0781100
C	4.2511140	-1.0087760	-0.6754120
C	4.5347600	-0.8289660	-2.0234230
C	4.4486900	0.4366140	-2.6214050
C	4.0681170	1.5317160	-1.8326840
C	3.7798830	1.3804520	-0.4819980
C	4.7874440	0.6213490	-4.0750820
S	3.4519150	-0.1153500	1.7821550
O	3.5490030	1.1449190	2.5057250
O	4.0380790	-1.3398380	2.3089300
H	-0.7089190	2.6291970	1.0962750
H	-5.6321400	-0.4119630	-0.2119090
H	-6.5236160	0.5855490	-1.3924930
H	-4.9890650	-0.2122570	-1.8346270
H	-2.1218730	4.5341640	0.7999150
H	-3.2191380	4.3627310	-0.5894530
H	-3.8436620	4.1609170	1.0391830

H	-0.2701570	-0.1973470	-1.5843070	H	-0.5481400	-2.2681020	0.5675700
H	2.8352550	0.9237210	-2.5162550	H	-2.1659440	-1.1008440	-2.2131470
H	1.6049640	2.8294420	-3.5064660	H	-2.6358970	-3.4866090	-2.6836100
H	0.0070330	4.1344950	-2.1232510	H	-3.6603100	-4.9209190	-0.9329990
H	-0.3403500	3.5256970	0.2614130	H	-4.2087110	-3.9530440	1.2880700
H	0.8947570	1.6201040	1.2455730	H	-3.7369410	-1.5663290	1.7512380
H	-2.6863410	1.4717300	-1.0926000	H	4.3180410	-1.9895430	-0.2215620
H	-3.3388180	3.0707020	0.6733330	H	4.8261260	-1.6857410	-2.6209190
H	-5.1828920	-0.1097130	2.8978230	H	3.9956670	2.5164010	-2.2811520
H	-4.5337090	-1.7264790	1.1426990	H	3.4864450	2.2309670	0.1202090
H	-3.9953690	3.3811350	3.0743990	H	4.5717470	-0.2805290	-4.6523520
H	-4.8724170	2.0943590	3.9308430	H	5.8564000	0.8364080	-4.1868690
H	-5.6821500	3.0454570	2.6824200	H	4.2367720	1.4585130	-4.5095980

Molecule **24(1,5)**

E = -1693.618149, H (0K) = -1693.234098,
H (298K) = -1693.206033,
G (298K) = -1693.292782 au.
Imaginary frequency = 0.

C	-0.1946510	0.0420150	1.3176900
C	-0.7682830	1.1187770	0.6698780
C	0.2157950	2.1777370	0.6865750
C	1.3554170	1.6803880	1.3401690
N	1.0756580	0.4149050	1.7242210
C	0.1067260	3.5665020	0.2454350
O	1.1217070	4.2419050	0.0347330
C	-1.2480780	4.2200380	0.0922260
C	2.6654770	2.3129800	1.6558760
C	-2.0781990	1.0826870	-0.0066210
C	-0.6861900	-1.3100400	1.5534260
N	-0.6692470	-2.3348650	0.6331230
N	-1.1790290	-3.4714110	1.1570790
N	-1.5051850	-3.2107690	2.3887770
C	-1.2180840	-1.9093740	2.6704790
C	-2.1977080	1.4962820	-1.3412560
C	-3.4185970	1.4147550	-2.0038040
C	-4.5429340	0.9129820	-1.3451980
C	-4.4355100	0.4972420	-0.0180630
C	-3.2132520	0.5826950	0.6471060
C	1.3862200	-1.4600320	-0.9840160
C	2.4579010	-2.0656760	-0.3226810
C	3.6562380	-1.3726850	-0.2467910
C	3.7982730	-0.0999520	-0.8249430

C	2.7032630	0.4679910	-1.4852560
C	1.4861220	-0.1998960	-1.5673940
C	5.1079930	0.6310110	-0.7210900
S	-0.1520420	-2.3259490	-1.0716120
O	0.0498520	-3.7369150	-1.3719880
O	-1.1404140	-1.5495740	-1.8057510
H	1.7280950	-0.1991090	2.1956470
H	-2.0425010	3.7005390	0.6260790
H	-1.1681910	5.2488400	0.4509650
H	-1.5130640	4.2575820	-0.9685430
H	3.2384720	1.6864220	2.3429110
H	3.2526390	2.4584160	0.7463720
H	2.5211320	3.2967470	2.1083260
H	-1.4087600	-1.4724900	3.6376200
H	-1.3228300	1.8661570	-1.8637120
H	-3.4912370	1.7333380	-3.0381750
H	-5.4936010	0.8456520	-1.8629340
H	-5.3042390	0.1090500	0.5028430
H	-3.1386630	0.2674810	1.6815150
H	2.3554830	-3.0455720	0.1283950
H	4.4971070	-1.8229510	0.2693900
H	2.7937330	1.4532690	-1.9275930
H	0.6355150	0.2534030	-2.0584910
H	5.4275600	0.7056220	0.3225250
H	5.0416860	1.6376170	-1.1367150
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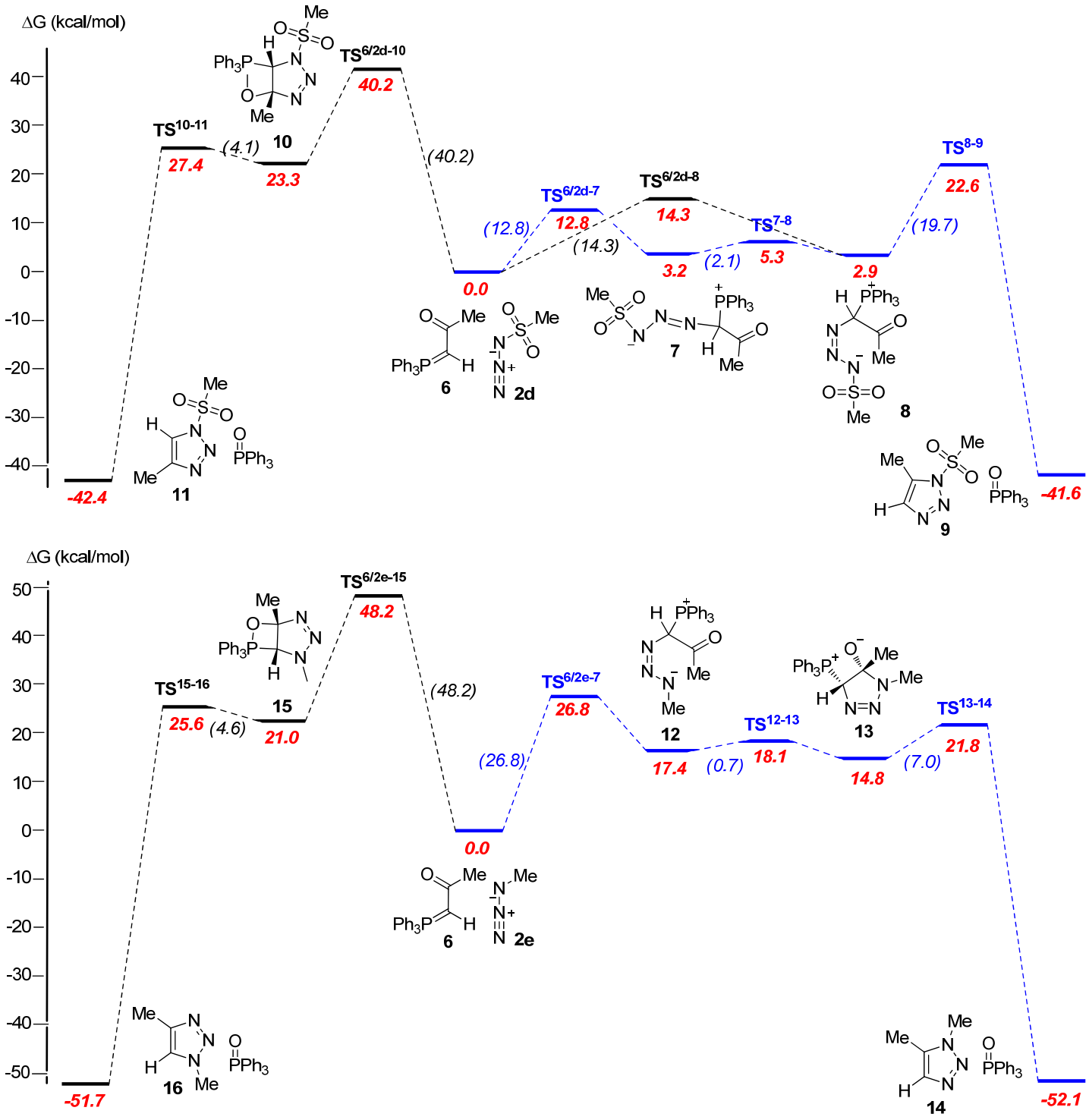

Figure S3 Relative Gibbs free energies for the energy profile of model reactions of acetylmethylidenephosphorane **6** with azides **2d,e**. (In kcal/mol, 298 K, DFT B3LYP-D3/6-311+G(d,p) level with SMD model for DCM)

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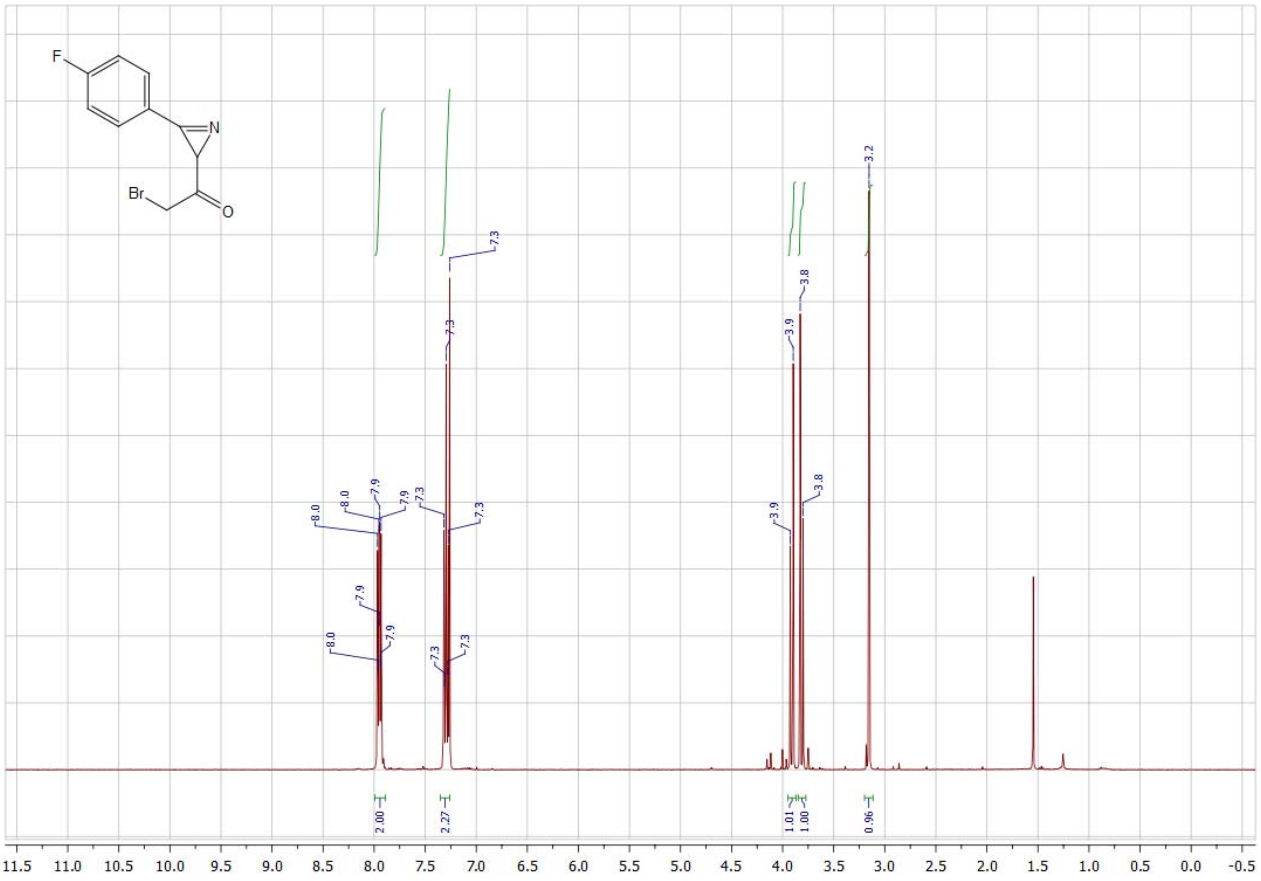
2-Bromo-1-(3-(4-fluorophenyl)-2H-azirin-2-yl)ethan-1-one, ^{1}H NMR (400 MHz, $CDCl_3$)



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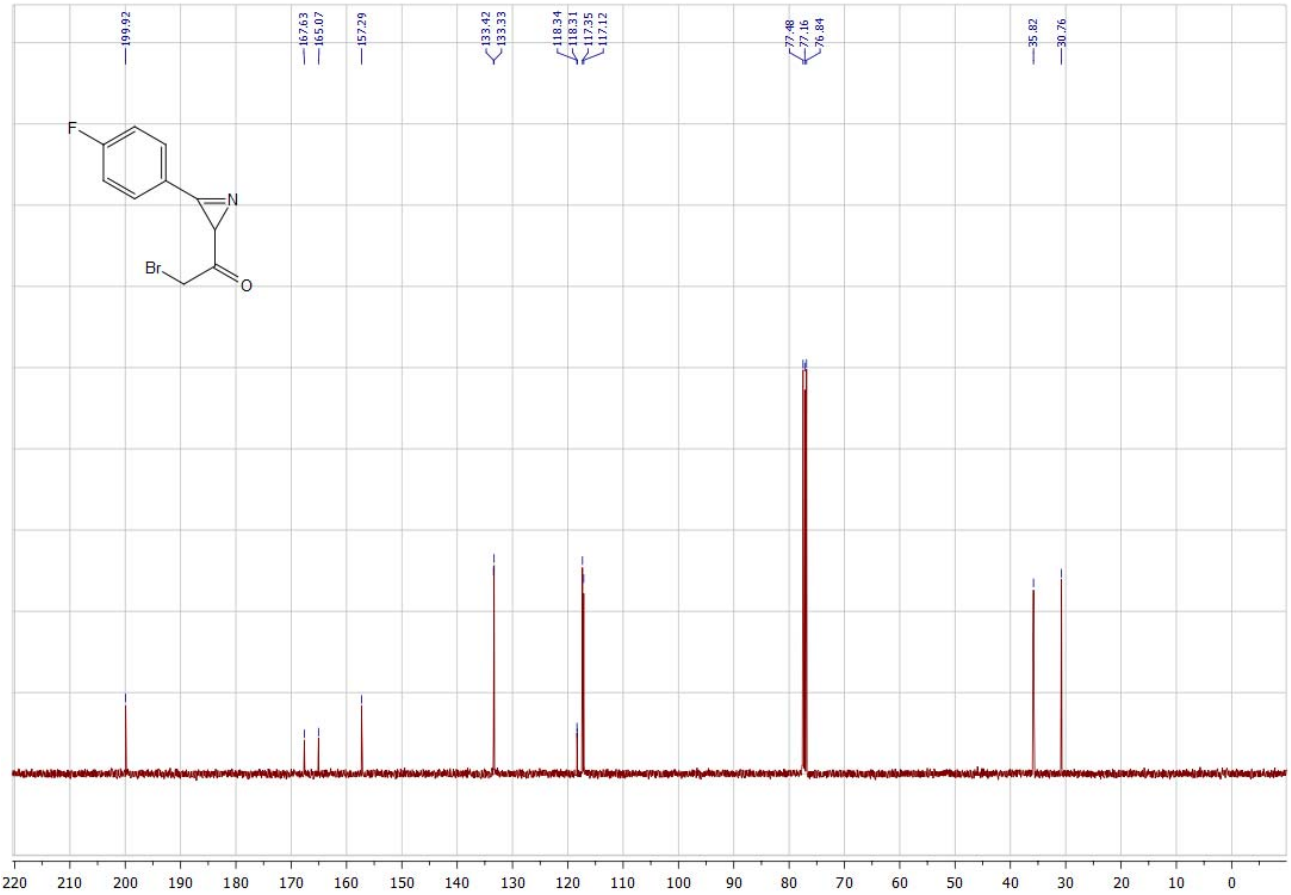

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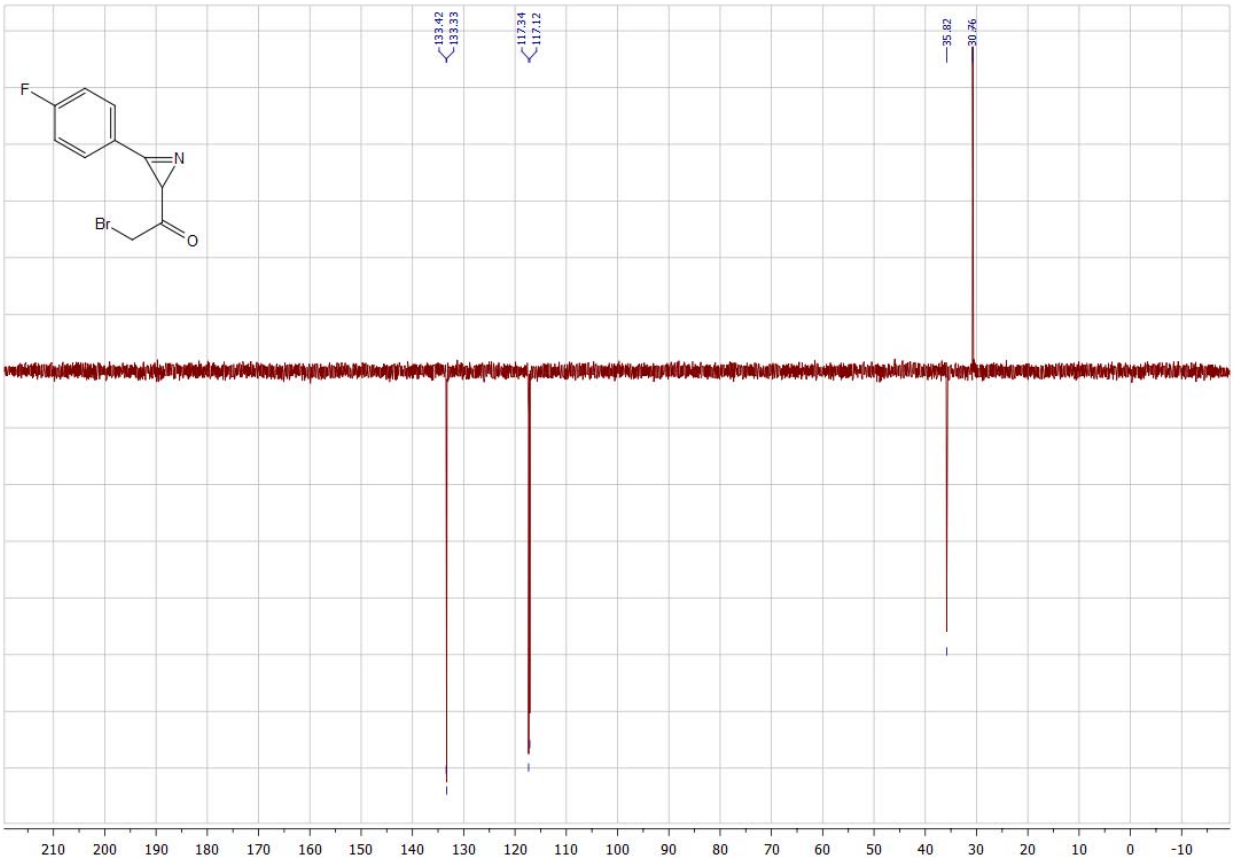

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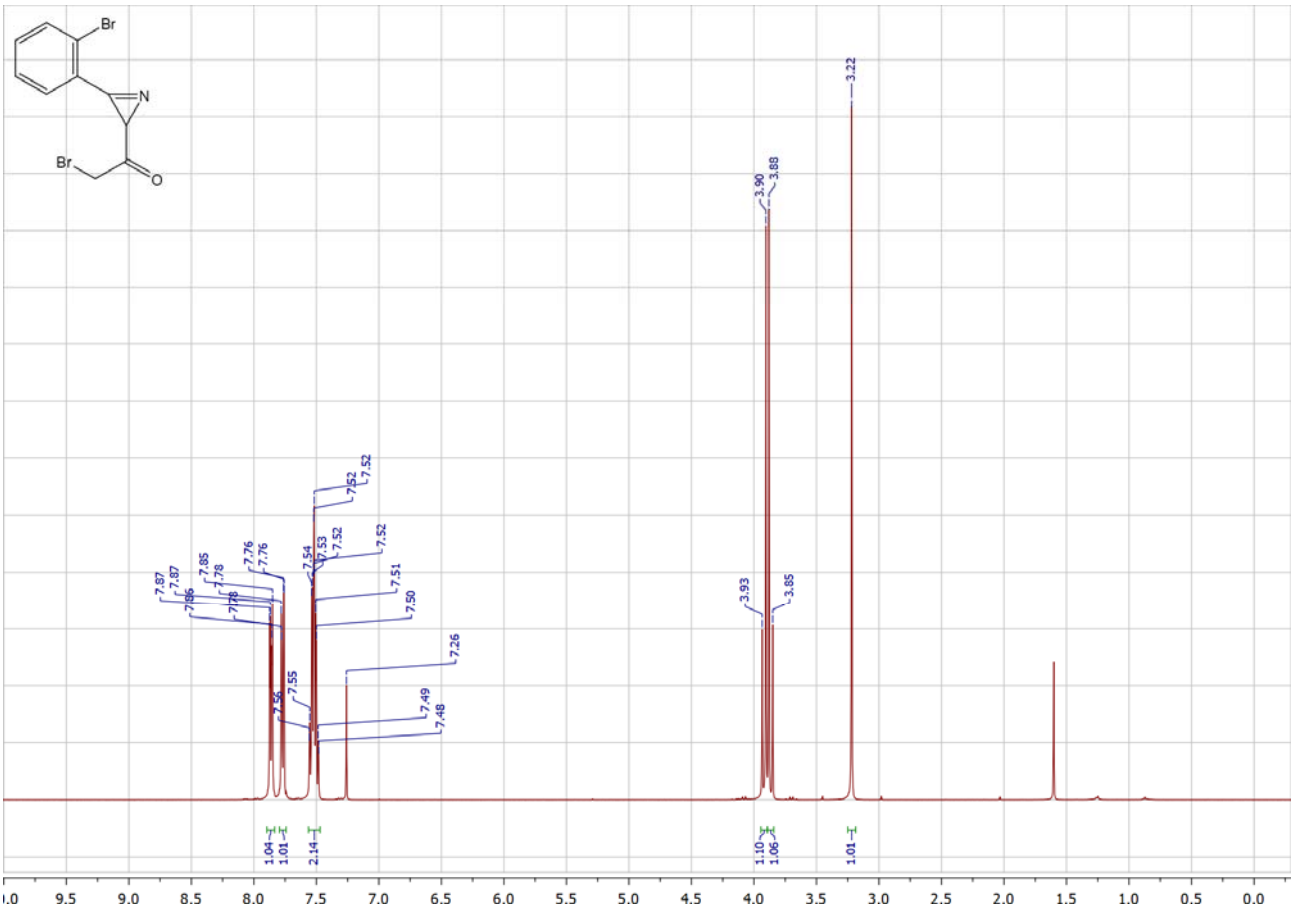

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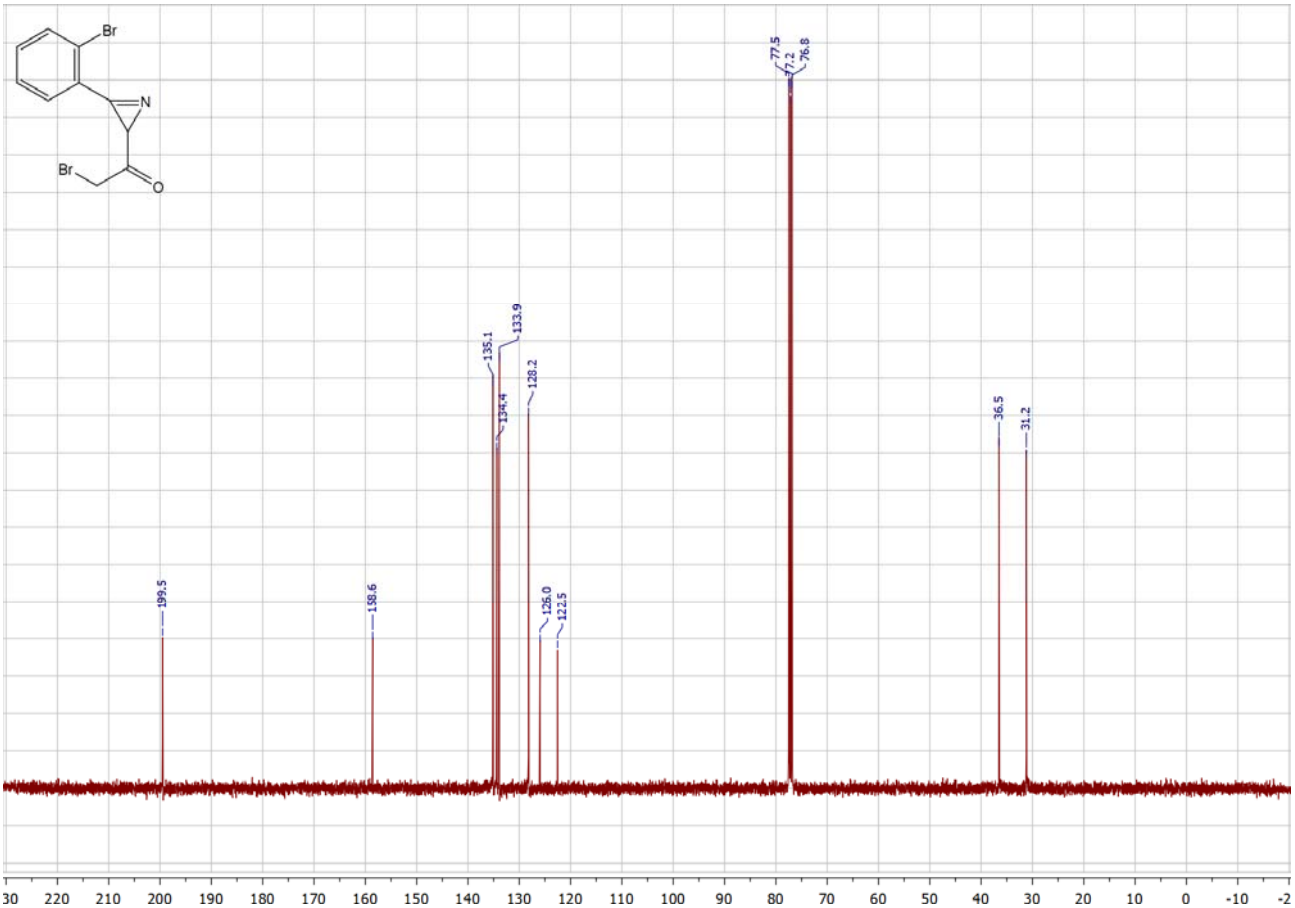

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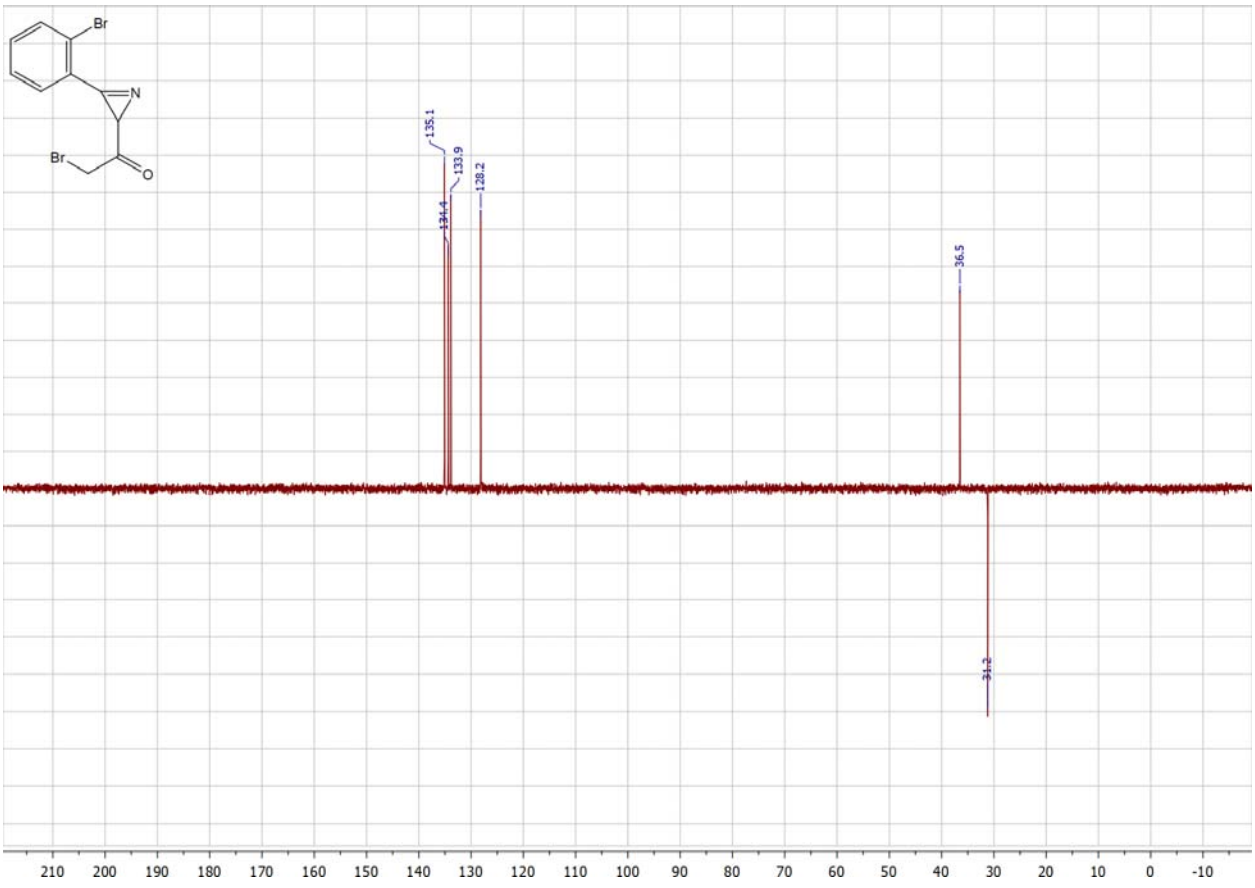
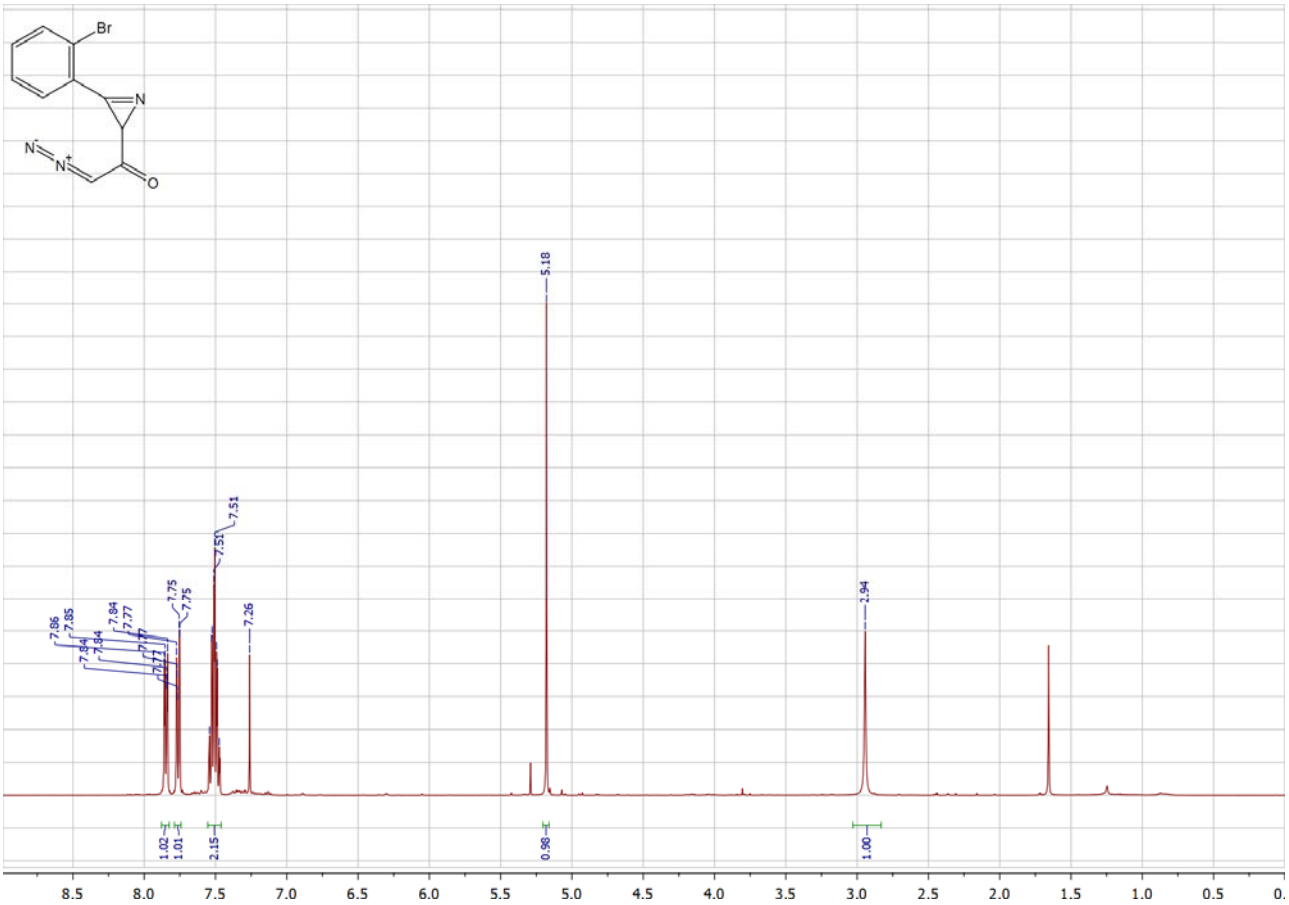


1-(3-(2-Bromophenyl)-2H-azirin-2-yl)-2-diazoethan-1-one, ^{1}H NMR (400 MHz, $CDCl_3$)



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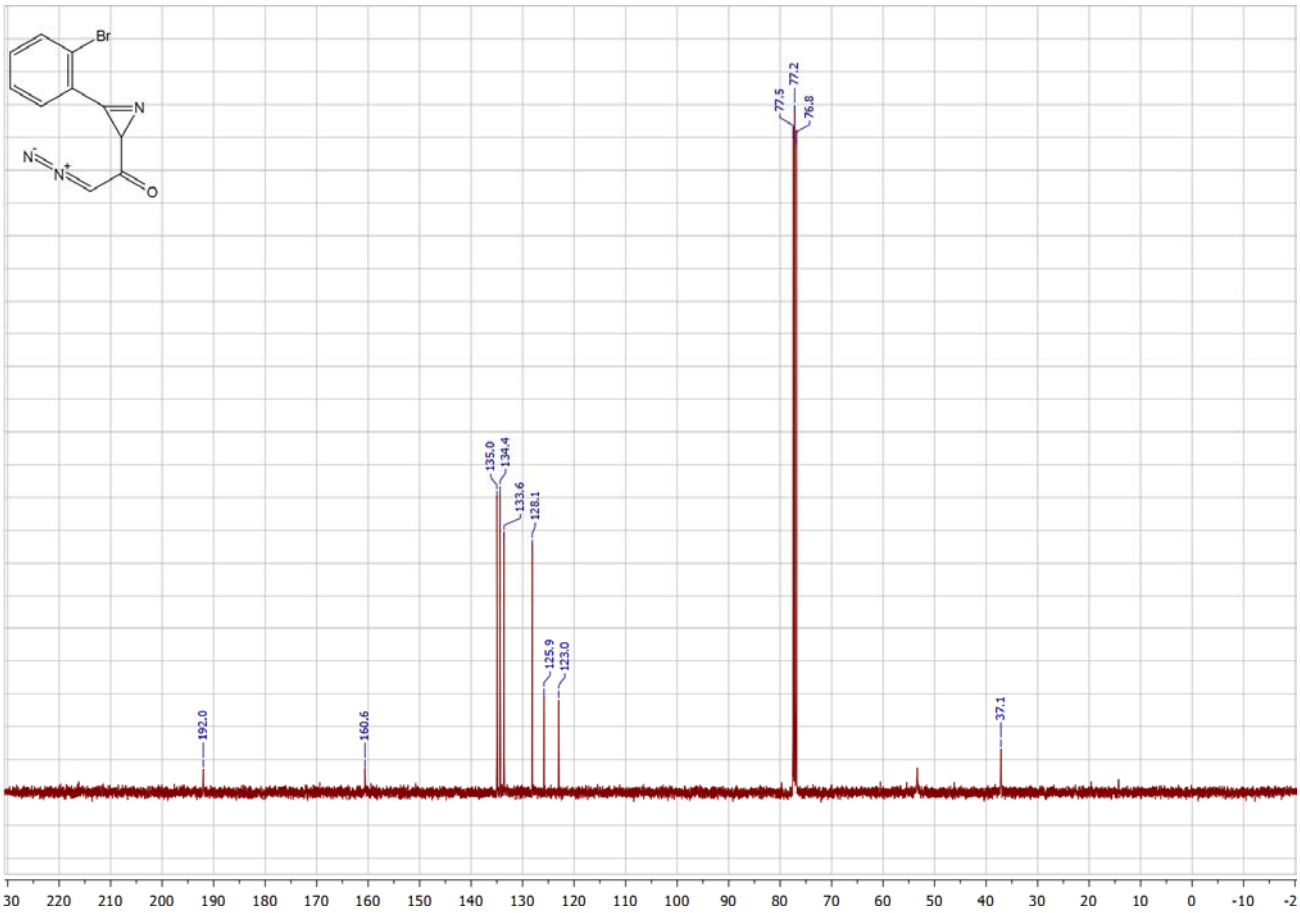

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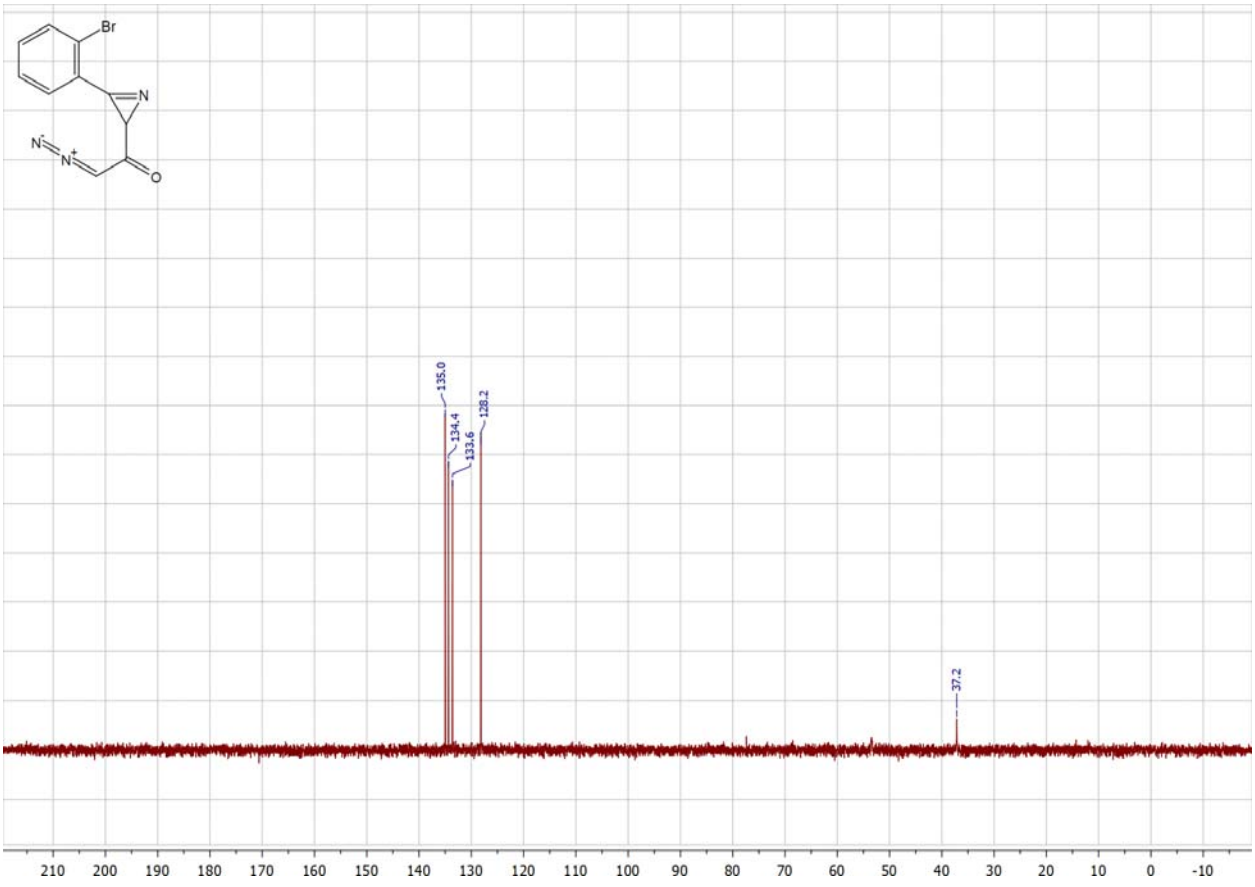

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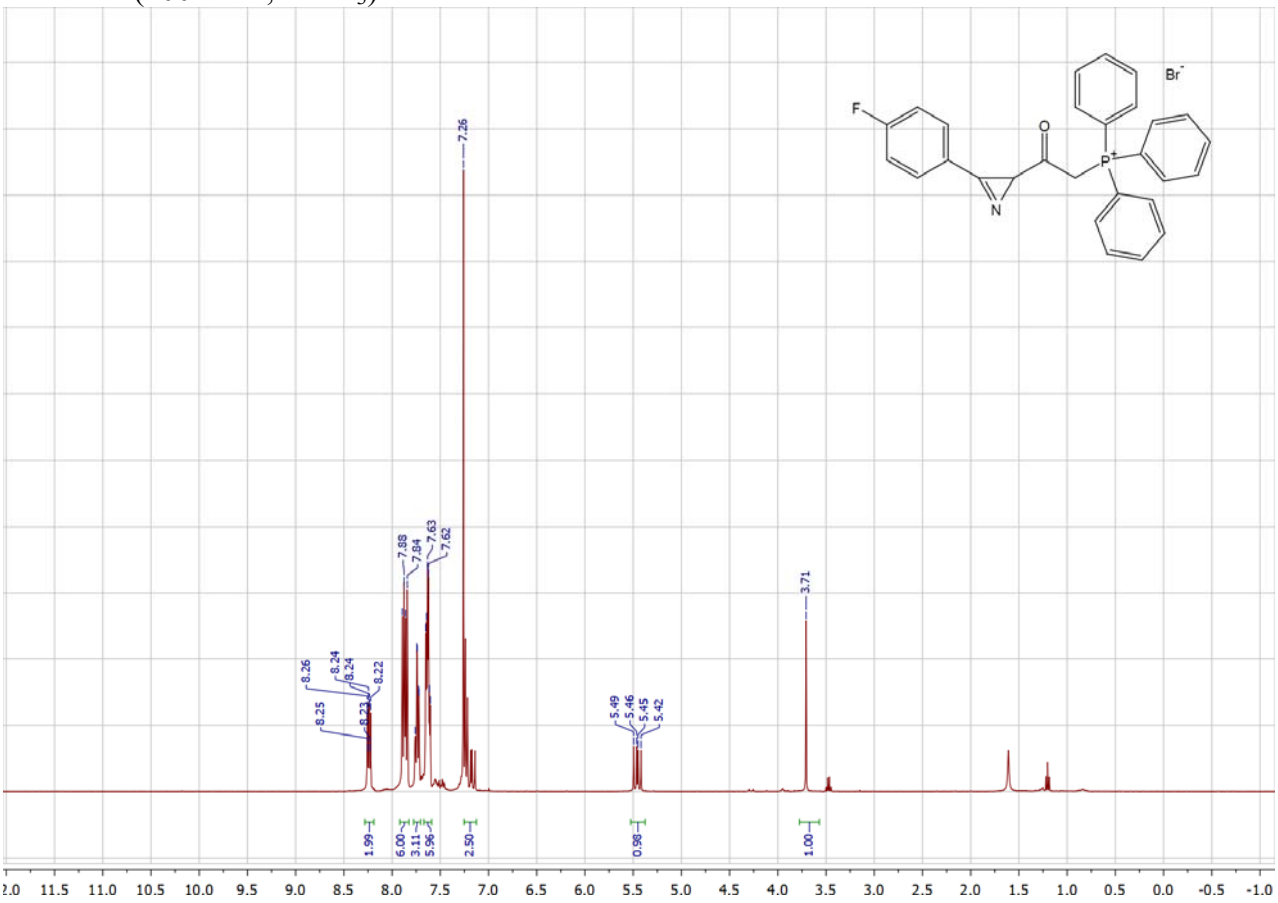
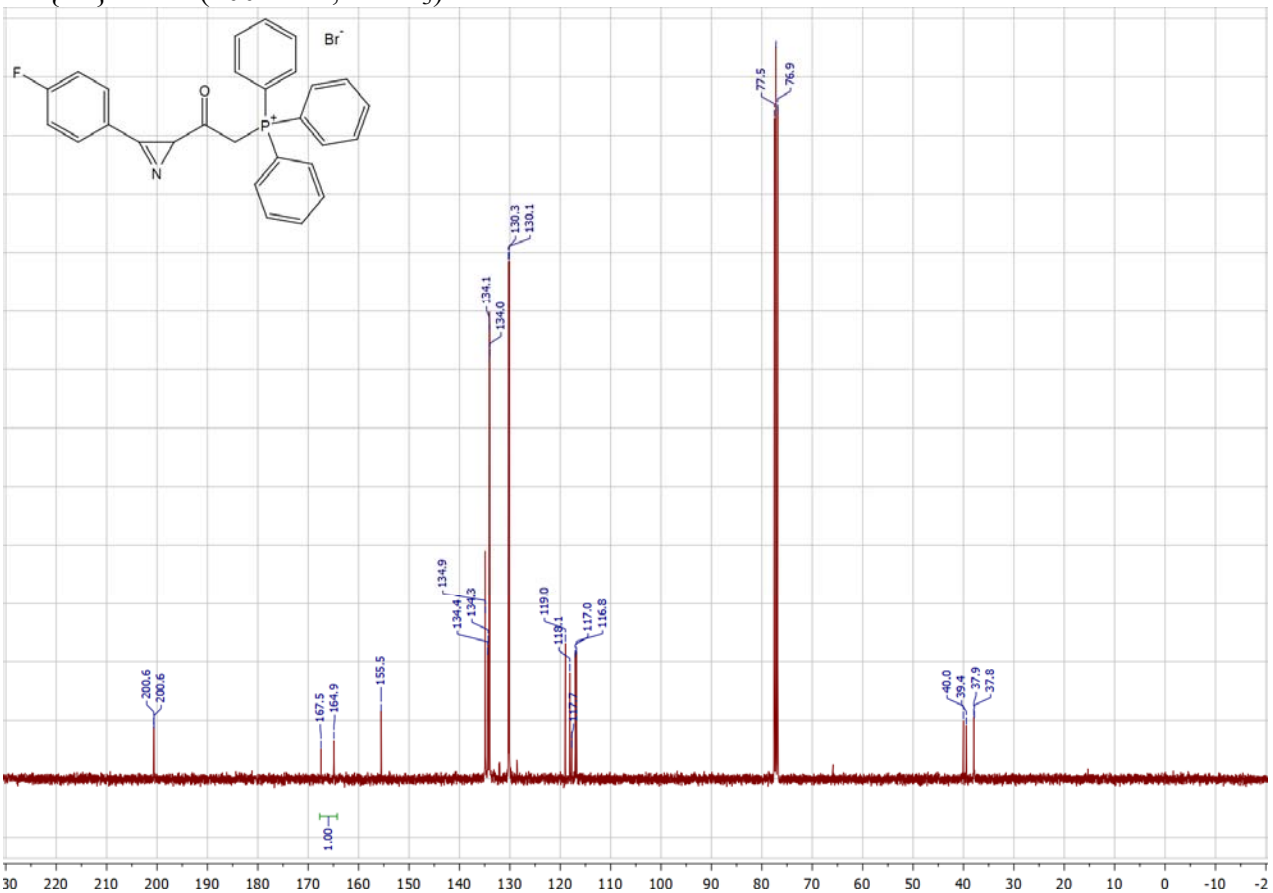
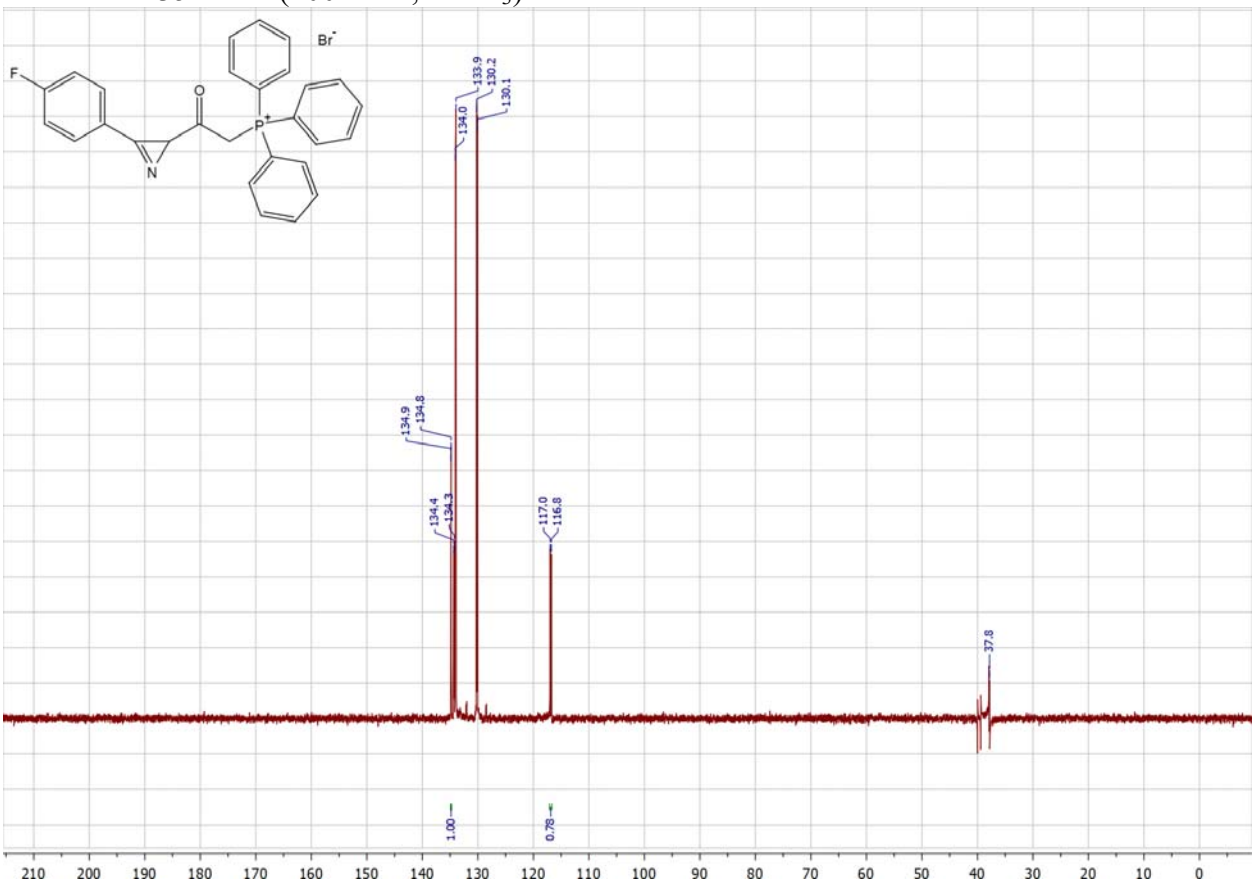
^{1}H NMR (400 MHz, $CDCl_3$)



