

Supporting Information

Smart Supramolecular Gels of Enolizable Amphiphilic Glycosylfuran

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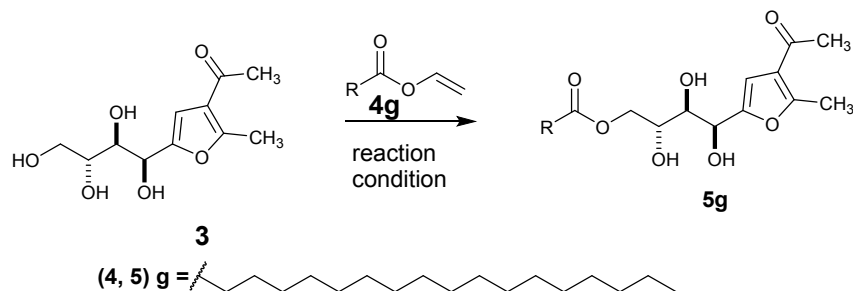
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Table of Contents

Table S1. Optimization of reaction condition	2
Table S2. Solvents/Oils used for gelation studies	2
Figure S1. (a) NMR and Mass spectral studies.	4
Figure S2. Images of gel formed by compound 5g	5
Figure S3. Optical microscopy image of (a-d) GH and (e-h) SGH respectively	5
Figure S4. FESEM image of (a-d) GH and (e-h) SGH respectively.	5
Figure S5. FETEM image of (a-f) Crystalline structure in water under neutral pH by glycosylfuran, 5g and (g,h) SGH respectively.	6
Figure S6. FTIR spectra of compound 5a-g	6
Figure S7. (a-f) XPS spectra of xerogel formed by GH and SGH	7
Figure S8-S23. NMR spectra	8
Figure S24. H ₂ S interaction/sensing studies	16

Table S1. Optimization of reaction condition

S. No	Solvent	Temperature (°C)	Time (h)	Yield (%) ^s
1	Dioxane	50	24	NR
2	Acetone	50	24	54
3	Acetonitrile	50	24	35
4	Isopropanol	50	24	38
5	<i>t</i> -BuOH	50	24	23
6	DMSO	50	24	Trace [#]
7	H ₂ O	50	24	Trace [#]
8	DCM	50	24	Trace [#]
9	DMF	50	24	Trace [#]
10	Toluene	50	24	10
11	Acetone	60	24	47
12	Acetone	70	24	Trace [#]
13	Acetone	50	48	78
14	Acetone	50	60	83
15	Acetone	50	72	79

Note: Reactions performed at <50 °C did not furnish the corresponding product in good yield, hence not shown in the optimization table. [#]observed trace product in TLC. ^sisolated yield after column chromatography.

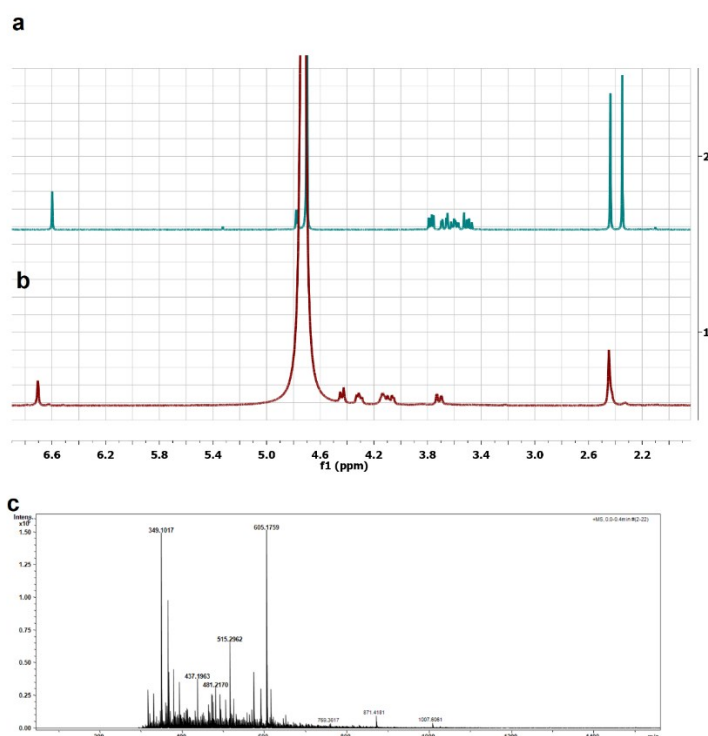
Table S2. Solvents/Oils used for gelation studies

S. No.	Solvent/vegetable oils	Observation Critical Gel Concentration (CGC wt/v%)						
		5a	5b	5c	5d	5e	5f	5g
1	Ethanol	S	S	S	S	S	S	S
2	<i>n</i> -Butanol	S	S	S	S	S	S	S

3	Octanol	S	S	S	S	S	S	S
4	Decanol	S	S	S	S	S	S	S
5	Dodecanol	S	S	S	S	S	S	S
6	Toluene	S	S	S	S	S	S	PG
7	Benzene	S	S	S	S	S	S	S
8	Diesel	S	S	S	S	S	S	S
9	1,2-Dichlorobenzene	S	S	S	S	S	PG	G
10	Chloroform	S	S	S	S	S	S	S
11	Hazelnut oil	S	S	S	PG	G (1)	G (1)	G(0.7)
12	Olive oil	S	PG	S	PG	G (1)	G (1)	G(0.8)
13	Heavy paraffin oil	S	PG	S	G(1)	G (1)	G (1)	G(0.6)
14	Light paraffin oil	S	S	S	PG	PG	PG	G (1)
15	Sesame oil	S	S	S	PG	PG	PG	PG
16	Linseed oil	S	S	S	PG	PG	G (1)	G (0.6)
17	H ₂ O	I	P	P	P	Crys	Crys	Crys
18	DMSO+ H ₂ O (1:9)*	S	P	S	P	P	PG	G (1)
19	DMF+ H ₂ O (1:1)	S	P	S	P	P	PG	PG
20	Ethylacetate	S	S	S	S	S	S	S
21	Cyclohexane	S	S	S	S	S	S	S
22	EPALO	S	S	S	S	S	PG	G (1)
23	Castor oil	S	S	S	S	S	S	PG

* Self-sorting gel under basic pH was observed even without using heating cooling cycle

NMR and mass spectral analysis



The addition of freshly prepared 1 wt/v% Na_2S solution into the solution of **5g** (1 wt/v%) dramatically accelerate the gelation process by encapsulating Na_2S and H_2S via the intermolecular interactions. Xerogel obtained from SGH is subjected to the mass spectral analysis. Mass spectral data reveals the enolization of **5g** along with the strongly interacted H_2O and Na_2S in xerogel state. Exact mass calculated for $\text{C}_{29}\text{H}_{51}\text{Na}_2\text{O}_8\text{S}$ $m/z = 605.3100$; found $m/z = 605.1759$

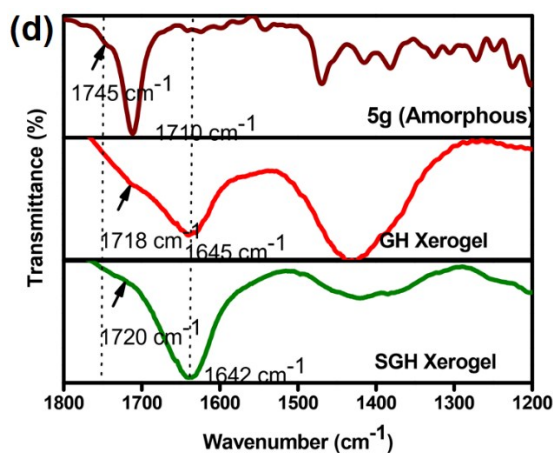


Figure S1. (a) ^1H NMR spectra of compound **3** in D_2O ; (b) ^1H NMR spectra of compound **3** in $\text{D}_2\text{O} + \text{NaOH}$ 1wt/v%; (c) Mass spectra of xerogel of SGH in MeOH and (d) FTIR spectral comparison of **5g** in amorphous state, GH xerogel and SGH xerogel.

