Supplementary Material

Methyl Nitrate Energetic Compounds based on Bicyclic Scaffolds of Furazan-Isofurazan (isoxazole): Syntheses, Crystal structures and Detonation Performances

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Table S1. Crystallographic parameters data for compound **1d** and **2e**

Compound	1d	2e
Formula	$C_6H_7N_7O_7$	$C_5H_6N_8O_7$
Molecular mass	289.19	290.18
Crystal system	Monoclinic	monoclinic
Space group	$P2_1$	$P2_1/c$
a/Å	7.1382(9)	15.3710(8)
b/Å	5.2760(7)	9.1833(4)
c/Å	15.469(2)	7.7679(4)
α/°	90	90
β/°	91.730(5)	91.405(4)
γ/°	90	90
Volume/Å^3	582.33(13)	1096.16(9)
Z	2	4
Temperature(K)	180(2)	150.0
ρ_{calc}(g/cm^3)	1.649	1.758
μ/mm^{-1}	0.848	1.447
F(000)	296.0	592.0
Crystal size	0.2 × 0.15 × 0.11	0.2 × 0.15 × 0.1
Reflections collected	5859	7421
Radiation	Ga Kα (λ = 0.134139)	Cu Kα (λ = 1.54178)
Goodness-of-fit on F^2	1.116	1.101
Final R indexes [I>=2σ (I)]	R_1 = 0.0832, wR_2 = 0.2490	R_1 = 0.0905, wR_2 = 0.2345
Final R indexes [all data]	R_1 =0.0877, wR_2 = 0.2533	R_1 =0.1006, wR_2 = 0.2469
Data/restraints/parameters	2095/11/198	2161/3/185

Table S2. Bond lengths for compound **1d**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	N3	1.304(8)	C6	O5	1.447(8)
C1	N2	1.373(7)	N1	O2	1.249(6)
C1	C2	1.442(8)	N1	O1	1.269(6)
C2	N4	1.297(8)	N1	N2	1.317(6)
C2	C3	1.472(8)	N3	O3	1.427(7)
C3	N5	1.308(8)	N4	O3	1.373(7)
C3	C4	1.407(8)	N5	O4	1.399(6)
C4	C5	1.321(9)	N6	O6	1.201(9)
C5	O4	1.377(8)	N6	O7	1.213(9)

Table S3. Bond angles for compound **1d**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N3	C1	N2	131.8(5)	O2	N1	O1	119.8(4)
N3	C1	C2	108.4(5)	O2	N1	N2	124.5(5)
N2	C1	C2	119.8(5)	O1	N1	N2	115.7(4)
N4	C2	C1	109.7(5)	N1	N2	C1	115.6(4)
N4	C2	C3	119.6(5)	C1	N3	O3	105.6(5)
C1	C2	C3	130.8(5)	C2	N4	O3	106.6(5)
N5	C3	C4	112.0(5)	C3	N5	O4	105.2(5)
N5	C3	C2	121.8(5)	O6	N6	O7	130.0(7)
C4	C3	C2	126.3(5)	O6	N6	O5	118.2(6)
C5	C4	C3	105.3(6)	O7	N6	O5	111.8(7)
C4	C5	O4	109.4(5)	N4	O3	N3	109.7(4)
C4	C5	C6	136.0(6)	C5	O4	N5	108.1(5)
O4	C5	C6	114.6(6)	N6	O5	C6	114.9(5)
O5	C6	C5	110.7(5)				

Table S4. Dihedral angles for compound **1d**.

Atom	Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Atom	Angle/°
C1	C2	C3	C4	167.944 (579)	C2	C1	N2	N1	-173.473 (461)
C1	N2	N1	O1	-176.933 (445)	O4	N5	C3	C2	-178.591 (476)
C4	C5	C6	O5	105.398 (870)	C6	C5	C4	C3	178.687 (717)
C5	C6	O5	N6	-80.092 (669)	C6	O5	N6	O7	177.559 (647)

Table S5. Hydrogen bonds for compound **1d**.

