D	mmClF Sequence No. Disorder Flag Model No. B _{average} B _{max} B _{max} B _{max} B _{asidor} E _{sovent} E _{sovent, lon} E _{sovent,}	A Companies A Companie	## AEtonsion_sp	Clic MW xlogp2 Resolution R _{free} R R _{free} -R Solvent T T _{ambient} B _{mean} pH Year EC code 178.141 -1.846 1.8 0.231 55 288 100 27.7 6.5 2001 3.2.1.23 280.329 2.783 2 0.26 0.22 0.04 45.18 298 100 40.4 7.2 2007 2.7.11.2 330.466 2.486 1.96 0.267 0.2291 0.0379 55.8 297 69 24.8 7 2004 308.339 1.802 2 0.259 0.21 0.049 42.19 278 294 7.2 2001 2.7.1.37 468.497 -0.726 1.8 0.216 0.194 0.022 59.3 277.15 100 28.36 8 2004 2.8.1.7 260.332 1.919 1.8 0.2383 0.2048 0.0335 44.5 77 27.484 8.5 2005 274.319 2.735 1.7 0.18908 0.16646 0.02262 50.18 288 93 13.031 7 2004 31.4.17 286.373 2.066 1.62 0.216 0.216 0.216 0 63.58 295 77 27.5 7 2006 13.1.9 365.269 2.864 1.73 0.232 0.232 0 63.54 295 77 27.5 7 2006 13.1.9 265.219 -2.419 1.96 0.1993 0.185 0.0143 50.1 289 293 6.7 2005 2.4.1.1 279.246 -1.996 1.96 0.2131 0.188 0.0251 49.87 280 293 6.7 2005 2.4.1.1 221.21 -2.132 1.7 0.21752 0.18618 0.03134 46.58 293 100 20.532 6.5 2007	de Keywords Macromolecule Beta-Galactosidase (E.C.3.2.1.23) Mitogen-activated protein kinase 1 (E.C.2.7.11.24) Mitogen-activated protein kinase 1 (E.C.2.7.1.37) Protein kinase, cell cycle, inhibition, TRANSFERASE PLP-binding enzyme, cysteine desulfurase, TRANSFERASE ESTROGEN RECEPTOR, LBD, GRIP PEPTIDE, HORMONE/GROWTH FACTOR RECEPTOR COMPLEX HUMAN ESTROGEN RECEPTOR ALPHA LIGAND-BINDING DOMAIN IN COMPLEX WITH OBCP-1M AND A GLUCOCORTICOID FO Oxidoreductase, InhA, Enoyl Acyl Carrier Reductase, Pyrrolidine Carboxamide Display Control Carrier Reductase, Pyrrolidine Carboxamide Coxidoreductase, InhA, Enoyl Acyl Carrier Reductase, Pyrrolidine Carboxamide Enoyl-[acyl-carrier-protein] reductase [NADH] (E.C.13.1.9) Oxidoreductase, InhA, Enoyl Acyl Carrier Reductase, Pyrrolidine Carboxamide Enoyl-[acyl-carrier-protein] reductase [NADH] (E.C.13.1.9) glycogenolysis, type 2 diabetes, TRANSFERASE Glycogen phosphorylase, muscle form (E.C.2.4.1.1) Lectin, CEL-III, Hemolysis, Hemagglutination, Pore-forming, Calcium, Magnesium, GalNac, TOXIN LECTIN, GLYCOPROTEIN, SIGNAL	Macromolecule Type Method Organism DPI Space Group Diffraction Source Refi HYDROLASE X-RAY DIFFRACTION 0.113 P 21 21 21 SYNCHROTRON TNT TRANSFERASE X-RAY DIFFRACTION 0.249 P 1.21 1 ROTATING ANODE CN3 TRANSCRIPTION, LIGAND BINDING X-RAY DIFFRACTION 0.229 P 31 SYNCHROTRON CN5 TRANSFERASE X-RAY DIFFRACTION P.21 21 21 SYNCHROTRON X-PI TRANSFERASE X-RAY DIFFRACTION 0.12 P 21 21 21 SYNCHROTRON CN5 REHORMONE/GROWTH FACTOR REC X-RAY DIFFRACTION 0.149 P 1.21 1 SYNCHROTRON REF OXIDOREDUCTASE X-RAY DIFFRACTION Mycobacterium tuberculosis P 62 2 2 SYNCHROTRON CN5 Hydrolase X-RAY DIFFRACTION Mycobacterium tuberculosis 0.105 P 21 21 21 SYNCHROTRON REF OXIDOREDUCTASE X-RAY DIFFRACTION Mycobacterium tuberculosis 0.093 P 62 2 2 SYNCHROTRON CN5 OXIDOREDUCTASE X-RAY DIFFRACTION Mycobacterium tuberculosis 0.112 P 62 2 2 SYNCHROTRON CN5 TRANSFERASE X-RAY DIFFRACTION Mycobacterium tuberculosis 0.112 P 62 2 2 SYNCHROTRON CN5 TRANSFERASE X-RAY DIFFRACTION Mycobacterium tuberculosis 0.112 P 62 2 2 SYNCHROTRON CN5 TRANSFERASE X-RAY DIFFRACTION P 43 21 2 SYNCHROTRON CN5 TRANSFERASE X-RAY DIFFRACTION N CN5 TRANSFERASE X-RAY DIFFRACTION TRANSFERASE X-RAY DIFFRACTION TRANSFE	Sugar Name OpenE	ACD/Labs Na 5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-one (non-preferred name) (3R,4S,5R,6F METHYL-4-(4-PHENYL-1H-PYRAZOL-3-YL)-1H-PYRROLE-2-CARBOXAMIDE N,N-DIMETH)-21-hydroxypregn-4-ene-3,20-dione (8S,9S,10R,1)-5-oxo-2,3,5,9b-tetrahydro-1H-pyrrolo[2,1-a]isoindol-9-yl]-3-pyridin-2-ylurea 1-[(9bR)-5-ox fructofuranosyl 3-O-octanoyl-alpha-D-glucopyranoside [(2R,3R,4S,5l-2S,5S)-5-(HYDROXYMETHYL)-8-METHYL-3-OXABICYCLO[3.3.1]NON-7-EN-2-YL]PHENOL 4-[(1S,2S,5S)-6]-CHLORO-2-METHYLPHENYL)-1-CYCLOHEXYL-5-OXOPYRROLIDINE-3-CARBOXAMIDE (3S)-N-(3-chle-2-methoxyphenyl)-3,5-dimethyl-1H-pyrazole-4-carboxylate ethyl 1-(4-methoxyphenyl)-3,5-dimethyl-1H-pyrazole-4-carboxylate (3S)-1-cycloh (3-BROMOPHENYL)-1-CYCLOHEXYL-5-OXOPYRROLIDINE-3-CARBOXAMIDE (3S)-1-cycloh (3-BROMOPHENYL)-1-CYCLOHEXYL-5-OXOPYRROLIDINE-3-CARBOXAMIDE (3S)-N-(3-bro-10xy(0xo)acetyl]-beta-D-glucopyranosylamine methyl 2-oxo-2-ylamino)-2-deoxy-alpha-D-galactopyranose N-[(2S,3R,4R)ylamino)-2-deoxy-alpha-D-galactopyranose	SMILES R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-one WL-4-(4-PHENYL-1H-PYRAZOL-3-YL)-1H-PYRROLE-2-CARBOXAMIDE CN(C=0 I3S,14S,17S)-17-(2-hydroxyethanoyl)-10,13-dimethyl-1,2,6,7,8,9,11,12,14,15,16,17-dodecahydrocyclopenta[a]phenanthren-3-one C1CC(C c0-1,2,3,9b-tetrahydrobenzo[f]pyrrolizin-9-yl]-3-pyridin-2-yl-urea C13=C(C R,6R)-2-[(2S,3S,4S,5R)-3,4-dihydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl]oxy-3,5-dihydroxy-6-(hydroxymethyl)oxan-4-yl] octanoate C(CCCC 0-5-(HYDROXYMETHYL)-8-METHYL-3-OXABICYCLO[3,3,1]NON-7-EN-2-YL]PHENOL C1[C@+ orto-2-methyl-phenyl)-1-cyclohexyl-5-oxo-pyrrolidine-3-carboxamide C1CCCC ethoxyphenyl)-3,5-dimethyl-pyrazole-4-carboxylate C2C(CCC omphenyl)-1-cyclohexyl-5-oxo-pyrrolidine-3-carboxamide C1CC(C omphenyl)-1-cyclohexyl-5-oxo-pyrrolidine-3-carboxamide C1CC(C omphenyl)-1-cyclohexyl-5-oxo-pyrrolidine-3-carboxamide C1CC(C omphenyl)-1-cyclohexyl-5-oxo-pyrrolidine-3-carboxamide C1CC(C omphenyl)-1-cyclohexyl-5-oxo-pyrrolidine-3-carboxamide C1CC(C omphenyl)-1-cyclohexyl-5-oxo-pyrrolidine-3-carboxamide C1CC(C 0-2-[[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]amino]ethanoate [C@@H 0-3,5R,6R)-2,4,5-trihydroxy-6-(hydroxymethyl)oxan-3-yl]ethanoamide C1C(C@H 0,5R,6R)-2,4,5-trihydroxy-6-(hydroxymethyl)oxan-3-yl]ethanoamide C1C(C@H 0,5R,6R)-2,4,5-trihydroxy-6-(hydroxymethyl)oxan-3-yl]ethanoamide	VHQ-R subset UHQ-R subset UHQ-R subset UHQ-R subset UHQ-R subset (Celliform)([C@H]([C@H]([C@GH](CO)O1)O)O)O)OOOOOOOOOOOOOOOOOOOOOOOOOOO
11017 A2G_2ccv_1_A_1101_G_	1 10.58 12.87 9.54 0.98493 10.0046 7.1842 3.2871 0.00710529 9.58187 9.58897529 1.89892 5.81942 8.30847 1.367347 40.83 31.84 2.57151 10.1279 7.5432 6.61396 5.59416 3.50285 9.09701 1.76794 3.11033 3.89008 3.38908 1.258087 1.2580	26.4319 3.9196 2.54305 17.06343 16.16248 30.266 24.43068 21.86753 4.8241 16.9369 7.4744471 0.074 0.97 10.58 18.86 21.58753 2.29.959 13.2002 24.3386 1.082071 0.172 0.077 0.78 0.97 10.58 18.88 20.4 271.42 29.959 13.2002 24.3386 1.082071 0.172 0.077 0.78 0.772 33.05 30.73 36.7347 378 216.6747 945.006 64.124 1.0844 1.1783 0.03369 6.66548 7.90546 2.1316 18.57746 17.63748 10.572 14.7378 10.572 14.738 1.08207 0.088 0.075 0.084 0.965 25.3 25.3 25.3015 16.00 44.7333 212.88 604.481 1.38539 3.9816 21.1200 25.1085 1.084	259.771	221.21 -2.132	LECTIN, SNAIL, HELIX POMATIA LECTIN, COLLAGEN, ACIDIC PH, COMPLEMENT, SUGAR-BINDING PROTEIN, GLYCOPROTEIN, POLYMORPHISM, INNATE IMML FICOLIN-1 enterotoxin, receptor, ligand, B-pentamer Lectin, CEL-III, Hemolysis, Hemagyliutination, Pore-forming, Calcium, Magnesium, METHYL-ALPHA-D-GALACTOPYLANOSIDE, TOXIN Hemolytic lectin CEL-III BETA/ALPHA BARREL, TIM barrel, HOMO-TETRAMER, METAL-BINDING PROTEIN, ISOMERASE L-rhamnose isomerase (E.C.5.3.1.14) Fatty acid-binding, LiPID TRANSPORT lectin, carbohydrate, SUGAR BINDING PROTEIN protein structure initiative, MCSG, Midwest Center for Structural (Probable transcriptional regulator phore) L-YSOZYME, ENZYME, SUBSTRATE COMPLEX, HYDROLASE LYSOZYME, ENZYME, SUBSTRATE COMPLEX, HYDROLASE Cyclosolic Neutral beta-Glycosylceramidase, Hydrolase protein-carbohydrate complex, glucose, galactose, periplasmic binding protein, SUGAR BINDING PROTEIN glucose binding protein, periplasmic binding protein, GBP, SUGAR BINDING PROTEIN glucose binding protein, periplasmic binding protein, disulfide, SUGAR BINDING PROTEIN glucose binding protein, periplasmic binding protein, disulfide, SUGAR BINDING PROTEIN glucose binding protein, periplasmic binding protein, 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3,6S)-2-(hydroxymethyl)-6-methoxy-oxane-3,4,5-triol [C@H]1(3,2,3,5,6-pentahydroxyhexanal C(-O)[C 6-(trifluoromethyl)pyrimidin-2-yl]sulfanyl-1-piperidin-1-yl-ethanone FC(F)(F) 3,2-(hydroxymethyl)oxane-2,3,4,5-tetrol C([C@G 3,-6-(hydroxymethyl)oxane-2,3,4,5-tetrol C([C@G 3,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol [C@GH 5,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol [C@GH 6,6R)-6	
