

Supporting Information

Liposome-based gene delivery systems containing a steroid derivative : computational and small angle X ray diffraction study

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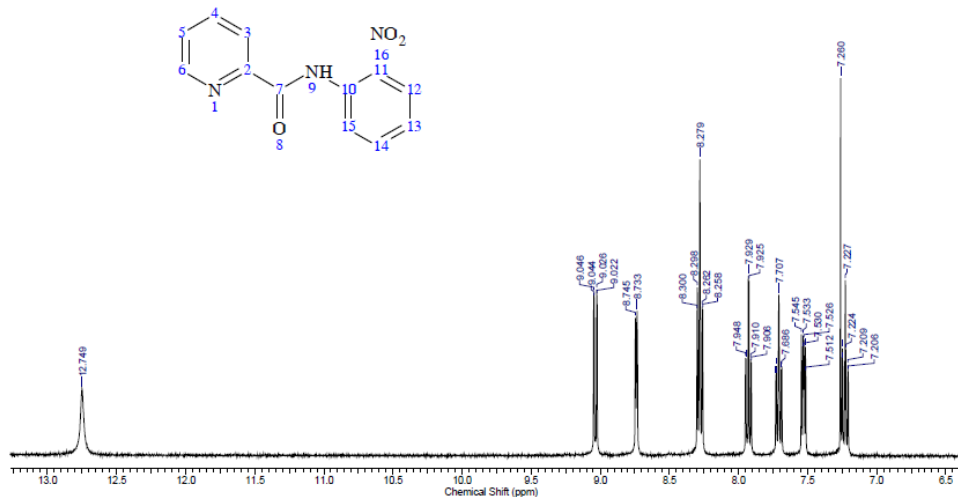
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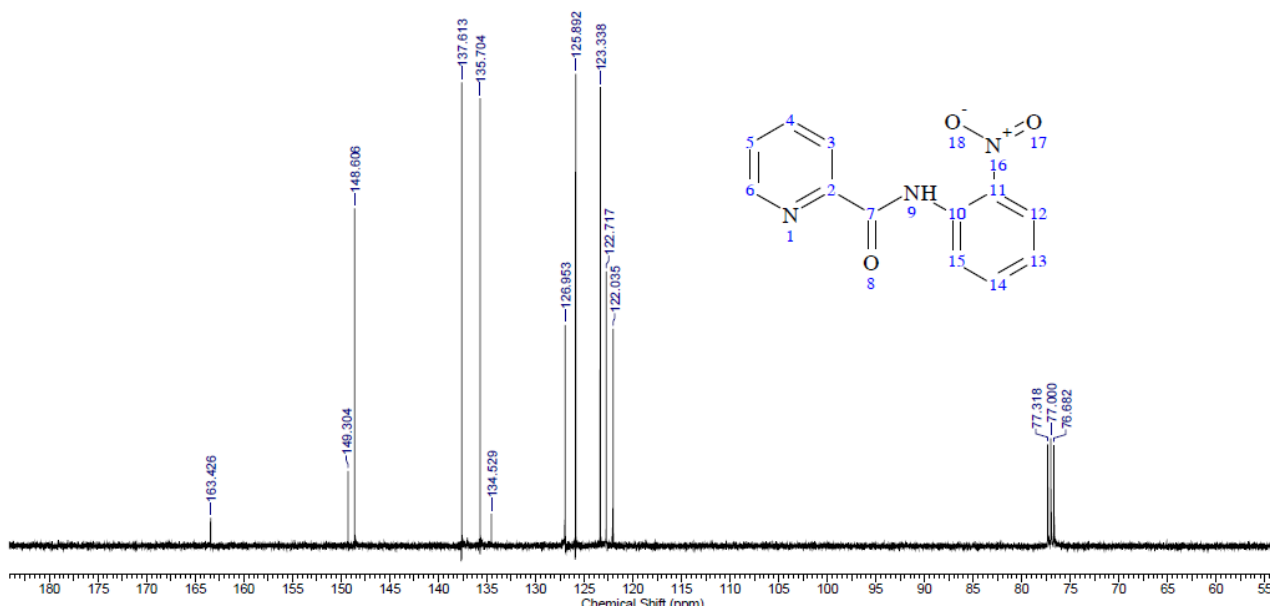
Synthetic protocols of Cholesteryl 2-(picolinamido)phenylcarbamate (CHOLp).

N-(2-nitrophenyl)picolinamide (**3**). A reaction mixture of 2-picolinic acid (**1**) (984 mg, 8 mmol) and 2,4,6-trichloro-1,3,5-triazine (1.46 g, 8 mmol) in THF (25 ml) was allowed to stir for 30' after which a solution of 2-nitroaniline (**2**) (1.10 g, 8 mmol) and triethylamine (2 ml) in THF (25 ml) was added. The resulting dark green mixture was refluxed for 20 h and thereafter cooled and diluted with 1:1 exane/ethylacetate (200 ml). The solution was washed with water (2x100 ml) and brine (100 ml), the organic extracts were dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. The dark green crude product was then purified over silica gel column (petrol ether/AcOEt, 6/4,v/v) to get the desired product as a yellow solid. (1.57 g, 81% yield).

