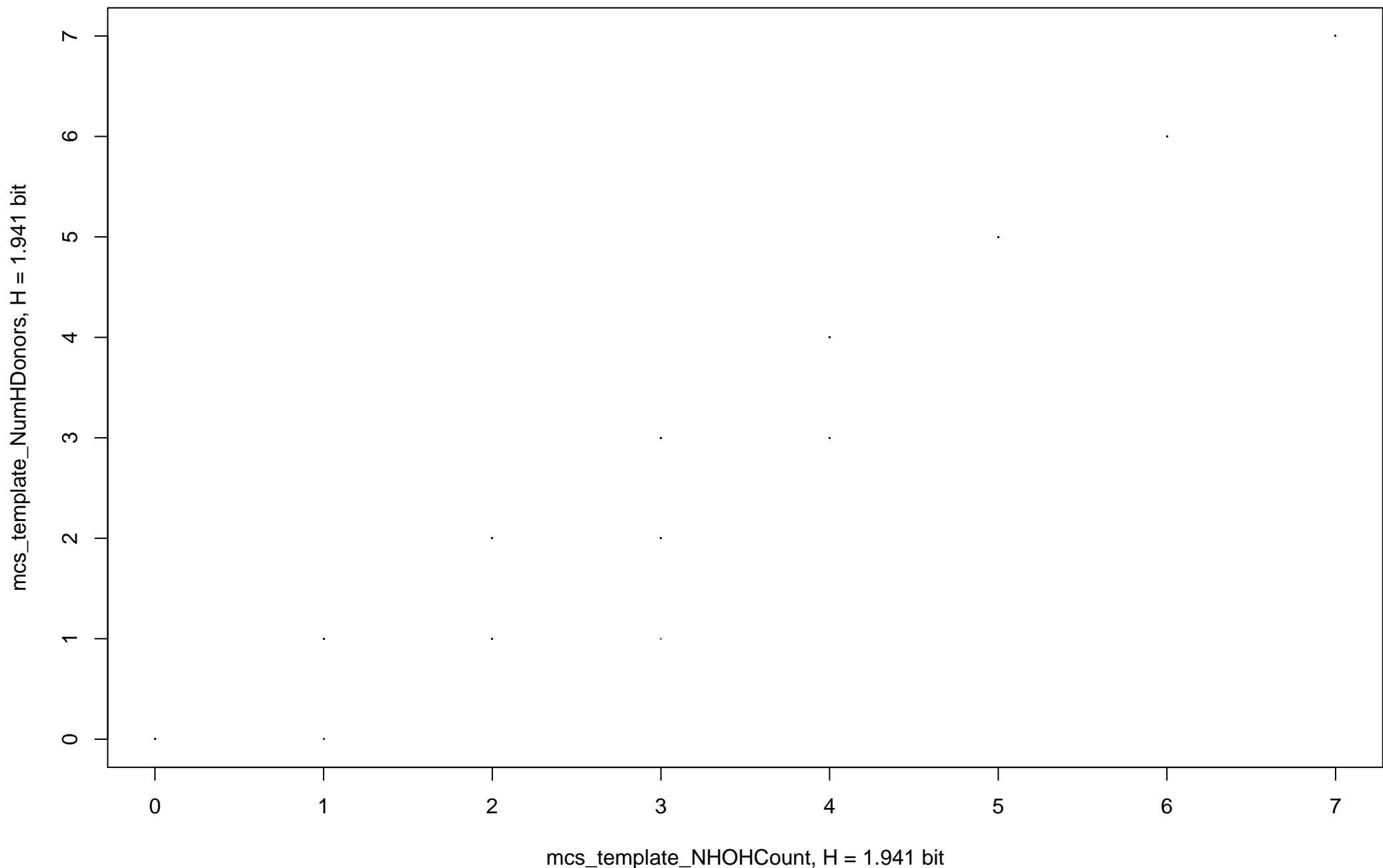
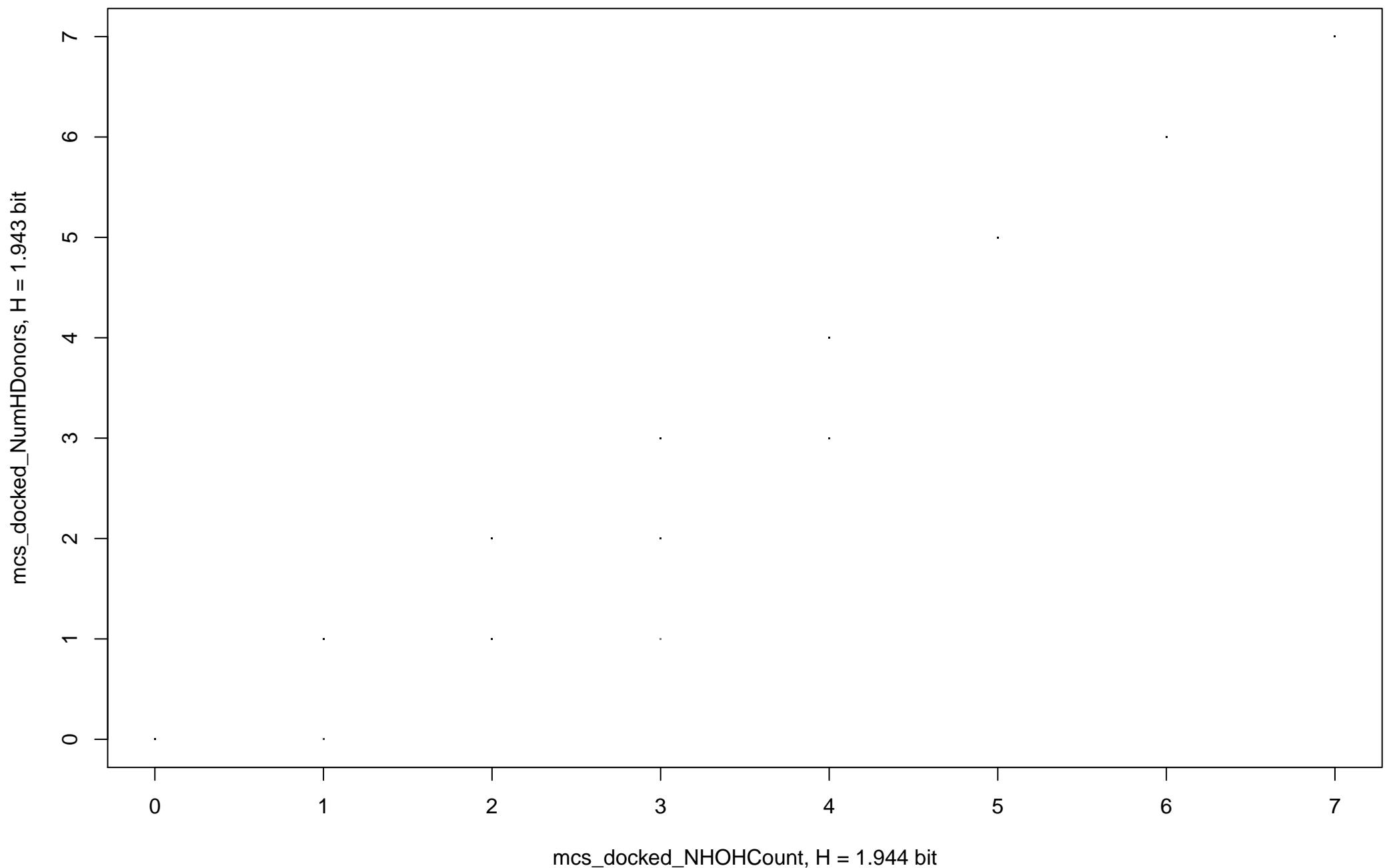


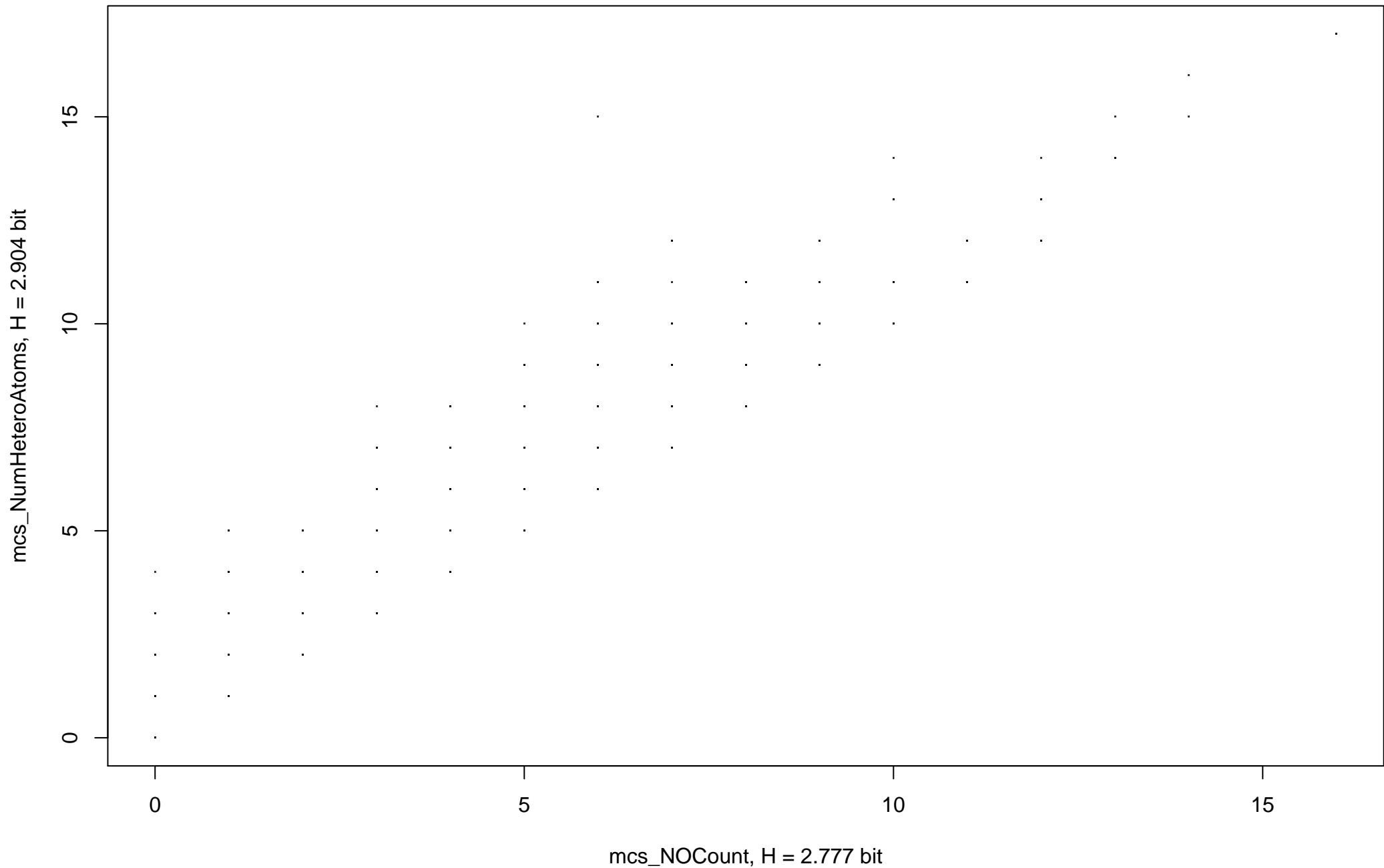
mcs_template_NHOHCount–mcs_template_NumHDonors, MI = 1.934 bit, normMI = 0.9966



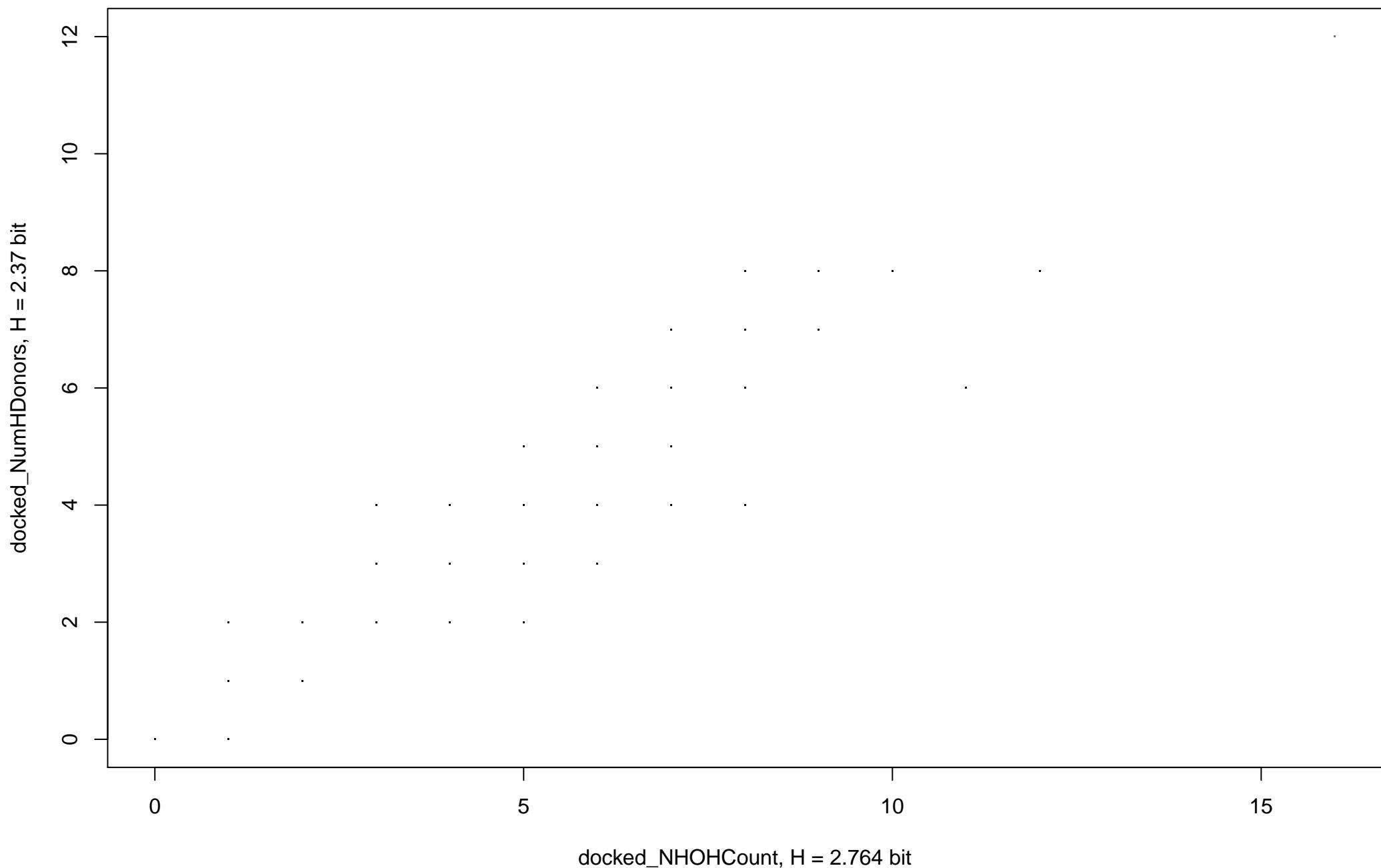
mcs_docked_NHOHCount-mcs_docked_NumHDonors, MI = 1.937 bit, normMI = 0.9966



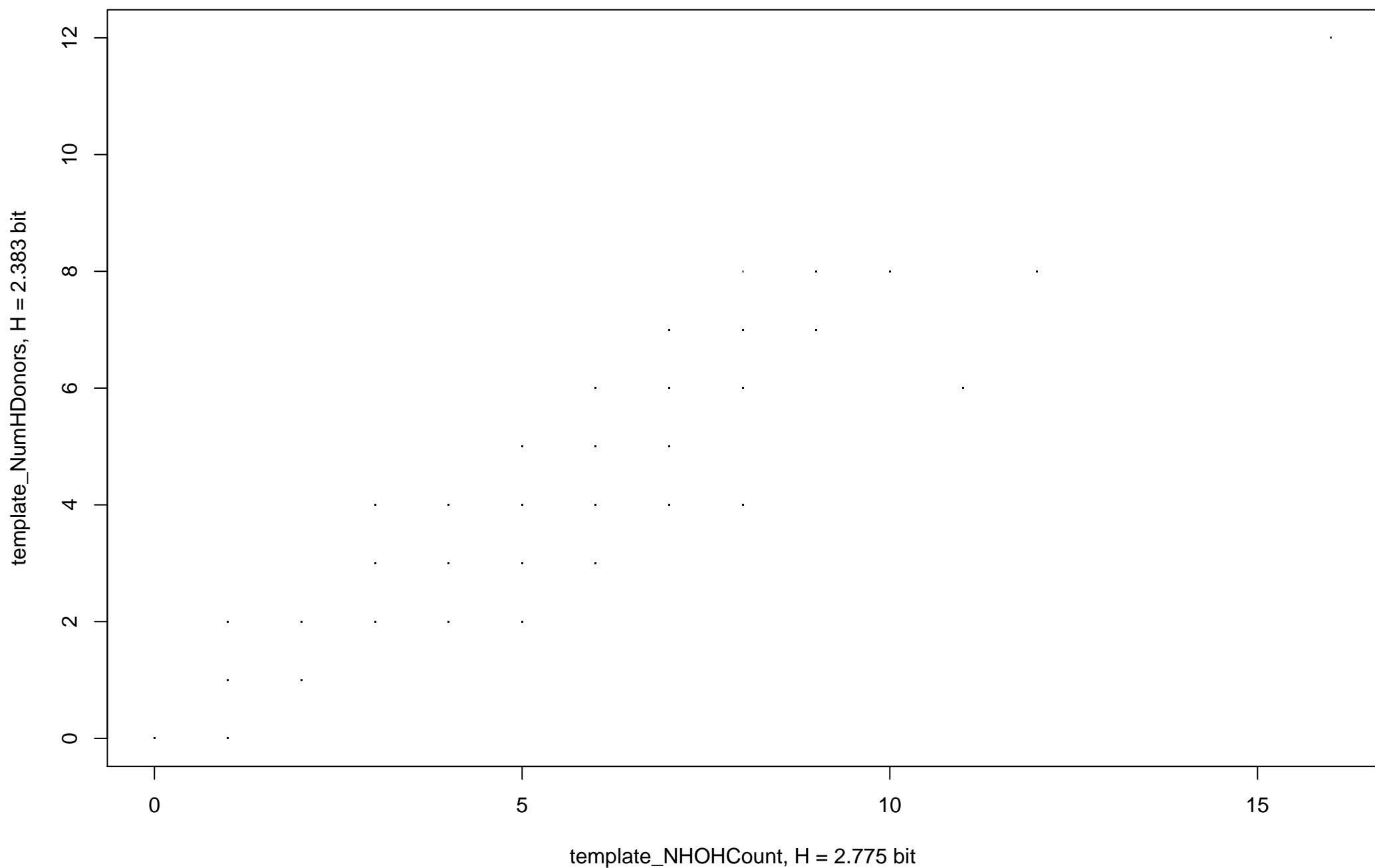
mcs_NOCount-mcs_NumHeteroAtoms, MI = 2.191 bit, normMI = 0.789



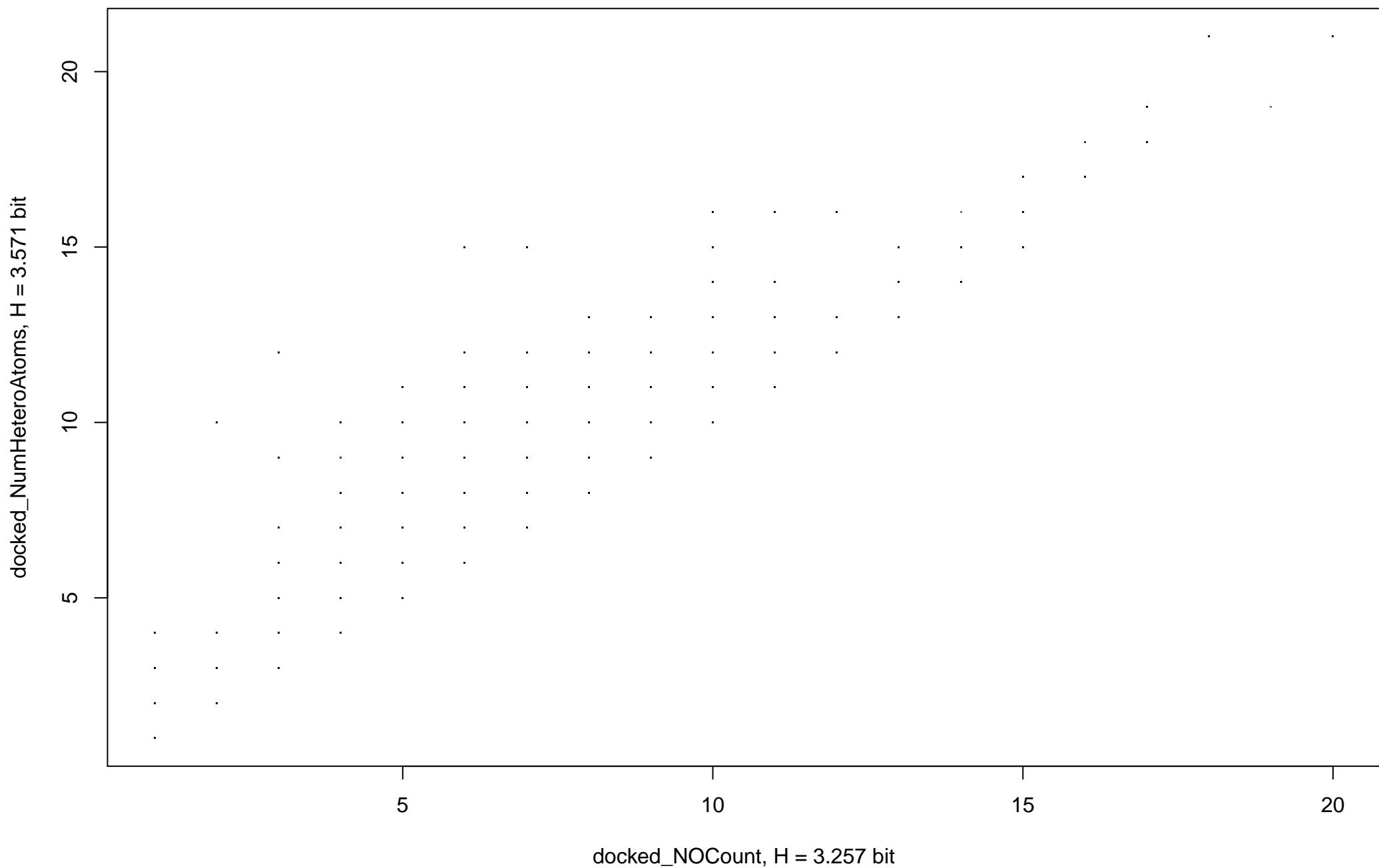
docked_NHOHCount-docked_NumHDonors, MI = 1.531 bit, normMI = 0.6458



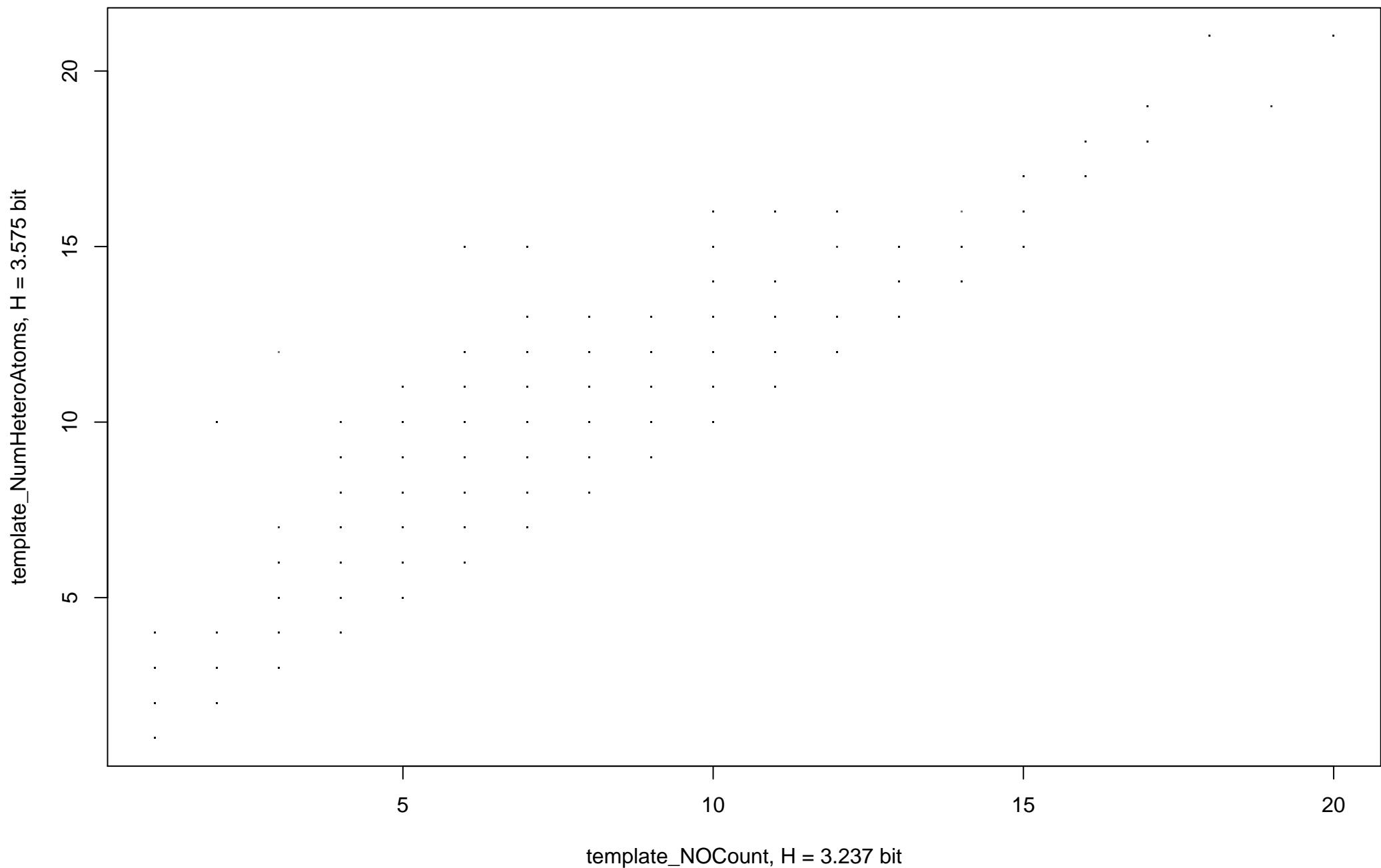
template_NHOHCount-template_NumHDonors, MI = 1.539 bit, normMI = 0.6457



docked_NOCount–docked_NumHeteroAtoms, MI = 1.552 bit, normMI = 0.4765

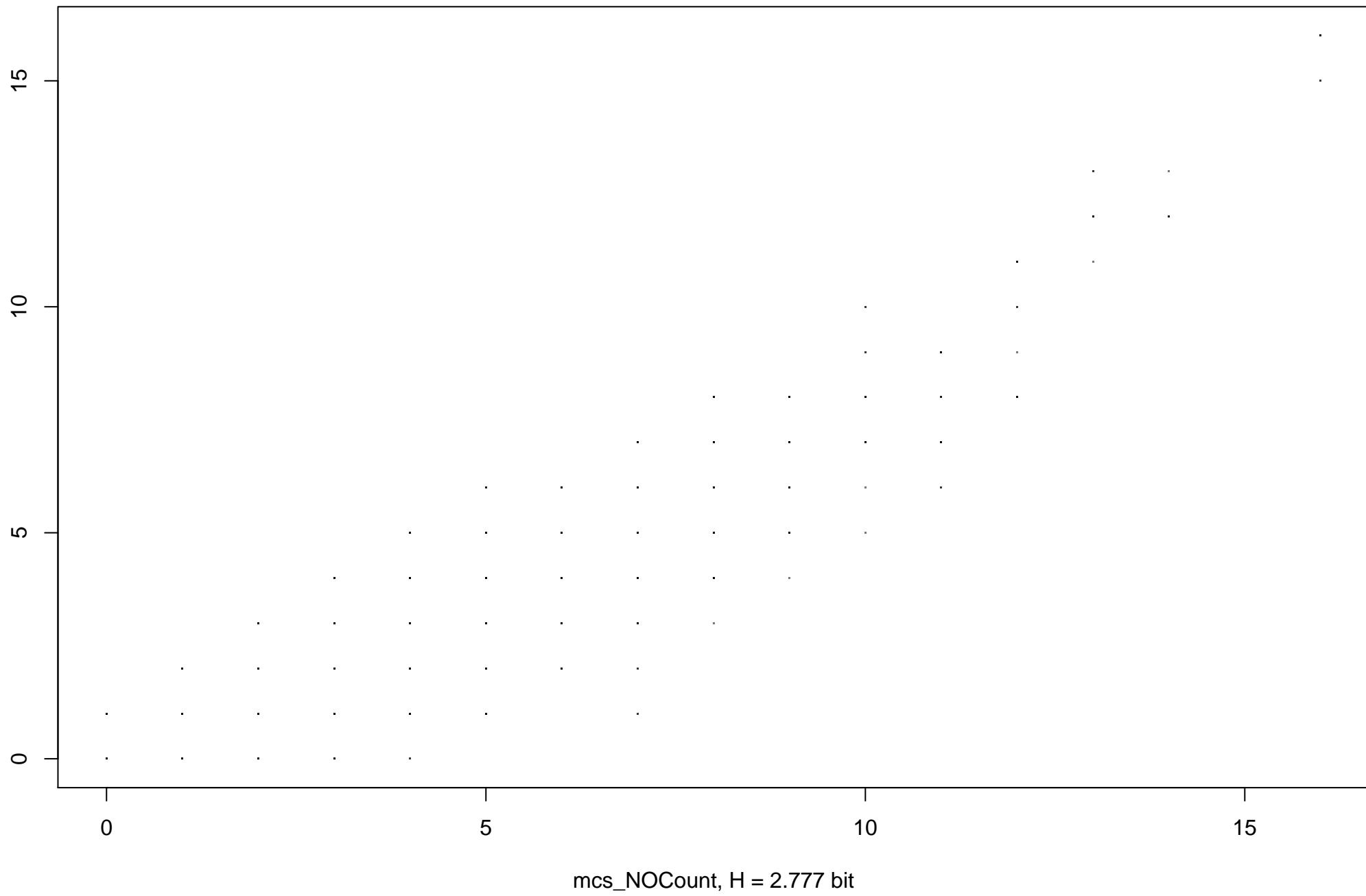


template_NOCount-template_NumHeteroAtoms, MI = 1.507 bit, normMI = 0.4655

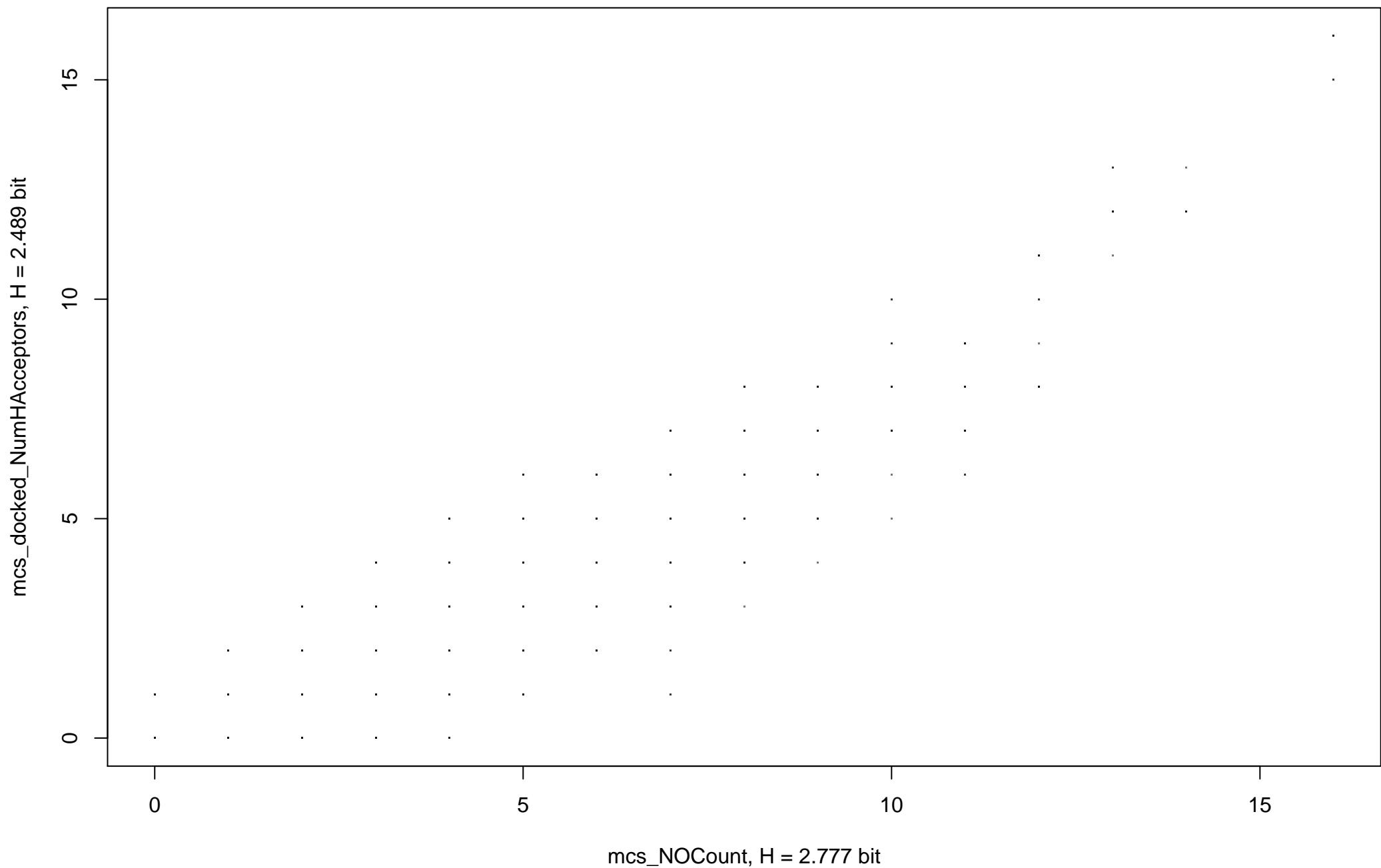


mcs_NOCount-mcs_template_NumHAcceptors, MI = 1.012 bit, normMI = 0.4067

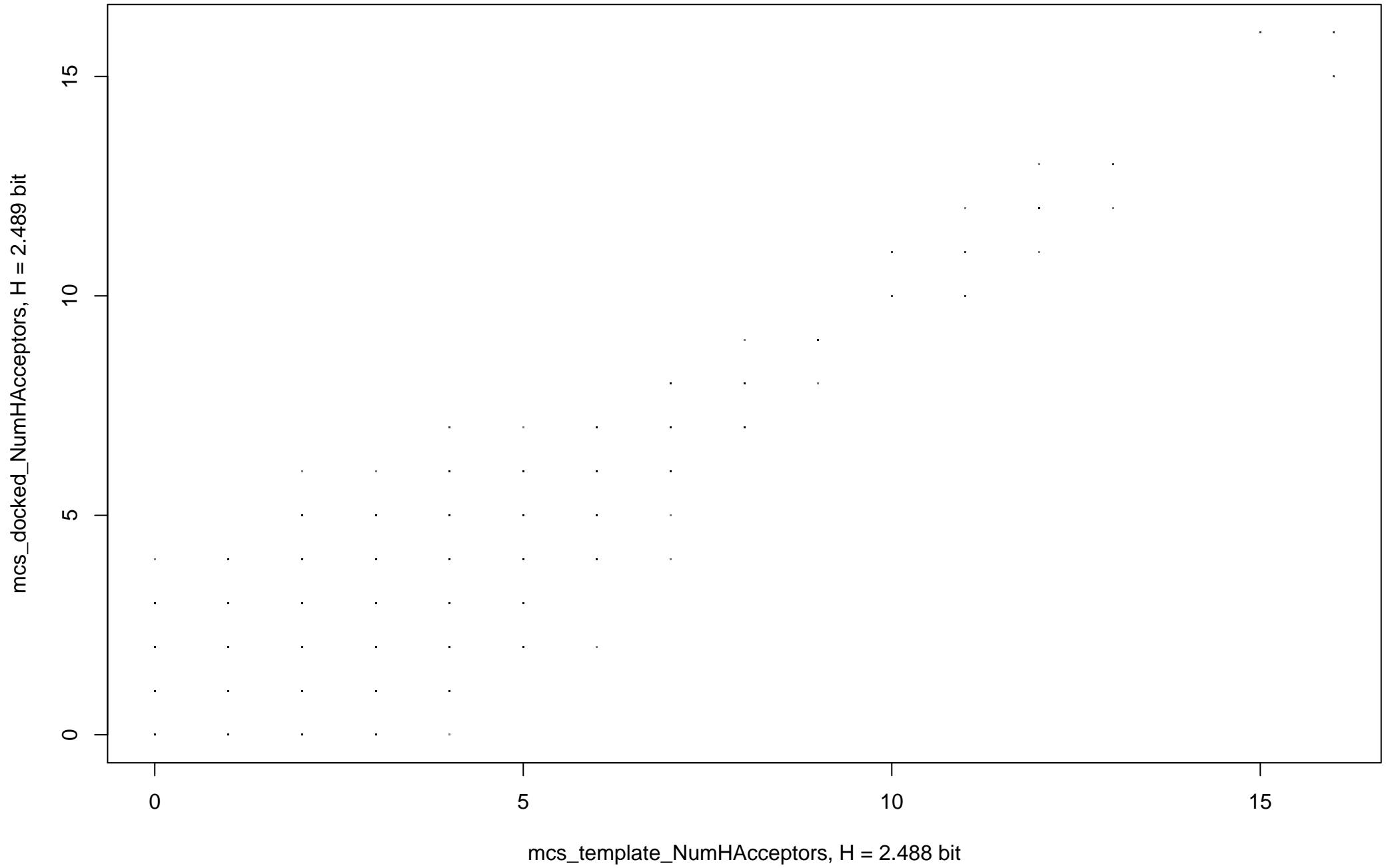
mcs_template_NumHAcceptors, H = 2.488 bit



mcs_NOCount-mcs_docked_NumHAcceptors, MI = 1.01 bit, normMI = 0.4058

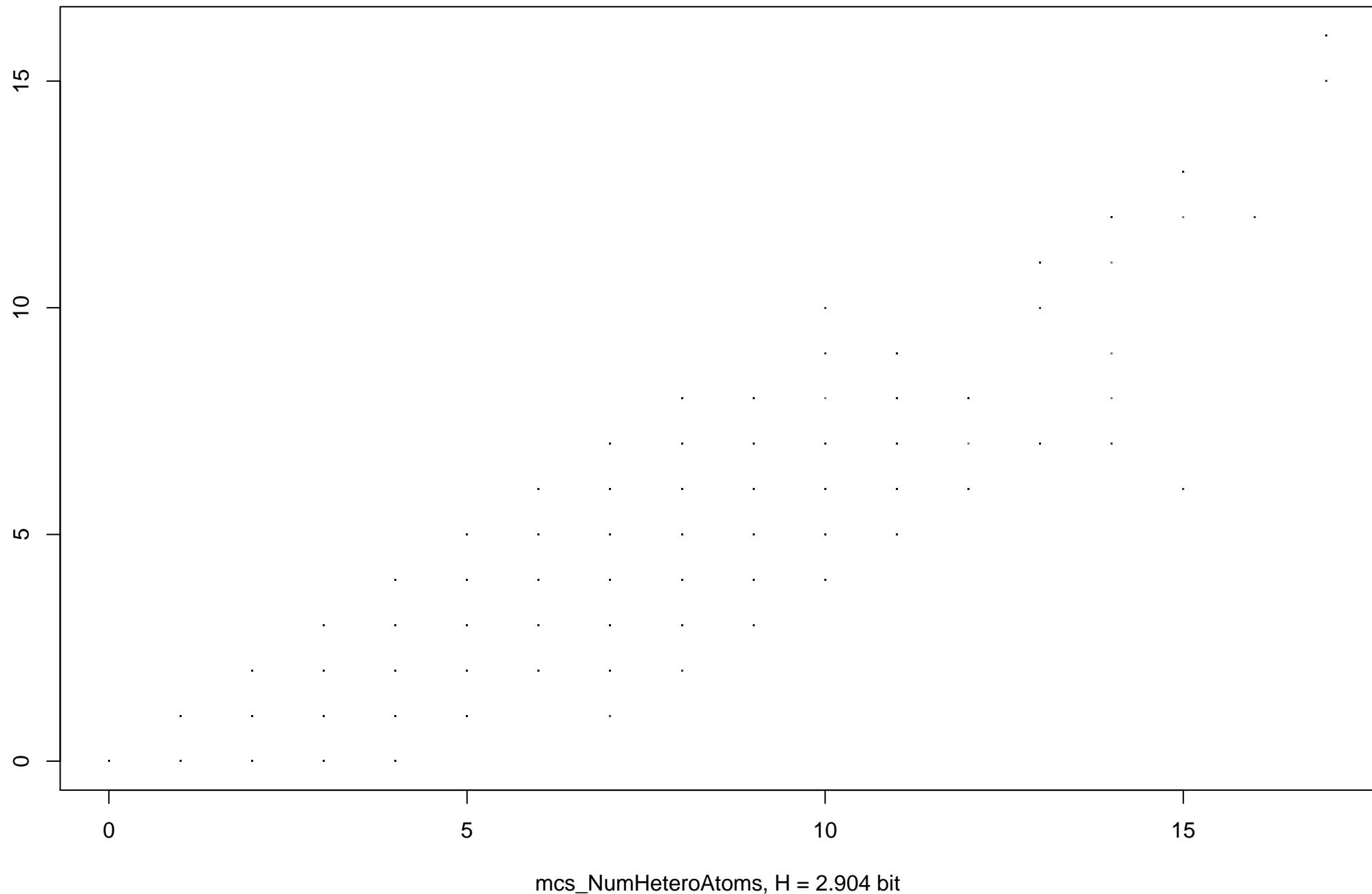


mcs_template_NumHAcceptors-mcs_docked_NumHAcceptors, MI = 1.006 bit, normMI = 0.4042

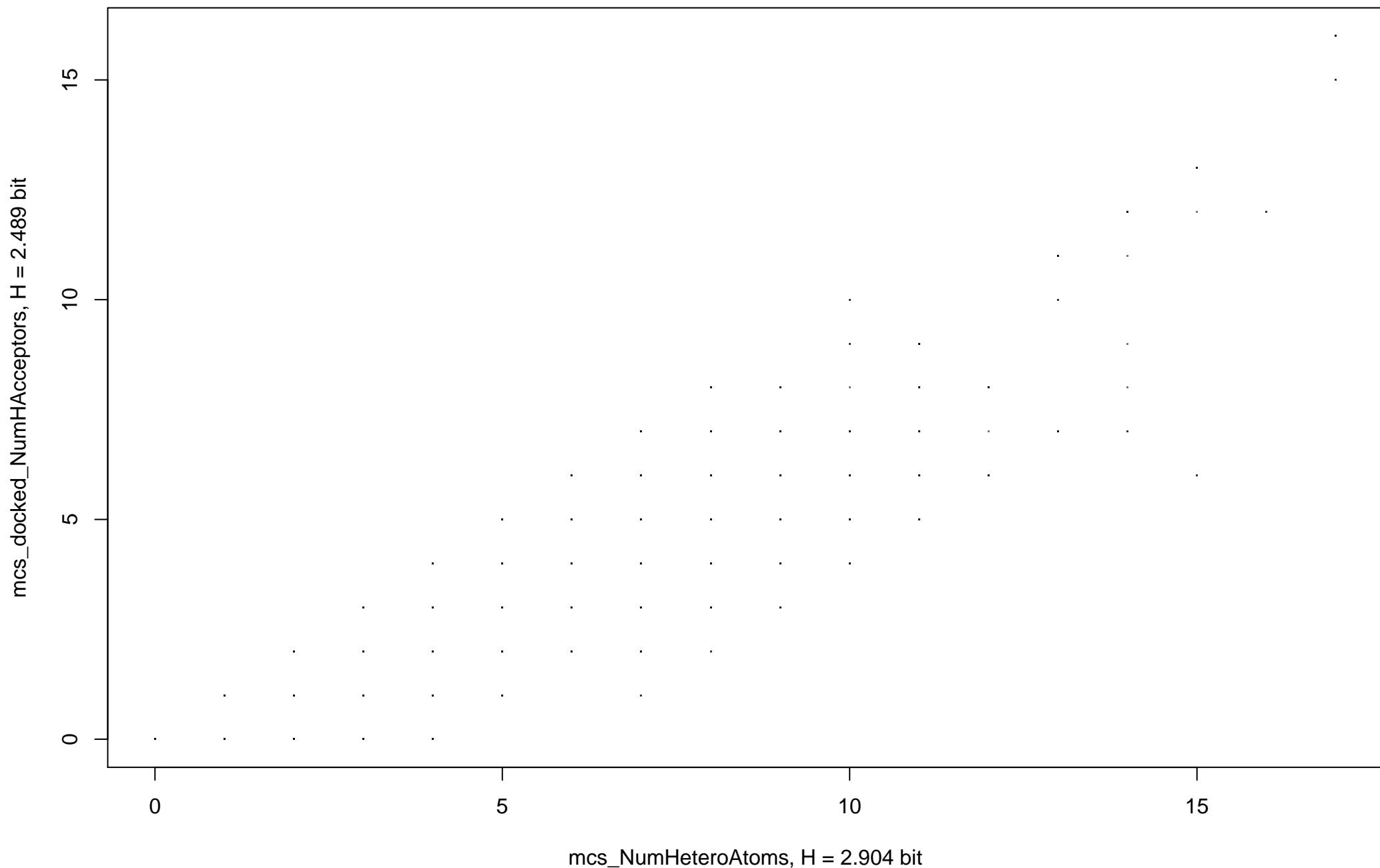


mcs_NumHeteroAtoms–mcs_template_NumHAcceptors, MI = 0.9415 bit, normMI = 0.3784

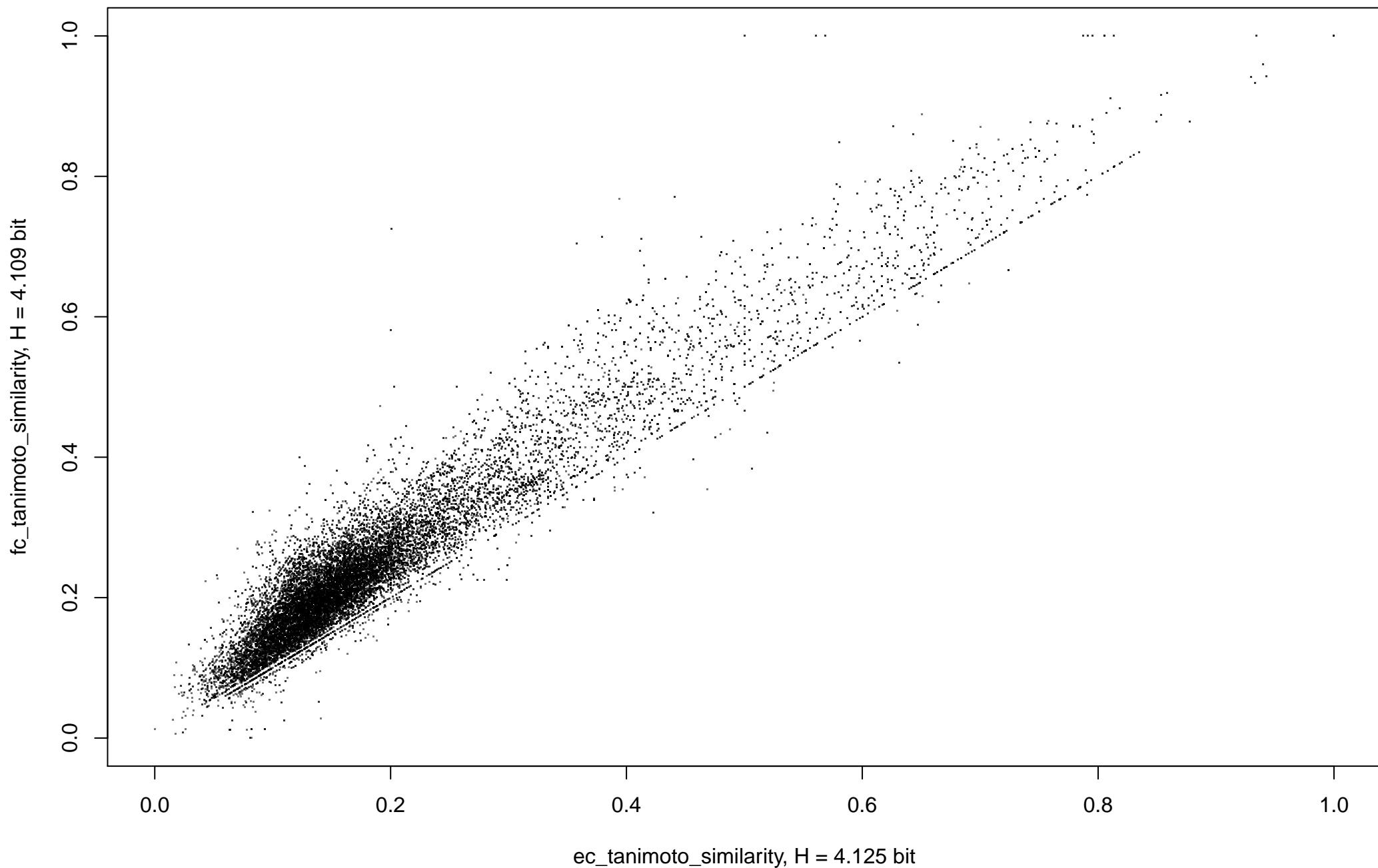
mcs_template_NumHAcceptors, H = 2.488 bit



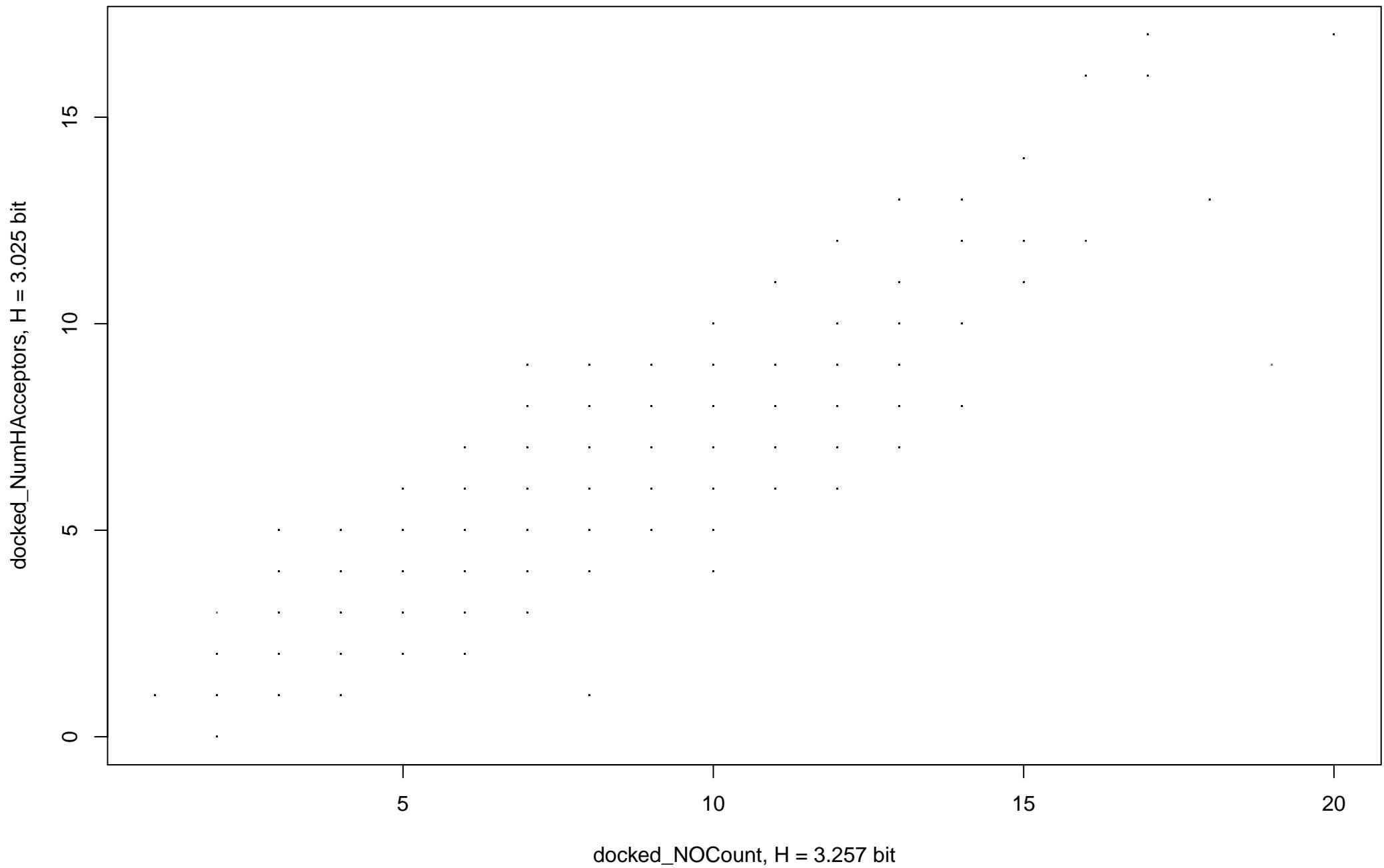
mcs_NumHeteroAtoms-mcs_docked_NumHAcceptors, MI = 0.9389 bit, normMI = 0.3772



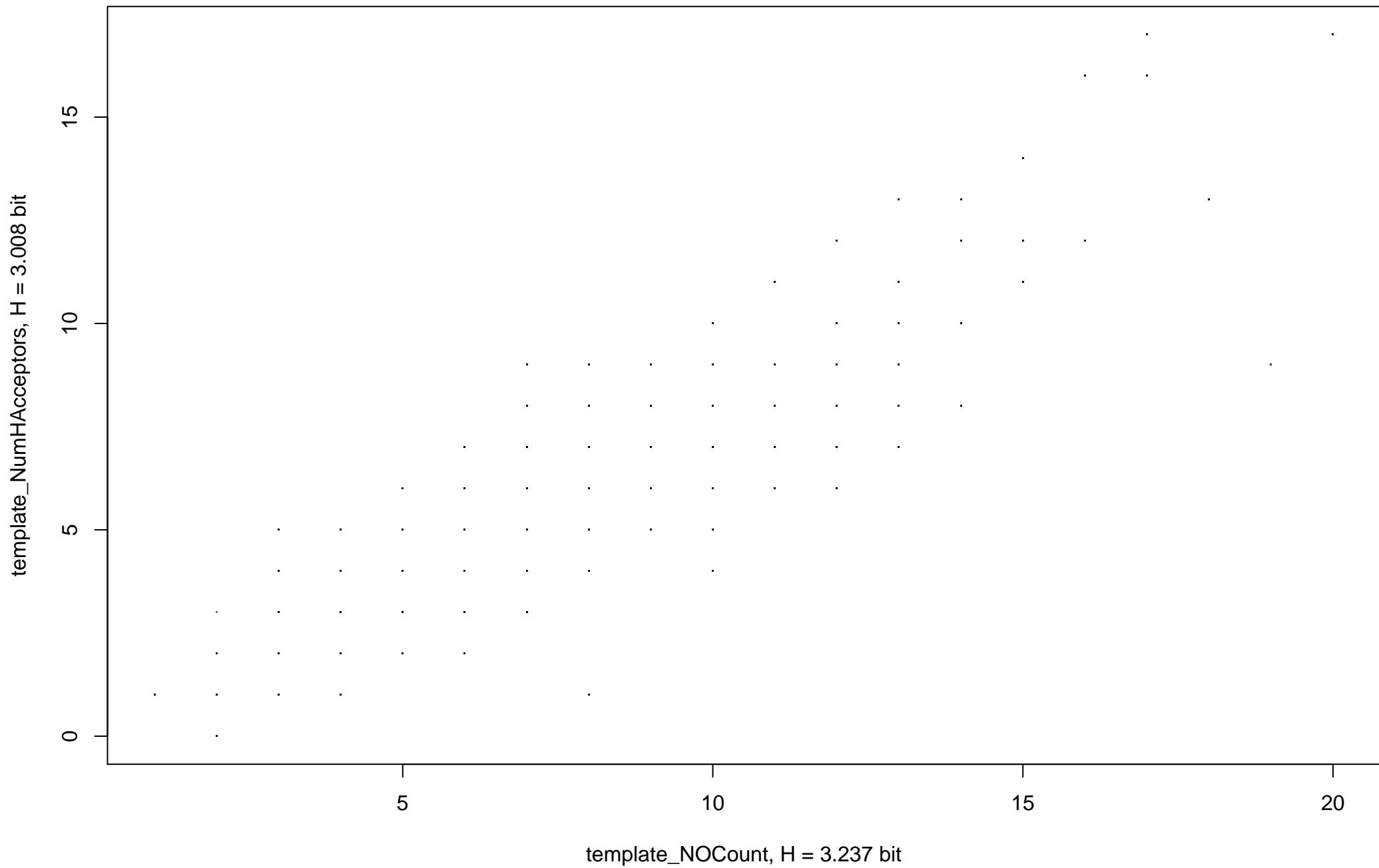
ec_tanimoto_similarity-fc_tanimoto_similarity, MI = 1.514 bit, normMI = 0.3685



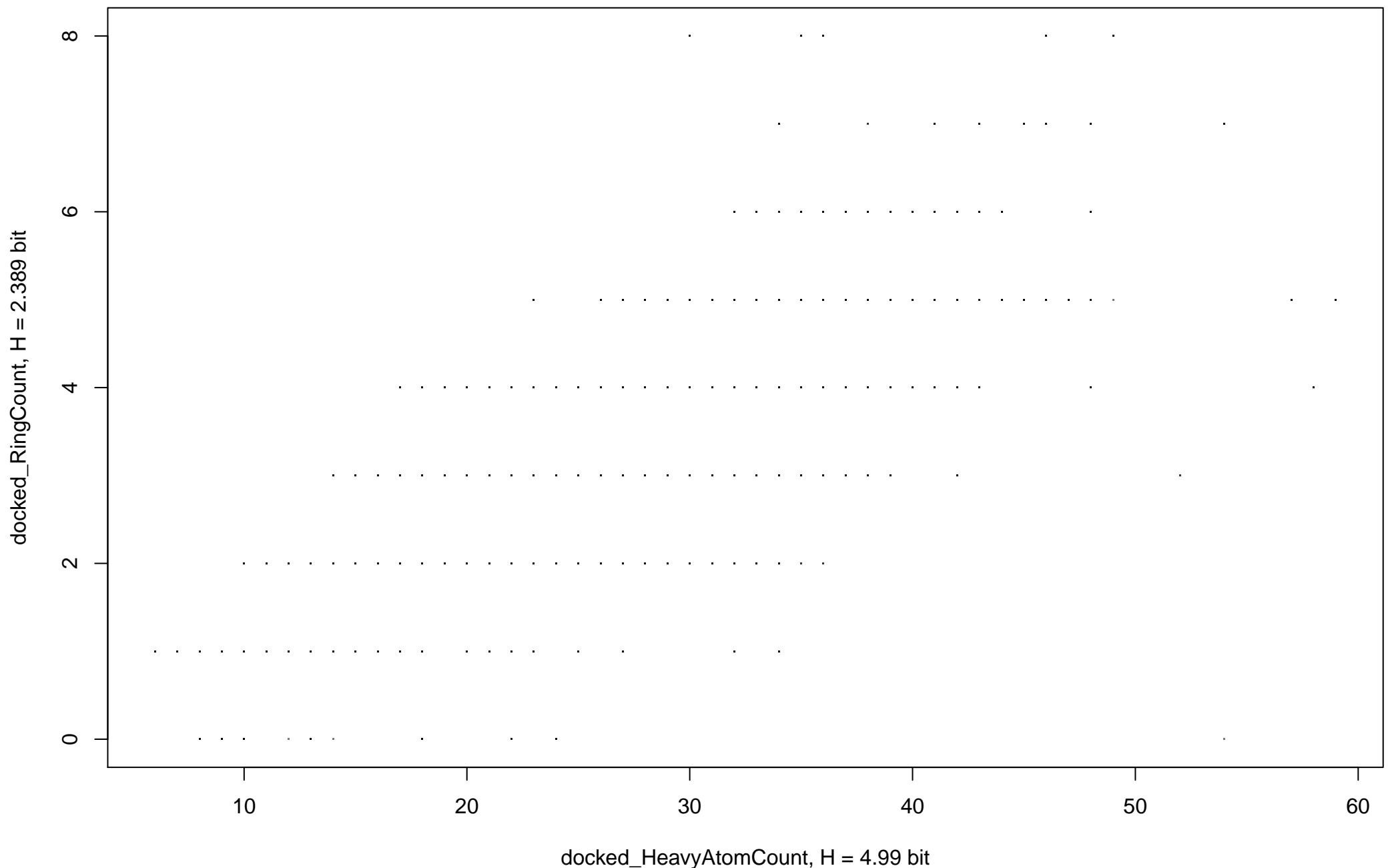
docked_NOCount-docked_NumHAcceptors, MI = 1.057 bit, normMI = 0.3494



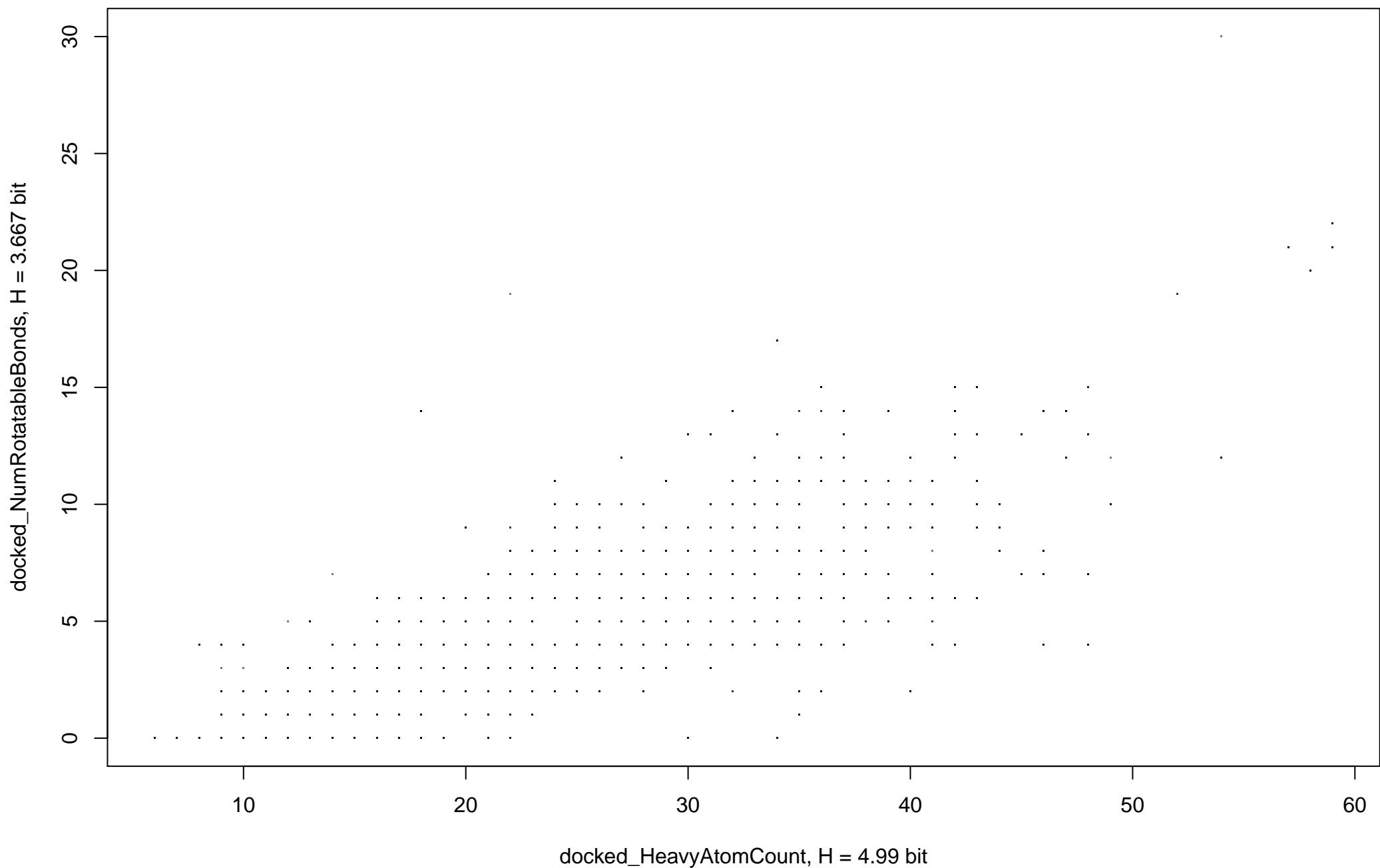
template_NOCount-template_NumHAcceptors, MI = 1.029 bit, normMI = 0.3422



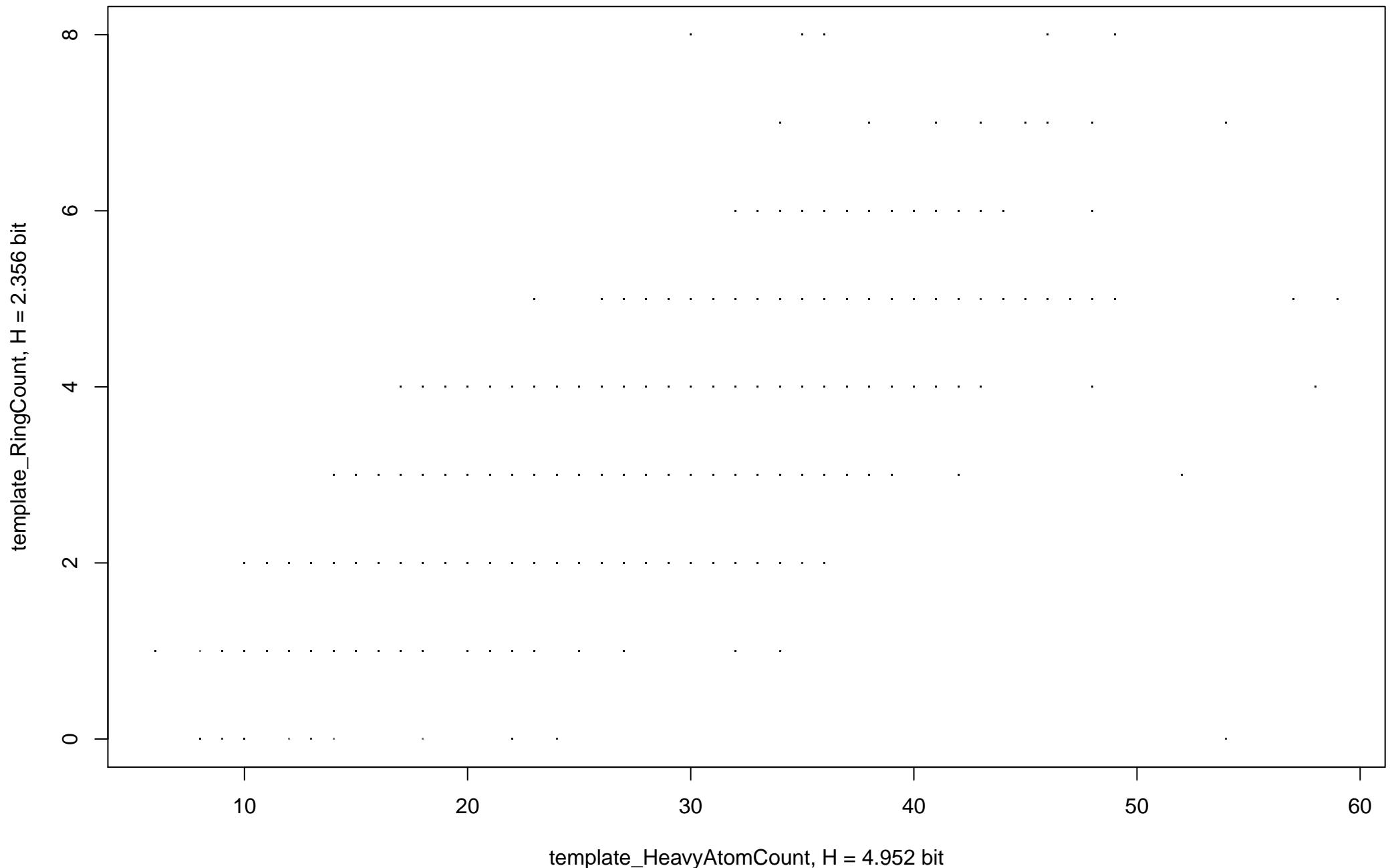
docked_HeavyAtomCount-docked_RingCount, MI = 0.8037 bit, normMI = 0.3364



docked_HeavyAtomCount-docked_NumRotatableBonds, MI = 1.184 bit, normMI = 0.3228

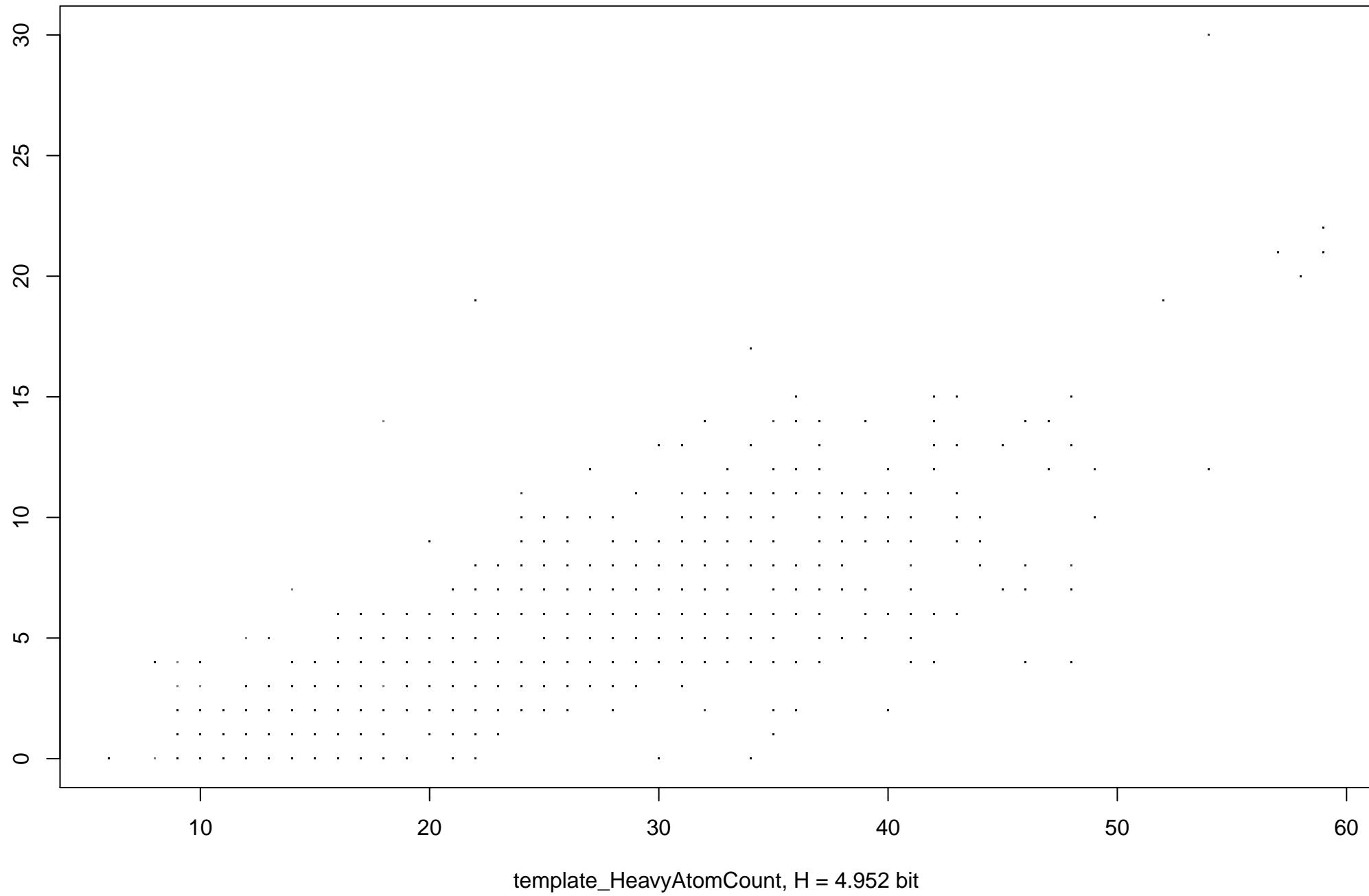


template_HeavyAtomCount–template_RingCount, MI = 0.7572 bit, normMI = 0.3214

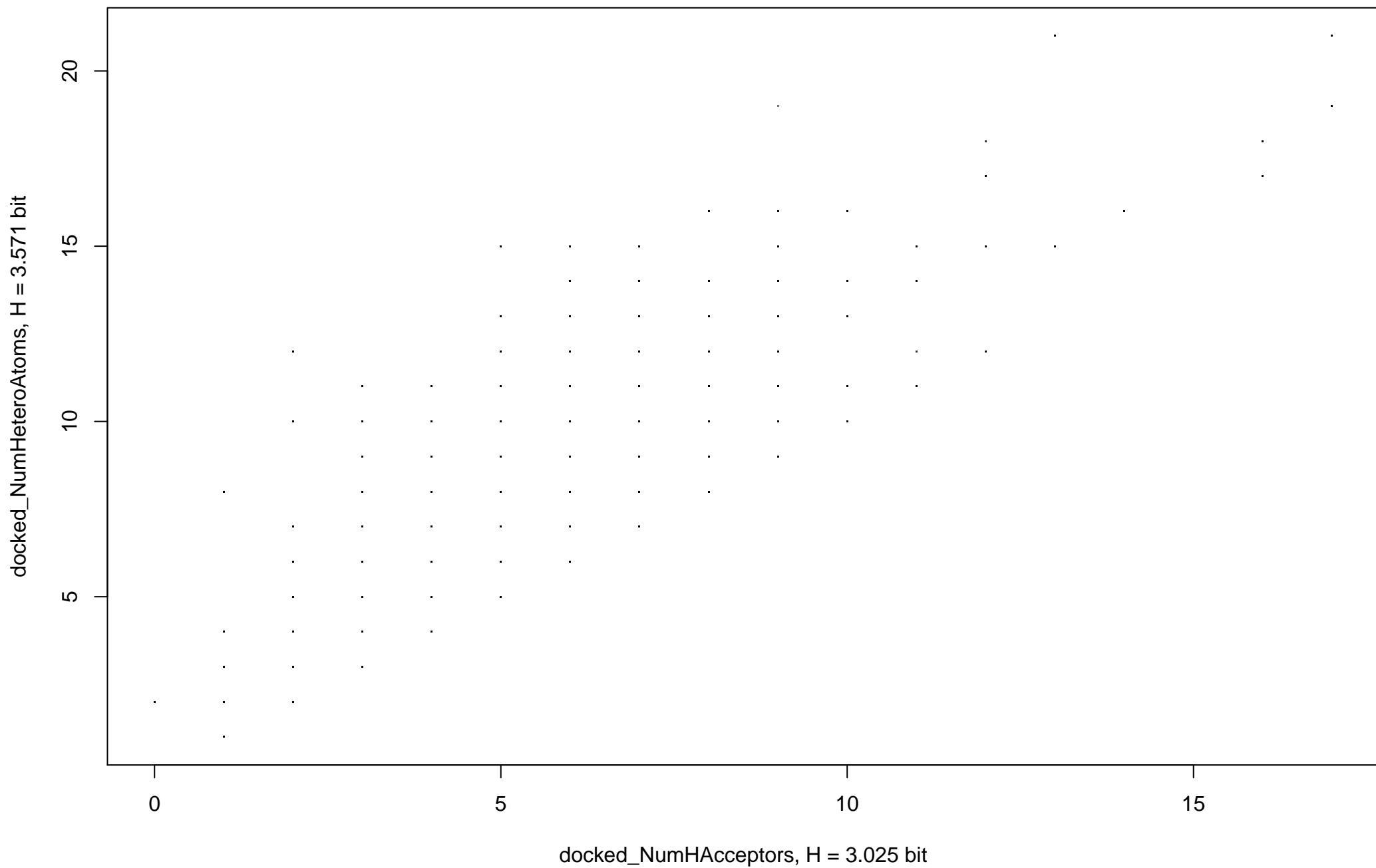


template_HeavyAtomCount-template_NumRotatableBonds, MI = 1.162 bit, normMI = 0.3168

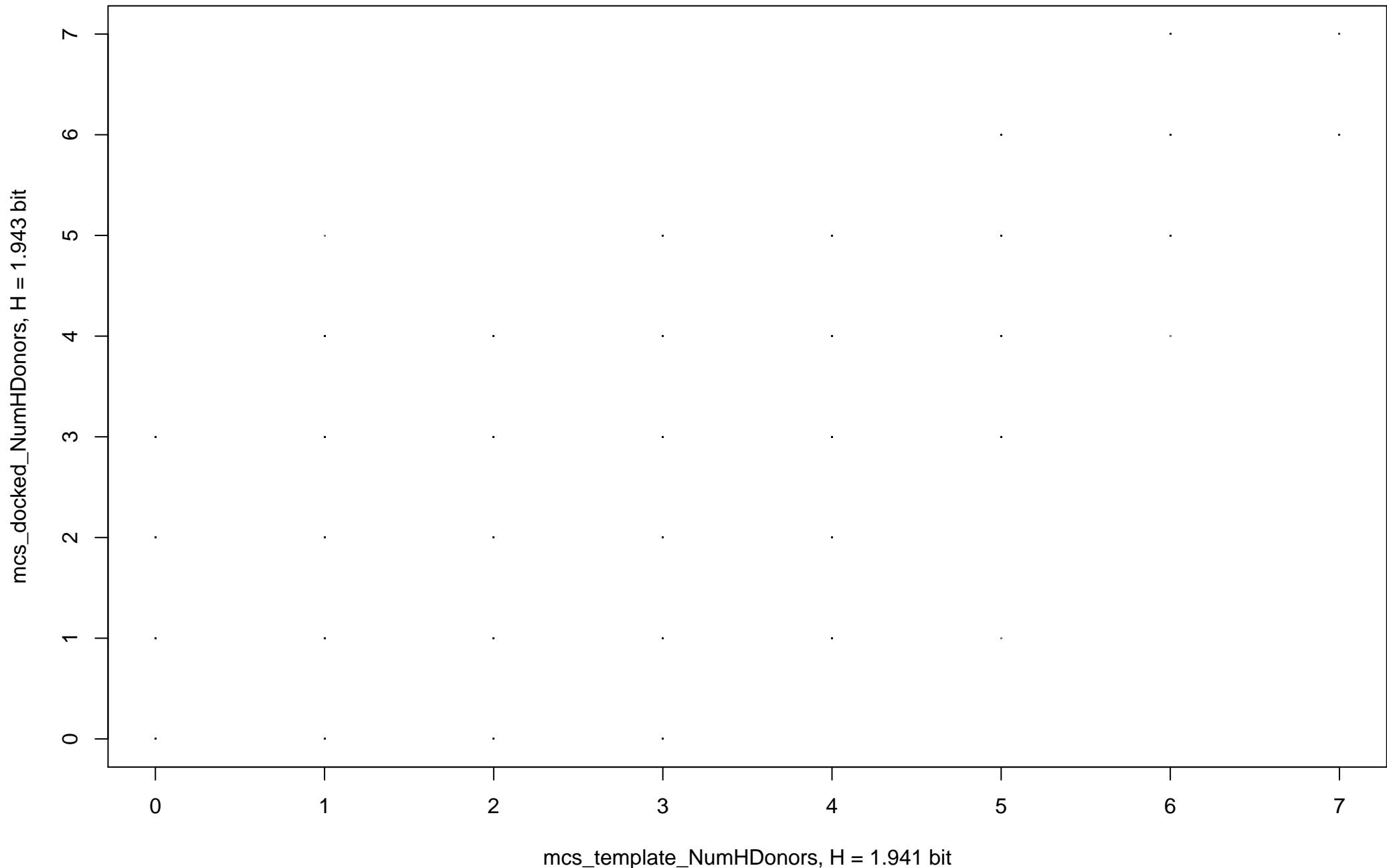
template_NumRotatableBonds, H = 3.668 bit



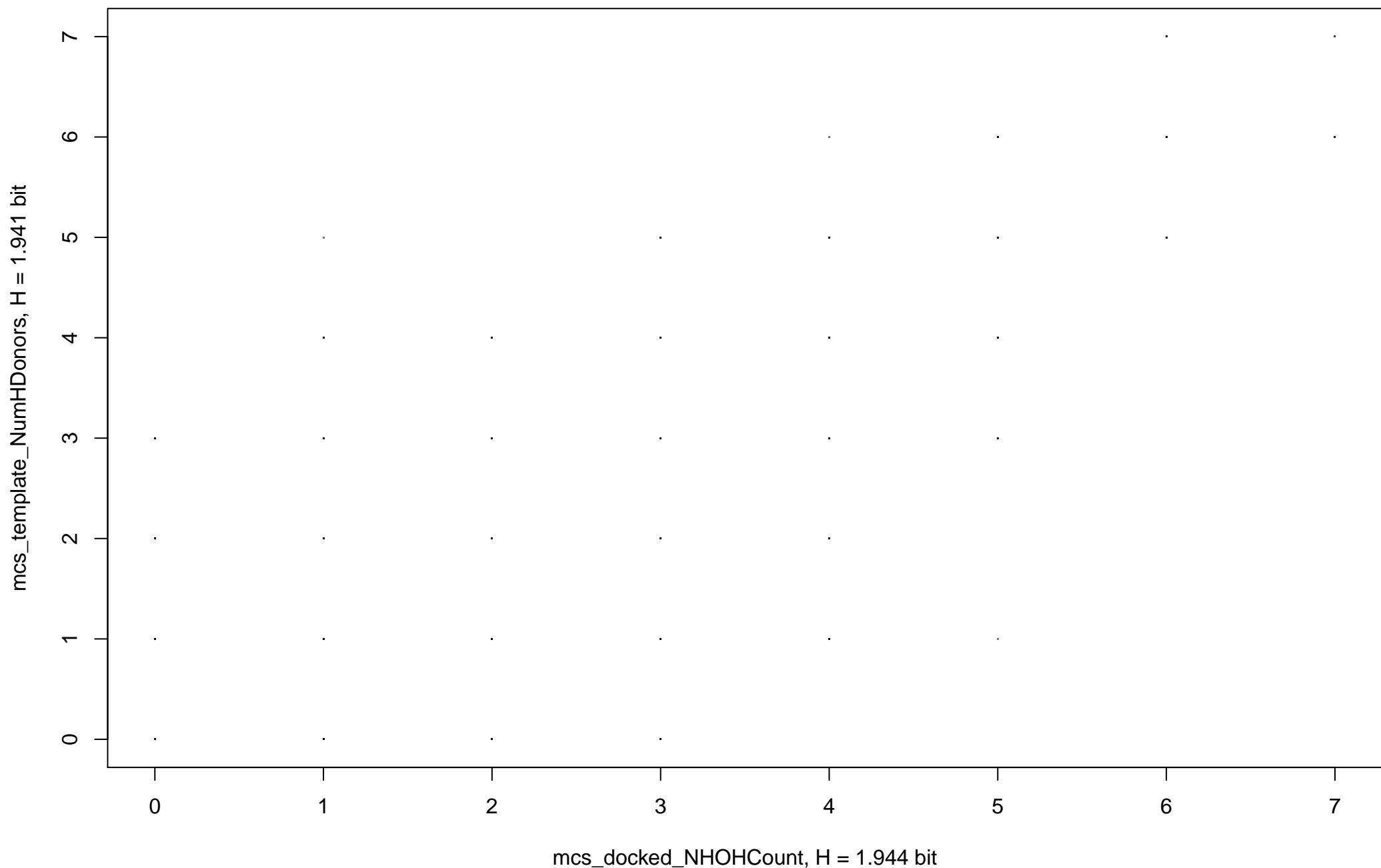
docked_NumHAcceptors-docked_NumHeteroAtoms, MI = 0.8788 bit, normMI = 0.2905



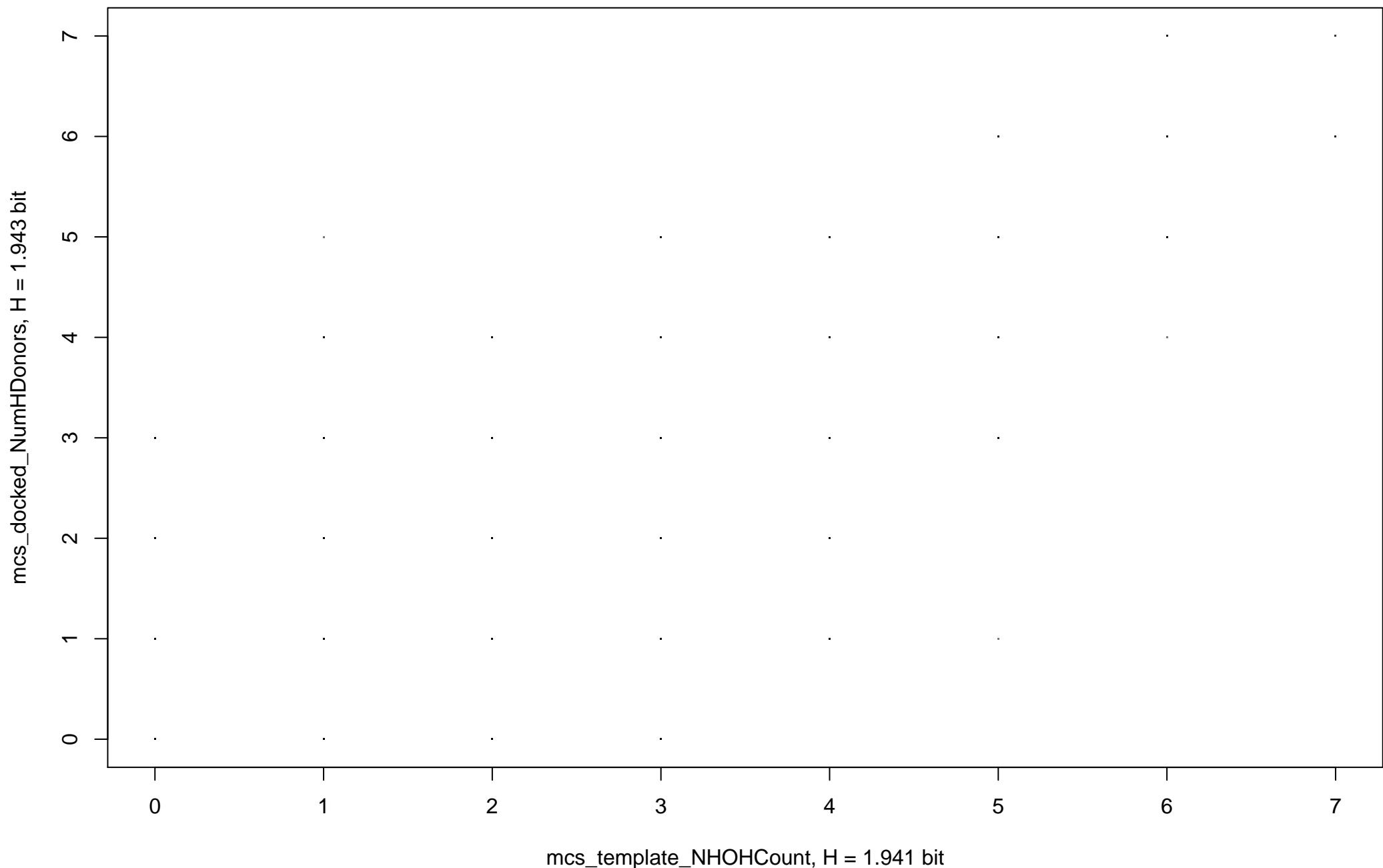
mcs_template_NumHDonors–mcs_docked_NumHDonors, MI = 0.5633 bit, normMI = 0.2902



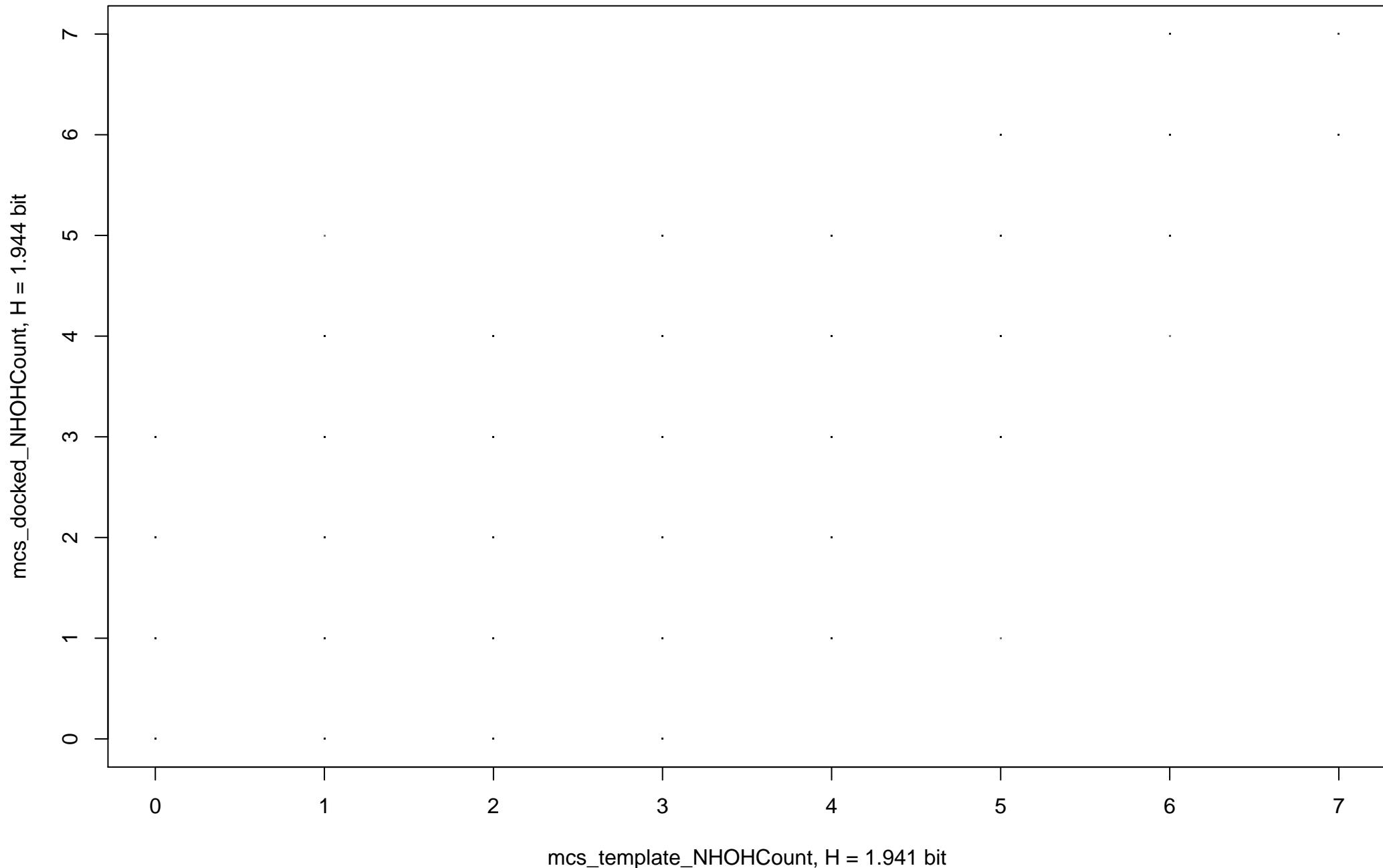
mcs_docked_NHOHCount-mcs_template_NumHDonors, MI = 0.5627 bit, normMI = 0.2899



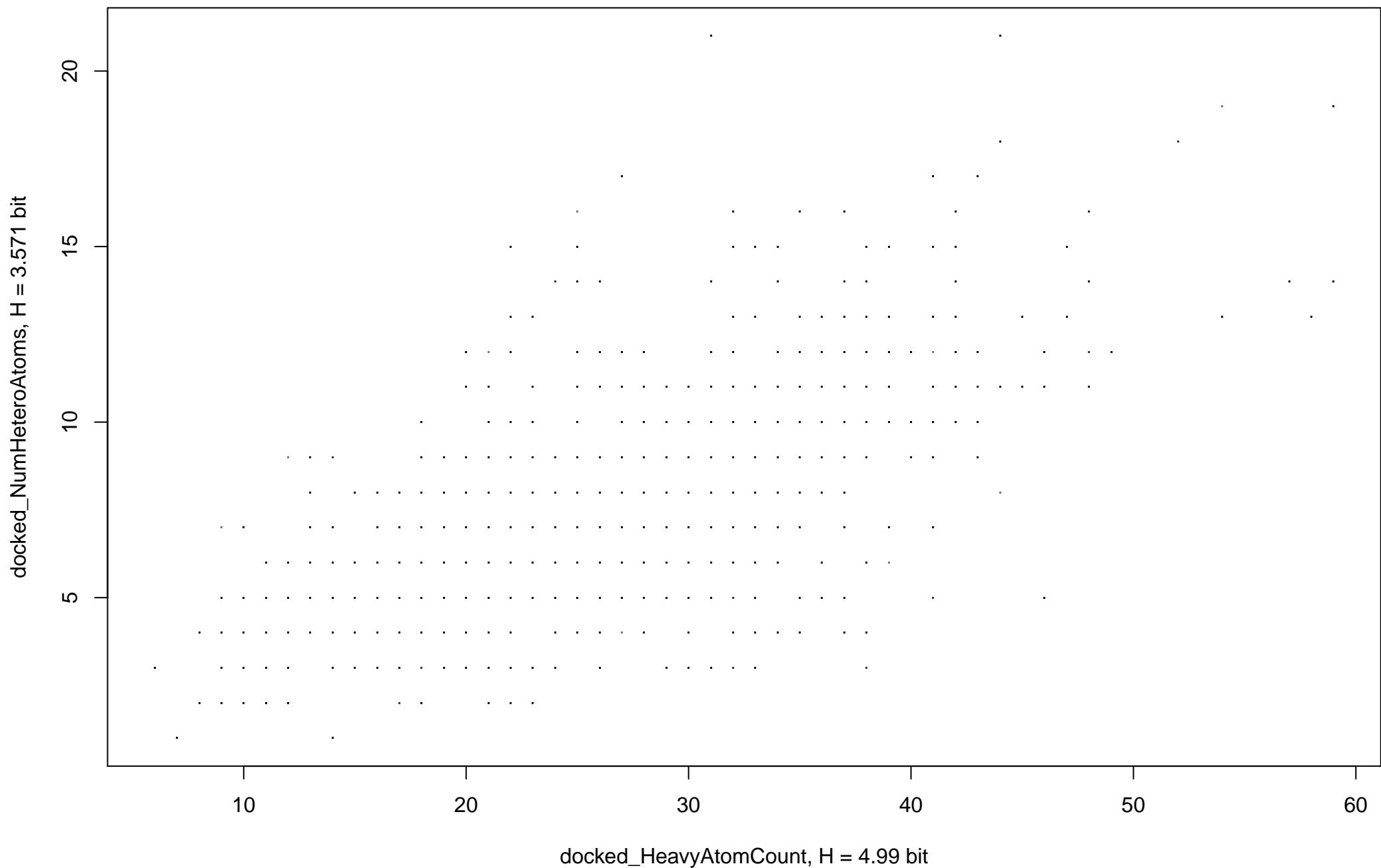
mcs_template_NHOHCount-mcs_docked_NumHDonors, MI = 0.5626 bit, normMI = 0.2898



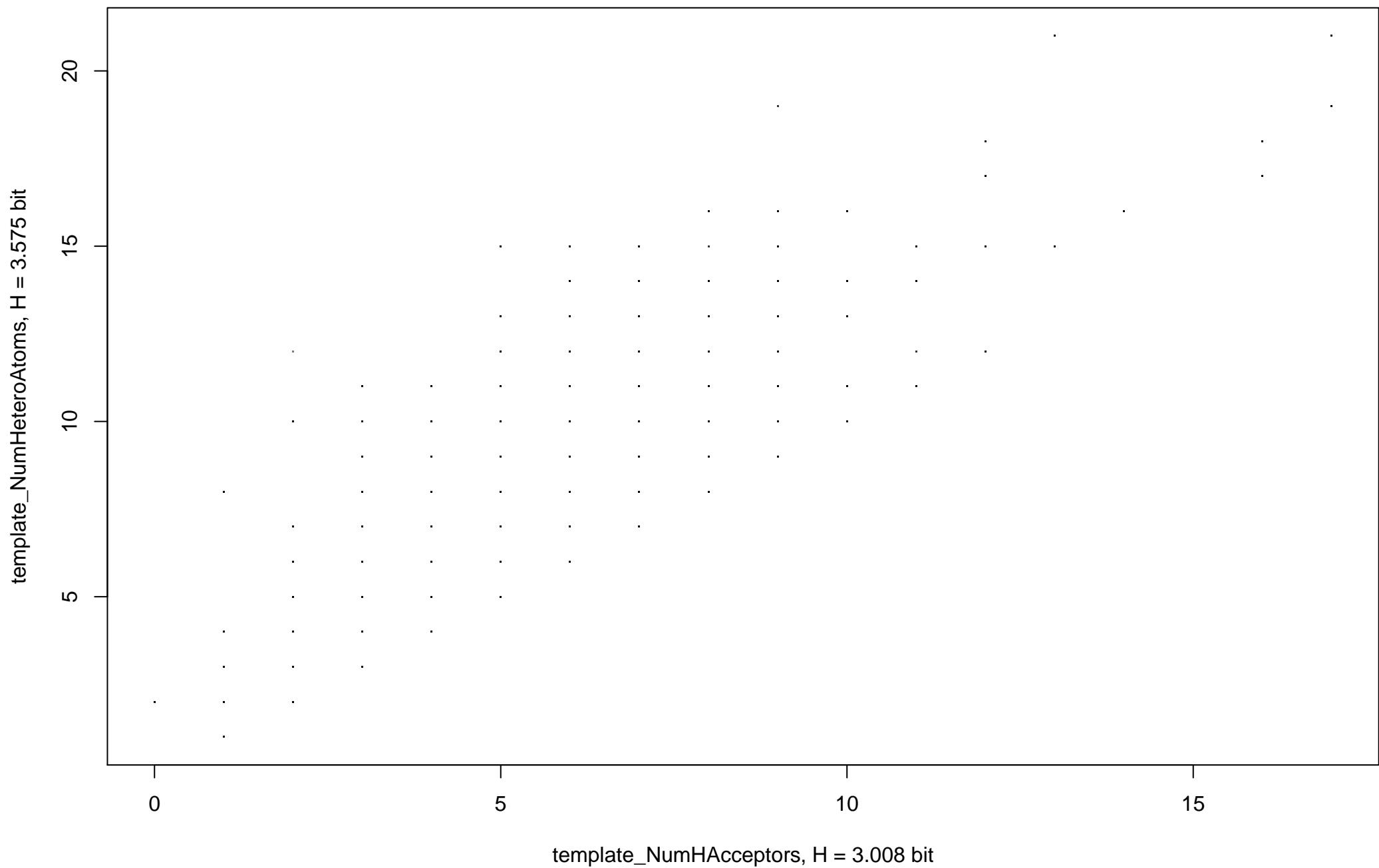
mcs_template_NHOHCount–mcs_docked_NHOHCount, MI = 0.5626 bit, normMI = 0.2898



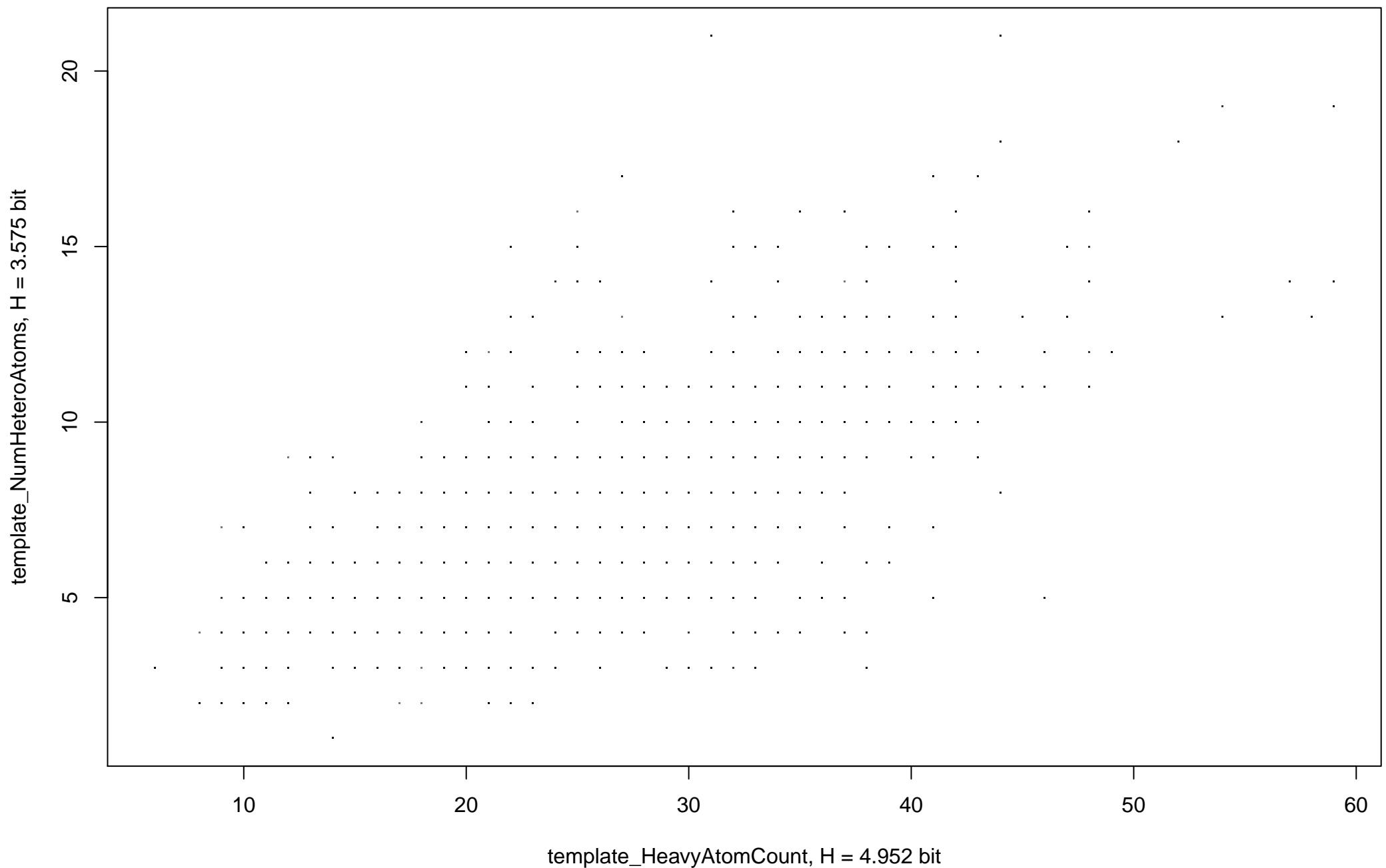
docked_HeavyAtomCount-docked_NumHeteroAtoms, MI = 1.018 bit, normMI = 0.2851



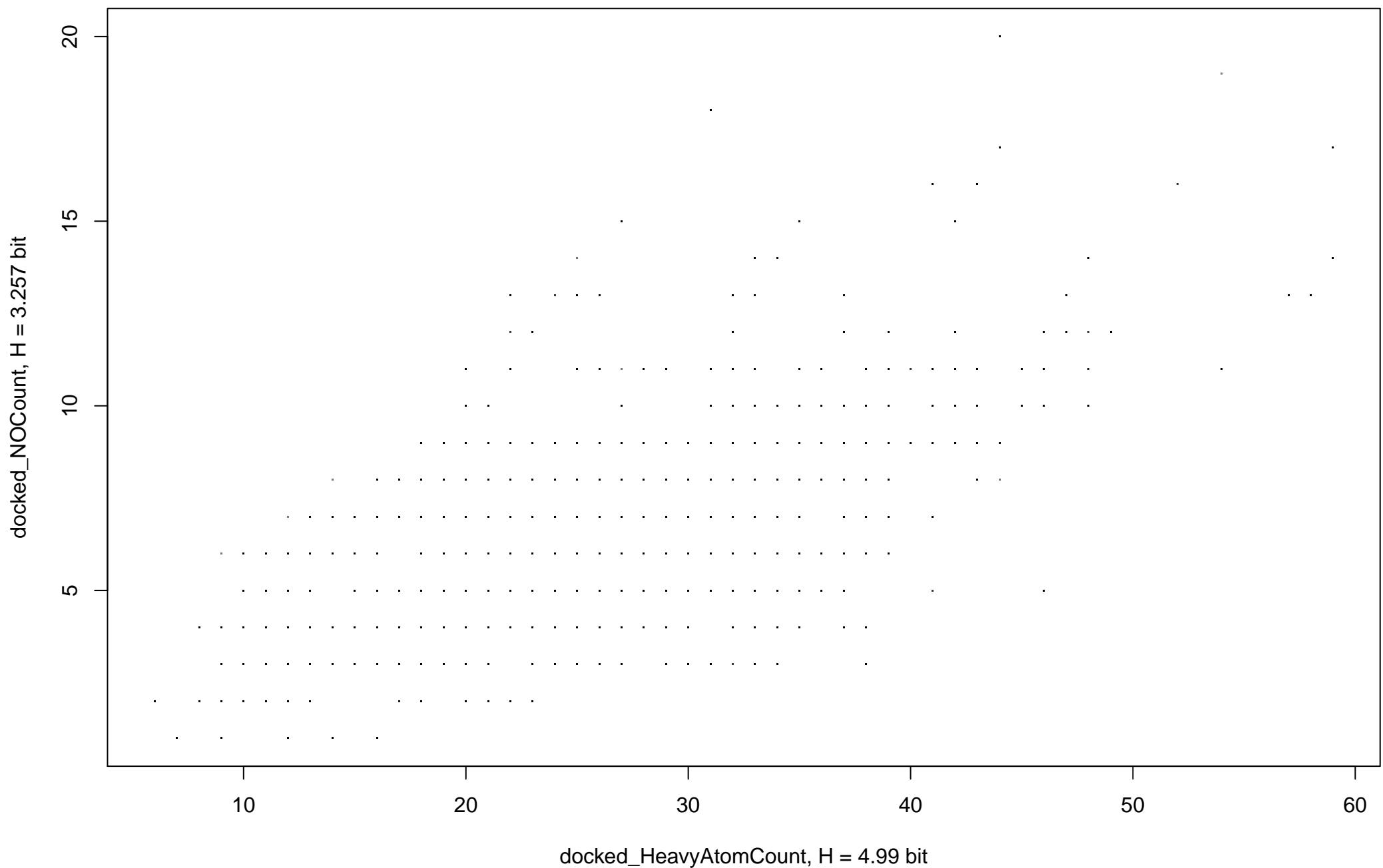
template_NumHAcceptors–template_NumHeteroAtoms, MI = 0.849 bit, normMI = 0.2823



template_HeavyAtomCount–template_NumHeteroAtoms, MI = 0.9942 bit, normMI = 0.2781

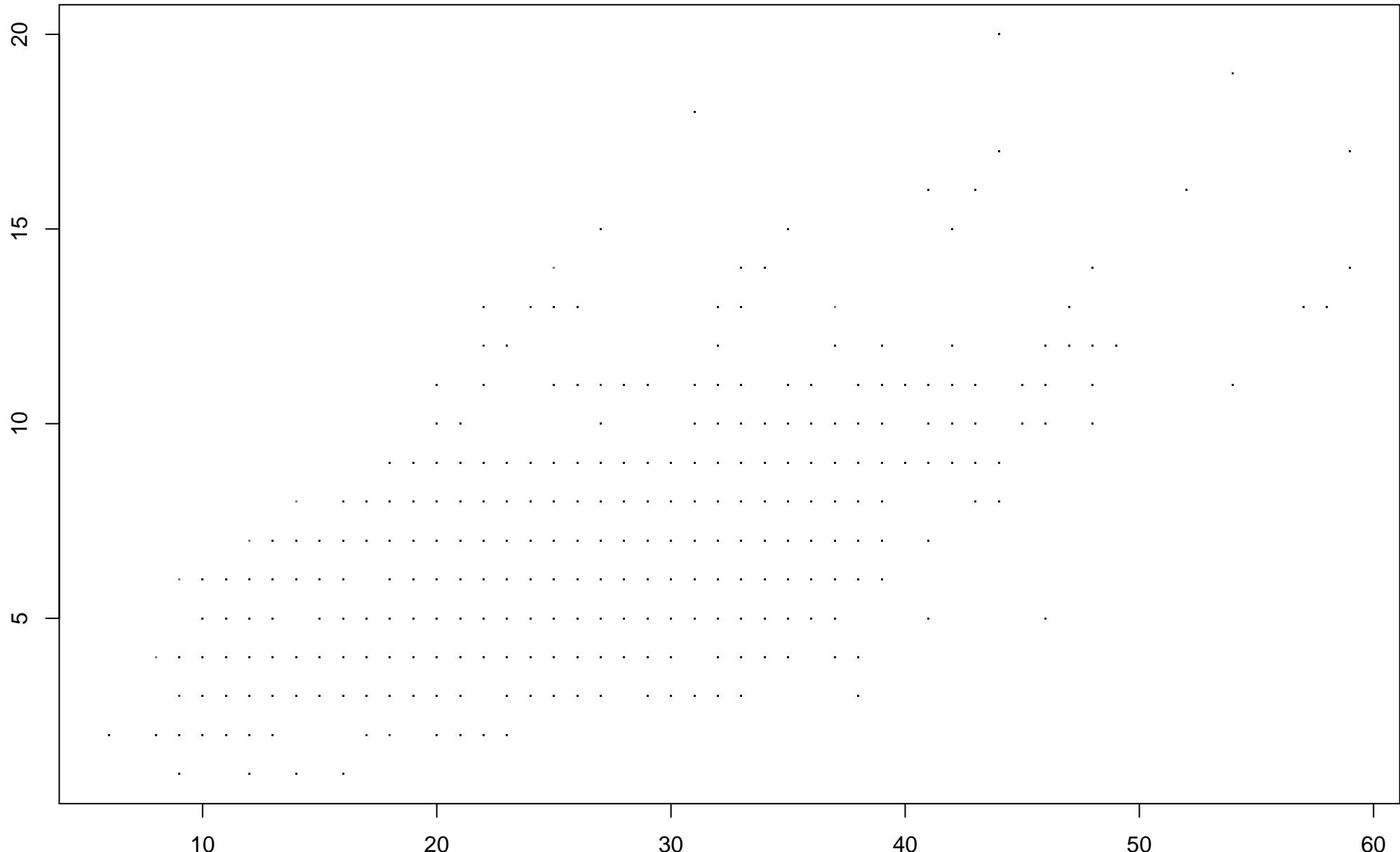


docked_HeavyAtomCount-docked_NOCount, MI = 0.895 bit, normMI = 0.2748



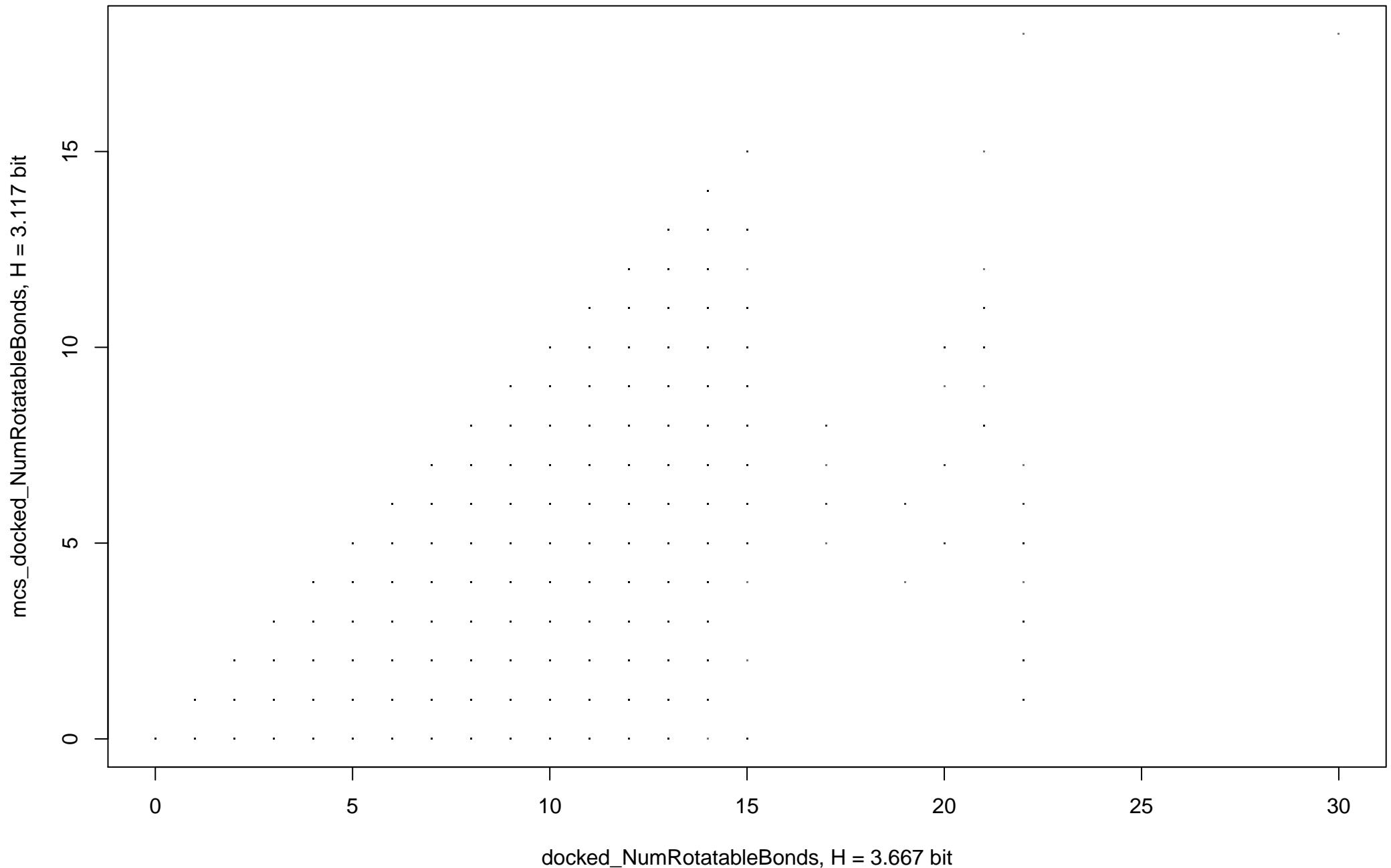
template_HeavyAtomCount–template_NOCount, MI = 0.8794 bit, normMI = 0.2717

template_NOCount, H = 3.237 bit

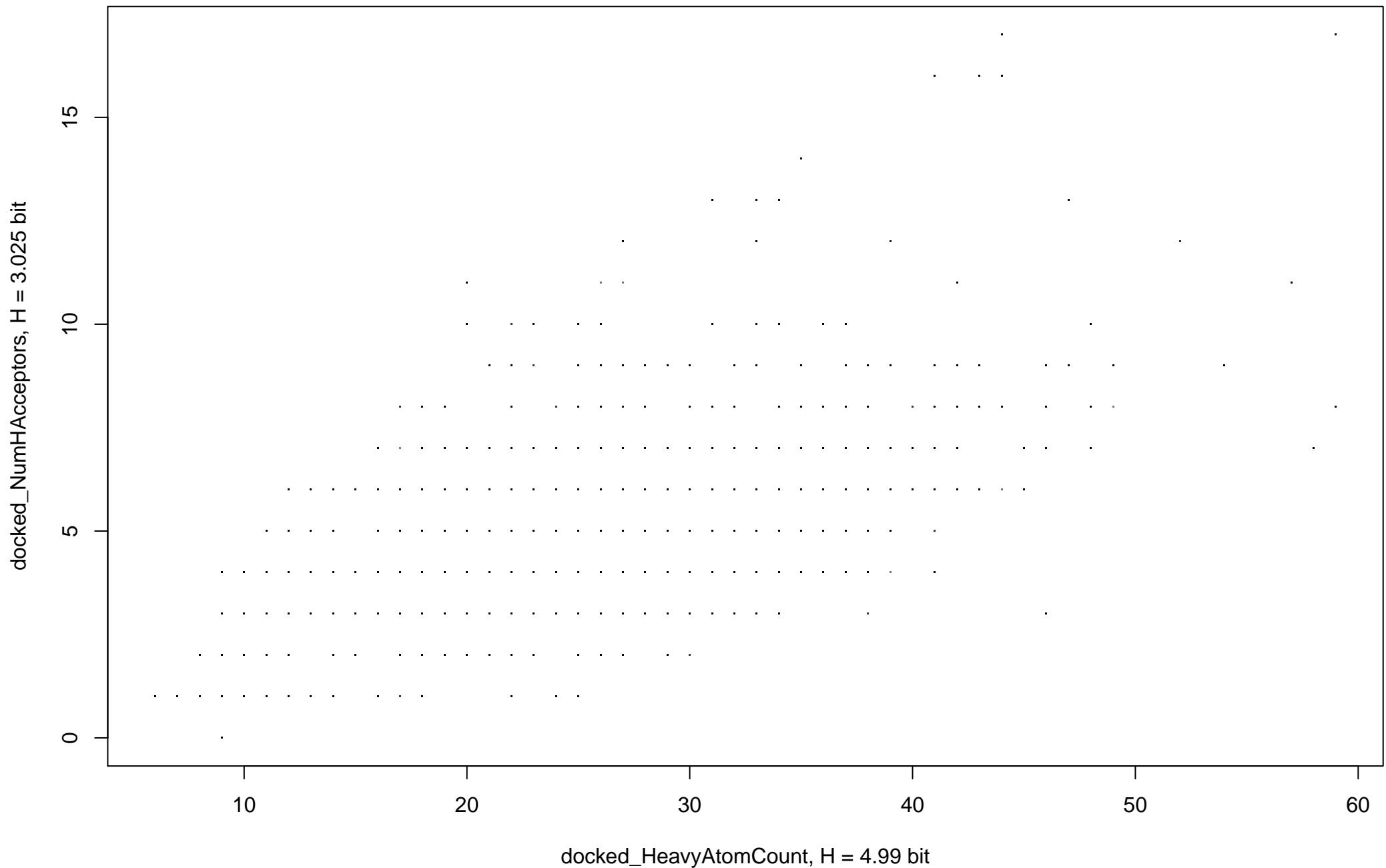


template_HeavyAtomCount, H = 4.952 bit

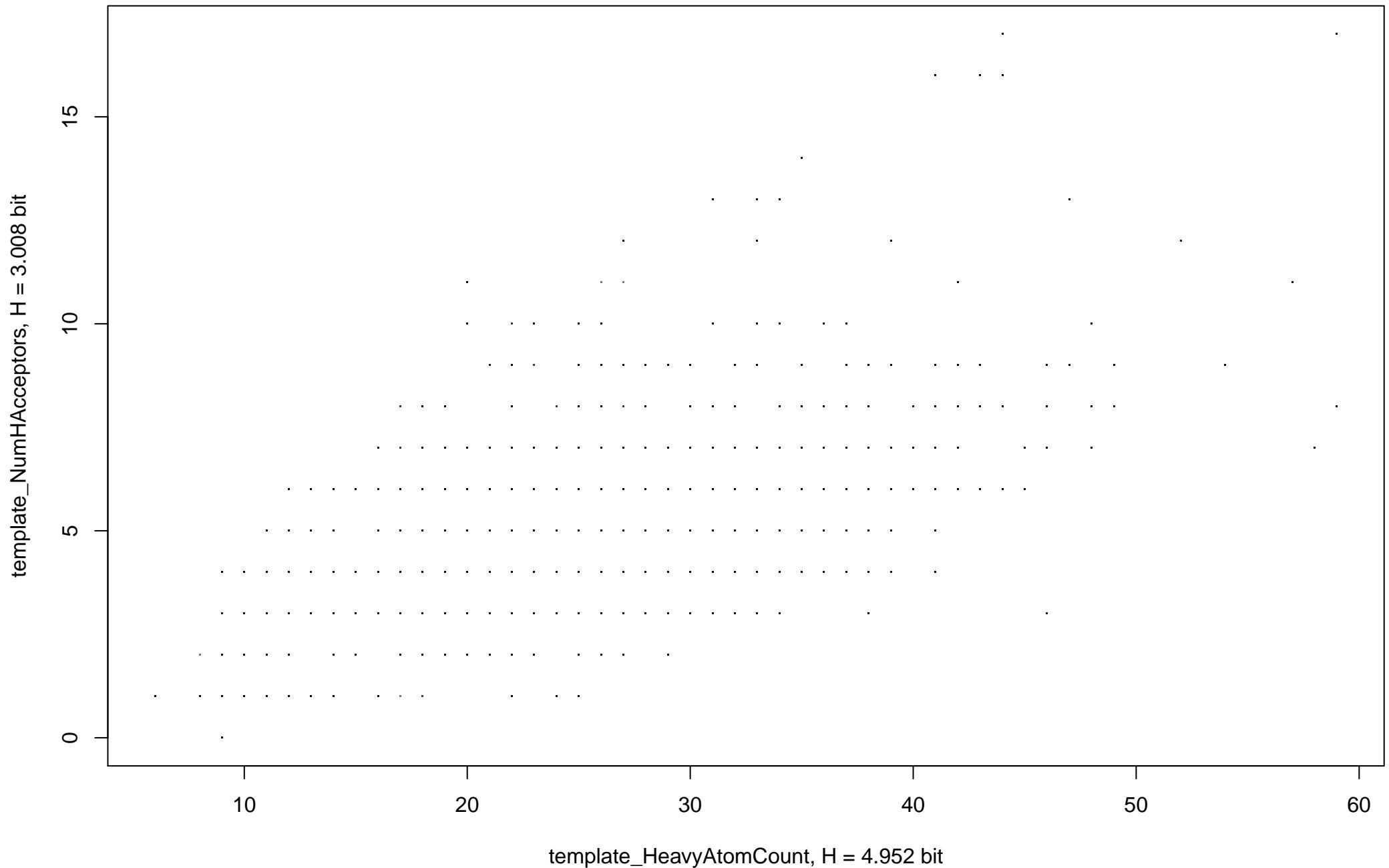
docked_NumRotatableBonds-mcs_docked_NumRotatableBonds, MI = 0.8093 bit, normMI = 0.2597



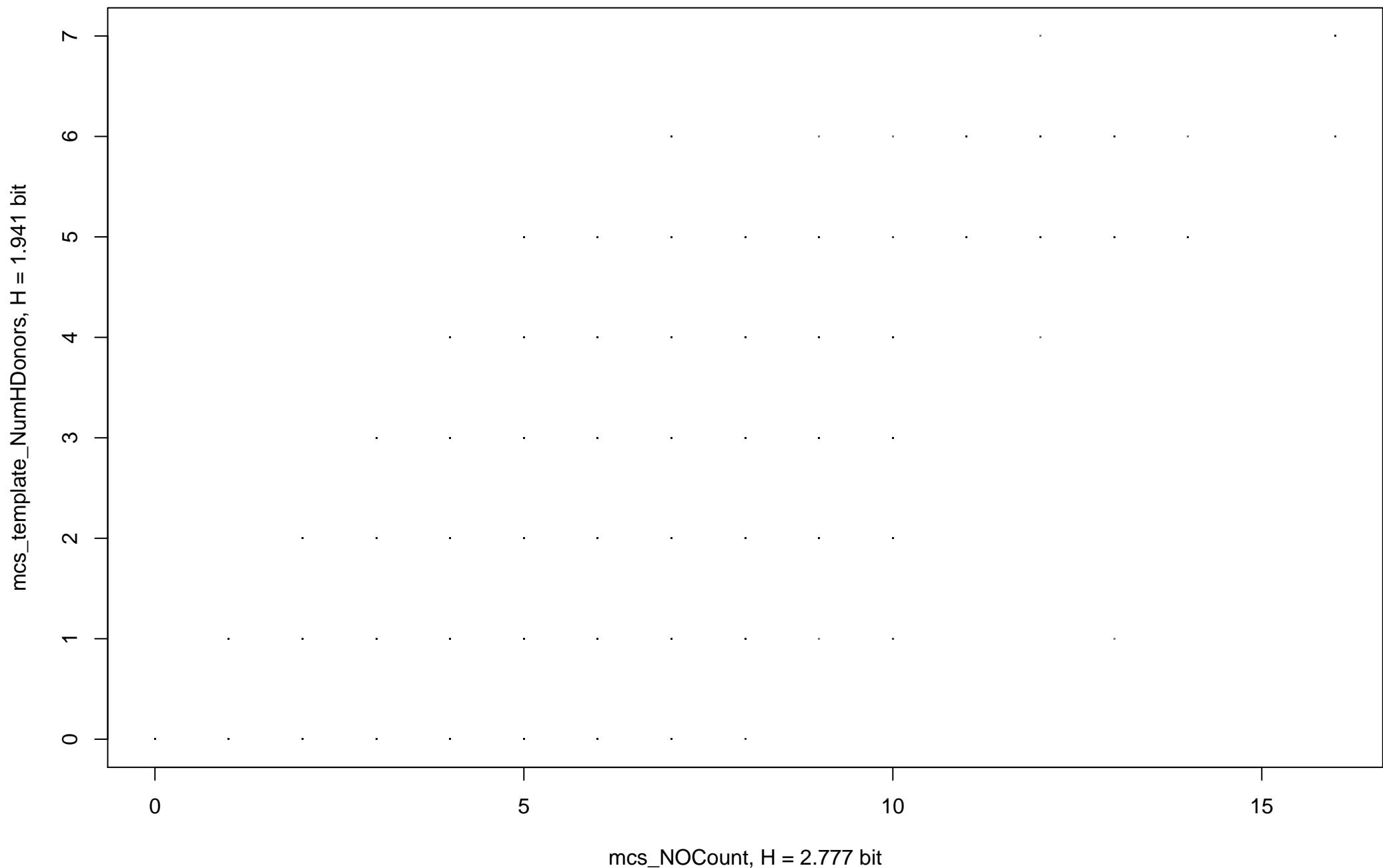
docked_HeavyAtomCount–docked_NumHAcceptors, MI = 0.7511 bit, normMI = 0.2483



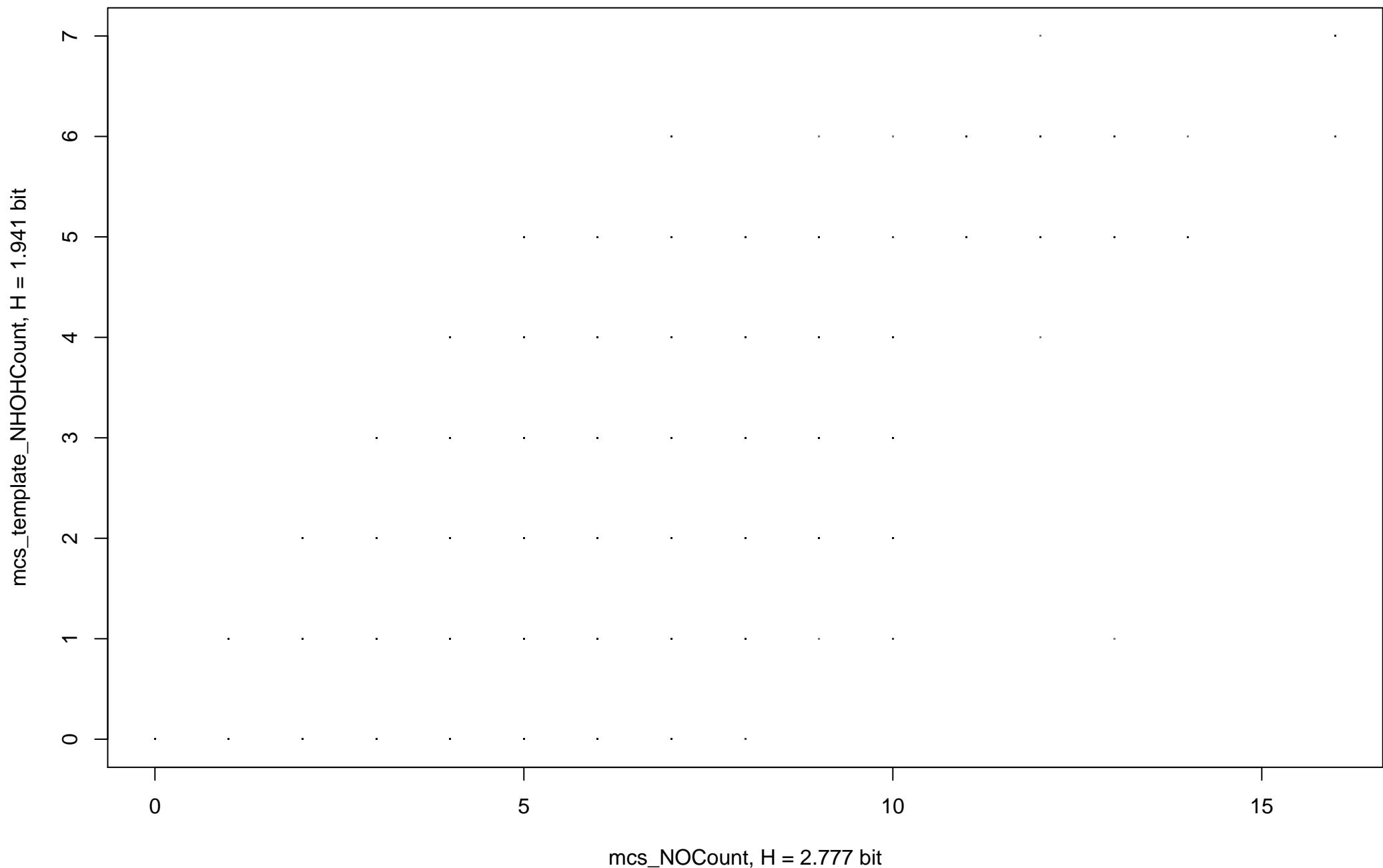
template_HeavyAtomCount–template_NumHAcceptors, MI = 0.7399 bit, normMI = 0.246



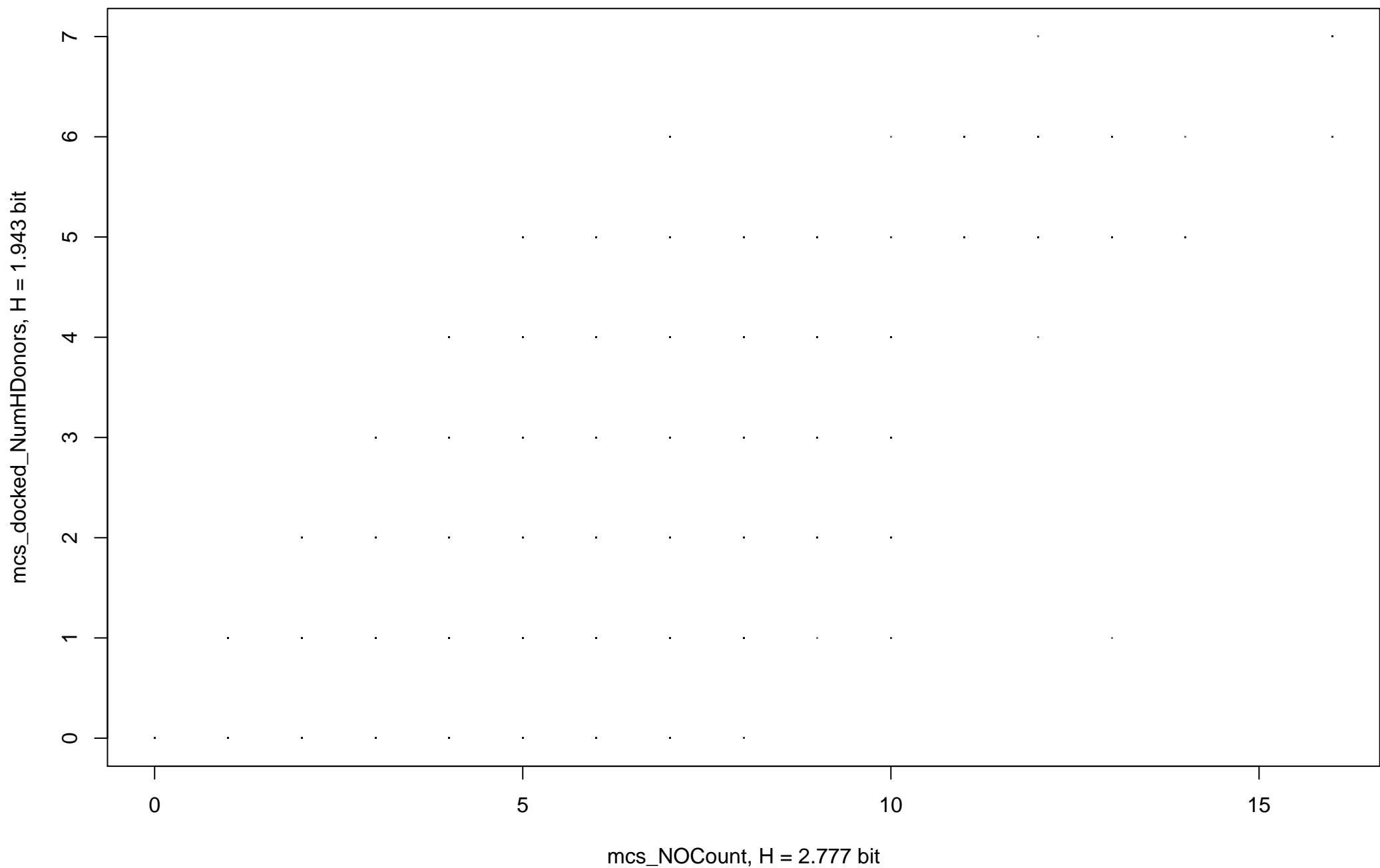
mcs_NOCount-mcs_template_NumHDonors, MI = 0.4677 bit, normMI = 0.241



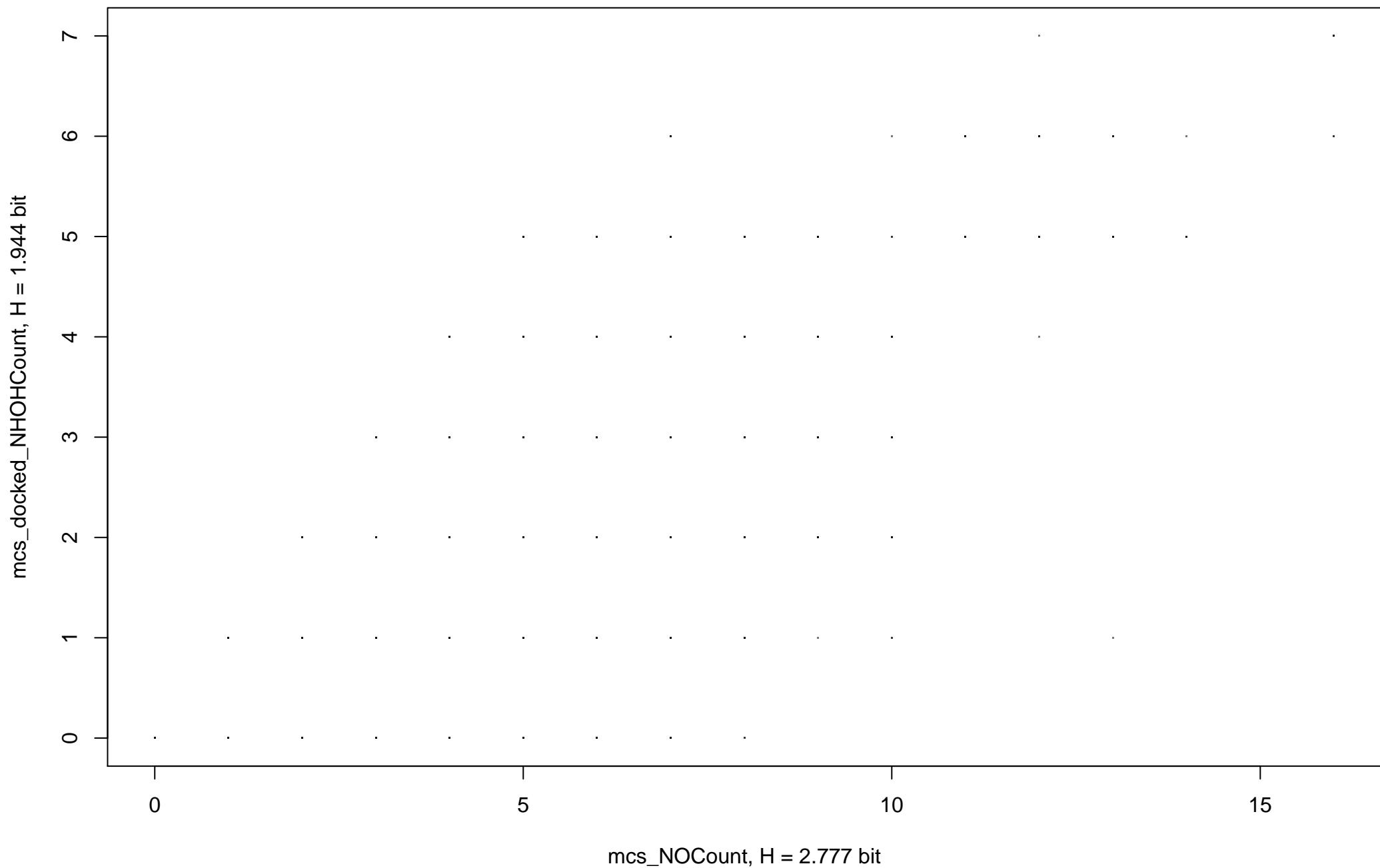
mcs_NOCount-mcs_template_NHOHCount, MI = 0.4678 bit, normMI = 0.241



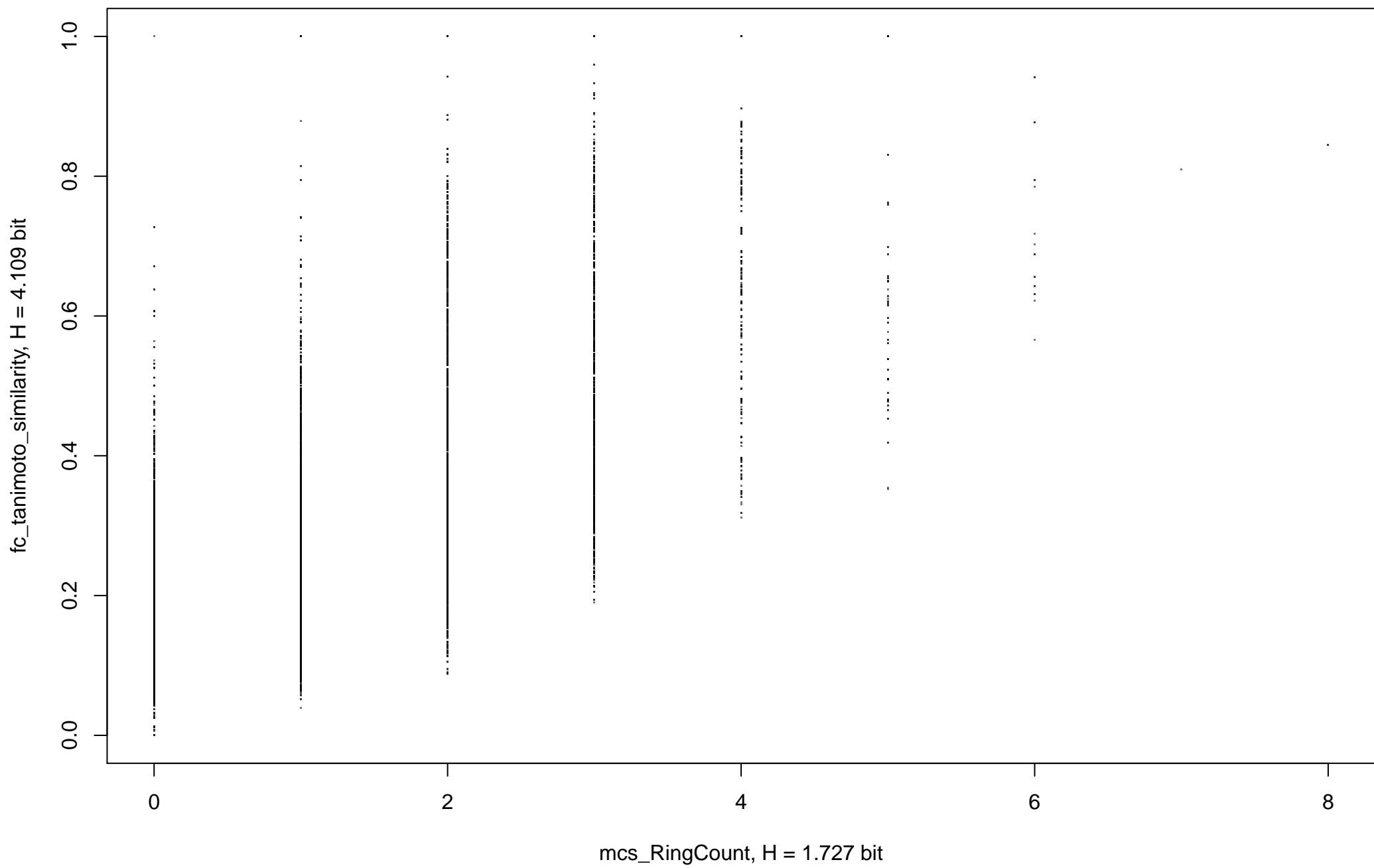
mcs_NOCount-mcs_docked_NumHDonors, MI = 0.4614 bit, normMI = 0.2374



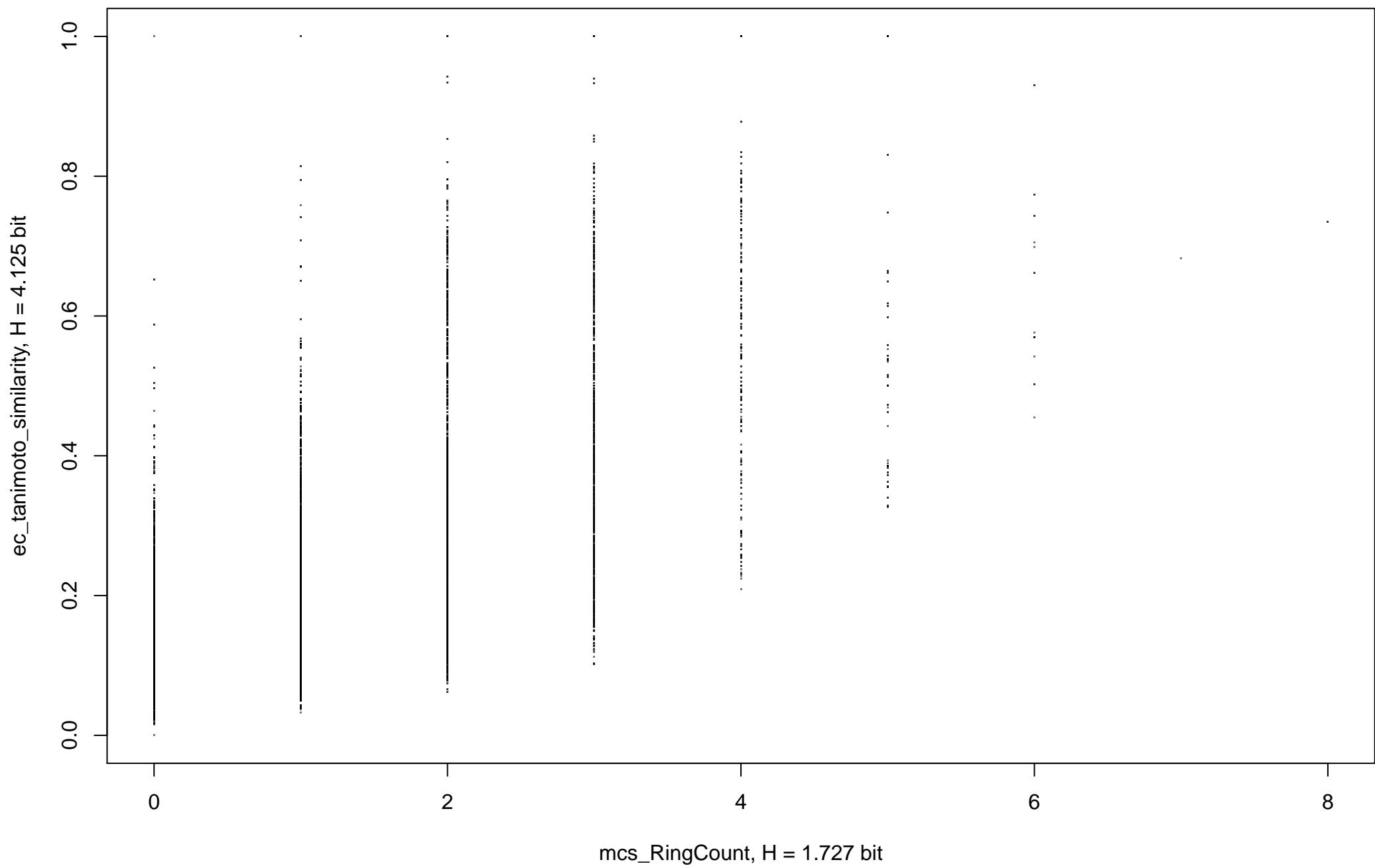
mcs_NOCount-mcs_docked_NHOHCount, MI = 0.4615 bit, normMI = 0.2374



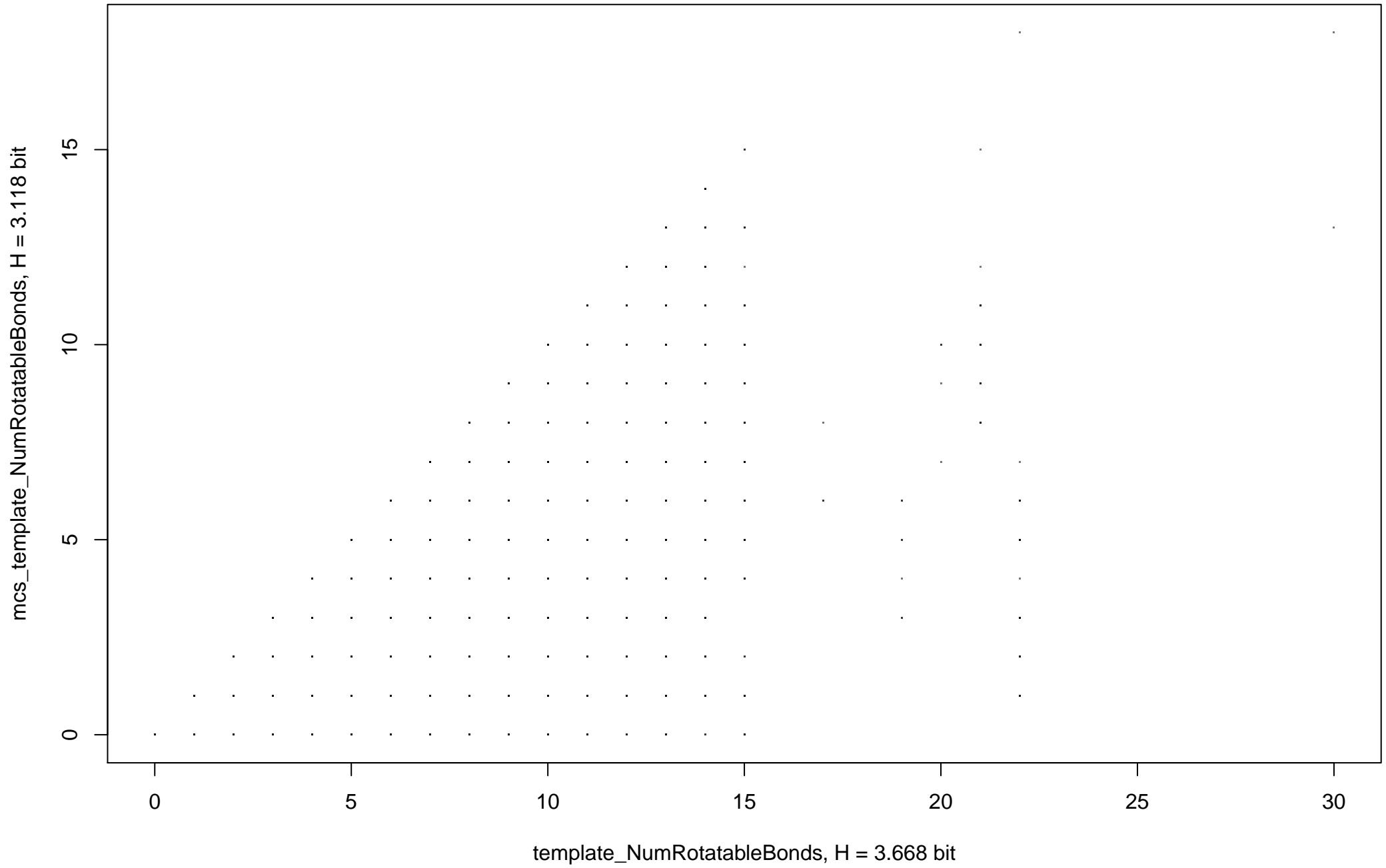
mcs_RingCount-fc_tanimoto_similarity, MI = 0.4053 bit, normMI = 0.2346



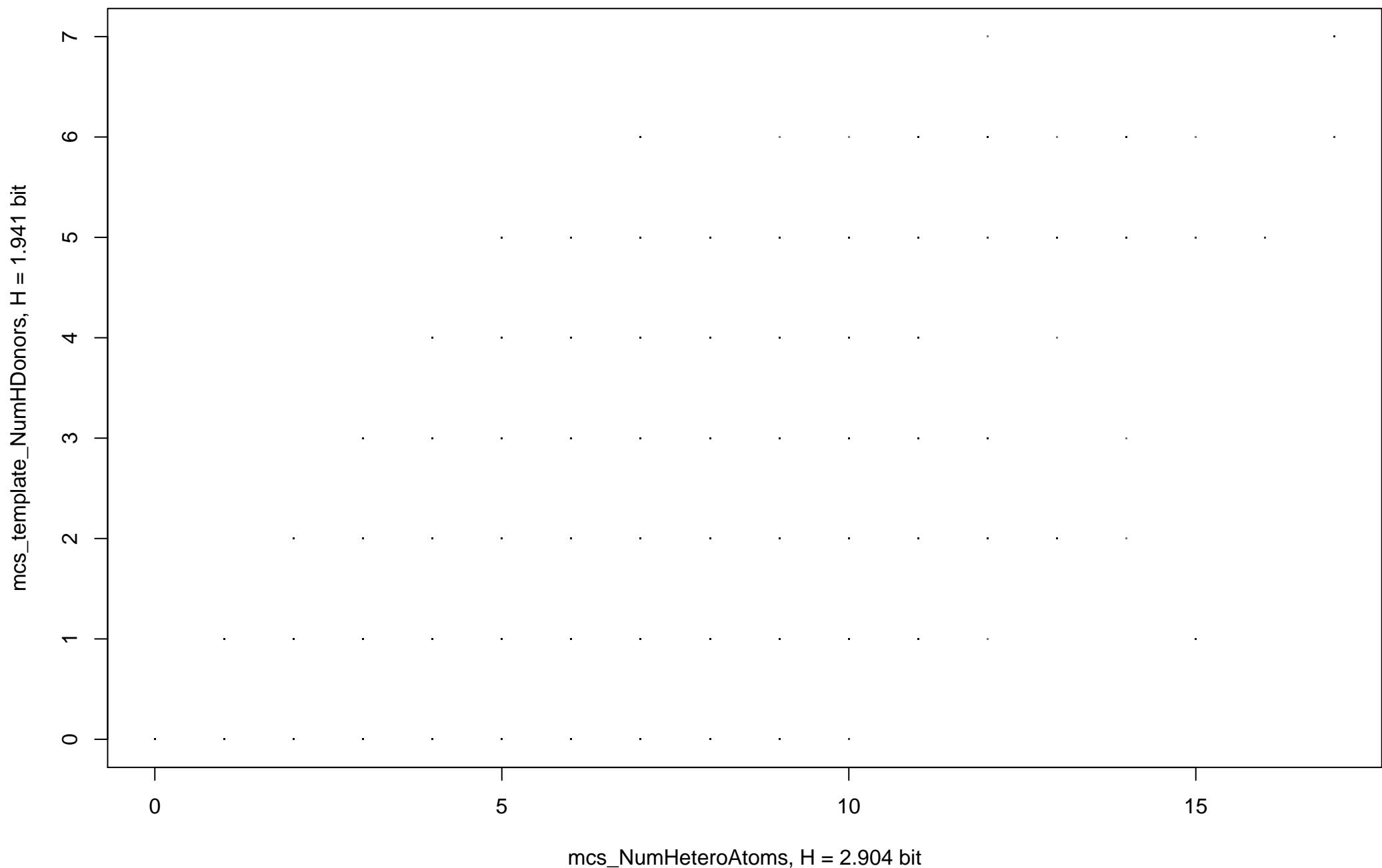
mcs_RingCount-ec_tanimoto_similarity, MI = 0.3942 bit, normMI = 0.2282



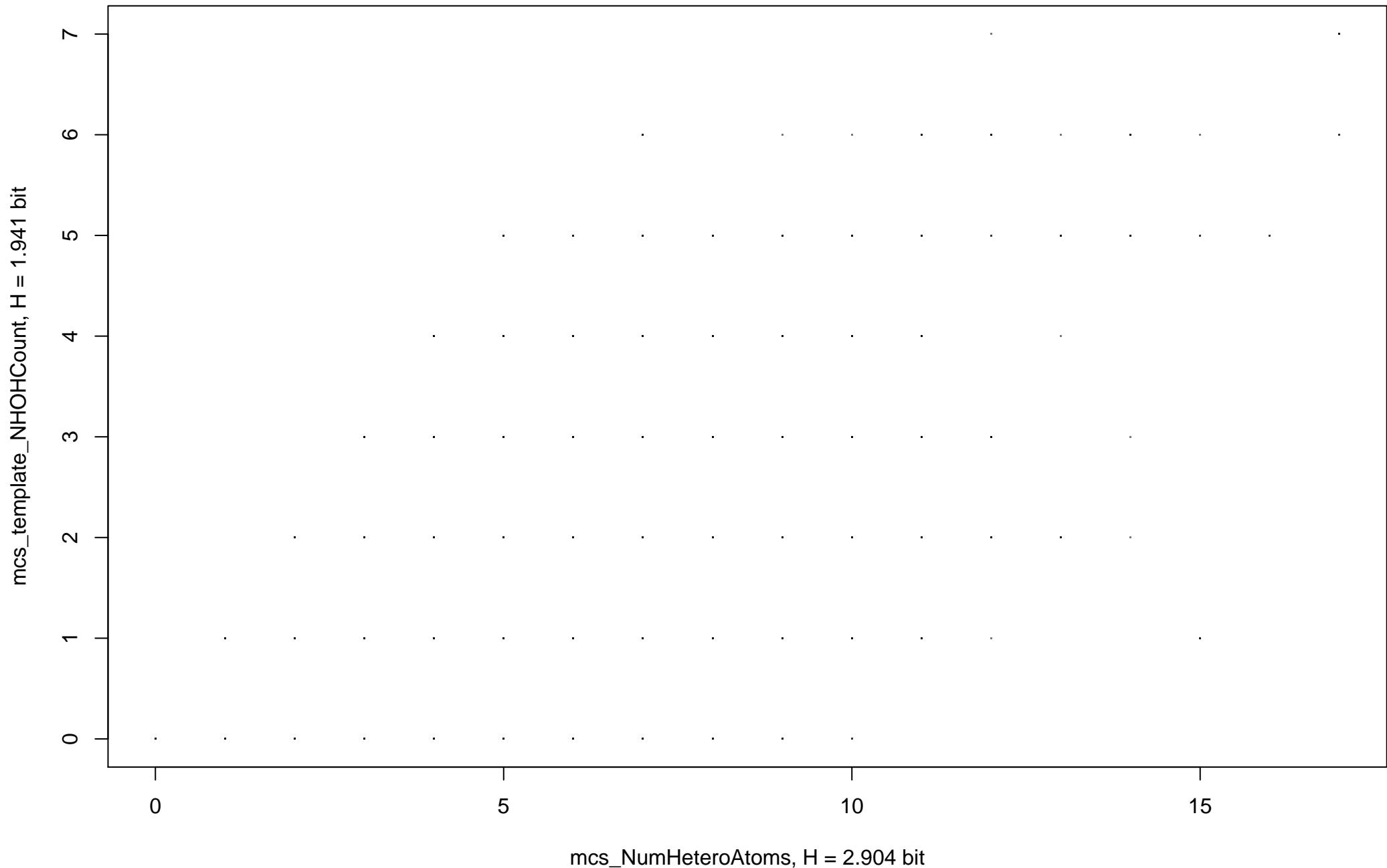
template_NumRotatableBonds-mcs_template_NumRotatableBonds, MI = 0.7054 bit, normMI = 0.2262



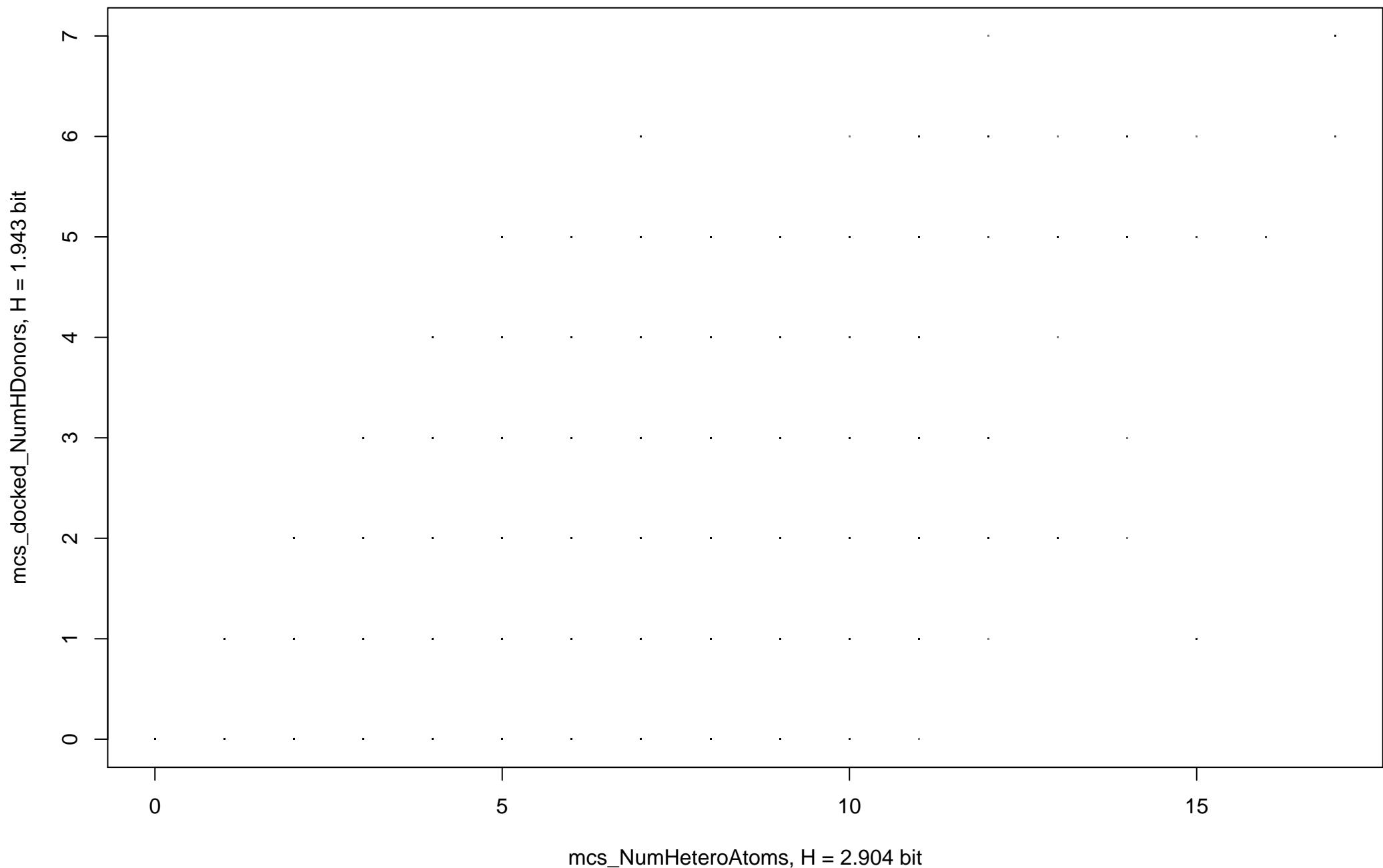
mcs_NumHeteroAtoms-mcs_template_NumHDonors, MI = 0.4177 bit, normMI = 0.2152



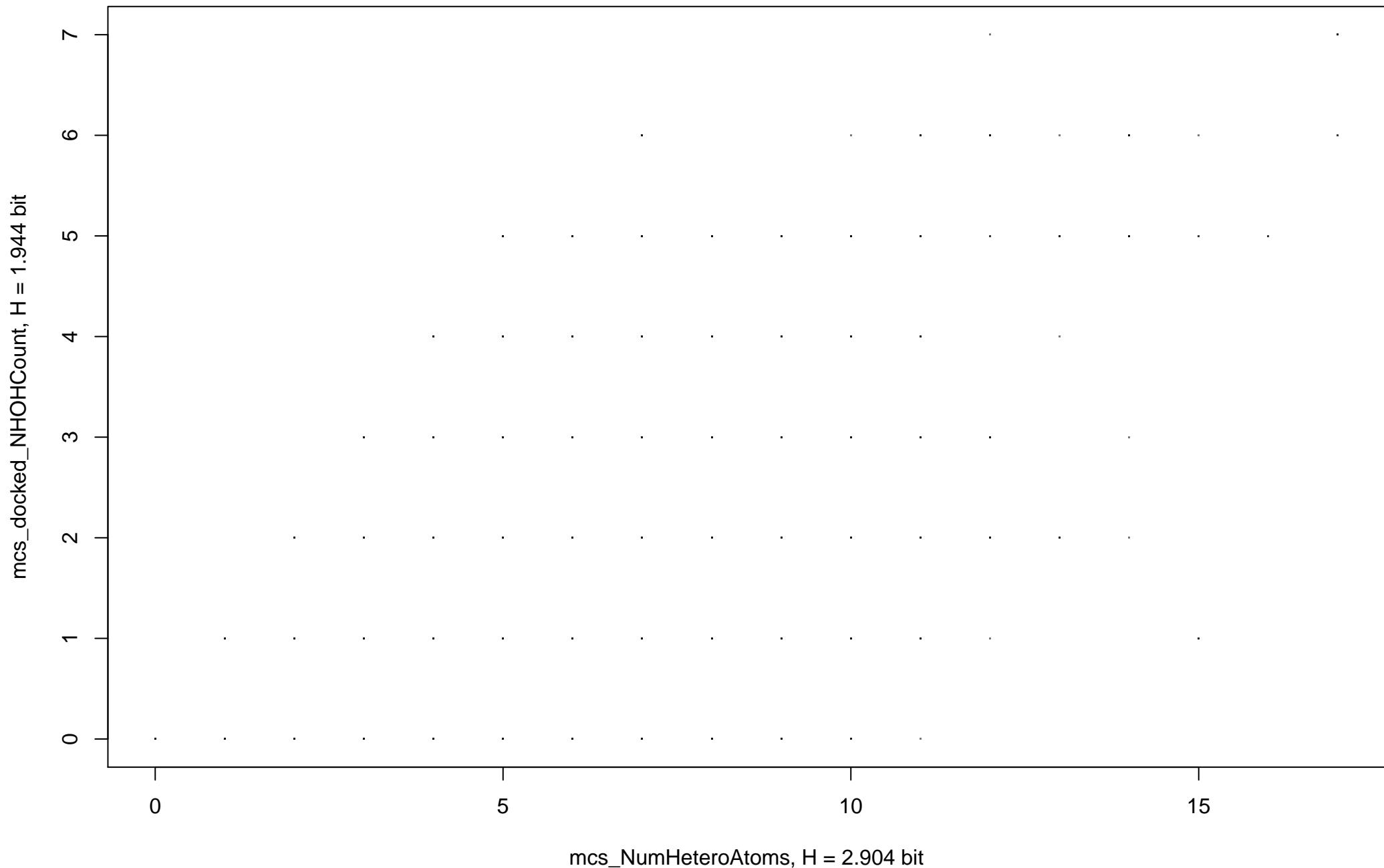
mcs_NumHeteroAtoms-mcs_template_NHOHCount, MI = 0.4176 bit, normMI = 0.2151



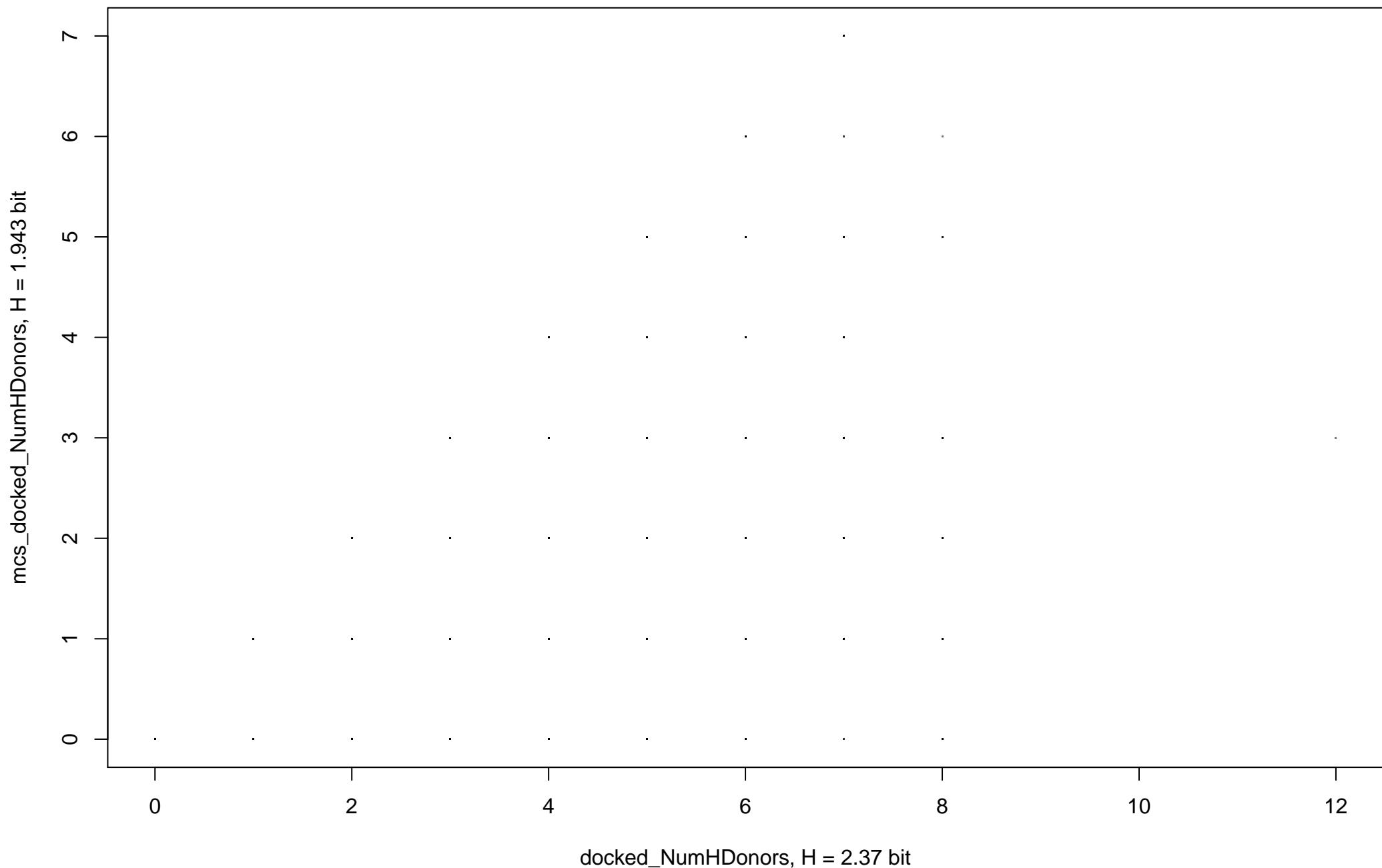
mcs_NumHeteroAtoms-mcs_docked_NumHDonors, MI = 0.4119 bit, normMI = 0.2119



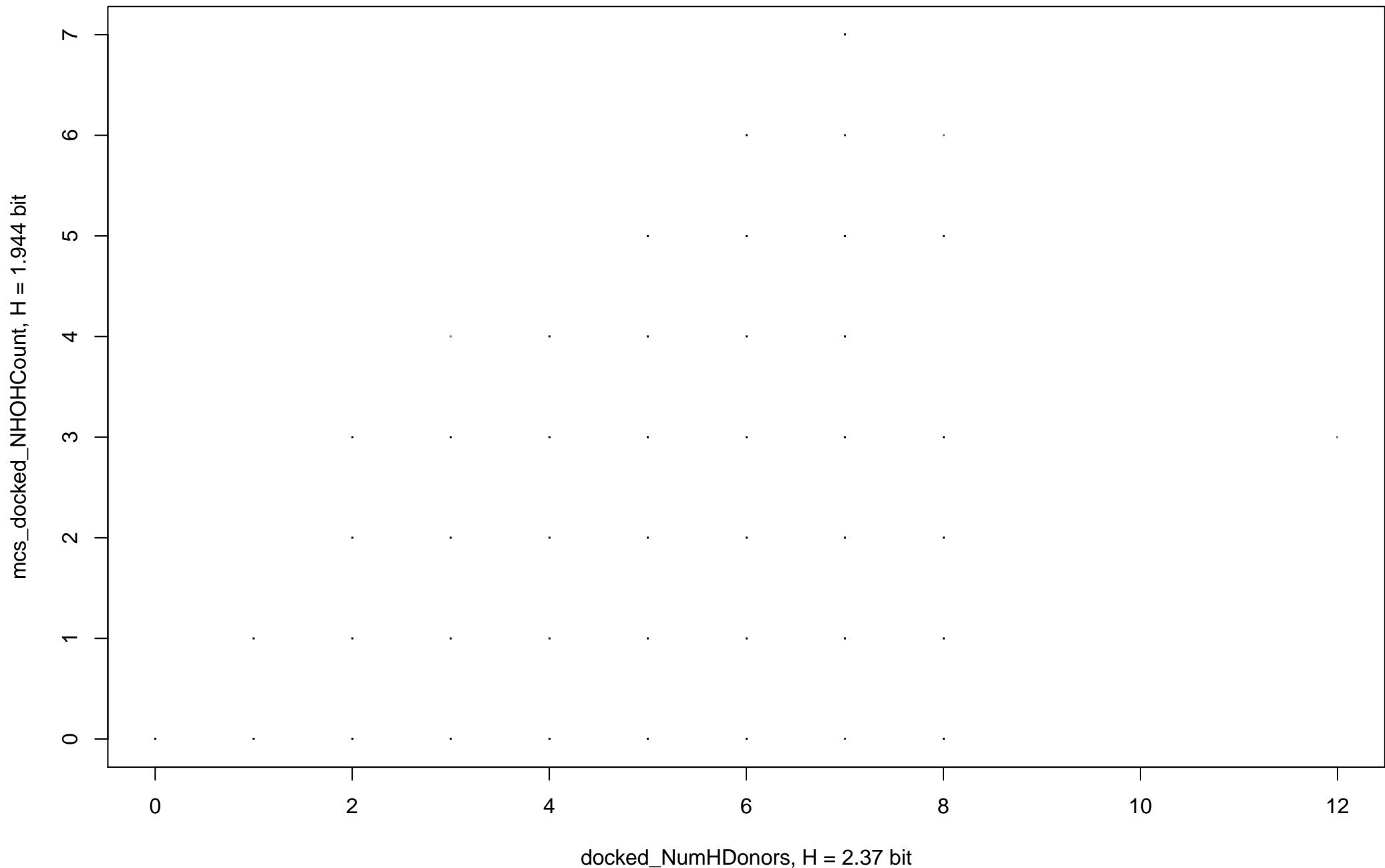
mcs_NumHeteroAtoms-mcs_docked_NHOHCount, MI = 0.4117 bit, normMI = 0.2118



docked_NumHDonors-mcs_docked_NumHDonors, MI = 0.3818 bit, normMI = 0.1965

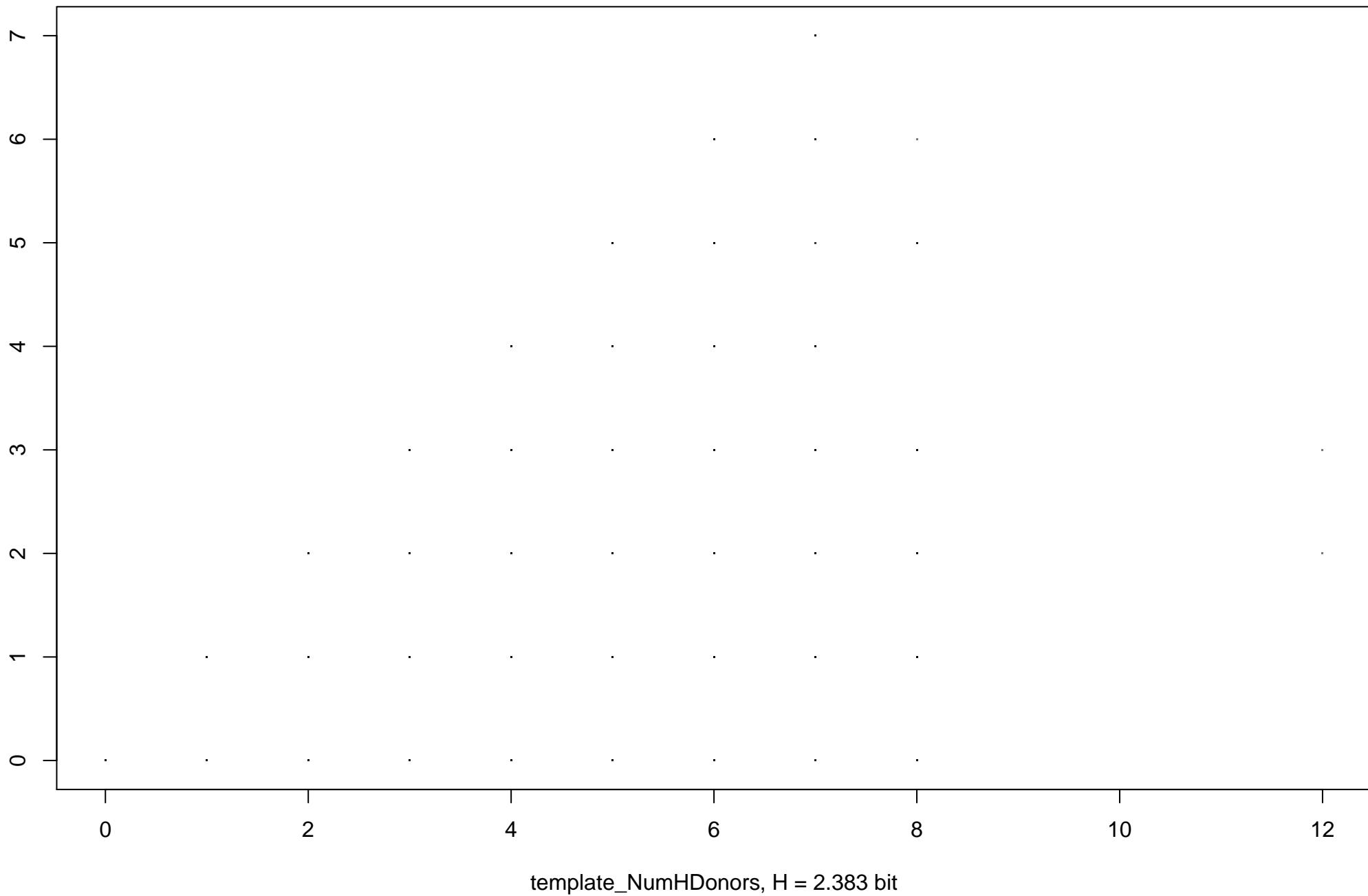


docked_NumHDonors-mcs_docked_NHOHCount, MI = 0.3802 bit, normMI = 0.1956

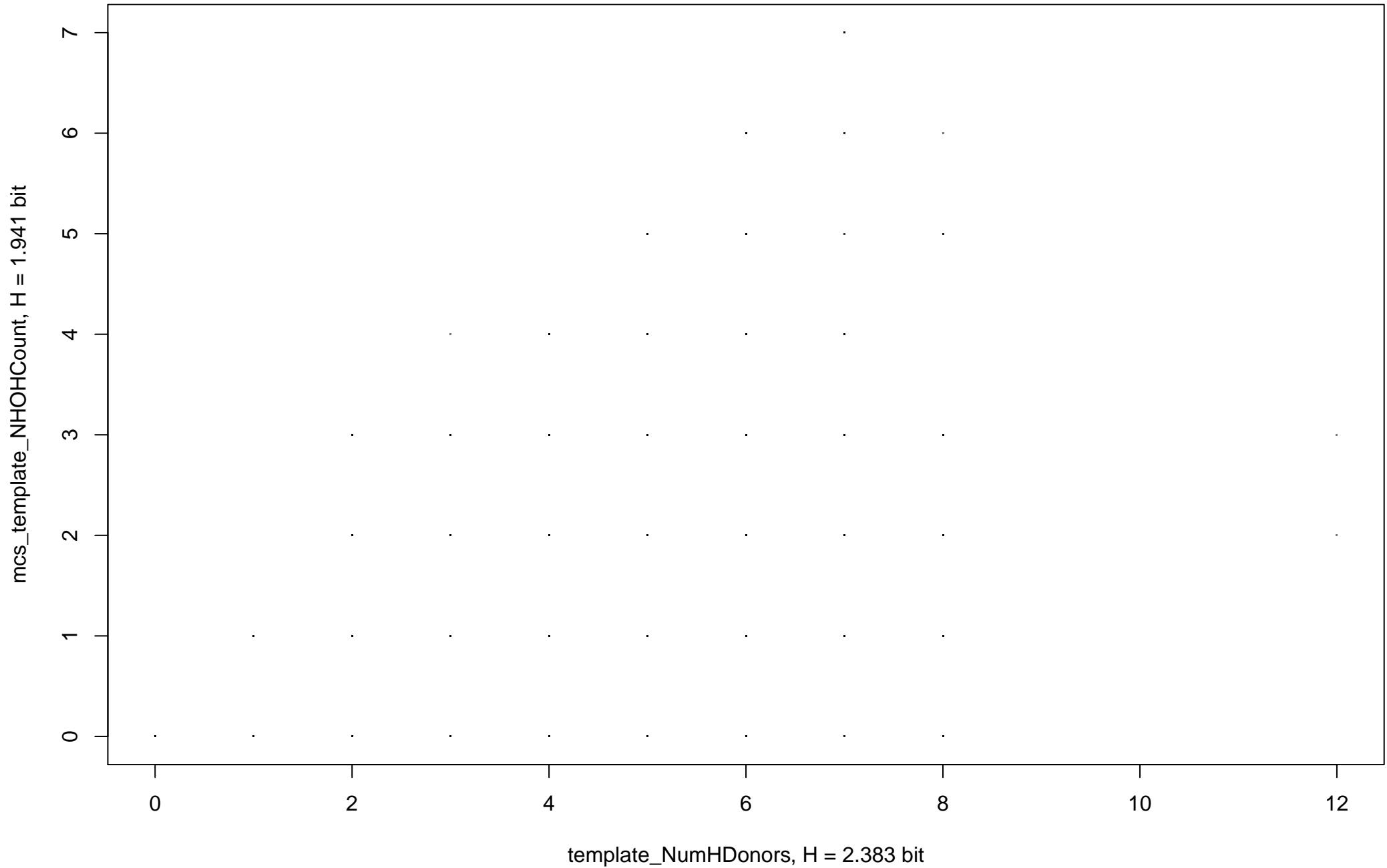


template_NumHDonors-mcs_template_NumHDonors, MI = 0.3652 bit, normMI = 0.1882

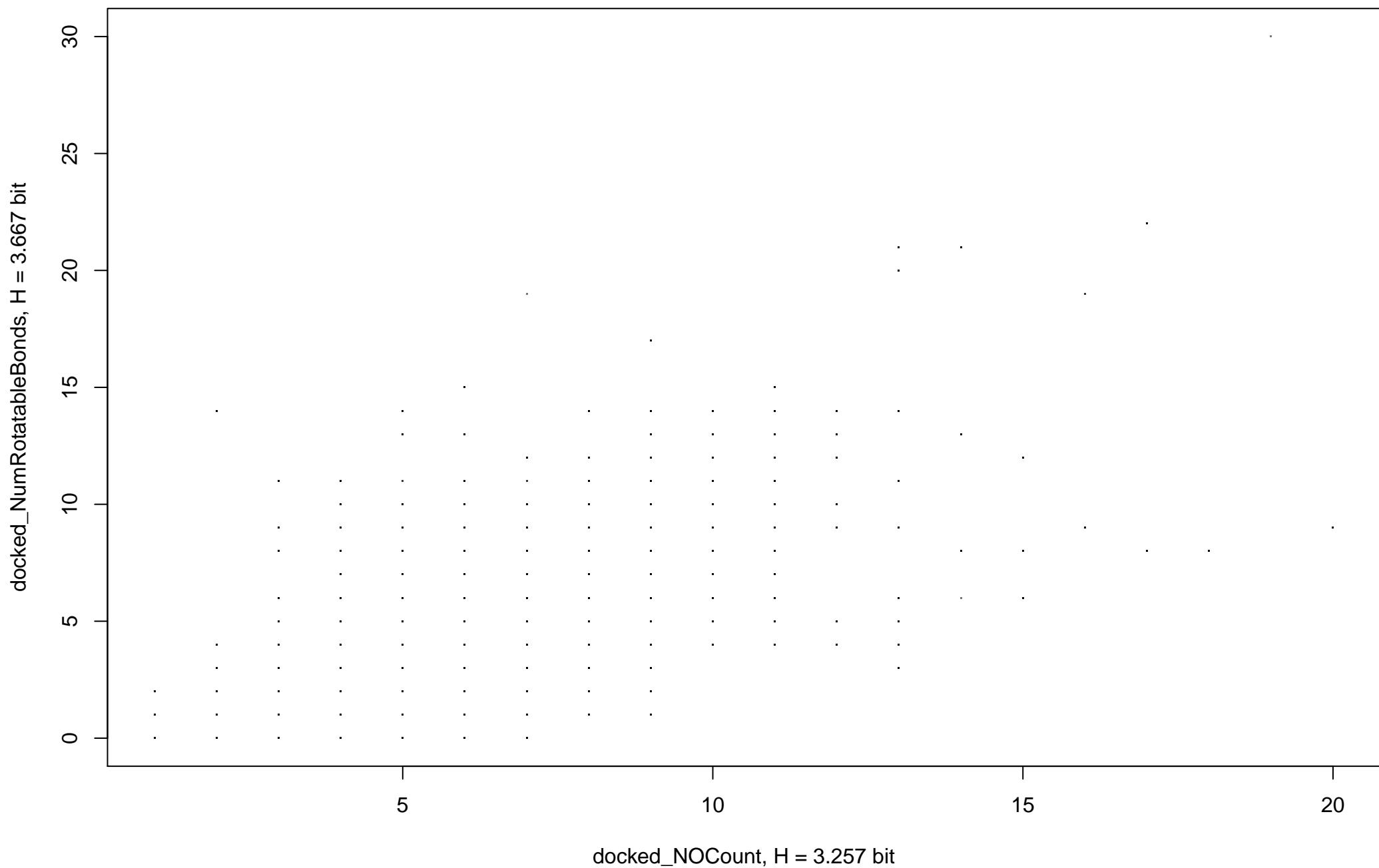
mcs_template_NumHDonors, H = 1.941 bit



template_NumHDonors-mcs_template_NHOHCount, MI = 0.3633 bit, normMI = 0.1871

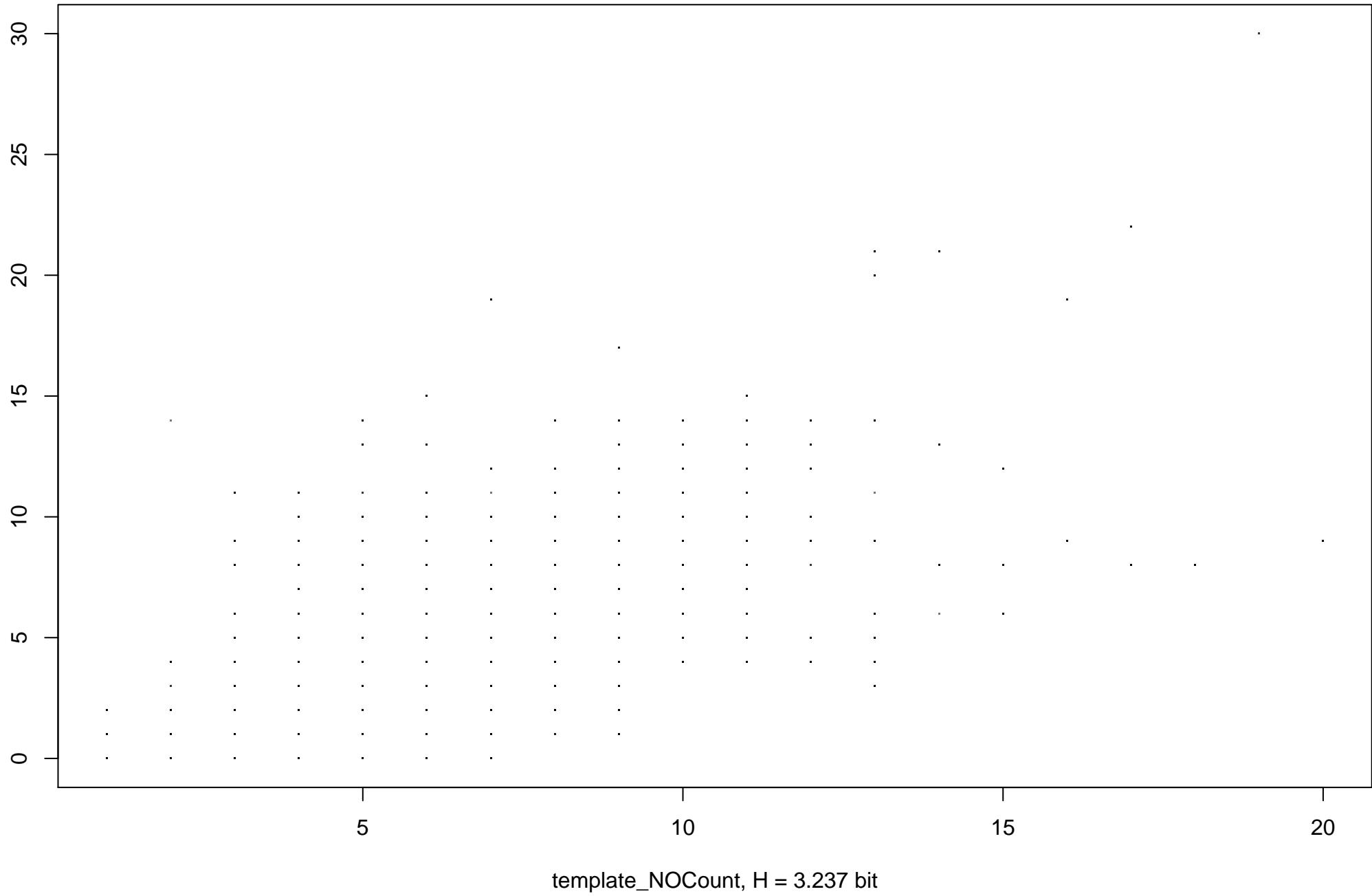


docked_NOCount-docked_NumRotatableBonds, MI = 0.596 bit, normMI = 0.183

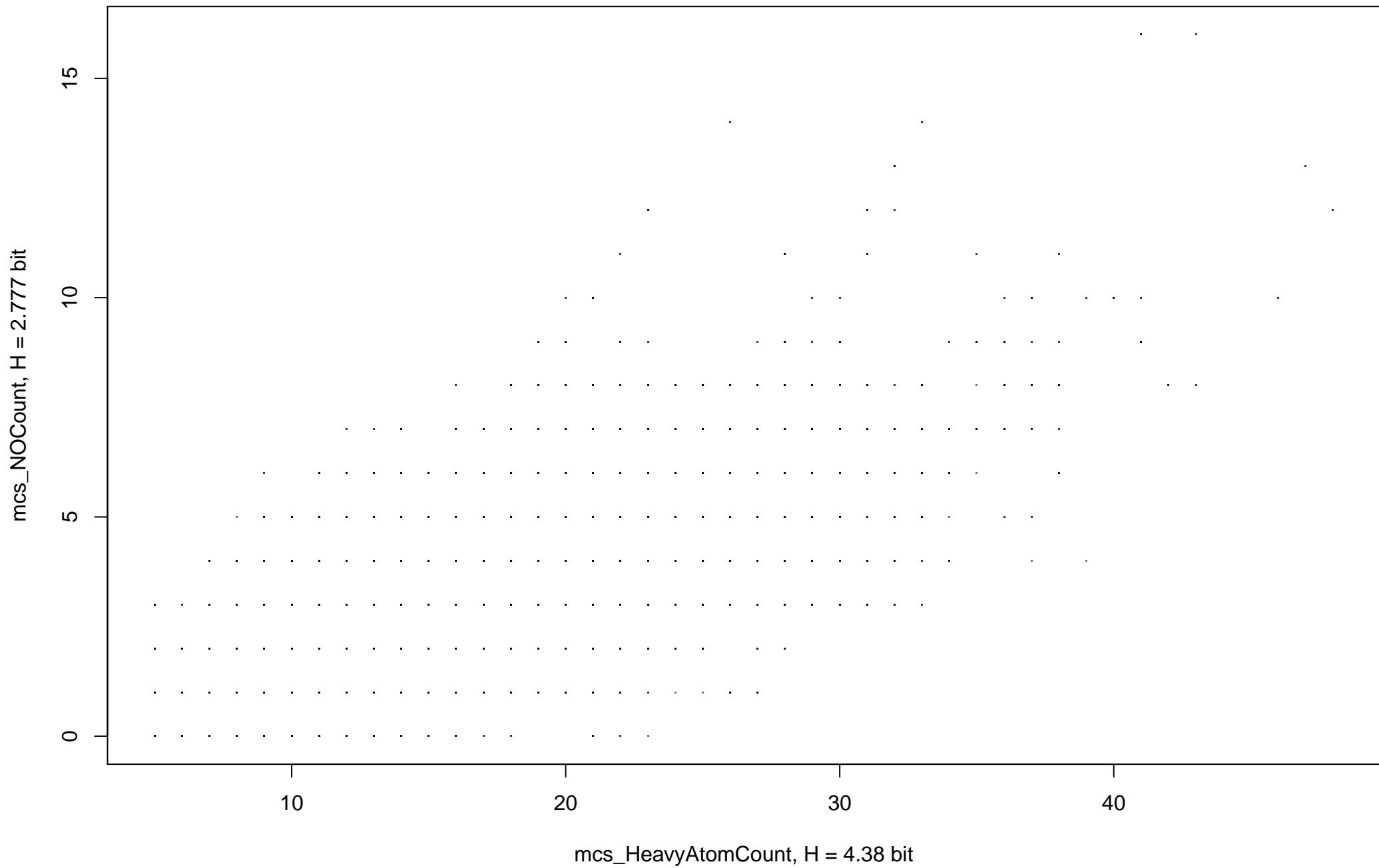


template_NOCount-template_NumRotatableBonds, MI = 0.5883 bit, normMI = 0.1818

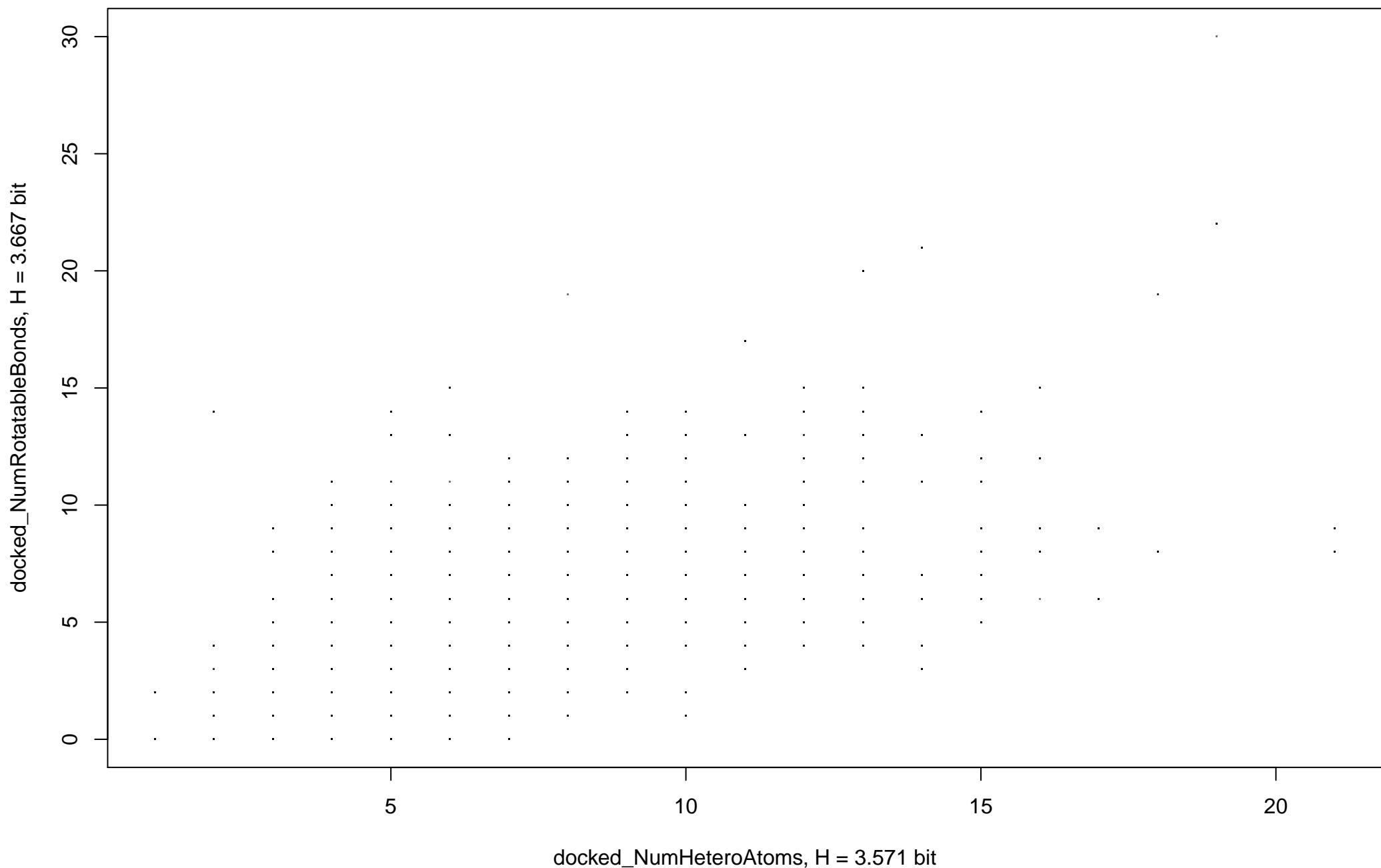
template_NumRotatableBonds, H = 3.668 bit



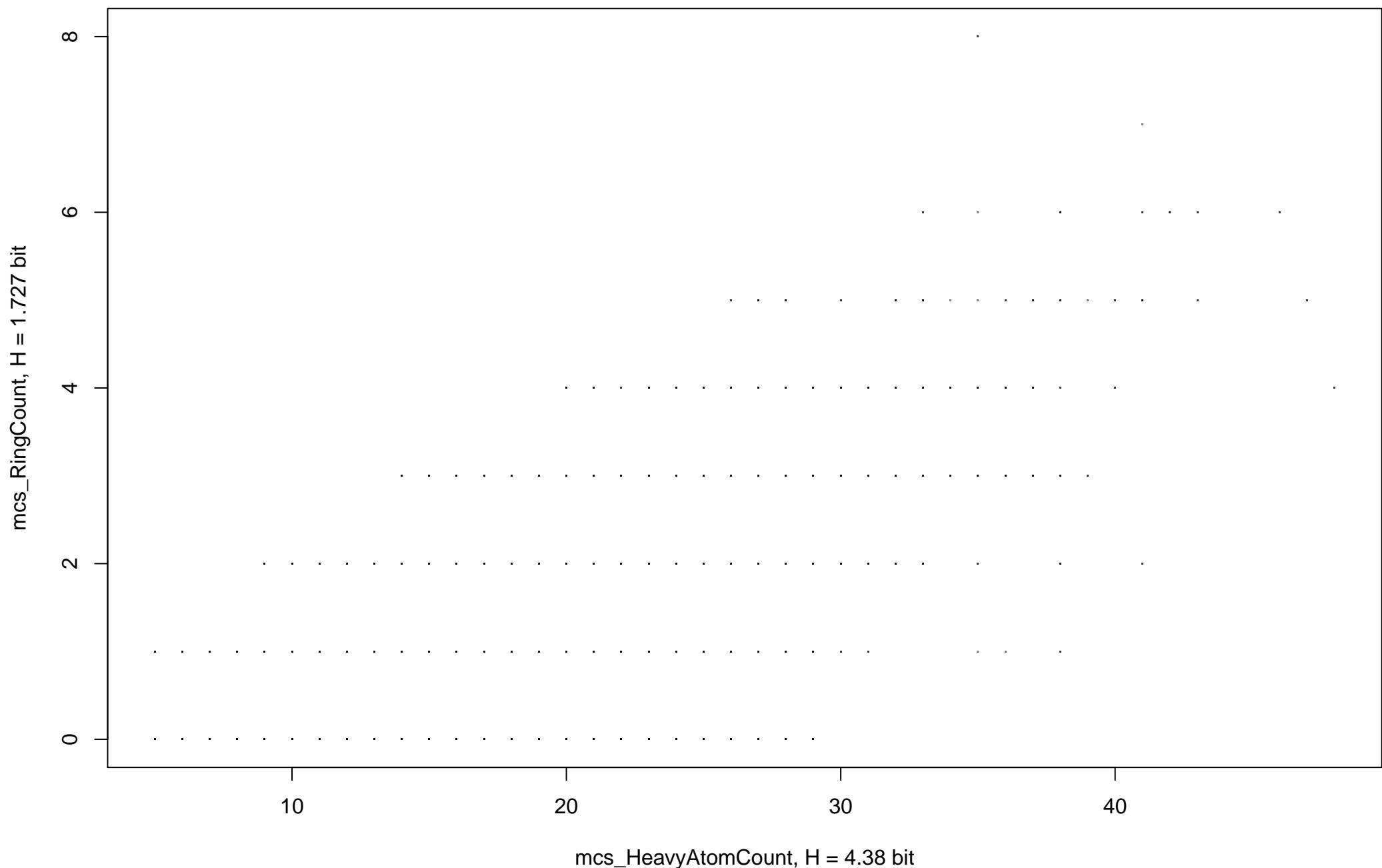
mcs_HeavyAtomCount-mcs_NOCount, MI = 0.5045 bit, normMI = 0.1817



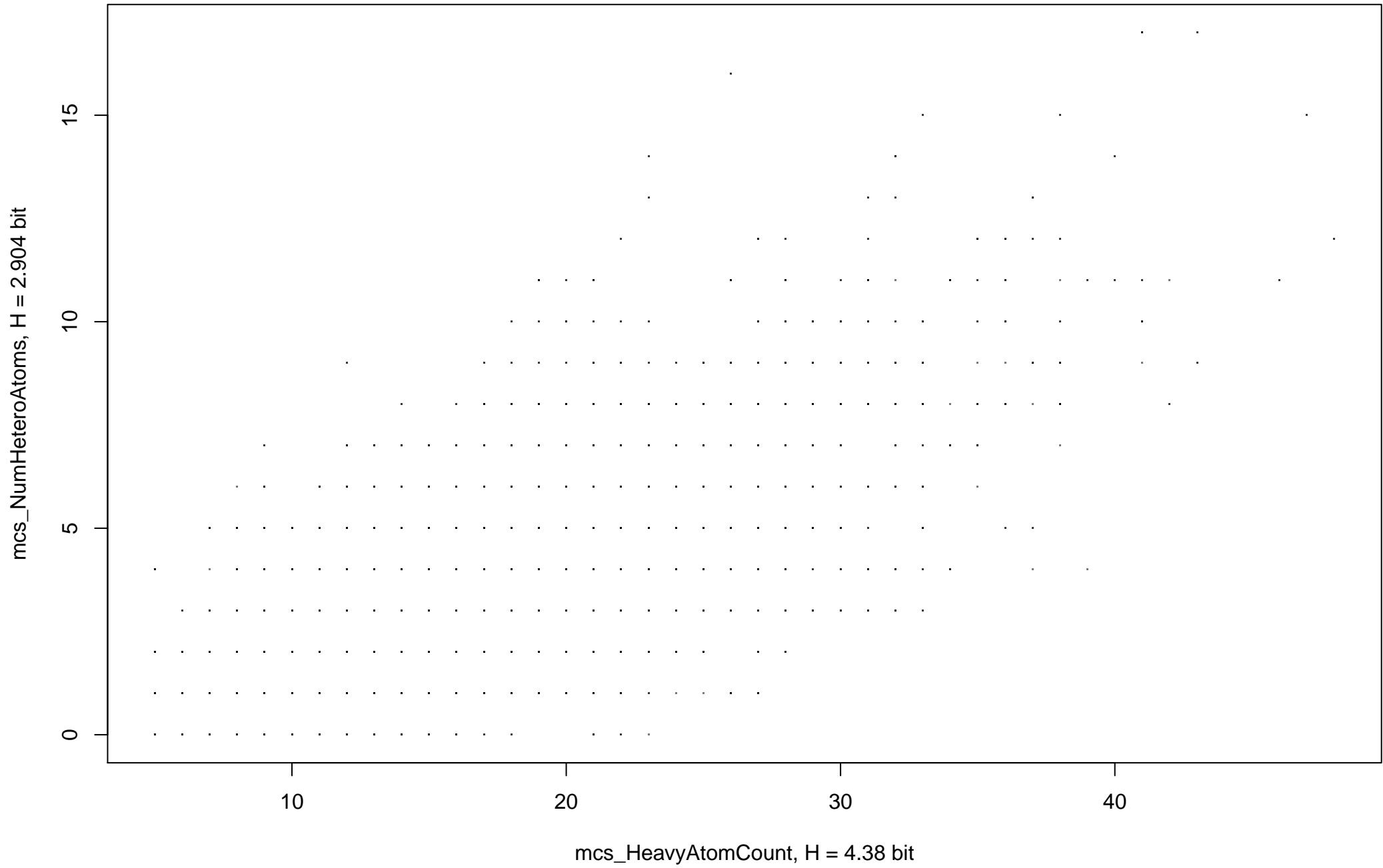
docked_NumHeteroAtoms–docked_NumRotatableBonds, MI = 0.633 bit, normMI = 0.1772



