Supporting Information

The extent of helical induction caused by introducing α-aminoisobutyric acid into an oligovaline sequence

Genichiro Tsuji,[a] Takashi Misawa,[a] Mitsunobu Doi,[b] and Yosuke Demizu[a,*]

[a]*Division of Organic Chemistry, National Institute of Health Sciences, Tokyo 158-8501, Japan*

[b]*Osaka University of Pharmaceutical Sciences, Osaka 569-1094, Japan*

demizu@nihs.go.jp

* To whom correspondence should be addressed. Tel & FAX: + 81-44-270-6578.

Supporting Information

Table S1. Crystal and experimental data.

Formula	$(C_{62}H_{112}N_{12}O_{15})$, $3(CH_4O)$
Fw	2627.41
cell setting	triclinic, *P*1
a	10.612(5) Å
b	17.232(8) Å
c	21.162(10) Å
α	88.192(7) °
β	87.296(7) °
γ	79.182(7) °
V	3796(3) $Å^3$
Z	1
T	100(2) K
Crystal description	block, 0.30×0.30×0.20 mm^3
D_X	1.149 g cm^{-3}
F(000)	1430
μ (MoKα)	0.083 mm^{-1}
Wavelength	0.71073 Å (MoKα)
θ_{max}	25.68 °
No of reflections (obs)	14000
No of reflections (I>2σ(I)	7867
Flack x parameter	0.6(16)
No of parameters	1660
*R*1	0.0922
wR	0.2264
Goodness of fit	1.007
$(\Delta/\sigma)_{max}$	0.011
Fraction θ-full	0.972
$\Delta\rho_{max}$	0.467 e $Å^{-3}$
$\Delta\rho_{min}$	–0.453 e $Å^{-3}$

Table S2. Atomic coorinates.

Atm	x	y	z	Ueq
Molecule A				
O1M	0.1551(7)	0.1524(4)	0.7063(3)	0.0460(17)
H1M	0.1836	0.1277	0.6696	0.069
C1M	0.1002(12)	0.2353(6)	0.6935(5)	0.055(3)
H1M1	0.0103	0.2463	0.7091	0.082
H1M2	0.1046	0.2462	0.6478	0.082
H1M3	0.1487	0.2690	0.7149	0.082
O2M	0.0845(11)	0.5705(6)	0.2015(5)	0.107(4)
H2M	0.1047	0.6118	0.1841	0.160
C2M	0.0942(17)	0.4974(7)	0.1797(7)	0.086(4)
H2M1	0.1595	0.4610	0.2026	0.129
H2M2	0.1188	0.4972	0.1344	0.129
H2M3	0.0112	0.4804	0.1859	0.129
O3M	0.212(2)	0.6591(11)	0.1386(9)	0.177(6)
H3M	0.1908	0.6486	0.1018	0.266
C3M	0.332(3)	0.7043(18)	0.1256(14)	0.185(12)
H3M1	0.3089	0.7583	0.1413	0.277
H3M2	0.3532	0.7061	0.0801	0.277
H3M3	0.4067	0.6759	0.1477	0.277
C1	0.2859(8)	-0.0847(5)	0.6730(4)	0.031(2)
C2	0.2401(11)	-0.0736(6)	0.6059(5)	0.049(3)
H2A	0.2031	-0.1191	0.5948	0.073
H2B	0.3128	-0.0691	0.5766	0.073
H2C	0.1747	-0.0253	0.6029	0.073
C3	0.3926(11)	-0.1554(6)	0.6798(5)	0.051(3)
H3A	0.3589	-0.2039	0.6745	0.077
H3B	0.4278	-0.1562	0.7218	0.077
H3C	0.4606	-0.1522	0.6473	0.077
C4	0.1722(9)	-0.0886(6)	0.7195(5)	0.046(2)
H4A	0.1399	-0.1374	0.7132	0.069
H4B	0.1038	-0.0429	0.7121	0.069
H4C	0.2002	-0.0881	0.7630	0.069
O1	0.3372(6)	-0.0122(4)	0.6810(3)	0.0364(14)
C5	0.3800(9)	0.0036(5)	0.7354(4)	0.035(2)
O5	0.3790(6)	-0.0375(3)	0.7842(3)	0.0355(14)
N11	0.4317(7)	0.0703(4)	0.7307(3)	0.0298(16)
H11	0.4317	0.0971	0.6946	0.036
C11	0.4872(8)	0.0971(5)	0.7862(4)	0.0294(19)
H11A	0.5596	0.0544	0.7988	0.035
C12	0.3940(8)	0.1122(5)	0.8424(4)	0.0278(19)
O12	0.4351(5)	0.1113(4)	0.8954(3)	0.0333(14)
C13	0.5439(9)	0.1698(6)	0.7672(4)	0.038(2)
H13	0.5901	0.1594	0.7252	0.045
C14	0.4410(10)	0.2443(5)	0.7594(4)	0.040(2)
H14A	0.3782	0.2344	0.7296	0.059
H14B	0.4814	0.2880	0.7432	0.059
H14C	0.3975	0.2582	0.8005	0.059
C15	0.6406(10)	0.1847(7)	0.8130(5)	0.052(3)
H15A	0.6745	0.2318	0.7991	0.079
H15B	0.7110	0.1390	0.8144	0.079
H15C	0.5991	0.1930	0.8552	0.079
N21	0.2693(7)	0.1244(4)	0.8329(3)	0.0295(16)
H21	0.2426	0.1249	0.7941	0.035
C21	0.1767(8)	0.1368(5)	0.8853(4)	0.0279(19)
H21A	0.1868	0.1860	0.9068	0.034
C22	0.1999(8)	0.0686(5)	0.9333(3)	0.0249(18)
O22	0.1728(5)	0.0815(3)	0.9896(3)	0.0303(13)
C23	0.0368(9)	0.1484(5)	0.8630(4)	0.036(2)
H23	0.0270	0.1912	0.8295	0.043
C24	0.0078(10)	0.0752(7)	0.8339(5)	0.055(3)
H24A	0.0704	0.0586	0.7991	0.082
H24B	-0.0789	0.0867	0.8176	0.082
H24C	0.0129	0.0326	0.8661	0.082
C25	-0.0564(9)	0.1766(6)	0.9167(4)	0.042(2)
H25A	-0.0346	0.2240	0.9344	0.063
H25B	-0.0519	0.1350	0.9497	0.063
H25C	-0.1436	0.1890	0.9012	0.063
N31	0.2510(7)	-0.0034(4)	0.9131(3)	0.0312(16)
H31	0.2696	-0.0099	0.8724	0.037
C31	0.2774(8)	-0.0730(5)	0.9566(4)	0.0279(18)
C32	0.3666(9)	-0.0568(5)	1.0065(4)	0.032(2)
O32	0.3511(6)	-0.0763(4)	1.0627(3)	0.0420(16)
C33	0.3488(10)	-0.1422(5)	0.9184(4)	0.039(2)
H33A	0.3676	-0.1892	0.9461	0.058
H33B	0.4293	-0.1294	0.9003	0.058
H33C	0.2954	-0.1525	0.8842	0.058
C34	0.1539(10)	-0.0923(6)	0.9864(5)	0.044(2)
H34A	0.1739	-0.1385	1.0149	0.065
H34B	0.0995	-0.1040	0.9531	0.065
H34C	0.1084	-0.0470	1.0104	0.065
N41	0.4649(7)	-0.0232(4)	0.9862(3)	0.0298(16)
H41	0.4735	-0.0118	0.9456	0.036
C41	0.5588(8)	-0.0048(6)	1.0288(4)	0.034(2)
H41A	0.5871	-0.0526	1.0562	0.041
C42	0.5006(8)	0.0616(5)	1.0708(4)	0.0296(19)
O42	0.5123(6)	0.0586(4)	1.1275(3)	0.0333(14)
C43	0.6766(8)	0.0129(6)	0.9908(4)	0.036(2)
H43	0.6467	0.0580	0.9609	0.044
C44	0.7700(9)	0.0387(6)	1.0341(4)	0.040(2)
H44A	0.7257	0.0838	1.0587	0.060
H44B	0.8412	0.0543	1.0086	0.060
H44C	0.8036	-0.0051	1.0629	0.060
C45	0.7416(10)	-0.0570(7)	0.9516(4)	0.048(3)
H45A	0.6791	-0.0724	0.9241	0.072
H45B	0.7750	-0.1016	0.9798	0.072
H45C	0.8125	-0.0421	0.9255	0.072
N51	0.4382(7)	0.1275(4)	1.0407(3)	0.0314(17)
H51	0.4312	0.1274	0.9995	0.038
C51	0.3824(8)	0.1984(5)	1.0756(4)	0.0290(19)
H51A	0.4534	0.2187	1.0951	0.035
C52	0.2908(8)	0.1768(5)	1.1289(4)	0.0295(19)
O52	0.2886(6)	0.2036(3)	1.1806(3)	0.0327(14)
C53	0.3138(9)	0.2627(5)	1.0319(4)	0.033(2)
H53	0.2492	0.2413	1.0081	0.040
C54	0.4103(11)	0.2905(6)	0.9857(4)	0.047(3)
H54A	0.3656	0.3319	0.9576	0.071
H54B	0.4542	0.2459	0.9604	0.071
H54C	0.4734	0.3116	1.0090	0.071
C55	0.2449(11)	0.3323(5)	1.0719(4)	0.048(3)
H55A	0.1827	0.3140	1.1018	0.072
H55B	0.2001	0.3739	1.0441	0.072
H55C	0.3081	0.3532	1.0954	0.072
N61	0.2073(7)	0.1295(4)	1.1146(3)	0.0298(16)
H61	0.2133	0.1088	1.0768	0.036
C61	0.1101(8)	0.1126(5)	1.1590(4)	0.0286(19)
C62	0.1665(8)	0.0806(5)	1.2225(4)	0.031(2)
O62	0.1195(6)	0.0995(3)	1.2728(3)	0.0370(15)
C63	0.0449(9)	0.0499(6)	1.1319(4)	0.037(2)
H63A	-0.0221	0.0379	1.1622	0.056
H63B	0.1087	0.0017	1.1242	0.056
H63C	0.0061	0.0697	1.0921	0.056
C64	0.0078(8)	0.1875(5)	1.1710(4)	0.035(2)
H64A	-0.0582	0.1751	1.2015	0.053
H64B	-0.0318	0.2066	1.1311	0.053
H64C	0.0485	0.2286	1.1879	0.053
N71	0.2742(7)	0.0224(4)	1.2148(3)	0.0318(17)
H71	0.3057	0.0081	1.1768	0.038
C71	0.3334(8)	-0.0141(5)	1.2707(4)	0.0289(19)
H71A	0.2662	-0.0325	1.2990	0.035
C72	0.3948(8)	0.0437(5)	1.3068(4)	0.0299(19)
O72	0.3800(6)	0.0484(4)	1.3635(3)	0.0391(15)
C73	0.4375(9)	-0.0875(5)	1.2514(4)	0.035(2)
H73	0.5019	-0.0708	1.2203	0.042
C74	0.3732(12)	-0.1497(6)	1.2219(5)	0.056(3)
H74A	0.3292	-0.1270	1.1840	0.084
H74B	0.3108	-0.1661	1.2526	0.084
H74C	0.4387	-0.1957	1.2102	0.084
C75	0.5055(11)	-0.1256(7)	1.3107(5)	0.058(3)