(2-(3-(4-Fluorophenyl)-2H-azirin-2-yl)-2-oxoethyl)triphenylphosphonium bromide (**1b**),
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



(2-(3-(4-Fluorophenyl)-2H-azirin-2-yl)-2-oxoethyl)triphenylphosphonium bromide (**1b**),
^{13}C DEPT 135 NMR (100 MHz, $CDCl_3$)



(2-(3-(4-Chlorophenyl)-2H-azirin-2-yl)-2-oxoethyl)triphenylphosphonium bromide (**1c**),
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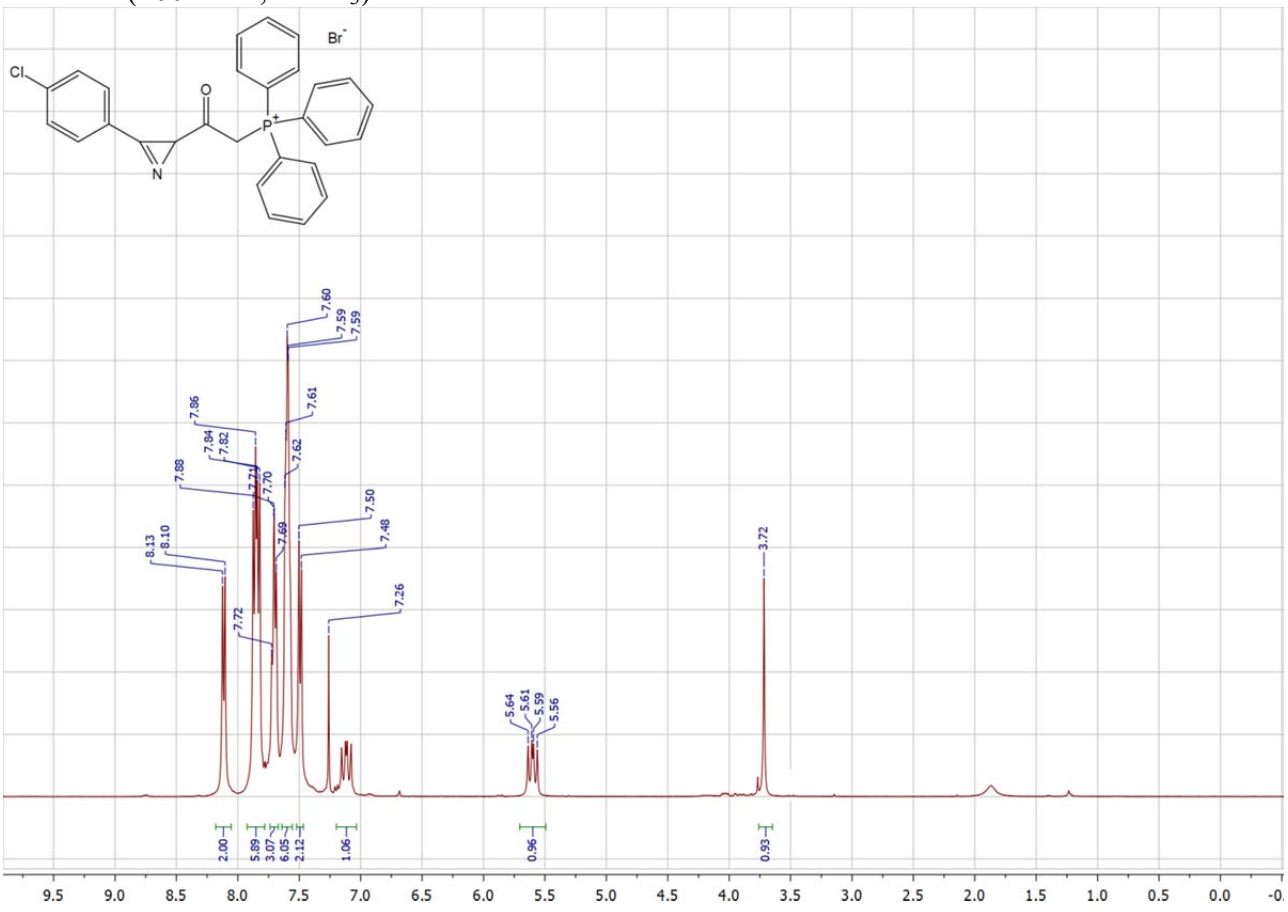

(2-(3-(4-Chlorophenyl)-2H-azirin-2-yl)-2-oxoethyl)triphenylphosphonium bromide (**1c**),
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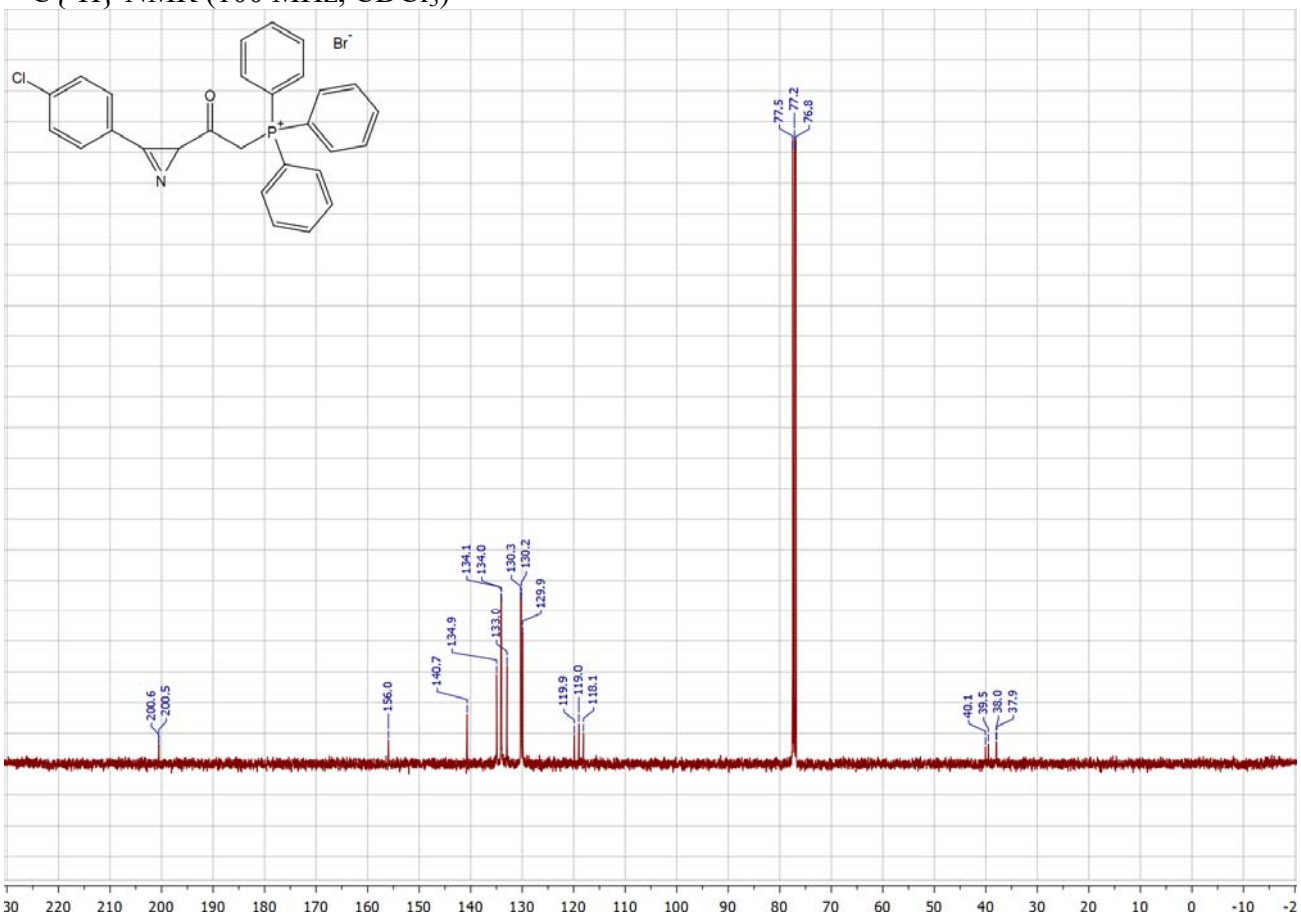

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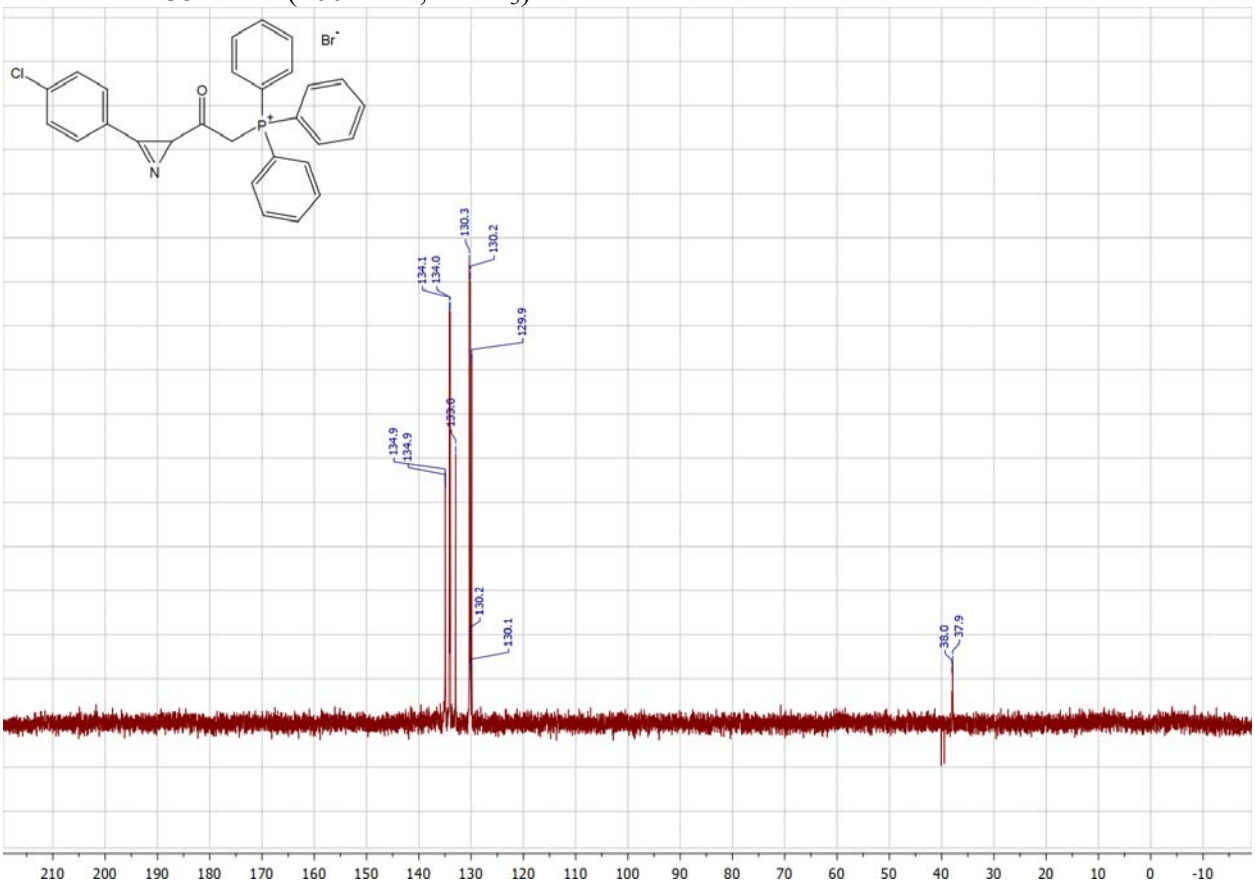

(2-(3-(4-Bromophenyl)-2H-azirin-2-yl)-2-oxoethyl)triphenylphosphonium bromide (**1d**),
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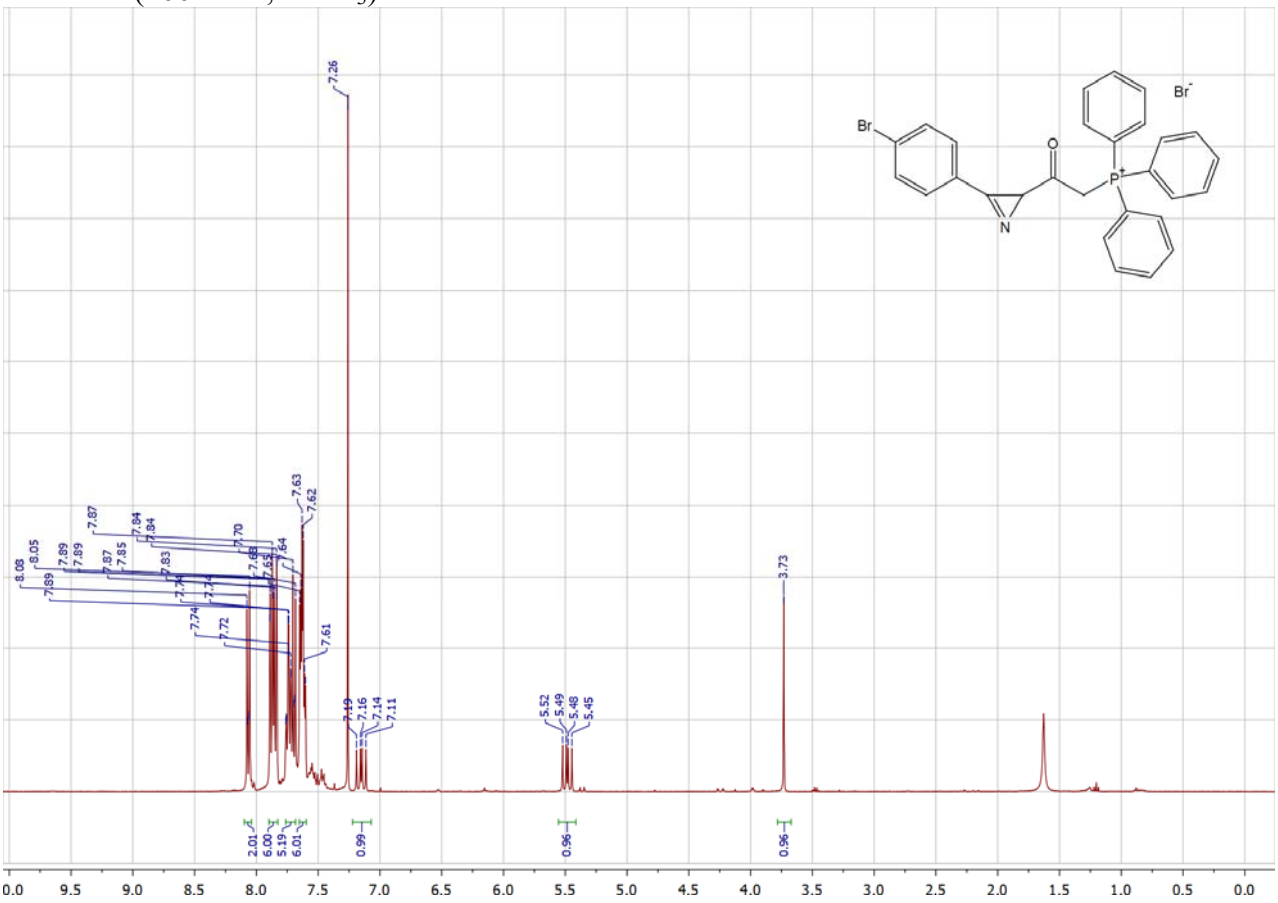

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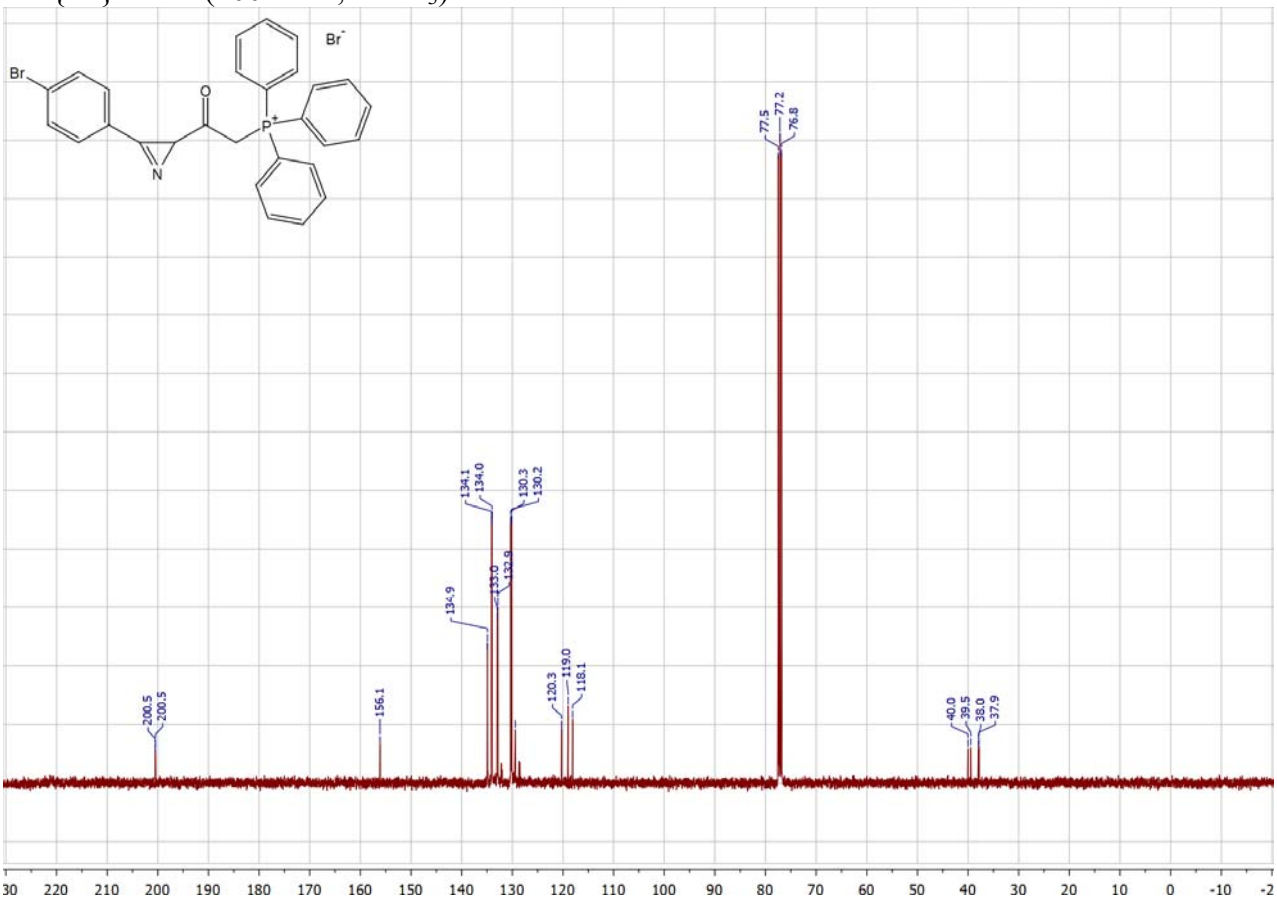

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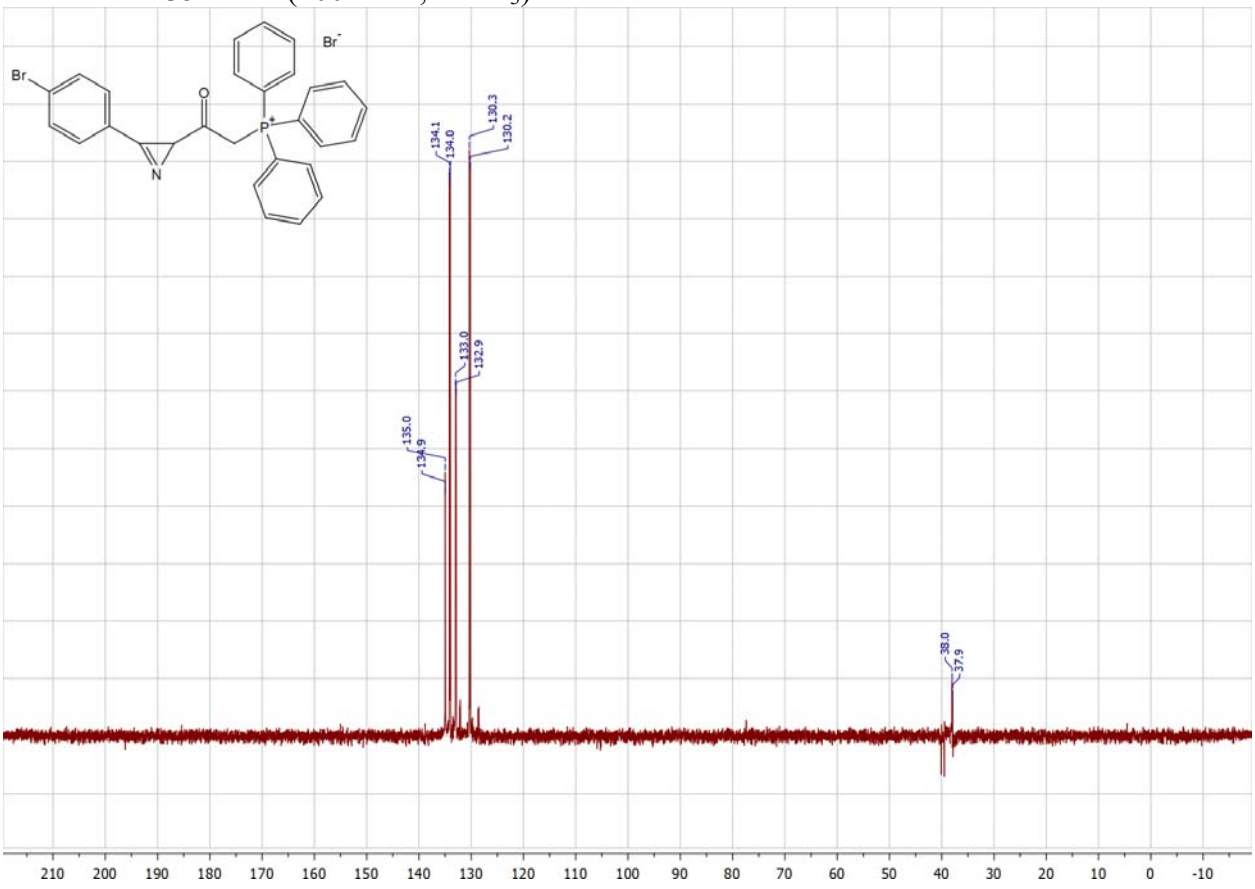

(2-Oxo-2-(3-(p-tolyl)-2H-azirin-2-yl)ethyl)triphenylphosphonium bromide (**1e**),
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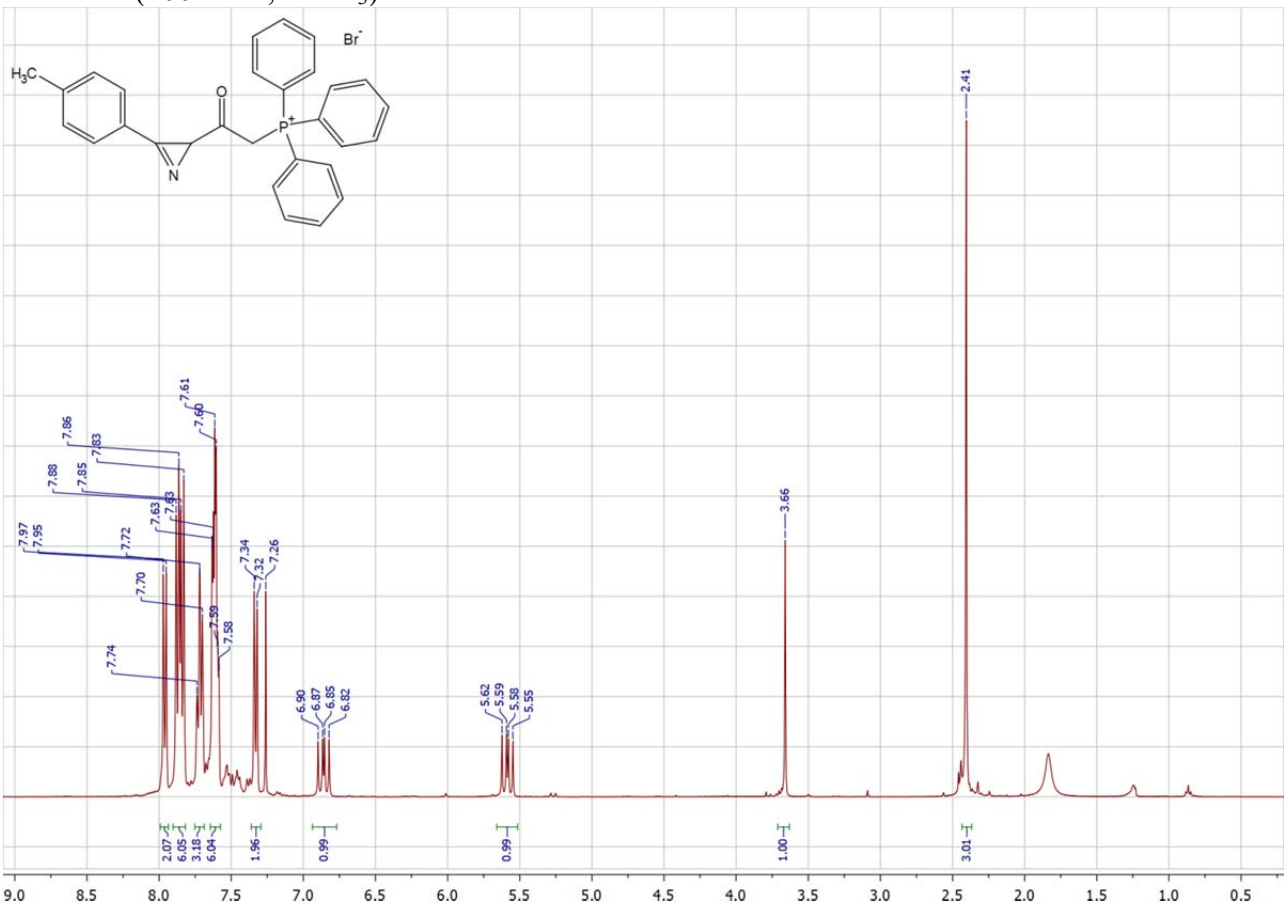

(2-Oxo-2-(3-(p-tolyl)-2H-azirin-2-yl)ethyl)triphenylphosphonium bromide (**1e**),
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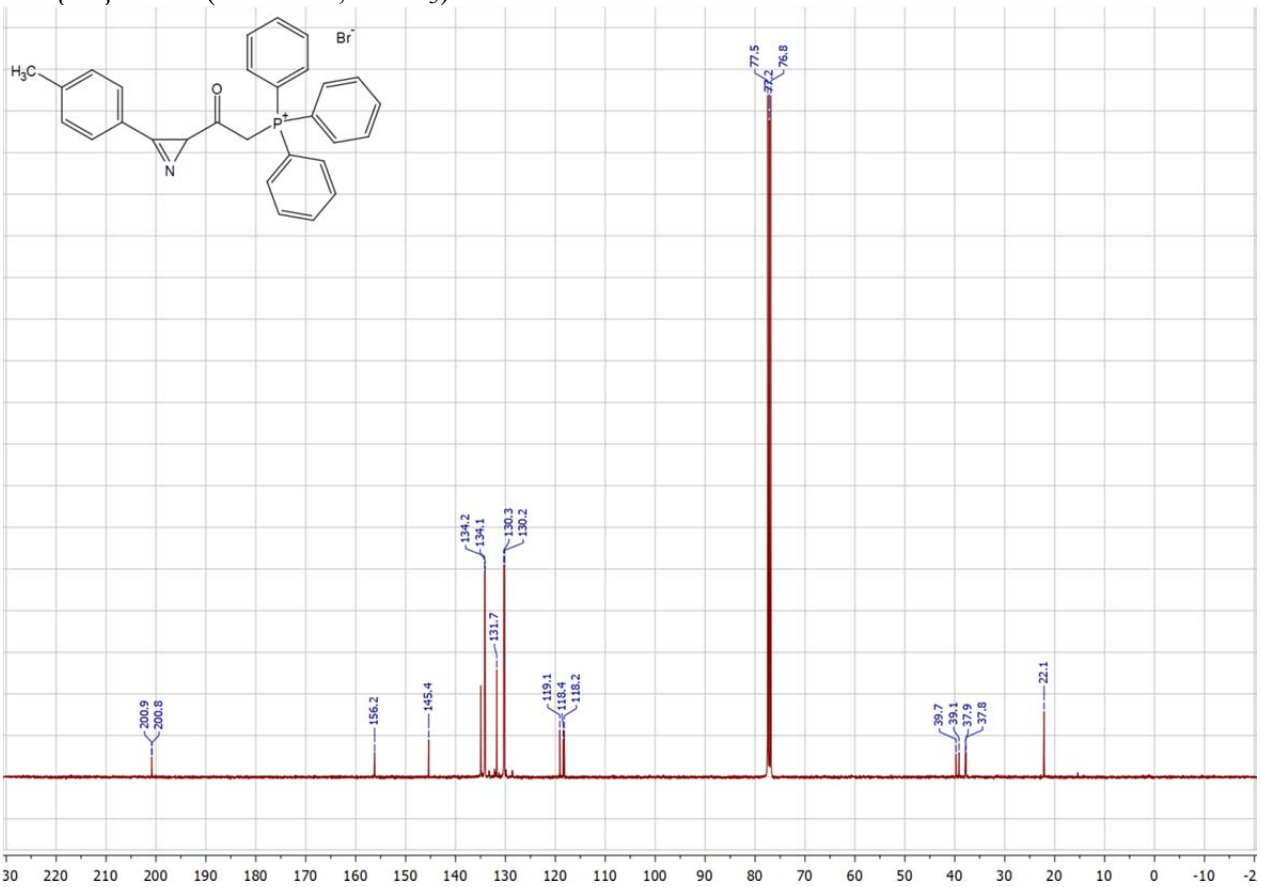

(2-Oxo-2-(3-(p-tolyl)-2H-azirin-2-yl)ethyl)triphenylphosphonium bromide (**1e**),
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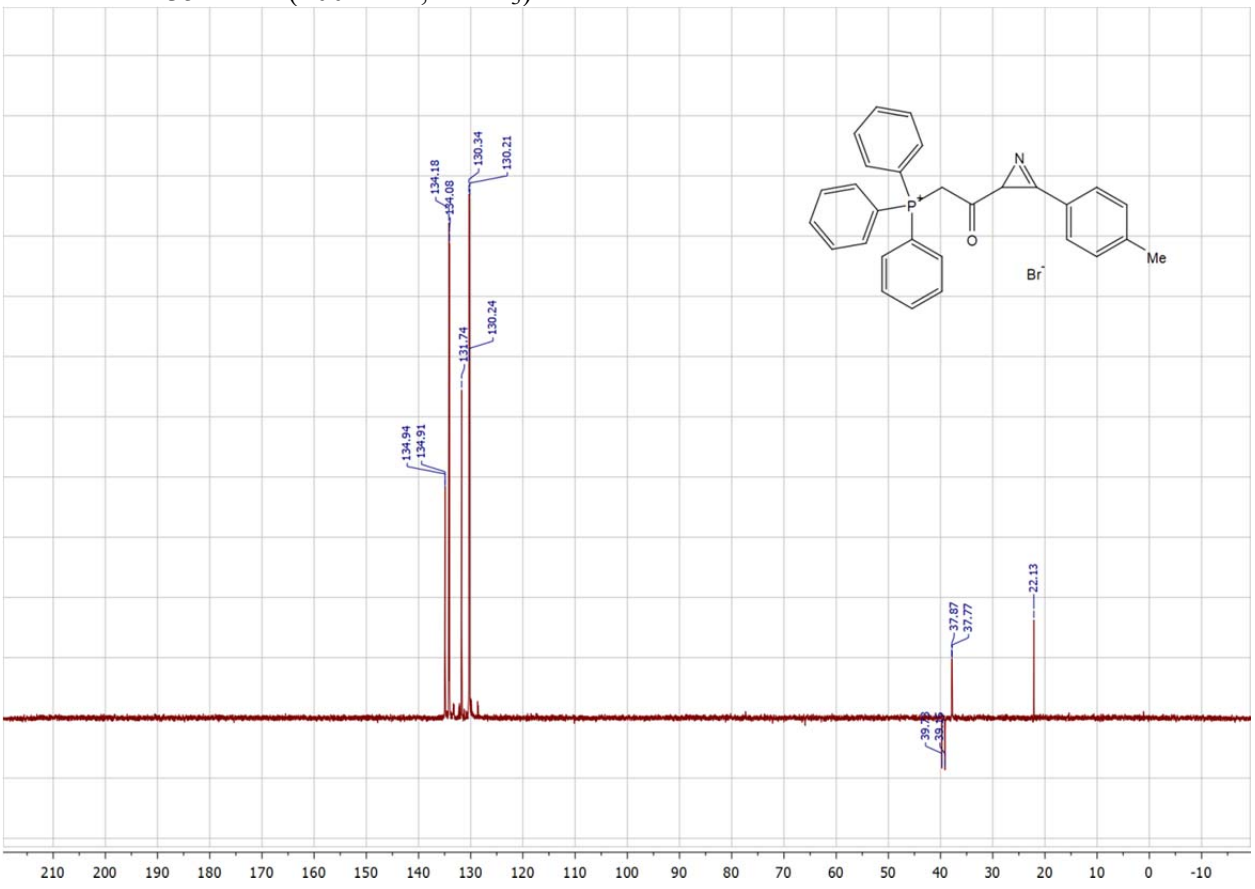
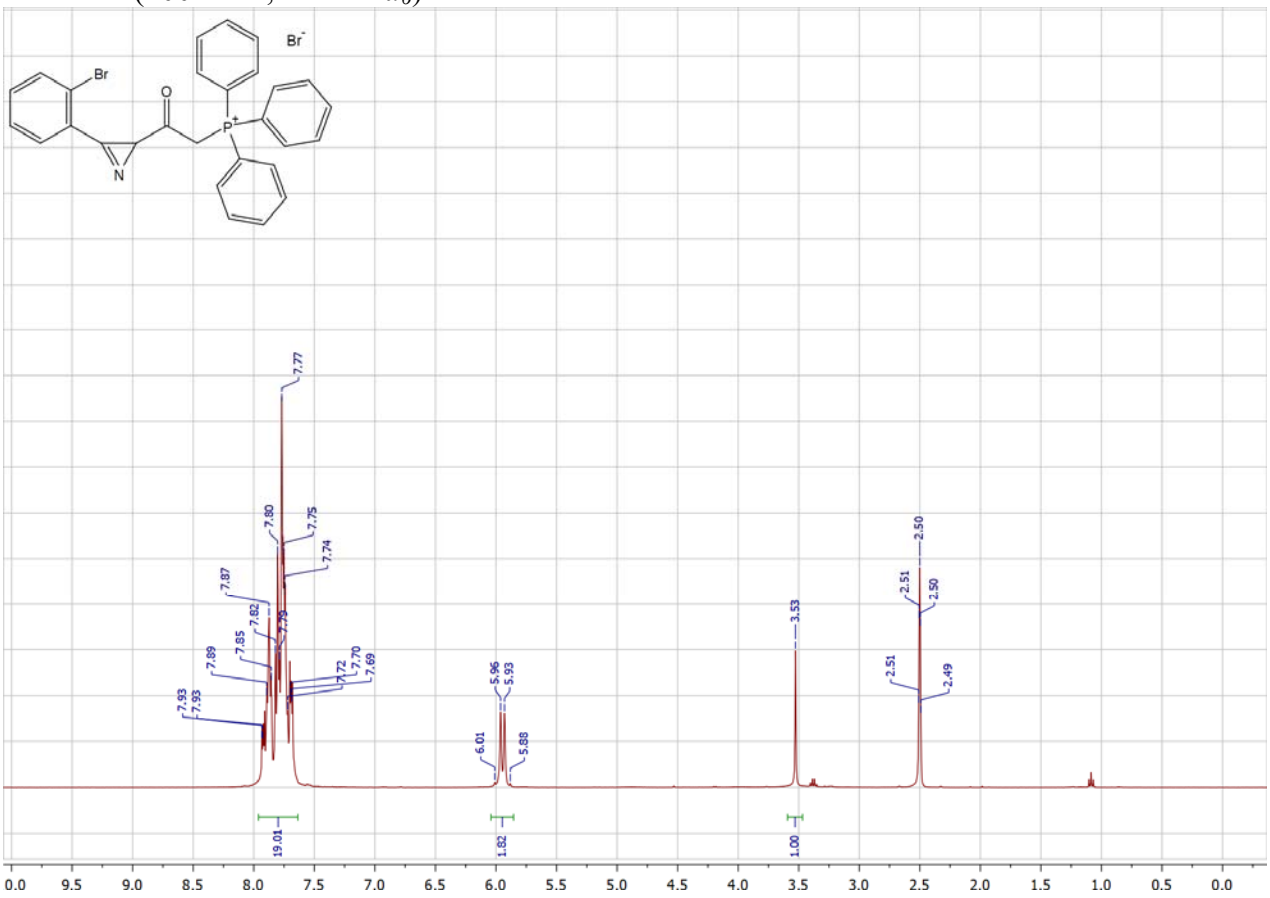
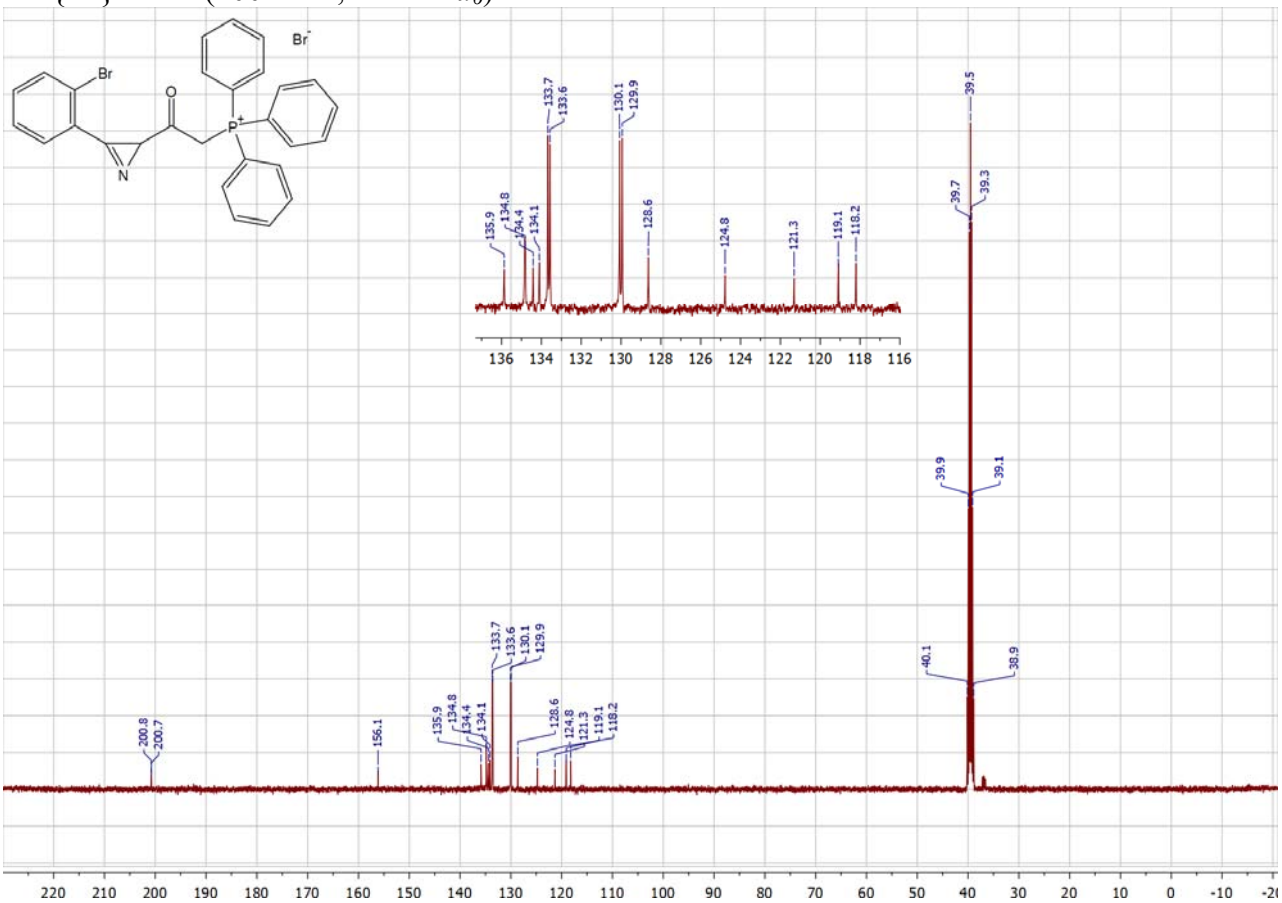


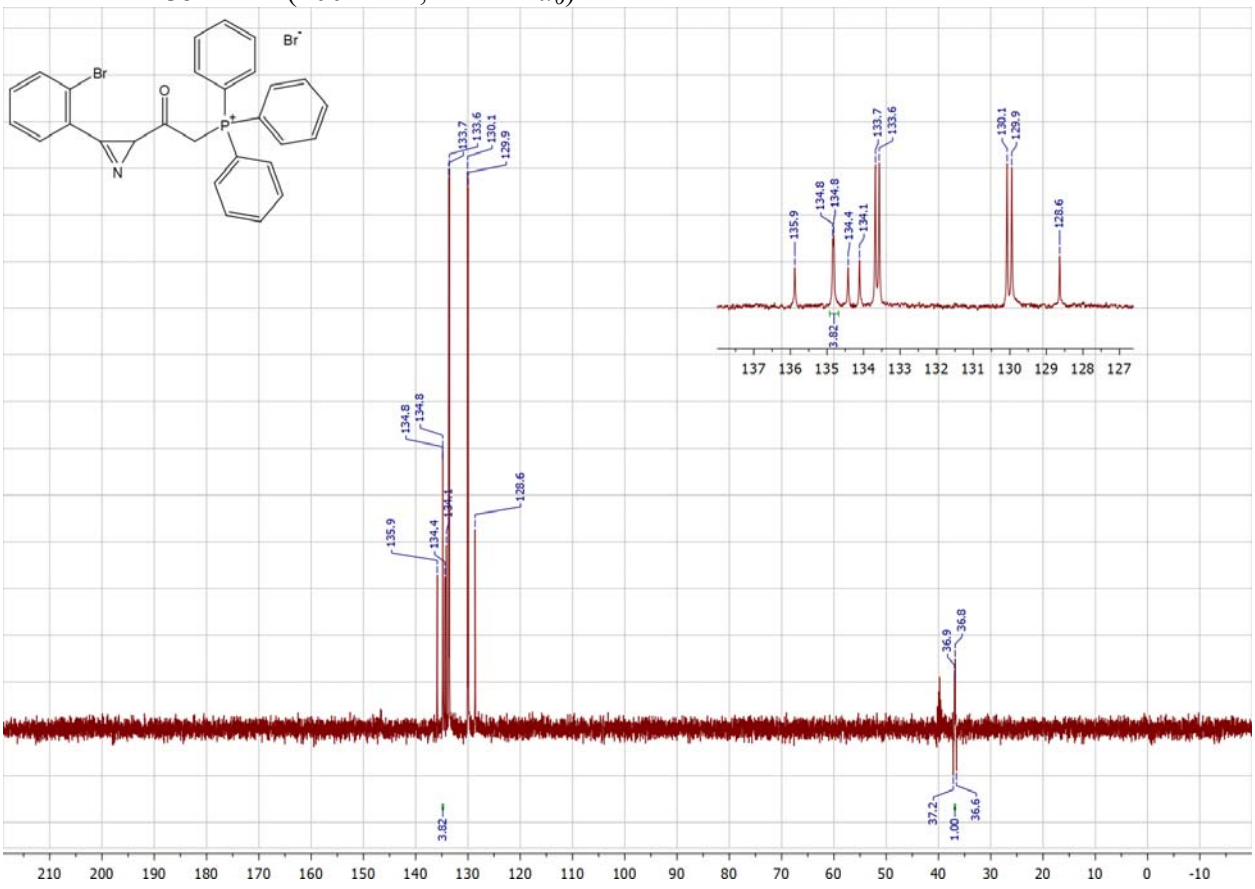
(2-(3-(2-Bromophenyl)-2H-azirin-2-yl)-2-oxoethyl)triphenylphosphonium bromide (**1g**),
^{1}H NMR (400 MHz, DMSO-d_6)



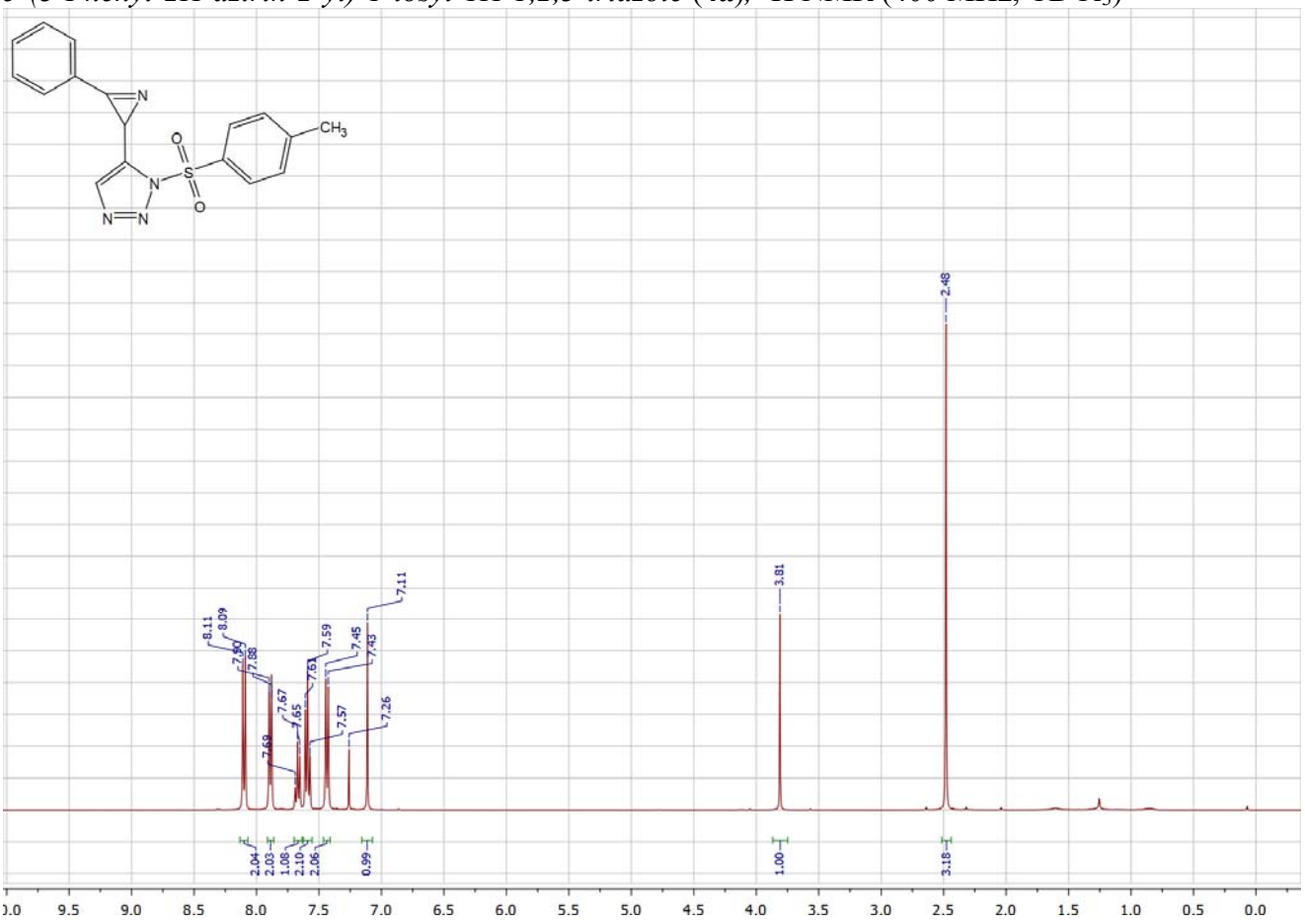
(2-(3-(2-Bromophenyl)-2H-azirin-2-yl)-2-oxoethyl)triphenylphosphonium bromide (**1g**),
^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6)



