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Supplementary

Anti-Inflammatory Flavonolignans from *Triticum aestivum* Linn. Hull

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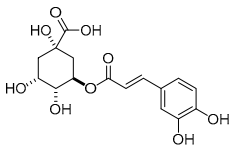
Table S1. Reported constituents of the aerial, hull, bran, and sprout part of *T. aestivum*.

Part	Compound name	Reference
Aerial	**Phenolic acid**	[10]
	3-*O*-caffeoylquinic acid (**1**)	
	4-*O*-caffeoylquinic acid (**2**)	
	5-*O*-caffeoylquinic acid (**3**)	
	3-*O*-feruoylquinic acid (**4**)	
	4-*O*-feruoylquinic acid (**5**)	
	5-*O*-feruoylquinic acid (**6**)	
	p-coumaric acid (**7**)	
	Flavonoid	
	isoorientin 6''-*O*-*β*-D-xylopyranoside (**8**)	
	isoorientin (**9**)	
	isoschaftoside (**10**)	
	isoscoparin 2''-*O*-*α*-L-rhamnopyranoside (**11**)	
	tricin 7-*O*-rutinoside (**12**)	
	luteolin 6-*C*-[6- glucopyranosyl -*O*-*E*-caffeoyl-*β*-D-glucopyranosyl(1''→2)-*β*-glucopyranoside] (**13**)	
	luteolin 6-*C*-[5-ribofuranosyl-*O*-*E*-feruoyl-*β*-D-ribofuranosyl(1''→2)-*β*-glucopyranoside] (**14**)	
	3',4',5'- *O*-trimethyltricetin 7-*O*-[*β*-D-glucuropyranosyl(1''→2)-*β*-D-glucopyranoside) (**15**)	
Hull (Bran)	**Oxyphytosterol**	[8, 11-13]
	stigmast-4-en-6*β*-ol-7-one (**16**)	
	stigmast-4,22-dien-6*β*-ol-3-one (**17**)	
	7-keto-*β*-sitosterol (**18**), 7-keto-stigmasterol (**19**)	
	7*β*-hydroxysitosterol (**20**),	
	7*β*-hydroxystigmasterol (**21**)	
	7-ketocholesterol (**22**),	
	7*β*-hydroxycholesterol (**23**),	
	7-ketocampesterol (**24**),	
	7*β*-hydroxycampesterol (**25**),	
	ergost-4-en-3,6-dione (**26**),	
	esgostane-3*β*,7*β*-diol (**27**),	

	7-ketocholesterol ferulate (**28**), 7-ketocampesterol (**29**), campesterol ferulate (**30**), stigmasterol ferulate (**31**), sitosterol ferulate (**32**), 3-*O*-glucopyranosyl-7-ketocampesterol (**33**), 3-*O*-glucopyranosyl-7-ketostigmasterol (**34**), 3-*O*-glucopyranosyl-7-ketositosterol (**35**), stigmasterol (**36**)	
	Flavonoid	
	Tricin (**37**)	
	Aliphatic compound	
	5-*n*-heptadecylresorcinol (**38**) 5-*n*-14′-(*Z*)-heneicosylresorcinol (**39**) 5-*n*-nonadecylresorcinol (**40**) 5-*n*-heneicosylresorcinol (**41**) 5-*n*-tricosylresorcinol (**42**) 1-*O*-(9*Z*,12*Z*,15*Z*-octadecatrienoate) glycerol (**43**) 2-linoleoylglycerol (**44**) 1-*O*-(9*Z*,12*Z*-octadecatrienoate) glycerol (**45**) pinellic acid (**46**)	
	Phenolic glycoside	
	Tachioside (**47**)	
Sprout	**Glycolipid**	[14,15]
	2-*α*-linolenoylglycerol 1-*O*-*β*-D-galactopyranoside (**48**), 3-*α*-linolenoylglycerol 1-*O*-*β*-D-galactopyranoside (**49**), 2,3-di-*α*-linolenoylglycerol 1-*O*-*β*-D-galactopyranoside (**50**), 2,3-di-*α*-linolenoylglycerol 1-*O*-(6-*O*-linolenoyl-*β*-D-galactopyranoside) (**51**), 2,3-di-*α*-linolenoylglycerol 1-*O*-[*α*-D-galactopyranoside-(1→6) *β*-D-galactopyranoside] (**52**)	
	Glyceride	
	trilinolenin (**53**),	

trilinolein (**54**)
Unsaturated fatty acid
α-linolenic (**55**),
α-linolenic acid methyl ester (**56**),
oleic acid (**57**),
12(*Z*)-actadecenoic acid (**58**)
Sterol
β-sitosterol (**59**)
daucosterol (**60**)
6′-*O*-linolenyl-daucosterol (**61**)
Alkaloid
(2*R*)-2-*O*-β-D-glucopyranosyl-4,7-dimethoxy-2*H*-1,4-benzoxazin-3(4*H*)-one (**62**)
adenosine (**63**)
Flavonoid
isoorientin (**9**)
triticumoside (**64**)
isoscoparin (**65**)
luteolin (**66**)
Tocopherol
α-tocopherol (**67**)

Phenolic acid



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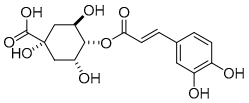

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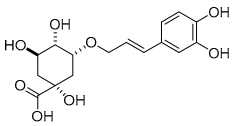

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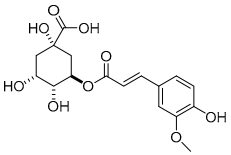

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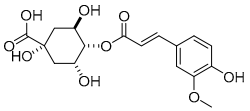

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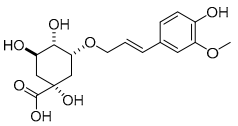

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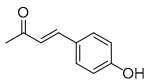

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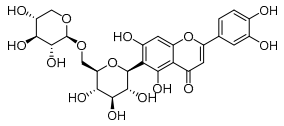
Flavonoid



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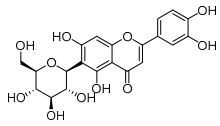

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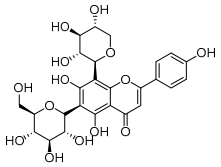

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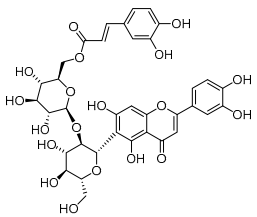

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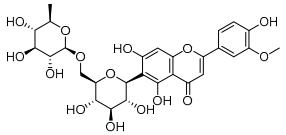

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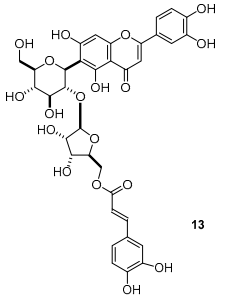

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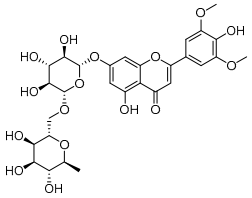

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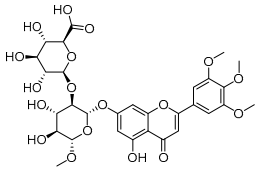

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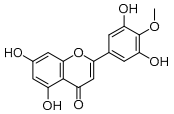

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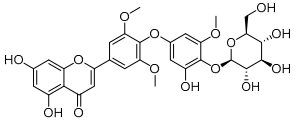

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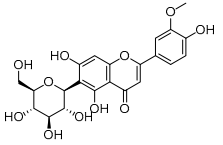

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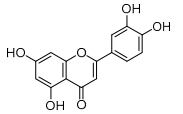