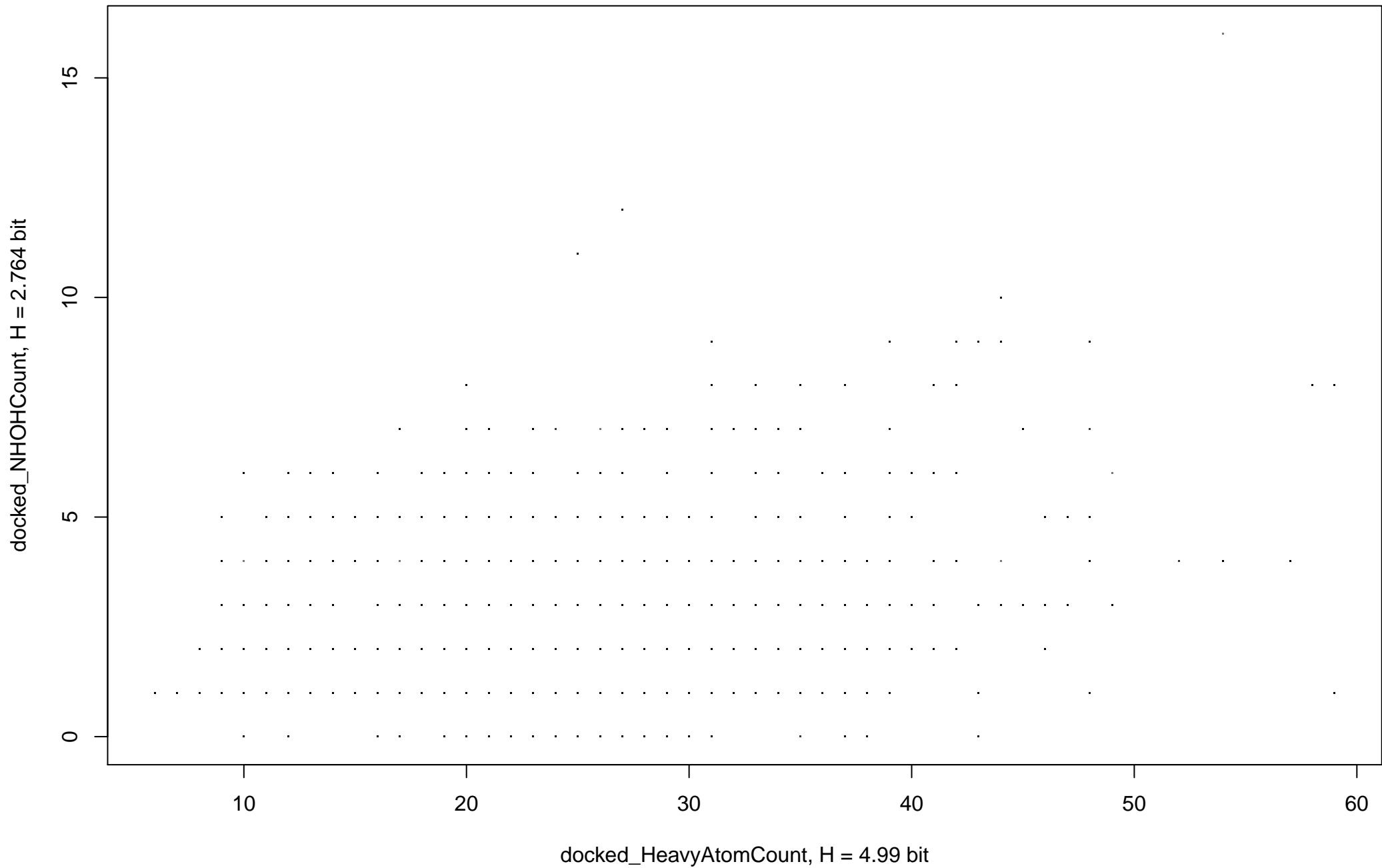
mcs_HeavyAtomCount–mcs_RingCount, MI = 0.3058 bit, normMI = 0.177



mcs_HeavyAtomCount–mcs_NumHeteroAtoms, MI = 0.5101 bit, normMI = 0.1756

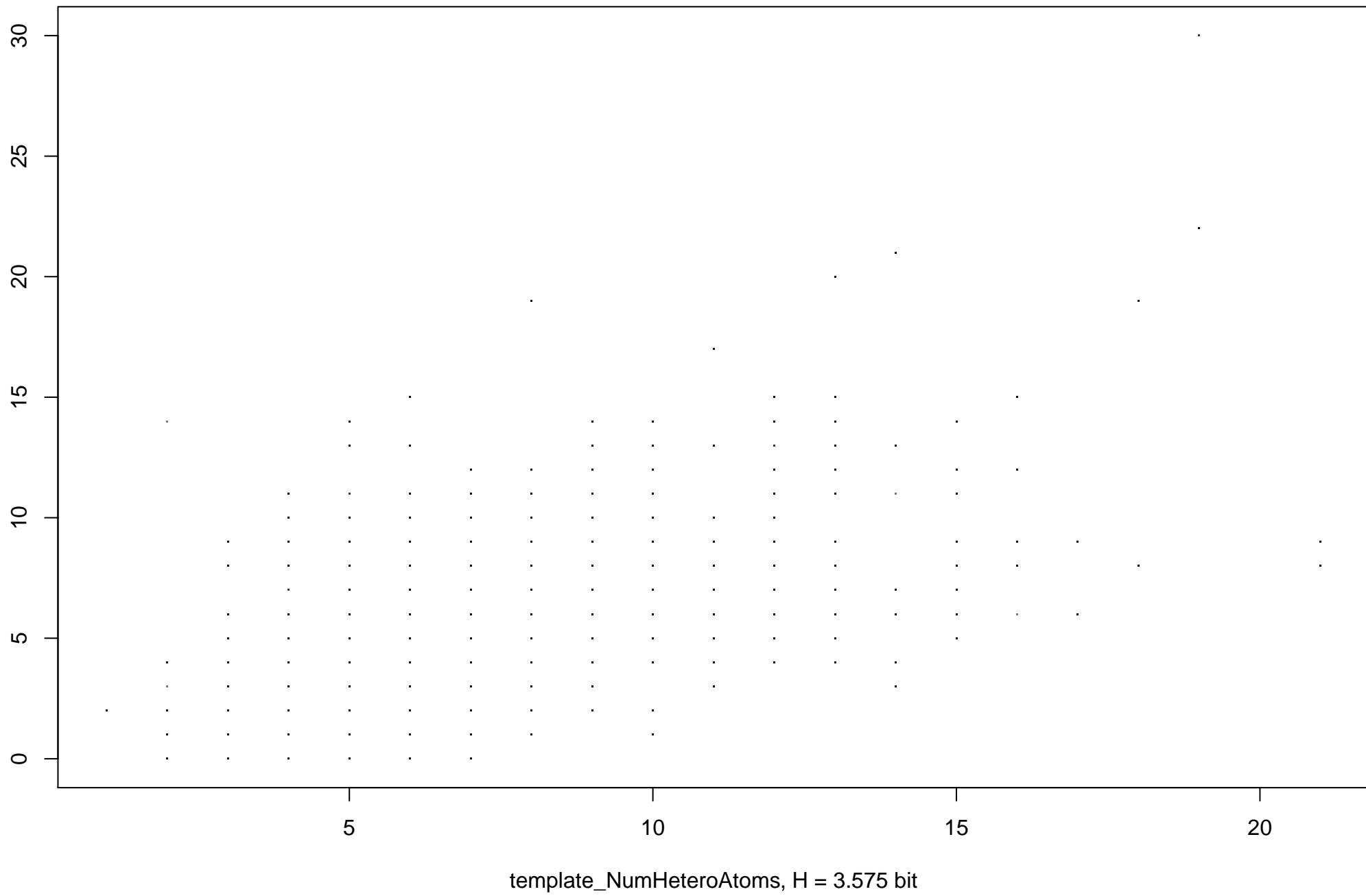


docked_HeavyAtomCount–docked_NHOHCount, MI = 0.4847 bit, normMI = 0.1754



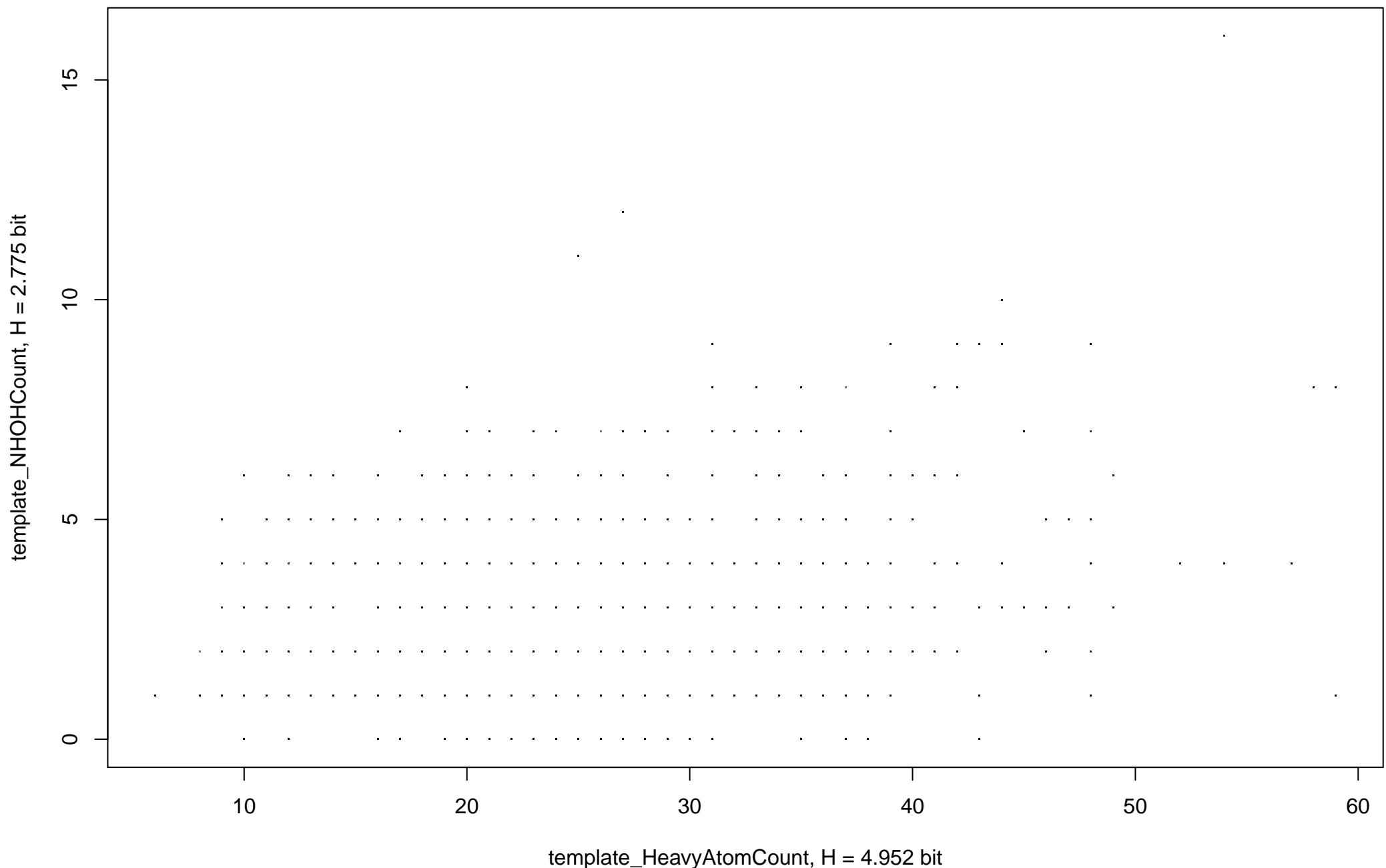
template_NumHeteroAtoms-template_NumRotatableBonds, MI = 0.6268 bit, normMI = 0.1753

template_NumRotatableBonds, H = 3.668 bit

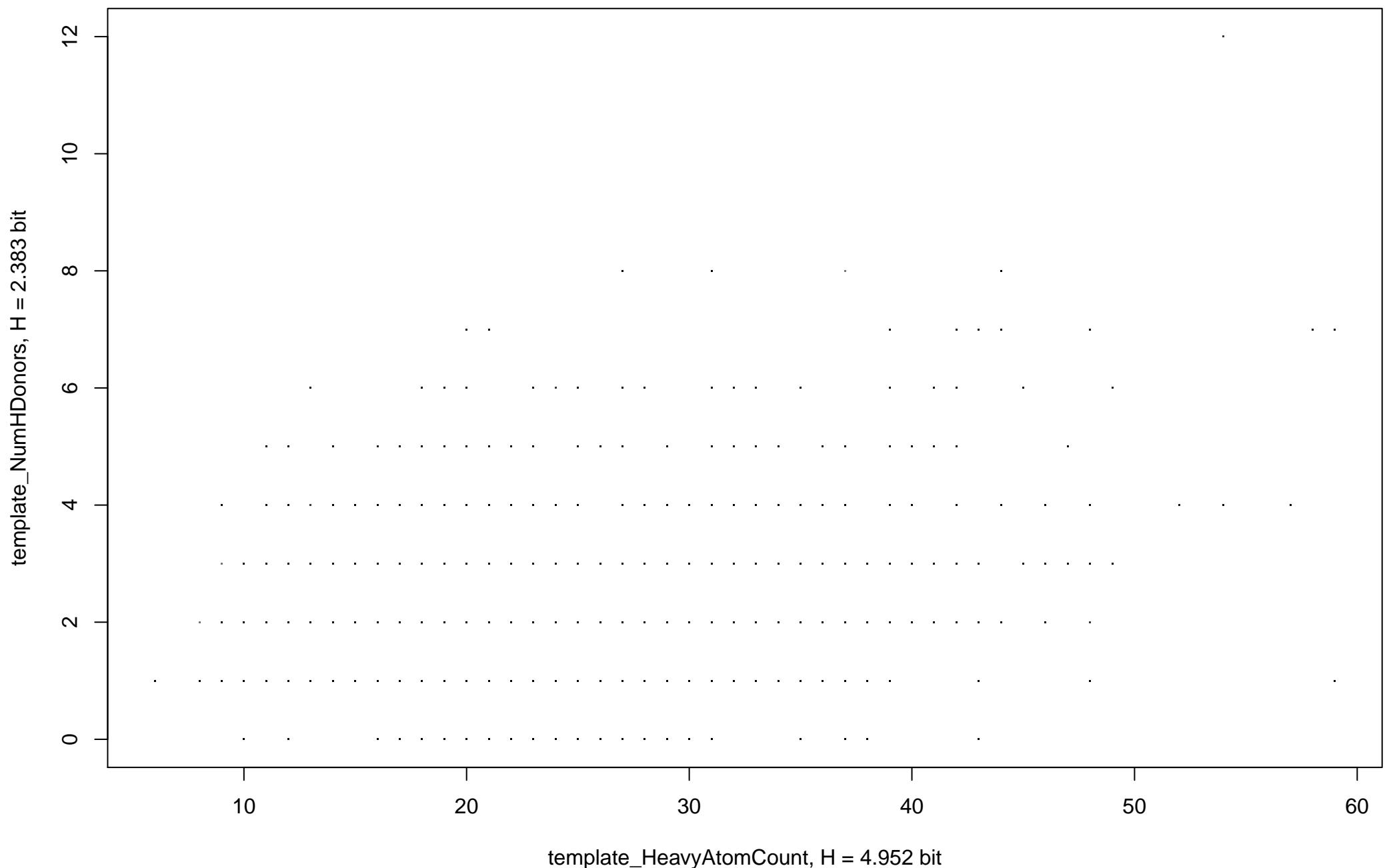


template_NumHeteroAtoms, H = 3.575 bit

template_HeavyAtomCount-template_NHOHCount, MI = 0.4829 bit, normMI = 0.174

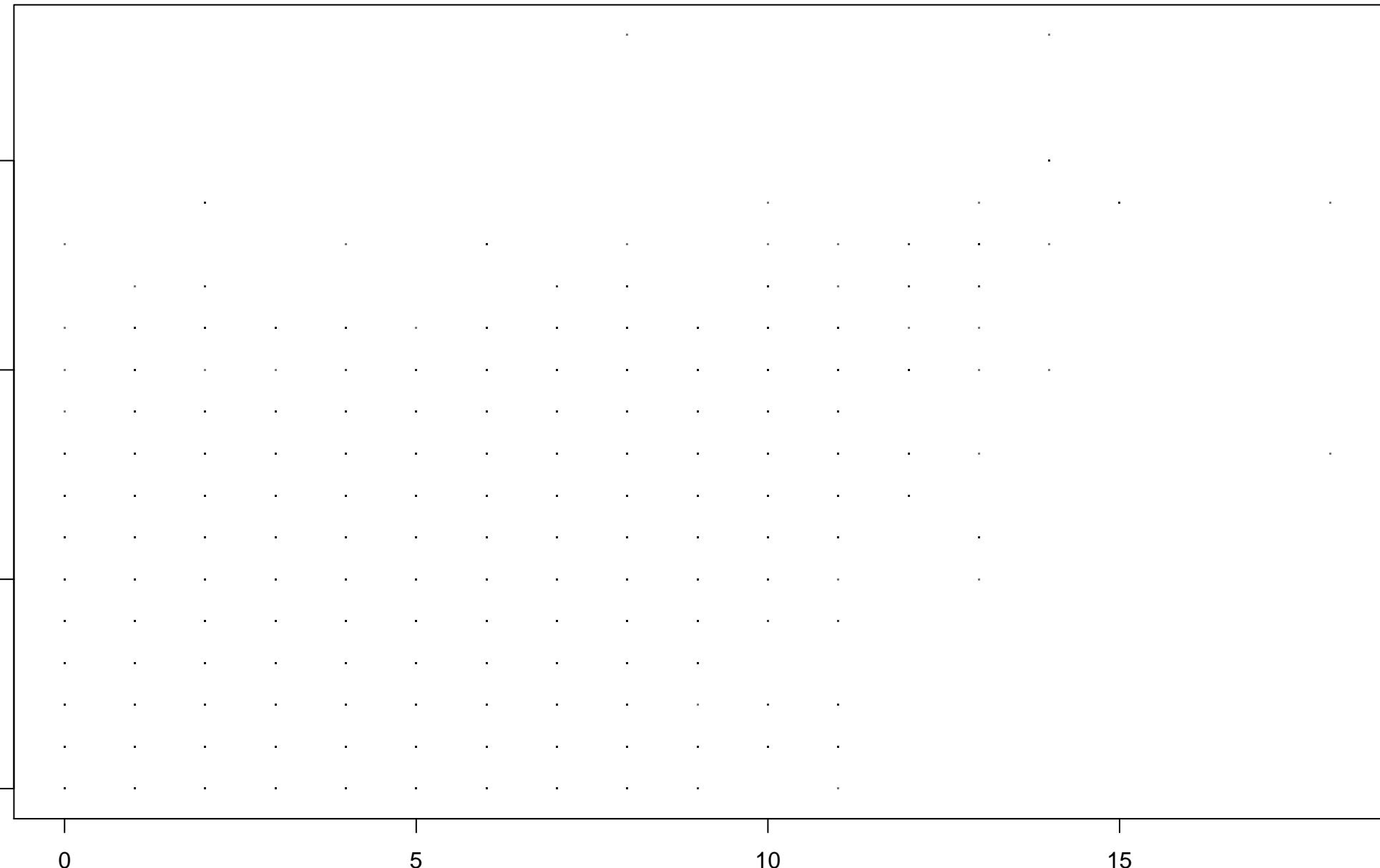


template_HeavyAtomCount-template_NumHDonors, MI = 0.4017 bit, normMI = 0.1686



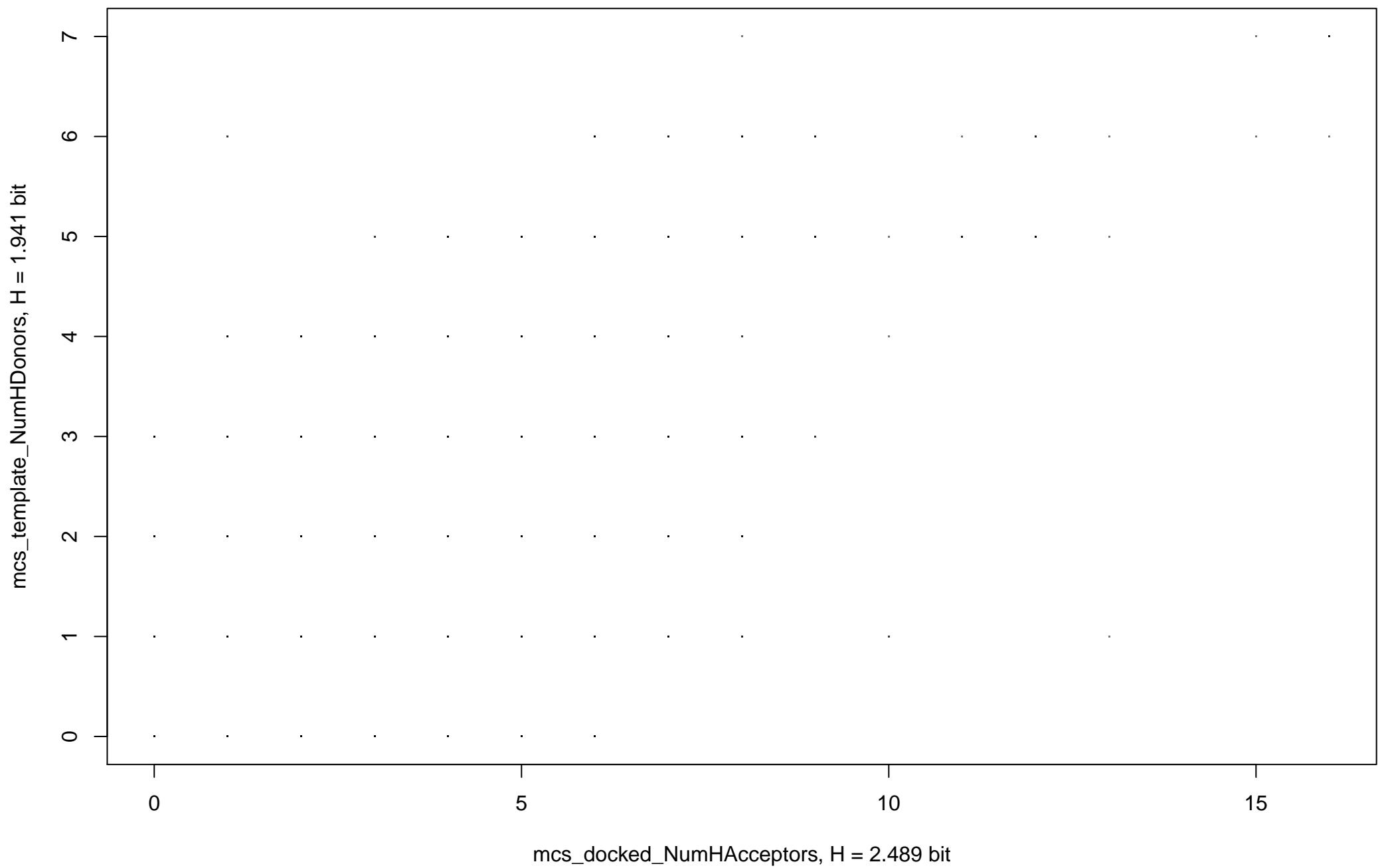
mcs_template_NumRotatableBonds–mcs_docked_NumRotatableBonds, MI = 0.5198 bit, normMI = 0.1668

mcs_docked_NumRotatableBonds, H = 3.117 bit

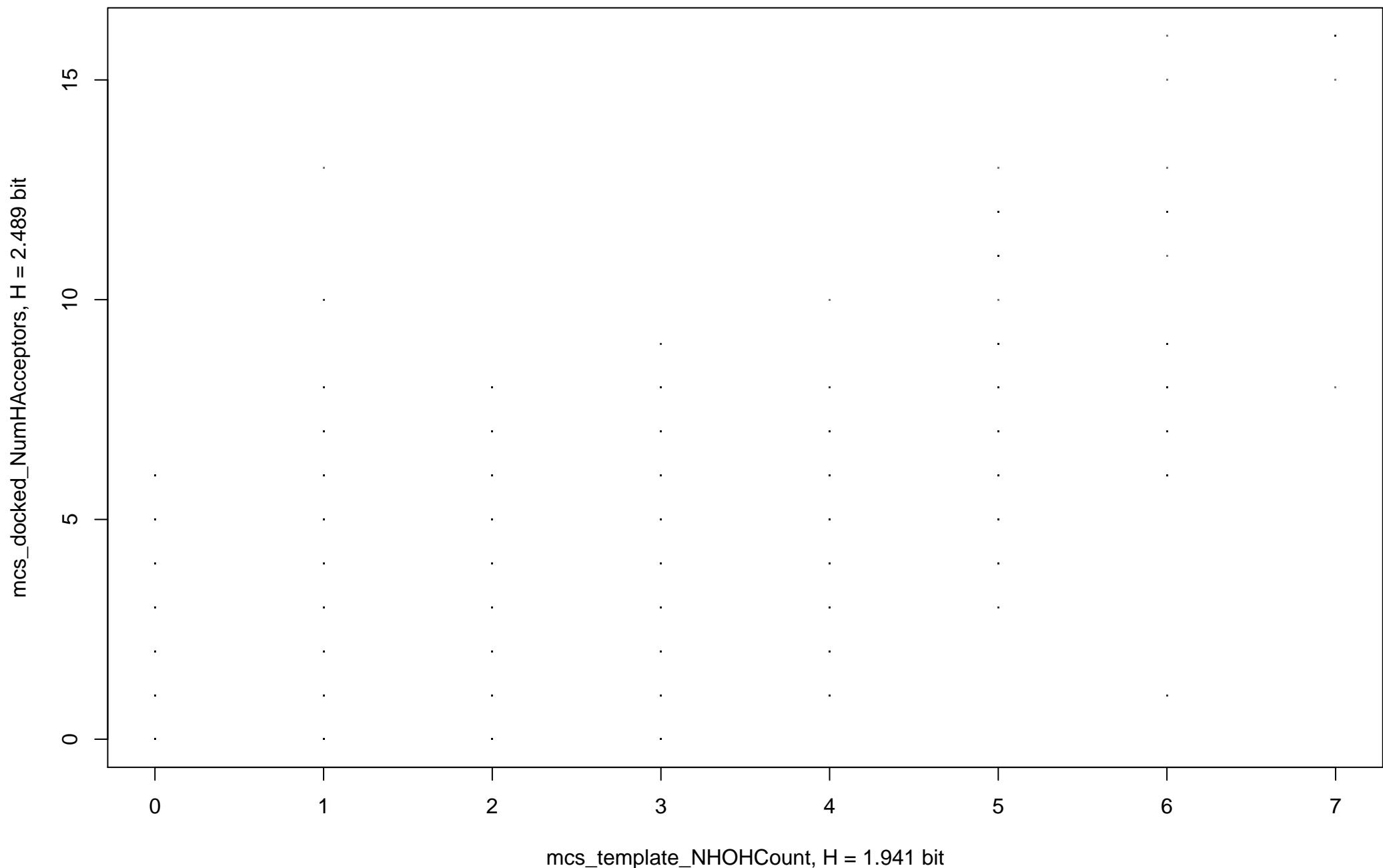


mcs_template_NumRotatableBonds, H = 3.118 bit

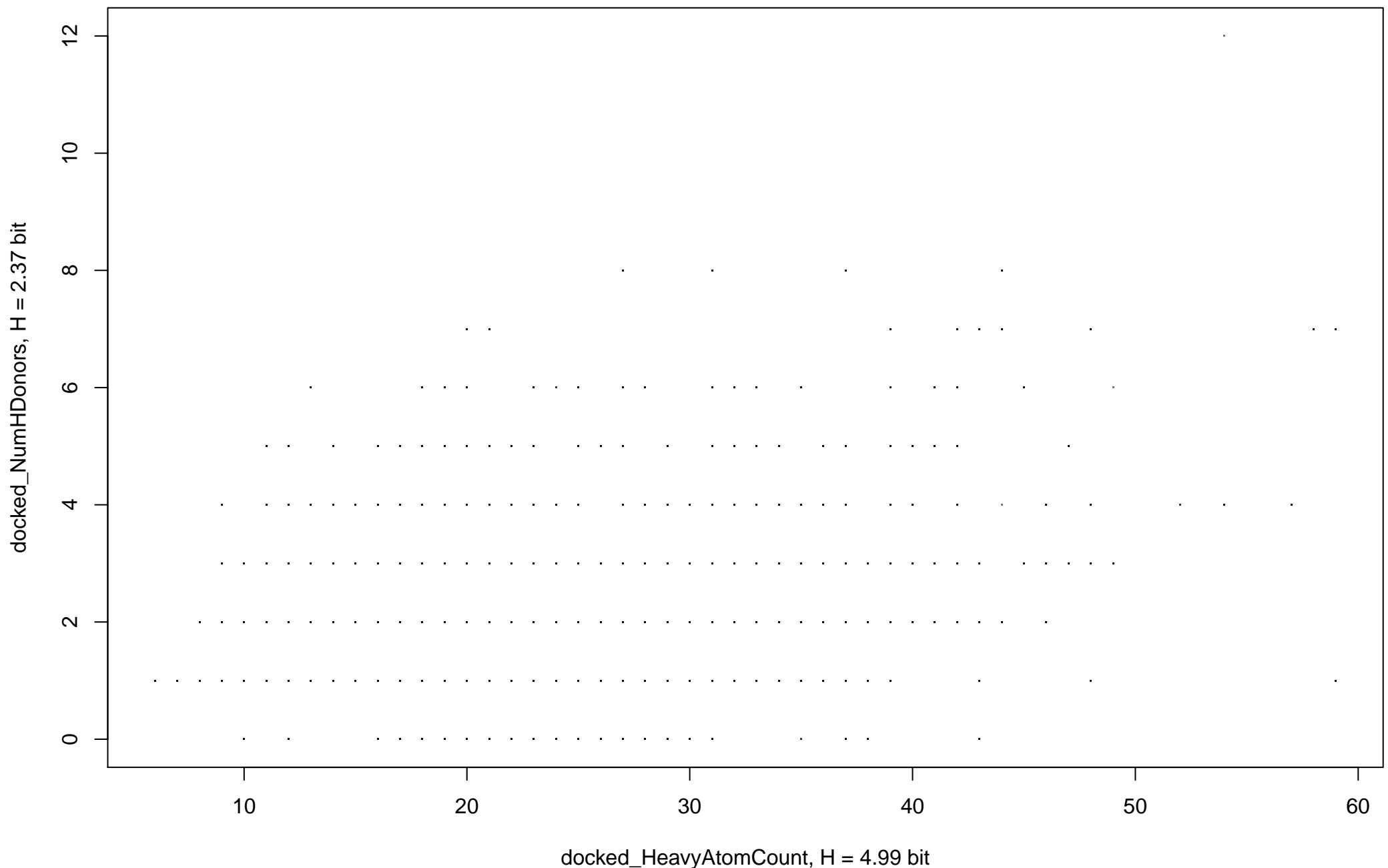
mcs_docked_NumHAcceptors–mcs_template_NumHDonors, MI = 0.3195 bit, normMI = 0.1646



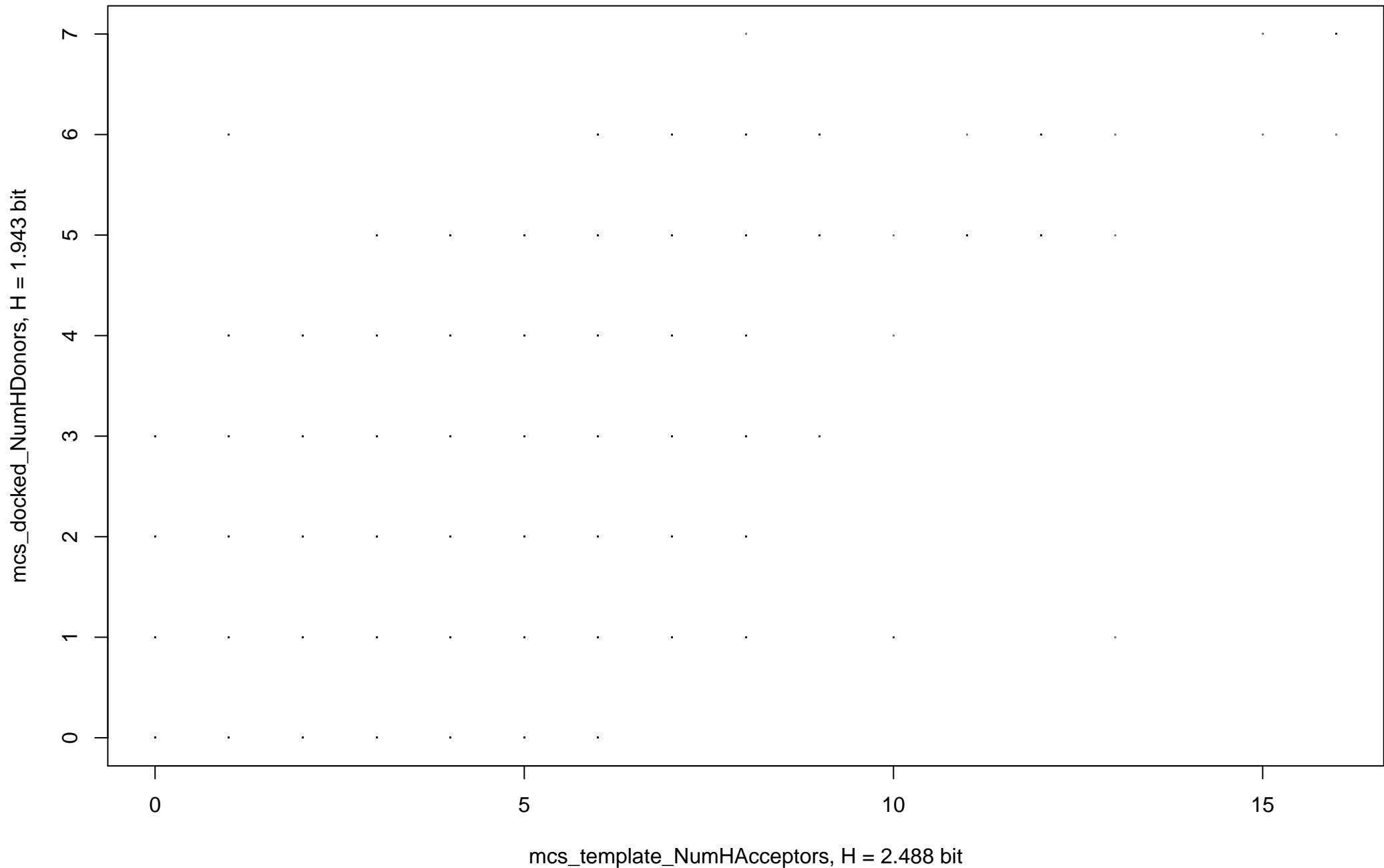
mcs_template_NHOHCount-mcs_docked_NumHAcceptors, MI = 0.319 bit, normMI = 0.1643



docked_HeavyAtomCount-docked_NumHDonors, MI = 0.3872 bit, normMI = 0.1634

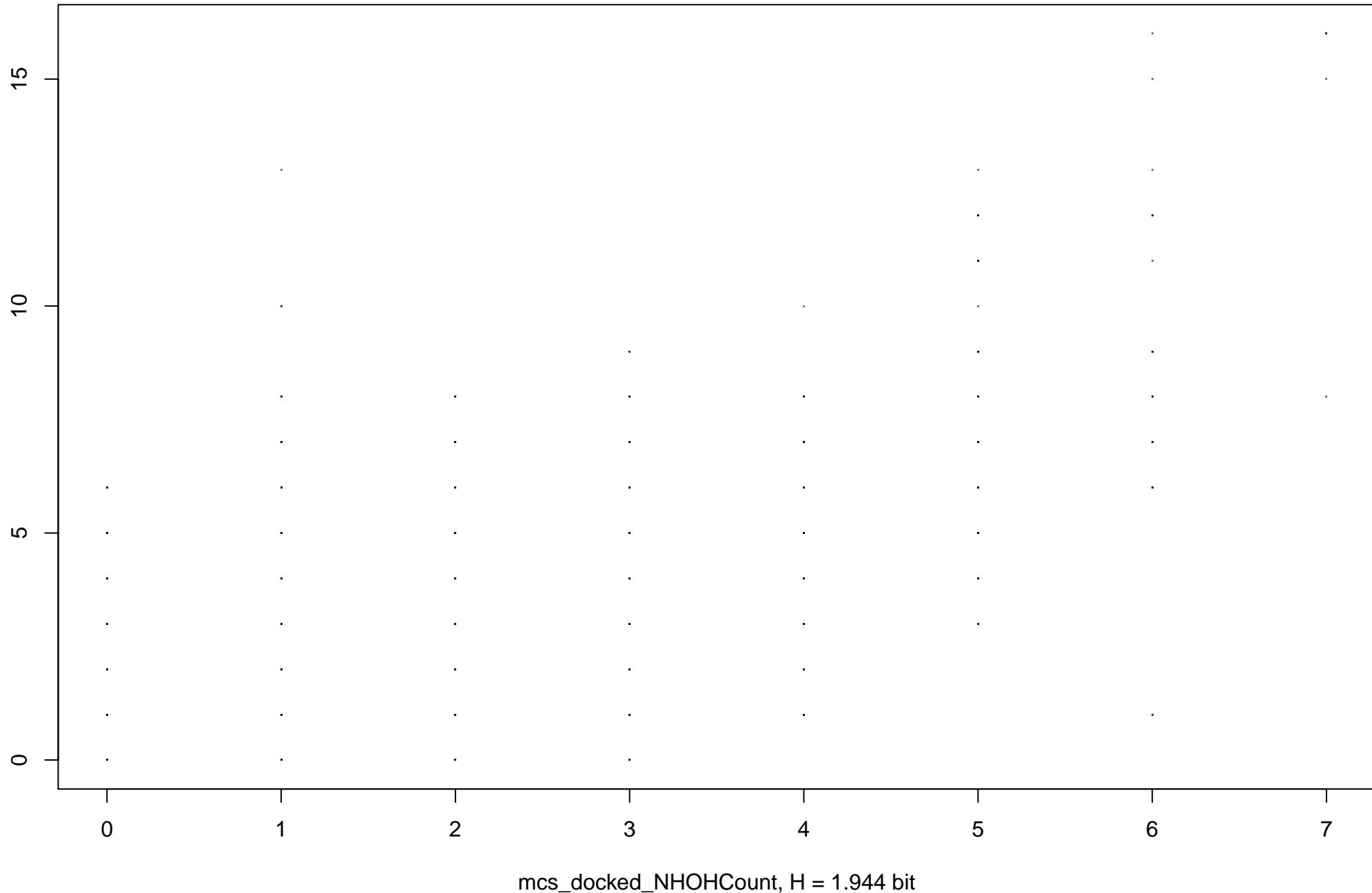


mcs_template_NumHAcceptors-mcs_docked_NumHDonors, MI = 0.3139 bit, normMI = 0.1616

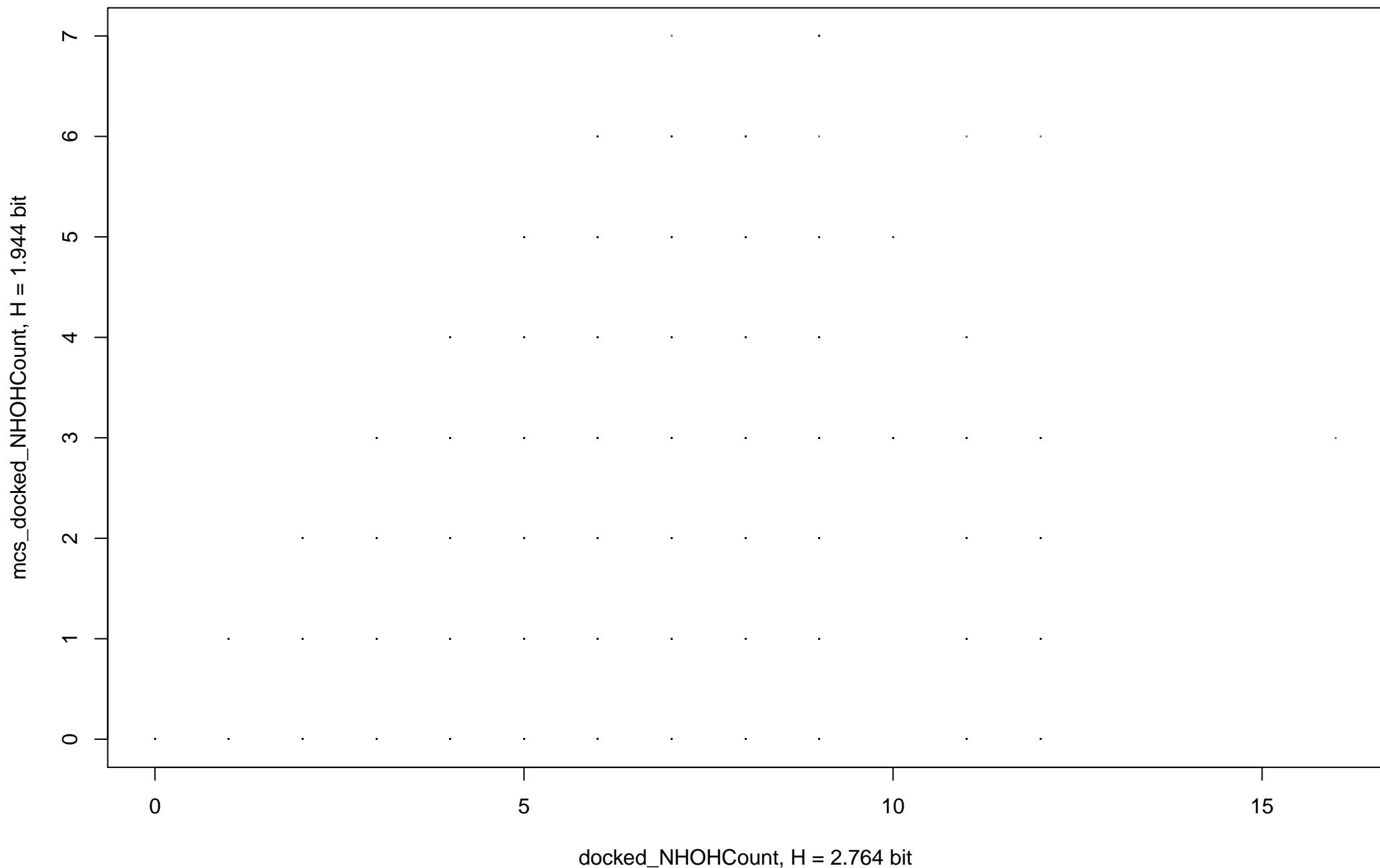


mcs_docked_NHOHCount-mcs_template_NumHAcceptors, MI = 0.3134 bit, normMI = 0.1612

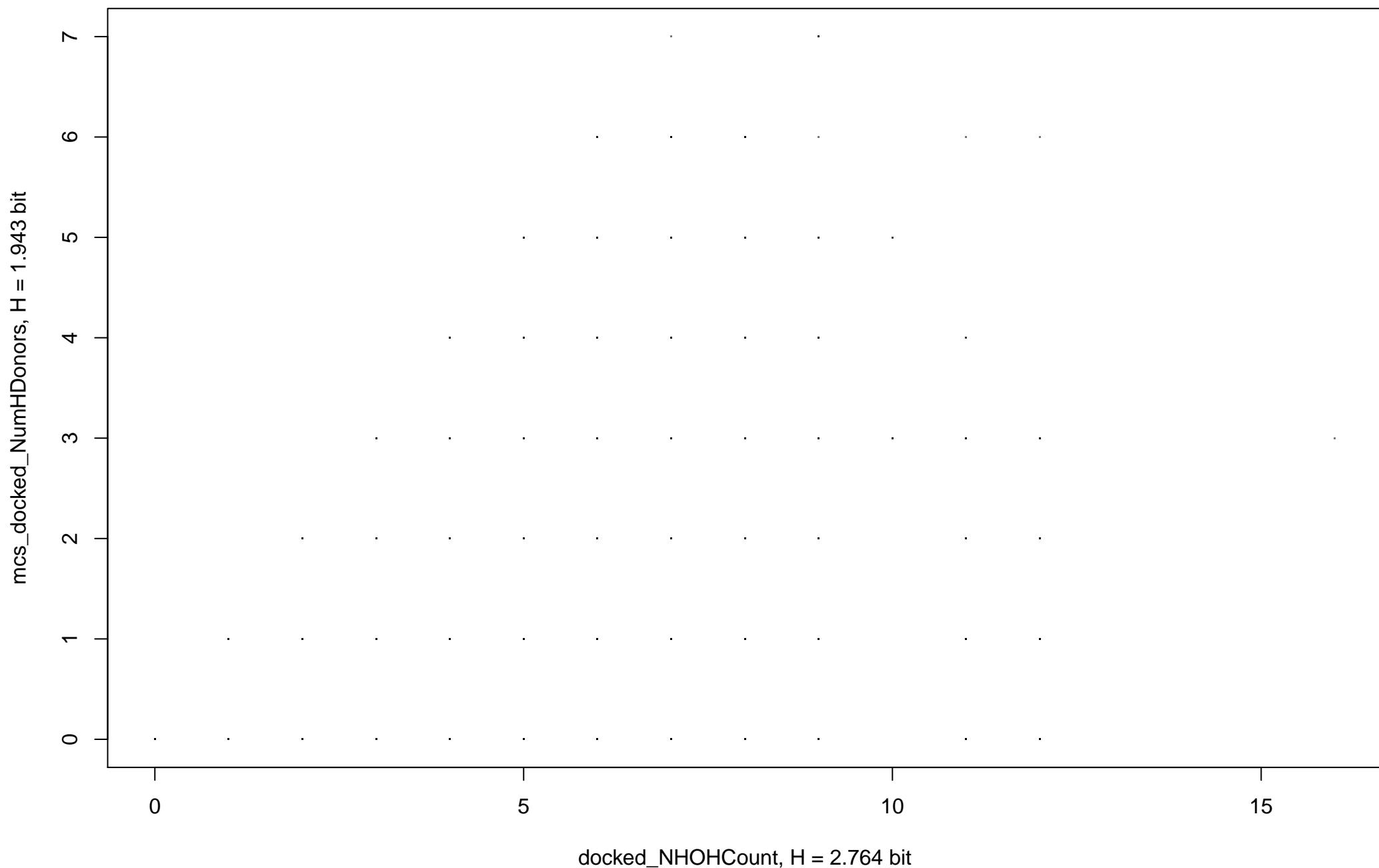
mcs_template_NumHAcceptors, H = 2.488 bit



docked_NHOHCount-mcs_docked_NHOHCount, MI = 0.3125 bit, normMI = 0.1608

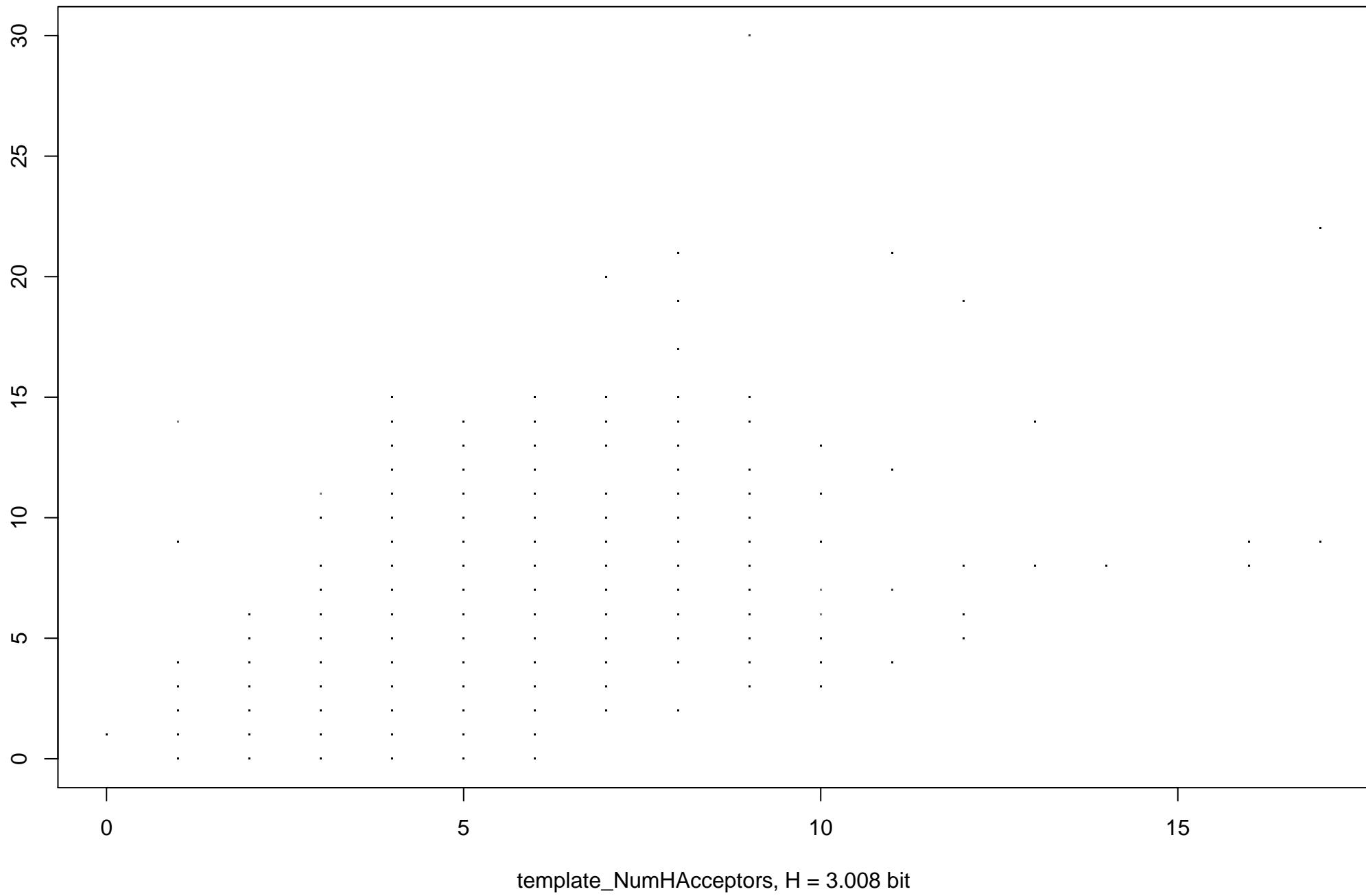


docked_NHOHCount-mcs_docked_NumHDonors, MI = 0.312 bit, normMI = 0.1606

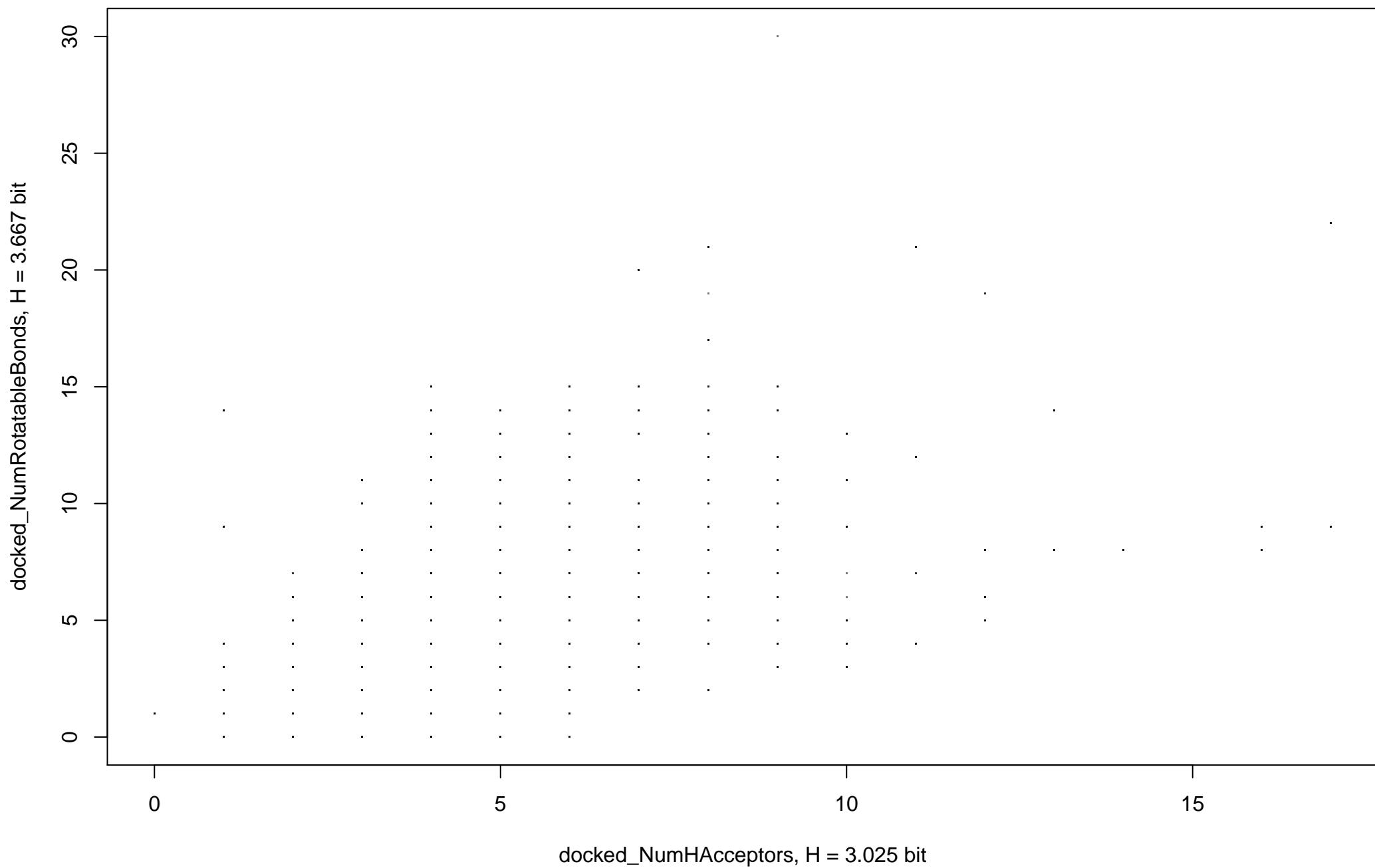


template_NumHAcceptors-template_NumRotatableBonds, MI = 0.4756 bit, normMI = 0.1581

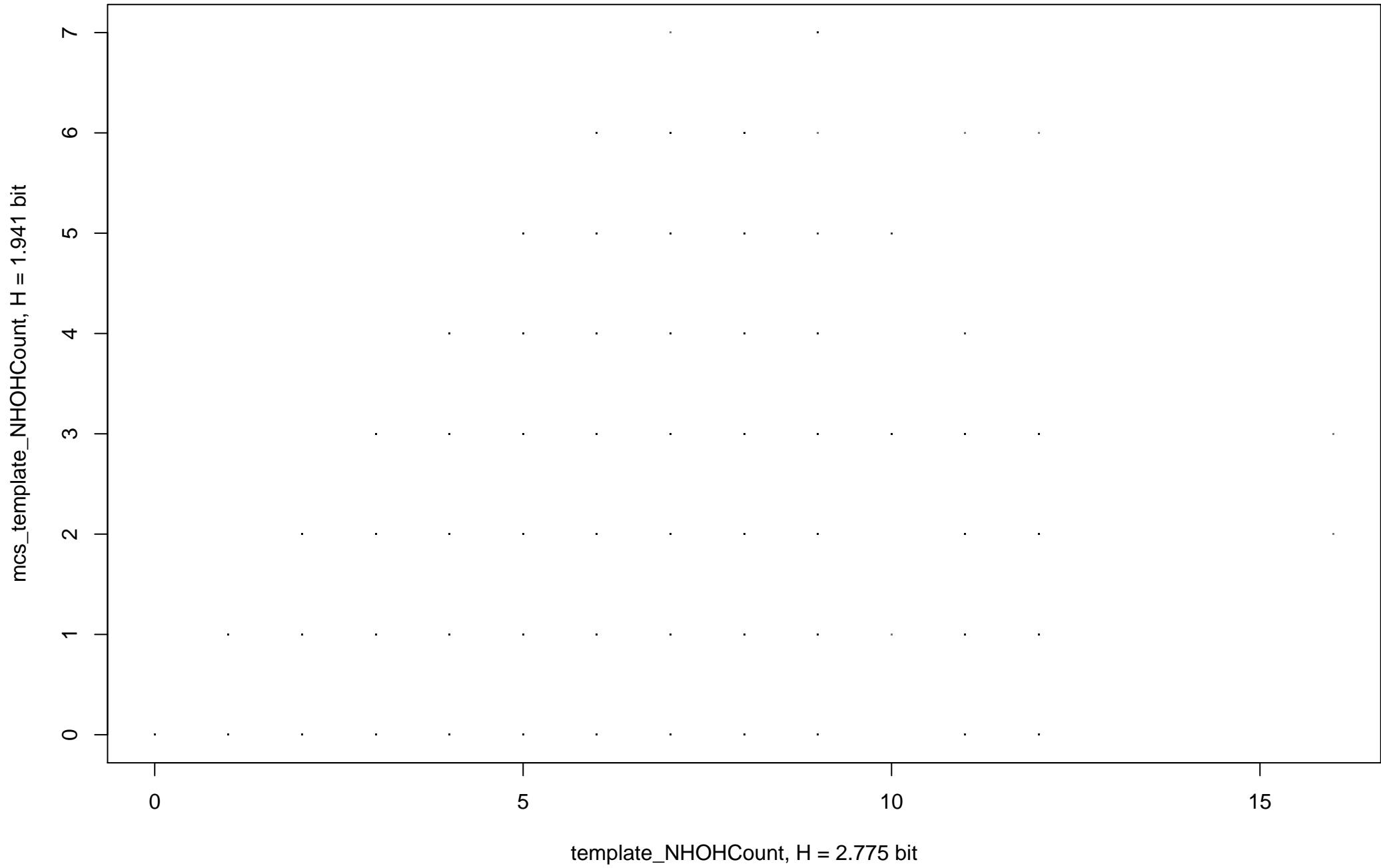
template_NumRotatableBonds, H = 3.668 bit



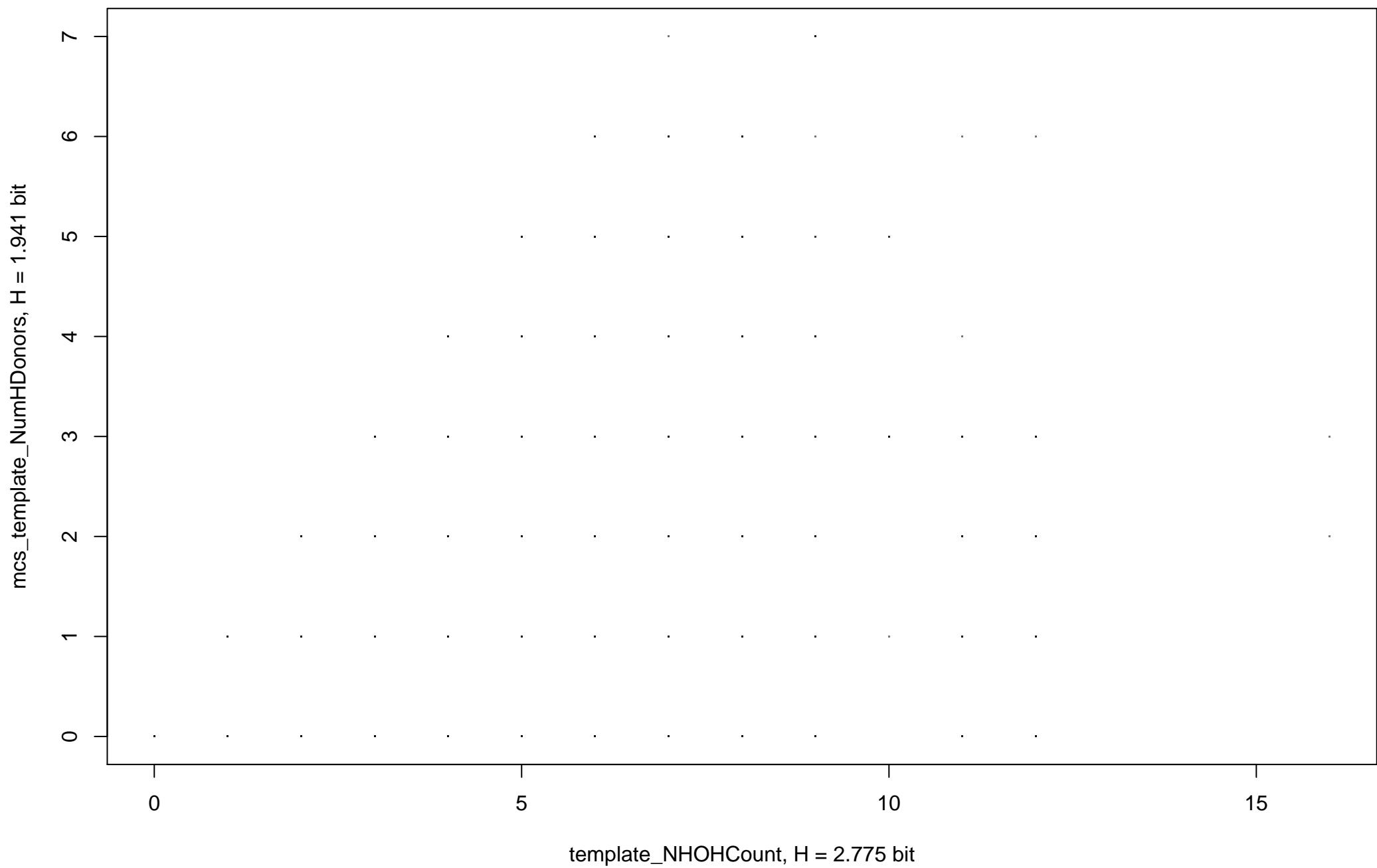
docked_NumHAcceptors-docked_NumRotatableBonds, MI = 0.4767 bit, normMI = 0.1576



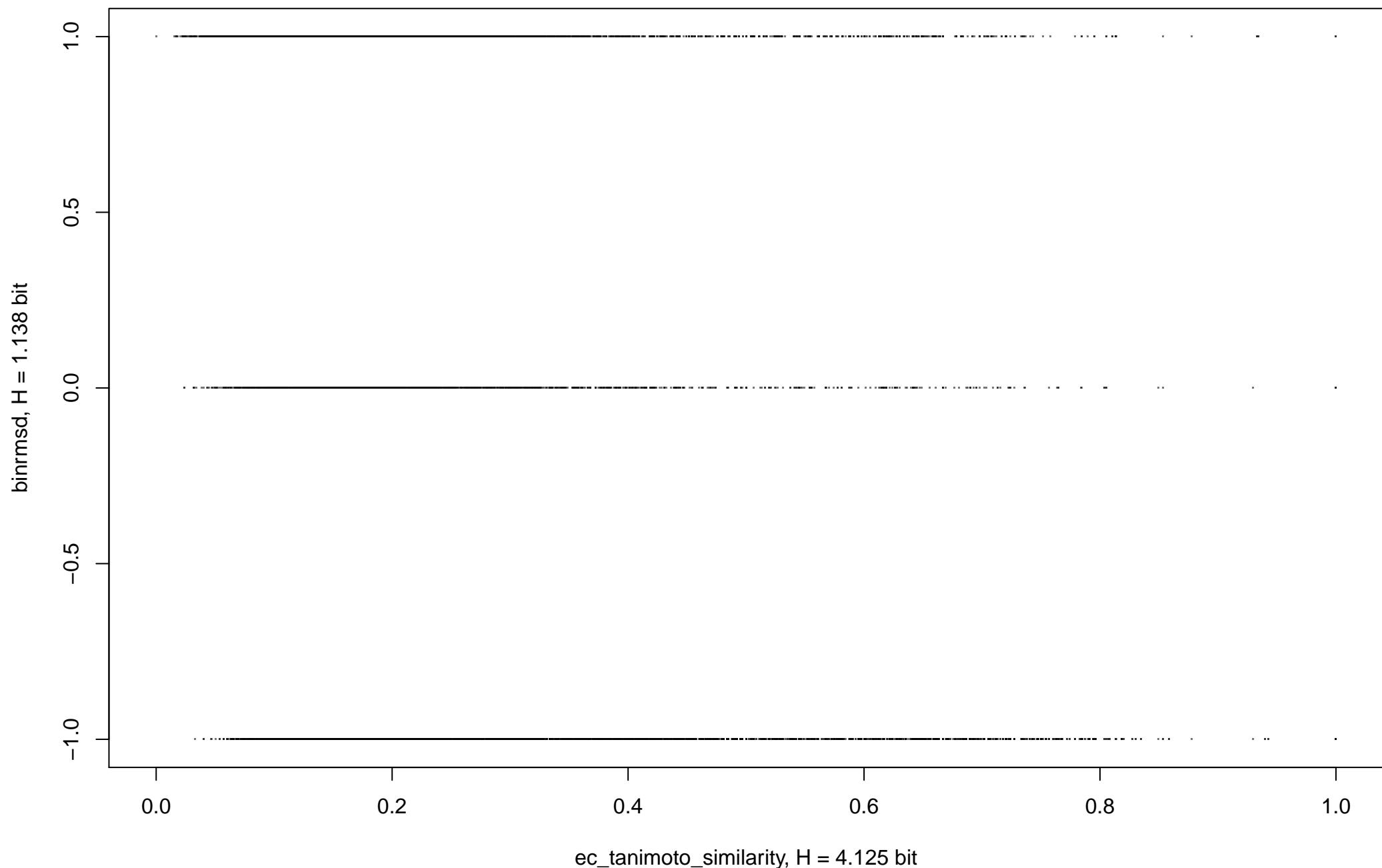
template_NHOHCount-mcs_template_NHOHCount, MI = 0.3046 bit, normMI = 0.1569



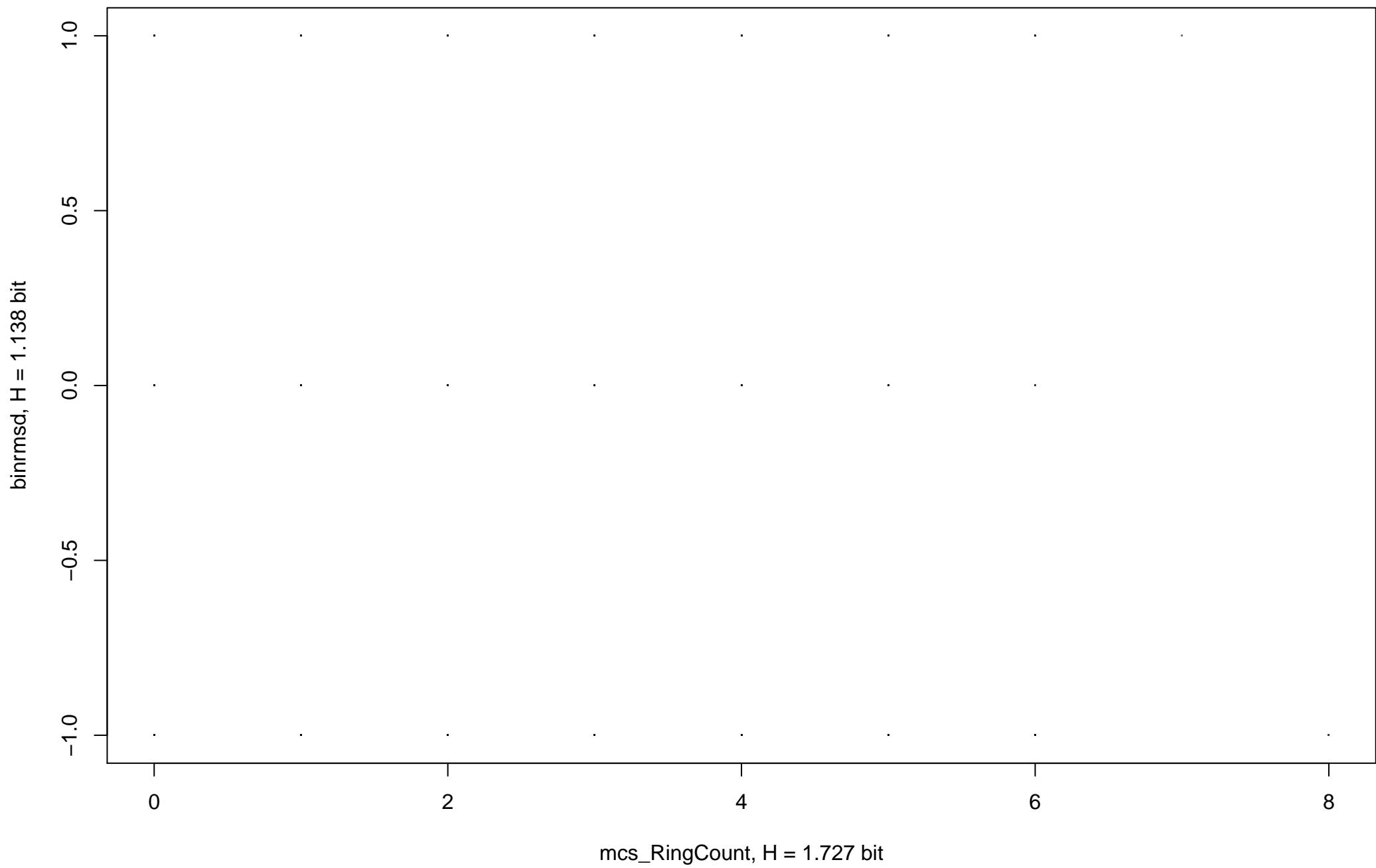
template_NHOHCount-mcs_template_NumHDonors, MI = 0.3042 bit, normMI = 0.1567



ec_tanimoto_similarity-binrmsd, MI = 0.1645 bit, normMI = 0.1446

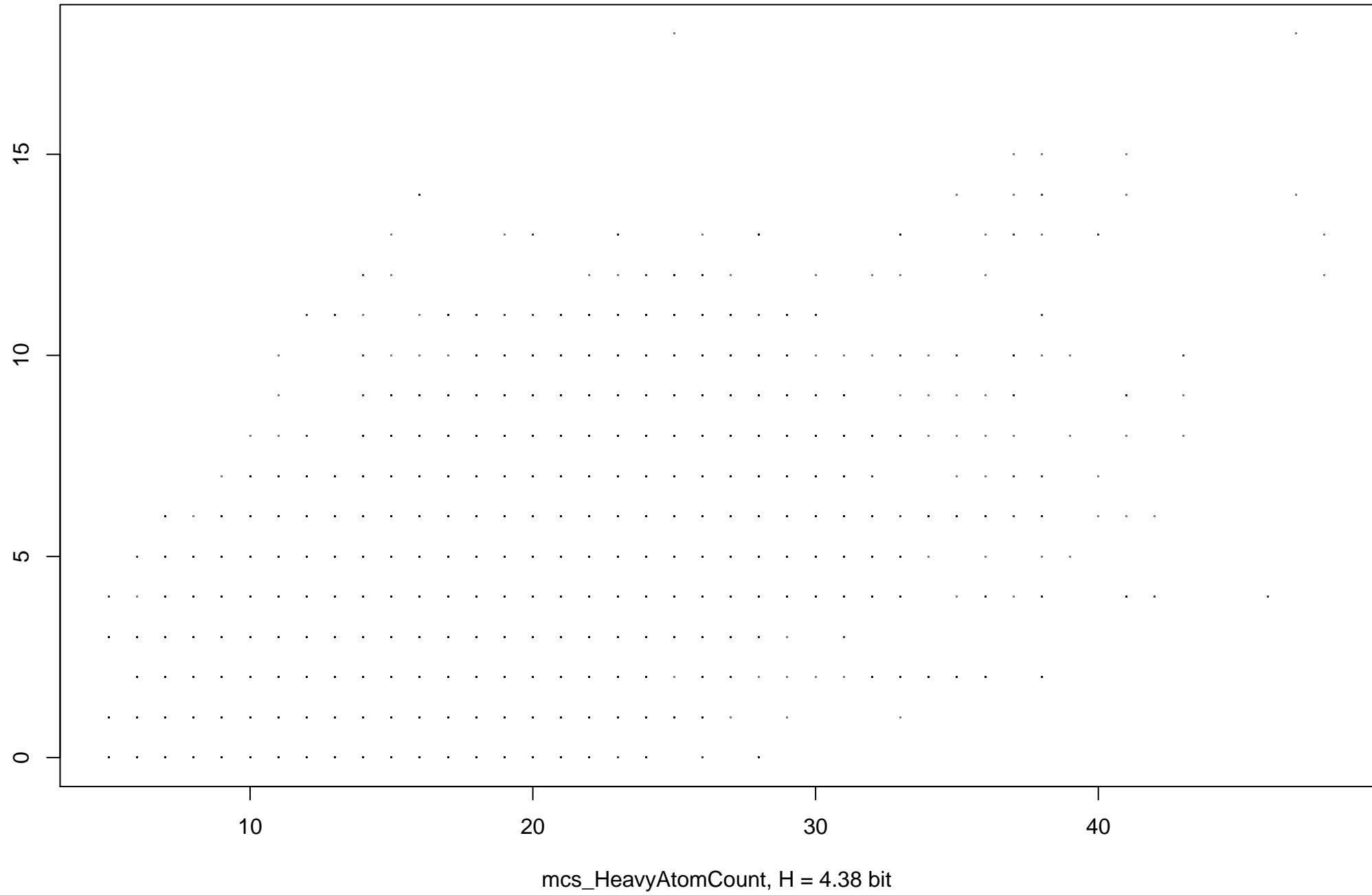


mcs_RingCount-binrmsd, MI = 0.1623 bit, normMI = 0.1426

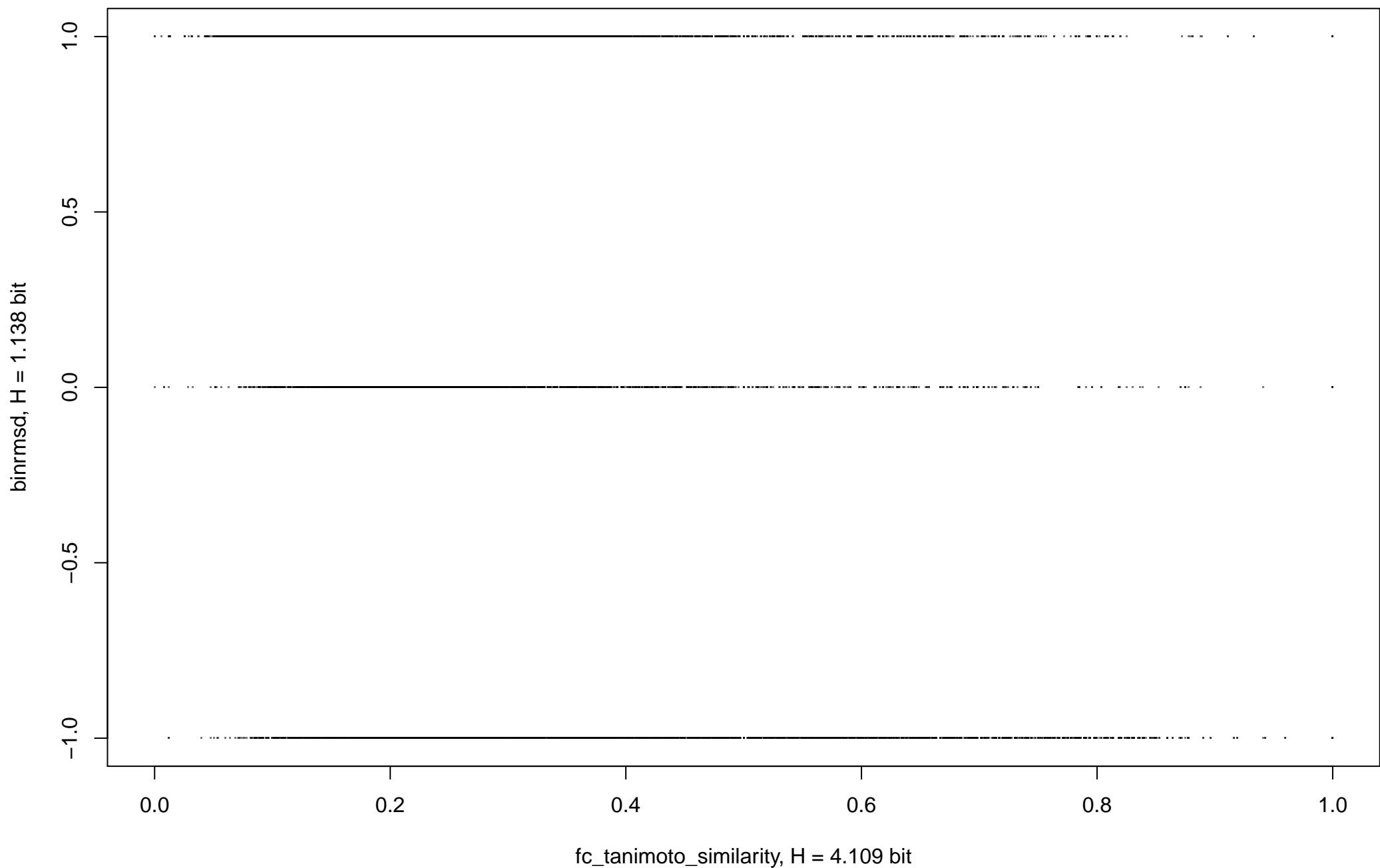


mcs_HeavyAtomCount–mcs_docked_NumRotatableBonds, MI = 0.4422 bit, normMI = 0.1419

mcs_docked_NumRotatableBonds, H = 3.117 bit

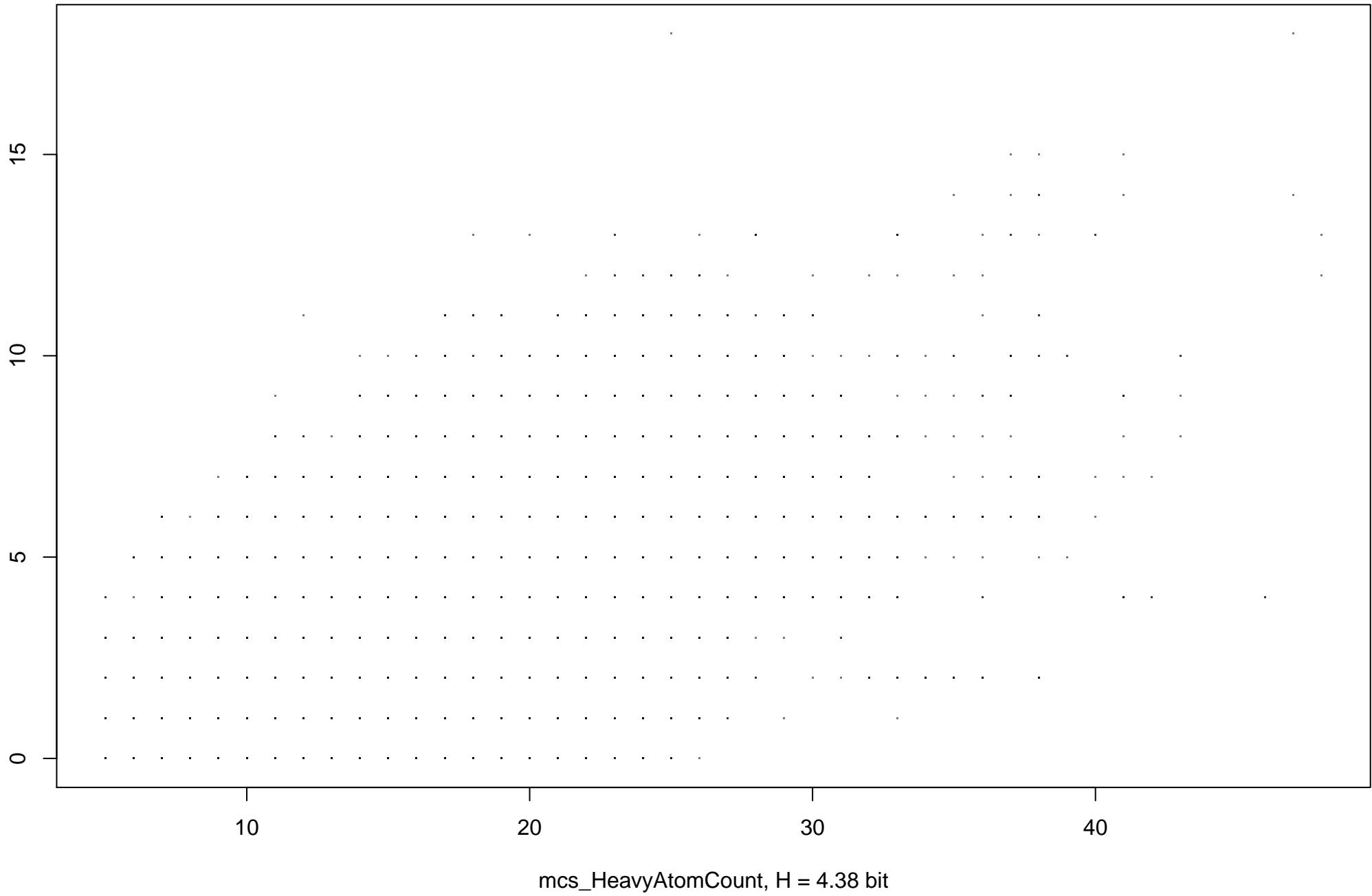


fc_tanimoto_similarity–binrmsd, MI = 0.1601 bit, normMI = 0.1406



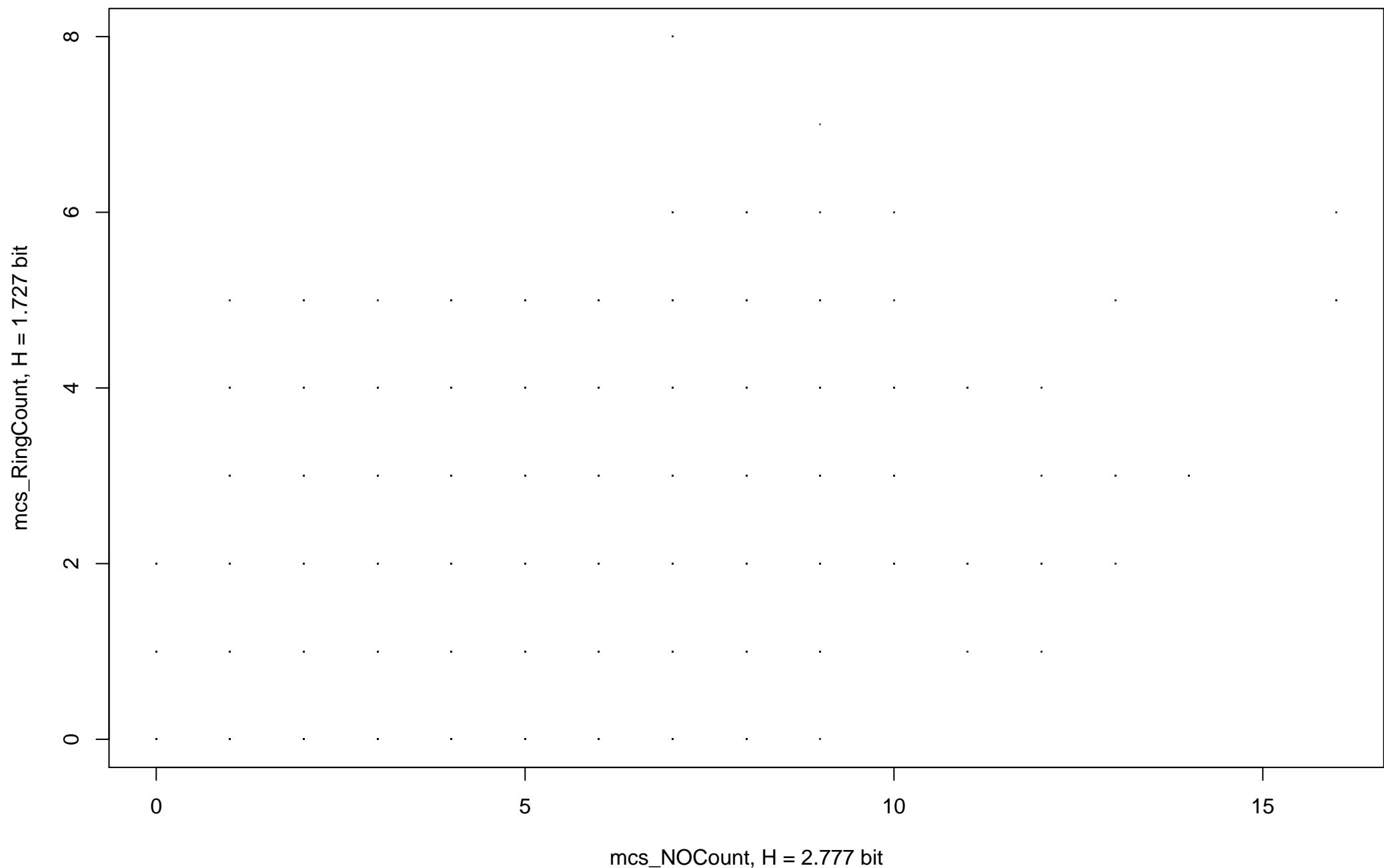
mcs_HeavyAtomCount–mcs_template_NumRotatableBonds, MI = 0.4342 bit, normMI = 0.1393

mcs_template_NumRotatableBonds, H = 3.118 bit



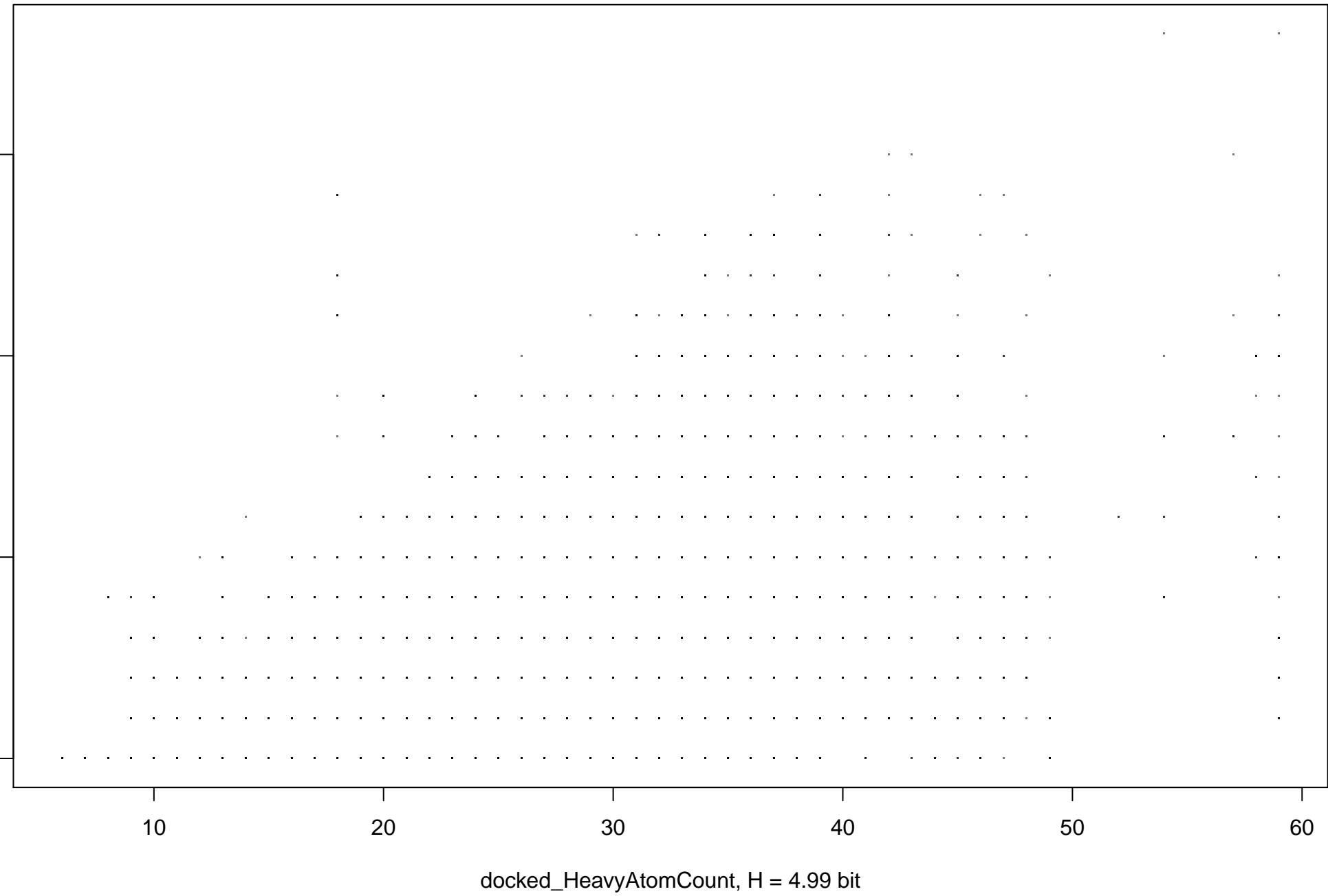
mcs_HeavyAtomCount, H = 4.38 bit

mcs_NOCount–mcs_RingCount, MI = 0.2391 bit, normMI = 0.1384



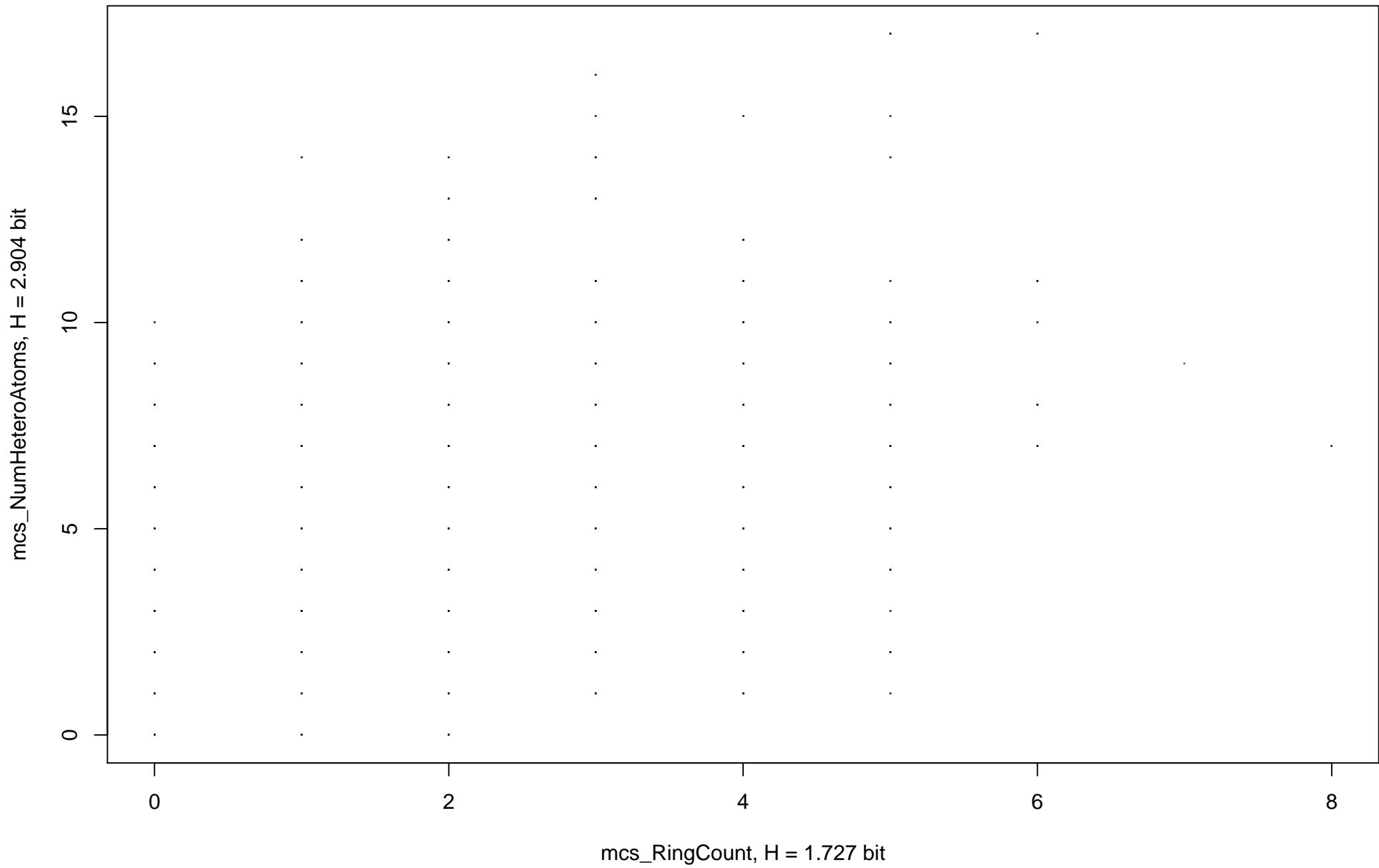
docked_HeavyAtomCount-mcs_docked_NumRotatableBonds, MI = 0.4298 bit, normMI = 0.1379

mcs_docked_NumRotatableBonds, H = 3.117 bit

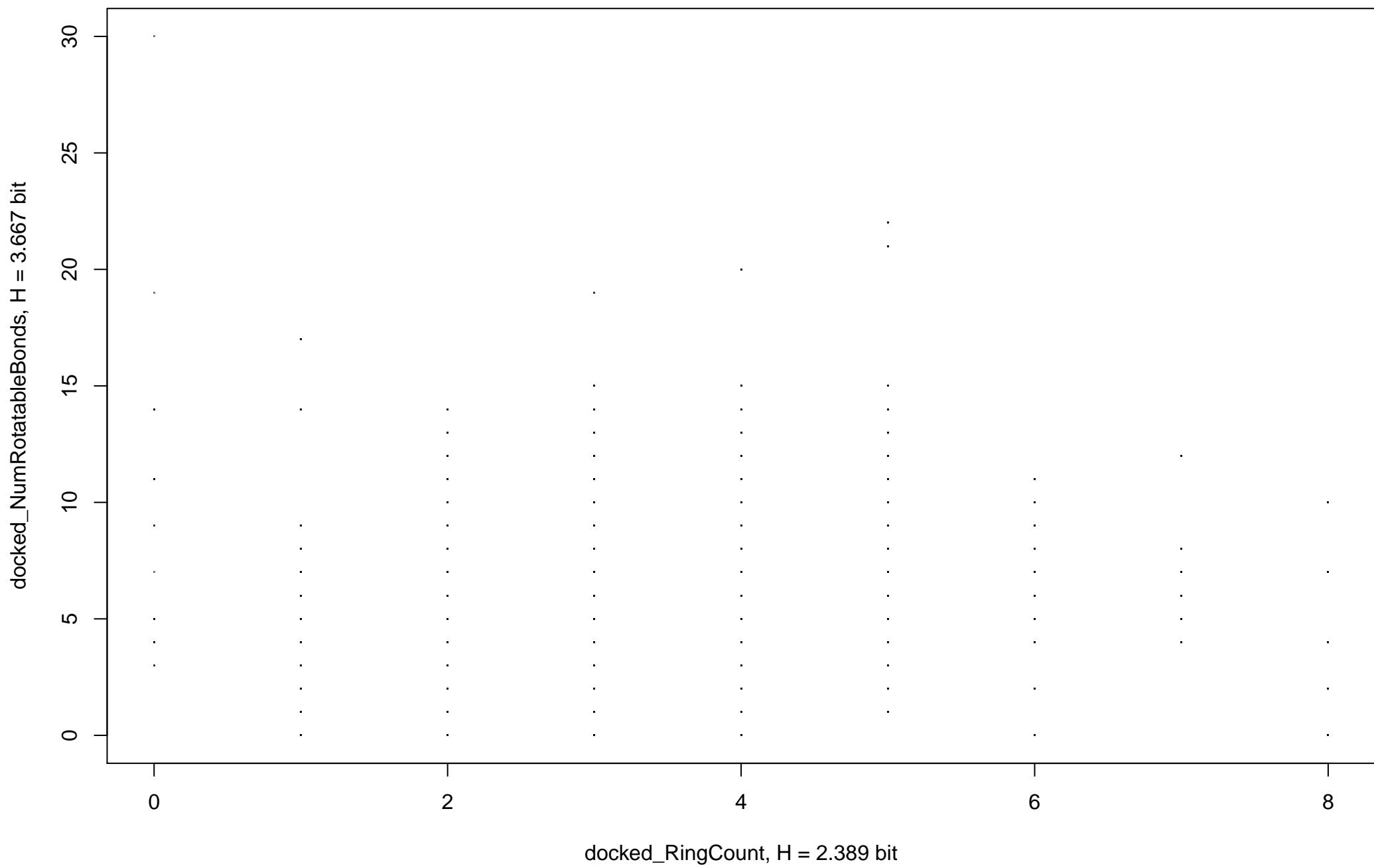


docked_HeavyAtomCount, H = 4.99 bit

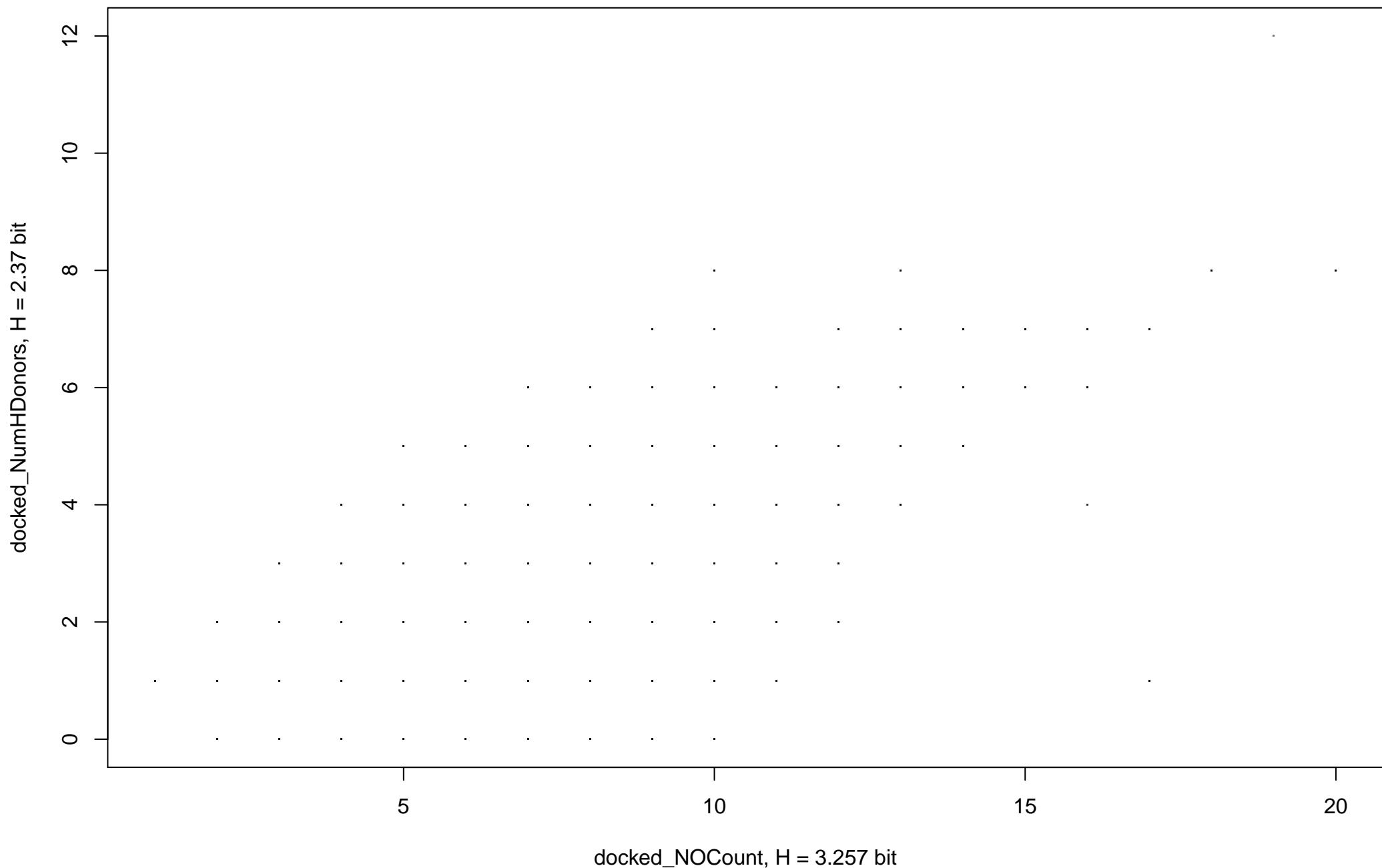
mcs_RingCount-mcs_NumHeteroAtoms, MI = 0.2376 bit, normMI = 0.1375



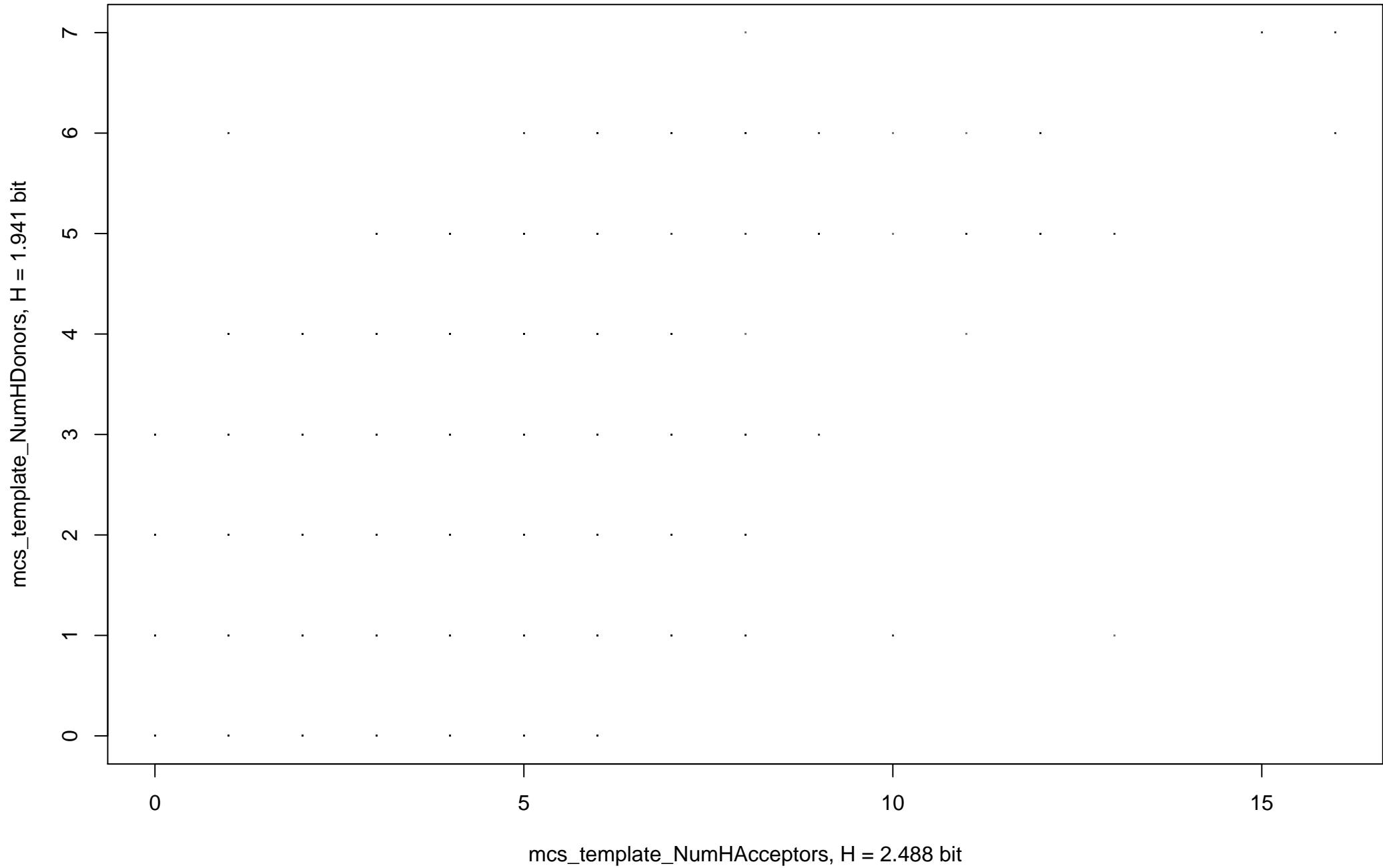
docked_RingCount–docked_NumRotatableBonds, MI = 0.327 bit, normMI = 0.1369



docked_NOCount–docked_NumHDonors, MI = 0.3178 bit, normMI = 0.1341

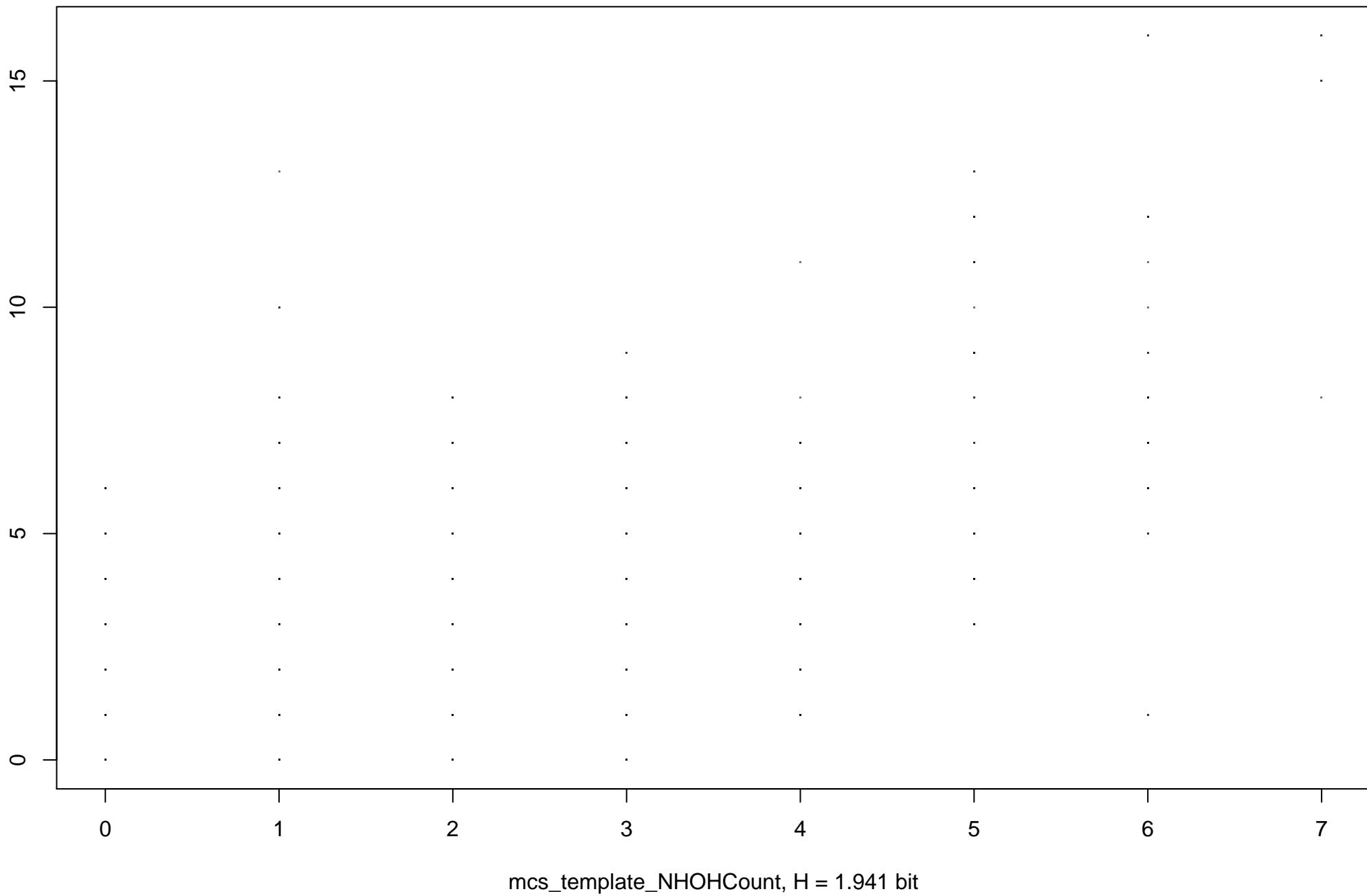


mcs_template_NumHAcceptors–mcs_template_NumHDonors, MI = 0.2564 bit, normMI = 0.1321



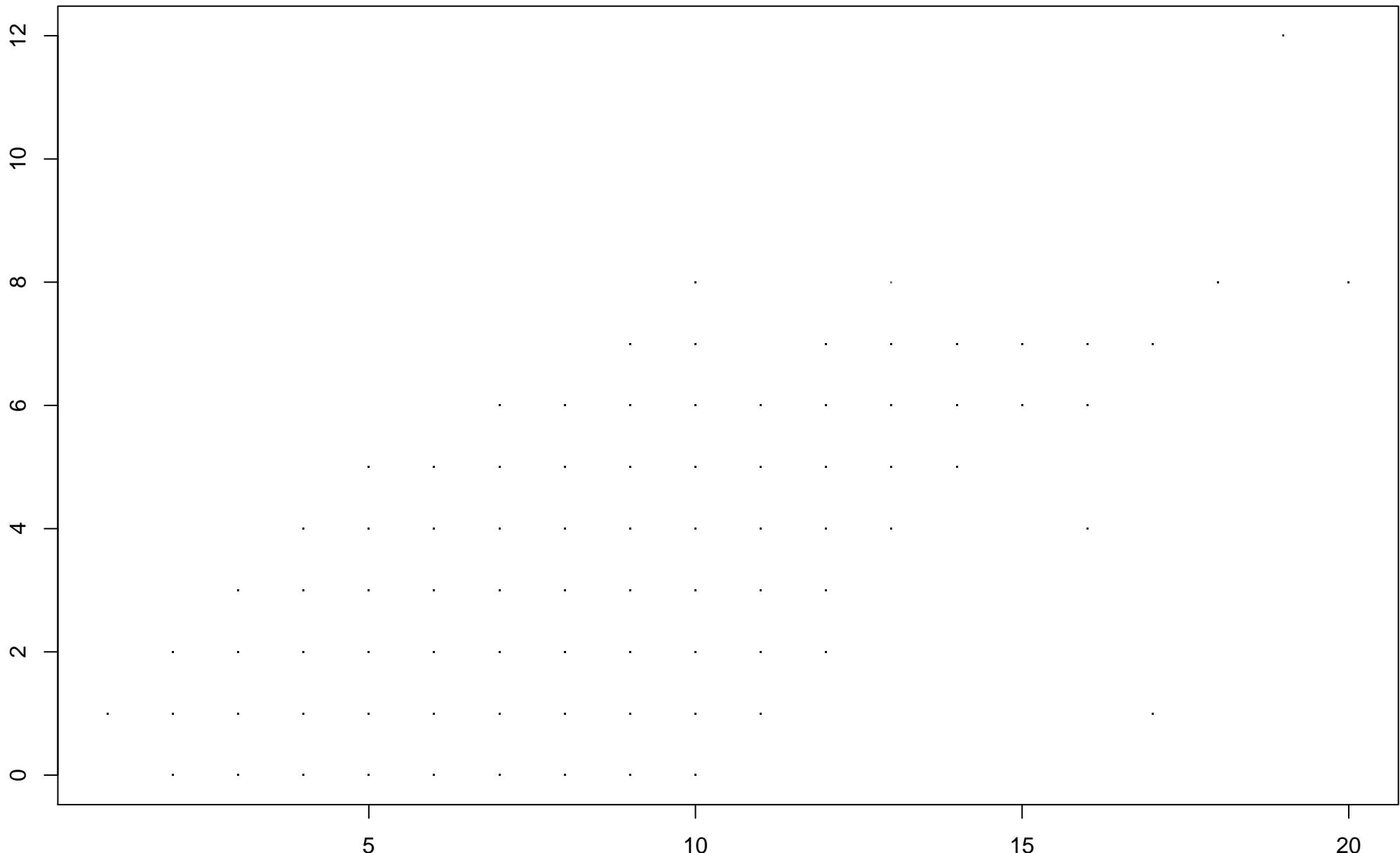
mcs_template_NHOHCount-mcs_template_NumHAcceptors, MI = 0.2562 bit, normMI = 0.132

mcs_template_NumHAcceptors, H = 2.488 bit



template_NOCount-template_NumHDonors, MI = 0.3141 bit, normMI = 0.1318

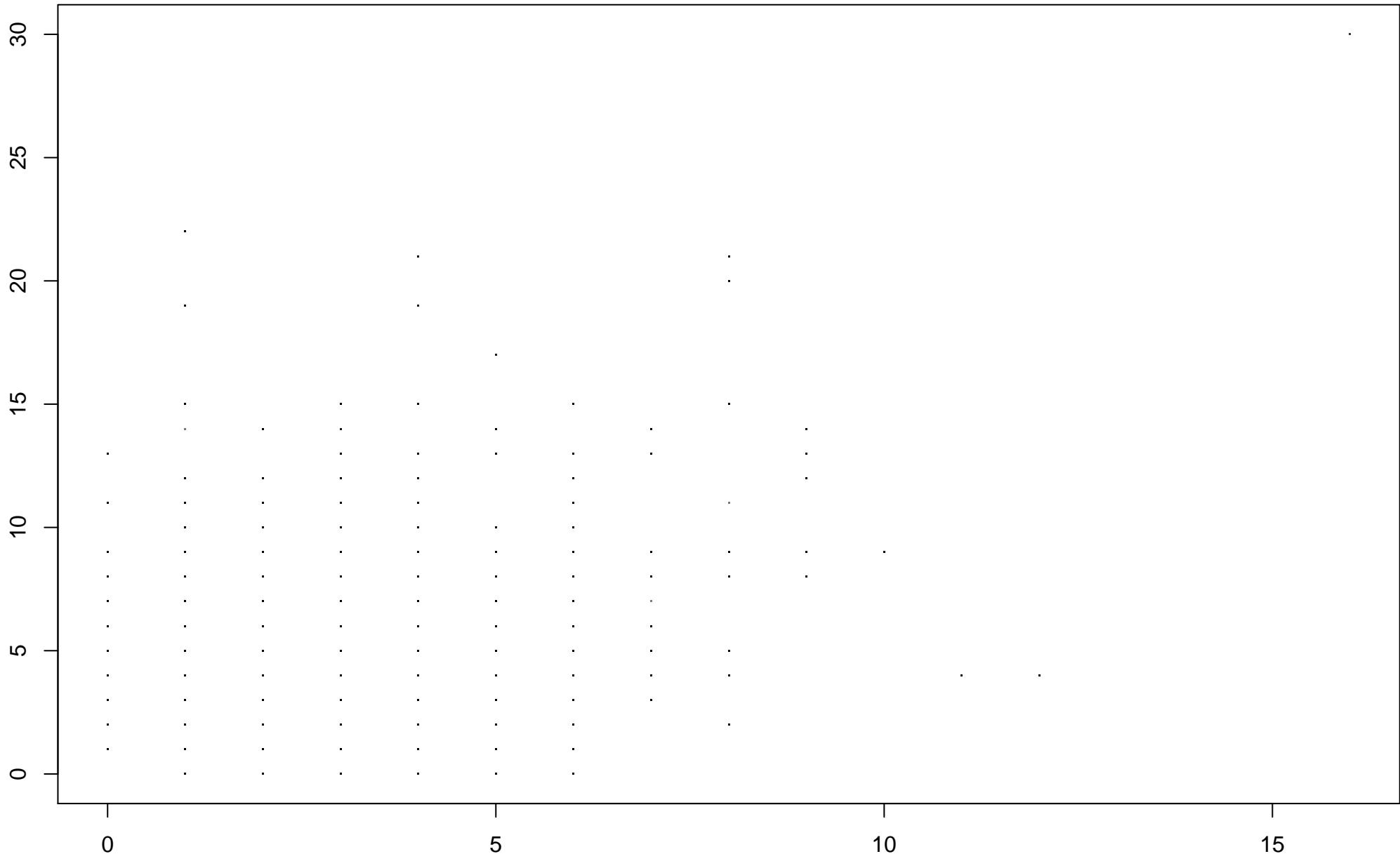
template_NumHDonors, H = 2.383 bit



template_NOCount, H = 3.237 bit

template_NHOHCount-template_NumRotatableBonds, MI = 0.3658 bit, normMI = 0.1318

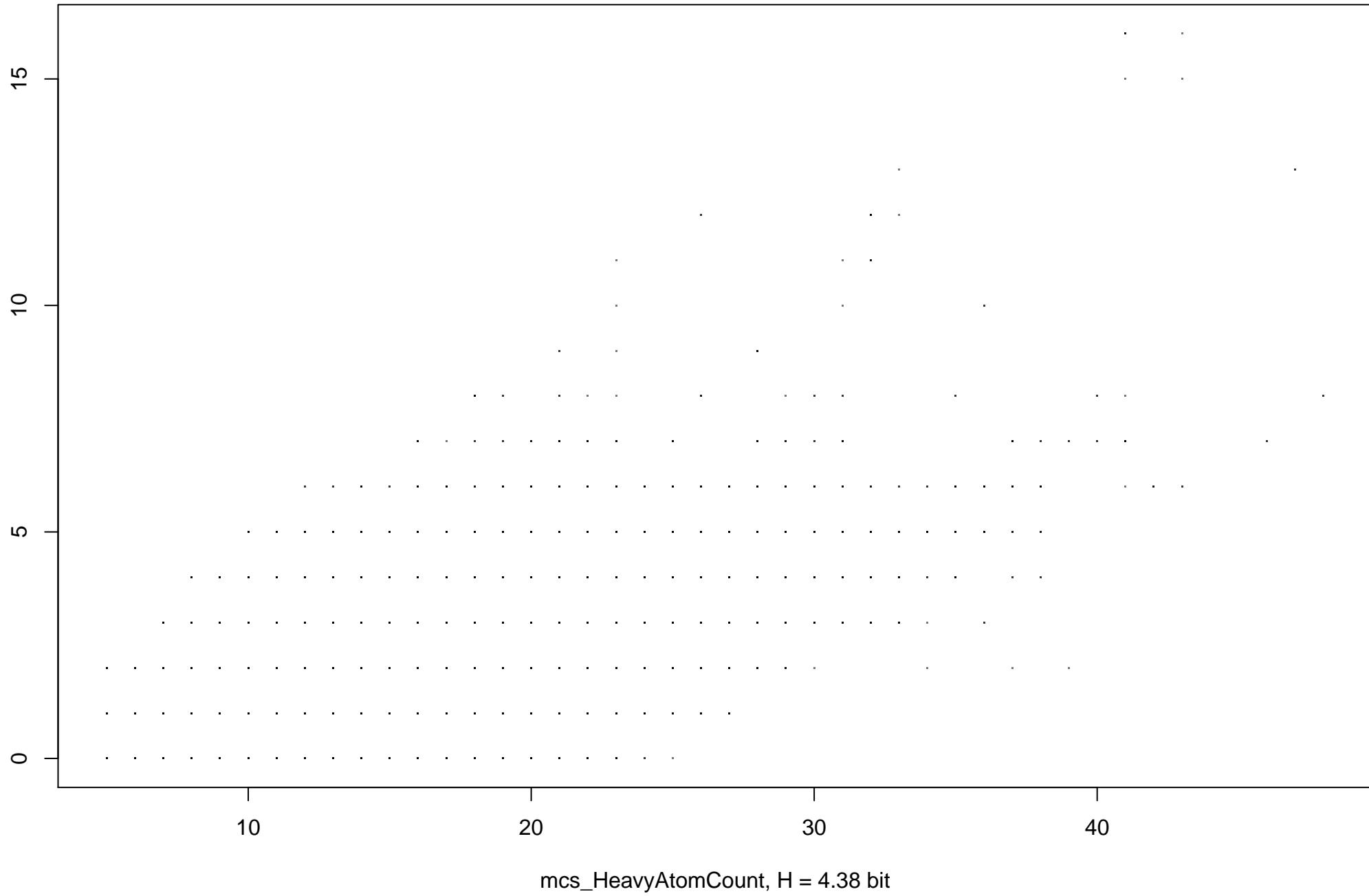
template_NumRotatableBonds, H = 3.668 bit



template_NHOHCount, H = 2.775 bit

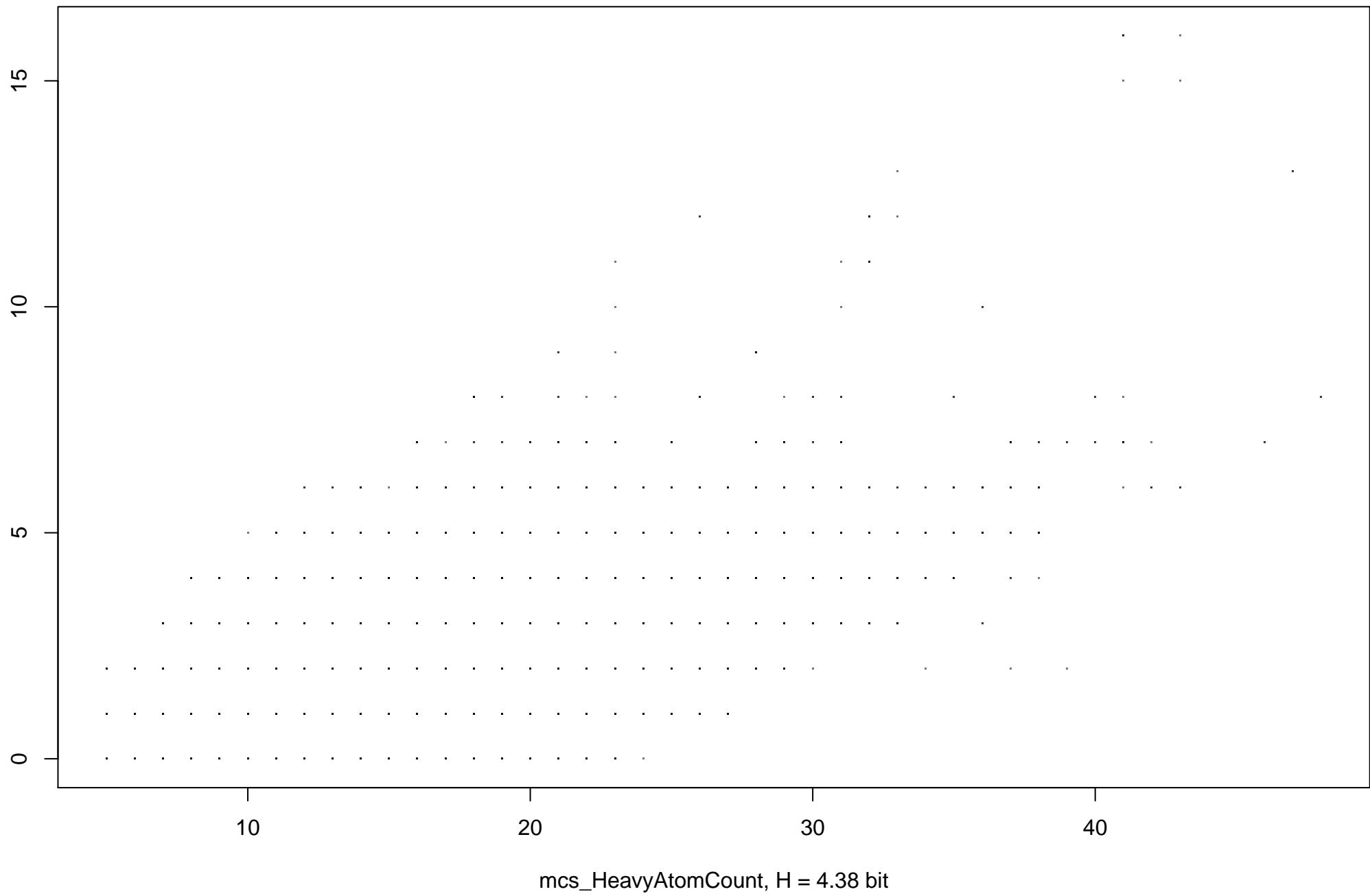
mcs_HeavyAtomCount-mcs_template_NumHAcceptors, MI = 0.3254 bit, normMI = 0.1308

mcs_template_NumHAcceptors, H = 2.488 bit



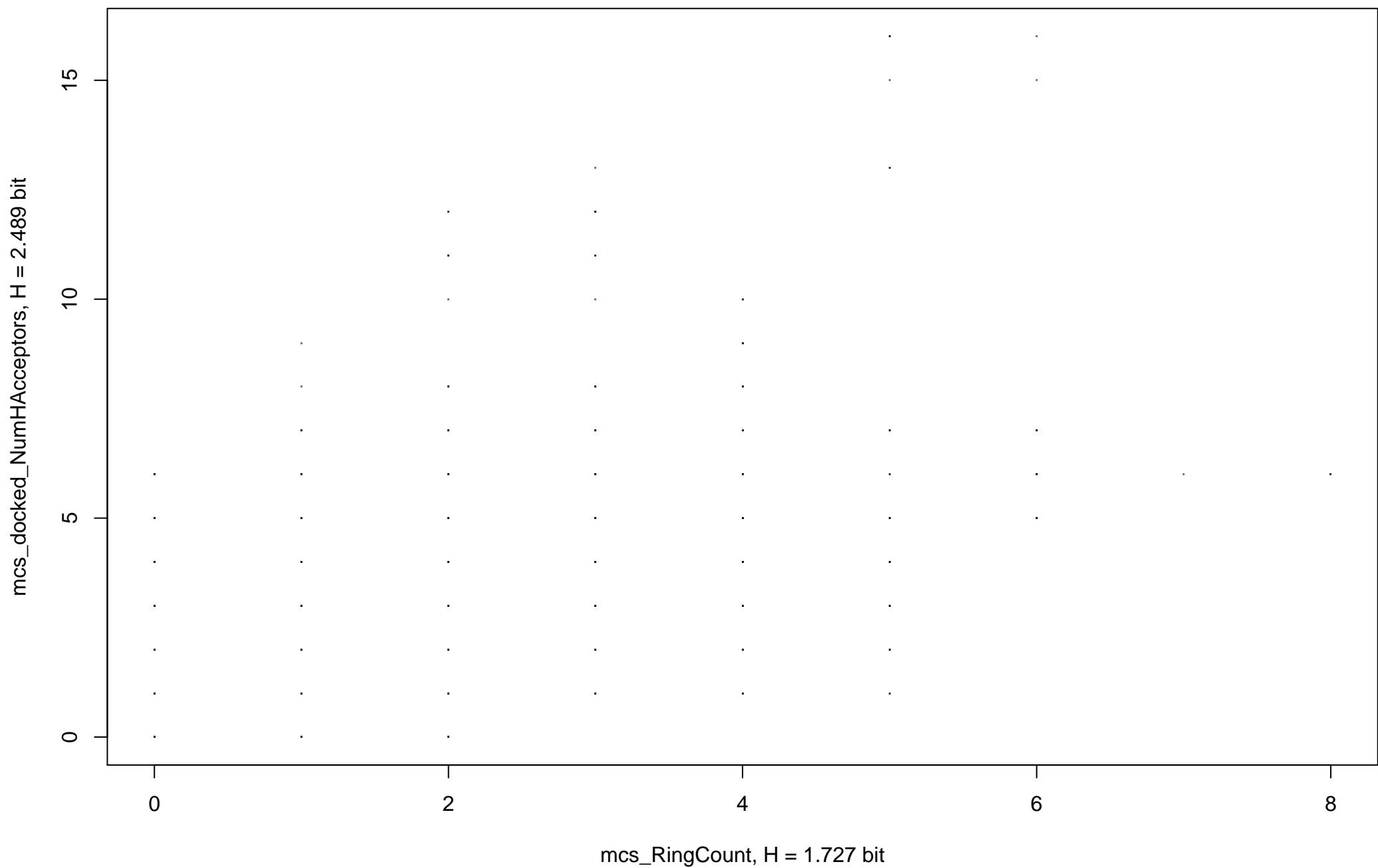
mcs_HeavyAtomCount-mcs_docked_NumHAcceptors, MI = 0.3245 bit, normMI = 0.1304

mcs_docked_NumHAcceptors, H = 2.489 bit



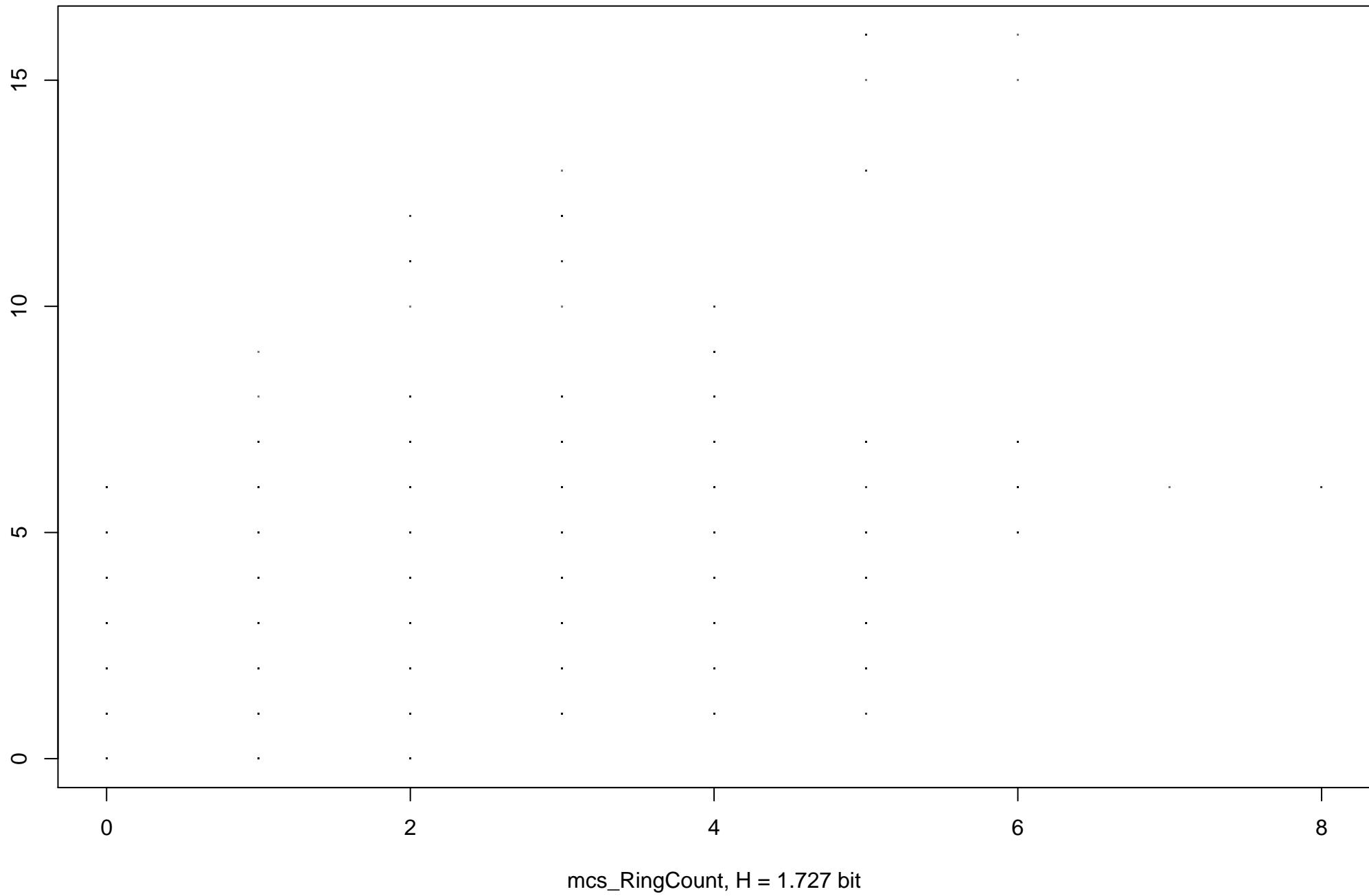
mcs_HeavyAtomCount, H = 4.38 bit

mcs_RingCount–mcs_docked_NumHAcceptors, MI = 0.2236 bit, normMI = 0.1294

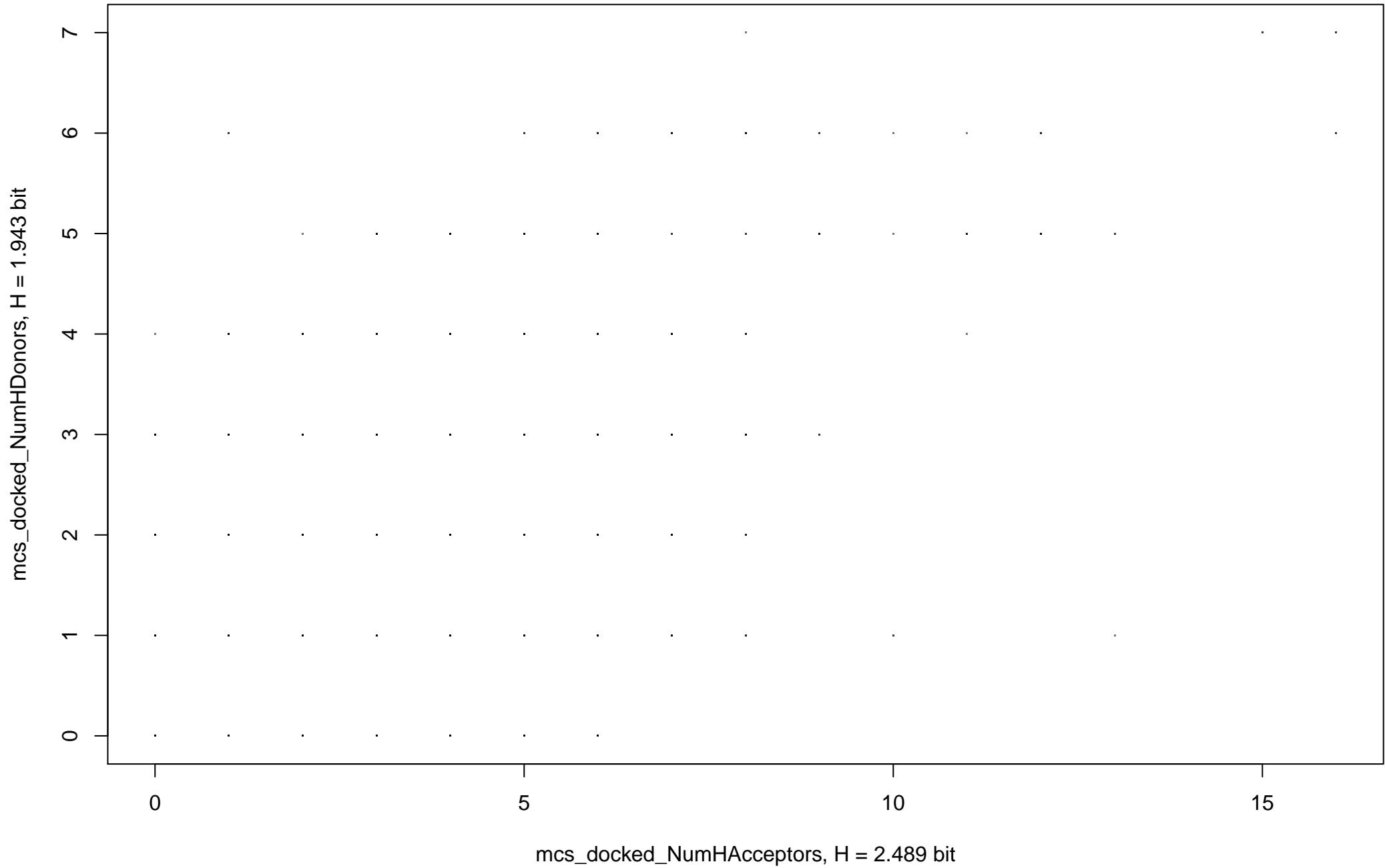


mcs_RingCount-mcs_template_NumHAcceptors, MI = 0.2227 bit, normMI = 0.1289

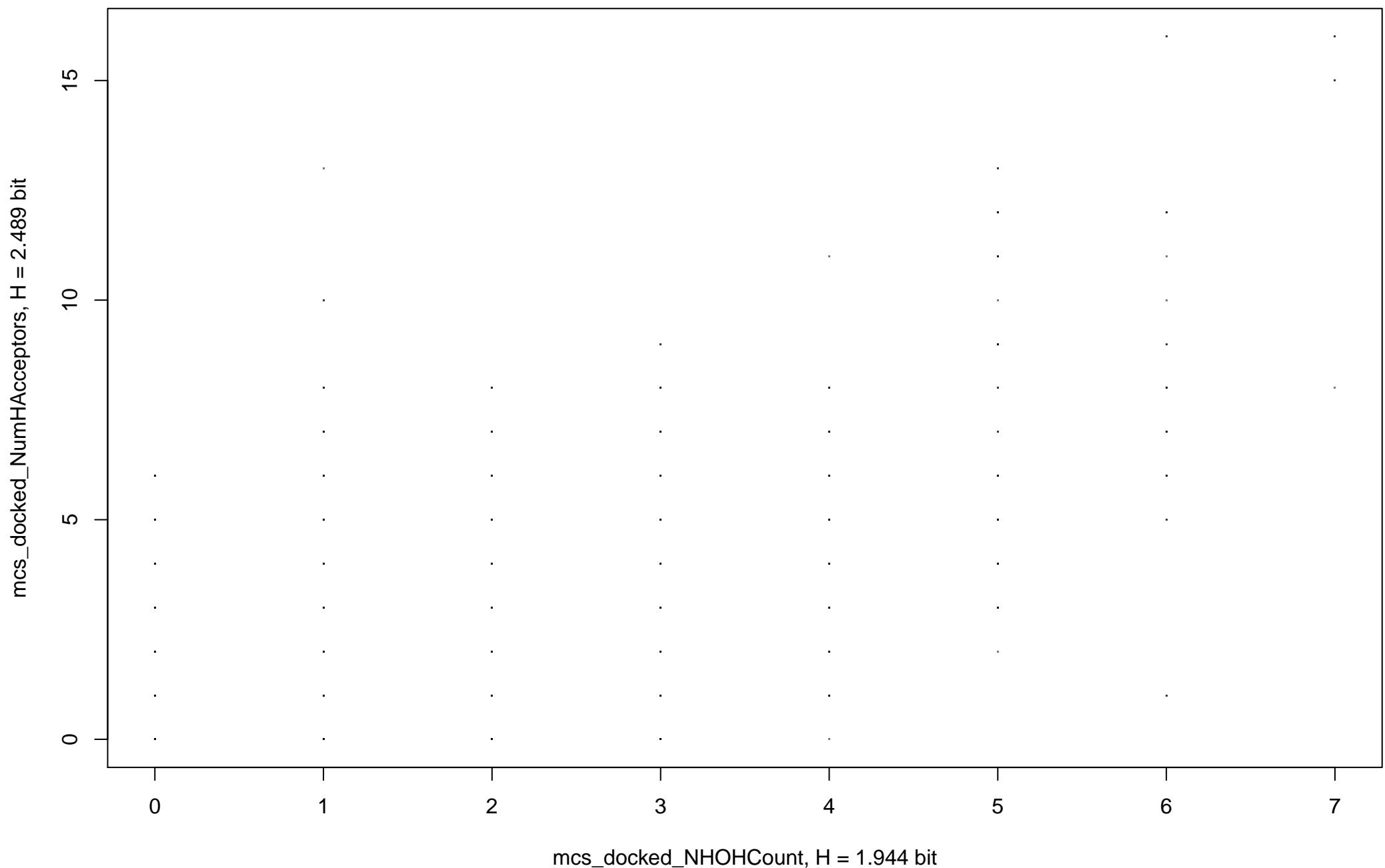
mcs_template_NumHAcceptors, H = 2.488 bit



mcs_docked_NumHAcceptors–mcs_docked_NumHDonors, MI = 0.2484 bit, normMI = 0.1278

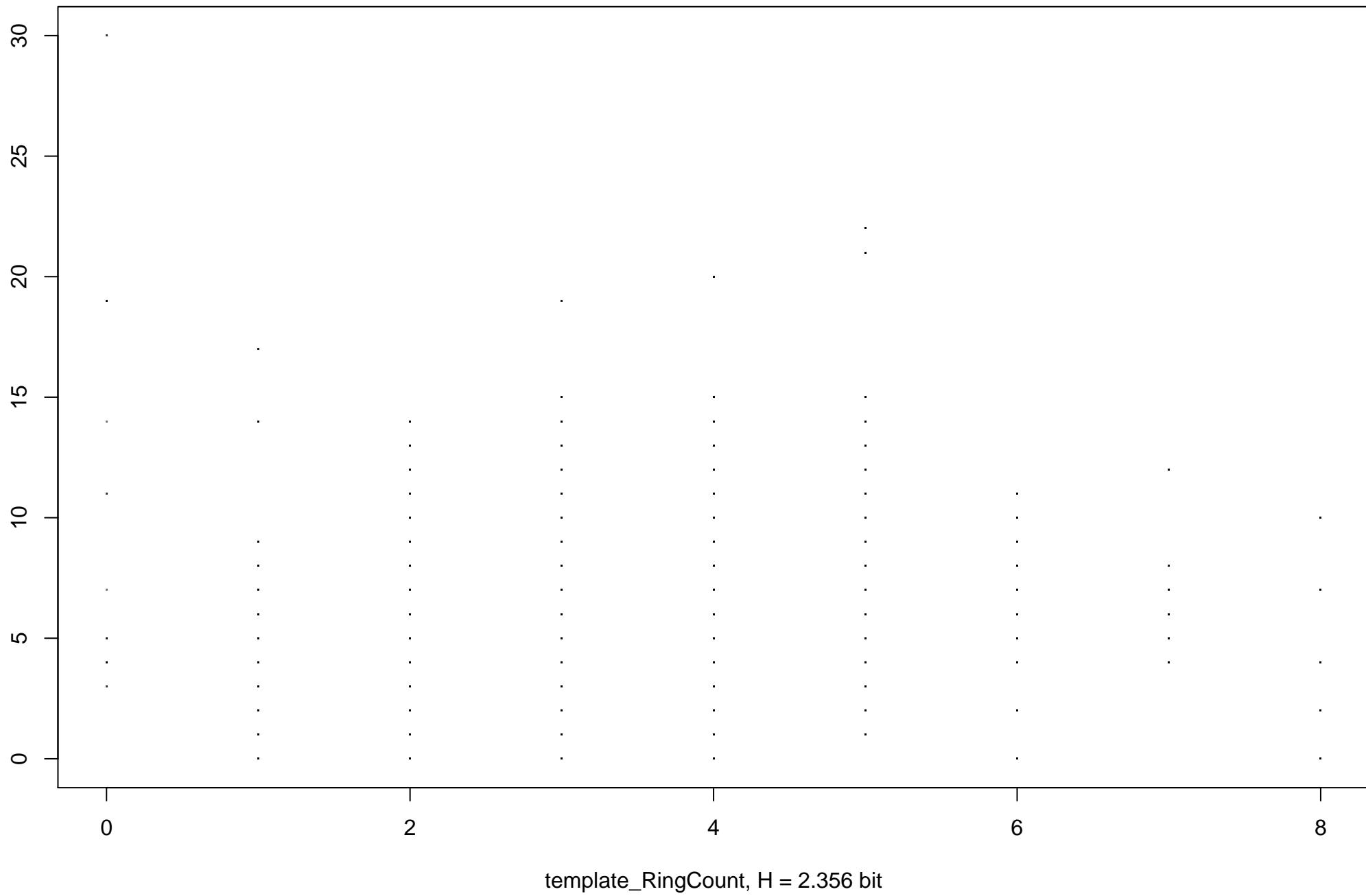


mcs_docked_NHOHCount-mcs_docked_NumHAcceptors, MI = 0.2482 bit, normMI = 0.1277



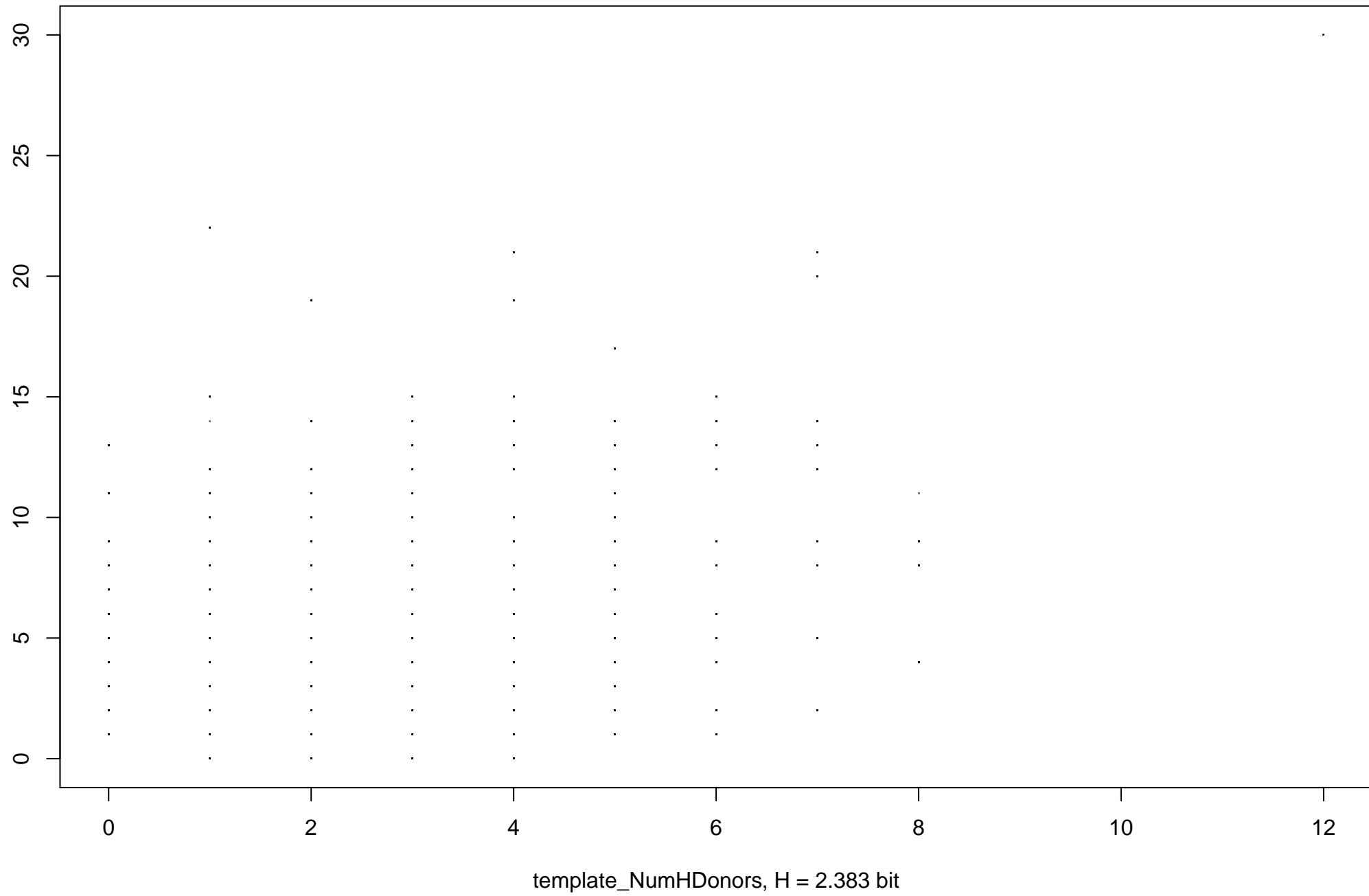
template_RingCount-template_NumRotatableBonds, MI = 0.2989 bit, normMI = 0.1269

template_NumRotatableBonds, H = 3.668 bit

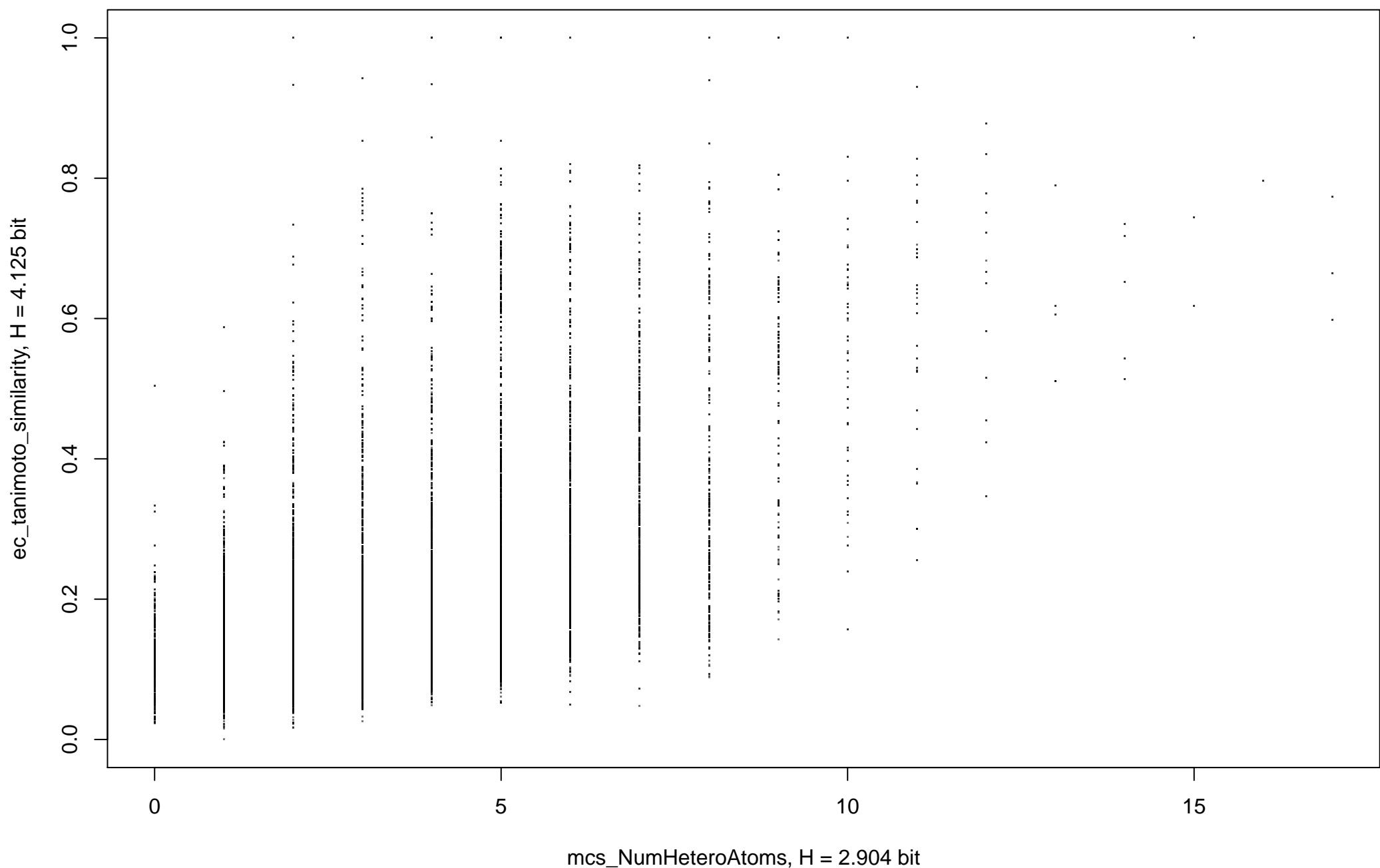


template_NumHDonors-template_NumRotatableBonds, MI = 0.3017 bit, normMI = 0.1266

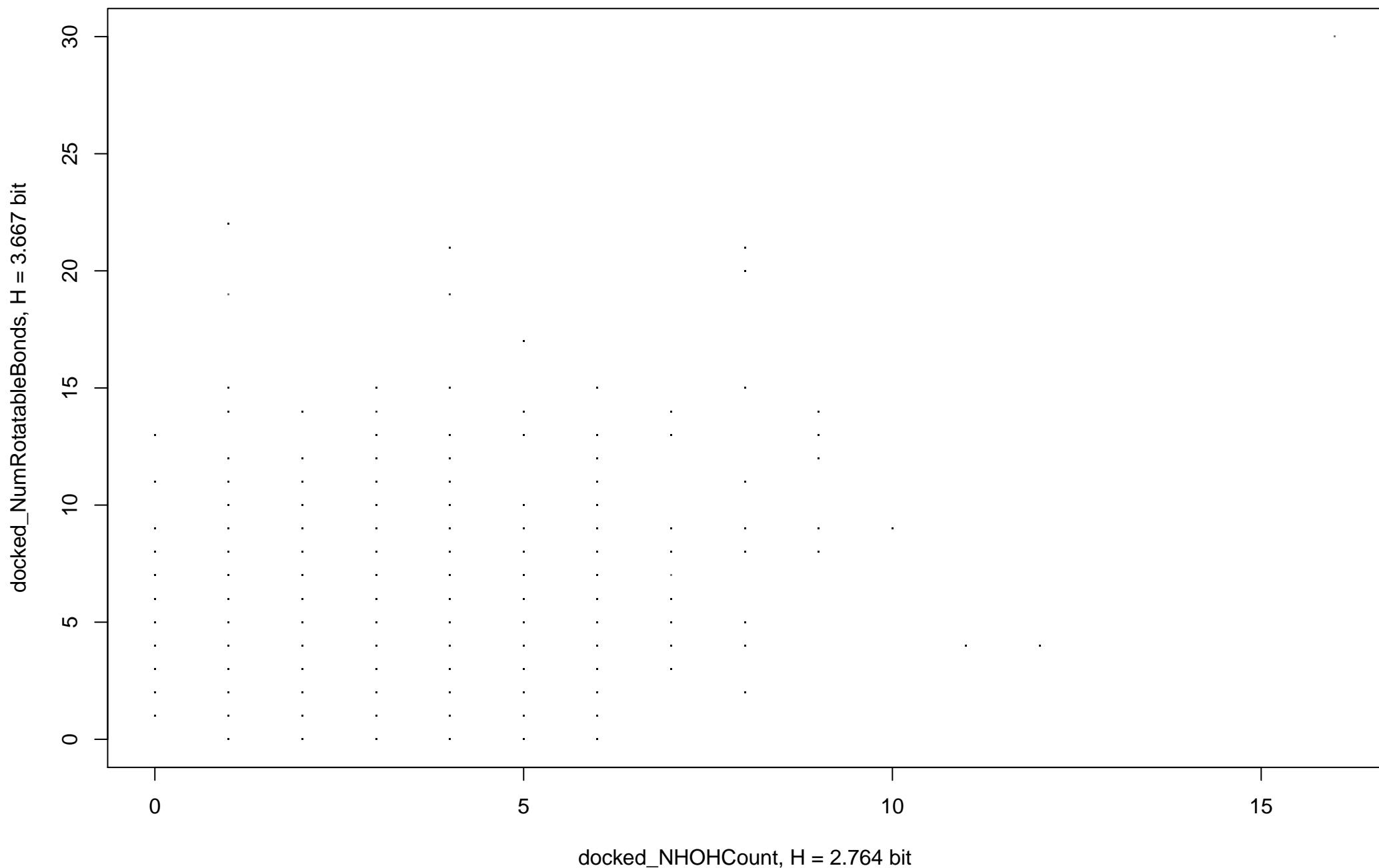
template_NumRotatableBonds, H = 3.668 bit



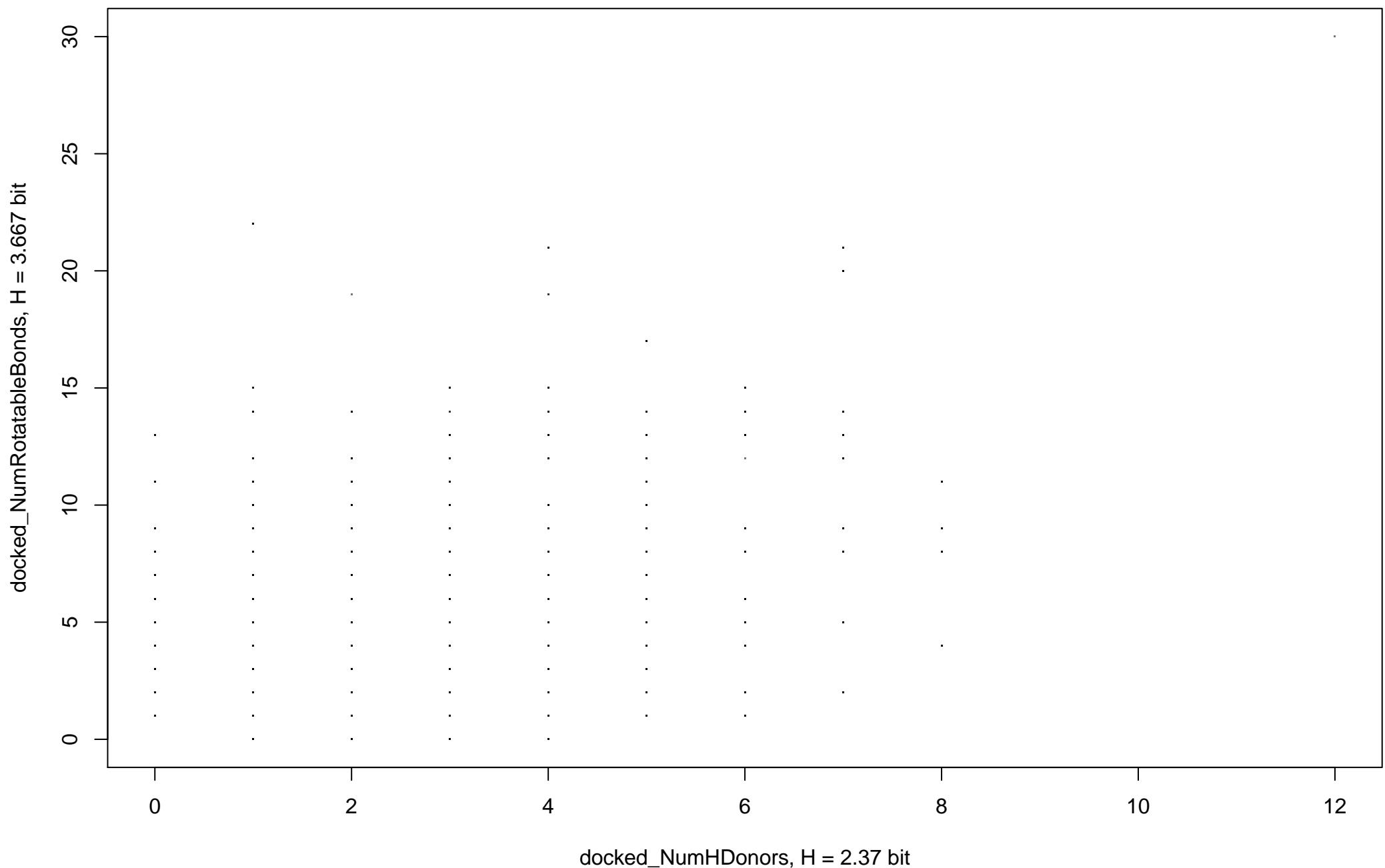
mcs_NumHeteroAtoms-ec_tanimoto_similarity, MI = 0.364 bit, normMI = 0.1253



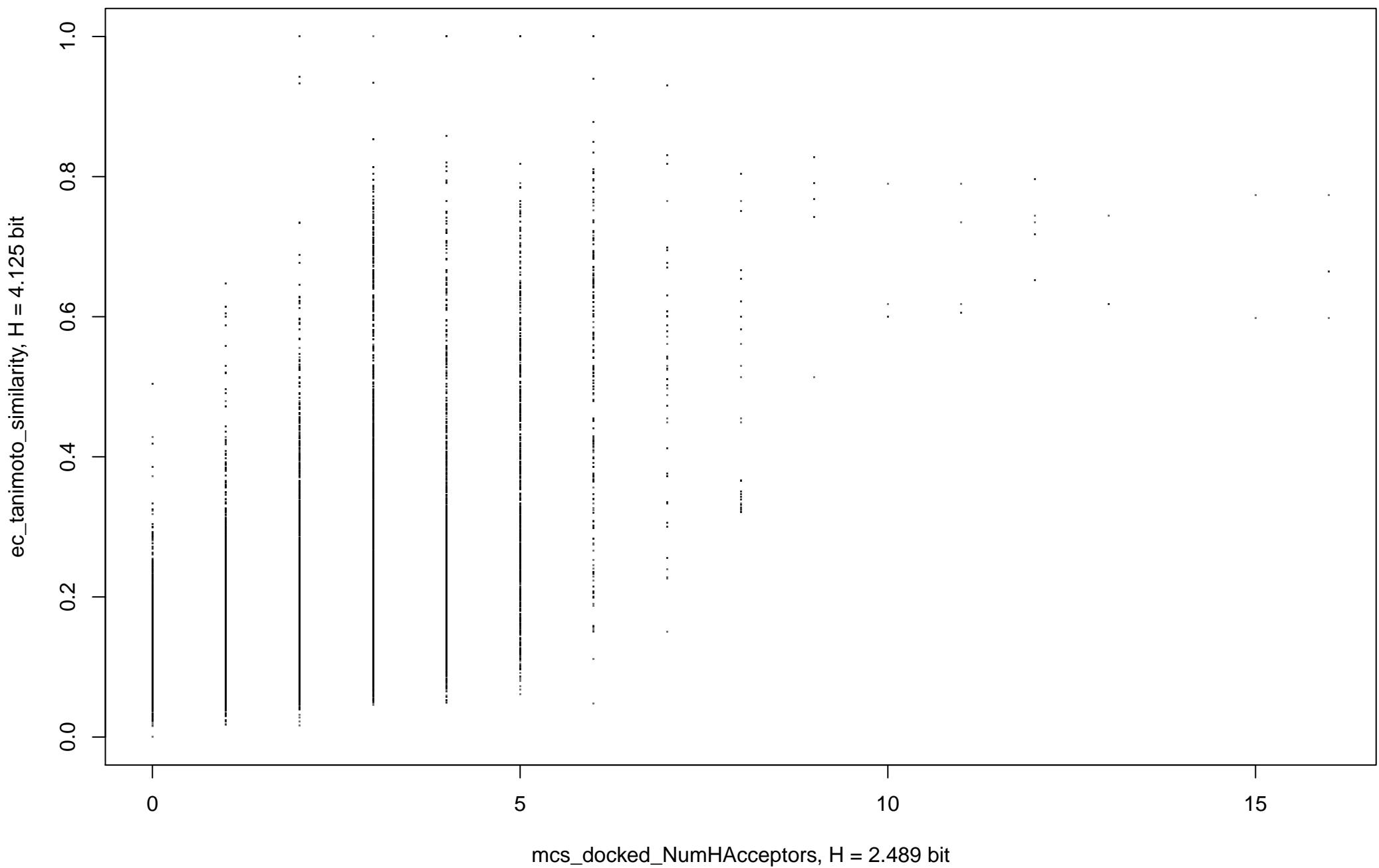
docked_NHOHCount–docked_NumRotatableBonds, MI = 0.3455 bit, normMI = 0.125



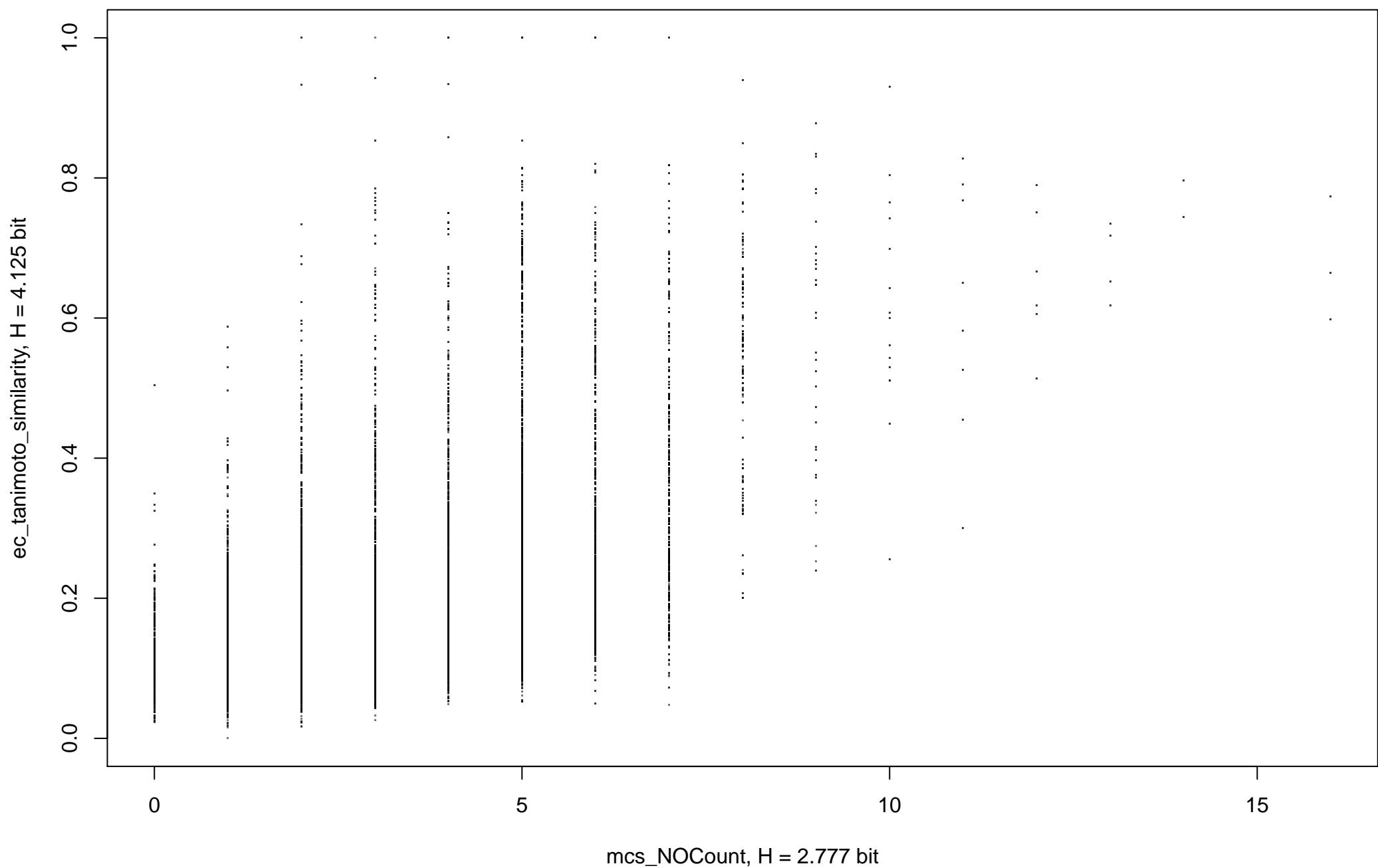
docked_NumHDonors–docked_NumRotatableBonds, MI = 0.2955 bit, normMI = 0.1247



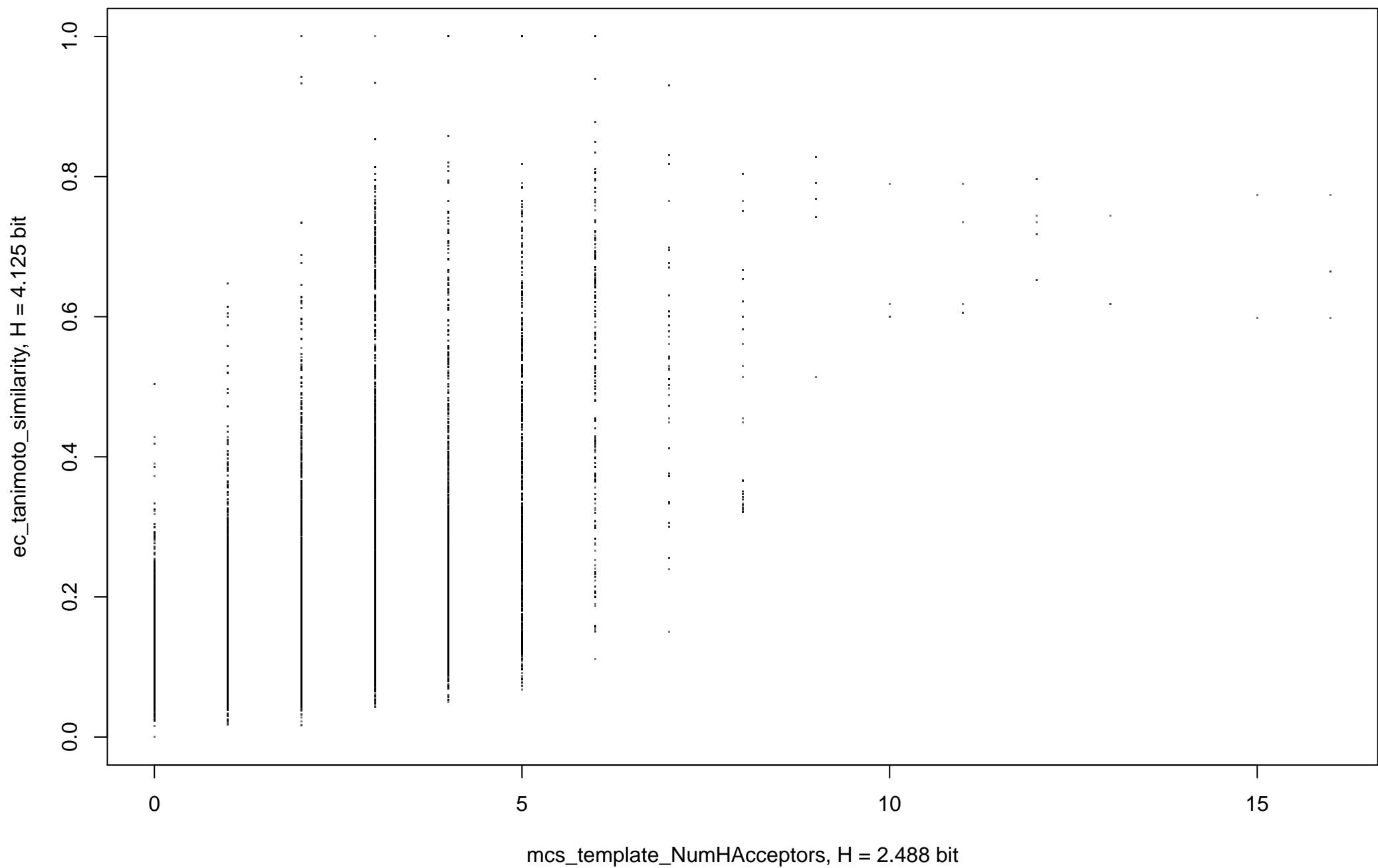
mcs_docked_NumHAcceptors–ec_tanimoto_similarity, MI = 0.2995 bit, normMI = 0.1203



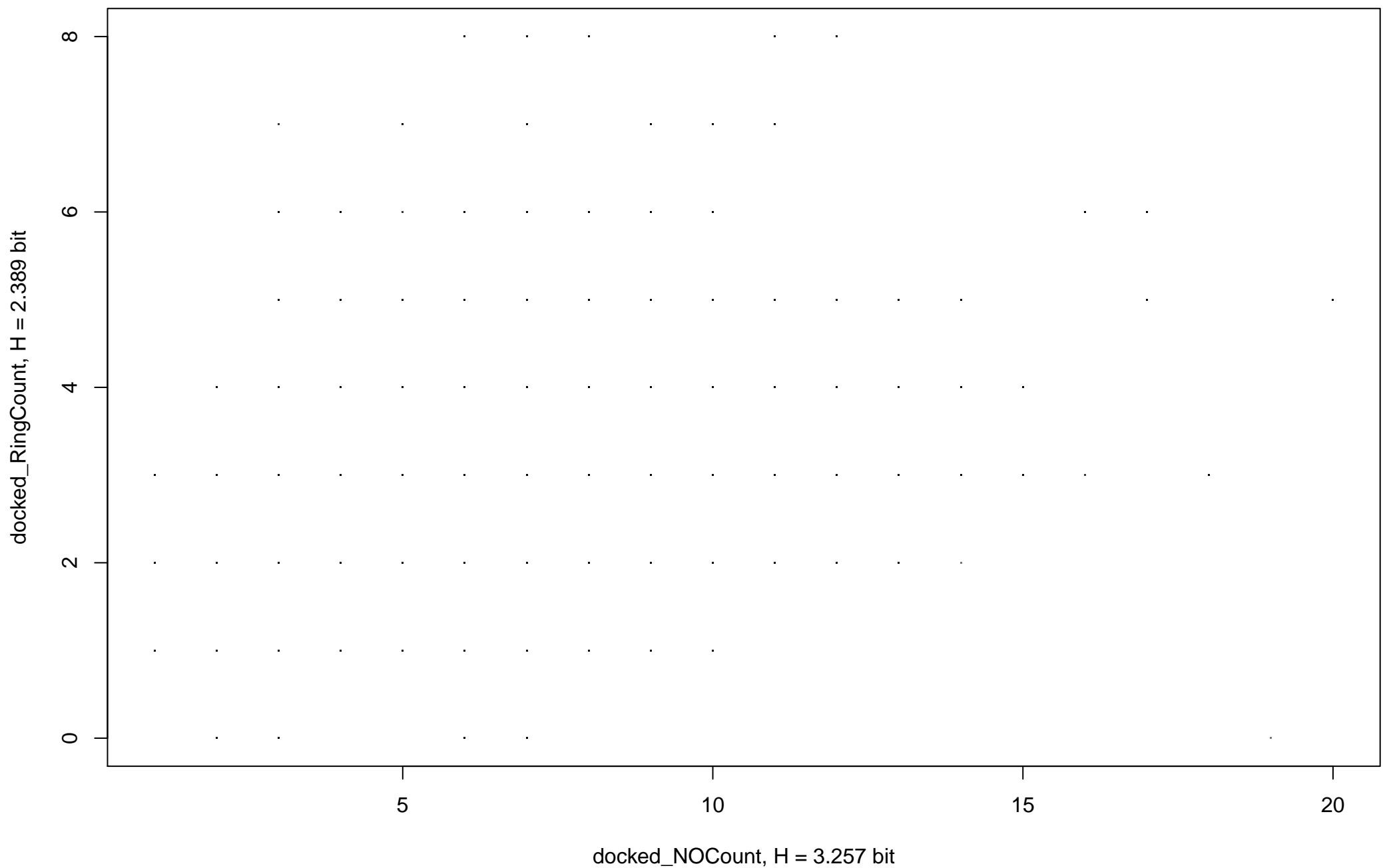
mcs_NOCount–ec_tanimoto_similarity, MI = 0.3339 bit, normMI = 0.1203



mcs_template_NumHAcceptors–ec_tanimoto_similarity, MI = 0.2977 bit, normMI = 0.1196

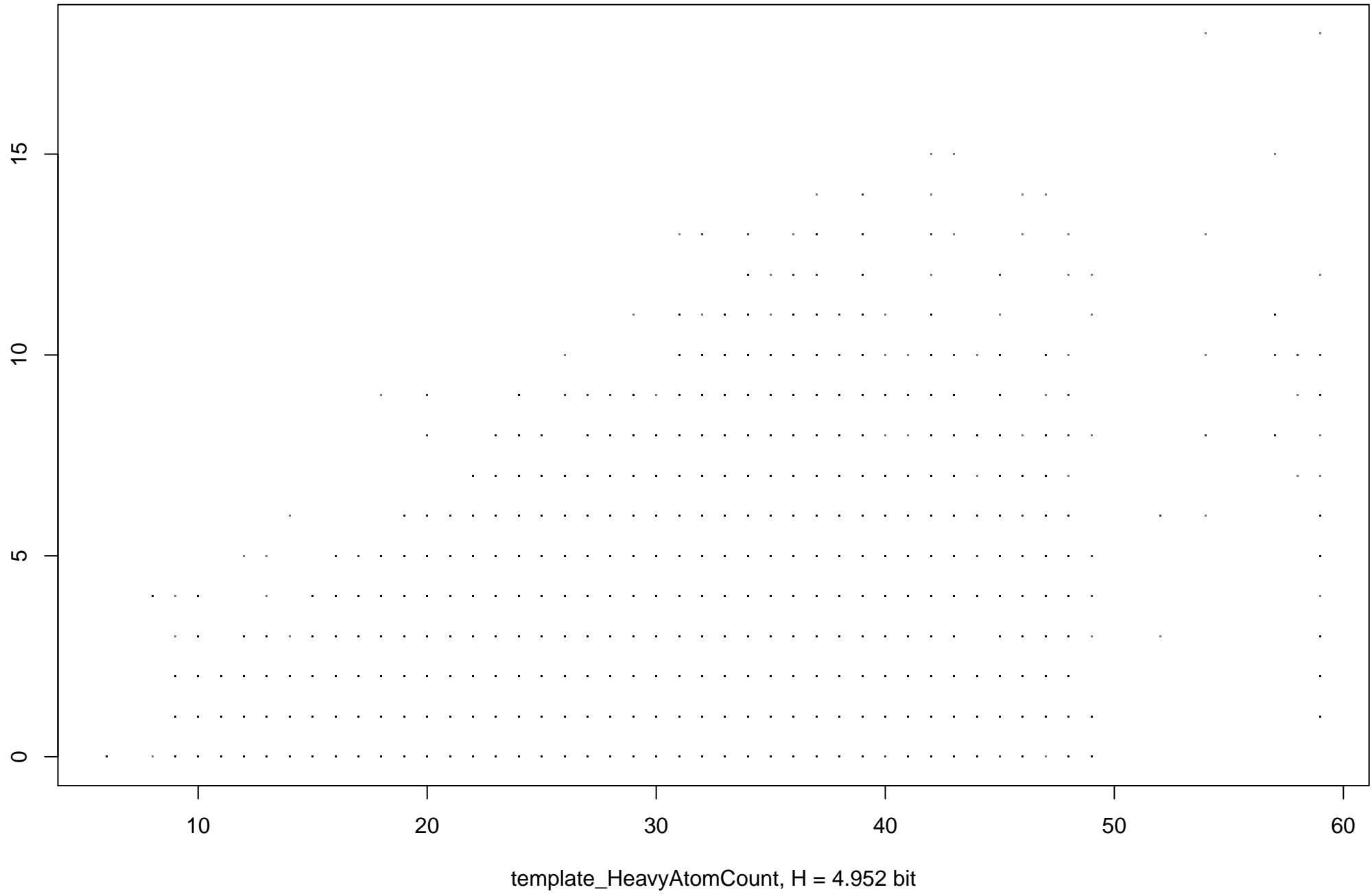


docked_NOCount-docked_RingCount, MI = 0.2853 bit, normMI = 0.1194



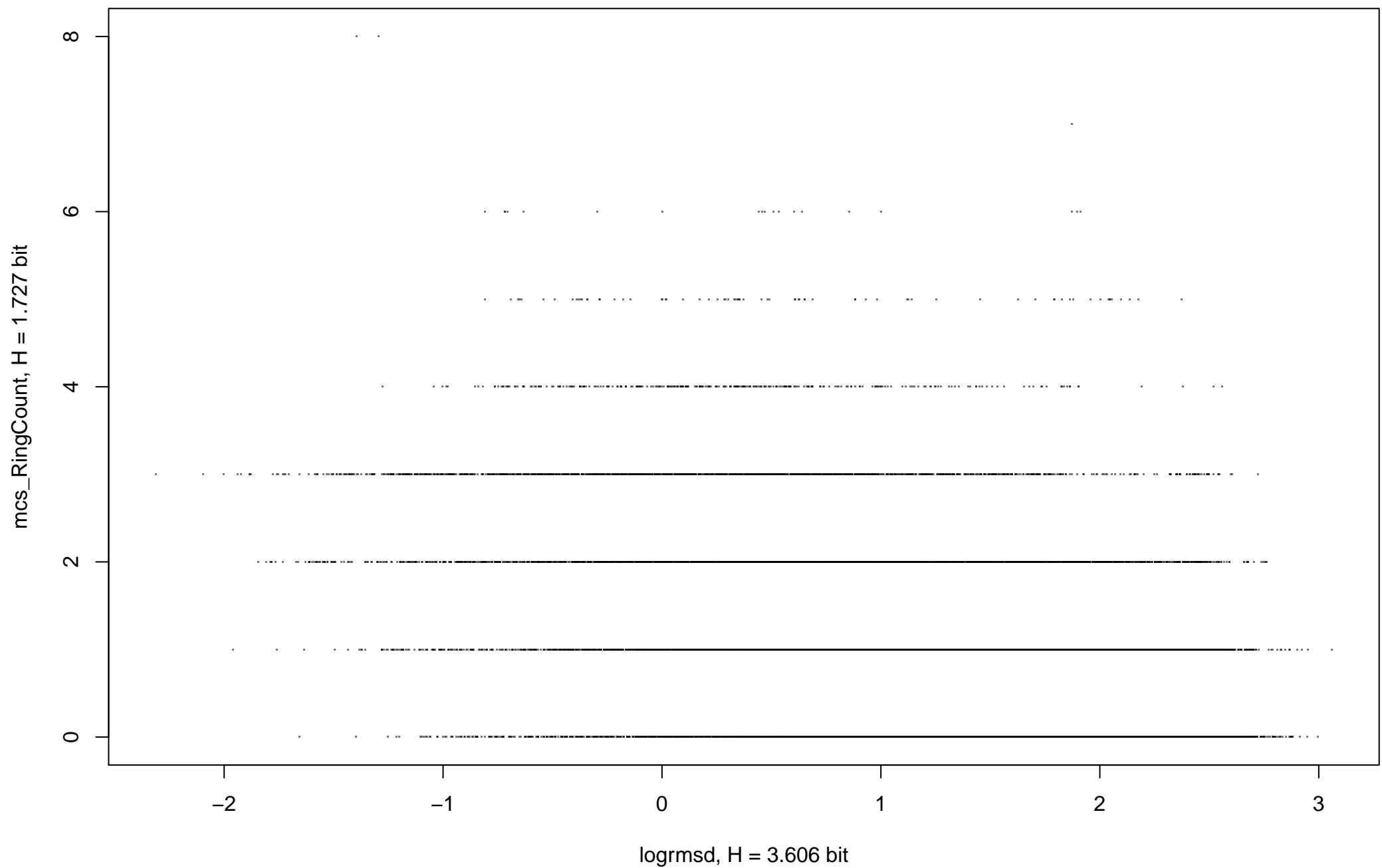
template_HeavyAtomCount-mcs_template_NumRotatableBonds, MI = 0.3703 bit, normMI = 0.1188

mcs_template_NumRotatableBonds, H = 3.118 bit

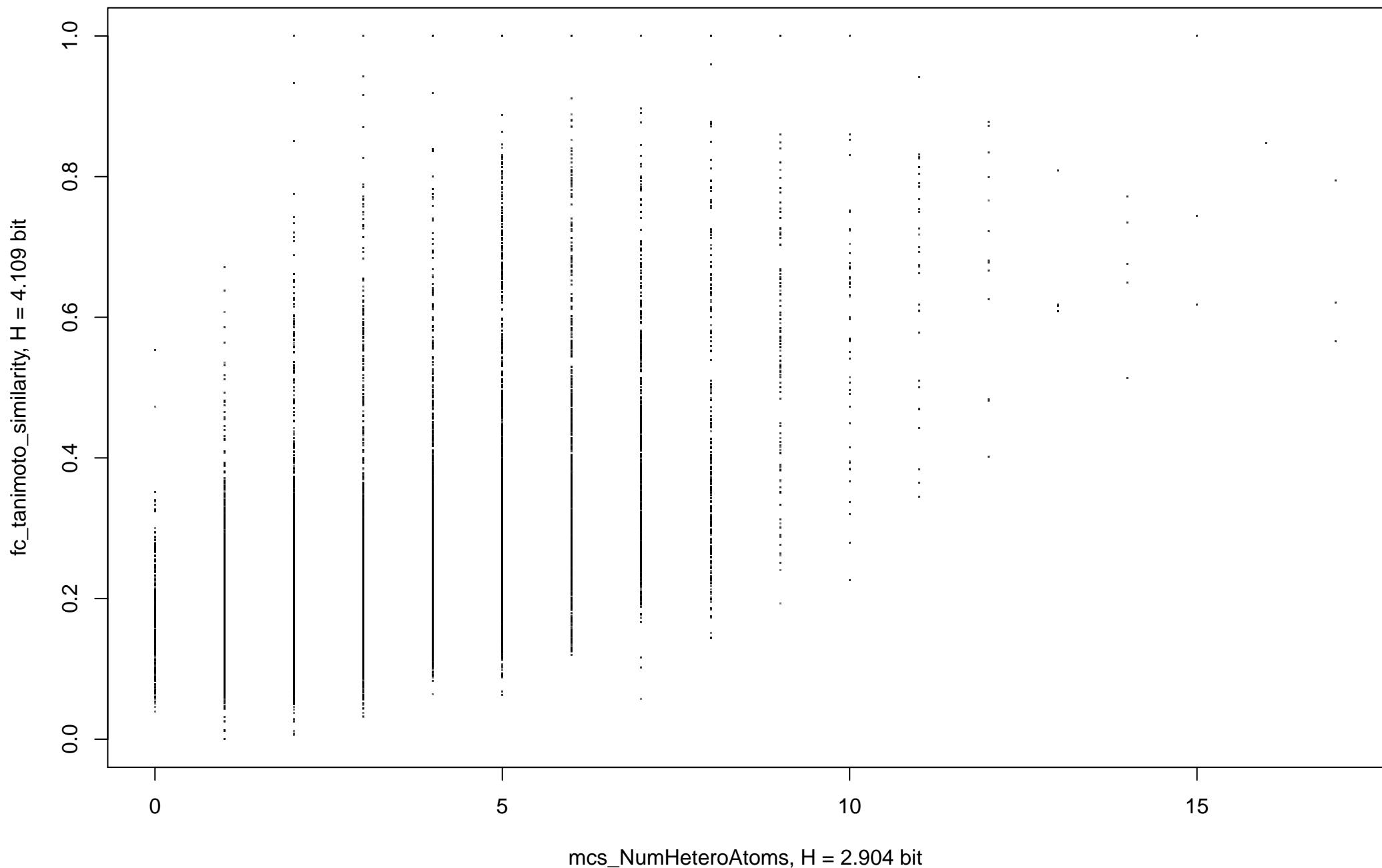


template_HeavyAtomCount, H = 4.952 bit

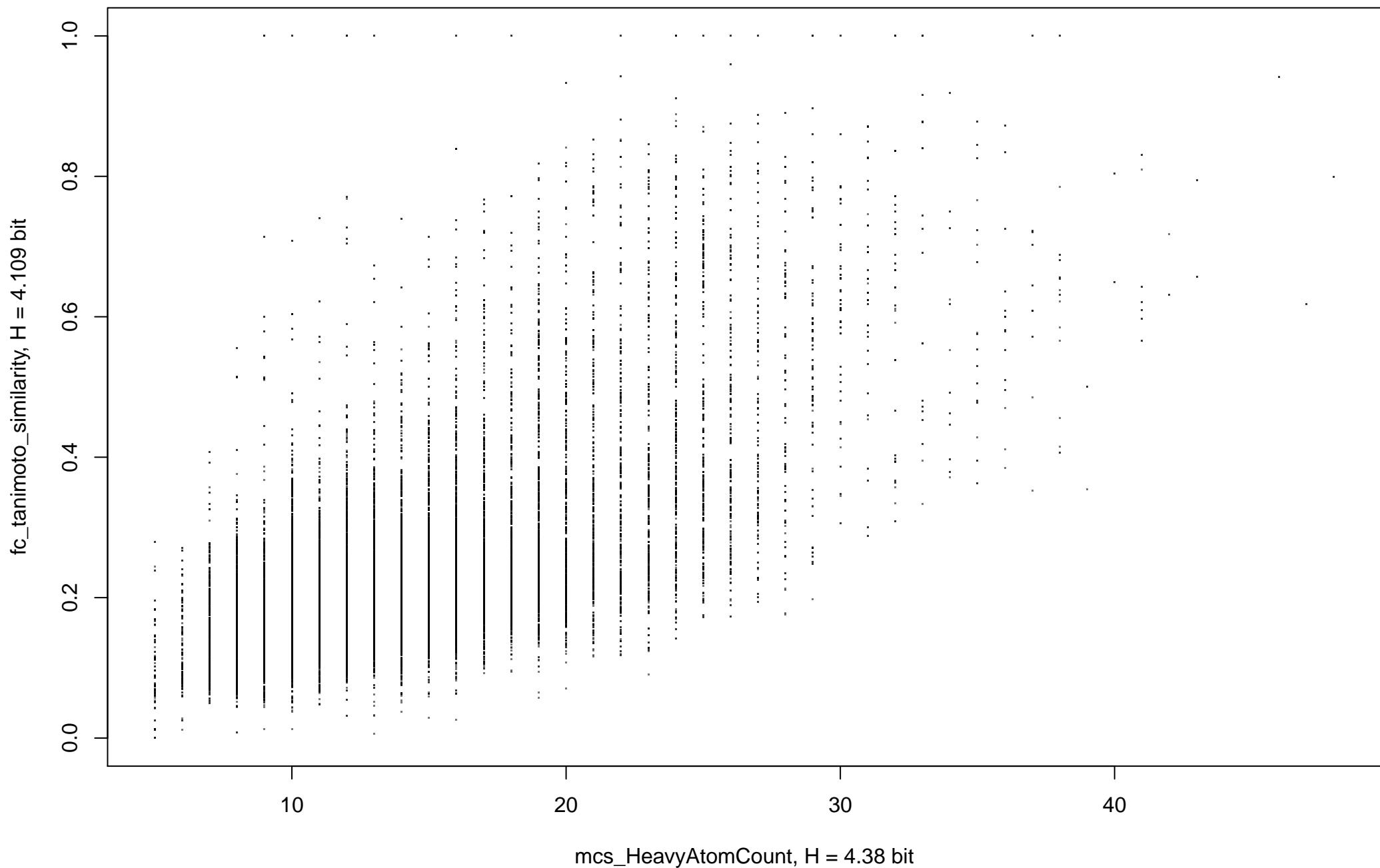
logrmsd-mcs_RingCount, MI = 0.1985 bit, normMI = 0.1149



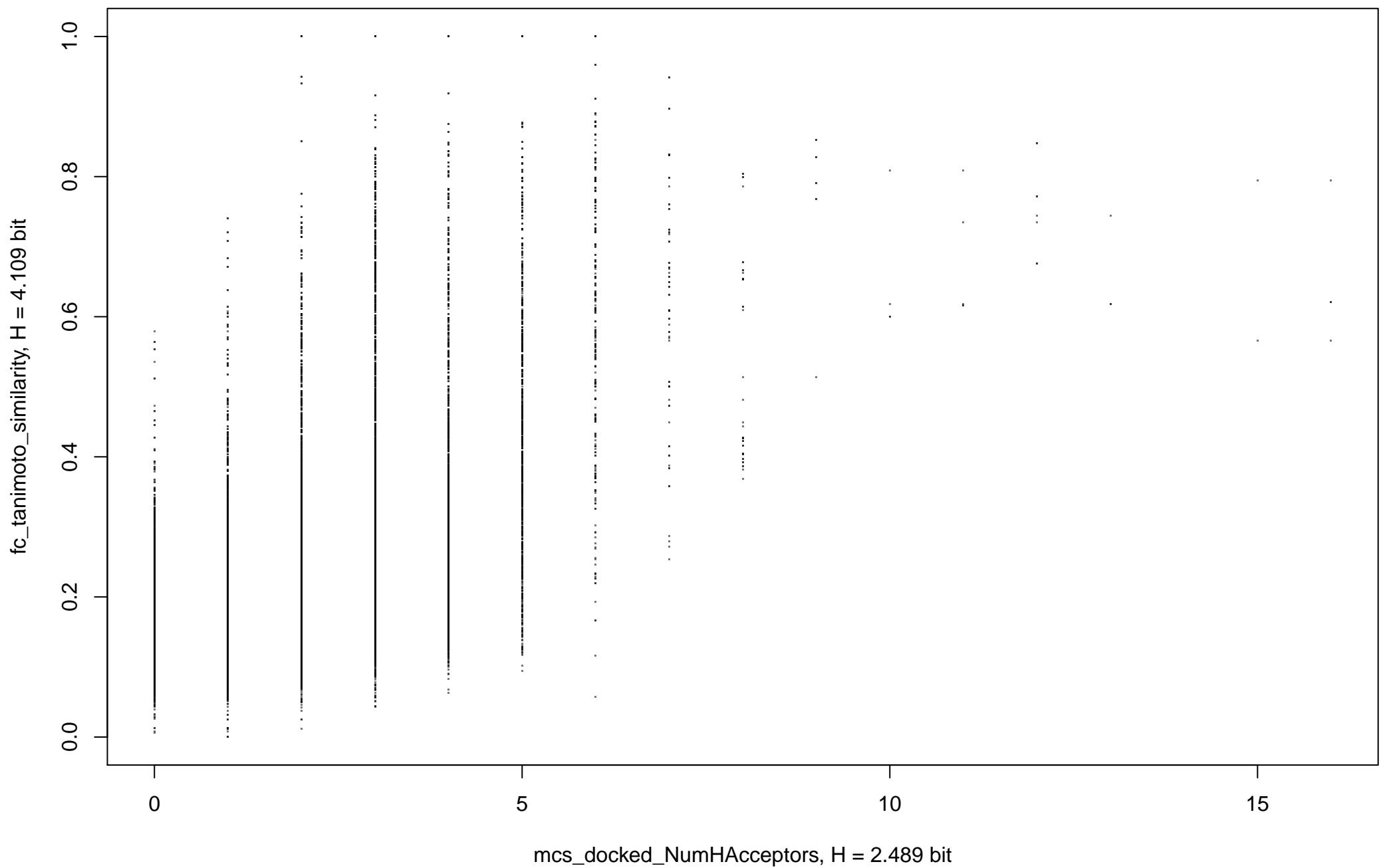
mcs_NumHeteroAtoms-fc_tanimoto_similarity, MI = 0.3325 bit, normMI = 0.1145



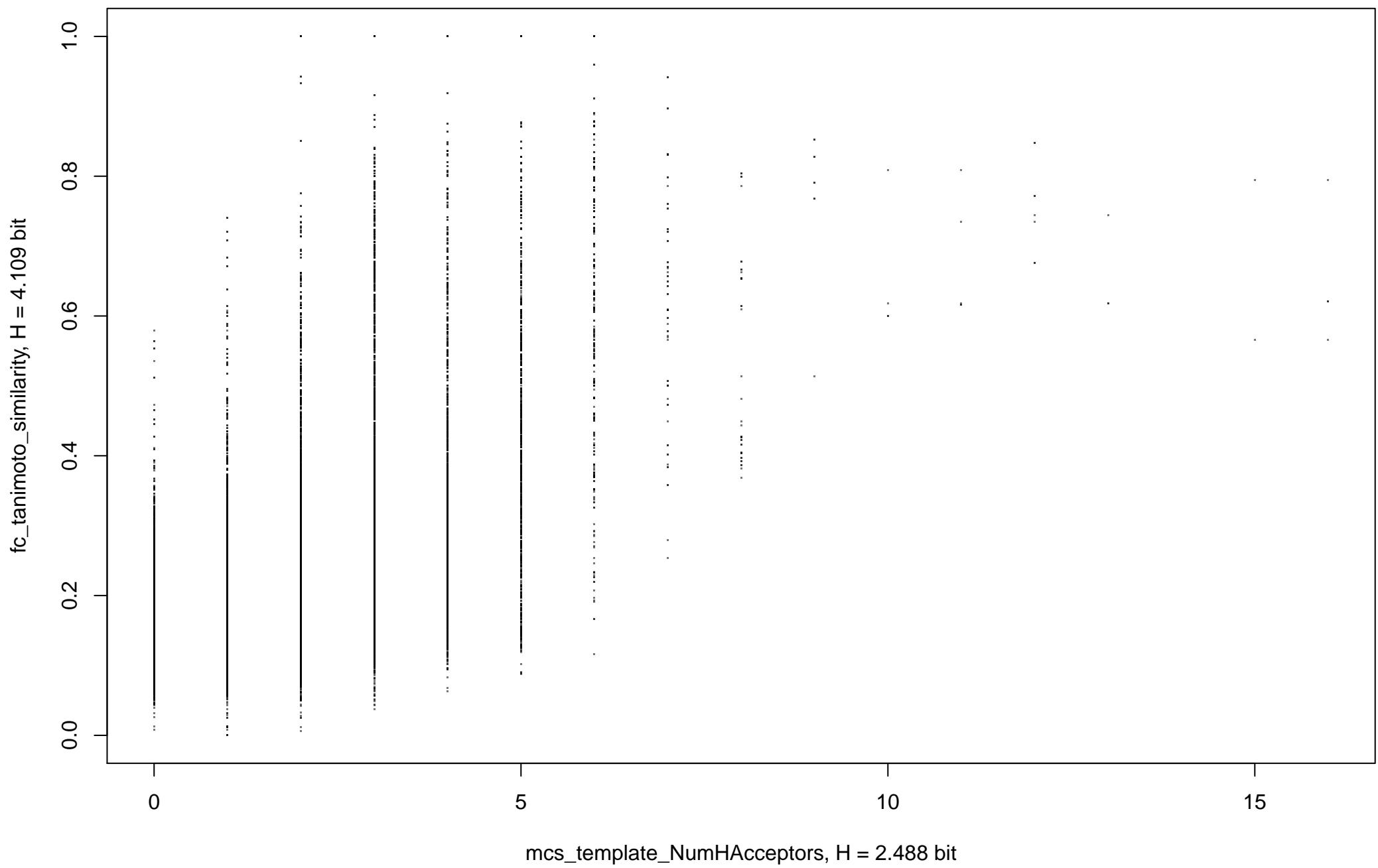
mcs_HeavyAtomCount-fc_tanimoto_similarity, MI = 0.4678 bit, normMI = 0.1139



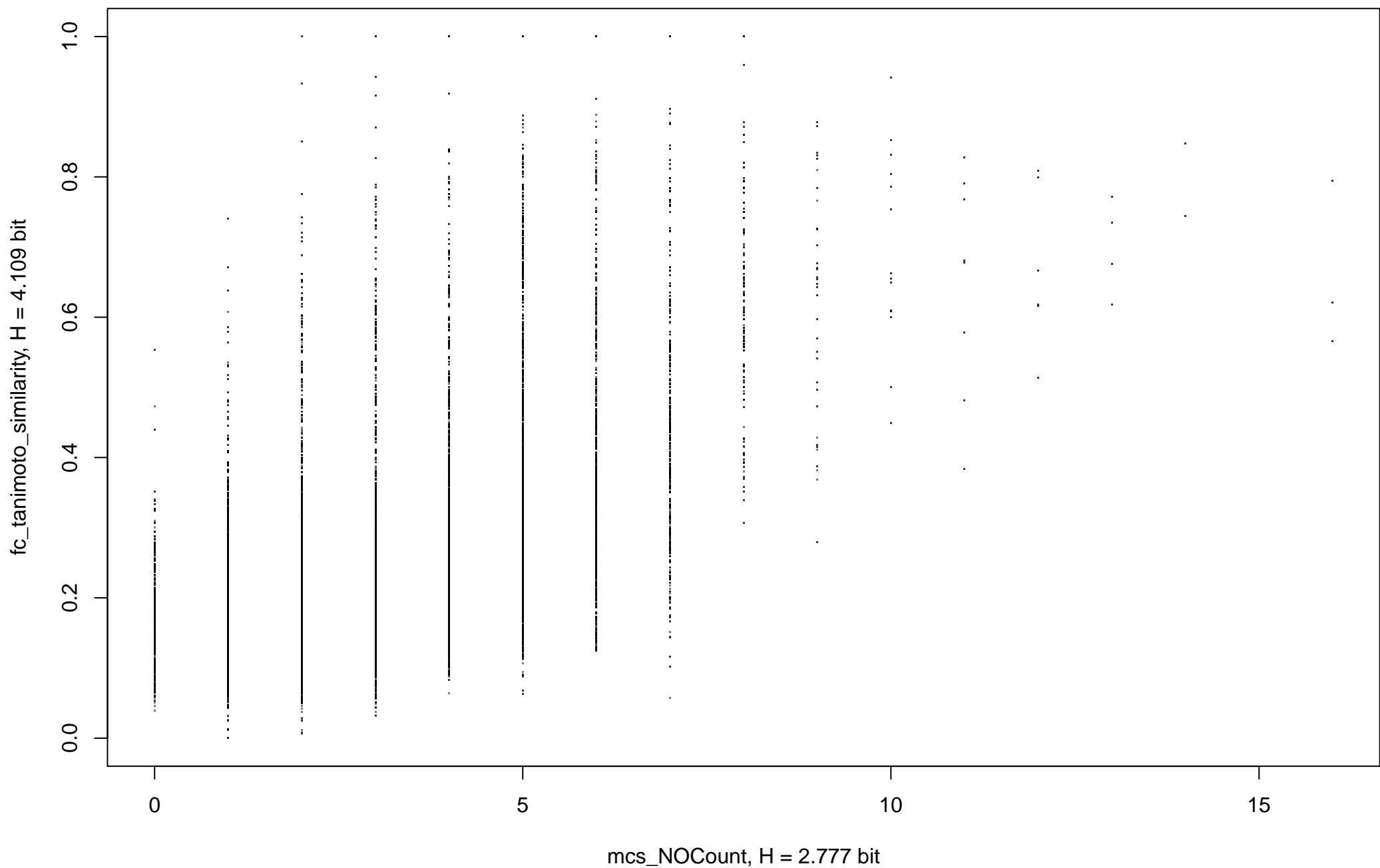
mcs_docked_NumHAcceptors-fc_tanimoto_similarity, MI = 0.2829 bit, normMI = 0.1136



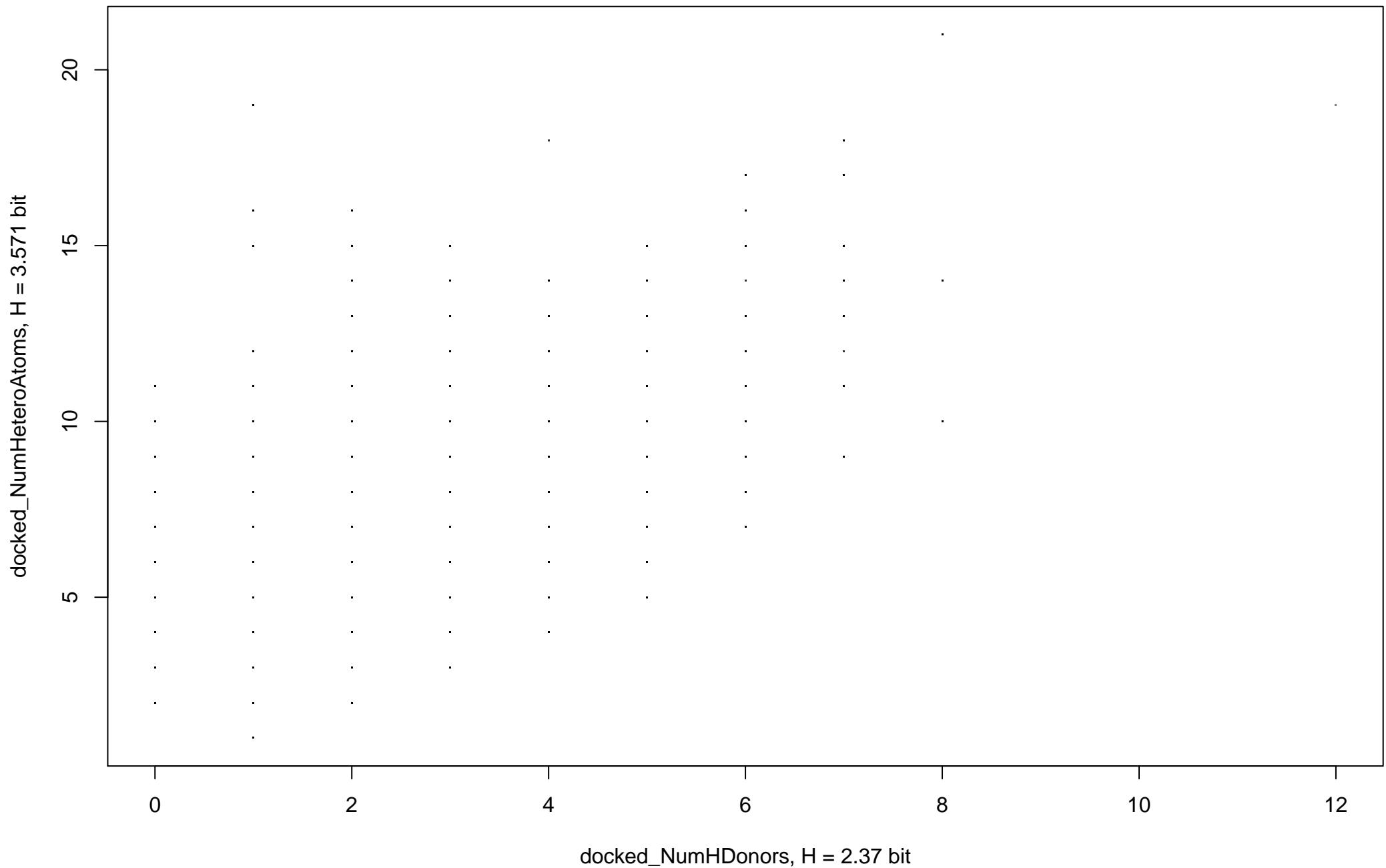
mcs_template_NumHAcceptors-fc_tanimoto_similarity, MI = 0.282 bit, normMI = 0.1133



