

Supporting Information for

New Sesquiterpene Glycosides from the Flowers of *Aster koraiensis* and their inhibition activities on EGF- and TPA-induced cell transformation

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Figure S1. HRESIMS spectrum of the new compound **1**.

Figure S2. ^1H NMR spectrum (600 MHz, methanol- d_4) of the new compound **1**.

Figure S3. ^{13}C NMR spectrum (150 MHz, methanol- d_4) of the new compound **1**.

Figure S4. HSQC spectrum (600 MHz, methanol- d_4) of the new compound **1**.

Figure S5. HMBC spectrum (600 MHz, methanol- d_4) of the new compound **1**.

Figure S6. COSY spectrum (600 MHz, methanol- d_4) of the new compound **1**.

Figure S7. NOESY spectrum (600 MHz, methanol- d_4) of the new compound **1**.

Figure S8. HRESIMS spectrum of the new compound **2**.

Figure S9. ^1H NMR spectrum (600 MHz, methanol- d_4) of the new compound **2**.

Figure S10. ^{13}C NMR spectrum (150 MHz, methanol- d_4) of the new compound **2**.

Figure S11. HSQC spectrum (600 MHz, methanol- d_4) of the new compound **2**.

Figure S12. HMBC spectrum (600 MHz, methanol- d_4) of the new compound **2**.

Figure S13. COSY spectrum (600 MHz, methanol- d_4) of the new compound **2**.

Figure S14. NOESY spectrum (600 MHz, methanol- d_4) of the new compound **2**.

Figure S15. ^1H NMR spectrum (700 MHz, DMSO- d_6) of the new compound **2**.

Figure S16. ^{13}C NMR spectrum (175 MHz, DMSO- d_6) of the new compound **2**.

Figure S17. HSQC spectrum (700 MHz, DMSO- d_6) of the new compound **2**.

Figure S18. HMBC spectrum (700 MHz, DMSO- d_6) of the new compound **2**.

Figure S19. COSY spectrum (700 MHz, DMSO- d_6) of the new compound **2**.

Figure S20. HRESIMS spectrum of the new compound **3**.

Figure S21. ^1H NMR spectrum (600 MHz, methanol- d_4) of the new compound **3**.

Figure S22. ^{13}C NMR spectrum (150 MHz, methanol- d_4) of the new compound **3**.

Figure S23. HSQC spectrum (600 MHz, methanol- d_4) of the new compound **3**.

Figure S24. HMBC spectrum (600 MHz, methanol- d_4) of the new compound **3**.

Figure S25. COSY spectrum (600 MHz, methanol- d_4) of the new compound **3**.

Figure S26. NOESY spectrum (600 MHz, methanol-*d*₄) of the new compound **3**.

Figure S27. HRESIMS spectrum of the new compound **4**.

Figure S28. ¹H NMR spectrum (600 MHz, methanol-*d*₄) of the new compound **4**.

Figure S29. ¹³C NMR spectrum (150 MHz, methanol-*d*₄) of the new compound **4**.

Figure S30. HSQC spectrum (600 MHz, methanol-*d*₄) of the new compound **4**.

Figure S31. HMBC spectrum (600 MHz, methanol-*d*₄) of the new compound **4**.

Figure S32. COSY spectrum (600 MHz, methanol-*d*₄) of the new compound **4**.

Figure S33. NOESY spectrum (600 MHz, methanol-*d*₄) of the new compound **4**.

Figure S1. HRESIMS spectrum of the new compound **1**.

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 20.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions

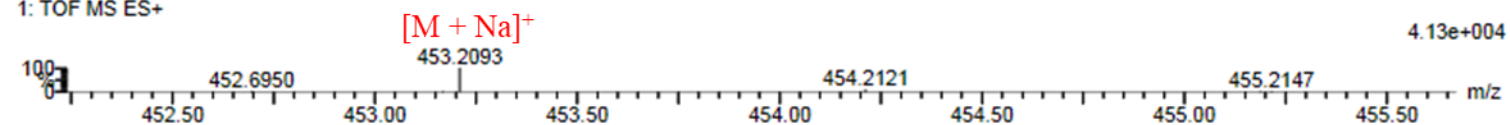
199 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)

Elements Used:

C: 0-100 H: 0-200 O: 0-50 Na: 0-1

20191216_SeoYH_Gyko7F-J18_pos_re 207 (2.326)

1: TOF MS ES+



Minimum: 15.00
Maximum: 100.00

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
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453.2093	100.00	453.2101	-0.8	-1.8	4.5	43.0	n/a	n/a	C21 H34 O9 Na
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Figure S2. ^1H NMR spectrum (600 MHz, methanol- d_4) of the new compound **1**.

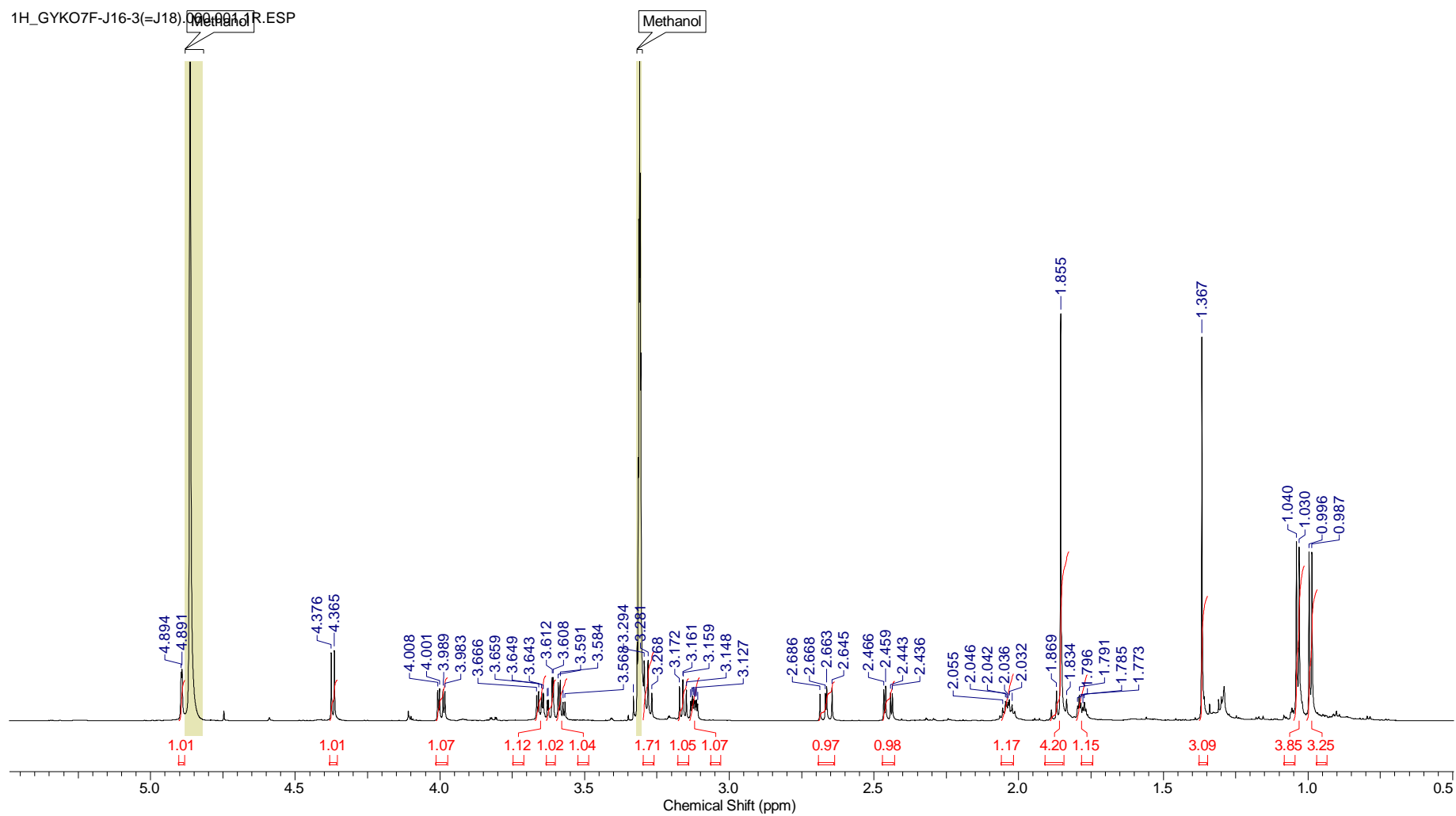


Figure S3. ^{13}C NMR spectrum (150 MHz, methanol- d_4) of the new compound **1**.

13C_GYKO7F-J16-3(=J18).061.001.1R.ESP

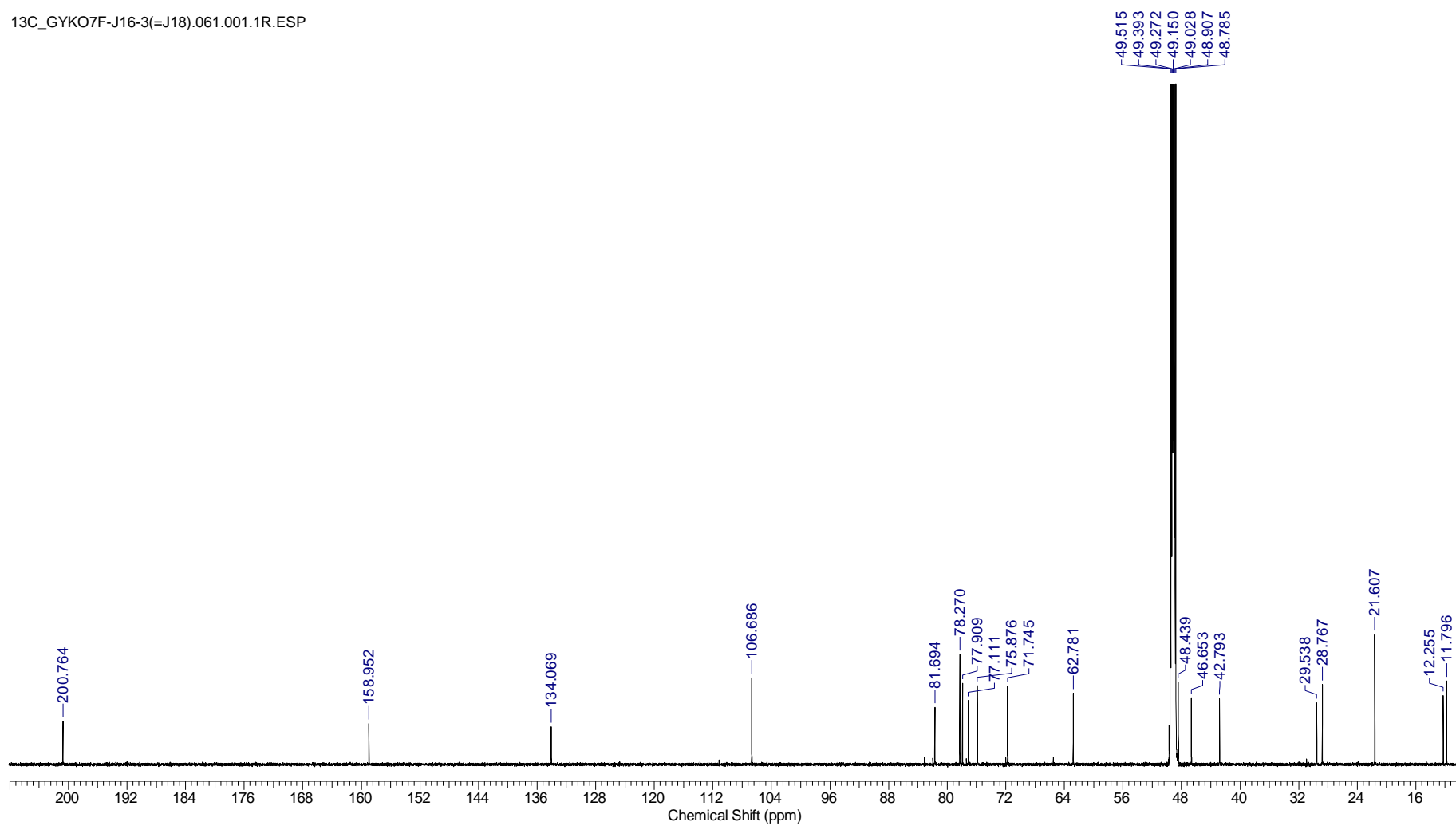


Figure S4. HSQC spectrum (600 MHz, methanol- d_4) of the new compound **1**.

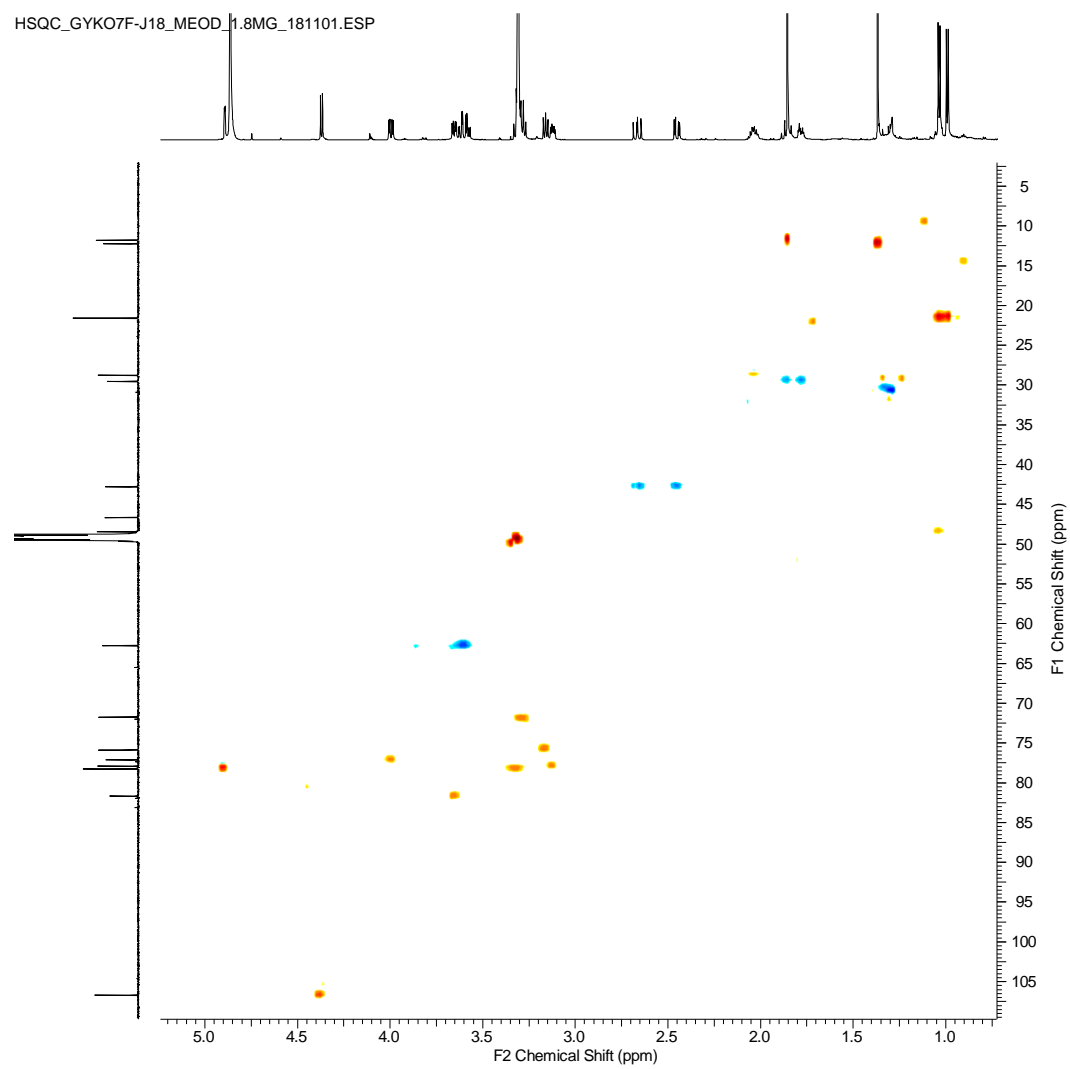


Figure S5. HMBC spectrum (600 MHz, methanol-*d*₄) of the new compound **1**.

