Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Novel Ammonium Dichloroacetates With Enhanced Herbicidal Activity For Weed Control

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Supporting Tables

Table S1. The solubilities of **ILs** in different solvents.

ILs	Solvents							
	Water (9.0)	Methanol (6.6)	DMSO (6.5)	Acetonitrile (6.2)	Acetone (5.1)	Isopropanol (4.3)	diethyl ether (2.8)	Toluene (2.3)
IL 1	+	+	+	+	+	+	−	−
IL 2	+	+	+	+	+	+	−	−
IL 3	+	+	+	+	+	+	−	−
IL 4	+	+	+	+	+	+	−	−
IL 5	+	+	+	+	+	+	−	−
IL 6	+	+	+	+	+	+	−	−
IL 7	+	+	+	+	+	+	−	−
IL 8	+	+	+	+	+	+	−	−
IL 9	+	+	+	+	+	+	−	−
IL 10	+	+	+	+	+	+	−	−
IL 11	+	+	+	+	+	+	−	−
IL 12	+	+	+	+	+	+	−	−
IL 13	+	+	+	+	+	+	±	±
IL14	+	+	+	+	+	+	±	±
IL 15	+	+	+	+	+	+	±	±

+, high solubility; ±, medium solubility; −, insoluble.

Table S2. Preliminary screening of herbicidal activity (percent inhibition rate %) of ammonium dichloroacetates ILs at 15 mg ml^{-1}. (21 days after treatment)

ILs	Grass weed		Broadleaf weeds									
	Eleusine indica (L.) Gaerth		*Amaranthus retroflexus L*		*Eclipta prostrata*		*Xanthium sibiricum Patrin ex Widder*		*Chenopodiumalbum L.*		*Solanum nigrum L.*	
	Pre-	*Post-*	*Pre-*	*Post-*	*Pre-*	*Post-*	*Pre-*	*Post-*	*Pre-*	*Post-*	*Pre-*	*Post-*
IL 1	0	0	0	0	0	0	0	0	0	0	0	0
IL 2	0	44	0	50	0	42	0	53	0	73	0	64
IL 3	0	10	0	80	0	4	0	64	0	78	0	59
IL 4	0	0	0	0	0	0	0	0	0	0	0	0
IL 5	0	5	0	0	0	0	0	0	0	0	0	0
IL 6	0	0	0	0	0	0	0	0	0	0	0	0
IL 7	0	0	0	0	0	0	0	0	0	0	0	0
IL 8	0	-44	0	-58	0	-35	0	-48	0	-54	0	-60
IL 9	0	47	0	46	0	56	0	62	0	43	0	38
IL 10	0	-28	0	-47	0	-30	0	-50	0	-68	0	-48
IL 11	0	-36	0	-53	0	-26	0	-56	0	-60	0	-39
IL 12	0	0	0	0	0	0	0	0	0	0	0	0
IL 13	0	80	0	100	0	100	0	100	0	100	0	100
IL14	0	82	0	100	0	100	0	100	0	100	0	100
IL 15	0	74	0	100	0	100	0	100	0	100	0	100

Post-, postemergence; *pre-*, preemergence.

Supporting Figures

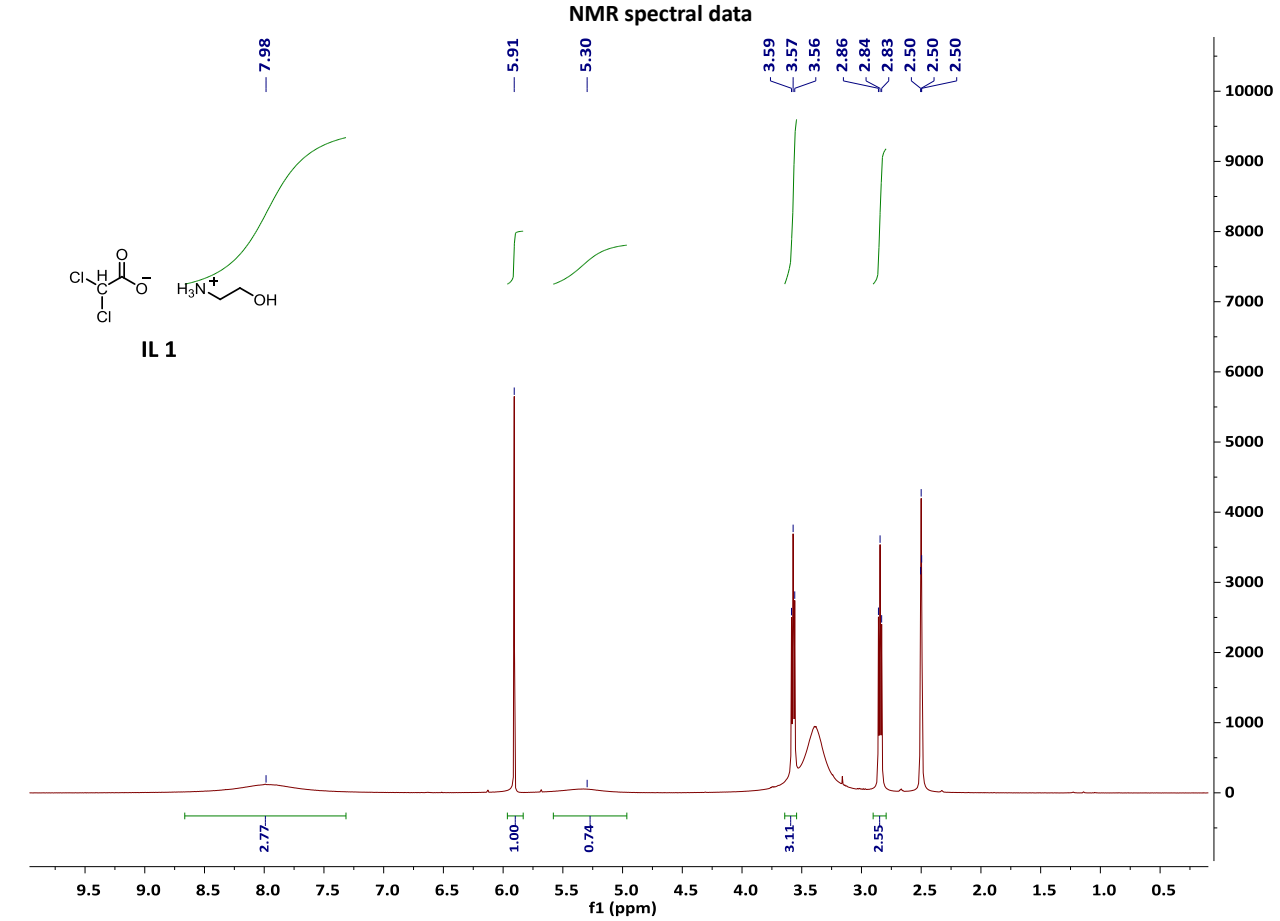

Fig. S1 ^{1}H NMR spectrum of **IL 1** in DMSO-d_6.

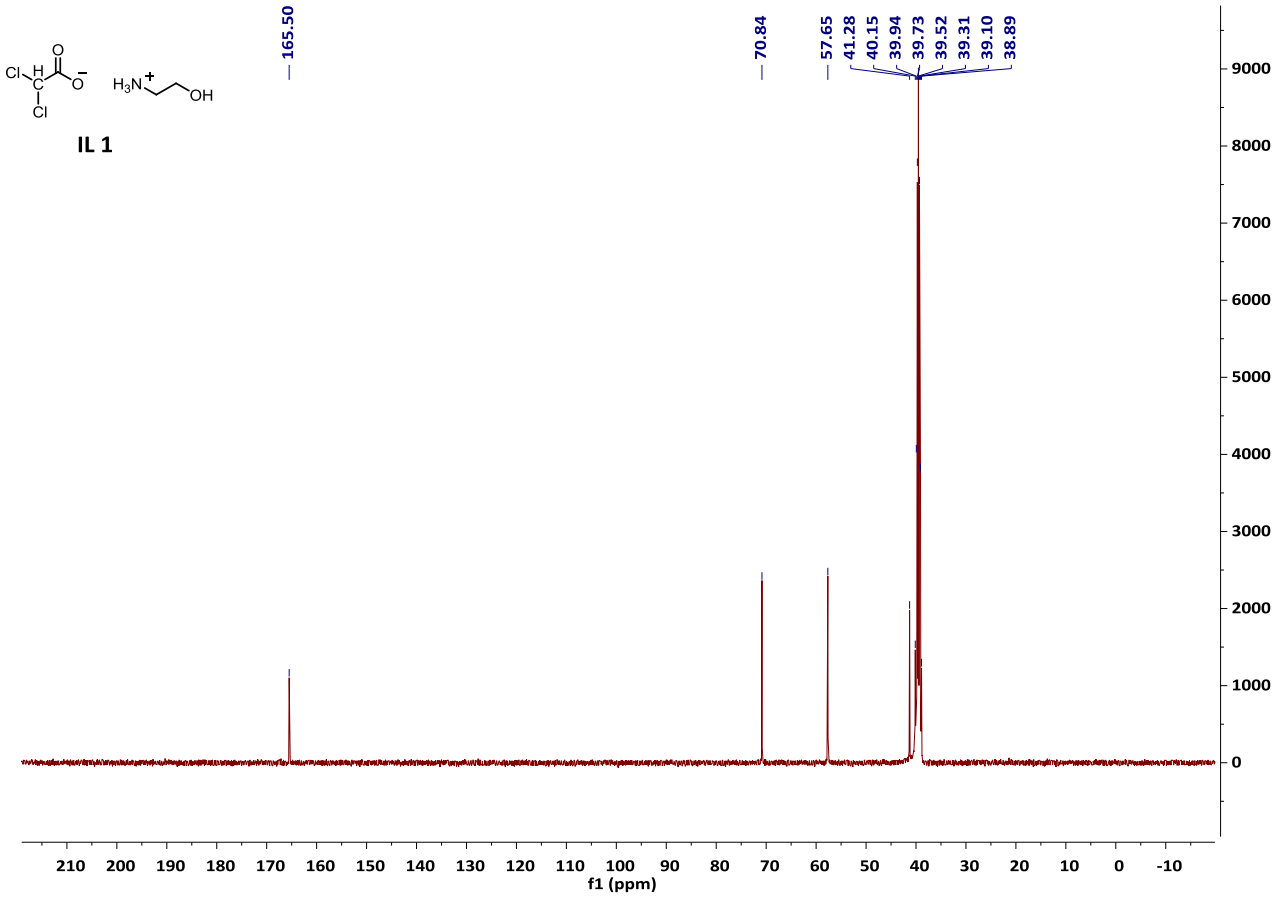

Fig. S2 ^{13}C NMR spectrum of **IL 1** in DMSO-d_6.

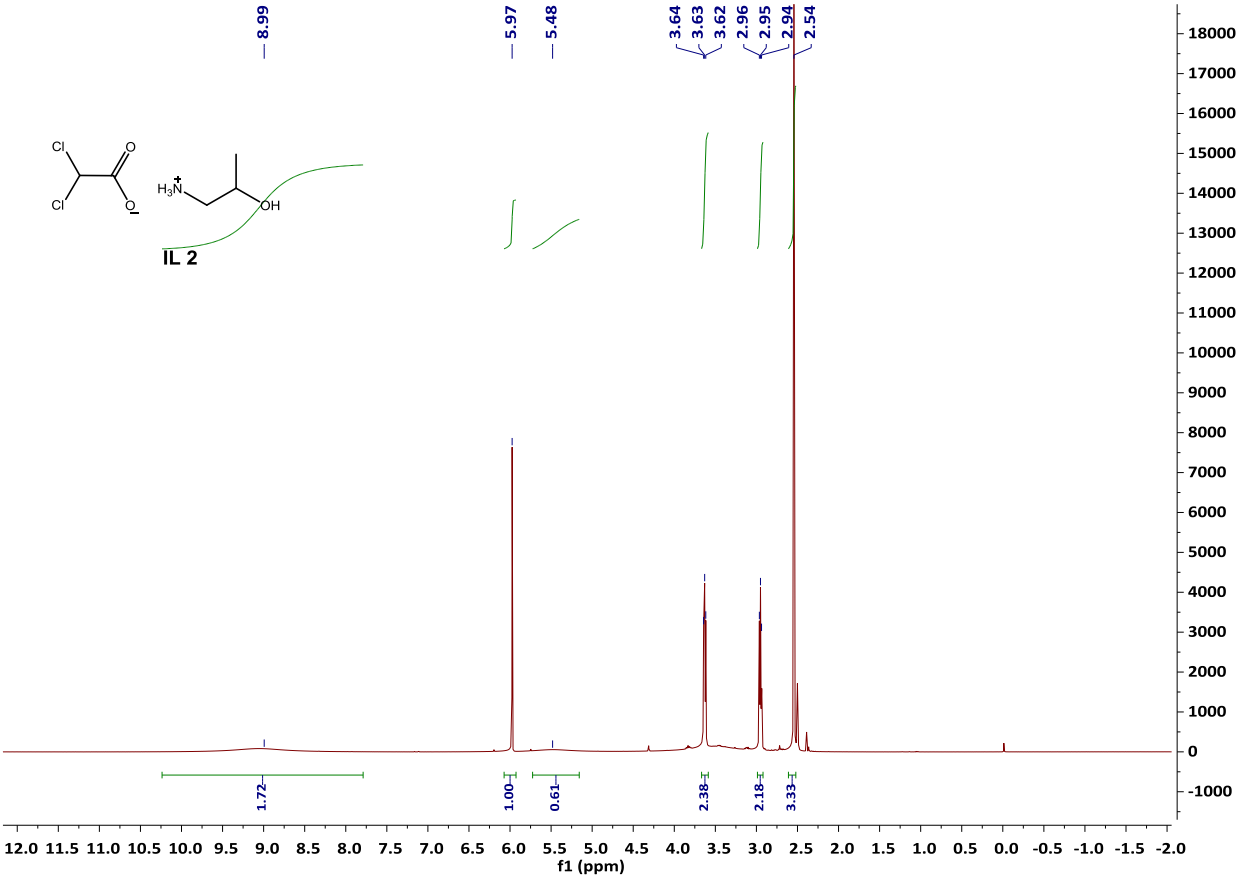

Fig. S3 ^{1}HNMR spectrum of **IL 2** in DMSO-d_6.

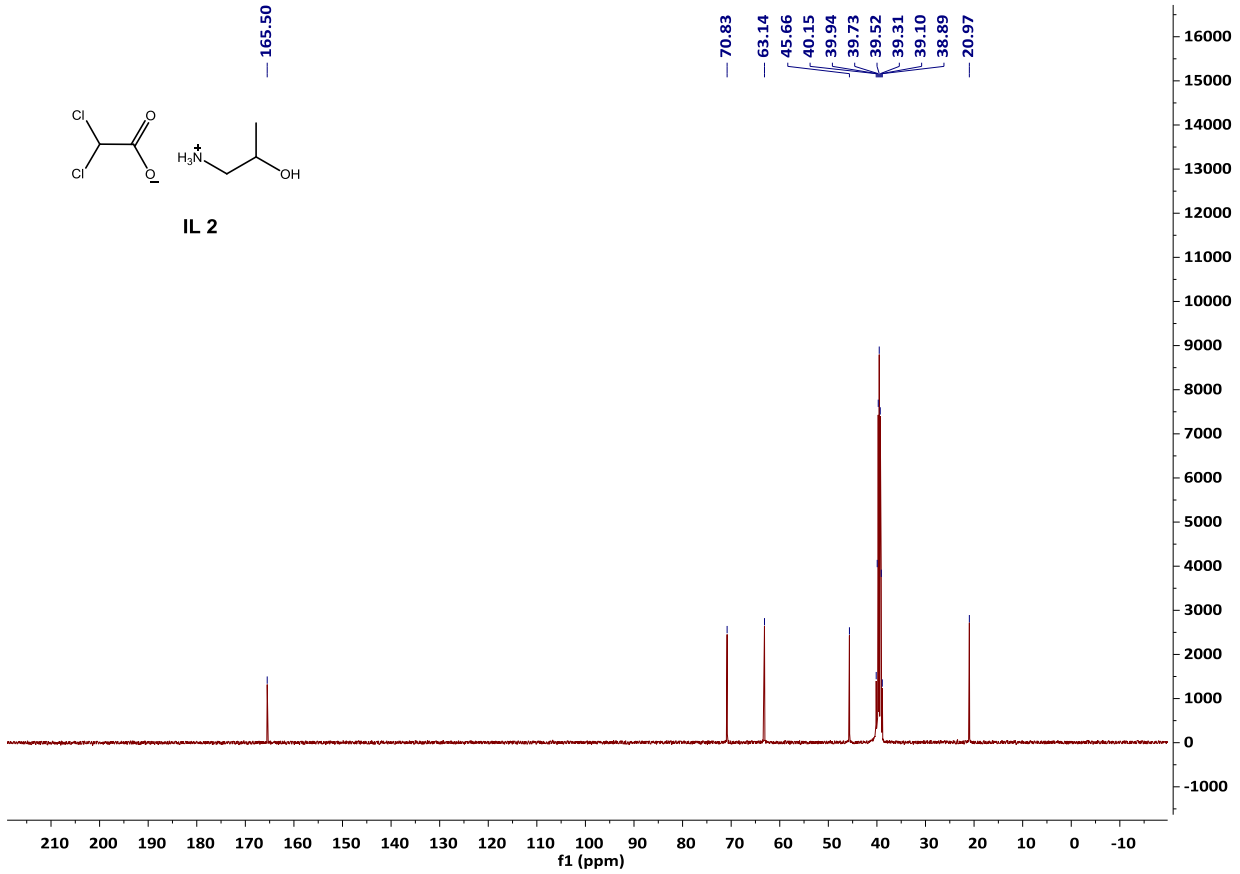

Fig. S4 ^{13}C NMR spectrum of **IL 2** in DMSO-d_6.