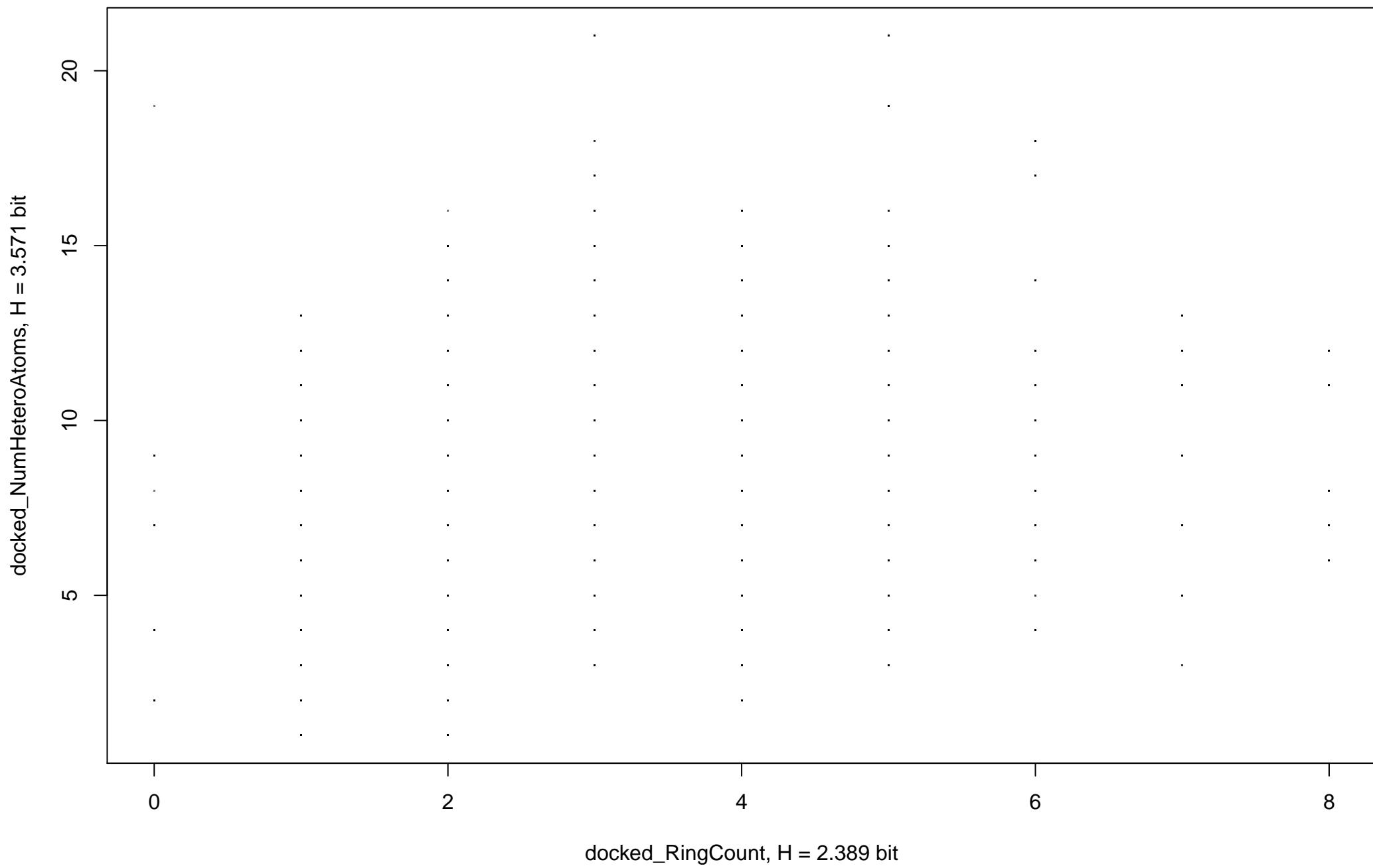
mcs_NOCount-fc_tanimoto_similarity, MI = 0.3139 bit, normMI = 0.113



docked_NumHDonors-docked_NumHeteroAtoms, MI = 0.2666 bit, normMI = 0.1125

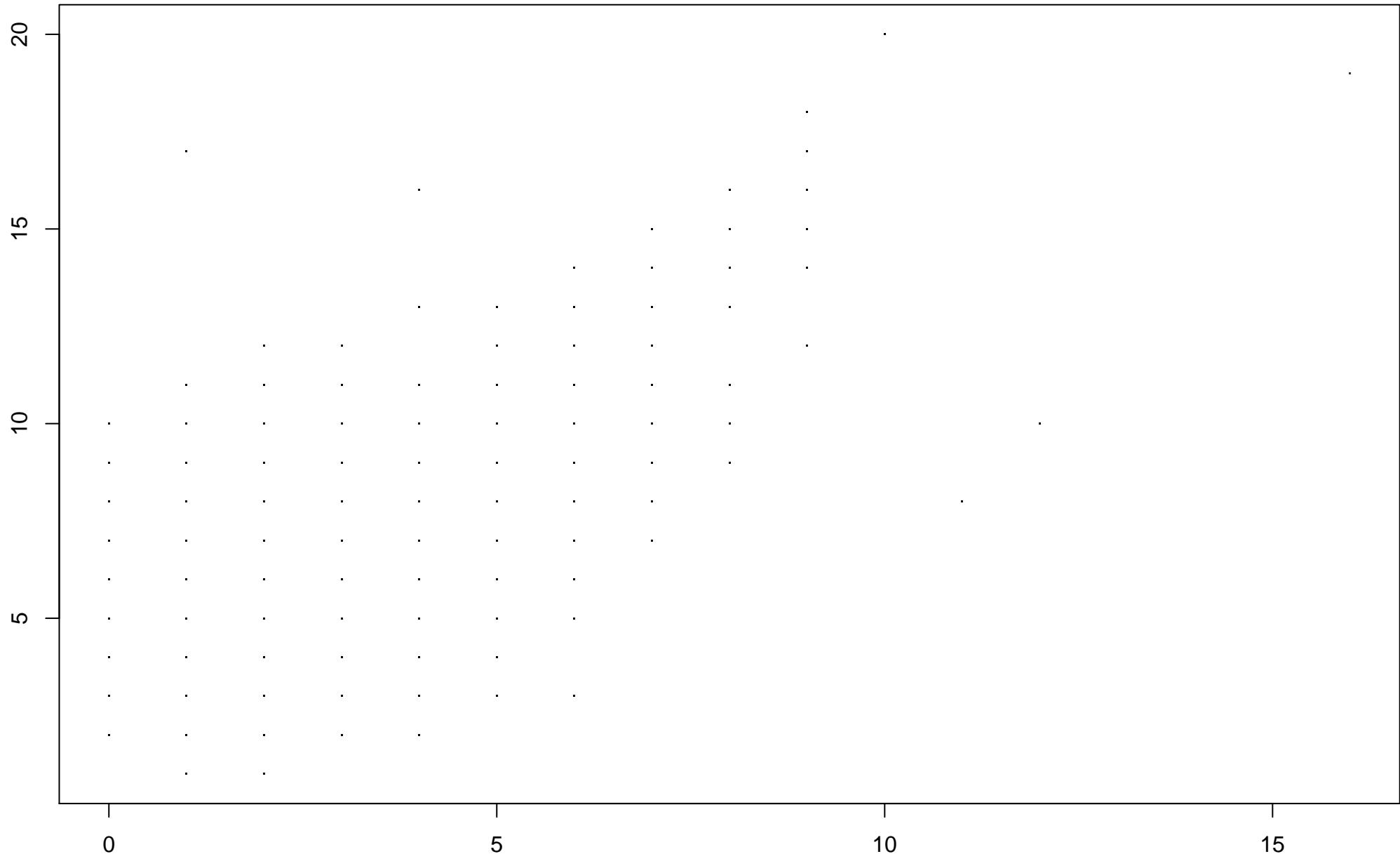


docked_RingCount–docked_NumHeteroAtoms, MI = 0.2686 bit, normMI = 0.1124



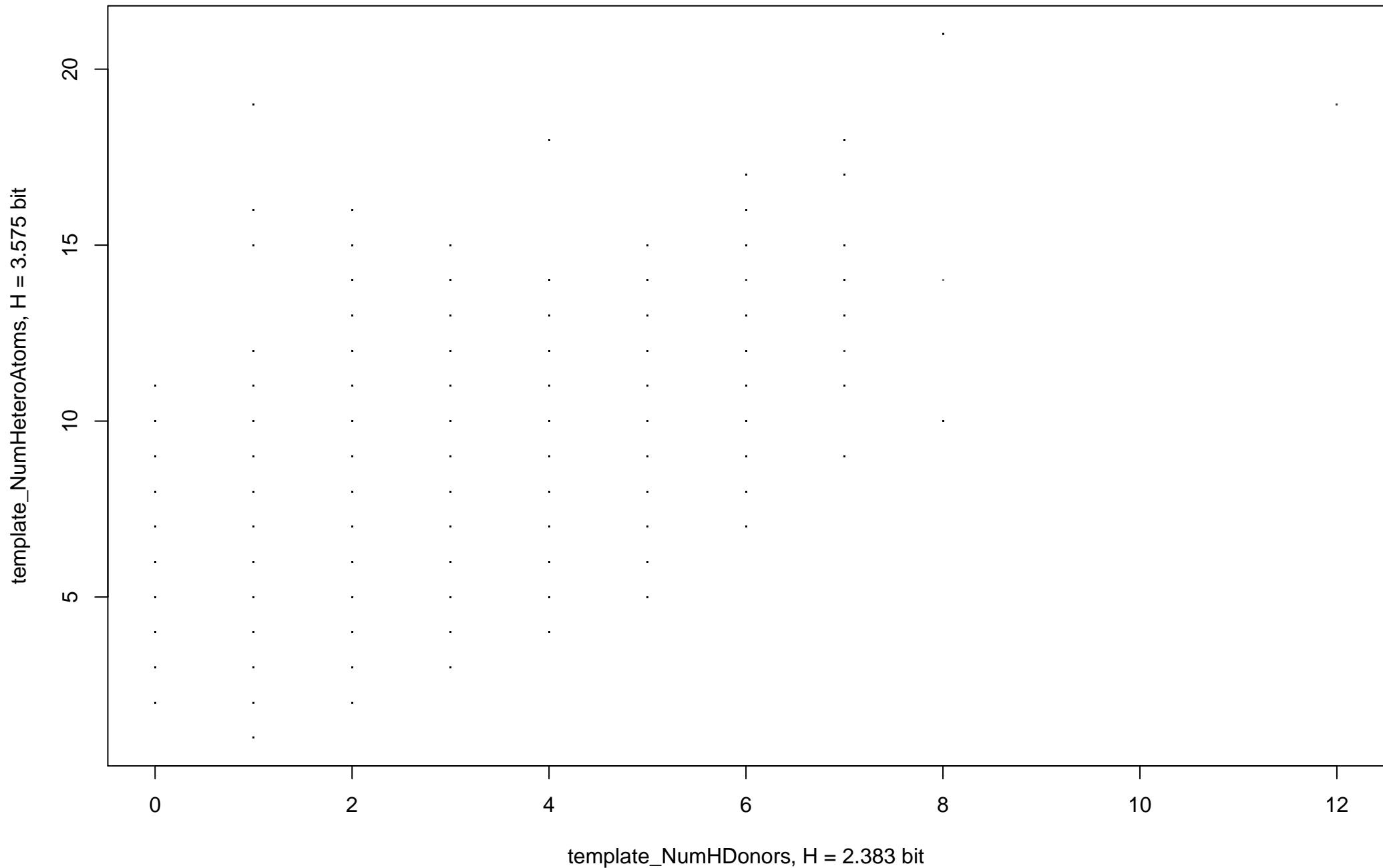
template_NHOHCount-template_NOCount, MI = 0.311 bit, normMI = 0.112

template_NOCount, H = 3.237 bit

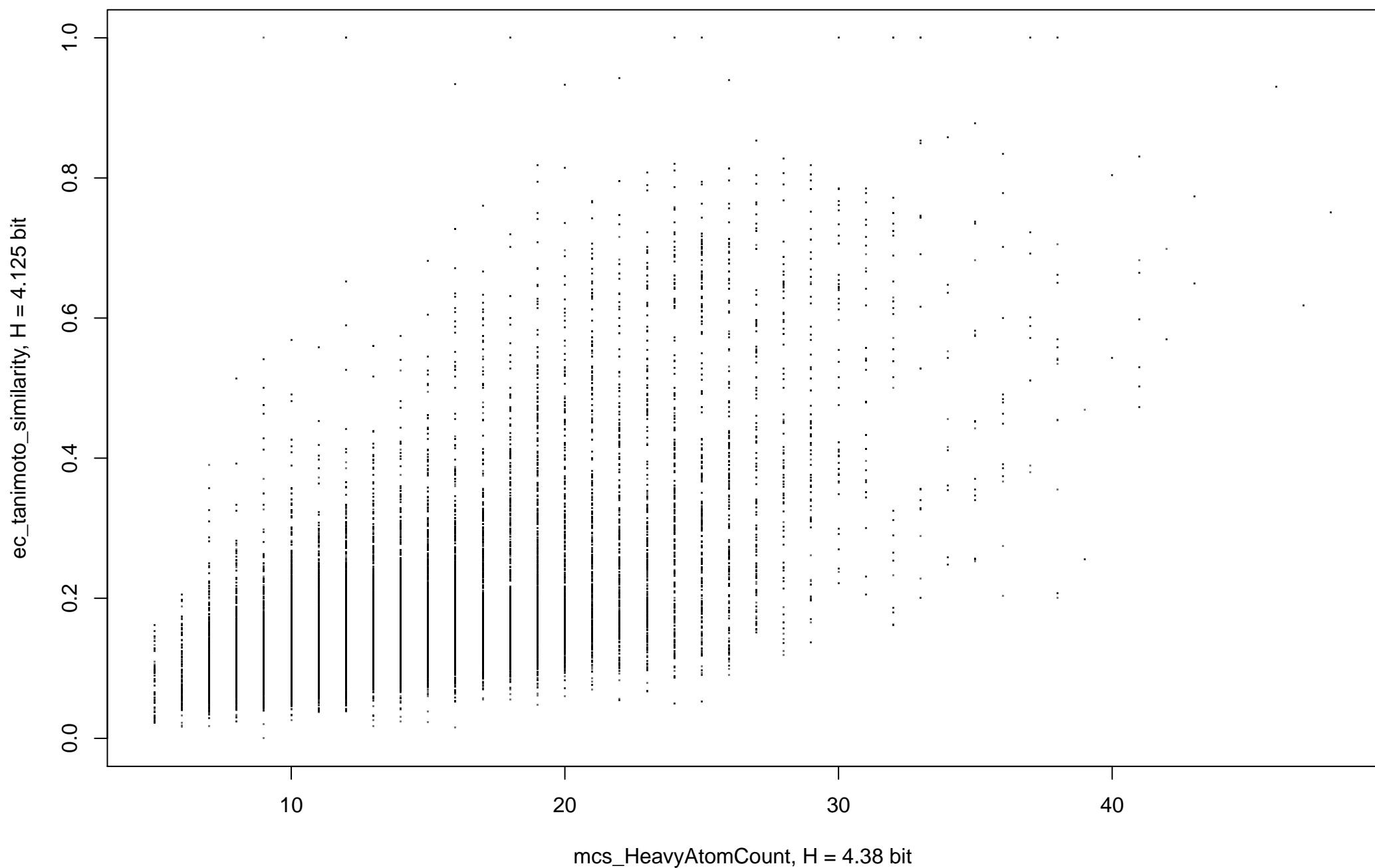


template_NHOHCount, H = 2.775 bit

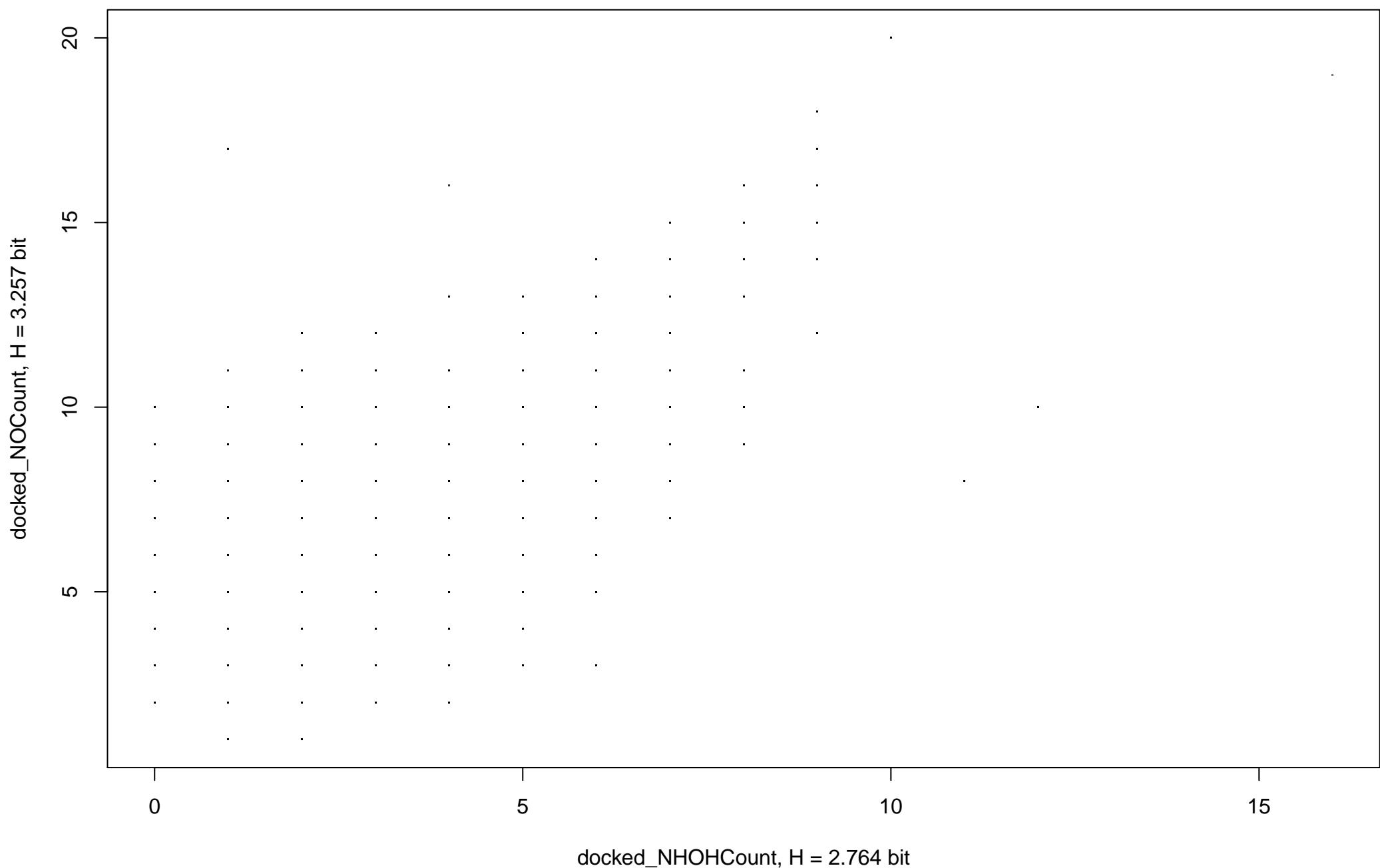
template_NumHDonors–template_NumHeteroAtoms, MI = 0.2642 bit, normMI = 0.1108



mcs_HeavyAtomCount–ec_tanimoto_similarity, MI = 0.4567 bit, normMI = 0.1107

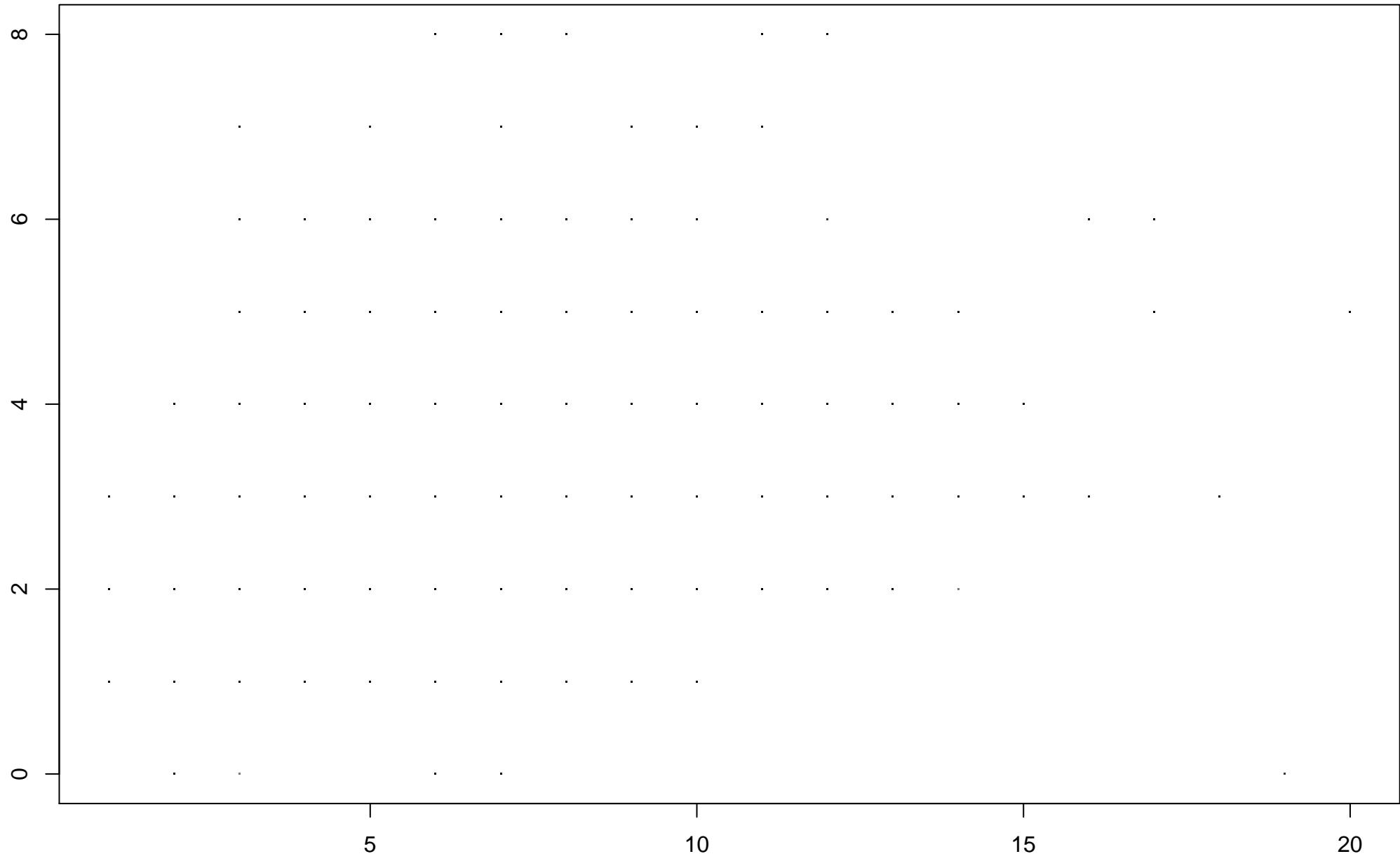


docked_NHOHCount–docked_NOCount, MI = 0.3015 bit, normMI = 0.1091



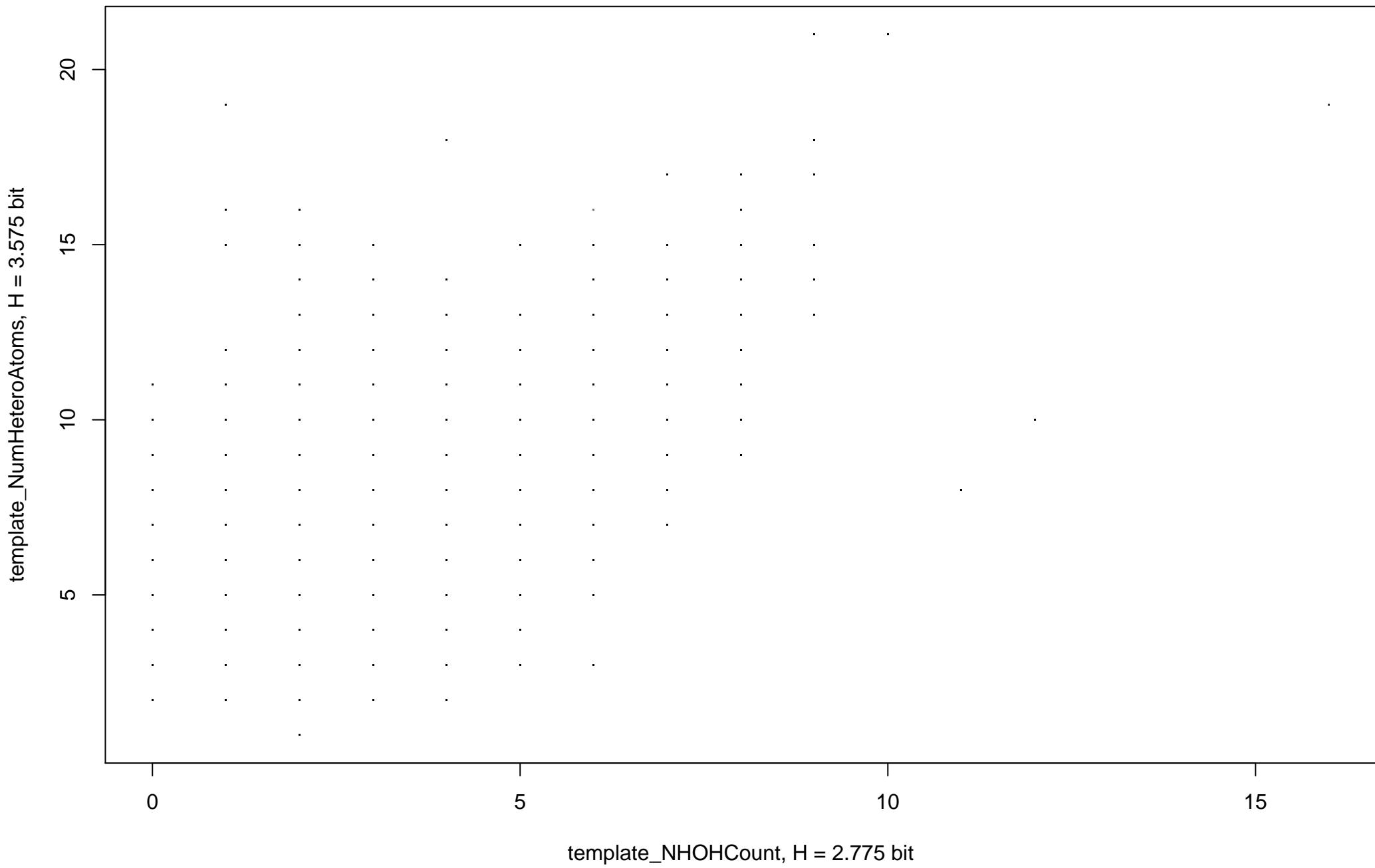
template_NOCount-template_RingCount, MI = 0.2511 bit, normMI = 0.1066

template_RingCount, H = 2.356 bit

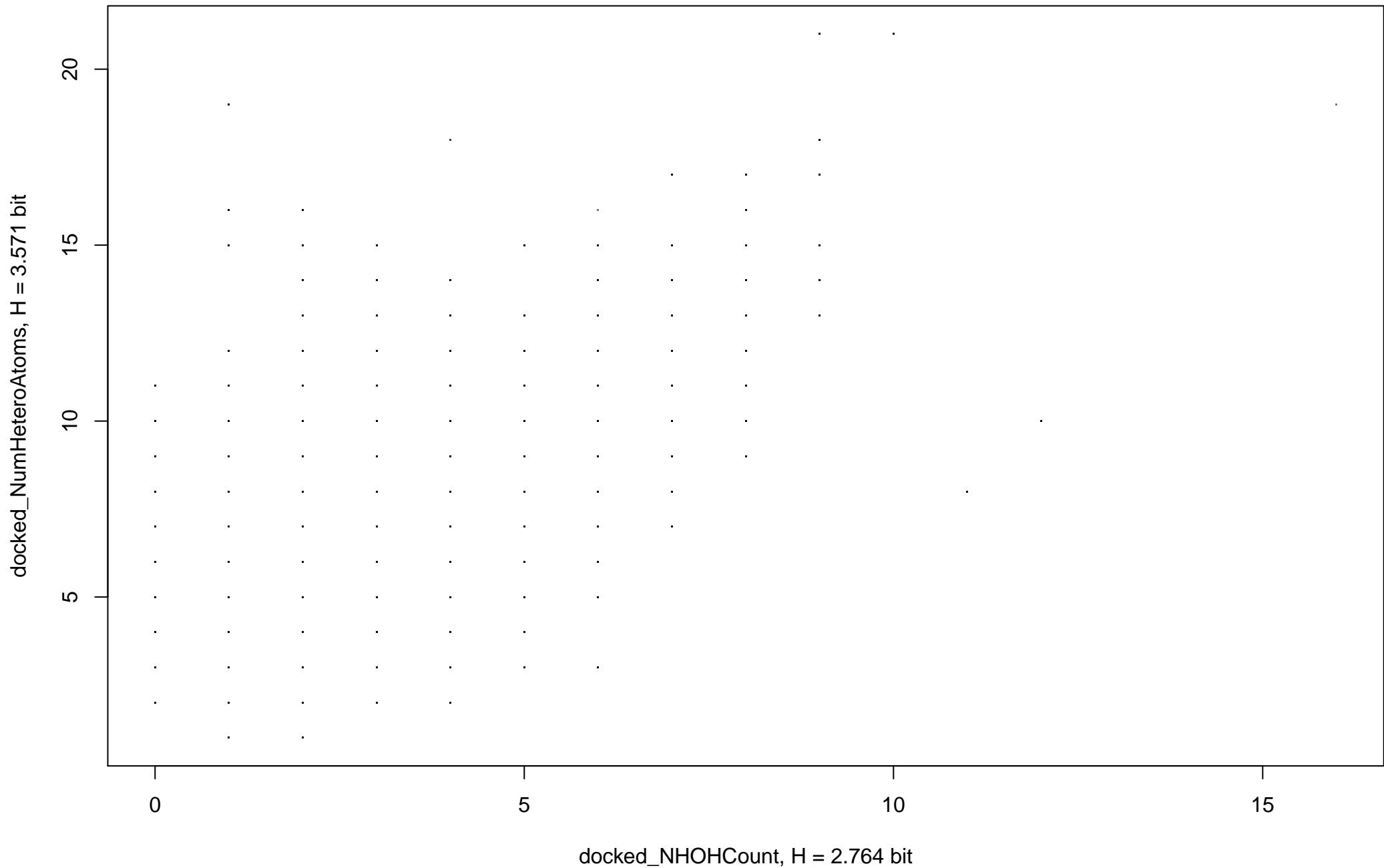


template_NOCount, H = 3.237 bit

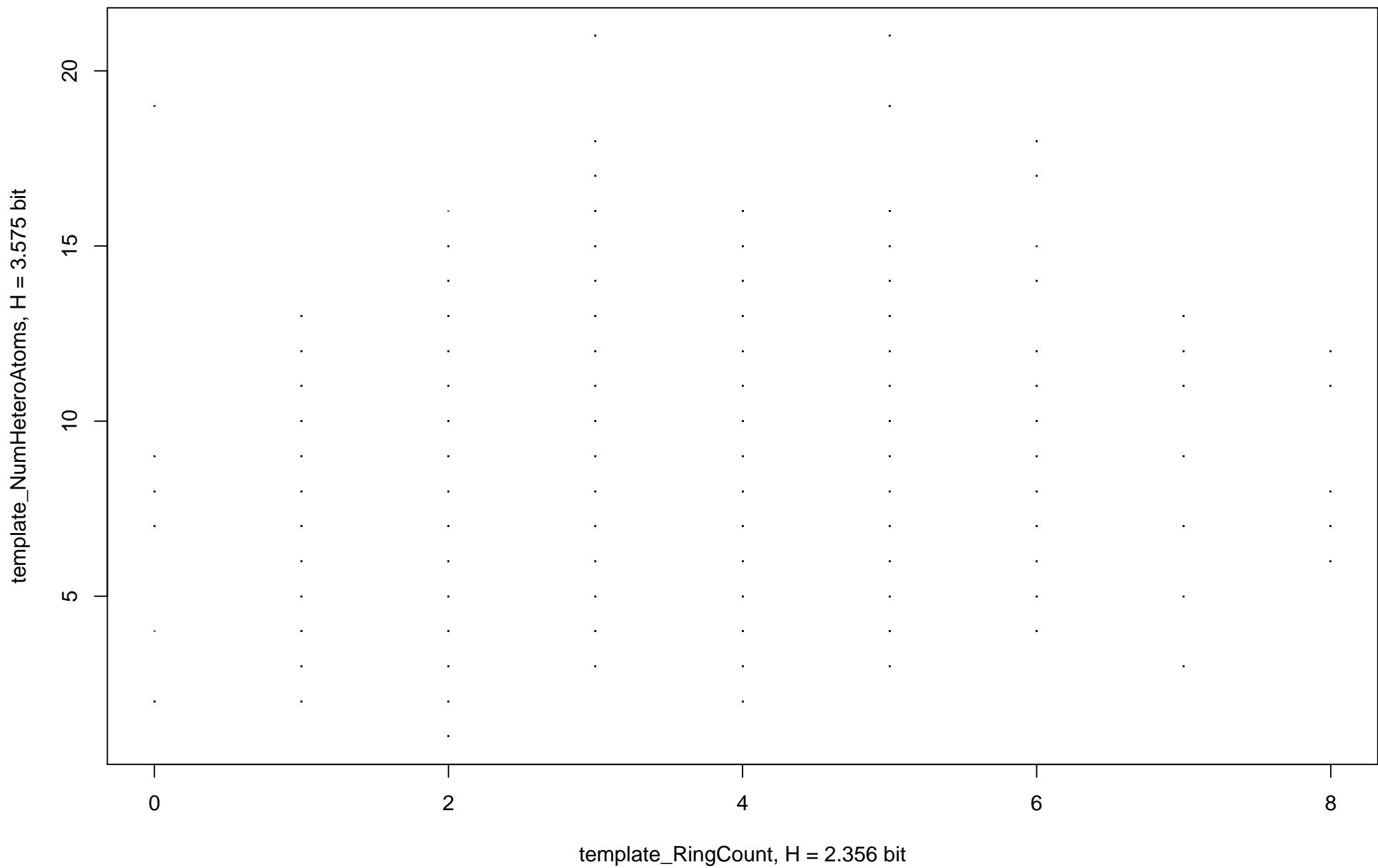
template_NHOHCount-template_NumHeteroAtoms, MI = 0.2891 bit, normMI = 0.1042



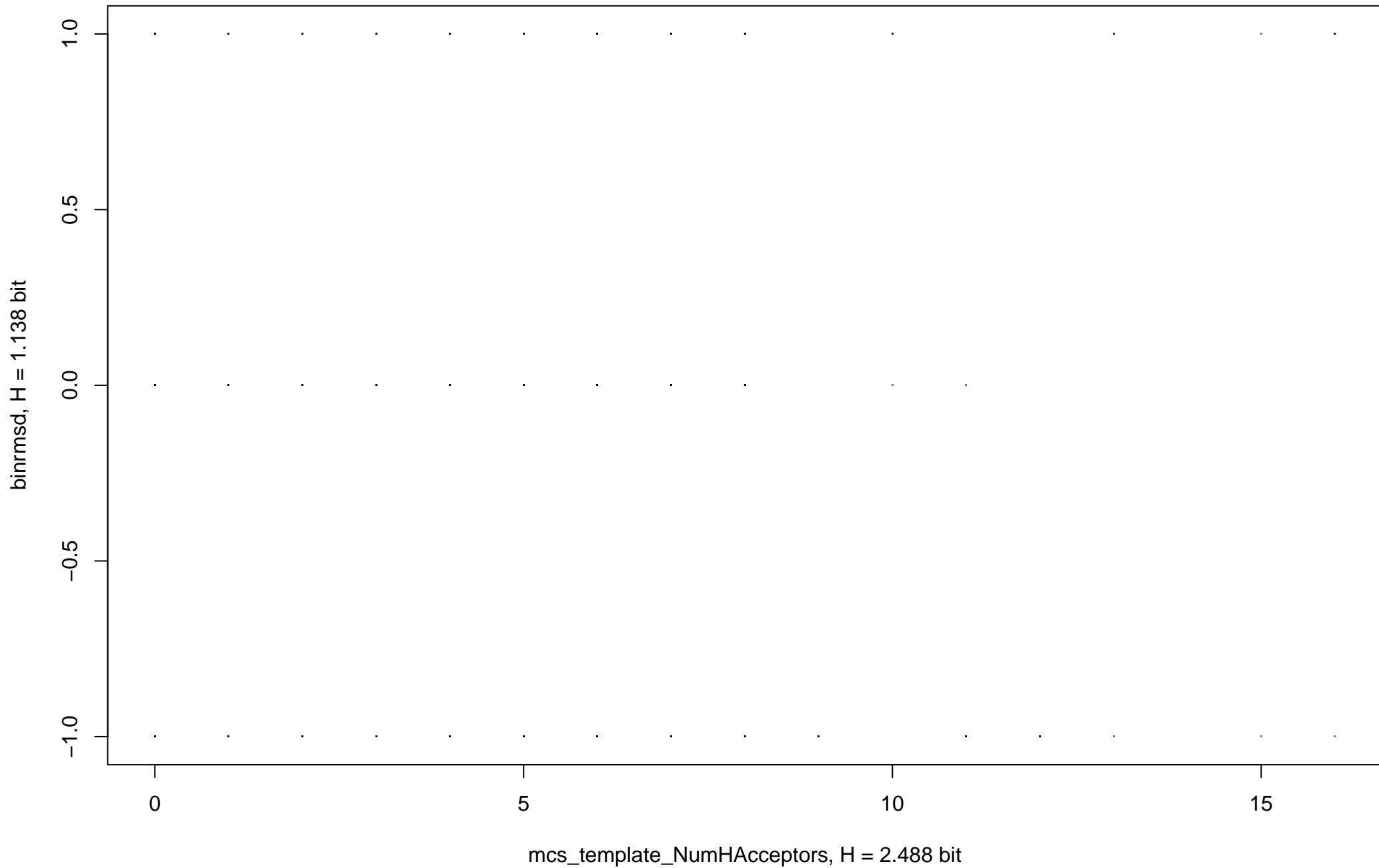
docked_NHOHCount–docked_NumHeteroAtoms, MI = 0.2776 bit, normMI = 0.1004



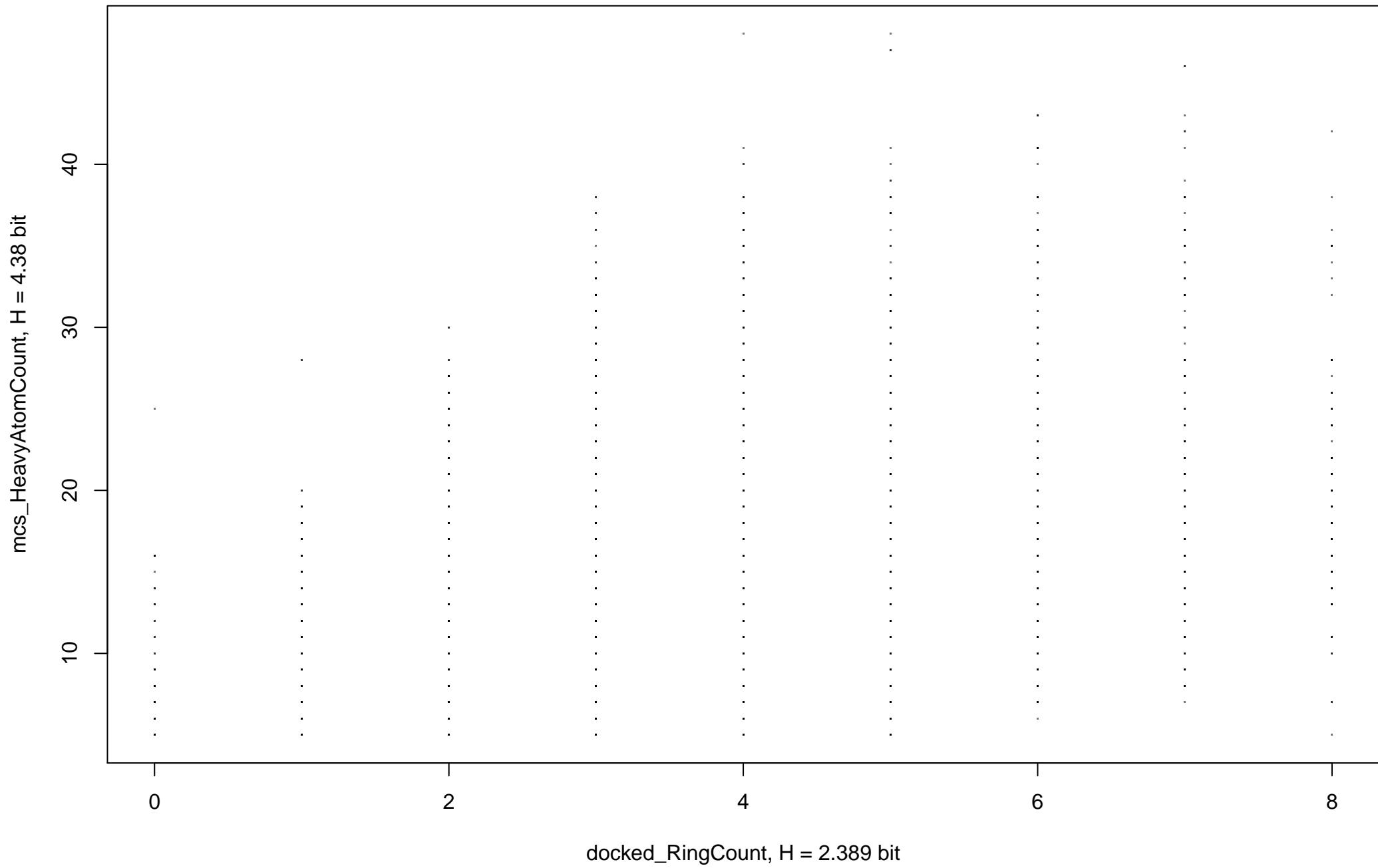
template_RingCount-template_NumHeteroAtoms, MI = 0.2356 bit, normMI = 0.09999



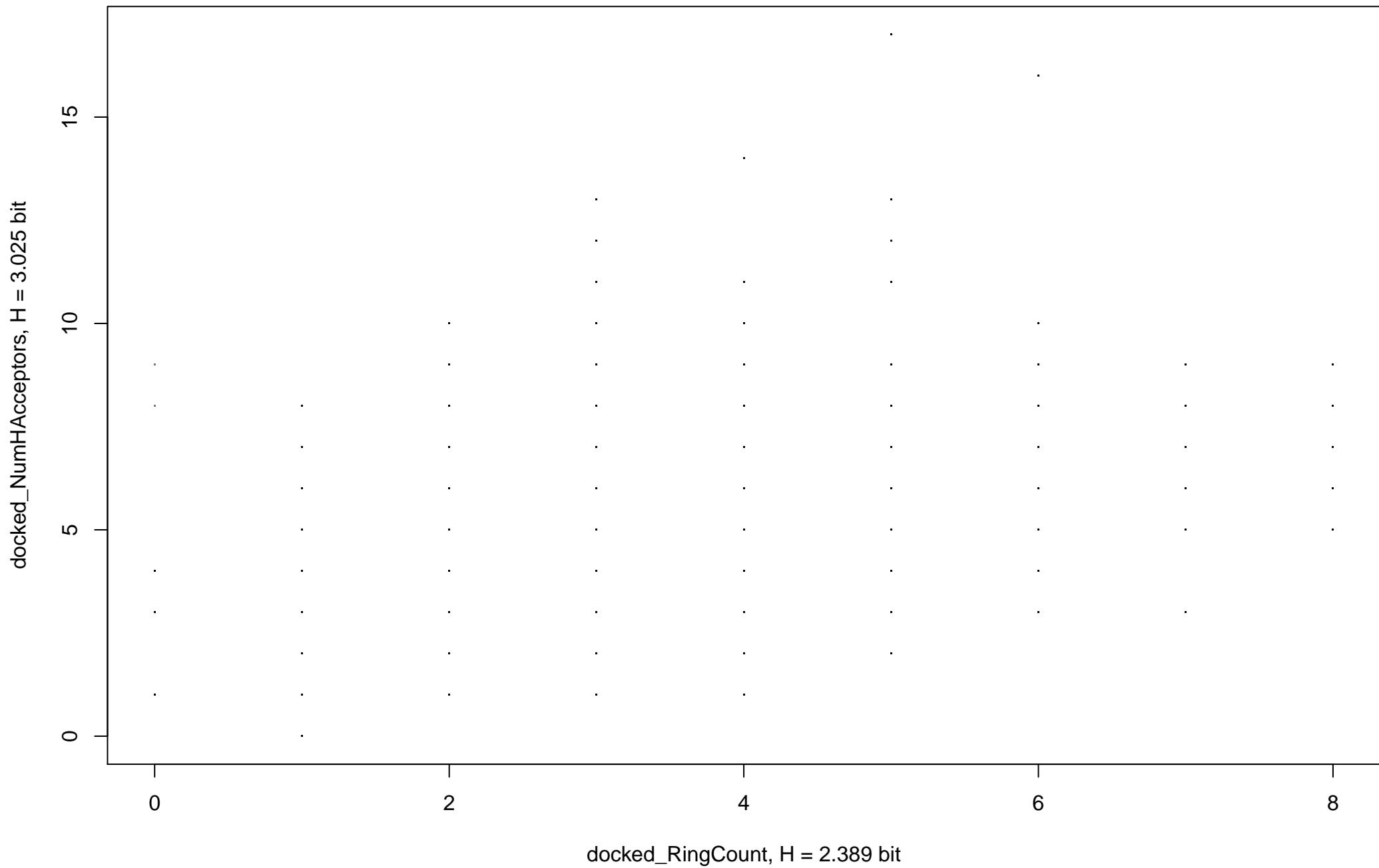
mcs_template_NumHAcceptors-binrmsd, MI = 0.1094 bit, normMI = 0.09616



docked_RingCount-mcs_HeavyAtomCount, MI = 0.2294 bit, normMI = 0.09604

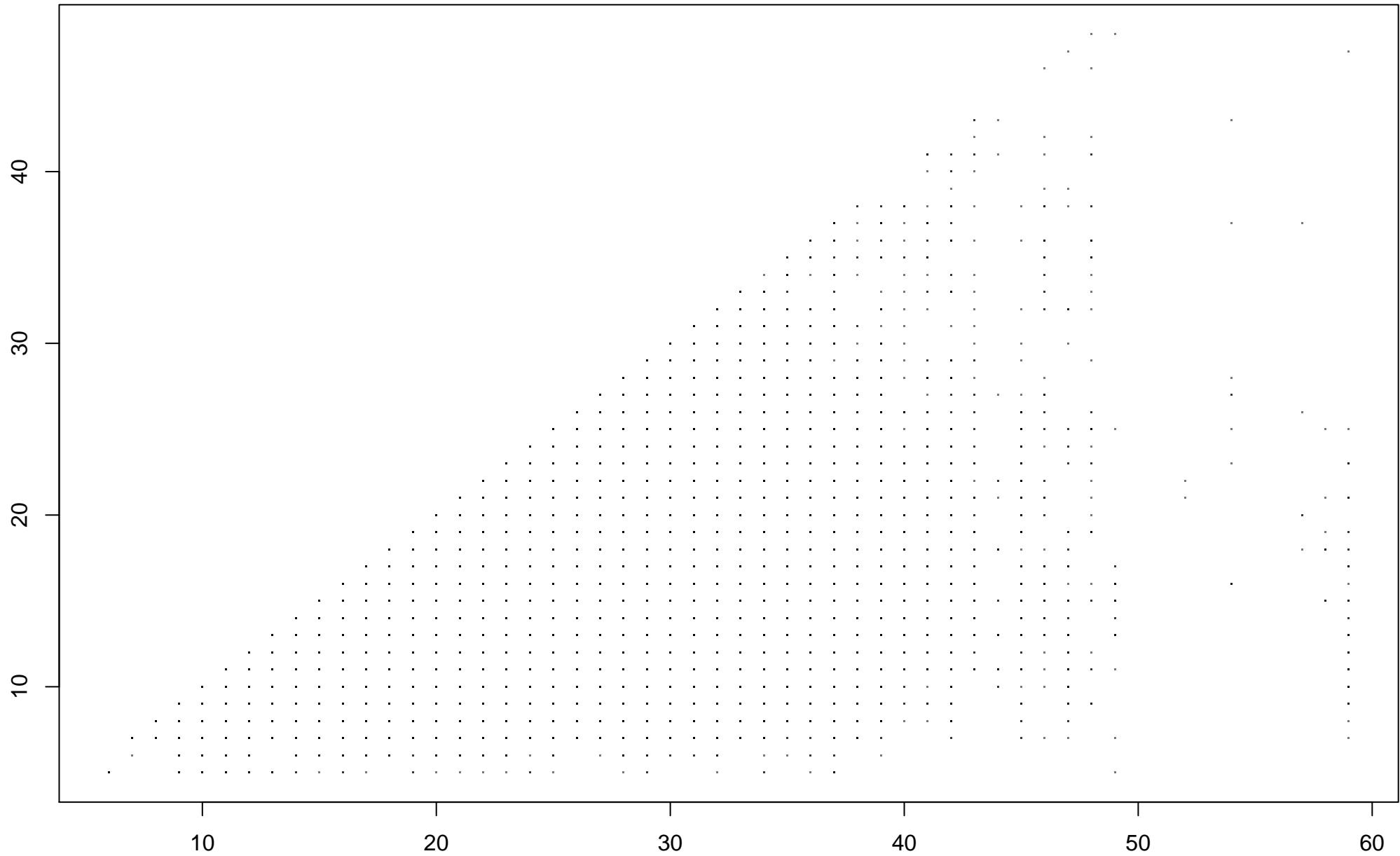


docked_RingCount-docked_NumHAcceptors, MI = 0.2293 bit, normMI = 0.09596



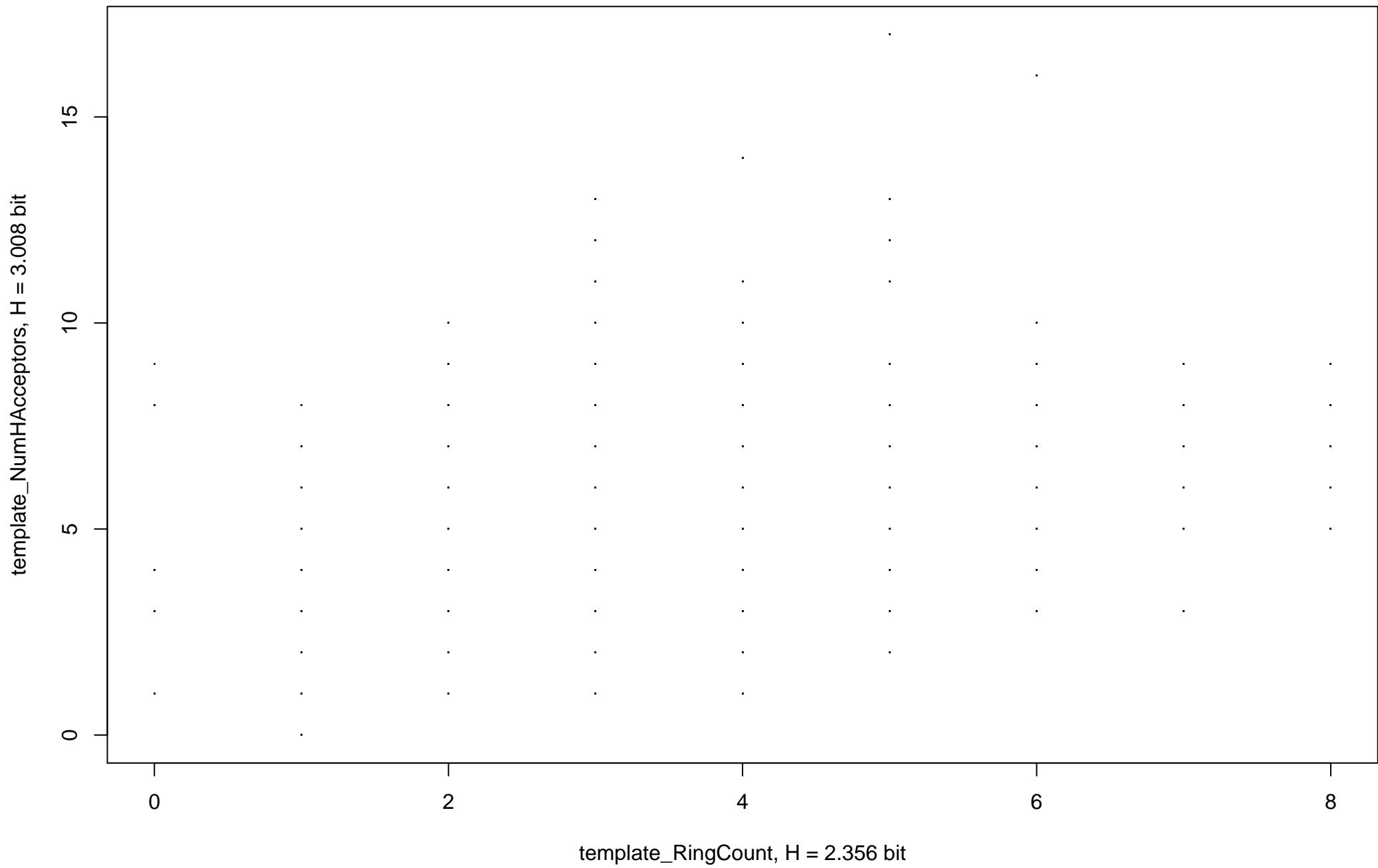
docked_HeavyAtomCount-mcs_HeavyAtomCount, MI = 0.4198 bit, normMI = 0.09584

mcs_HeavyAtomCount, H = 4.38 bit

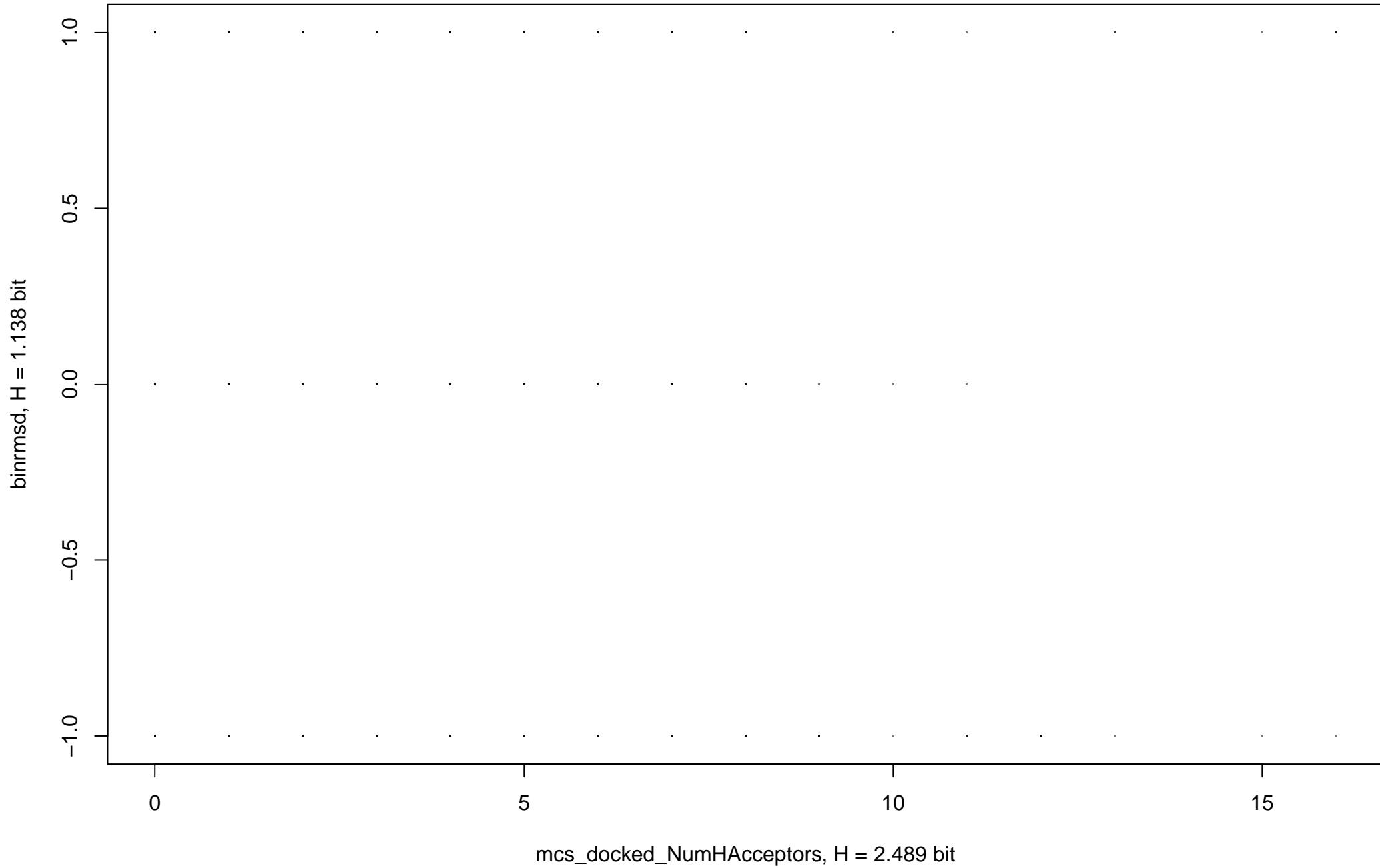


docked_HeavyAtomCount, H = 4.99 bit

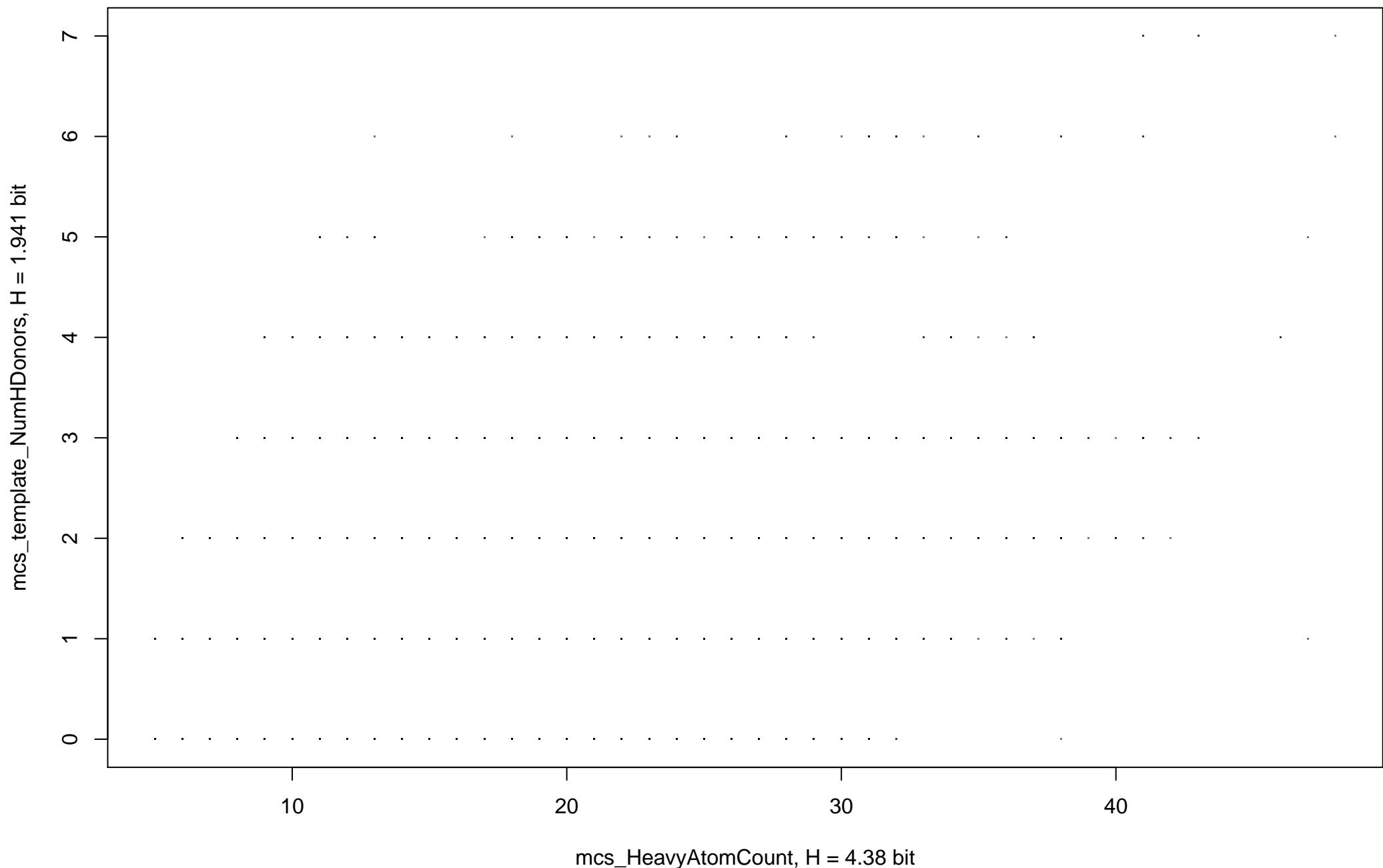
template_RingCount-template_NumHAcceptors, MI = 0.2238 bit, normMI = 0.09501



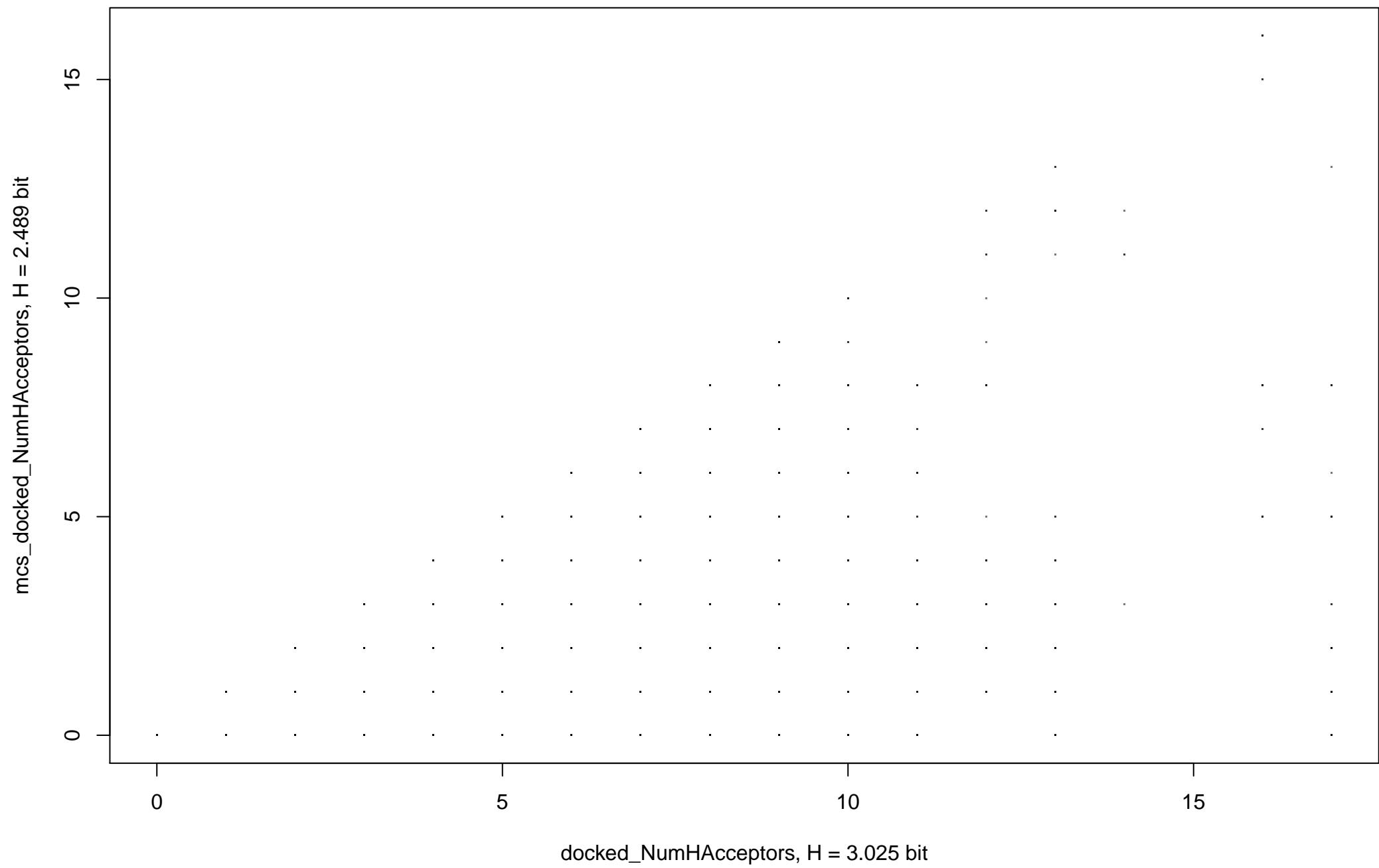
mcs_docked_NumHAcceptors–binrmsd, MI = 0.108 bit, normMI = 0.09494



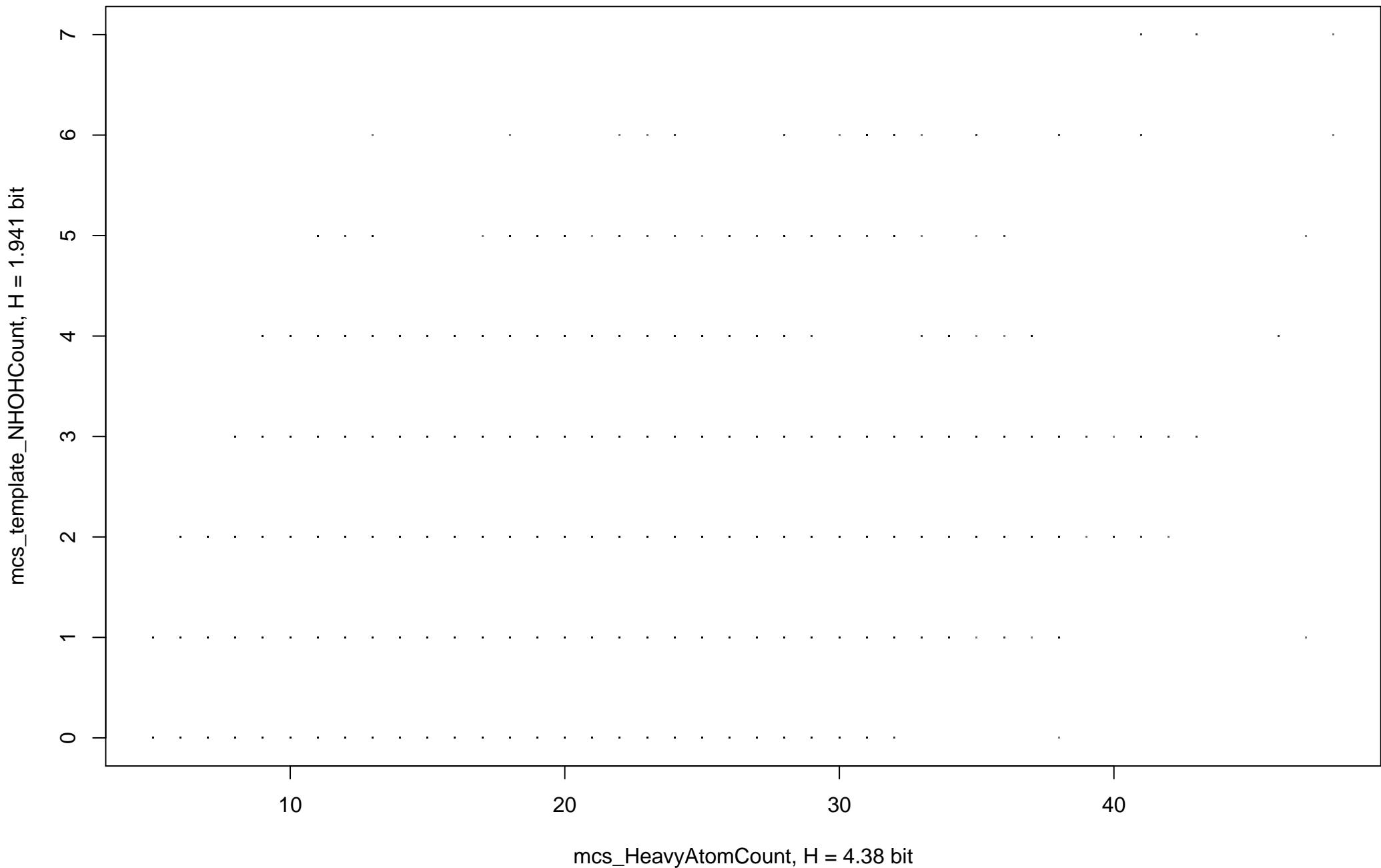
mcs_HeavyAtomCount-mcs_template_NumHDonors, MI = 0.1782 bit, normMI = 0.09183



docked_NumHAcceptors-mcs_docked_NumHAcceptors, MI = 0.2286 bit, normMI = 0.09182

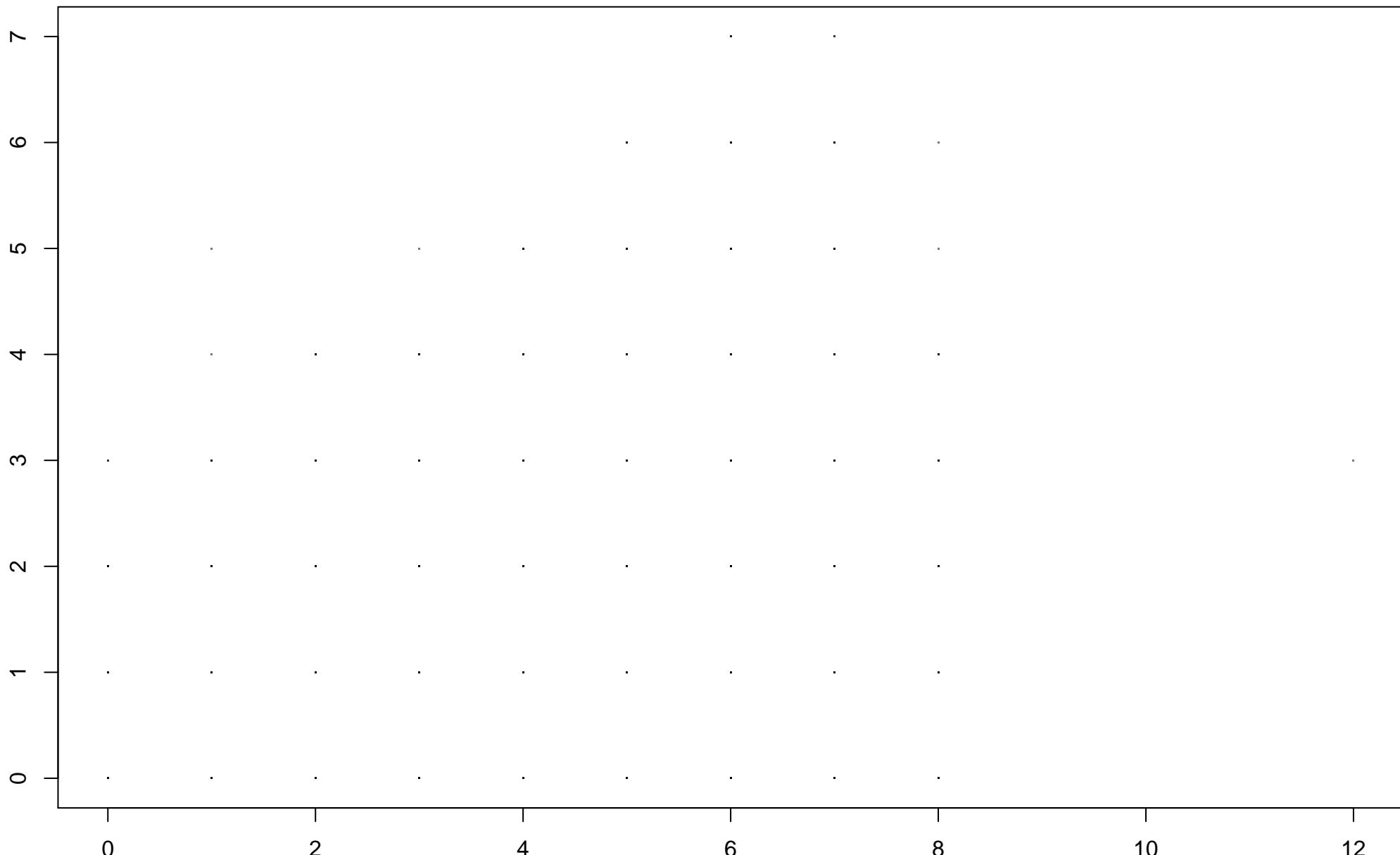


mcs_HeavyAtomCount-mcs_template_NHOHCount, MI = 0.1782 bit, normMI = 0.0918



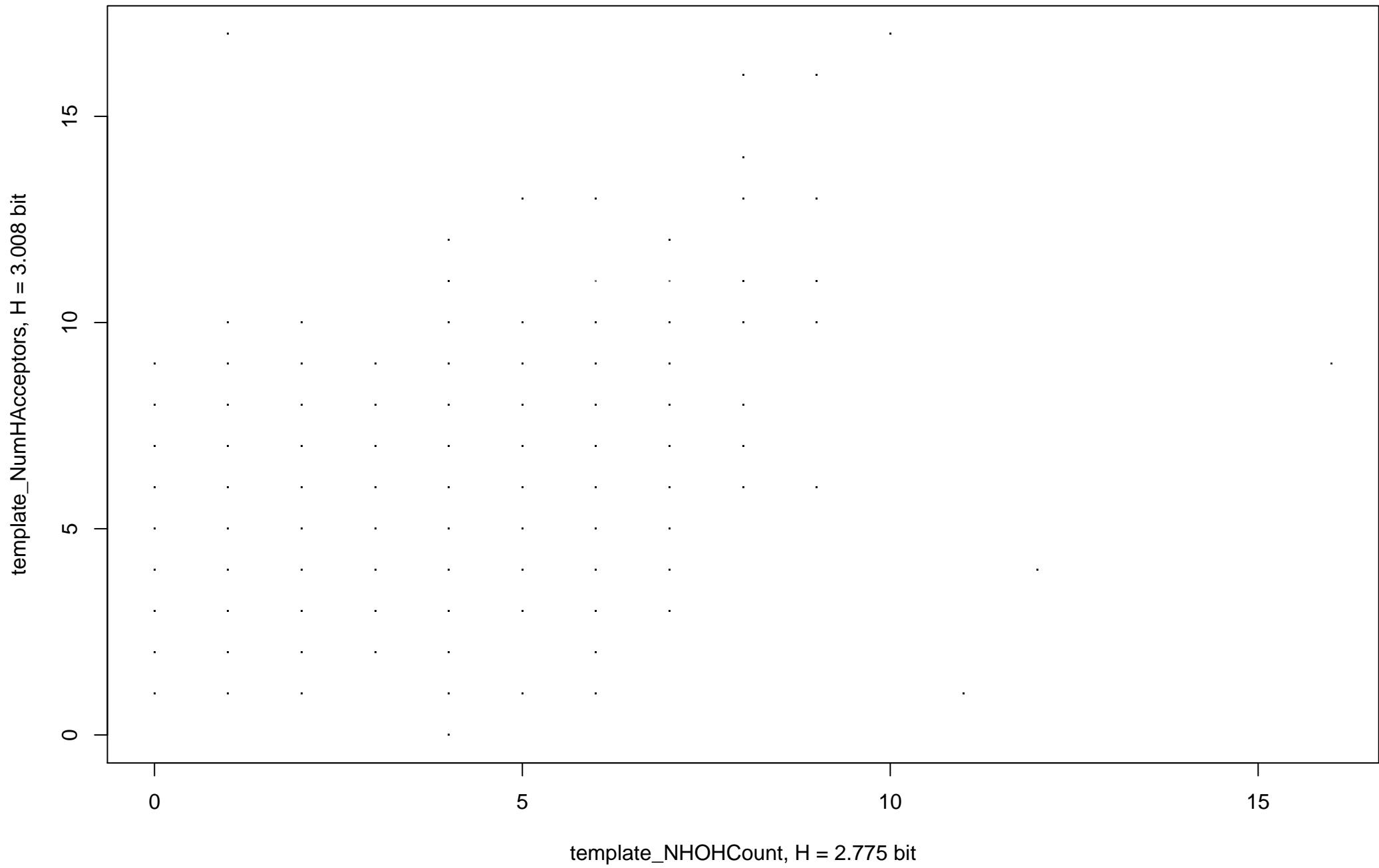
docked_NumHDonors-mcs_template_NumHDonors, MI = 0.1776 bit, normMI = 0.09153

mcs_template_NumHDonors, H = 1.941 bit

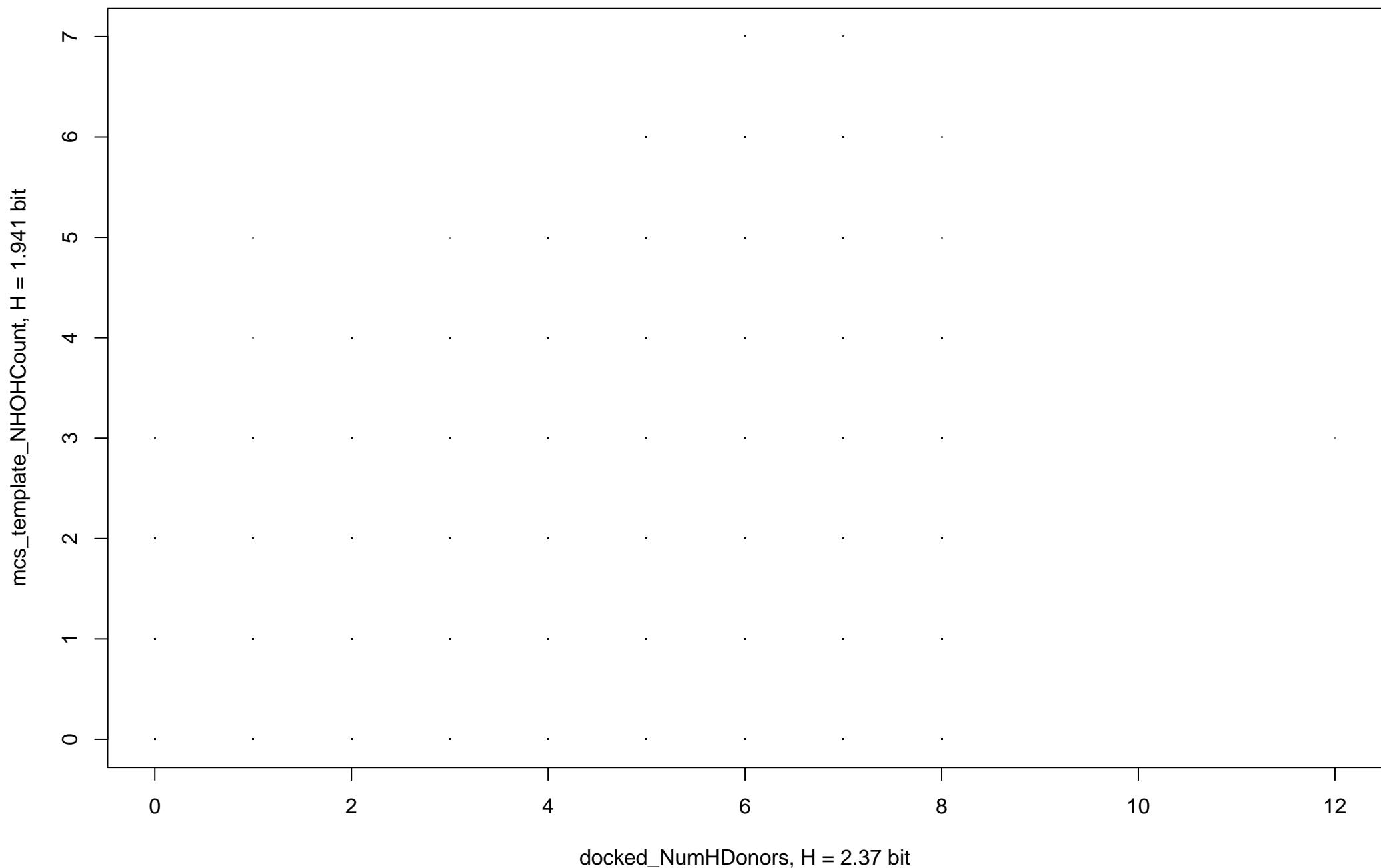


docked_NumHDonors, H = 2.37 bit

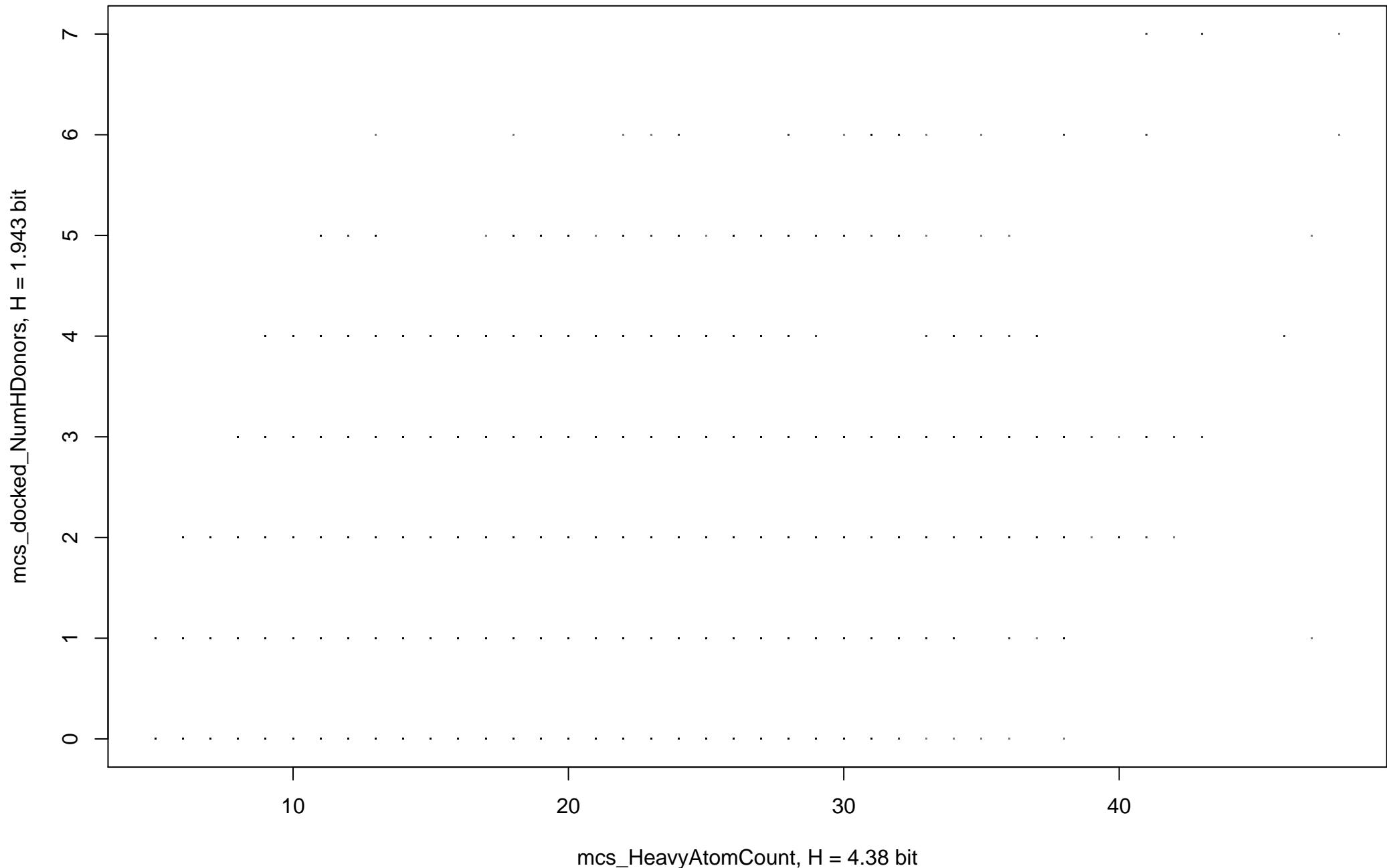
template_NHOHCount-template_NumHAcceptors, MI = 0.2534 bit, normMI = 0.09132



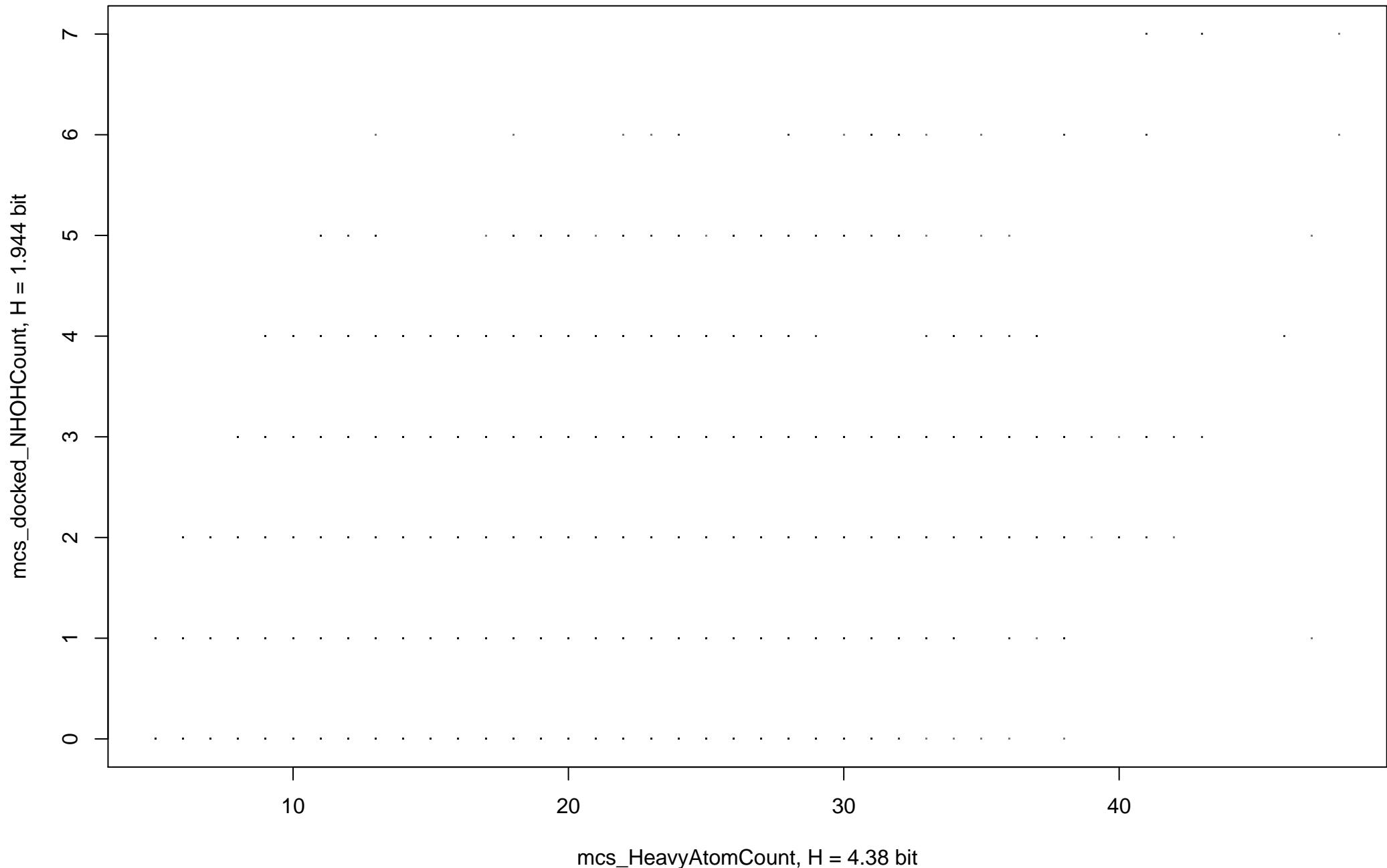
docked_NumHDonors-mcs_template_NHOHCount, MI = 0.1772 bit, normMI = 0.09129



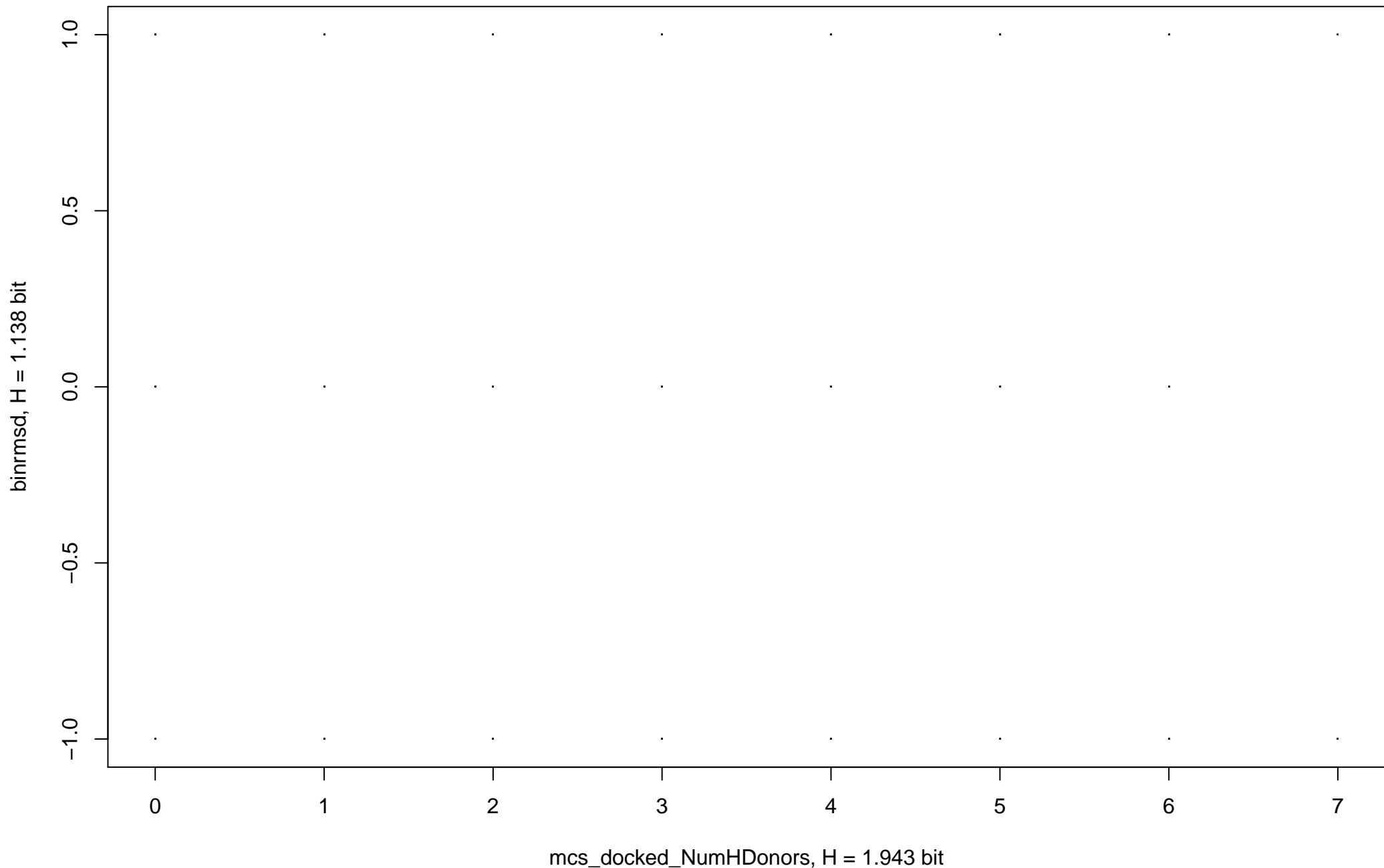
mcs_HeavyAtomCount-mcs_docked_NumHDonors, MI = 0.1773 bit, normMI = 0.09124



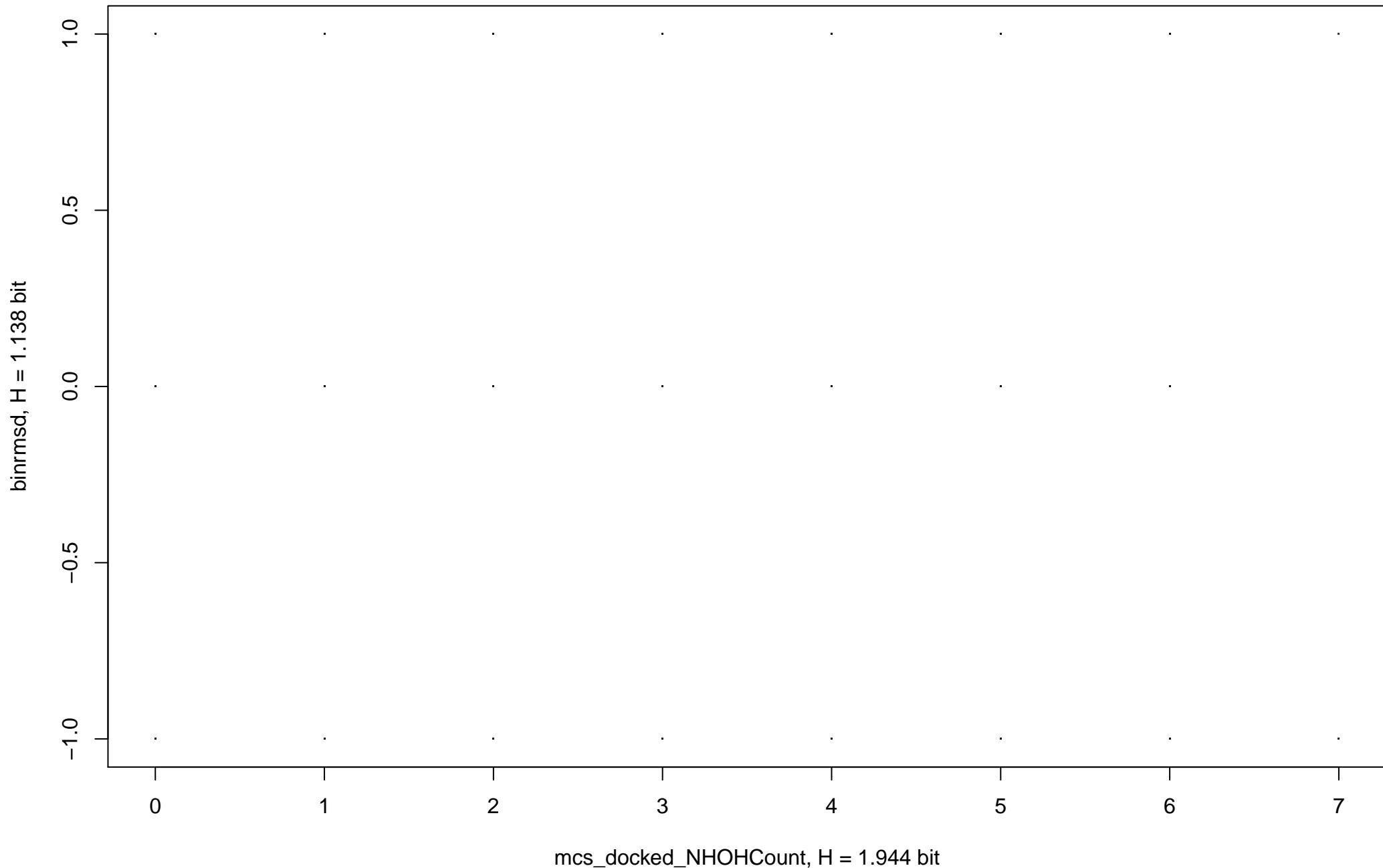
mcs_HeavyAtomCount–mcs_docked_NHOHCount, MI = 0.1773 bit, normMI = 0.0912



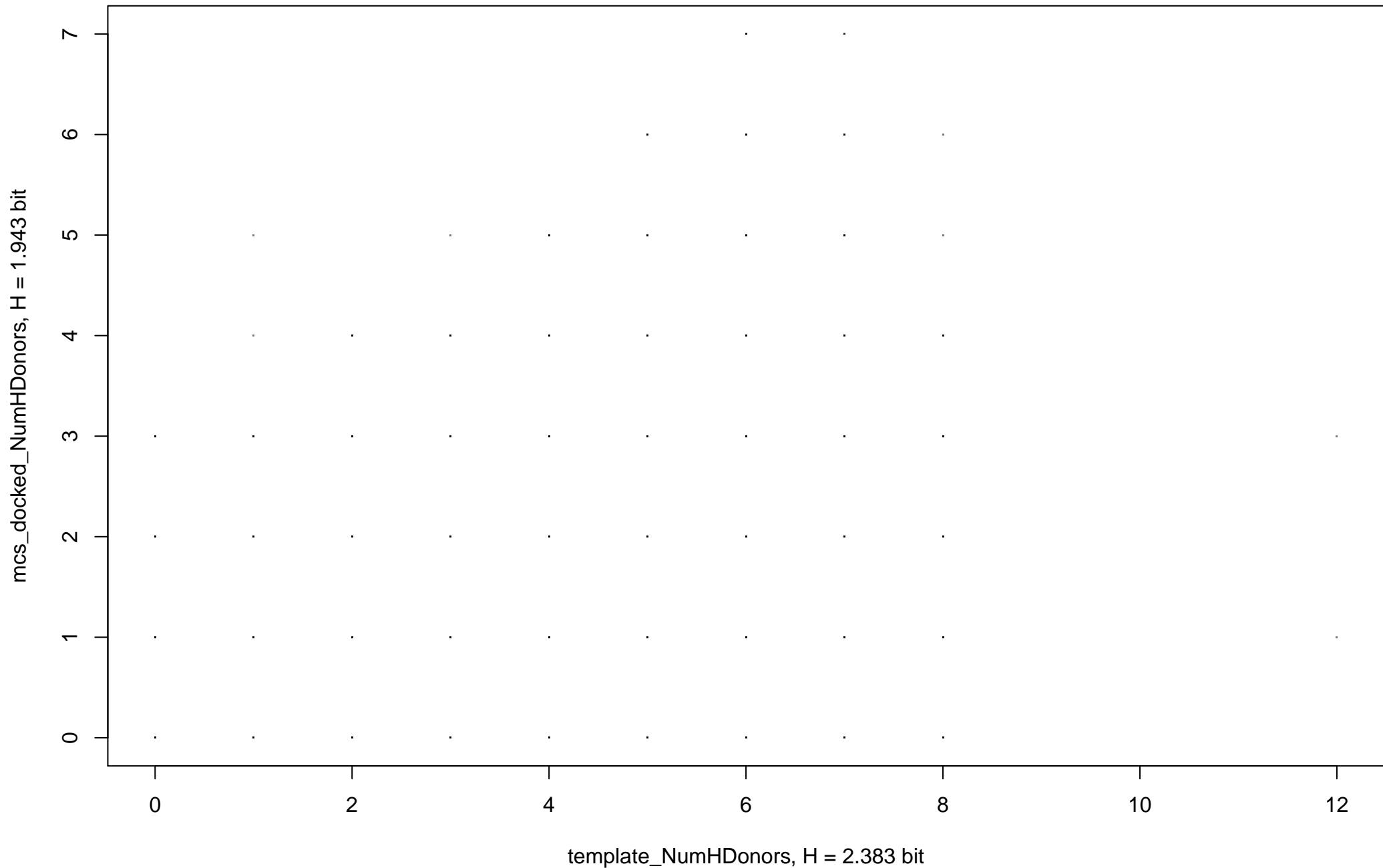
mcs_docked_NumHDonors–binrmsd, MI = 0.09984 bit, normMI = 0.08772



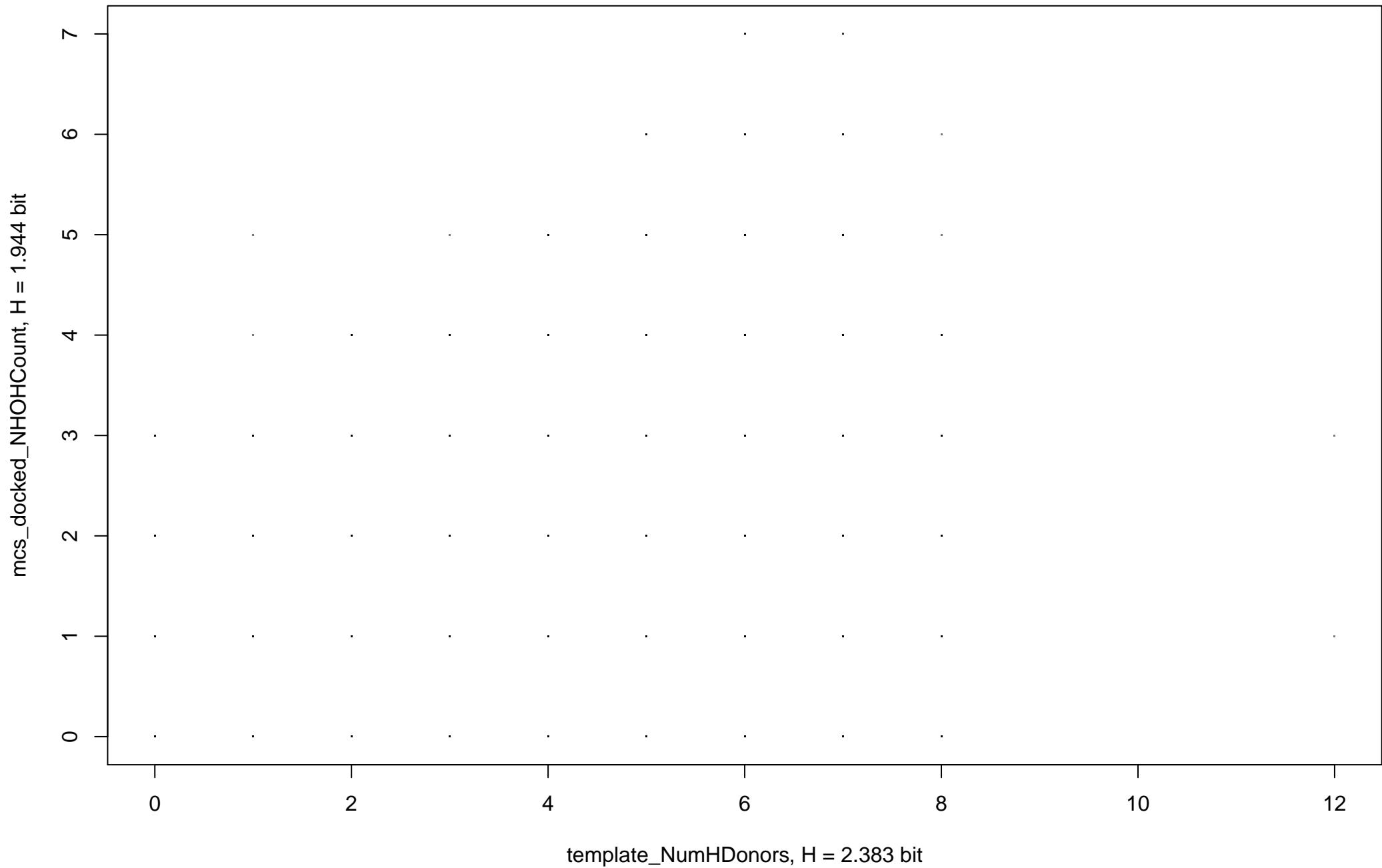
mcs_docked_NHOHCount-binrmsd, MI = 0.09977 bit, normMI = 0.08766



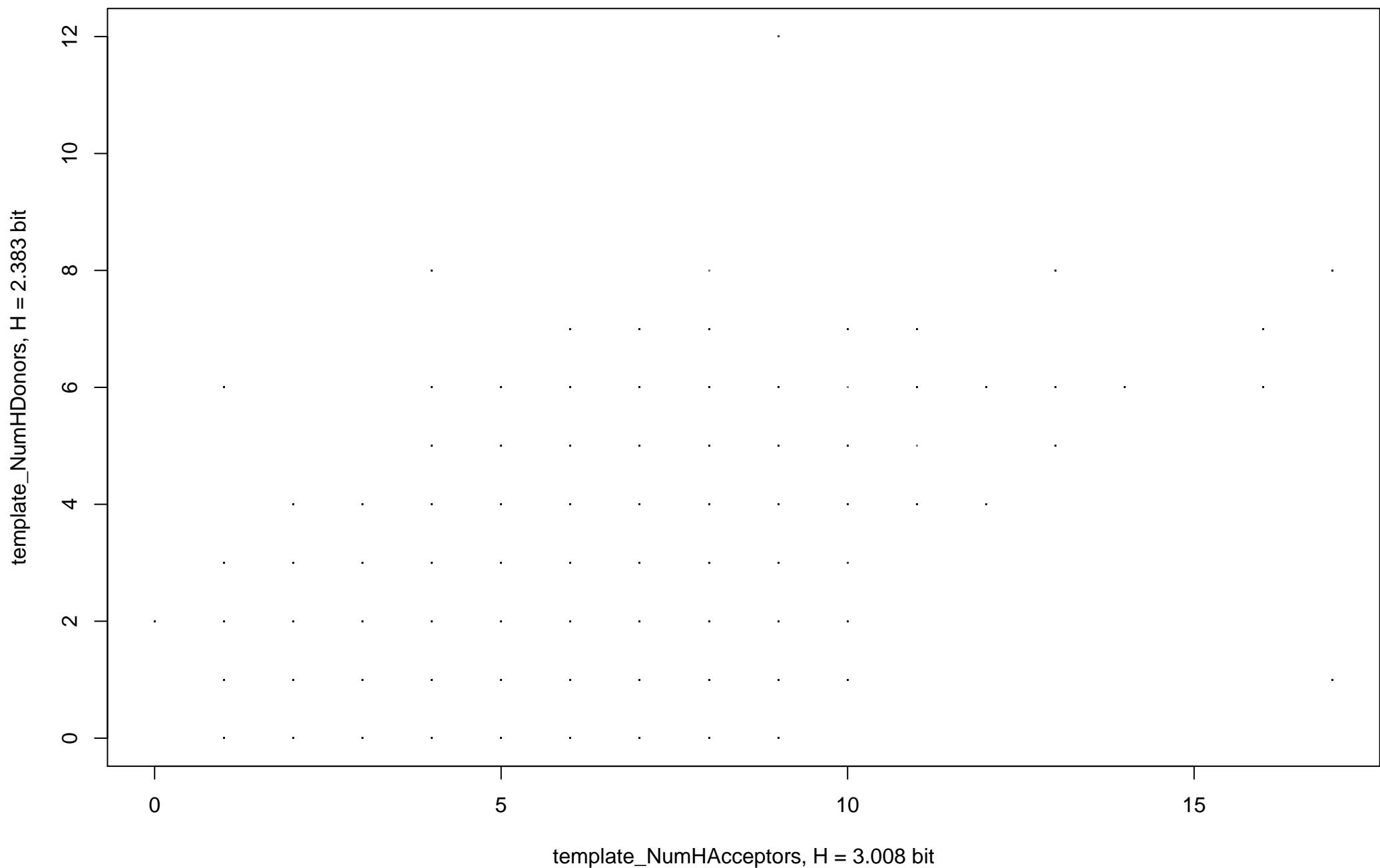
template_NumHDonors-mcs_docked_NumHDonors, MI = 0.1696 bit, normMI = 0.08727



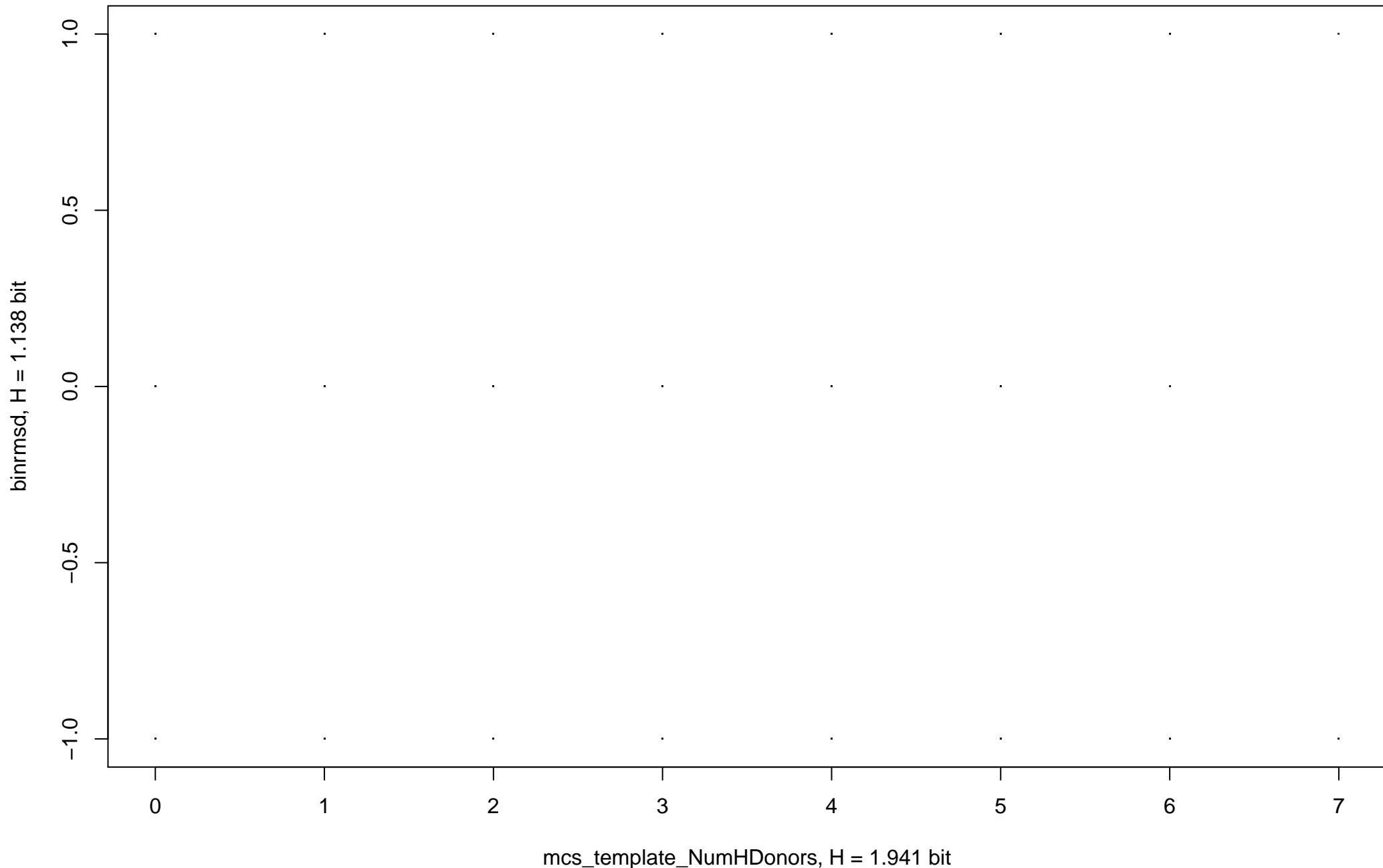
template_NumHDonors-mcs_docked_NHOHCount, MI = 0.1693 bit, normMI = 0.0871



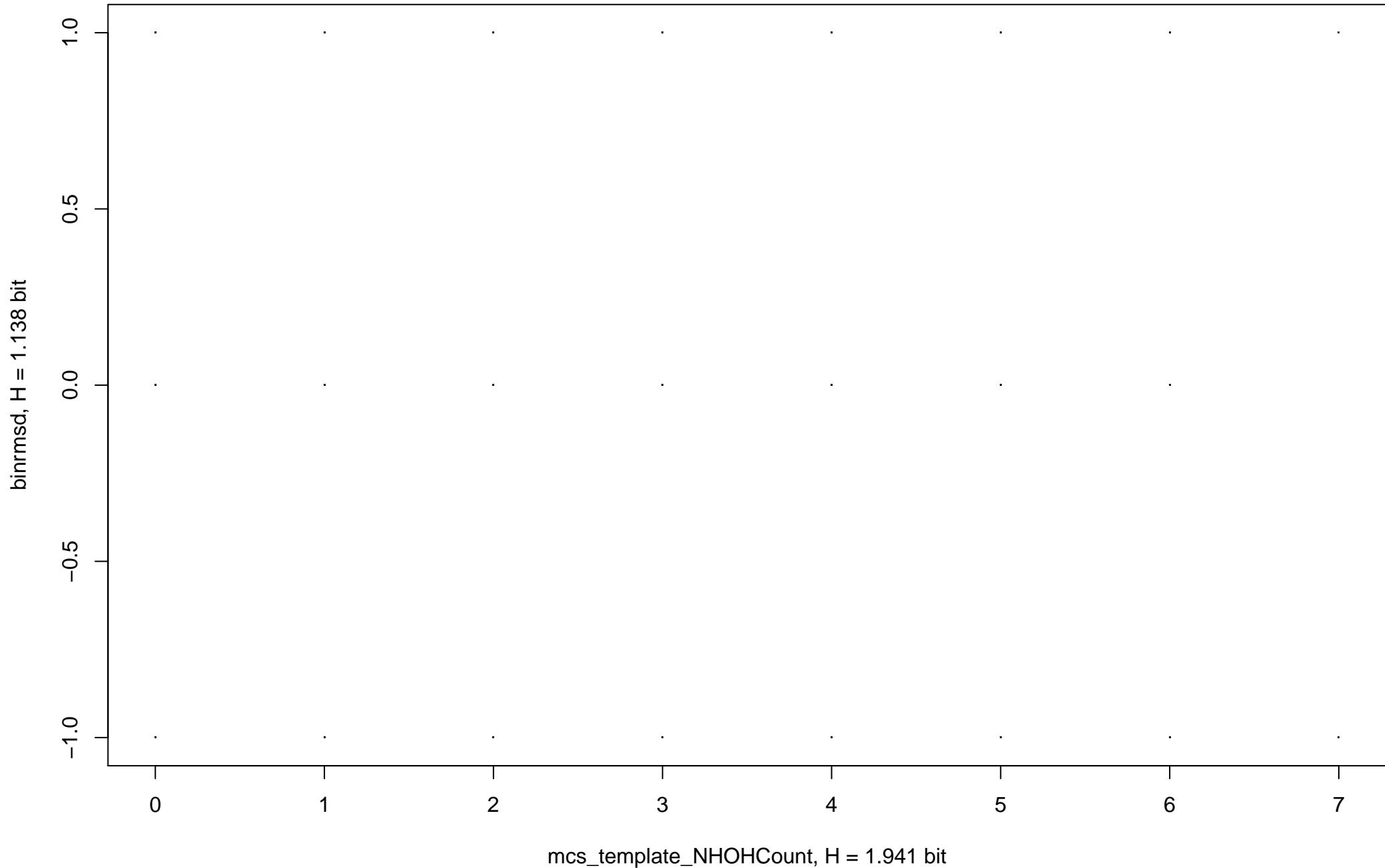
template_NumHAcceptors-template_NumHDonors, MI = 0.2073 bit, normMI = 0.08697



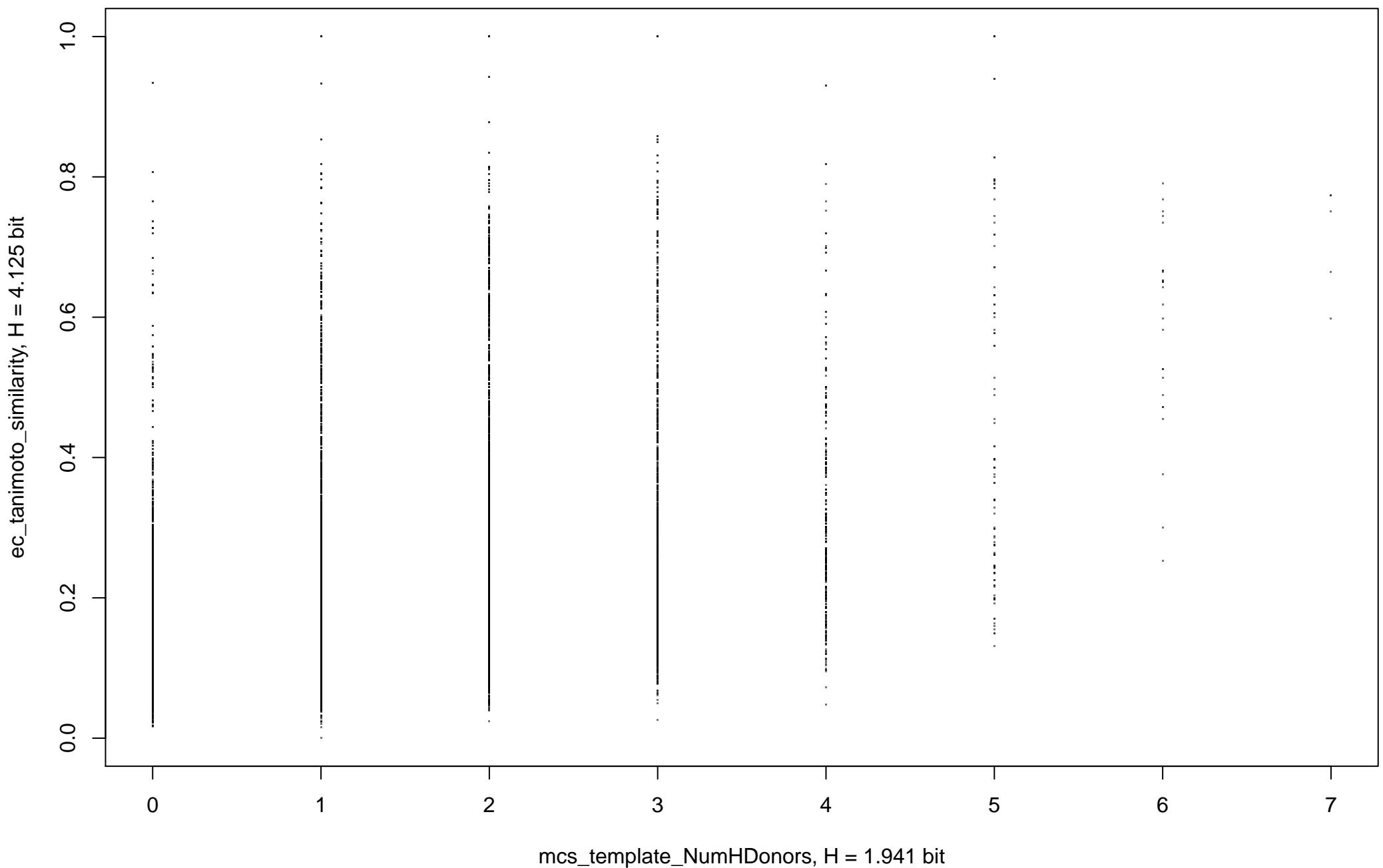
mcs_template_NumHDonors–binrmsd, MI = 0.0981 bit, normMI = 0.0862



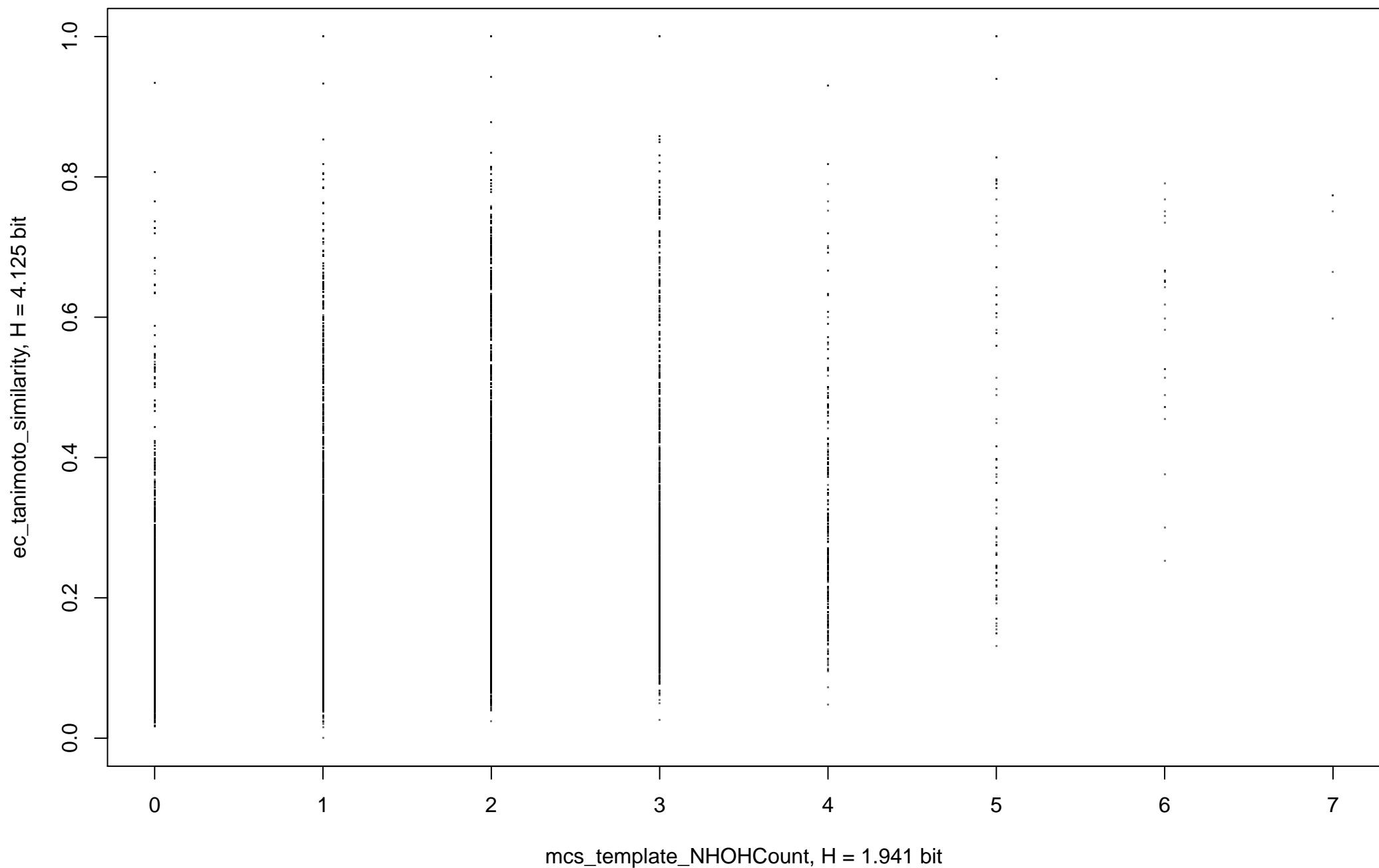
mcs_template_NHOHCount-binrmsd, MI = 0.09788 bit, normMI = 0.08601



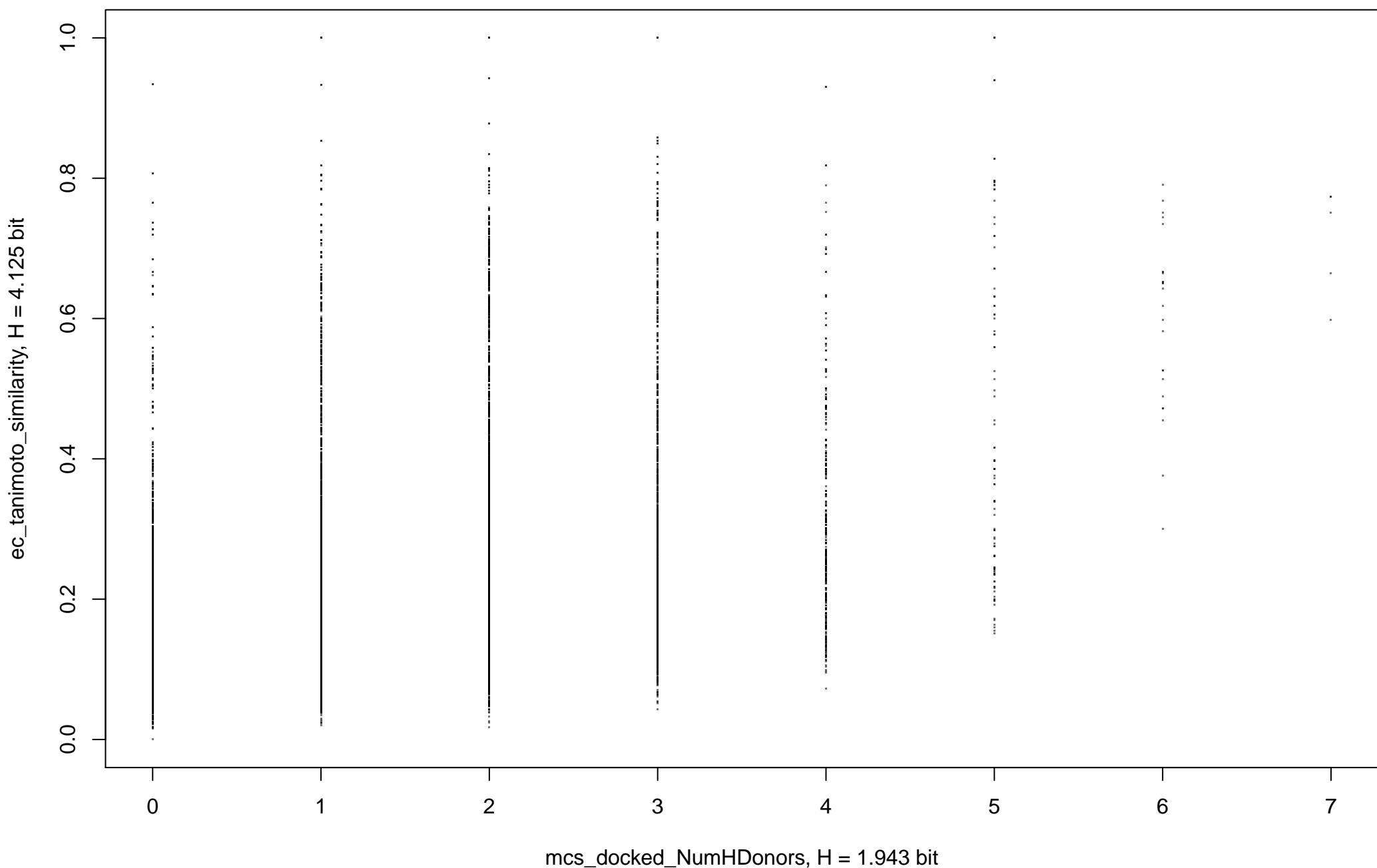
mcs_template_NumHDonors–ec_tanimoto_similarity, MI = 0.1666 bit, normMI = 0.08585



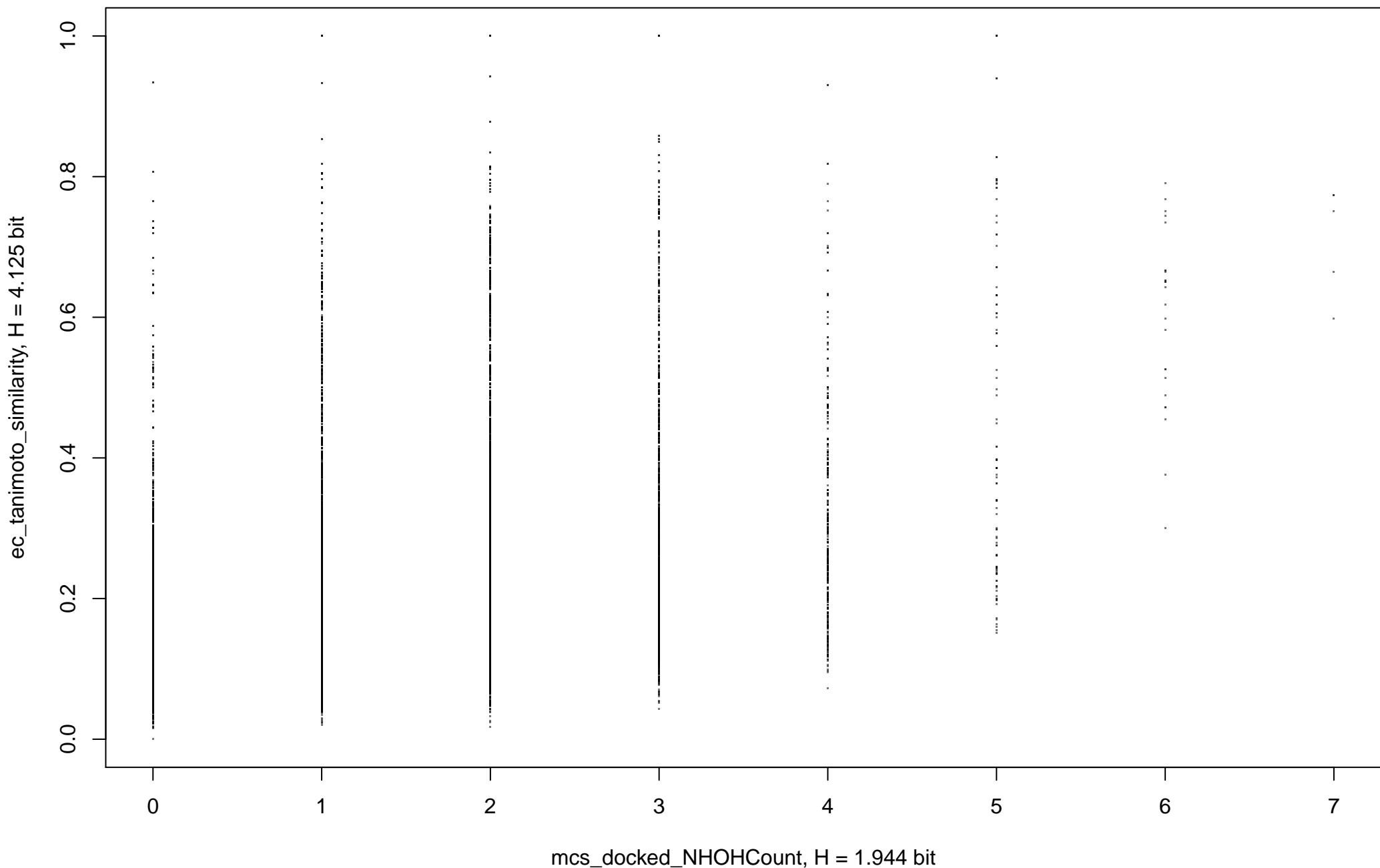
mcs_template_NHOHCount–ec_tanimoto_similarity, MI = 0.1665 bit, normMI = 0.08576



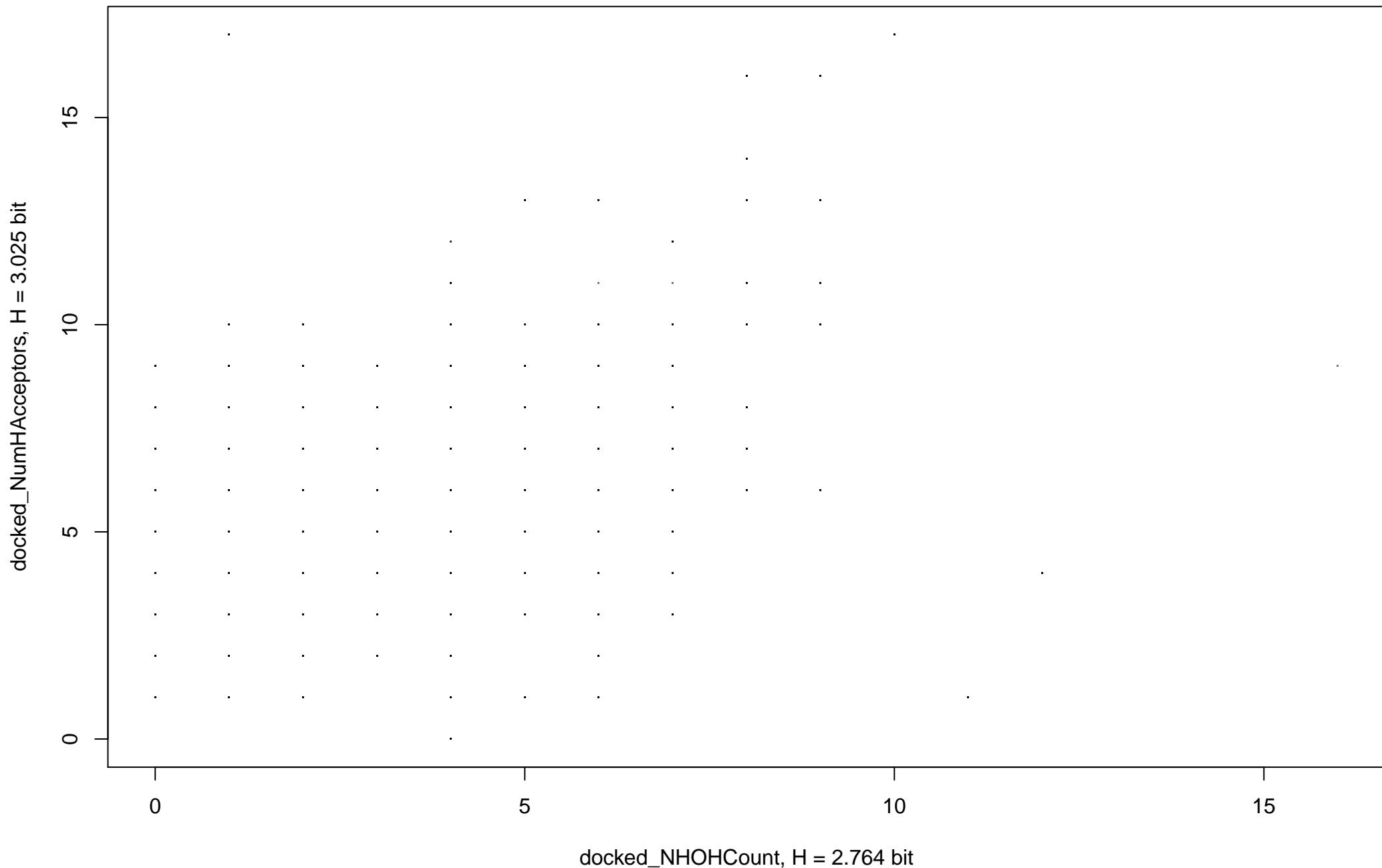
mcs_docked_NuHDonors–ec_tanimoto_similarity, MI = 0.1665 bit, normMI = 0.08566



mcs_docked_NHOHCount–ec_tanimoto_similarity, MI = 0.1663 bit, normMI = 0.08557

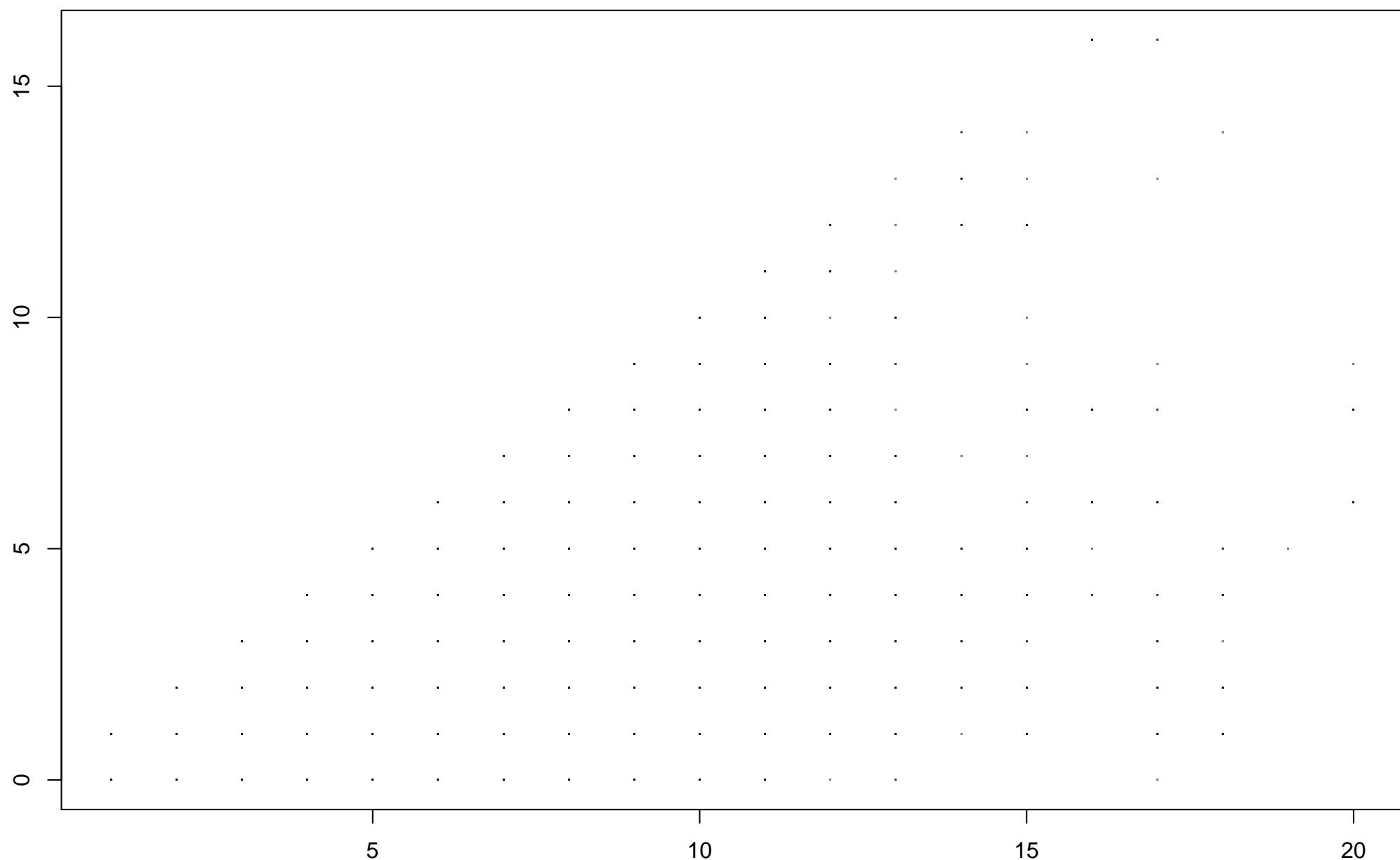


docked_NHOHCount–docked_NumHAcceptors, MI = 0.2358 bit, normMI = 0.08528



docked_NOCount-mcs_NOCount, MI = 0.2367 bit, normMI = 0.08526

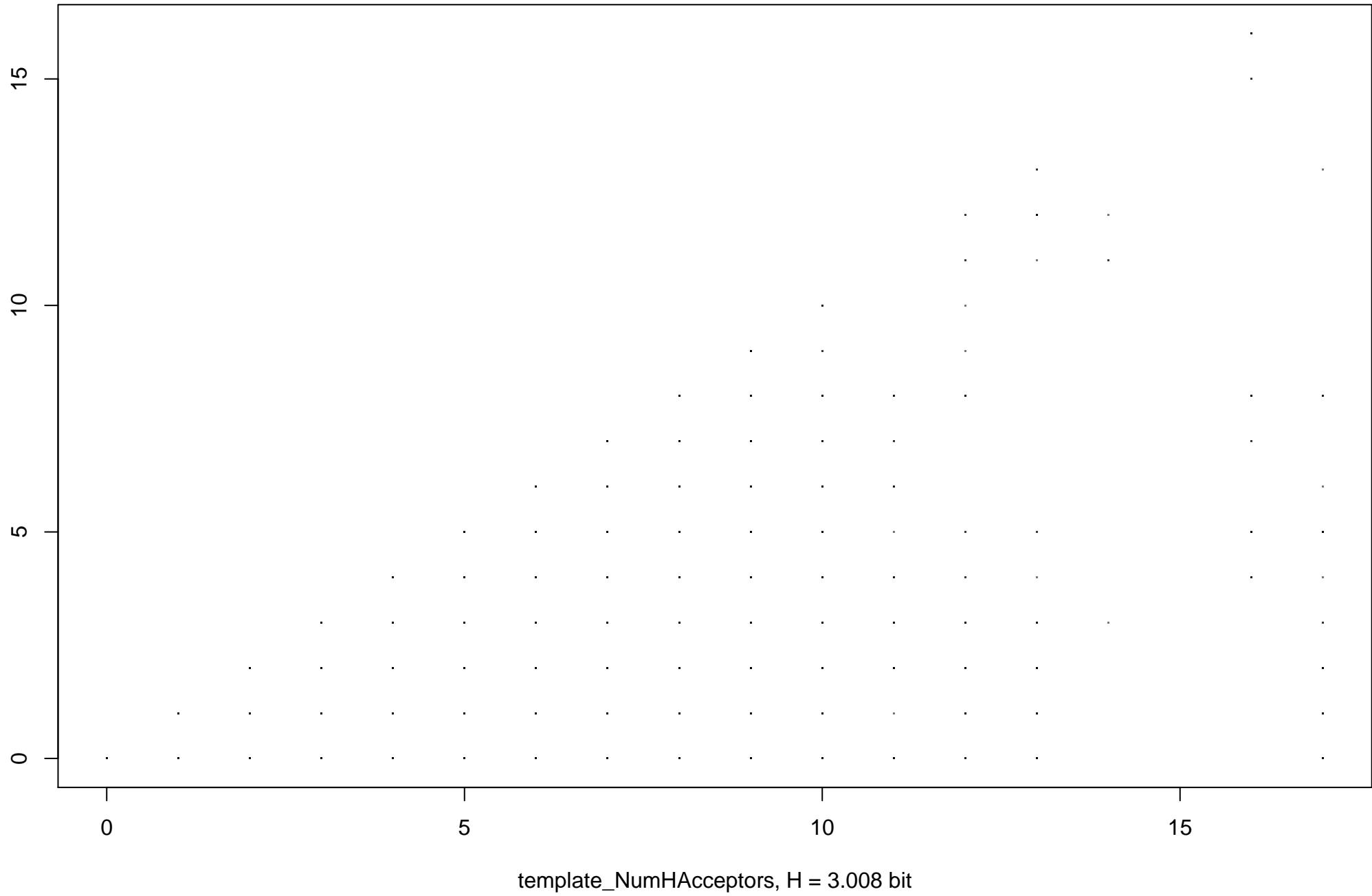
mcs_NOCount, H = 2.777 bit



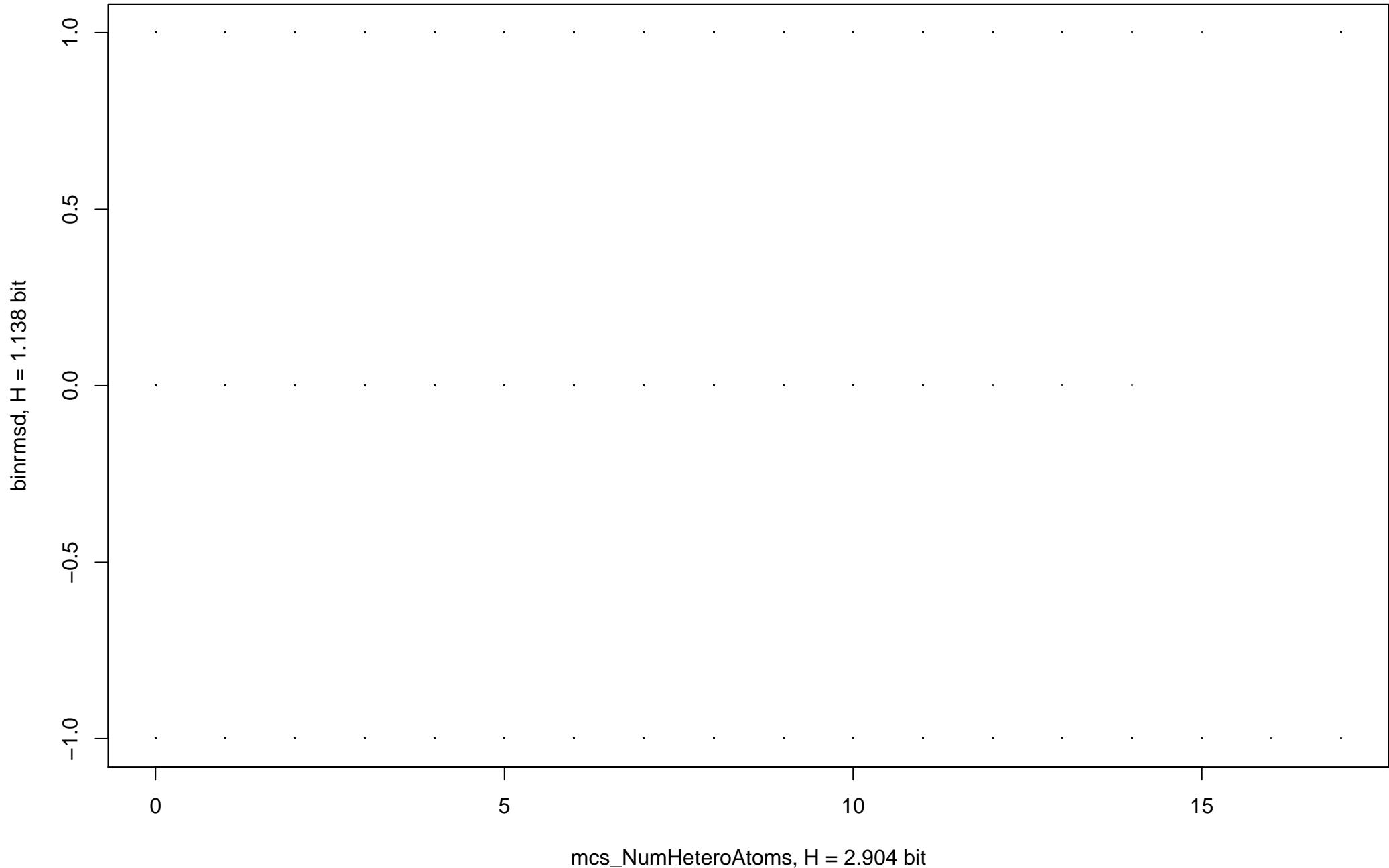
docked_NOCount, H = 3.257 bit

template_NumHAcceptors-mcs_template_NumHAcceptors, MI = 0.2119 bit, normMI = 0.08516

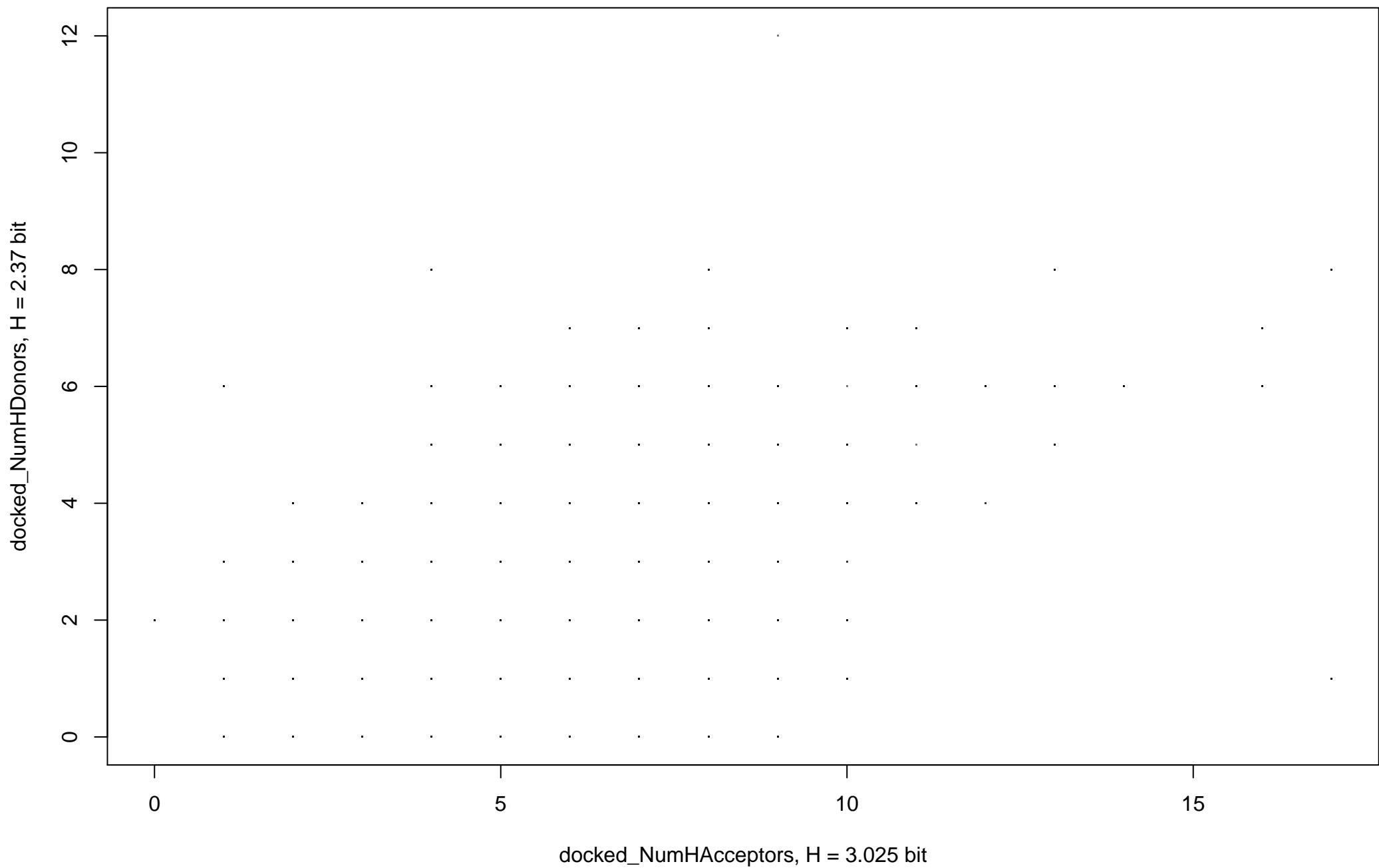
mcs_template_NumHAcceptors, H = 2.488 bit



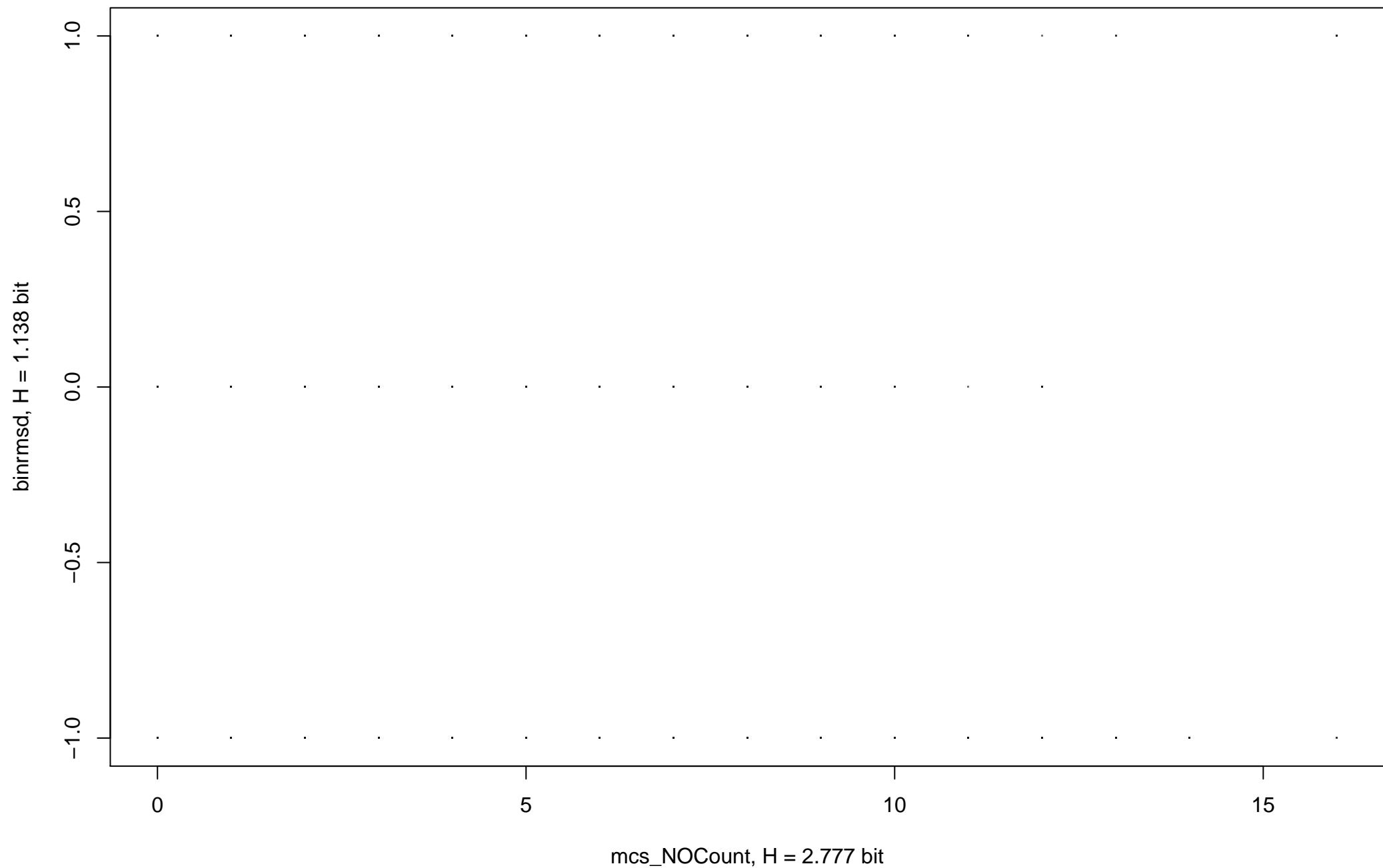
mcs_NumHeteroAtoms-binrmsd, MI = 0.09672 bit, normMI = 0.08498



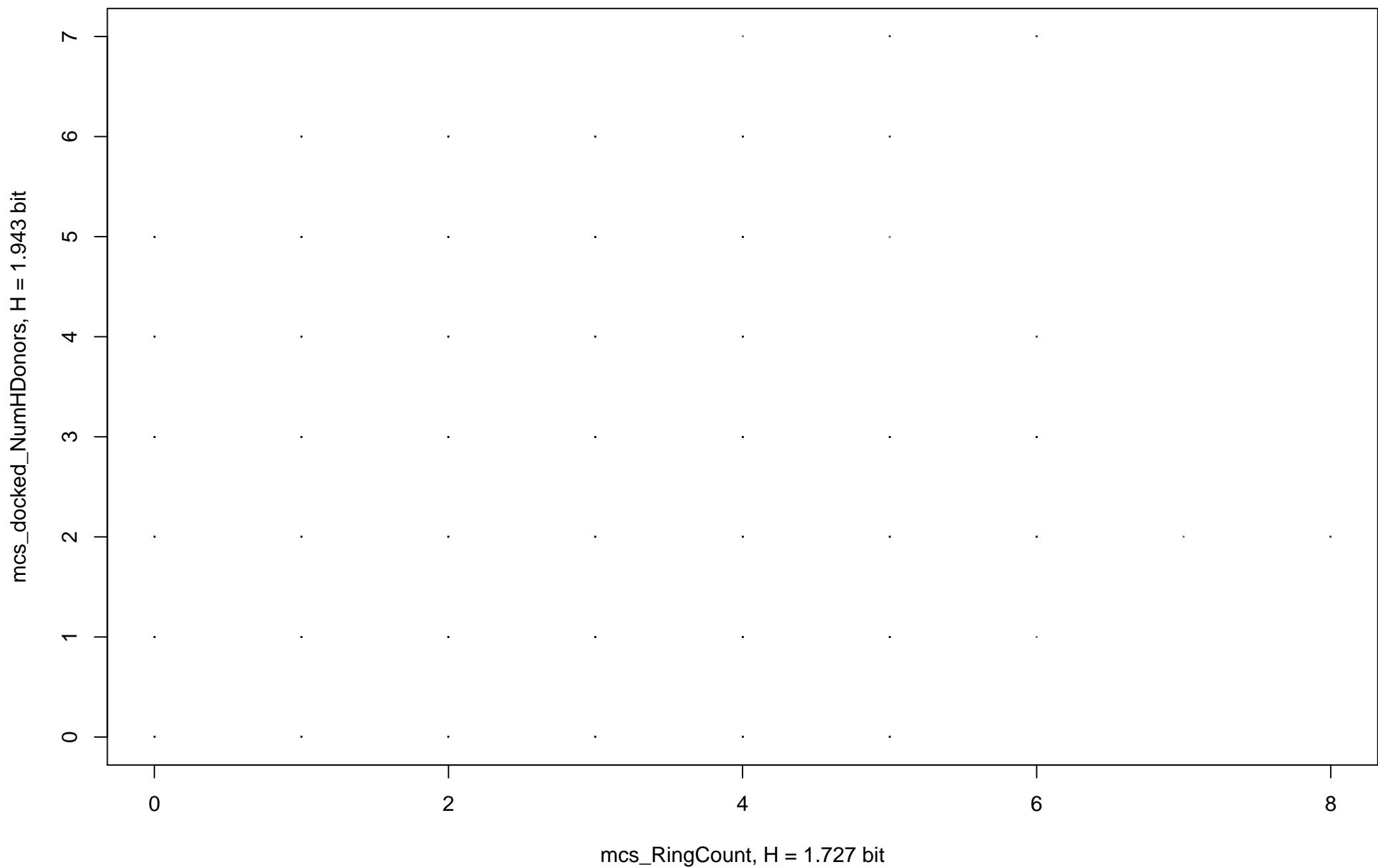
docked_NumHAcceptors-docked_NumHDonors, MI = 0.1973 bit, normMI = 0.08325



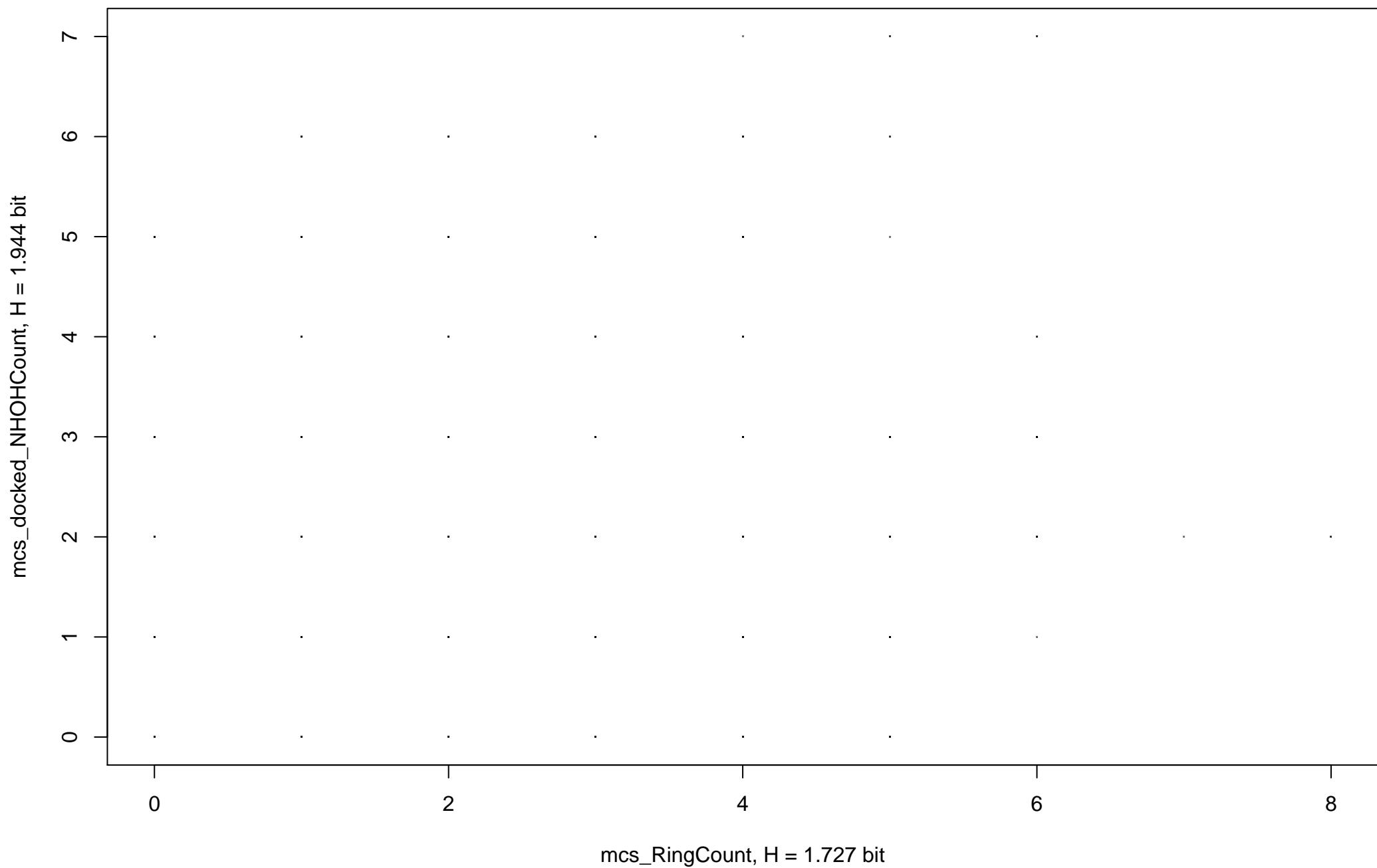
mcs_NOCount-binrmsd, MI = 0.09438 bit, normMI = 0.08293



mcs_RingCount-mcs_docked_NumHDonors, MI = 0.1416 bit, normMI = 0.08198

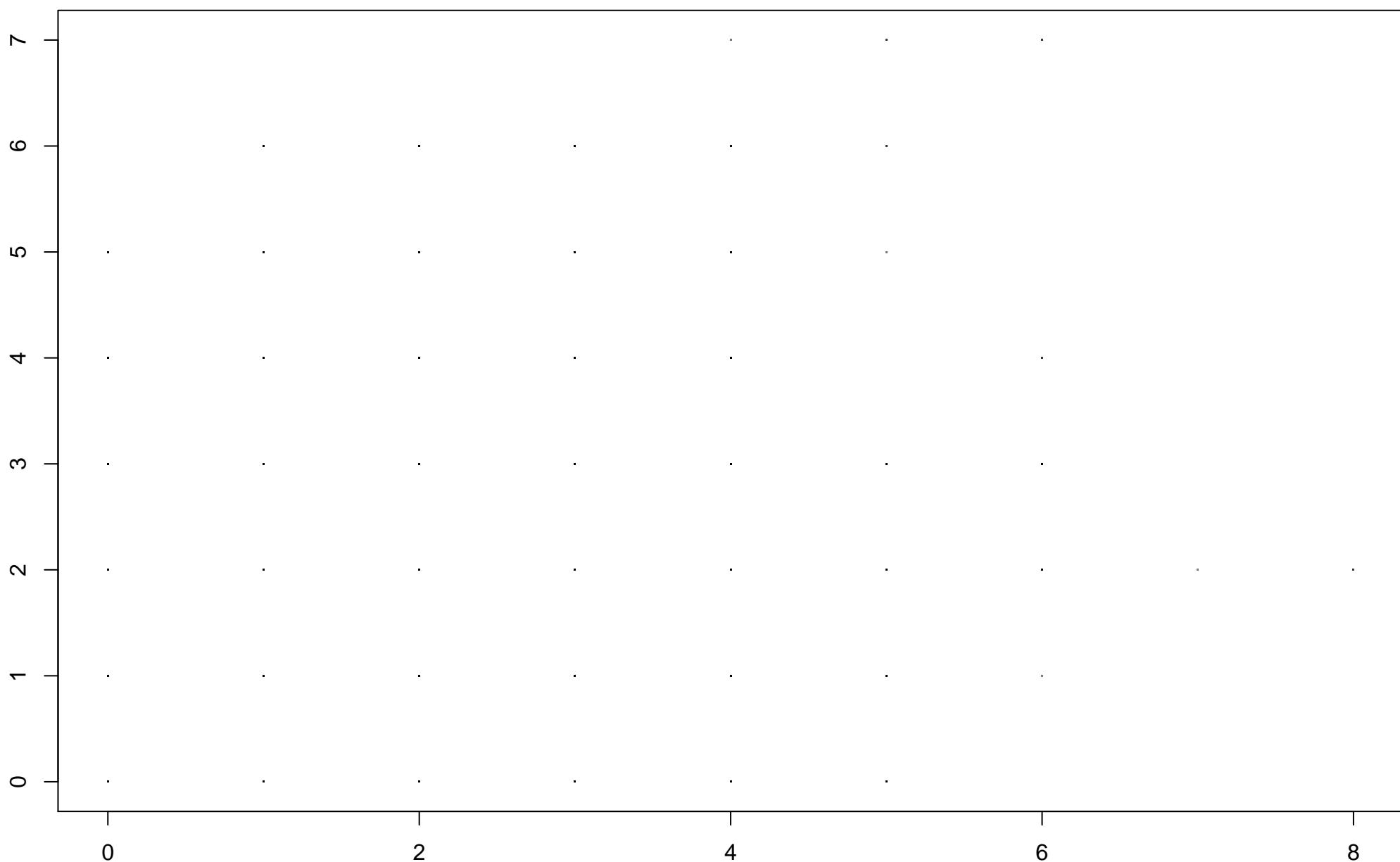


mcs_RingCount-mcs_docked_NHOHCount, MI = 0.1413 bit, normMI = 0.08177



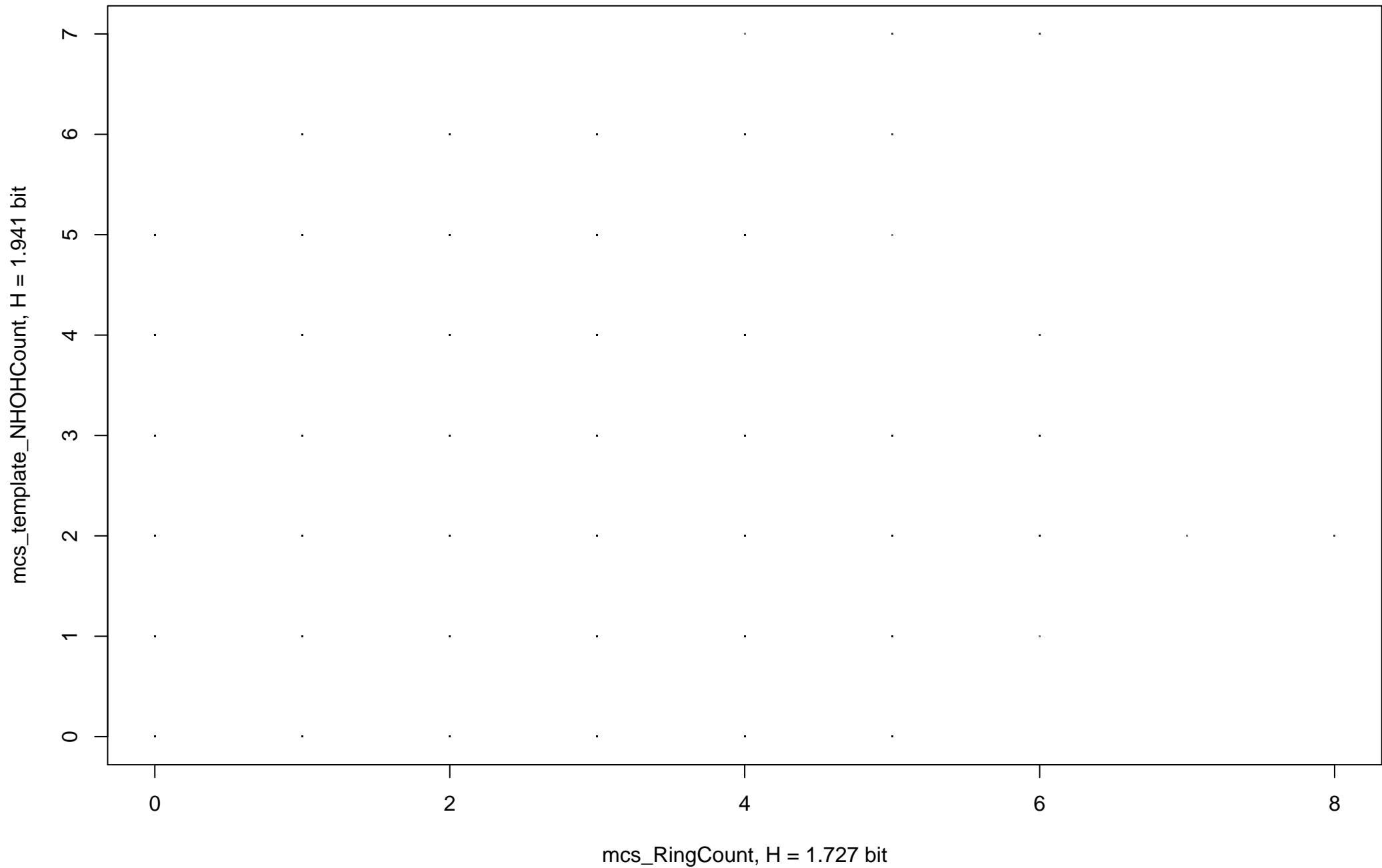
mcs_RingCount–mcs_template_NumHDonors, MI = 0.1398 bit, normMI = 0.08093

mcs_template_NumHDonors, H = 1.941 bit

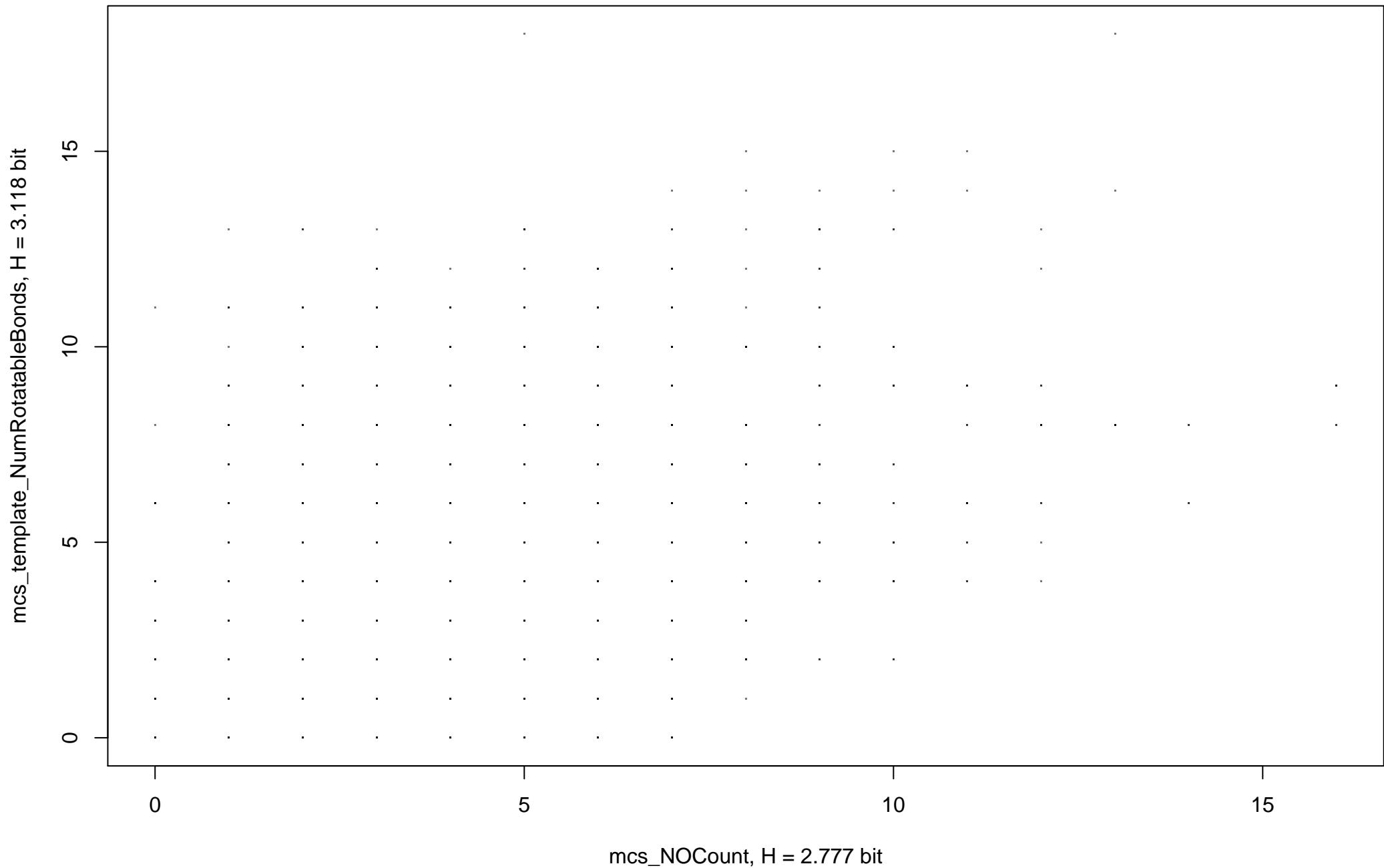


mcs_RingCount, H = 1.727 bit

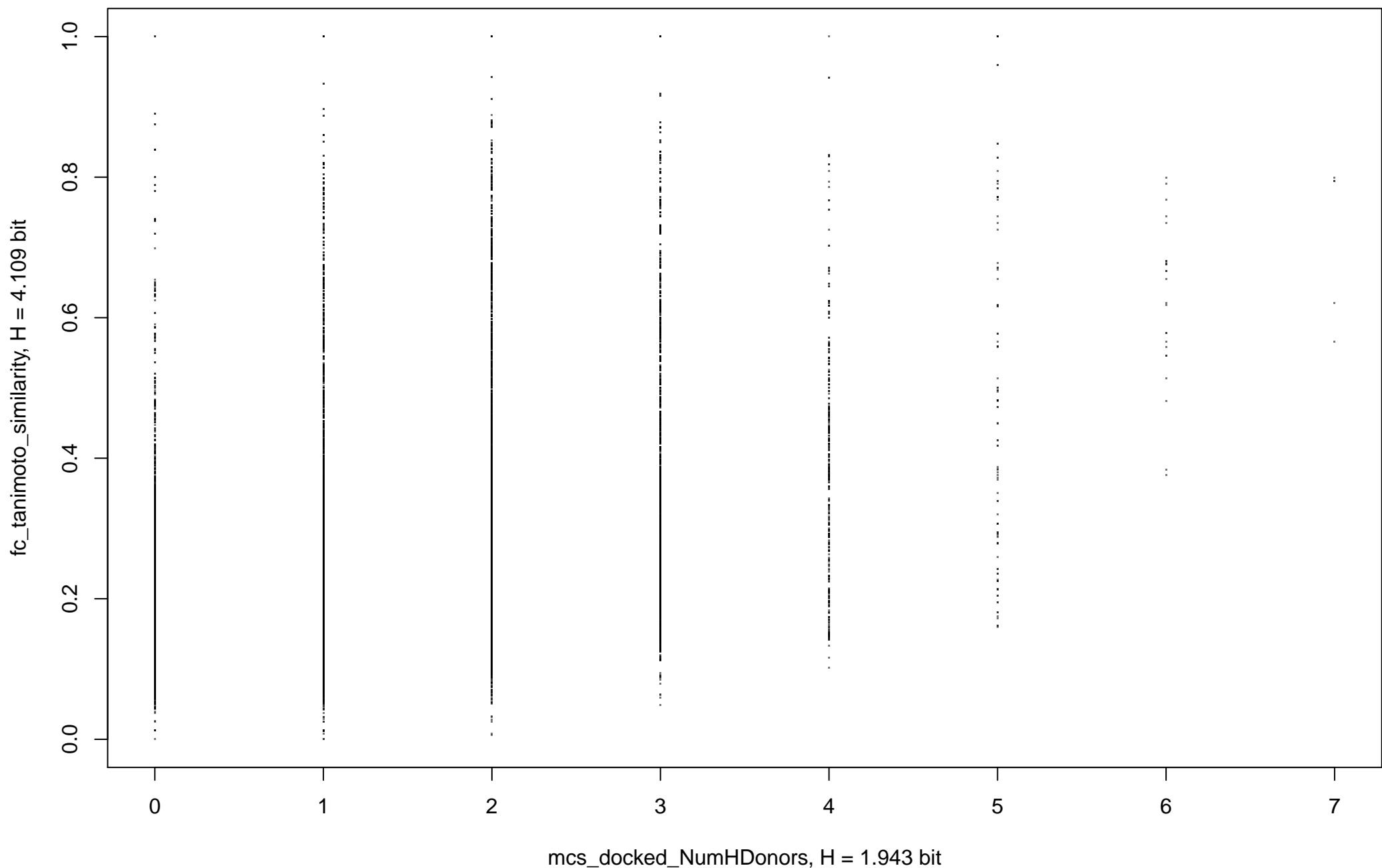
mcs_RingCount-mcs_template_NHOHCount, MI = 0.1394 bit, normMI = 0.08072



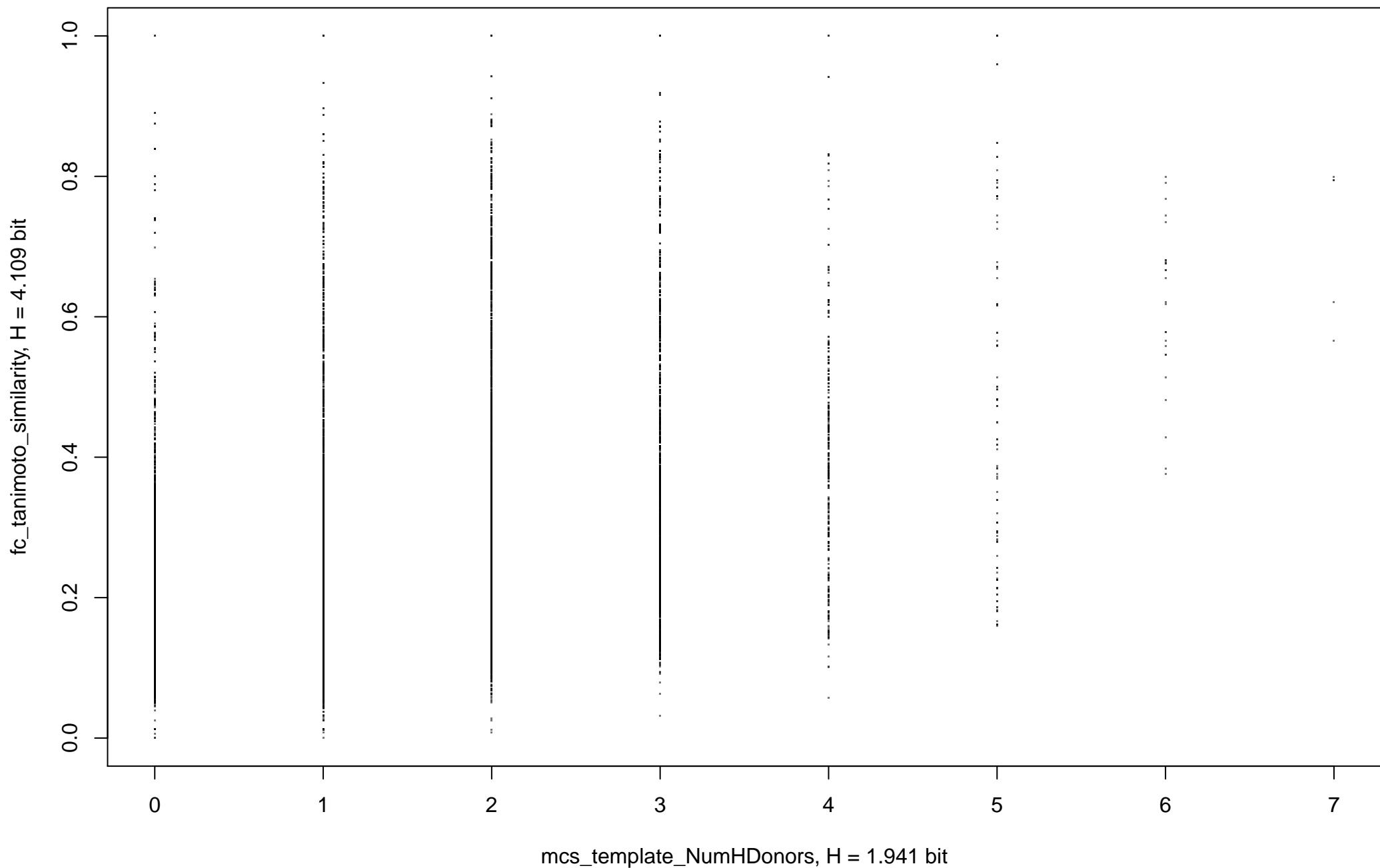
mcs_NOCount-mcs_template_NumRotatableBonds, MI = 0.2232 bit, normMI = 0.08038



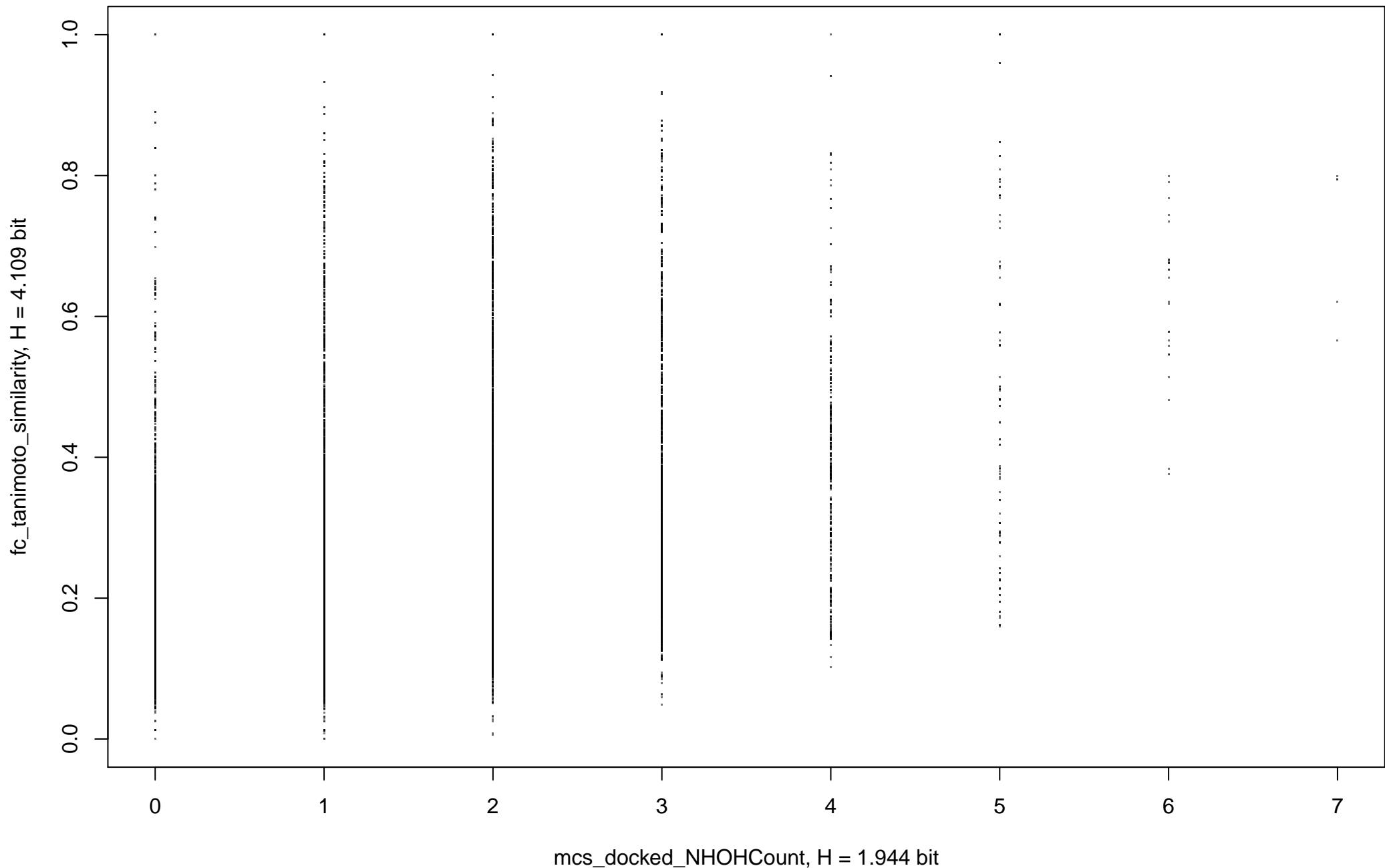
mcs_docked_NuHDonors-fc_tanimoto_similarity, MI = 0.1561 bit, normMI = 0.08031



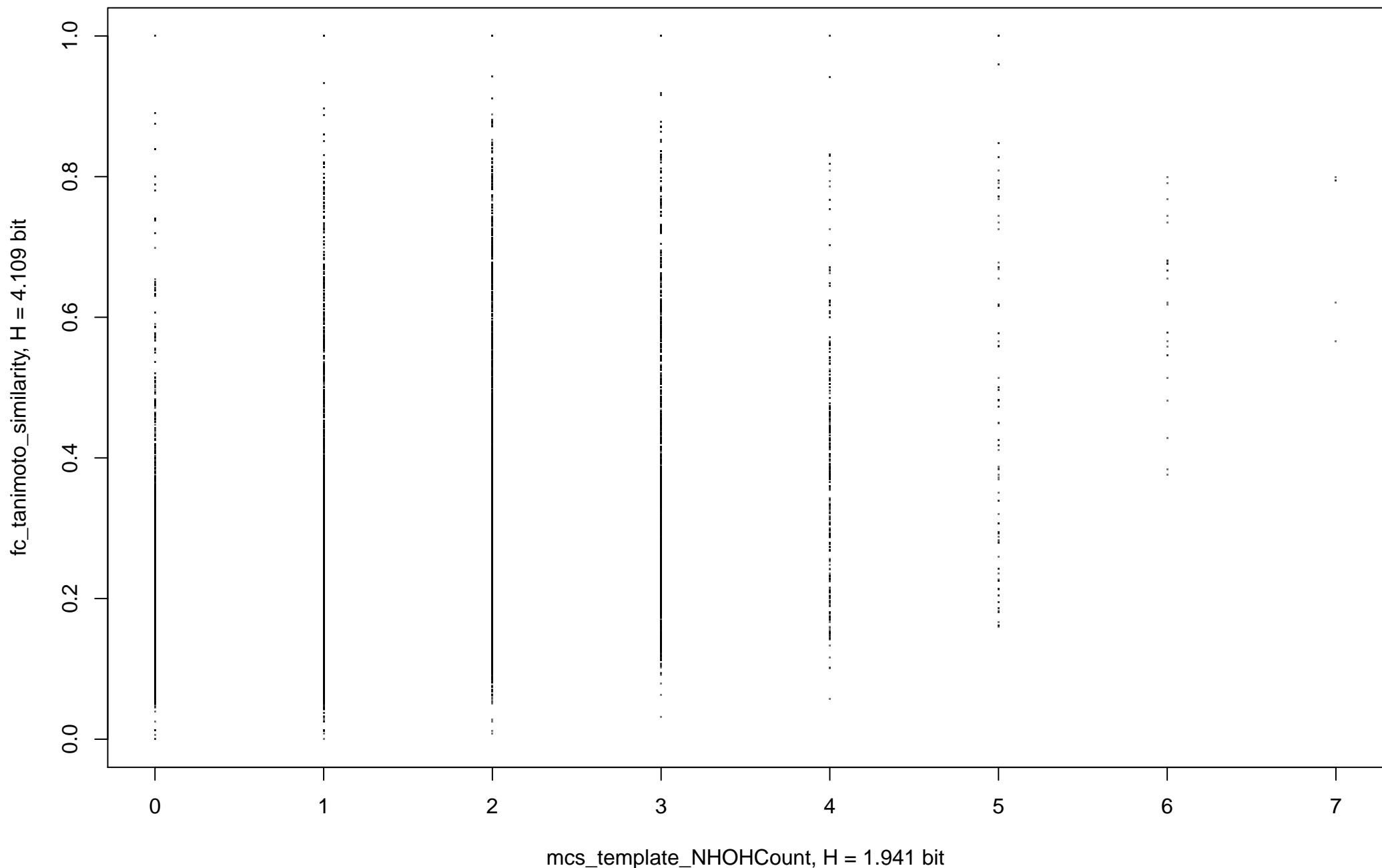
mcs_template_NumHDonors-fc_tanimoto_similarity, MI = 0.1557 bit, normMI = 0.08024



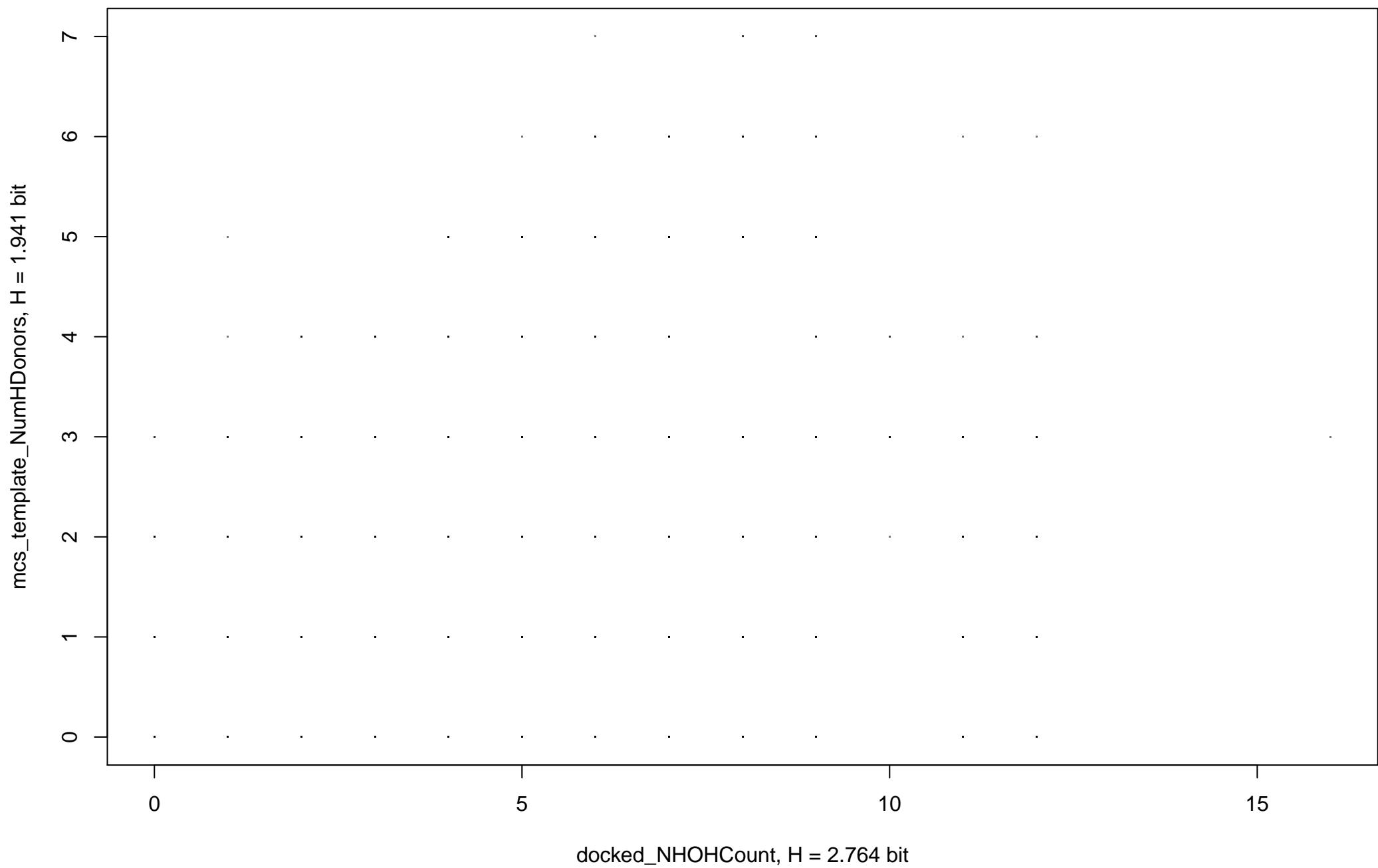
mcs_docked_NHOHCount–fc_tanimoto_similarity, MI = 0.156 bit, normMI = 0.08024



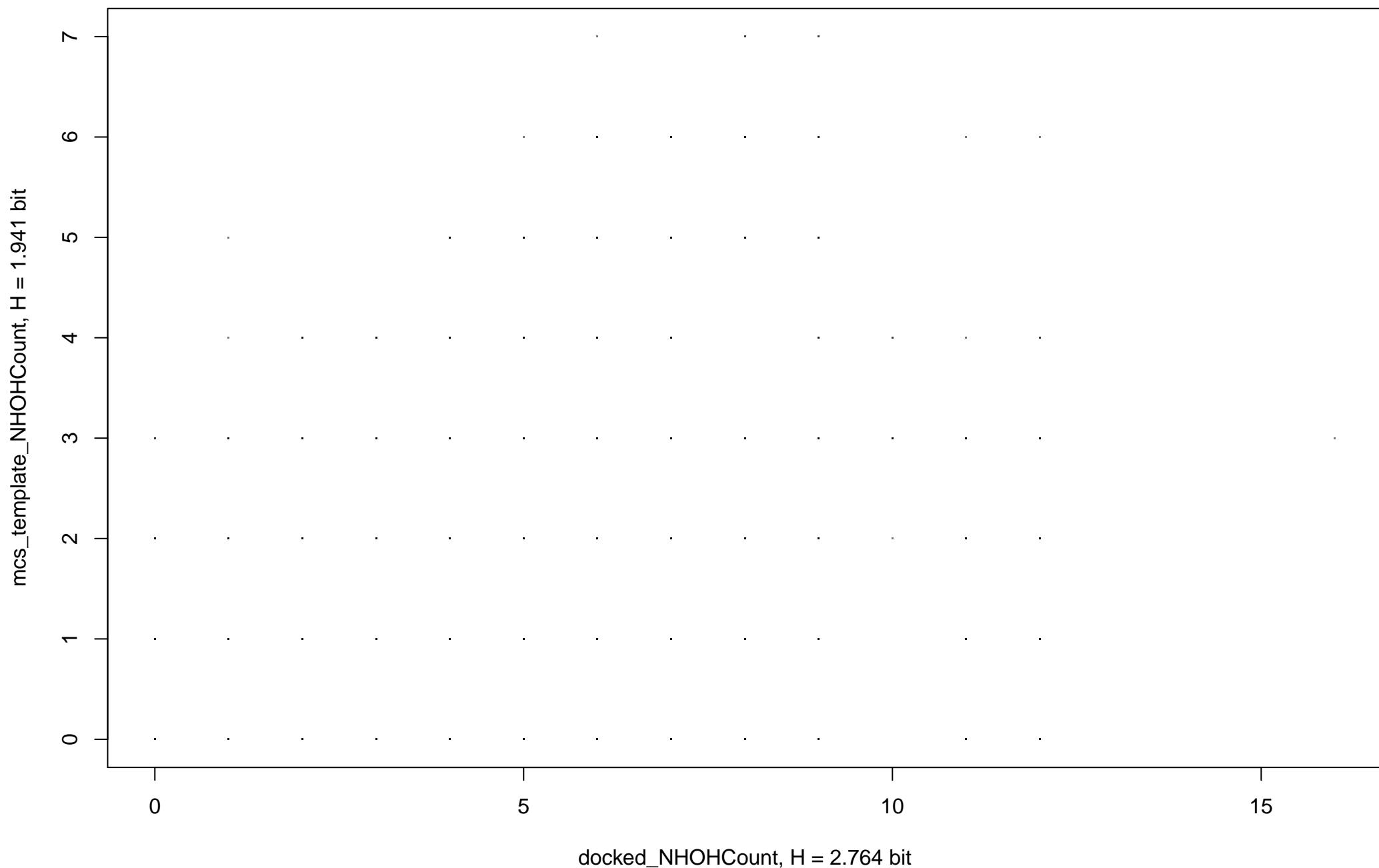
mcs_template_NHOHCount-fc_tanimoto_similarity, MI = 0.1556 bit, normMI = 0.08017



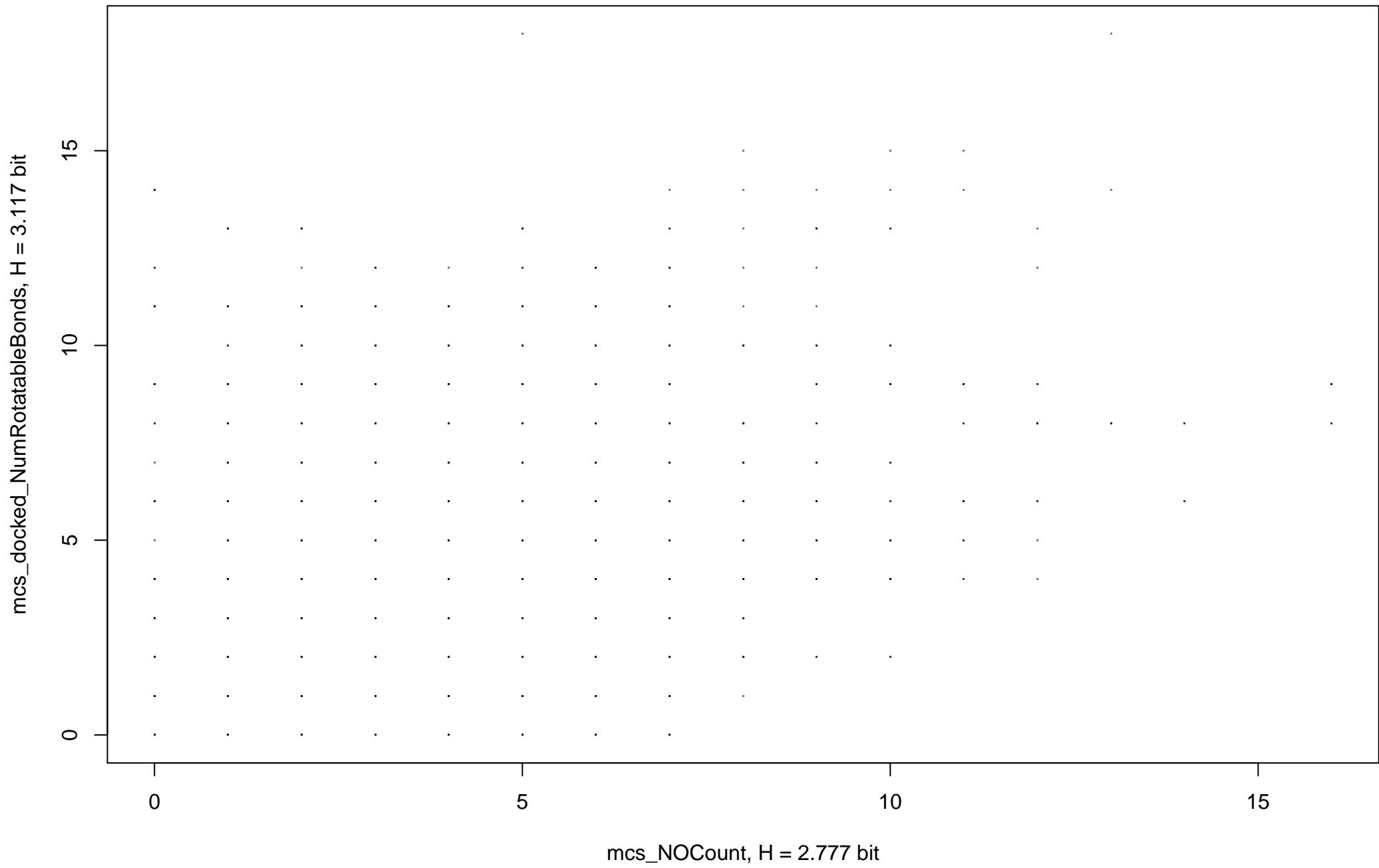
docked_NHOHCount-mcs_template_NumHDonors, MI = 0.1546 bit, normMI = 0.07966



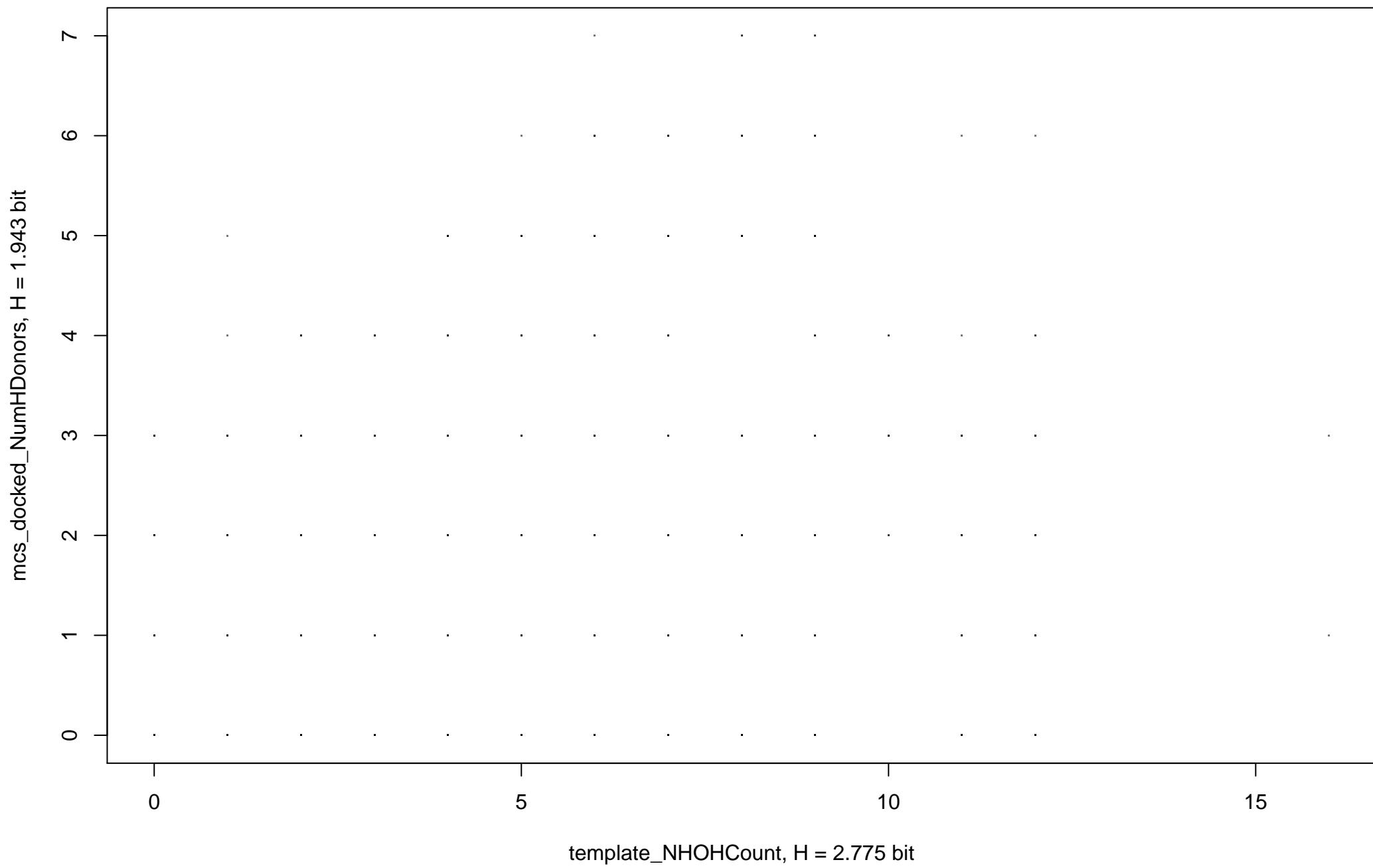
docked_NHOHCount-mcs_template_NHOHCount, MI = 0.1546 bit, normMI = 0.07961