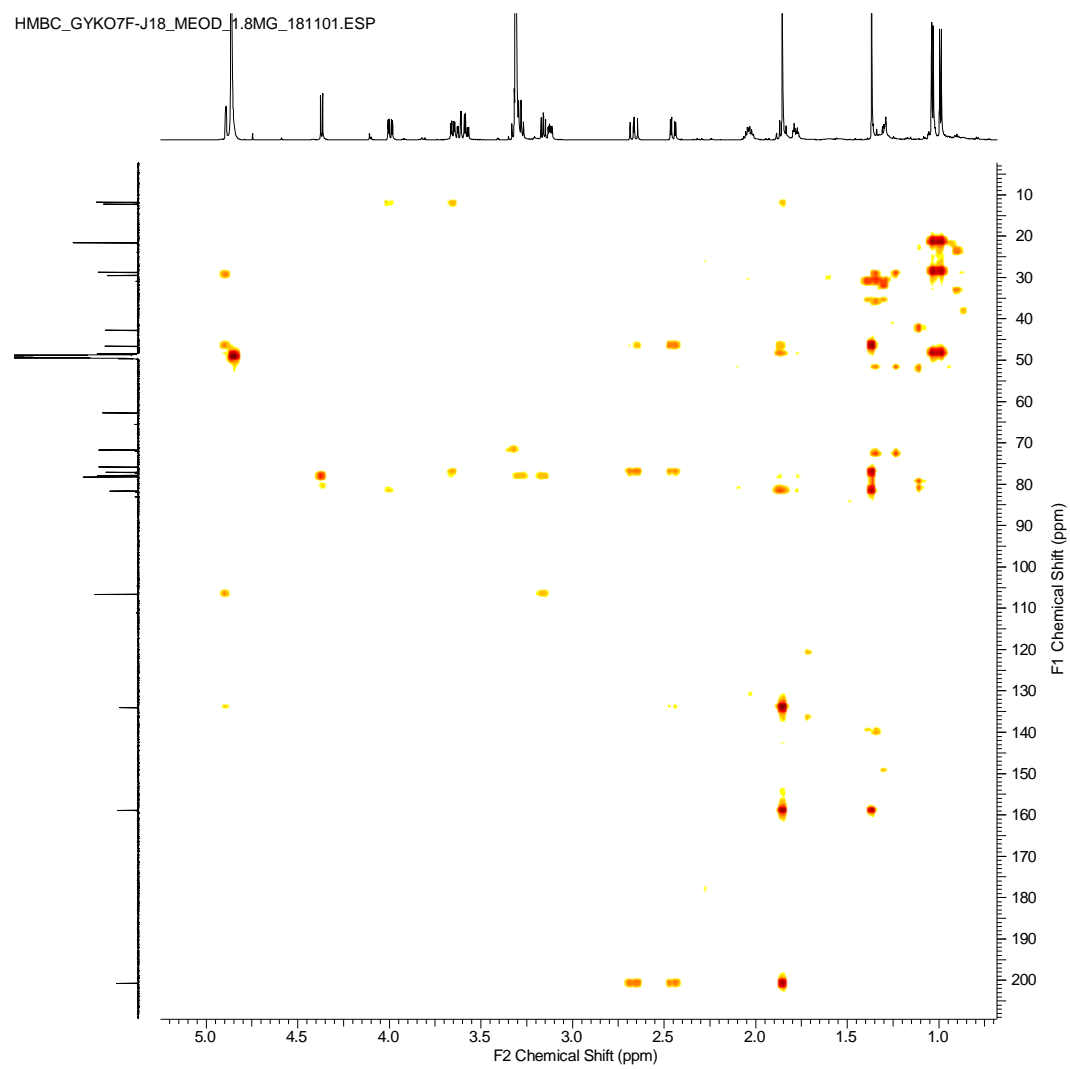


Figure S6. COSY spectrum (600 MHz, methanol-*d*₄) of the new compound **1**.

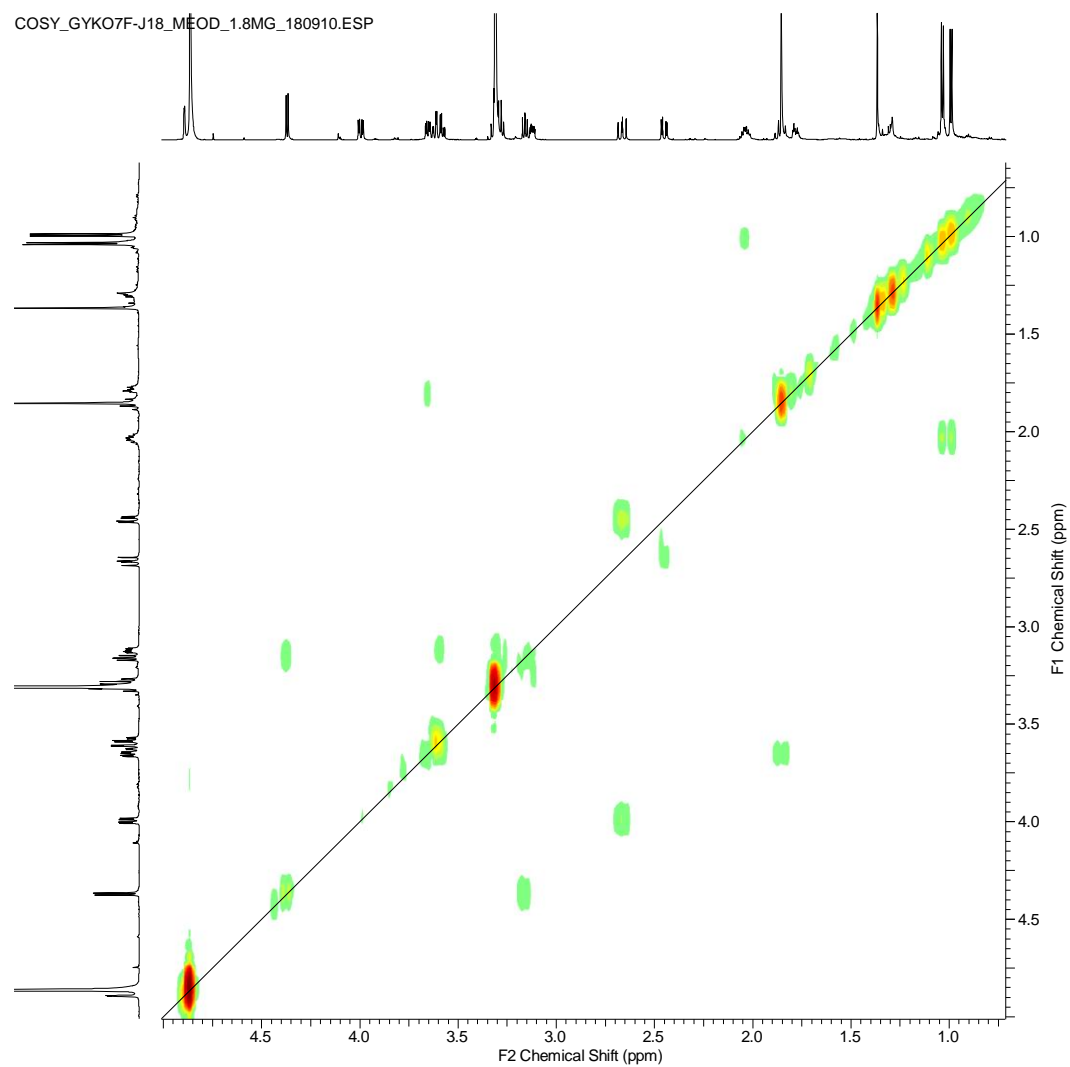


Figure S7. NOESY spectrum (600 MHz, methanol- d_4) of the new compound **1**.

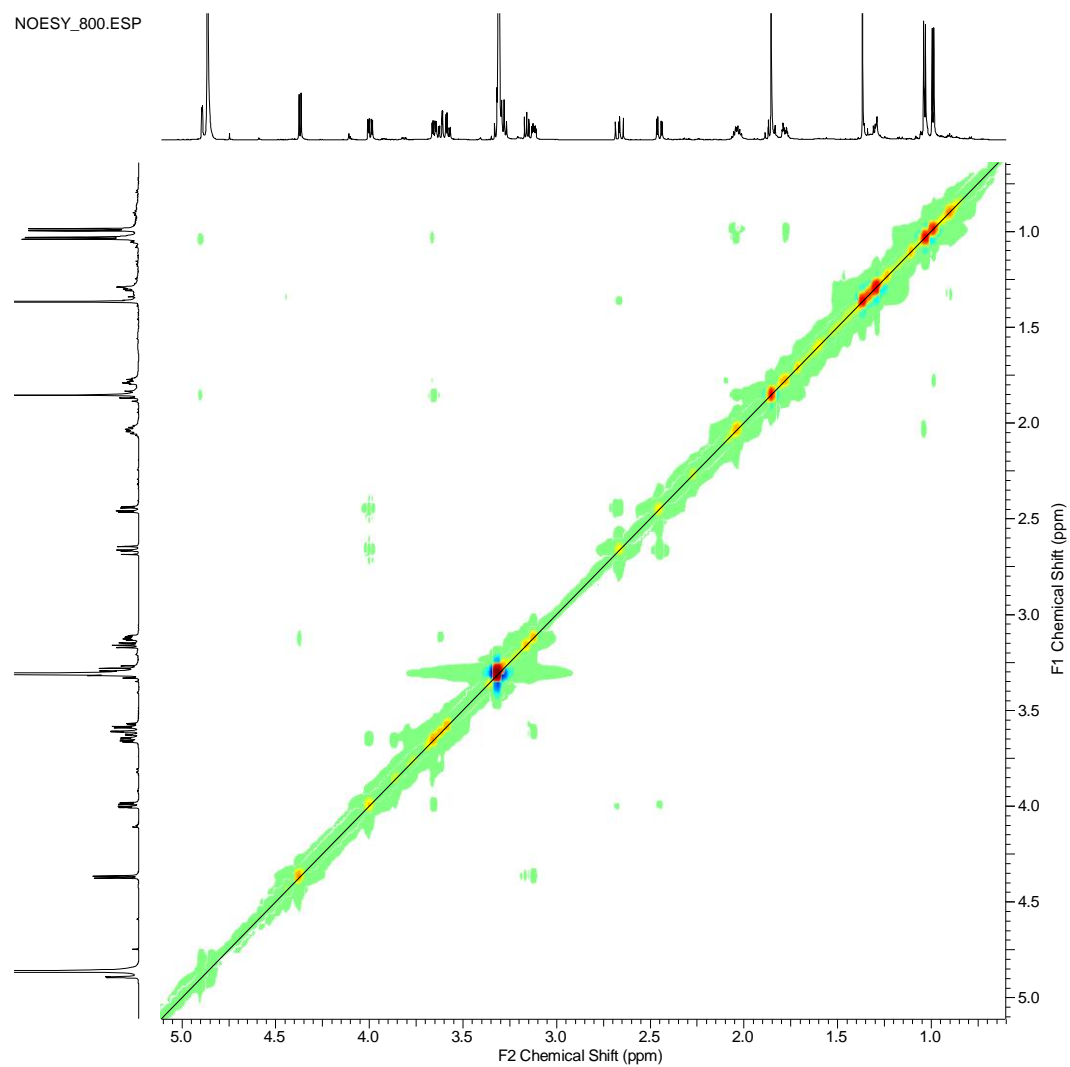


Figure S8. HRESIMS spectrum of the new compound **2**.

Multiple Mass Analysis: 4 mass(es) processed

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

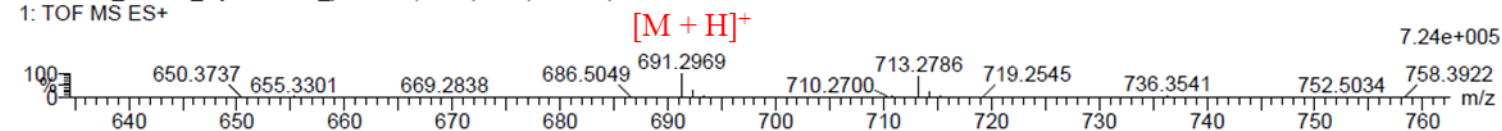
927 formula(e) evaluated with 4 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-500 H: 0-1000 O: 0-200

20191216_SeoYH_Gyko7F-J22_pos 328 (3.685) Cm (327:331)

1: TOF MS ES+



Minimum: 15.00

Maximum: 100.00

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
691.2969	100.00	691.2966	0.3	0.4	12.5	102.6	0.024	97.68	C35 H47 O14
		691.3001	-3.2	-4.6	34.5	106.4	3.761	2.32	C53 H39 O
692.3008	28.64	---							
713.2786	85.06	713.2809	-2.3	-3.2	15.5	121.6	0.282	75.42	C37 H45 O14
		713.2751	3.5	4.9	24.5	122.7	1.403	24.58	C44 H41 O9
714.2817	22.36	---							

Figure S9. ^1H NMR spectrum (600 MHz, methanol- d_4) of the new compound **2**.