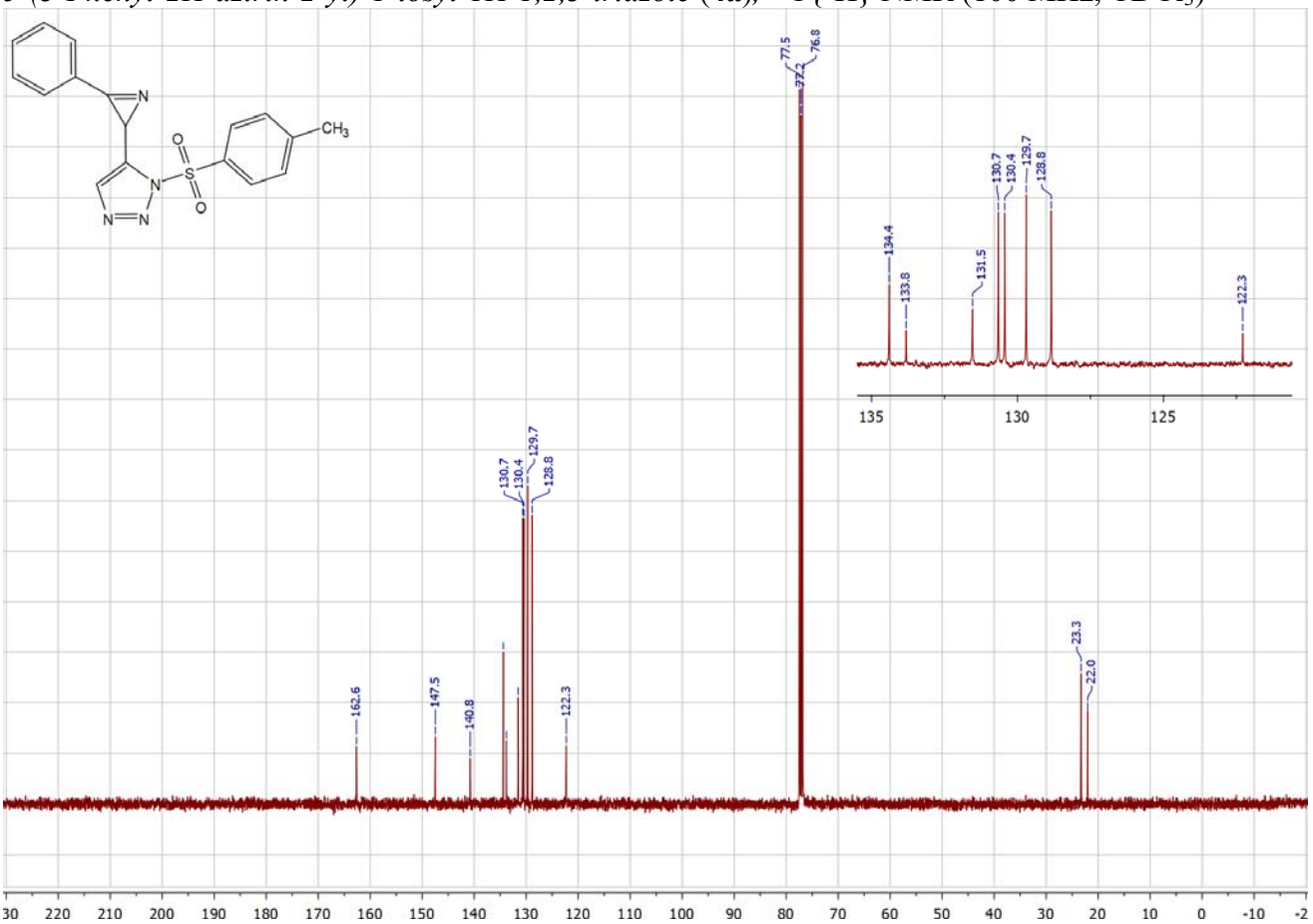
(2-(3-(2-Bromophenyl)-2H-azirin-2-yl)-2-oxoethyl)triphenylphosphonium bromide (**1g**),
^{13}C DEPT 135 NMR (100 MHz, DMSO-d_6)



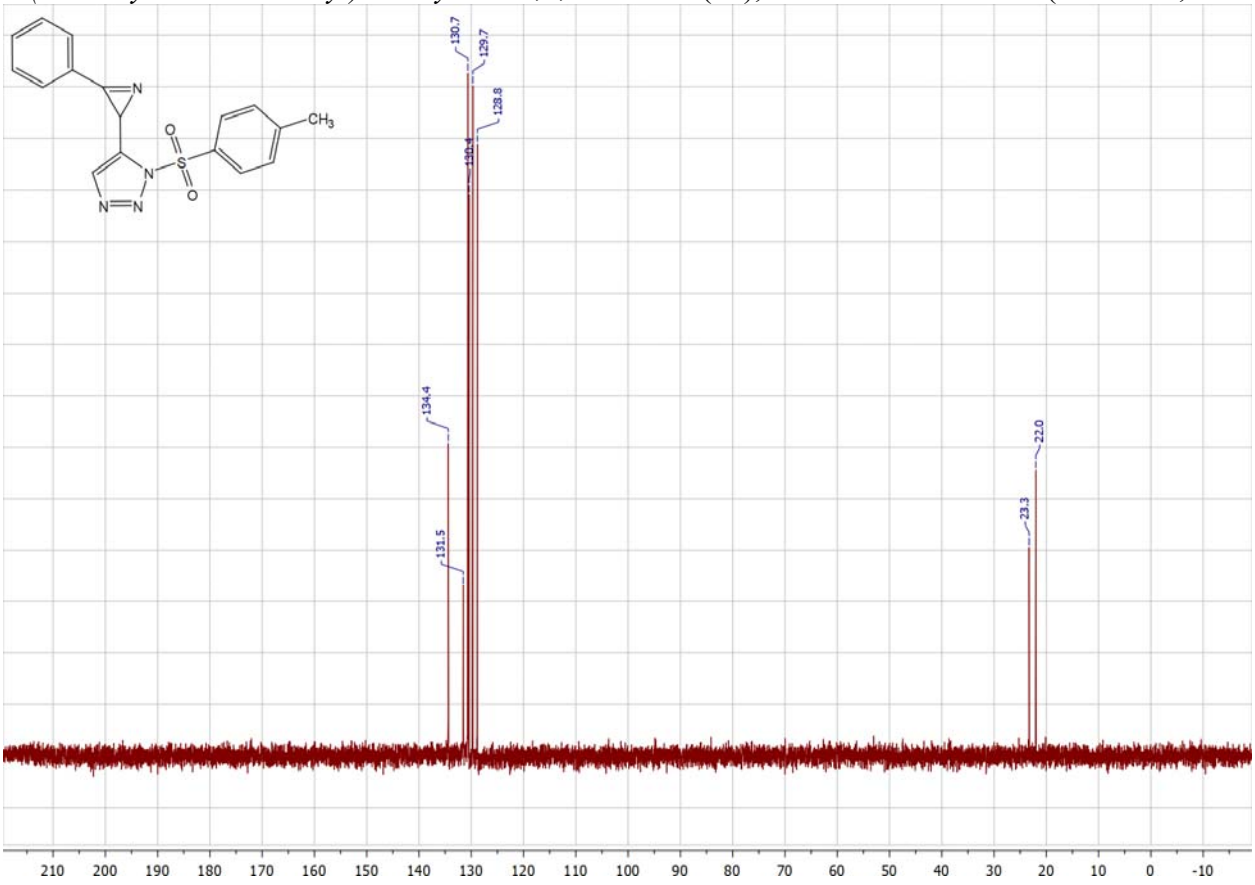
5-(3-Phenyl-2H-azirin-2-yl)-1-tosyl-1H-1,2,3-triazole (**4a**), ^{1}H NMR (400 MHz, $CDCl_3$)



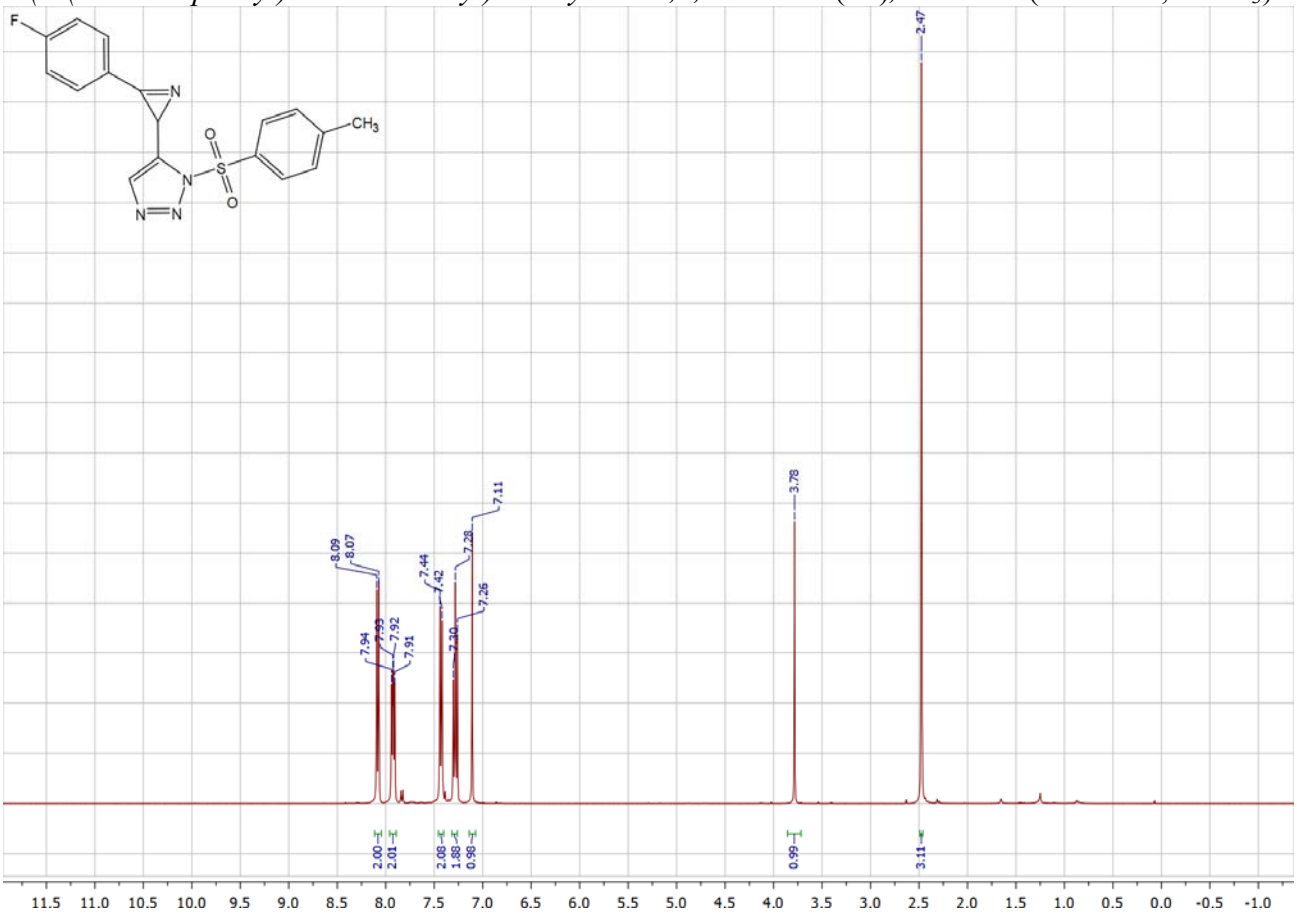
5-(3-Phenyl-2H-azirin-2-yl)-1-tosyl-1H-1,2,3-triazole (**4a**), $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



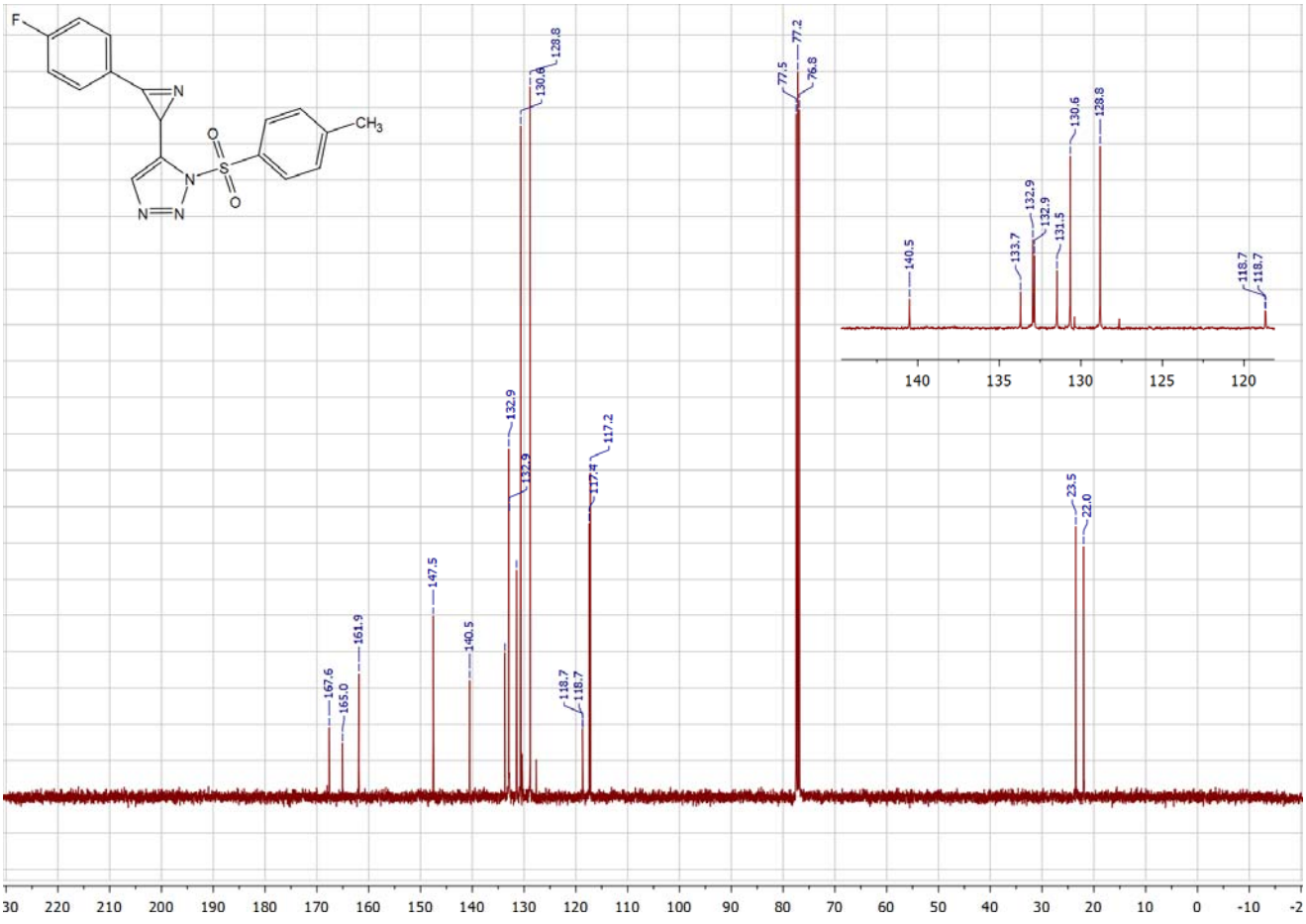
5-(3-Phenyl-2H-azirin-2-yl)-1-tosyl-1H-1,2,3-triazole (**4a**), ^{13}C DEPT 135 NMR (100 MHz, $CDCl_3$)



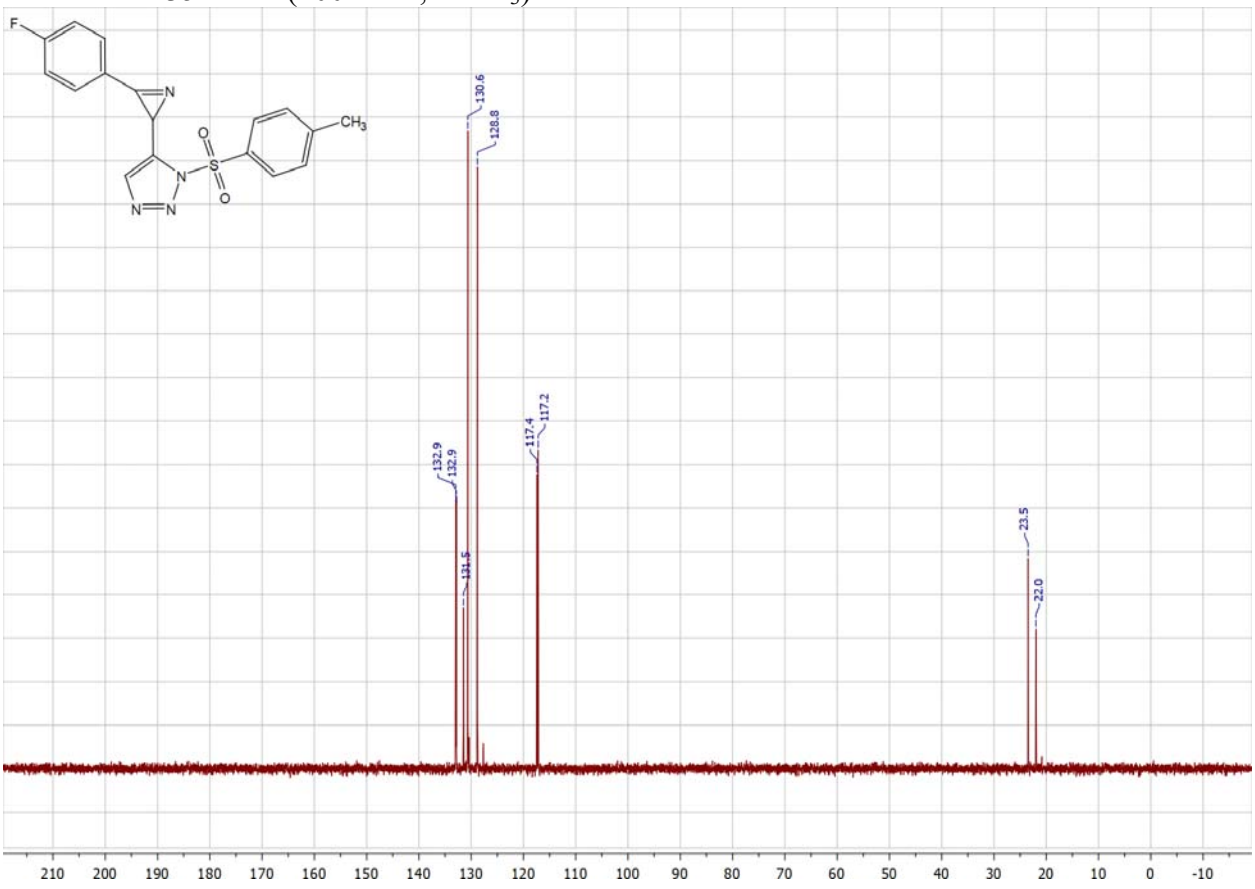
5-(3-(4-Fluorophenyl)-2H-azirin-2-yl)-1-tosyl-1H-1,2,3-triazole (**4b**), ^{1}H NMR (400 MHz, $CDCl_3$)



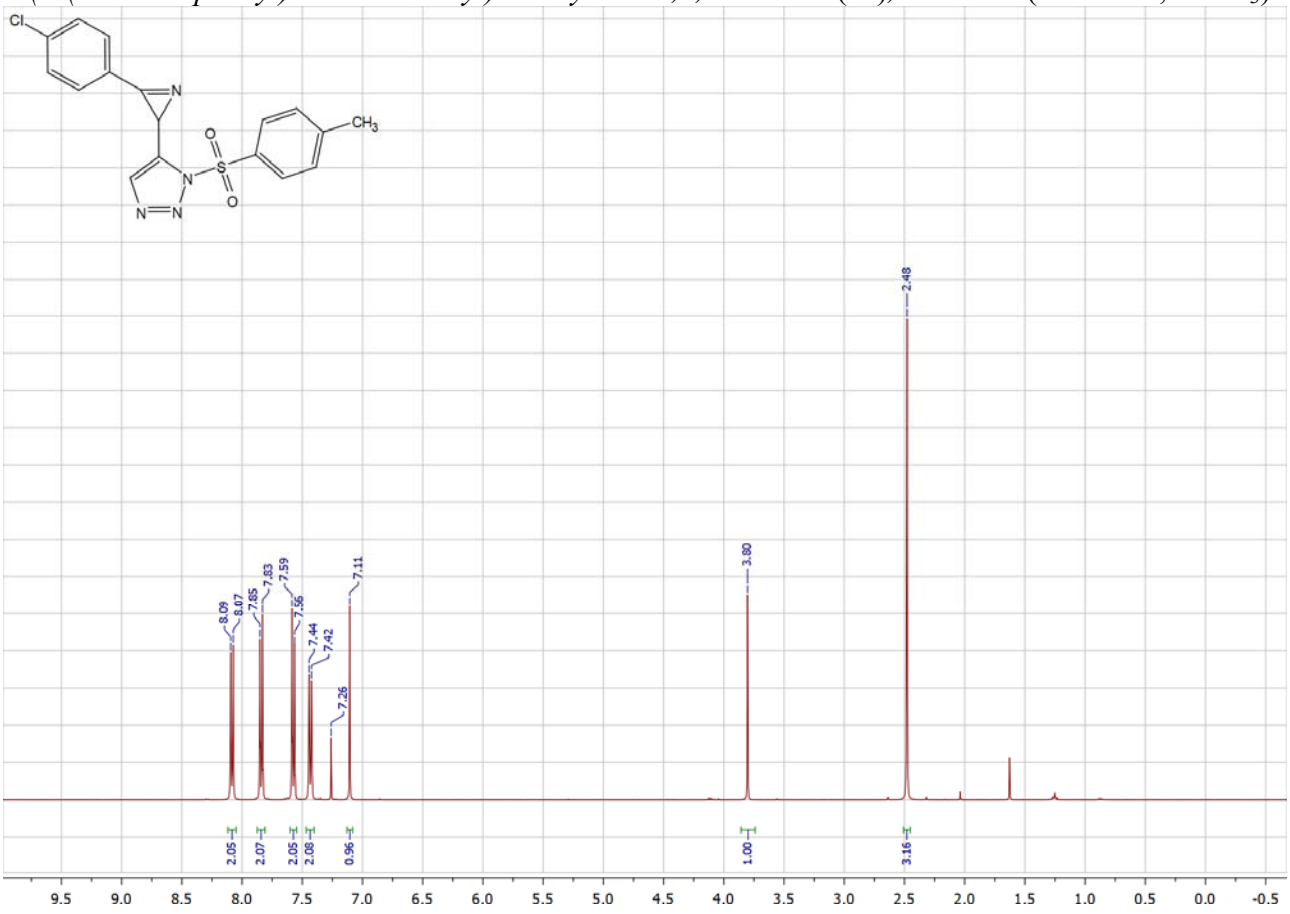
5-(3-(4-Fluorophenyl)-2H-azirin-2-yl)-1-tosyl-1H-1,2,3-triazole (**4b**), $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



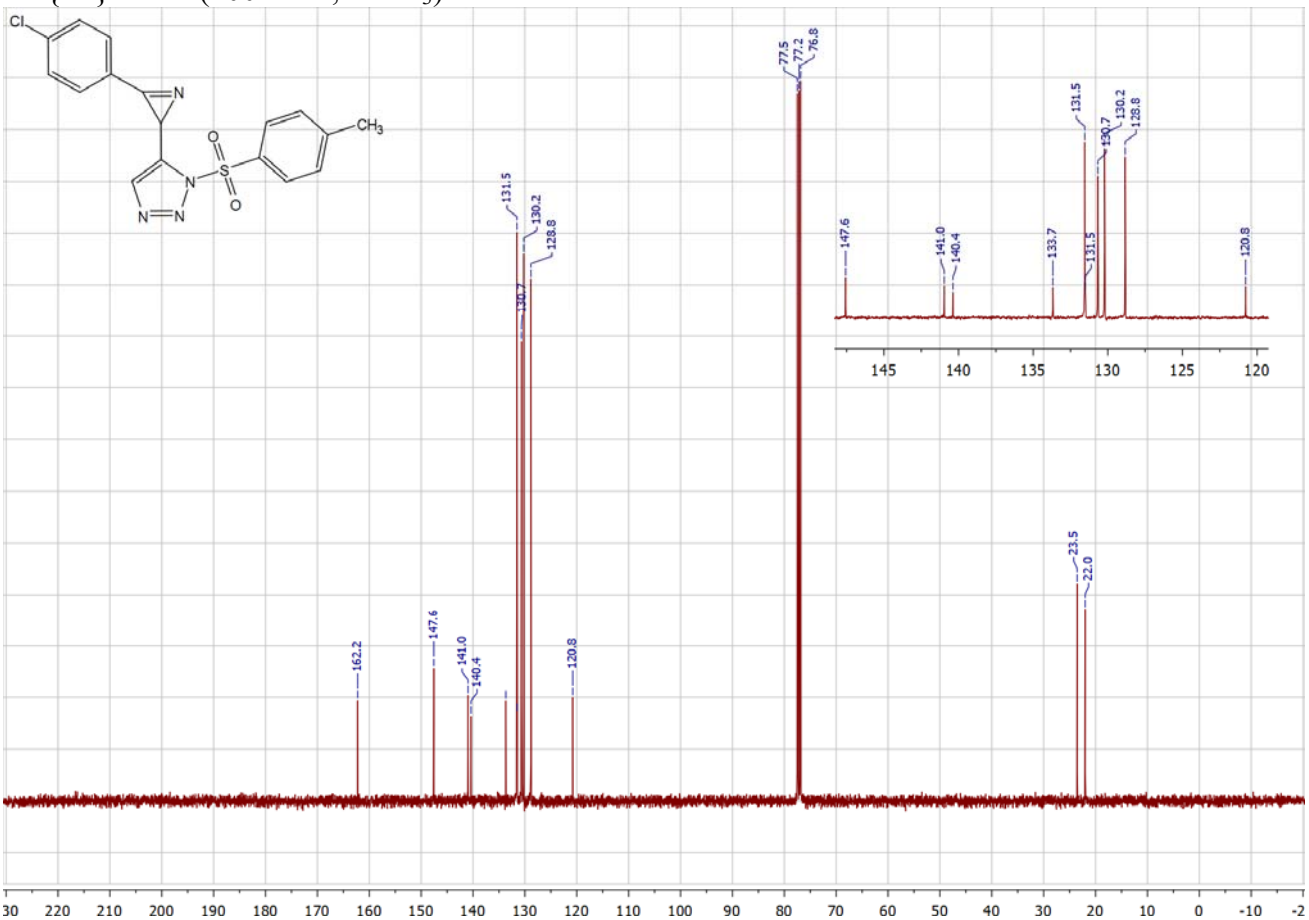
5-(3-(4-Fluorophenyl)-2H-azirin-2-yl)-1-tosyl-1H-1,2,3-triazole (**4b**),
^{13}C DEPT 135 NMR (100 MHz, $CDCl_3$)



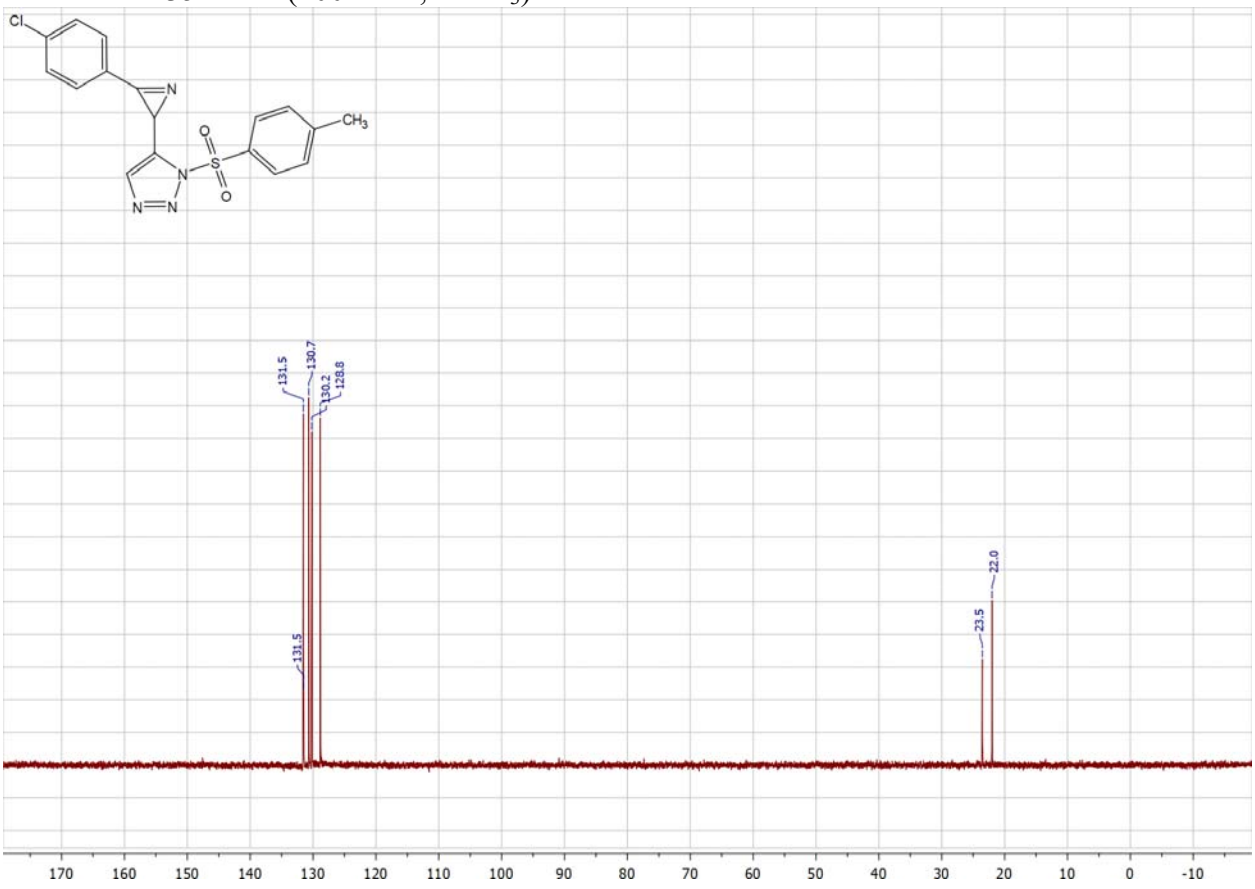
5-(3-(4-Chlorophenyl)-2H-azirin-2-yl)-1-tosyl-1H-1,2,3-triazole (**4c**), ^{1}H NMR (400 MHz, $CDCl_3$)



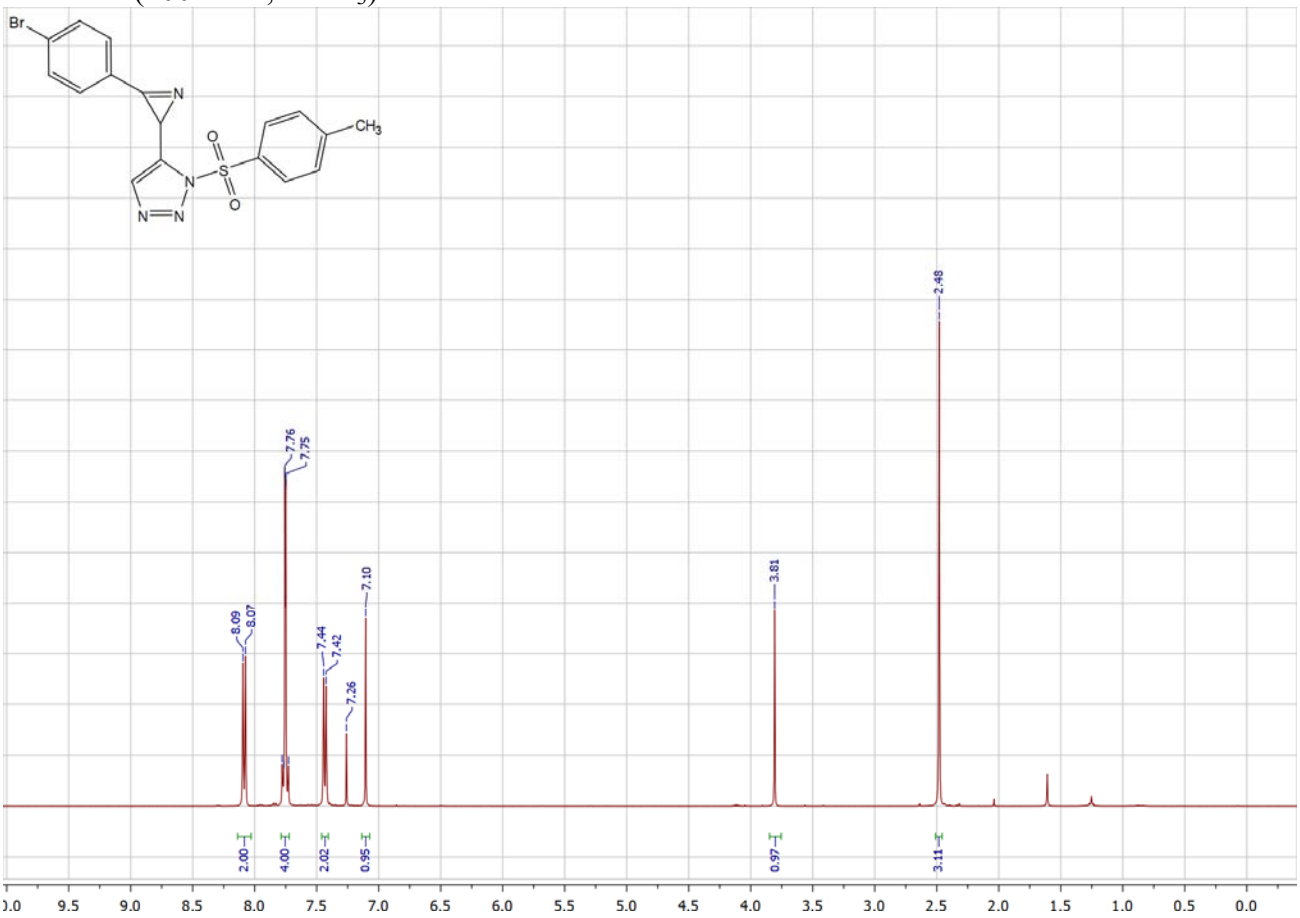
5-(3-(4-Chlorophenyl)-2H-azirin-2-yl)-1-tosyl-1H-1,2,3-triazole (**4c**),
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



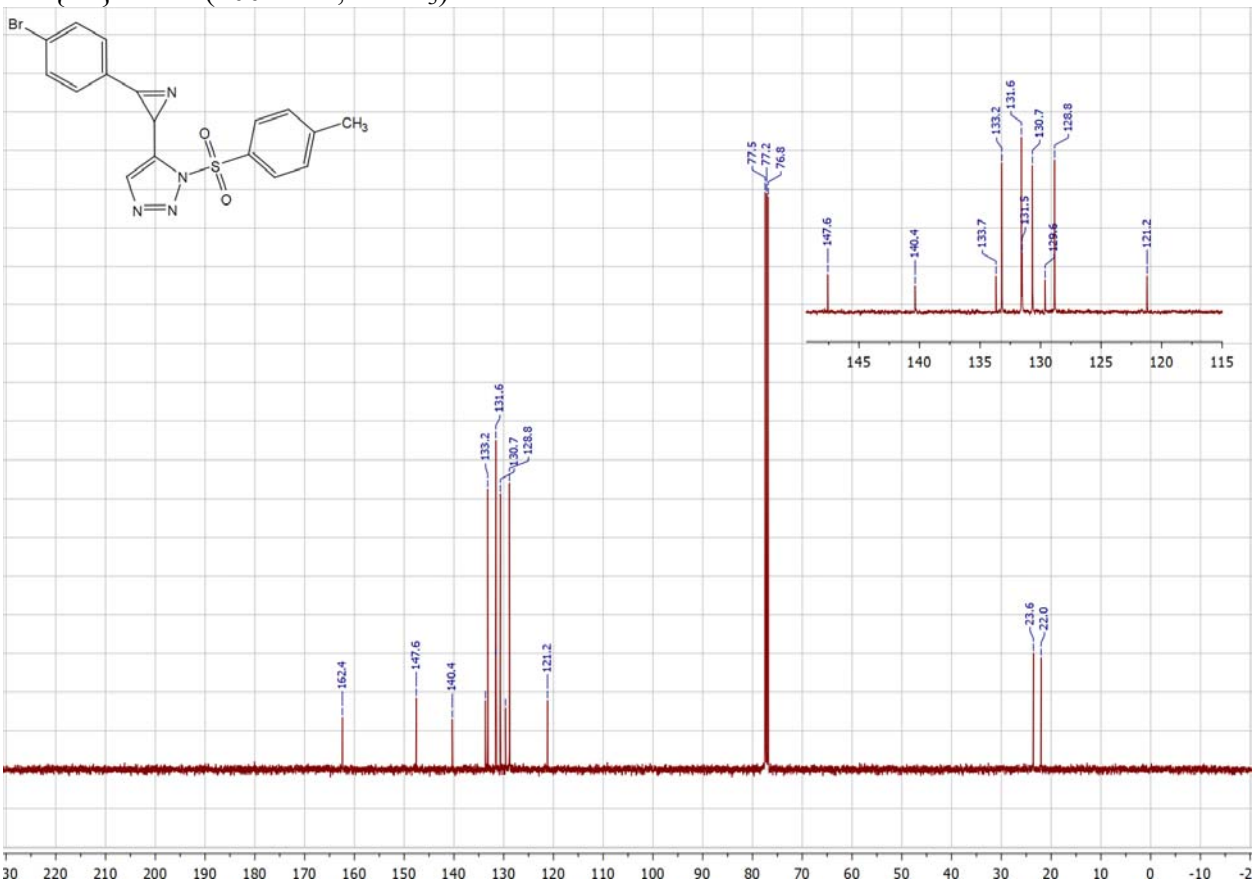
5-(3-(4-Chlorophenyl)-2H-azirin-2-yl)-1-tosyl-1H-1,2,3-triazole (**4c**),
^{13}C DEPT 135 NMR (100 MHz, $CDCl_3$)



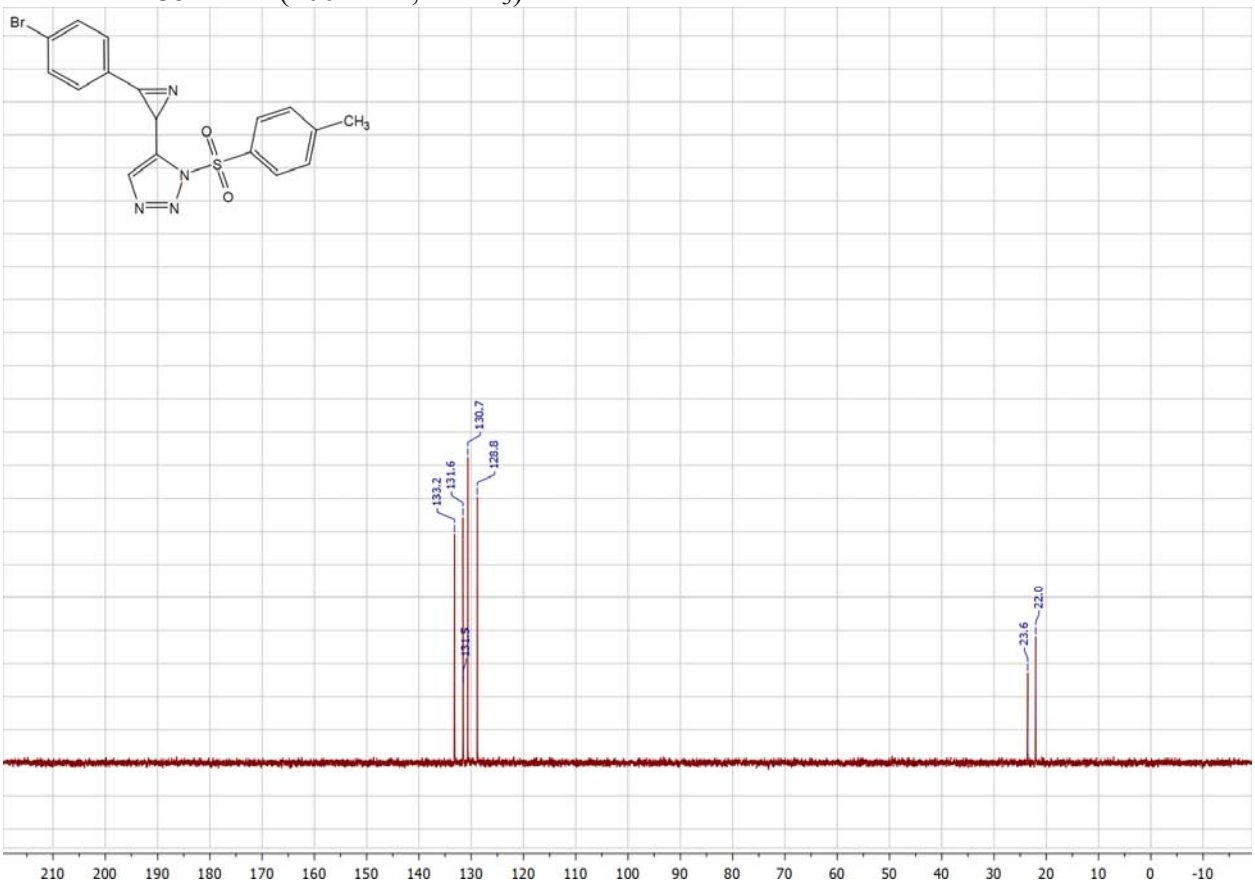
5-(3-(4-Bromophenyl)-2H-azirin-2-yl)-1-tosyl-1H-1,2,3-triazole (**4d**),
^{1}H NMR (400 MHz, $CDCl_3$)



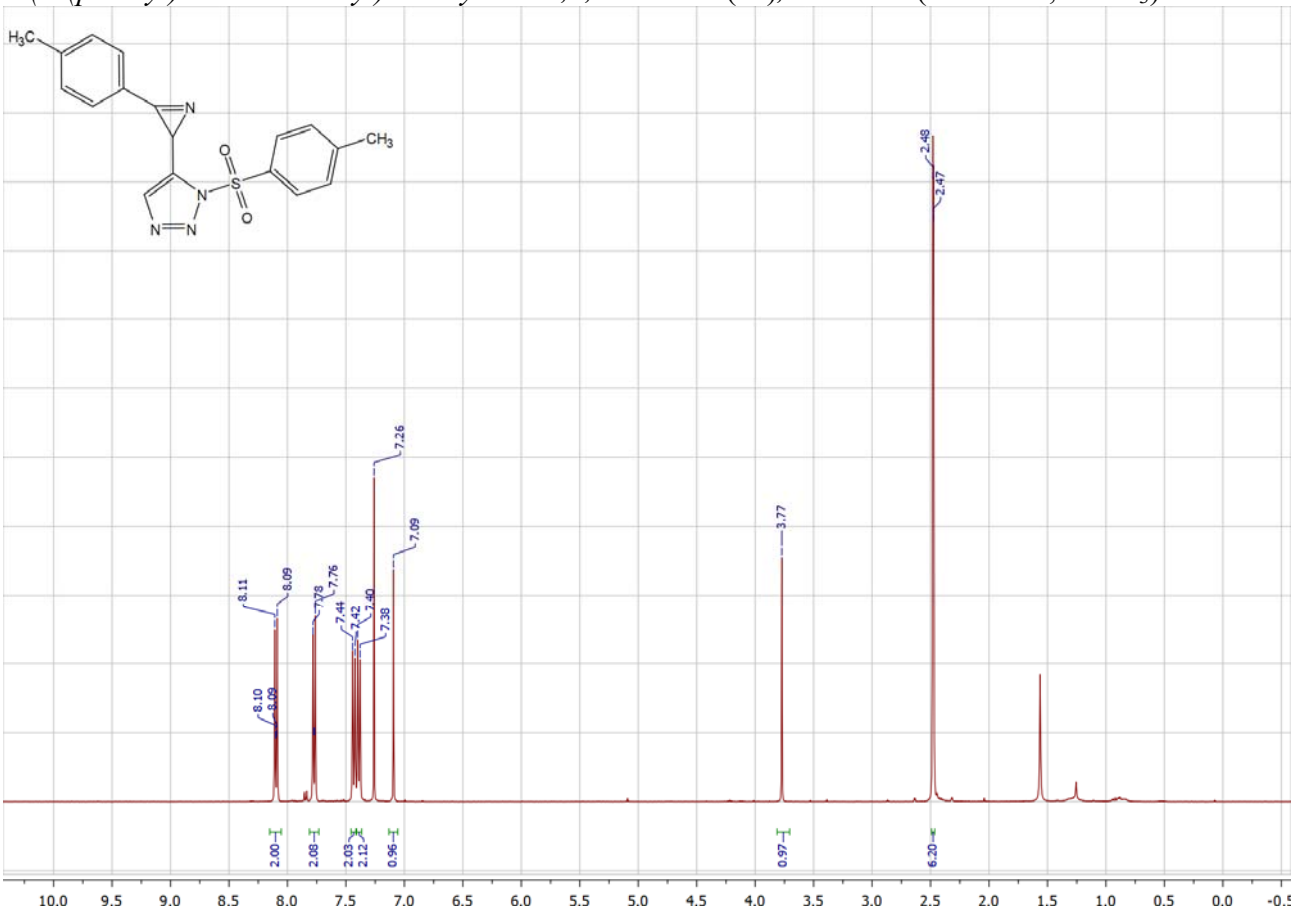
5-(3-(4-Bromophenyl)-2H-azirin-2-yl)-1-tosyl-1H-1,2,3-triazole (**4d**),
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



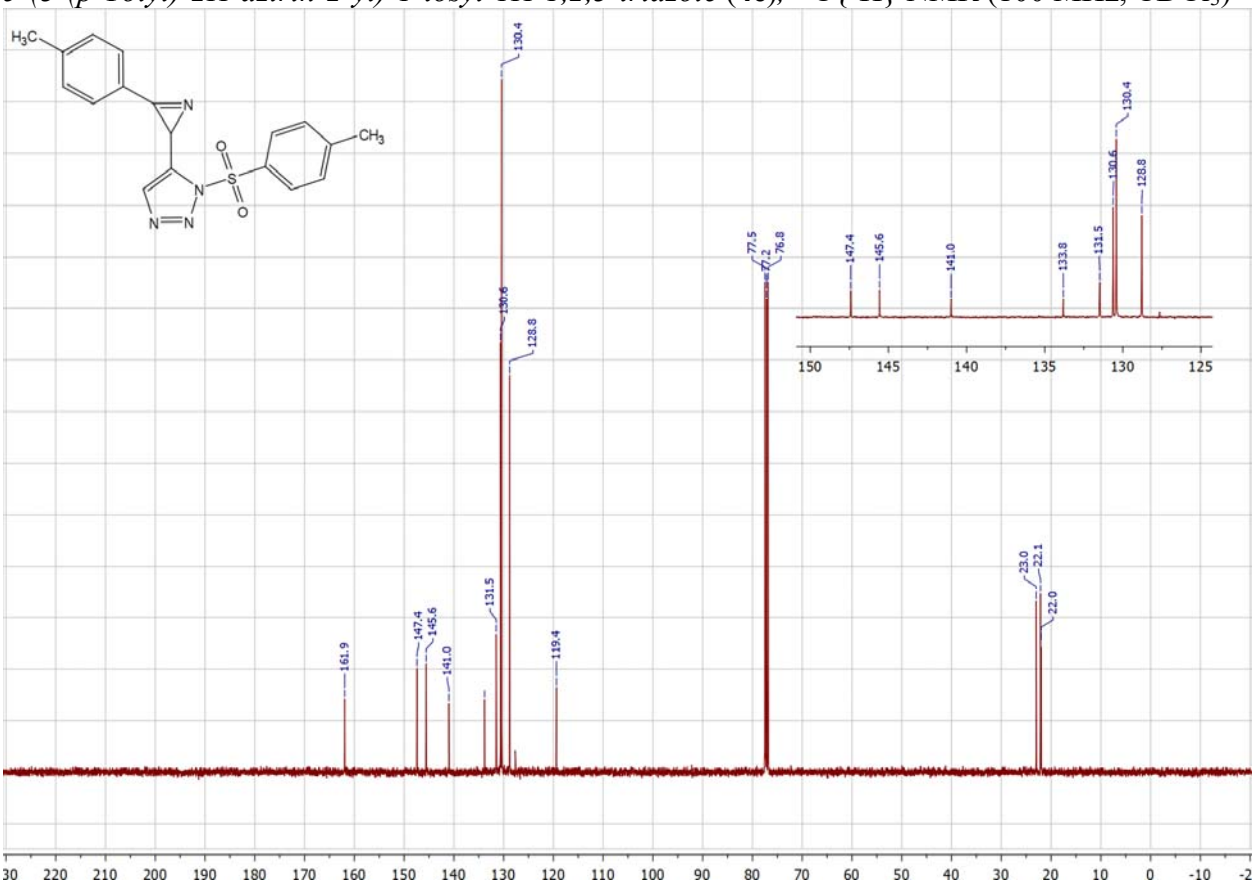
5-(3-(4-Bromophenyl)-2H-azirin-2-yl)-1-tosyl-1H-1,2,3-triazole (**4d**),
^{13}C DEPT 135 NMR (100 MHz, $CDCl_3$)



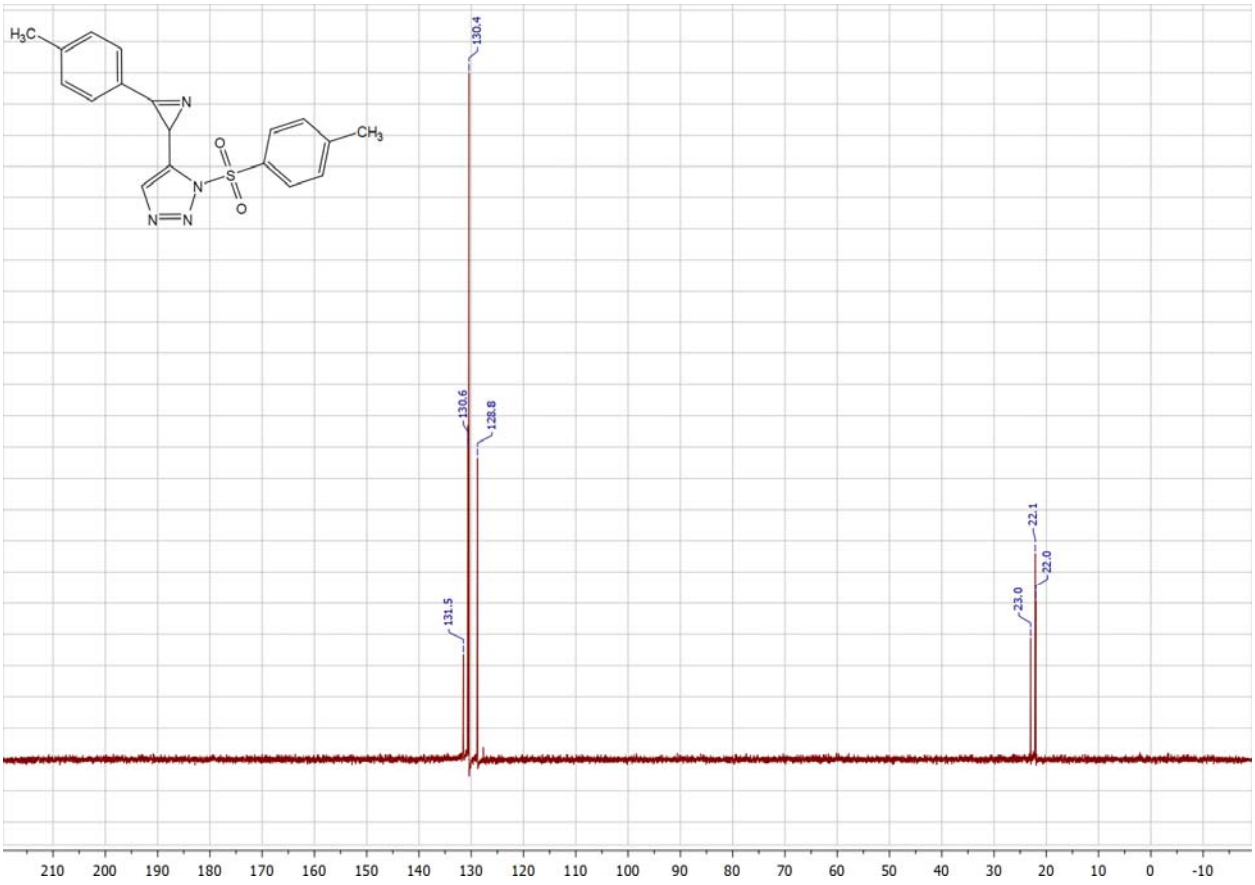
5-(3-(p-Tolyl)-2H-azirin-2-yl)-1-tosyl-1H-1,2,3-triazole (**4e**), ^{1}H NMR (400 MHz, $CDCl_3$)