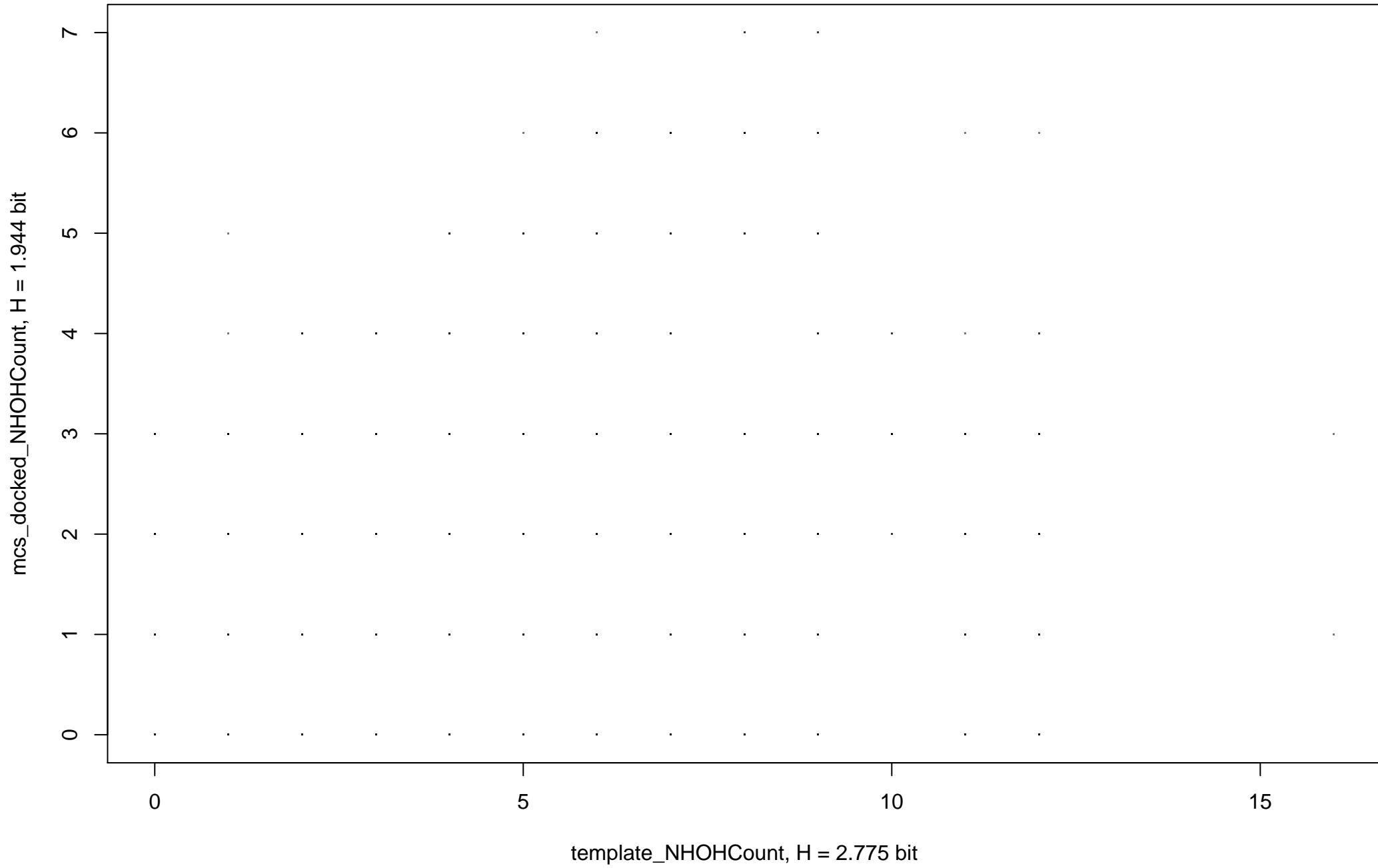
mcs_NOCount-mcs_docked_NumRotatableBonds, MI = 0.2176 bit, normMI = 0.07836



template_NHOHCount-mcs_docked_NumHDonors, MI = 0.1522 bit, normMI = 0.07832

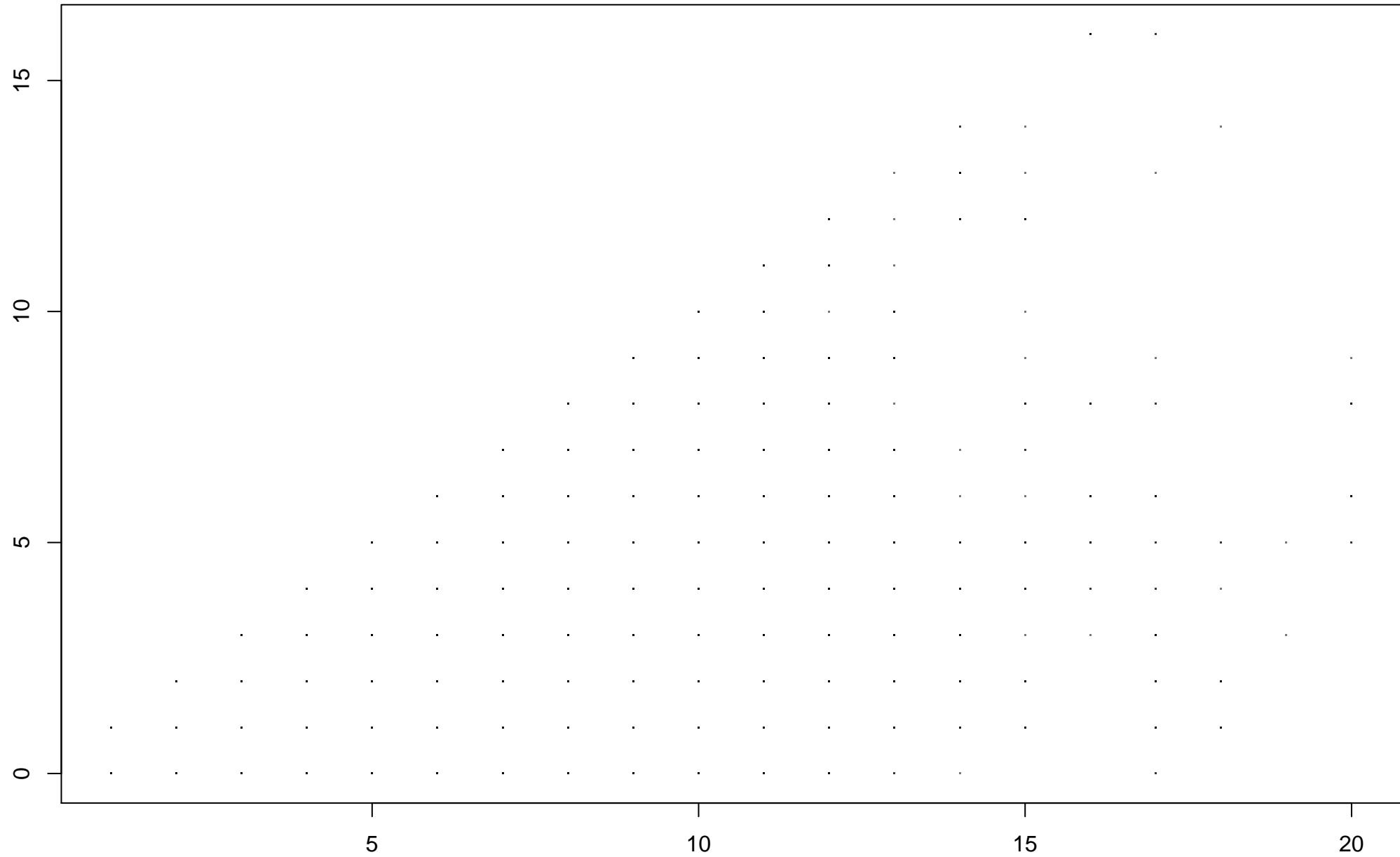


template_NHOHCount-mcs_docked_NHOHCount, MI = 0.1521 bit, normMI = 0.07827



template_NOCount-mcs_NOCount, MI = 0.2128 bit, normMI = 0.07666

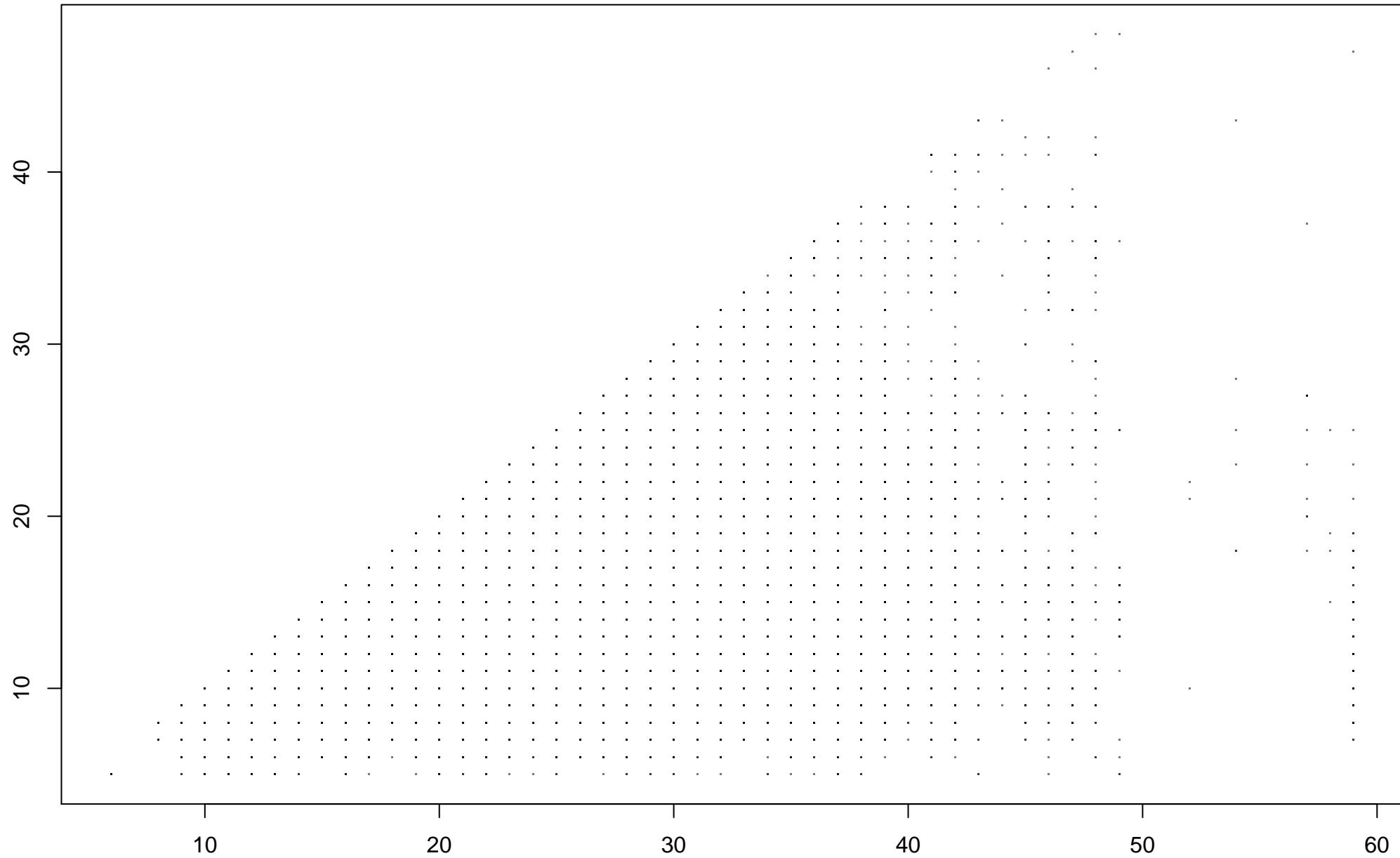
mcs_NOCount, H = 2.777 bit



template_NOCount, H = 3.237 bit

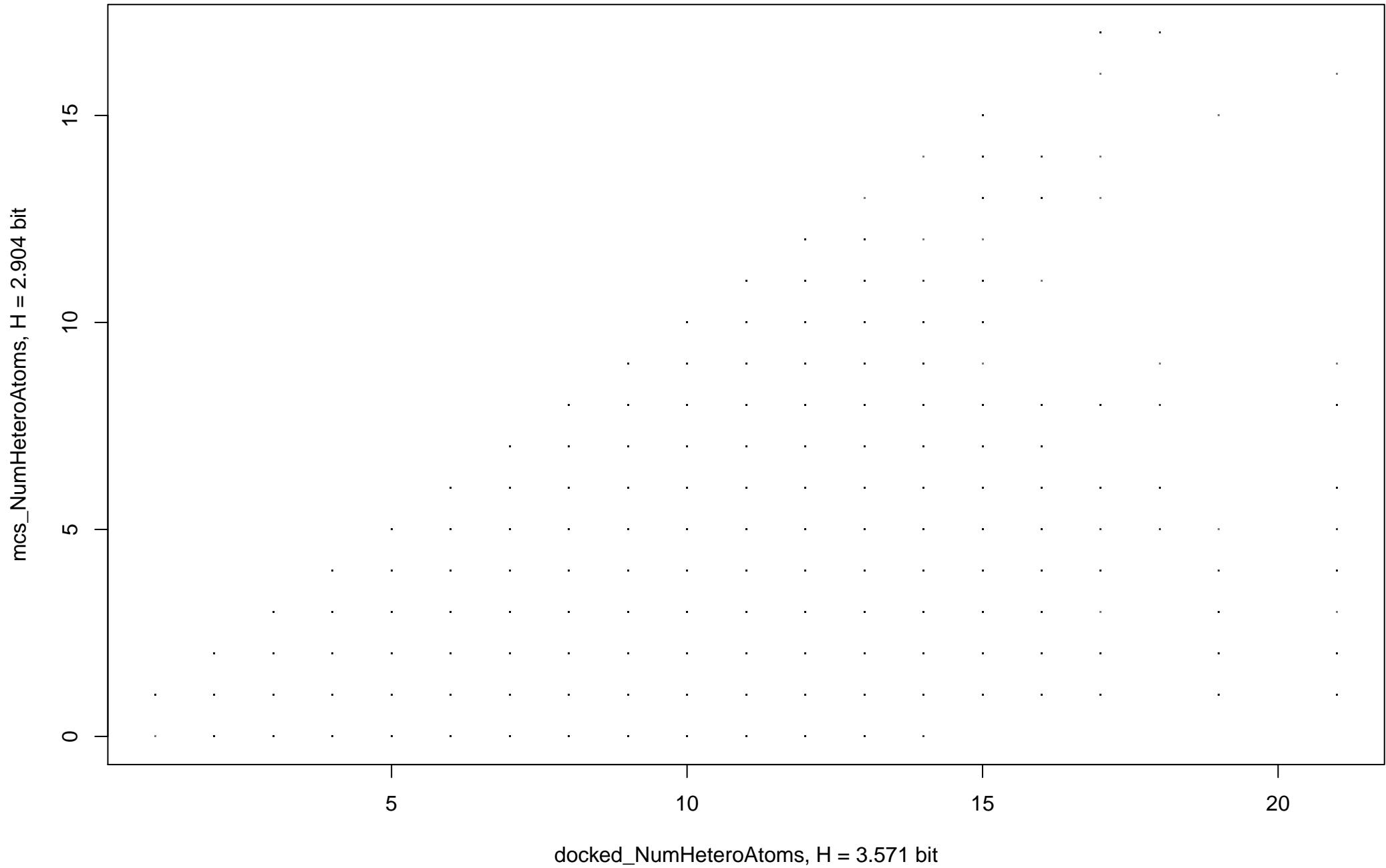
template_HeavyAtomCount–mcs_HeavyAtomCount, MI = 0.3355 bit, normMI = 0.07659

mcs_HeavyAtomCount, H = 4.38 bit



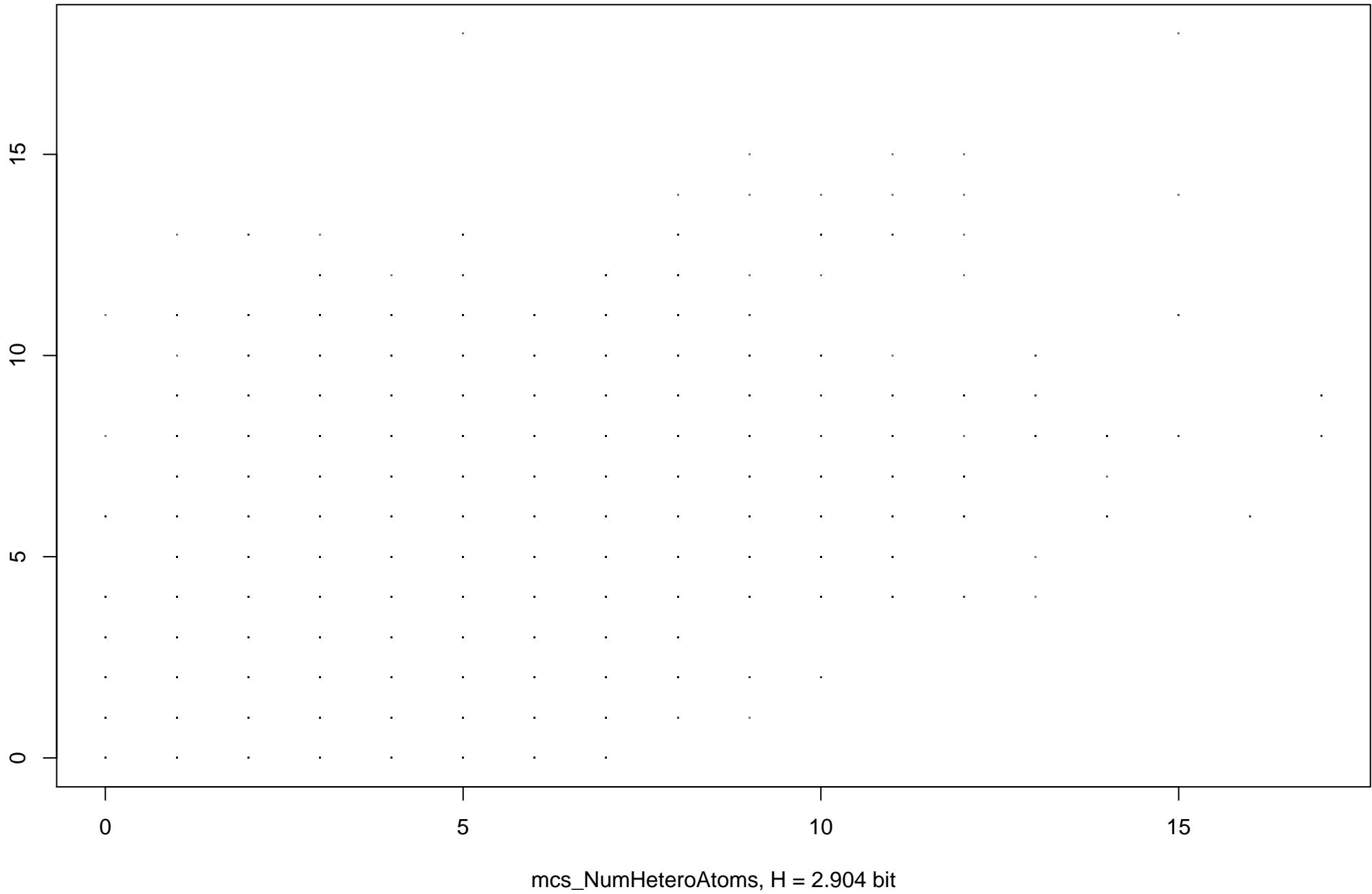
template_HeavyAtomCount, H = 4.952 bit

docked_NumHeteroAtoms-mcs_NumHeteroAtoms, MI = 0.2202 bit, normMI = 0.07581

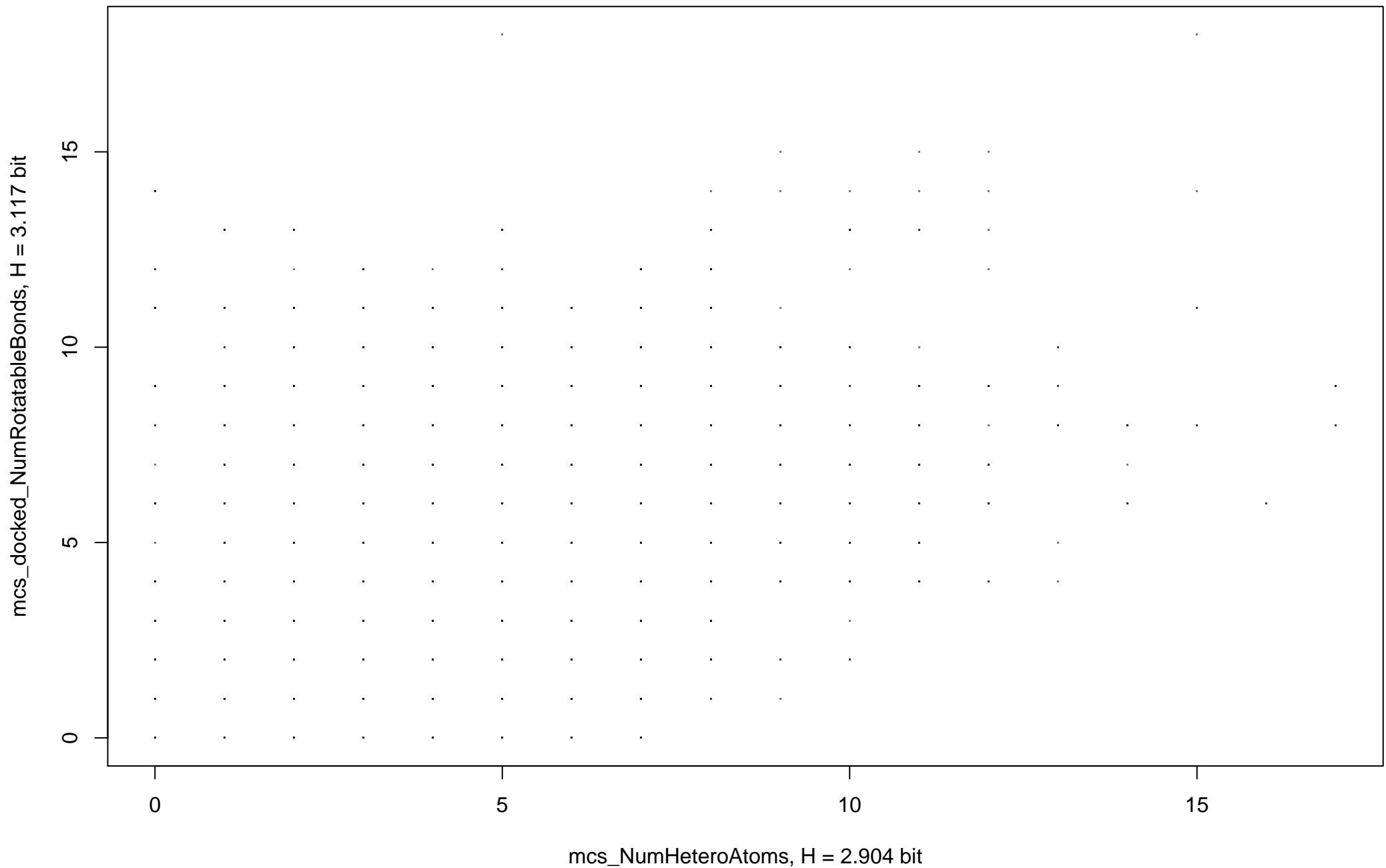


mcs_NumHeteroAtoms–mcs_template_NumRotatableBonds, MI = 0.2187 bit, normMI = 0.0753

mcs_template_NumRotatableBonds, H = 3.118 bit

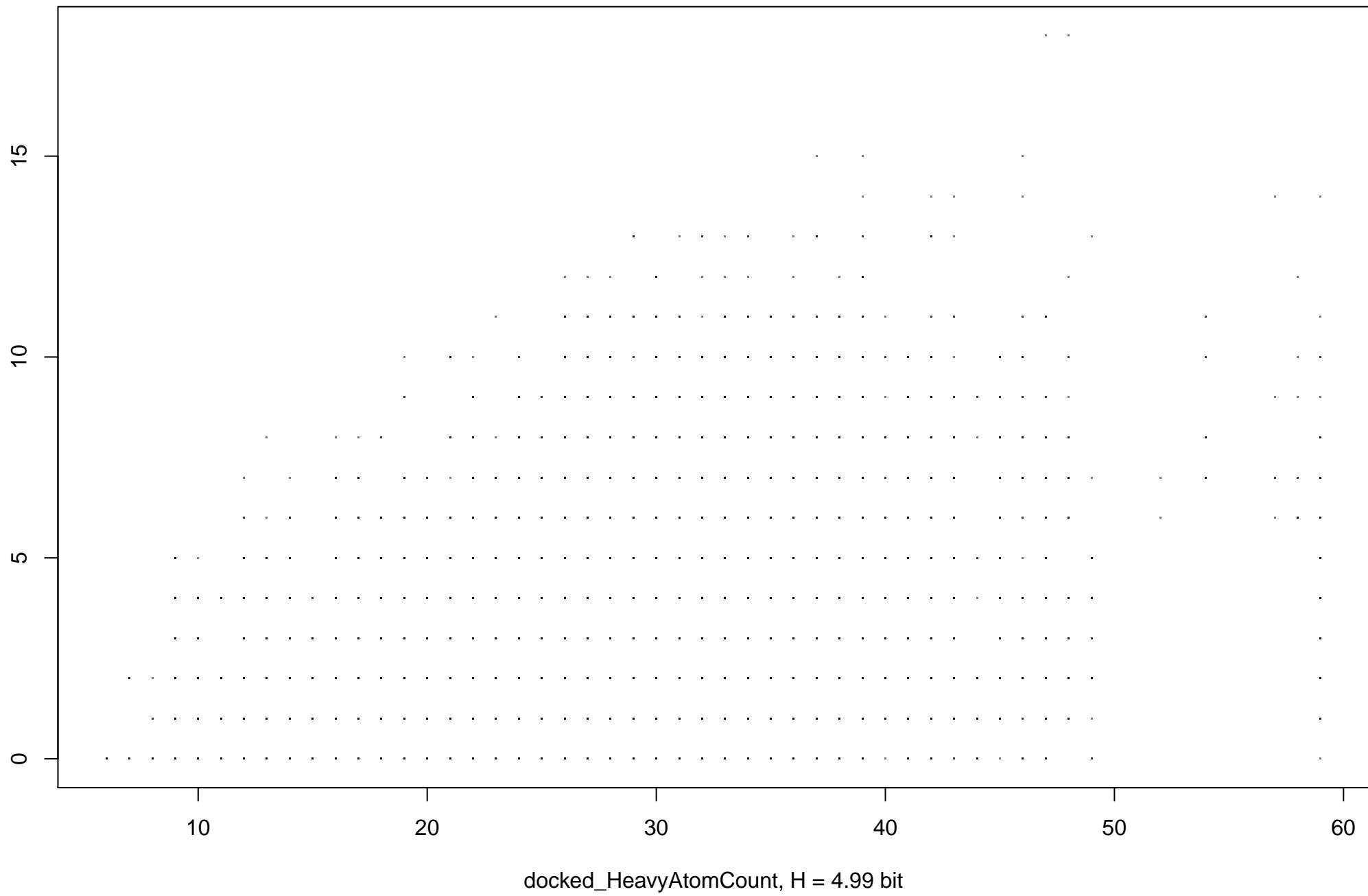


mcs_NumHeteroAtoms–mcs_docked_NumRotatableBonds, MI = 0.215 bit, normMI = 0.07404



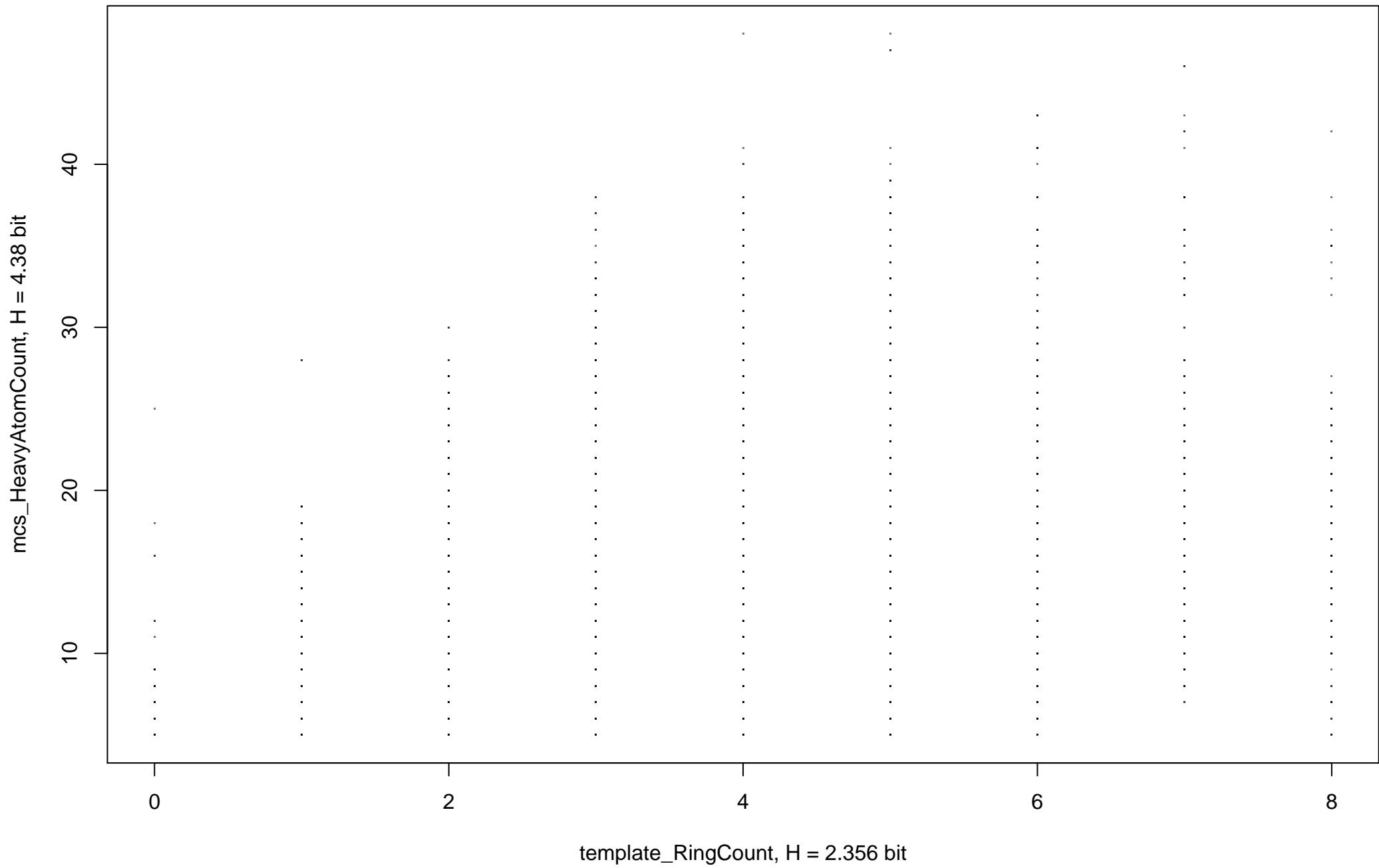
docked_HeavyAtomCount–mcs_template_NumRotatableBonds, MI = 0.2242 bit, normMI = 0.07192

mcs_template_NumRotatableBonds, H = 3.118 bit

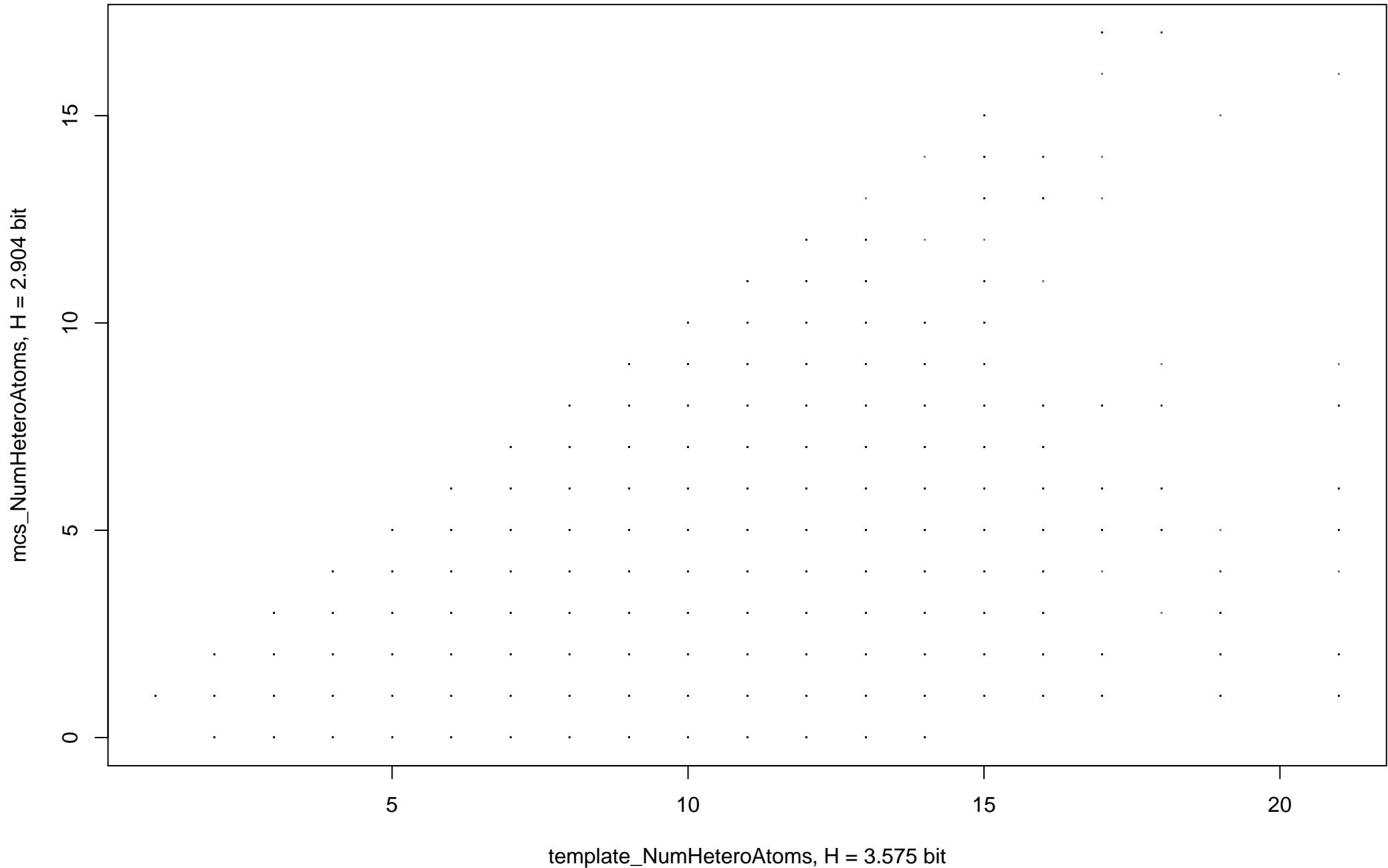


docked_HeavyAtomCount, H = 4.99 bit

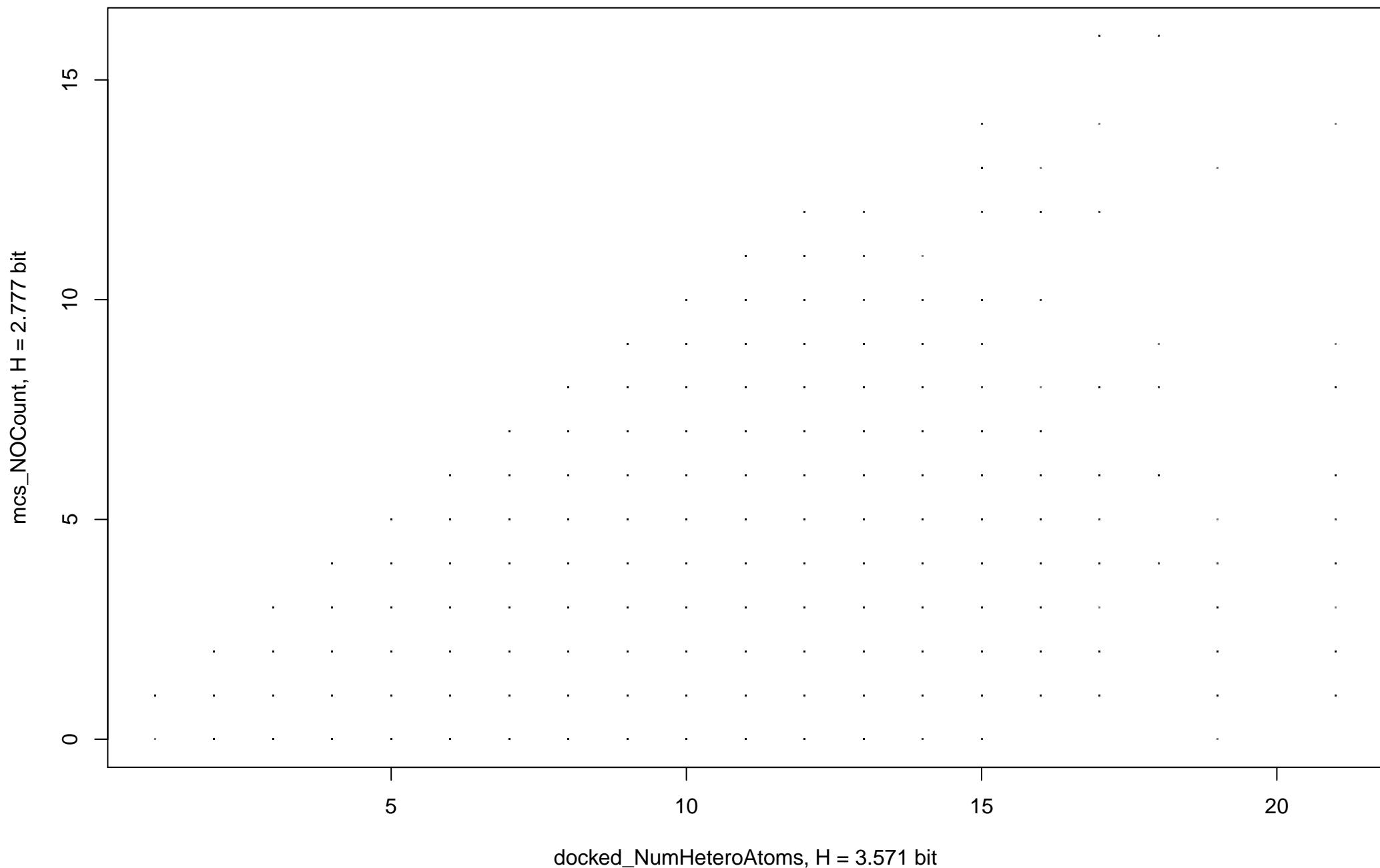
template_RingCount-mcs_HeavyAtomCount, MI = 0.1694 bit, normMI = 0.07189



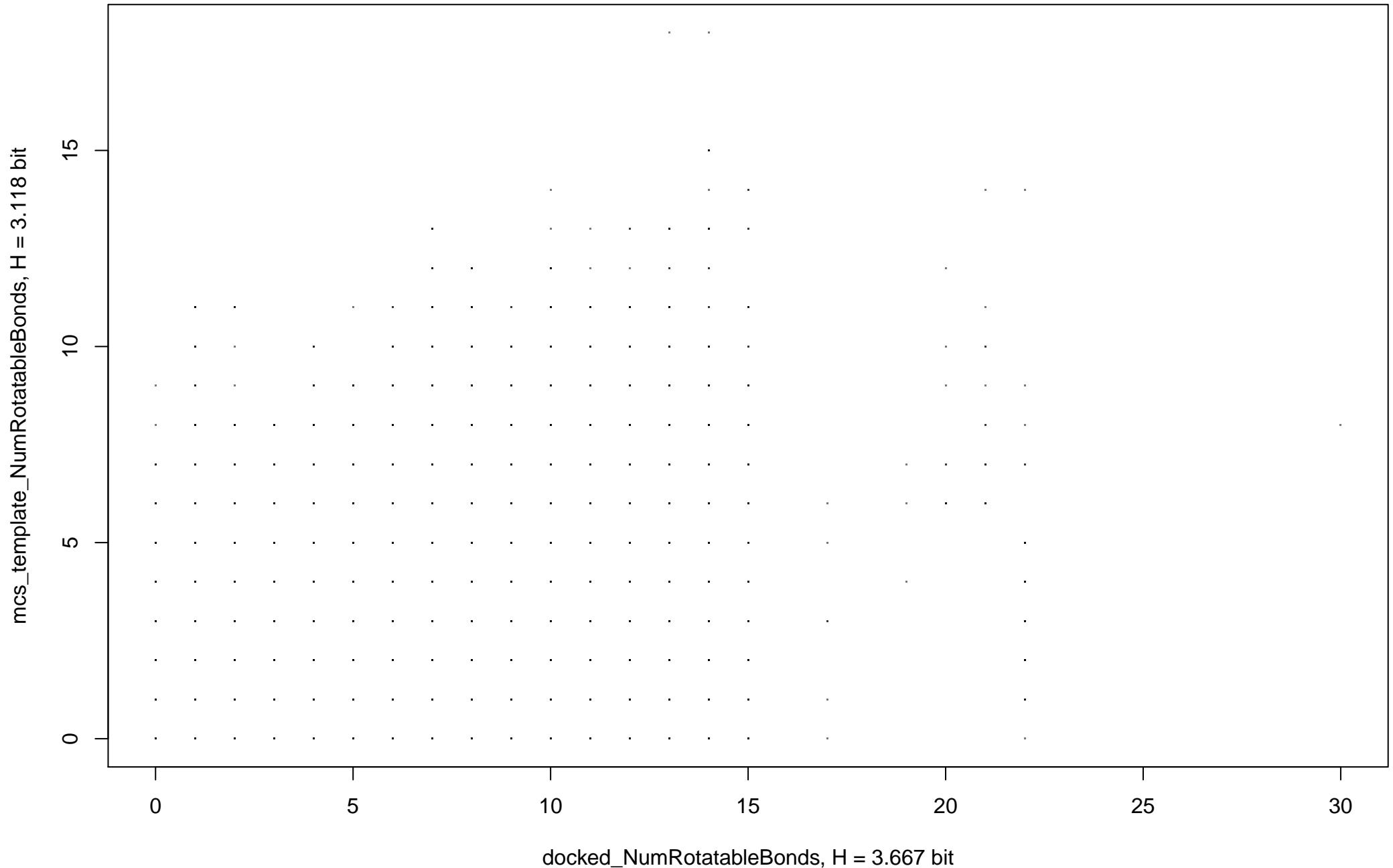
template_NumHeteroAtoms–mcs_NumHeteroAtoms, MI = 0.1978 bit, normMI = 0.06811



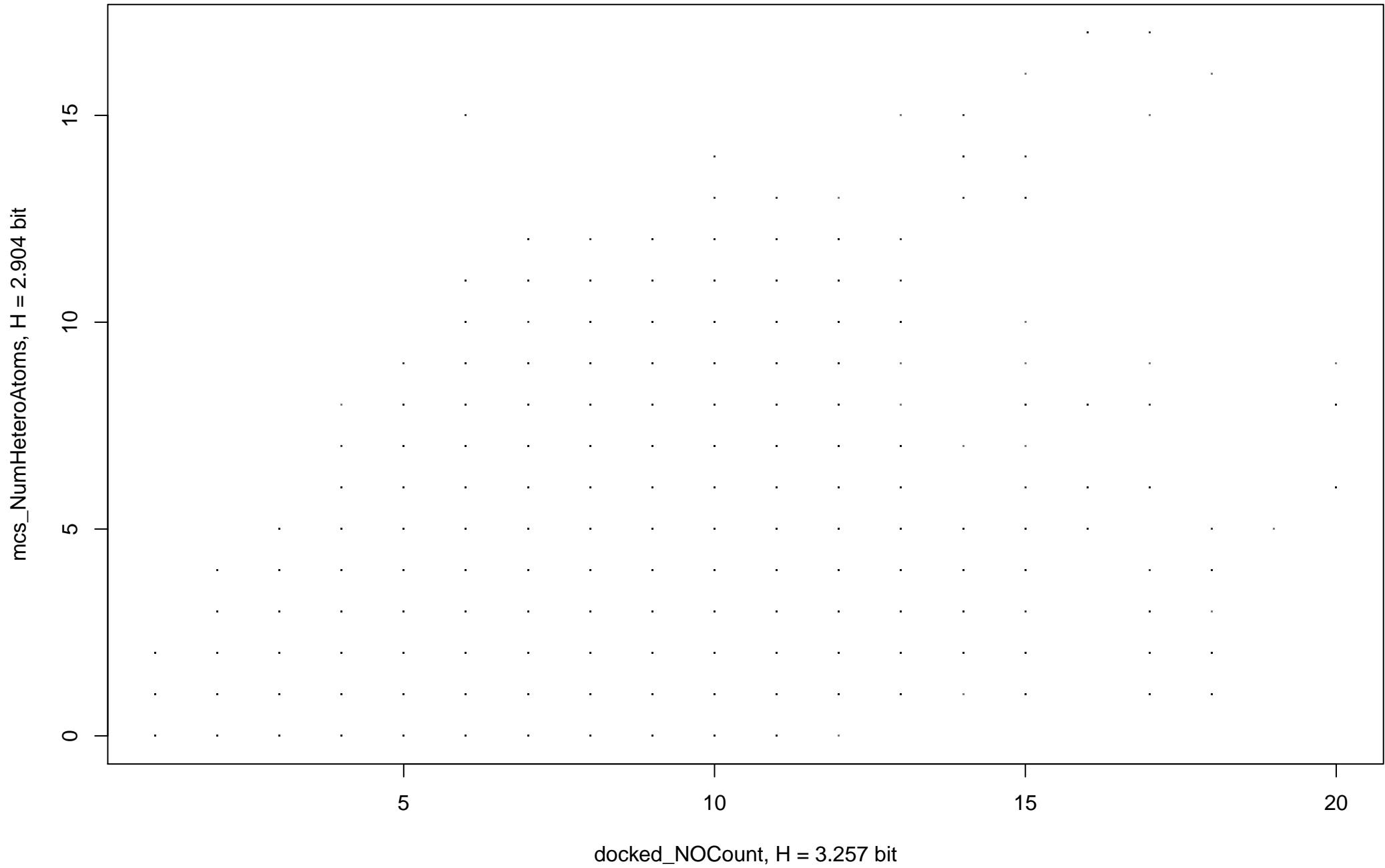
docked_NumHeteroAtoms-mcs_NOCount, MI = 0.185 bit, normMI = 0.06663



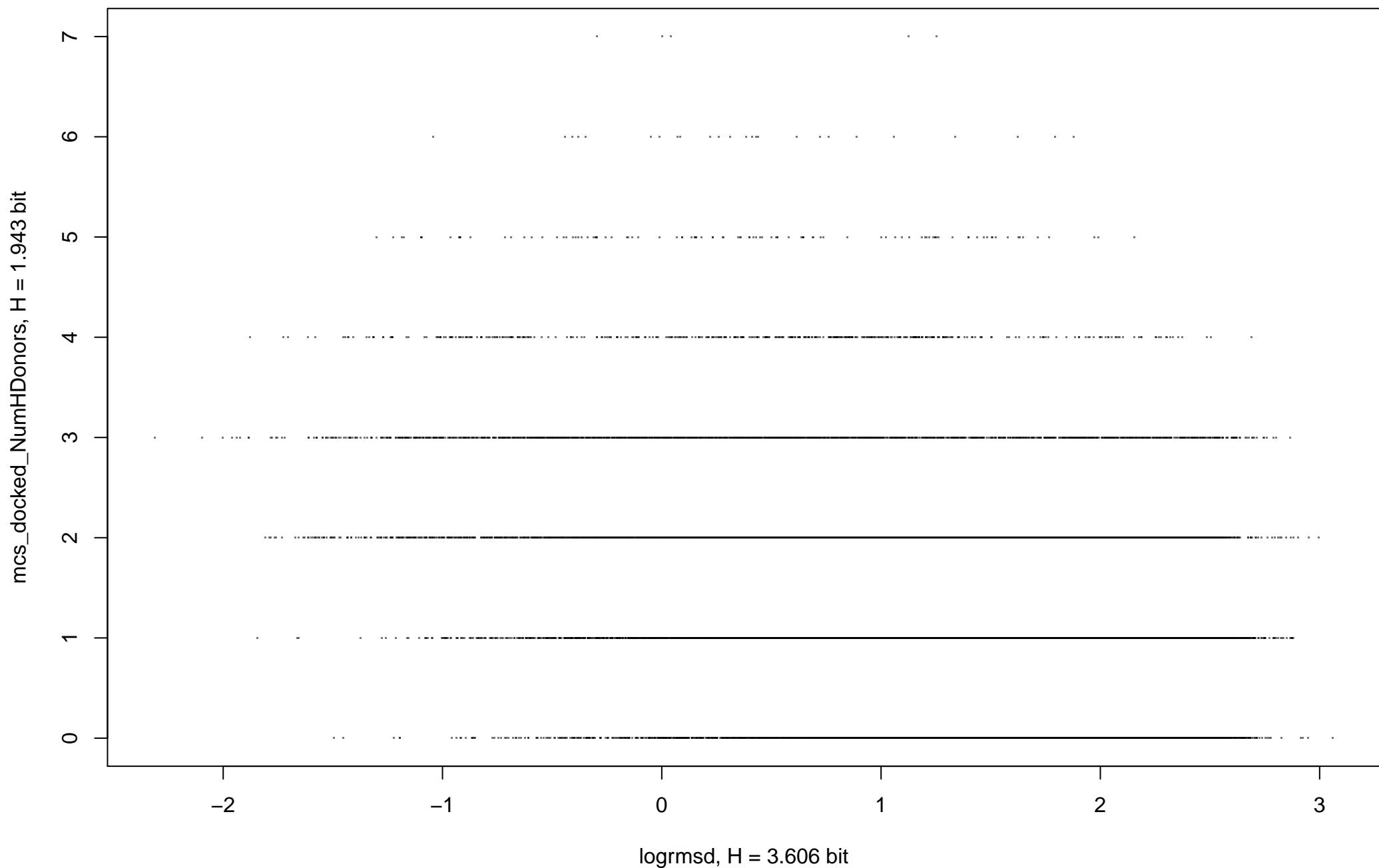
docked_NumRotatableBonds–mcs_template_NumRotatableBonds, MI = 0.2056 bit, normMI = 0.06592



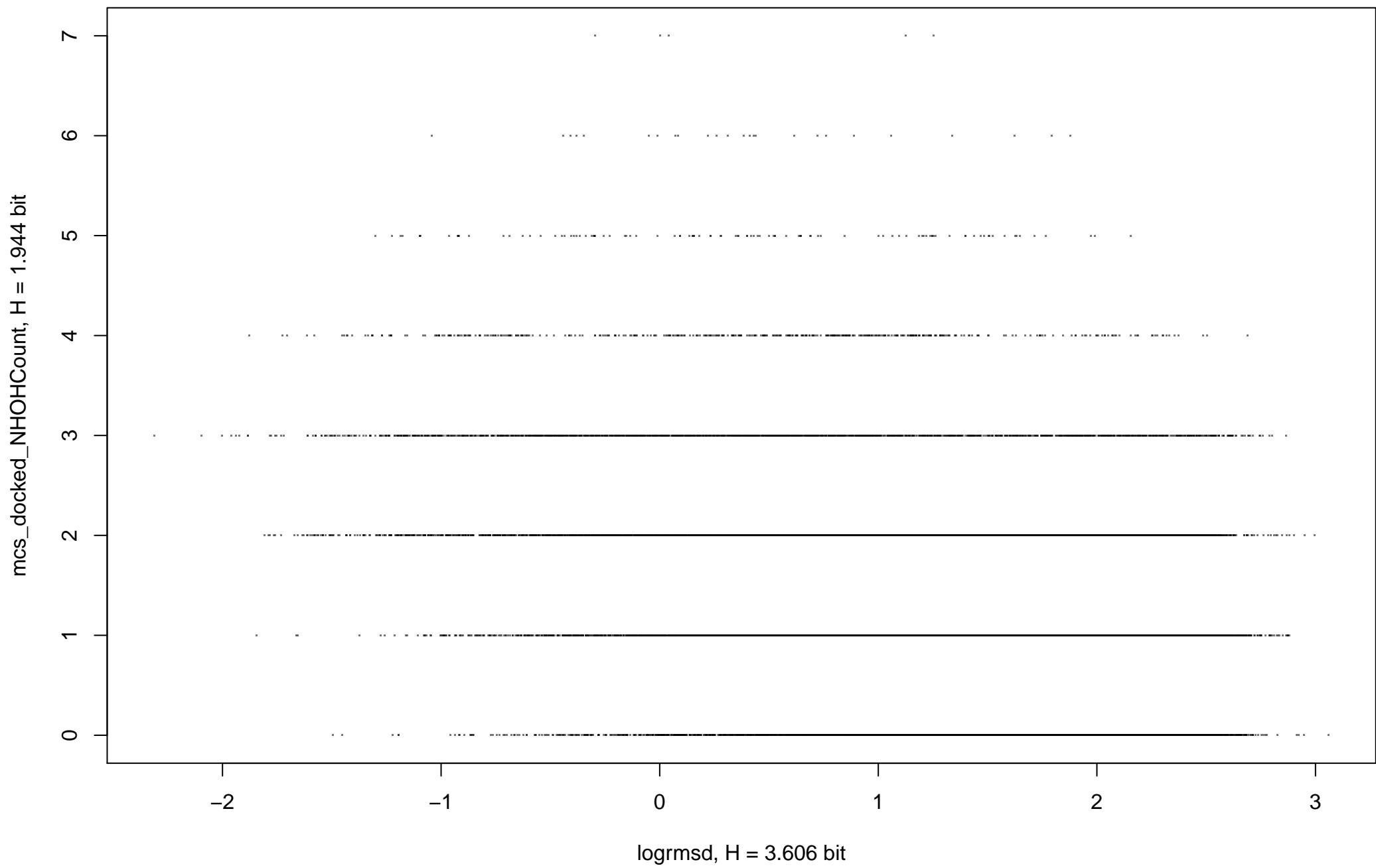
docked_NOCount-mcs_NumHeteroAtoms, MI = 0.1892 bit, normMI = 0.06513



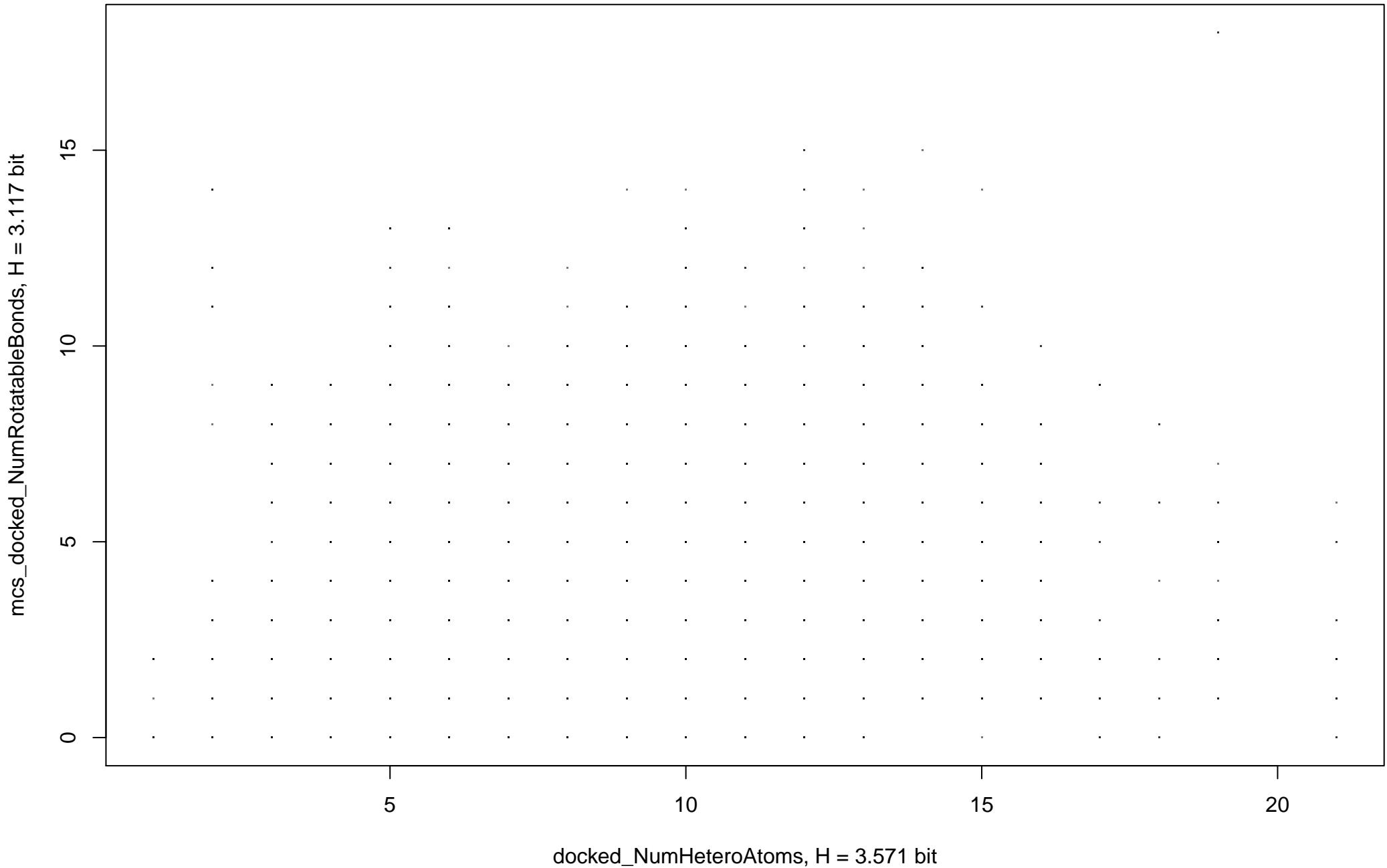
logrmsd-mcs_docked_NumHDonors, MI = 0.1249 bit, normMI = 0.06428



logrmsd-mcs_docked_NHOHCount, MI = 0.1248 bit, normMI = 0.06421

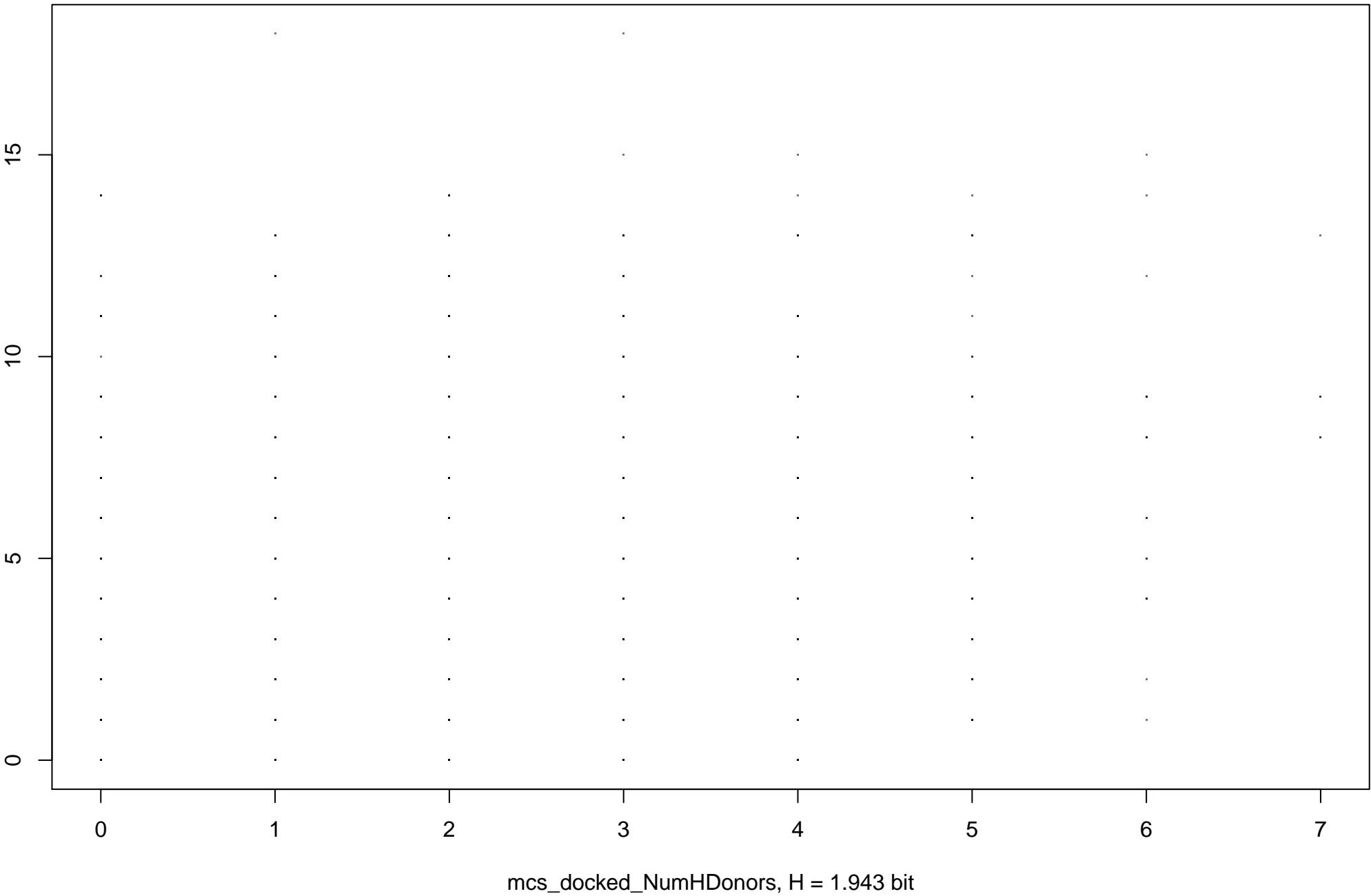


docked_NumHeteroAtoms–mcs_docked_NumRotatableBonds, MI = 0.1998 bit, normMI = 0.0641



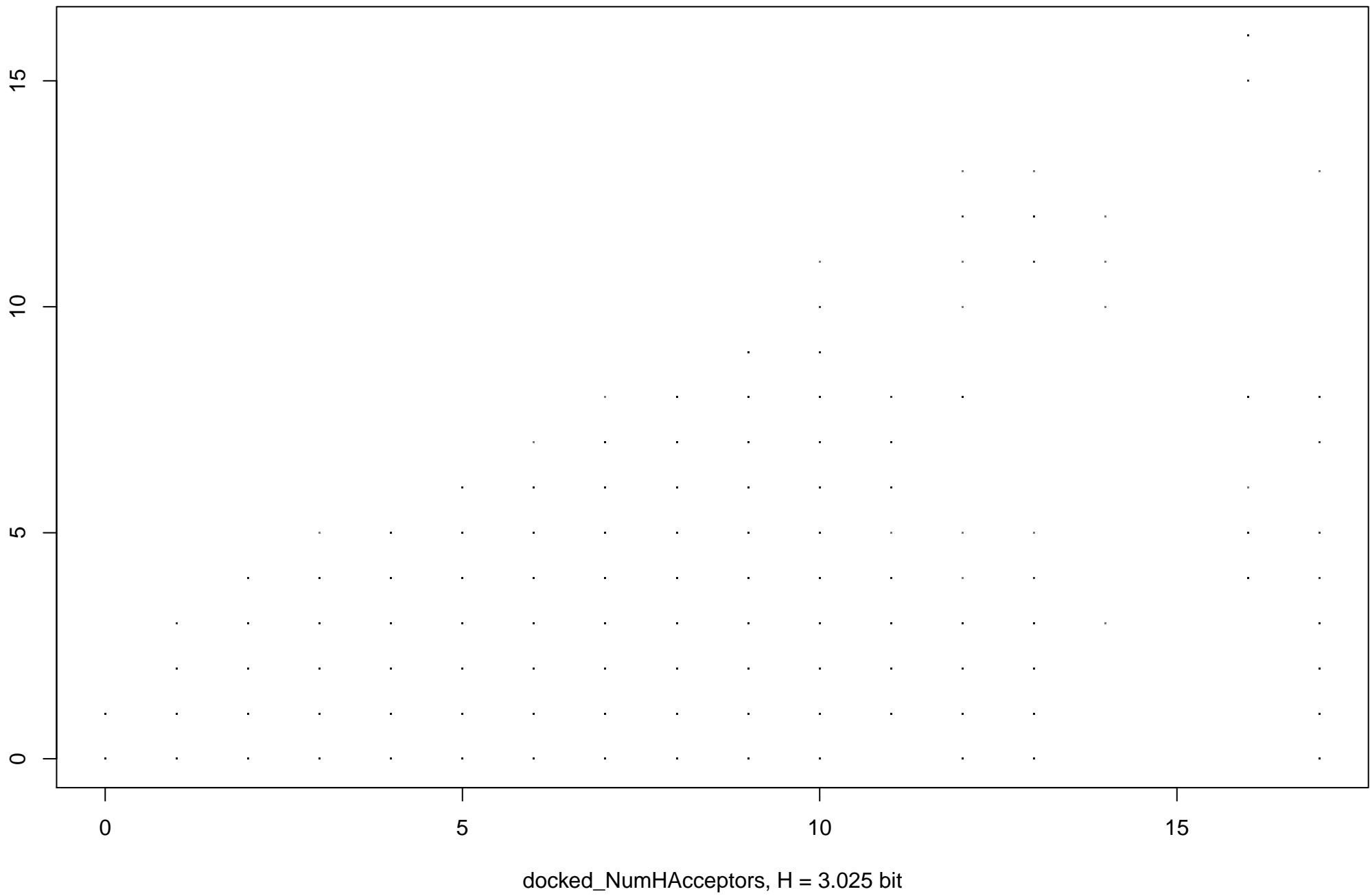
mcs_docked_NumHDonors–mcs_docked_NumRotatableBonds, MI = 0.1234 bit, normMI = 0.06349

mcs_docked_NumRotatableBonds, H = 3.117 bit



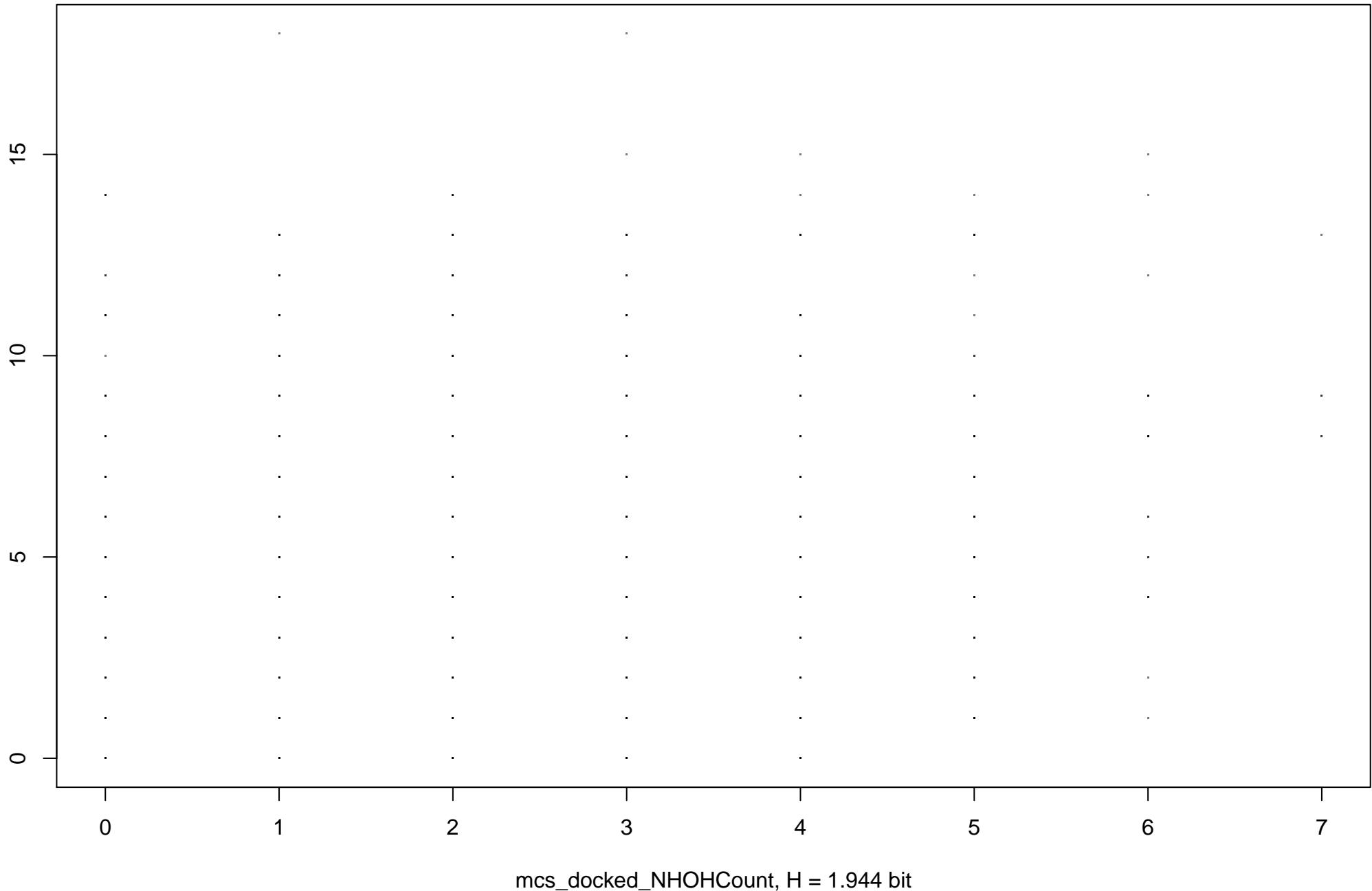
docked_NumHAcceptors-mcs_template_NumHAcceptors, MI = 0.158 bit, normMI = 0.06349

mcs_template_NumHAcceptors, H = 2.488 bit

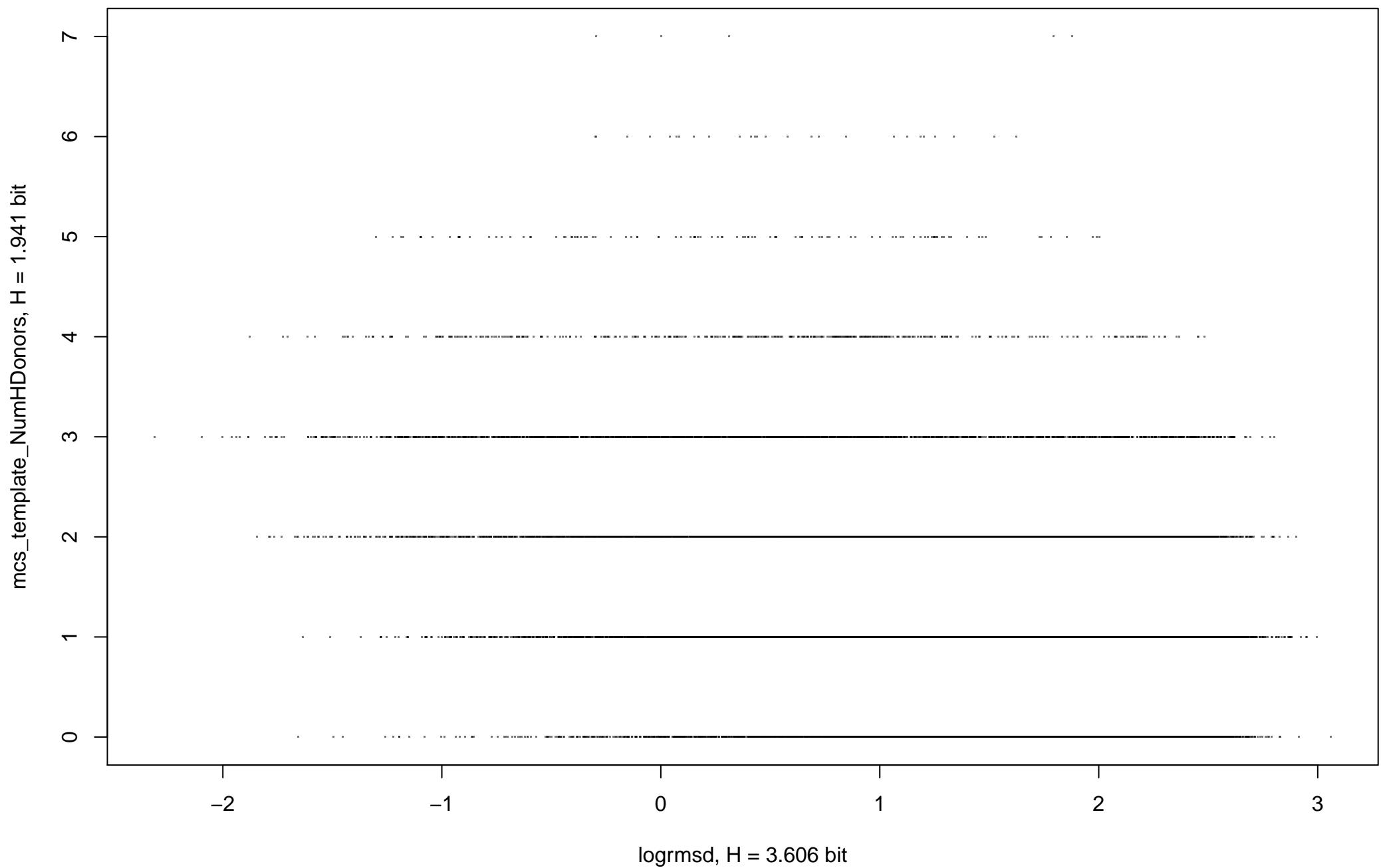


mcs_docked_NHOHCount-mcs_docked_NumRotatableBonds, MI = 0.123 bit, normMI = 0.06328

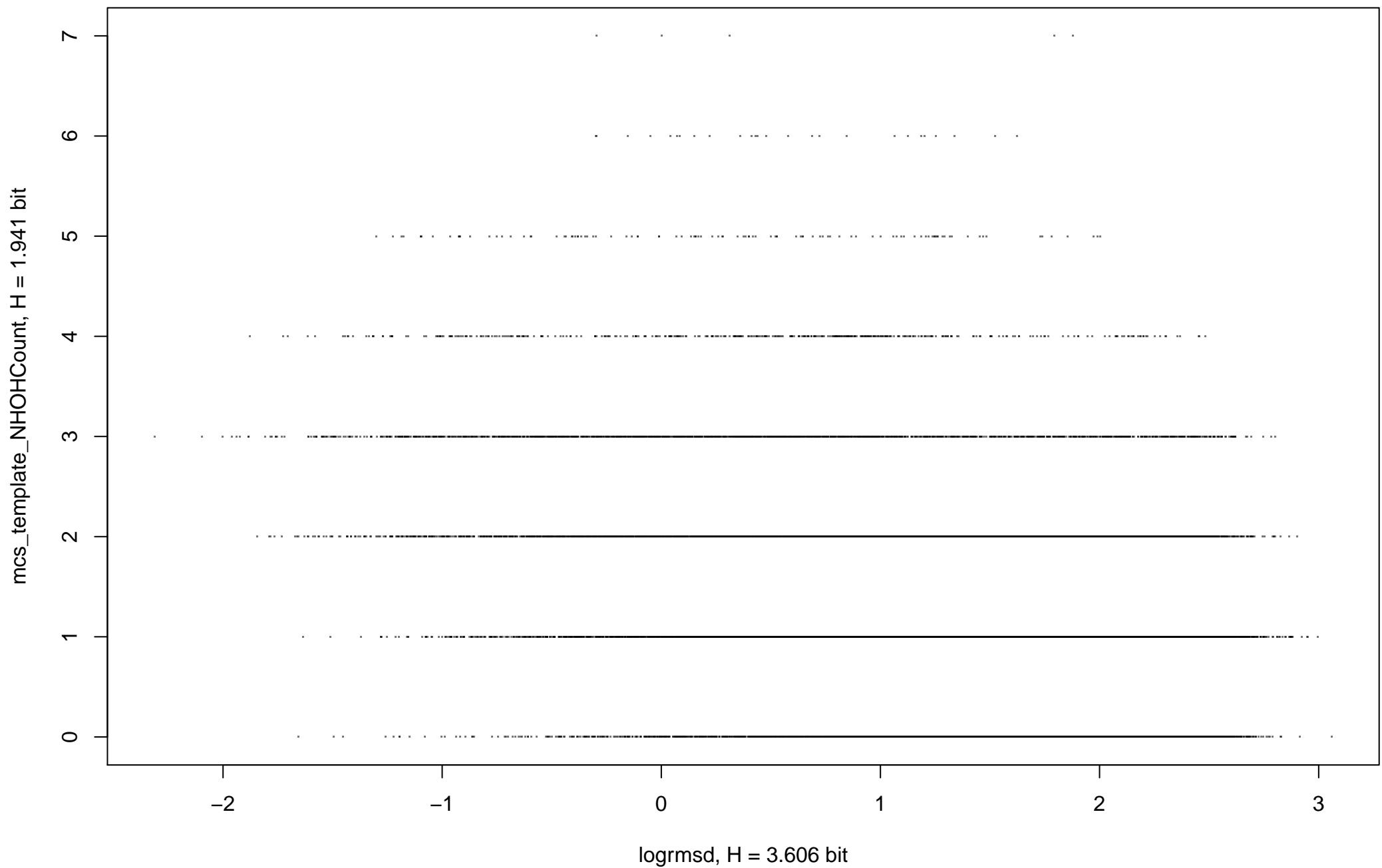
mcs_docked_NumRotatableBonds, H = 3.117 bit



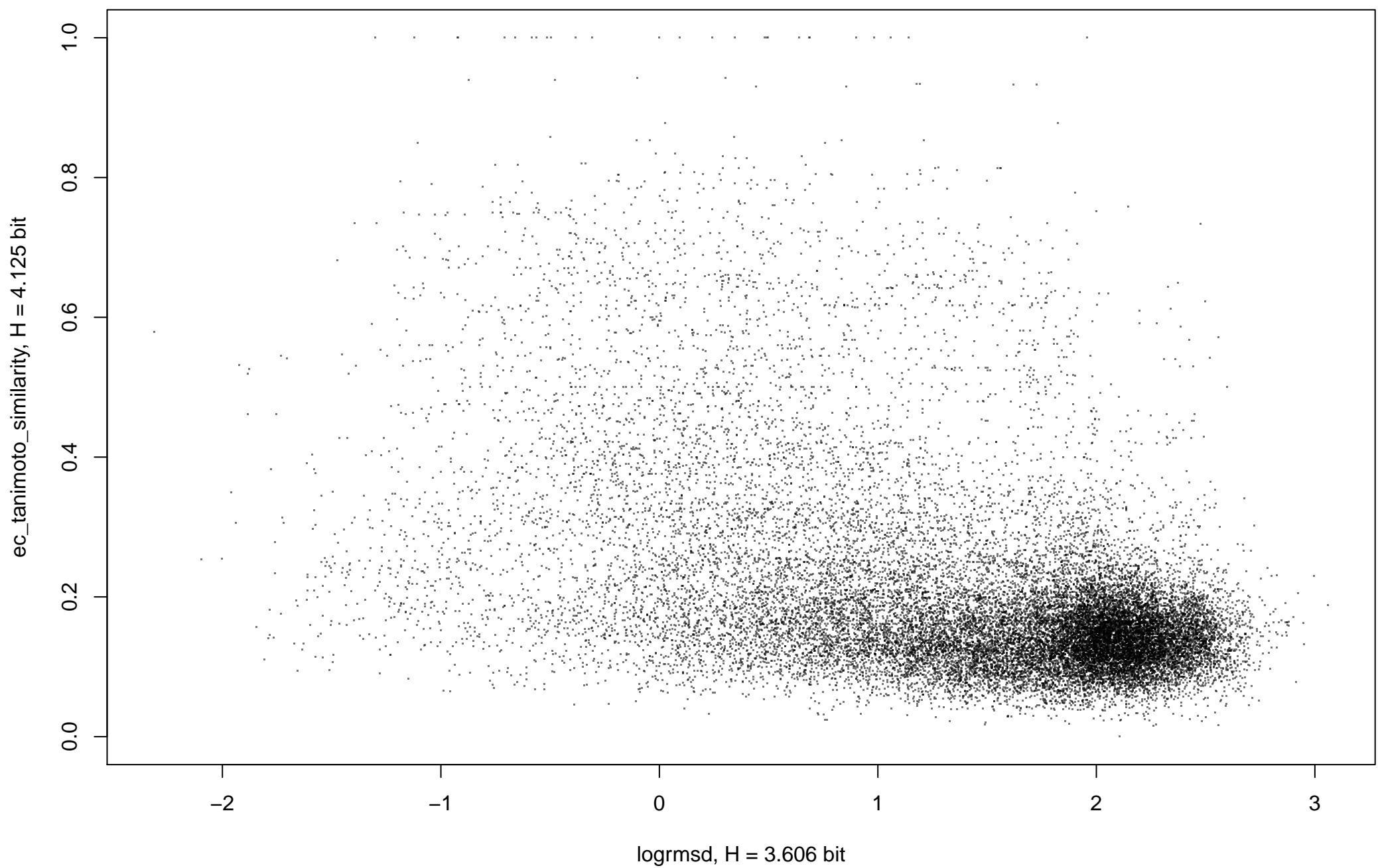
logrmsd-mcs_template_NumHDonors, MI = 0.1224 bit, normMI = 0.06309



logrmsd-mcs_template_NHOHCount, MI = 0.1222 bit, normMI = 0.06294

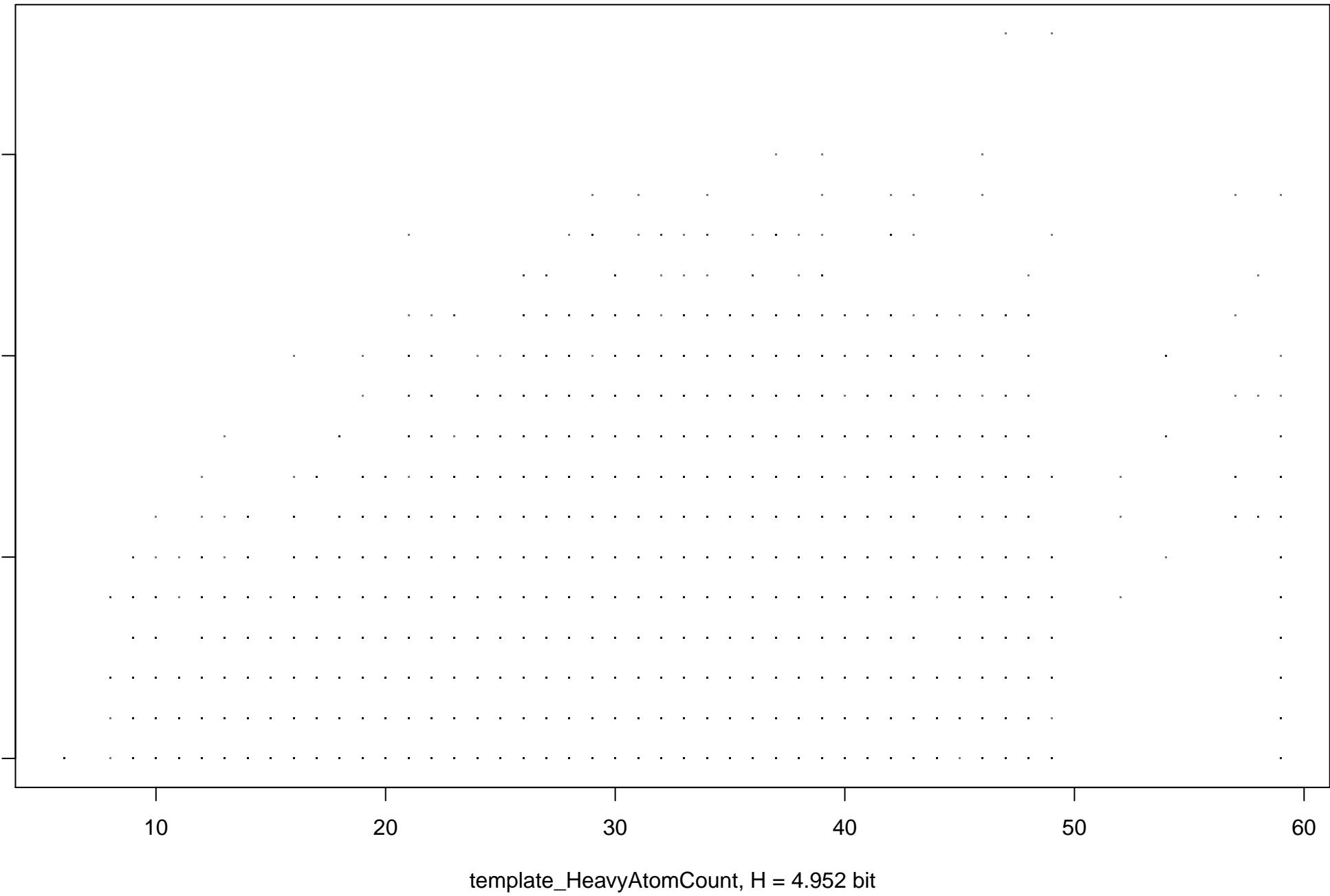


logrmsd-ec_tanimoto_similarity, MI = 0.226 bit, normMI = 0.06267

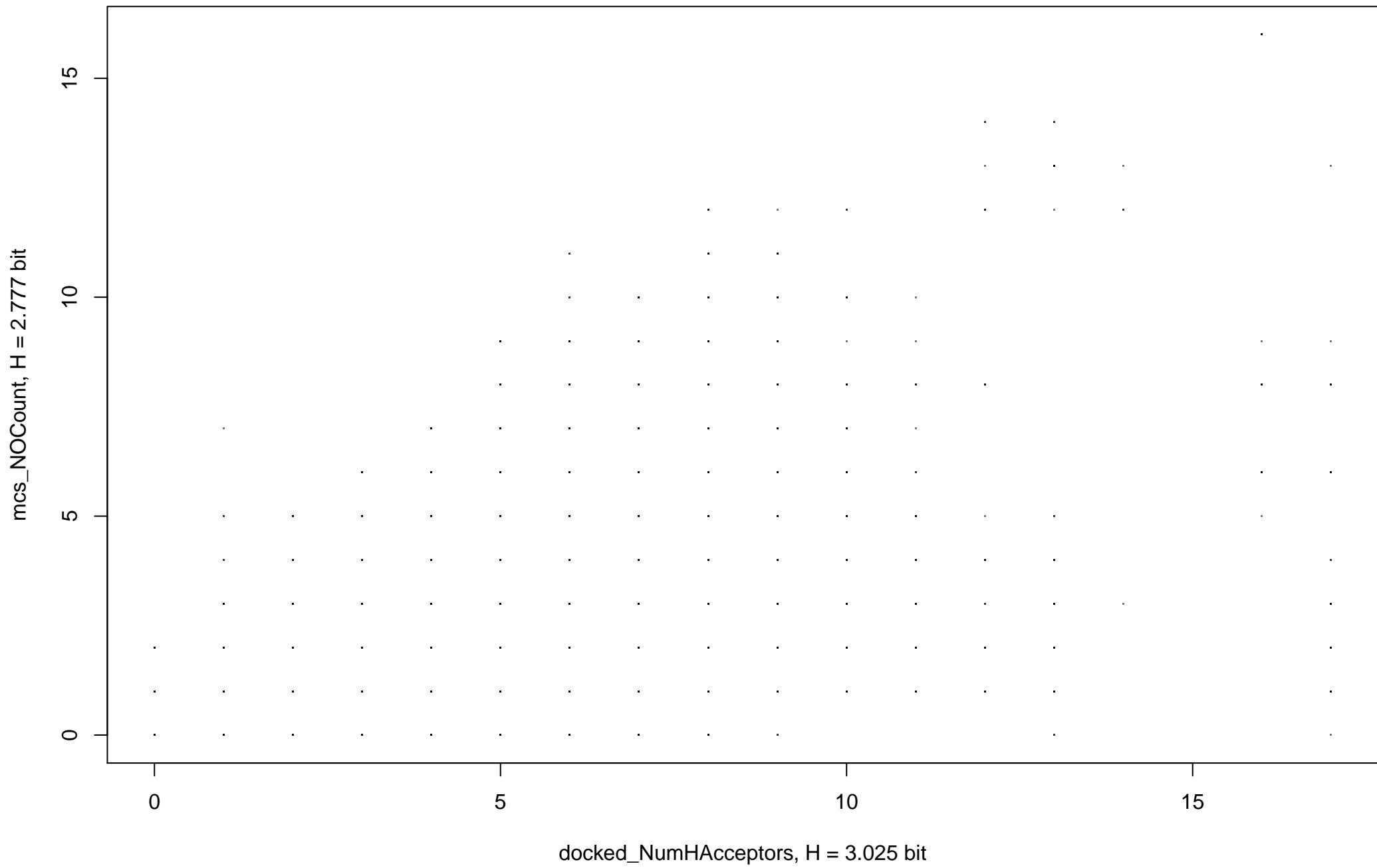


template_HeavyAtomCount-mcs_docked_NumRotatableBonds, MI = 0.1914 bit, normMI = 0.06143

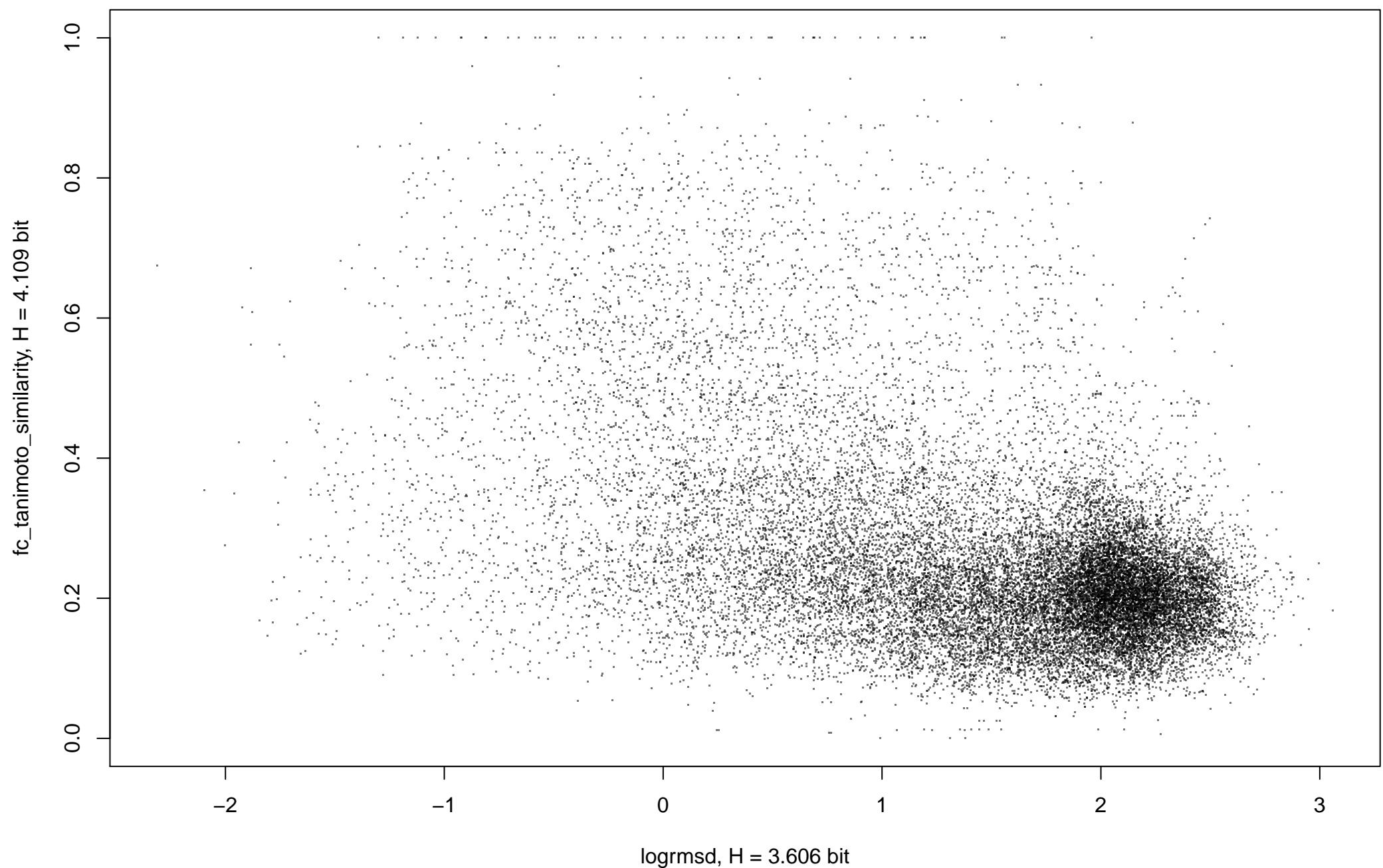
mcs_docked_NumRotatableBonds, H = 3.117 bit



docked_NumHAcceptors–mcs_NOCount, MI = 0.1694 bit, normMI = 0.06101

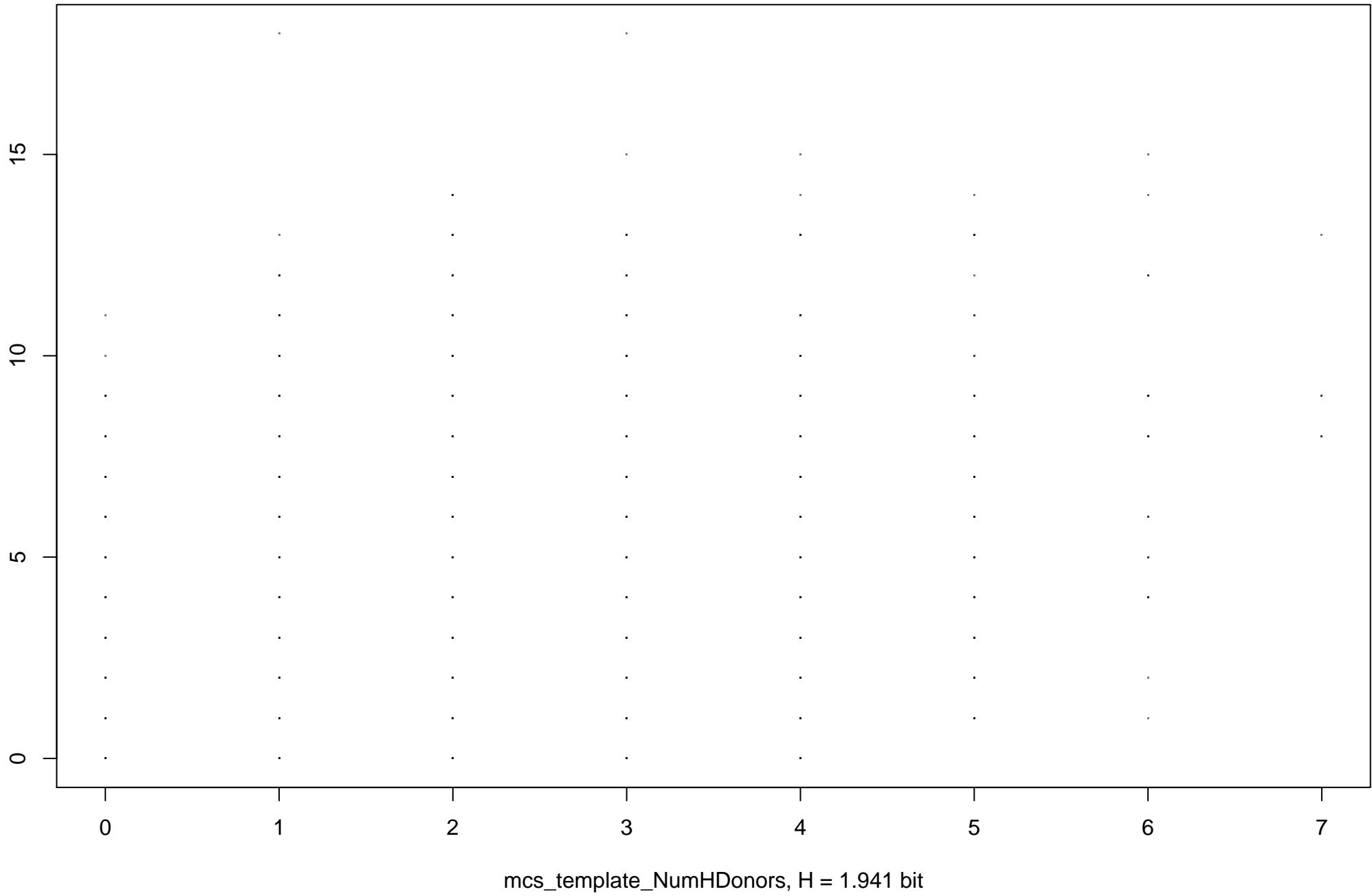


logrmsd-fc_tanimoto_similarity, MI = 0.2158 bit, normMI = 0.05983

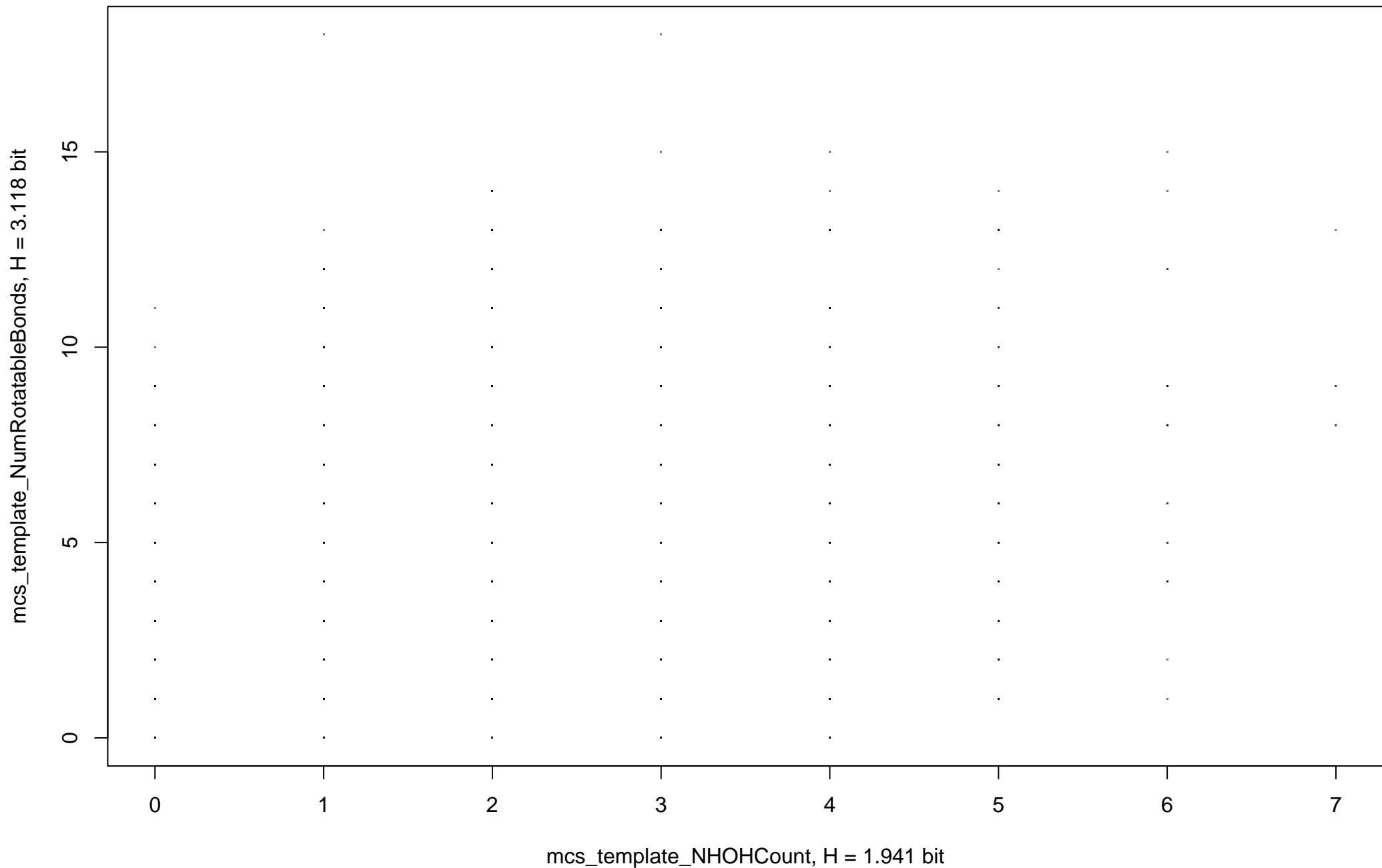


mcs_template_NumHDonors-mcs_template_NumRotatableBonds, MI = 0.1161 bit, normMI = 0.05981

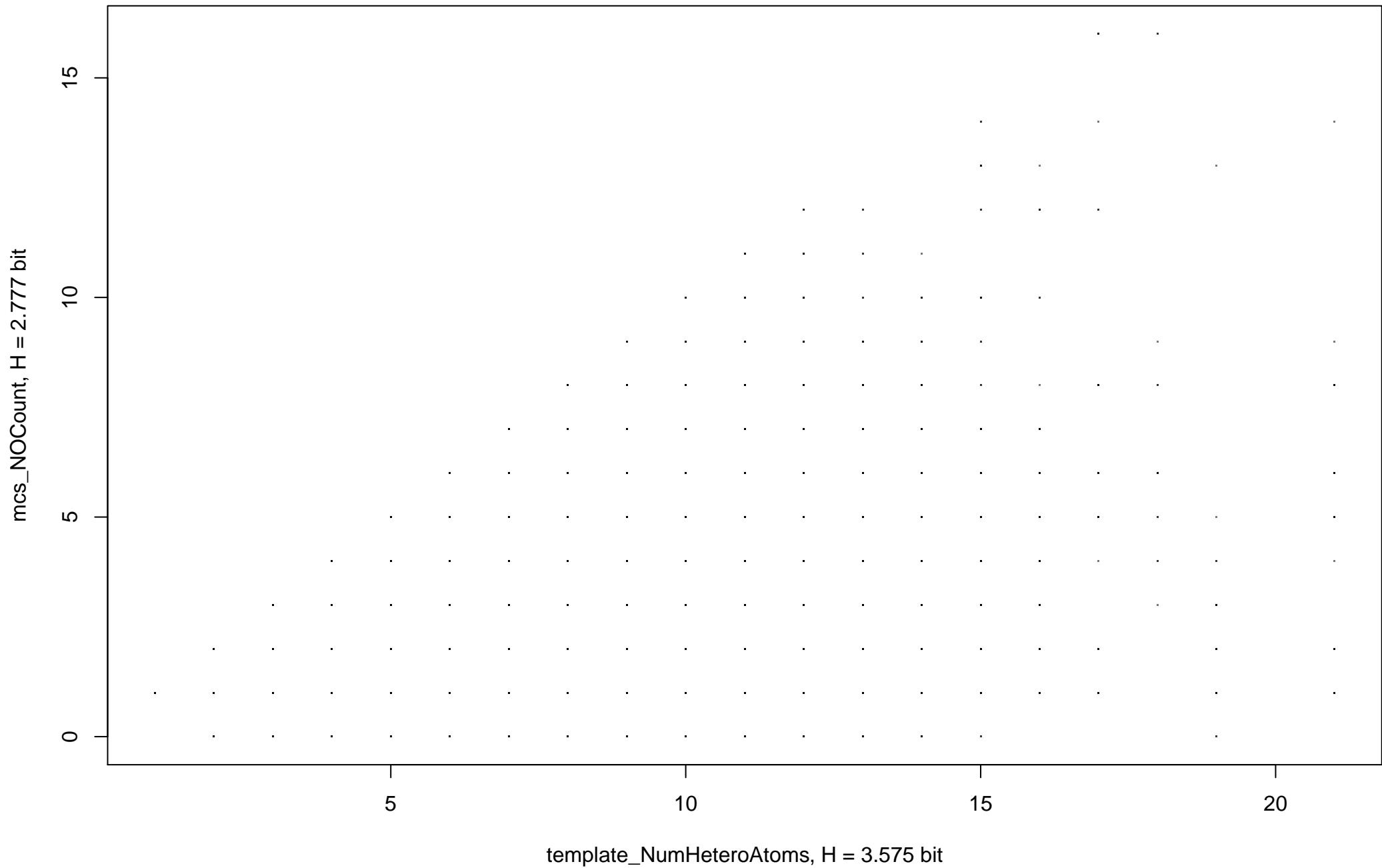
mcs_template_NumRotatableBonds, H = 3.118 bit



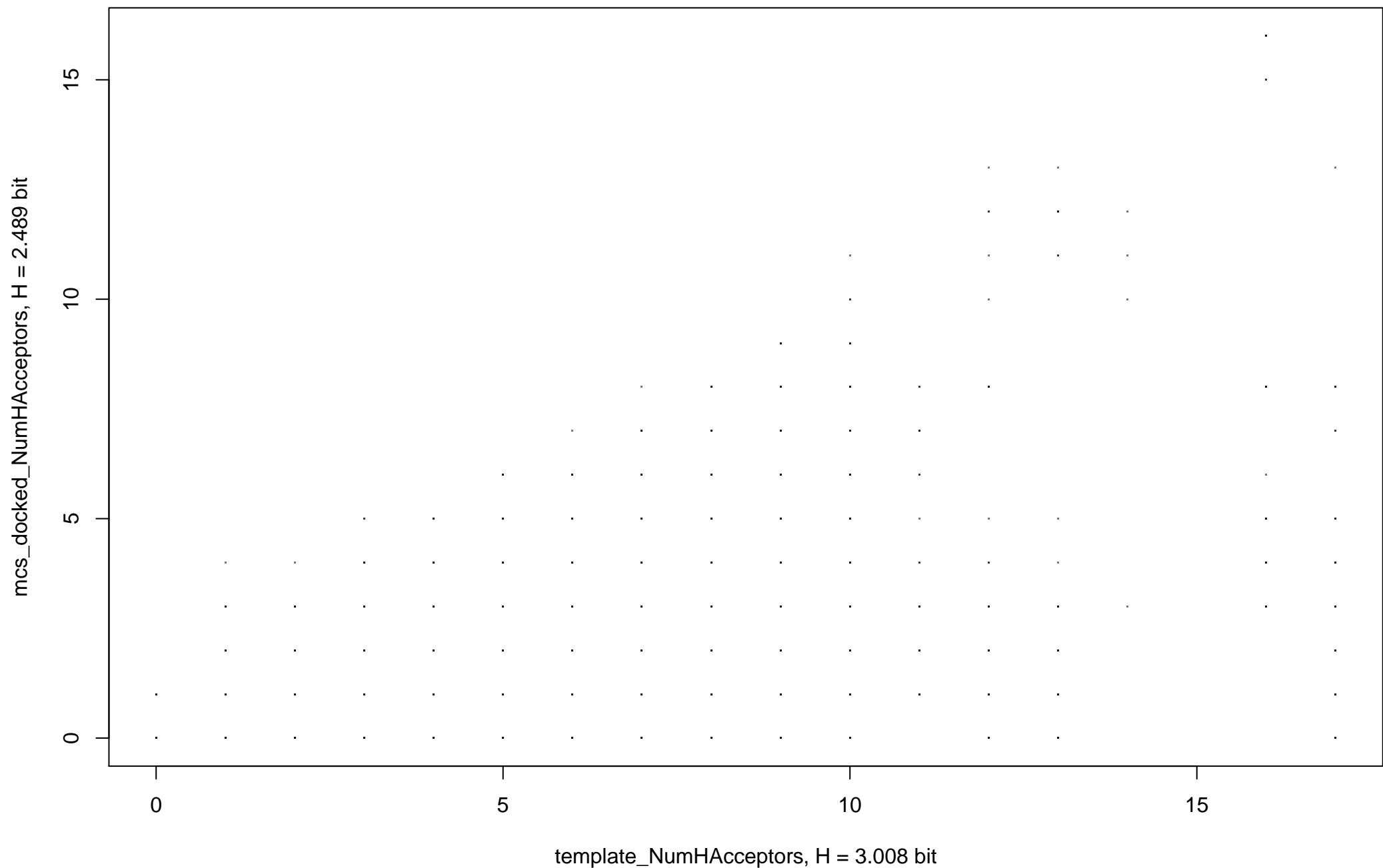
mcs_template_NHOHCount–mcs_template_NumRotatableBonds, MI = 0.1157 bit, normMI = 0.05962



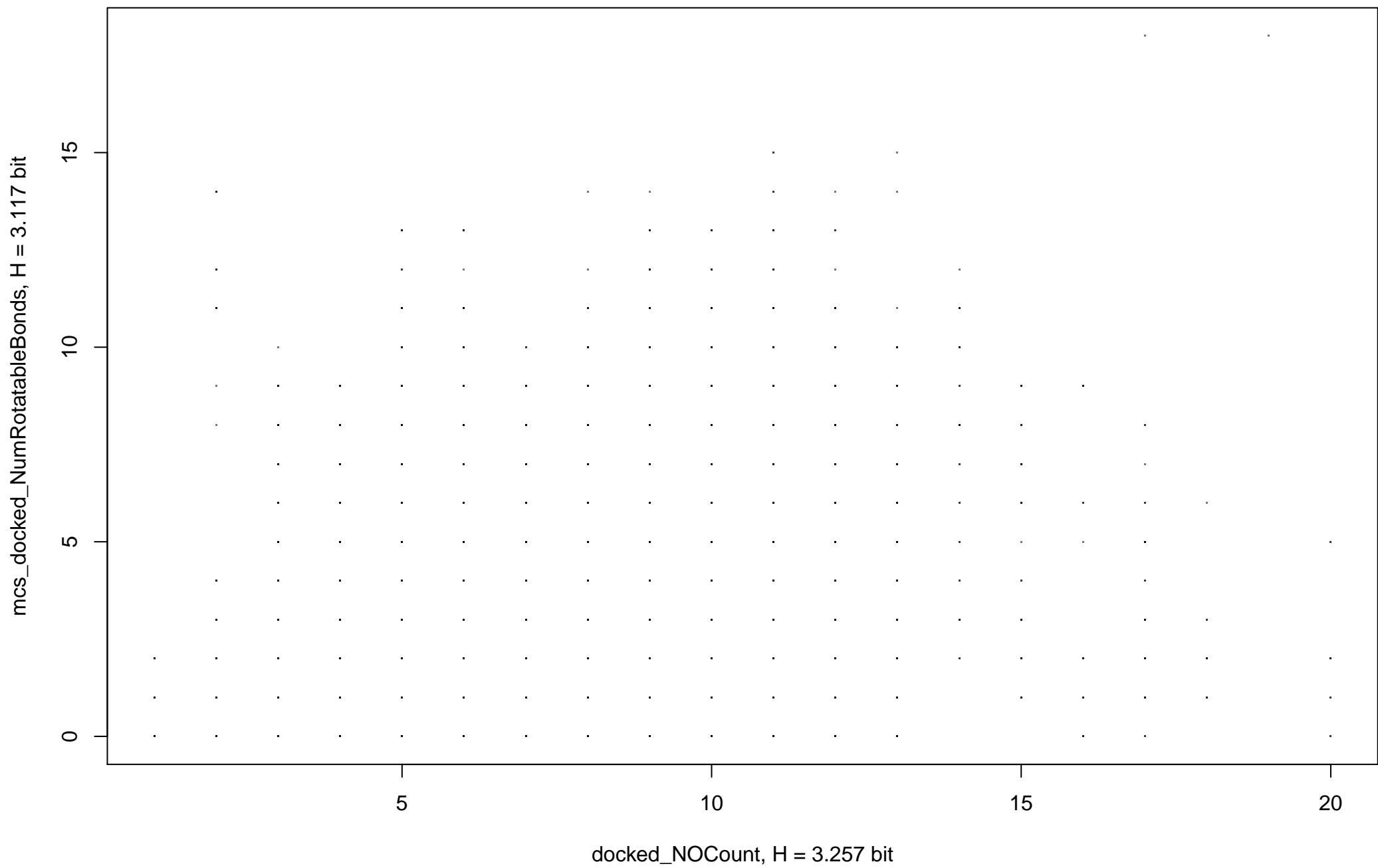
template_NumHeteroAtoms-mcs_NOCount, MI = 0.1645 bit, normMI = 0.05925



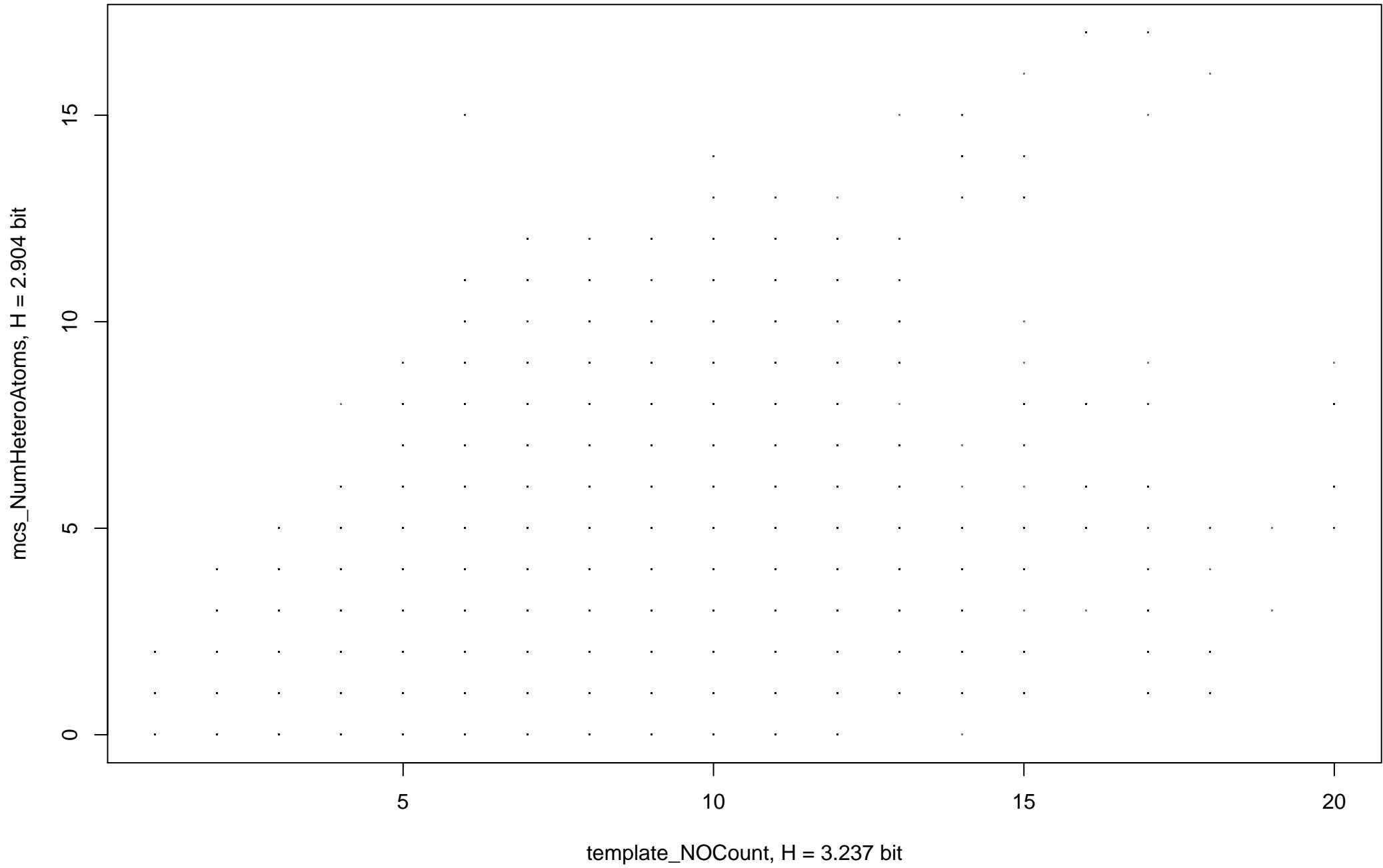
template_NumHAcceptors-mcs_docked_NumHAcceptors, MI = 0.1463 bit, normMI = 0.05878



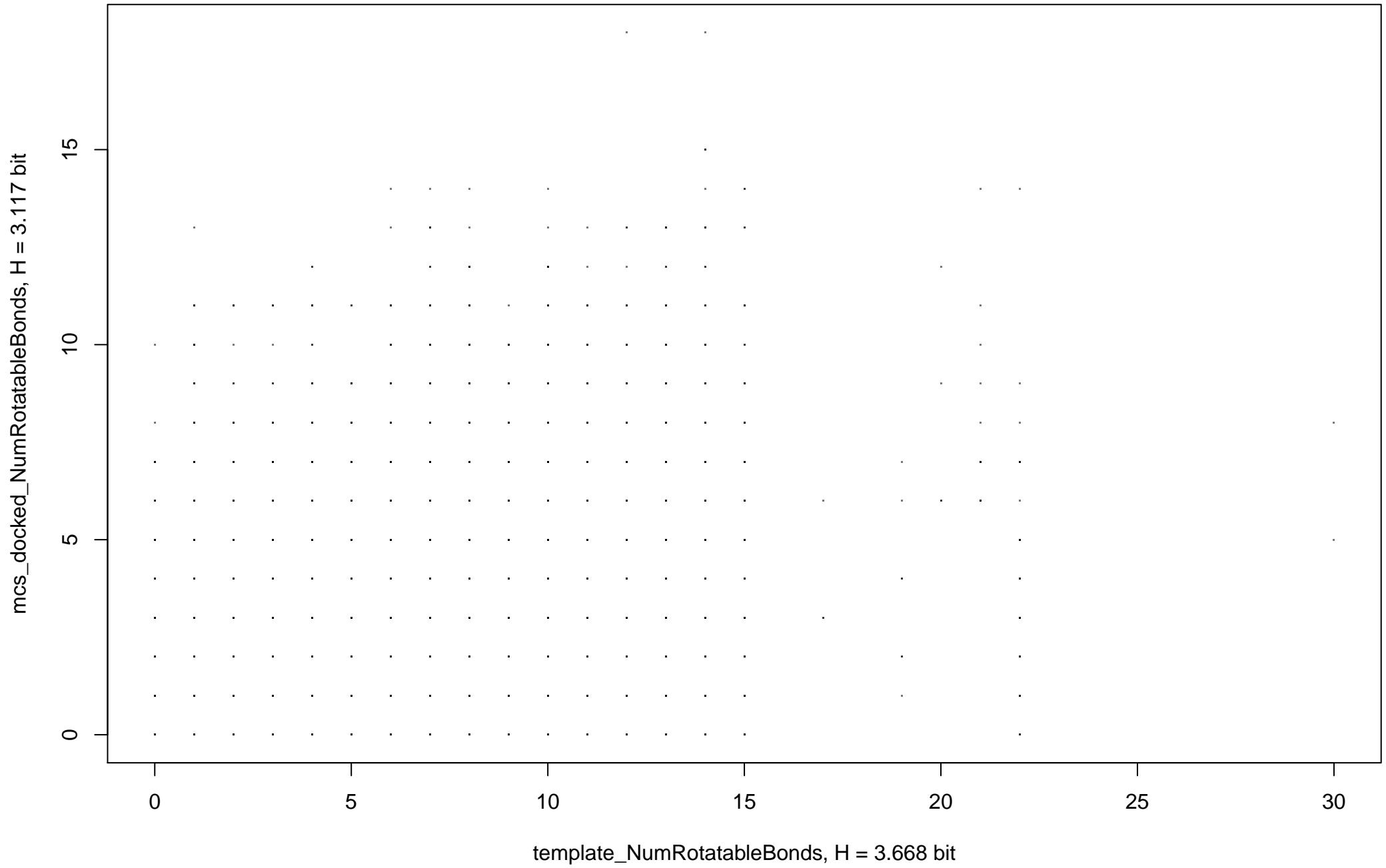
docked_NOCOUNT-mcs_docked_NumRotatableBonds, MI = 0.1831 bit, normMI = 0.05873



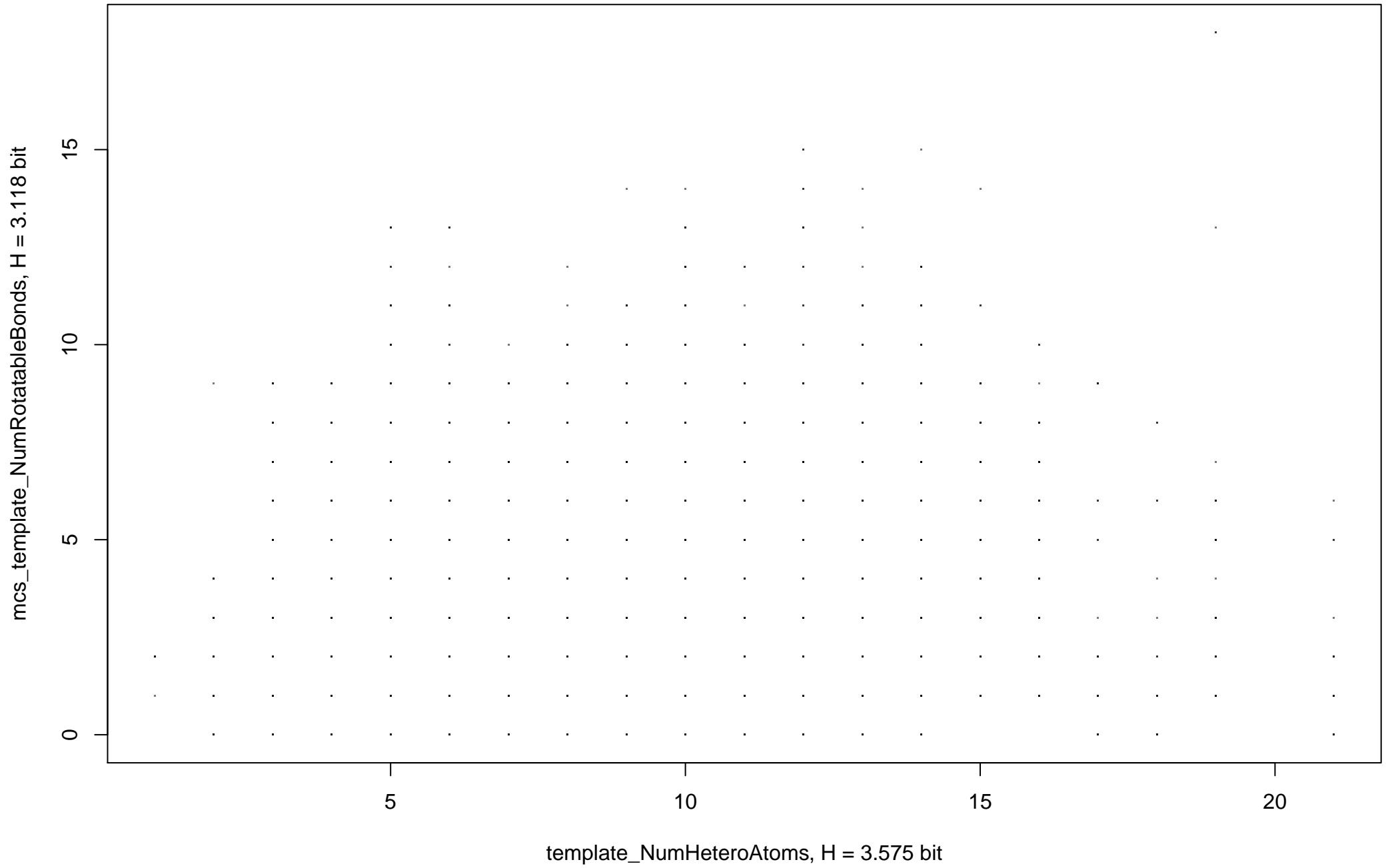
template_NOCount-mcs_NumHeteroAtoms, MI = 0.1703 bit, normMI = 0.05862



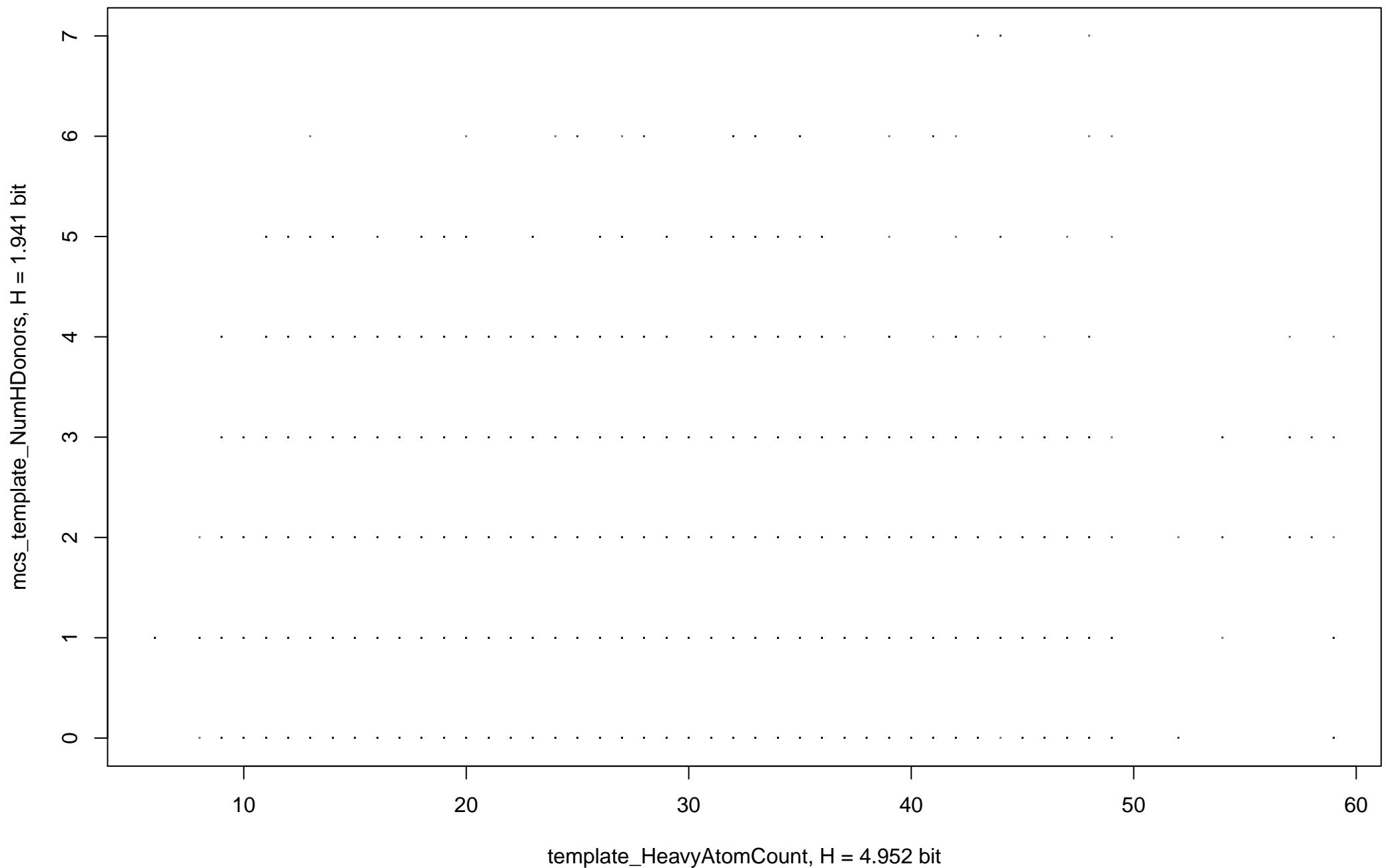
template_NumRotatableBonds-mcs_docked_NumRotatableBonds, MI = 0.1808 bit, normMI = 0.058



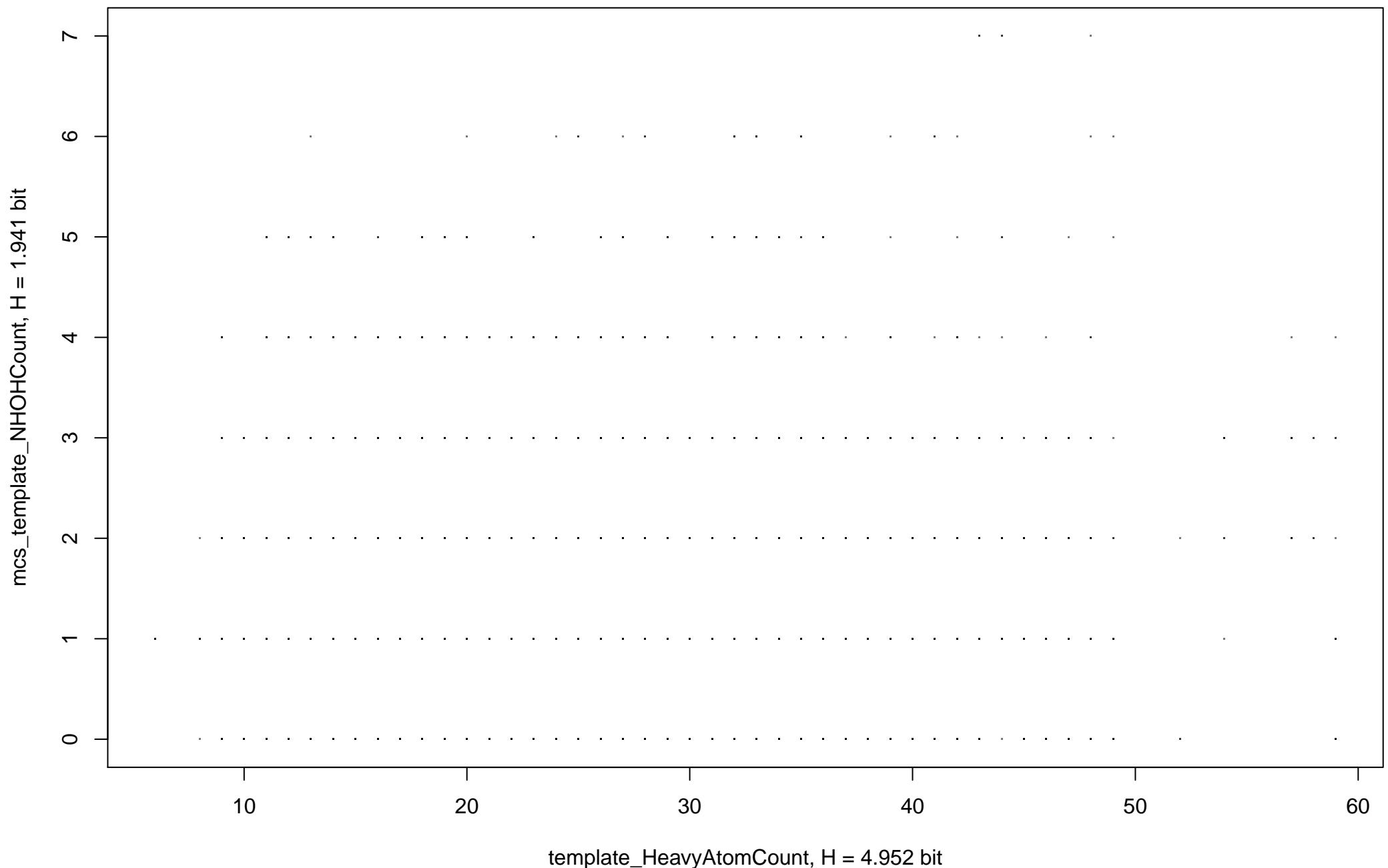
template_NumHeteroAtoms–mcs_template_NumRotatableBonds, MI = 0.1799 bit, normMI = 0.05771



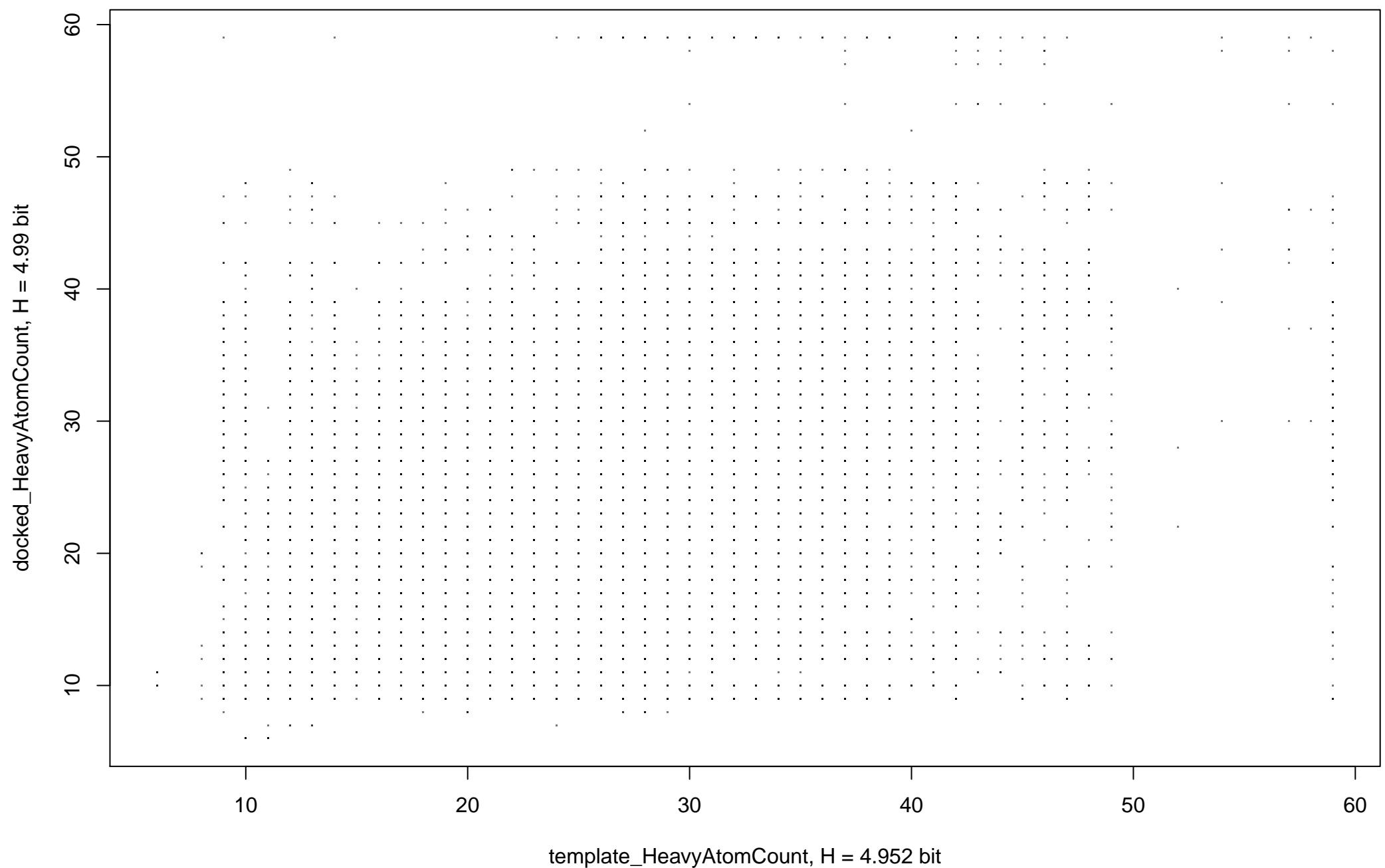
template_HeavyAtomCount-mcs_template_NumHDonors, MI = 0.1119 bit, normMI = 0.05764



template_HeavyAtomCount-mcs_template_NHOHCount, MI = 0.1119 bit, normMI = 0.05764

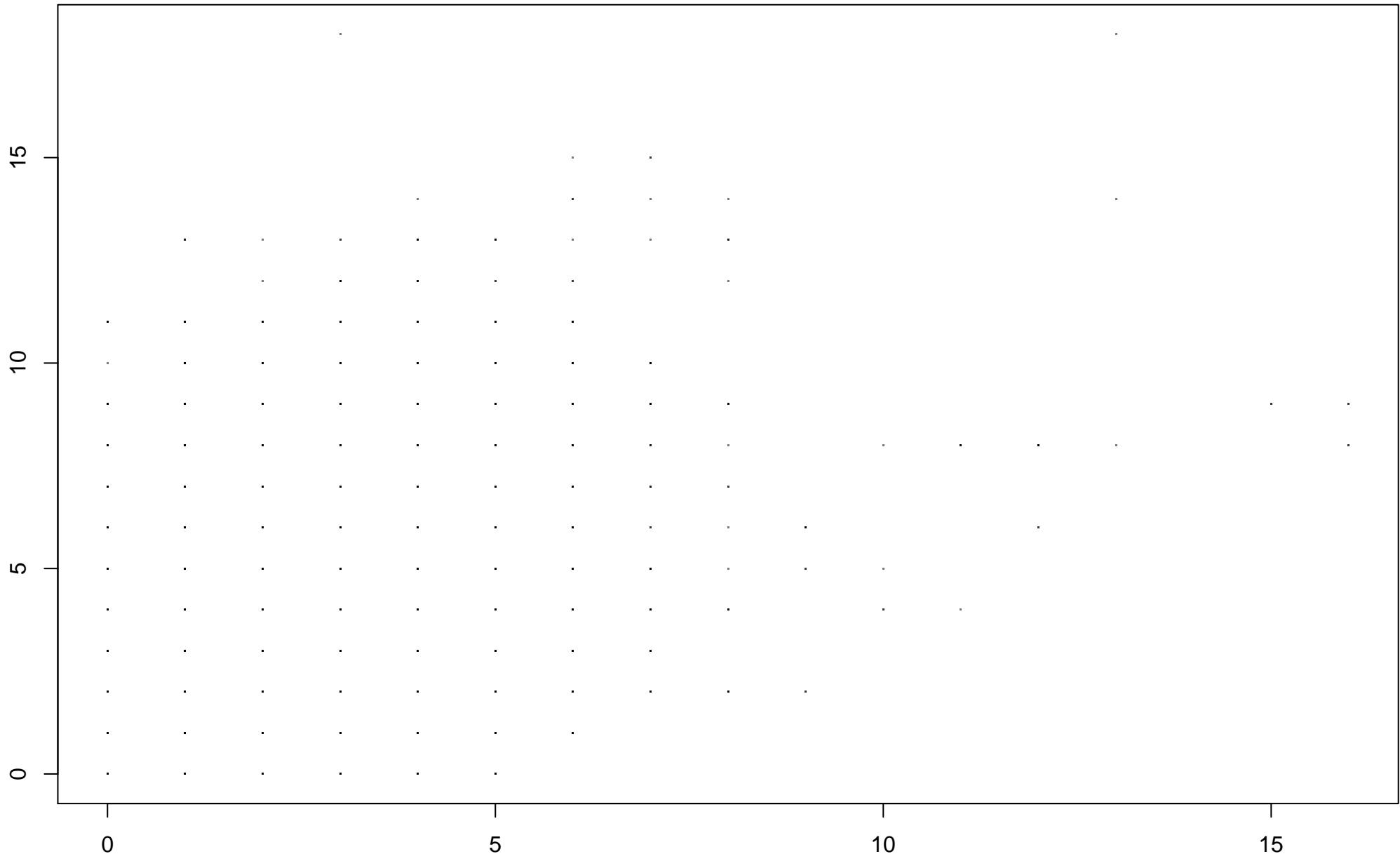


template_HeavyAtomCount-docked_HeavyAtomCount, MI = 0.2835 bit, normMI = 0.05725



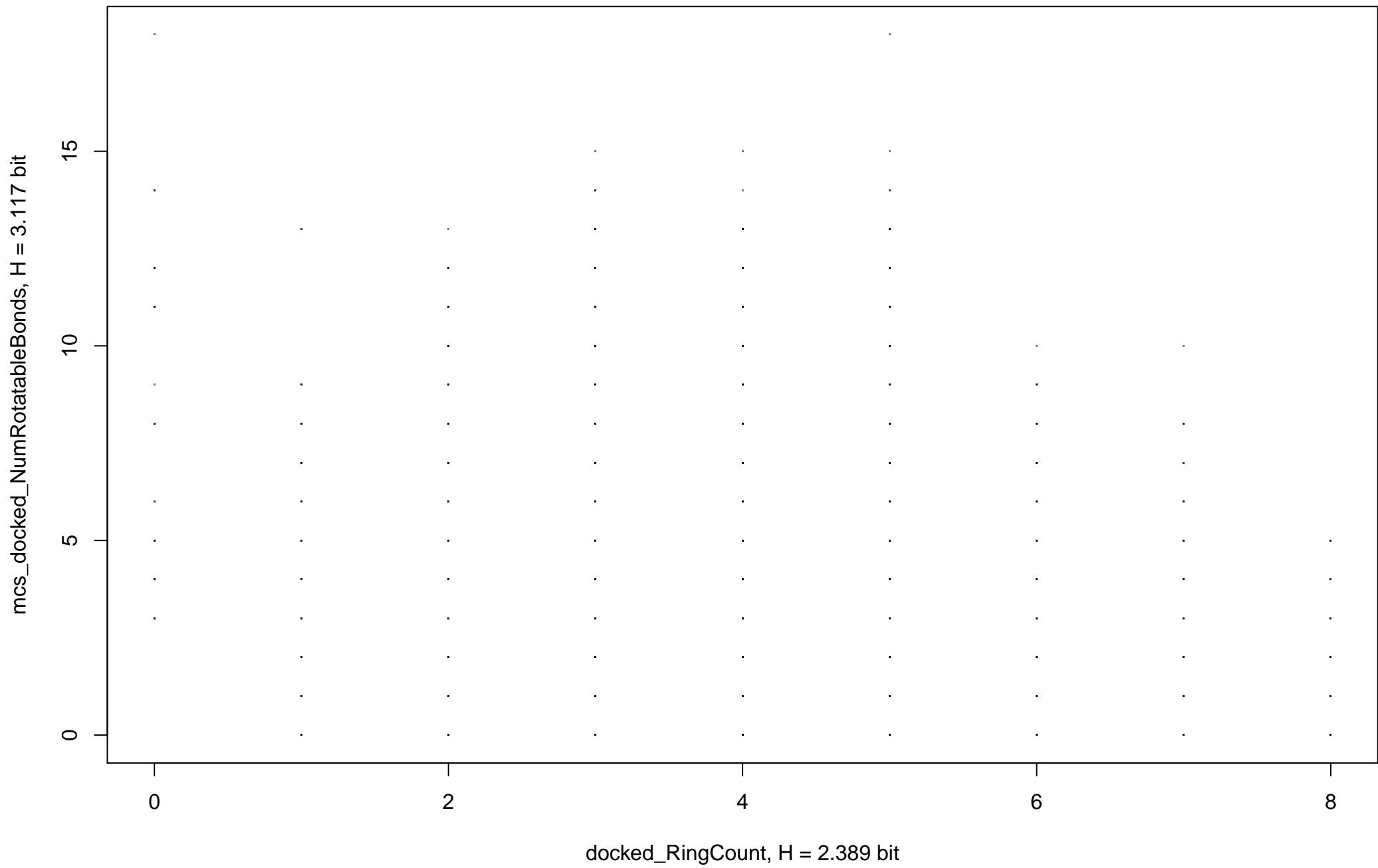
mcs_docked_NumHAcceptors-mcs_template_NumRotatableBonds, MI = 0.1399 bit, normMI = 0.05621

mcs_template_NumRotatableBonds, H = 3.118 bit



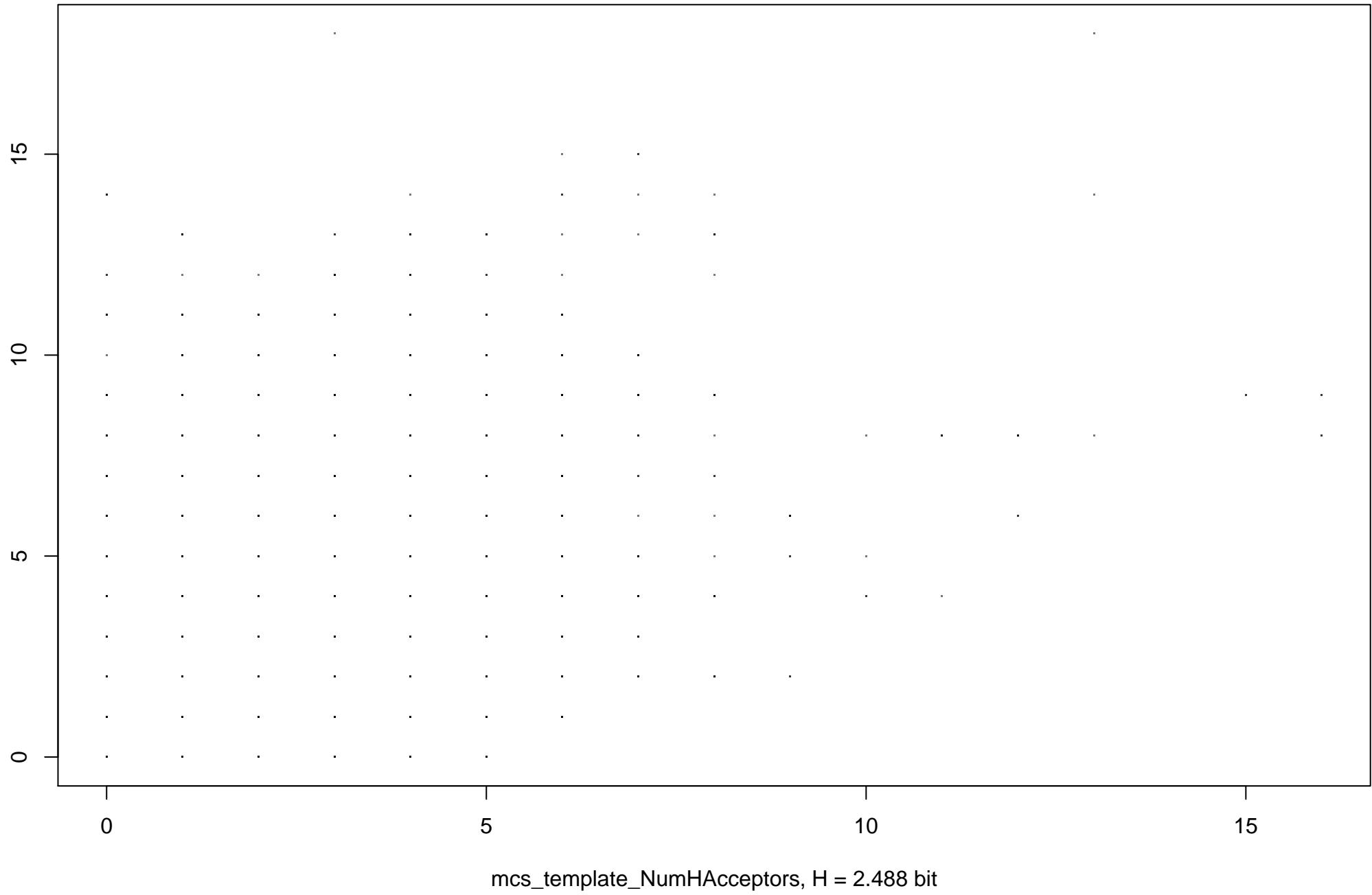
mcs_docked_NumHAcceptors, H = 2.489 bit

docked_RingCount-mcs_docked_NumRotatableBonds, MI = 0.1342 bit, normMI = 0.05619

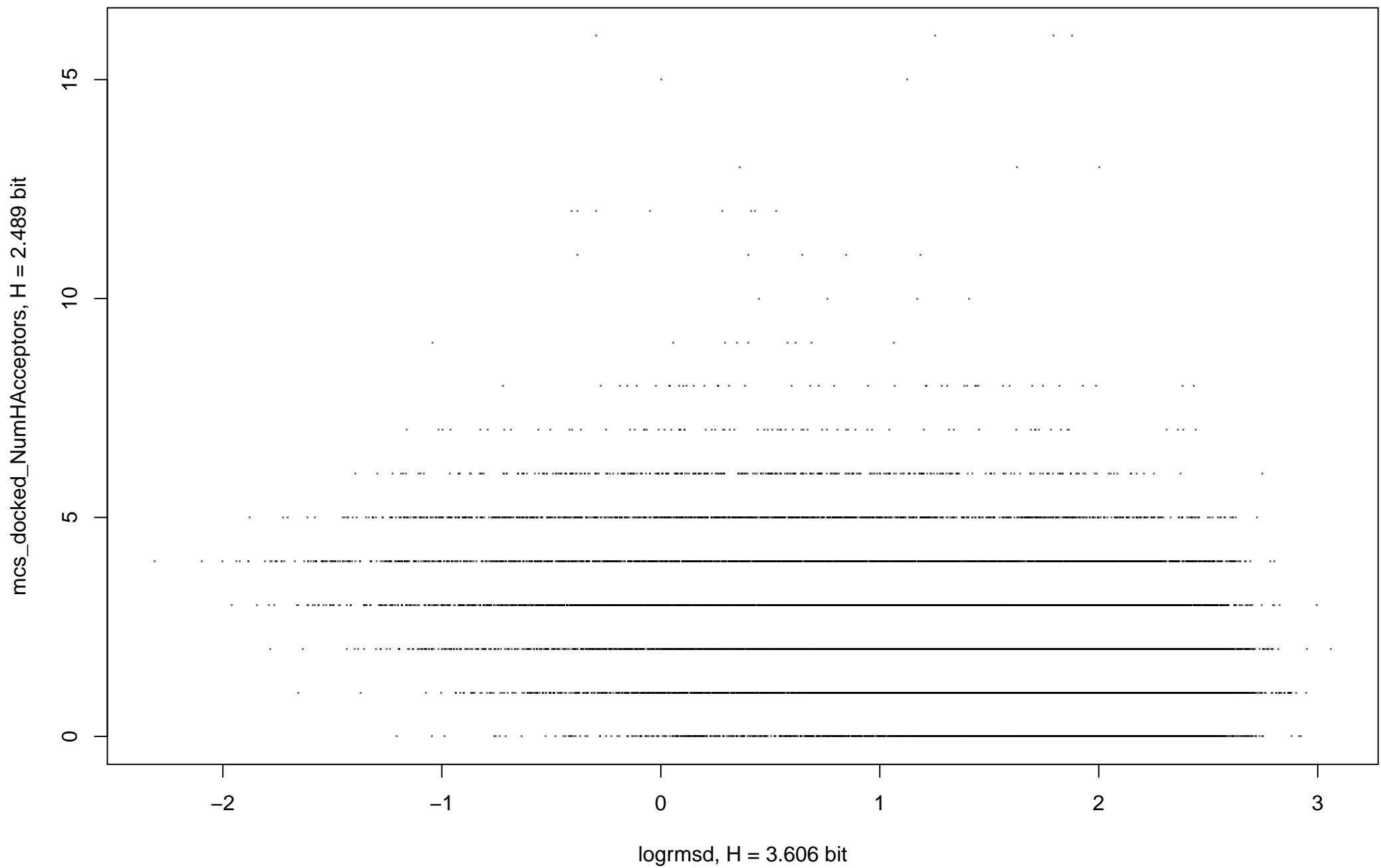


mcs_template_NumHAcceptors-mcs_docked_NumRotatableBonds, MI = 0.1385 bit, normMI = 0.05566

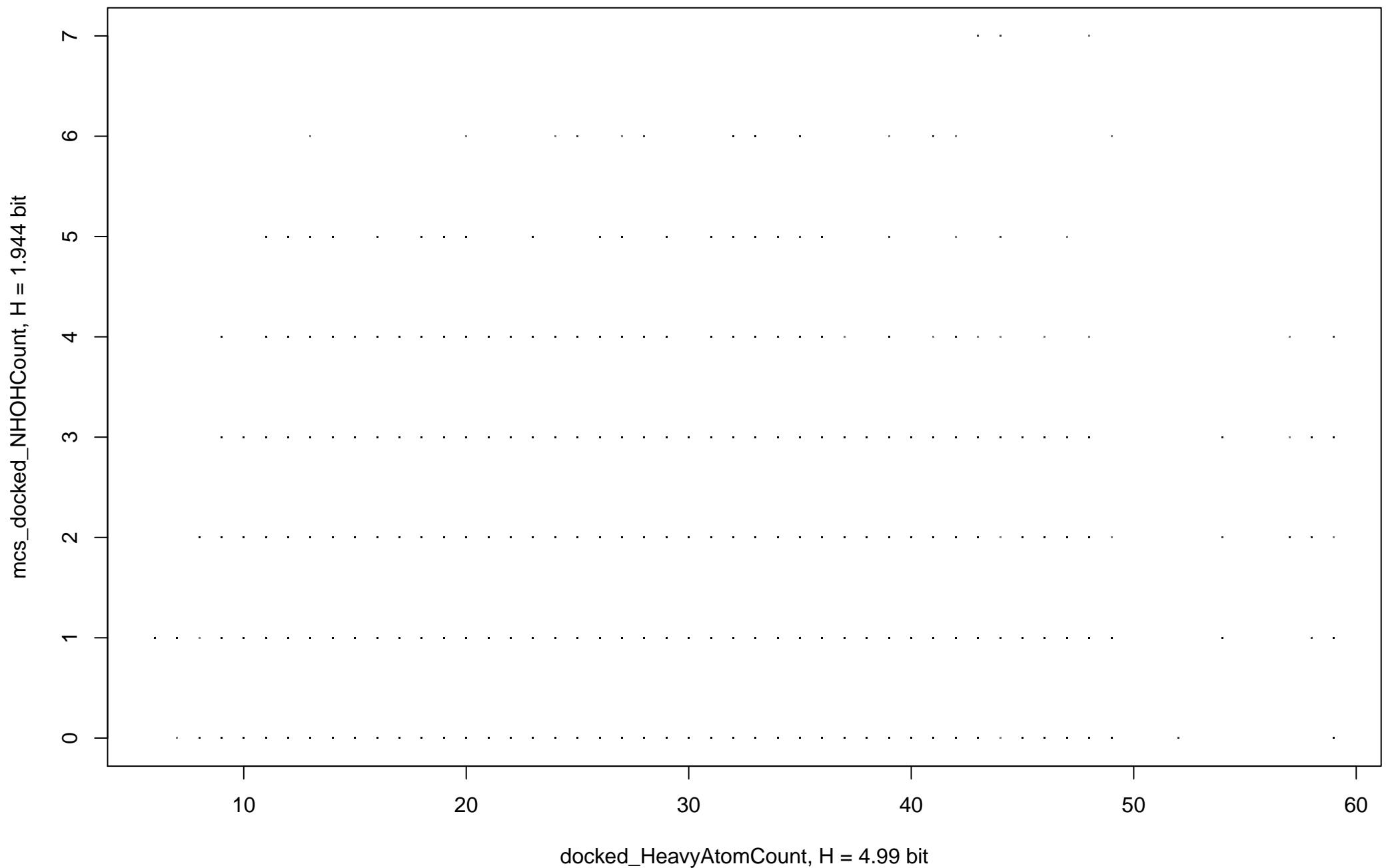
mcs_docked_NumRotatableBonds, H = 3.117 bit



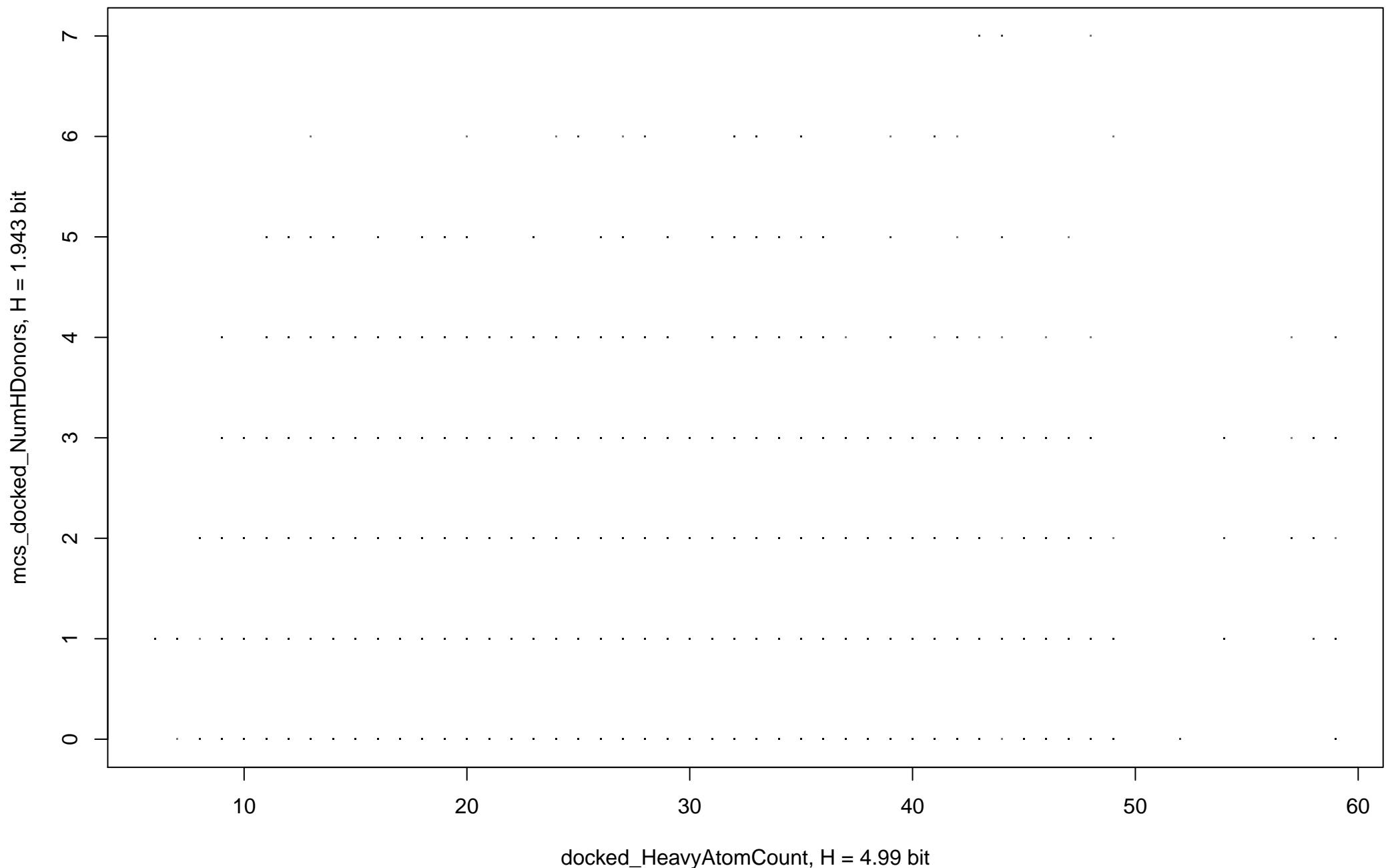
logrmsd-mcs_docked_NumHAcceptors, MI = 0.1385 bit, normMI = 0.05566



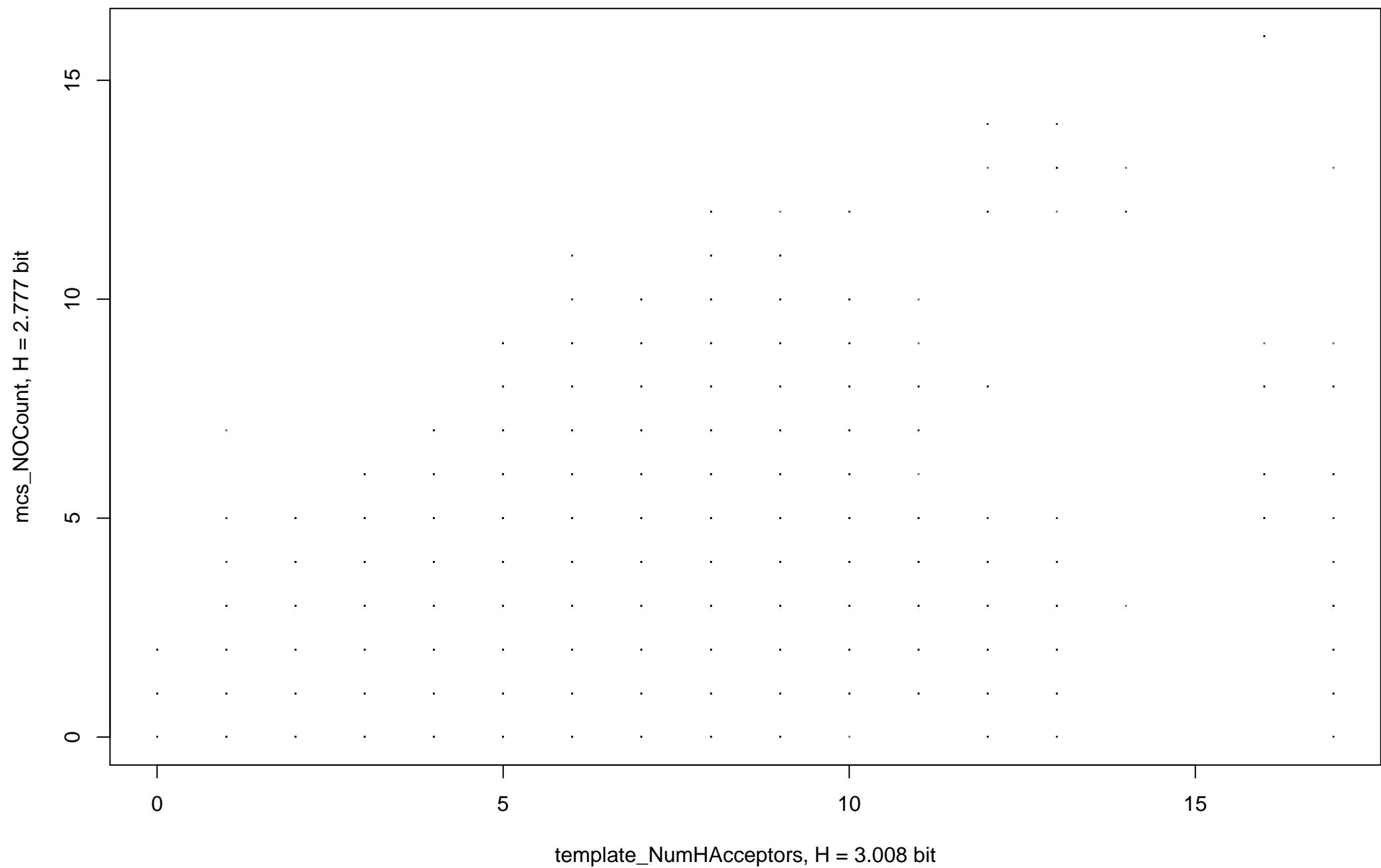
docked_HeavyAtomCount-mcs_docked_NHOHCount, MI = 0.1081 bit, normMI = 0.05563



docked_HeavyAtomCount-mcs_docked_NumHDonors, MI = 0.108 bit, normMI = 0.0556

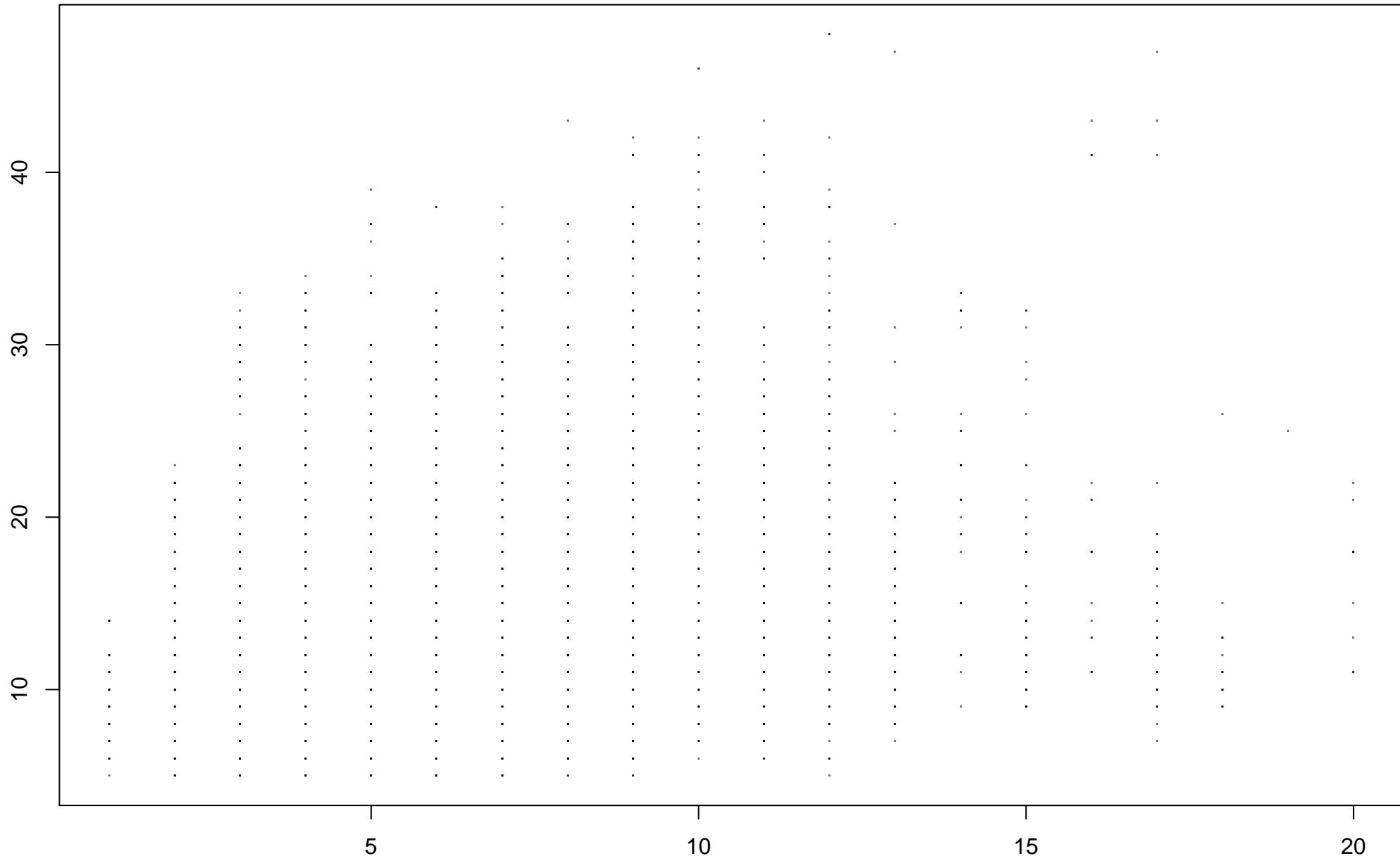


template_NumHAcceptors-mcs_NOCount, MI = 0.154 bit, normMI = 0.05548



docked_NOCount-mcs_HeavyAtomCount, MI = 0.1806 bit, normMI = 0.05546

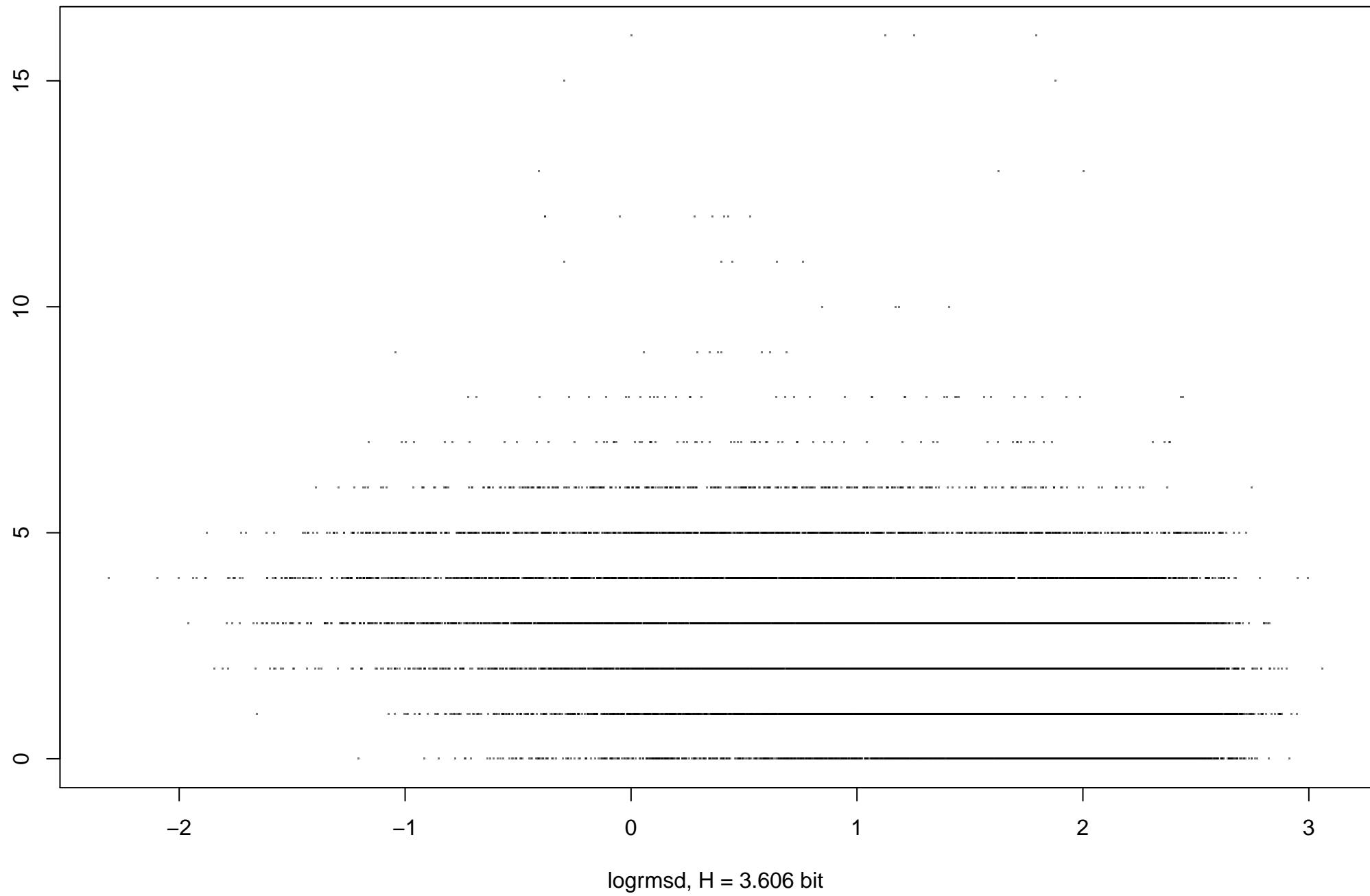
mcs_HeavyAtomCount, H = 4.38 bit



docked_NOCount, H = 3.257 bit

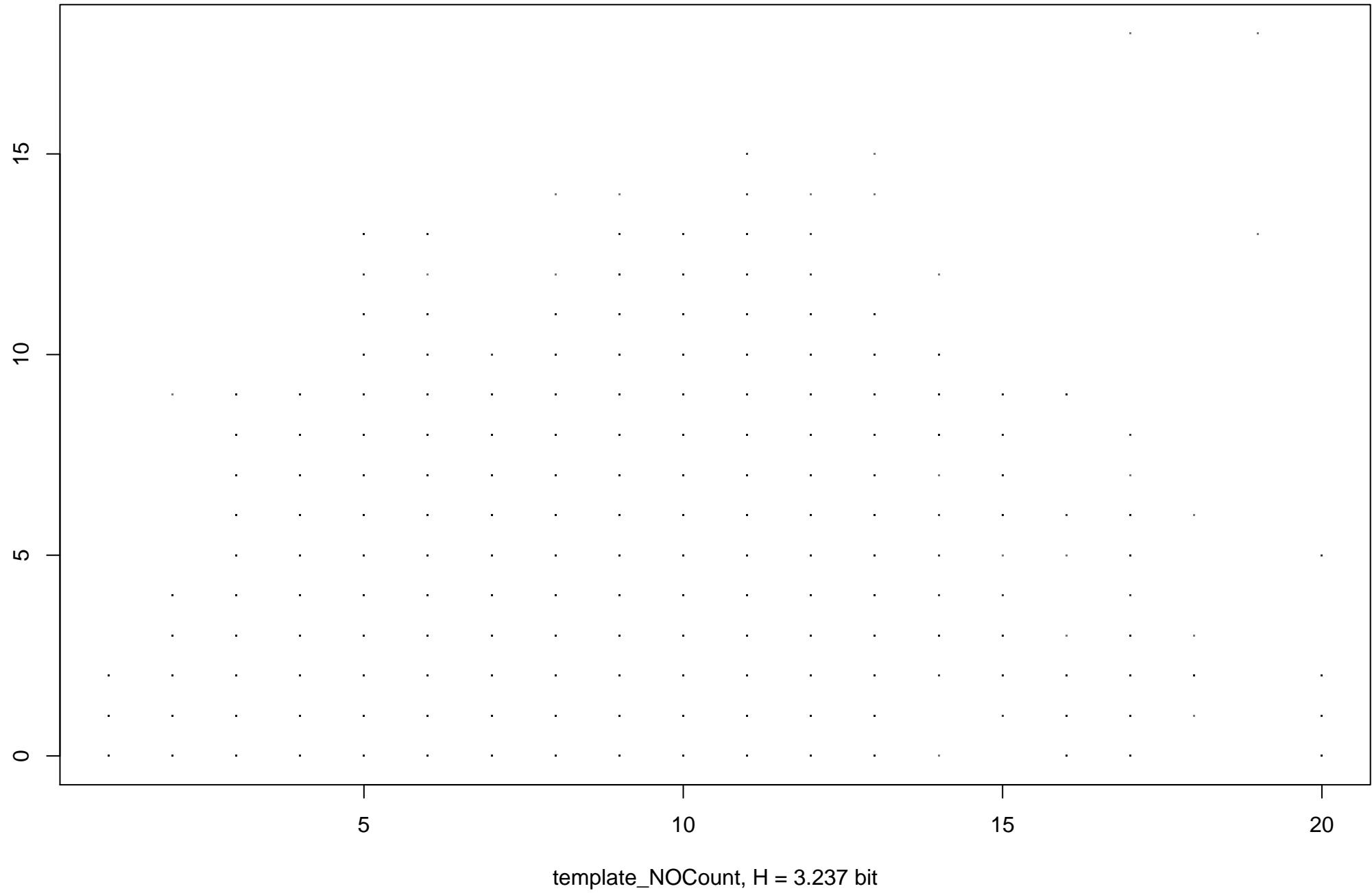
logrmsd-mcs_template_NumHAcceptors, MI = 0.1376 bit, normMI = 0.0553

mcs_template_NumHAcceptors, H = 2.488 bit

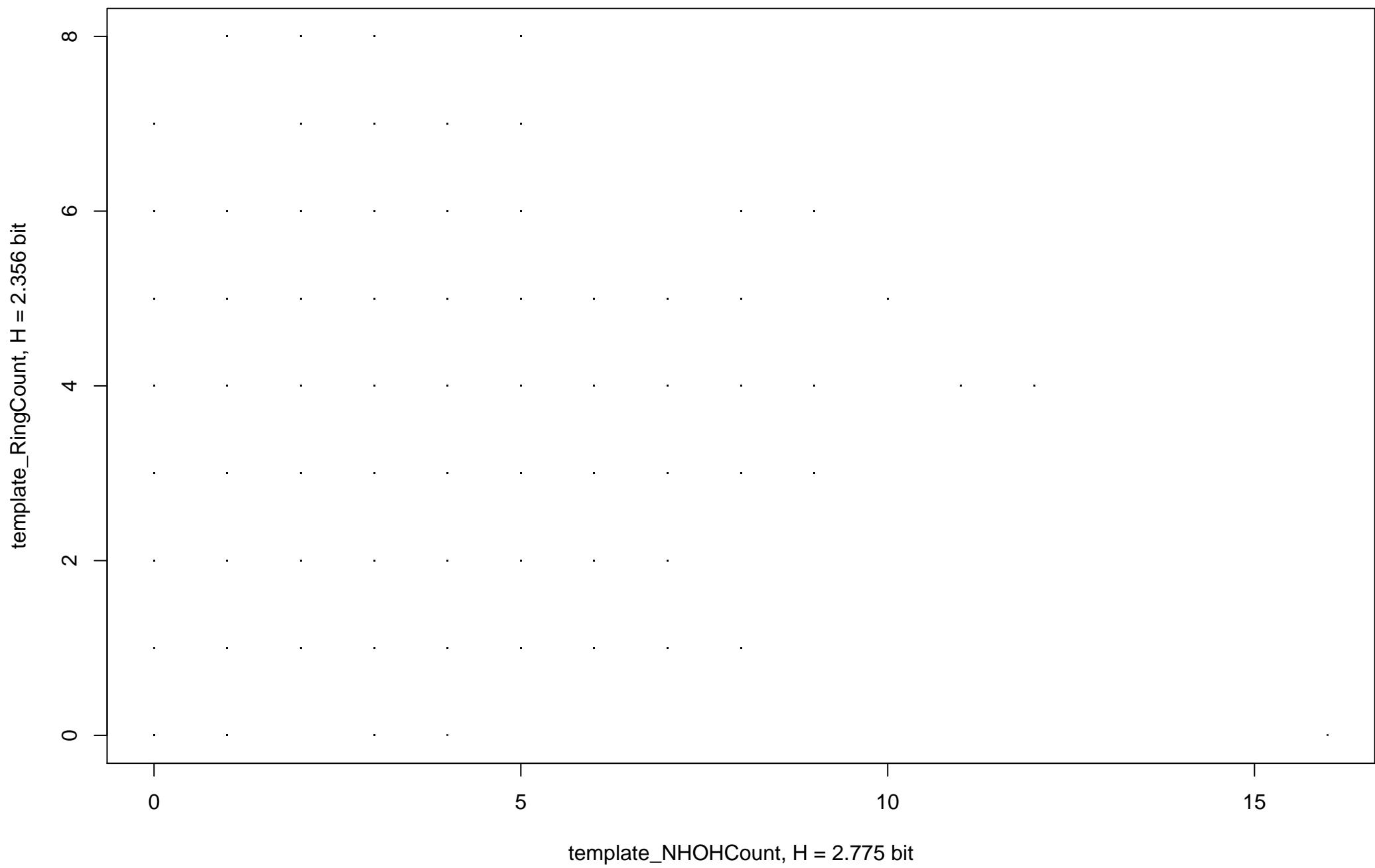


template_NOCount-mcs_template_NumRotatableBonds, MI = 0.1673 bit, normMI = 0.05364

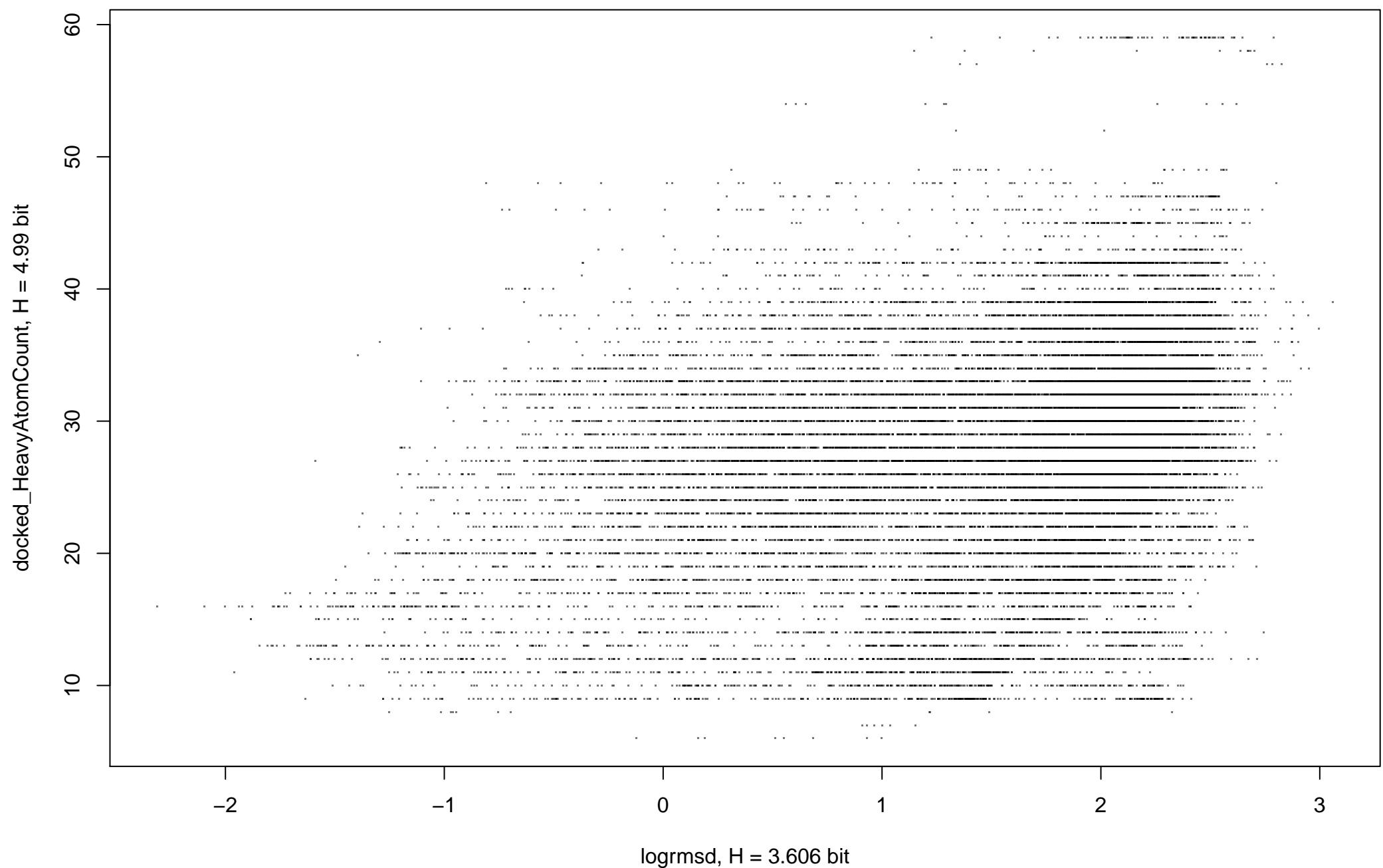
mcs_template_NumRotatableBonds, H = 3.118 bit



template_NHOHCount-template_RingCount, MI = 0.1236 bit, normMI = 0.05244

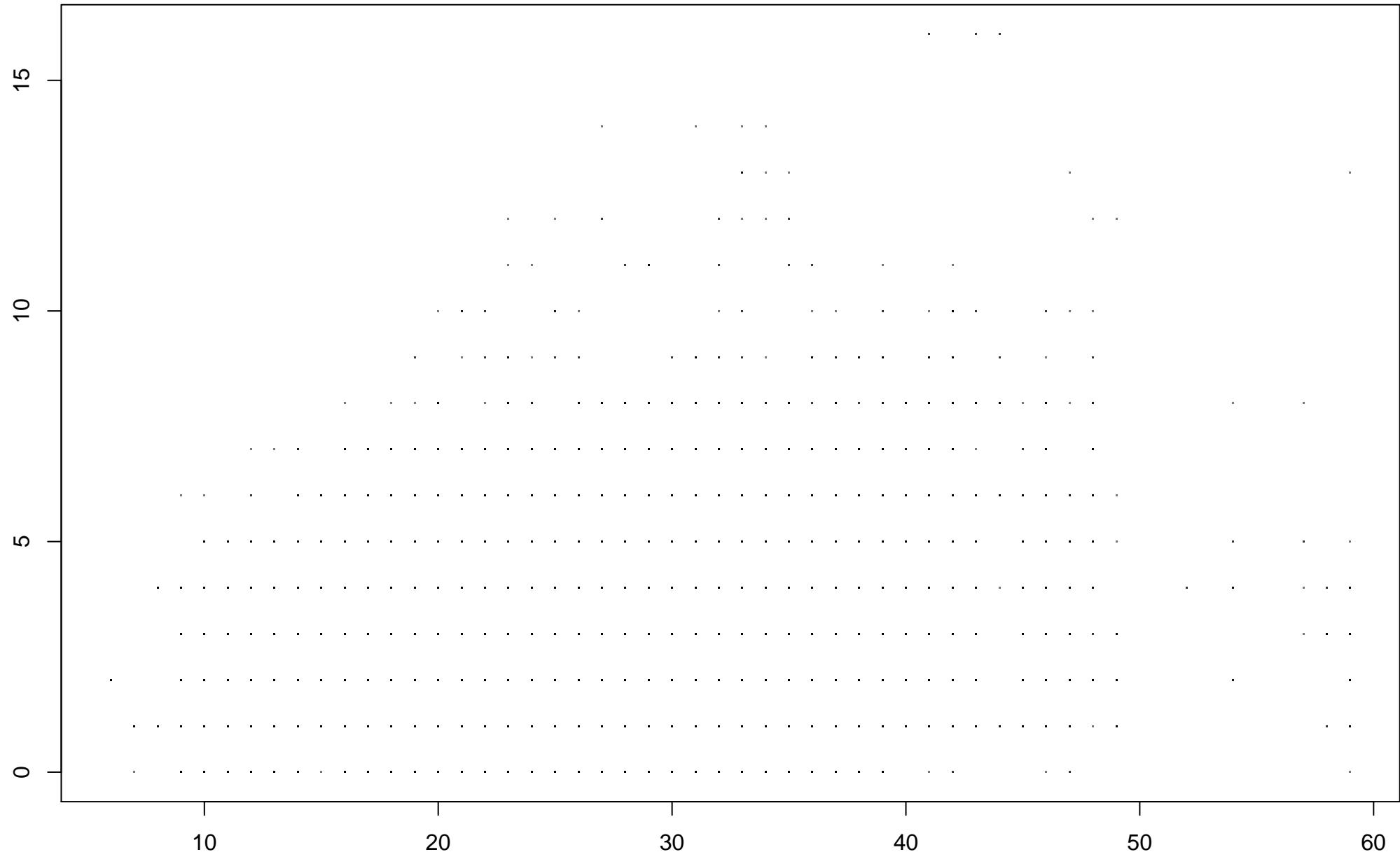


logrmsd-docked_HeavyAtomCount, MI = 0.189 bit, normMI = 0.05242



docked_HeavyAtomCount-mcs_NOCount, MI = 0.1435 bit, normMI = 0.05169

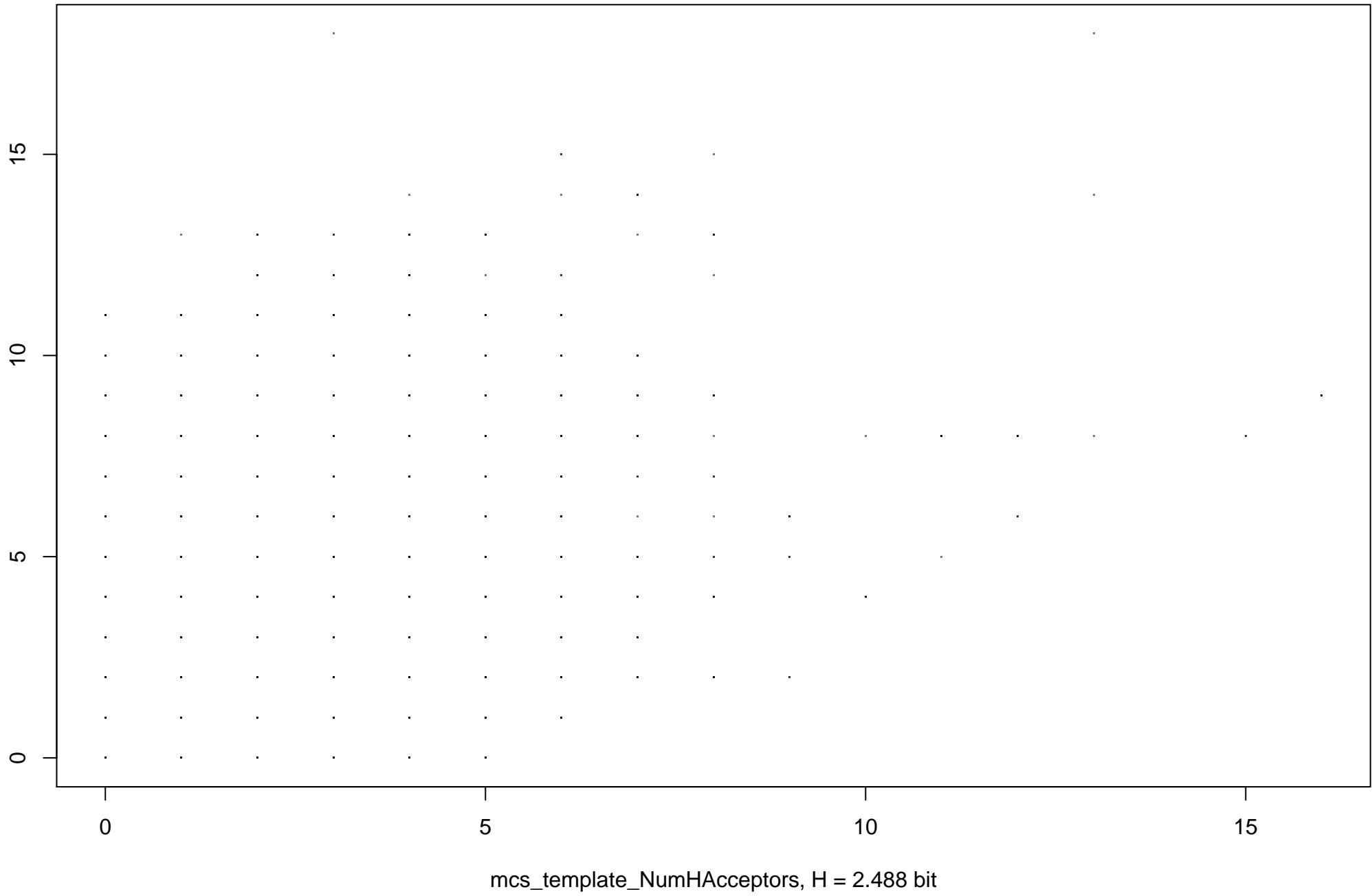
mcs_NOCount, H = 2.777 bit



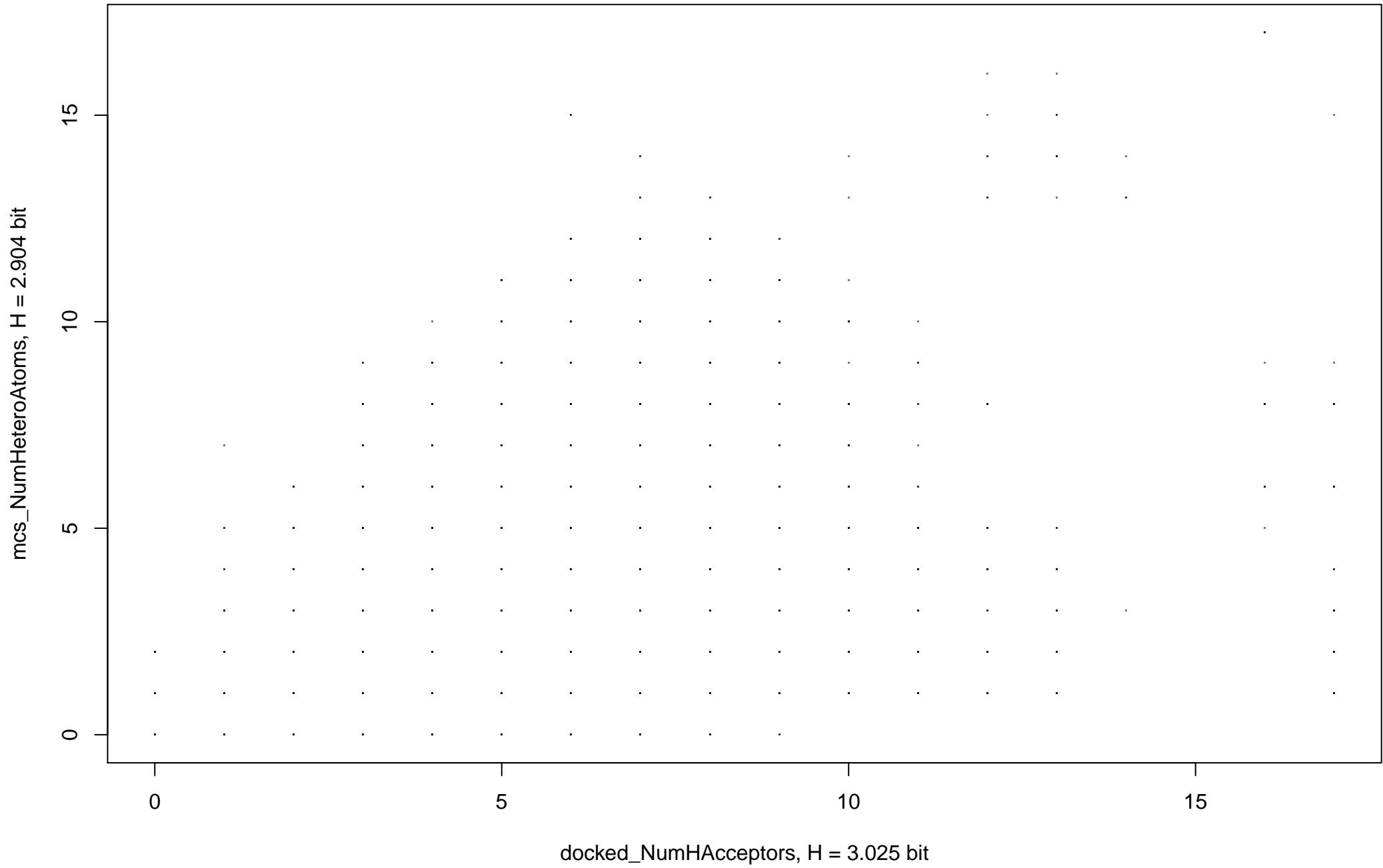
docked_HeavyAtomCount, H = 4.99 bit

mcs_template_NumHAcceptors-mcs_template_NumRotatableBonds, MI = 0.1279 bit, normMI = 0.0514

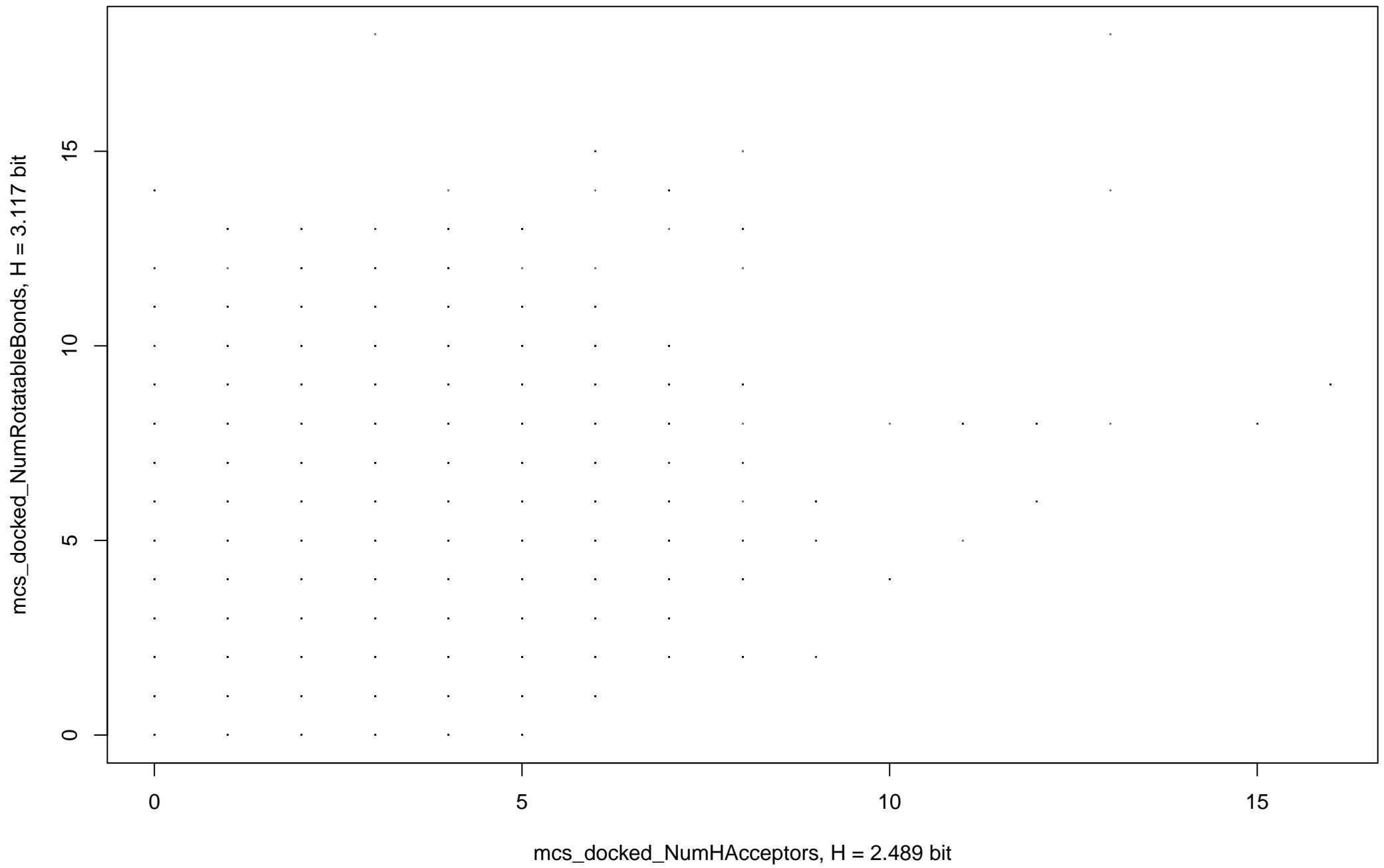
mcs_template_NumRotatableBonds, H = 3.118 bit



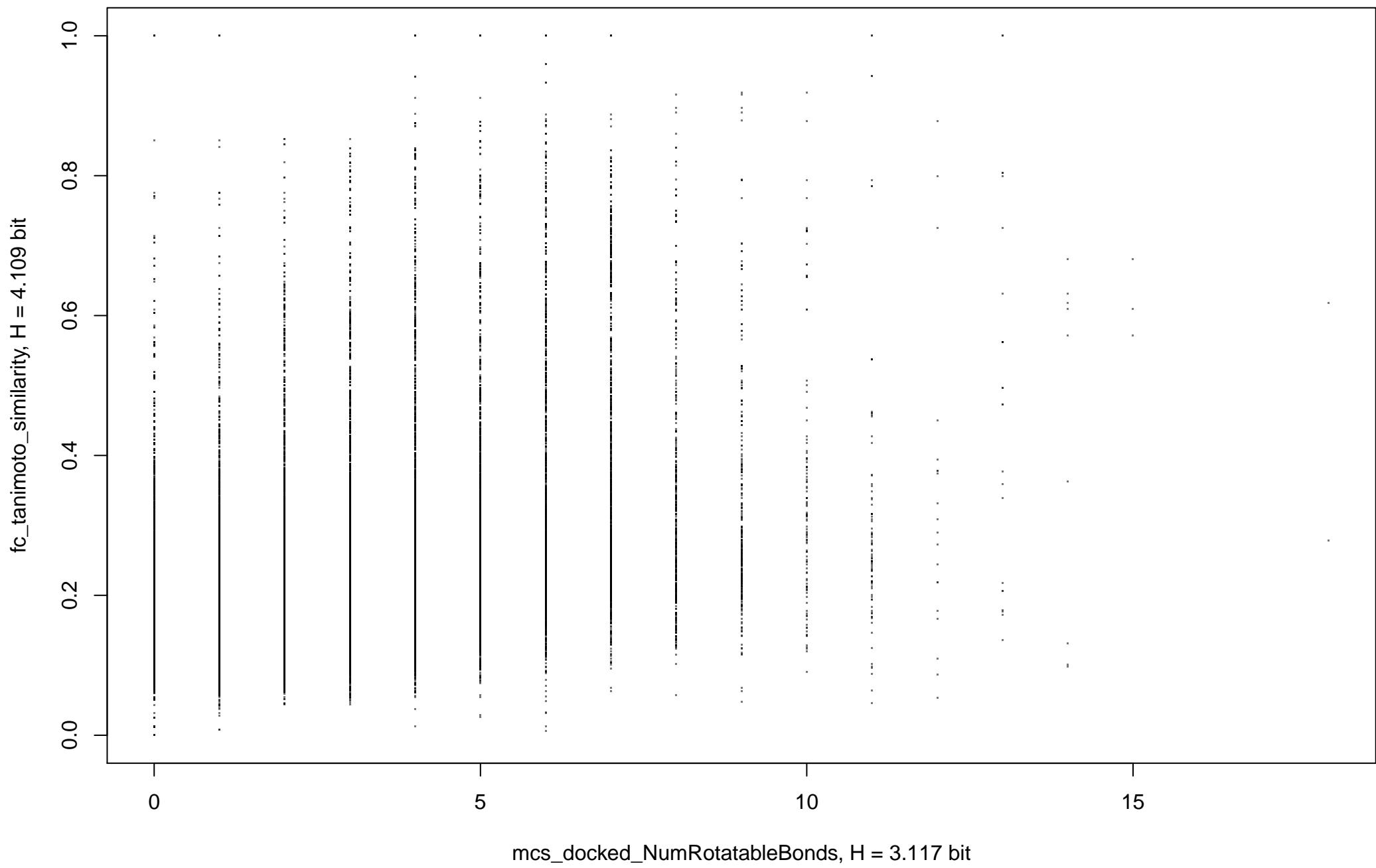
docked_NumHAcceptors-mcs_NumHeteroAtoms, MI = 0.1477 bit, normMI = 0.05085



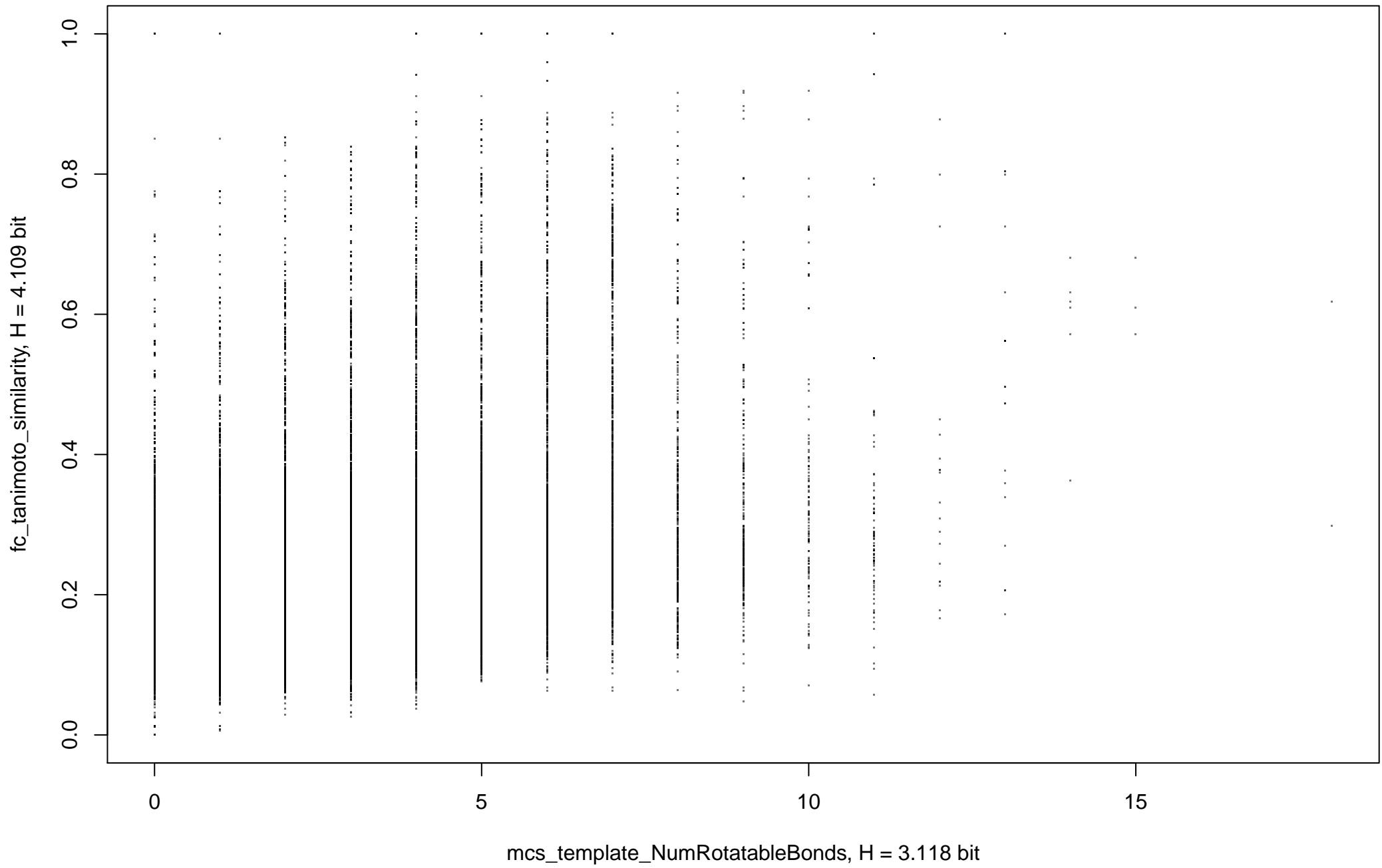
mcs_docked_NumHAcceptors-mcs_docked_NumRotatableBonds, MI = 0.1255 bit, normMI = 0.05044



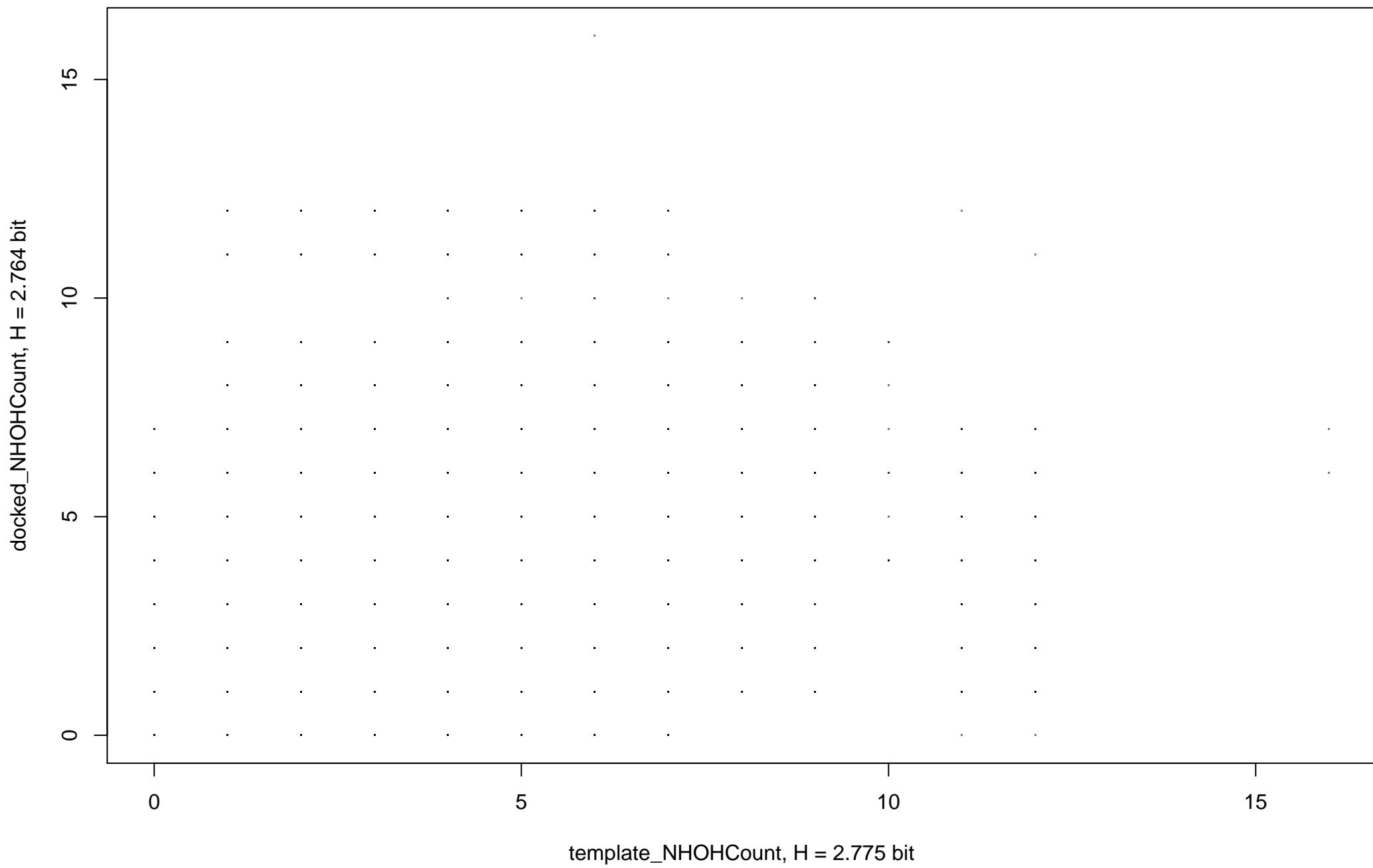
mcs_docked_NumRotatableBonds-fc_tanimoto_similarity, MI = 0.1571 bit, normMI = 0.05039



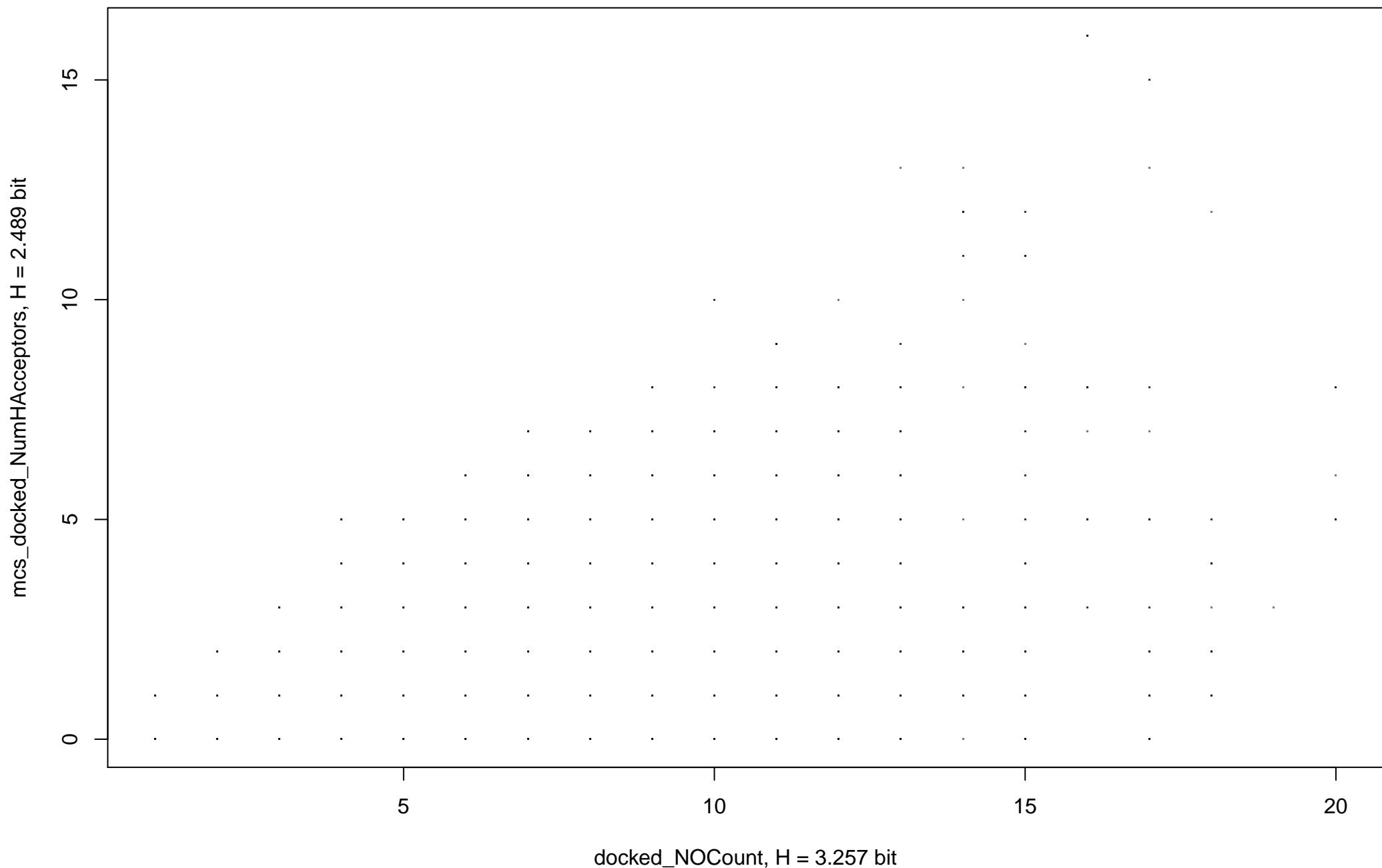
mcs_template_NumRotatableBonds-fc_tanimoto_similarity, MI = 0.1566 bit, normMI = 0.05023