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Prostacyclin synthase, enzyme-inhibitor complex, cybaca, cytochrome p450, Endoplasmic reticulum, Fatty acid biosynthesis, Heme, Iron Prostacyclin synthase (E.C.5.1.99.4) Extractioi dioxygenase, 2,3-dihydroxybiphenyl, Non-heme iron, Anaerobic, PCB biodegradation, OXIDOREDUCTASE Extractioi dioxygenase, 2,3-Dihydroxybiphenyl, non-heme iron, Anaerobic, PCB biodegradation, OXIDOREDUCTASE Extractioi dioxygenase, 2,3-Dihydroxybiphenyl, non-heme iron, Anaerobic, PCB biodegradation, OXIDOREDUCTASE Extractioi dioxygenase, 2,3-Dihydroxybiphenyl, non-heme iron, Anaerobic, PCB biodegradation, OXIDOREDUCTASE Extractioi dioxygenase, protein substrate complex, Oxidoreductase 1,2-dihydroxynaphthalene dioxygenase (E.C.1.13.11.39) four repetitions of beta-alpha-beta-beta-beta motifs, OXIDOREDUCTASE 1,2-dihydroxynaphthalene dioxygenase (E.C.1.13.11.39) Extractioi dioxygenase, 2,3-Dihydroxybiphenyl, non-heme iron, Anaerobic, PCB biodegradation, OXIDOREDUCTASE 1,2-dihydroxynaphthalene dioxygenase 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13OXIDOREDUCTASE X-RAY DIFFRACTION 0.175 P 21 21 21 SYNCHROTRON CNS OXIDOREDUCTASE X-RAY DIFFRACTION 0.118 P 1 SYNCHROTRON SHE Nydrolase X-RAY DIFFRACTION 0.118 P 1 SYNCHROTRON SHE Nydrolase X-RAY DIFFRACTION 0.175 P 21 21 21 SYNCHROTRON SHE Nydrolase X-RAY DIFFRACTION 0.177 P 61 ROTATING ANODE X-P 14 Hydrolase X-RAY DIFFRACTION 0.177 P 61 ROTATING ANODE CNS OXIDOREDUCTASE X-RAY DIFFRACTION 0.077 P 1 21 1 SYNCHROTRON REF Nydrolase X-RAY DIFFRACTION 0.095 P 1 21 1 SYNCHROTRON REF Nydrolase X-RAY DIFFRACTION 0.095 P 1 21 1 SYNCHROTRON REF Nydrolase X-RAY DIFFRACTION 0.095 P 1 21 1 SYNCHROTRON REF Nydrolase X-RAY DIFFRACTION 0.095 P 1 21 1 SYNCHROTRON REF Nydrolase X-RAY DIFFRACTION 0.095 P 1 21 1 SYNCHROTRON REF Nydrolase X-RAY DIFFRACTION 0.095 P 1 21 1 SYNCHROTRON REF Nydrolase X-RAY DIFFRACTION 0.095 P 1 21 1 SYNCHROTRON REF Nydrolase X-RAY DIFFRACTION 0.095 P 1 21 1 SYNCHROTRON REF Nydrolase X-RAY DIFFRACTION 0.095 P 1 21 1 SYNCHROTRON REF Nydrolase X-RAY DIFFRACTION 0.095 P 1 21 1 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92555 CBF_1p4j_1_998_E_	1 20.8473 26.42 16.7 2.99918 1 16.6113 16.74 14.14 1.23905 1 16.6113 16.74 14.14 1.23905 1 1 16.6113 16.74 14.14 1.23905 1 1 20.8478 27.31 11.59 4.64648 1 1 20.8478 27.31 11.59 4.64648 1 1 20.8478 27.31 11.59 4.64648 1 1 22.6152 19.66 9.04 2.90024 11.8326 8.25644 6.07648 4.35208 7.89565 12.24773 1.69873 4.22814 6.17112 1 42.1068 43.3 41.47 0.360621 9 1 1 34.082 20.51 8.64 3.27052 1 1 22.458 22.99 4.48006 1 1 29.4532 45.86 22.99 4.48006 1 1 29.4532 45.86 22.99 4.48006 1 1 25.78 20.19 1.2563 2.264 4.0458 3.46034 2.24862 2.238366 4.63228 1.31747 1.83008 3.21686 1 1 2.78 20.19 7.39 3.37123 12.3464 9.82574 5.31708 10.2617 1.04798 11.50597 1.87367 7.58845 12.1947 1 1 1.2578 20.19 1.2578 20.19 1.2578	-2.81944 3.2992 5.248 6.3268 12.1792 5.248 6.3268 12.1792 5.248 5.2982 5.3142 1.3148 1.4.2868 2.2142 2.2142 2.21428 2.21422 2.2142 2.2142 2.2142 2.2142 2.2142 2.2142 2.2142 2.2142 2.2142	541,049 535,119 7,2947 61,335 4,355 5,93 2 3,2 2 6 7 1 1 1 15 8 13 no no 791,54 788,495 4,80694 62,711 14,715 3,045 4 6,4 1 8 111 2 2 2 23 11 22 no no 812,218 803,306 14,3346 149,251 19,715 8,912 4 6,4 1 8 11 2 2 2 23 11 22 no no 768,15 766,994 1,45367 19,443 6,493 1,156 4 6,4 1 8 11 2 2 2 23 11 22 no no 6515,34 506,333 24,49 766,404 16,791 9,007 6 6 6 26 3 5 4 4 31 6 21 yes no 169,501 151,182 47,6641 2068,72 19,17 18,319 5 6,2 9 3 4 3 3 5 31 8 23 yes no 37,148 37,151 1,7136 21,783 2,544 0,003 1 1 1 0 0 0 0 0 0 5 5 2 6 no no 299,865 275,509 31,6255 518,106 18,843 24,356 4 52,3 4 6 8 1 1 1 19 10 16 no no 64,099 62,204 2,32892 17,369 2,717 1,895 2 3 6 2 3 2 2 16 6 13 yes no 454,061 452,99 5,9036 100,982 16,929 1,112 3 4 6 0 3 5 3 5 2 6 6 20 yes no 43,382 41,533 3,3743 109,396 2,679 1,849 1 1 1 0 0 0 0 0 0 4 2 2 4 no no 40,928 40,532 12,8091 45,495 3,94 0,396 1 1,15 1 1 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	223.182 -3.504	glycogen Phosphorylase, structure, catalytic site, new allostenc site, IRANS-ERASE Slycogen phosphorylase (E. C.2.4.1.1) TRANS-ERASE Slycogen phosphorylase (E. C.2.4.1.1) Beta sandwich, HYDROLASE ENDOGLUCANASE, CELLULIOSE DEGRADATION, CLYCOSIDE HYDROLASE FAMILY 5 Periplasmic binding protein, cellulose, thermophilic proteins, cellobiose binding protein, SUGAR BINDING PROTEIN Jaipha/beta-hydrolase, luciferase, OXIDOREDUCTASE Photoprotein, obelin, bioluminescence, calcium binding, EF-hand, aequorin, Structural Genomics, PSI, Protein Structure Initiative, South Obelin CLYCOGEN METABOLISM, GLYCOGEN PHOSPHORYLASE B, INHIBITION, CENTRAL CAVITY, DRUG BINDING SITE, TRANSFER GLYCOGEN PHOSPHORYLASE (E.C.2.4.1.1) Lind edhagenase alpha/beta-hydrolase halocarbons GLYCOGEN PHOSPHORYLASE, INHIBITOR BINDING, AMIDOCARBAMATE, TRANSFERASE GLYCOGEN PHOSPHORYLASE, INHIBITOR BINDING, AMIDOCARBAMATE, TRANSFERASE GLYCOGEN PHOSPHORYLASE, INHIBITOR BINDING, AMIDOCARBAMATE, TRANSFERASE Methionine aminopeptidase, complex, HYDROLASE 3D-STRUCTURE, ATP-BINDING, CHAPERONE, HEAT SHOCK, INHIBITOR, MULTIGENE FAMILY, CHAPERONE/COMPLEX HORMONE HO	TRANSFERASE X-RAY DIFFRACTION P43 21 2 SYNCHROTRON CNS HYDROLASE X-RAY DIFFRACTION 0.174 C 1 2 1 SYNCHROTRON REF ENDOGLUCANASE X-RAY DIFFRACTION 0.169 P 21 21 21 SYNCHROTRON REF SUGAR BINDING PROTEIN X-RAY DIFFRACTION 0.078 P 41 21 2 SYNCHROTRON REF OXIDOREDUCTASE X-RAY DIFFRACTION 0.144 P 1 2 1 1 SYNCHROTRON REF GLYCOGEN METABOLISM X-RAY DIFFRACTION P43 21 2 SYNCHROTRON X-P HYDROLASE X-RAY DIFFRACTION 0.142 P 21 21 2 ROTATING ANODE CNS TRANSFERASE X-RAY DIFFRACTION 0.142 P 21 21 2 ROTATING ANODE CNS TRANSFERASE X-RAY DIFFRACTION 0.142 P 21 21 2 ROTATING ANODE CNS TRANSFERASE X-RAY DIFFRACTION 0.166 P 1 21 1 ROTATING ANODE CNS CHAPERONE X-RAY DIFFRACTION 0.016 P 1 21 1 ROTATING ANODE CNS HORMONE X-RAY DIFFRACTION 0.081 P 43 2 2 SYNCHROTRON X-P HORMONE X-RAY DIFFRACTION 0.0157 I 2 1 3 PRO HORMONE X-RAY DIFFRACTION 0.152 I 2 1 3 PRO HORMONE X-RAY DIFFRACTION 0.152 I 2 1 3 PRO HORMONE X-RAY DIFFRACTION 0.152 I 2 1 3 PRO HORMONE X-RAY DIFFRACTION 0.152 I 2 1 3 PRO HORMONE X-RAY DIFFRACTION 0.152 I 2 1 3 PRO Transport Protein X-RAY DIFFRACTION 0.143 I 2 1 3 PRO OXIDOREDUCTASE X-RAY DIFFRACTION 0.161 P 2 1 2 1 2 SYNCHROTRON CNS OXIDOREDUCTASE X-RAY DIFFRACTION 0.161 P 2 1 2 1 2 SYNCHROTRON CNS OXIDOREDUCTASE X-RAY DIFFRACTION 0.161 P 2 1 2 1 2 SYNCHROTRON CNS OXIDOREDUCTASE X-RAY DIFFRACTION 0.245 P 2 1 2 1 2 SYNCHROTRON CNS OXIDOREDUCTASE X-RAY DIFFRACTION 0.245 P 2 1 2 1 2 SYNCHROTRON CNS OXIDOREDUCTASE X-RAY DIFFRACTION 0.245 P 2 1 2 1 2 SYNCHROTRON CNS OXIDOREDUCTASE X-RAY DIFFRACTION 0.245 P 2 1 2 1 2 SYNCHROTRON CNS OXIDOREDUCTASE X-RAY DIFFRACTION 0.245 P 2 1 2 1 2 SYNCHROTRON CNS OXIDOREDUCTASE X-RAY DIFFRACTION 0.245 P 2 1 2 1 2 SYNCHROTRON CNS OXIDOREDUCTASE X-RAY DIFFRACTION 0.245 P 2 1 2 1 2 SYNCHROTRON CNS OXIDOREDUCTASE X-RAY DIFFRACTION 0.245 P 2 1 2 1 2 SYNCHROTRON CNS OXIDOREDUCTASE X-RAY DIFFRACTION 0.245 P 2 1 2 1 2 SYNCHROTRON CNS OXIDOREDUCTASE X-RAY DIFFRACTION 0.245 P 2 1 2 1 2 SYNCHROTRON CNS	1 C-(1-HYDROGYL-BETA-D-GLUCOPYRANOSYL) FORMAMIDE	N-[((2R,3R,4\$,58,6R)-2,3,4,5-tetrahydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-carboxamide (non-preferred name) (2R,3R,4\$,58,6R)-2,3,4,5-tetrahydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-carboxamide (non-preferred name) (2R,3R,4\$,58,6R)-2-glucopyranose) (2R,3S,4\$,5F,6N,2YL-5-(4-HYDROXYPHENYL)PYRAZIN-2-YL]-2-(4-HYDROXYPHENYL)ACETAMIDE 2-(4-hydroxymosyl-beta-D-glucopyranose) (2R,3S,4\$,5F,6N,2YL-5-(4-HYDROXYPHENYL)PYRAZIN-2-YL]-2-(4-HYDROXYPHENYL)ACETAMIDE 2-(4-hydroxymosyl-benyl-1-4-fluorobenzyl)-2-(4-hydroxypiperidin-1-yl)-2-oxoethyl]-1H-indole-2-carboxamide 5-chloro-N-[(2,2-dichloropropane) (2S)-1,2-dichloropropane (2S)-1,2-dichloropropane (2S)-1,2-dichloropropane (2S)-1,3-thiazol-2-ylethanediamide N'-cyclopentyl-N'-1,3-thiazol-2-ylethanediamide N'-cyclopentyl-N'-1,3-thiazol-2-ylethanediamide N'-cyclopentyl-N'-1,4-ENZODIOXIN-6-YL)-3-METHYL-1H-PYRAZOL-5-YL]-6-ETHYLBENZENE-1,3-DIOL 4-[4-(2,3-dihyleth)-1,2-DICHLOF-1,1-DICHLOF-1	O1(C@R)	
143593 DFR 9xia 1 389 E DFR 9xia 1 A 389 B B 156523 DOG 1lke 1 500 B DOG 1lke 1 A 500 B B 1lke DOG A 500 B 157704 DR4 1zjp 1 1 J DR4 1zjp 1 A J 1zjp DR4 A 1 J 157706 DR5 288u 1 2 J DR5 288u 1 A 2 J 288u DR5 A 2 J 158589 DTL 1h16 1 A 9009 W DTL 1h16 1 A 9009 L 1h16 DTL A 9009 L 158591 DTL 1h17 1 A 9009 W DTL 1h17 1 A 9009 L 1h17 DTL A 9009 L 159283 DTX 1lnm 1 700 B DTX 1lnm 1 A 700 B 1lnm DTX A 700 B 180283 ESM 1lhw 1 301 E ESM 1lhw 1 301 E ESM 1lhw 1 301 E ETX 3bby 1 A 218 E ETX 3bby ETX A 218 E 180767 ETX 2d19 1 1006 K ETX 2d19 1 A 1006 K 2d19 ETX A 1006 K 180770 ETX 2fd6 1 403 L ETX 2fd6 2fd6 ETX H 403 L 2fd6 ETX H 400 L 2fd6 ETX H 400 L 2fd6 ETX H 400 L	1 12,5417 16,45 7.41 2,56556 14, 43,992 14,550 8,92694 7,61106 6,69929 18,4852 25,18449 3,63024 -5,81144 -14,1195 14,5621 8,264 8,115 14,562 1		406.302	1/8.185 -1.7 1.9 0.141 55.93 1990 5.3.1.5 390.519 2.444 1.9 0.24753 0.18808 51.1 298 298 33.566 8 2002 350.408 0.606 1.59 0.232 46.03 113 2005 356.326 -4.002 1.69 0.232 46.37 113 2005 122.121 -2.552 1.53 0.163 0.145 0.018 51.48 100 17.1 7.3 2002 2.3.1.54 122.121 -2.552 1.75 0.173 0.148 0.025 51.54 100 19 7.3 2002 2.3.1.54 374.519 3.685 1.9 0.24454 0.20637 0.03817 51.1 298 298 30.722 7.8 2002 90.1218 -0.266 1.85 0.195 0.161 0.034 53.46 277 100 16.365 8 2007 90.1218 -0.266 1.75 0.231 43.9 298 160 25.27 6 2005 3.1.3.2 90.1218 -0.266 <td>D-XYLOSE ISOMERASE (IC. C. S. 3.1.5) COMPLEX WITH INACTIVATOR PIERIS BRASSICAE, LIPOCALIN, ANTICALIN, GENETICAL ENGINEERING, DIGOXIGENIN, LIGAND BINDING PROTEIN GTB, ABOO (H), blood group, Hantigen, glycosyltransferase, retaining GTB, Blood