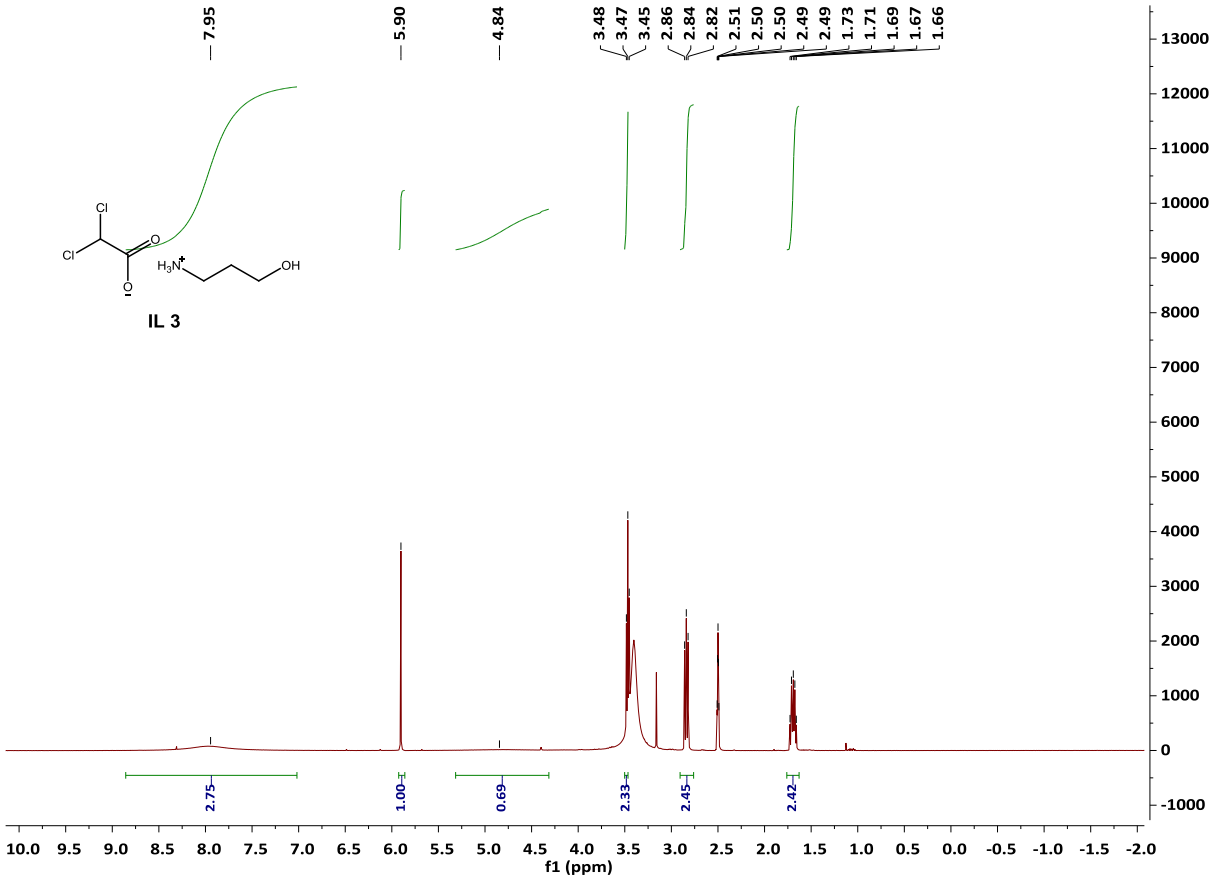

Fig. S5 ^{1}HNMR spectrum of **IL 3** in DMSO-d_6.

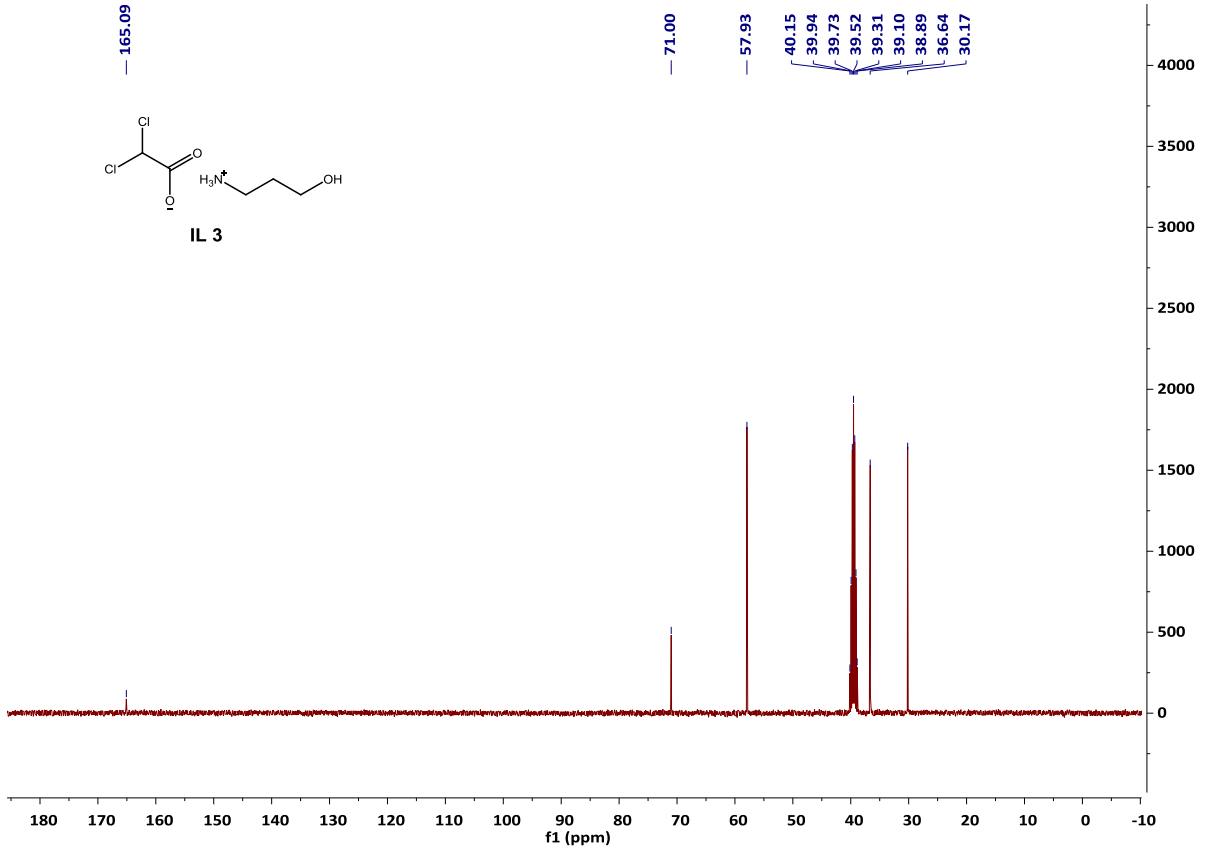

Fig. S6 ^{13}C NMR spectrum of **IL 3** in DMSO-d_6.

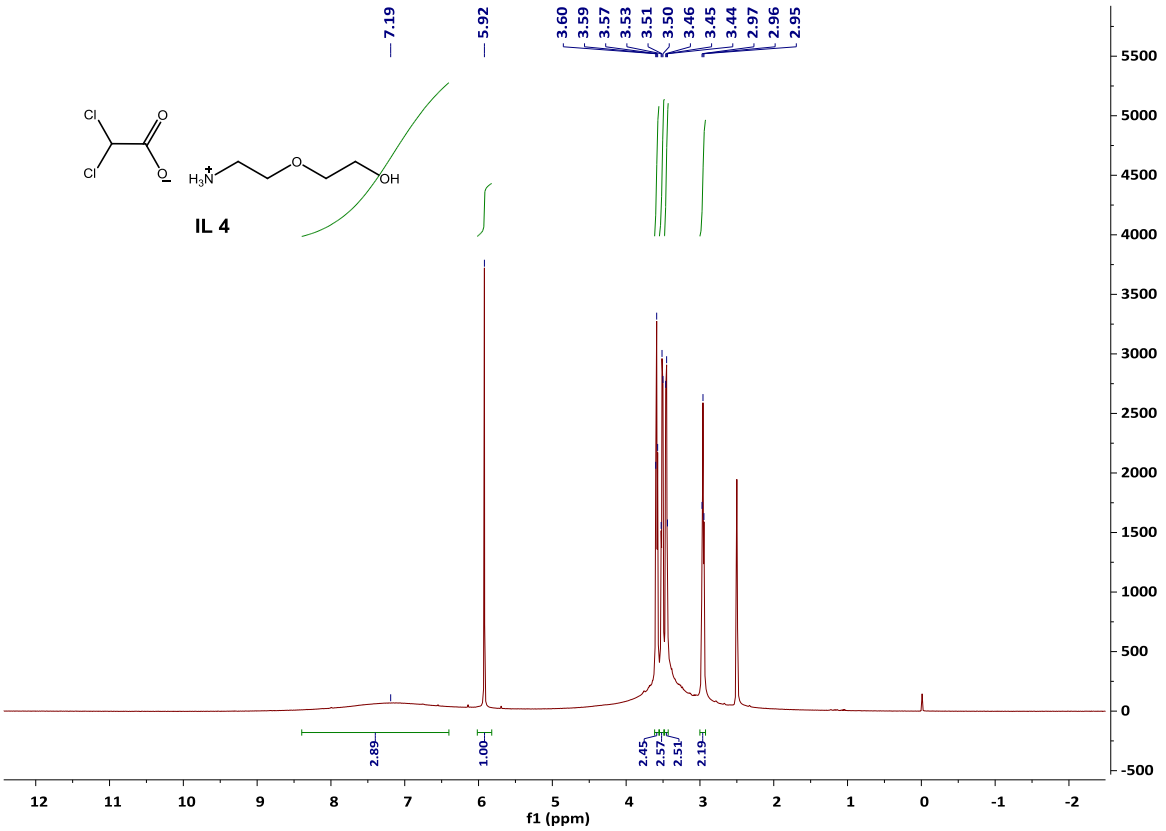

Fig. S7 ^{1}HNMR spectrum of **IL 4** in DMSO-d_6.

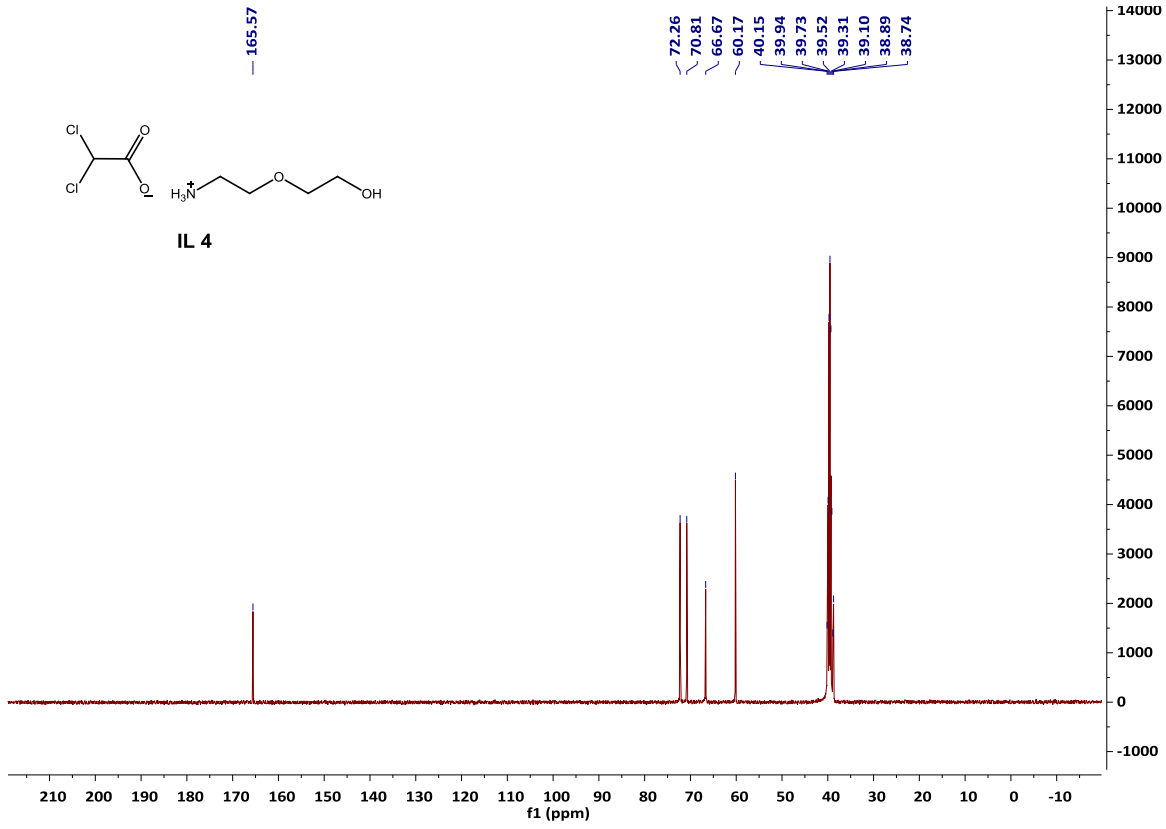

Fig. S8 ^{13}C NMR spectrum of **IL 4** in DMSO-d_6.

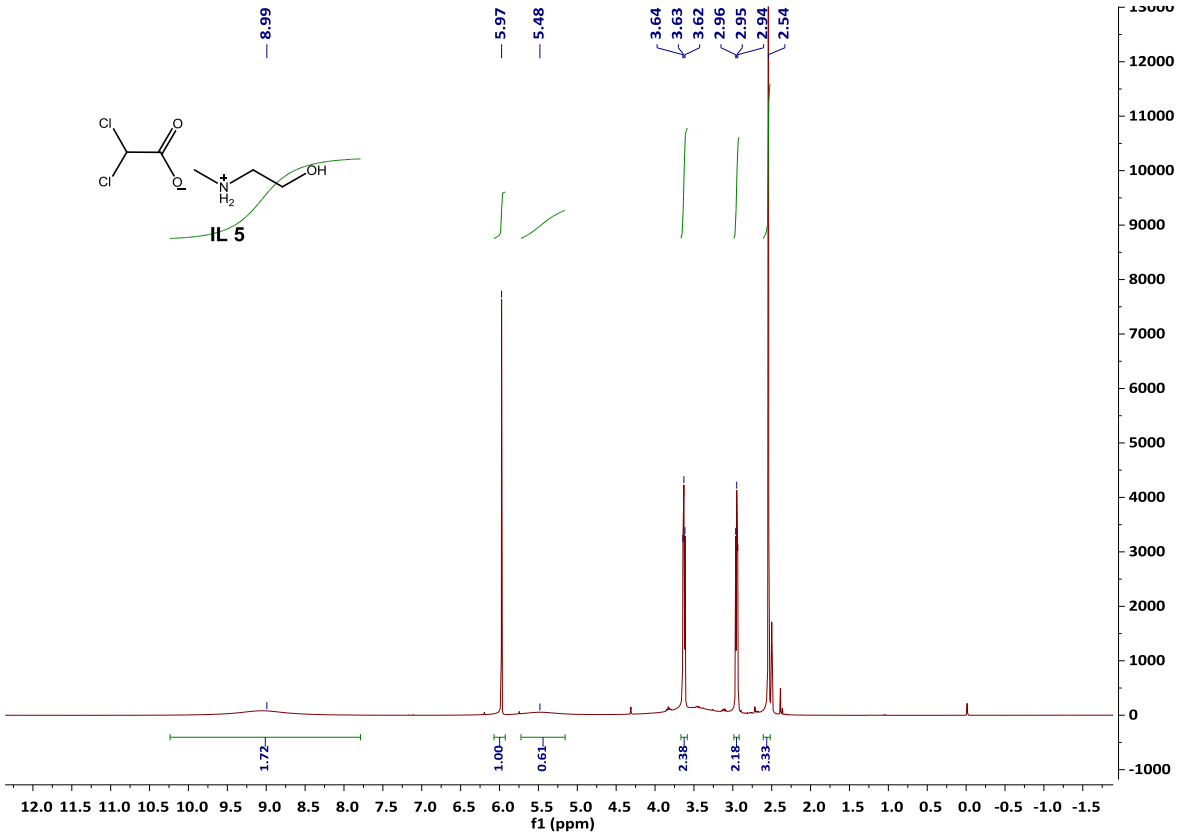

Fig. S9 ^{1}HNMR spectrum of **IL 5** in DMSO-d_6.

