

# Supporting Information

for

## Total synthesis of elansolids B1 and B2

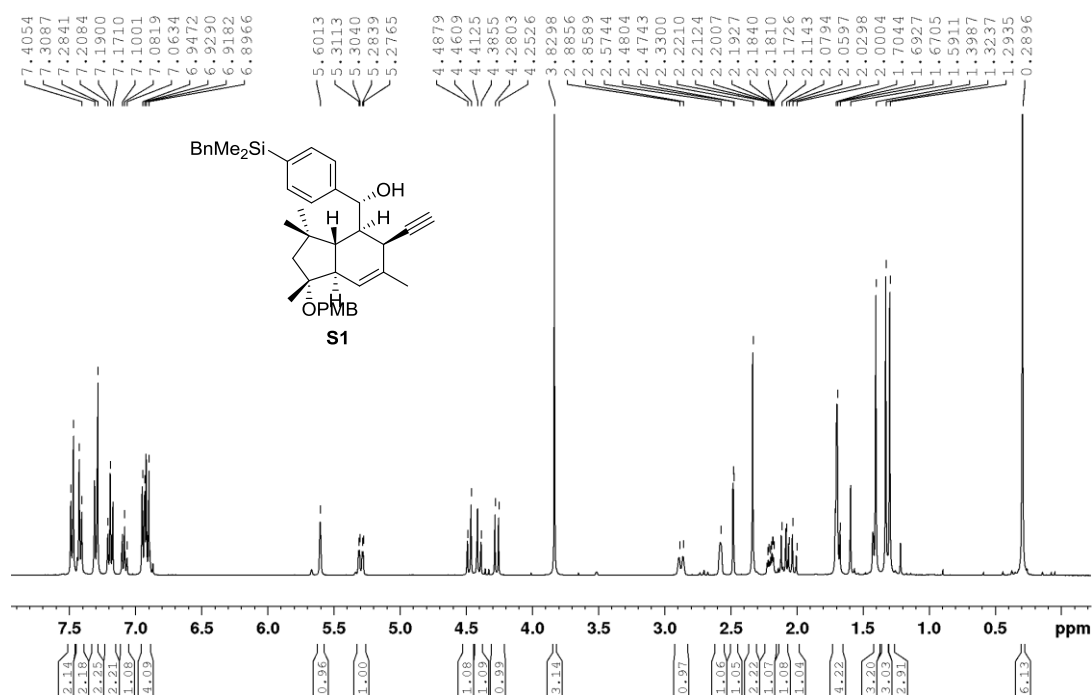
Liang-Liang Wang and Andreas Kirschning\*

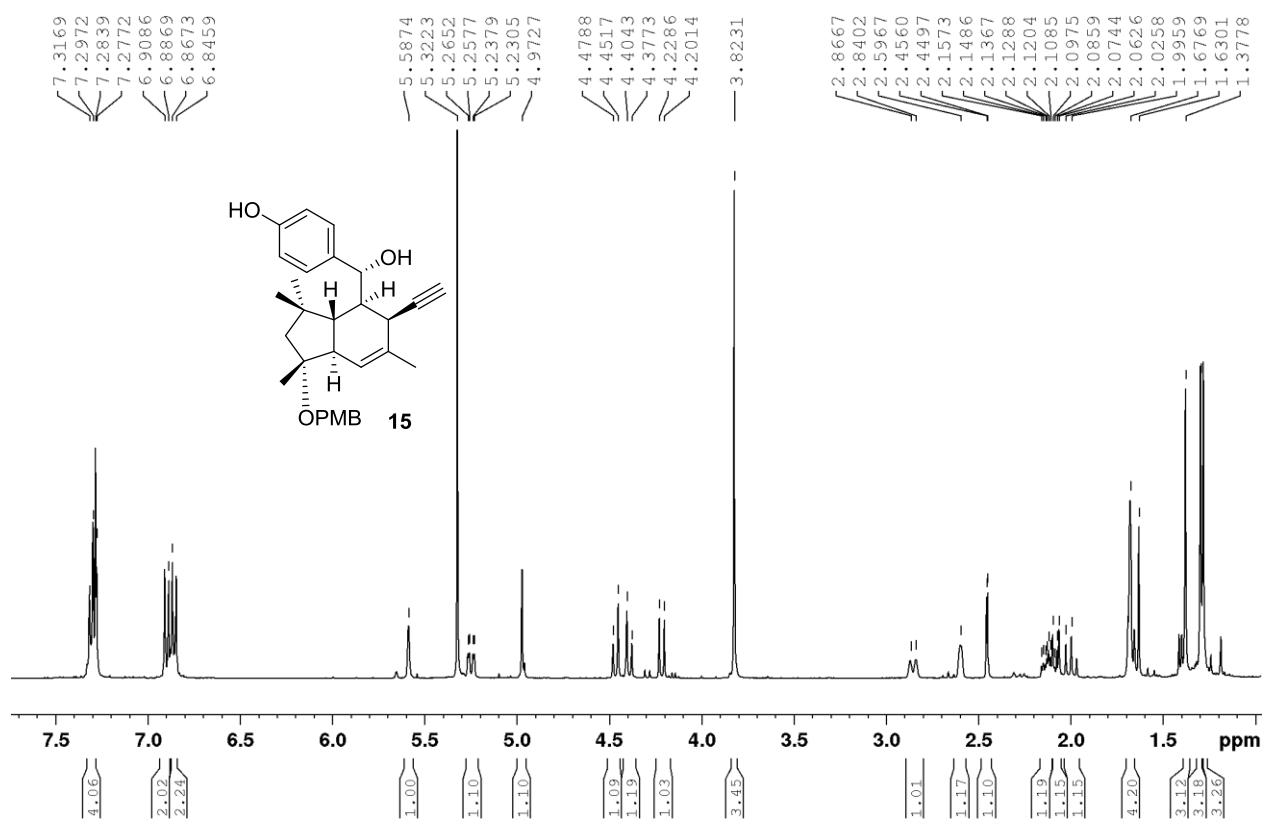
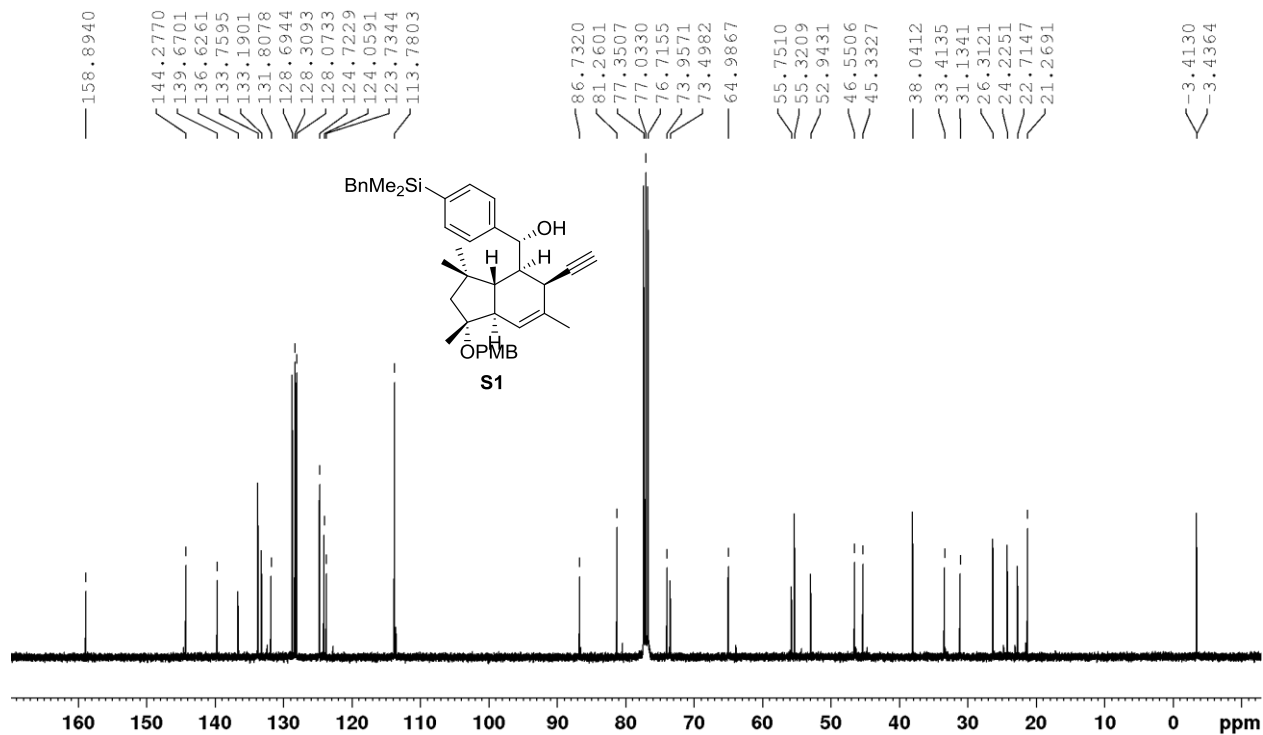
Address: Institute of Organic Chemistry and Center of Biomolecular Drug Research (BMWZ), Leibniz University Hannover, Schneiderberg 1b, 30167 Hannover, Germany

