Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

SUPPORTING INFORMATION

Efficient Syntheses of *alpha*- and *beta*-*C*-Nucleosides and the Origin of Anomeric Selectivity[†]

Tongchao Liu,[a,b,‡] *Zhengdan Zhu,*[b,c,e,‡] *Huanming Ren,*[b,d] *Yabin Chen,*[b] *Guohua Chen,*[d] *Maosheng Cheng,*[a] *Dongmei Zhao,*[a,*] *Jingkang Shen*[b,e], *Weiliang Zhu,*[b,c,e*] *Bing Xiong*[b,e*] *and Yue-Lei Chen*[b,e*]

[a] Key Laboratory of Structure-Based Drug Design and Discovery of Ministry of Education, Shenyang Pharmaceutical University, 103 Wenhua Lu, Shenyang 110016, P. R. China.

[b] State Key Laboratory of Drug Research, Shanghai Institute of Materia Medica, Chinese Academy of Sciences, 555 Zuchongzhi Road, Shanghai 201203; P. R. China.

[c] CAS Key Laboratory of Receptor Research, Drug Discovery and Design Center, Shanghai Institute of Materia Medica, Chinese Academy of Sciences, 555 Zuchongzhi Road, Shanghai 201203; P. R. China.

[d] School of Pharmacy, China Pharmaceutical University, 24 Tongjiaxiang, Nanjing 210009, P. R. China.

[e] University of Chinese Academy of Sciences, No.19A Yuquan Road, Beijing 100049, P. R. China.

[†] Dedicated to the memory of Professor Qi-Zhuo Wang (1922-2018).

[‡] T. L. and Z. Z. contributed equally to this work.

E-mail: D. Z.: dongmeiz-67@163.com; W.Z.: wlzhu@simm.ac.cn; B. X.: bxiong@simm.ac.cn; Y.-L. C.: chenyuelei@gmail.com

Table of Contents

1. General.

All solvents were dried and purified prior to use: Et_2O and THF were distilled from potassium, and DCM was distilled from CaH_2. All other commercially available reagents were used as received. All moisture sensitive reactions were performed under N_2 (ca. +1.1 bar) in heating-gun (500-600 °C)/vacuum dried glassware sealed with rubber septa. Flash chromatography was performed on silica gel (300-400 mesh ASTM), and monitored by thin layer chromatography (TLC) on HSGF-254 (10-40 μm) TLC plates. NMR data were collected on a *Varian* Mercury-300 High Performance Digital FT-NMR, a *Varian* Mercury-400 High Performance Digital FT-NMR, a Bruker Ultrashield 500 NMR, or an Agilent 1260 Prospekt 2 Bruker Ascend 600 NMR. Spectra from solutions in $CDCl_3$ (δC = 77.0 ppm) are calibrated relative to TMS (δH = 0.00 ppm). HRMS were carried out on a *Thermo Finnigan* MAT-95 spectrometer (for EI), or on a *Waters*, Q-Tof Ultima Global spectrometer (for ESI). Melting points were measured on an uncorrected SGW X-4 micro melting point apparatus. HPLC analysis was performed on a Gilson HPLC system (306 pump, UV/vis-156 Detector, 215 liquid handle) with a YMC-ODS column (4.6 x 50 mm, 5 μm). Unless otherwise mentioned, a common HPLC condition was applied: solvent A = H_2O containing 0.1% (v/v) TFA, solvent B = MeCN containing 0.1% (v/v) TFA; flow rate = 2.5 mL/min; Gradient (B%): 0-0.5 min (4% isostatic), 0.5-4.5 min (4% - 95%), 4.5-6.1 min (95% isostatic), 6.1-6.3 min (95% - 4%), 6.3-8.0 min (4% isostatic); peaks were identified at 254 nm and 214 nm.

2. Experimental procedures and characterization of products.

General Procedure A:

A solution of compound **12a** or **12b** (0.64 mmol) in THF (5 mL) was cooled to -30 ^oC and treated with LDA (0.83 mmol). The mixture was kept at -30 ^oC for 50 min, cooled to -78 ^oC, treated with *n*-BuLi (1.60 mmol), stirred for 5 min, and then treated with a solution of **16a**, **16b**, **18a**, **18b**, **19**, **3**, **35** or **38** (1.92 mmol) in THF (10 mL). The solution was stirred at -78 ^oC for 2 h, quenched with sat. aq. NH_4Cl (10 mL), warmed to RT, and extracted with ethyl acetate (10 mL x 4). Combined organic phases were washed with

sat. aq. $NaHCO_3$ (10 mL) and brine (20 mL), dried with Na_2SO_4, and concentrated to dryness to afford crude products **20**, **20a**/**b**, **23a**/**b**, **25a**/**b**, **28a**/**b**, **30a**/**b**, **33a**/**b**, **36** or **39**, respectively.

General Procedure B:

Crude **20a**/**b**, **25a**/**b** or **30a** obtained from **General Procedure A** was dissolved in DCM (10 mL), cooled to -78 ^{o}C, stirred with Et_3SiH (2.56 mmol) for 5 min, and treated with TMSOTf (1.28 mmol). The mixture was then stirred at -78 ^{o}C for 2 h, before quenched by sat. aq. $NaHCO_3$ (5 mL) and extracted with DCM (10 mL x 3). Combined organic phases were washed with brine, dried with Na_2SO_4, concentrated, and purified with flash chromatography on silica gel (4:1, 60 - 90 ^{o}C petroleum ether – EtOAc) to afford products **21a**/**b**, **26a**/**b** or **31a**, respectively.

General Procedure C:

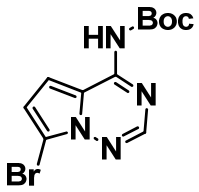
Crude **20a**/**b**, **25a**/**b**, or **30a**/**b** obtained from **General Procedure A** was dissolved in DCM (10 mL), cooled to 0 ^{o}C, stirred with Et_3SiH (2.56 mmol) for 5 min, and treated with $BF_3{\cdot}Et_2O$ (1.28 mmol). The mixture was then warmed to RT and stirred for 1 h, before quenched by sat. aq. $NaHCO_3$ and extracted with DCM (10 mL x 3). Combined organic phases were washed with brine, dried with Na_2SO_4, concentrated, and purified with flash chromatography on silica gel (25:1, DCM : MeOH) to afford products **22a**/**b**, **27a**/**b**, **32** or **4a**, respectively.

General Procedure D:

Crude **23a**/**b**, **28a**/**b** or **33a**/**b** obtained from **General Procedure A** was dissolved in MeCN (10 mL), cooled to -40 ^{o}C, stirred with Et_3SiH (2.56 mmol) for 5 min, and treated with $BF_3{\cdot}Et_2O$ (1.28 mmol). The mixture was then warmed to RT and stirred for 2 h, before quenched by sat. aq. $NaHCO_3$ (10 mL) and extracted with DCM (10 mL x 3). Combined organic phases were washed with brine, dried with Na_2SO_4, concentrated, and purified with flash chromatography on silica gel (25:1, DCM : MeOH) to afford products **24a**/**b**, **29a**/**b**, **34** or **4b**, respectively.

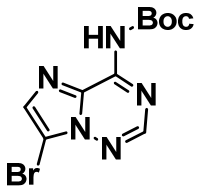
General Procedure E:

Crude **25a**/**b**, **30a**/**b**, **36** or **39** obtained from **General Procedure A** was dissolved in DCM (10 mL), cooled to -10 °C, stirred with Et_3SiH (2.56 mmol) for 5 min, and treated with $BF_3 \cdot Et_2O$ (1.28 mmol). The mixture was then stirred at -10 °C for 2 h, before quenched by sat. aq. $NaHCO_3$ (5 mL) and extracted with DCM (10 mL x 3). Combined organic phases were washed with brine, dried with Na_2SO_4, concentrated, and purified with flash chromatography on silica gel (4:1, 60 - 90 °C petroleum ether – EtOAc) to afford products **26a/b**, **31a/b**, **37** or **40**, respectively.



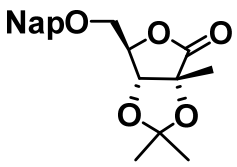
Preparation of compound 12a

A suspension of compound **1a** (5.0 g, 23.47 mmol) in THF (100 mL) was mixed with TEA (16.3 mL, 0.12 mol) and DMAP (287 mg, 2.35 mmol). Boc_2O (15.4 g, 70.42 mmol) was then slowly added to the above suspension at RT. The resulting mixture was stirred at RT overnight, treated with aq. NaOH (3 M, 100 mL), heated at 60 °C for 6 h, and cooled to RT. The organic phase was separated and the aqueous phase was washed with ethyl acetate (20 mL x 3). Combined organic phases were washed with brine (100 mL), dried with Na_2SO_4, concentrated to dryness, and purified with flash chromatography on silica gel (10 : 1，60 - 90 °C petroleum ether - EtOAc) to afford product **12a** (white solid, 6.6 g, 90%). M.p. 180.0 °C (decomposition) (60 - 90 °C petroleum ether – EtOAc)；R_f 0.21 (10:1，60 - 90 °C petroleum ether : EtOAc); HPLC t_R 2.79 min; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (s, 1H, ArH), 8.24 (s, 1H, NH), 7.39 (d, J = 4.8 Hz, 1H, ArH), 6.90 (d, J = 4.8 Hz, 1H, ArH), 1.58 (s, 9H, $C(CH_3)_3$); ^{13}C-NMR (126 MHz, $CDCl_3$) δ 151.52 (C=O), 150.60 (ArC), 147.00 (ArC), 116.57 (ArC), 115.34 (ArC), 108.71 (ArC), 103.35 (ArC), 83.13 ($C(CH_3)_3$), 28.29 ($C(CH_3)_3$); HRMS (ESI^+) calcd. For $C_{11}H_{13}BrN_4NaO_2^+$ 335.0114, found 335.0119.



Preparation of compound 12b

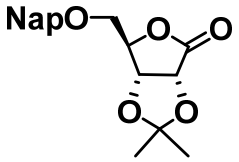
A suspension of compound **1b** (5.0 g，23.36 mmol) in THF (100 mL) was mixed with TEA (16.3 mL, 0.12 mol) and DMAP (287 mg, 2.35 mmol). Boc_2O (15.4 g, 70.42 mmol) was then slowly added to the above suspension at RT. The resulting mixture was stirred at RT overnight, treated with aq. NaOH (3 M, 100 mL), heated at 60 ^oC for 6 h, and cooled to RT. The organic phase was separated and the aqueous phase was washed with ethyl acetate (20 mL x 3). Combined organic phases were washed with brine (100 mL), dried with Na_2SO_4, concentrated to dryness, and purified with flash chromatography on silica gel (10 : 1，60 - 90 ^oC petroleum ether - EtOAc) to afford product **12b** (white solid, 6.3 g, 86%). M.p. 160.5 – 163.8 ^oC (60 - 90 ^oC petroleum ether – EtOAc); R_f 0.29 (5:1, 60 - 90 ^oC petroleum ether – EtOAc); HPLC t_R 2.72 min; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.62 (s, 1H, ArH), 8.58 (s, 1H, NH), 7.70 (s, 1H, ArH), 1.57 (s, 9H, $C(CH_3)_3$); ^{13}C-NMR (126 MHz, $CDCl_3$) δ 149.51 (C=O), 149.41 (ArC), 148.68 (ArC), 133.48 (ArC), 129.16 (ArC), 103.44 (ArC), 83.87 ($C(CH_3)_3$), 28.14 ($C(CH_3)_3$); HRMS (ESI^+) calcd. For $C_{10}H_{12}BrN_5NaO_2^+$ 336.0067, found 336.0058.



Preparation of compound 16a

A solution of **17a** (10.0 g, 49.46 mmol) in DMF (100 mL) was cooled to 0 ^oC, treated with NaH (60% in mineral oil, 3.0 g, 74.18 mmol), stirred for 30 min, and treated with 2-(bromomethyl)naphthalene (16.4 g, 74.18 mmol). The suspension was warmed to RT and stirred for 3 h, before cold water (200 mL) was

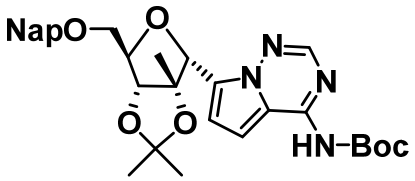
added. The reaction mixture was then extracted with ethyl acetate (100 mL x 4). Combined organic phases were washed with brine (100 mL), dried with Na_2SO_4, concentrated to dryness, and purified with flash chromatography on silica gel (4:1，60 - 90 °C petroleum ether – EtOAc to afford product **16a** (white solid, 15.1 g, 89%). M.p. 68.8 – 70.2 °C (60 - 90 °C petroleum ether – EtOAc); R_f 0.27 (5:1, 60 - 90 °C petroleum ether – EtOAc); $[\alpha]_D^{20}$ -15.46 (*c* 0.705 $CHCl_3$); HPLC t_R 3.81 min; ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.87 – 7.80 (m, 3H, ArH), 7.72 (s, 1H, ArH), 7.53 – 7.45 (m, 2H, ArH), 7.40 (dd, *J* = 8.4, 1.6 Hz, 1H, ArH), 4.72 (d, *J* = 11.9 Hz, 1H, OC$\underline{H}_2$-), 4.65 (d, *J* = 11.9 Hz, 1H, OC$\underline{H}_2$-), 4.57 (t, *J* = 2.6 Hz, 1H, H-4), 4.51 (s, 1H, H-3), 3.76 (dd, *J* = 10.9, 3.0 Hz, 1H, H-5a), 3.73 (dd, *J* = 10.9, 2.6 Hz, 1H, H-5b), 1.58 (s, 3H, 2-CH_3), 1.43 (s, 3H, OC(C$\underline{H}_3$)$_2$O), 1.40 (s, 3H, OC(C$\underline{H}_3$)$_2$O); ^{13}C-NMR (126 MHz, $CDCl_3$) δ 176.43 ($\underline{C}$=O), 134.41 (ArC), 133.27 (2 x ArC), 128.63 (ArC), 128.02 (ArC), 127.86 (ArC), 127.14 (ArC), 126.47 (ArC), 126.35 (ArC), 125.80 (ArC), 112.90 (O$\underline{C}$(CH$_3$)$_2$O), 82.98 (C-2), 82.84 (C-3), 82.02 (C-4), 74.13 (O$\underline{C}$H$_2$-), 69.33 (C-5), 26.98 (OC($\underline{C}$H$_3$)$_2$O), 26.88 (OC($\underline{C}$H$_3$)$_2$O), 19.95 (2-$\underline{C}$H$_3$); HRMS (ESI^+) calcd. For $C_{20}H_{22}NaO_5^+$ 365.1359, found 365.1366.



Preparation of compound 16b

A solution of **17b** (10.0 g, 53.14 mmol) in DMF (100 mL) was cooled to 0 °C, treated with NaH (60% in mineral oil, 3.2 g, 79.71 mmol), stirred for 30 min, and treated with 2-(bromomethyl)naphthalene (17.6 g, 79.71 mmol). The suspension was warmed to RT and stirred for 3 h, before cold water (200 mL) was added. The reaction mixture was then extracted with ethyl acetate (100 mL x 4). Combined organic phases were washed with brine (100 mL), dried with Na_2SO_4, concentrated to dryness, and purified with flash chromatography on silica gel (4:1，60 - 90 °C petroleum ether – EtOAc to afford product **16b** (white solid, 15.9 g, 91%). M.p. 105.4 – 106.8 °C (60 - 90 °C petroleum ether – EtOAc); R_f 0.22 (5:1, 60 - 90 °C

petroleum ether – EtOAc); $[\alpha]_D^{20}$ -41.67 (*c* 0.240 $CHCl_3$); HPLC t_R 3.65 min; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.86 – 7.81 (m, 3H, ArH), 7.69 (s, 1H, ArH), 7.51 – 7.47 (m, 2H, ArH), 7.37 (dd, *J* = 8.4, 1.4 Hz, 1H, ArH), 4.81 (d, *J* = 5.5 Hz, 1H, H-2), 4.73 (d, *J* = 2.2 Hz, 1H, H-3), 4.71 (d, *J* = 4.0 Hz, 1H, OC$\underline{H}_2$-), 4.65 (t, *J* = 1.8 Hz, 1H, H-4), 4.62 (d, *J* = 11.9 Hz, 1H, OC$\underline{H}_2$-), 3.75 (dd, *J* = 10.7, 2.3 Hz, 1H, H-5a), 3.70 (dd, *J* = 10.7, 1.8 Hz, 1H, H-5b), 1.47 (s, 3H, OC(C$\underline{H}_3$)$_2$O), 1.36 (s, 3H, OC(C$\underline{H}_3$)$_2$O); ^{13}C NMR (126 MHz, $CDCl_3$) δ 174.47 (1-$\underline{C}$=O), 134.46 (ArC), 133.29 (ArC), 133.28 (ArC), 128.72 (ArC), 128.04 (ArC), 127.87 (ArC), 126.93 (ArC), 126.50 (ArC), 126.37 (ArC), 125.58 (ArC), 113.31 ((O$\underline{C}$(CH$_3$)$_2$O), 81.23 (C-4), 78.54 (C-3), 75.87 (C-2), 74.19 (O$\underline{C}$H$_2$-), 69.17 (C-5), 26.95 (OC($\underline{C}$H$_3$)$_2$O), 25.76 (OC($\underline{C}$H$_3$)$_2$O); HRMS (ESI^+) calcd. For $C_{19}H_{20}NaO_5^+$ 351.1203, found 351.1209.



Preparation of compound 21a

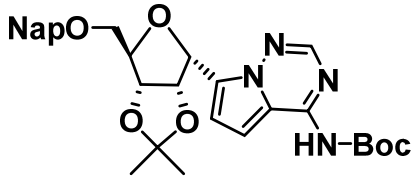
Method 1:

From compound **12a** (0.64 mmol) and **16a** (1.92 mmol), **general procedure A** yielded crude **20a**, then crude **20a** was dissolved in MeCN (10 mL), cooled to -40 °C, stirred with Et_3SiH (2.56 mmol) for 5 min, and treated with $BF_3 \cdot Et_2O$ (1.28 mmol). The mixture was then stirred at -40 °C for 2 h, before quenched by sat. aq. $NaHCO_3$ (5 mL) and extracted with DCM (10 mL x 3). Combined organic phases were washed with brine, dried with Na_2SO_4, concentrated, and purified with flash chromatography on silica gel (4:1, 60 - 90 °C petroleum ether – EtOAc) to afford product **21a** (colorless amorphous solid, 183 mg, 0.33 mmol, 51%). R_f 0.71 (1:1, 60 - 90 °C petroleum ether – EtOAc); $[\alpha]_D^{20}$ -100.48 (*c* 0.210 $CHCl_3$); HPLC t_R 3.74 min; ^{1}H-NMR (500 MHz, $CDCl_3$) δ 8.16 (s, 1H, ArH), 7.85 – 7.82 (m, 4H, ArH), 7.54 – 7.47 (m, 3H, ArH), 7.21 (d, *J* = 4.2 Hz, 1H, ArH), 7.05 (d, *J* = 3.7 Hz, 1H, ArH), 5.86 (s, 1H, H-1'), 4.80 (d, *J* = 12.3 Hz, 1H, Nap-C$\underline{H}_2$-), 4.75 (d, *J* = 12.2 Hz, 1H, Nap-C$\underline{H}_2$-), 4.64 (s, 1H, H-3'), 4.40 (t, *J* = 4.1 Hz, 1H,

H-4'), 3.79 – 3.76 (m, 2H, H-5'a, H-5'b), 1.59 (s, 3H, 2'-C$\underline{H}_3$), 1.57 (s, 9H, C(C$\underline{H}_3$)$_3$), 1.47 (s, 3H, OC(C$\underline{H}_3$)$_2$O), 1.38 (s, 3H, OC(C$\underline{H}_3$)$_2$O), N$\underline{H}$ is missing; Selected NOESY (500 MHz, $CDCl_3$): δ (^{1}H) / δ (^{1}H) = 5.86 / 3.79 – 3.76 (H-1' / H-5'a, H-5'b); ^{13}C-NMR (126 MHz, $CDCl_3$) δ 151.24 (C=O), 150.25 (ArC), 146.05 (ArC), 135.40 (ArC), 133.39 (ArC), 133.15 (ArC), 129.26 (ArC), 128.37 (ArC), 127.98 (ArC), 127.83 (ArC), 126.64 (ArC), 126.28 (ArC), 126.08 (ArC), 125.76 (ArC), 115.10 (ArC), 114.08 (ArC), 113.06 (O$\underline{C}$(CH$_3$)$_2$O), 105.22 (ArC), 91.13 (C-2'), 89.49 (C-3'), 83.31 (C-4'), 82.67 ($\underline{C}$(CH$_3$)$_3$), 80.48 (C-1'), 73.93 (Nap-$\underline{C}$H$_2$-), 71.41 (C-5'), 28.27 (C($\underline{C}$H$_3$)$_3$), 27.76 (OC($\underline{C}$H$_3$)$_2$O), 27.52 (OC($\underline{C}$H$_3$)$_2$O), 23.08 (2'-$\underline{C}$H$_3$); HRMS (ESI$^+$) calcd. For $C_{31}H_{37}N_4O_6^+$ 561.2708, found 561.2701.

Method 2:

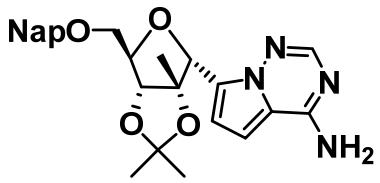
From compound **12a** (0.64 mmol) and **16a** (1.92 mmol), **general procedure A** and then **general procedure B** yielded product **21a** (colorless amorphous solid, 269 mg, 0.48 mmol, 75%). ^{1}H-NMR of product **21a** obtained from method 2 was identical to that from method 1.



Preparation of compound 21b

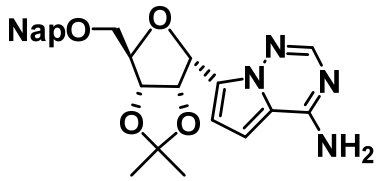
From compound **12a** (0.64 mmol) and **16b** (1.92 mmol), **general procedure A** and then **general procedure B** yielded product **21b** (white amorphous solid, 287 mg, 0.52 mmol, 82%). R_f 0.46 (2:1, 60 - 90 ^{o}C petroleum ether – EtOAc); [α]$_D^{20}$ -131.30 (*c* 0.115 $CHCl_3$); HPLC t_R 3.62 min; ^{1}H-NMR (500 MHz, $CDCl_3$) δ 8.16 (s, 1H, ArH), 7.85 – 7.81 (m, 4H, ArH), 7.50 – 7.45 (m, 3H, ArH), 7.19 (d, *J* = 3.6 Hz, 1H, ArH), 7.02 (s, 1H, ArH), 5.89 (s, 1H, H-1'), 5.11 (s, 1H, H-2'), 4.96 (d, *J* = 5.9 Hz, 1H, H-3'), 4.78 (d, *J* = 12.3 Hz, 1H, Nap-C$\underline{H}_2$-), 4.72 (d, *J* = 12.3 Hz, 1H, Nap-C$\underline{H}_2$-), 4.42 (t, *J* = 3.5 Hz, 1H, H-4'), 3.75 (dd, *J* = 10.2, 3.8 Hz, 1H, H-5'a), 3.71 (dd, *J* = 10.2, 4.2 Hz, 1H, H-5'b), 1.56 (s, 9H, C(C$\underline{H}_3$)$_3$), 1.40 (s, 3H, OC(C$\underline{H}_3$)$_2$O), 1.28 (s, 3H, OC(C$\underline{H}_3$)$_2$O), N$\underline{H}$ is missing; Selected NOESY (500 MHz, $CDCl_3$): δ (^{1}H) / δ

(^{1}H) = 5.89 / 3.75, 3.71 (H-1' / H-5'a, H-5'b); ^{13}C-NMR (126 MHz, $CDCl_3$) δ 151.08 (ArC), 150.20 (C=O), 146.26 (ArC), 135.42 (ArC), 133.40 (ArC), 133.16 (ArC), 129.05 (ArC), 128.42 (ArC), 128.01 (ArC), 127.84 (ArC), 126.57 (ArC), 126.31 (ArC), 126.10 (ArC), 125.67 (ArC), 115.00 (ArC), 113.33 (ArC), 112.79 (O<u>C</u>$(CH_3)_2$O), 105.03 (ArC), 83.58 (C-3'), 82.97 (C-4'), 82.71 (<u>C</u>$(CH_3)_3$), 81.57 (C-2'), 77.25 (C-1'), 73.88 (Nap-<u>C</u>H_2-), 71.44 (C-5'), 28.28 (C(<u>C</u>$H_3)_3$), 26.38 (OC(<u>C</u>$H_3)_2$O), 25.18 (OC(<u>C</u>$H_3)_2$O); HRMS (ESI$^+$) calcd. For $C_{30}H_{35}N_4O_6^+$ 547.2551, found 547.2565.