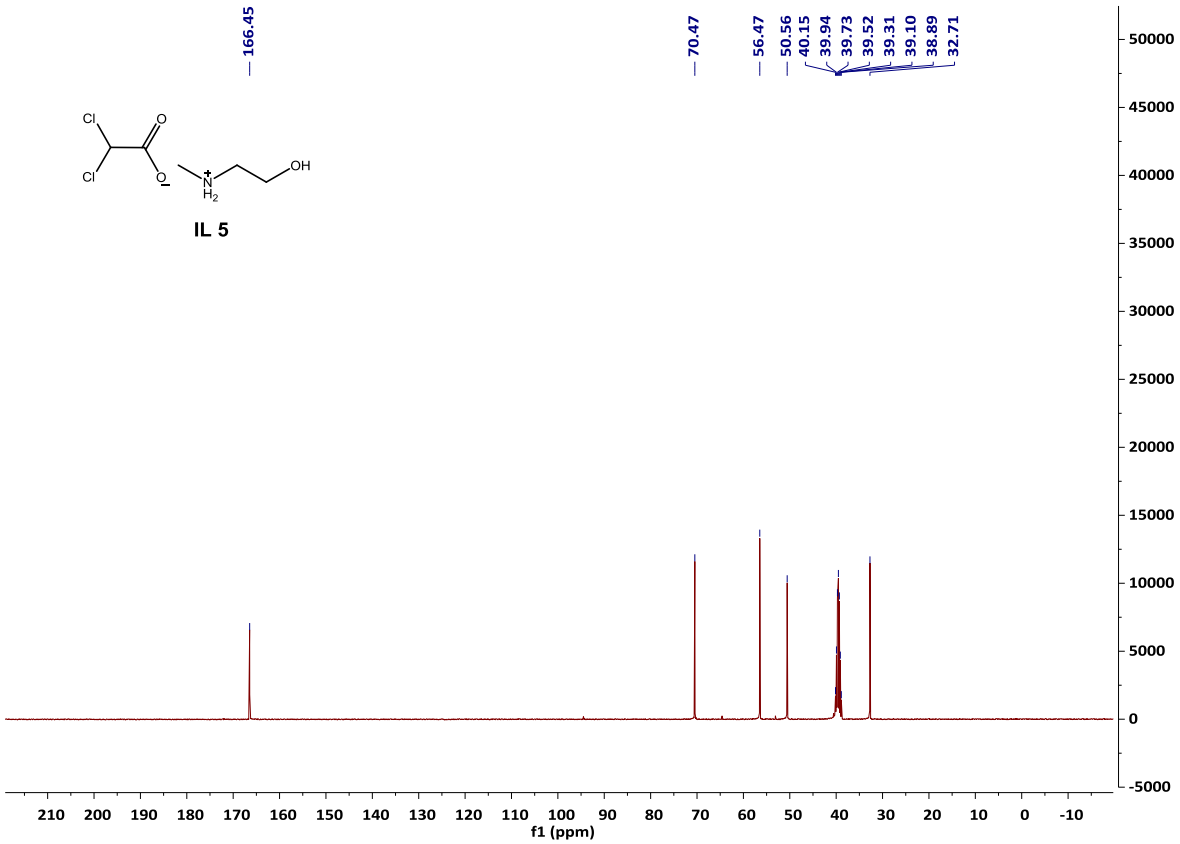

Fig. S10 ^{13}C NMR spectrum of **IL 5** in DMSO-d_6.

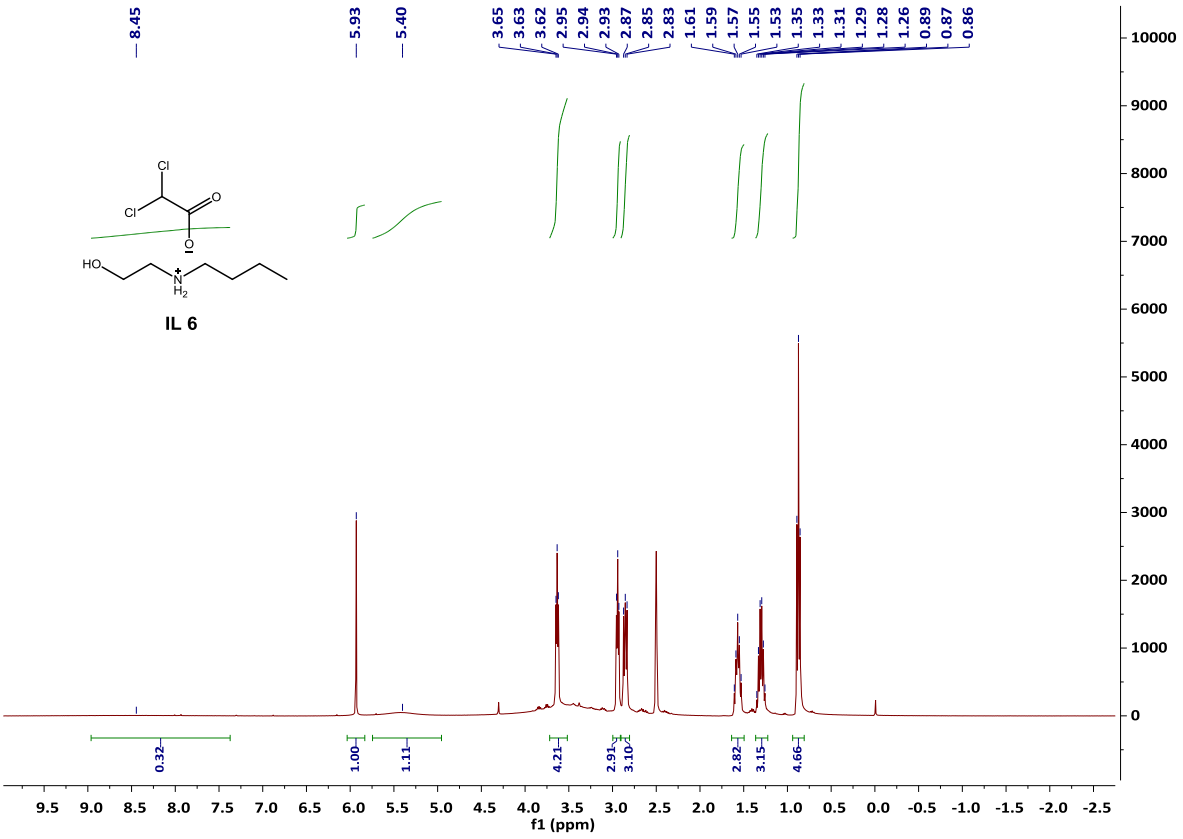

Fig. S11 ^{1}HNMR spectrum of **IL 6** in DMSO-d_6.

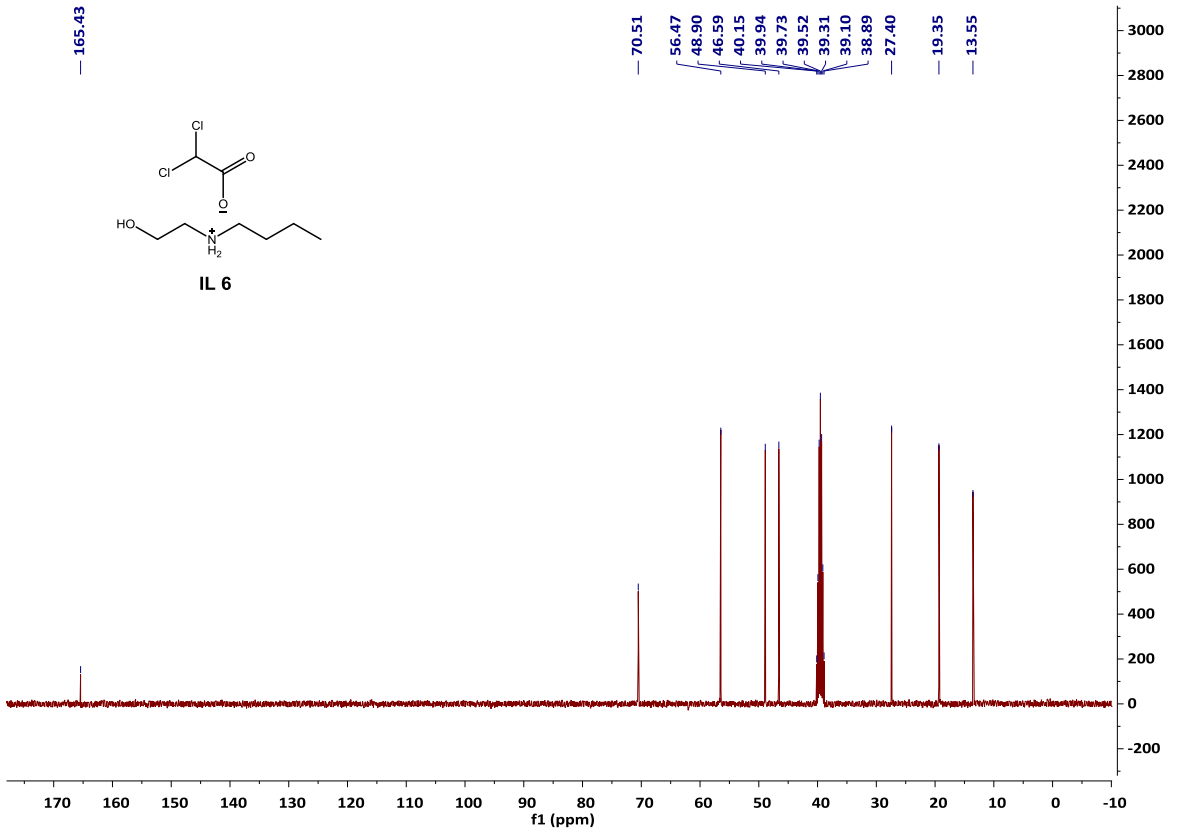

Fig. S12 ^{13}C NMR spectrum of **IL 6** in DMSO-d_6.

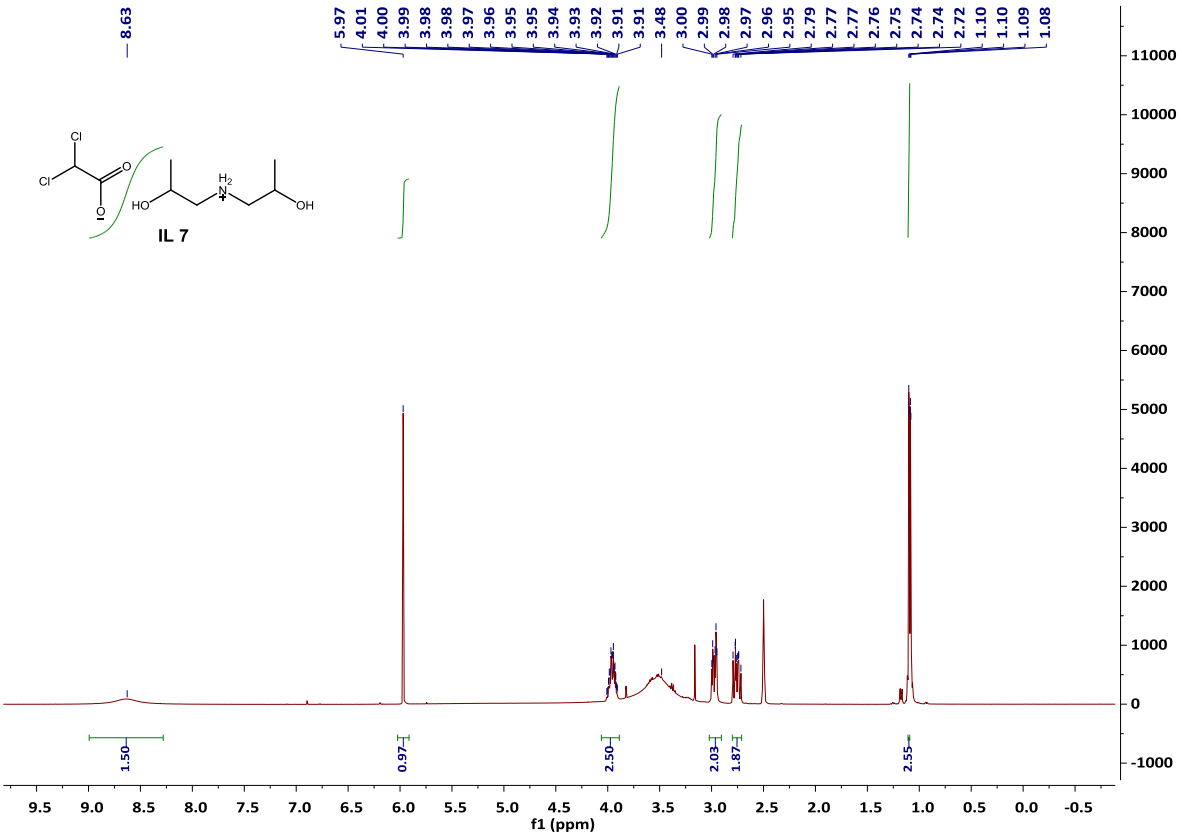

Fig. S13 ^{1}HNMR spectrum of **IL 7** in DMSO-d_6.

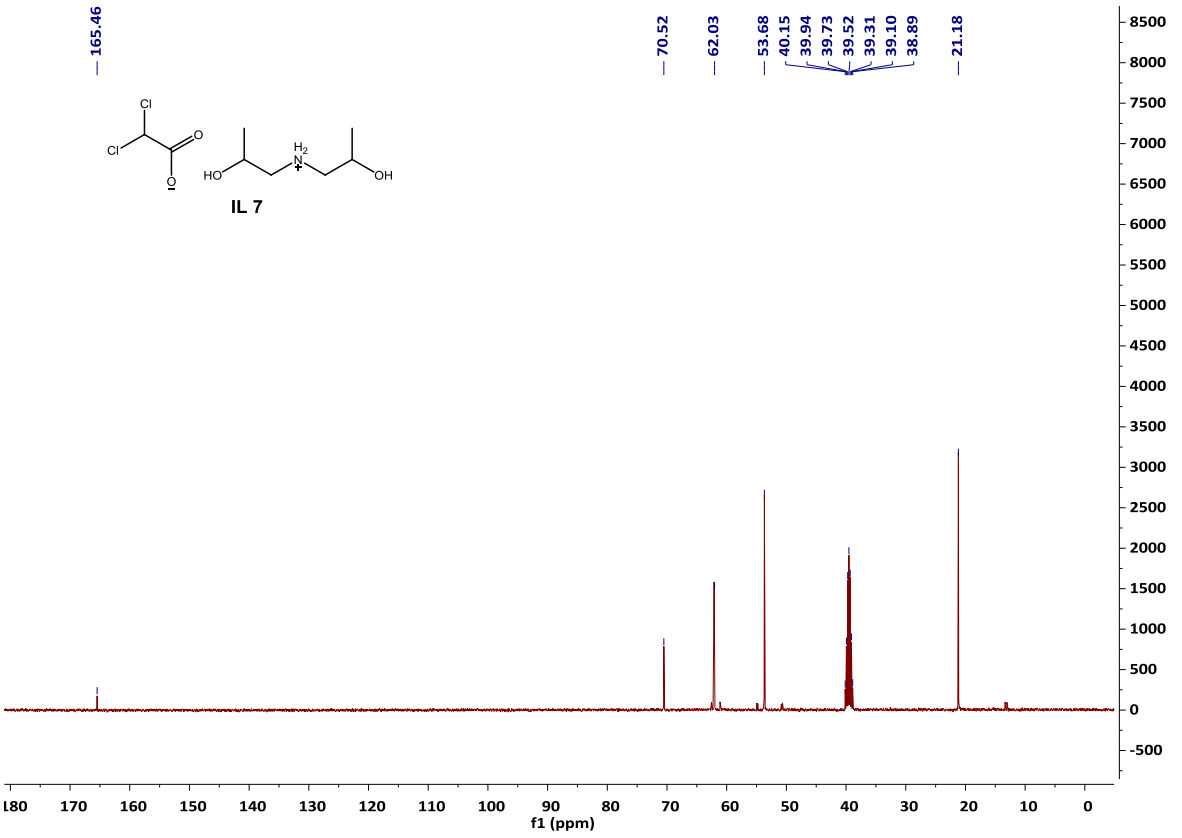

Fig. S14 ^{13}C NMR spectrum of **IL 7** in DMSO-d_6.

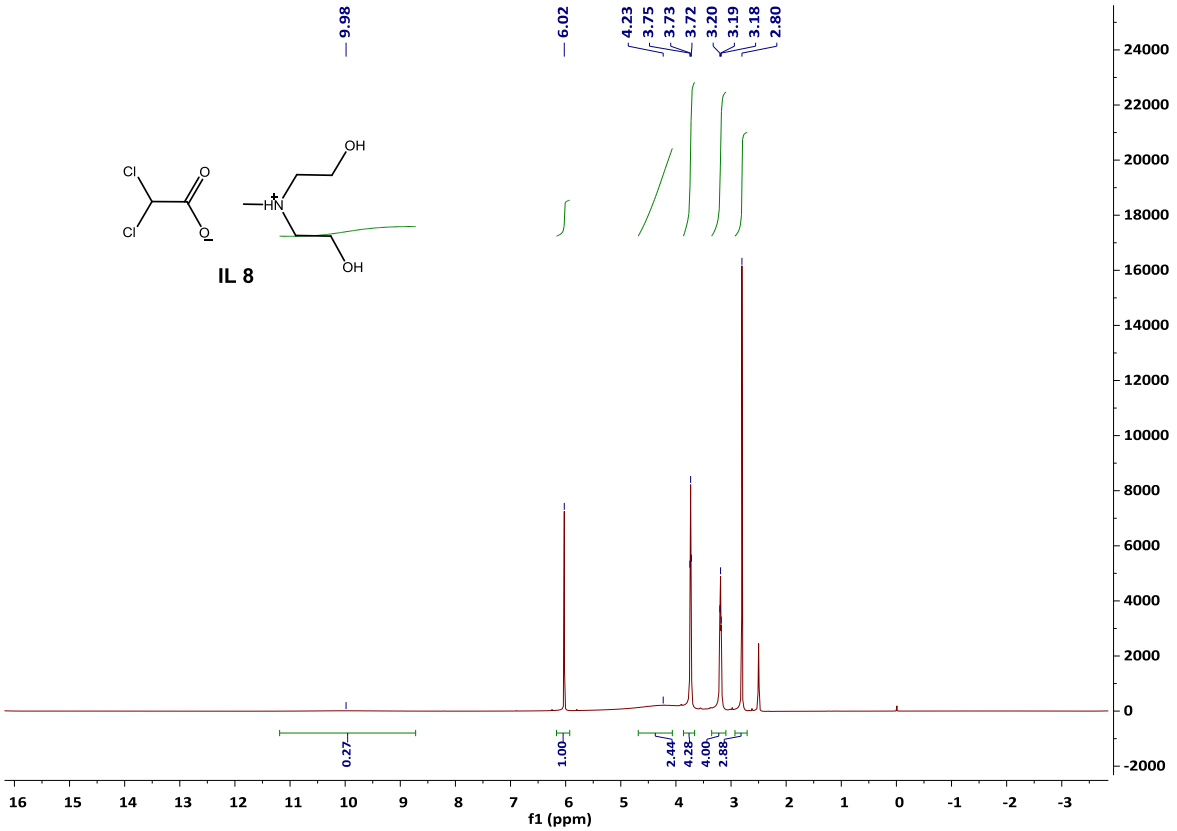

Fig. S15 ^{1}HNMR spectrum of **IL 8** in DMSO-d_6.

