

**Supplemental Information for:**  
**Growth Inhibition of Colon Cancer and Melanoma Cells by Versiol**  
**Derivatives from *Paraconiothyrium* sp.**

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<sup>§</sup>Natural Products Discovery Group, University of Oklahoma, Norman, OK 73019, United States

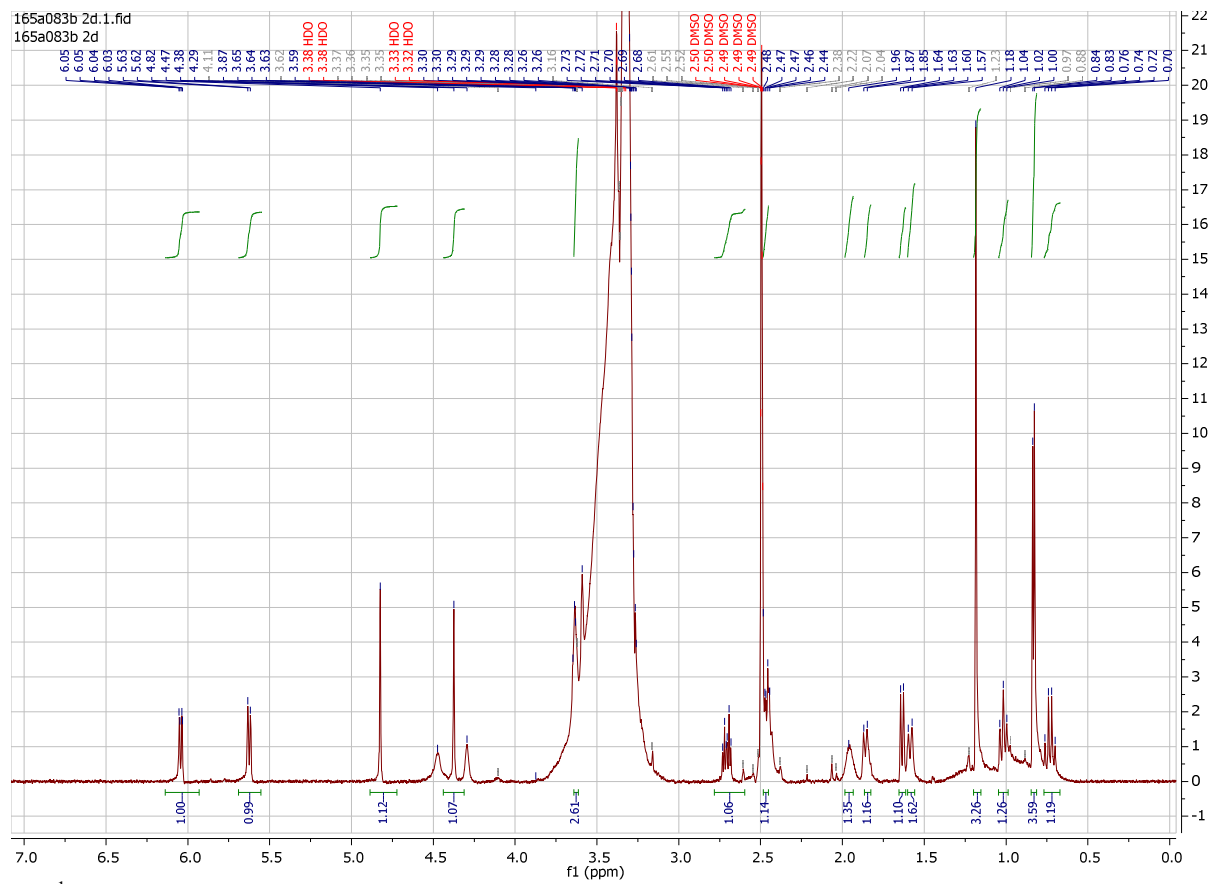
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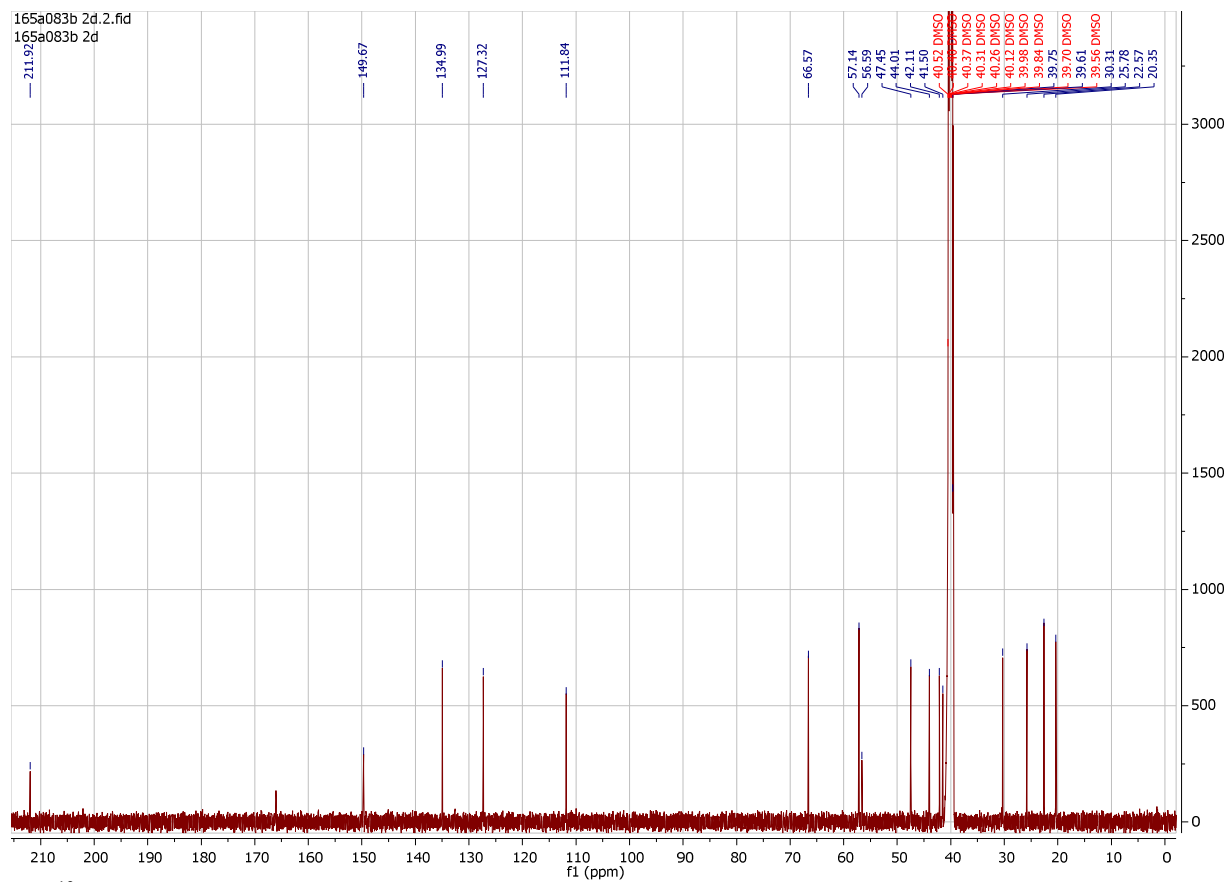
List of Supporting Information

- S1. <sup>1</sup>H NMR spectrum (600 MHz) of compound **1** in DMSO-*d*<sub>6</sub>.
- S2. <sup>13</sup>C NMR spectrum (150 MHz) of compound **1** in DMSO-*d*<sub>6</sub>.
- S3. COSY spectrum of compound **1** in DMSO-*d*<sub>6</sub>.
- S4. HSQC spectrum of compound **1** in DMSO-*d*<sub>6</sub>.
- S5. HMBC spectrum of compound **1** in DMSO-*d*<sub>6</sub>.
- S6. ROESY spectrum of compound **1** in DMSO-*d*<sub>6</sub>.
- S7. <sup>1</sup>H NMR spectrum (600 MHz) of compound **3** in DMSO-*d*<sub>6</sub>.
- S8. <sup>13</sup>C NMR spectrum (150 MHz) of compound **3** in DMSO-*d*<sub>6</sub>.
- S9. COSY spectrum of compound **3** in DMSO-*d*<sub>6</sub>.
- S10. HSQC spectrum of compound **3** in DMSO-*d*<sub>6</sub>.
- S11. HMBC spectrum of compound **3** in DMSO-*d*<sub>6</sub>.
- S12. ROESY spectrum of compound **3** in DMSO-*d*<sub>6</sub>.
- S13. <sup>1</sup>H NMR spectrum (600 MHz) of compound **4** in DMSO-*d*<sub>6</sub>.
- S14. <sup>13</sup>C NMR spectrum (150 MHz) of compound **4** in DMSO-*d*<sub>6</sub>.
- S15. COSY spectrum of compound **4** in DMSO-*d*<sub>6</sub>.
- S16. HSQC spectrum of compound **4** in DMSO-*d*<sub>6</sub>.
- S17. HMBC spectrum of compound **4** in DMSO-*d*<sub>6</sub>.
- S18. ROESY spectrum of compound **4** in DMSO-*d*<sub>6</sub>.
- S19. <sup>1</sup>H NMR spectrum (600 MHz) of compound **5** in DMSO-*d*<sub>6</sub>.
- S20. <sup>13</sup>C NMR spectrum (150 MHz) of compound **5** in DMSO-*d*<sub>6</sub>.
- S21. COSY spectrum of compound **5** in DMSO-*d*<sub>6</sub>.
- S22. HSQC spectrum of compound **5** in DMSO-*d*<sub>6</sub>.
- S23. HMBC spectrum of compound **5** in DMSO-*d*<sub>6</sub>.
- S24. ROESY spectrum of compound **5** in DMSO-*d*<sub>6</sub>.
- S25. <sup>1</sup>H NMR spectrum (600 MHz) of compound **6** in DMSO-*d*<sub>6</sub>.
- S26. <sup>13</sup>C NMR spectrum (150 MHz) of compound **6** in DMSO-*d*<sub>6</sub>.
- S27. COSY spectrum of compound **6** in DMSO-*d*<sub>6</sub>.
- S28. HSQC spectrum of compound **6** in DMSO-*d*<sub>6</sub>.
- S29. HMBC spectrum of compound **6** in DMSO-*d*<sub>6</sub>.
- S30. ROESY spectrum of compound **6** in DMSO-*d*<sub>6</sub>.
- S31. <sup>1</sup>H NMR spectrum (600 MHz) of compound **7** in DMSO-*d*<sub>6</sub>.
- S32. <sup>13</sup>C NMR spectrum (150 MHz) of compound **7** in DMSO-*d*<sub>6</sub>.
- S33. COSY spectrum of compound **7** in DMSO-*d*<sub>6</sub>.
- S34. HSQC spectrum of compound **7** in DMSO-*d*<sub>6</sub>.
- S35. HMBC spectrum of compound **7** in DMSO-*d*<sub>6</sub>.
- S36. ROESY spectrum of compound **7** in DMSO-*d*<sub>6</sub>.
- S37. <sup>1</sup>H NMR spectrum (600 MHz) of compound **8** in DMSO-*d*<sub>6</sub>.
- S38. <sup>13</sup>C NMR spectrum (150 MHz) of compound **8** in DMSO-*d*<sub>6</sub>.
- S39. COSY spectrum of compound **8** in DMSO-*d*<sub>6</sub>.
- S40. HSQC spectrum of compound **8** in DMSO-*d*<sub>6</sub>.
- S41. HMBC spectrum of compound **8** in DMSO-*d*<sub>6</sub>.
- S42. ROESY spectrum of compound **8** in DMSO-*d*<sub>6</sub>.
- S43. <sup>1</sup>H NMR spectrum (600 MHz) of compound **10** in DMSO-*d*<sub>6</sub>.
- S44. <sup>13</sup>C NMR spectrum (150 MHz) of compound **10** in DMSO-*d*<sub>6</sub>.
- S45. COSY spectrum of compound **10** in DMSO-*d*<sub>6</sub>.
- S46. HSQC spectrum of compound **10** in DMSO-*d*<sub>6</sub>.
- S47. HMBC spectrum of compound **10** in DMSO-*d*<sub>6</sub>.
- S48. ROESY spectrum of compound **10** in DMSO-*d*<sub>6</sub>.
- S49. Proposed biosynthesis of cratellenone E (**1**) and isoverisol A (**3**) via the common C14 heptaketide.

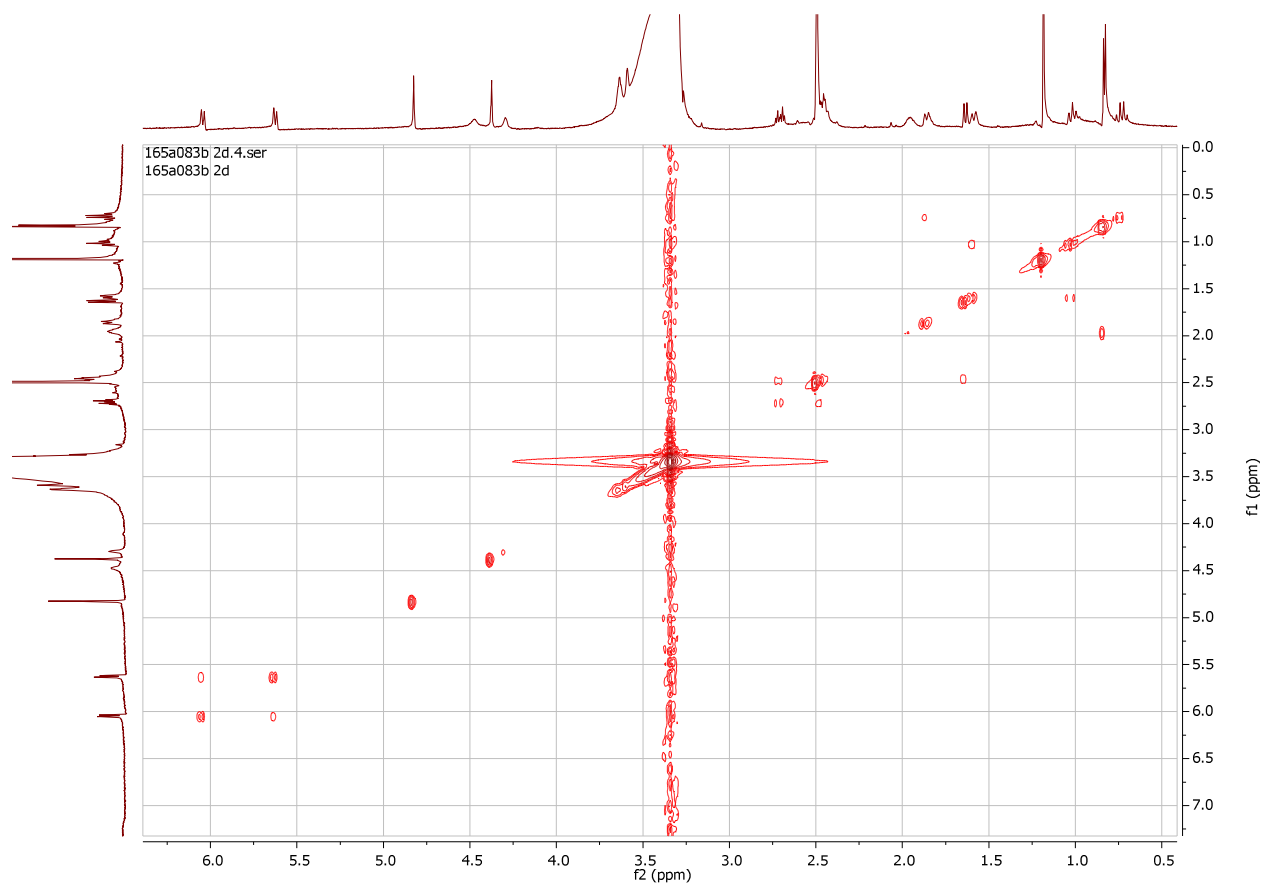
- S50.  $\Delta\delta$  ( $\delta_S - \delta_R$ ) values obtained from MTPA esters for compound **4**.
- S51. Cytotoxicity of *Paraconiothyrium* sp. fractions in COLO205, KM12 colon tumor cells.
- S52. Cytotoxicity of compounds from *Paraconiothyrium* sp. in COLO205, KM12 colon tumor cells.
- S53. NCI 60 cell single dose test of compound **8**.
- S54. Compound **8** NCI-60 mean bar graphs in single dose test.
- S55. NCI 60 cell single dose test of compound **9**.
- S56. Compound **9** NCI-60 mean bar graphs in single dose test.
- S57. NCI 60 cell single dose test of compound **10**.
- S58. Compound **10** NCI-60 mean bar graphs in single dose test.
- S59. NCI 60 cell 5-dose test of compound **8**.
- S60. Compound **8** mean bar graphs in 5-dose test.
- S61. NCI 60 cell 5-dose test of *Paraconiothyrium* sp. extract.
- S62. *Paraconiothyrium* sp. extract NCI-60 mean bar graphs in 5-dose test.
- S63. Comparison of experimental and calculated  $^{13}\text{C}$  and  $^1\text{H}$  chemical shifts in DMSO- $d_6$  for **1a** and **1b** and their statistical parameters.



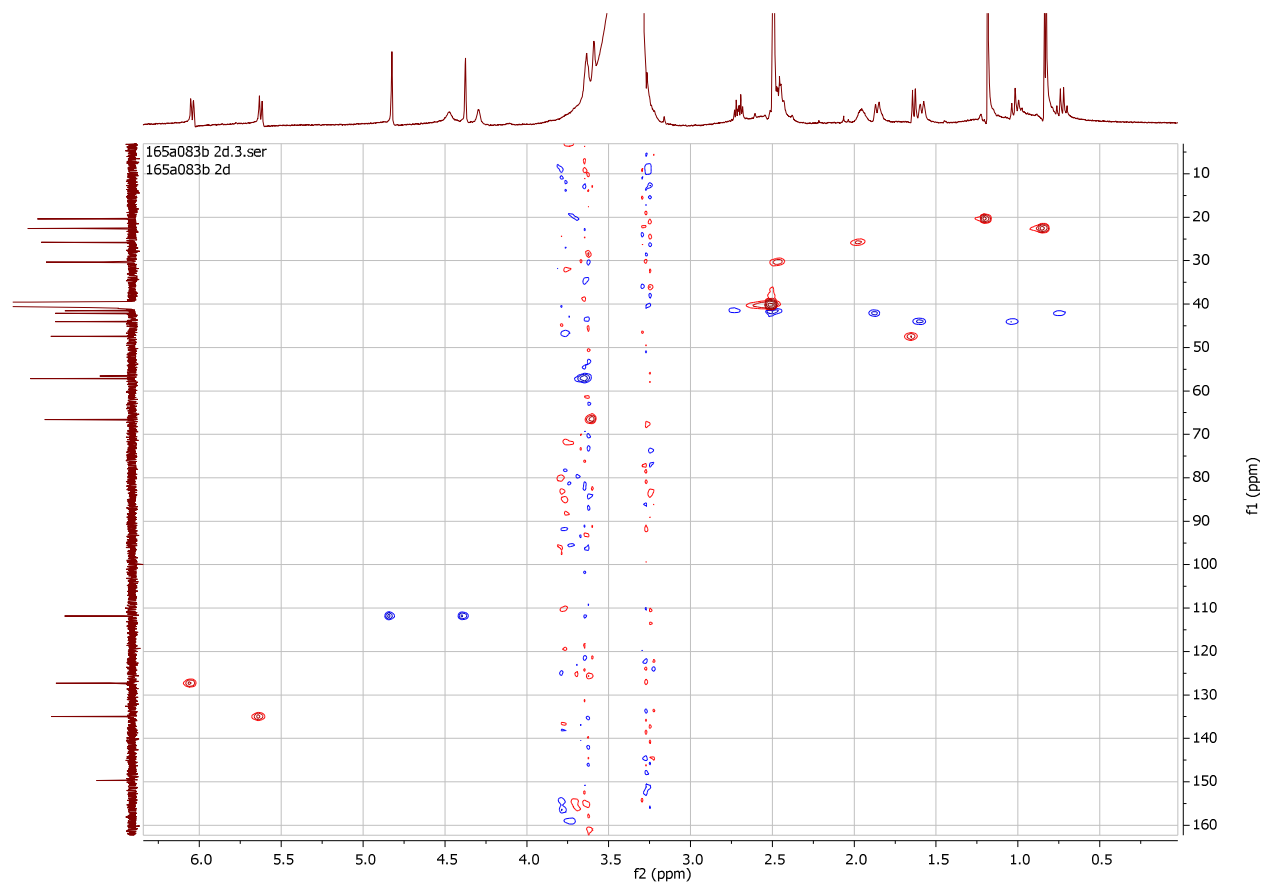
S1.  $^1\text{H}$  NMR spectrum (600 MHz) of compound **1** in  $\text{DMSO}-d_6$ .



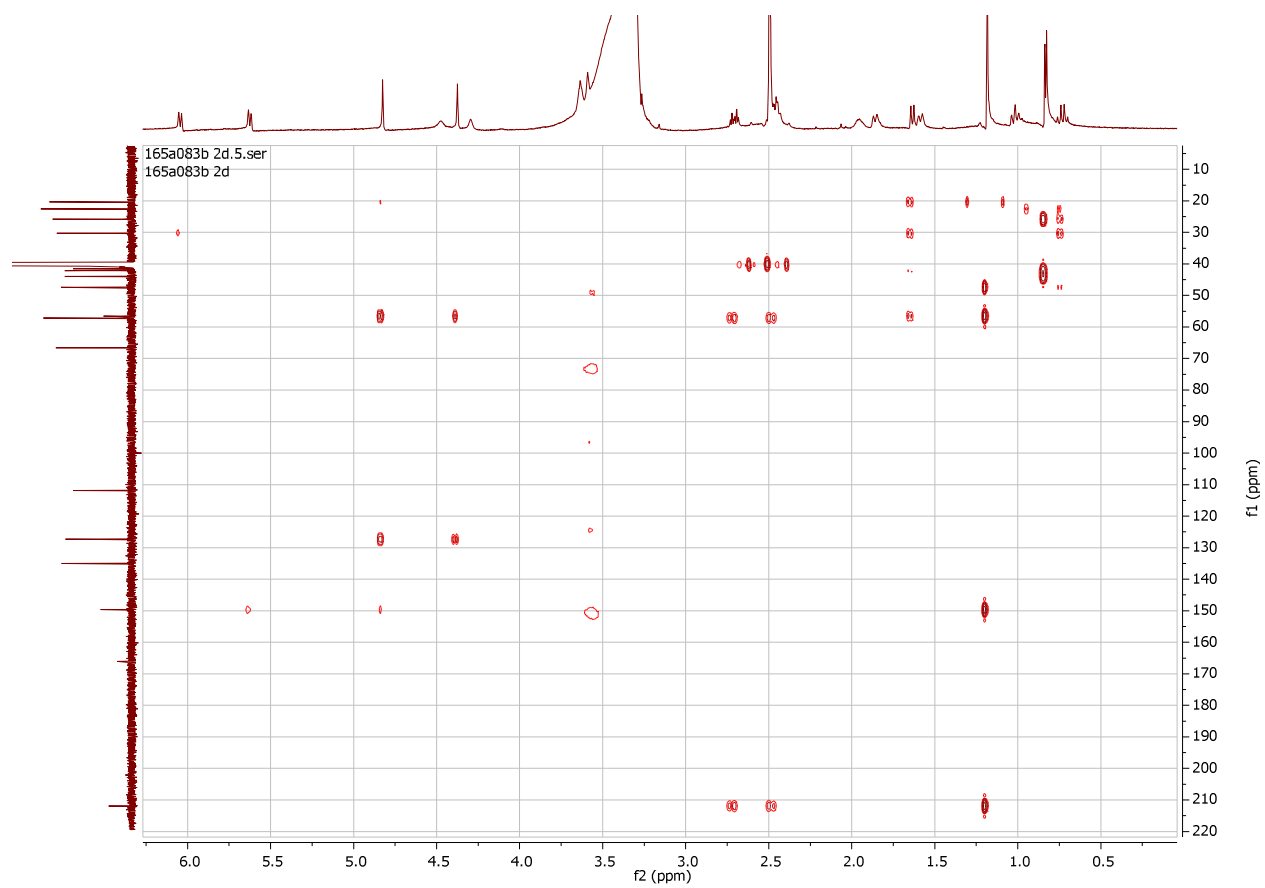
S2.  $^{13}\text{C}$  NMR spectrum (150 MHz) of compound **1** in  $\text{DMSO-}d_6$ .



S3. COSY spectrum of compound **1** in DMSO- $d_6$ .

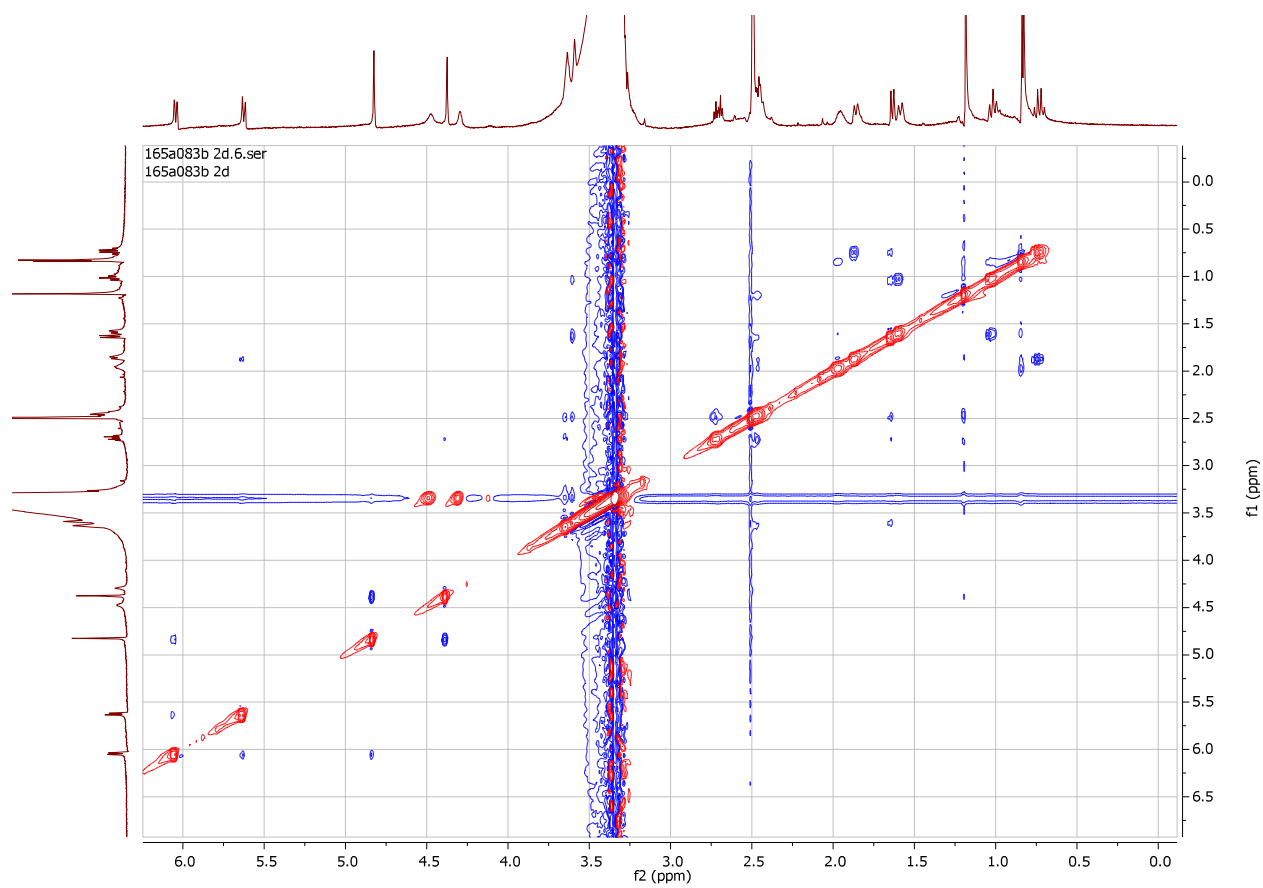


S4. HSQC spectrum of compound **1** in DMSO- $d_6$ .