group, ABO((H), glycosyltransferase, retaining ABO blood group (transferase A, alpha 1-3-N-acetylgalactosaminyltransferase); transferase B, alpha 1-3-galactosyltransferase) LYASE, GLYCYL RADICAL ENZYME, TRANSFERASE, ACYLTRANSFERASE, ACETYLATION FORMATE ACETYLTRANSFERASE 1 (E. C. 2.3.1.54) PIERIS BRASSICAE, LIPOCALIN, ANTICALIN, GENETICAL ENGINEERING, DIGOXIGENIN, DIGITOXIGENIN, LIGAND BINDING PROTEIN SHBG, 2-Methoxyestradiol, TRANSPORT PROTEIN NP, 416804.1, glutathione S-transferase, N-terminal domain, Structural Genomics, Joint Center for Structural Genomics, PSI, Protein Structural Genomics</td> <td> SOMERASE(INTRAMOLECULAR O) X-RAY DIFFRACTION 12 2 2</td> <td>1 3-DEOXY-3-METHYL-D-FRUCTOSE 3 -3-deox 5</td> <td>/-3-methyl-beta-D-fructofuranose ,5beta,8alpha,12beta)-3,12,14-trihydroxycard-20(22)-enolide ,5beta,8alpha,12beta)-3,12,14-trihydroxycard-20(22)-enolide 9-(beta-D-galactopyranosyloxy)nonanoate 4-O-beta-D-galactopyranosyl-beta-D-glucopyranoside (2S,3R,4S,5F-butane-1,2,3,4-tetrol (2S,3S)-butar -butane-1,2,3,4-tetrol (2S,3S)-butar ,5beta,8alpha)-3,14-dihydroxycard-20(22)-enolide ,17beta)-2-methoxyestra-1(10),2,4-triene-3,17-diol (2S,3S)-butar (2S,4S)-6,8R (8R,9S,13S,1 (2FTHOXYET (2FTHOXYE</td> <td>(C)OCC (C)COCC (C)COCC</td> <td>((\text{UC@H})((\text{LC@})(\text{CO})(\text{O})(\text{O})\text{O})\text{O}(\text{O}</td>	D-XYLOSE ISOMERASE (IC. C. S. 3.1.5) COMPLEX WITH INACTIVATOR PIERIS BRASSICAE, LIPOCALIN, ANTICALIN, GENETICAL ENGINEERING, DIGOXIGENIN, LIGAND BINDING PROTEIN GTB, ABOO (H), blood group, Hantigen, glycosyltransferase, retaining GTB, Blood group, ABO((H), glycosyltransferase, retaining ABO blood group (transferase A, alpha 1-3-N-acetylgalactosaminyltransferase); transferase B, alpha 1-3-galactosyltransferase) LYASE, GLYCYL RADICAL ENZYME, TRANSFERASE, ACYLTRANSFERASE, ACETYLATION FORMATE ACETYLTRANSFERASE 1 (E. C. 2.3.1.54) PIERIS BRASSICAE, LIPOCALIN, ANTICALIN, GENETICAL ENGINEERING, DIGOXIGENIN, DIGITOXIGENIN, LIGAND BINDING PROTEIN SHBG, 2-Methoxyestradiol, TRANSPORT PROTEIN NP, 416804.1, glutathione S-transferase, N-terminal domain, Structural Genomics, Joint Center for Structural Genomics, PSI, Protein Structural Genomics	SOMERASE(INTRAMOLECULAR O) X-RAY DIFFRACTION 12 2 2	1 3-DEOXY-3-METHYL-D-FRUCTOSE 3 -3-deox 5	/-3-methyl-beta-D-fructofuranose ,5beta,8alpha,12beta)-3,12,14-trihydroxycard-20(22)-enolide ,5beta,8alpha,12beta)-3,12,14-trihydroxycard-20(22)-enolide 9-(beta-D-galactopyranosyloxy)nonanoate 4-O-beta-D-galactopyranosyl-beta-D-glucopyranoside (2S,3R,4S,5F-butane-1,2,3,4-tetrol (2S,3S)-butar -butane-1,2,3,4-tetrol (2S,3S)-butar ,5beta,8alpha)-3,14-dihydroxycard-20(22)-enolide ,17beta)-2-methoxyestra-1(10),2,4-triene-3,17-diol (2S,3S)-butar (2S,4S)-6,8R (8R,9S,13S,1 (2FTHOXYET (2FTHOXYE	(C)OCC (C)COCC	((\text{UC@H})((\text{LC@})(\text{CO})(\text{O})(\text{O})\text{O})\text{O}(\text{O}
201700 GAL jiz7 1, A 2001 E GAL jiz7 1, A 2001 E 1 z7 GAL A 2001 E 201814 GAL rdk_1 1 1 C GAL rdk_1 1 1 C C C C C C C	1 19.5608 31.31 10.74 5.03122 6.10625 3.98978 5.80251 4.9467 2.83376 19.3919 -1.06231 -11.2939 -15.1203	-3.75716 10.23169 3.8264 22.4513 20.2777 41.978 30.5841 22.7677 4.3004 21.4371 3.0594 0.072 0.072 0.093 0.063 10.0 10.68 19.868 20 431.07 40.062 435.644 10.062 43.073 5.06901 4.0573 5.06901 4.06901	495.47	180.157 -2.341 1.5 0.219 55 288 100 20.7 6.5 2001 3.2.1.23 180.157 -2.341 1.8 0.23642 0.20315 0.03327 49.07 293.4 100 21.962 6 2007 3.2.1.21 180.157 -2.341 1.78 0.225 0.193 0.032 51.28 293 100 17.6 6 2007 3.2.1.21 180.157 -2.341 1.49 0.226 0.203 0.02369 42.28 113 22.49 2006 180.157 -2.341 2 0.267 0.217 57.22 295 92 7 1999 3.4.24.6 180.157 -2.341 2 0.167 43.59 1993 180.157 -2.341 2 0.207 0.179 0.028 57.12 298 293 5.7 2001 3.2.1.8 180.157 -2.341 1.75 0.217 0.169 0.048 44.01 277 277 6 2003 51.33 180.157 -2.341 1.75 0.217 0.169 0.048 44.01 277 277 6 2003 51.33 180.157 -2.341 1.9 0.20521 0.16904 0.03617 48.86 298 100 15.561 2004 2.4.2.36 180.157 -2.341 1.9 0.20521 0.16904 0.03617 48.86 298 100 13.109 2004 2.4.2.36 180.157 -2.341 1.7 0.194 0.185 0.009 57.86 293 293 25.3 7.3 2003 180.157 -2.341 1.7 0.194 0.185 0.009 57.86 293 293 25.3 7.3 2003 180.157 -2.341 1.59 0.229 45.77 291 113 7.5 2005 180.157 -2.341 1.85 0.245 0.196 0.049 63.5 298 100 7.5 2005 180.157 -2.341 1.56 0.205 0.176 0.029 52 290 100 19.486 5.6 2005 180.157 -2.341 1.56 0.205 0.176 0.029 52 290 100 19.486 5.6 2005 180.157 -2.341 1.50 0.245 0.187 44 43 289 26.2 8.1 1998 180.157 -2.341 1.8 0.267 0.182 45.16 100 16 7.5 2005 180.157 -2.341 1.8 0.267 0.182 45.16 100 16 7.5 2005 180.157 -2.341 1.8 0.267 0.182 45.16 100 16 7.5 2005 180.157 -2.341 1.8 0.267 0.182 45.16 100 16 7.5 2005 180.157 -2.341 1.8 0.267 0.182 45.16 100 16 7.5 2005 180.157 -2.341 1.8 0.266 0.176 44.415 277 277 6 2003 5.1.33 180.157 -2.341 1.8 0.266 0.176 44.415	Beta-Galactosidase (E. C.3.2.1.23) C-TYPE LECTIN, CALCIUM-BINDING PROTEIN CHORNO (Soutral beta-Glycosylceramidase, Hydrolase) Novel Cytosolic Neutral beta-Glycosylceramidase, Hydrolase beta trefici, TOXIN PROTEIN-CARBOHYDRATE INTERACTION, GLYCOSIDE HYDROLASE, CBM32, GH84C, HYDROLASE BETA TREFOIL, JELLY-ROLL, TOXIN GALACTOSE-BINDING PROTEIN GALACTOSE-BINDING PROTEIN GALACTOSE-BINDING PROTEIN GALACTOSE-BINDING PROTEIN GALACTOSE-BINDING PROTEIN GALACTOSE-GLUCOSE-BINDING PROTEIN GALACTOSE GLUCOSE-BINDING PROTEIN COMPLEXED WITH D-GALACTOSE GALACTOSE GLUCOSE-BINDING FROTEIN GALACTOSE GLUCOSE-	HYDROLASE	E	galactopyranose (2R,3R,4S,5F) -galactopyranose (2R,3R,4S,5F)	[C@@H 3,6R)-6-(hydroxymethyl)oxane-2,3.4,5-tetrol [C@H]1(1,0)-1,000000000000000000000000000000000	1 (C@@H (C@H (C@@H (CO@H (CO@H (CO)O1)O)O)O)O O O O O O O O O O O O O O O
Control Cont	1 1/20 1/2	-1.9.5125	366.458	180.157 -2.341 1.7 0.22132 0.17897 0.04235 39.19 295 100 14.432 6.3 2006 2.71.6 180.157 -2.341 1.5 0.22807 0.18909 0.03898 38.64 295 100 15.952 6.3 2006 2.71.6 180.157 -2.341 1.76 0.235 0.211 0.024 48 287 6.7 2001 2.41.1 180.157 -2.341 1.4 0.228 0.205 0.023 58.49 298 100 6 2003 180.157 -2.341 1.93 0.235 0.1926 0.0424 47.09 289 100 20.205 6.7 2007 2.41.1 180.157 -2.341 1.9 0.258 0.213 0.045 59.11 298 110 6.5 1999 2.71.1 180.157 -2.341 1.7 0.209 44.5 293 100 7 2001 1.1.5 180.157 -2.341 1.8 0.198 0.166 0.032 39 290 100 17.6 7 2001 1.1.5 180.157 -2.341 1.94 0.19 55.7 295 120 21.4 7.5 2001 2.4.11 180.157 -2.341 2 0.218 0.179 0.039 50.17 295 298 31.5 6.7 2002 2.4.11 180.157 -2.341 2 0.235 0.207 0.028 50.3 298 298 33.8 6.7 2002 2.4.11 180.157 -2.341 2 0.218 0.168 0.055 44.18 277 277 6 2003 2.4.11 180.157 -2.341 1.75 0.218 0.168 0.055 44.18 277 277 6 2003 2.4.11 180.157 -2.341 1.6 0.20697 0.152 0.024 56.27 295 120 18.3 7.5 2003 2.4.11 180.157 -2.341 1.6 0.20697 0.18744 0.01963 45.3 293 90 13.51 6.5 2003 2.4.15 180.157 -2.341 1.6 0.20697 0.18744 0.01963 45.3 293 90 13.51 6.5 2003 2.4.15 180.157 -2.341 1.6 0.20697 0.18744 0.01963 45.3 293 90 13.51 6.5 2003 2.4.15 180.157 -2.341 1.8 0.177 48.7 291 100 6.5 2004 5.3.15 180.157 -2.341 1.9 0.256 0.234 0.022 56.63 100 2.3086 5.6 2005 2.4.11 180.157 -2.341 1.9 0.256 0.234 0.022 56.63 100 2.3086 5.6 2005 2.4.11 180.157 -2.341 1.9 0.256 0.234 0.022 56.63 100 100 15.6 2005 2.4.11 180.157 -2.341 1.75 0.188 0.15 0.0382 33.17	galactokinase, ATP analogue, galactose, Structural Genomics, NPPSFA, National Project on Protein Structural and Functional Analyses Probable galactokinase (E.C.2.7.1.6) galactokinase, ADP analogue, galactose, Structural Genomics, NPPSFA, National Project on Protein Structural and Functional Analyses Probable galactokinase (E.C.2.7.1.6) GLYCOGEN METABOLISM, GLYCOGEN PHOSPHORYLASE B, INHIBITION, CENTRAL, CAVITY, DEGIDINION STE, TRANSFERGLYCOGEN PHOSPHORYLASE (E.C.2.4.1.1) collectin, c-type lectin, alpha-helical coiled coil, carbohydrate recognition domain, SIGNALING PROTEIN Clycogen phosphorylase, muscle form (E.C.2.4.1.1) STRUCTURALLY HOMOLOGOUS DOMAINS, TRANSFERASE HEXOKINASE TYPE (E.C.2.7.1.1) SOR FAMILY, OXIDOREDUCTASE x-ray diffraction, endoglucanase, family 9, cellutiose, cellulose binding domain, (alpha-alpha)6-barrel, HYDROLASE Endoglucanase (E.C.2.4.1.19) ytype 2 diabetes, glycogen phosphorylase, structure, inhibitor, new allosteric site, Transferase glycogen phosphorylase(E.C.2.4.1.1) ytype 2 diabetes, glycogen phosphorylase, structure, inhibitor, new allosteric site, Transferase glycogen phosphorylase(E.C.2.4.1.1) MUTAROTASE, EPIMERASE, GALACTOSE METABOLISM, ISOMERASE GALACTOSE MUTAROTASE, EPIMERASE, GALACTOSE METABOLISM, ISOMERASE GALACTOSE MUTAROTASE, EPIMERASE, GALACTOSE METABOLISM, ISOMERASE glycosyltransferase, transferase, cyclodextin Cyclomatiotextrin glucanotransferase precursor (E.C.2.4.1.19) xylose isomerase, hydrice shift, atomic resolution, tim barrel alpha-beta, RIKEN Structural Genomics/Proteomics Initiative, RSGI, Structural Genomics, PHOTOSYNTHESIS SINGERASE(INTRAMOLECULAR OXIDOREDUCTSE) Glycosph Phosphorylase, Iransferase protein-carbohydrate complex, glucose, galactose, periplasmic binding protein, SUGAR BINDING PROTEIN Glycogen phosphorylase, Iransferase protein-carbohydrate complex, glucose, galactose, pe	Transferase	S	(2S,3R,4S,5F) 0-galactopyranose (2S,3R,4S,5F) 0-glucopyranose (2S,3R,4S,5F) 0-glucopyranose (2S,3R,4S,5S)	C@H11	([C@@H]([C@H]([C@H](CO)O1)O)O)O
