Grassypeptolides A–C, Cytotoxic Bis-Thiazoline Containing Marine Cyclodepsipeptides

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Contents

Table S1. NMR Spectral Data for Grassypeptolide B (**2**) in $CDCl_3$ (600 MHz)

C/H no.		δ_H (*J* in Hz)	δ_C[a]	^{1}H–^{1}H COSY	HMBC[b]	ROESY
Maba	1		172.7, s			
	2	2.55, qd (7.0, 6.8)	45.5, d	H-3, H_3-5	1, 3, 4, 5	H-3, H_3-4, H_3-5
	3	4.27, m	48.3, d	H-2, H_3-4, NH	1, 2, 4, 6	H-2, H_3-4, H_3-5, H-31/35, H52/56
	4	1.22, d (6.7)	19.5, q	H-3	2, 3	H-2, H-3
	5	1.15, d (7.0)	14.5, q		1, 2, 3	H-2, H-3, H-52/56
	NH	7.31, m		H-3		
Thr	6		169.6, s			
	7	4.49, dd (7.9, 6.7)	58.8, d	H-8, NH	6, 8, 9, 10	H_3-9, H-31/35, NH
	8	4.03, m	68.5, d	H-7, H_3-9	6	H_3-9
	9	1.29, d (6.4)	19.7, q	H-8	7, 8	H-7, H-8, H_3-16, H_3-22
	OH	5.02, br[c]				
	NH	7.13, d (7.9)		H-7	10	H-7
N-Me-Leu	10		170.3, s			
	11	5.02, br	56.1, d	H-12a, H-12b		
	12a	1.89, m	36.4, t	H-11, H-12b	10, 11, 13, 15	H-12b, H_3-14, H_3-16
	12b	1.76, ddd (–14.3, 7.9, 6.5)		H-11, H-12a, H-13	10, 11, 13, 15	H-12a, H_3-14, H_3-15
	13	1.59, m	24.8, d	H-12b, H_3-14, H_3-15	12, 14	H_3-14, H_3-15, H_3-16
	14	1.02, d (6.6)	23.0, q	H-13	12, 13, 15	H-12a, H-12b, H-13, H_3-22
	15	0.96, d (6.4)	21.9, q	H-13	12, 13, 14	H-12b, H-13
	16	3.22, s	31.6, q		11, 17	H_3-9, H-12a, H-13, H-18, H-25, H-31/35, H_3-45
Ala-thn-ca	17		170.2, s			
	18	5.347, dd (10.4, 10.4)	77.6, d	H-19a, H-19b	20	H_3-16, H-19a, H-19b
	19a	3.71, dd (–10.5, 10.4)	33.3, t	H-18, H-19b	17, 18, 20	H-18, H-19b
	19b	3.33, dd (–10.5, 10.4)		H-18, H-19a	17, 20	H-18, H-19a
	20		178.9, s			
	21	4.90, dq (7.5, 7.1)	48.2, d	H_3-22, NH	20, 22, 24	H_3-22, H-31/35, NH
	22	1.65, d (7.1)	18.0, q	H-21	20, 21	H_3-9, H_3-14, H-21, H-41a, H-41b, H-43, NH
	NH	7.73, d (7.5)		H-21	21, 22, 24	H-21, H_3-22, H-25, H_2-26
N-Me-Phe-thn-ca	24		170.4, s			
	25	5.351, m	78.8, d	H_2-26	24, 27	H_3-16, H_2-26, NH (Ala)
	26	3.77, m (2H)	37.6, t	H-25	24, 25, 27	H-25, H-31/35, H-52/56, NH (Ala)
	27		177.5, s			
	28	3.91, dd (10.1, 3.2)	68.9, d	H-29a, H-29b		H-31/35, H_3-36
	29a	3.65, dd (–13.4, 10.1)	34.9, t	H-28, H-29b	27, 28, 30, 31/35	H-31/35
	29b	3.48, dd (–13.4, 3.2)		H-28, H-29a	28, 30, 31/35	H-31/35, H_3-36
	30		138.2, s			
	31/35	7.43, m	129.8, d	H-32/34	29, 30, 33	H-3, H-7, H_3-16, H-21, H_2-26, H-28, H-29a, H-29b, H_3-36, H-38, H-43, H-44, H_3-45, H_3-47, H-49
	32/34	7.36, m	127.1, d	H-31/35, H-33		
	33	7.43, m	128.6, d	H-32/34	31/35	
	36	2.81, s	39.3, q		28, 37	H-28, H-29b, H-31/35, H-38
Pro	37		172.9, s			
	38	4.81, dd (8.4, 4.2)	57.0, d	H-39a, H-39b	37, 39, 40, 41	H-31/35, H_3-36, H-39a, H-39b, H52/56
	39a	2.11, m	27.4, t	H-38, H-39b, H-40a, H-40b	37, 38, 41	H-38
	39b	2.06, m		H-38, H-39a, H-40a, H-40b	37, 40	H-38
	40a	2.18, m	24.6, t	H-39a, H-39bH-40b, H-41a, H-41b	38, 39, 41	H-40b
	40b	1.93, m		H-39a, H-39b, H-40a, H-41a, H-41b	38, 39, 41	H-40a
	41a	3.76, m	47.4, t	H-40a, H-40b, H-41b	39, 40	H_3-22, H-43
	41b	3.67, m		H-40a, H-40b, H-41a	39, 40	H_3-22, H_3-36, H-43
N-Me-Val	42		168.1, s			
	43	4.98, d (10.9)	60.0, d	H-44	42, 44, 45, 46, 47, 48	H_3-22, H-31/35, H-41a, H-41b, H-44, H_3-45, H_3-46, H-50a
	44	2.47, dqq (10.9, 6.6, 6.4)	27.1, d	H-43, H_3-45, H_3-46	43, 45, 46	H-31/35, H-43, H_3-45, H_3-46, H_3-47
	45	1.01, d (6.4)	19.2, q	H-44	43, 44, 46	H_3-16, H-31/35, H-43, H-44
	46	0.93, d (6.6)	17.9, q	H-44	43, 44, 45	H-43, H-44, H_3-47
	47	3.20, s	30.1, q		43, 48	H-31/35, H_3-46, H-49, H-54
Pla	48		171.0, s			
	49	5.40, dd (9.9, 3.0)	72.0, d	H-50a, H-50b	1, 48, 50, 51	H-31/35, H_3-47, H-50a, H-50b, H-52/56
	50a	3.17, dd (–14.3, 9.9)	37.0, t	H-49, H-50b	48, 49, 51, 52/56	H-43, H-49, H-50b, H-52/56
	50b	3.06, dd (–14.3, 2.7)		H-49, H-50a	48, 51, 52/56	H-49, H-50a, H-52/56
	51		135.7, s			
	52/56	7.27, m	129.1, d	H-53/55	50, 54, 52/56	H-3, H_3-5, H_2-26, H-38, H-49, H-50a, H-50b
	53/55	7.36, m	128.5, d	H-52/56, H-54	51, 53/55	
	54	7.32, m	126.8, d	H-52/56		H_3-47

[a]Multiplicity derived from edited-HSQC. [b]Protons showing long-range correlation to indicated carbon. [c]OH signal assigned by default.

Table S2. Distance Constraints Used for Molecular Modeling of Grassypeptolide C (**3**)

Atom 1	Atom 2	Constant	Lower (Å)	Upper (Å)	Pwr
H7A	H1	2	3.5	5	2
H1	P9	2	3.5	5	2
H1	H43A	2	3.5	5	2
H1	P46	2	3.5	5	2
H7A	P14	2	3.5	5	2
H7A	P16	2	3.5	5	2
H7A	P46	2	3.5	5	2
H8A	P16	2	3.5	5	2
H8A	P46	2	3.5	5	2
H11A	H2	2	2.5	3.5	2
H2	P12	2	3.5	6	2
H2	P16	2	3.5	5	2
H11A	P16	2	3.5	5	2
H11A	P50	2	3.5	6	2
P12	P16	2	3.5	6	2
H13A	P16	2	3.5	5	2
P14	P16	2	3.5	5	2
P15	P16	2	3.5	5	2
H18A	P9	2	3.5	5	2
H18A	H13A	2	3.5	5	2
H18A	P15	2	3.5	5	2
H18A	P16	2	3.5	5	2
H21A	H18A	2	3.5	5	2
H21A	P16	2	3.5	5	2
P9	P22	2	3.5	6	2
H25A	H5	2	3.5	5	2
H25A	H21A	2	3.5	5	2
H28A	P36	2	3.5	5	2
P3135	P36	2	3.5	5	2
H38A	P3135	2	3.5	5	2
H44A	P3135	2	3.5	5	2
P3135	P45	2	3.5	5	2
P36	P39	2	3.5	6	2
H38A	P36	2	3.5	5	2
P36	P41	2	3.5	6	2
H43A	P22	2	3.5	6	2
H43A	P41	2	2.5	4.5	2
H43A	P47	2	3.5	5	2
H43A	P50	2	3.5	6	2
H44A	P47	2	3.5	5	2
P46	P47	2	3.5	5	2
H49A	H43A	2	3.5	5	2
H49A	P46	2	3.5	5	2
P15	P50	2	3.5	6	2
P40	P50	2	3.5	7	2
H11A	P5	2	3.5	5	2
P22	P19	2	3.5	7	2
H5	H28A	2	3.5	5	2
H28A	H38A	2	3.5	5	2
H49A	P47	2	2.5	3.5	2

Table S3. Angle Constraints Used in Molecular Modeling of Grassypeptolide C (**3**)

Atom 1	Atom 2	Atom 3	Atom 4	Const	Value (°)	Pwr
H1	N1	C3	H3A	0.005	180	2
H2	N2	C7	H7A	0.005	180	2
H5	N5	C21	H21A	0.005	180	2
H1	N1	C6	O3	2	180	2
H2	N2	C10	O5	2	180	2
C16	N3	C17	O6	2	180	2
H5	N5	C24	O7	2	180	2
C36	N7	C37	O8	2	0	2
C41	N8	C42	O9	2	180	2
C47	N9	C48	O10	2	180	2

Table S4. Energies and Constraint Violations[a] of Grassypeptolide C (**3**) Molecular Models

Struc 1[b]	Energy 60.12 kcal/mol		
Atom 1	Atom 2	Range (Å)	Violation (Å)
H7A	P14	3.5-5	1.715
H7A	P16	3.5-5	1.053
H8A	P46	3.5-5	2.453
H18A	P15	3.5-5	1.141
H21A	P16	3.5-5	2.249
H43A	P22	3.5-6	1.182
P15	P50	3.5-6	1.61
H11A	P5	3.5-5	2.133

Struc 2	Energy 62.76 kcal/mol		
Atom 1	Atom 2	Range (Å)	Violation (Å)
H1	P46	3.5-5	1.14
H7A	P14	3.5-5	2.537
H8A	P46	3.5-5	1.817
H18A	P9	3.5-5	1.768
H21A	P16	3.5-5	2.363
P15	P50	3.5-6	1.091
H11A	P5	3.5-5	2.286

Struc 3	Energy 38.46 kcal/mol		
Atom 1	Atom 2	Range (Å)	Violation (Å)
P14	P16	3.5-5	1.11
P15	P16	3.5-5	1.111
H18A	P9	3.5-5	1.012
H18A	H13A	3.5-5	1.139
H18A	P15	3.5-5	1.257
H44A	P3135	3.5-5	1.012

Struc 4	Energy 37.82 kcal/mol		
Atom 1	Atom 2	Range (Å)	Violation (Å)
H7A	P14	3.5-5	2.157
H18A	H13A	3.5-5	1.57

Struc 5	Energy 60.65 kcal/mol		
Atom 1	Atom 2	Range (Å)	Violation (Å)
H7A	H1	3.5-5	1.116
H43A	H1	3.5-5	1.062
H7A	P14	3.5-5	2.558
H7A	P16	3.5-5	1.14
H18A	P15	3.5-5	1.17
H21A	P16	3.5-5	1.125
P9	P22	3.5-6	1.415
H44A	P3135	3.5-5	1.552
H11A	P5	3.5-5	1.865

Struc 6	Energy 33.93 kcal/mol		
Atom 1	Atom 2	Range (Å)	Violation (Å)
H7A	P14	3.5-5	2.575

Struc 7	Energy 37.01 kcal/mol		
Atom 1	Atom 2	Range (Å)	Violation (Å)
P15	P16	3.5-5	1.126
H18A	P9	3.5-5	1.001
H18A	P15	3.5-5	1.098
H44A	P3135	3.5-5	1.067

Struc 8	Energy 32.67 kcal/mol		
Atom 1	Atom 2	Range (Å)	Violation (Å)
H18A	P9	3.5-5	1.037

Struc 9	Energy 30.62 kcal/mol		
Atom 1	Atom 2	Range (Å)	Violation (Å)
H18A	P9	3.5-5	1.319

Struc 10	Energy 35.22 kcal/mol		
Atom 1	Atom 2	Range (Å)	Violation (Å)
H7A	P14	3.5-5	2.057

[a]Only violations of > 1 Å to the upper bound of constraints are shown. [b]Members of the higher energy conformational family are shown in red, while members of the lower energy conformational family are shown in blue.

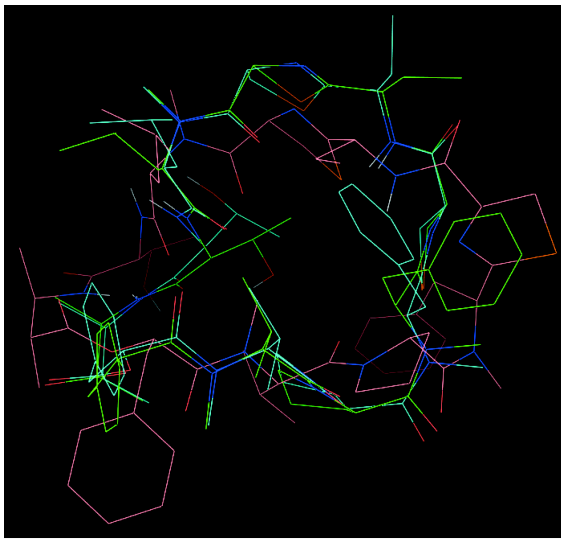


Figure S1. Higher-energy conformational family of grassypeptolide C (**3**) molecular models.

Table S5. Atom coordinates for modeled grassypeptolide C (**3**) structure 1

Atom number	Atom name[a,b]	x	y	z	Atom type[c]	Charge[d]
1	C11	−1.391	1.4867	−3.2106	C.3	0.1336
2	C10	−0.4116	0.9916	−2.19	C.2	0.2042
3	N2	0.8906	1.28	−2.4053	N.am	−0.2613
4	O5	−0.8124	0.3228	−1.2526	O.2	−0.3944
5	N3	−1.5557	2.9248	−2.9873	N.am	−0.2542
6	C12	−2.7346	0.7089	−3.1896	C.3	−0.0099
7	C13	−3.6585	1.0191	−4.401	C.3	−0.0425
8	C14	−3.0272	0.5708	−5.7514	C.3	−0.0625
9	C15	−5.0062	0.2777	−4.1921	C.3	−0.0625
10	C7	1.9099	0.6884	−1.5572	C.3	0.1563
11	C6	3.0143	0.175	−2.45	C.2	0.2046
12	N1	2.6439	−0.6933	−3.4218	N.am	−0.2796
13	C8	2.344	1.7204	−0.4859	C.3	0.0924
14	C9	1.1835	2.0526	0.4848	C.3	−0.0346
15	O4	3.4398	1.2294	0.3077	O.3	−0.3874
16	O3	4.1588	0.5626	−2.2769	O.2	−0.3944
17	C3	3.6121	−1.2448	−4.3719	C.3	0.0598
18	C16	−1.2848	3.8764	−4.0621	C.3	0.0254
19	C17	−1.8942	3.3438	−1.7327	C.2	0.1909
20	C18	−2.0315	4.7949	−1.3271	C.3	0.1002
21	O6	−2.1193	2.5424	−0.8389	O.2	−0.3959
22	C4	3.1454	−0.8824	−5.8067	C.3	−0.0395
23	C2	3.737	−2.7837	−4.1718	C.3	0.08
24	C1	2.3803	−3.4286	−4.3133	C.2	0.2415
25	C5	4.3258	−3.0803	−2.7667	C.3	−0.0418
26	O1	1.6279	−3.3278	−3.2123	O.3	−0.2498
27	O2	2.0218	−3.9612	−5.3516	O.2	−0.3699
28	C49	0.2103	−3.4902	−3.3902	C.3	0.1852
29	C48	−0.3492	−2.9799	−2.0793	C.2	0.2166
30	N9	−0.2715	−3.5935	−0.863	N.am	−0.252
31	O10	−0.8669	−1.8846	−2.183	O.2	−0.3933
32	C50	−0.3163	−4.8634	−3.8932	C.3	0.0292
33	C51	−1.8059	−5.085	−3.5788	C.ar	−0.0379
34	C56	−2.2483	−6.3207	−3.0895	C.ar	−0.0601
35	C55	−3.592	−6.5148	−2.7561	C.ar	−0.0686
36	C54	−4.5105	−5.4749	−2.9198	C.ar	−0.0687
37	C53	−4.0843	−4.2501	−3.4388	C.ar	−0.0686
38	C52	−2.7423	−4.0636	−3.7827	C.ar	−0.0601
39	C43	−0.8145	−2.8767	0.31	C.3	0.1359
40	C47	0.3554	−4.9125	−0.7578	C.3	0.0255
41	C42	−0.1295	−3.23	1.6242	C.2	0.2068
42	C44	−2.3738	−2.9968	0.4277	C.3	−0.0061
43	C46	−3.1531	−2.0422	−0.5223	C.3	−0.0584
44	C45	−2.8421	−4.4604	0.2351	C.3	−0.0584
45	N4	−2.4653	4.8053	0.052	N.2	−0.3321
46	C20	−1.4658	4.9759	0.8185	C.2	0.1014

Table S5. Continued

47	S1	0.1511	5.2564	0.1632	S.3	–0.0465
48	C19	–0.7163	5.6227	–1.3807	C.3	0.043
49	C21	–1.6692	4.9511	2.3088	C.3	0.1158
50	N5	–0.7944	3.9596	2.9372	N.am	–0.2623
51	C22	–3.1336	4.5889	2.6854	C.3	–0.013
52	C23	–3.3924	4.7362	4.2083	C.3	–0.0602
53	C24	–0.1097	4.2335	4.0745	C.2	0.1895
54	C25	0.5631	3.0775	4.7783	C.3	0.1001
55	O7	–0.0347	5.3478	4.5672	O.2	–0.396
56	N6	–0.0594	1.8557	4.3257	N.2	–0.332
57	C27	0.8072	0.9329	4.2252	C.2	0.1037
58	S2	2.4944	1.2362	4.6706	S.3	–0.0463
59	C26	2.0854	2.9964	4.499	C.3	0.043
60	C28	0.3758	–0.4179	3.7067	C.3	0.128
61	N7	0.5433	–1.4562	4.7301	N.am	–0.2484
62	C29	–1.0624	–0.3488	3.1117	C.3	0.0238
63	C30	–2.185	–0.411	4.1553	C.ar	–0.0376
64	C31	–2.5815	–1.6387	4.6999	C.ar	–0.06
65	C32	–3.5588	–1.6854	5.6985	C.ar	–0.0686
66	C33	–4.1704	–0.5073	6.1359	C.ar	–0.0687
67	C34	–3.8115	0.7159	5.5634	C.ar	–0.0686
68	C35	–2.8361	0.7571	4.5635	C.ar	–0.06
69	C37	1.1191	–2.6734	4.4709	C.2	0.2073
70	C38	1.7517	–3.1847	3.178	C.3	0.134
71	C36	0.0844	–1.2197	6.1025	C.3	0.0266
72	O8	1.2125	–3.4759	5.3878	O.2	–0.3941
73	C39	3.18	–2.6121	2.9859	C.3	–0.0104
74	C40	3.399	–2.679	1.4561	C.3	–0.0281
75	C41	2.0241	–2.2627	0.8871	C.3	0.0369
76	N8	1.1638	–2.9029	1.8738	N.am	–0.2498
77	O9	–0.7914	–3.7662	2.4987	O.2	–0.3942
78	H11A	–0.8738	1.2396	–4.1521	H	0.0802
79	H2	1.1998	1.8335	–3.183	H	0.1884
80	H12B	–2.5272	–0.3708	–3.2043	H	0.0315
81	H12A	–3.2716	0.9308	–2.2559	H	0.0315
82	H13A	–3.8634	2.103	–4.4357	H	0.0298
83	H14C	–2.6969	–0.4781	–5.6893	H	0.0232
84	H14A	–3.7646	0.6561	–6.5625	H	0.0232
85	H14B	–2.1657	1.1924	–6.0323	H	0.0232
86	H15B	–5.4772	0.5946	–3.2487	H	0.0232
87	H15C	–4.835	–0.8091	–4.1539	H	0.0232
88	H15A	–5.6988	0.5003	–5.017	H	0.0232
89	H7A	1.4806	–0.1624	–1.0224	H	0.0826
90	H1	1.6849	–0.9747	–3.5132	H	0.1856
91	H8A	2.6143	2.6462	–1.0131	H	0.0639
92	H9A	0.3219	2.4604	–0.0576	H	0.0257
93	H9C	0.8626	1.1539	1.0283	H	0.0257

