

## Antiproliferative and cytotoxic effects of *Boerhaavia diffusa*-derived sitosteryl oleate and its derivatives in human glioblastoma (U-87) cells

Rakhi Srivastava<sup>1</sup>, Nalini Yadav<sup>1</sup>, Lucky<sup>1</sup>, Daman Saluja<sup>1</sup> and Madhu Chopra<sup>1,2\*</sup>

<sup>1</sup>Dr. B. R. Ambedkar Center for Biomedical Research, University of Delhi, Delhi 110007, India

<sup>2</sup>Delhi School of Public Health, Institution of Eminence, University of Delhi, Delhi 1100007, India

Received 16 June 2025; revised received 27 February 2026; accepted 11 March 2026

### Supplementary Tables

Supplementary Table 1 — <sup>1</sup>H- and <sup>13</sup>C-NMR, and <sup>1</sup>H, <sup>1</sup>H- COSY Data of isolated sitosteryl oleate (1) in CDCl<sub>3</sub> (δ in ppm)

Position	<sup>13</sup> C-NMR	<sup>1</sup> H-NMR	<sup>1</sup> H, <sup>1</sup> H-COSY
1	37.23	1.14 (m)	
2	27.21	1.81 (m)	H-C(3)
3	74.1	4.15 (m, 1H)	H-C(2), H-C(4)
4	38.15	2.7 (m)	H-C(3)
5	140.65	—	
6	122	5.36 (m)	H-C(4), H-C(7)
7	31.91	1.98 (m)	H-C(6)
8	31.85		
9	50.12		
10	36.49	—	
11	21.07		
12	39.77	1.23, 2.02	
13	42.31		
14	56.75	1.09 (m)	
15	24.80		
16	28.23		
17	56.05		
18	11.84	0.68 (s, 3H)	
19	19.38	0.98 (s, 3H)	
20	36.13		
21	18.77	0.89 (m)	
22	33.94		
23	26.08		
24	45.83	0.93 (m)	
25	29.18		
26	19.80	0.84 (m)	
27	19.02	0.80 (m)	
28	23.06		
29	11.96	0.82 (m)	
1'	180	—	
2'	34.28	2.31 (m)	H-C(3')
3'	25.62	1.28 (m)	H-C(2')
4'	29.28		
5'	29.47		
6'	29.51		
7'	29.62		
8'	27.16		
9'	130.16	5.36 (m)	
10'	130.21	5.36 (m)	

(Contd.)

Supplementary Table 1 — <sup>1</sup> H- and <sup>13</sup> C-NMR, and <sup>1</sup> H, <sup>1</sup> H- COSY Data of isolated sitosteryl oleate (1) in CDCl <sub>3</sub> (δ in ppm) (Contd.)					
Position	<sup>13</sup> C-NMR	<sup>1</sup> H-NMR	<sup>1</sup> H, <sup>1</sup> H-COSY		
11'	21.19				
12'	29.69				
13'	29.75				
14'	29.75				
15'	29.75				
16'	31.82				
17'	22.68				
18'	14.10	0.89 (m)			

Supplementary Table 2 — <sup>1</sup> H- and <sup>13</sup> C-NMR, and HRMS Data of synthesised sitosteryl esters 2a, 2b, 2c, 2d, 2e, 2f, 2g, 2h, 2i, 2j in CDCl <sub>3</sub> (δ in ppm)					
Compound No.	Name	Description	<sup>1</sup> H NMR (400MHz, CDCl <sub>3</sub> ) (ppm)	<sup>13</sup> C NMR (400MHz, CDCl <sub>3</sub> ) (ppm)	HRMS
2a	17-(5-ethyl-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-10,13-dimethyl-1H-cyclopenta[a]phenanthren-3-yl acetate	White shiny crystals, yield: 59%	0.675 (d, 3H), 0.77-0.85 (m, 10H), 0.90 (m, 1H) 0.93 (t, 5H), 1.01 (s, 6H), 1.24 (t, 3H), 1.42-1.52 (m, 6H), 1.56 (s, 3H), 1.61-1.69 (m, 3H), 1.83-1.86 (m, 3H), 1.94 (s, 1H), 1.98 (s, 1H), 2.01(s, 1H), 2.24 (t, <i>J</i> =8Hz, 2H), 2.30 (d, <i>J</i> =8Hz, 2H), 4.62 (m,1H), 5.35 (s, 1H)	11.93, 12.06, 13.72, 18.63, 18.86, 19.06, 19.11, 19.41, 19.90, 21.10, 21.17, 21.30, 23.14, 25.49, 26.14, 29.00, 29.22, 31.97, 34.01, 36.68, 38.25, 42.39, 45.91, 50.10, 56.00, 56.11, 56.77, 73.76, 122.66, 139.80, 173.24	calculated for C <sub>31</sub> H <sub>52</sub> O <sub>2</sub> [M] <sup>+</sup> 456.74, found [M] <sup>+</sup> 456.7416
2b	17-(5-ethyl-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-10,13-dimethyl-1H-cyclopenta[a]phenanthren-3-yl propionate	White shiny crystals, yield: 78%	0.675 (d, 3H), 0.75-0.85 (m, 10H), 0.89-0.92 (m, 3H), 1.01 (s, 6H), 1.05-1.27 (m, 12H), 1.42-1.57 (m, 9H), 1.83-1.86 (m, 3H), 1.94-2.01 (m, 2H), 2.26-2.31 (m, 4H), 4.56-4.63 (m, 1H), 5.36 (s, 1H)	11.93, 12.06, 18.86, 19.11, 19.40, 19.90, 21.11, 23.14, 24.37, 25.49, 26.14, 27.87, 28.01, 28.32, 29.22, 31.94, 34.01, 36.24, 36.68, 37.08, 38.23, 39.80, 40.59, 42.39, 45.91, 50.10, 51.31, 56.11, 56.77, 73.83, 122.66, 139.81, 174.04	calculated for C <sub>32</sub> H <sub>54</sub> O <sub>2</sub> [M + Na] <sup>+</sup> 493.402, found [M + Na] <sup>+</sup> 493.4010
2c	17-(5-ethyl-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-10,13-dimethyl-1H-cyclopenta[a]phenanthren-3-yl butyrate	White shiny crystals, yield: 76%	0.67 (m, 3H), 0.75-0.85 (m, 11H), 0.90-0.95 (m, 8H), 1.01 (s, 6H), 1.13-1.16 (m, 5H), 1.41-1.49 (m, 4H), 1.52-1.56 (m, 3H), 1.58-1.68 (m, 5H), 1.83-1.86 (m, 3H), 1.92-2.01 (m, 2H), 2.24 (t, 2H), 2.30 (d, 2H), 4.56-4.63 (m, 1H), 5.36 (s, 1H)	11.94, 12.07, 18.86, 19.11, 19.41, 19.91, 21.10, 23.13, 24.37, 25.50, 26.11, 27.90, 28.33, 29.20, 31.93, 34.00, 36.24, 36.67, 37.08, 38.24, 39.79, 40.61, 42.39, 45.89, 50.09, 51.31, 56.10, 56.76, 56.86, 73.75, 122.67, 139.79, 173.25	calculated for C <sub>32</sub> H <sub>56</sub> O <sub>2</sub> [M + Na] <sup>+</sup> 507.4183, found [M + Na] <sup>+</sup> 507.4165
2d	17-(5-ethyl-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-10,13-dimethyl-1H-cyclopenta[a]phenanthren-3-yl pentanoate	White shiny crystals, yield: 62%	0.67 (m, 3H), 0.75-0.85 (m, 11H), 0.90 (t, 7H), 1.01 (s, 6H), 1.09-1.19 (m, 5H), 1.27-1.36 (m, 4H), 1.41-1.49 (m, 4H), 1.52-1.61 (m, 7H), 1.83-1.85 (m, 3H), 1.93-2.01 (m, 2H), 2.26 (t, 2H), 2.31 (s, 2H), 4.57-4.61 (m, 1H), 5.35 (d, 1H)	11.94, 12.06, 13.84, 18.86, 19.10, 19.41, 19.91, 21.10, 22.34, 23.13, 24.37, 26.11, 27.23, 27.89, 28.33, 29.20, 31.98, 34.00, 34.53, 36.24, 36.68, 37.08, 38.23, 39.79, 42.39, 45.90, 50.09, 56.10, 56.76, 73.76, 122.67, 139.80, 173.44	calculated for C <sub>34</sub> H <sub>58</sub> O <sub>2</sub> [M + Na] <sup>+</sup> 521.43298, found [M + Na] <sup>+</sup> 521.4268

(Contd.)