Donor atom	Accept atom	Length/Å	Angle/°
N7-H6	O3	3.353	108.324 (142)
N7-H6	N1	3.051	108.149 (130)
N7-H7	N1	2.995	169.925 (234)
N7-H8	N5	2.595	115.475 (251)
N7-H6	N3	2.281	103.966 (143)
N7-H6	O2	2.193	98.846 (157)
N7-H7	O3	2.684	112.926 (357)
C6-H6A	O5	3.215	156.366 (221)
C6-H6A	O3	3.021	122.229 (380)
C6-H6B	O4	2.752	149.719 (431)
C6-H6A	N4	2.512	148.970 (403)

Table S6. Bond lengths for compound **2e**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O7	N7	1.2715	N7	N6	1.3105
O4	C2	1.3609	N6	C5	1.3815
O4	C3	1.3561	N5	C5	1.3059
O5	N5	1.3986	N4	C4	1.2952
O5	N4	1.3657	N3	N2	1.4005
O3	N1	1.4103	N3	C3	1.2877
O3	C1	1.4557	N2	C2	1.2763
O2	N1	1.2004	C4	C5	1.4412
O6	N7	1.2466	C4	C3	1.4543
O1	N1	1.1982	C2	C1	1.4850

Table S7. Dihedral angles for compound **2e**.

Atom	Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Atom	Angle/°
C5	N6	N7	O6	2.025 (6)	O4	C3	C4	C5	170.362 (3)
C5	N5	O5	N4	1.614 (4)	C3	O4	C2	C1	176.690 (3)
O4	C2	C1	O3	72.788 (4)	C2	C1	O3	N1	170.315 (4)
N2	O2	C1	O3	-111.138 (4)					

Table S8. Bond angles for compound **2e**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C3	O4	C2	102.0	N4	C4	C5	109.9
N4	O5	N5	111.6	N4	C4	C3	121.3
N1	O3	C1	112.0	C5	C4	C3	128.7
O7	N7	N6	114.8	N6	C5	C4	120.4
O6	N7	O7	120.1	N5	C5	N6	131.5
O6	N7	N6	125.1	N5	C5	C4	108.1
N7	N6	C5	116.1	O4	C2	C1	119.3
O2	N1	O3	117.3	N2	C2	O4	113.0
O1	N1	O3	112.7	N2	C2	C1	127.6
O1	N1	O2	130.0	O4	C3	C4	118.2
C5	N5	O5	105.0	N3	C3	O4	112.7
C4	N4	O5	105.3	N3	C3	C4	129.0
C3	N3	N2	106.0	O3	C1	C2	105.9
C2	N2	N3	106.2				

Table S9. Hydrogen bonds for compound **2e**.

Donor atom	Accept atom	Length/Å	Angle/°
N8-H3	N2	3.087	126.613 (4)
N8-H4	O6	2.760	124.258 (3)
N8-H5	N7	2.726	132.993 (4)
N8-H4	N7	2.718	150.521 (3)
N8-H2	N5	2.366	150.480 (4)
N8-H2	N3	2.239	157.061 (3)
N8-H5	O7	2.127	135.438 (4)
C1-H1B	O1	2.911	152.932 (4)
C1-H1A	N4	2.772	162.022 (6)

Table S10. Kinetic parameters and enthalpies of thermal decomposition of **1d**, **2e** and **3e**[a].

	β_i (K min^{-1})	T_p (K)	E_k (kJ mol^{-1})	r	log A_k (s^{-1})
1d	2.5	405.81	148.5712	0.997	15.51
	5	412.27			
	10	417.91			
	15	422.51			
3e	2.5	399.97	148.9869	0.992	16.12
	5	400.51			
	10	406.11			
	15	411.03			
2e	2.5	397.97	186.907	0.996	21.87
	5	402.51			
	10	406.74			
	15	410.34			

[a] E_k is the apparent activation energy; r is the liner correlation coefficient; A_k is pre-exponential factor.