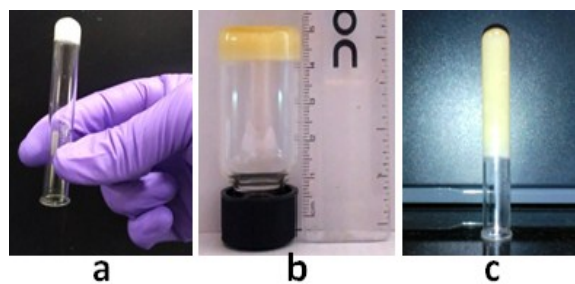


Figure S2. Images of gel formed by compound **5g** in a) 1 wt/v% of Na_2S under self-sorting condition (SGH); b) 1 wt/v% of NaOH under self-sorting condition (GH); c) 1 wt/v% of Na_2S under the influence of heating cooling cycle.

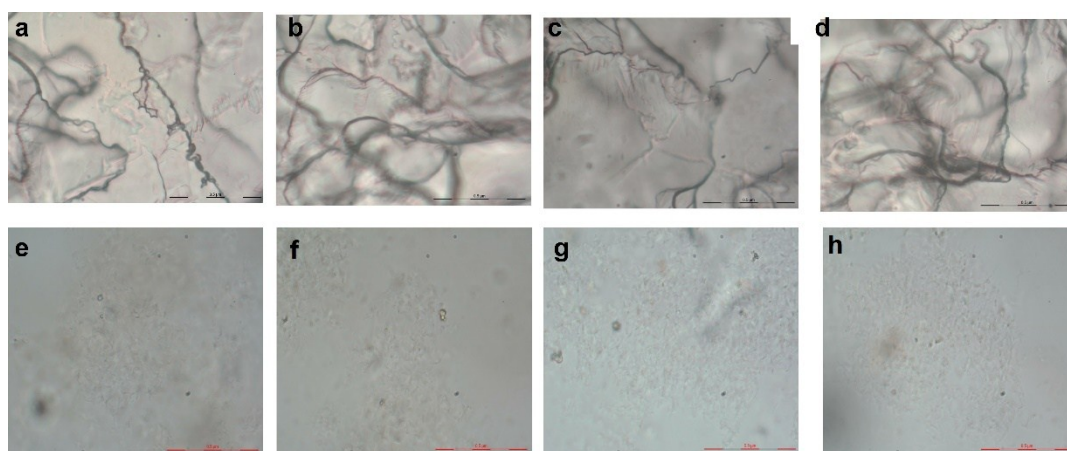


Figure S3. Optical microscopy image of (a-d) GH and (e-h) SGH respectively

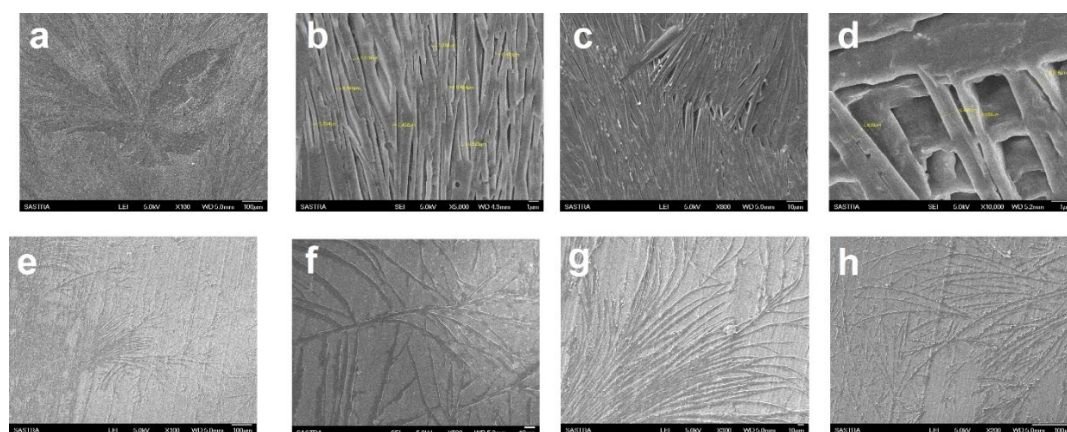


Figure S4 FESEM image of (a-d) GH and (e-h) SGH respectively.

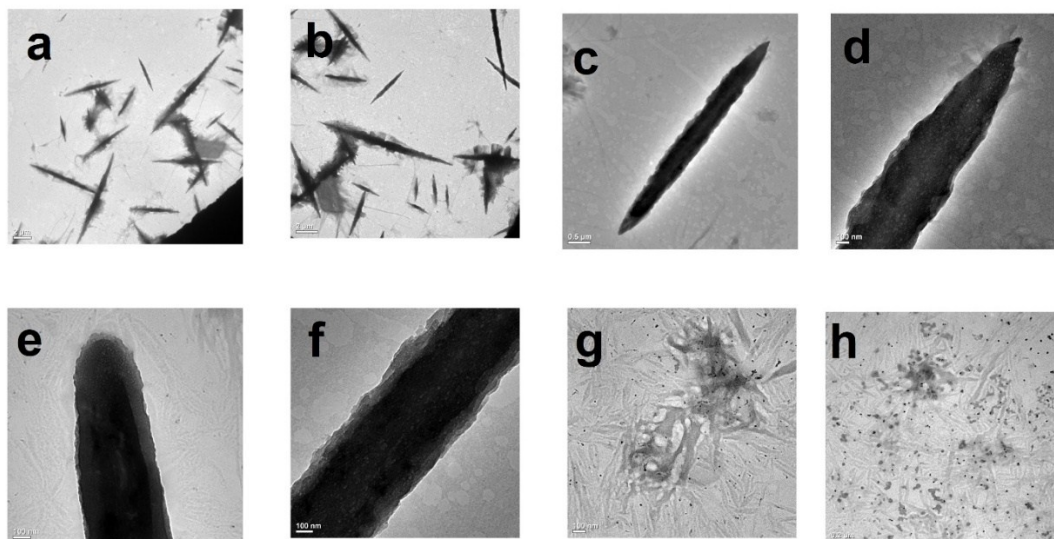


Figure S5 FETEM image of (a-f) Crystalline structure in water under neutral pH by glycosylfuran, 5g and (g,h) SGH respectively.