Supplementary Table 2 — <sup>1</sup>H- and <sup>13</sup>C-NMR, and HRMS Data of synthesised sitosteryl esters 2a, 2b, 2c, 2d, 2e, 2f, 2g, 2h, 2i, 2j in CDCl<sub>3</sub> (δ in ppm) (Contd.)

Compound No.	Name	Description	<sup>1</sup> H NMR (400MHz, CDCl <sub>3</sub> ) (ppm)	<sup>13</sup> C NMR (400MHz, CDCl <sub>3</sub> ) (ppm)	HRMS
2e	17-(5-ethyl-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-10,13-dimethyl-1H-cyclopenta[a]phenanthren-3-yl hexanoate	White shiny crystals, yield: 85%	0.67 (m, 3H), 0.75-0.85 (m, 10H), 0.86-0.91 (m, 7H), 1.00 (s, 6H), 1.12-1.15 (m, 3H), 1.27-1.31 (m, 7H), 1.41-1.66 (m, 13H), 1.82-1.86 (m, 3H), 1.93-2.01 (m, 2H), 2.25 (t, 2H), 2.28 (d, 2H), 4.56-4.64 (m, 1H), 5.35 (d, 1H)	11.94, 12.06, 12.35, 14.03, 18.86, 19.10, 19.41, 19.91, 21.10, 21.31, 22.42, 23.12, 24.37, 26.10, 27.89, 28.33, 29.19, 31.38, 31.98, 34.00, 34.77, 36.24, 36.68, 37.07, 38.23, 39.79, 42.38, 45.89, 50.08, 56.09, 56.76, 73.77, 122.67, 139.79, 173.46	calculated for C <sub>35</sub> H <sub>60</sub> O <sub>2</sub> [M + Na] <sup>+</sup> 535.4490, found [M + Na] <sup>+</sup> 535.4424
2f	17-(5-ethyl-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-10,13-dimethyl-1H-cyclopenta[a]phenanthren-3-yl octanoate	White shiny crystals, yield: 60%	0.66 (m, 3H), 0.75-0.91 (m, 16H), 1.00 (s, 6H), 0.13 (m, 3H), 1.27 (t, 13H), 1.41-1.49 (m, 4H), 1.53-1.61 (m, 8H), 1.82-1.86 (m, 3H), 1.93-2.01 (m, 2H), 2.23-2.39 (m, 4H), 4.56-4.64 (m, 1H), 5.35 (d, 1H).	11.94, 12.06, 14.17, 18.86, 19.10, 19.41, 19.91, 21.10, 22.69, 23.12, 24.37, 25.15, 26.10, 27.88, 28.33, 29.02, 29.16, 31.75, 31.93, 31.98, 34.00, 34.81, 36.24, 36.68, 37.07, 38.23, 39.79, 42.38, 45.89, 50.08, 51.31, 56.09, 56.76, 73.77, 122.67, 139.79, 173.48	calculated for C <sub>37</sub> H <sub>64</sub> O <sub>2</sub> [M + Na] <sup>+</sup> 563.4803, found [M + Na] <sup>+</sup> 563.4767
2g	17-(5-ethyl-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-10,13-dimethyl-1H-cyclopenta[a]phenanthren-3-yl nonanoate	White shiny crystals, yield: 82%	0.66 (m, 3H), 0.75-0.91 (m, 17H), 1.01 (s, 6H), 1.12-1.16 (m, 3H), 1.26 (d, 14H), 1.41-1.61 (m, 11H), 1.82-1.86 (m, 3H), 1.92-2.01 (m, 2H), 2.25 (t, 2H), 2.29 (d, 2H), 4.56-4.64 (m, 1H), 5.35 (d, 1H)	11.94, 12.06, 12.12, 18.78, 18.86, 19.06, 19.10, 19.41, 19.91, 20.30, 21.10, 21.30, 22.73, 23.13, 24.37, 25.15, 25.50, 26.11, 27.89, 28.33, 29.21, 29.31, 31.90, 31.93, 31.98, 34.81, 36.24, 36.68, 37.08, 38.23, 39.79, 42.38, 45.90, 50.09, 51.31, 56.10, 56.76, 73.35, 122.66, 139.80, 173.45	calculated for C <sub>38</sub> H <sub>66</sub> O <sub>2</sub> [M + Na] <sup>+</sup> 577.4959, found [M + Na] <sup>+</sup> 577.4746
2h	17-(5-ethyl-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-10,13-dimethyl-1H-cyclopenta[a]phenanthren-3-yl decanoate	White shiny crystals, yield: 85%	0.66 (m, 3H), 0.75-0.91 (m, 17H), 1.01 (s, 6H), 1.12-1.16 (m, 3H), 1.25-1.28 (m, 17H), 1.41-1.49 (m, 3H), 1.52-1.63 (m, 7H), 1.82-1.86 (m, 3H), 1.93-2.01 (m, 3H), 2.25 (t, 2H), 2.29 (d, 2H), 4.56-4.64 (m, 1H), 5.35 (d, 1H)	11.94, 12.06, 12.12, 12.35, 14.20, 18.86, 19.11, 19.41, 19.91, 21.10, 21.30, 22.76, 23.13, 24.37, 25.16, 25.50, 26.11, 27.89, 28.33, 29.20, 29.35, 29.51, 31.95, 34.00, 34.81, 36.24, 36.68, 37.08, 38.24, 39.79, 40.60, 42.39, 45.90, 50.09, 51.31, 55.99, 56.10, 56.76, 56.86, 73.75, 122.66, 139.80, 173.45	calculated for C <sub>39</sub> H <sub>68</sub> O <sub>2</sub> [M] <sup>+</sup> 568.5219, found [M] <sup>+</sup> 568.7569

(Contd.)

Supplementary Table 2 — <sup>1</sup>H- and <sup>13</sup>C-NMR, and HRMS Data of synthesised sitosteryl esters 2a, 2b, 2c, 2d, 2e, 2f, 2g, 2h, 2i, 2j in CDCl<sub>3</sub> (δ in ppm) (Contd.)