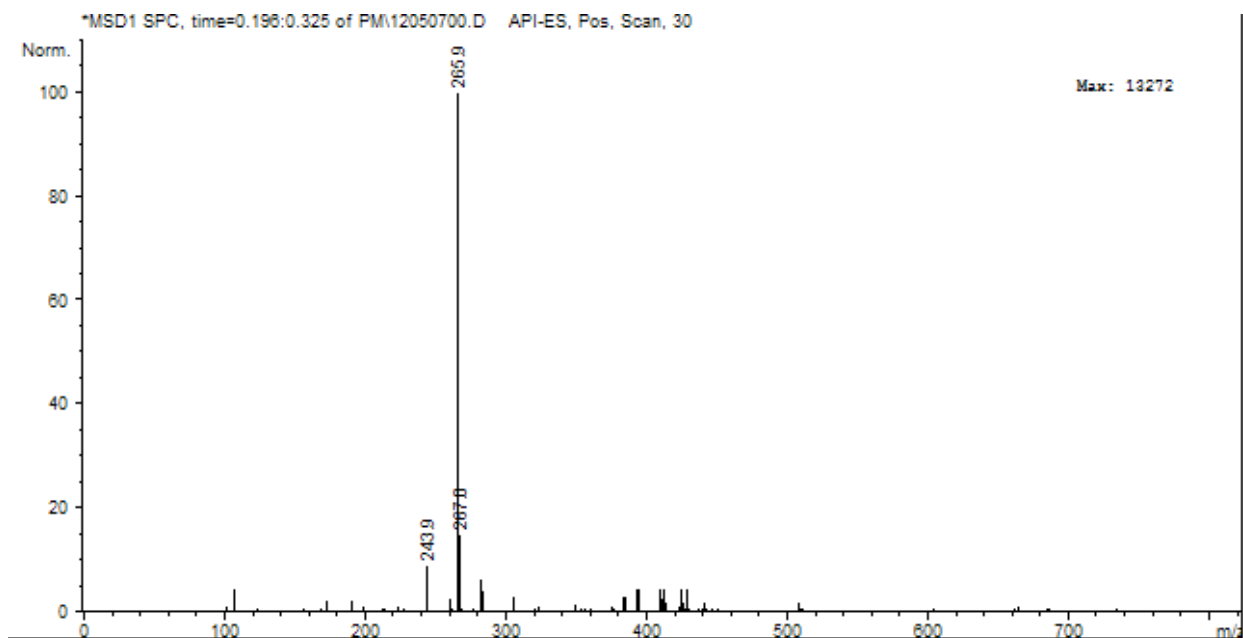
¹H NMR (400M, CDCl₃): δ = 7.23 (m, 1H); 7.53 (m, 1H); 7.71 (m, 1H); 7.93 (m, 1H); 8.28 (m, 2H); 8.74 (d, 1H, J = 4.8 Hz); 9.03 (d, 1H, J = 8.0); 12.75 (bs, 1 H).



^{13}C -NMR (400 M, CDCl_3): δ =122.04; 122.72; 123.34; 125.89; 126.95; 134.53; 135.70; 137.61; 148.61; 149.30; 163.43.

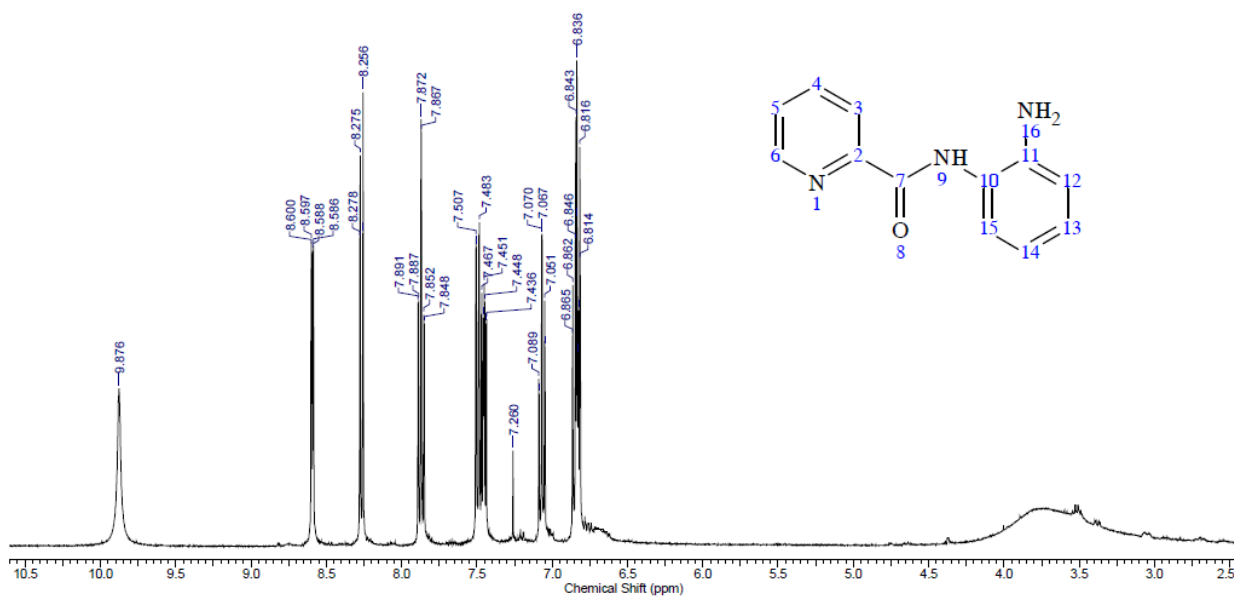


HRMS(ESI⁺): m/z 265.9($\text{M}^+ + \text{Na}$).