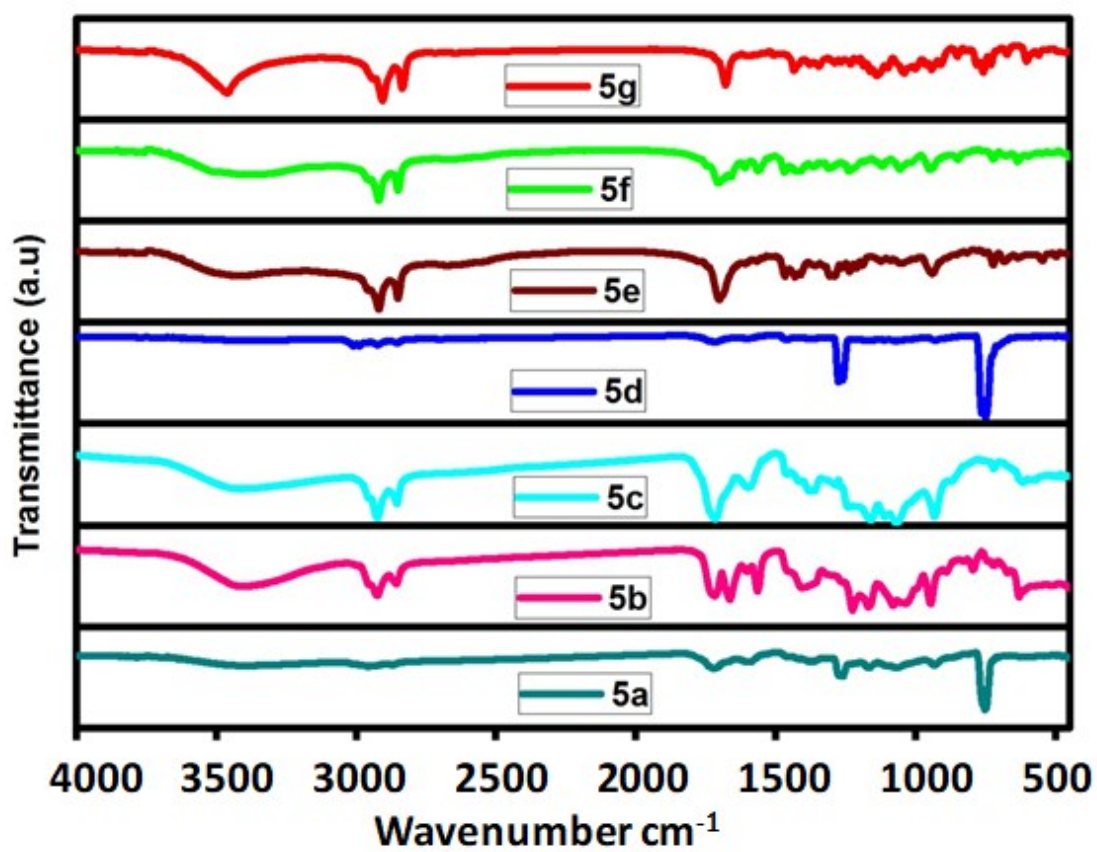


Figure S6 FTIR spectra of compound 5a-g

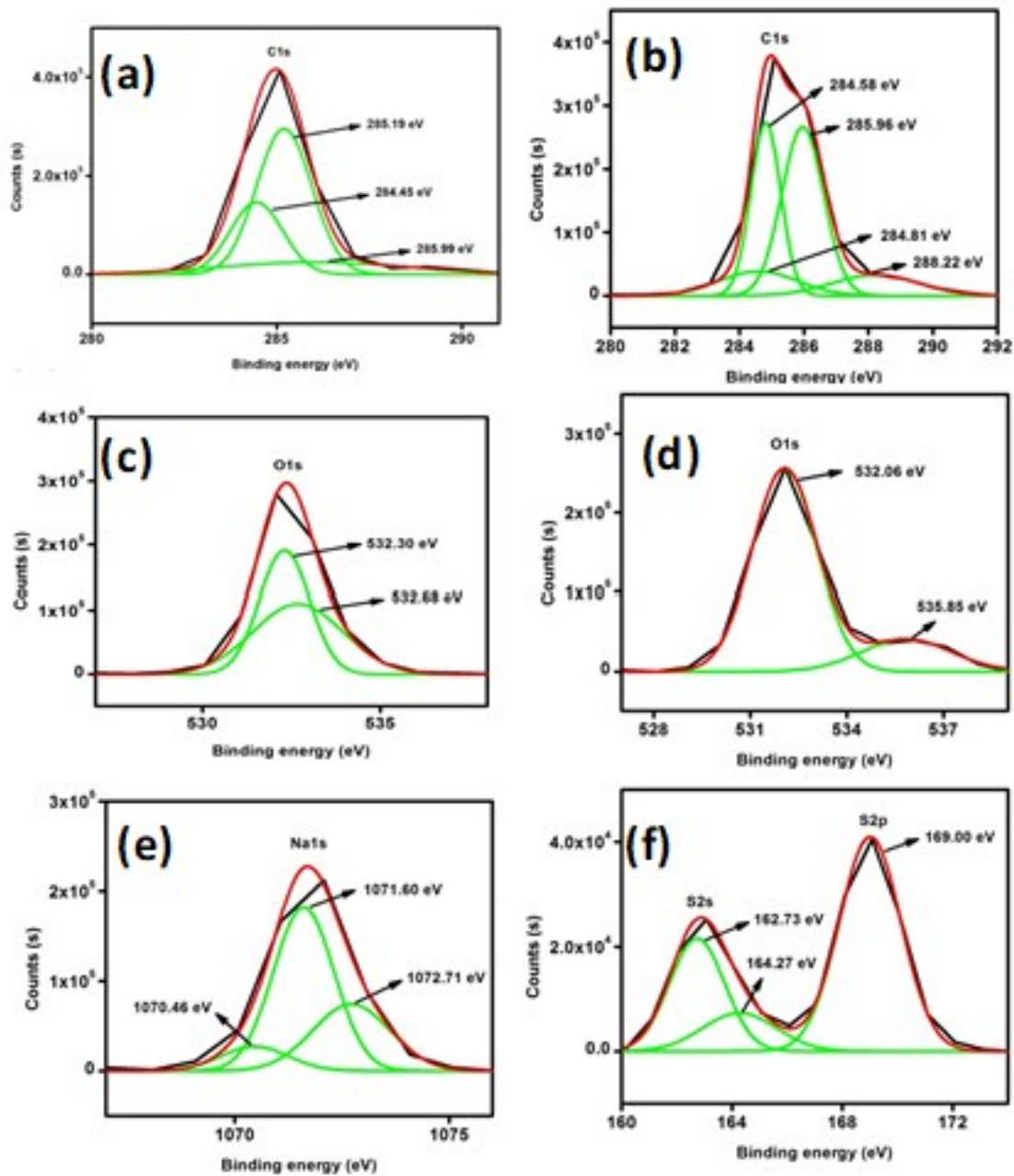


Figure S7. (a-f) XPS spectra of xerogel formed by GH and SGH

NMR spectra

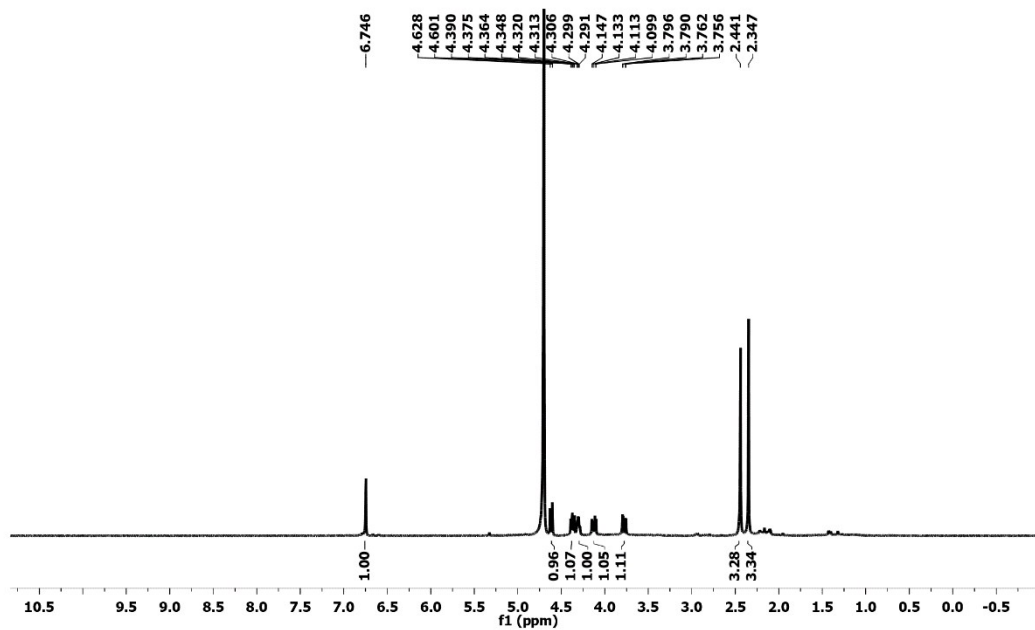


Figure S8. ^1H NMR of compound, **3** in D_2O

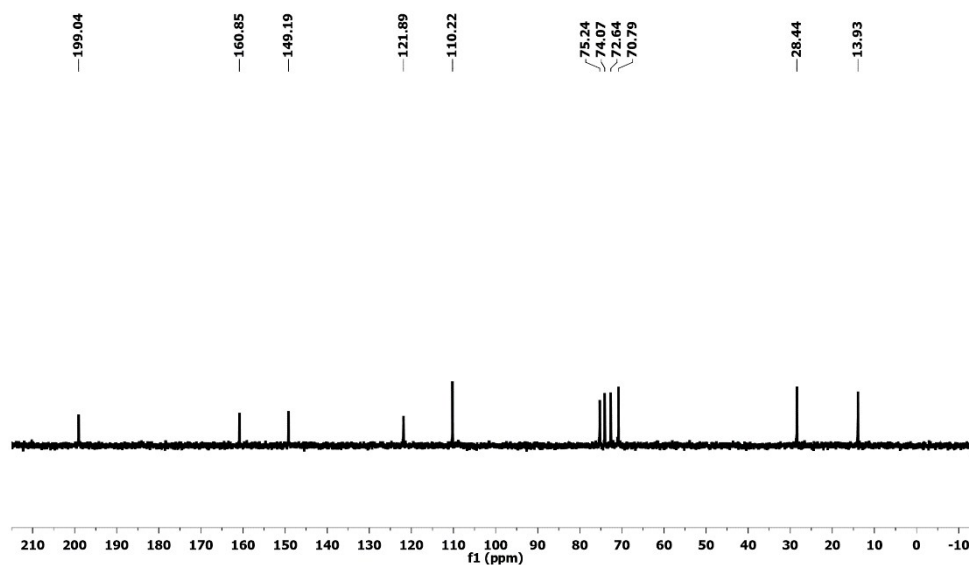


Figure S9. ^{13}C NMR of compound, **3** in D_2O