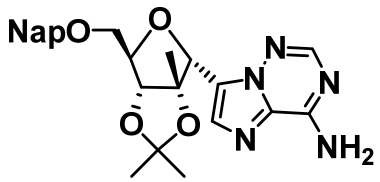
Preparation of compound 22a

From compound **12a** (0.64 mmol) and **16a** (656 mg, 1.92 mmol), **general procedure A** and then **general procedure C** yielded product **22a** (colorless amorphous solid, 168 mg, 0.36 mmol, 57%). R_f 0.41 (15 : 1, DCM : MeOH); $[\alpha]_D^{20}$ -112.31 (*c* 0.195 $CHCl_3$); HPLC t_R 3.22 min; ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.90 (s, 1H, ArH), 7.86 – 7.83 (m, 4H, nap-H), 7.55 – 7.47 (m, 3H, nap-H), 6.92 (d, *J* = 4.5 Hz, 1H, ArH), 6.66 (d, *J* = 4.5 Hz, 1H, ArH), 5.83 (s, 1H, H-1'), 5.65 (br s, 2H, N<u>H</u>$_2$), 4.81 – 4.74 (m, 2H, Nap-C<u>H</u>$_2$-), 4.64 (s, 1H, H-3'), 4.38 (t, *J* = 4.3 Hz, 1H, H-4'), 3.77 (dd, *J* = 4.4, 1.3 Hz, 2H, H-5'a, H-5'b), 1.58 (s, 3H, 2'-C<u>H</u>$_3$), 1.52 (s, 3H, OC(C<u>H</u>$_3)_2$O), 1.40 (s, 3H, OC(C<u>H</u>$_3)_2$O); Selected NOESY (500 MHz, $CDCl_3$): δ (^{1}H) / δ (^{1}H) = 5.83 / 3.77 (H-1' / H-5'a, H-5'b); ^{13}C NMR (151 MHz, $CDCl_3$) δ 155.29 (ArC), 146.89 (ArC), 135.42 (Nap-C), 133.38 (Nap-C), 133.13 (Nap-C), 128.38 (Nap-C), 128.01 (Nap-C), 127.91 (ArC), 127.83 (Nap-C), 126.64 (Nap-C), 126.26 (Nap-C), 126.06 (Nap-C), 125.79 (Nap-C), 114.15 (ArC), 113.02 (O<u>C</u>$(CH_3)_2$O), 112.70 (ArC), 100.59 (ArC), 90.94 (C-2'), 89.41 (C-3'), 83.13 (C-4'), 80.13 (C-1'), 73.90 (Nap-<u>C</u>H_2-), 71.26 (C-5'), 27.86 (OC(<u>C</u>$H_3)_2$O), 27.59 (OC(<u>C</u>$H_3)_2$O), 22.95 (2'-<u>C</u>H_3); HRMS (ESI$^+$) calcd. For $C_{26}H_{28}N_4NaO_4^+$ 483.2003, found 483.1994.



Preparation of compound 22b

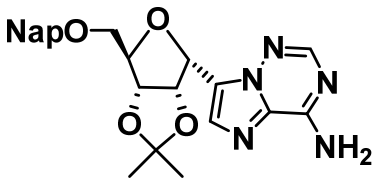
From compound **12a** (0.64 mmol) and **16b** (1.92 mmol), **general procedure A** and then **general procedure C** yielded product **22b** (white amorphous solid, 169 mg, 0.38 mmol, 59%). R_f 0.40 (15 : 1, DCM : MeOH); $[\alpha]_D^{20}$ -120.65 (*c* 0.155 $CHCl_3$); HPLC t_R 3.15 min; ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.92 (s, 1H, ArH), 7.85 – 7.81 (m, 4H, nap-H), 7.52 – 7.46 (m, 3H, nap-H), 6.90 (d, *J* = 4.5 Hz, 1H, ArH), 6.64 (d, *J* = 4.5 Hz, 1H, ArH), 5.88 (d, *J* = 4.0 Hz, 1H, H-1'), 5.63 (br s, 2H, N$\underline{H_2}$), 5.08 (dd, *J* = 5.9, 4.1 Hz, 1H, H-2'), 4.95 (dd, *J* = 6.0, 0.8 Hz, 1H, H-3'), 4.80 – 4.71 (m, 2H, Nap-C$\underline{H_2}$-), 4.42 (t, *J* = 4.2 Hz, 1H, H-4'), 3.75 – 3.69 (m, 2H, H-5'a, H-5'b), 1.46 (s, 3H, OC(C$\underline{H_3}$)$_2$O), 1.30 (s, 3H, OC(C$\underline{H_3}$)$_2$O); Selected NOESY (500 MHz, $CDCl_3$): δ (^{1}H) / δ (^{1}H) = 5.88 / 3.75 – 3.69 (H-1' / H-5'a, H-5'b); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.29 (ArC), 147.12 (ArC), 135.45 (Nap-C), 133.40 (Nap-C), 133.16 (Nap-C), 128.41 (Nap-C), 128.02 (Nap-C), 127.82 (Nap-C), 127.63 (ArC), 126.59 (Nap-C), 126.27 (Nap-C), 126.07 (Nap-C), 125.72 (Nap-C), 114.07 (ArC), 112.77 (O$\underline{C}$(CH$_3$)$_2$O), 111.98 (ArC), 100.38 (ArC), 83.59 (C-3'), 82.84 (C-4'), 81.61 (C-2'), 76.76 (C-1'), 73.85 (Nap-$\underline{C}$H$_2$-), 71.19 (C-5'), 26.42 (OC($\underline{C}$H$_3$)$_2$O), 25.15 (OC($\underline{C}$H$_3$)$_2$O); HRMS (ESI$^+$) calcd. For $C_{25}H_{27}N_4O_4^+$ 447.2027, found 447.2036.



Preparation of compound 24a

From compound **12b** (0.64 mmol) and **16a** (1.92 mmol), **general procedure A** and then **general procedure D** yielded product **24a** (colorless amorphous solid, 162 mg, 0.35 mmol, 55%). R_f 0.63 (15 : 1, DCM : MeOH); $[\alpha]_D^{20}$ -92.00 (*c* 0.125 $CHCl_3$); HPLC t_R 3.36 min; ^{1}H-NMR (500 MHz, $CDCl_3$) δ 8.10 (s,

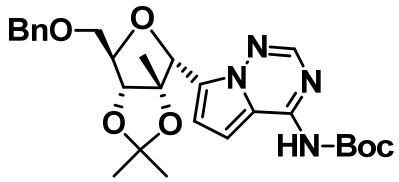
1H, ArH), 7.87 – 7.81 (m, 4H, nap-H), 7.77 (s, 1H, ArH), 7.56 – 7.51 (m, 1H, nap-H), 7.50 – 7.45 (m, 2H, nap-H), 5.68 (s, 1H, H-1'), 4.80 (d, *J* = 12.1 Hz, 1H, Nap-C$\underline{H}_2$-), 4.75 (d, *J* = 12.1 Hz, 1H, Nap-C$\underline{H}_2$-), 4.67 (s, 1H, H-3'), 4.37 (t, *J* = 3.8 Hz, 1H, H-4'), 3.80 (dd, *J* = 10.3, 3.8 Hz, 1H, H-5'a), 3.76 (dd, *J* = 10.3, 4.1 Hz, 1H, H-5'b), 1.57 (s, 3H, 2'-C$\underline{H}_3$), 1.50 (s, 3H, OC(C$\underline{H}_3$)$_2$O), 1.40 (s, 3H, OC(C$\underline{H}_3$)$_2$O), NH_2 are missing; Selected NOESY (500 MHz, $CDCl_3$): δ (^{1}H) / δ (^{1}H) = 5.68 / 3.80, 3.76 (H-1' / H-5'a, H-5'b); ^{13}C-NMR (126 MHz, $CDCl_3$) δ 153.84 (ArC), 148.80 (ArC), 135.34 (Nap-C), 133.41 (Nap-C), 133.19 (Nap-C), 132.74 (ArC), 128.48 (ArC), 128.44 (Nap-C), 128.01 (Nap-C), 127.86 (Nap-C), 126.97 (ArC), 126.73 (Nap-C), 126.32 (Nap-C), 126.13 (Nap-C), 125.80 (Nap-C), 113.24 (O$\underline{C}$(CH$_3$)$_2$O), 90.84 (C-2'), 89.47 (C-3'), 83.54 (C-4'), 79.74 (C-1'), 74.01 (Nap-$\underline{C}$H$_2$-), 71.60 (C-5'), 27.90 (OC($\underline{C}$H$_3$)$_2$O), 27.62 (OC($\underline{C}$H$_3$)$_2$O), 22.77 (2'-$\underline{C}$H$_3$); HRMS (ESI$^+$) calcd. For $C_{25}H_{28}N_5O_4^+$ 462.2136, found 462.2133.



Preparation of compound 24b

From compound **12b** (0.64 mmol) and **16b** (1.92 mmol), **general procedure A** and then **general procedure D** yielded product **24b** (white amorphous solid, 155 mg, 0.35 mmol, 54%). R_f 0.60 (15 : 1, DCM : MeOH); $[\alpha]_D^{20}$ -62.14 (*c* 0.140 $CHCl_3$); HPLC t_R 3.29 min; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.10 (s, 1H, ArH), 7.83 (dd, *J* = 15.5, 8.4 Hz, 4H, nap-H), 7.74 (s, 1H, ArH), 7.51 – 7.45 (m, 3H, nap-H), 5.79 (d, *J* = 4.1 Hz, 1H, H-1'), 5.07 (dd, *J* = 5.8, 4.2 Hz, 1H, H-2'), 4.98 (d, *J* = 6.0 Hz, 1H, H-3'), 4.78 (d, *J* = 12.3 Hz, 1H, Nap-C$\underline{H}_2$-), 4.72 (d, *J* = 12.3 Hz, 1H, Nap-C$\underline{H}_2$-), 4.41 (t, *J* = 3.7 Hz, 1H, H-4'), 3.76 (dd, *J* = 10.3, 3.6 Hz, 1H, H-5'a), 3.71 (dd, *J* = 10.3, 4.0 Hz, 1H, H-5'b), 1.45 (s, 3H, OC(C$\underline{H}_3$)$_2$O), 1.31 (s, 3H, OC(C$\underline{H}_3$)$_2$O), NH_2 are missing; Selected NOESY (500 MHz, $CDCl_3$): δ (^{1}H) / δ (^{1}H) = 5.79 / 3.76, 3.71 (H-1' / H-5'a, H-5'b); ^{13}C NMR (151 MHz, $CDCl_3$) δ 153.85 (ArC), 148.84 (ArC), 135.32 (Nap-C), 133.37 (Nap-C), 133.15 (Nap-C), 131.92 (ArC), 128.46 (Nap-C), 128.41 (ArC), 127.99 (Nap-C), 127.83

(Nap-C), 126.75 (ArC), 126.63 (Nap-C), 126.32 (Nap-C), 126.13 (Nap-C), 125.69 (Nap-C), 112.97 (O<u>C</u>(CH$_3$)$_2$O), 83.63 (C-3'), 83.08 (C-4'), 81.64 (C-2'), 76.02 (C-1'), 73.90 (Nap-<u>C</u>H$_2$-), 71.54 (C-5'), 26.39 (OC(<u>C</u>H$_3$)$_2$O), 25.13 (OC(<u>C</u>H$_3$)$_2$O); HRMS (ESI$^+$) calcd. For $C_{24}H_{25}N_5NaO_4^+$ 470.1799, found 470.1806.



Preparation of compound 26a

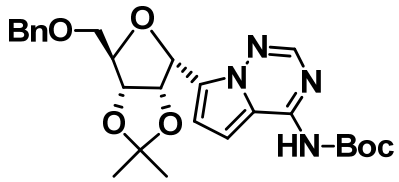
Method 1:

From compound **12a** (0.64 mmol) and **18a**[1] (1.92 mmol), **general procedure A** and then **general procedure B** yielded product **26a** (colorless amorphous solid, 252 mg, 0.49 mmol, 77%). R_f 0.39 (4:1, 60 - 90 °C petroleum ether – EtOAc); [α] $_D^{20}$ -118.18 (*c* 0.110 $CHCl_3$); HPLC t_R 3.38 min; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.16 (s, 1H, ArH), 7.40 – 7.30 (m, 5H, Bn-H), 7.25 (d, *J* = 4.7 Hz, 1H, ArH), 7.04 (s, 1H, ArH), 5.80 (s, 1H, H-1'), 4.64 – 4.58 (m, 3H, H-3', Bn-C<u>H</u>$_2$-), 4.37 (t, *J* = 4.2 Hz, 1H, H-4'), 3.71 (d, *J* = 4.2 Hz, 2H, H-5'a, H-5'b), 1.59 (s, 3H, 2'-C<u>H</u>$_3$), 1.57 (s, 9H, C(C<u>H</u>$_3$)$_3$), 1.45 (s, 3H, OC(C<u>H</u>$_3$)$_2$O), 1.37 (s, 3H, OC(C<u>H</u>$_3$)$_2$O), NH is missing; Selected NOESY (500 MHz, $CDCl_3$): δ (^{1}H) / δ (^{1}H) = 5.80 / 3.71 (H-1' / H-5'a, H-5'b); ^{13}C NMR (126 MHz, $CDCl_3$) δ 151.39 (ArC), 150.46 (C=O), 145.89 (ArC), 137.89 (Bn-C), 129.29 (ArC), 128.53 (2 x Bn-C), 127.85 (2 x Bn-C), 127.79 (Bn-C), 115.14 (ArC), 114.02 (ArC), 113.01 (O<u>C</u>(CH$_3$)$_2$O), 105.87 (ArC), 91.08 (C-2'), 89.43 (C-3'), 83.20 (C-4'), 82.56 (<u>C</u>(CH$_3$)$_3$), 80.47 (C-1'), 73.78 (Bn-<u>C</u>H$_2$-), 71.17 (C-5'), 28.26 (C(<u>C</u>H$_3$)$_3$), 27.71 (OC(<u>C</u>H$_3$)$_2$O), 27.46 (OC(<u>C</u>H$_3$)$_2$O), 23.09 (2'-<u>C</u>H$_3$); HRMS (ESI$^+$) calcd. For $C_{27}H_{34}N_4NaO_6^+$ 533.2371, found 533.2382.

[1] (a) B. Thomas, C. Aesop, G. Benjamin R., K. Choung U., M. Samuel E., S. Oliver L., W. Andrew W., J. Xu and L. Zhang, WO2011035250A1, 2011. (b) R. Pontiggia, O. Pontiggia, M. Simian, J. M. Montserrat, J. W. Engels and A. M. Iribarren, *Bioorg. Med. Chem. Lett.*, 2010, **20**, 2806-2808.

Method 2:

From compound **12a** (0.64 mmol) and **18a** (1.92 mmol), **general procedure A** and then **general procedure E** yielded product **26a** (colorless amorphous solid, 242 mg, 0.47 mmol, 74%). ^{1}H-NMR of product **26a** obtained from method 2 was identical to that from method 1.



Preparation of compound 26b

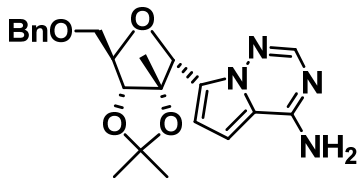
Method 1:

From compound **12a** (0.64 mmol) and **18b**[2] (1.92 mmol), **general procedure A** and then **general procedure B** yielded product **26b** (colorless amorphous solid, 248 mg, 0.50 mmol, 78%). R_f 0.32 (4:1, 60 - 90 ^{o}C petroleum ether – EtOAc); $[\alpha]_D^{20}$ -123.08 (*c* 0.130 $CHCl_3$); HPLC t_R 3.30 min; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.17 (s, 1H, ArH), 7.38 – 7.27 (m, 5H, Bn-H), 7.23 (d, *J* = 4.7 Hz, 1H, ArH), 7.08 – 6.95 (m, 1H, ArH), 5.91 – 5.78 (m, 1H, H-1'), 5.14 – 5.07 (m, 1H, H-2'), 4.94 (d, *J* = 6.0 Hz, 1H, H-3'), 4.63 – 4.55 (m, 2H, Bn-C$\underline{H}_2$-), 4.40 (t, *J* = 3.9 Hz, 1H, H-4'), 3.71 – 3.65 (m, 2H, H-5'a, H-5'b), 1.57 (s, 9H, C(C$\underline{H}_3$)$_3$), 1.39 (s, 3H, OC(C$\underline{H}_3$)$_2$O), 1.28 (s, 3H, OC(C$\underline{H}_3$)$_2$O), NH is missing; Selected NOESY (500 MHz, $CDCl_3$): δ (^{1}H) / δ (^{1}H) = 5.91 – 5.78 / 3.71 – 3.65 (H-1' / H-5'a, H-5'b); ^{13}C NMR (126 MHz, $CDCl_3$) δ 151.21 (ArC), 150.37 (C=O), 146.11 (ArC), 137.95 (Bn-C), 129.09 (ArC), 128.59 (2 x Bn-C), 127.88 (Bn-C), 127.74 (2 x Bn-C), 115.02 (ArC), 113.30 (ArC), 112.77 (O$\underline{C}$(CH$_3$)$_2$O), 105.59 (ArC), 83.54 (C-3'), 82.93 (C-4'), 82.66 ($\underline{C}$(CH$_3$)$_3$), 81.55 (C-2'), 77.26 (C-1'), 73.75 (Bn-$\underline{C}$H$_2$-), 71.33 (C-5'), 28.28 (C($\underline{C}$H$_3$)$_3$), 26.37 (OC($\underline{C}$H$_3$)$_2$O), 25.19 (OC($\underline{C}$H$_3$)$_2$O); HRMS (ESI^{+}) calcd. For $C_{26}H_{32}N_4NaO_6^{+}$ 519.2214, found 519.2228.

Method 2:

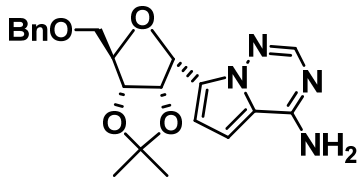
[2] (a) M. Shiozaki, *Carbohyd. Res.*, 2001, **335**, 147-150. (b) V. E. Marquez, M. I. Lim, C. K. H. Tseng, A. Markovac, M. A. Priest, M. S. Khan and B. Kaskar, *J. Org. Chem.*, 1988, **53**, 5709-5714.

From compound **12a** (0.64 mmol) and **18b** (1.92 mmol), **general procedure A** and then **general procedure E** yielded product **26b** (colorless amorphous solid, 242 mg, 0.49 mmol, 76%). ^{1}H-NMR of product **26b** obtained from method 2 was identical to that from method 1.



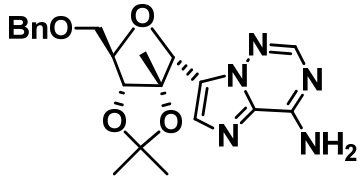
Preparation of compound 27a

From compound **12a** (0.64 mmol) and **18a** (1.92 mmol), **general procedure A** and then **general procedure C** yielded product **27a** (colorless amorphous solid, 144 mg, 0.35 mmol, 55%). R_f 0.44 (15 : 1, DCM : MeOH); $[\alpha]_D^{20}$ -114.86 (*c* 0.175 $CHCl_3$); HPLC t_R 2.91 min; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.90 (s, 1H, ArH), 7.41 – 7.28 (m, 5H, Bn-H), 6.91 (d, *J* = 4.5 Hz, 1H, ArH), 6.66 (d, *J* = 4.5 Hz, 1H, ArH), 5.77 (s, 3H, H-1', $N\underline{H}_2$), 4.64 – 4.58 (m, 3H, H-3', Bn-$C\underline{H}_2$-), 4.35 (t, *J* = 4.4 Hz, 1H, H-4'), 3.71 (d, *J* = 4.5 Hz, 2H, H-5'a, H-5'b), 1.58 (s, 3H, 2'-CH_3), 1.50 (s, 3H, OC($C\underline{H}_3$)$_2$O), 1.40 (s, 3H, OC($C\underline{H}_3$)$_2$O); Selected NOESY (600 MHz, $CDCl_3$): δ (^{1}H) / δ (^{1}H) = 5.77 / 3.71 (H-1' / H-5'a, H-5'b); ^{13}C NMR (151 MHz, $CDCl_3$) δ 155.31 (ArC), 146.85 (ArC), 137.93 (Bn-C), 128.57 (2 x Bn-C), 127.90 (3 x Bn-C, ArC), 114.15 (ArC), 113.00 (O$\underline{C}$(CH_3)$_2$O), 112.66 (ArC), 100.61 (ArC), 90.90 (C-2'), 89.38 (C-3'), 83.04 (C-4'), 80.10 (C-1'), 73.78 (Bn-$\underline{C}H_2$-), 71.03 (C-5'), 27.84 (OC($\underline{C}H_3$)$_2$O), 27.56 (OC($\underline{C}H_3$)$_2$O), 22.98 (2'-$\underline{C}H_3$); HRMS (ESI^+) calcd. For $C_{22}H_{26}N_4NaO_4^+$ 433.1846, found 433.1848.



Preparation of compound 27b

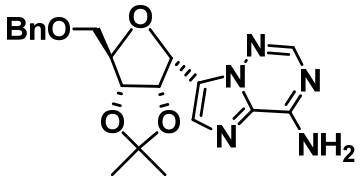
From compound **12a** (0.64 mmol) and **18b** (1.92 mmol), **general procedure A** and then **general procedure C** yielded product **27b** (colorless amorphous solid, 150 mg, 0.38 mmol, 59%). R_f 0.54 (15 : 1, DCM : MeOH); $[\alpha]_D^{20}$ -105.45 (*c* 0.110 $CHCl_3$); HPLC t_R 2.83 min; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.93 (s, 1H, ArH), 7.38 – 7.29 (m, 5H, Bn-H), 6.89 (d, *J* = 4.5 Hz, 1H, ArH), 6.65 (d, *J* = 4.5 Hz, 1H, ArH), 5.84 (d, *J* = 4.0 Hz, 1H, H-1'), 5.42 (br s, 2H, N$\underline{H}_2$), 5.06 (dd, *J* = 5.9, 4.1 Hz, 1H, H-2'), 4.95 – 4.93 (m, 1H, H-3'), 4.63 – 4.56 (m, 2H, Bn-C$\underline{H}_2$-), 4.38 (t, *J* = 4.2 Hz, 1H, H-4'), 3.69 – 3.64 (m, 2H, H-5'a, H-5'b), 1.45 (s, 3H, OC(C$\underline{H}_3$)$_2$O), 1.30 (s, 3H, OC(C$\underline{H}_3$)$_2$O); Selected NOESY (600 MHz, $CDCl_3$): δ (^{1}H) / δ (^{1}H) = 5.84 / 3.69 – 3.64 (H-1' / H-5'a, H-5'b); ^{13}C NMR (151 MHz, $CDCl_3$) δ 155.16 (ArC), 147.14 (ArC), 137.98 (Bn-C), 128.61 (2 x Bn-C), 127.89 (Bn-C), 127.80 (2 x Bn-C), 127.68 (ArC), 114.02 (ArC), 112.75 (O$\underline{C}$(CH$_3$)$_2$O), 112.03 (ArC), 100.33 (ArC), 83.57 (C-3'), 82.80 (C-4'), 81.59 (C-2'), 76.73 (C-1'), 73.74 (Bn-$\underline{C}$H$_2$-), 71.13 (C-5'), 26.41 (OC($\underline{C}$H$_3$)$_2$O), 25.15 (OC($\underline{C}$H$_3$)$_2$O); HRMS (ESI$^+$) calcd. For $C_{21}H_{25}N_4O_4^+$ 397.1870, found 397.1875.



Preparation of compound 29a

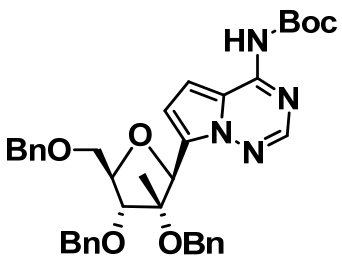
From compound **12b** (0.64 mmol) and **18a** (1.92 mmol), **general procedure A** and then **general procedure D** yielded product **29a** (colorless amorphous solid, 147 mg, 0.36 mmol, 56%). R_f 0.48 (15 : 1, DCM : MeOH); $[\alpha]_D^{20}$ -69.52 (*c* 0.105 $CHCl_3$); HPLC t_R 3.10 min; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.11 (s, 1H, ArH), 7.76 (s, 1H, ArH), 7.40 – 7.31 (m, 5H, Bn-H), 5.63 (s, 1H, H-1'), 4.65 – 4.58 (m, 3H, H-3', Bn-C$\underline{H}_2$-), 4.35 – 4.33 (m, 1H, H-4'), 3.75 – 3.70 (m, 2H, H-5'a, H-5'b), 1.57 (s, 3H, 2'-C$\underline{H}_3$), 1.49 (s, 3H, OC(C$\underline{H}_3$)$_2$O), 1.40 (s, 3H, OC(C$\underline{H}_3$)$_2$O), NH_2 are missing; Selected NOESY (500 MHz, $CDCl_3$): δ (^{1}H) / δ (^{1}H) = 5.63 / 3.75 – 3.70 (H-1' / H-5'a, H-5'b); ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.75 (ArC), 148.81 (ArC), 137.86 (Bn-C), 132.76 (ArC), 128.63 (2 x Bn-C), 128.44 (ArC), 127.98 (Bn-C), 127.94 (2 x

Bn-C), 126.99 (ArC), 113.22 (O<u>C</u>$(CH_3)_2$O), 90.83 (C-2'), 89.44 (C-3'), 83.48 (C-4'), 79.75 (C-1'), 73.88 (Bn-<u>C</u>H_2-), 71.43 (C-5'), 27.87 (OC(<u>C</u>$H_3)_2$O), 27.59 (OC(<u>C</u>$H_3)_2$O), 22.79 (2'-<u>C</u>H_3); HRMS (ESI^+) calcd. For $C_{21}H_{26}N_5O_4^+$ 412.1979, found 412.1985.