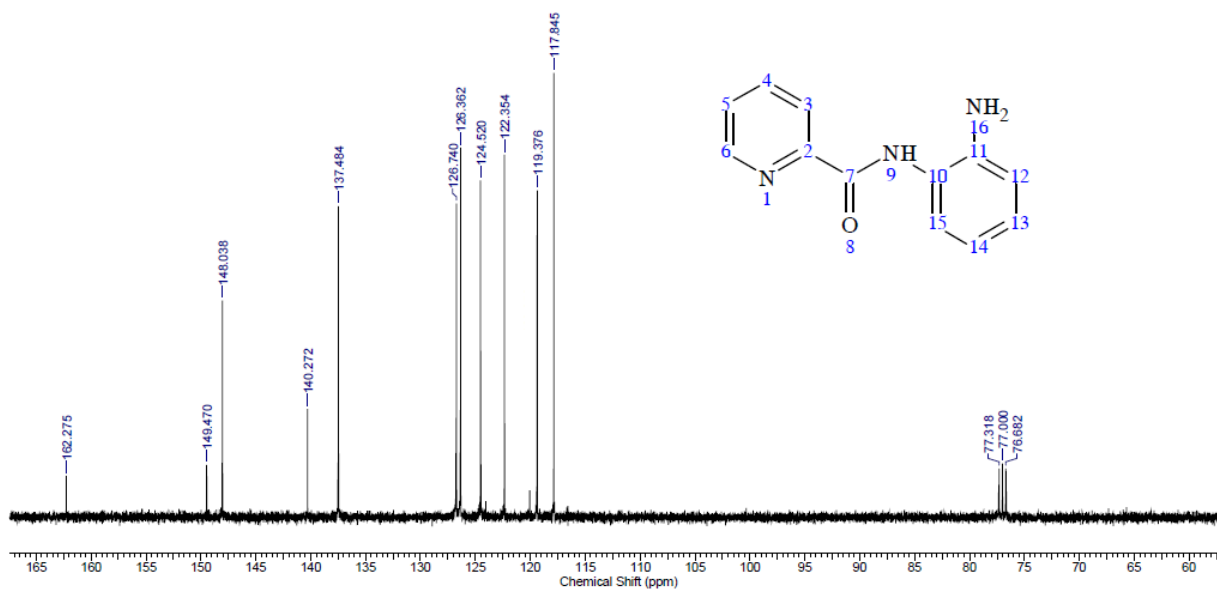


N-(2-aminophenyl)picolinamide (**4**). To a solution of *N*-(2-nitrophenyl)picolinamide (**3**) (243 mg, 1 mmol) in 10 ml of dry MeOH, 10%Pd/C-catalyst (243 mg) was added and the mixture stirred and refluxed under H₂ atmosphere. After 3h the solution was filtered through Celite and the solvent was evaporated under reduced pressure. The resulting yellow-brown oil was used directly without purification (173 mg).

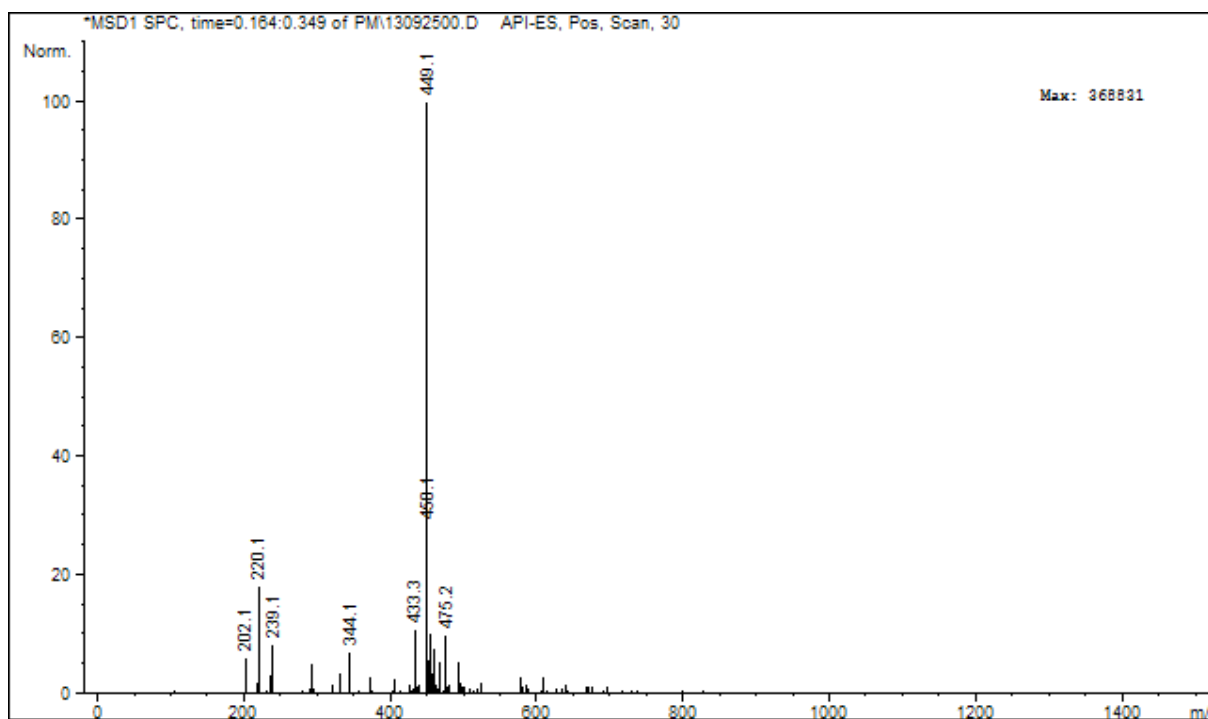
¹H NMR (400M, CDCl₃): δ = 3.76 (bs, -NH₂); 6.84 (m, 2H); 7.07 (m, 1H); 7.47 (m, 2H); 7.87 (m, 1H); 8.27 (m, 1H); 8.60 (m, 1H); 9.88 (bs, -NH).



¹³C-NMR (400 M, CDCl₃): δ = 117.85; 119.38; 122.35; 124.52; 126.36; 126.74; 137.48; 140.27; 148.04; 149.47; 162.28.