1H_GYKO7F-J22_MEOD_181019.ESP

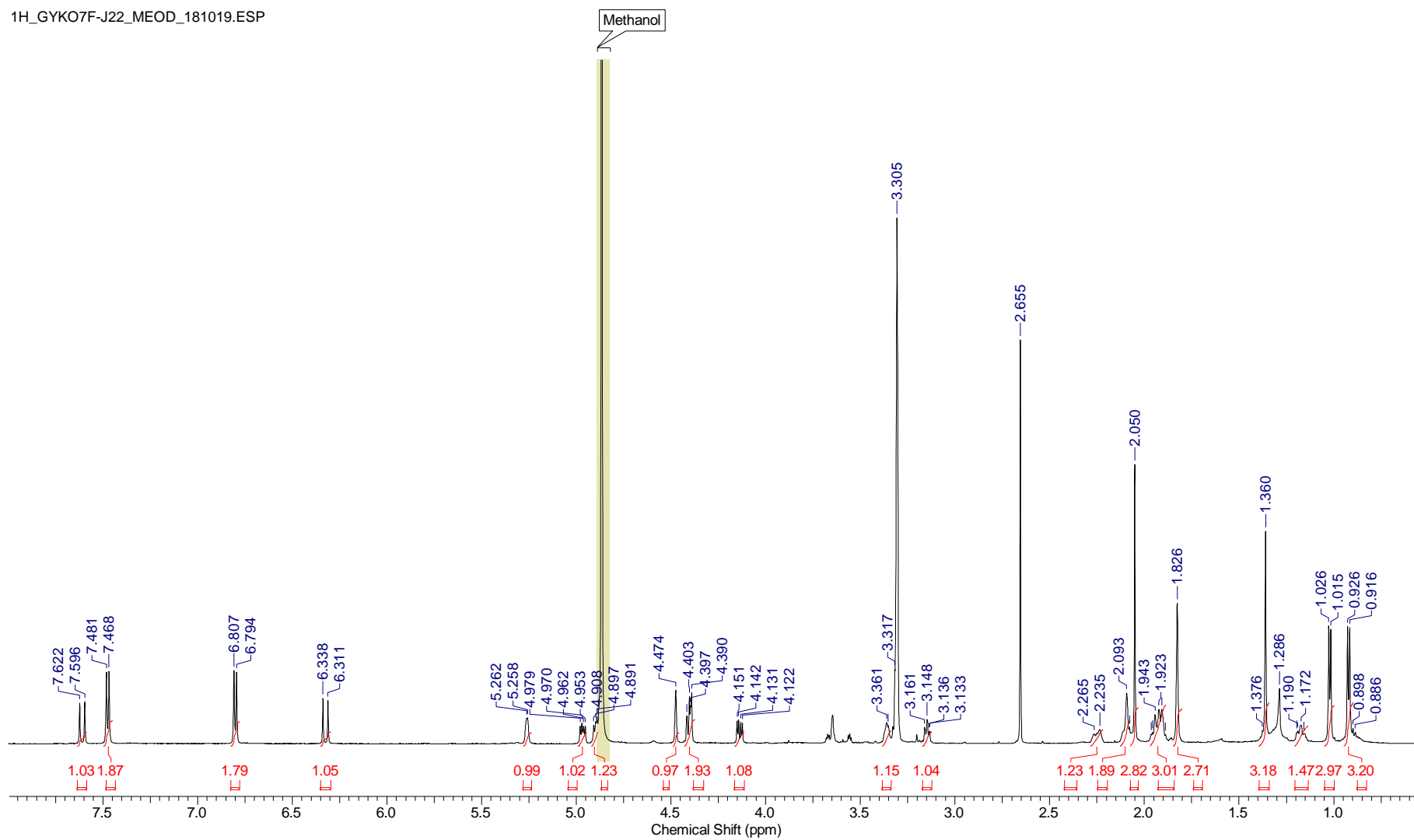


Figure S10. ^{13}C NMR spectrum (150 MHz, methanol- d_4) of the new compound **2**.

13C_GYKO7F-J22_MEOD_3.ESP

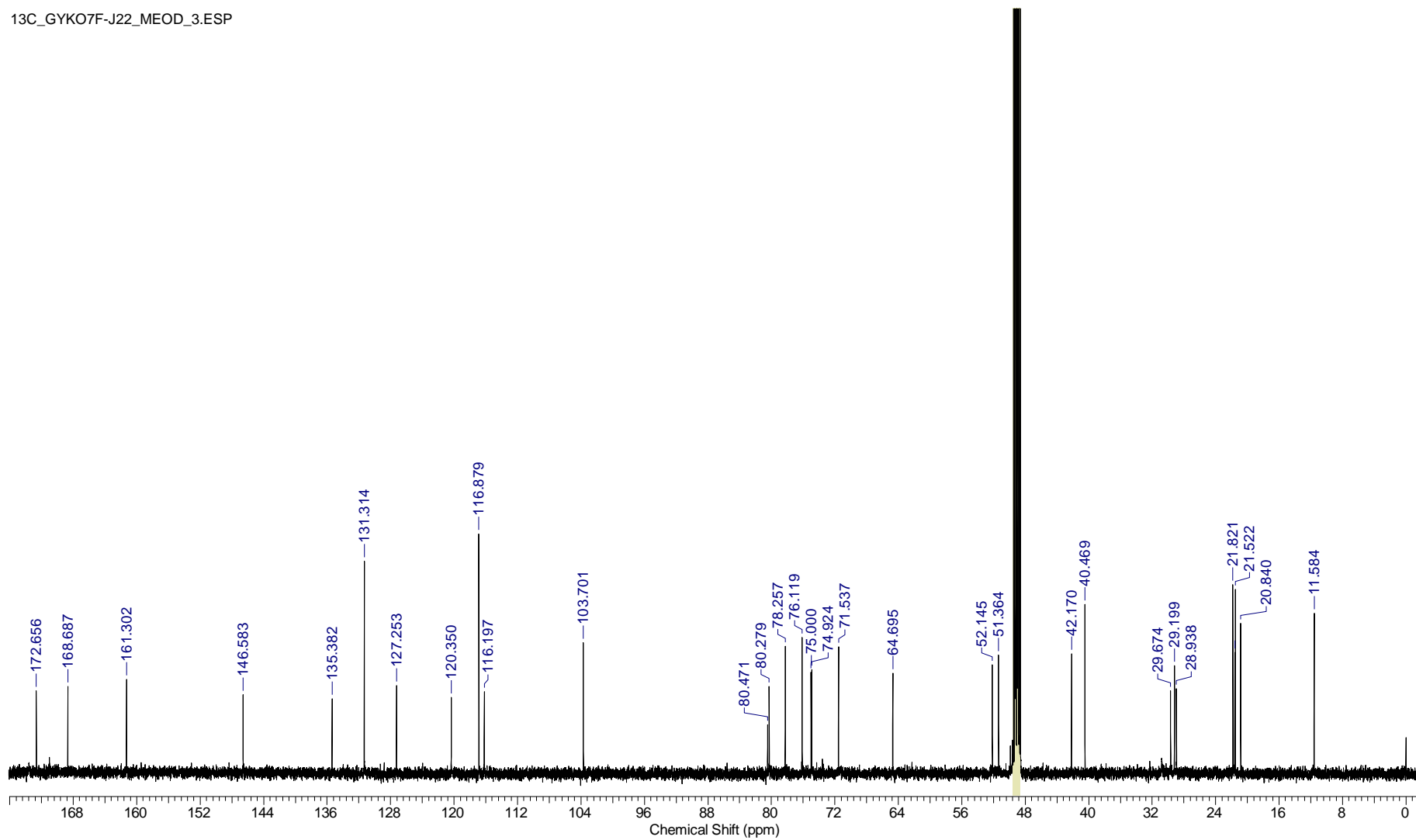


Figure S11. HSQC spectrum (600 MHz, methanol-*d*₄) of the new compound **2**.

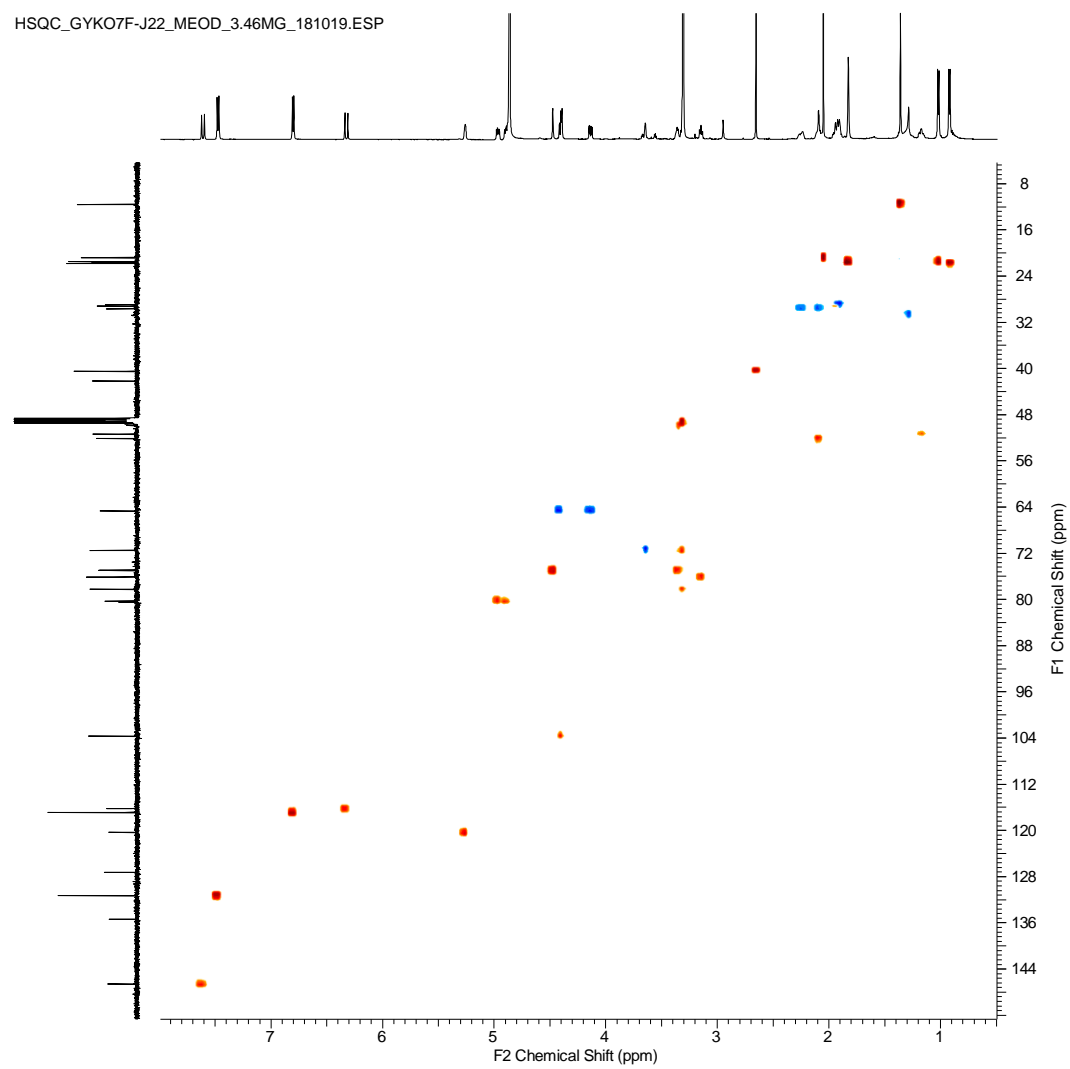


Figure S12. HMBC spectrum (600 MHz, methanol- d_4) of the new compound **2**.

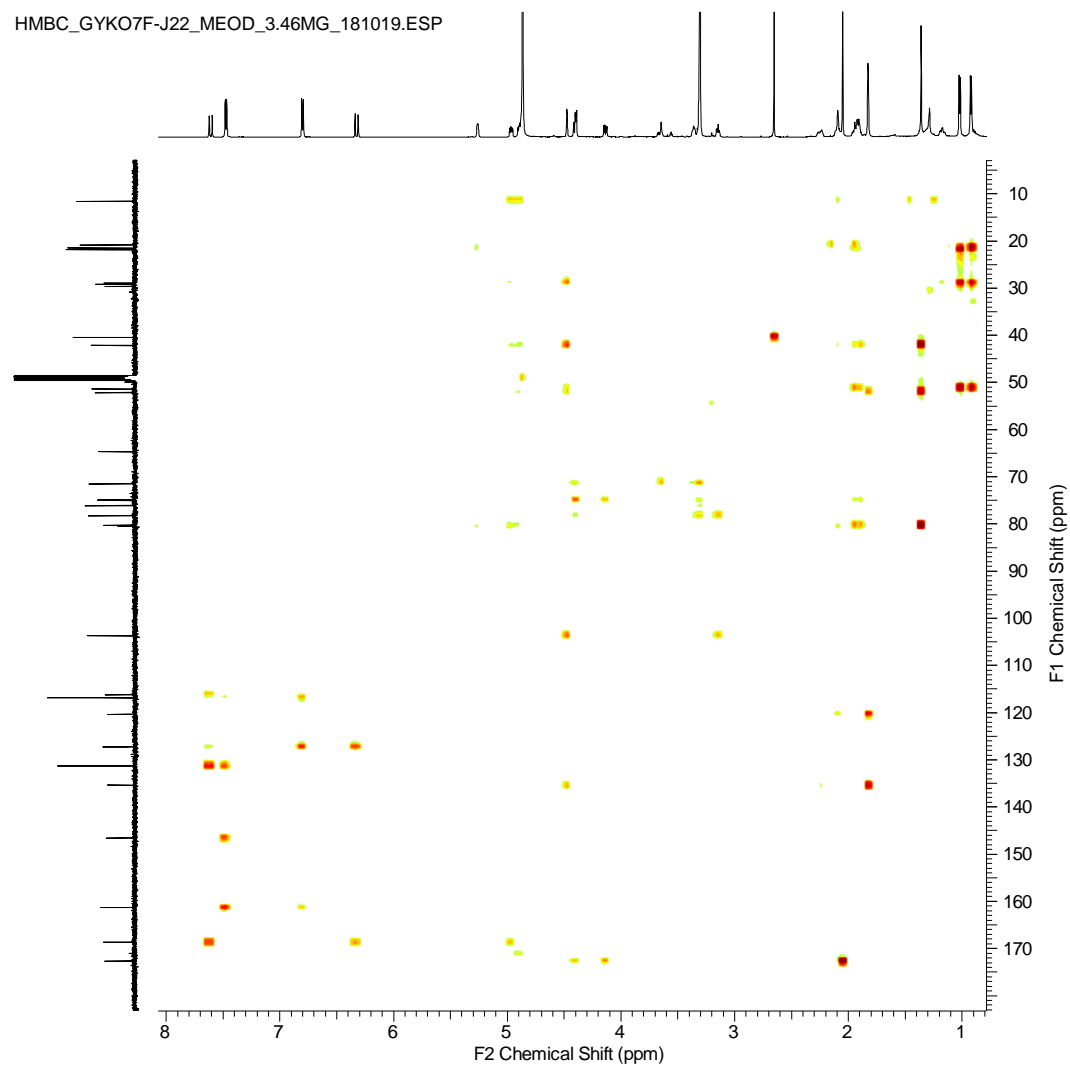


Figure S13. COSY spectrum (600 MHz, methanol- d_4) of the new compound **2**.