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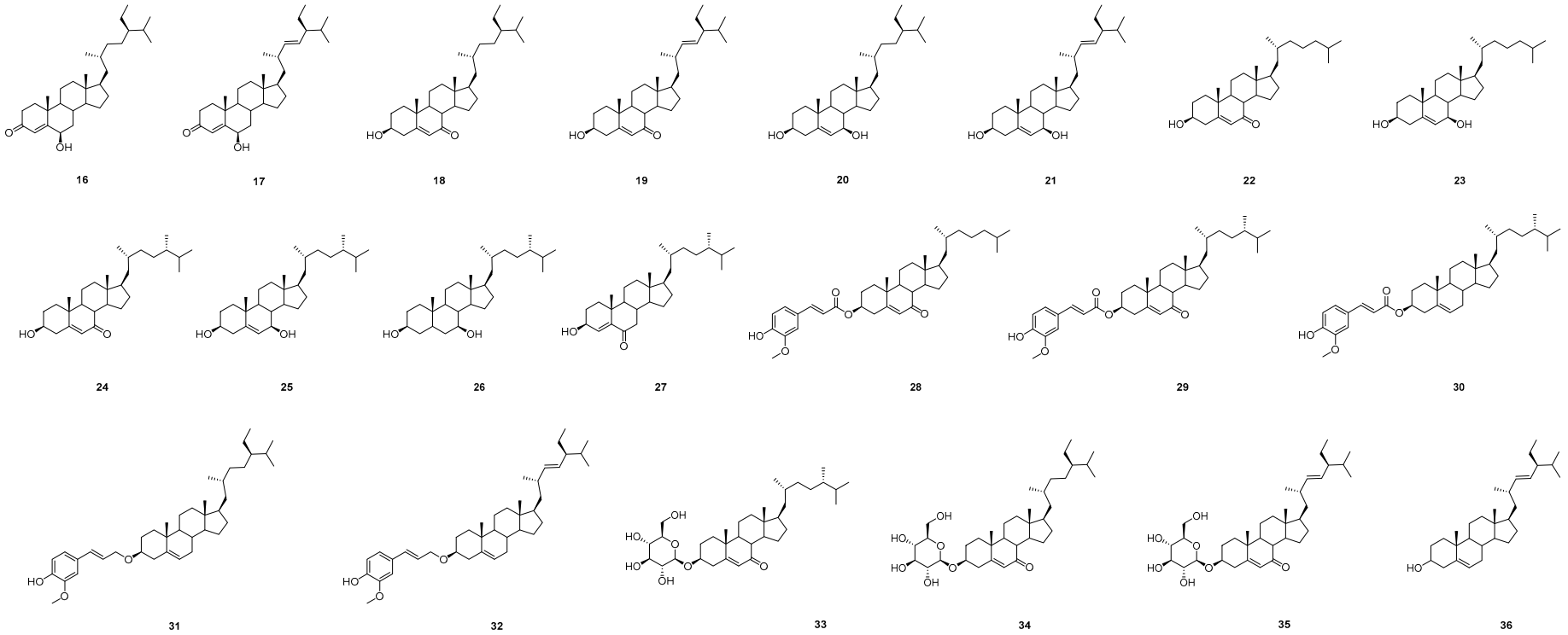
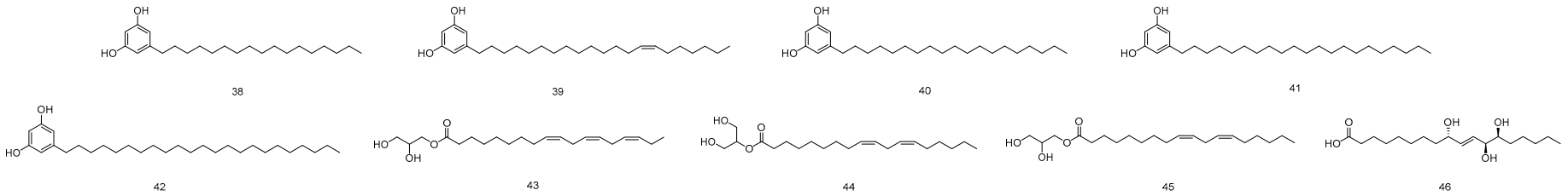
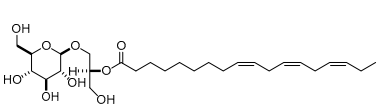
Oxyphytosterol



Aliphatic compound



Glycolipid



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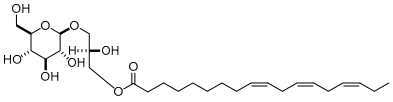

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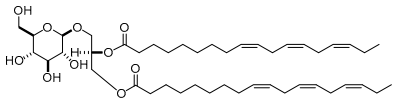

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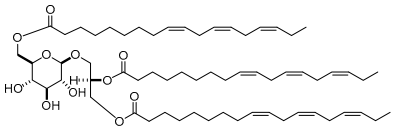

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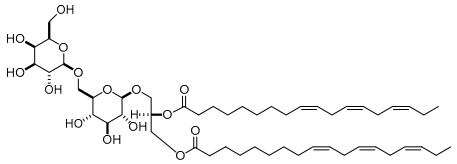

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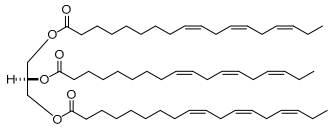
Glyceride



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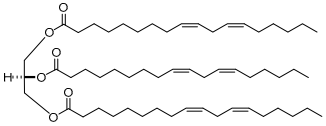

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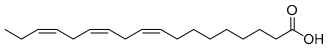
Unsaturated fatty acid



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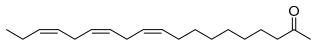

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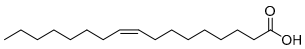

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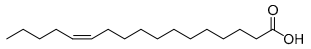

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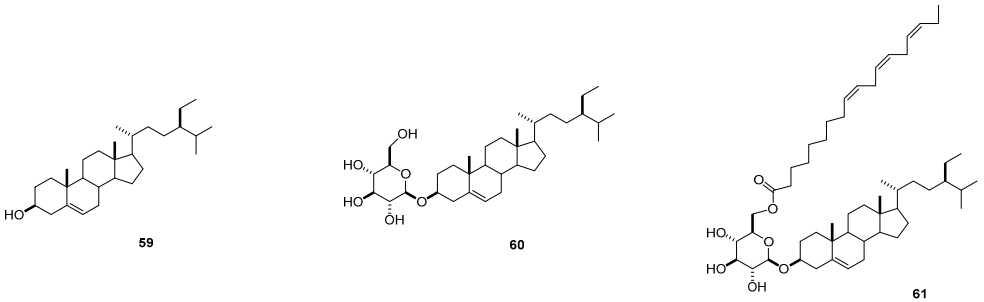
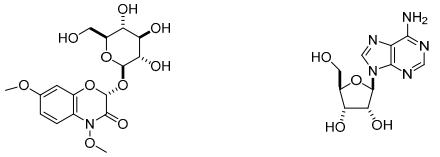
Sterol



59 60 61

Alkaloid



62 63

Tocopherol

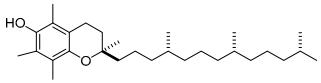


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Figure S1. The chemical structures of reported constituents of the aerial, hull, bran, and sprout part of *T. aestivum*.

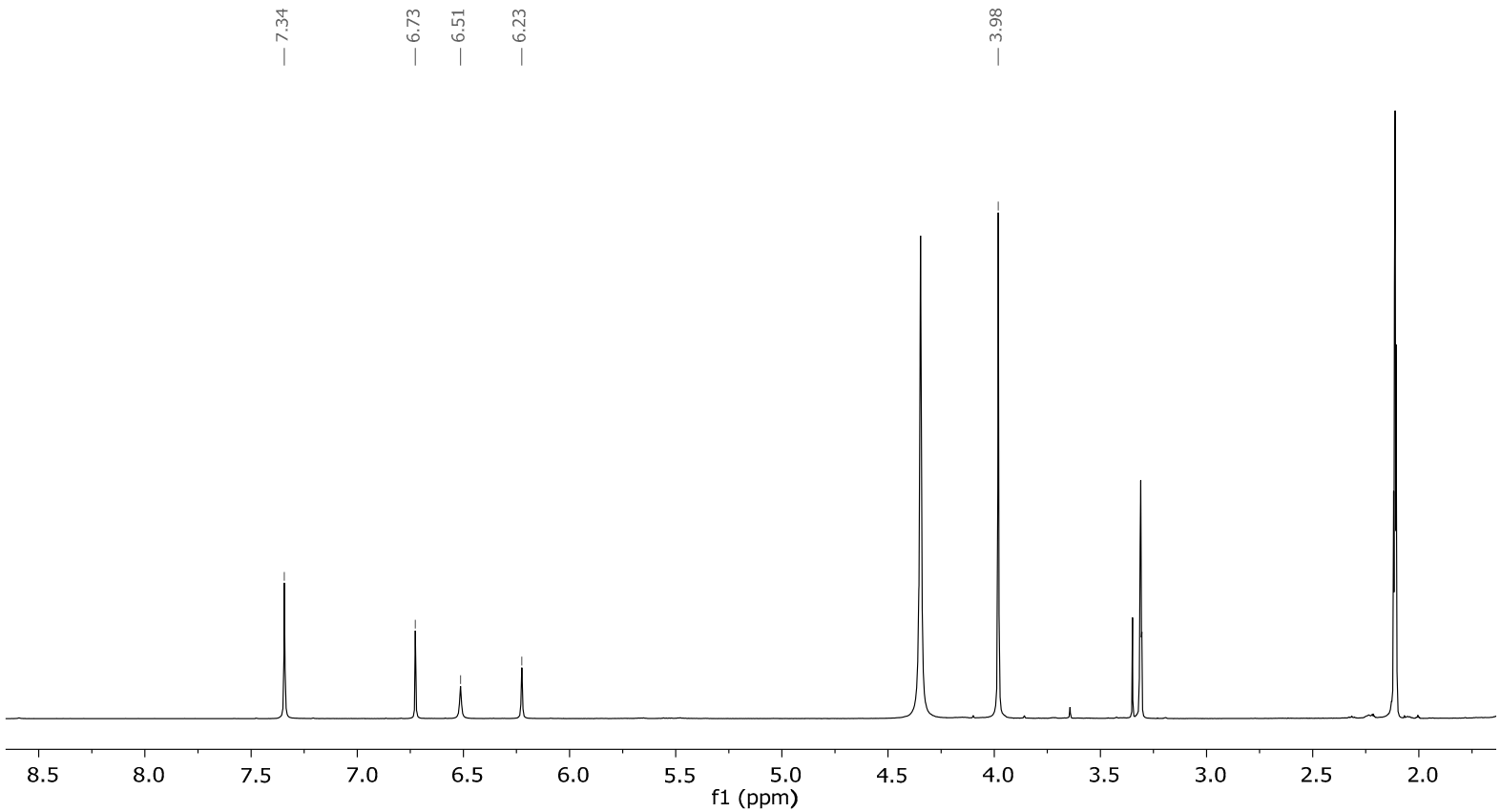

Figure S2. ^{1}H NMR (600 MHz) spectrum of compound **1** in methanol-d_4/acetone-d_6 (1:1).