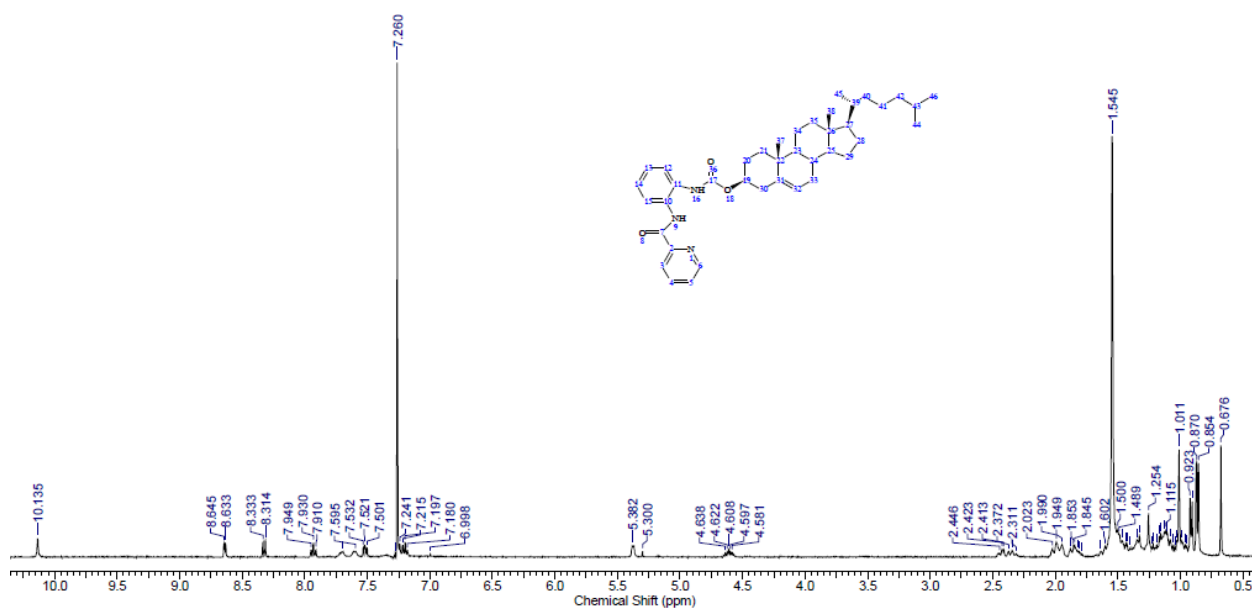


HRMS(ESI⁺): m/z 449.1 (2M⁺ + Na).

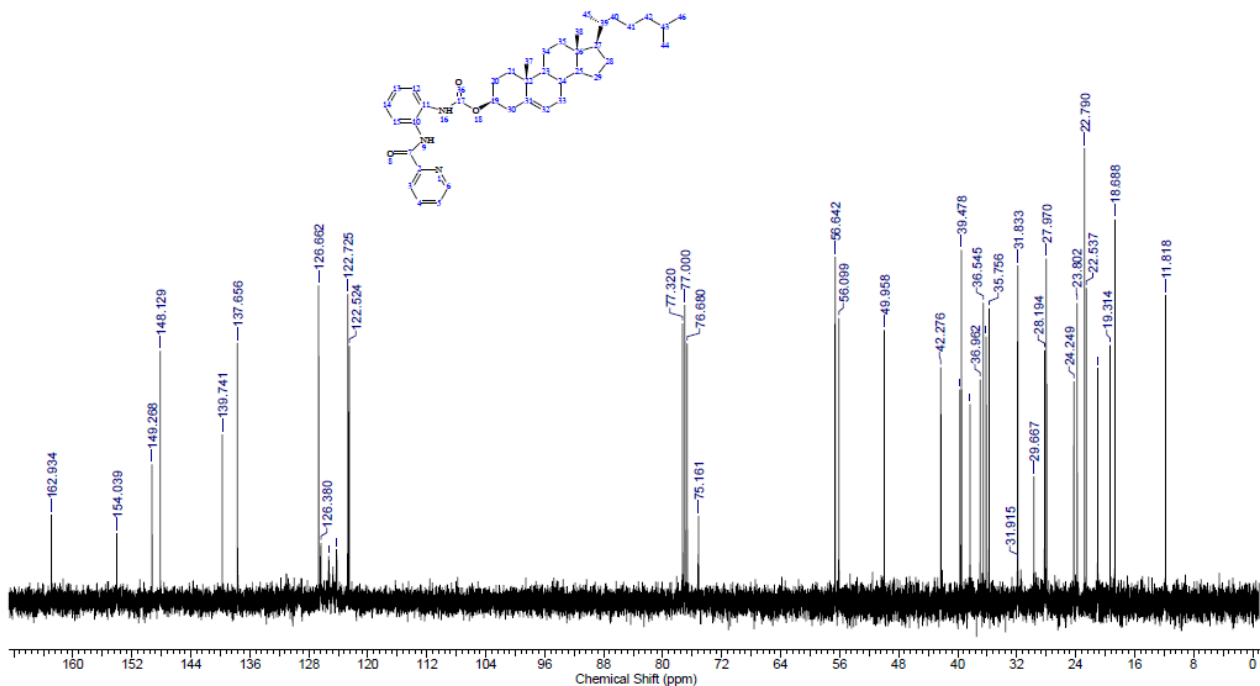


Cholesteryl 2-(picolinamido)phenylcarbamate (6). Cholesterylchloroformate (5) (449.12 mg, 1 mmol) was dissolved in a suspension of potassium carbonate (691.05 mg, 5 mmol) in THF(15 ml) and DCM. A solution of *N*-(2-aminophenyl)picolinamide (4) (213 mg, 1 mmol) in THF (2 ml) was added and the reaction mixture was refluxed overnight. After being cooled, it was filtered and the solvent was removed under reduced pressure. The crude product was then purified over silica gel column (petrol ether/AcOEt, 7/3) to get the desired product as a white solid (294.3 g, 47% yield).