H75A	0.5474	-0.0871	1.3305	0.086
H75B	0.5701	-0.1717	1.2984	0.086
H75C	0.4421	-0.1422	1.3408	0.086
N81	0.4618(7)	0.0878(4)	1.2721(3)	0.0315(17)
H81	0.4697	0.0820	1.2309	0.038
C81	0.5234(10)	0.1464(7)	1.3016(4)	0.044(2)
H81A	0.5871	0.1183	1.3319	0.053
C82	0.4213(10)	0.2030(6)	1.3385(4)	0.041(2)
O82	0.4428(7)	0.2228(4)	1.3924(3)	0.0497(18)
C83	0.5937(10)	0.1883(7)	1.2517(4)	0.049(3)
H83	0.5321	0.2110	1.2186	0.059
C84	0.7047(12)	0.1305(8)	1.2201(5)	0.067(3)
H84A	0.6712	0.0871	1.2021	0.100
H84B	0.7674	0.1091	1.2517	0.100
H84C	0.7462	0.1582	1.1864	0.100
C85	0.6457(13)	0.2542(7)	1.2790(5)	0.062(3)
H85A	0.6908	0.2802	1.2455	0.094
H85B	0.7057	0.2330	1.3119	0.094
H85C	0.5749	0.2927	1.2976	0.094
N91	0.3127(8)	0.2326(4)	1.3109(3)	0.0369(18)
H91	0.3010	0.2141	1.2738	0.044
C91	0.2106(10)	0.2937(5)	1.3371(4)	0.041(2)
C92	0.1750(11)	0.2682(6)	1.4033(4)	0.047(3)
O92	0.1534(8)	0.3139(4)	1.4478(3)	0.055(2)
C93	0.0979(11)	0.3039(6)	1.2977(4)	0.046(3)
H93A	0.0300	0.3449	1.3155	0.069
H93B	0.0667	0.2540	1.2967	0.069
H93C	0.1219	0.3198	1.2546	0.069
C94	0.2622(15)	0.3714(6)	1.3395(5)	0.067(4)
H94A	0.1947	0.4129	1.3570	0.100
H94B	0.2882	0.3871	1.2967	0.100
H94C	0.3364	0.3635	1.3664	0.100
N101	0.1521(8)	0.1929(4)	1.4106(3)	0.0360(18)
H101	0.1702	0.1602	1.3789	0.043
C101	0.0986(9)	0.1660(5)	1.4697(4)	0.034(2)
H10A	0.0428	0.2135	1.4888	0.040
C102	0.1985(8)	0.1353(5)	1.5175(4)	0.033(2)
O102	0.1708(7)	0.1323(4)	1.5743(3)	0.0451(17)
C103	0.0120(10)	0.1063(6)	1.4616(4)	0.042(2)
H103	-0.0198	0.0918	1.5048	0.051
C104	0.0832(11)	0.0299(6)	1.4312(5)	0.048(3)
H10B	0.1572	0.0071	1.4562	0.073
H10C	0.1129	0.0418	1.3880	0.073
H10D	0.0251	-0.0079	1.4299	0.073
C105	-0.1038(11)	0.1450(8)	1.4255(6)	0.063(3)
H10E	-0.1598	0.1067	1.4202	0.095
H10F	-0.0755	0.1633	1.3838	0.095
H10G	-0.1512	0.1901	1.4491	0.095
N111	0.3244(7)	0.1118(4)	1.4960(3)	0.0305(16)
H111	0.3428	0.1094	1.4550	0.037
C111	0.4264(9)	0.0910(5)	1.5398(4)	0.033(2)
H11B	0.3981	0.0573	1.5750	0.039
C112	0.4573(9)	0.1661(5)	1.5672(4)	0.032(2)
O112	0.4712(6)	0.1694(4)	1.6235(3)	0.0392(15)
C113	0.5465(9)	0.0438(6)	1.5045(4)	0.038(2)
H113	0.5635	0.0727	1.4642	0.046
C114	0.5237(10)	-0.0374(6)	1.4893(5)	0.043(2)
H11C	0.4487	-0.0322	1.4631	0.064
H11D	0.5083	-0.0662	1.5287	0.064
H11E	0.5993	-0.0663	1.4662	0.064
C115	0.6637(10)	0.0354(7)	1.5453(5)	0.050(3)
H11F	0.6788	0.0879	1.5553	0.075
H11G	0.7392	0.0063	1.5222	0.075
H11H	0.6482	0.0064	1.5847	0.075
N121	0.4709(7)	0.2256(4)	1.5261(3)	0.0334(17)
H121	0.4653	0.2186	1.4853	0.040
C121	0.4946(9)	0.3016(5)	1.5471(4)	0.037(2)
C122	0.6068(10)	0.2895(6)	1.5910(5)	0.044(2)
O122	0.6103(7)	0.3296(4)	1.6359(3)	0.0510(18)
C123	0.3731(11)	0.3475(7)	1.5798(5)	0.055(3)
H12A	0.3895	0.3982	1.5937	0.082
H12B	0.3483	0.3168	1.6165	0.082
H12C	0.3034	0.3569	1.5501	0.082
C124	0.5346(11)	0.3456(7)	1.4880(5)	0.050(3)
H12D	0.5516	0.3971	1.4999	0.074
H12E	0.4655	0.3534	1.4581	0.074
H12F	0.6126	0.3146	1.4682	0.074
O125	0.7015(7)	0.2317(4)	1.5722(3)	0.0475(17)
C125	0.8110(11)	0.2155(8)	1.6128(6)	0.064(3)
H12G	0.8755	0.1723	1.5953	0.097
H12H	0.7825	0.2002	1.6553	0.097
H12I	0.8487	0.2630	1.6151	0.097

Molecule-B

C1	-0.1022(10)	0.8202(6)	0.1709(5)	0.044(2)
C2	-0.2123(10)	0.8869(7)	0.1883(5)	0.053(3)
H2A	-0.1839	0.9377	0.1820	0.079
H2B	-0.2394	0.8807	0.2328	0.079
H2C	-0.2845	0.8856	0.1615	0.079
C3	0.0144(10)	0.8203(6)	0.2073(6)	0.054(3)
H3A	0.0430	0.8709	0.2001	0.081
H3B	0.0829	0.7771	0.1931	0.081
H3C	-0.0057	0.8129	0.2525	0.081
C4	-0.0683(11)	0.8216(7)	0.1008(5)	0.055(3)
H4A	-0.0370	0.8704	0.0893	0.083
H4B	-0.1448	0.8195	0.0772	0.083
H4C	-0.0012	0.7759	0.0905	0.083
O1	-0.1479(6)	0.7432(4)	0.1811(3)	0.0408(15)
C5	-0.1808(9)	0.7194(6)	0.2398(4)	0.040(2)
O5	-0.1835(6)	0.7552(4)	0.2864(3)	0.0406(16)
N11	-0.2121(8)	0.6468(5)	0.2368(3)	0.0401(19)
H11	-0.2071	0.6228	0.2005	0.048
C11	-0.2542(9)	0.6094(5)	0.2946(4)	0.036(2)
H11A	-0.3332	0.6445	0.3120	0.043
C12	-0.1530(9)	0.5997(5)	0.3447(4)	0.033(2)
O12	-0.1930(6)	0.5998(3)	0.4001(3)	0.0371(15)
C13	-0.2910(10)	0.5285(6)	0.2792(4)	0.043(2)
H13	-0.2262	0.5027	0.2468	0.052
C14	-0.4179(12)	0.5436(9)	0.2496(5)	0.071(4)
H14A	-0.4157	0.5802	0.2133	0.107
H14B	-0.4845	0.5670	0.2806	0.107
H14C	-0.4369	0.4937	0.2353	0.107
C15	-0.2876(15)	0.4731(9)	0.3350(6)	0.078(4)
H15A	-0.2025	0.4649	0.3530	0.116
H15B	-0.3052	0.4223	0.3217	0.116
H15C	-0.3528	0.4956	0.3671	0.116
N21	-0.0309(7)	0.5954(4)	0.3282(3)	0.0340(17)
H21	-0.0060	0.5939	0.2879	0.041
C21	0.0619(9)	0.5932(5)	0.3757(4)	0.035(2)
H21A	0.0604	0.5435	0.4012	0.042
C22	0.0266(9)	0.6588(5)	0.4203(4)	0.037(2)
O22	0.0556(6)	0.6480(4)	0.4771(3)	0.0389(15)
C23	0.1955(9)	0.5860(6)	0.3475(5)	0.046(2)
H23	0.2091	0.5424	0.3165	0.055
C24	0.2956(10)	0.5634(7)	0.3987(5)	0.056(3)
H24A	0.3821	0.5590	0.3792	0.084
H24B	0.2861	0.5126	0.4186	0.084
H24C	0.2821	0.6042	0.4309	0.084
C25	0.2205(11)	0.6605(7)	0.3124(6)	0.062(3)
H25A	0.3093	0.6517	0.2953	0.093
H25B	0.2068	0.7045	0.3417	0.093
H25C	0.1616	0.6731	0.2777	0.093
N31	-0.0308(7)	0.7295(4)	0.3985(3)	0.0306(16)
H31	-0.0487	0.7352	0.3583	0.037
C31	-0.0657(8)	0.7990(5)	0.4399(4)	0.031(2)
C32	-0.1539(8)	0.7774(5)	0.4954(4)	0.031(2)
O32	-0.1442(6)	0.8009(4)	0.5492(3)	0.0420(16)
C33	-0.1416(10)	0.8652(5)	0.4000(4)	0.039(2)
H33A	-0.1667	0.9125	0.4255	0.059
H33B	-0.2186	0.8486	0.3856	0.059
H33C	-0.0882	0.8771	0.3633	0.059
C34	0.0523(9)	0.8236(6)	0.4623(5)	0.041(2)
H34A	0.0273	0.8694	0.4895	0.061
H34B	0.1045	0.8376	0.4258	0.061