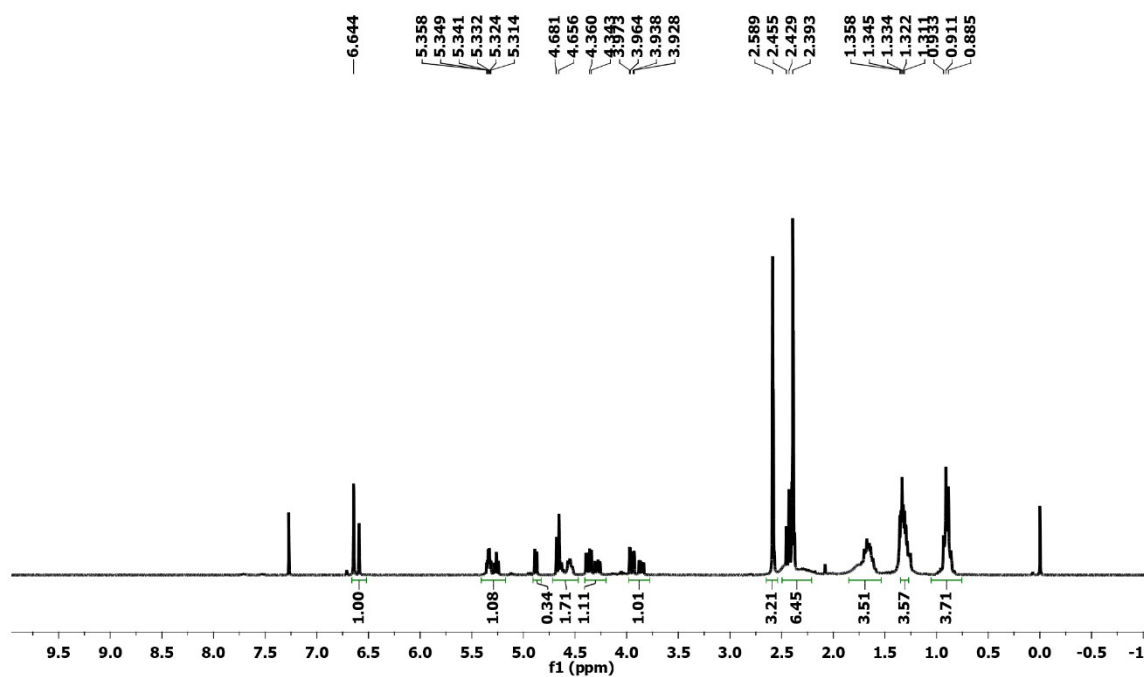


Figure S10. ^1H NMR of compound, **5a** in CDCl_3

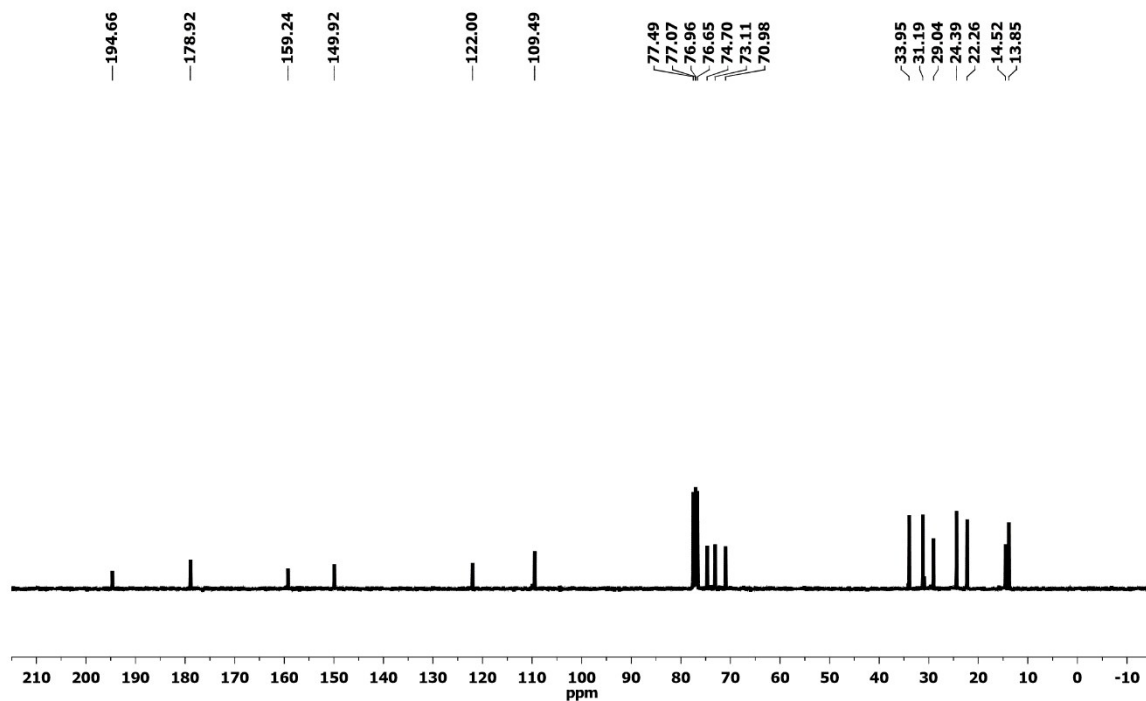


Figure S11. ^{13}C NMR of compound, **5a** in CDCl_3

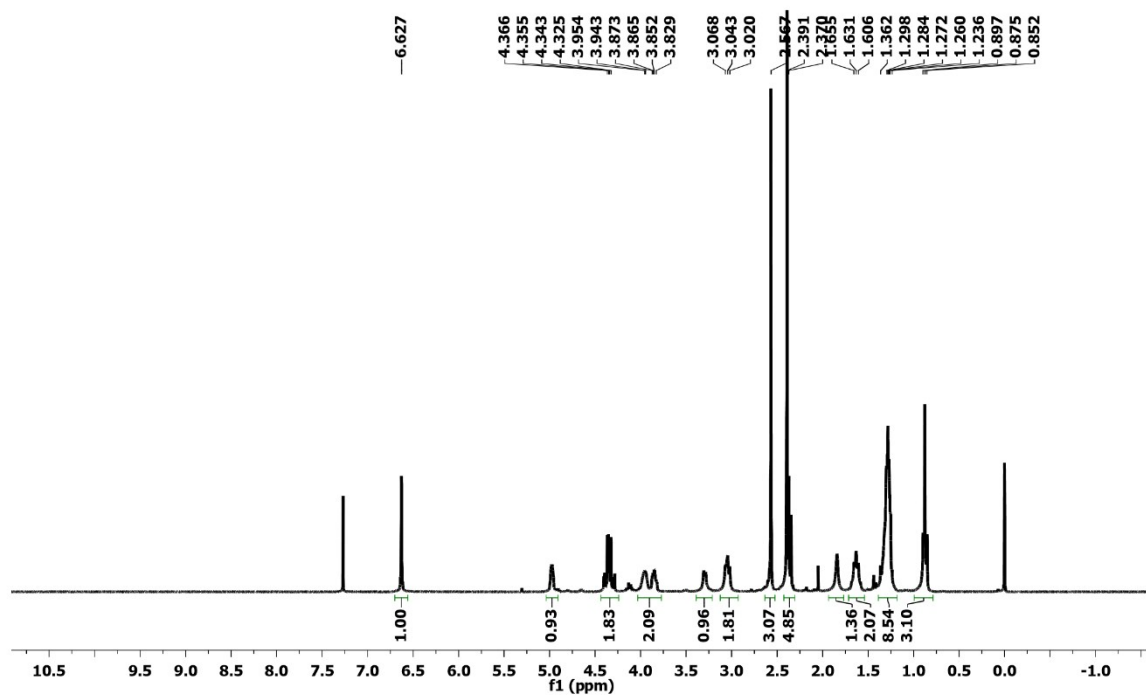


Figure S12. ^1H NMR of compound, **5b** in CDCl_3

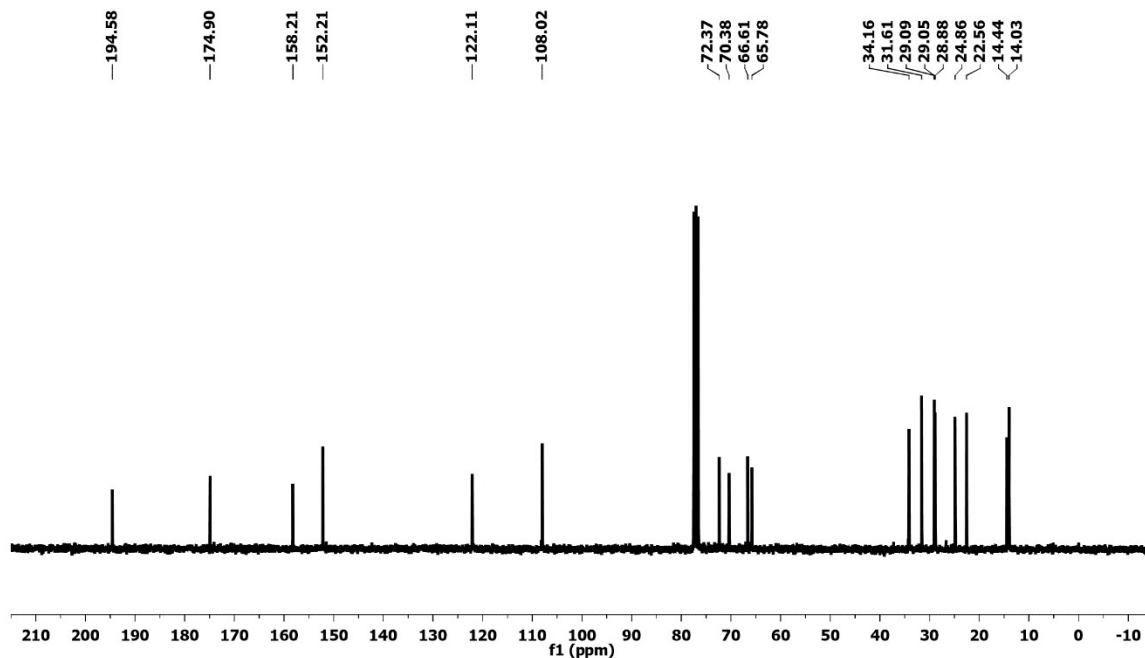


Figure S13. ^{13}C NMR of compound, **5b** in CDCl_3

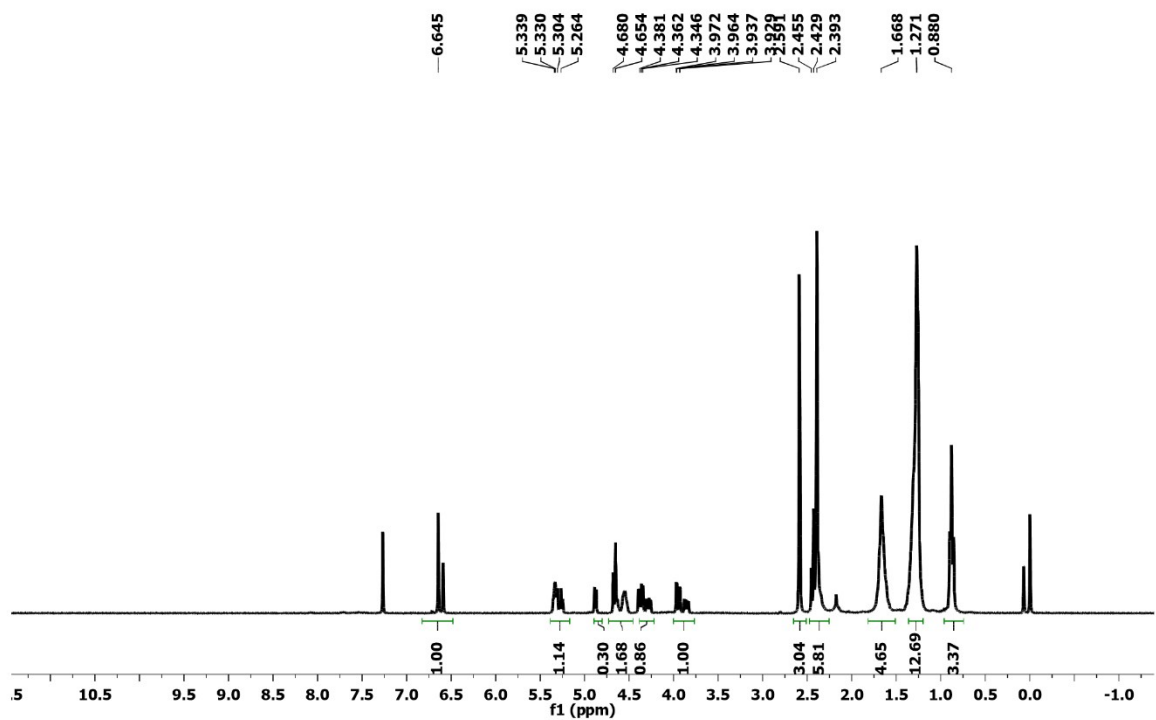