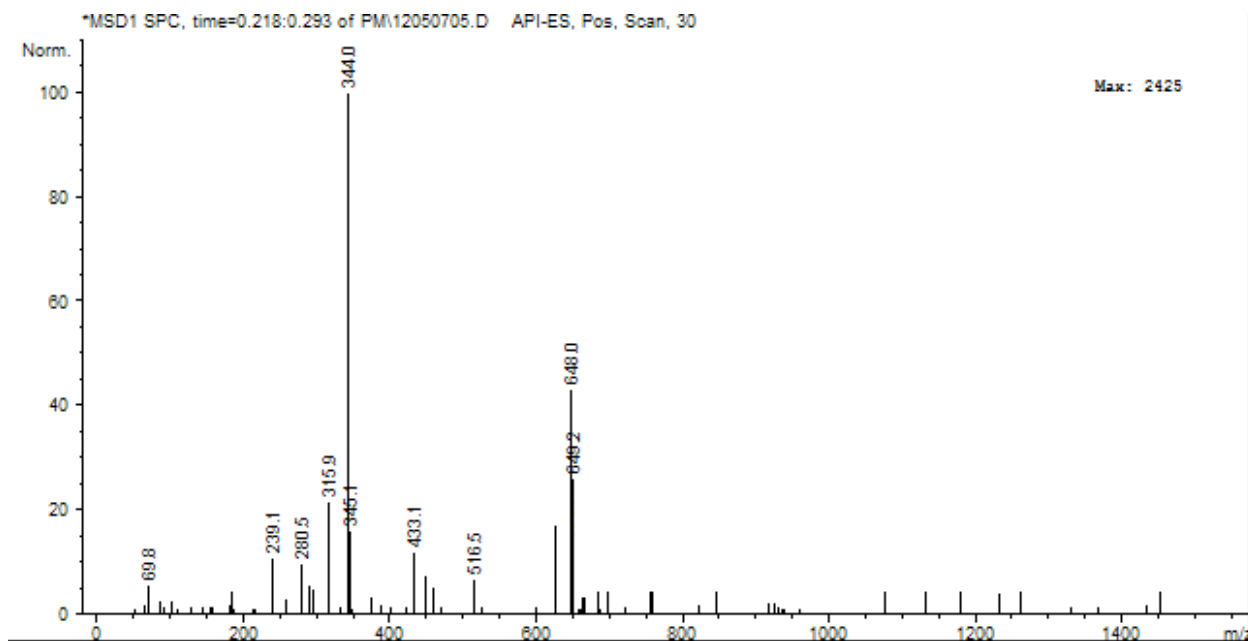
¹H NMR (400M, CDCl₃): δ = 0.67 (s, 3H); 0.86–1.67 (m, 22H); 0.86 (6H, d, J = 6.4 Hz); 0.91 (d, 3H, J = 6.4 Hz); 1.01 (s, 3H); 4.56-4.66 (1H, m, cholesterol 3-H1); 5.35-5.40 (1H, m, cholesterol 6-H1); 7.17-7.29 (2H, m, ArH); 7.39 (1H, broad, -NH); 7.50-7.54 (1H, m, ArH); 7.58-7.64 (1H, m, ArH); 7.67-7.74 (1H, m, ArH); 7.90-7.96 (1H, m, ArH); 8.32 (1H, d, J=7.6, ArH); 8.64 (1H, d, J = 4.8, ArH); 10.14 (1H, s, NH).



¹³C-NMR (400 M, CDCl₃): δ = 11.82; 18.69; 19.31; 21.01; 22.54; 22.79; 23.80; 24.25; 27.97; 28.19; 29.67; 31.83; 31.88; 35.76; 36.15; 36.55; 36.96; 38.34; 39.48; 39.69; 42.28; 49.96; 56.10; 56.64; 75.16; 122.52; 122.73; 124.24; 124.74; 125.31; 126.38; 126.66; 137.66; 139.74; 148.13; 149.27; 154.04; 162.93.



HRMS(ESI⁺): m/z 648.0 (M⁺ + 22.9).



CHOLp.gro

101

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CHOLp.itp

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26	68	1	1.0920e-01	2.8225e+05
27	76	1	1.0920e-01	2.8225e+05
27	75	1	1.0920e-01	2.8225e+05
27	74	1	1.0920e-01	2.8225e+05
31	78	1	1.0090e-01	3.4326e+05
79	84	1	1.0870e-01	2.8811e+05
80	85	1	1.0870e-01	2.8811e+05
81	86	1	1.0870e-01	2.8811e+05
82	87	1	1.0870e-01	2.8811e+05
88	90	1	1.0090e-01	3.4326e+05
93	98	1	1.0870e-01	2.8811e+05
94	99	1	1.0870e-01	2.8811e+05
95	100	1	1.0870e-01	2.8811e+05
96	101	1	1.0880e-01	2.8694e+05
1	10	1	1.5350e-01	2.5363e+05
1	2	1	1.5350e-01	2.5363e+05
2	3	1	1.5350e-01	2.5363e+05
3	4	1	1.5350e-01	2.5363e+05
3	29	1	1.4390e-01	2.5230e+05
4	5	1	1.5080e-01	2.7472e+05
5	6	1	1.3240e-01	4.9346e+05
5	10	1	1.5080e-01	2.7472e+05
6	7	1	1.5080e-01	2.7472e+05
7	8	1	1.5350e-01	2.5363e+05
8	14	1	1.5350e-01	2.5363e+05
8	9	1	1.5350e-01	2.5363e+05