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C. 2.1.1-) untiple domain, beta-alpha-barrel, alpha-amylase-family, complex with glucose, HYDROLASE DIABETES, GLYCOGEN METABOLISM, PHOSPHORYLASE A, INHIBITION, ALLOSTERIC SITE, CRYSTAL STRUCTURE, TRANSFE GLYCOGEN PHOSPHORYLASE GLYCOGEN PHOSPHORYLASE, GLUCOPYRANOSE SPIROHYDANTOIN, WATER STRUCTURE, INHIBITOR BINDING, ANTH-IYPE GLYCOGEN PHOSPHORYLASE GLYCOGEN PHOSPHORYLASE, GLUCOPYRANOSE SPIROHYDANTOIN, WATER STRUCTURE, INHIBITOR BINDING, ANTH-IYPE GLYCOGEN PHOSPHORYLASE GLYCOGEN PHOSPHORYLASE GLUCOPYRANOSE SPIROHYDANTOIN, WATER STRUCTURE, INHIBITOR BINDING, ANTH-IYPE GLYCOGEN PHOSPHORYLASE B COMPLEX, LECTIN, SACCHARIDE lectin, carbohydrate recognition, glucose, sugar binding protein Beta-prism-1 fold, Post translational protein, glacose-specific, SUGAR BINDING PROTEIN OXIDOREDUCTASE(FLAVOPROTEIN) OXIDOREDUCTASE(FLAVOPROTEIN) OXIDOREDUCTASE(FLAVOPROTEIN) OXIDOREDUCTASE(FLAVOPROTEIN) Insulin, HORNIONE, GLUCOSE METABOLISM UPOCALIN, BETA-BARREL, Transport Protein Major Urinary Protein Major Urinary Protein Methionine aminopeptidase, pita bread, hydrolase protein-product complex, TRANSFERASE Umonen-1,2-epoxide hydrolase hydrophotin, amphipilie, protein surfactant, SURFACE ACTIVE PROTEIN PROTEINS PROTEIN	Hydrolase	1 ALPHA-D-GLUCOSE alpha-1 1 ALPHA-D-GLUCOSE alpha-1 1 ALPHA-D-GLUCOSE alpha-1 3.8	(2S,3R,4S,5S) -glucopyranose (2S,3R,4S,5S) -glucopyranose (2S,3R,4S,5S) -glucopyranose (2S,3R,4S,5S) -glucopyranose (2S,3R,4S,5S) -glucopyranose (2S,3R,4S,5S) -glucopyranose (2S,3R,4S,5S) -glucopyranoside (2S,3R,4S,5S) -glpta-D-glucopyranoside (2R,3S,4S,5F) -glucopyranoside (2R,3R,4S,5F) -glucopyranoside (2R,3R,4S,5F) -glucopyranoside (2R,3S,4S,5F) -glucopyranoside (2R,3S,4S	C@H]10	([C@@H]([C@H]([C@@H](CO@H](CO)O1)O)O)O no no ([C@@H]([C@H]([C@@H](CO)O1)OO)OO no no ([C@@H]([C@H]([C@H](CO)O1)OO)OOC no no ([C@@H]([C@H]([C@H](CO)O1)OO)OOC yes yes yes ([C@@H]([C@H]([C@H]((CO)O1)OO)OOC no no no cCCCCCC (C=C1)O no no no no cCCCCCCC([C@H](O)[C@H](O)[C@H](O)C@H](OO)OOC no no no no cCCCCCC no no no no no cCCCCCCC([C@H](O)[C@H](O)[C@H](O)[C@H](O1)CO no no no no cCCCCCCC([C@H](O)[C@H](O)[C@H](O)[C@H](O1)CO no no no no cCCCCCCC([C@H](O)[C@H](O)[C@H](O)[C@H](O1)CO no no no no no cCCCCCCC([C@H](O)[C@H](O)[C@H](O)[C@H](O1)CO no no no no no no no no no cCCCCCC([C@H](O)[C@H](O)[C@H](O)[C@H](O1)CO no no no no no no no no no n
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INTEBEta-lactamases SHV-1 (E.C.3.5.2.6) Antibiotic resistance, bactamase inhibitor, HYDROLASE, BETA-LACTAM HYDROLASE,	TRANSPORT PROTEIN X-RAY DIFFRACTION 0.196 P 43 21 2 ROTATING ANODE CNS hydrolase X-RAY DIFFRACTION 0.094 P 21 21 21 ROTATING ANODE CNS hydrolase X-RAY DIFFRACTION 0.089 P 21 21 21 SYNCHROTRON CNS HYDROLASE X-RAY DIFFRACTION 0.089 P 21 21 21 SYNCHROTRON CNS HYDROLASE X-RAY DIFFRACTION 0.099 P 21 21 21 SYNCHROTRON CNS HYDROLASE X-RAY DIFFRACTION 0.099 P 21 21 21 SYNCHROTRON CNS HYDROLASE X-RAY DIFFRACTION 0.017 P 31 2 1 SYNCHROTRON CNS HYDROLASE X-RAY DIFFRACTION 0.17 P 31 2 1 SYNCHROTRON CNS HYDROLASE X-RAY DIFFRACTION 0.143 P 1 21 1 ROTATING ANODE CNS HYDROLASE X-RAY DIFFRACTION 0.143 P 1 21 1 ROTATING ANODE CNS HYDROLASE X-RAY DIFFRACTION 0.1447 P 21 21 21 ROTATING ANODE CNS HYDROLASE X-RAY DIFFRACTION 0.1447 P 21 21 21 ROTATING ANODE CNS HYDROLASE X-RAY DIFFRACTION 0.145 P 21 21 21 ROTATING ANODE CNS HYDROLASE X-RAY DIFFRACTION 0.15 P 21 21 21 ROTATING ANODE CNS HYDROLASE X-RAY DIFFRACTION 0.15 P 21 21 21 ROTATING ANODE CNS HYDROLASE X-RAY DIFFRACTION 0.089 P 31 2 1 ROTATING ANODE CNS HYDROLASE X-RAY DIFFRACTION 0.156 P 21 21 21 SYNCHROTRON REPORTED TO SYNCHROTRON CNS HYDROLASE X-RAY DIFFRACTION 0.156 P 21 21 21 SYNCHROTRON REPORTED TO SYNCHROTRON REPORTED TO SYNCHROTRON CNS HYDROLASE X-RAY DIFFRACTION 0.156 P 21 21 21 SYNCHROTRON REPORTED TO SYNCHROTRON CNS HYDROLASE X-RAY DIFFRACTION 0.131 P 21 21 21 ROTATING ANODE CNS HYDROLASE X-RAY DIFFRACTION 0.131 P 21 21 21 ROTATING ANODE CNS HYDROLASE X-RAY DIFFRACTION 0.131 P 21 21 21 ROTATING ANODE CNS HYDROLASE X-RAY DIFFRACTION 0.131 P 21 21 21 ROTATING ANODE CNS HYDROLASE X-RAY DIFFRACTION 0.131 P 21 21 21 ROTATING ANODE CNS HYDROLASE X-RAY DIFFRACTION 0.131 P 21 21 21 ROTATING ANODE CNS HYDROLASE X-RAY DIFFRACTION 0.131 P 21 21 21 ROTATING ANODE CNS HYDROLASE X-RAY DIFFRACTION 0.131 P 21 21 21 ROTATING ANODE CNS HYDROLASE X-RAY DIFFRACTION 0.131 P 21 21 21 ROTATING ANODE CNS HYDROLASE X-RAY DIFFRACTION 0.131 P 21 21 21 ROTATING ANODE CNS HYDROLASE X-RAY DIFFRACTION 0	0 (3S,4R,5R,5S)-3,4,5-1RINTDROXY-6-(HYDROXYME1HYL)TETRAHYDRO-2H-PYRAN-2-ONE	ky-6-methylheptan-3-one hexylhexyl 4-O-alpha-D-glucopyranosyl-beta-D-glucopyranoside hexylhexyl 4-O-alpha-D-glucopyranosyl-beta-D-glucopyranose hexplexylhexyl 4-O-alpha-D-glucopyranose hexplexylhexylexylhexylexyllhexylexylexylexylexylexylexylexylexylexyl	-6-METHYL-HEPTAN-3-ONE CC(CCC 5.6R)-2-[(2R,3S,4R,5R,6R)-6-(6-cyclohexylhexoxy)-4,5-dihydroxy-2-(hydroxymethyl)oxan-3-yl]oxy-6-(hydroxymethyl)oxane-3,4,5-triol C@H]1(5.6R)-2-[(2R,3S,4R,5R,6R)-6-(6-cyclohexylhexoxy)-4,5-dihydroxy-2-(hydroxymethyl)oxan-3-yl]oxy-6-(hydroxymethyl)oxane-3,4,5-triol C@H]1(5.6R)-2-[(2R,3S,4R,5R,6R)-6-(6-cyclohexylhexoxy)-4,5-dihydroxy-2-(hydroxymethyl)oxan-3-yl]oxy-6-(hydroxymethyl)oxane-3,4,5-triol C@H]1(5.6R)-2-[(2R,3S,4R,5R,6R)-6-(6-cyclohexylhexoxy)-4,5-dihydroxy-2-(hydroxymethyl)oxan-3-yl]oxy-6-(hydroxymethyl)oxane-3,4,5-triol C@H]1(5.6R)-6-(hydroxymethyl)-5-[(2S,3S,4S,5S,6R)-3,4,5-trihydroxy-2-(hydroxymethyl)oxan-2-yl]oxy-oxane-2,3,4-triol C@@H (5.6R)-4-(hydroxymethyl)-2-methoxy-oxan-3-yl]ethanamide C@@H (5.6R)-4-(hydroxymethyl)-6-[(2R,3S,4R,5R,6S)-4,5-6-trihydroxy-2-(hydroxymethyl)oxan-3-yl]oxy-oxane-3,4,5-triol C@H]1(7.6R)-2-(hydroxymethyl)-6-[(2R,3S,4R,5R,6S)-4,5-6-trihydroxy-2-(hydroxymethyl)oxan-3-yl]oxy-oxane-3,4,5-triol C@H]1(7.6R)-2-(hydroxymethyl)-6-[(2R,3S,4R,5R,6S)-4,5-6-trihydroxy-2-(hydroxymethyl)oxan-3-yl]oxy-oxane-3,4,5-triol C@H]1(7.6R)-2-(hydroxymethyl)-6-[(2R,3S,4R,5R,6S)-4,5-6-trihydroxy-2-(hydroxymethyl)oxan-3-yl]oxy-oxane-3,4,5-triol C@H]1(7.6R)-2-(hydroxymethyl)-6-[(2R,3S,4R,5R,6S)-4,5-6-trihydroxy-2-(hydroxymethyl)oxan-3-yl]oxy-oxane-3,4,5-triol C@H]1(7.6R)-2-(hydroxymethyl)-6-[(2R,3S,4R,5R,6S)-4,5-6-trihydroxy-2-(hydroxymethyl)oxan-3-yl]oxy-oxane-3,4,5-triol C@H]1(7.6R)-2-(hydroxymethyl)-6-[(2R,3S,4R,5R,6S)-4,5-6-trihydroxy-2-(hydroxymethyl)oxan-3-yl]oxy-oxane-3,4,5-triol C@H]1(7.6R)-2-(hydroxymethyl)-6-[(2R,3S,4R,5R,6S)-4,5-6-trihydroxy-2-(hydroxymethyl)oxan-3-yl]oxy-oxane-3,4,5-triol C@H]1(7.6R)-2-(hydroxymethyl)-6-[(2R,3S,4R,5R,6S)-4,5-6-trihydroxy-2-(hydroxymethyl)oxan-3-yl]oxy-oxane-3,4,5-triol C@H]1(7.6R)-6-(hydroxymethyl)-6-[(2R,3S,4R,5R,6S)-4,5-6-trihydroxy-2-(hydroxymethyl)oxan-3-yl]oxy-oxane-3,4,5-triol C@H]1(7.6R)-6-(hydroxymethyl)-6-[(2R,3S,4R,5R,6S)-4,5-6-trihydroxy-2-(hydroxymethyl)-6-[(2R,3S,4R,5R,6S)-4,5-6-trihydroxy-2-(hydroxymethyl)-6-[(2	C(CC)=0)(O)C
184948 MAN 2guc 1 C 1 C MAN 2guc 1 A 122 C 2guc MAN A 122 C 284959 MAN 2gud 1 C 5 MAN 2gud 1 B 123 2gud MAN B 123 284960 MAN 2gud 1 C 6 J MAN 2gud 1 B 124 J 2gud MAN B 124 J 286078 MBG 2vmg 1 A 1179 B MBG 2vmg 1 A 1179 C 2vmg MBG A 1179 C 286751 ME2 1pjx 1 471 D ME2 1pjx 1 A 471 D 1pjx ME2 A 471 D 288255 MFU 1rdi 1 1 1 C MFU 1rdi 1 1 1 C 1rdi MFU 1 1 C 288259 MFU 2bt9 1 A 1091 D MFU 2bt9 1 A 1091 D 2bt9 MFU A 1091 D 288260 MFU 2bt9 1 A 1092 E MFU 2bt9 1 B 1089 F 288260 MFU 2bt9 1 B 1089 F 2bt9 MFU B 1089 F 288262 MFU 2bt9 1 B 1090 G MFU 2bt9 1 C 1090 H 2bt9 MFU B 1090 G 288263 MFU 2bt9 1 C 1091 I MFU 2bt9 1 C 1091 I 2bt9 MFU C 1090 H 288264 MFU 2bt9 1 C 1091 I MFU 2bt9 1 C 1091 I 2bt9 MFU C 1091 I 355709 MGC 1 G 155 I MGC 1 G 1	1 20.5133 28.07 13.4 4.01908 5.94032 3.78922 2.9151 1.16623 7.73248 8.88871 -1.04137 -1.99147 -3.8039 8.735 10.06 7.83 0.747085 5.73784 3.48132 2.41016 2.18602 3.75387 5.64169 -1.03654 -2.21466 -2.43991 11.6567 19.72 9.21 2.77127 5.55512 3.44942 1.77271 1.51903 8.15009 9.66982 11.6567 19.72 9.21 2.77127 5.55512 3.44942 1.77271 1.51903 8.15009 9.66982 11.6567 19.72 9.21 2.77127 5.65512 3.44942 1.77271 1.51903 8.15009 9.66982 12.6567 1.65		358.518 357.718 4.29521 72.948 0.999 0.8 1 2.2 1 5 6 1 1 12 6 12 no no 352.099 352.086 0.0121897 0.606 0.432 0.003 1 2.2 1 5 6 1 1 1 12 6 12 no no 435.673 438.615 -6.36575 6.881 17.204 2.242 2 3.2 1 4 6 1 1 1 13 6 14 no no 352.097 349.629 0.804473 11.256 0.001 0.448 1 2.2 1 3 5 1 1 1 12 5 14 no no 356.656 369.655 0.00486159 0.485 0.322 0.001 1 2.2 1 3 5 1 1 1 12 5 14 no no 356.656 369.655 0.00486159 0.485 0.322 0.001 1 2.2 1 3 5 1 1 1 12 5 14 no no 448.613 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	180.157 -2.341 1.79 0.1887 0.1507 0.038 48.43 293 100 17.984 6.5 2006 180.157 -2.341 0.94 0.15607 0.1355 0.02057 48.3 293 100 8.641 6.5 2006 180.157 -2.341 0.94 0.15607 0.1355 0.02057 48.3 293 100 8.641 6.5 2006 194.184 -2.036 