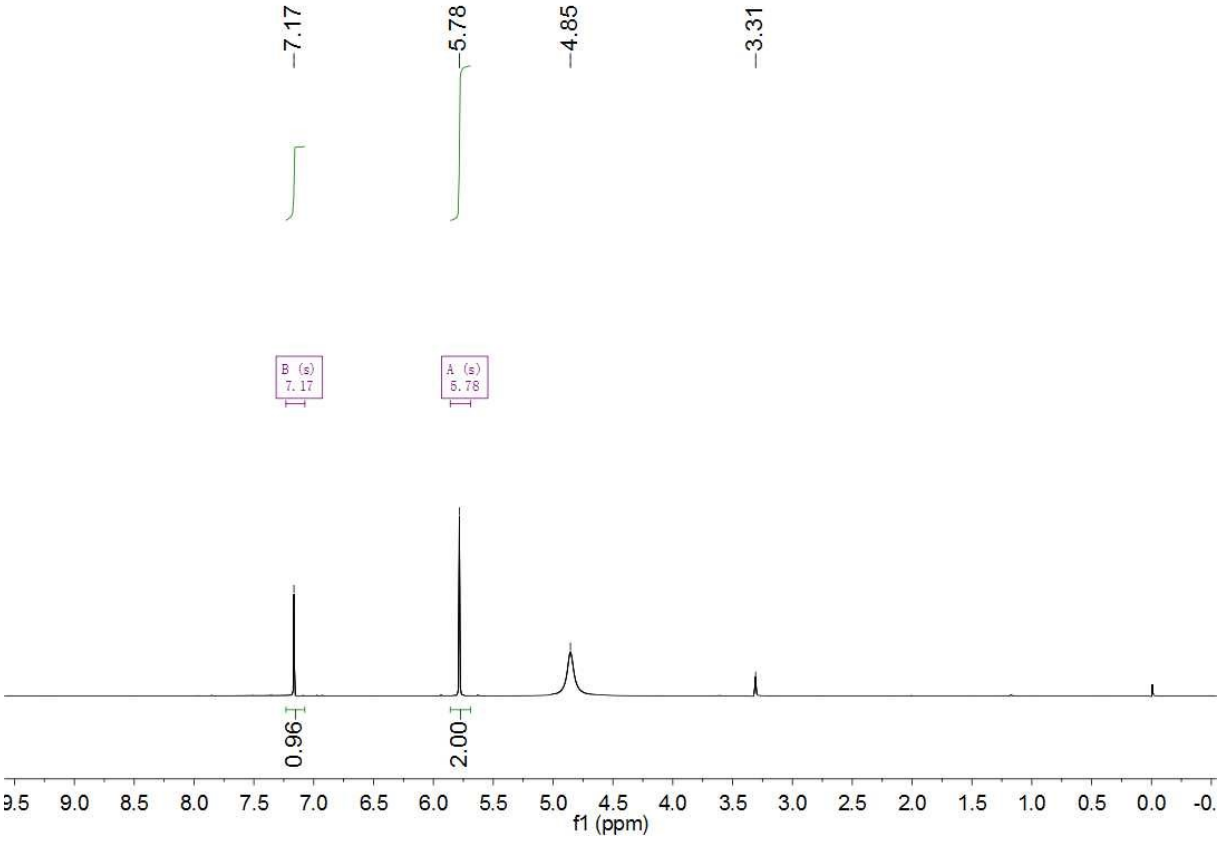

Figure S1. ^{1}H NMR (CD_3OD-d_6, 500 MHz) data of compound **1d.**