Table S5. Continued

94	H9B	1.5183	2.802	1.2151	H	0.0257
95	H4	4.2166	1.0445	–0.2095	H	0.2101
96	H3A	4.6178	–0.8115	–4.2339	H	0.0582
97	H16B	–0.1961	4.0062	–4.151	H	0.0488
98	H16C	–1.7569	4.8576	–3.9261	H	0.0488
99	H16A	–1.6588	3.4717	–5.0111	H	0.0488
100	H18A	–2.8446	5.247	–1.9138	H	0.0619
101	H4C	2.1479	–1.2987	–6.0139	H	0.0253
102	H4A	3.8529	–1.2701	–6.5559	H	0.0253
103	H4B	3.0902	0.2127	–5.9083	H	0.0253
104	H2A	4.4167	–3.2039	–4.9328	H	0.0574
105	H5B	4.3618	–4.1665	–2.597	H	0.0258
106	H5A	3.7108	–2.6213	–1.9771	H	0.0258
107	H5C	5.3441	–2.6713	–2.6873	H	0.0258
108	H49A	–0.0742	–2.7595	–4.1673	H	0.0918
109	H50B	0.3091	–5.6595	–3.4715	H	0.048
110	H50A	–0.2366	–4.9266	–4.9898	H	0.048
111	H56A	–1.5502	–7.142	–2.9642	H	0.0557
112	H55A	–3.9231	–7.473	–2.3676	H	0.0599
113	H54A	–5.5508	–5.6177	–2.6455	H	0.0559
114	H53A	–4.7972	–3.4427	–3.5745	H	0.0599
115	H52A	–2.4413	–3.1147	–4.2121	H	0.0557
116	H43A	–0.5903	–1.7999	0.2273	H	0.0805
117	H47B	–0.315	–5.678	–1.1676	H	0.0488
118	H47C	1.3146	–4.9401	–1.2945	H	0.0488
119	H47A	0.5626	–5.1986	0.2814	H	0.0488
120	H44A	–2.6936	–2.6888	1.4374	H	0.0343
121	H46A	–2.7784	–1.0108	–0.434	H	0.0234
122	H46C	–3.0804	–2.3647	–1.5676	H	0.0234
123	H46B	–4.2206	–2.0291	–0.26	H	0.0234
124	H45B	–2.6394	–4.7775	–0.7946	H	0.0234
125	H45A	–3.9241	–4.5449	0.4211	H	0.0234
126	H45C	–2.3142	–5.1351	0.9252	H	0.0234
127	H19A	–0.0543	5.4087	–2.2283	H	0.0448
128	H19B	–0.955	6.6981	–1.3742	H	0.0448
129	H21A	–1.4633	5.9788	2.6371	H	0.0854
130	H5	–0.8199	3.0244	2.5808	H	0.1896
131	H22B	–3.3402	3.5515	2.3711	H	0.032
132	H22A	–3.8324	5.2532	2.1514	H	0.032
133	H23A	–4.4383	4.4783	4.4375	H	0.0233
134	H23B	–3.2099	5.7739	4.5279	H	0.0233
135	H23C	–2.7384	4.0723	4.7917	H	0.0233
136	H25A	0.3748	3.1445	5.8627	H	0.0619
137	H26A	2.6742	3.6201	5.1891	H	0.0448
138	H26B	2.3092	3.293	3.4644	H	0.0448
139	H28A	1.0681	–0.5746	2.8816	H	0.088
140	H29A	–1.1783	0.5323	2.4622	H	0.0485

Table S5. Continued

141	H29B	–1.2264	–1.2068	2.4693	H	0.0485
142	H31A	–2.1309	–2.564	4.3532	H	0.0557
143	H32A	–3.8426	–2.6378	6.1358	H	0.0599
144	H33A	–4.9239	–0.5429	6.9169	H	0.0559
145	H34A	–4.2902	1.633	5.893	H	0.0599
146	H35A	–2.5877	1.7015	4.098	H	0.0557
147	H38A	1.8234	–4.2843	3.2246	H	0.0802
148	H36C	–0.4715	–0.2761	6.2014	H	0.0489
149	H36A	–0.5651	–2.0347	6.4557	H	0.0489
150	H36B	0.9621	–1.16	6.7638	H	0.0489
151	H39B	3.9425	–3.1744	3.5493	H	0.0313
152	H39A	3.2208	–1.5588	3.3057	H	0.0313
153	H40A	3.611	–3.7221	1.1663	H	0.0287
154	H40B	4.223	–2.036	1.1047	H	0.0287
155	H41B	1.9368	–1.1737	0.9249	H	0.0524
156	H41A	1.9009	–2.6165	–0.1456	H	0.0524
157	P5	4.4722	–3.153	–2.4205	Du	0
158	P4	3.0303	–0.7854	–6.1594	Du	0
159	P9	0.9009	2.1388	0.7286	Du	0
160	P12	–2.8994	0.28	–2.7301	Du	0
161	P14	–2.8758	0.4568	–6.0947	Du	0
162	P15	–5.337	0.0953	–4.1399	Du	0
163	P16	–1.204	4.1119	–4.3628	Du	0
164	P22	–3.5863	4.4023	2.2612	Du	0
165	P23	–3.4622	4.7748	4.5857	Du	0
166	P29	–1.2023	–0.3372	2.4657	Du	0
167	P3135	–2.3593	–0.4312	4.2256	Du	0
168	P36	–0.0248	–1.1569	6.4736	Du	0
169	P39	3.5817	–2.3666	3.4275	Du	0
170	P40	3.917	–2.8791	1.1355	Du	0
171	P41	1.9189	–1.8951	0.3897	Du	0
172	P46	–3.3598	–1.8016	–0.7539	Du	0
173	P45	–2.9593	–4.8192	0.1839	Du	0
174	P47	0.5207	–5.2722	–0.7269	Du	0
175	P50	0.0363	–5.2931	–4.2306	Du	0
176	P19	–0.5046	6.0534	–1.8013	Du	0

[a]Atom nomenclature as in Figure 1a. [b]Pseudoatoms used in modeling are designated by "P" followed by the number of the relevant carbon atom(s). [c]Tripos forcefield atom type. [d]Gasteiger-Huckel charges.

Table S6. Atom coordinates for modeled grassypeptolide C (**3**) structure 2

Atom number	Atom name[a,b]	x	y	z	Atom type[c]	Charge[d]
1	N2	–0.3831	–2.485	–1.7662	N.am	–0.2613
2	C7	–1.7327	–1.9583	–1.681	C.3	0.1563
3	C6	–2.3187	–1.8701	–3.0673	C.2	0.2046
4	N1	–1.5124	–1.3071	–4.0001	N.am	–0.2796
5	C3	–1.8924	–1.2228	–5.411	C.3	0.0598
6	C8	–2.4565	–2.8475	–0.6357	C.3	0.0924
7	H8A	–1.7274	–3.0274	0.1732	H	0.0639
8	C9	–3.6625	–2.1426	0.0273	C.3	–0.0346
9	O3	–3.4403	–2.2982	–3.2872	O.2	–0.3944
10	H1	–0.6009	–0.9753	–3.7448	H	0.1856
11	C2	–1.7415	0.2421	–5.9176	C.3	0.08
12	C1	–0.3357	0.7312	–5.6616	C.2	0.2415
13	C4	–0.9845	–2.2005	–6.2033	C.3	–0.0395
14	C5	–2.7635	1.1465	–5.1806	C.3	–0.0418
15	O1	–0.1527	1.2073	–4.4229	O.3	–0.2498
16	O2	0.5329	0.6627	–6.5163	O.2	–0.3699
17	C49	1.2017	1.2668	–3.94	C.3	0.1852
18	C48	1.0767	1.5709	–2.4572	C.2	0.2166
19	C50	2.2395	2.1334	–4.7056	C.3	0.0292
20	C51	3.4997	2.3252	–3.8461	C.ar	–0.0379
21	C52	3.9336	3.6044	–3.4798	C.ar	–0.0601
22	C53	5.0348	3.7633	–2.6335	C.ar	–0.0686
23	C54	5.7333	2.6439	–2.1739	C.ar	–0.0687
24	C55	5.3392	1.3664	–2.58	C.ar	–0.0686
25	C56	4.2317	1.2103	–3.4182	C.ar	–0.0601
26	H50B	2.5772	1.6322	–5.626	H	0.048
27	H50A	1.7907	3.0873	–5.0059	H	0.048
28	N9	0.5161	2.6851	–1.8977	N.am	–0.252
29	O10	1.4872	0.6712	–1.749	O.2	–0.3933
30	C43	0.3576	2.7304	–0.4256	C.3	0.1359
31	C47	0.0271	3.7607	–2.7657	C.3	0.0255
32	C42	–0.881	3.5068	–0.0009	C.2	0.2068
33	C44	1.6539	3.213	0.2984	C.3	–0.0061
34	C45	2.2117	4.5304	–0.3019	C.3	–0.0584
35	C46	2.7579	2.1166	0.31	C.3	–0.0584
36	H44A	1.4023	3.4097	1.3532	H	0.0343
37	N8	–2.1233	3.0281	–0.2703	N.am	–0.2498
38	O9	–0.7451	4.5672	0.5875	O.2	–0.3942
39	C38	–3.3182	3.7803	0.0973	C.3	0.134
40	C39	–4.4218	2.7893	–0.3559	C.3	–0.0104
41	C40	–3.7648	1.9985	–1.5059	C.3	–0.0281
42	C41	–2.337	1.7692	–0.9689	C.3	0.0369
43	C37	–3.6558	4.2182	1.5161	C.2	0.2073
44	N7	–3.368	3.5976	2.7007	N.am	–0.2484
45	H41A	–2.3332	0.959	–0.2281	H	0.0524
46	H41B	–1.6475	1.5445	–1.7928	H	0.0524

Table S6. Continued

47	H40A	−4.2876	1.0591	−1.7509	H	0.0287
48	H40B	−3.7277	2.6392	−2.403	H	0.0287
49	H39B	−4.6491	2.0809	0.4567	H	0.0313
50	H39A	−5.3555	3.2919	−0.6572	H	0.0313
51	O8	−4.3318	5.236	1.5383	O.2	−0.3941
52	C28	−2.4464	2.4588	2.8013	C.3	0.128
53	C27	−3.1283	1.3052	3.4962	C.2	0.1037
54	C36	−3.9041	4.2154	3.9178	C.3	0.0266
55	C29	−1.1938	3.0048	3.5441	C.3	0.0238
56	C30	0.0971	2.1734	3.5273	C.ar	−0.0376
57	C35	1.2287	2.7513	4.1163	C.ar	−0.06
58	C34	2.4444	2.0651	4.1684	C.ar	−0.0686
59	C33	2.5308	0.7719	3.6512	C.ar	−0.0687
60	C32	1.4036	0.1889	3.0683	C.ar	−0.0686
61	C31	0.2021	0.8951	2.9664	C.ar	−0.06
62	H29B	−1.4384	3.1791	4.6025	H	0.0485
63	H29A	−0.9379	3.9758	3.0923	H	0.0485
64	S2	−4.8217	0.9499	3.1077	S.3	−0.0463
65	C26	−4.5005	−0.6805	3.8233	C.3	0.043
66	C25	−3.3997	−0.4157	4.878	C.3	0.1001
67	N6	−2.5043	0.5908	4.345	N.2	−0.332
68	C24	−2.6916	−1.7052	5.2229	C.2	0.1895
69	N5	−1.6778	−2.1167	4.4268	N.am	−0.2623
70	O7	−3.0696	−2.3311	6.2008	O.2	−0.396
71	H26A	−5.4087	−1.1252	4.2581	H	0.0448
72	H26B	−4.119	−1.3328	3.0236	H	0.0448
73	C21	−0.8702	−3.2886	4.7736	C.3	0.1158
74	C20	−0.603	−4.085	3.5276	C.2	0.1014
75	C22	0.4167	−2.7402	5.4485	C.3	−0.013
76	C23	1.2177	−3.8318	6.2075	C.3	−0.0602
77	S1	−1.9498	−4.5199	2.4662	S.3	−0.0465
78	C19	−0.7621	−5.5798	1.5983	C.3	0.043
79	C18	0.6297	−4.9693	1.9094	C.3	0.1002
80	N4	0.5895	−4.4159	3.242	N.2	−0.3321
81	C17	0.9677	−3.7973	1.0155	C.2	0.1909
82	C10	0.5778	−1.9411	−0.9912	C.2	0.2042
83	C11	1.8834	−2.6726	−0.9424	C.3	0.1336
84	O5	0.4223	−0.935	−0.3164	O.2	−0.3944
85	N3	1.6033	−3.9048	−0.1873	N.am	−0.2542
86	H2	−0.2239	−3.3124	−2.31	H	0.1884
87	C12	2.9919	−1.8097	−0.2841	C.3	−0.0099
88	C13	4.3451	−2.5431	−0.0975	C.3	−0.0425
89	C15	4.9704	−2.9455	−1.4608	C.3	−0.0625
90	C14	5.3013	−1.5985	0.6782	C.3	−0.0625
91	H12A	3.1663	−0.9116	−0.8957	H	0.0315
92	H12B	2.6507	−1.4801	0.7058	H	0.0315
93	H13A	4.1917	−3.4491	0.5134	H	0.0298

Table S6. Continued

94	H19A	–0.989	–5.6327	0.524	H	0.0448
95	H19B	–0.8422	–6.5865	2.0377	H	0.0448
96	H5	–1.4032	–1.5686	3.6357	H	0.1896
97	H22B	1.0487	–2.2598	4.6847	H	0.032
98	H22A	0.1208	–1.9648	6.1746	H	0.032
99	O6	0.6214	–2.7169	1.4628	O.2	–0.3959
100	C16	1.9961	–5.2238	–0.6755	C.3	0.0254
101	H7A	–1.6843	–0.9512	–1.2587	H	0.0826
102	H3A	–2.9348	–1.5458	–5.5768	H	0.0582
103	O57	–2.8994	–4.0917	–1.2046	O.3	–0.3874
104	H3	–2.191	–4.6048	–1.5776	H	0.2101
105	H9C	–3.3368	–1.2385	0.5649	H	0.0257
106	H9A	–4.128	–2.829	0.7526	H	0.0257
107	H9B	–4.4028	–1.8661	–0.7353	H	0.0257
108	H2A	–1.9476	0.2885	–7.0007	H	0.0574
109	H4B	0.0784	–1.9487	–6.0688	H	0.0253
110	H4A	–1.1433	–3.2277	–5.8395	H	0.0253
111	H4C	–1.2225	–2.1673	–7.2776	H	0.0253
112	H5C	–3.7912	0.8501	–5.4373	H	0.0258
113	H5A	–2.6112	2.1991	–5.462	H	0.0258
114	H5B	–2.6421	1.0508	–4.0913	H	0.0258
115	H49A	1.5668	0.2293	–4.0224	H	0.0918
116	H52A	3.4173	4.485	–3.848	H	0.0557
117	H53A	5.3479	4.758	–2.3315	H	0.0599
118	H54A	6.5801	2.7655	–1.5057	H	0.0559
119	H55A	5.8937	0.496	–2.2451	H	0.0599
120	H56A	3.949	0.2117	–3.7341	H	0.0557
121	H43A	0.1455	1.7278	–0.0174	H	0.0805
122	H47A	–0.6657	3.3836	–3.53	H	0.0488
123	H47C	–0.5052	4.5435	–2.2103	H	0.0488
124	H47B	0.8735	4.2575	–3.2548	H	0.0488
125	H45C	2.5182	4.3714	–1.3424	H	0.0234
126	H45B	3.0913	4.8644	0.2699	H	0.0234
127	H45A	1.4617	5.3336	–0.2816	H	0.0234
128	H46B	2.3527	1.1505	0.6489	H	0.0234
129	H46A	3.5694	2.3966	0.9958	H	0.0234
130	H46C	3.1931	1.9866	–0.6903	H	0.0234
131	H38A	–3.3214	4.6581	–0.5686	H	0.0802
132	H28A	–2.1513	2.074	1.8296	H	0.088
133	H36A	–4.9752	4.444	3.8024	H	0.0489
134	H36B	–3.8136	3.5506	4.7896	H	0.0489
135	H36C	–3.3593	5.1478	4.1308	H	0.0489
136	H35A	1.1668	3.7493	4.54	H	0.0557
137	H34A	3.3175	2.5344	4.6109	H	0.0599
138	H33A	3.4666	0.2238	3.7014	H	0.0559
139	H32A	1.4677	–0.8209	2.693	H	0.0599
140	H31A	–0.6311	0.4346	2.4498	H	0.0557

Table S6. Continued

141	H25A	–3.8482	0.0141	5.79	H	0.0619
142	H21A	–1.3758	–3.9596	5.4795	H	0.0854
143	H23A	0.5996	–4.277	7.0029	H	0.0233
144	H23B	2.1097	–3.3823	6.6718	H	0.0233
145	H23C	1.5482	–4.6341	5.5324	H	0.0233
146	H18A	1.4169	–5.7303	1.886	H	0.0619
147	H11A	2.1329	–2.8322	–2.0051	H	0.0802
148	H15A	5.9719	–3.3737	–1.3074	H	0.0232
149	H15C	5.0602	–2.0659	–2.1162	H	0.0232
150	H15B	4.357	–3.7014	–1.9704	H	0.0232
151	H14C	4.8718	–1.3412	1.6598	H	0.0232
152	H14A	5.4564	–0.6682	0.111	H	0.0232
153	H14B	6.2725	–2.0866	0.8401	H	0.0232
154	H16C	1.1636	–5.9377	–0.5971	H	0.0488
155	H16A	2.85	–5.5956	–0.0906	H	0.0488
156	H16B	2.2902	–5.1857	–1.7326	H	0.0488
157	P4	–0.7625	–2.4479	–6.3953	Du	0
158	P5	–3.0148	1.3667	–4.9969	Du	0
159	P9	–3.9559	–1.9778	0.1941	Du	0
160	P12	2.9085	–1.1958	–0.0949	Du	0
161	P15	5.1297	–3.047	–1.798	Du	0
162	P14	5.5336	–1.3653	0.8703	Du	0
163	P16	2.1013	–5.573	–0.8068	Du	0
164	P22	0.5847	–2.1123	5.4297	Du	0
165	P23	1.4192	–4.0978	6.4024	Du	0
166	P29	–1.1882	3.5775	3.8474	Du	0
167	P3135	0.2678	2.092	3.4949	Du	0
168	P36	–4.0493	4.3808	4.2409	Du	0
169	P39	–5.0023	2.6864	–0.1002	Du	0
170	P40	–4.0076	1.8491	–2.077	Du	0
171	P41	–1.9903	1.2517	–1.0105	Du	0
172	P46	3.0384	1.8445	0.3182	Du	0
173	P45	2.357	4.8565	–0.4514	Du	0
174	P47	–0.0991	4.0615	–2.9983	Du	0
175	P50	2.1839	2.3598	–5.3159	Du	0
176	P19	–0.9156	–6.1096	1.2809	Du	0

[a]Atom nomenclature as in Figure 1a. [b]Pseudoatoms used in modeling are designated by "P" followed by the number of the relevant carbon atom(s). [c]Tripos forcefield atom type. [d]Gasteiger-Huckel charges.

Table S7. Atom coordinates for modeled grassypeptolide C (**3**) structure 3

Atom number	Atom name[a,b]	x	y	z	Atom type[c]	Charge[d]
1	N2	–3.1374	–2.2402	–1.762	N.am	–0.2613
2	C7	–3.6879	–2.7154	–3.0309	C.3	0.1563
3	C6	–4.636	–1.7092	–3.6517	C.2	0.2046
4	N1	–4.3306	–0.3862	–3.6765	N.am	–0.2796
5	C3	–5.2769	0.592	–4.2197	C.3	0.0598
6	O3	–5.6716	–2.1472	–4.1294	O.2	–0.3944
7	C2	–5.9729	1.3634	–3.0612	C.3	0.08
8	C1	–5.0264	2.2802	–2.3264	C.2	0.2415
9	O1	–3.9706	1.6852	–1.7485	O.3	–0.2498
10	O2	–5.2384	3.4829	–2.2852	O.2	–0.3699
11	C49	–3.1718	2.5597	–0.9226	C.3	0.1852
12	C48	–1.9036	1.8136	–0.5635	C.2	0.2166
13	N9	–0.7801	1.8627	–1.3341	N.am	–0.252
14	O10	–1.9224	1.1848	0.4828	O.2	–0.3933
15	C43	0.4252	1.1869	–0.8361	C.3	0.1359
16	C47	–0.7747	2.6234	–2.5907	C.3	0.0255
17	C42	1.6591	1.9884	–1.1848	C.2	0.2068
18	N8	1.8738	3.2113	–0.6261	N.am	–0.2498
19	C38	3.0915	3.953	–0.9175	C.3	0.134
20	C39	3.1333	4.9623	0.2552	C.3	–0.0104
21	C40	1.6269	5.2148	0.5275	C.3	–0.0281
22	C41	0.9393	3.8391	0.3106	C.3	0.0369
23	C37	4.3455	3.1835	–1.3321	C.2	0.2073
24	N7	5.1969	2.3822	–0.6075	N.am	–0.2484
25	O8	4.5797	3.3407	–2.5219	O.2	–0.3941
26	C28	5.0402	2.1043	0.8366	C.3	0.128
27	C27	5.9674	0.9866	1.2658	C.2	0.1037
28	C36	6.3238	1.7828	–1.3447	C.3	0.0266
29	S2	7.275	1.2482	2.433	S.3	–0.0463
30	C26	7.3025	–0.5557	2.6137	C.3	0.043
31	C25	6.7233	–1.1092	1.2844	C.3	0.1001
32	N6	5.7718	–0.1612	0.7549	N.2	–0.332
33	C24	6.043	–2.444	1.4791	C.2	0.1895
34	N5	4.8354	–2.6306	0.8906	N.am	–0.2623
35	O7	6.6057	–3.2896	2.1564	O.2	–0.396
36	C21	4.0827	–3.8761	1.0519	C.3	0.1158
37	C20	2.8357	–3.566	1.8411	C.2	0.1014
38	S1	2.9575	–3.3134	3.5913	S.3	–0.0465
39	C19	1.3796	–2.4417	3.4136	C.3	0.043
40	C18	0.6843	–3.189	2.2461	C.3	0.1002
41	N4	1.706	–3.4804	1.2642	N.2	–0.3321
42	C17	–0.4981	–2.4422	1.6752	C.2	0.1909
43	C10	–3.395	–2.8795	–0.5958	C.2	0.2042
44	C11	–2.6887	–2.4011	0.6536	C.3	0.1336
45	O5	–4.1475	–3.8375	–0.5128	O.2	–0.3944
46	N3	–1.3967	–3.0652	0.8592	N.am	–0.2542