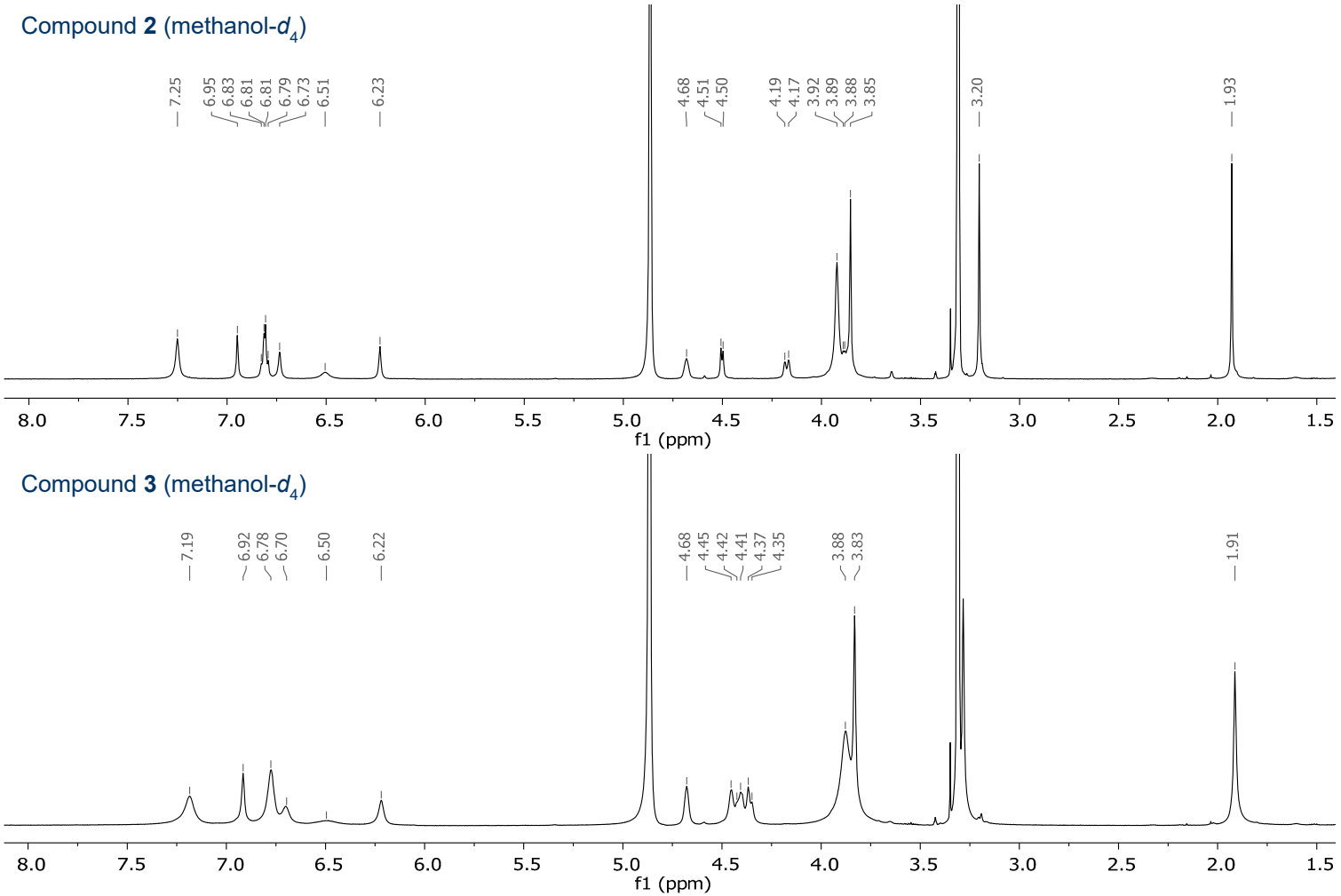

Figure S3. ^{1}H NMR (600 MHz) spectra of compounds **2** (top) and **3** (bottom) in methanol-d_4.

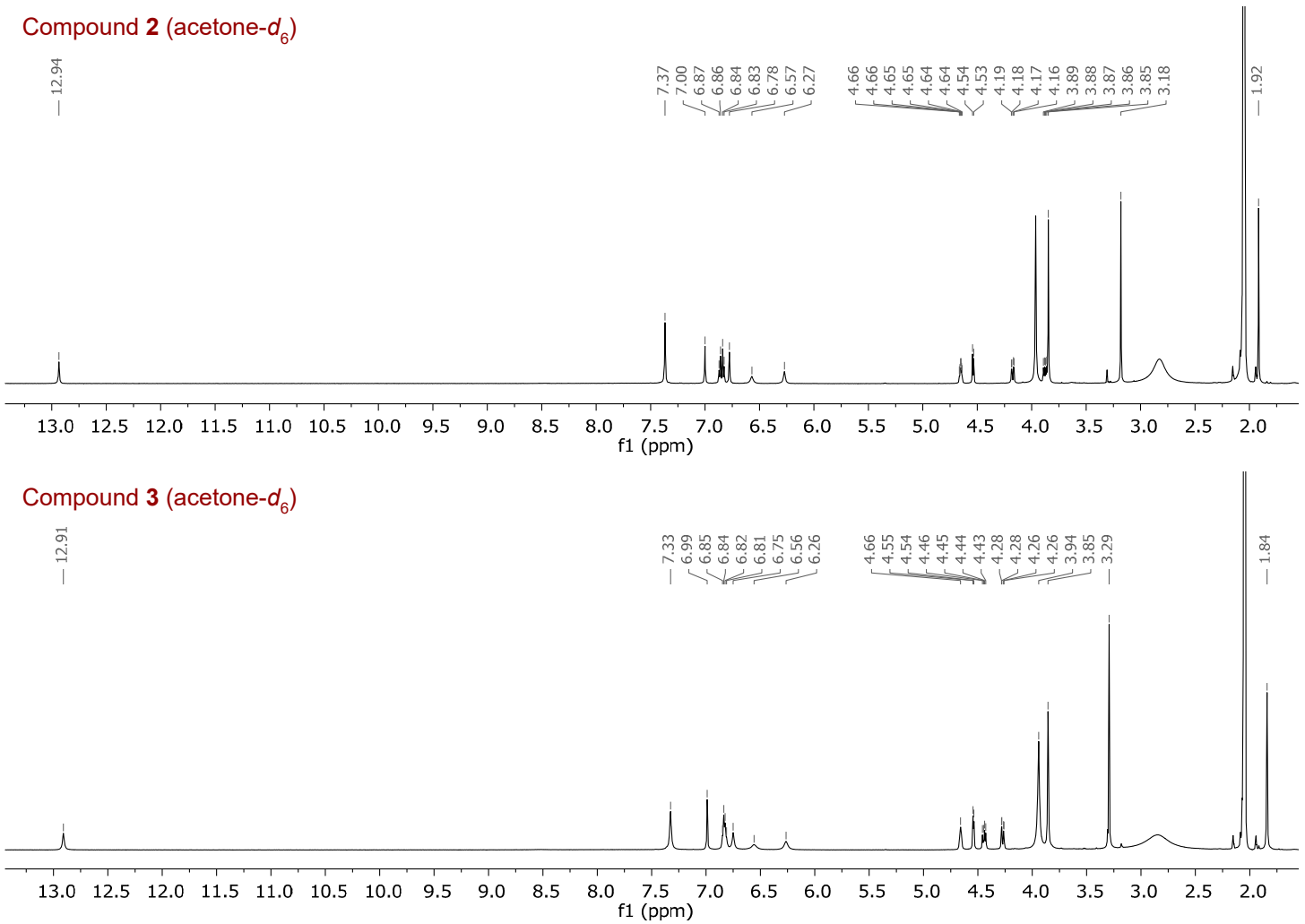

Figure S4. ^{1}H NMR (600 MHz) spectra of compounds **2** (top) and **3** (bottom) in acetone-d_6.