Compound No.	Name	Description	<sup>1</sup> H NMR (400MHz, CDCl <sub>3</sub> ) (ppm)	<sup>13</sup> C NMR (400MHz, CDCl <sub>3</sub> ) (ppm)	HRMS
2i	17-(5-ethyl-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-10,13-dimethyl-1H-cyclopenta[a]phenanthren-3-yl undecanoate	White shiny crystals, yield: 83%	0.67 (m, 3H), 0.75-0.91 (m, 17H), 1.00 (s, 6H), 1.12-1.15 (m, 3H), 1.24 (m, 20H), 1.41-1.45 (m, 4H), 1.59 (m, 6H), 1.84 (d, 3H), 1.93-2.01 (m, 3H), 2.25 (t, 2H), 2.29 (d, 2H), 4.56-4.64 (m, 1H), 5.35 (d, 1H)	11.94, 12.06, 12.35, 14.21, 18.86, 19.11, 19.41, 19.91, 20.03, 21.10, 21.31, 22.77, 23.13, 24.37, 25.16, 26.11, 27.89, 28.33, 29.01, 29.20, 29.35, 29.40, 29.55, 29.64, 31.98, 33.78, 34.00, 34.81, 36.24, 36.68, 37.08, 38.24, 38.90, 39.79, 42.38, 45.89, 50.09, 51.31, 56.07, 56.76, 73.75, 122.67, 139.79	calculated for C <sub>40</sub> H <sub>70</sub> O <sub>2</sub> [M + Na] <sup>+</sup> 605.5272, found [M + Na] <sup>+</sup> 605.5097
2j	17-(5-ethyl-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-10,13-dimethyl-1H-cyclopenta[a]phenanthren-3-yl benzoate	White shiny crystals, yield: 62%	0.69 (d, 6H), 0.71-0.84 (m, 14H), 1.25 (m, 8H), 1.38-1.84 (m, 14H), 2.45 (t, 2H), 4.8 (m, 1H), 5.37 (m, 2H), 7.26 (m, 2H), 7.43 (m, 1H), 8.05 (m, 2H)	11.95, 19.47, 21.13, 23.14, 24.38, 27.96, 31.96, 36.74, 37.11, 38.29, 39.81, 42.40, 45.90, 50.11, 50.91, 56.77, 74.71, 122.88, 128.57, 129.45, 129.63, 130.28, 133.85, 139.73, 171.97	calculated for C <sub>36</sub> H <sub>54</sub> O <sub>2</sub> [M] + H 519.419, found [M] + H 519.1384

## Supplementary Figures

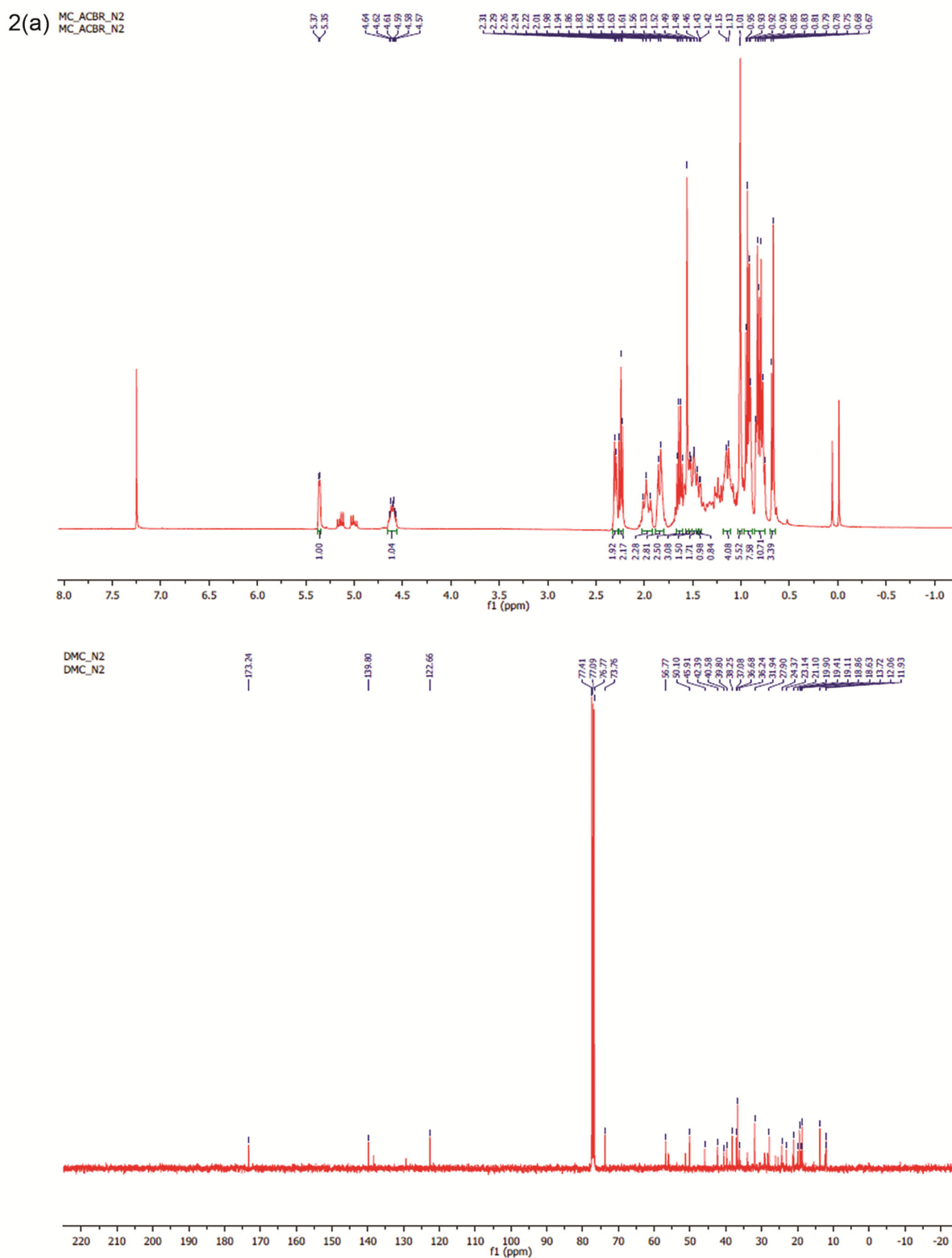


Fig. S1 —  $^1\text{H}$ NMR spectra of newly synthesised compound. 17-(5-ethyl-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-10,13-dimethyl-1H-cyclopenta[a]phenanthren-3-yl acetate (2a).