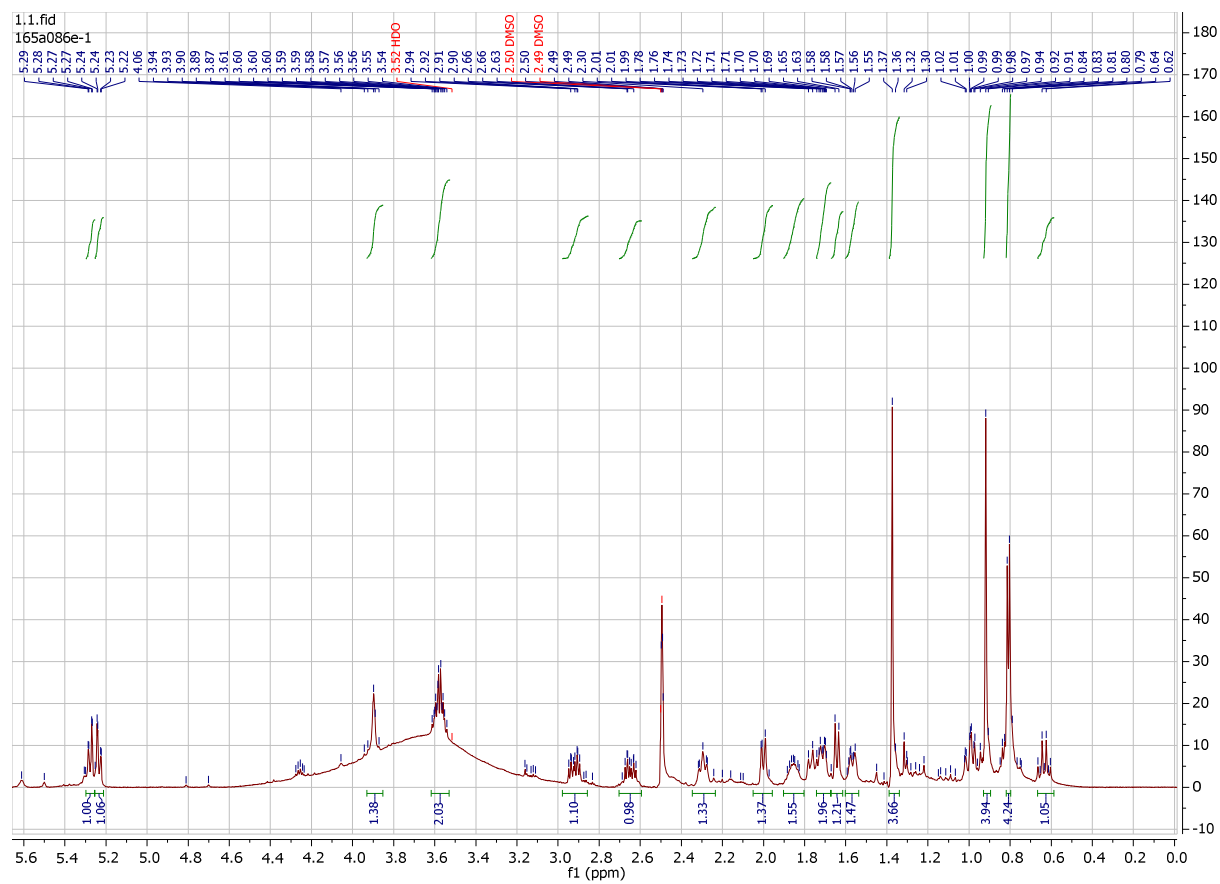


S5. HMBC spectrum of compound **1** in  $\text{DMSO-}d_6$ .

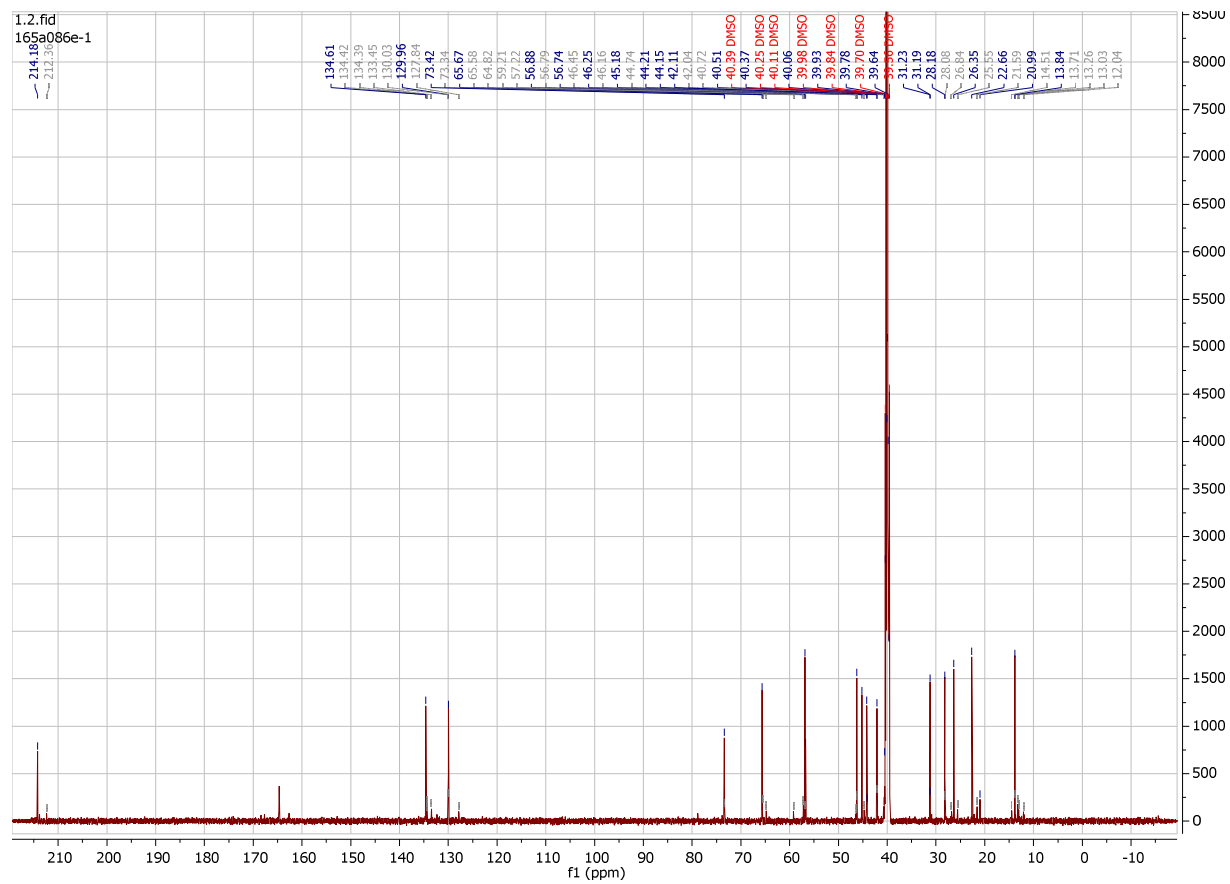




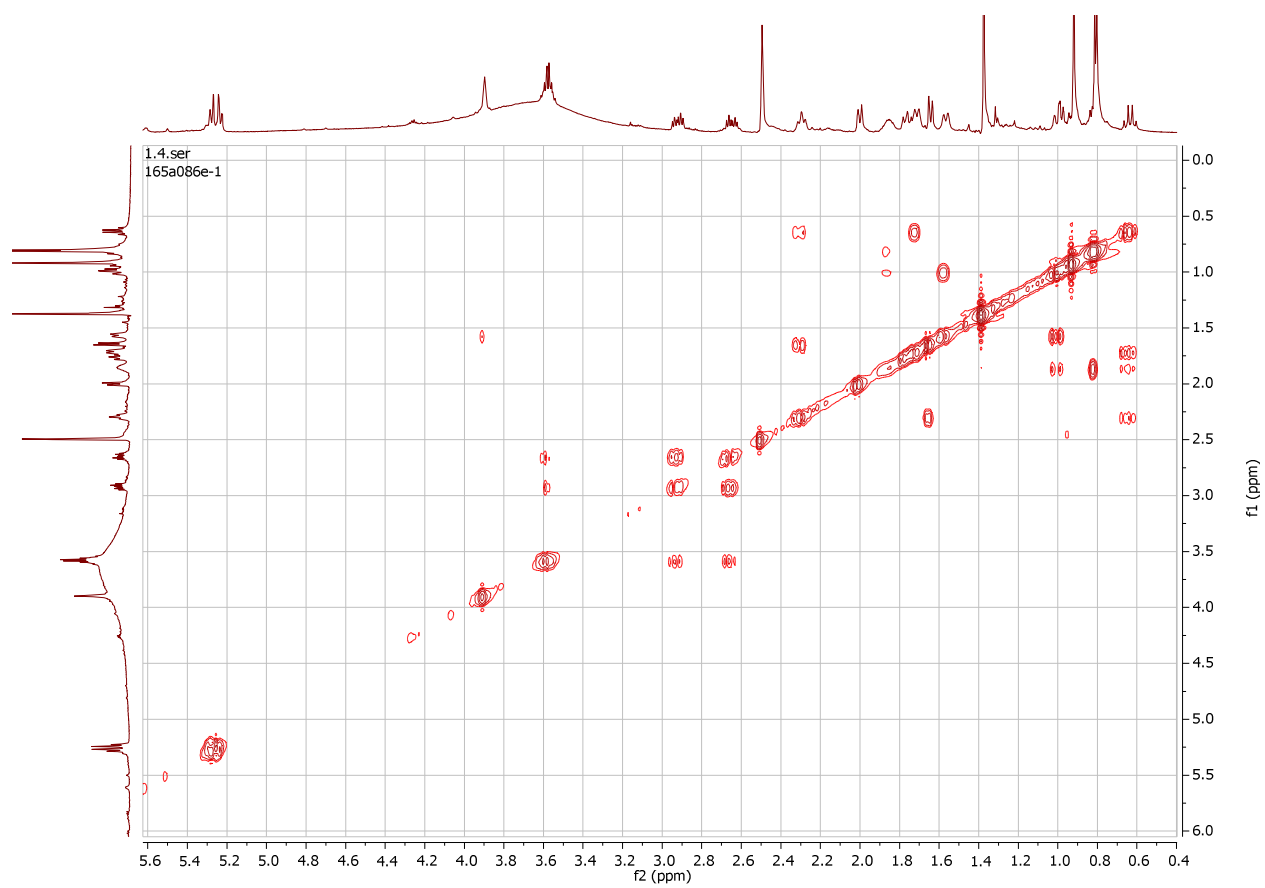
S6. ROESY spectrum of compound **1** in DMSO- $d_6$ .



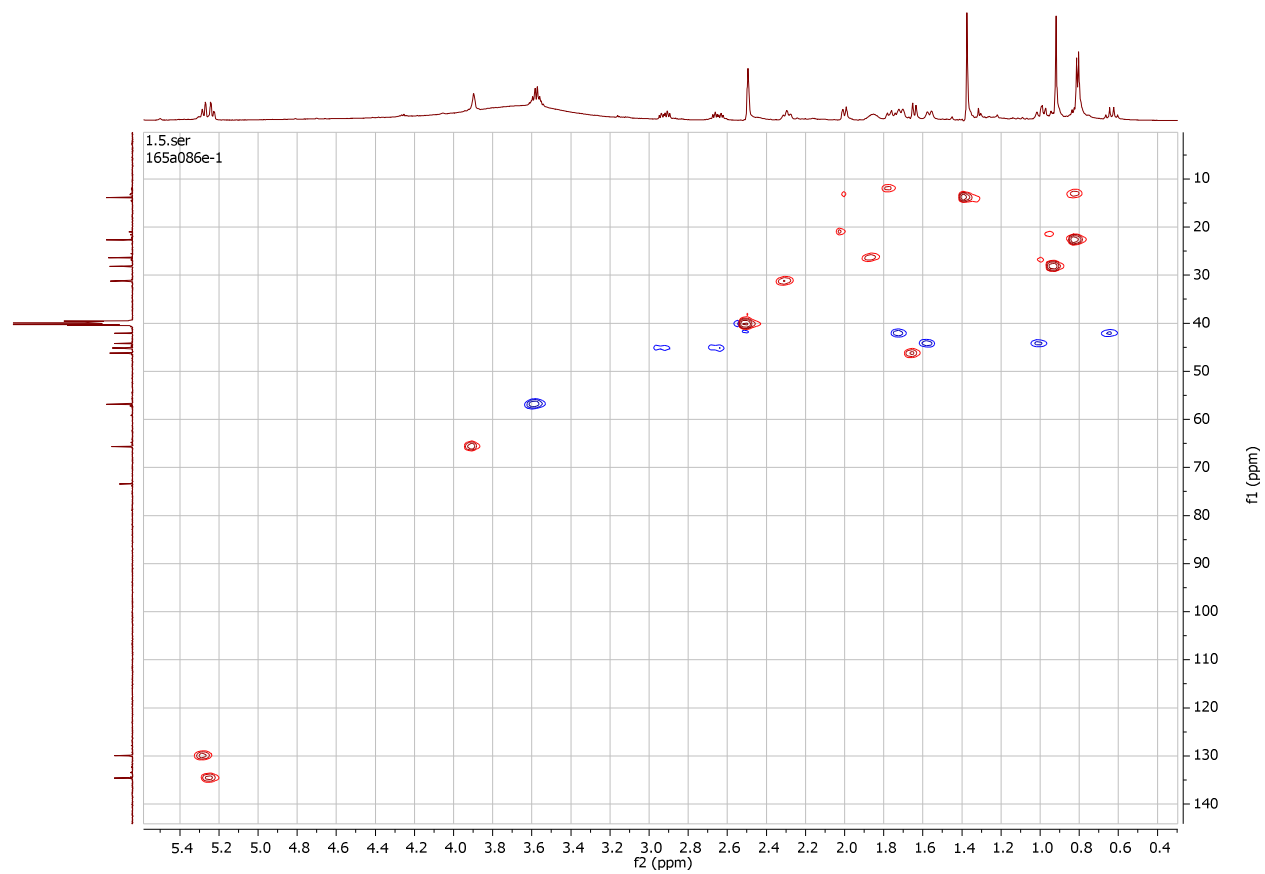
S7.  $^1\text{H}$  NMR spectrum (600 MHz) of compound **3** in  $\text{DMSO}-d_6$ .



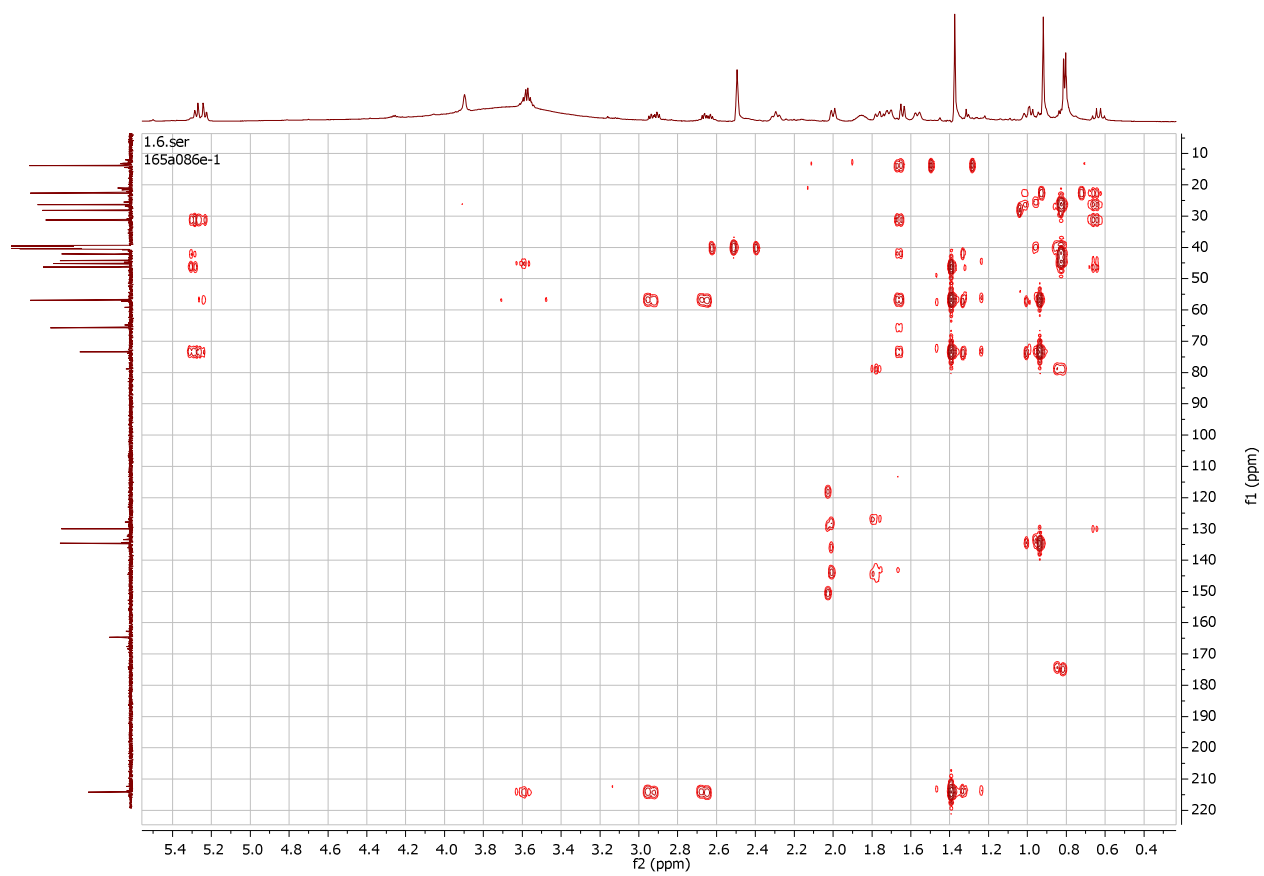
S8.  $^{13}\text{C}$  NMR spectrum (150 MHz) of compound **3** in  $\text{DMSO-}d_6$ .



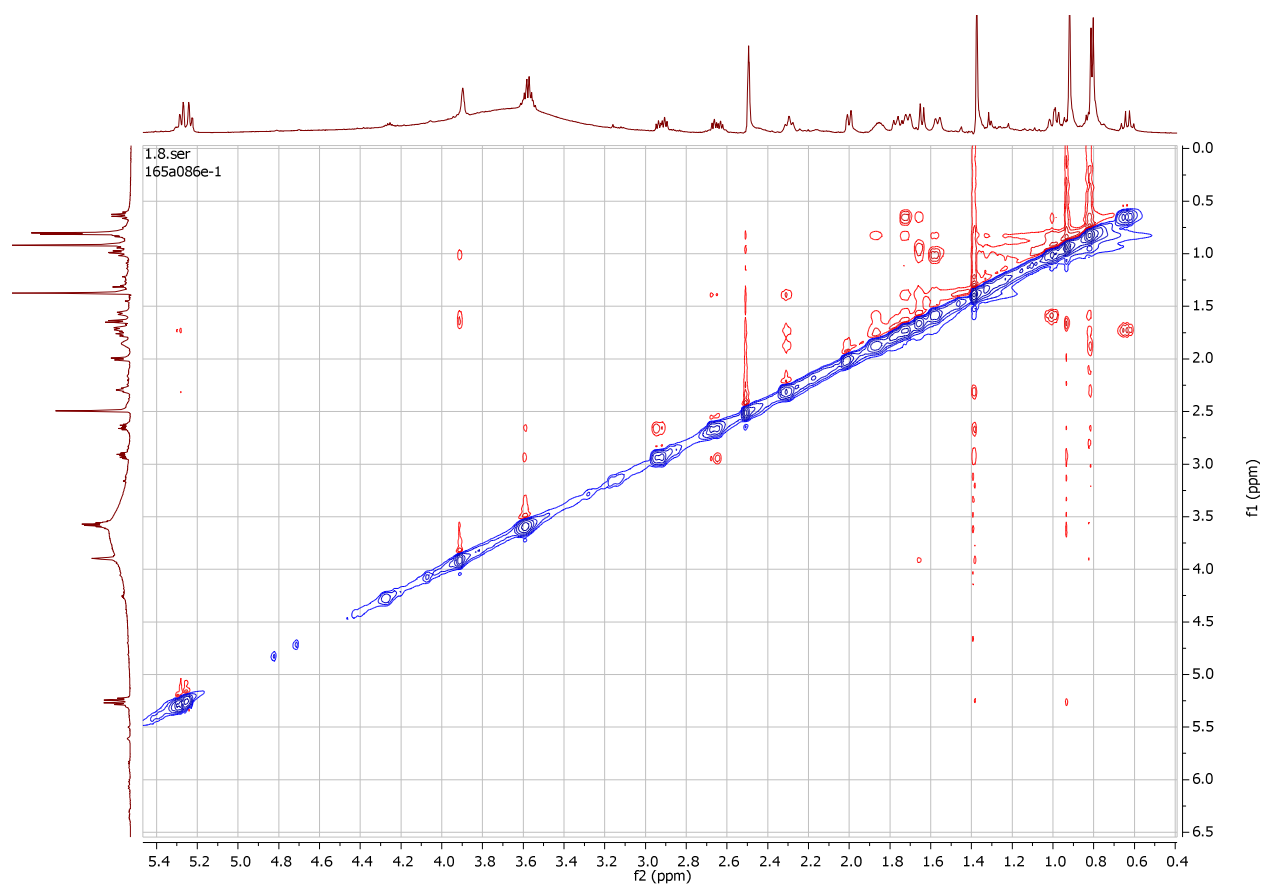
S9. COSY spectrum of compound **3** in DMSO- $d_6$ .



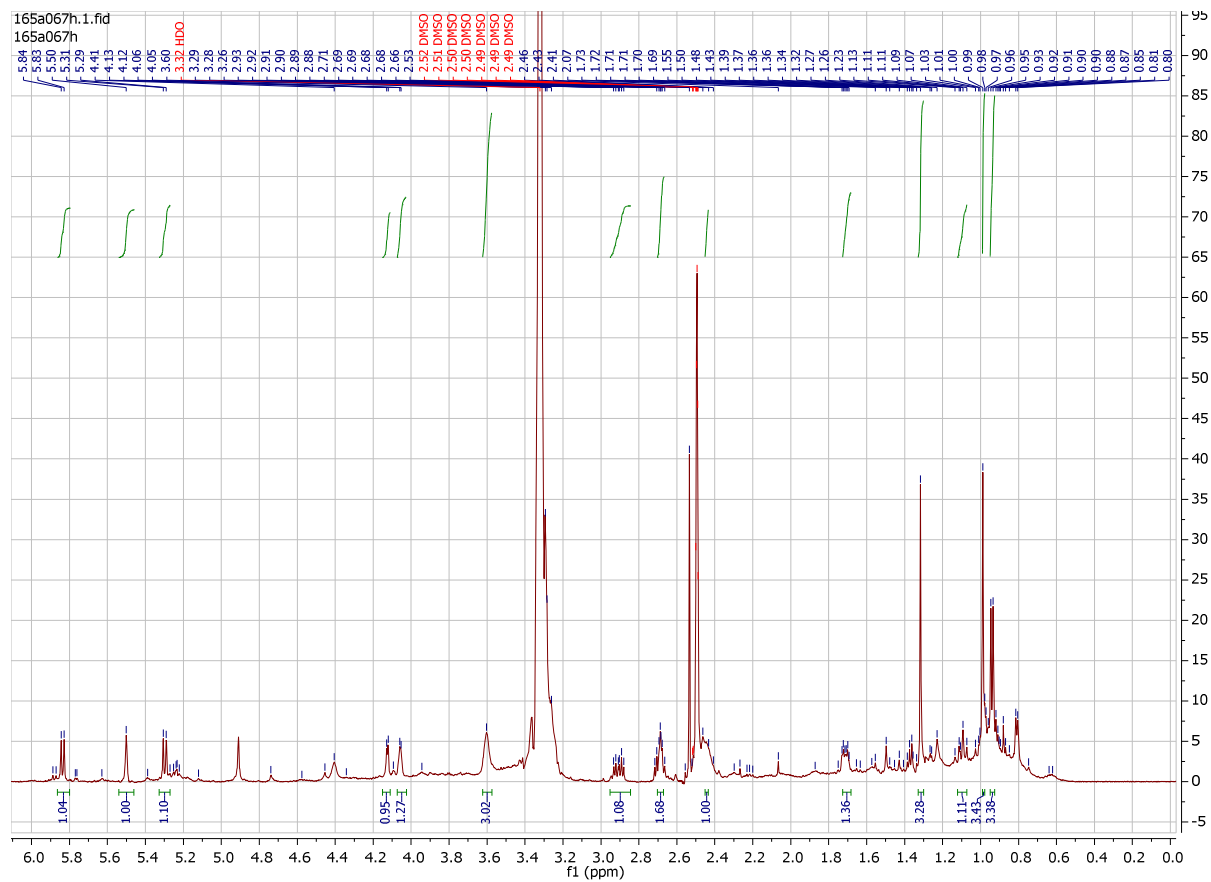
S10. HSQC spectrum of compound **3** in  $\text{DMSO}-d_6$ .



S11. HMBC spectrum of compound **3** in DMSO- $d_6$ .

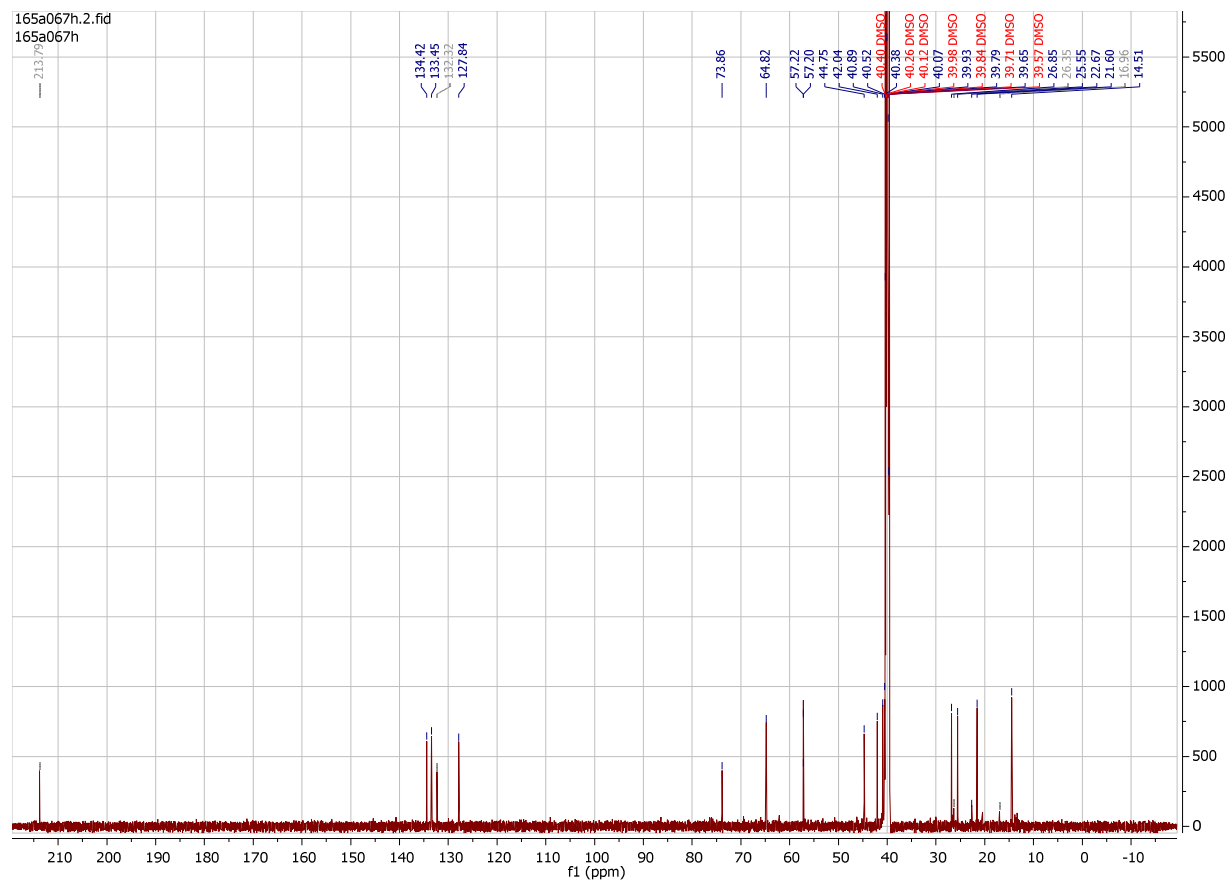


S12. ROESY spectrum of compound **3** in DMSO- $d_6$ .