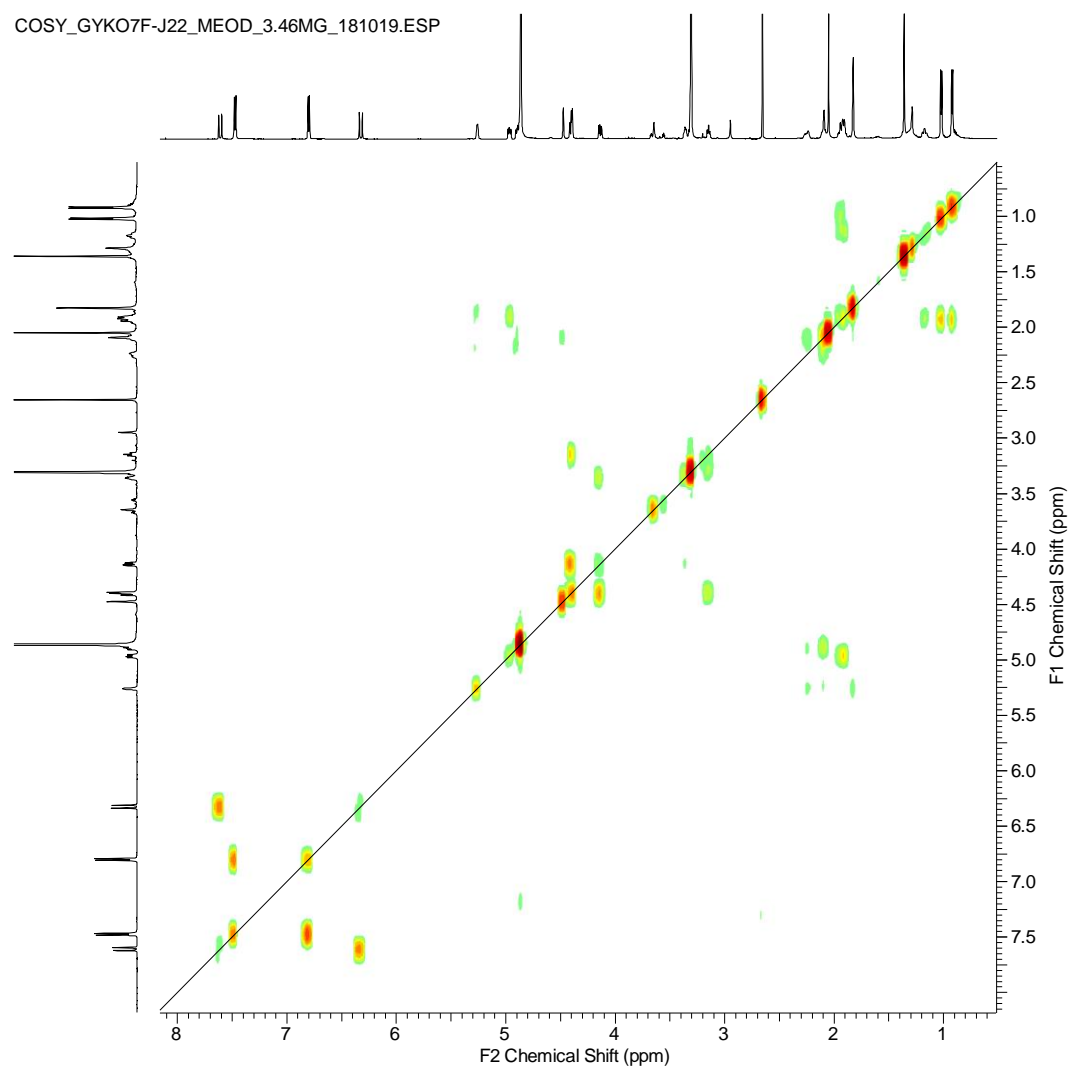


Figure S14. NOESY spectrum (600 MHz, methanol- d_4) of the new compound **2**.

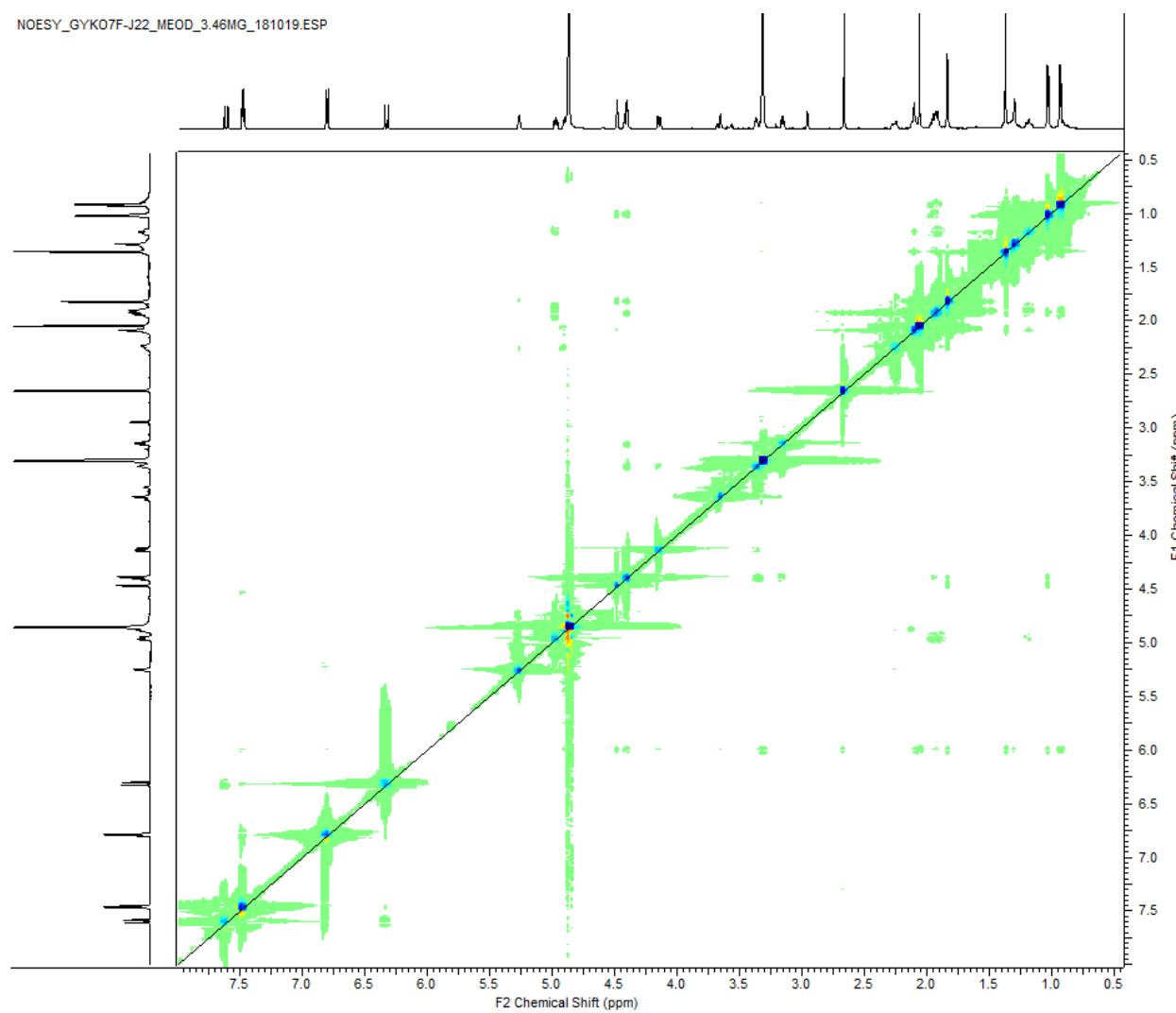


Figure S15. ^1H NMR spectrum (700 MHz, $\text{DMSO-}d_6$) of the new compound **2**.

1H_J22_DMSO.ESP

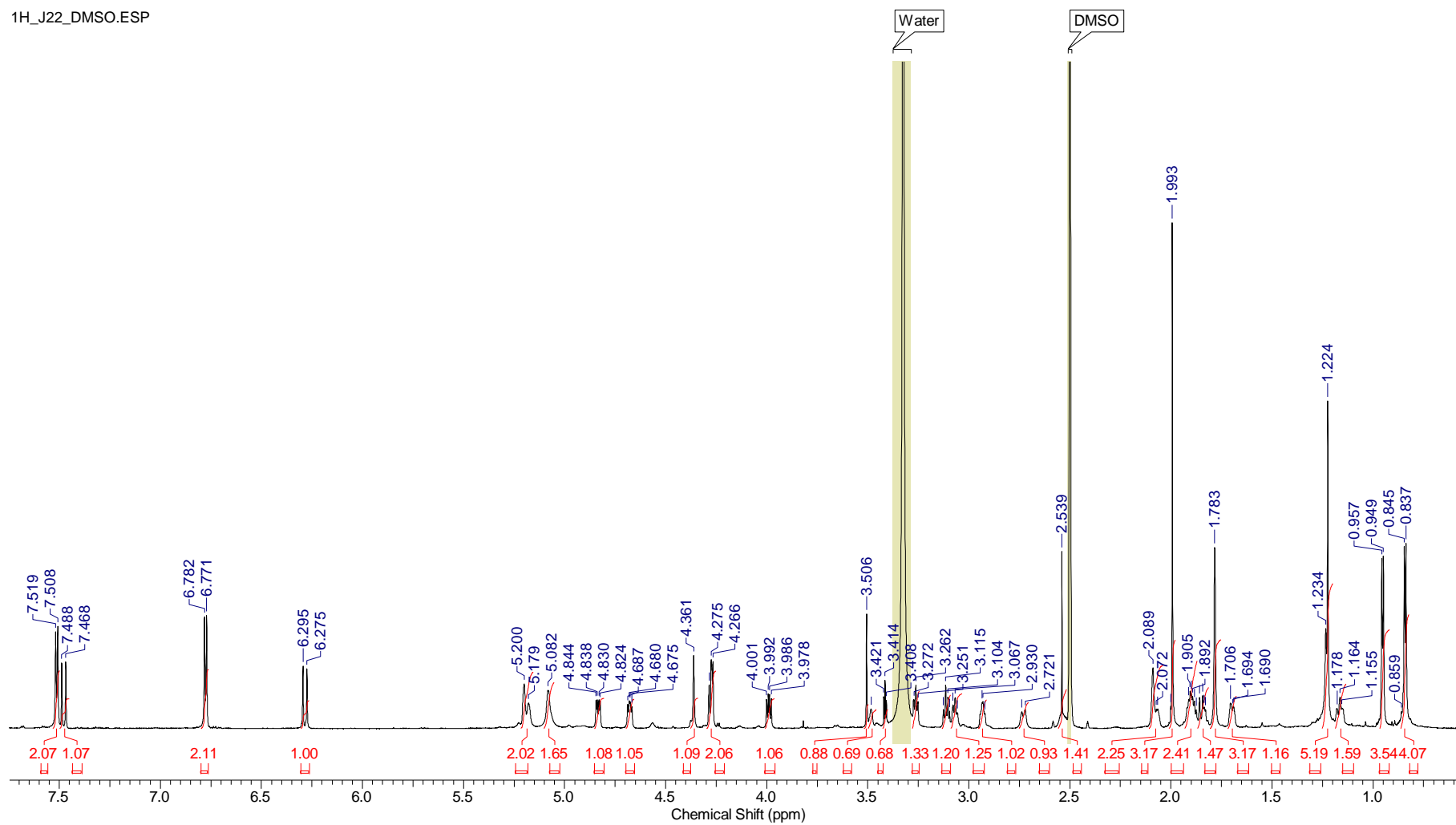


Figure S16. ^{13}C NMR spectrum (175 MHz, $\text{DMSO}-d_6$) of the new compound **2**.