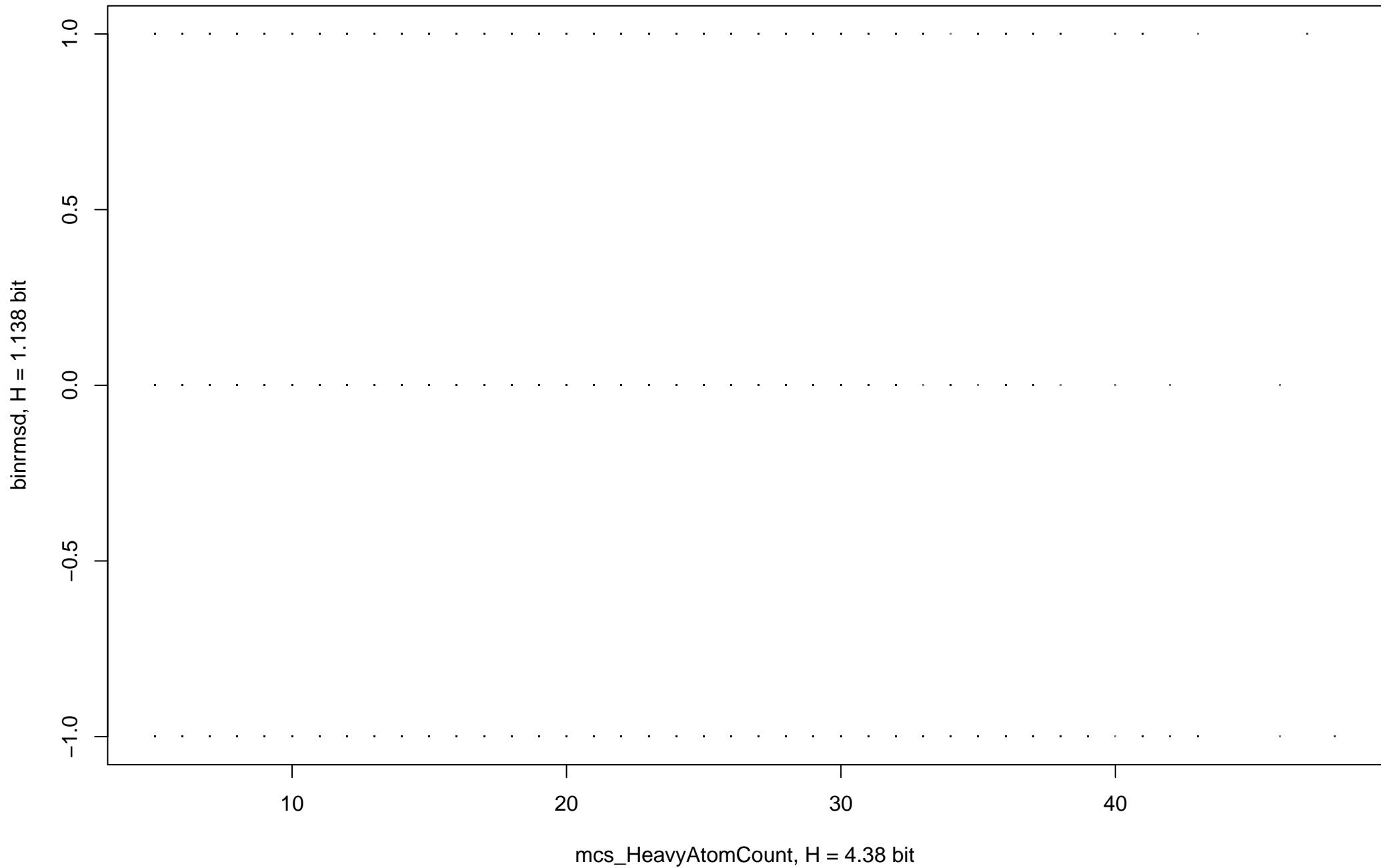
template_NHOHCount-docked_NHOHCount, MI = 0.1384 bit, normMI = 0.05006



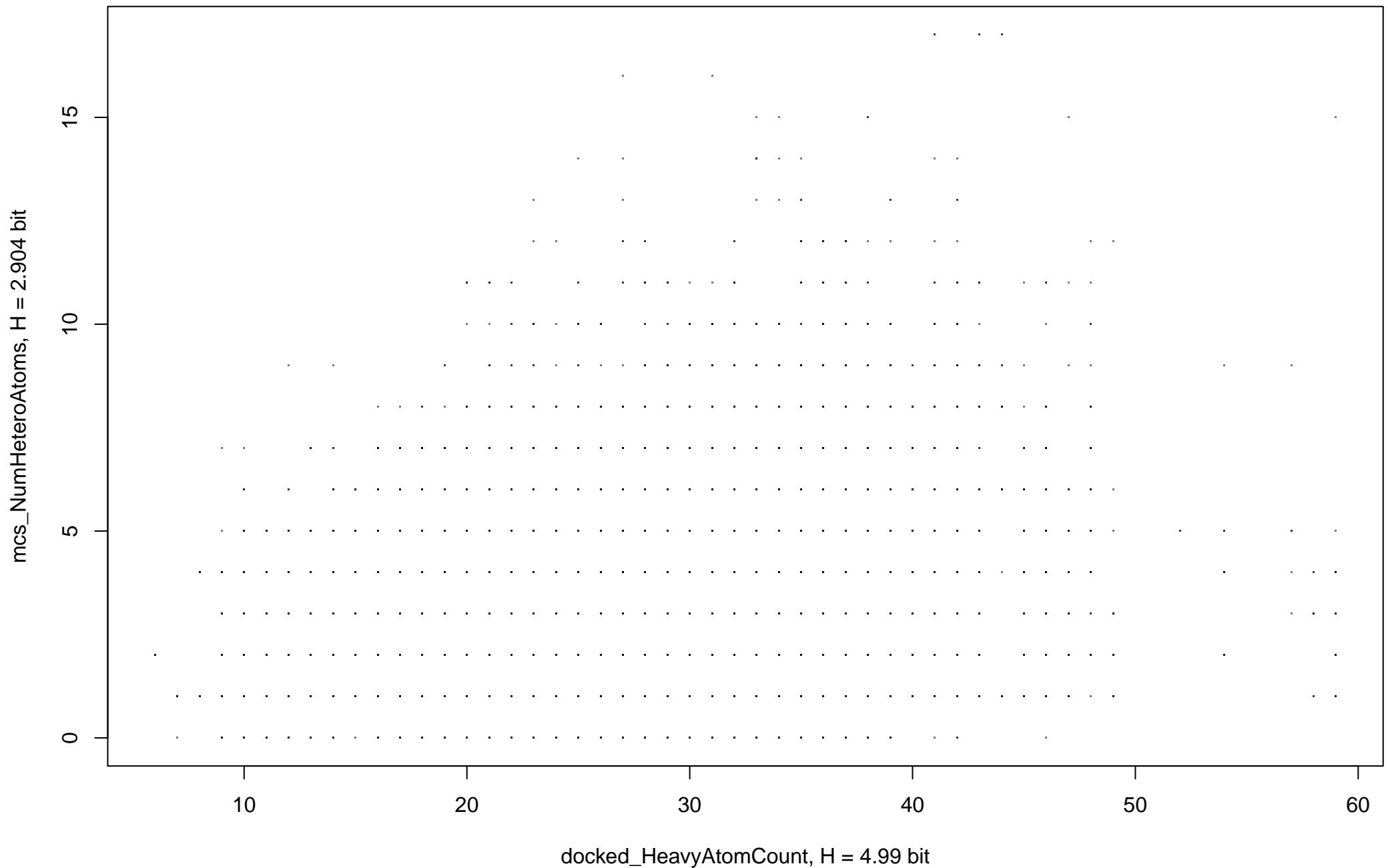
docked_NOCount-mcs_docked_NumHAcceptors, MI = 0.1243 bit, normMI = 0.04994



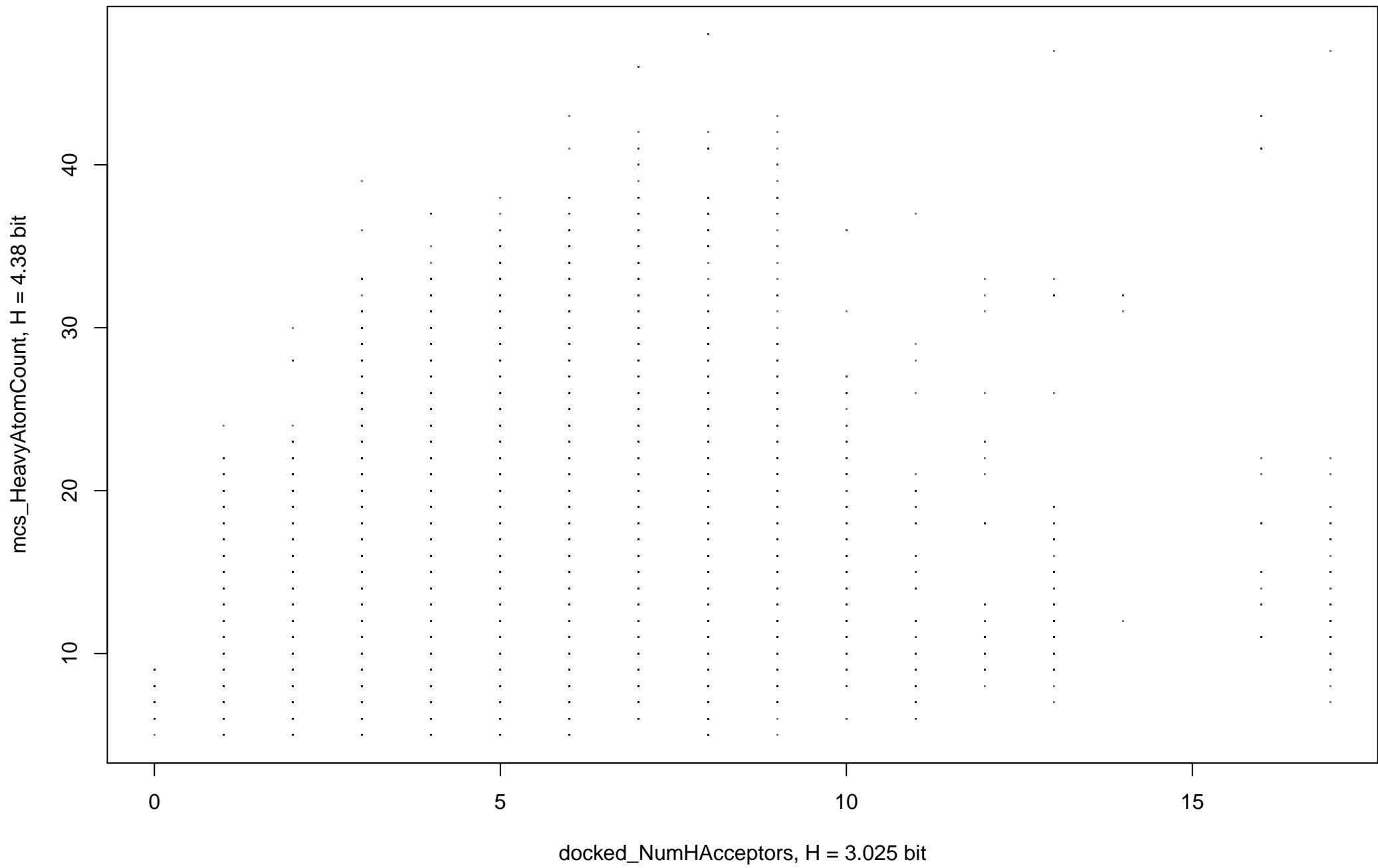
mcs_HeavyAtomCount–binrmsd, MI = 0.05609 bit, normMI = 0.04928



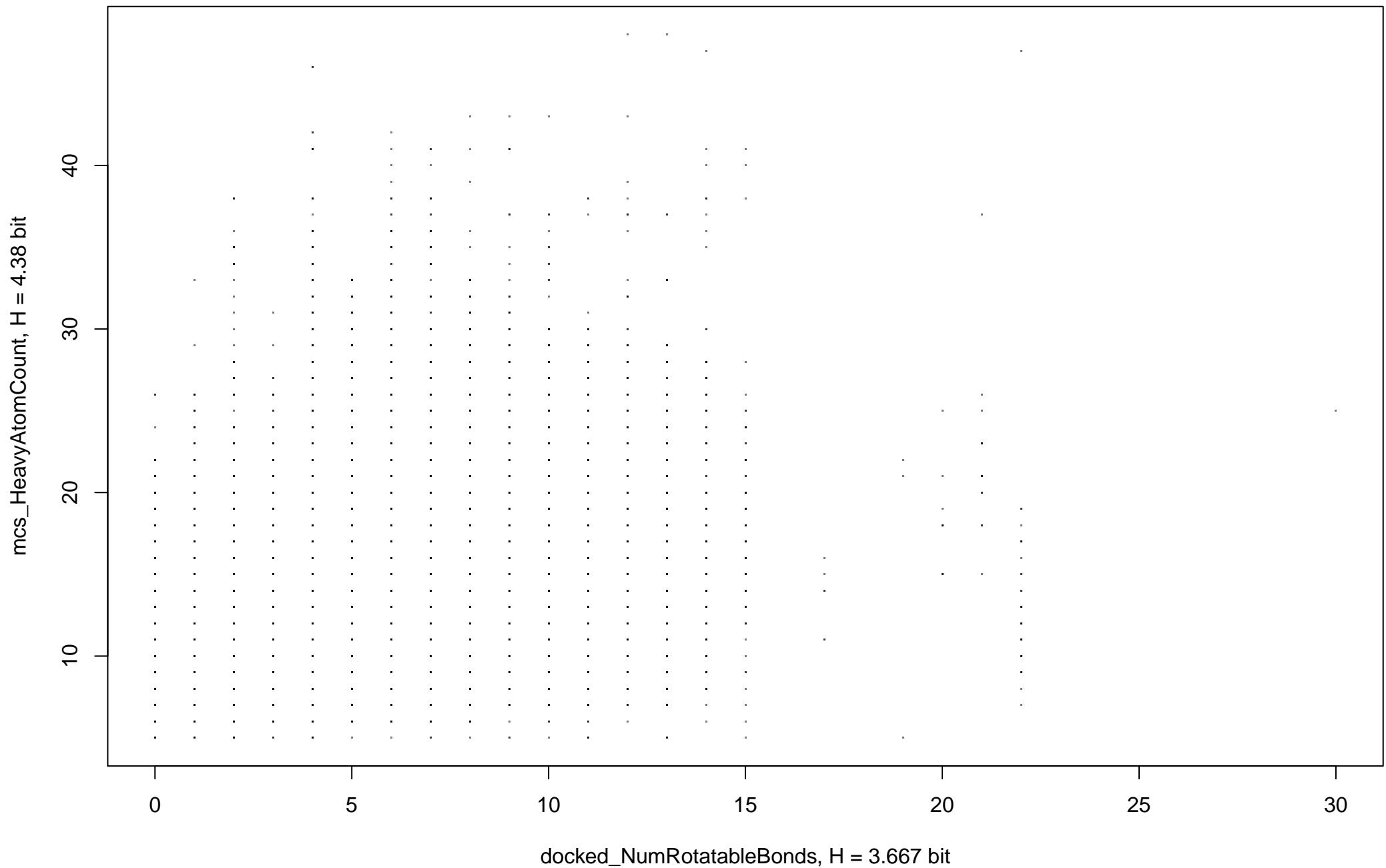
docked_HeavyAtomCount-mcs_NumHeteroAtoms, MI = 0.1408 bit, normMI = 0.04847



docked_NumHAcceptors-mcs_HeavyAtomCount, MI = 0.146 bit, normMI = 0.04827

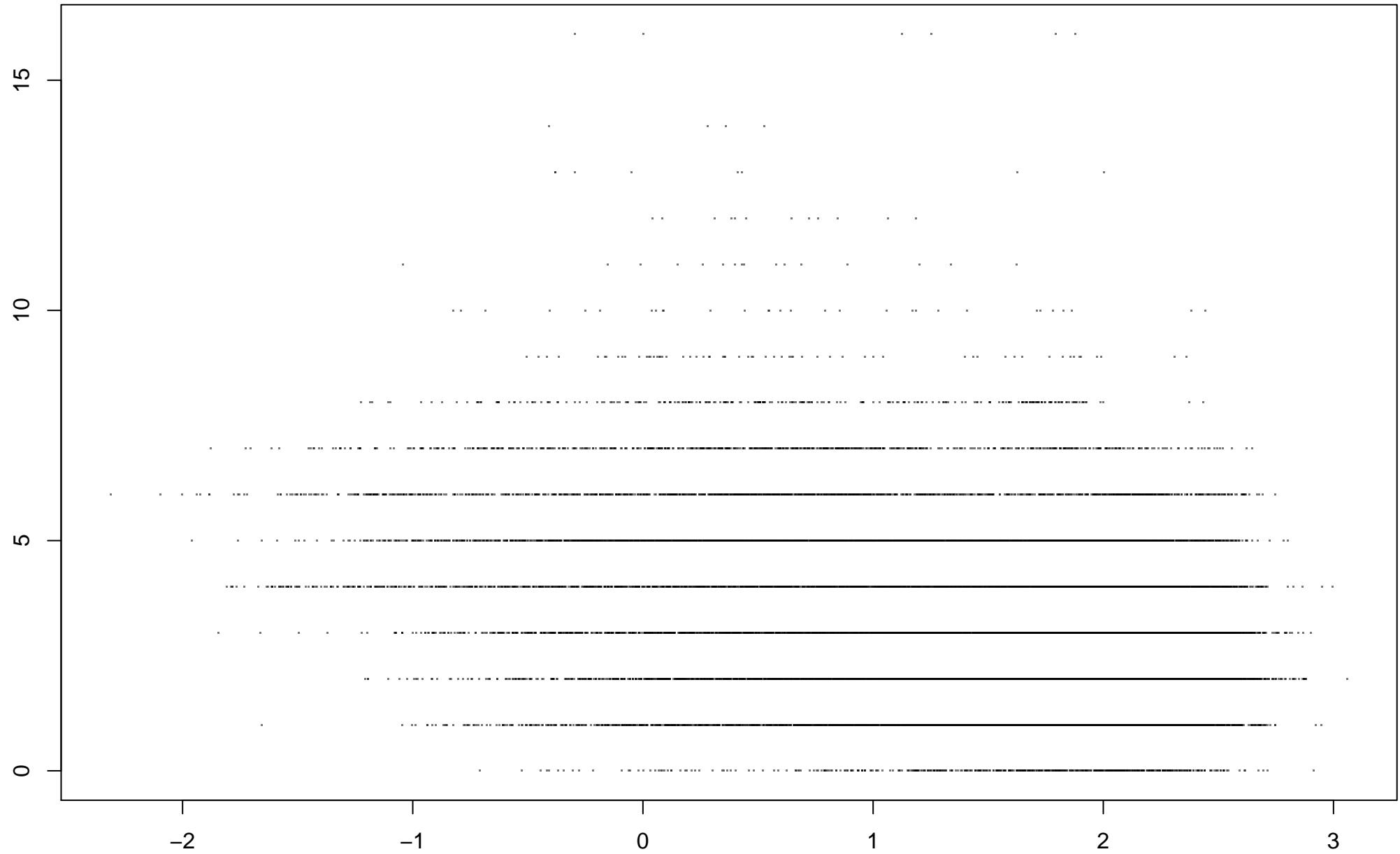


docked_NumRotatableBonds-mcs_HeavyAtomCount, MI = 0.1765 bit, normMI = 0.04814



logrmsd-mcs_NOCount, MI = 0.131 bit, normMI = 0.04718

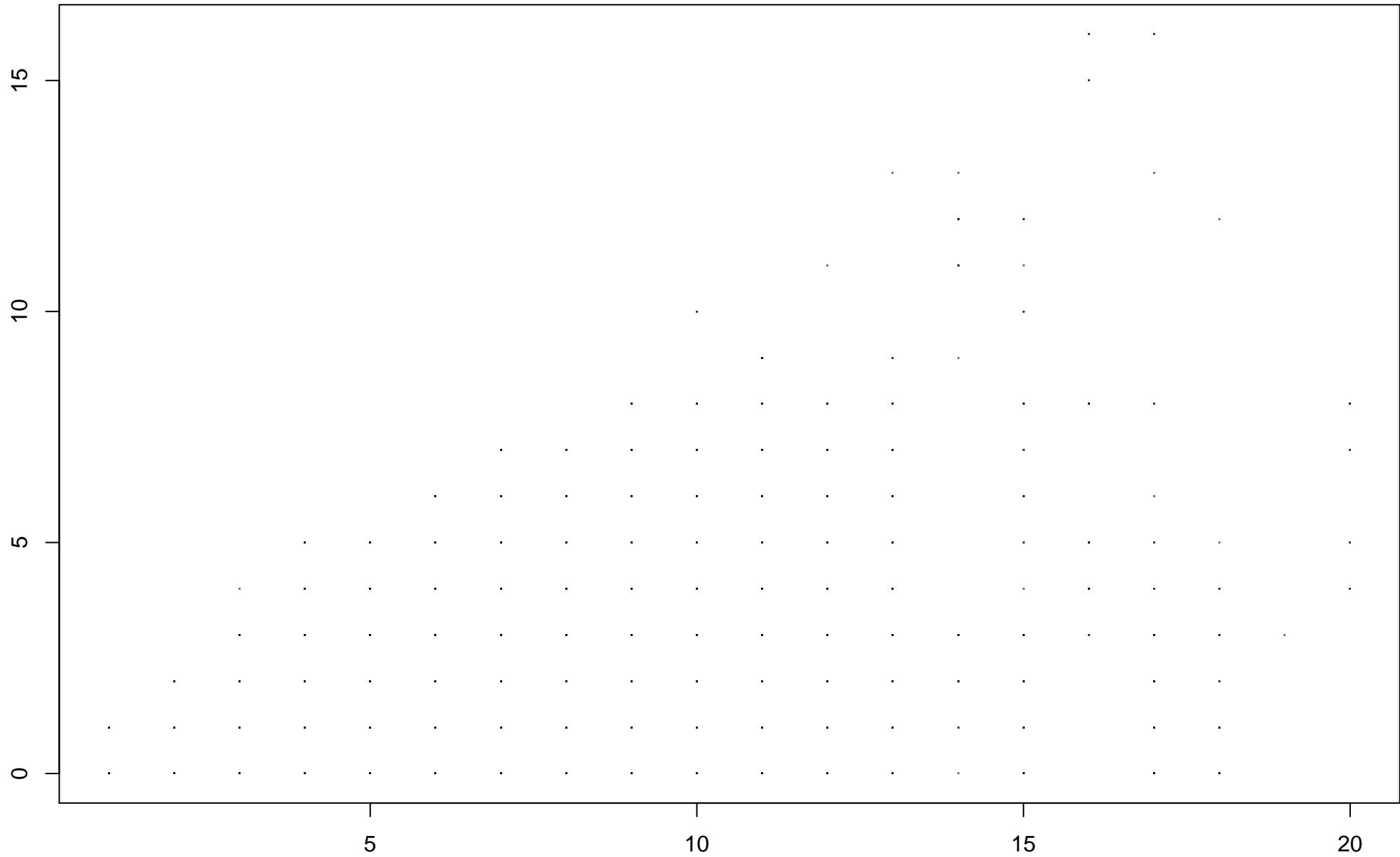
mcs_NOCount, $H = 2.777$ bit



logrmsd, $H = 3.606$ bit

docked_NOCount-mcs_template_NumHAcceptors, MI = 0.1164 bit, normMI = 0.04679

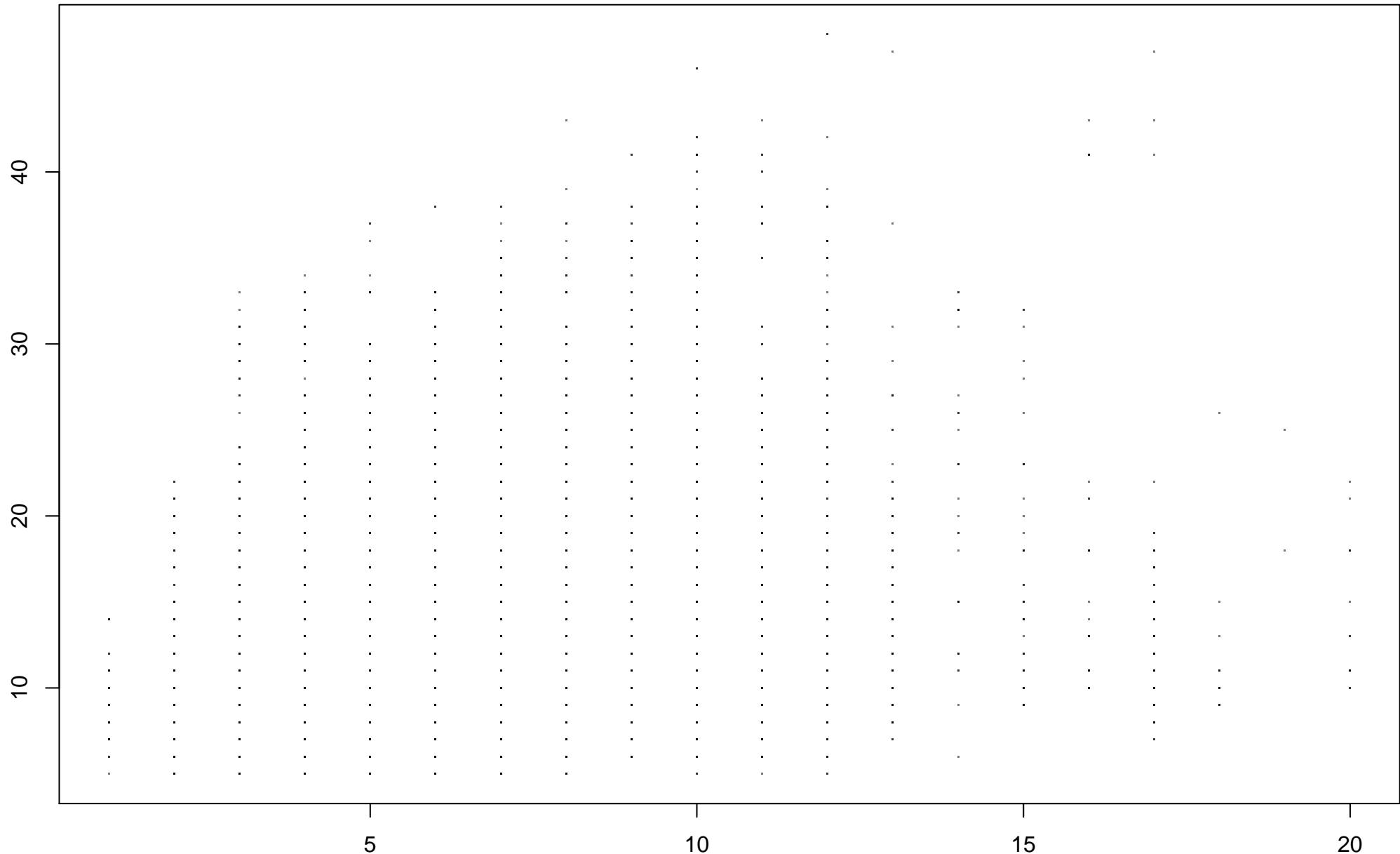
mcs_template_NumHAcceptors, H = 2.488 bit



docked_NOCount, H = 3.257 bit

template_NOCount-mcs_HeavyAtomCount, MI = 0.1513 bit, normMI = 0.04676

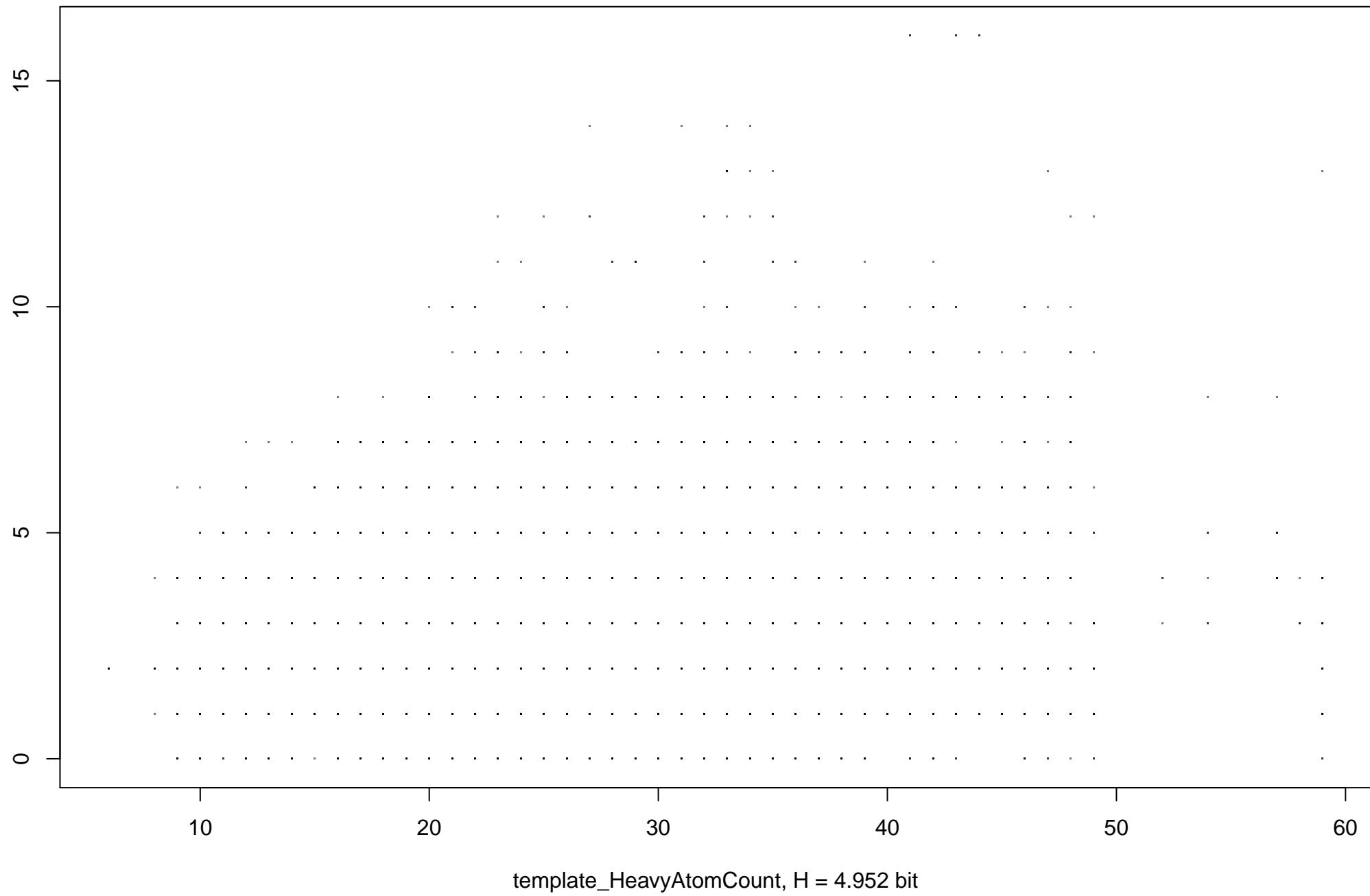
mcs_HeavyAtomCount, H = 4.38 bit



template_NOCount, H = 3.237 bit

template_HeavyAtomCount-mcs_NOCount, MI = 0.1294 bit, normMI = 0.04659

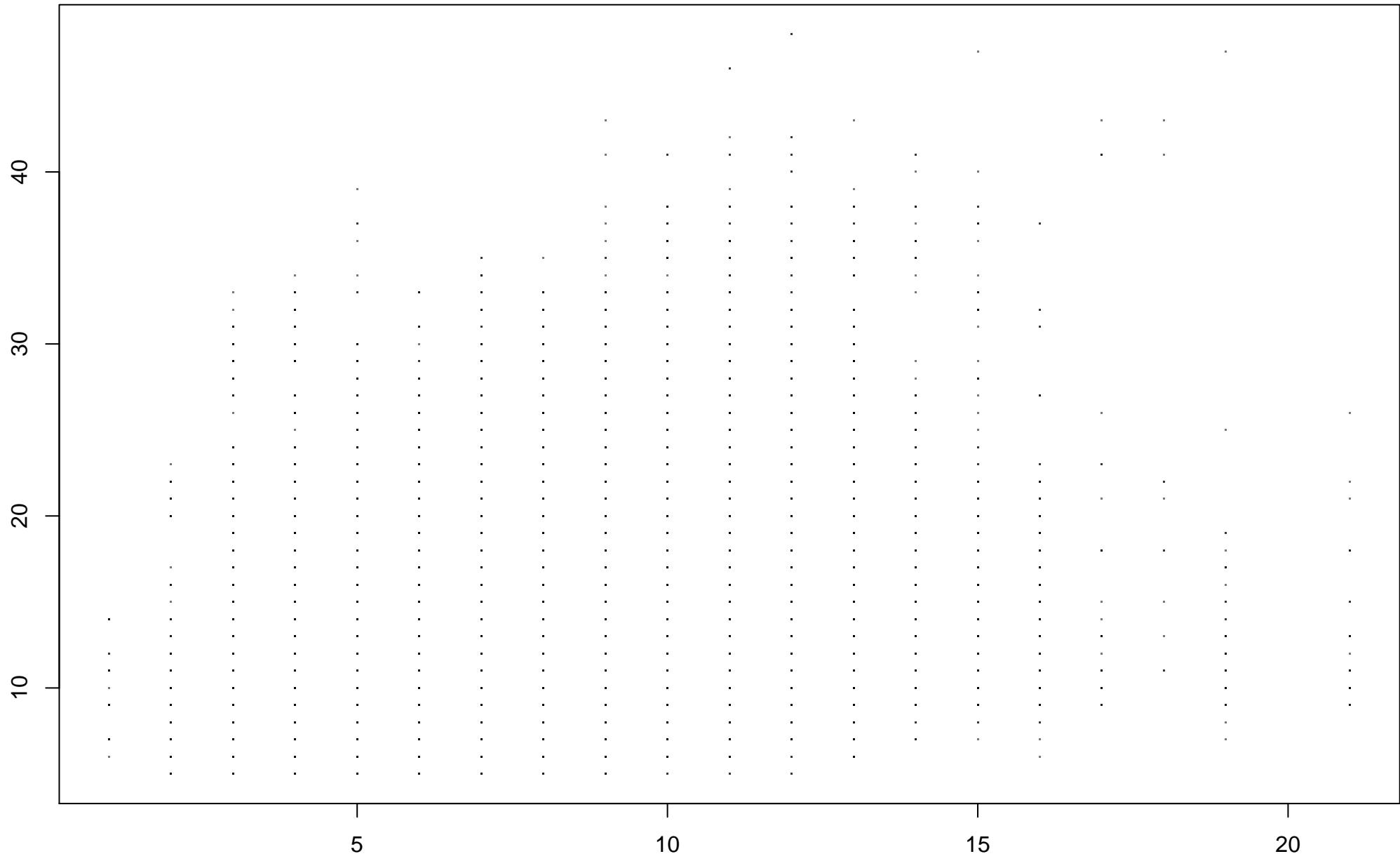
mcs_NOCount, H = 2.777 bit



template_HeavyAtomCount, H = 4.952 bit

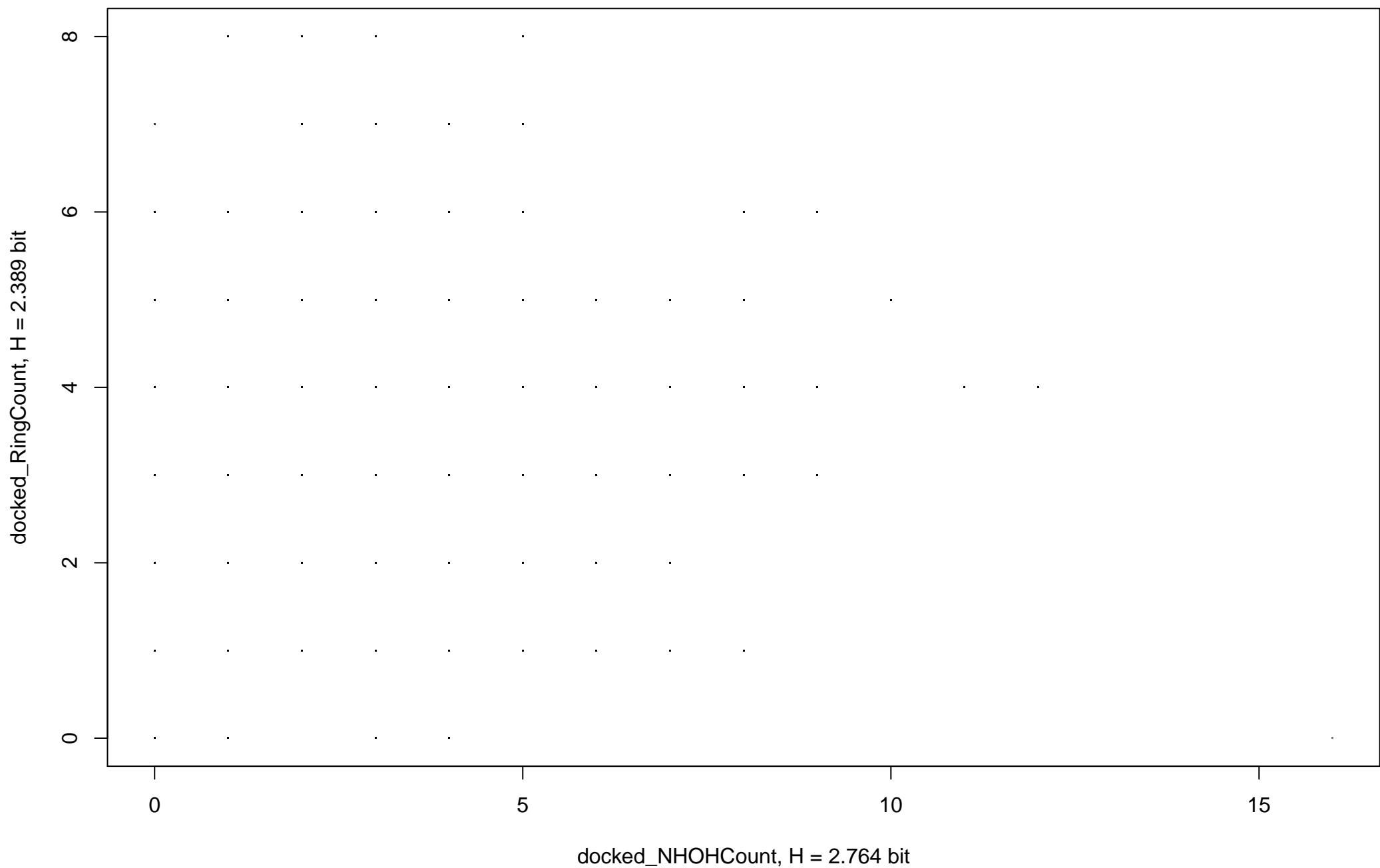
docked_NumHeteroAtoms-mcs_HeavyAtomCount, MI = 0.1656 bit, normMI = 0.04636

mcs_HeavyAtomCount, H = 4.38 bit

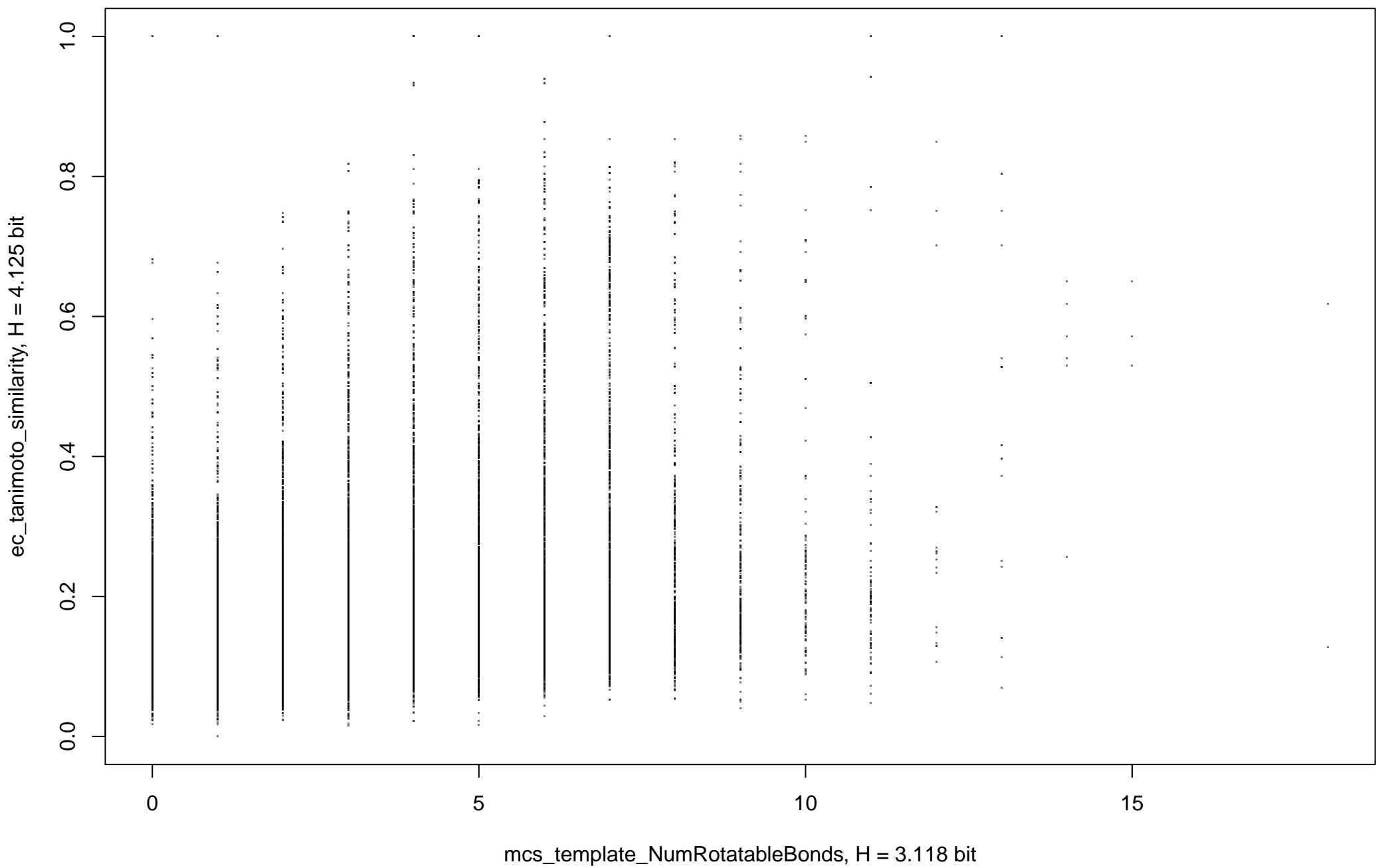


docked_NumHeteroAtoms, H = 3.571 bit

docked_NHOHCount–docked_RingCount, MI = 0.1103 bit, normMI = 0.04617

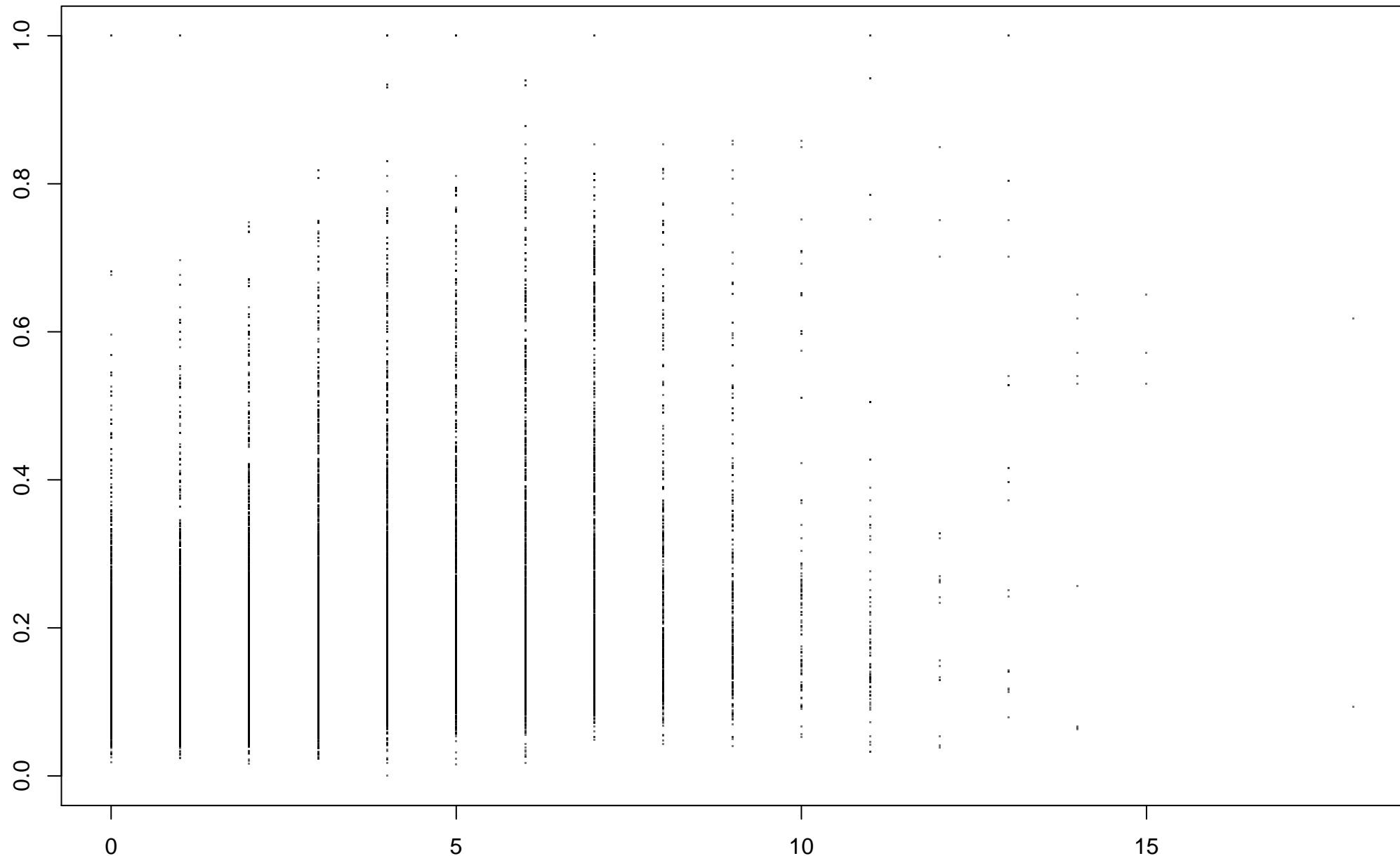


mcs_template_NumRotatableBonds–ec_tanimoto_similarity, MI = 0.1438 bit, normMI = 0.04612



mcs_docked_NumRotatableBonds–ec_tanimoto_similarity, MI = 0.1433 bit, normMI = 0.04597

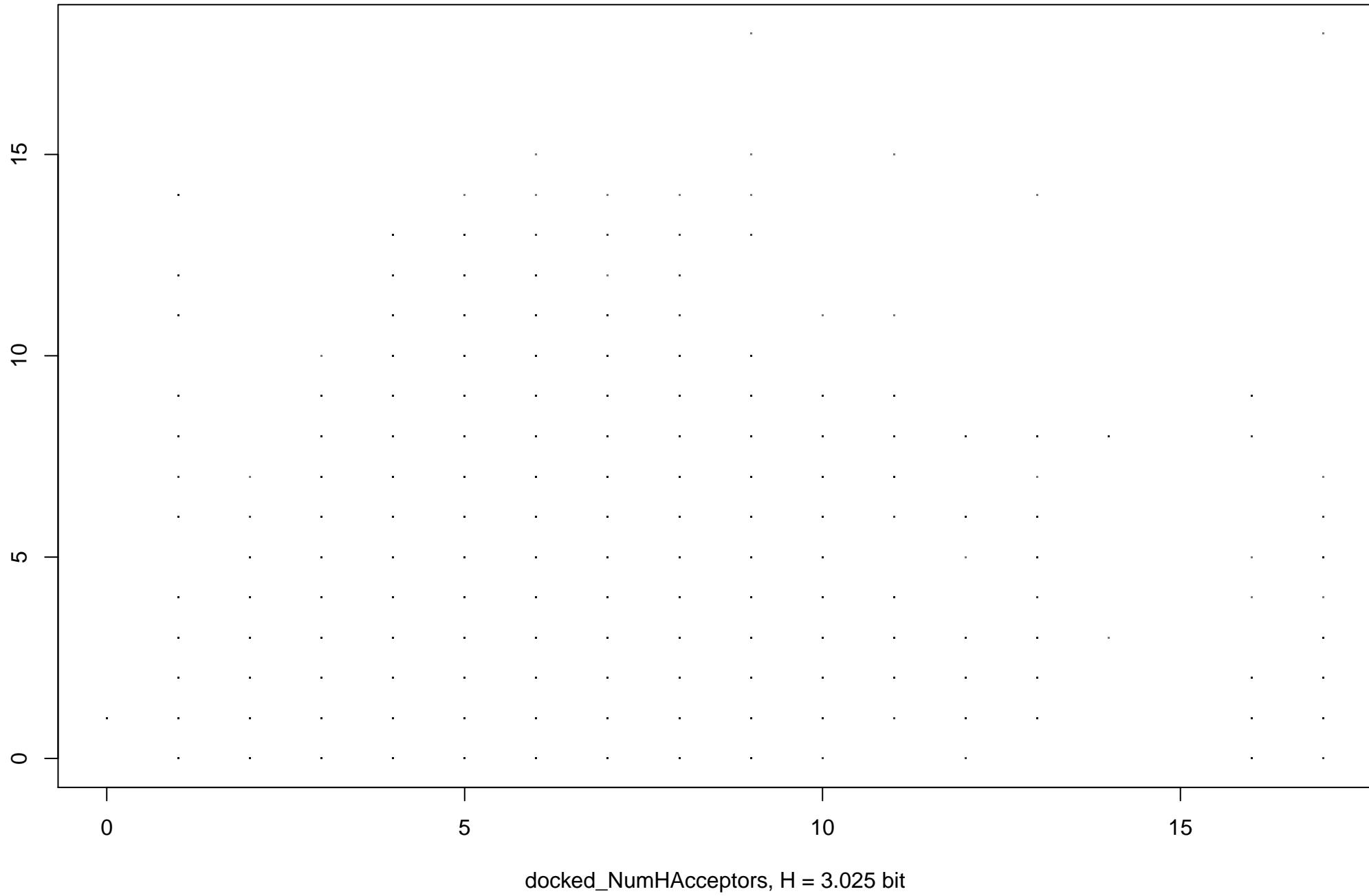
ec_tanimoto_similarity, H = 4.125 bit



mcs_docked_NumRotatableBonds, H = 3.117 bit

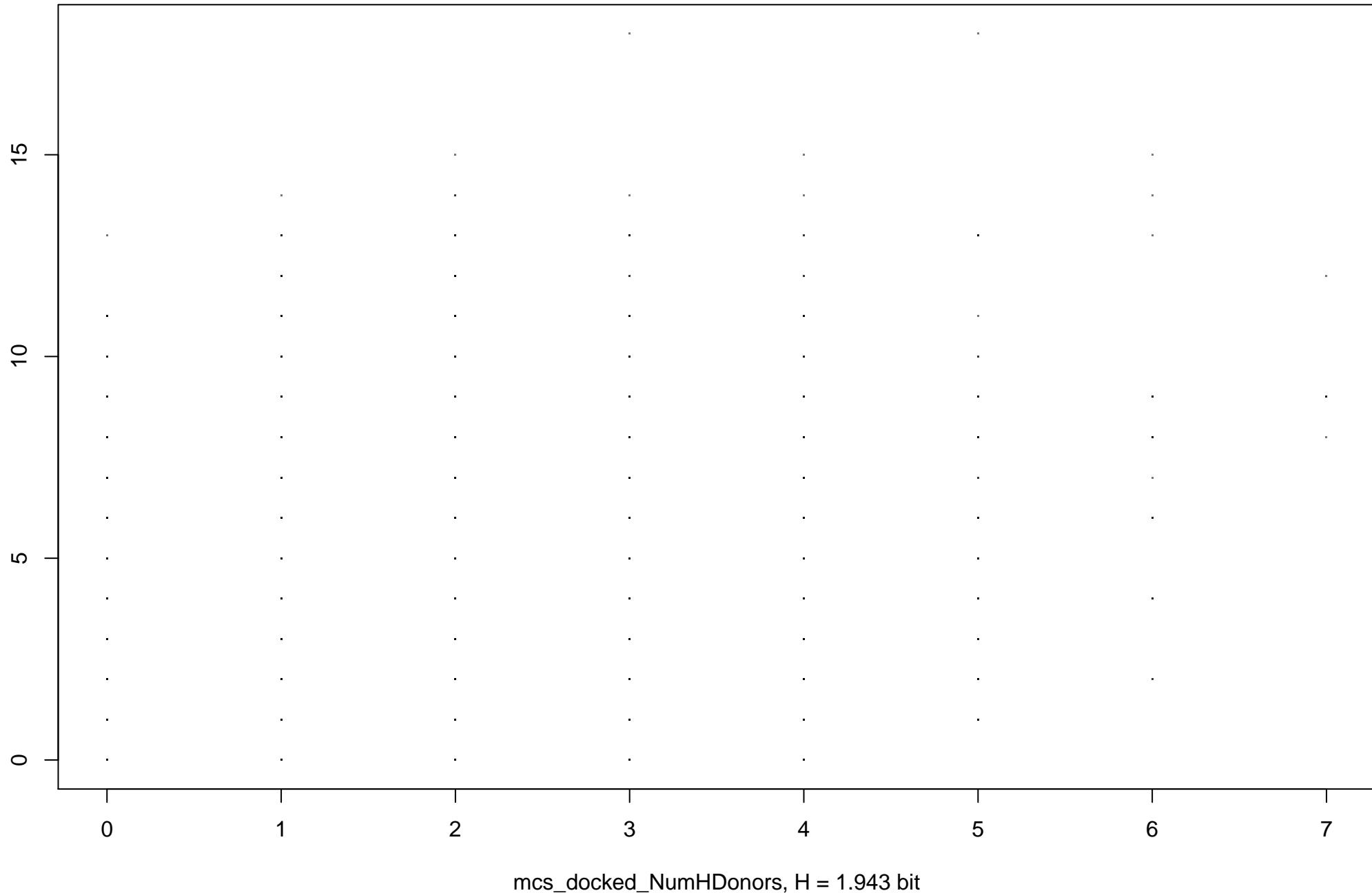
docked_NumHAcceptors-mcs_docked_NumRotatableBonds, MI = 0.1387 bit, normMI = 0.04584

mcs_docked_NumRotatableBonds, H = 3.117 bit

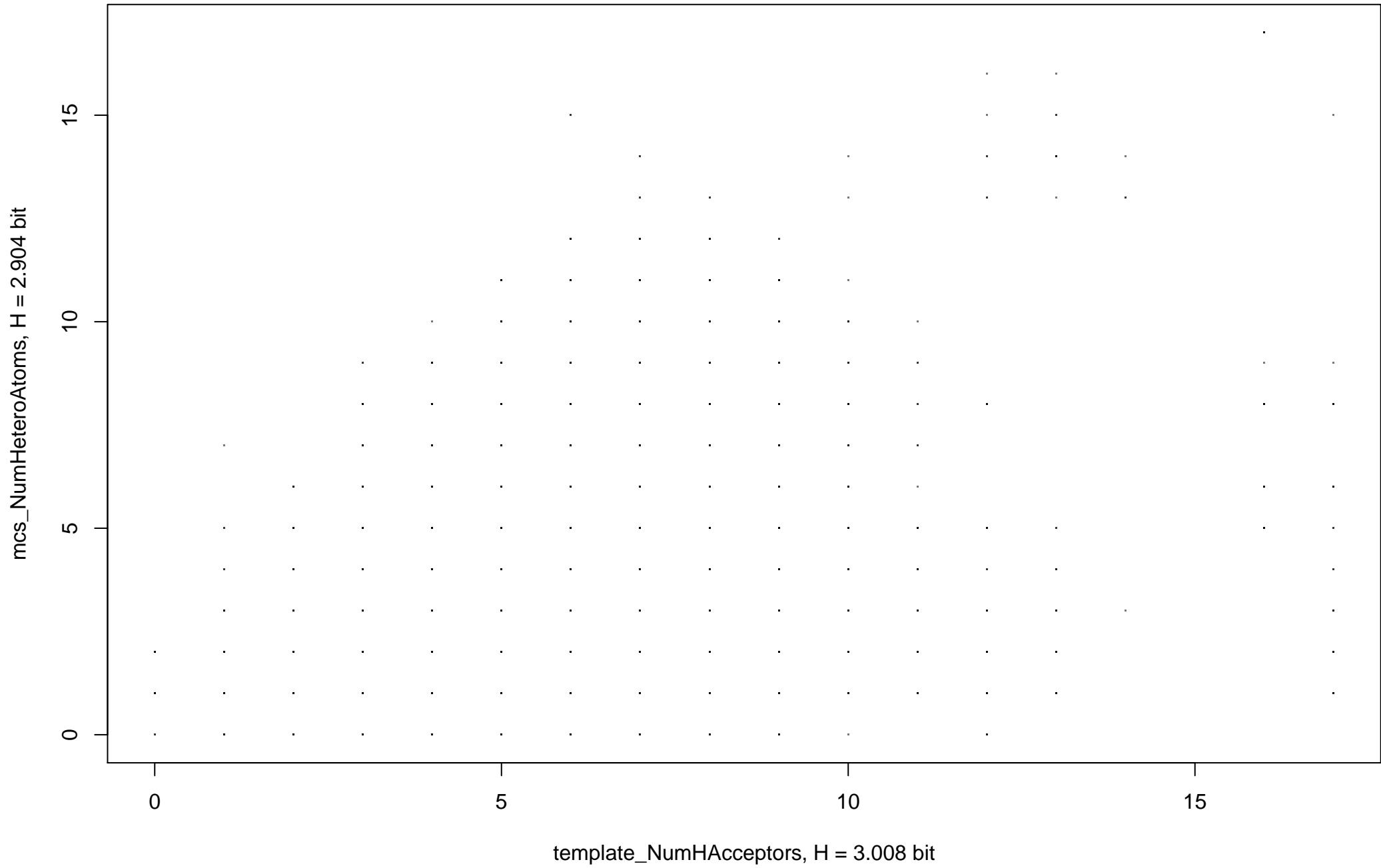


mcs_docked_NumHDonors–mcs_template_NumRotatableBonds, MI = 0.08898 bit, normMI = 0.04579

mcs_template_NumRotatableBonds, H = 3.118 bit

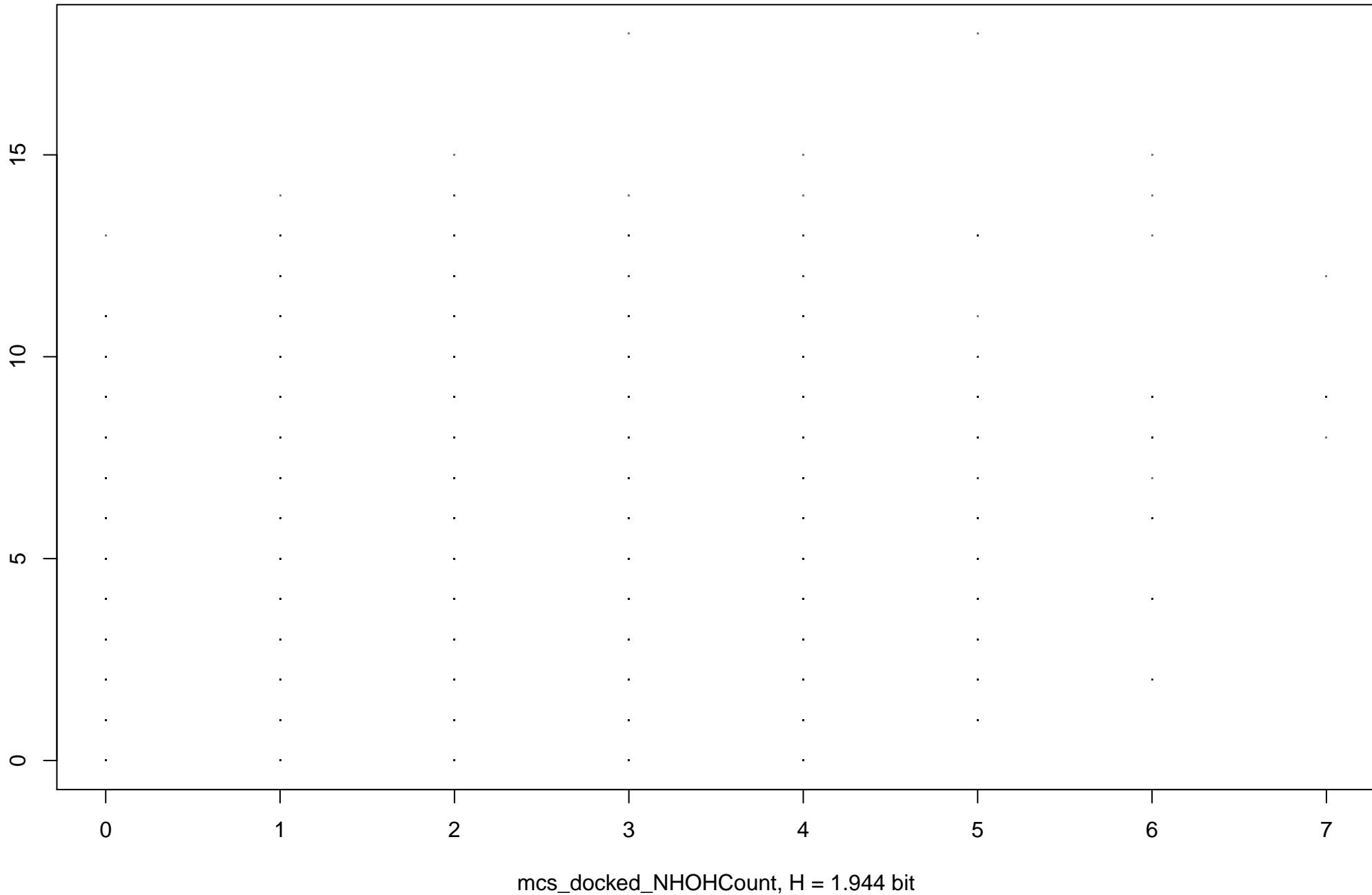


template_NumHAcceptors-mcs_NumHeteroAtoms, MI = 0.1327 bit, normMI = 0.0457

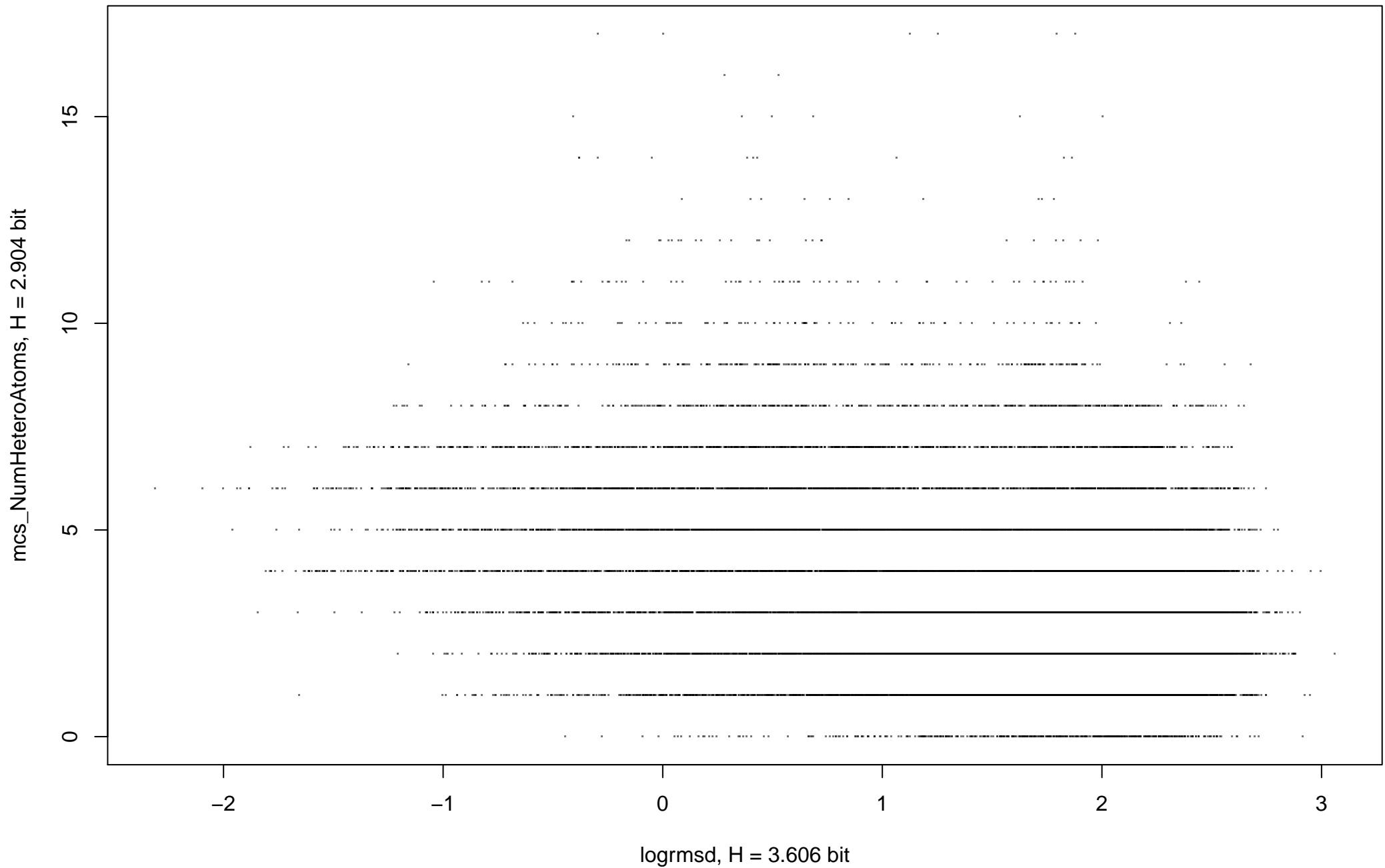


mcs_docked_NHOHCount–mcs_template_NumRotatableBonds, MI = 0.08883 bit, normMI = 0.04569

mcs_template_NumRotatableBonds, H = 3.118 bit

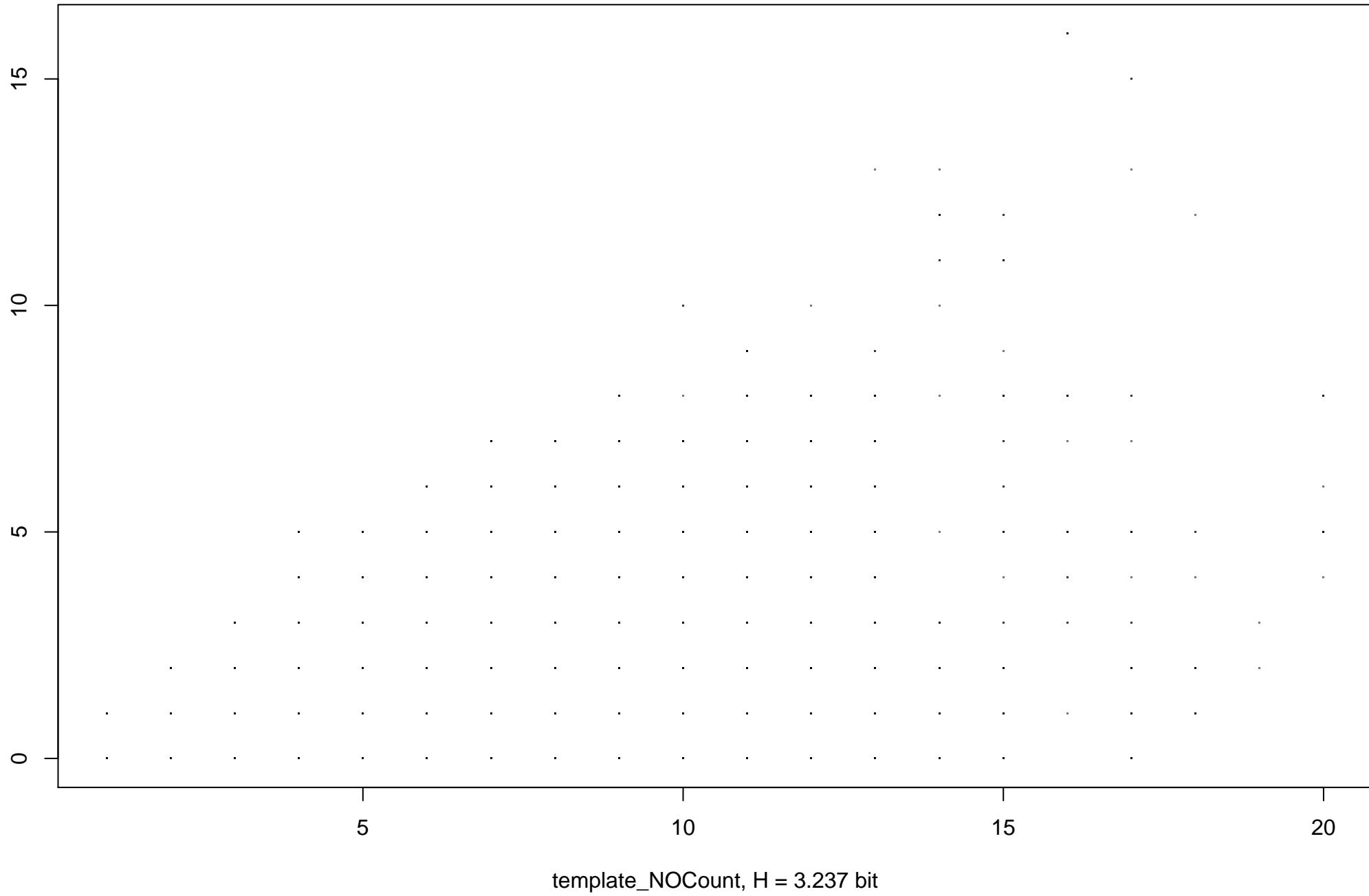


logrmsd-mcs_NumHeteroAtoms, MI = 0.1318 bit, normMI = 0.04538



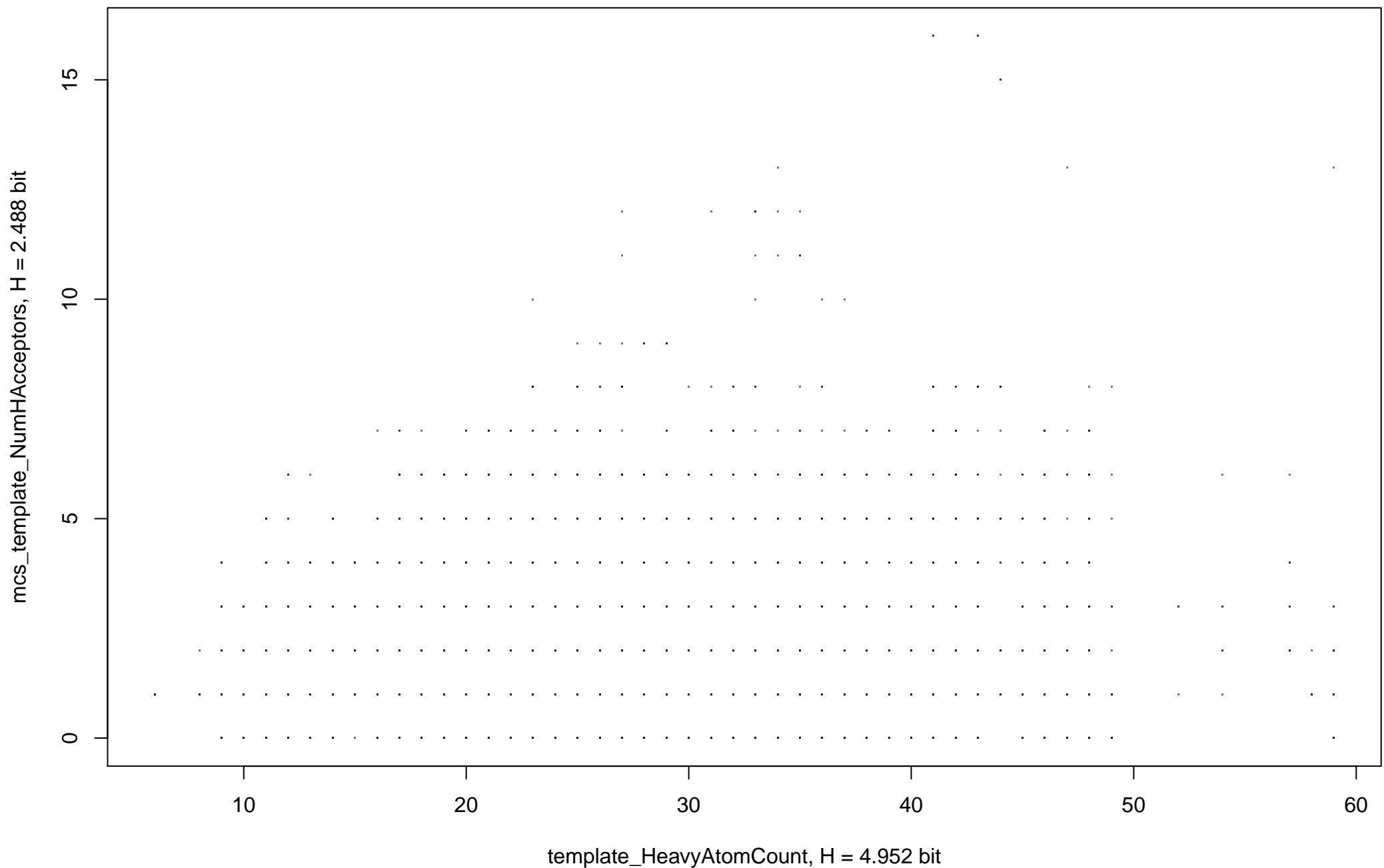
template_NOCount-mcs_template_NumHAcceptors, MI = 0.1115 bit, normMI = 0.04483

mcs_template_NumHAcceptors, H = 2.488 bit

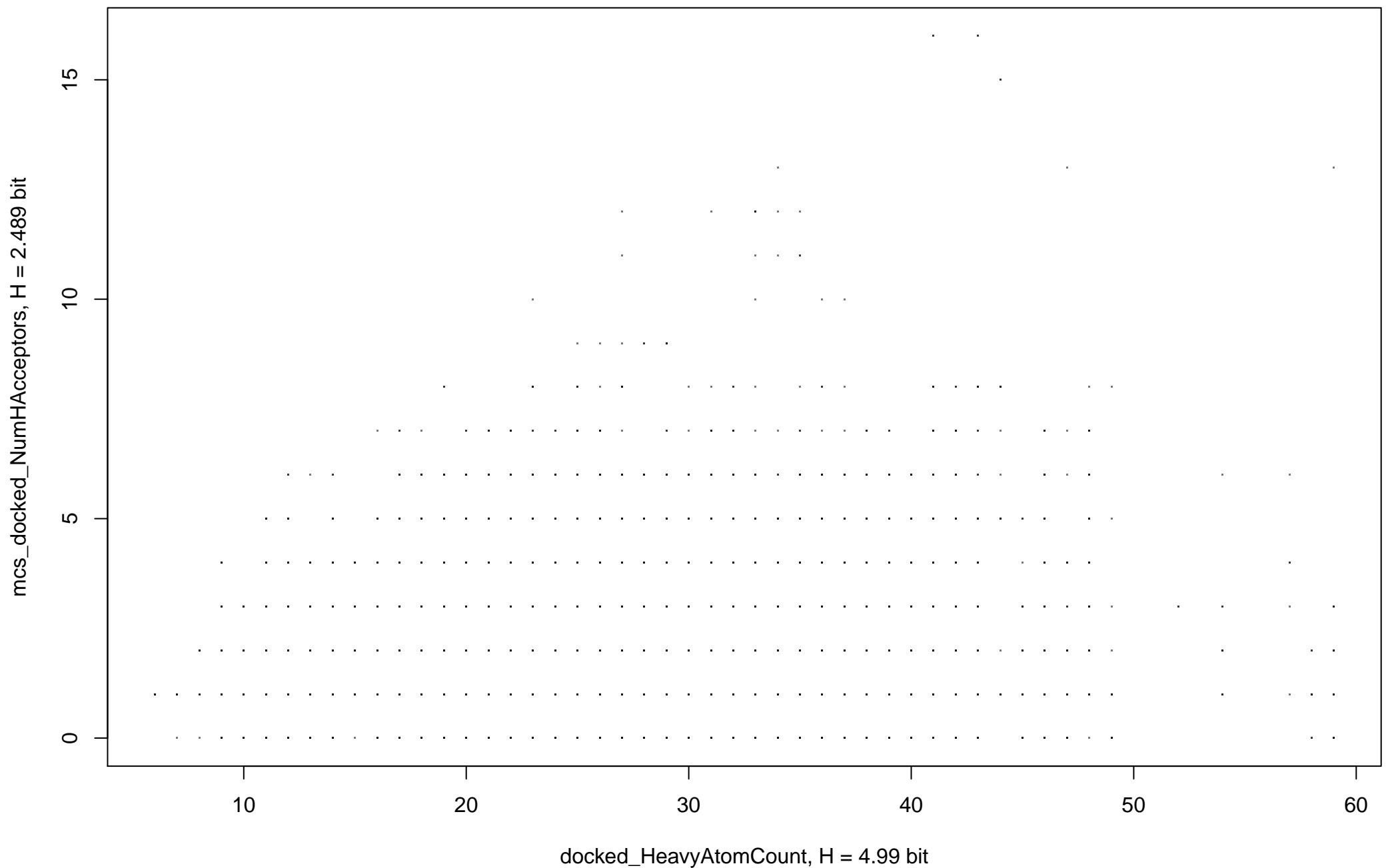


template_NOCount, H = 3.237 bit

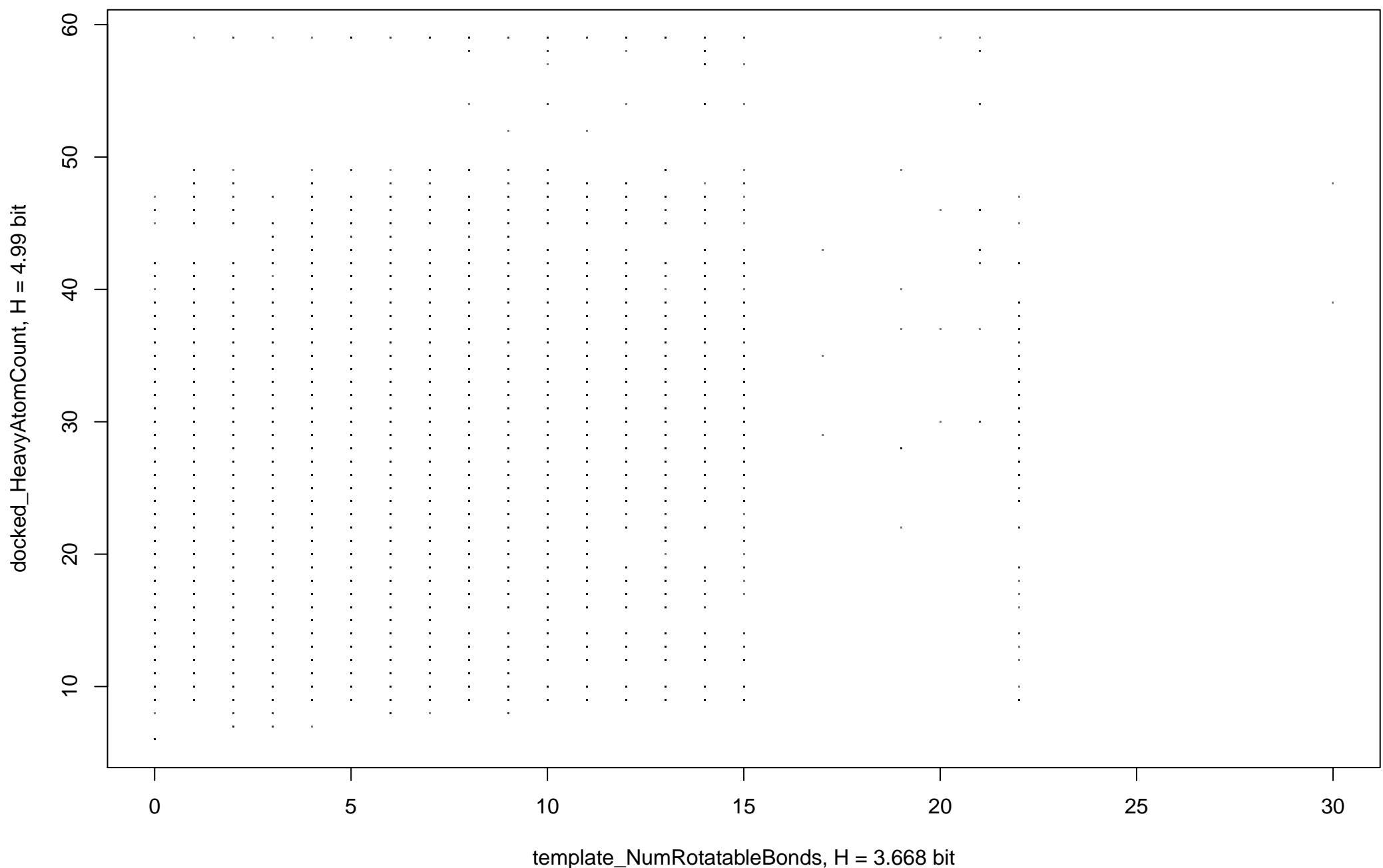
template_HeavyAtomCount-mcs_template_NumHAcceptors, MI = 0.11 bit, normMI = 0.04419



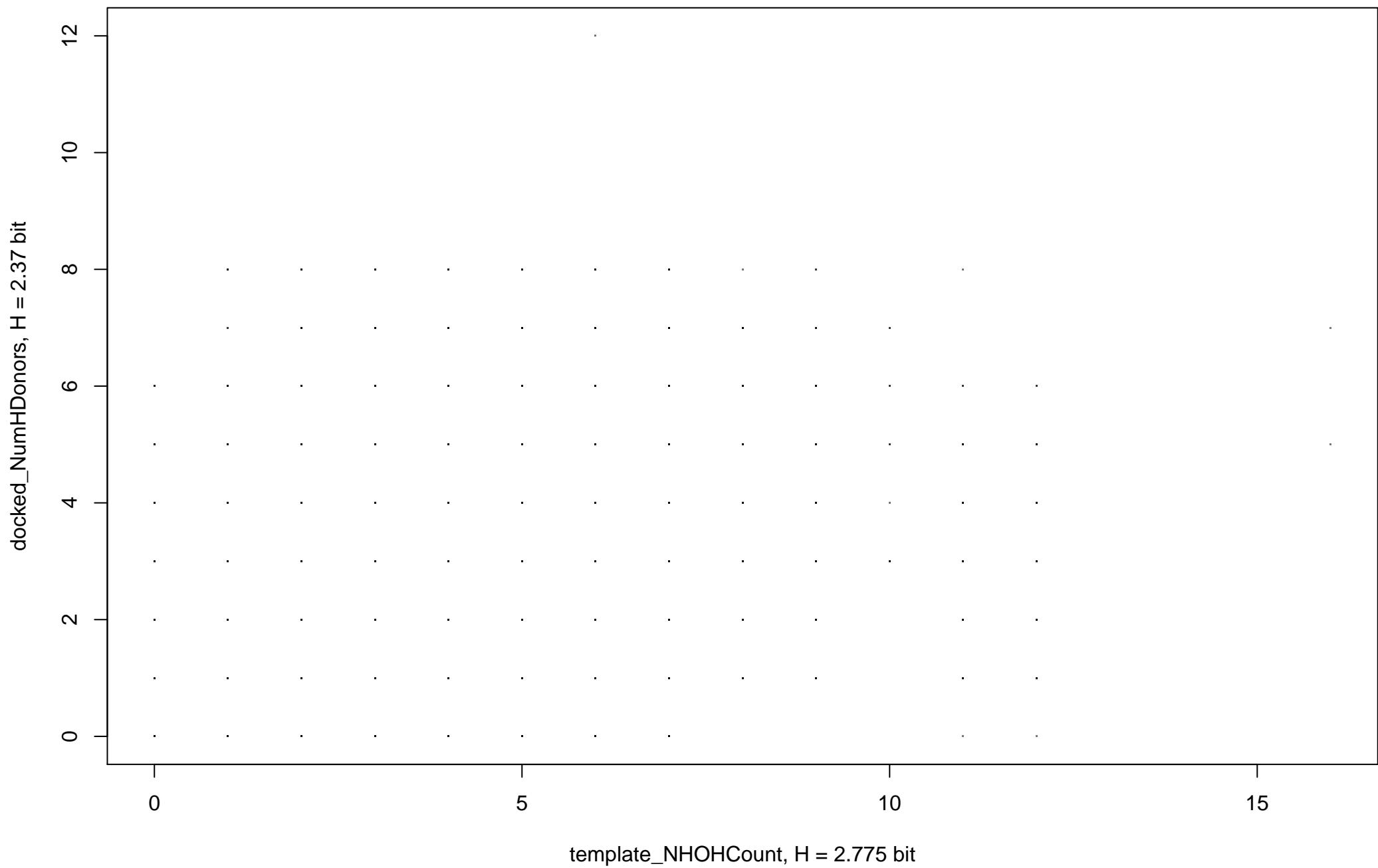
docked_HeavyAtomCount-mcs_docked_NumHAcceptors, MI = 0.1097 bit, normMI = 0.04406



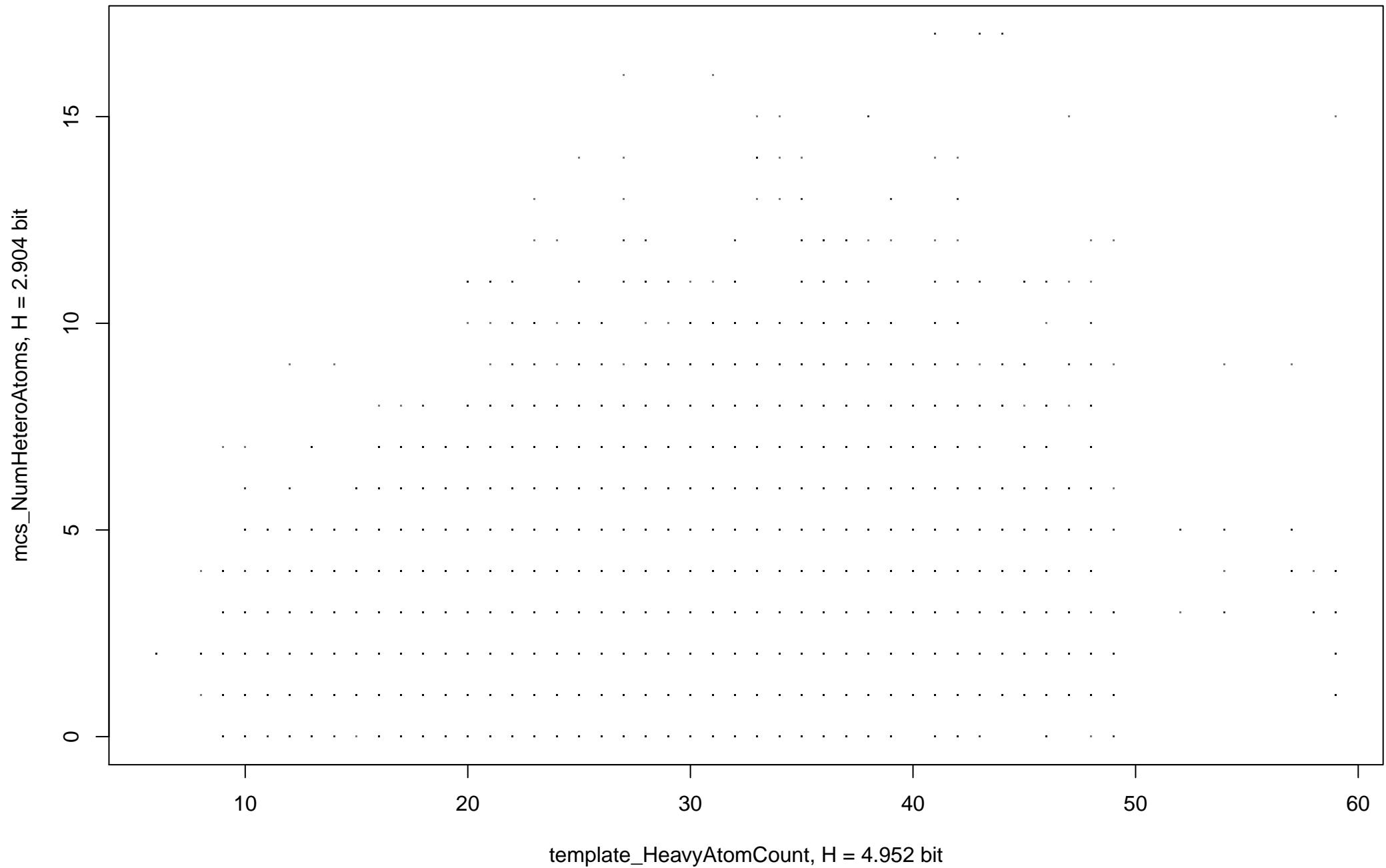
template_NumRotatableBonds-docked_HeavyAtomCount, MI = 0.1612 bit, normMI = 0.04393



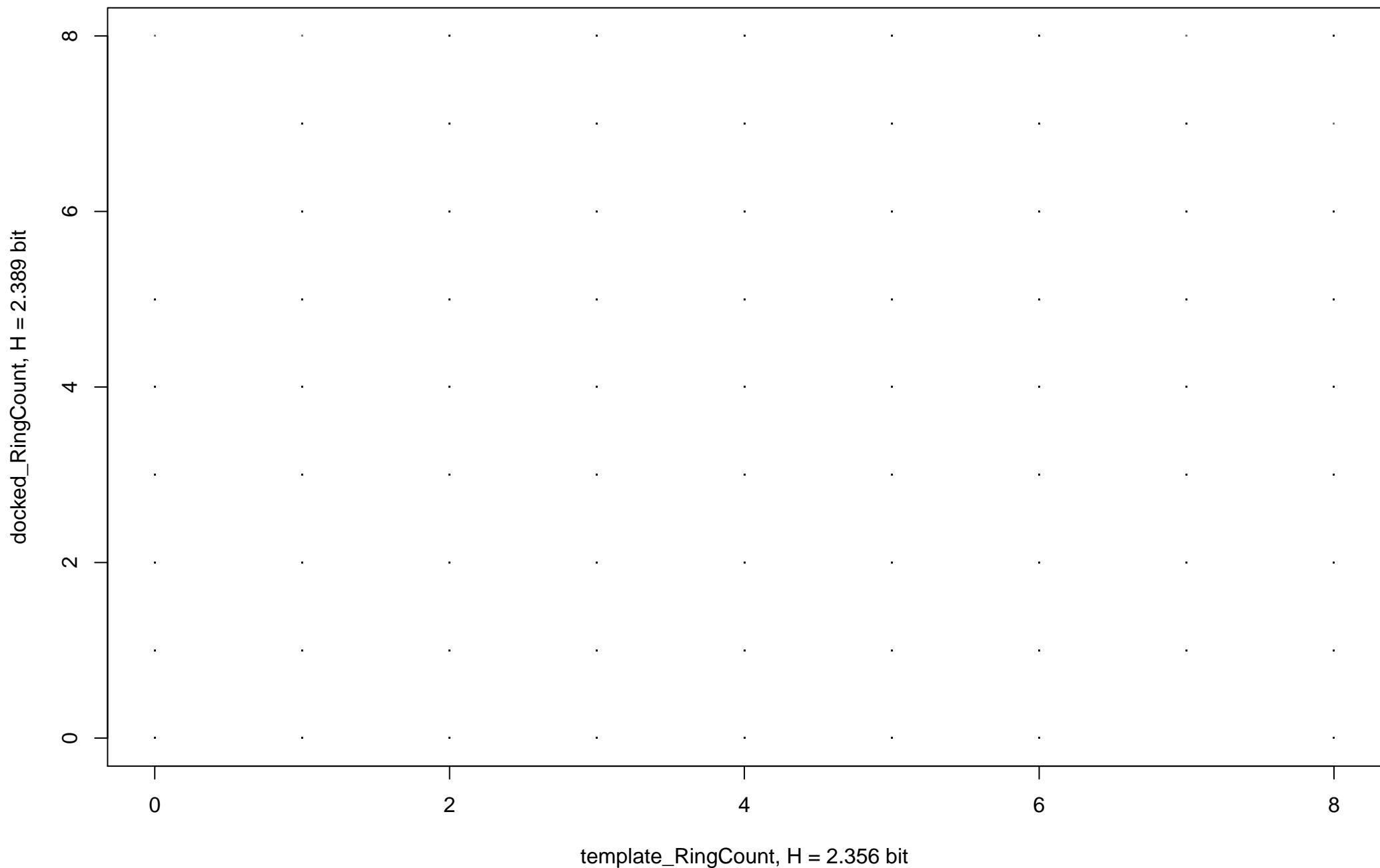
template_NHOHCount-docked_NumHDonors, MI = 0.1038 bit, normMI = 0.04381



template_HeavyAtomCount-mcs_NumHeteroAtoms, MI = 0.1271 bit, normMI = 0.04377

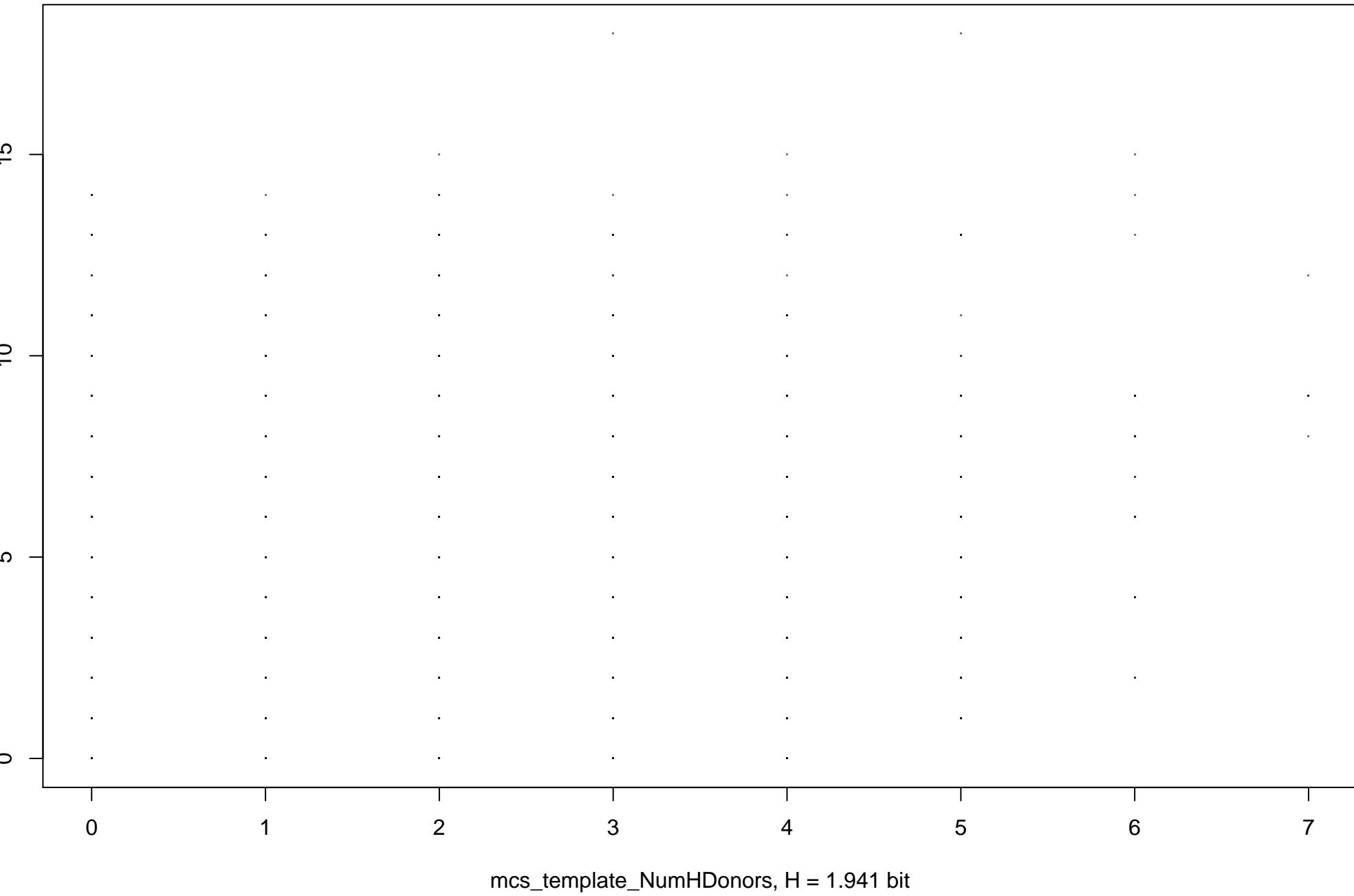


template_RingCount–docked_RingCount, MI = 0.103 bit, normMI = 0.04373



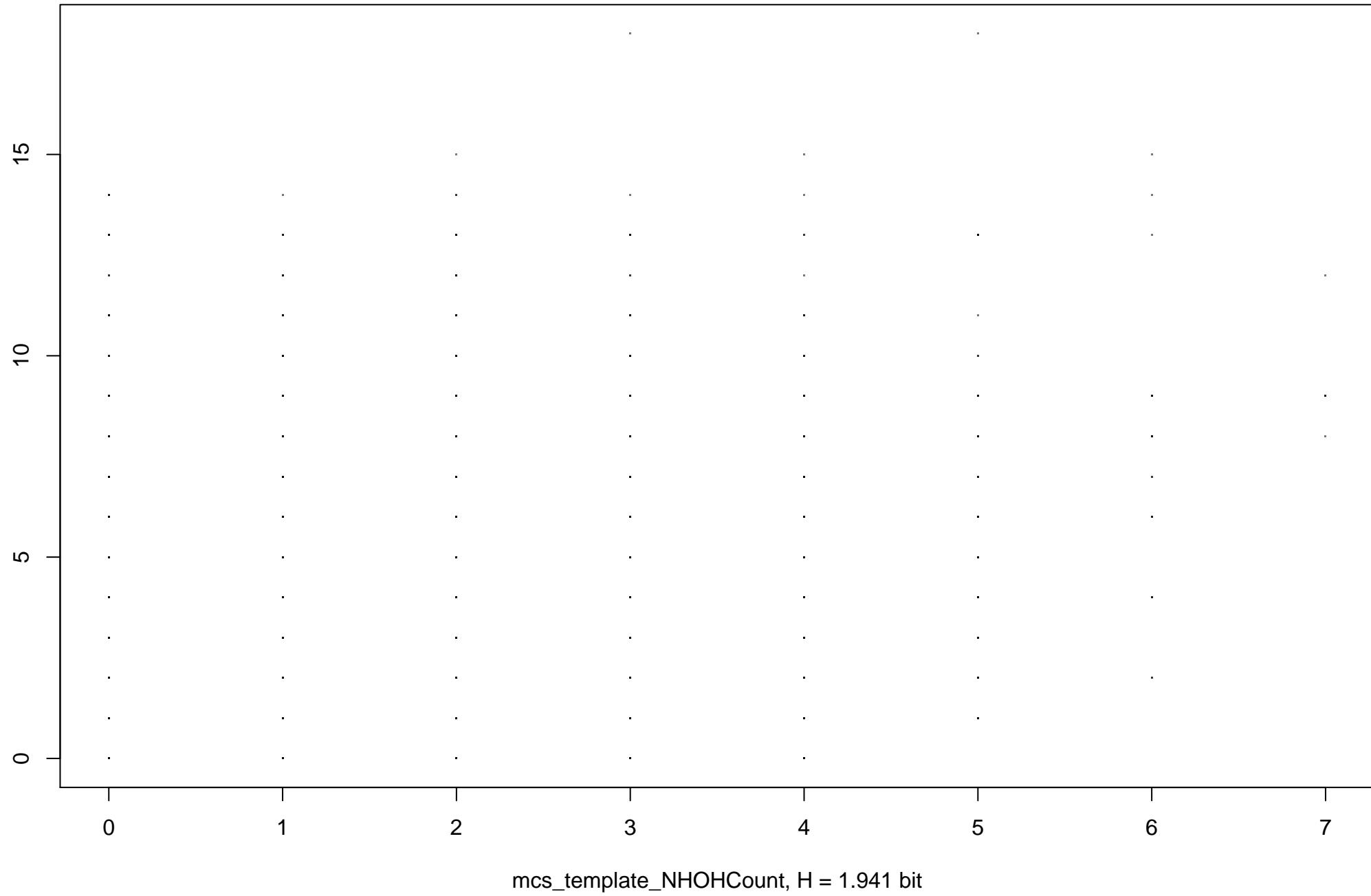
mcs_template_NumHDonors–mcs_docked_NumRotatableBonds, MI = 0.08457 bit, normMI = 0.04358

mcs_docked_NumRotatableBonds, H = 3.117 bit



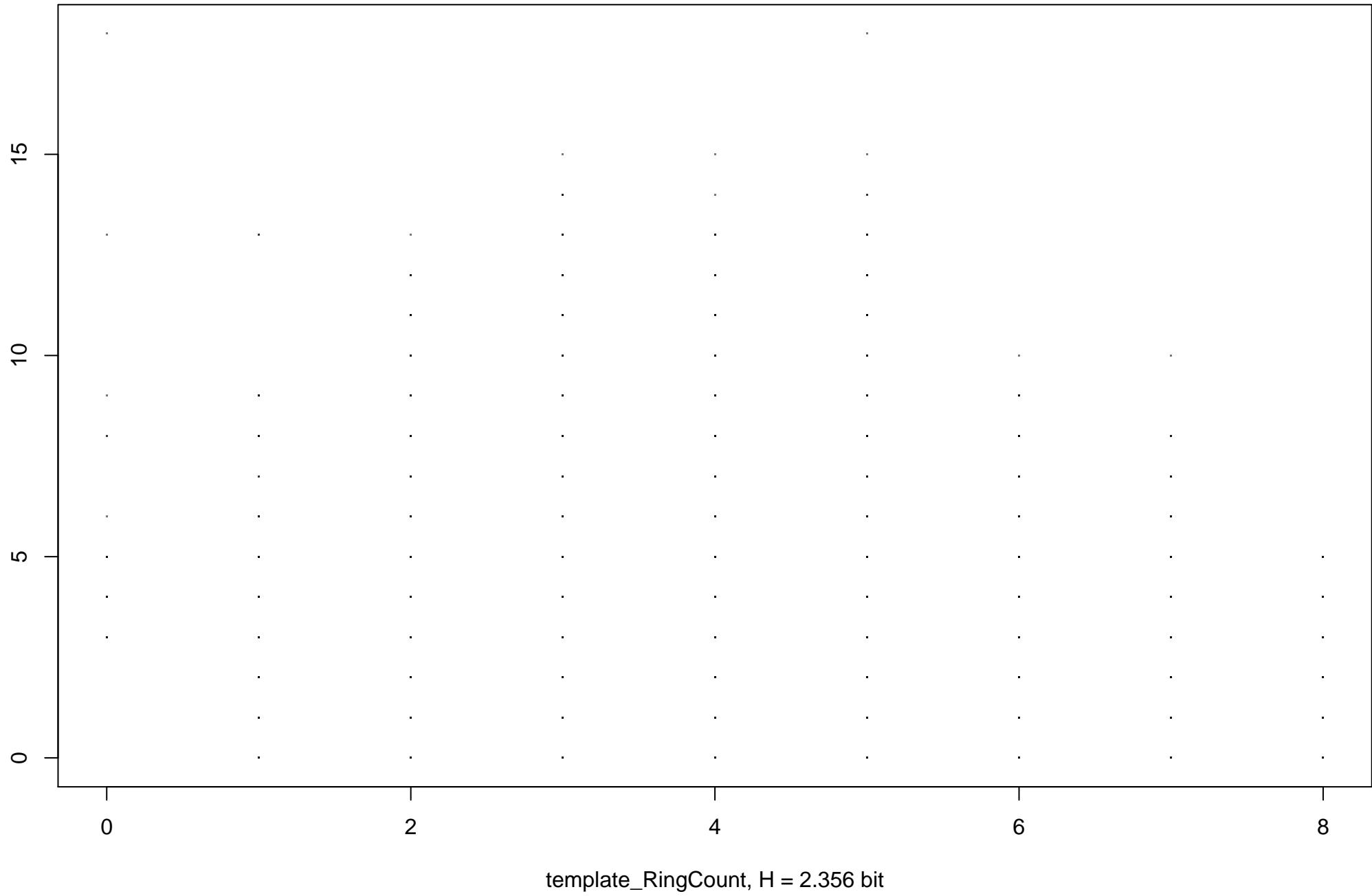
mcs_template_NHOHCount-mcs_docked_NumRotatableBonds, MI = 0.08456 bit, normMI = 0.04355

mcs_docked_NumRotatableBonds, H = 3.117 bit



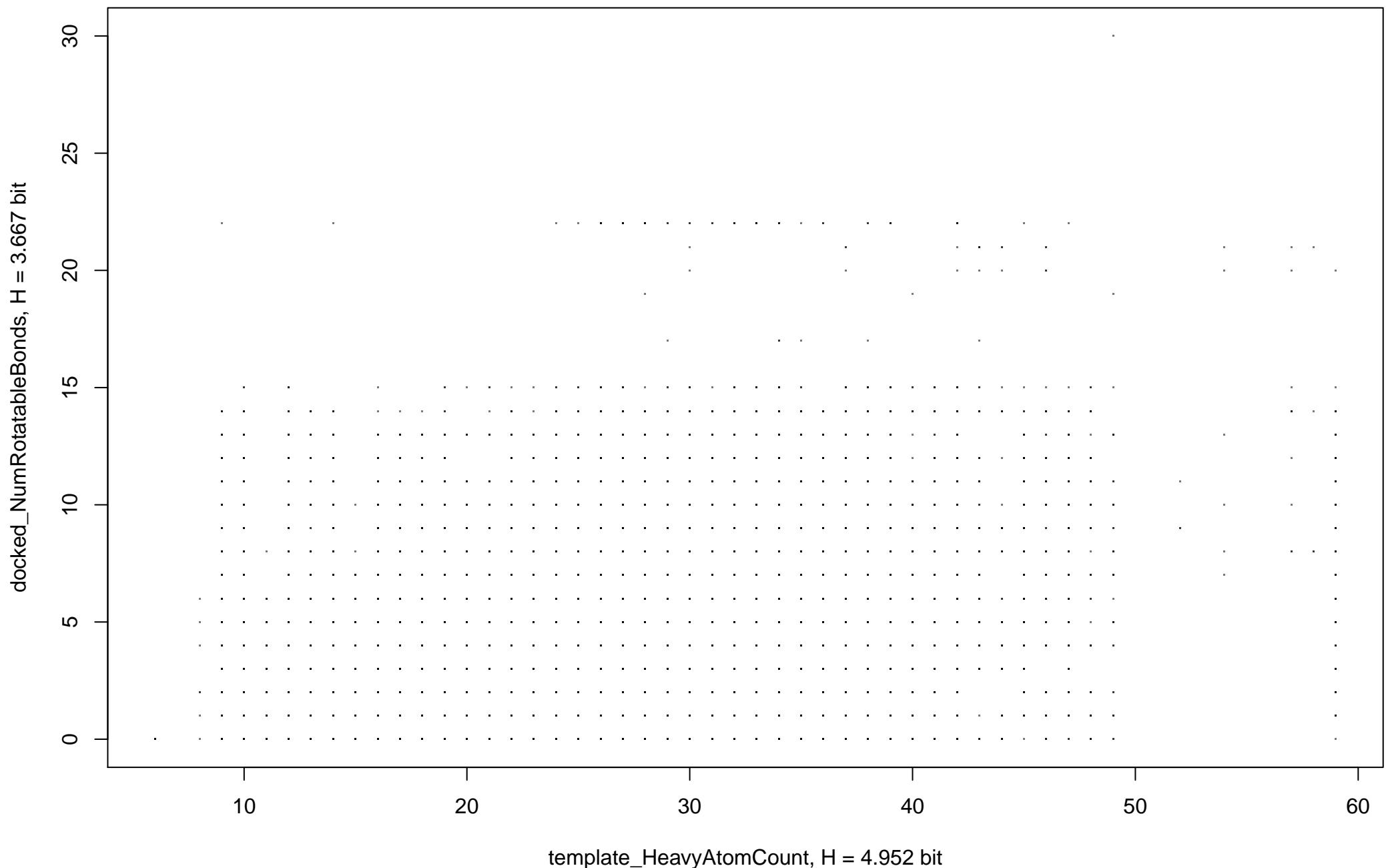
template_RingCount-mcs_template_NumRotatableBonds, MI = 0.1018 bit, normMI = 0.04323

mcs_template_NumRotatableBonds, H = 3.118 bit

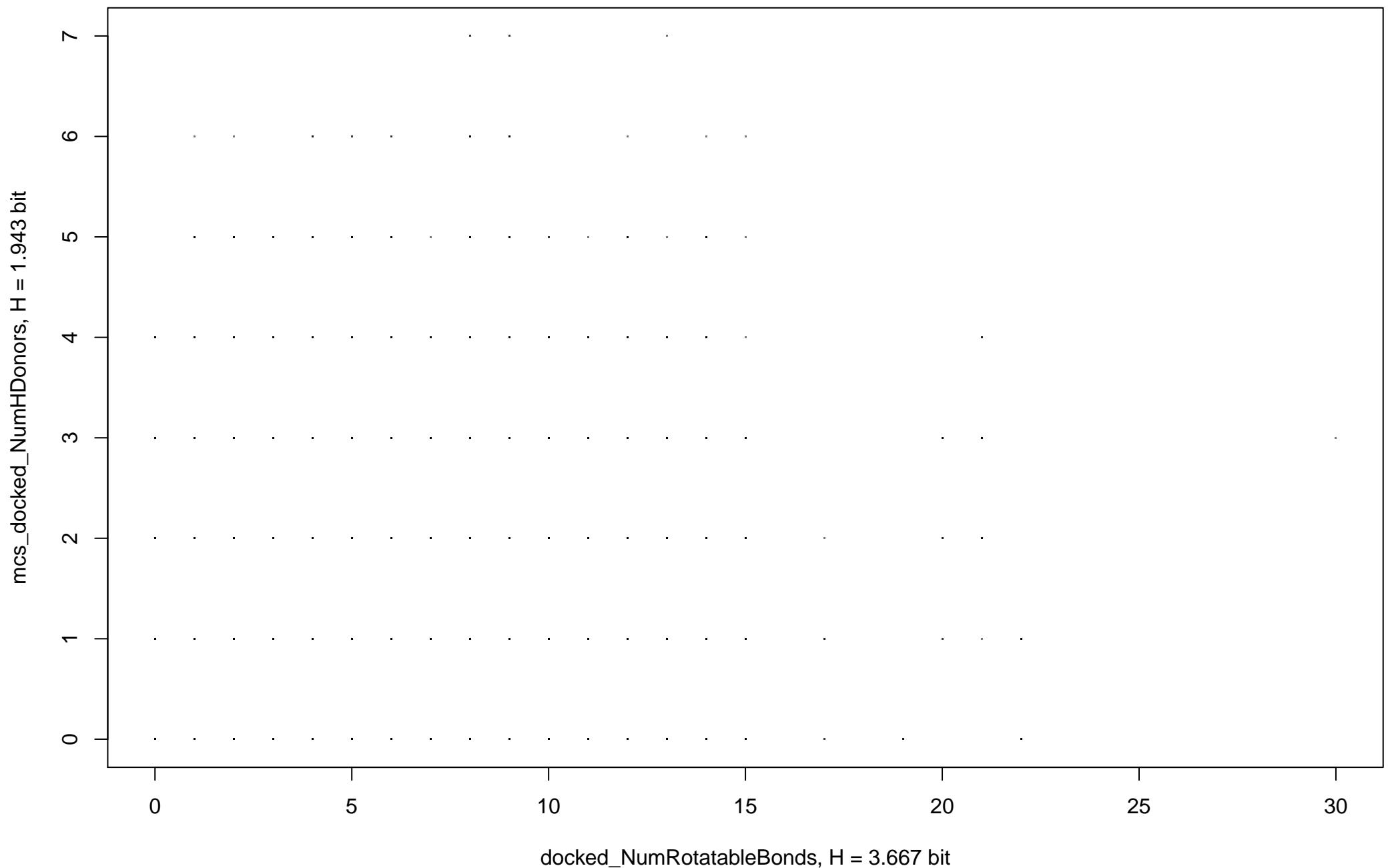


template_RingCount, H = 2.356 bit

template_HeavyAtomCount-docked_NumRotatableBonds, MI = 0.1583 bit, normMI = 0.04316

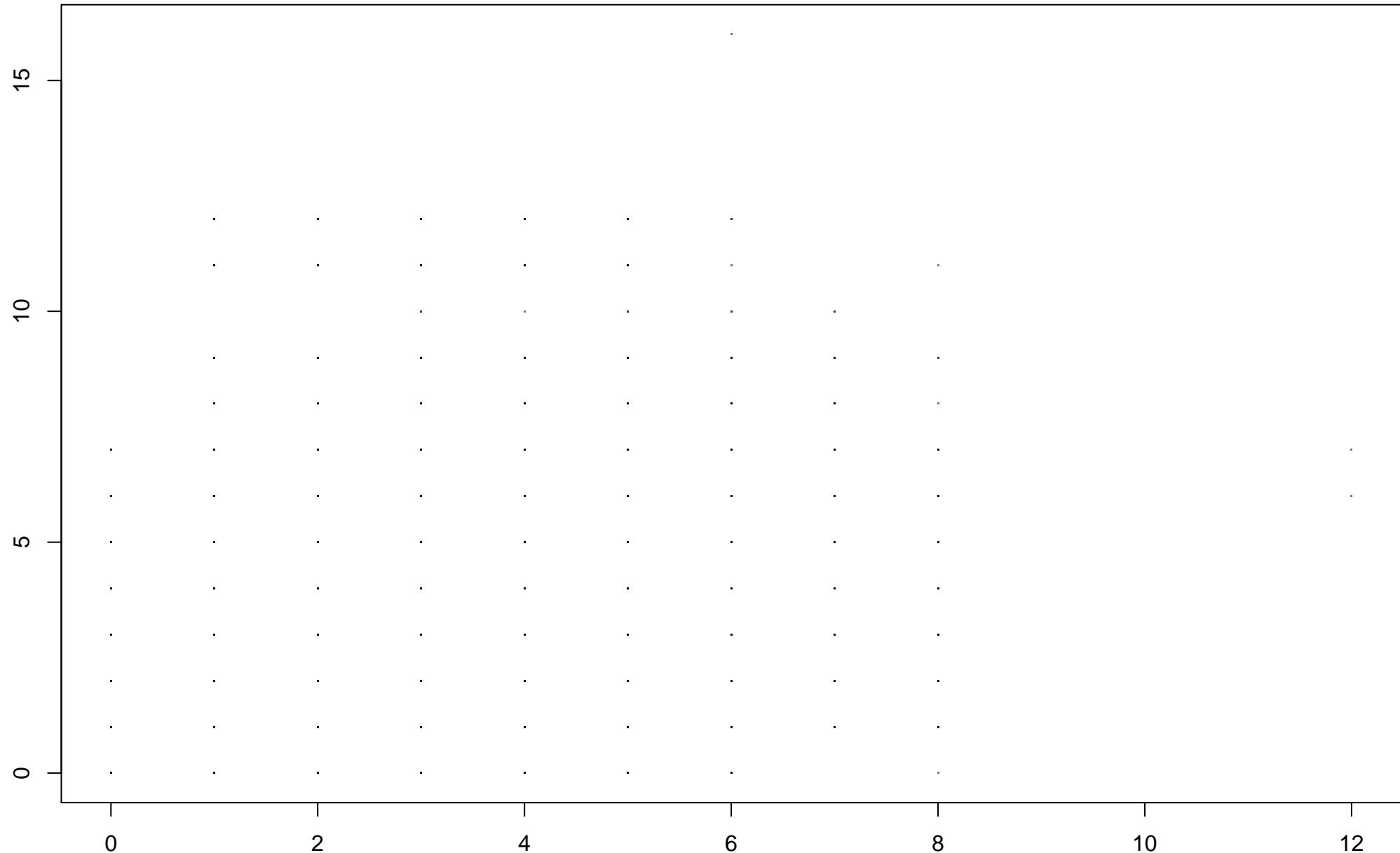


docked_NumRotatableBonds-mcs_docked_NumHDonors, MI = 0.08364 bit, normMI = 0.04304



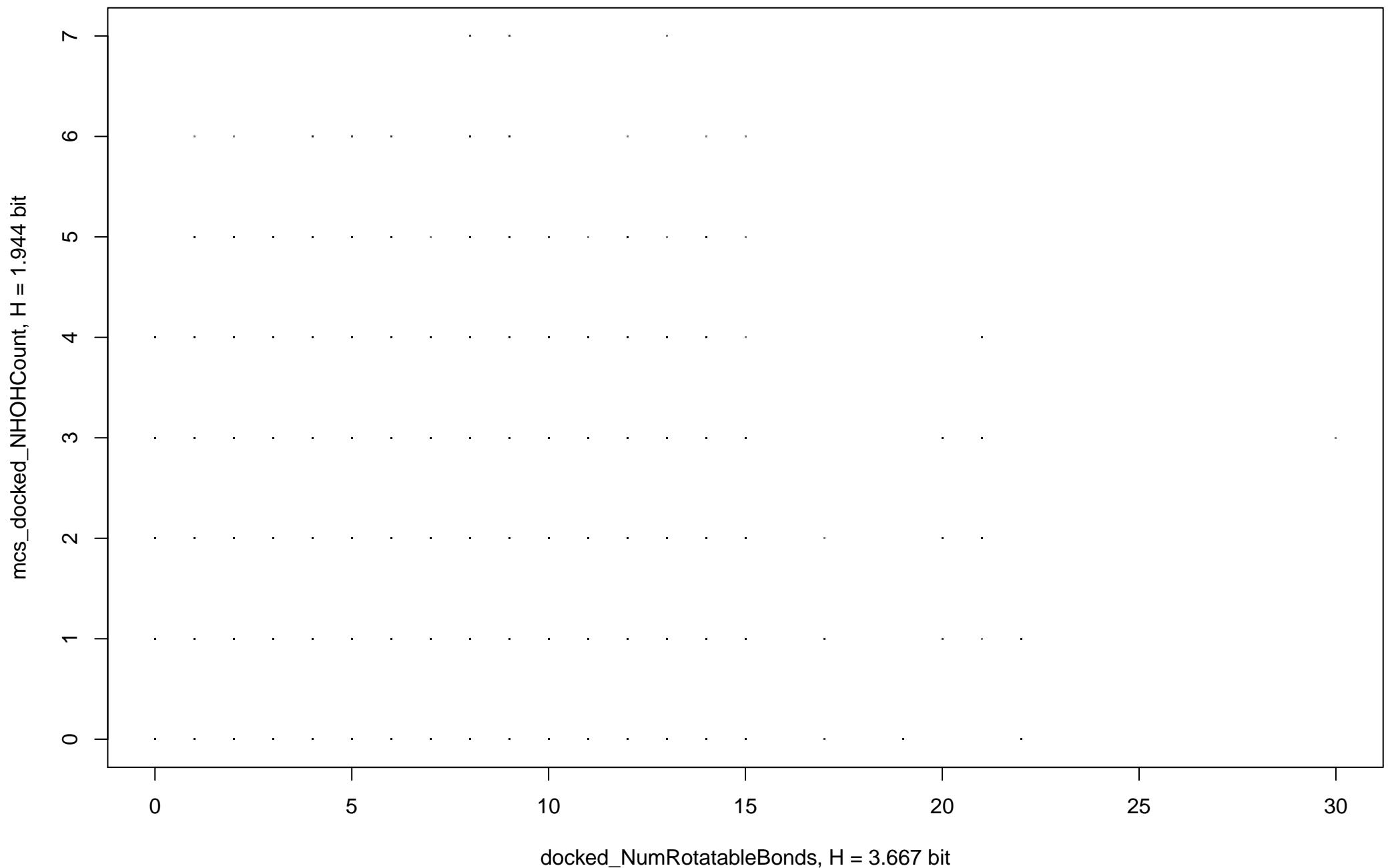
template_NumHDonors-docked_NHOHCount, MI = 0.1024 bit, normMI = 0.04297

docked_NHOHCount, H = 2.764 bit

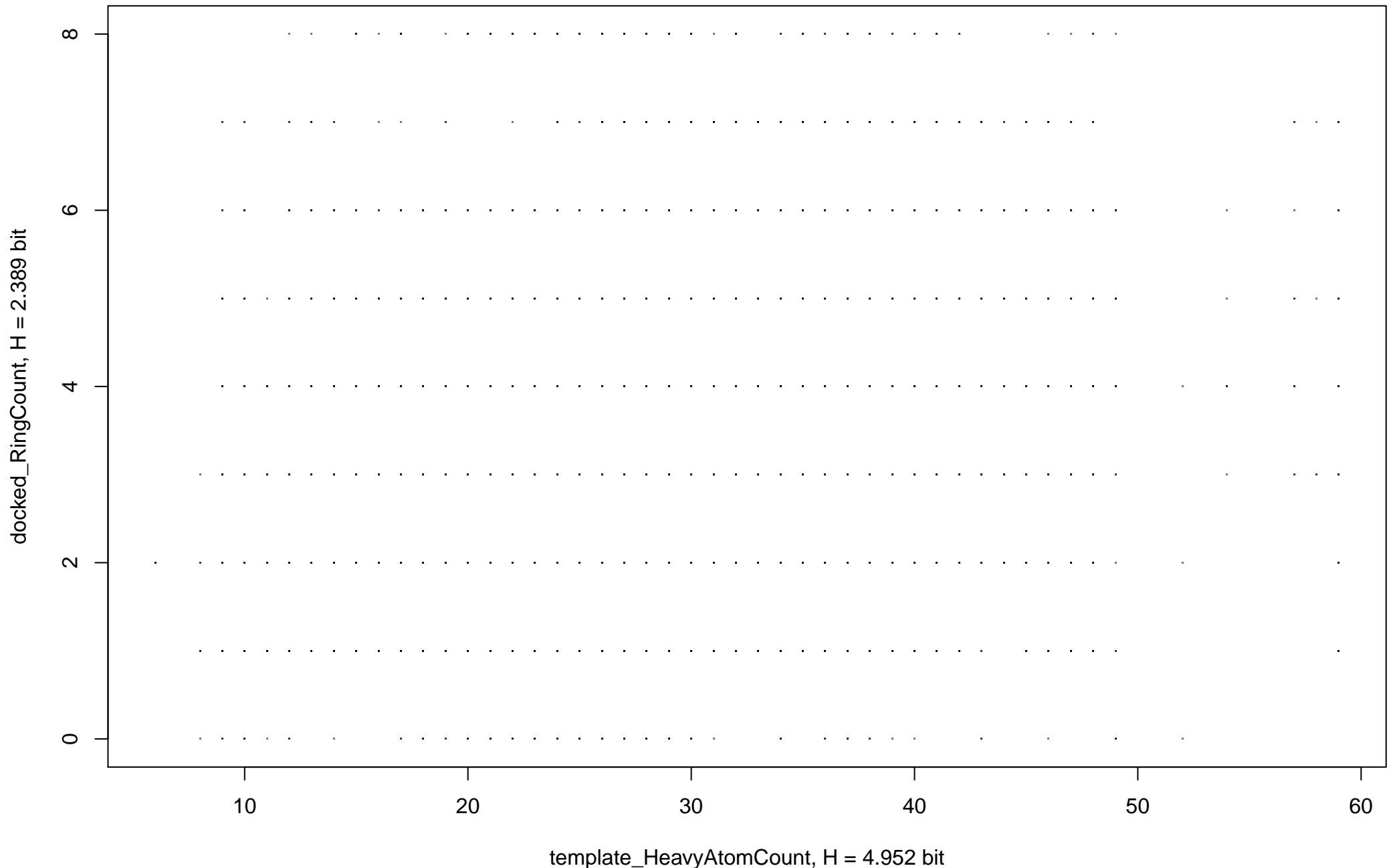


template_NumHDonors, H = 2.383 bit

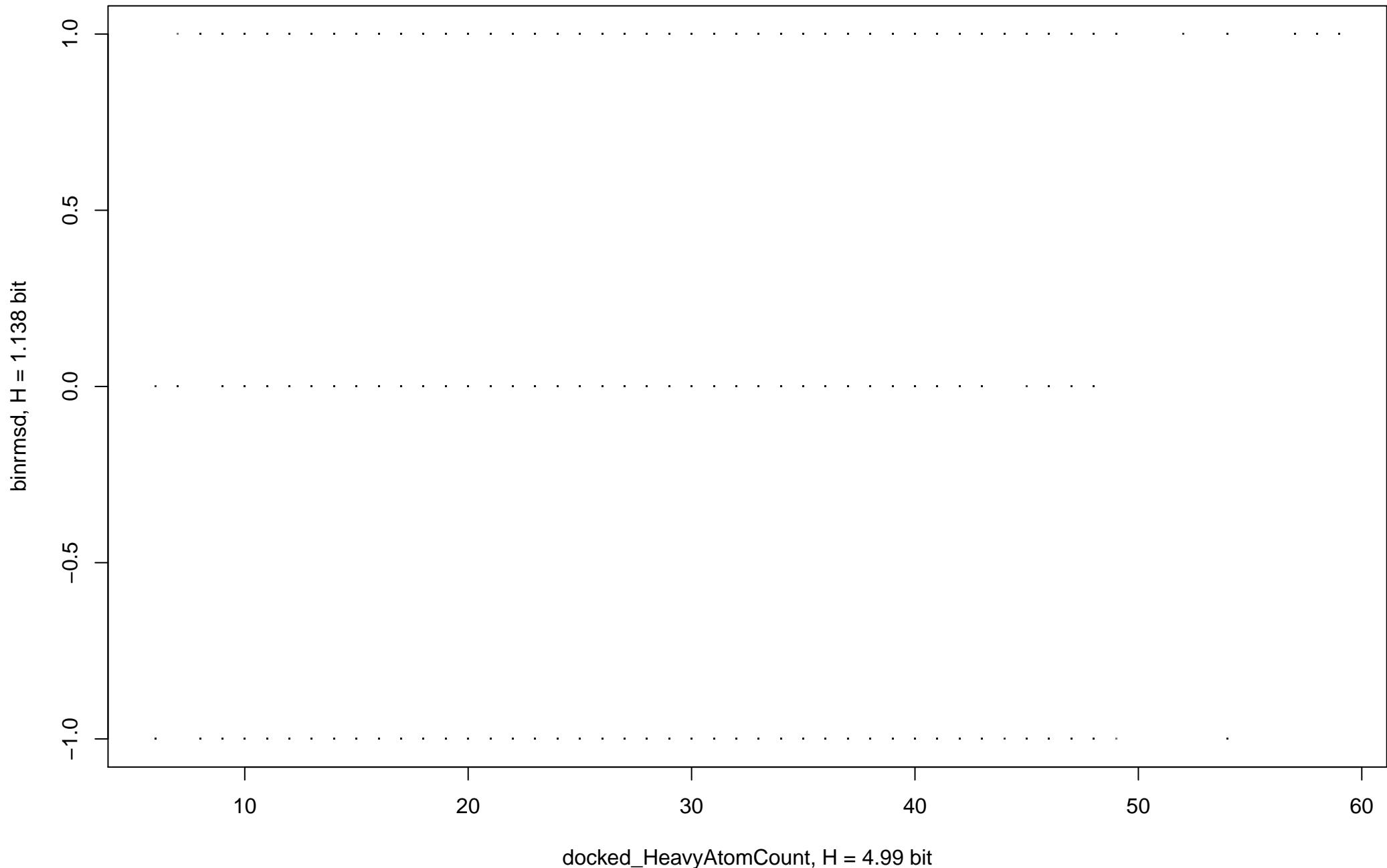
docked_NumRotatableBonds-mcs_docked_NHOHCount, MI = 0.08339 bit, normMI = 0.0429



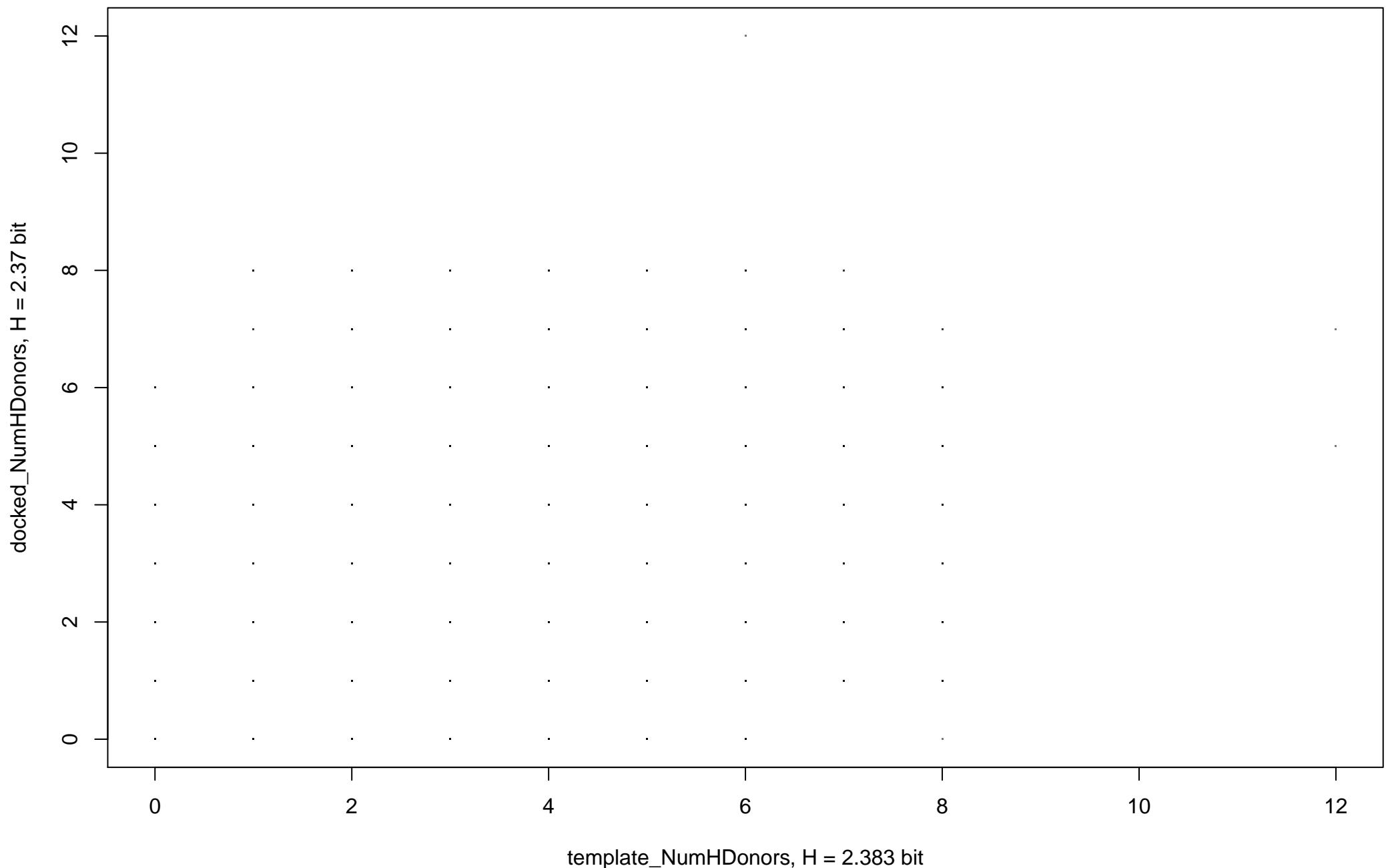
template_HeavyAtomCount-docked_RingCount, MI = 0.1009 bit, normMI = 0.04225



docked_HeavyAtomCount–binrmsd, MI = 0.04805 bit, normMI = 0.04222

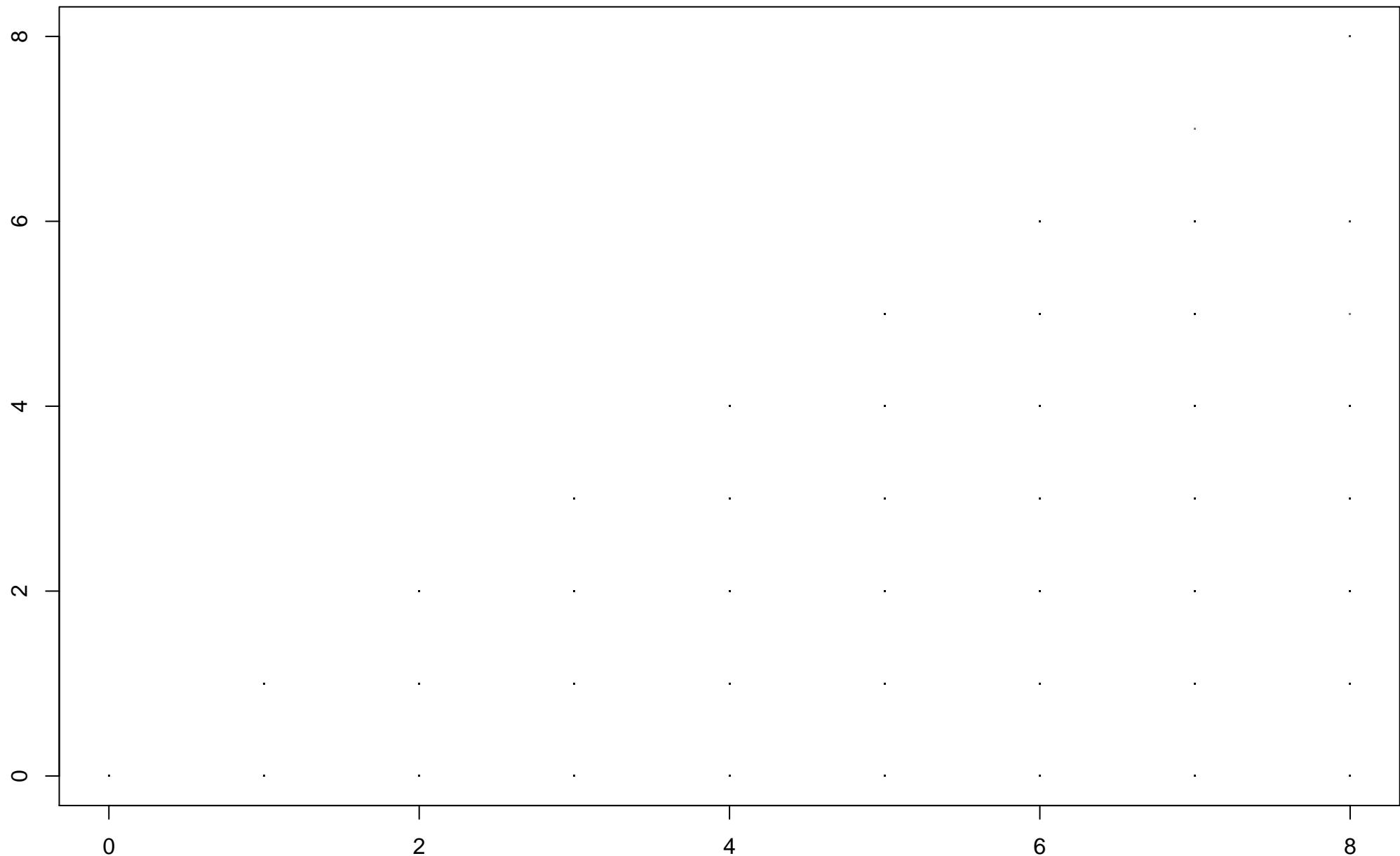


template_NumHDonors-docked_NumHDonors, MI = 0.09998 bit, normMI = 0.04218



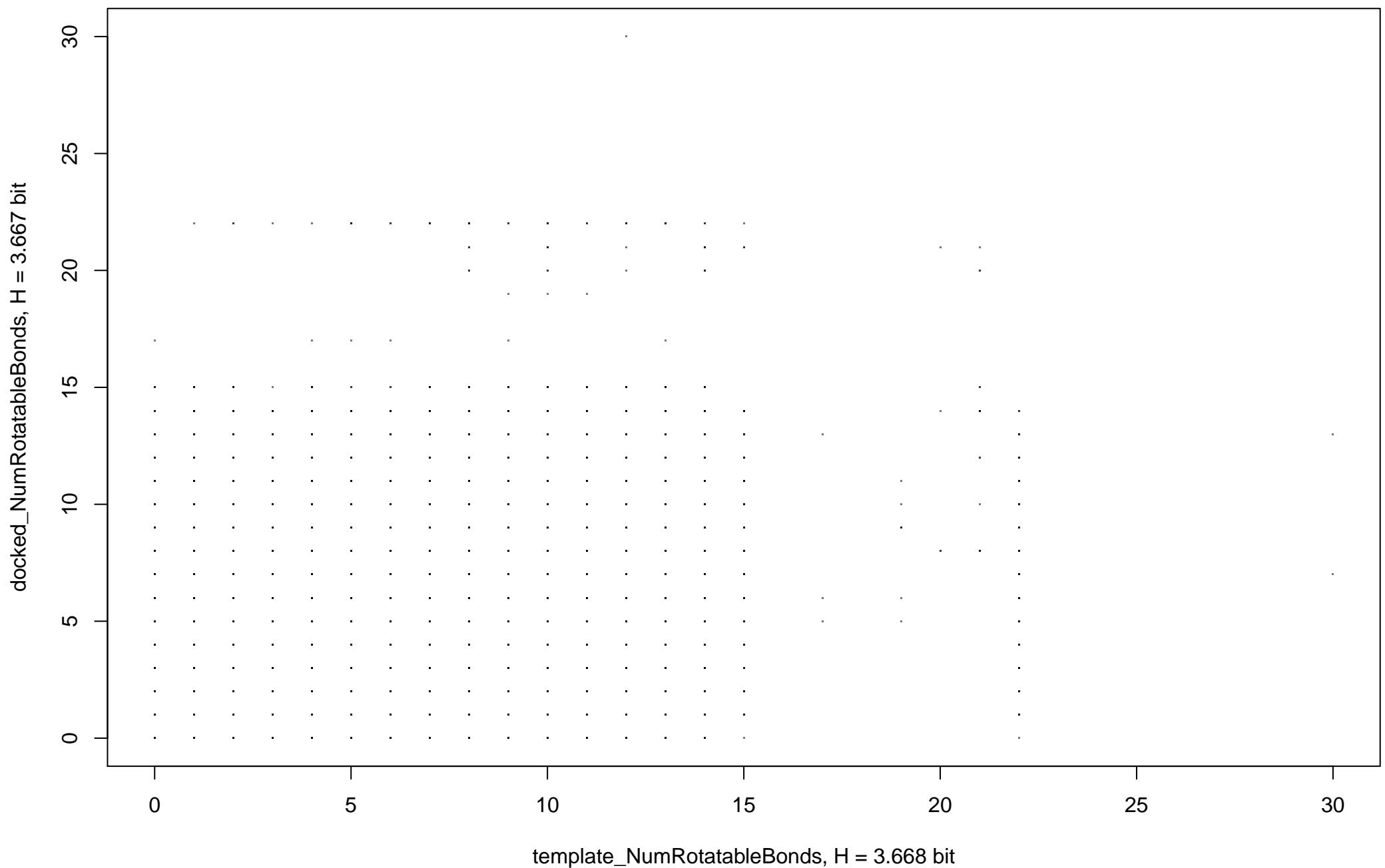
docked_RingCount-mcs_RingCount, MI = 0.07284 bit, normMI = 0.04217

mcs_RingCount, H = 1.727 bit

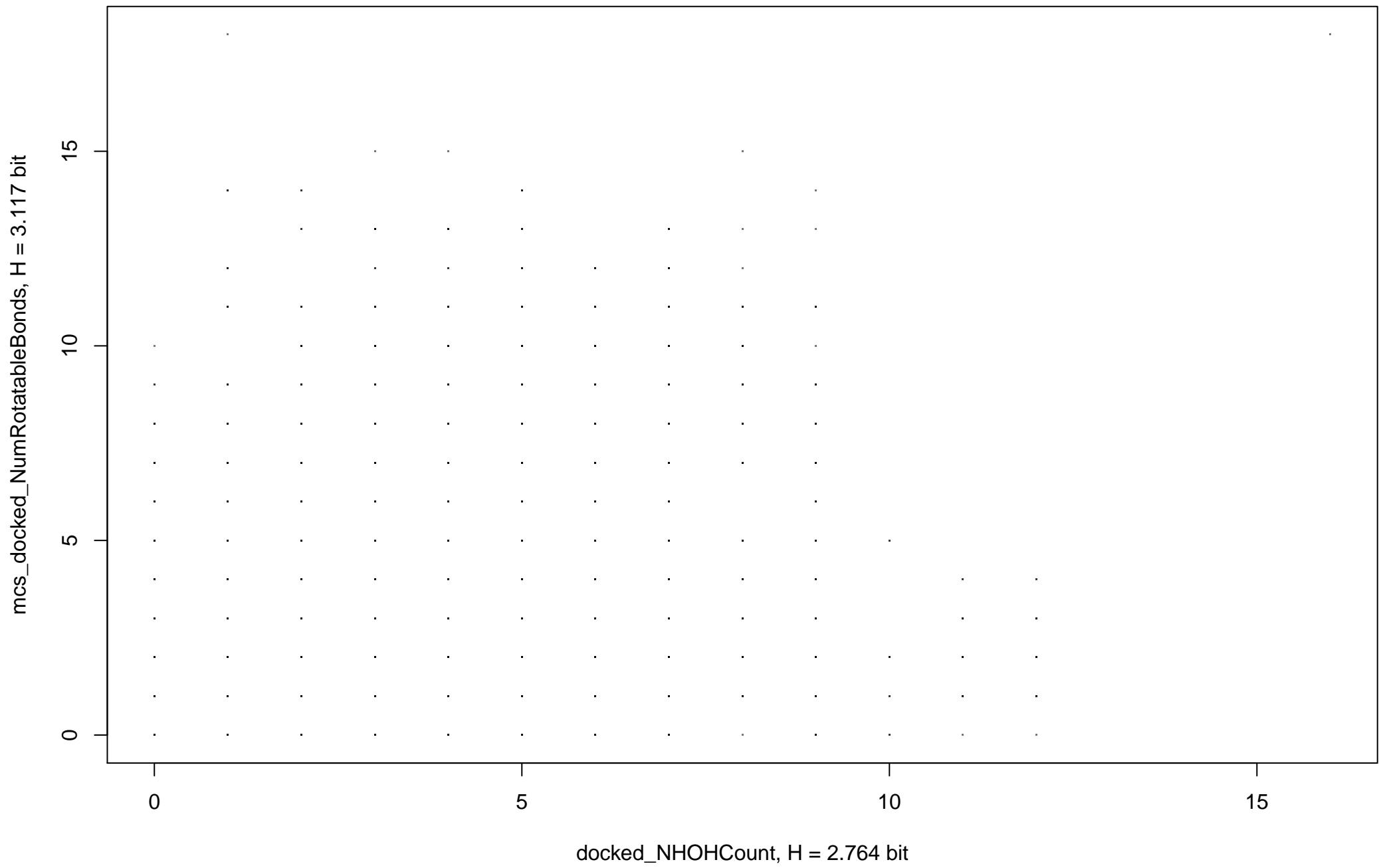


docked_RingCount, H = 2.389 bit

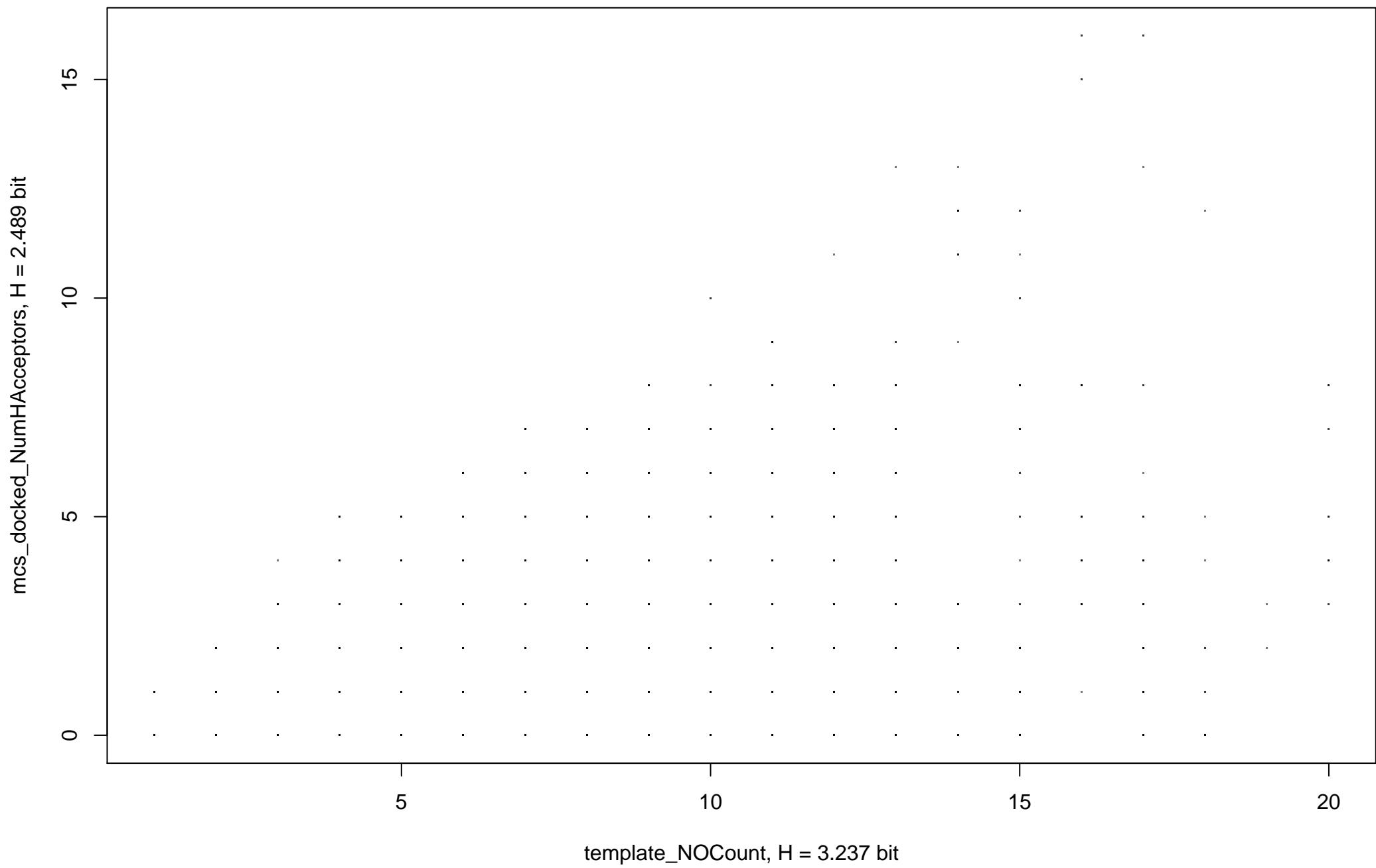
template_NumRotatableBonds-docked_NumRotatableBonds, MI = 0.1544 bit, normMI = 0.04212



docked_NHOHCount-mcs_docked_NumRotatableBonds, MI = 0.1155 bit, normMI = 0.04178

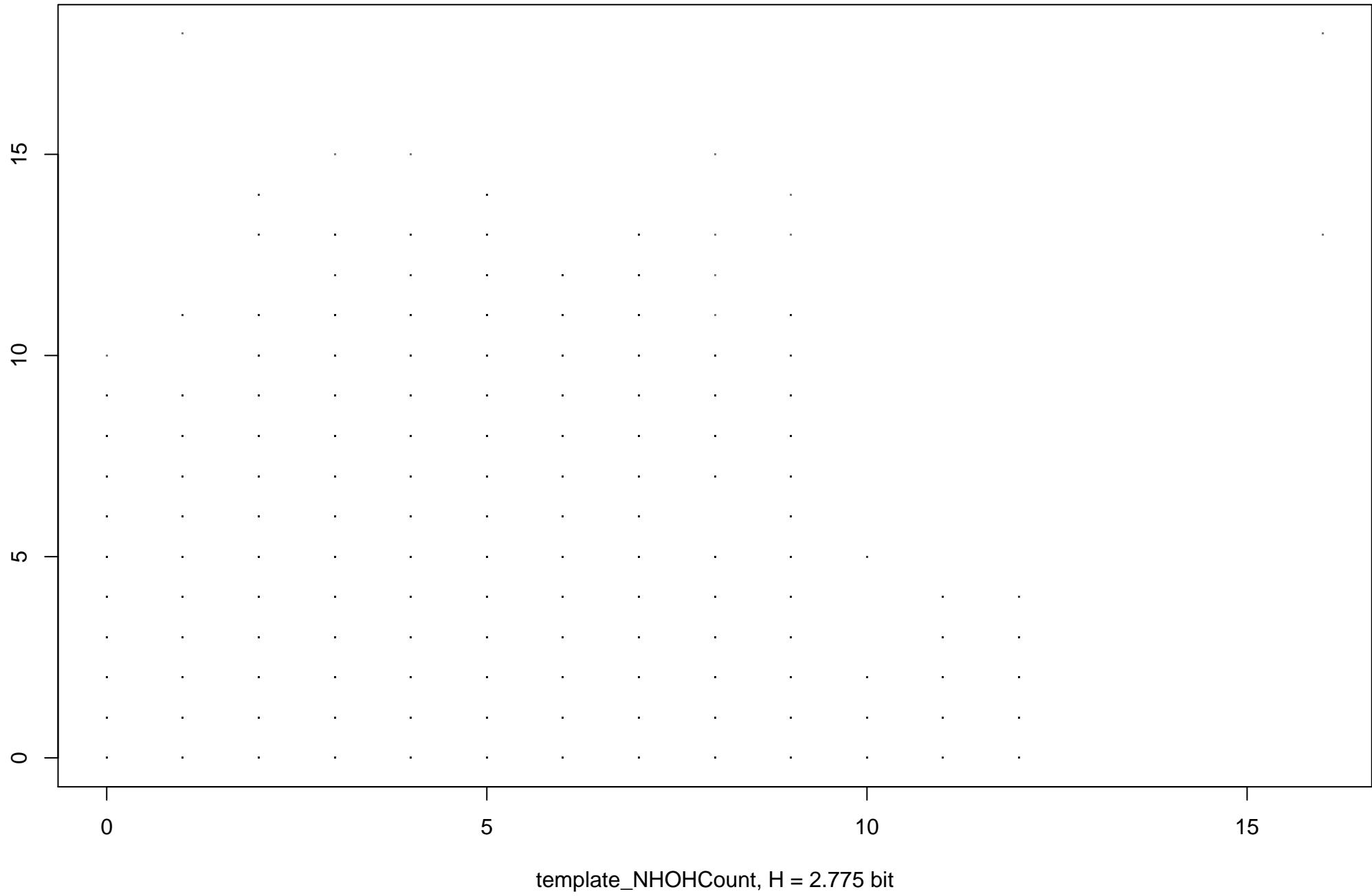


template_NOCount-mcs_docked_NumHAcceptors, MI = 0.1029 bit, normMI = 0.04132

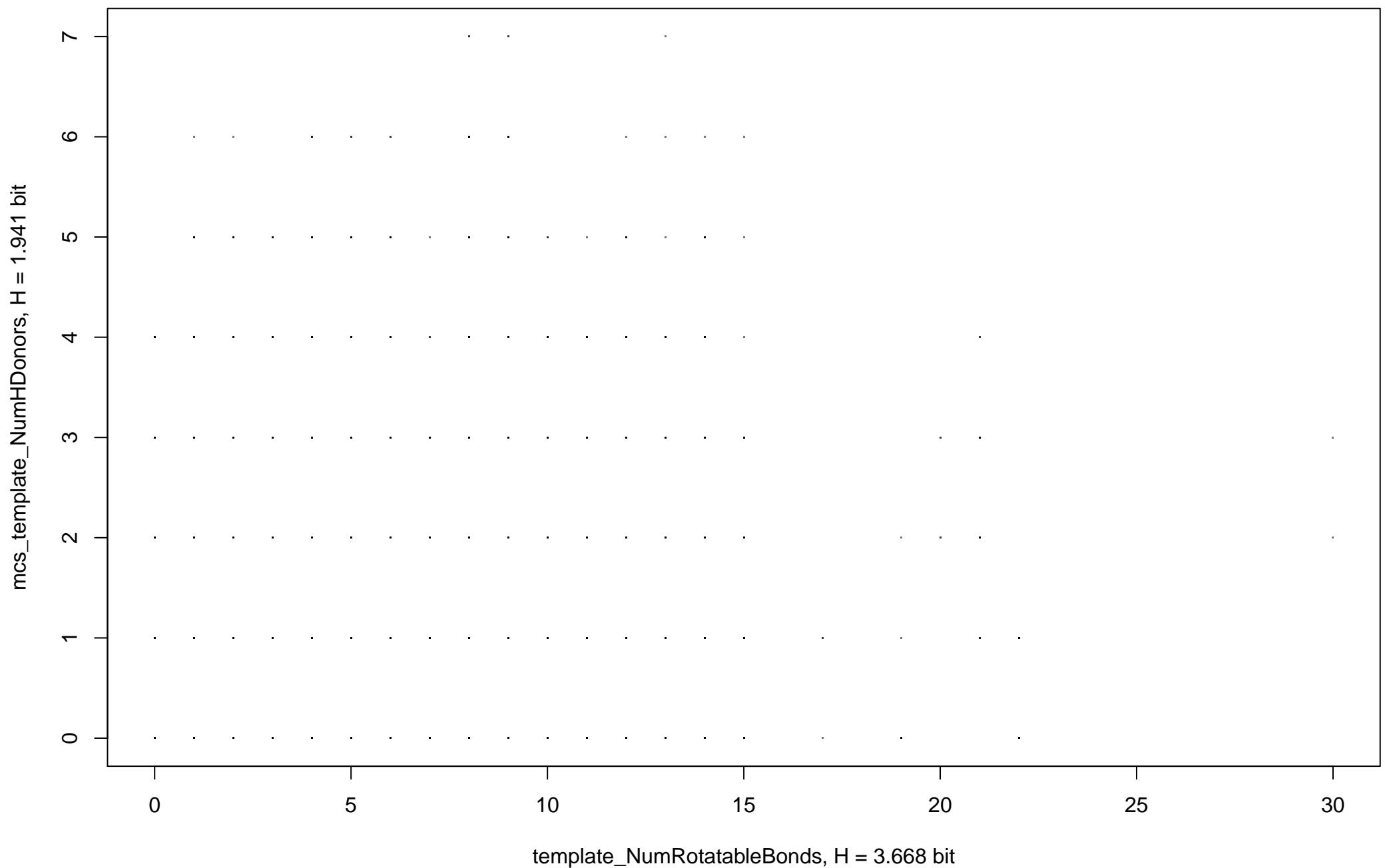


template_NHOHCount–mcs_template_NumRotatableBonds, MI = 0.1138 bit, normMI = 0.04102

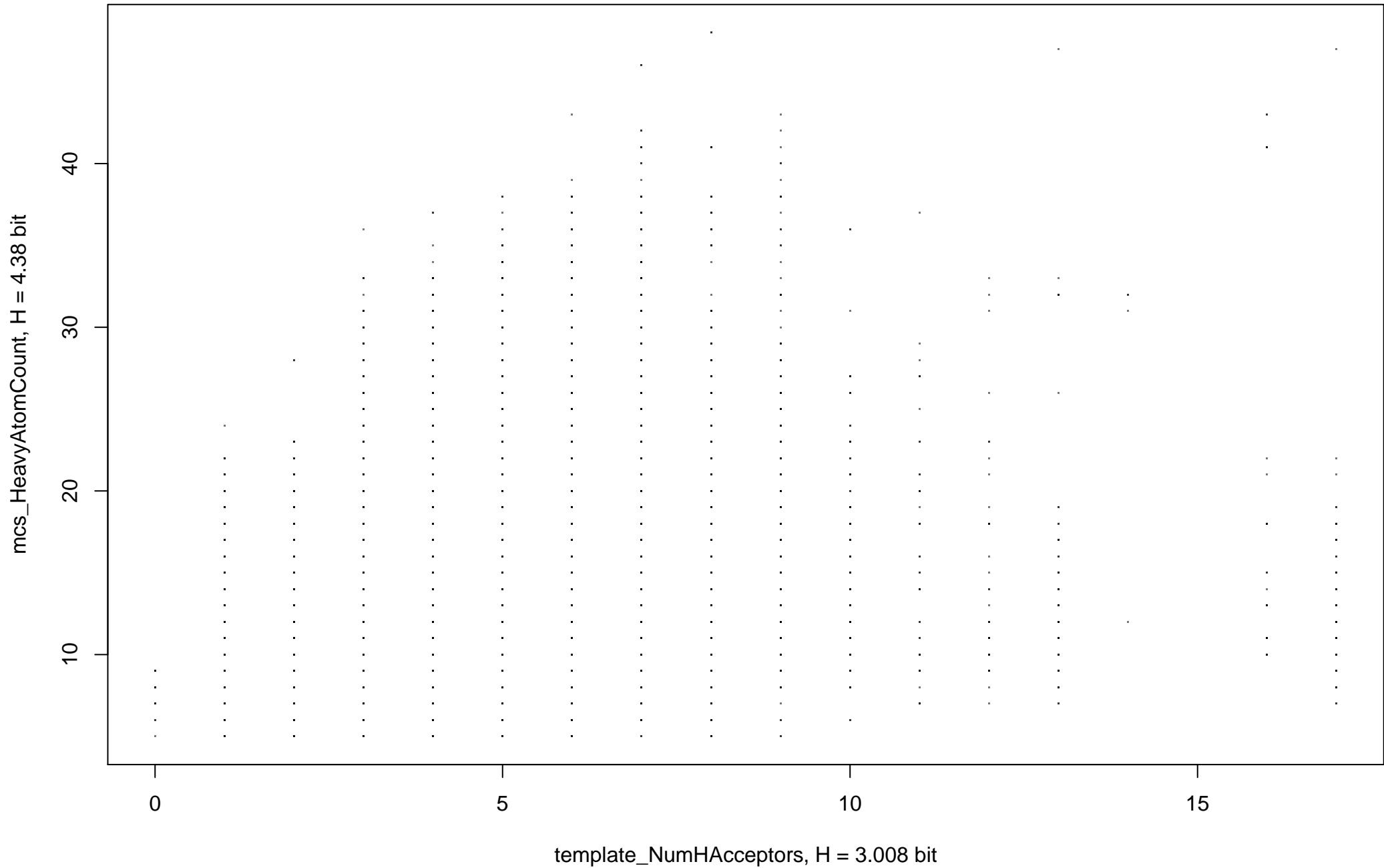
mcs_template_NumRotatableBonds, H = 3.118 bit



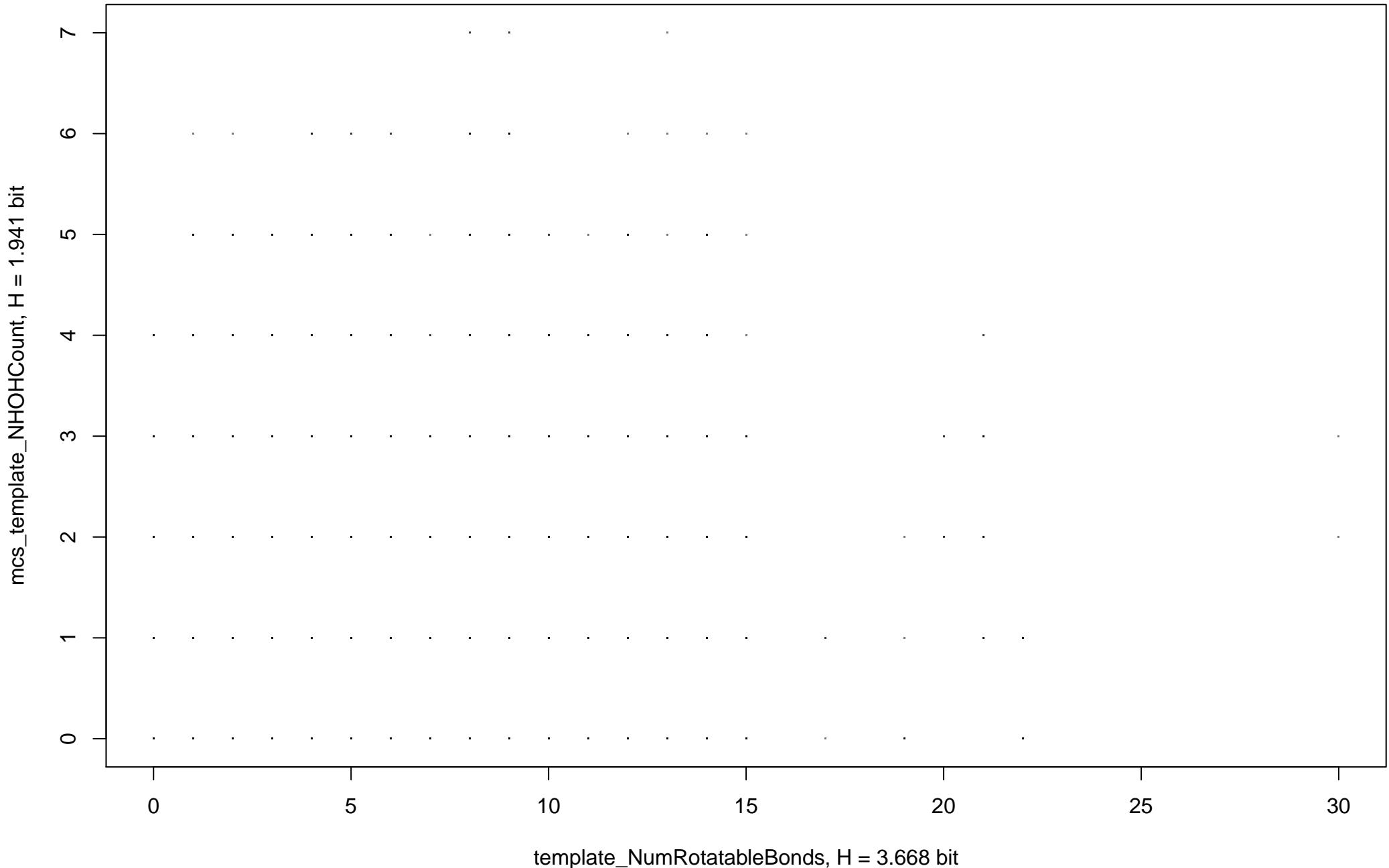
template_NumRotatableBonds-mcs_template_NumHDonors, MI = 0.07951 bit, normMI = 0.04097



template_NumHAcceptors-mcs_HeavyAtomCount, MI = 0.123 bit, normMI = 0.0409

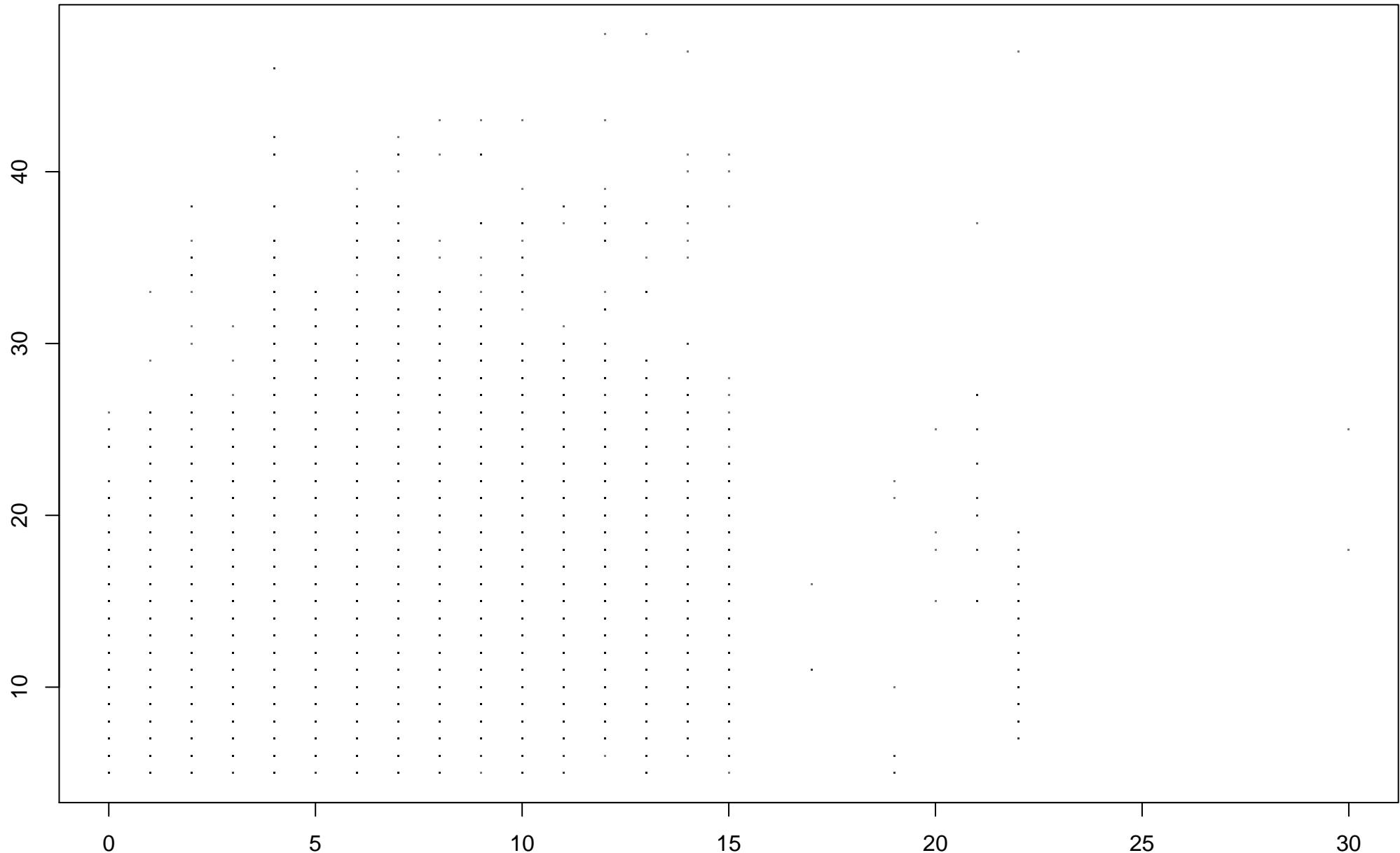


template_NumRotatableBonds–mcs_template_NHOHCount, MI = 0.07926 bit, normMI = 0.04083



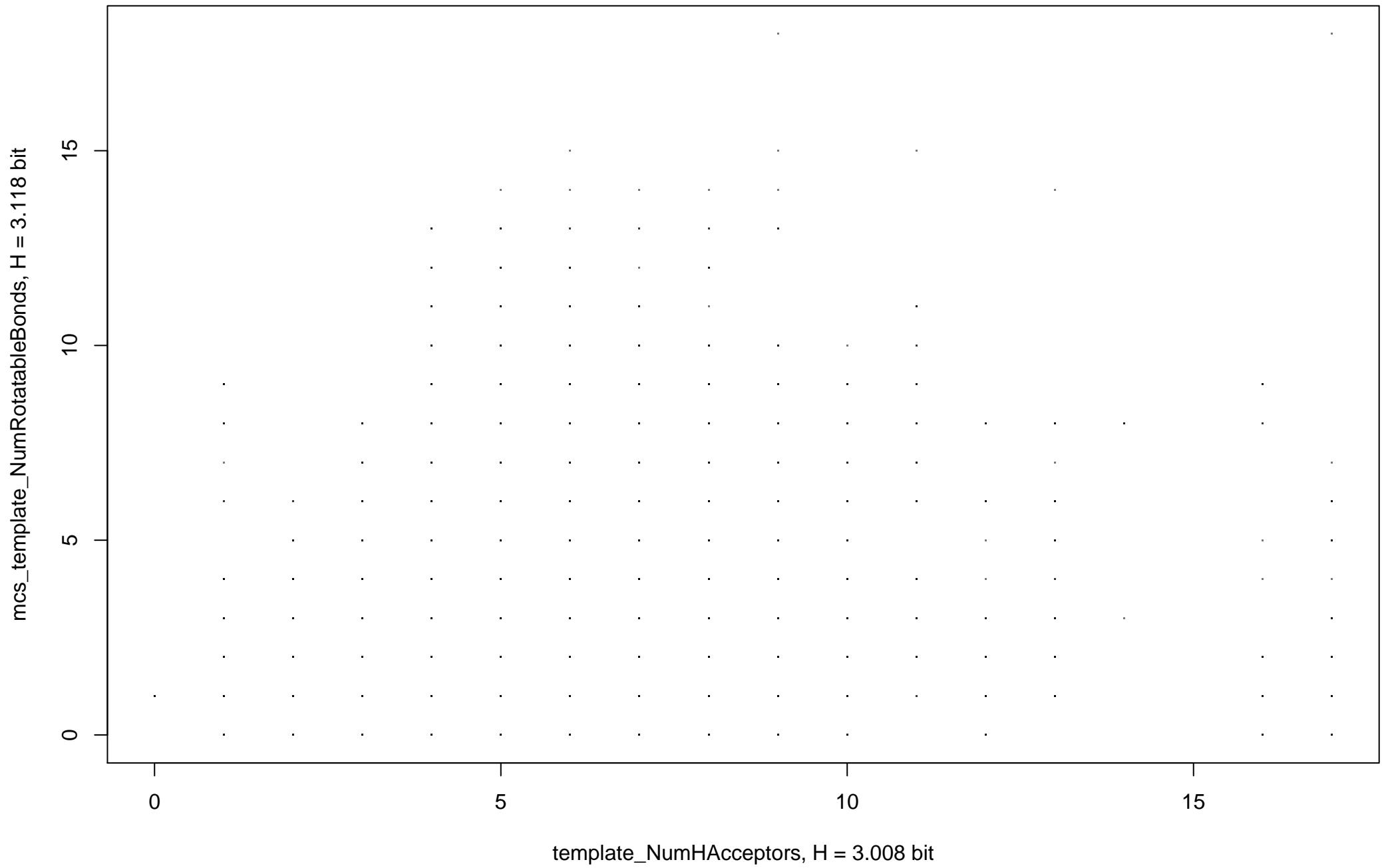
template_NumRotatableBonds-mcs_HeavyAtomCount, MI = 0.1473 bit, normMI = 0.04016

mcs_HeavyAtomCount, H = 4.38 bit

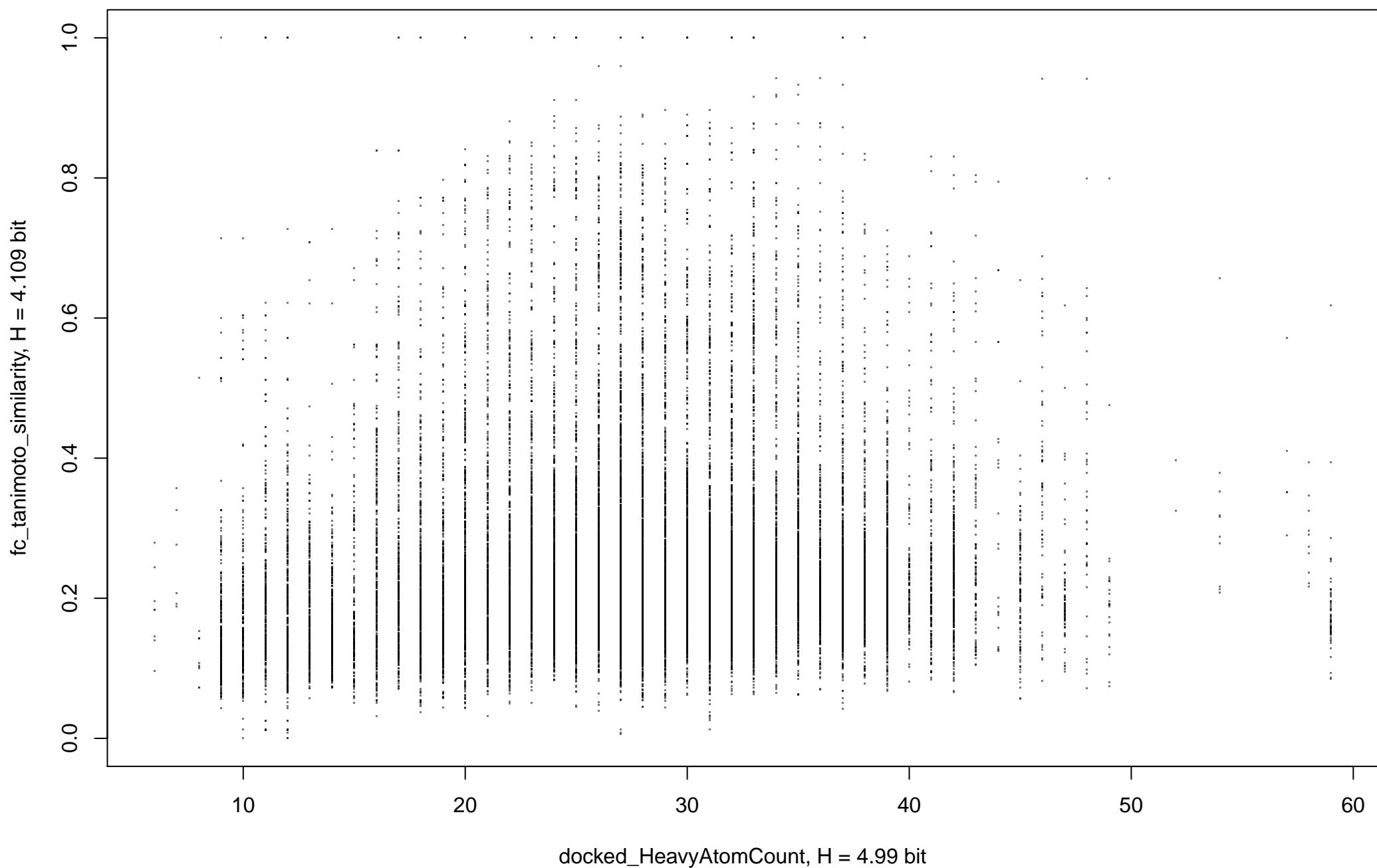


template_NumRotatableBonds, H = 3.668 bit

template_NumHAcceptors-mcs_template_NumRotatableBonds, MI = 0.1208 bit, normMI = 0.04015

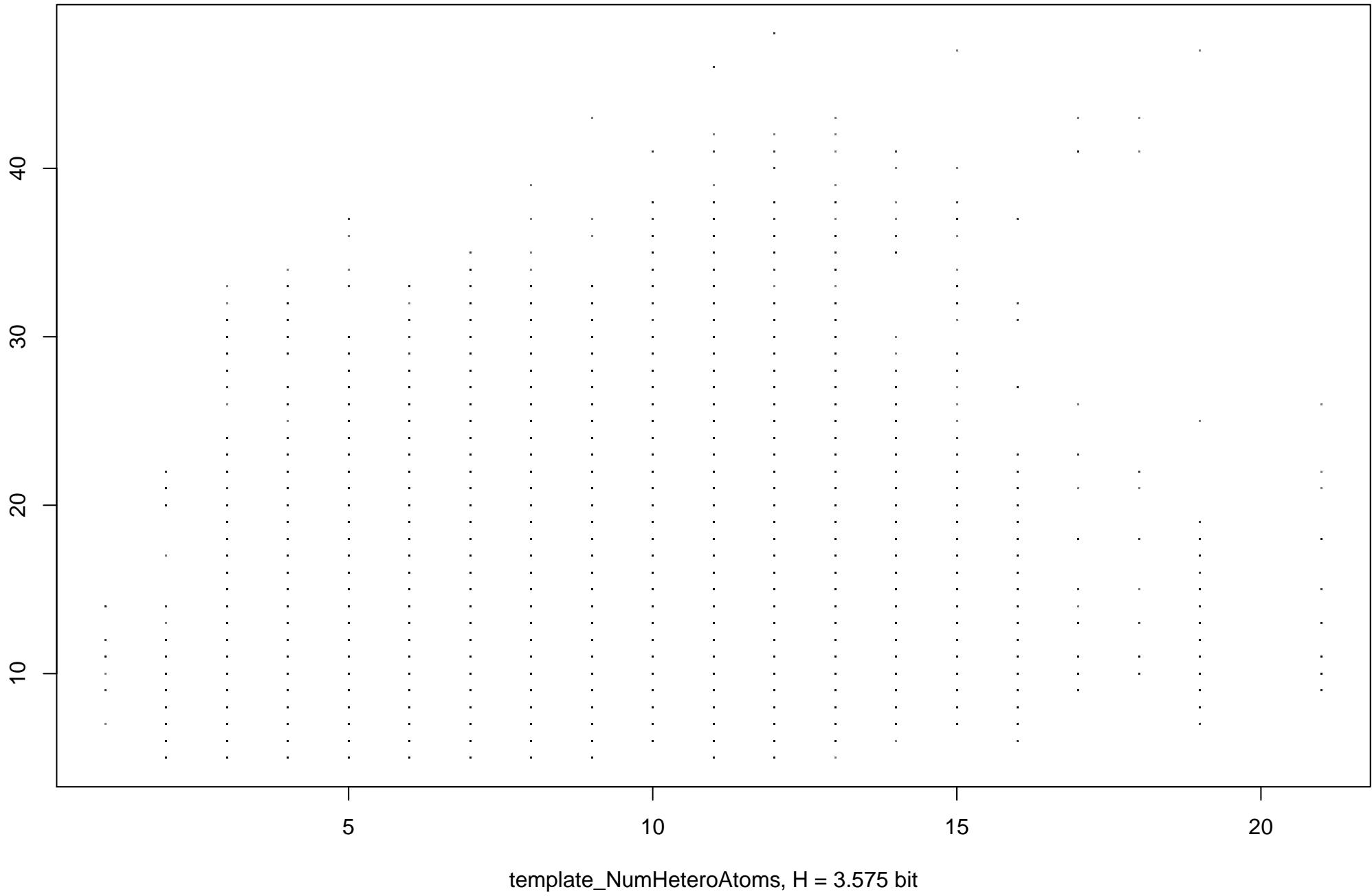


docked_HeavyAtomCount-fc_tanimoto_similarity, MI = 0.1619 bit, normMI = 0.03941



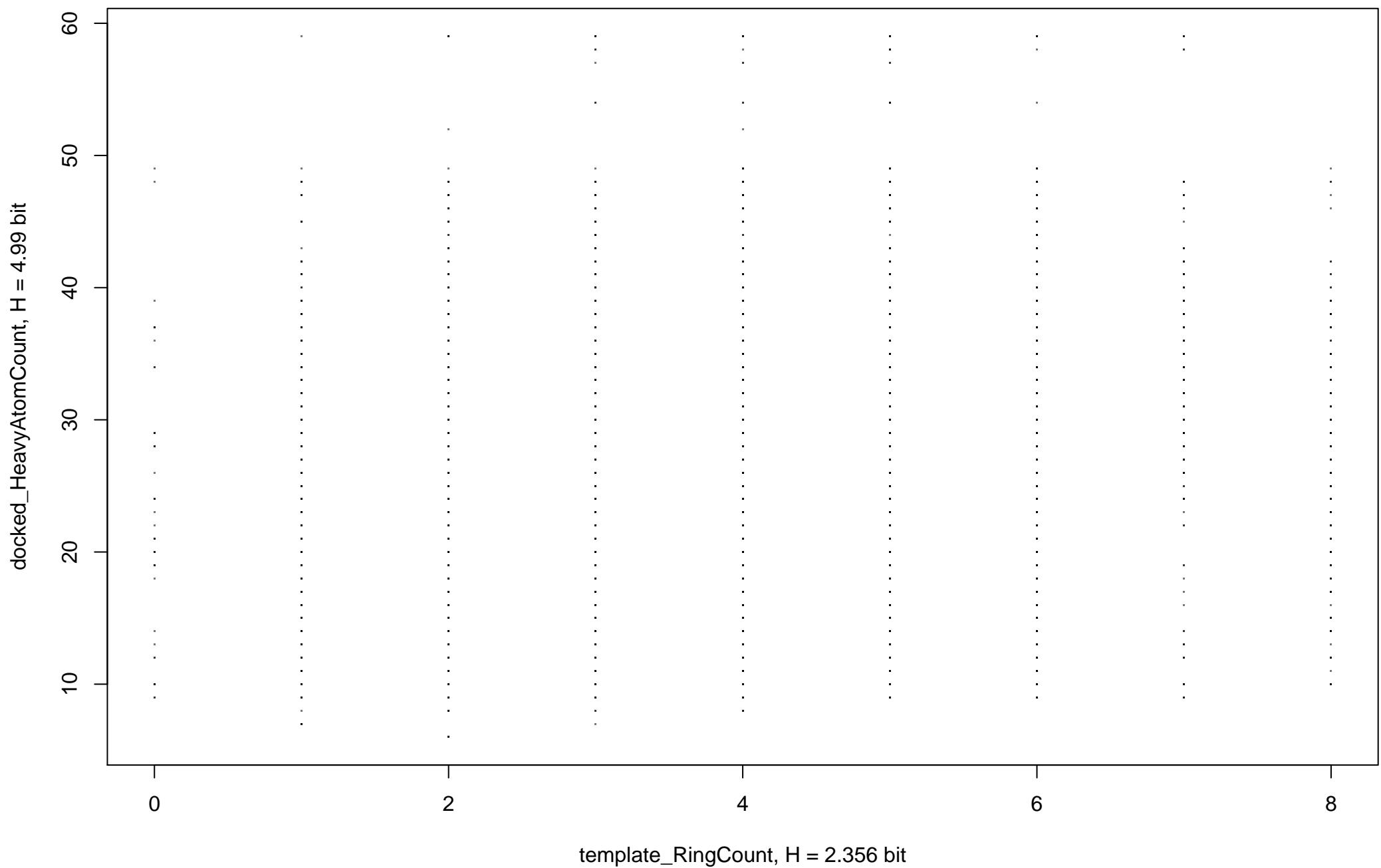
template_NumHeteroAtoms-mcs_HeavyAtomCount, MI = 0.1383 bit, normMI = 0.0387

mcs_HeavyAtomCount, H = 4.38 bit

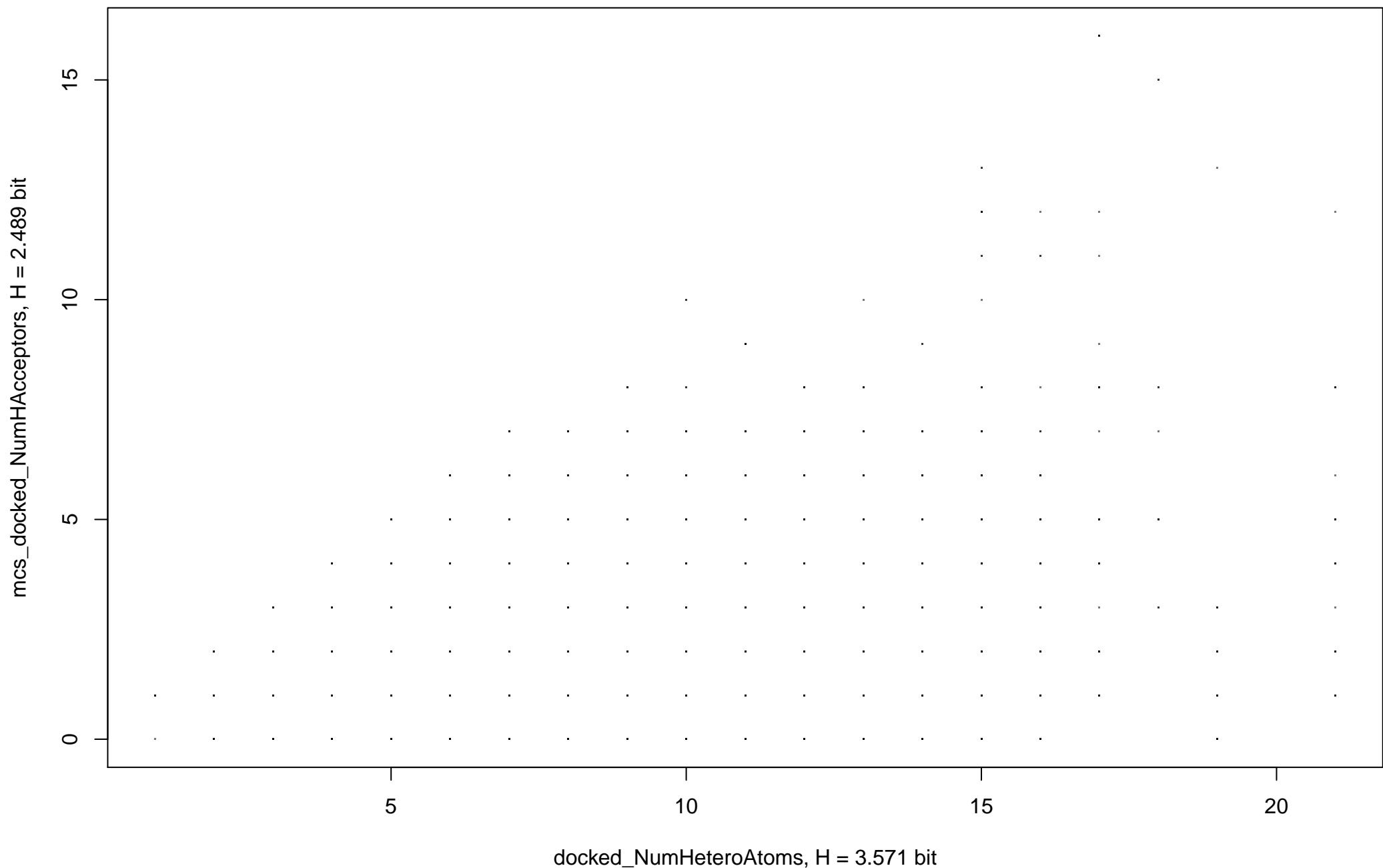


template_NumHeteroAtoms, H = 3.575 bit

template_RingCount-docked_HeavyAtomCount, MI = 0.09047 bit, normMI = 0.0384

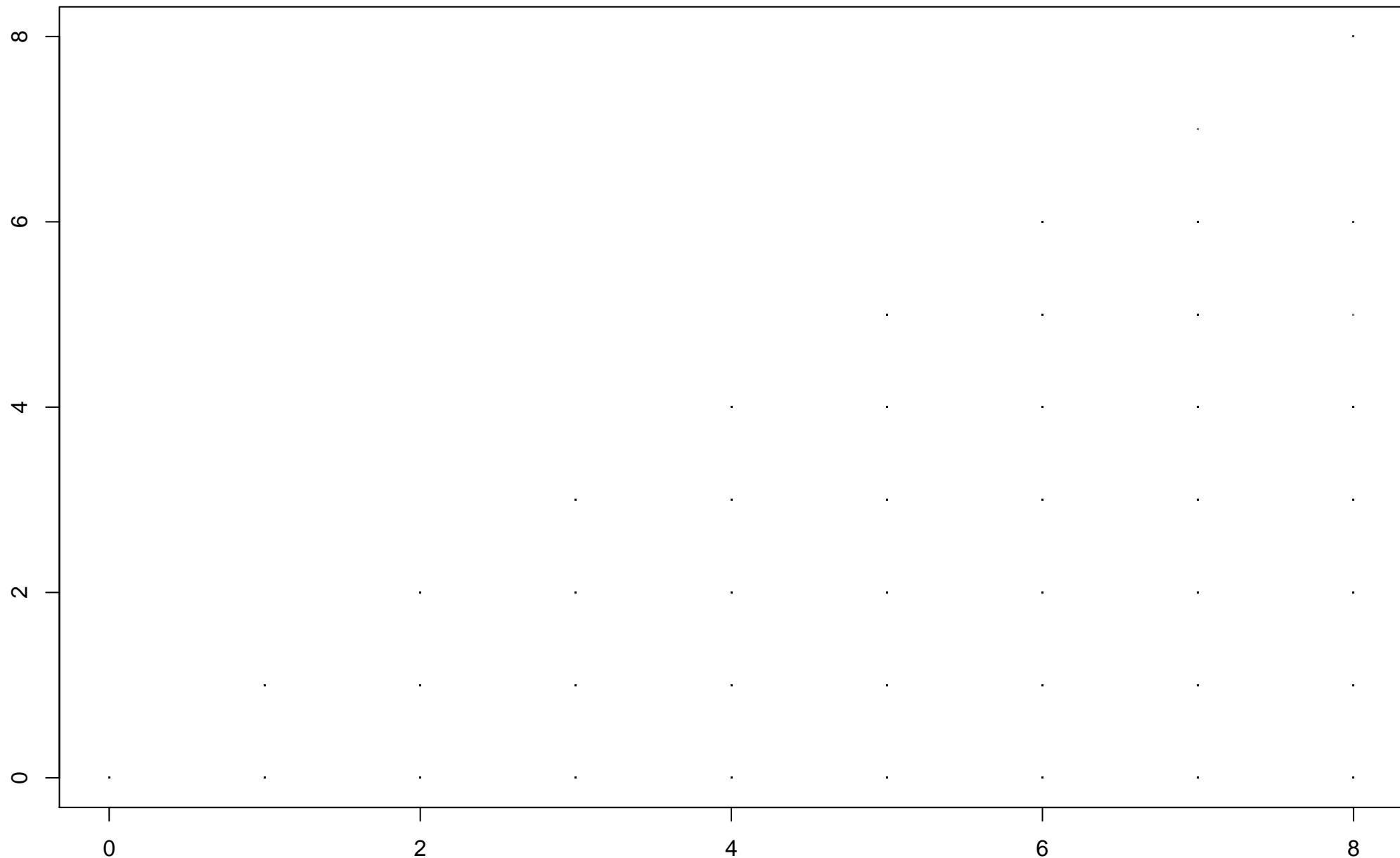


docked_NumHeteroAtoms-mcs_docked_NumHAcceptors, MI = 0.09304 bit, normMI = 0.03738



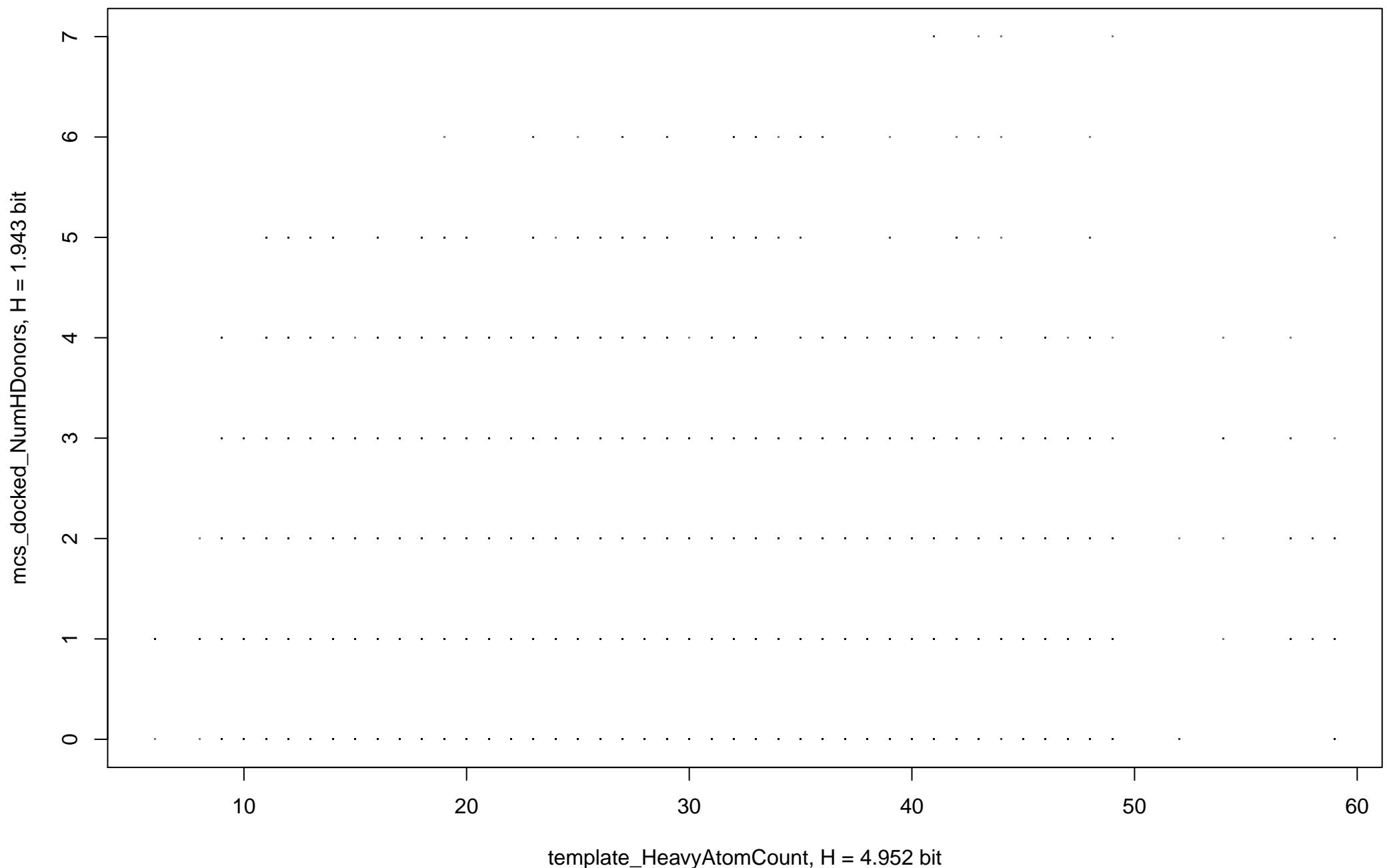
template_RingCount-mcs_RingCount, MI = 0.06404 bit, normMI = 0.03707

mcs_RingCount, H = 1.727 bit



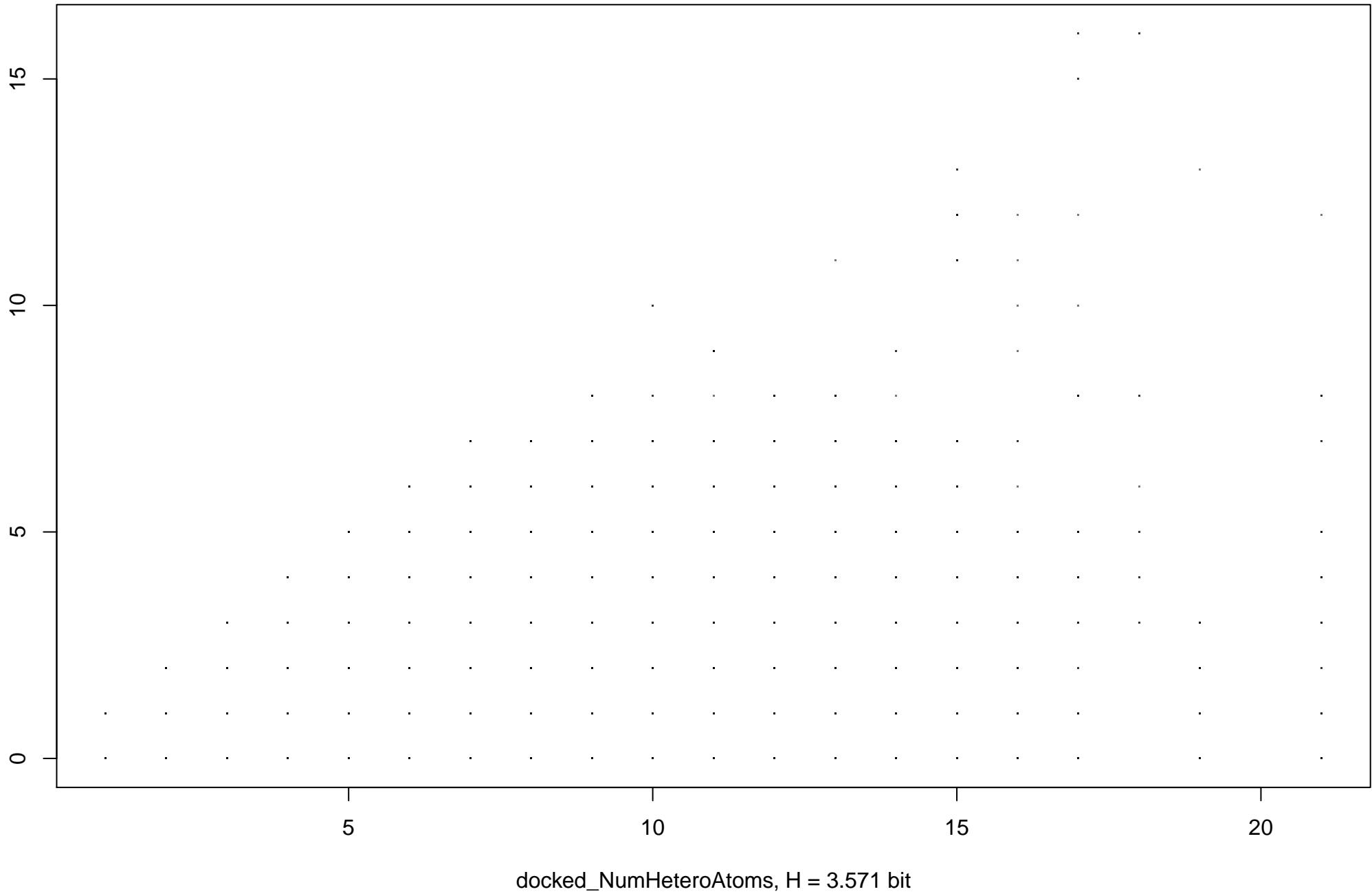
template_RingCount, H = 2.356 bit

template_HeavyAtomCount-mcs_docked_NumHDonors, MI = 0.07182 bit, normMI = 0.03696



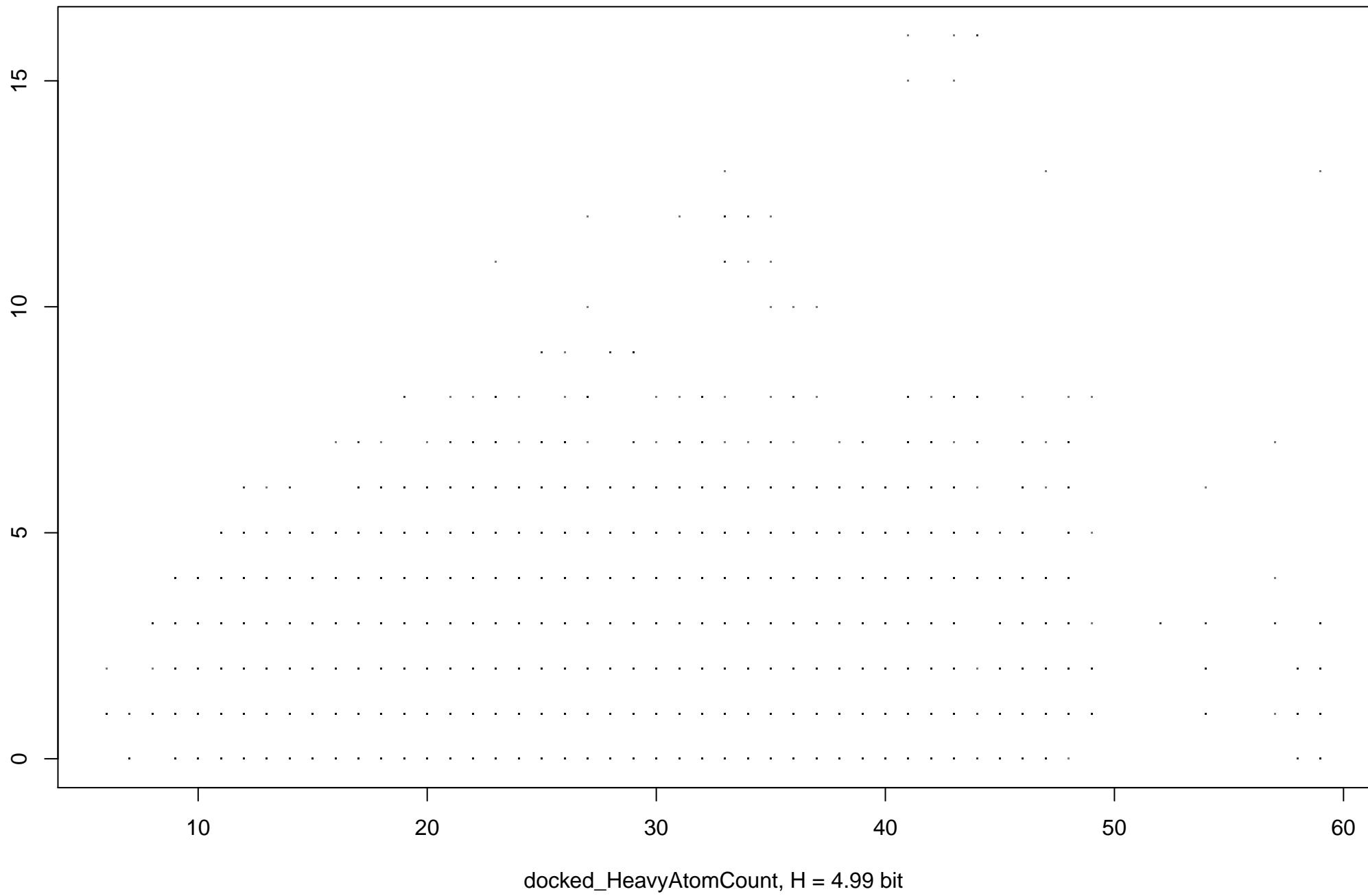
docked_NumHeteroAtoms-mcs_template_NumHAcceptors, MI = 0.09192 bit, normMI = 0.03694

mcs_template_NumHAcceptors, H = 2.488 bit

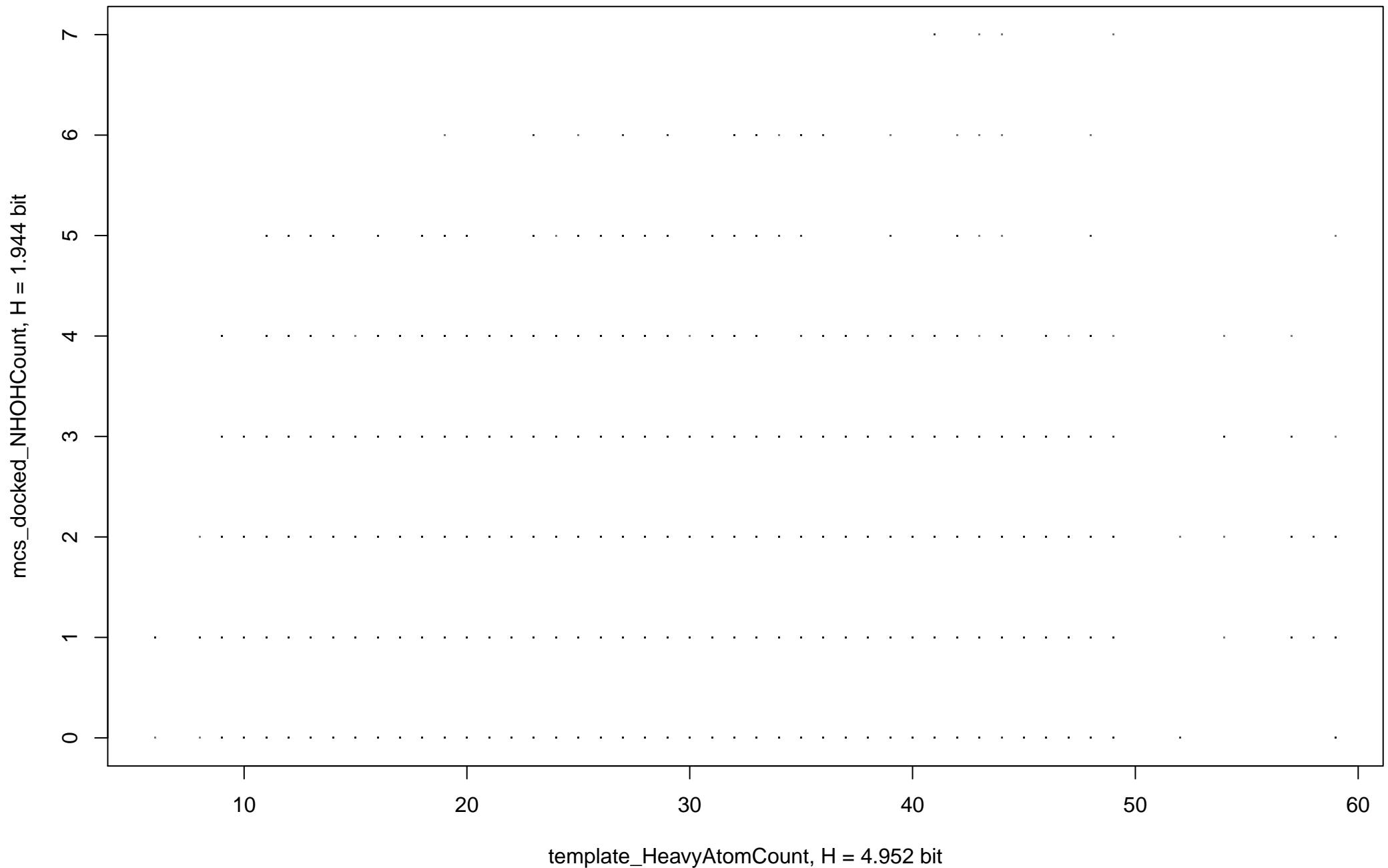


docked_HeavyAtomCount-mcs_template_NumHAcceptors, MI = 0.09187 bit, normMI = 0.03692