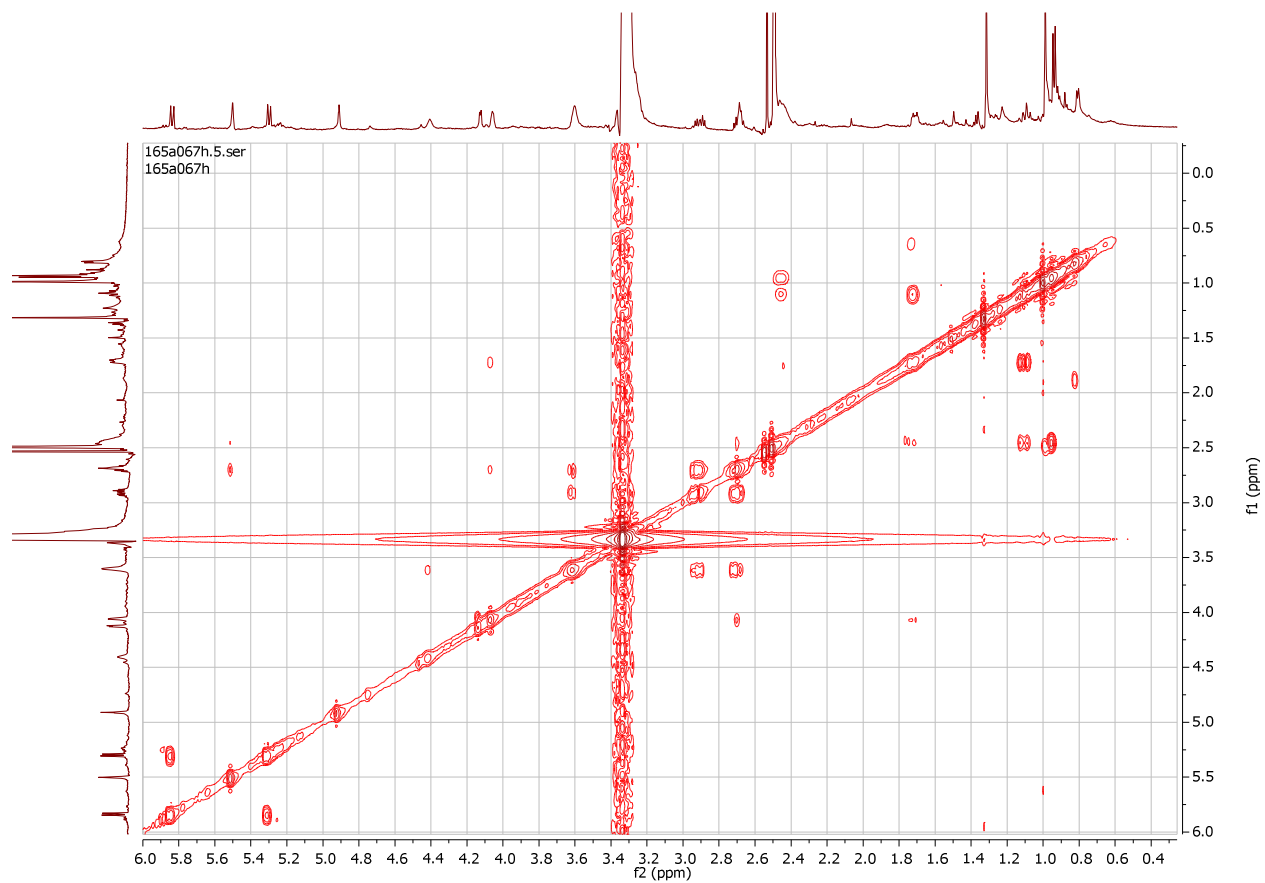


S13.  $^1\text{H}$  NMR spectrum (600 MHz) of compound **4** in  $\text{DMSO}-d_6$ .

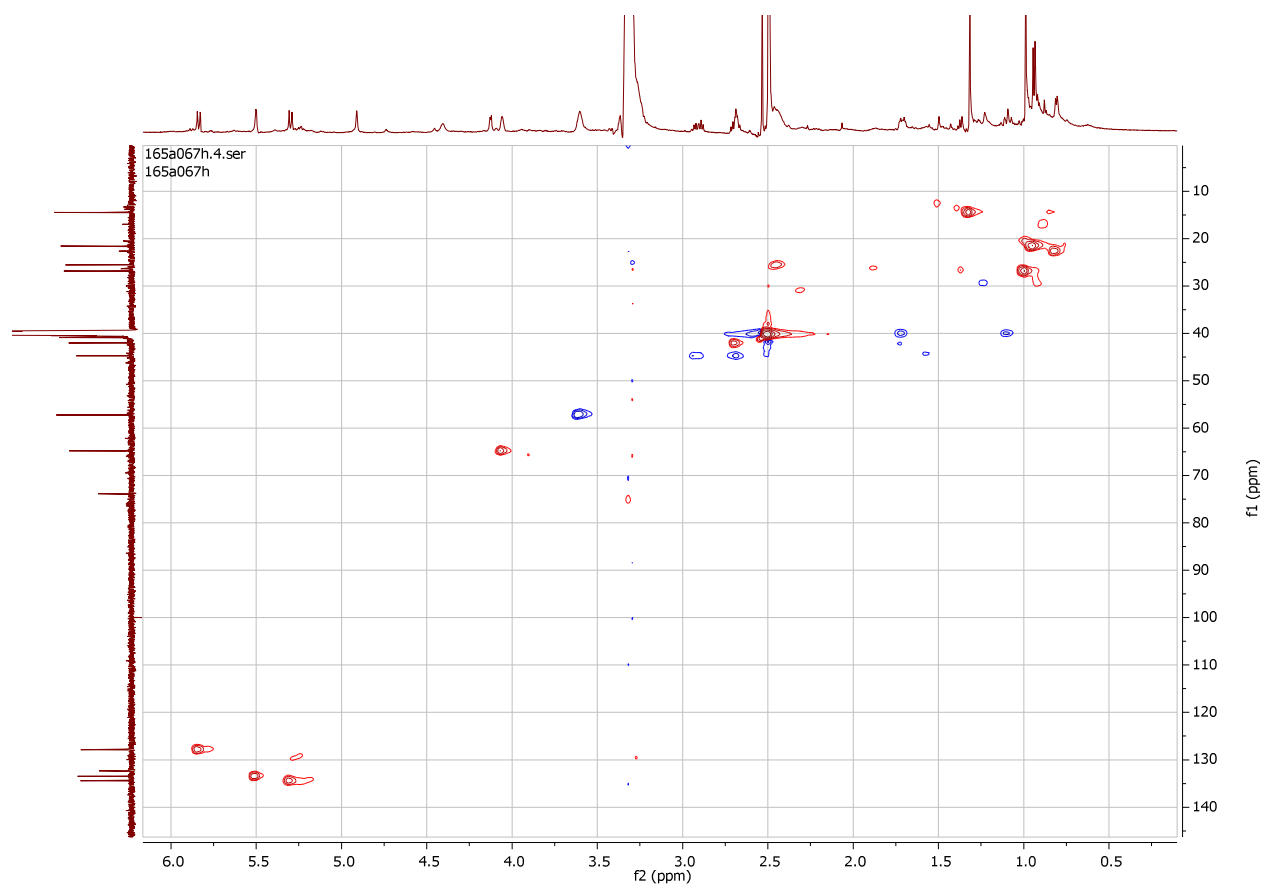




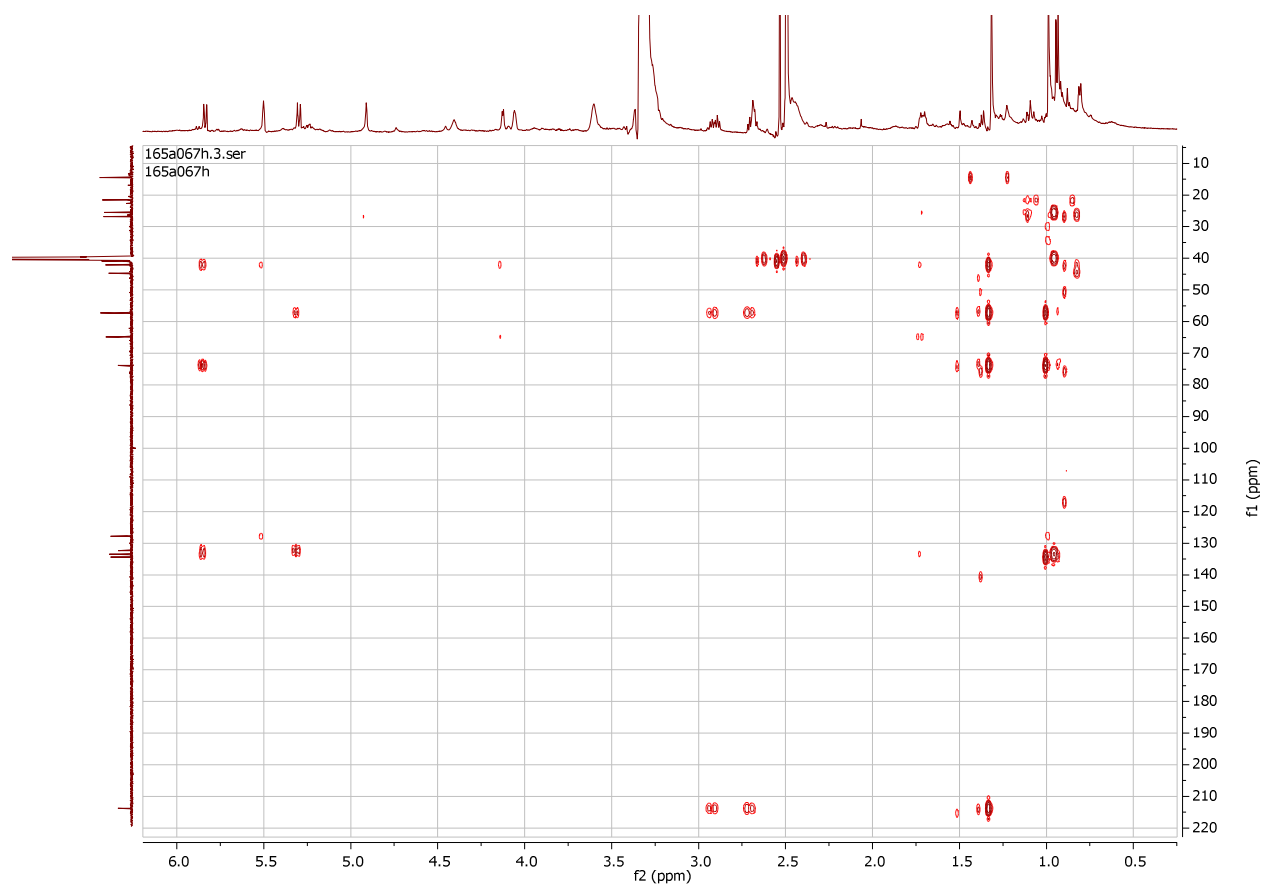
S14.  $^{13}\text{C}$  NMR spectrum (150 MHz) of compound **4** in  $\text{DMSO-}d_6$ .



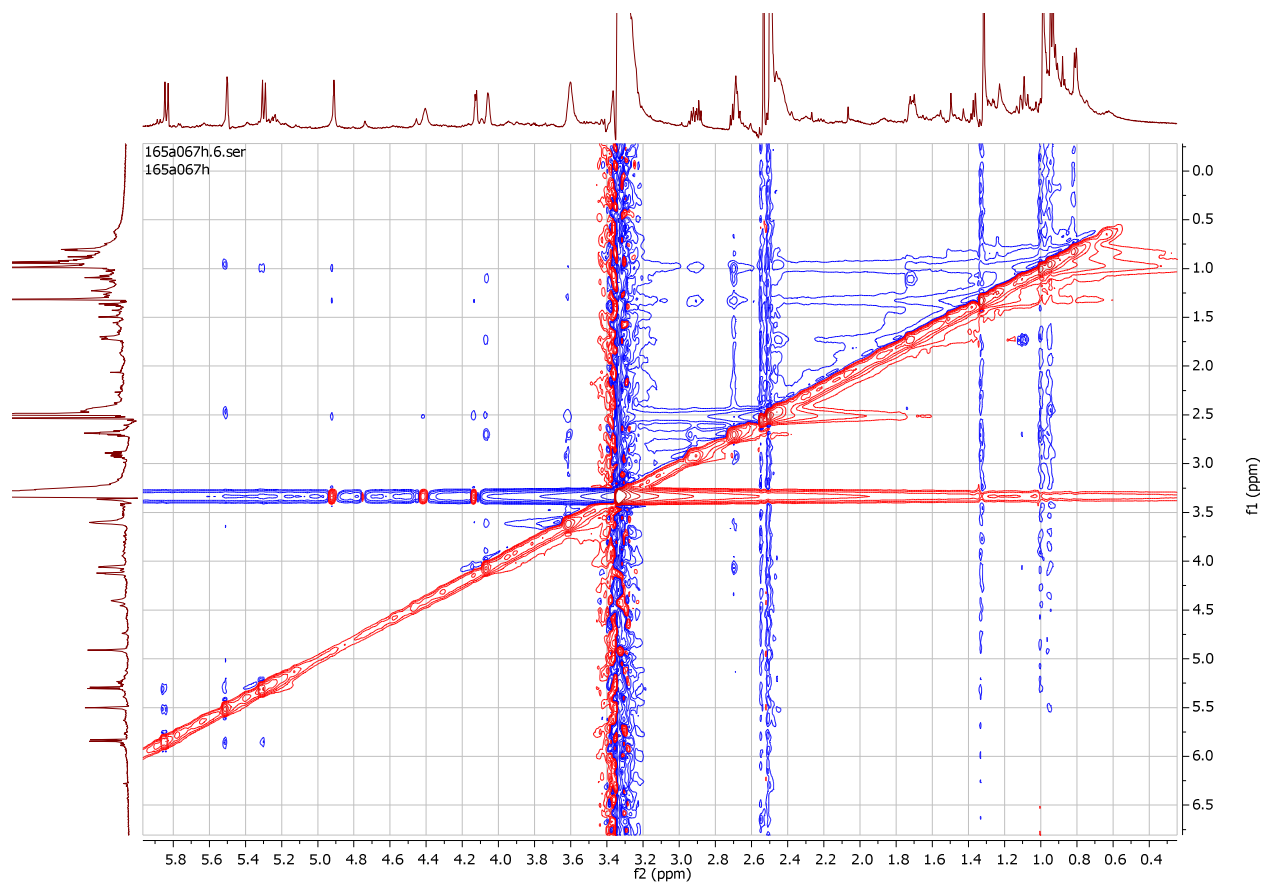
S15. COSY spectrum of compound **4** in DMSO- $d_6$ .



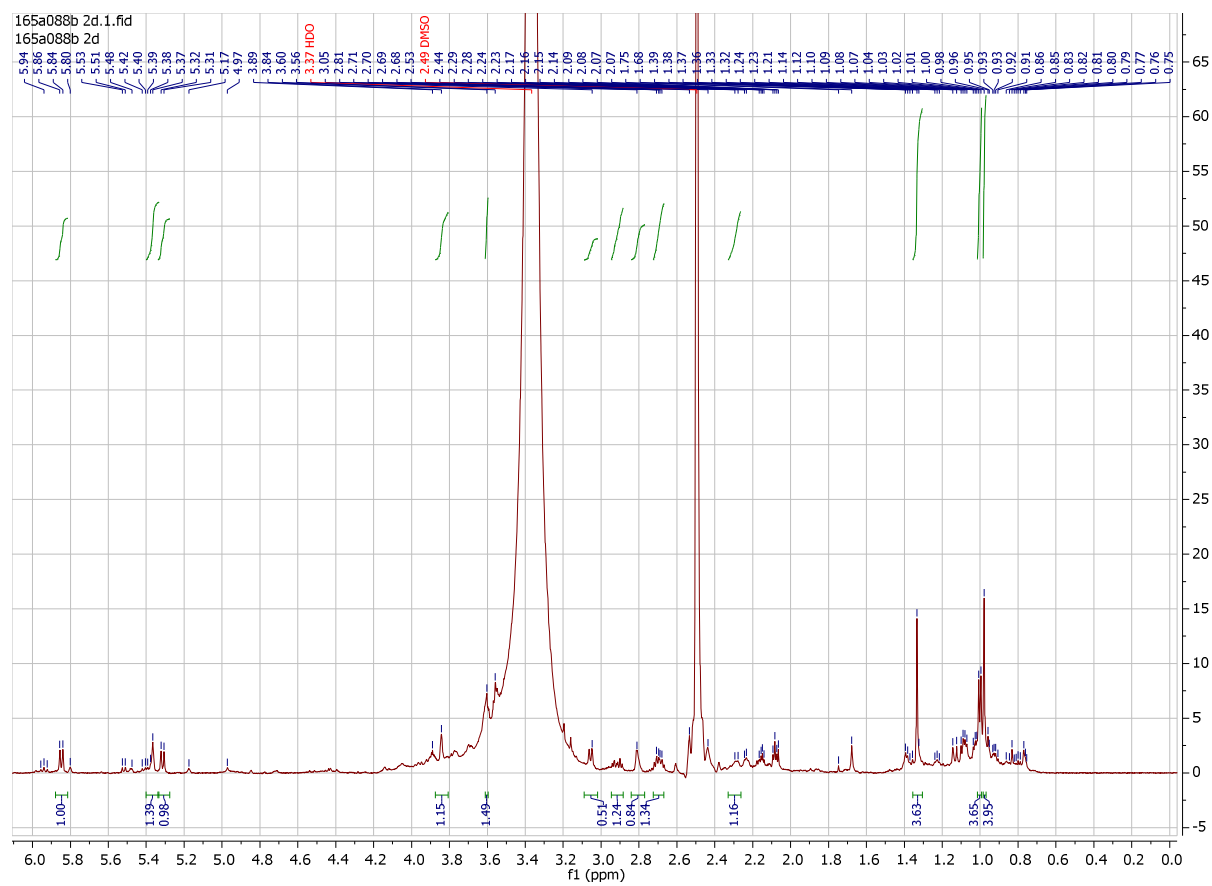
S16. HSQC spectrum of compound **4** in DMSO- $d_6$ .



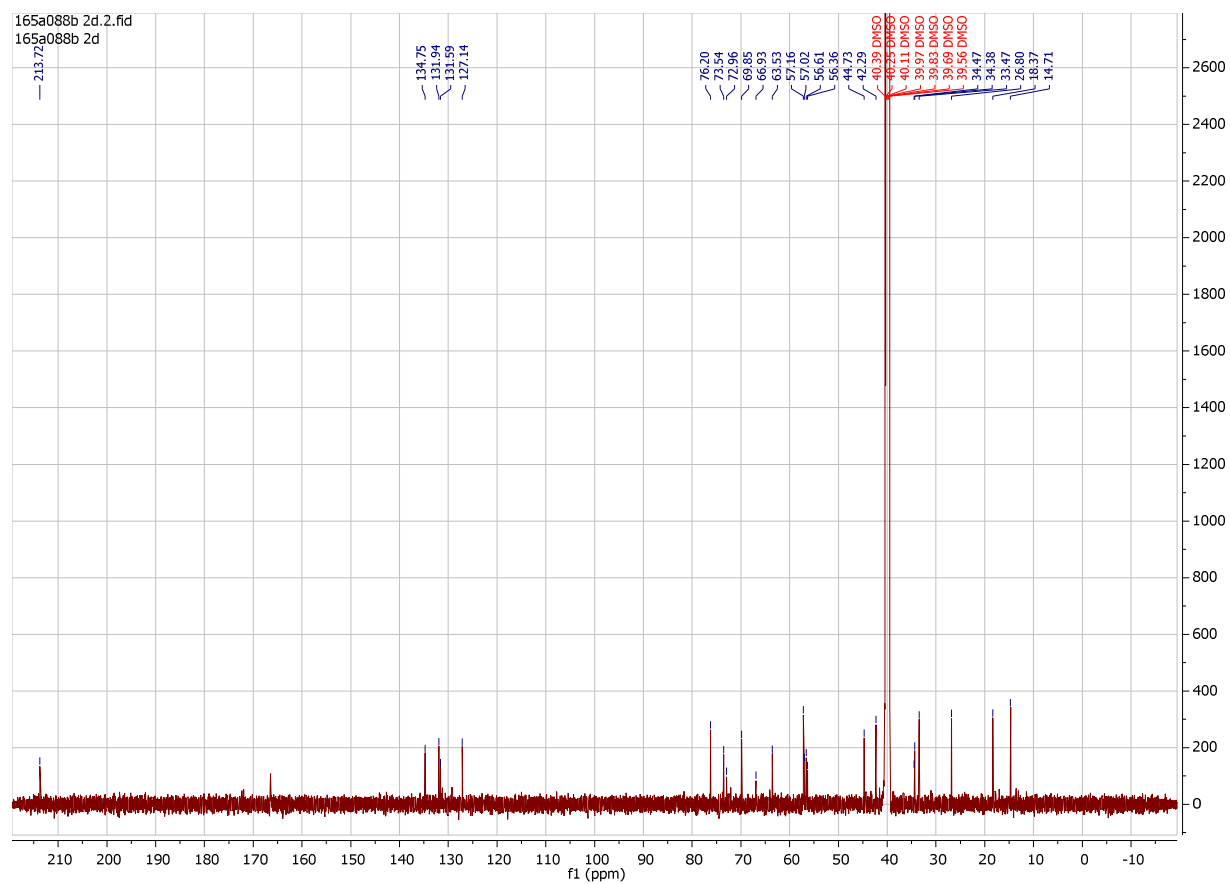
S17. HMBC spectrum of compound **4** in DMSO- $d_6$ .



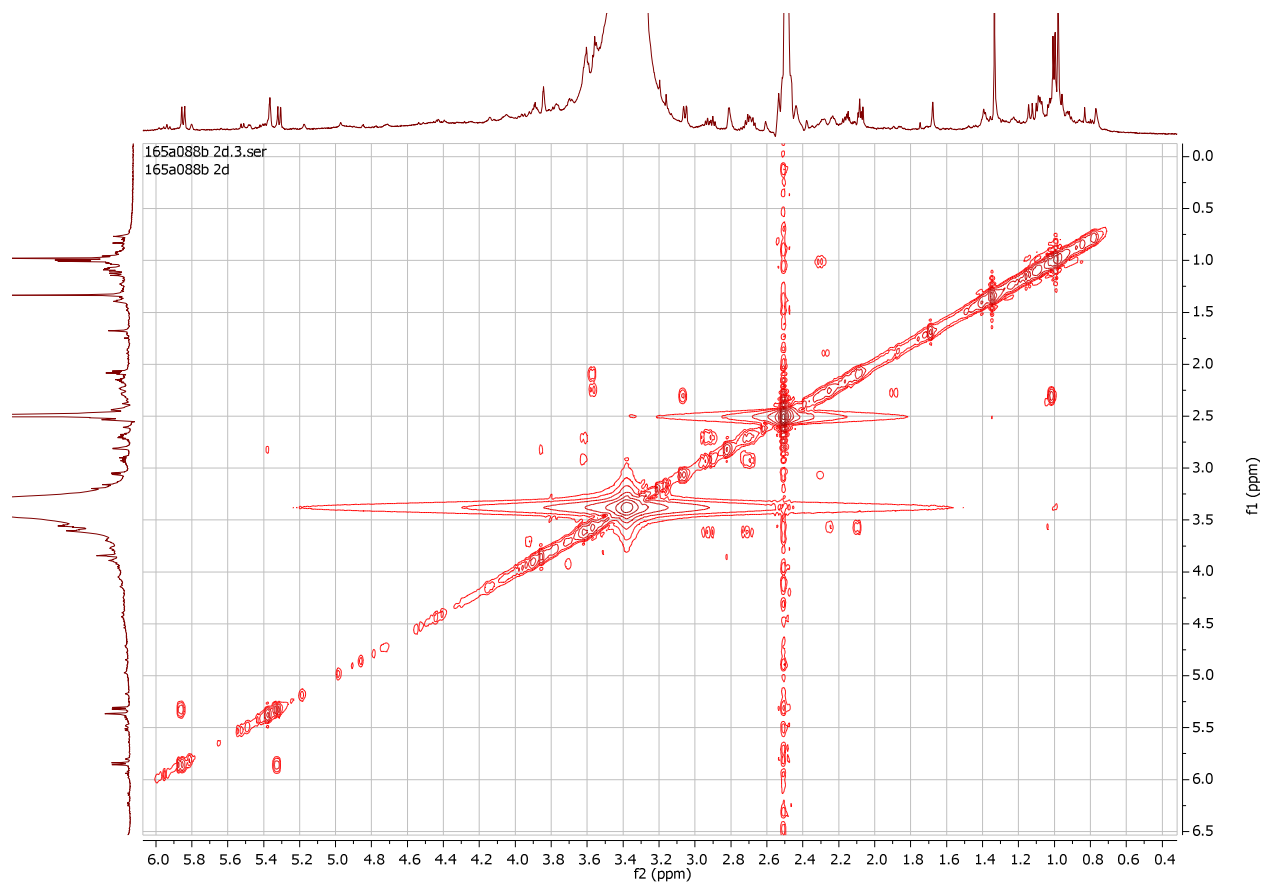
S18. ROESY spectrum of compound **4** in DMSO- $d_6$ .



S19.  $^1\text{H}$  NMR spectrum (600 MHz) of compound **5** in  $\text{DMSO-}d_6$ .

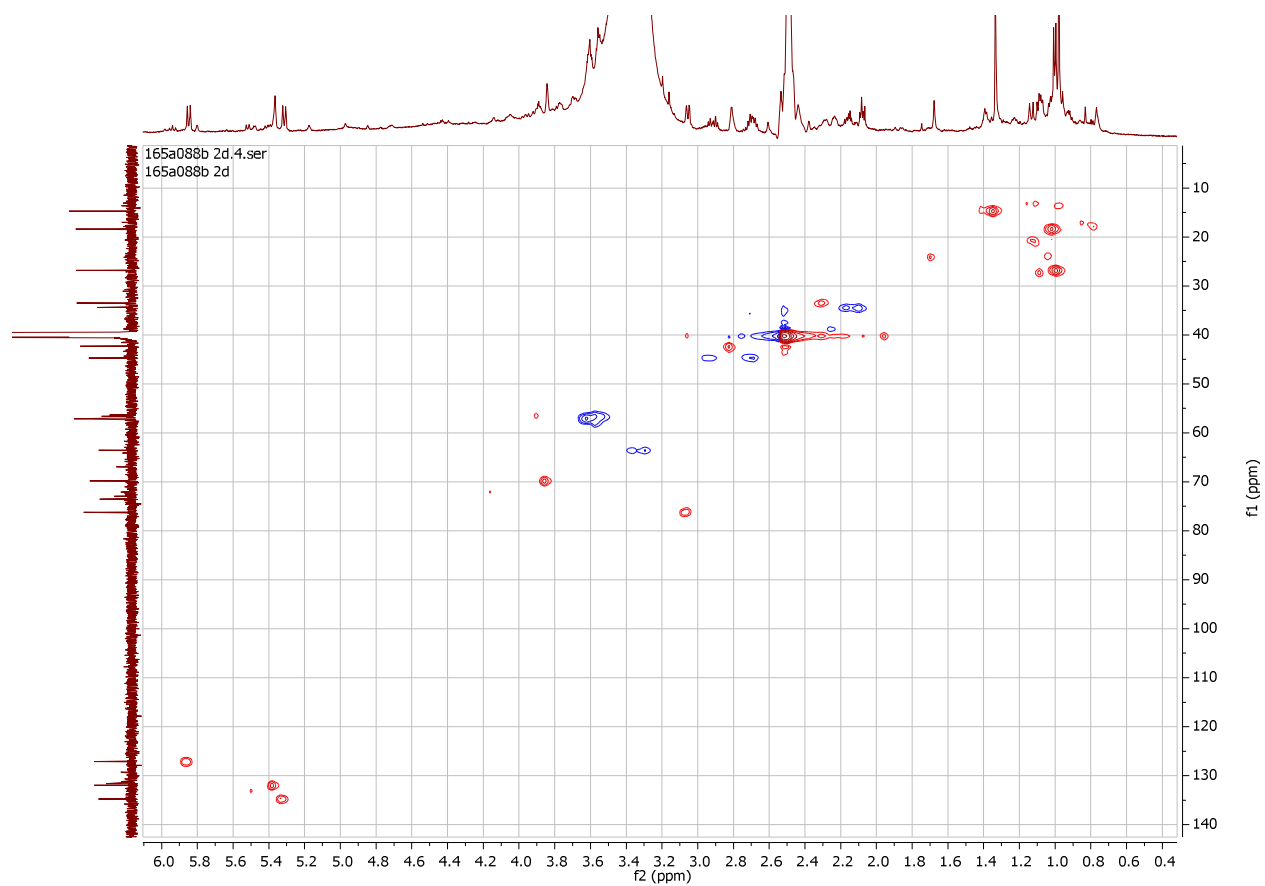


S20.  $^{13}\text{C}$  NMR spectrum (150 MHz) of compound **5** in  $\text{DMSO}-d_6$ .