Table S7. Continued

47	O6	−0.6439	−1.2827	2.0308	O.2	−0.3959
48	C16	−1.1743	−4.4597	0.4609	C.3	0.0254
49	O9	2.4593	1.4954	−1.9619	O.2	−0.3942
50	C5	−6.6287	0.3844	−2.0513	C.3	−0.0418
51	C4	−4.5522	1.5507	−5.2006	C.3	−0.0395
52	C8	−2.5233	−3.0649	−3.997	C.3	0.0924
53	O4	−3.0172	−3.7134	−5.1833	O.3	−0.3874
54	C9	−1.5112	−4.0248	−3.3159	C.3	−0.0346
55	C12	−3.4741	−2.7304	1.9524	C.3	−0.0099
56	C13	−4.9391	−2.2173	1.9801	C.3	−0.0425
57	C15	−5.5358	−2.5055	3.3837	C.3	−0.0625
58	C14	−5.0328	−0.7049	1.6464	C.3	−0.0625
59	C22	3.8079	−4.4977	−0.3442	C.3	−0.013
60	C23	3.1368	−5.8935	−0.2485	C.3	−0.0602
61	C29	3.6778	1.5688	1.347	C.3	0.0238
62	C30	3.7097	1.3224	2.862	C.ar	−0.0376
63	C31	3.4963	2.3828	3.7503	C.ar	−0.06
64	C32	3.5608	2.1717	5.1303	C.ar	−0.0686
65	C33	3.8363	0.8959	5.6297	C.ar	−0.0687
66	C34	4.0334	−0.1692	4.7469	C.ar	−0.0686
67	C35	3.9504	0.0416	3.3677	C.ar	−0.06
68	C44	0.3998	−0.3043	−1.2891	C.3	−0.0061
69	C46	0.2369	−0.4771	−2.8241	C.3	−0.0584
70	C45	1.6034	−1.1319	−0.7651	C.3	−0.0584
71	C50	−3.9276	2.9611	0.378	C.3	0.0292
72	C51	−2.9673	3.7106	1.3174	C.ar	−0.0379
73	C52	−2.506	3.121	2.501	C.ar	−0.0601
74	C53	−1.5754	3.7844	3.306	C.ar	−0.0686
75	C54	−1.1209	5.0563	2.9484	C.ar	−0.0687
76	C55	−1.6062	5.6662	1.7887	C.ar	−0.0686
77	C56	−2.5342	4.9991	0.9838	C.ar	−0.0601
78	H2	−2.5161	−1.4604	−1.7887	H	0.1884
79	H7A	−4.264	−3.6413	−2.8797	H	0.0826
80	H1	−3.4827	−0.0266	−3.2851	H	0.1856
81	H3A	−6.0868	0.0985	−4.7846	H	0.0582
82	H2A	−6.7749	1.986	−3.4964	H	0.0574
83	H49A	−2.9093	3.4876	−1.4512	H	0.0918
84	H43A	0.4494	1.1498	0.2644	H	0.0805
85	H47C	−1.6593	2.3804	−3.1976	H	0.0488
86	H47A	0.1038	2.3844	−3.2066	H	0.0488
87	H47B	−0.752	3.7064	−2.4022	H	0.0488
88	H38A	2.7928	4.5719	−1.7808	H	0.0802
89	H39B	3.6826	5.8854	0.0059	H	0.0313
90	H39A	3.5871	4.5315	1.1544	H	0.0313
91	H40B	1.4412	5.6386	1.5276	H	0.0287
92	H40A	1.2514	5.9278	−0.2263	H	0.0287
93	H41A	0.8616	3.2998	1.2666	H	0.0524

Table S7. Continued

94	H41B	–0.0693	3.971	–0.102	H	0.0524
95	H28A	5.333	3.0043	1.3969	H	0.088
96	H36B	6.0338	0.7744	–1.6759	H	0.0489
97	H36A	7.2248	1.7102	–0.7187	H	0.0489
98	H36C	6.6423	2.3562	–2.2274	H	0.0489
99	H26B	8.3174	–0.9274	2.8229	H	0.0448
100	H26A	6.6456	–0.8049	3.4606	H	0.0448
101	H25A	7.5257	–1.2164	0.5355	H	0.0619
102	H5	4.4192	–1.9001	0.3442	H	0.1896
103	H21A	4.6354	–4.6242	1.64	H	0.0854
104	H19B	0.796	–2.459	4.3473	H	0.0448
105	H19A	1.5983	–1.3993	3.1375	H	0.0448
106	H18A	0.2852	–4.1299	2.6562	H	0.0619
107	H11A	–2.5585	–1.3123	0.5756	H	0.0802
108	H16A	–1.3726	–5.1295	1.3101	H	0.0488
109	H16C	–1.831	–4.782	–0.3555	H	0.0488
110	H16B	–0.1485	–4.6099	0.1013	H	0.0488
111	H5A	–7.3707	–0.2515	–2.5584	H	0.0258
112	H5B	–7.1373	0.9479	–1.2534	H	0.0258
113	H5C	–5.8718	–0.2648	–1.5882	H	0.0258
114	H4A	–3.746	2.0996	–4.6927	H	0.0253
115	H4C	–4.1102	0.9681	–6.0235	H	0.0253
116	H4B	–5.2606	2.2798	–5.6237	H	0.0253
117	H8A	–1.9952	–2.1404	–4.281	H	0.0639
118	H4	–3.6185	–3.1703	–5.6825	H	0.2101
119	H9B	–2.0162	–4.9527	–3.0069	H	0.0257
120	H9C	–1.0521	–3.5628	–2.4287	H	0.0257
121	H9A	–0.7067	–4.2832	–4.0211	H	0.0257
122	H12A	–2.9365	–2.2917	2.8084	H	0.0315
123	H12B	–3.4858	–3.8238	2.0919	H	0.0315
124	H13A	–5.5324	–2.7764	1.2397	H	0.0298
125	H15C	–4.9845	–1.9445	4.1545	H	0.0232
126	H15A	–5.4636	–3.5805	3.6134	H	0.0232
127	H15B	–6.5943	–2.21	3.4186	H	0.0232
128	H14B	–4.7515	–0.5167	0.6003	H	0.0232
129	H14C	–4.3631	–0.1323	2.3053	H	0.0232
130	H14A	–6.0632	–0.3455	1.7833	H	0.0232
131	H22B	3.1756	–3.8212	–0.9379	H	0.032
132	H22A	4.7706	–4.6021	–0.8709	H	0.032
133	H23B	2.9601	–6.2942	–1.2592	H	0.0233
134	H23A	2.1713	–5.8346	0.2749	H	0.0233
135	H23C	3.7881	–6.5952	0.2954	H	0.0233
136	H29B	2.8951	2.2986	1.2154	H	0.0485
137	H29A	3.3824	0.6673	0.7931	H	0.0485
138	H31A	3.278	3.3762	3.3701	H	0.0557
139	H32A	3.3969	2.9987	5.8143	H	0.0599
140	H33A	3.8957	0.733	6.7012	H	0.0559

Table S7. Continued

141	H34A	4.2517	–1.1588	5.1347	H	0.0599
142	H35A	4.073	–0.7903	2.6851	H	0.0557
143	H44A	–0.4836	–0.7476	–0.8042	H	0.0343
144	H46A	–0.7187	–0.0535	–3.1658	H	0.0234
145	H46B	0.2446	–1.5436	–3.0889	H	0.0234
146	H46C	1.0569	0.0094	–3.3698	H	0.0234
147	H45C	1.422	–2.1938	–0.9865	H	0.0234
148	H45A	2.548	–0.8397	–1.2444	H	0.0234
149	H45B	1.7045	–1.0209	0.3246	H	0.0234
150	H50B	–4.3249	2.0561	0.8617	H	0.048
151	H50A	–4.7846	3.6176	0.1661	H	0.048
152	H52A	–2.863	2.1417	2.8033	H	0.0557
153	H53A	–1.2049	3.3112	4.2103	H	0.0599
154	H54A	–0.3939	5.5694	3.5704	H	0.0559
155	H55A	–1.2609	6.6578	1.5126	H	0.0599
156	H56A	–2.9153	5.4881	0.0932	H	0.0557
157	P5	–6.7933	0.1439	–1.8	Du	0
158	P4	–4.3723	1.7825	–5.4466	Du	0
159	P9	–1.2584	–4.2662	–3.1522	Du	0
160	P12	–3.2111	–3.0577	2.4501	Du	0
161	P15	–5.6808	–2.5783	3.7288	Du	0
162	P14	–5.0593	–0.3315	1.5629	Du	0
163	P16	–1.1174	–4.8405	0.3519	Du	0
164	P22	3.9731	–4.2117	–0.9044	Du	0
165	P23	2.9732	–6.2413	–0.2296	Du	0
166	P29	3.1388	1.4829	1.0043	Du	0
167	P3135	3.6755	1.293	3.0276	Du	0
168	P36	6.6336	1.6136	–1.5407	Du	0
169	P39	3.6349	5.2085	0.5802	Du	0
170	P40	1.3463	5.7832	0.6506	Du	0
171	P41	0.3962	3.6354	0.5823	Du	0
172	P45	1.8915	–1.3515	–0.6354	Du	0
173	P46	0.1943	–0.5292	–3.2082	Du	0
174	P47	–0.7691	2.8237	–2.9354	Du	0
175	P50	–4.5547	2.8369	0.5139	Du	0
176	P19	1.1971	–1.9292	3.7424	Du	0

[a]Atom nomenclature as in Figure 1a. [b]Pseudoatoms used in modeling are designated by "P" followed by the number of the relevant carbon atom(s). [c]Tripos forcefield atom type. [d]Gasteiger-Huckel charges.

Table S8. Atom coordinates for modeled grassypeptolide C (**3**) structure 4

Atom number	Atom name[a,b]	x	y	z	Atom type[c]	Charge[d]
1	O1	–4.4747	2.0782	–0.2663	O.3	–0.2498
2	C49	–3.9852	0.8485	–0.8441	C.3	0.1852
3	C48	–2.8144	0.2553	–0.0819	C.2	0.2166
4	C50	–3.6715	1.0303	–2.3594	C.3	0.0292
5	C51	–3.5995	–0.3345	–3.0651	C.ar	–0.0379
6	C52	–2.3808	–1.0061	–3.2123	C.ar	–0.0601
7	C53	–2.3103	–2.2129	–3.9135	C.ar	–0.0686
8	C54	–3.4706	–2.7754	–4.4506	C.ar	–0.0687
9	C55	–4.6991	–2.1345	–4.2702	C.ar	–0.0686
10	C56	–4.7623	–0.922	–3.5772	C.ar	–0.0601
11	N9	–2.9466	–0.5342	1.0246	N.am	–0.252
12	O10	–1.7125	0.5164	–0.5338	O.2	–0.3933
13	C47	–4.2811	–0.8374	1.5501	C.3	0.0255
14	C43	–1.7296	–1.0931	1.6379	C.3	0.1359
15	C42	–1.852	–2.5883	1.8541	C.2	0.2068
16	C44	–1.2765	–0.2702	2.8886	C.3	–0.0061
17	C46	–0.9214	1.1829	2.4744	C.3	–0.0584
18	C45	–2.2978	–0.2261	4.0604	C.3	–0.0584
19	N8	–2.0921	–3.4383	0.8165	N.am	–0.2498
20	O9	–1.6853	–3.0175	2.9832	O.2	–0.3942
21	C38	–2.1879	–4.8766	1.0496	C.3	0.134
22	C39	–3.2499	–5.1194	–0.0583	C.3	–0.0104
23	C40	–2.6899	–4.2974	–1.2412	C.3	–0.0281
24	C41	–2.2982	–2.9698	–0.5517	C.3	0.0369
25	C37	–1.0044	–5.7987	0.7588	C.2	0.2073
26	N7	0.3252	–5.5371	0.5497	N.am	–0.2484
27	O8	–1.3577	–6.9665	0.6898	O.2	–0.3941
28	C36	1.1814	–6.6963	0.2639	C.3	0.0266
29	C28	0.9263	–4.2029	0.6571	C.3	0.128
30	C27	1.7045	–3.939	–0.6108	C.2	0.1037
31	C29	1.8393	–4.0829	1.9144	C.3	0.0238
32	C30	1.0433	–4.0471	3.2295	C.ar	–0.0376
33	C31	1.0543	–2.9038	4.0387	C.ar	–0.06
34	C32	0.2677	–2.8394	5.1926	C.ar	–0.0686
35	C33	–0.5183	–3.9328	5.565	C.ar	–0.0687
36	C34	–0.4936	–5.0972	4.793	C.ar	–0.0686
37	C35	0.302	–5.1593	3.6455	C.ar	–0.06
38	S2	0.8787	–3.6646	–2.1554	S.3	–0.0463
39	C26	2.4345	–2.9252	–2.7193	C.3	0.043
40	C25	3.5161	–3.6335	–1.8632	C.3	0.1001
41	N6	2.9729	–3.9227	–0.557	N.2	–0.332
42	C24	4.7394	–2.7841	–1.6304	C.2	0.1895
43	N5	4.5943	–1.7136	–0.8133	N.am	–0.2623
44	O7	5.796	–3.11	–2.1482	O.2	–0.396
45	C21	5.7481	–0.933	–0.37	C.3	0.1158
46	C20	5.5639	0.5298	–0.6684	C.2	0.1014

Table S8. Continued

47	C22	5.8725	−1.0999	1.1686	C.3	−0.013
48	C23	6.0739	−2.5866	1.5621	C.3	−0.0602
49	S1	6.9595	1.6103	−0.8331	S.3	−0.0465
50	C19	5.7816	2.78	−1.5612	C.3	0.043
51	C18	4.4215	2.417	−0.9098	C.3	0.1002
52	N4	4.3822	0.98	−0.7707	N.2	−0.3321
53	C17	3.2453	3.0523	−1.6159	C.2	0.1909
54	N3	1.979	2.551	−1.5502	N.am	−0.2542
55	O6	3.5051	4.0652	−2.2448	O.2	−0.3959
56	C11	0.9015	3.2938	−2.2189	C.3	0.1336
57	C10	0.7358	4.5738	−1.4402	C.2	0.2042
58	C16	1.715	1.3298	−0.7809	C.3	0.0254
59	C12	1.0867	3.5387	−3.7468	C.3	−0.0099
60	C13	1.322	2.2489	−4.5876	C.3	−0.0425
61	C15	2.7451	1.6414	−4.4473	C.3	−0.0625
62	C14	0.2418	1.1759	−4.2995	C.3	−0.0625
63	N2	0.3365	4.4491	−0.1509	N.am	−0.2613
64	O5	0.9808	5.6409	−1.9806	O.2	−0.3944
65	C7	0.1614	5.6176	0.7086	C.3	0.1563
66	C6	−1.3105	5.9082	0.9203	C.2	0.2046
67	C8	0.8844	5.4173	2.0669	C.3	0.0924
68	O4	0.7385	6.6289	2.8293	O.3	−0.3874
69	C9	2.3846	5.084	1.8472	C.3	−0.0346
70	N1	−2.1123	4.8928	1.3164	N.am	−0.2796
71	O3	−1.7238	7.0404	0.7226	O.2	−0.3944
72	C3	−3.566	5.0292	1.3838	C.3	0.0598
73	C2	−4.1741	4.4529	0.0707	C.3	0.08
74	C1	−3.5986	3.094	−0.2533	C.2	0.2415
75	O2	−2.4078	2.979	−0.4977	O.2	−0.3699
76	C5	−3.8931	5.3799	−1.1443	C.3	−0.0418
77	C4	−4.1017	4.2711	2.6285	C.3	−0.0395
78	H49A	−4.849	0.1718	−0.8111	H	0.0918
79	H50A	−2.7335	1.5806	−2.5323	H	0.048
80	H50B	−4.4745	1.6244	−2.8228	H	0.048
81	H52A	−1.4776	−0.5974	−2.7809	H	0.0557
82	H53A	−1.3555	−2.7135	−4.0398	H	0.0599
83	H54A	−3.4178	−3.7083	−5.0034	H	0.0559
84	H55A	−5.6054	−2.5789	−4.6699	H	0.0599
85	H56A	−5.7234	−0.4369	−3.4396	H	0.0557
86	H47B	−4.226	−1.4234	2.4777	H	0.0488
87	H47C	−4.8274	0.0937	1.7655	H	0.0488
88	H47A	−4.8648	−1.4437	0.843	H	0.0488
89	H43A	−0.8603	−1.0501	0.9596	H	0.0805
90	H44A	−0.3534	−0.7271	3.2783	H	0.0343
91	H46A	−1.8144	1.6699	2.061	H	0.0234
92	H46B	−0.571	1.7662	3.3398	H	0.0234
93	H46C	−0.1271	1.1929	1.7146	H	0.0234

Table S8. Continued

94	H45C	−2.612	−1.2313	4.3746	H	0.0234
95	H45A	−3.1868	0.3576	3.7824	H	0.0234
96	H45B	−1.8381	0.2632	4.9335	H	0.0234
97	H38A	−2.6149	−5.1272	2.0353	H	0.0802
98	H39A	−3.4197	−6.1749	−0.325	H	0.0313
99	H39B	−4.2187	−4.6903	0.2529	H	0.0313
100	H40B	−3.428	−4.1747	−2.0503	H	0.0287
101	H40A	−1.7975	−4.7985	−1.65	H	0.0287
102	H41A	−3.1654	−2.3033	−0.6298	H	0.0524
103	H41B	−1.4148	−2.4906	−0.9956	H	0.0524
104	H36C	0.8232	−7.2082	−0.6426	H	0.0489
105	H36B	1.1648	−7.4084	1.1029	H	0.0489
106	H36A	2.2299	−6.4184	0.0849	H	0.0489
107	H28A	0.2165	−3.3813	0.7016	H	0.088
108	H29B	2.4333	−3.1585	1.8277	H	0.0485
109	H29A	2.5486	−4.9215	1.9704	H	0.0485
110	H31A	1.6748	−2.0522	3.7788	H	0.0557
111	H32A	0.2656	−1.9391	5.7995	H	0.0599
112	H33A	−1.1438	−3.8785	6.4506	H	0.0559
113	H34A	−1.0922	−5.9544	5.0856	H	0.0599
114	H35A	0.3411	−6.0837	3.0841	H	0.0557
115	H26A	2.5888	−3.0669	−3.8002	H	0.0448
116	H26B	2.384	−1.8482	−2.4997	H	0.0448
117	H25A	3.7916	−4.5995	−2.3191	H	0.0619
118	H5	3.7027	−1.4893	−0.4135	H	0.1896
119	H21A	6.6841	−1.2543	−0.8518	H	0.0854
120	H22B	4.9563	−0.7196	1.6534	H	0.032
121	H22A	6.7239	−0.5043	1.5367	H	0.032
122	H23B	6.189	−2.6752	2.6539	H	0.0233
123	H23A	6.9777	−2.9898	1.0795	H	0.0233
124	H23C	5.2083	−3.1939	1.2549	H	0.0233
125	H19A	6.0831	3.8236	−1.3799	H	0.0448
126	H19B	5.7435	2.5885	−2.6453	H	0.0448
127	H18A	4.399	2.8256	0.1093	H	0.0619
128	H11A	−0.0696	2.7838	−2.1116	H	0.0802
129	H16A	0.6424	1.1621	−0.645	H	0.0488
130	H16B	2.152	1.3959	0.2271	H	0.0488
131	H16C	2.1042	0.4415	−1.2969	H	0.0488
132	H12B	0.1602	4.0194	−4.1072	H	0.0315
133	H12A	1.8988	4.2476	−3.9623	H	0.0315
134	H13A	1.2315	2.5568	−5.6409	H	0.0298
135	H15C	2.8879	0.8571	−5.2071	H	0.0232
136	H15A	2.8995	1.1779	−3.4662	H	0.0232
137	H15B	3.5125	2.4152	−4.5993	H	0.0232
138	H14A	−0.766	1.6167	−4.3529	H	0.0232
139	H14C	0.4003	0.7578	−3.2962	H	0.0232
140	H14B	0.3075	0.3554	−5.0284	H	0.0232

Table S8. Continued

141	H2	0.1495	3.547	0.2384	H	0.1884
142	H7A	0.5956	6.4927	0.2095	H	0.0826
143	H8A	0.41	4.5835	2.6127	H	0.0639
144	H4	1.1353	6.5726	3.6926	H	0.2101
145	H9C	2.8786	5.9011	1.3003	H	0.0257
146	H9B	2.8916	4.952	2.8156	H	0.0257
147	H9A	2.4964	4.1532	1.2709	H	0.0257
148	H1	−1.74	3.9827	1.4678	H	0.1856
149	H3A	−3.8752	6.0859	1.4578	H	0.0582
150	H2A	−5.2696	4.3816	0.1854	H	0.0574
151	H5A	−4.3131	6.3833	−0.9734	H	0.0258
152	H5C	−2.8124	5.4791	−1.3276	H	0.0258
153	H5B	−4.3584	4.9611	−2.0507	H	0.0258
154	H4B	−5.19	4.4067	2.7278	H	0.0253
155	H4C	−3.6151	4.6615	3.5355	H	0.0253
156	H4A	−3.89	3.1935	2.5524	H	0.0253
157	P5	−3.828	5.6079	−1.4506	Du	0
158	P4	−4.2317	4.0873	2.9386	Du	0
159	P9	2.7555	5.0021	1.7956	Du	0
160	P12	1.0295	4.1335	−4.0348	Du	0
161	P15	3.1	1.4834	−4.4242	Du	0
162	P14	−0.0194	0.91	−4.2258	Du	0
163	P22	5.8401	−0.612	1.5951	Du	0
164	P23	6.125	−2.953	1.6628	Du	0
165	P29	2.4909	−4.04	1.899	Du	0
166	P3135	1.0079	−4.068	3.4315	Du	0
167	P16	1.6329	0.9998	−0.5716	Du	0
168	P36	1.406	−7.0116	0.1817	Du	0
169	P39	−3.8192	−5.4326	−0.036	Du	0
170	P40	−2.6127	−4.4866	−1.8501	Du	0
171	P41	−2.2901	−2.3969	−0.8127	Du	0
172	P46	−0.8375	1.543	2.3718	Du	0
173	P45	−2.5456	−0.2035	4.3635	Du	0
174	P47	−4.6394	−0.9245	1.6954	Du	0
175	P50	−3.604	1.6025	−2.6776	Du	0
176	P19	5.9133	3.2061	−2.0126	Du	0

[a]Atom nomenclature as in Figure 1a. [b]Pseudoatoms used in modeling are designated by "P" followed by the number of the relevant carbon atom(s). [c]Tripos forcefield atom type. [d]Gasteiger-Huckel charges.