Preparation of compound 29b

From compound **12b** (0.64 mmol) and **18b** (1.92 mmol), **general procedure A** and then **general procedure D** yielded product **29b** (colorless amorphous solid, 140 mg, 0.35 mmol, 55%). R_f 0.51 (15 : 1, DCM : MeOH); $[\alpha]_D^{20}$ -93.91 (*c* 0.115 $CHCl_3$); HPLC t_R 2.92 min; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.12 (s, 1H, ArH), 7.74 (s, 1H, ArH), 7.37 – 7.29 (m, 5H, Bn-H), 5.76 (d, *J* = 4.1 Hz, 1H, H-1'), 5.06 (dd, *J* = 5.9, 4.2 Hz, 1H, H-2'), 4.97 (d, *J* = 6.0 Hz, 1H, H-3'), 4.64 – 4.55 (m, 2H, Bn-C<u>H</u>$_2$-), 4.39 (t, *J* = 3.7 Hz, 1H, H-4'), 3.71 (dd, *J* = 10.2, 3.7 Hz, 1H, H-5'a), 3.67 (dd, *J* = 10.2, 3.9 Hz, 1H, H-5'b), 1.45 (s, 3H, OC(C<u>H</u>$_3)_2$O), 1.31 (s, 3H, OC(C<u>H</u>$_3)_2$O), NH_2 are missing; Selected NOESY (600 MHz, $CDCl_3$): δ (^{1}H) / δ (^{1}H) = 5.76 / 3.71, 3.67 (H-1' / H-5'a, H-5'b); ^{13}C NMR (151 MHz, $CDCl_3$) δ 153.74 (ArC), 148.86 (ArC), 137.88 (Bn-C), 132.05 (ArC), 128.64 (2 x Bn-C), 128.38 (ArC), 127.95 (Bn-C), 127.77 (2 x Bn-C), 126.80 (ArC), 112.96 (O<u>C</u>$(CH_3)_2$O), 83.62 (C-3'), 83.06 (C-4'), 81.66 (C-2'), 76.05 (C-1'), 73.78 (Bn-<u>C</u>H_2-), 71.53 (C-5'), 26.39 (OC(<u>C</u>$H_3)_2$O), 25.15 (OC(<u>C</u>$H_3)_2$O); HRMS (ESI^+) calcd. For $C_{20}H_{24}N_5O_4^+$ 398.1823, found 398.1828.



Preparation of compound 31a

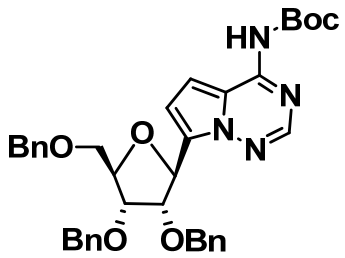
Method 1:

From compound **12a** (0.64 mmol) and **19**[3] (1.92 mmol), **general procedure A** and then **general procedure E** yielded product **31a** (colorless amorphous solid, 337 mg, 0.52 mmol, 81%). R_f 0.44 (4:1, 60 - 90 ^{o}C petroleum ether – EtOAc); $[\alpha]_D^{20}$ 24.52 (*c* 0.155 $CHCl_3$); HPLC t_R 4.10 min; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.15 (s, 2H, ArH, N<u>H</u>), 7.43 – 7.25 (m, 15H, Bn-H), 7.10 (dd, *J* = 21.6, 4.0 Hz, 2H, ArH), 5.94 (s, 1H, H-1'), 4.86 (dd, *J* = 55.4, 12.0 Hz, 2H, Bn-C<u>H</u>$_2$-), 4.69 – 4.57 (m, 4H, 2 x Bn-C<u>H</u>$_2$-), 4.42 (d, *J* = 8.3 Hz, 1H, H-4'), 4.06 (d, *J* = 8.7 Hz, 1H, H-3'), 3.91 (d, *J* = 10.5 Hz, 1H, H-5'a), 3.72 (dd, *J* = 10.9, 3.2 Hz, 1H, H-5'b), 1.57 (s, 9H, C(C<u>H</u>$_3$)$_3$), 1.01 (s, 3H, 2'-C<u>H</u>$_3$); Selected NOESY (600 MHz, $CDCl_3$): δ (^{1}H) / δ (^{1}H) = 7.10 / 3.91, 3.72, 4.06 (ArH / H-5'a, H-5'b, H-3'); ^{13}C NMR (151 MHz, $CDCl_3$) δ 151.20 (ArC), 150.35 (C=O), 146.02 (ArC), 139.76 (Bn-C), 138.30 (Bn-C), 138.26 (Bn-C), 132.14 (ArC), 128.55 (2 x Bn-C), 128.42 (2 x Bn-C), 128.32 (3 x Bn-C), 127.97 (2 x Bn-C), 127.95 (2 x Bn-C), 127.81 (Bn-C), 127.26 (2 x Bn-C), 127.21 (Bn-C), 115.10 (ArC), 112.41 (ArC), 105.63 (ArC), 85.18 (C-2'), 82.81 (<u>C</u>(CH$_3$)$_3$), 82.17 (C-3'), 79.39 (C-4'), 77.97 (C-1'), 73.59 (2 x Bn-<u>C</u>H$_2$-), 69.17 (C-5'), 65.91 (Bn-<u>C</u>H$_2$-), 28.26 (C(<u>C</u>H$_3$)$_3$), 17.47 (2-<u>C</u>H$_3$); HRMS (ESI$^+$) calcd. For $C_{38}H_{42}N_4NaO_6^+$ 673.2997, found 673.3004.

Method 2:

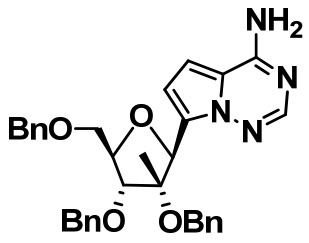
From compound **12a** (0.64 mmol) and **19** (1.92 mmol), **general procedure A** and then **general procedure B** yielded product **31a** (colorless amorphous solid, 333 mg, 0.51 mmol, 80%). ^{1}H-NMR of product **31a** obtained from method 2 was identical to that from method 1.

[3] A. Tokarenko, L. Postova Slavetinska, B. Klepetarova and M. Hocek, *Eur. J. Org. Chem.*, 2015, 7962-7983.



Preparation of compound 31b

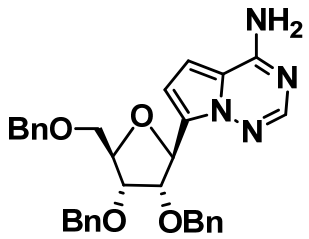
From compound **12a** (0.64 mmol) and **3**[4] (1.92 mmol), **general procedure A** and then **general procedure E** yielded product **31b** (colorless amorphous solid, 355 mg, 0.56 mmol, 87%). R_f 0.32 (4:1, 60 - 90 °C petroleum ether – EtOAc); $[\alpha]_D^{20}$ 69.49 (*c* 0.495 $CHCl_3$); HPLC t_R 3.97 min; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.77 (s, 1H, NH), 8.20 (s, 1H, ArH), 7.33 – 7.25 (m, 15H, Bn-H), 7.15 (d, *J* = 4.7 Hz, 1H, ArH), 6.93 – 6.81 (m, 1H, ArH), 5.74 (d, *J* = 3.6 Hz， 1H, H-1'), 4.73 (t, *J* = 10.2 Hz, 2H, Bn-CH_2-), 4.62 – 4.51 (m, 3H, Bn-CH_2-, Bn-CH_2-), 4.43 – 4.39 (m, 2H, H-4', Bn-CH_2-), 4.23 – 4.20 (m, 1H, H-2'), 4.11 (dd, *J* = 6.7, 4.9 Hz, 1H, H-3'), 3.82 – 3.76 (m, 1H, H-5'a), 3.66 (dd, *J* = 10.8, 3.9 Hz, 1H, H-5'b), 1.57 (s, 9H, C(CH_3)$_3$); Selected NOESY (500 MHz, $CDCl_3$): δ (^{1}H) / δ (^{1}H) = 6.93 – 6.81 / 3.82 – 3.76, 3.66 (ArH / H-5'a, H-5'b); ^{13}C NMR (126 MHz, $CDCl_3$) δ 151.45 (ArC), 150.55 (C=O), 145.98 (ArC), 138.34 (Bn-C), 137.97 (Bn-C), 137.95 (Bn-C), 131.06 (ArC), 128.45 (2 x Bn-C), 128.42 (2 x Bn-C), 128.37 (2 x Bn-C), 128.22 (2 x Bn-C), 127.96 (2 x Bn-C), 127.83 (2 x Bn-C), 127.71 (2 x Bn-C), 127.67 (Bn-C), 115.71 (ArC), 112.24 (ArC), 106.04 (ArC), 82.76 (C(CH$_3$)$_3$), 80.63 (C-4'), 79.12 (C-2'), 77.23 (C-3'), 76.36 (C-1'), 73.48 (Bn-CH_2-), 72.13 (Bn-CH_2-), 71.70 (Bn-CH_2-), 69.70 (C-5'), 28.27 (C(CH_3)$_3$); HRMS (ESI$^+$) calcd. For $C_{37}H_{40}N_4NaO_6^+$ 659.2840, found 659.2854.



[4] (a) B. Bernet, S. E. Mangholz, K. Briner and A. Vasella, *Helv. Chim. Acta*, 2003, **86**, 1488-1521. (b) S. E. Mangholz and A. Vasella, *Helv. Chim. Acta*, 1995, **78**, 1020-1035.

Preparation of compound 32

From compound **12a** (0.64 mmol) and **19** (1.92 mmol), **general procedure A** and then **general procedure C** yielded product **32** (colorless amorphous solid, 229 mg, 0.42 mmol, 65%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (s, 1H), 7.51 – 7.20 (m, 15H), 6.90 (d, *J* = 4.5 Hz, 1H), 6.53 (d, *J* = 4.5 Hz, 1H), 5.91 (s, 1H), 5.65 (br s, 2H), 4.92 (d, *J* = 12.1 Hz, 1H), 4.81 (d, *J* = 12.1 Hz, 1H), 4.76 – 4.54 (m, 4H), 4.41 (dt, *J* = 8.4, 2.4 Hz, 1H), 4.08 (d, *J* = 8.7 Hz, 1H), 3.91 (dd, *J* = 10.9, 2.4 Hz, 1H), 3.72 (dd, *J* = 10.3, 4.2 Hz, 1H), 1.03 (s, 3H). NMR data was parallel to literature report.[5]

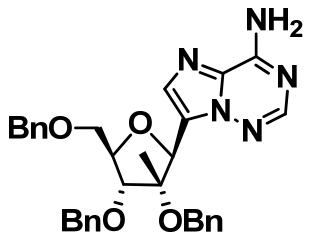


Preparation of compound 4a

From compound **12a** (0.64 mmol) and **3** (1.92 mmol), **general procedure A** and then **general procedure C** yielded product **4a** (colorless amorphous solid, 209 mg, 0.39 mmol, 61%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.90 (s, 1H), 7.34 – 7.24 (m, 15H), 6.68 (d, *J* = 4.5 Hz, 1H), 6.50 (d, *J* = 4.5 Hz, 1H), 5.72（br s, 2H） 5.68 (d, *J* = 4.2 Hz, 1H), 4.73 (q, *J* = 12.3 Hz, 2H), 4.60 (d, *J* = 12.0 Hz, 1H), 4.58 – 4.49 (m, 2H), 4.44 (d, *J* = 11.9 Hz, 1H), 4.40 (dt, *J* = 6.9, 3.8 Hz, 1H), 4.27 (t, *J* = 4.6 Hz, 1H), 4.12 (dd, *J* = 6.4, 5.1 Hz, 1H), 3.78 (dd, *J* = 10.7, 3.4 Hz, 1H), 3.66 (dd, *J* = 10.7, 4.1 Hz, 1H). NMR data was parallel to literature report.[6]

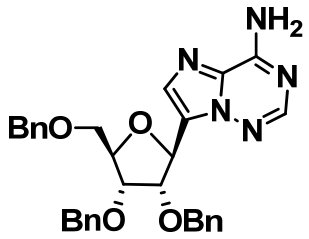
[5] Y. S. Babu, P. Chand, P. Kotian; M. Wu and V. S. Kumar, US 20090227524A1, 2009.

[6] J. M. LEE and M. CHOI, WO2014035140A2, 2014.



Preparation of compound 34

From compound **12b** (0.64 mmol) and **19** (1.92 mmol), **general procedure A** and then **general procedure D** yielded product **34** (colorless amorphous solid, 212 mg, 0.38 mmol, 60%). ^{1}H-NMR (500 MHz, $CDCl_3$) δ 8.08 (s, 1H), 7.74 (s, 1H), 7.50 – 7.22 (m, 15H), 5.75 (s, 1H), 4.83 (t, *J* = 8.3 Hz, 2H), 4.69 – 4.62 (m, 3H), 4.58 (d, *J* = 11.9 Hz, 1H), 4.44 – 4.38 (m, 1H), 4.08 (d, *J* = 8.4 Hz, 1H), 3.89 (dd, *J* = 10.9, 2.6 Hz, 1H), 3.71 (dd, *J* = 10.9, 3.5 Hz, 1H), 1.10 (s, 3H). NMR data was parallel to literature report.[7]

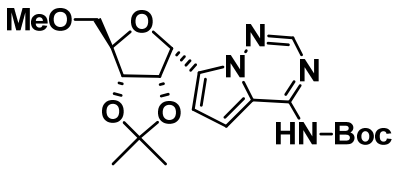


Preparation of compound 4b

From compound **12b** (0.64 mmol) and **3** (1.92 mmol), **general procedure A** and then **general procedure D** yielded product **4b** (colorless amorphous solid, 203 mg, 0.38 mmol, 59%). ^{1}H-NMR (400 MHz, CD_3OD) δ 7.97 (s, 1H), 7.46 (s, 1H), 7.33 – 7.26 (m, 10H), 7.22 – 7.18 (m, 5H), 5.45 (d, *J* = 5.2 Hz, 1H), 4.66 (d, *J* = 12.1 Hz, 1H), 4.61 (d, *J* = 2.9 Hz, 1H), 4.58 (d, *J* = 3.2 Hz, 1H), 4.51 (dd, *J* = 12.0, 5.1 Hz, 3H), 4.43 (t, *J* = 5.1 Hz, 1H), 4.31 – 4.26 (m, 1H), 4.20 (t, *J* = 5.2 Hz, 1H), 3.71 (dd, *J* = 10.7, 3.7 Hz, 1H), 3.62 (dd, *J* = 10.8, 4.2 Hz, 1H). NMR data was parallel to literature report.[6] ^{1}H NMR was also measured in $CDCl_3$ for better resolution: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (s, 1H), 7.48 (s, 1H), 7.37 – 7.23 (m, 15H), 5.62 – 5.52 (m, 1H), 4.74 – 4.62 (m, 2H), 4.58 (dd, *J* = 11.9, 3.3 Hz, 2H), 4.55 – 4.47 (m, 2H), 4.40

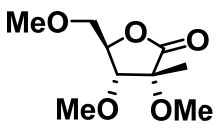
[7] A. CHO, C. U. KIM, J. PARRISH and J. XU, WO2009132123A1, 2009.

(dt, *J* = 5.6, 3.9 Hz, 1H), 4.35 (t, *J* = 5.0 Hz, 1H), 4.15 (t, *J* = 5.4 Hz, 1H), 3.74 (dd, *J* = 10.7, 3.7 Hz, 1H), 3.63 (dd, *J* = 10.7, 4.0 Hz, 1H), NH_2 are missing.



Preparation of compound 37

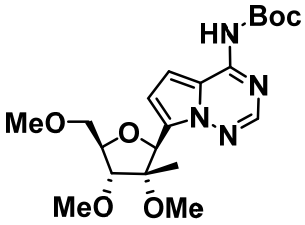
From compound **12a** (0.64 mmol) and compound **35**[8] (1.92 mmol), **general procedure A** and then **general procedure E** yielded product **37** (colorless oil, 194 mg, 0.46 mmol, 72%). R_f 0.31 (2:1, 60 - 90 ^oC petroleum ether – EtOAc); $[\alpha]_D^{20}$ -97.50 (*c* 0.160 $CHCl_3$); HPLC t_R 2.80 min; ^1H NMR (500 MHz, Chloroform-*d*) δ 8.16 (s, 1H, ArH), 7.87 (br s, 1H, N<u>H</u>), 7.18 (d, *J* = 4.1 Hz, 1H, ArH), 7.06 – 6.90 (m, 1H, ArH), 5.82 – 5.68 (m, 1H, H-1'), 5.11 – 5.05 (m, 1H, H-2'), 4.91 (d, *J* = 5.9 Hz, 1H, H-3'), 4.38 (t, *J* = 3.9 Hz, 1H, H-4'), 3.62 – 3.58 (m, 2H, H-5'a, H-5'b), 3.40 (s, 3H, 5'-OC<u>H</u>$_3$), 1.56 (s, 9H, C(C<u>H</u>$_3$)$_3$), 1.38 (s, 3H, OC(C<u>H</u>$_3$)$_2$O), 1.28 (s, 3H, OC(C<u>H</u>$_3$)$_2$O); Selected NOESY (500 MHz, $CDCl_3$): δ (^1H) / δ (^1H) = 5.82 – 5.68 / 3.62 – 3.58 (H-1' / H-5'a, H-5'b); ^{13}C NMR (151 MHz, $CDCl_3$) δ 151.06 (ArC), 150.16 (C=O), 146.24 (ArC), 129.06 (ArC), 114.93 (ArC), 113.27 (ArC), 112.78 (O<u>C</u>(CH$_3$)$_2$O), 104.97 (ArC), 83.42 (C-3'), 82.84 (C-4'), 82.71 (<u>C</u>(CH$_3$)$_3$), 81.47 (C-2'), 77.23 (C-1'), 73.92 (C-5'), 59.65 (5'-O<u>C</u>H$_3$), 28.27 (C(<u>C</u>H$_3$)$_3$), 26.35 (OC(<u>C</u>H$_3$)$_2$O), 25.16 (OC(<u>C</u>H$_3$)$_2$O); HRMS (ESI$^+$) calcd. For $C_{20}H_{29}N_4O_6^+$ 421.2082, found 421.2075.



Preparation of compound 38

[8] L. Hough, J. K. N. Jones and D. L. Mitchell, *Can. J. Chem.*, 1958, **36**, 1720-1728.

A suspension of NaH (60% in mineral oil, 1.0 g, 25.90 mmol) in DMF (20 mL) was cooled to 0 °C. To this suspension, a solution of 2-*C*-methyl D-ribonic acid *gamma*-lactone (1.0 g, 0.62 mmol) in DMF (5 mL) was added dropwise. The mixture was stirred at 0 °C for 30 min, treated with CH_3I (1.7 mL, 27.75 mmol), warmed to RT, and stirred at this temperature for 3 h before cold water (60 mL) was added. The mixture was then extracted with ethyl acetate (10 mL x 3). Combined organic phases were washed with brine (100 mL), dried with Na_2SO_4, concentrated to dryness, and purified with flash chromatography on silica gel (5:1， 60 - 90 °C petroleum ether – EtOAc to afford product **38** (colorless oil, 806 mg, 64%). R_f 0.47 (2:1, 60 - 90 °C petroleum ether – EtOAc); $[\alpha]_D^{20}$ 101.63 (*c* 0.735 $CHCl_3$); ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.40 (ddd, *J* = 8.0, 3.7, 2.3 Hz, 1H, H-4'), 3.76 – 3.71 (m, 2H, H-3', H-5'a), 3.60 (dd, *J* = 11.6, 3.7 Hz, 1H, H-5'b), 3.54 (s, 3H, OC$\underline{H}_3$), 3.39 (s, 3H, OC$\underline{H}_3$), 3.38 (s, 3H, OC$\underline{H}_3$), 1.52 (s, 3H, 2-C$\underline{H}_3$); ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.48 (C=O), 82.63 (C-3'), 79.88 (C-4'), 77.09 (C-2'), 70.12 (C-5'), 59.92 (O$\underline{C}H_3$), 59.58 (O$\underline{C}H_3$), 52.88 (O$\underline{C}H_3$), 17.95 (2'-$\underline{C}H_3$). HRMS (ESI^+) calcd. For $C_9H_{17}O_5^+$ 205.1071, found 205.1065.



Preparation of compound 40

From compound **12a** (0.64 mmol) and compound **38** (1.92 mmol), **general procedure A** and then **general procedure E** yielded product **40** (colorless oil, 214 mg, 0.51 mmol, 79%). R_f 0.38 (1:1, 60 - 90 °C petroleum ether – EtOAc); $[\alpha]_D^{20}$ 85.60 (*c* 0.125 $CHCl_3$); HPLC t_R 2.62 min; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.15 (s, 2H, N$\underline{H}$, ArH), 7.21 (d, *J* = 4.6 Hz, 1H, ArH), 7.13 – 6.99 (m, 1H, ArH), 5.85 (s, 1H, H-1'), 4.19 (dt, *J* = 8.6, 2.8 Hz, 1H, H-4'), 3.82 (dd, *J* = 11.0, 2.1 Hz, 1H, H-5'a), 3.72 (d, *J* = 8.8 Hz, 1H, H-3'), 3.66 (dd, *J* = 11.0, 3.6 Hz, 1H, H-5'b), 3.52 (s, 3H, OC$\underline{H}_3$), 3.51 (s, 3H, OC$\underline{H}_3$), 3.49 (s, 3H, OC$\underline{H}_3$), 1.56 (s, 9H, C(C$\underline{H}_3$)$_3$), 1.03 (s, 3H, 2'-C$\underline{H}_3$); Selected NOESY (500 MHz, $CDCl_3$): δ (^{1}H) / δ (^{1}H) = 7.13 –

6.99 / 3.82, 3.72, 3.66 (ArH / H-5'a, H-3', H-5'b); ^{13}C NMR (126 MHz, $CDCl_3$) δ 151.31 (ArC), 150.41 (C=O), 146.04 (ArC), 132.22 (ArC), 115.15 (ArC), 112.25 (ArC), 105.91 (ArC), 84.77 (C-2'), 84.41 (C-3'), 82.79 ($\underline{C}(CH_3)_3$), 79.05 (C-4'), 76.47 (C-1'), 72.11 (C-5'), 60.03 ($O\underline{C}H_3$), 59.44 ($O\underline{C}H_3$), 51.34 ($O\underline{C}H_3$), 28.27 ($C(\underline{C}H_3)_3$), 16.46 (2'-$\underline{C}H_3$); HRMS (ESI^+) calcd. For $C_{20}H_{31}N_4O_6^+$ 423.2238, found 423.2248.

3. DFT Studies.

3.1 Computational Details.

All calculations were carried out with the Gaussian 09 program package.[9] Geometry optimization were performed at the M06-2*X*/6-31G(d,p) level,[10] using the SMD (Solvation Model based on Density) method[11] for dichloromethane to incorporate solvent effects. Freqency analysis was conducted at the same level of theory to confirm the obtained geometries as local energy minima or transition states, and to acquire the the thermal corrections to Gibbs free energies. The larger basis sets, 6-311+G(d,p), were applied to upgrade the precision of single-point energies to triple-ζ quality. Finally, the Gibbs free energies were obtained by adding the thermal corrections, acquired from the frequencies calculated previously, to the precise single-point energies. The M06-2*X* calculated energies and optimized geometris are summarized in Table S1 and Fig. S1-S4.

According to experimental results, the dehydroxylation processes of hemiketal intermediates **25b**, **30b**, **36** and **39** were not related to the anomeric stereoselectivity of products **26b**, **31b**, **37** and **40**. Thus, the conformers of hemiketal intermediates **25b**, **30b**, **36** and **39** with lower free energies were used simply to

[9] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, et al. Gaussian 09, Revision C.01., Gaussian, Inc.: Wallingford, CT, 2009.

[10] (a) Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.,* 2008, **120,** 215-241. (b) R. Ditchfield, W. J. Hehre and J. A. Pople, *J. Chem. Phys.,* 1971, **54,** 724.

[11] A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B.,* 2009, **113,** 6378-6396.

describe the energy profiles (Fig. 1 in manuscript). The detail information of the high energy anomers of the hemiketals is included in Table S1. Meanwhile, the calculation yielded a different conformation of Et_3SiH in **TS-39-40** from that in other transition structures. Thus, the new conformer of Et_3SiH was used to replace the silane in **TS-39**-*alpha*-**40** to yield a new transition structure ***TS-39**-*alpha*-**40**. The calculation result suggested that **TS-39**-*alpha*-**40** is indeed more stable than ***TS-39**-*alpha*-**40**. Information of ***TS-39**-*alpha*-**40** is included in Table S1, too.

Table S1. Summary of M06-2*X* calculated energies for optimized geometries.

Geometry	Single-point Energy[a] (a.u.)	Thermal correction of Gibbs Free Energy[b] (a.u.)	Gibbs Free Energy[c] (a.u.)	IF[d] (cm^{-1})
BF_3	-324.563487	-0.013068	-324.576555	
$[HO(BF_3)_2]^-$	-725.2015801	0.006607	-725.1949731	
$HSiEt_3$	-527.7108455	0.171698	-527.5391475	
$HOSiEt_3$	-602.9963804	0.176082	-602.8202984	
25b	-1755.44973	0.509347	-1754.940383	
***25b**[e]	-1755.444997	0.506042	-1754.938955	
25b-cation	-1679.425592	0.49306	-1678.932532	
TS-25b-26b	-2207.129402	0.686231	-2206.443171	346.8775i
TS-25b-*beta*-**26b**	-2207.12766	0.688083	-2206.439577	325.2567i
26b	-1680.210433	0.501595	-1679.708838	
beta-**26b**	-1680.21406	0.505785	-1679.708275	
30b	-2179.355613	0.651859	-2178.703754	
***30b**[e]	-2179.351545	0.655849	-2178.695696	
30b-cation	-2103.335745	0.640557	-2102.695188	
TS-30b-*alpha*-**31b**	-2631.039632	0.836067	-2630.203565	352.9678i

TS-30b-31b	-2631.043803	0.835582	-2630.208221	312.8068i
alpha-**31b**	-2104.119535	0.649005	-2103.470530	
31b	-2104.122601	0.651223	-2103.471378	
36	-1524.421934	0.428537	-1523.993397	
***36**[e]	-1524.418964	0.429443	-1523.989521	
36-cation	-1448.397765	0.414358	-1447.983407	
TS-36-37	-1976.107259	0.60957	-1975.497689	-352.6338i
TS-36-*beta*-**37**	-1976.099366	0.608698	-1975.490668	-214.2035i
37	-1449.186442	0.423813	-1448.762629	
beta- **37**	-1449.184051	0.424371	-1448.75968	
39	-1525.586736	0.447176	-1525.13956	
***39**[e]	-1525.582237	0.45004	-1525.132197	
39-cation	-1449.561368	0.434461	-1449.126907	
TS-39-*alpha*-**40**	-1977.271403	0.630504	-1976.640899	-317.7540i
***TS-39**-*alpha*-**40**[f]	-1977.26792	0.63012	-1976.6378	-386.2618i
TS-39-40	-1977.274435	0.625623	-1976.648812	-348.6006i
alpha-**40**	-1450.347954	0.443812	-1449.904142	
40	-1450.352048	0.444593	-1449.907455	

a) Single-point energies were calculated at the M06-2*X*/6-311+G(d,p) level.