9	10	1	1.5350e-01	2.5363e+05
9	11	1	1.5350e-01	2.5363e+05
10	19	1	1.5350e-01	2.5363e+05
11	12	1	1.5350e-01	2.5363e+05
12	13	1	1.5350e-01	2.5363e+05
13	18	1	1.5350e-01	2.5363e+05
13	17	1	1.5350e-01	2.5363e+05
13	14	1	1.5350e-01	2.5363e+05
14	15	1	1.5350e-01	2.5363e+05
15	16	1	1.5350e-01	2.5363e+05
16	17	1	1.5350e-01	2.5363e+05
17	20	1	1.5350e-01	2.5363e+05
20	22	1	1.5350e-01	2.5363e+05
20	21	1	1.5350e-01	2.5363e+05
22	23	1	1.5350e-01	2.5363e+05
23	24	1	1.5350e-01	2.5363e+05
24	25	1	1.5350e-01	2.5363e+05
25	27	1	1.5350e-01	2.5363e+05
25	26	1	1.5350e-01	2.5363e+05
28	29	1	1.3430e-01	3.4418e+05
28	31	1	1.3450e-01	4.0016e+05
28	30	1	1.2140e-01	5.4225e+05
31	77	1	1.4220e-01	3.1154e+05
77	83	1	1.3870e-01	4.0033e+05
77	79	1	1.3870e-01	4.0033e+05
79	80	1	1.3870e-01	4.0033e+05
80	81	1	1.3870e-01	4.0033e+05
81	82	1	1.3870e-01	4.0033e+05
82	83	1	1.3870e-01	4.0033e+05
83	88	1	1.4220e-01	3.1154e+05
88	89	1	1.3450e-01	4.0016e+05
89	92	1	1.4870e-01	2.9263e+05
89	91	1	1.2140e-01	5.4225e+05
92	97	1	1.3420e-01	4.0426e+05
92	93	1	1.3870e-01	4.0033e+05
93	94	1	1.3870e-01	4.0033e+05
94	95	1	1.3870e-01	4.0033e+05
95	96	1	1.3870e-01	4.0033e+05
96	97	1	1.3420e-01	4.0426e+05

```
[ pairs ]
; ai aj funct
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1 42 1
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2 32 1
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37 3 1
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4 36 1
4 35 1
5 41 1
5 40 1
38 5 1
37 5 1
5 44 1
5 43 1
5 42 1
5 45 1
5 34 1
6 46 1
6 33 1
6 32 1
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7 45 1
8 59 1
8 58 1
8 48 1
8 47 1
8 39 1
38 9 1
37 9 1
9 44 1
9 43 1
9 42 1
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10 35 1
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10 47 1
10 46 1
10 39 1
10 33 1
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91	97	1
91	93	1
92	95	1
93	96	1
94	97	1

[angles]

;	ai	aj	ak	funct	theta	cth
	1	2	36	1	1.1005e+02	3.8802e+02
	1	2	35	1	1.1005e+02	3.8802e+02
	2	3	34	1	1.1007e+02	3.8794e+02
	2	1	38	1	1.1005e+02	3.8802e+02
	2	1	37	1	1.1005e+02	3.8802e+02
	3	4	33	1	1.1005e+02	3.8802e+02
	3	4	32	1	1.1005e+02	3.8802e+02
	3	2	36	1	1.1005e+02	3.8802e+02
	3	2	35	1	1.1005e+02	3.8802e+02
	4	3	34	1	1.1007e+02	3.8794e+02

5	6	39	1	1.2094e+02	4.1873e+02
5	4	33	1	1.1049e+02	3.9355e+02
5	4	32	1	1.1049e+02	3.9355e+02
6	7	41	1	1.1049e+02	3.9355e+02
6	7	40	1	1.1049e+02	3.9355e+02
7	8	46	1	1.1005e+02	3.8802e+02
7	6	39	1	1.1730e+02	3.8208e+02
8	14	51	1	1.1005e+02	3.8802e+02
8	9	45	1	1.1005e+02	3.8802e+02
8	7	41	1	1.1005e+02	3.8802e+02
8	7	40	1	1.1005e+02	3.8802e+02
9	11	48	1	1.1005e+02	3.8802e+02
9	11	47	1	1.1005e+02	3.8802e+02
9	8	46	1	1.1005e+02	3.8802e+02
10	1	38	1	1.1005e+02	3.8802e+02
10	1	37	1	1.1005e+02	3.8802e+02
10	19	44	1	1.1005e+02	3.8802e+02
10	19	43	1	1.1005e+02	3.8802e+02
10	19	42	1	1.1005e+02	3.8802e+02
10	9	45	1	1.1005e+02	3.8802e+02
11	9	45	1	1.1005e+02	3.8802e+02
11	12	50	1	1.1005e+02	3.8802e+02
11	12	49	1	1.1005e+02	3.8802e+02
12	11	48	1	1.1005e+02	3.8802e+02
12	11	47	1	1.1005e+02	3.8802e+02
13	12	50	1	1.1005e+02	3.8802e+02
13	12	49	1	1.1005e+02	3.8802e+02
13	18	54	1	1.1005e+02	3.8802e+02
13	18	53	1	1.1005e+02	3.8802e+02
13	18	52	1	1.1005e+02	3.8802e+02
13	17	55	1	1.1005e+02	3.8802e+02
13	14	51	1	1.1005e+02	3.8802e+02
14	15	59	1	1.1005e+02	3.8802e+02
14	15	58	1	1.1005e+02	3.8802e+02
14	8	46	1	1.1005e+02	3.8802e+02
15	16	57	1	1.1005e+02	3.8802e+02
15	16	56	1	1.1005e+02	3.8802e+02
15	14	51	1	1.1005e+02	3.8802e+02
16	17	55	1	1.1005e+02	3.8802e+02
16	15	59	1	1.1005e+02	3.8802e+02
16	15	58	1	1.1005e+02	3.8802e+02
17	20	60	1	1.1005e+02	3.8802e+02
17	16	57	1	1.1005e+02	3.8802e+02
17	16	56	1	1.1005e+02	3.8802e+02
20	17	55	1	1.1005e+02	3.8802e+02
20	22	65	1	1.1005e+02	3.8802e+02
20	22	64	1	1.1005e+02	3.8802e+02
20	21	63	1	1.1005e+02	3.8802e+02
20	21	62	1	1.1005e+02	3.8802e+02
20	21	61	1	1.1005e+02	3.8802e+02
21	20	60	1	1.1005e+02	3.8802e+02
22	20	60	1	1.1005e+02	3.8802e+02
22	23	67	1	1.1005e+02	3.8802e+02
22	23	66	1	1.1005e+02	3.8802e+02
23	22	65	1	1.1005e+02	3.8802e+02
23	22	64	1	1.1005e+02	3.8802e+02
23	24	72	1	1.1005e+02	3.8802e+02
23	24	71	1	1.1005e+02	3.8802e+02
24	23	67	1	1.1005e+02	3.8802e+02
24	23	66	1	1.1005e+02	3.8802e+02
24	25	73	1	1.1005e+02	3.8802e+02
25	24	72	1	1.1005e+02	3.8802e+02
25	24	71	1	1.1005e+02	3.8802e+02
25	27	76	1	1.1005e+02	3.8802e+02
25	27	75	1	1.1005e+02	3.8802e+02
25	27	74	1	1.1005e+02	3.8802e+02
25	26	70	1	1.1005e+02	3.8802e+02
25	26	69	1	1.1005e+02	3.8802e+02
25	26	68	1	1.1005e+02	3.8802e+02