Table S9. Atom coordinates for modeled grassypeptolide C (**3**) structure 5

Atom number	Atom name[a,b]	x	y	z	Atom type[c]	Charge[d]
1	N9	1.6987	0.713	0.5826	N.am	–0.252
2	C43	1.3947	0.4147	1.9988	C.3	0.1359
3	C42	1.088	–1.0551	2.1936	C.2	0.2068
4	C44	0.2384	1.301	2.5833	C.3	–0.0061
5	C46	–0.9984	1.3819	1.6462	C.3	–0.0584
6	C45	–0.1527	0.9251	4.0441	C.3	–0.0584
7	N8	2.0457	–2.0142	2.2507	N.am	–0.2498
8	O9	–0.0827	–1.3881	2.2542	O.2	–0.3942
9	C38	1.6326	–3.4065	2.2879	C.3	0.134
10	C39	2.9308	–4.0792	1.7838	C.3	–0.0104
11	C40	4.0577	–3.1563	2.3077	C.3	–0.0281
12	C41	3.4709	–1.7258	2.1869	C.3	0.0369
13	C37	1.2732	–3.7803	3.7071	C.2	0.2073
14	N7	0.288	–4.6365	4.115	N.am	–0.2484
15	O8	1.9838	–3.2382	4.5398	O.2	–0.3941
16	C36	0.1807	–4.8236	5.57	C.3	0.0266
17	C28	–0.6634	–5.2815	3.1817	C.3	0.128
18	C27	–0.0208	–6.1463	2.1194	C.2	0.1037
19	C29	–1.7787	–4.362	2.583	C.3	0.0238
20	C30	–2.4392	–3.3866	3.5757	C.ar	–0.0376
21	C31	–2.7818	–3.7821	4.8739	C.ar	–0.06
22	C32	–3.2894	–2.8602	5.7938	C.ar	–0.0686
23	C33	–3.5012	–1.5337	5.4113	C.ar	–0.0687
24	C34	–3.2274	–1.1428	4.0987	C.ar	–0.0686
25	C35	–2.7276	–2.0725	3.1826	C.ar	–0.06
26	S2	0.4098	–7.8451	2.4098	S.3	–0.0463
27	C26	0.3379	–8.0186	0.6004	C.3	0.043
28	C25	0.7852	–6.624	0.1014	C.3	0.1001
29	N6	0.1937	–5.6432	0.976	N.2	–0.332
30	C24	0.3676	–6.247	–1.2981	C.2	0.1895
31	N5	0.1054	–4.9302	–1.4841	N.am	–0.2623
32	O7	0.2978	–7.0992	–2.1691	O.2	–0.396
33	C21	–0.2179	–4.368	–2.7933	C.3	0.1158
34	C20	–1.507	–3.5913	–2.745	C.2	0.1014
35	C22	0.8955	–3.3418	–3.1422	C.3	–0.013
36	C23	2.2912	–4.0156	–3.1891	C.3	–0.0602
37	N4	–1.9292	–3.1105	–3.8435	N.2	–0.3321
38	C18	–2.9978	–2.1788	–3.5792	C.3	0.1002
39	C19	–3.6902	–2.6101	–2.2591	C.3	0.043
40	S1	–2.3721	–3.2957	–1.2215	S.3	–0.0465
41	C17	–2.2309	–0.8779	–3.4457	C.2	0.1909
42	N3	–2.1158	0.0442	–4.445	N.am	–0.2542
43	O6	–1.6597	–0.7326	–2.3767	O.2	–0.3959
44	C11	–1.2062	1.1785	–4.2411	C.3	0.1336
45	C16	–2.8147	–0.163	–5.7112	C.3	0.0254
46	C10	–1.5241	1.8108	–2.9201	C.2	0.2042

Table S9. Continued

47	C12	0.2849	0.751	−4.2856	C.3	−0.0099
48	C13	0.7357	0.0739	−5.6073	C.3	−0.0425
49	C15	0.6027	1.02	−6.8327	C.3	−0.0625
50	C14	2.2191	−0.3511	−5.4413	C.3	−0.0625
51	N2	−2.7258	2.4	−2.775	N.am	−0.2613
52	O5	−0.6988	1.7758	−2.0227	O.2	−0.3944
53	C7	−2.9813	3.1866	−1.5781	C.3	0.1563
54	C8	−4.4781	3.1125	−1.1912	C.3	0.0924
55	O4	−4.7763	4.0165	−0.114	O.3	−0.3874
56	C9	−4.834	1.6476	−0.8137	C.3	−0.0346
57	C6	−2.4023	4.5336	−1.94	C.2	0.2046
58	N1	−1.0468	4.5845	−2.0205	N.am	−0.2796
59	O3	−3.1435	5.4691	−2.1947	O.2	−0.3944
60	C3	−0.3678	5.6615	−2.7345	C.3	0.0598
61	C2	1.0979	5.8407	−2.2361	C.3	0.08
62	C1	1.8517	4.5269	−2.2671	C.2	0.2415
63	O1	1.8353	3.8454	−1.1093	O.3	−0.2498
64	O2	2.4047	4.1431	−3.2853	O.2	−0.3699
65	C49	2.3713	2.5025	−1.126	C.3	0.1852
66	C48	2.1263	1.9756	0.2769	C.2	0.2166
67	O10	2.3296	2.8006	1.1537	O.2	−0.3933
68	C50	3.8911	2.4013	−1.4311	C.3	0.0292
69	C51	4.6892	3.2711	−0.4495	C.ar	−0.0379
70	C56	4.9162	4.6236	−0.7285	C.ar	−0.0601
71	C55	5.6499	5.4156	0.1592	C.ar	−0.0686
72	C54	6.1563	4.8606	1.3375	C.ar	−0.0687
73	C53	5.9258	3.5127	1.6257	C.ar	−0.0686
74	C52	5.1986	2.7205	0.7326	C.ar	−0.0601
75	C5	1.0886	6.4306	−0.8027	C.3	−0.0418
76	C4	−0.3973	5.2616	−4.2359	C.3	−0.0395
77	C47	1.4634	−0.2575	−0.4984	C.3	0.0255
78	H43A	2.2911	0.6521	2.5848	H	0.0805
79	H44A	0.5985	2.335	2.6735	H	0.0343
80	H46C	−1.4911	0.4117	1.5078	H	0.0234
81	H46B	−1.7422	2.083	2.056	H	0.0234
82	H46A	−0.6858	1.7532	0.6604	H	0.0234
83	H45C	0.7487	0.891	4.6761	H	0.0234
84	H45B	−0.8366	1.6818	4.4614	H	0.0234
85	H45A	−0.6588	−0.0457	4.1178	H	0.0234
86	H38A	0.8309	−3.5379	1.5641	H	0.0802
87	H39A	2.95	−4.0567	0.6806	H	0.0313
88	H39B	3.0273	−5.1235	2.1222	H	0.0313
89	H40B	4.2484	−3.3972	3.3665	H	0.0287
90	H40A	5.0017	−3.2768	1.7514	H	0.0287
91	H41A	3.8243	−1.0892	3.0132	H	0.0524
92	H41B	3.7246	−1.2713	1.2168	H	0.0524
93	H36B	−0.4815	−5.6508	5.8602	H	0.0489

Table S9. Continued

94	H36A	–0.1944	–3.8978	6.034	H	0.0489
95	H36C	1.1676	–5.0534	6.003	H	0.0489
96	H28A	–1.2295	–6.043	3.7399	H	0.088
97	H29A	–1.3854	–3.7802	1.7416	H	0.0485
98	H29B	–2.5874	–4.9862	2.1685	H	0.0485
99	H31A	–2.6652	–4.8119	5.1817	H	0.0557
100	H32A	–3.5219	–3.1752	6.8064	H	0.0599
101	H33A	–3.8798	–0.8121	6.1284	H	0.0559
102	H34A	–3.4034	–0.1169	3.7901	H	0.0599
103	H35A	–2.5725	–1.7584	2.1556	H	0.0557
104	H26B	0.9806	–8.8339	0.235	H	0.0448
105	H26A	–0.7071	–8.21	0.3109	H	0.0448
106	H25A	1.883	–6.541	0.1724	H	0.0619
107	H5	0.185	–4.2909	–0.7163	H	0.1896
108	H21A	–0.296	–5.1238	–3.5912	H	0.0854
109	H22B	0.6766	–2.8764	–4.1166	H	0.032
110	H22A	0.9049	–2.5394	–2.3838	H	0.032
111	H23B	2.5512	–4.4425	–2.2081	H	0.0233
112	H23A	3.0612	–3.276	–3.4582	H	0.0233
113	H23C	2.3003	–4.8214	–3.9395	H	0.0233
114	H18A	–3.7325	–2.2062	–4.3938	H	0.0619
115	H19B	–4.2106	–1.7752	–1.7656	H	0.0448
116	H19A	–4.4063	–3.4249	–2.452	H	0.0448
117	H11A	–1.3483	2.004	–4.9566	H	0.0802
118	H16C	–2.6366	0.6578	–6.4175	H	0.0488
119	H16B	–2.4836	–1.0996	–6.1845	H	0.0488
120	H16A	–3.9003	–0.1896	–5.5354	H	0.0488
121	H12A	0.9105	1.6434	–4.1222	H	0.0315
122	H12A	0.4743	0.0434	–3.4646	H	0.0315
123	H13A	0.1312	–0.8329	–5.7799	H	0.0298
124	H15C	1.0247	0.5384	–7.7278	H	0.0232
125	H15A	1.1423	1.9616	–6.65	H	0.0232
126	H15B	–0.4458	1.2581	–7.0504	H	0.0232
127	H14A	2.569	–0.877	–6.3407	H	0.0232
128	H14B	2.8474	0.5379	–5.2769	H	0.0232
129	H14C	2.337	–1.0212	–4.5768	H	0.0232
130	H2	–3.3868	2.4158	–3.5289	H	0.1884
131	H7A	–2.3896	2.8089	–0.7357	H	0.0826
132	H8A	–5.0848	3.419	–2.0578	H	0.0639
133	H4	–4.2869	3.8165	0.6768	H	0.2101
134	H9A	–4.6602	0.9723	–1.667	H	0.0257
135	H9C	–4.2143	1.3014	0.0291	H	0.0257
136	H9B	–5.8922	1.58	–0.5217	H	0.0257
137	H1	–0.4905	3.7819	–1.798	H	0.1856
138	H3A	–0.9291	6.609	–2.6628	H	0.0582
139	H2A	1.6218	6.5579	–2.8908	H	0.0574
140	H49A	1.7992	1.9472	–1.8786	H	0.0918

Table S9. Continued

141	H50B	4.1258	2.7053	–2.4615	H	0.048
142	H50A	4.2073	1.3506	–1.3405	H	0.048
143	H56A	4.5251	5.0675	–1.6376	H	0.0557
144	H55A	5.8271	6.4627	–0.0665	H	0.0599
145	H54A	6.7272	5.4747	2.0272	H	0.0559
146	H53A	6.3118	3.0811	2.5444	H	0.0599
147	H52A	5.0301	1.6736	0.965	H	0.0557
148	H5A	2.1197	6.5275	–0.4298	H	0.0258
149	H5C	0.615	7.4242	–0.8041	H	0.0258
150	H5B	0.5213	5.7771	–0.1213	H	0.0258
151	H4A	0.1012	4.2948	–4.3988	H	0.0253
152	H4C	0.1026	6.0254	–4.8515	H	0.0253
153	H4B	–1.439	5.166	–4.5804	H	0.0253
154	H47A	2.2404	–0.207	–1.2737	H	0.0488
155	H47B	0.4801	–0.0706	–0.9438	H	0.0488
156	H47C	1.4695	–1.3041	–0.1711	H	0.0488
157	P5	1.0853	6.5762	–0.4517	Du	0
158	P4	–0.4118	5.1621	–4.6102	Du	0
159	P9	–4.9222	1.2846	–0.7199	Du	0
160	P12	0.6924	0.8434	–3.7934	Du	0
161	P15	0.5737	1.2527	–7.1427	Du	0
162	P14	2.5845	–0.4534	–5.3981	Du	0
163	P16	–3.0068	–0.2105	–6.0458	Du	0
164	P22	0.7907	–2.7079	–3.2502	Du	0
165	P23	2.6376	–4.18	–3.2019	Du	0
166	P29	–1.9864	–4.3832	1.955	Du	0
167	P3135	–2.6189	–3.2852	3.6687	Du	0
168	P36	0.1639	–4.8673	5.9657	Du	0
169	P39	2.9886	–4.5901	1.4014	Du	0
170	P40	4.625	–3.337	2.5589	Du	0
171	P41	3.7744	–1.1802	2.115	Du	0
172	P45	–0.2489	0.8424	4.4184	Du	0
173	P46	–1.3064	1.416	1.4081	Du	0
174	P47	1.3966	–0.5272	–0.7962	Du	0
175	P50	4.1665	2.0279	–1.901	Du	0
176	P19	–4.3084	–2.6	–2.1088	Du	0

[a]Atom nomenclature as in Figure 1a. [b]Pseudoatoms used in modeling are designated by "P" followed by the number of the relevant carbon atom(s). [c]Tripos forcefield atom type. [d]Gasteiger-Huckel charges.

Table S10. Atom coordinates for modeled grassypeptolide C (**3**) structure 6

Atom number	Atom name[a,b]	x	y	z	Atom type[c]	Charge[d]
1	N3	–1.9268	3.7971	–2.205	N.am	–0.2542
2	C11	–3.1637	3.201	–2.7334	C.3	0.1336
3	C10	–4.0972	3.0108	–1.5659	C.2	0.2042
4	N2	–3.7916	2.0402	–0.675	N.am	–0.2613
5	C12	–3.8127	4.108	–3.8146	C.3	–0.0099
6	C13	–2.861	4.4673	–4.9898	C.3	–0.0425
7	C15	–2.4518	3.2212	–5.8227	C.3	–0.0625
8	C14	–3.5772	5.5031	–5.8975	C.3	–0.0625
9	O5	–5.0654	3.7467	–1.452	O.2	–0.3944
10	C7	–4.6254	1.8328	0.5059	C.3	0.1563
11	C6	–5.4891	0.6039	0.3227	C.2	0.2046
12	N1	–4.9102	–0.5842	0.0235	N.am	–0.2796
13	C8	–3.7481	1.7768	1.7812	C.3	0.0924
14	C9	–2.9561	3.1023	1.9435	C.3	–0.0346
15	O4	–4.609	1.5478	2.9107	O.3	–0.3874
16	O3	–6.6986	0.7352	0.4347	O.2	–0.3944
17	C3	–5.7239	–1.7531	–0.3221	C.3	0.0598
18	C2	–5.6398	–1.9836	–1.8615	C.3	0.08
19	C1	–4.258	–2.3999	–2.2975	C.2	0.2415
20	C4	–5.2674	–2.9935	0.4924	C.3	–0.0395
21	C5	–6.0271	–0.698	–2.6405	C.3	–0.0418
22	O1	–3.2609	–1.8437	–1.5927	O.3	–0.2498
23	O2	–4.0989	–3.1941	–3.2122	O.2	–0.3699
24	C16	–1.9509	5.0806	–1.4946	C.3	0.0254
25	C17	–0.7392	3.1553	–2.4062	C.2	0.1909
26	C18	0.5789	3.7313	–1.9308	C.3	0.1002
27	N4	0.6175	3.8742	–0.4942	N.2	–0.3321
28	C20	1.8143	3.7562	–0.084	C.2	0.1014
29	S1	3.1316	3.4424	–1.2277	S.3	–0.0465
30	C19	1.804	2.8544	–2.3075	C.3	0.043
31	O6	–0.6777	2.0872	–2.992	O.2	–0.3959
32	C21	2.0931	3.8957	1.3888	C.3	0.1158
33	N5	3.2765	3.1172	1.7378	N.am	–0.2623
34	C22	0.9012	3.4017	2.2598	C.3	–0.013
35	C23	0.5345	1.9073	2.0351	C.3	–0.0602
36	C24	4.2372	3.603	2.5579	C.2	0.1895
37	C25	5.2635	2.5953	3.0066	C.3	0.1001
38	O7	4.2908	4.7545	2.9597	O.2	–0.396
39	C26	6.3054	2.2705	1.9058	C.3	0.043
40	S2	6.7634	0.5443	2.2207	S.3	–0.0463
41	C27	5.1241	0.3759	2.8831	C.2	0.1037
42	N6	4.4903	1.405	3.2708	N.2	–0.332
43	C28	4.4166	–0.9543	3.0062	C.3	0.128
44	N7	5.351	–2.0021	2.5763	N.am	–0.2484
45	C29	3.8423	–1.1054	4.455	C.3	0.0238
46	C30	2.8778	–2.2816	4.7182	C.ar	–0.0376

Table S10. Continued

47	C31	3.1061	–3.5676	4.2145	C.ar	–0.06
48	C32	2.2105	–4.6113	4.4647	C.ar	–0.0686
49	C33	1.075	–4.3888	5.2461	C.ar	–0.0687
50	C34	0.8384	–3.1147	5.766	C.ar	–0.0686
51	C35	1.7345	–2.0742	5.5034	C.ar	–0.06
52	C37	5.2456	–2.6205	1.3599	C.2	0.2073
53	C36	6.4457	–2.4448	3.4531	C.3	0.0266
54	C38	4.3165	–2.3044	0.1911	C.3	0.134
55	O8	6.0552	–3.4922	1.0805	O.2	–0.3941
56	C39	4.9145	–1.1117	–0.5959	C.3	–0.0104
57	C40	3.7475	–0.6379	–1.4847	C.3	–0.0281
58	C41	2.5469	–0.7004	–0.5167	C.3	0.0369
59	N8	2.9262	–1.8624	0.2802	N.am	–0.2498
60	C42	2.0134	–2.568	0.9929	C.2	0.2068
61	C43	0.5445	–2.1777	0.9801	C.3	0.1359
62	O9	2.36	–3.5345	1.6491	O.2	–0.3942
63	N9	–0.0854	–2.5928	–0.2881	N.am	–0.252
64	C44	–0.2518	–2.6968	2.2226	C.3	–0.0061
65	C46	–1.5666	–1.8985	2.4623	C.3	–0.0584
66	C45	–0.587	–4.2137	2.1777	C.3	–0.0584
67	C48	–1.0648	–1.7999	–0.8199	C.2	0.2166
68	C49	–1.9233	–2.1821	–2.0134	C.3	0.1852
69	O10	–1.3524	–0.7246	–0.3159	O.2	–0.3933
70	C47	0.2359	–3.8798	–0.9199	C.3	0.0255
71	C50	–1.5779	–1.3731	–3.2918	C.3	0.0292
72	C51	–0.263	–1.8251	–3.9416	C.ar	–0.0379
73	C52	–0.1861	–3.0833	–4.5503	C.ar	–0.0601
74	C53	0.999	–3.5044	–5.1604	C.ar	–0.0686
75	C54	2.1114	–2.659	–5.185	C.ar	–0.0687
76	C55	2.0358	–1.3951	–4.5941	C.ar	–0.0686
77	C56	0.8607	–0.9914	–3.9543	C.ar	–0.0601
78	H11A	–3.0279	2.201	–3.1732	H	0.0802
79	H2	–2.9872	1.4557	–0.8041	H	0.1884
80	H12A	–4.7133	3.6076	–4.2079	H	0.0315
81	H12B	–4.138	5.051	–3.3492	H	0.0315
82	H13A	–1.9455	4.9383	–4.5922	H	0.0298
83	H15B	–3.3456	2.6941	–6.1892	H	0.0232
84	H15A	–1.8498	2.5206	–5.228	H	0.0232
85	H15C	–1.8448	3.5269	–6.6887	H	0.0232
86	H14C	–3.8263	6.4104	–5.3242	H	0.0232
87	H14A	–2.9285	5.792	–6.7366	H	0.0232
88	H14B	–4.5096	5.0736	–6.2956	H	0.0232
89	H7A	–5.3215	2.6779	0.6219	H	0.0826
90	H1	–3.9171	–0.6711	–0.0655	H	0.1856
91	H8A	–3.0317	0.9459	1.6821	H	0.0639
92	H9A	–3.6419	3.9624	1.9733	H	0.0257
93	H9B	–2.3744	3.0918	2.877	H	0.0257