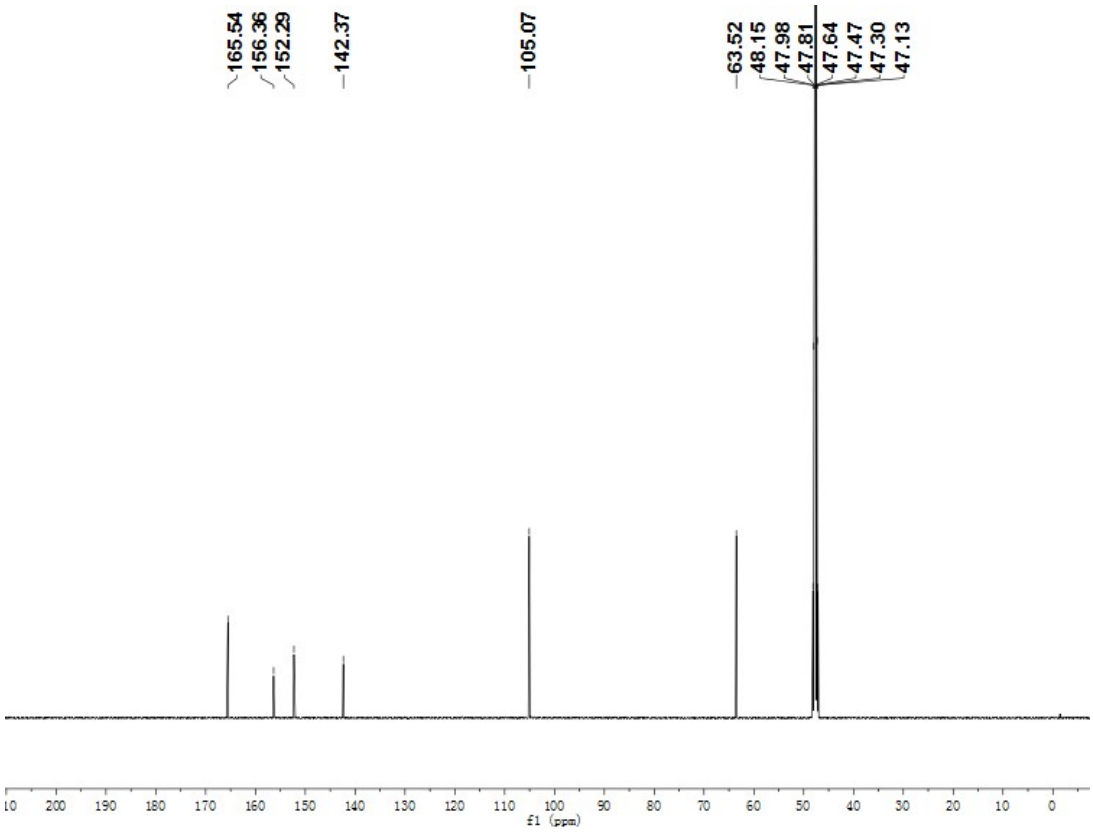

Figure S2. ^{13}C NMR (CD_3OD-d_6, 125 MHz) data of compound **1d**.