13C_J22_DMSO.ESP

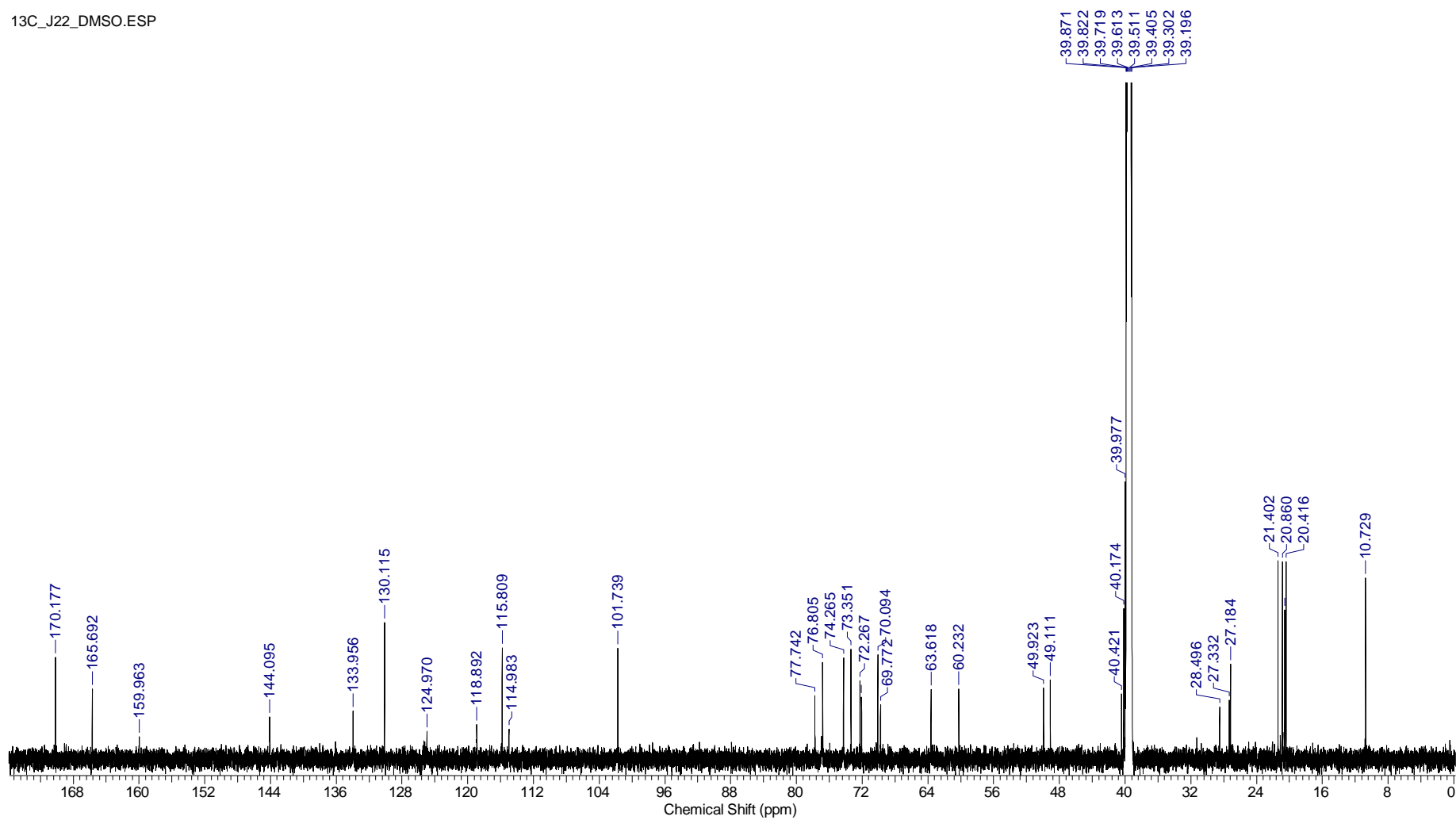


Figure S17. HSQC spectrum (700 MHz, DMSO-*d*₆) of the new compound **2**.

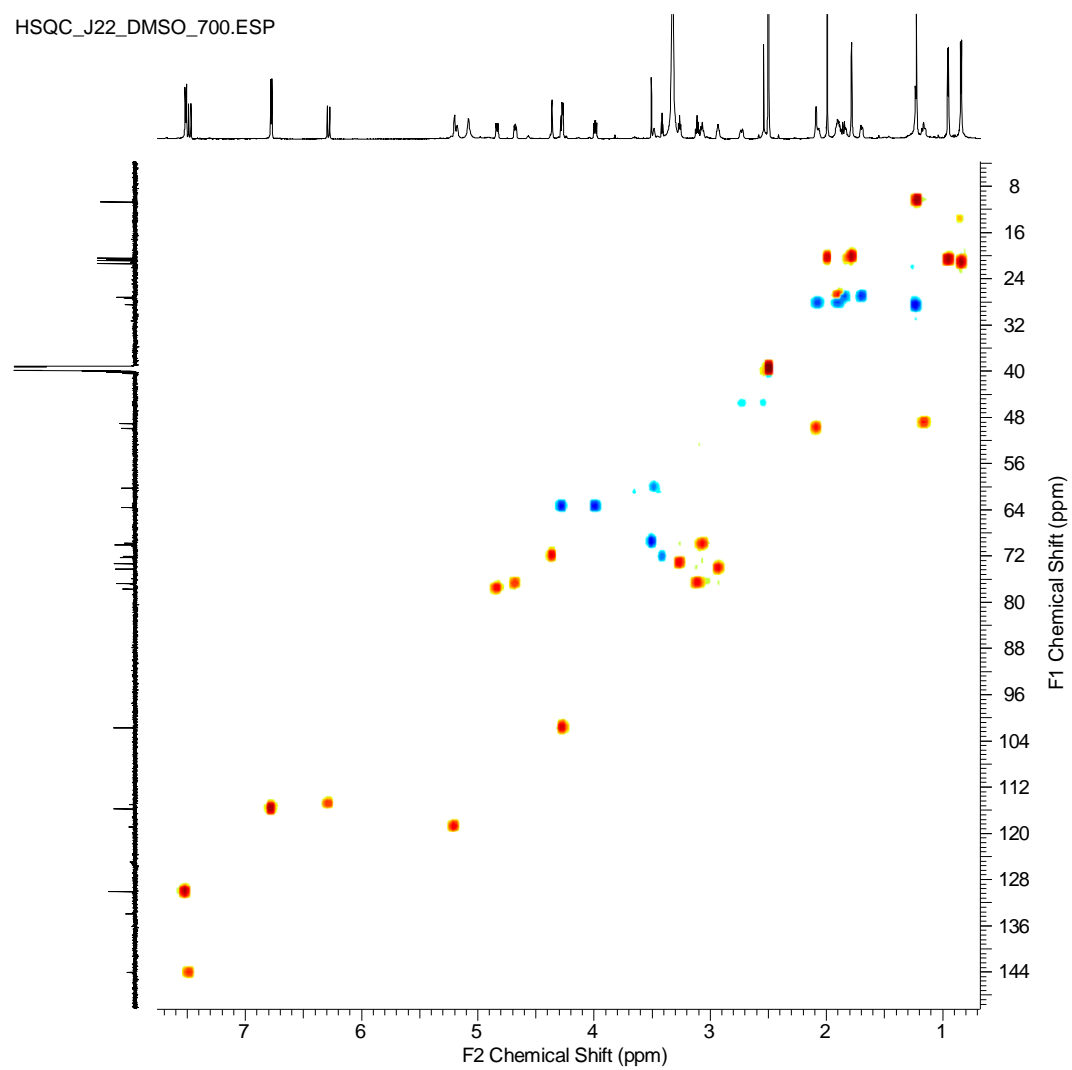


Figure S18. HMBC spectrum (700 MHz, DMSO- d_6) of the new compound **2**.

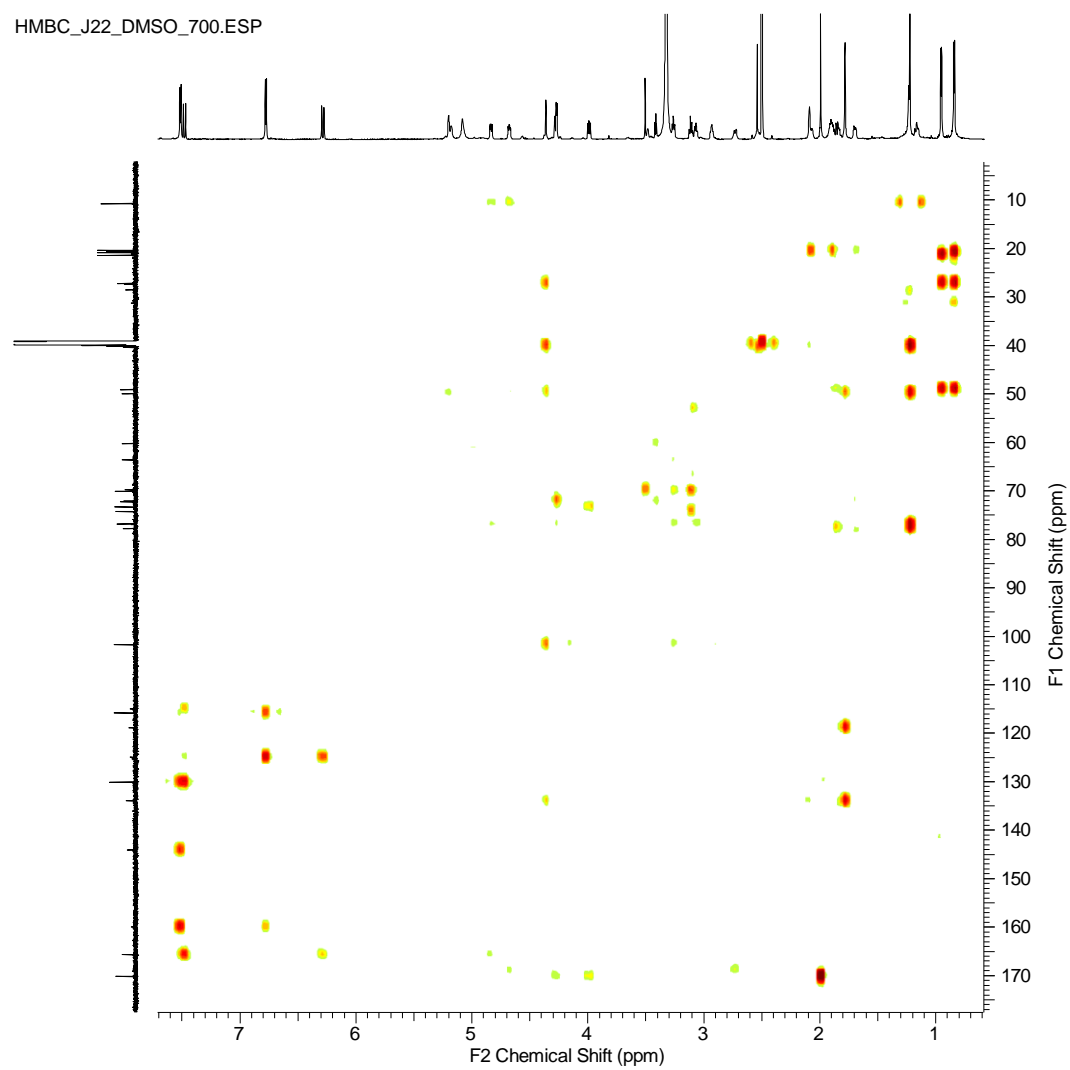


Figure S19. COSY spectrum (700 MHz, DMSO-*d*₆) of the new compound **2**.

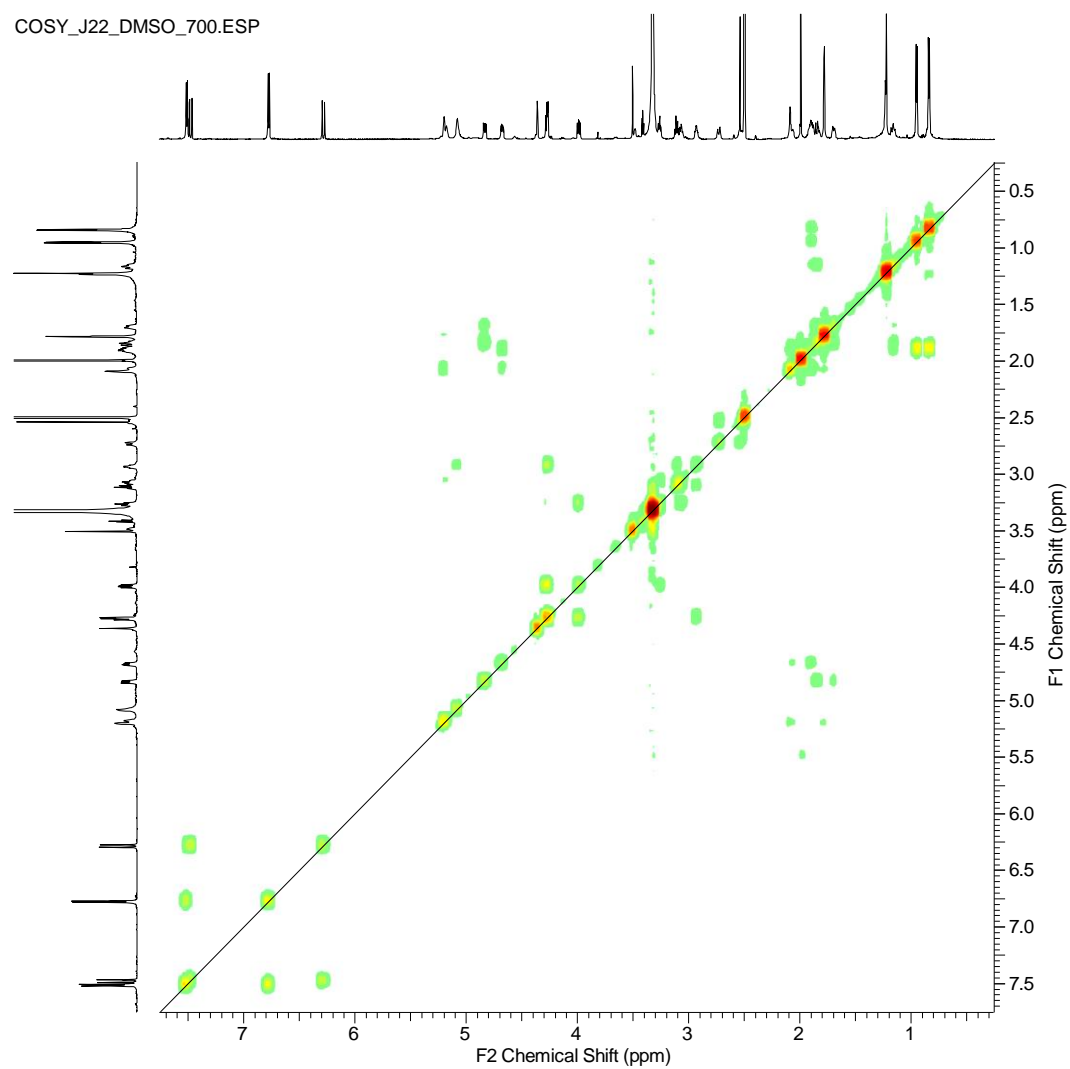


Figure S20. HRESIMS spectrum of the new compound **3**.

Multiple Mass Analysis: 2 mass(es) processed

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 20.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions

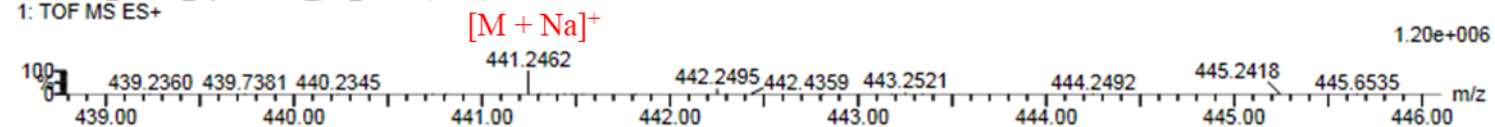
385 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)

Elements Used:

C: 0-100 H: 0-200 O: 0-50 Na: 0-1

20191216_SeoYH_Gyko7F-J17_pos_re 244 (2.743)

1: TOF MS ES+



Minimum: 15.00
Maximum: 100.00

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
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441.2462	100.00	441.2464	-0.2	-0.5	2.5	145.5	n/a	n/a	C21 H38 O8 Na
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Figure S21. ^1H NMR spectrum (600 MHz, methanol- d_4) of the new compound **3**.