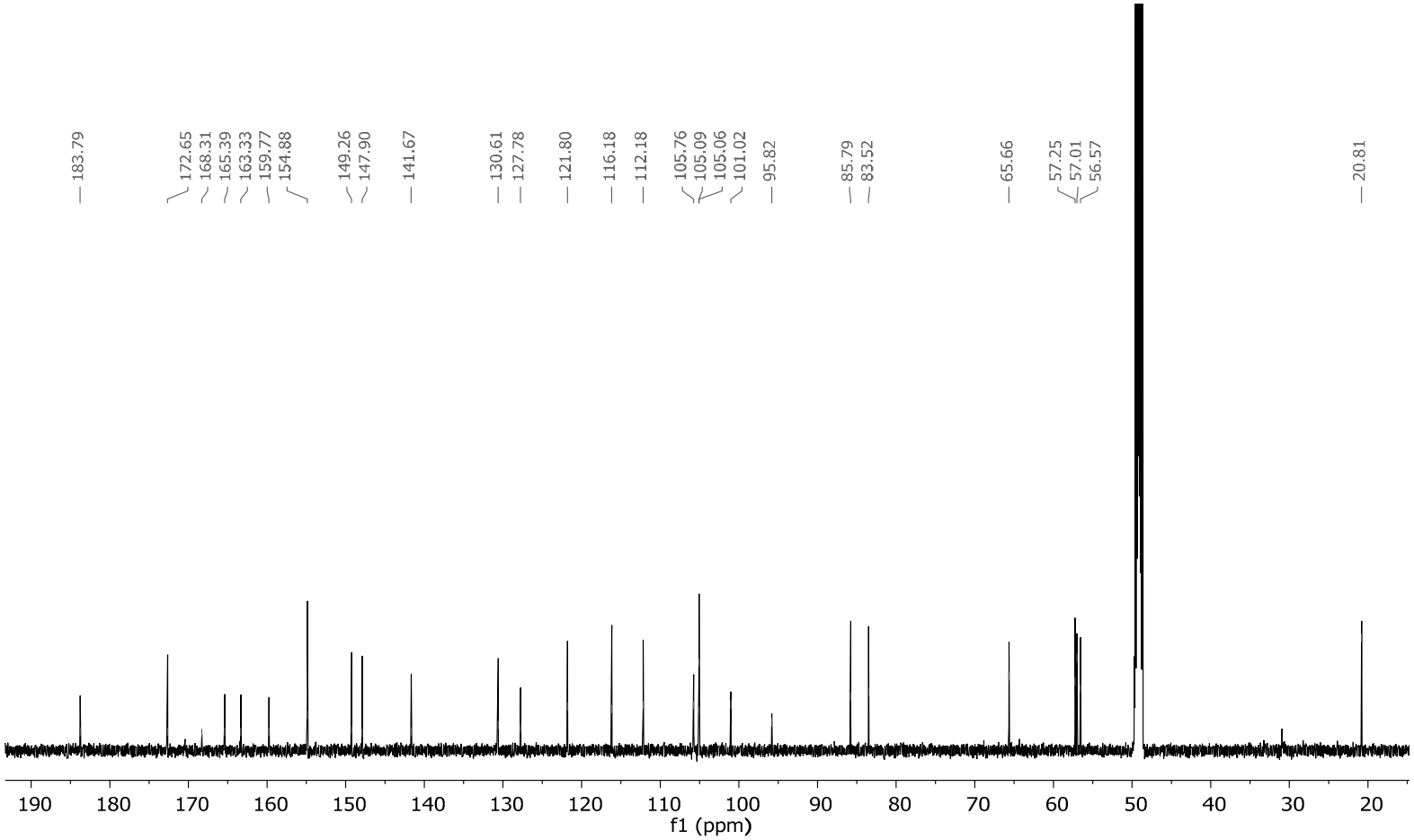

Figure S5. ^{13}C NMR (150 MHz) spectrum of compound **2** in methanol-d_4.

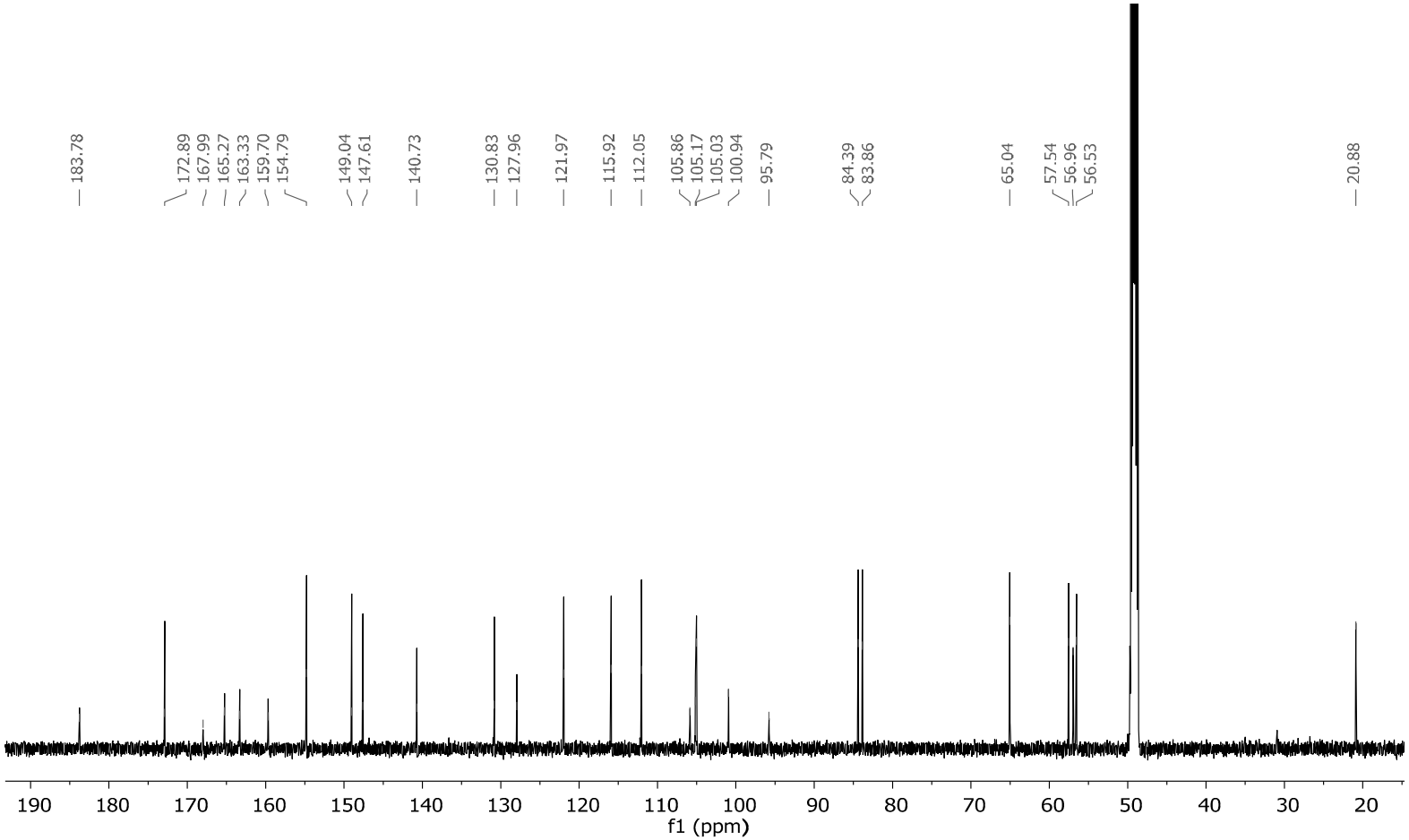

Figure S6. ^{13}C NMR (150 MHz) spectrum of compound **3** in methanol-d_4.