S21. COSY spectrum of compound **5** in DMSO- $d_6$ .

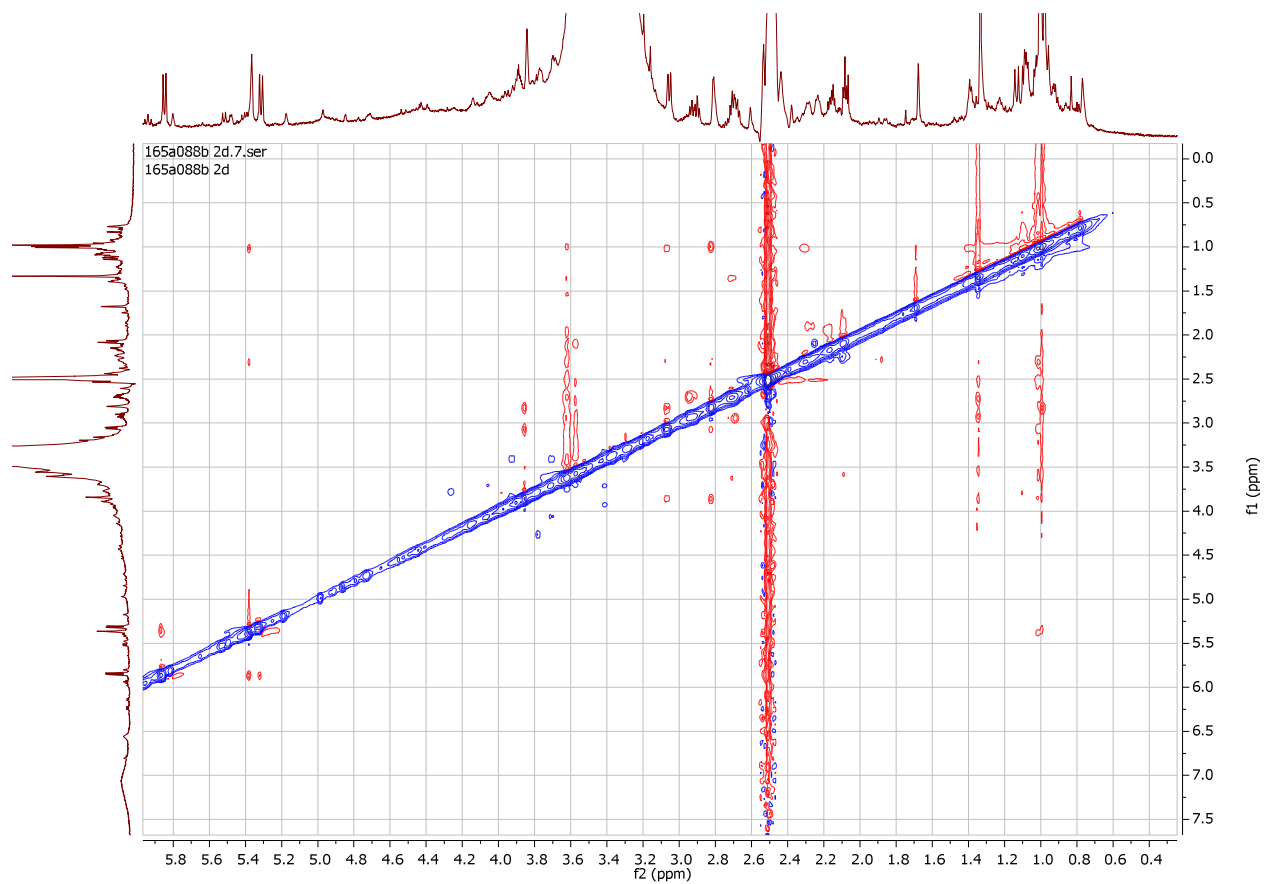




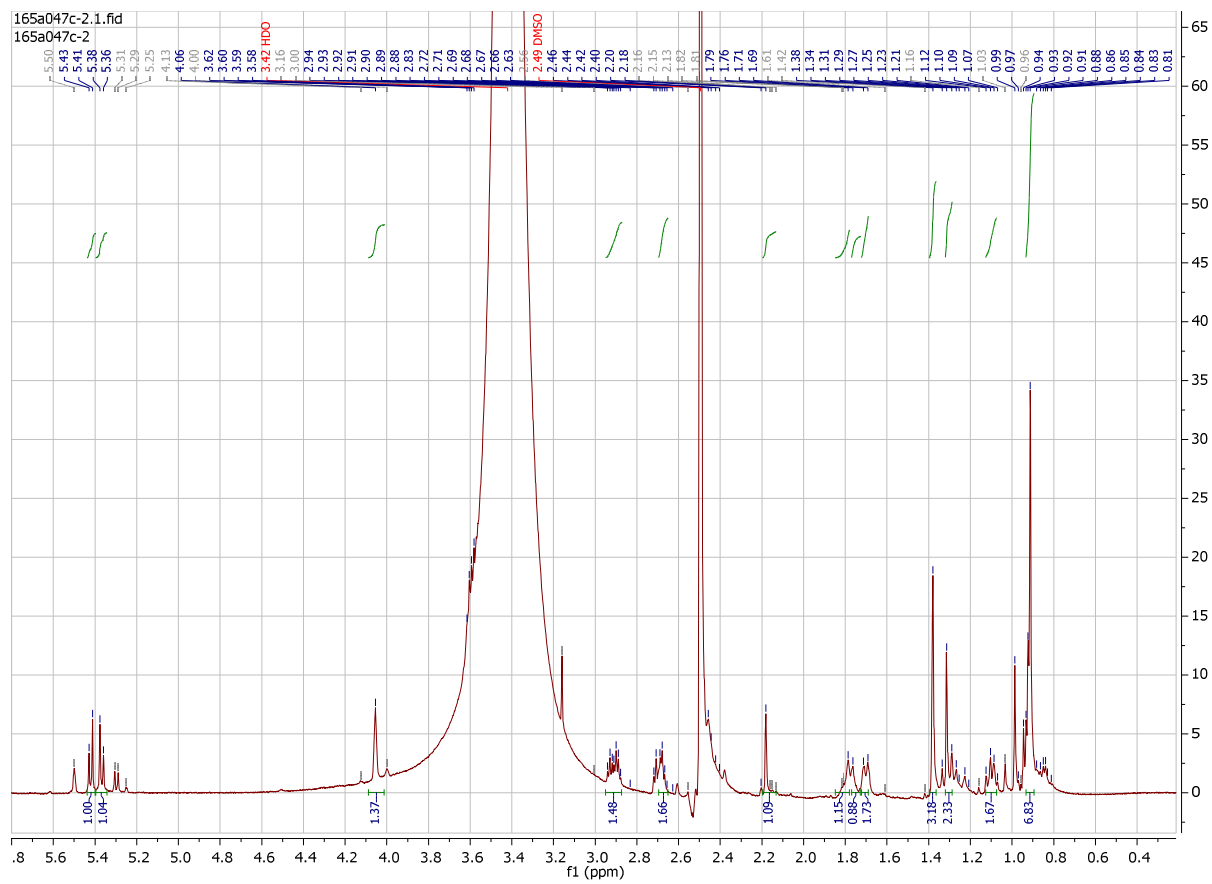
S22. HSQC spectrum of compound **5** in DMSO- $d_6$ .



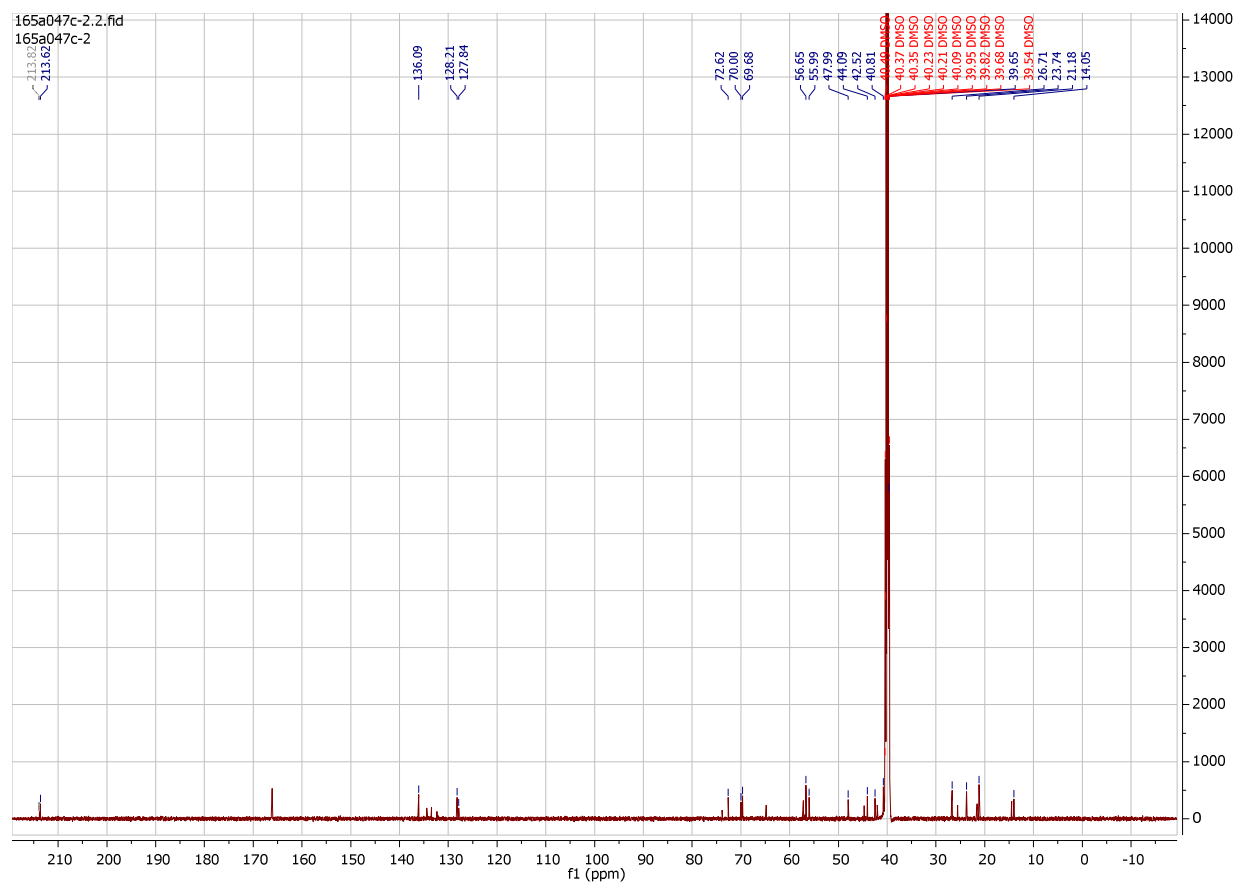
S23. HMBC spectrum of compound **5** in DMSO- $d_6$ .



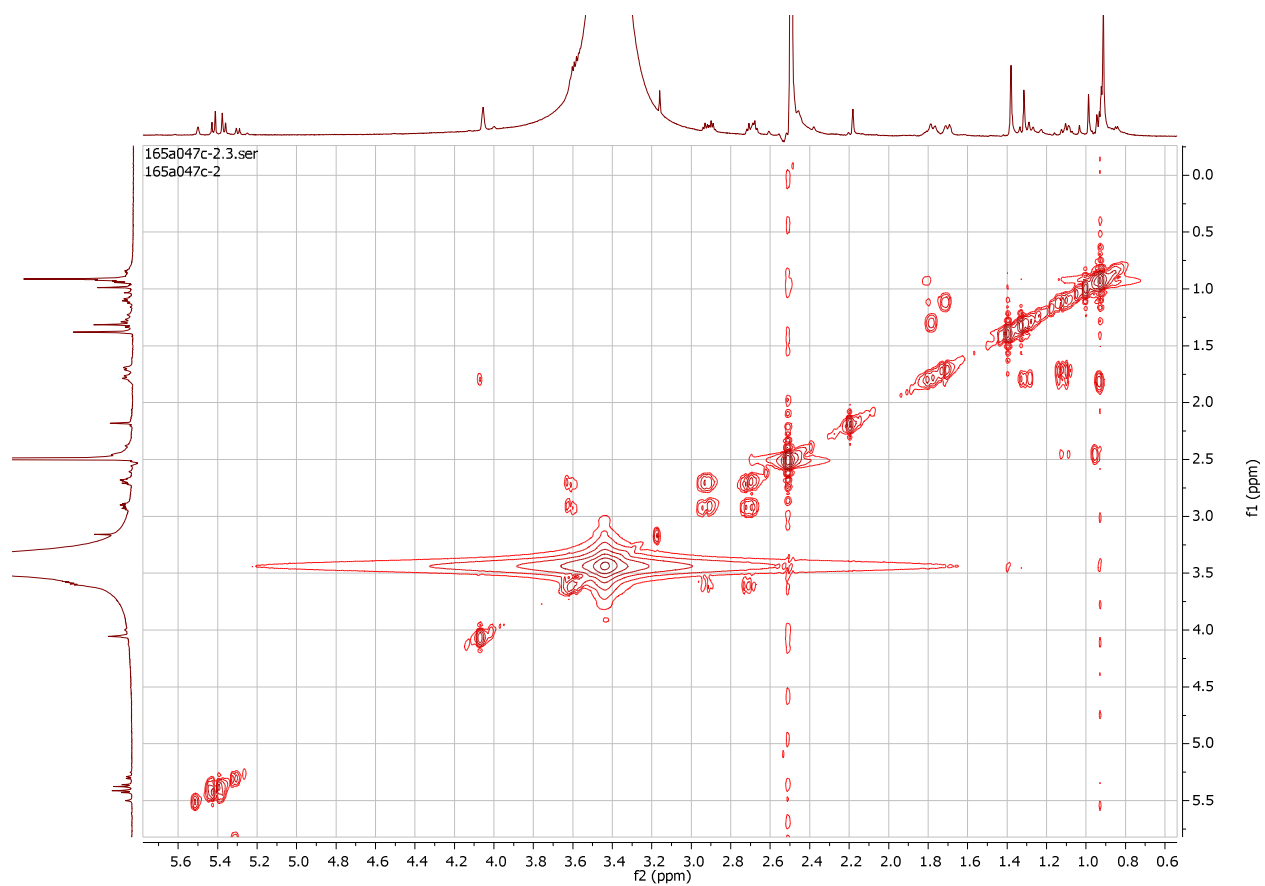
S24. ROESY spectrum of compound **5** in DMSO- $d_6$ .



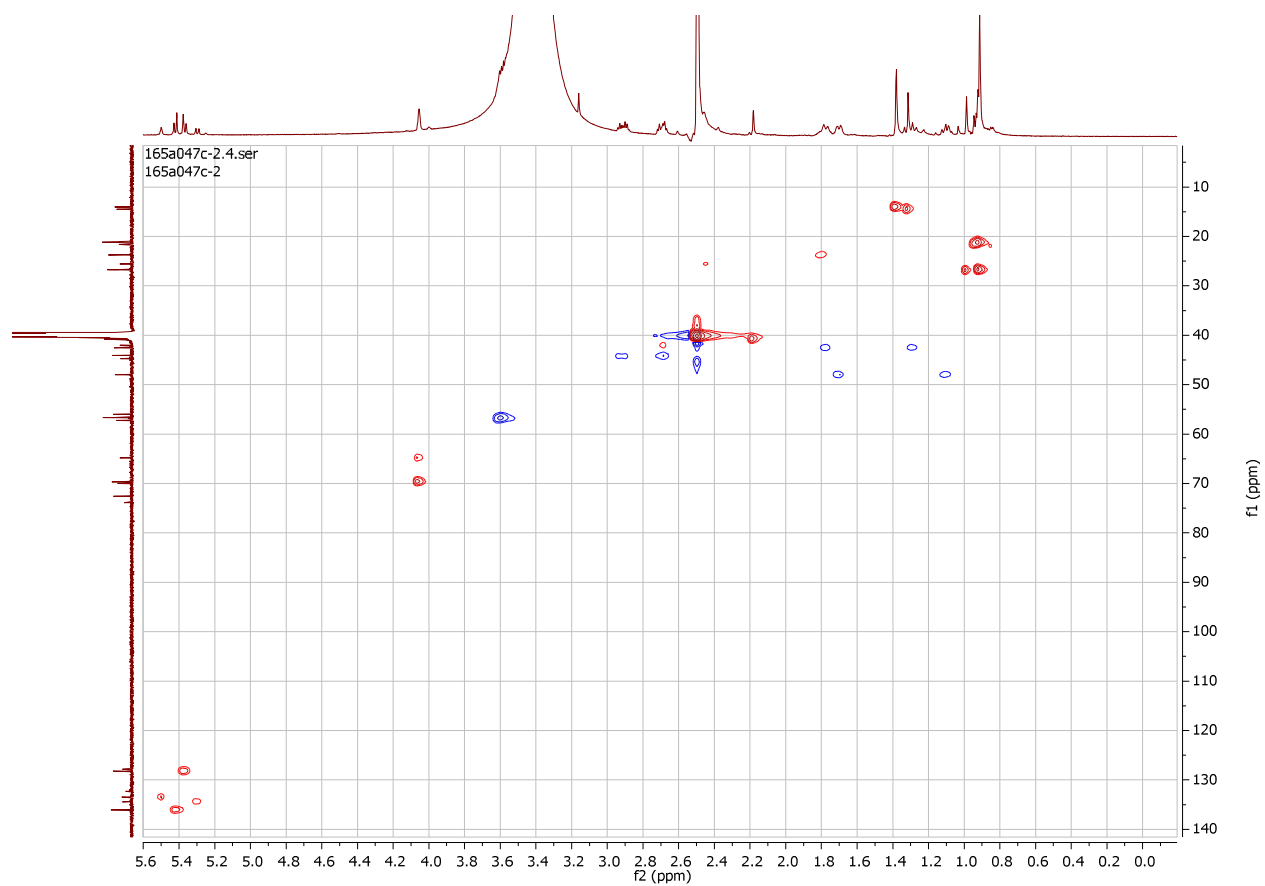
S25.  $^1\text{H}$  NMR spectrum (600 MHz) of compound **6** in  $\text{DMSO}-d_6$ .



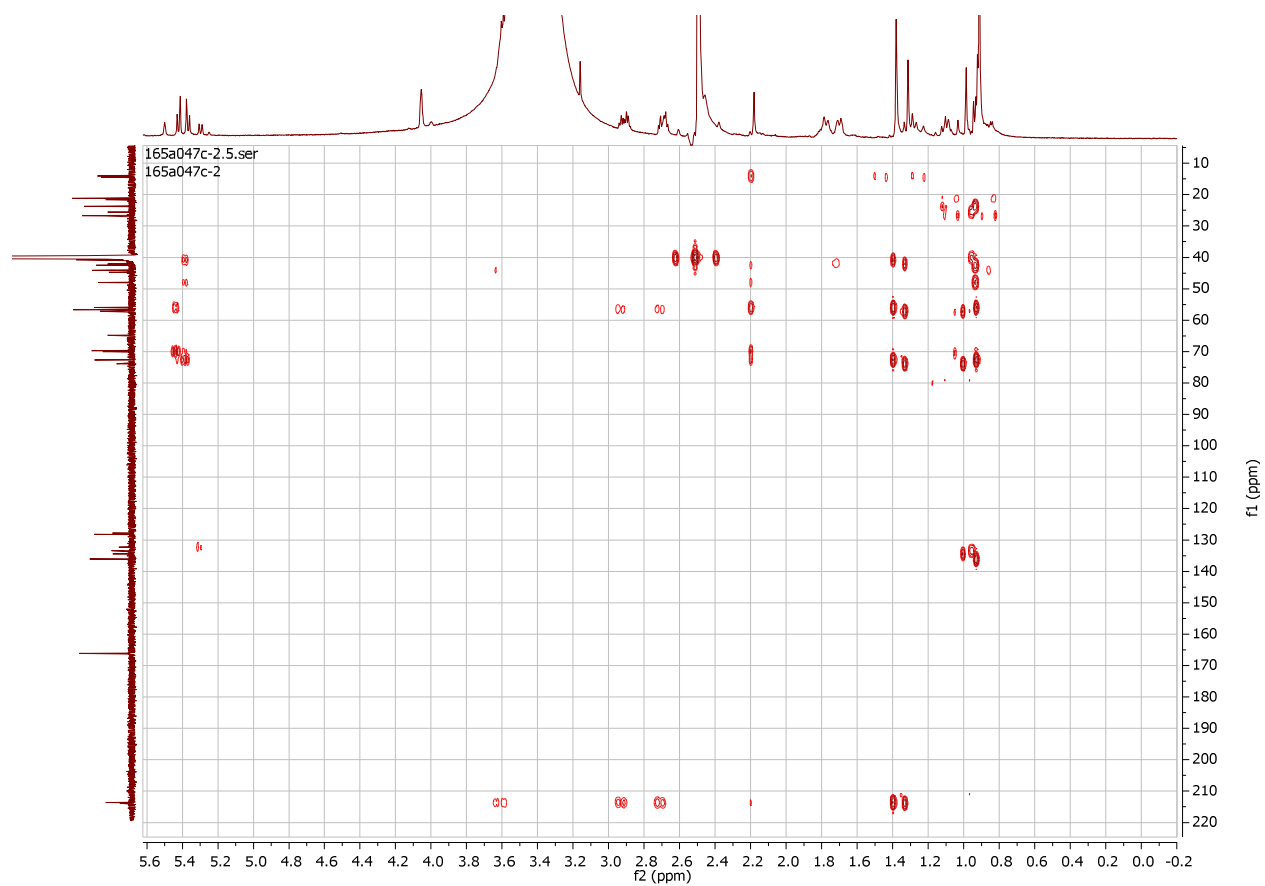
S26.  $^{13}\text{C}$  NMR spectrum (150 MHz) of compound **6** in  $\text{DMSO}-d_6$ .



S27. COSY spectrum of compound **6** in DMSO- $d_6$ .

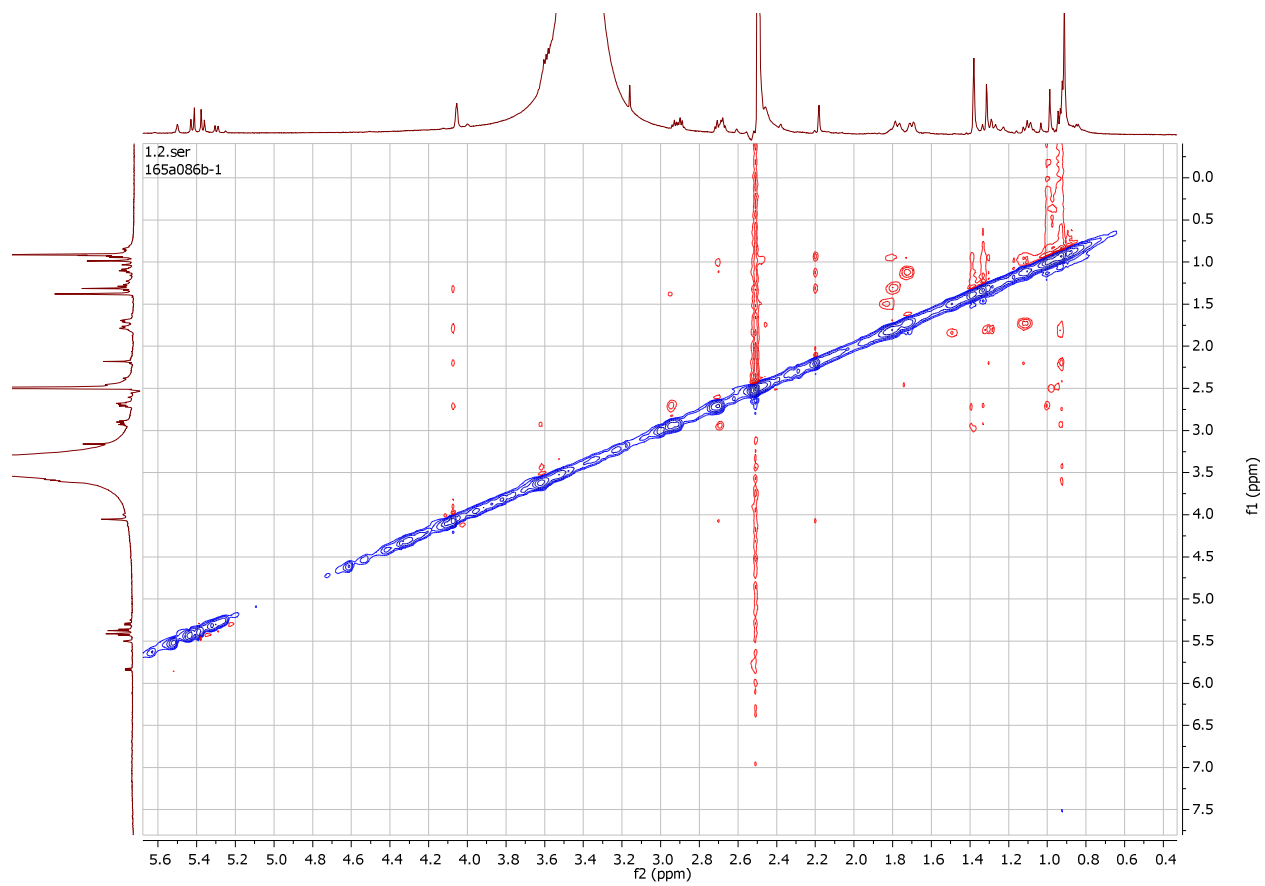


S28. HSQC spectrum of compound **6** in DMSO- $d_6$ .