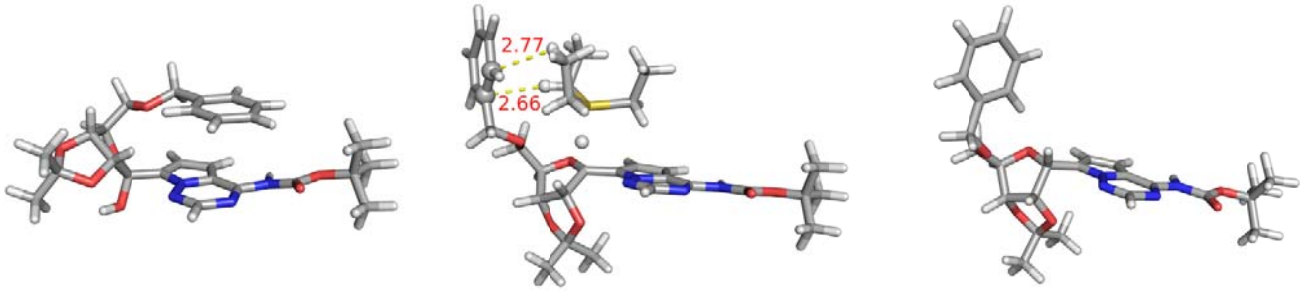
b) Thermal corrections of Gibbs free energies were calculated at the M06-2*X*/6-31G(d,p) level.

c) Gibbs free energies were obtained by adding the associated values in a) and b).

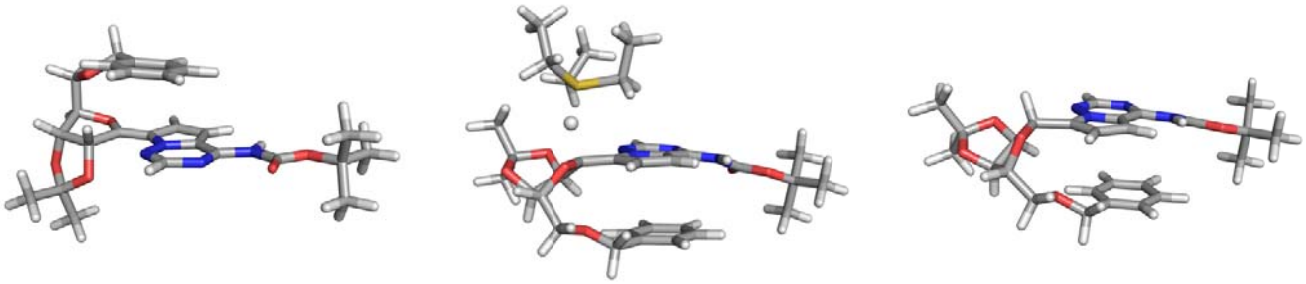
d) Imaginary frequencies were calculated at the M06-2*X*/6-31G(d,p) level for trafensition states.

e) Anomer of the hemiketal intermediate with higher free energy.

f) A transition state in which Et_3SiH adopts similar conformation with that in **TS-39-40**.

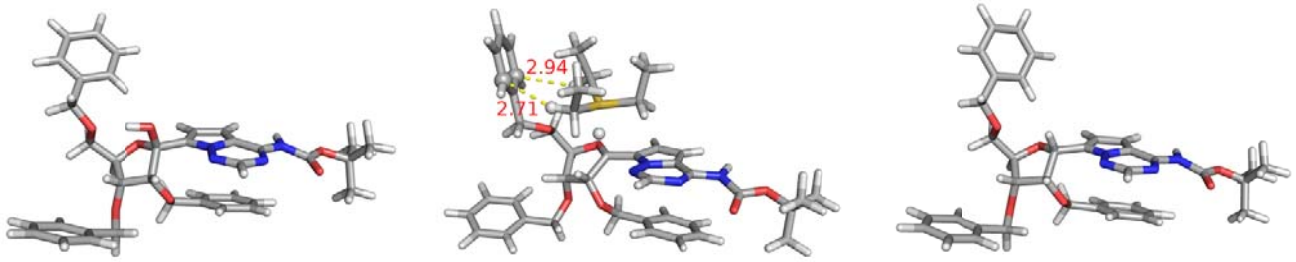


25b **TS-25b-26b** **26b**

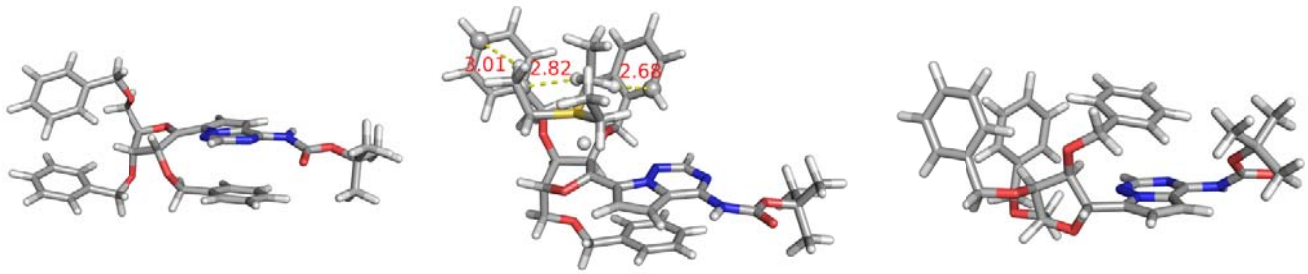


25b-cation **TS-25b-*beta*-26b** *beta*-**26b**

Fig. S1 Geometries optimimzed at the M06-2*X*/6-31G(d,p) level with SMD method for dichloromethane involved in the reduction reaction of hemiketal **25b**.

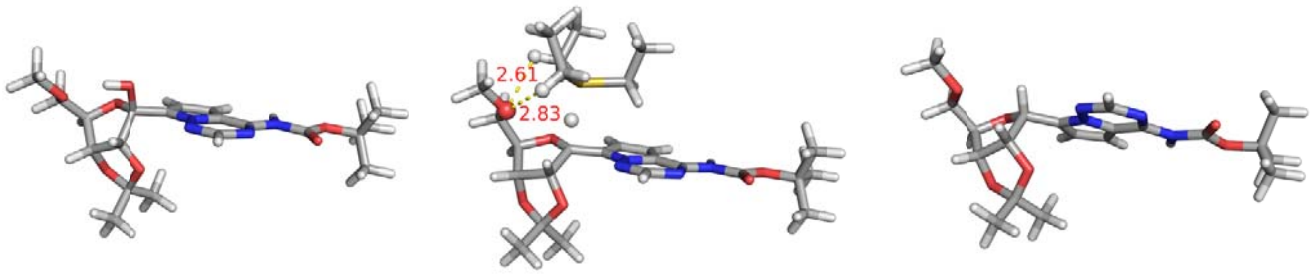


30b **TS-30b-*alpha*-31b** *alpha*-**31b**

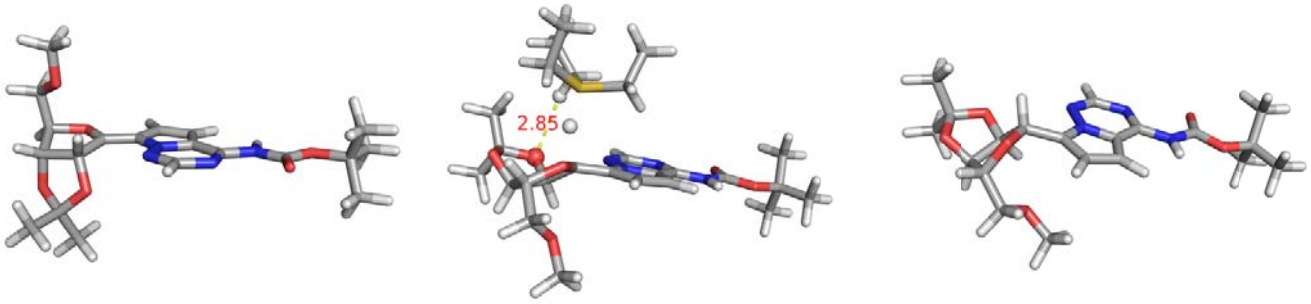


30b-cation **TS-30b-31b** **31b**

Fig. S2 Geometries optimimzed at the M06-2*X*/6-31G(d,p) level with SMD method for dichloromethane involved in the reduction reaction of hemiketal **30b**.

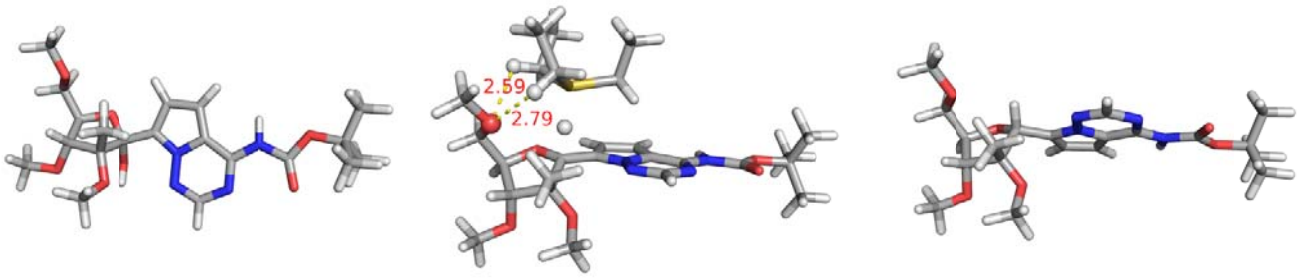


36 **TS-36-37** **37**

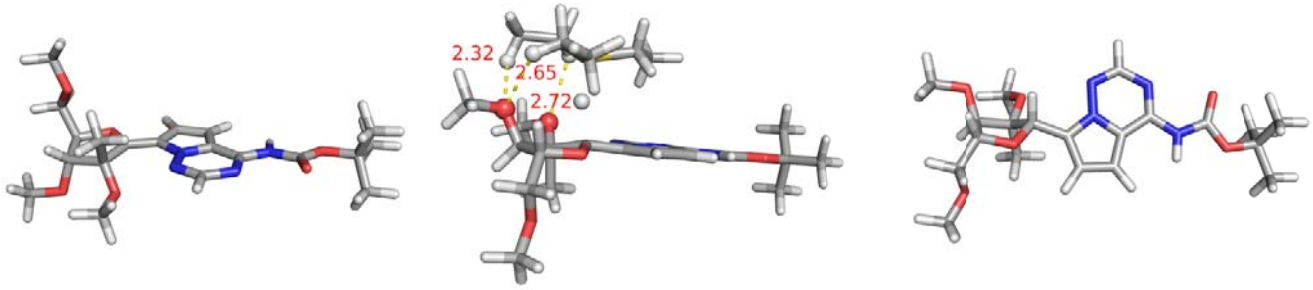


36-cation **TS-36-*beta*-37** *beta*-**37**

Fig. S3 Geometries optimimzed at the M06-2*X*/6-31G(d,p) level with SMD method for dichloromethane involved in the reduction reaction of hemiketal **36**.



39 **TS-39-*alpha*-40** *alpha*-**40**



39-cation **TS-39-40** **40**

Fig. S4 Geometries optimimzed at the M06-2*X*/6-31G(d,p) level with SMD method for dichloromethane involved in the reduction reaction of hemiketal **39**.

3.2 Cartesian Coordiantes of All Optimized Geometries.

BF_3

B	-0.65239100	-0.14851500	0.00000000
F	-1.30887800	0.99091300	0.00000000
F	0.66288600	-0.14851500	0.00000000
F	-1.30887800	-1.28794300	0.00000000

$[HO(BF_3)_2]^-$

B	1.97111200	-1.84860300	-0.01919300
F	0.77077000	-1.32884900	0.41963000
F	2.97425500	-1.69678100	0.92822400
F	1.84325700	-3.15589400	-0.43359800
O	2.45600800	-1.02374800	-1.22260900
H	3.18061400	-0.43555400	-0.96172600
B	1.50657100	-0.38189000	-2.24198600
F	0.50184300	-1.29991000	-2.45107700
F	2.26063700	-0.15376500	-3.37990600
F	1.03842900	0.80859200	-1.71650400

$HSiEt_3$

Si	-0.00130900	0.00157300	-1.03387700
H	-0.00239100	0.00628600	-2.52791800
C	-1.32820500	1.22125600	-0.45388000
H	-0.92813100	2.23924700	-0.54818200
H	-2.16786800	1.16489900	-1.15780400
C	-1.84533200	0.98667100	0.97119400
H	-1.04262700	1.04528400	1.71358800
H	-2.60264400	1.72738400	1.24924600
H	-2.30646300	-0.00218300	1.06554400
C	-0.38624400	-1.76205500	-0.46263200
H	0.10397000	-2.45366800	-1.15917900
H	-1.46327500	-1.94244900	-0.57354900
C	0.06092800	-2.08370500	0.96875700
H	-0.41661000	-1.42748000	1.70349000
H	-0.18368500	-3.11542300	1.24296700
H	1.14397500	-1.96460200	1.07912700
C	1.72054600	0.53776300	-0.45606300
H	2.40237700	-0.31715900	-0.55337700
H	2.09252800	1.29553100	-1.15673000
C	1.77542000	1.09783900	0.97102800
H	2.79540600	1.38181100	1.25080700
H	1.14926900	1.99137400	1.06767200

H	1.42376400	0.36992200	1.70928000

$HOSiEt_3$

Si	-0.01209100	-0.00115000	-1.03341200
C	-1.33526800	1.20823100	-0.44712800
H	-0.93985500	2.22791700	-0.54468000
H	-2.17508500	1.14734200	-1.15279200
C	-1.85373900	0.97305000	0.97733600
H	-1.05166700	1.03543000	1.72030800
H	-2.61354500	1.71068000	1.25611100
H	-2.31078800	-0.01767400	1.07234900
C	-0.41049800	-1.75503100	-0.46134500
H	0.07302100	-2.44479900	-1.16548000
H	-1.48942400	-1.93536000	-0.55768200
C	0.05349100	-2.08159900	0.96458900
H	-0.40862800	-1.42243900	1.70656900
H	-0.19485500	-3.11117600	1.24270200
H	1.13883000	-1.97036200	1.05936000
C	1.70413800	0.52434100	-0.47496500
H	2.38245600	-0.33374200	-0.56807700
H	2.06424300	1.26963500	-1.19572400
C	1.77721600	1.10659000	0.94239600
H	2.80129500	1.38826300	1.20813700
H	1.15735400	2.00523300	1.03229500
H	1.42960200	0.39207000	1.69588900
O	0.07281800	0.03970100	-2.70932600
H	-0.71215300	-0.27698400	-3.17363200

25b

C	4.42328200	-1.47406100	-0.30451400
C	3.31716400	-2.40623000	-0.81780200
C	2.04610100	-2.00420000	0.01969100
O	2.46954600	-0.94375100	0.86821100
C	3.67920800	-0.35165400	0.40330700
O	5.09258300	-2.27693900	0.65313900
C	3.42144900	0.81775400	-0.52974700
O	3.73765500	-3.70862400	-0.44881900
C	0.88449900	-1.51244100	-0.80285300
N	0.37812500	-2.22382300	-1.83851200
C	-0.71635900	-1.55840300	-2.38189600
C	-0.91034800	-0.39955600	-1.63981100
C	0.09103800	-0.38059000	-0.65503600
N	0.86011000	-3.40572700	-2.29719000
C	0.21278200	-3.87435600	-3.32485700
N	-0.85100500	-3.33188700	-3.98079600
C	-1.29578400	-2.18685500	-3.52052700
O	2.98245500	0.29701100	-1.76689300
C	5.01251900	-3.61568100	0.21094300
C	6.11126100	-3.93907000	-0.78916900
C	5.01051900	-4.52498000	1.41884900
C	2.30341600	1.24034200	-2.56566600
C	1.66628700	0.55001400	-3.74457300
C	0.55691400	1.13357200	-4.36125900
C	-0.05524500	0.51748400	-5.44911300
C	0.43487500	-0.69566700	-5.93217400
C	1.54270300	-1.28087200	-5.32249400
C	2.15751700	-0.66094700	-4.23473200
H	5.10241200	-1.11830100	-1.08634000
H	3.13567300	-2.34701300	-1.88924500
H	4.23382400	-0.00453500	1.28001000
H	2.65542000	1.46960700	-0.08643700
H	4.34230200	1.40648600	-0.65925300
H	-1.67932900	0.34236200	-1.80589000
H	0.25054400	0.37729900	0.09856700
H	0.57858700	-4.82286100	-3.70398100
H	6.00051800	-4.96551900	-1.14676000

H	6.05778800	-3.26560900	-1.64933900
H	7.09013400	-3.83110100	-0.31562000
H	4.84627300	-5.55955600	1.10894300
H	5.97072300	-4.46018200	1.93595000
H	4.21700400	-4.21835600	2.10524000
H	1.52165400	1.74073000	-1.97485500
H	3.00554000	2.01884800	-2.90646000
H	0.16158200	2.07012400	-3.97410000
H	-0.92672200	0.97491700	-5.90944100
H	-0.05617100	-1.19136500	-6.76399500
H	1.92690600	-2.22699000	-5.69223300
H	3.02133700	-1.11658500	-3.76021000
N	-2.34650000	-1.52767600	-4.11618400
C	-2.84486200	-1.72340400	-5.39876300
O	-2.48060100	-2.56861000	-6.17834800
O	-3.79050900	-0.79737600	-5.60139300
C	-4.55032900	-0.77490800	-6.85327500
C	-5.52027300	0.37818700	-6.63468800
C	-3.61937400	-0.48155500	-8.02351500
C	-5.30590800	-2.08776700	-7.02531400
H	-6.14921300	0.50384000	-7.51977300
H	-6.16425000	0.17949000	-5.77352300
H	-4.97593800	1.31025300	-6.45841500
H	-4.21702800	-0.34579200	-8.92976000
H	-3.06175600	0.44249900	-7.84249100
H	-2.91698900	-1.29910000	-8.18941700
H	-5.99874100	-1.99393700	-7.86644300
H	-4.62627200	-2.91750400	-7.22184000
H	-5.88855000	-2.30774500	-6.12565500
H	-2.68757000	-0.69736500	-3.64731700
O	1.59405900	-3.06345000	0.78954300
H	2.29269500	-3.74007600	0.75546100

***25b**

C	3.72330000	-2.49486500	-0.86972000
C	2.24907700	-2.65193300	-1.27432100
C	1.63062300	-1.22891400	-1.04576900
O	2.66549000	-0.44230400	-0.47732500
C	3.94887700	-0.99180200	-0.77106000
O	3.75011000	-3.04771000	0.43485700
C	4.54781300	-0.39453600	-2.02851300
O	1.73041600	-3.62749200	-0.39983800
C	0.49606000	-1.22036900	-0.06694500
N	-0.65049000	-1.90834000	-0.28668700
C	-1.50965800	-1.74657100	0.79441900
C	-0.87603000	-0.92331500	1.71628700
C	0.37915600	-0.60069900	1.17034300
N	-0.91636000	-2.67998500	-1.36944300
C	-2.07710000	-3.26298300	-1.32355200
N	-3.03035500	-3.19242300	-0.34957500
C	-2.75067600	-2.44354400	0.68780400
O	3.78073000	-0.82270700	-3.14591300
C	2.75921400	-4.05739400	0.49299100
C	3.31430300	-5.39094300	0.01494600
C	2.20180200	-4.10653300	1.89835000
C	4.26046100	-0.33091500	-4.38672500
C	4.00890700	1.14821800	-4.59416000
C	4.75398200	1.83738700	-5.55367100
C	4.50709100	3.18348400	-5.80838900
C	3.51874000	3.85926400	-5.09428500
C	2.78044800	3.17940900	-4.12877200
C	3.02076900	1.82906800	-3.88007600
H	4.42712600	-2.99552300	-1.54410700
H	2.09428000	-2.95171000	-2.31391500
H	4.60770000	-0.75892500	0.07079700
H	4.54966000	0.69951800	-1.95238400

H	5.58477700	-0.74102800	-2.14051600
H	-1.27603300	-0.59719700	2.66643900
H	1.14459400	0.01860400	1.61416200
H	-2.31459500	-3.88546300	-2.17971500
H	2.52383700	-6.14564000	0.01306300
H	3.70552200	-5.29585400	-1.00237100
H	4.12014000	-5.72323200	0.67444900
H	1.38610400	-4.83154700	1.94960500
H	2.98191100	-4.40385700	2.60350700
H	1.82308000	-3.11810700	2.16930900
H	5.33348200	-0.54777100	-4.48125800
H	3.73654100	-0.90864700	-5.15518300
H	5.53178100	1.31400900	-6.10502300
H	5.09019100	3.70697300	-6.56001100
H	3.32732400	4.91004300	-5.28829500
H	2.01139100	3.69958200	-3.56590000
H	2.44082800	1.30818600	-3.12209300
N	-3.62621000	-2.29594900	1.73654200
C	-4.86592200	-2.90439800	1.90705800
O	-5.38351600	-3.67876100	1.14207700
O	-5.35969000	-2.46852600	3.07190300
C	-6.66405500	-2.93372300	3.54871000
C	-6.81417600	-2.19936700	4.87409300
C	-7.75444100	-2.51190700	2.57144300
C	-6.62848200	-4.44095500	3.77063900
H	-7.76271800	-2.47321700	5.34299700
H	-5.99934000	-2.46554600	5.55324100
H	-6.80119000	-1.11723500	4.71699000
H	-8.73213700	-2.72729000	3.01216700
H	-7.69463100	-1.43596700	2.38164300
H	-7.67102500	-3.04717200	1.62510700
H	-7.55171400	-4.75012400	4.26918200
H	-6.54214000	-4.98142200	2.82761800
H	-5.78554300	-4.70713200	4.41539100
H	-3.34184400	-1.67916400	2.48749800
O	1.17172200	-0.67427000	-2.24280600
H	1.91475800	-0.73502400	-2.86988000

25b-cation

C	4.64569400	-1.23727600	0.02086200
C	3.19026700	-1.02608900	-0.44814300
C	2.46963100	-0.87672200	0.88252100
O	3.27452800	-0.96458000	1.90015700
C	4.65930600	-0.75955300	1.46532700
O	4.77436000	-2.64185600	-0.00041900
C	4.91304000	0.73473000	1.58459300
O	2.79926700	-2.24361200	-1.03558800
C	1.11321000	-0.73816200	1.13117900
N	0.16145400	-0.53955100	0.13807600
C	-1.05151900	-0.36681800	0.71794300
C	-0.90660200	-0.46307500	2.12425800
C	0.42657600	-0.68097900	2.37454100
N	0.42174300	-0.46439300	-1.17454000
C	-0.63894000	-0.22600400	-1.90260600
N	-1.91149500	-0.04584500	-1.48045700
C	-2.13531400	-0.11071400	-0.18962500
N	-3.36917100	0.08092200	0.35313300
O	3.99554400	1.37153400	0.71753300
C	3.92634800	-3.13802000	-1.02523900
C	4.61527900	-3.08496500	-2.37787600
C	3.45446800	-4.51728300	-0.63190300
C	-4.55734400	0.38377200	-0.33125100
C	3.02590700	2.20159200	1.34960500
C	1.93657300	2.50029200	0.35101900
C	0.60990400	2.61073000	0.77100700
C	-0.39876300	2.89953000	-0.14685900
C	-0.08825100	3.07581400	-1.49459800

C	1.23576800	2.97004500	-1.91760300
C	2.24390500	2.68489600	-1.00005100
O	-4.65023400	0.52870800	-1.52162300
O	-5.51788500	0.47694800	0.58418600
C	-6.90205700	0.77575600	0.18474200
C	-7.63713900	0.78240200	1.51717100
C	-6.96143300	2.14675400	-0.47595200
C	-7.42520000	-0.33431700	-0.71742900
H	5.38817000	-0.72757000	-0.60018300
H	3.02159800	-0.16896100	-1.10016600
H	5.29566100	-1.35881600	2.11558200
H	4.78715900	1.05782700	2.62321400
H	5.93891200	0.95223400	1.26945800
H	-1.70676000	-0.37608000	2.84572100
H	0.90229700	-0.80449300	3.33757800
H	-0.46184000	-0.15697200	-2.96999300
H	-3.46238000	-0.01037200	1.35855000
H	3.93261500	-3.43488100	-3.15559700
H	4.91676900	-2.06063800	-2.61641100
H	5.50245600	-3.72254000	-2.37015700
H	2.73483700	-4.88712600	-1.36544000
H	4.30321500	-5.20415500	-0.59558000
H	2.98080900	-4.47333600	0.35126700
H	2.60044700	1.69498300	2.22804000
H	3.50872100	3.12551100	1.69675800
H	0.36612700	2.46162700	1.82076200
H	-1.42820100	2.98293600	0.19065600
H	-0.87595300	3.28858800	-2.21093600
H	1.48381100	3.10790800	-2.96565200
H	3.27498300	2.59880100	-1.32955300
H	-8.69505000	0.99945900	1.35014400
H	-7.55338300	-0.19199900	2.00646800
H	-7.22428900	1.54689600	2.18123200
H	-8.00821400	2.40676400	-0.65659400
H	-6.52846900	2.90417700	0.18420100
H	-6.43138200	2.15455400	-1.42905500
H	-8.49408100	-0.17774800	-0.88720500
H	-6.91712600	-0.34036600	-1.68240000
H	-7.29362300	-1.30745200	-0.23525900