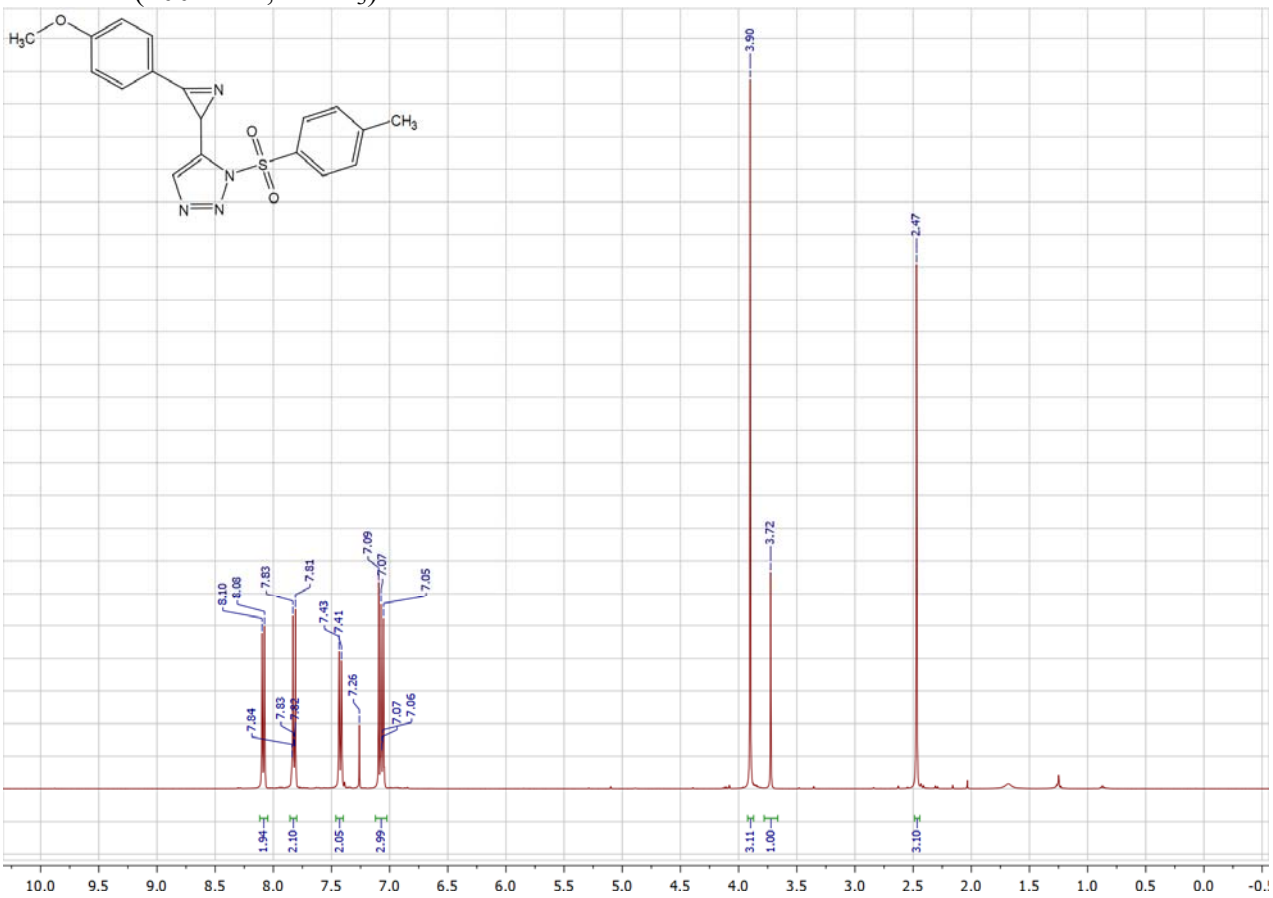
5-(3-(p-Tolyl)-2H-azirin-2-yl)-1-tosyl-1H-1,2,3-triazole (**4e**), ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



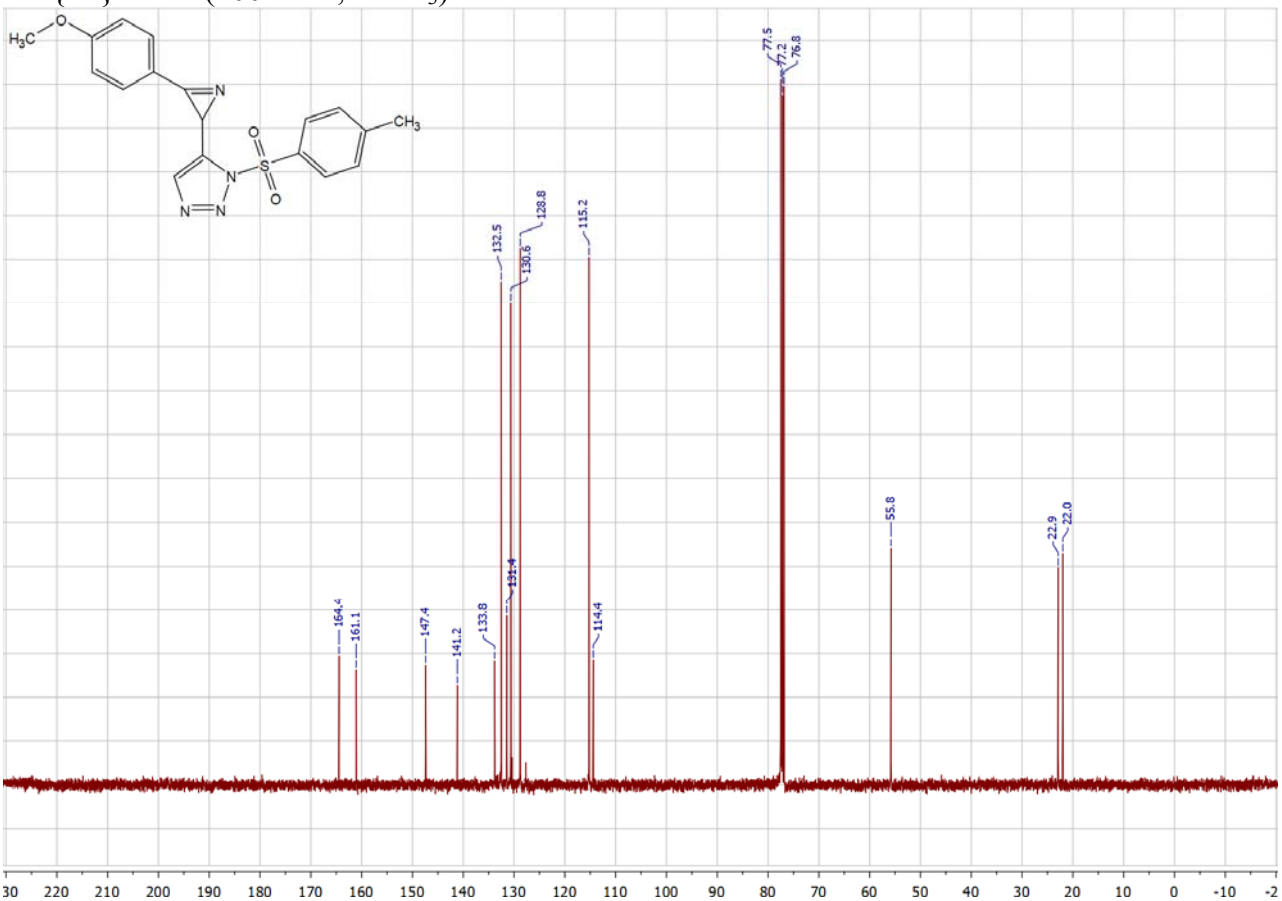
5-(3-(p-Tolyl)-2H-azirin-2-yl)-1-tosyl-1H-1,2,3-triazole (**4e**),
^{13}C DEPT 135 NMR (100 MHz, $CDCl_3$)



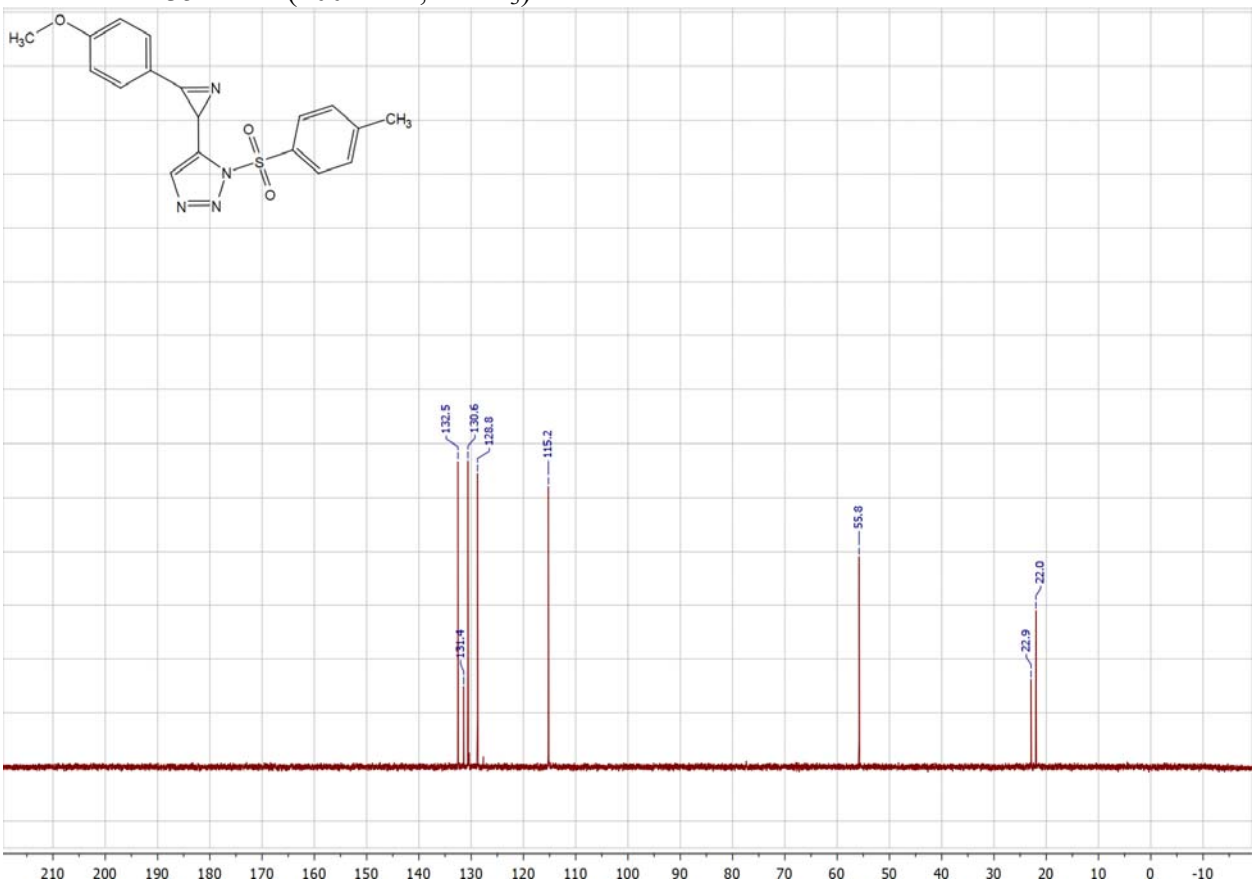
5-(3-(4-Methoxyphenyl)-2H-azirin-2-yl)-1-tosyl-1H-1,2,3-triazole (**4f**),
^{1}H NMR (400 MHz, $CDCl_3$)



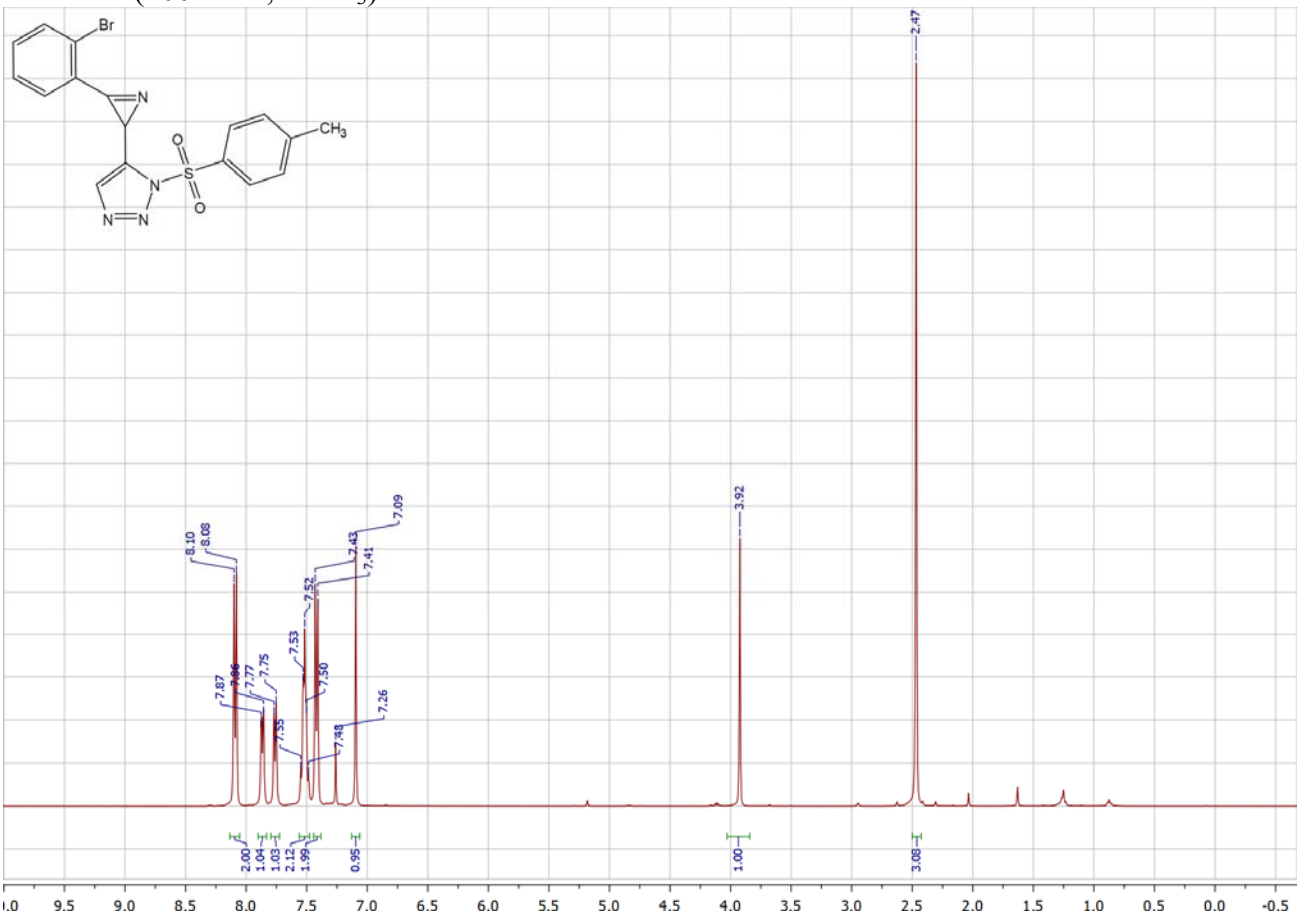
5-(3-(4-Methoxyphenyl)-2H-azirin-2-yl)-1-tosyl-1H-1,2,3-triazole (**4f**),
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



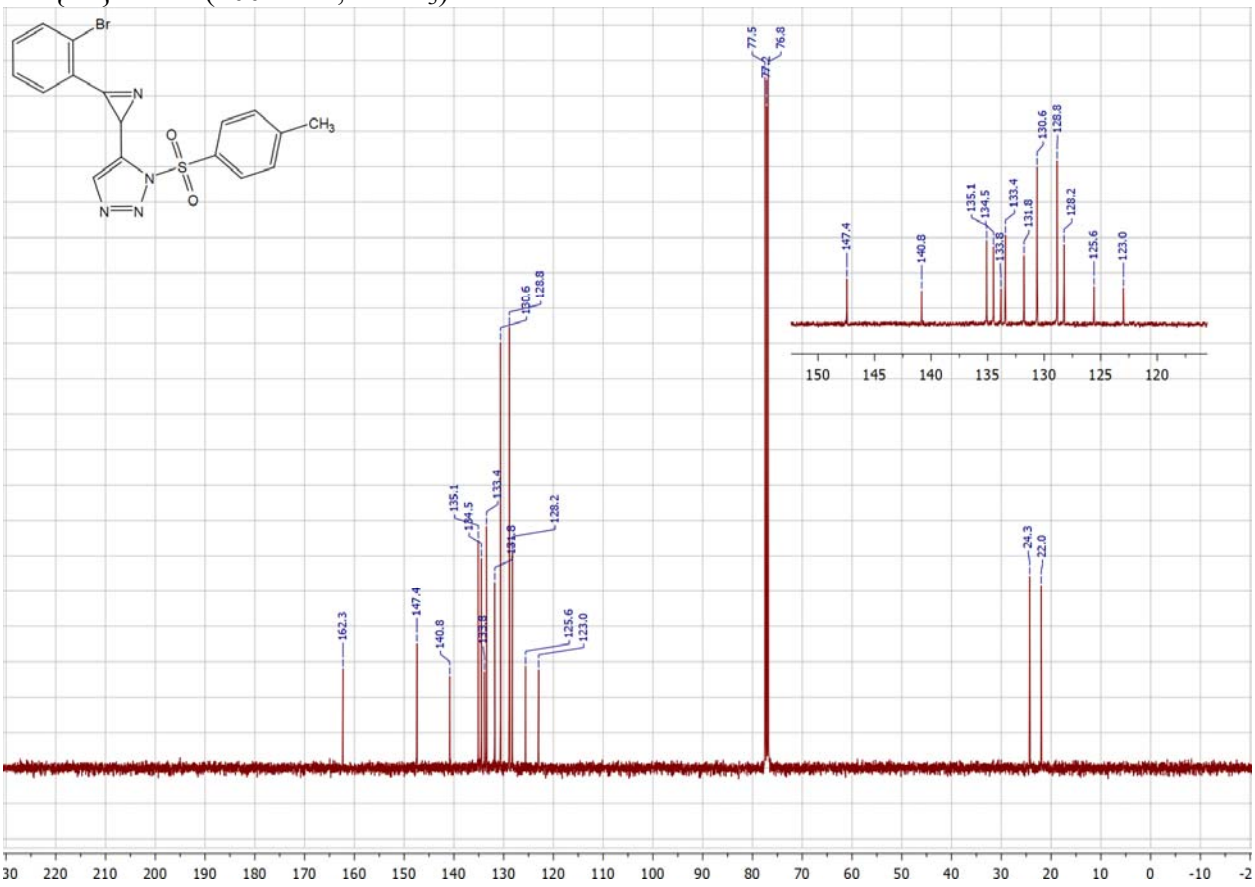
5-(3-(4-Methoxyphenyl)-2H-azirin-2-yl)-1-tosyl-1H-1,2,3-triazole (**4f**),
^{13}C DEPT 135 NMR (100 MHz, $CDCl_3$)



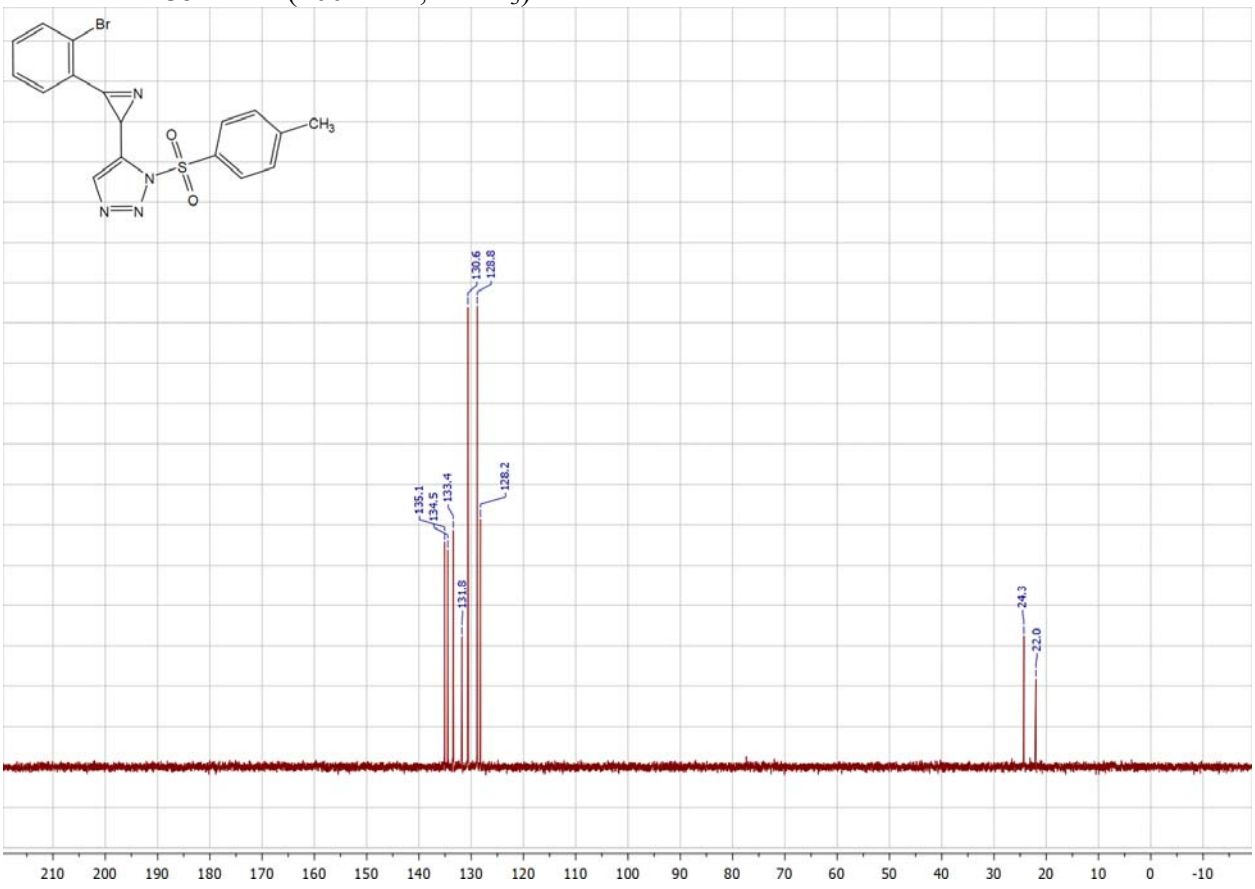
5-(3-(2-Bromophenyl)-2H-azirin-2-yl)-1-tosyl-1H-1,2,3-triazole (**4g**),
^{1}H NMR (400 MHz, $CDCl_3$)



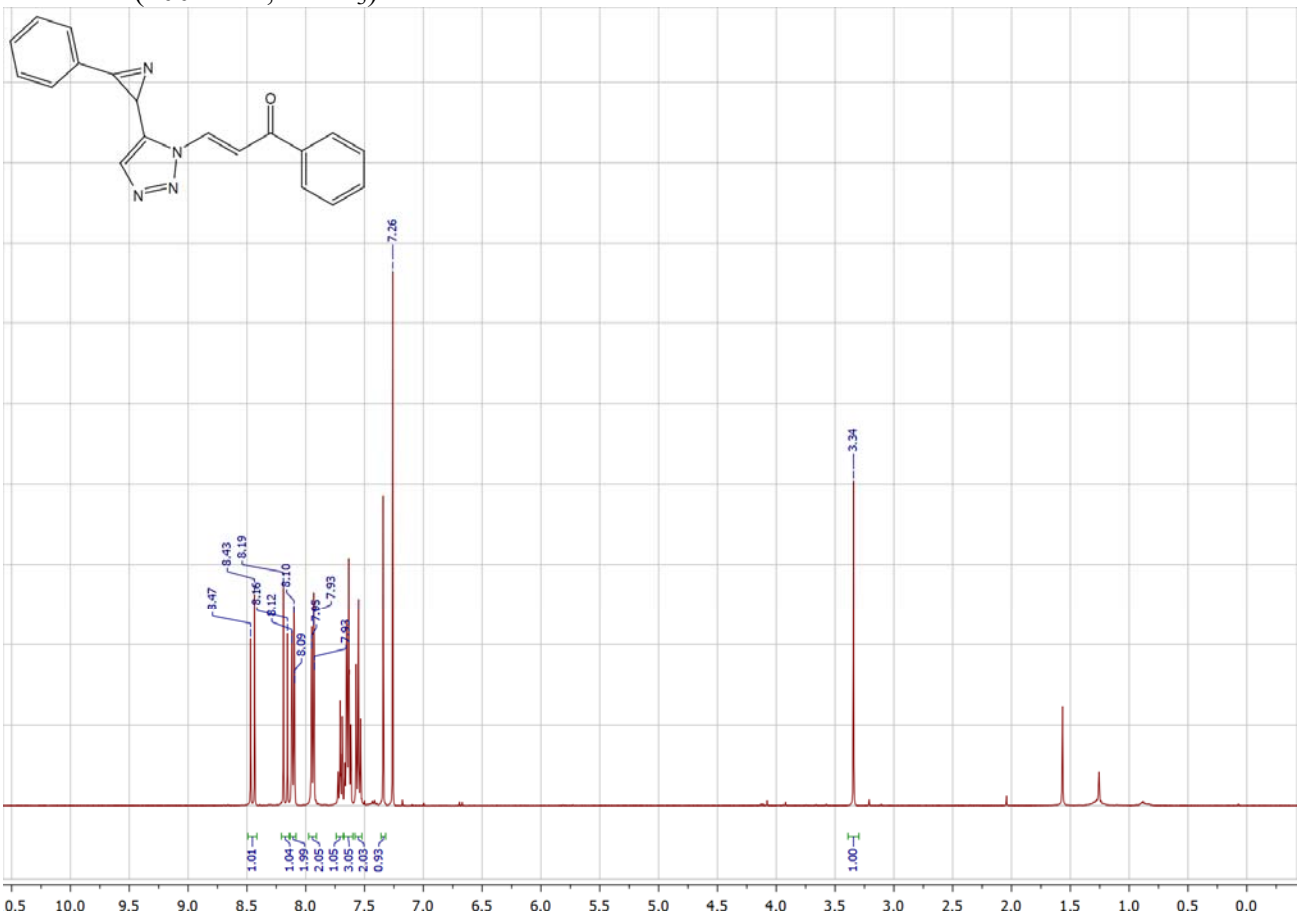
5-(3-(2-Bromophenyl)-2H-azirin-2-yl)-1-tosyl-1H-1,2,3-triazole (**4g**),
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



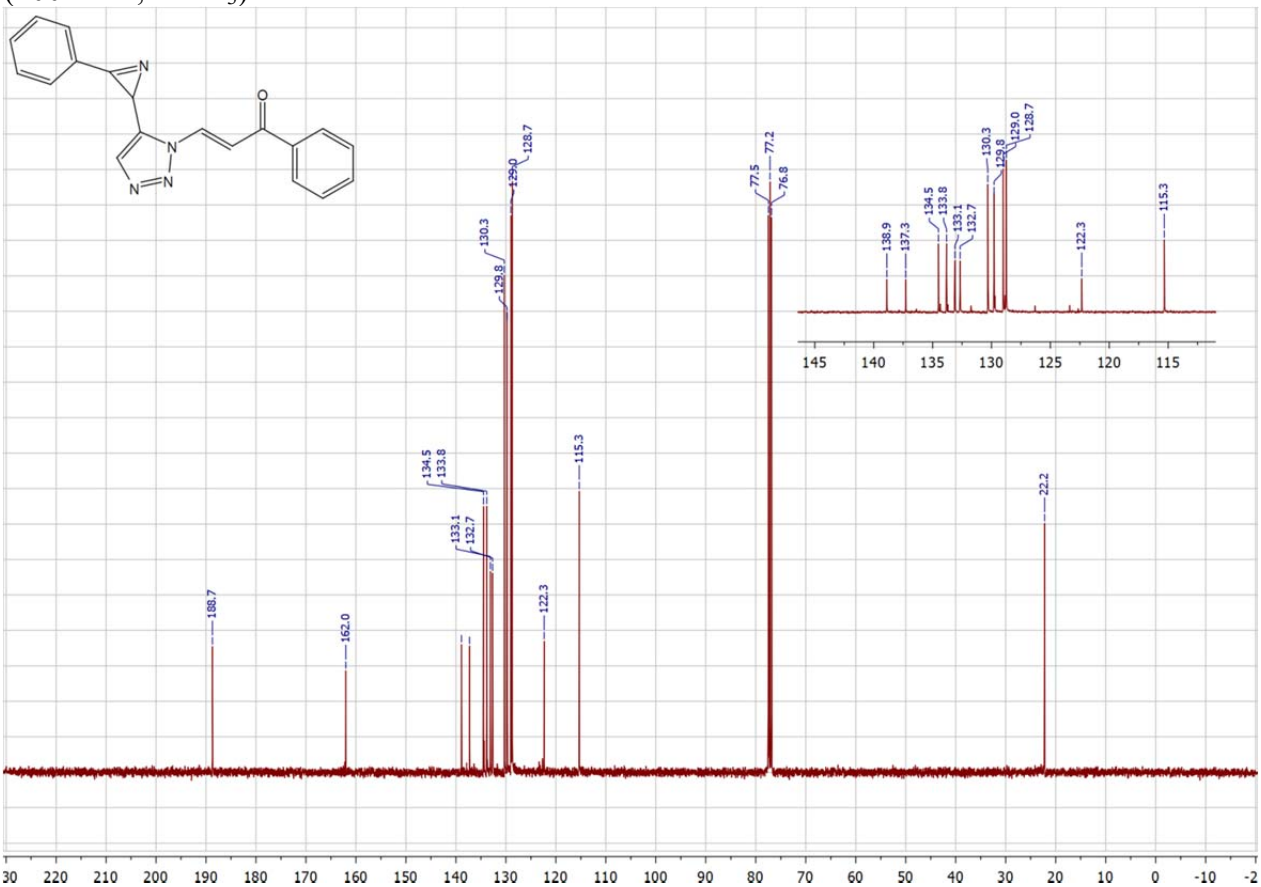
5-(3-(2-Bromophenyl)-2H-azirin-2-yl)-1-tosyl-1H-1,2,3-triazole (**4g**),
^{13}C DEPT 135 NMR (100 MHz, $CDCl_3$)



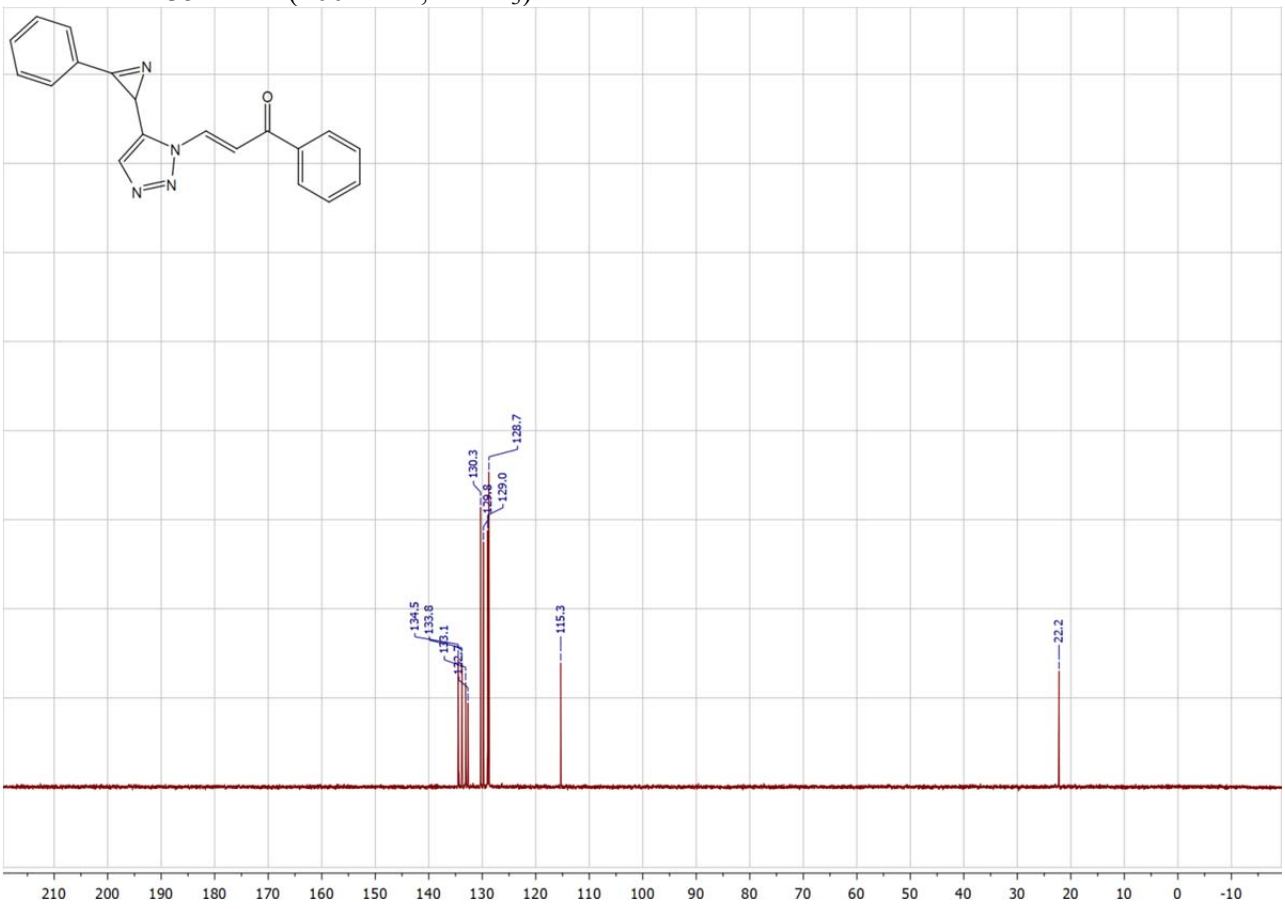
(E)-1-phenyl-3-(5-(3-phenyl-2H-azirin-2-yl)-1H-1,2,3-triazol-1-yl)prop-2-en-1-one (**4h**), ^{1}H NMR (400 MHz, $CDCl_3$)



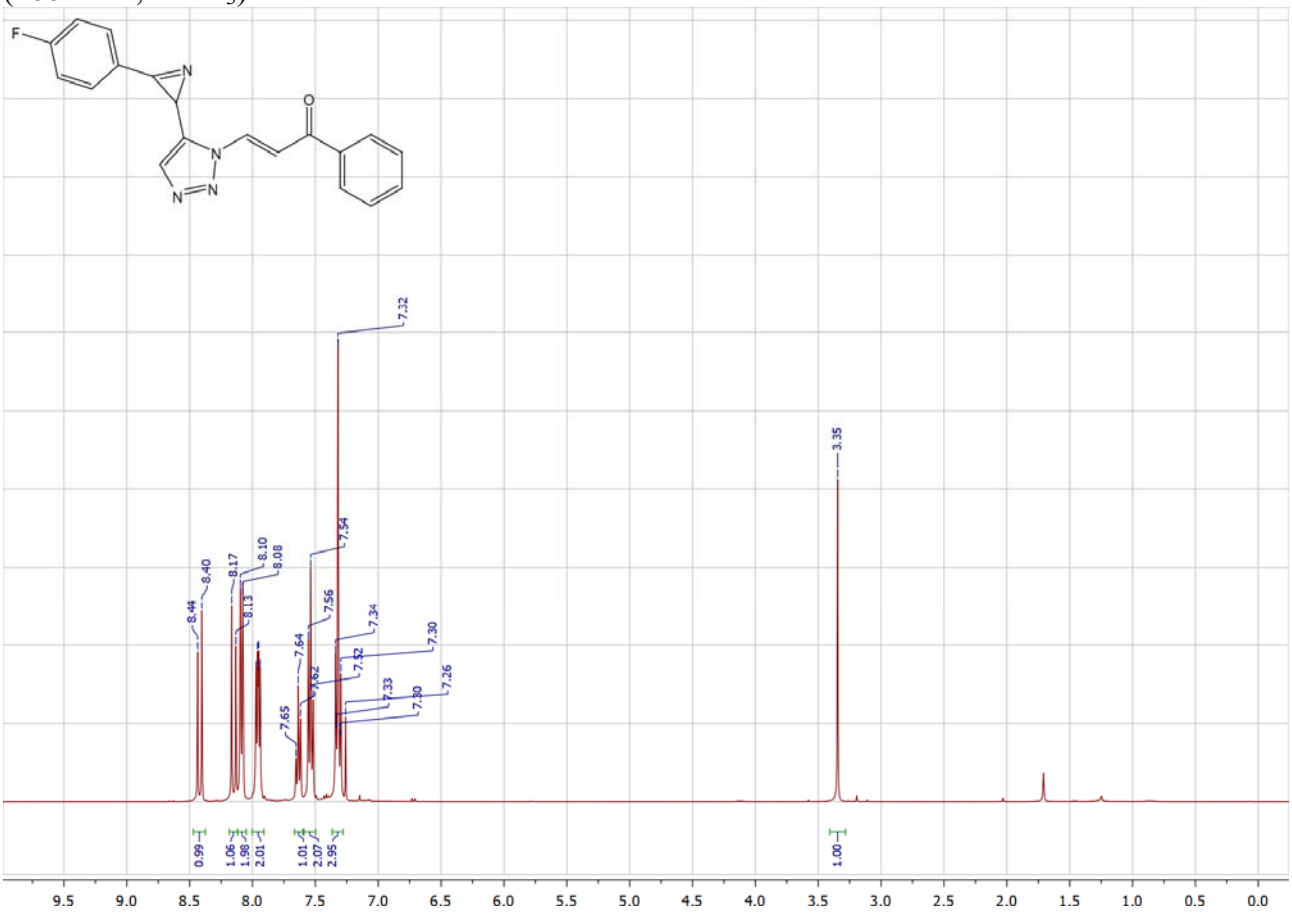
(E)-1-phenyl-3-(5-(3-phenyl-2H-azirin-2-yl)-1H-1,2,3-triazol-1-yl)prop-2-en-1-one (**4h**), $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



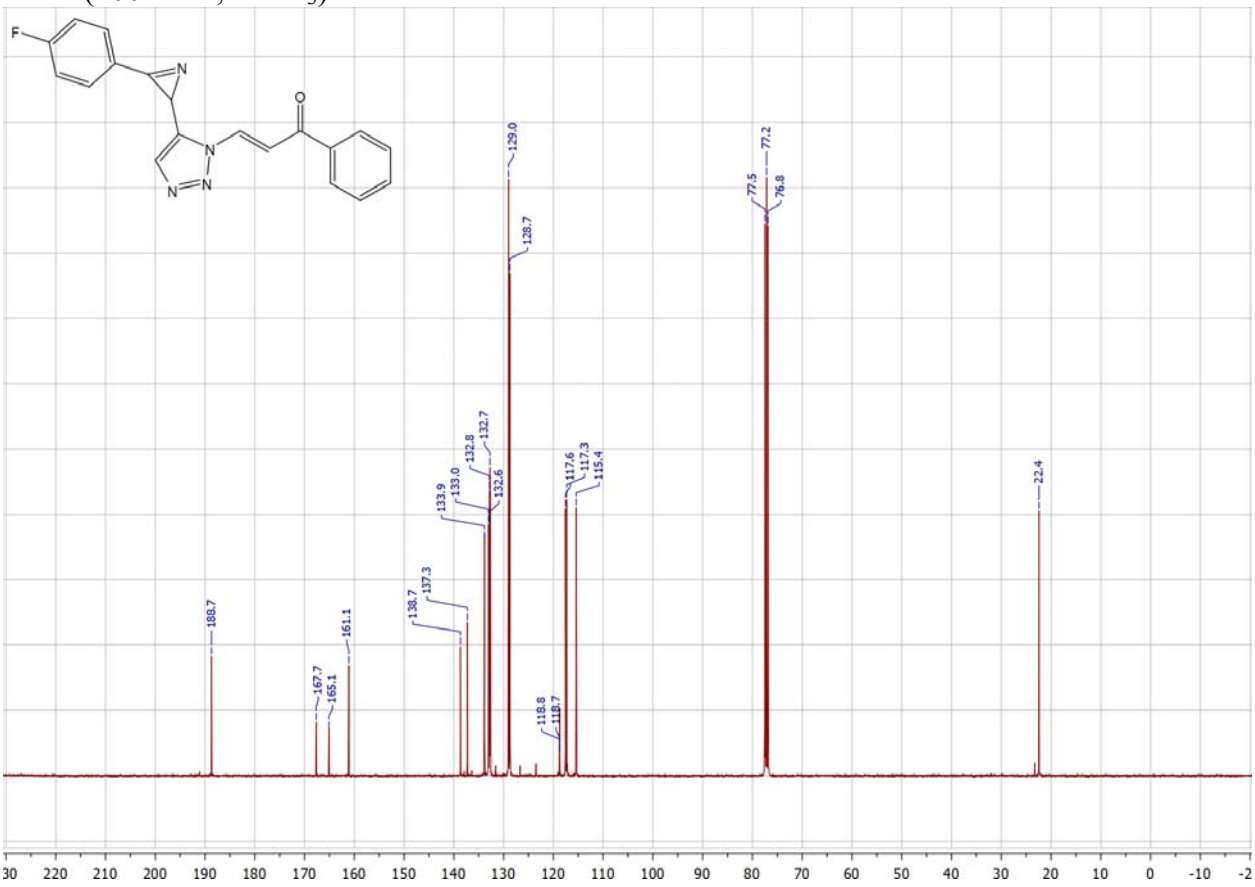
(E)-1-phenyl-3-(5-(3-phenyl-2H-azirin-2-yl)-1H-1,2,3-triazol-1-yl)prop-2-en-1-one (**4h**),
^{13}C DEPT 135 NMR (100 MHz, $CDCl_3$)



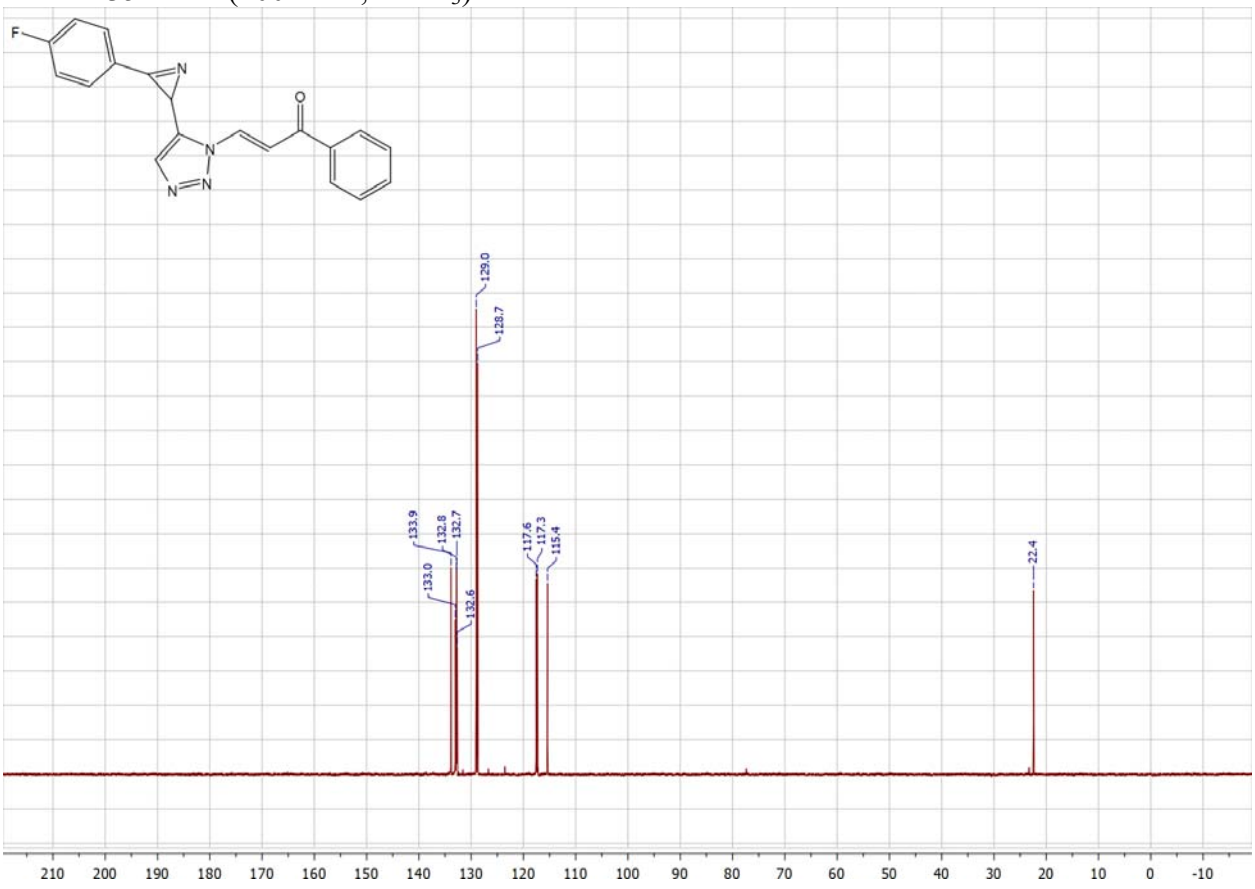
(E)-3-(5-(3-(4-Fluorophenyl)-2H-azirin-2-yl)-1H-1,2,3-triazol-1-yl)-1-phenylprop-2-en-1-one (**4i**), ^{1}H NMR (400 MHz, $CDCl_3$)



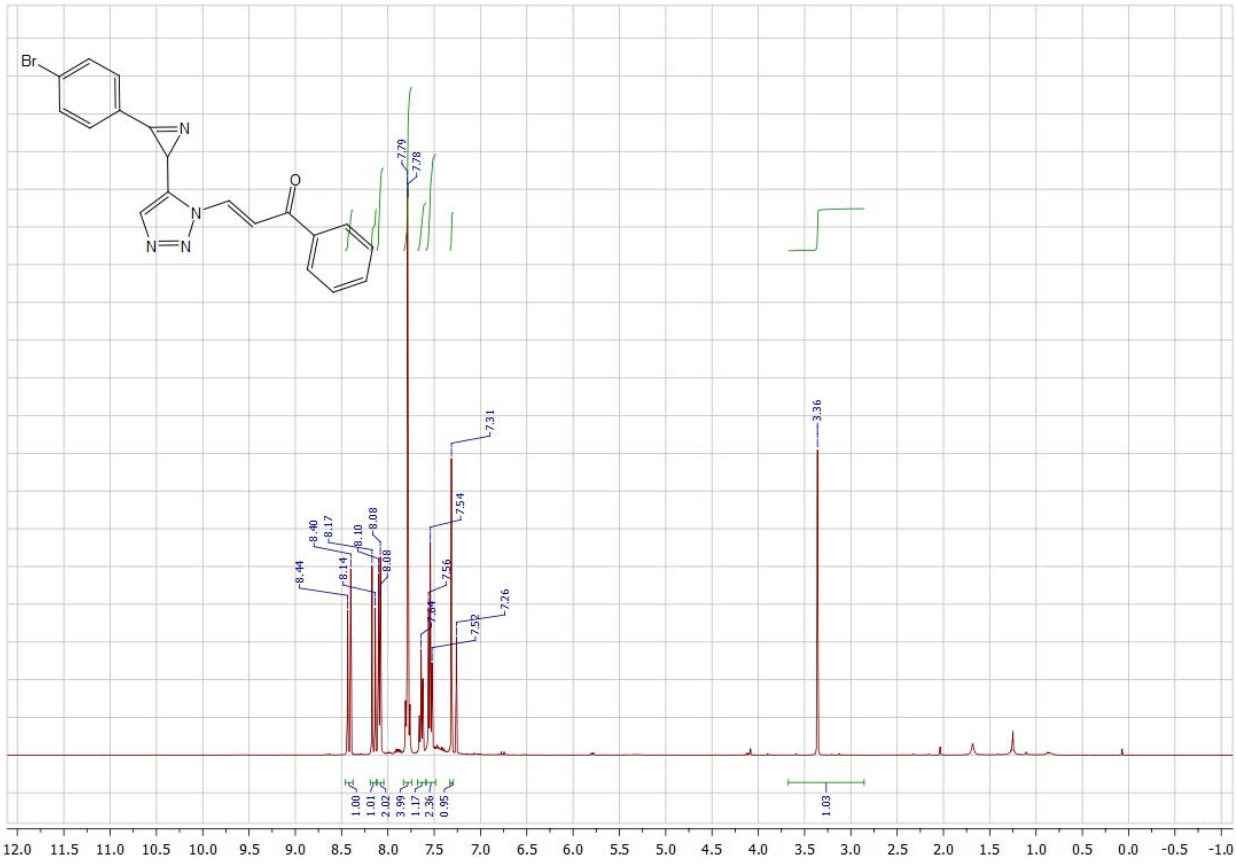
(E)-3-(5-(3-(4-Fluorophenyl)-2H-azirin-2-yl)-1H-1,2,3-triazol-1-yl)-1-phenylprop-2-en-1-one (**4i**), ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