H34C	0.1023	0.7799	0.4864	0.061
N41	-0.2472(6)	0.7392(4)	0.4816(3)	0.0289(16)
H41	-0.2555	0.7289	0.4417	0.035
C41	-0.3345(8)	0.7138(5)	0.5282(4)	0.0310(19)
H41A	-0.3719	0.7603	0.5547	0.037
C42	-0.2646(8)	0.6485(5)	0.5725(4)	0.0247(17)
O42	-0.2803(6)	0.6507(3)	0.6298(3)	0.0319(13)
C43	-0.4437(9)	0.6864(5)	0.4982(4)	0.037(2)
H43	-0.4057	0.6481	0.4647	0.044
C44	-0.5217(9)	0.6437(6)	0.5446(5)	0.043(2)
H44A	-0.5912	0.6272	0.5226	0.065
H44B	-0.5583	0.6793	0.5787	0.065
H44C	-0.4661	0.5971	0.5624	0.065
C45	-0.5288(10)	0.7554(6)	0.4657(5)	0.054(3)
H45A	-0.5994	0.7367	0.4464	0.080
H45B	-0.4781	0.7785	0.4329	0.080
H45C	-0.5639	0.7954	0.4970	0.080
N51	-0.1910(7)	0.5874(4)	0.5446(3)	0.0296(16)
H51	-0.1807	0.5871	0.5031	0.036
C51	-0.1272(8)	0.5207(5)	0.5824(4)	0.0272(18)
H51A	-0.1942	0.4989	0.6083	0.033
C52	-0.0389(7)	0.5485(5)	0.6267(4)	0.029(2)
O52	-0.0284(6)	0.5192(3)	0.6806(3)	0.0308(13)
C53	-0.0529(8)	0.4543(5)	0.5396(4)	0.032(2)
H53	0.0091	0.4766	0.5107	0.039
C54	0.0210(10)	0.3882(5)	0.5807(4)	0.041(2)
H54A	0.0811	0.4097	0.6059	0.061
H54B	0.0689	0.3468	0.5535	0.061
H54C	-0.0394	0.3659	0.6090	0.061
C55	-0.1463(10)	0.4215(6)	0.5004(5)	0.046(2)
H55A	-0.1935	0.4641	0.4741	0.068
H55B	-0.2070	0.3992	0.5285	0.068
H55C	-0.0987	0.3801	0.4731	0.068
N61	0.0283(6)	0.6031(4)	0.6057(3)	0.0307(16)
H61	0.0199	0.6203	0.5662	0.037
C61	0.1138(8)	0.6352(5)	0.6443(4)	0.033(2)
C62	0.0476(8)	0.6585(5)	0.7079(4)	0.0286(19)
O62	0.0927(6)	0.6440(4)	0.7592(3)	0.0380(15)
C63	0.2355(9)	0.5727(6)	0.6554(4)	0.038(2)
H63A	0.2932	0.5948	0.6816	0.057
H63B	0.2793	0.5573	0.6147	0.057
H63C	0.2114	0.5262	0.6771	0.057
C64	0.1518(9)	0.7078(5)	0.6115(4)	0.038(2)
H64A	0.2098	0.7292	0.6380	0.058
H64B	0.0747	0.7479	0.6048	0.058
H64C	0.1953	0.6930	0.5706	0.058
N71	-0.0738(7)	0.7061(4)	0.7024(3)	0.0319(17)
H71	-0.1062	0.7182	0.6650	0.038
C71	-0.1454(8)	0.7352(5)	0.7602(4)	0.032(2)
H71A	-0.0877	0.7611	0.7851	0.038
C72	-0.1836(8)	0.6703(5)	0.8008(4)	0.0270(18)
O72	-0.1719(6)	0.6673(4)	0.8575(3)	0.0385(15)
C73	-0.2631(9)	0.7999(5)	0.7425(4)	0.039(2)
H73	-0.3171	0.7758	0.7141	0.047
C74	-0.3423(12)	0.8252(7)	0.8016(5)	0.059(3)
H74A	-0.3667	0.7788	0.8233	0.088
H74B	-0.4198	0.8627	0.7904	0.088
H74C	-0.2920	0.8505	0.8296	0.088
C75	-0.2234(12)	0.8700(6)	0.7075(5)	0.055(3)
H75A	-0.1720	0.8520	0.6692	0.082
H75B	-0.1723	0.8956	0.7349	0.082
H75C	-0.3001	0.9079	0.6957	0.082
N81	-0.2355(7)	0.6157(4)	0.7705(3)	0.0330(17)
H81	-0.2479	0.6205	0.7296	0.040
C81	-0.2696(9)	0.5497(5)	0.8073(4)	0.035(2)
H81A	-0.3419	0.5709	0.8378	0.042
C82	-0.1584(10)	0.5060(5)	0.8451(4)	0.036(2)
O82	-0.1718(7)	0.4878(4)	0.8999(3)	0.0488(18)
C83	-0.3171(10)	0.4922(6)	0.7631(4)	0.045(2)
H83	-0.2494	0.4760	0.7291	0.054
C84	-0.4406(11)	0.5342(8)	0.7322(5)	0.065(3)
H84A	-0.4240	0.5816	0.7088	0.097
H84B	-0.5082	0.5495	0.7651	0.097
H84C	-0.4685	0.4984	0.7030	0.097
C85	-0.3417(13)	0.4190(8)	0.7993(6)	0.069(4)
H85A	-0.2626	0.3925	0.8189	0.104
H85B	-0.3694	0.3830	0.7702	0.104
H85C	-0.4091	0.4341	0.8323	0.104
N91	-0.0447(8)	0.4880(4)	0.8117(3)	0.0353(18)
H91	-0.0395	0.5053	0.7723	0.042
C91	0.0697(10)	0.4404(5)	0.8394(4)	0.041(2)
C92	0.1022(10)	0.4794(5)	0.8998(4)	0.041(2)
O92	0.1362(9)	0.4373(5)	0.9462(3)	0.069(2)
C93	0.1850(10)	0.4408(6)	0.7921(5)	0.046(2)
H93A	0.2625	0.4093	0.8097	0.069
H93B	0.1975	0.4953	0.7844	0.069
H93C	0.1680	0.4182	0.7521	0.069
C94	0.0493(14)	0.3561(6)	0.8559(5)	0.065(3)
H94A	0.1270	0.3256	0.8743	0.098
H94B	0.0314	0.3306	0.8174	0.098
H94C	-0.0234	0.3581	0.8865	0.098
N101	0.0923(7)	0.5567(5)	0.8970(4)	0.0396(19)
H101	0.0594	0.5842	0.8639	0.048
C101	0.1368(10)	0.5967(6)	0.9499(5)	0.050(3)
H10A	0.2099	0.5587	0.9681	0.059
C102	0.0353(11)	0.6149(6)	1.0023(5)	0.049(3)
O102	0.0701(8)	0.6234(5)	1.0557(4)	0.072(2)
C103	0.1911(10)	0.6714(7)	0.9271(6)	0.061(3)
H103	0.2238	0.6941	0.9646	0.074
C104	0.0880(11)	0.7319(7)	0.9004(6)	0.063(3)
H10B	0.0185	0.7459	0.9325	0.095
H10C	0.0547	0.7108	0.8635	0.095
H10D	0.1228	0.7791	0.8876	0.095
C105	0.3060(12)	0.6455(8)	0.8794(6)	0.068(3)
H10E	0.3709	0.6056	0.8995	0.102
H10F	0.3438	0.6915	0.8663	0.102
H10G	0.2758	0.6231	0.8422	0.102
N111	-0.0877(8)	0.6205(5)	0.9902(3)	0.042(2)
H111	-0.1091	0.6146	0.9512	0.050
C111	-0.1876(10)	0.6360(6)	1.0399(4)	0.043(2)
H11B	-0.1517	0.6642	1.0734	0.052
C112	-0.2204(10)	0.5615(6)	1.0717(4)	0.043(3)
O112	-0.2530(7)	0.5614(4)	1.1277(3)	0.0457(17)
C113	-0.3071(12)	0.6952(8)	1.0154(5)	0.065(3)
H113	-0.2743	0.7378	0.9902	0.078
C114	-0.3773(13)	0.6582(7)	0.9751(6)	0.071(4)
H11C	-0.3204	0.6338	0.9405	0.107
H11D	-0.4467	0.6975	0.9577	0.107
H11E	-0.4140	0.6175	0.9990	0.107
C115	-0.3870(16)	0.7323(10)	1.0675(7)	0.093(5)
H11F	-0.3350	0.7575	1.0947	0.139
H11G	-0.4237	0.6922	1.0922	0.139
H11H	-0.4565	0.7723	1.0509	0.139
N121	-0.2120(9)	0.4973(5)	1.0354(4)	0.051(2)
H121	-0.1894	0.5003	0.9950	0.062
C121	-0.2397(12)	0.4239(6)	1.0623(5)	0.055(3)
C122	-0.3792(14)	0.4382(7)	1.0930(6)	0.064(3)
O122	-0.4156(11)	0.3986(6)	1.1326(5)	0.096(3)
C123	-0.2419(16)	0.3700(8)	1.0072(6)	0.085(4)
H12A	-0.2605	0.3192	1.0232	0.127
H12B	-0.1582	0.3615	0.9844	0.127
H12C	-0.3086	0.3945	0.9785	0.127
C124	-0.1546(13)	0.3860(7)	1.1118(7)	0.076(4)
H12D	-0.1816	0.3370	1.1267	0.115
H12E	-0.1596	0.4219	1.1472	0.115
H12F	-0.0661	0.3740	1.0944	0.115
O125	-0.4540(9)	0.4950(5)	1.0597(5)	0.082(3)
C125	-0.5889(17)	0.5130(12)	1.0844(10)	0.115(6)
H12G	-0.6379	0.5547	1.0581	0.172
H12H	-0.5915	0.5307	1.1281	0.172
H12I	-0.6267	0.4653	1.0834	0.172

Table S3. Bond lengths (Å) & angles (°)*.

Lengths

Solvents

O1M	- C1M	1.460(12)
O2M	- C2M	1.339(17)
O3M	- C3M	1.62(4)

Molecule A

C1	- C2	1.517(14)
C1	- C3	1.508(13)
C1	- C4	1.531(13)
C1	- O1	1.471(12)
O1	- C5	1.312(11)
C5	- O5	1.234(10)
C5	- N11	1.362(12)
N11	- C11	1.463(11)
C11	- C12	1.508(12)
C11	- C13	1.524(14)
C12	- O12	1.221(11)
C12	- N21	1.324(11)
C13	- C14	1.531(13)
C13	- C15	1.506(15)
N21	- C21	1.440(11)
C21	- C22	1.521(11)
C21	- C23	1.554(13)
C22	- O22	1.230(9)
C22	- N31	1.332(10)
C23	- C24	1.509(16)
C23	- C25	1.501(12)
N31	- C31	1.481(11)
C31	- C32	1.517(13)
C31	- C33	1.521(12)
C31	- C34	1.516(14)
C32	- O32	1.237(11)
C32	- N41	1.333(12)
N41	- C41	1.459(12)
C41	- C42	1.493(12)
C41	- C43	1.528(13)
C42	- O42	1.211(11)
C42	- N51	1.359(10)
C43	- C44	1.515(14)
C43	- C45	1.521(14)
N51	- C51	1.461(11)
C51	- C52	1.537(12)
C51	- C53	1.520(12)
C52	- O52	1.199(11)
C52	- N61	1.361(12)
C53	- C54	1.515(14)
C53	- C55	1.538(12)
N61	- C61	1.427(11)
C61	- C62	1.541(12)
C61	- C63	1.527(14)
C61	- C64	1.542(11)
C62	- O62	1.183(10)
C62	- N71	1.379(10)
N71	- C71	1.437(11)
C71	- C72	1.529(13)
C71	- C73	1.566(11)
C72	- O72	1.206(11)
C72	- N81	1.319(12)
C73	- C74	1.537(16)
C73	- C75	1.543(14)
N81	- C81	1.471(14)
C81	- C82	1.519(13)
C81	- C83	1.508(15)
C82	- O82	1.244(11)
C82	- N91	1.324(13)
C83	- C84	1.534(15)
C83	- C85	1.495(18)
N91	- C91	1.464(11)
C91	- C92	1.507(12)
C91	- C93	1.470(15)
C91	- C94	1.542(16)
C92	- O92	1.232(11)
C92	- N101	1.367(13)
N101	- C101	1.448(11)
C101	- C102	1.511(12)
C101	- C103	1.521(15)
C102	- O102	1.226(11)
C102	- N111	1.381(11)
C103	- C104	1.534(14)
C103	- C105	1.512(15)
N111	- C111	1.445(11)
C111	- C112	1.531(13)
C111	- C113	1.550(12)
C112	- O112	1.212(11)
C112	- N121	1.348(11)
C113	- C114	1.511(15)
C113	- C115	1.529(14)
N121	- C121	1.465(12)
C121	- C122	1.524(14)
C121	- C123	1.528(14)
C121	- C124	1.526(14)
C122	- O122	1.198(13)
C122	- O125	1.331(12)
O125	- C125	1.457(14)