Figure S14. ^1H NMR of compound, **5c** in CDCl_3

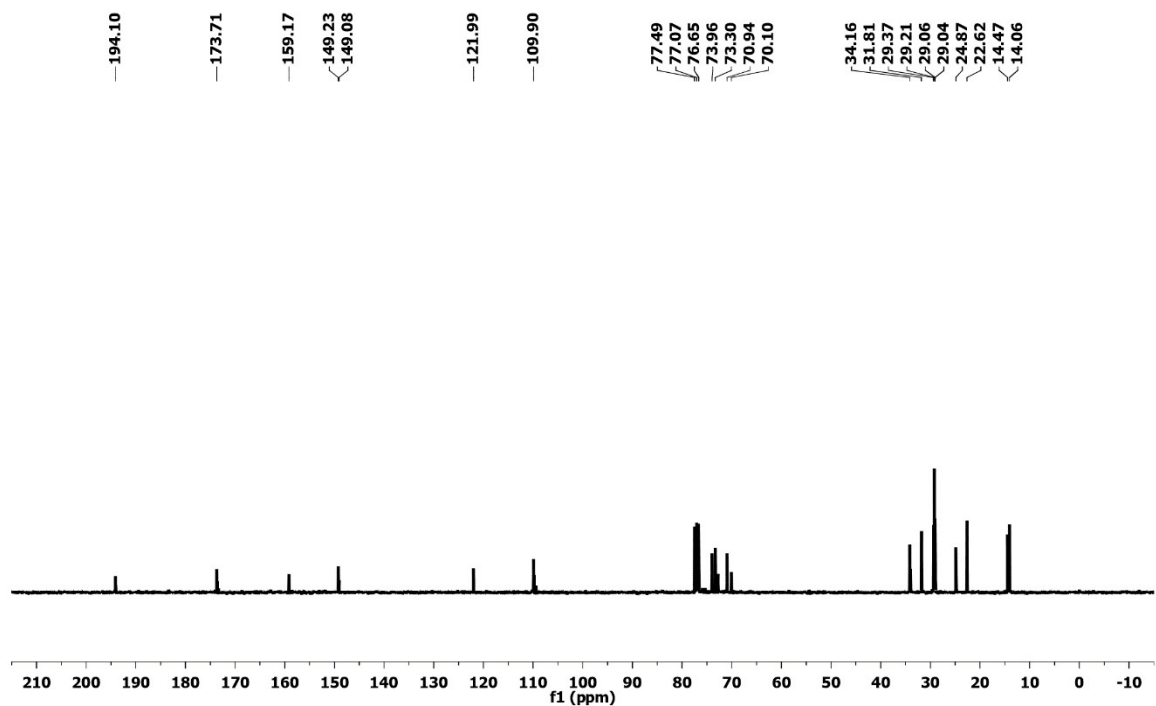


Figure S15. ^{13}C NMR of compound, **5c** in CDCl_3

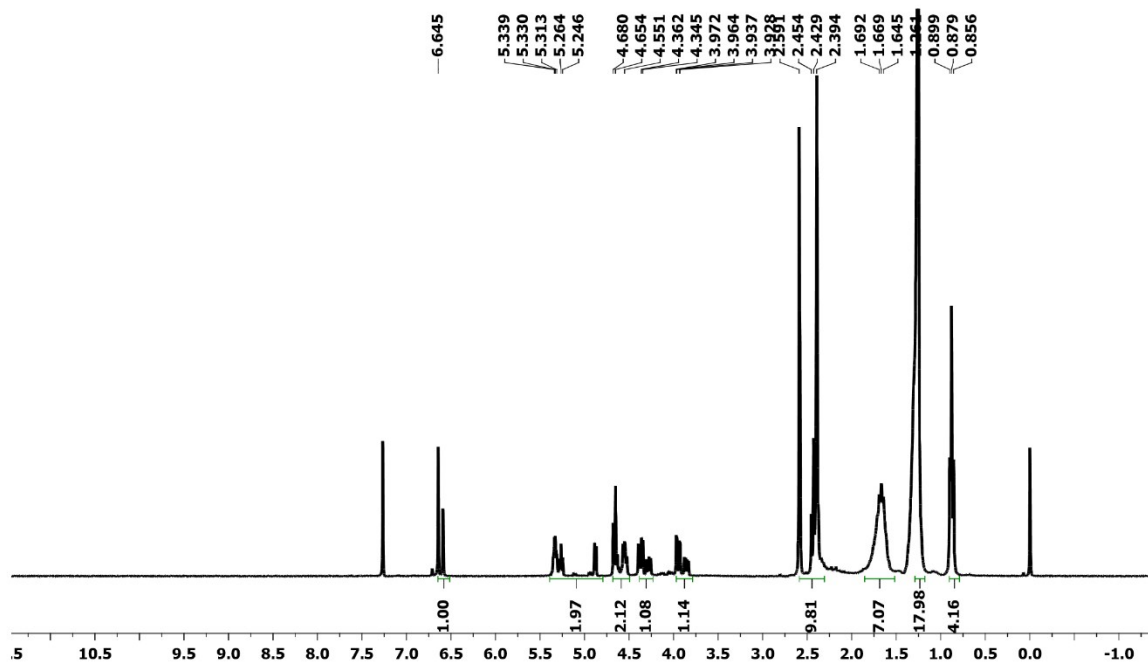


Figure S16. ^1H NMR of compound, **5d** in CDCl_3

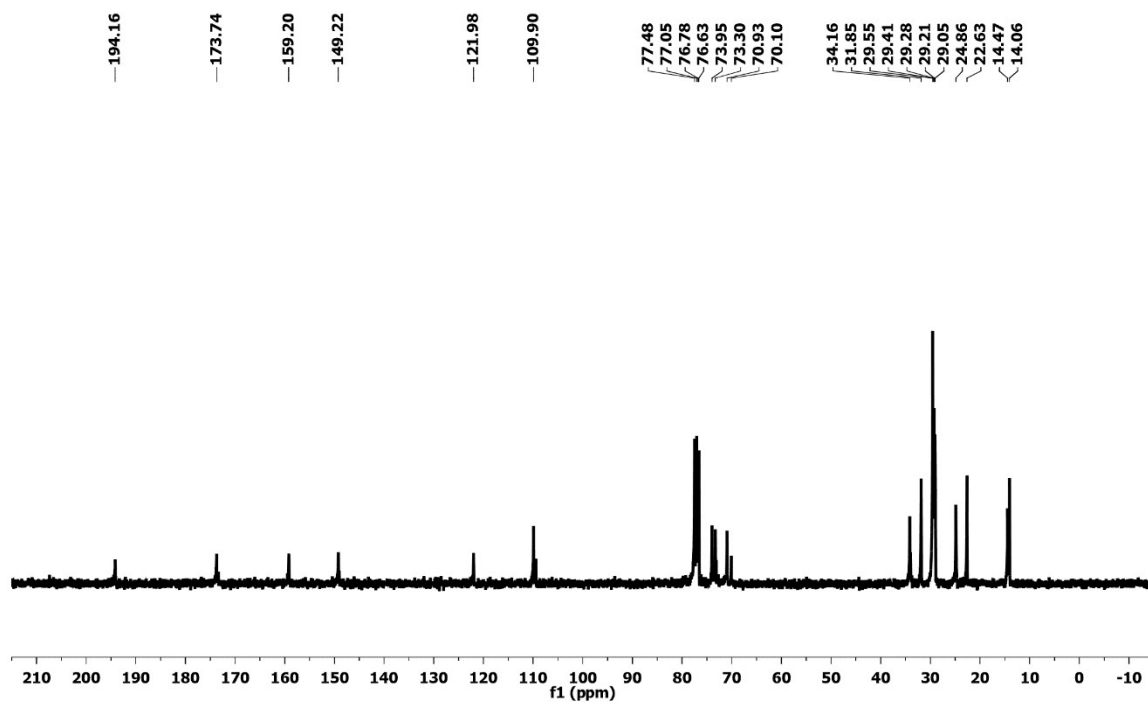


Figure S17. ^{13}C NMR of compound, **5d** in CDCl_3

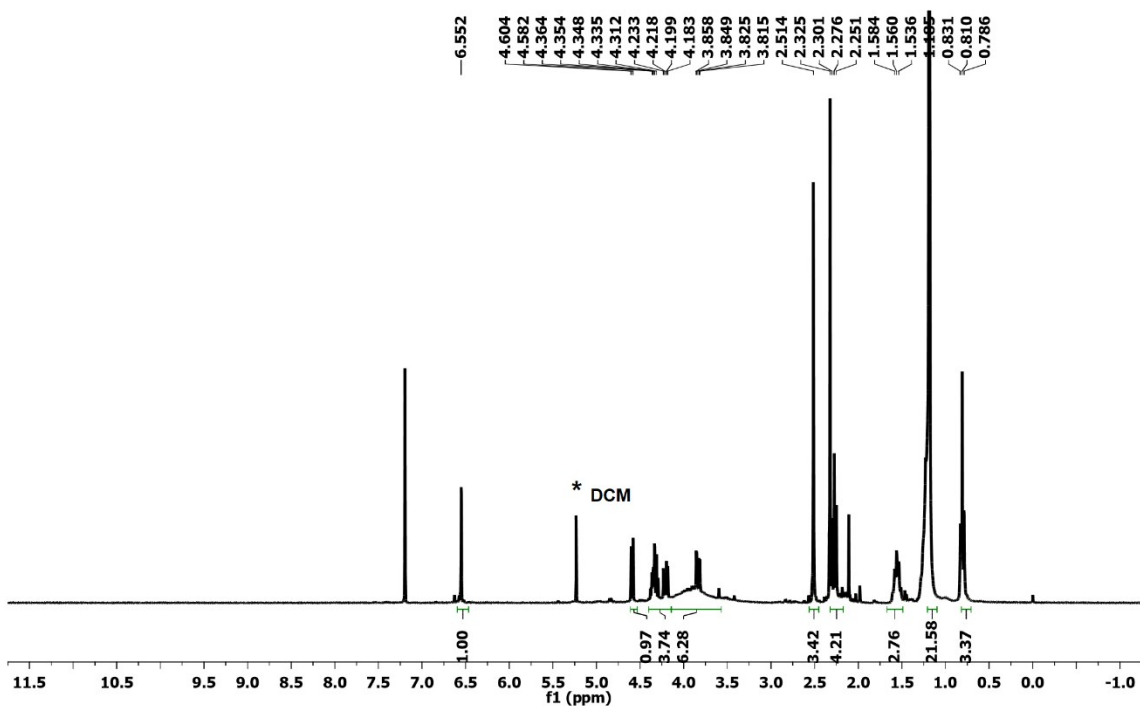