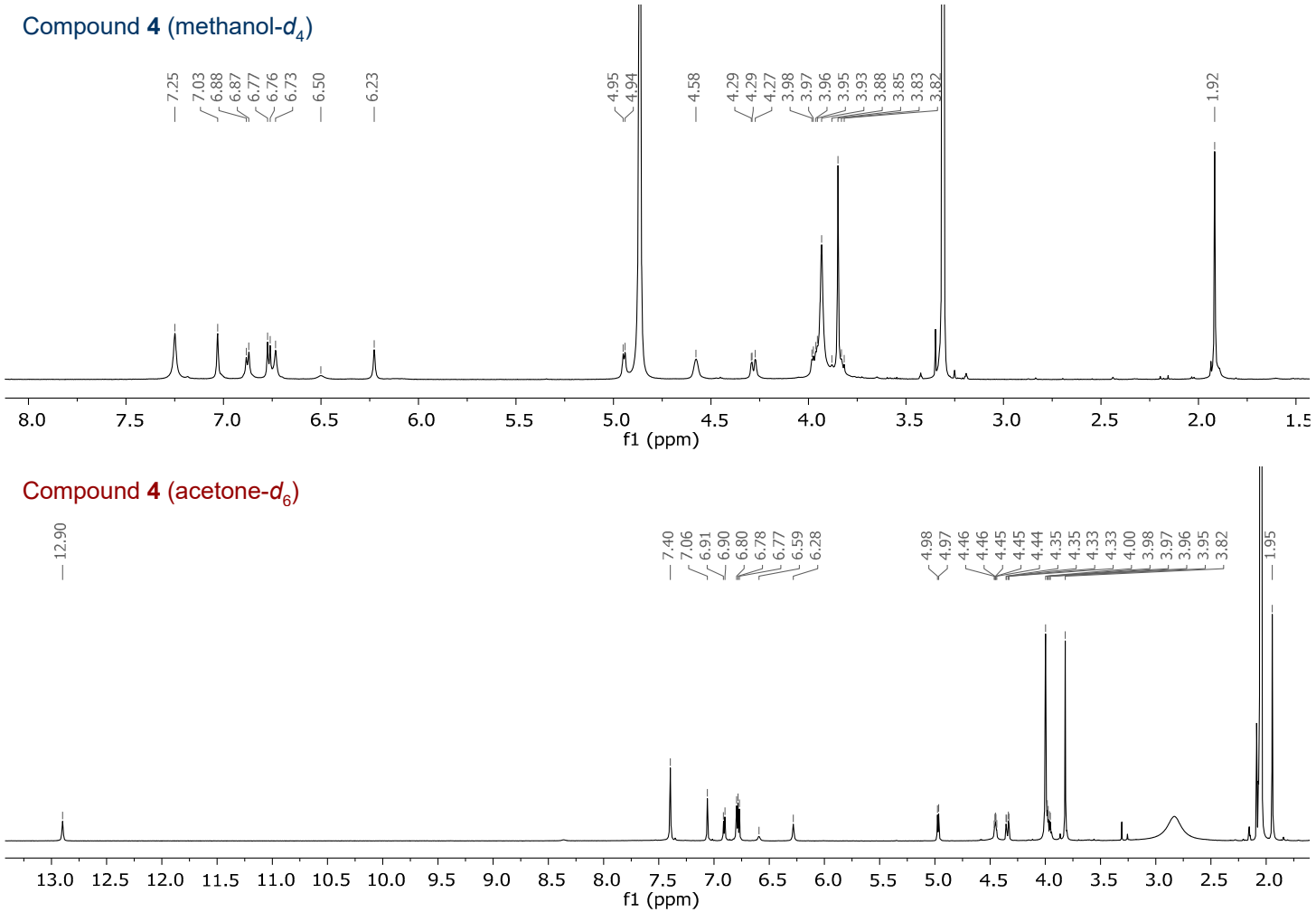

Figure S7. ^{1}H NMR (600 MHz) spectra of compound **4** in methanol-d_4 (top) and acetone-d_6 (bottom).

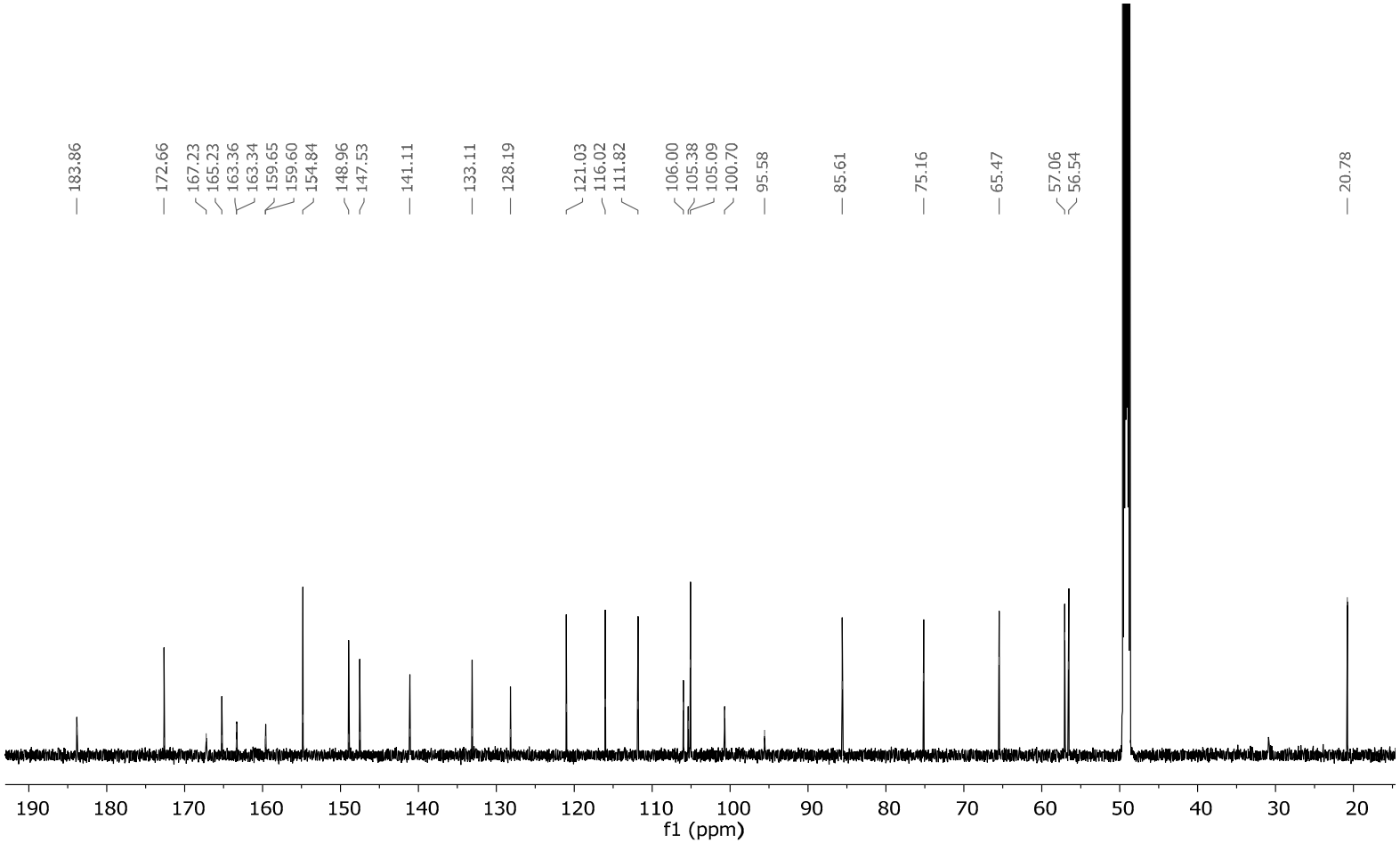

Figure S8. ^{13}C NMR (150 MHz) spectrum of compound **4** in methanol-d_4.

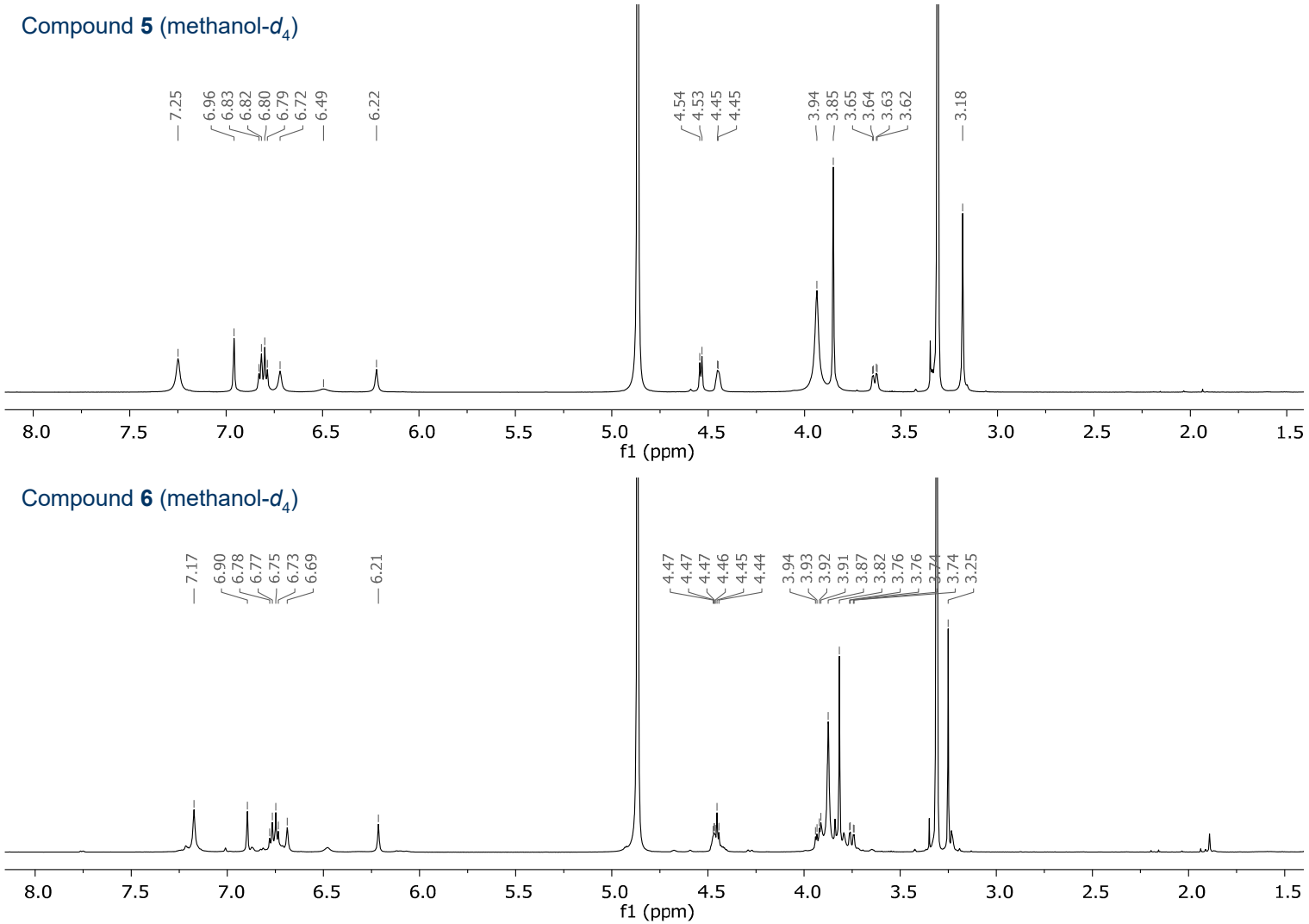

Figure S9. 1H NMR (600 MHz) spectra of compounds 5 (top) and 6 (bottom) in methanol-d4.