TS-25b-26b

C	3.67094700	-2.37675900	-1.01704000
C	2.14786600	-2.54841900	-1.16605300
C	1.65064200	-1.27737100	-0.43622400
O	2.63364000	-0.45903200	-0.15479500
C	3.89050200	-0.89349600	-0.77490900
O	3.92144200	-3.07144800	0.18753300
C	4.18024400	-0.11172800	-2.03344900
O	1.82554600	-3.68909200	-0.42614200
C	0.54023000	-1.25652100	0.46613600
N	-0.59794700	-1.96927600	0.21145400
C	-1.48964300	-1.78111500	1.23747700
C	-0.90006000	-0.92321900	2.17621800
C	0.35875500	-0.58840700	1.68552400
N	-0.83734100	-2.65077000	-0.92847800
C	-2.02210900	-3.20035000	-0.96008700
N	-2.98817700	-3.15900000	-0.00897100
C	-2.74112400	-2.46222300	1.07551000
O	3.30514900	-0.55303200	-3.05220500
C	2.99546500	-4.14320900	0.28221500
C	3.52510400	-5.39030400	-0.40188000
C	2.64623900	-4.34725600	1.73820500
C	3.84036000	-0.42395900	-4.37394600
C	3.84680400	1.00364900	-4.86232300
C	4.82765900	1.90438300	-4.43328000
C	4.76924000	3.24478800	-4.80602000
C	3.73758100	3.69709900	-5.62735200

C	2.77497800	2.80093300	-6.08742200
C	2.83241700	1.46172500	-5.70537900
H	4.24365700	-2.76221400	-1.86571900
H	1.78025700	-2.60818800	-2.18938900
H	4.65937600	-0.70885700	-0.02328600
H	4.07976300	0.96411400	-1.84317700
H	5.22585100	-0.31639700	-2.30299800
H	-1.34441600	-0.59613500	3.10545900
H	1.09629700	0.04740100	2.15452200
H	-2.25075600	-3.75686700	-1.86216800
H	2.77031300	-6.17939400	-0.36877000
H	3.76384200	-5.18052300	-1.44821600
H	4.42662000	-5.73886100	0.10750800
H	1.87988400	-5.11974400	1.83111900
H	3.53251300	-4.66156900	2.29417600
H	2.26943800	-3.41156500	2.15839000
H	4.85430500	-0.84698900	-4.38711800
H	3.19915900	-1.03966700	-5.00955200
H	5.64408200	1.55557700	-3.80585900
H	5.53215800	3.93557100	-4.46057600
H	3.69283300	4.74187300	-5.91882100
H	1.98018700	3.14249200	-6.74396400
H	2.08455800	0.76088200	-6.06774500
Si	0.20691800	0.57073500	-2.42023900
H	0.93344900	-0.62989400	-1.73734300
C	-1.36114100	0.79372200	-1.39861400
H	-1.79142300	-0.19373400	-1.19969500
H	-1.09132600	1.22049900	-0.42379500
C	-2.43144300	1.65835100	-2.08687600
H	-2.82412100	1.15542600	-2.97533100
H	-3.27437500	1.83750900	-1.41254400
H	-2.04741300	2.63408600	-2.39962800
C	1.40134300	2.00794100	-2.23092900
H	2.19756300	1.89515600	-2.97563800
H	1.87863400	1.90904400	-1.24608100
C	0.75092600	3.39448000	-2.34745400
H	-0.00895700	3.54764500	-1.57486600
H	1.50163500	4.18274400	-2.23366700
H	0.27213100	3.53824300	-3.32136000
C	-0.11193200	0.00738800	-4.18132500
H	0.81819200	-0.44145700	-4.55165800
H	-0.86006300	-0.79478400	-4.16315400
C	-0.55867700	1.14372200	-5.11447300
H	-0.66181300	0.78624000	-6.14428200
H	-1.52391800	1.55888300	-4.81252300
H	0.16696700	1.96257700	-5.11943200
N	-3.64395800	-2.35069300	2.09244200
C	-4.95915000	-2.83262700	2.12330800
O	-5.51064400	-3.40821600	1.22154500
O	-5.45759100	-2.52276400	3.31903400
C	-6.83936900	-2.88284100	3.66605900
C	-6.98210500	-2.33077600	5.07723500
C	-7.80832400	-2.19149400	2.71519200
C	-6.99061100	-4.39847500	3.65655000
H	-7.98515600	-2.54456500	5.45470600
H	-6.25127100	-2.79193400	5.74723100
H	-6.83068500	-1.24774200	5.08289400
H	-8.82761000	-2.33101000	3.08612700
H	-7.60124600	-1.11773900	2.68054800
H	-7.74402200	-2.60249100	1.70720300
H	-7.97974500	-4.65888600	4.04362400
H	-6.89271100	-4.80313700	2.64829000
H	-6.23764200	-4.85783300	4.30379700
H	-3.35071700	-1.84806100	2.92204700

TS-25b-*beta*-**26b**

C	4.47006500	-1.49290800	-0.26041600

C	3.32712600	-2.26905600	-0.95481700	H	0.67186600	-4.72529200	-3.77927100
C	2.07896900	-1.63429300	-0.28627500	H	5.74486800	-5.00826500	-1.32066500
O	2.41956700	-0.75952700	0.64624700	H	5.98573100	-3.28593100	-1.65850100
C	3.80177500	-0.32843300	0.44945700	H	6.86724900	-4.05869700	-0.32065700
O	4.94551500	-2.42770400	0.68149600	H	4.46310900	-5.71432300	0.78684700
C	3.72702900	0.89940000	-0.44048600	H	5.56302800	-4.75345900	1.79532200
O	3.54885900	-3.61421900	-0.63222500	H	3.81099200	-4.44323900	1.85967000
C	0.83937500	-1.35772700	-0.92961300	H	1.66150300	1.79825200	-1.72162700
N	0.34612400	-2.12373700	-1.94903300	H	3.05033700	2.19677800	-2.75046400
C	-0.80696500	-1.55782000	-2.42211100	H	0.09969800	2.04801200	-3.59378800
C	-1.08165100	-0.41162700	-1.66061100	H	-1.03020500	0.93026300	-5.49308900
C	-0.05924100	-0.29480500	-0.72882700	H	-0.04666500	-1.12222100	-6.49338800
N	0.90472300	-3.26574500	-2.39623200	H	2.10527800	-2.00331100	-5.62190500
C	0.25888900	-3.79604500	-3.40285700	H	3.25707800	-0.85013400	-3.75767100
N	-0.84507900	-3.32136000	-4.02919500	Si	0.77429100	-4.10710100	1.12529200
C	-1.36808900	-2.21095700	-3.56460000	H	1.68309300	-2.96687400	0.56399200
O	3.22101800	0.43886000	-1.67710200	C	1.00403100	-4.01449500	2.99327700
C	4.78556600	-3.70898800	0.09959500	H	2.04733000	-3.76153600	3.21547300
C	5.91835800	-4.03213100	-0.86187500	H	0.40080700	-3.18297900	3.37809800
C	4.64230100	-4.72309200	1.20792600	C	0.62863600	-5.32475900	3.70246700
C	2.42285500	1.36888200	-2.38887700	H	1.25143600	-6.15574500	3.35551100
C	1.74809100	0.66547300	-3.54119400	H	0.76894800	-5.23856500	4.78433000
C	0.54625500	1.16652900	-4.04844400	H	-0.41656900	-5.59827000	3.52739500
C	-0.09026100	0.53672000	-5.11543900	C	-0.96569500	-3.61480400	0.59102700
C	0.46285400	-0.61187400	-5.68104000	H	-1.13094400	-3.94807900	-0.44176400
C	1.66412500	-1.11350800	-5.18270200	H	-1.04191200	-2.51996500	0.58217600
C	2.30875800	-0.47182600	-4.12573100	C	-2.05473600	-4.18883900	1.51163300
H	5.24709600	-1.16078100	-0.95581500	H	-1.92461800	-3.84320300	2.54193300
H	3.25556800	-2.11898800	-2.03249100	H	-3.04912400	-3.87313700	1.18157400
H	4.22914900	-0.11730200	1.42950100	H	-2.04418300	-5.28323400	1.52379100
H	3.05892100	1.64272700	0.01183200	C	1.32771100	-5.73610100	0.36851800
H	4.72560200	1.34152200	-0.55229100	H	1.69988200	-5.53074200	-0.64061300
H	-1.91645500	0.25947000	-1.80664200	H	2.17911900	-6.11956000	0.94127400
H	0.06863400	0.48134500	0.01260500	C	0.20143000	-6.77931500	0.32638500

H	0.55829400	-7.71934400	-0.10581800
H	-0.18464900	-7.00446600	1.32605400
H	-0.63974100	-6.43570100	-0.28454500
N	-2.44371300	-1.60988000	-4.15226300
C	-2.90585000	-1.81912800	-5.45717000
O	-2.47526000	-2.64359900	-6.22209200
O	-3.87704600	-0.93422000	-5.67546700
C	-4.57850700	-0.90315200	-6.96658500
C	-5.58960600	0.21685500	-6.76761700
C	-3.59657800	-0.55572600	-8.07836300
C	-5.28251900	-2.23389400	-7.20167900
H	-6.17848100	0.34511900	-7.67924100
H	-6.26783200	-0.01992400	-5.94330900
H	-5.08068300	1.15904500	-6.54573900
H	-4.15174800	-0.40576900	-9.00868400
H	-3.06876700	0.37374000	-7.84340200
H	-2.86846700	-1.35264400	-8.23388100
H	-5.93551000	-2.14121600	-8.07400800
H	-4.56907200	-3.03818200	-7.38416300
H	-5.90137800	-2.49165900	-6.33712200
H	-2.83547600	-0.80312300	-3.68030800

26b

C	3.91575700	-2.56593200	-0.77033700
C	2.44977000	-2.70332200	-1.21059300
C	1.86703100	-1.27706700	-0.96886800
O	2.91825300	-0.47077100	-0.44529700
C	4.18231900	-1.06931300	-0.72521100
O	3.88365100	-3.07921900	0.55131300
C	4.75391100	-0.54532800	-2.02632500
O	1.90146900	-3.68684900	-0.35747800
C	0.74500100	-1.25272700	0.01425500
N	-0.44192000	-1.83039800	-0.27572200
C	-1.30882100	-1.71710400	0.80656700
C	-0.63063700	-1.03253800	1.80798300
C	0.65278700	-0.74584900	1.30522400
N	-0.73601800	-2.45501400	-1.44327500
C	-1.94081200	-2.94371000	-1.48174500
N	-2.90313300	-2.91107200	-0.51629200
C	-2.58927300	-2.31424400	0.60856900
O	3.90133400	-0.98354900	-3.06815400
C	2.89490900	-4.09325600	0.58620700
C	3.47492600	-5.43292900	0.15434400
C	2.28482000	-4.12835700	1.97026100
C	4.18444800	-0.39356700	-4.31819200
C	3.63804700	1.01321700	-4.45900600
C	3.97361100	1.76624800	-5.58775100
C	3.44827400	3.04202300	-5.76822700
C	2.58574100	3.58375900	-4.81490900
C	2.25646000	2.84145600	-3.68410700
C	2.77747200	1.55976300	-3.50687700
H	4.62442000	-3.11046300	-1.40480500
H	2.32636000	-2.99923400	-2.25310400
H	4.86003900	-0.81930600	0.09692800
H	4.80197900	0.55092500	-1.98795300
H	5.77312600	-0.93305700	-2.17486900
H	-1.02137100	-0.76814700	2.78076000
H	1.45071900	-0.22334900	1.81248500
H	-2.20602400	-3.44640700	-2.40596300
H	2.68814500	-6.19133700	0.13744800
H	3.90302300	-5.35663300	-0.84938600
H	4.25637200	-5.74915400	0.85018400
H	1.47688800	-4.86340000	2.00041100
H	3.04119700	-4.40747800	2.70813000
H	1.88284500	-3.14247400	2.21510400
H	5.26820200	-0.39638800	-4.50750300
H	3.72241700	-1.04056300	-5.07166100

H	4.64883100	1.34623800	-6.33022900
H	3.71325500	3.61589700	-6.65114600
H	2.17588200	4.57955000	-4.95268300
H	1.58932800	3.25822800	-2.93549100
H	2.53014400	0.98563600	-2.61799100
H	1.53219800	-0.87362600	-1.93301000
N	-3.47569700	-2.22525400	1.65495700
C	-4.76872300	-2.73448700	1.72976100
O	-5.32971000	-3.36824300	0.87171700
O	-5.25796300	-2.38841500	2.92596500
C	-6.62181200	-2.76237300	3.30753500
C	-6.75249800	-2.16667200	4.70272400
C	-7.62170100	-2.12055600	2.35297400
C	-6.75114500	-4.27998800	3.35390500
H	-7.74839800	-2.37568800	5.10154700
H	-6.00849400	-2.59937800	5.37729800
H	-6.60961700	-1.08285000	4.67100600
H	-8.63331700	-2.27666200	2.73846000
H	-7.44238900	-1.04312100	2.28856000
H	-7.55634900	-2.55449000	1.35470900
H	-7.72407300	-4.54157700	3.78003300
H	-6.67535700	-4.71784600	2.35793400
H	-5.97186400	-4.70563900	3.99325100
H	-3.15962800	-1.73232000	2.48138800

beta-**26b**

C	4.42090300	-1.46765700	-0.30762500
C	3.31309200	-2.41110200	-0.81283900
C	2.06429500	-1.99398300	0.00820600
O	2.47657600	-0.95024900	0.88535800
C	3.67742400	-0.34720600	0.40269000
O	5.10424900	-2.26575600	0.64185200
C	3.40225700	0.82044300	-0.52830800
O	3.74596000	-3.70922500	-0.44545800
C	0.88457900	-1.52753100	-0.79631800
N	0.37293300	-2.23583700	-1.83047400
C	-0.72371800	-1.56931100	-2.37280700
C	-0.91228500	-0.41034700	-1.63020400
C	0.09030800	-0.39474100	-0.64632600
N	0.84753500	-3.42317400	-2.28552200
C	0.19663600	-3.89194300	-3.31079600
N	-0.86329000	-3.34498300	-3.96914400
C	-1.30374200	-2.19706100	-3.51031600
O	2.95981400	0.30067000	-1.76474600
C	5.01234800	-3.61052900	0.20473900
C	6.12106700	-3.93685400	-0.78656000
C	5.01592000	-4.51022500	1.42122600
C	2.28745500	1.24731000	-2.56413900
C	1.64967200	0.55949000	-3.74443900
C	0.54816700	1.15028700	-4.36846800
C	-0.06594400	0.53386400	-5.45515600
C	0.41440600	-0.68657300	-5.92978500
C	1.51465300	-1.27869400	-5.31302600
C	2.13135700	-0.65857000	-4.22648500
H	5.08996100	-1.10878100	-1.09753500
H	3.14215700	-2.35292200	-1.88767300
H	4.23571000	0.00672700	1.27443900
H	2.63380000	1.46554100	-0.07895900
H	4.31697500	1.41802400	-0.66278400
H	-1.67859300	0.33472100	-1.79501700
H	0.25192500	0.36237600	0.10766600
H	0.55603400	-4.84468800	-3.68551800
H	6.01109300	-4.96317900	-1.14550700
H	6.07337600	-3.26396500	-1.64785000
H	7.09862100	-3.83070600	-0.30925700
H	4.87085500	-5.54968500	1.11758500
H	5.96948900	-4.42732500	1.94842800

H	4.20563400	-4.21349600	2.09098900
H	1.50638200	1.75140800	-1.97522100
H	2.99361700	2.02308100	-2.90344900
H	0.16042500	2.09277300	-3.98806300
H	-0.93105800	0.99732200	-5.92145700
H	-0.07816000	-1.18231200	-6.76074000
H	1.89097200	-2.23069600	-5.67575100
H	2.98810200	-1.12014500	-3.74511400
H	1.77004700	-2.85452200	0.62202500
N	-2.35093000	-1.53461300	-4.10947500
C	-2.84539400	-1.72942000	-5.39378000
O	-2.48742700	-2.58130200	-6.16888100
O	-3.78078000	-0.79448600	-5.60376700
C	-4.53446500	-0.76938500	-6.85926300
C	-5.49080900	0.39700300	-6.65153100
C	-3.59511100	-0.49405300	-8.02716300
C	-5.30539000	-2.07372200	-7.02726600
H	-6.11604300	0.52380100	-7.53906600
H	-6.13933500	0.21266600	-5.79057100
H	-4.93562300	1.32373500	-6.48079100
H	-4.18771700	-0.34430000	-8.93450400
H	-3.01888400	0.41793700	-7.84327200
H	-2.90934800	-1.32548700	-8.19312100
H	-5.99119400	-1.97723000	-7.87384300
H	-4.63468800	-2.91312300	-7.21346200
H	-5.89677100	-2.28009700	-6.13007300
H	-2.68510000	-0.69845000	-3.64605700

30b

C	2.41622100	-3.31731600	-1.81033100
C	0.97872800	-3.05308300	-1.28602100
C	0.98382500	-1.51032400	-1.09410400
O	2.31819800	-1.17555200	-0.76121800
C	3.23958300	-2.10755100	-1.33606700
O	2.99616600	-4.48763000	-1.28707000
O	0.63774700	-3.80864200	-0.15299800
C	0.12487000	-1.01633500	0.02989500
N	-1.18551400	-1.34101400	0.14982700
C	-1.69493600	-0.79811100	1.32249300
C	-0.67208200	-0.09572800	1.94519400
C	0.46293700	-0.23678800	1.12914700
N	-1.89673000	-2.11085500	-0.71044200
C	-3.11629800	-2.34232700	-0.32121200
N	-3.73619400	-1.93778200	0.82529000
C	-3.03199000	-1.18502700	1.63291600
H	2.39916100	-3.35469800	-2.90809900
H	0.21897300	-3.30085600	-2.02765900
H	3.93641800	-2.43070600	-0.55400500
H	-0.73739300	0.43095300	2.88712800
H	1.45098000	0.16116600	1.30969800
H	-3.70924100	-2.94787200	-0.99844700
N	-3.52163400	-0.75834600	2.84426500
C	-4.65362500	-1.21699500	3.51059200
O	-5.44633600	-2.01975500	3.08467500
O	-4.68450000	-0.60730000	4.70108000
C	-5.78189400	-0.85953500	5.63826300
C	-5.42857700	0.04066600	6.81443400
C	-7.10600300	-0.43482400	5.01447900
C	-5.77995900	-2.32380900	6.06079500
H	-6.18264400	-0.06464600	7.59860500
H	-4.45392600	-0.23374200	7.22762900
H	-5.39532800	1.08770800	6.50050300
H	-7.88718700	-0.47126900	5.77930200
H	-7.03628500	0.59253000	4.64437500
H	-7.39104800	-1.09190900	4.19231100
H	-6.52271700	-2.46762500	6.85071200
H	-6.02706900	-2.97973700	5.22545300

H	-4.79985000	-2.60247700	6.45969500
H	-2.92588400	-0.14048300	3.38216800
C	1.39670800	-3.65716100	1.03896900
H	2.03114900	-4.54393900	1.16519300
H	2.05889200	-2.78548300	0.99095600
C	2.43090100	-5.67779500	-1.81873800
H	2.82069100	-6.48416500	-1.18880900
H	1.33919100	-5.66905700	-1.71065300
C	2.82174300	-5.90796400	-3.26202400
C	4.13503700	-5.66331900	-3.67443600
C	1.89204300	-6.37286500	-4.19198500
C	4.51304700	-5.88821000	-4.99443700
H	4.85494800	-5.28821800	-2.95172700
C	2.27074100	-6.60712900	-5.51355300
H	0.86563600	-6.55097800	-3.88013300
C	3.58094900	-6.36417900	-5.91720200
H	5.53538800	-5.69378000	-5.30496400
H	1.53926100	-6.97107400	-6.22867200
H	3.87508400	-6.54124000	-6.94723700
C	0.46439600	-3.50189100	2.22175800
C	0.96113800	-3.01268400	3.43360200
C	-0.88804100	-3.83140200	2.12779700
C	0.11562700	-2.83463400	4.52484600
H	2.01343800	-2.74817400	3.51335800
C	-1.73665900	-3.65491400	3.22099200
H	-1.27544400	-4.20079800	1.18370200
C	-1.24013800	-3.14766800	4.41892200
H	0.51192600	-2.43974900	5.45569100
H	-2.79332000	-3.89270300	3.12445900
H	-1.90479200	-2.99375000	5.26407000
C	4.02332400	-1.42929600	-2.44200400
O	3.11891000	-1.06800800	-3.47492000
H	4.52371000	-0.53896600	-2.04166800
C	3.66146600	-0.14919000	-4.40986000
C	3.79320200	1.25402500	-3.85566500
H	4.63540900	-0.50990700	-4.76739900
H	2.97305100	-0.15423100	-5.26102500
C	4.72505400	2.13426400	-4.40925800
C	2.96711800	1.69464500	-2.81911000
C	4.82331900	3.44323700	-3.94352400
H	5.37696000	1.79138900	-5.20942200
C	3.07239600	3.00154000	-2.34777900
H	2.24849900	1.00993600	-2.37677100
C	3.99708900	3.87966100	-2.90925200
H	5.55085900	4.12010100	-4.38122700
H	2.42874800	3.33336300	-1.53858800
H	4.07707900	4.89746900	-2.54013300
H	4.78440100	-2.11860100	-2.83424600
O	0.59007700	-0.87425500	-2.28046700
H	1.33294600	-0.96006500	-2.90866900

***30b**

C	-2.34637100	-0.26151700	-1.30548800
C	-1.09406500	-0.25436900	-0.41182200
C	-0.00815300	-0.31465600	-1.52645300
O	-0.46223300	0.68440200	-2.43364900
C	-1.89390300	0.62140300	-2.48918300
O	-2.62290400	-1.57376200	-1.74466600
C	-2.43536900	2.03710000	-2.45638100
O	-1.13824300	-1.33827600	0.46897300
C	1.45880000	-0.13660000	-1.28474400
N	2.05643400	0.88442200	-0.62062100
C	3.44582300	0.73872700	-0.65607100
C	3.71983900	-0.40559500	-1.39924200
C	2.48589500	-0.94134900	-1.78121000
N	1.42051100	1.89592900	0.00855300
C	2.20050000	2.79429700	0.53584400

N	3.55618600	2.79500400	0.56022000	H	-2.20266100	0.13594500	-3.42538600
C	4.16723900	1.76544800	0.01389800	H	-2.30554700	2.44103300	-1.44559200
N	5.54866900	1.79128900	0.06248100	H	-1.87512500	2.66850500	-3.16037600
O	-3.80057200	1.97761100	-2.82907300	H	4.70254400	-0.79093500	-1.62332600
C	6.44427500	0.75779300	0.32476600	H	2.32066800	-1.83184100	-2.37302400
C	-4.61116400	2.93635600	-2.16202500	H	1.69685700	3.61775600	1.02936200
C	-4.87083800	2.52396700	-0.73302400	H	5.93930900	2.70960000	0.24866700
C	-4.30672700	3.20531100	0.34511300	H	-4.14590700	3.93090700	-2.20229800
C	-4.48174500	2.73690500	1.64785500	H	-5.54736100	2.97577800	-2.72699600
C	-5.22196600	1.58083500	1.87865400	H	-3.71870500	4.10163900	0.16140900
C	-5.79656700	0.89678100	0.80578300	H	-4.03015400	3.26974400	2.47919500
C	-5.61997500	1.36832000	-0.49028700	H	-5.35088100	1.20970800	2.89088100
O	7.63738600	0.95878900	0.33384900	H	-6.36972500	-0.01062200	0.97715600
O	5.81875500	-0.38296300	0.58616700	H	-6.05408500	0.82792500	-1.32929400
C	6.58153300	-1.62005000	0.80966000	H	5.93479300	-3.63461200	1.19462400
C	5.48499800	-2.65087900	1.03704800	H	4.89216600	-2.39381300	1.91997300
C	7.39295100	-1.95392200	-0.43548200	H	4.82128500	-2.70375100	0.16855500
C	7.45199900	-1.47623200	2.05154700	H	7.86976100	-2.92848800	-0.29782300
C	-3.96431600	-1.74040200	-2.15615200	H	6.74060300	-2.01486400	-1.31218800
C	-4.89032000	-2.08235400	-1.00574700	H	8.16982100	-1.20989300	-0.61614400
C	0.07673900	-1.83810800	1.00964900	H	7.87881200	-2.45282100	2.29779300
C	0.82992300	-0.87281600	1.89871500	H	8.26470000	-0.76761800	1.89111100
C	-4.38718000	-2.37204300	0.26214400	H	6.84799000	-1.14457900	2.90167400
C	-5.25547900	-2.72358700	1.29645200	H	-4.32735700	-0.83901400	-2.67419700
C	-6.62824400	-2.79152100	1.07222200	H	-3.96882800	-2.55862000	-2.88508200
C	-7.13535600	-2.49366900	-0.19384400	H	-0.22952200	-2.71326200	1.59235100
C	-6.27019200	-2.13813800	-1.22469000	H	0.73782300	-2.19755100	0.21100500
C	0.15246900	-0.02520500	2.77898500	H	-3.31532500	-2.30954500	0.42901100
C	0.86260900	0.84313200	3.60300900	H	-4.85520200	-2.94536600	2.28162200
C	2.25734200	0.87319500	3.55859200	H	-7.30106000	-3.06978400	1.87768500
C	2.93864600	0.02430000	2.68897400	H	-8.20485500	-2.53810900	-0.37698400
C	2.22417000	-0.84612100	1.86684300	H	-6.66648900	-1.90671000	-2.21155700
H	-3.19378700	0.16679100	-0.75472000	H	-0.93323500	-0.02994500	2.78649500
H	-0.10835500	-1.31473900	-1.97616800	H	0.32706200	1.50470600	4.27749300

H	2.80875200	1.55948800	4.19430200
H	4.02426100	0.04511200	2.63173300
H	2.75732100	-1.48736700	1.16663400
O	-1.14970000	0.97246500	0.24306300
H	-0.26264300	1.38475600	0.28617800