26	25	73	1	1.1005e+02	3.8802e+02
27	25	73	1	1.1005e+02	3.8802e+02
28	31	78	1	1.1846e+02	4.1179e+02
29	3	34	1	1.0882e+02	4.2543e+02
32	4	33	1	1.0835e+02	3.2995e+02
35	2	36	1	1.0835e+02	3.2995e+02
37	1	38	1	1.0835e+02	3.2995e+02
40	7	41	1	1.0835e+02	3.2995e+02
42	19	44	1	1.0835e+02	3.2995e+02
42	19	43	1	1.0835e+02	3.2995e+02
43	19	44	1	1.0835e+02	3.2995e+02
47	11	48	1	1.0835e+02	3.2995e+02
49	12	50	1	1.0835e+02	3.2995e+02
52	18	54	1	1.0835e+02	3.2995e+02
52	18	53	1	1.0835e+02	3.2995e+02
53	18	54	1	1.0835e+02	3.2995e+02
56	16	57	1	1.0835e+02	3.2995e+02
58	15	59	1	1.0835e+02	3.2995e+02
61	21	63	1	1.0835e+02	3.2995e+02
61	21	62	1	1.0835e+02	3.2995e+02
62	21	63	1	1.0835e+02	3.2995e+02

64	22	65	1	1.0835e+02	3.2995e+02
66	23	67	1	1.0835e+02	3.2995e+02
68	26	70	1	1.0835e+02	3.2995e+02
68	26	69	1	1.0835e+02	3.2995e+02
69	26	70	1	1.0835e+02	3.2995e+02
71	24	72	1	1.0835e+02	3.2995e+02
74	27	76	1	1.0835e+02	3.2995e+02
74	27	75	1	1.0835e+02	3.2995e+02
75	27	76	1	1.0835e+02	3.2995e+02
77	31	78	1	1.1594e+02	3.9631e+02
77	79	84	1	1.2001e+02	4.0551e+02
79	80	85	1	1.2001e+02	4.0551e+02
80	81	86	1	1.2001e+02	4.0551e+02
80	79	84	1	1.2001e+02	4.0551e+02
81	82	87	1	1.2001e+02	4.0551e+02
81	80	85	1	1.2001e+02	4.0551e+02
82	81	86	1	1.2001e+02	4.0551e+02
83	88	90	1	1.1594e+02	3.9631e+02
83	82	87	1	1.2001e+02	4.0551e+02
89	88	90	1	1.1846e+02	4.1179e+02
92	93	98	1	1.2001e+02	4.0551e+02
93	94	99	1	1.2001e+02	4.0551e+02
94	95	100	1	1.2001e+02	4.0551e+02
94	93	98	1	1.2001e+02	4.0551e+02
95	96	101	1	1.2109e+02	4.0367e+02
95	94	99	1	1.2001e+02	4.0551e+02
96	95	100	1	1.2001e+02	4.0551e+02
97	96	101	1	1.1594e+02	4.3363e+02
1	10	19	1	1.1063e+02	5.2894e+02
1	10	9	1	1.1063e+02	5.2894e+02
1	10	5	1	1.1144e+02	5.3162e+02
1	2	3	1	1.1063e+02	5.2894e+02
2	3	4	1	1.1063e+02	5.2894e+02
2	3	29	1	1.0842e+02	5.6718e+02
2	1	10	1	1.1063e+02	5.2894e+02
3	4	5	1	1.1144e+02	5.3162e+02
3	29	28	1	1.1514e+02	5.3246e+02
4	5	6	1	1.2342e+02	5.3831e+02
4	5	10	1	1.1652e+02	5.2467e+02
4	3	29	1	1.0842e+02	5.6718e+02
5	6	7	1	1.2342e+02	5.3831e+02
5	10	19	1	1.1144e+02	5.3162e+02
5	10	9	1	1.1144e+02	5.3162e+02
6	7	8	1	1.1144e+02	5.3162e+02
6	5	10	1	1.2342e+02	5.3831e+02
7	8	14	1	1.1063e+02	5.2894e+02
7	8	9	1	1.1063e+02	5.2894e+02
8	14	15	1	1.1063e+02	5.2894e+02
8	14	13	1	1.1063e+02	5.2894e+02
8	9	10	1	1.1063e+02	5.2894e+02
8	9	11	1	1.1063e+02	5.2894e+02
9	10	19	1	1.1063e+02	5.2894e+02
9	11	12	1	1.1063e+02	5.2894e+02
9	8	14	1	1.1063e+02	5.2894e+02
10	9	11	1	1.1063e+02	5.2894e+02
11	12	13	1	1.1063e+02	5.2894e+02
12	13	18	1	1.1063e+02	5.2894e+02
12	13	17	1	1.1063e+02	5.2894e+02
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13	17	20	1	1.1063e+02	5.2894e+02
13	17	16	1	1.1063e+02	5.2894e+02
13	14	15	1	1.1063e+02	5.2894e+02
14	15	16	1	1.1063e+02	5.2894e+02
14	13	18	1	1.1063e+02	5.2894e+02
14	13	17	1	1.1063e+02	5.2894e+02
15	16	17	1	1.1063e+02	5.2894e+02
16	17	20	1	1.1063e+02	5.2894e+02
17	13	18	1	1.1063e+02	5.2894e+02
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20	22	23	1	1.1063e+02	5.2894e+02
21	20	22	1	1.1063e+02	5.2894e+02
22	23	24	1	1.1063e+02	5.2894e+02
23	24	25	1	1.1063e+02	5.2894e+02
24	25	27	1	1.1063e+02	5.2894e+02
24	25	26	1	1.1063e+02	5.2894e+02
26	25	27	1	1.1063e+02	5.2894e+02
28	31	77	1	1.2371e+02	5.3798e+02
29	28	31	1	1.0928e+02	6.4166e+02
29	28	30	1	1.2333e+02	6.3538e+02
30	28	31	1	1.2203e+02	6.3455e+02
31	77	83	1	1.1989e+02	5.6877e+02
31	77	79	1	1.1989e+02	5.6877e+02
77	83	88	1	1.1989e+02	5.6877e+02
77	83	82	1	1.1997e+02	5.6216e+02
77	79	80	1	1.1997e+02	5.6216e+02
79	80	81	1	1.1997e+02	5.6216e+02
79	77	83	1	1.1997e+02	5.6216e+02
80	81	82	1	1.1997e+02	5.6216e+02
81	82	83	1	1.1997e+02	5.6216e+02

82	83	88	1	1.1989e+02	5.6877e+02
83	88	89	1	1.2371e+02	5.3798e+02
88	89	92	1	1.1514e+02	5.7296e+02
88	89	91	1	1.2203e+02	6.3455e+02
89	92	97	1	1.1794e+02	5.6660e+02
89	92	93	1	1.2014e+02	5.4091e+02
91	89	92	1	1.2344e+02	5.7463e+02
92	97	96	1	1.1586e+02	5.7396e+02
92	93	94	1	1.1997e+02	5.6216e+02
93	94	95	1	1.1997e+02	5.6216e+02
93	92	97	1	1.2263e+02	5.7873e+02
94	95	96	1	1.1997e+02	5.6216e+02
95	96	97	1	1.2263e+02	5.7873e+02

[dihedrals]

;i	j	k	l	func	C0	...	C5					
1	10	19	44	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
1	10	19	43	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
1	10	19	42	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
1	10	9	45	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
1	2	3	34	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	0.00000	;
2	3	4	33	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