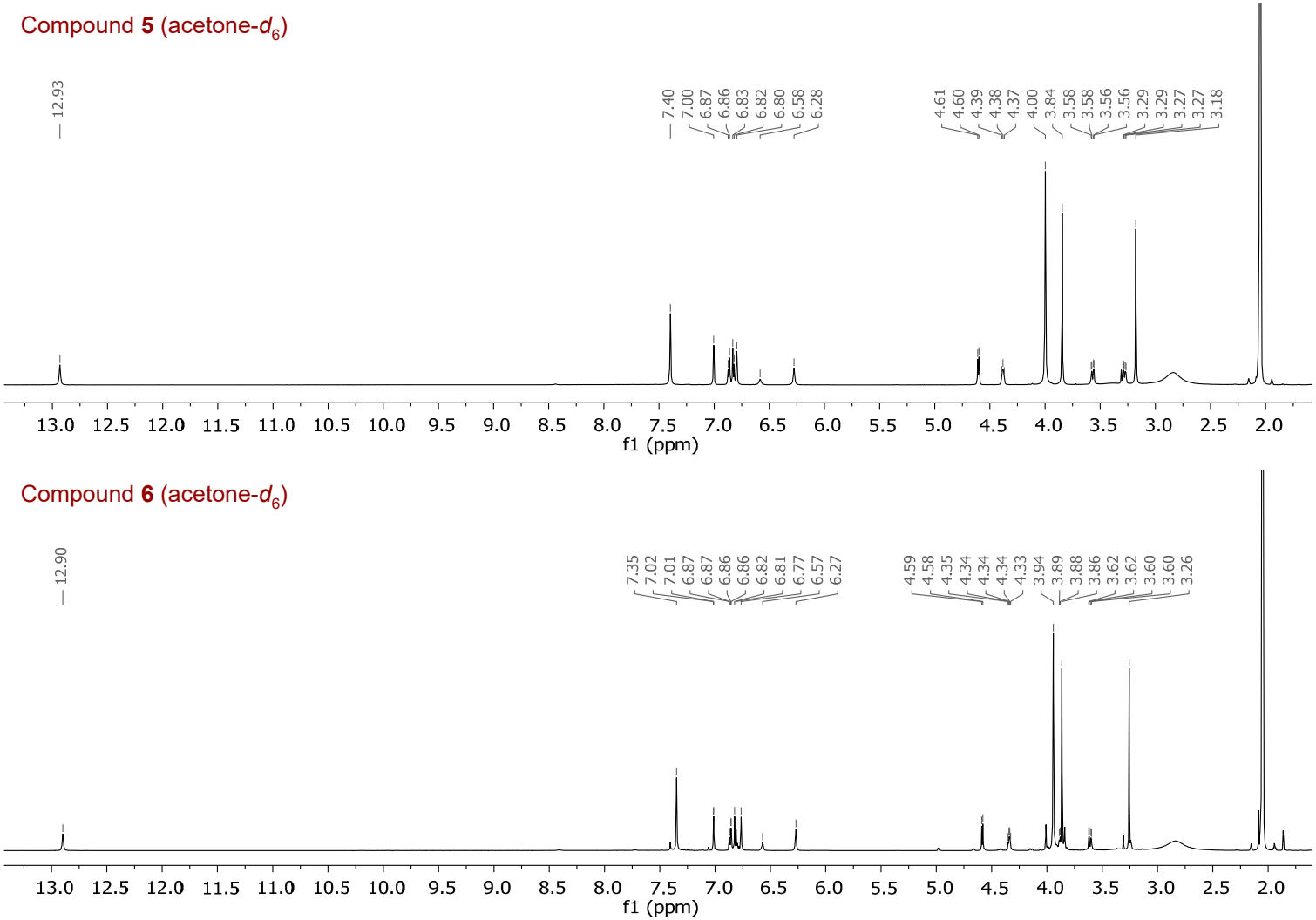

Figure S10. ^{1}H NMR (600 MHz) spectra of compounds **5** (top) and **6** (bottom) in acetone-d_6.

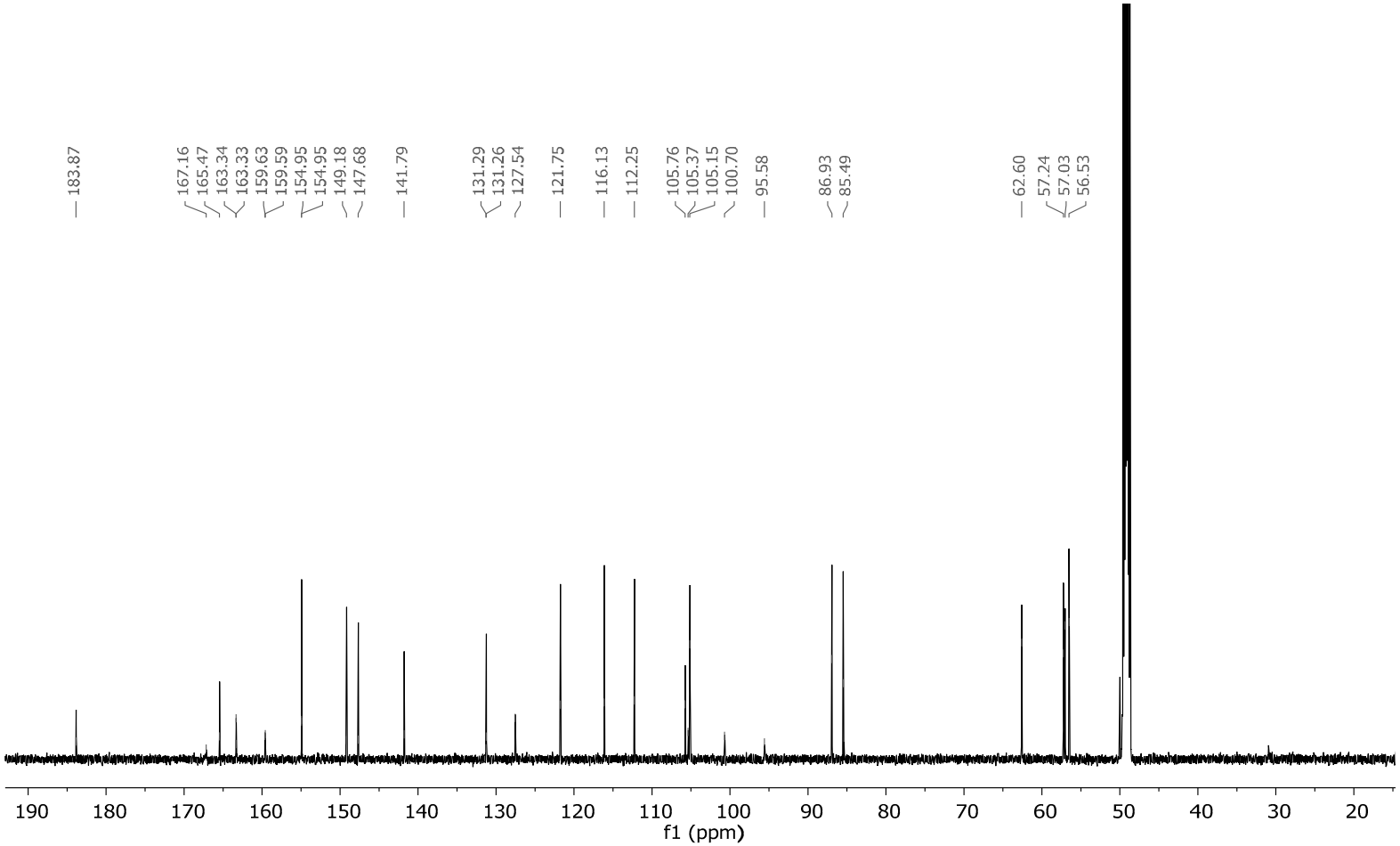

Figure S11. ^{13}C NMR (150 MHz) spectrum of compound **5** in methanol-d_4.