1.9 0.296 0.233 37.07 113 24.57 2008 148.202 0.063 0.85 0.1284 0.1206 0.0078 43.34 120 6.5 2003 3.1.8.2 178.185 -1.118 1.8 0.244 0.196 0.048 52.24 100 20.9 7.4 1995 178.185 -1.118 0.94 0.1201 25.7 100 2005 178.185 -1.118 0.94 0.1201 25.7 100 2005 178.185 -1.118 0.94 0.1201 25.7 100 2005 178.185 -	griffthsin, iectins, domain swapping, mannose binding, HIV, SARS, SUGAR BINDING PROTEIN griffthsin, iectins, domain swapping, mannose binding, HIV, SARS, SUGAR BINDING PROTEIN griffthsin, iectins, domain swapping, mannose binding, HIV, SARS, SUGAR BINDING PROTEIN CARBOHYDRATE-BINDING MODULE, SUGAR-BINDING PROTEIN, GALACTOSE, FUCOSIDASE, CLOSTRIDIUM PERFIRIORS FIBRONECTIN TYPE III DOMAIN PROTEIN PHOSPHOTRIESTERASE (PTE), NITROGEN-CALCIUM COORDINATION, BETA-PROPELLER, BOND-LENGTH AND BOND-ANGLE DISSOPROPYLFLUOROPHOSPHATASE (E.C.3.1.8.2) C-TYPE LECTIN, CALCIUM-BINDING PROTEIN LECTIN, SUGAR RECOGNITION, BETA-PROPELLER AID beta sheet protein, Beta-prison I fold, Galactose-specific, SUGAR BINDING PROTEIN AID beta sheet protein, Beta-prison I fold, Galactose-specific, SUGAR BINDING PROTEIN AID beta sheet protein, Beta-prison I fold, Galactose-specific, SUGAR BINDING PROTEIN AID beta sheet protein, Beta-prison I fold, Galactose-specific, SUGAR BINDING PROTEIN AID beta sheet protein, Beta-prison I fold, Galactose-specific, SUGAR BINDING PROTEIN AID beta sheet protein, Beta-prison I fold, Galactose-specific, SUGAR BINDING PROTEIN AID beta sheet protein, Beta-prison I fold, Galactose-specific, SUGAR BINDING PROTEIN AID beta sheet protein, Beta-prison I fold, Galactose-specific, SUGAR BINDING PROTEIN AID beta sheet protein, Beta-prison I fold, Galactose-specific, SUGAR BINDING PROTEIN C-TYPE LECTIN, CALCIUM-BINDING PROTEIN AND SE-BINDING PROTEIN-C LECTIN, CALCIUM-BINDING PROTEIN LECTIN,	SUGAR BINDING PROTEIN X-RAY DIFFRACTION 0.132 P 1 21 1 ROTATING ANODE REF	1 ALPHA-D-MANNOSE alpha-1	D-mannopyranose (2S,3S,4S,5S) D-mannopyranose (2S,3S,4S,5S) D-mannopyranose (2S,3S,4S,5S) D-mannopyranose (2S,3S,4S,5S) D-mannopyranoside (2R,3R,4S,5F) DXY-2-(2-METHOXYETHOXY)ETHANE (2R,3S,4R,5S) D-d-deoxy-alpha-L-galactopyranoside (2R,3S,4R,5S) D-d-deoxy-alpha-L-galactopyranoside (2R,3S,4R,5S) D-deoxy-alpha-L-galactopyranoside (2R,3S,4R,5S) D-deoxy-alpha-D-galactopyranosyl-(1->4)-alpha-D-glucopyranose (2S,3R,4R,5S) D-deoxy-alpha-D-glucopyranosyl-(1->4)-alpha-D-glucopyranose (2S,3R,4R,5S) D-deoxy-alpha-D-mannopyranoside (2R,3S,4S,5S) alpha-D-mannopyranoside (2R,3S,4S,5S)	C@H11((IC@H)(IC@H)(IC@@H](IC@@H](CO)O1)O)OOOOOOOOOOOOOOOOOOOOOOOOOOOOOOO
Note	1 13.6977 13.99 7.99 2.83316 8.82797 6.5442 4.58637 3.84652 -3.20139 7.04191 -1.50277 -3.36133 3.98676 1 18.6708 21.68 16.19 1.39983 9.1498 6.41018 4.45926 3.45399 -3.31245 6.76644 1.81788 -3.92557 4.70952 1 24.6865 51.88 28.65 6.16768 8.73874 6.24439 5.866 4.38507 -3.16969 7.54203 -1.60904 -2.14835 -3.72217 1 28.6851 34.6 22.71 3.62211 7.36211 7.67411 4.76184 -3.6.0677 4.8.4001 12.3324 -1.30788 4.59256 -4.52028 1 3.284 34.06 30.58 0.889443 9.78611 7.67411 4.76184 -3.6.0677 4.8.4001 12.3324 -1.30788 4.59256 -4.52028 1 22.2359 28.69 0 5.59749 -2.83865 -8.93366 -10.7558 3.82214 -1.33329 -1.10444 -1.50021 1 3.195 18.44 10.48 2.35217 7.21691 4.84053 4.06053 1.99854 -8.34658 10.34512 -0.770099 -1.96191 -3.21215 1 2.1867 14.4 10.49 1.1953 -1.26026 -2.6765 -2.6		401.721 39.95.51 4.83238 79.848 0.641 2.17 2 3.2 1 4 6 1 1 1 33 6 14 no no 404.228 401.858 4.34688 46.273 1.446 2.37 2 3.2 1 4 6 1 1 1 13 6 14 no no 404.228 401.858 4.34688 46.273 1.446 2.37 2 3.2 1 4 6 1 1 1 13 6 14 no no 404.228 1.528 2 3.99.727 3.50027 52.33 1.228 1.526 2 3.2 1 4 6 1 1 1 13 6 14 no no 404.228 1.756 2 3.2 1 4 6 1 1 1 13 6 14 no no 404.228 1.756 2 3.2 1 4 6 1 1 1 13 6 14 no no 404.228 1.756 2 3.2 1 4 6 1 1 1 13 6 14 no no 404.228 1.756 2 3.2 1 4 6 1 1 1 13 6 14 no no 404.228 1.756 2 3.2 1 1 4 6 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	194.184 2.036 1.77 0.16991 0.14173 0.02818 52.02 295 277 11.688 4.5 2002 194.184 2.036 1.8 0.205 0.198 0.007 53.45 295 295 295 6.5 2004 194.184 2.036 1.7 0.215 0.191 0.024 52.42 297 293 6.5 2003 194.184 2.036 1.9 0.204 0.185 0.019 60.2 298 298 298 26 7.3 2004 152.149 1.552 1.9 0.204 0.1843 38.09 1995 143.156 2.471 1.8 0.224 51.8 100 18.11 8.1 1999 182.173 3.896 1.9 0.199 0.155 0.04436 39.48 100 18.11 6.5 2007 1.1.341 182.173 3.896 1.9 0.202 0.1761 0.0259 52.22 293 100 5 2002 1.1.163 182.173 3.896 1.9 0.228 50.5 300 100 35.6 6 2005 1.14.13 182.173 3.896 1.9 0.228 50.5 280 100 27.8 6 2005 1.14.13 182.173 3.896 1.9 0.228 50.5 280 100 27.8 6 2005 1.14.13 221.21 2.132 1.4 0.217 0.187 0.03 42.68 298 100 7.5 2001 221.21 2.2132 1.95 0.218 0.198 0.02 69.6 298 100 24.6 6 2002 221.52 221.21 2.132 2 0.352 0.342 0.01 59.84 293 100 34.3 7.5 2002 221.21 2.132 2 0.229 0.1891 0.0399 53.1 298 100 29.4 5.5 2003 221.21 2.132 2 0.258 0.211 0.047 53.6 298 100 29.4 5.5 2003 221.21 2.132 2 0.258 0.211 0.047 53.6 298 100 29.4 5.5 2003 221.21 2.132 2 0.195 0.163 0.032 39.67 277 100 22.5 8 2003 221.21 2.132 1.75 0.187 0.174 0.01235 54.4 100 21.94 7 2007 221.21 2.2132 1.4 0.23157 0.21313 0.01844 55.54 298 100 20.214 8 2006 24.2.12 22.126 0.343 1.85 0.215 0.18029 0.02876 47.18 277 100 20.214 8 2006 24.2.12 22.126 0.343 1.85 0.215 0.18029 0.02876 47.18 277 100 20.214 8 2006 24.2.12 22.126 0.343 1.85 0.215 0.18029 0.02876 47.18 277 100 20.214 8 2006 24.2.12 22.126 0.343 1.85 0.215 0.18029 0.02876 47.18	legume lectin, SUGAR BINDING PROTEIN lectin, soform 1 lectin, carbohydrate, SUGAR BINDING PROTEIN lectin, mannose, carbohydrate, SUGAR BINDING PROTEIN Agglutinin alpha chain, Agglutinin beta-3 chain HORMONE LYASE SCYTAL.ONE DEHYDRATASE COMPLEXED WITH CYCLOPROPYLAMIDE LYASE 17 AD, SUGAR, POLYOL, FLAVIN, OXIDASE, FLAVOPROTEIN, OXIDOREDUCTASE 17 AD, SUGAR, POLYOL, FLAVIN, OXIDASE, FLAVOPROTEIN, OXIDOREDUCTASE 18 AD, SUGAR, POLYOL, FLAVIN, OXIDASE, FLAVOPROTEIN, OXIDOREDUCTASE 19 Carbonydrate complex, OXIDOREDUCTASE 20 Aviderductase enzyme-inhibitor complex, OXIDOREDUCTASE 21 ACRA complex, SUGAR BINDING PROTEIN 22 Carbonydrate complex, SUGAR BINDING PROTEIN 23 Major Capsit Protein Vp54, PBCV-1, Chlorella virus, Jelly roll motif, Glycoprotein, Viral protein 24 beta-sandwich, alphafapha barrel, TRANSFERASE 25 Lectors, Naccessificate, Sugarda, Sug	SUGAR BINDING PROTEIN X-RAY DIFFRACTION 0.162 12 2 2 SYNCHROTRON REF	1 1 1 1 1 1 1 1 1 1	(2R,3S,4S,5S alpha-D-mannopyranoside (2R,3S,4S,5S) alpha-D-mannopyranoside (2R,3S,4S,	C@H]1(, S.6S)-2-(hydroxymethyl)-6-methoxy-oxane-3,4,5-triol C@M]1(, S.6S)-1-(hydroxymethyl)-2,2-dichloro-3-methyl-1-[(S)-methylsulfinyl]cyclopropane-1-carboxamide C[C@@ R]-hexane-1,2,3,4,5,6-hexol C[C@ C@ R]-hexane-1,2,3,4,5,6-hexol OC[C@ C@ R]-hexane-1,2,3,4,5,6-hexol OC[C@ C@ R]-hexane-1,2,3,4,5,6-hexol OC[C@ C@ R]-R,5,6R)-2,4,5-trihydroxy-6-(hydroxymethyl)oxan-3-ylethanamide C@ R,5,6R)-2,4,5-trihydroxy-6-(hydroxymethyl)oxan-3-ylethanamide CR R,5,6R)-2,4	(C@H (C@H (C@@H (C@@H (CO)O1)O)O)OC
490861 NCA 2r6v 1 A 174 C	1 15.7927 25.49 12.45 2.92075 1 15.7922 15.66 14.61 0.564442 5.4234 4.88794 4.92371 4.17447 2.81967 1.3548 0.984075 1.32173 6.47858 1 125.524 126.1 124.94 0.364421 5.65212 5.22165 5.02273 4.29168 1.41141 2.88027 0.778508 1.52878 2.16278 1 125.524 126.1 124.94 0.364421 5.65212 5.22165 5.02273 4.29168 1.41141 2.88027 0.778508 1.52878 2.16278 1 15.0444 18.27 12.16 2.37891 1 16.0444 18.27 12.16 2.37891 1 17.0452 2.414 12.81 3.75785 5.44653 4.86935 1.43966 1.59623 2.48243 1.04936 4.80764 1.45046 2.00071 1 13.13089 22.044 12.81 3.75785 5.44653 4.89695 4.81787 4.07866 1.59623 2.48243 1.04936 1.45046 2.00071 1 13.111 17.56 11.17 1.94096 5.34597 4.896037 3.44229 2.58888 0.85341 0.878735 1.38801 2.74826 1.3211 17.56 1.17 1.94096 5.34597 4.896037 3.44229 2.58888 0.85341 0.878735 1.38801 2.74826 1.45046 2.00071 1 24.1013 33.57 16.51 4.93887 9.9898 7.43332 6.7713 5.23579 2.28484 7.50063 1.52553 3.17489 4.2822 1.45046 2.00071 1 2.503947 35.35 18.92 5.18431 1.26932 1.15020 1	-5,38865 0,760272 0.054 3,22607 3,86007 -0.947 4,81822 0,96816 281190 -0.9486 0.042 0.062 12562 12562 151 59.778 6.273 7,0744 7,77124 2,35164 1.51066 2,89482 4,40488 -7.771 4,40464 2,89488 -0.0002 2,90009 -0.5318 0.145 0.062 0.0687 0.576 16 16.04 16.044 16 16.025 1.0567 0.0671 0.0650 0.0671 0.0650 0.0671 0.0650 0.0671 0.0650 0.0671 0.0650 0.0671 0.0650 0.0671 0.0650 0.0671 0.0650 0.0671 0.0650 0.0671 0.0650 0.0671 0.0650 0.0671 0.0650 0.0671 0.0650 0.0671 0.0671 0.0650 0.0671 0.06	59.064 59.026 0.0483957 1.697 1.622 0.038 1 1 1 2 1 2 1 1 9 3 6 yes no 61.071 51.114 -0.0782951 0.112 0.864 -0.043 1 1 2 1 2 1 2 1 1 9 3 6 yes no 61.071 51.114 -0.0782951 0.112 0.864 -0.043 1 1 2 1 2 1 2 1 1 9 3 6 yes no 38.676 40.275 0.891535 0.005 3.434 0.0599 1 1 2 1 2 1 2 1 1 9 3 6 yes no 38.325 36.327 0.194847 4.506 0.109 -0.002 1 1 2 2 1 2 1 1 9 3 6 yes no 44.084 44.183 -0.20291 0.01 1.094 -0.099 1 1 1 2 1 2 1 2 1 1 9 3 6 yes no 259.283 2807.72 46.71916 18.581 39.409 -1.479 2 3.2 2 5 6 1 1 1 5 7 15 no no 284.046 282.329 -2.90742 32.042 46.836 1.719 2 3.2 2 5 6 1 1 1 15 7 15 no no 