2	3	4	32	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
38	1	2	3	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
37	1	2	3	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
4	5	6	39	3	55.64720	0.00000	-55.64720	0.00000	0.00000	0.00000	0.00000	;
4	3	2	36	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
4	3	2	35	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
5	6	7	41	3	6.40152	-9.58136	0.00000	6.35968	0.00000	0.00000	0.00000	;
5	6	7	40	3	6.40152	-9.58136	0.00000	6.35968	0.00000	0.00000	0.00000	;
38	1	10	5	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	0.00000	;
37	1	10	5	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	0.00000	;
5	10	19	44	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	0.00000	;
5	10	19	43	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	0.00000	;
5	10	19	42	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	0.00000	;
5	10	9	45	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	0.00000	;
5	4	3	34	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	0.00000	;
6	7	8	46	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	0.00000	;
6	5	4	33	3	6.40152	-9.58136	0.00000	6.35968	0.00000	0.00000	0.00000	;
6	5	4	32	3	6.40152	-9.58136	0.00000	6.35968	0.00000	0.00000	0.00000	;
7	8	14	51	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
7	8	9	45	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
8	14	15	59	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
8	14	15	58	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
8	9	11	48	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
8	9	11	47	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
8	7	6	39	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
38	1	10	9	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
37	1	10	9	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
9	10	19	44	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
9	10	19	43	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
9	10	19	42	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
9	11	12	50	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
9	11	12	49	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
9	8	14	51	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
9	8	7	41	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
9	8	7	40	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
10	1	2	36	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
10	1	2	35	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
10	9	11	48	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
10	9	11	47	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
10	9	8	46	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
10	5	6	39	3	55.64720	0.00000	-55.64720	0.00000	0.00000	0.00000	0.00000	;
10	5	4	33	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
10	5	4	32	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
11	9	8	46	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
12	11	9	45	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
12	13	18	54	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
12	13	18	53	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
12	13	18	52	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
12	13	17	55	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
12	13	14	51	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
13	12	11	48	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
13	12	11	47	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
13	17	20	60	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
13	17	16	57	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
13	17	16	56	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
13	14	15	59	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
13	14	15	58	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
13	14	8	46	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
14	15	16	57	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
14	15	16	56	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
14	13	12	50	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
14	13	12	49	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
14	13	18	54	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
14	13	18	53	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
14	13	18	52	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
14	13	17	55	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
14	8	9	45	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;
14	8	7	41	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	0.00000	;