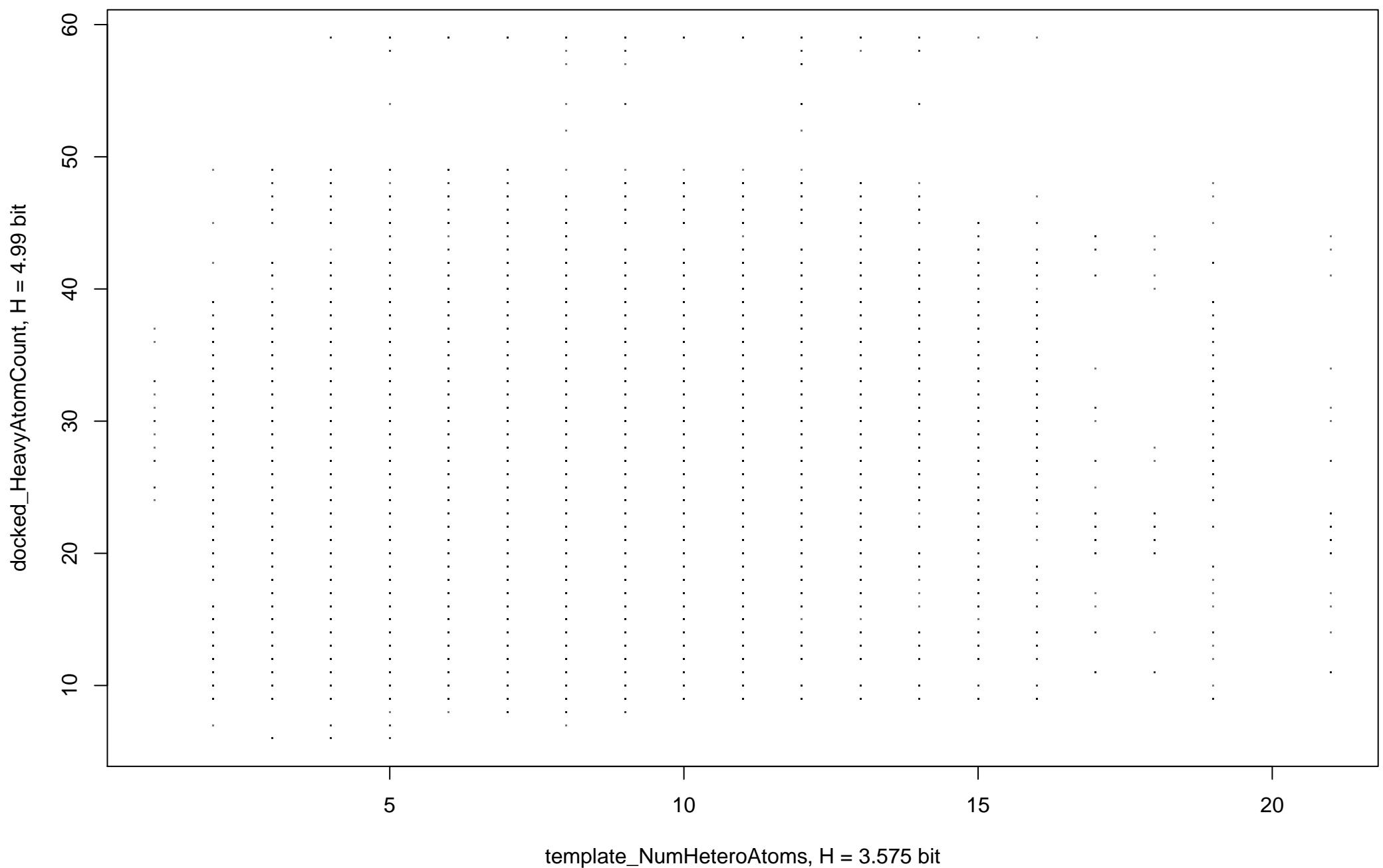
mcs_template_NumHAcceptors, H = 2.488 bit



template_HeavyAtomCount-mcs_docked_NHOHCount, MI = 0.0716 bit, normMI = 0.03683

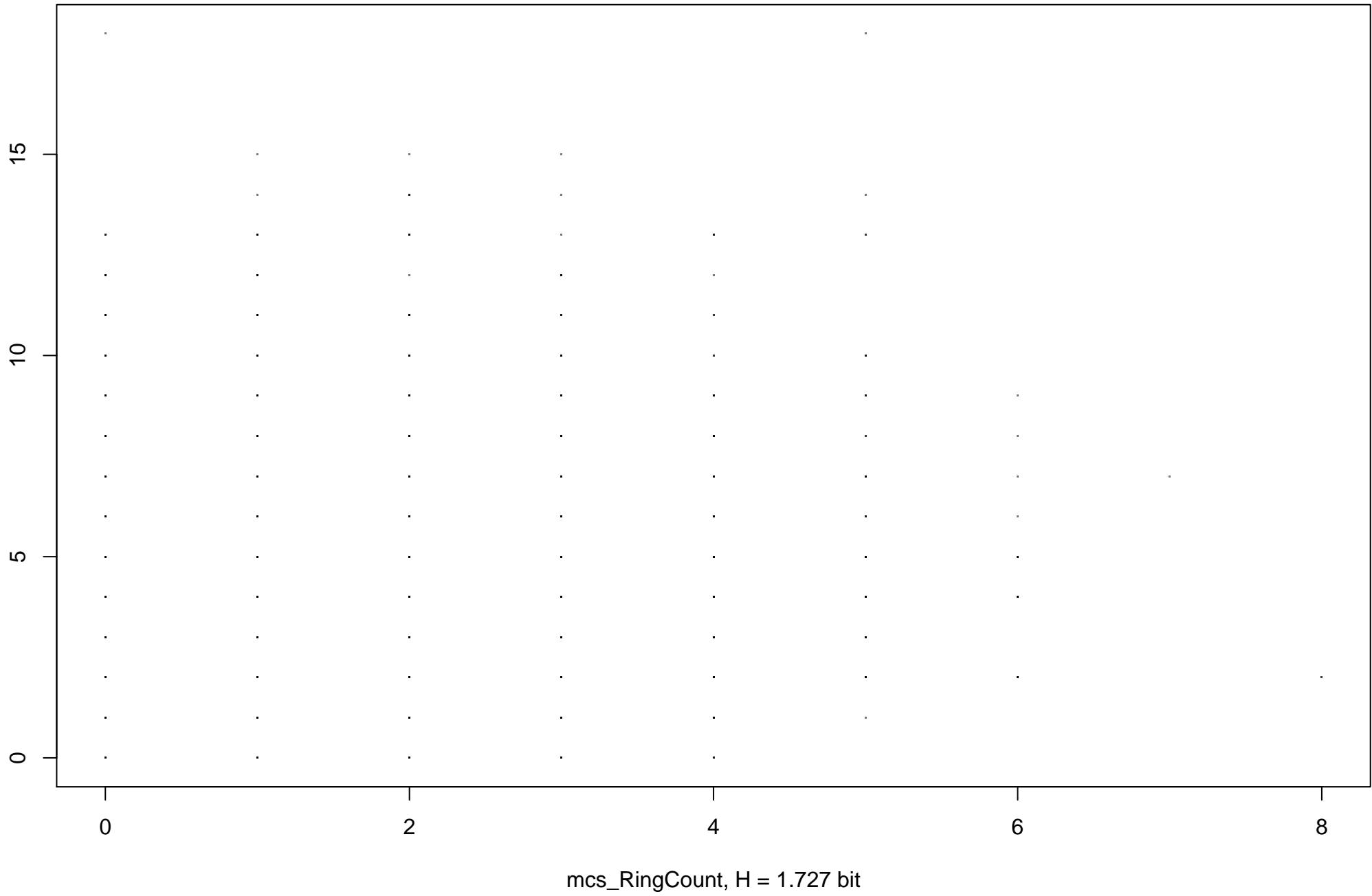


template_NumHeteroAtoms-docked_HeavyAtomCount, MI = 0.1314 bit, normMI = 0.03676

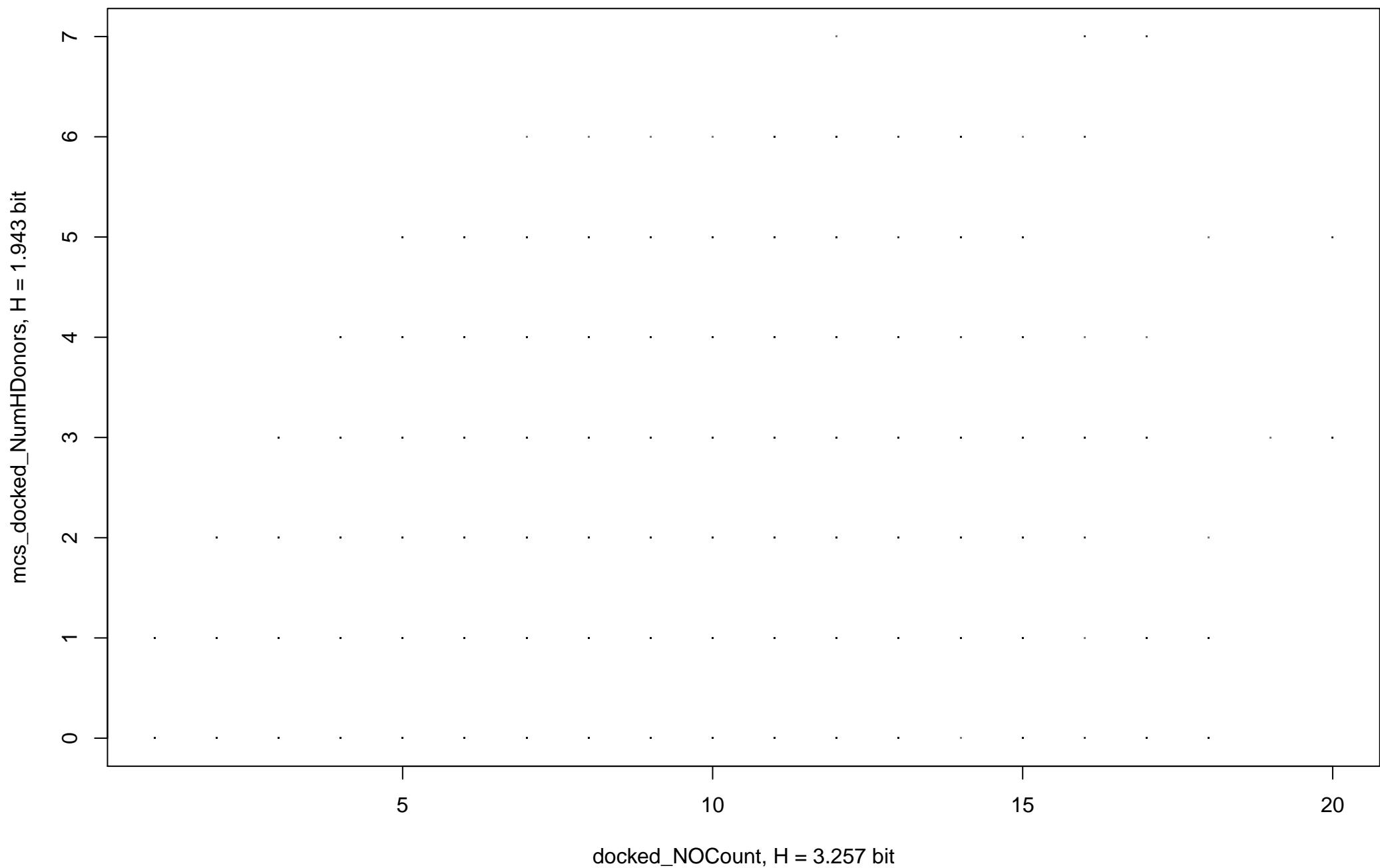


mcs_RingCount-mcs_template_NumRotatableBonds, MI = 0.0619 bit, normMI = 0.03583

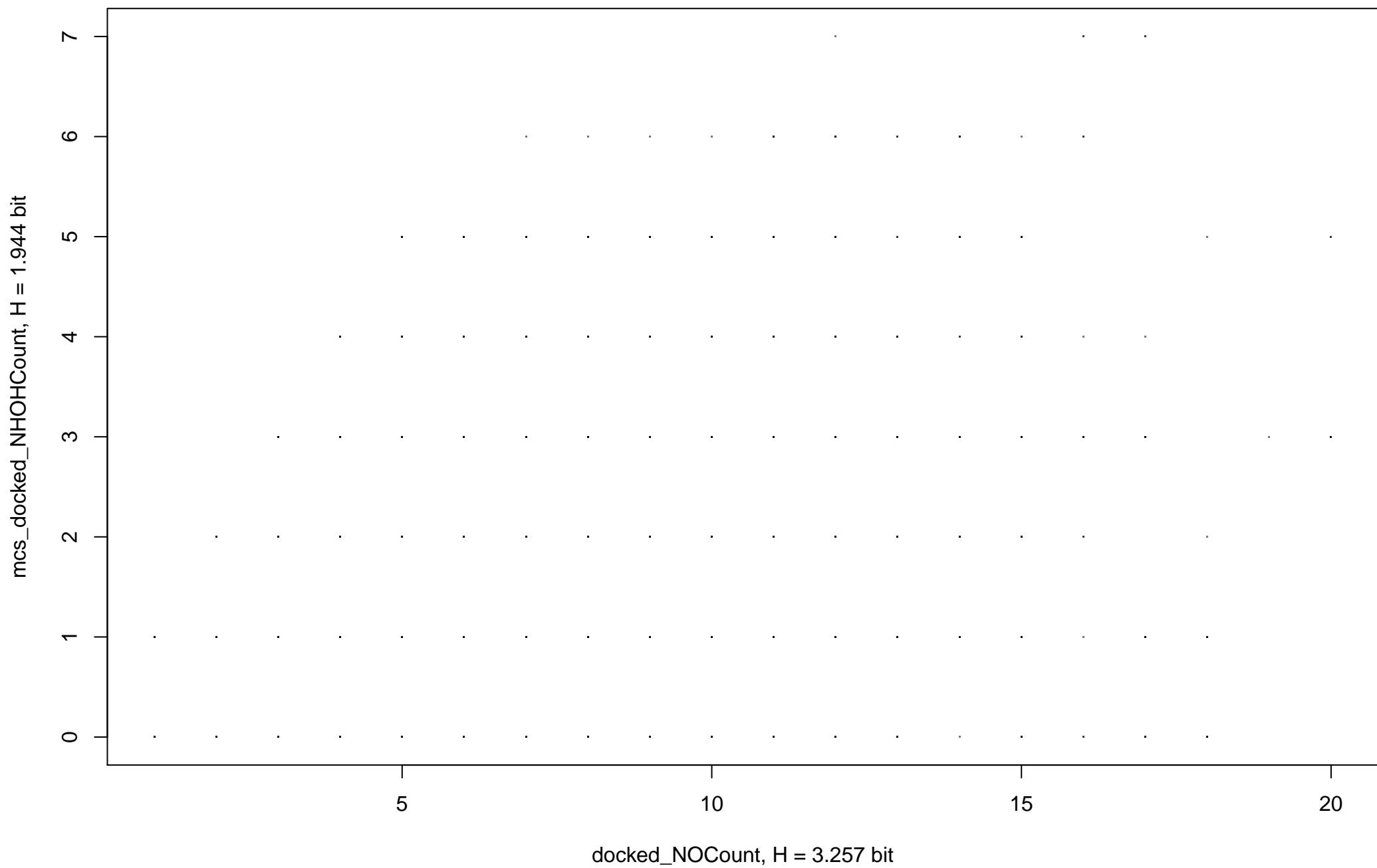
mcs_template_NumRotatableBonds, H = 3.118 bit



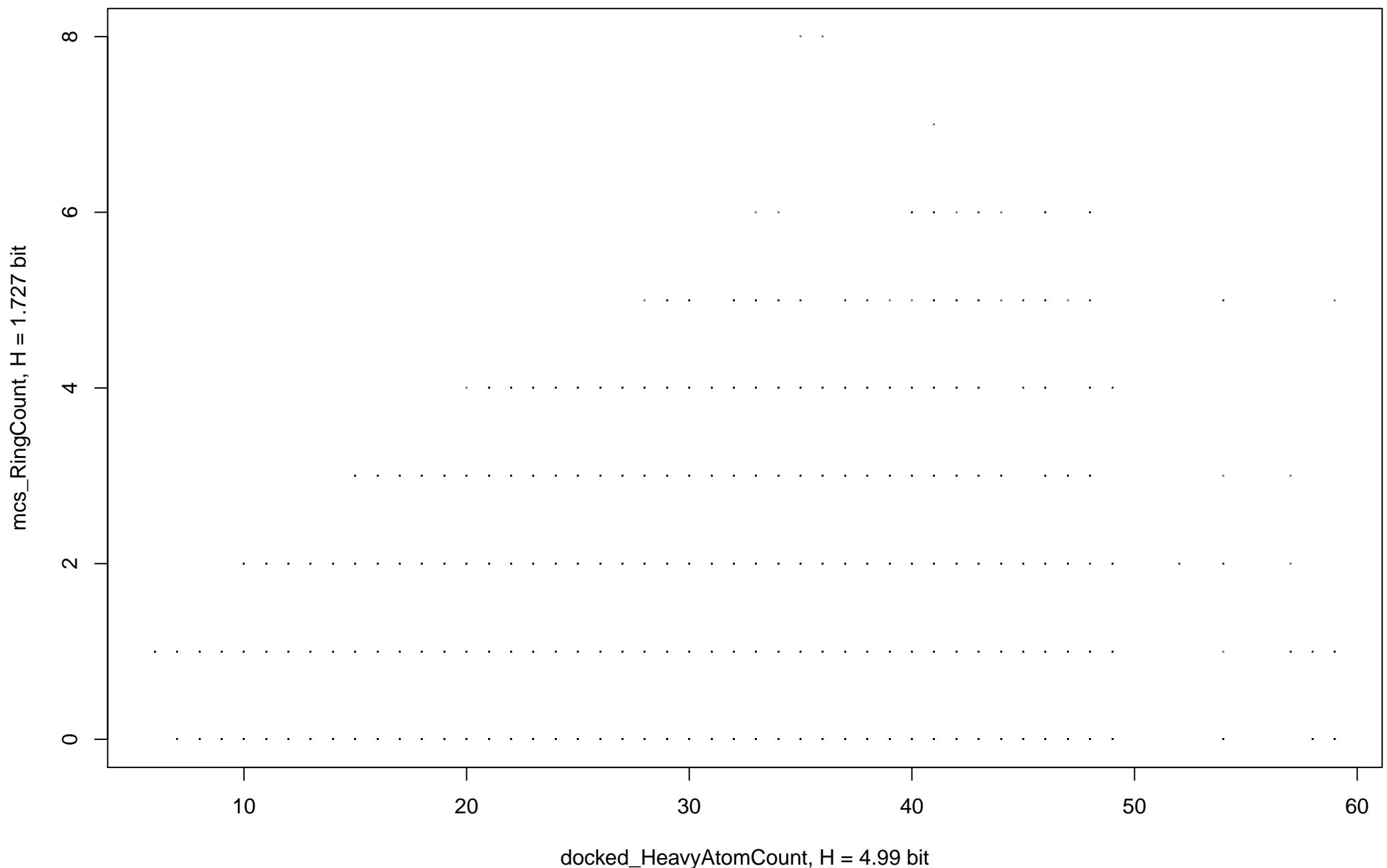
docked_NOCount-mcs_docked_NumHDonors, MI = 0.06934 bit, normMI = 0.03568



docked_NOCount-mcs_docked_NHOHCount, MI = 0.06925 bit, normMI = 0.03562

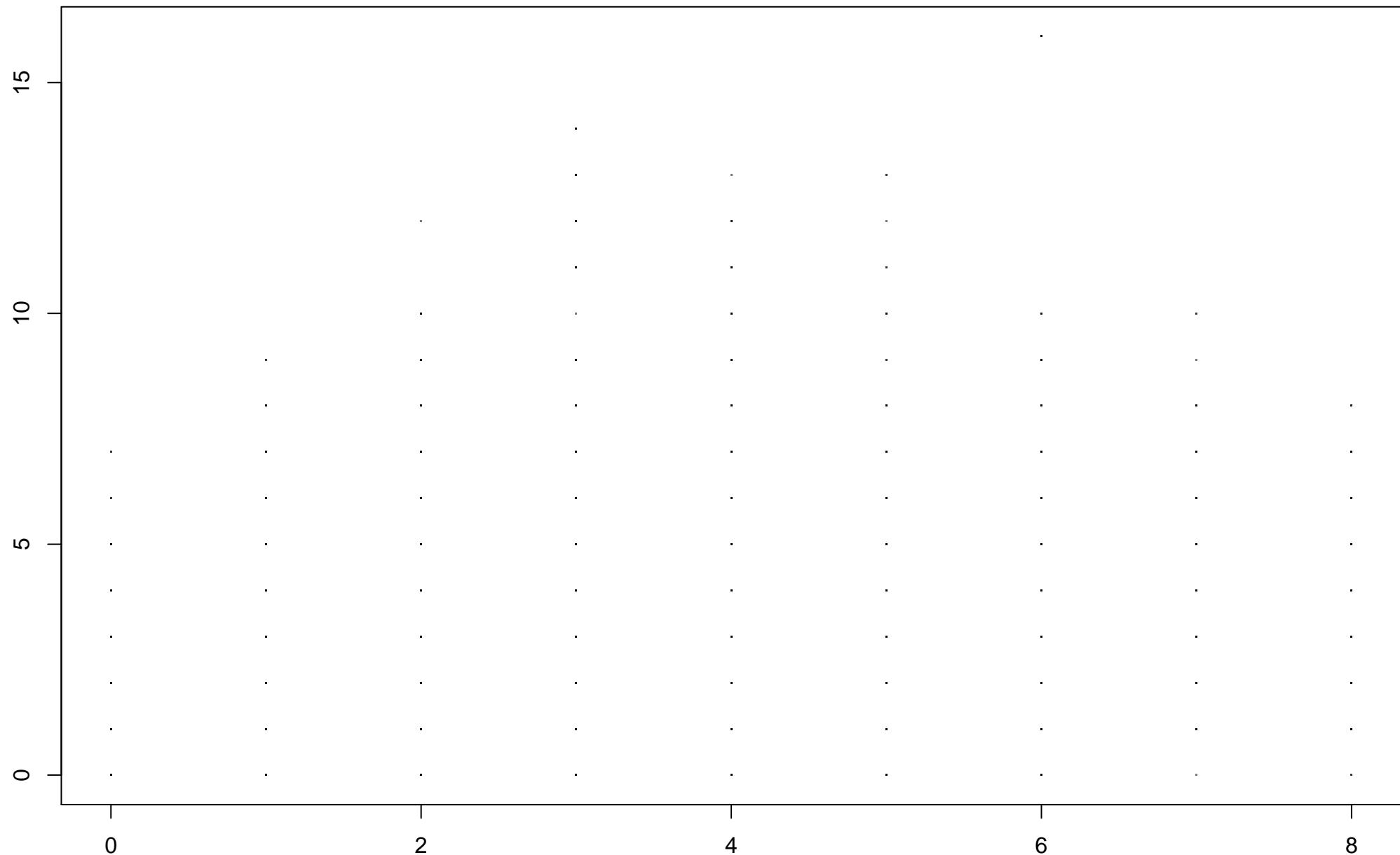


docked_HeavyAtomCount–mcs_RingCount, MI = 0.06143 bit, normMI = 0.03556



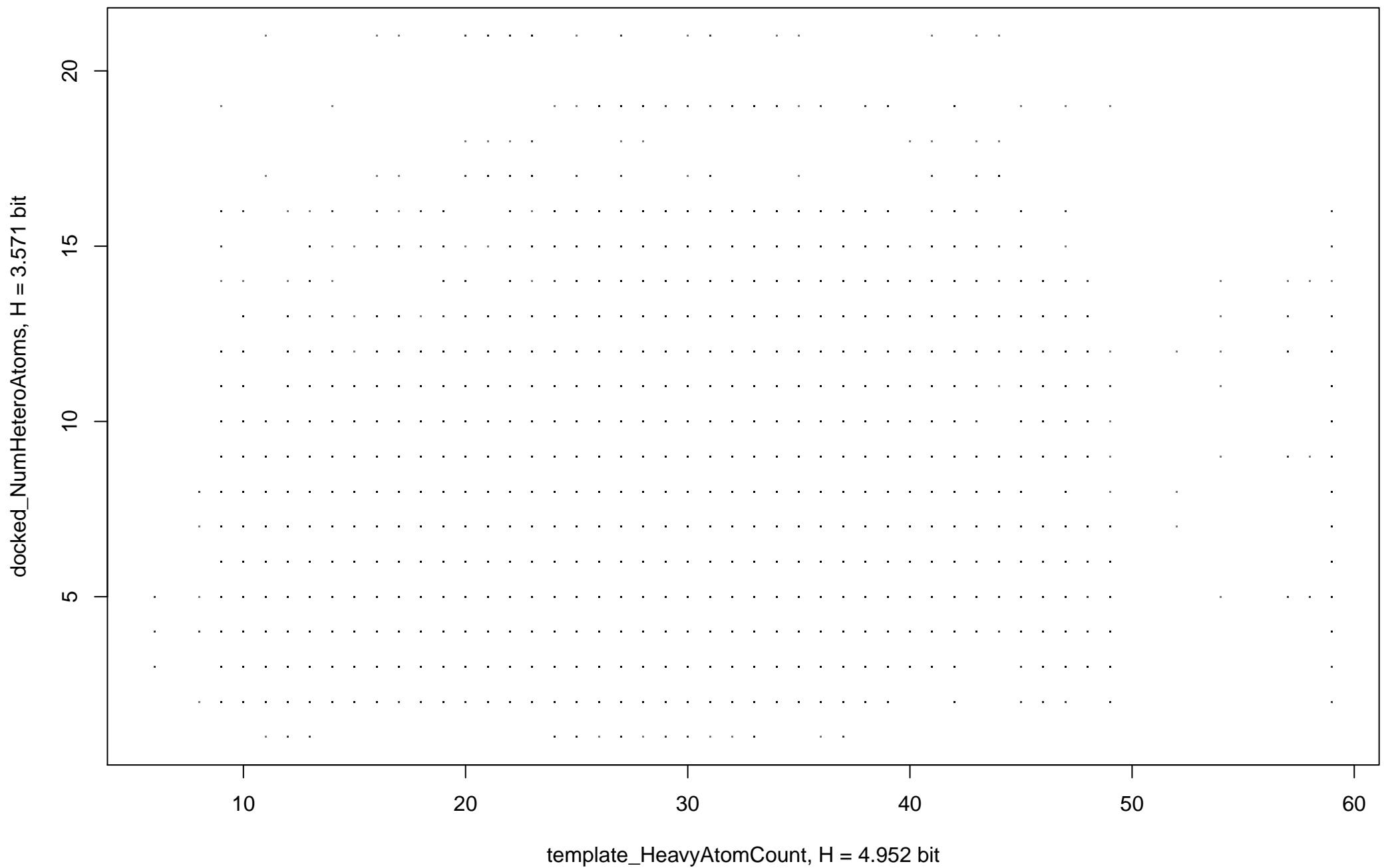
docked_RingCount-mcs_NOCount, MI = 0.08495 bit, normMI = 0.03556

mcs_NOCount, H = 2.777 bit

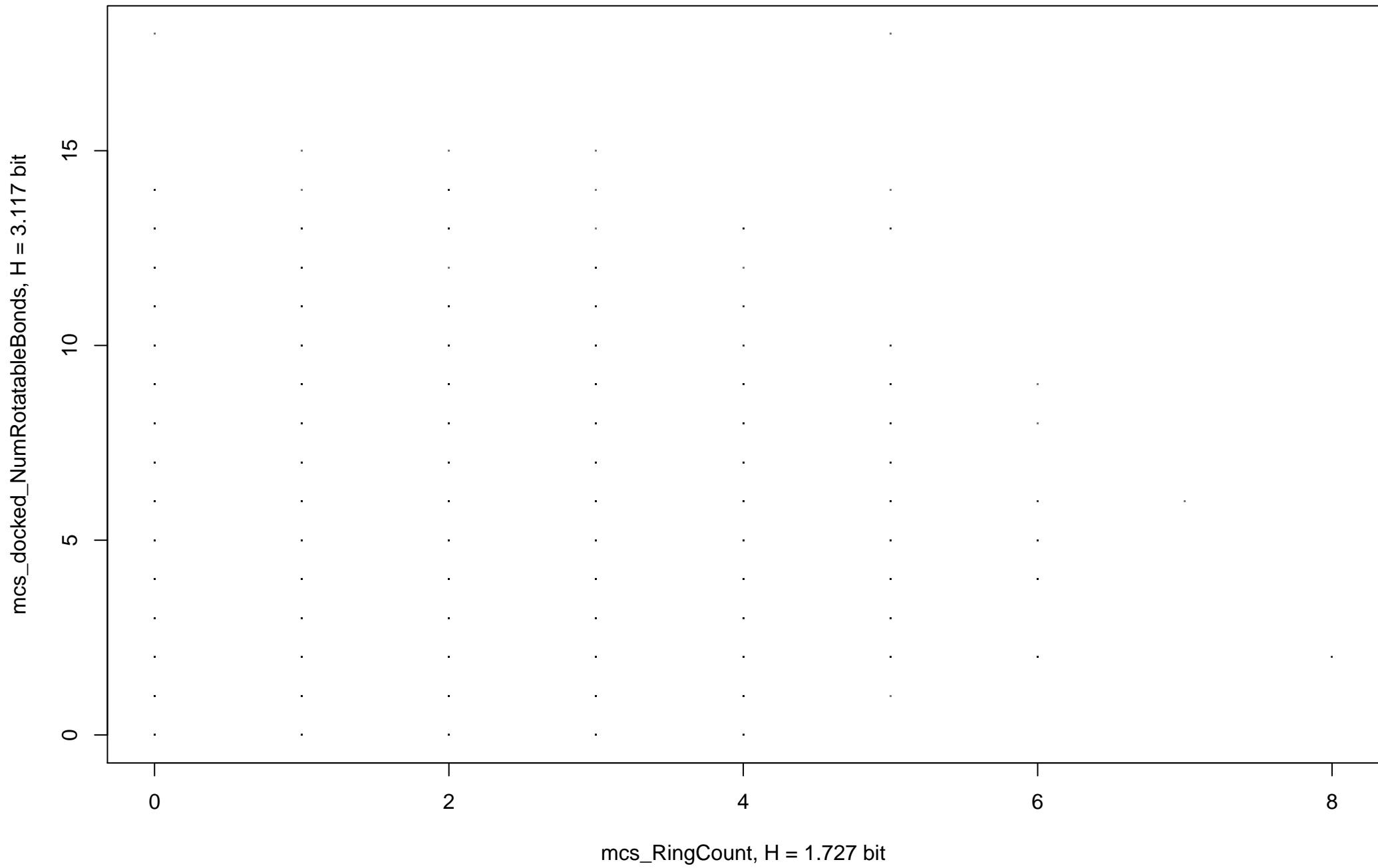


docked_RingCount, H = 2.389 bit

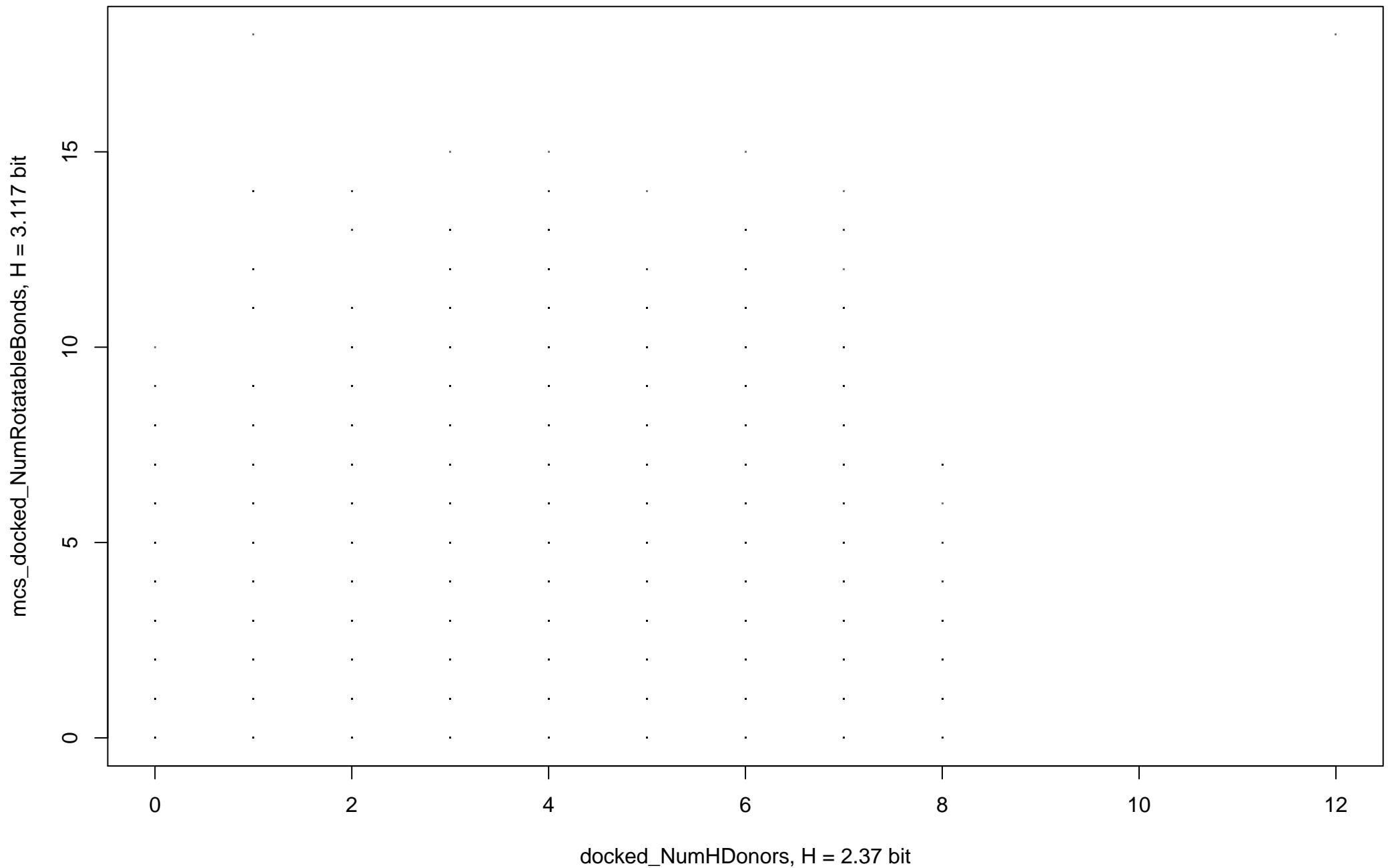
template_HeavyAtomCount-docked_NumHeteroAtoms, MI = 0.1265 bit, normMI = 0.03543



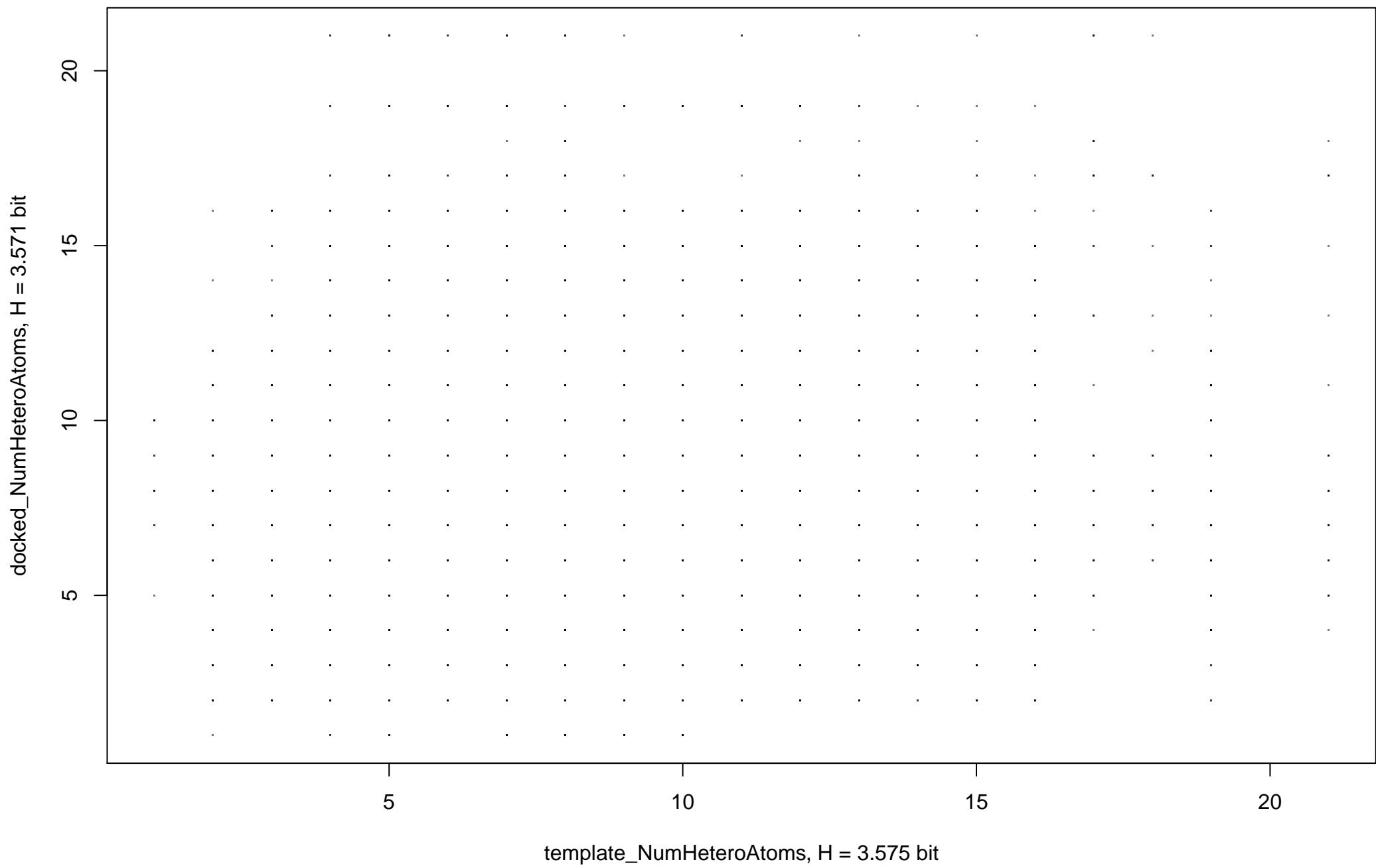
mcs_RingCount–mcs_docked_NumRotatableBonds, MI = 0.06118 bit, normMI = 0.03542



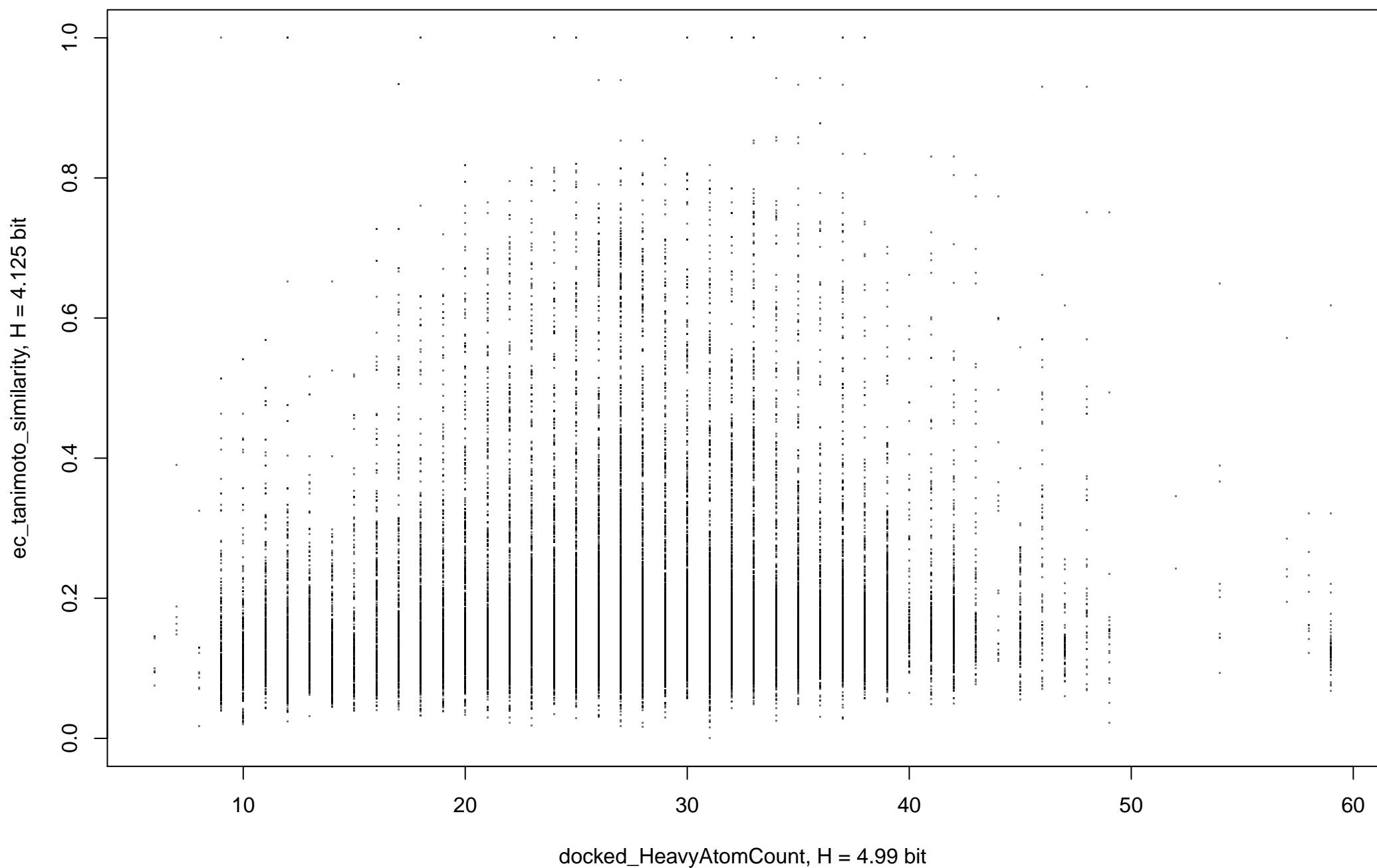
docked_NumHDonors-mcs_docked_NumRotatableBonds, MI = 0.08364 bit, normMI = 0.03529



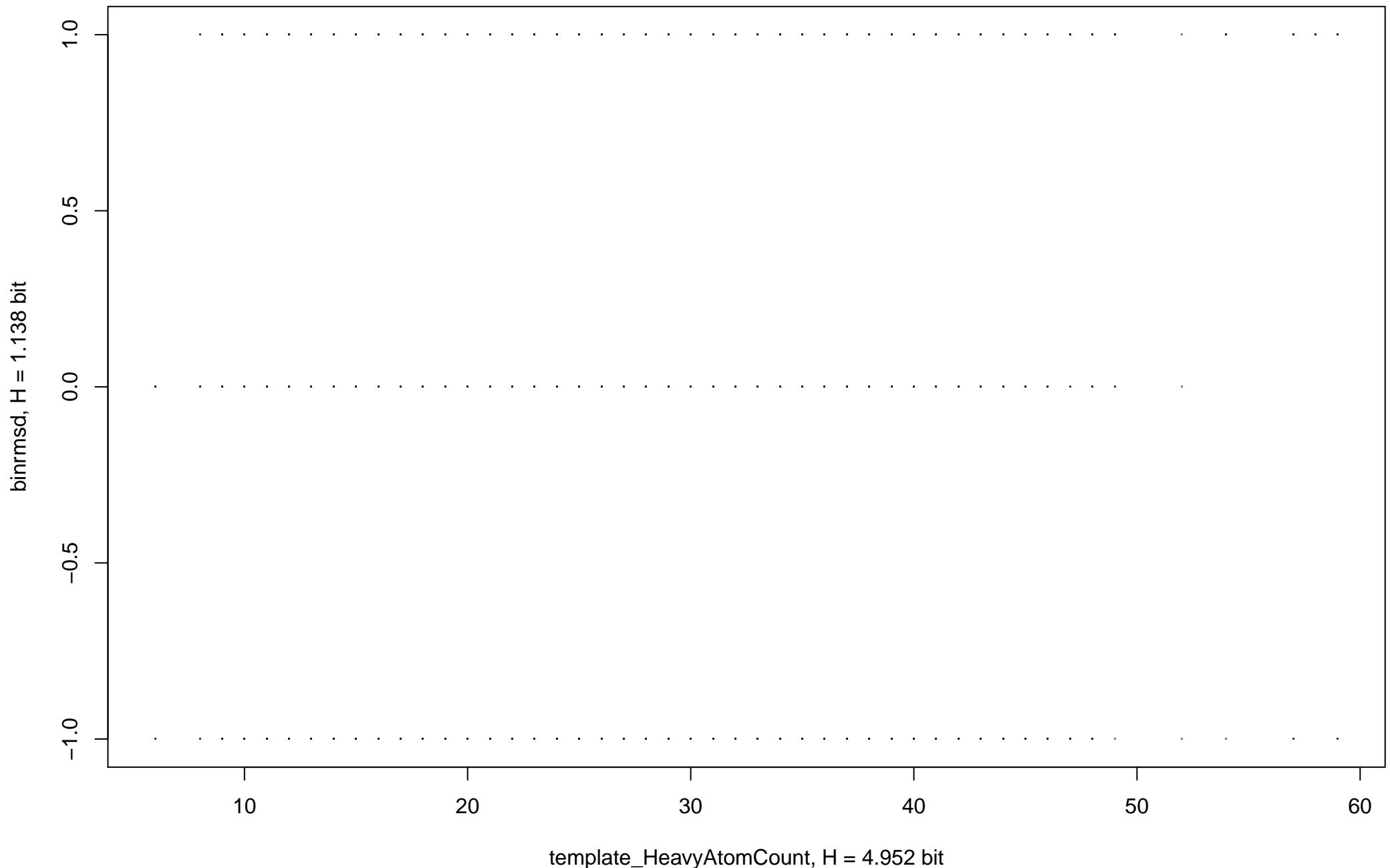
template_NumHeteroAtoms-docked_NumHeteroAtoms, MI = 0.1255 bit, normMI = 0.03514



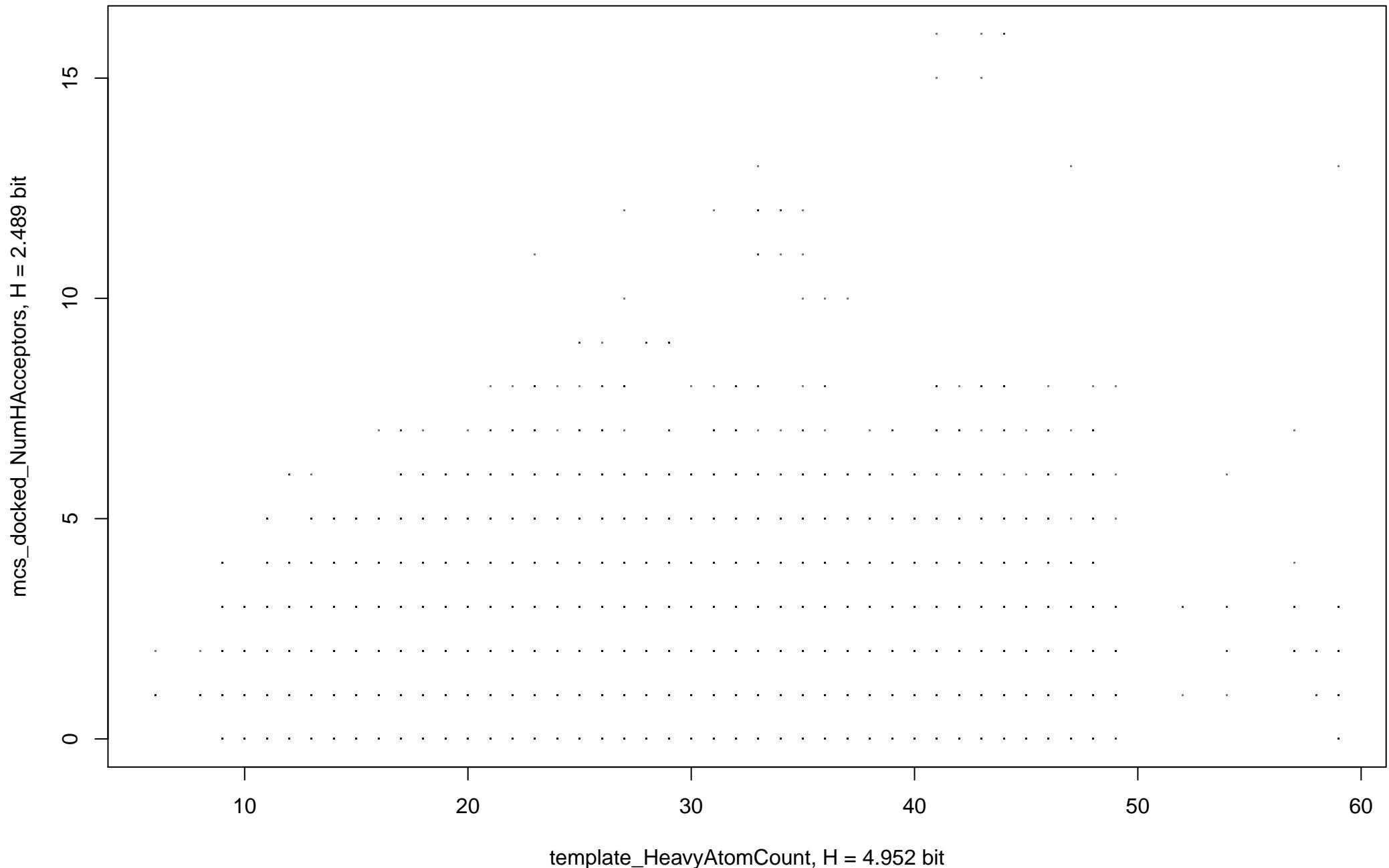
docked_HeavyAtomCount–ec_tanimoto_similarity, MI = 0.1438 bit, normMI = 0.03486



template_HeavyAtomCount–binrmsd, MI = 0.03956 bit, normMI = 0.03476

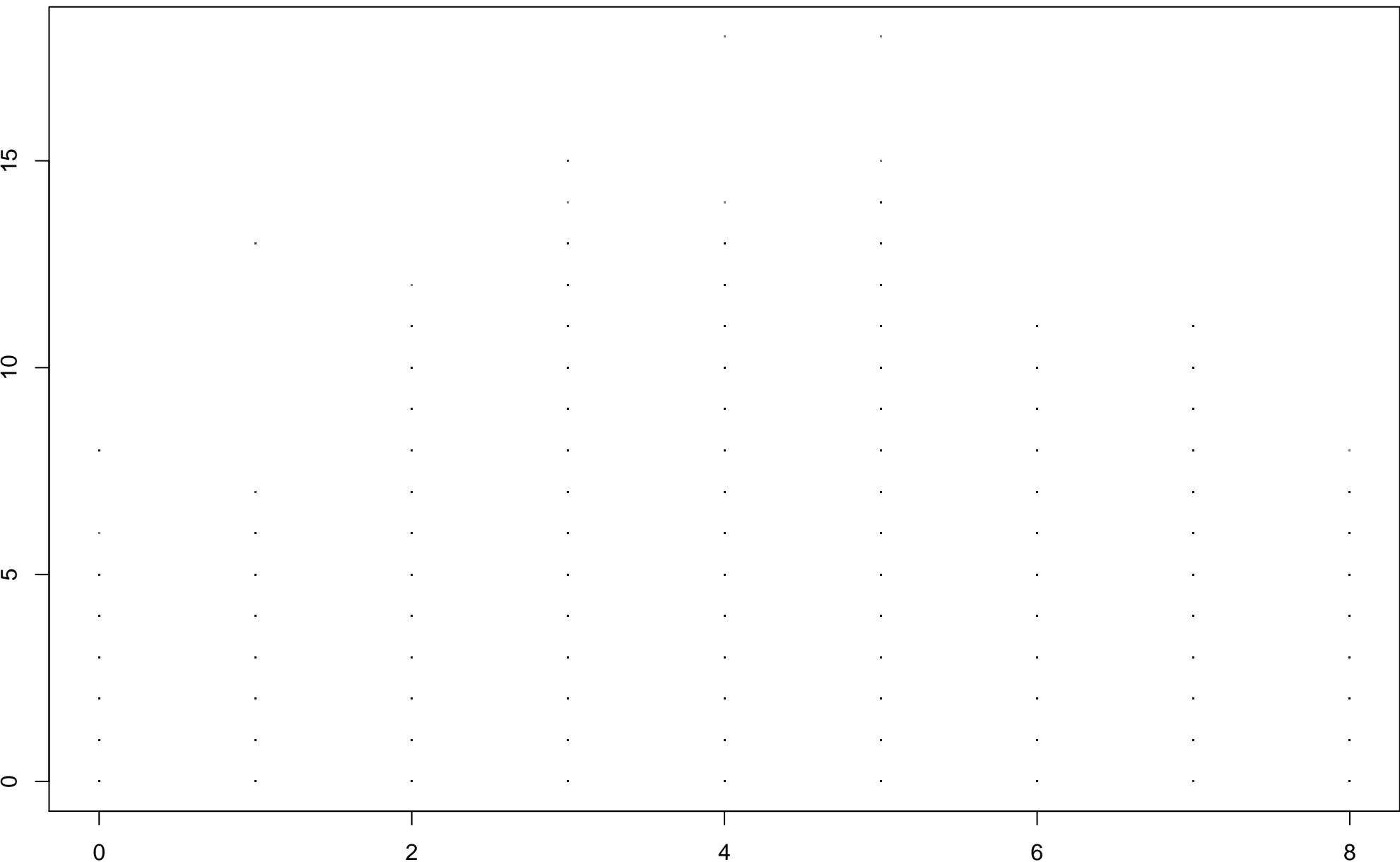


template_HeavyAtomCount-mcs_docked_NumHAcceptors, MI = 0.08625 bit, normMI = 0.03465



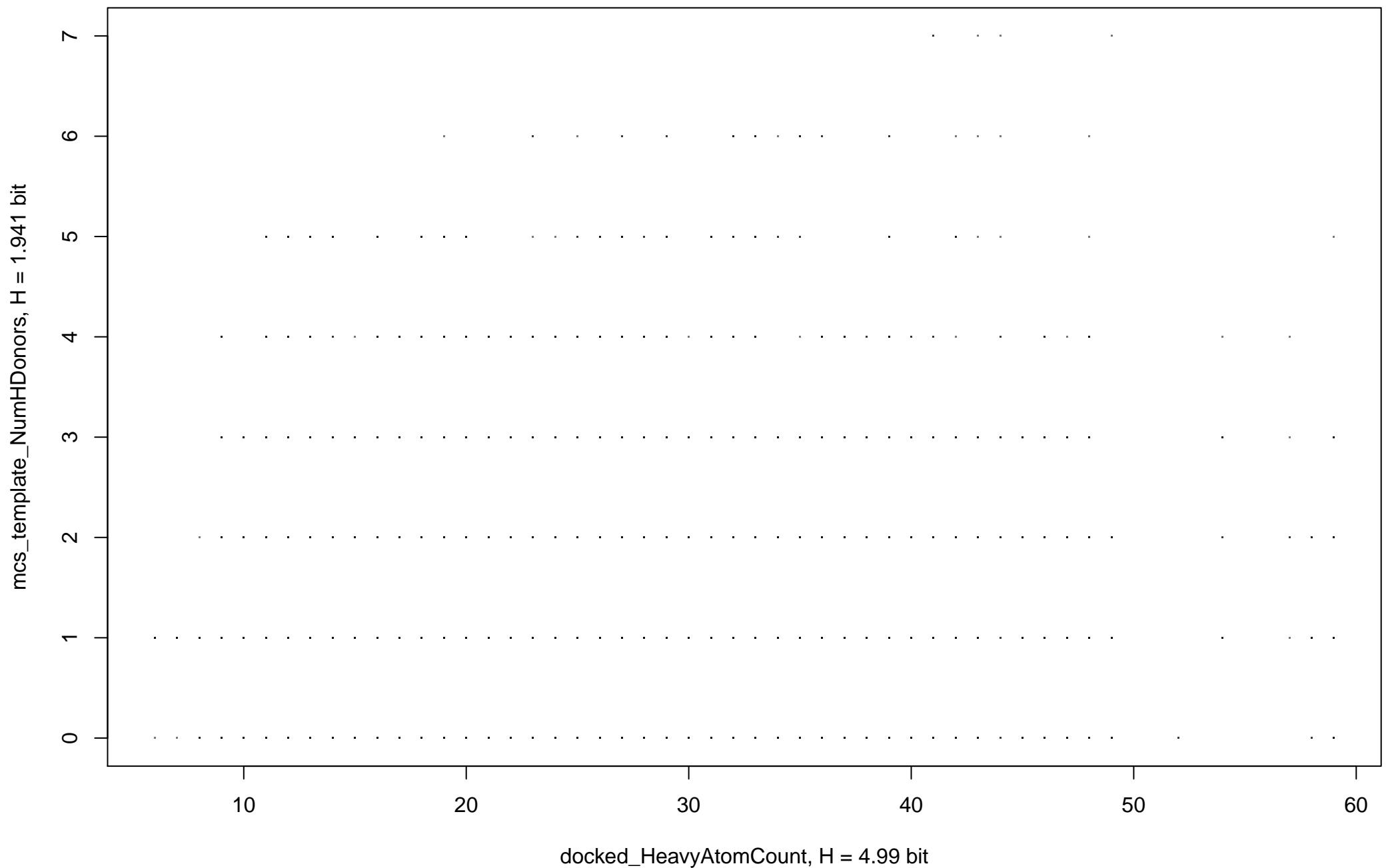
docked_RingCount-mcs_template_NumRotatableBonds, MI = 0.08263 bit, normMI = 0.03458

mcs_template_NumRotatableBonds, H = 3.118 bit

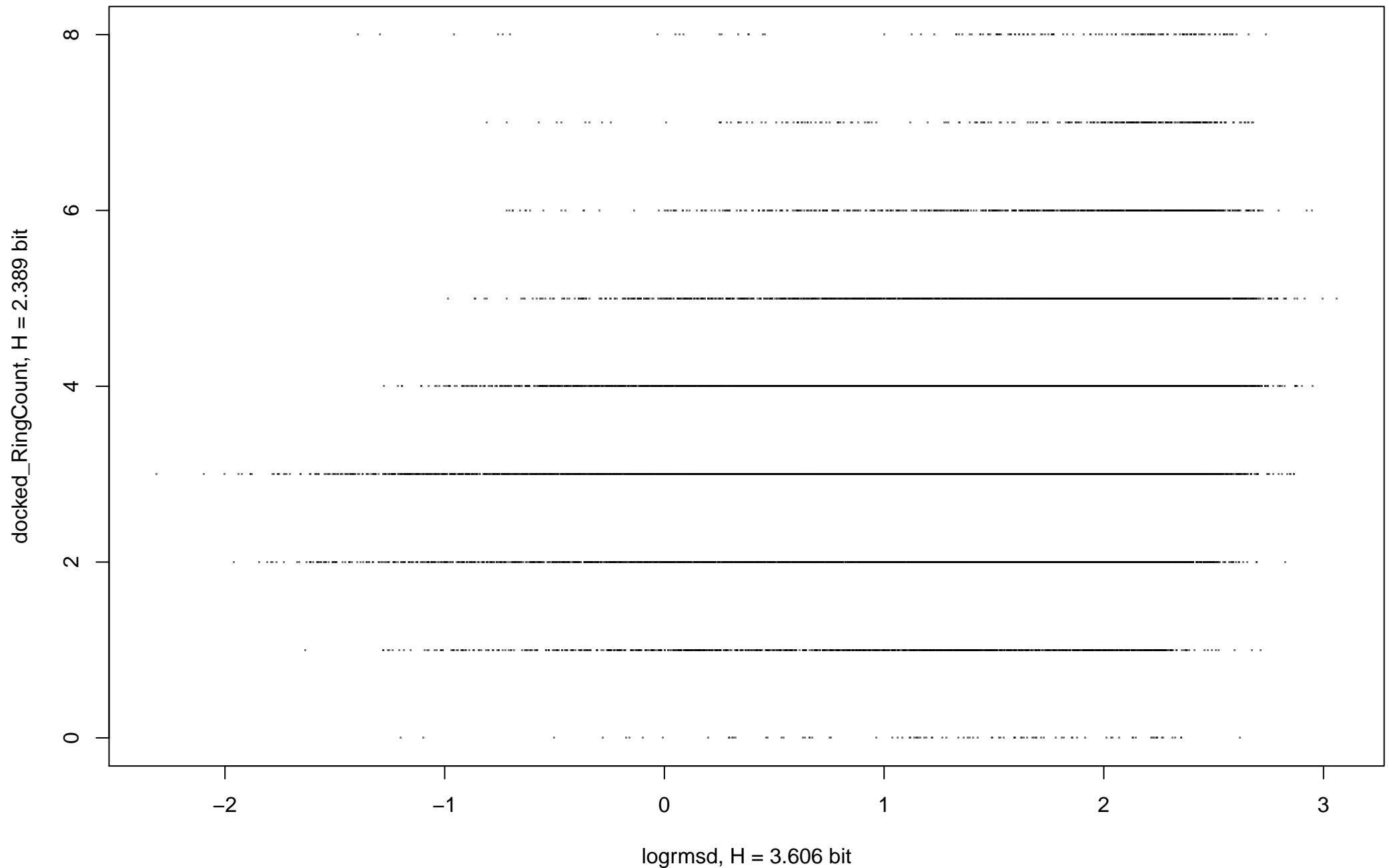


docked_RingCount, H = 2.389 bit

docked_HeavyAtomCount-mcs_template_NumHDonors, MI = 0.06695 bit, normMI = 0.0345

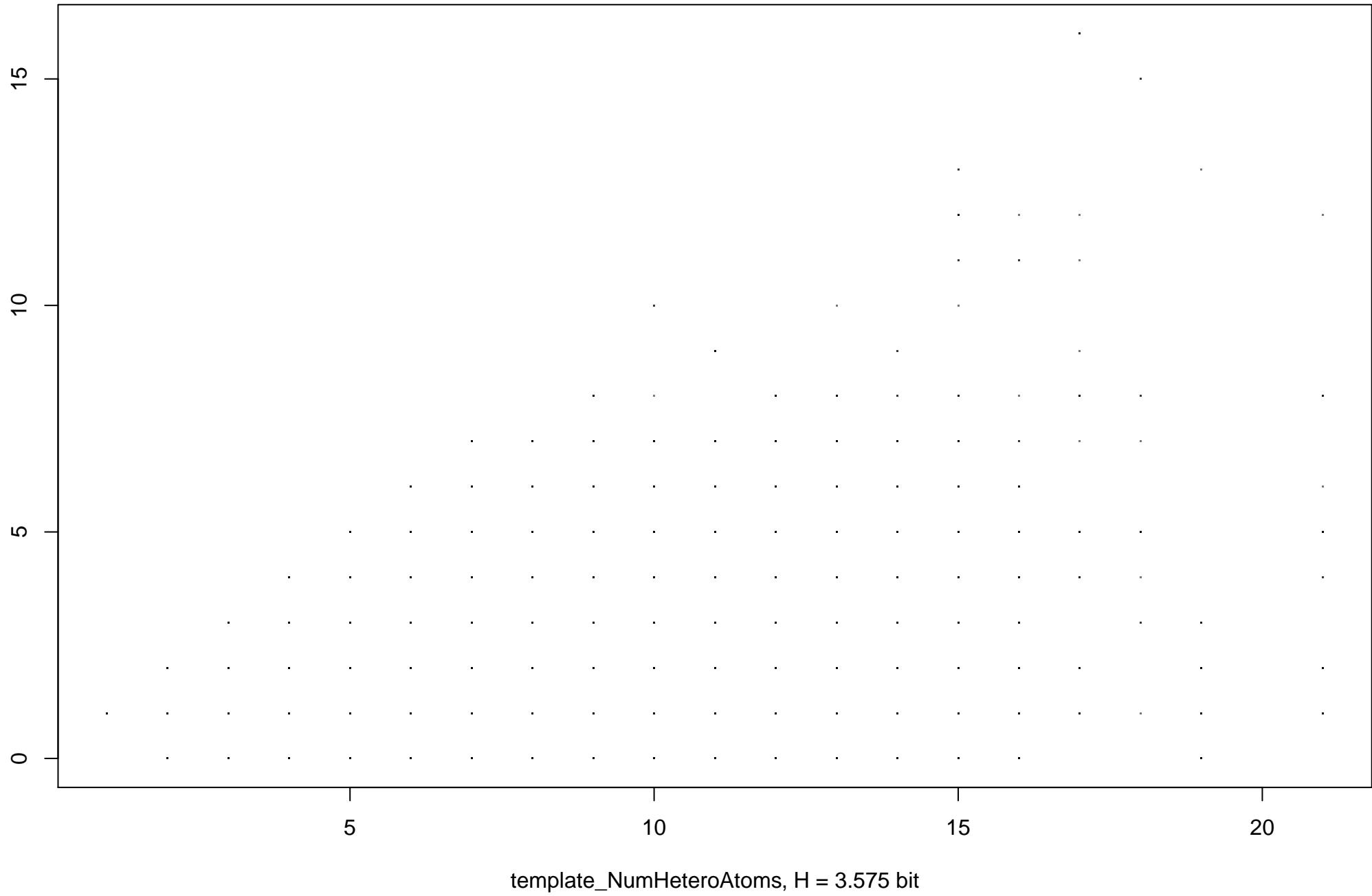


logrmsd-docked_RingCount, MI = 0.0824 bit, normMI = 0.03449



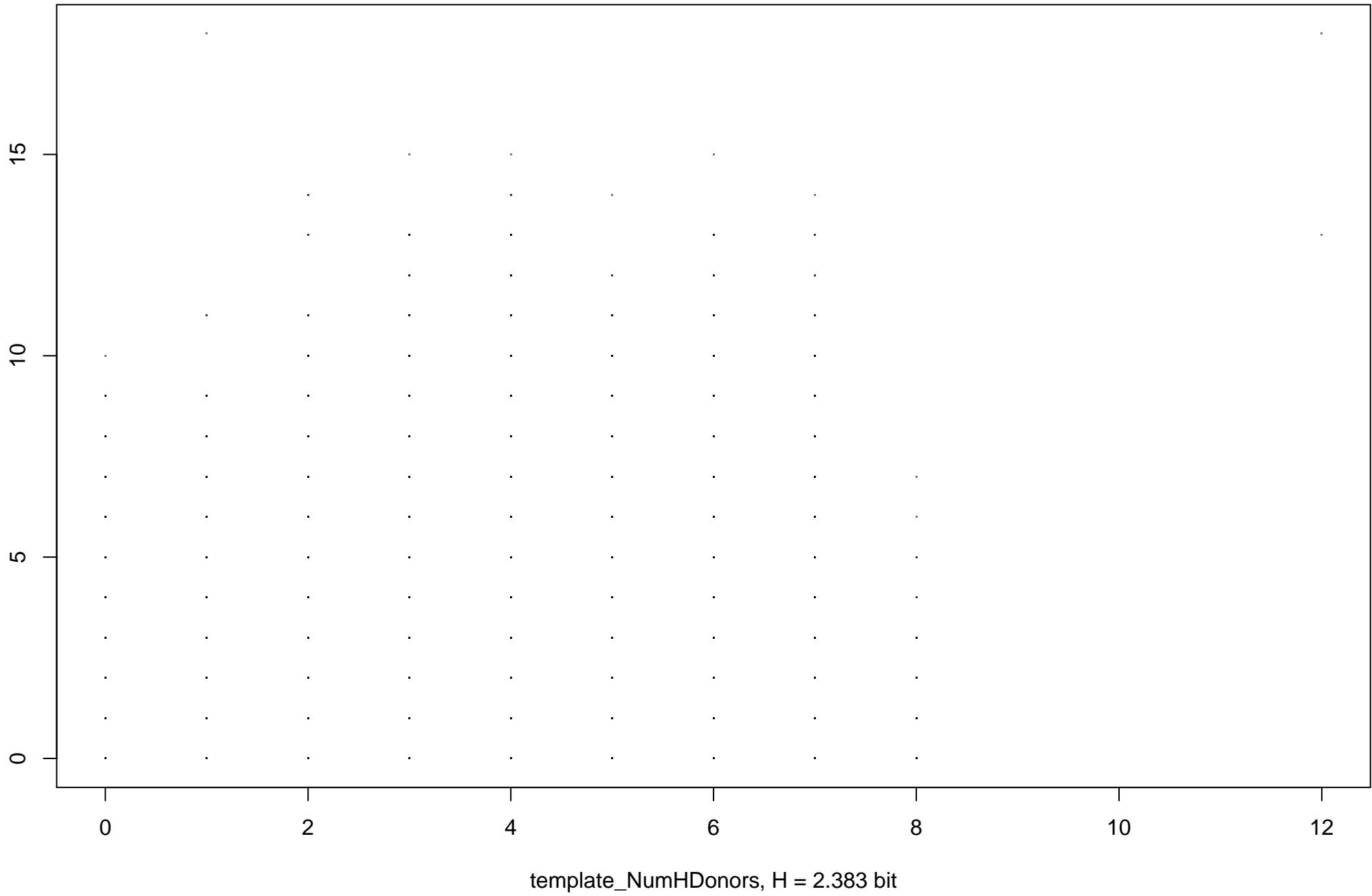
template_NumHeteroAtoms-mcs_template_NumHAcceptors, MI = 0.08581 bit, normMI = 0.03449

mcs_template_NumHAcceptors, H = 2.488 bit

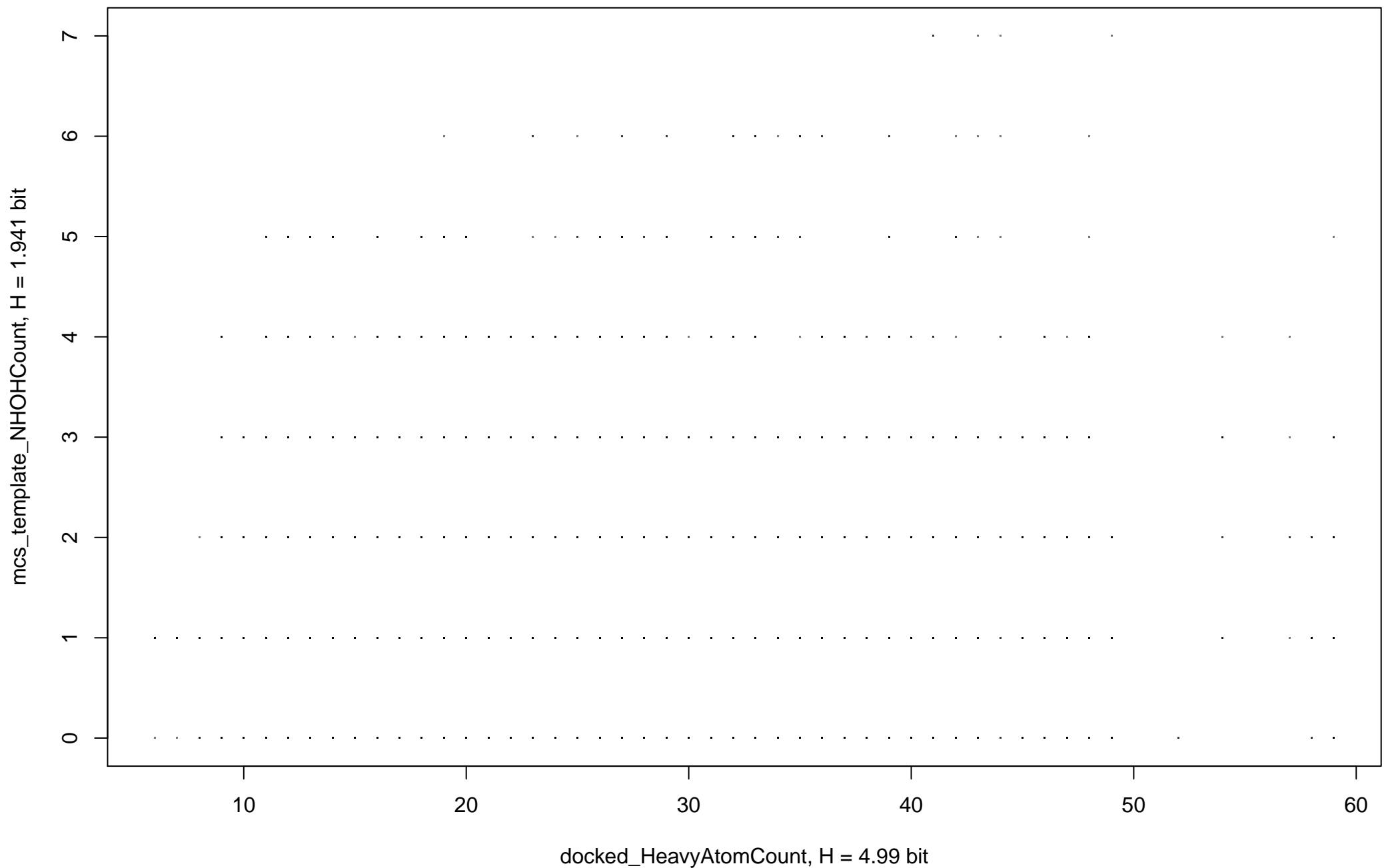


template_NumHDonors-mcs_template_NumRotatableBonds, MI = 0.08205 bit, normMI = 0.03443

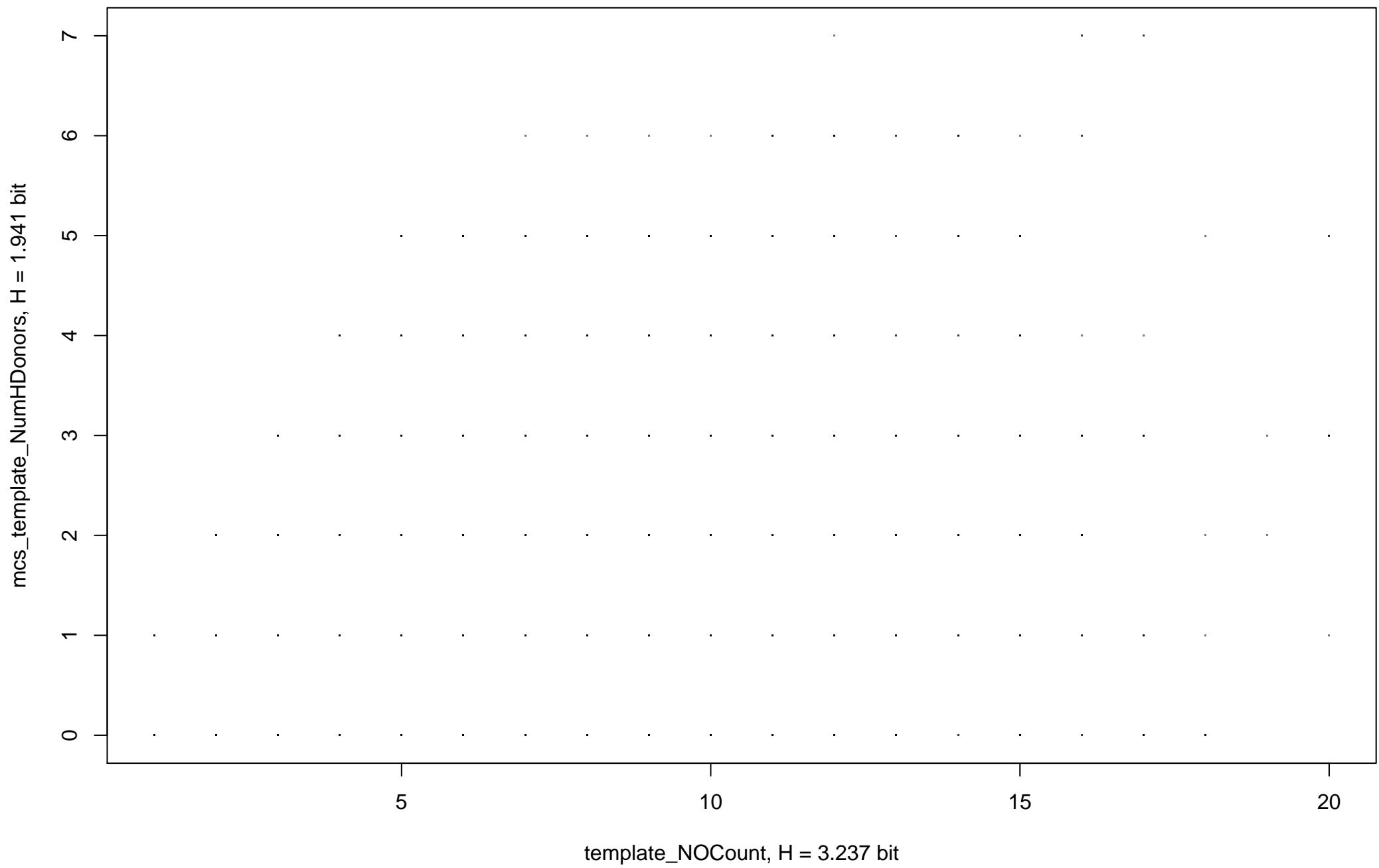
mcs_template_NumRotatableBonds, H = 3.118 bit



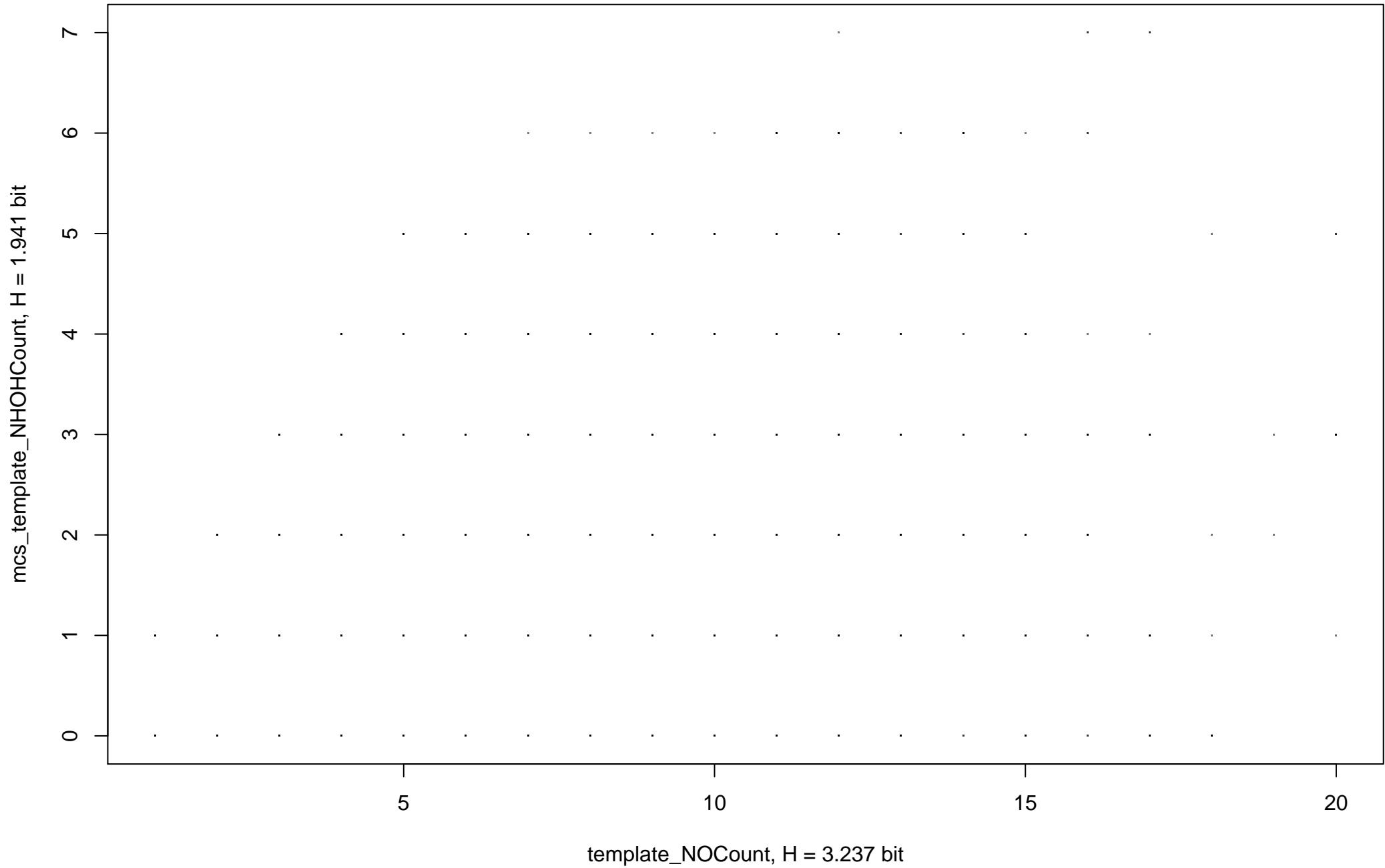
docked_HeavyAtomCount-mcs_template_NHOHCount, MI = 0.06666 bit, normMI = 0.03434



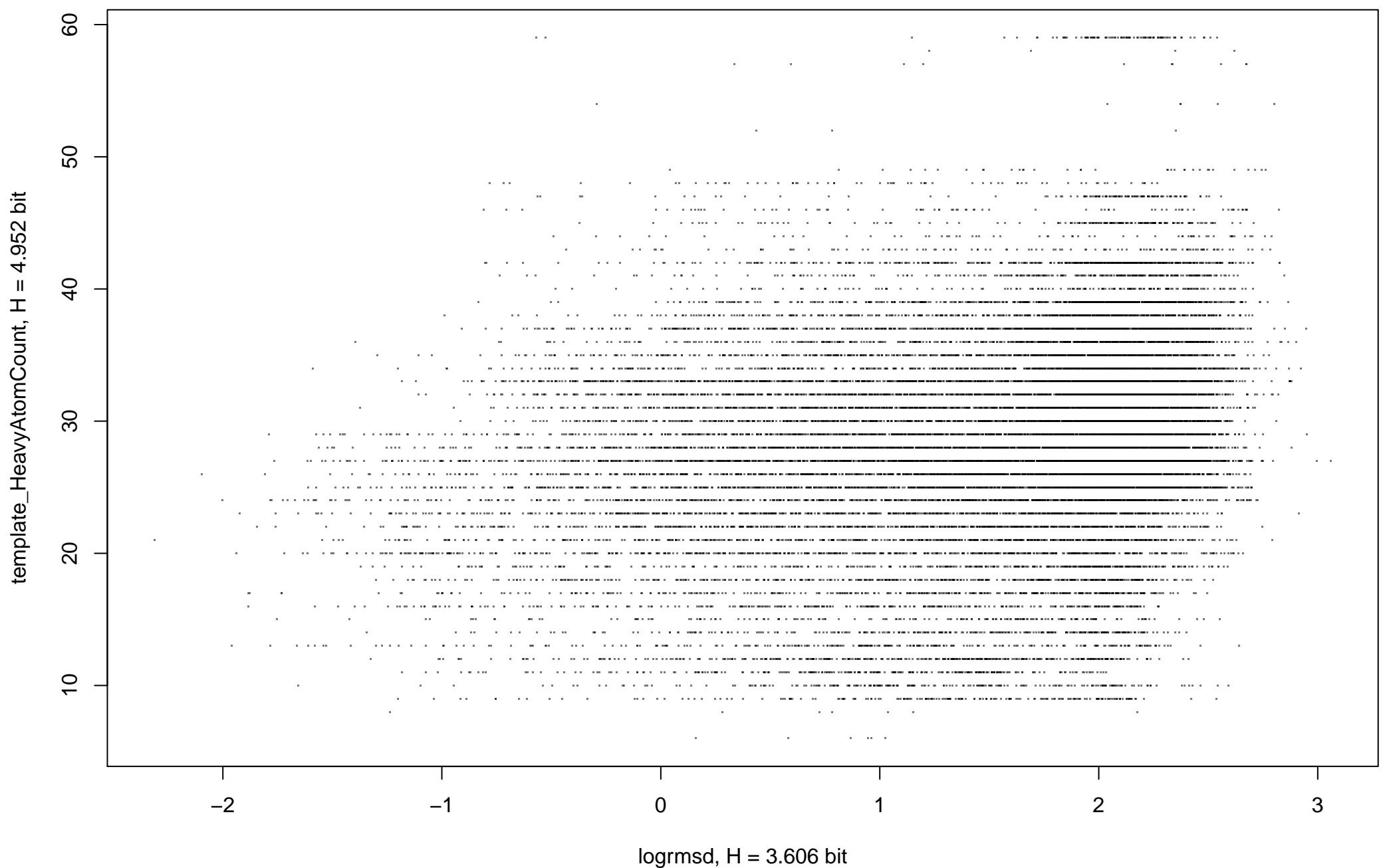
template_NOCount-mcs_template_NumHDonors, MI = 0.06584 bit, normMI = 0.03393



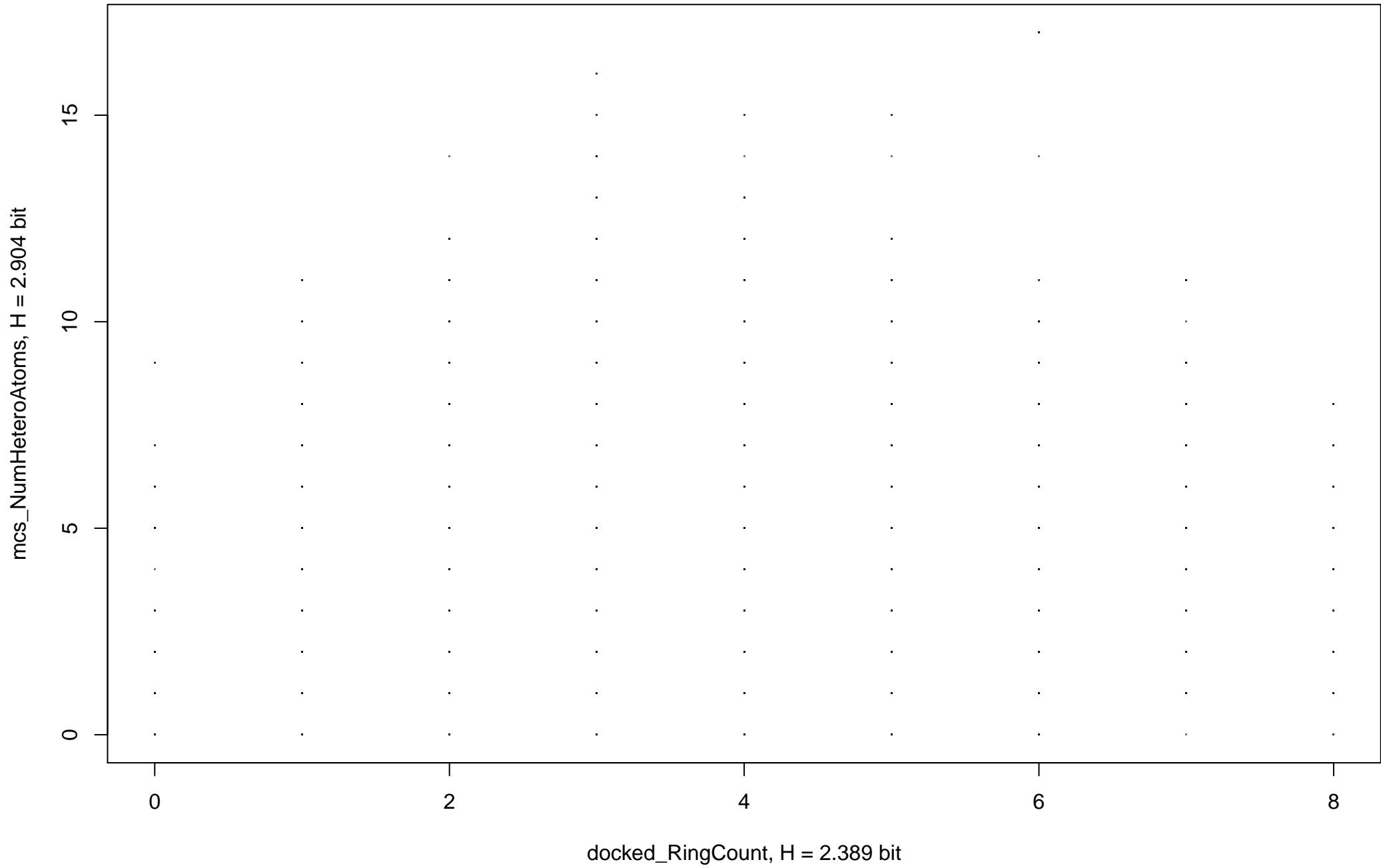
template_NOCount-mcs_template_NHOHCount, MI = 0.0657 bit, normMI = 0.03384



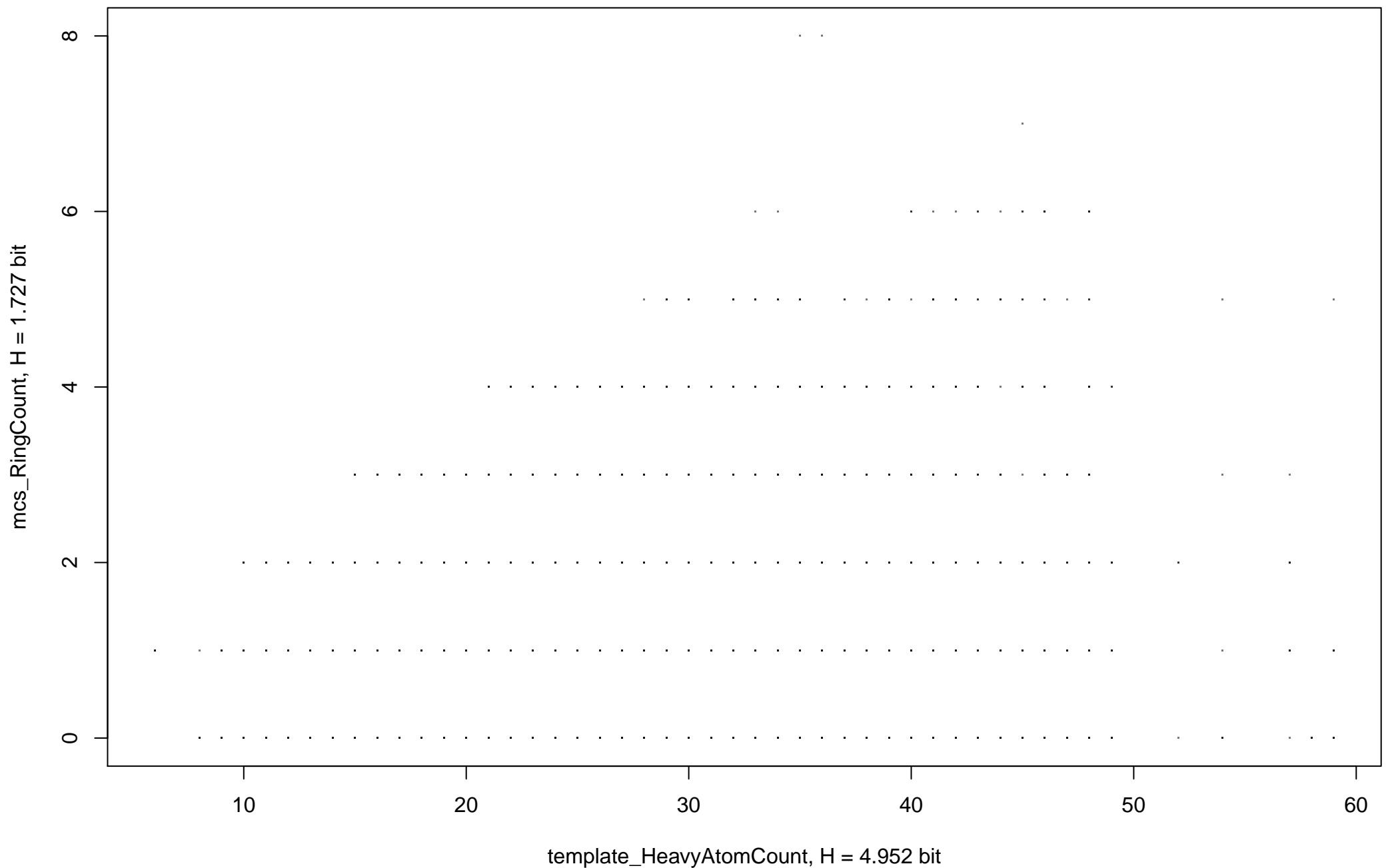
logrmsd-template_HeavyAtomCount, MI = 0.1202 bit, normMI = 0.03333



docked_RingCount-mcs_NumHeteroAtoms, MI = 0.07916 bit, normMI = 0.03313

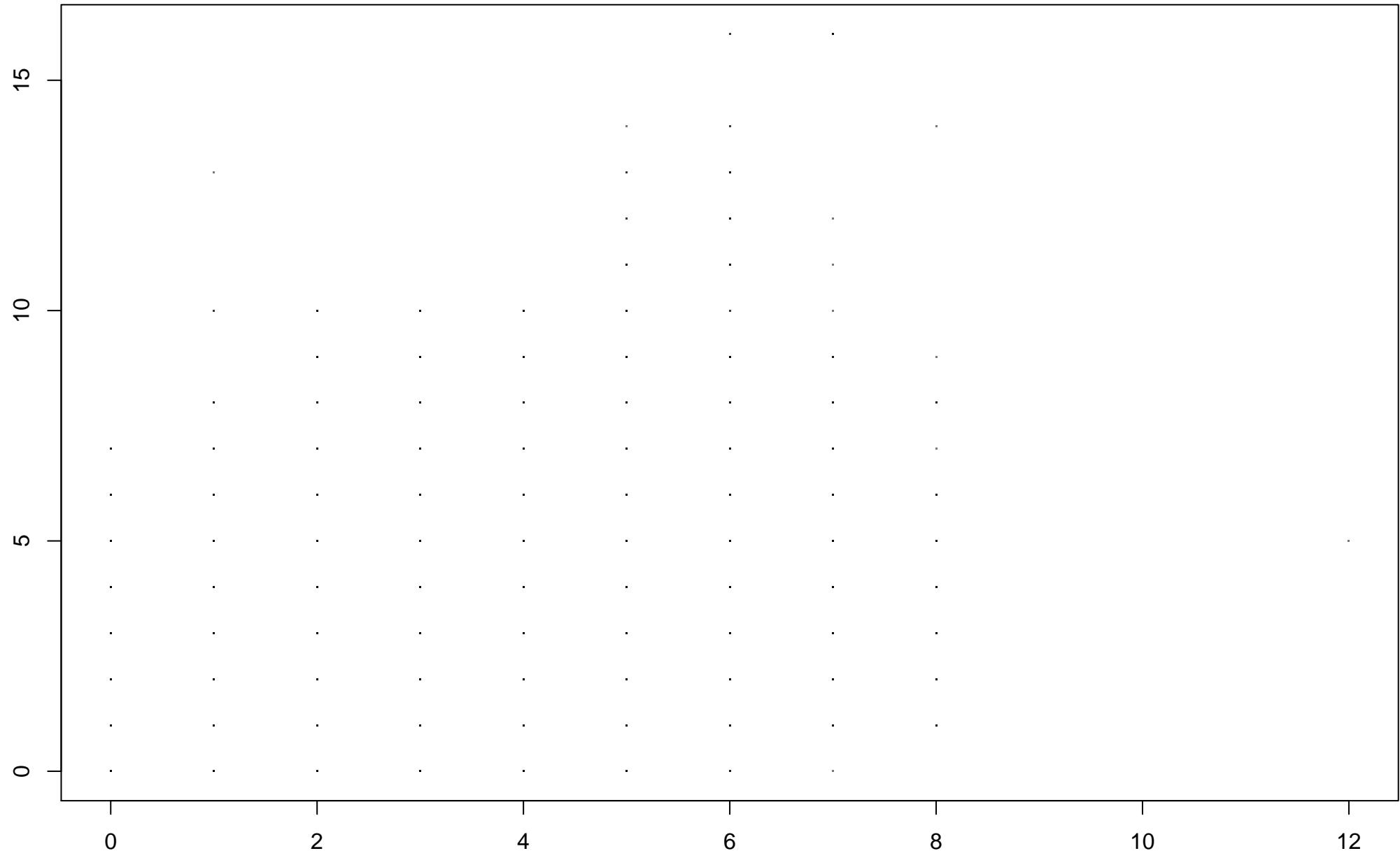


template_HeavyAtomCount–mcs_RingCount, MI = 0.0572 bit, normMI = 0.03311



docked_NumHDonors-mcs_NOCount, MI = 0.0779 bit, normMI = 0.03286

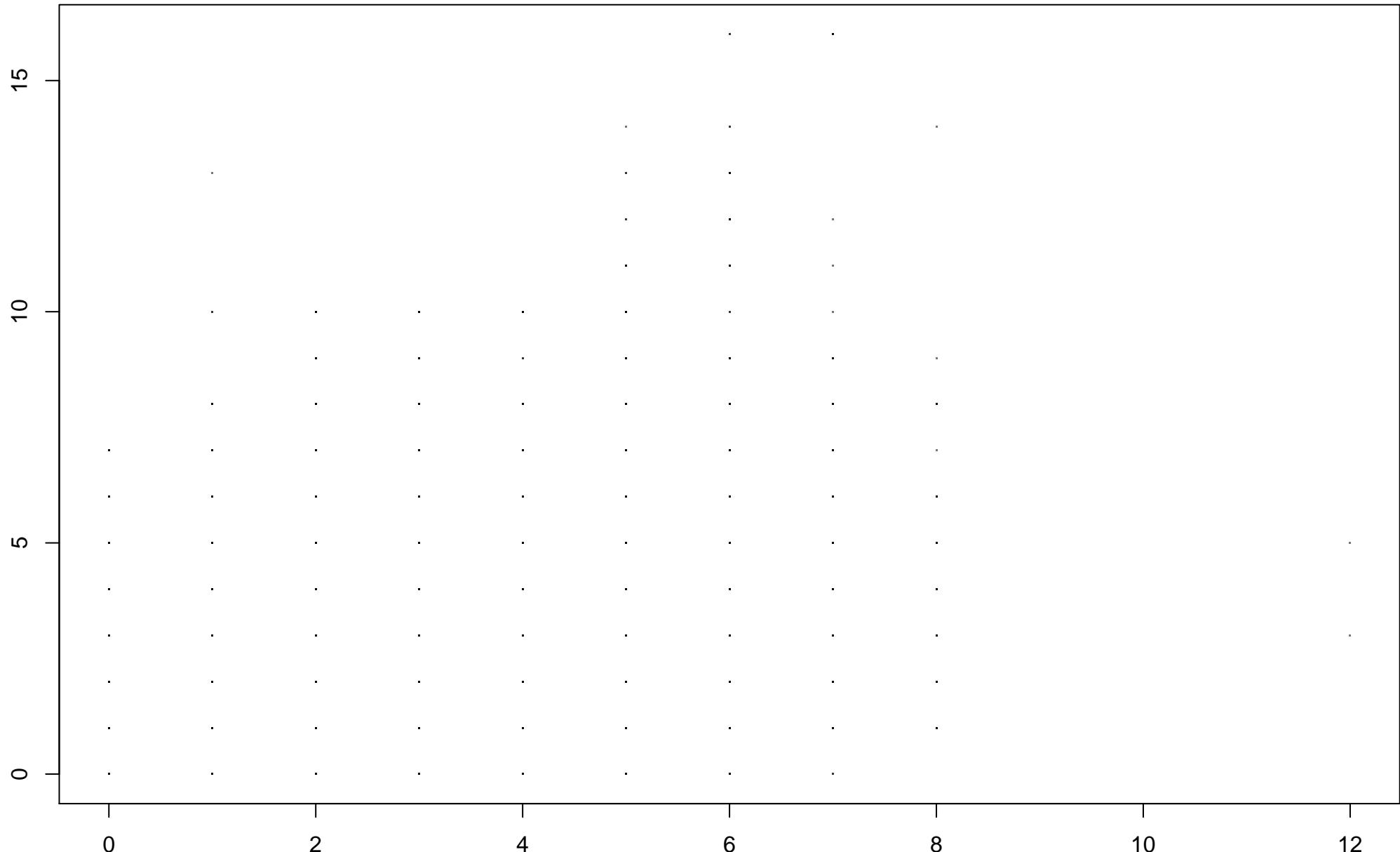
mcs_NOCount, H = 2.777 bit



docked_NumHDonors, H = 2.37 bit

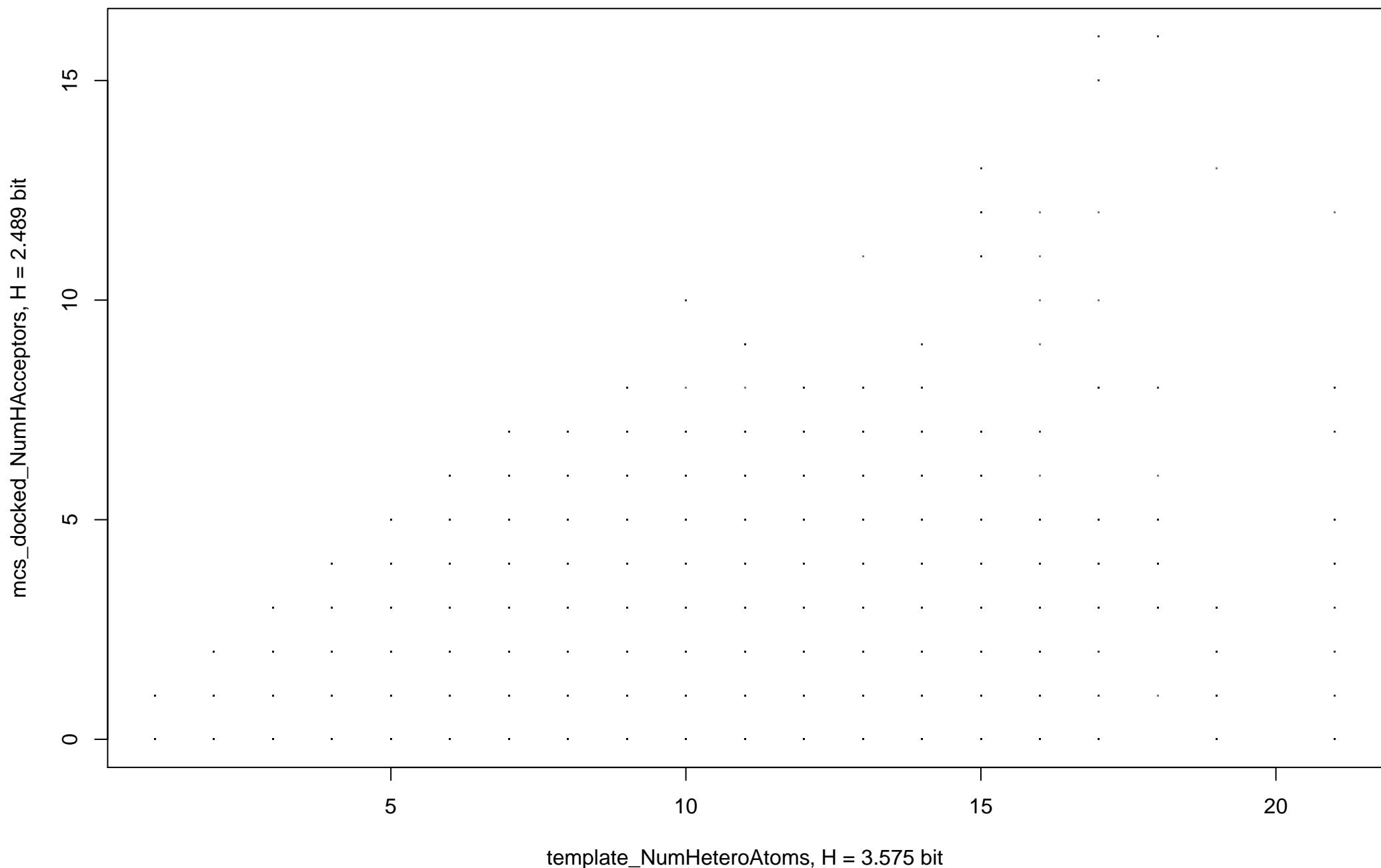
template_NumHDonors-mcs_NOCount, MI = 0.07757 bit, normMI = 0.03255

mcs_NOCount, H = 2.777 bit

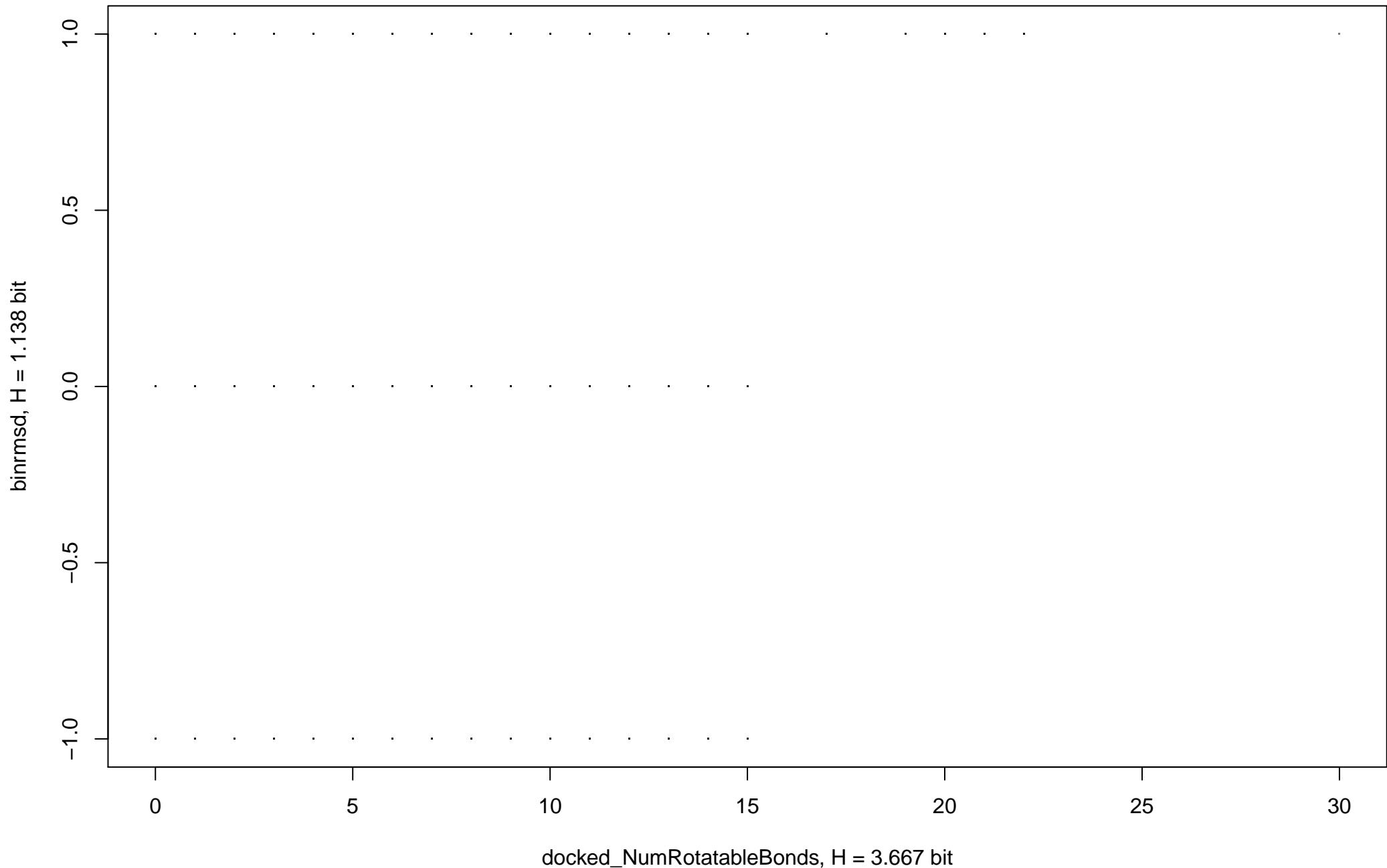


template_NumHDonors, H = 2.383 bit

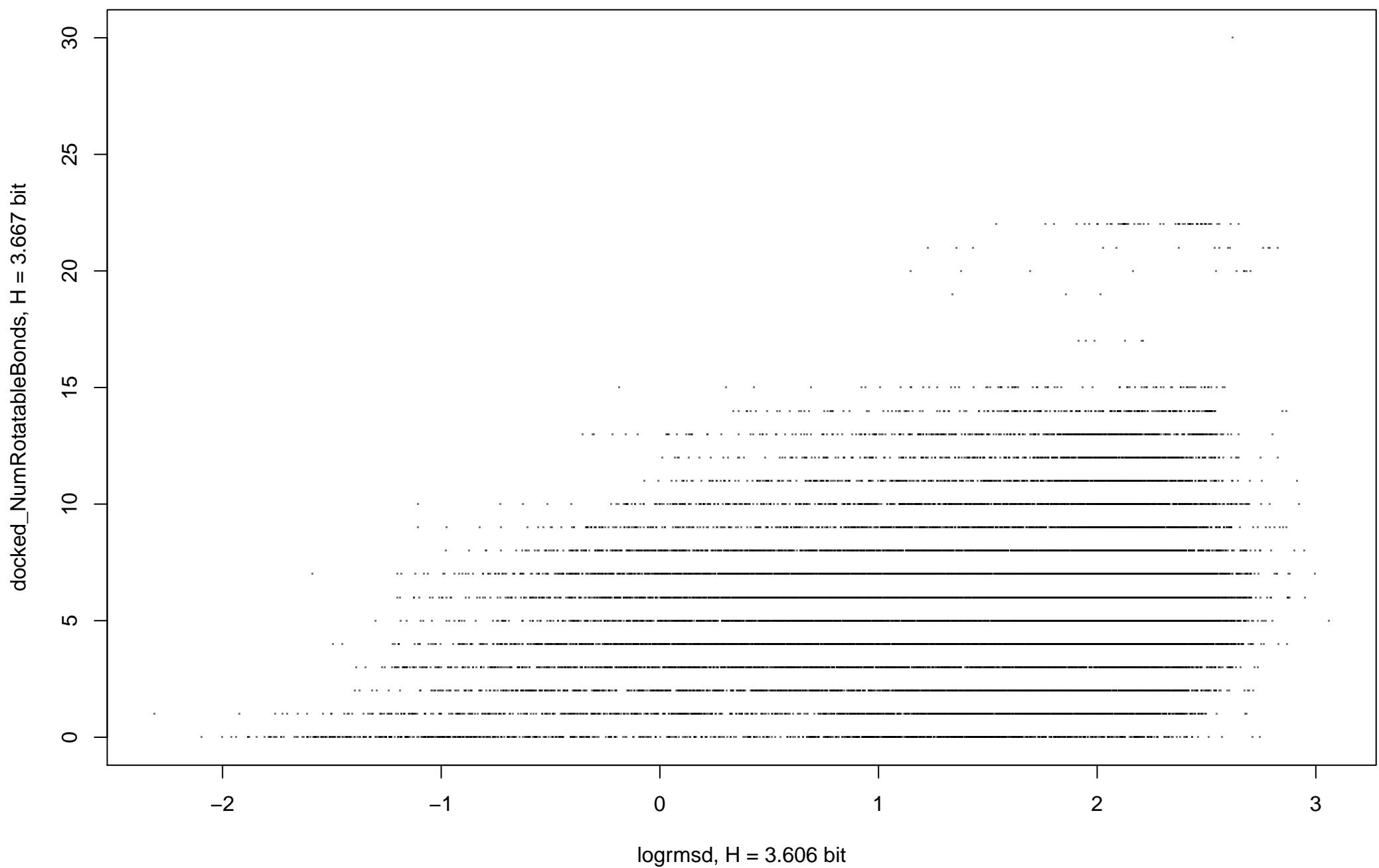
template_NumHeteroAtoms-mcs_docked_NumHAcceptors, MI = 0.0804 bit, normMI = 0.0323



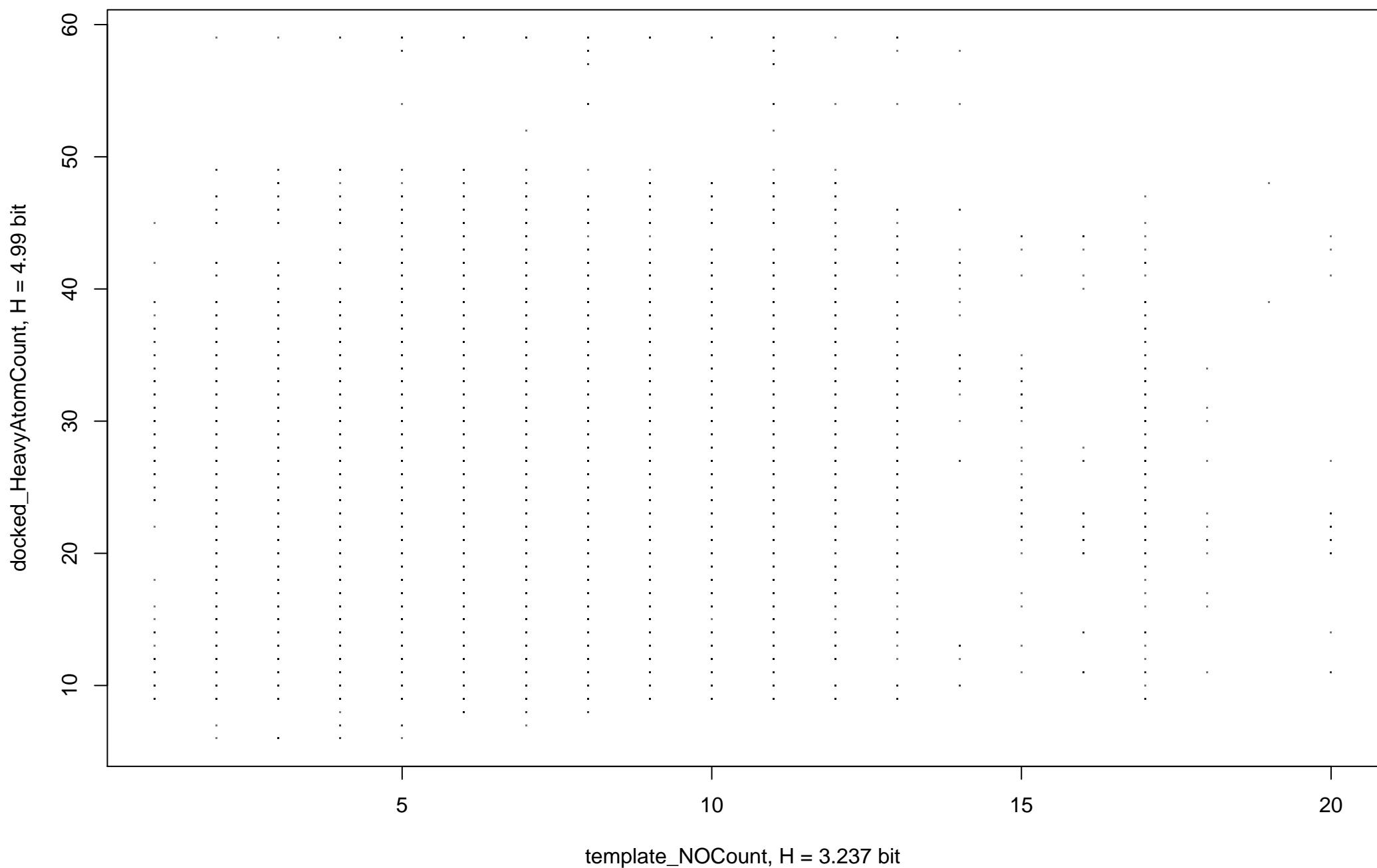
docked_NumRotatableBonds–binrmsd, MI = 0.03652 bit, normMI = 0.03209



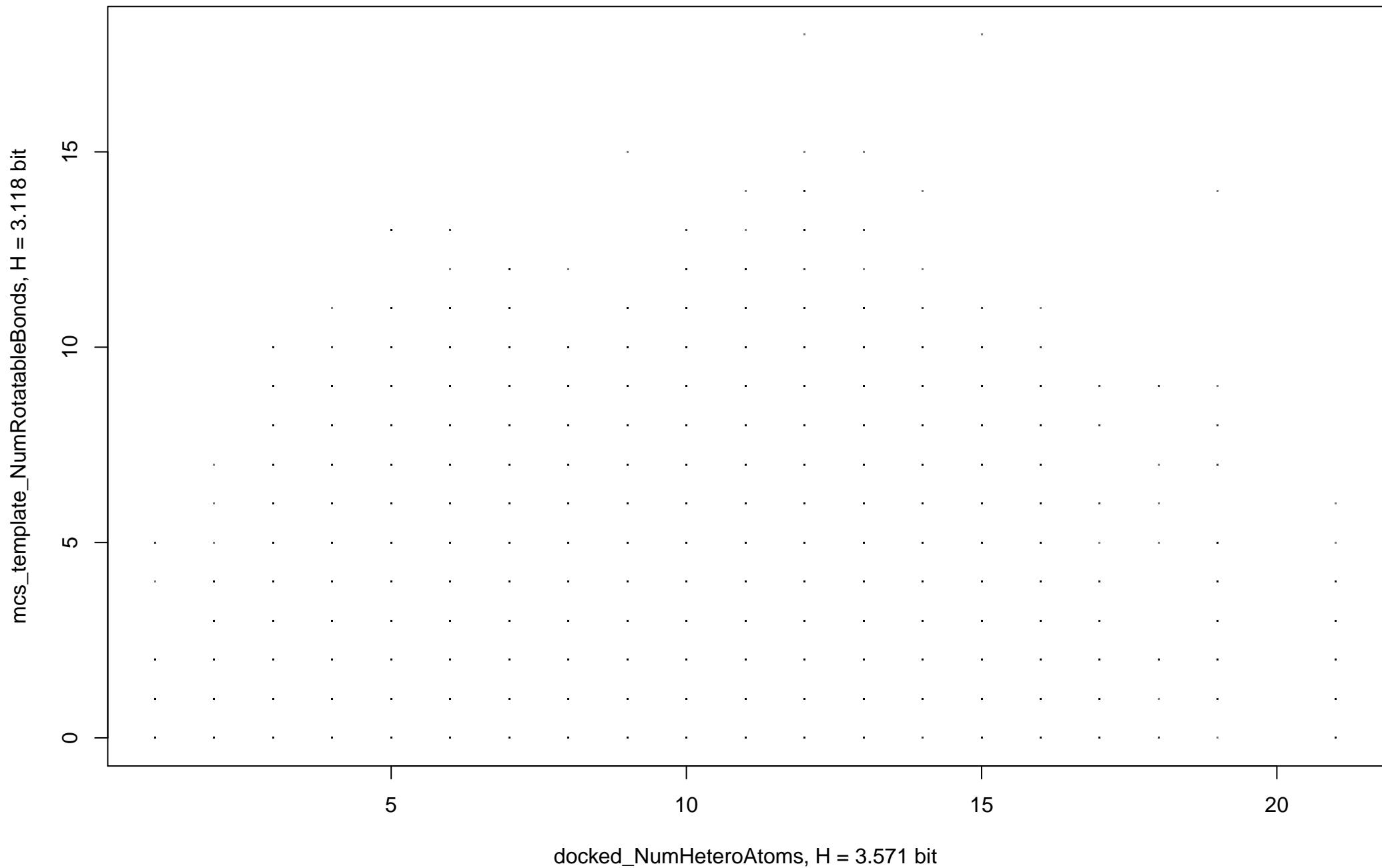
logrmsd-docked_NumRotatableBonds, MI = 0.1152 bit, normMI = 0.03195



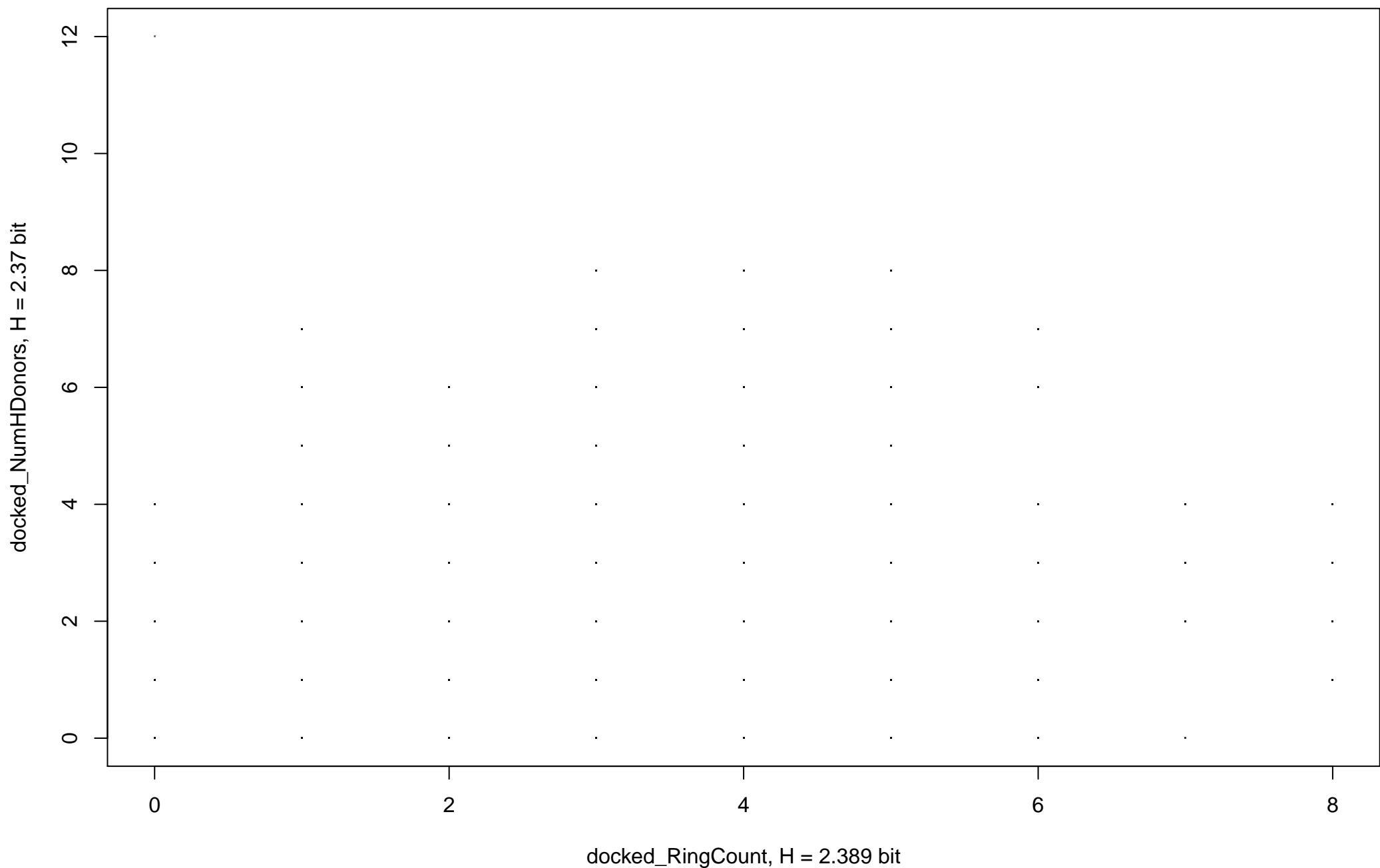
template_NOCount-docked_HeavyAtomCount, MI = 0.1032 bit, normMI = 0.0319



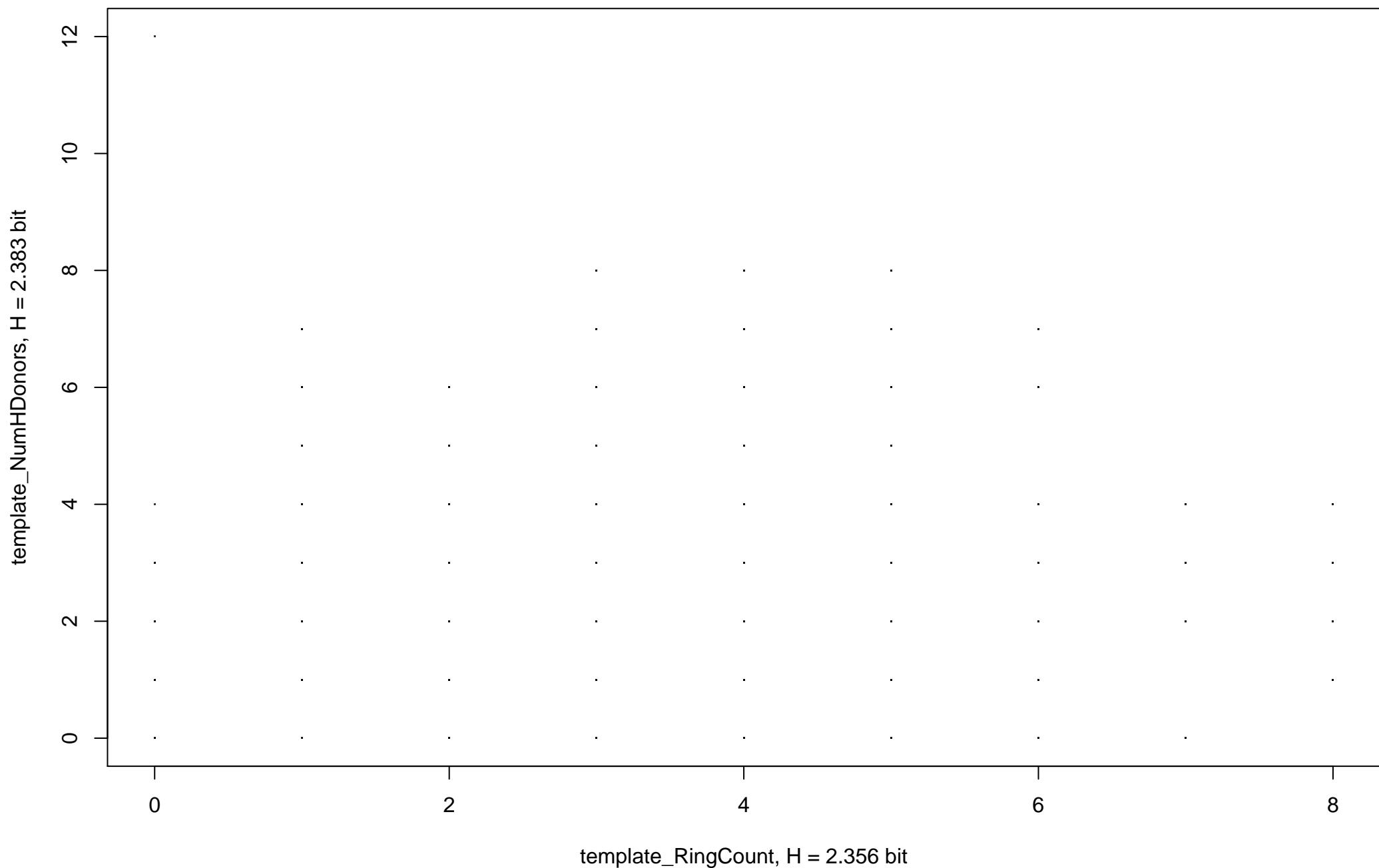
docked_NumHeteroAtoms–mcs_template_NumRotatableBonds, MI = 0.09904 bit, normMI = 0.03176



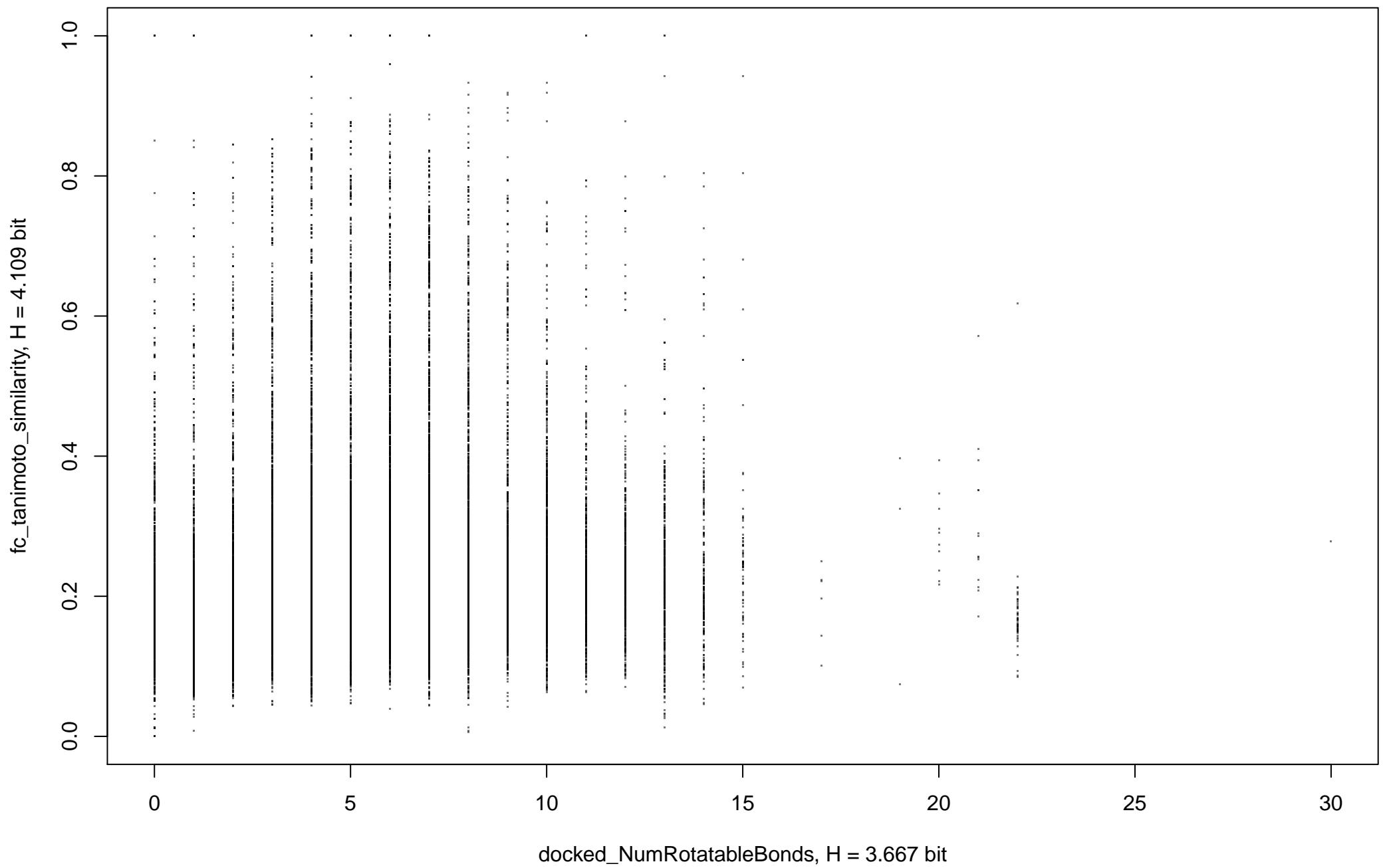
docked_RingCount–docked_NumHDonors, MI = 0.07511 bit, normMI = 0.03169



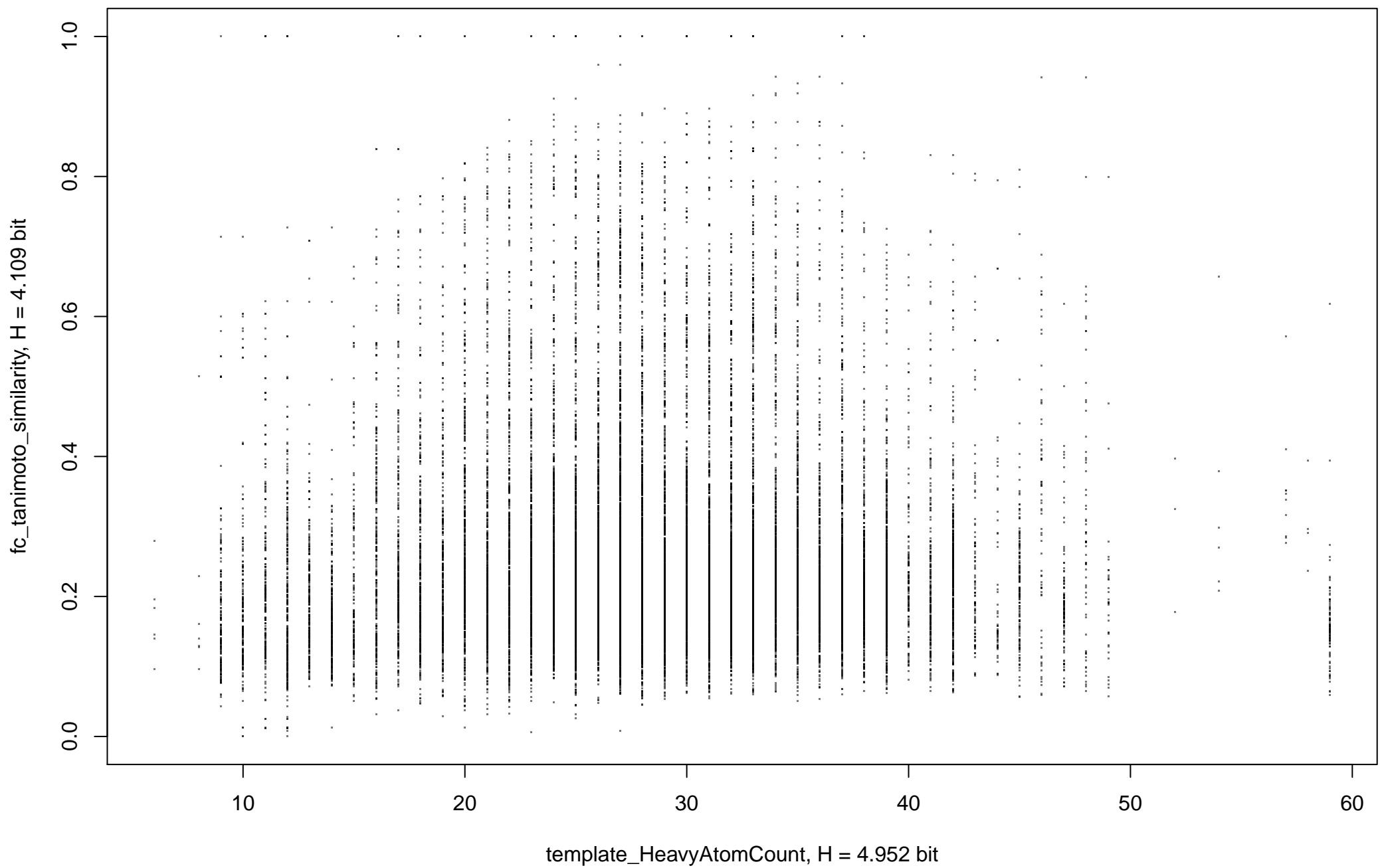
template_RingCount-template_NumHDonors, MI = 0.07388 bit, normMI = 0.03136



docked_NumRotatableBonds-fc_tanimoto_similarity, MI = 0.1146 bit, normMI = 0.03124

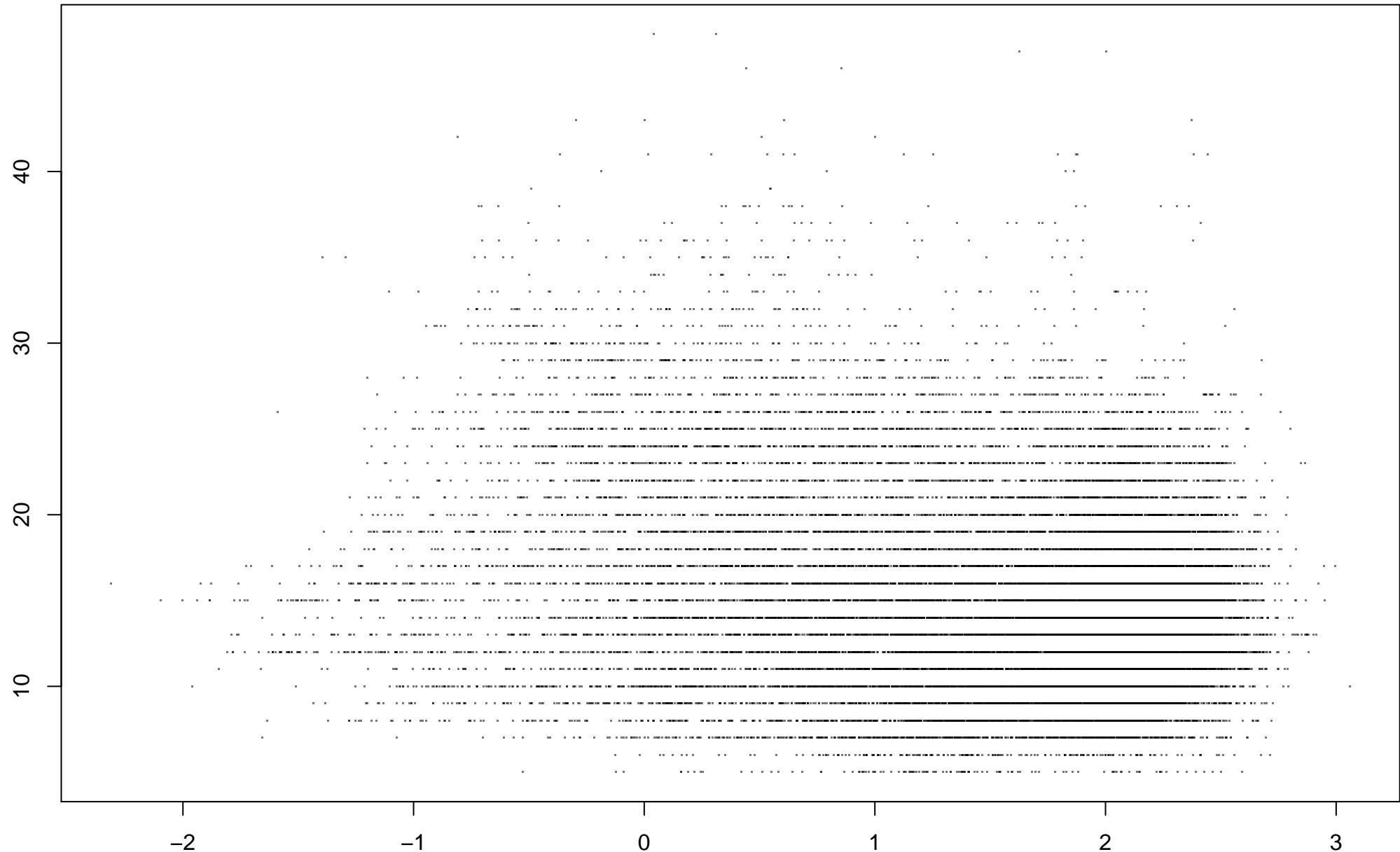


template_HeavyAtomCount-fc_tanimoto_similarity, MI = 0.1277 bit, normMI = 0.03108



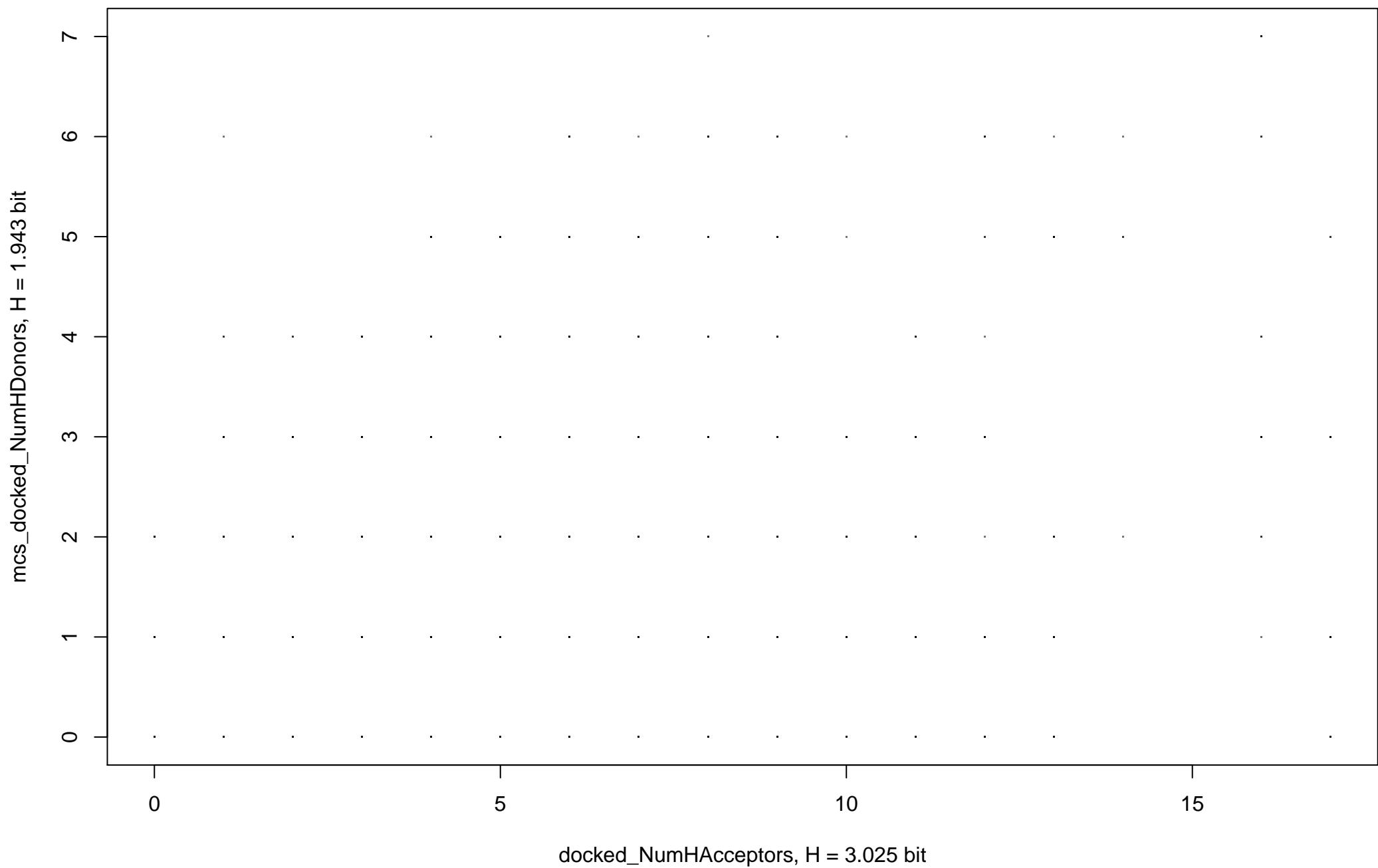
logrmsd-mcs_HeavyAtomCount, MI = 0.1115 bit, normMI = 0.03093

mcs_HeavyAtomCount, H = 4.38 bit

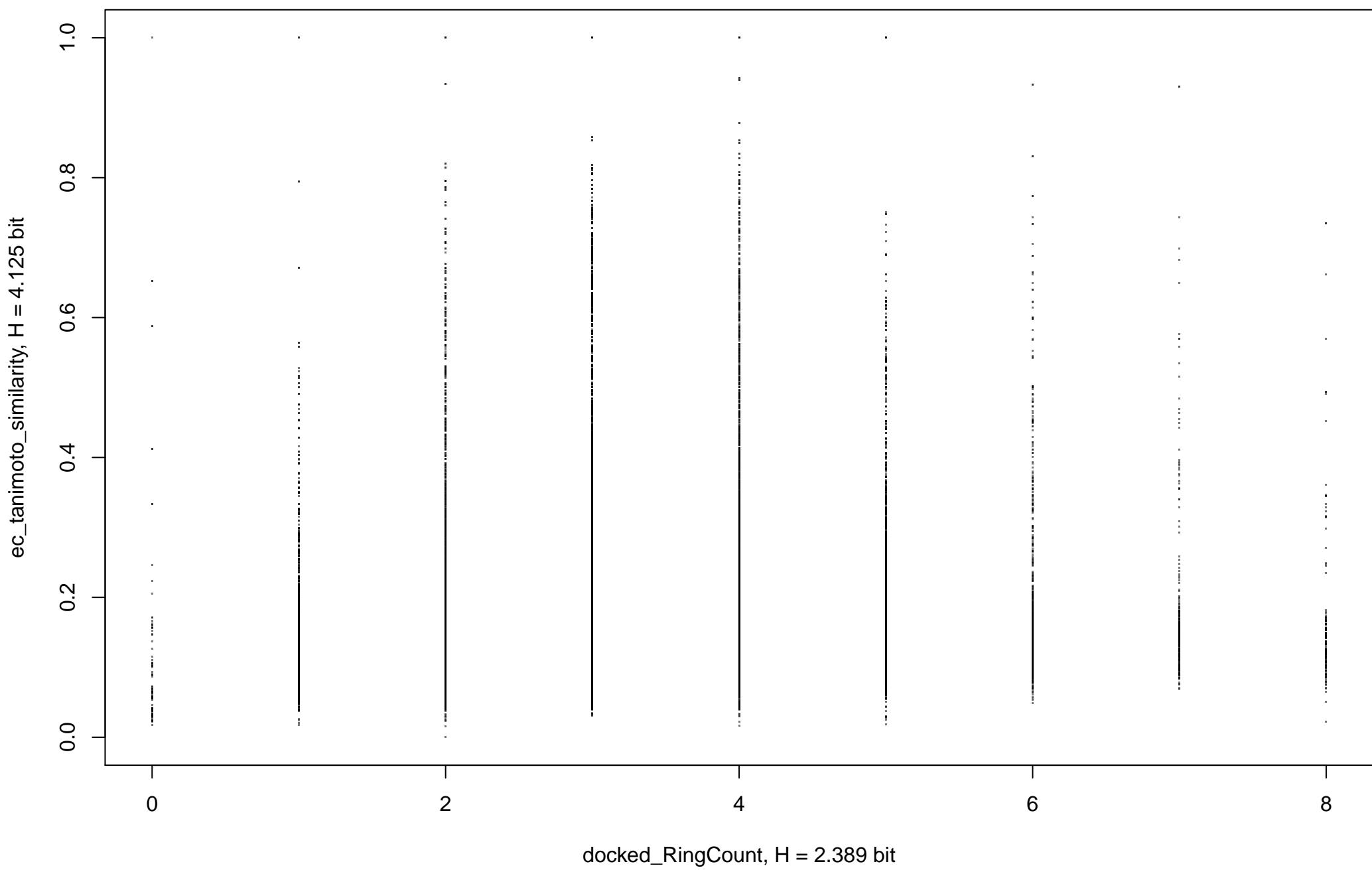


logrmsd, H = 3.606 bit

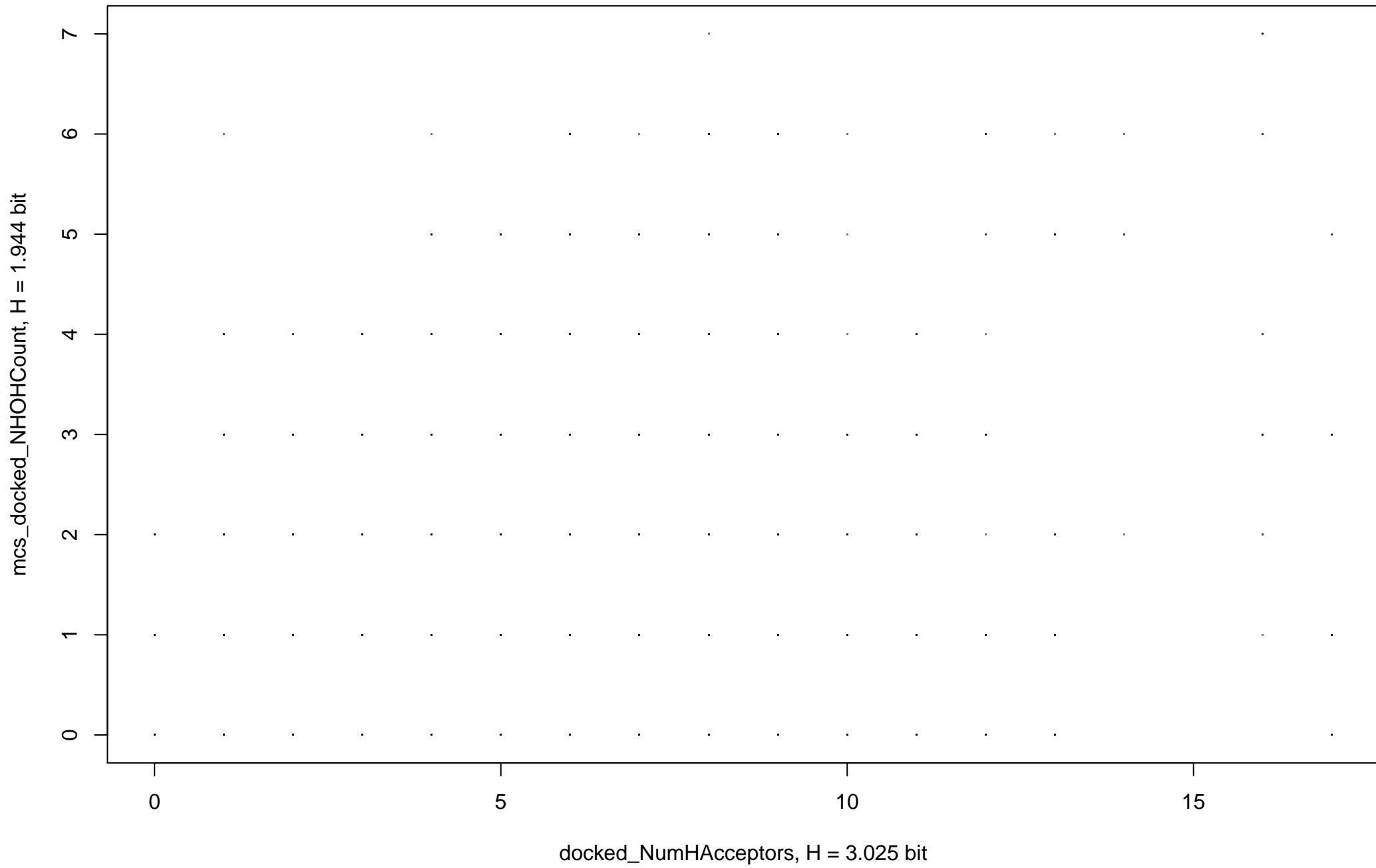
docked_NumHAcceptors-mcs_docked_NumHDonors, MI = 0.05938 bit, normMI = 0.03055



docked_RingCount-ec_tanimoto_similarity, MI = 0.07297 bit, normMI = 0.03054

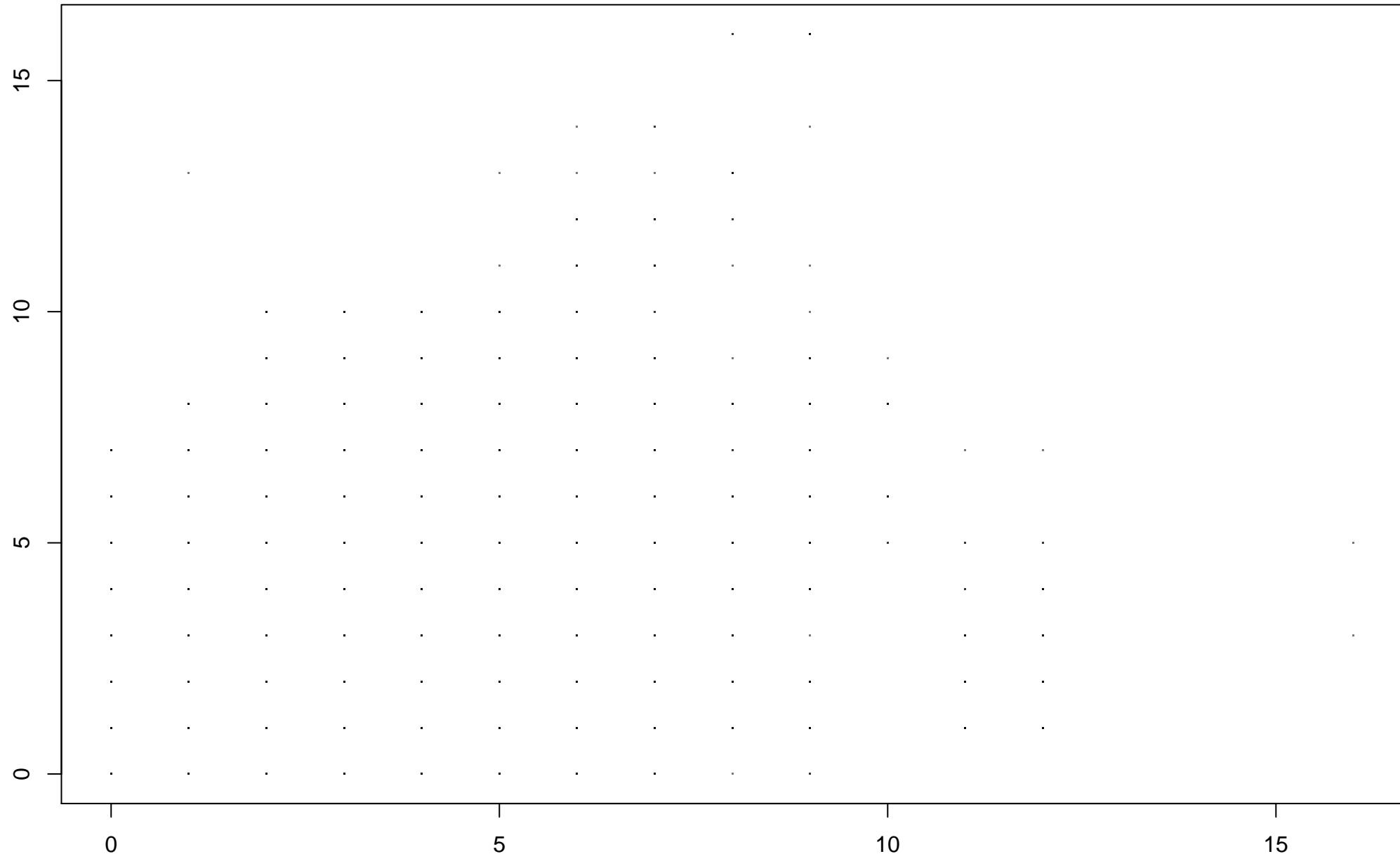


docked_NumHAcceptors–mcs_docked_NHOHCount, MI = 0.05923 bit, normMI = 0.03047



template_NHOHCount-mcs_NOCount, MI = 0.08396 bit, normMI = 0.03025

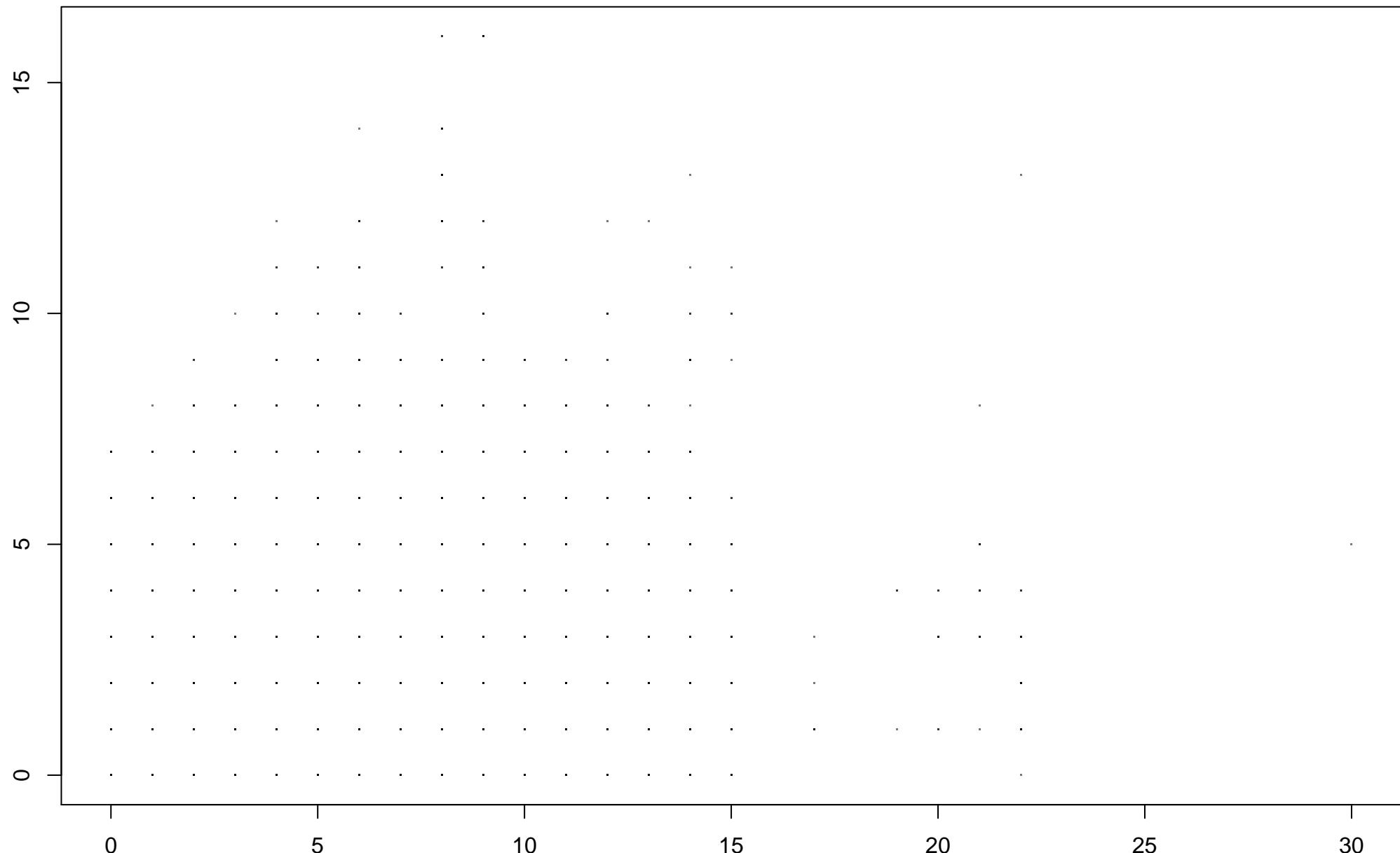
mcs_NOCount, H = 2.777 bit



template_NHOHCount, H = 2.775 bit

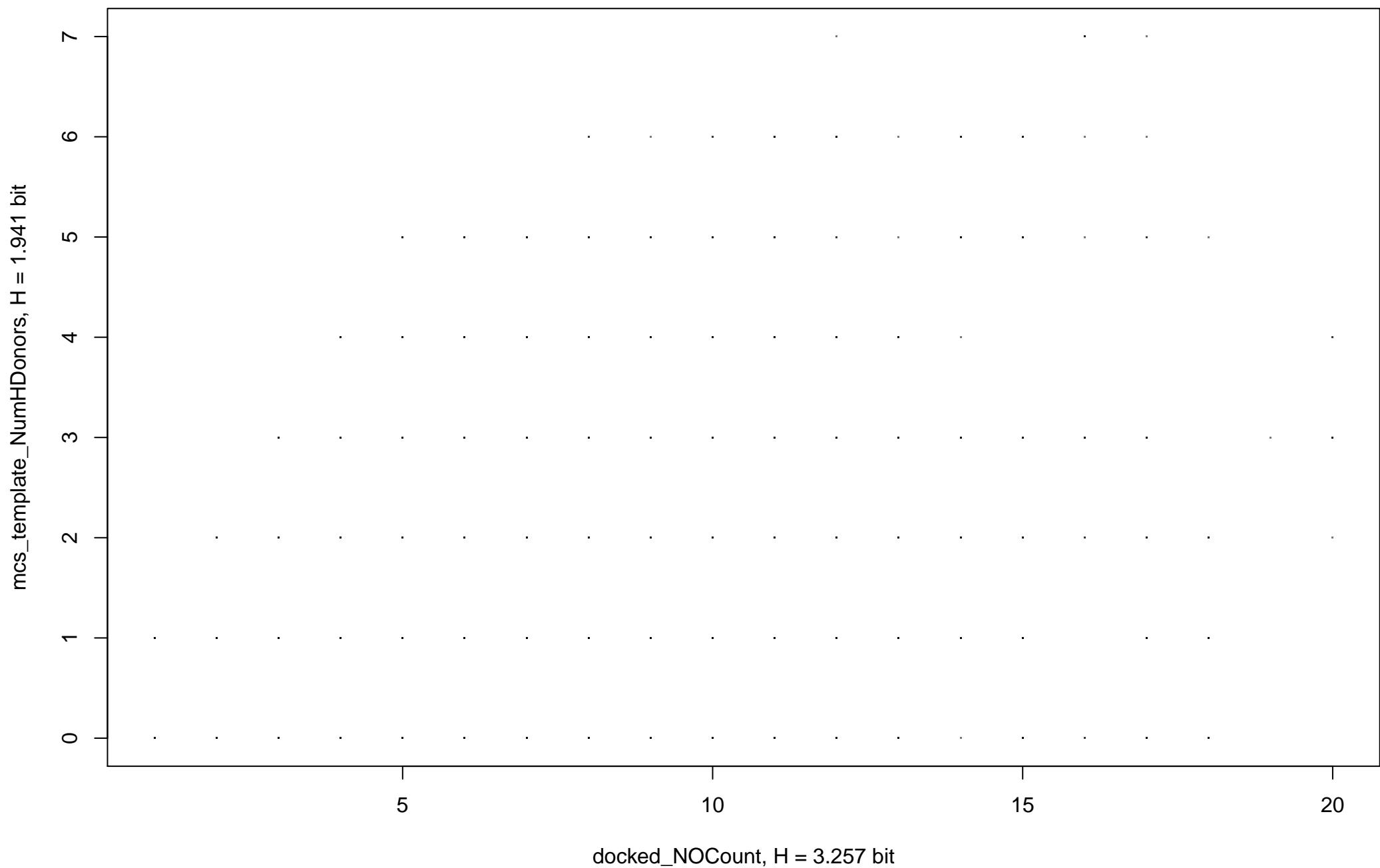
docked_NumRotatableBonds-mcs_NOCount, MI = 0.08337 bit, normMI = 0.03003

mcs_NOCount, H = 2.777 bit

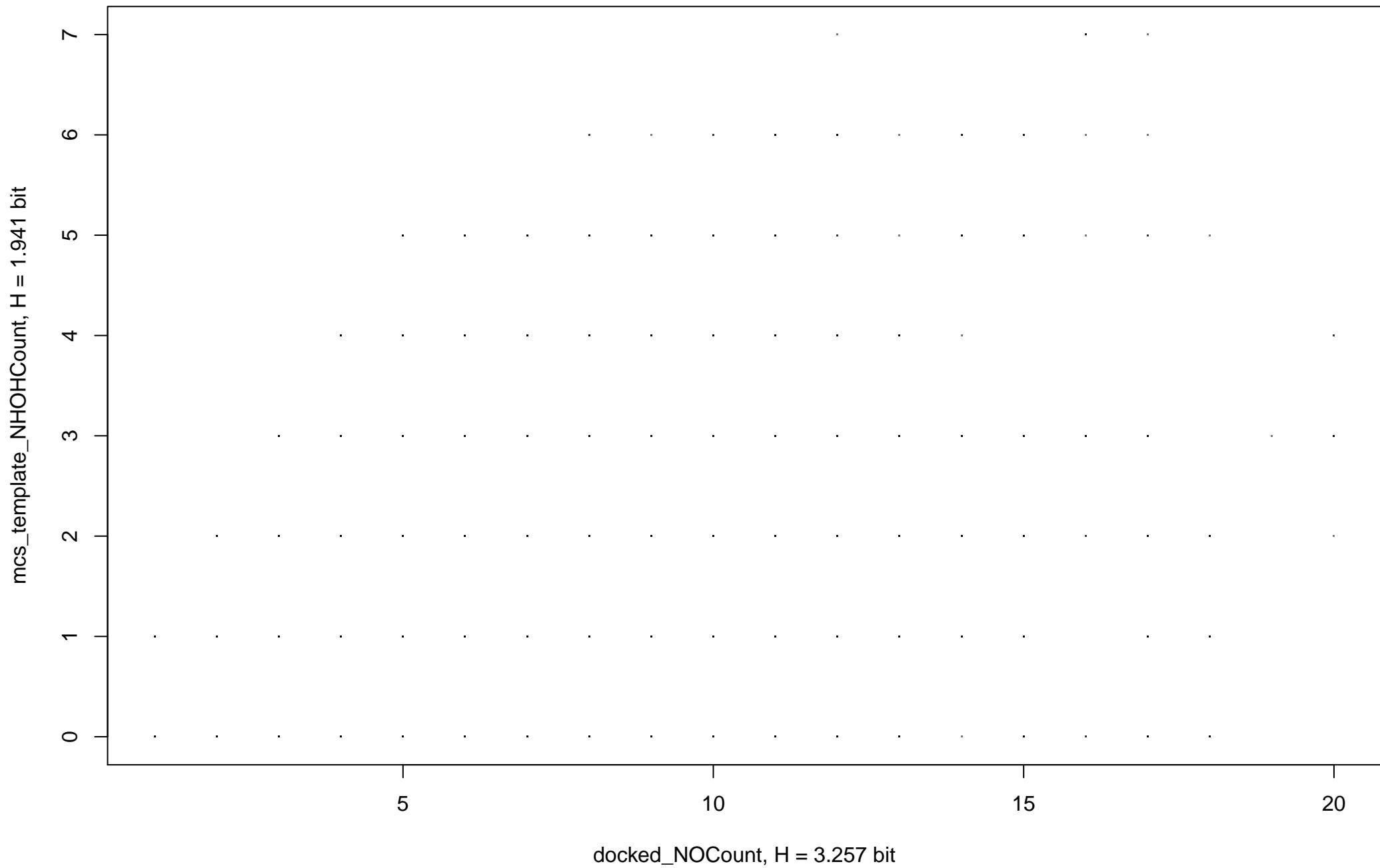


docked_NumRotatableBonds, H = 3.667 bit

docked_NOCOUNT-mcs_template_NumHDonors, MI = 0.05795 bit, normMI = 0.02986

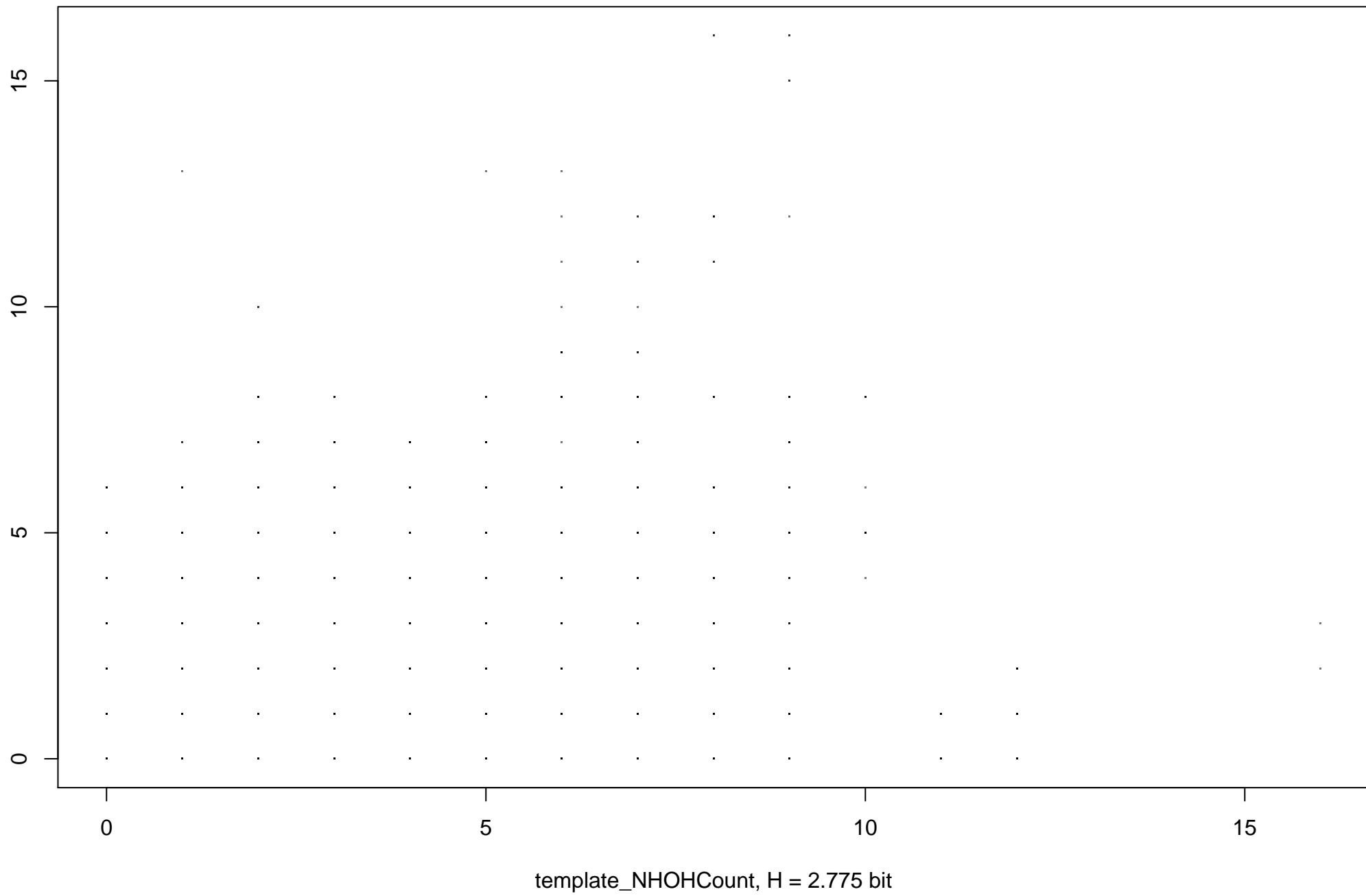


docked_NOCount-mcs_template_NHOHCount, MI = 0.05787 bit, normMI = 0.02981



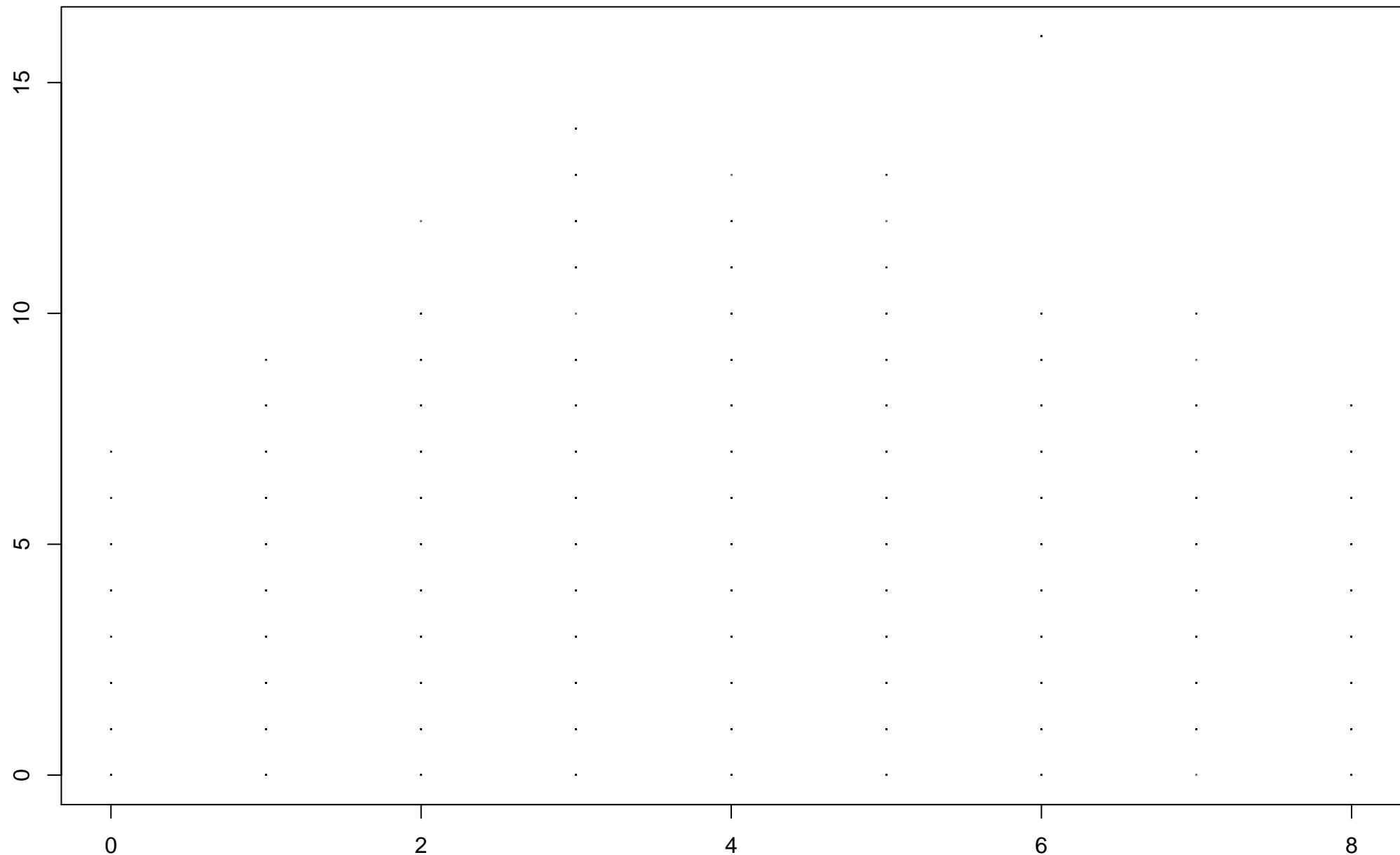
template_NHOHCount-mcs_template_NumHAcceptors, MI = 0.07402 bit, normMI = 0.02975

mcs_template_NumHAcceptors, H = 2.488 bit



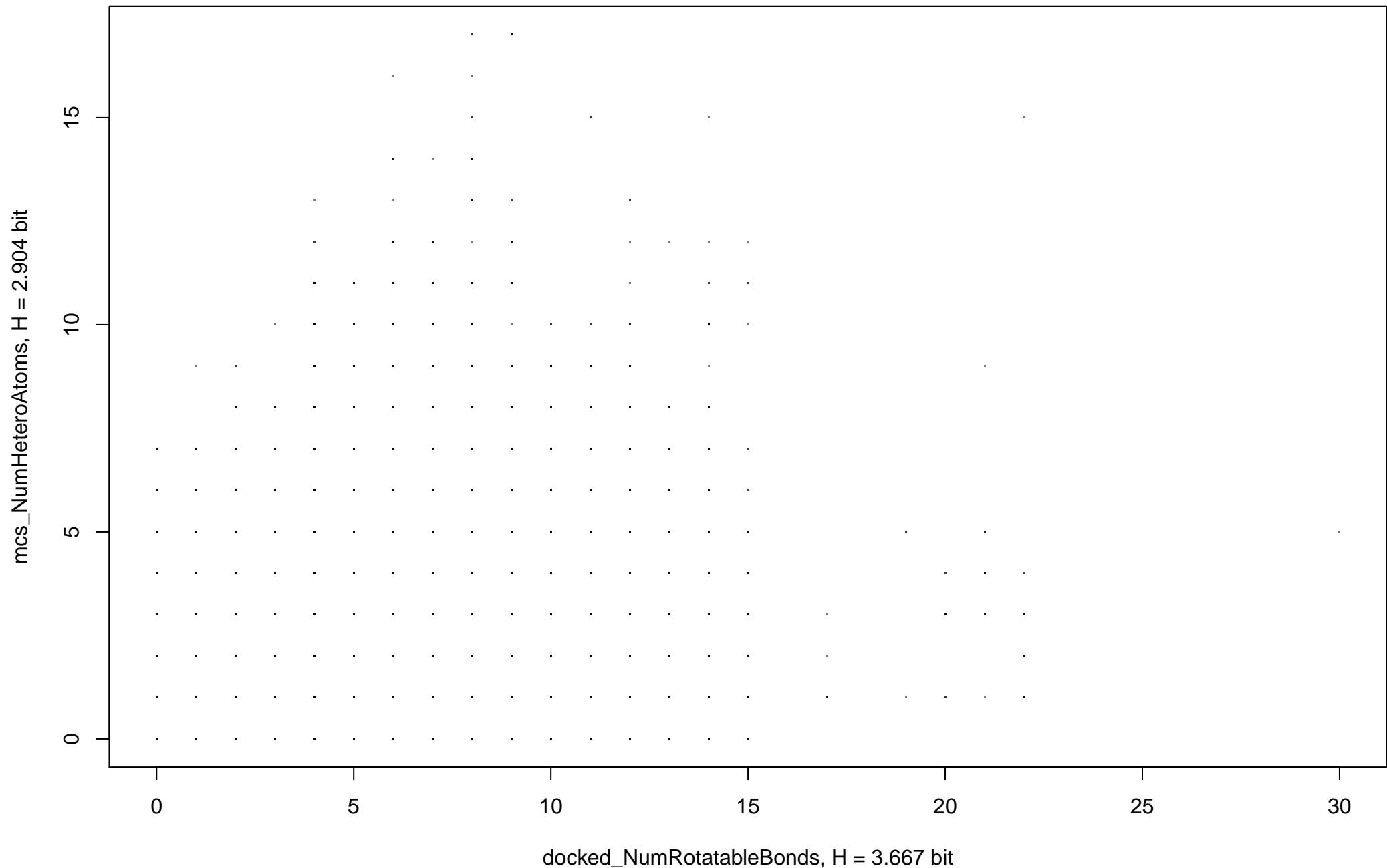
template_RingCount–mcs_NOCount, MI = 0.06993 bit, normMI = 0.02968

mcs_NOCount, H = 2.777 bit

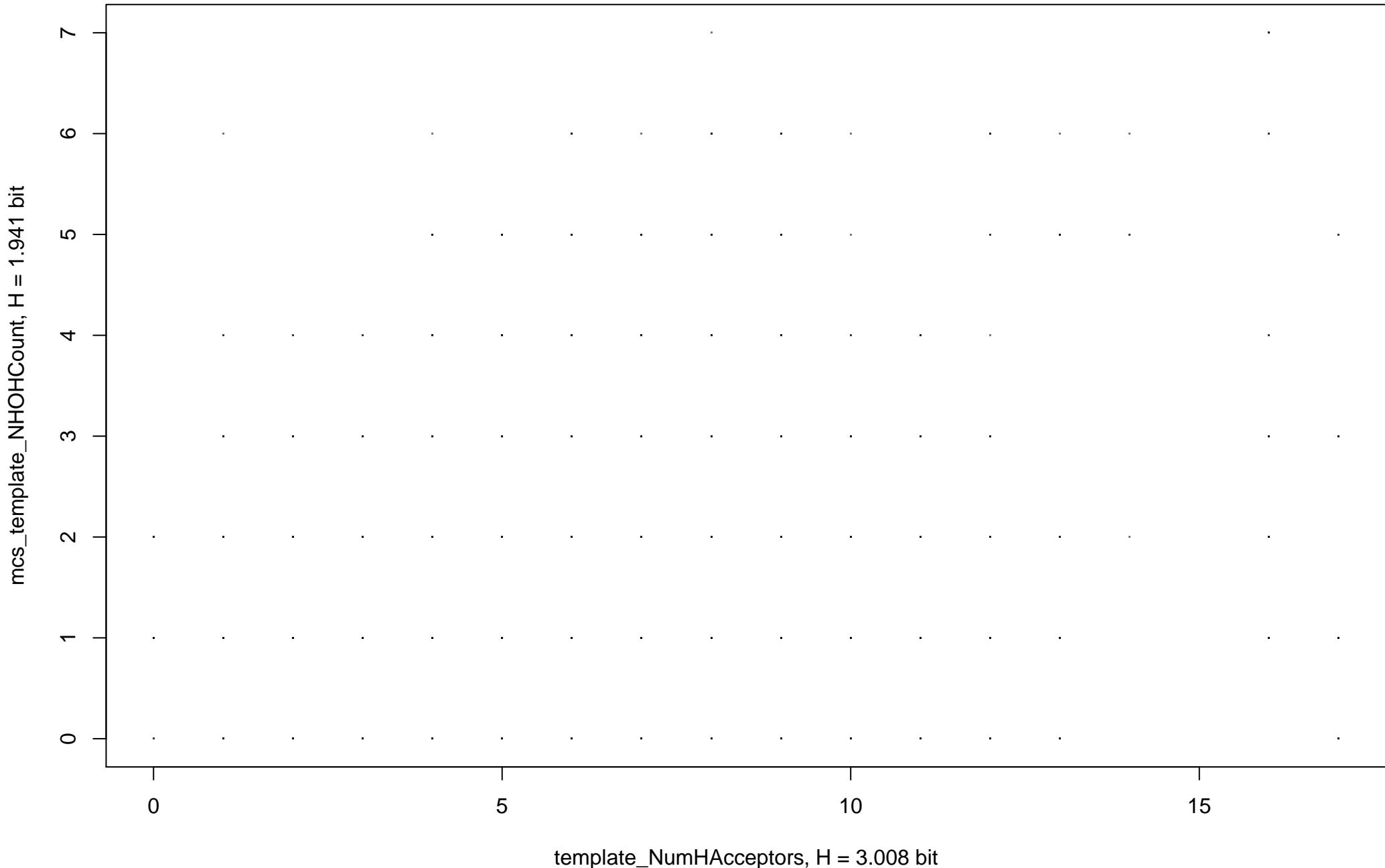


template_RingCount, H = 2.356 bit

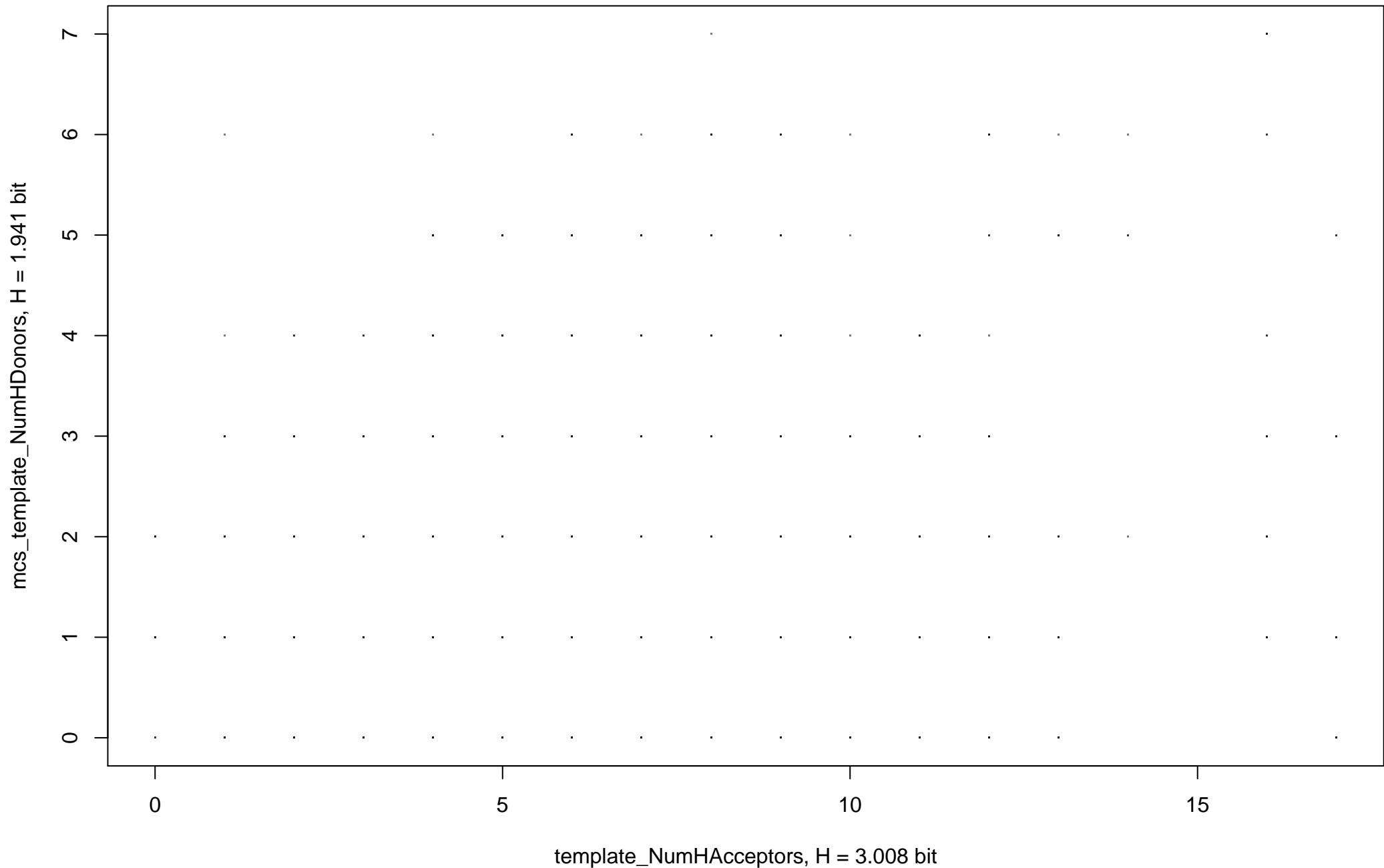
docked_NumRotatableBonds-mcs_NumHeteroAtoms, MI = 0.08569 bit, normMI = 0.0295



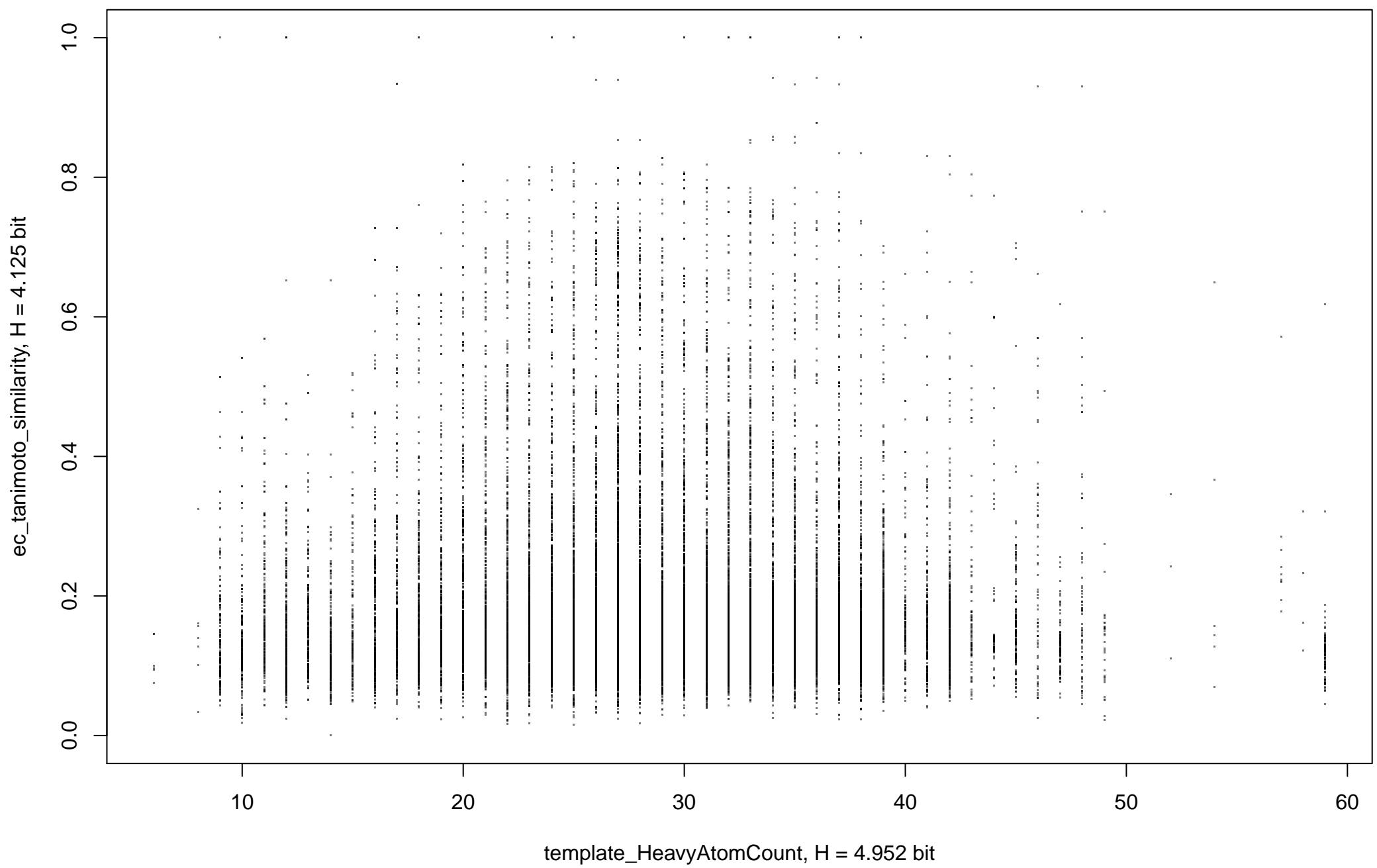
template_NumHAcceptors-mcs_template_NHOHCount, MI = 0.05719 bit, normMI = 0.02946



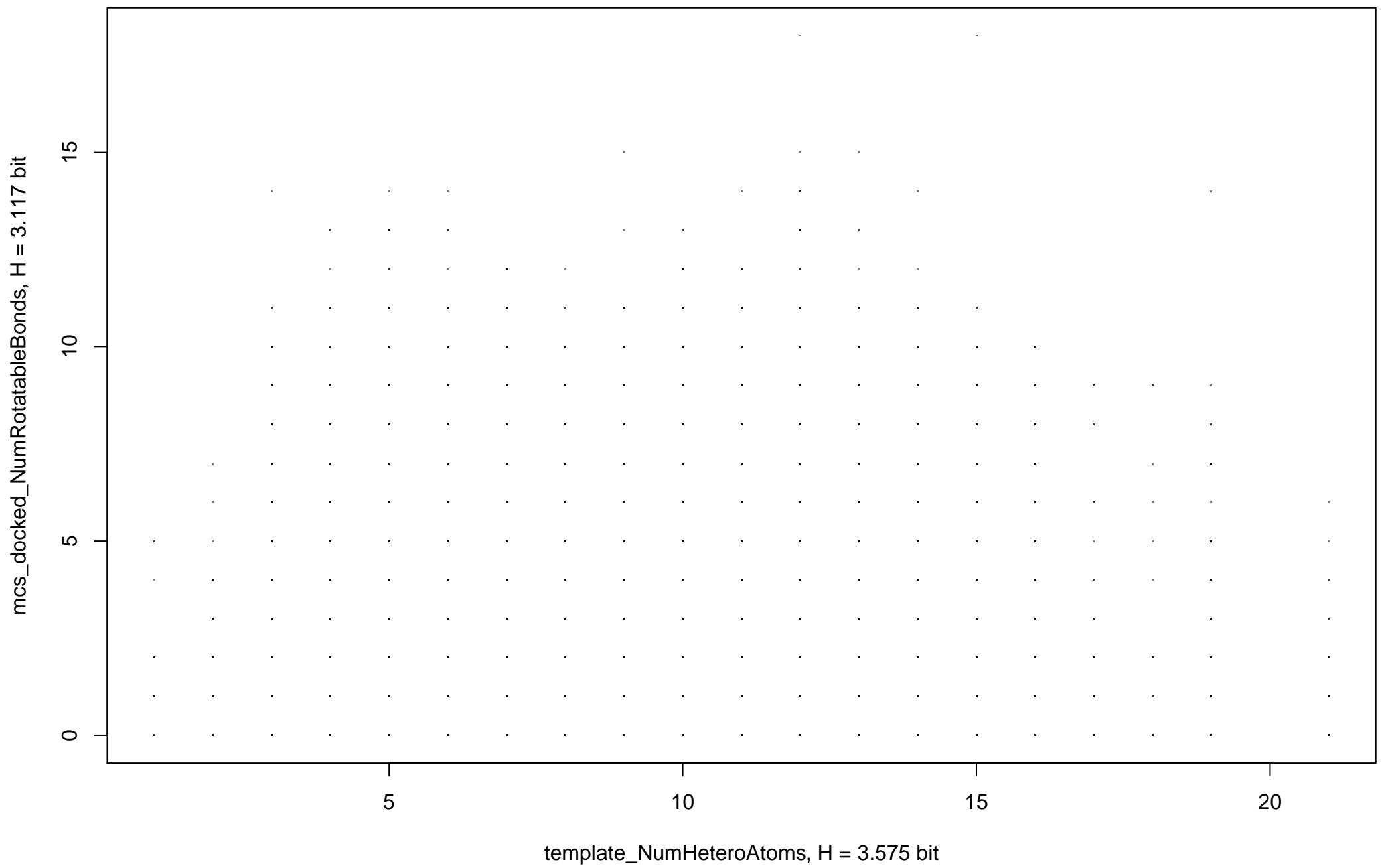
template_NumHAcceptors-mcs_template_NumHDonors, MI = 0.05715 bit, normMI = 0.02945



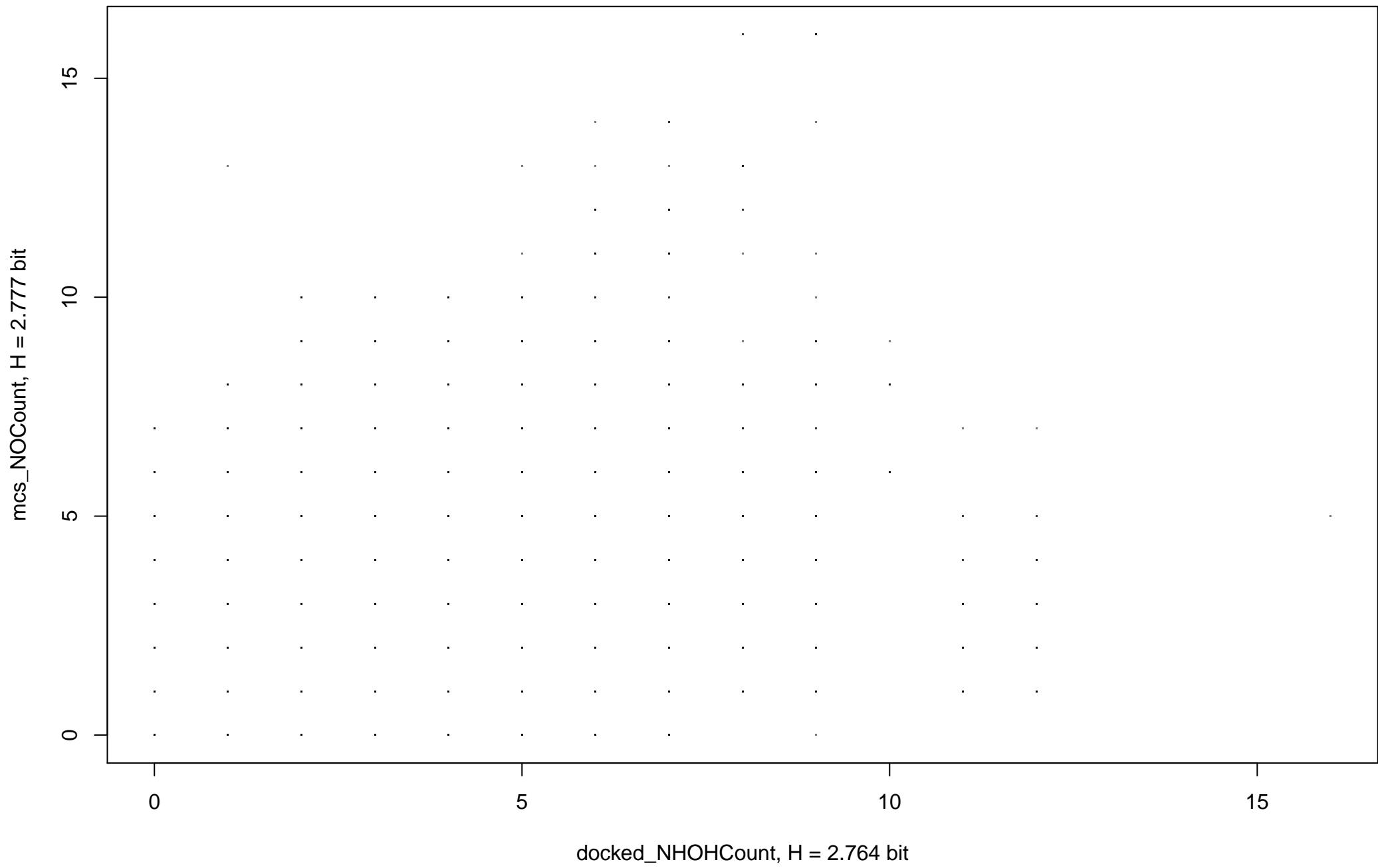
template_HeavyAtomCount–ec_tanimoto_similarity, MI = 0.1213 bit, normMI = 0.02941



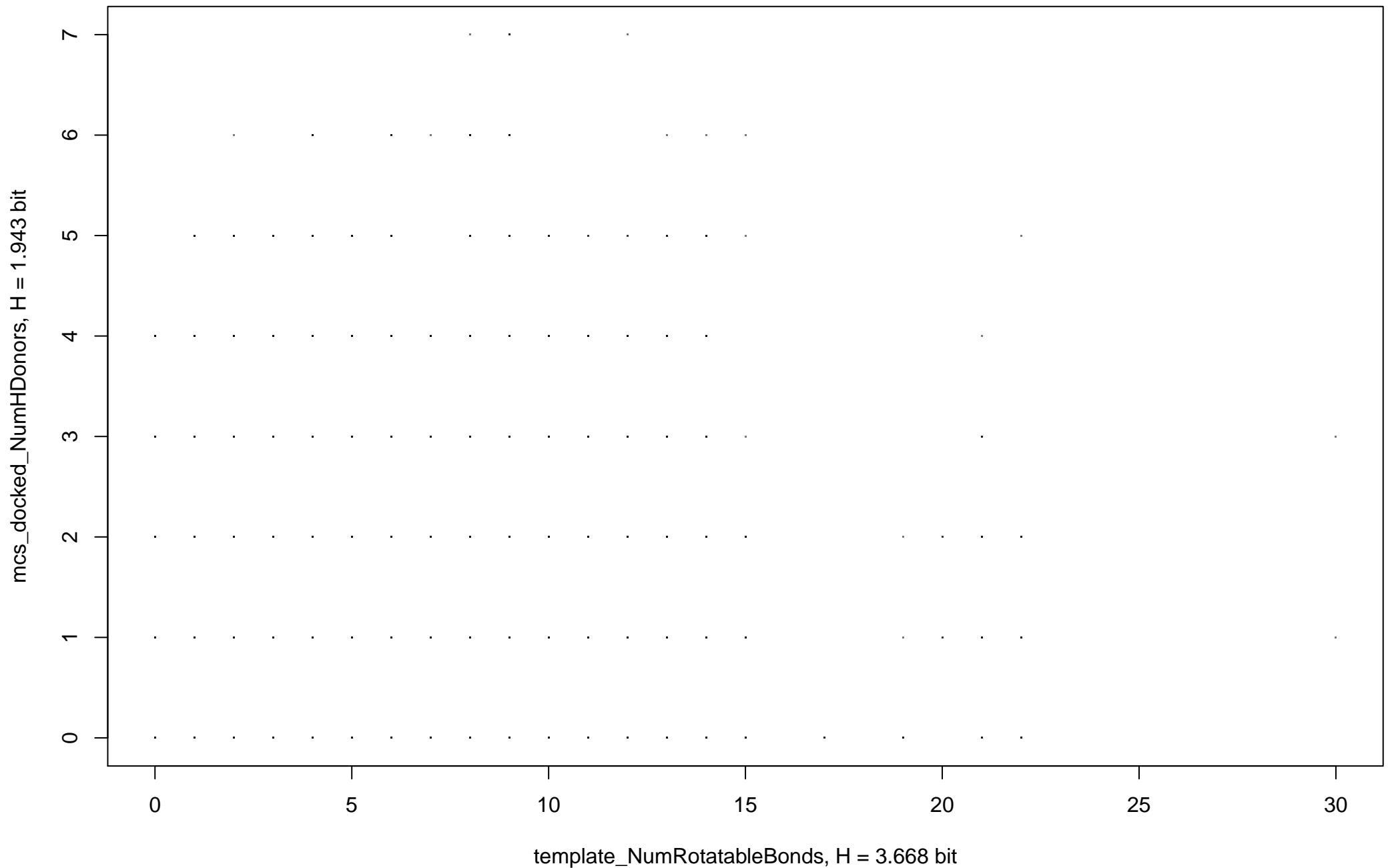
template_NumHeteroAtoms–mcs_docked_NumRotatableBonds, MI = 0.09133 bit, normMI = 0.0293



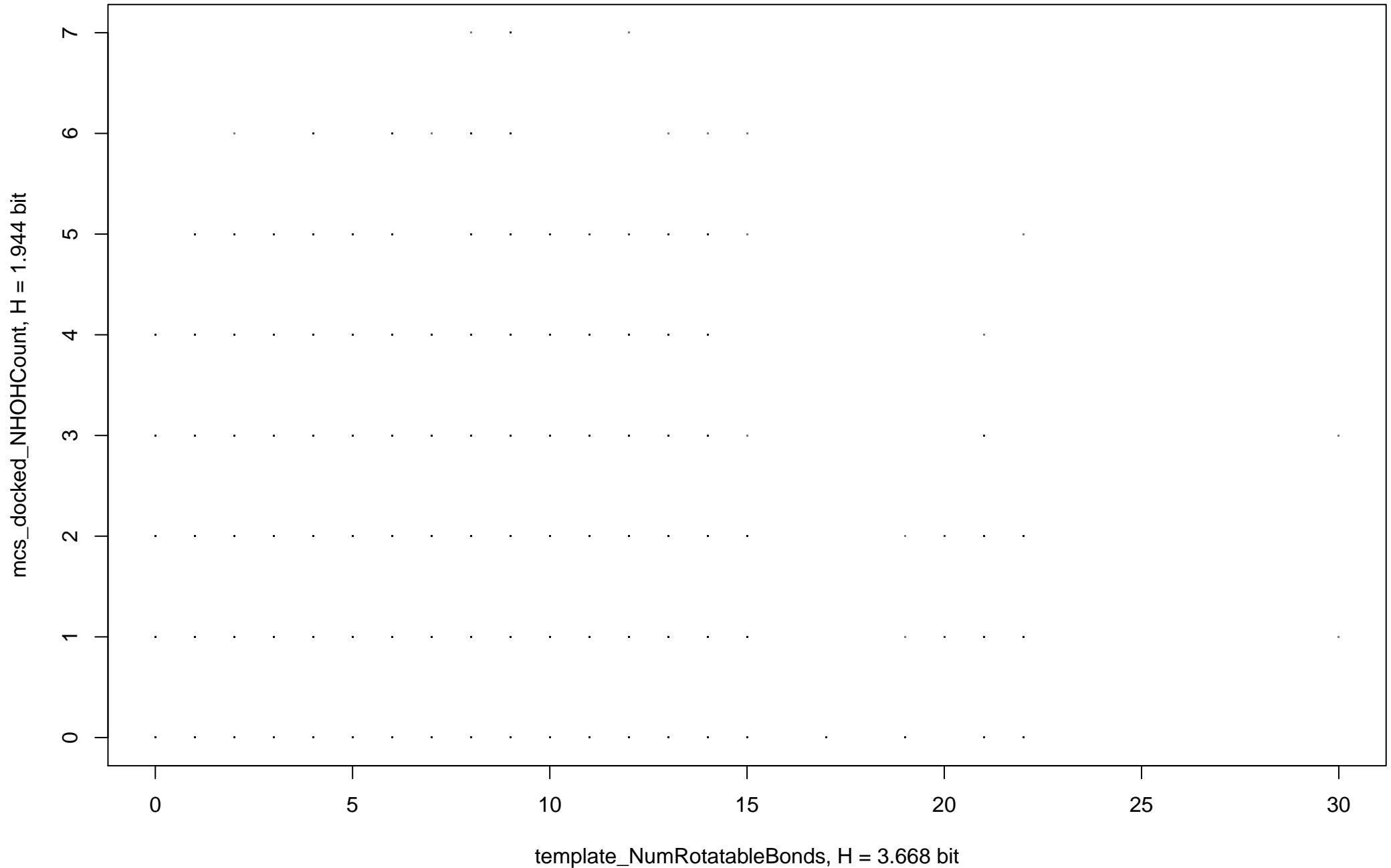
docked_NHOHCount–mcs_NOCount, MI = 0.08078 bit, normMI = 0.02922