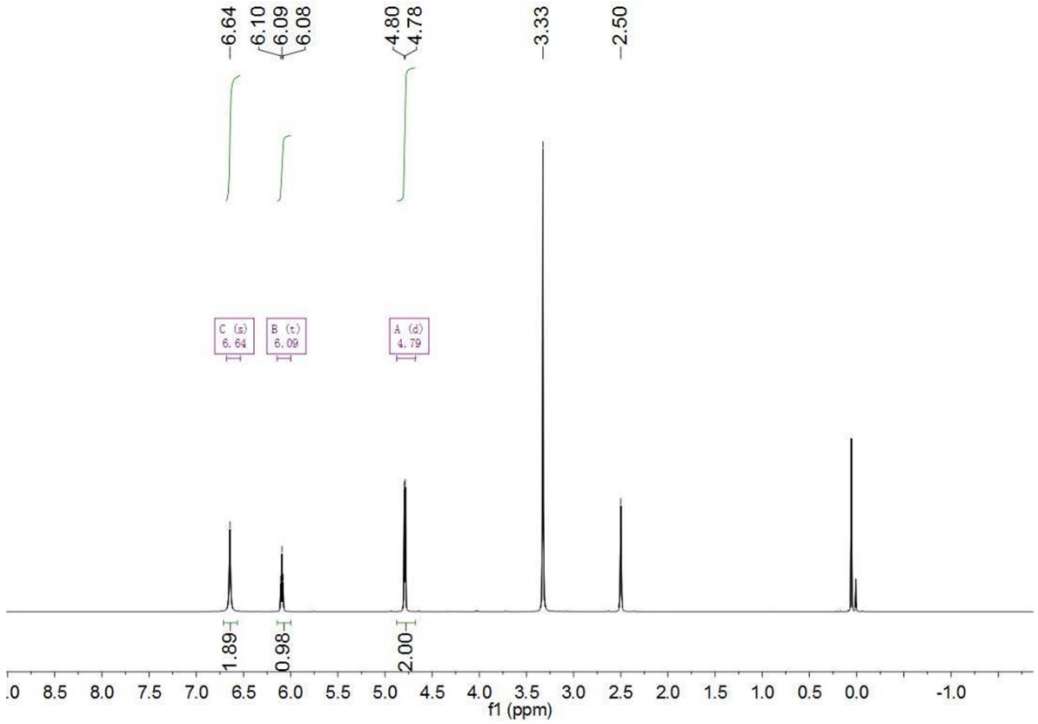

Figure S3. ^{1}H NMR (DMSO-d_6, 500 MHz) data of compound **2b.**

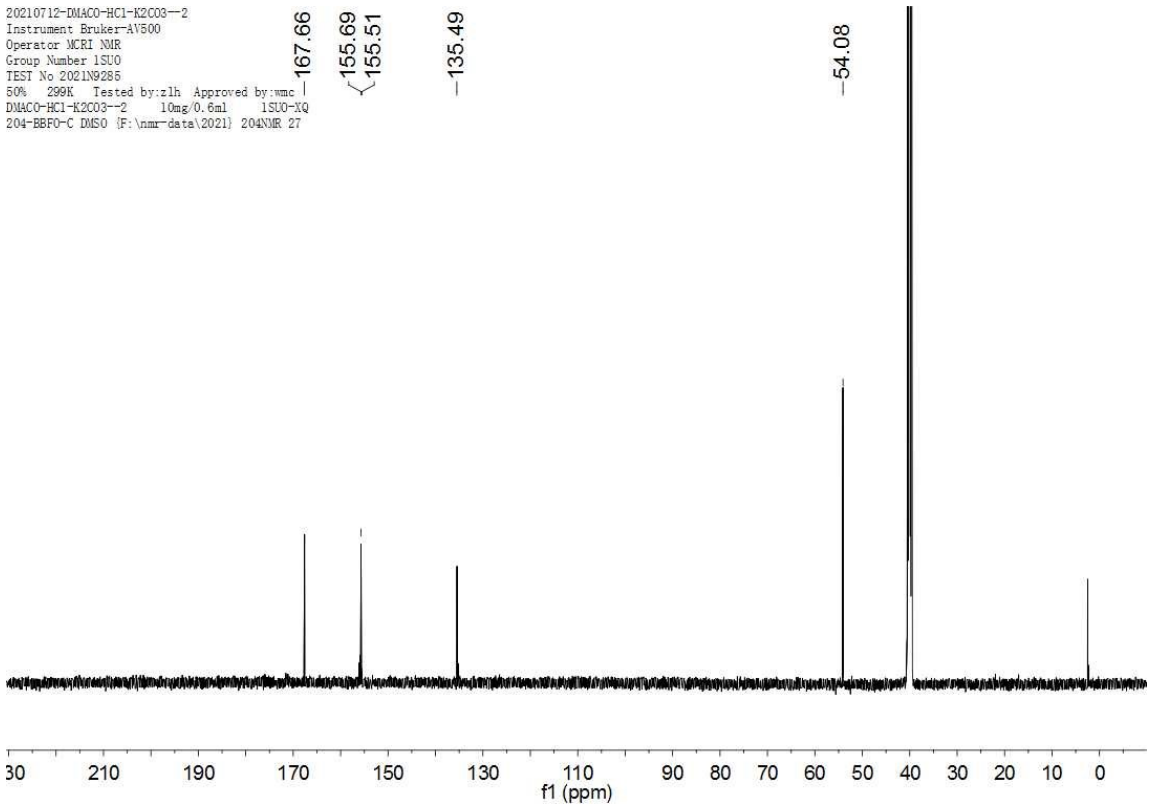