276.298 275.048 1.6581 10.27 1.453 1.25 2 3.2 2 5 6 1 1 1 15 7 15 no no 276.298 275.048 1.6581 10.27 1.453 1.25 2 3.2 2 5 6 1 1 1 15 7 15 no no 284.466 280.912 2.8838 220.909 14.34 7.554 2 3.2 2 5 6 1 1 1 15 7 15 no no 284.466 280.912 2.8838 220.909 14.34 7.554 2 3.2 2 5 6 1 1 1 15 7 15 no no 284.466 280.912 2.8838 220.909 14.34 7.554 2 3.2 2 5 6 1 1 1 15 7 15 no no 284.466 280.912 2.8838 220.909 14.34 7.554 2 3.2 2 5 6 1 1 1 15 7 15 no no 284.466 280.912 2.8838 220.909 14.34 7.554 2 3.2 2 5 6 1 1 1 15 7 15 no no 284.466 280.912 2.8838 220.909 14.34 7.554 2 3.2 2 5 6 1 1 1 15 7 15 no no 284.466 280.912 2.8838 220.909 14.34 7.554 2 3.2 2 5 6 1 1 1 15 7 15 no no 284.466 280.912 2.8838 220.909 14.34 7.554 2 3.2 2 5 6 1 1 1 15 7 15 no no 284.466 280.912 2.8838 220.909 14.34 7.554 2 3.2 2 5 6 1 1 1 15 7 15 no no 286.566 243.688 23.8643 67.875 1.497 22.878 2 3.2 2 5 6 1 1 1 15 7 15 no no 286.566 243.688 23.8643 67.875 1.497 22.878 2 3.2 2 5 6 1 1 1 15 7 15 no no 286.566 243.688 23.8643 67.875 1.497 22.878 2 3.2 2 5 6 1 1 1 15 7 15 no no 286.566 243.688 23.8643 67.875 1.497 22.878 2 3.2 2 5 6 6 1 1 1 15 7 15 no no 286.566 243.688 23.8643 67.875 1.497 22.878 2 3.2 2 5 6 6 1 1 1 15 7 15 no no 286.566 243.688 23.8645 51.334 4.799 2 3.3 2 2 5 6 6 1 1 1 15 7 15 no no 286.566 243.688 23.8645 51.334 4.799 2 3.3 2 2 5 6 6 1 1 1 15 7 15 no no 286.566 243.688 23.8645 51.334 4.799 2 3.3 2 2 5 6 6 1 1 1 15 7 15 no no 286.566 243.688 23.8645 51.334	122.126 -0.343	NP_142786.1, FMN-binding protein, Flavin reductase like domain, Structural Genomics, Joint Center for Structural Genomics, CSG, Pn Uncharacterized protein PH0856 siz', sirtuin, siz'Zm, Sir'1, p53, nicothamide, HVDROLASE beta-alpha-barrel, Structural Genomics, P58, Protein Structural Genomics, P58, P58, P58, P58, P58, P58, P58, P58	HYDROLASE	Dyridin Spridin Dyridin Dyridin Spridin Spri	pyridine-3-cai pyridi	N1=CC= rboxamide	CC(=C1)C(=O)N
51448/ NIZ_1v08_1_A_1502_C NTZ_1v08_1_A_1502_C 1v08 NTZ A 1502_C C 514493 NTZ_1e6q_1_M_999_KA NTZ_1e6q_1_M_999_K 1e6q NTZ_M 999_K H 514496 NTZ_2fb_1_A_1446_F NTZ_2fb_1_A_1001_B OC9_2qhv_1_A_1001_B 2qhv OC9_A 1446_C 1446_C 2fb_NTZ_A 1446_C 1444	1 21 6494 27.83 18.42 2.97972		333.203 331.652 7.44118 29.484 1.618 1.551 1 2 1 4 7 1 3 144 8 10 yes no 355.657 365.728 0.543044 16.132 5.352 -0.071 1 2 1 4 7 1 3 144 8 10 yes no 6.818 1.551 1 2 1 4 7 1 3 144 8 10 yes no 6.818 1.551 1 2 1 4 7 1 3 144 8 10 yes no 6.818 1.551 1 2 1 4 7 1 3 144 8 10 yes no 6.818 1.551 1 2 1 4 7 1 3 144 8 10 yes no 6.818 1.551 1 2 1 4 7 1 3 144 8 10 yes no 6.818 1.551 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	2U2.169 -3.633 1.9 0.205 0.175 0.02985 57.5 100 22.38 7.5 2004 3.2.1.21 202.169 -3.633 1.35 0.146 50 100 16.2 7 2000 3.2.3.1 202.169 -3.633 1.87 0.22 0.184 0.03542 47 100 27.52 7 2006 3.2.1.21 130.23 3.127 1.6 0.237 0.21 0.027 50.47 298 110 21.959 7 2007 114.23 4.892 2 53.37 100 20.83 2007 146.229 1.362 1.7 0.2 0.19 0.01 49.57 291 100 24.9 4.8 2006 246.219 -1.044 1.92 0.2 0.182 0.018 48.96 289 298 29.8 6.8 2004 2.4.1.1 374.441 3.011 1.7 0.2 46.71 100 2004 41.9 202	EL IA-GLUCUSIDASE, GLYCUSIDE HYDROLASE, DIMBOA-GLUCOSIDE, INHIBITOR, PEST DEFENSE, FAMILY GH1, HYDROLASI BETA-GLUCOSIDASE (E.C.3.2.1.21) HYDROLASE, FAMILY 1 GLYCOSYL HYDROLASE, GLUCOSINOLATE, MYROSINASE, ITM BARREL, D-GLUCOONO-1, 5-LACTONE, MYROSINASE (E.C.3.2.1.21) TANNSFERASE, HYDROLASE, INHIBITOR, GLYCOSIDASE, DOLYSACCHARIDE DEGRADATION, TRANSITION STATE MIMIC, CARBOH BETA-GLUCOSIDASE A (E.C.3.2.1.21) ILIPOMINISTERASE, HYDROLASE, INHIBITOR, GLYCOSIDASE, DOLYSACCHARIDE DEGRADATION, TRANSITION STATE MIMIC, CARBOH BETA-GLUCOSIDASE A (E.C.3.2.1.21) ILIPOMINISTERASE, HYDROLASE, INHIBITOR, GLYCOSIDASE, DOLYSACCHARIDE DEGRADATION, TRANSITION STATE MIMIC, CARBOH BETA-GLUCOSIDASE A (E.C.3.2.1.21) ILIPOMINISTERASE, HYDROLASE, INHIBITOR, GLYCOSIDASE, DOLYSACCHARIDE DEGRADATION, TRANSITION STATE MIMIC, CARBOH BETA-GLUCOSIDASE A (E.C.3.2.1.21) ILIPOMINISTERASE, INHIBITOR, GLYCOSIDASE, DOLYSACCHARIDE DEGRADATION, TRANSITION STATE MIMIC, CARBOH BETA-GLUCOSIDASE A (E.C.3.2.1.21) ILIPOMINISTERASE, INHIBITOR, GLYCOSIDASE, DOLYSACCHARIDE DEGRADATION, TRANSITION STATE MIMIC, CARBOH BETA-GLUCOSIDASE A (E.C.2.3.1.21) ILIPOMINISTERASE, INHIBITOR, GLYCOSIDASE, DOLYSACCHARIDE DEGRADATION, TRANSITION STATE MIMIC, CARBOH BETA-GLUCOSIDASE A (E.C.2.3.1.21) ILIPOMINISTERASE, ENDRE OF TRANSFERASE, DOLYSACCHARIDE, DOLYSACCHA	HYDROLASE	1.1.24 0 NOJIRIMYCINE TETRAZOLE (\$R,6R)	I-1-OL OCTAN-1-OL octane octane IE-1,8-DIOL OCTANE-1,8 5-anhydro-1-(5-methyl-1,3,4-oxadiazol-2-yl)-D-glucitol (2R,3S,4S,5F) S(3-METHYLBENZYL)PYRIMIDINE-4,6-DICARBOXAMIDE N,N'-bis[(3-math)	S)-5-(hydroxymethyl)-5,6,7,8-tetrahydro-[1,2,3,4]tetrazolo[5,1-f]pyridine-6,7,8-triol C12=NN S)-5-(hydroxymethyl)-5,6,7,8-tetrahydro-[1,2,3,4]tetrazolo[5,1-f]pyridine-6,7,8-triol C12=NN C12=N	N=N N 1 C@@H (C@H (C@H (C@H (C@H () C@H (C@H (C@H (C@H (C@H (C@H (C@H (C@H ())))
PGO 2 PGO 3 PGO 4	1	3,3898 0.09222 2.0276 0.000 0.00000 0.00000 0.00000 0.0000 0.00000 0.0000 0.0000 0.0000 0.0000 0.000	110.948 111.037 -0.144806 0.997 1.427 -0.099 1 1 1 2 2 2 0 0 0 5 2 8 no no 98.553 96.642 4.42244 30.577 5.485 1.911 1 1 1 2 2 2 0 0 0 5 2 8 no no 99.556 92.658 -0.282712 59.632 10.663 -0.102 1 1 1 1 2 2 2 0 0 0 5 2 8 no no 10 10.965 12.8 128.114 0.6532 0.622 0.501 0.104 1 1 1 1 2 2 2 0 0 0 5 2 8 no no 10 10.965 106.831 -0.099 4.217 20.769 0.134 1 1 1 1 2 2 2 0 0 0 5 2 8 no no 10 10.965 106.831 -0.099 4.217 20.769 0.134 1 1 1 1 2 2 2 0 0 0 5 2 8 no no 10 10.966 10.477 1.79253 23.138 3.157 -0.004 1 1 1 1 2 2 2 0 0 0 5 2 8 no no 10 10.946 10.477 1.79253 23.138 3.157 -0.004 1 1 1 1 2 2 2 0 0 0 5 2 8 no no 10 10.945 1.53739 12.686 0.339 1.019 1 1 1 1 2 2 2 0 0 0 5 2 8 no no 10 10.984 19.276 0.26596 3.194 0.009 0.119 1 1 1 1 2 2 2 0 0 0 5 2 8 no no 142.181 142.727 2.22641 0.573 17.248 -0.546 1 1 1 1 2 2 2 0 0 0 5 2 8 no no 142.181 142.727 2.22641 0.573 17.248 -0.546 1 1 1 1 2 2 2 0 0 0 5 2 8 no no 75.205 72.014 6.46177 38.054 0.001 3.191 3 3 3 1 0 2 1 1 1 10 2 8 yes no 175.205 72.014 6.46177 38.054 0.001 3.191 3 3 3 1 0 2 1 1 1 10 2 8 yes no 175.205 72.714 6.46177 38.054 0.001 3.191 3 3 3 1 0 2 1 1 1 10 2 8 yes no 175.205 67.2 2.71012 11.137 -0.04 1.952 3 3 3 1 0 2 1 1 1 10 2 8 yes no 175.055 72.014 6.9554 2.8278 2.5225 0.218 1.533 3 3 1 0 2 1 1 1 10 2 8 yes no 176.682 167.46 -0.10428 2.525 0.218 1.53 3 3 1 0 2 1 1 1 10 2 8 yes no 176.682 167.46 -0.10428 2.725 3.786 0.266 1 1 1 2 1 1 1 2 2 2 1 1 1 2 8 yes no 177.112 177.615 -0.328055 5.376 5.698 -0.503 1 1 1 2 1 1 1 2 2 2 1 1 1 2 8 yes no 177.112 177.615 -0.328055 5.376 5.698 -0.503 1 1 1 2 1 1 1 2 2 2 1 1 1 2 8 yes no 177.112 177.615 -0.328055 5.376 5.698 -0.503 1 1 1 2 2 1 1 1 2 2 1 1 1 2 8 yes no 177.112 177.615 -0.328055 5.376 5.698 -0.503 1 1 1 2 1 1 1 2 2 1 1 1 1 2 3 14 yes no 273.392 274.155 3.2288 28.181 6.143 -0.763 3 3 2 0 3 1 1 1 2 2 1 1 1 2 3 14 yes no 273.392 274.155 3.2288 28.181 6.143 -0.763 3 3 2 0 3 3 1 1 1 1 1 2 3 14 yes no 273.392 274.155 3.2288 28.181 6.143 -0.763 3 3 3 2 0 3 3 1 1 1 1 1 2 3 14 yes no 273.392 274.155 3.2288 28.181 6.143 -0.763 3 3	76.095 0.748 1.0 0.209 0.172 0.03/19 44.39 100 17.74 2006 76.095 -0.748 1.26 0.162 0.141 0.021 34.11 277 100 10.501 4.5 2007 76.095 -0.748 1.65 0.222 0.193 0.029 52.97 293 100 22 5.6 2007 76.095 -0.748 1.7 0.197 0.168 0.029 46.49 277 100 19.685 7.5 2008 76.095 -0.748 1.08 0.166 44.45 293 100 32 6 2000 76.095 -0.748 1.55 0.2486 44.38 291 110 23 49 2000 1.1.14 76.095 -0.748 1.8 0.23 0.195 0.035 44.82 278 100 7 49 2007 41.14 4.9 2001 1.1.14 4.9 2001 1.1.14	PP_001095275.1, Putative monoxygenase, Antibiotic biosynthesis monoxygenase. Antibiotic biosynthesis monoxygenase. Antibiotic biosynthesis monoxygenase Uncharacterized conserved protein, STRUCTURAL GENOMICS, UNKNOWN FUNCTION, NPPSFA, National Project on Protein Structuu Universal stress protein family NP_786286.1, putative carboxylesterase, Structural Genomics, JoSG, Protein Structural Universal stress protein family NP_786286.1, putative carboxylesterase, Structural Genomics, JoSG, Protein Structural Universal stress protein family NP_786286.1, putative carboxylesterase, Structural Genomics, JoSG, Protein Structural Universal Stress protein family NP_786286.1, putative carboxylesterase, Structural Genomics, JoSG, Protein Structural Universal Stress protein family NP_786286.1, putative carboxylesterase, Structural Genomics, JoSG, Protein Structural Universal Stress protein family NP_786286.1, putative carboxylesterase, Structural Genomics, JoSG, Protein Structural Universal Stress protein family NP_786286.1, putative carboxylesterase, Structural Genomics, JoSG, Protein Structural Universal Structural Genomics, JoSG, Protein Structural Genomics, JoSG, Pr	OXIDOREDUCTASE X-RAY DIFFRACTION Shewanella loihica	S-1,2-PROPANEDIOL (2S)-pr	(2S)-propane opane-1,2-diol (2S)-propane opane-1,2-diol <t< td=""><td> C(C@H</td><td> </td></t<>	C(C@H	