30b-cation

C	2.78589600	-2.90490900	-1.60037200
C	1.36653500	-2.52373900	-1.06635200
C	1.69618600	-1.68420700	0.15848300
O	2.96737000	-1.50942100	0.32317600
C	3.73051300	-1.96912500	-0.84732100
O	3.12845100	-4.23466700	-1.31825200
O	0.52909300	-3.60318000	-0.79355200
C	0.82859800	-1.22204600	1.13761700
N	-0.55508800	-1.25003500	1.00595700
C	-1.11564600	-0.97683800	2.20907200
C	-0.08820200	-0.73579500	3.15255100
C	1.10596300	-0.86383400	2.48513500
N	-1.21731700	-1.41126400	-0.14940100
C	-2.51729300	-1.34148500	-0.01695400
N	-3.22552600	-1.17380000	1.12258700
C	-2.54925700	-1.01526900	2.23481900
H	2.84472600	-2.70281300	-2.67488600
H	0.85356000	-1.88579800	-1.79127200
H	4.61334000	-2.47863800	-0.46012900
H	-0.23640900	-0.50697900	4.19845700
H	2.10135000	-0.77790300	2.89844500
H	-3.08251100	-1.44449900	-0.93643500
N	-3.15639600	-0.90319300	3.44924000
C	-4.46359900	-1.30935300	3.75732500
O	-5.23634600	-1.79548100	2.97273900
O	-4.65080400	-1.07074500	5.05201400
C	-5.92392700	-1.42390100	5.69883600
C	-5.70631400	-0.96746200	7.13401100
C	-7.06420600	-0.64760400	5.05299800
C	-6.12654800	-2.93194300	5.63189400
H	-6.59759200	-1.18861800	7.72657000
H	-4.85364400	-1.48756600	7.57923800
H	-5.52112300	0.10958900	7.17028600
H	-7.97386000	-0.80467100	5.63944200
H	-6.83868700	0.42287300	5.05161200
H	-7.24744700	-0.97780200	4.03005700
H	-7.01993200	-3.19697800	6.20420900
H	-6.25990600	-3.27262200	4.60403900
H	-5.27149700	-3.44949200	6.07744800
H	-2.57632800	-0.66956200	4.24757000
C	0.83238700	-4.41960000	0.34905500
H	0.90207400	-5.44990000	-0.01677200
H	1.80719100	-4.16259900	0.77623600
C	2.72620700	-5.14775600	-2.33390400
H	2.87138500	-6.14133900	-1.89862900
H	1.65704400	-5.03005600	-2.55183000
C	3.54150000	-5.00990700	-3.60282700
C	4.82721900	-4.46598300	-3.57586700
C	3.01786500	-5.46031600	-4.81665300
C	5.57778100	-4.37116300	-4.74605500
H	5.23626900	-4.11360300	-2.63295400
C	3.77475000	-5.38377300	-5.98382000
H	2.01342200	-5.87597400	-4.84661400
C	5.05572700	-4.83462100	-5.95199700
H	6.57253800	-3.93689300	-4.71478300
H	3.36011800	-5.74406500	-6.92048800
H	5.64116300	-4.76429400	-6.86363800
C	-0.24945500	-4.30491000	1.39797400
C	0.08354300	-4.17150000	2.74564000
C	-1.59812800	-4.34460800	1.02919000

C	-0.91427000	-4.08334300	3.71763600
H	1.13040600	-4.12845600	3.03800500
C	-2.59537700	-4.24142500	1.99526000
H	-1.85951400	-4.43574700	-0.02156800
C	-2.25494100	-4.11357400	3.34384700
H	-0.64036100	-3.97927400	4.76342900
H	-3.64044100	-4.24850500	1.70001700
H	-3.03600300	-4.03016800	4.09527100
C	4.07501700	-0.74126300	-1.65545000
O	2.84362300	-0.21903000	-2.10470900
H	4.62073600	-0.00699300	-1.04818800
C	2.98293700	0.76563200	-3.12444300
C	3.55188700	0.17778500	-4.39430200
H	1.97386500	1.15430700	-3.28741200
H	3.61583400	1.58973100	-2.76817400
C	4.69302400	0.71739700	-4.98493000
C	2.95954800	-0.95642100	-4.96072700
C	5.23528900	0.14074500	-6.13346400
H	5.16404500	1.59003800	-4.53925500
C	3.50450000	-1.54009400	-6.09988800
H	2.06815000	-1.38023600	-4.50255300
C	4.64582400	-0.99161500	-6.68780200
H	6.12455800	0.56974700	-6.58498400
H	3.04528000	-2.42594600	-6.52844400
H	5.07321700	-1.44951300	-7.57477500
H	4.71577400	-1.05717500	-2.49001100

TS-30b-*alpha*-**31b**

C	2.47433400	-2.95624100	-1.59401500
C	1.08258600	-2.46473600	-1.07353700
C	1.47996400	-1.34592100	-0.07908400
O	2.78039000	-1.20684800	-0.00288400
C	3.46569900	-1.90877700	-1.09382400
O	2.83654500	-4.20741300	-1.07305600
O	0.28372600	-3.45292600	-0.50613800
C	0.72991700	-1.04231500	1.10578300
N	-0.63585900	-1.00480500	1.07445000
C	-1.11048200	-0.74385800	2.33484600
C	-0.01322800	-0.58640800	3.19098300
C	1.13270400	-0.75576100	2.41791400
N	-1.38638100	-1.11994500	-0.03972100
C	-2.67000000	-1.03323100	0.19083800
N	-3.29531400	-0.87482500	1.38283900
C	-2.53755900	-0.74303800	2.44605800
H	2.46566700	-2.97801000	-2.68868800
H	0.50628600	-2.03416700	-1.89346500
H	4.34380300	-2.36784300	-0.63610200
H	-0.06157200	-0.39653300	4.25391000
H	2.15977300	-0.72409600	2.75311100
H	-3.30278900	-1.10350700	-0.68709600
Si	0.71075800	1.39009000	-1.31847000
H	1.02102800	-0.10113500	-0.94761300
C	-0.39178600	2.01162600	0.07942200
H	-1.40337000	1.60958400	-0.04785700
H	-0.00881800	1.61771200	1.03083500
C	-0.43289900	3.54672300	0.15678400
H	-0.81883100	3.99306900	-0.76510000
H	-1.07879900	3.87626200	0.97636800
H	0.56336800	3.96329500	0.33521000
C	2.35626000	2.29700000	-1.31488000
H	3.13388000	1.62181700	-1.68236300
H	2.61262000	2.55060600	-0.27874200
C	2.33454100	3.56007100	-2.19137100
H	1.56953800	4.27307300	-1.86671100
H	3.29975600	4.07498800	-2.15458300
H	2.13616600	3.30643900	-3.23845700
C	-0.15868900	1.27757900	-2.97746600

H	0.60325700	1.13489600	-3.75025500	H	4.91963500	-4.55401900	-2.43895400
H	-0.77514500	0.36997600	-2.97151200	C	3.14981100	-6.19717400	-5.46424500
C	-1.03092000	2.49791000	-3.30513800	H	1.43433000	-6.35424300	-4.17165400
H	-1.51366000	2.37951700	-4.28019900	C	4.46915400	-5.76536900	-5.58592100
H	-1.82163300	2.63327600	-2.56048800	H	6.13213300	-4.83068700	-4.58642700
H	-0.44253700	3.42052300	-3.33915500	H	2.64770300	-6.65775600	-6.30949700
N	-3.06822700	-0.61167900	3.69844100	H	4.99826900	-5.89003300	-6.52553200
C	-4.35599000	-0.98973700	4.09420100	C	-0.37975700	-4.02362200	1.74307700
O	-5.19675700	-1.45452200	3.36795500	C	-0.04370800	-3.98326500	3.09655000
O	-4.45098800	-0.75298100	5.40233500	C	-1.72795700	-4.02693000	1.37524900
C	-5.68225000	-1.08803500	6.13016000	C	-1.03842200	-3.94457200	4.07289600
C	-5.36157000	-0.64283300	7.54965200	H	1.00391600	-3.97090600	3.38891800
C	-6.85256900	-0.29174200	5.56718400	C	-2.72312400	-3.97292200	2.34861500
C	-5.91475000	-2.59276600	6.07405900	H	-1.99065600	-4.05110700	0.32196500
H	-6.21018800	-0.86175000	8.20267900	C	-2.38075600	-3.93200200	3.70086500
H	-4.48345100	-1.17279000	7.92880000	H	-0.76251700	-3.91108700	5.12276700
H	-5.16503800	0.43234100	7.57960000	H	-3.76789100	-3.94822200	2.05364300
H	-7.72170000	-0.43628100	6.21514200	H	-3.15932700	-3.88840200	4.45788300
H	-6.61036500	0.77504400	5.55301500	C	3.87190700	-0.92924100	-2.17319700
H	-7.11096400	-0.61451100	4.55826800	O	2.70959400	-0.52940200	-2.87582800
H	-6.77156500	-2.84567200	6.70491200	H	4.39197700	-0.07400300	-1.72395700
H	-6.12264500	-2.92722400	5.05654900	C	2.85160000	-0.38491200	-4.28962400
H	-5.03975400	-3.12490600	6.45981200	C	3.29697400	0.99593000	-4.71580400
H	-2.42972500	-0.39265300	4.45430000	H	3.55012200	-1.14853000	-4.65871100
C	0.71025800	-4.09942800	0.70012800	H	1.86669300	-0.60046500	-4.71425700
H	0.92633500	-5.14587900	0.45591400	C	4.51462400	1.52962200	-4.27766100
H	1.63666200	-3.66445200	1.08840900	C	2.50059000	1.75568400	-5.57584900
C	2.36669900	-5.30437800	-1.84917900	C	4.91405900	2.80220200	-4.67540800
H	2.53893100	-6.18835900	-1.22690800	H	5.16624800	0.94373100	-3.63547200
H	1.28603400	-5.21928800	-2.02122400	C	2.90494000	3.02575300	-5.98789500
C	3.10221200	-5.44209300	-3.16500800	H	1.55661300	1.34783500	-5.93031200
C	4.42567400	-5.01329700	-3.29112100	C	4.10932100	3.55396600	-5.53183300
C	2.46780200	-6.02826200	-4.26145900	H	5.85971200	3.20404800	-4.32445500
C	5.10449300	-5.17013700	-4.49730700	H	2.27594800	3.60200000	-6.65944300

H	4.42465700	4.54422100	-5.84544600
H	4.57349800	-1.44934600	-2.83926800

TS-30b-31b

C	2.15978700	1.05548200	-0.11696800
C	0.75674100	0.39295800	-0.10160800
C	0.62545400	-0.04958700	-1.55420400
O	1.80242300	-0.12501400	-2.13901200
C	2.87686000	0.31994800	-1.24663000
O	2.07489100	2.41033200	-0.48478600
O	-0.26585000	1.25048300	0.28152300
C	-0.38004500	-0.89951500	-2.12768000
N	-1.52289200	-1.30542600	-1.48731100
C	-2.25964200	-2.09013700	-2.33962800
C	-1.57845300	-2.18226300	-3.55998600
C	-0.40875400	-1.44495000	-3.42114400
N	-1.82540000	-1.07788900	-0.19194200
C	-2.93989400	-1.63889400	0.18986000
N	-3.79193000	-2.40432500	-0.53733400
C	-3.46441200	-2.63725500	-1.78483300
N	-4.22105600	-3.40969200	-2.62295400
C	-5.36610700	-4.18716500	-2.39348800
O	-5.91636600	-4.72149700	-3.33000700
O	-5.68958900	-4.24958300	-1.12011300
C	-6.86988000	-5.01065200	-0.68328700
C	-6.68794200	-6.48442900	-1.02017700
C	-6.85456300	-4.79086100	0.82254400
C	-8.12517100	-4.41517200	-1.30694900
C	1.92261800	3.32809000	0.59376500
C	2.16180300	4.72021300	0.06861400
C	-0.56939100	1.16236300	1.67705400
C	-1.60911700	2.20607700	1.97560200
C	1.27032600	5.75232200	0.36444800
C	1.50545600	7.04525500	-0.10313900
C	2.63337300	7.31178000	-0.87500200
C	3.52635000	6.28299500	-1.17762500
C	3.29176100	4.99447300	-0.70769900
C	-2.89420800	2.07114400	1.44202400
C	-3.85067600	3.06026100	1.64769100
C	-3.53117800	4.19477000	2.39540100
C	-2.25649500	4.33128000	2.93899900
C	-1.29836900	3.33906700	2.72779200
H	2.68100100	0.93230500	0.84003700
H	0.77305400	-0.53095900	0.49334700
H	3.51901100	0.99184600	-1.81920800
H	-1.90426200	-2.73404900	-4.43039500
H	0.35873200	-1.28966000	-4.16687700
H	-3.20472800	-1.46467700	1.22815300
H	-3.94117600	-3.43473900	-3.59750700
H	-7.48962800	-7.05629900	-0.54457400
H	-6.72522600	-6.65690300	-2.09633400
H	-5.73185800	-6.84612100	-0.62997400
H	-7.70111900	-5.30905600	1.27992000
H	-5.92913900	-5.18001700	1.25647300
H	-6.92780300	-3.72455100	1.05344500
H	-9.00233400	-4.88841300	-0.85654300
H	-8.17342900	-3.34117400	-1.10447400
H	-8.15387000	-4.58056000	-2.38458000
H	0.91837200	3.25635900	1.02537400
H	2.65548400	3.08072300	1.37678200
H	-0.93684000	0.15000800	1.89110100
H	0.33707700	1.34097500	2.27202100
H	0.38478100	5.54050700	0.96038700
H	0.80462800	7.84048500	0.13161500
H	2.81620100	8.31662100	-1.24303000
H	4.40662600	6.48870500	-1.77922100
H	3.98341200	4.18992500	-0.94313000

H	-3.13096200	1.19058700	0.84980100
H	-4.84481400	2.94909300	1.22586500
H	-4.27680600	4.96737800	2.55491200
H	-2.00472700	5.20918800	3.52584200
H	-0.30165000	3.44698900	3.14921200
Si	-0.32901200	2.70901700	-2.69873100
H	0.11049200	1.37542600	-2.01816800
C	-1.20259700	3.68422100	-1.35637100
H	-1.88695800	2.97902300	-0.87201900
H	-0.46830700	3.95589200	-0.59164000
C	-1.97974900	4.91977200	-1.82909500
H	-2.75891900	4.65065600	-2.54958500
H	-2.47490900	5.40484500	-0.98116400
H	-1.33049200	5.66340500	-2.30021900
C	1.23313600	3.46400900	-3.42668000
H	1.42973100	2.98852400	-4.39587700
H	2.07151100	3.21688000	-2.76701900
C	1.13802300	4.98922600	-3.58590500
H	0.99399700	5.47489500	-2.61467500
H	2.05608500	5.39471200	-4.02341200
H	0.30566900	5.28240700	-4.23502200
C	-1.51400100	2.09897400	-4.02892000
H	-1.11703100	1.16979900	-4.45731000
H	-2.46958600	1.83582900	-3.55776900
C	-1.72837400	3.12777100	-5.15068700
H	-2.43894800	2.75592800	-5.89540500
H	-2.11989600	4.07510000	-4.76683200
H	-0.79003100	3.34502400	-5.67123800
C	3.61918700	-0.93079600	-0.80568600
O	2.73048900	-1.77157600	-0.09942400
H	4.04796500	-1.43766600	-1.67732400
C	2.26869600	-2.90214000	-0.82882800
C	1.00414400	-3.42310800	-0.19320100
H	2.06845300	-2.63614300	-1.87488400
H	3.04855400	-3.67805300	-0.82726500
C	0.07515800	-4.11231800	-0.97606000
C	0.75679900	-3.25661600	1.17194100
C	-1.08446400	-4.63037500	-0.40400600
H	0.25921200	-4.23606800	-2.04108900
C	-0.40565900	-3.77152900	1.74342100
H	1.47692800	-2.71984100	1.78234500
C	-1.32855600	-4.45956900	0.95827500
H	-1.80043200	-5.16473300	-1.02281100
H	-0.59083800	-3.63364700	2.80453700
H	-2.23818800	-4.85475500	1.40062000
H	4.43875300	-0.63684000	-0.14156000

alpha-**31b**

C	2.50283900	-3.34071300	-1.79526400
C	1.07006100	-3.00307900	-1.28161600
C	1.18368300	-1.48858700	-0.98523200
O	2.54528900	-1.24900300	-0.64309300
C	3.38034300	-2.14879000	-1.37268000
O	3.03023000	-4.51846500	-1.22905400
O	0.63863600	-3.80839900	-0.21300600
C	0.35207000	-0.99042600	0.15066200
N	-0.98324300	-1.20079000	0.21595300
C	-1.48460000	-0.69493400	1.41071600
C	-0.42399200	-0.12951100	2.10414400
C	0.72030700	-0.31368600	1.30818500
N	-1.72850300	-1.83018800	-0.72688700
C	-2.97791300	-1.97435500	-0.39293200
N	-3.59540200	-1.61237300	0.76830100
C	-2.85548900	-0.99424400	1.65648300
H	2.48203200	-3.42087800	-2.88937300
H	0.32354900	-3.16406500	-2.06077200
H	4.17206100	-2.49693300	-0.70033100

H	-0.47358600	0.34011900	3.07673100	H	0.94227000	-6.66656500	-3.81548900
H	1.73220800	-0.01464200	1.54021200	C	3.69660500	-6.51718900	-5.80213200
H	-3.60117400	-2.46219400	-1.13522000	H	5.62909400	-5.79955500	-5.17443900
H	0.93747200	-0.95013300	-1.91247000	H	1.66885700	-7.16044600	-6.13266600
N	-3.34502300	-0.64050100	2.89182200	H	4.01400900	-6.72664000	-6.81908300
C	-4.52945600	-1.06828400	3.48420900	C	0.40424600	-3.61567500	2.17135500
O	-5.38638900	-1.72921600	2.95248400	C	0.89775800	-3.25741800	3.42929800
O	-4.52923800	-0.61453300	4.74286700	C	-0.96634800	-3.82652500	2.01657000
C	-5.67571200	-0.86450600	5.62043200	C	0.03450000	-3.09246300	4.50853300
C	-5.26680600	-0.16634800	6.91035900	H	1.96460100	-3.08600500	3.55643600
C	-6.92699700	-0.22233600	5.03349300	C	-1.83282500	-3.66342800	3.09778600
C	-5.84145900	-2.36259200	5.84678500	H	-1.35071400	-4.09127000	1.03619100
H	-6.05425900	-0.28345700	7.65926600	C	-1.33748100	-3.28799100	4.34376400
H	-4.34261100	-0.59822900	7.30494500	H	0.42982700	-2.79826500	5.47639200
H	-5.10762300	0.90132400	6.73487900	H	-2.90152900	-3.80583600	2.95540400
H	-7.73411400	-0.27959600	5.76935400	H	-2.01526200	-3.14311500	5.18003500
H	-6.73994100	0.83234400	4.81058100	C	3.99944600	-1.42924100	-2.55428900
H	-7.24589700	-0.73067600	4.12301000	O	2.94296600	-1.04908900	-3.41605500
H	-6.61036400	-2.52629100	6.60733400	H	4.55447600	-0.54984300	-2.20100000
H	-6.14140700	-2.87317600	4.93105100	C	3.31844000	-0.11248100	-4.40072700
H	-4.90496300	-2.79643300	6.21001500	C	3.38320000	1.31104200	-3.88353000
H	-2.70254200	-0.16290200	3.51276200	H	4.28135800	-0.39248400	-4.85342300
C	1.36214200	-3.76830300	1.00915100	H	2.55950000	-0.17755800	-5.18812100
H	1.93173900	-4.70124000	1.11093800	C	3.87568800	2.31821000	-4.71804100
H	2.08443500	-2.94411800	1.01924200	C	2.92423100	1.64470800	-2.60917500
C	2.44800700	-5.70150900	-1.75514100	C	3.90306900	3.64144000	-4.28903600
H	2.79279300	-6.50740600	-1.09839900	H	4.23534000	2.06050500	-5.71198800
H	1.35418000	-5.65938300	-1.68367400	C	2.95939400	2.97053900	-2.17648800
C	2.87657600	-5.97516400	-3.18064600	H	2.55726900	0.86115700	-1.95064700
C	4.19510300	-5.72909000	-3.57477300	C	3.44352600	3.97177400	-3.01400700
C	1.97265300	-6.48585700	-4.11235000	H	4.28492800	4.41525400	-4.94831000
C	4.60304700	-5.99664900	-4.87805900	H	2.60525700	3.21988400	-1.18050600
H	4.89477500	-5.31754400	-2.85203700	H	3.46649400	5.00333800	-2.67648500
C	2.38126300	-6.76262200	-5.41634300	H	4.70113600	-2.09902100	-3.07555900

31b

C	-2.33009000	-0.62196600	-1.67031100
C	-0.99559400	-0.86635300	-0.97296000
C	-0.01114600	-0.86181600	-2.16199800
O	-0.54767900	0.10984000	-3.05932400
C	-1.93076000	0.35149300	-2.78167800
O	-2.80796100	-1.84045200	-2.20801600
C	-2.11018800	1.80593400	-2.37942600
O	-1.03918200	-2.04842400	-0.21856600
C	1.40585100	-0.51214600	-1.84075700
N	1.76304100	0.62268900	-1.18707000
C	3.14866300	0.65264500	-0.99707900
C	3.66904100	-0.49667700	-1.58391300
C	2.58255300	-1.21304400	-2.10287200
N	0.91445200	1.60487300	-0.80613000
C	1.49412700	2.61656900	-0.23079500
N	2.81552400	2.77105300	0.05399900
C	3.62107600	1.79313300	-0.29358100
N	4.96359700	1.98480100	-0.00546300
O	-3.49719300	2.08397200	-2.41839500
C	5.89767100	1.08796800	0.50011300
C	-3.88005800	3.11567700	-1.52250600
C	-3.85350400	2.63849700	-0.08797000
C	-3.03618500	3.23628700	0.87025700
C	-2.99412000	2.73930300	2.17362100
C	-3.76427900	1.63273400	2.52294900
C	-4.58227700	1.02512100	1.56792600
C	-4.62727600	1.53022200	0.27279000
O	7.03772100	1.43549700	0.71402400
O	5.36846200	-0.10892800	0.72962800
C	6.21763400	-1.21865900	1.18622700
C	5.23380100	-2.37526900	1.29289200
C	7.28584600	-1.51255800	0.14044200
C	6.81053000	-0.89350400	2.55148700
C	-4.21143100	-1.83838900	-2.36859600
C	-4.95362200	-2.02023300	-1.05807600
C	0.12716600	-2.32499000	0.54545000
C	0.52647700	-1.20566900	1.48005400
C	-4.31274000	-2.57238800	0.05271300
C	-5.01581500	-2.77324300	1.23979900
C	-6.36244700	-2.42499600	1.32848500
C	-7.00299100	-1.86281700	0.22415700
C	-6.30017600	-1.65961200	-0.96130500
C	-0.43214300	-0.56845800	2.27348100
C	-0.05899700	0.45884500	3.13516000
C	1.27583400	0.85910700	3.21572400
C	2.23410800	0.23307800	2.42182200
C	1.85576900	-0.79063300	1.55365700
H	-3.06638100	-0.18632200	-0.98446300
H	-0.78426700	0.00055900	-0.33711100
H	-0.01352700	-1.86013300	-2.62393600
H	-2.52063700	0.15125500	-3.68537200
H	-1.69692200	1.96299200	-1.37389500
H	-1.56186000	2.45715800	-3.07492800
H	4.71234600	-0.77145100	-1.60950700
H	2.62182900	-2.16018700	-2.62420800
H	0.83243400	3.42085100	0.07336200
H	5.21401200	2.95296000	0.16827900
H	-3.23389500	3.99656300	-1.64510100
H	-4.89661500	3.39857200	-1.81306400
H	-2.42585100	4.09275100	0.59341900
H	-2.35231800	3.21159000	2.91149400
H	-3.72783700	1.24176300	3.53561000
H	-5.18297700	0.15846700	1.82937900
H	-5.25726100	1.05334700	-0.47517800
H	5.76799800	-3.28220000	1.58817100

H	4.46817400	-2.16343800	2.04482300	C	-1.55589000	-2.21887100	0.61185700
H	4.74420100	-2.55361600	0.33053900	C	-1.06880100	-1.48794800	1.68762900
H	7.83566800	-2.41029700	0.43690000	C	0.16567000	-0.94944000	1.28193300
H	6.82458800	-1.70309800	-0.83381300	N	-0.74572500	-2.73628900	-1.62020900
H	7.99287500	-0.68719400	0.04818000	C	-1.83991200	-3.42549700	-1.74933000
H	7.28694700	-1.79316400	2.95185200	N	-2.85764100	-3.58682000	-0.85438400
H	7.55543300	-0.10016600	2.48800100	C	-2.71612200	-2.99251700	0.30392700
H	6.01941900	-0.59058500	3.24442300	O	3.68696300	-0.10653800	-2.88479100
H	-4.54943800	-0.91375800	-2.86150200	C	3.04866400	-3.89360300	0.21170000
H	-4.44107700	-2.67012800	-3.04337200	C	3.79543500	-5.05825400	-0.42144600
H	-0.12538100	-3.22316800	1.11817000	C	2.46442100	-4.21891100	1.56880600
H	0.97068000	-2.57472600	-0.11134900	C	4.09912400	0.65225000	-4.00899500
H	-3.25780400	-2.82326900	-0.01985500	H	4.60041000	-2.31606800	-1.57412000
H	-4.50910400	-3.20288300	2.09934000	H	2.29977900	-2.46492800	-2.43076400
H	-6.90837400	-2.58418600	2.25355900	H	4.43879500	-0.33602200	0.34259600
H	-8.04955400	-1.57962500	0.28705900	H	4.10355100	1.37020600	-1.48729500
H	-6.79925800	-1.21492500	-1.81975700	H	5.41015800	0.19090900	-1.78310000
H	-1.47465100	-0.87101500	2.19635800	H	-1.55226100	-1.35744900	2.64572200
H	-0.81077600	0.95059400	3.74553700	H	0.82813500	-0.32581100	1.86389400
H	1.56388200	1.66218000	3.88726500	H	-1.95642200	-3.93216600	-2.70160300
H	3.27487600	0.54515900	2.46207100	H	3.11760100	-5.90373200	-0.56274300
H	2.60159000	-1.25546000	0.91151400	H	4.19245900	-4.76605700	-1.39827400
				H	4.62437900	-5.36994900	0.21910200
36				H	1.75104700	-5.04165600	1.47933200
C	3.81735600	-2.02669500	-0.86444800	H	3.25693400	-4.51272600	2.26150100
C	2.38883100	-2.31713400	-1.35187800	H	1.94896700	-3.33741200	1.95771400
C	1.57015900	-1.04703600	-0.93081100	H	5.17590900	0.53382700	-4.18226400
O	2.47100700	-0.24047100	-0.18679900	H	3.55110900	0.27734400	-4.87478200
C	3.82043500	-0.53955900	-0.53640100	N	-3.67588500	-3.06994700	1.28528800
O	3.89307300	-2.76384800	0.34326100	C	-4.85298200	-3.81223900	1.27727600
C	4.32144100	0.31206900	-1.68772600	O	-5.24526000	-4.50463100	0.37215700
O	1.99603100	-3.48125200	-0.66125600	O	-5.45262800	-3.61196700	2.45691800
C	0.41558100	-1.34968400	-0.02408400	C	-6.71650300	-4.28190200	2.77046900
N	-0.62845200	-2.11751200	-0.41968500	C	-7.00976400	-3.79240800	4.18209500