Molecule B

C1	- C2	1.518(14)
C1	- C3	1.488(16)
C1	- C4	1.510(15)
C1	- O1	1.502(13)
O1	- C5	1.347(11)
C5	- O5	1.176(11)
C5	- N11	1.357(14)
N11	- C11	1.455(11)
C11	- C12	1.528(13)
C11	- C13	1.564(14)
C12	- O12	1.228(11)
C12	- N21	1.315(12)
C13	- C14	1.487(16)
C13	- C15	1.492(16)
N21	- C21	1.435(12)
C21	- C22	1.478(12)
C21	- C23	1.497(13)
C22	- O22	1.254(11)
C22	- N31	1.334(10)
C23	- C24	1.543(15)
C23	- C25	1.523(16)
N31	- C31	1.486(11)
C31	- C32	1.547(12)
C31	- C33	1.524(12)
C31	- C34	1.497(14)
C32	- O32	1.236(11)
C32	- N41	1.335(12)
N41	- C41	1.436(11)
C41	- C42	1.543(11)
C41	- C43	1.504(14)
C42	- O42	1.217(11)
C42	- N51	1.324(10)
C43	- C44	1.516(14)
C43	- C45	1.519(13)
N51	- C51	1.456(10)
C51	- C52	1.505(13)
C51	- C53	1.553(11)
C52	- O52	1.234(10)
C52	- N61	1.337(11)
C53	- C54	1.528(12)
C53	- C55	1.519(15)
N61	- C61	1.443(12)
C61	- C62	1.518(12)
C61	- C63	1.541(12)
C61	- C64	1.522(13)
C62	- O62	1.207(11)
C62	- N71	1.399(10)
N71	- C71	1.461(10)
C71	- C72	1.493(12)
C71	- C73	1.561(11)
C72	- O72	1.211(11)
C72	- N81	1.366(12)
C73	- C74	1.503(14)
C73	- C75	1.513(14)
N81	- C81	1.450(11)
C81	- C82	1.522(13)
C81	- C83	1.550(14)
C82	- O82	1.201(11)
C82	- N91	1.358(12)
C83	- C84	1.537(15)
C83	- C85	1.513(17)
N91	- C91	1.467(12)
C91	- C92	1.545(13)
C91	- C93	1.545(14)
C91	- C94	1.536(14)
C92	- O92	1.229(11)
C92	- N101	1.316(12)
N101	- C101	1.474(14)
C101	- C102	1.507(15)
C101	- C103	1.560(17)
C102	- O102	1.227(14)
C102	- N111	1.327(15)
C103	- C104	1.482(15)
C103	- C105	1.553(16)
N111	- C111	1.452(12)
C111	- C112	1.521(15)
C111	- C113	1.569(15)
C112	- O112	1.219(11)
C112	- N121	1.354(13)
C113	- C114	1.401(19)
C113	- C115	1.448(19)
N121	- C121	1.445(14)
C121	- C122	1.567(19)
C121	- C123	1.517(17)
C121	- C124	1.471(18)
C122	- O122	1.162(17)
C122	- O125	1.342(15)
O125	- C125	1.48(2)

Angles

Molecule A

C2	-C1	-C3	112.1(8)
C2	-C1	-C4	110.0(8)
C2	-C1	-O1	101.8(7)
C3	-C1	-C4	112.3(8)
C3	-C1	-O1	109.2(7)
C4	-C1	-O1	111.1(7)
C1	-O1	-C5	121.1(7)
O1	-C5	-O5	125.3(8)
O1	-C5	-N11	111.1(8)
O5	-C5	-N11	123.6(8)
C5	-N11	-C11	119.5(7)
N11	-C11	-C12	113.6(7)
N11	-C11	-C13	108.7(7)
C12	-C11	-C13	111.8(7)
C11	-C12	-O12	119.4(8)
C11	-C12	-N21	118.8(8)
O12	-C12	-N21	121.8(8)
C11	-C13	-C14	112.7(8)
C11	-C13	-C15	112.1(8)
C14	-C13	-C15	109.7(8)
C12	-N21	-C21	120.8(7)
N21	-C21	-C22	111.2(7)
N21	-C21	-C23	111.8(7)
C22	-C21	-C23	109.7(7)
C21	-C22	-O22	119.3(6)
C21	-C22	-N31	118.8(7)
O22	-C22	-N31	121.9(7)
C21	-C23	-C24	112.6(8)
C21	-C23	-C25	110.0(8)
C24	-C23	-C25	111.9(8)
C22	-N31	-C31	122.4(7)
N31	-C31	-C32	108.9(7)
N31	-C31	-C33	107.7(7)
N31	-C31	-C34	111.1(7)
C32	-C31	-C33	107.3(7)
C32	-C31	-C34	111.4(8)
C33	-C31	-C34	110.4(8)
C31	-C32	-O32	121.6(8)
C31	-C32	-N41	116.5(8)
O32	-C32	-N41	121.9(8)
C32	-N41	-C41	122.4(8)
N41	-C41	-C42	111.1(7)
N41	-C41	-C43	110.1(7)
C42	-C41	-C43	111.9(7)
C41	-C42	-O42	122.7(8)
C41	-C42	-N51	115.3(8)
O42	-C42	-N51	121.9(8)
C41	-C43	-C44	110.6(7)
C41	-C43	-C45	111.9(7)
C44	-C43	-C45	111.2(8)
C42	-N51	-C51	121.2(7)
N51	-C51	-C52	109.3(7)
N51	-C51	-C53	111.2(7)
C52	-C51	-C53	111.2(7)
C51	-C52	-O52	121.2(8)
C51	-C52	-N61	117.8(7)
O52	-C52	-N61	120.9(8)
C51	-C53	-C54	109.8(7)
C51	-C53	-C55	109.0(7)
C54	-C53	-C55	109.7(8)
C52	-N61	-C61	121.9(7)
N61	-C61	-C62	111.7(7)
N61	-C61	-C63	108.9(7)
N61	-C61	-C64	110.4(7)
C62	-C61	-C63	108.2(7)
C62	-C61	-C64	109.0(7)
C63	-C61	-C64	108.5(7)
C61	-C62	-O62	124.6(8)
C61	-C62	-N71	112.6(7)
O62	-C62	-N71	122.7(8)
C62	-N71	-C71	117.9(7)
N71	-C71	-C72	111.6(7)
N71	-C71	-C73	109.1(7)
C72	-C71	-C73	109.9(7)
C71	-C72	-O72	120.9(8)
C71	-C72	-N81	116.0(7)
O72	-C72	-N81	123.2(8)
C71	-C73	-C74	109.8(7)
C71	-C73	-C75	109.8(8)
C74	-C73	-C75	107.8(8)
C72	-N81	-C81	120.7(8)
N81	-C81	-C82	108.7(8)
N81	-C81	-C83	110.0(9)
C82	-C81	-C83	112.4(8)
C81	-C82	-O82	119.9(8)
C81	-C82	-N91	118.4(9)
O82	-C82	-N91	121.6(8)
C81	-C83	-C84	110.8(8)
C81	-C83	-C85	111.4(10)
C84	-C83	-C85	109.0(9)
C82	-N91	-C91	125.3(8)
N91	-C91	-C92	108.4(7)
N91	-C91	-C93	109.9(8)
N91	-C91	-C94	108.5(7)

C92 -C91 -C93	109.8(7)	C32 -C31 -C33	108.8(7)	O102-C102-N111	121.8(10)
C92 -C91 -C94	109.4(8)	C32 -C31 -C34	112.2(7)	C101-C103-C104	110.3(10)
C93 -C91 -C94	110.8(9)	C33 -C31 -C34	110.1(8)	C101-C103-C105	108.6(9)
C91 -C92 -O92	123.1(8)	C31 -C32 -O32	120.4(8)	C104-C103-C105	113.1(10)
C91 -C92 -N101	116.3(8)	C31 -C32 -N41	117.4(7)	C102-N111-C111	121.4(9)
O92 -C92 -N101	120.2(9)	O32 -C32 -N41	121.9(8)	N111-C111-C112	113.6(8)
C92 -N101-C101	121.0(7)	C32 -N41 -C41	123.7(7)	N111-C111-C113	110.5(9)
N101-C101-C102	113.5(7)	N41 -C41 -C42	111.4(7)	C112-C111-C113	113.9(9)
N101-C101-C103	113.7(8)	N41 -C41 -C43	111.7(7)	C111-C112-O112	119.9(8)
C102-C101-C103	110.3(8)	C42 -C41 -C43	110.4(7)	C111-C112-N121	117.4(9)
C101-C102-O102	121.8(8)	C41 -C42 -O42	122.3(8)	O112-C112-N121	122.7(8)
C101-C102-N111	118.4(8)	C41 -C42 -N51	116.2(7)	C111-C113-C114	111.3(10)
O102-C102-N111	119.8(8)	O42 -C42 -N51	121.4(8)	C111-C113-C115	111.2(11)
C101-C103-C104	112.7(8)	C41 -C43 -C44	112.9(8)	C114-C113-C115	111.7(11)
C101-C103-C105	109.3(9)	C41 -C43 -C45	110.3(8)	C112-N121-C121	120.7(9)
C104-C103-C105	112.5(9)	C44 -C43 -C45	111.0(8)	N121-C121-C122	109.6(9)
C102-N111-C111	120.9(7)	C42 -N51 -C51	120.2(7)	N121-C121-C123	106.4(9)
N111-C111-C112	109.7(7)	N51 -C51 -C52	109.6(7)	N121-C121-C124	116.1(9)
N111-C111-C113	109.0(7)	N51 -C51 -C53	111.1(7)	C122-C121-C123	105.7(10)
C112-C111-C113	110.5(7)	C52 -C51 -C53	111.1(7)	C122-C121-C124	106.2(10)
C111-C112-O112	119.9(8)	C51 -C52 -O52	119.3(8)	C123-C121-C124	112.3(10)
C111-C112-N121	117.2(7)	C51 -C52 -N61	118.7(7)	C121-C122-O122	124.9(13)
O112-C112-N121	122.9(8)	O52 -C52 -N61	122.0(8)	C121-C122-O125	109.1(11)
C111-C113-C114	110.0(8)	C51 -C53 -C54	109.6(7)	O122-C122-O125	125.2(12)
C111-C113-C115	110.3(8)	C51 -C53 -C55	109.9(7)	C122-O125-C125	113.7(12)
C114-C113-C115	109.2(8)	C54 -C53 -C55	109.7(8)		
C112-N121-C121	122.0(7)	C52 -N61 -C61	123.5(7)		
N121-C121-C122	110.8(7)	N61 -C61 -C62	109.8(7)		
N121-C121-C123	109.9(7)	N61 -C61 -C63	109.8(7)		
N121-C121-C124	106.6(7)	N61 -C61 -C64	110.0(7)		
C122-C121-C123	110.8(8)	C62 -C61 -C63	108.8(7)		
C122-C121-C124	107.1(8)	C62 -C61 -C64	109.1(7)		
C123-C121-C124	111.6(8)	C63 -C61 -C64	109.2(7)		
C121-C122-O122	123.4(9)	C61 -C62 -O62	126.5(8)		
C121-C122-O125	112.2(9)	C61 -C62 -N71	112.9(7)		
O122-C122-O125	124.3(9)	O62 -C62 -N71	120.3(8)		
C122-O125-C125	115.3(8)	C62 -N71 -C71	118.3(7)		
Molecule B		N71 -C71 -C72	112.5(7)		
C2 -C1 -C3	113.1(9)	N71 -C71 -C73	109.3(7)		
C2 -C1 -C4	111.3(9)	C72 -C71 -C73	112.3(7)		
C2 -C1 -O1	108.4(8)	C71 -C72 -O72	121.9(8)		
C3 -C1 -C4	109.9(9)	C71 -C72 -N81	116.2(7)		
C3 -C1 -O1	110.5(8)	O72 -C72 -N81	122.0(8)		
C4 -C1 -O1	103.2(8)	C71 -C73 -C74	109.1(8)		
C1 -O1 -C5	120.3(7)	C71 -C73 -C75	112.3(7)		
O1 -C5 -O5	126.3(8)	C74 -C73 -C75	111.1(8)		
O1 -C5 -N11	108.9(8)	C72 -N81 -C81	118.4(7)		
O5 -C5 -N11	124.8(9)	N81 -C81 -C82	112.2(7)		
C5 -N11 -C11	119.0(8)	N81 -C81 -C83	109.8(7)		
N11 -C11 -C12	111.7(7)	C82 -C81 -C83	110.3(8)		
N11 -C11 -C13	109.9(7)	C81 -C82 -O82	122.1(8)		
C12 -C11 -C13	111.7(7)	C81 -C82 -N91	114.8(8)		
C11 -C12 -O12	116.3(8)	O82 -C82 -N91	123.1(8)		
C11 -C12 -N21	120.7(8)	C81 -C83 -C84	109.7(8)		
O12 -C12 -N21	122.9(8)	C81 -C83 -C85	111.0(9)		
C11 -C13 -C14	109.0(9)	C84 -C83 -C85	109.9(9)		
C11 -C13 -C15	113.4(9)	C82 -N91 -C91	121.9(8)		
C14 -C13 -C15	112.3(9)	N91 -C91 -C92	110.1(7)		
C12 -N21 -C21	120.2(8)	N91 -C91 -C93	108.2(8)		
N21 -C21 -C22	112.4(7)	N91 -C91 -C94	111.2(7)		
N21 -C21 -C23	112.0(8)	C92 -C91 -C93	106.1(7)		
C22 -C21 -C23	113.3(8)	C92 -C91 -C94	109.3(7)		
C21 -C22 -O22	119.7(8)	C93 -C91 -C94	111.8(8)		
C21 -C22 -N31	119.0(8)	C91 -C92 -O92	119.0(8)		
O22 -C22 -N31	121.3(8)	C91 -C92 -N101	116.3(8)		
C21 -C23 -C24	110.9(8)	O92 -C92 -N101	124.7(9)		
C21 -C23 -C25	113.7(9)	C92 -N101-C101	119.2(8)		
C24 -C23 -C25	108.8(9)	N101-C101-C102	112.2(9)		
C22 -N31 -C31	122.3(7)	N101-C101-C103	112.0(9)		
N31 -C31 -C32	108.3(7)	C102-C101-C103	112.1(9)		
N31 -C31 -C33	106.6(7)	C101-C102-O102	118.1(10)		
N31 -C31 -C34	110.7(7)	C101-C102-N111	120.1(10)		