STATE TAKE Typo 1	1 21,2592 24,28 17.33 2,2033 1,1498 5,07143 4,16844 3,48948 0,6869 1,44066 2,09776 0,700646 1,35227 4,18572 1,185	14.4788	273.116	100.127 0.041 1.39 0.171 0.148 0.023 51.36 298 100 6 2005 1.11.1.5 1.50 1.	MAJOR URINARY PROTEIN 1 sequenced ligand binding site, Oxidoreoluctase hydrolase, aminopeptidase, metal binding, protease EC 3.4.11.18 CARBOHYDRATE KINASE, RIBOSE, NUCLEOTIDE BINDING, TRANSFERASE EC 3.4.11.18 BETÄALPHA BARREL, TIM barrie, HOMO-TETRAMER, METAL-BINDING PROTEIN, ISOMERASE BETÄALPHA BARREL, TIM barrie, HOMO-TETRAMER, METAL-BINDING PROTEIN, ISOMERASE CIS-TRANS ISOMERASE CIS-TRANS ISOMERASE CIS-TRANS ISOMERASE CIS-TRANS ISOMERASE CIS-TRANS LIGHT AND ARRIED A	Oxidoreductase	2-ISOBUTYL-3-METHOXYPYRAZINE 2-meth	bxy-3-(2-methylpropyl)pyrazine 2-methoxy-3-N-4-YLMETHANOL N-4-YLMETHANOL PYRIDIN-4-Y ETHYLPHENYL)-1H-1,2,3-TRIAZOLE 4-(3-METHYL) bribofuranose (2S,3R,4S,5F bry-L-mannose (2R,3R,4S,5F bry-L-mannose (2R,3R,4S,5F bry-L-glo-methylpyridin-2-yl)propyl]formamide N-hydroxy-N-cyclohexyl-3-phenylpropyl (2S)-1-(3,3-dimethyl-2-oxopentanoyl)piperidine-2-carboxylate (1-cyclohexyl-BETA-D-GLUCOPYRANOSE bry-BETA-D-GLUCOPYRANOSE (2R,3R,4R,5E br-G-actylamino)-2-deoxy-1-seleno-beta-D-glucopyranoside (2R,3S,4S,5S br-G-actylamino)-2-deoxy-1-seleno-beta-D-glucopyranoside (2S,3R,4R,5F br-HYL-5-THIO-ALPHA-D-RIBOFURANOSE (2S,3R,4R,5F br-Hyl-5-THIO-ALPHA-D-RIBOFURANOSE (2S,3R,4S,5S br-Hyl-1-pregn-4-ene-3,20-dione (8S,9S,10R,1 br-Hyl-1-pregn-4-ene	N1=CC= N1=CC= N1	No
	1 1178 14.07 9.93 11.032 1 7.37217 9.59 5.78 1.116 13.4627 9.34996 4.26713 2.71468 .19.6636 22.37828 1 38.1213 44.76 34.87 3.00877 1 22.9778 25.81 20.01 16.2986 13.7175 9.60038 2.37313 3.61246 24.6434 21.0094 2.25666 4.97419 .5.51004 1 22.9778 25.81 20.01 16.2986 13.7712 9.6278 2.25785 3.80952 2.60.0925 22.28658 2.37253 1.46.8667 1.59652 1 36.9165 29.64 23.6 14.0996 13.7712 9.6278 2.25785 3.80952 2.60.0925 22.28658 2.37253 1.46.8667 1.59652 1 30.0074 31.74 27.89 1.08887 27.00143 13.5315 9.34848 2.19017 -3.90766 2.5.9615 22.05384 2.40833 1.43.4383 1.58103 1 31.7396 34.06 28.39 1.46656 13.5701 9.42727 2.2.6574 4.09933 2.5.9762 21.87687 2.37327 1.44.889 1.5.9033 1 31.7396 33.0 2.728 1.87112 1 30.5087 33.6 27.28 1.87112 1 30.5087 33.6 27.28 1.87112 1 30.5087 3.35 5.359 1.70654 13.4606 9.32276 1.74211 3.54683 -24.1793 20.63247 2.37339 1.35508 -15.5765 1 36.8017 38.56 34.13 12.4249 13.5182 9.35966 2.49588 4.10355 2.5.4207 21.31715 2.38888 1.45.645 1.5.9332 1.4.8603 49.27 4.737 0.42232 1.3.599 9.39966 2.49588 4.10355 2.5.4207 21.31715 2.38888 1.45.645 1.5.9332 1.3.5799 2.4.901 2.3.0018 1.4.3141 1.6.0018 1.3.5799 3.3.99 3.2.43 1.3.5018 9.3.999 9.3.9966 2.49588 4.10355 2.5.4207 21.31715 2.3.3818 1.4.5454 1.5.9332 1.3.5799 9.3.5966 2.49588 4.10355 2.5.4207 21.31715 2.3.3818 1.4.5454 1.5.9332 1.3.5799 9.3.5966 2.49588 4.10355 2.5.4207 21.31715 2.3.3818 1.4.5454 1.5.9332 1.3.5799 9.3.5966 2.49588 4.10355 2.5.4207 21.31715 2.3.3818 1.4.5454 1.5.9332 1.3.5799 9.3.5966 2.49588 4.10355 2.5.4207 21.31715 2.3.3818 1.4.5454 1.5.9332 1.3.5799 9.3.5966 2.49588 4.10355 2.5.4207 21.31715 2.3.3818 1.4.5454 1.5.9332 1.3.5799 9.3.5966 2.49588 4.10355 2.5.51056 21.58134 2.3.8033 1.3.9006 1.5.5765 1.5.5		940.739 939.004 2.53343 67.975 26.166 1.735 5 7.2 1 8 11 2 2 2 23 11 22 no no 934.866 923.594 13.9623 94.782 4.596 11.272 5 7.2 1 8 11 2 2 2 23 11 22 no no 934.866 923.594 9.5529 9.07725 20.599 1.421 9.968 5 7.2 1 8 11 2 2 2 23 11 22 no no 941.303 926.205 23.8629 96.509 1.635 15.098 5 7.2 1 8 11 2 2 2 23 11 22 no no 935.602 932.414 3.269 18.789 13.329 3.521 5 7.2 1 8 11 2 2 2 23 11 22 no no 958.895 99.5754 64.3911 3893.82 3.004 18.341 5 7.2 1 8 11 2 2 2 23 11 22 no no 964.846 982.366 4.586.36 4.3911 3893.82 3.004 18.341 5 7.2 1 8 11 2 2 2 23 11 22 no no 975.166 953.855 72.3103 3241.54 23.765 21.281 5 7.2 1 8 11 2 2 2 23 11 22 no no 9848.955 925.479 34.7439 362.17 4.956 23.476 5 7.2 1 8 11 2 2 2 23 11 22 no no 975.166 953.85 72.3103 3241.54 23.765 21.281 5 7.2 1 8 11 2 2 2 23 11 22 no no 9848.955 925.479 34.7439 362.17 4.956 23.476 5 7.2 1 8 11 2 2 2 23 11 22 no no 9853.82 921.651 5.0967 3.341 9.865 3.32.113 34.39 19.809 5 7.2 1 8 11 2 2 2 23 11 22 no no 9853.82 921.651 5.0967 29.669 1.487 32.669 5 7.2 1 8 11 2 2 2 23 11 22 no no 9948.955 925.479 34.7439 362.17 4.956 23.476 5 7.2 1 8 11 2 2 2 23 11 22 no no 9948.955 925.479 34.7439 362.17 4.956 23.476 5 7.2 1 8 11 2 2 2 23 11 22 no no 9948.955 925.479 34.7439 362.17 4.956 23.476 5 7.2 1 8 11 2 2 2 23 11 22 no no 9948.955 925.479 34.7439 362.17 4.956 23.476 5 7.2 1 8 11 2 2 2 23 11 22 no no 9948.955 925.479 34.7439 362.17 4.956 23.476 5 7.2 1 8 11 2 2 2 2 3 11 22 no no 9948.955 925.479 34.7439 362.17 4.956 23.476 5 7.2 1 8 11 2 2 2 2 3 11 22 no no 9948.955 925.479 34.7439 362.17 4.956 23.476 5 7.2 1 8 11 2 2 2 2 3 11 22 no no 9948.955 925.479 34.7439 362.17 4.956 23.476 5 7.2 1 8 11 2 2 2 2 3 11 22 no no 9948.955 925.479 34.7439 362.17 4.956 23.476 5 7.2 1 8 11 2 2 2 2 3 11 22 no no 9948.955 925.479 34.7439 362.17 4.956 23.476 5 7.2 1 8 11 2 2 2 2 3 11 22 no no 9948.955 925.479 34.7439 362.17 4.956 23.476 5 7.2 1 8 11 2 2 2 2 3 11 22 no no 9948.955 925.479 34.7439 362.17 4.956 23.476 5 7.2 1 8 11 2 2 2 2 3 11 22 no no 9948.955 925.479 34.7439 362.17 4.956 23.476	342.299	agular iram, would adjustment, in, in, in, in, in, in, in, in, in, in	TRANSFERASE X-RAY DIFFRACTION P.1.21 SYNCHROTRON REF TRANSFERASE X-RAY DIFFRACTION D.0.79 C.1.21 SYNCHROTRON CNS HYDROLASE X-RAY DIFFRACTION D.0.79 C.1.21 SYNCHROTRON CNS TRANSFERASE/DNA X-RAY DIFFRACTION D.1.17 P.21.21.21 ROTATING ANODE CNS TRANSFERASE/DNA X-RAY DIFFRACTION D.1.45 P.21.21.21 ROTATING ANODE CNS TRANSFERASE/DNA X-RAY DIFFRACTION D.1.45 P.21.21.21 SYNCHROTRON CNS TRANSFERASE/DNA X-RAY DIFFRACTION D.1.46 P.21.21.21 SYNCHROTRON CNS TRANSFERASE/DNA X-RAY DIFFRACTION D.1.7 P.21.21.21 ROTATING ANODE CNS TRANSFERASE/DNA X-RAY DIFFRACTION D.1.56 P.61 ROTATING ANODE CNS TRANSFERASE X-RAY DIFFRACTION D.1.56 P.61 ROTATING ANODE CNS TRANSFERASE X-RAY DIFFRACTION D.1.27 P.61 ROTATING ANODE CNS TRANSFERASE X-RAY DIFFRACTION D.1.27 P.61 ROTATING ANODE CNS TRANSFERASE X-RAY DIFFRACTION D.1.46 P.61 ROTATING ANODE CNS TRANSFERASE X-RAY DIFFRACTION D.1.46 P.61 ROTATING ANODE CNS TRANSFERASE X-RAY DIFFRACTION D.1.46 P.61 ROTATING ANODE CNS TRANSFERASE/DNA X-RAY DIFFRACTION D.1.46 P.61 SYNCHROTRON CNS TRANSFERASE/DNA X-RAY	SUCROSE Deta-D	fructofuranosyl alpha-D-glucopyranoside	Comparisor Com	

Column ID	Column name	Originating from	Evalenation
Column ID	Column name	Originating from	Explanation
Α	Values identifying ligand instance:	our own assignment	sequential assignment of numerical ID
В	PCCD Ligand Instance ID ₂₀₀₈	Ligand Expo (see Note)	Ligand Instance ID from 2008 download (Note: In our internal nomenclature, we inverted the sequence of substrings PDB ID and Ligand ID)
C D	PCCD Ligand Instance ID ₂₀₁₀ PDB ID	Ligand Expo (see Note) Ligand Expo Instance ID	Ligand Instance ID from 2010 download (Note: In our internal nomenclature, we inverted the sequence of substrings PDB ID and Ligand ID) PDB ID
E	Ligand ID	Ligand Expo Instance ID	Chemical Component Identifier (3-letter-code), also known as Ligand ID or HET ID
F G	Chain ID Residue	Ligand Expo Instance ID Ligand Expo Instance ID	Chain ID Residue ID number of the ligand instance
Н	mmCIF Asym ID	Ligand Expo Instance ID	mmCIF Asym ID
J	mmCIF Sequence No. Disorder Flag	Ligand Expo Instance ID Ligand Expo Instance ID	mmCIF sequence number Disorder Flag (for structures modeled with disorder)
K	Model No.	Ligand Expo Instance ID	Model number
	B value statistics:		
L	Baverage	Ligand Expo PDBML file	Average B value of ligand instance atoms
M	B _{max}	Ligand Expo PDBML file	Largest B value among ligand instance atoms
N	Bmin	Ligand Expo PDBML file Ligand Expo PDBML file	Smallest B value among ligand instance atoms Standard deviation of B values of ligand instance atoms
0	B _{stddev}	Ligania Expo PDBINIL IIIe	Standard deviation of B values of ligand instance atoms
_	Solvent model QC energies:		Values in kcal/mol, relative to vacuum X-ray conformational energy
D D	Esolvent,H	G09 solvent model runs G09 solvent model runs	Conformational energy of ligand with unmodified heavy-atom crystal coordinates and hydrogens added by CACTVS, calculated in IEFPCM solvent model Solvent model conformational energy of ligand after optimization of hydrogens (all other internal coordinates kept fixed)
	Esolvent,In	G09 solvent model runs	Solvent model conformational energy of ligand after optimization of bond lenghts between heavy atoms (bond angles and torsions kept fixed)
S	Esolvent,ang	G09 solvent model runs	Solvent model conformational energy of ligand after optimization of bond angles (torsions kept fixed)
T	Esolvent,tor	G09 solvent model runs	Solvent model conformational energy of ligand after optimization of torsions (full unconstrained optimization)
U	$\Delta E_{solvent,ang-tor}$	G09 solvent model runs	Energy difference between angle-optimized and torsion-optimized solvent model conformations ([S]-[T]), "solvent conformational energy"
	Vacuum QC energies:		Values in kcal/mol, relative to vacuum X-ray conformational energy