Table S10. Continued

94	H9C	−2.2616	3.2335	1.1	H	0.0257
95	H4	−4.1287	1.4707	3.7286	H	0.2101
96	H3A	−6.79	−1.5904	−0.0868	H	0.0582
97	H2A	−6.3445	−2.7896	−2.1313	H	0.0574
98	H4B	−4.2148	−3.2456	0.2982	H	0.0253
99	H4C	−5.8872	−3.8675	0.2386	H	0.0253
100	H4A	−5.377	−2.7838	1.5679	H	0.0253
101	H5B	−5.3047	0.1111	−2.4509	H	0.0258
102	H5A	−6.0364	−0.9031	−3.7227	H	0.0258
103	H5C	−7.0299	−0.3548	−2.3428	H	0.0258
104	H16A	−2.9771	5.4345	−1.322	H	0.0488
105	H16C	−1.4302	5.8516	−2.0802	H	0.0488
106	H16B	−1.4889	5.0031	−0.5022	H	0.0488
107	H18A	0.7152	4.7285	−2.3767	H	0.0619
108	H19B	2.0742	2.9189	−3.3729	H	0.0448
109	H19A	1.6294	1.8038	−2.0316	H	0.0448
110	H21A	2.2352	4.969	1.5979	H	0.0854
111	H5	3.306	2.1585	1.4546	H	0.1896
112	H22A	0.0196	4.0265	2.0425	H	0.032
113	H22B	1.1592	3.5435	3.3226	H	0.032
114	H23A	−0.3533	1.648	2.6304	H	0.0233
115	H23C	0.3081	1.7073	0.9767	H	0.0233
116	H23B	1.3472	1.2398	2.3573	H	0.0233
117	H25A	5.7517	2.9047	3.9456	H	0.0619
118	H26A	5.8492	2.3118	0.9042	H	0.0448
119	H26B	7.1773	2.9415	1.9371	H	0.0448
120	H28A	3.5386	−0.8921	2.3557	H	0.088
121	H29A	3.2814	−0.1832	4.6753	H	0.0485
122	H29B	4.639	−1.1691	5.2076	H	0.0485
123	H31A	3.9798	−3.7815	3.6184	H	0.0557
124	H32A	2.3968	−5.5973	4.0504	H	0.0599
125	H33A	0.382	−5.1998	5.4471	H	0.0559
126	H34A	−0.043	−2.9335	6.3736	H	0.0599
127	H35A	1.5291	−1.096	5.9255	H	0.0557
128	H36C	7.3867	−2.506	2.8844	H	0.0489
129	H36B	6.248	−3.4324	3.8918	H	0.0489
130	H36A	6.6378	−1.7313	4.2654	H	0.0489
131	H38A	4.2836	−3.1832	−0.4753	H	0.0802
132	H39B	5.8144	−1.3822	−1.1722	H	0.0313
133	H39A	5.1644	−0.2917	0.0927	H	0.0313
134	H40A	3.9038	0.3608	−1.9237	H	0.0287
135	H40B	3.6113	−1.3734	−2.294	H	0.0287
136	H41B	2.5069	0.1973	0.1186	H	0.0524
137	H41A	1.6115	−0.8111	−1.0843	H	0.0524
138	H43A	0.5575	−1.0831	1.0949	H	0.0805
139	H44A	0.383	−2.5122	3.1026	H	0.0343
140	H46A	−1.365	−0.8196	2.5392	H	0.0234

Table S10. Continued

141	H46B	–2.0425	–2.2185	3.4025	H	0.0234
142	H46C	–2.2845	–2.0667	1.6469	H	0.0234
143	H45A	–1.3366	–4.4173	1.4004	H	0.0234
144	H45B	0.3017	–4.8298	1.9846	H	0.0234
145	H45C	–1.0129	–4.5312	3.1421	H	0.0234
146	H49A	–1.8791	–3.2593	–2.2185	H	0.0918
147	H47B	1.0876	–4.3864	–0.4477	H	0.0488
148	H47C	0.5143	–3.7189	–1.9709	H	0.0488
149	H47A	–0.6084	–4.5817	–0.8695	H	0.0488
150	H50A	–1.5576	–0.3043	–3.036	H	0.048
151	H50B	–2.3623	–1.5078	–4.0521	H	0.048
152	H52A	–1.0498	–3.7405	–4.554	H	0.0557
153	H53A	1.0547	–4.4876	–5.6173	H	0.0599
154	H54A	3.031	–2.9823	–5.663	H	0.0559
155	H55A	2.8899	–0.7259	–4.6339	H	0.0599
156	H56A	0.8264	–0.0225	–3.4731	H	0.0557
157	P5	–6.1237	–0.3823	–2.8388	Du	0
158	P4	–5.1597	–3.299	0.7016	Du	0
159	P9	–2.7593	3.4292	1.9834	Du	0
160	P12	–4.4256	4.3293	–3.7786	Du	0
161	P15	–2.3467	2.9139	–6.0353	Du	0
162	P14	–3.7548	5.7587	–6.1188	Du	0
163	P16	–1.9654	5.4297	–1.3015	Du	0
164	P22	0.5894	3.785	2.6826	Du	0
165	P23	0.434	1.5317	1.9882	Du	0
166	P29	3.9602	–0.6762	4.9415	Du	0
167	P3135	2.7544	–2.4387	4.7719	Du	0
168	P36	6.7575	–2.5566	3.6805	Du	0
169	P39	5.4894	–0.837	–0.5398	Du	0
170	P40	3.7575	–0.5063	–2.1089	Du	0
171	P41	2.0592	–0.3069	–0.4829	Du	0
172	P46	–1.8973	–1.7016	2.5295	Du	0
173	P45	–0.6826	–4.5928	2.1757	Du	0
174	P47	0.3311	–4.229	–1.096	Du	0
175	P50	–1.96	–0.906	–3.544	Du	0
176	P19	1.8518	2.3613	–2.7023	Du	0

[a]Atom nomenclature as in Figure 1a. [b]Pseudoatoms used in modeling are designated by "P" followed by the number of the relevant carbon atom(s). [c]Tripos forcefield atom type. [d]Gasteiger-Huckel charges.

Table S11. Atom coordinates for modeled grassypeptolide C (**3**) structure 7

Atom number	Atom name[a,b]	x	y	z	Atom type[c]	Charge[d]
1	N5	–2.9829	–1.9969	4.1826	N.am	–0.2623
2	C21	–2.4573	–0.9092	5.0087	C.3	0.1158
3	C20	–0.988	–0.7572	4.7078	C.2	0.1014
4	C22	–3.2666	0.3902	4.7536	C.3	–0.013
5	C23	–4.7485	0.2157	5.1748	C.3	–0.0602
6	N4	–0.5624	0.2403	4.0451	N.2	–0.3321
7	C18	0.8746	0.1479	3.9087	C.3	0.1002
8	C19	1.2395	–1.358	3.9803	C.3	0.043
9	S1	0.1516	–1.9849	5.2859	S.3	–0.0465
10	C17	1.418	0.8436	2.6817	C.2	0.1909
11	N3	1.4249	2.2056	2.5845	N.am	–0.2542
12	O6	1.9082	0.1322	1.8183	O.2	–0.3959
13	C11	2.2911	2.8049	1.5613	C.3	0.1336
14	C10	1.7929	4.1726	1.1447	C.2	0.2042
15	C16	0.8227	3.0151	3.6484	C.3	0.0254
16	C12	3.6919	2.8265	2.2442	C.3	–0.0099
17	C13	4.9119	2.9927	1.2946	C.3	–0.0425
18	C15	5.0162	1.8312	0.2674	C.3	–0.0625
19	C14	4.9383	4.3701	0.5819	C.3	–0.0625
20	N2	0.8209	4.2401	0.2033	N.am	–0.2613
21	O5	2.2581	5.1608	1.6907	O.2	–0.3944
22	C7	0.2067	5.5159	–0.1664	C.3	0.1563
23	C6	0.5361	5.9149	–1.5902	C.2	0.2046
24	C8	–1.329	5.4324	0.0415	C.3	0.0924
25	C9	–1.6784	4.9498	1.4763	C.3	–0.0346
26	O4	–1.9567	6.6956	–0.2397	O.3	–0.3874
27	N1	0.4738	5.0057	–2.5971	N.am	–0.2796
28	O3	0.8479	7.0806	–1.781	O.2	–0.3944
29	C3	0.8293	5.3786	–3.9696	C.3	0.0598
30	C2	2.1994	4.7566	–4.3673	C.3	0.08
31	C1	2.1206	3.2647	–4.574	C.2	0.2415
32	O1	1.7507	2.5552	–3.4973	O.3	–0.2498
33	C49	1.8461	1.1248	–3.6598	C.3	0.1852
34	C4	–0.3023	4.9554	–4.9426	C.3	–0.0395
35	C5	3.2818	5.0645	–3.2992	C.3	–0.0418
36	O2	2.3804	2.7716	–5.6614	O.2	–0.3699
37	C48	1.1842	0.5096	–2.4438	C.2	0.2166
38	C50	3.3266	0.6527	–3.7408	C.3	0.0292
39	C51	3.3721	–0.8824	–3.6614	C.ar	–0.0379
40	C52	3.8382	–1.5318	–2.5115	C.ar	–0.0601
41	C53	3.8065	–2.9267	–2.4258	C.ar	–0.0686
42	C54	3.3378	–3.684	–3.5022	C.ar	–0.0687
43	C55	2.904	–3.0434	–4.6655	C.ar	–0.0686
44	C56	2.9309	–1.6481	–4.7468	C.ar	–0.0601
45	N9	–0.1288	0.1433	–2.4259	N.am	–0.252
46	O10	1.9031	0.3279	–1.4735	O.2	–0.3933

Table S11. Continued

47	C43	–0.6413	–0.5189	–1.219	C.3	0.1359
48	C42	–1.6963	–1.5399	–1.5857	C.2	0.2068
49	C47	–0.9785	0.3705	–3.6025	C.3	0.0255
50	C44	–1.0533	0.5761	–0.1896	C.3	–0.0061
51	C45	–1.5921	–0.0032	1.1446	C.3	–0.0584
52	C46	–2.0417	1.6224	–0.7737	C.3	–0.0584
53	N8	–1.3633	–2.6716	–2.2652	N.am	–0.2498
54	O9	–2.847	–1.3198	–1.2465	O.2	–0.3942
55	C38	–2.3771	–3.6598	–2.6016	C.3	0.134
56	C39	–1.515	–4.9113	–2.8979	C.3	–0.0104
57	C40	–0.2229	–4.2867	–3.4901	C.3	–0.0281
58	C41	0.0038	–2.9737	–2.6906	C.3	0.0369
59	C37	–3.6351	–3.7546	–1.739	C.2	0.2073
60	N7	–3.8202	–4.2312	–0.4629	N.am	–0.2484
61	O8	–4.6085	–3.3129	–2.3327	O.2	–0.3941
62	C28	–2.7381	–4.7966	0.3706	C.3	0.128
63	C36	–5.1922	–4.1624	0.0718	C.3	0.0266
64	C27	–3.2014	–4.9544	1.8042	C.2	0.1037
65	N6	–3.5242	–3.8981	2.4342	N.2	–0.332
66	C25	–3.9256	–4.2265	3.7824	C.3	0.1001
67	C26	–3.3555	–5.6216	4.1522	C.3	0.043
68	S2	–3.2908	–6.5405	2.5902	S.3	–0.0463
69	C24	–3.4393	–3.1517	4.7261	C.2	0.1895
70	O7	–3.4736	–3.369	5.9267	O.2	–0.396
71	C29	–1.4399	–3.9731	0.5694	C.3	0.0238
72	C30	–0.4679	–4.7089	1.5019	C.ar	–0.0376
73	C31	0.3478	–5.7299	1.0012	C.ar	–0.06
74	C32	1.2027	–6.4322	1.8555	C.ar	–0.0686
75	C33	1.2502	–6.11	3.2146	C.ar	–0.0687
76	C34	0.4518	–5.0779	3.7145	C.ar	–0.0686
77	C35	–0.3927	–4.3693	2.8554	C.ar	–0.06
78	H5	–2.9779	–1.873	3.1879	H	0.1896
79	H21A	–2.5156	–1.1252	6.0865	H	0.0854
80	H22B	–3.2348	0.6482	3.6846	H	0.032
81	H22A	–2.8178	1.2213	5.3225	H	0.032
82	H23B	–4.8178	–0.0288	6.2461	H	0.0233
83	H23A	–5.3058	1.1482	4.9918	H	0.0233
84	H23C	–5.2207	–0.5937	4.5963	H	0.0233
85	H18A	1.3513	0.6332	4.7733	H	0.0619
86	H19A	2.3008	–1.5358	4.2139	H	0.0448
87	H19B	0.9795	–1.8733	3.043	H	0.0448
88	H11A	2.3092	2.1787	0.659	H	0.0802
89	H16A	0.6943	4.0661	3.3617	H	0.0488
90	H16C	1.4715	3.0013	4.5358	H	0.0488
91	H16B	–0.1772	2.6478	3.9129	H	0.0488
92	H12B	3.7118	3.6105	3.0185	H	0.0315
93	H12A	3.8465	1.8685	2.7683	H	0.0315

Table S11. Continued

94	H13A	5.8014	2.9378	1.9472	H	0.0298
95	H15C	4.8881	0.8587	0.7685	H	0.0232
96	H15B	4.2566	1.9238	–0.5208	H	0.0232
97	H15A	6.0042	1.8464	–0.2149	H	0.0232
98	H14C	4.8833	5.1858	1.3194	H	0.0232
99	H14B	4.0959	4.4631	–0.1162	H	0.0232
100	H14A	5.8721	4.4816	0.01	H	0.0232
101	H2	0.4639	3.4105	–0.2228	H	0.1884
102	H7A	0.5757	6.3267	0.4812	H	0.0826
103	H8A	–1.7436	4.7189	–0.6846	H	0.0639
104	H9B	–1.287	3.9381	1.6634	H	0.0257
105	H9A	–1.25	5.6321	2.226	H	0.0257
106	H9C	–2.7708	4.9253	1.6073	H	0.0257
107	H4	–1.6725	7.3866	0.349	H	0.2101
108	H1	0.2182	4.051	–2.4367	H	0.1856
109	H3A	0.9536	6.4709	–4.0712	H	0.0582
110	H2A	2.5228	5.2119	–5.3203	H	0.0574
111	H49A	1.3474	0.7864	–4.5797	H	0.0918
112	H4C	–0.0403	5.219	–5.979	H	0.0253
113	H4B	–0.4826	3.8717	–4.8895	H	0.0253
114	H4A	–1.2341	5.4749	–4.6704	H	0.0253
115	H5C	3.3755	6.1509	–3.1466	H	0.0258
116	H5A	3.0189	4.5961	–2.3394	H	0.0258
117	H5B	4.2583	4.6696	–3.6215	H	0.0258
118	H50A	3.9022	1.1082	–2.9208	H	0.048
119	H50B	3.8018	0.9645	–4.6834	H	0.048
120	H52A	4.225	–0.9589	–1.6747	H	0.0557
121	H53A	4.1465	–3.4224	–1.5217	H	0.0599
122	H54A	3.3125	–4.7674	–3.435	H	0.0559
123	H55A	2.5447	–3.6299	–5.5055	H	0.0599
124	H56A	2.6035	–1.1608	–5.6596	H	0.0557
125	H43A	0.1392	–1.11	–0.7149	H	0.0805
126	H47A	–2.0451	0.2497	–3.3665	H	0.0488
127	H47B	–0.8612	1.398	–3.9786	H	0.0488
128	H47C	–0.7388	–0.3416	–4.4055	H	0.0488
129	H44A	–0.1244	1.1046	0.0793	H	0.0343
130	H45C	–1.6964	0.8223	1.863	H	0.0234
131	H45A	–0.8873	–0.7375	1.5614	H	0.0234
132	H45B	–2.5764	–0.4766	1.0248	H	0.0234
133	H46C	–2.963	1.1461	–1.136	H	0.0234
134	H46A	–2.3227	2.3492	0.0012	H	0.0234
135	H46B	–1.5781	2.1757	–1.6034	H	0.0234
136	H38A	–2.7024	–3.3318	–3.6038	H	0.0802
137	H39A	–1.2613	–5.4654	–1.9871	H	0.0313
138	H39B	–2.0057	–5.612	–3.5943	H	0.0313
139	H40B	–0.4114	–4.0341	–4.5477	H	0.0287
140	H40A	0.638	–4.9732	–3.4463	H	0.0287

Table S11. Continued

141	H41A	0.6806	–3.1589	–1.8431	H	0.0524
142	H41B	0.44	–2.1941	–3.3296	H	0.0524
143	H28A	–2.4986	–5.8	–0.011	H	0.088
144	H36A	–5.9761	–4.2043	–0.6985	H	0.0489
145	H36C	–5.4128	–5.0069	0.7405	H	0.0489
146	H36B	–5.3074	–3.2217	0.6308	H	0.0489
147	H25A	–5.0282	–4.2499	3.7973	H	0.0619
148	H26B	–2.3226	–5.5358	4.5212	H	0.0448
149	H26A	–3.9651	–6.1436	4.9059	H	0.0448
150	H29A	–1.6753	–2.9647	0.9362	H	0.0485
151	H29B	–0.8879	–3.8645	–0.3518	H	0.0485
152	H31A	0.3187	–5.9803	–0.055	H	0.0557
153	H32A	1.8288	–7.2279	1.4639	H	0.0599
154	H33A	1.9068	–6.6604	3.8812	H	0.0559
155	H34A	0.488	–4.8312	4.7704	H	0.0599
156	H35A	–0.9965	–3.555	3.2364	H	0.0557
157	P5	3.5509	5.1389	–3.0358	Du	0
158	P4	–0.5857	4.8552	–5.1797	Du	0
159	P9	–1.7692	4.8318	1.8323	Du	0
160	P12	3.7791	2.7395	2.8934	Du	0
161	P14	4.9504	4.7102	0.4044	Du	0
162	P15	5.0496	1.543	0.0109	Du	0
163	P16	0.6629	3.2384	3.9368	Du	0
164	P22	–3.0263	0.9348	4.5035	Du	0
165	P23	–5.1148	0.1752	5.2781	Du	0
166	P29	–1.2816	–3.4146	0.2922	Du	0
167	P3135	–0.3389	–4.7676	1.5907	Du	0
168	P36	–5.5654	–4.1443	0.2243	Du	0
169	P39	–1.6335	–5.5387	–2.7907	Du	0
170	P40	0.1133	–4.5036	–3.997	Du	0
171	P41	0.5603	–2.6765	–2.5863	Du	0
172	P45	–1.72	–0.1306	1.4831	Du	0
173	P46	–2.288	1.8903	–0.9128	Du	0
174	P47	–1.2151	0.4354	–3.9169	Du	0
175	P50	3.852	1.0363	–3.8021	Du	0
176	P19	1.6402	–1.7046	3.6285	Du	0

[a]Atom nomenclature as in Figure 1a. [b]Pseudoatoms used in modeling are designated by "P" followed by the number of the relevant carbon atom(s). [c]Tripos forcefield atom type. [d]Gasteiger-Huckel charges.

Table S12. Atom coordinates for modeled grassypeptolide C (**3**) structure 8

Atom number	Atom name[a,b]	x	y	z	Atom type[c]	Charge[d]
1	C3	5.4197	2.4264	2.4965	C.3	0.0598
2	C2	5.3682	1.6122	3.825	C.3	0.08
3	N1	4.0555	2.7757	2.0848	N.am	–0.2796
4	C1	4.7777	0.2382	3.6304	C.2	0.2415
5	C4	6.1471	1.6654	1.3544	C.3	–0.0395
6	C5	4.527	2.3629	4.8916	C.3	–0.0418
7	O1	3.8196	0.1794	2.6969	O.3	–0.2498
8	O2	5.1741	–0.7211	4.2742	O.2	–0.3699
9	C49	3.177	–1.0988	2.5268	C.3	0.1852
10	C48	2.4477	–0.9245	1.2086	C.2	0.2166
11	C50	2.2051	–1.3367	3.7123	C.3	0.0292
12	C51	1.3183	–2.5669	3.4818	C.ar	–0.0379
13	C52	–0.0621	–2.4272	3.301	C.ar	–0.0601
14	C53	–0.875	–3.553	3.1458	C.ar	–0.0686
15	C54	–0.3056	–4.8291	3.1431	C.ar	–0.0687
16	C55	1.0771	–4.9735	3.2844	C.ar	–0.0686
17	C56	1.8841	–3.8465	3.4641	C.ar	–0.0601
18	N9	2.65	–1.699	0.0988	N.am	–0.252
19	O10	1.6758	0.0215	1.1892	O.2	–0.3933
20	C47	3.5805	–2.8317	0.1486	C.3	0.0255
21	C43	1.9826	–1.3124	–1.1563	C.3	0.1359
22	C42	1.5286	–2.5201	–1.9589	C.2	0.2068
23	C44	2.8605	–0.3143	–1.9887	C.3	–0.0061
24	C46	2.9264	1.0918	–1.3291	C.3	–0.0584
25	C45	4.3058	–0.8159	–2.261	C.3	–0.0584
26	N8	0.5261	–3.3232	–1.5224	N.am	–0.2498
27	O9	2.0592	–2.7382	–3.036	O.2	–0.3942
28	C38	0.1082	–4.4694	–2.3191	C.3	0.134
29	C39	–1.1116	–4.9763	–1.5097	C.3	–0.0104
30	C40	–0.7996	–4.5111	–0.0693	C.3	–0.0281
31	C41	–0.1483	–3.1171	–0.2453	C.3	0.0369
32	C37	–0.2169	–4.3218	–3.7993	C.2	0.2073
33	N7	–0.9487	–3.3371	–4.4034	N.am	–0.2484
34	O8	0.2017	–5.2445	–4.4824	O.2	–0.3941
35	C36	–1.1758	–3.4758	–5.8448	C.3	0.0266
36	C28	–1.4941	–2.1909	–3.6672	C.3	0.128
37	C27	–2.9652	–2.0524	–3.9629	C.2	0.1037
38	C29	–0.7177	–0.8582	–3.8913	C.3	0.0238
39	C30	–0.3635	–0.5741	–5.3563	C.ar	–0.0376
40	C35	0.8037	–1.1079	–5.9166	C.ar	–0.06
41	C34	1.107	–0.8868	–7.2629	C.ar	–0.0686
42	C33	0.2514	–0.1173	–8.0555	C.ar	–0.0687
43	C32	–0.8982	0.4446	–7.4939	C.ar	–0.0686
44	C31	–1.1942	0.2289	–6.145	C.ar	–0.06
45	S2	–4.0603	–3.4332	–3.8007	S.3	–0.0463
46	C26	–5.3548	–2.1833	–3.5869	C.3	0.043