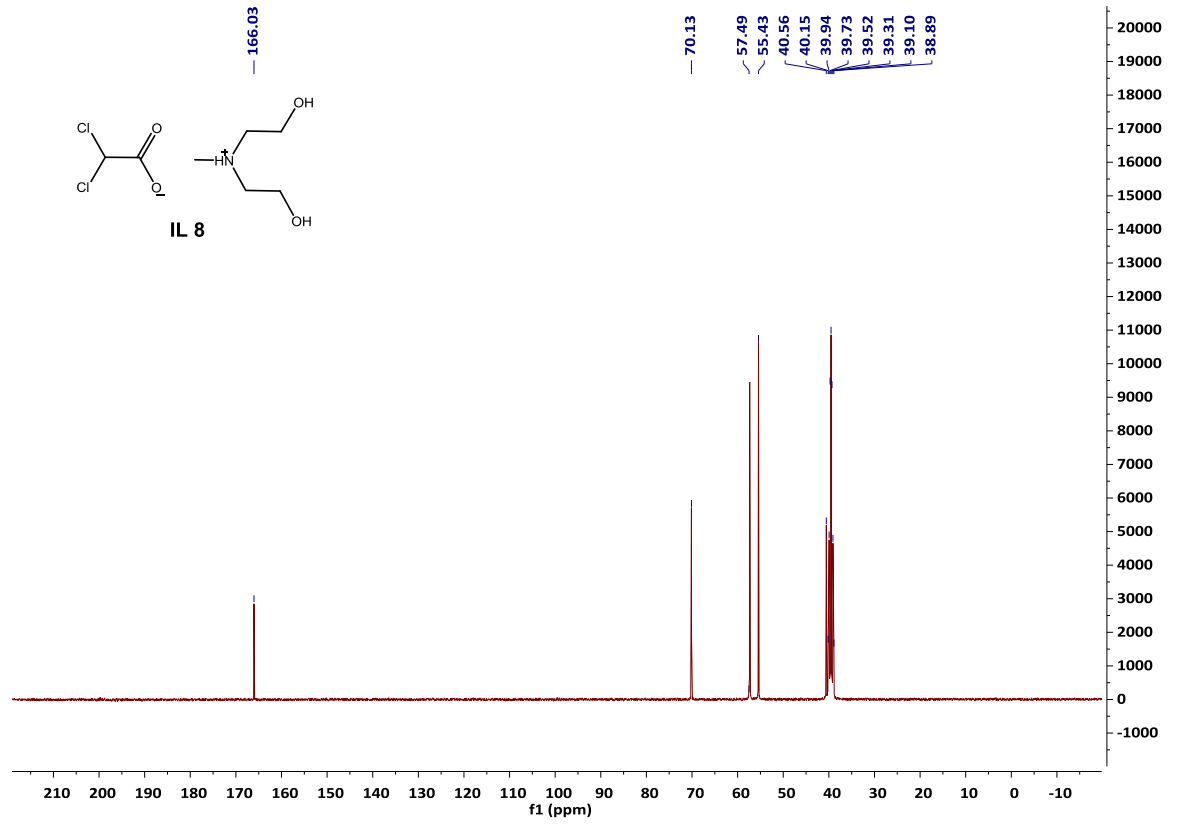

Fig. S16 ^{13}C NMR spectrum of **IL 8** in DMSO-d_6.

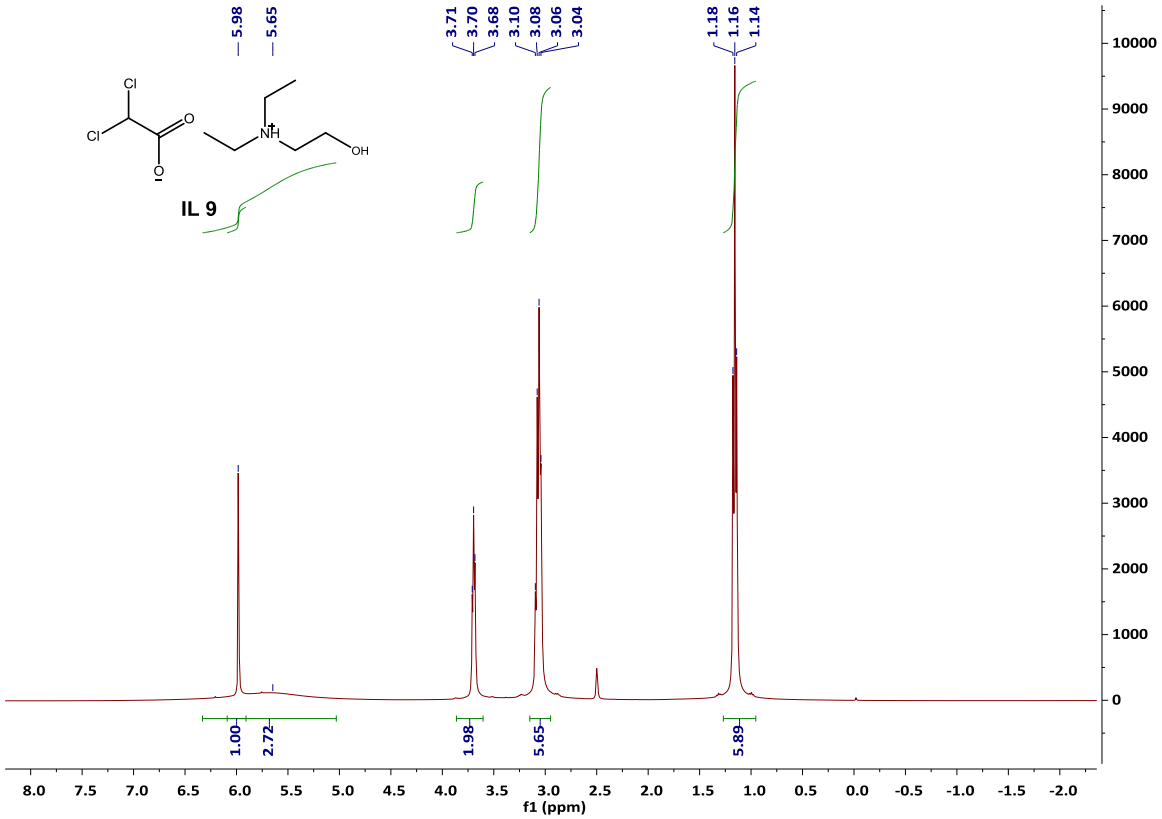

Fig. S17 ^{1}HNMR spectrum of **IL 9** in DMSO-d_6.

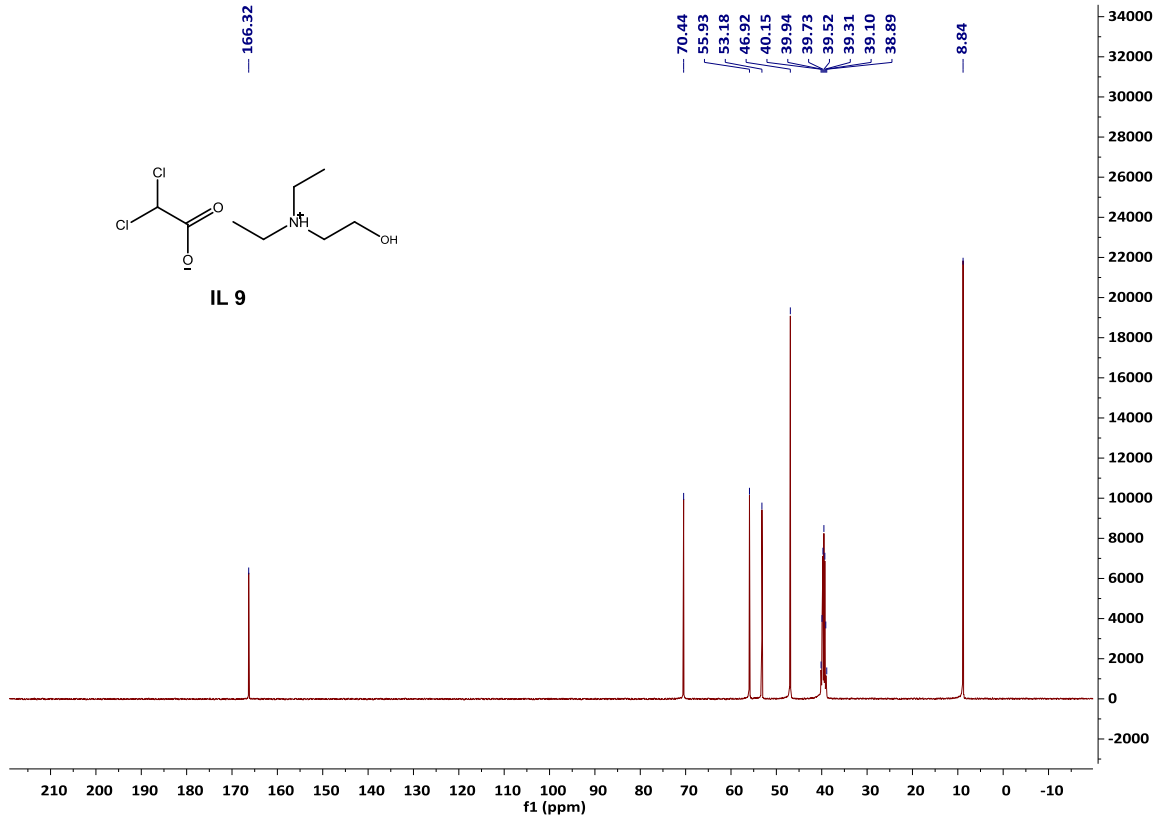

Fig. S18 ^{13}C NMR spectrum of **IL 9** in DMSO-d_6.

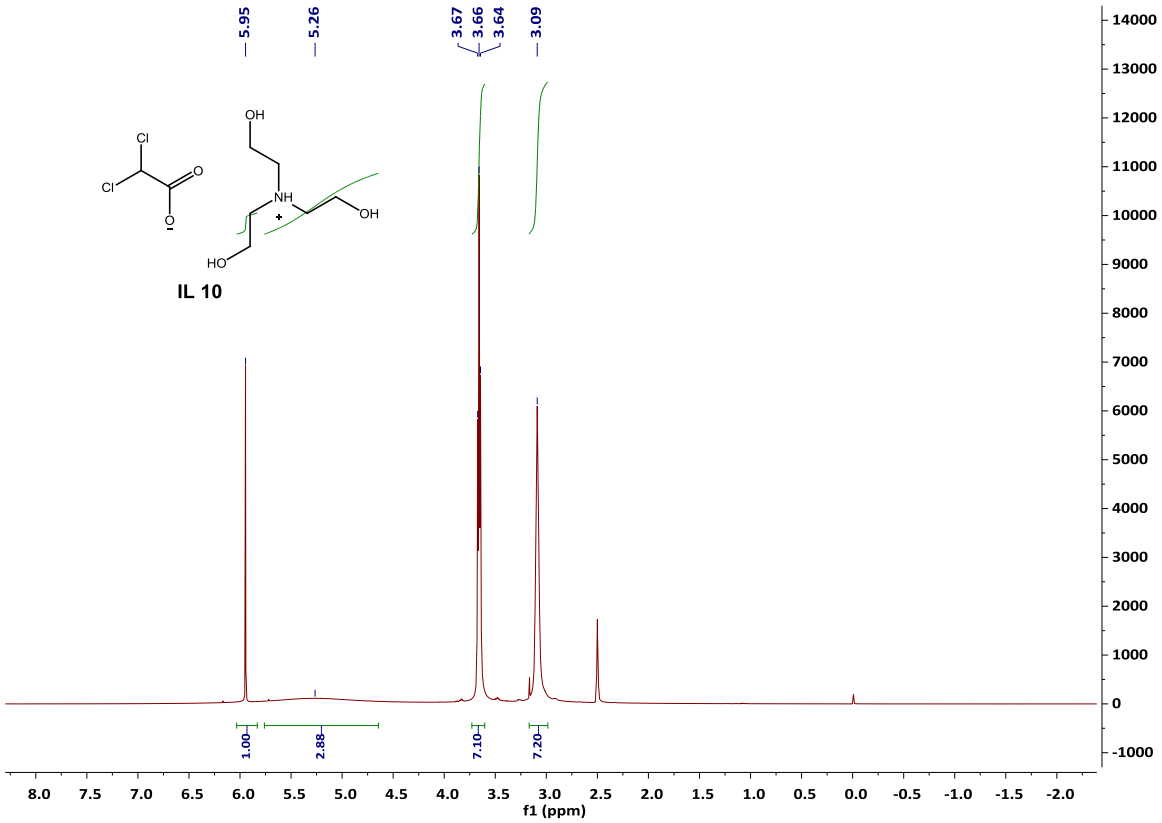

Fig. S19 ^{1}HNMR spectrum of **IL 10** in DMSO-d_6.

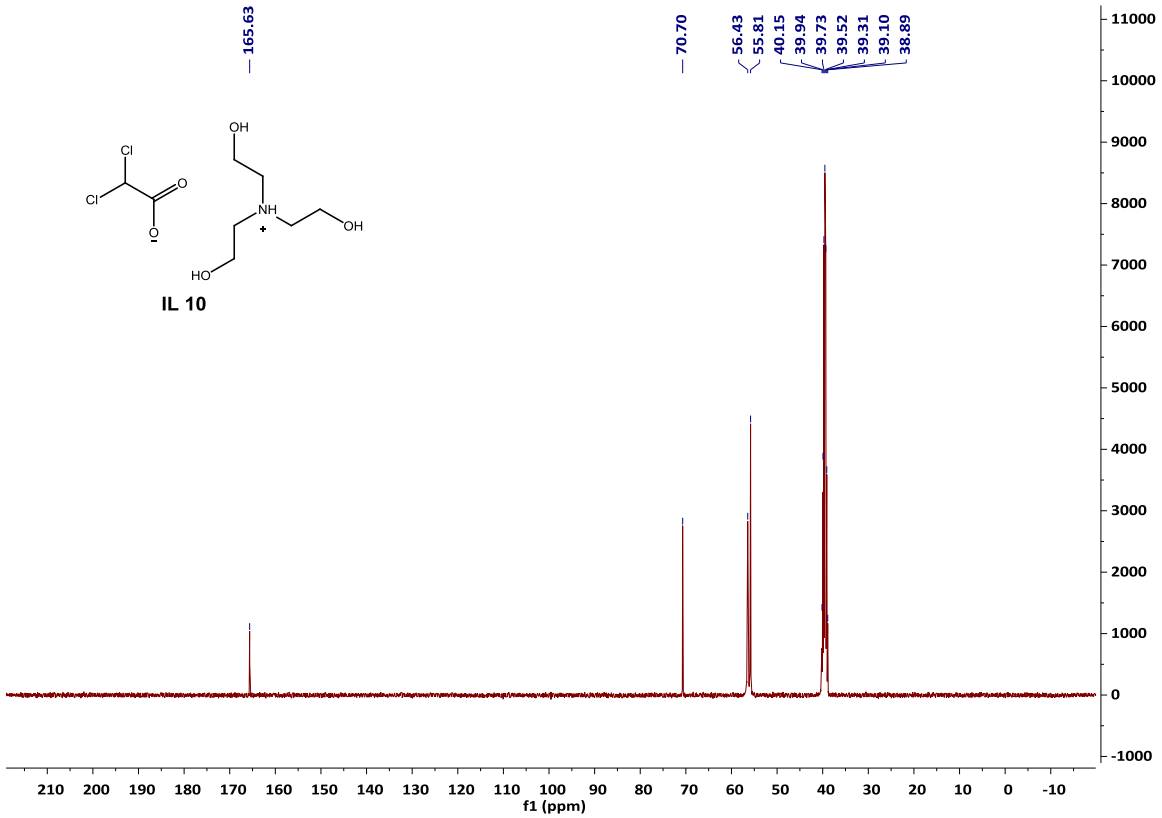

Fig. S20 ^{13}C NMR spectrum of **IL 10** in DMSO-d_6.