Figure S4. ^{13}C NMR (DMSO-d_6, 125 MHz) data of compound **2b**.

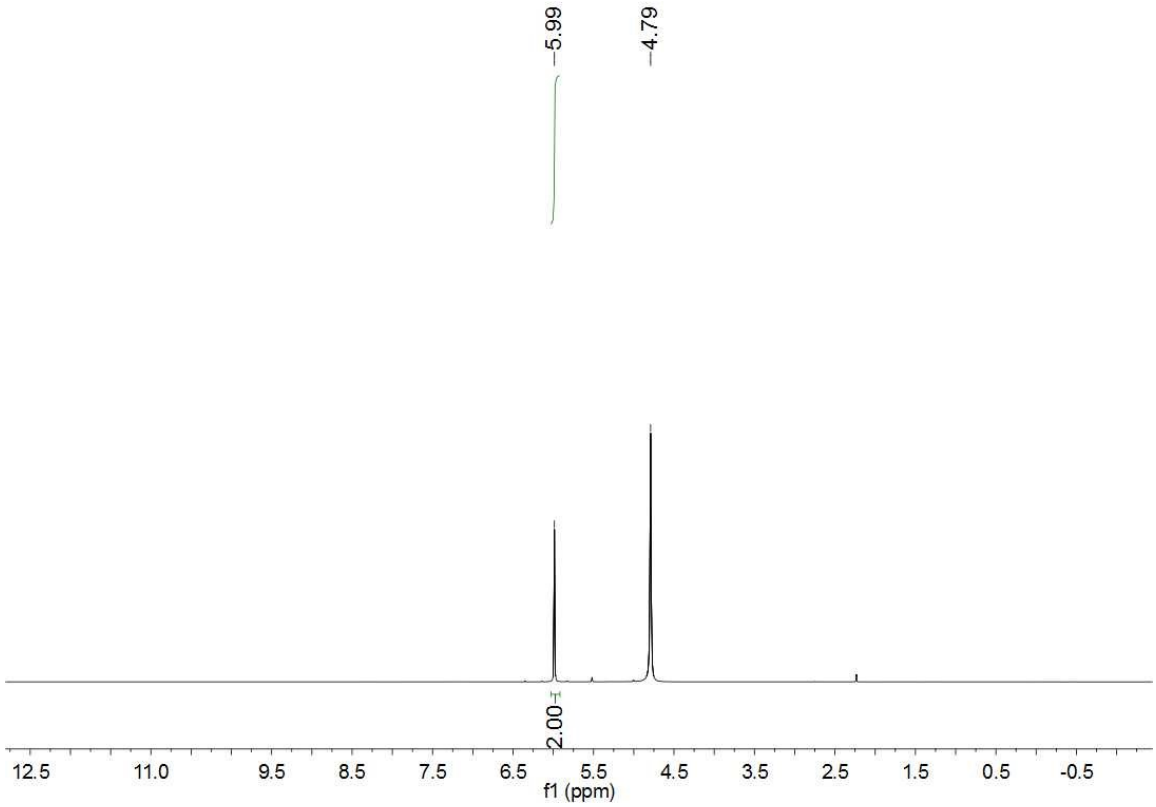

Figure S5. ^{1}H NMR (D_2O, 500 MHz) data of compound **2e**.