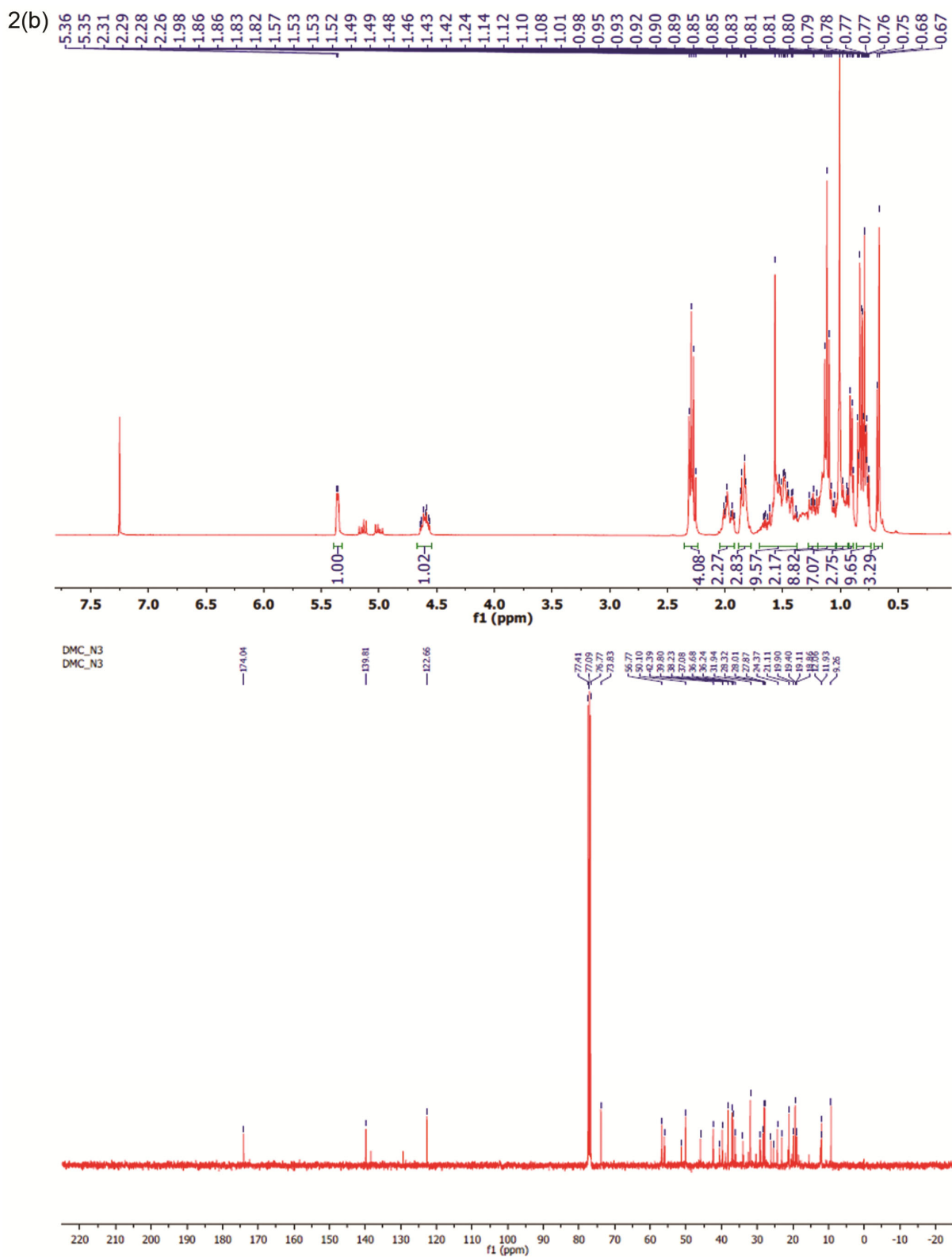


Fig. S2 — <sup>1</sup>H NMR spectra of newly synthesised compound. 17-(5-ethyl-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-10,13-dimethyl-1H-cyclopenta[a]phenanthren-3-yl propionate (2b).

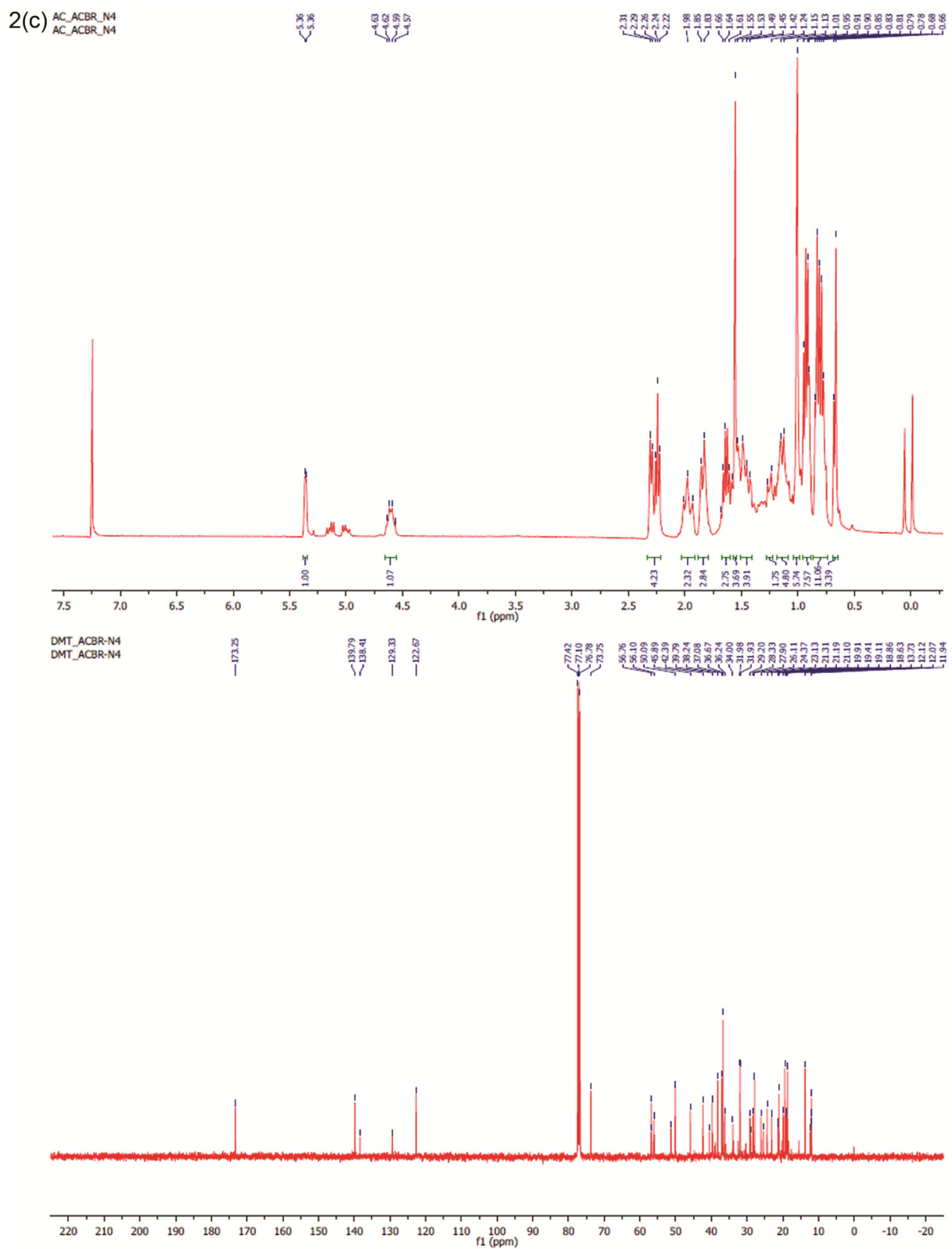


Fig. S3 — <sup>1</sup>HNMR spectra of newly synthesised compound. 17-(5-ethyl-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-10,13-dimethyl-1H-cyclopenta[a]phenanthren-3-yl butyrate (2c).