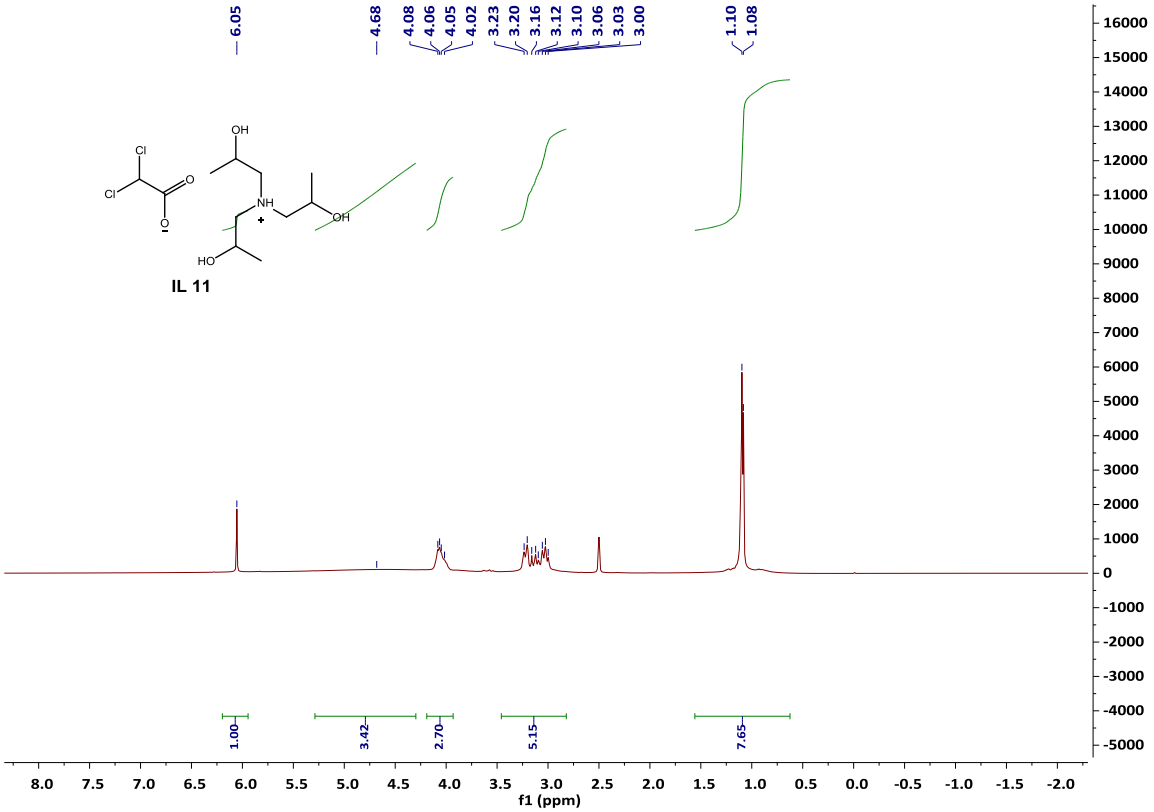

Fig. S21 ^{1}HNMR spectrum of **IL 11** in DMSO-d_6.

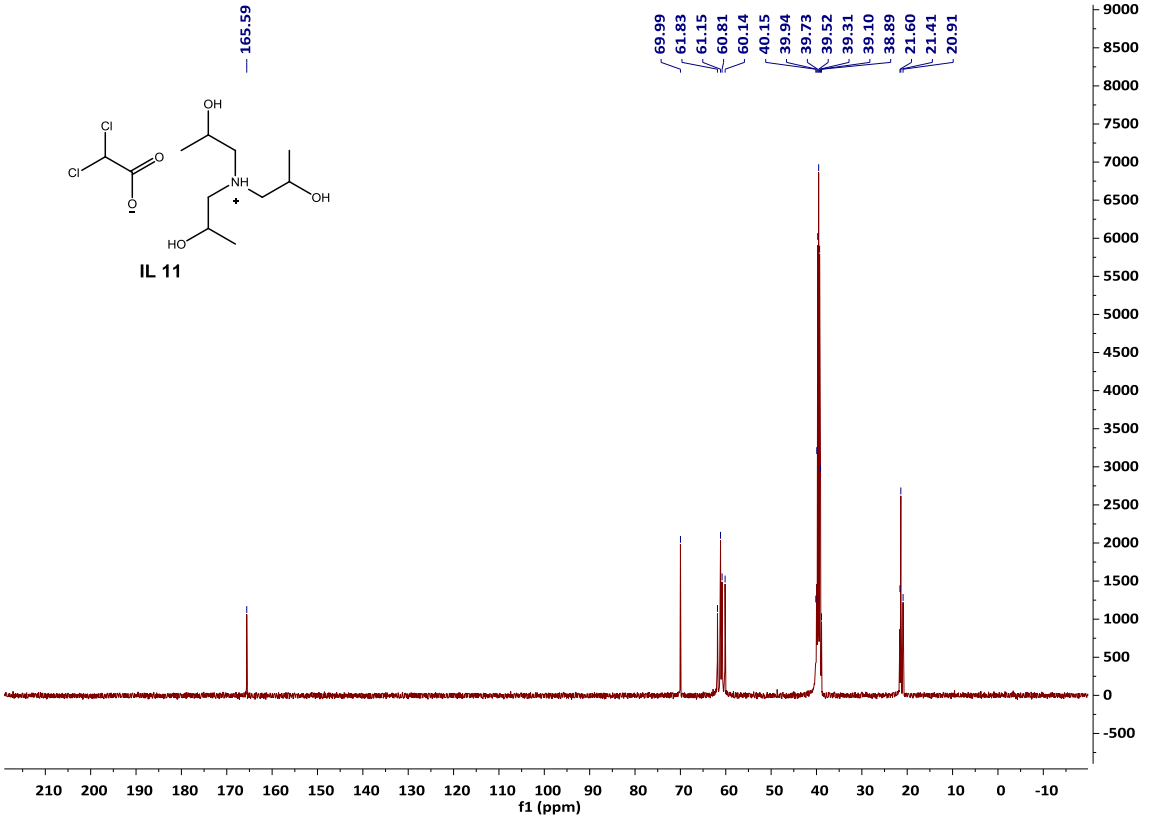

Fig. S22 ^{13}C NMR spectrum of **IL 11** in DMSO-d_6.

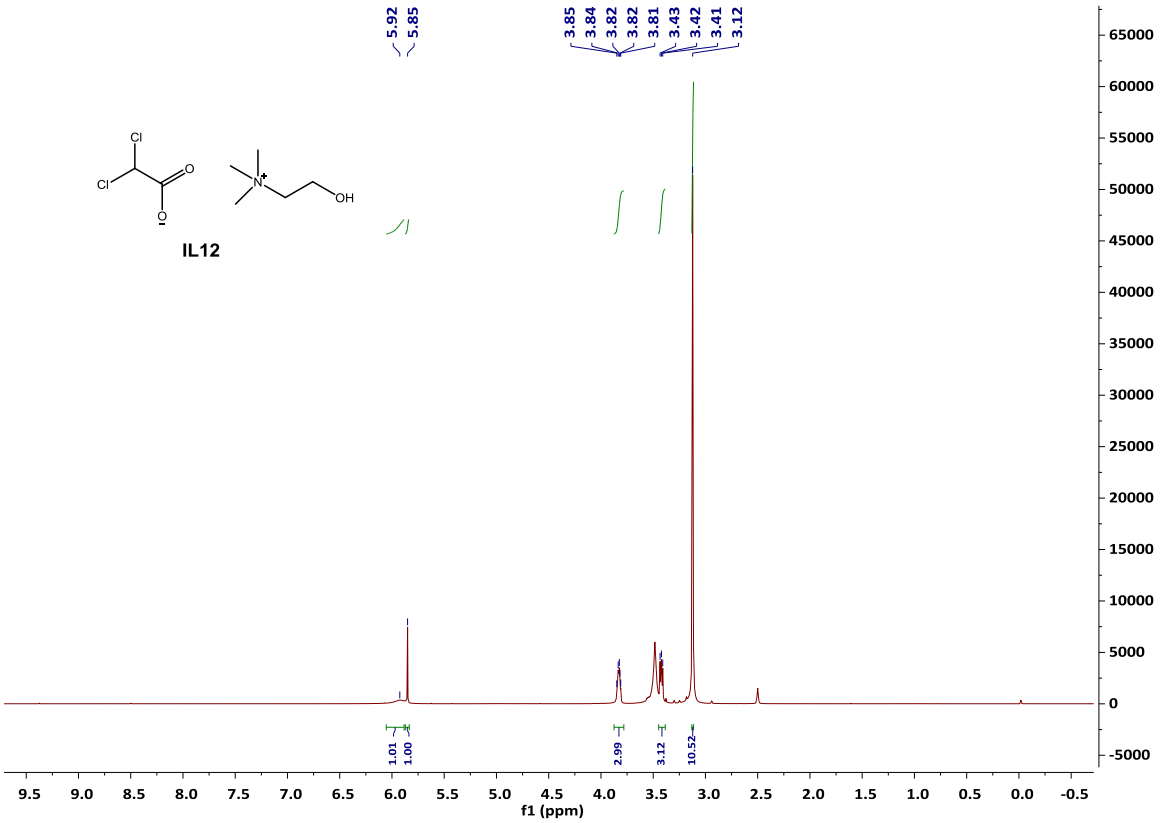

Fig. S23 ^{1}HNMR spectrum of **IL 12** in DMSO-d_6.

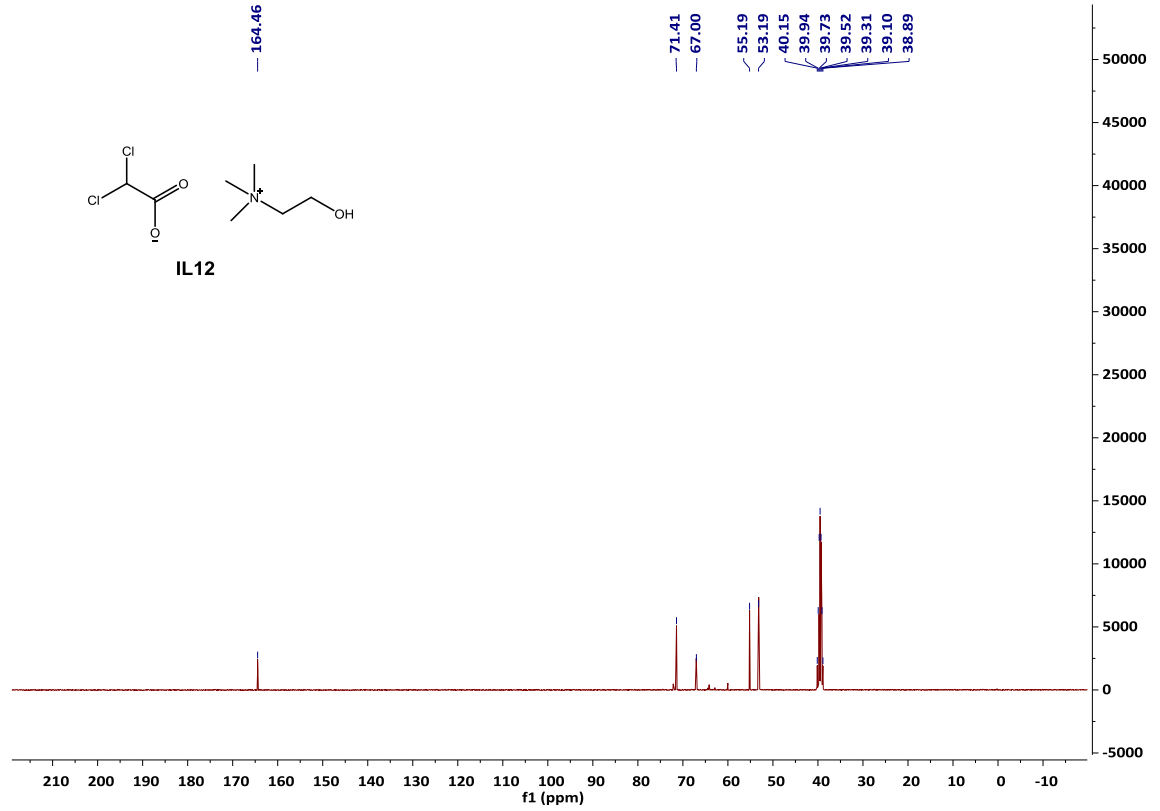

Fig. S24 ^{13}C NMR spectrum of **IL 12** in DMSO-d_6.

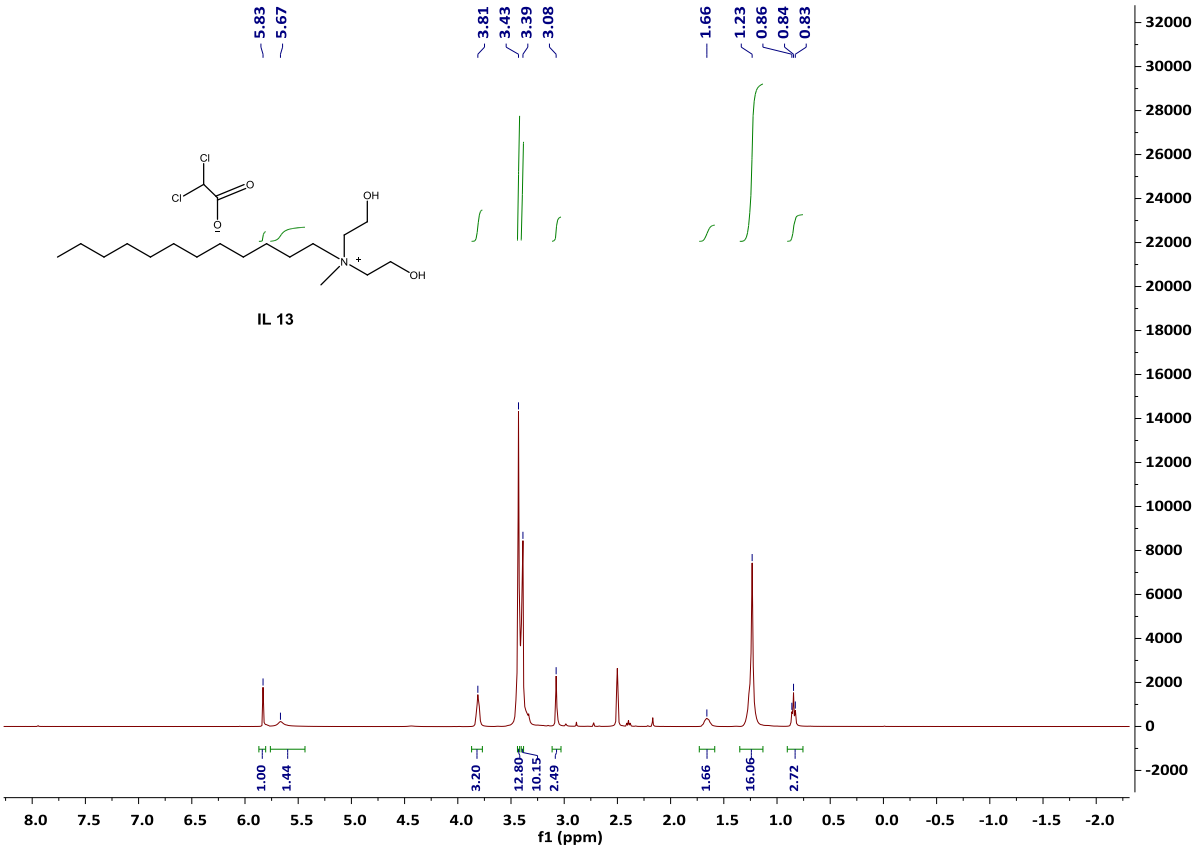

Fig. S25 ^{1}HNMR spectrum of **IL 13** in DMSO-d_6.