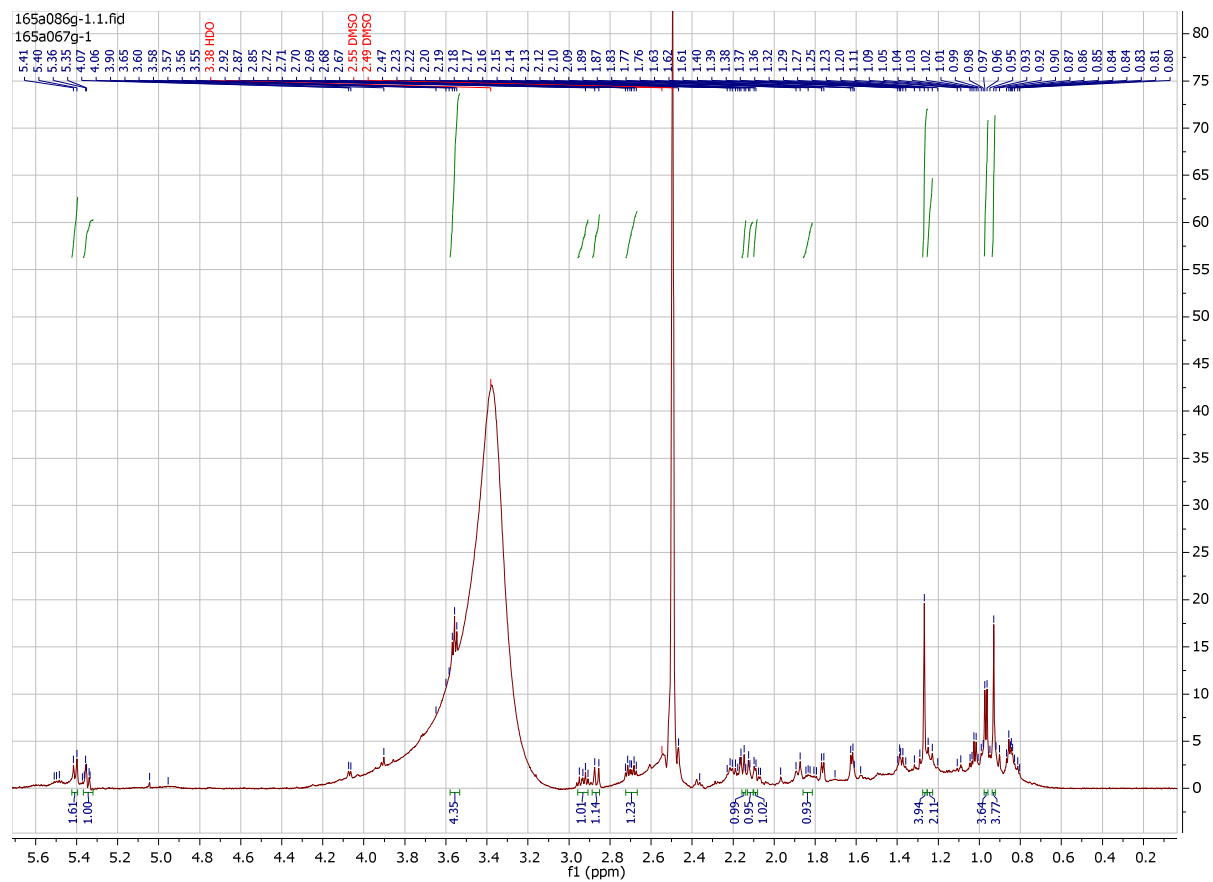


S29. HMBC spectrum of compound **6** in DMSO- $d_6$ .

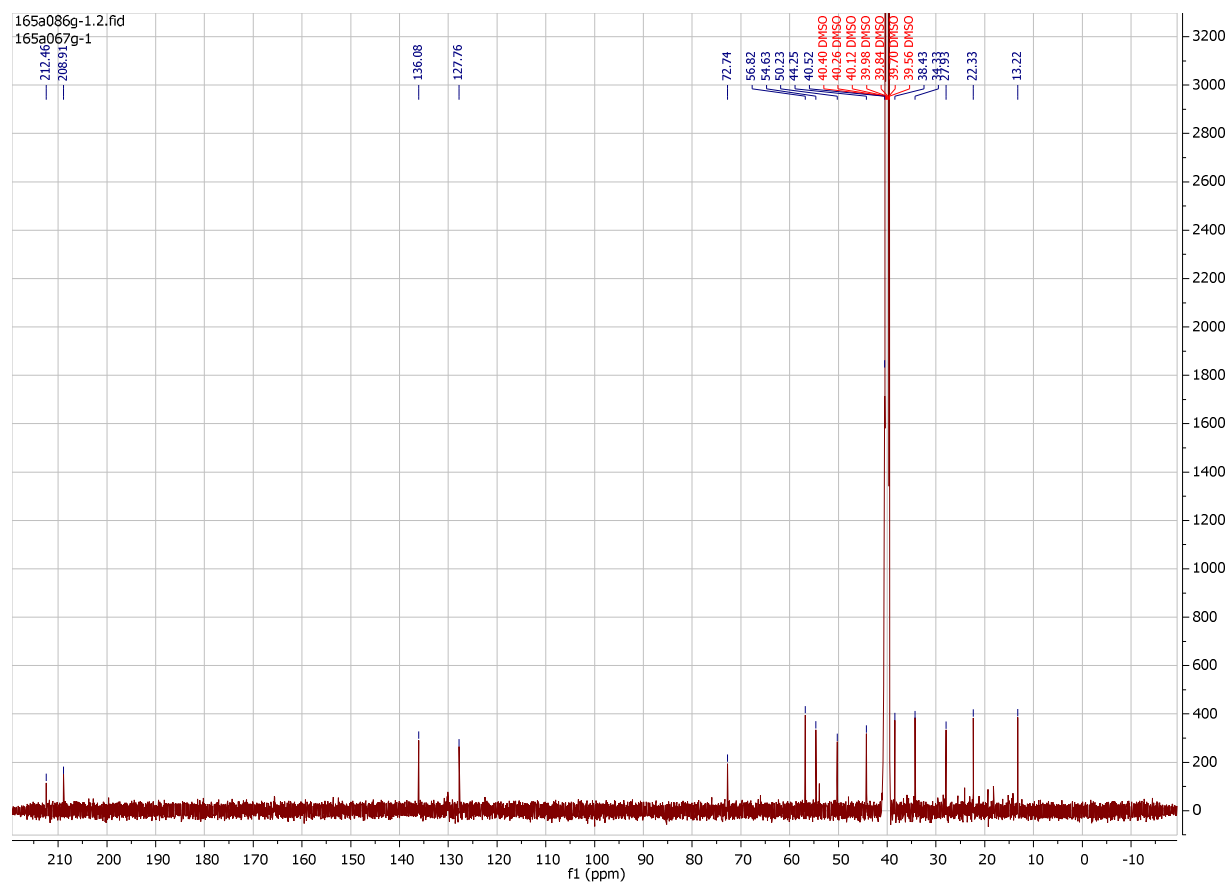




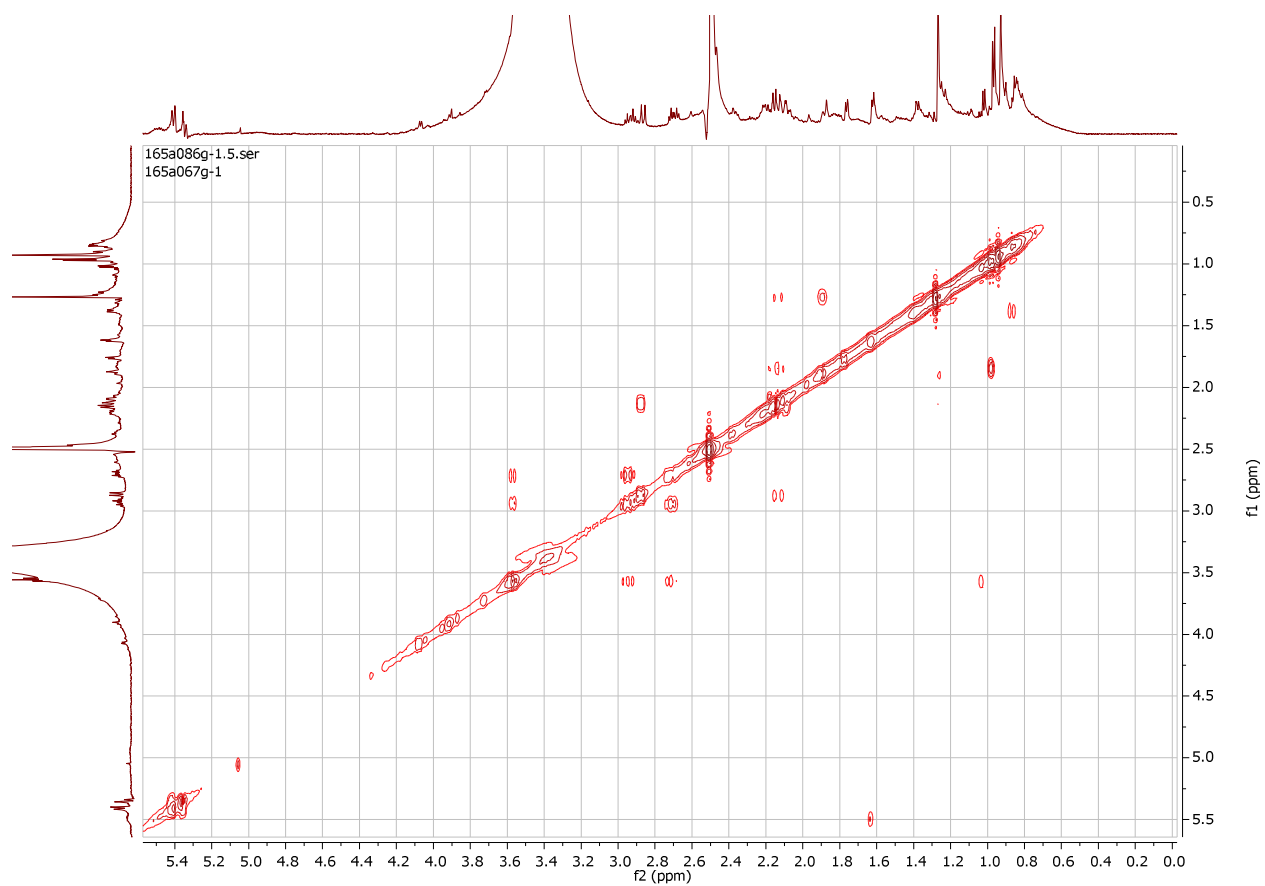
S30. ROESY spectrum of compound **6** in DMSO- $d_6$ .



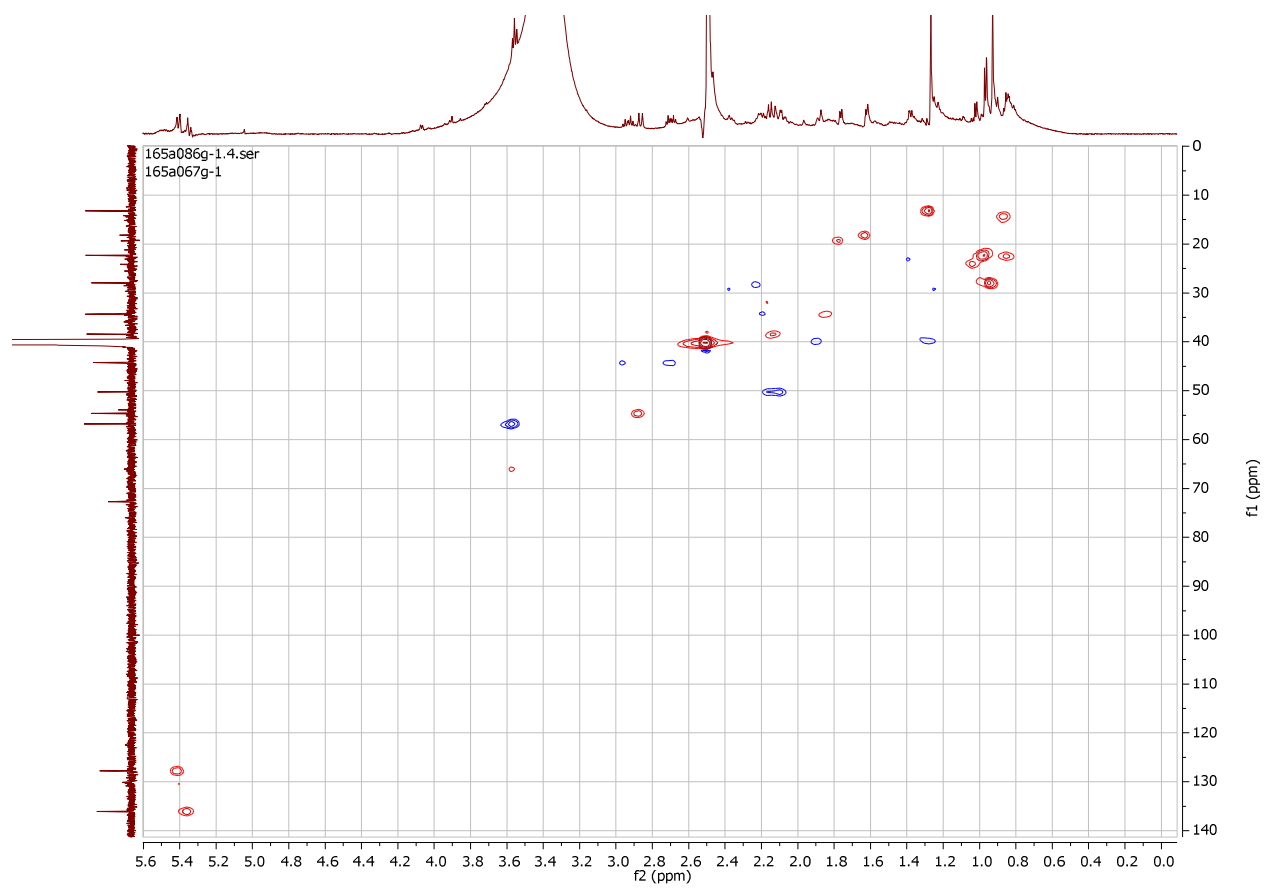
S31.  $^1\text{H}$  NMR spectrum (600 MHz) of compound **7** in  $\text{DMSO}-d_6$ .



S32.  $^{13}\text{C}$  NMR spectrum (150 MHz) of compound **7** in  $\text{DMSO-}d_6$ .



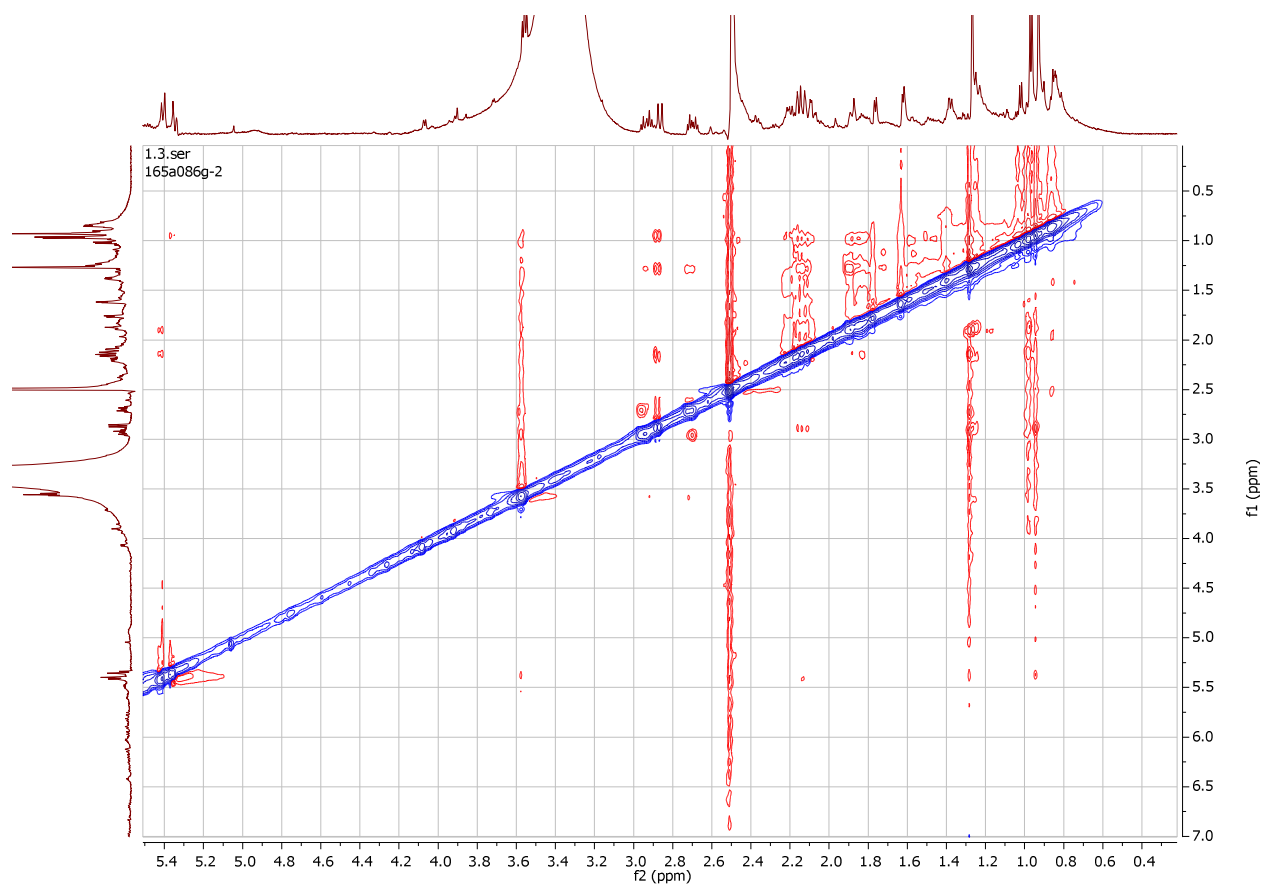
S33. COSY spectrum of compound **7** in DMSO- $d_6$ .



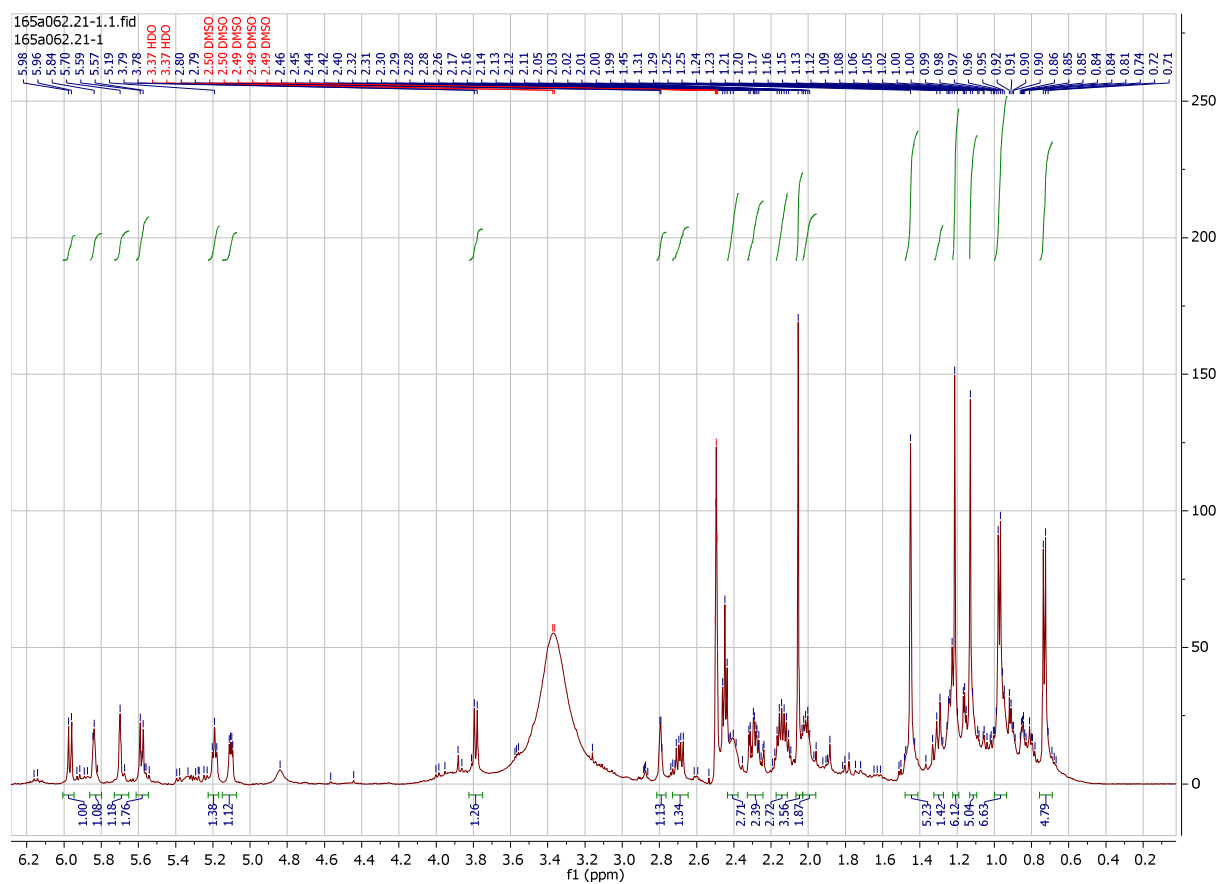
S34. HSQC spectrum of compound **7** in DMSO- $d_6$ .



S35. HMBC spectrum of compound **7** in DMSO-*d*<sub>6</sub>.

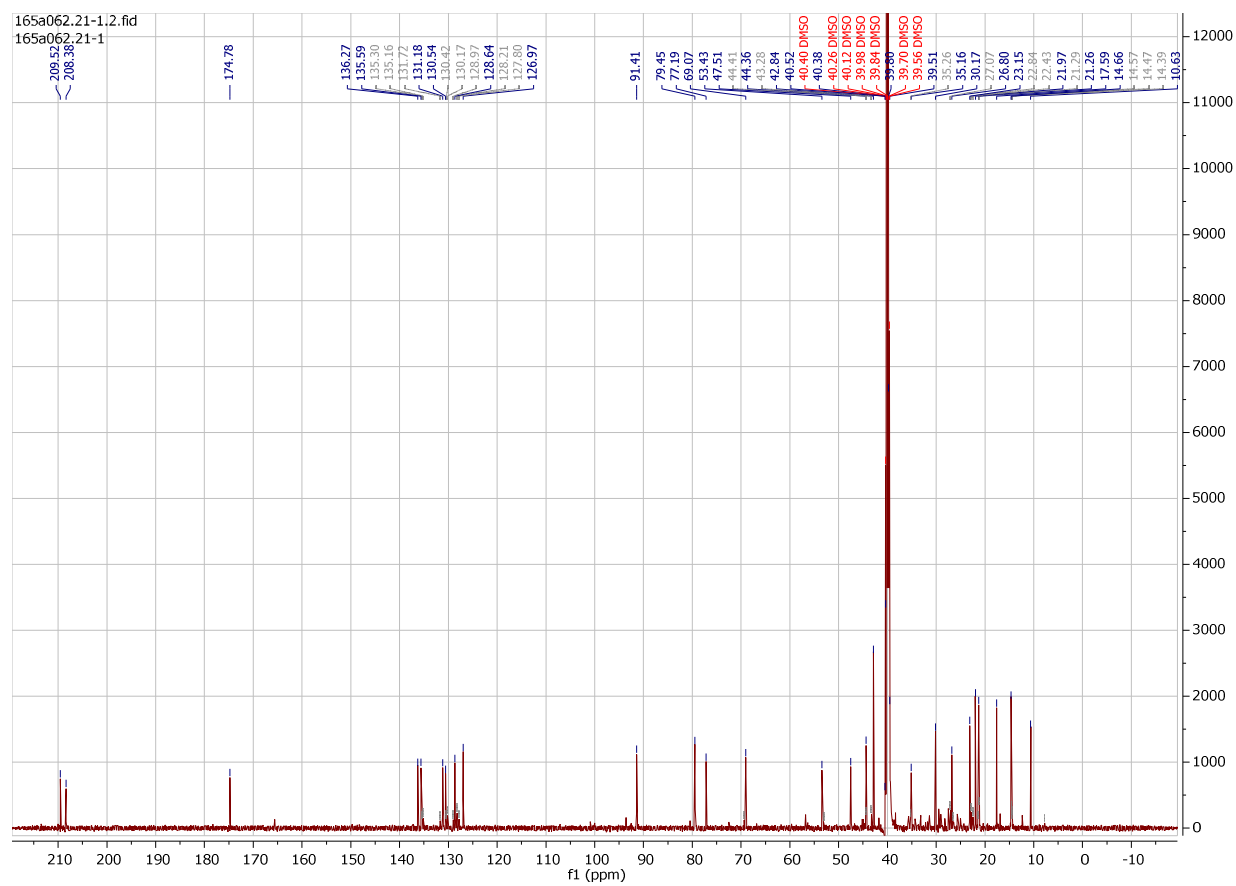


S36. ROESY spectrum of compound **7** in DMSO- $d_6$ .

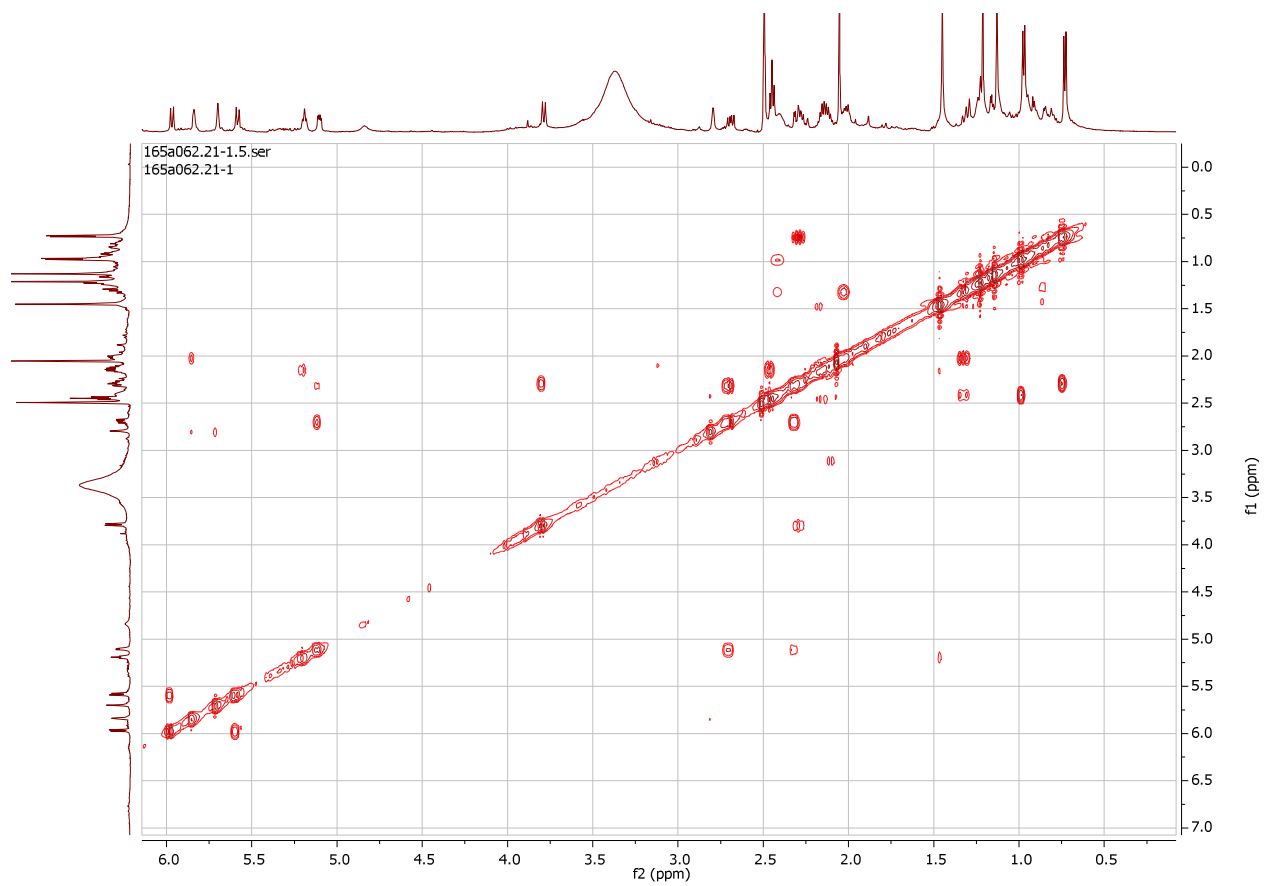


S37.  $^1\text{H}$  NMR spectrum (600 MHz) of compound **8** in  $\text{DMSO}-d_6$ .