*PARST: Nardelli, M. (1995). J. Appl. Cryst. 28, 659.

Table S4. Torsion angles (°)*.

Molecule A

C5	O1	C1	C2	175.7(8)	C5	O1	C1	C3	-65.7(10)	C5	O1	C1	C4	58.7(10)
C1	O1	C5	O5	-2.0(14)	C1	O1	C5	N11	175.4(7)	C125	O125	C122	O122	3.9(15)
C125	O125	C122	C121	-178.6(8)	O1	C5	N11	C11	-178.8(7)	O5	C5	N11	C11	-1.4(13)
C12	C11	N11	C5	-57.7(10)	C13	C11	N11	C5	177.1(8)	N11	C11	C12	O12	158.1(8)
N11	C11	C12	N21	-20.5(11)	C13	C11	C12	O12	-78.5(10)	C13	C11	C12	N21	103.0(9)
N11	C11	C13	C14	75.4(9)	N11	C11	C13	C15	-160.3(8)	C12	C11	C13	C14	-50.8(9)
C12	C11	C13	C15	73.5(10)	O12	C12	N21	C21	-0.3(13)	C11	C12	N21	C21	178.2(7)
C22	C21	N21	C12	-56.1(10)	C23	C21	N21	C12	-179.0(7)	N21	C21	C22	O22	148.8(8)
N21	C21	C22	N31	-30.2(11)	C23	C21	C22	O22	-87.1(9)	C23	C21	C22	N31	93.9(9)
N21	C21	C23	C24	65.4(9)	N21	C21	C23	C25	-169.0(7)	C22	C21	C23	C24	-58.3(9)
C22	C21	C23	C25	67.2(9)	O22	C22	N31	C31	0.7(13)	C21	C22	N31	C31	179.7(7)
C32	C31	N31	C22	-57.6(10)	C33	C31	N31	C22	-173.7(8)	C34	C31	N31	C22	65.4(10)
N31	C31	C32	O32	139.0(8)	N31	C31	C32	N41	-43.4(10)	C33	C31	C32	O32	-104.8(9)
C33	C31	C32	N41	72.8(9)	C34	C31	C32	O32	16.1(12)	C34	C31	C32	N41	-166.3(8)
O32	C32	N41	C41	-1.9(13)	C31	C32	N41	C41	-179.5(8)	C42	C41	N41	C32	-70.1(10)
C43	C41	N41	C32	165.5(8)	N41	C41	C42	O42	131.3(9)	N41	C41	C42	N51	-51.6(10)
C43	C41	C42	O42	-105.2(10)	C43	C41	C42	N51	71.8(10)	N41	C41	C43	C44	175.3(8)
N41	C41	C43	C45	-60.1(10)	C42	C41	C43	C44	51.3(10)	C42	C41	C43	C45	175.9(7)
O42	C42	N51	C51	0.3(13)	C41	C42	N51	C51	-176.8(7)	C52	C51	N51	C42	-54.7(10)
C53	C51	N51	C42	-177.9(8)	N51	C51	C52	O52	138.1(8)	N51	C51	C52	N61	-45.4(10)
C53	C51	C52	O52	-98.8(9)	C53	C51	C52	N61	77.8(9)	N51	C51	C53	C54	-65.8(9)
N51	C51	C53	C55	174.0(8)	C52	C51	C53	C54	172.1(7)	C52	C51	C53	C55	51.9(10)
O52	C52	N61	C61	3.0(12)	C51	C52	N61	C61	-173.6(7)	C62	C61	N61	C52	-53.2(10)
C63	C61	N61	C52	-172.6(8)	C64	C61	N61	C52	68.3(10)	N61	C61	C62	O62	137.8(9)
N61	C61	C62	N71	-46.7(10)	C63	C61	C62	O62	-102.3(10)	C63	C61	C62	N71	73.2(9)
C64	C61	C62	O62	15.5(12)	C64	C61	C62	N71	-169.0(7)	O62	C62	N71	C71	-2.4(12)
C61	C62	N71	C71	-178.0(7)	C72	C71	N71	C62	-68.2(10)	C73	C71	N71	C62	170.1(7)
N71	C71	C72	O72	134.9(8)	N71	C71	C72	N81	-44.1(10)	C73	C71	C72	O72	-103.9(9)
C73	C71	C72	N81	77.1(9)	N71	C71	C73	C74	-63.7(9)	N71	C71	C73	C75	177.9(8)
C72	C71	C73	C74	173.6(7)	C72	C71	C73	C75	55.3(10)	O72	C72	N81	C81	0.0(14)
C71	C72	N81	C81	179.0(8)	C82	C81	N81	C72	-56.7(11)	C83	C81	N81	C72	179.9(8)
N81	C81	C82	O82	136.2(9)	N81	C81	C82	N91	-46.6(11)	C83	C81	C82	O82	-101.9(10)
C83	C81	C82	N91	75.4(12)	N81	C81	C83	C84	-64.5(11)	N81	C81	C83	C85	173.9(9)
C82	C81	C83	C84	174.3(8)	C82	C81	C83	C85	52.7(12)	O82	C82	N91	C91	3.9(15)
C81	C82	N91	C91	-173.4(9)	C92	C91	N91	C82	-52.2(12)	C93	C91	N91	C82	-172.3(9)
C94	C91	N91	C82	66.4(11)	N91	C91	C92	O92	138.5(11)	N91	C91	C92	N101	-49.2(12)
C93	C91	C92	O92	-101.4(12)	C93	C91	C92	N101	70.9(11)	C94	C91	C92	O92	20.4(15)
C94	C91	C92	N101	-167.4(10)	O92	C92	N101	C101	1.9(15)	C91	C92	N101	C101	-170.6(9)
C102	C101	N101	C92	-85.7(11)	C103	C101	N101	C92	147.0(9)	N101	C101	C102	O102	158.1(8)
N101	C101	C102	N111	-20.6(11)	C103	C101	C102	O102	-73.0(11)	C103	C101	C102	N111	108.4(9)
N101	C101	C103	C104	62.2(10)	N101	C101	C103	C105	-63.7(10)	C102	C101	C103	C104	-66.7(9)
C102	C101	C103	C105	167.4(8)	O102	C102	N111	C111	-6.2(12)	C101	C102	N111	C111	172.5(7)
C112	C111	N111	C102	-76.0(10)	C113	C111	N111	C102	162.9(7)	N111	C111	C112	O112	134.8(9)
N111	C111	C112	N121	-46.8(11)	C113	C111	C112	O112	-105.0(10)	C113	C111	C112	N121	73.4(10)
N111	C111	C113	C114	-70.9(9)	N111	C111	C113	C115	168.5(8)	C112	C111	C113	C114	168.5(7)
C112	C111	C113	C115	47.9(10)	O112	C112	N121	C121	-4.5(14)	C111	C112	N121	C121	177.1(8)
C122	C121	N121	C112	51.2(11)	C123	C121	N121	C112	-71.7(11)	C124	C121	N121	C112	167.3(9)
N121	C121	C122	O122	-143.1(10)	N121	C121	C122	O125	39.4(11)	C123	C121	C122	O122	-20.9(14)
C123	C121	C122	O125	161.6(8)	C124	C121	C122	O122	101.1(11)	C124	C121	C122	O125	-76.5(10)

Molecule B

C5	O1	C1	C2	-65.3(11)	C5	O1	C1	C3	59.2(11)	C5	O1	C1	C4	176.6(8)
C1	O1	C5	O5	3.7(15)	C1	O1	C5	N11	-176.9(8)	C125	O125	C122	O122	9.3(19)
C125	O125	C122	C121	179.6(11)	O1	C5	N11	C11	-178.5(8)	O5	C5	N11	C11	0.9(15)
C12	C11	N11	C5	-58.2(11)	C13	C11	N11	C5	177.3(8)	N11	C11	C12	O12	151.5(8)
N11	C11	C12	N21	-25.4(11)	C13	C11	C12	O12	-85.0(9)	C13	C11	C12	N21	98.1(9)
N11	C11	C13	C14	-75.8(10)	N11	C11	C13	C15	158.4(10)	C12	C11	C13	C14	159.8(8)
C12	C11	C13	C15	33.9(12)	O12	C12	N21	C21	-2.1(12)	C11	C12	N21	C21	174.6(7)
C22	C21	N21	C12	-52.7(10)	C23	C21	N21	C12	178.4(8)	N21	C21	C22	O22	146.5(8)
N21	C21	C22	N31	-36.4(12)	C23	C21	C22	O22	-85.3(11)	C23	C21	C22	N31	91.9(11)
N21	C21	C23	C24	-166.1(8)	N21	C21	C23	C25	70.9(11)	C22	C21	C23	C24	65.4(10)
C22	C21	C23	C25	-57.7(11)	O22	C22	N31	C31	-1.0(14)	C21	C22	N31	C31	-178.1(8)
C32	C31	N31	C22	-56.9(10)	C33	C31	N31	C22	-173.9(8)	C34	C31	N31	C22	66.4(11)
N31	C31	C32	O32	142.1(8)	N31	C31	C32	N41	-43.9(10)	C33	C31	C32	O32	-102.4(9)
C33	C31	C32	N41	71.6(9)	C34	C31	C32	O32	19.7(12)	C34	C31	C32	N41	-166.3(8)
O32	C32	N41	C41	-7.5(13)	C31	C32	N41	C41	178.6(7)	C42	C41	N41	C32	-66.7(10)
C43	C41	N41	C32	169.3(8)	N41	C41	C42	O42	132.2(8)	N41	C41	C42	N51	-51.2(10)
C43	C41	C42	O42	-103.0(9)	C43	C41	C42	N51	73.6(10)	N41	C41	C43	C44	168.1(7)
N41	C41	C43	C45	-67.0(9)	C42	C41	C43	C44	43.5(10)	C42	C41	C43	C45	168.3(7)