Table S12. Continued

47	C25	−4.851	−0.9368	−4.3619	C.3	0.1001
48	N6	−3.4091	−0.9144	−4.3053	N.2	−0.332
49	C24	−5.286	0.3322	−3.6708	C.2	0.1895
50	N5	−4.4493	0.7824	−2.7055	N.am	−0.2623
51	O7	−6.3286	0.8784	−3.9939	O.2	−0.396
52	C21	−4.6968	2.0154	−1.9671	C.3	0.1158
53	C20	−4.6495	1.6459	−0.5089	C.2	0.1014
54	C22	−3.61	3.0588	−2.3466	C.3	−0.013
55	C23	−3.673	3.4099	−3.8556	C.3	−0.0602
56	S1	−5.9217	0.6297	0.1879	S.3	−0.0465
57	C19	−4.6913	0.2741	1.4695	C.3	0.043
58	C18	−3.8507	1.5768	1.5614	C.3	0.1002
59	N4	−3.6838	2.0533	0.2086	N.2	−0.3321
60	C17	−2.515	1.3879	2.251	C.2	0.1909
61	N3	−1.671	2.432	2.4958	N.am	−0.2542
62	O6	−2.2355	0.2503	2.5924	O.2	−0.3959
63	C11	−0.4355	2.1544	3.2512	C.3	0.1336
64	C10	0.6004	3.2499	3.0966	C.2	0.2042
65	C16	−2.0587	3.7823	2.062	C.3	0.0254
66	C12	−0.7483	1.7954	4.7393	C.3	−0.0099
67	C13	−1.9266	2.5725	5.409	C.3	−0.0425
68	C15	−2.2868	1.9075	6.7674	C.3	−0.0625
69	C14	−1.623	4.0771	5.6492	C.3	−0.0625
70	N2	1.2892	3.3265	1.9305	N.am	−0.2613
71	O5	0.7494	4.0578	3.9986	O.2	−0.3944
72	C7	2.2212	4.4287	1.6783	C.3	0.1563
73	C6	3.6557	4.069	2.0066	C.2	0.2046
74	C8	2.0821	4.9517	0.2207	C.3	0.0924
75	O4	2.8371	6.1636	0.037	O.3	−0.3874
76	C9	0.6014	5.2647	−0.121	C.3	−0.0346
77	O3	4.4184	5.0011	2.2107	O.2	−0.3944
78	H3A	6.0271	3.3264	2.6963	H	0.0582
79	H2A	6.3991	1.4909	4.2012	H	0.0574
80	H1	3.4235	2.0199	1.9158	H	0.1856
81	H4B	6.1948	2.3082	0.4616	H	0.0253
82	H4C	5.6264	0.7378	1.0772	H	0.0253
83	H4A	7.1738	1.4096	1.659	H	0.0253
84	H5C	3.4748	2.4462	4.5772	H	0.0258
85	H5B	4.9281	3.3754	5.0537	H	0.0258
86	H5A	4.5589	1.8174	5.8478	H	0.0258
87	H49A	3.9222	−1.9043	2.4982	H	0.0918
88	H50B	1.5931	−0.4339	3.8581	H	0.048
89	H50A	2.7666	−1.501	4.6448	H	0.048
90	H52A	−0.5115	−1.4427	3.2829	H	0.0557
91	H53A	−1.9476	−3.4353	3.0269	H	0.0599
92	H54A	−0.9357	−5.7057	3.0291	H	0.0559
93	H55A	1.5243	−5.9622	3.2568	H	0.0599

Table S12. Continued

94	H56A	2.9541	–3.9711	3.5946	H	0.0557
95	H47C	3.2421	–3.5602	0.9002	H	0.0488
96	H47B	3.6334	–3.3666	–0.8097	H	0.0488
97	H47A	4.6031	–2.5049	0.3874	H	0.0488
98	H43A	1.0332	–0.7906	–0.9558	H	0.0805
99	H44A	2.3886	–0.1635	–2.9737	H	0.0343
100	H46C	3.4729	1.0438	–0.3781	H	0.0234
101	H46A	1.9161	1.4872	–1.1426	H	0.0234
102	H46B	3.4532	1.8003	–1.9872	H	0.0234
103	H45B	4.8128	–0.1302	–2.9583	H	0.0234
104	H45C	4.8884	–0.8392	–1.3304	H	0.0234
105	H45A	4.3149	–1.8176	–2.7128	H	0.0234
106	H38A	0.9252	–5.201	–2.2075	H	0.0802
107	H39B	–2.0421	–4.4958	–1.8462	H	0.0313
108	H39A	–1.2454	–6.0682	–1.5853	H	0.0313
109	H40A	–0.0585	–5.2058	0.3614	H	0.0287
110	H40B	–1.6942	–4.4951	0.5736	H	0.0287
111	H41B	–0.9086	–2.3238	–0.31	H	0.0524
112	H41A	0.5324	–2.9097	0.5916	H	0.0524
113	H36C	–1.7634	–4.3881	–6.0305	H	0.0489
114	H36A	–0.2224	–3.558	–6.3882	H	0.0489
115	H36B	–1.7419	–2.6312	–6.2633	H	0.0489
116	H28A	–1.4997	–2.3583	–2.5871	H	0.088
117	H29A	0.2271	–0.9066	–3.3529	H	0.0485
118	H29B	–1.2586	–0.0033	–3.4562	H	0.0485
119	H35A	1.4822	–1.7013	–5.3113	H	0.0557
120	H34A	2.0074	–1.314	–7.6934	H	0.0599
121	H33A	0.4799	0.0448	–9.1043	H	0.0559
122	H32A	–1.5607	1.0498	–8.1049	H	0.0599
123	H31A	–2.0722	0.6923	–5.7122	H	0.0557
124	H26A	–5.4166	–1.9754	–2.5066	H	0.0448
125	H26B	–6.3329	–2.5388	–3.9456	H	0.0448
126	H25A	–5.1581	–0.9557	–5.4202	H	0.0619
127	H5	–3.6076	0.2817	–2.4924	H	0.1896
128	H21A	–5.6841	2.4547	–2.1784	H	0.0854
129	H22B	–2.6097	2.6558	–2.1158	H	0.032
130	H22A	–3.7581	3.9765	–1.7527	H	0.032
131	H23B	–2.9032	4.1583	–4.1019	H	0.0233
132	H23A	–4.6602	3.8242	–4.1126	H	0.0233
133	H23C	–3.4961	2.5137	–4.4694	H	0.0233
134	H19B	–5.162	–0.002	2.4258	H	0.0448
135	H19A	–4.0829	–0.5673	1.1012	H	0.0448
136	H18A	–4.4428	2.3224	2.1139	H	0.0619
137	H11A	0.0553	1.2718	2.8094	H	0.0802
138	H16A	–2.2276	3.8088	0.9774	H	0.0488
139	H16B	–2.9756	4.1038	2.5761	H	0.0488
140	H16C	–1.3004	4.5471	2.2698	H	0.0488

Table S12. Continued

141	H12B	0.1653	1.8946	5.3473	H	0.0315
142	H12A	–1.0266	0.7289	4.7658	H	0.0315
143	H13A	–2.8262	2.4957	4.7765	H	0.0298
144	H15B	–3.1357	2.4258	7.2401	H	0.0232
145	H15C	–1.424	1.9489	7.449	H	0.0232
146	H15A	–2.5733	0.8541	6.6228	H	0.0232
147	H14A	–1.5175	4.6215	4.7031	H	0.0232
148	H14C	–2.4469	4.5518	6.204	H	0.0232
149	H14B	–0.6994	4.1927	6.2364	H	0.0232
150	H2	1.1537	2.6523	1.2009	H	0.1884
151	H7A	2.0016	5.268	2.3579	H	0.0826
152	H8A	2.4452	4.1847	–0.4834	H	0.0639
153	H4	3.77	6.0481	0.1861	H	0.2101
154	H9C	0.5354	5.714	–1.1235	H	0.0257
155	H9A	–0.012	4.3514	–0.1194	H	0.0257
156	H9B	0.184	5.9747	0.6093	H	0.0257
157	P5	4.3206	2.5463	5.1596	Du	0
158	P4	6.3317	1.4852	1.0659	Du	0
159	P9	0.2358	5.3467	–0.2112	Du	0
160	P12	–0.4307	1.3117	5.0566	Du	0
161	P15	–2.3777	1.7429	7.104	Du	0
162	P14	–1.5546	4.4553	5.7145	Du	0
163	P16	–2.1679	4.1532	1.9411	Du	0
164	P22	–3.1839	3.3161	–1.9343	Du	0
165	P23	–3.6865	3.4987	–4.228	Du	0
166	P29	–0.5158	–0.4549	–3.4046	Du	0
167	P3135	–0.295	–0.5045	–5.5117	Du	0
168	P36	–1.2426	–3.5257	–6.2273	Du	0
169	P39	–1.6438	–5.282	–1.7158	Du	0
170	P40	–0.8764	–4.8504	0.4675	Du	0
171	P41	–0.1881	–2.6168	0.1408	Du	0
172	P45	4.672	–0.929	–2.3338	Du	0
173	P46	2.9474	1.4438	–1.1693	Du	0
174	P47	3.8262	–3.1439	0.1593	Du	0
175	P50	2.1799	–0.9675	4.2514	Du	0
176	P19	–4.6225	–0.2846	1.7635	Du	0

[a]Atom nomenclature as in Figure 1a. [b]Pseudoatoms used in modeling are designated by "P" followed by the number of the relevant carbon atom(s). [c]Tripos forcefield atom type. [d]Gasteiger-Huckel charges.

Table S13. Atom coordinates for modeled grassypeptolide C (**3**) structure 9

Atom number	Atom name[a,b]	x	y	z	Atom type[c]	Charge[d]
1	N2	–0.0735	3.3824	2.9465	N.am	–0.2613
2	C7	0.5318	3.4135	4.2771	C.3	0.1563
3	C6	–0.2392	2.466	5.1731	C.2	0.2046
4	C8	2.038	3.0321	4.2308	C.3	0.0924
5	O4	2.6239	3.1307	5.5402	O.3	–0.3874
6	C9	2.8132	3.9097	3.2125	C.3	–0.0346
7	N1	–0.4508	1.1967	4.7485	N.am	–0.2796
8	O3	–0.6597	2.8841	6.2409	O.2	–0.3944
9	C3	–1.3526	0.2914	5.4611	C.3	0.0598
10	C2	–2.7329	0.299	4.7369	C.3	0.08
11	C1	–2.5786	0.1099	3.2433	C.2	0.2415
12	C4	–0.7546	–1.1382	5.5096	C.3	–0.0395
13	C5	–3.4725	1.6441	4.9759	C.3	–0.0418
14	O1	–3.1967	–0.9497	2.705	O.3	–0.2498
15	O2	–1.9203	0.9027	2.5914	O.2	–0.3699
16	C49	–3.218	–0.9809	1.2585	C.3	0.1852
17	C48	–1.8581	–0.9608	0.5784	C.2	0.2166
18	N9	–0.9581	–1.9802	0.6912	N.am	–0.252
19	C50	–4.1618	0.1301	0.7063	C.3	0.0292
20	C51	–5.4796	0.1942	1.4936	C.ar	–0.0379
21	C56	–5.8345	1.3506	2.1994	C.ar	–0.0601
22	C55	–7.0065	1.3847	2.9605	C.ar	–0.0686
23	C54	–7.8453	0.2682	3.004	C.ar	–0.0687
24	C53	–7.5159	–0.8761	2.2726	C.ar	–0.0686
25	C52	–6.3441	–0.9066	1.5113	C.ar	–0.0601
26	O10	–1.6136	0.0191	–0.1077	O.2	–0.3933
27	C43	0.2853	–1.914	–0.0956	C.3	0.1359
28	C42	0.6282	–3.287	–0.6358	C.2	0.2068
29	C47	–1.2786	–3.1445	1.5221	C.3	0.0255
30	C44	1.4676	–1.2304	0.6655	C.3	–0.0061
31	C46	1.1885	0.2871	0.8495	C.3	–0.0584
32	C45	1.7719	–1.855	2.0567	C.3	–0.0584
33	N8	–0.0516	–3.8407	–1.6763	N.am	–0.2498
34	O9	1.5649	–3.8801	–0.1298	O.2	–0.3942
35	C41	–1.1788	–3.1686	–2.3125	C.3	0.0369
36	C40	–1.8352	–4.3812	–3.0177	C.3	–0.0281
37	C39	–1.232	–5.5887	–2.2585	C.3	–0.0104
38	C38	0.2665	–5.1931	–2.1282	C.3	0.134
39	C37	0.9801	–5.3752	–3.4687	C.2	0.2073
40	N7	2.0481	–4.6949	–3.9905	N.am	–0.2484
41	O8	0.5176	–6.2823	–4.1438	O.2	–0.3941
42	C36	2.5264	–5.1281	–5.3094	C.3	0.0266
43	C28	2.7092	–3.578	–3.3089	C.3	0.128
44	C27	2.8056	–2.4422	–4.2952	C.2	0.1037
45	C29	4.0966	–3.9766	–2.7329	C.3	0.0238
46	C30	3.9479	–4.9101	–1.5232	C.ar	–0.0376

Table S13. Continued

47	C35	4.1965	−4.4468	−0.2248	C.ar	−0.06
48	C34	4.0126	−5.291	0.8742	C.ar	−0.0686
49	C33	3.5871	−6.6078	0.6814	C.ar	−0.0687
50	C32	3.3665	−7.0843	−0.6136	C.ar	−0.0686
51	C31	3.5614	−6.2415	−1.7113	C.ar	−0.06
52	N6	3.9398	−1.9383	−4.5721	N.2	−0.332
53	C25	3.7822	−0.8745	−5.5376	C.3	0.1001
54	C26	2.4288	−1.0719	−6.2695	C.3	0.043
55	S2	1.3254	−1.8174	−5.0444	S.3	−0.0463
56	C24	3.845	0.4725	−4.8528	C.2	0.1895
57	N5	3.2809	0.6161	−3.6296	N.am	−0.2623
58	O7	4.3994	1.3877	−5.4411	O.2	−0.396
59	C21	3.2367	1.9127	−2.9568	C.3	0.1158
60	C20	1.7932	2.3424	−2.9461	C.2	0.1014
61	C22	3.8567	1.7932	−1.5392	C.3	−0.013
62	C23	5.3436	1.3617	−1.6181	C.3	−0.0602
63	S1	0.8212	2.1371	−4.415	S.3	−0.0465
64	C19	−0.5956	2.3171	−3.3035	C.3	0.043
65	C18	−0.0811	3.2554	−2.179	C.3	0.1002
66	N4	1.2812	2.8561	−1.9024	N.2	−0.3321
67	C17	−0.9822	3.2598	−0.962	C.2	0.1909
68	N3	−0.7054	4.011	0.1422	N.am	−0.2542
69	O6	−1.9876	2.5696	−1.0251	O.2	−0.3959
70	C11	−1.6893	4.0105	1.236	C.3	0.1336
71	C10	−1.0613	4.2406	2.593	C.2	0.2042
72	C16	0.5147	4.8271	0.1774	C.3	0.0254
73	C12	−2.9431	4.8711	0.8942	C.3	−0.0099
74	C13	−2.6614	6.2664	0.2587	C.3	−0.0425
75	C15	−3.9795	6.8484	−0.3245	C.3	−0.0625
76	C14	−2.055	7.2774	1.2704	C.3	−0.0625
77	O5	−1.4459	5.1552	3.3033	O.2	−0.3944
78	H2	0.1986	2.6527	2.3208	H	0.1884
79	H7A	0.4234	4.4195	4.7131	H	0.0826
80	H8A	2.1436	1.9788	3.9235	H	0.0639
81	H4	2.6017	4.0169	5.8852	H	0.2101
82	H9A	2.6548	4.9787	3.4208	H	0.0257
83	H9B	2.4803	3.6984	2.1865	H	0.0257
84	H9C	3.8899	3.6909	3.2717	H	0.0257
85	H1	−0.0961	0.8794	3.8705	H	0.1856
86	H3A	−1.5168	0.6159	6.5027	H	0.0582
87	H2A	−3.3607	−0.5063	5.156	H	0.0574
88	H4B	−1.3821	−1.8024	6.1243	H	0.0253
89	H4A	−0.6918	−1.5606	4.4985	H	0.0253
90	H4C	0.256	−1.1049	5.9447	H	0.0253
91	H5C	−4.4813	1.5999	4.5422	H	0.0258
92	H5A	−3.5785	1.8478	6.0525	H	0.0258
93	H5B	−2.9306	2.4827	4.5122	H	0.0258

Table S13. Continued

94	H49A	–3.6802	–1.9439	1.0004	H	0.0918
95	H50B	–4.3954	–0.0647	–0.3528	H	0.048
96	H50A	–3.6666	1.1107	0.7534	H	0.048
97	H56A	–5.2032	2.2332	2.1641	H	0.0557
98	H55A	–7.265	2.2793	3.5188	H	0.0599
99	H54A	–8.7506	0.2898	3.6026	H	0.0559
100	H53A	–8.1713	–1.7415	2.2959	H	0.0599
101	H52A	–6.1123	–1.7934	0.9314	H	0.0557
102	H43A	0.1539	–1.3101	–1.007	H	0.0805
103	H47C	–0.3934	–3.7692	1.7067	H	0.0488
104	H47B	–1.6668	–2.8519	2.5063	H	0.0488
105	H47A	–2.0253	–3.7699	1.0105	H	0.0488
106	H44A	2.3748	–1.3247	0.0416	H	0.0343
107	H46A	0.3217	0.4092	1.5072	H	0.0234
108	H46C	0.9699	0.7828	–0.1086	H	0.0234
109	H46B	2.0479	0.7955	1.3133	H	0.0234
110	H45A	0.8969	–1.7551	2.7108	H	0.0234
111	H45B	2.044	–2.9175	1.9984	H	0.0234
112	H45C	2.6142	–1.3265	2.5297	H	0.0234
113	H41A	–1.8807	–2.7582	–1.5708	H	0.0524
114	H41B	–0.8673	–2.3825	–3.0182	H	0.0524
115	H40B	–2.9369	–4.3627	–2.9779	H	0.0287
116	H40A	–1.5227	–4.4186	–4.0747	H	0.0287
117	H39A	–1.4217	–6.5495	–2.7628	H	0.0313
118	H39B	–1.6899	–5.6463	–1.2549	H	0.0313
119	H38A	0.7383	–5.8335	–1.3651	H	0.0802
120	H36C	3.4238	–4.5809	–5.6343	H	0.0489
121	H36B	2.7837	–6.1984	–5.2937	H	0.0489
122	H36A	1.7412	–4.9598	–6.0626	H	0.0489
123	H28A	2.1212	–3.1399	–2.5081	H	0.088
124	H29A	4.7031	–4.4775	–3.5023	H	0.0485
125	H29B	4.6398	–3.0699	–2.4216	H	0.0485
126	H35A	4.5269	–3.4266	–0.0562	H	0.0557
127	H34A	4.1983	–4.9224	1.8783	H	0.0599
128	H33A	3.4297	–7.2593	1.5353	H	0.0559
129	H32A	3.0441	–8.1094	–0.7668	H	0.0599
130	H31A	3.4107	–6.6283	–2.7128	H	0.0557
131	H25A	4.6097	–0.9483	–6.2626	H	0.0619
132	H26B	2.0164	–0.1358	–6.6765	H	0.0448
133	H26A	2.5382	–1.8055	–7.0844	H	0.0448
134	H5	2.8317	–0.1463	–3.1651	H	0.1896
135	H21A	3.7802	2.7005	–3.5026	H	0.0854
136	H22B	3.7836	2.7603	–1.0142	H	0.032
137	H22A	3.3015	1.0412	–0.9598	H	0.032
138	H23B	5.927	2.1002	–2.1897	H	0.0233
139	H23A	5.4364	0.3807	–2.1098	H	0.0233
140	H23C	5.7691	1.2863	–0.6049	H	0.0233

Table S13. Continued

141	H19B	–1.4783	2.7163	–3.827	H	0.0448
142	H19A	–0.822	1.315	–2.9049	H	0.0448
143	H18A	–0.0478	4.2851	–2.5685	H	0.0619
144	H11A	–2.0747	2.9893	1.369	H	0.0802
145	H16A	0.6363	5.3702	1.1234	H	0.0488
146	H16B	0.5087	5.5787	–0.6251	H	0.0488
147	H16C	1.4054	4.1958	0.068	H	0.0488
148	H12B	–3.5281	4.2993	0.1542	H	0.0315
149	H12A	–3.5778	4.9811	1.7882	H	0.0315
150	H13A	–1.9692	6.1501	–0.5911	H	0.0298
151	H15A	–4.7269	6.9679	0.4742	H	0.0232
152	H15B	–3.7967	7.8289	–0.7903	H	0.0232
153	H15C	–4.3919	6.1791	–1.0964	H	0.0232
154	H14A	–1.9325	8.2645	0.7984	H	0.0232
155	H14C	–2.7159	7.389	2.1435	H	0.0232
156	H14B	–1.0654	6.9543	1.6154	H	0.0232
157	P5	–3.6635	1.9768	5.0356	Du	0
158	P4	–0.606	–1.4893	5.5225	Du	0
159	P9	3.0083	4.1227	2.9596	Du	0
160	P12	–3.553	4.6402	0.9712	Du	0
161	P15	–4.3052	6.992	–0.4708	Du	0
162	P14	–1.9046	7.536	1.5191	Du	0
163	P16	0.8502	5.0482	0.1888	Du	0
164	P22	3.5425	1.9008	–0.987	Du	0
165	P23	5.7109	1.2557	–1.6348	Du	0
166	P29	4.6714	–3.7737	–2.962	Du	0
167	P3135	3.9688	–5.0275	–1.3845	Du	0
168	P39	–1.5558	–6.0979	–2.0088	Du	0
169	P40	–2.2298	–4.3907	–3.5263	Du	0
170	P41	–1.374	–2.5704	–2.2945	Du	0
171	P46	1.1132	0.6625	0.904	Du	0
172	P45	1.8517	–1.9997	2.413	Du	0
173	P50	–4.031	0.523	0.2003	Du	0
174	P36	2.6495	–5.2464	–5.6635	Du	0
175	P47	–1.3618	–3.4637	1.7412	Du	0
176	P19	–1.1501	2.0156	–3.366	Du	0

[a]Atom nomenclature as in Figure 1a. [b]Pseudoatoms used in modeling are designated by "P" followed by the number of the relevant carbon atom(s). [c]Tripos forcefield atom type. [d]Gasteiger-Huckel charges.