V W	Evacuum,H	G09 vacuum runs	Vacuum conformational energy of ligand after optimization of hydrogens (all other internal coordinates kept fixed)
X	Evacuum,len Evacuum,ang	G09 vacuum runs G09 vacuum runs	Vacuum conformational energy of ligand after optimization of bond lenghts between heavy atoms (bond angles and torsions kept fixed) Vacuum conformational energy of ligand after optimization of bond angles (torsions kept fixed)
Υ	Evacuum,tor	G09 vacuum runs	Vacuum conformational energy of ligand after optimization of torsions (full unconstrained optimization)
Z	ΔE _{vacuum,H-len}	G09 vacuum runs	Energy difference between hydrogen-optimized and bond-length-optimized vacuum conformations ([V]-[W])
	ΔEvacuum,len-ang	G09 vacuum runs	Energy difference between bond-length-optimized and angle-optimized vacuum conformations ([W]-[X]) Energy difference between angle-optimized and torsion-optimized vacuum conformations ([W]-[X]) "vacuum conformational energy"
AB AC	ΔEvacuum,ang-tor	G09 vacuum runs G09 vacuum runs	Energy difference between angle-optimized and torsion-optimized vacuum conformations ([X]-[Y]), "vacuum conformational energy" Energy difference between bond-length-optimized and torsion-optimized vacuum conformations ([W]-[Y])
AD	E _{GEM}	MacroModel & G09 global E min. runs	Vacuum conf. E of lowest of (up to) three QC-reoptimized, OPLS-2001-calculated, lowest-energy ligand conformations ("global" energy minimum)
AE	ΔE _{vacuum,len-GEM}	G09 vacuum runs	Energy difference between bond-length-optimized and "global" energy minimum vacuum conformations ([W]-[AD])
AF	ΔE _{vacuum} ,ang-GEM	G09 vacuum runs	Energy difference between angle-optimized and "global" energy minimum vacuum conformations ([X]-[AD])
AG AH	AEvacuum,tor-GEM	G09 vacuum runs OpenEye Omega runs	Energy difference between torsion-optimized and "global" energy minimum vacuum conformations ([Y]-[AD]) Molecular mechanics MMFF94s energy difference between crystal conformation and lowest-energy conformation from Omega conformational search
, u I			
ΔΙ	Comparison solvent model, vacuum QC e		Difference between solvent and vacuum conformational energies (ILII IAPI)
AI	$\Delta \Delta E_{ang-tor}$	G09 solvent and vacuum runs	Difference between solvent and vacuum conformational energies ([U]-[AB])
Λ.1	Residue-specific crystallographic "quality"		Deal areas D feator of lineard instance
AJ AK	RSR ₂₀₀₈ RSR ₂₀₁₀	Manual extraction from EDS late 2008 Parsed from 2010 download from EDS	Real -space R-factor of ligand instance Real -space R-factor of ligand instance
AL	RSCC ₂₀₀₈	Manual extraction from EDS late 2008	Real-space correlation coefficient of ligand instance
AM	RSCC ₂₀₁₀	Parsed from 2010 download from EDS	Real-space correlation coefficient of ligand instance
AN	OWAB ₂₀₀₈	Manual extraction from EDS late 2008	Occupancy-weighted average B-factor of ligand instance atoms Occupancy-weighted average B factor of ligand instance atoms
AO AP	OWAB ₂₀₁₀	Parsed from 2010 download from EDS Calculated from PDBML file	Occupancy-weighted average B-factor of ligand instance atoms Occupancy-weighted average B-factor of ligand instance atoms
, u			Designation moralists and age of rector of rigative moralists
A C	Results of torsional sampling around cryst		Number of compling iterations achieved for compling around linear any stal conformation using accusate distribution of transfer of the standard of the standar
AQ AR	n _{torsion} E _{torsion.min}	Maestro runs using MMFF94s Maestro runs using MMFF94s	Number of sampling iterations achieved for sampling around ligand crystal conformation using gaussian distribution of torsional perturbations Minimum of MMFF94s energies of torsion-sampled conformations around ligand crystal conformation, using gaussian distribution of torsional perturbations
AS	Etorsion,max	Maestro runs using MMFF94s	Maximum of MMFF94s energies of torsion-sampled conformations around ligand crystal conformation, using gaussian distribution of torsional perturbations
AT	E _{torsion,avg}	Maestro runs using MMFF94s	Arithmetic mean of MMFF94s energies of torsion-sampled conformations around ligand crystal conformation, using gaussian distribution of torsional perturbations
AU	Etorsion,median	Maestro runs using MMFF94s	Median of MMFF94s energies of torsion-sampled conformations around ligand crystal conformation, using gaussian distribution of torsional perturbations
AV AW	Etorsion,SP ΔEtorsion,avg-SP	Maestro runs using MMFF94s Maestro runs using MMFF94s	MMFF94s energy of ligand instance crystal conformation (after optimization of added hydrogens) MMFF94s energy difference between arithmetic mean of sampled conformations and ligand crystal conformation ([AT]-[AV])
AX	Δ⊑torsion,avg-SP ΔEtorsion,max-SP	Maestro runs using MMFF94s	MMFF94s energy difference between maximum E among sampled conformations and ligand crystal conformation ([AS]-[AV])
AY	$\Delta E_{torsion,SP-min}$	Maestro runs using MMFF94s	MMFF94s energy difference between ligand crystal conformation and minimum E among sampled conformations ([AV]-[AR])
AZ	$\Delta E_{torsion,median}$ -SP	Maestro runs using MMFF94s	MMFF94s energy difference between median of sampled conformations and ligand crystal conformation ([AU]-[AV])
	Ligand molecule properties:		All properties calculated by CACTVS
BA	n _{rot}	PCCD ligand (prototype) structure	Number of freely rotatable bonds Number of freely rotatable bonds partially accounted macrosyclic single bonds
BB BC	n _{rot_eff}	PCCD ligand (prototype) structure PCCD ligand (prototype) structure	Number of freely rotatable bonds + partially accounted macrocyclic single bonds Number of possible tautomers
BD	n _{hdonors}	PCCD ligand (prototype) structure PCCD ligand (prototype) structure	Number of hydrogen bond donors
BE	nhacceptors	PCCD ligand (prototype) structure	Number of hydrogen bond acceptors
BF	n _{ringsystems}	PCCD ligand (prototype) structure	Number of ring systems
BG	n _{rings}	PCCD ligand (prototype) structure	Number of rings (smallest number of smallest rings) Number of heavy (non hydrogen) atoms
BH BI	nheavy_atoms nheteroatoms	PCCD ligand (prototype) structure PCCD ligand (prototype) structure	Number of heavy (non-hydrogen) atoms Number of hetero atomes
BJ	nheteroatoms nhydrogens	PCCD ligand (prototype) structure	Number of hydrogen atoms
BK	aromatic	PCCD ligand (prototype) structure	Boolean: Is molecule aromatic?
BL BM	macrocyclic MW	PCCD ligand (prototype) structure PCCD ligand (prototype) structure	Boolean: Is molecule a macrocycle? Molecular weight
BN	xlogp2	PCCD ligand (prototype) structure	Octanol/water partition coefficient, calculated by XLOGP v. 2.0 algorithm
	Crystallographic properties of the entire Pl		All values taken as is from PDBML files; no cross-check vs. original publication
BO BD	Resolution	PDBML file	Crystallographic resolution
BP BQ	R _{free}	PDBML file PDBML file	R _{free} R value
BR	R _{free} -R	PDBML file	R _{free} - R
BS BT	Solvent T	PDBML file PDBML file	Solvent content of crystal Temperature during crystal growth / co-crystallization
BU	Tambient	PDBML file	Temperature during data collection
BV	B _{mean}	PDBML file	Average B value (of entire PDB structure)
BW BX	pH Year	PDBML file PDBML file	pH value Year of publication
BY	EC code	PDBML file	EC code of protein
BZ CA	Keywords Macromolecule	PDBML file PDBML file	Keywords associated with PDB structure Protein name
CB CC	Macromolecule Type Method	PDBML file PDBML file	Protein type Experimental method used (here for all: X-ray diffraction)
CD	Organism	PDBML file	Organism that was source of protein (if given)
CE CF	DPI Space Group	PDBML file PDBML file	Diffraction-component precision index (or: diffraction-data precision indicator) of the experimental data Space group of crystal
CG	Diffraction Source	PDBML file	Source of X-ray beam
СН	Refinement Program	PDBML file	Software used for structure refinement
	Various ligand molecule properties/identifi		
CI CJ	Sugar Name	manual assignment Ligand Expo mmCIF file	Boolean: Is ligand molecule a sugar? (Heuristically determined from ligand molecule name [next column].) Ligand molecule name
CK	OpenEye Name	Ligand Expo mmCIF file	OpenEye ligand molecule name (calculated IUPAC name)
CL CM	ACD/Labs Name SMILES	Ligand Expo mmCIF file PCCD ligand (prototype) structure	ACD Labs ligand molecule name (calculated IUPAC name) SMILES string of ligand molecule (calculated by CACTVS)
		g (prototypo) ottuotuto	
CN	HQ subset membership: VHQ-R subset		member of the "Very High-Quality set with Results" (VHQ-R) subset
CO	UHQ-R subset		member of the "Ultra High-Quality subset with Results" (UHQ-R) subset
	Abbreviations used:	Electron Density Comes	Unneala Elastran Dansity Sarvar, http://ada.hma.uu.co/ada/
	PCCD	Electron Density Server PDB Chemical Component Dictionary	Uppsala Electron Density Server, http://eds.bmc.uu.se/eds/ http://deposit.rcsb.org/cc_dict_tut.html
	QC	quantum-chemical (or quantum chemistry)	
	Notes:		
	Greenish entries are used in manuscript fig	gures	