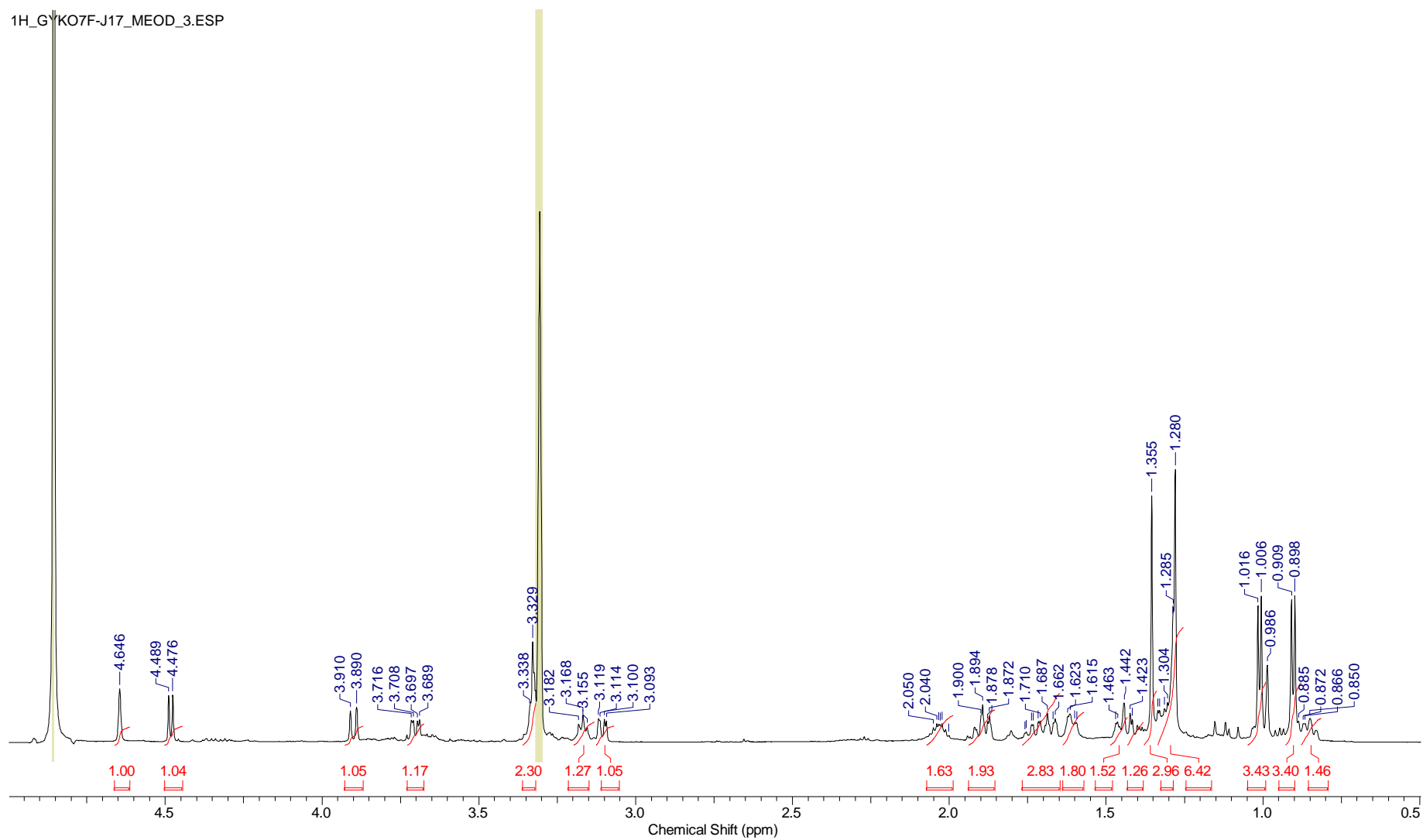


Figure S22. ^{13}C NMR spectrum (150 MHz, methanol- d_4) of the new compound **3**.

13C_GYKO7F-J17_MEOD_3.ESP

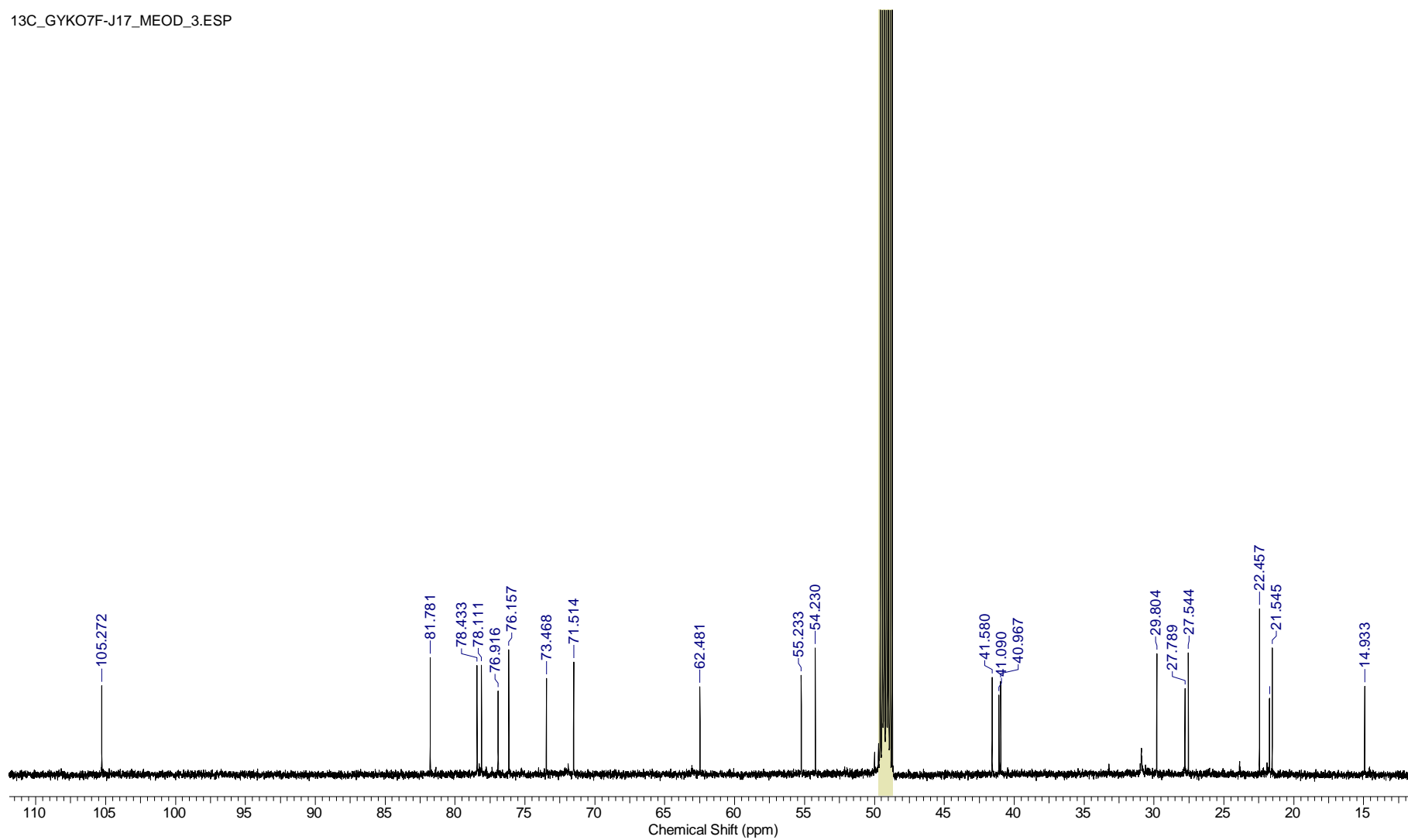


Figure S23. HSQC spectrum (600 MHz, methanol-*d*₄) of the new compound **3**.

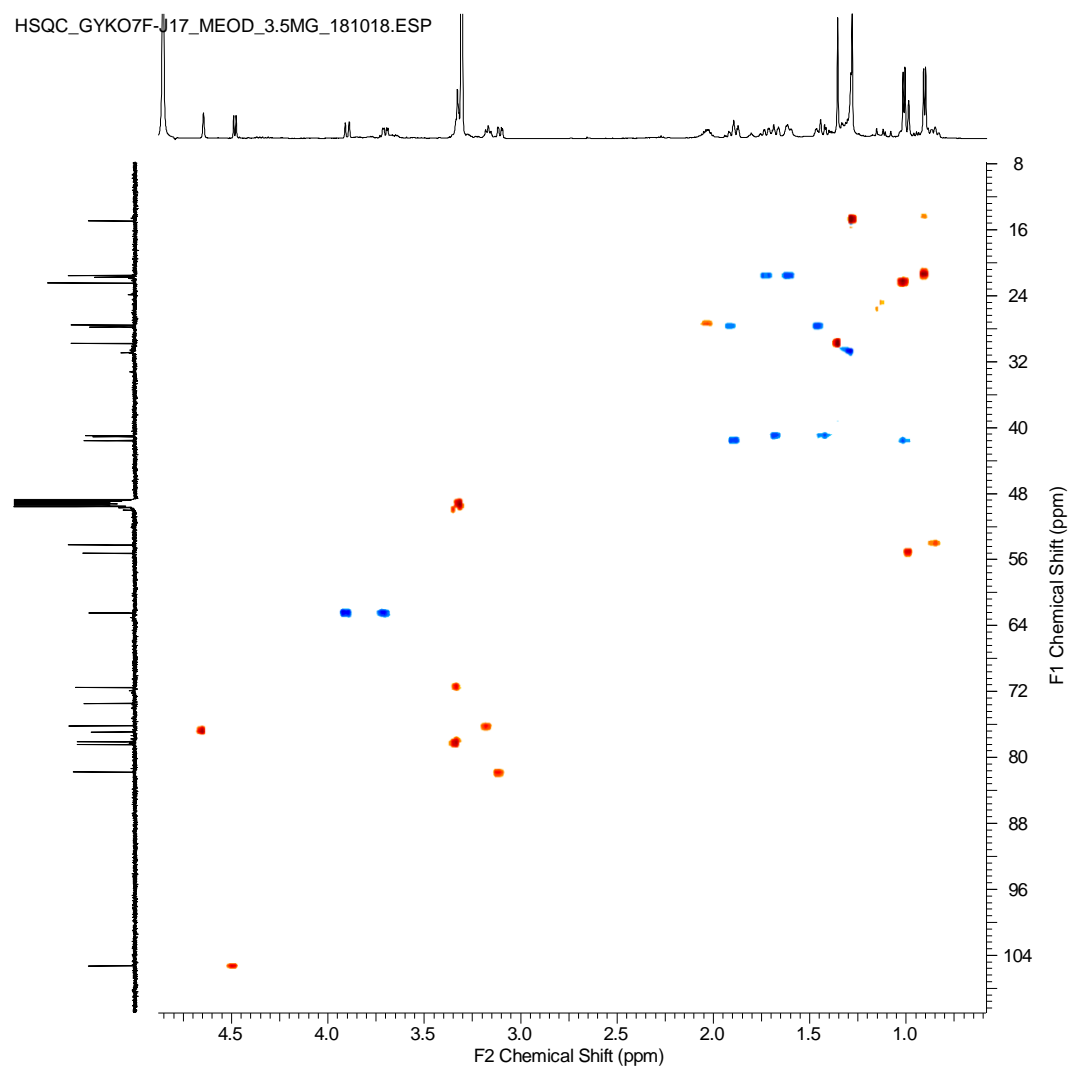


Figure S24. HMBC spectrum (600 MHz, methanol-*d*₄) of the new compound **3**.

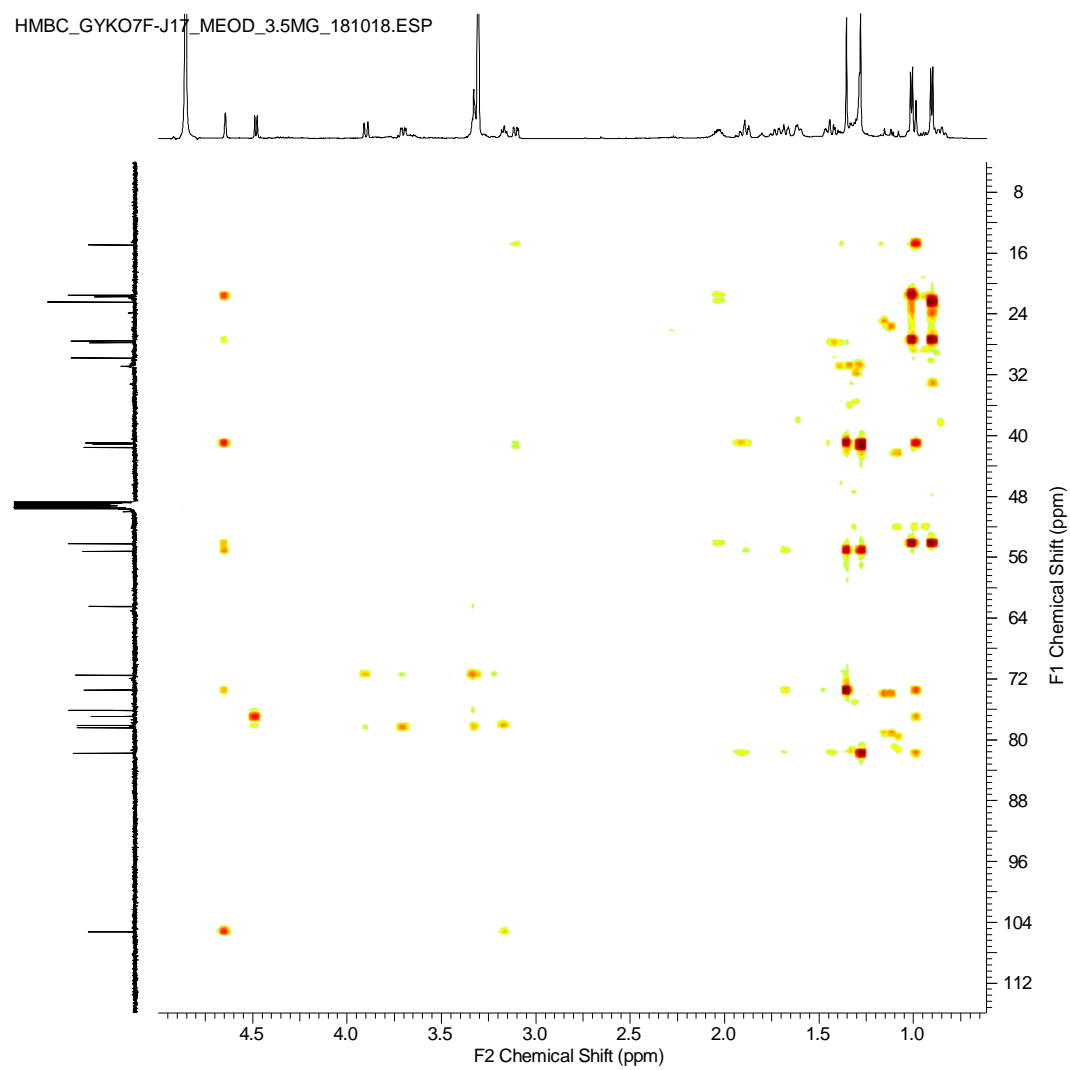


Figure S25. COSY spectrum (600 MHz, methanol-*d*₄) of the new compound **3**.