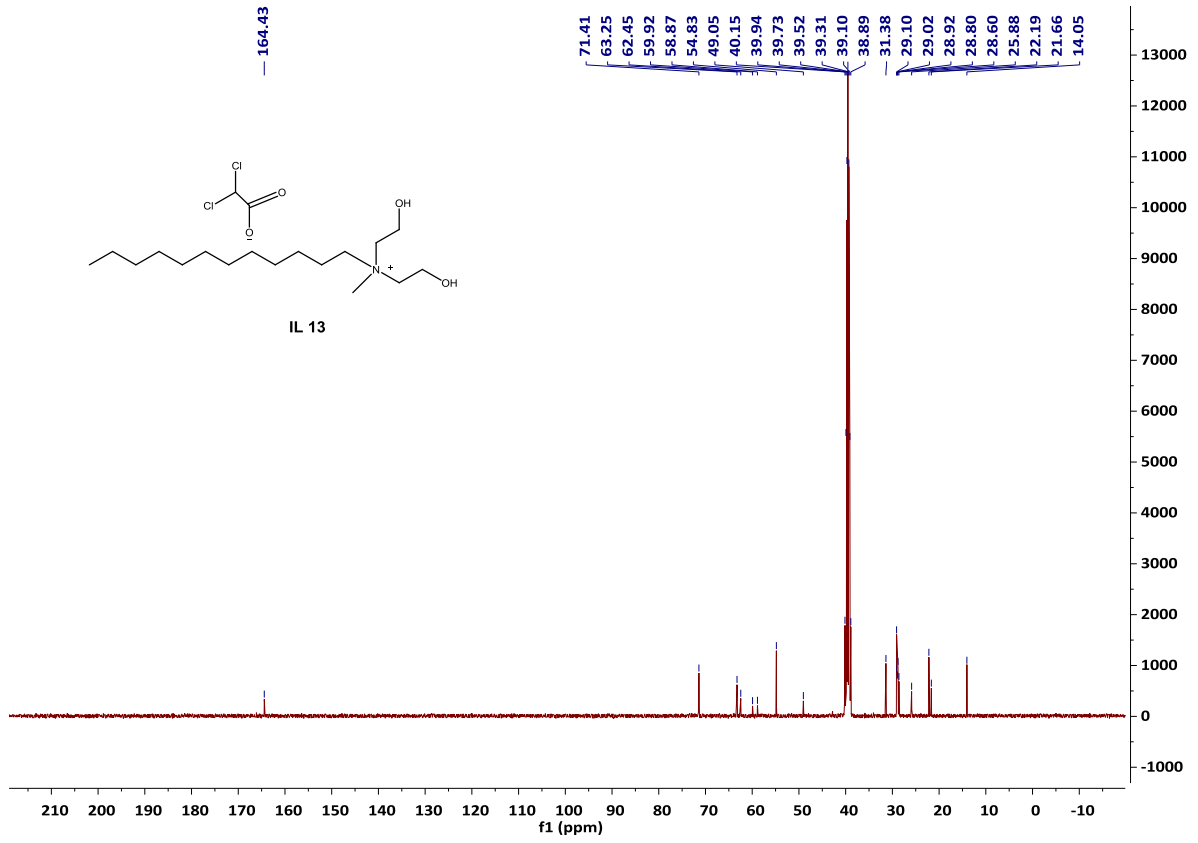

Fig. S26 ^{13}C NMR spectrum of **IL 13** in DMSO-d_6.

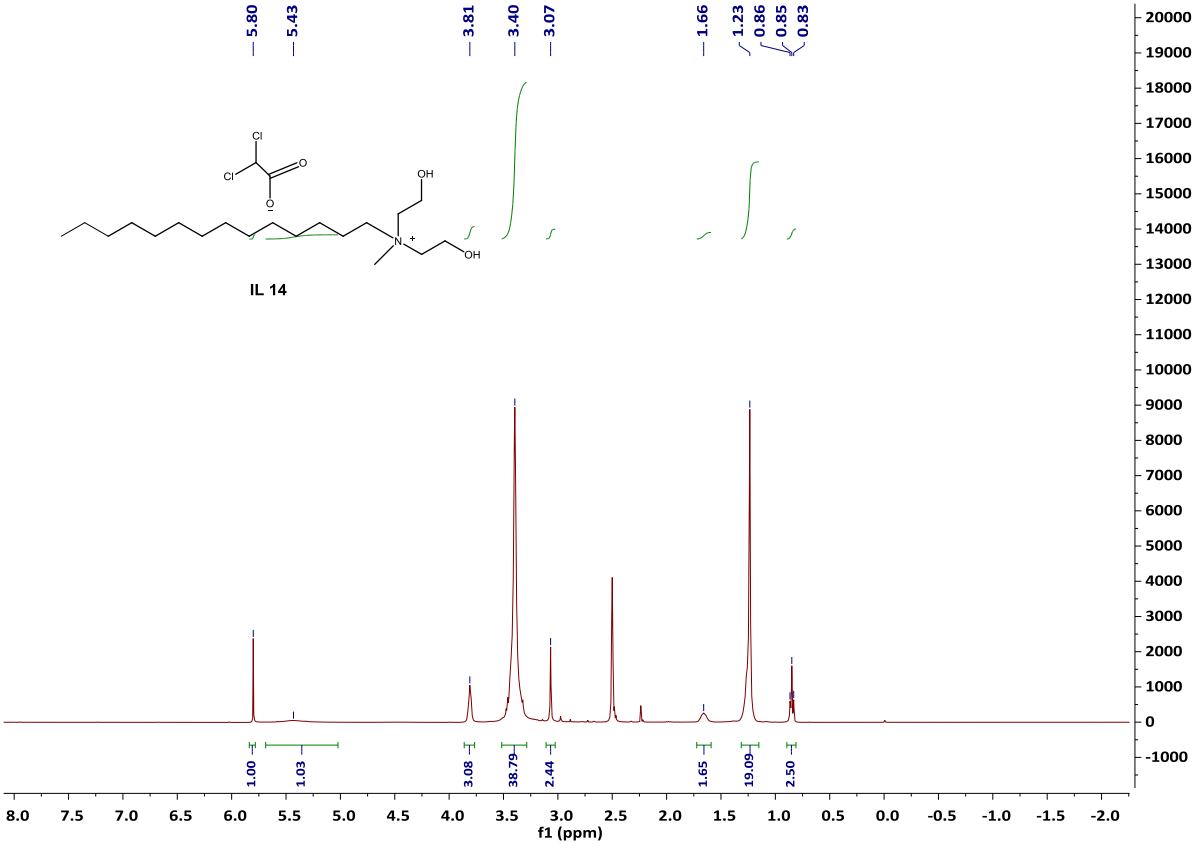

Fig. S27 ^{1}HNMR spectrum of **IL 14** in DMSO-d_6.

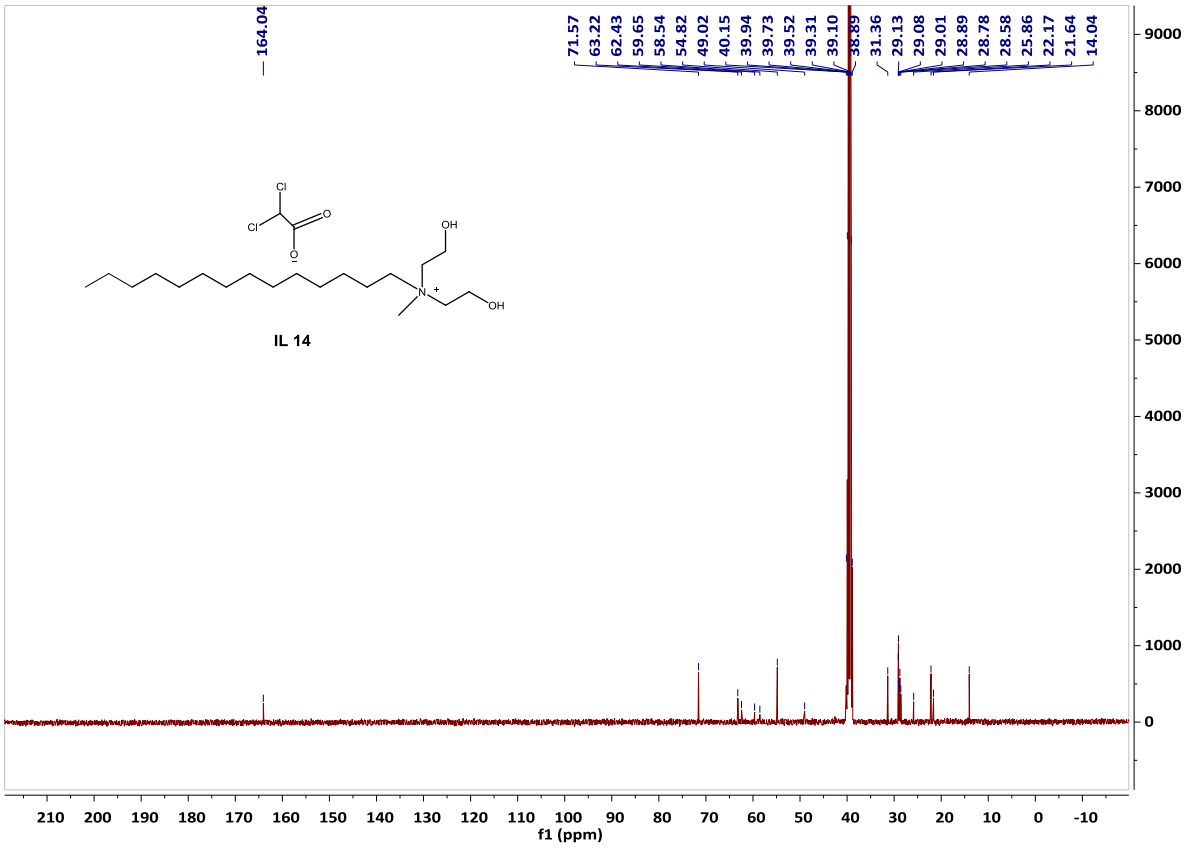

Fig. S28 ^{13}C NMR spectrum of **IL 14** in DMSO-d_6.

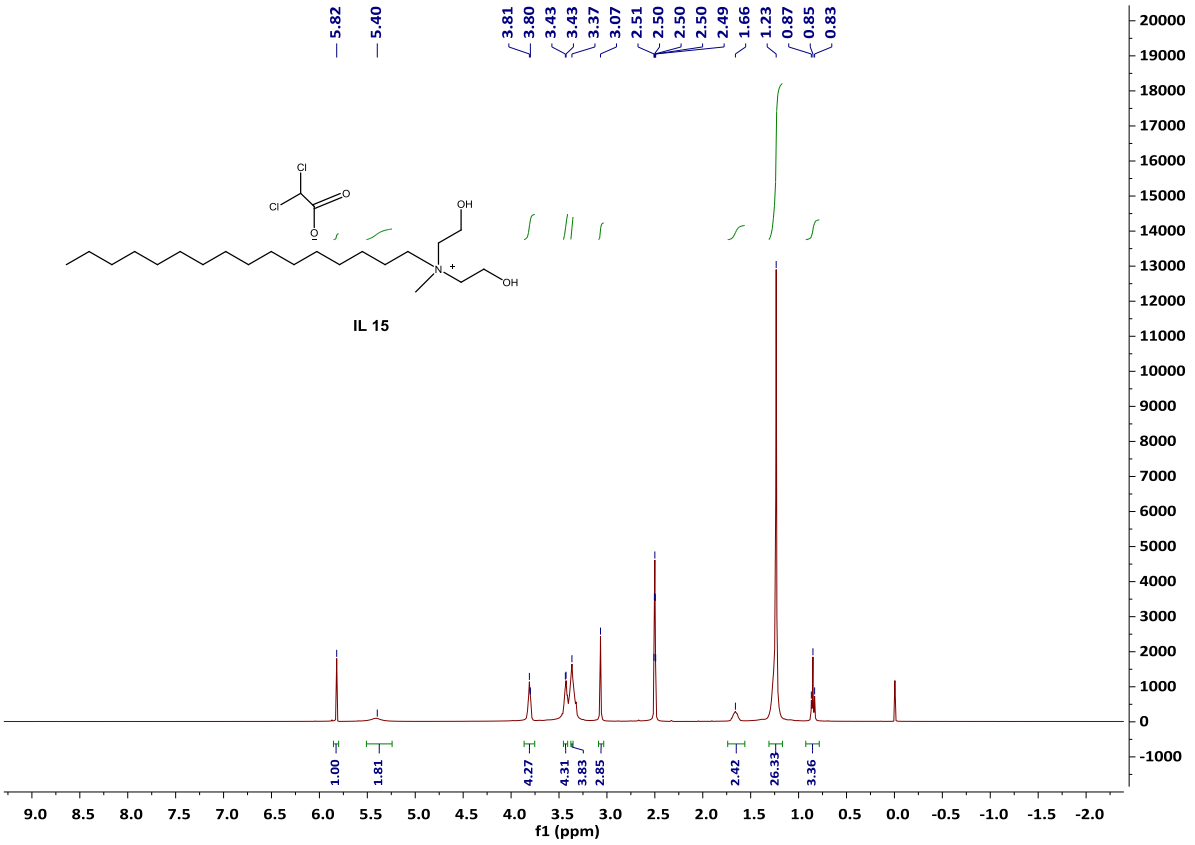

Fig. S29 ^{1}HNMR spectrum of **IL 15** in DMSO-d_6.

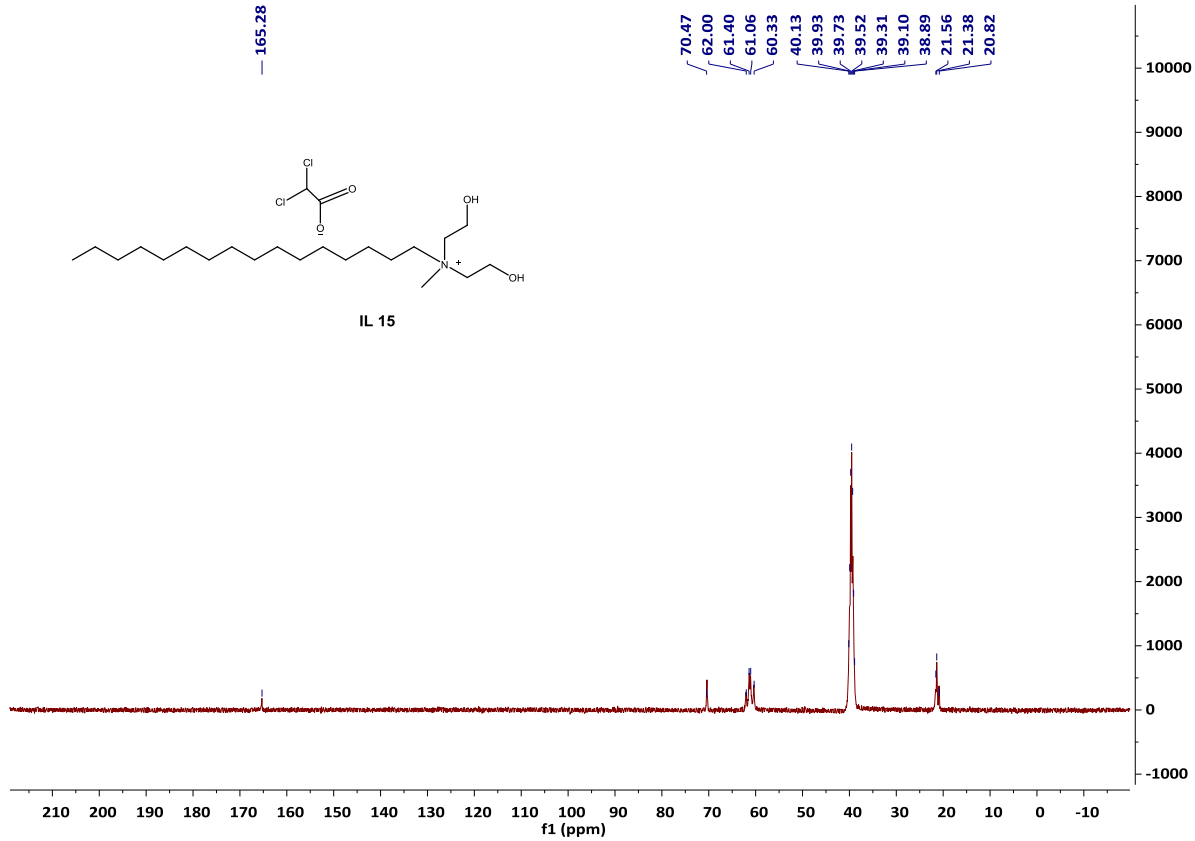

Fig. S30 ^{13}C NMR spectrum of **IL 15** in DMSO-d_6.

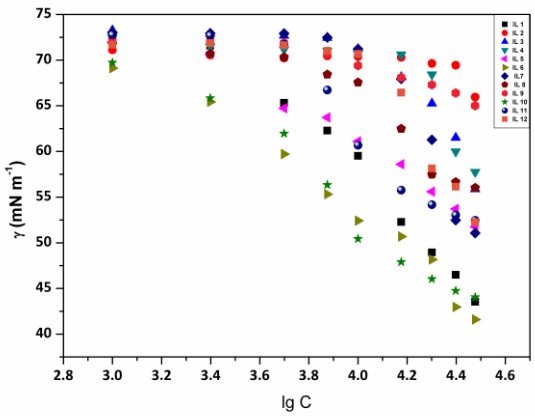

Fig. S31 Surface tension ($\gamma_{[mN\ m^{-1}]}$) data *vs*. the logarithm of concentration (C mg L^{-1}) isotherms measured at 298 K for aqueous solutions of **ILs 1-12**.