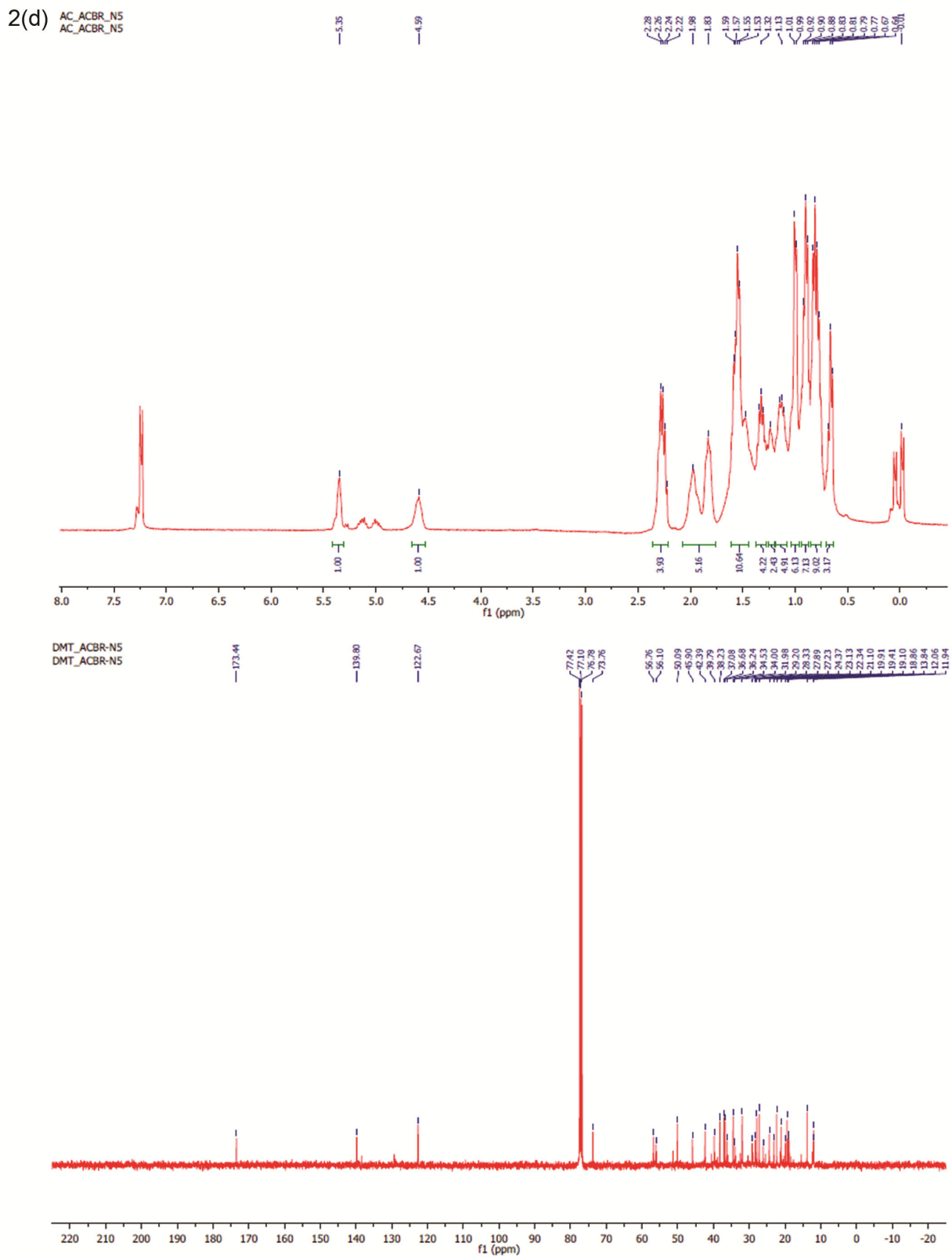


Fig. S4 — <sup>1</sup>HNMR spectra of newly synthesised compound. 17-(5-ethyl-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-10,13-dimethyl-1H-cyclopenta[a]phenanthren-3-yl pentanoate (2d).

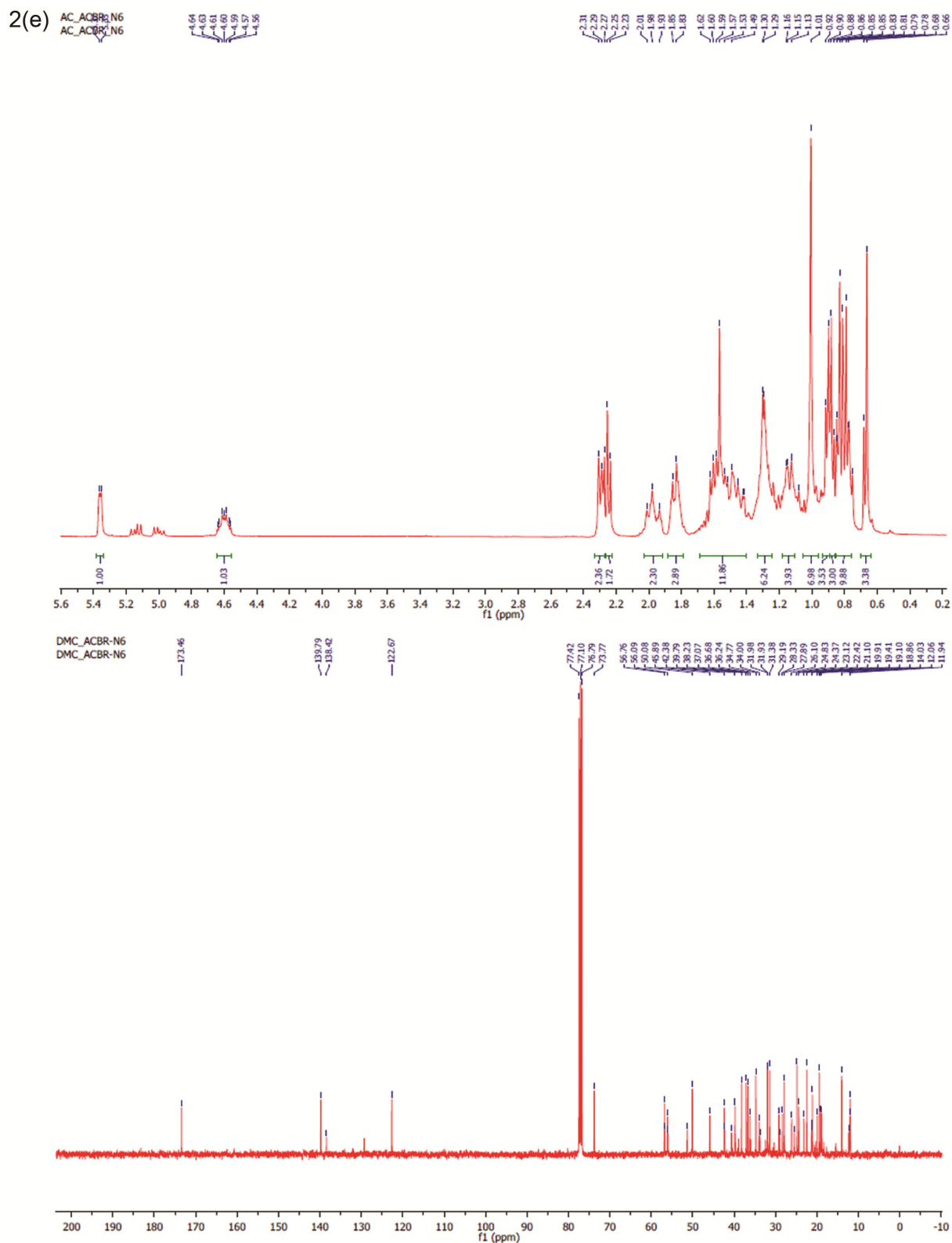


Fig. S5 —  $^1\text{H}$ NMR spectra of newly synthesised compound. 17-(5-ethyl-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-10,13-dimethyl-1H-cyclopenta[a]phenanthren-3-yl hexanoate (2e).