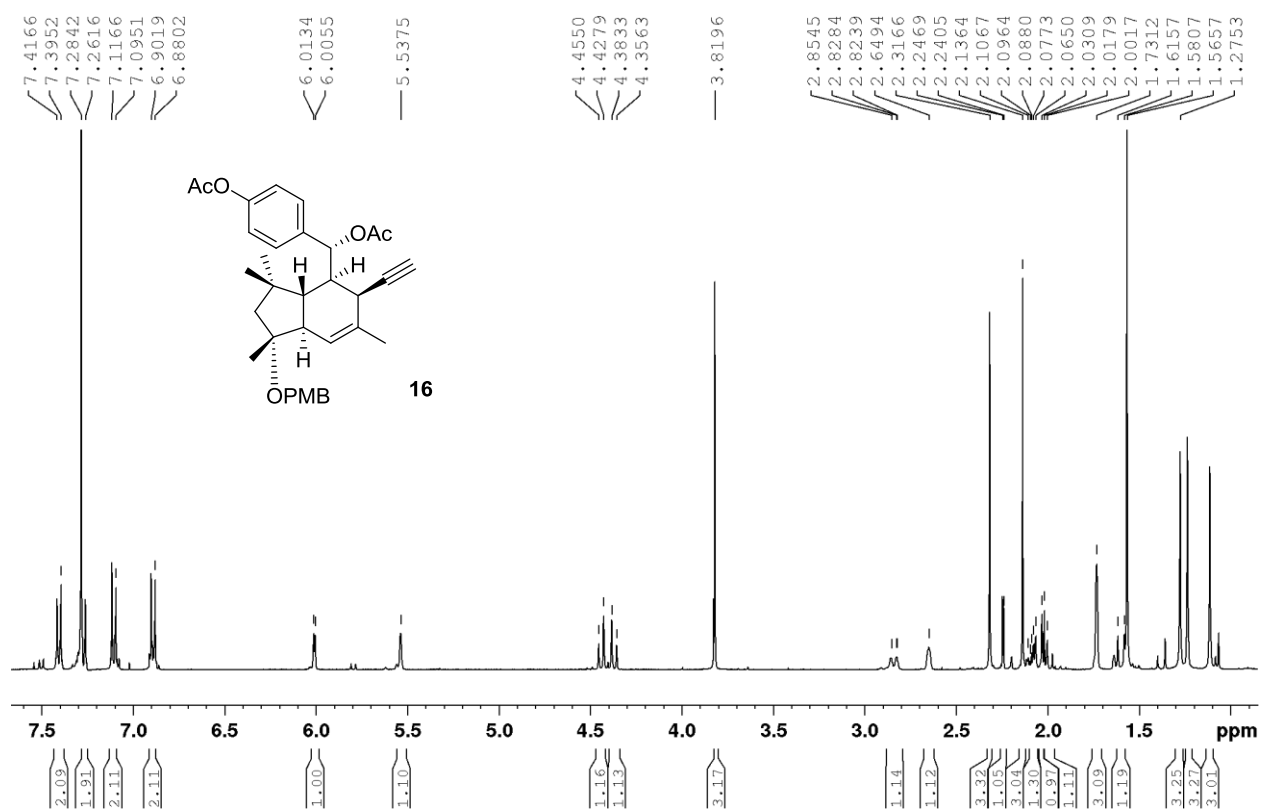
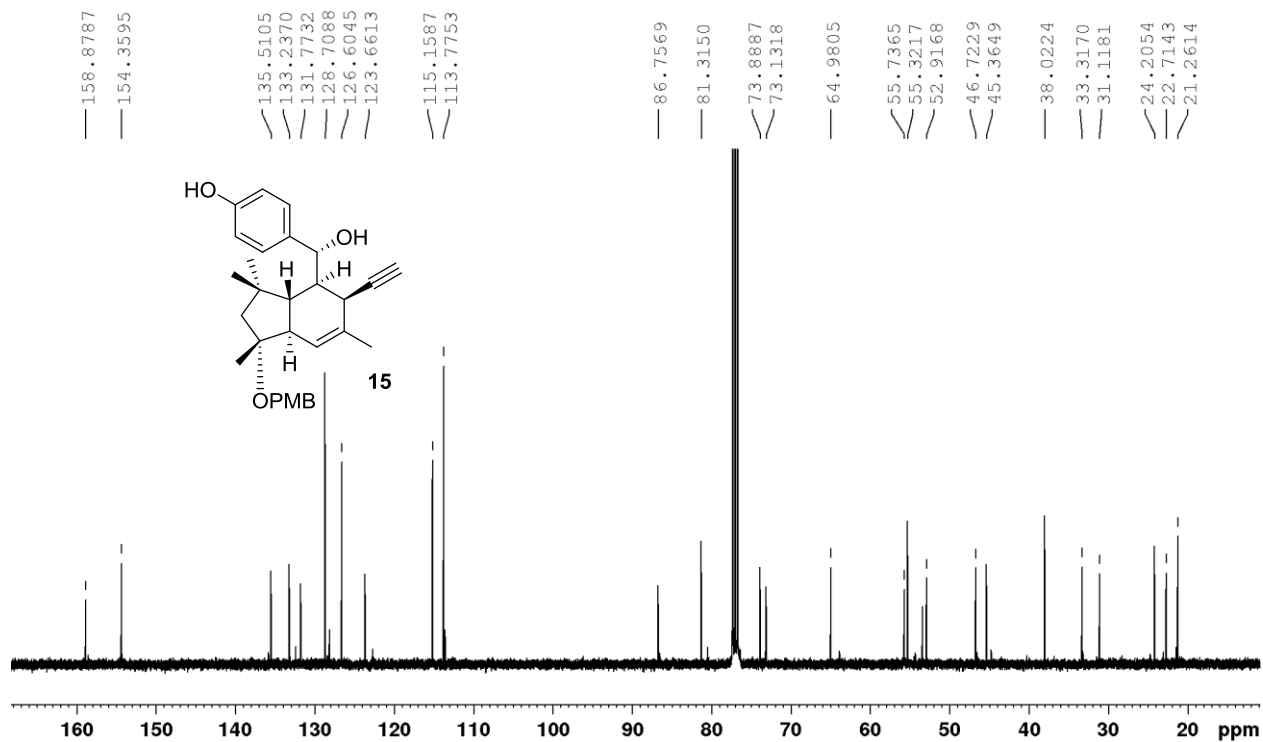
Email: Andreas Kirschning - [andreas.kirschning@oci.uni-hannover.de](mailto:andreas.kirschning@oci.uni-hannover.de)

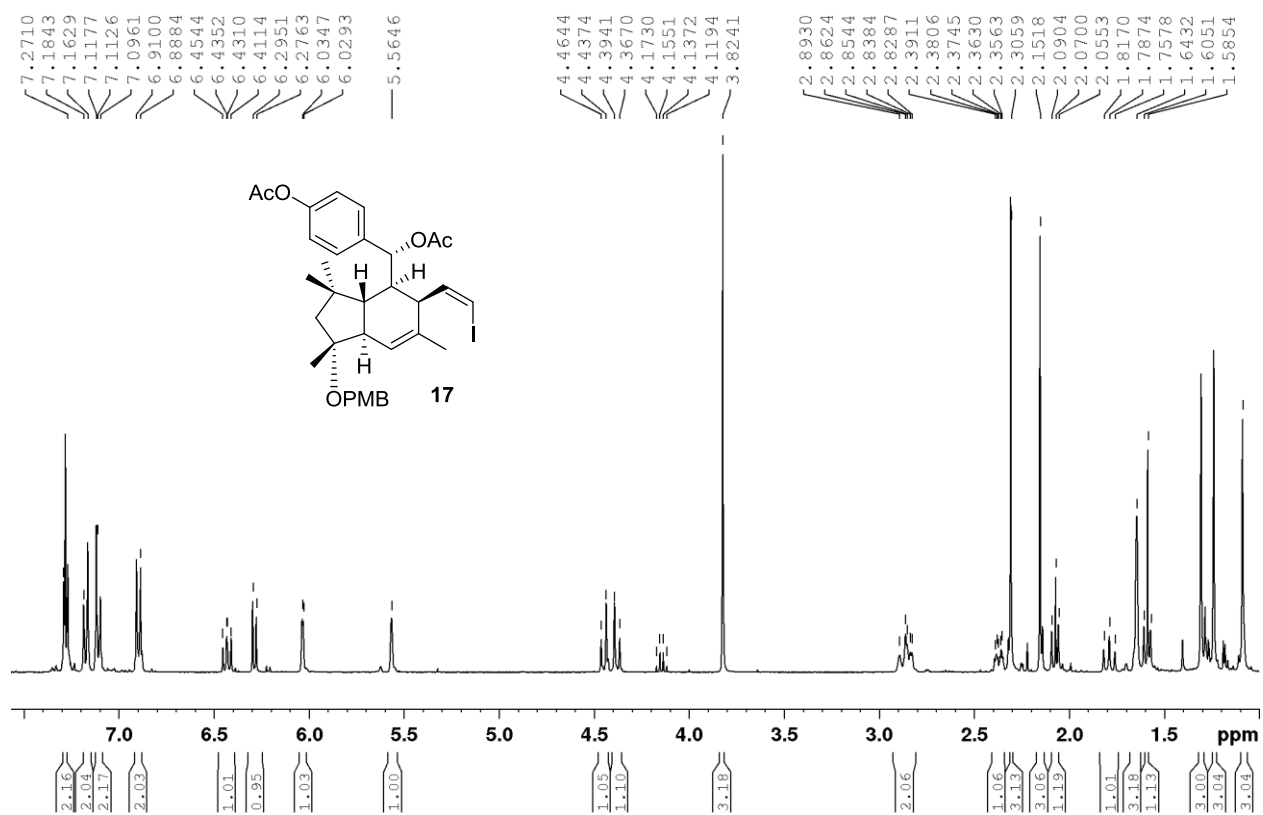
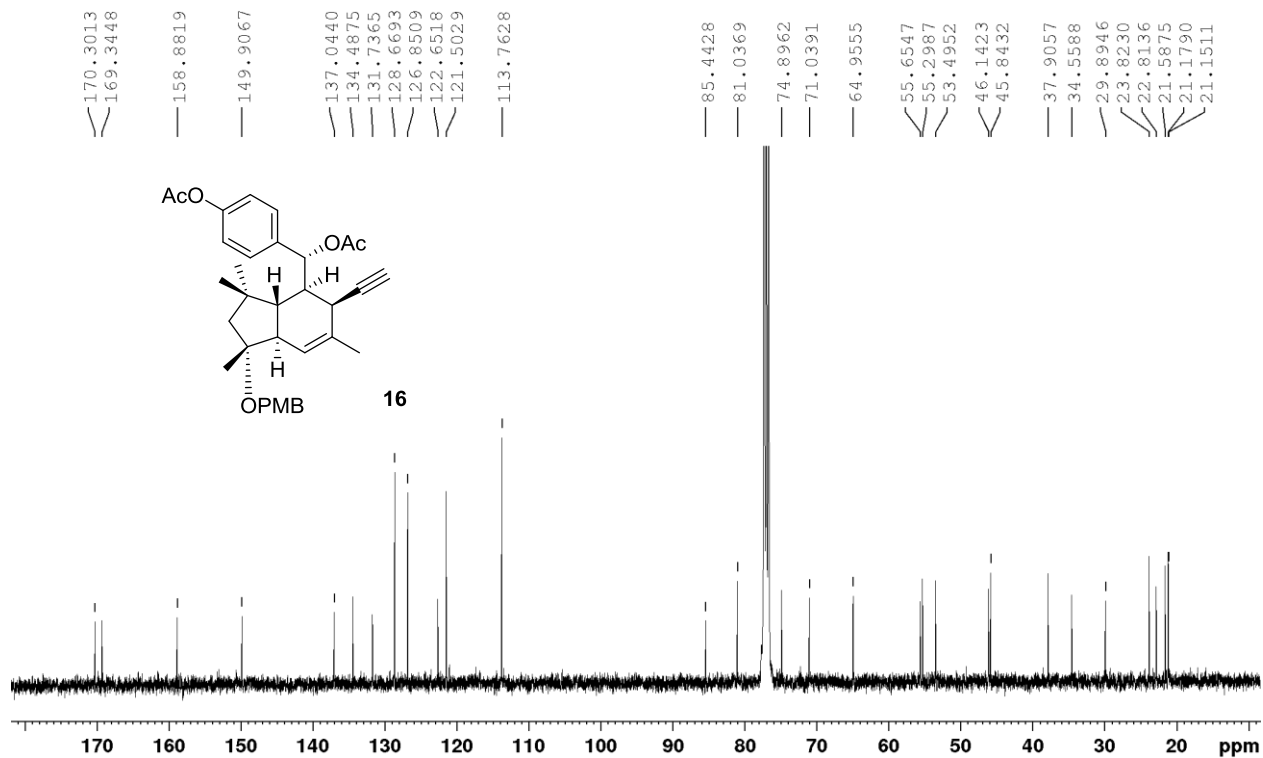
\*Corresponding author