C	-7.80191400	-3.82229600	1.80464800	O	3.08303700	0.31592300	-1.68935600
C	-6.52270800	-5.79357200	2.75591800	C	4.99682400	-3.75361600	0.10356500
H	-7.94995300	-4.22363600	4.53528600	C	6.14577200	-4.05839000	-0.84330600
H	-6.21003000	-4.09128900	4.86559300	C	4.89048700	-4.72594500	1.25667100
H	-7.09765400	-2.70249400	4.19926500	C	2.58302800	1.36173600	-2.48997500
H	-8.76510400	-4.22232200	2.13455100	H	5.18510600	-1.20052900	-1.05373800
H	-7.86742600	-2.73011200	1.80339300	H	3.15688900	-2.27718000	-1.94170900
H	-7.60711500	-4.17083600	0.78982400	H	4.30943500	-0.16969300	1.34259300
H	-7.42204400	-6.27134400	3.15505700	H	2.81410800	1.42877200	0.04148800
H	-6.34838800	-6.16578700	1.74601500	H	4.49367600	1.31669400	-0.54574700
H	-5.67643000	-6.07154200	3.39136000	H	-1.64613900	0.20675800	-1.85003900
H	-3.50093400	-2.55318300	2.13829800	H	0.40156900	0.39141400	-0.08178400
H	3.87435600	1.71695000	-3.86839200	H	0.36128300	-5.21107900	-3.27725200
O	1.07341600	-0.35963300	-2.03740700	H	6.02014500	-5.05387700	-1.27556000
H	1.84398300	-0.17568900	-2.60544900	H	6.17446700	-3.32814800	-1.65686400
				H	7.09375900	-4.02322600	-0.30100500
***36**				H	4.72188600	-5.73721000	0.87920400
C	4.47594100	-1.56853700	-0.30505500	H	5.81456000	-4.71761200	1.83917800
C	3.35431100	-2.43837100	-0.88250900	H	4.06026000	-4.43230300	1.90387600
C	2.10708500	-2.08018500	0.01054400	H	1.74159300	1.87163100	-2.00064000
O	2.51506100	-1.01850400	0.85312200	H	3.36244400	2.10449500	-2.70989500
C	3.75858400	-0.45559700	0.44167900	N	-2.59860500	-1.95950500	-3.77874500
O	5.09080400	-2.44469500	0.62550500	C	-3.44878700	-2.47797600	-4.75098300
C	3.54790300	0.76246800	-0.43616800	O	-3.32991200	-3.54698600	-5.29467300
O	3.76478400	-3.77061200	-0.64555900	O	-4.40698600	-1.56814400	-4.96203300
C	0.91181000	-1.61713300	-0.77968500	C	-5.46748300	-1.82262200	-5.94052200
N	0.32864500	-2.41929000	-1.70264700	C	-6.31357000	-0.56018100	-5.85227600
C	-0.78052500	-1.78437400	-2.25288200	C	-4.86527100	-1.96805000	-7.33319400
C	-0.88800900	-0.53729400	-1.64816300	C	-6.27802600	-3.04430100	-5.52471700
C	0.17174000	-0.44274700	-0.72927700	H	-7.15145800	-0.63006200	-6.55089600
N	0.76247200	-3.65639100	-2.05567000	H	-6.71053100	-0.43277400	-4.84125900
C	0.03346700	-4.22256000	-2.97266500	H	-5.71752300	0.31997800	-6.11029500
N	-1.08245800	-3.74249300	-3.59063300	H	-5.67360100	-1.99523500	-8.06970400
C	-1.48232400	-2.54571600	-3.23281200	H	-4.22597300	-1.10914100	-7.55881500

H	-4.27973900	-2.88365400	-7.42211300	H	4.23742500	-0.29713400	1.61025800
H	-7.14862100	-3.13252200	-6.18109900	H	4.21392500	1.81305000	0.24298800
H	-5.68962800	-3.95954100	-5.59914700	H	5.77048200	0.95630200	0.08061100
H	-6.63468400	-2.92942400	-4.49655800	H	-2.19724400	-0.39552300	-1.30511000
H	-2.85215500	-1.04496600	-3.42557300	H	-0.07114500	0.22924100	0.21811700
H	2.23403600	0.92169800	-3.42628500	H	1.41304300	-3.46981500	-4.89965900
O	1.72708800	-3.16512200	0.79196900	H	4.70962000	-5.43399900	-1.07032100
H	2.30529300	-3.90223100	0.52827800	H	5.72204700	-3.97739700	-1.04544000
				H	5.61526600	-5.01020900	0.40093300
36-cation				H	2.51457500	-5.43842400	0.31265500
C	4.55913800	-1.62376800	-0.10383200	H	3.40578300	-4.98083600	1.77920300
C	3.53042400	-1.89694200	-1.21698800	H	2.06931800	-3.95587900	1.19639400
C	2.36991600	-1.02266100	-0.76063300	H	4.29591200	2.76691000	-1.97170900
O	2.66503800	-0.29399200	0.26916600	H	5.92452700	2.06204600	-2.17607000
C	4.11188500	-0.31631300	0.52835600	N	-2.62627200	-2.03818300	-3.81468000
O	4.30098800	-2.67515700	0.80181100	C	-3.40328200	-2.54989600	-4.86760000
C	4.69541600	0.90452400	-0.14434200	O	-2.98206500	-3.21550100	-5.77620400
O	3.17327200	-3.24910800	-1.08220500	O	-4.65479900	-2.15528300	-4.65220600
C	1.06455900	-1.00574400	-1.22955400	C	-5.72430500	-2.52675100	-5.59211500
N	0.63897000	-1.69674300	-2.35855000	C	-6.95138300	-1.87621900	-4.96980400
C	-0.69812600	-1.52099800	-2.50381300	C	-5.43050200	-1.93423800	-6.96407800
C	-1.17030600	-0.69791100	-1.45337900	C	-5.87184400	-4.04237500	-5.62664200
C	-0.08286800	-0.37647800	-0.67723200	H	-7.82974200	-2.08654600	-5.58507700
N	1.43689600	-2.37336000	-3.19932300	H	-7.12681600	-2.27171600	-3.96556000
C	0.79577600	-2.91533200	-4.20187900	H	-6.82132400	-0.79235800	-4.90541600
N	-0.52985000	-2.86358500	-4.46590900	H	-6.29741400	-2.09520700	-7.61104800
C	-1.28351900	-2.17445100	-3.64239100	H	-5.25825800	-0.85685500	-6.88286600
O	4.45623100	0.74353600	-1.52058500	H	-4.56113000	-2.40397000	-7.42543400
C	3.87161000	-3.80059200	0.05109800	H	-6.76477200	-4.29931900	-6.20334800
C	5.05716600	-4.60687900	-0.44739400	H	-5.00857500	-4.51963900	-6.09193600
C	2.90023800	-4.59584100	0.89061700	H	-5.99593800	-4.43307900	-4.61236600
C	4.84925200	1.87144700	-2.28183900	H	-3.13506200	-1.49292200	-3.12809500
H	5.59506800	-1.59541500	-0.45267600	H	4.62379000	1.65100300	-3.32608700
H	3.85186400	-1.64794700	-2.22815000				

TS-36-37

C	3.66271900	-2.43469000	-1.07834900
C	2.14124900	-2.67579200	-1.15449500
C	1.60493900	-1.35221300	-0.56502700
O	2.56622800	-0.48932800	-0.34979900
C	3.83629400	-0.93117100	-0.93662500
O	3.99687200	-3.04162000	0.15245900
C	4.10613700	-0.21759400	-2.23656600
O	1.88100800	-3.72691400	-0.26783600
C	0.46511000	-1.24394700	0.29506600
N	-0.66205500	-1.98497400	0.07491000
C	-1.61464100	-1.64817700	1.00346500
C	-1.07594600	-0.66440600	1.84391900
C	0.21442800	-0.40514800	1.38993200
N	-0.83174800	-2.83649700	-0.95831800
C	-2.01731800	-3.38467100	-0.98422200
N	-3.04914000	-3.18542200	-0.12763000
C	-2.86472300	-2.33452800	0.85471800
O	3.19423900	-0.67942300	-3.20894500
C	3.11676000	-4.13598800	0.34908500
C	3.62695800	-5.38438600	-0.34878200
C	2.89262900	-4.31545400	1.83196600
C	3.60511500	-0.30574700	-4.51432600
H	4.21410700	-2.84993600	-1.92673400
H	1.75117500	-2.87309100	-2.15222800
H	4.60027200	-0.68041400	-0.19890600
H	4.02938300	0.87021700	-2.10148000
H	5.13961800	-0.45389000	-2.52973900
H	-1.57444500	-0.20669600	2.68674400
H	0.92615000	0.29533200	1.80330800
H	-2.18811000	-4.07965300	-1.79882100
H	2.90124400	-6.19320500	-0.23790500
H	3.77608400	-5.19463900	-1.41552900
H	4.57678000	-5.69540400	0.09281300
H	2.15404200	-5.10173700	2.00217100
H	3.82858600	-4.60184500	2.31713200
H	2.53167500	-3.37998400	2.26527400
H	4.58487400	-0.74164900	-4.74830300
H	2.86668900	-0.68812100	-5.21995200
Si	0.17711700	0.22387500	-2.75613500
H	0.89768400	-0.88644900	-1.93594500
C	-1.50833800	0.40758800	-1.93344500
H	-1.93255500	-0.59204800	-1.78435100
H	-1.39162900	0.85636500	-0.93830900
C	-2.48088300	1.23261200	-2.79368800
H	-2.64062600	0.76069700	-3.76859000
H	-3.45716000	1.31476400	-2.30651800
H	-2.11597800	2.24794500	-2.97163700
C	1.26689400	1.73880000	-2.52894000
H	2.08707000	1.68472200	-3.25329100
H	1.72863400	1.66389300	-1.53488500
C	0.53282800	3.08142500	-2.65304000
H	-0.26177700	3.17381400	-1.90633300
H	1.22429900	3.91596900	-2.50181700
H	0.07876900	3.20655300	-3.64107300
C	0.03908600	-0.43822700	-4.51063000
H	0.81972400	-1.19185700	-4.66049500
H	-0.91641600	-0.97047900	-4.59599800
C	0.13911000	0.65522000	-5.58314200
H	0.06925000	0.22730600	-6.58791700
H	-0.66533900	1.39166900	-5.48406300
H	1.08946900	1.19530400	-5.51790600
N	-3.83999100	-2.05212300	1.76592800
C	-5.13959400	-2.57379800	1.81475400
O	-5.61043900	-3.34483800	1.01971400
O	-5.72757900	-2.05129600	2.88981300
C	-7.11592800	-2.39995100	3.22189200
C	-7.36488900	-1.59743900	4.49078000

C	-8.04281300	-1.94450600	2.10195000	C	6.08538000	-3.78948900	-0.45523600
C	-7.22014100	-3.89441900	3.49817200	C	4.54853100	-4.83858700	1.25079000
H	-8.38497500	-1.77276800	4.84148400	C	3.67761700	1.98801500	-1.89617700
H	-6.66822400	-1.89865600	5.27804300	H	5.28107300	-1.02574600	-0.31945900
H	-7.24027000	-0.52782000	4.30039900	H	3.56932500	-1.88655000	-1.83864900
H	-9.07941000	-2.07124400	2.42662600	H	3.72748100	-0.34454700	1.94956600
H	-7.87894500	-0.88500400	1.88377800	H	3.04991100	1.70588600	0.64059000
H	-7.88856200	-2.52610800	1.19225900	H	4.78643400	1.34616800	0.43674500
H	-8.21896600	-4.11402300	3.88591500	H	-1.88344900	-0.26229900	-2.41193600
H	-7.06039300	-4.48172300	2.59331100	H	-0.05199800	0.38709900	-0.54014000
H	-6.48682000	-4.19084100	4.25411000	H	1.09833800	-5.34224900	-3.30604700
H	-3.60934100	-1.40183500	2.50798000	H	6.07126800	-4.71024500	-1.04251600
H	3.67558500	0.78564100	-4.61290400	H	6.21520900	-2.94764400	-1.14061600
				H	6.93396500	-3.82103000	0.23211000
TS-36-*beta*-**37**				H	4.46675100	-5.76088500	0.67101800
C	4.40569900	-1.44612700	0.18406200	H	5.38512700	-4.93515900	1.94673300
C	3.44947800	-2.17196000	-0.78920400	H	3.63042600	-4.68283000	1.81981400
C	2.07098100	-1.63811600	-0.32151200	H	2.94547900	2.73279000	-1.55823700
O	2.18765000	-0.73481700	0.61706000	H	4.68513000	2.41356600	-1.80366600
C	3.58176500	-0.36924300	0.86913300	Si	0.80829600	-3.95423200	1.36566600
O	4.74770900	-2.47158500	1.09103700	H	1.71019700	-3.05117800	0.50115500
C	3.76882400	0.98596300	0.22551800	C	1.30341100	-3.51979100	3.13359300
O	3.68414100	-3.53608400	-0.58556500	H	2.24582600	-4.01828500	3.38778000
C	0.89033500	-1.52276500	-1.11280000	H	1.51531600	-2.44262900	3.15373600
N	0.52529000	-2.46848500	-2.03194900	C	0.23510300	-3.85078000	4.18540500
C	-0.62999600	-2.07511900	-2.65469200	H	-0.00432100	-4.91877800	4.19908600
C	-1.01806000	-0.83829800	-2.11618800	H	0.57856900	-3.57840200	5.18808800
C	-0.07785900	-0.50511000	-1.14949200	H	-0.69295900	-3.30287800	3.99562300
N	1.16919700	-3.63666900	-2.22078400	C	-0.95351200	-3.42187200	0.96156100
C	0.60484700	-4.39358000	-3.12496800	H	-1.04547400	-3.31087300	-0.12691900
N	-0.51025900	-4.13682800	-3.85106500	H	-1.14862400	-2.43183000	1.39179100
C	-1.12915200	-2.99981000	-3.63023100	C	-2.00166000	-4.43764300	1.44612000
O	3.56070600	0.78989100	-1.15214700	H	-1.96755800	-4.58094000	2.52987400
C	4.78919400	-3.66697800	0.33090000	H	-3.01306700	-4.10758100	1.19053500

H	-1.84996200	-5.41604000	0.97931400	O	3.90036800	-2.68564000	0.40725200
C	1.14519000	-5.72924700	0.82548800	C	4.27832100	0.26856000	-1.82026100
H	0.31700200	-6.04118800	0.17695000	O	2.02355000	-3.47279500	-0.58527000
H	2.04063100	-5.72498700	0.19506900	C	0.46535800	-1.32699400	0.02066700
C	1.30821200	-6.71489400	1.98856300	N	-0.60802600	-2.03506900	-0.39593800
H	1.52317700	-7.72413000	1.62380800	C	-1.51041500	-2.20047400	0.65107100
H	2.12996300	-6.42143900	2.65078900	C	-0.97421500	-1.56069600	1.76183300
H	0.39913400	-6.77221200	2.59649400	C	0.26034000	-1.01706900	1.36015500
N	-2.26167000	-2.64170200	-4.29961500	N	-0.77334500	-2.53044400	-1.64768000
C	-2.94268300	-3.37973200	-5.27743700	C	-1.88441500	-3.18872600	-1.80313700
O	-2.62955500	-4.47490300	-5.66488400	N	-2.86143900	-3.43686800	-0.88532900
O	-3.97577300	-2.63811900	-5.67303800	C	-2.67691300	-2.95090700	0.31894000
C	-4.89878300	-3.13373200	-6.70381500	O	3.55808700	-0.22480700	-2.92863100
C	-5.88952700	-1.98637100	-6.83975400	C	3.07569500	-3.83368300	0.31083600
C	-4.14455500	-3.35557900	-8.00867800	C	3.84711700	-5.00916700	-0.27249000
C	-5.59426300	-4.39462000	-6.20730800	C	2.49165300	-4.12356500	1.67628000
H	-6.64407500	-2.23980200	-7.58858800	C	3.86885200	0.46329500	-4.12009700
H	-6.39242800	-1.79946000	-5.88690400	H	4.61592700	-2.33711800	-1.52800400
H	-5.37840200	-1.07231500	-7.15464300	H	2.32207300	-2.50400200	-2.38004600
H	-4.86601100	-3.57326300	-8.80127200	H	4.49367000	-0.24630200	0.25056300
H	-3.59477000	-2.45134900	-8.28641100	H	4.07715200	1.33968000	-1.66933900
H	-3.44683900	-4.19028300	-7.93283600	H	5.36193900	0.14106400	-1.97425300
H	-6.37484100	-4.67362100	-6.92077800	H	-1.42777400	-1.49158700	2.74075500
H	-4.89552100	-5.22655000	-6.11275900	H	0.95112300	-0.44972100	1.96662600
H	-6.06695600	-4.21001900	-5.23807700	H	-2.04648500	-3.59484200	-2.79611100
H	-2.66632500	-1.73772600	-4.08350400	H	3.18502200	-5.87150400	-0.38392400
H	3.48419400	1.74215900	-2.94128700	H	4.24558000	-4.75028700	-1.25790500
				H	4.67687400	-5.28148700	0.38484900
37				H	1.78970500	-4.95834000	1.61031700
C	3.83373500	-2.00629200	-0.83564100	H	3.28616300	-4.38557000	2.37946600
C	2.40404700	-2.32026100	-1.30807100	H	1.96279200	-3.23853200	2.03747900
C	1.60359300	-1.04378000	-0.90097500	H	4.93801700	0.38098000	-4.36064400
O	2.50789000	-0.18563900	-0.21432000	H	3.28716600	0.00920000	-4.92452200
C	3.84346000	-0.50483700	-0.59055100	N	-3.59218600	-3.14431600	1.32594800

C	-4.82584200	-3.78484300	1.25115600	N	0.72624000	-3.69747400	-2.02664100
O	-5.30172700	-4.29091800	0.26631600	C	-0.01777400	-4.26907500	-2.92846800
O	-5.37387000	-3.72543000	2.47071700	N	-1.12376000	-3.77843400	-3.55554700
C	-6.69543000	-4.30602000	2.71894900	C	-1.50241800	-2.56805400	-3.21846600
C	-6.91257600	-4.01774400	4.19822600	O	3.07597000	0.31750200	-1.65307500
C	-7.74168400	-3.59283900	1.87086100	C	5.02913200	-3.75572100	0.09329300
C	-6.66073900	-5.80790000	2.46328900	C	6.16743900	-4.03115500	-0.87934000
H	-7.88406100	-4.40766600	4.51265300	C	4.97987900	-4.73461600	1.24577100
H	-6.13381400	-4.49538600	4.79936000	C	2.58432500	1.37389400	-2.44383900
H	-6.89147300	-2.94072100	4.38673500	H	5.15983900	-1.18451400	-1.04537100
H	-8.73691600	-3.93361500	2.17043700	H	3.18509300	-2.32534900	-1.93375700
H	-7.68627800	-2.51224000	2.03396100	H	4.28997400	-0.20220800	1.37764400
H	-7.60435200	-3.80209200	0.80946800	H	2.74745300	1.38150600	0.09885400
H	-7.60369000	-6.24766200	2.80092900	H	4.43814300	1.32690200	-0.46156700
H	-6.52892800	-6.03011500	1.40385900	H	-1.62173000	0.20568700	-1.86813200
H	-5.84599800	-6.26849800	3.03016800	H	0.43343800	0.38107900	-0.11084200
H	-3.36588800	-2.75445400	2.23295100	H	0.28716500	-5.27160200	-3.20972700
H	3.60923000	1.52826100	-4.04562300	H	6.05348900	-5.02670600	-1.31517100
H	1.24131400	-0.55622900	-1.81463300	H	6.16186900	-3.29683000	-1.69012800
				H	7.12826900	-3.97836500	-0.36092300
beta- **37**				H	4.83748200	-5.74926900	0.86659800
C	4.47057700	-1.57636400	-0.28978400	H	5.91376200	-4.69879200	1.81198200
C	3.35801100	-2.47081200	-0.86595100	H	4.14780100	-4.47524900	1.90424100
C	2.11468500	-2.10076900	-0.01176800	H	1.73035000	1.87029000	-1.96187900
O	2.51168600	-1.08152000	0.89641000	H	3.36244900	2.12603600	-2.63616200
C	3.73867800	-0.48521200	0.47591800	N	-2.60724300	-1.97163300	-3.77723300
O	5.12127300	-2.44429100	0.62212600	C	-3.47313800	-2.49625000	-4.73208800
C	3.50625800	0.74467000	-0.38081100	O	-3.39331800	-3.58959500	-5.23294200
O	3.78495100	-3.79494900	-0.60698300	O	-4.39728600	-1.56094300	-4.98095800
C	0.92177800	-1.63950800	-0.79447100	C	-5.46663100	-1.81353900	-5.95005300
N	0.31931100	-2.44328300	-1.70170800	C	-6.25333900	-0.51036700	-5.92433700
C	-0.78726000	-1.80190600	-2.25369600	C	-4.87228200	-2.05358800	-7.33297600
C	-0.87317200	-0.54701300	-1.66257400	C	-6.33172700	-2.97506700	-5.47671800
C	0.19311500	-0.45603500	-0.75074800	H	-7.08968500	-0.57181100	-6.62518900

H	-6.64914900	-0.32022400	-4.92275700	H	3.60203600	1.96122900	-0.42182000
H	-5.61540900	0.32877200	-6.21565800	H	5.24230900	1.31787200	-0.16825500
H	-5.68164800	-2.07768600	-8.06848600	H	-1.60470000	-1.29786200	-3.28850600
H	-4.19415100	-1.23672700	-7.59788100	H	0.57465700	-0.05717700	-2.26355500
H	-4.32930500	-2.99807800	-7.37823500	H	-0.43031100	-5.90117400	0.28558700
H	-7.20596100	-3.05671400	-6.12913800	H	4.30149100	2.79857000	-2.57926000
H	-5.78447900	-3.91784500	-5.50575200	H	5.93153000	2.11113300	-2.35669100
H	-6.68200300	-2.79381800	-4.45614800	N	-2.92290200	-3.99301000	-2.83456300
H	-2.83300700	-1.03853700	-3.45525800	C	-3.89343700	-4.95834600	-3.08796200
H	2.25550300	0.94868100	-3.39433200	O	-3.98205500	-6.03117200	-2.54603500
H	1.83854500	-2.99127300	0.56739400	O	-4.69538800	-4.46685400	-4.03977200
				C	-5.82693300	-5.25312900	-4.53603500
39				C	-6.43891500	-4.33144600	-5.58239500
C	4.42004300	-1.45051000	-0.16303500	C	-5.32424600	-6.53843600	-5.18178800
C	3.31986500	-2.34739100	-0.79883400	C	-6.81353800	-5.51561800	-3.40480200
C	2.03233700	-1.66551900	-0.23977600	H	-7.31206600	-4.81155000	-6.03157800
O	2.33038000	-0.30198300	-0.30745300	H	-6.75410000	-3.38876800	-5.12630100
C	3.68476300	-0.11788000	0.11663600	H	-5.71451100	-4.11532600	-6.37274000
O	4.89184400	-2.05074800	1.02046100	H	-6.16165700	-7.03881400	-5.67650600
C	4.25171100	1.08902900	-0.59425400	H	-4.56754000	-6.30927500	-5.93809300
O	3.32708100	-3.66667100	-0.31287900	H	-4.89840500	-7.21833600	-4.44330200
C	0.78304000	-1.86641200	-1.05471600	H	-7.71843500	-5.96917000	-3.81940200
N	0.03965200	-3.00218900	-1.00060100	H	-6.39444100	-6.19183700	-2.65903100
C	-1.01936200	-2.91238000	-1.89968500	H	-7.09274500	-4.57482400	-2.92089200
C	-0.93082300	-1.68051600	-2.53467700	H	-3.01029600	-3.14536500	-3.38132000
C	0.19741200	-1.03525000	-2.00213000	H	4.93122800	1.60384200	-3.74340600
N	0.26767400	-4.07472900	-0.19909000	C	4.44779200	-4.44707200	-0.68545000
C	-0.59620000	-5.03423200	-0.34575100	H	4.40844300	-5.35739000	-0.08416700
N	-1.67330600	-5.09702300	-1.18106000	H	4.41087700	-4.72597300	-1.74496100
C	-1.87896800	-4.05197500	-1.94320500	H	5.38837800	-3.92581800	-0.47657900
O	4.35436600	0.81063500	-1.97012400	C	6.05686100	-1.42267000	1.51007000
C	4.90772700	1.88856800	-2.68970600	H	5.87368600	-0.37888400	1.80131400
H	5.25331500	-1.29692900	-0.86422800	H	6.37872100	-1.97719900	2.39371000
H	3.70546800	0.06023000	1.19984000	H	6.86231200	-1.43874900	0.76152100