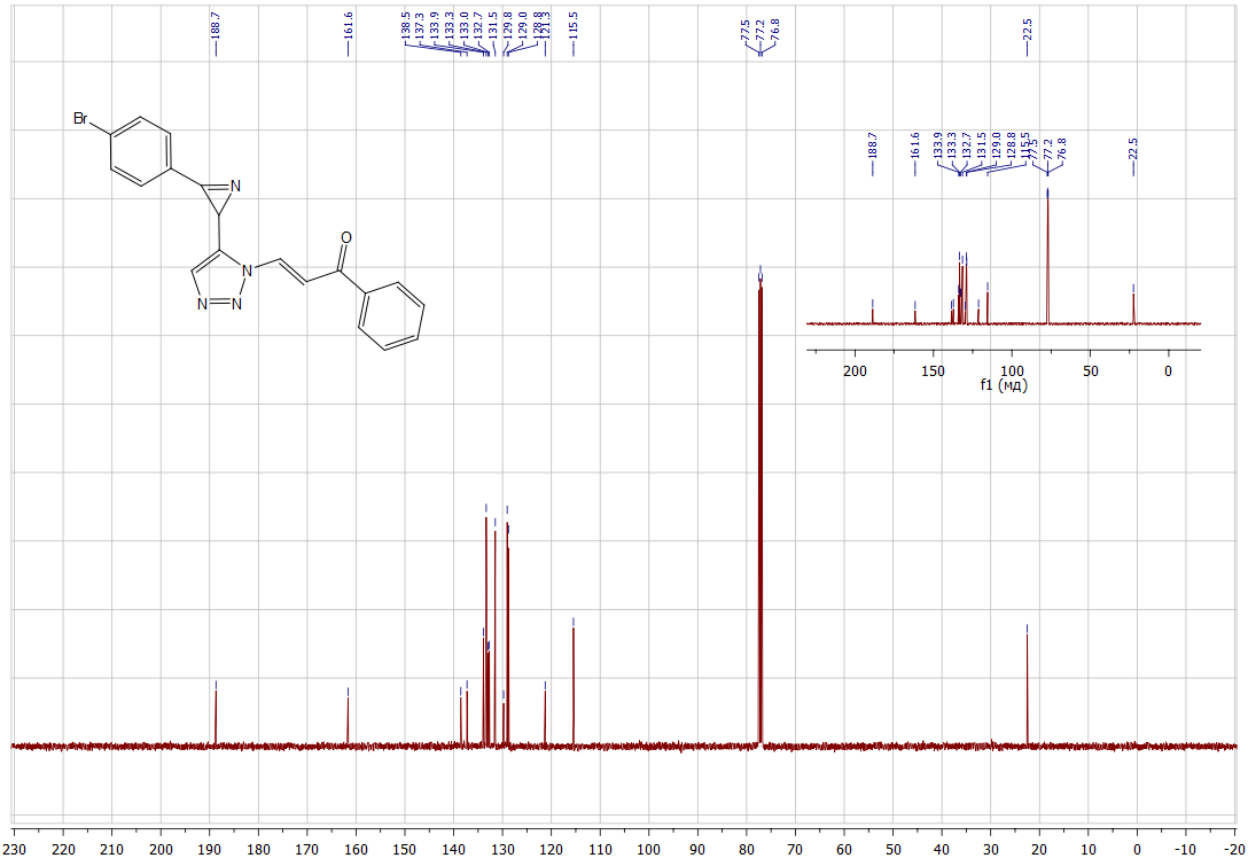
(E)-3-(5-(3-(4-Fluorophenyl)-2H-azirin-2-yl)-1H-1,2,3-triazol-1-yl)-1-phenylprop-2-en-1-one (**4i**), ^{13}C DEPT 135 NMR (100 MHz, $CDCl_3$)



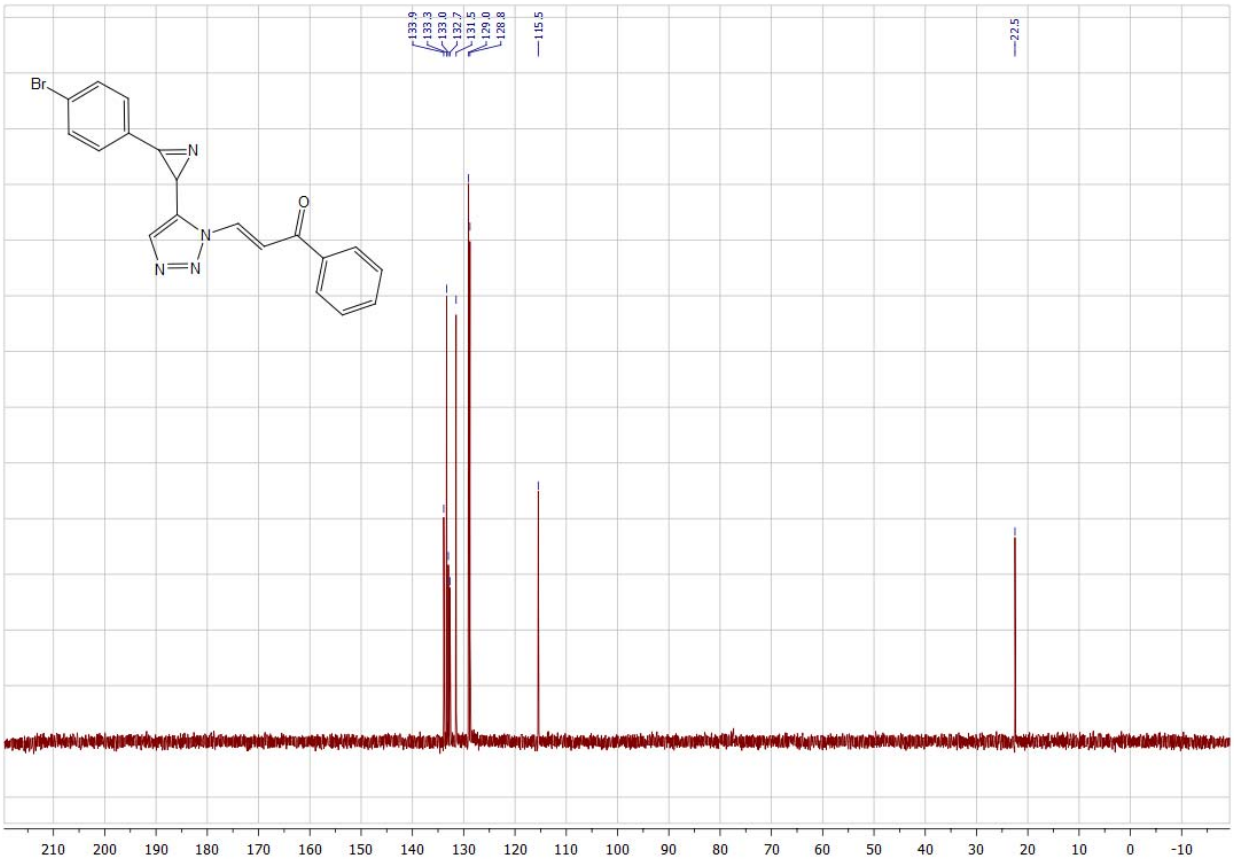
(E)-3-(5-(3-(4-Bromophenyl)-2H-azirin-2-yl)-1H-1,2,3-triazol-1-yl)-1-phenylprop-2-en-1-one (**4j**), ^{1}H NMR (400 MHz, $CDCl_3$)



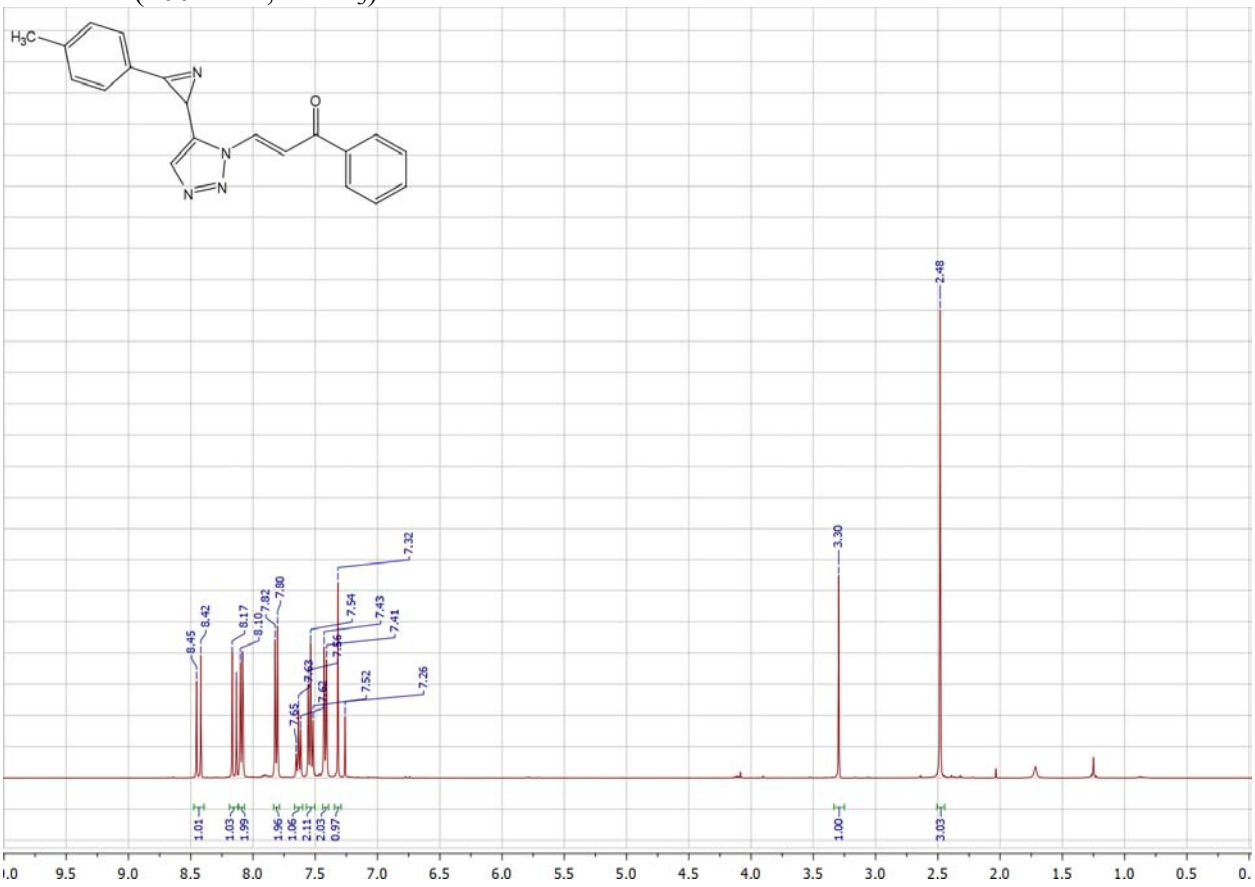
(E)-3-(5-(3-(4-Bromophenyl)-2H-azirin-2-yl)-1H-1,2,3-triazol-1-yl)-1-phenylprop-2-en-1-one (**4j**), $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



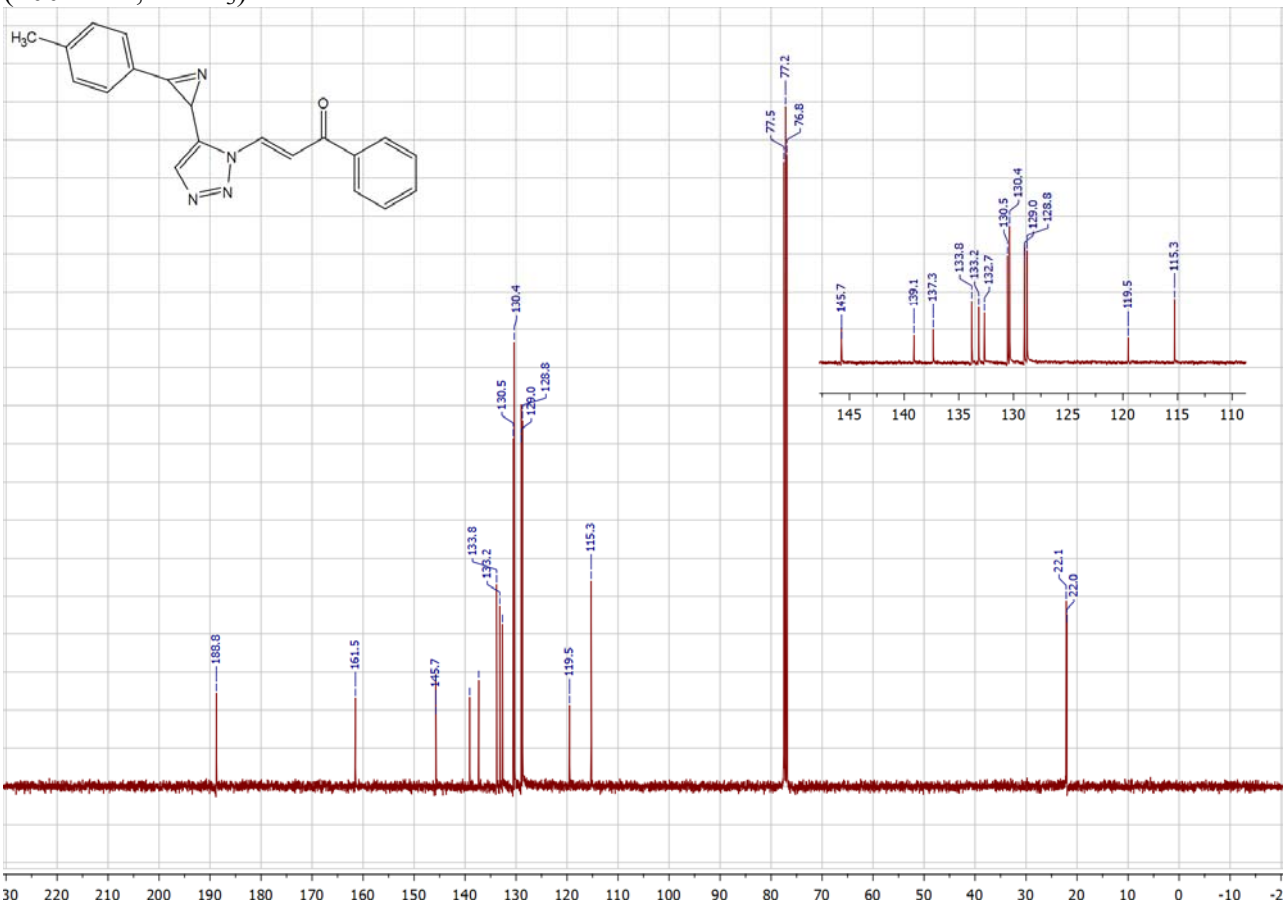
(E)-3-(5-(3-(4-Bromophenyl)-2H-azirin-2-yl)-1H-1,2,3-triazol-1-yl)-1-phenylprop-2-en-1-one (**4j**), ^{13}C DEPT 135 NMR (100 MHz, $CDCl_3$)



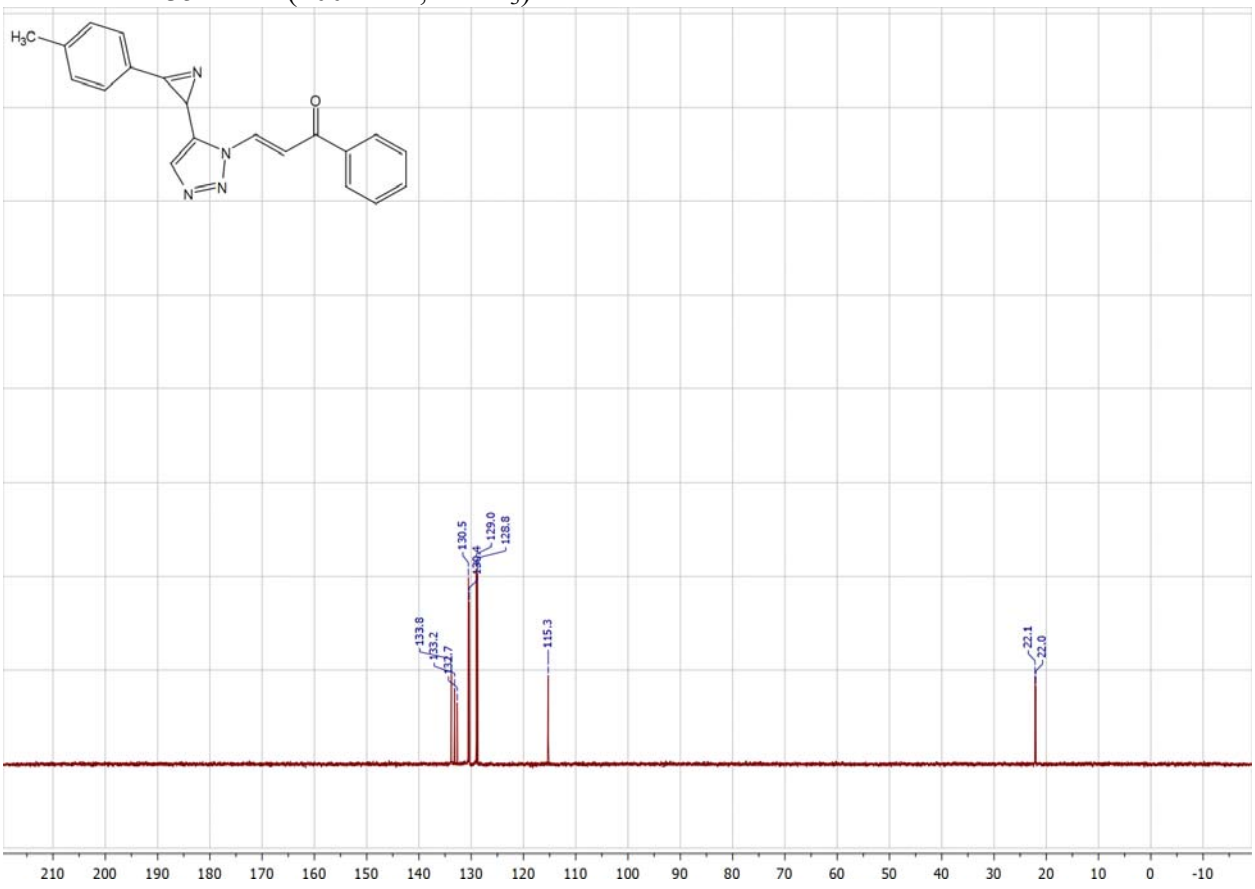
(E)-1-Phenyl-3-(5-(3-(p-tolyl)-2H-azirin-2-yl)-1H-1,2,3-triazol-1-yl)prop-2-en-1-one (**4k**), ^{1}H NMR (400 MHz, $CDCl_3$)



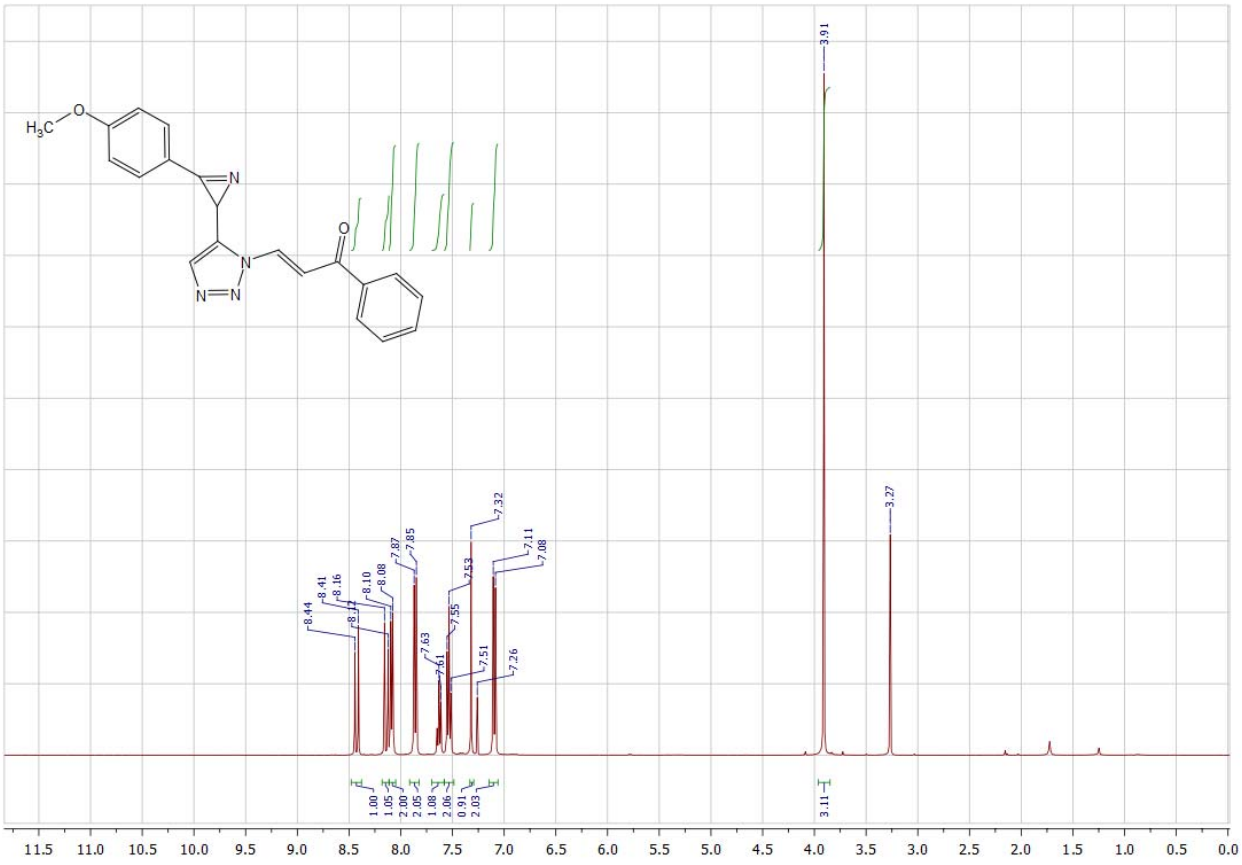
(E)-1-Phenyl-3-(5-(3-(p-tolyl)-2H-azirin-2-yl)-1H-1,2,3-triazol-1-yl)prop-2-en-1-one (**4k**), $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



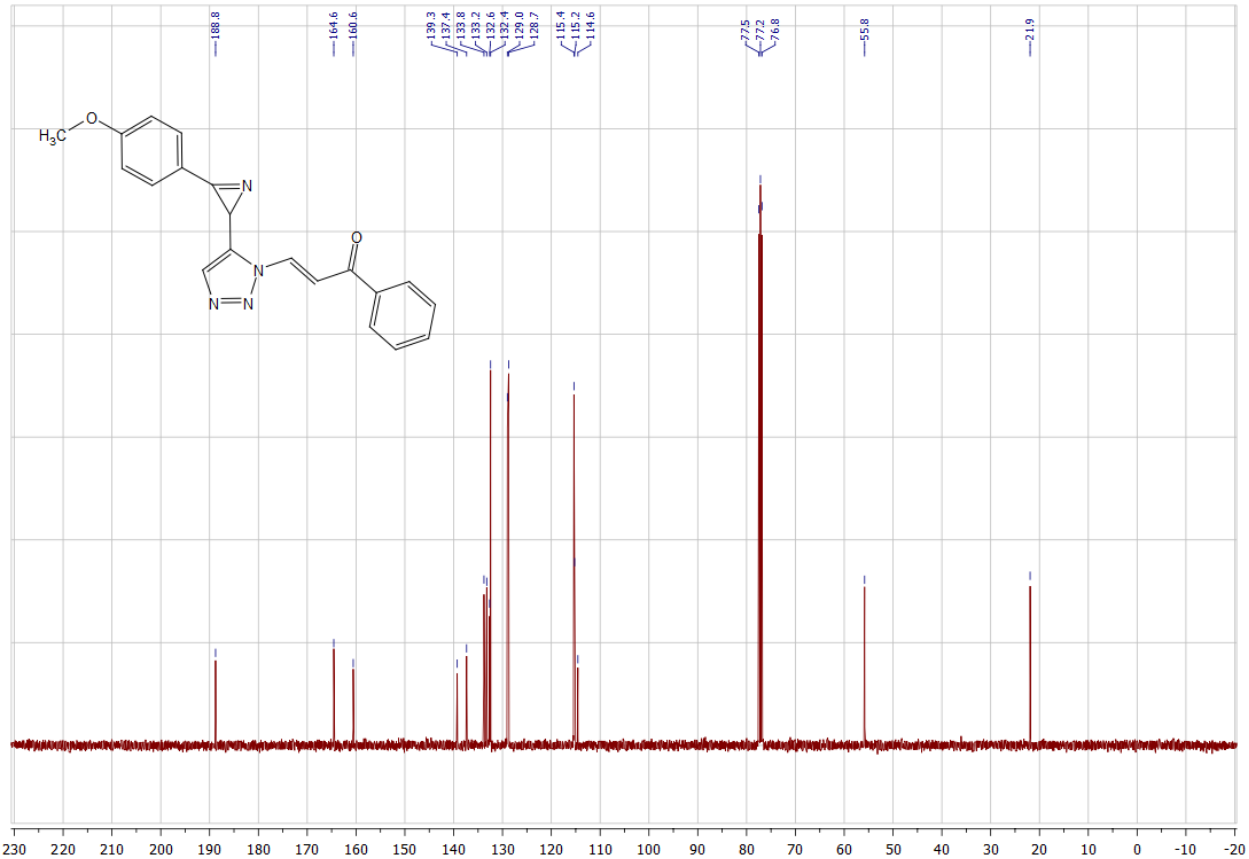
(E)-1-Phenyl-3-(5-(3-(p-tolyl)-2H-azirin-2-yl)-1H-1,2,3-triazol-1-yl)prop-2-en-1-one (**4k**),
^{13}C DEPT 135 NMR (100 MHz, $CDCl_3$)



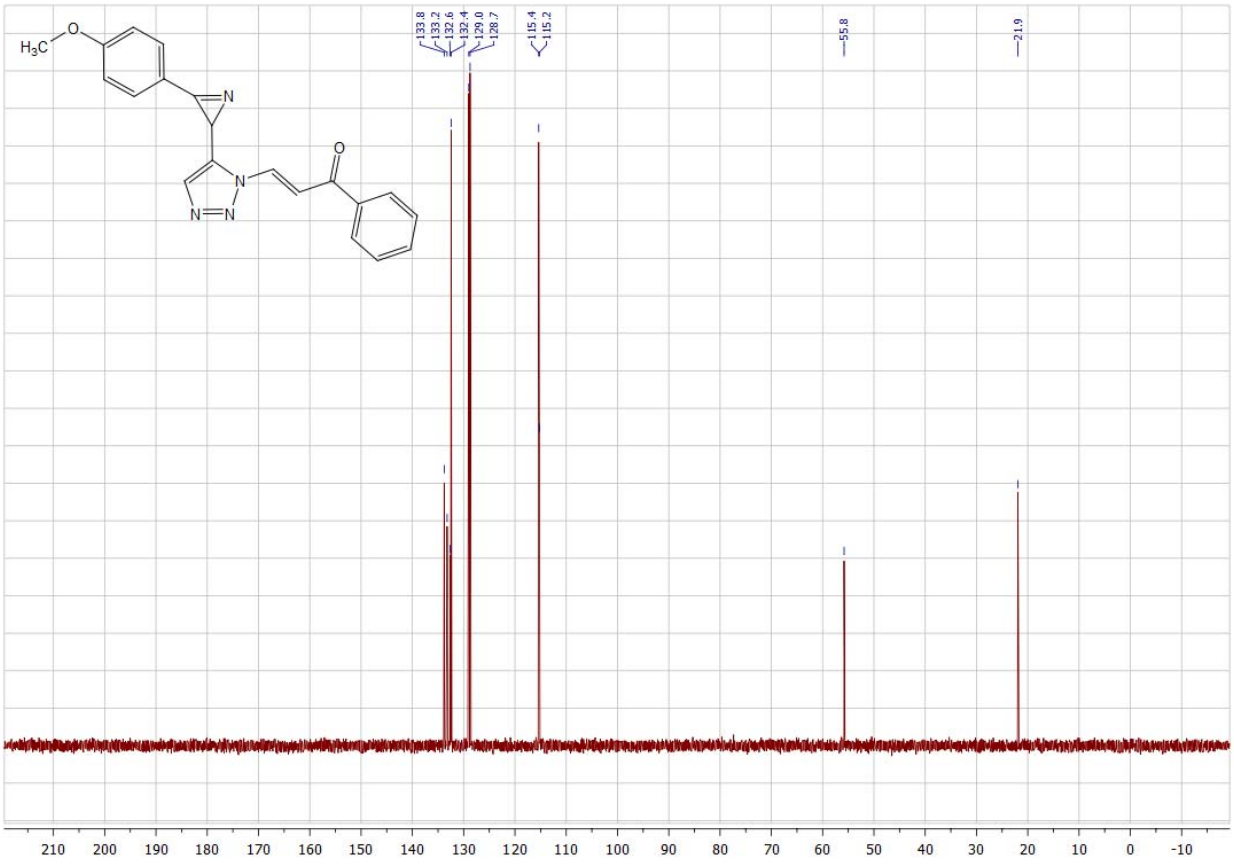
(E)-3-(5-(3-(4-methoxyphenyl)-2H-azirin-2-yl)-1H-1,2,3-triazol-1-yl)-1-phenylprop-2-en-1-one (**4l**), ^{1}H NMR (400 MHz, $CDCl_3$)



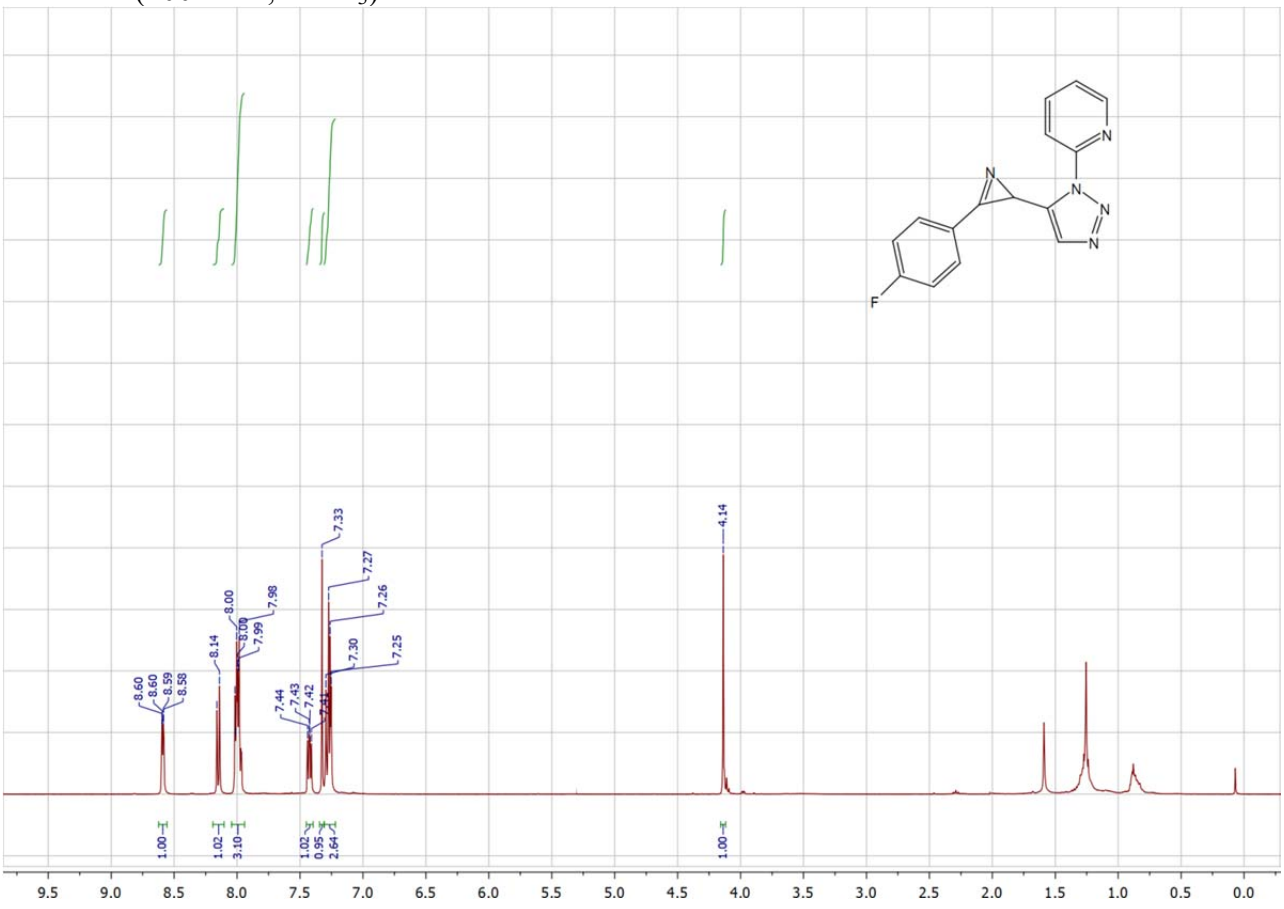
(E)-3-(5-(3-(4-methoxyphenyl)-2H-azirin-2-yl)-1H-1,2,3-triazol-1-yl)-1-phenylprop-2-en-1-one (**4l**), $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



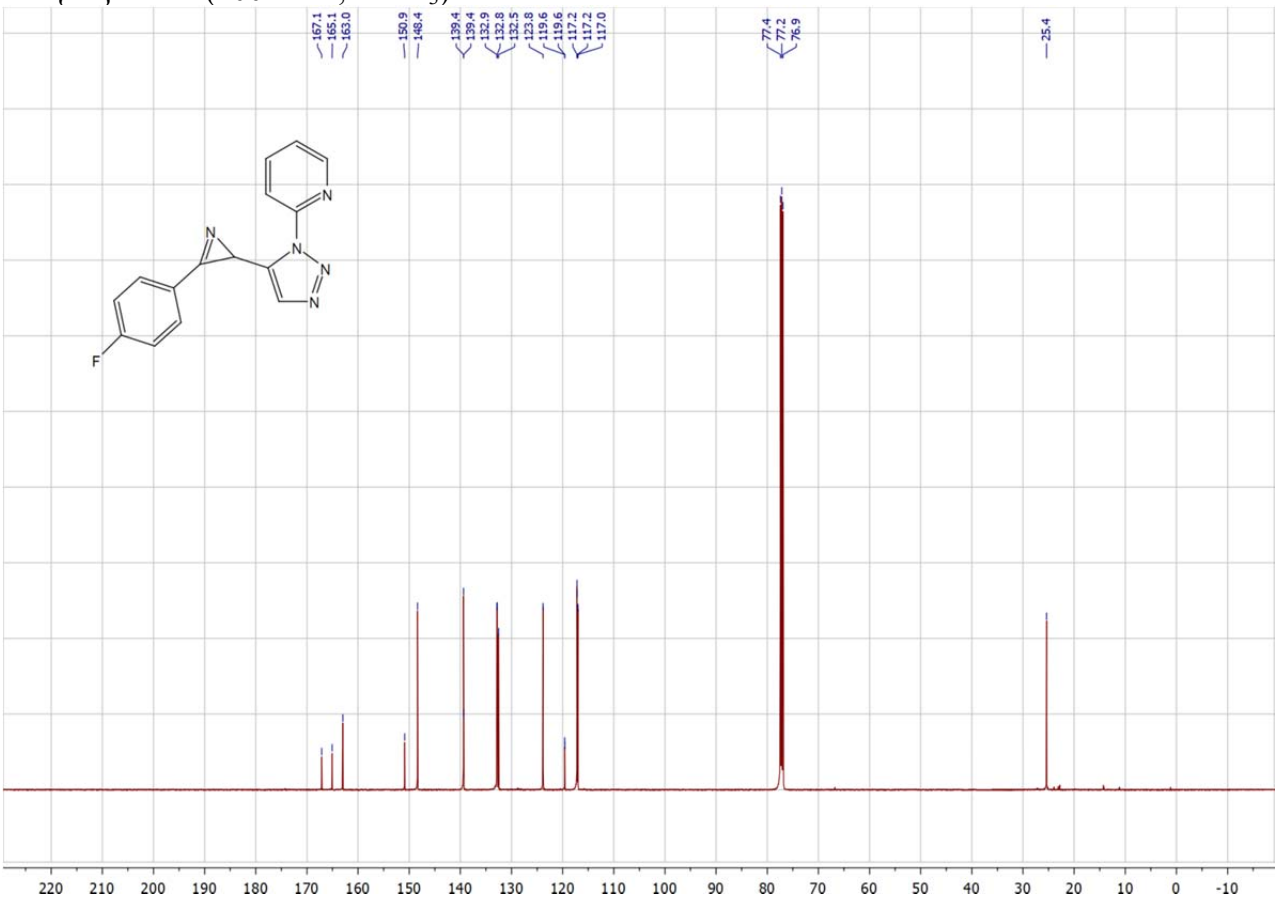
(E)-3-(5-(3-(4-methoxyphenyl)-2H-azirin-2-yl)-1H-1,2,3-triazol-1-yl)-1-phenylprop-2-en-1-one (**4l**), ^{13}C DEPT 135 NMR (100 MHz, $CDCl_3$)



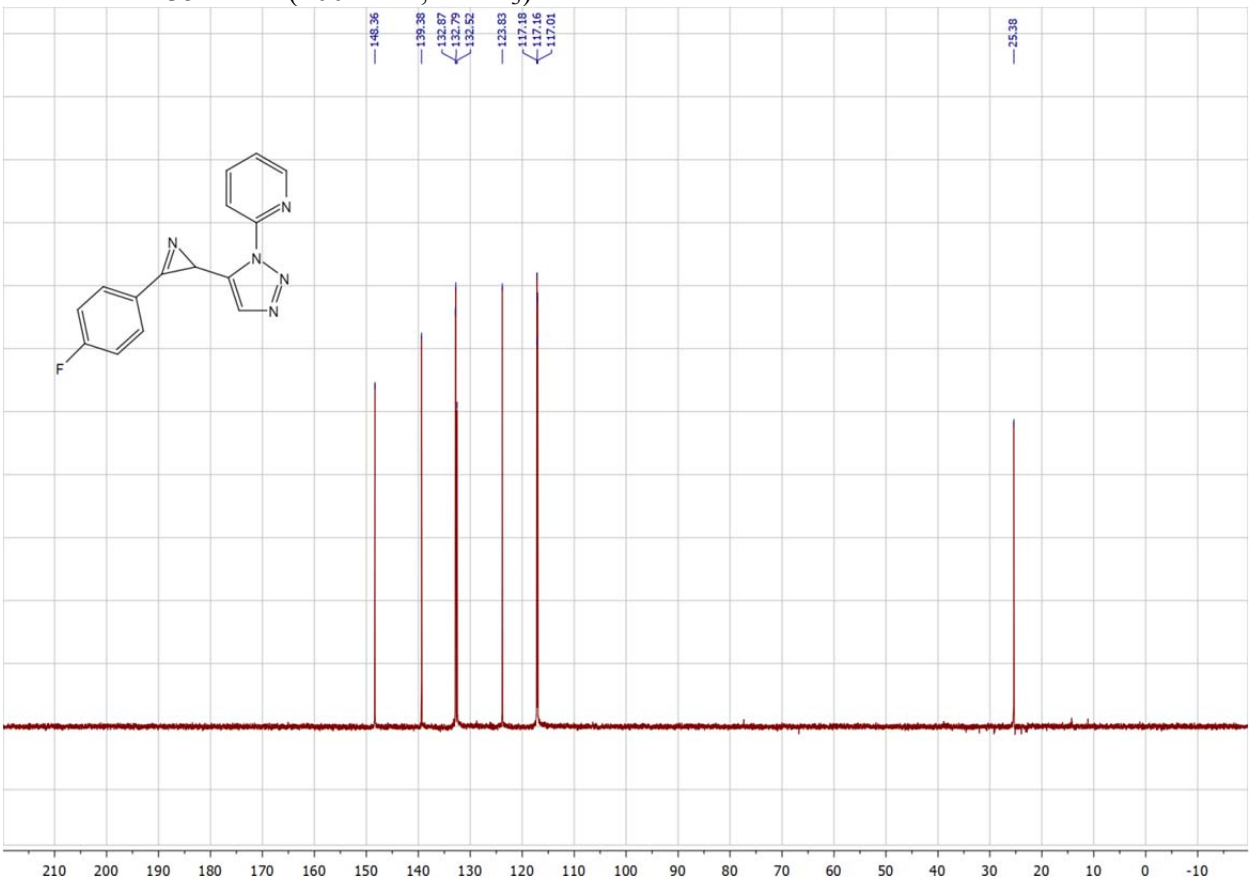
2-(5-(3-(4-Fluorophenyl)-2H-azirin-2-yl)-1H-1,2,3-triazol-1-yl)pyridine (**5a**),
^{1}H NMR (400 MHz, $CDCl_3$)



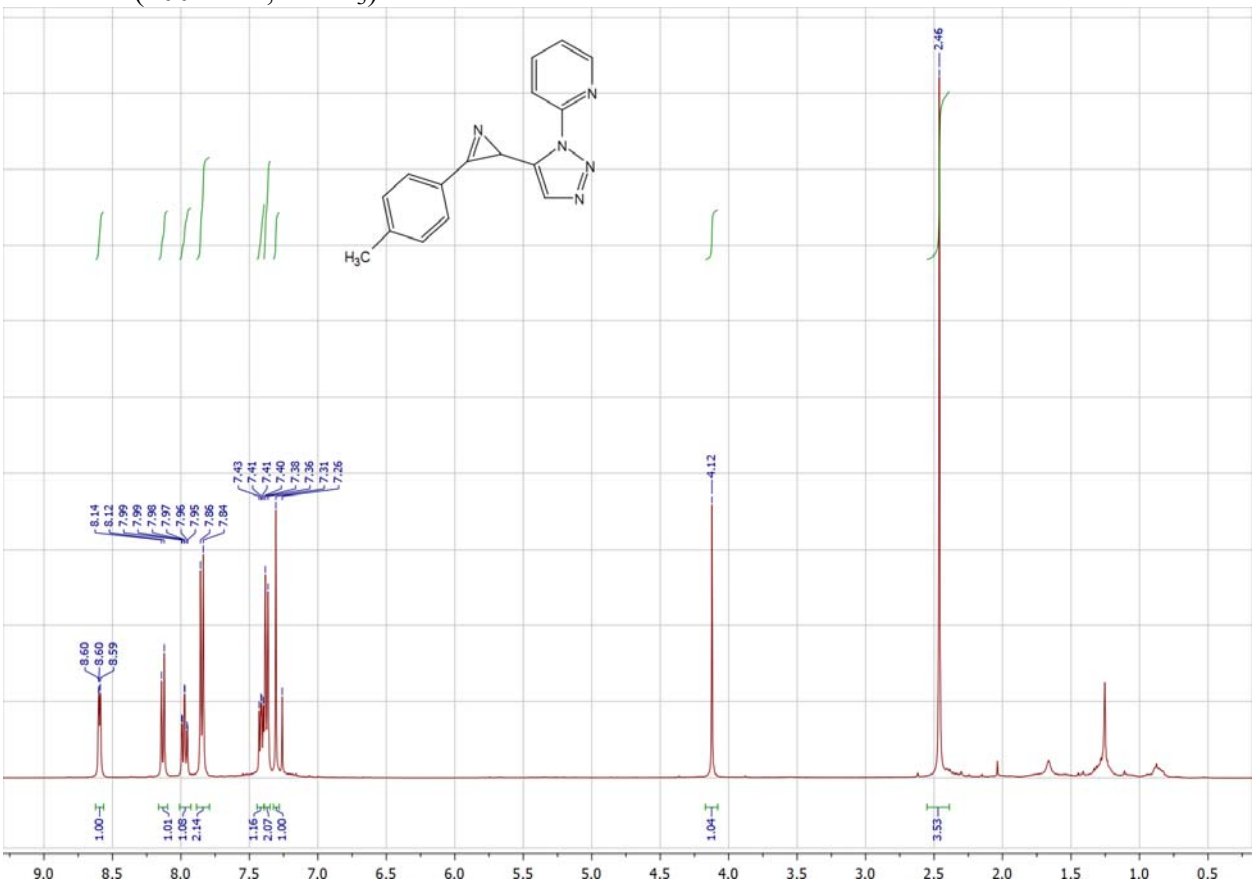
2-(5-(3-(4-Fluorophenyl)-2H-azirin-2-yl)-1H-1,2,3-triazol-1-yl)pyridine (**5a**),
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



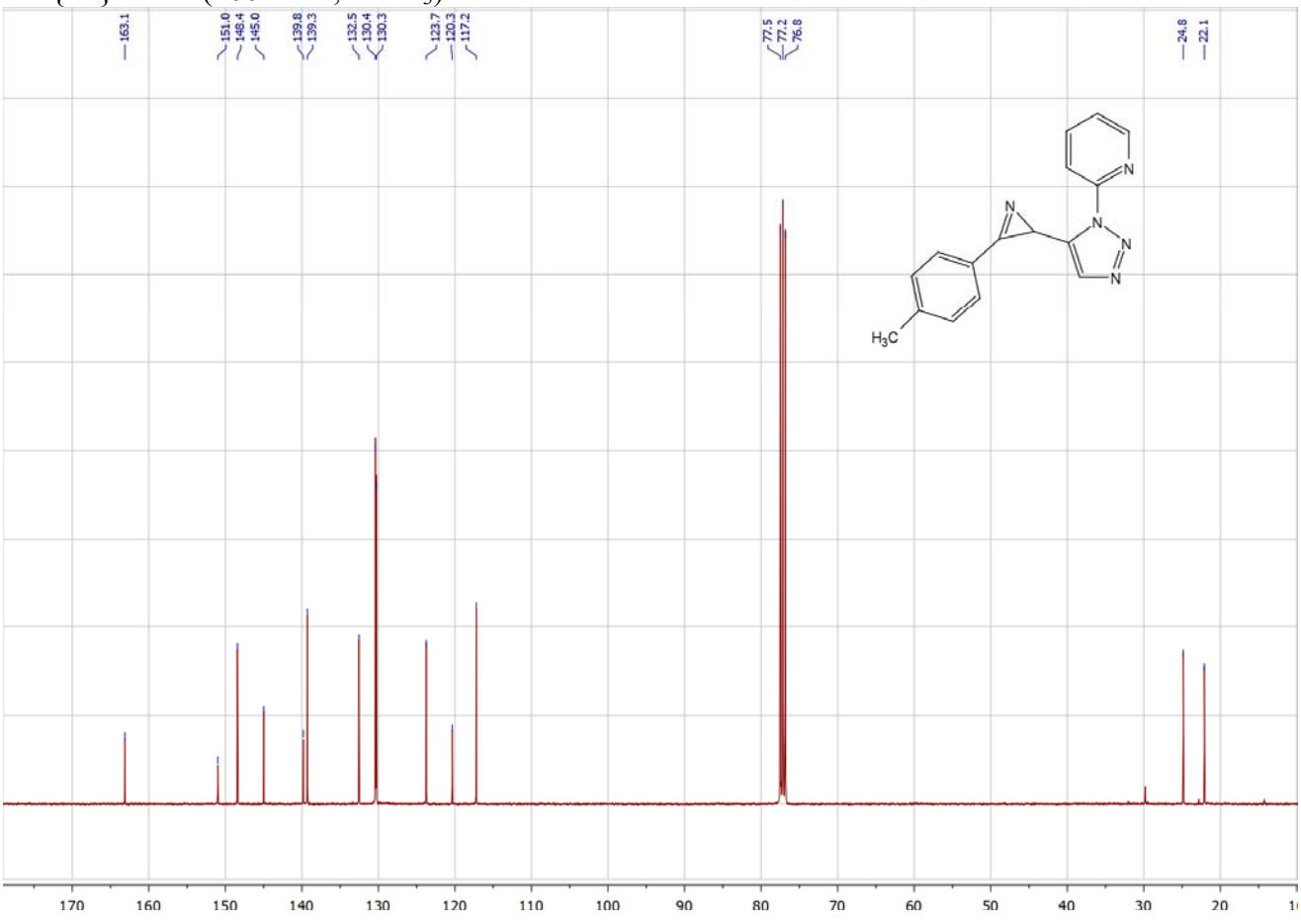
2-(5-(3-(4-Fluorophenyl)-2H-azirin-2-yl)-1H-1,2,3-triazol-1-yl)pyridine (**5a**),
^{13}C DEPT 135 NMR (100 MHz, $CDCl_3$)



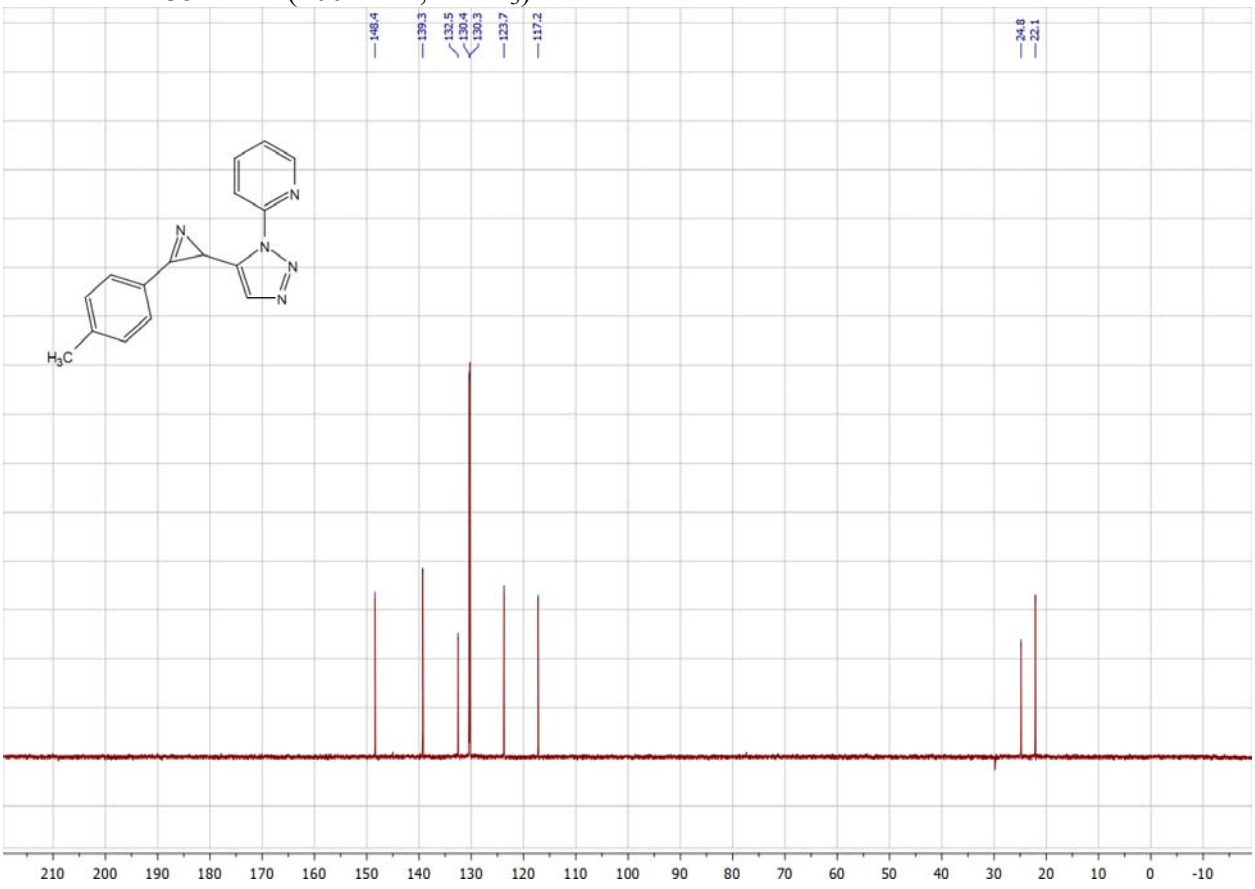
2-(5-(3-(p-Tolyl)-2H-azirin-2-yl)-1H-1,2,3-triazol-1-yl)pyridine (**5b**),
^{1}H NMR (400 MHz, $CDCl_3$)