Post-emergence Herbicidal activity

Chenopodium album L. (C. album)

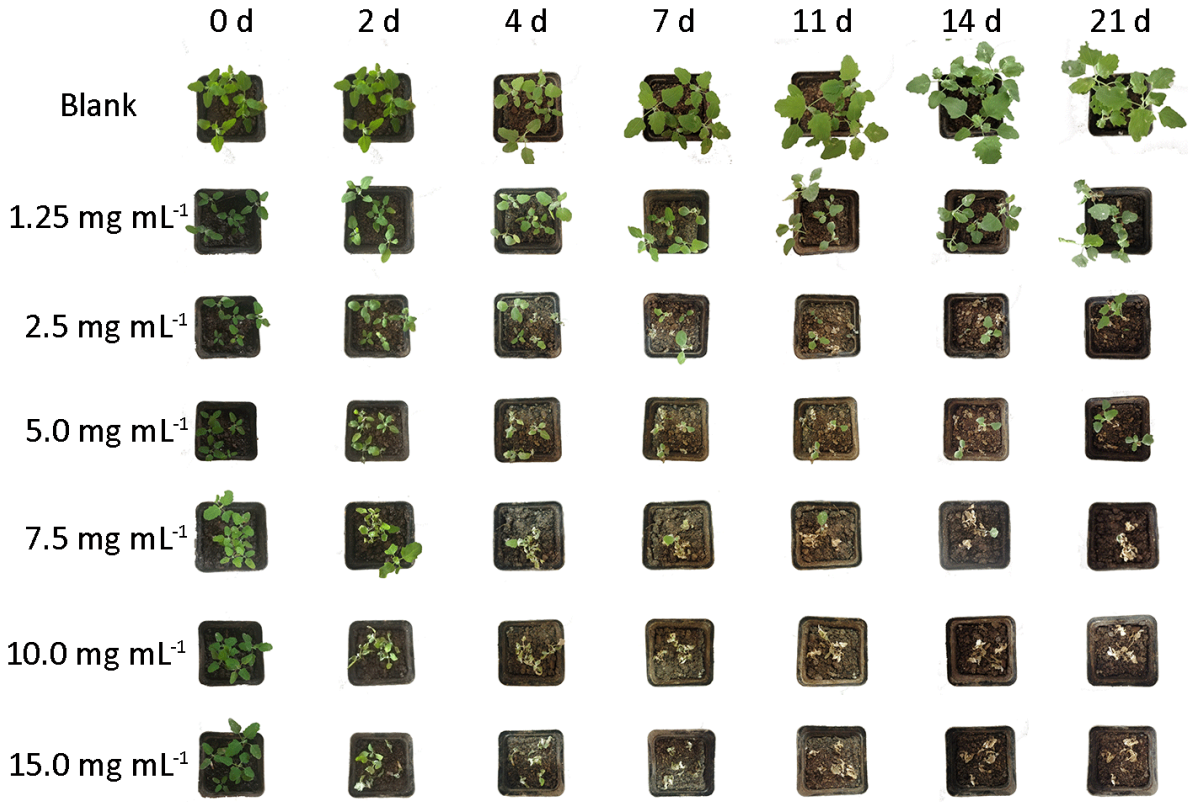

Fig. S32 Digital photographs of *Chenopodium album L.* after spraying with **IL 13** in different concentrations.

Chenopodium album L. (C. album)

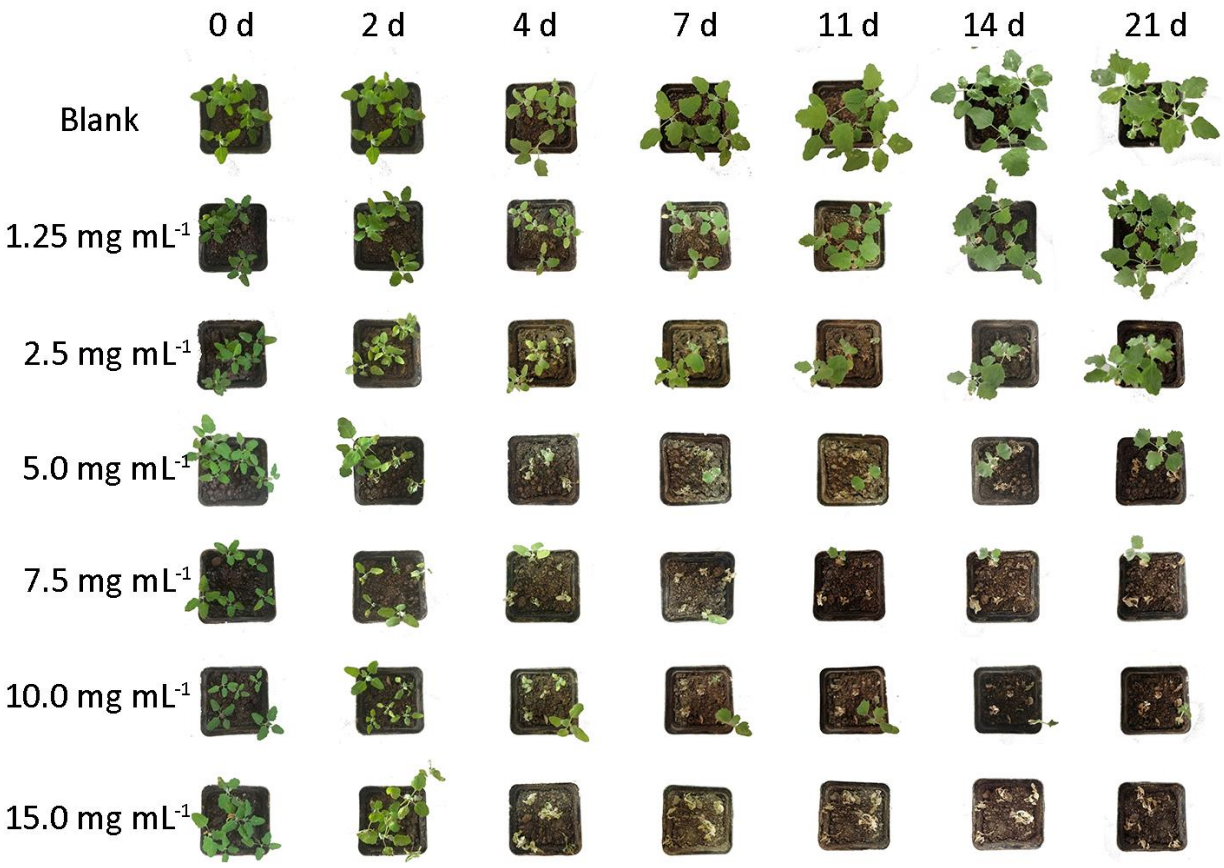

Fig. S33 Digital photographs of *Chenopodium album L.* after spraying with **IL 14** in different concentrations.

Chenopodium album L. (C. album)

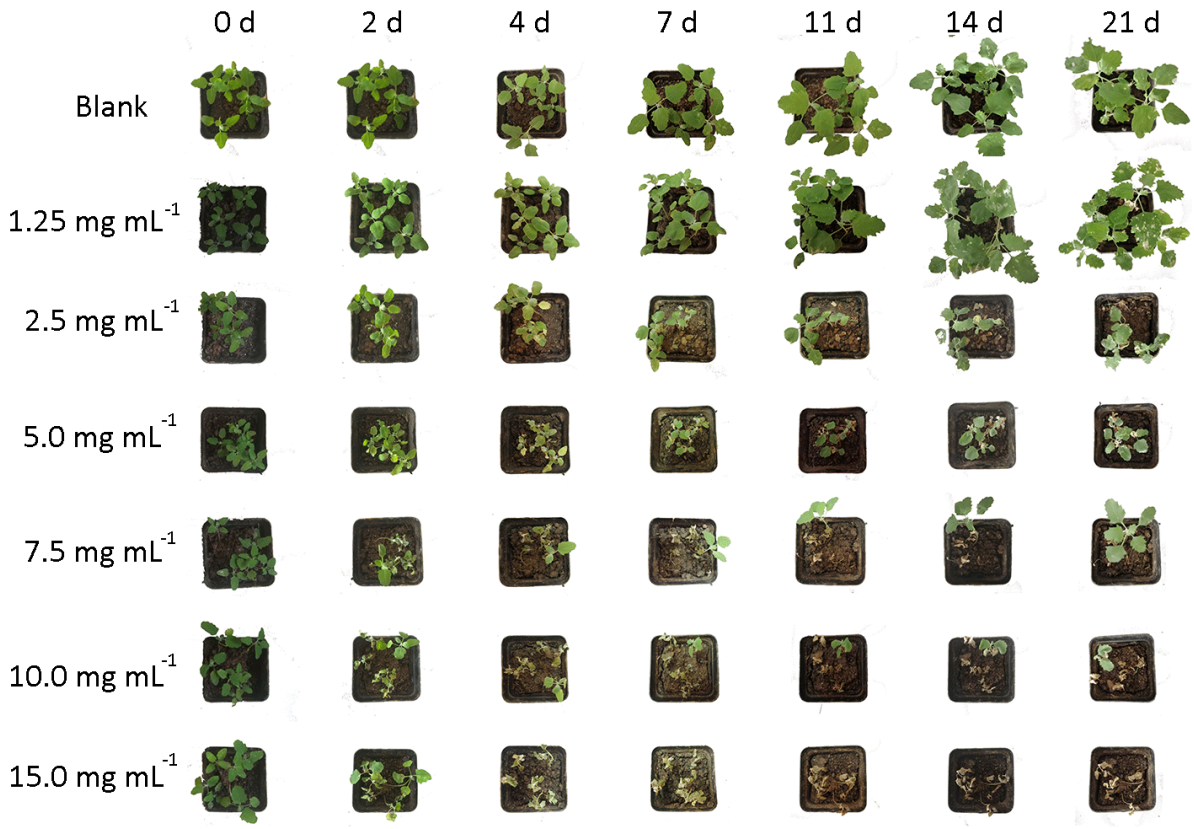

Fig. S34 Digital photographs of *Chenopodium album L.* after spraying with **IL 15** in different concentrations.

Chenopodium album L. (C. album)

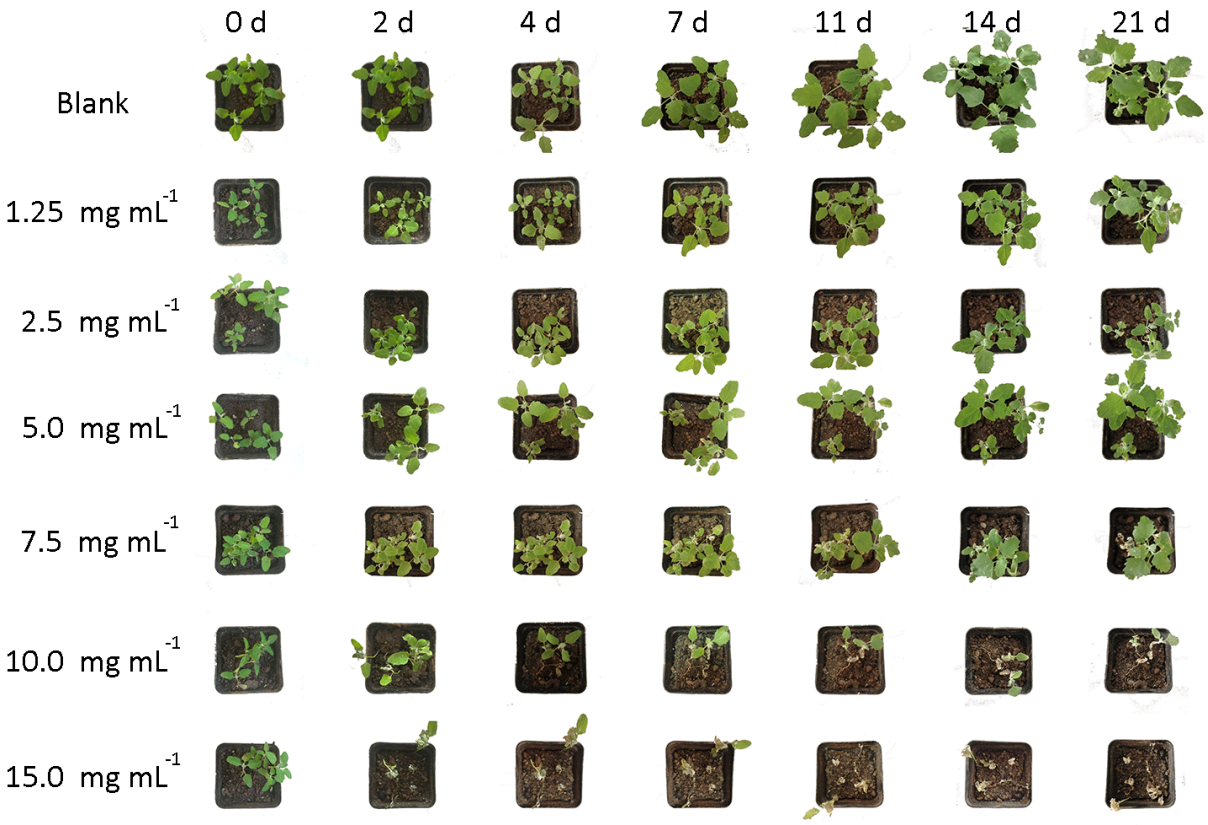

Fig. S35 Digital photographs of *Chenopodium album L.* after spraying with DCA in different concentrations.

Solanum nigrum L. (S. nigrum)

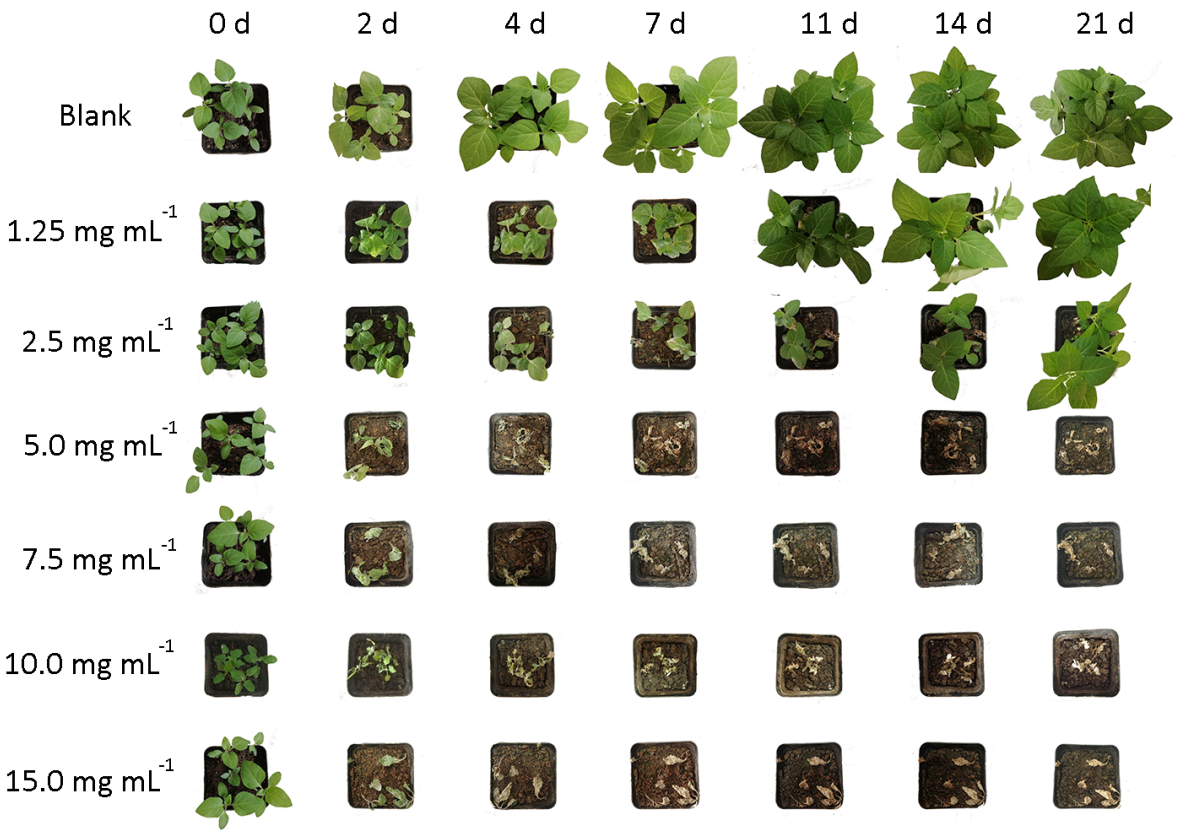

Fig. S36 Digital photographs of *Solanum nigrum L.* after spraying with **IL13** in different concentrations.

Solanum nigrum L. (S. nigrum)

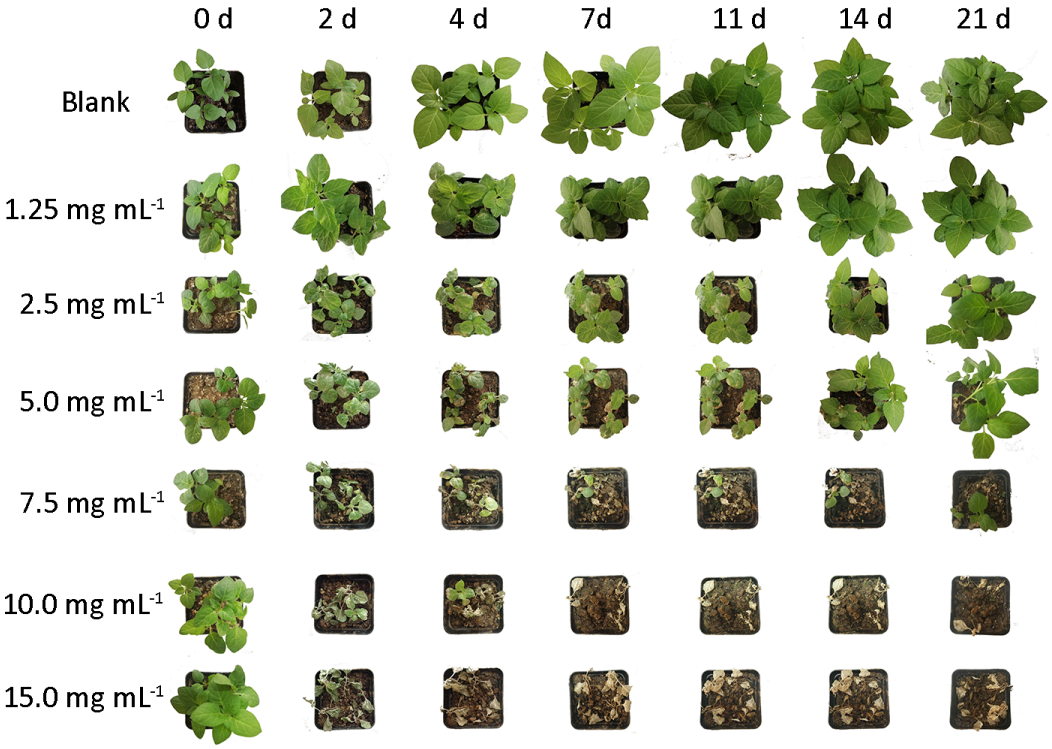

Fig. S37 Digital photographs of *Solanum nigrum L.* after spraying with **IL14** in different concentrations.