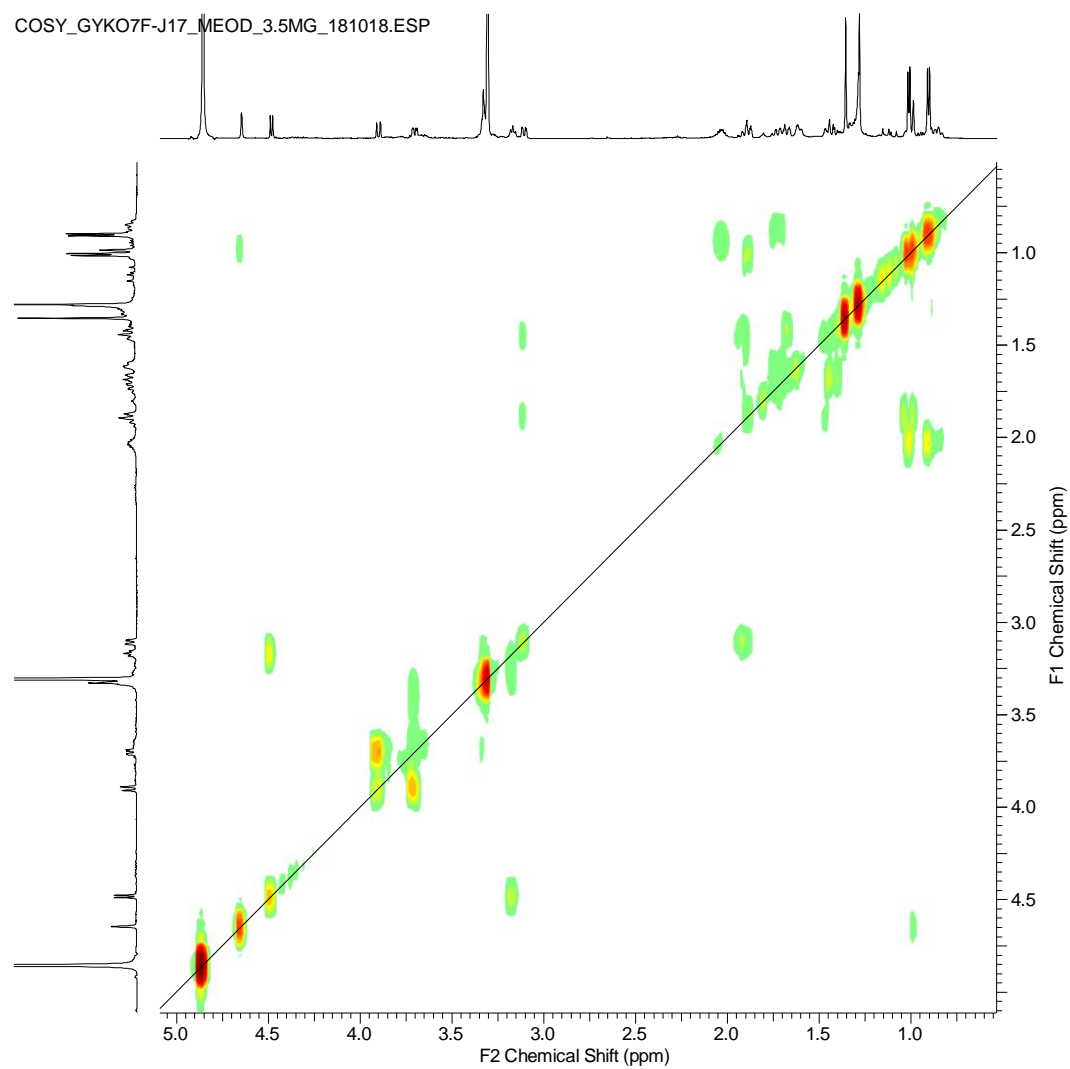


Figure S26. NOESY spectrum (600 MHz, methanol- d_4) of the new compound **3**.

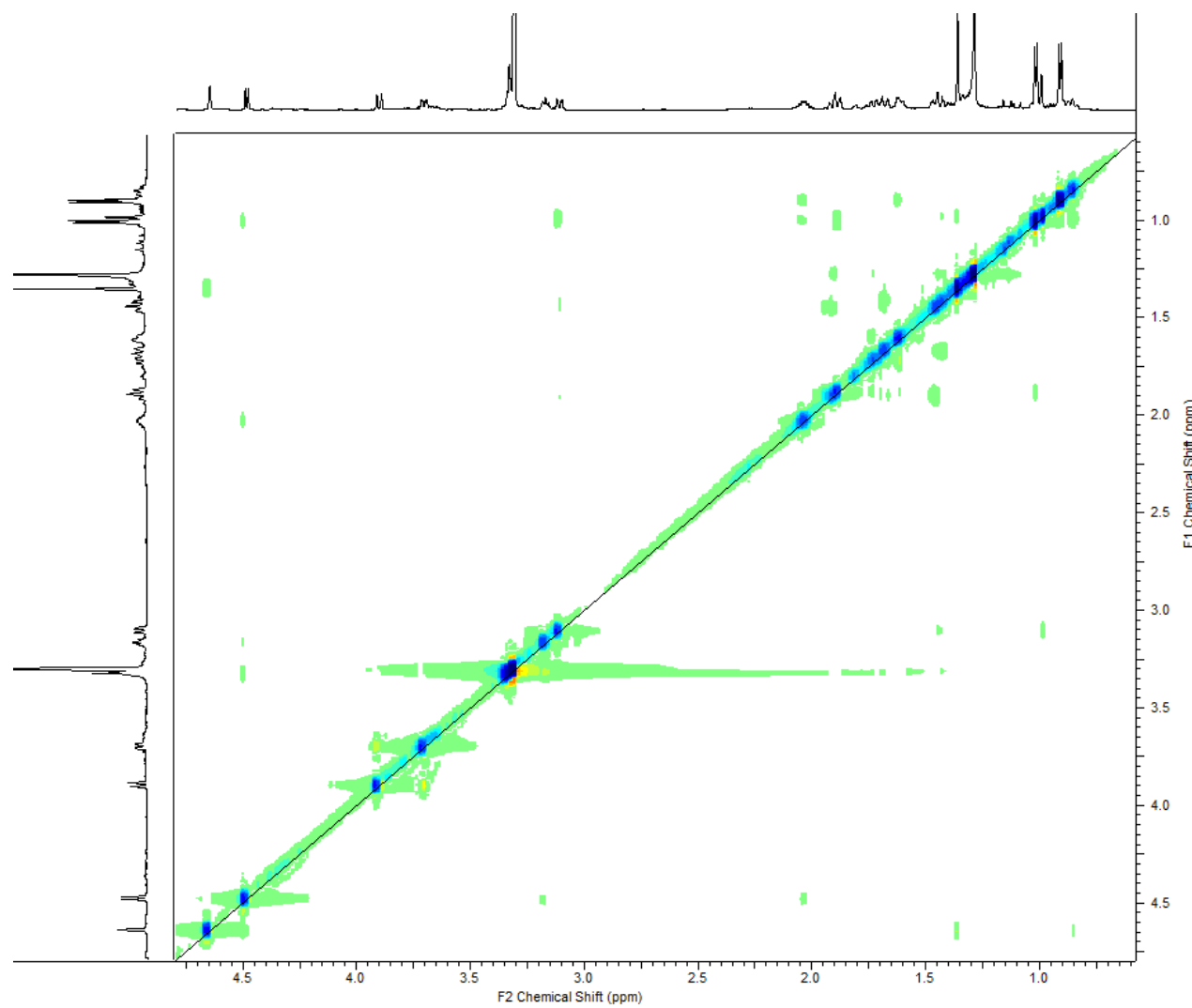


Figure S27. HRESIMS spectrum of the new compound 4.

Multiple Mass Analysis: 2 mass(es) processed

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 20.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions

652 formula(e) evaluated with 2 results within limits (up to 20 closest results for each mass)

Elements Used:

C: 0-100 H: 0-200 O: 0-50 Na: 0-1

20191216_SeoYH_Gyko7F-J19_pos_re 231 (2.600)

1: TOF MS ES+



Minimum: 15.00
Maximum: 100.00

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
587.3036	100.00	587.3009	2.7	4.6	15.5	63.1	1.273	28.00	C36 H43 O7
		587.3043	-0.7	-1.2	3.5	62.1	0.328	72.00	C27 H48 O12 Na

Figure S28. ^1H NMR spectrum (600 MHz, methanol- d_4) of the new compound **4**.

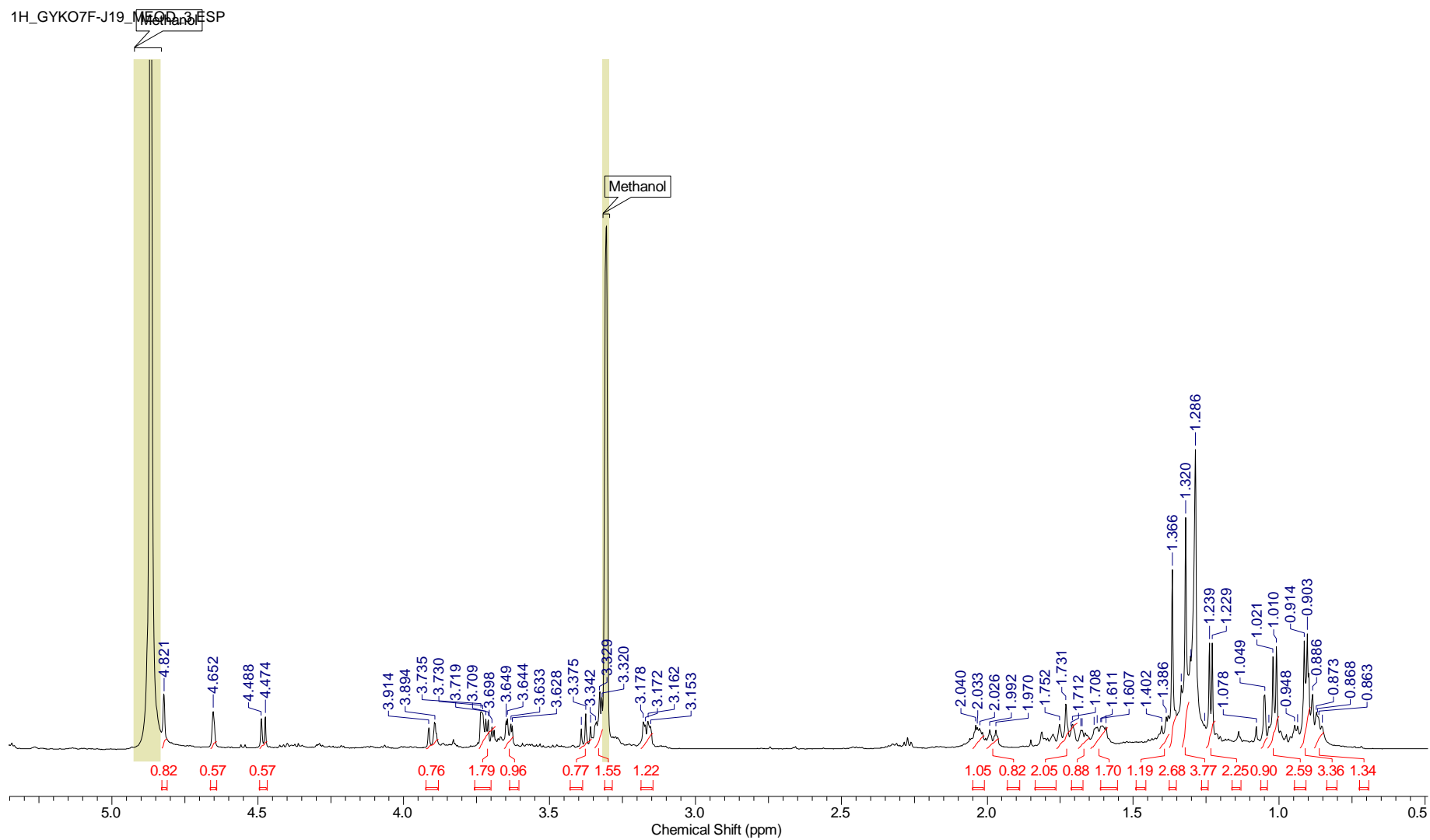


Figure S29. ^{13}C NMR spectrum (150 MHz, methanol- d_4) of the new compound **4**.