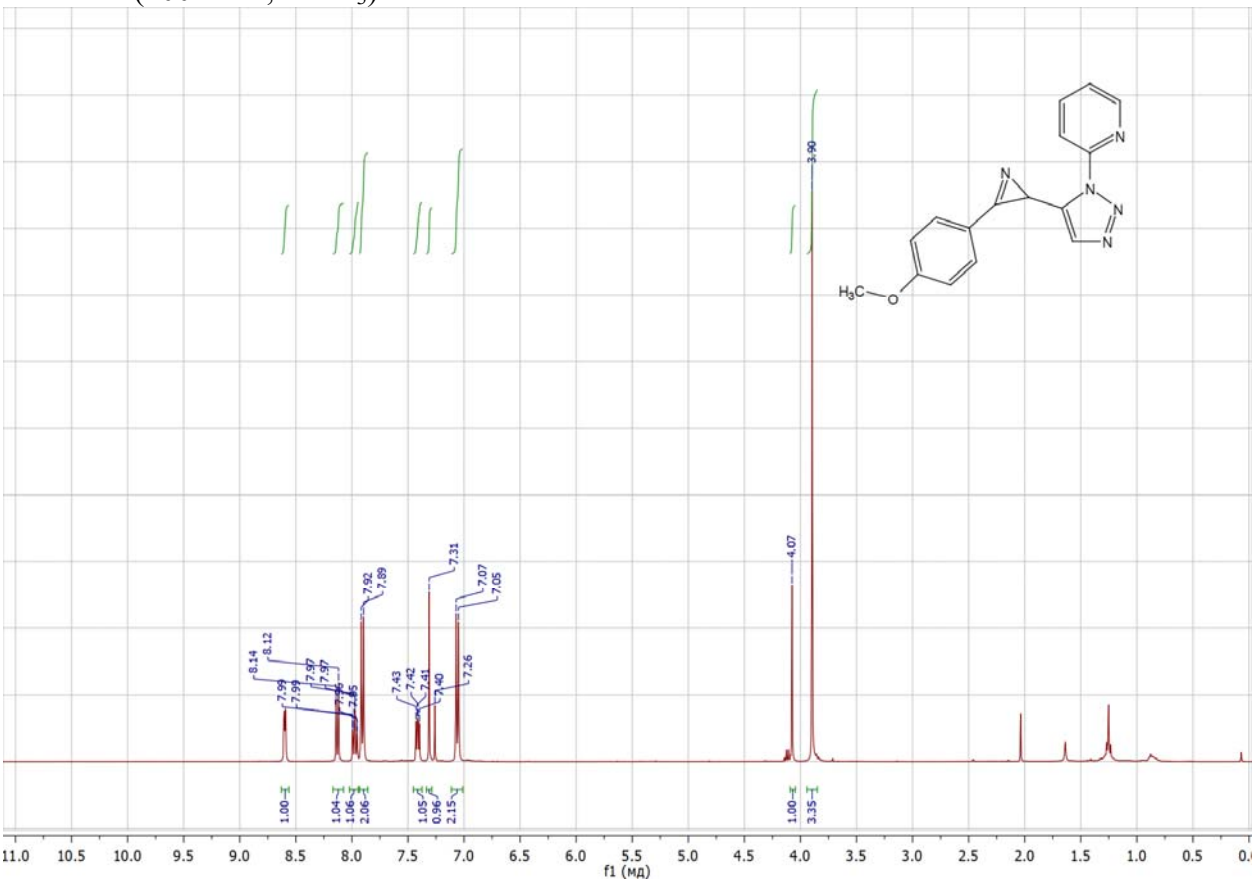
2-(5-(3-(p-Tolyl)-2H-azirin-2-yl)-1H-1,2,3-triazol-1-yl)pyridine (**5b**),
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



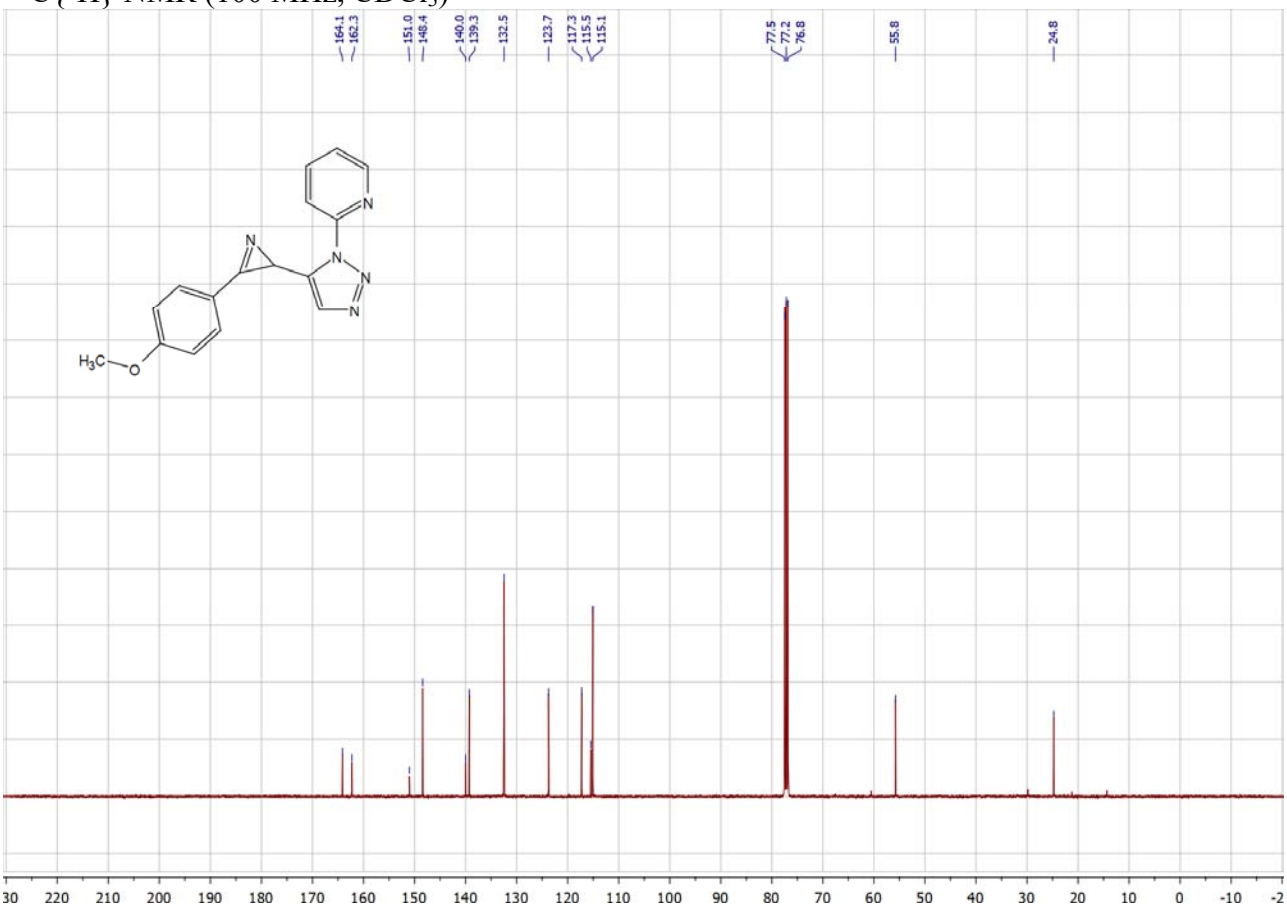
2-(5-(3-(p-Tolyl)-2H-azirin-2-yl)-1H-1,2,3-triazol-1-yl)pyridine (**5b**),
^{13}C DEPT 135 NMR (100 MHz, $CDCl_3$)



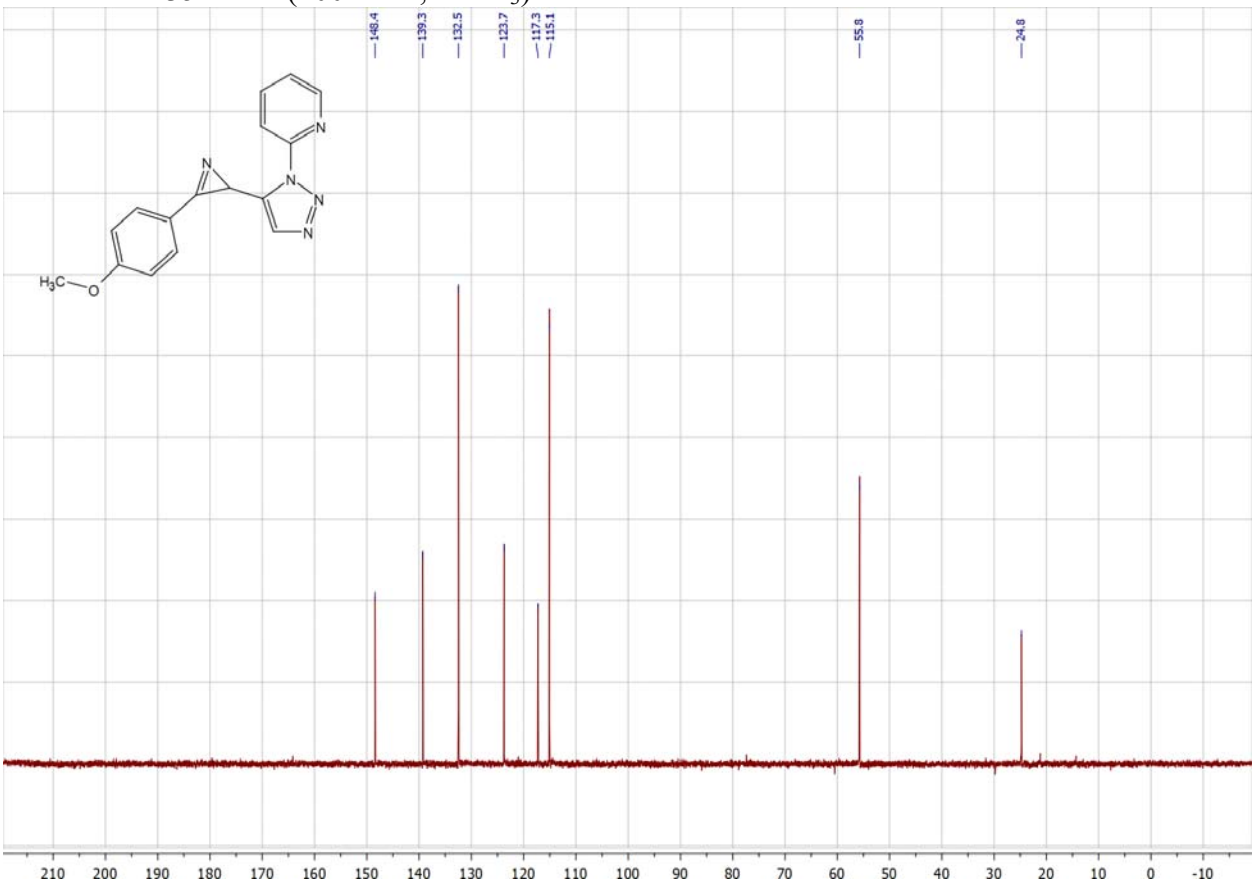
2-(5-(3-(4-Methoxyphenyl)-2H-azirin-2-yl)-1H-1,2,3-triazol-1-yl)pyridine (**5c**),
^{1}H NMR (400 MHz, $CDCl_3$)



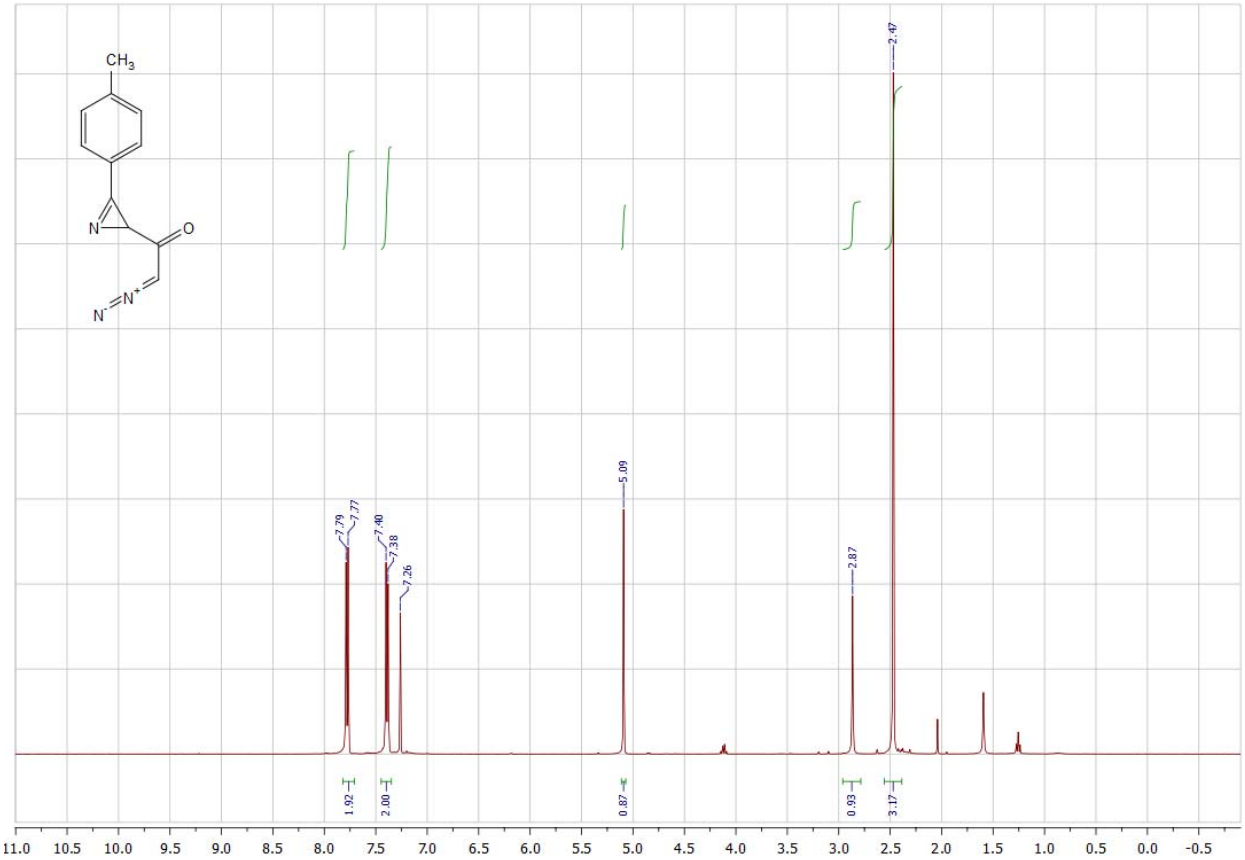
2-(5-(3-(4-Methoxyphenyl)-2H-azirin-2-yl)-1H-1,2,3-triazol-1-yl)pyridine (**5c**),
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



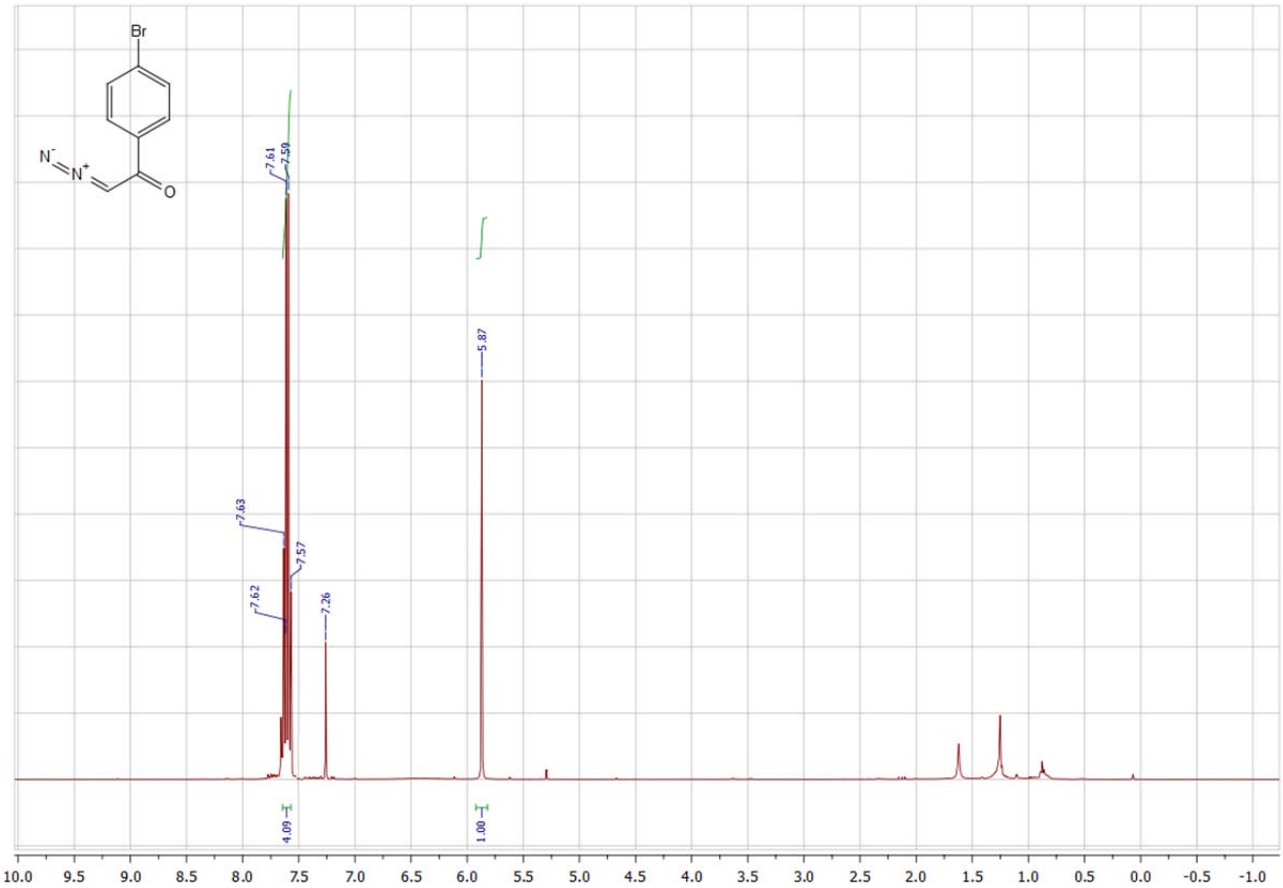
2-(5-(3-(4-Methoxyphenyl)-2H-azirin-2-yl)-1H-1,2,3-triazol-1-yl)pyridine (**5c**),
^{13}C DEPT 135 NMR (100 MHz, $CDCl_3$)



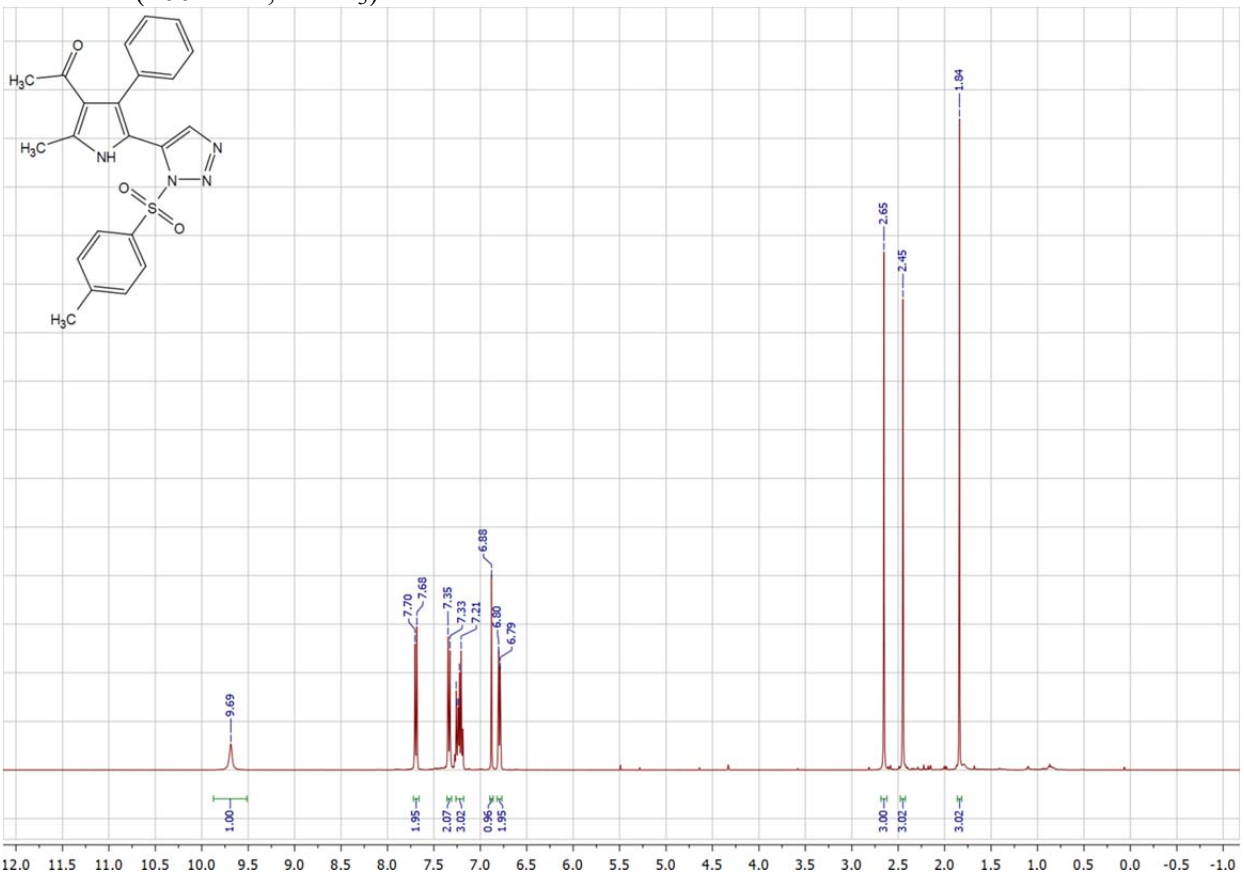
2-Diazo-1-(3-(p-tolyl)-2H-azirin-2-yl)ethan-1-one (**17**), ^{1}H NMR (400 MHz, $CDCl_3$)



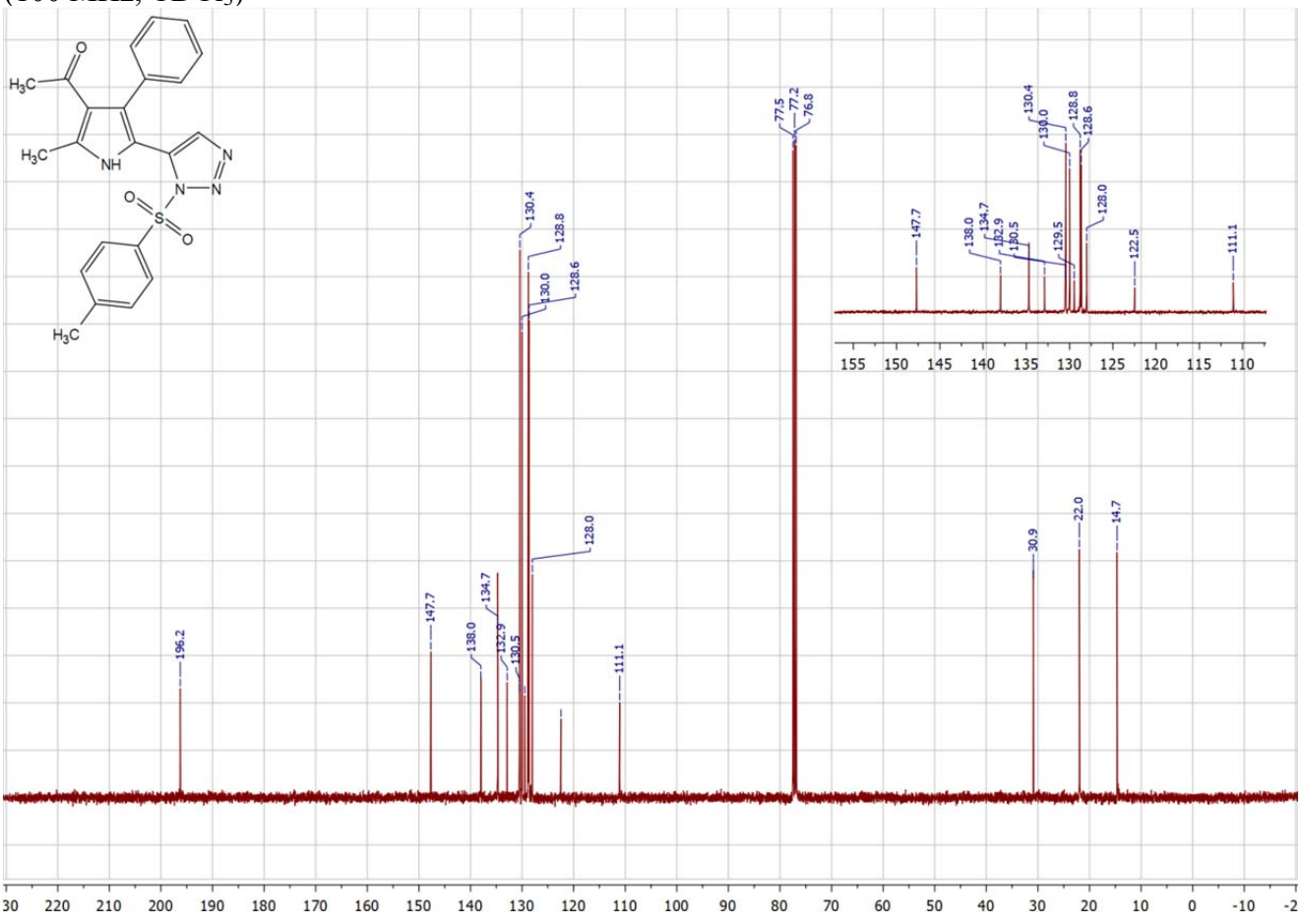
1-(4-Bromophenyl)-2-diazoethan-1-one (***19***), ^{1}H NMR (400 MHz, $CDCl_3$)



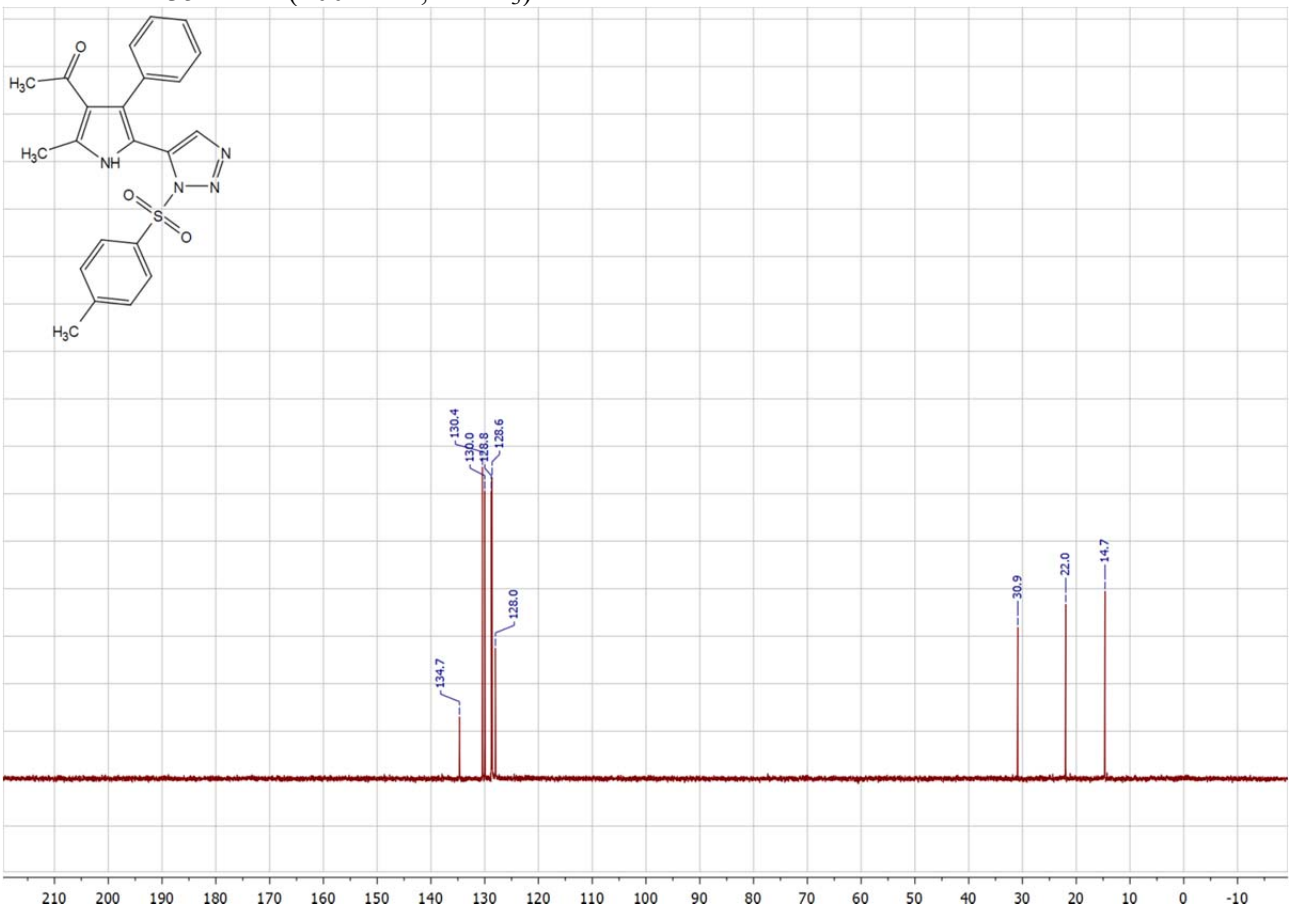
1-(2-Methyl-4-phenyl-5-(1-tosyl-1H-1,2,3-triazol-5-yl)-1H-pyrrol-3-yl)ethan-1-one (**20a**), ^{1}H NMR (400 MHz, $CDCl_3$)



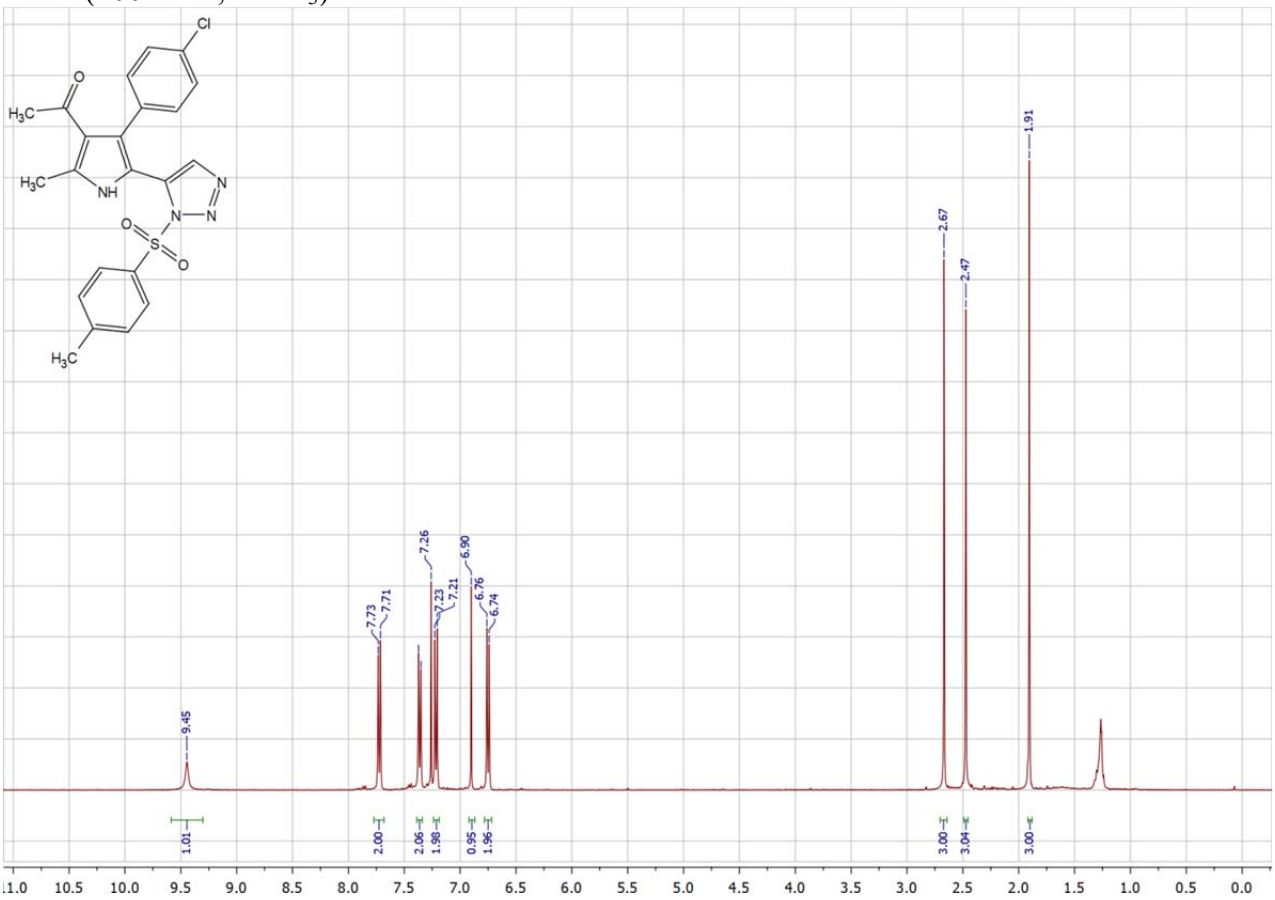
1-(2-Methyl-4-phenyl-5-(1-tosyl-1H-1,2,3-triazol-5-yl)-1H-pyrrol-3-yl)ethan-1-one (**20a**), ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



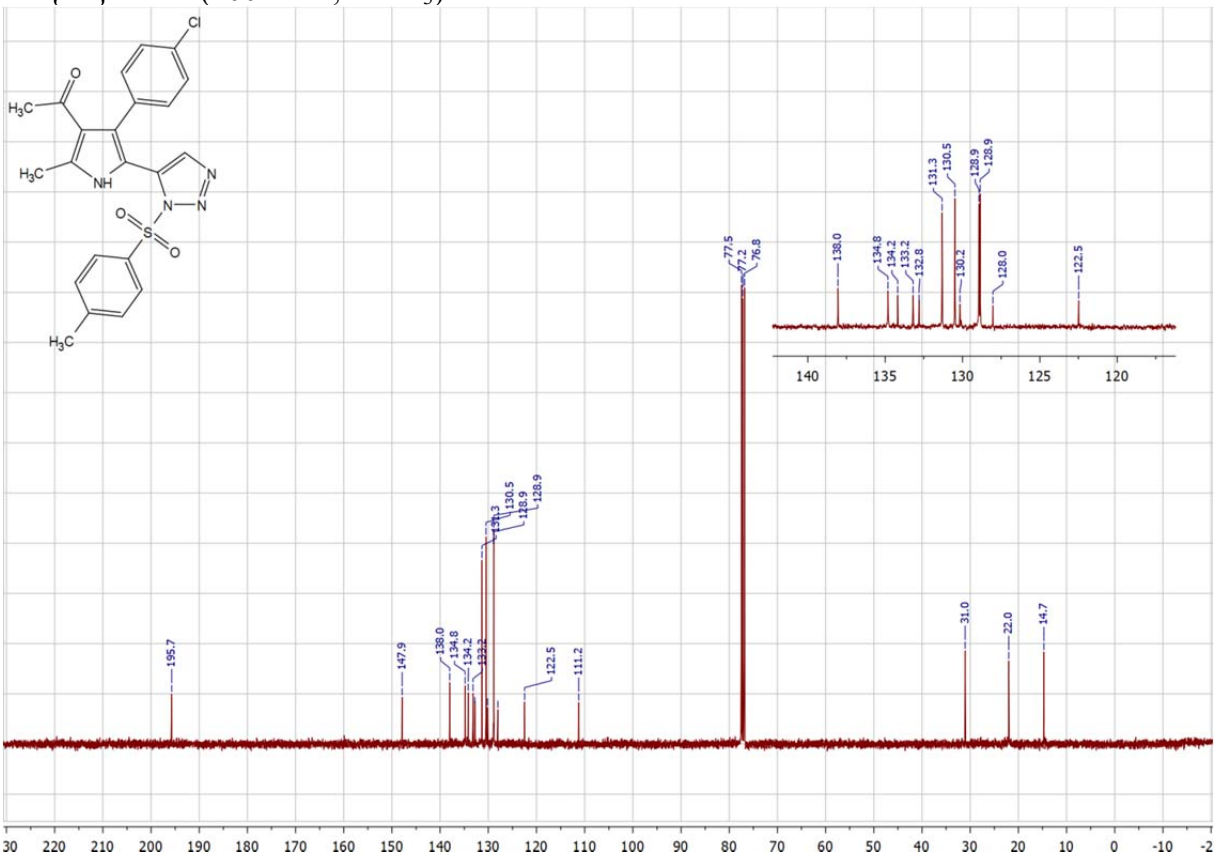
1-(2-Methyl-4-phenyl-5-(1-tosyl-1H-1,2,3-triazol-5-yl)-1H-pyrrol-3-yl)ethan-1-one (**20a**),
^{13}C DEPT 135 NMR (100 MHz, $CDCl_3$)



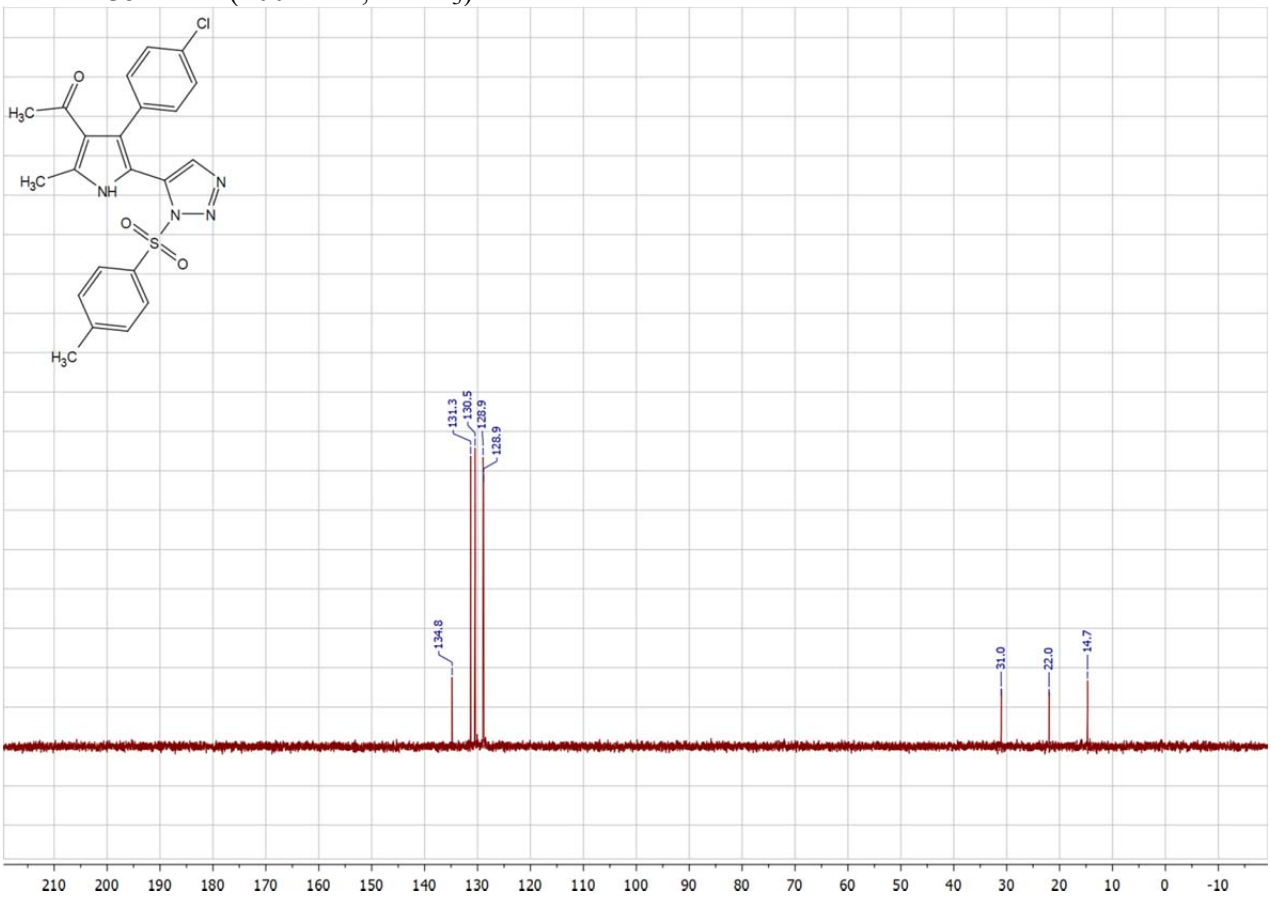
1-(4-(4-Chlorophenyl)-2-methyl-5-(1-tosyl-1H-1,2,3-triazol-5-yl)-1H-pyrrol-3-yl)ethan-1-one (**20b**), ^{1}H NMR (400 MHz, $CDCl_3$)



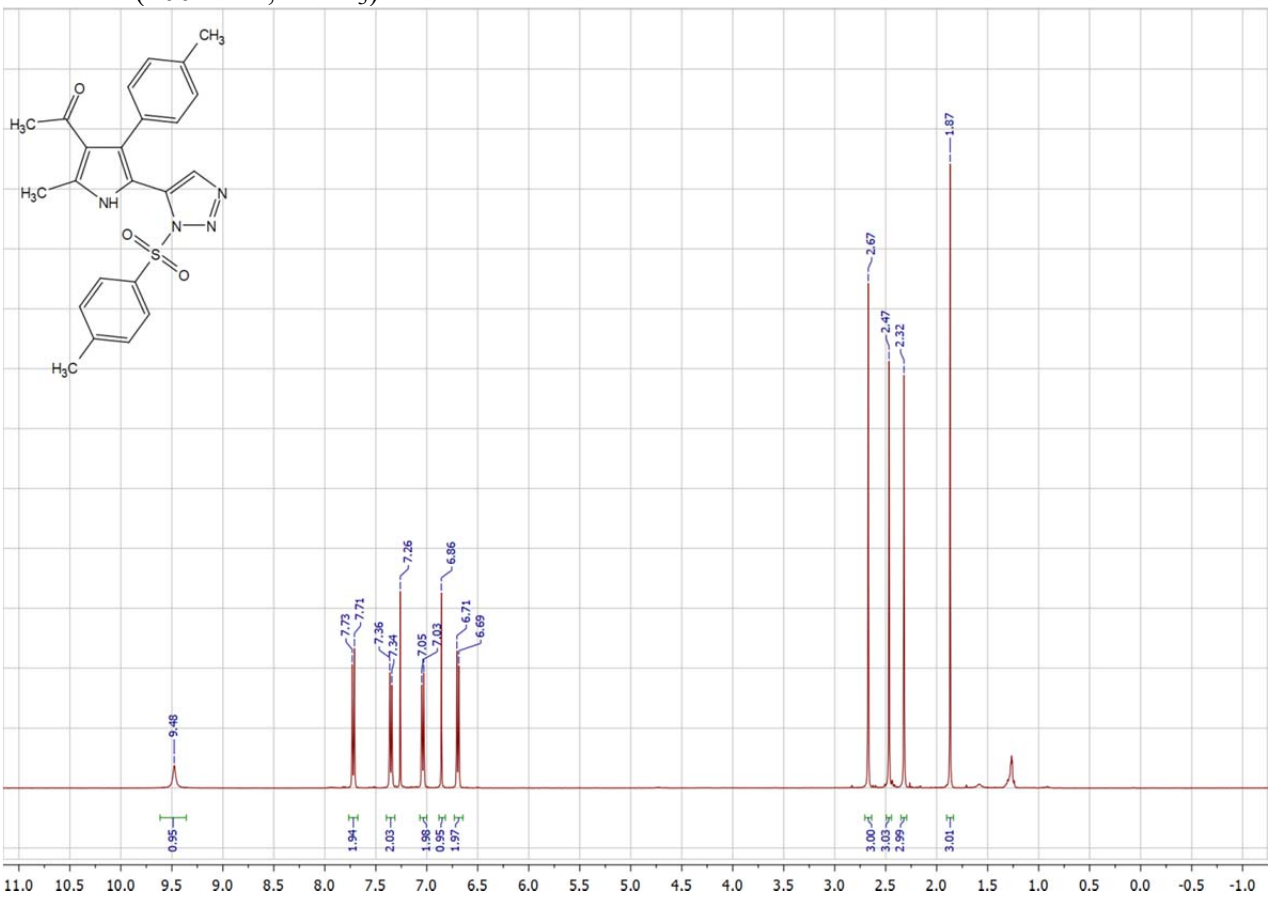
1-(4-(4-Chlorophenyl)-2-methyl-5-(1-tosyl-1H-1,2,3-triazol-5-yl)-1H-pyrrol-3-yl)ethan-1-one (**20b**), $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



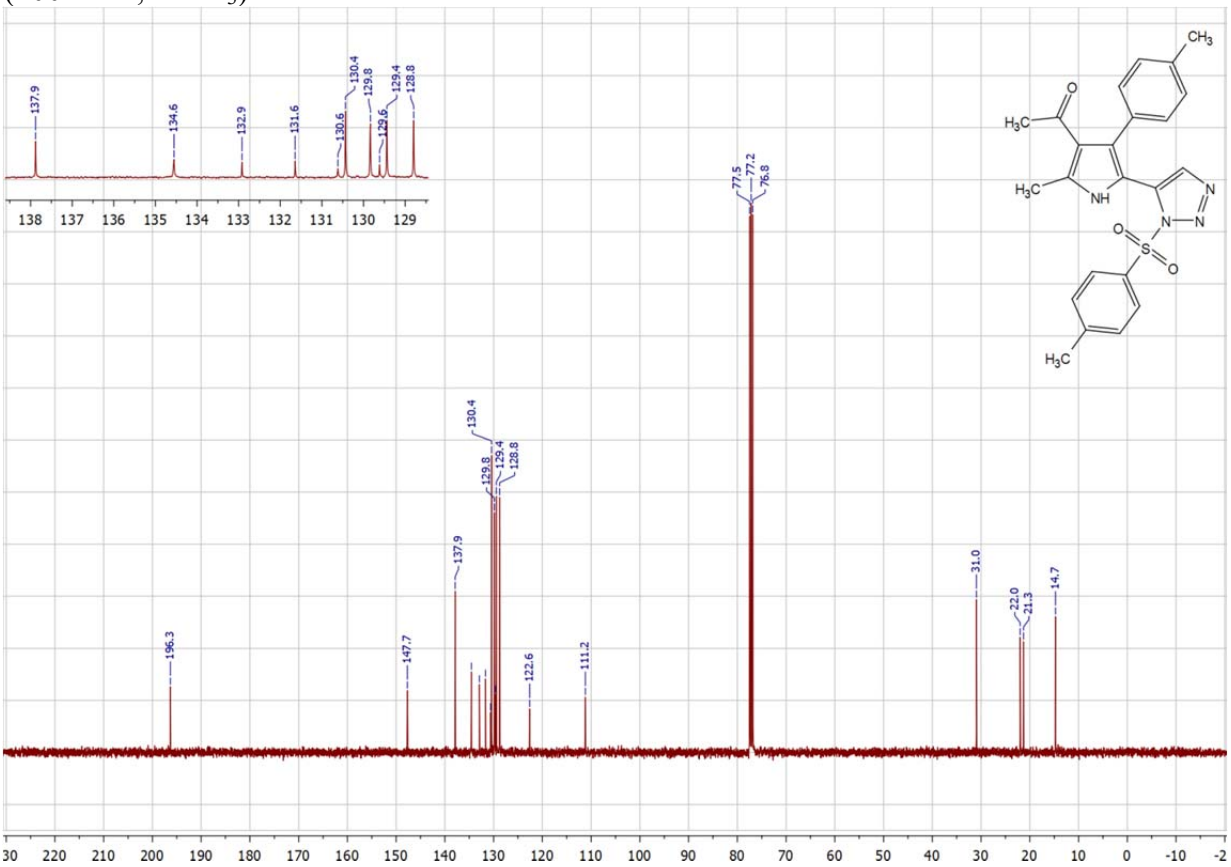
1-(4-(4-Chlorophenyl)-2-methyl-5-(1-tosyl-1H-1,2,3-triazol-5-yl)-1H-pyrrol-3-yl)ethan-1-one (**20b**), ^{13}C DEPT 135 NMR (100 MHz, $CDCl_3$)