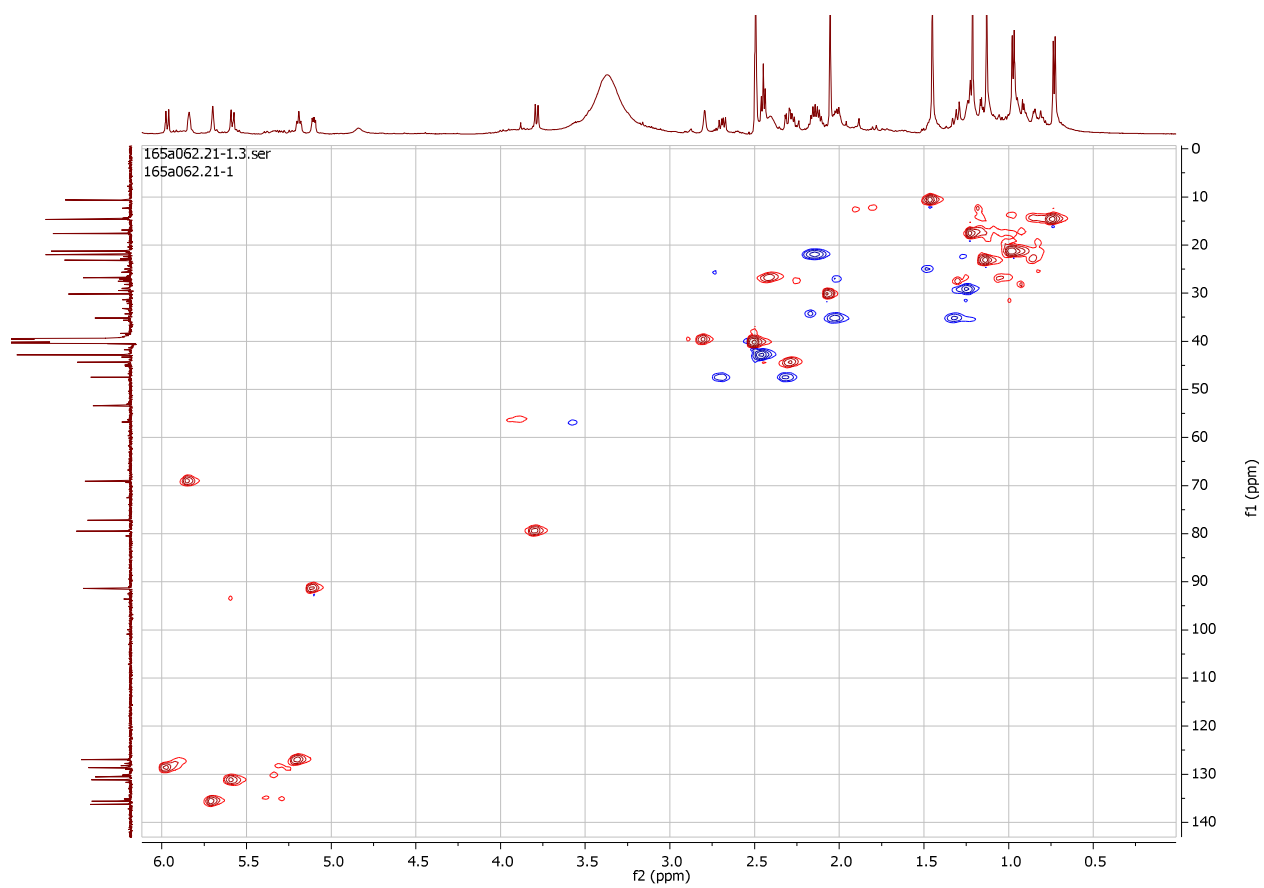




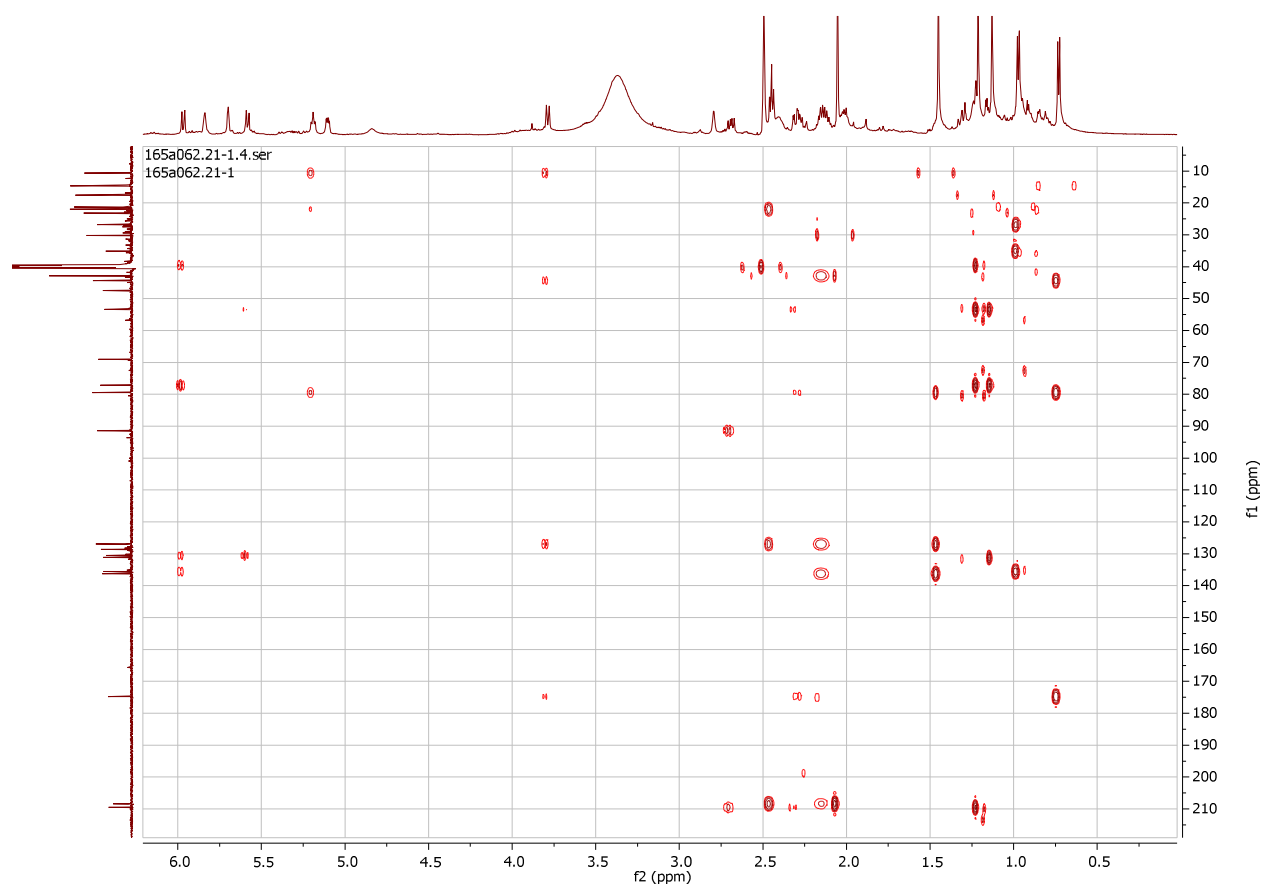
S38.  $^{13}\text{C}$  NMR spectrum (150 MHz) of compound **8** in  $\text{DMSO}-d_6$ .



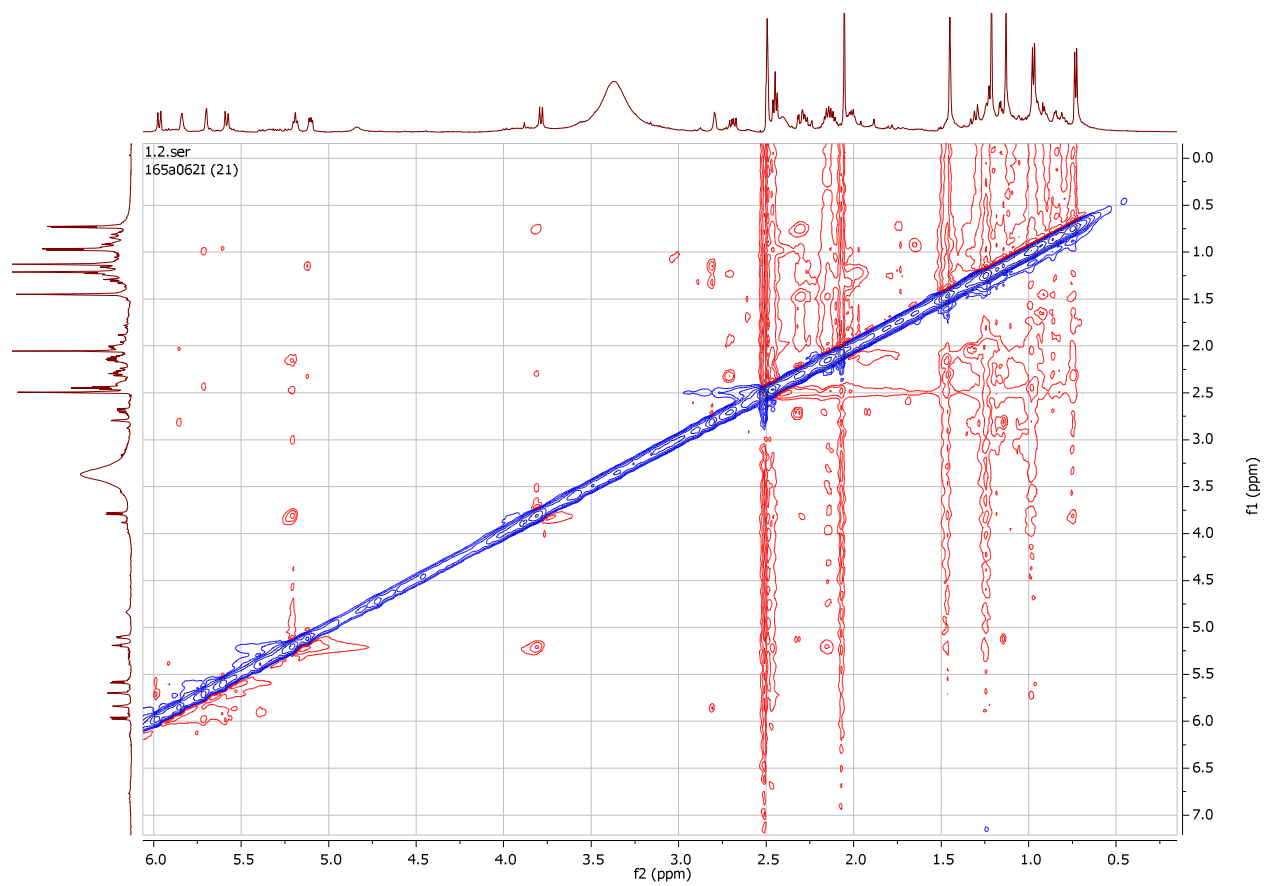
S39. COSY spectrum of compound **8** in DMSO- $d_6$ .



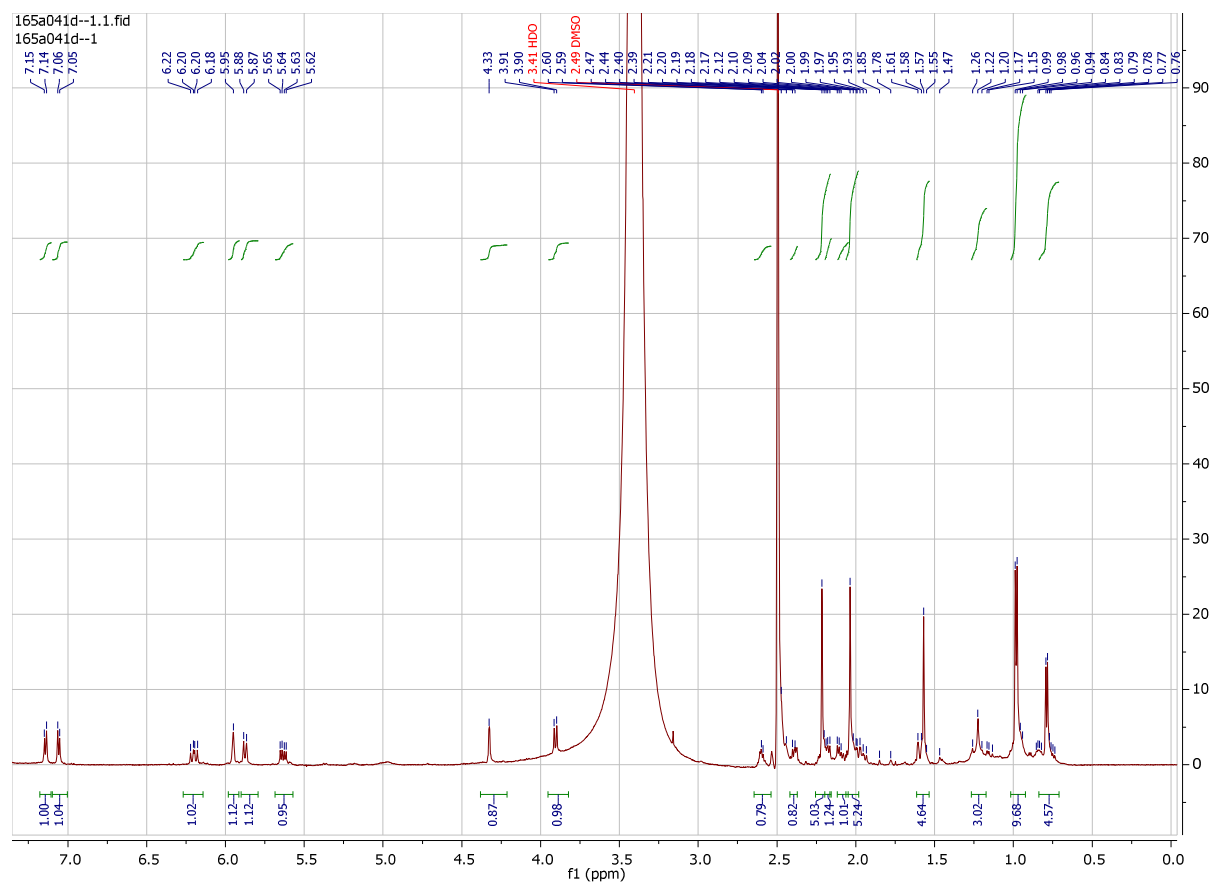
S40. HSQC spectrum of compound **8** in DMSO- $d_6$ .



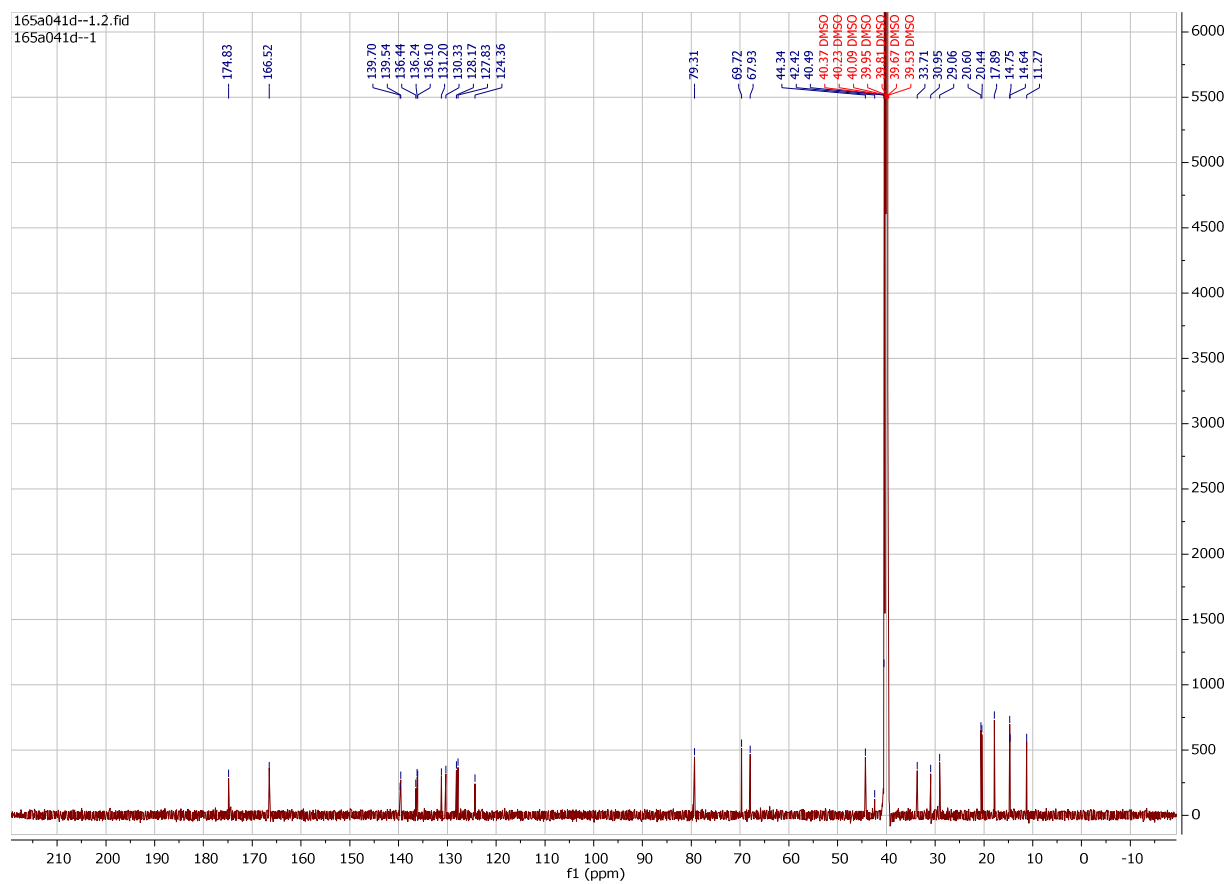
S41. HMBC spectrum of compound **8** in DMSO- $d_6$ .



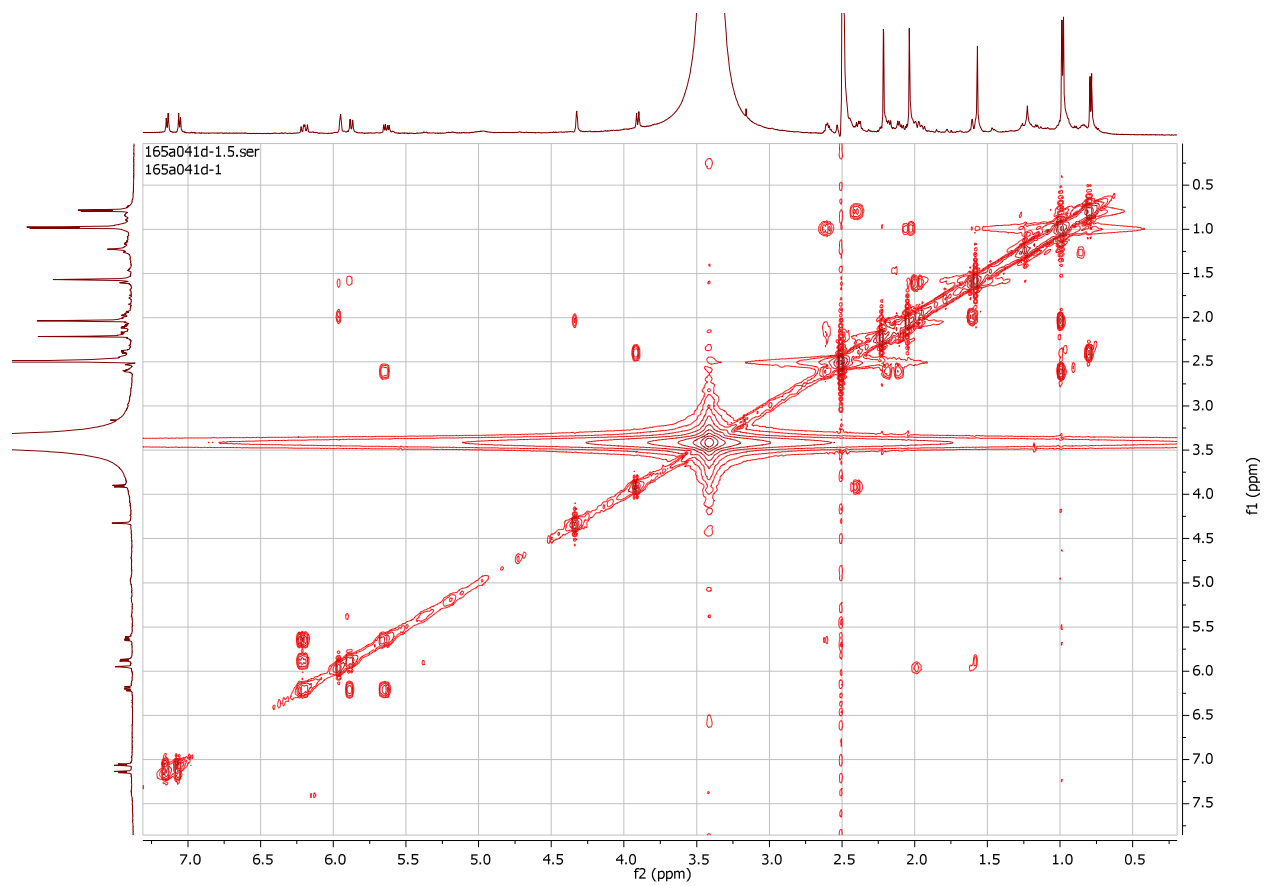
S42. ROESY spectrum of compound **8** in DMSO- $d_6$ .



S43.  $^1\text{H}$  NMR spectrum (600 MHz) of compound **10** in  $\text{DMSO}-d_6$ .

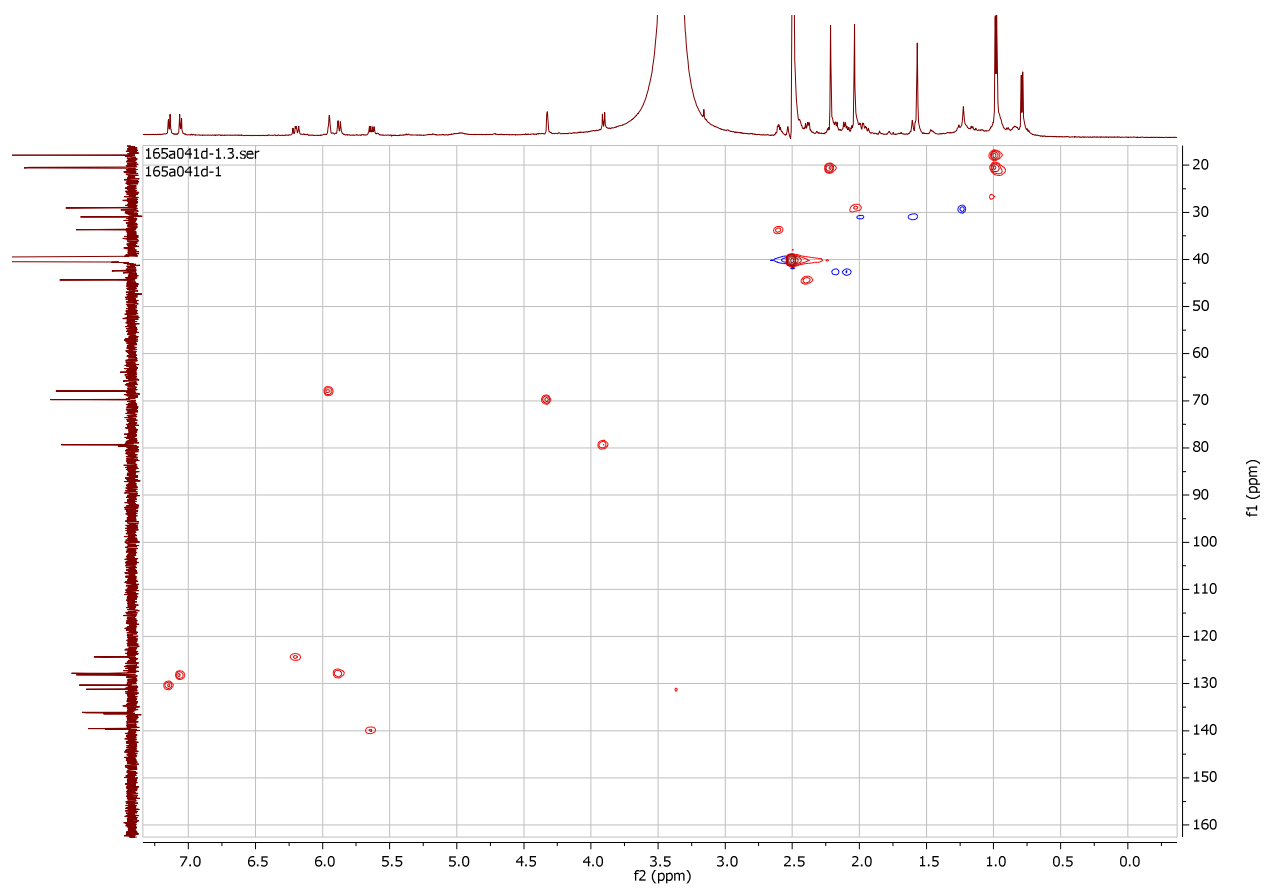


S44.  $^{13}\text{C}$  NMR spectrum (150 MHz) of compound **10** in  $\text{DMSO}-d_6$ .

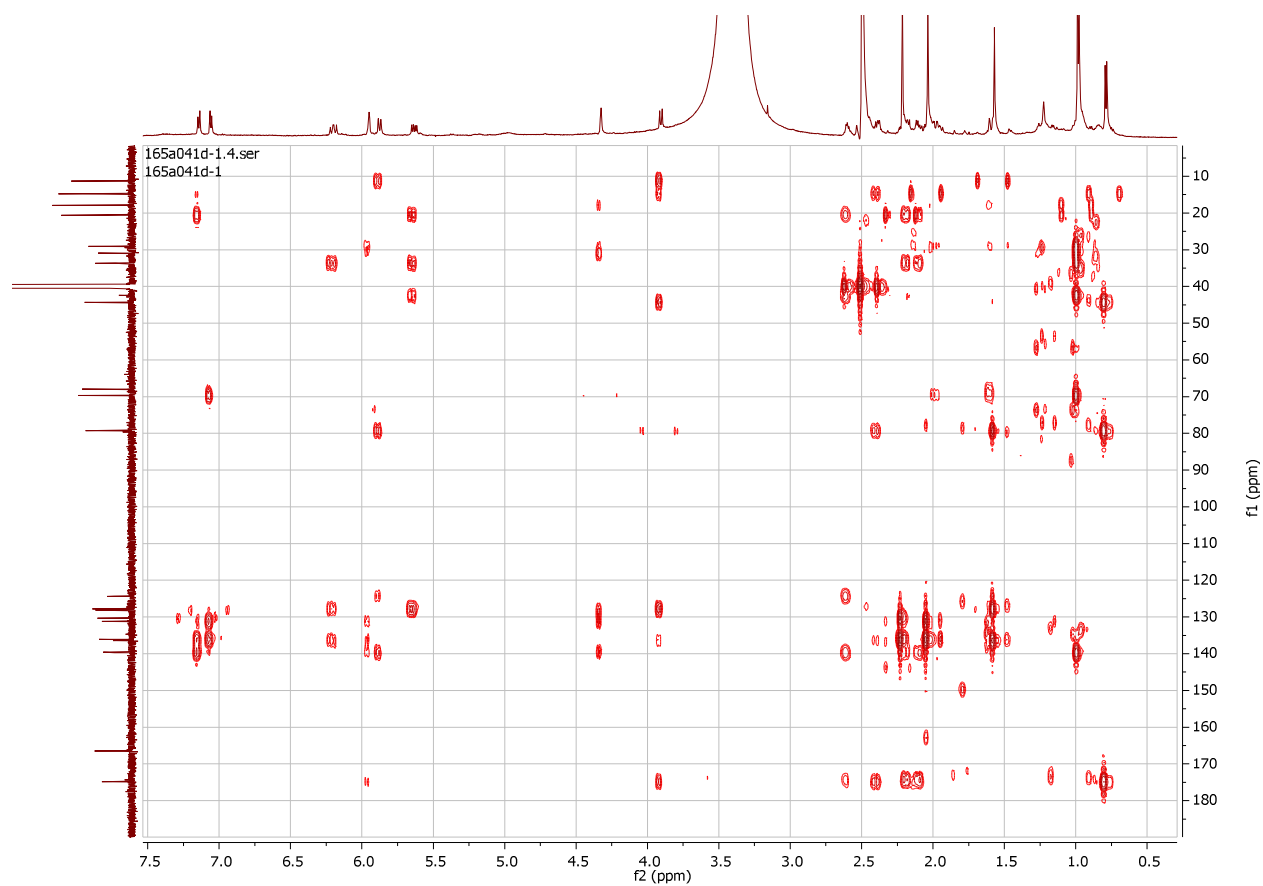


S45. COSY spectrum of compound **10** in DMSO- $d_6$ .