O42	C42	N51	C51	0.3(13)	C41	C42	N51	C51	-176.4(7)	C52	C51	N51	C42	-60.1(10)
C53	C51	N51	C42	176.7(7)	N51	C51	C52	O52	142.5(8)	N51	C51	C52	N61	-39.1(10)
C53	C51	C52	O52	-94.3(9)	C53	C51	C52	N61	84.1(9)	N51	C51	C53	C54	175.7(7)
N51	C51	C53	C55	-63.6(9)	C52	C51	C53	C54	53.4(9)	C52	C51	C53	C55	174.1(7)
O52	C52	N61	C61	-2.9(12)	C51	C52	N61	C61	178.7(7)	C62	C61	N61	C52	-47.5(10)
C63	C61	N61	C52	72.2(10)	C64	C61	N61	C52	-167.6(7)	N61	C61	C62	O62	134.0(9)
N61	C61	C62	N71	-50.7(9)	C63	C61	C62	O62	13.8(12)	C63	C61	C62	N71	-171.0(7)
C64	C61	C62	O62	-105.3(10)	C64	C61	C62	N71	69.9(9)	O62	C62	N71	C71	-2.0(12)
C61	C62	N71	C71	-177.6(7)	C72	C71	N71	C62	-66.0(10)	C73	C71	N71	C62	168.5(7)
N71	C71	C72	O72	135.5(9)	N71	C71	C72	N81	-46.1(10)	C73	C71	C72	O72	-100.7(10)
C73	C71	C72	N81	77.7(9)	N71	C71	C73	C74	175.6(8)	N71	C71	C73	C75	-60.7(9)
C72	C71	C73	C74	50.0(10)	C72	C71	C73	C75	173.7(7)	O72	C72	N81	C81	-4.0(13)
C71	C72	N81	C81	177.6(7)	C82	C81	N81	C72	-52.8(10)	C83	C81	N81	C72	-175.9(8)
N81	C81	C82	O82	133.4(9)	N81	C81	C82	N91	-47.9(10)	C83	C81	C82	O82	-103.8(10)
C83	C81	C82	N91	74.9(10)	N81	C81	C83	C84	-63.6(10)	N81	C81	C83	C85	174.8(9)
C82	C81	C83	C84	172.2(8)	C82	C81	C83	C85	50.6(11)	O82	C82	N91	C91	3.7(13)
C81	C82	N91	C91	-174.9(7)	C92	C91	N91	C82	-57.0(11)	C93	C91	N91	C82	-172.5(8)
C94	C91	N91	C82	64.3(10)	N91	C91	C92	O92	138.8(10)	N91	C91	C92	N101	-41.9(12)
C93	C91	C92	O92	-104.3(11)	C93	C91	C92	N101	74.9(11)	C94	C91	C92	O92	16.4(14)
C94	C91	C92	N101	-164.3(10)	O92	C92	N101	C101	6.6(16)	C91	C92	N101	C101	-172.6(9)
C102	C101	N101	C92	-85.3(11)	C103	C101	N101	C92	147.6(9)	N101	C101	C102	O102	156.5(9)
N101	C101	C102	N111	-22.8(13)	C103	C101	C102	O102	-76.5(12)	C103	C101	C102	N111	104.3(11)
N101	C101	C103	C104	64.7(12)	N101	C101	C103	C105	-59.8(11)	C102	C101	C103	C104	-62.5(13)
C102	C101	C103	C105	173.0(9)	O102	C102	N111	C111	-0.8(15)	C101	C102	N111	C111	178.4(9)
C112	C111	N111	C102	-90.7(11)	C113	C111	N111	C102	139.8(10)	N111	C111	C112	O112	146.8(9)
N111	C111	C112	N121	-33.4(13)	C113	C111	C112	O112	-85.5(12)	C113	C111	C112	N121	94.3(11)
N111	C111	C113	C114	74.7(12)	N111	C111	C113	C115	-160.2(11)	C112	C111	C113	C114	-54.6(12)
C112	C111	C113	C115	70.5(13)	O112	C112	N121	C121	-1.1(16)	C111	C112	N121	C121	179.1(10)
C122	C121	N121	C112	57.3(13)	C123	C121	N121	C112	171.1(11)	C124	C121	N121	C112	-63.1(14)
N121	C121	C122	O122	-156.9(13)	N121	C121	C122	O125	32.8(13)	C123	C121	C122	O122	88.8(15)
C123	C121	C122	O125	-81.5(11)	C124	C121	C122	O122	-30.7(17)	C124	C121	C122	O125	159.0(10)

*PLATON: Spek, A. L. (2009). Acta Cryst. D65, 148-155.

Table S5. Hydrogen bond geometries*.

Nr	Typ	Res	Donor	---	H....Acceptor	[ARU]	D - H	H...A	D...A	D - H...A
Molecule A										
1		3	O1M_1	--H1M_1	..O102_1	[1554.01]	0.91	2.03	2.819(9)	145
2		4	O2M_1	--H2M_1	..O3M_1	[1555.05]	0.85	1.76	2.53(2)	151
3		5	O3M_1	--H3M_1	..O102_2	[1554.02]	0.85	1.77	2.53(2)	147
4		1	N11_1	--H11_1	..O112_1	[1554.01]	0.88	2.00	2.859(9)	164
5		1	N21_1	--H21_1	..O1M_1	[1555.03]	0.88	2.12	2.981(9)	167
7	Intra	1	N31_1	--H31_1	..O5_1	[ ]	0.88	2.17	3.014(9)	161
9	Intra	1	N41_1	--H41_1	..O12_1	[ ]	0.88	2.32	2.944(9)	128
11	Intra	1	N51_1	--H51_1	..O12_1	[ ]	0.88	2.23	3.099(9)	172
12	Intra	1	N61_1	--H61_1	..O22_1	[ ]	0.88	2.00	2.856(9)	162
14	Intra	1	N81_1	--H81_1	..O42_1	[ ]	0.88	2.25	3.122(9)	173
15	Intra	1	N91_1	--H91_1	..O52_1	[ ]	0.88	2.00	2.850(9)	162
17	Intra	1	N101_1	--H101_1	..N91_1	[ ]	0.88	2.51	2.799(10)	100
18	Intra	1	N111_1	--H111_1	..O72_1	[ ]	0.88	2.22	3.033(9)	154
20	Intra	1	N121_1	--H121_1	..O82_1	[ ]	0.88	1.99	2.862(9)	170
Molecule B										
21		2	N11_2	--H11_2	..O112_2	[1554.02]	0.88	2.02	2.869(10)	161
22		2	N21_2	--H21_2	..O2M_1	[1555.04]	0.88	2.04	2.905(13)	167
24	Intra	2	N31_2	--H31_2	..O5_2	[ ]	0.88	2.11	2.912(9)	151
26	Intra	2	N41_2	--H41_2	..O12_2	[ ]	0.88	2.38	2.954(9)	123
28	Intra	2	N51_2	--H51_2	..O12_2	[ ]	0.88	2.19	3.059(9)	169
29	Intra	2	N61_2	--H61_2	..O22_2	[ ]	0.88	1.97	2.822(9)	163
31	Intra	2	N71_2	--H71_2	..O42_2	[ ]	0.88	2.51	3.045(10)	120
32	Intra	2	N81_2	--H81_2	..O42_2	[ ]	0.88	2.19	3.061(9)	172
33	Intra	2	N91_2	--H91_2	..O52_2	[ ]	0.88	1.95	2.813(9)	167
35	Intra	2	N101_2	--H101_2	..O62_2	[ ]	0.88	2.45	3.239(11)	149
37	Intra	2	N111_2	--H111_2	..O72_2	[ ]	0.88	2.23	3.026(9)	150
39	Intra	2	N121_2	--H121_2	..O82_2	[ ]	0.88	2.03	2.884(11)	165

Translation of ARU-Code to CIF and Equivalent Position Code

```
==========================================================
  [ 1554.] = [  1_554] = x,y,-1+z
  [ 1465.] = [  1_465] = -1+x,1+y,z
```

*PLATON: Spek, A. L. (2009). Acta Cryst. D65, 148-155.

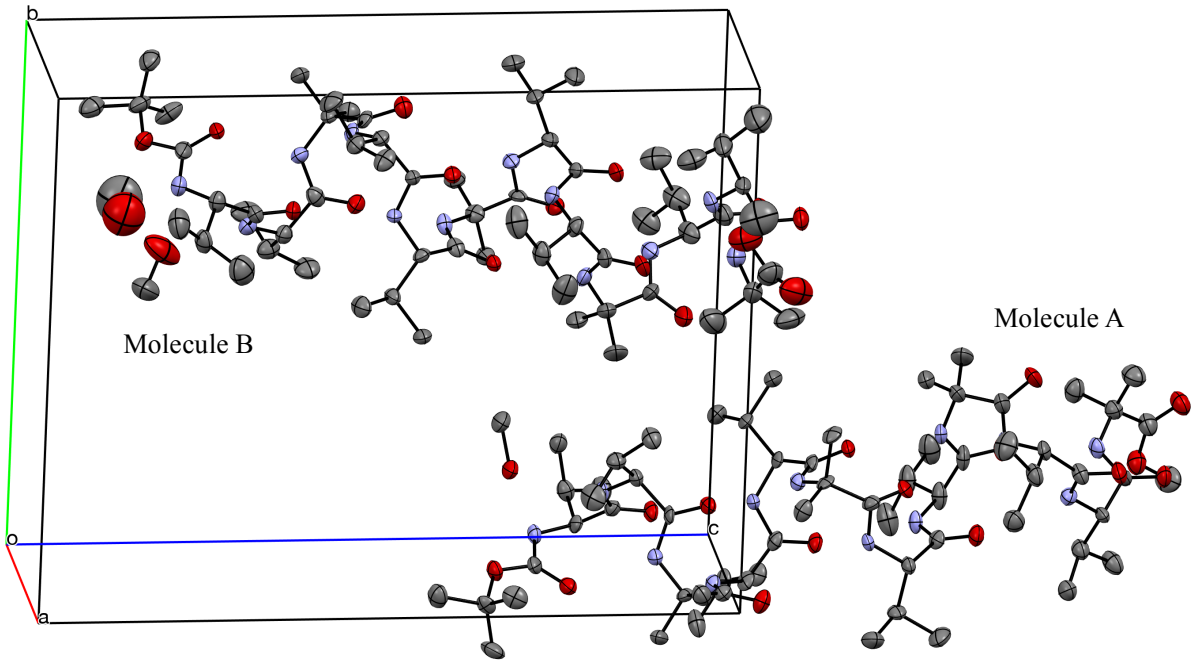

Figure S1. Molecular structures (ORTEP, helix side).

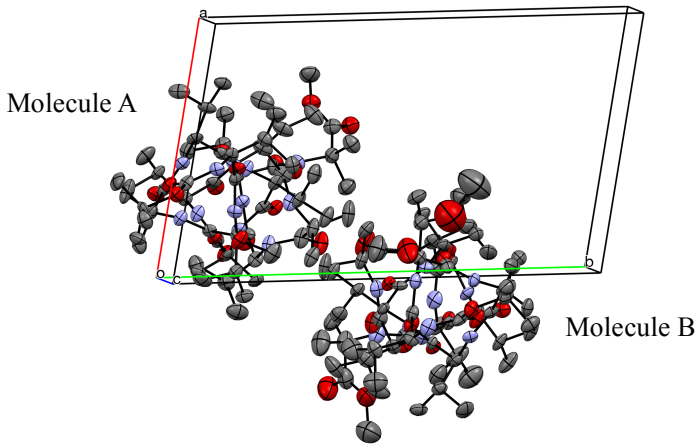

Figure S2. Molecular structures (ORTEP, helix top).