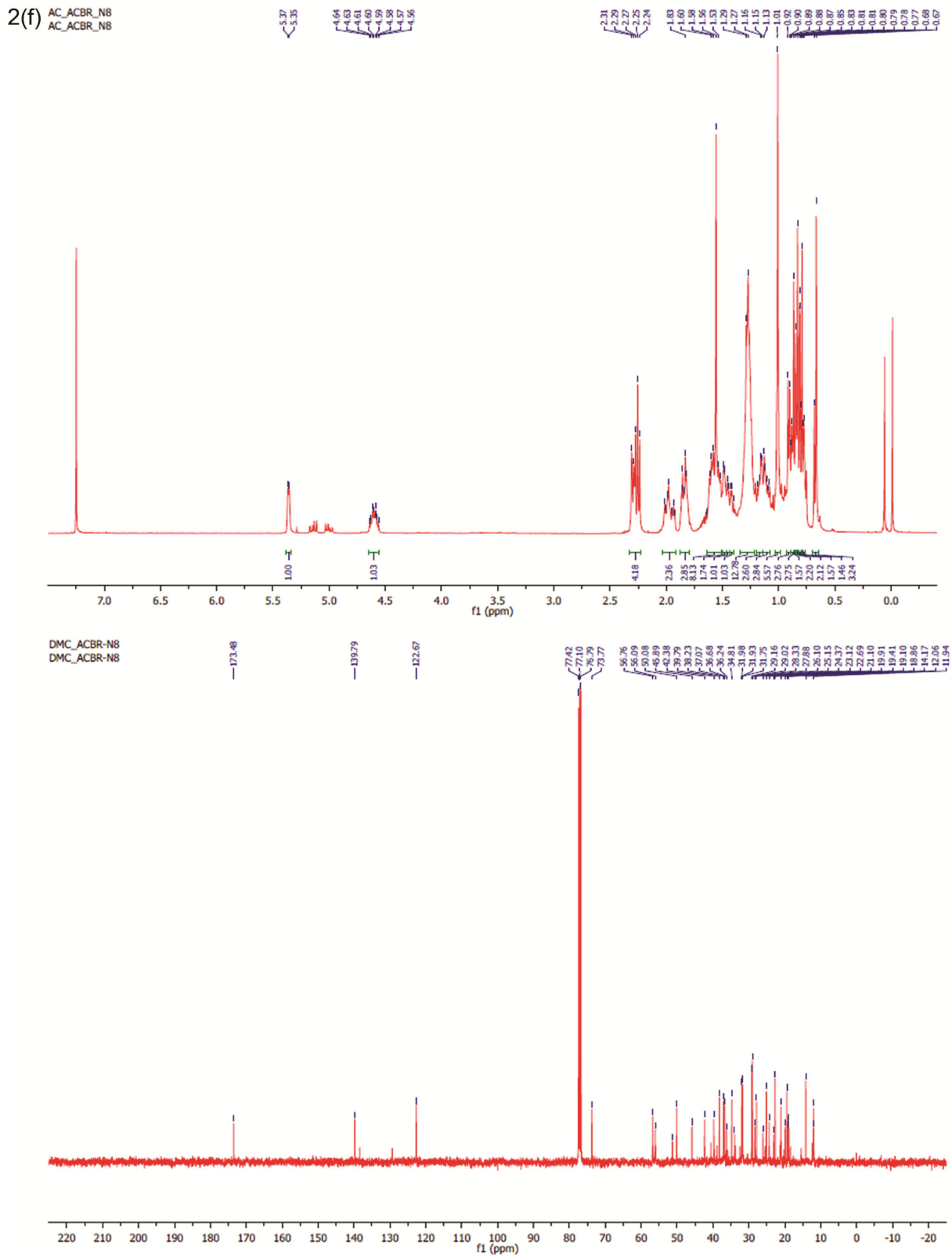


Fig. S6 — 1H NMR spectra of newly synthesised compound. 17-(5-ethyl-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-10,13-dimethyl-1H-cyclopenta[a]phenanthren-3-yl octanoate (2f).

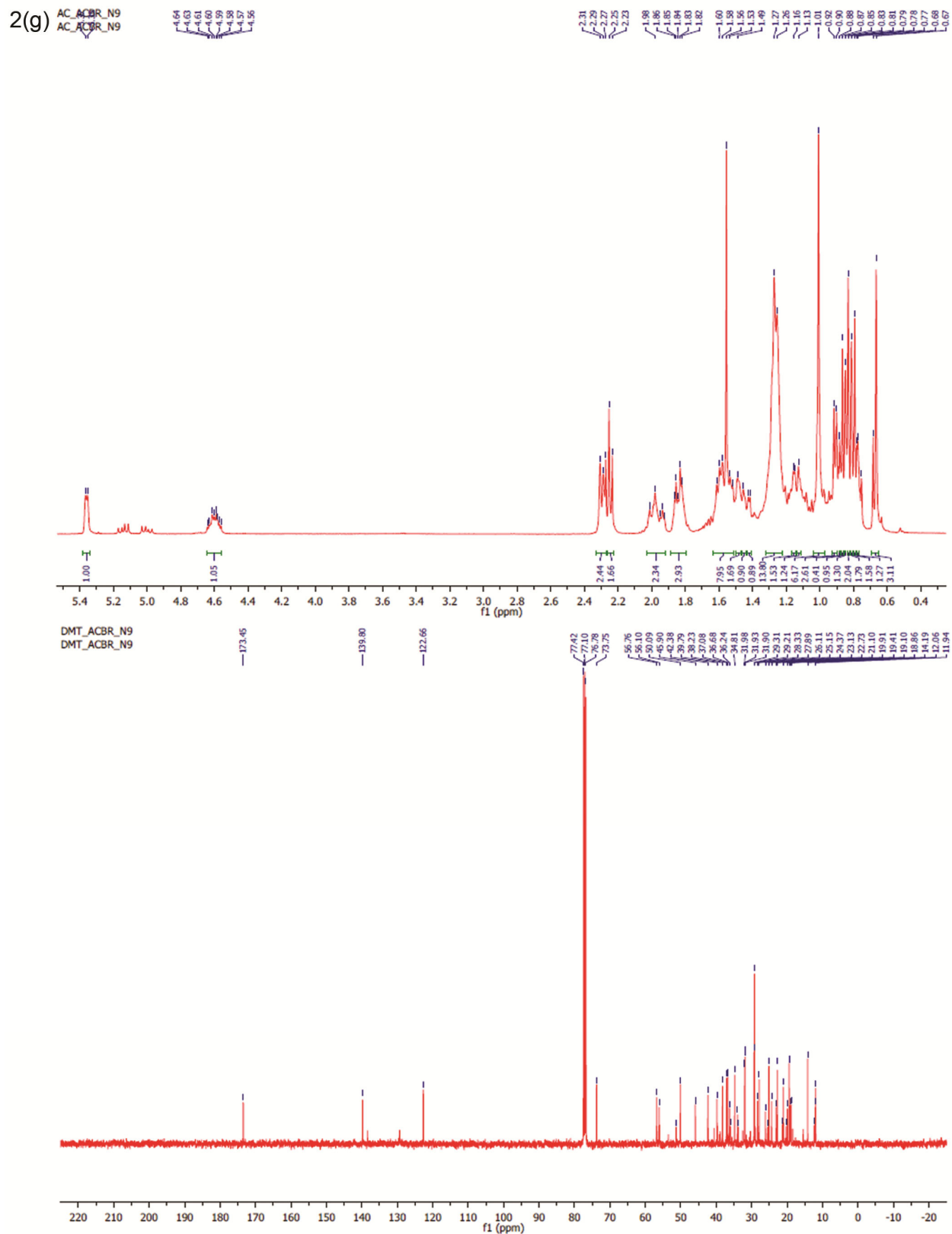


Fig. S7 — <sup>1</sup>HNMR spectra of newly synthesised compound. 17-(5-ethyl-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-10,13-dimethyl-1H-cyclopenta[a]phenanthren-3-yl nonanoate (2g).