Table S14. Atom coordinates for modeled grassypeptolide C (**3**) structure 10

Atom number	Atom name[a,b]	x	y	z	Atom type[c]	Charge[d]
1	N7	–4.5134	4.3308	–0.0025	N.am	–0.2484
2	C28	–3.5328	4.0194	–1.0513	C.3	0.128
3	C27	–2.4282	5.0439	–1.0768	C.2	0.1037
4	C29	–4.115	3.9654	–2.503	C.3	0.0238
5	C30	–5.5067	3.3144	–2.5985	C.ar	–0.0376
6	C31	–5.6791	1.9673	–2.2678	C.ar	–0.06
7	C32	–6.9496	1.3857	–2.2537	C.ar	–0.0686
8	C33	–8.0641	2.1403	–2.6277	C.ar	–0.0687
9	C34	–7.8961	3.4684	–3.0275	C.ar	–0.0686
10	C35	–6.6233	4.0467	–3.023	C.ar	–0.06
11	N6	–1.4398	4.8062	–1.838	N.2	–0.332
12	C25	–0.4947	5.8953	–1.7599	C.3	0.1001
13	C26	–0.6909	6.5903	–0.39	C.3	0.043
14	S2	–2.4866	6.5415	–0.1277	S.3	–0.0463
15	C36	–5.6504	5.2192	–0.2632	C.3	0.0266
16	C24	0.8901	5.3248	–1.919	C.2	0.1895
17	N5	1.0296	4.0041	–1.6603	N.am	–0.2623
18	O7	1.7989	6.0563	–2.2781	O.2	–0.396
19	C21	2.3031	3.3149	–1.8445	C.3	0.1158
20	C20	2.724	2.7277	–0.5234	C.2	0.1014
21	C22	2.1228	2.2201	–2.9303	C.3	–0.013
22	C23	1.6116	2.8229	–4.2641	C.3	–0.0602
23	N4	3.3054	1.5981	–0.5082	N.2	–0.3321
24	C18	3.6744	1.2593	0.8462	C.3	0.1002
25	C19	2.6915	2.009	1.7856	C.3	0.043
26	S1	2.4266	3.6115	0.9841	S.3	–0.0465
27	C17	3.6903	–0.2387	1.0579	C.2	0.1909
28	N3	4.5879	–1.0461	0.4238	N.am	–0.2542
29	O6	2.878	–0.6849	1.8501	O.2	–0.3959
30	C16	5.5492	–0.4724	–0.5229	C.3	0.0254
31	C11	4.5874	–2.4843	0.7192	C.3	0.1336
32	C10	4.257	–3.1635	–0.5821	C.2	0.2042
33	C12	5.9227	–2.9943	1.3341	C.3	–0.0099
34	C13	6.2129	–2.5046	2.7856	C.3	–0.0425
35	C15	6.5822	–0.9988	2.8765	C.3	–0.0625
36	C14	5.0522	–2.8465	3.7594	C.3	–0.0625
37	N2	2.9919	–2.9992	–1.0344	N.am	–0.2613
38	O5	5.1181	–3.8019	–1.1669	O.2	–0.3944
39	C7	2.5481	–3.6426	–2.2653	C.3	0.1563
40	C6	1.7822	–4.9018	–1.9191	C.2	0.2046
41	C8	1.7579	–2.6381	–3.1408	C.3	0.0924
42	O4	1.2791	–3.3275	–4.3087	O.3	–0.3874
43	C9	2.6604	–1.4371	–3.5315	C.3	–0.0346
44	N1	0.7667	–4.8479	–1.0229	N.am	–0.2796
45	O3	2.1359	–5.9452	–2.4472	O.2	–0.3944
46	C3	0.1346	–6.0719	–0.5235	C.3	0.0598

Table S14. Continued

47	C2	0.5471	−6.275	0.9659	C.3	0.08
48	C1	−0.0846	−5.2466	1.8712	C.2	0.2415
49	C4	−1.405	−6.0051	−0.7059	C.3	−0.0395
50	C5	2.0887	−6.2003	1.132	C.3	−0.0418
51	O1	−0.1171	−4.0037	1.3673	O.3	−0.2498
52	O2	−0.538	−5.5607	2.9611	O.2	−0.3699
53	C49	−0.6862	−2.9929	2.2253	C.3	0.1852
54	C48	−0.9152	−1.8228	1.2857	C.2	0.2166
55	C50	0.3163	−2.6394	3.3594	C.3	0.0292
56	N9	−2.1463	−1.3017	0.9807	N.am	−0.252
57	O10	0.1089	−1.3918	0.778	O.2	−0.3933
58	C51	−0.1904	−1.4939	4.2505	C.ar	−0.0379
59	C52	0.5429	−0.3089	4.386	C.ar	−0.0601
60	C53	0.0825	0.7239	5.2068	C.ar	−0.0686
61	C54	−1.1339	0.5917	5.8813	C.ar	−0.0687
62	C55	−1.8738	−0.5861	5.7501	C.ar	−0.0686
63	C56	−1.3921	−1.6306	4.9559	C.ar	−0.0601
64	C43	−2.2462	−0.2411	−0.0399	C.3	0.1359
65	C47	−3.3533	−1.8465	1.6119	C.3	0.0255
66	C42	−3.0922	0.9011	0.5128	C.2	0.2068
67	C44	−2.7778	−0.8202	−1.3929	C.3	−0.0061
68	C45	−2.3051	0.0555	−2.5921	C.3	−0.0584
69	C46	−2.3043	−2.2816	−1.6294	C.3	−0.0584
70	C37	−4.4544	3.7756	1.2473	C.2	0.2073
71	C38	−3.3742	2.9137	1.8931	C.3	0.134
72	C39	−2.2693	3.8538	2.4332	C.3	−0.0104
73	C40	−1.1006	2.9029	2.7524	C.3	−0.0281
74	C41	−1.1169	1.9324	1.5514	C.3	0.0369
75	N8	−2.5421	1.8983	1.2508	N.am	−0.2498
76	O9	−4.291	0.9135	0.2864	O.2	−0.3942
77	O8	−5.3398	4.0547	2.0426	O.2	−0.3941
78	H28A	−3.0759	3.0439	−0.8589	H	0.088
79	H29A	−4.1666	4.9831	−2.9212	H	0.0485
80	H29B	−3.4341	3.4014	−3.1611	H	0.0485
81	H31A	−4.8203	1.3625	−2.0251	H	0.0557
82	H32A	−7.0696	0.3489	−1.9547	H	0.0599
83	H33A	−9.0546	1.6965	−2.61	H	0.0559
84	H34A	−8.7561	4.0521	−3.3413	H	0.0599
85	H35A	−6.5141	5.0746	−3.3515	H	0.0557
86	H25A	−0.7142	6.5894	−2.5883	H	0.0619
87	H26A	−0.2092	6.0044	0.4087	H	0.0448
88	H26B	−0.3006	7.6195	−0.3762	H	0.0448
89	H36B	−5.7797	5.9363	0.5625	H	0.0489
90	H36C	−6.5745	4.6307	−0.3629	H	0.0489
91	H36A	−5.503	5.8289	−1.1632	H	0.0489
92	H5	0.2407	3.4599	−1.3685	H	0.1896
93	H21A	3.112	3.9932	−2.1604	H	0.0854

Table S14. Continued

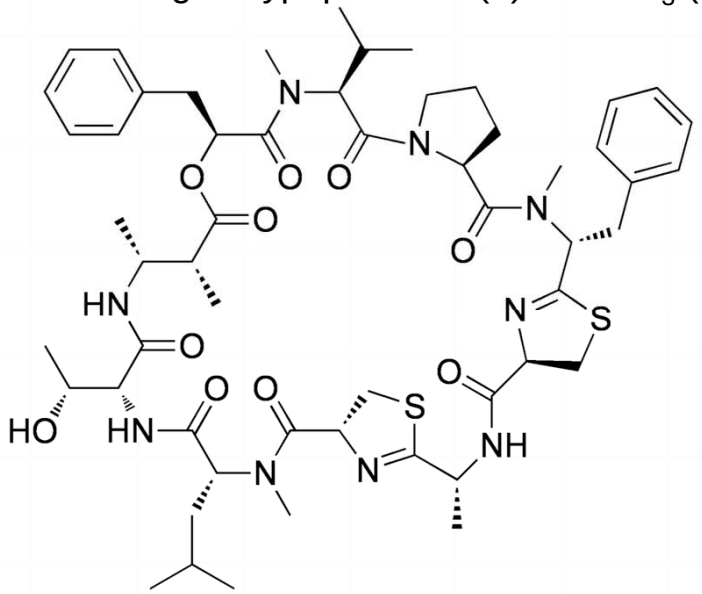
94	H22A	3.0884	1.7192	−3.11	H	0.032
95	H22B	1.3992	1.4691	−2.5721	H	0.032
96	H23B	1.526	2.0322	−5.0261	H	0.0233
97	H23C	2.3122	3.5894	−4.6299	H	0.0233
98	H23A	0.6208	3.2843	−4.1302	H	0.0233
99	H18A	4.6863	1.6502	1.0335	H	0.0619
100	H19A	3.0725	2.1178	2.8129	H	0.0448
101	H19B	1.7155	1.5052	1.8093	H	0.0448
102	H16B	6.2788	0.1622	−0.001	H	0.0488
103	H16C	6.1082	−1.2557	−1.0545	H	0.0488
104	H16A	5.0418	0.1164	−1.2985	H	0.0488
105	H11A	3.7775	−2.8065	1.3903	H	0.0802
106	H12A	5.8693	−4.0964	1.3619	H	0.0315
107	H12B	6.7743	−2.7299	0.6893	H	0.0315
108	H13A	7.1059	−3.0596	3.123	H	0.0298
109	H15B	6.9225	−0.7582	3.8959	H	0.0232
110	H15C	7.3959	−0.7578	2.1757	H	0.0232
111	H15A	5.7209	−0.3576	2.654	H	0.0232
112	H14B	5.3834	−2.7131	4.7992	H	0.0232
113	H14C	4.1869	−2.1878	3.5955	H	0.0232
114	H14A	4.7333	−3.892	3.6231	H	0.0232
115	H2	2.3241	−2.4637	−0.5118	H	0.1884
116	H7A	3.4207	−3.977	−2.8419	H	0.0826
117	H8A	0.9087	−2.2543	−2.5568	H	0.0639
118	H4	0.7569	−2.7693	−4.8758	H	0.2101
119	H9C	3.5263	−1.7847	−4.1152	H	0.0257
120	H9B	2.0929	−0.7165	−4.1396	H	0.0257
121	H9A	3.0264	−0.9205	−2.6308	H	0.0257
122	H1	0.4892	−3.9858	−0.5996	H	0.1856
123	H3A	0.4782	−6.9626	−1.0778	H	0.0582
124	H2A	0.2031	−7.2738	1.2869	H	0.0574
125	H4C	−1.8402	−5.1624	−0.1511	H	0.0253
126	H4B	−1.8744	−6.9354	−0.3497	H	0.0253
127	H4A	−1.6429	−5.8749	−1.7731	H	0.0253
128	H5A	2.465	−5.1949	0.8888	H	0.0258
129	H5B	2.5817	−6.9306	0.4719	H	0.0258
130	H5C	2.3661	−6.4273	2.1733	H	0.0258
131	H49A	−1.6154	−3.3653	2.6729	H	0.0918
132	H50A	1.2877	−2.392	2.9066	H	0.048
133	H50B	0.4802	−3.506	4.0173	H	0.048
134	H52A	1.4809	−0.1792	3.8613	H	0.0557
135	H53A	0.6692	1.6308	5.3182	H	0.0599
136	H54A	−1.5022	1.4006	6.5045	H	0.0559
137	H55A	−2.8223	−0.6907	6.2679	H	0.0599
138	H56A	−1.9598	−2.5529	4.8989	H	0.0557
139	H43A	−1.2578	0.1639	−0.2986	H	0.0805
140	H47B	−4.2668	−1.3784	1.2219	H	0.0488

Table S14. Continued

141	H47A	–3.4616	–2.9246	1.4226	H	0.0488
142	H47C	–3.3264	–1.6593	2.696	H	0.0488
143	H44A	–3.8799	–0.8526	–1.3806	H	0.0343
144	H45A	–2.8358	–0.2304	–3.5137	H	0.0234
145	H45C	–1.2243	–0.0727	–2.7625	H	0.0234
146	H45B	–2.4876	1.1214	–2.4007	H	0.0234
147	H46A	–1.2156	–2.349	–1.5147	H	0.0234
148	H46B	–2.772	–2.9716	–0.9149	H	0.0234
149	H46C	–2.5705	–2.621	–2.6426	H	0.0234
150	H38A	–3.8293	2.3834	2.7466	H	0.0802
151	H39A	–1.9367	4.5333	1.6385	H	0.0313
152	H39B	–2.593	4.4494	3.3026	H	0.0313
153	H40B	–1.3561	2.3615	3.6762	H	0.0287
154	H40A	–0.134	3.415	2.888	H	0.0287
155	H41A	–0.7015	0.9618	1.861	H	0.0524
156	H41B	–0.5608	2.3484	0.6979	H	0.0524
157	P5	2.4709	–6.1842	1.178	Du	0
158	P4	–1.7858	–5.9909	–0.758	Du	0
159	P9	2.8818	–1.1406	–3.6285	Du	0
160	P12	6.3218	–3.4131	1.0256	Du	0
161	P15	6.6798	–0.6245	2.9085	Du	0
162	P14	4.7679	–2.931	4.0059	Du	0
163	P16	5.8096	–0.3257	–0.7847	Du	0
164	P22	2.2438	1.5941	–2.841	Du	0
165	P23	1.4863	2.9686	–4.5954	Du	0
166	P29	–3.8003	4.1923	–3.0411	Du	0
167	P3135	–5.6672	3.2186	–2.6883	Du	0
168	P36	–5.9524	5.4653	–0.3212	Du	0
169	P39	–2.2648	4.4913	2.4705	Du	0
170	P40	–0.7451	2.8883	3.2821	Du	0
171	P41	–0.6312	1.6551	1.2794	Du	0
172	P45	–2.1826	0.2728	–2.8923	Du	0
173	P46	–2.186	–2.6472	–1.6907	Du	0
174	P47	–3.6849	–1.9874	1.7801	Du	0
175	P50	0.8839	–2.949	3.4619	Du	0
176	P19	2.394	1.8115	2.3111	Du	0

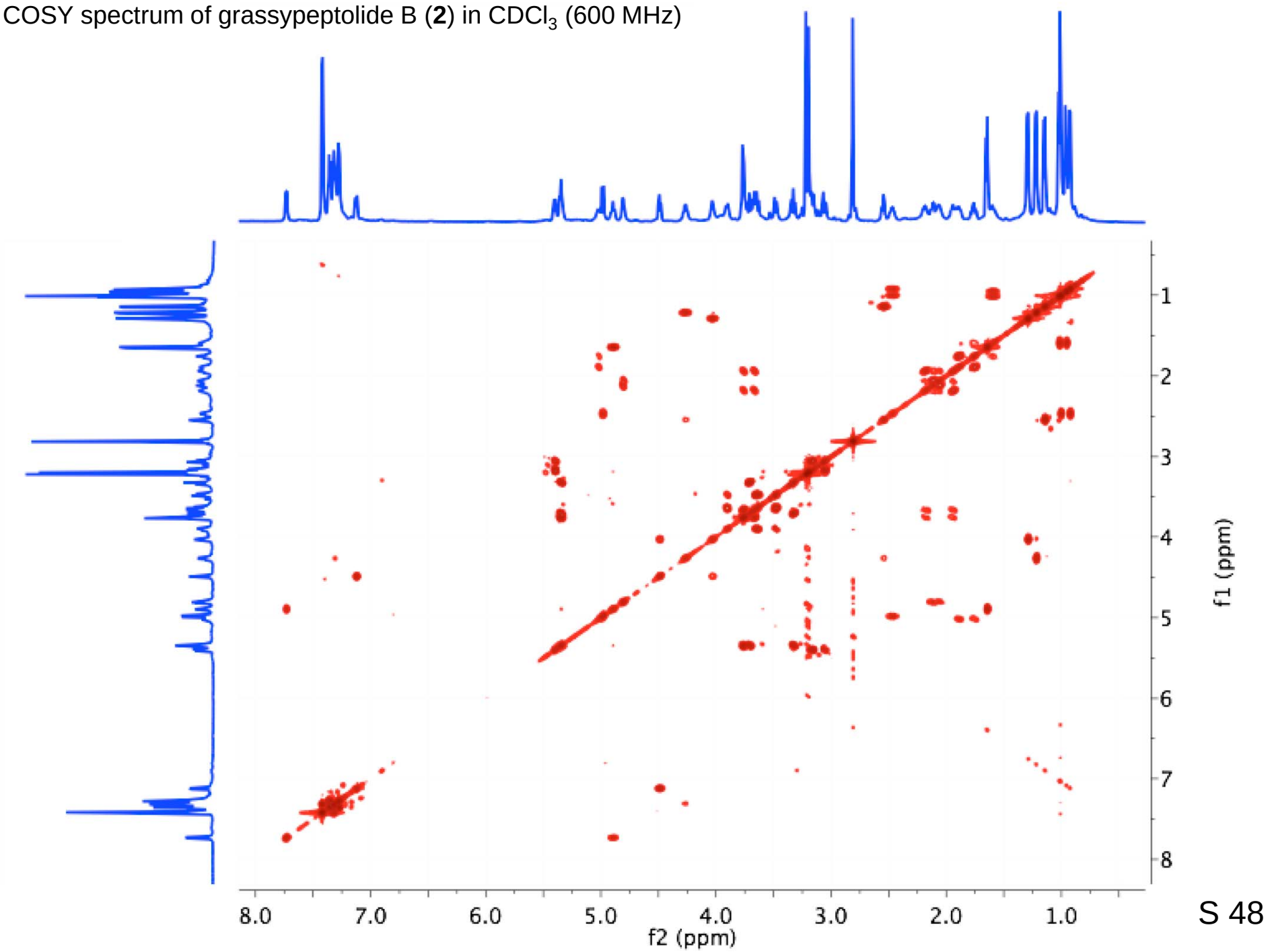
[a]Atom nomenclature as in Figure 1a. [b]Pseudoatoms used in modeling are designated by "P" followed by the number of the relevant carbon atom(s). [c]Tripos forcefield atom type. [d]Gasteiger-Huckel charges.