13C_GYKO7F-J19_MEOD_3.ESP

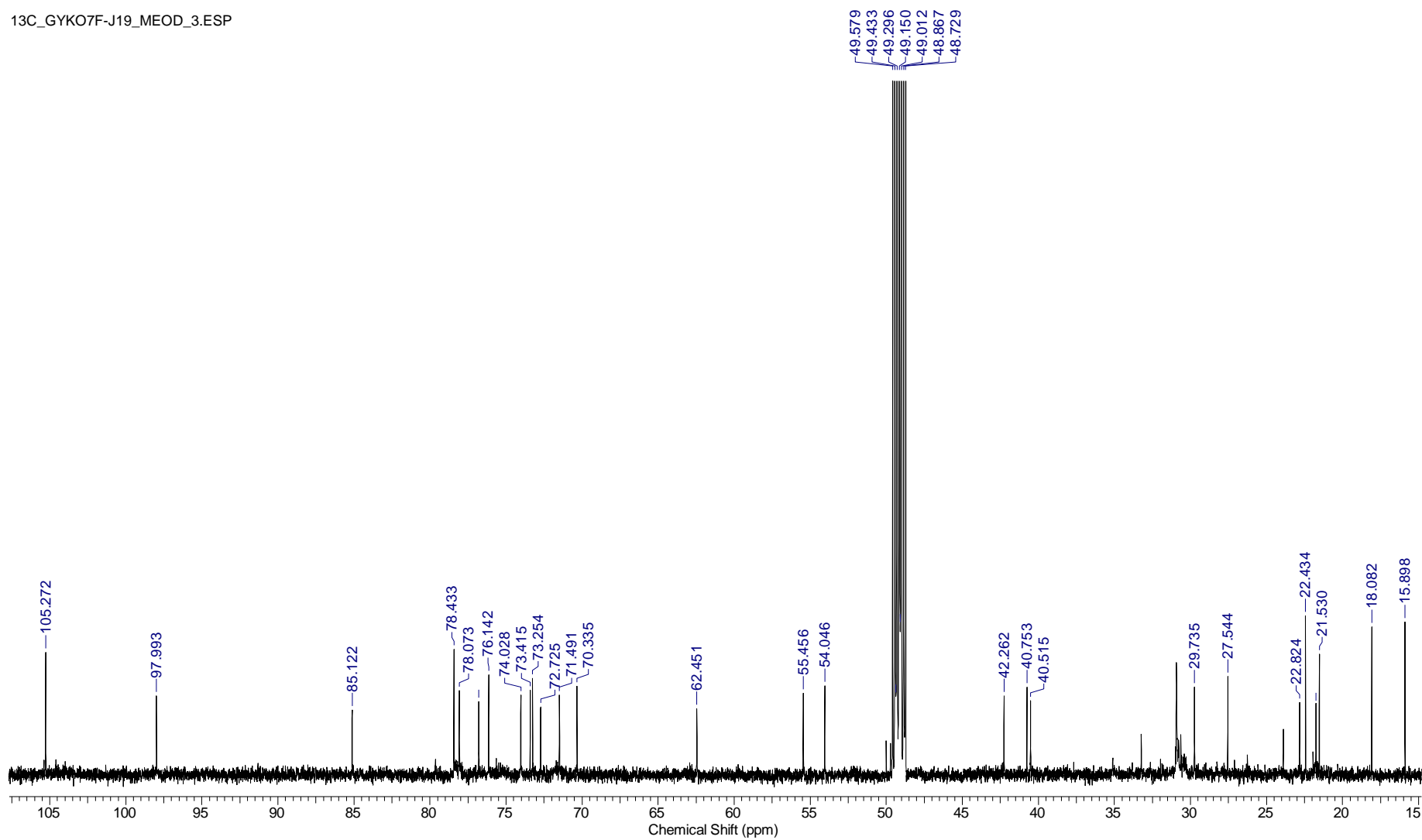


Figure S30. HSQC spectrum (600 MHz, methanol- d_4) of the new compound 4.

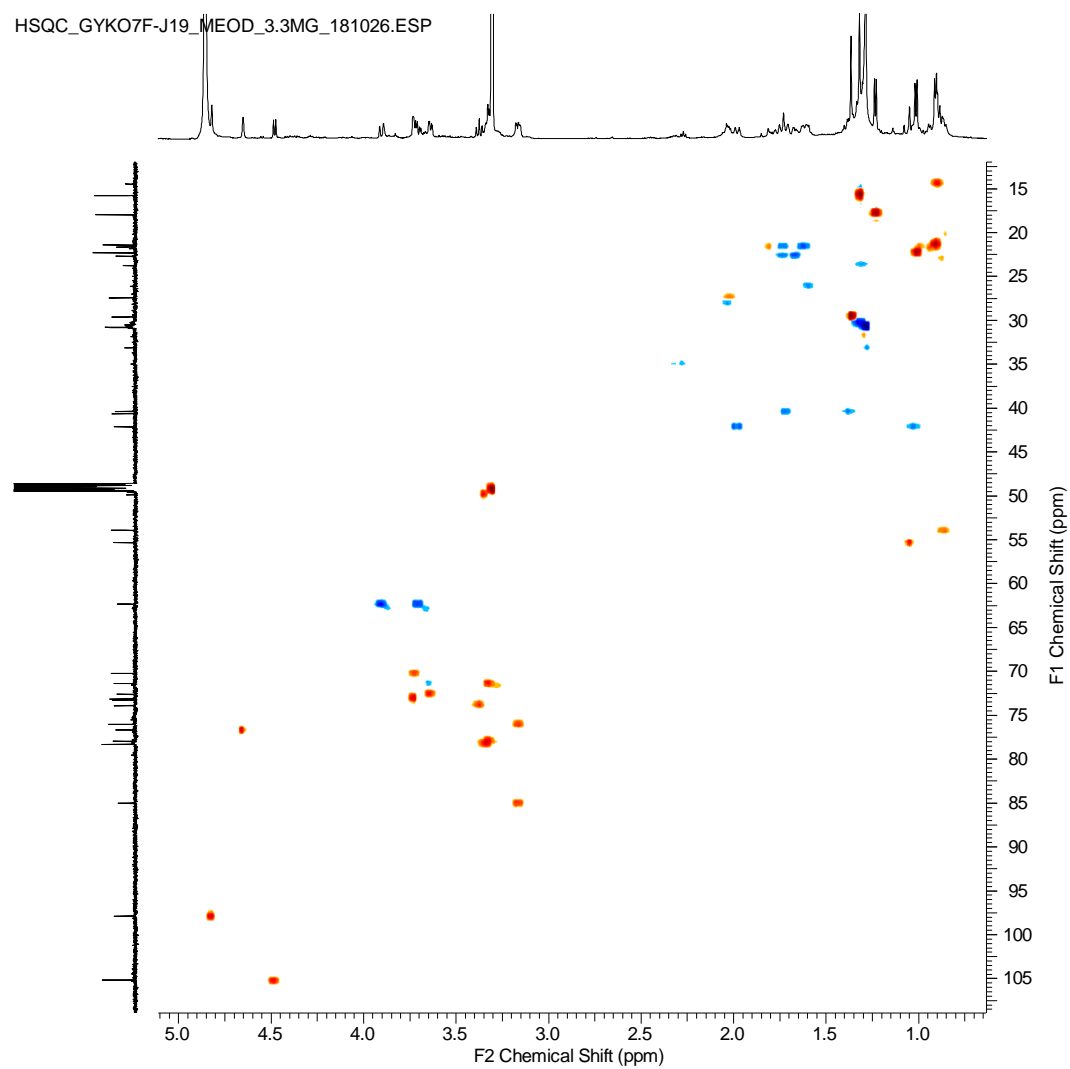


Figure S31. HMBC spectrum (600 MHz, methanol-*d*₄) of the new compound **4**.

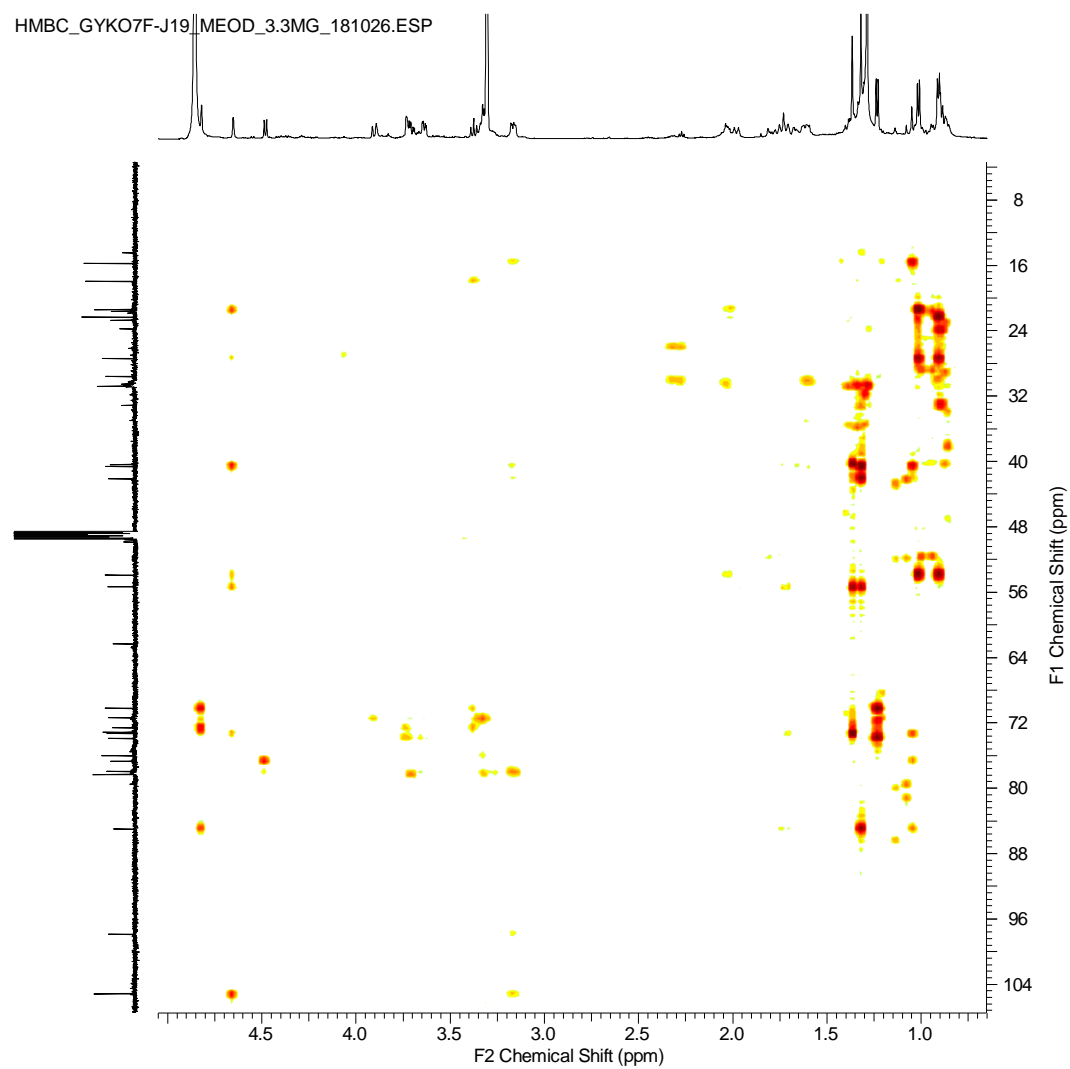


Figure S32. COSY spectrum (600 MHz, methanol-*d*₄) of the new compound **4**.

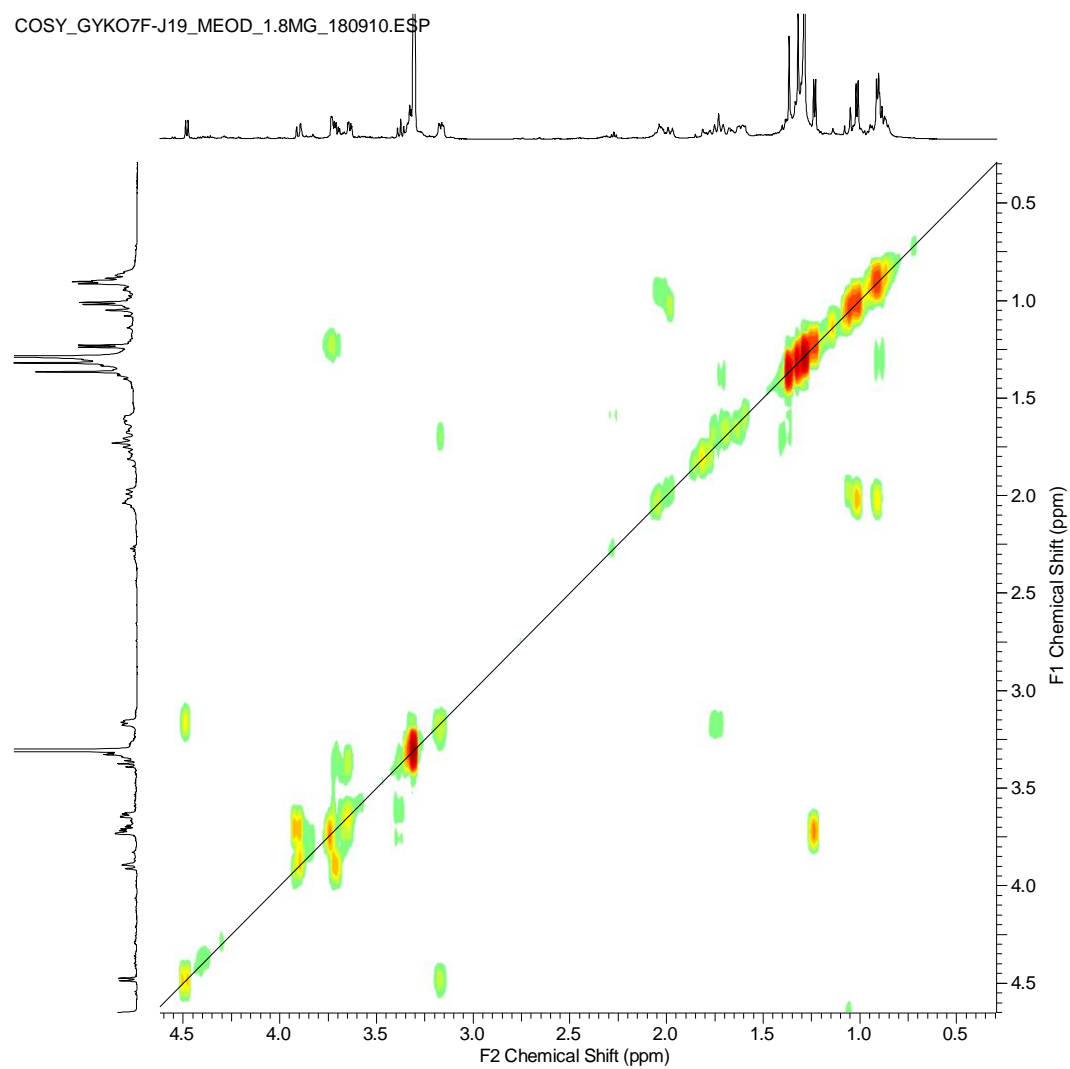


Figure S33. NOESY spectrum (600 MHz, methanol- d_4) of the new compound **4**.