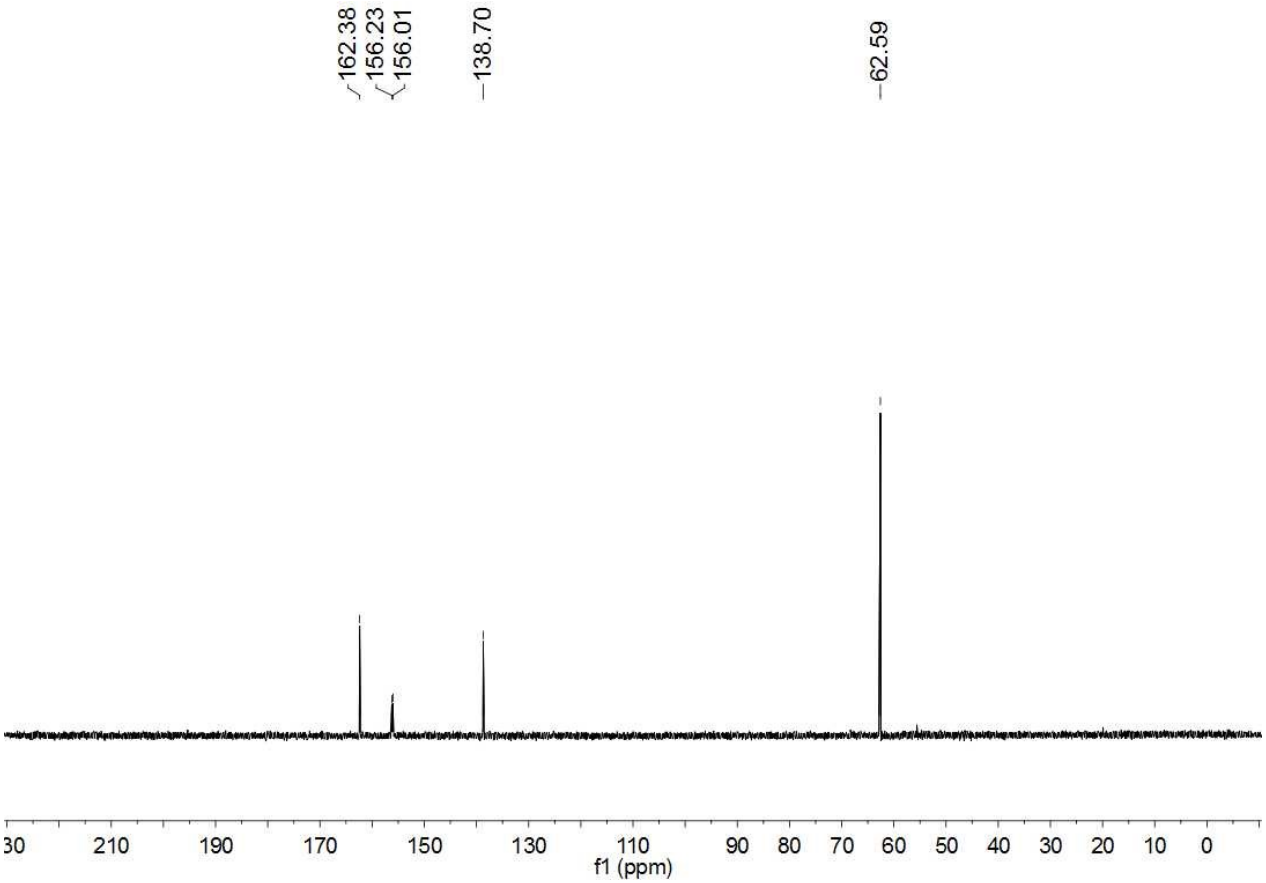

Figure S6. ^{13}C NMR (D_2O, 125 MHz) data of compound **2e**.