Figure S18. ^1H NMR of compound, **5e** in CDCl_3

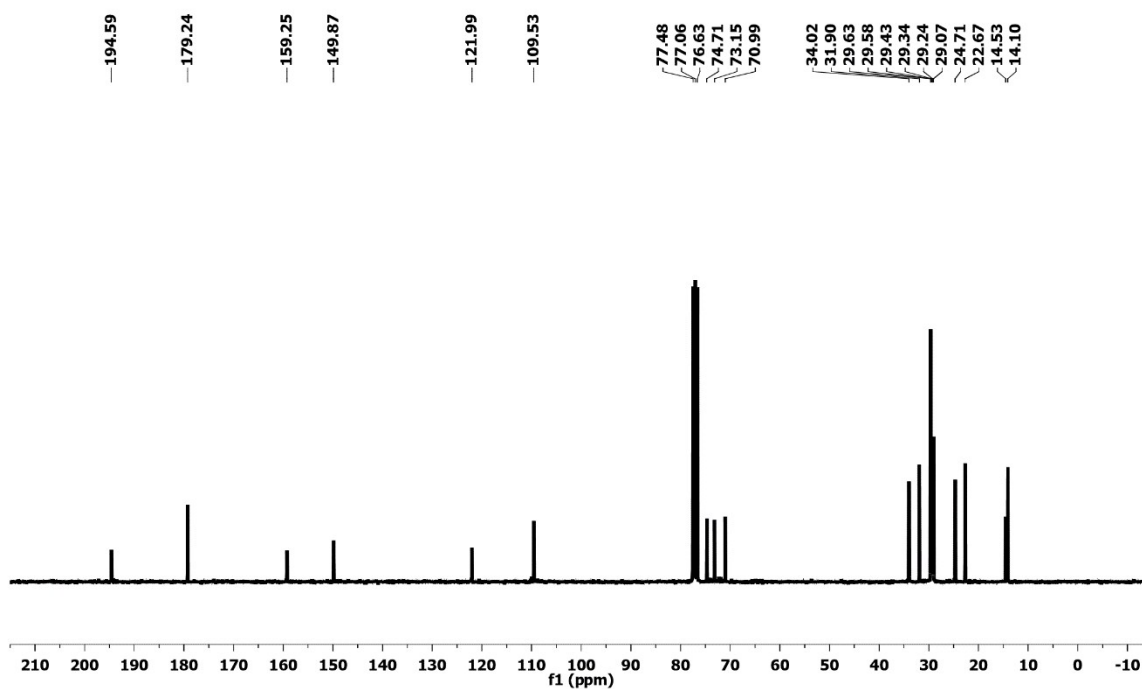


Figure S19. ^{13}C NMR of compound, **5e** in CDCl_3

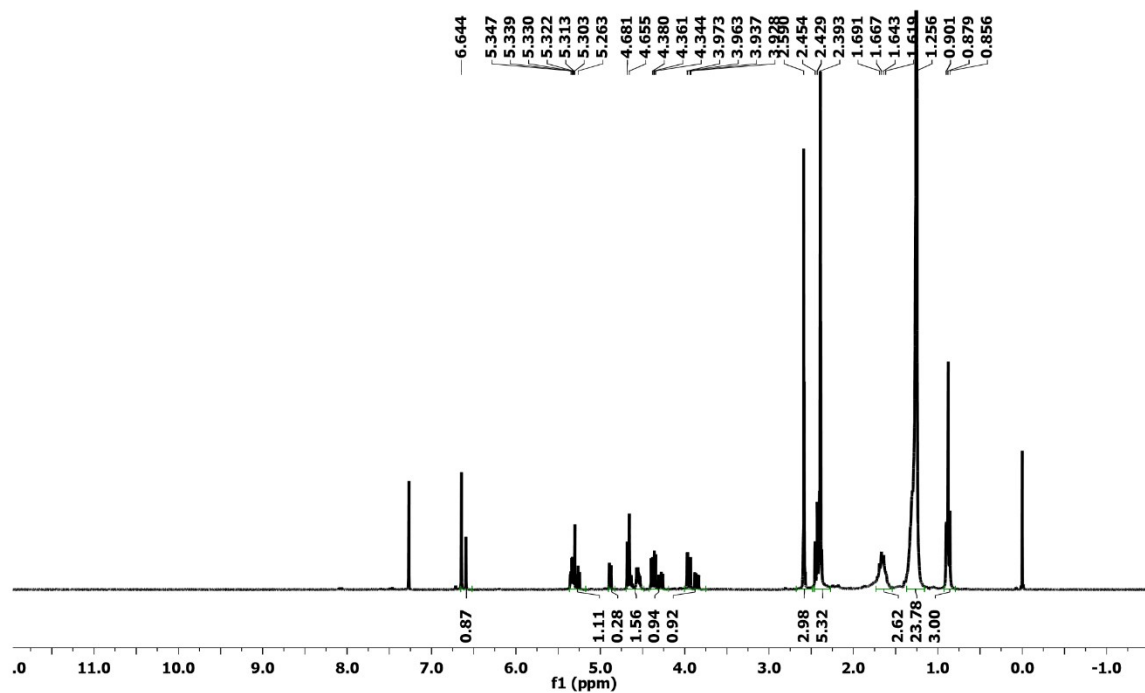


Figure S20. ^1H NMR of compound, **5f** in CDCl_3 at 300 K

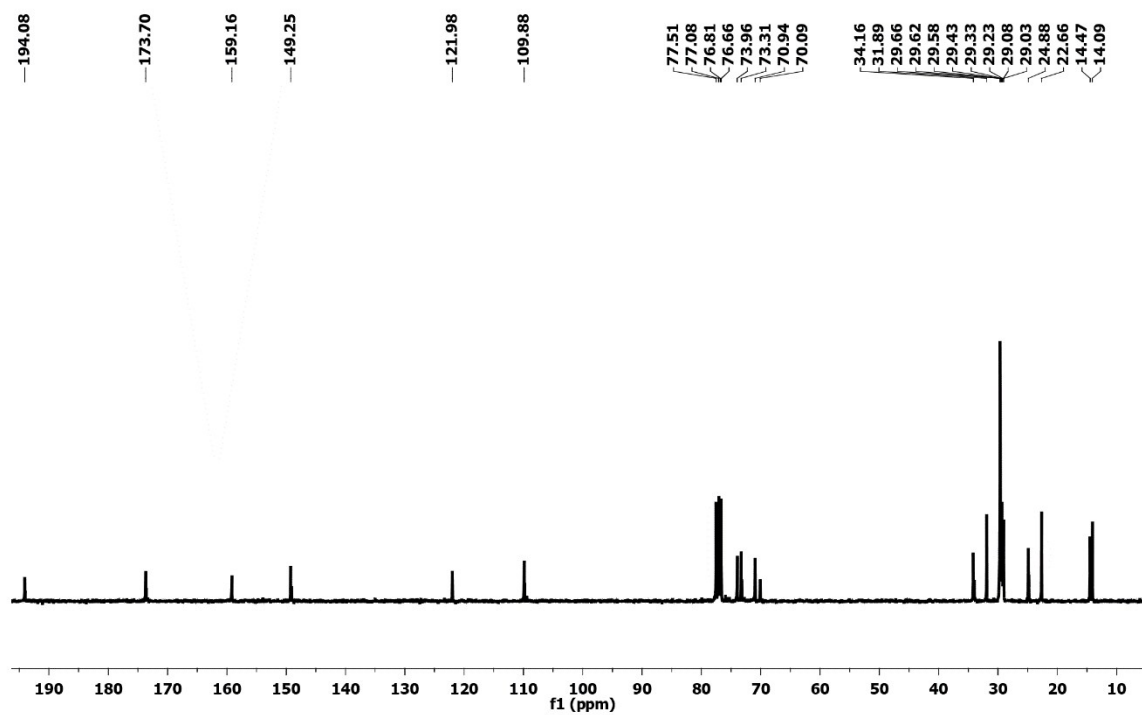


Figure S21. ^{13}C NMR of compound, **5f** in CDCl_3 at 300 K

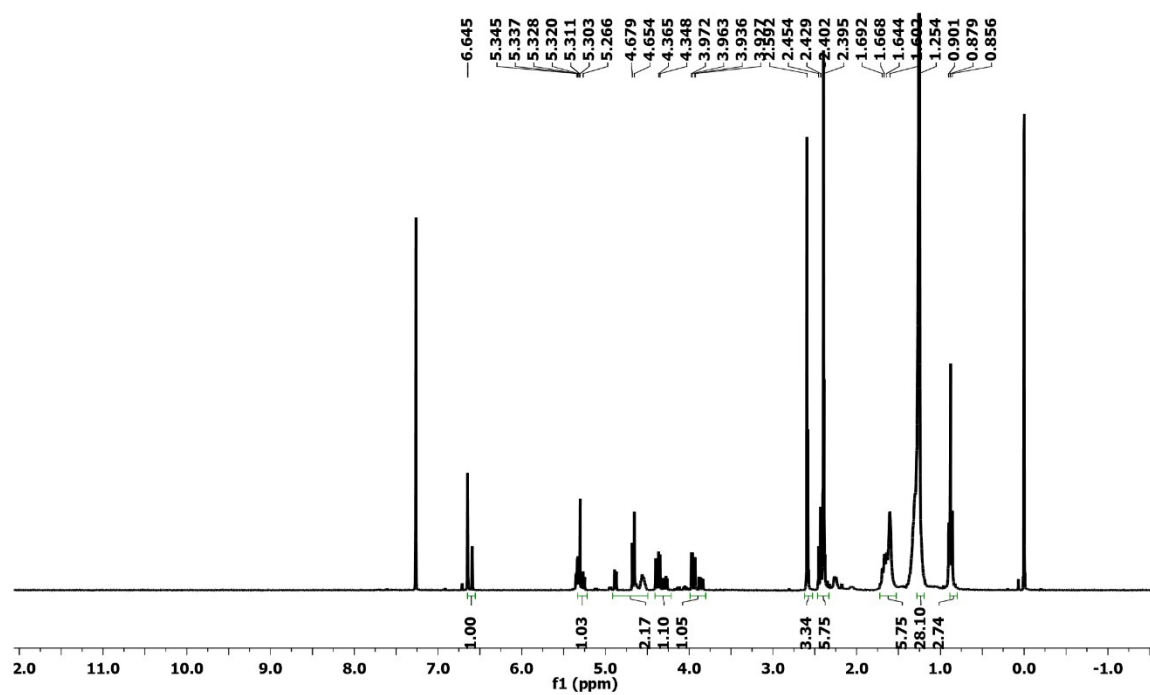