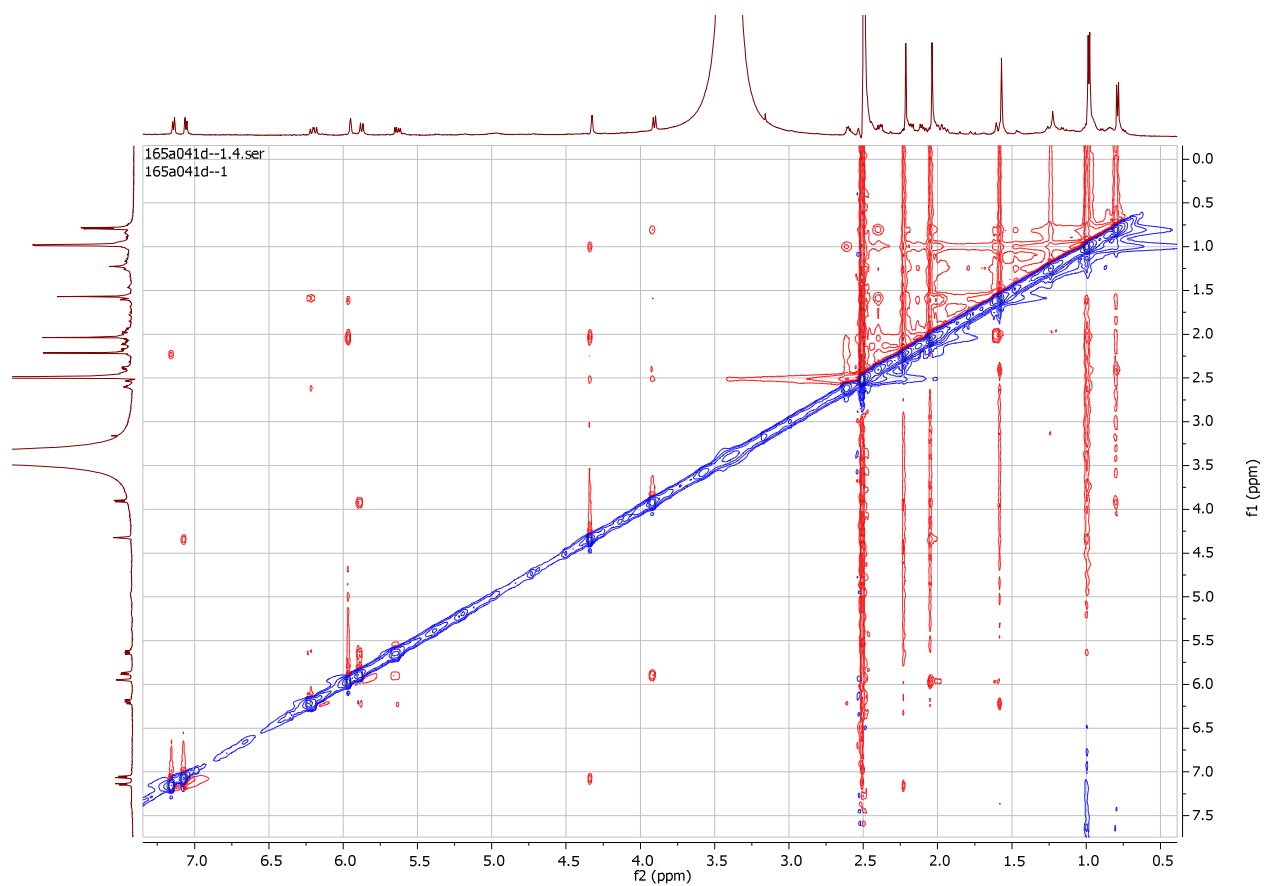




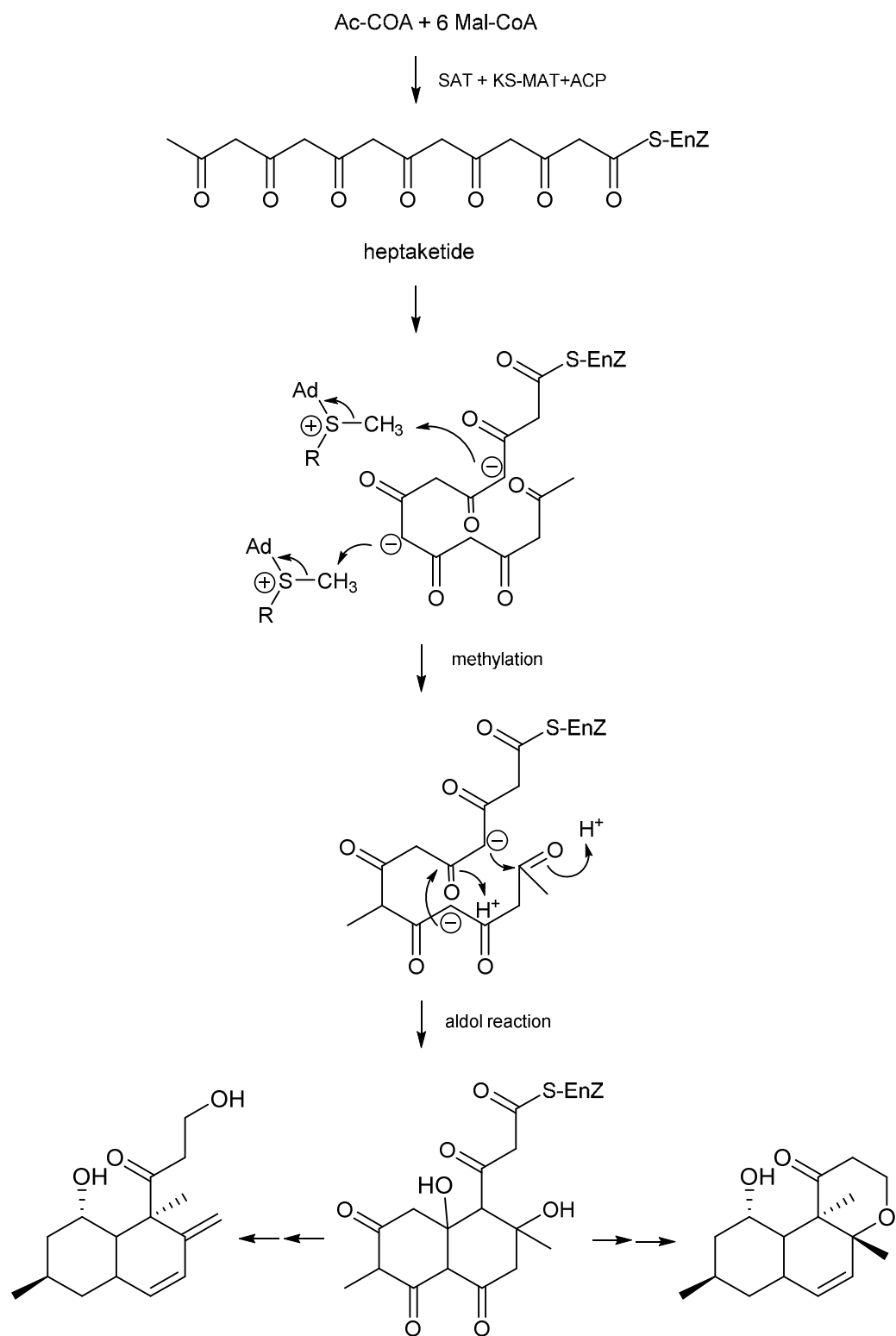
S46. HSQC spectrum of compound **10** in DMSO- $d_6$ .



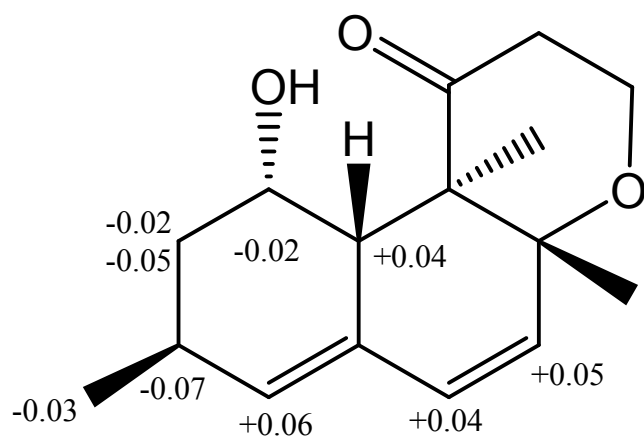
S47. HMBC spectrum of compound **10** in DMSO- $d_6$ .



S48. ROESY spectrum of compound **10** in DMSO- $d_6$ .



S49. Proposed biosynthesis of cratellenone E (**1**) and isoversiol A (**3**) via the common C14 heptaketide

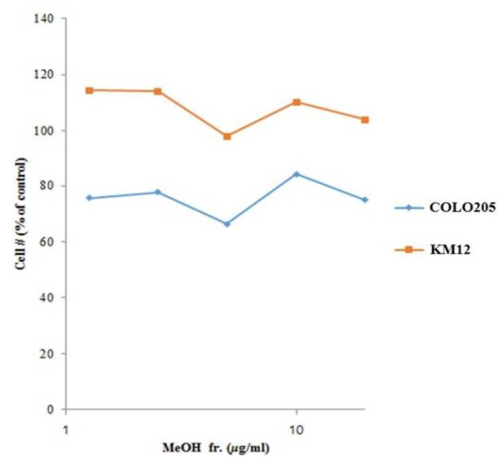
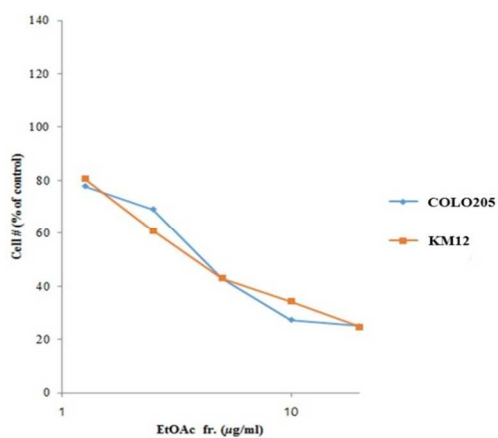
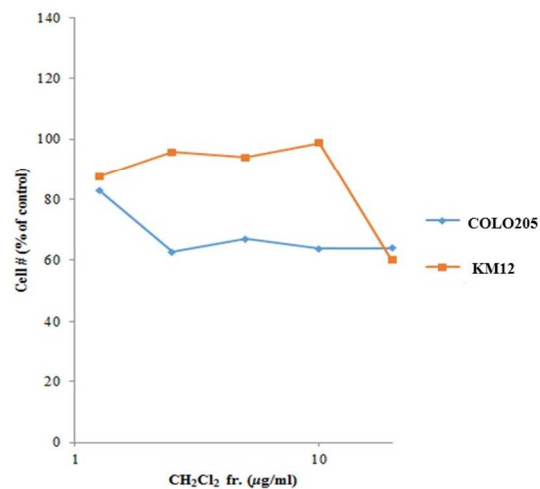
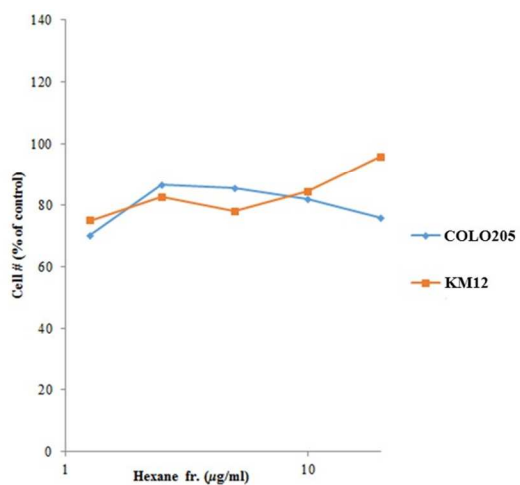


4a R = (*S*)-MTPA ester

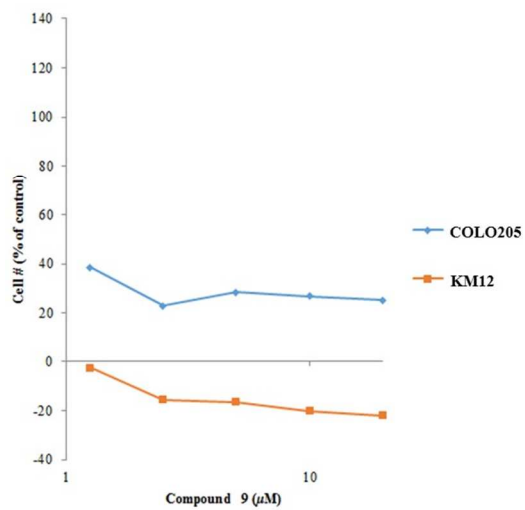
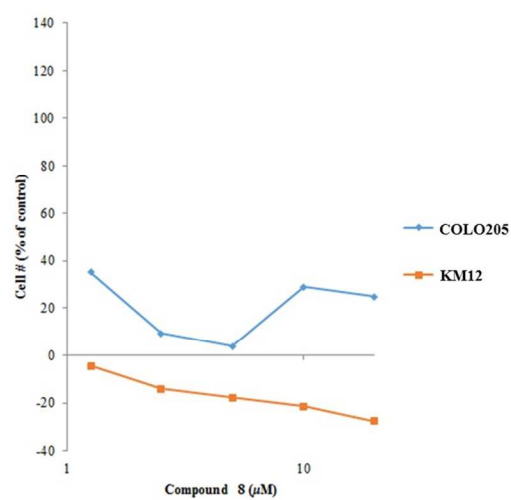
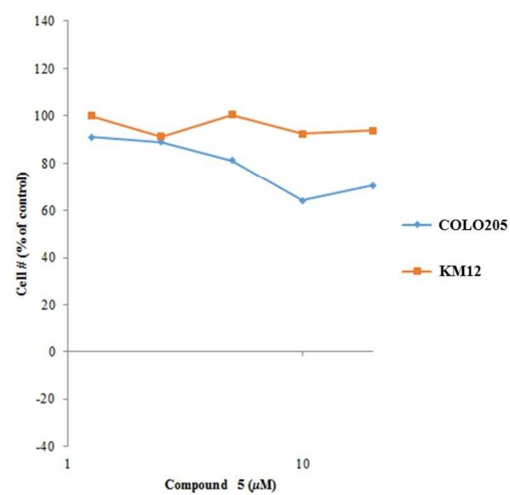
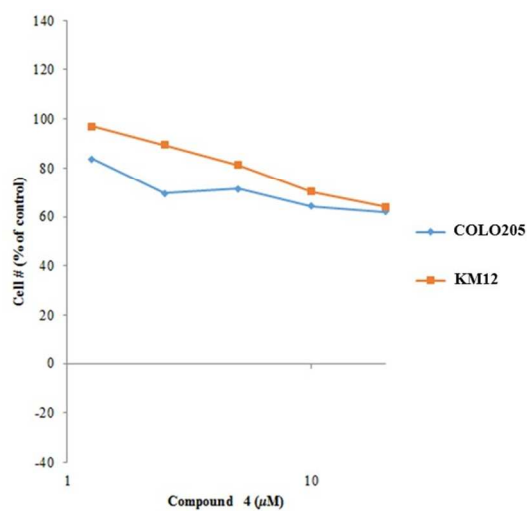
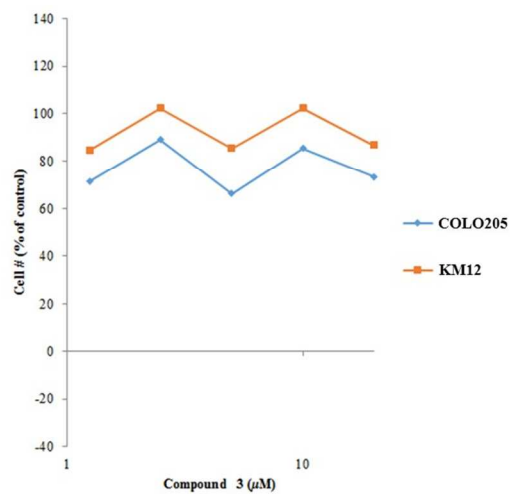
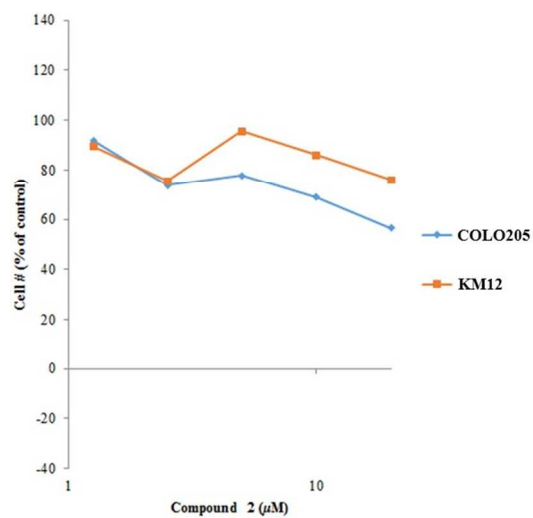
4b R = (*R*)-MTPA ester

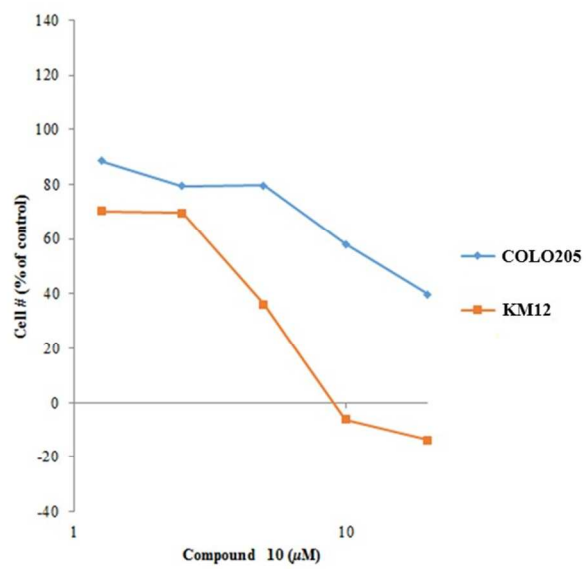
S50.  $\Delta\delta$  ( $\delta_S$ - $\delta_R$ ) values obtained from MTPA esters for compound **4**

Preparation of (*S*)-MTPA ester and (*R*)-MTPA ester. The absolute configuration of 1-OH in compound **4** was determined according to the modified Mosher's method. In brief, compound **4** (1 mg) was transferred into a 5 mL glass vial, followed by adding dry pyridine,  $\text{CHCl}_3$ , (*R*)-(-)- $\alpha$ -methoxy- $\alpha$ -trifluoromethylphenylacetyl (MTPA) chloride, and then carefully shaken to mix at room temperature. Every 30 min, the reactant was subjected to TLC analysis (*n*-hexane-EtOAc = 5:1) to estimate to the conversion to the (*S*)-MTPA ester derivative (**4a**). In the same manner described above, another portion of compound **4** (1 mg) was reacted with (*S*)-(+)-MTPA chloride to afford the (*R*)-MTPA ester (**4b**).



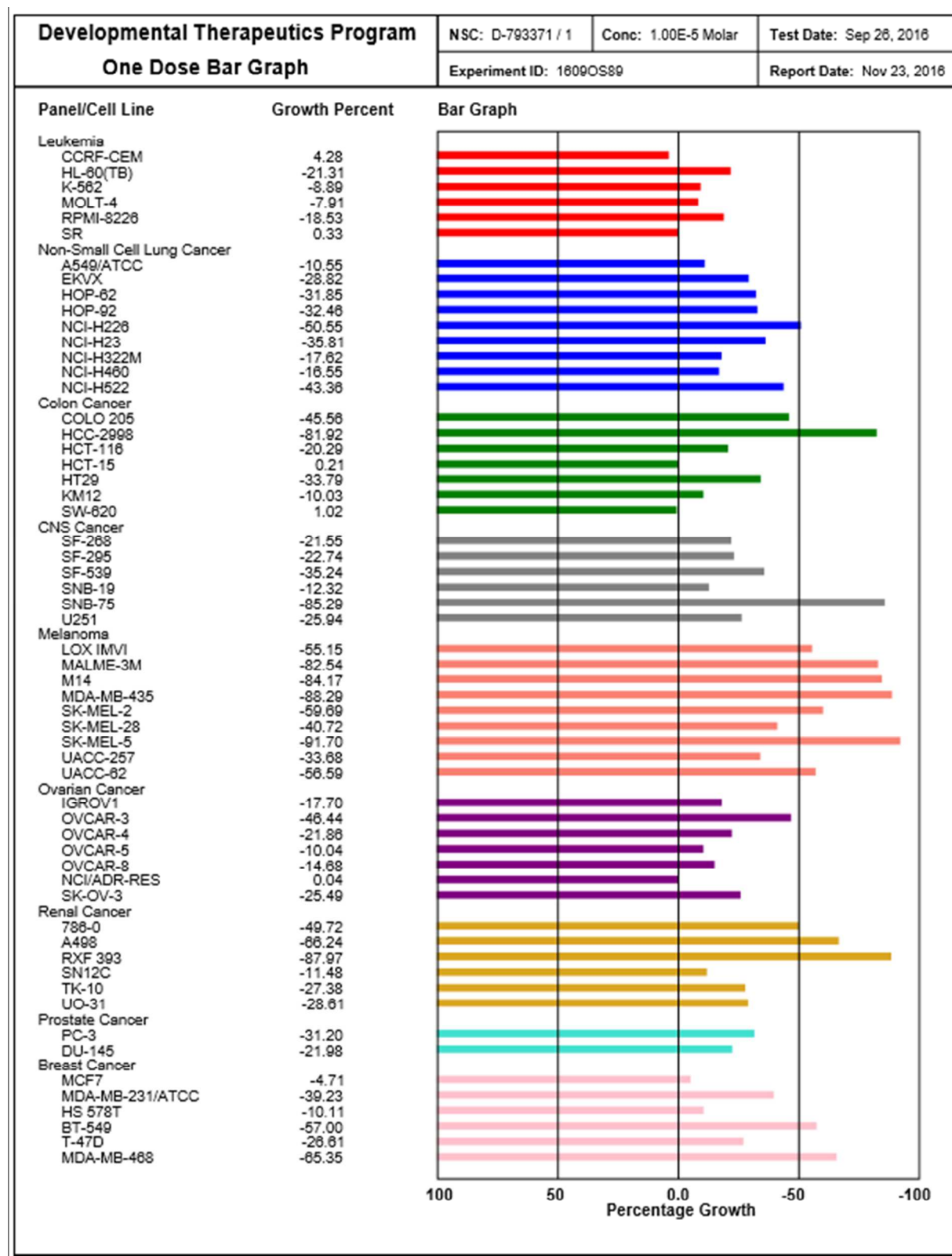
S51. Cytotoxicity of *Paraconiothyrium* sp. fractions in COLO205, KM12 colon tumor cells.



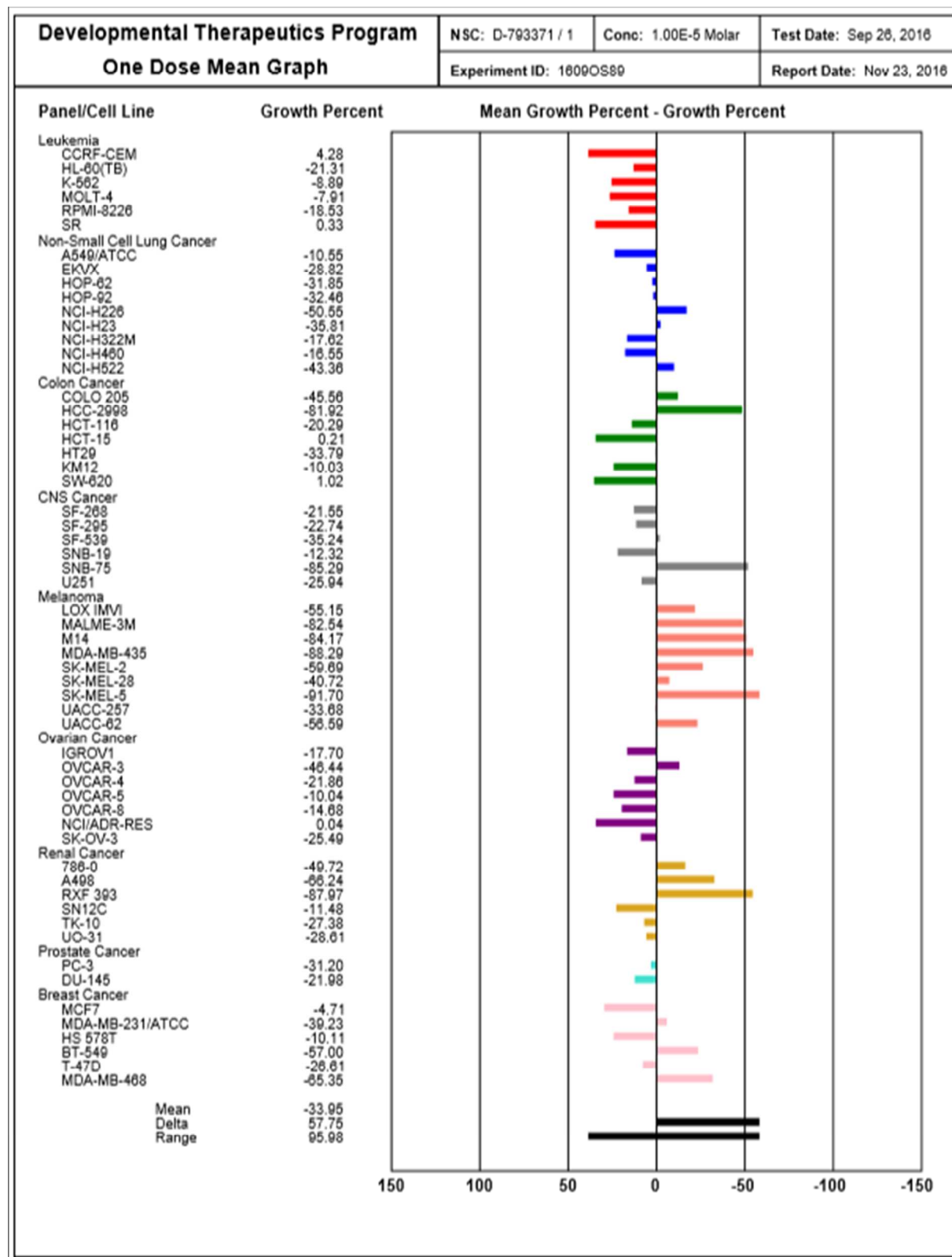


S52. Cytotoxicity of compounds from *Paraconiothyrium* sp. in COLO205, KM12 colon tumor cells.