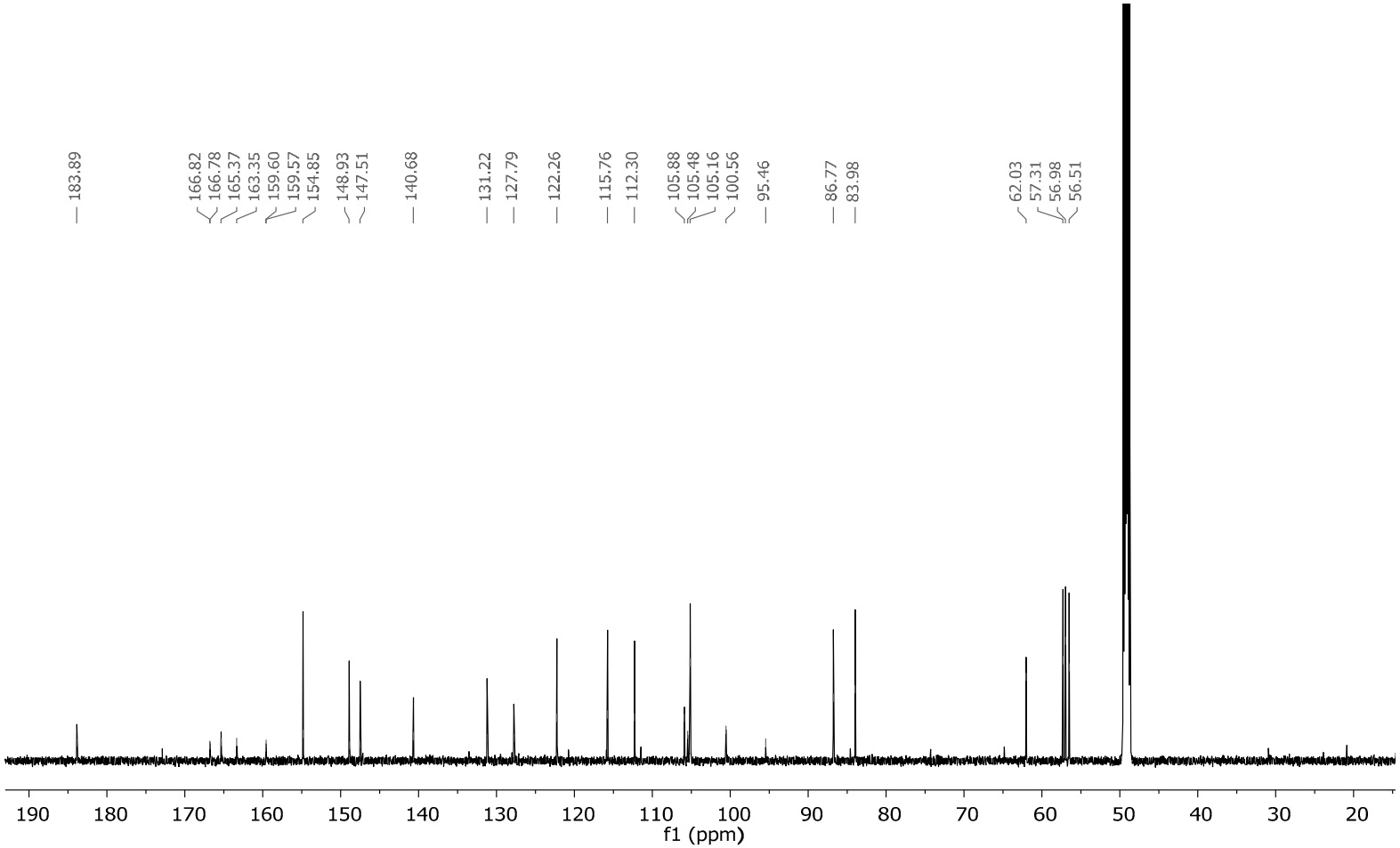

Figure S12. ^{13}C NMR (150 MHz) spectrum of compound **6** in methanol-d_4.

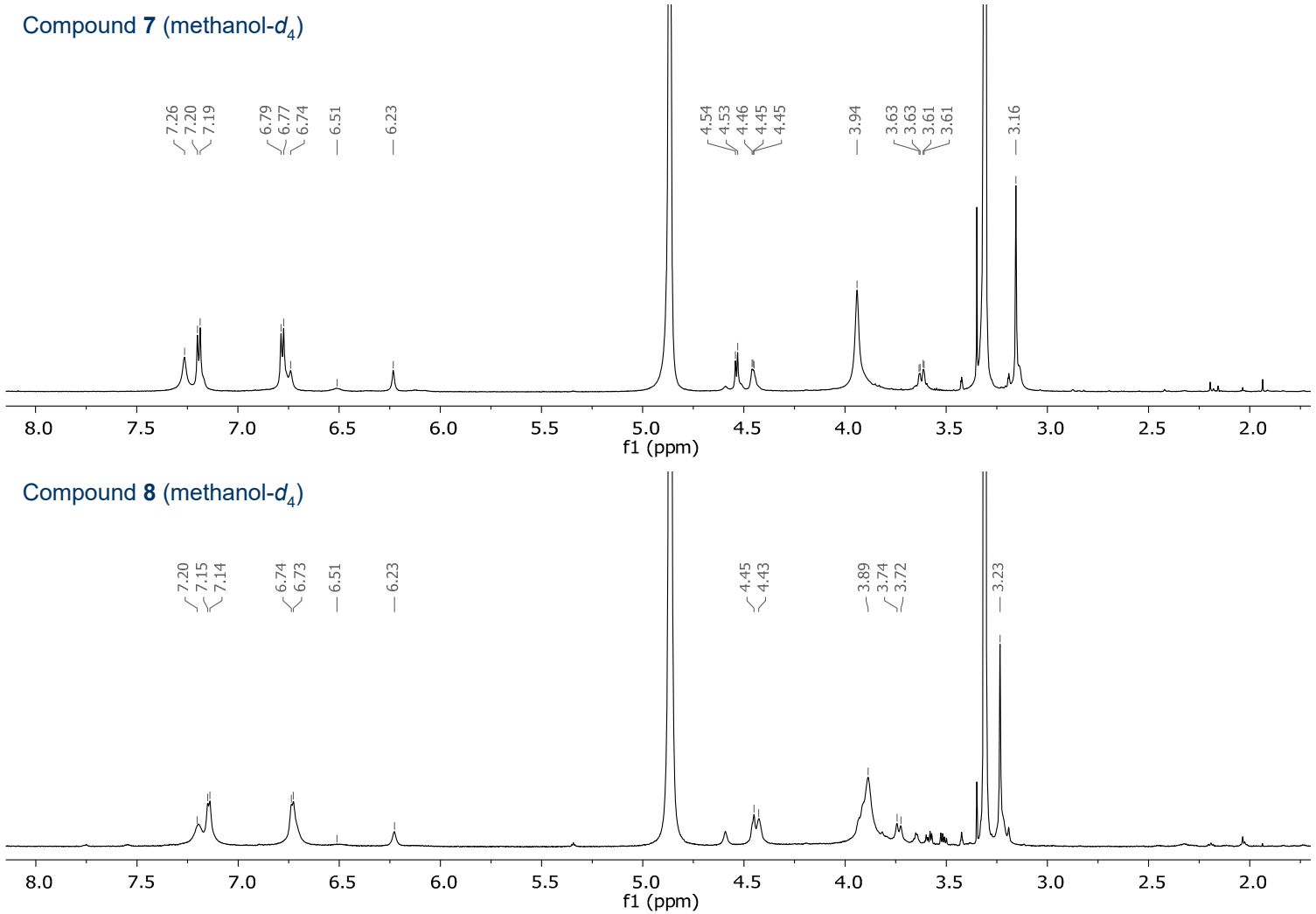

Figure S13. ^{1}H NMR (600 MHz) spectra of compounds **7** (top) and **8** (bottom) in methanol-d_4.

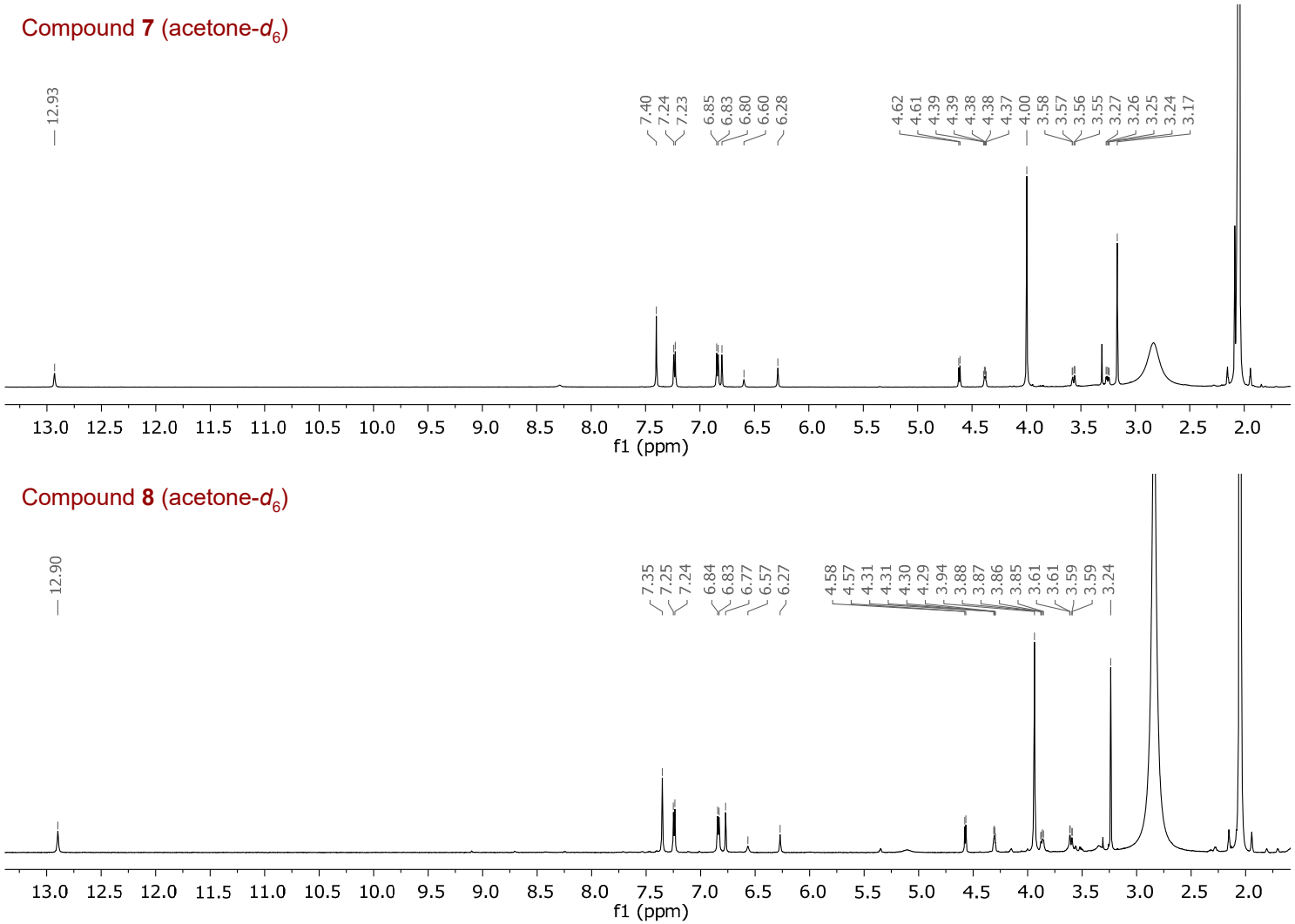

Figure S14. ^{1}H NMR (600 MHz) spectra of compounds **7** (top) and **8** (bottom) in acetone-d_6.