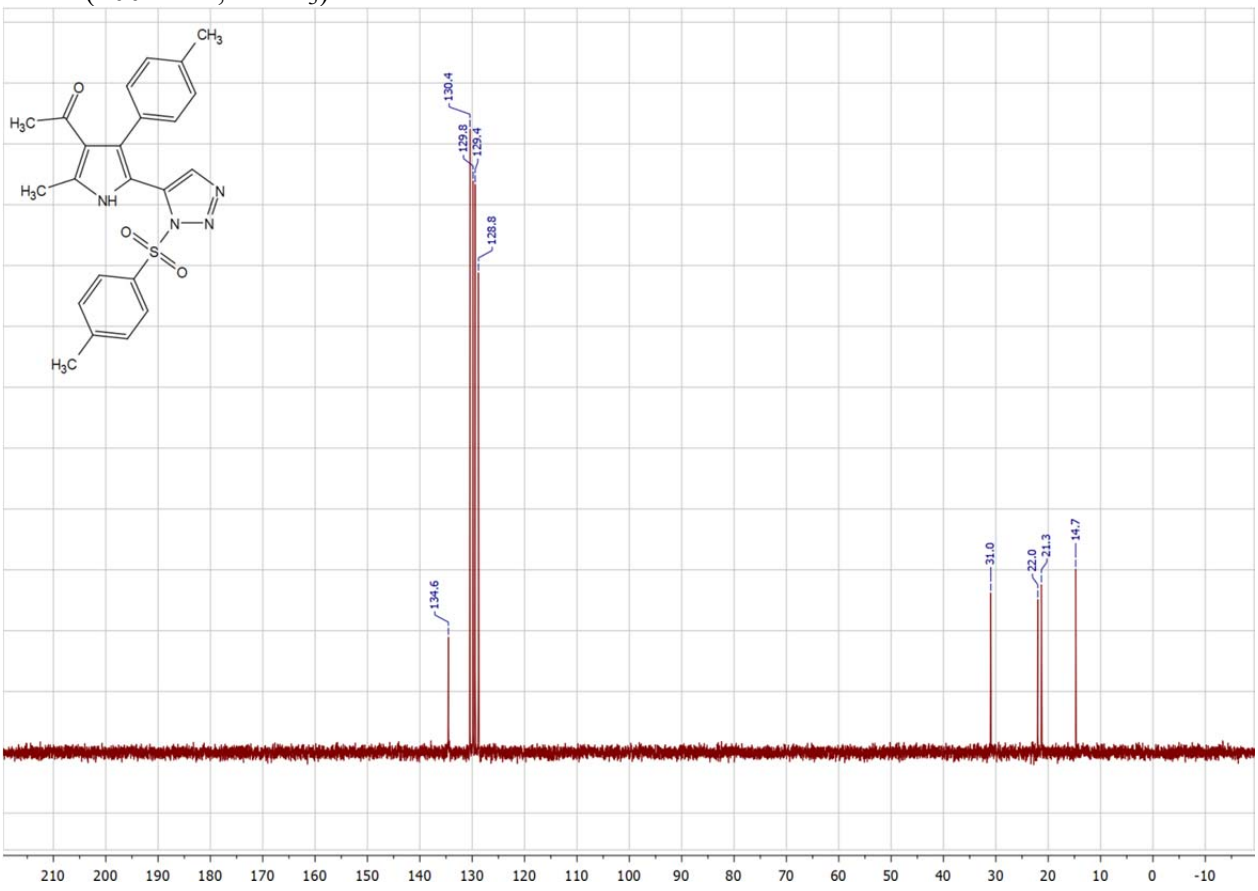
1-(2-Methyl-4-(p-tolyl)-5-(1-tosyl-1H-1,2,3-triazol-5-yl)-1H-pyrrol-3-yl)ethan-1-one (**20c**), ^{1}H NMR (400 MHz, $CDCl_3$)



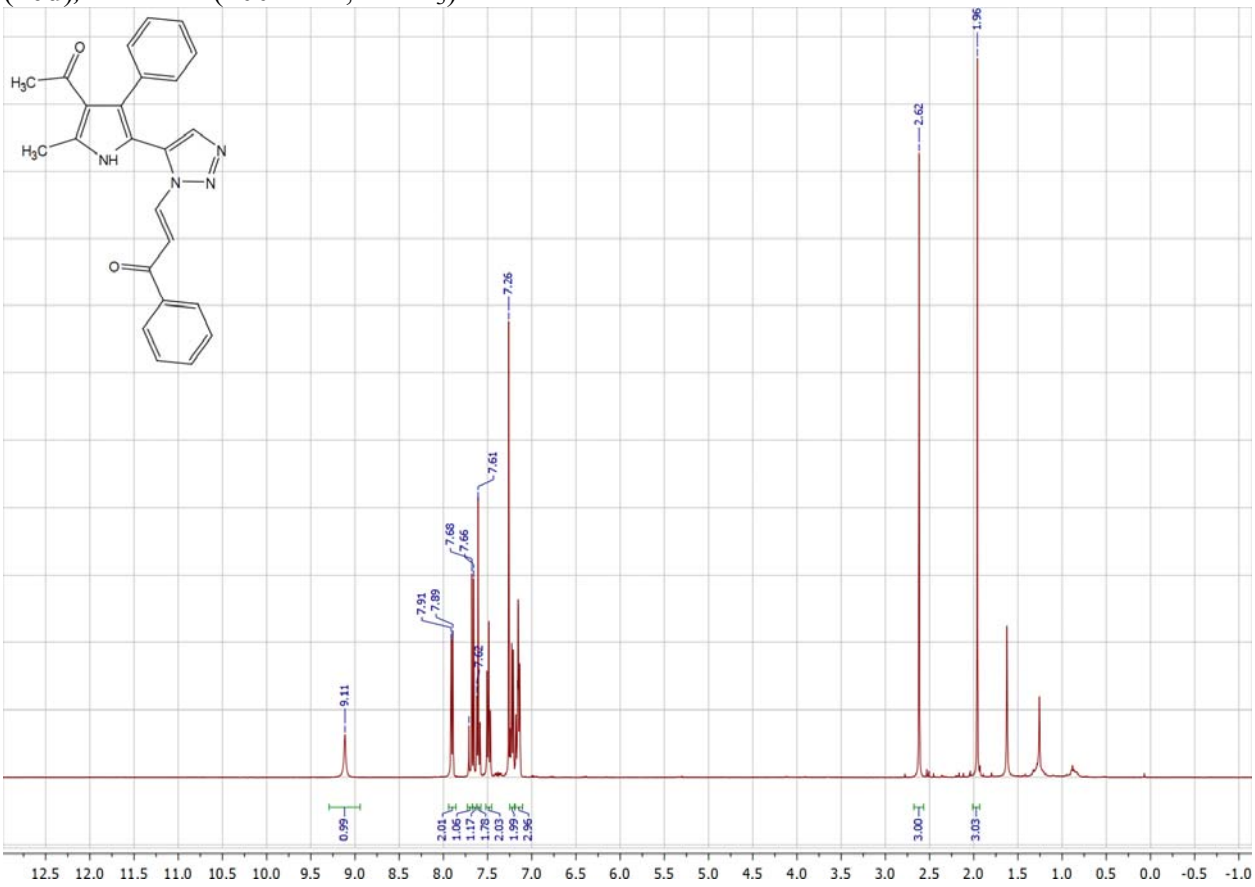
1-(2-Methyl-4-(p-tolyl)-5-(1-tosyl-1H-1,2,3-triazol-5-yl)-1H-pyrrol-3-yl)ethan-1-one (**20c**), $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



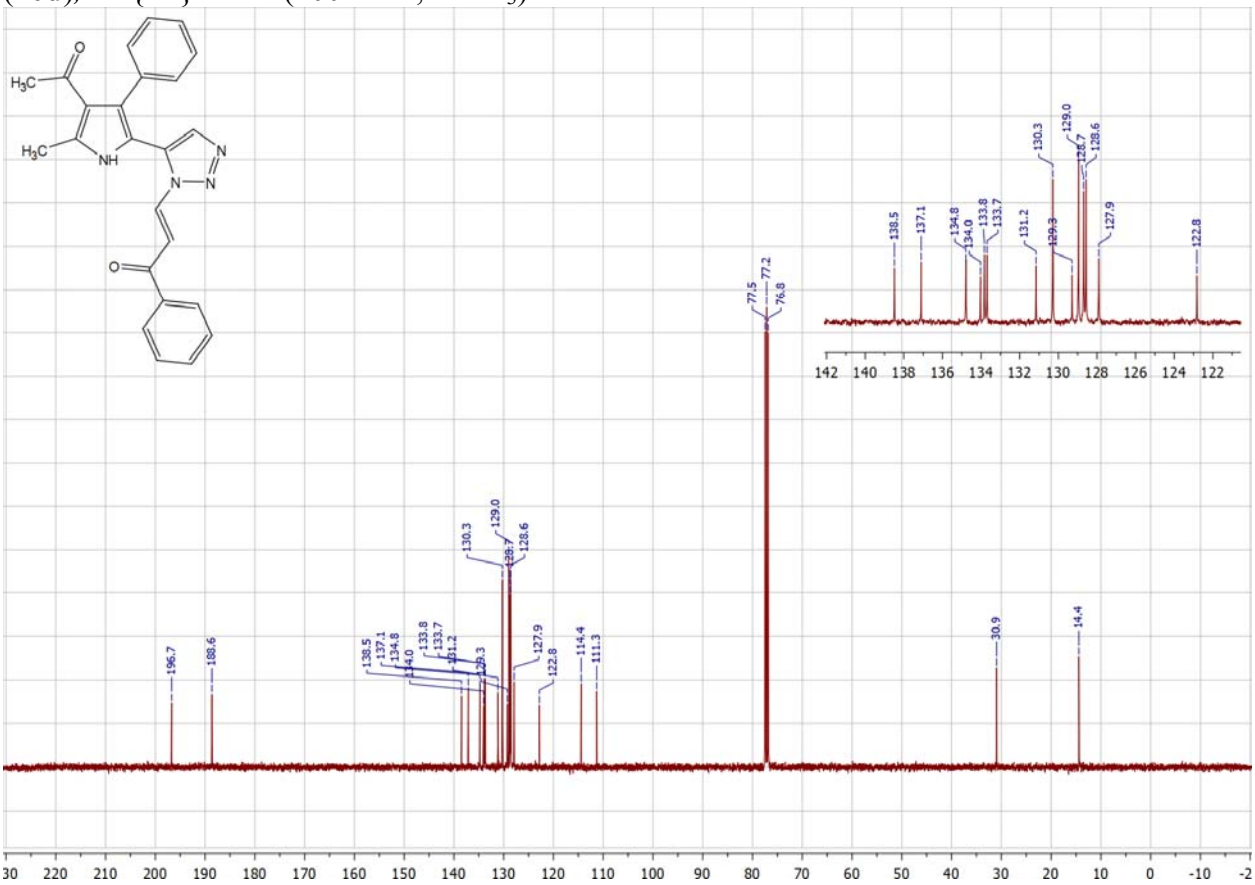
1-(2-Methyl-4-(p-tolyl)-5-(1-tosyl-1H-1,2,3-triazol-5-yl)-1H-pyrrol-3-yl)ethan-1-one (**20c**), ^{13}C DEPT 135 NMR (100 MHz, $CDCl_3$)



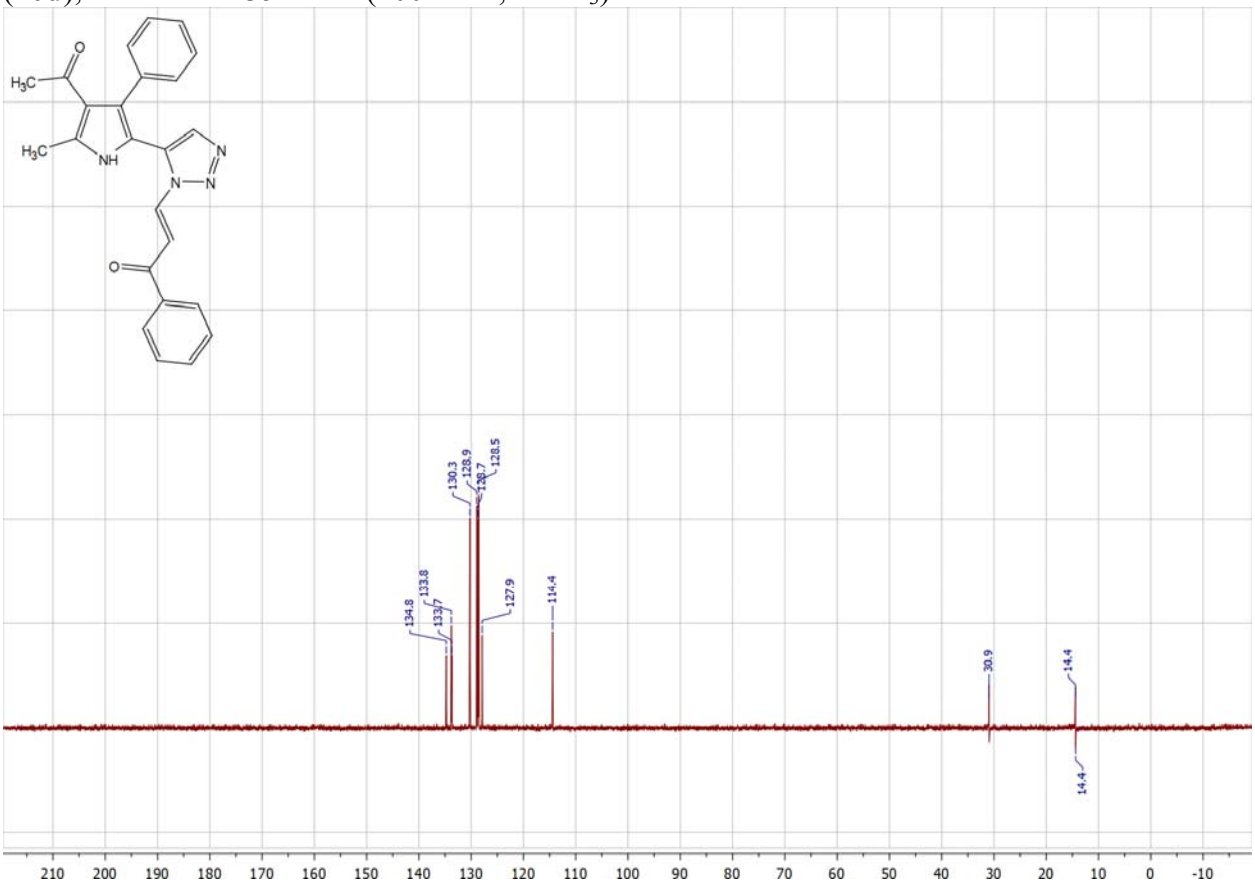
(E)-3-(5-(4-Acetyl-5-methyl-3-phenyl-1H-pyrrol-2-yl)-1H-1,2,3-triazol-1-yl)-1-phenylprop-2-en-1-one (**20d**), ^{1}H NMR (400 MHz, $CDCl_3$)



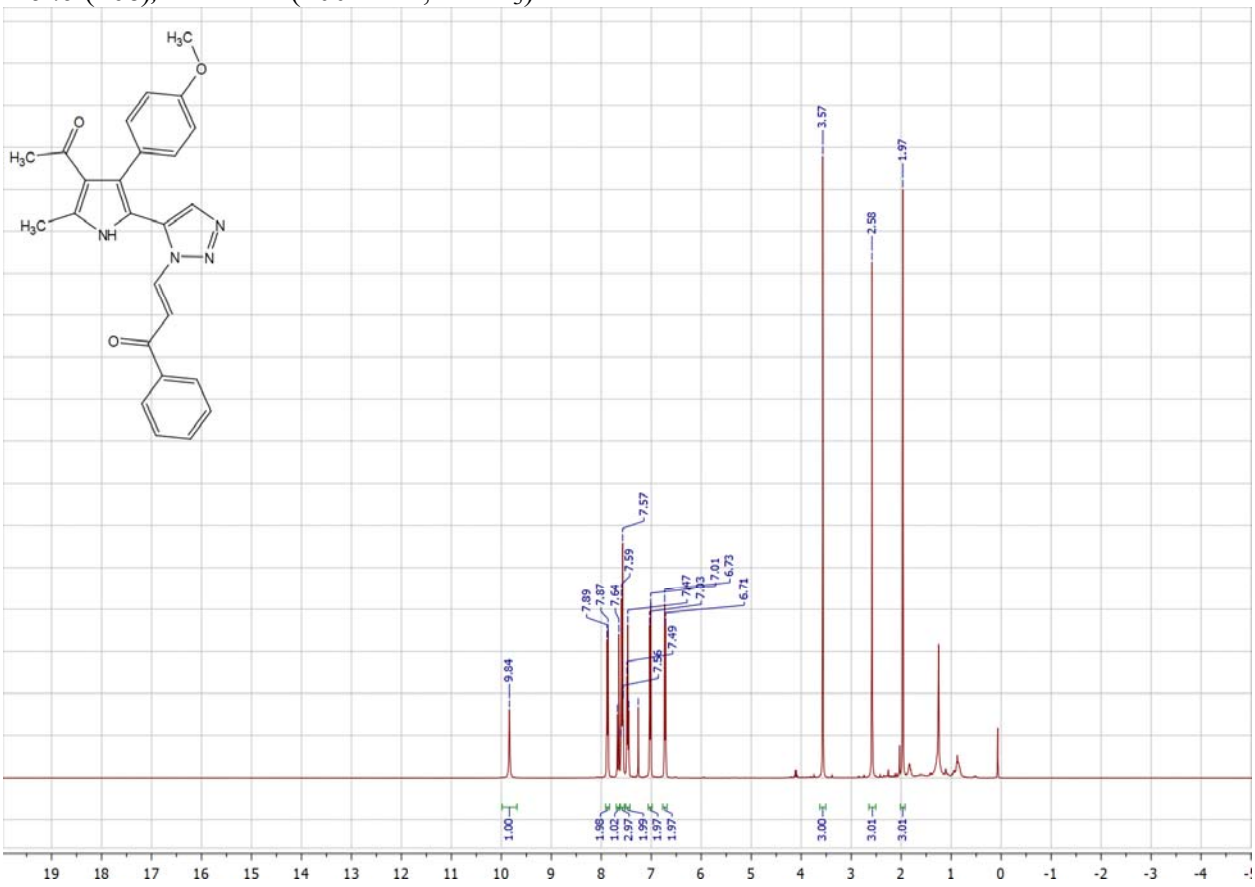
(E)-3-(5-(4-Acetyl-5-methyl-3-phenyl-1H-pyrrol-2-yl)-1H-1,2,3-triazol-1-yl)-1-phenylprop-2-en-1-one (**20d**), $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



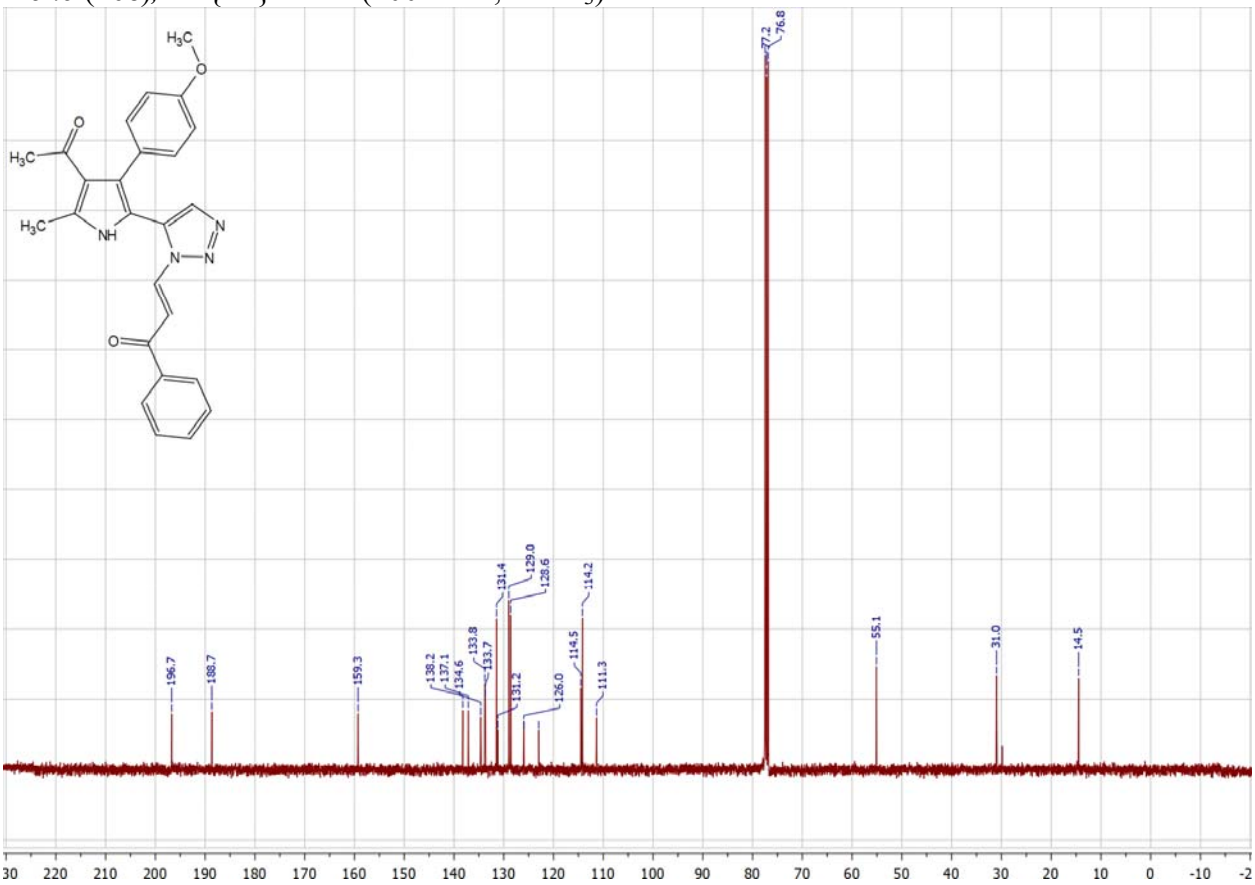
(E)-3-(5-(4-Acetyl-5-methyl-3-phenyl-1H-pyrrol-2-yl)-1H-1,2,3-triazol-1-yl)-1-phenylprop-2-en-1-one (**20d**), ^{13}C DEPT 135 NMR (100 MHz, $CDCl_3$)



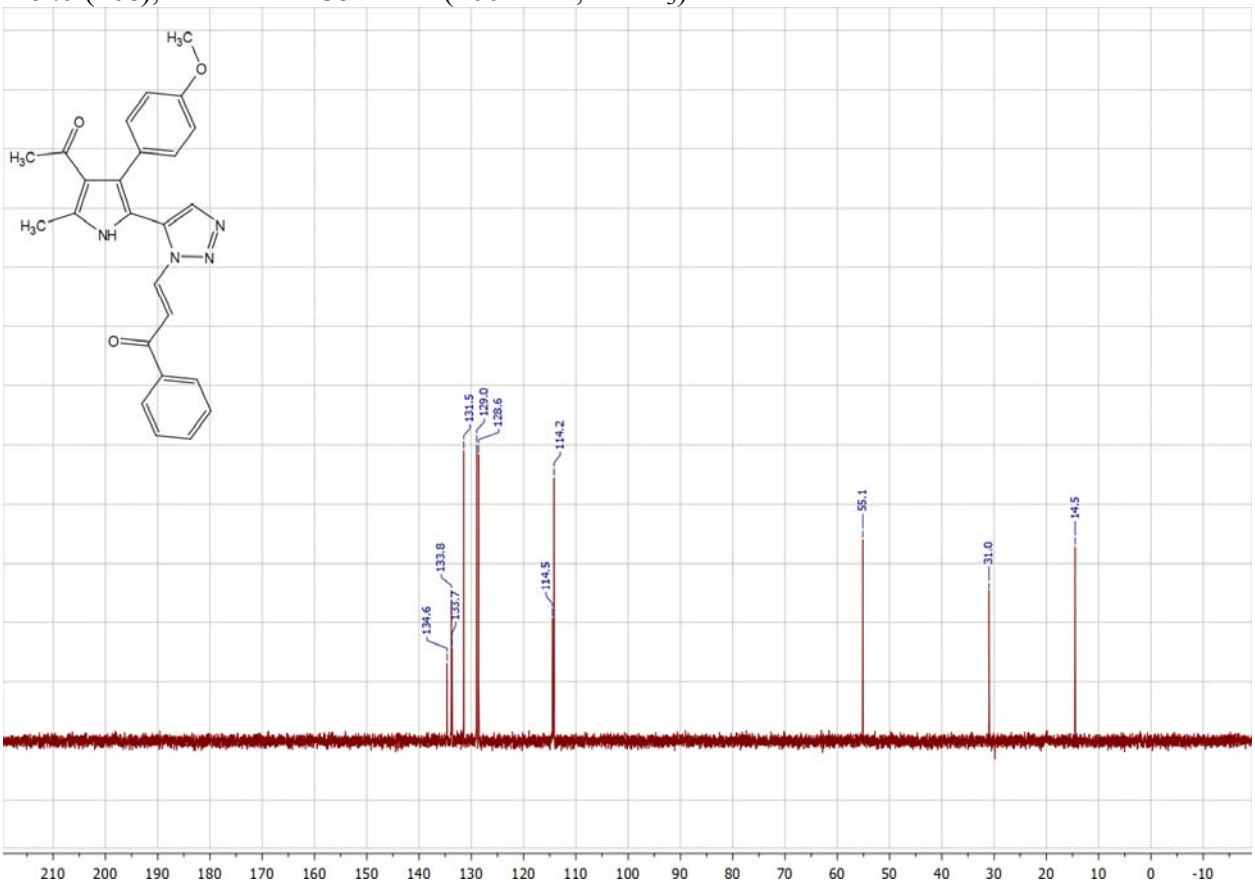
(E)-3-(5-(4-Acetyl-3-(4-methoxyphenyl)-5-methyl-1H-pyrrol-2-yl)-1H-1,2,3-triazol-1-yl)-1-phenylprop-2-en-1-one (**20e**), ^{1}H NMR (400 MHz, $CDCl_3$)



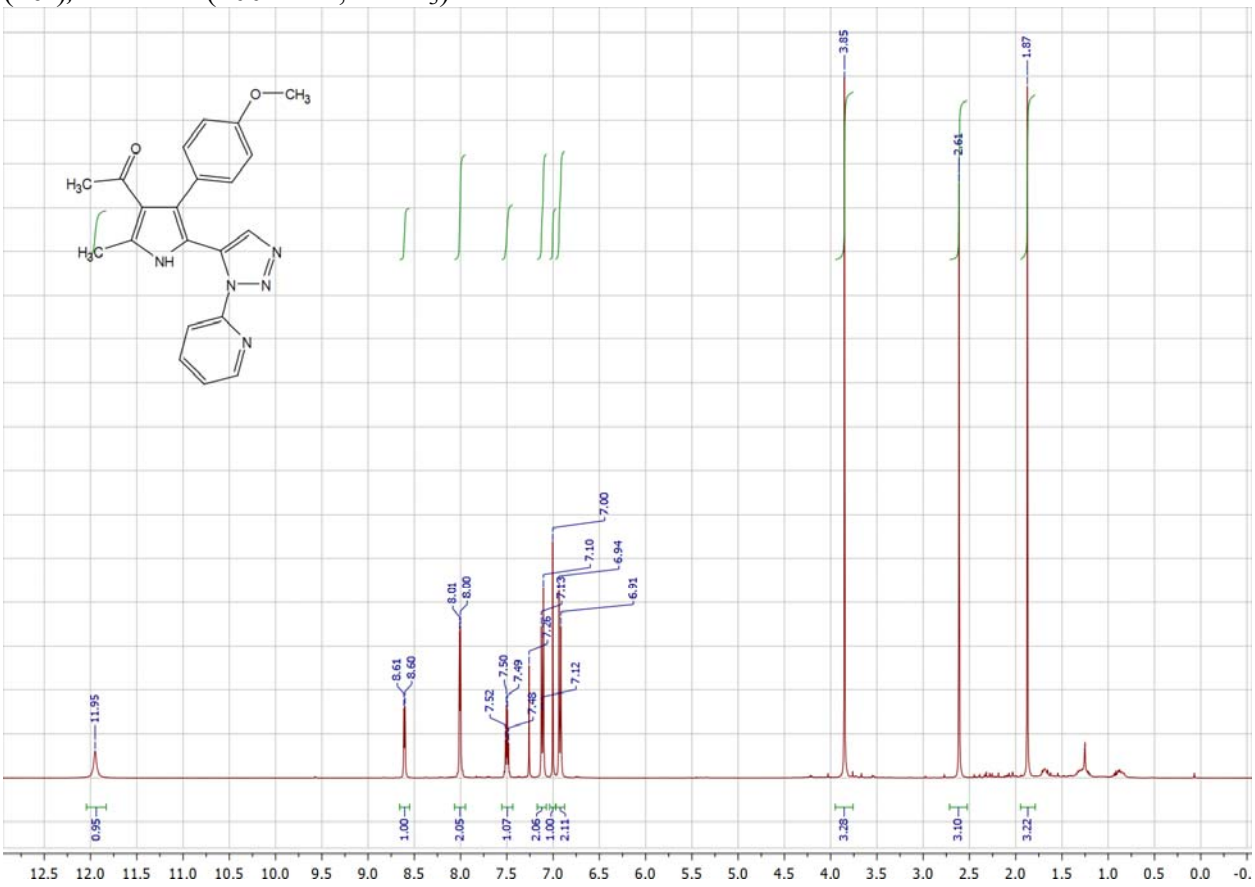
(E)-3-(5-(4-Acetyl-3-(4-methoxyphenyl)-5-methyl-1H-pyrrol-2-yl)-1H-1,2,3-triazol-1-yl)-1-phenylprop-2-en-1-one (**20e**), ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



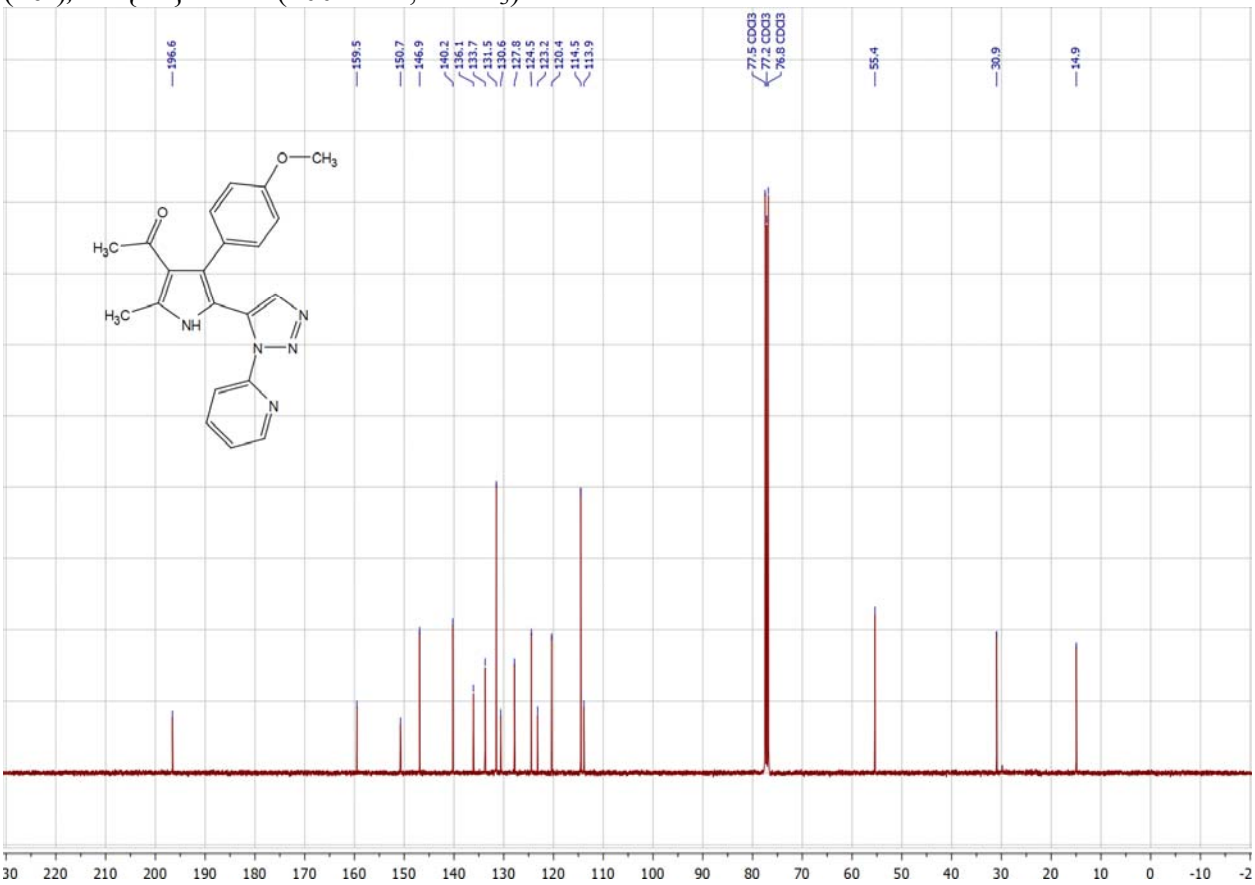
(E)-3-(5-(4-Acetyl-3-(4-methoxyphenyl)-5-methyl-1H-pyrrol-2-yl)-1H-1,2,3-triazol-1-yl)-1-phenylprop-2-en-1-one (**20e**), ^{13}C DEPT 135 NMR (100 MHz, $CDCl_3$)



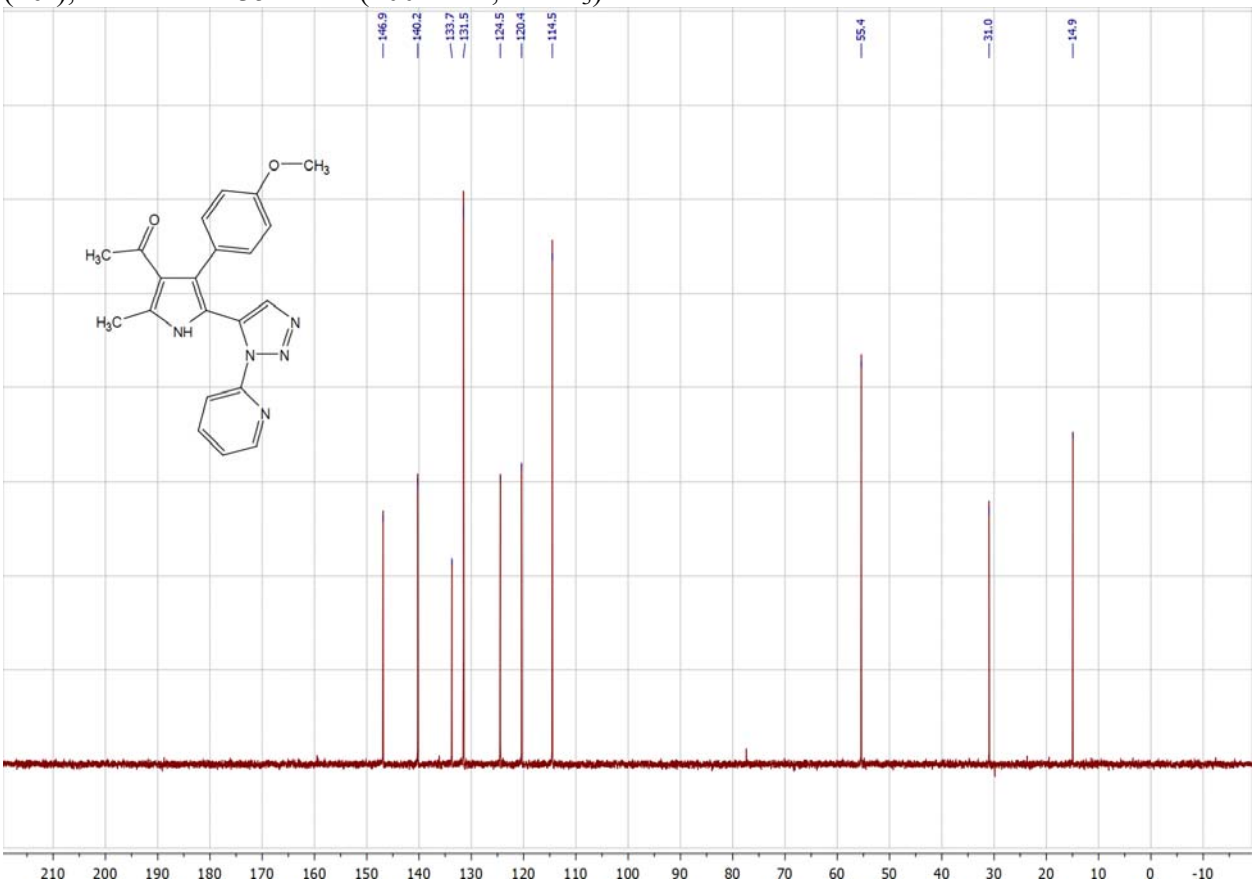
1-(4-(4-Methoxyphenyl)-2-methyl-5-(1-(pyridin-2-yl)-1H-1,2,3-triazol-5-yl)-1H-pyrrol-3-yl)ethan-1-one (**20f**), ^{1}H NMR (400 MHz, $CDCl_3$)



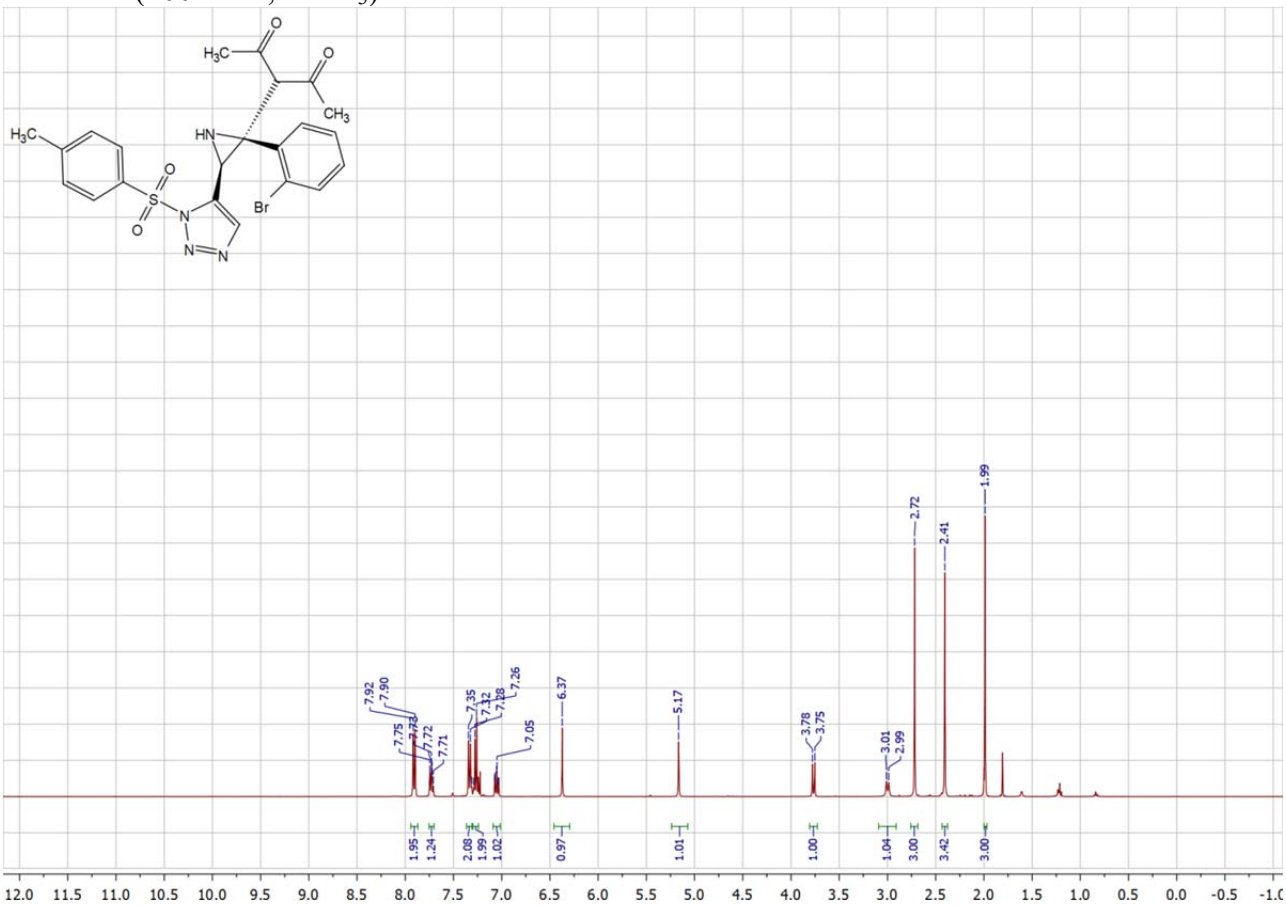
1-(4-(4-Methoxyphenyl)-2-methyl-5-(1-(pyridin-2-yl)-1H-1,2,3-triazol-5-yl)-1H-pyrrol-3-yl)ethan-1-one (**20f**), $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



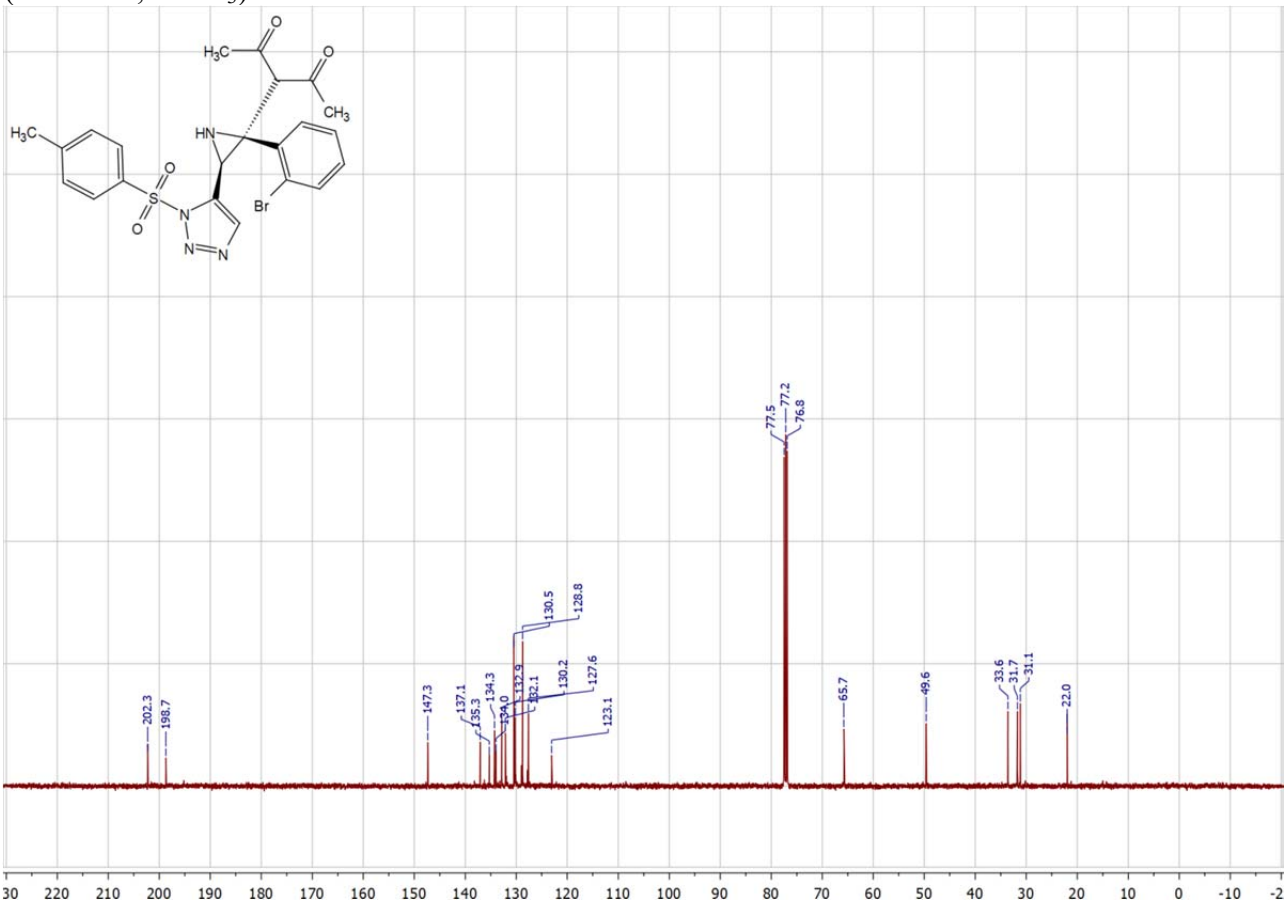
1-(4-(4-Methoxyphenyl)-2-methyl-5-(1-(pyridin-2-yl)-1H-1,2,3-triazol-5-yl)-1H-pyrrol-3-yl)ethan-1-one (**20f**), ^{13}C DEPT 135 NMR (100 MHz, $CDCl_3$)



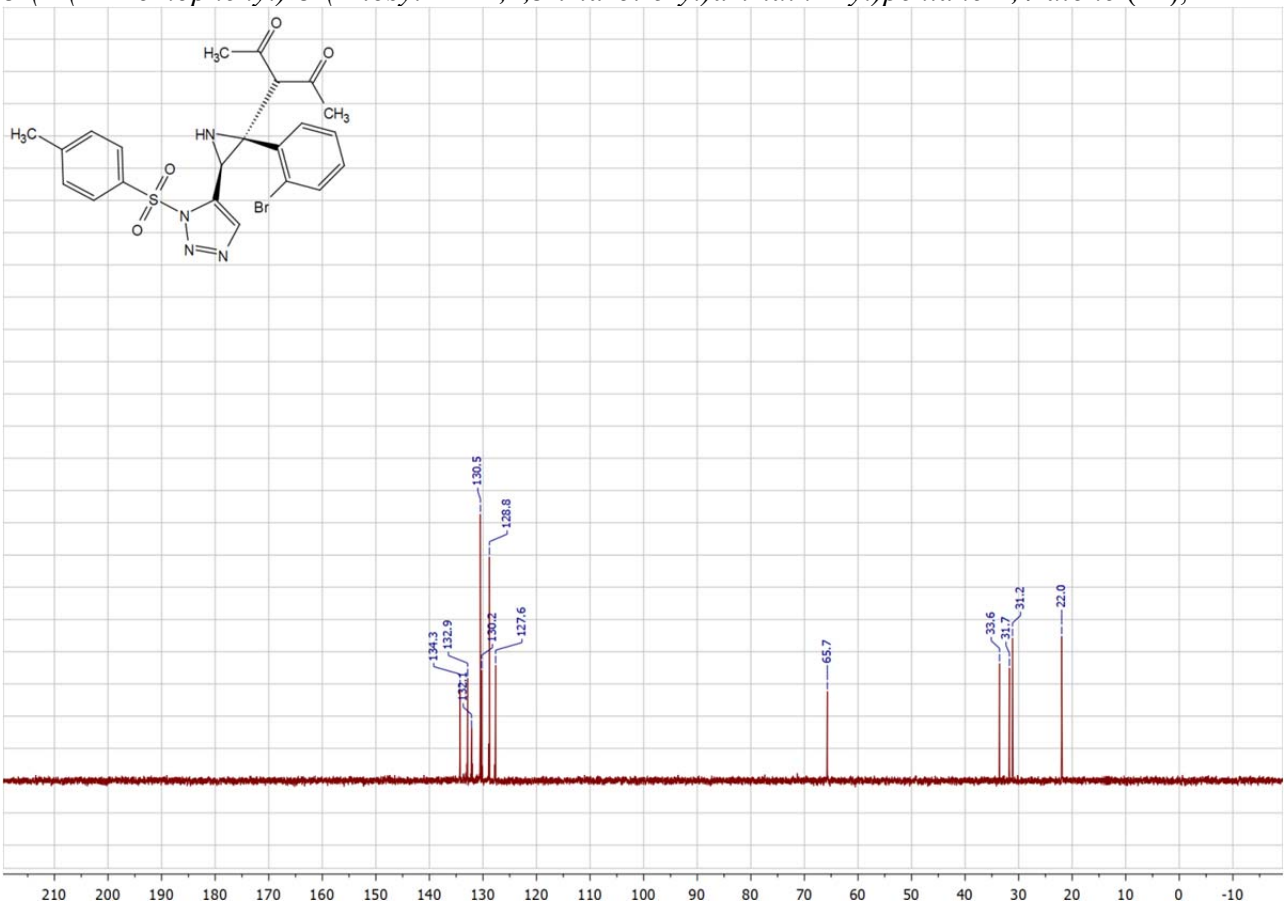
3-(2-(2-Bromophenyl)-3-(1-tosyl-1H-1,2,3-triazol-5-yl)aziridin-2-yl)pentane-2,4-dione (**21**), ^{1}H NMR (400 MHz, $CDCl_3$)



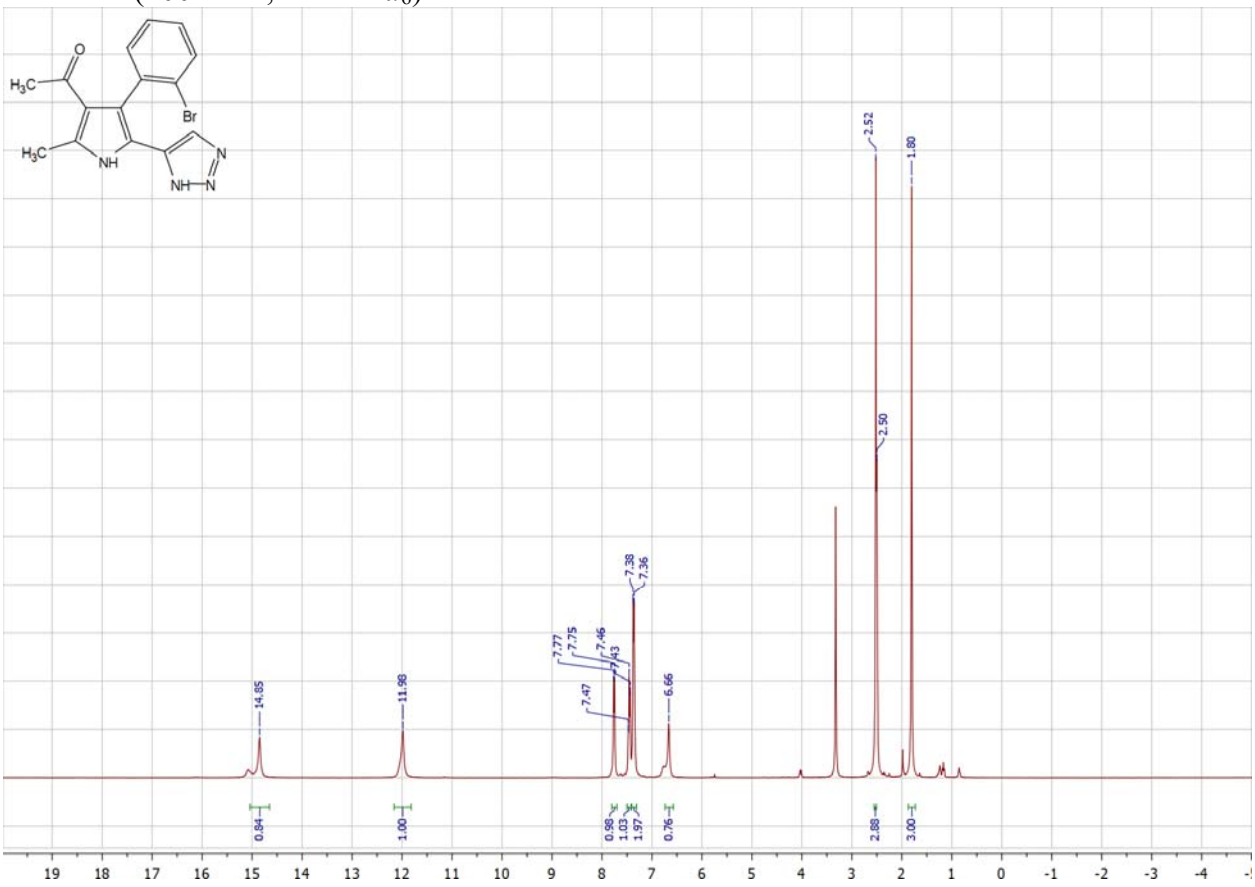
3-(2-(2-Bromophenyl)-3-(1-tosyl-1H-1,2,3-triazol-5-yl)aziridin-2-yl)pentane-2,4-dione (**21**), $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