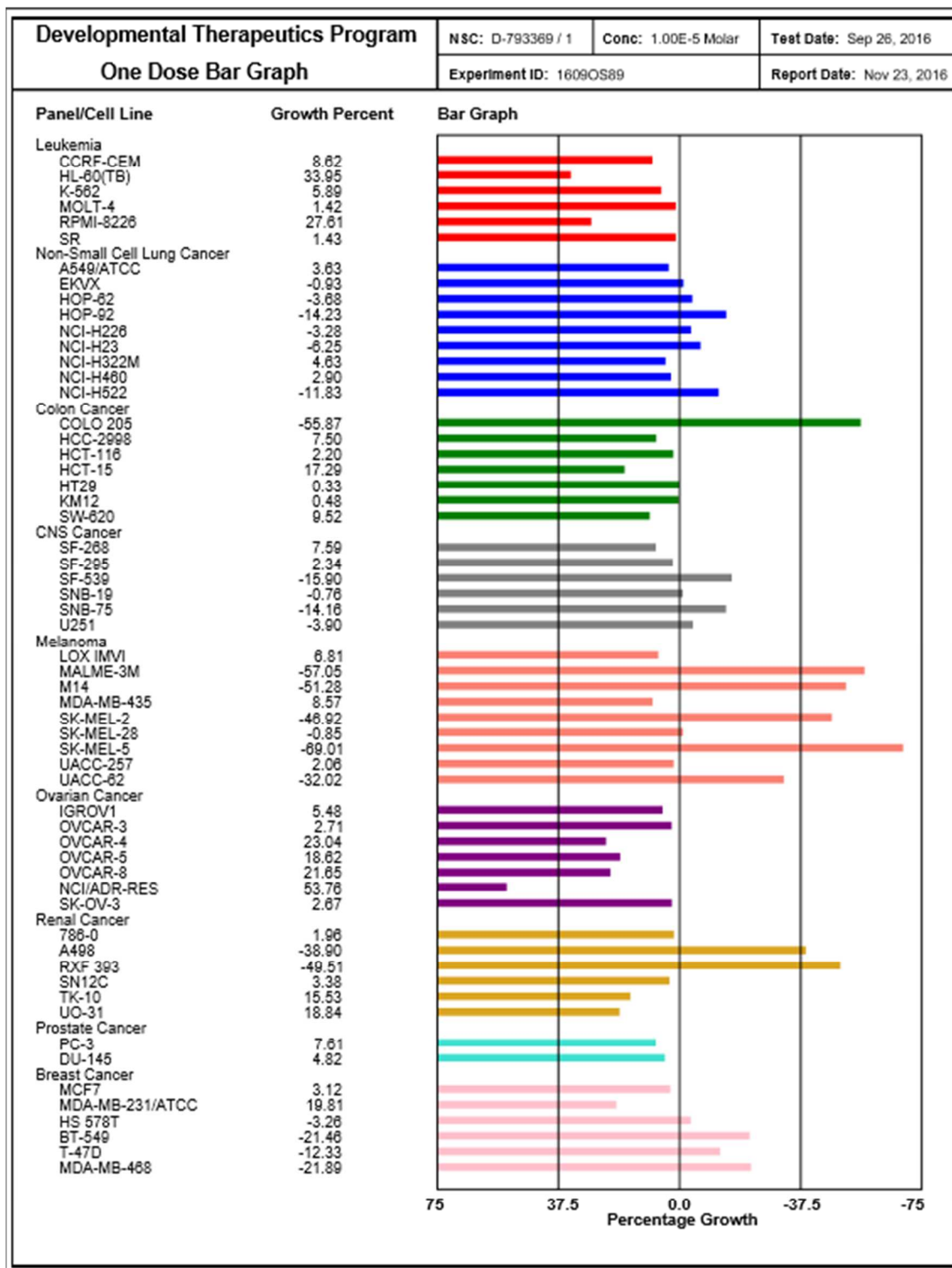




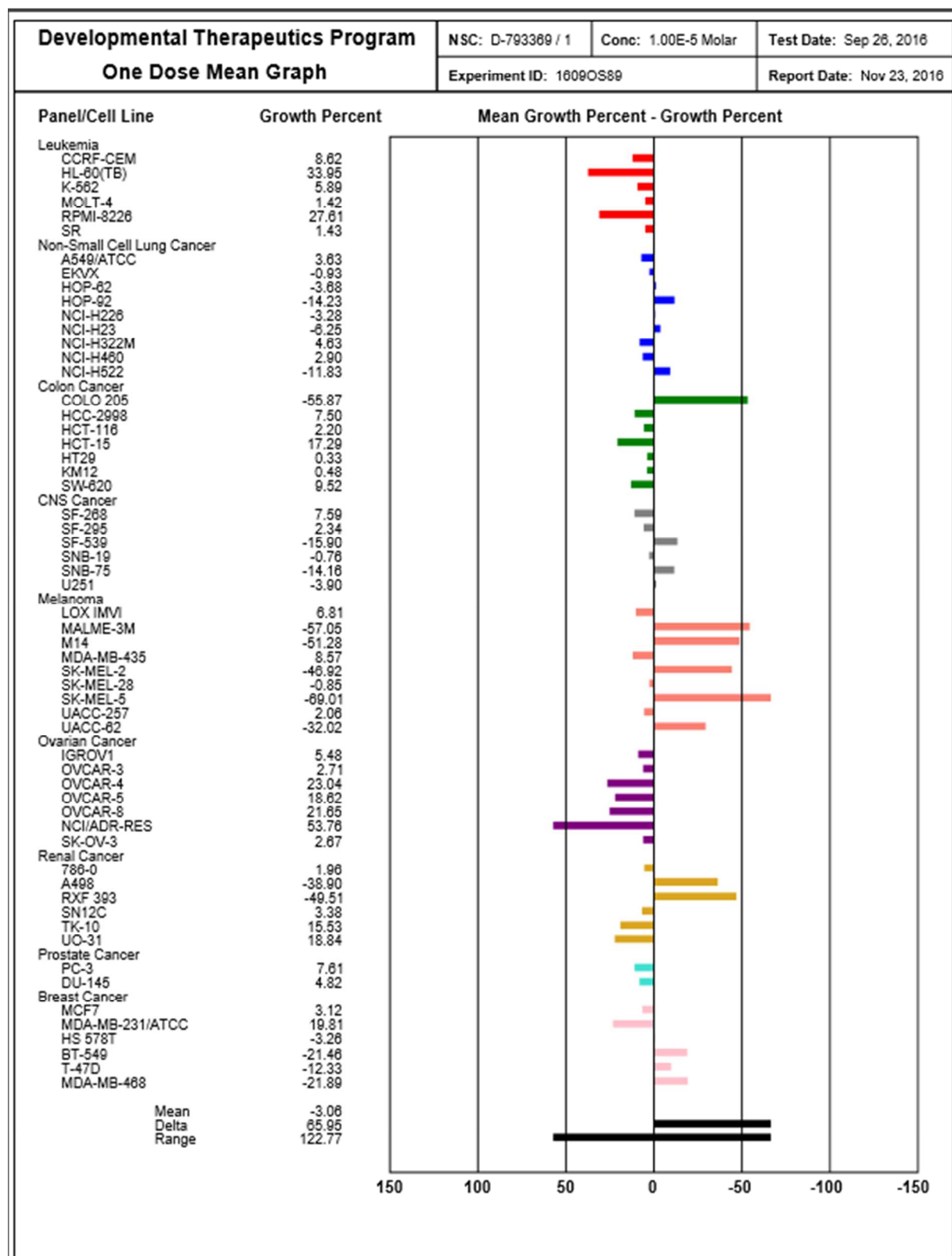
S53. NCI 60 cell single dose test of compound 8.



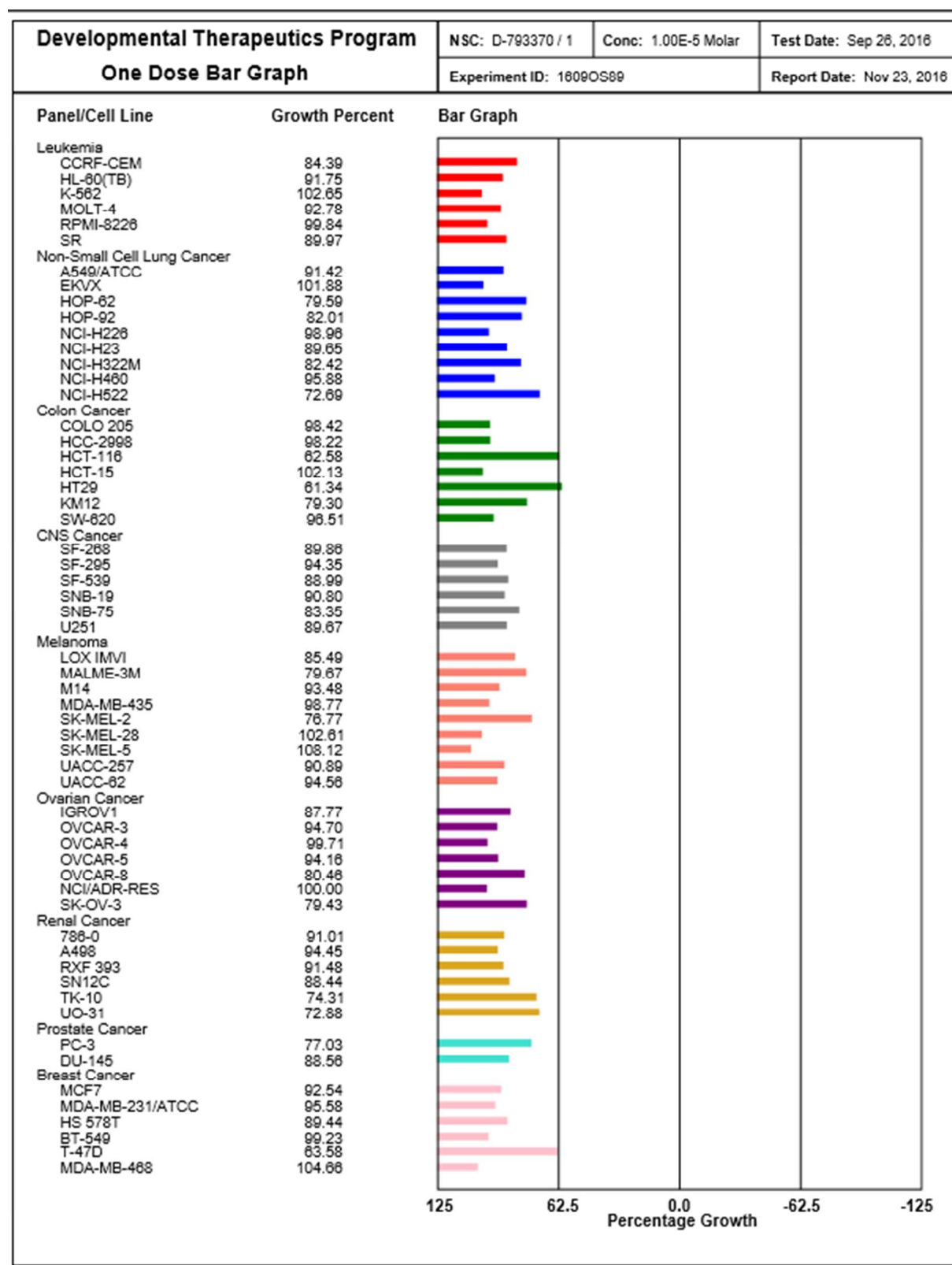
S54. Compound 8 NCI-60 mean bar graphs in single dose test.



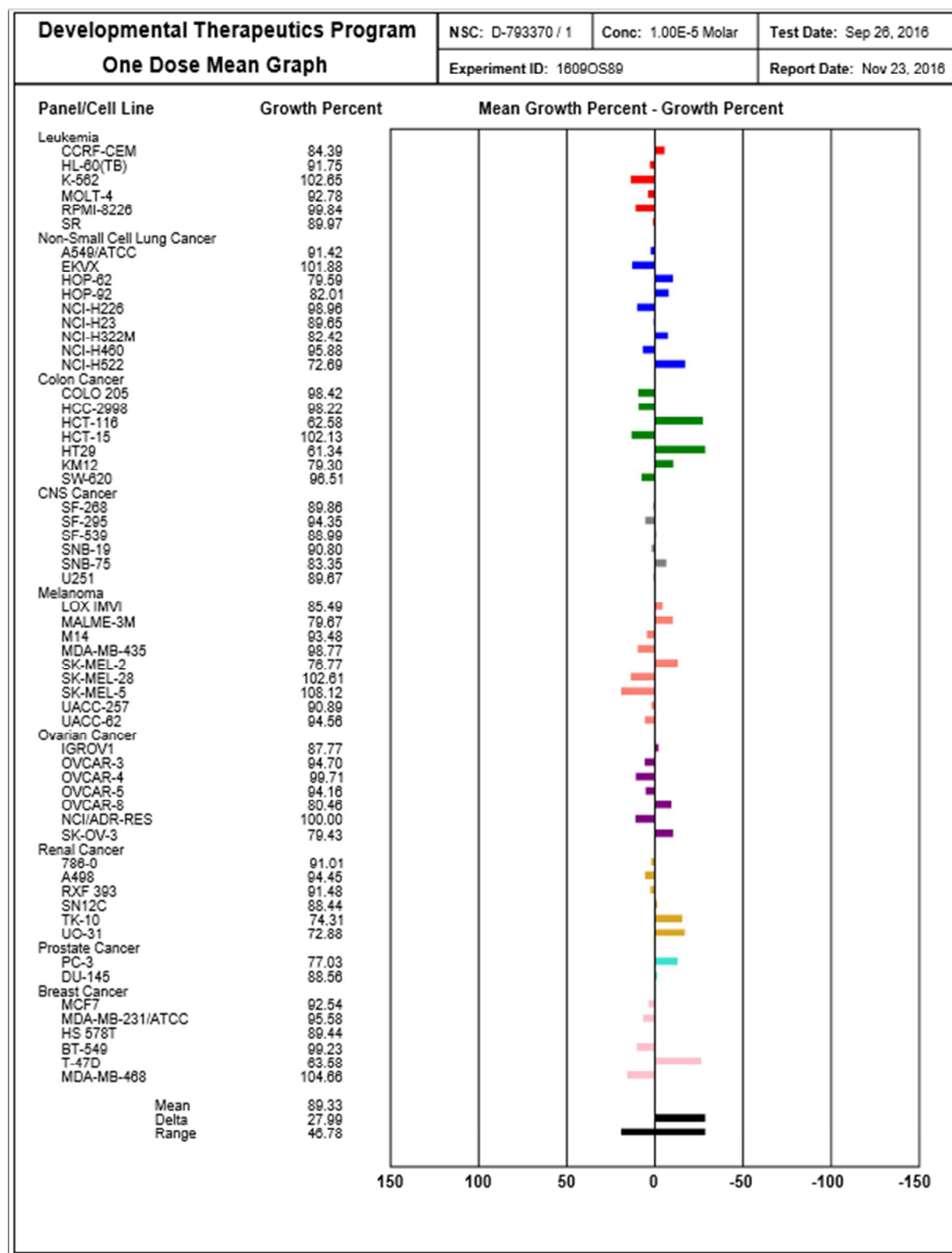
S55. NCI 60 cell single dose test of compound 9.



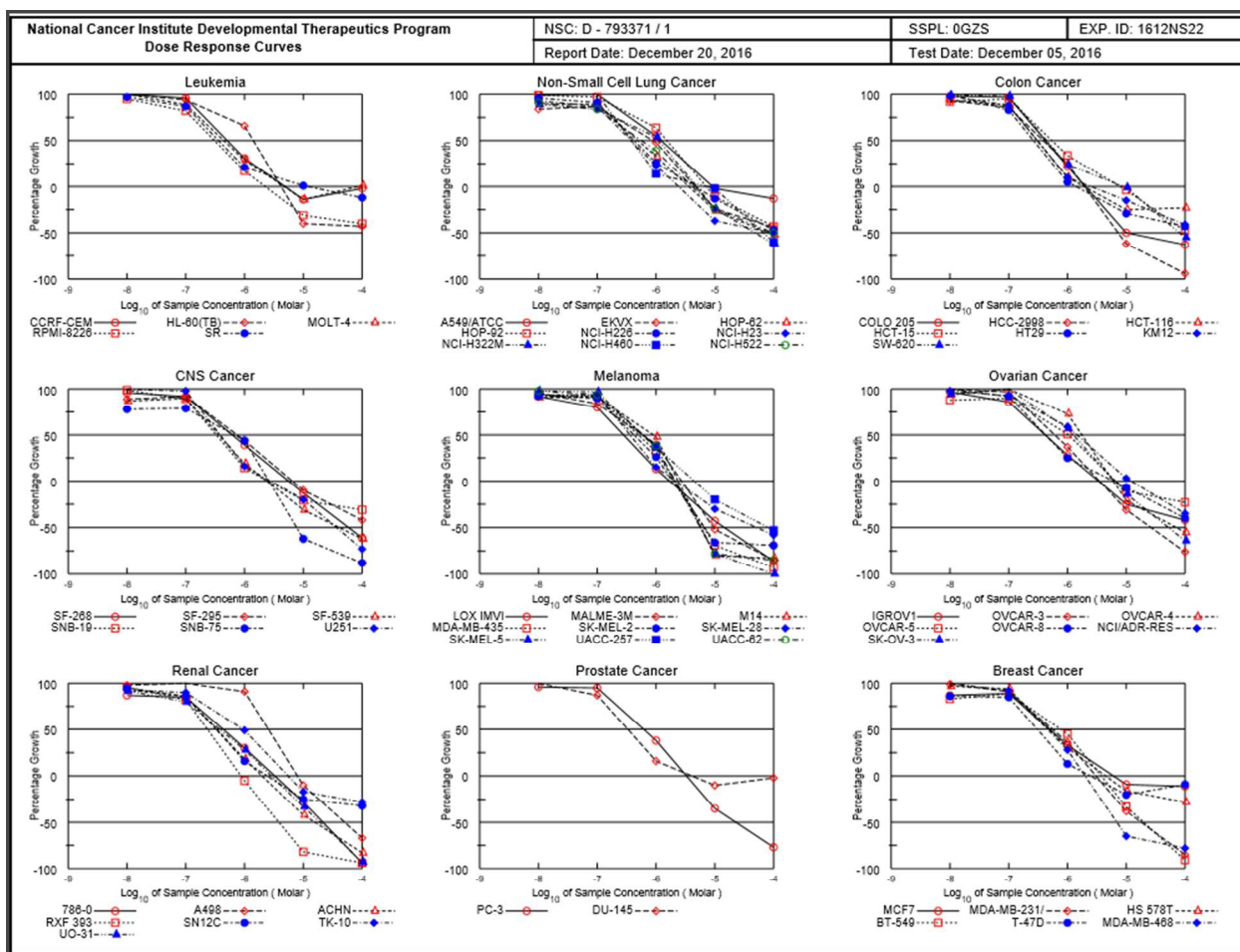
S56. Compound 9 NCI-60 mean bar graphs in single dose test.



S57. NCI 60 cell single dose test of compound 10.

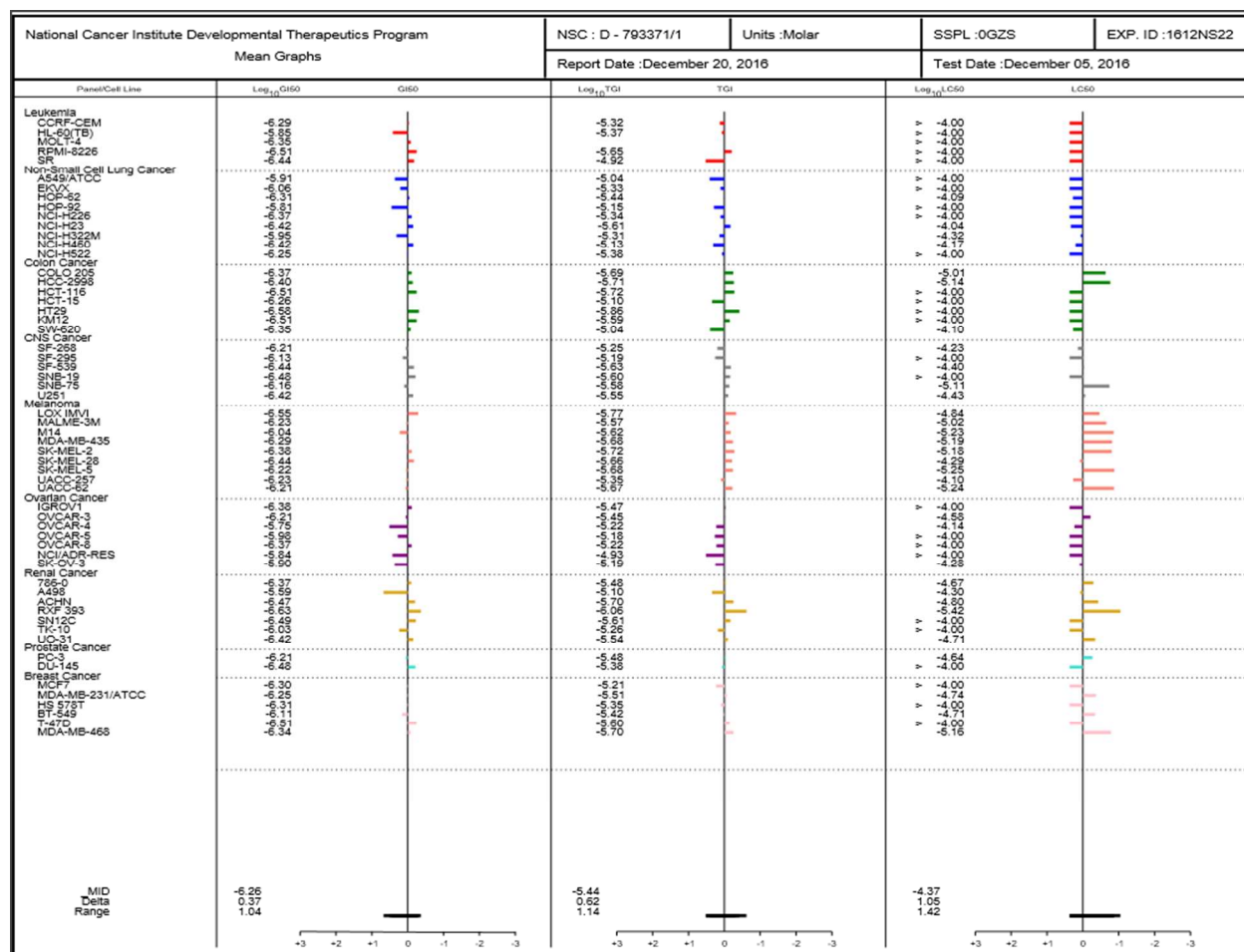


S58. Compound **10** NCI-60 mean bar graphs in single dose test.



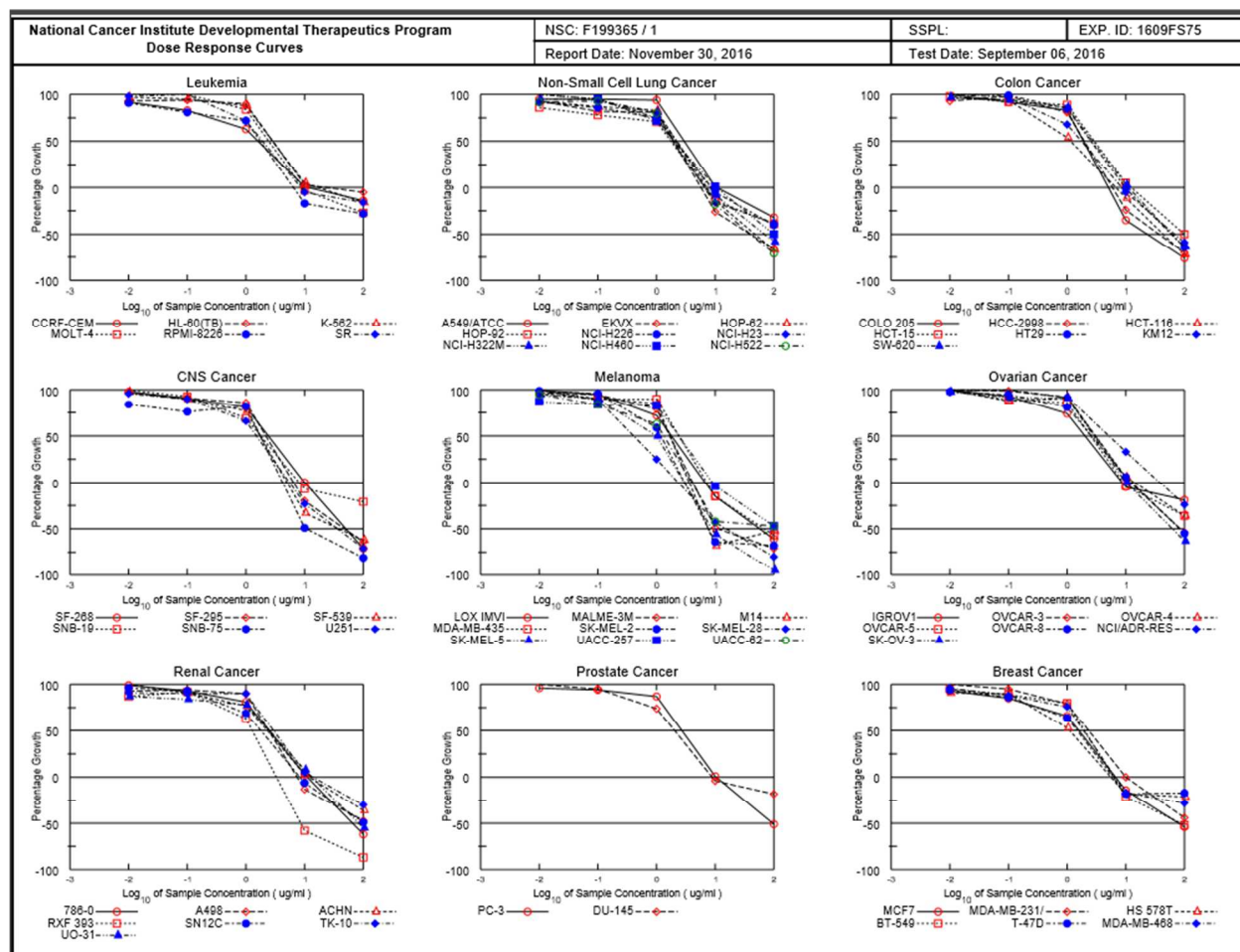
S59. NCI 60 cell 5-dose test of compound 8.





S60. Compound **8** NCI-60 mean bar graphs in 5-dose test.

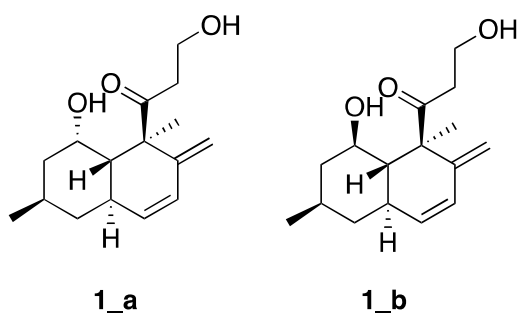




S61. NCI 60 cell 5-dose test of *Paraconiothyrium* sp. extract.



**S63.** Comparison of experimental and calculated  $^{13}\text{C}$  and  $^1\text{H}$  chemical shifts in  $\text{DMSO-}d_6$  for **1a** and **1b** and their statistical parameters.



Position	$\delta_{\text{C exp.}}$	$\delta_{\text{C calc.}}$		$\delta_{\text{H exp.}}$	$\delta_{\text{H calc.}}$	
		<b>1a</b>	<b>1b</b>		<b>1a</b>	<b>1b</b>
1	66.5	68.3	69.3	3.60	3.55	3.45
2	44.0	43.2	42.5	1.04	1.10	1.05
				1.60	1.55	1.75
3	25.7	27.8	31.4	1.96	1.86	1.56
4	42.1	41.6	39.8	0.74	0.75	0.91
				1.87	1.82	1.75
5	30.3	31.9	35.2	2.46	2.47	2.02
6	134.9	132.5	132.6	5.63	5.56	5.61
7	127.3	123.4	124.6	6.04	6.10	6.09
8	149.6	148.6	146.6			
9	56.6	59.9	56.0			
10	47.4	47.7	48.9	1.64	1.70	1.94
11	211.9	216.7	216.4			
12	41.5	39.8	40.6	2.49	2.32	2.27
				2.72	2.80	2.89

13	57.2	59.0	59.4	3.64	3.65	3.76
14	22.5	20.8	18.7	0.84	0.87	0.98
15	111.8	108.1	110.4	4.30	4.32	4.41
				4.80	4.87	4.93
16	20.2	20.0	17.0	1.20	1.27	1.18
MAE	<b>2.0</b>	2.7		<b>0.06</b>	0.16	
R <sup>2</sup>	<b>0.9981</b>	0.9969		<b>0.9982</b>	0.9850	
DP4	<b>99.9%</b>	0.1%		<b>100.0%</b>	0.0%	