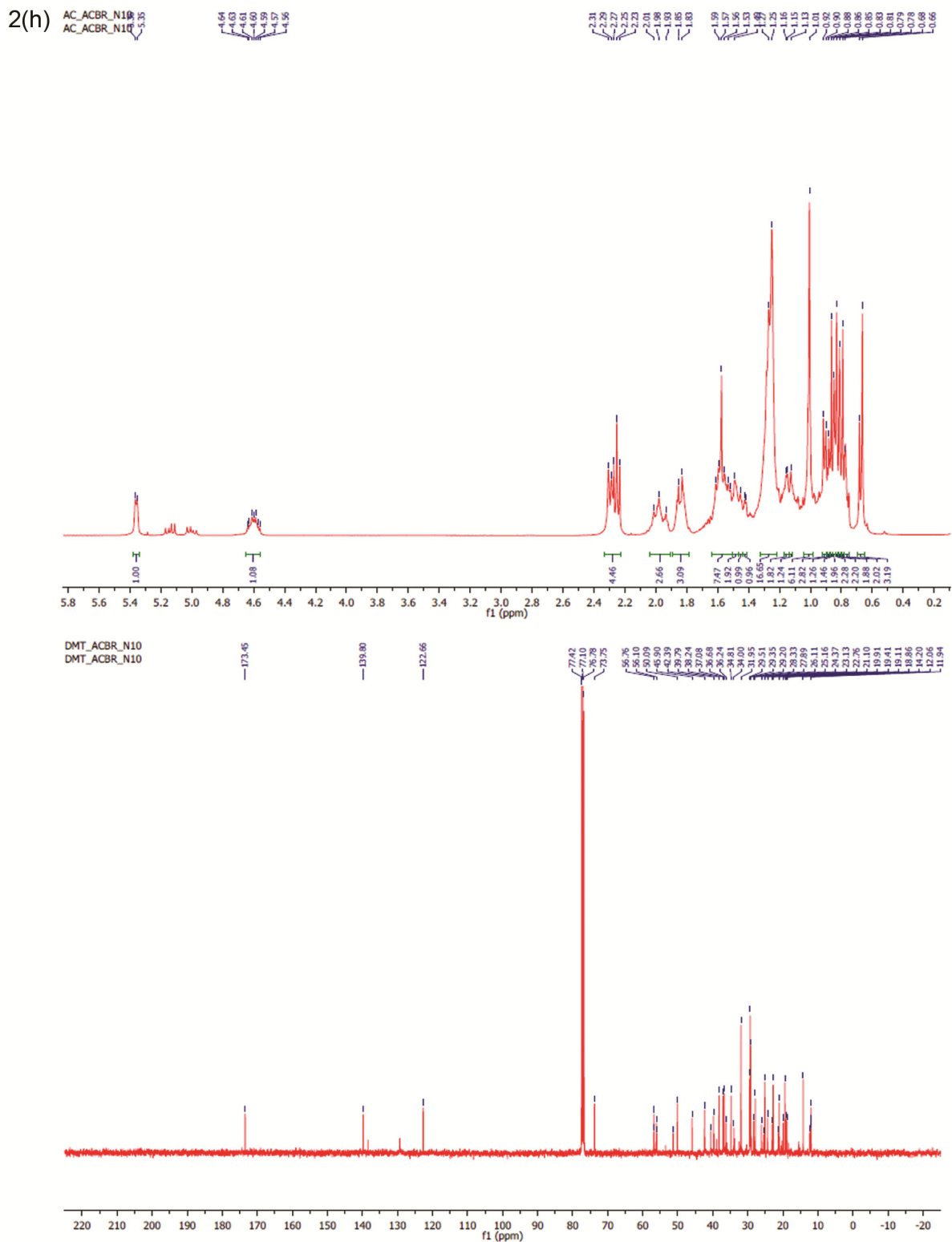


Fig. S8 — <sup>1</sup>HNMR spectra of newly synthesised compound. 17-(5-ethyl-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-10,13-dimethyl-1H-cyclopenta[a]phenanthren-3-yl decanoate (2h).

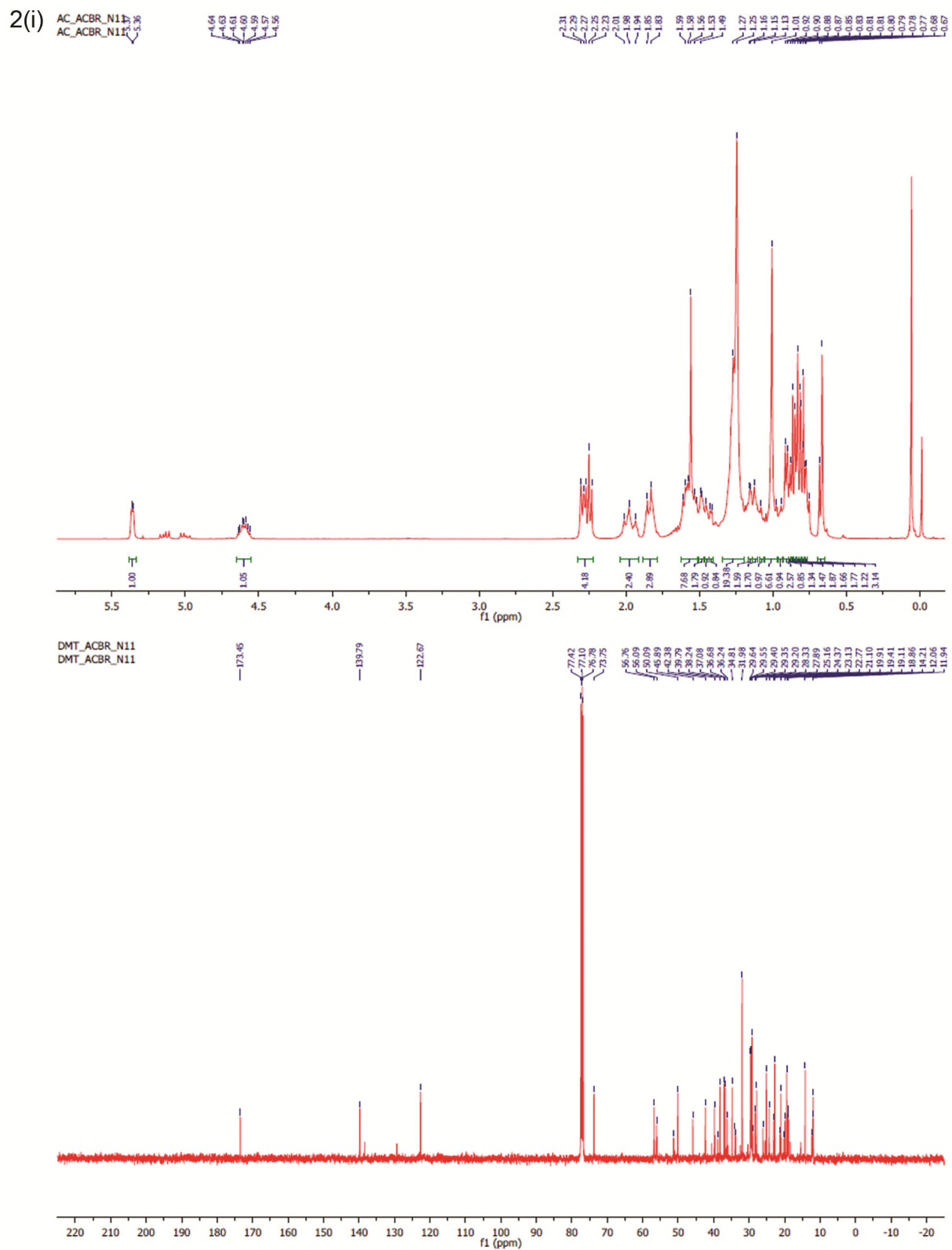


Fig. S9 — <sup>1</sup>HNMR spectra of newly synthesised compound. 17-(5-ethyl-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-10,13-dimethyl-1H-cyclopenta[a]phenanthren-3-yl undecanoate (2i).