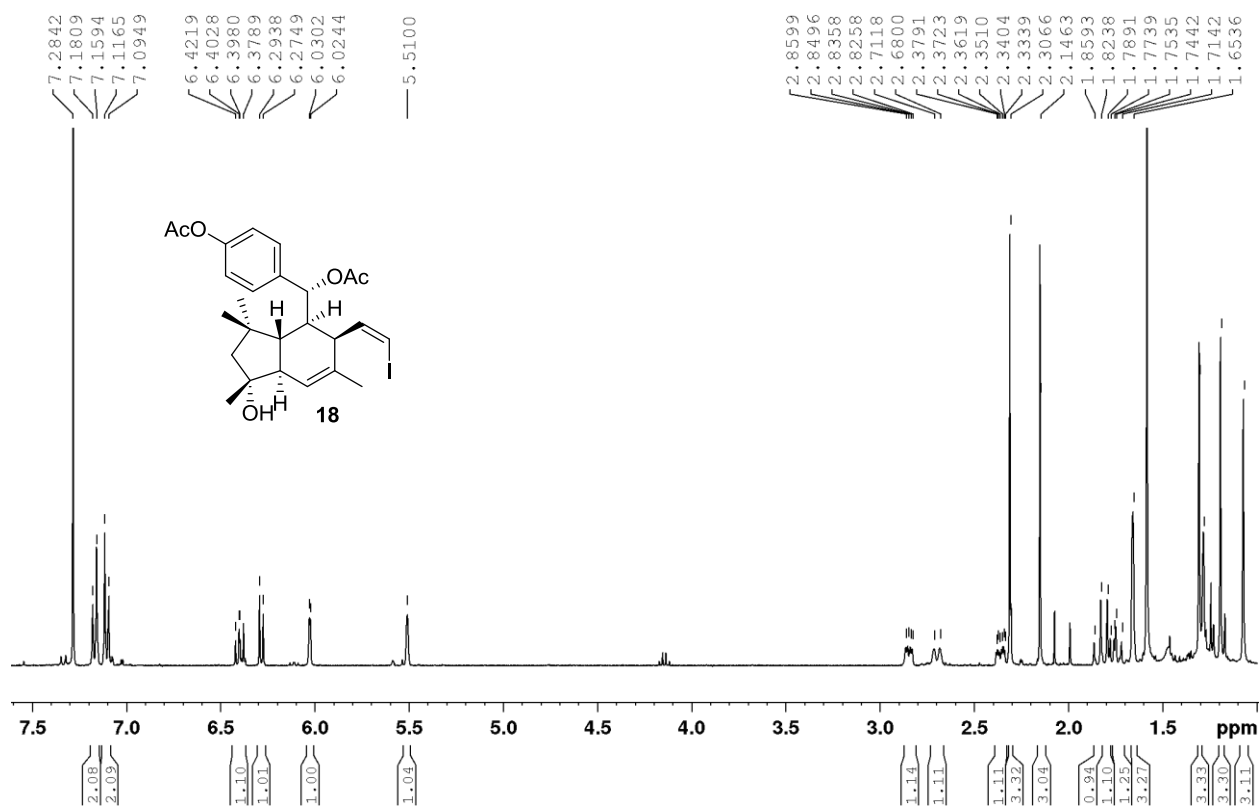
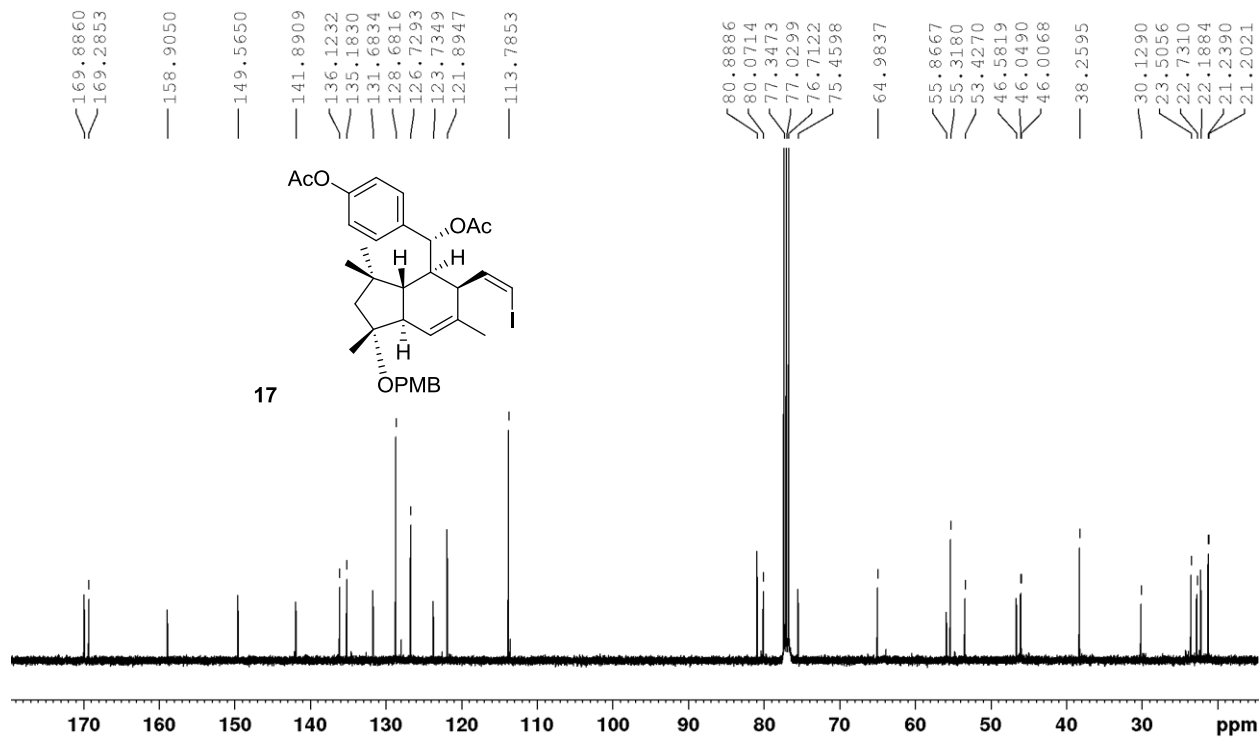
### $^1\text{H}$ and $^{13}\text{C}$ NMR spectra of synthesized compounds