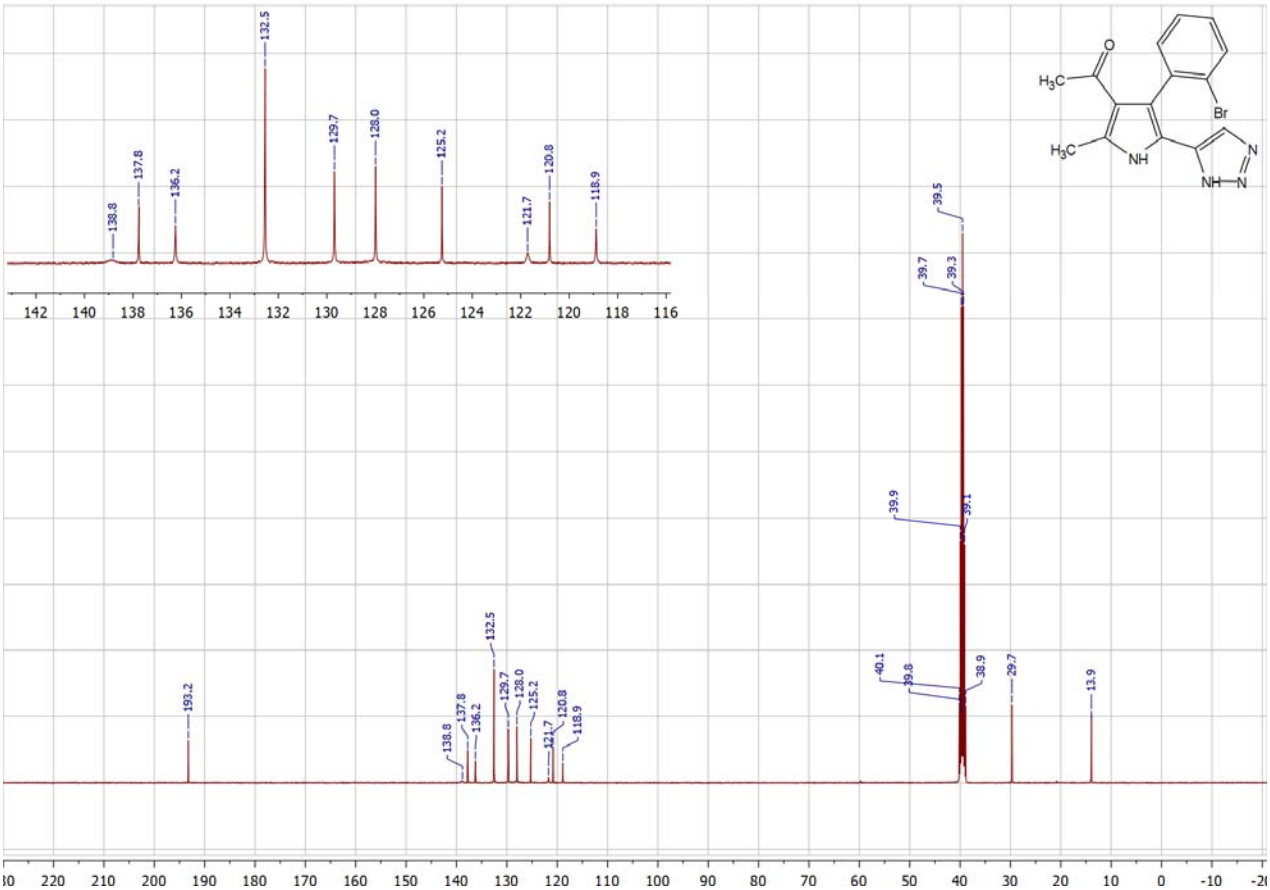
3-(2-(2-Bromophenyl)-3-(1-tosyl-1H-1,2,3-triazol-5-yl)aziridin-2-yl)pentane-2,4-dione (**21**), ^{13}C DEPT



1-(4-(2-Bromophenyl)-2-methyl-5-(1H-1,2,3-triazol-5-yl)-1H-pyrrol-3-yl)ethan-1-one (**22**), ^{1}H NMR (400 MHz, DMSO-d_6)

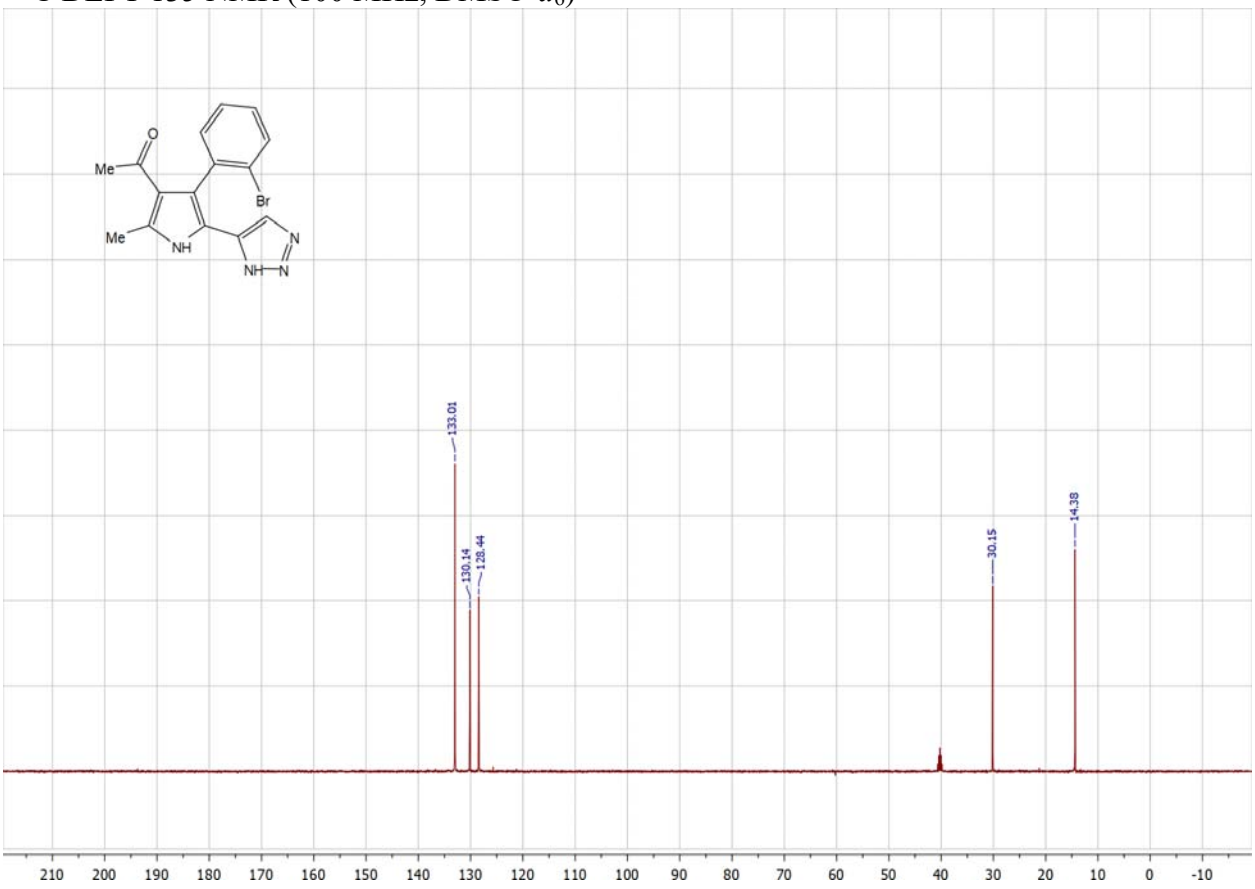


1-(4-(2-Bromophenyl)-2-methyl-5-(1H-1,2,3-triazol-5-yl)-1H-pyrrol-3-yl)ethan-1-one (**22**), ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6)

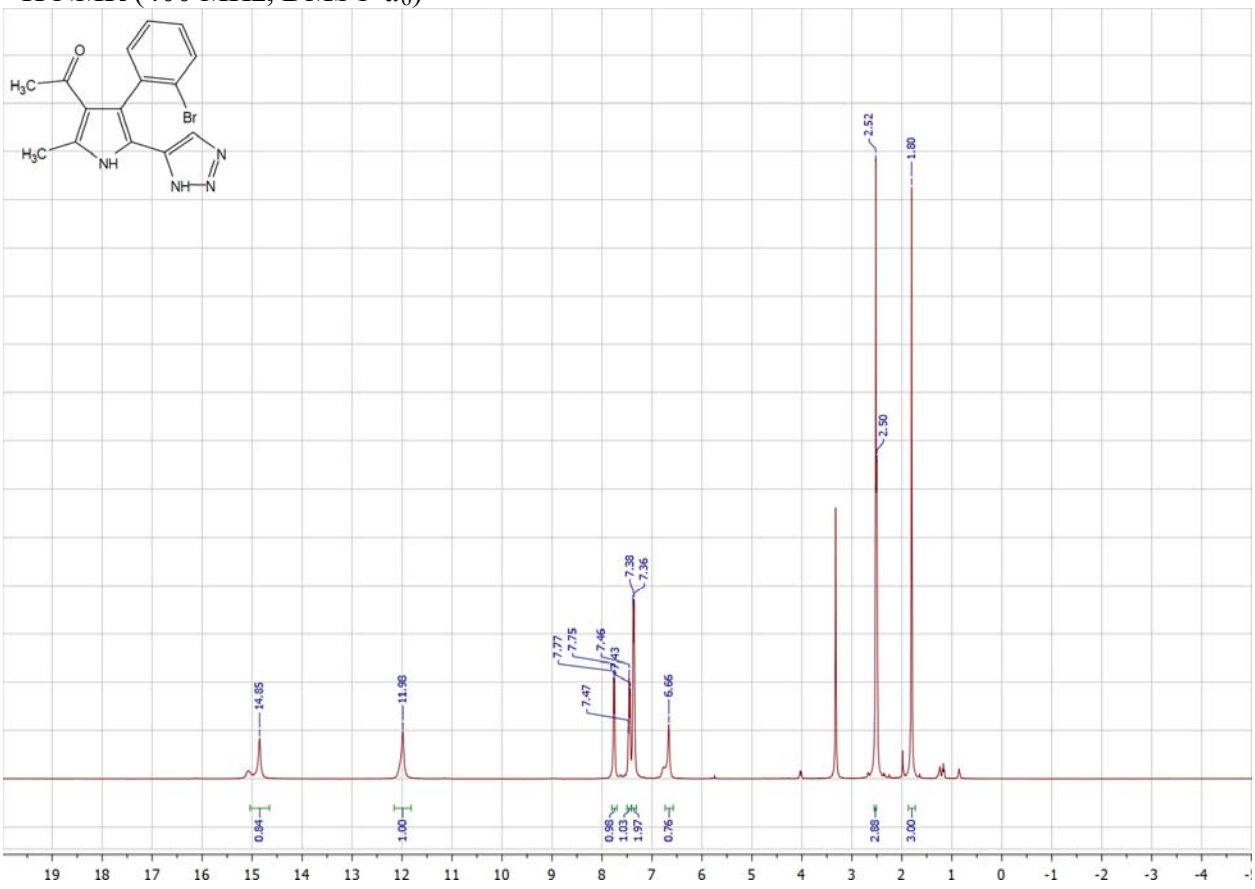


1-(4-(2-Bromophenyl)-2-methyl-5-(1H-1,2,3-triazol-5-yl)-1H-pyrrol-3-yl)ethan-1-one (**22**),

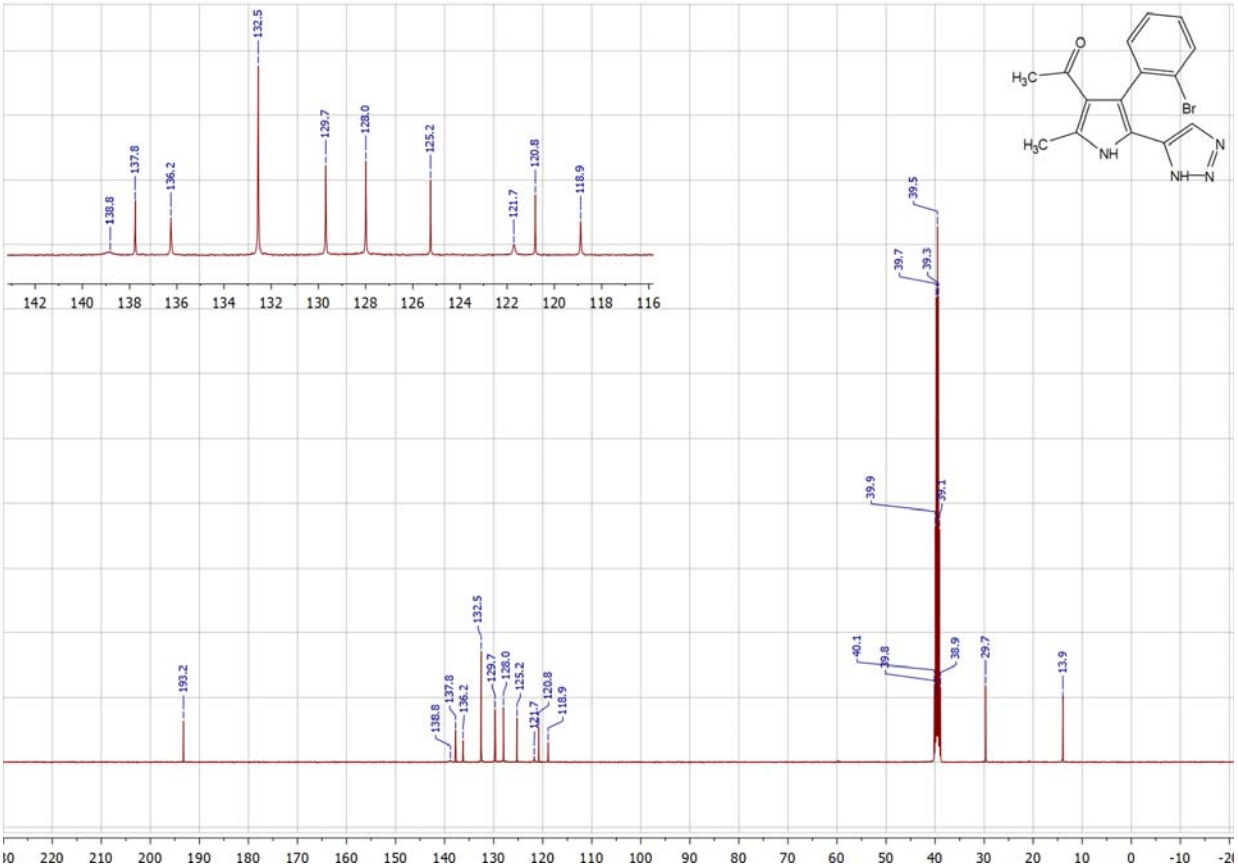
^{13}C DEPT 135 NMR (100 MHz, DMSO-d_6)



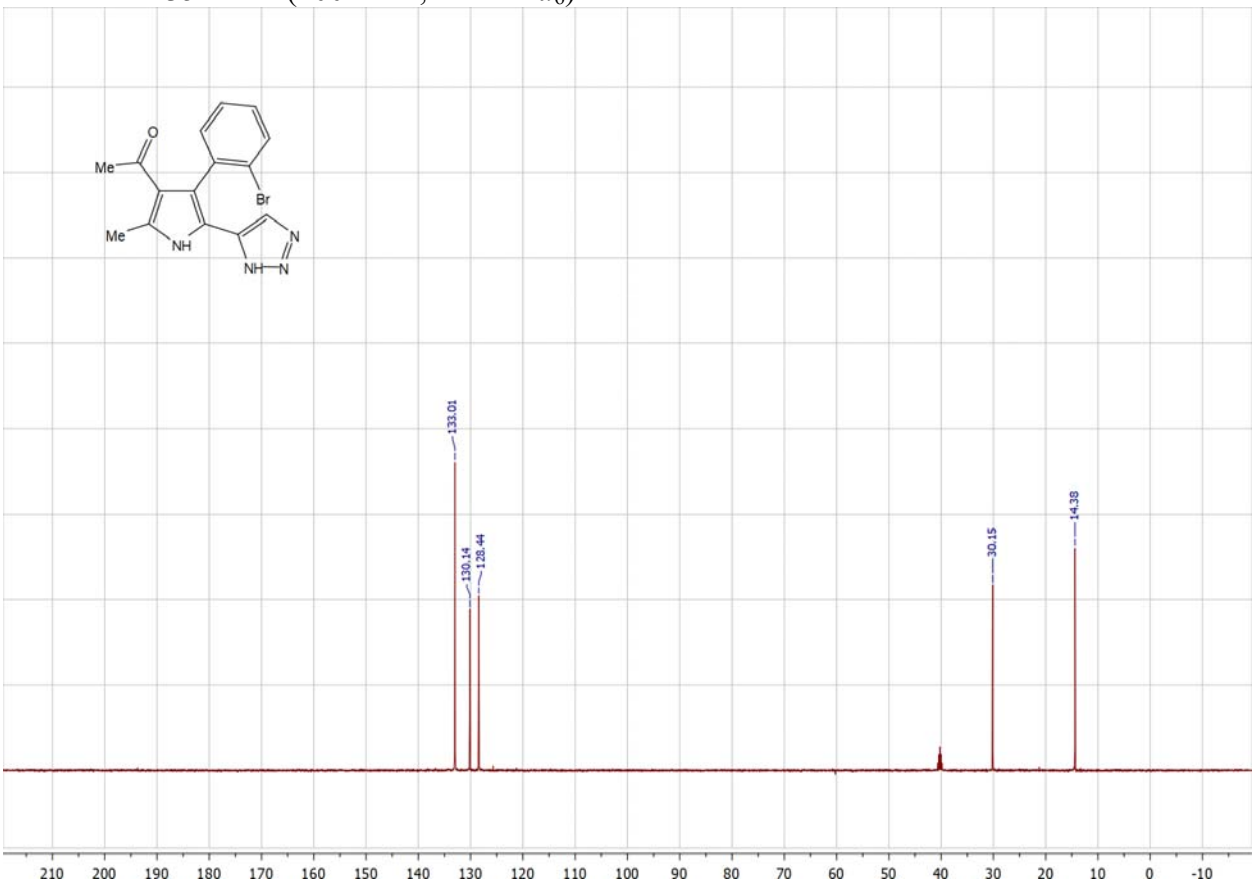
1-(2-Methyl-4-phenyl-5-(1H-1,2,3-triazol-5-yl)-1H-pyrrol-3-yl)ethan-1-one (**23a**),
^{1}H NMR (400 MHz, DMSO-d_6)



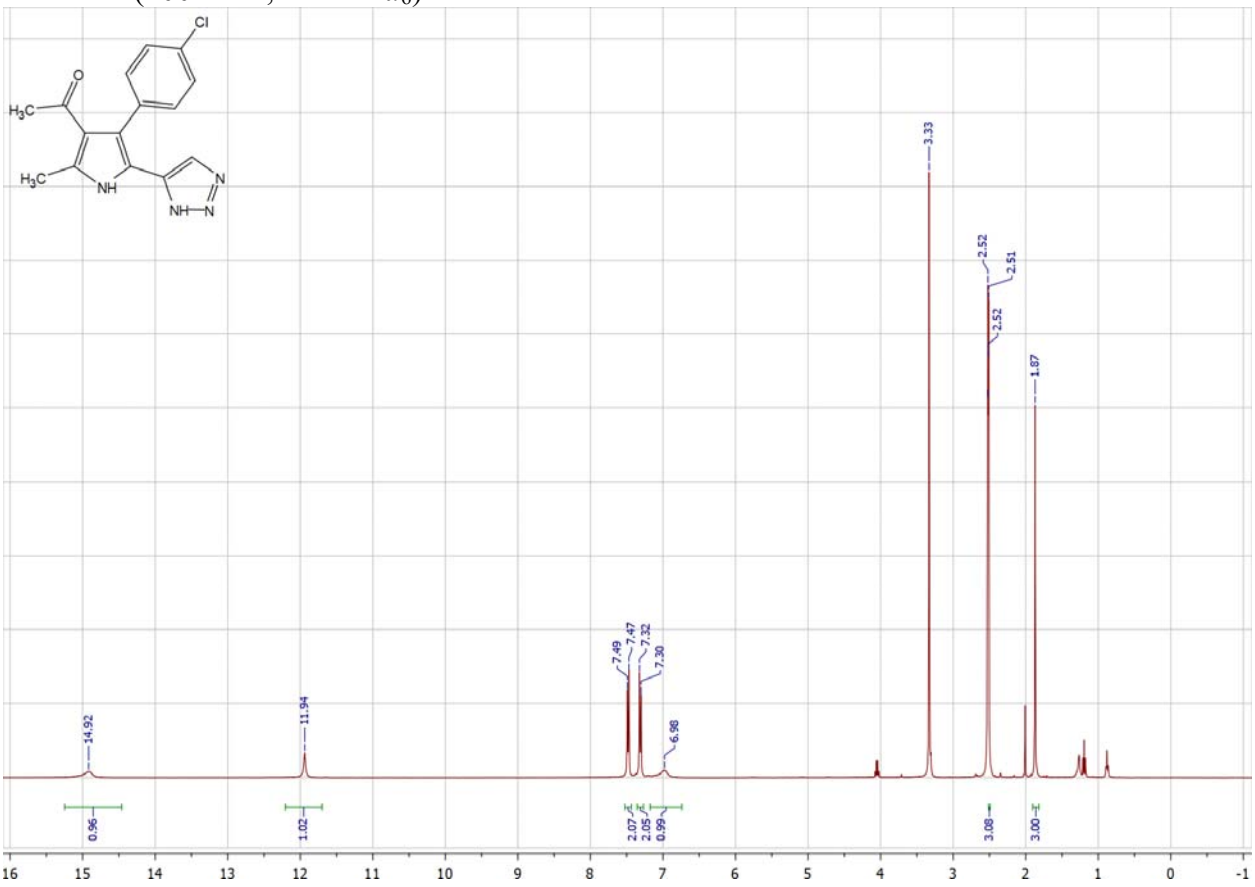
1-(2-Methyl-4-phenyl-5-(1H-1,2,3-triazol-5-yl)-1H-pyrrol-3-yl)ethan-1-one (**23a**),
^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6)



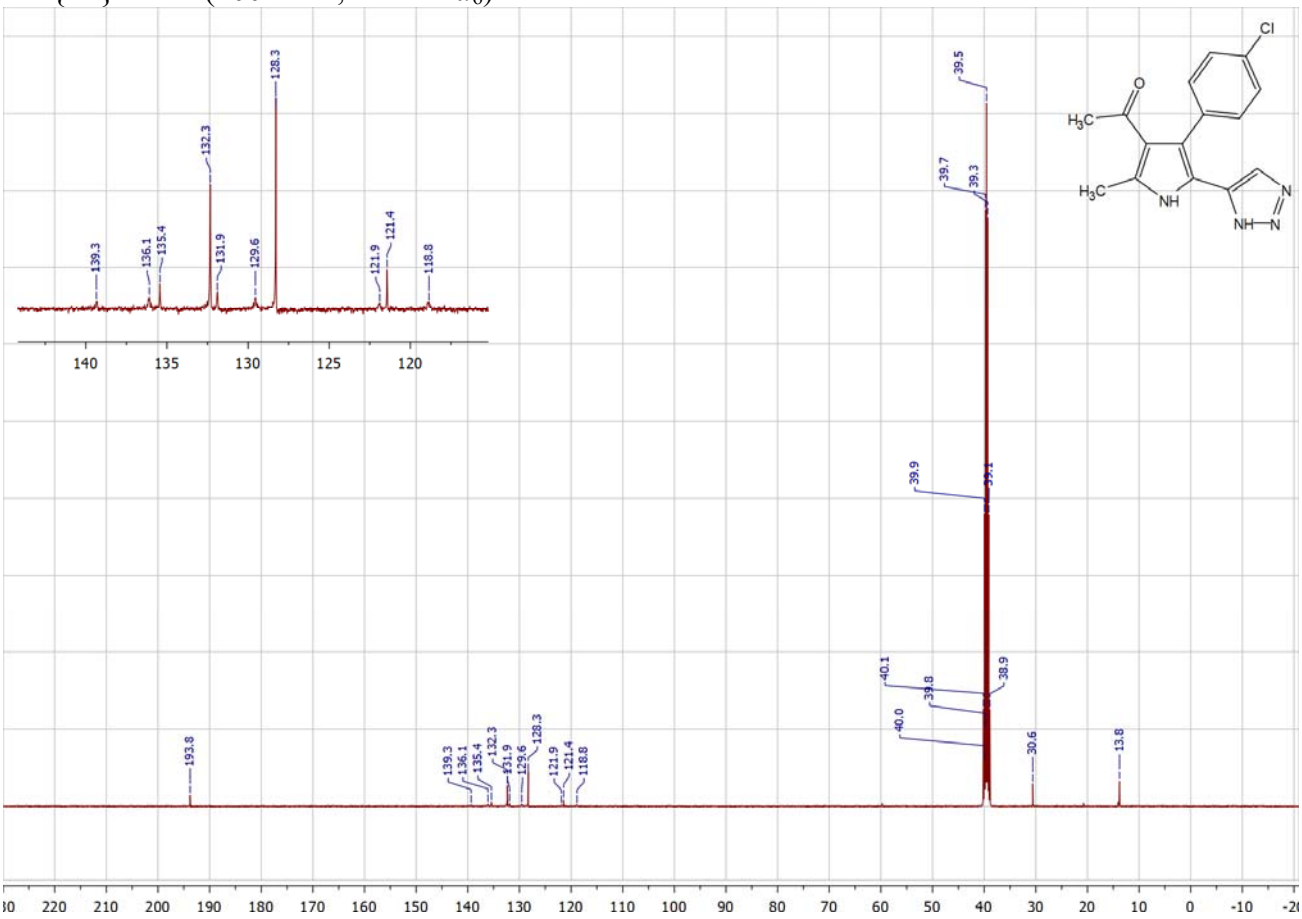
1-(2-Methyl-4-phenyl-5-(1H-1,2,3-triazol-5-yl)-1H-pyrrol-3-yl)ethan-1-one (**23a**),
^{13}C DEPT 135 NMR (100 MHz, DMSO-d_6)



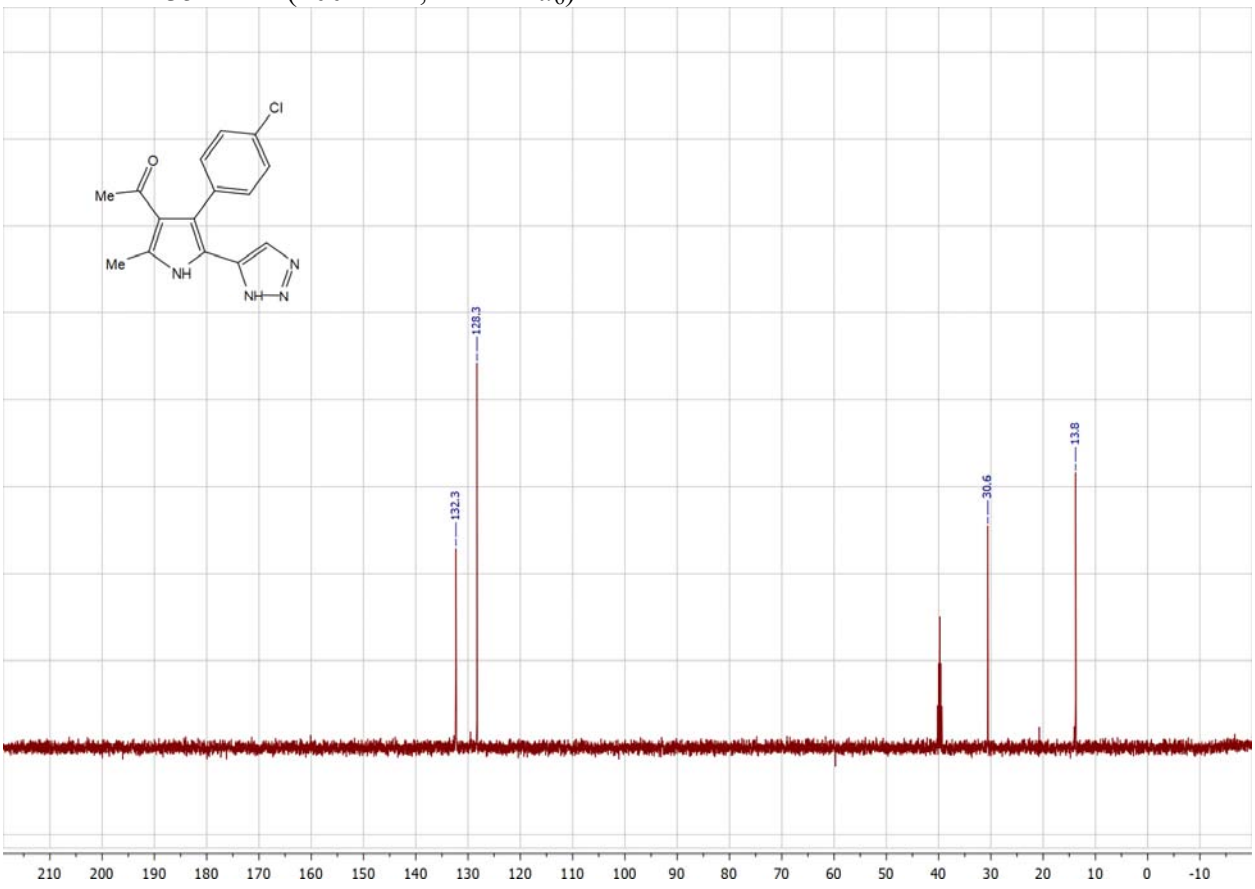
1-(4-(4-Chlorophenyl)-2-methyl-5-(1H-1,2,3-triazol-5-yl)-1H-pyrrol-3-yl)ethan-1-one (**23b**), ^{1}H NMR (400 MHz, DMSO-d_6)



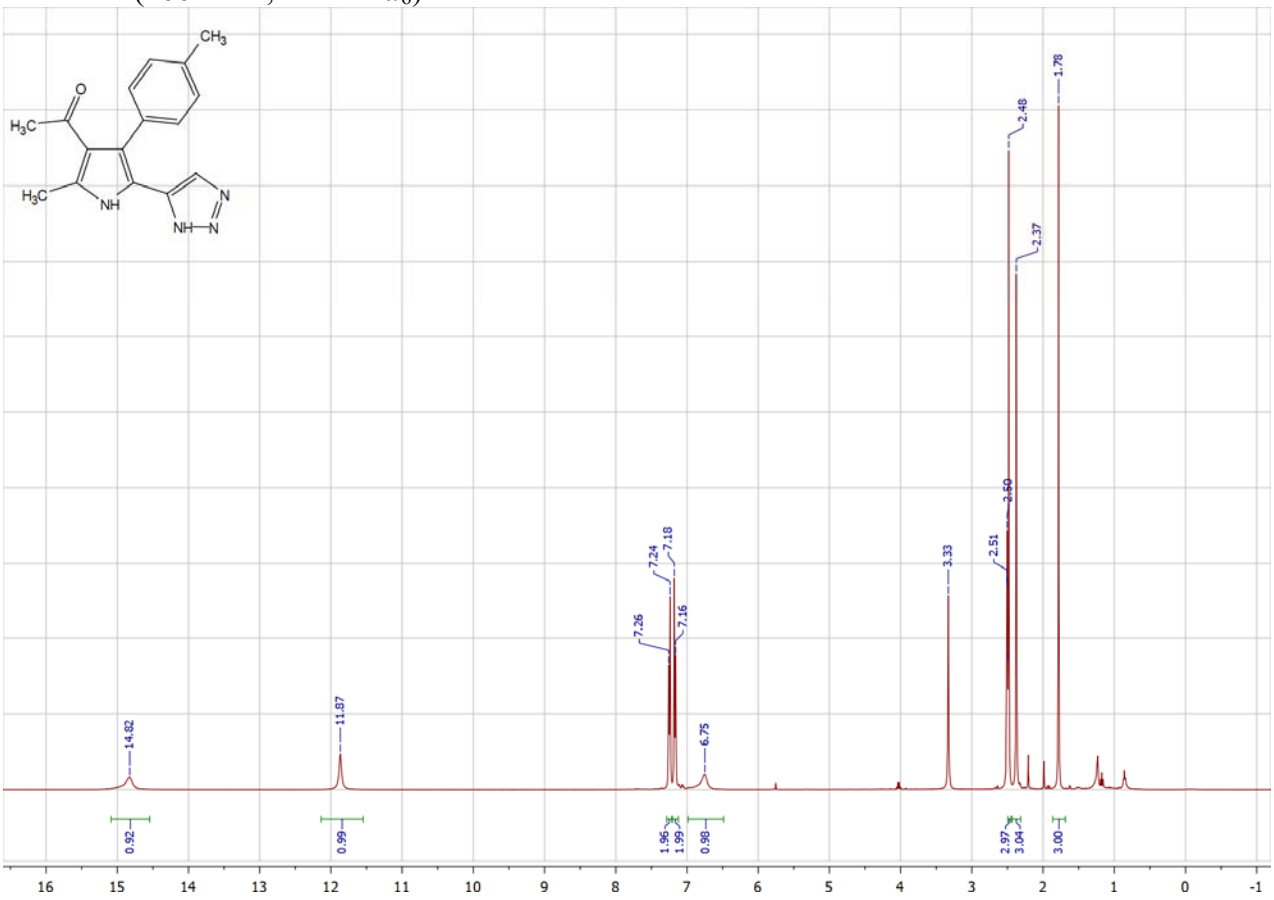
1-(4-(4-Chlorophenyl)-2-methyl-5-(1H-1,2,3-triazol-5-yl)-1H-pyrrol-3-yl)ethan-1-one (**23b**), ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6)



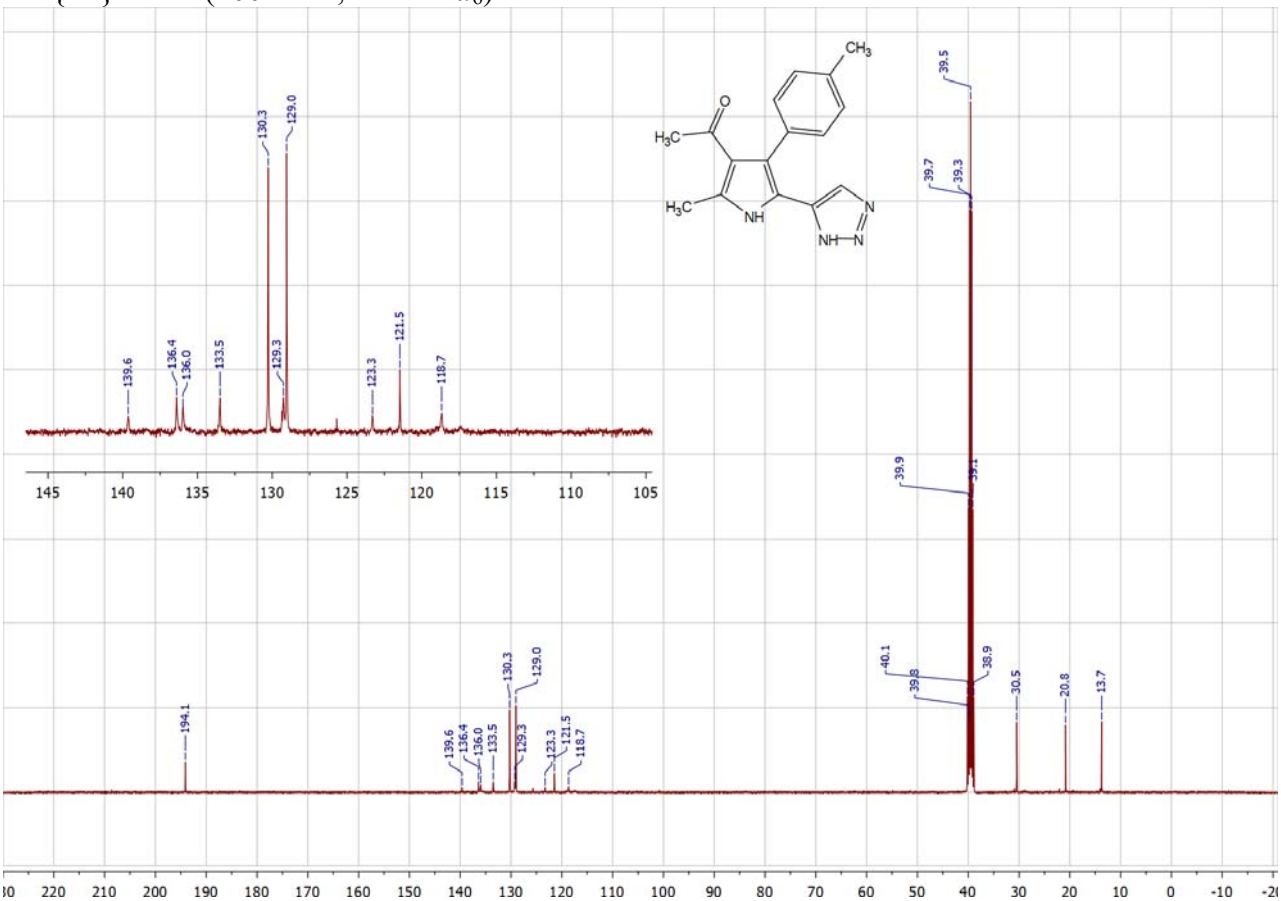
1-(4-(4-Chlorophenyl)-2-methyl-5-(1H-1,2,3-triazol-5-yl)-1H-pyrrol-3-yl)ethan-1-one (**23b**), ^{13}C DEPT 135 NMR (100 MHz, DMSO-d_6)



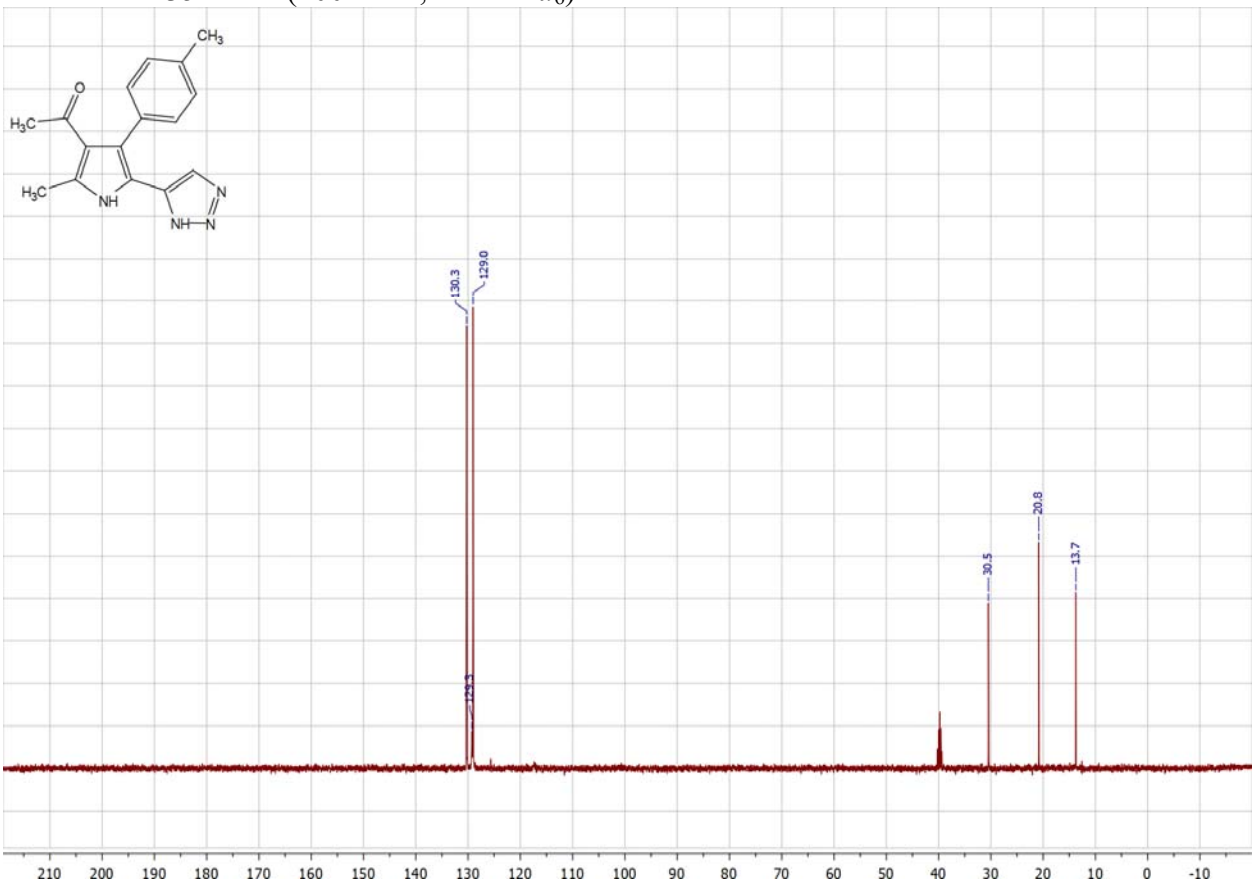
1-(2-Methyl-4-(p-tolyl)-5-(1H-1,2,3-triazol-5-yl)-1H-pyrrol-3-yl)ethan-1-one (**23c**),
^{1}H NMR (400 MHz, DMSO-d_6)



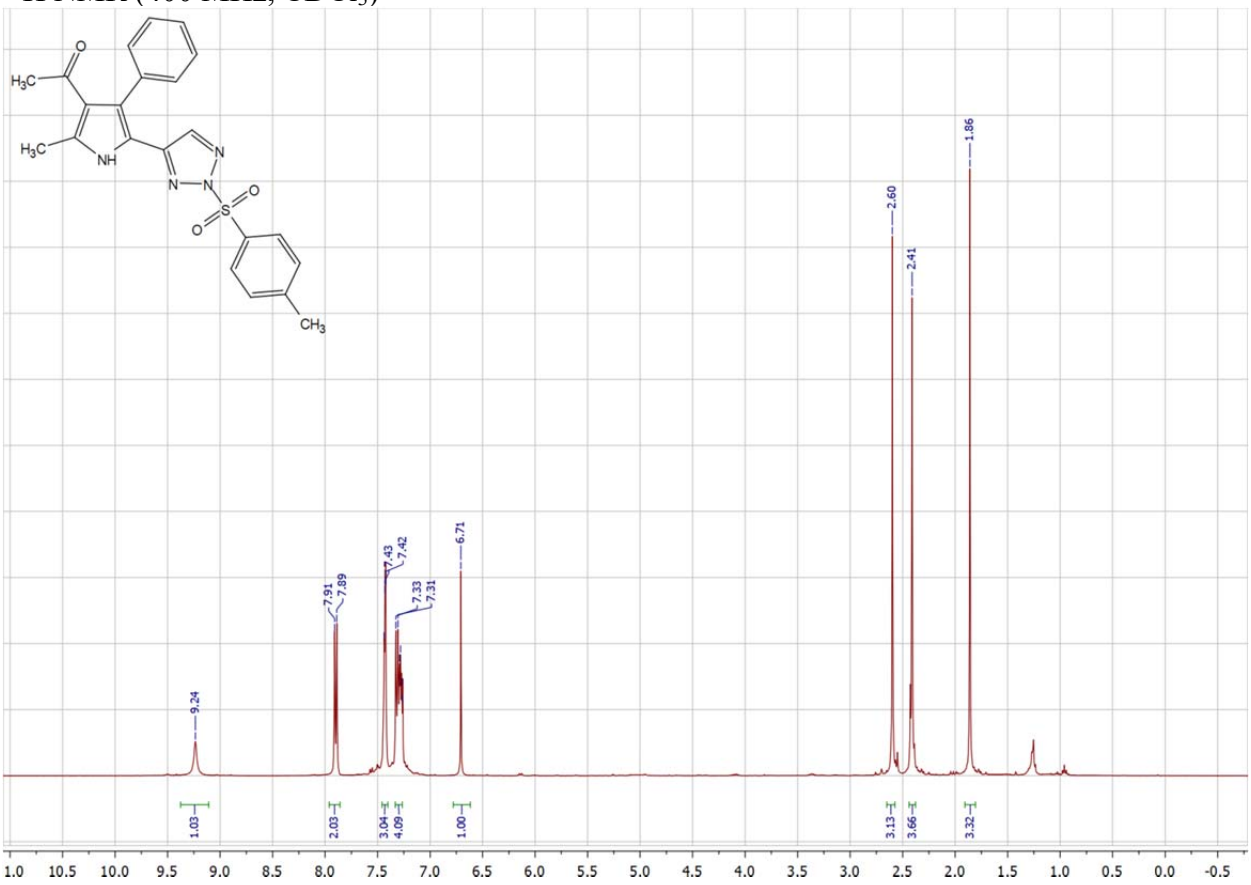
1-(2-Methyl-4-(p-tolyl)-5-(1H-1,2,3-triazol-5-yl)-1H-pyrrol-3-yl)ethan-1-one (**23c**),
^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6)



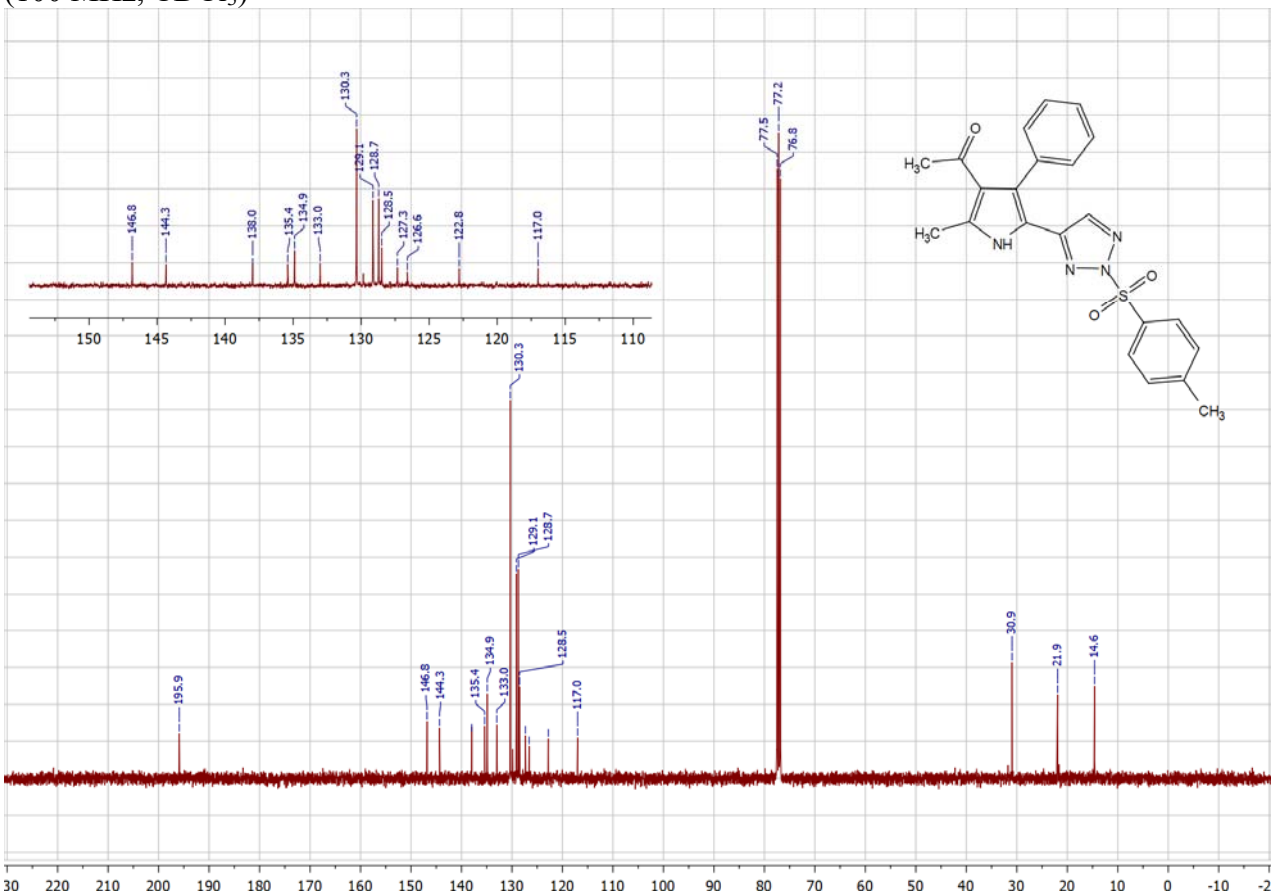
1-(2-Methyl-4-(p-tolyl)-5-(1H-1,2,3-triazol-5-yl)-1H-pyrrol-3-yl)ethan-1-one (**23c**),
^{13}C DEPT 135 NMR (100 MHz, DMSO-d_6)



1-(2-Methyl-4-phenyl-5-(2-tosyl-2H-1,2,3-triazol-4-yl)-1H-pyrrol-3-yl)ethan-1-one (**24**), ^{1}H NMR (400 MHz, $CDCl_3$)



1-(2-Methyl-4-phenyl-5-(2-tosyl-2H-1,2,3-triazol-4-yl)-1H-pyrrol-3-yl)ethan-1-one (**24**), $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



1-(2-Methyl-4-phenyl-5-(2-tosyl-2H-1,2,3-triazol-4-yl)-1H-pyrrol-3-yl)ethan-1-one (**24**),
^{13}C DEPT 135 NMR (100 MHz, $CDCl_3$)