Figure S22. ^1H NMR of compound, **5g** in CDCl_3

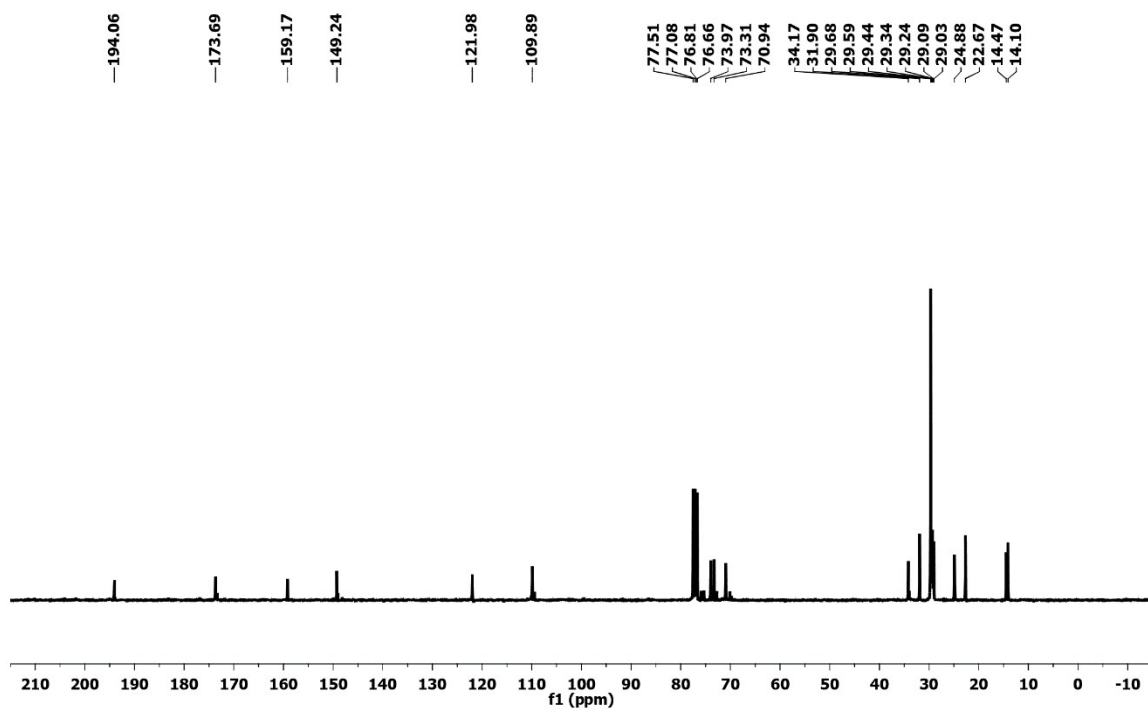


Figure S23. ^{13}C NMR of compound, **5g** in CDCl_3

H₂S interaction/sensing studies

The sensing response H₂S generated from Na₂S has been calculated using the equation, $S = R_a/R_g$, where R_a represents the resistance at the ambient atmosphere and R_g is the resistance of the sensing element in the presence of the target gas.