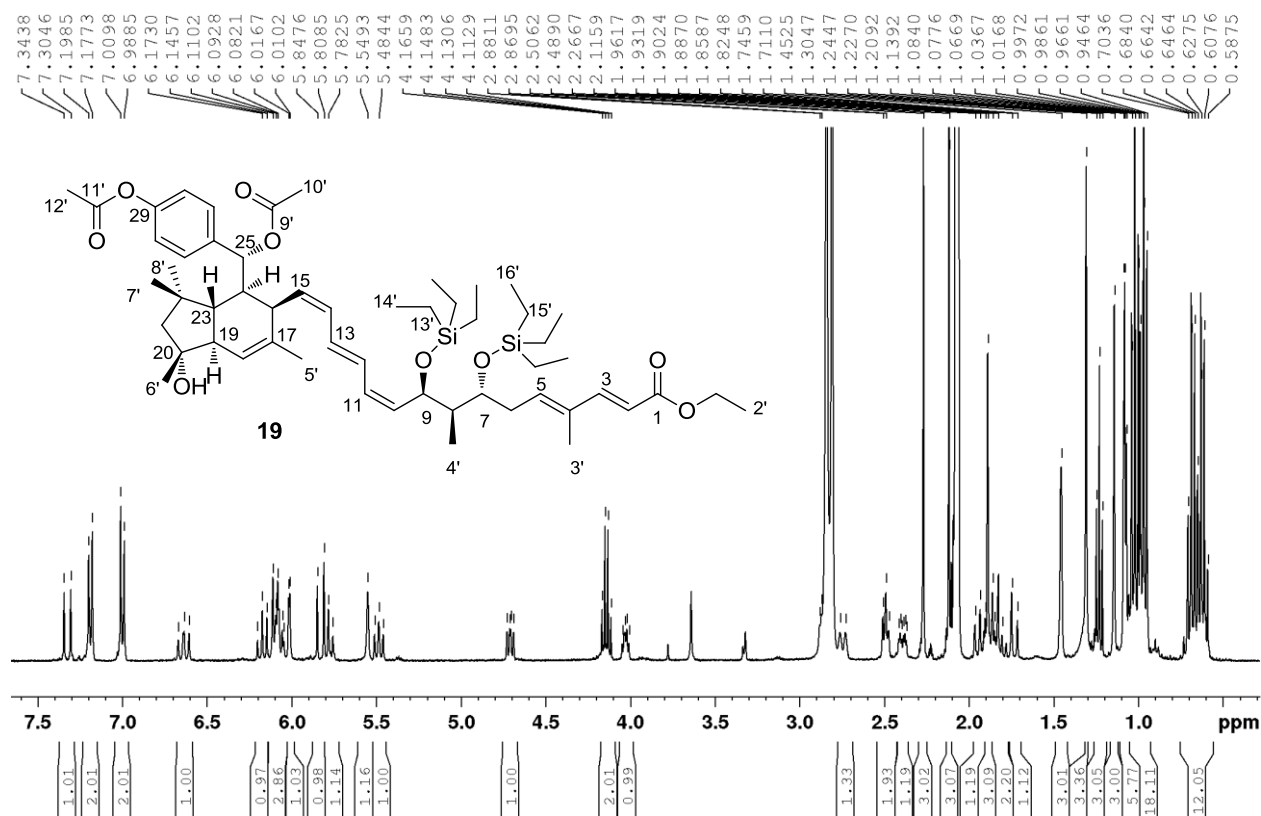
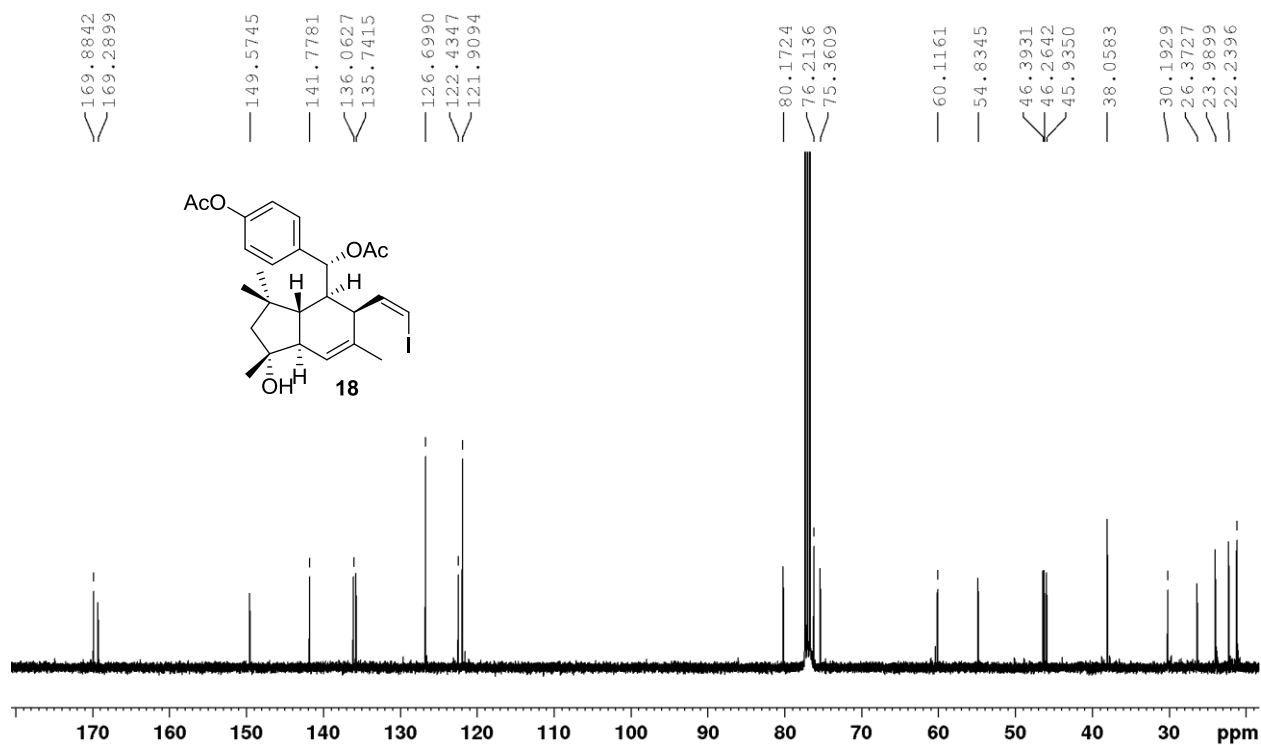