Solanum nigrum L. (S. nigrum)

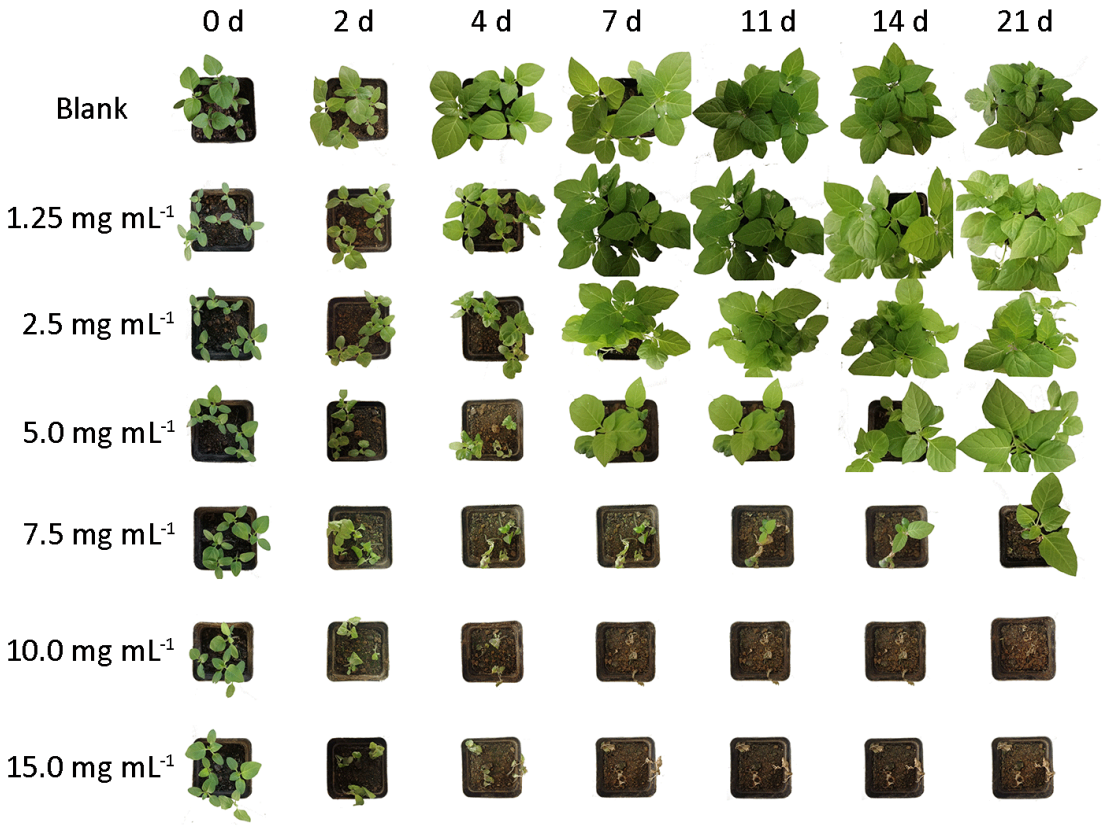

Fig. S38 Digital photographs of *Solanum nigrum L.* after spraying with **IL 15** in different concentrations.

Solanum nigrum L. (S. nigrum)

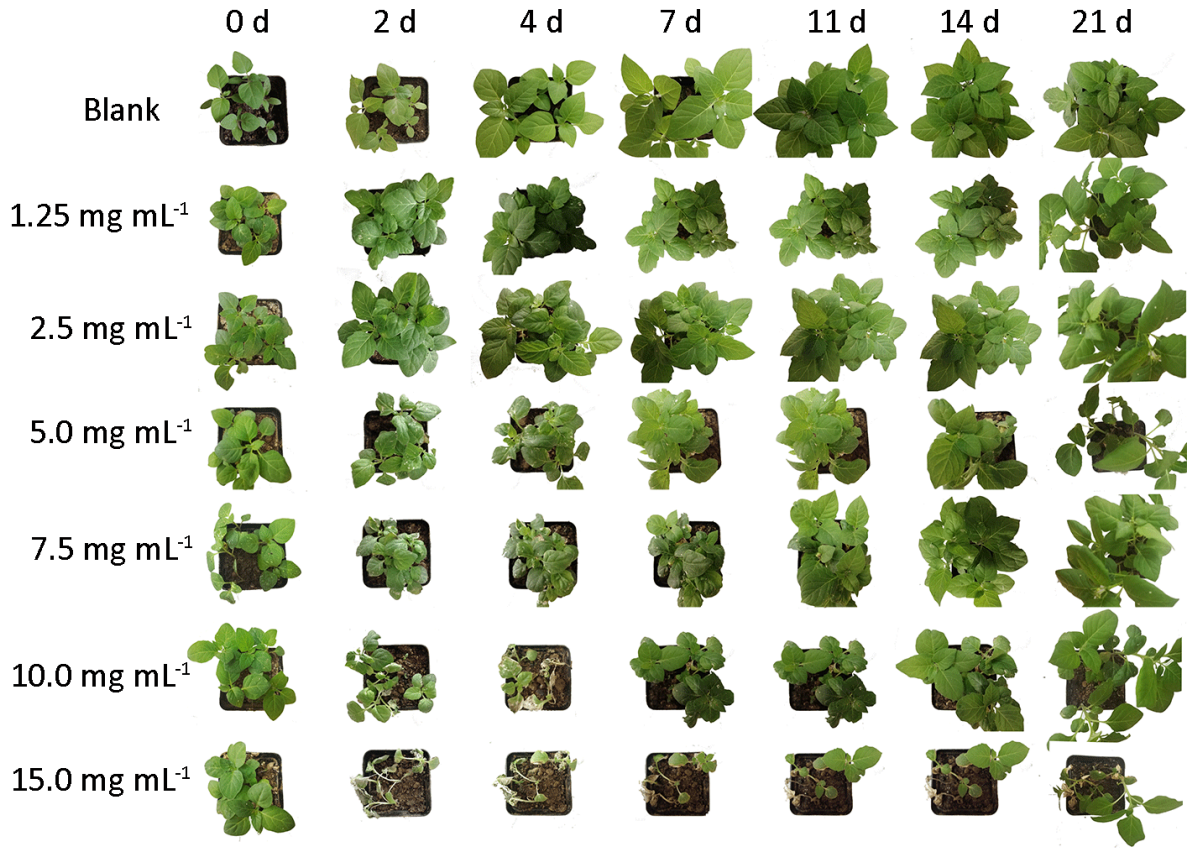

Fig. S39 Digital photographs of *Solanum nigrum L.* after spraying with DCA in different concentrations.

Xanthium sibiricum Patrin ex Widder (*X. sibiricum*)

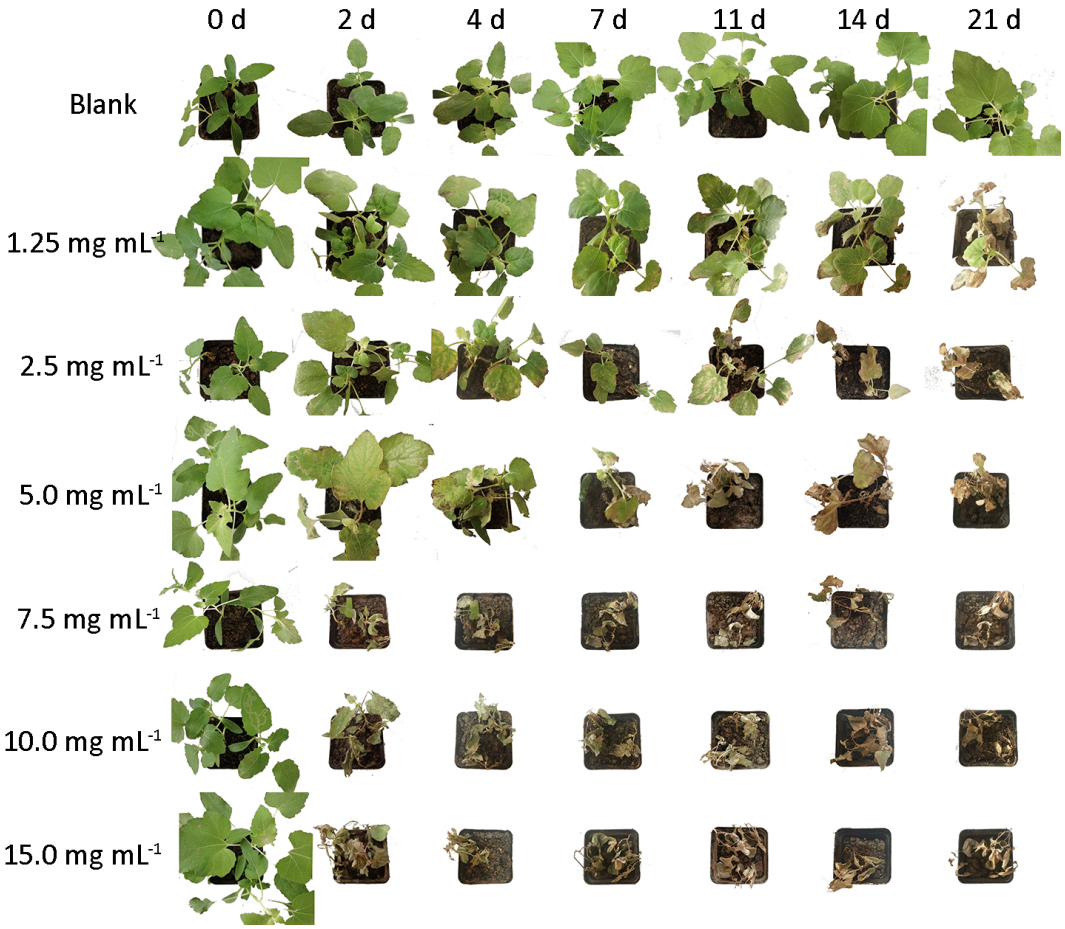

Fig. S40 Digital photographs of *Xanthium sibiricum Patrin ex Widder* after spraying with **IL 13** in different concentrations.

Xanthium sibiricum Patrin ex Widder (*X. sibiricum*)

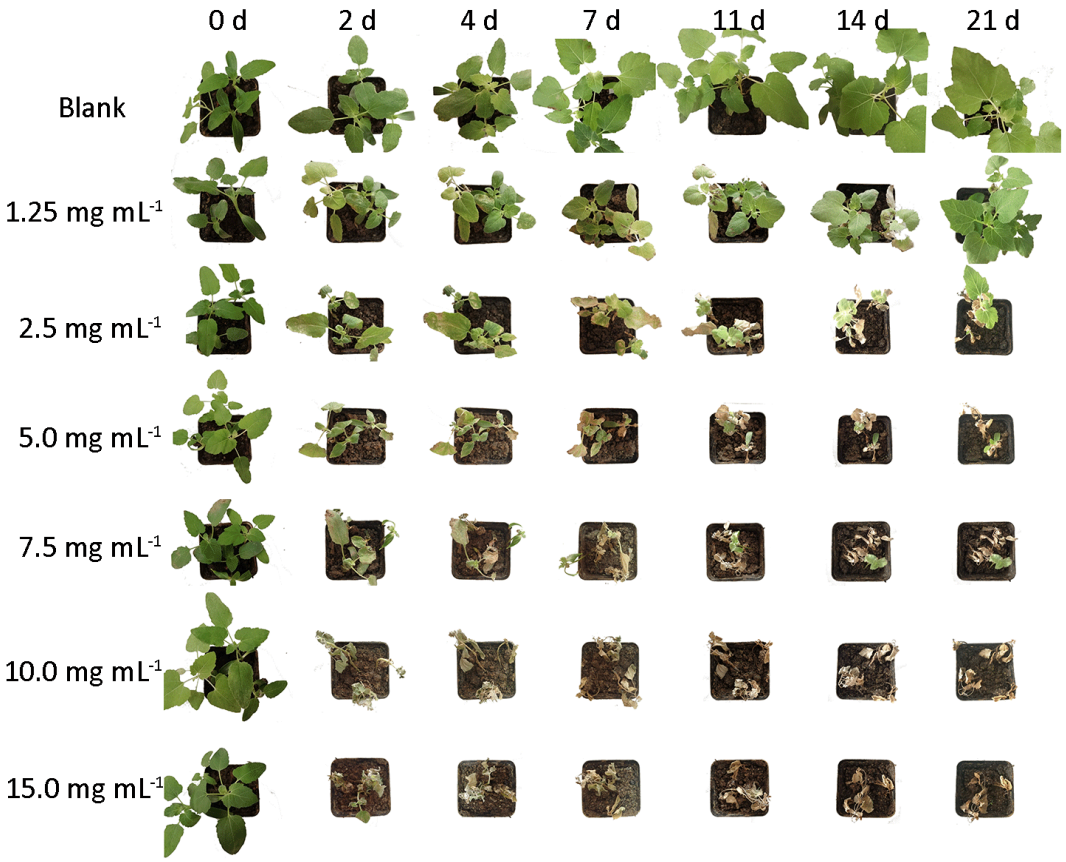

Fig. S41 Digital photographs of *Xanthium sibiricum Patrin ex Widder* after spraying with **IL 14** in different concentrations.

Xanthium sibiricum Patrin ex Widder (*X. sibiricum*)

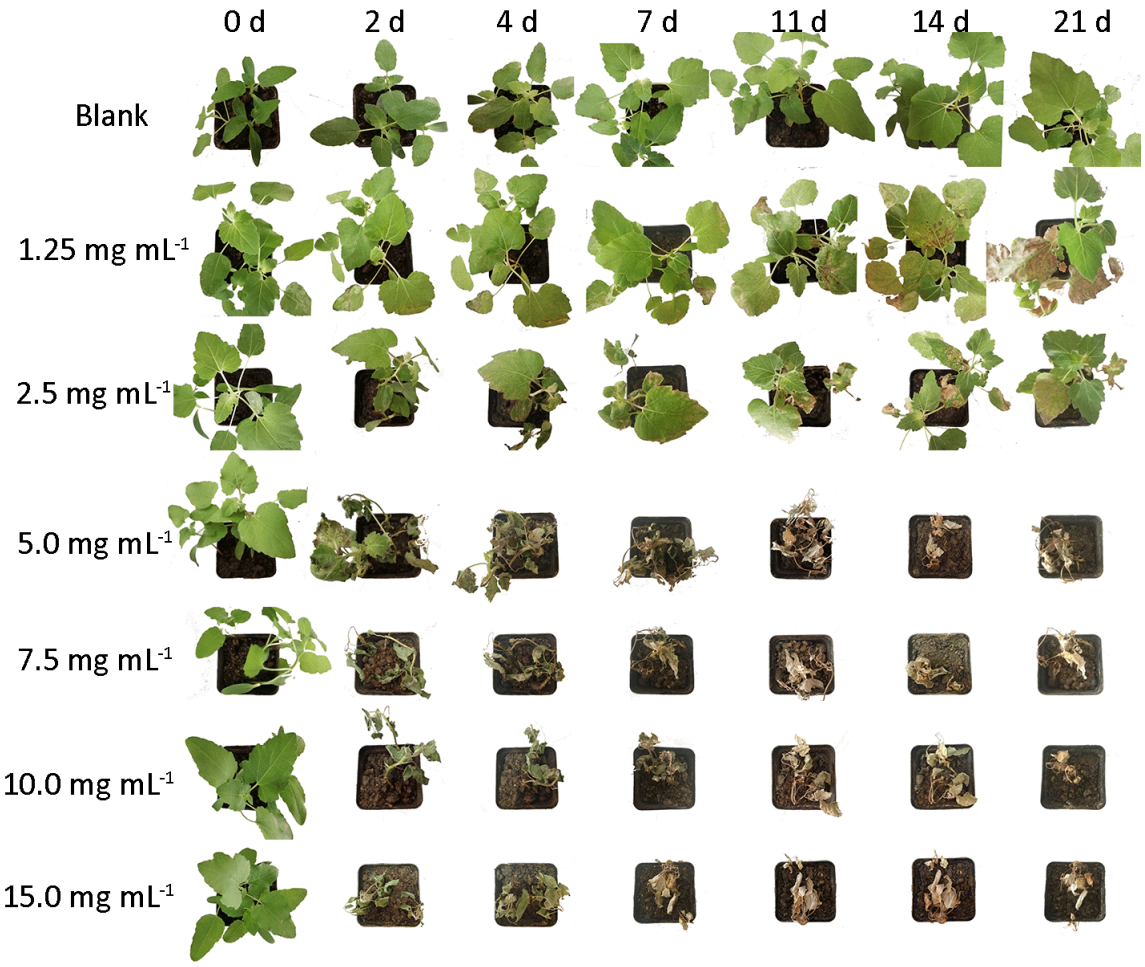

Fig. S42 Digital photographs of *Xanthium sibiricum Patrin ex Widder* after spraying with **IL 15** in different concentrations.

Xanthium sibiricum Patrin ex Widder (*X. sibiricum*)

Fig. S43 Digital photographs of *Xanthium sibiricum Patrin ex Widder* after spraying with DCA in different concentrations.