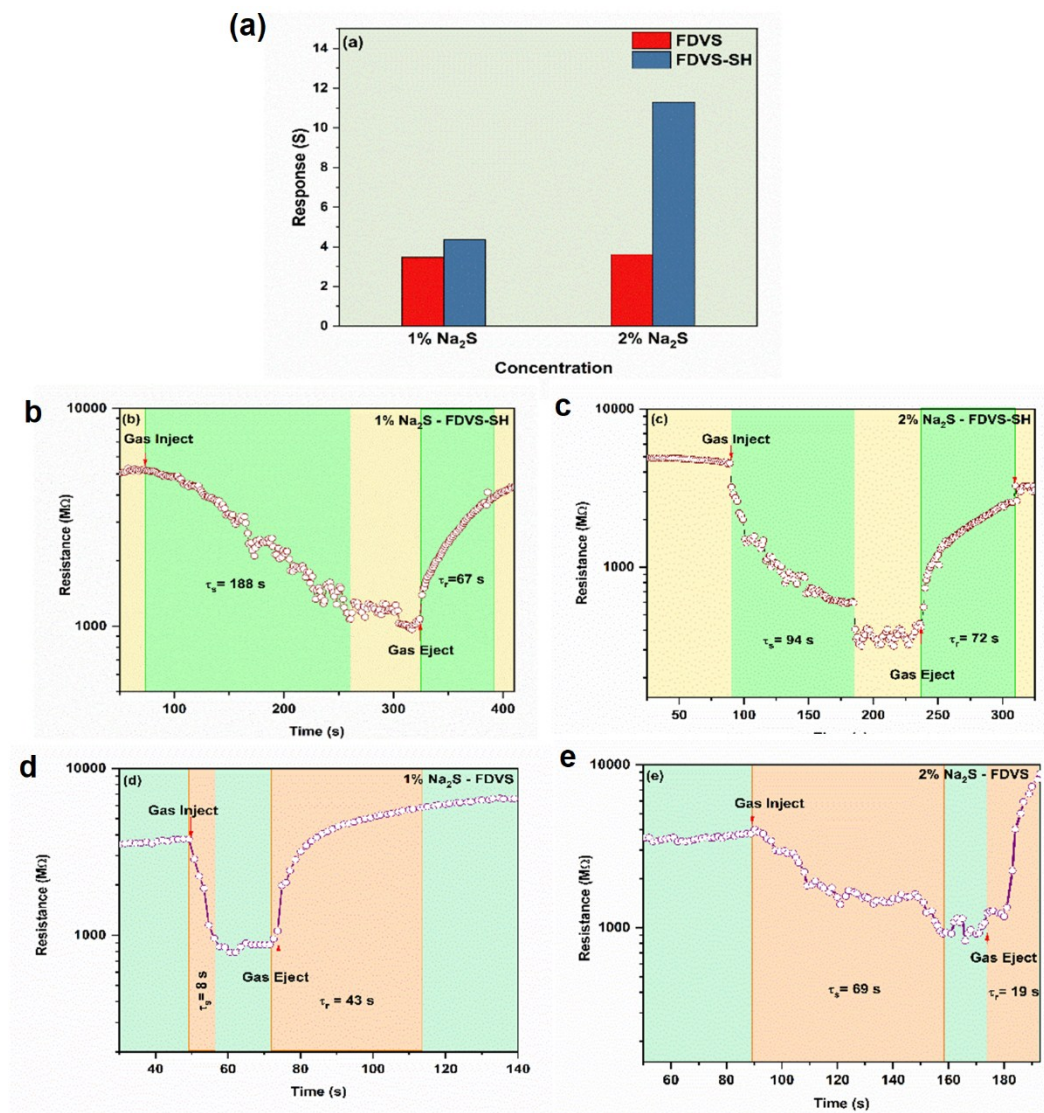


Figure S24. (a) representation of H₂S Sensing characteristics of **5g** in amorphous state (red) and xerogel of GH in assembled state (blue) towards 1% and 2% of Na₂S concentration. (b-e) shows the transient responses GH & amorphous 5g sensing elements towards 1% and 2% of Na₂S concentration dissolved in water.