^{1}H NMR spectrum of grassypeptolide B (**2**) in $CDCl_3$ (600 MHz)

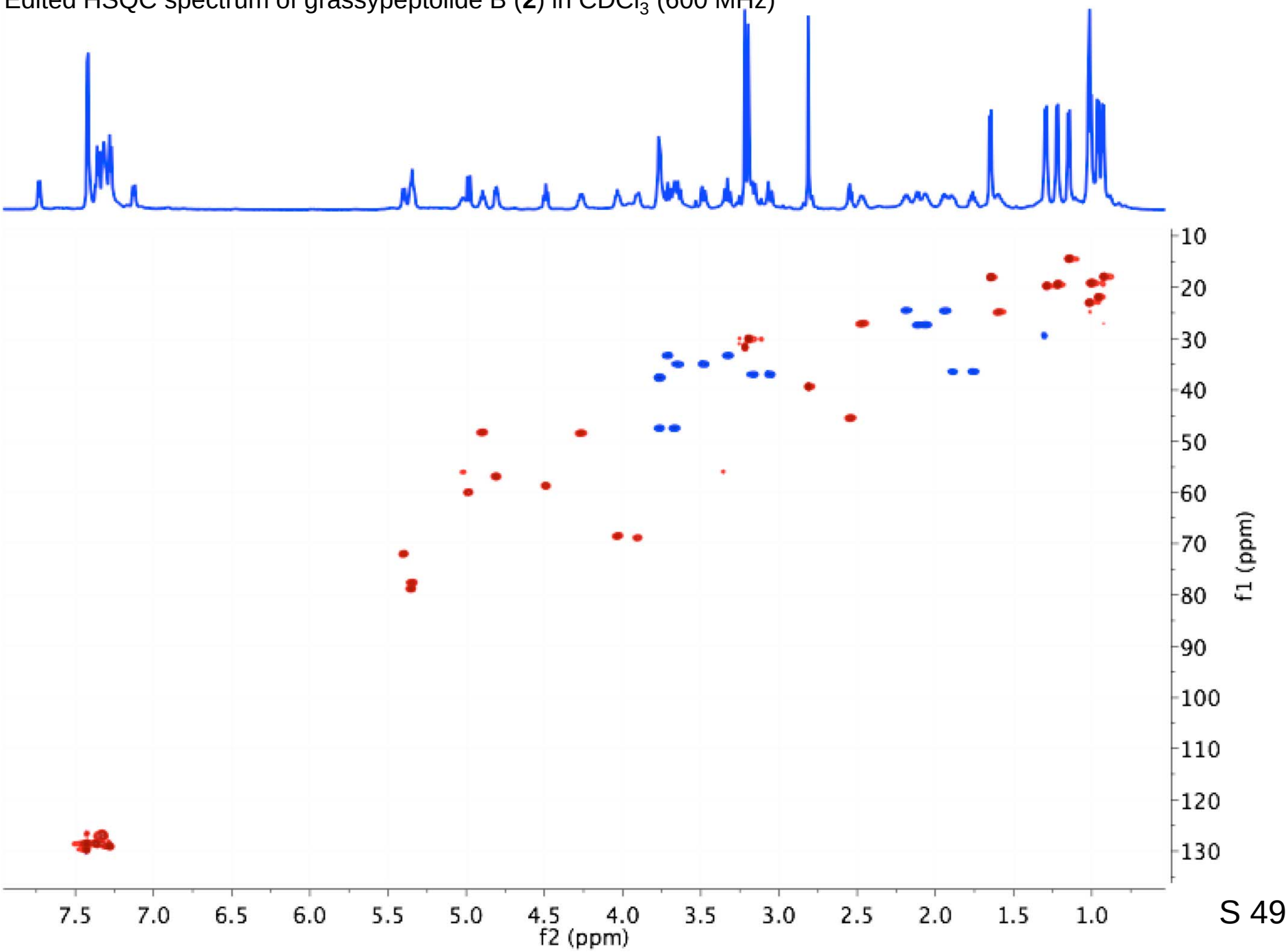


2

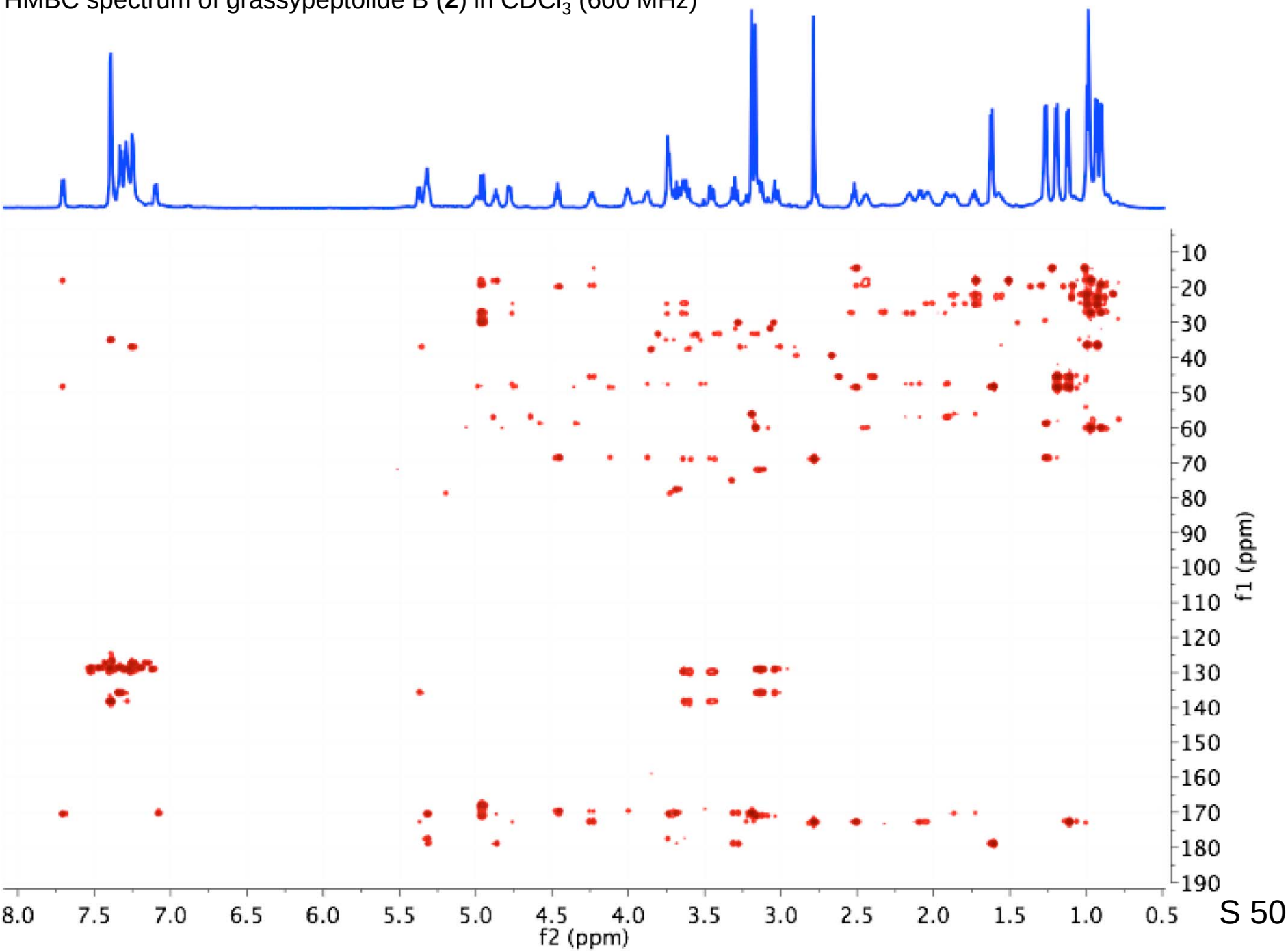
COSY spectrum of grassypeptolide B (**2**) in $CDCl_3$ (600 MHz)



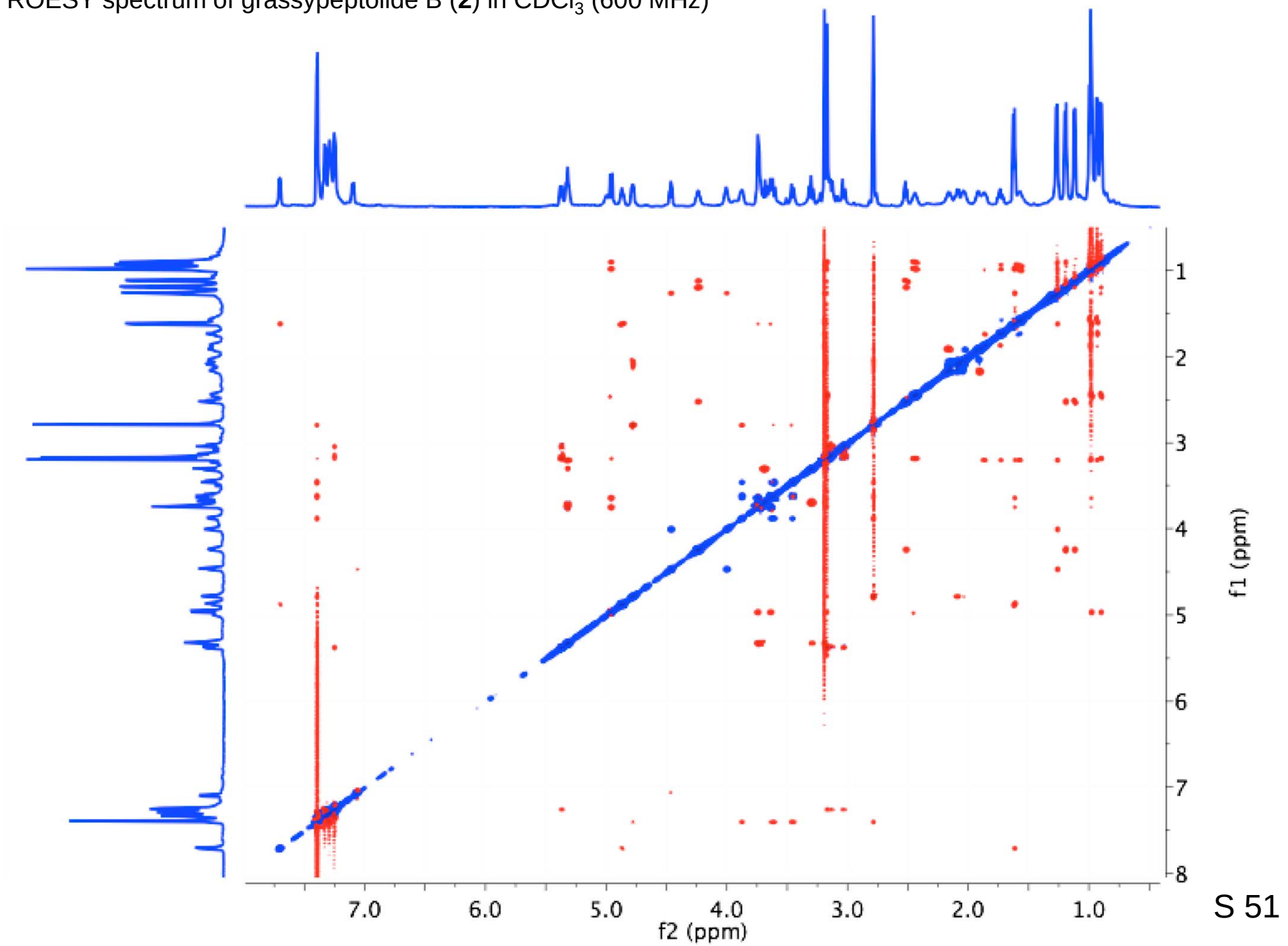
Edited HSQC spectrum of grassypeptolide B (**2**) in $CDCl_3$ (600 MHz)



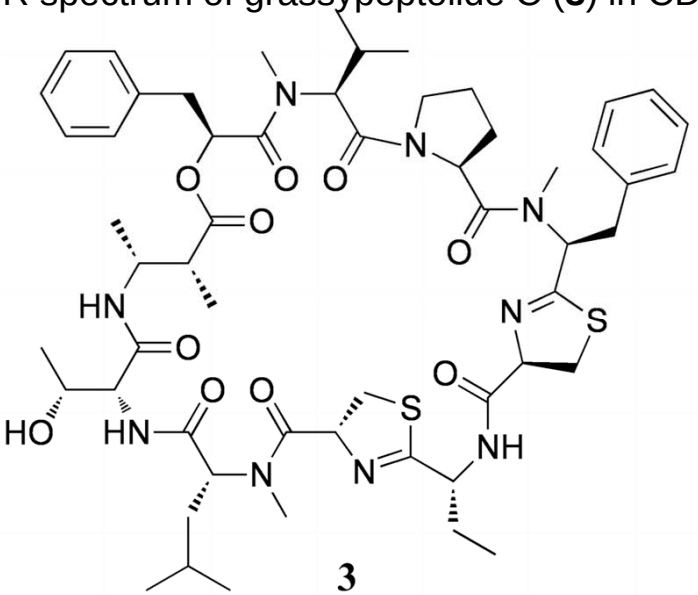
HMBC spectrum of grassypeptolide B (**2**) in $CDCl_3$ (600 MHz)



ROESY spectrum of grassypeptolide B (**2**) in $CDCl_3$ (600 MHz)

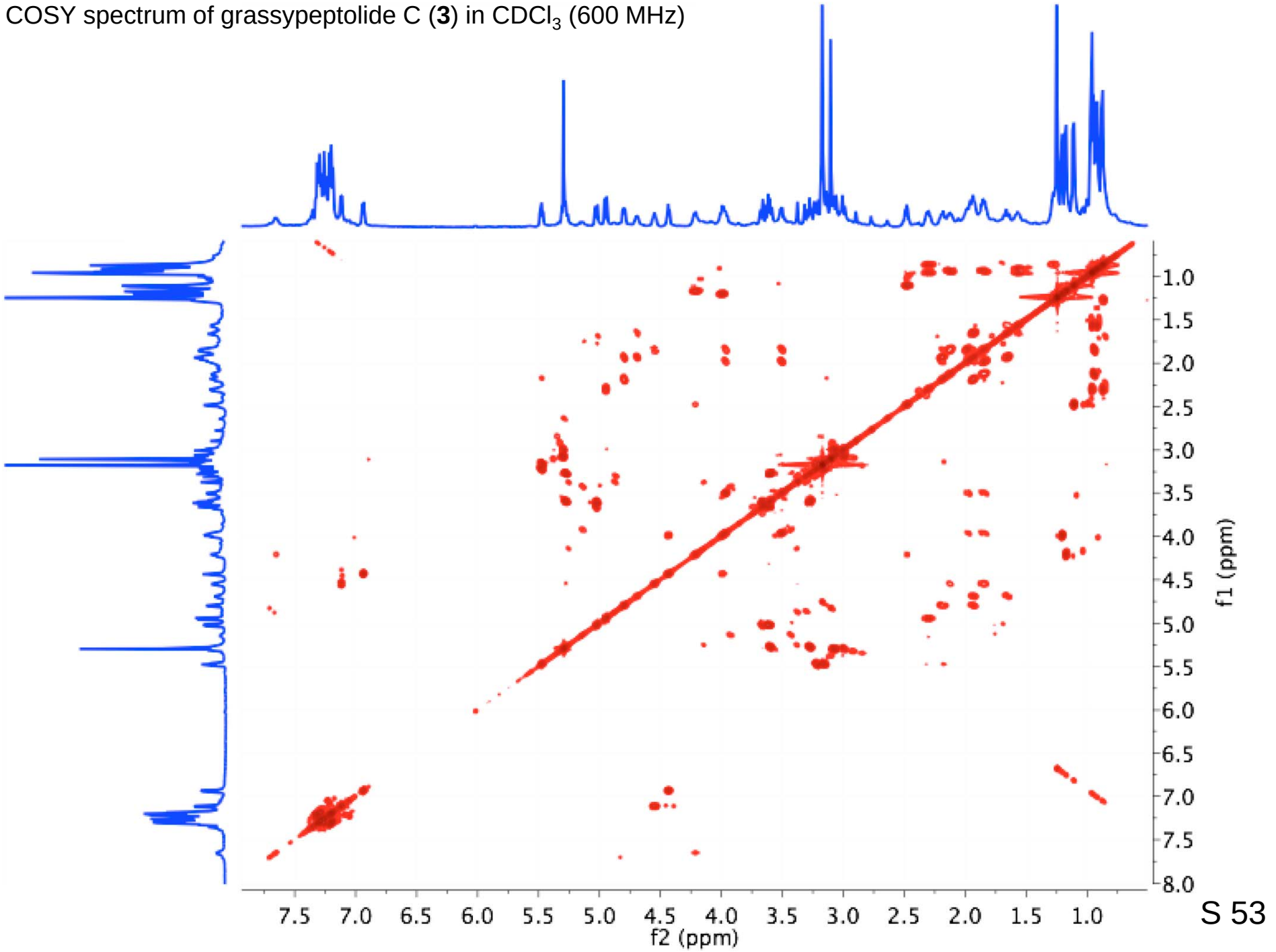


^{1}H NMR spectrum of grassypeptolide C (**3**) in $CDCl_3$ (600 MHz)

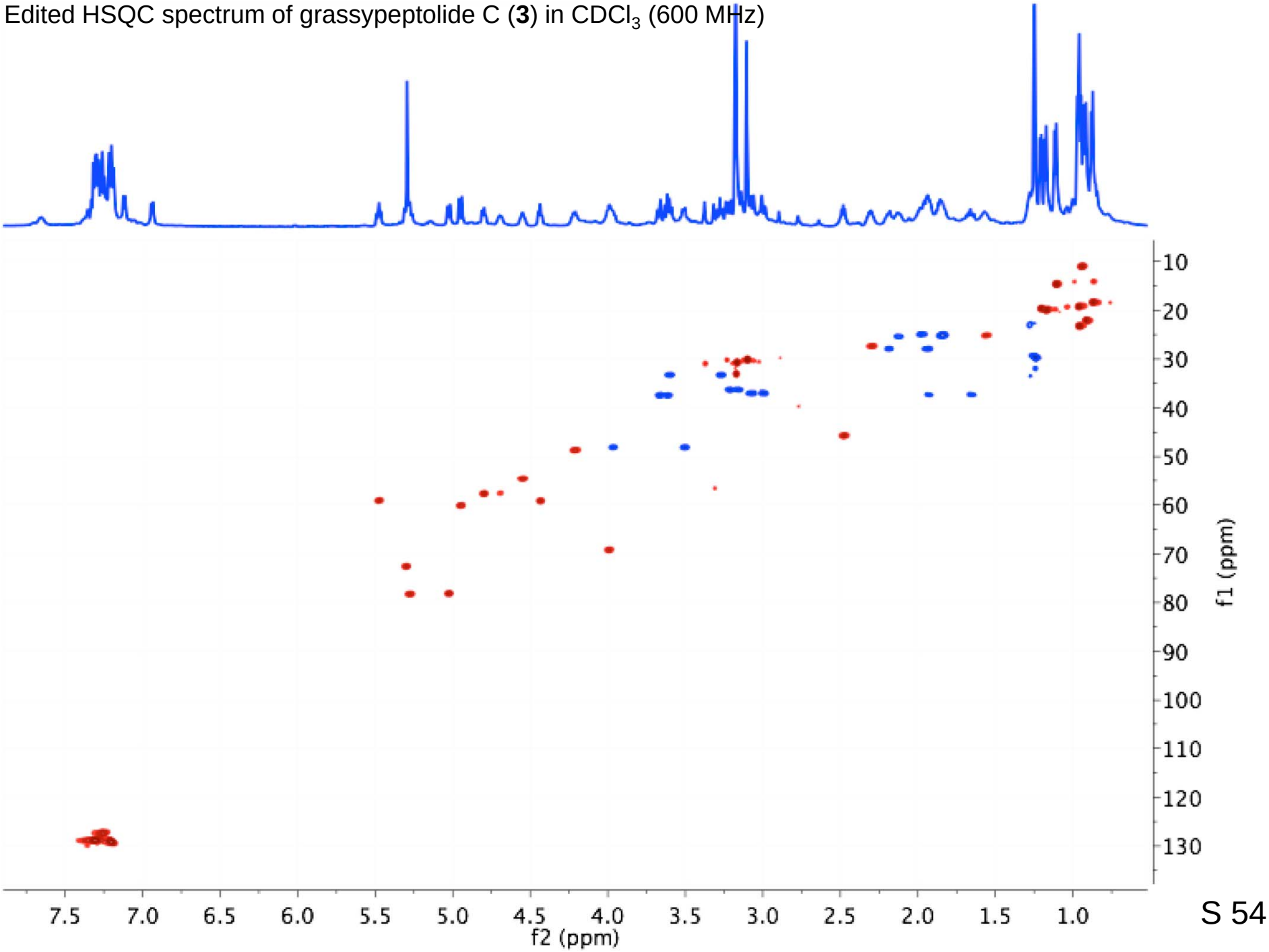


3

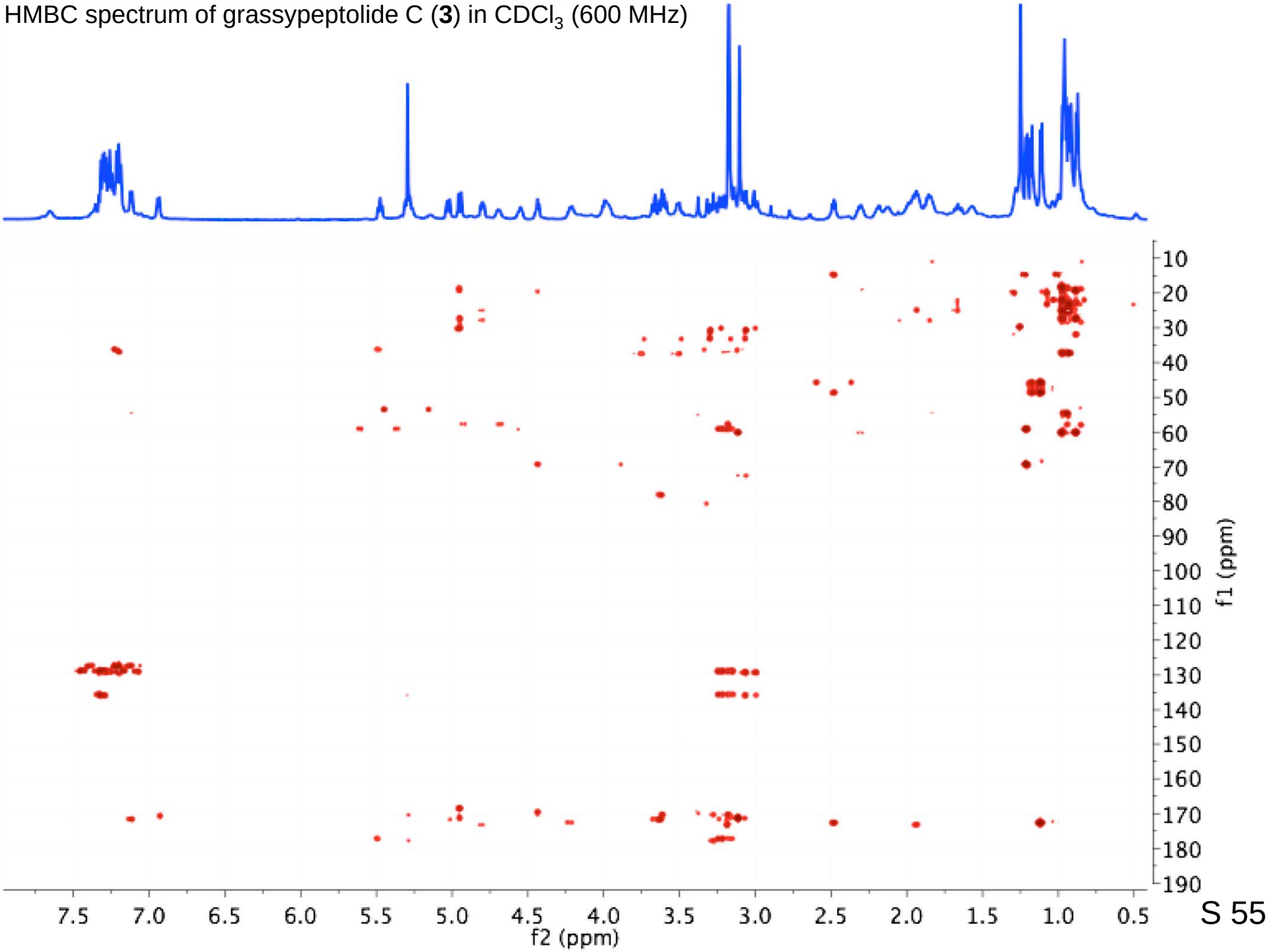
COSY spectrum of grassypeptolide C (**3**) in $CDCl_3$ (600 MHz)



Edited HSQC spectrum of grassypeptolide C (**3**) in $CDCl_3$ (600 MHz)



HMBC spectrum of grassypeptolide C (**3**) in $CDCl_3$ (600 MHz)



ROESY spectrum of grassypeptolide C (**3**) in $CDCl_3$ (600 MHz)