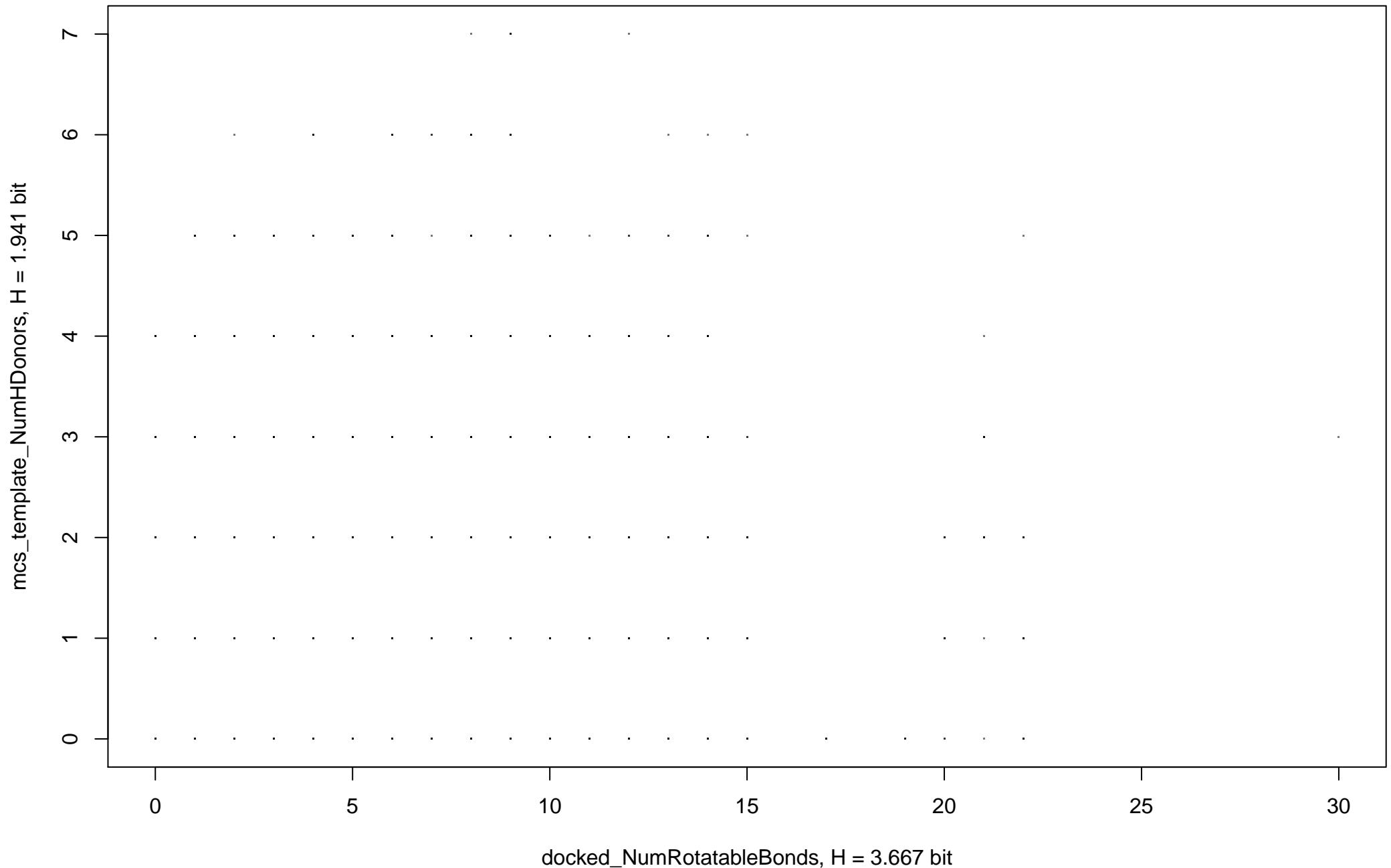
template_NumRotatableBonds-mcs_docked_NumHDonors, MI = 0.05634 bit, normMI = 0.02899



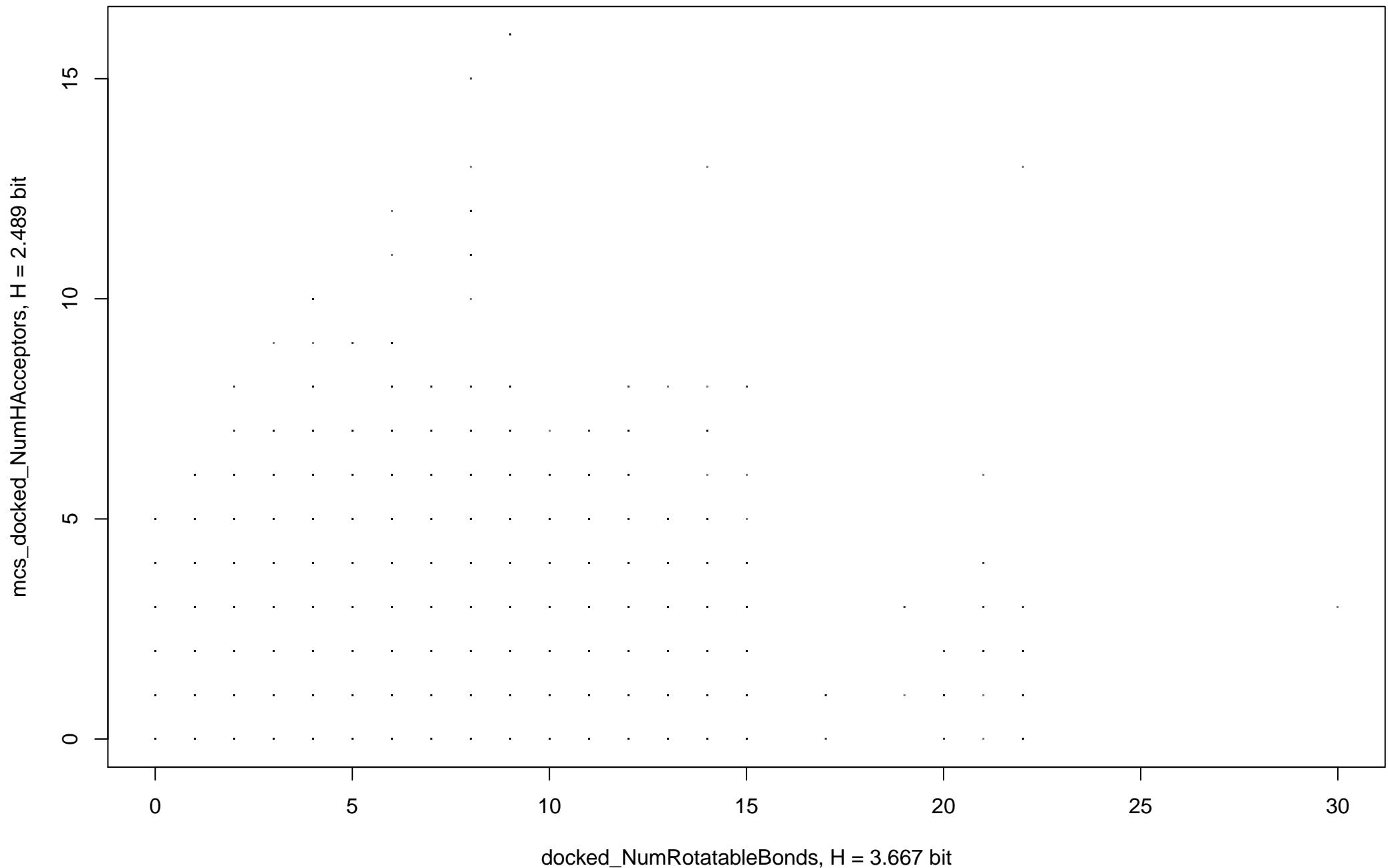
template_NumRotatableBonds-mcs_docked_NHOHCount, MI = 0.05617 bit, normMI = 0.02889



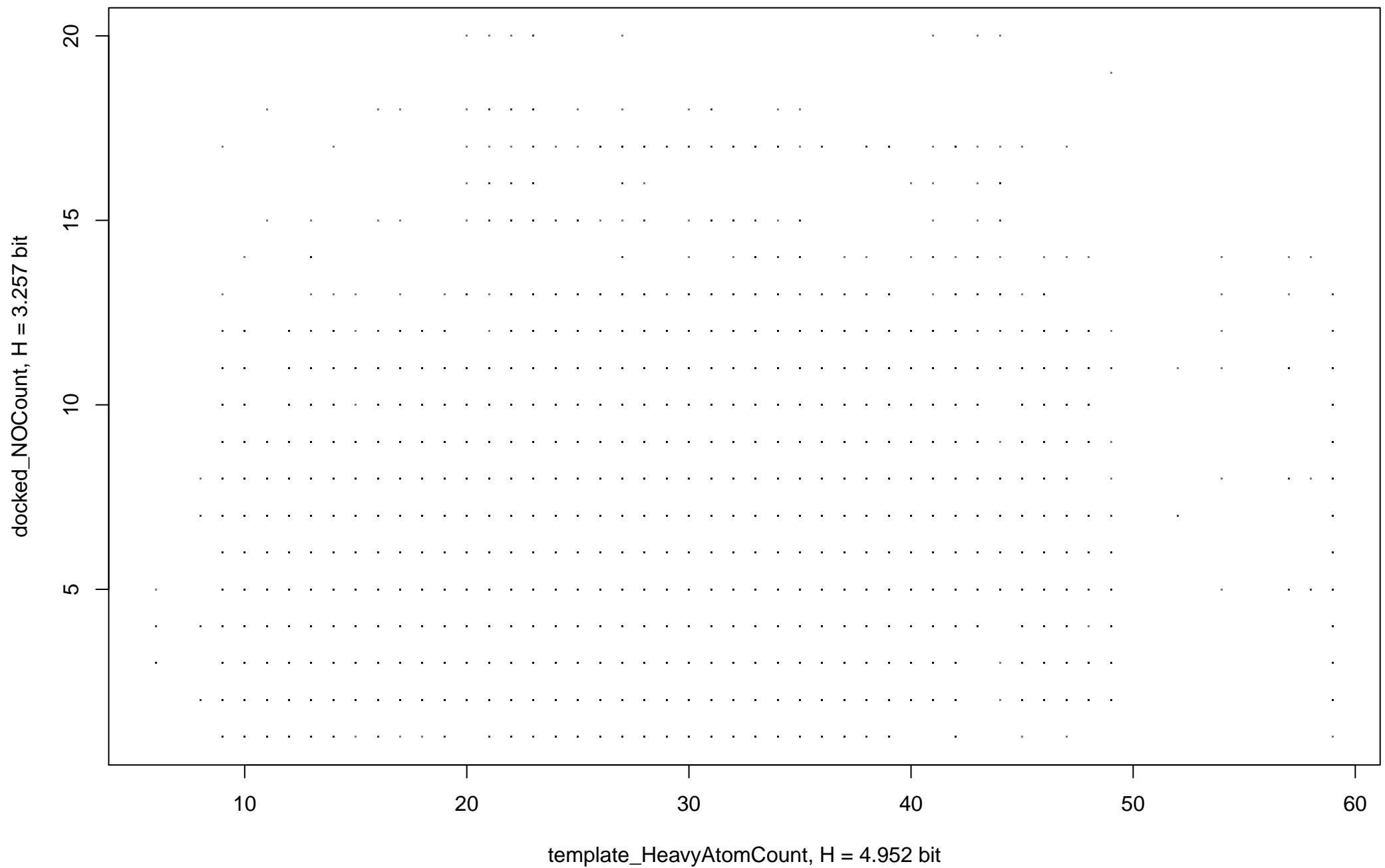
docked_NumRotatableBonds-mcs_template_NumHDonors, MI = 0.05537 bit, normMI = 0.02853



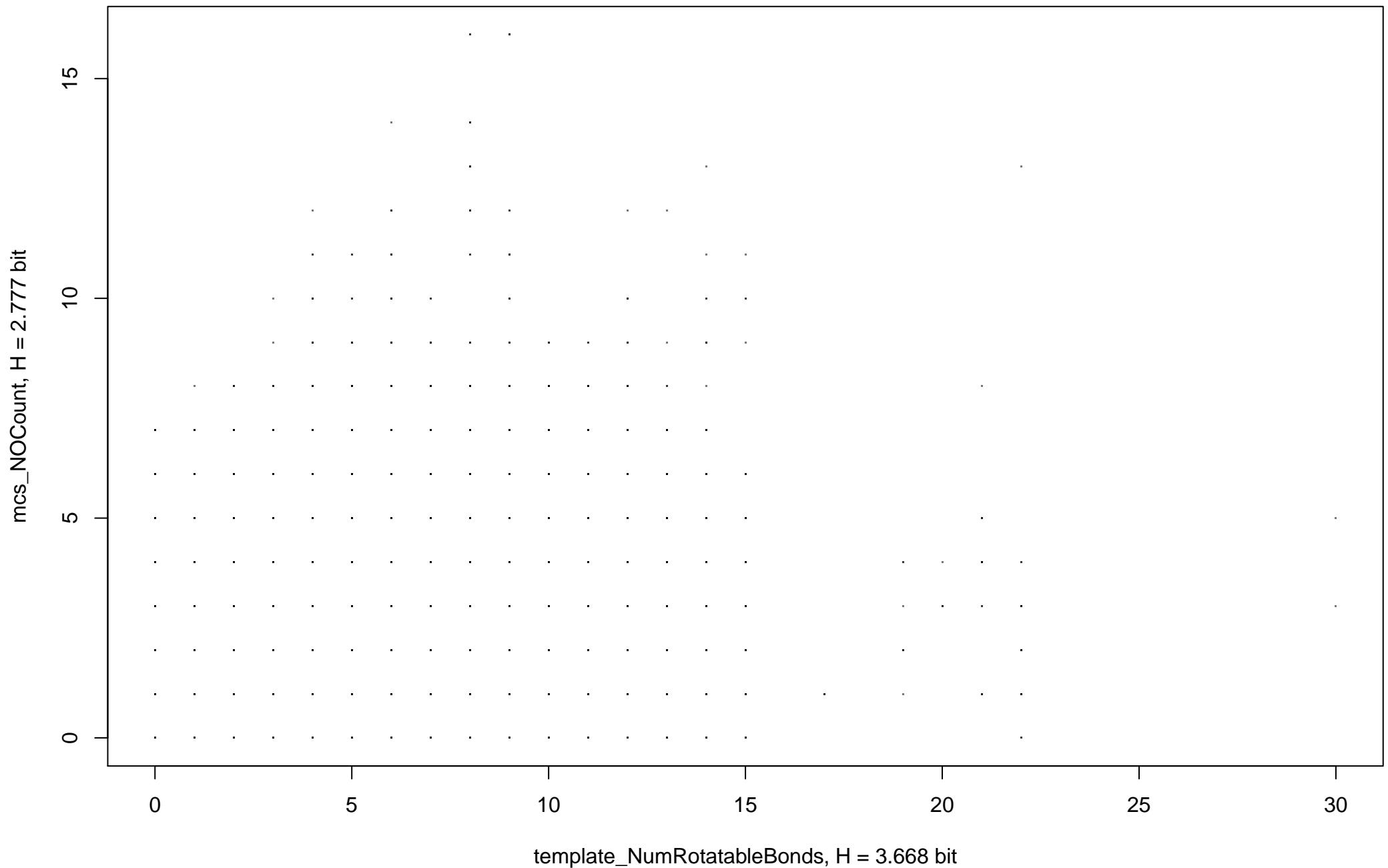
docked_NumRotatableBonds-mcs_docked_NumHAcceptors, MI = 0.07094 bit, normMI = 0.0285



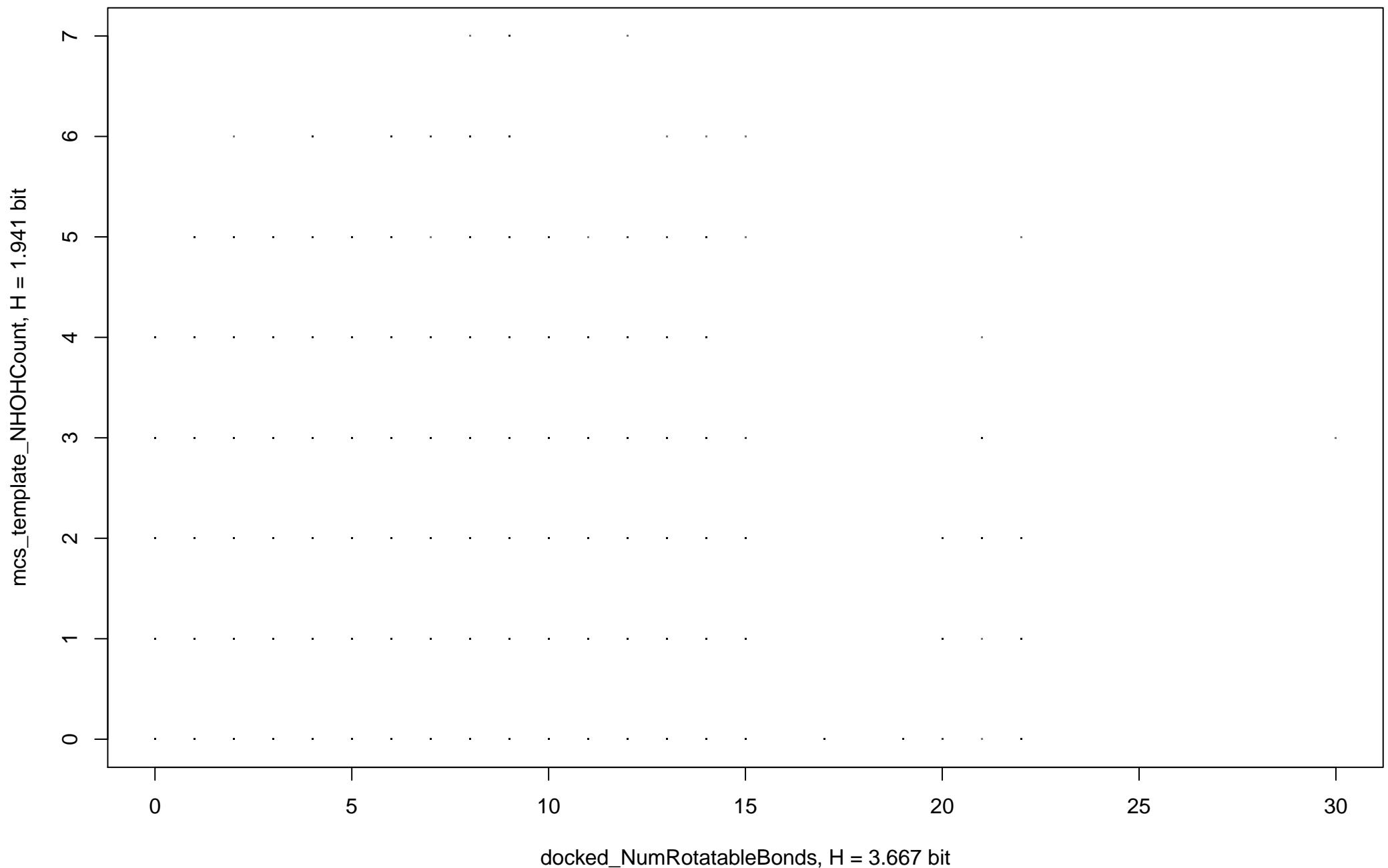
template_HeavyAtomCount-docked_NOCount, MI = 0.09267 bit, normMI = 0.02845



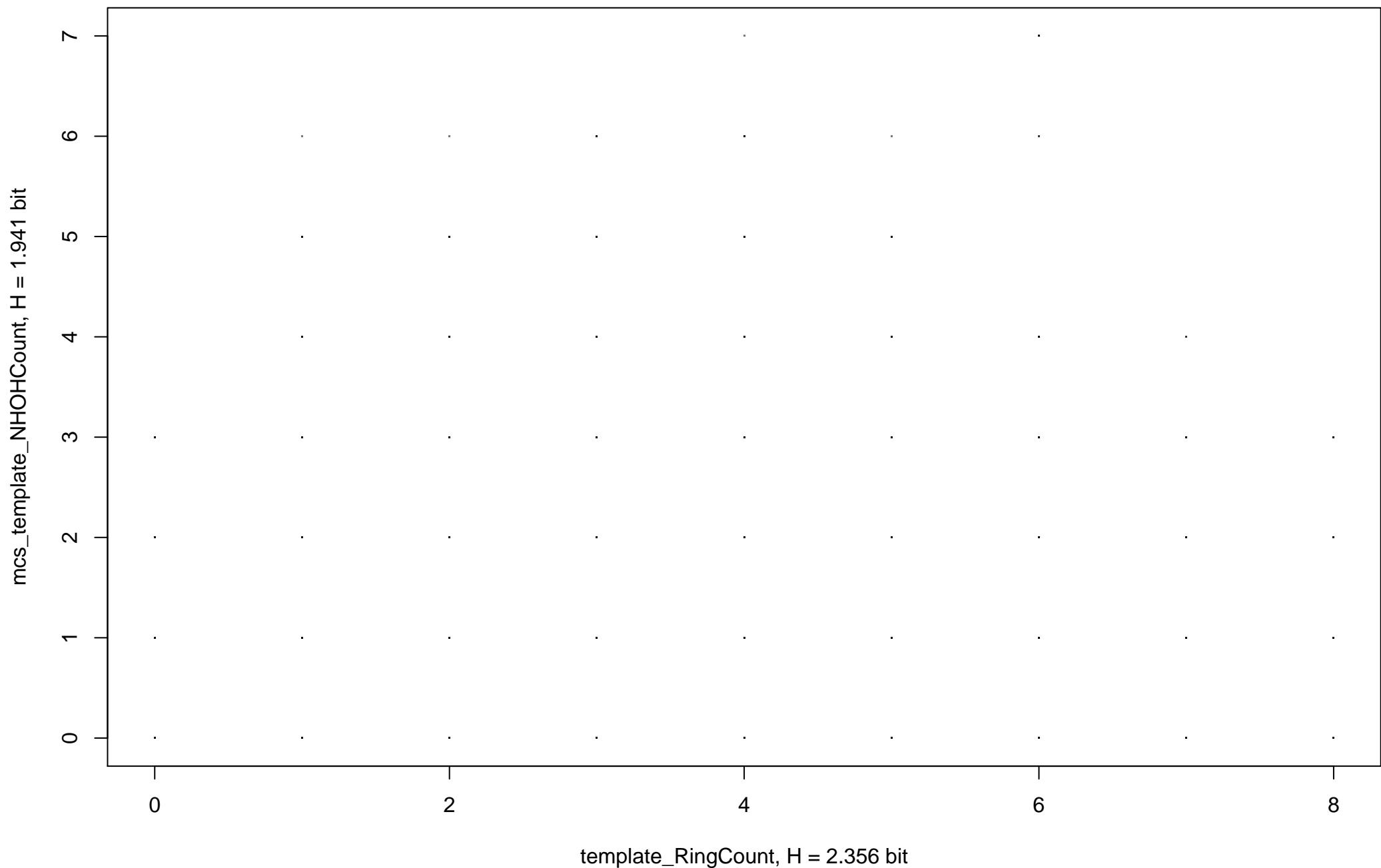
template_NumRotatableBonds-mcs_NOCount, MI = 0.07899 bit, normMI = 0.02845



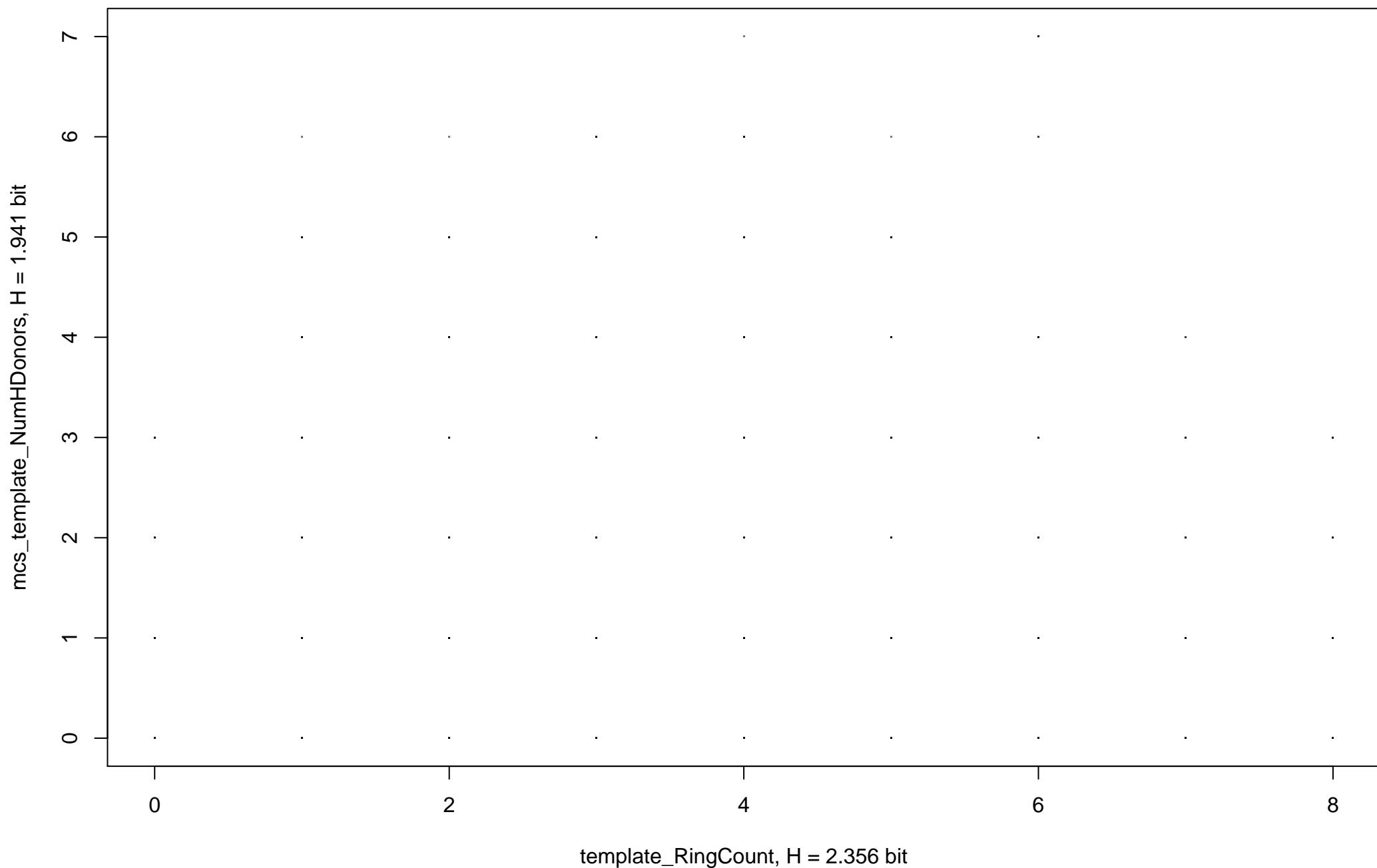
docked_NumRotatableBonds-mcs_template_NHOHCount, MI = 0.05509 bit, normMI = 0.02837



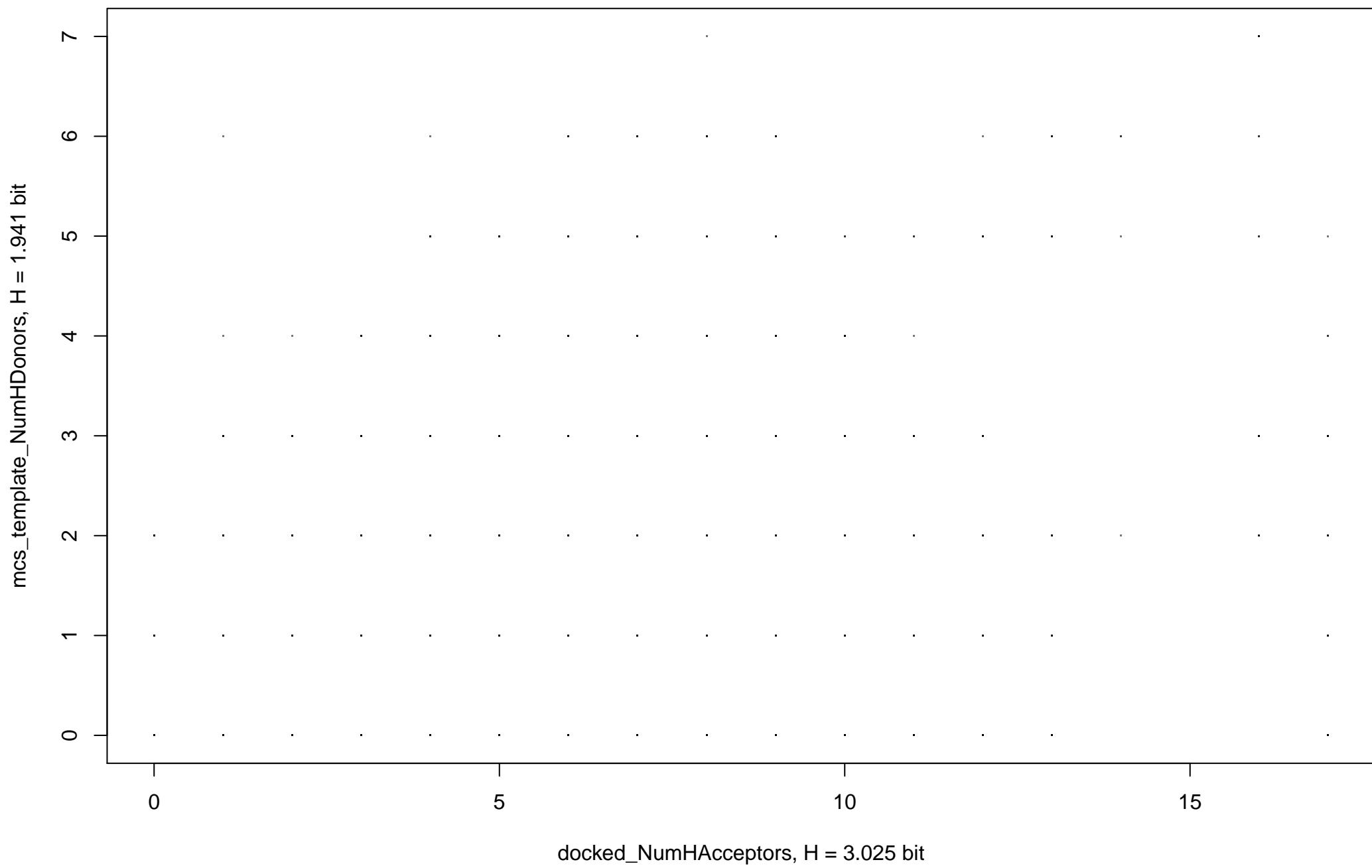
template_RingCount-mcs_template_NHOHCount, MI = 0.05482 bit, normMI = 0.02824



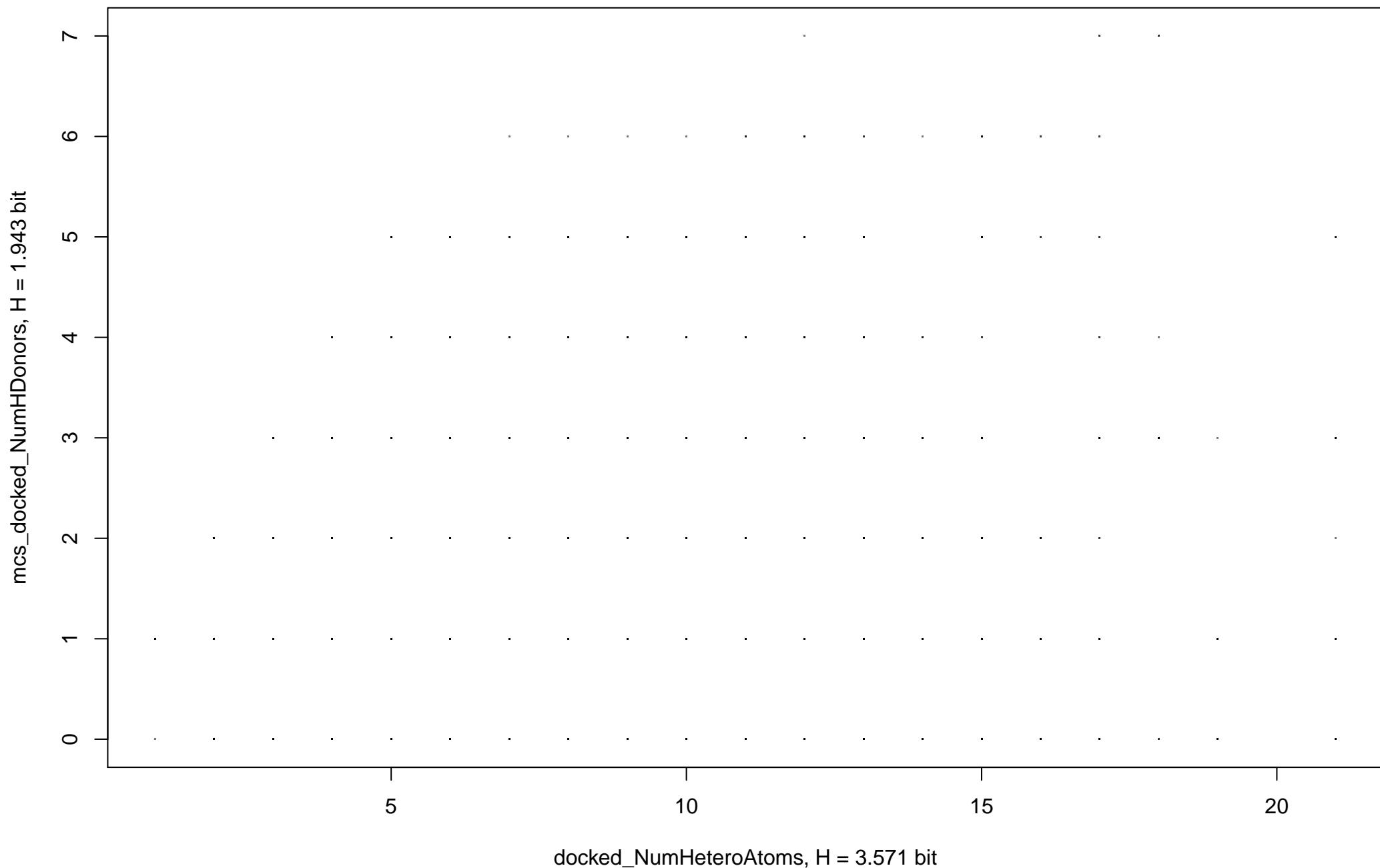
template_RingCount-mcs_template_NumHDonors, MI = 0.05468 bit, normMI = 0.02818



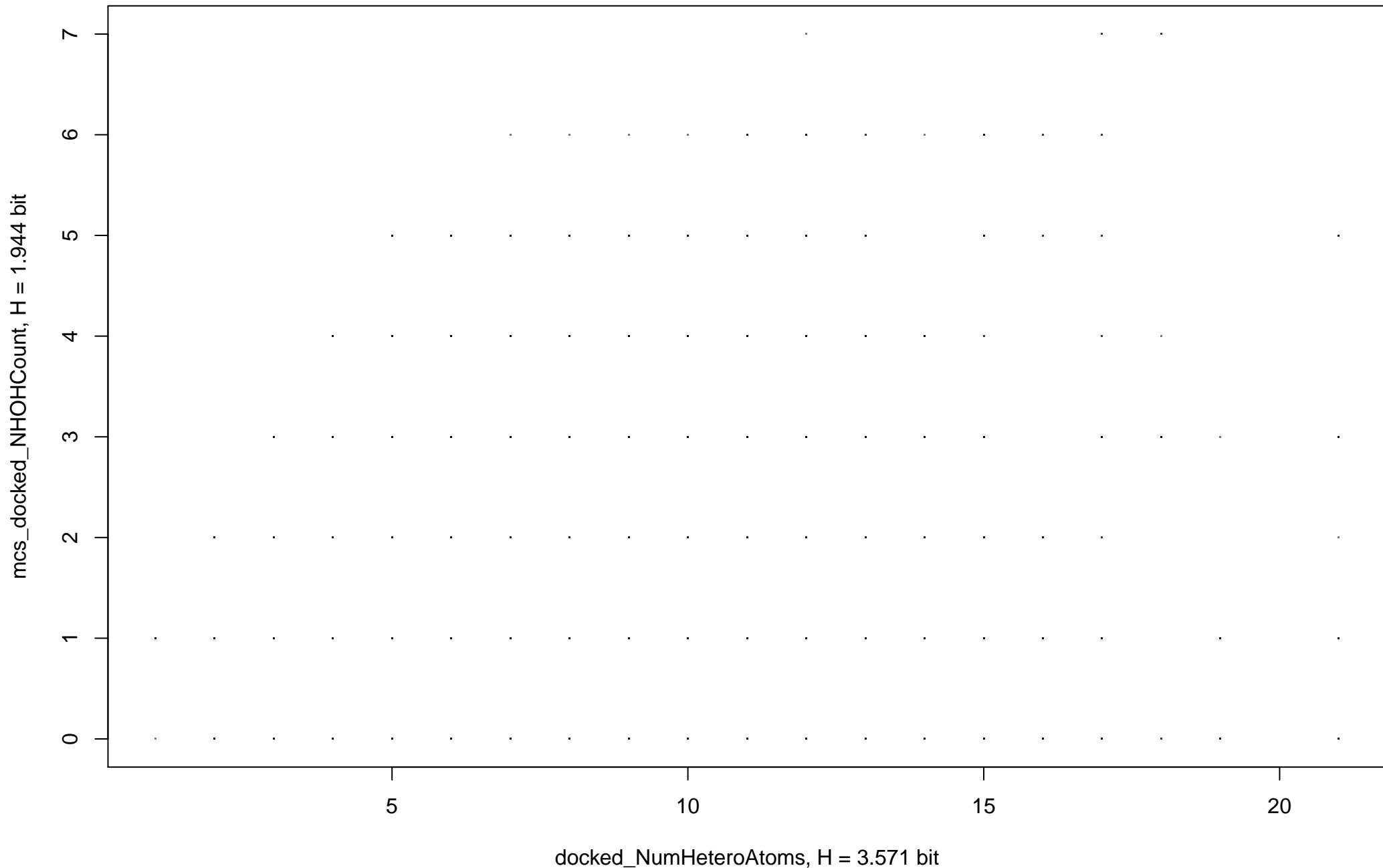
docked_NumHAcceptors-mcs_template_NumHDonors, MI = 0.05435 bit, normMI = 0.02801



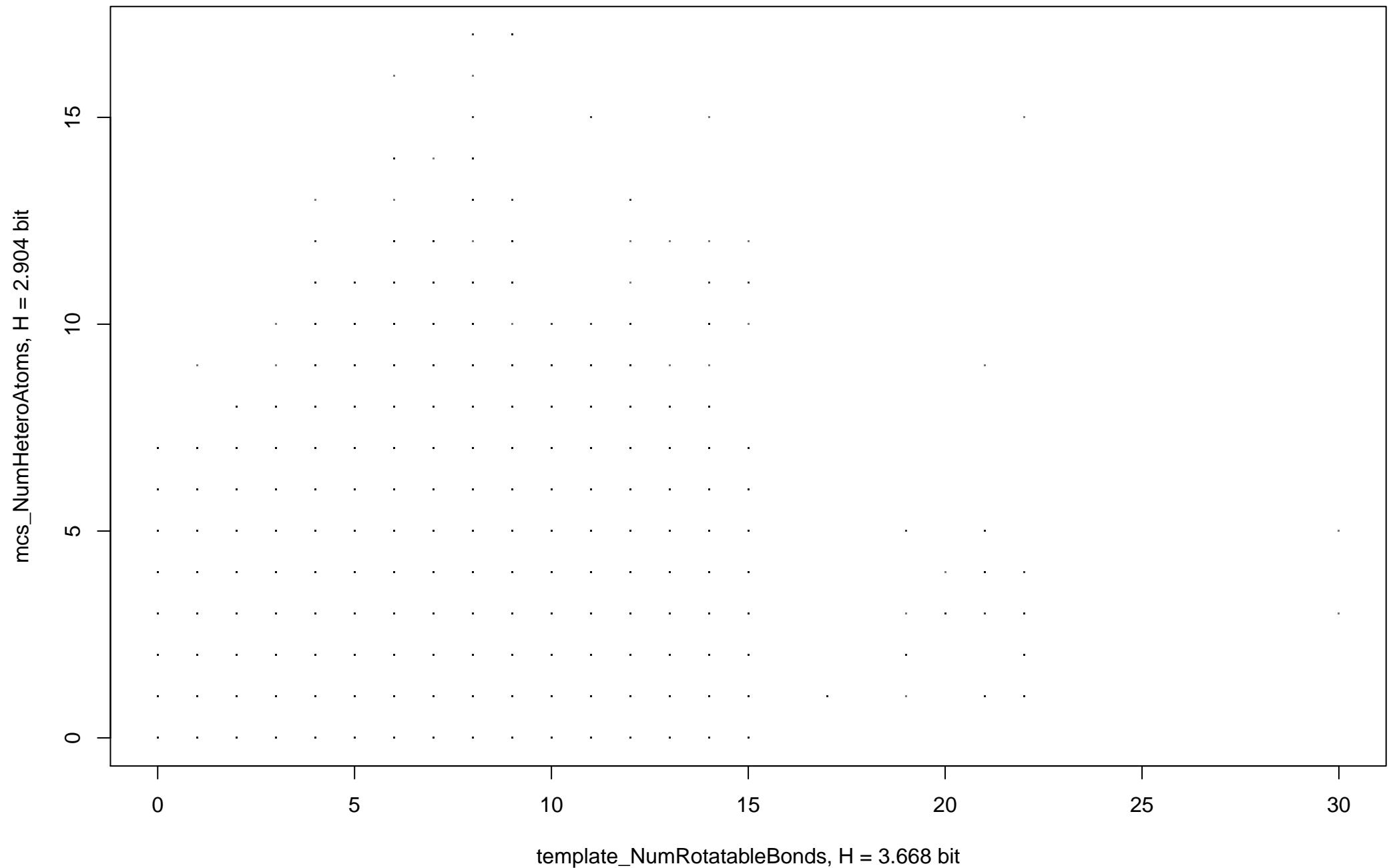
docked_NumHeteroAtoms-mcs_docked_NumHDonors, MI = 0.05442 bit, normMI = 0.028



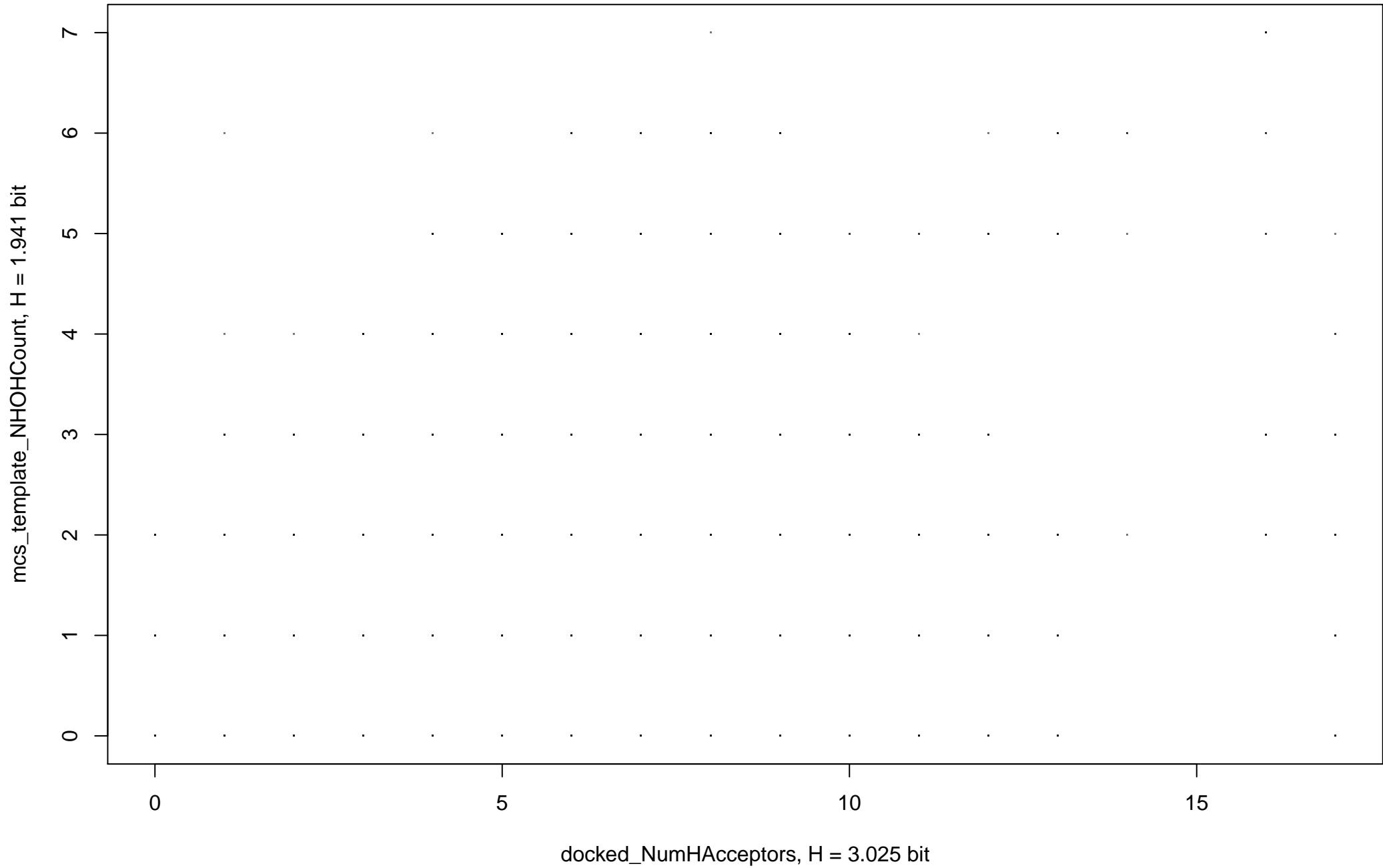
docked_NumHeteroAtoms-mcs_docked_NHOHCount, MI = 0.05426 bit, normMI = 0.02791



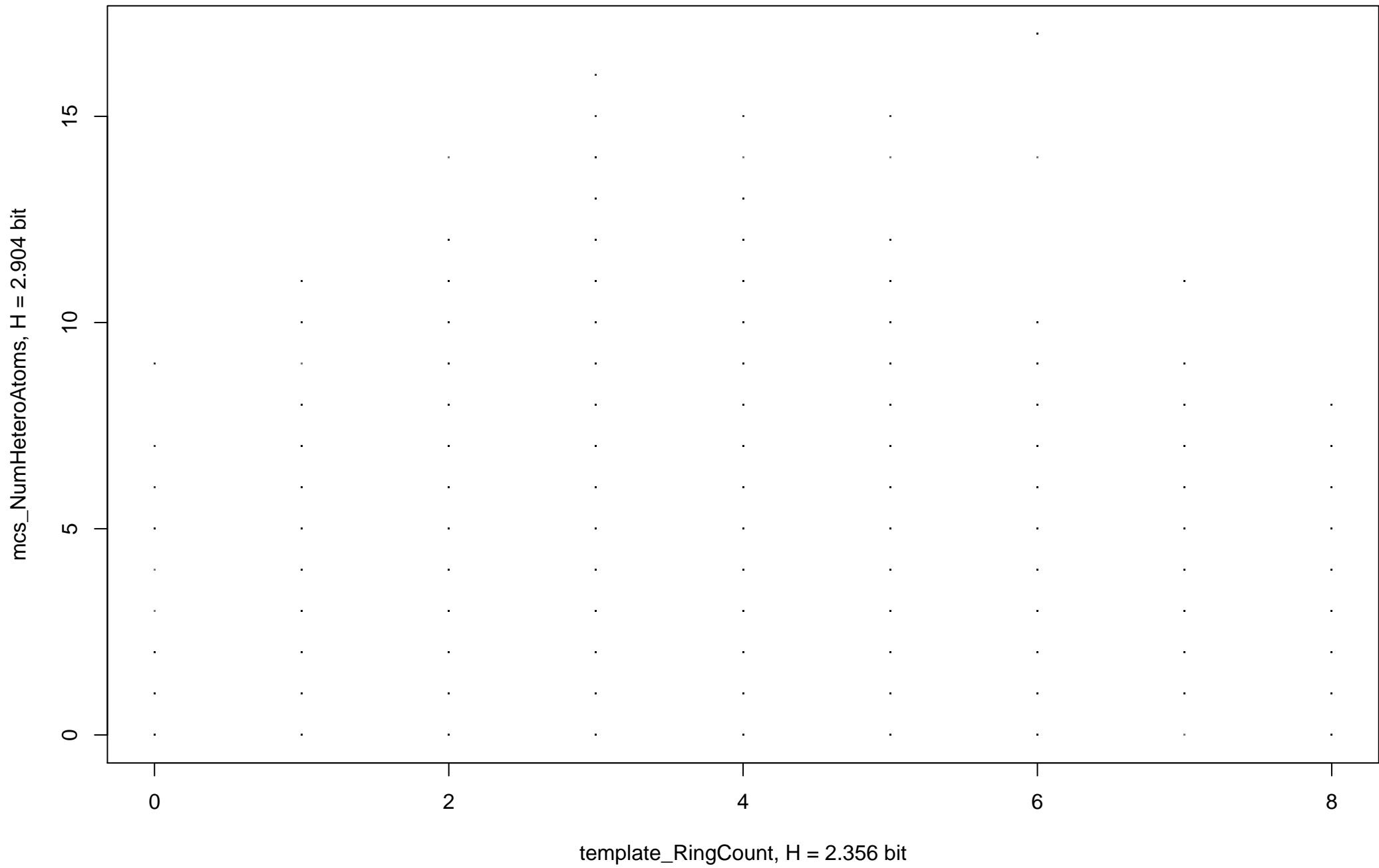
template_NumRotatableBonds-mcs_NumHeteroAtoms, MI = 0.08101 bit, normMI = 0.02789



docked_NumHAcceptors-mcs_template_NHOHCount, MI = 0.05407 bit, normMI = 0.02785

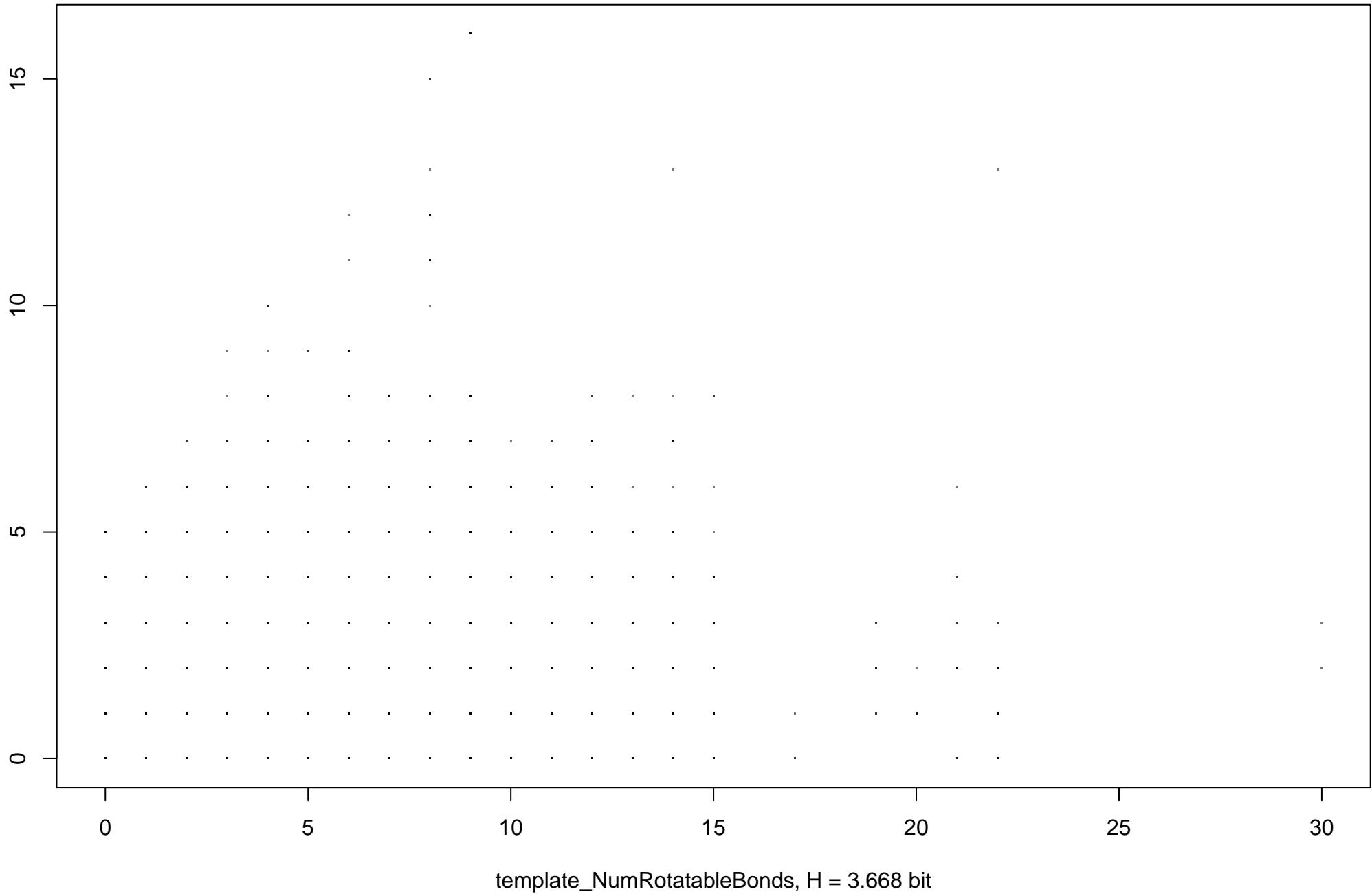


template_RingCount-mcs_NumHeteroAtoms, MI = 0.06538 bit, normMI = 0.02775



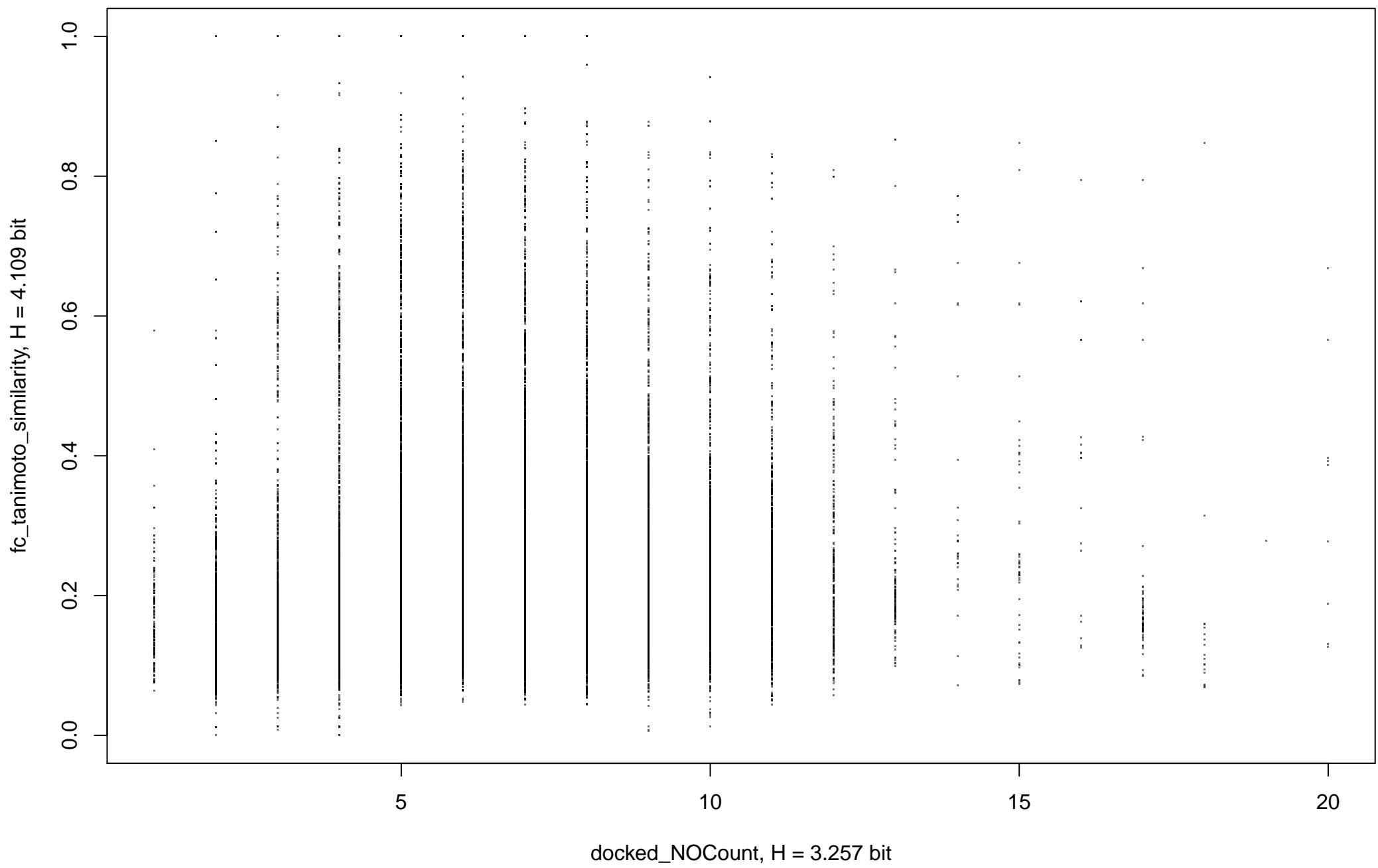
template_NumRotatableBonds–mcs_template_NumHAcceptors, MI = 0.06871 bit, normMI = 0.02762

mcs_template_NumHAcceptors, H = 2.488 bit



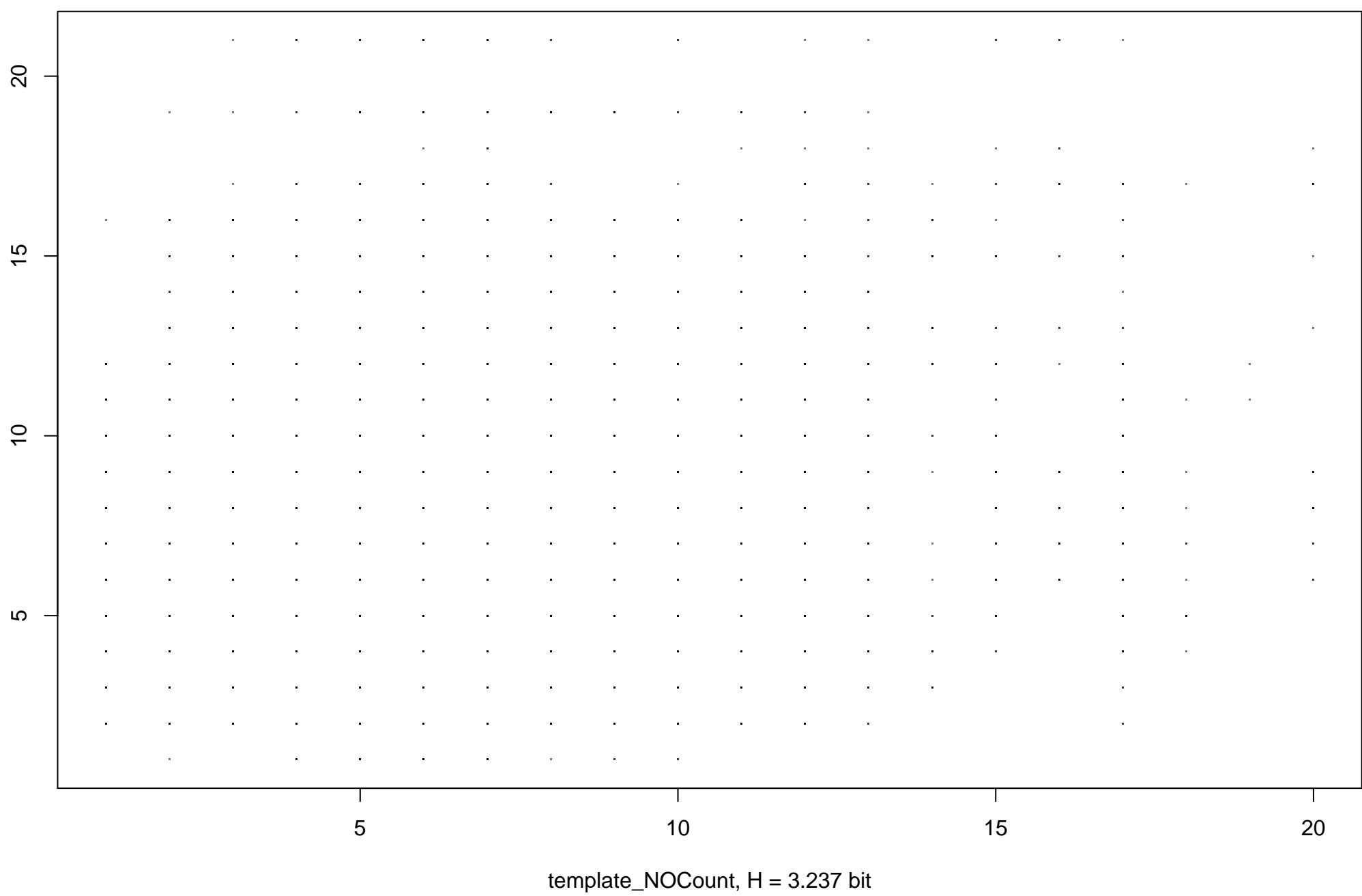
template_NumRotatableBonds, H = 3.668 bit

docked_NOCount-fc_tanimoto_similarity, MI = 0.08982 bit, normMI = 0.02758

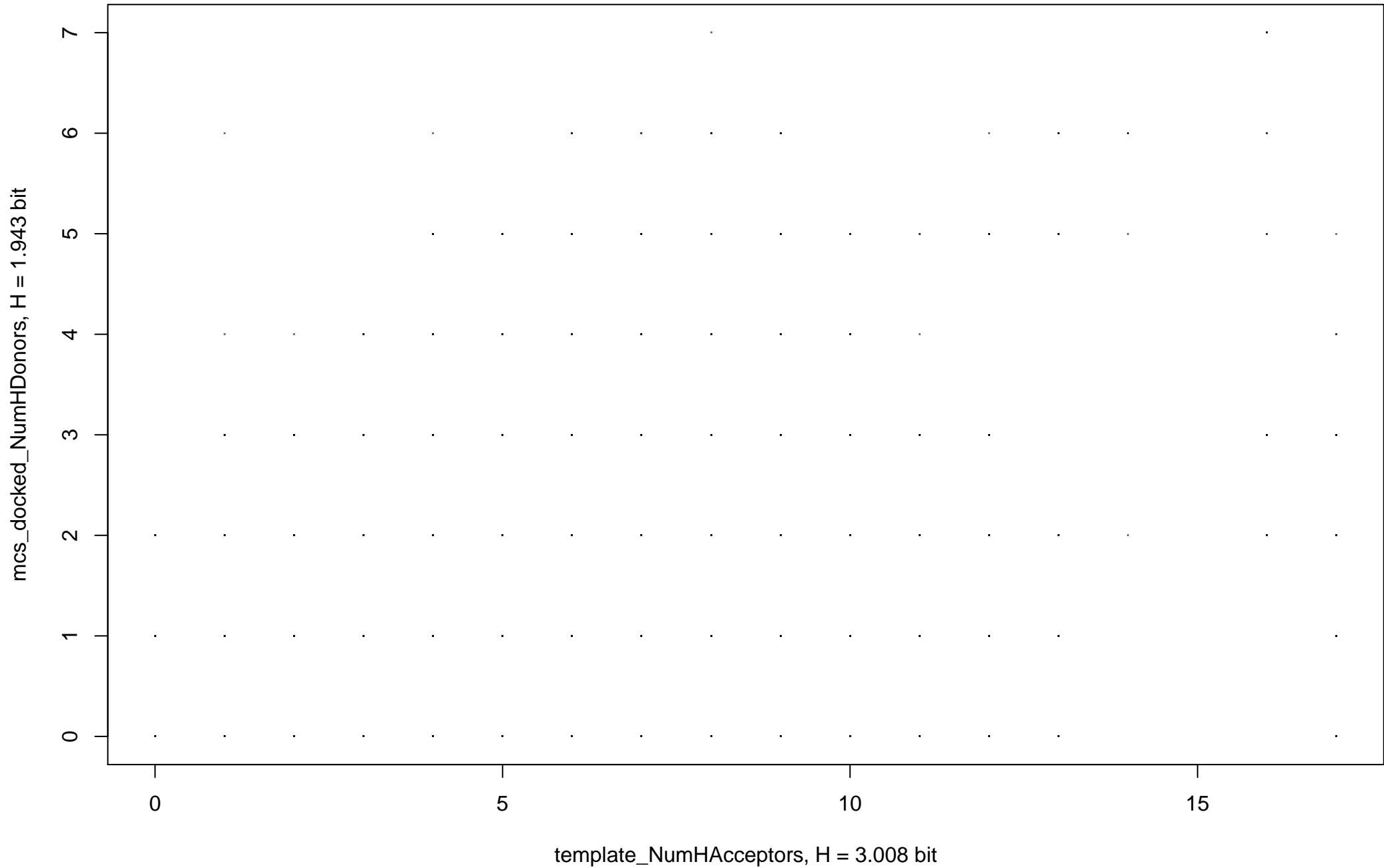


template_NOCount-docked_NumHeteroAtoms, MI = 0.08897 bit, normMI = 0.02749

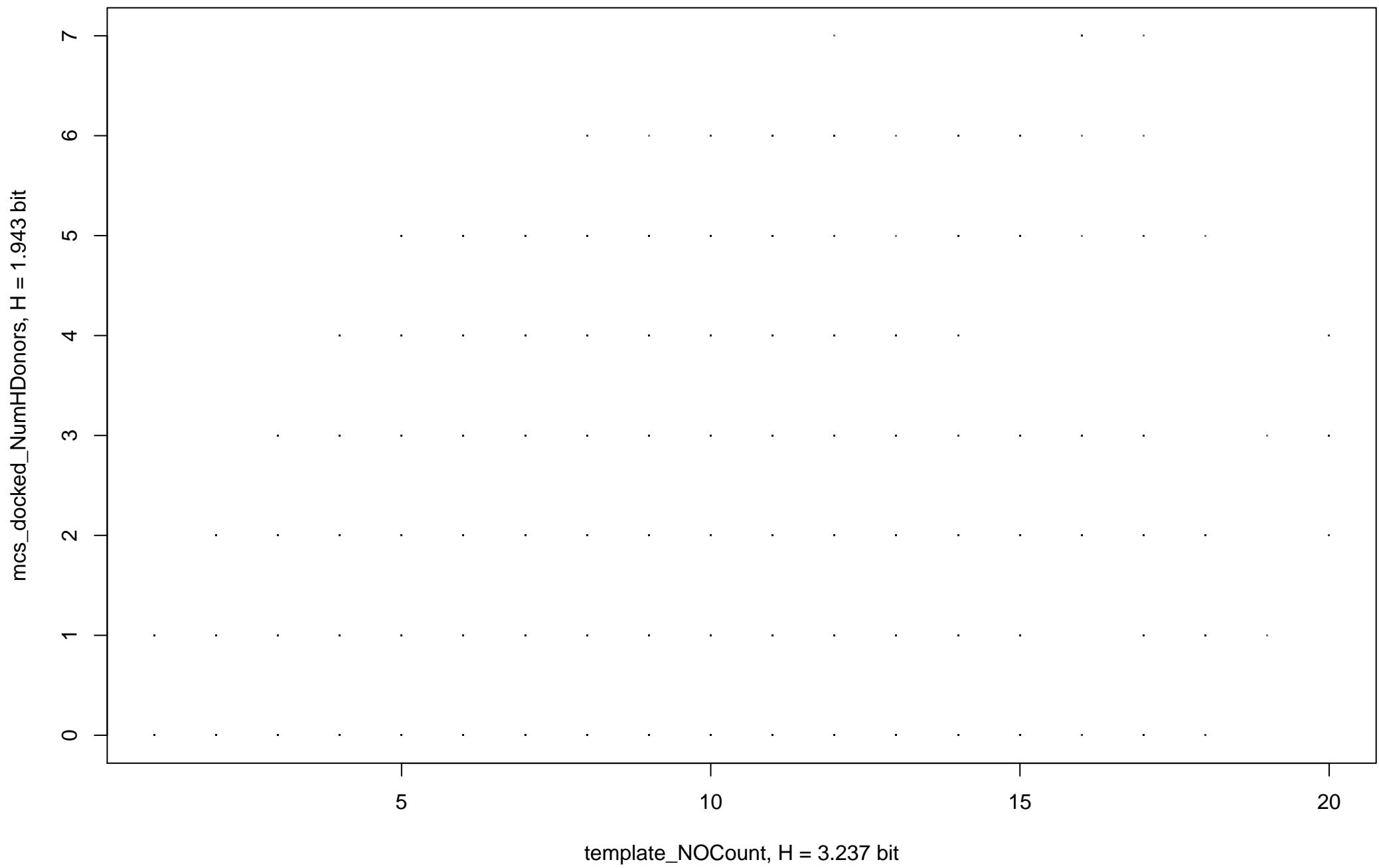
docked_NumHeteroAtoms, H = 3.571 bit



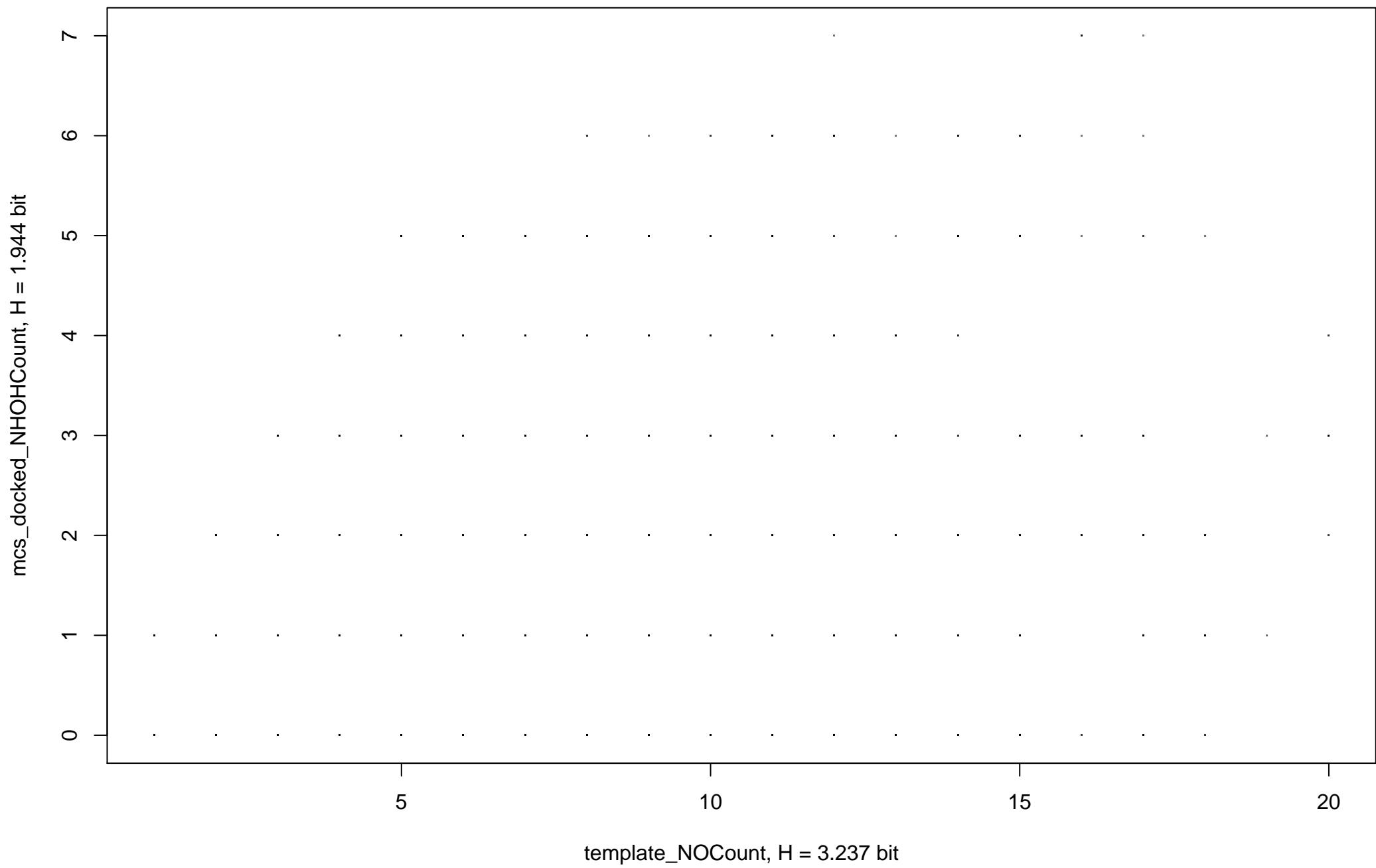
template_NumHAcceptors-mcs_docked_NumHDonors, MI = 0.0534 bit, normMI = 0.02748



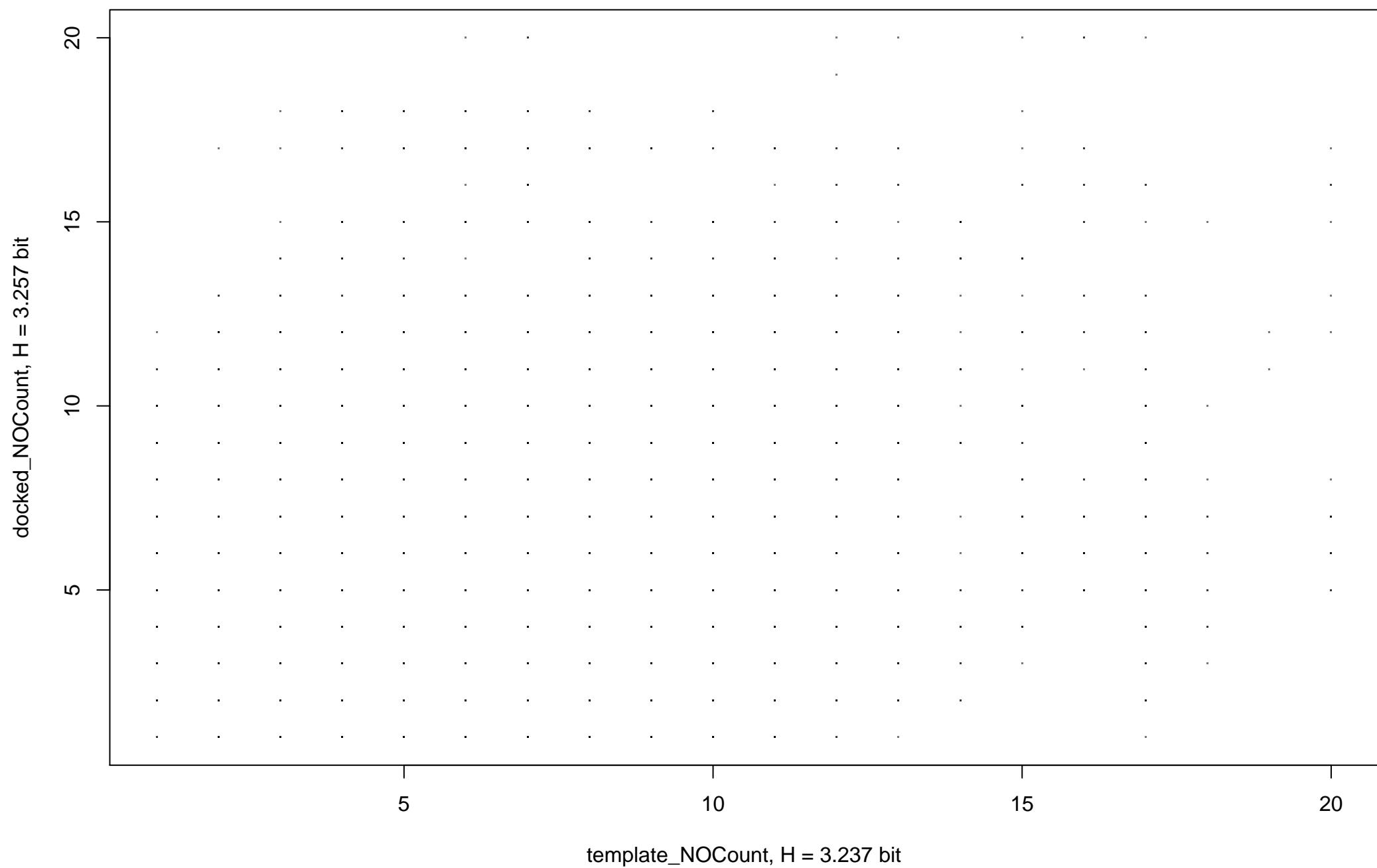
template_NOCount-mcs_docked_NumHDonors, MI = 0.05338 bit, normMI = 0.02747



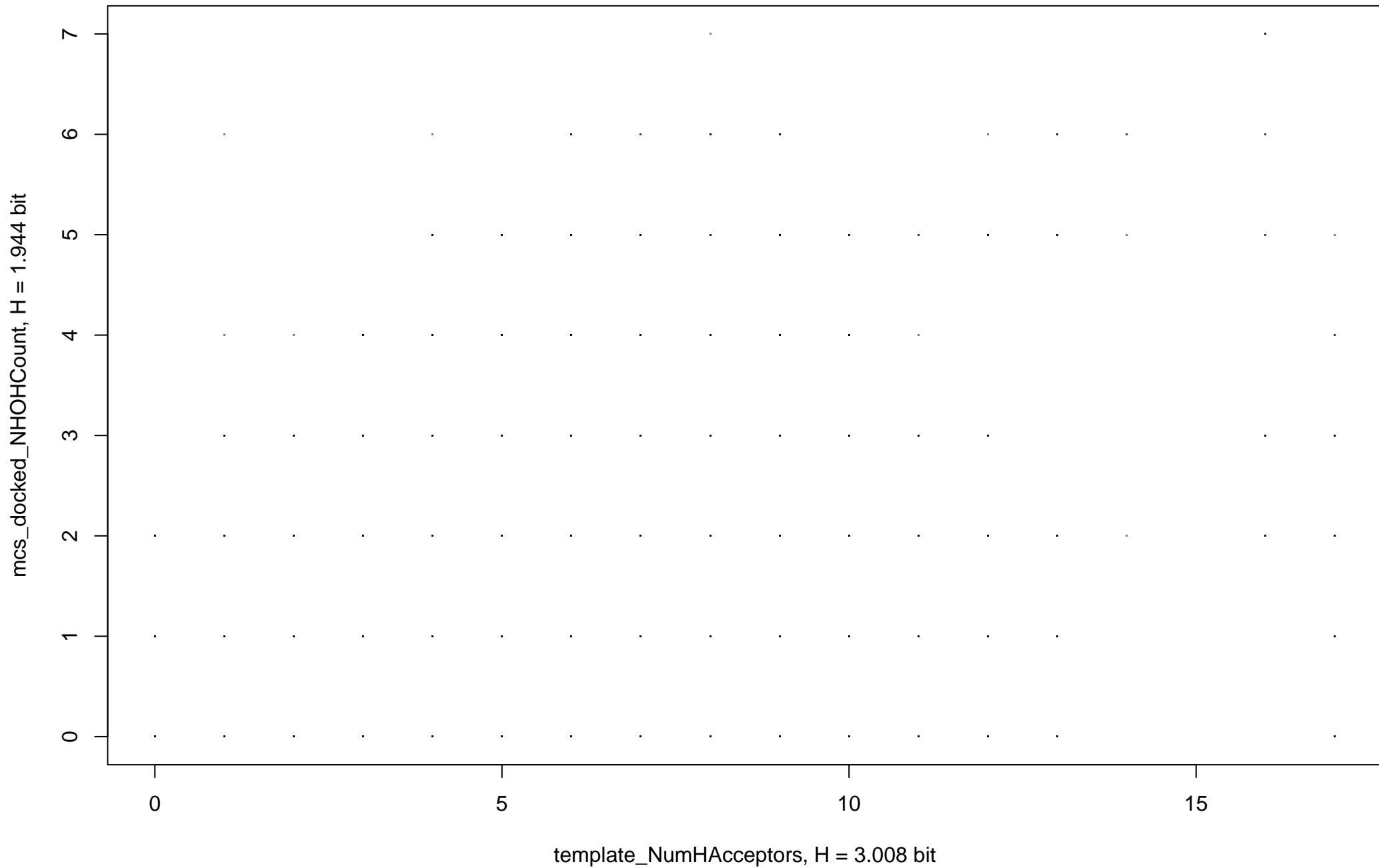
template_NOCount-mcs_docked_NHOHCount, MI = 0.05335 bit, normMI = 0.02744



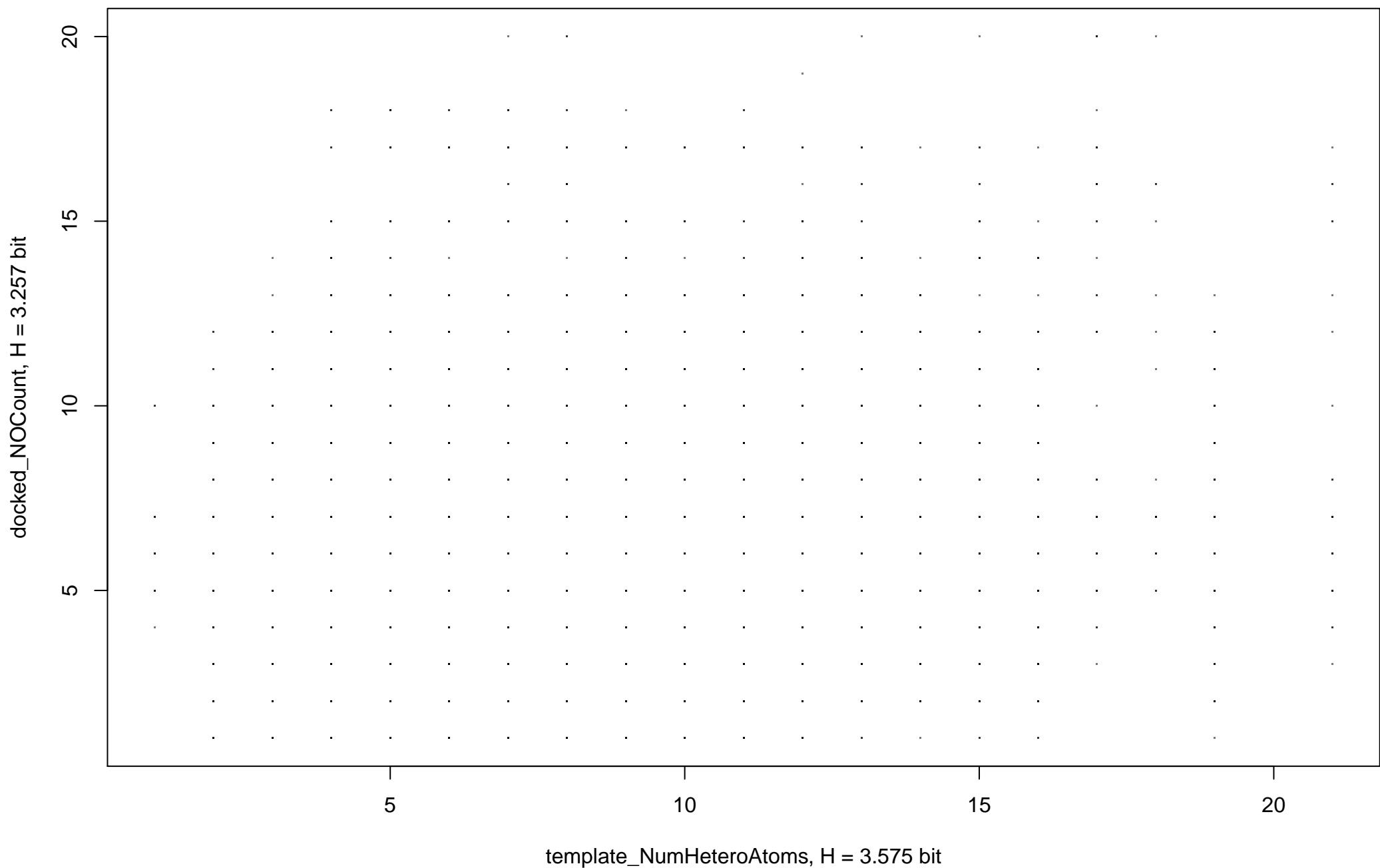
template_NOCount–docked_NOCount, MI = 0.08841 bit, normMI = 0.02731



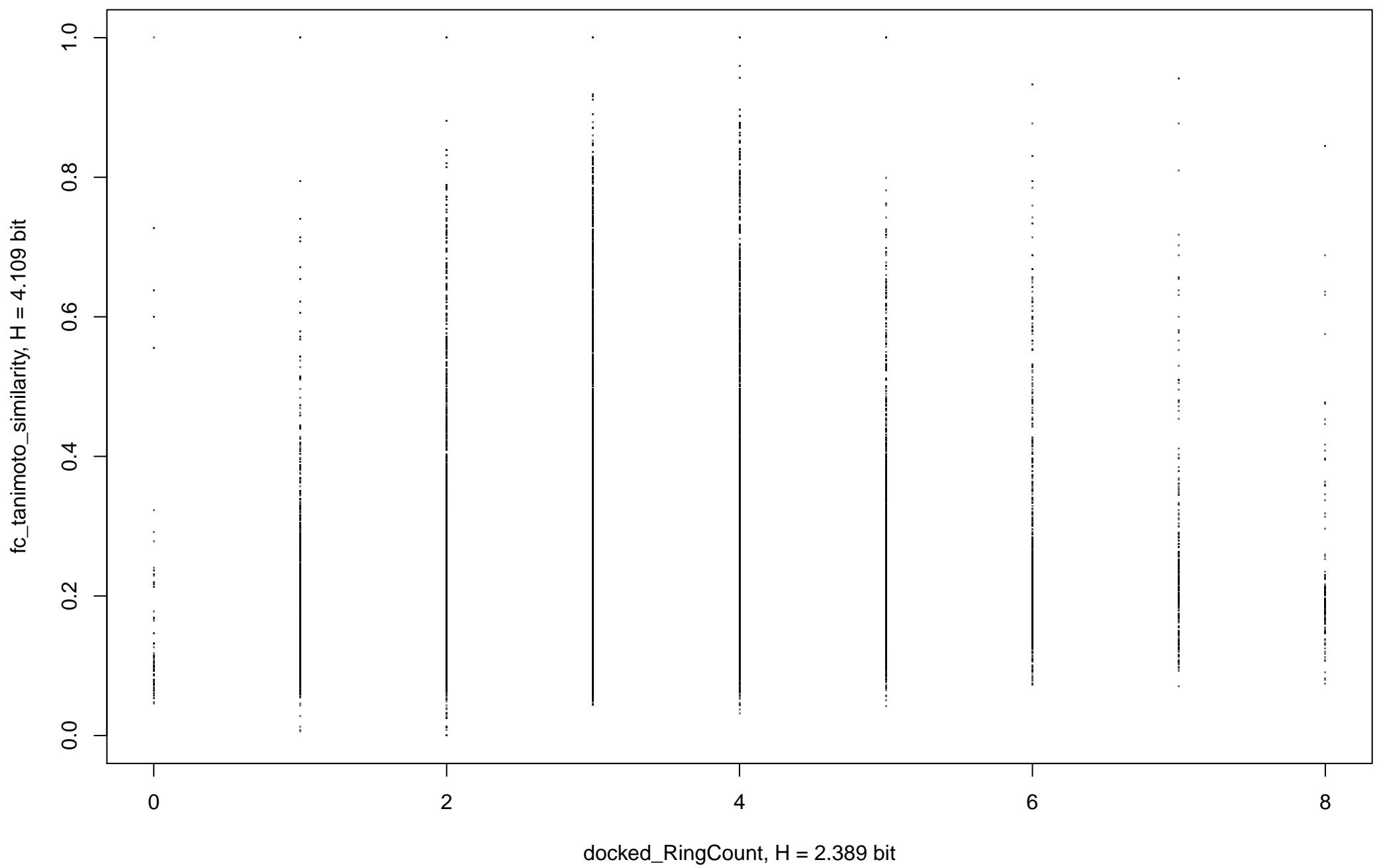
template_NumHAcceptors-mcs_docked_NHOHCount, MI = 0.05309 bit, normMI = 0.02731



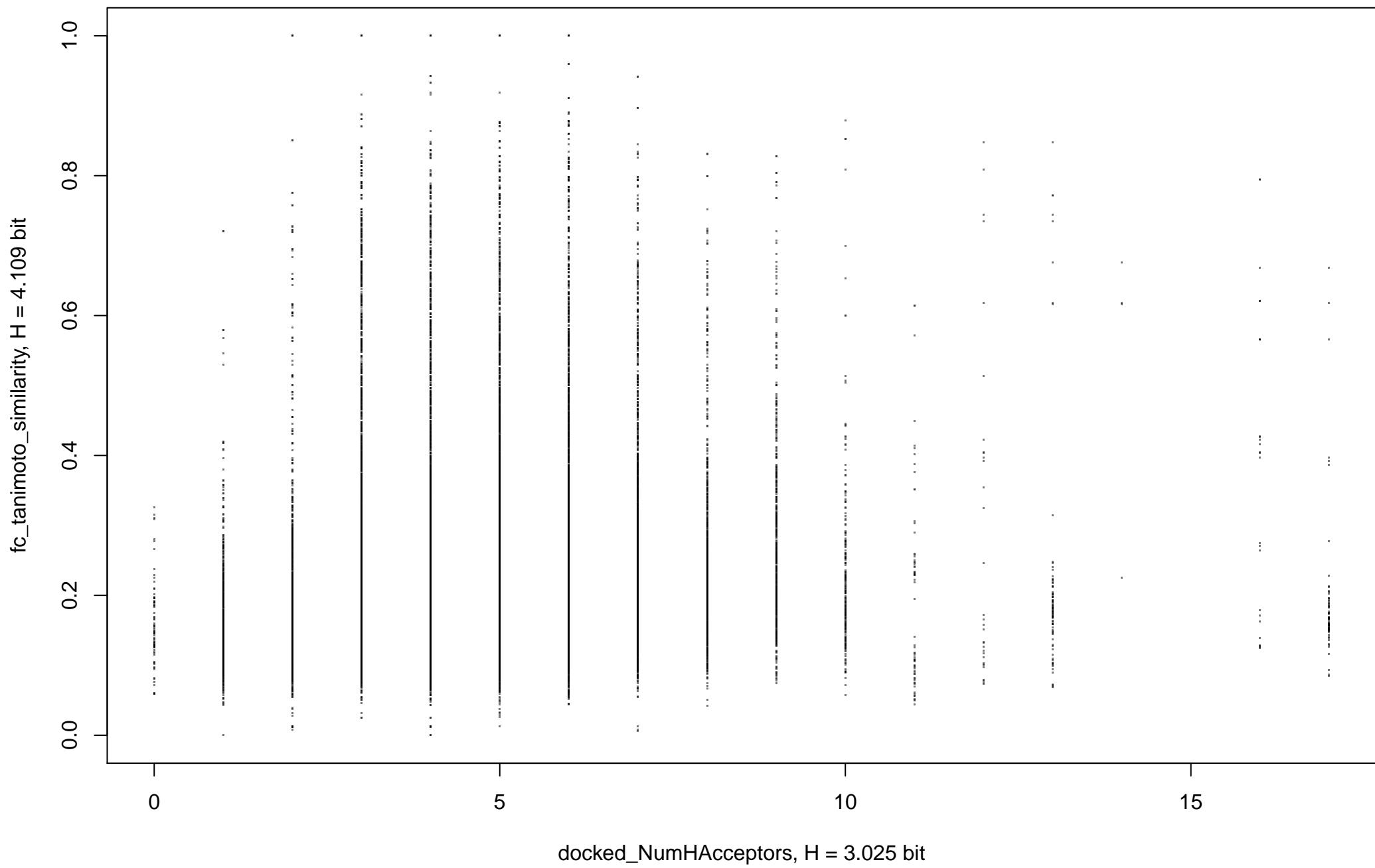
template_NumHeteroAtoms-docked_NOCount, MI = 0.08886 bit, normMI = 0.02728



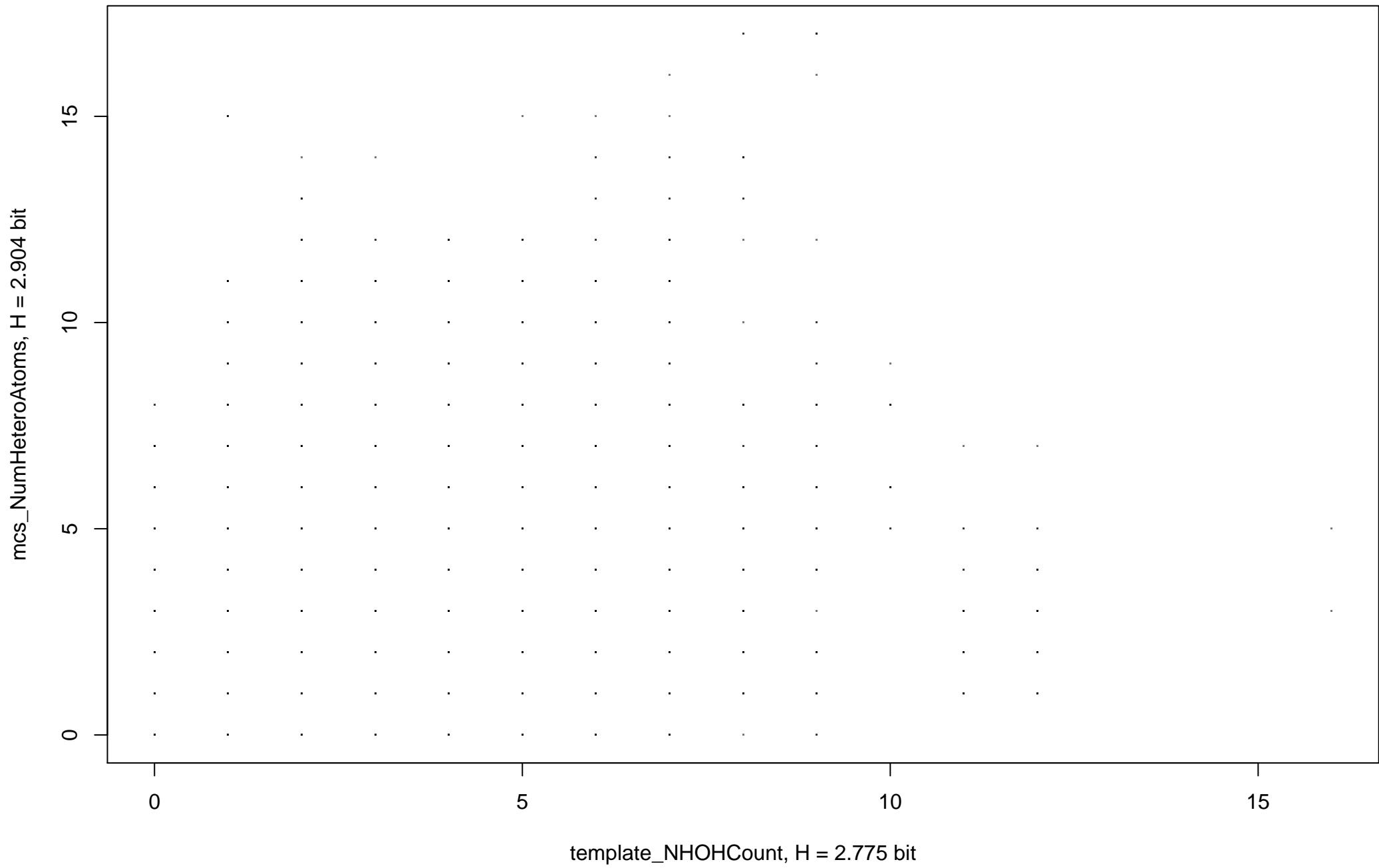
docked_RingCount-fc_tanimoto_similarity, MI = 0.0651 bit, normMI = 0.02725



docked_NumHAcceptors–fc_tanimoto_similarity, MI = 0.082 bit, normMI = 0.0271

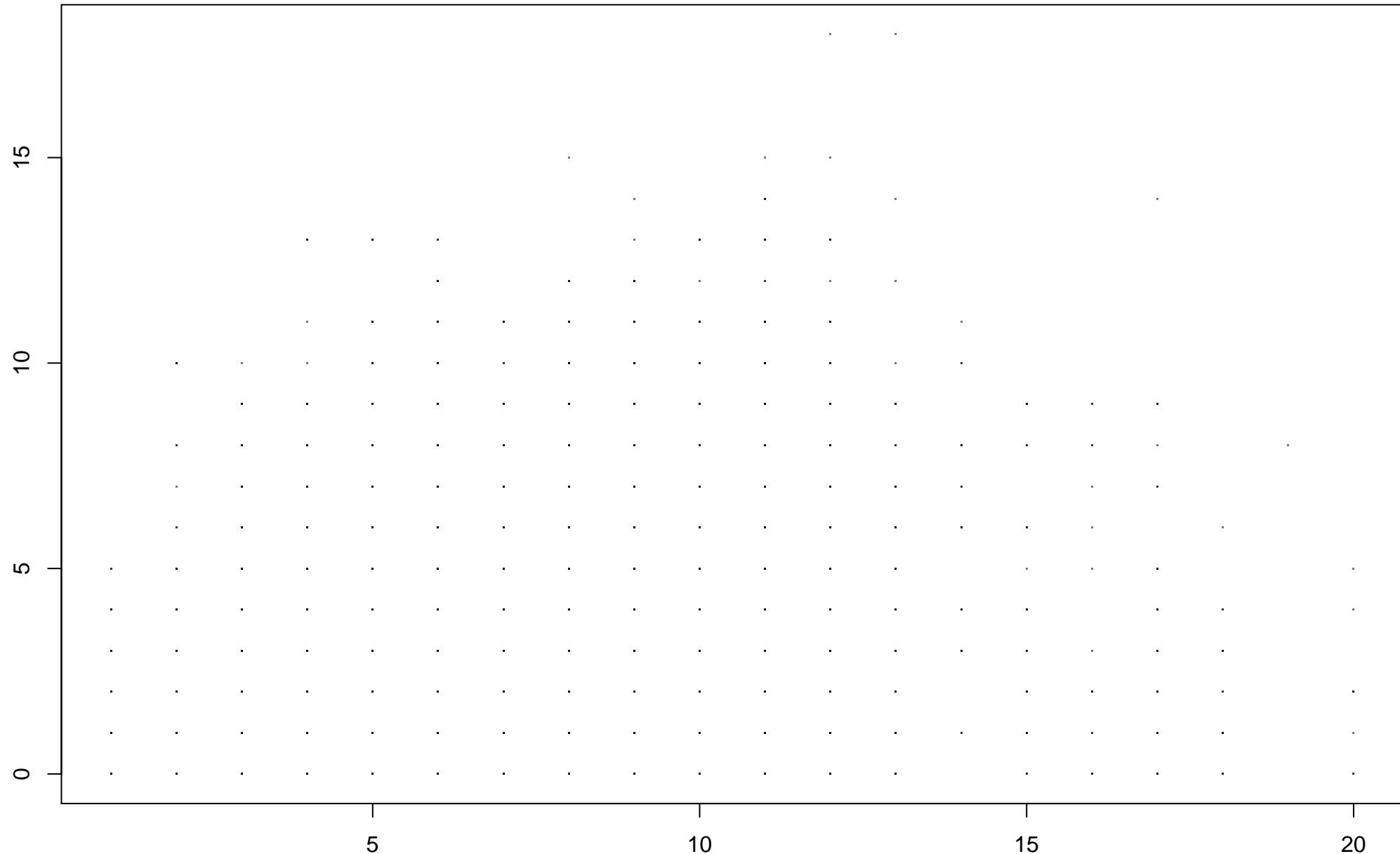


template_NHOHCount-mcs_NumHeteroAtoms, MI = 0.07397 bit, normMI = 0.02665



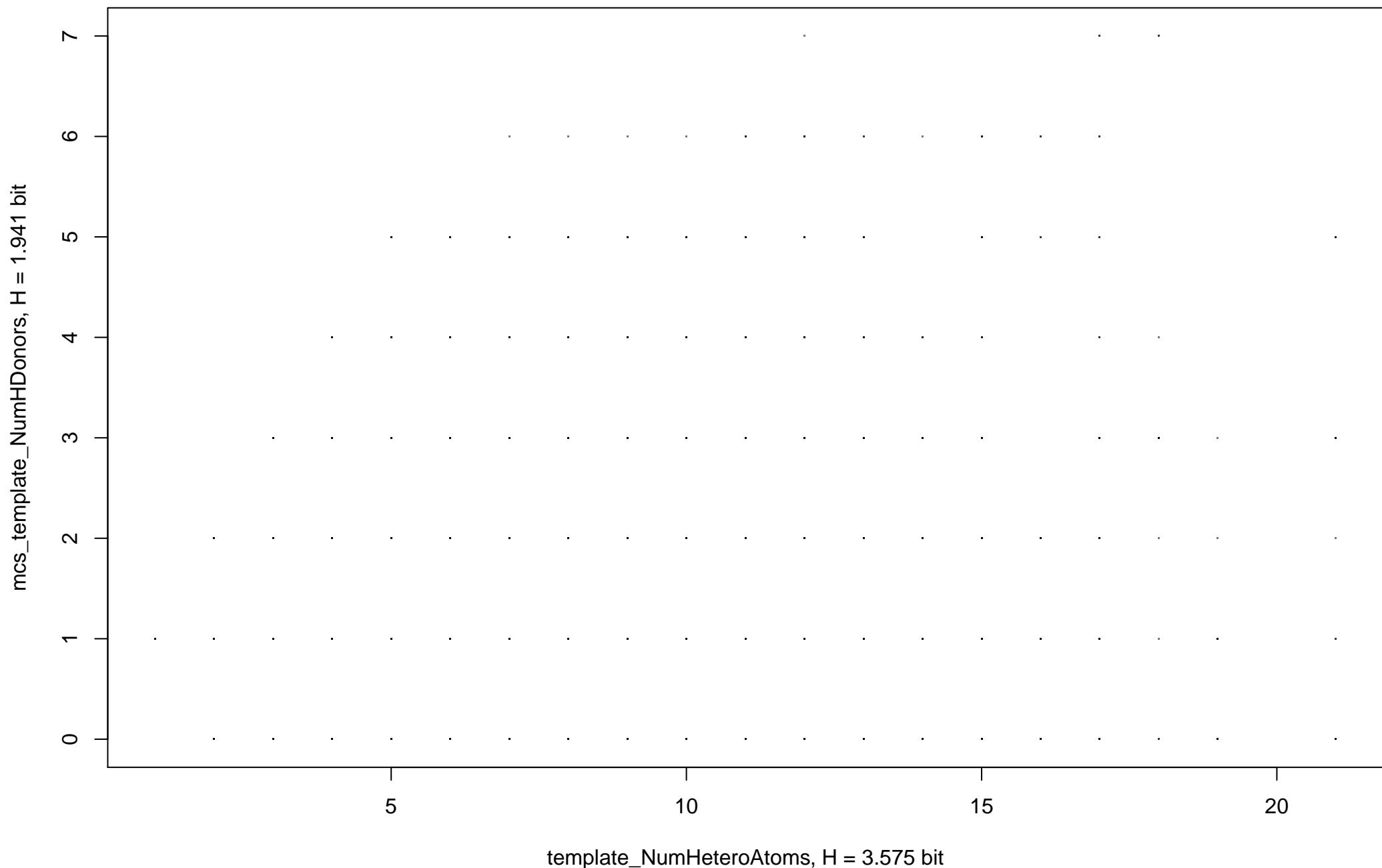
docked_NOCOUNT-mcs_template_NumRotatableBonds, MI = 0.08304 bit, normMI = 0.02663

mcs_template_NumRotatableBonds, H = 3.118 bit

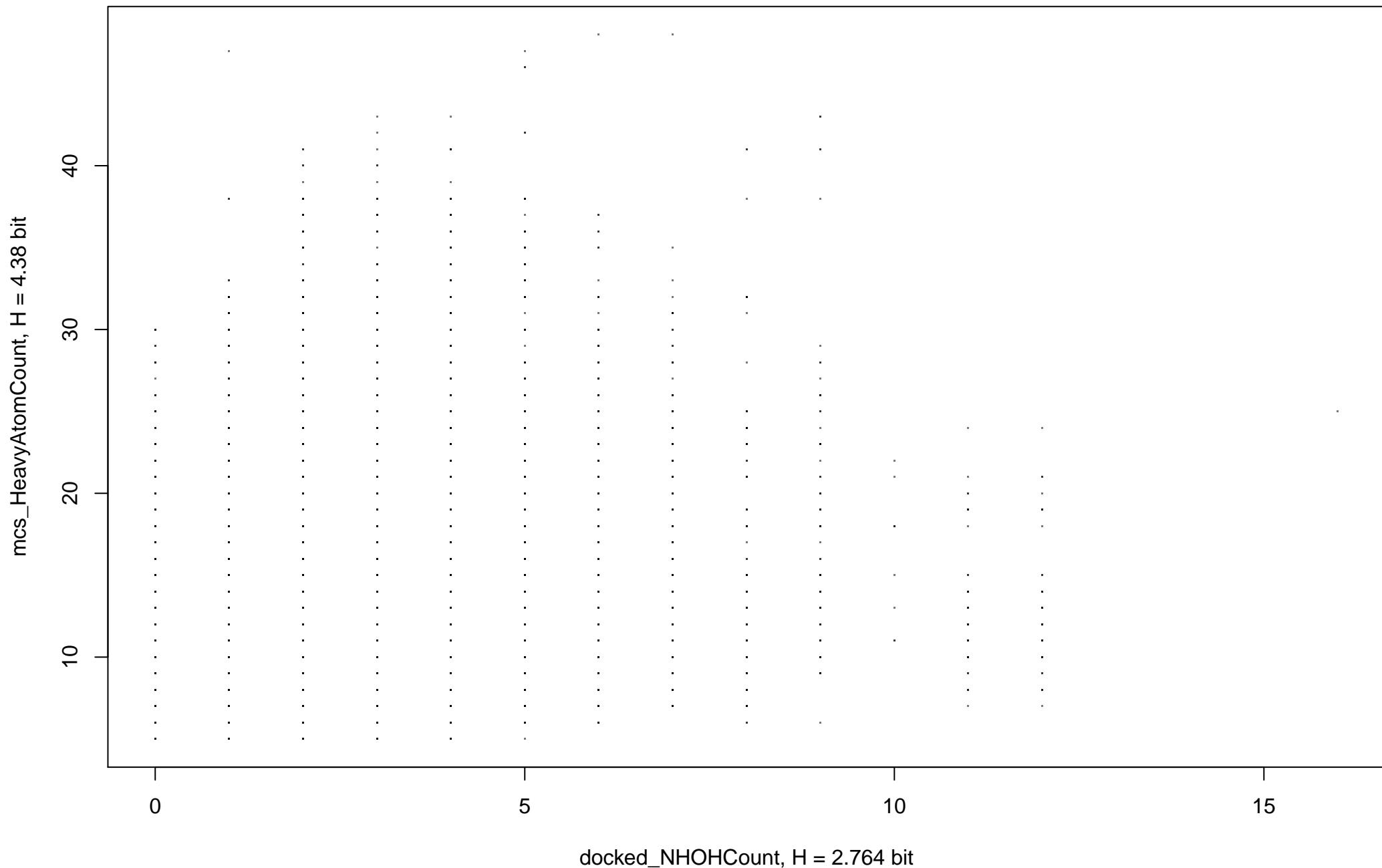


docked_NOCOUNT, H = 3.257 bit

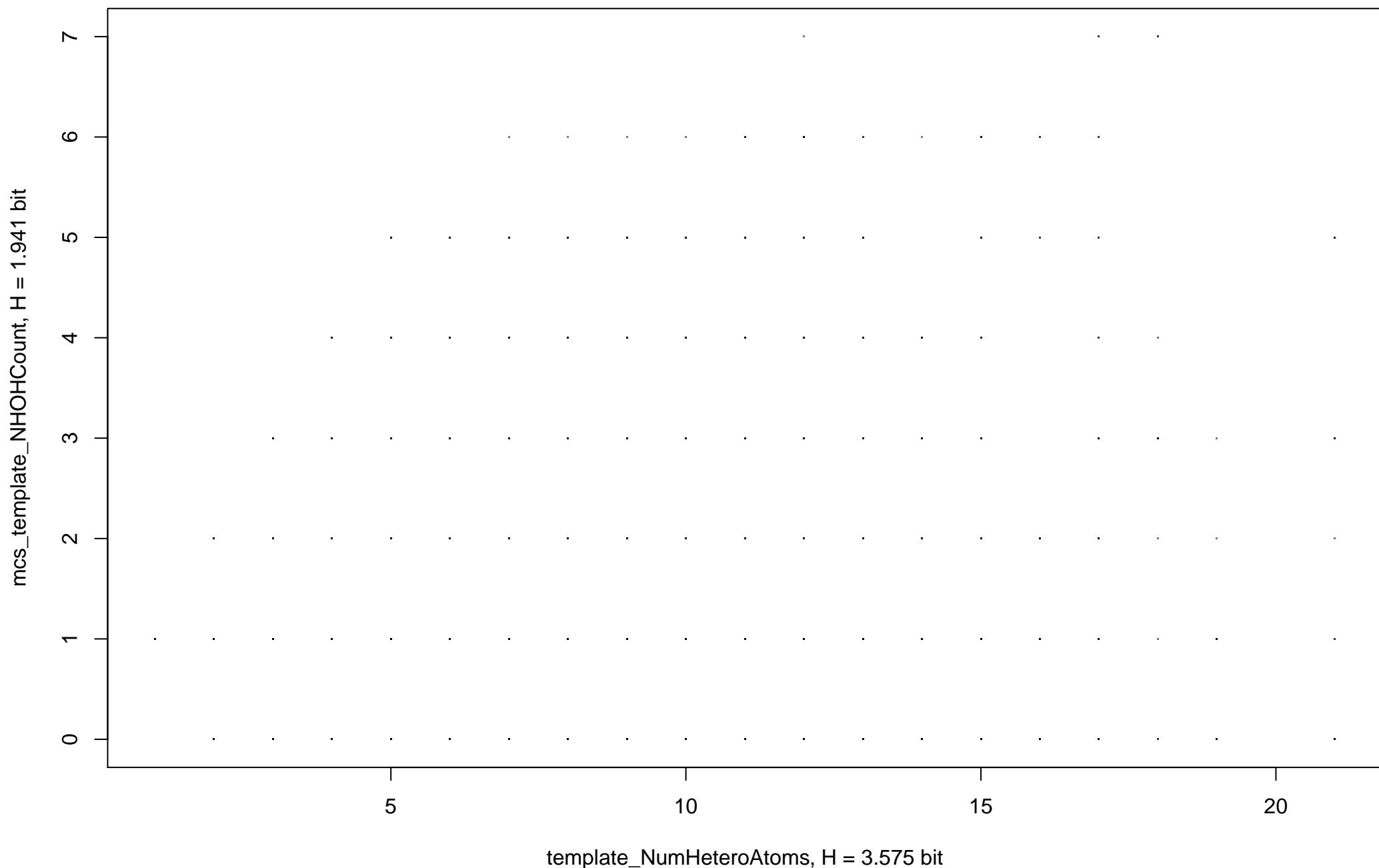
template_NumHeteroAtoms-mcs_template_NumHDonors, MI = 0.05153 bit, normMI = 0.02655



docked_NHOHCount-mcs_HeavyAtomCount, MI = 0.07332 bit, normMI = 0.02652

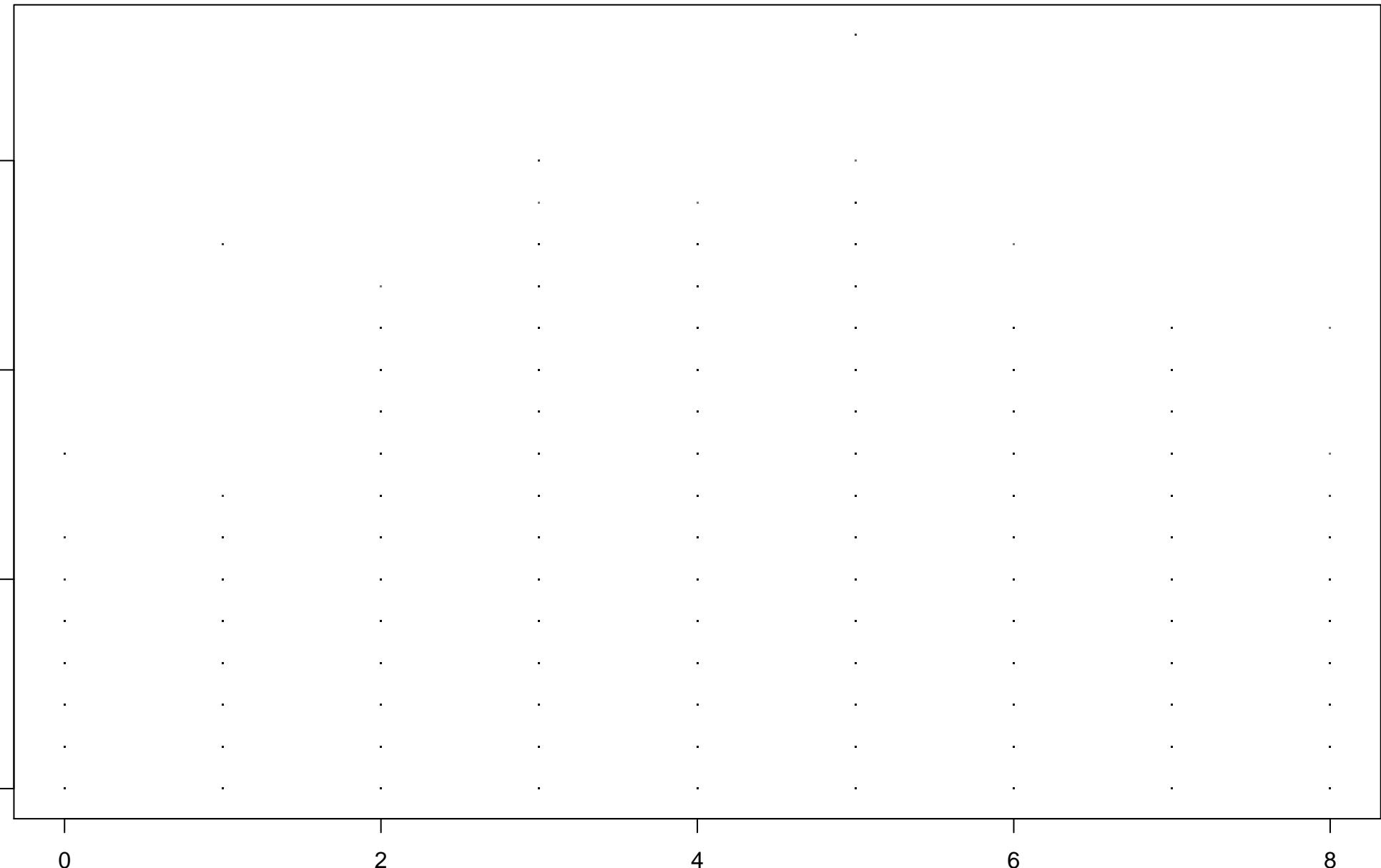


template_NumHeteroAtoms-mcs_template_NHOHCount, MI = 0.05138 bit, normMI = 0.02647



template_RingCount-mcs_docked_NumRotatableBonds, MI = 0.06198 bit, normMI = 0.02631

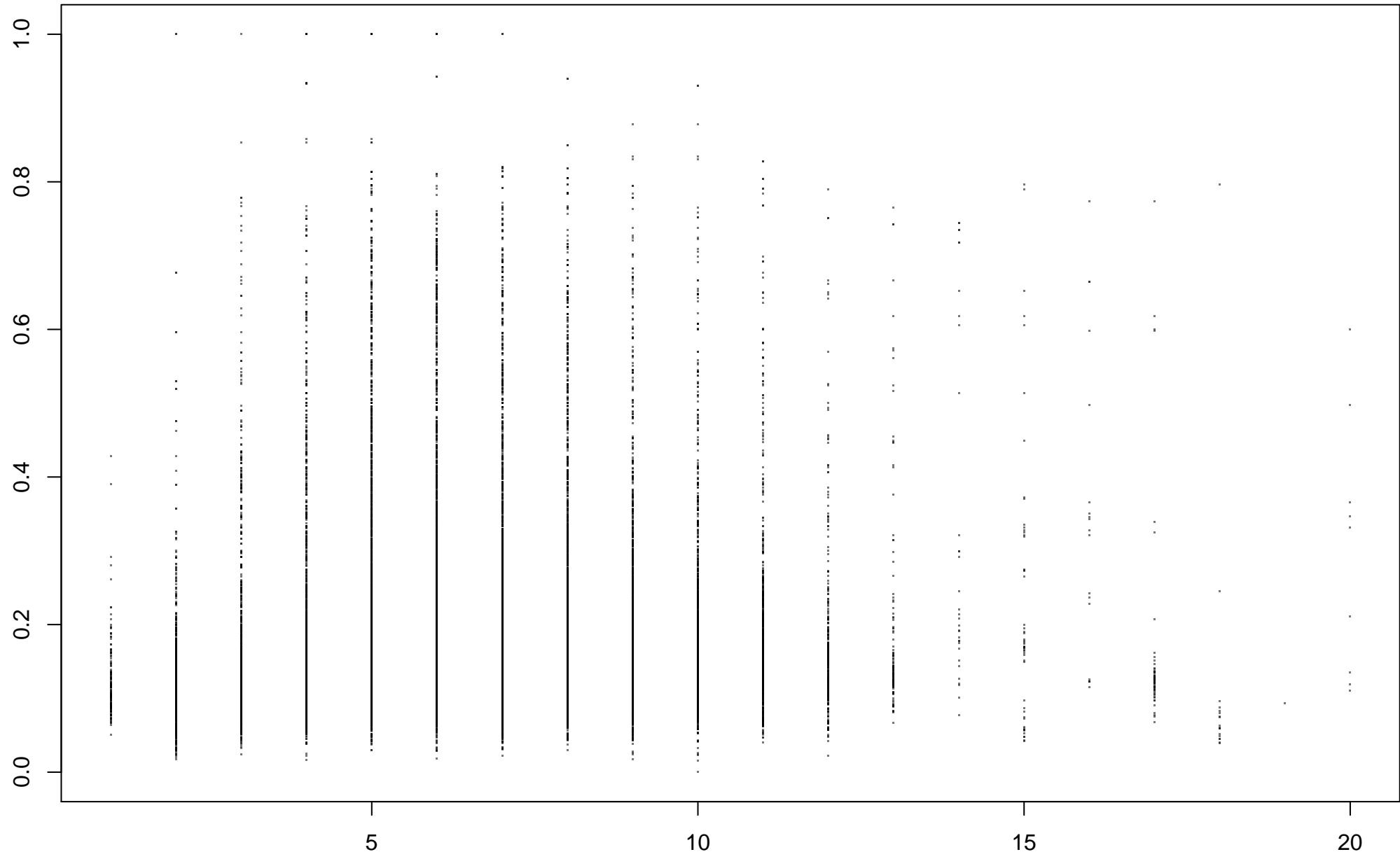
mcs_docked_NumRotatableBonds, H = 3.117 bit



template_RingCount, H = 2.356 bit

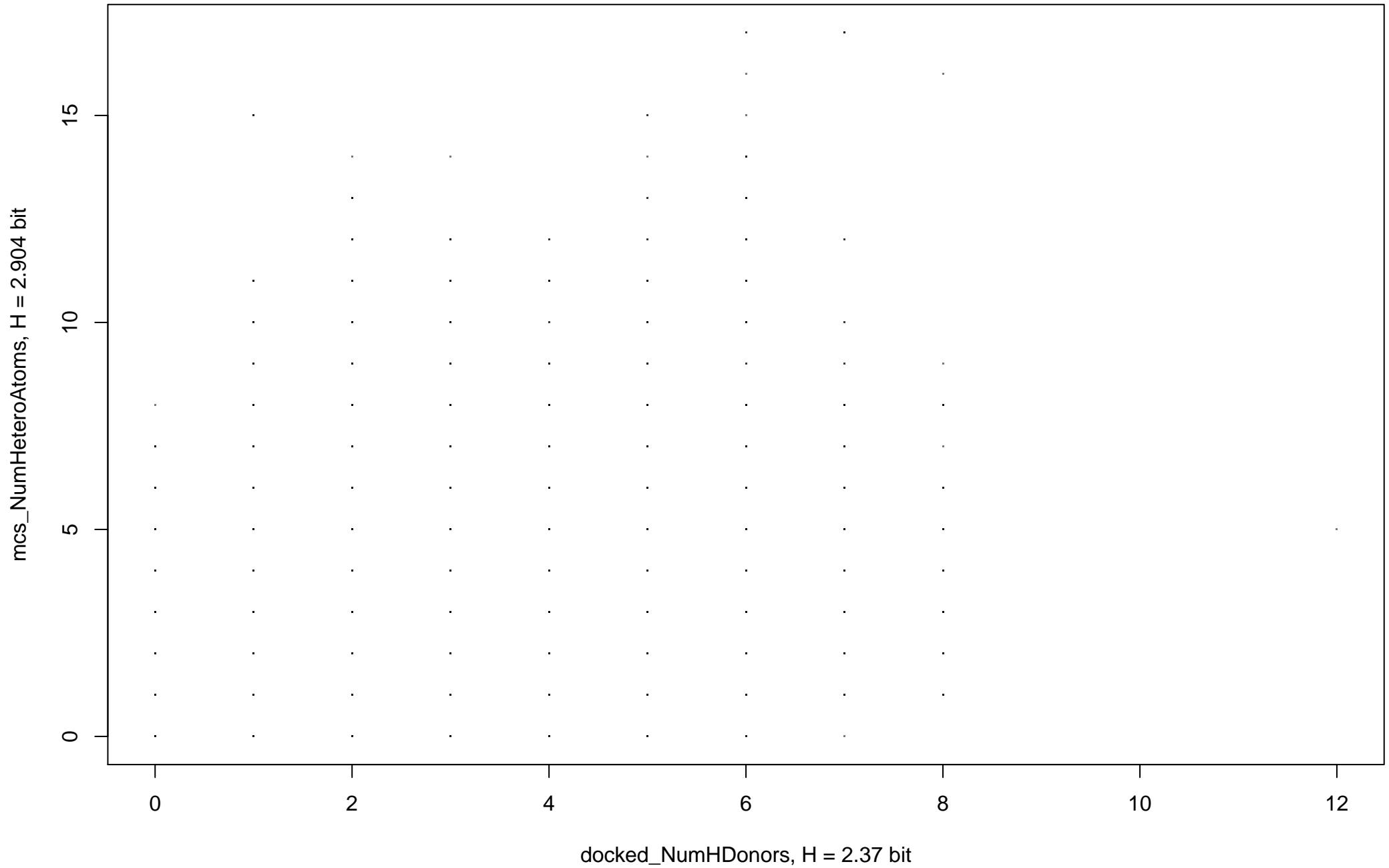
docked_NOCOUNT-ec_tanimoto_similarity, MI = 0.08555 bit, normMI = 0.02627

ec_tanimoto_similarity, H = 4.125 bit

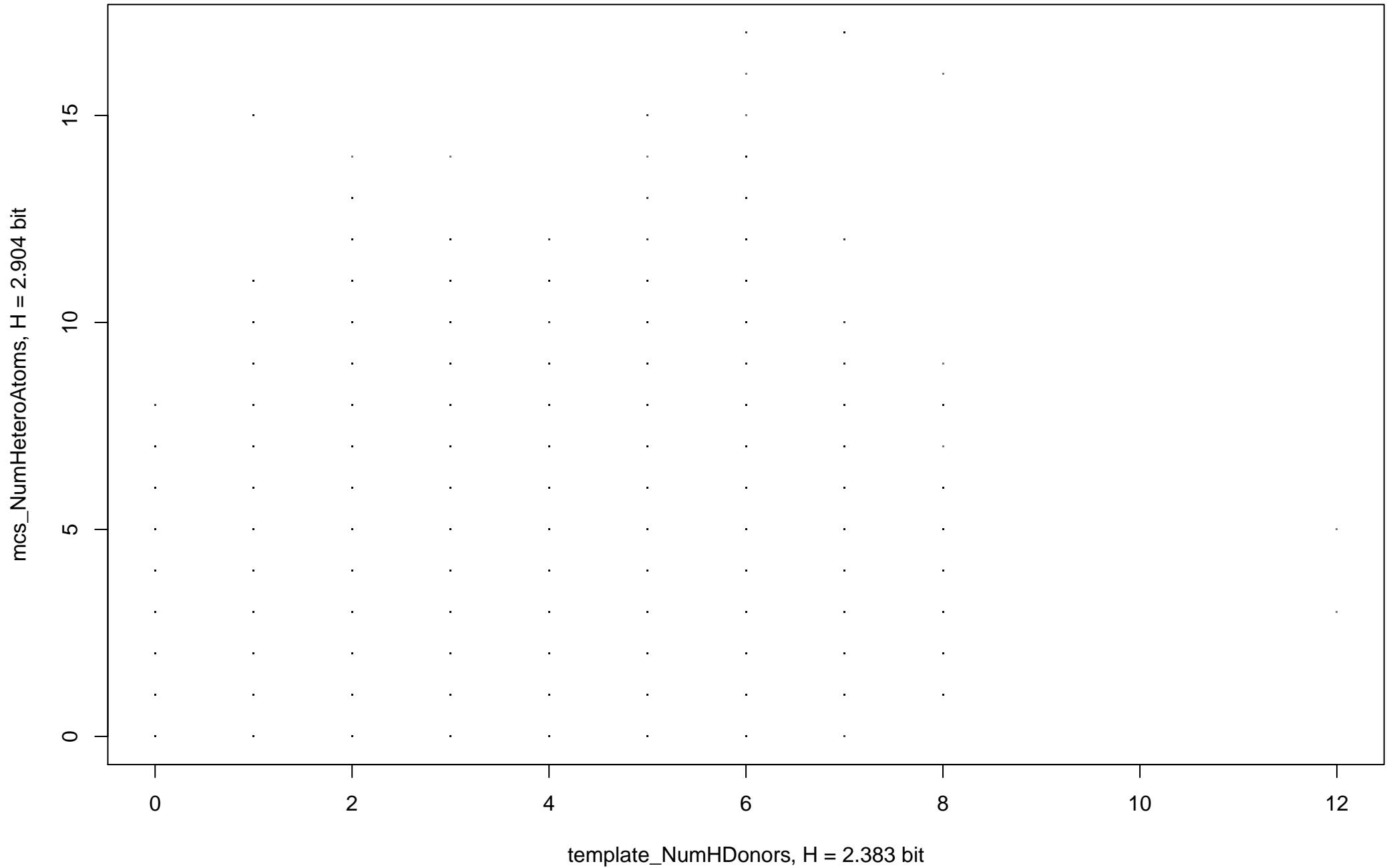


docked_NOCOUNT, H = 3.257 bit

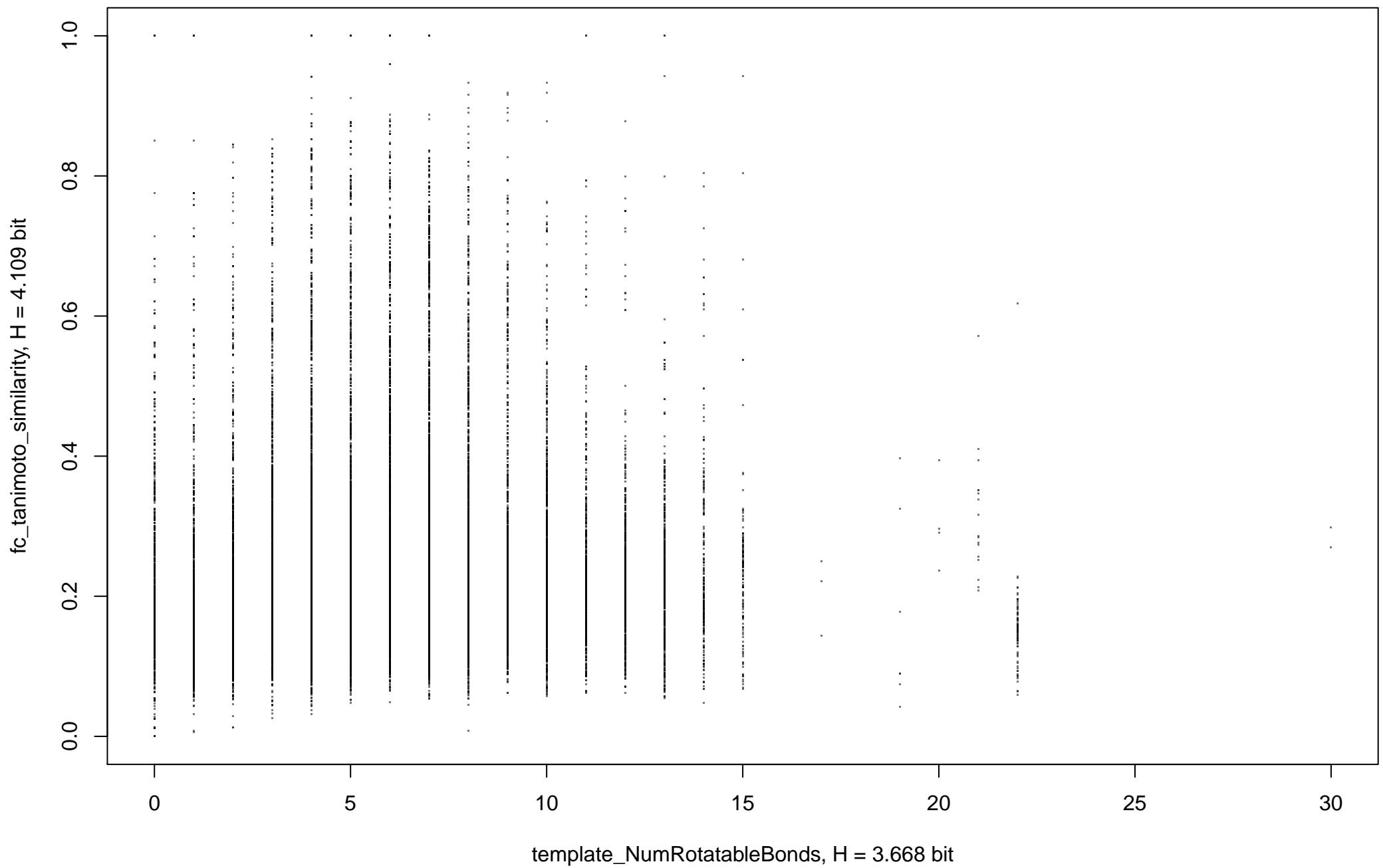
docked_NumHDonors-mcs_NumHeteroAtoms, MI = 0.06206 bit, normMI = 0.02618



template_NumHDonors-mcs_NumHeteroAtoms, MI = 0.06217 bit, normMI = 0.02609

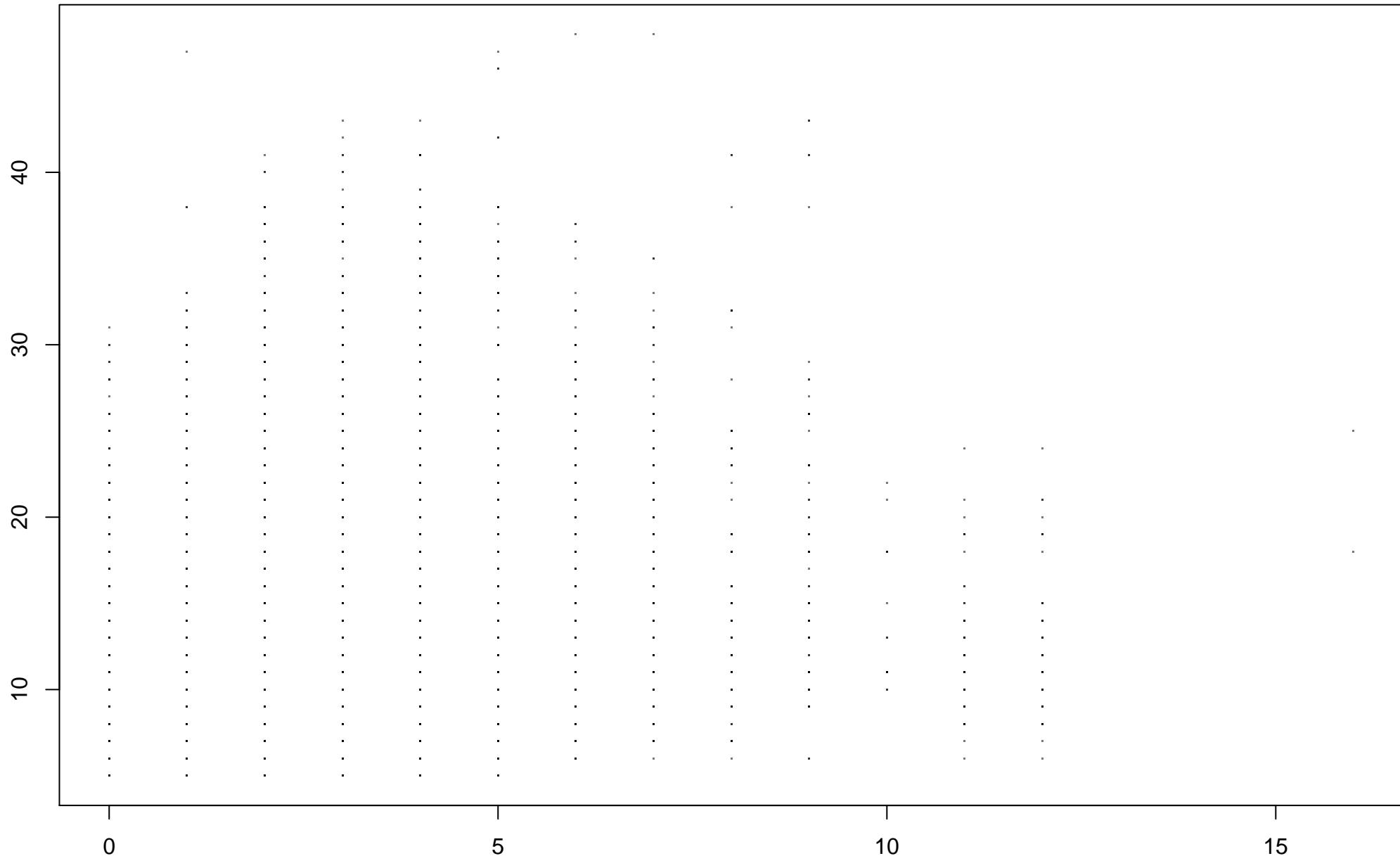


template_NumRotatableBonds-fc_tanimoto_similarity, MI = 0.09568 bit, normMI = 0.02608



template_NHOHCount-mcs_HeavyAtomCount, MI = 0.07214 bit, normMI = 0.02599

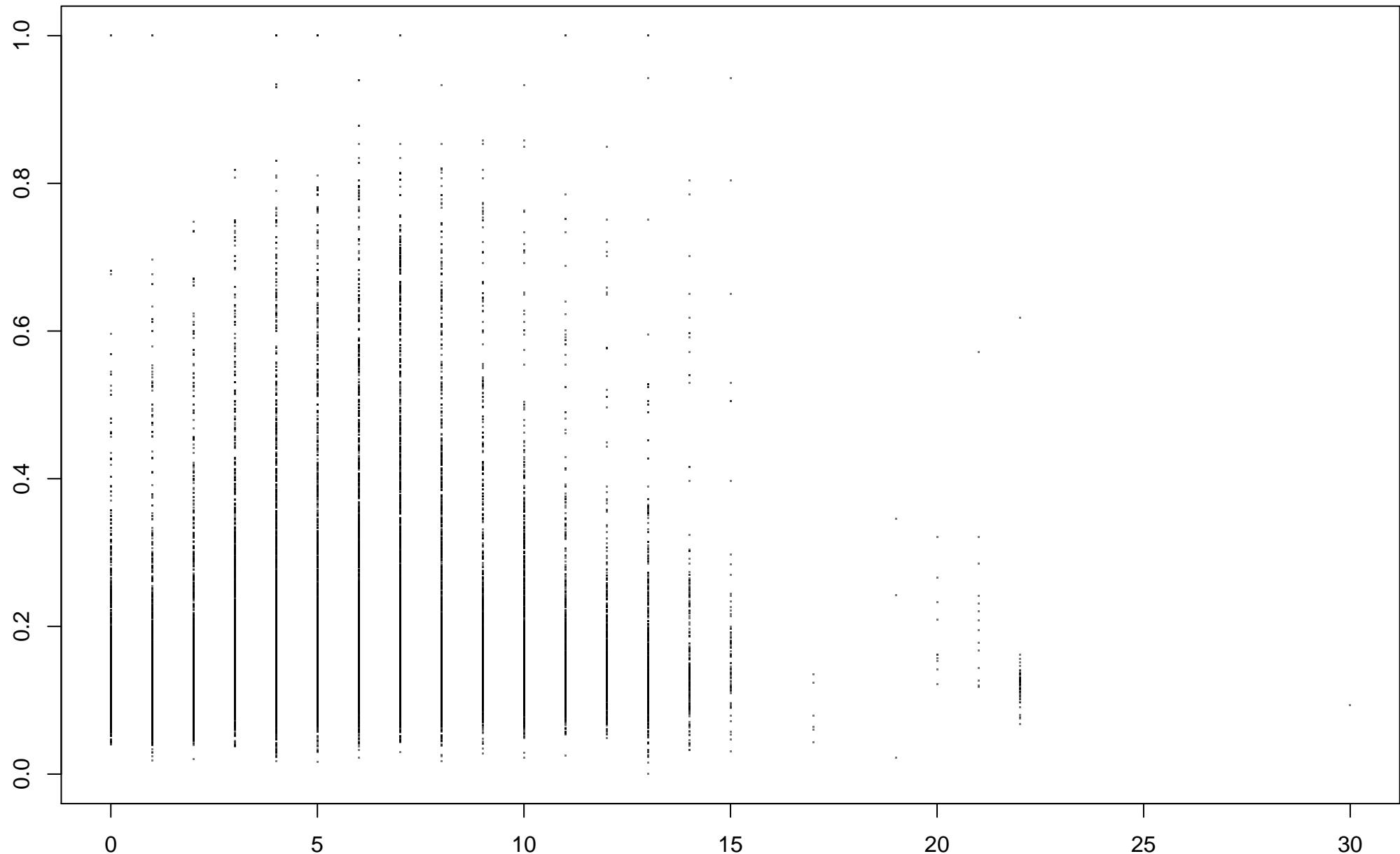
mcs_HeavyAtomCount, H = 4.38 bit



template_NHOHCount, H = 2.775 bit

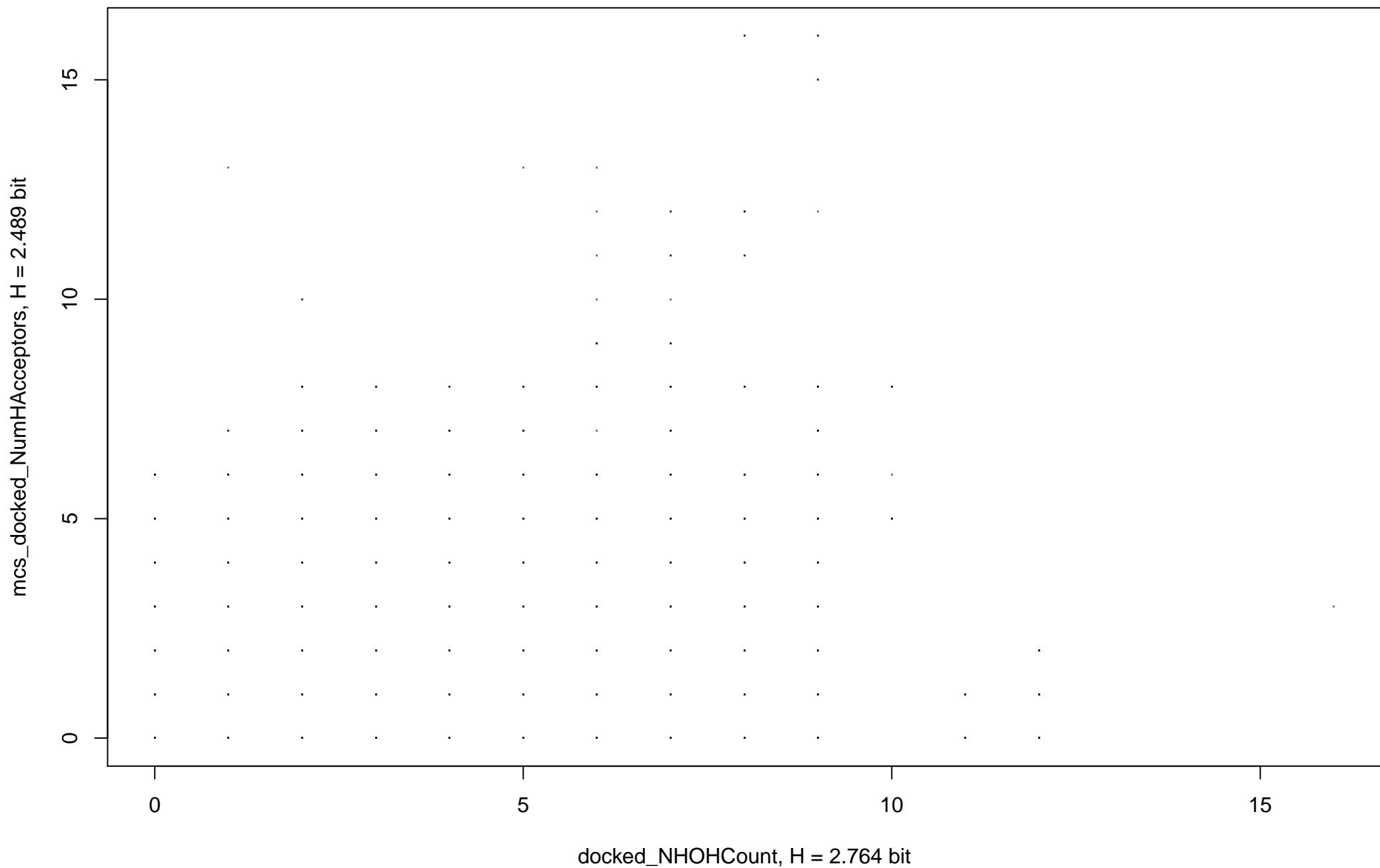
docked_NumRotatableBonds–ec_tanimoto_similarity, MI = 0.09529 bit, normMI = 0.02599

ec_tanimoto_similarity, H = 4.125 bit

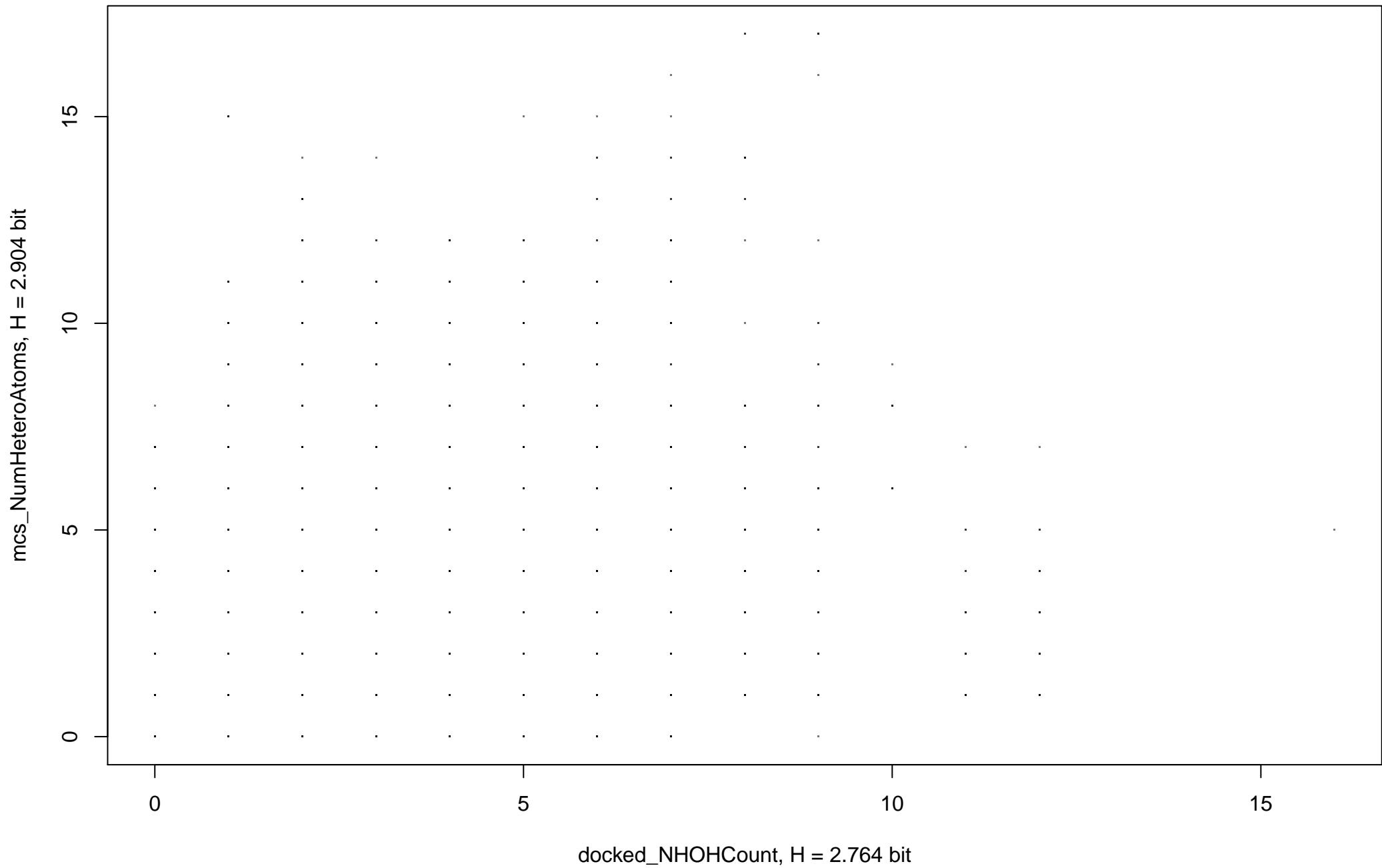


docked_NumRotatableBonds, H = 3.667 bit

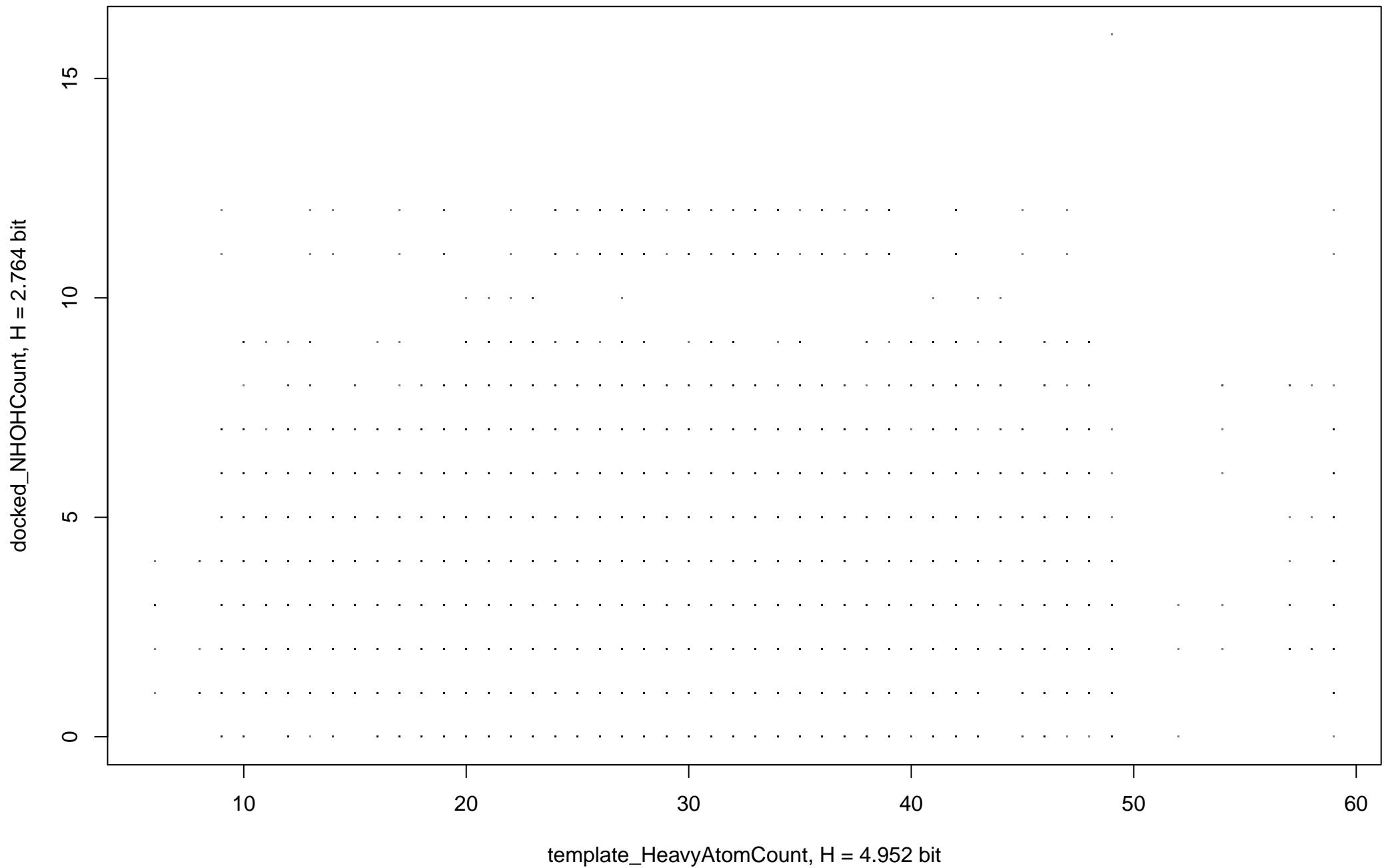
docked_NHOHCount–mcs_docked_NumHAcceptors, MI = 0.06459 bit, normMI = 0.02595



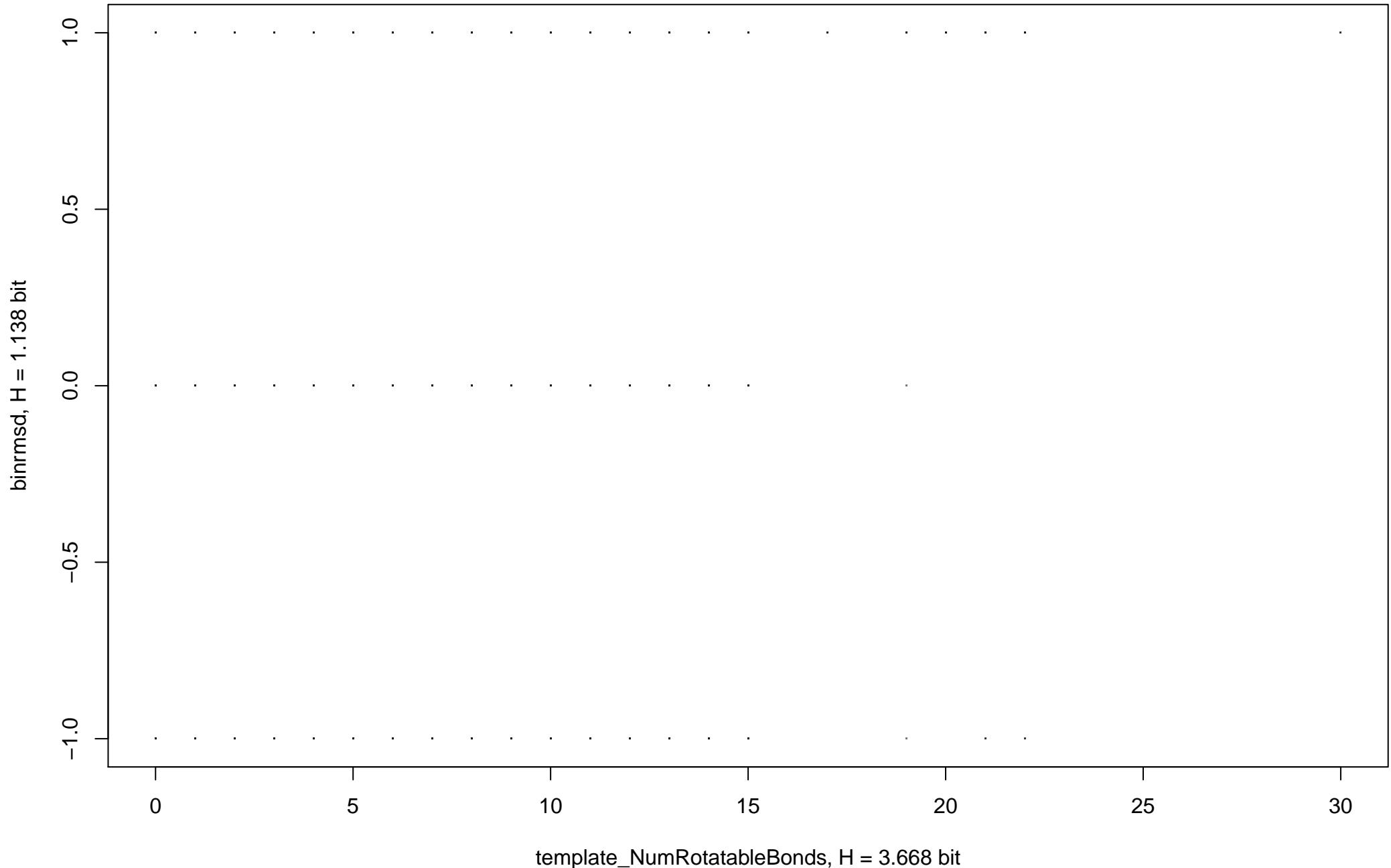
docked_NHOHCount-mcs_NumHeteroAtoms, MI = 0.07027 bit, normMI = 0.02542



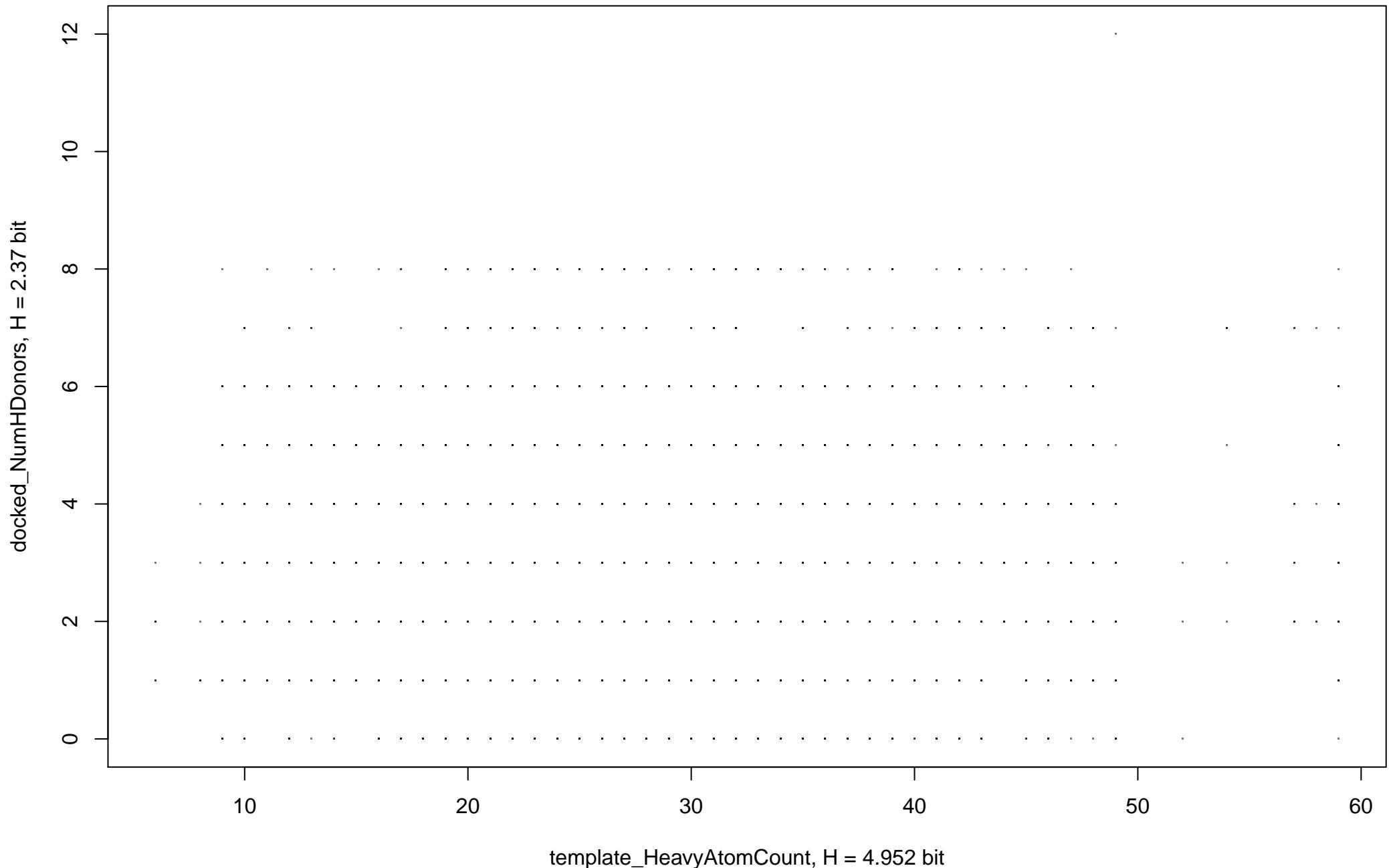
template_HeavyAtomCount-docked_NHOHCount, MI = 0.06985 bit, normMI = 0.02527



template_NumRotatableBonds-binrmsd, MI = 0.02836 bit, normMI = 0.02492

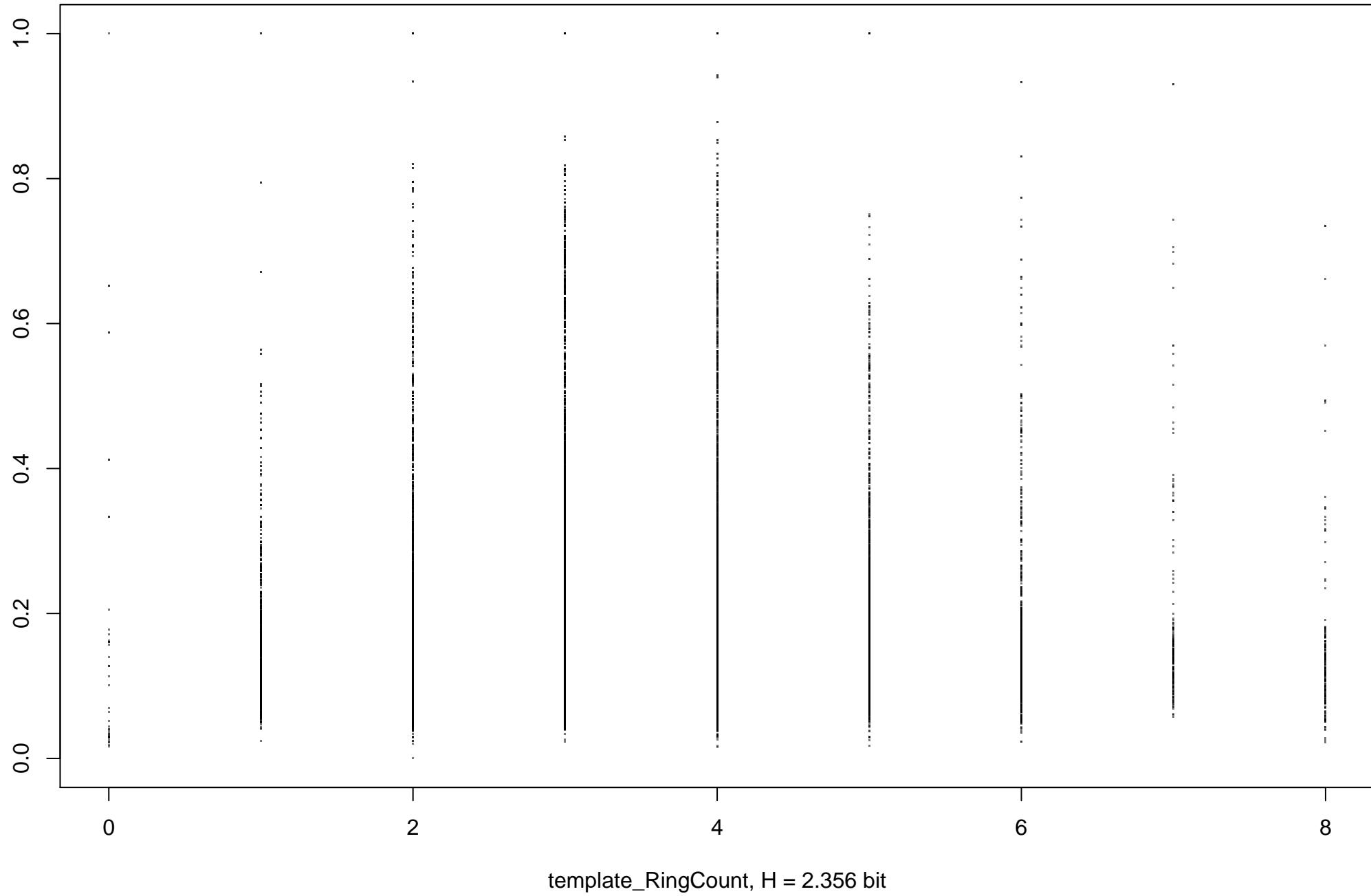


template_HeavyAtomCount-docked_NumHDonors, MI = 0.05867 bit, normMI = 0.02475



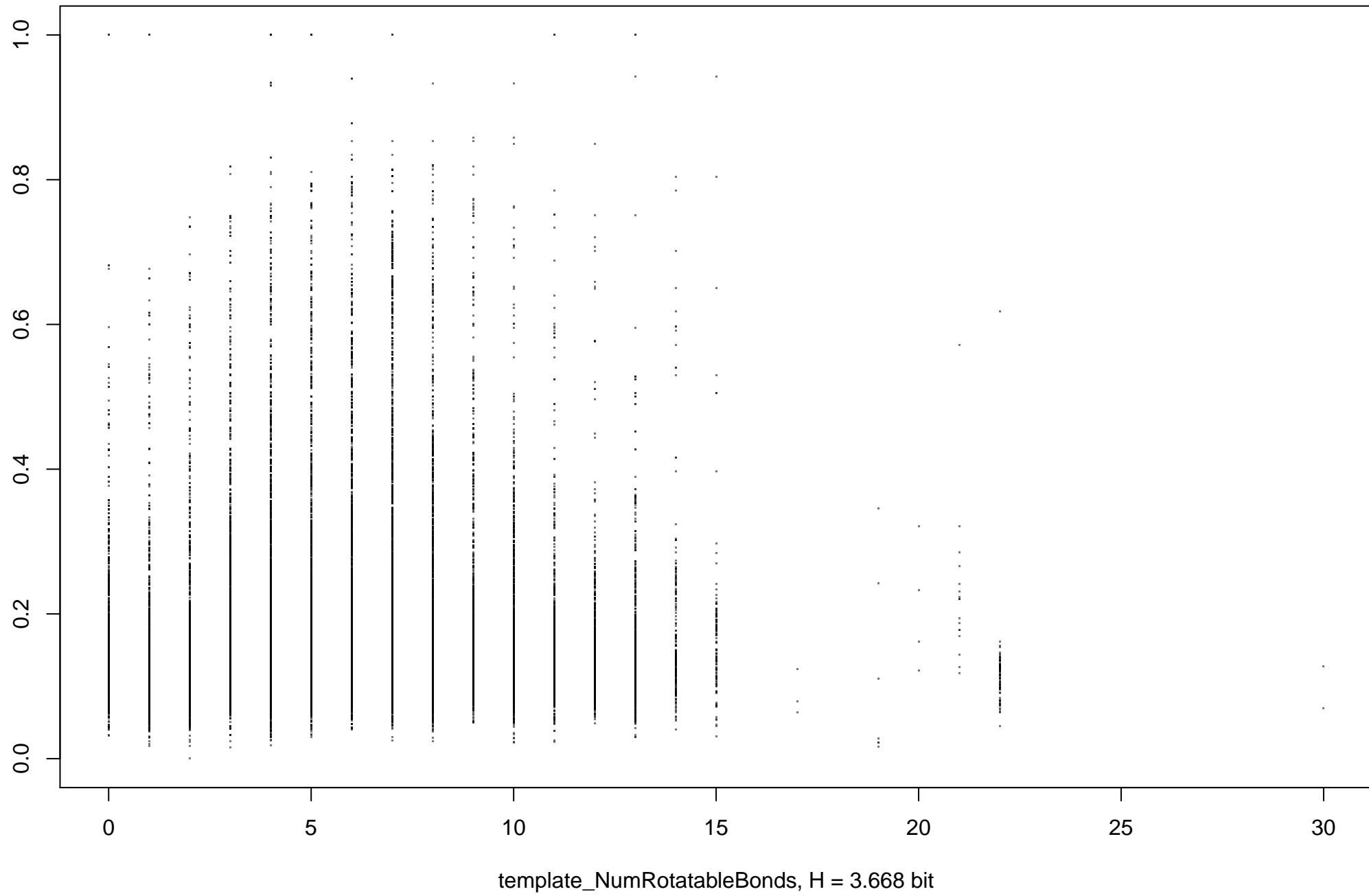
template_RingCount-ec_tanimoto_similarity, MI = 0.05796 bit, normMI = 0.0246

ec_tanimoto_similarity, H = 4.125 bit



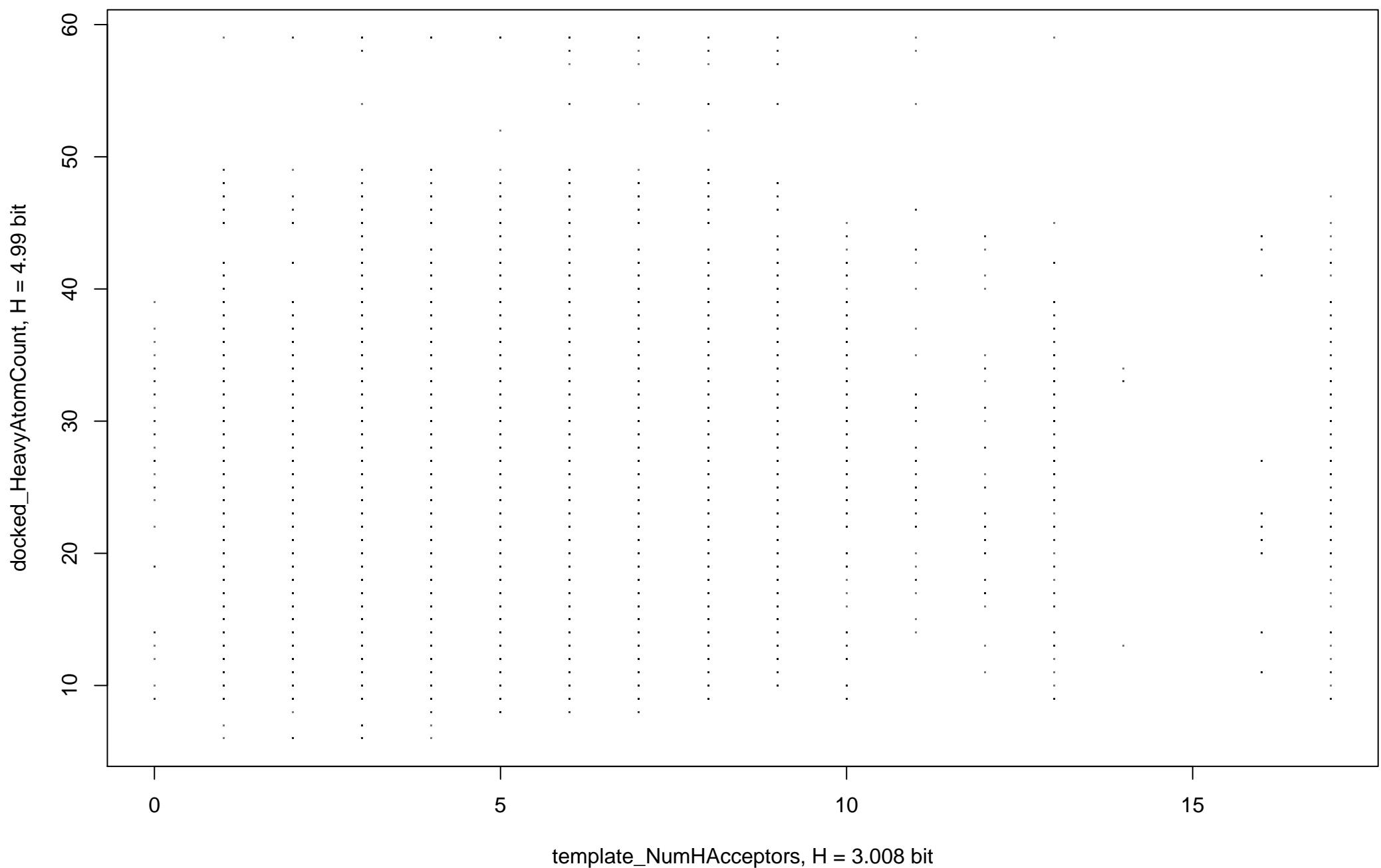
template_NumRotatableBonds–ec_tanimoto_similarity, MI = 0.08981 bit, normMI = 0.02448

ec_tanimoto_similarity, H = 4.125 bit

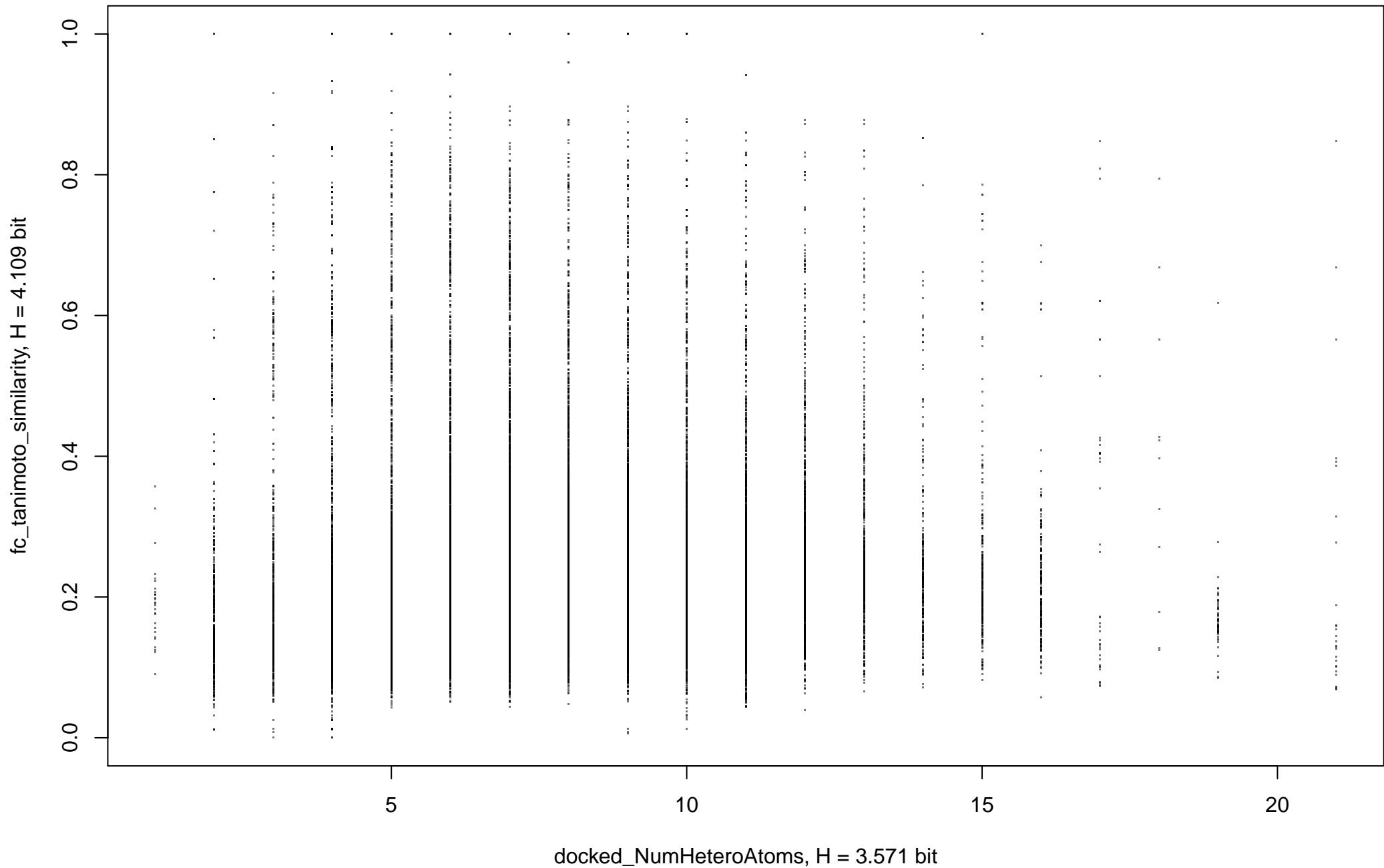


template_NumRotatableBonds, H = 3.668 bit

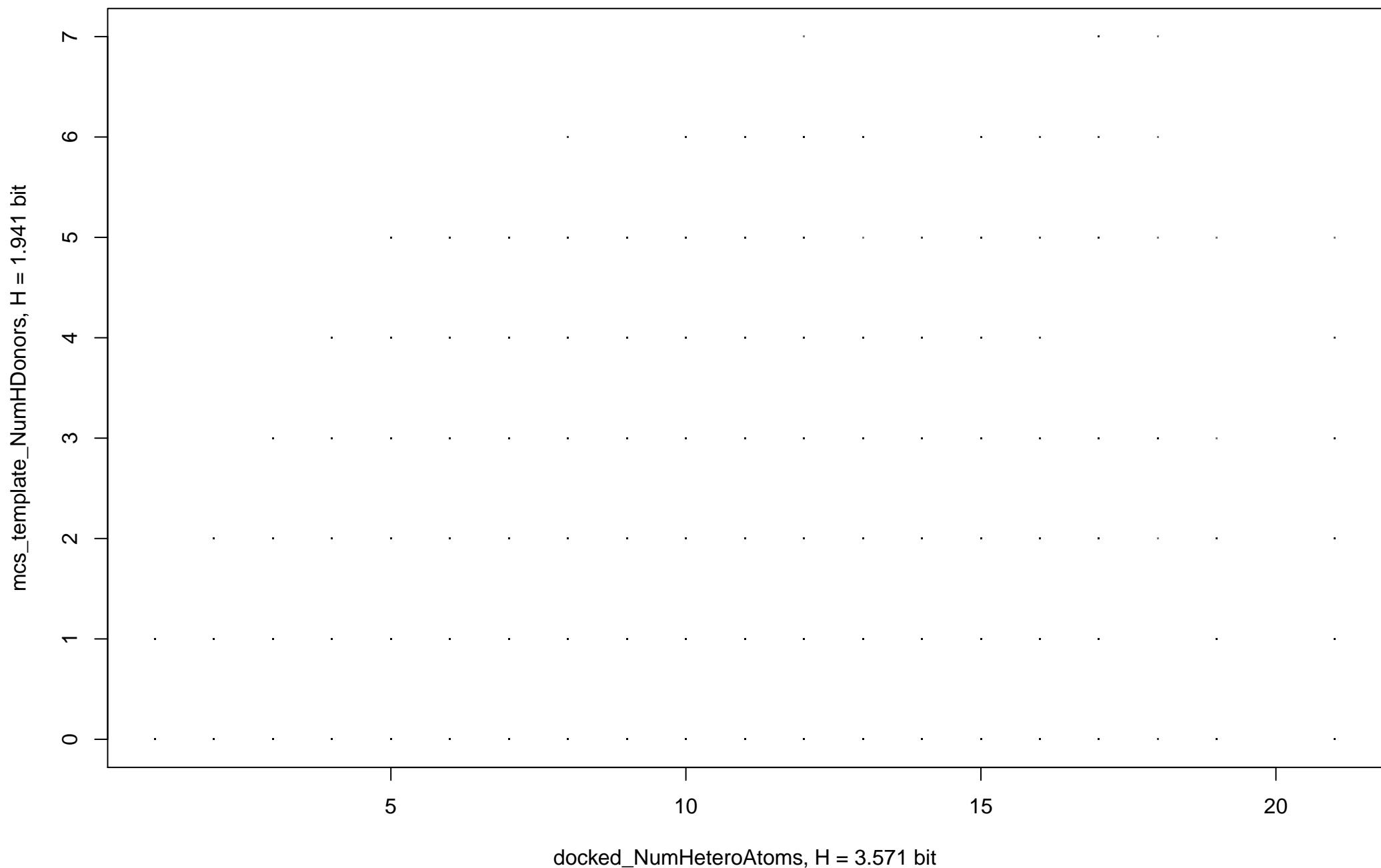
template_NumHAcceptors-docked_HeavyAtomCount, MI = 0.07359 bit, normMI = 0.02447



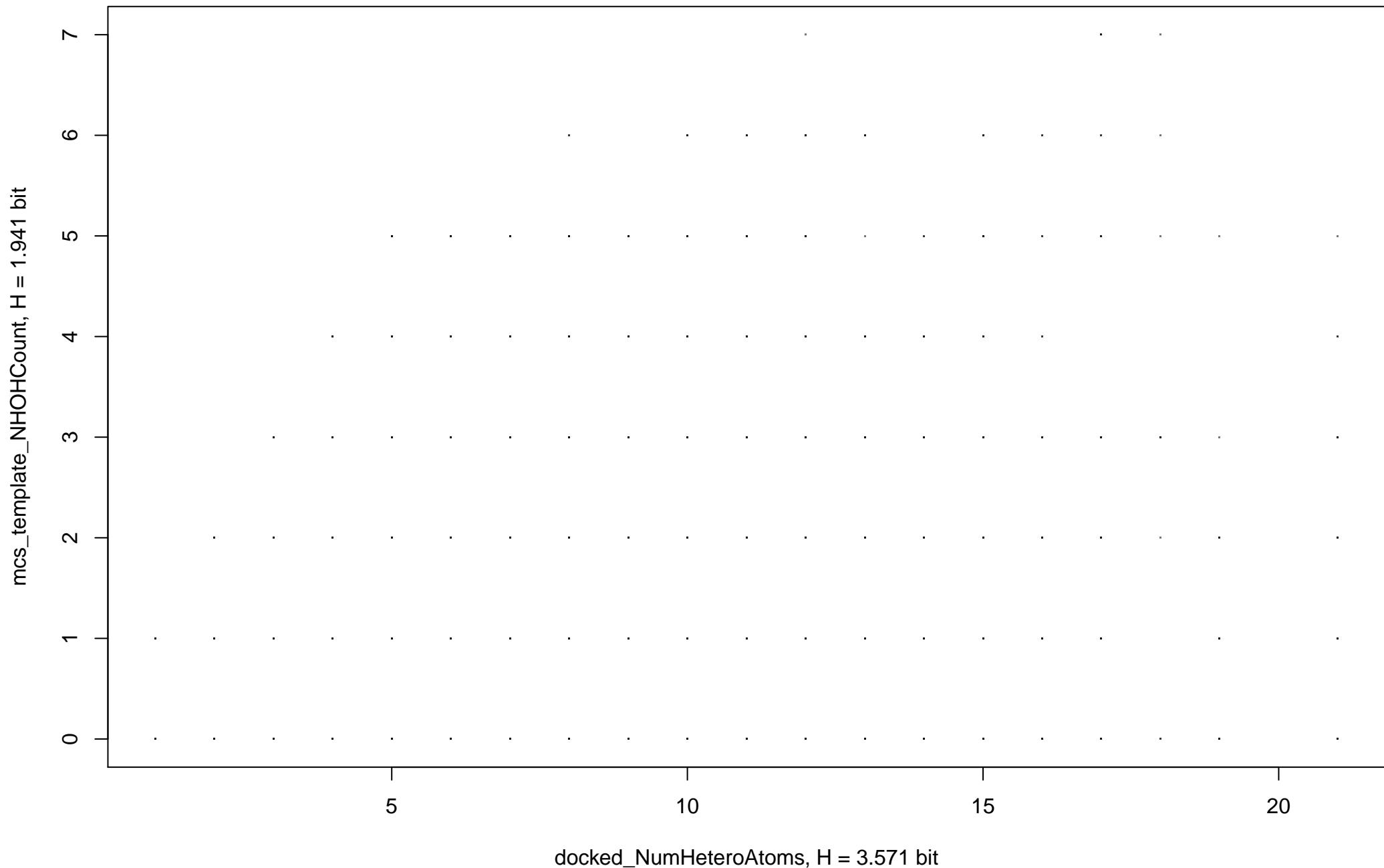
docked_NumHeteroAtoms-fc_tanimoto_similarity, MI = 0.08712 bit, normMI = 0.02439



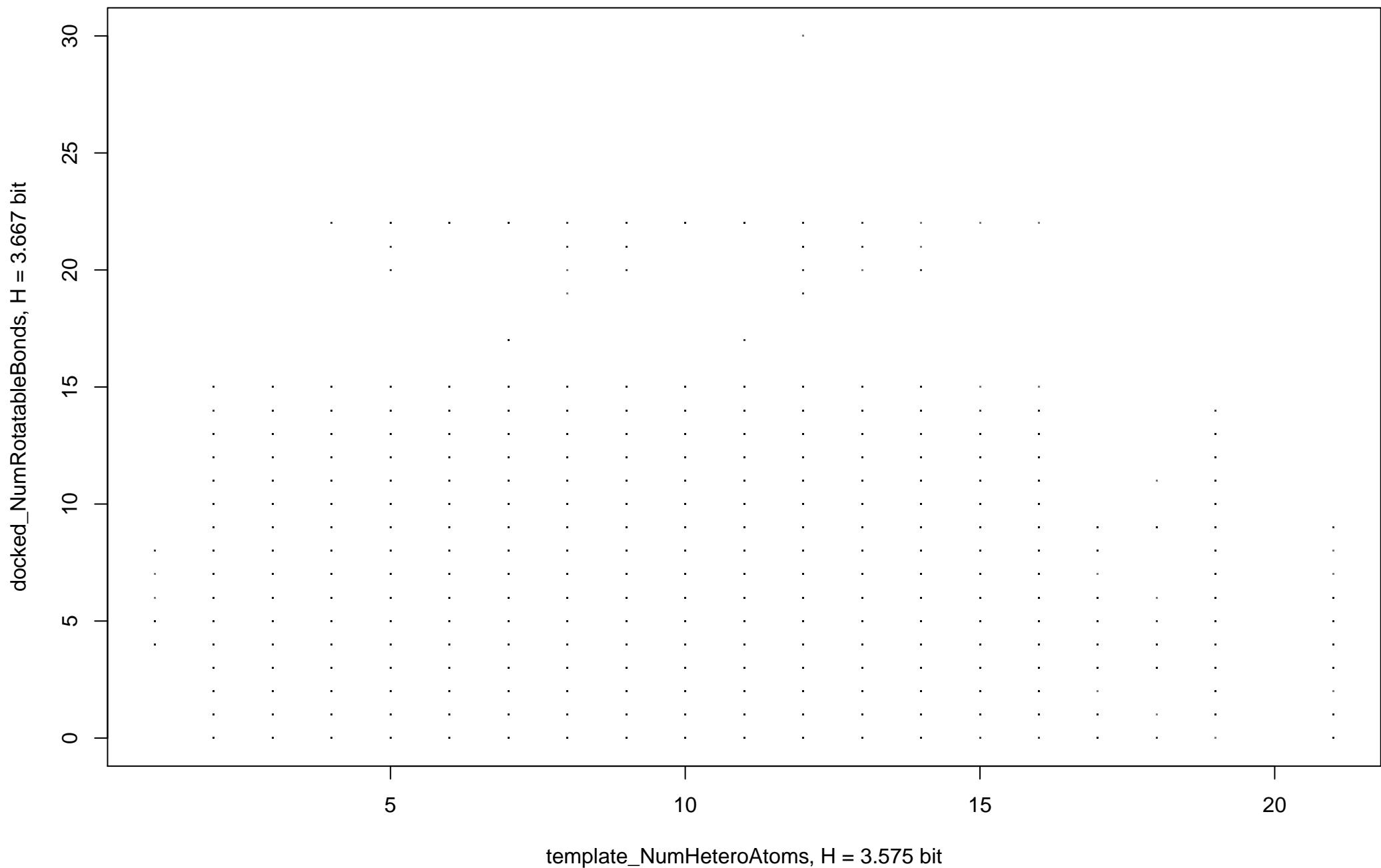
docked_NumHeteroAtoms-mcs_template_NumHDonors, MI = 0.04721 bit, normMI = 0.02433



docked_NumHeteroAtoms-mcs_template_NHOHCount, MI = 0.04697 bit, normMI = 0.02419

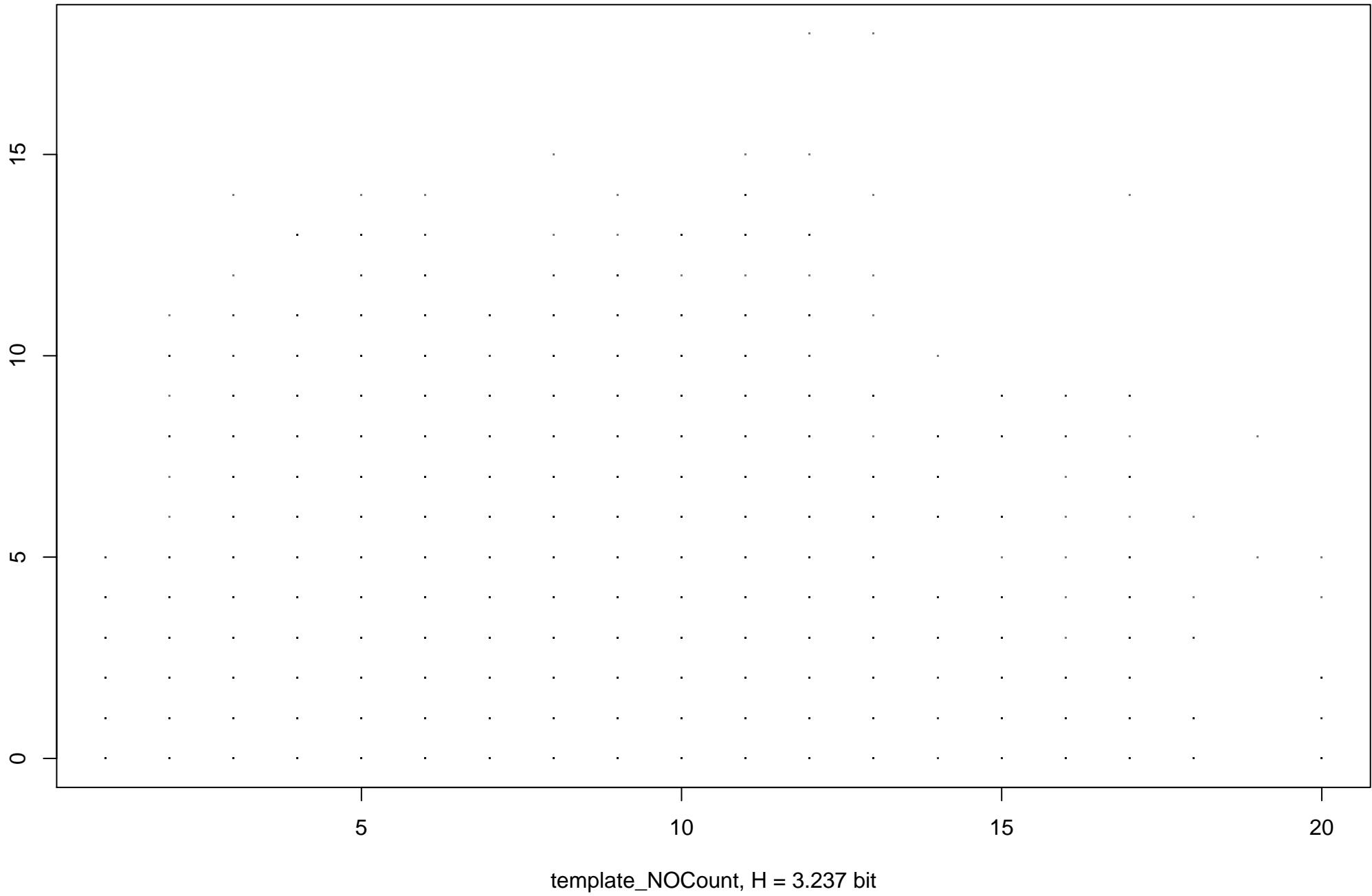


template_NumHeteroAtoms-docked_NumRotatableBonds, MI = 0.08626 bit, normMI = 0.02413



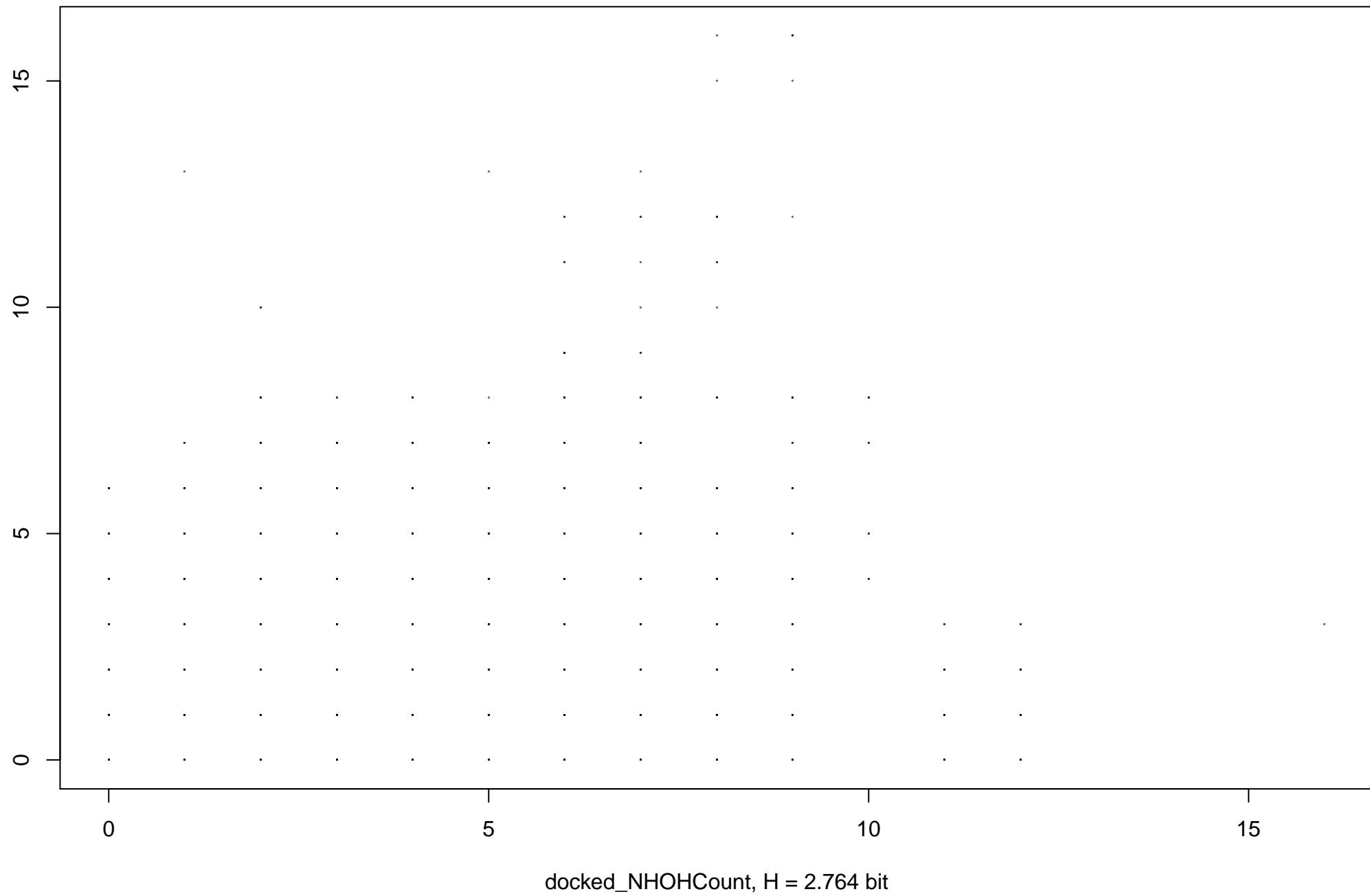
template_NOCount-mcs_docked_NumRotatableBonds, MI = 0.0746 bit, normMI = 0.02393

mcs_docked_NumRotatableBonds, H = 3.117 bit

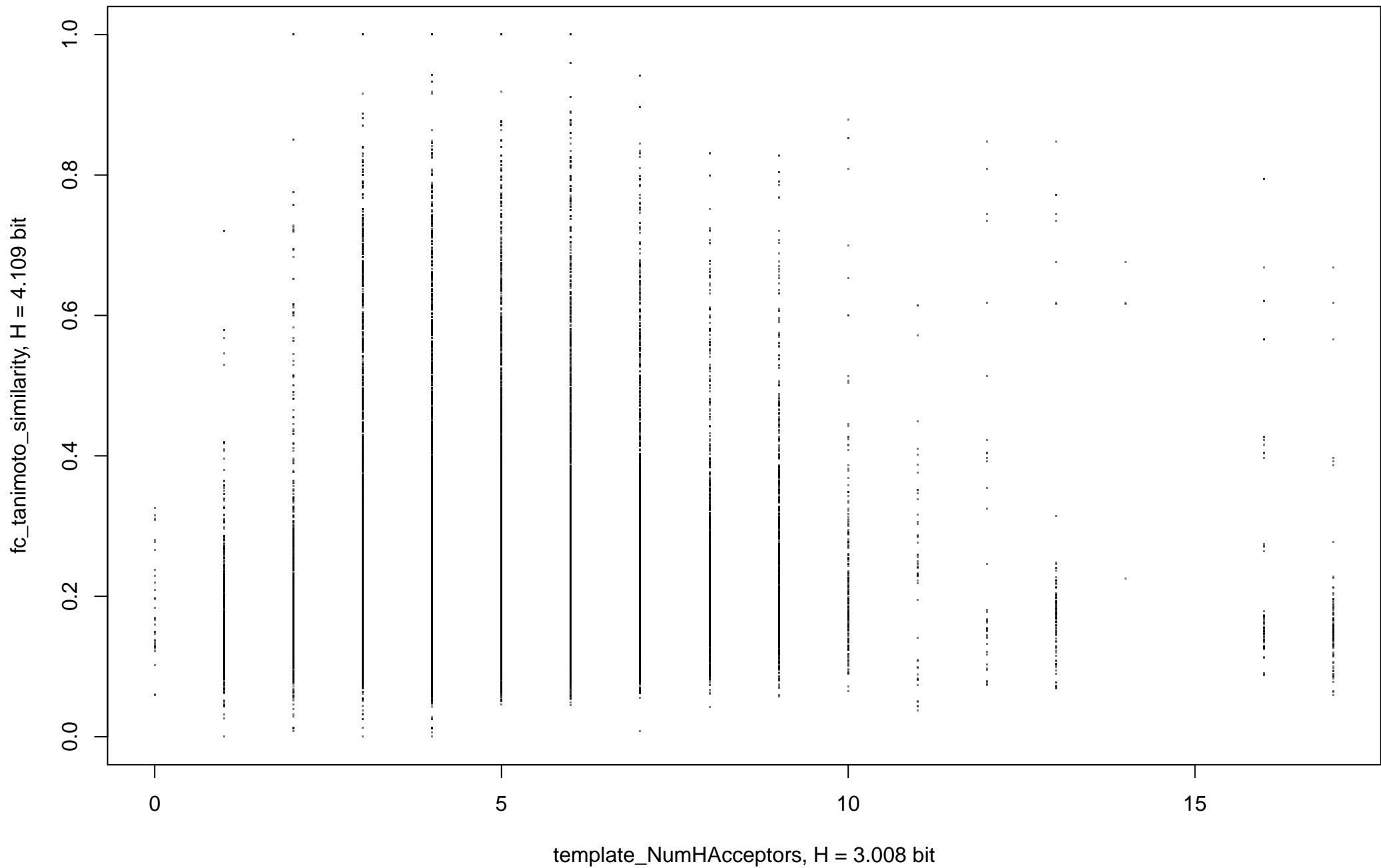


docked_NHOHCount-mcs_template_NumHAcceptors, MI = 0.05924 bit, normMI = 0.02381

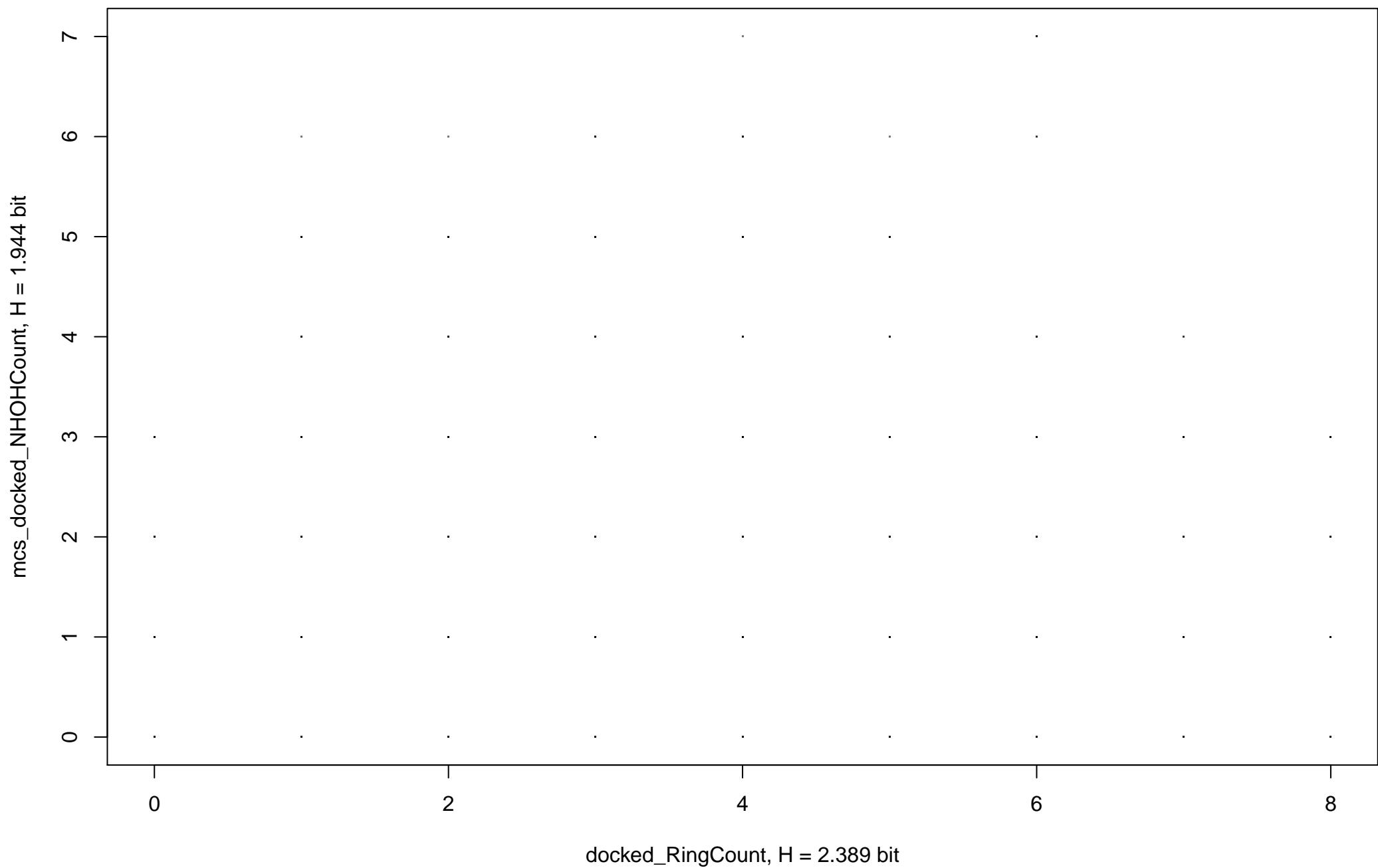
mcs_template_NumHAcceptors, H = 2.488 bit



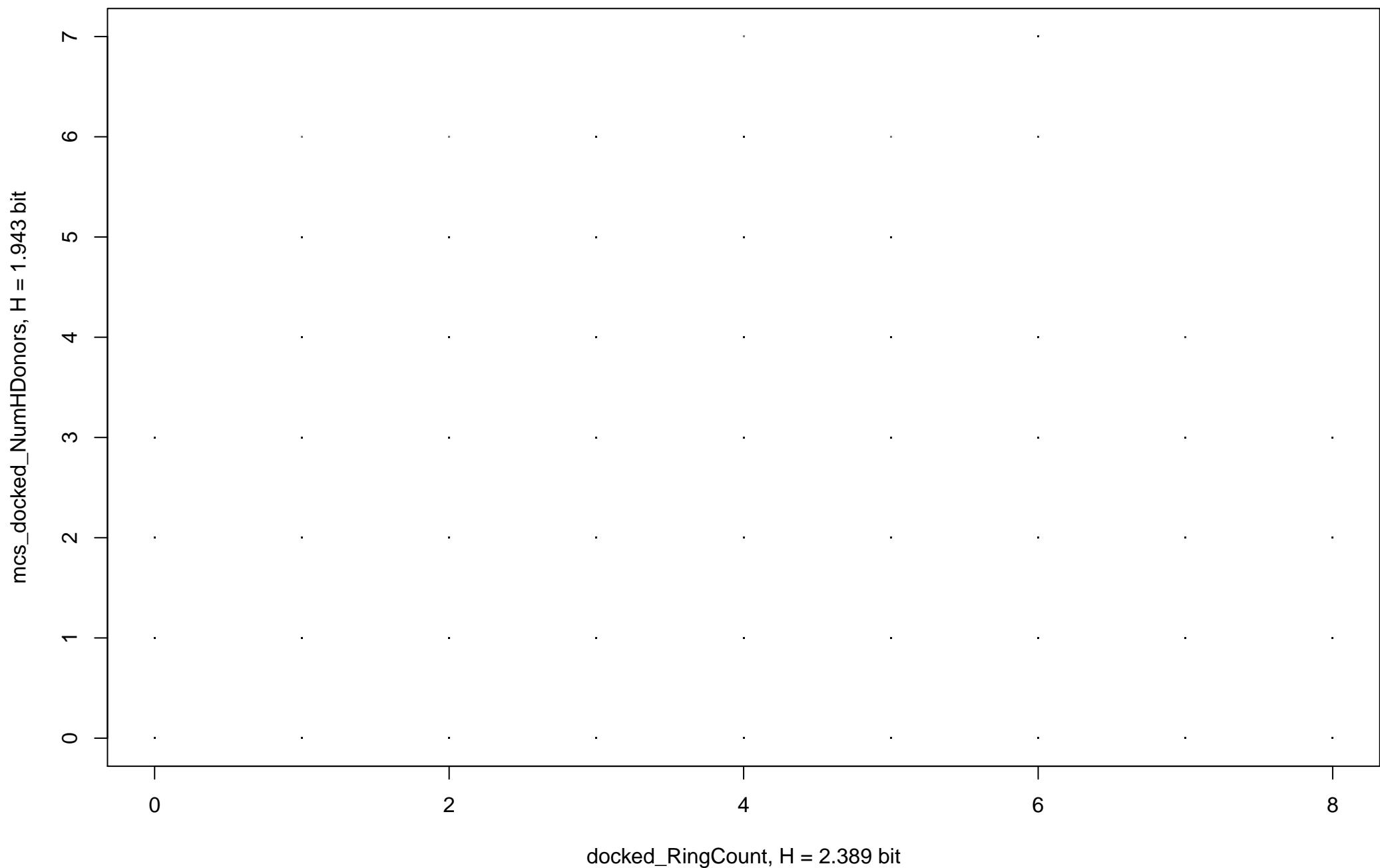
template_NumHAcceptors-fc_tanimoto_similarity, MI = 0.07126 bit, normMI = 0.02369



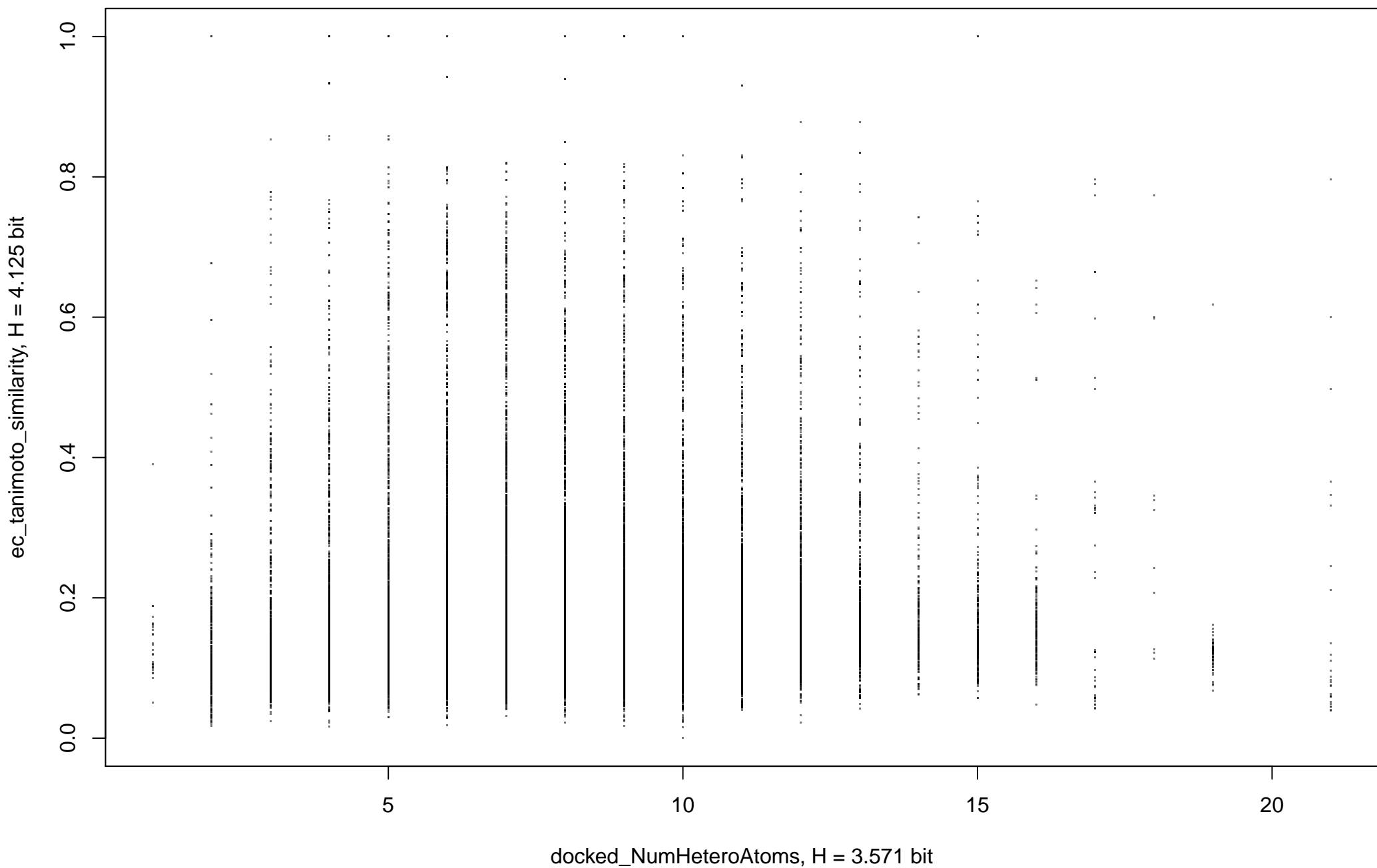
docked_RingCount–mcs_docked_NHOHCount, MI = 0.04586 bit, normMI = 0.02359