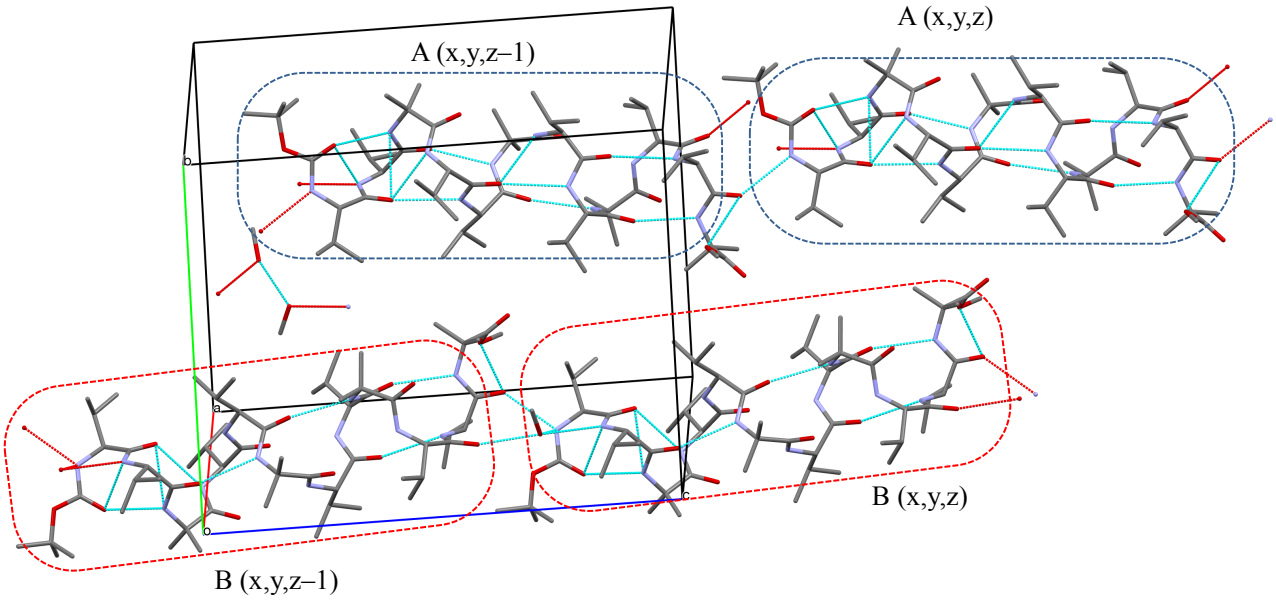

Figure S3. Molecular packing (head-to-tail).

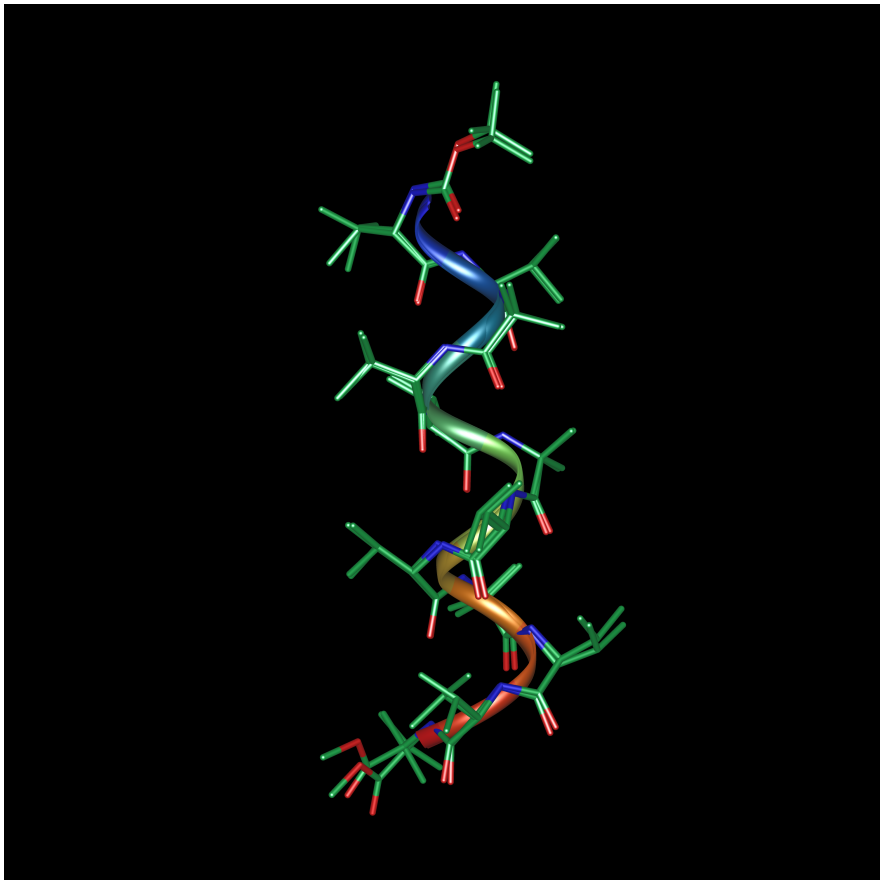

Figure S4. Molecular fitting (RMS=0.138 Å).