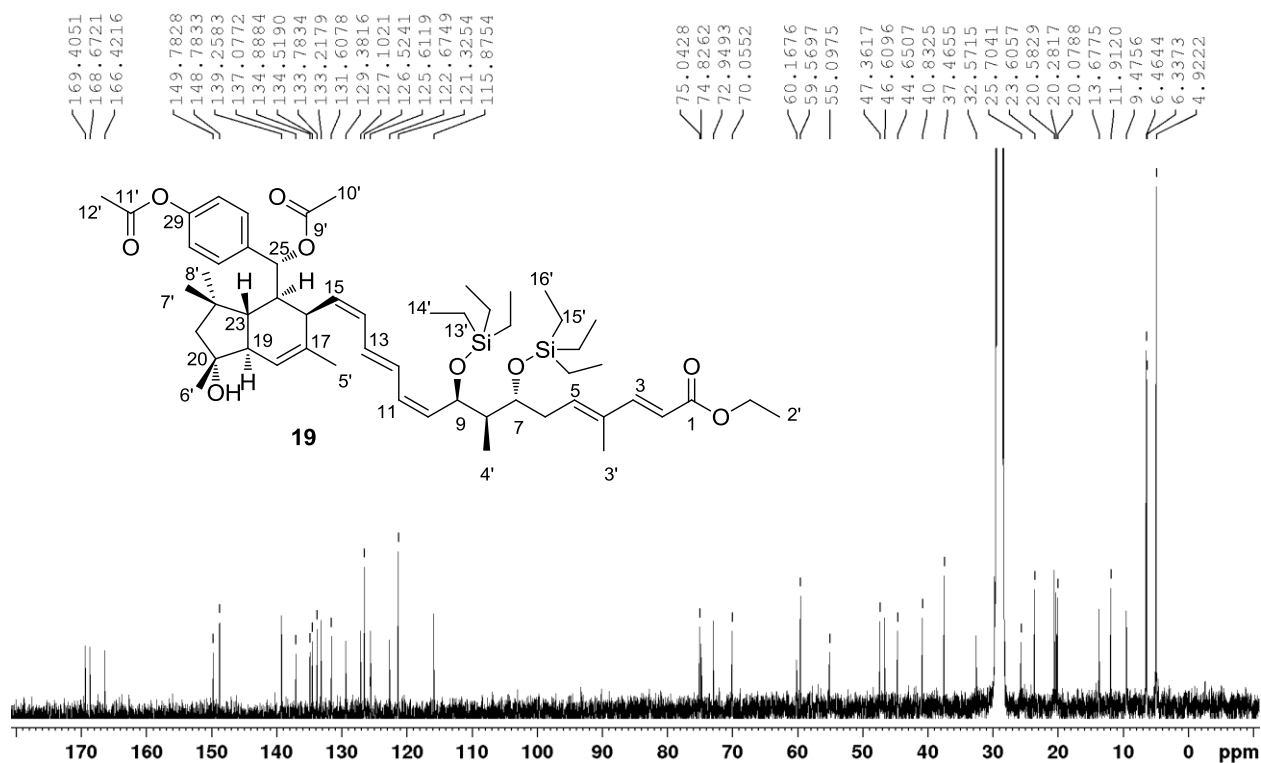




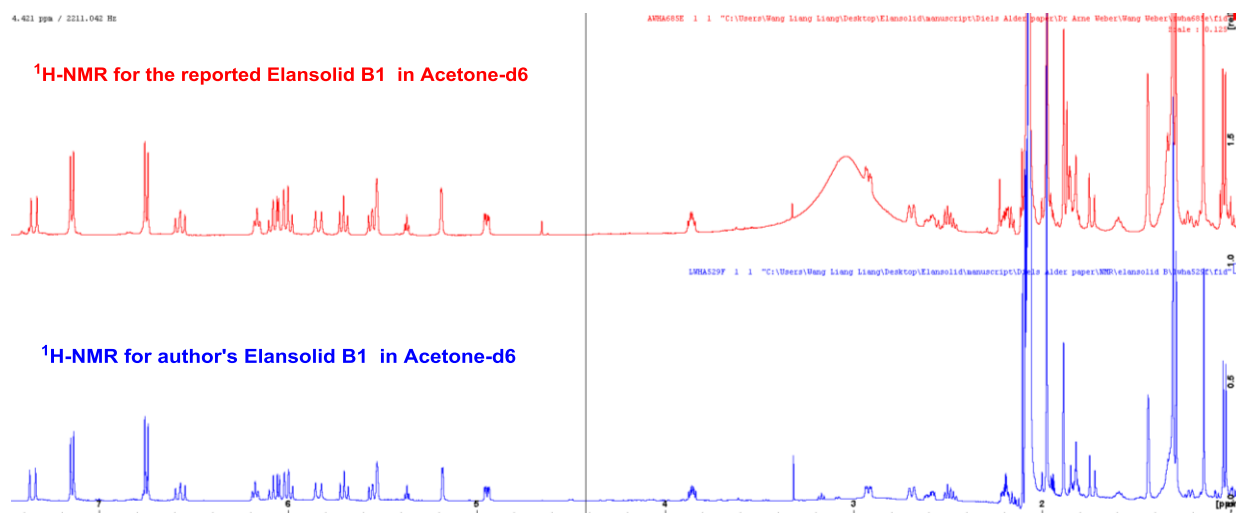




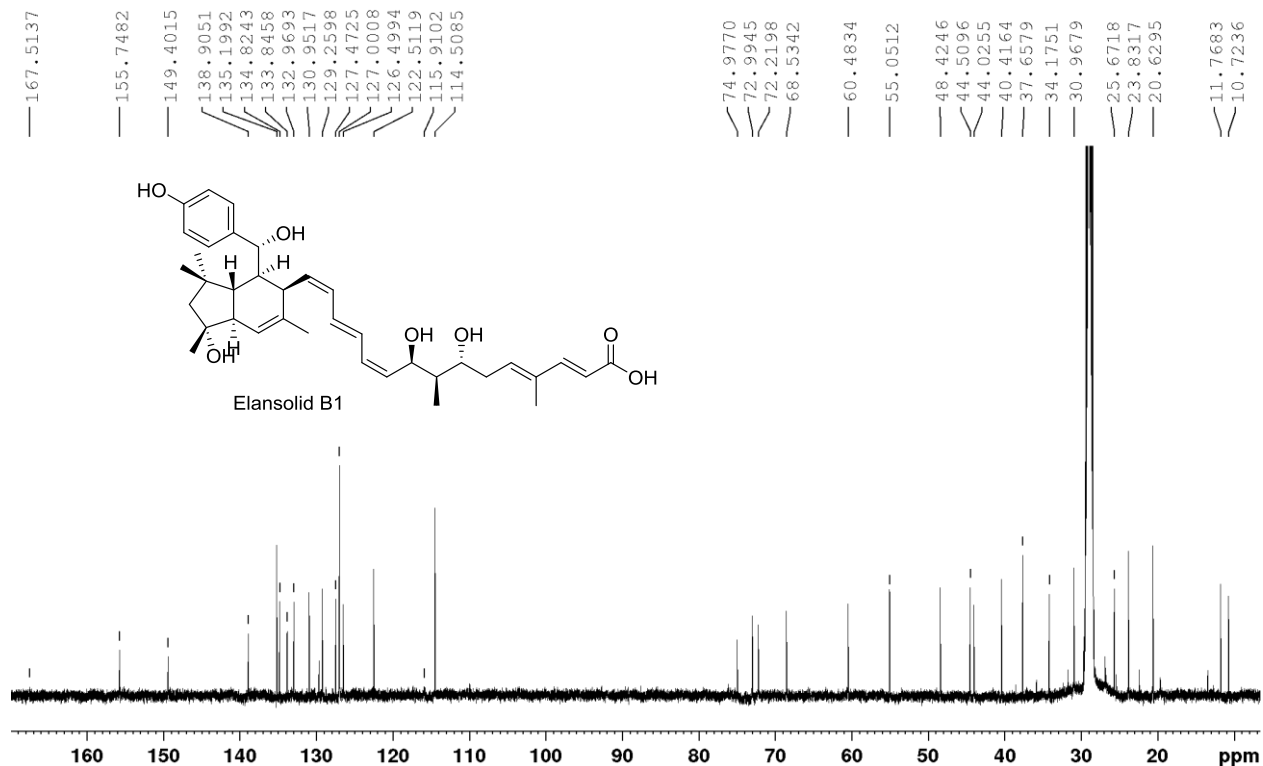
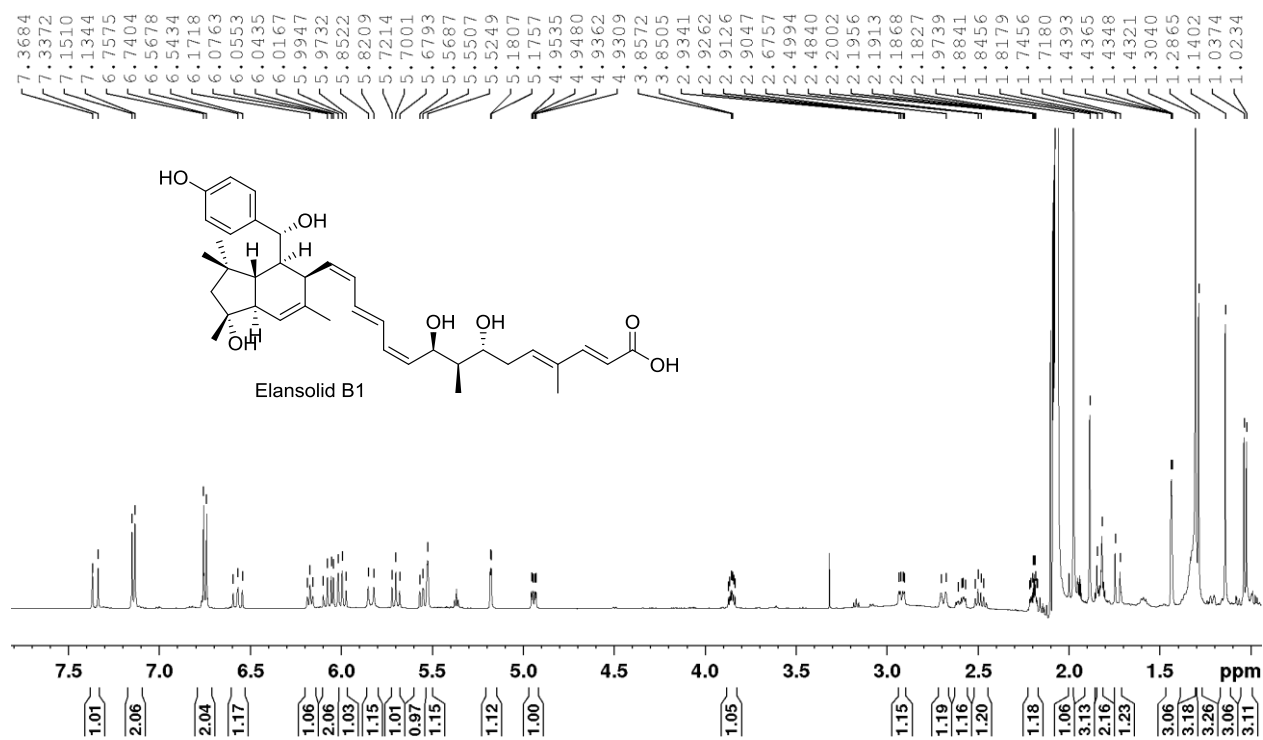




**Elansolid B1: Comparison of  $^1\text{H}$  NMR spectra of the synthetic sample (blue) with the reported one (red) [S1]**