C	3.37185400	-2.27432800	-2.31777300	H	4.80310700	0.59548800	-4.44029900
H	2.60562800	-2.92239600	-2.75348900	H	3.11016500	0.40683300	-4.97405000
H	3.20532300	-1.24377200	-2.64100700	N	-3.51317900	-2.63634700	2.20132500
H	4.35313900	-2.58694900	-2.68524900	C	-4.72611900	-3.28892500	2.39599900
O	1.84610900	-2.03205000	1.09726100	O	-5.29323100	-3.98149800	1.58879500
H	2.12640300	-2.95933600	1.16778900	O	-5.13735700	-2.99672900	3.63579500
				C	-6.39989800	-3.53885600	4.14307300
***39**				C	-6.46631300	-2.96847300	5.55316100
C	3.78762800	-2.07777800	-1.01451900	C	-7.56171500	-3.02638000	3.30032400
C	2.27561000	-2.45612600	-1.17330900	C	-6.33282700	-5.06124700	4.18198200
C	1.51030800	-1.11089200	-0.83597200	H	-7.37745800	-3.31463200	6.04780100
O	2.47667100	-0.25235600	-0.26091200	H	-5.60375900	-3.29527700	6.14066200
C	3.78934200	-0.56855400	-0.71171000	H	-6.47785900	-1.87532200	5.52493800
O	4.35122300	-2.80901400	0.05009500	H	-8.50271700	-3.31339500	3.77845300
C	4.20131200	0.30272100	-1.88375300	H	-7.52829900	-1.93451600	3.23717000
O	1.87815000	-3.37419900	-0.17831400	H	-7.53904900	-3.44359900	2.29302500
C	0.43053900	-1.25874000	0.20369900	H	-7.22135100	-5.44347900	4.69267800
N	-0.67944300	-2.01546600	0.02884300	H	-6.29558500	-5.48596700	3.17825300
C	-1.49869800	-1.91722800	1.15072100	H	-5.44997400	-5.38508000	4.74150100
C	-0.87766100	-1.06140800	2.05019800	H	-3.19718000	-2.07179400	2.98029100
C	0.32738100	-0.65674200	1.45110200	H	3.57559400	1.80348800	-3.96307800
N	-0.95444700	-2.79176900	-1.04753500	C	1.98572600	-2.94743800	-2.58655100
C	-2.06906600	-3.45329800	-0.95105900	H	0.91821800	-3.13225100	-2.71115600
N	-2.96937200	-3.46332500	0.07361500	H	2.30855000	-2.20152000	-3.31516200
C	-2.68685800	-2.70556700	1.10428900	H	2.54594000	-3.86434100	-2.78888800
O	3.43126600	-0.04464200	-3.02080800	C	2.21299900	-4.72902000	-0.39574800
C	3.75293500	0.73827000	-4.15697700	H	1.54690600	-5.19641800	-1.13196500
H	4.33565800	-2.28966600	-1.94415200	H	3.25387000	-4.85367600	-0.71265500
H	4.47344800	-0.35718100	0.11739300	H	2.08009400	-5.23533600	0.56343600
H	4.04930500	1.36196700	-1.63250600	C	5.76058600	-2.83473500	-0.00157500
H	5.26964100	0.14403000	-2.09420400	H	6.19896700	-1.82899200	0.06819900
H	-1.25436000	-0.76861600	3.02034600	H	6.10474700	-3.42212900	0.85204600
H	1.06991900	0.00895900	1.86452100	H	6.11723100	-3.30474800	-0.92914700
H	-2.30928600	-4.07821900	-1.80483900	O	0.91742000	-0.51902700	-1.95206100

H	1.64755800	-0.26973300	-2.54875900

39-cation

C	3.95262700	-2.17751900	-1.21563900
C	2.47913400	-2.68960000	-1.04090300
C	1.88218500	-1.63011900	-0.13052700
O	2.65984500	-0.61300100	0.04378600
C	3.94848400	-0.74855200	-0.64435300
O	4.81326900	-3.01402900	-0.49640700
C	4.05759000	0.37560800	-1.64549200
O	2.41102500	-3.87474700	-0.30566400
C	0.67219500	-1.61442400	0.56343300
N	-0.34346800	-2.56722800	0.51880500
C	-1.32317200	-2.20117300	1.38849100
C	-0.95848700	-0.99025000	2.01810300
C	0.26411400	-0.63209300	1.50599700
N	-0.38675000	-3.64776600	-0.27777100
C	-1.46942400	-4.36641700	-0.13768300
N	-2.51495700	-4.14595600	0.69188900
C	-2.46010500	-3.07787700	1.45050600
O	3.04280700	0.20783600	-2.59908500
C	3.08167500	1.19697400	-3.61017600
H	4.22298700	-2.16039900	-2.27963000
H	4.70770000	-0.63774600	0.13404400
H	3.96579400	1.34493500	-1.13438400
H	5.05819400	0.32327500	-2.10203800
H	-1.54020900	-0.46165500	2.75980100
H	0.85207700	0.23651900	1.76645900
H	-1.52273400	-5.24341100	-0.77287300
H	4.03065900	1.16142400	-4.16100600
H	2.25871300	0.99089300	-4.29618200
N	-3.44865800	-2.74858100	2.32691500
C	-4.67651100	-3.40478300	2.50908400
O	-5.06044100	-4.34427600	1.86349000
O	-5.30317600	-2.78405400	3.50467000
C	-6.63291200	-3.23411700	3.94383900
C	-6.94909100	-2.27201800	5.07926800
C	-7.63122000	-3.07612800	2.80445300
C	-6.54713900	-4.66648900	4.45454600
H	-7.93270300	-2.50551000	5.49429700
H	-6.20410200	-2.35947700	5.87490900
H	-6.95917800	-1.24017800	4.71753700
H	-8.63613600	-3.27930900	3.18537800
H	-7.61070800	-2.05099600	2.42302000
H	-7.42144000	-3.76840100	1.98813900
H	-7.50120500	-4.93462400	4.91704200
H	-6.34218300	-5.36927800	3.64624700
H	-5.76336600	-4.75124000	5.21299600
H	-3.29837300	-1.94200000	2.92212100
H	2.95545900	2.20083400	-3.18447700
C	1.75654900	-2.69371400	-2.39233700
H	0.71616500	-2.99610000	-2.28068600
H	1.81318500	-1.69634000	-2.83185600
H	2.26762800	-3.38782200	-3.06431200
C	2.61508900	-5.06800100	-1.04215600
H	1.76824000	-5.28170800	-1.70383900
H	3.54246600	-5.02744800	-1.62402600
H	2.69733100	-5.86537500	-0.30191900
C	6.16979300	-2.83639900	-0.86575900
H	6.52288800	-1.81569100	-0.66489500
H	6.75728500	-3.53300100	-0.26613300
H	6.31958000	-3.05652200	-1.93097100

TS-39-*alpha*-**40**

C	3.80704300	-2.08911700	-1.06212600
C	2.28829800	-2.49637400	-1.12961900
C	1.62078100	-1.25591000	-0.47463700
O	2.48785500	-0.32258400	-0.17970800

C	3.81336900	-0.58798100	-0.73047900	H	1.84824900	2.18380800	-2.55092600
O	4.42447800	-2.82809300	-0.04553100	H	1.39875100	1.82662200	-0.89208900
C	4.09909600	0.35654100	-1.87178700	C	0.09020300	3.26001100	-1.84977000
O	1.97921100	-3.51929200	-0.22341300	H	-0.73269200	3.13239500	-1.13947900
C	0.48353900	-1.28525900	0.40555900	H	0.66078300	4.14004200	-1.53738000
N	-0.59694900	-2.10715600	0.24032400	H	-0.34654900	3.48195800	-2.82888800
C	-1.49249100	-1.88640000	1.25845600	C	0.12479000	0.15959000	-4.31887600
C	-0.97640500	-0.88503700	2.08923000	H	1.02894500	-0.40325200	-4.57395400
C	0.24847800	-0.50632300	1.54782600	H	-0.72185400	-0.49016600	-4.57293200
N	-0.79120100	-2.94559100	-0.79862500	C	0.06591700	1.46148100	-5.13100000
C	-1.91079700	-3.61242500	-0.72878200	H	0.09143900	1.25575200	-6.20549200
N	-2.86046300	-3.55815700	0.23869200	H	-0.85134300	2.02378300	-4.92597300
C	-2.66397500	-2.71385000	1.22277700	H	0.91291500	2.11578700	-4.89810300
O	3.25942800	0.05107300	-2.96091400	N	-3.54894400	-2.57682800	2.25294900
C	3.65124000	0.75086400	-4.12998900	C	-4.76603600	-3.24725600	2.42532600
H	4.29179300	-2.27153900	-2.03016200	O	-5.23518500	-4.04738900	1.65826100
H	4.50737600	-0.37788200	0.08755400	O	-5.28192900	-2.82457300	3.57904000
H	3.95579700	1.39683900	-1.54426900	C	-6.57869100	-3.33193100	4.04699100
H	5.15735400	0.22818700	-2.14635200	C	-6.76990500	-2.58979000	5.36198800
H	-1.44089300	-0.49958200	2.98587400	C	-7.66833700	-2.95801000	3.05040200
H	0.93536800	0.23148600	1.93737700	C	-6.48977900	-4.83426500	4.28313300
H	-2.09478400	-4.29344500	-1.55253000	H	-7.71584500	-2.89122600	5.81877800
H	4.68781100	0.50740100	-4.39623600	H	-5.95739000	-2.82353400	6.05552500
H	2.99289600	0.43974000	-4.94263000	H	-6.79059500	-1.50945400	5.19424400
Si	0.09997400	0.46047400	-2.46374200	H	-8.64284700	-3.20665500	3.48015000
H	0.88083000	-0.71607300	-1.81268200	H	-7.64635500	-1.88221900	2.85218800
C	-1.63305900	0.30300300	-1.74050000	H	-7.55363500	-3.49835100	2.11012100
H	-1.91863400	-0.75516000	-1.76695900	H	-7.40716900	-5.17026100	4.77475900
H	-1.62073400	0.60239200	-0.68398200	H	-6.37499100	-5.38163600	3.34701500
C	-2.67147300	1.12146400	-2.52612900	H	-5.64597700	-5.06378200	4.94063000
H	-2.72382300	0.79251600	-3.56909700	H	-3.30666200	-1.92602000	2.99103800
H	-3.66981100	1.00112000	-2.09473000	H	3.57073600	1.83701800	-3.98913500
H	-2.43938200	2.19051000	-2.52594100	C	1.88437800	-2.78838200	-2.57168900
C	0.98859200	2.01488500	-1.89268700	H	0.81317600	-2.97945600	-2.64033500

H	2.16161900	-1.94584000	-3.20664300	H	5.27143200	0.11504900	-1.98666400
H	2.43451600	-3.66655800	-2.91793900	H	-1.28029100	-0.66360100	3.18931900
C	2.31617100	-4.83661300	-0.62802800	H	1.05623900	0.10297200	2.07813500
H	1.60473300	-5.22162400	-1.36698400	H	-2.19921200	-4.15618100	-1.54371800
H	3.33449500	-4.89121400	-1.02692900	H	5.06308900	-0.42325800	-4.17577200
H	2.25875200	-5.44973500	0.27287400	H	3.48760200	-0.16832300	-4.96517300
C	5.83263100	-2.87868600	-0.18762100	Si	0.11722500	0.48148000	-2.50577500
H	6.28847100	-1.88070200	-0.13645300	H	0.86496200	-0.69351400	-1.78111100
H	6.21436300	-3.48094900	0.63801000	C	-1.69645900	0.27814000	-2.03799600
H	6.11428100	-3.34654900	-1.14014200	H	-2.26439000	0.70193500	-2.87887000
				H	-1.93033200	-0.79249600	-2.03958100
*** TS-39**-*alpha*-**40**				C	-2.15037700	0.93734600	-0.73166200
C	3.79306200	-2.13920900	-0.95972500	H	-2.08673100	2.02735400	-0.79837700
C	2.26672600	-2.50864400	-1.07411700	H	-3.19087300	0.68461000	-0.50453800
C	1.61166000	-1.24811800	-0.44531300	H	-1.54138500	0.63059300	0.12371200
O	2.48929100	-0.32281500	-0.15714400	C	0.91217800	2.04765700	-1.82564200
C	3.82943000	-0.63542100	-0.64347400	H	1.50673600	1.78354000	-0.94155100
O	4.35799000	-2.88527500	0.08194400	H	0.10631700	2.69310200	-1.45504400
C	4.19882400	0.26466400	-1.79753000	C	1.77172800	2.81216100	-2.83959900
O	1.90762000	-3.52289500	-0.17603600	H	1.16699200	3.18762300	-3.67064100
C	0.48855100	-1.27448000	0.45593600	H	2.25890800	3.67352700	-2.37202900
N	-0.61408500	-2.06433600	0.28604900	H	2.55058400	2.17159500	-3.26173300
C	-1.45160800	-1.90851400	1.36443200	C	0.35145100	0.19818400	-4.34390400
C	-0.86982200	-0.98822100	2.24377500	H	0.03877700	1.12338800	-4.84818300
C	0.33389700	-0.58913600	1.66926800	H	1.42061800	0.08742100	-4.54874500
N	-0.85788500	-2.84883900	-0.78447200	C	-0.44364800	-0.99089100	-4.89441800
C	-1.97625200	-3.51594500	-0.69724100	H	-0.25888900	-1.12857800	-5.96397400
N	-2.88785600	-3.49684500	0.30758500	H	-0.17494000	-1.92473700	-4.39037700
C	-2.64436200	-2.70388400	1.32356100	H	-1.52013700	-0.84468300	-4.76286400
O	3.43623400	-0.09116100	-2.92919700	N	-3.49681600	-2.59403300	2.38389800
C	4.12981300	0.15263400	-4.14328100	C	-4.73004200	-3.23471100	2.55421200
H	4.30253700	-2.34259000	-1.91111300	O	-5.23778200	-3.98877700	1.76539000
H	4.48849300	-0.42986700	0.20414900	O	-5.21093100	-2.84401500	3.73396100
H	4.04322400	1.32035400	-1.53225200	C	-6.51054300	-3.33560200	4.21046000

C	-6.65281600	-2.64179600	5.55759500	C	5.33437900	-1.09444900	-0.81496800
C	-7.61095700	-2.89376700	3.25406300	O	1.49870500	-3.98283000	-0.43797500
C	-6.45733700	-4.84798400	4.38530900	C	0.82149800	-0.86063200	-0.12137800
H	-7.59245700	-2.94233900	6.02775800	N	-0.43528900	-1.21843000	-0.54995700
H	-5.82722800	-2.91798200	6.21943100	C	-1.29552000	-0.16870700	-0.33178200
H	-6.65580800	-1.55550400	5.43234400	C	-0.58263400	0.88148100	0.25592900
H	-8.58254200	-3.12945700	3.69752800	C	0.72940100	0.44680600	0.38428400
H	-7.56123400	-1.81247400	3.09441000	N	-0.79482800	-2.40125800	-1.09528400
H	-7.53324500	-3.40221000	2.29248200	C	-2.05641300	-2.47016500	-1.41888600
H	-7.37371700	-5.17946600	4.88185400	N	-3.01958200	-1.52507700	-1.27419800
H	-6.37541300	-5.36044400	3.42611300	C	-2.65418500	-0.38723300	-0.73763800
H	-5.60711700	-5.12571600	5.01527600	O	4.89677000	-1.02861500	-2.14657800
H	-3.21911700	-1.98330600	3.14341900	C	5.85340400	-0.42106600	-2.99173400
H	4.36398600	1.21786300	-4.26404800	H	4.39693100	-3.46622500	-1.42445200
C	1.88329300	-2.80589100	-2.51970600	H	4.66327700	-1.93535800	1.03377400
H	0.81675100	-3.02429000	-2.58122400	H	5.50116100	-0.08964300	-0.39919700
H	2.13534200	-1.95642600	-3.15598800	H	6.27865000	-1.65545200	-0.73271400
H	2.45271400	-3.67198800	-2.86548600	H	-0.98394300	1.84301300	0.54254000
C	2.24064200	-4.84588600	-0.56672600	H	1.56125000	0.99618300	0.80220900
H	1.54610700	-5.22483900	-1.32466400	H	-2.36505400	-3.41181400	-1.85999500
H	3.26892900	-4.91413800	-0.93622000	H	6.06767200	0.60799700	-2.67443600
H	2.14984600	-5.45518300	0.33402300	H	6.79212400	-0.99104600	-3.00008200
C	5.76948000	-2.95967800	-0.00763800	Si	1.61638300	-3.04358600	2.67571300
H	6.23963800	-1.96929900	0.05899400	H	1.85550100	-2.48463900	1.23187700
H	6.11017700	-3.56550000	0.83314000	C	3.26818900	-2.83474200	3.54132200
H	6.07917500	-3.43515400	-0.94765400	H	3.20214200	-3.33332500	4.51780600
				H	4.03072800	-3.37660300	2.96971100
TS-39-40				C	3.65652800	-1.36170900	3.72596400
C	3.82043700	-3.17883500	-0.53528700	H	2.95773400	-0.85062500	4.39530600
C	2.31519300	-2.95699200	-0.89993300	H	4.65710000	-1.26222300	4.15729700
C	2.00591100	-1.67947500	-0.11063800	H	3.65059900	-0.81586900	2.77492900
O	3.10532900	-0.98442700	0.08963100	C	0.31463600	-1.83667600	3.29507200
C	4.29745400	-1.81969100	0.00719200	H	0.61807700	-0.81936900	3.01614300
O	3.89583500	-4.17463500	0.44955700	H	0.31810400	-1.86221800	4.39327700

C	-1.09042800	-2.14325900	2.76222800	C	5.21700800	-4.63580500	0.66910200
H	-1.47534200	-3.07855500	3.17970900	H	5.87318100	-3.84347700	1.05398300
H	-1.79940900	-1.34942100	3.01625600	H	5.15613000	-5.43316900	1.41219800
H	-1.09361200	-2.25588900	1.67262800	H	5.64988400	-5.03354700	-0.25799800
C	0.95301000	-4.79321700	2.58322600	C	2.16000100	-2.62155900	-2.38722600
H	0.41865700	-4.95484300	3.53112600	H	1.10988800	-2.45750500	-2.63383300
H	0.19258300	-4.82352800	1.79402800	H	2.74544100	-1.73164700	-2.62774500
C	1.99821900	-5.89230300	2.37372900	H	2.54751700	-3.44996100	-2.98583500
H	1.53375300	-6.88345100	2.39422000				
H	2.50553400	-5.76519200	1.41506900	*alpha*- **40**			
H	2.75869900	-5.87070200	3.16209900	C	3.78060200	-2.13032600	-1.04346600
N	-3.52805300	0.64171700	-0.53407800	C	2.23594400	-2.39662500	-1.11459700
C	-4.88986200	0.67684300	-0.85824400	C	1.62589500	-1.02390800	-0.67028300
O	-5.49548000	-0.20217600	-1.41450600	O	2.67819100	-0.26342600	-0.09875300
O	-5.35923200	1.85061600	-0.43653000	C	3.91113800	-0.63513700	-0.70011300
C	-6.77056600	2.20532000	-0.63633200	O	4.35136400	-2.92656500	-0.02790100
C	-6.85463800	3.59353400	-0.01819500	C	4.24696200	0.25021200	-1.88399900
C	-7.08239700	2.25852600	-2.12643400	O	1.82892300	-3.35233400	-0.15935300
C	-7.66020400	1.22333000	0.11503700	C	0.55236400	-1.12054300	0.36430600
H	-7.87613800	3.97236000	-0.10413400	N	-0.71864800	-1.46628500	0.05414200
H	-6.58261700	3.56031700	1.04048800	C	-1.50661800	-1.47286600	1.20279300
H	-6.18183000	4.28460600	-0.53366000	C	-0.68959900	-1.11298900	2.26704500
H	-8.08725100	2.66770800	-2.26379000	C	0.59312200	-0.89458500	1.73563500
H	-6.37273900	2.91656500	-2.63681700	N	-1.17292400	-1.76801100	-1.18849800
H	-7.04418200	1.26797900	-2.58099300	C	-2.43859600	-2.06660500	-1.22647600
H	-8.69483700	1.57458700	0.06730600	N	-3.33239900	-2.11864700	-0.19940600
H	-7.61050400	0.22463500	-0.32023200	C	-2.87109800	-1.82698100	0.99358300
H	-7.36339300	1.17346400	1.16687800	O	3.32442000	0.00859500	-2.92139200
H	-3.16889100	1.47845000	-0.08876200	C	3.58553000	0.79371100	-4.06347300
H	5.43496300	-0.40493100	-3.99928500	H	4.25658500	-2.35805600	-2.00873800
C	1.50657800	-5.16740500	-1.21317500	H	4.69068200	-0.49440300	0.05707100
H	2.52826700	-5.52235300	-1.39516000	H	4.21151100	1.30621400	-1.57552500
H	0.97013600	-5.91642100	-0.62766900	H	5.27430500	0.02897700	-2.21903600
H	0.98808300	-5.02797100	-2.16839500	H	-0.99278700	-1.02288400	3.30102000

H	1.47986100	-0.59796400	2.27599700	H	6.01553800	-3.52994700	-1.11833500
H	-2.82593700	-2.30746600	-2.21124200	H	1.23186100	-0.51739600	-1.56190700
H	4.58337800	0.58222700	-4.47288300				
H	2.83228200	0.54565500	-4.81380000	**40**			
N	-3.67756600	-1.84348400	2.10613800	C	3.81994800	-3.20232600	-0.75192200
C	-5.02100300	-2.19757200	2.18367300	C	2.41690600	-2.79856500	-1.28615200
O	-5.70851900	-2.56722400	1.26529800	C	1.91733200	-1.93254200	-0.10371000
O	-5.39253600	-2.05086400	3.46089500	O	3.05541400	-1.16975200	0.25353200
C	-6.76038400	-2.36795800	3.87737500	C	4.18457200	-2.04255100	0.20984000
C	-6.73512400	-2.05418500	5.36702600	O	3.70545400	-4.42412700	-0.05793700
C	-7.74960600	-1.46374200	3.15202600	C	5.41305500	-1.24387100	-0.16272700
C	-7.04241600	-3.84707400	3.64361200	O	1.52830000	-3.87809500	-1.41159900
H	-7.71628200	-2.25581700	5.80433300	C	0.79942200	-0.99082200	-0.39354300
H	-5.99180800	-2.67357400	5.87663700	N	-0.50562000	-1.33842900	-0.25474600
H	-6.48894000	-1.00174000	5.53367900	C	-1.32097500	-0.27281100	-0.62466100
H	-8.74251500	-1.59631400	3.59142700	C	-0.49352100	0.77795900	-0.99909200
H	-7.45978500	-0.41538700	3.27127200	C	0.82711900	0.32323600	-0.85064500
H	-7.80191400	-1.70130100	2.08914100	N	-0.96542500	-2.53076200	0.20206100
H	-8.01076500	-4.09964000	4.08507500	C	-2.26236000	-2.61135600	0.24250100
H	-7.07060000	-4.08413400	2.57957900	N	-3.18777500	-1.67576700	-0.11665600
H	-6.27461100	-4.45788900	4.12786500	C	-2.72265200	-0.52623400	-0.53915000
H	-3.25002300	-1.57961900	2.98546000	O	5.32728700	-0.84752700	-1.51001100
H	3.52340100	1.86638200	-3.83328500	C	6.43109300	-0.06441200	-1.90308800
C	1.79663100	-2.76436000	-2.52852100	H	4.55578600	-3.29495500	-1.56357200
H	0.71226900	-2.89916800	-2.55999800	H	4.34166200	-2.47856400	1.20803100
H	2.07604500	-1.96047800	-3.21300600	H	5.49029500	-0.36572500	0.49723400
H	2.28303300	-3.68415700	-2.86516200	H	6.30734100	-1.86732700	0.00080200
C	2.11483700	-4.70129100	-0.47139100	H	-0.81352900	1.75428700	-1.33540700
H	1.40022300	-5.11008800	-1.19674600	H	1.73297700	0.87947200	-1.04522000
H	3.13309800	-4.83223100	-0.85186600	H	-2.65364100	-3.55388300	0.61051200
H	2.01980500	-5.26075900	0.46262800	H	6.49465900	0.86215000	-1.31547200
C	5.74944800	-3.04890600	-0.16619900	H	7.37599500	-0.61443900	-1.78741700
H	6.25966000	-2.07646900	-0.11588700	N	-3.55302700	0.49631800	-0.93187000
H	6.10415500	-3.66982900	0.65900300	C	-4.94450300	0.50020300	-0.97662500

O	-5.66483700	-0.40319700	-0.63389400	H	-3.10913200	1.34509200	-1.26172500
O	-5.31969000	1.68709900	-1.46689300	H	6.29496700	0.19035300	-2.95601700
C	-6.74045600	2.00346800	-1.63340700	C	1.86446300	-4.81357100	-2.41577600
C	-6.70343900	3.41621600	-2.19986700	H	2.90558700	-5.14811900	-2.32843000
C	-7.37314300	1.04089600	-2.63149600	H	1.20823000	-5.67500800	-2.27310700
C	-7.43946200	1.98251900	-0.27943400	H	1.69893500	-4.41217700	-3.42338700
H	-7.72269200	3.76907700	-2.37663700	C	4.96197400	-5.00073600	0.22160200
H	-6.21435100	4.09881500	-1.49928400	H	5.57438500	-4.36917100	0.88076300
H	-6.15802500	3.43538000	-3.14758400	H	4.78044400	-5.95291800	0.72424400
H	-8.38541900	1.38384200	-2.86417700	H	5.52745300	-5.18481700	-0.70333100
H	-6.79460000	1.02598700	-3.56013700	C	2.54458000	-1.98487500	-2.56741000
H	-7.43083100	0.02883900	-2.22969000	H	1.55254200	-1.74061300	-2.95746500
H	-8.45570800	2.36965000	-0.39692800	H	3.09456600	-1.06298900	-2.36475800
H	-7.49369500	0.97143500	0.12570300	H	3.09732000	-2.54106200	-3.33006300
H	-6.90840700	2.62514600	0.42934500	H	1.62444200	-2.62599800	0.69997600

The end