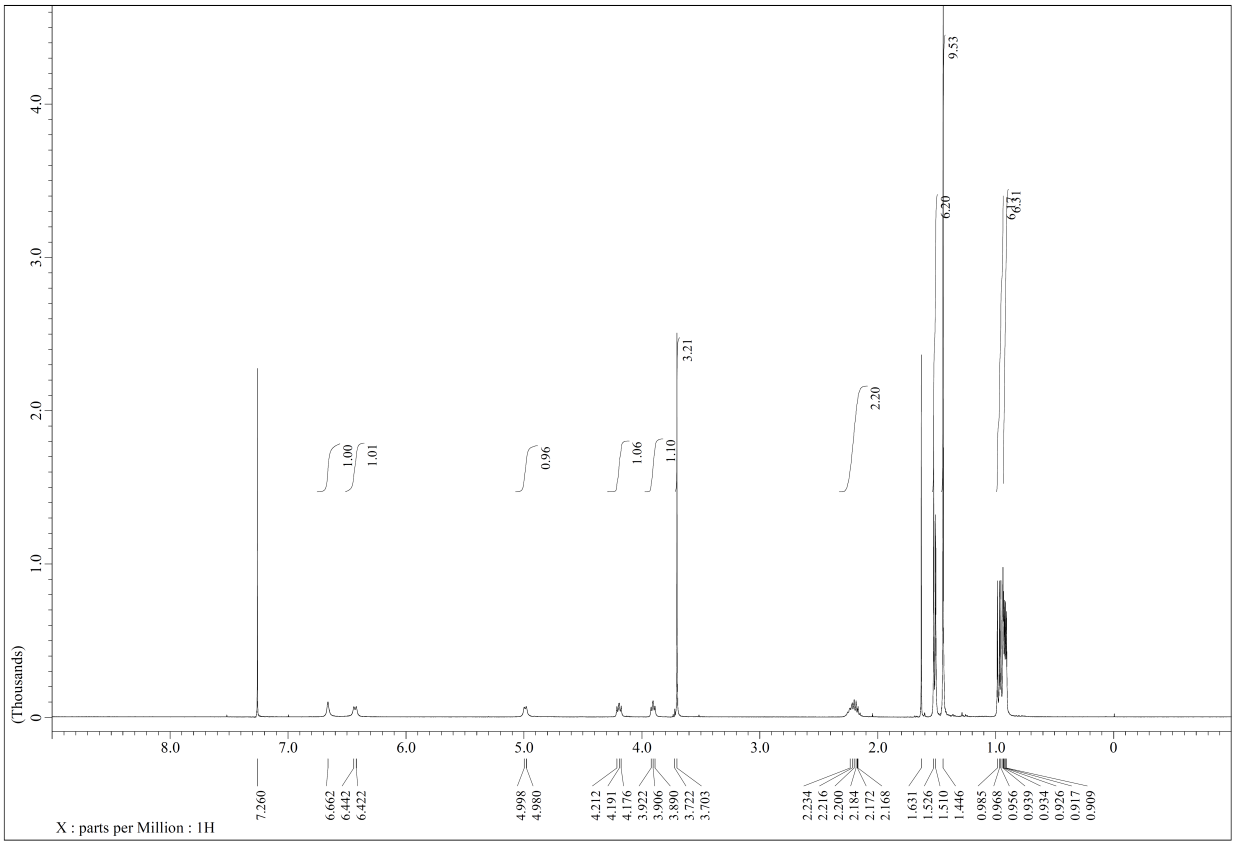

Figure S5. **^{1}H NMR of tripeptide 1**

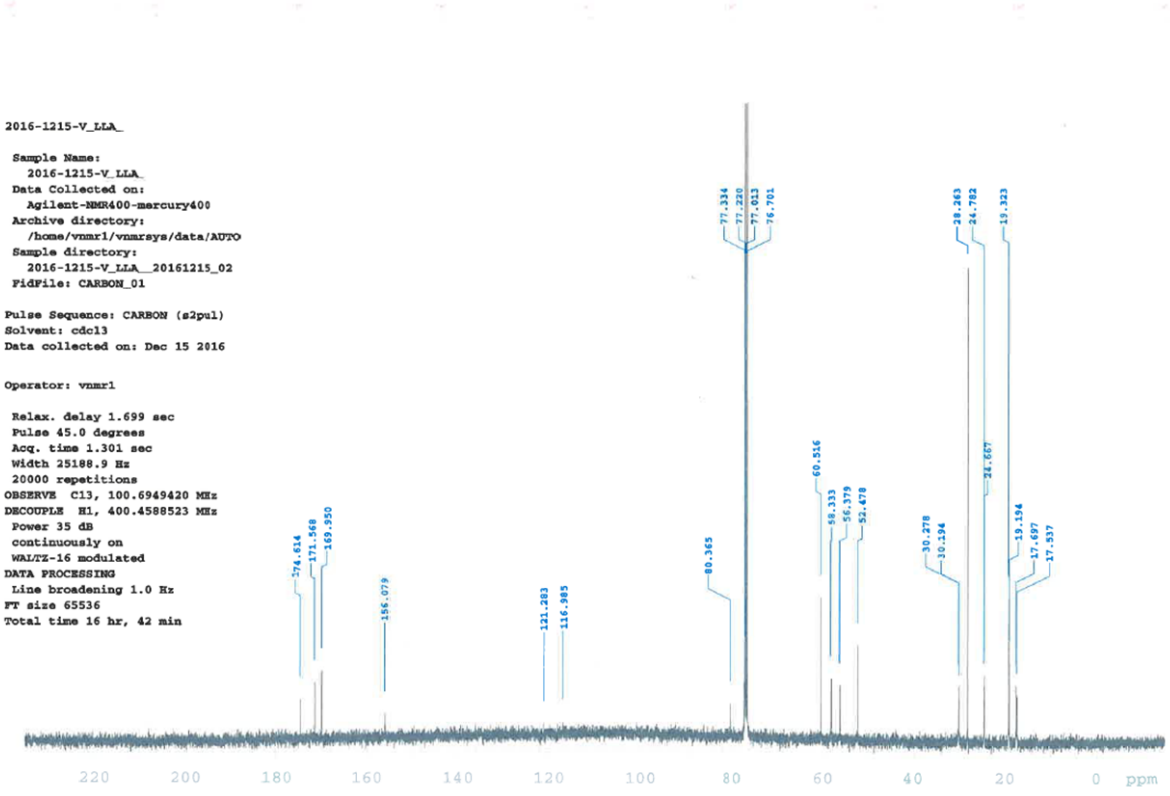

Figure S6. ^{13}C NMR of tripeptide 1

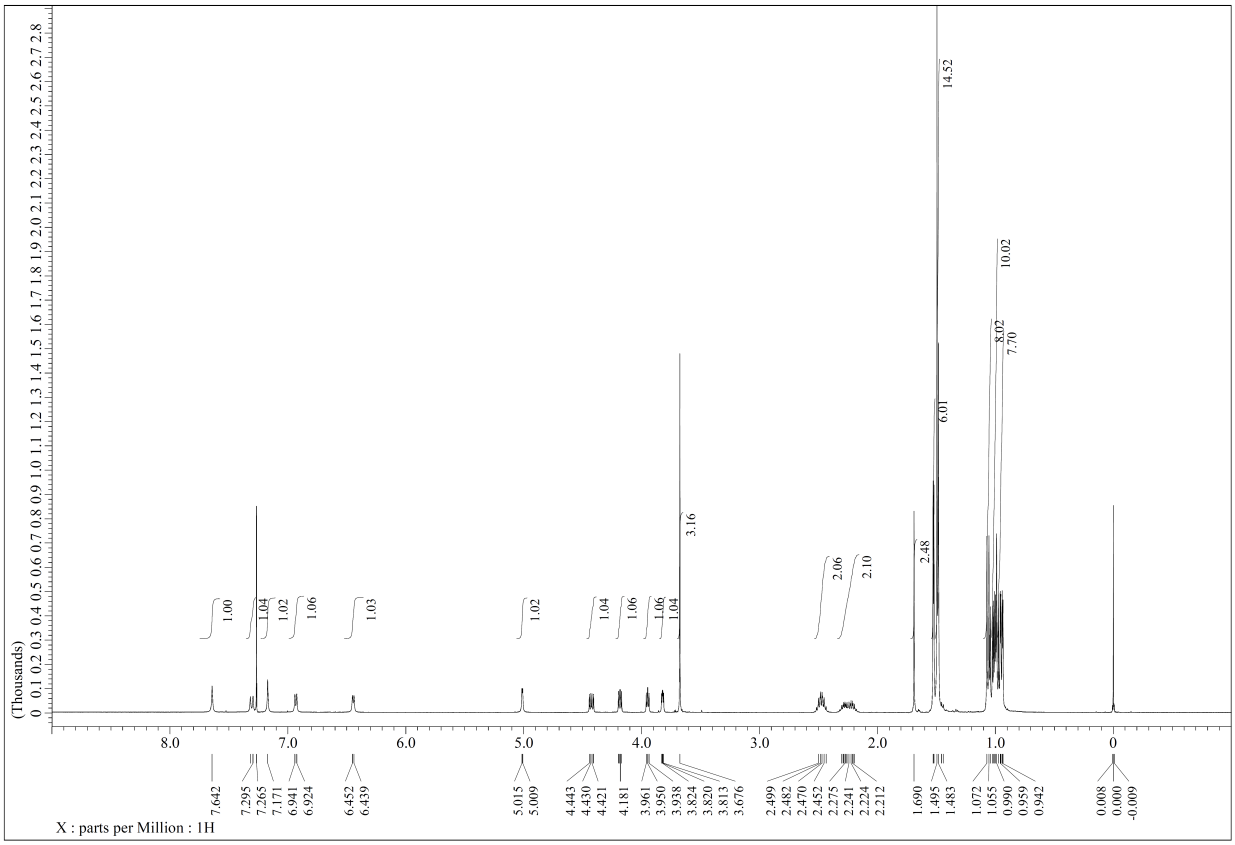

Figure S7. **^{1}H NMR of hexapeptide 2**

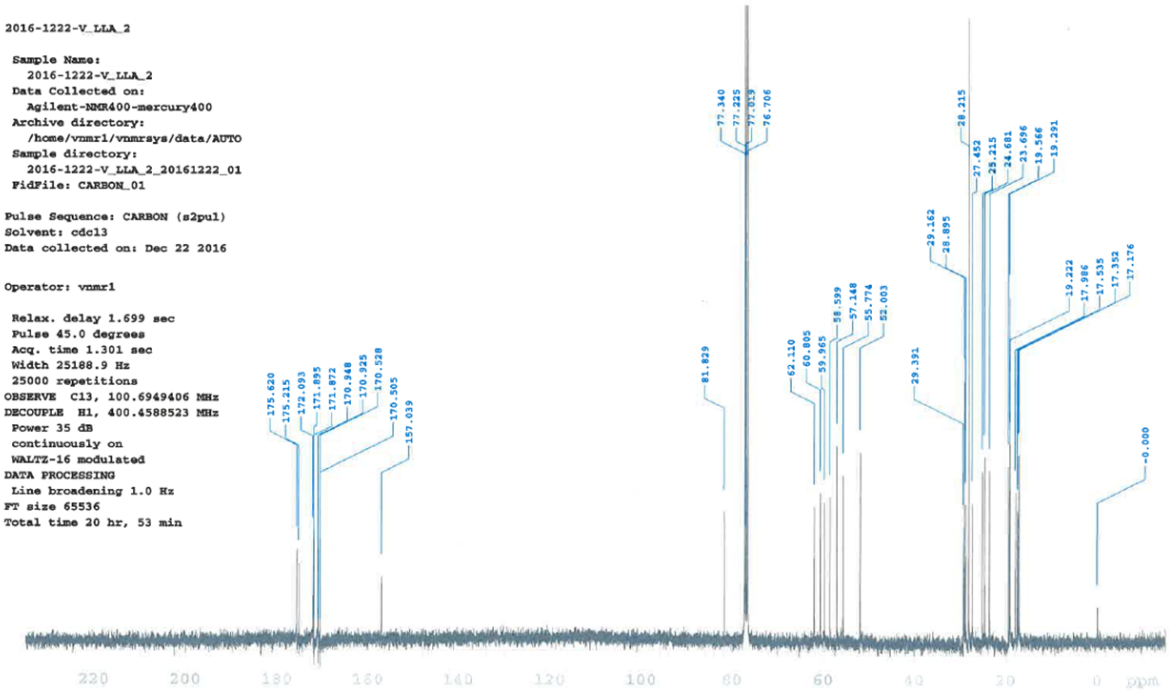

Figure S8. ^{13}C NMR of hexapeptide 2

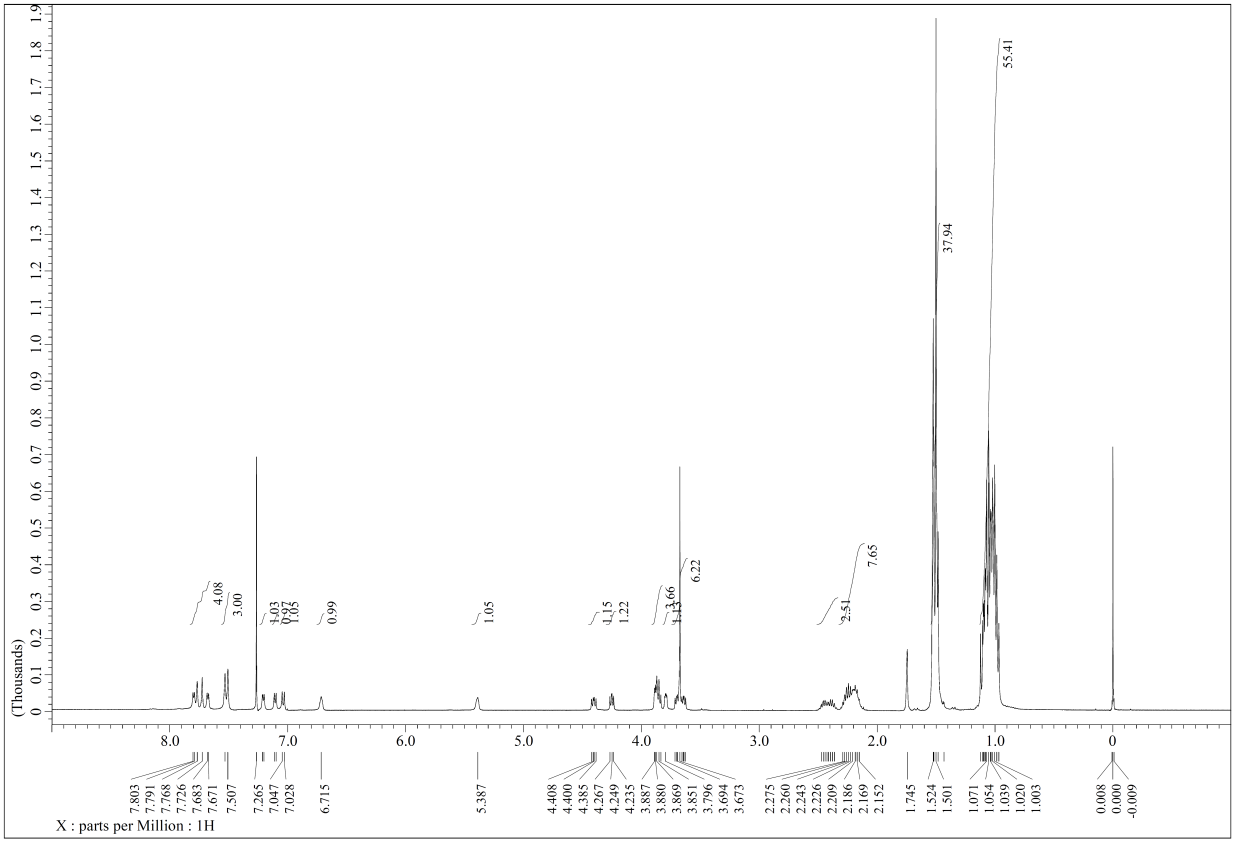

Figure S9. **^{1}H NMR of dodecapeptide 3**

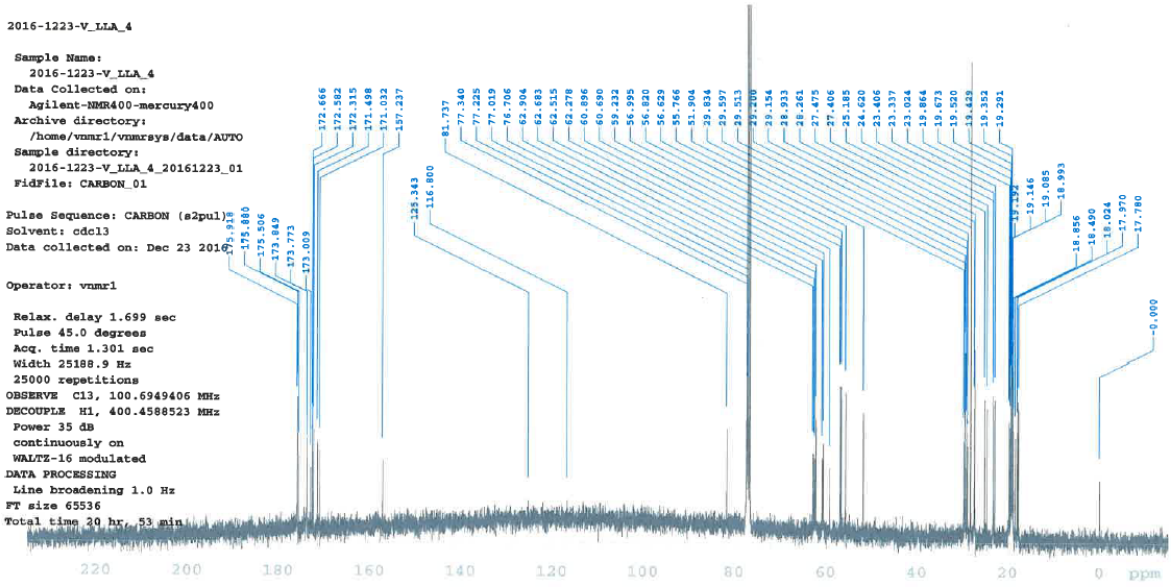

Figure S10. ^{13}C NMR of dodecapeptide 3