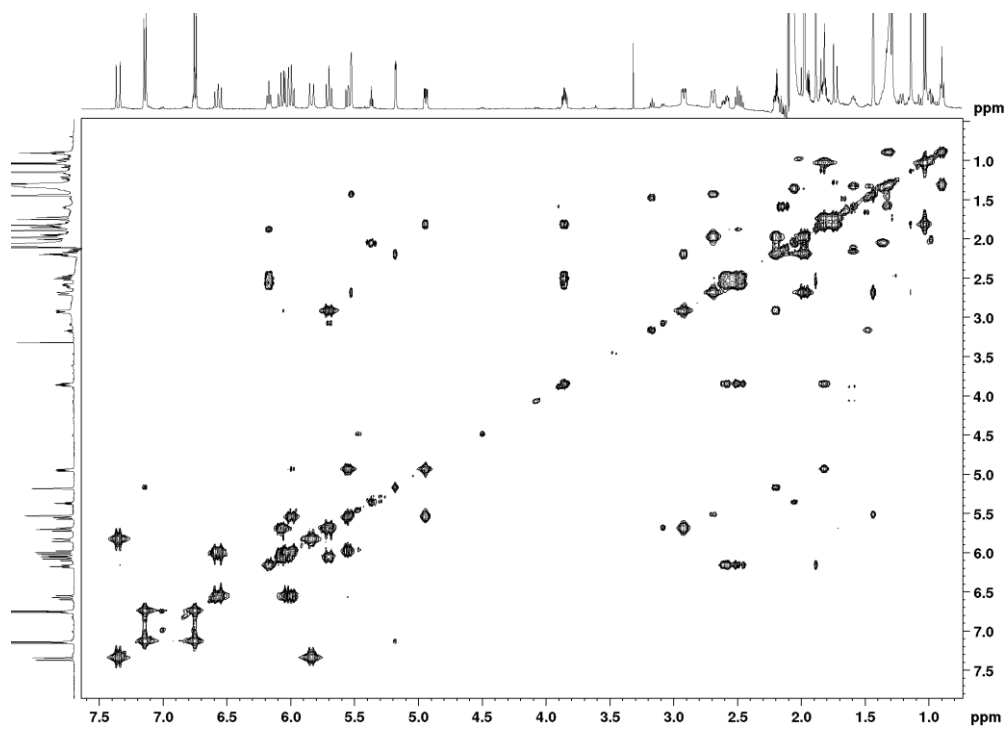


**Elansolid B1:  $^1\text{H}$ ,  $^{13}\text{C}$  NMR in acetone- $d_6$**

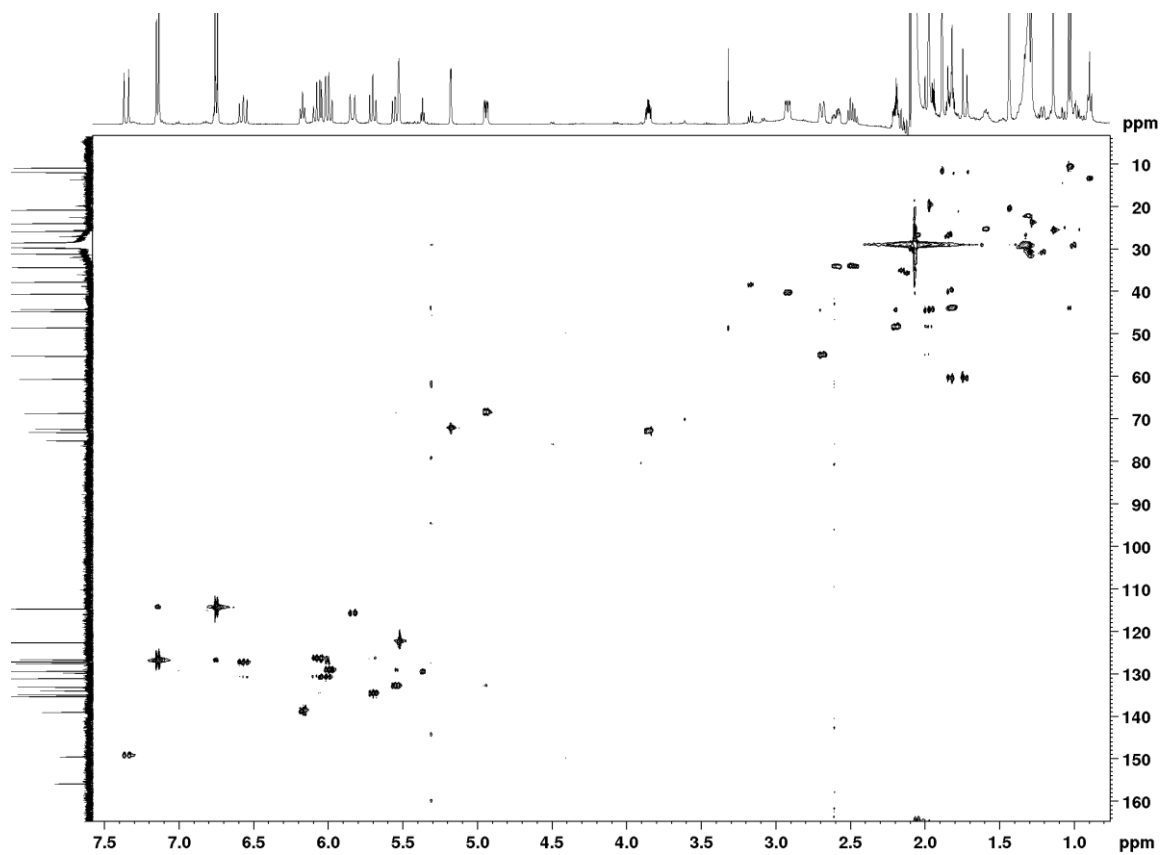




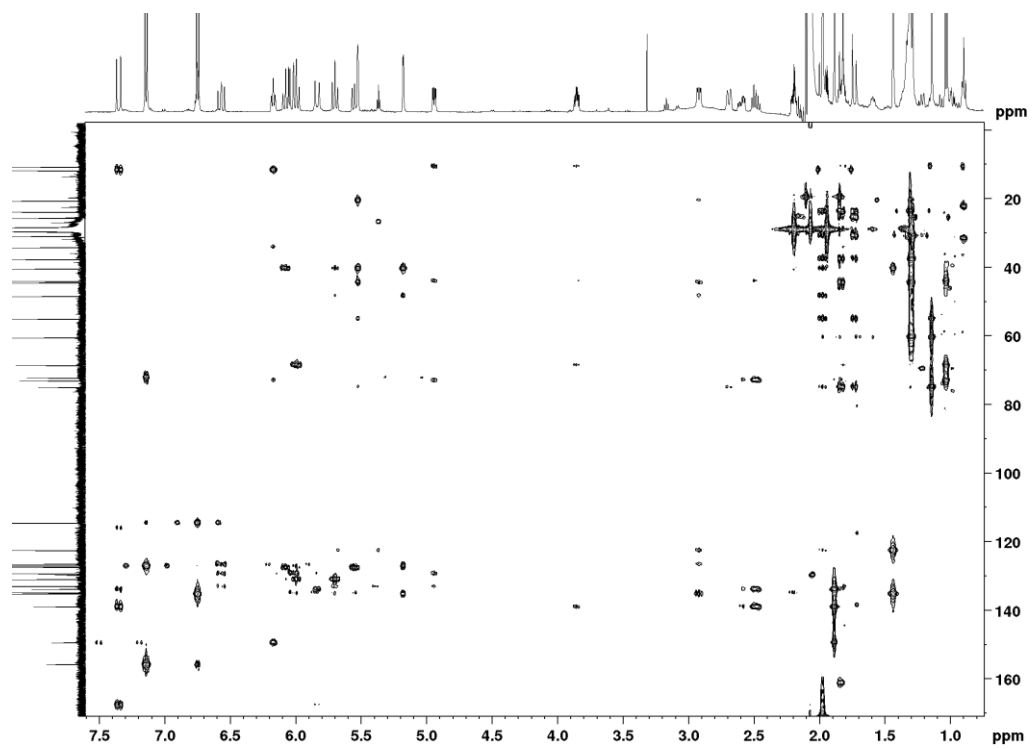
Elansolid B1:  $^1\text{H}$ - $^1\text{H}$  COSY in acetone- $d_6$



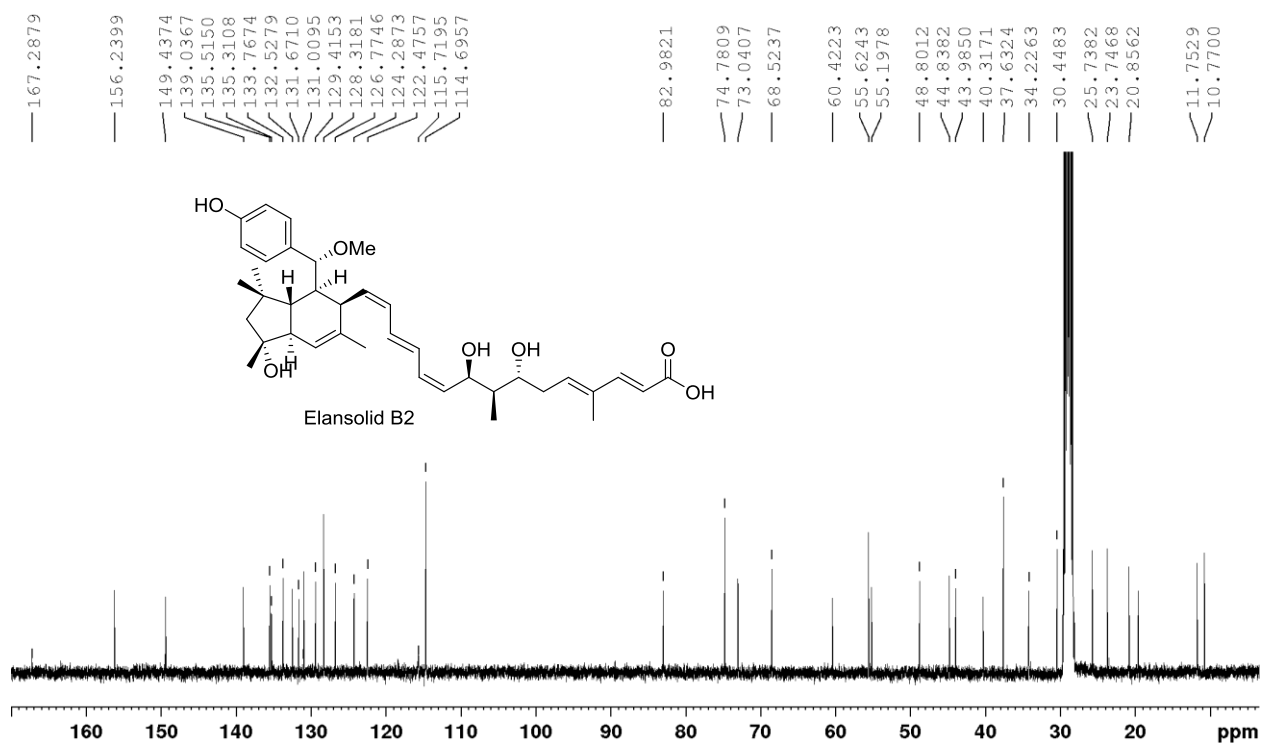
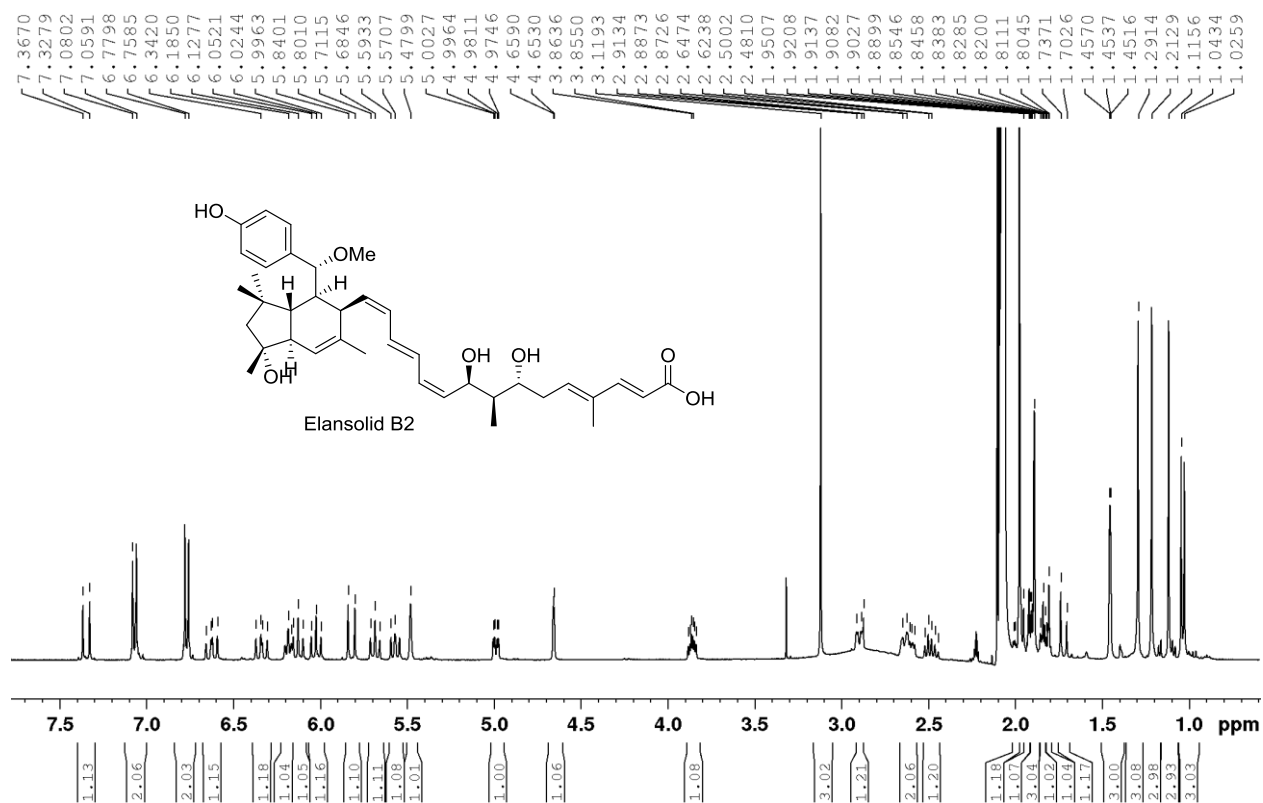
Elansolid B1:  $^1\text{H}$ - $^{13}\text{C}$  HSQC in acetone- $d_6$