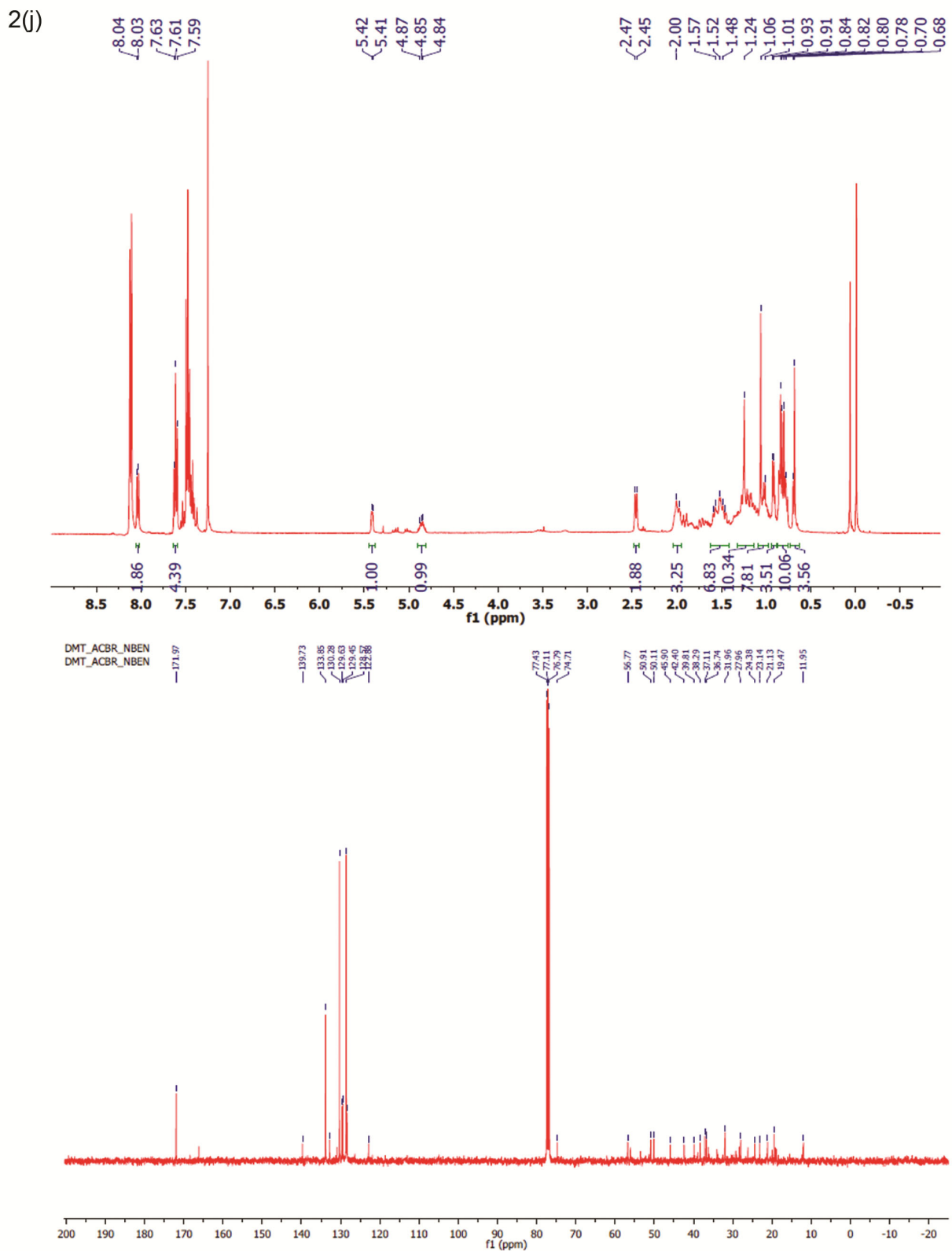


Fig. S10 — <sup>1</sup>HNMR spectra of newly synthesised compound. 17-(5-ethyl-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro10,13-dimethyl-1H-cyclopenta[a]phenanthren-3-yl benzoate (2j).

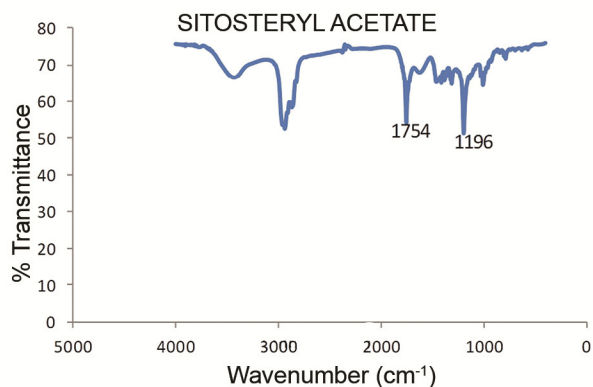


Fig. S11 — IR spectra of representative newly synthesised compound. 17-(5-ethyl-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-10,13-dimethyl-1H-cyclopenta[a]phenanthren-3-yl acetate (2a).

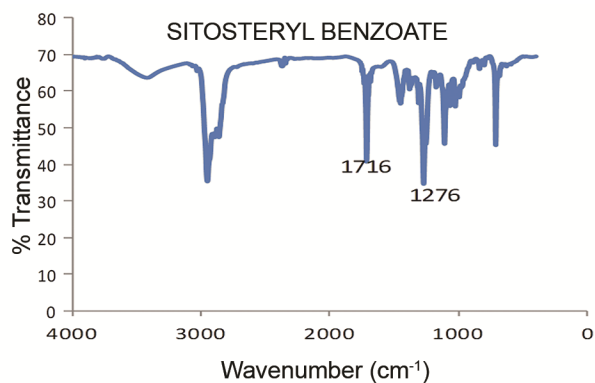


Fig. S12 — IR spectra of representative newly synthesised compound. 17-(5-ethyl-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-10,13-dimethyl-1H-cyclopenta[a]phenanthren-3-yl benzoate (2j).

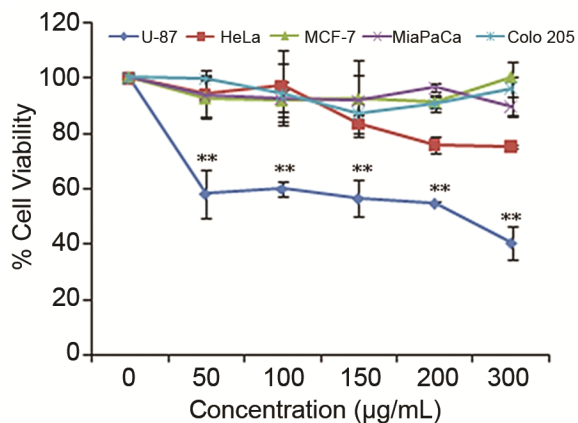


Fig. S13 — Effect of sitosteryl oleate (BDPT-3) on different cell lines. Cultured cells were treated with or without sitosteryl oleate (BDPT-3) under different concentrations for 72h. Cell viability was analysed by MTT assay.