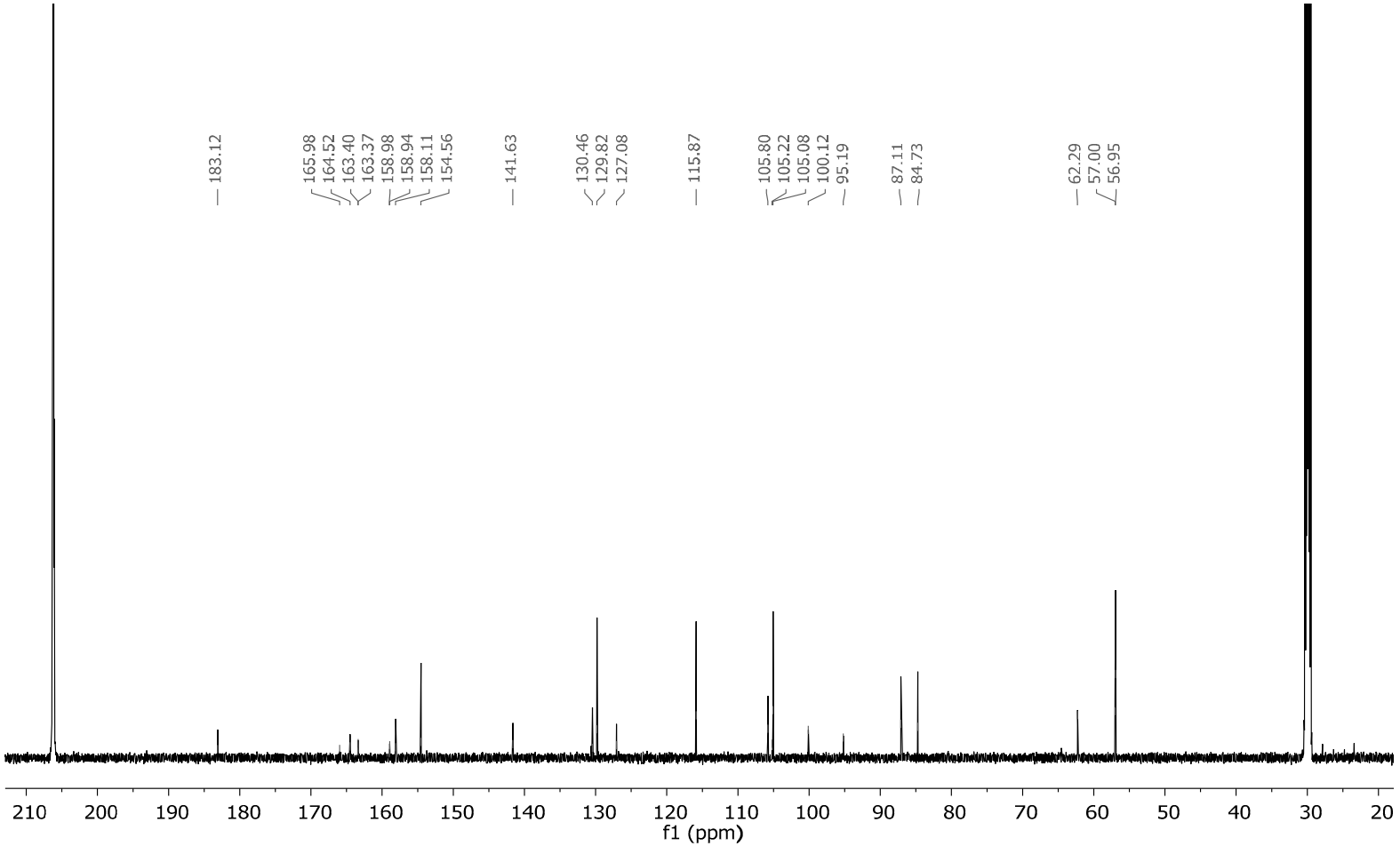

Figure S15. ^{13}C NMR (150 MHz) spectrum of compound **7** in acetone-d_6.

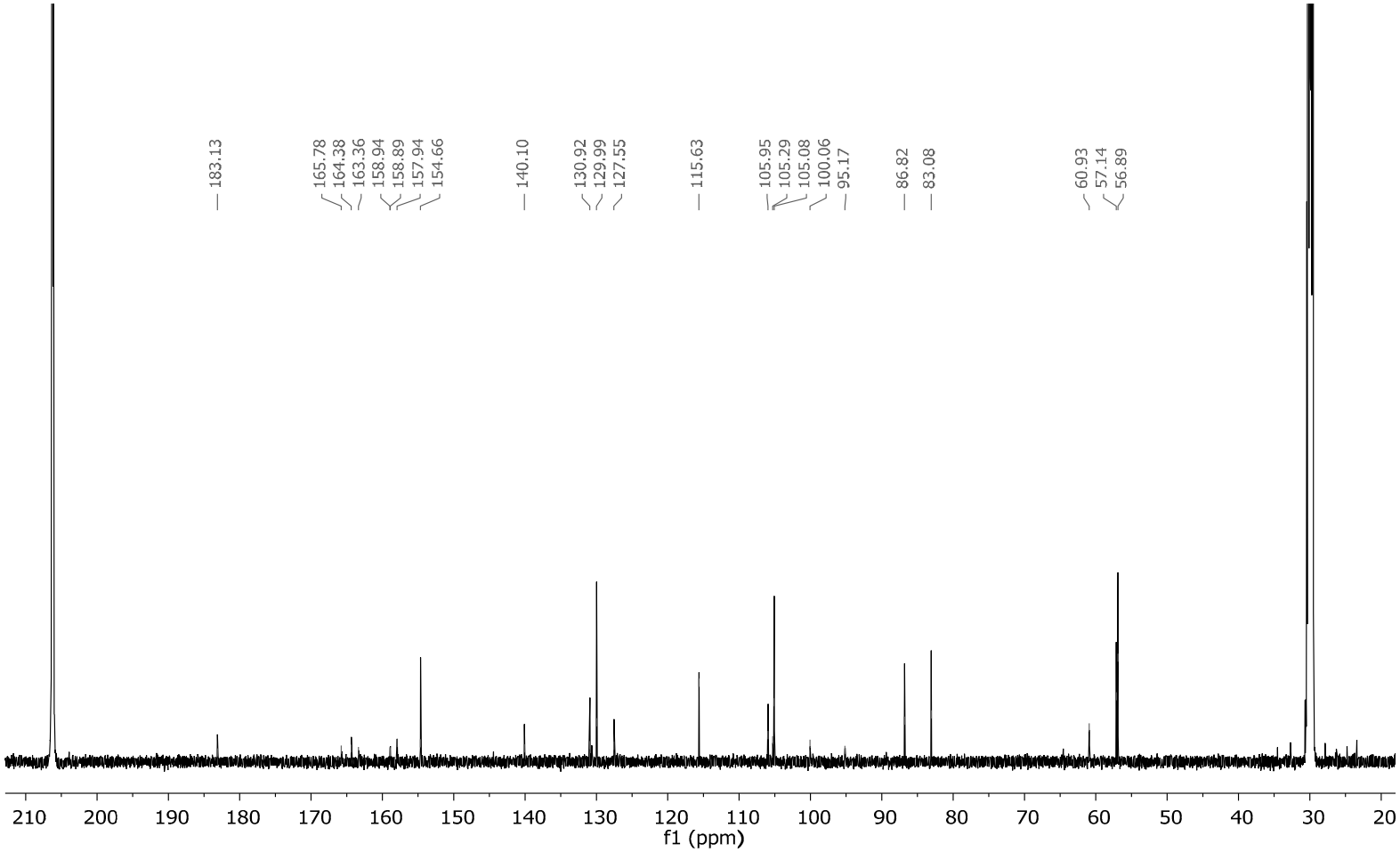

Figure S16. ^{13}C NMR (150 MHz) spectrum of compound **8** in acetone-d_6.