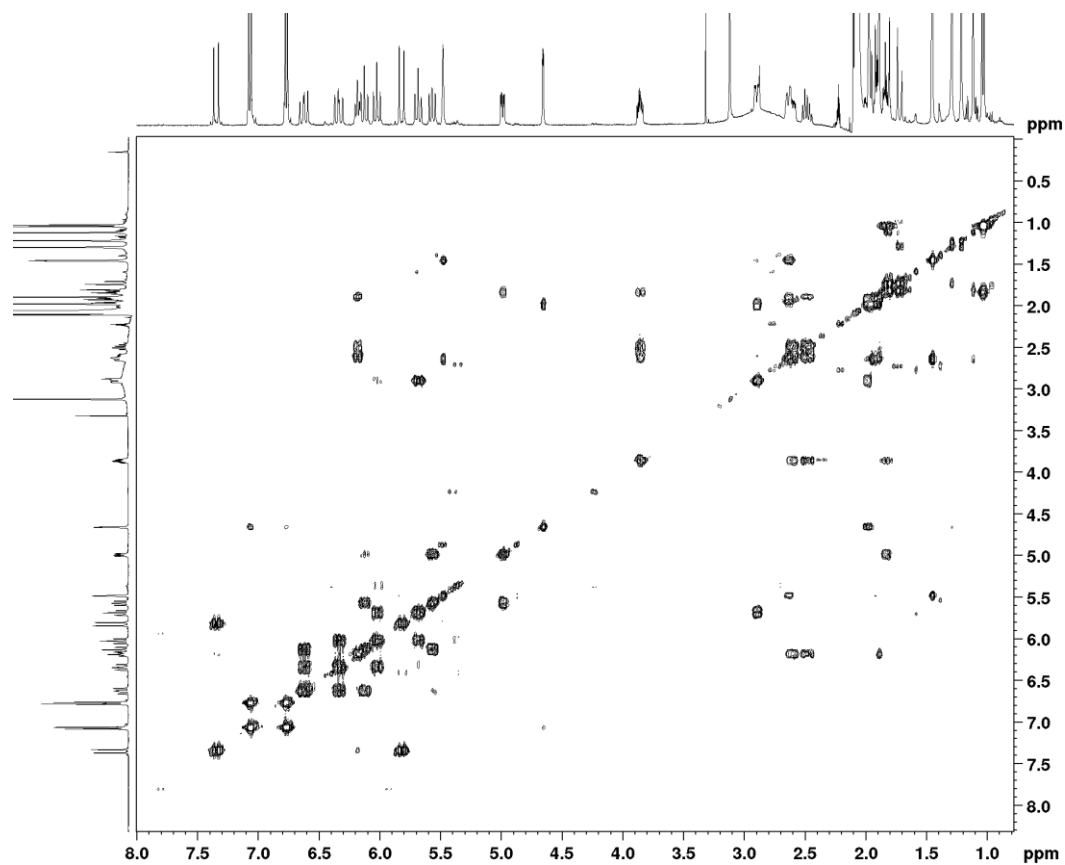
Elansolid B1:  $^1\text{H}$ - $^{13}\text{C}$  HMBC in acetone- $d_6$



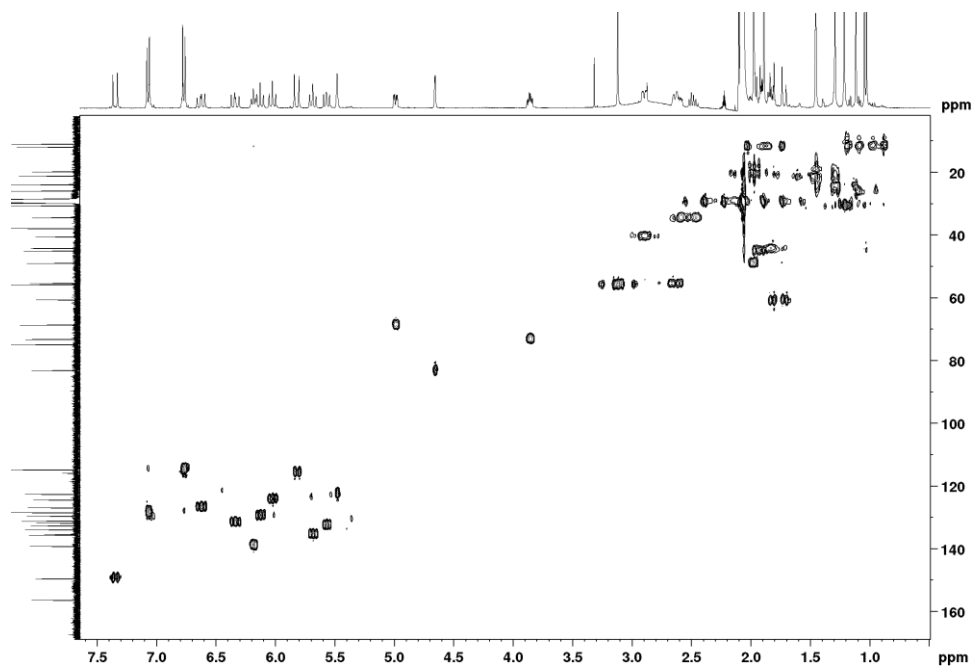
**Elansolid B2:  $^1\text{H}$ ,  $^{13}\text{C}$  NMR in acetone- $d_6$**



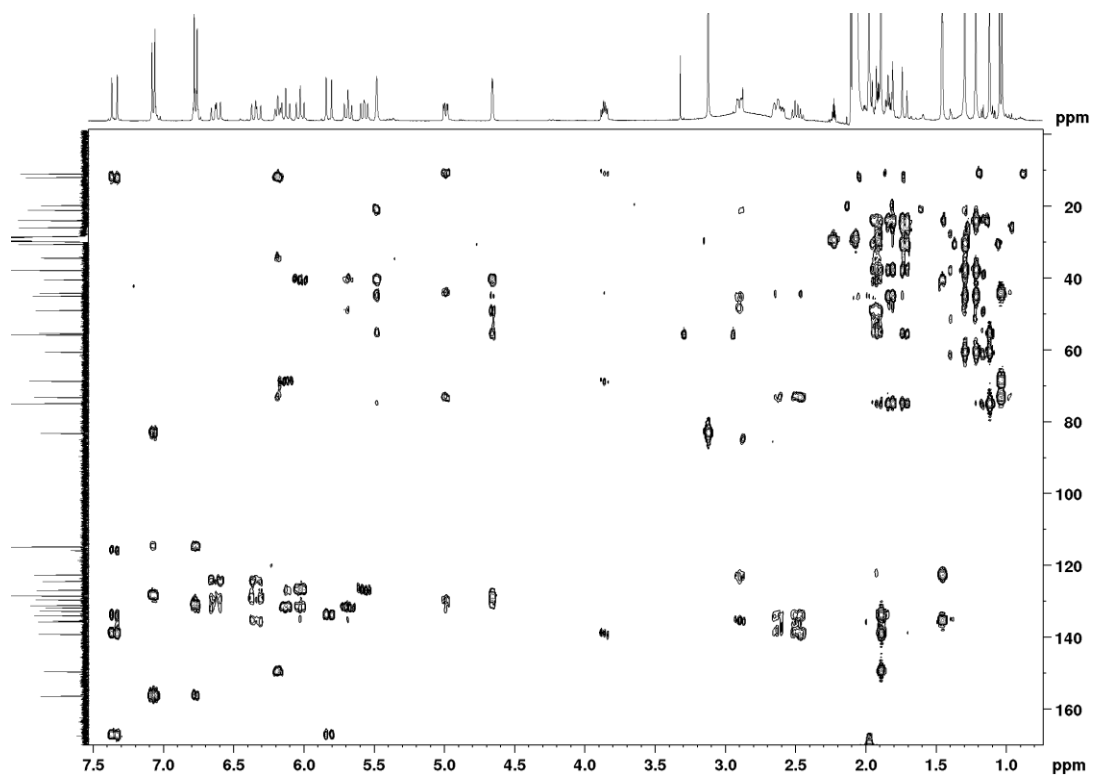
Elansolid B2:  $^1\text{H}$ - $^1\text{H}$  COSY in acetone- $d_6$



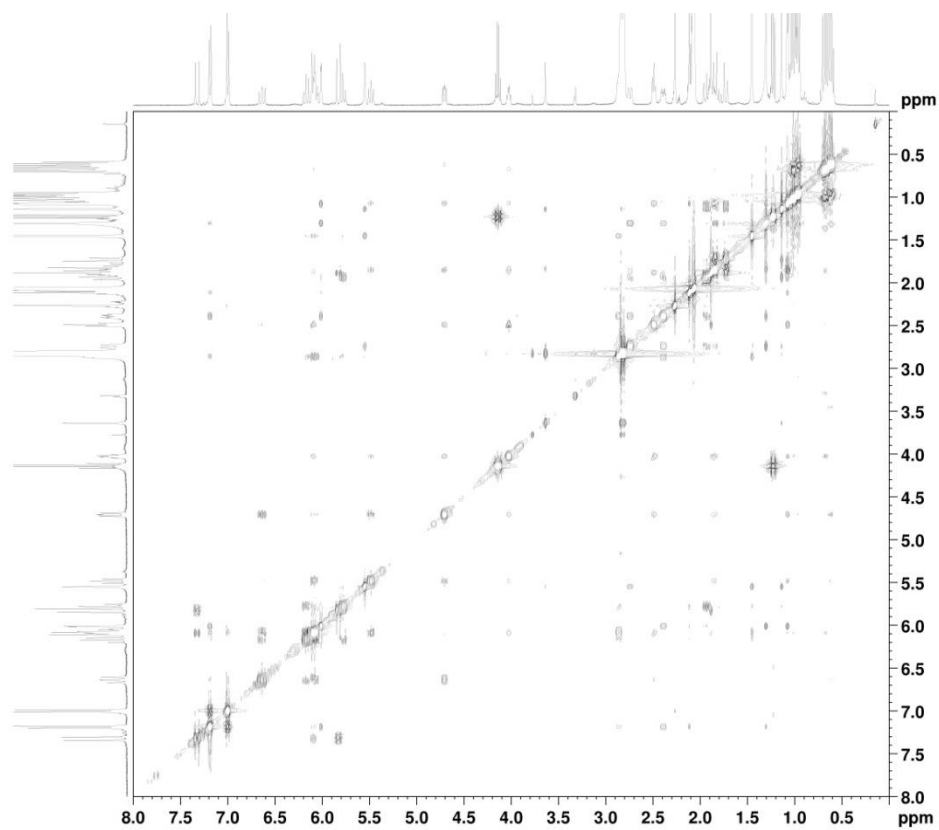
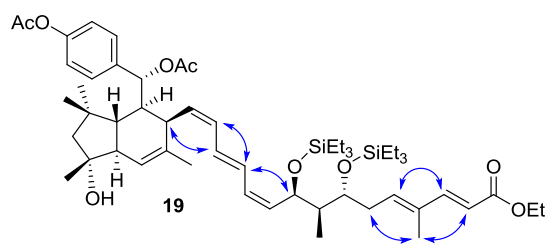
Elansolid B2:  $^1\text{H}$ - $^{13}\text{C}$  HSQC in acetone- $d_6$



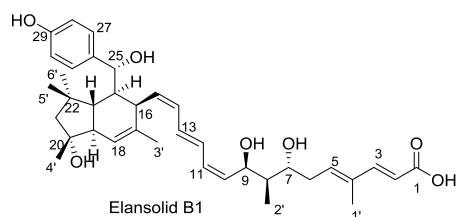
Elansolid B2:  $^1\text{H}$ - $^{13}\text{C}$  HMBC in acetone- $d_6$



Selective key nOe for compound **19**



**Elansolid B1: Comparison of  $^1\text{H}$ ,  $^{13}\text{C}$  NMR spectra for the author's sample and the reported one**



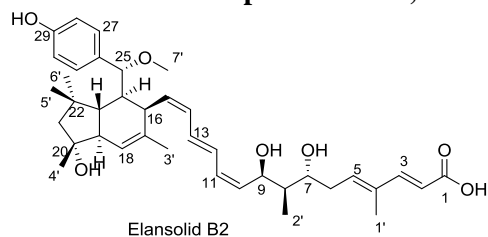
Elansolid B1: 500 MHz $^1\text{H}$ NMR (acetone- $d_6$ ) (author's sample)				Elans. B1: 600 MHz $^1\text{H}$ NMR (acetone- $d_6$ ) (ref.: Angew. Chem. Int. Ed. 2011, 50, 532-536)			
H	$\delta_{\text{H}}$	m	J(Hz)	H	$\delta_{\text{H}}$	m	J(Hz)
-				-			
2	5.84	d	15.7	2	5.82	d	15.7
3	7.35	d	15.6	3	7.33	d	15.8
-				-			
5	6.17	t	7.23	5	6.17	t	7.23br
6a	2.59	ddd	4.2, 6.8, 15.3	6a	2.58	ddd	4.0, 7.1, 15.3
6b	2.51-2.47	m	-	6b	2.47	dt	7.6, 15.3
7	3.87-3.84	m	-	7	3.84	td	4.2, 7.2
8	1.83-1.80	m	-	8	1.80	ddq	3.7, 6.6, 7.0
9	4.94	ddd	0.9, 3.6, 8.6	9	4.93	dd	3.3, 8.8br
10	5.55	dd	9.5, 10.9	10	5.53	dd	9.0, 10.5
11	5.99	dd	10.8, 11.0	11	5.98	t	11.0
12	6.57	dd	12.2, 13.6	12	6.55	dd	11.9, 14.1
13	6.09-6.02	m	-	13	6.02	t	11.7, 14.1
14	overlap			14	6.06	t	11.0
15	5.70	t	10.5	15	5.68	t	10.8
16	2.92	dd	4.0, 10.8	16	2.91	dd	4.0, 10.6
-				-			
18	5.52	s	-	18	5.51	s	br
19	2.69	d	12.6	19	2.67	dq	1.5, 12.6
-				-			
21a	1.83;	d;	13.8;	21a	1.82;	d;	13.8;
21b	1.73	d	13.8	21b	1.72	d	13.8
-				-			
23	1.99-1.95	m	-	23		dd	11.3, 12.5
24	2.22-2.18	m	-	24	2.19	ddd	3.1, 4.1, 11.5
25	5.18	d	2.5	25	5.16	d	2.6
-				-			
27	7.14	d	8.3	27	7.13	d	8.4
28	6.75	d	8.5	28	6.73	d	8.4
-				-			
1'	1.88	s	-	1'	1.87	s	-
2'	1.03	d	7.0	2'	1.01	d	7.0
3'	1.44	dd	1.4, 2.2	3'	1.42	q	1.0br
4'	1.14	s	-	4'	1.13	s	-
5'	1.30	s	-	5'	1.29	s	-
6'	1.29	s	-	6'	1.27	s	-

Elansolid B1: 125 MHz <sup>13</sup> C NMR (acetone- <i>d</i> <sub>6</sub> ) (author's sample )		Elans. B1: 125 MHz <sup>1</sup> H NMR (acetone- <i>d</i> <sub>6</sub> ) (ref.: Org.Lett. 2016, 16, 568-571)	
C	δ <sub>C</sub>	C	δ <sub>C</sub>
1	167.5	1	-
2	115.9	2	-
3	149.4	3	150.2
4	133.8	4	134.8
5	138.9	5	139.7
6	34.1	6	35.1
7	73.0	7	73.9
8	44.0	8	44.9
9	68.5	9	69.4
10	132.9	10	133.9
11	129.3	11	130.2
12	127.5	12	128.3
13	130.9	13	131.9
14	126.5	14	127.4
15	134.8	15	135.7
16	40.4	16	41.3
17	135.2	17	136.1
18	122.5	18	123.4
19	55.1	19	55.9
20	74.9	20	75.9
21	60.5	21	61.4
22	37.7	22	38.6
23	44.5	23	45.4
24	48.4	24	49.3
25	72.2	25	73.1
26	135.2	26	136.1
27	127.0	27	127.9
28	114.5	28	115.4
29	155.7	29	156.7
1'	11.8	1'	12.7
2'	10.7	2'	11.6
3'	20.6	3'	21.5
4'	25.7	4'	26.6
5'	30.9	5'	31.9
6'	23.8	6'	24.7

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**Elansolid B2: Comparison of  $^1\text{H}$ ,  $^{13}\text{C}$  NMR spectra for the author's sample and the reported one**



Elansolid B2: 400MHz $^1\text{H}$ NMR (acetone- $d_6$ ) (author's sample )				Elans. B2: 600MHz $^1\text{H}$ NMR (acetone- $d_6$ ) (ref.: Angew. Chem. Int. Ed. 2011, 50, 532-536)			
H	$\delta_{\text{H}}$	m	J(Hz)	H	$\delta_{\text{H}}$	m	J(Hz)
-				-			
2	5.82	t	15.7	2	5.80	d	15.4
3	7.35	d	15.7	3	7.33	d	15.4
-				-			
5	6.18	t	7.2	5	6.17	t	7.2br
6a	2.60-2.58	m		6a	2.59	ddd	3.7, 7, 15.4
6b	2.52-2.44	m		6b	2.47	dt	7.7, 15.4
7	3.88-3.84	m	-	7	3.85	ddd	4, 7, 8
8	1.85-1.82	m	-	8	1.81	ddq	3.7, 6.8, 7.2
9	4.99	ddd	0.9, 3.5, 8.6	9	4.98	ddd	1, 3.2, 8.8
10	5.57	dd	9.7, 10.1	10	5.55	dd	8.8, 11
11	6.13	t	11.2	11	6.11	t	11.2
12	6.63	dd	11.5, 14.6	12	6.61	dd	11.5, 14.6
13	6.34	dd	11.5, 14.6	13	6.32	dd	11.5, 14.6
14	6.02	t	11.2	14	6.01	t	11.2
15	5.68	t	10.8	15	5.67	t	10.8
16	2.90	dd	3.3, 10.6	16	2.88	dd	3.5, 10.5
-				-			
18	5.48	s	-	18	5.47	s	-
19	2.64-2.62	m	-	19	2.63	dtq	1.8, 2, 12.1
-				-			
21a	1.82	d	13.5	21a	1.81	d	14.0
21b	1.72	d	13.8	21b	1.71	d	14.0
-				-			
23	1.95-1.91	m	-	23	1.91	t	12.2
24	2.01-1.97	m	-	24	1.97	m	2.6, 3.8, 11.4
25	4.66	d	2.4	25	4.64	d	2.6
-				-			
27	7.07	d	8.4	27	7.05	d	8.5
28	6.77	d	8.5	28	6.75	d	8.5
-				-			
1'	1.89	s	-	1'	1.87	s	-
2'	1.03	d	7.0	2'	1.02	d	7.0
3'	1.45	dd	1.3, 2.1	3'	1.44	dt	1, 1.3
4'	1.12	s	-	4'	1.10	s	-
5'	1.29	s	-	5'	1.28	s	-
6'	1.21	s	-	6'	1.20	s	-
7'	3.12	s	-	7'	3.10	s	-

Elansolid B2: 100 MHz <sup>13</sup> C NMR (acetone- d <sub>6</sub> ) (author's sample )		Elansolid B2: 150 MHz <sup>13</sup> C NMR (acetone- d <sub>6</sub> ) (ref.:Angew. Chem. Int. Ed. 2011, 50, 532-536)	
C	δ <sub>C</sub>	C	δ <sub>C</sub>
1	167.3	1	168.1
2	115.7	2	116.5
3	149.4	3	150.4
4	133.8	4	134.7
5	139.0	5	139.9
6	34.2	6	35.2
7	73.0	7	74.1
8	44.0	8	44.9
9	68.5	9	69.5
10	132.5	10	133.4
11	129.4	11	130.3
12	126.8	12	127.7
13	131.6	13	132.6
14	124.3	14	125.2
15	135.5	15	136.4
16	40.3	16	41.2
17	135.3	17	136.2
18	122.5	18	123.3
19	55.2	19	56.1
20	74.8	20	75.8
21	60.4	21	61.4
22	37.6	22	38.5
23	44.8	23	45.8
24	48.8	24	49.7
25	82.9	25	83.9
26	131.0	26	131.9
27	128.3	27	129.2
28	114.7	28	115.6
29	156.2	29	157.2
1'	11.8	1'	12.6
2'	10.8	2'	11.6
3'	20.9	3'	21.7
4'	25.7	4'	26.6
5'	23.7	5'	24.6
6'	30.4	6'	31.3
7'	55.6	7'	56.5

#### 4. References SI:

- [S1] A. Weber, R. Dehn, N. Schläger, B. Dieter, A. Kirschning, *Org. Lett.* **2014**, *16*, 568-571.  
[S2] L.L.Wang, D. Candito, G. Dräger, J. Hermann, R. Müller, A. Kirschning, *Chem. Eur. J.* **2017**,  
DOI:10.1002/chem.201605884.