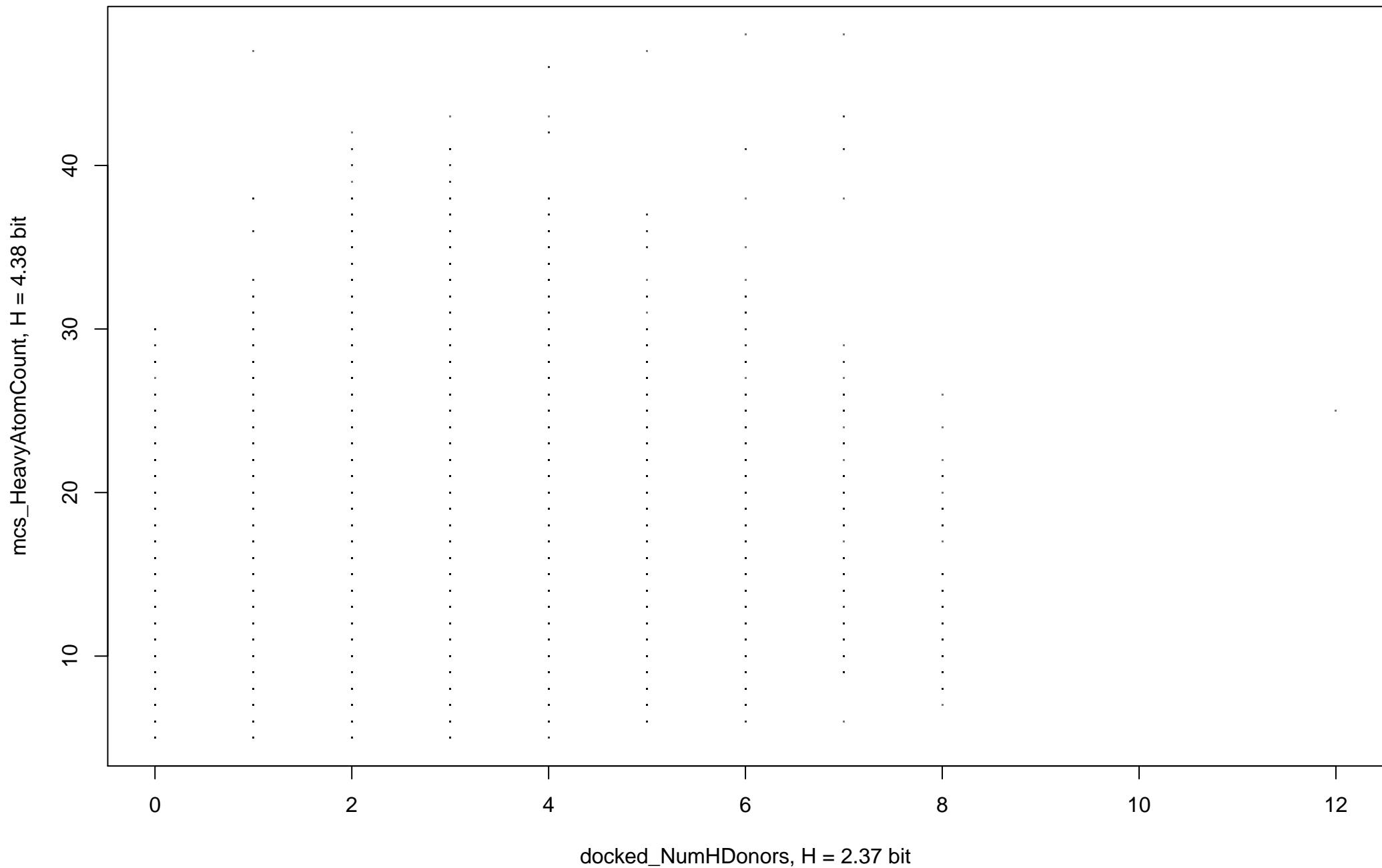
docked_RingCount-mcs_docked_NumHDonors, MI = 0.04577 bit, normMI = 0.02356



docked_NumHeteroAtoms–ec_tanimoto_similarity, MI = 0.0839 bit, normMI = 0.02349

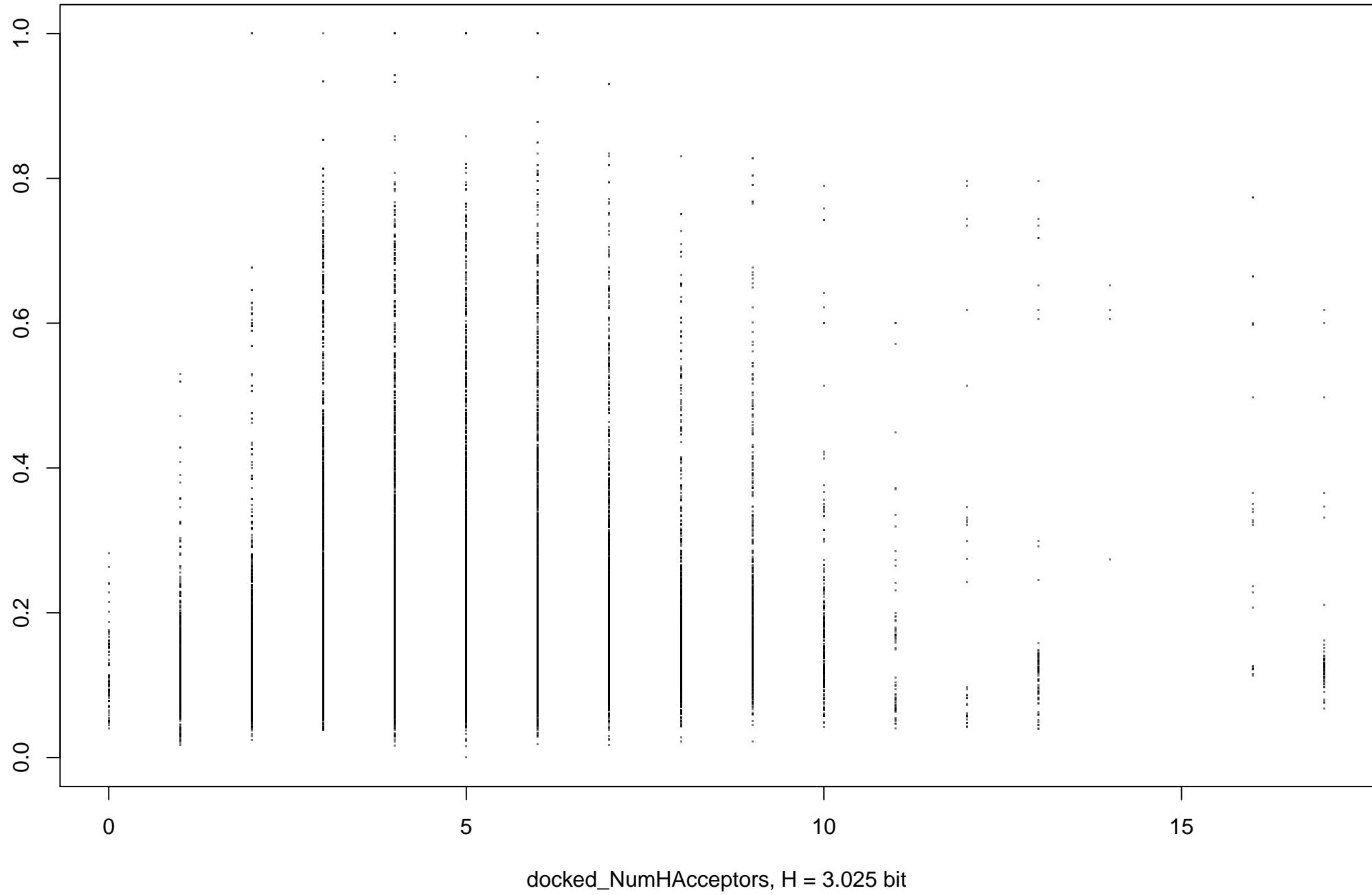


docked_NumHDonors-mcs_HeavyAtomCount, MI = 0.05534 bit, normMI = 0.02335



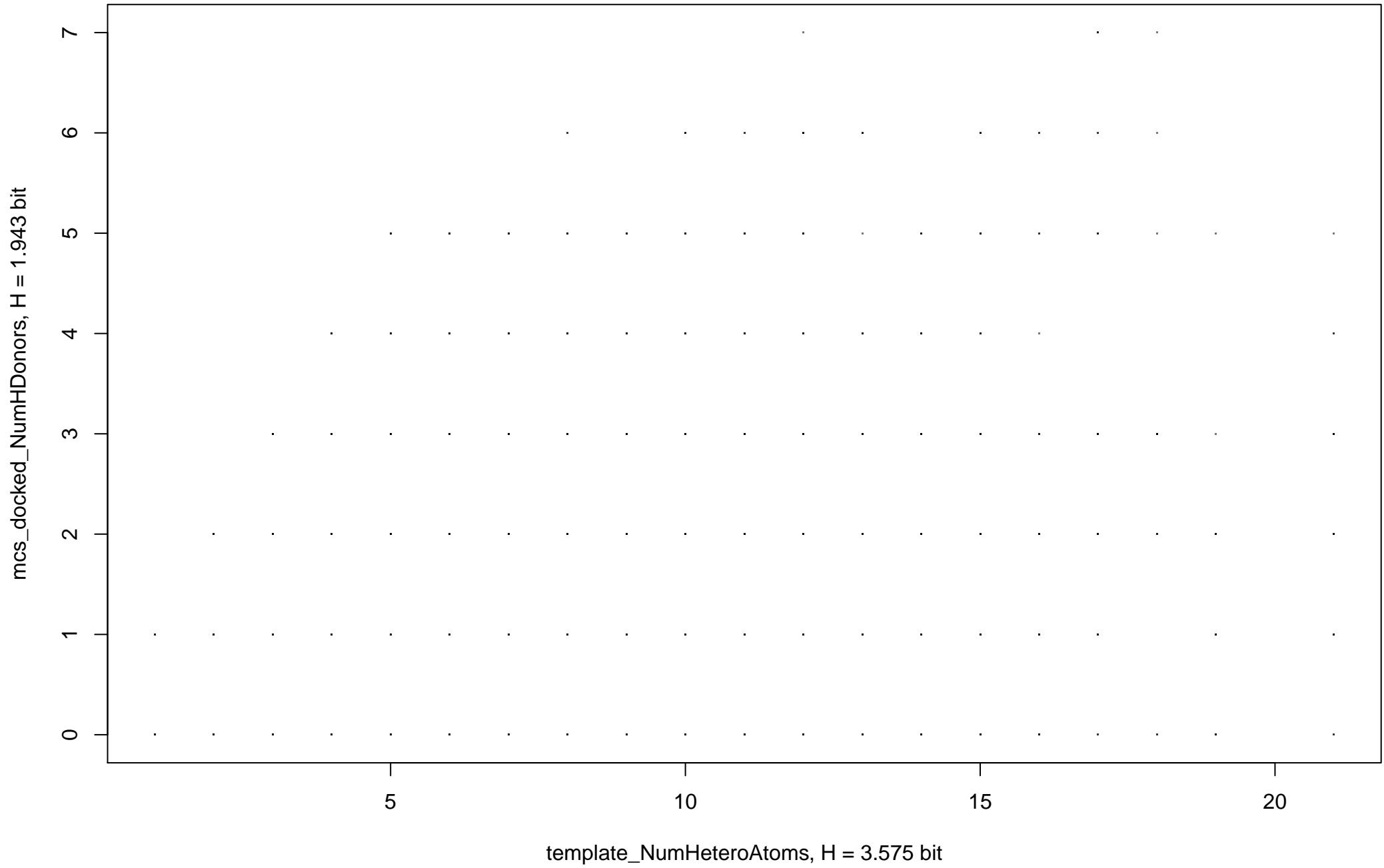
docked_NumHAcceptors-ec_tanimoto_similarity, MI = 0.07052 bit, normMI = 0.02331

ec_tanimoto_similarity, H = 4.125 bit

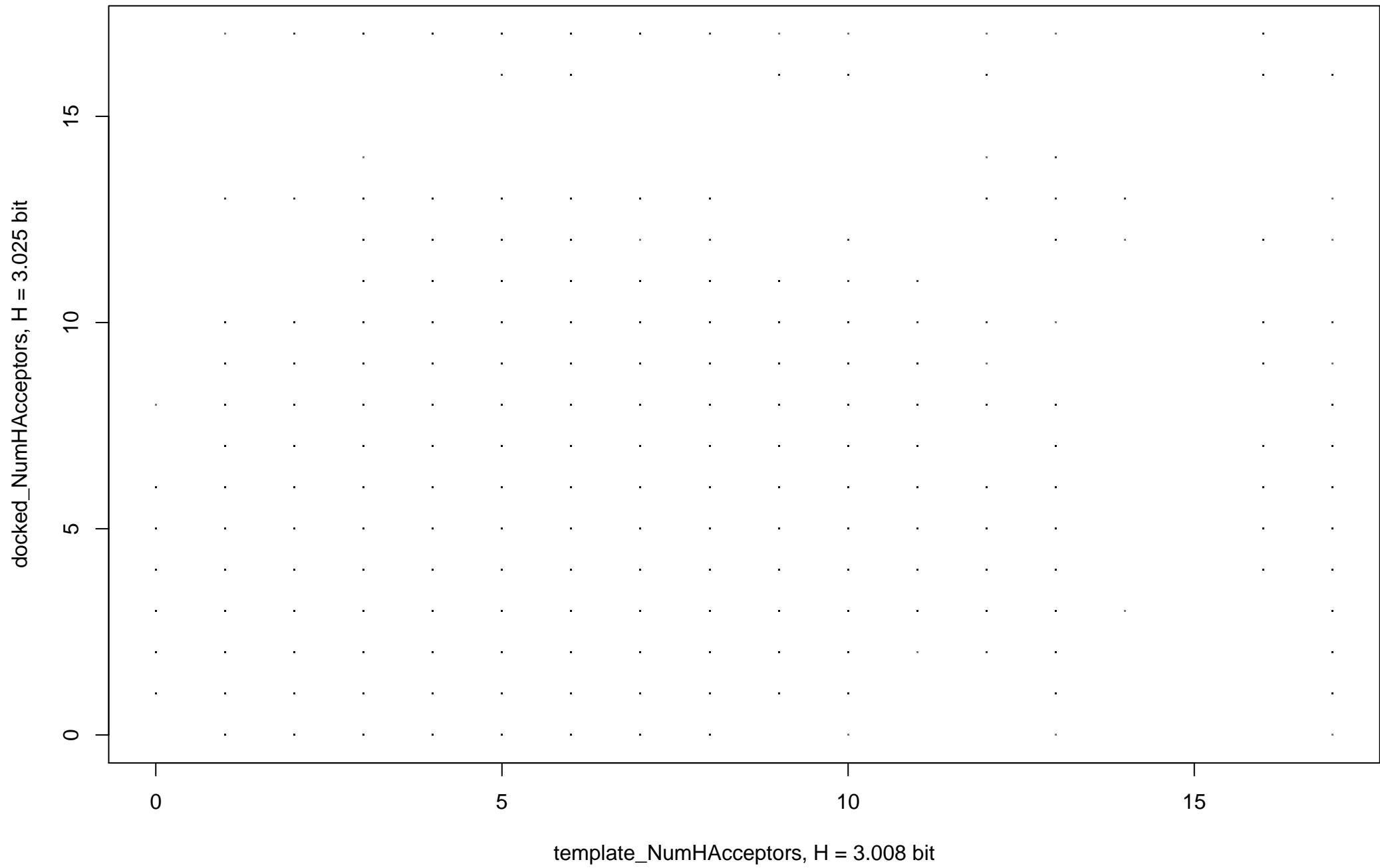


docked_NumHAcceptors, H = 3.025 bit

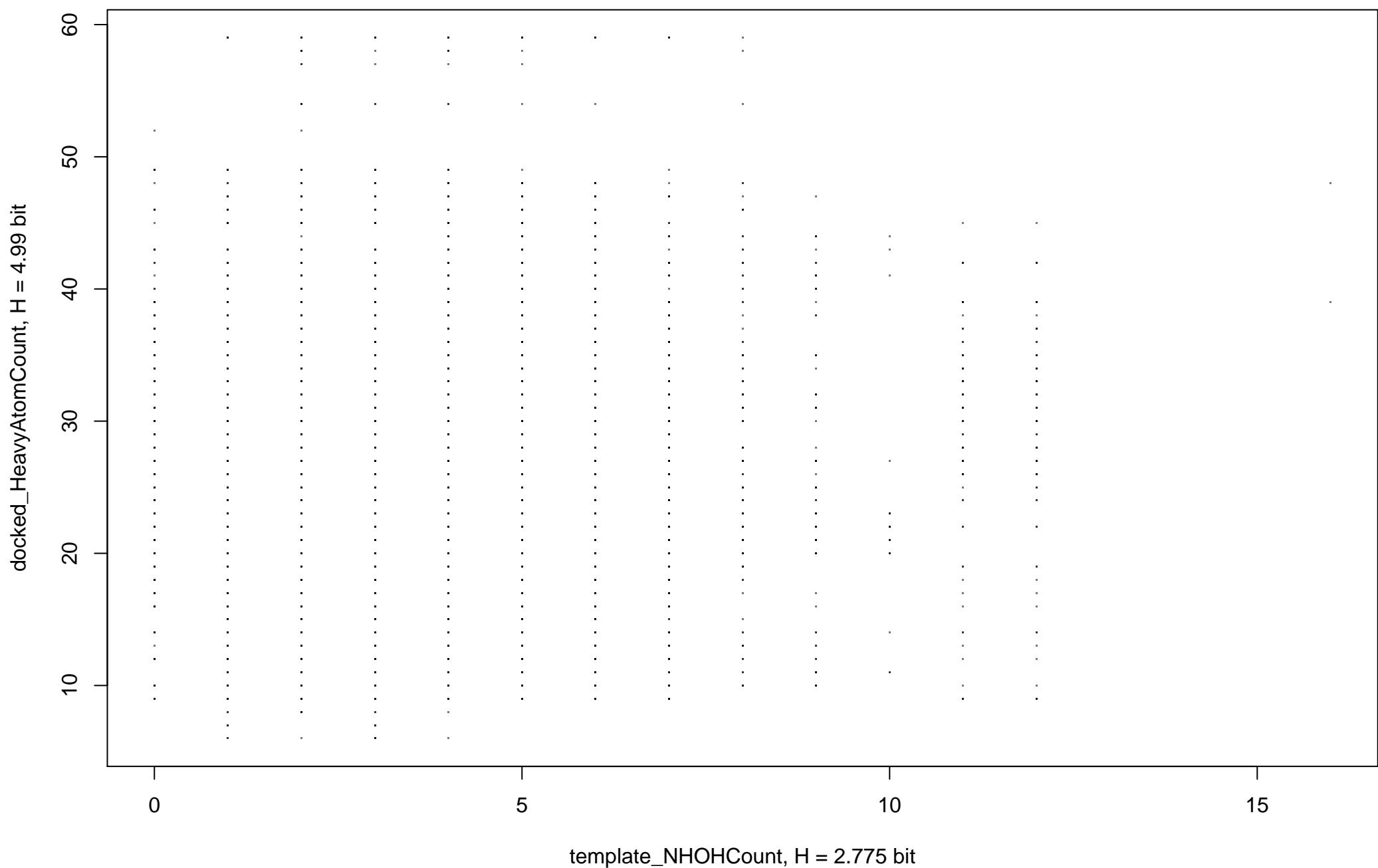
template_NumHeteroAtoms-mcs_docked_NumHDonors, MI = 0.04522 bit, normMI = 0.02327



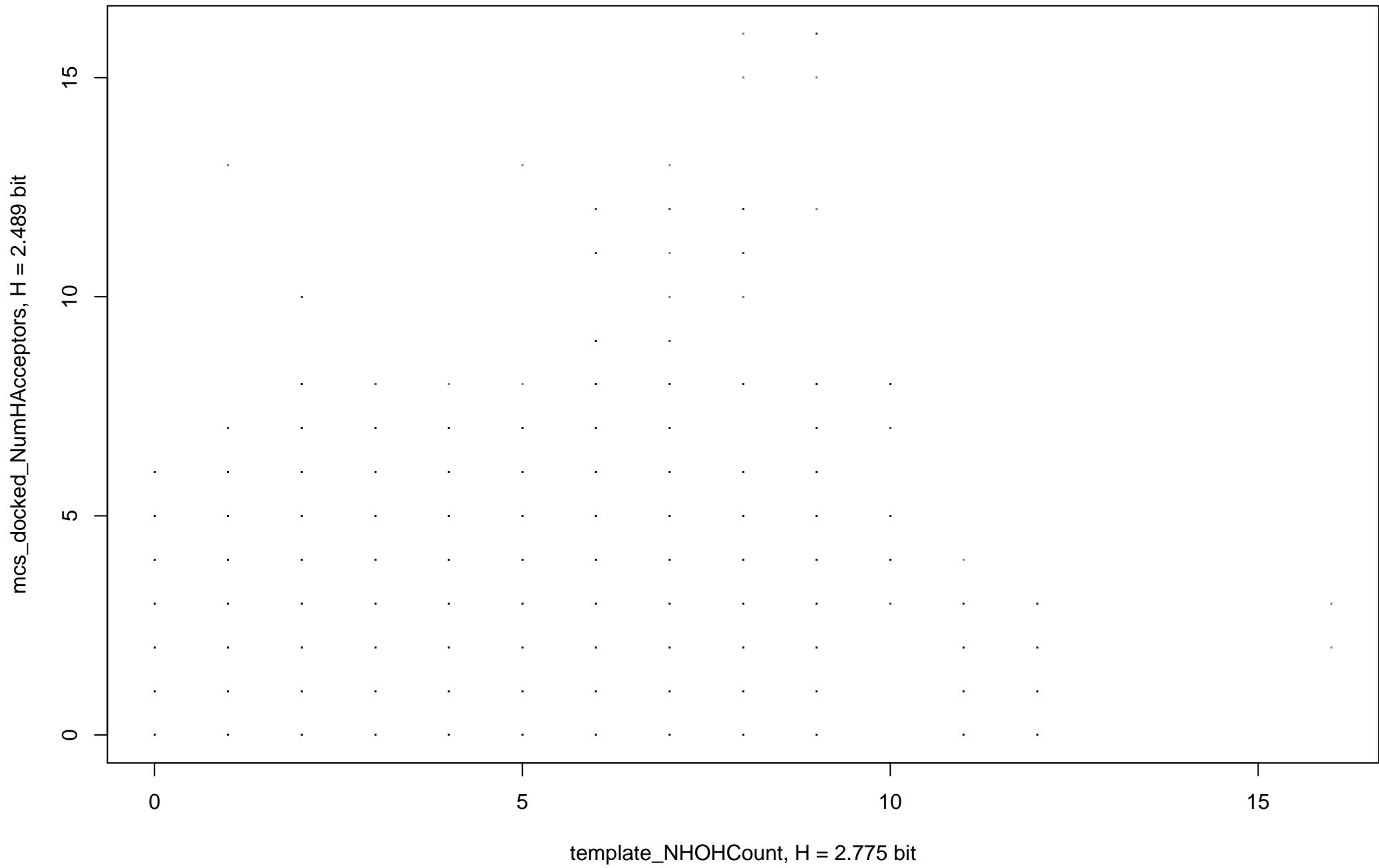
template_NumHAcceptors-docked_NumHAcceptors, MI = 0.06996 bit, normMI = 0.02326



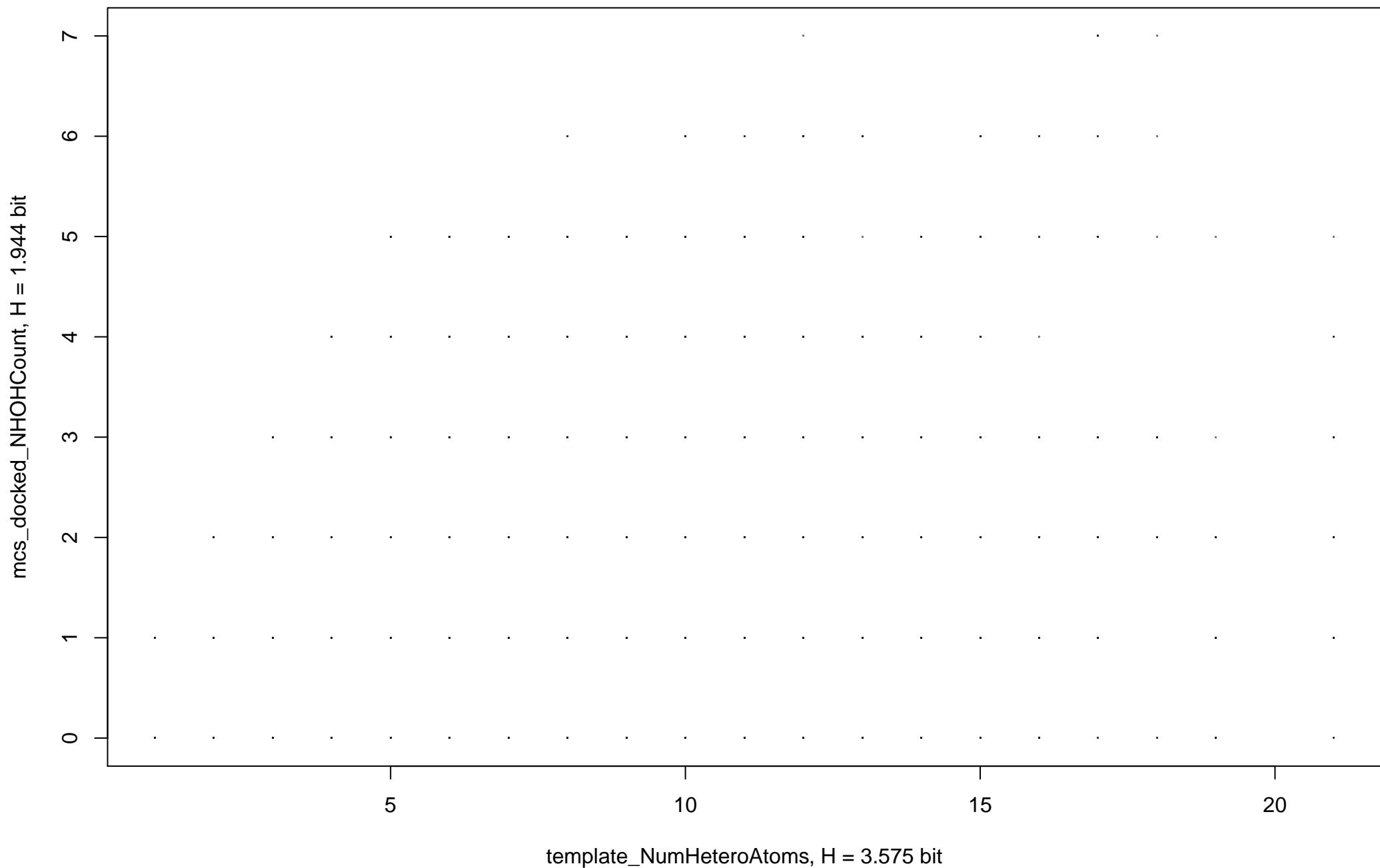
template_NHOHCount–docked_HeavyAtomCount, MI = 0.0644 bit, normMI = 0.0232



template_NHOHCount-mcs_docked_NumHAcceptors, MI = 0.05775 bit, normMI = 0.0232

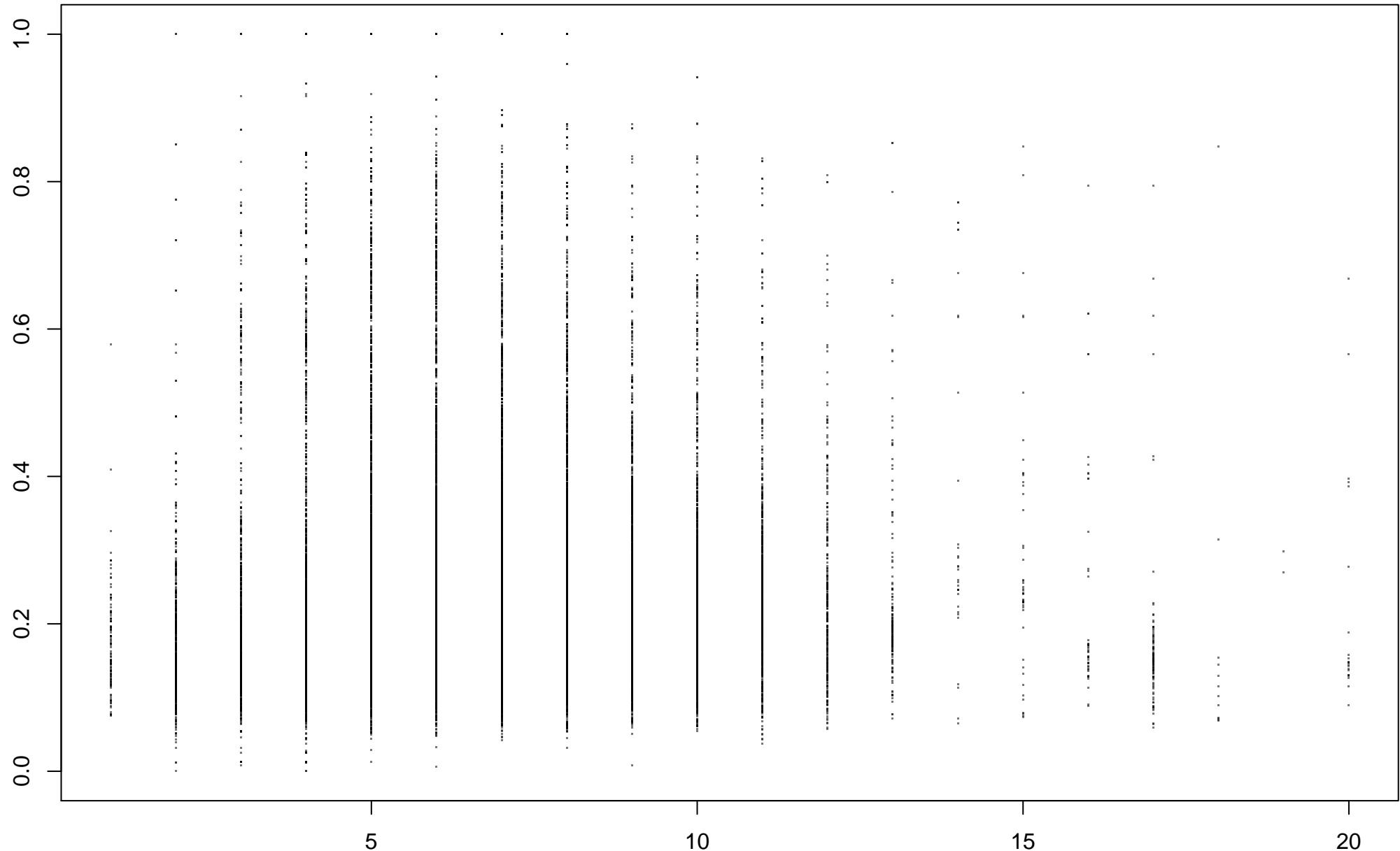


template_NumHeteroAtoms-mcs_docked_NHOHCount, MI = 0.04502 bit, normMI = 0.02316



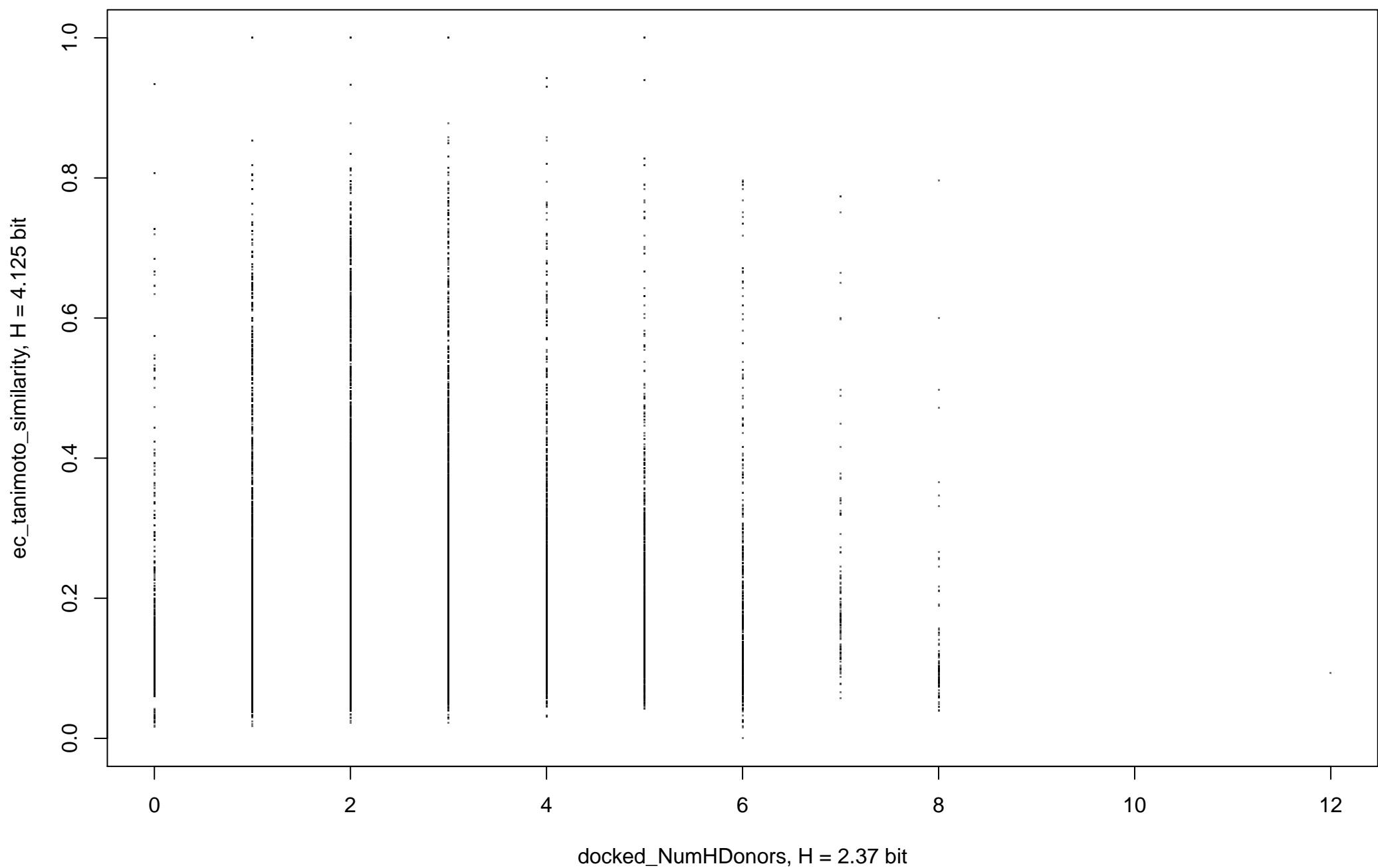
template_NOCount-fc_tanimoto_similarity, MI = 0.07485 bit, normMI = 0.02313

fc_tanimoto_similarity, $H = 4.109$ bit

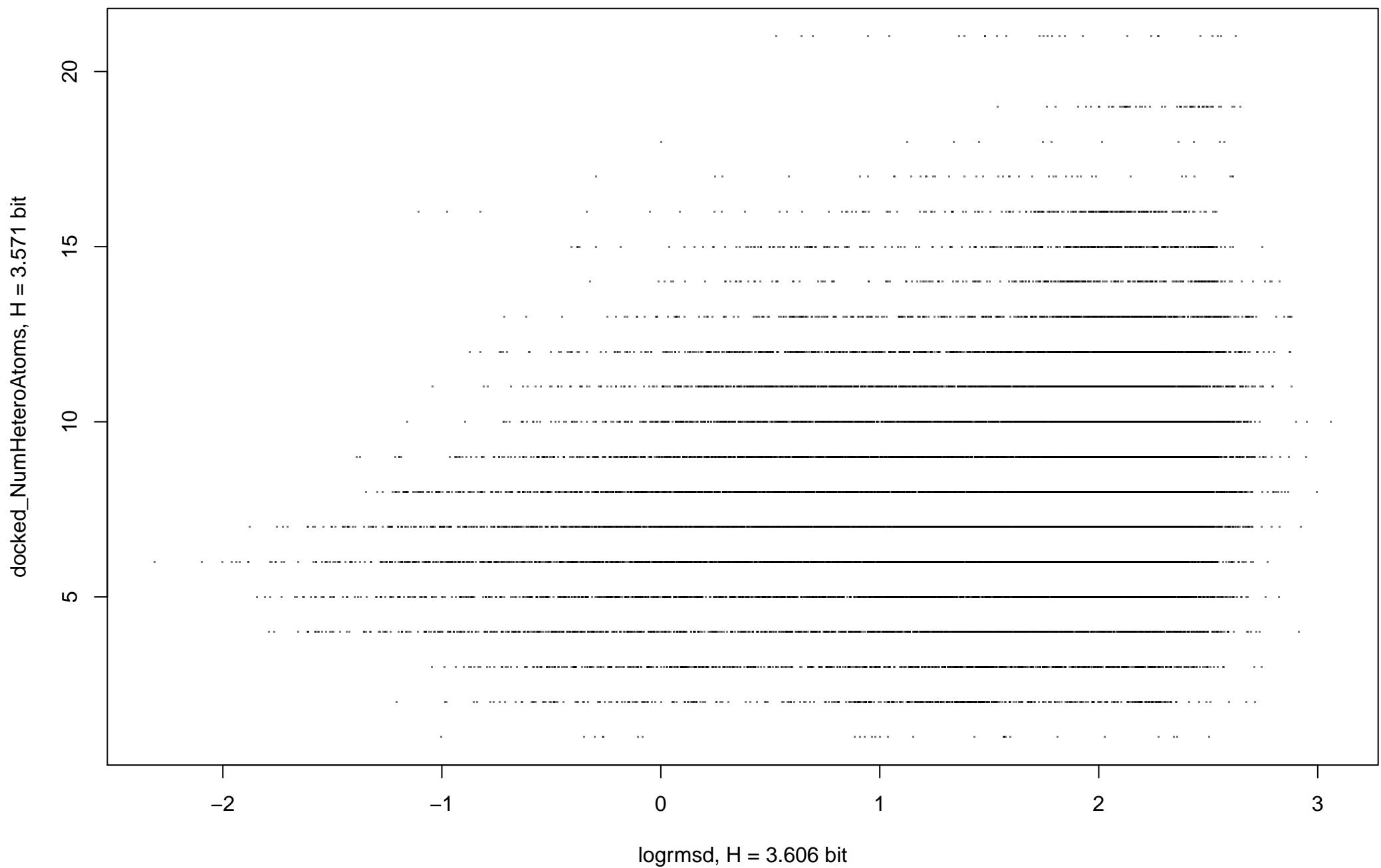


template_NOCount, $H = 3.237$ bit

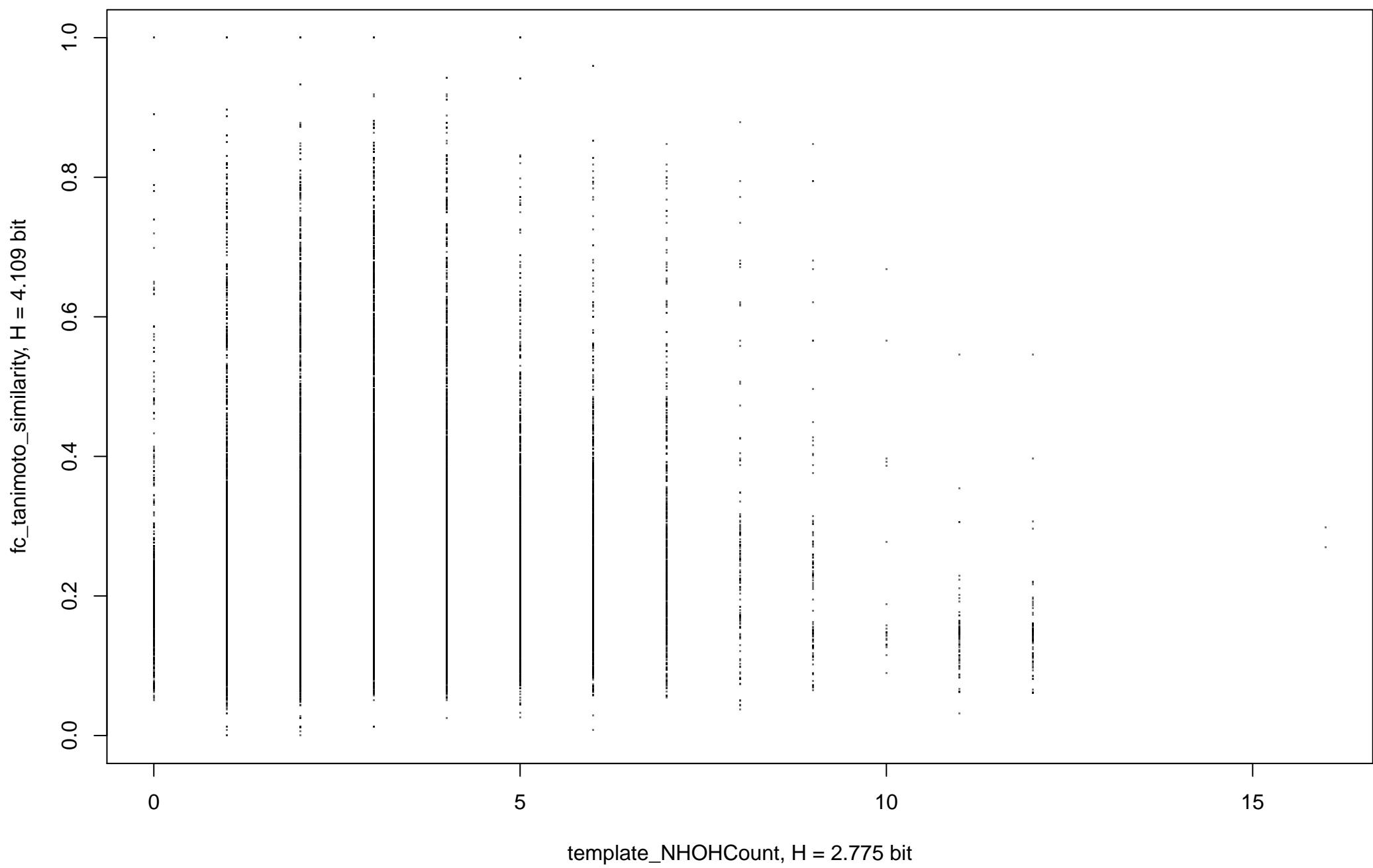
docked_NuHDonors-ec_tanimoto_similarity, MI = 0.05455 bit, normMI = 0.02302



logrmsd-docked_NumHeteroAtoms, MI = 0.08185 bit, normMI = 0.02292

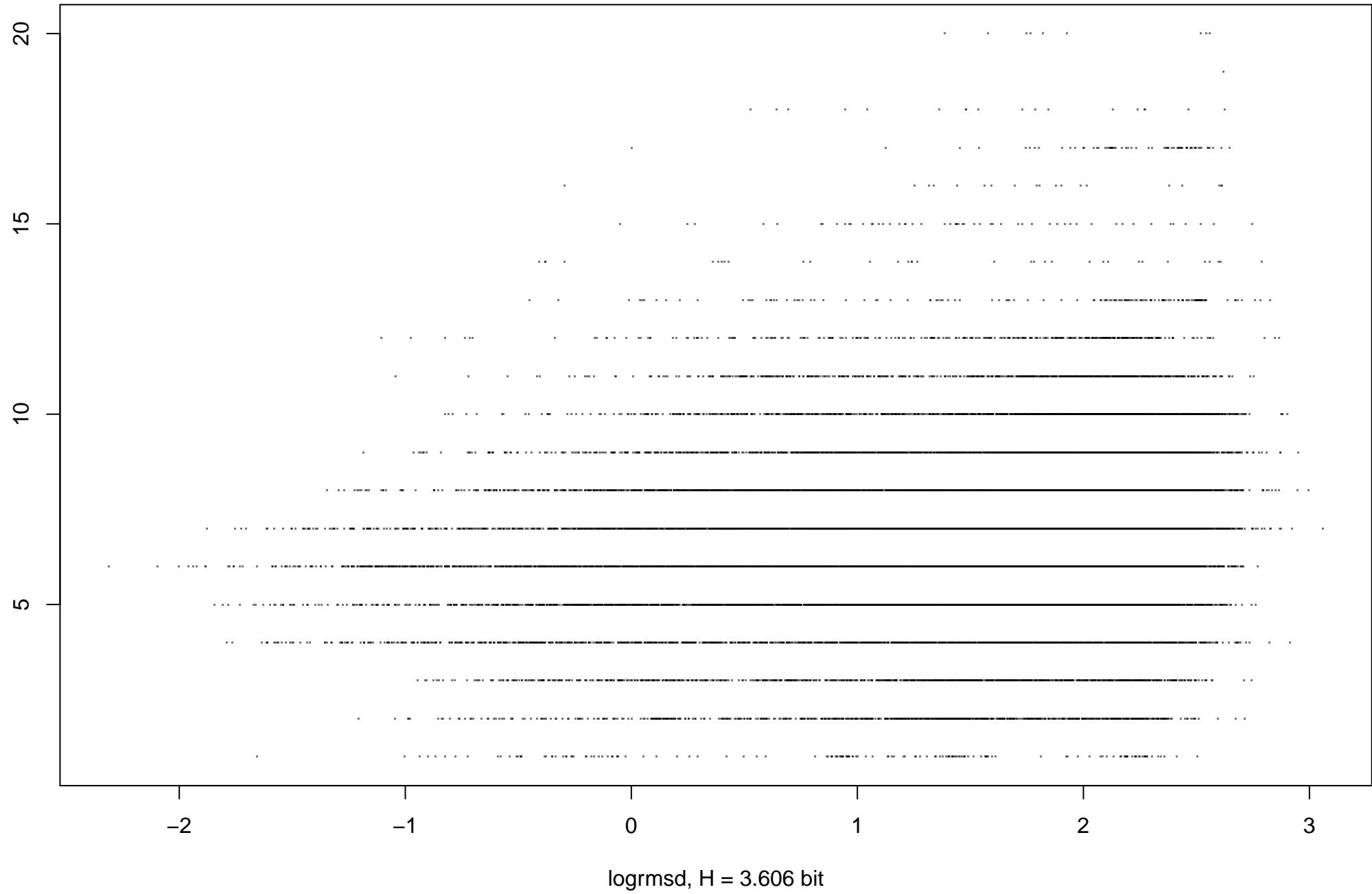


template_NHOHCount-fc_tanimoto_similarity, MI = 0.06321 bit, normMI = 0.02278



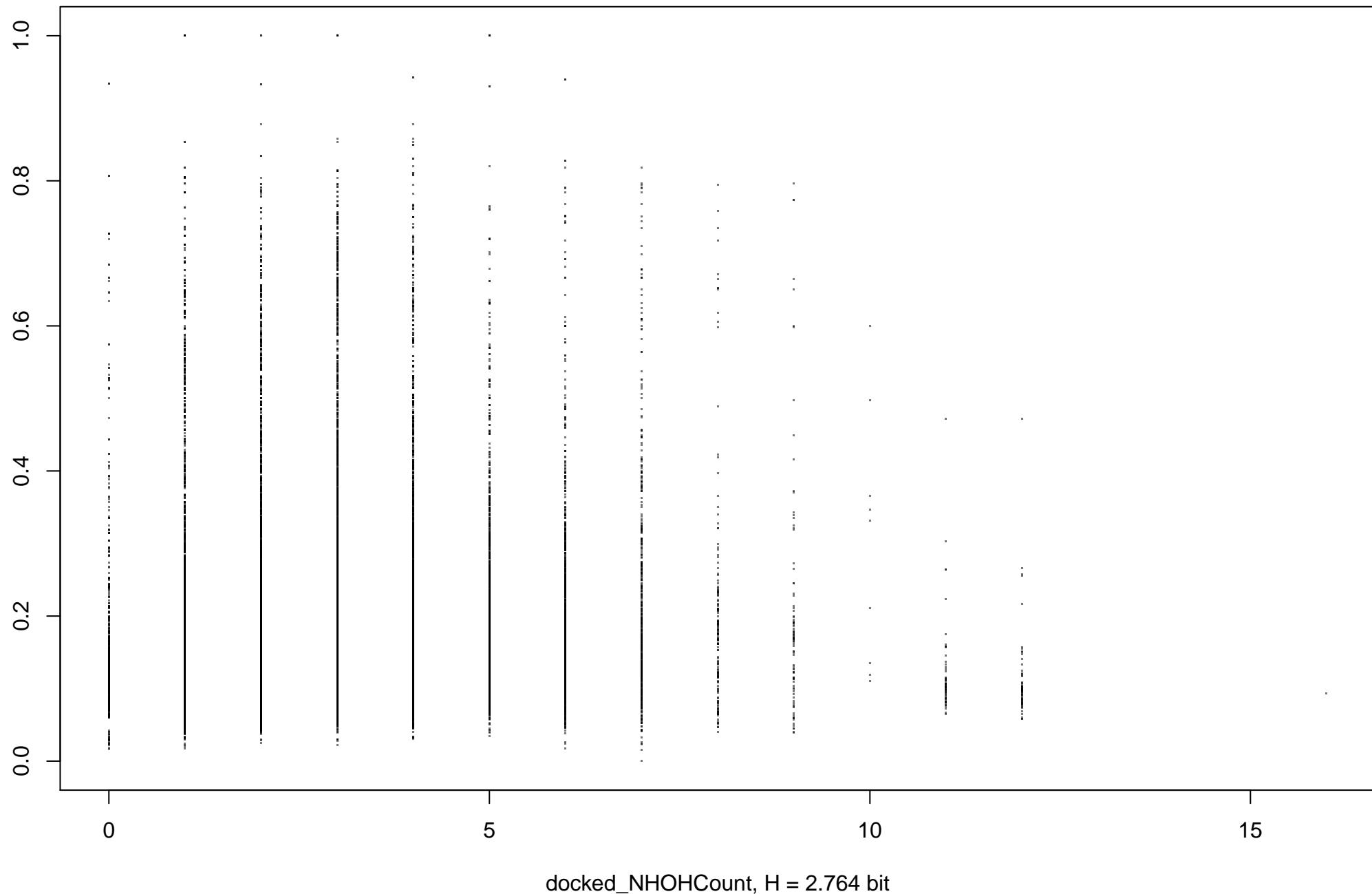
logrmsd-docked_NOCount, MI = 0.07417 bit, normMI = 0.02277

docked_NOCount, H = 3.257 bit

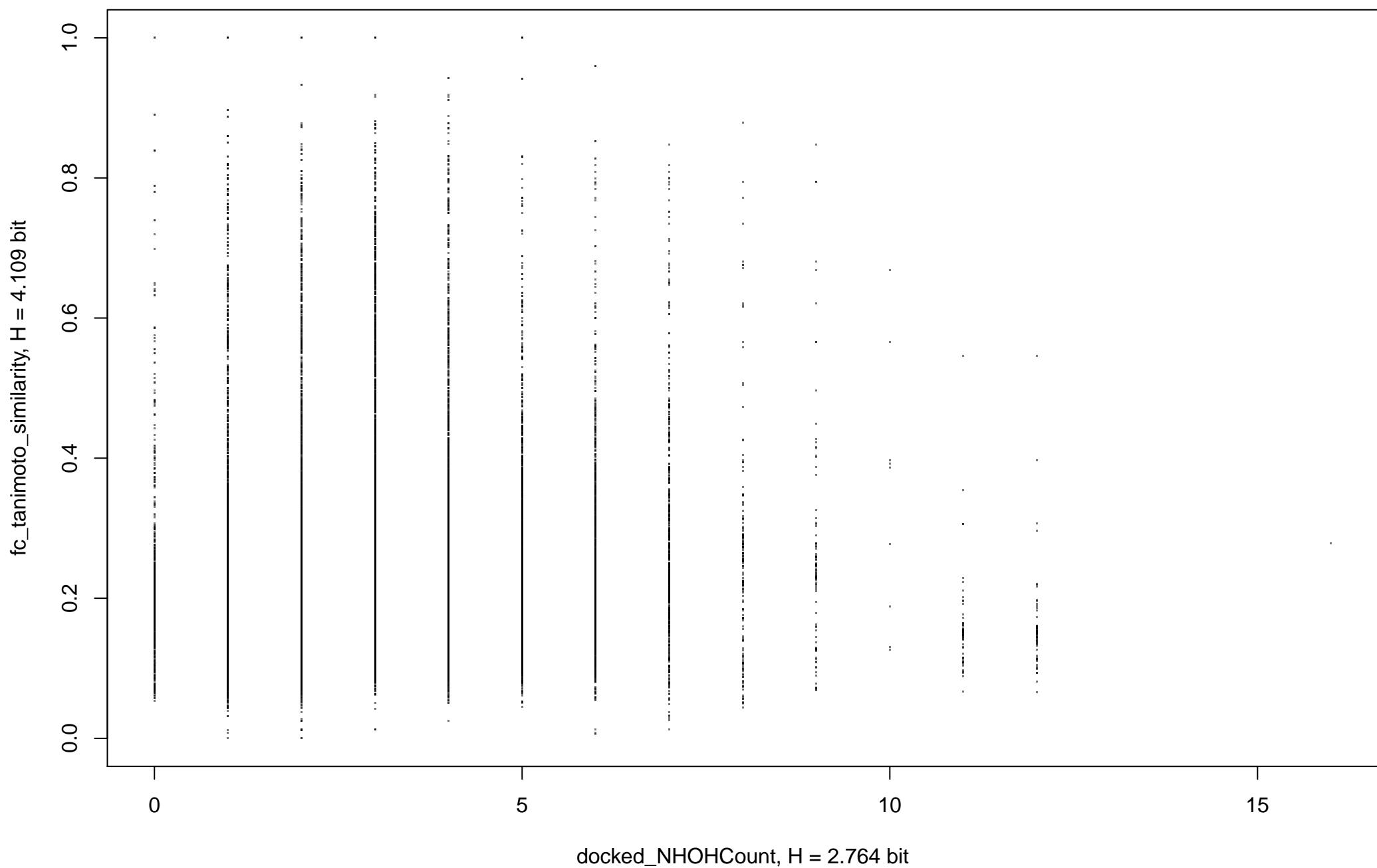


docked_NHOHCount–ec_tanimoto_similarity, MI = 0.06245 bit, normMI = 0.02259

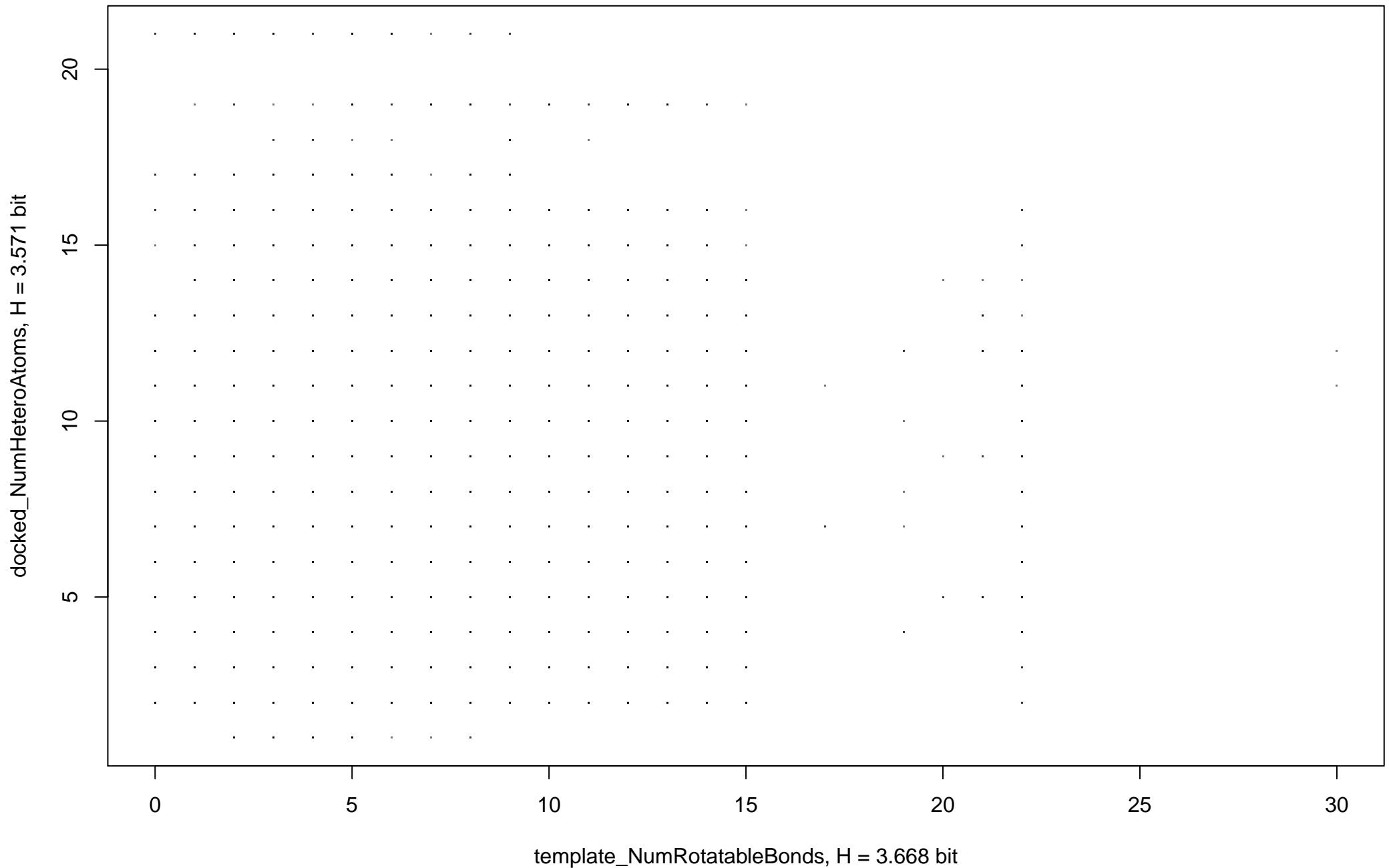
ec_tanimoto_similarity, H = 4.125 bit



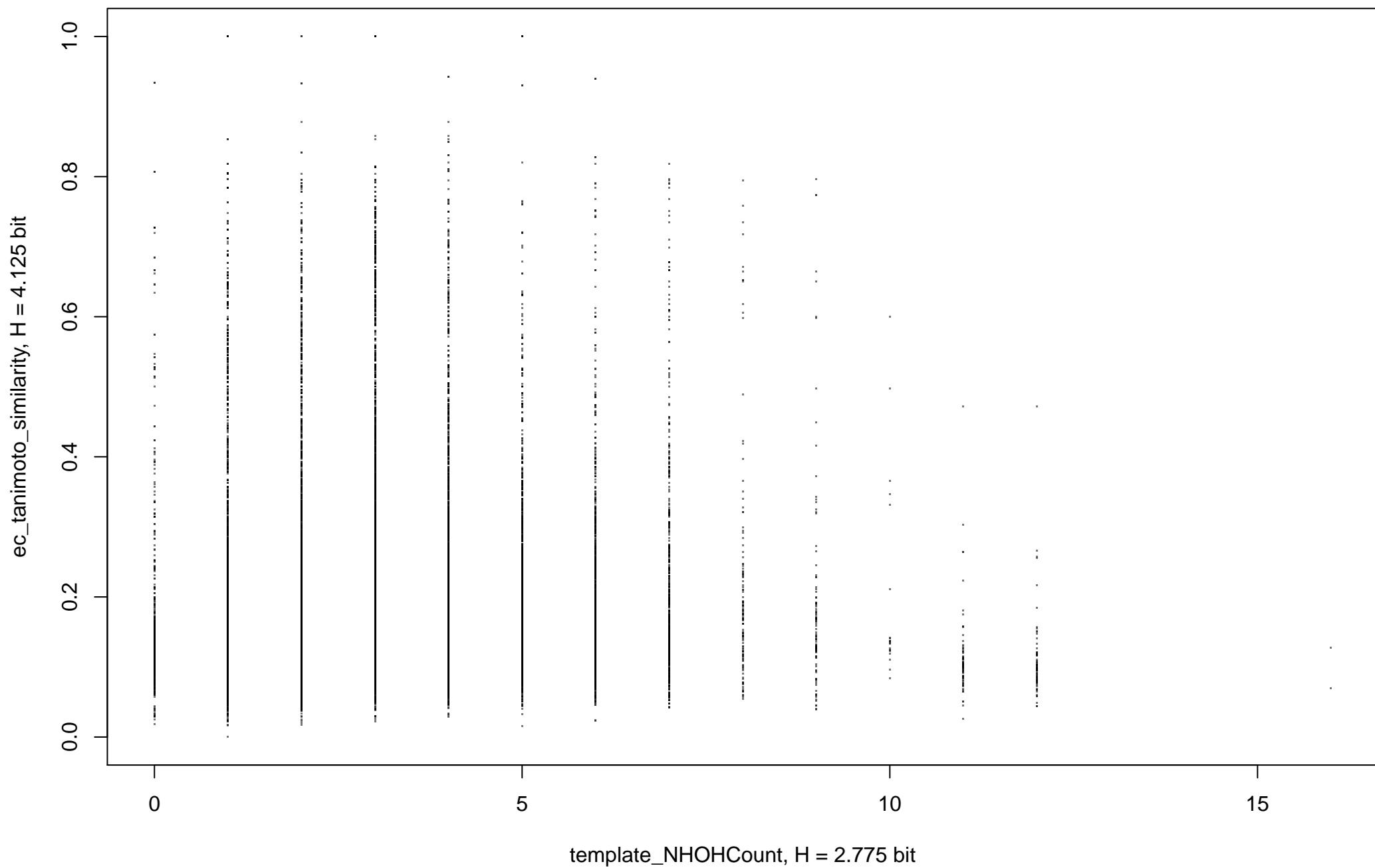
docked_NHOHCount-fc_tanimoto_similarity, MI = 0.06229 bit, normMI = 0.02253



template_NumRotatableBonds-docked_NumHeteroAtoms, MI = 0.08004 bit, normMI = 0.02241

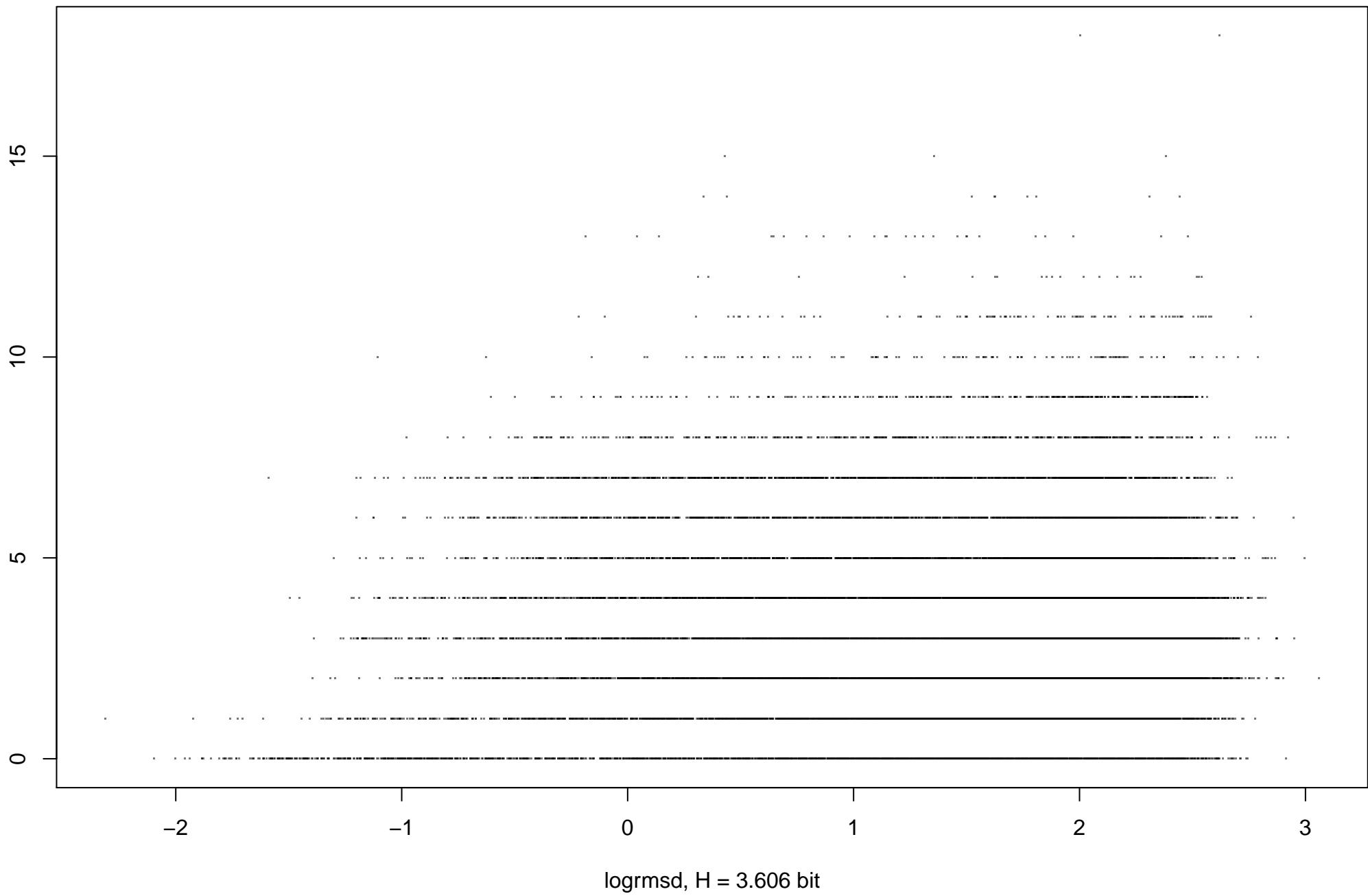


template_NHOHCount–ec_tanimoto_similarity, MI = 0.06215 bit, normMI = 0.0224



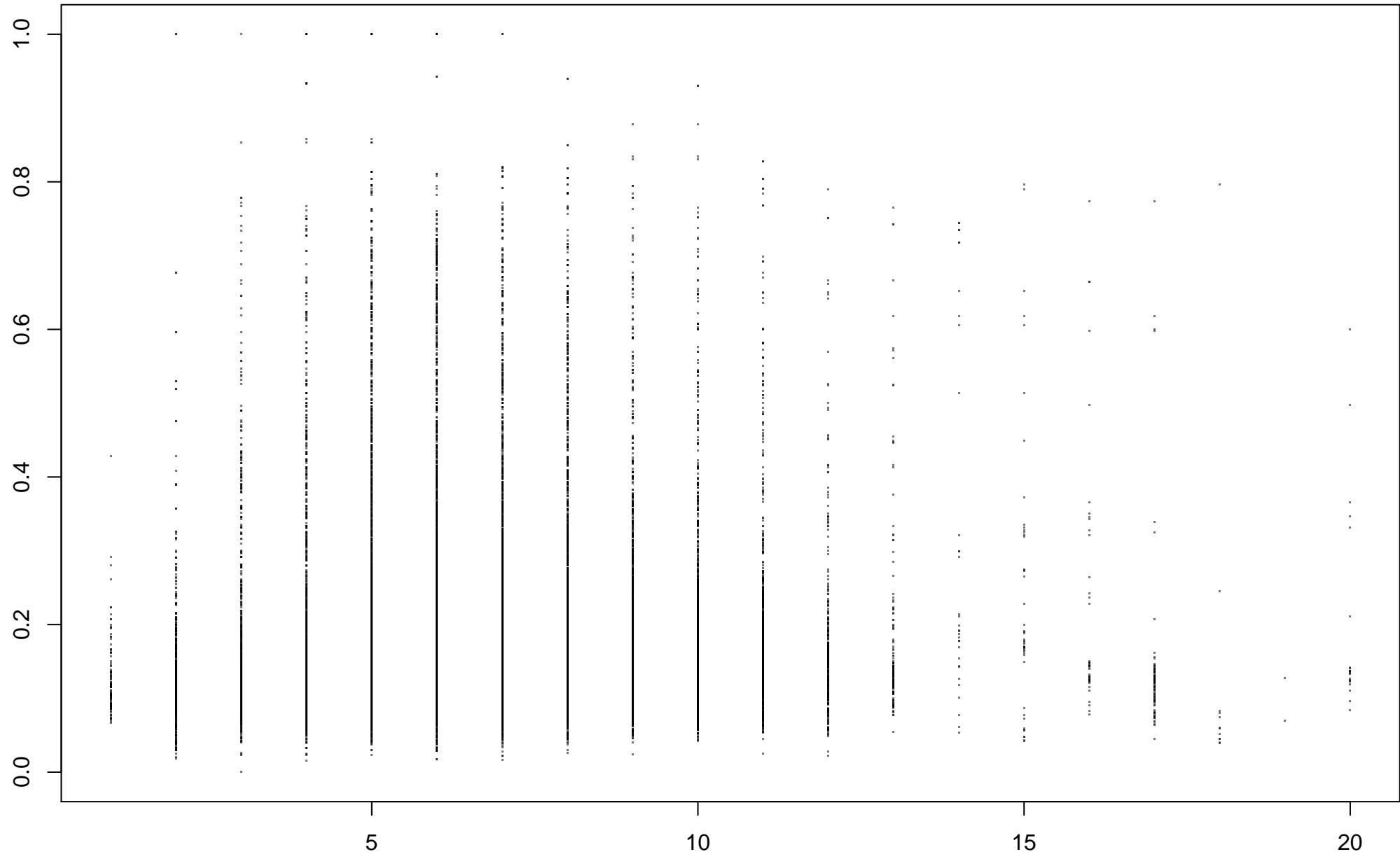
logrmsd-mcs_docked_NumRotatableBonds, MI = 0.06952 bit, normMI = 0.02231

mcs_docked_NumRotatableBonds, H = 3.117 bit



template_NOCount-ec_tanimoto_similarity, MI = 0.07177 bit, normMI = 0.02217

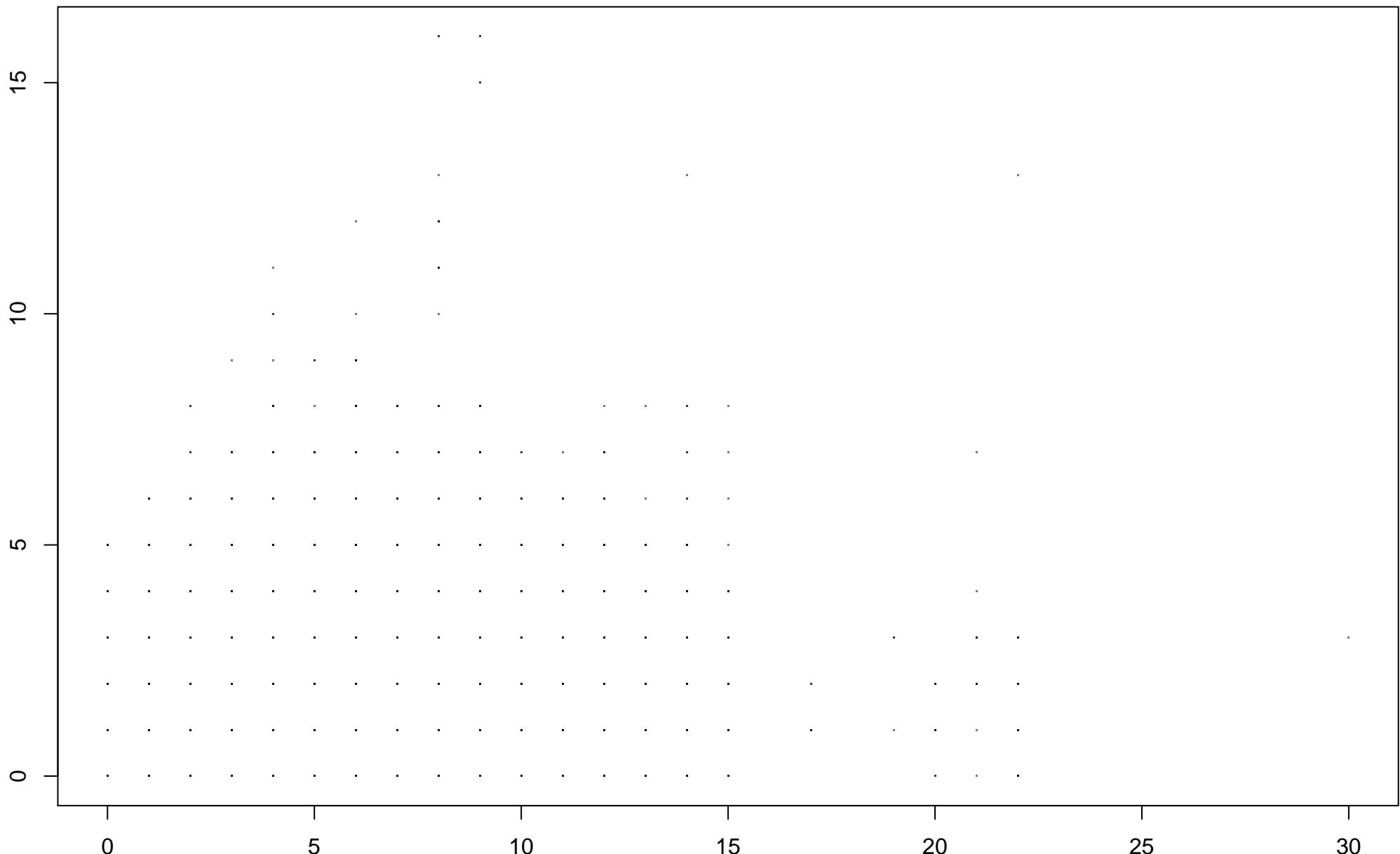
ec_tanimoto_similarity, H = 4.125 bit



template_NOCount, H = 3.237 bit

docked_NumRotatableBonds-mcs_template_NumHAcceptors, MI = 0.05514 bit, normMI = 0.02216

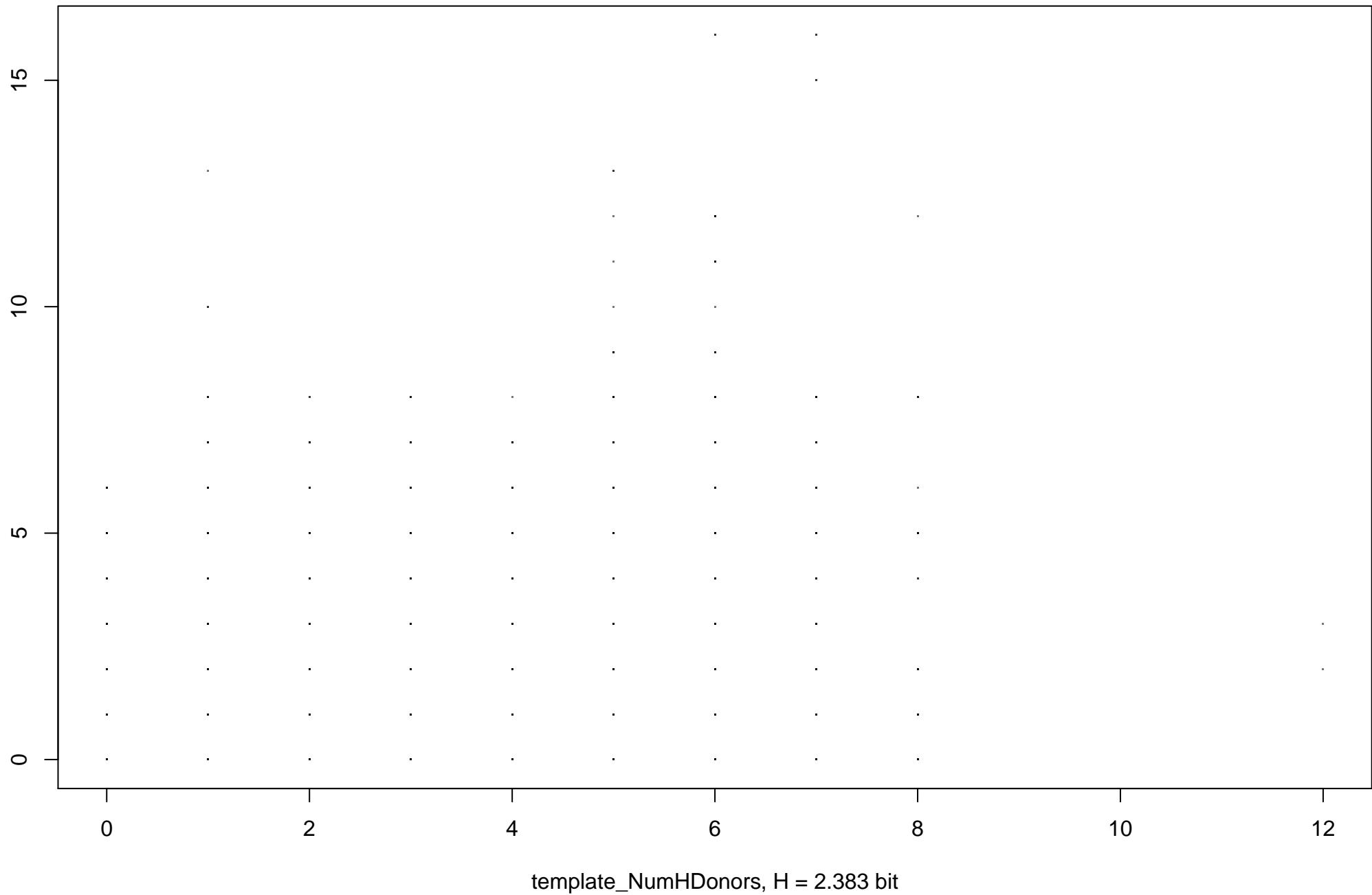
mcs_template_NumHAcceptors, H = 2.488 bit



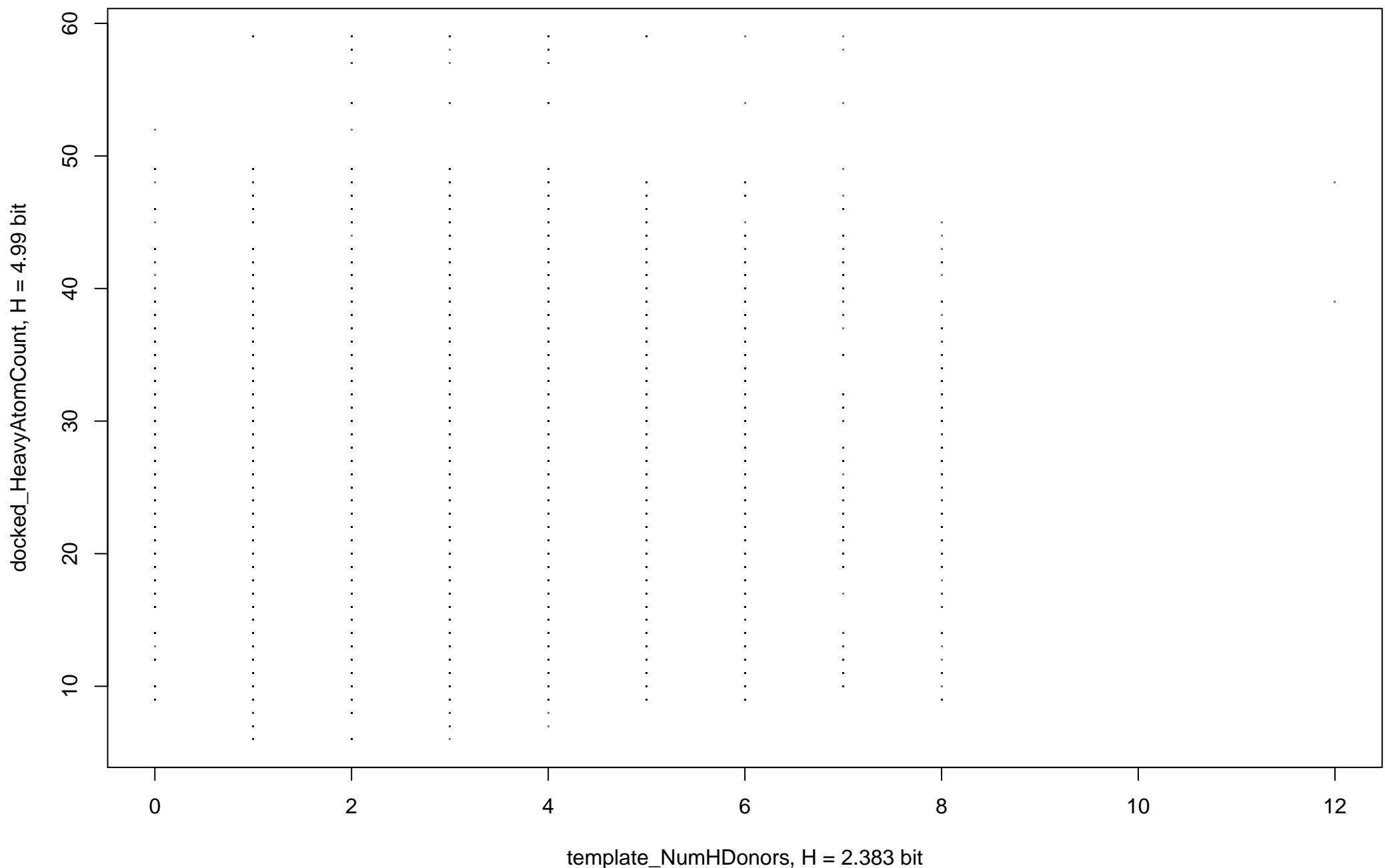
docked_NumRotatableBonds, H = 3.667 bit

template_NumHDonors-mcs_template_NumHAcceptors, MI = 0.0527 bit, normMI = 0.02212

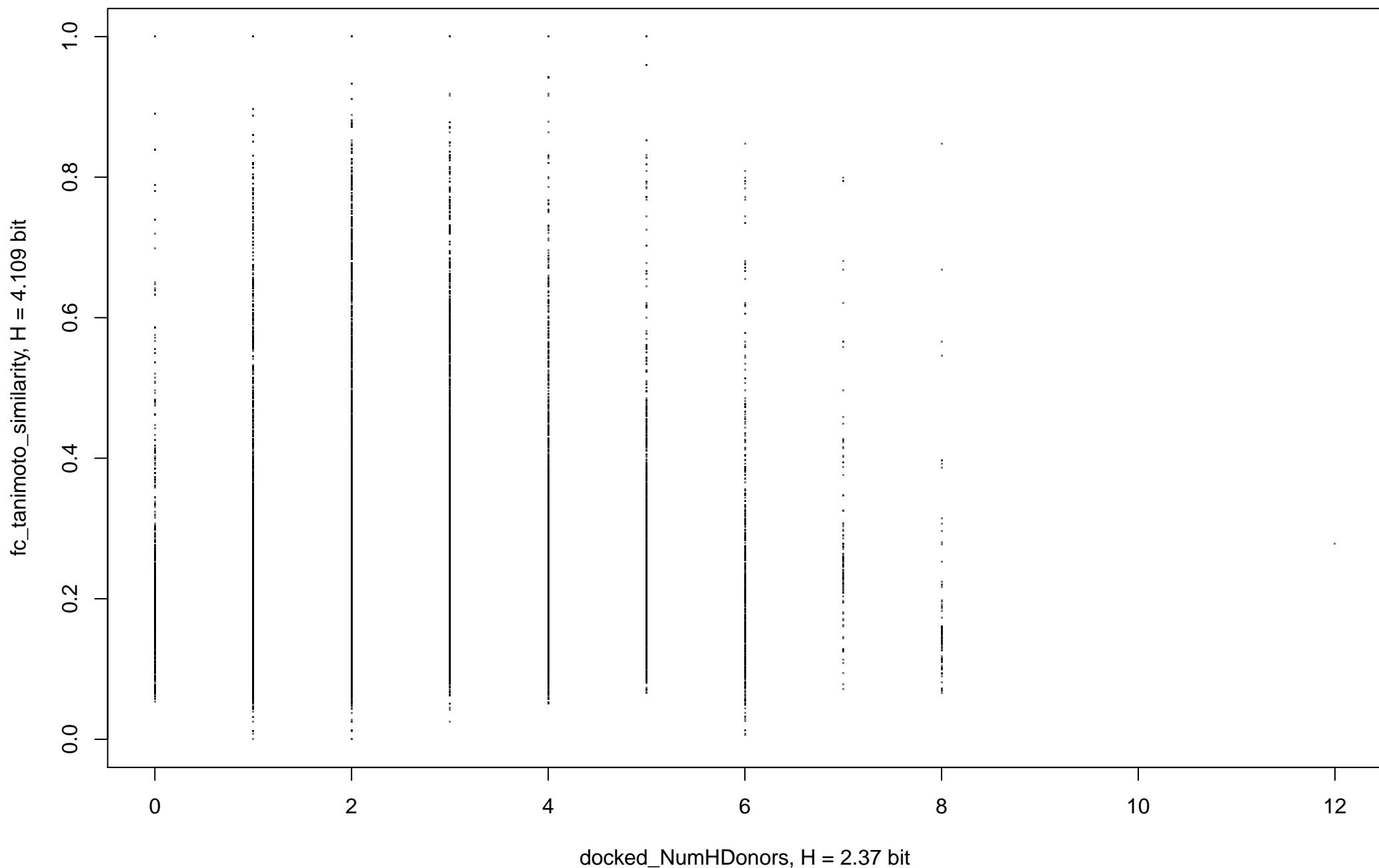
mcs_template_NumHAcceptors, H = 2.488 bit



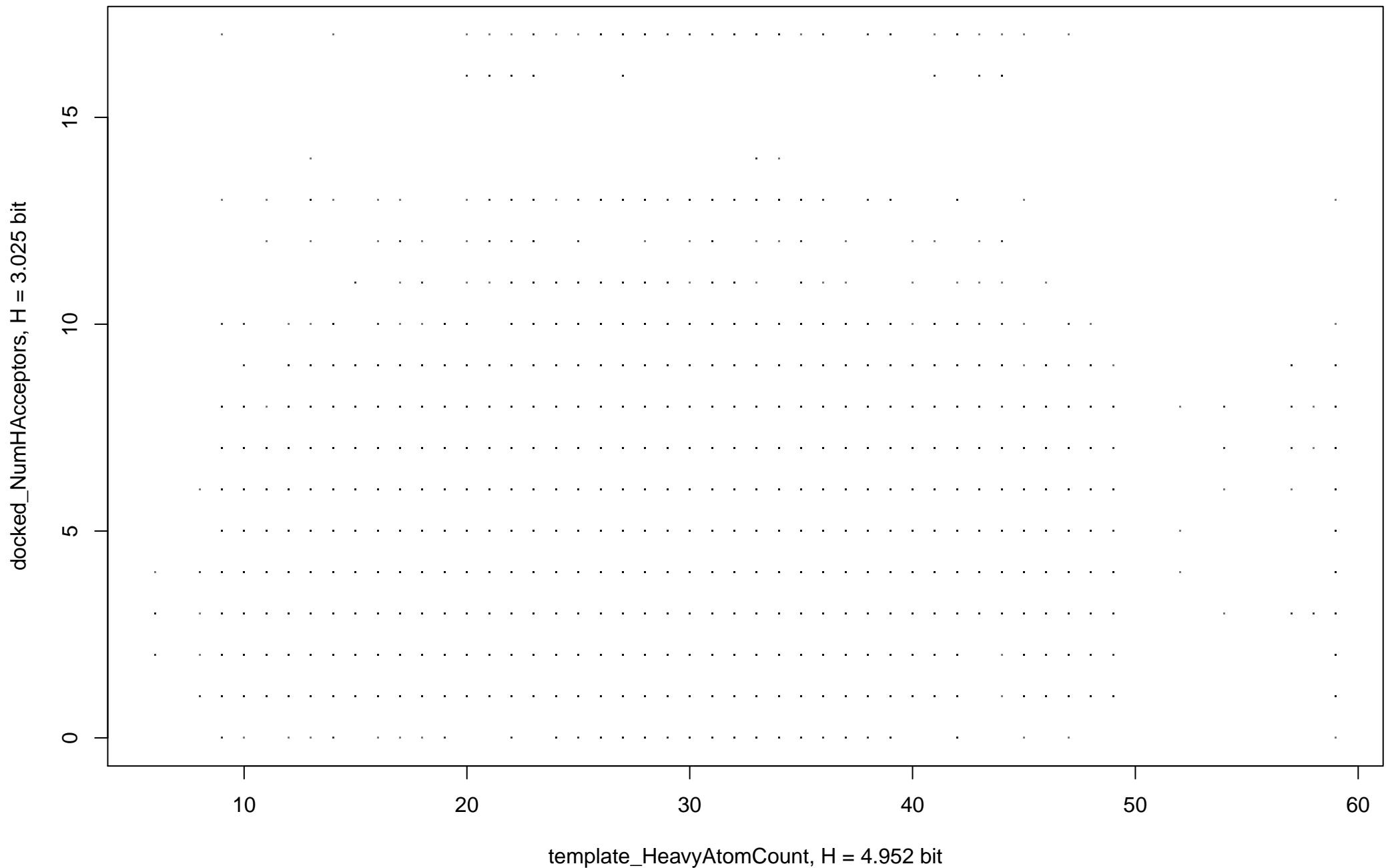
template_NumHDonors-docked_HeavyAtomCount, MI = 0.05219 bit, normMI = 0.0219



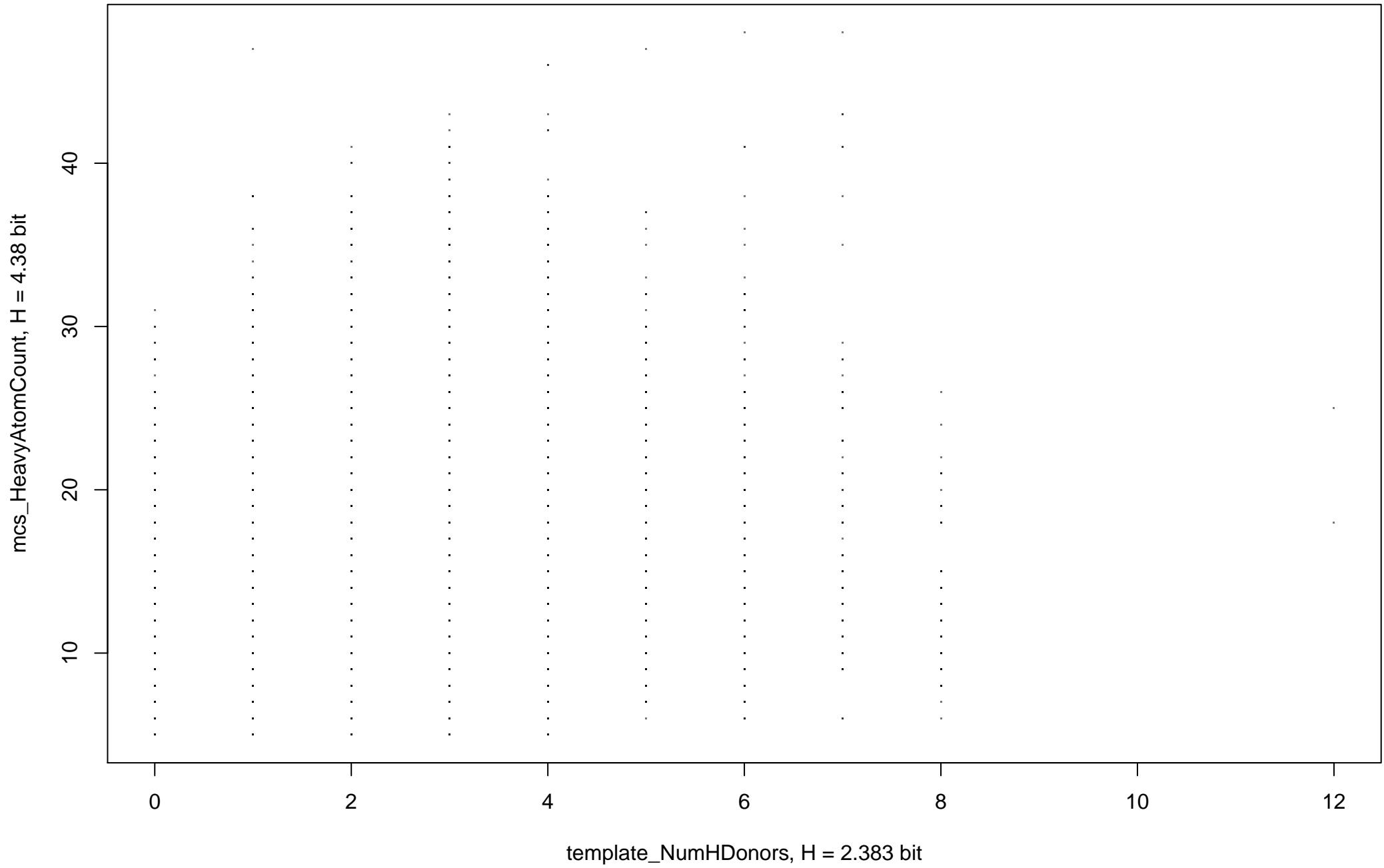
docked_NuHDonors-fc_tanimoto_similarity, MI = 0.05145 bit, normMI = 0.02171



template_HeavyAtomCount-docked_NumHAcceptors, MI = 0.06566 bit, normMI = 0.0217

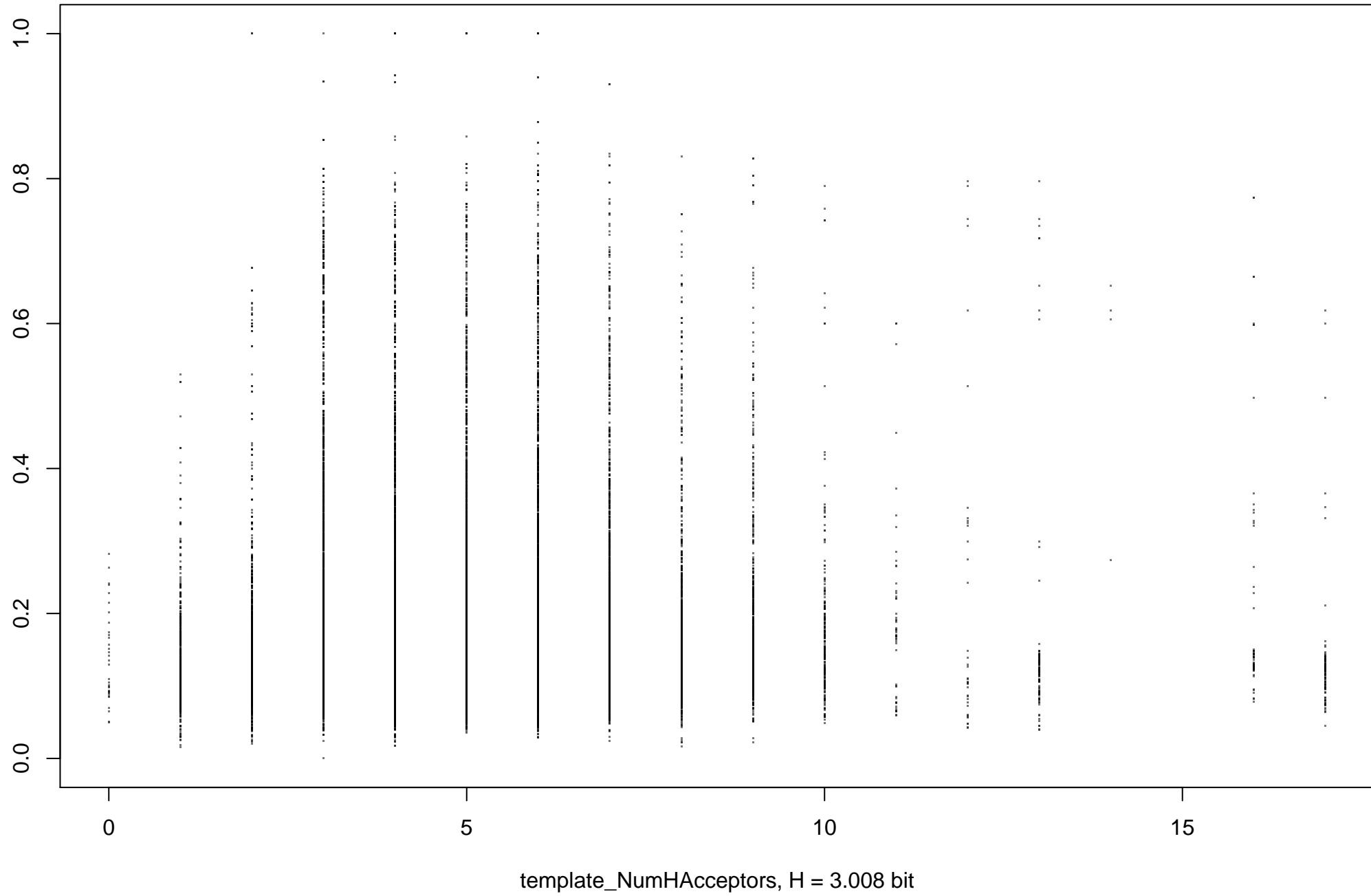


template_NumHDonors-mcs_HeavyAtomCount, MI = 0.0507 bit, normMI = 0.02127



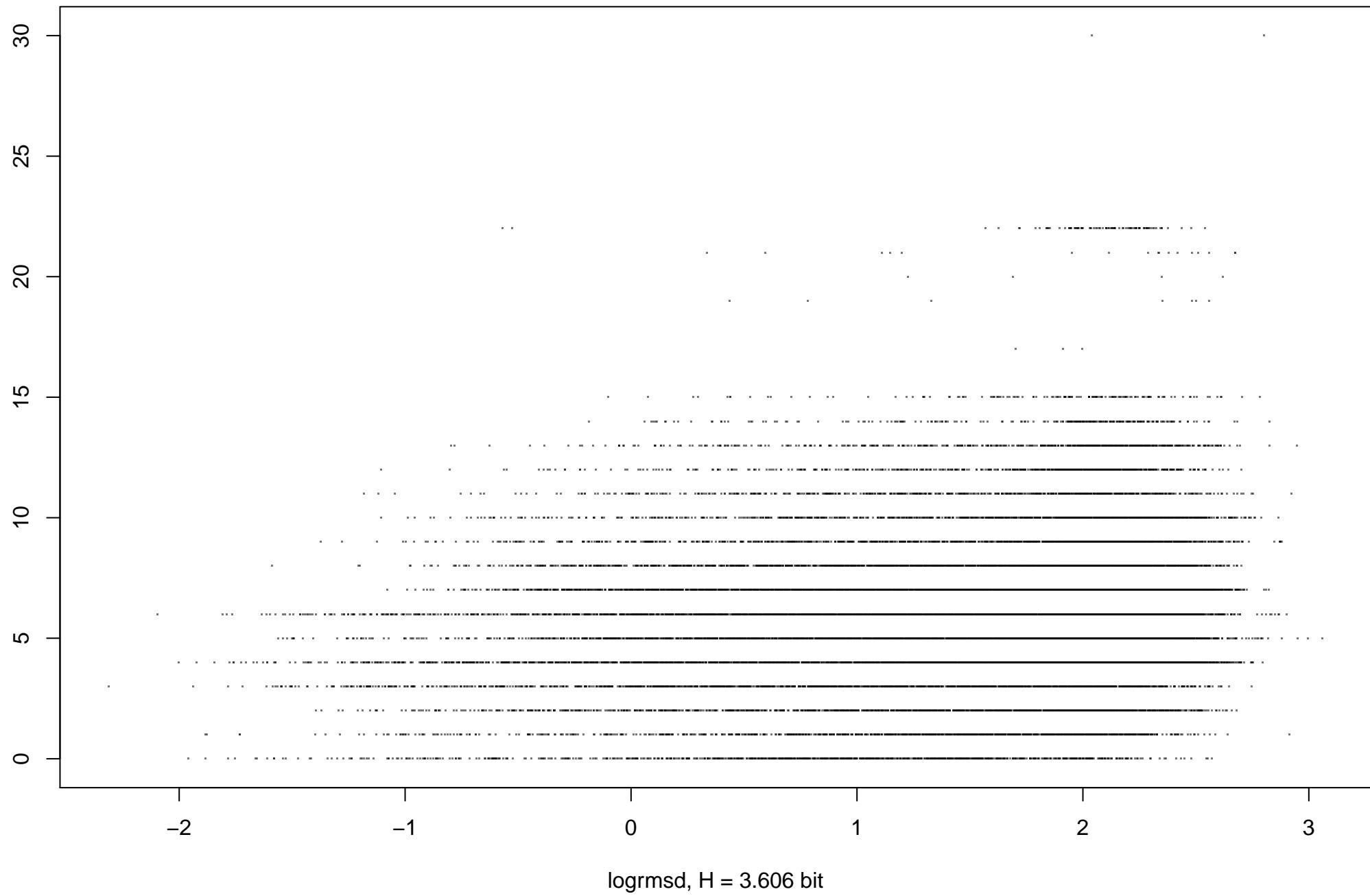
template_NumHAcceptors–ec_tanimoto_similarity, MI = 0.06173 bit, normMI = 0.02052

ec_tanimoto_similarity, H = 4.125 bit



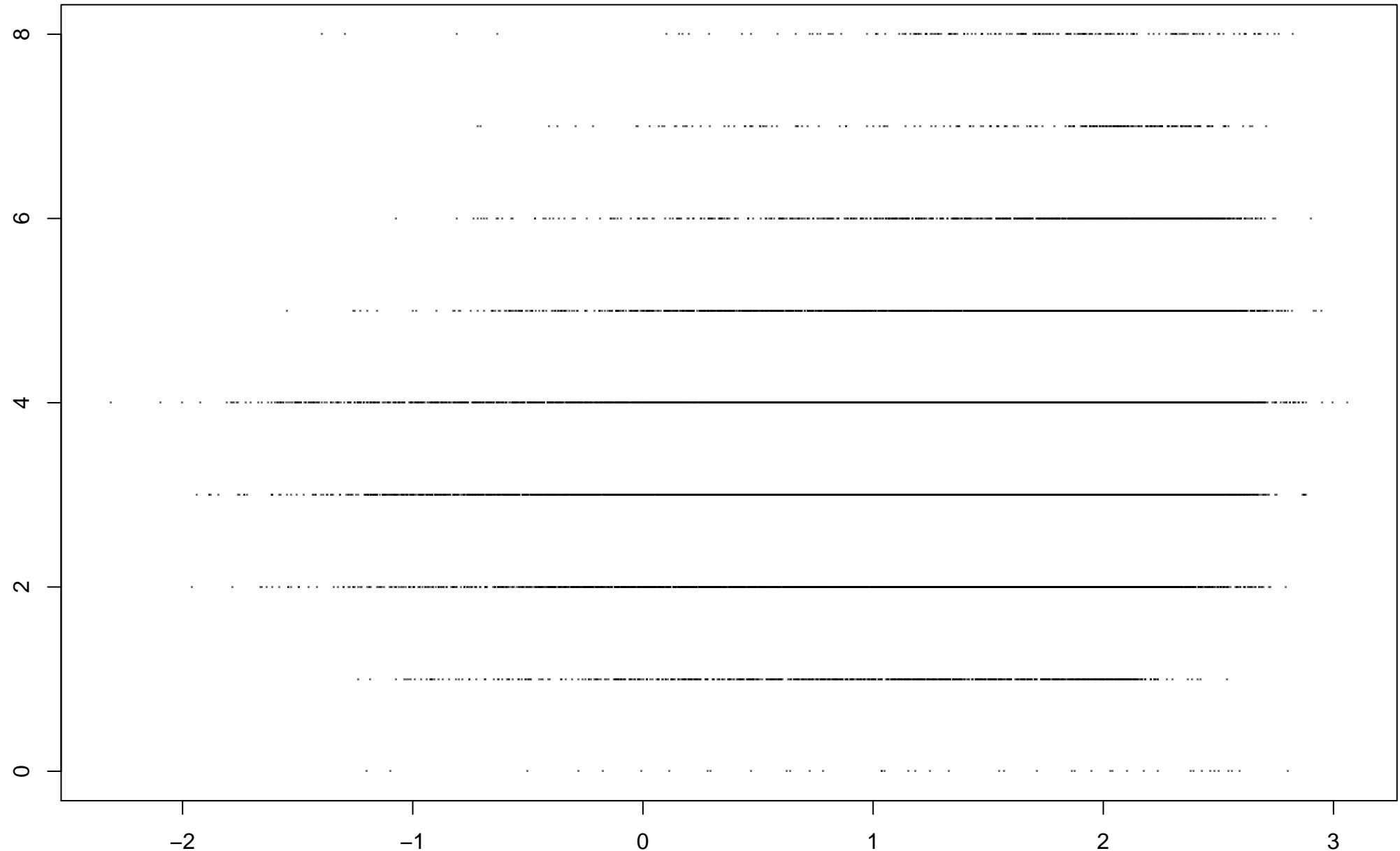
logrmsd-template_NumRotatableBonds, MI = 0.07394 bit, normMI = 0.02051

template_NumRotatableBonds, H = 3.668 bit



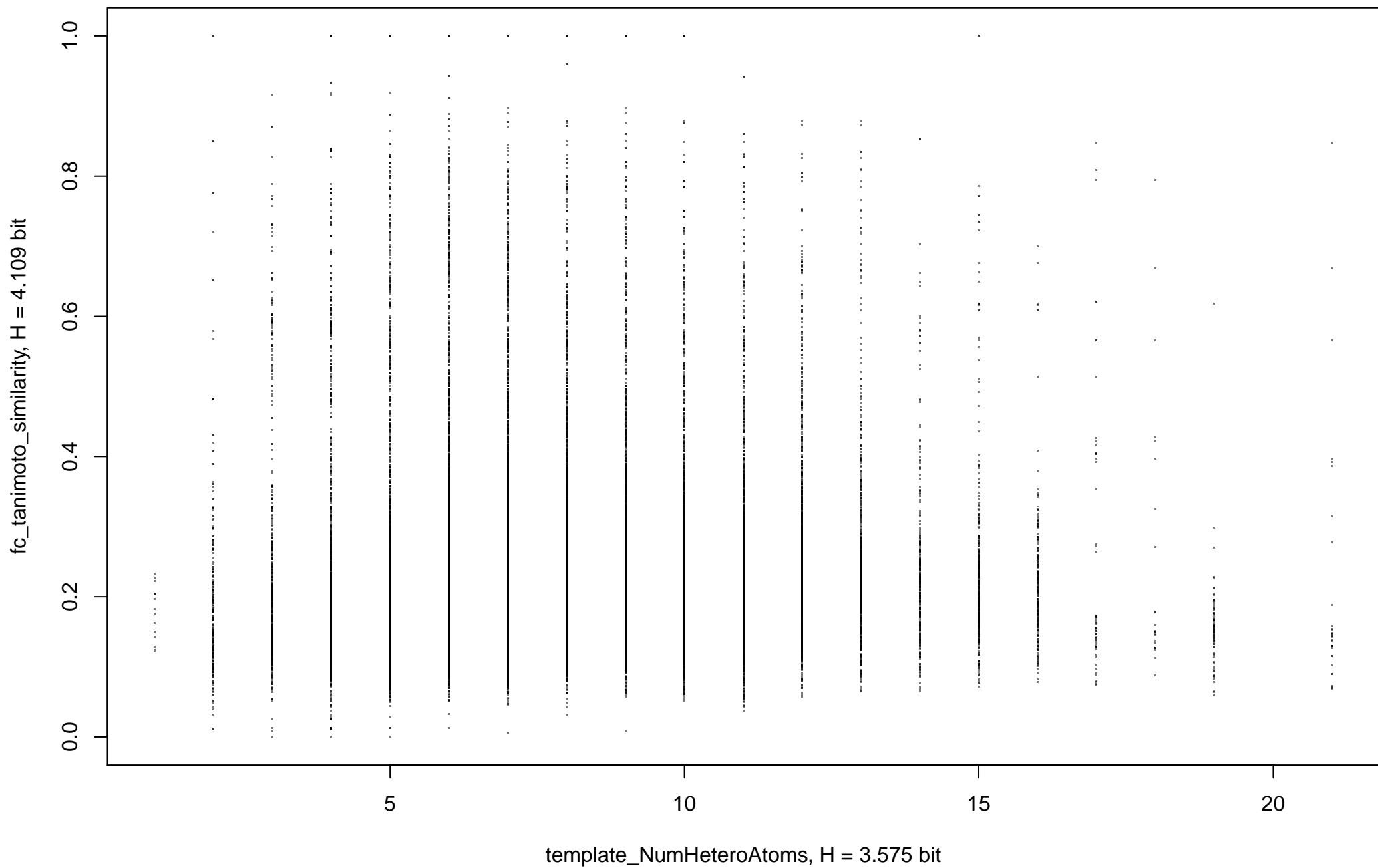
logrmsd-template_RingCount, MI = 0.04813 bit, normMI = 0.02043

template_RingCount, H = 2.356 bit

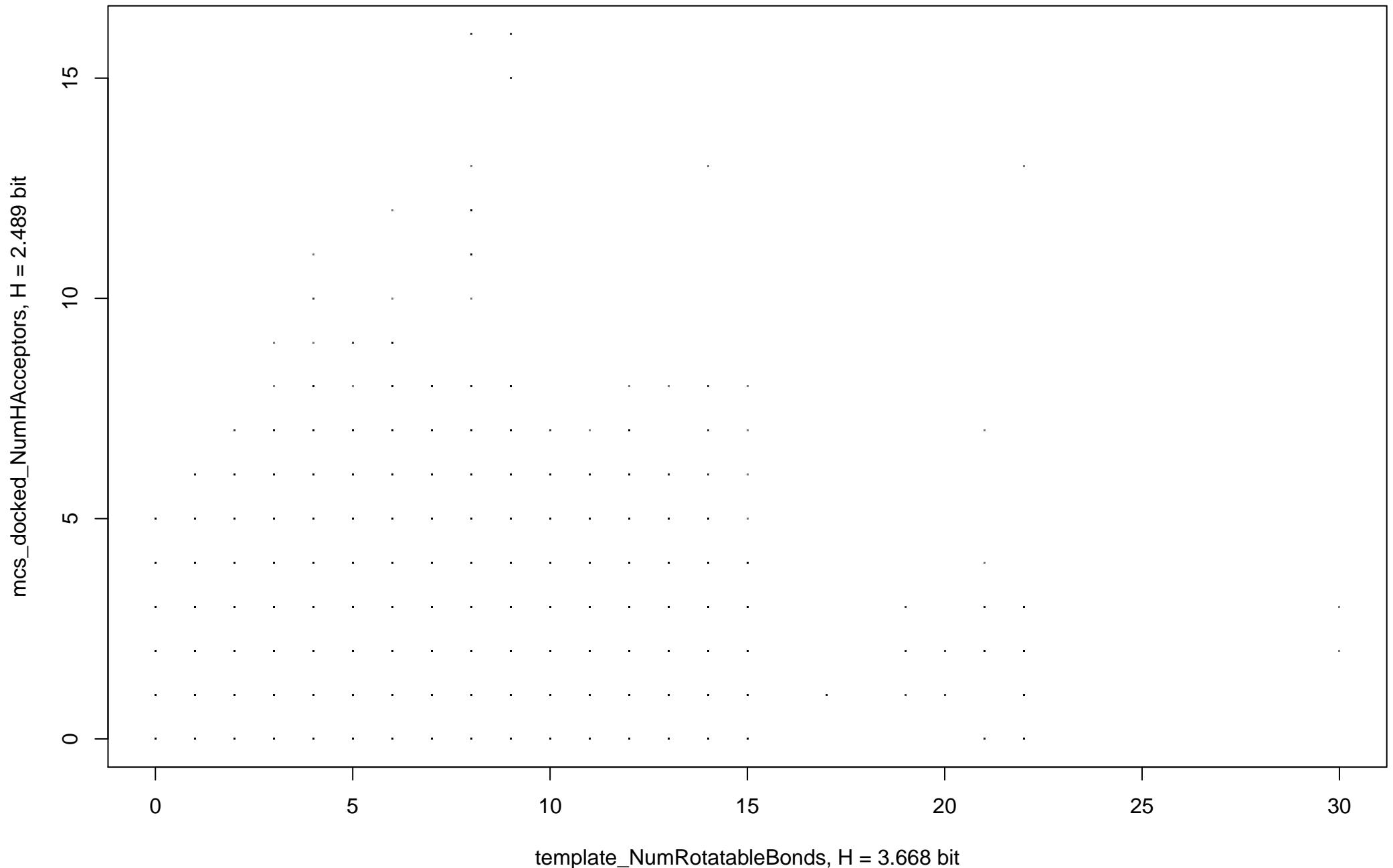


logrmsd, H = 3.606 bit

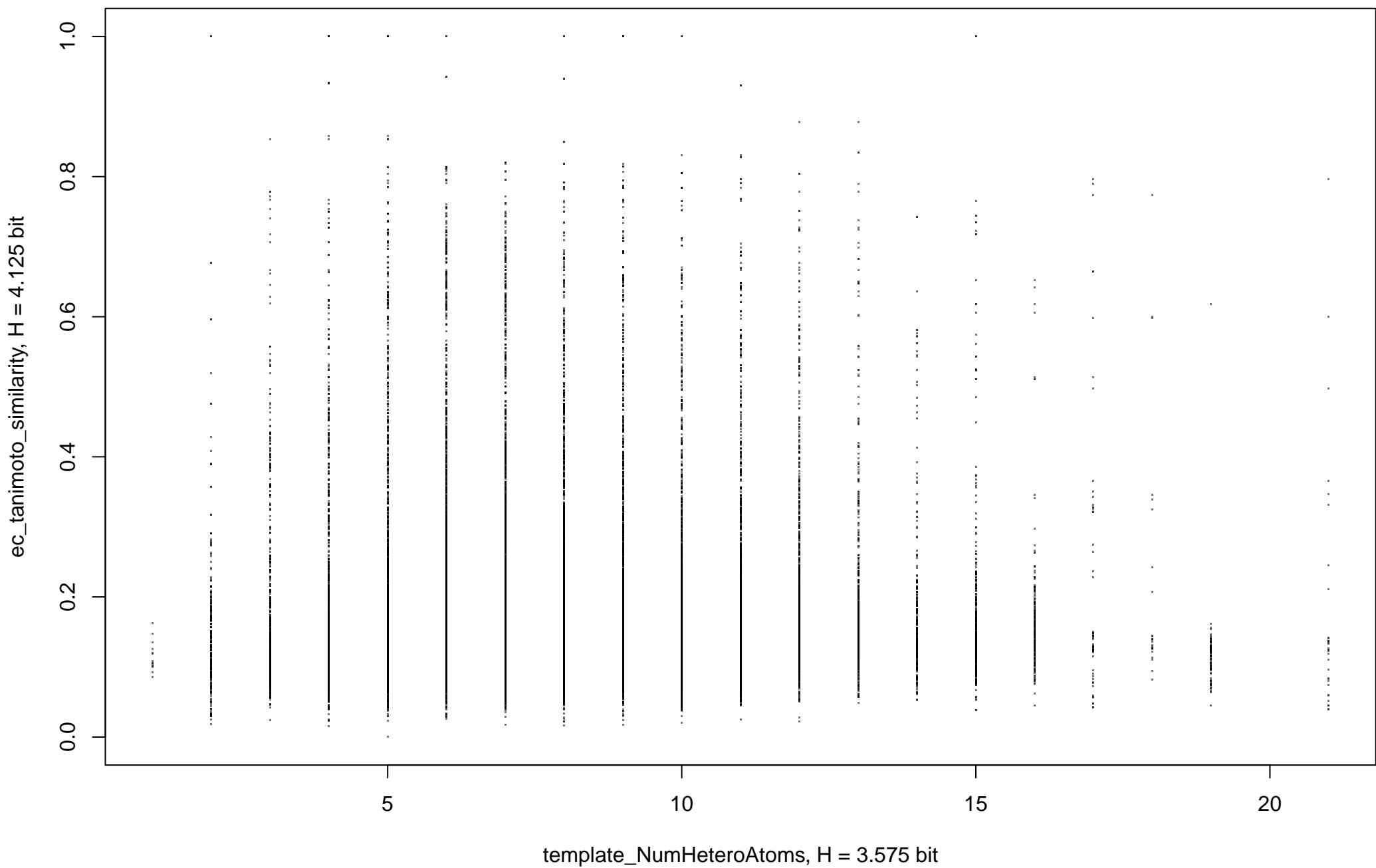
template_NumHeteroAtoms-fc_tanimoto_similarity, MI = 0.07282 bit, normMI = 0.02037



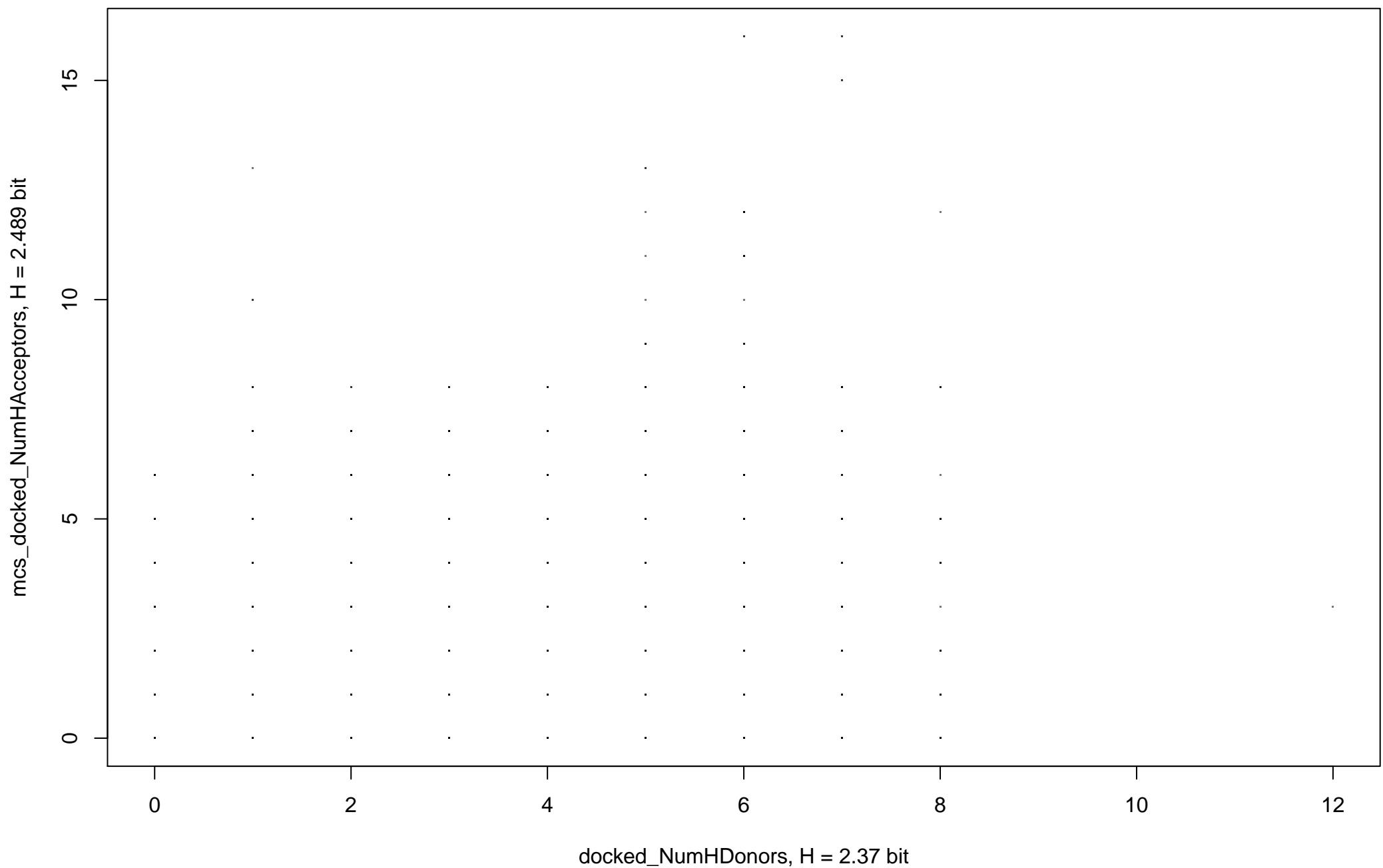
template_NumRotatableBonds-mcs_docked_NumHAcceptors, MI = 0.05051 bit, normMI = 0.02029



template_NumHeteroAtoms–ec_tanimoto_similarity, MI = 0.07239 bit, normMI = 0.02025

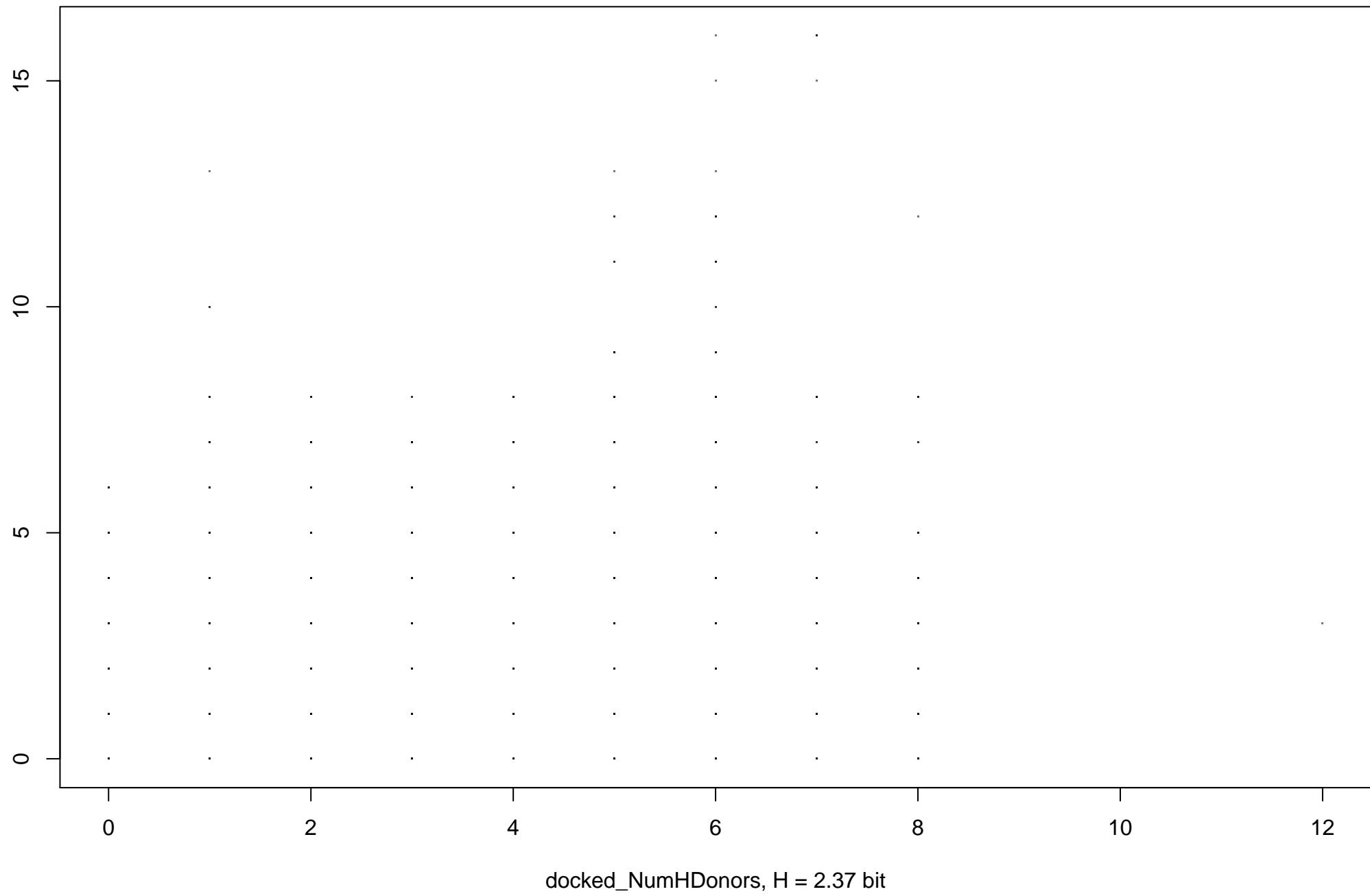


docked_NumHDonors-mcs_docked_NumHAcceptors, MI = 0.04778 bit, normMI = 0.02016



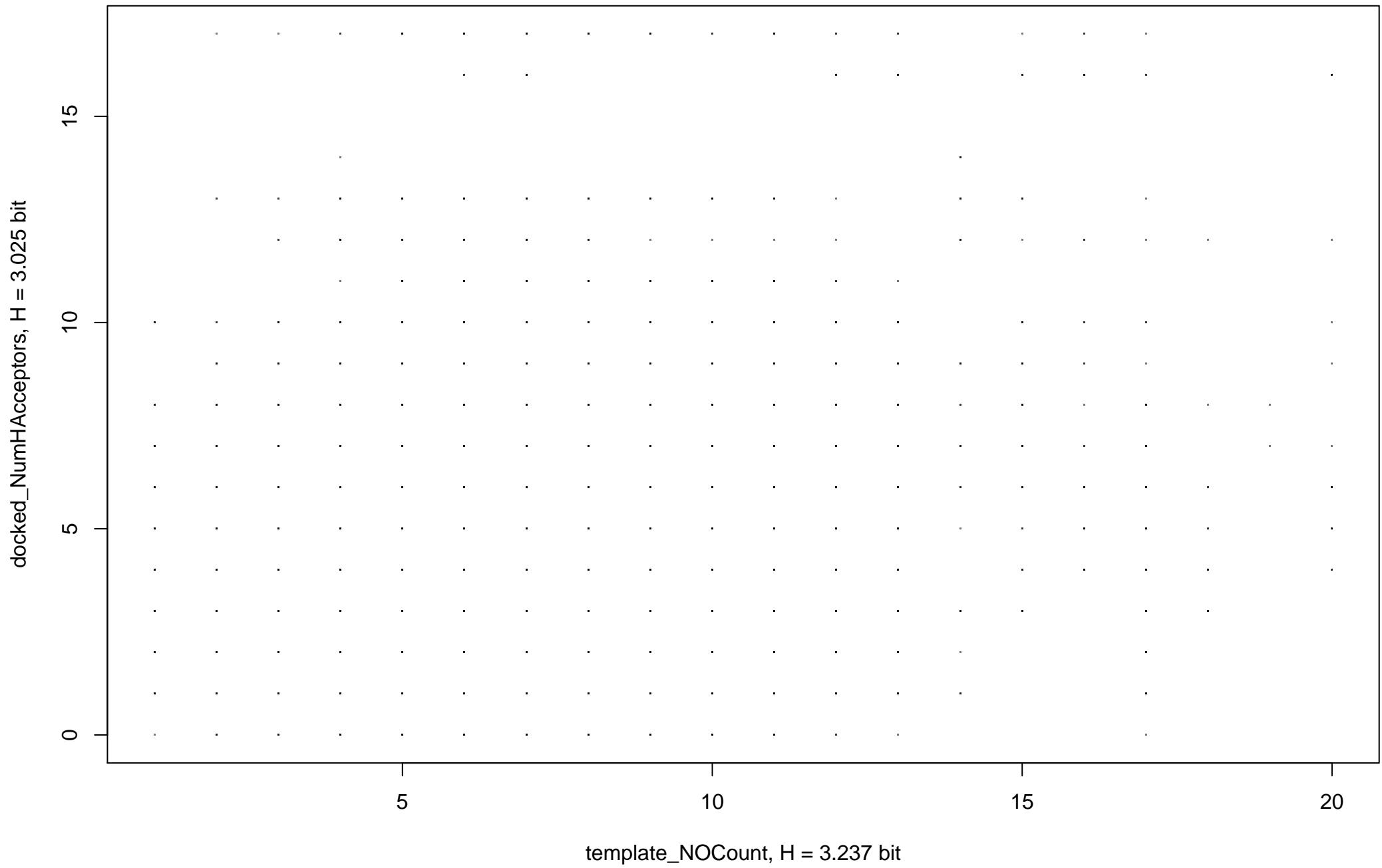
docked_NumHDonors–mcs_template_NumHAcceptors, MI = 0.04774 bit, normMI = 0.02014

mcs_template_NumHAcceptors, H = 2.488 bit

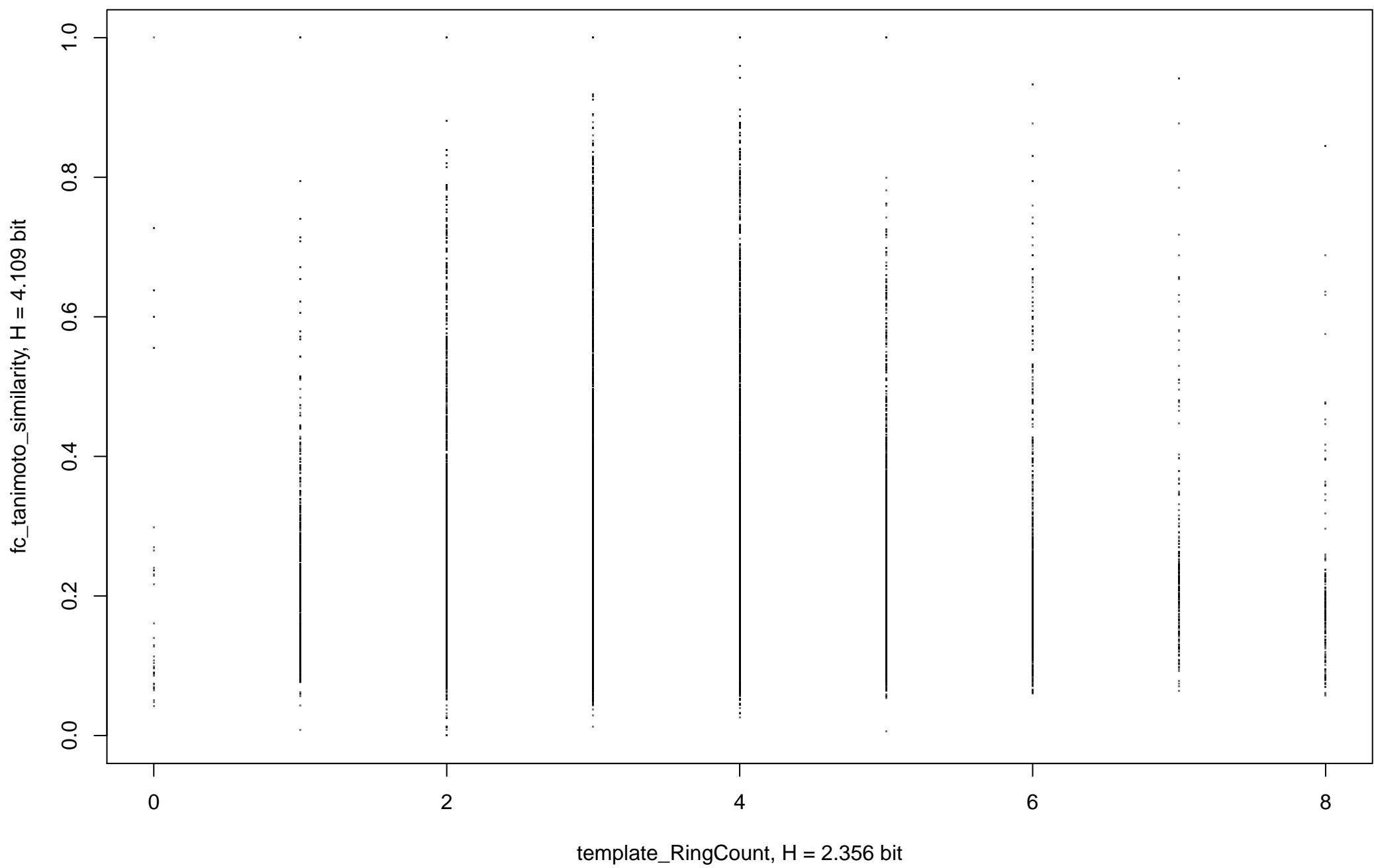


docked_NumHDonors, H = 2.37 bit

template_NOCount-docked_NumHAcceptors, MI = 0.05943 bit, normMI = 0.01964

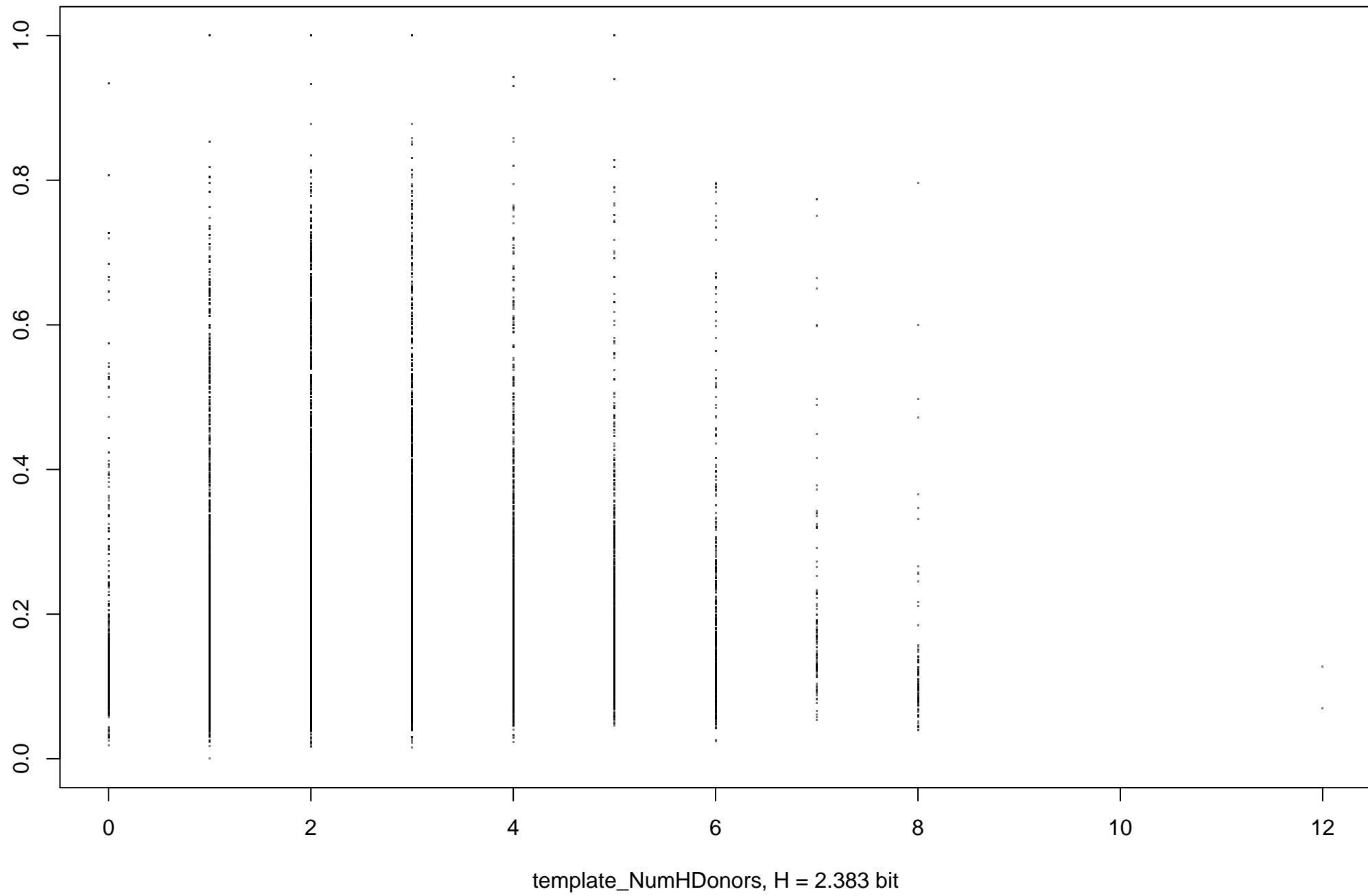


template_RingCount-fc_tanimoto_similarity, MI = 0.04607 bit, normMI = 0.01955



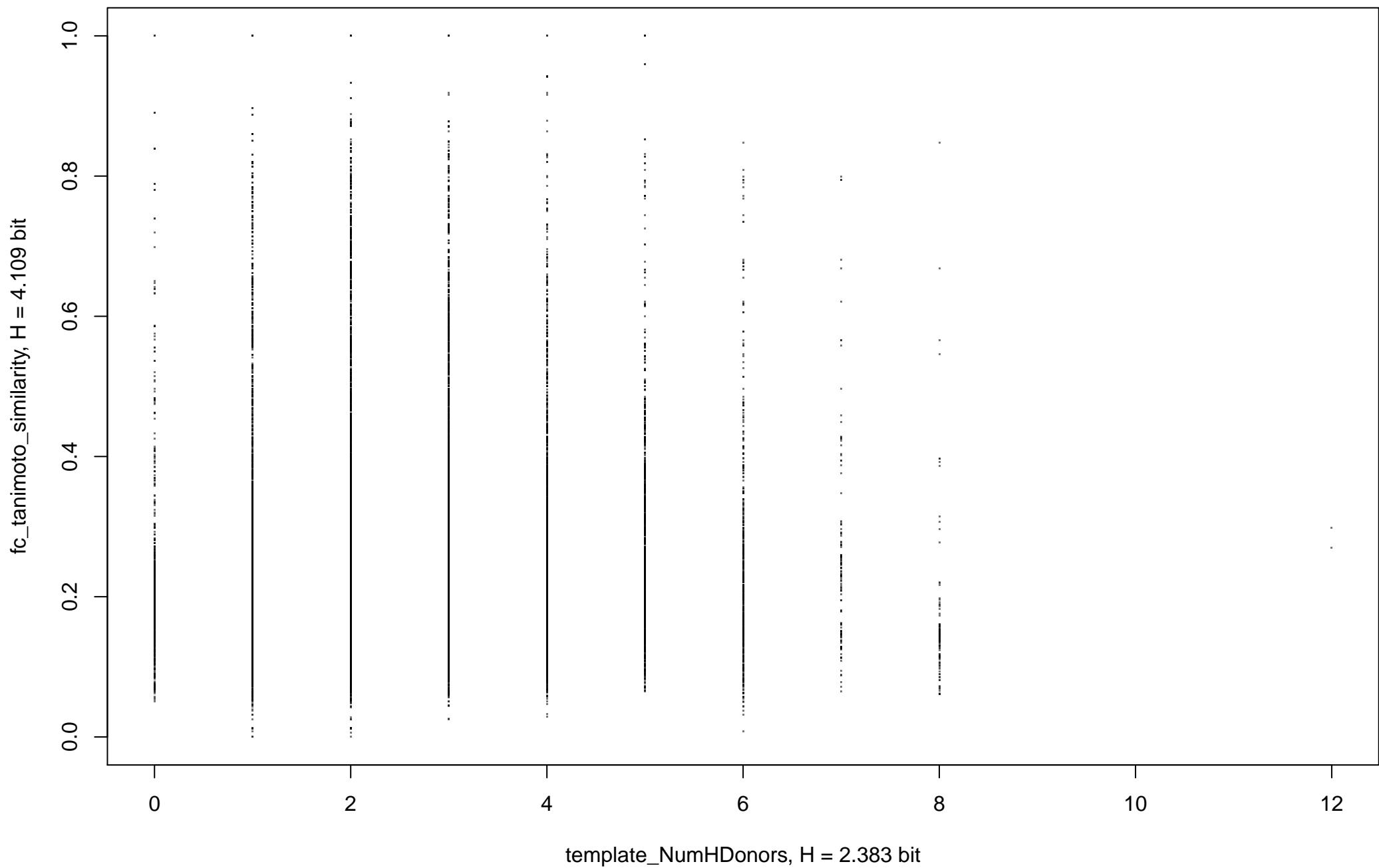
template_NumHDonors-ec_tanimoto_similarity, MI = 0.04621 bit, normMI = 0.01939

ec_tanimoto_similarity, H = 4.125 bit



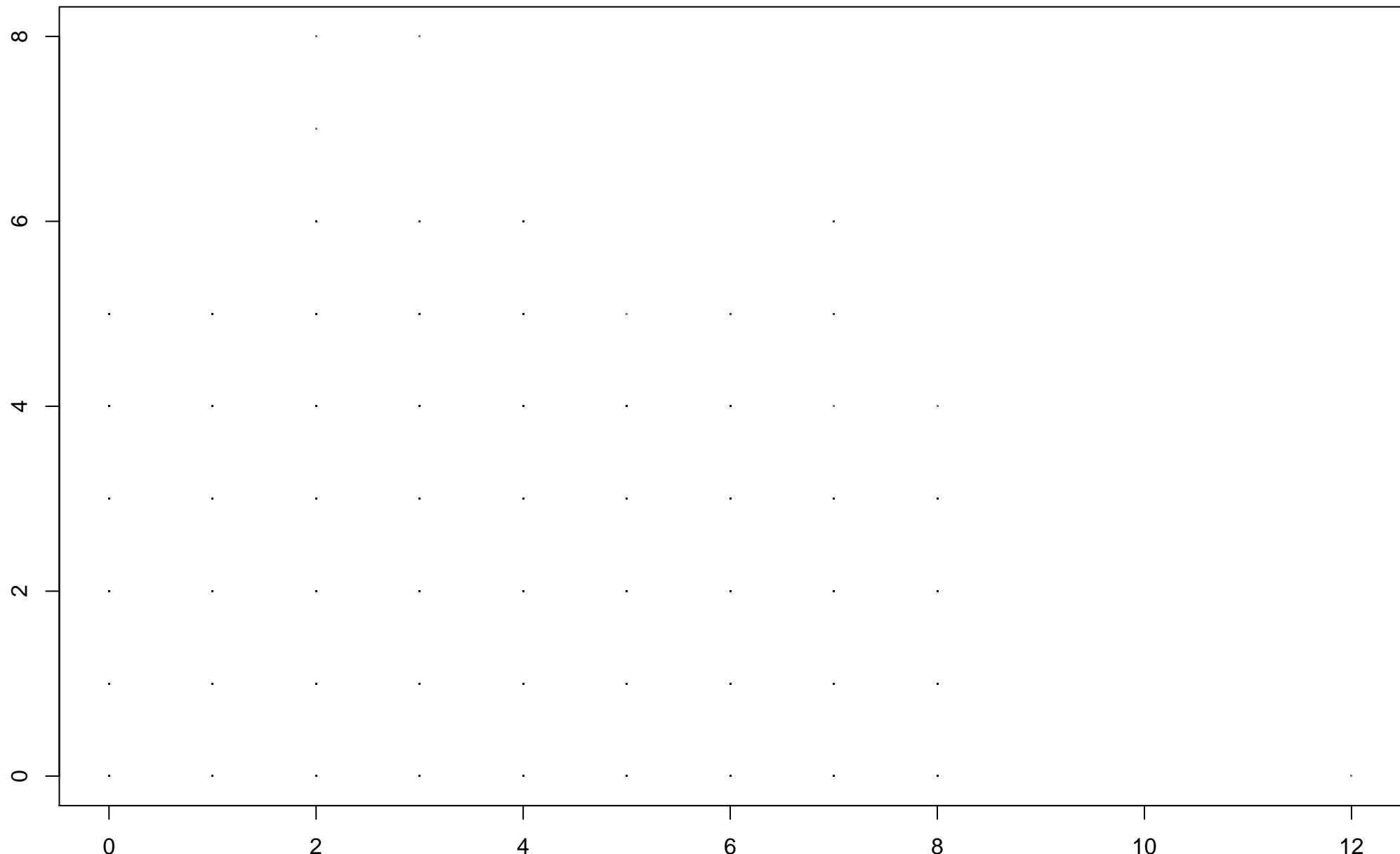
template_NumHDonors, H = 2.383 bit

template_NumHDonors-fc_tanimoto_similarity, MI = 0.04571 bit, normMI = 0.01918



docked_NumHDonors–mcs_RingCount, MI = 0.03288 bit, normMI = 0.01904

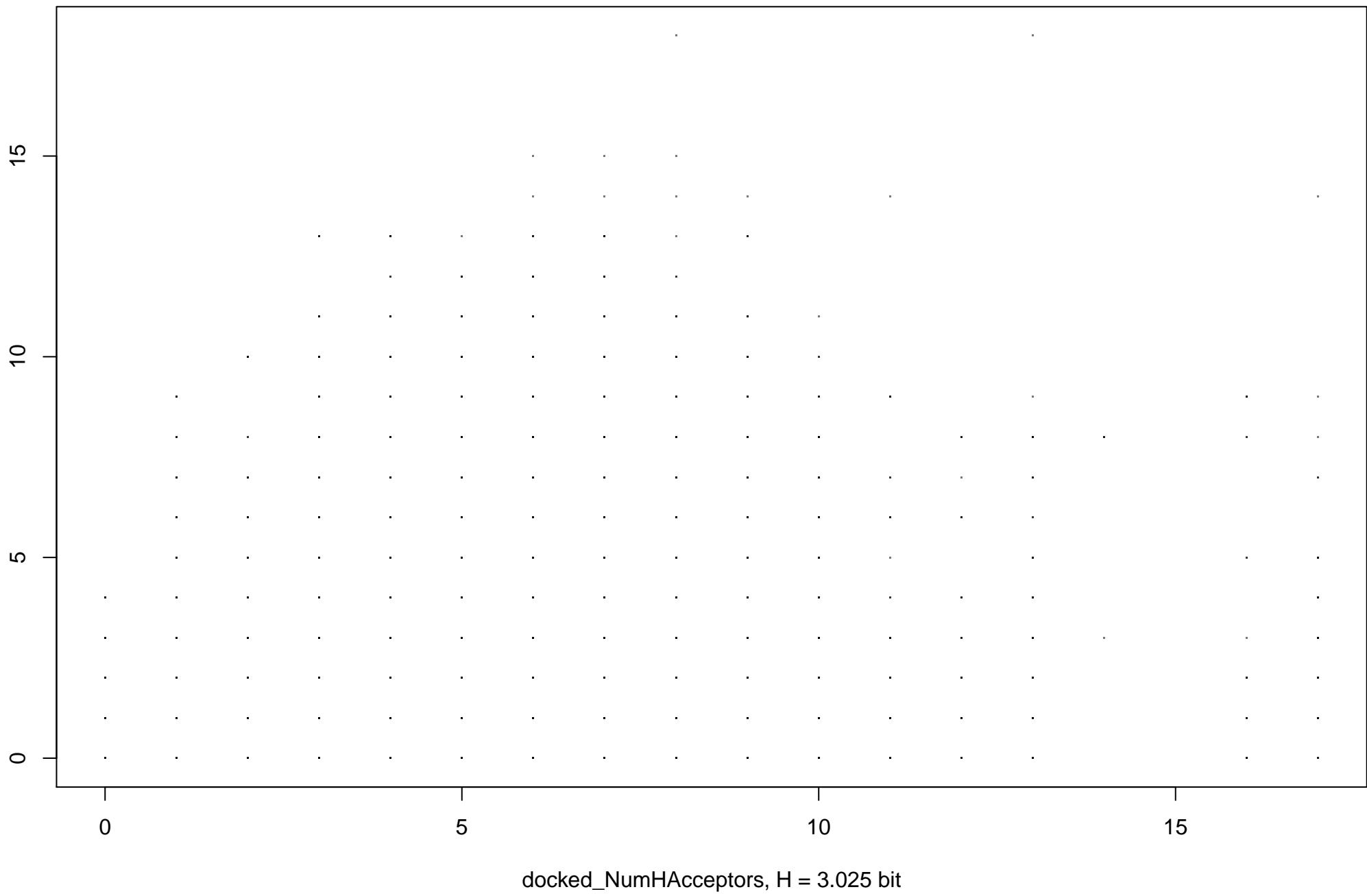
mcs_RingCount, H = 1.727 bit



docked_NumHDonors, H = 2.37 bit

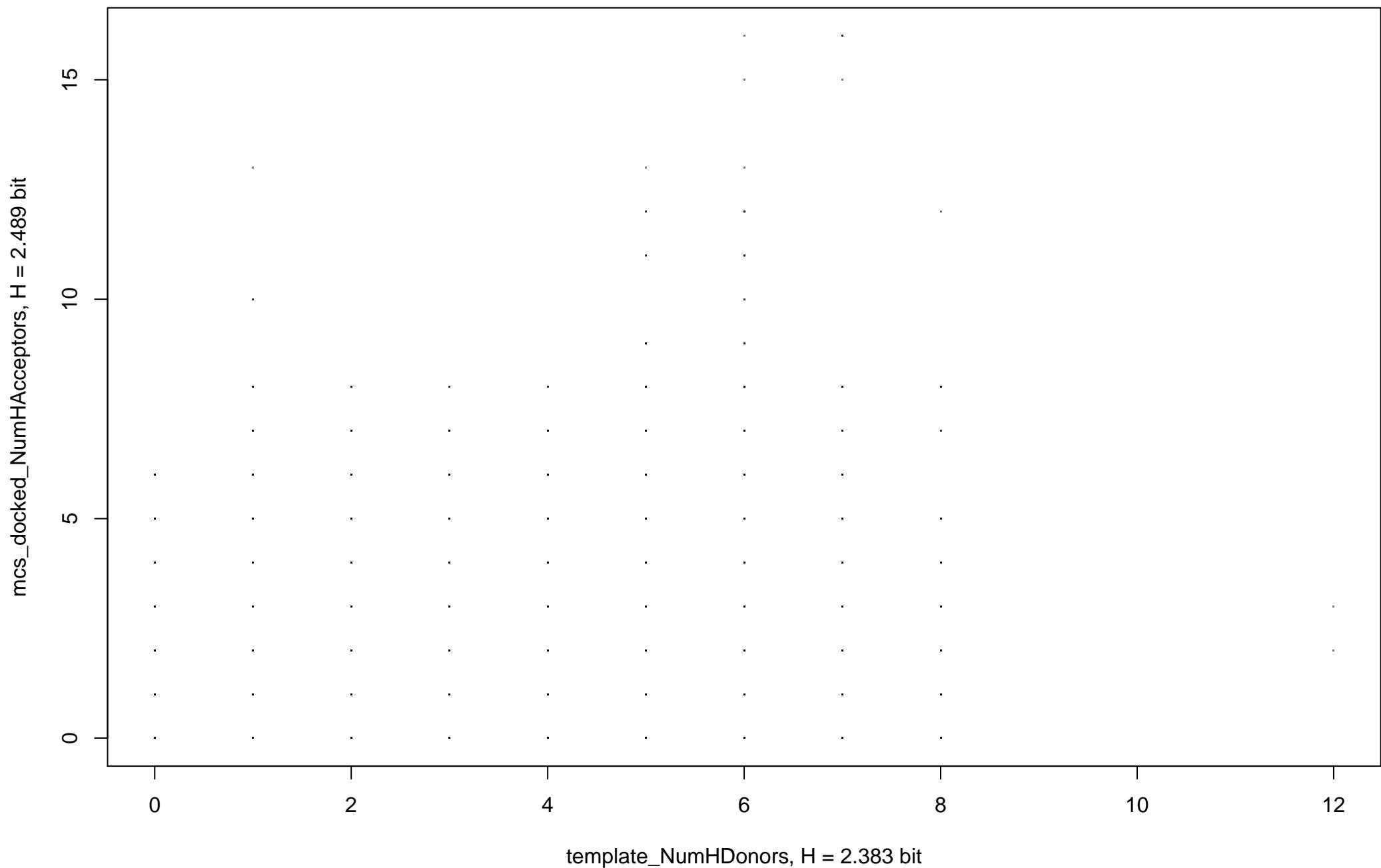
docked_NumHAcceptors-mcs_template_NumRotatableBonds, MI = 0.05757 bit, normMI = 0.01903

mcs_template_NumRotatableBonds, H = 3.118 bit

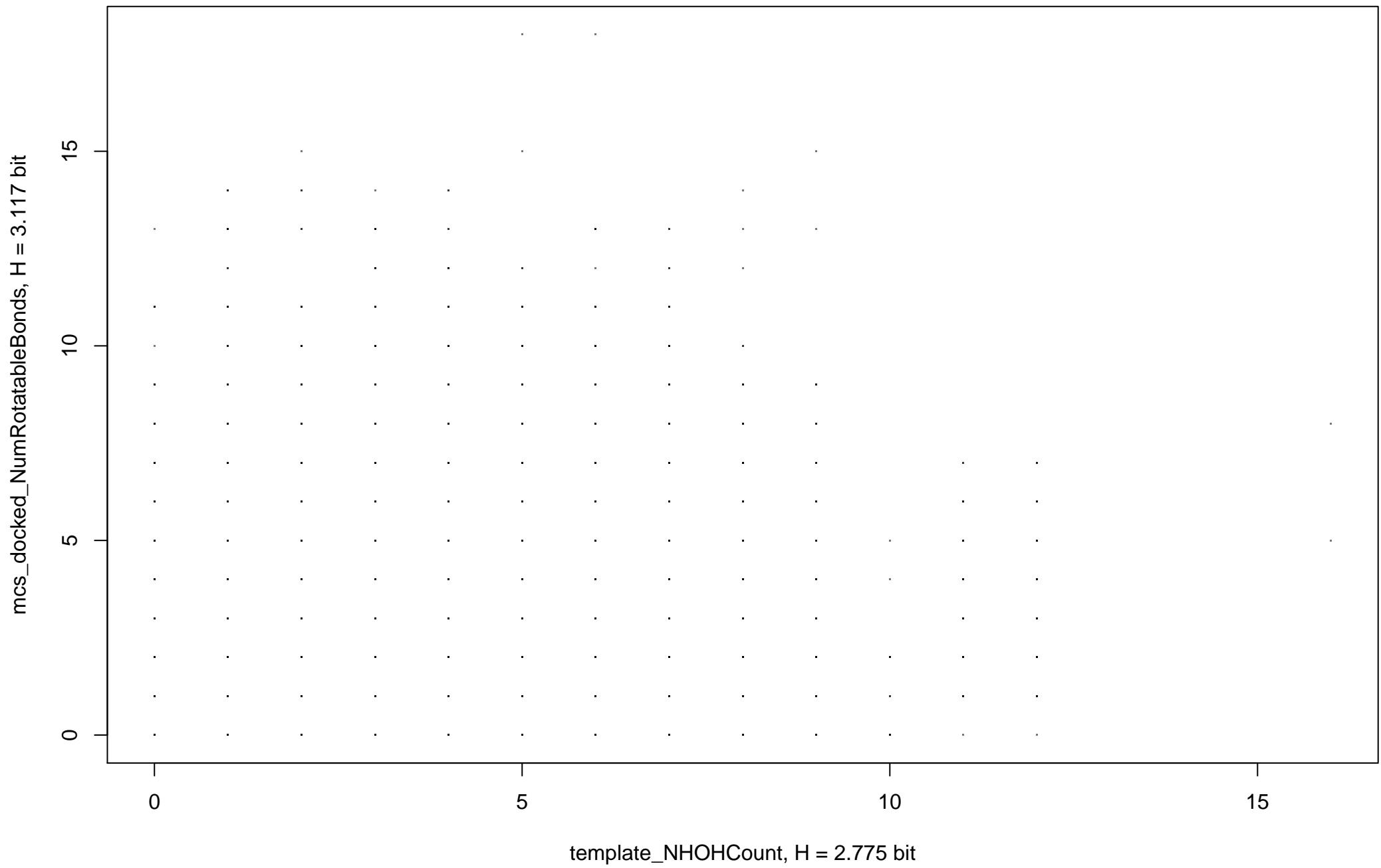


docked_NumHAcceptors, H = 3.025 bit

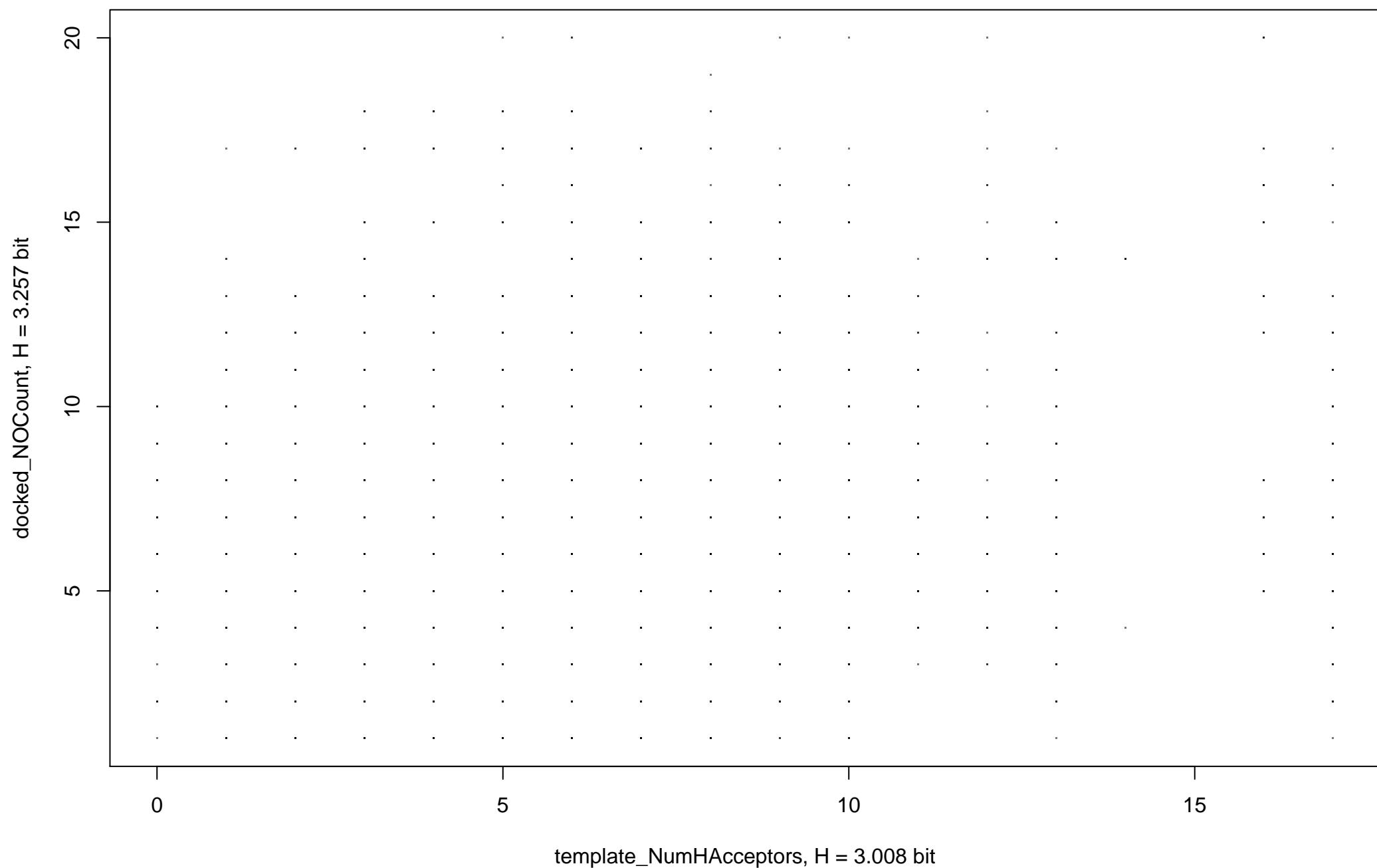
template_NumHDonors-mcs_docked_NumHAcceptors, MI = 0.04528 bit, normMI = 0.019



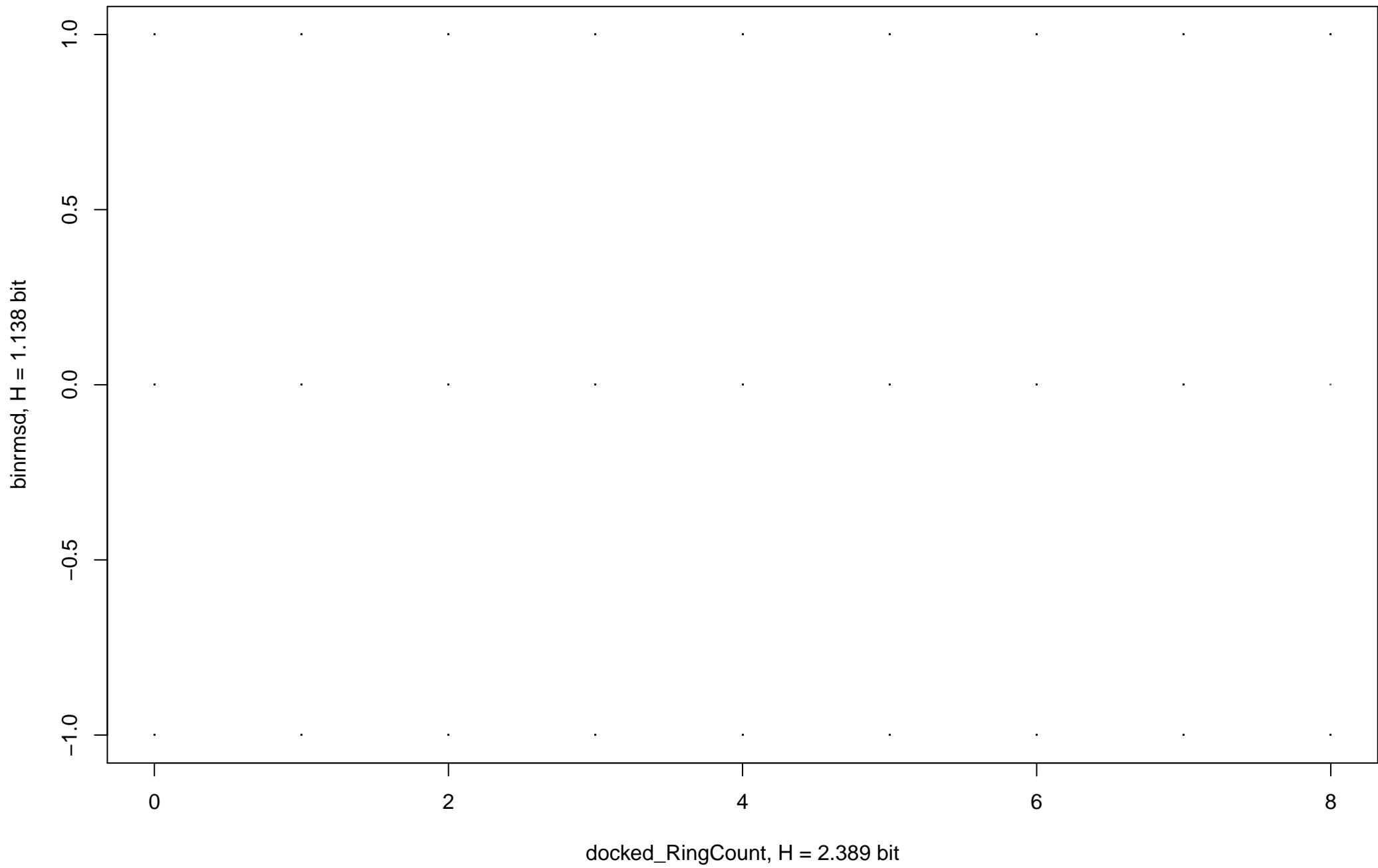
template_NHOHCount-mcs_docked_NumRotatableBonds, MI = 0.05254 bit, normMI = 0.01893



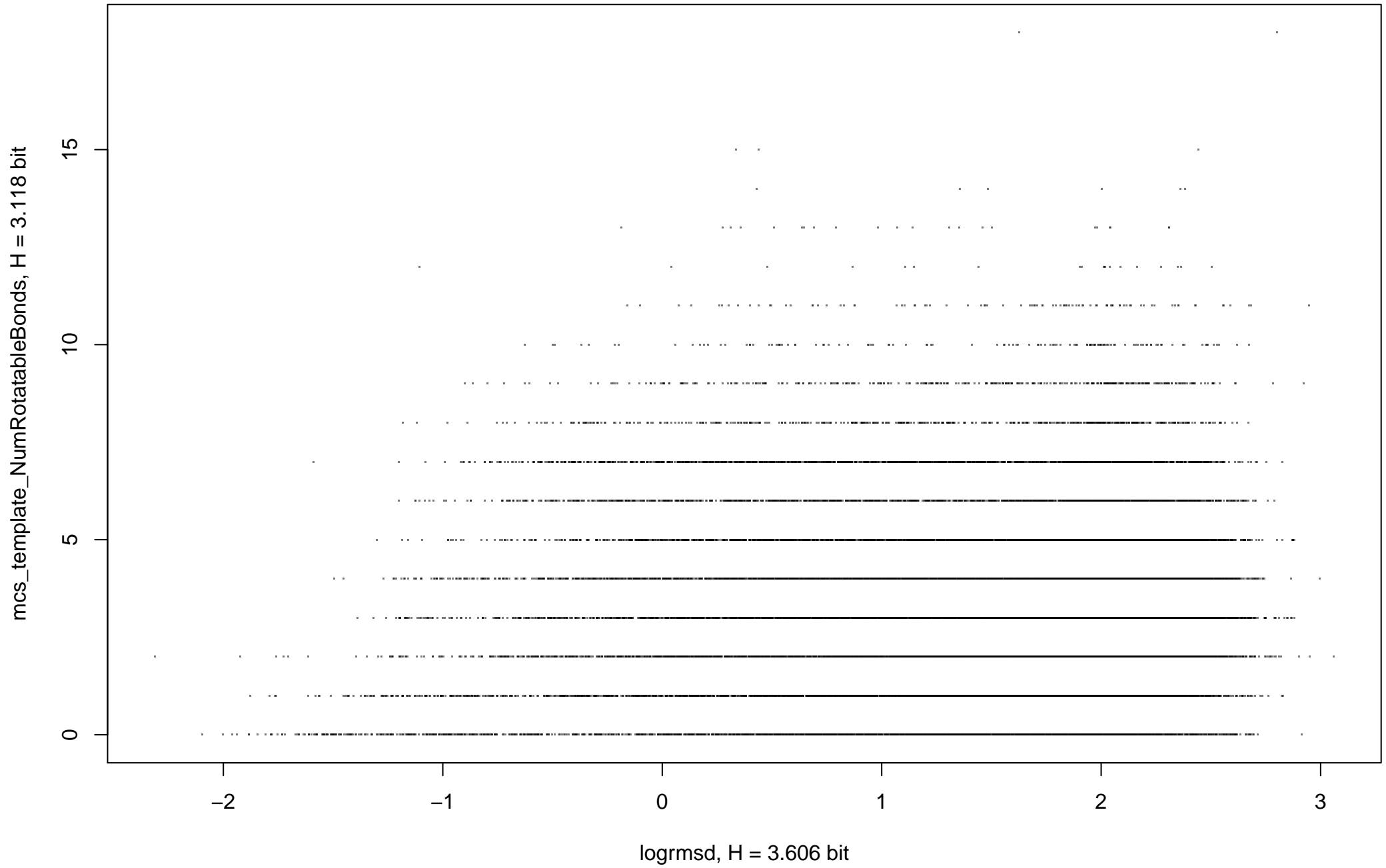
template_NumHAcceptors-docked_NOCount, MI = 0.05612 bit, normMI = 0.01866



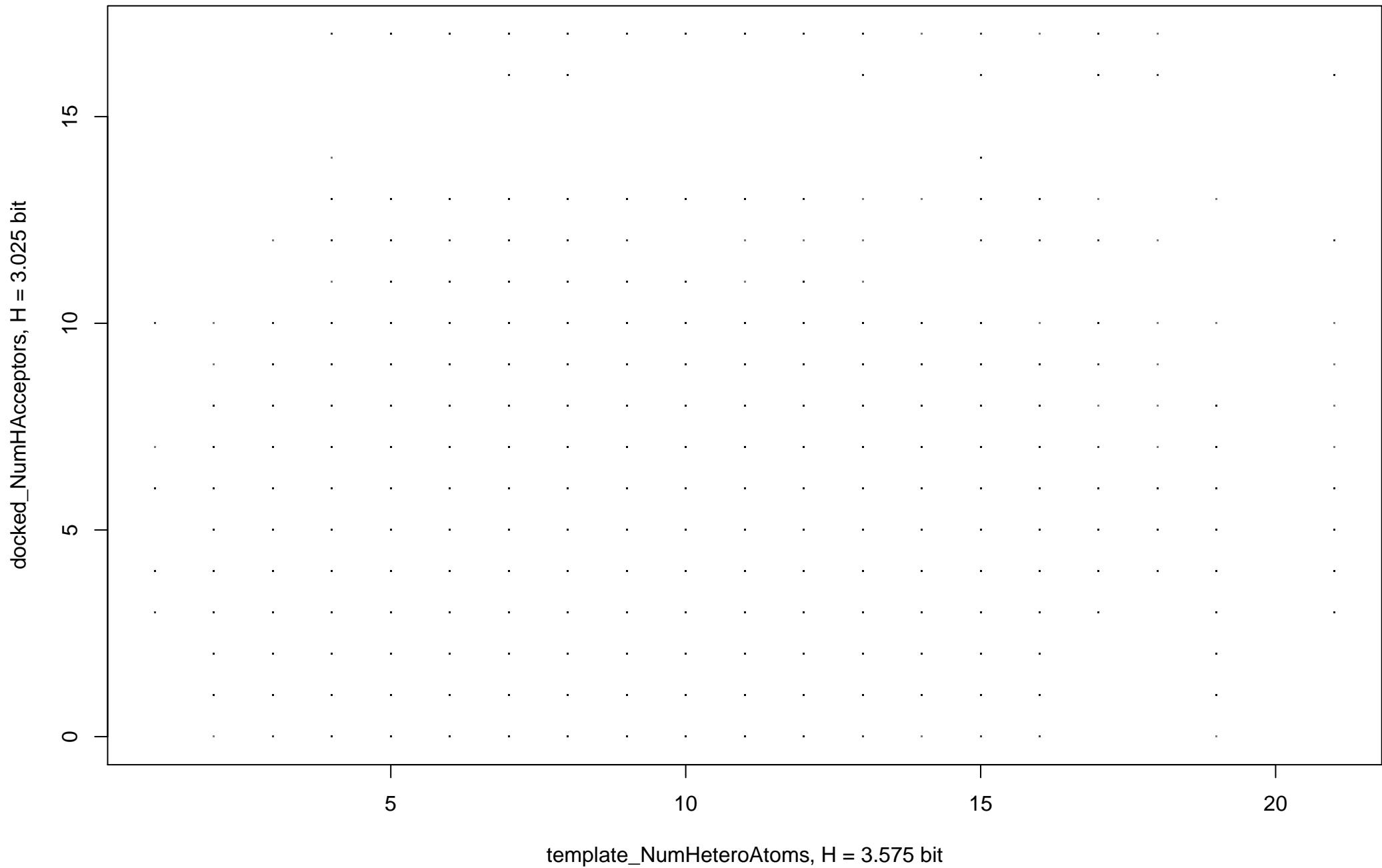
docked_RingCount–binrmsd, MI = 0.02113 bit, normMI = 0.01856



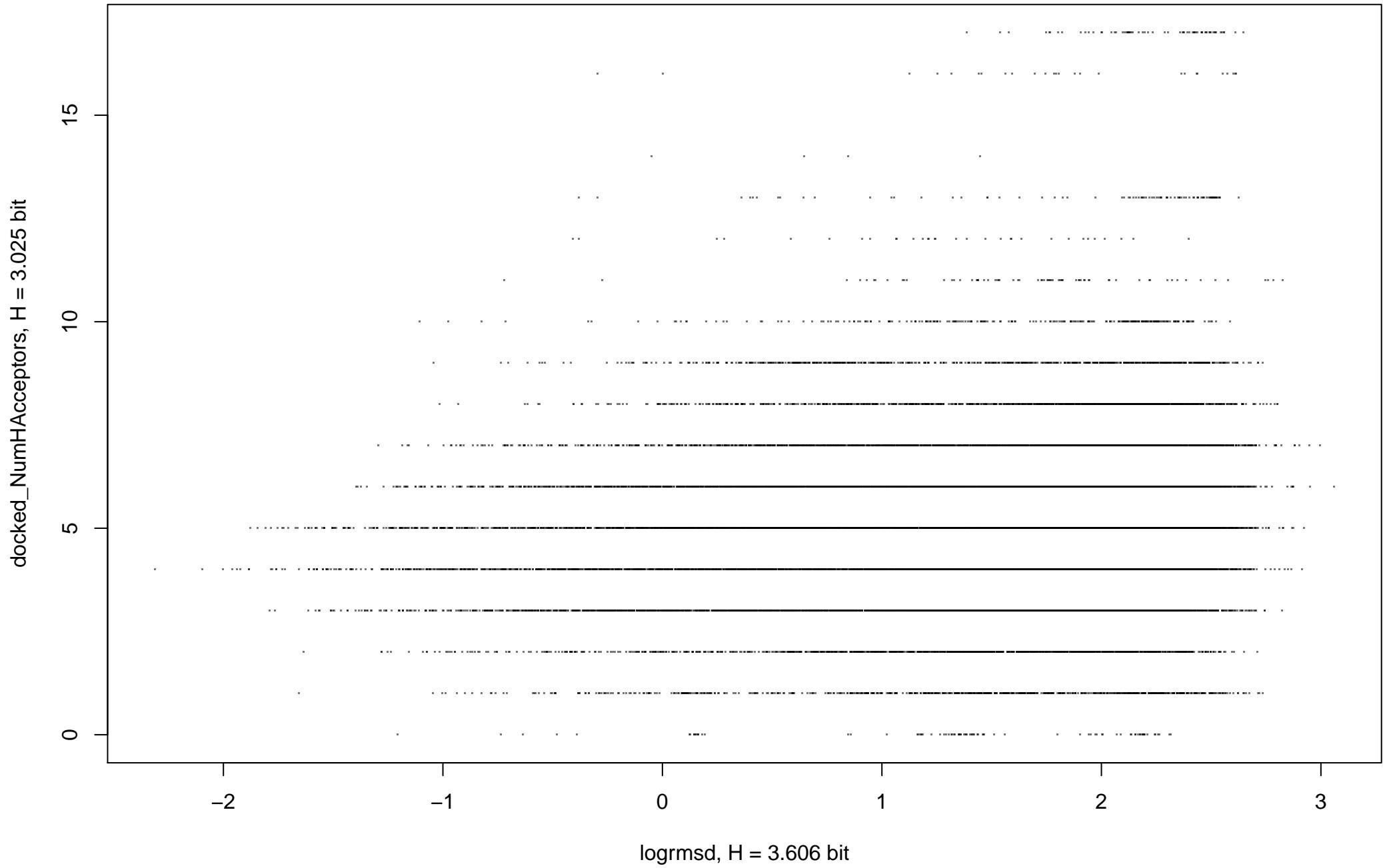
logrmsd-mcs_template_NumRotatableBonds, MI = 0.05713 bit, normMI = 0.01832



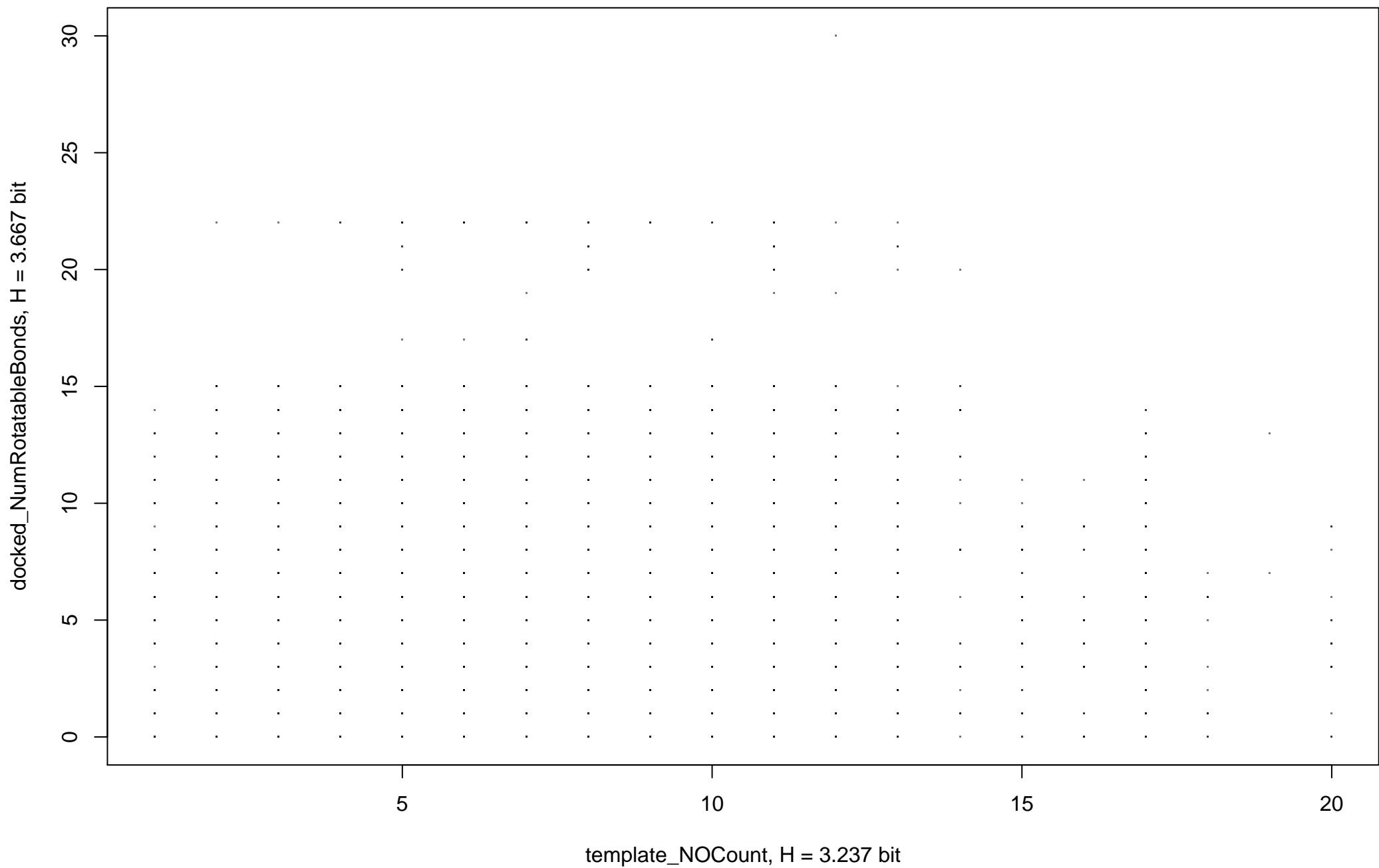
template_NumHeteroAtoms-docked_NumHAcceptors, MI = 0.05523 bit, normMI = 0.01825



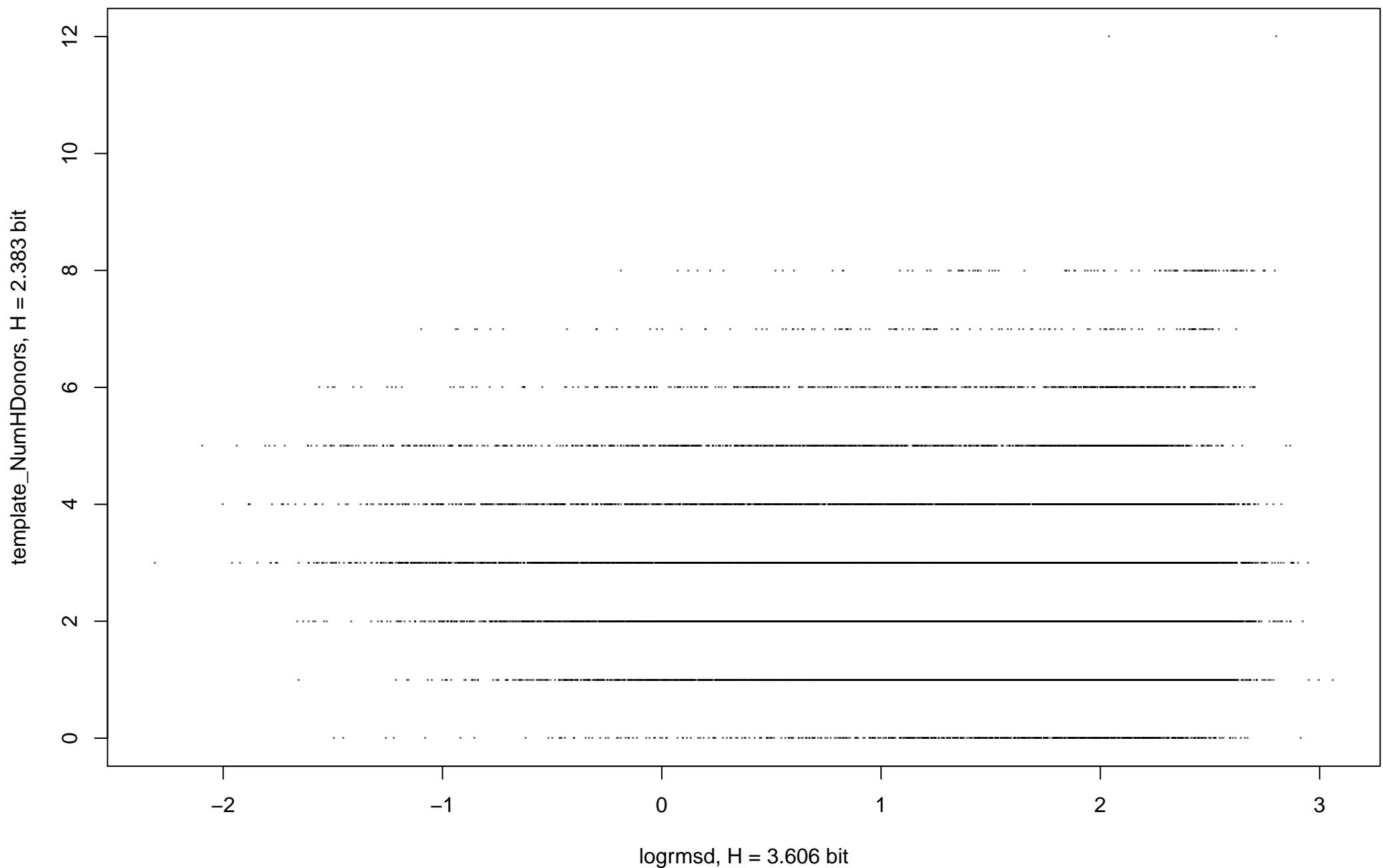
logrmsd-docked_NumHAcceptors, MI = 0.0547 bit, normMI = 0.01808



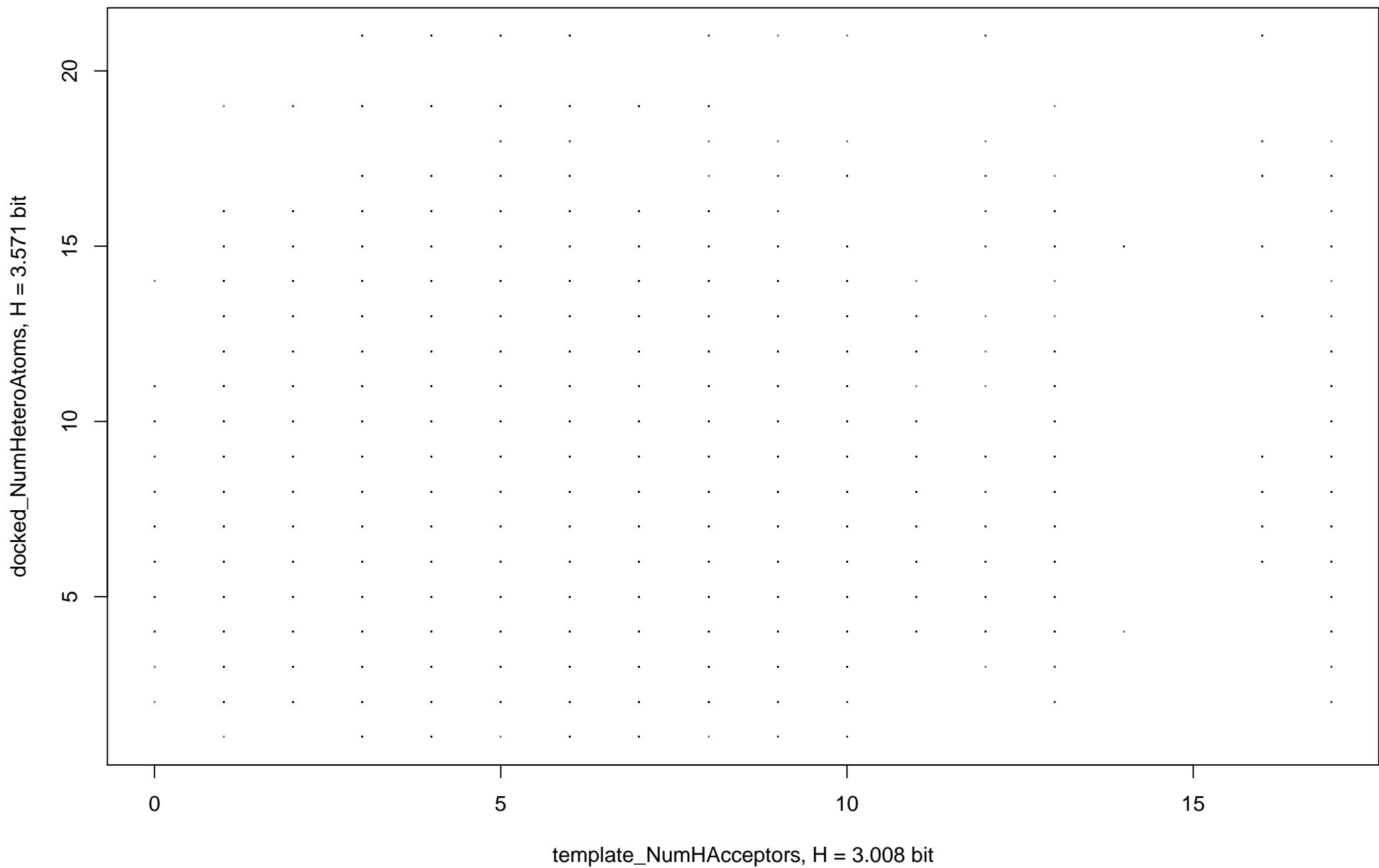
template_NOCount-docked_NumRotatableBonds, MI = 0.0579 bit, normMI = 0.01789



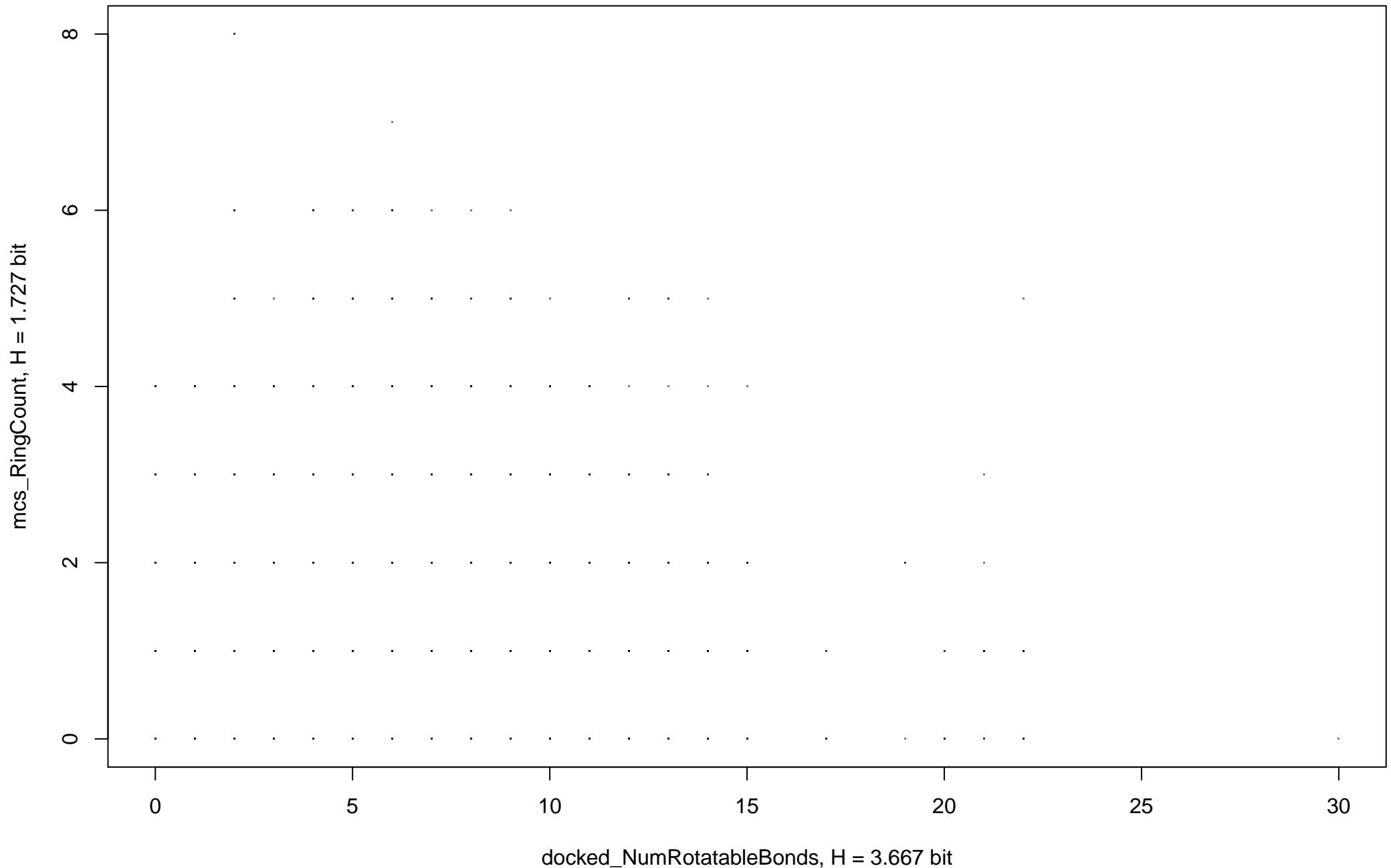
logrmsd-template_NumHDonors, MI = 0.04242 bit, normMI = 0.0178



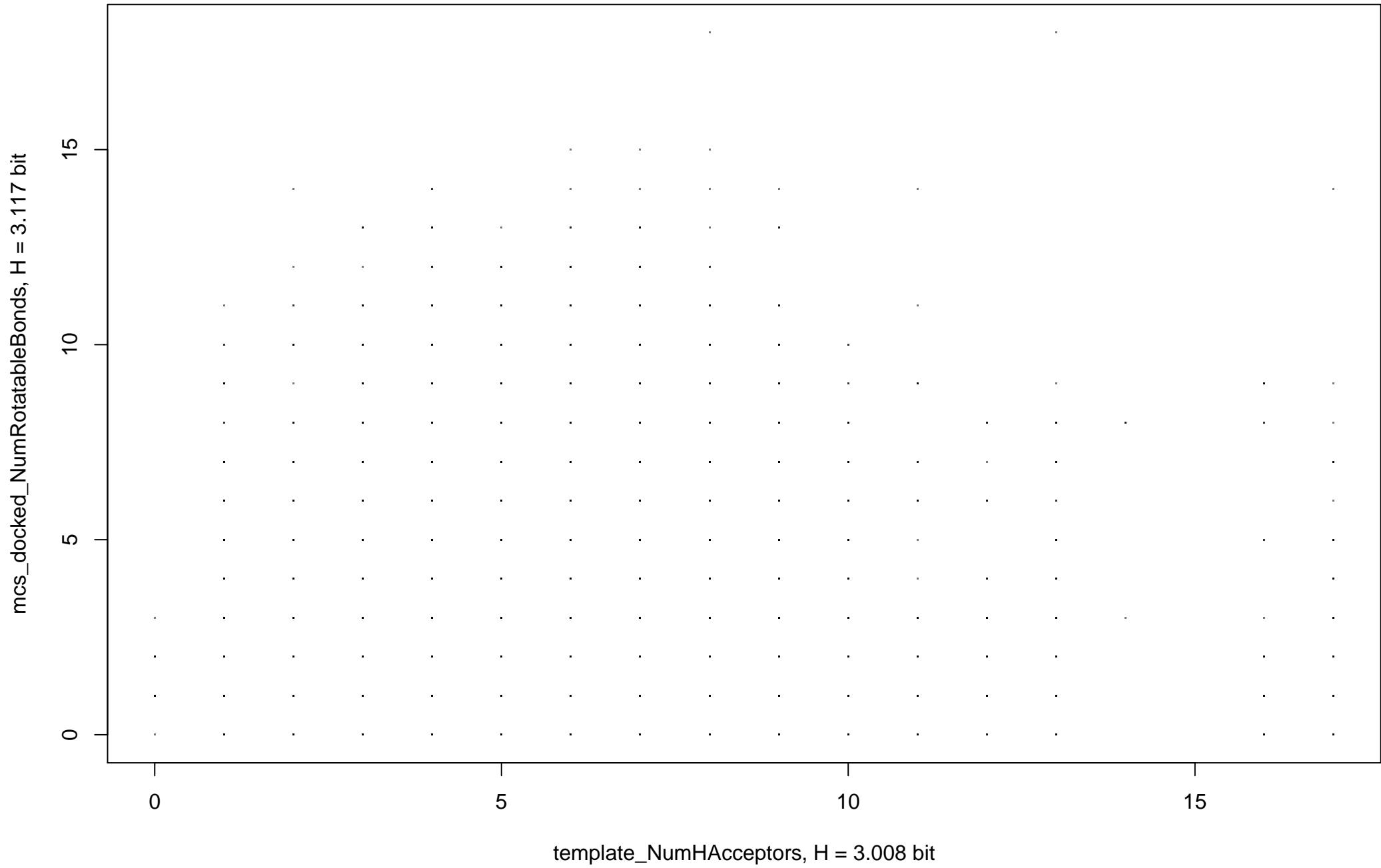
template_NumHAcceptors-docked_NumHeteroAtoms, MI = 0.05331 bit, normMI = 0.01772



docked_NumRotatableBonds–mcs_RingCount, MI = 0.03001 bit, normMI = 0.01737

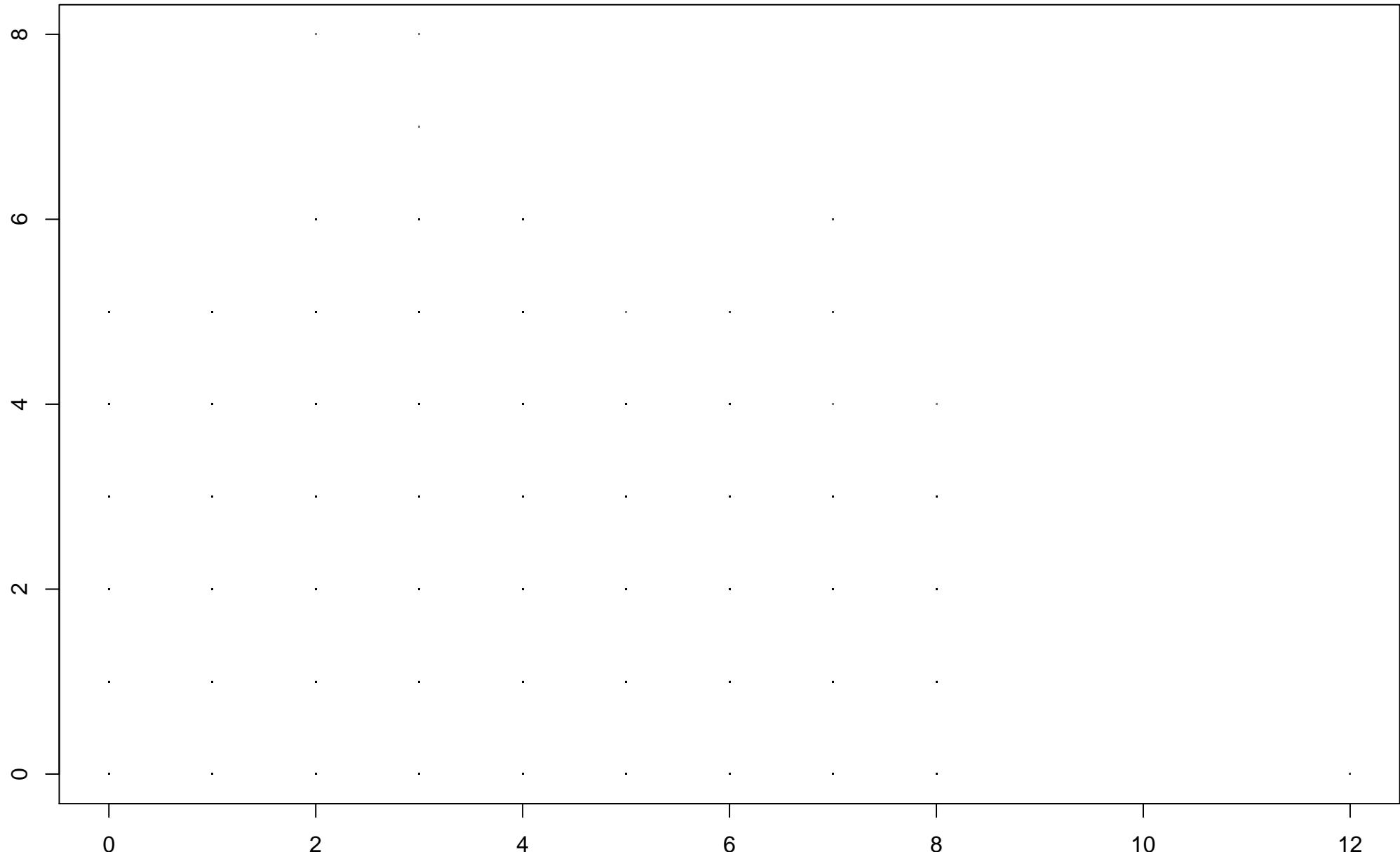


template_NumHAcceptors-mcs_docked_NumRotatableBonds, MI = 0.0521 bit, normMI = 0.01732



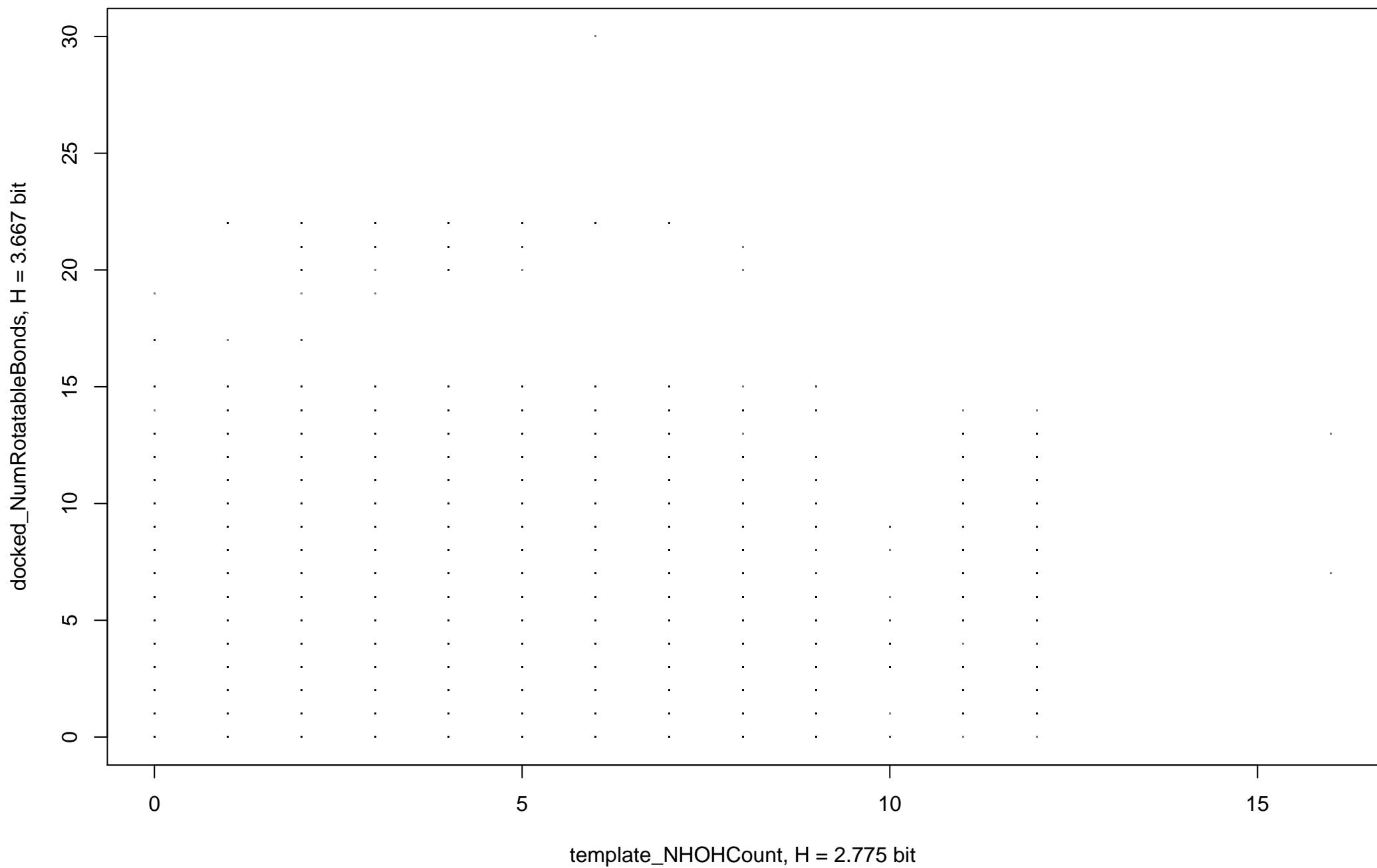
template_NumHDonors-mcs_RingCount, MI = 0.02983 bit, normMI = 0.01727

mcs_RingCount, H = 1.727 bit

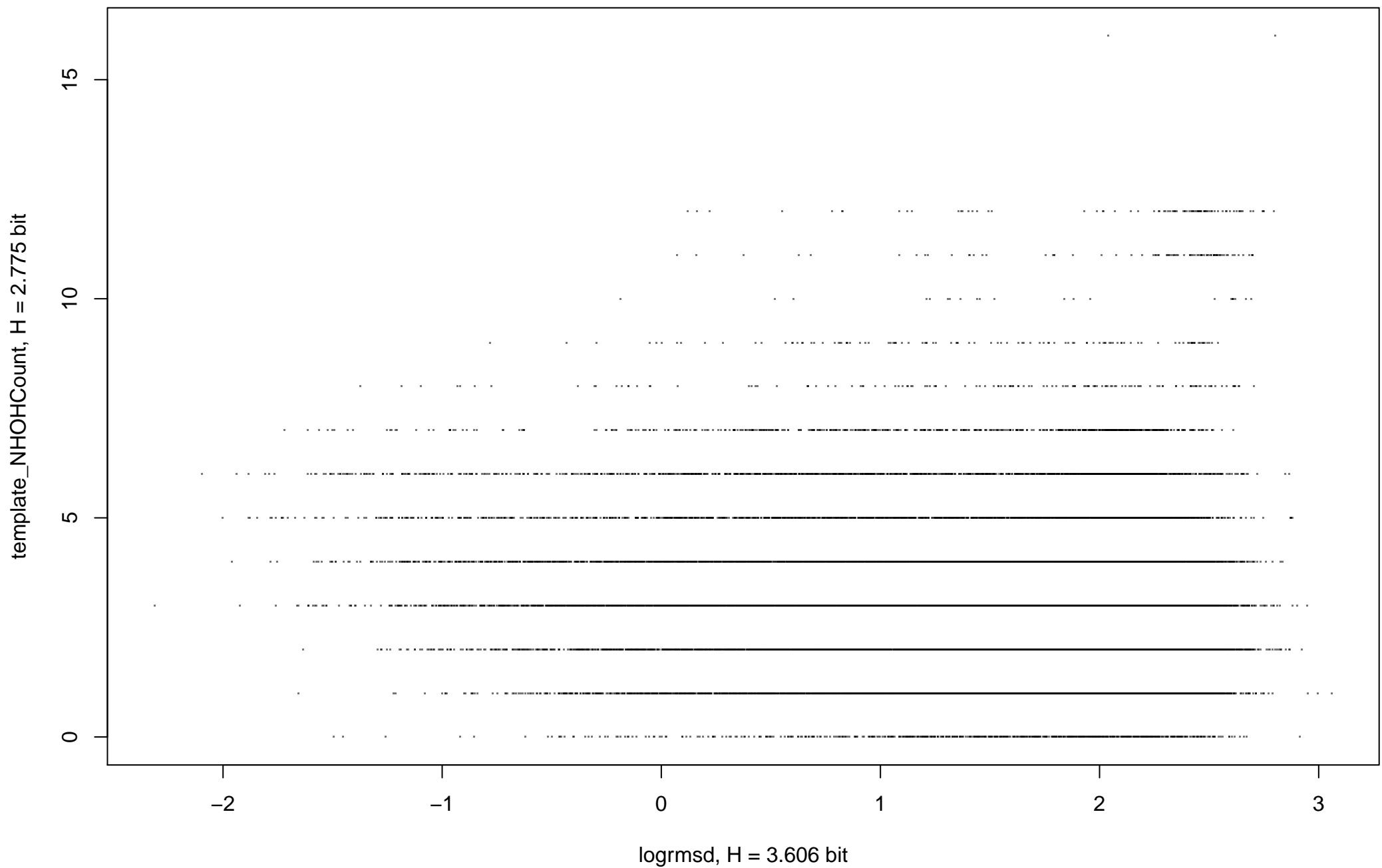


template_NumHDonors, H = 2.383 bit

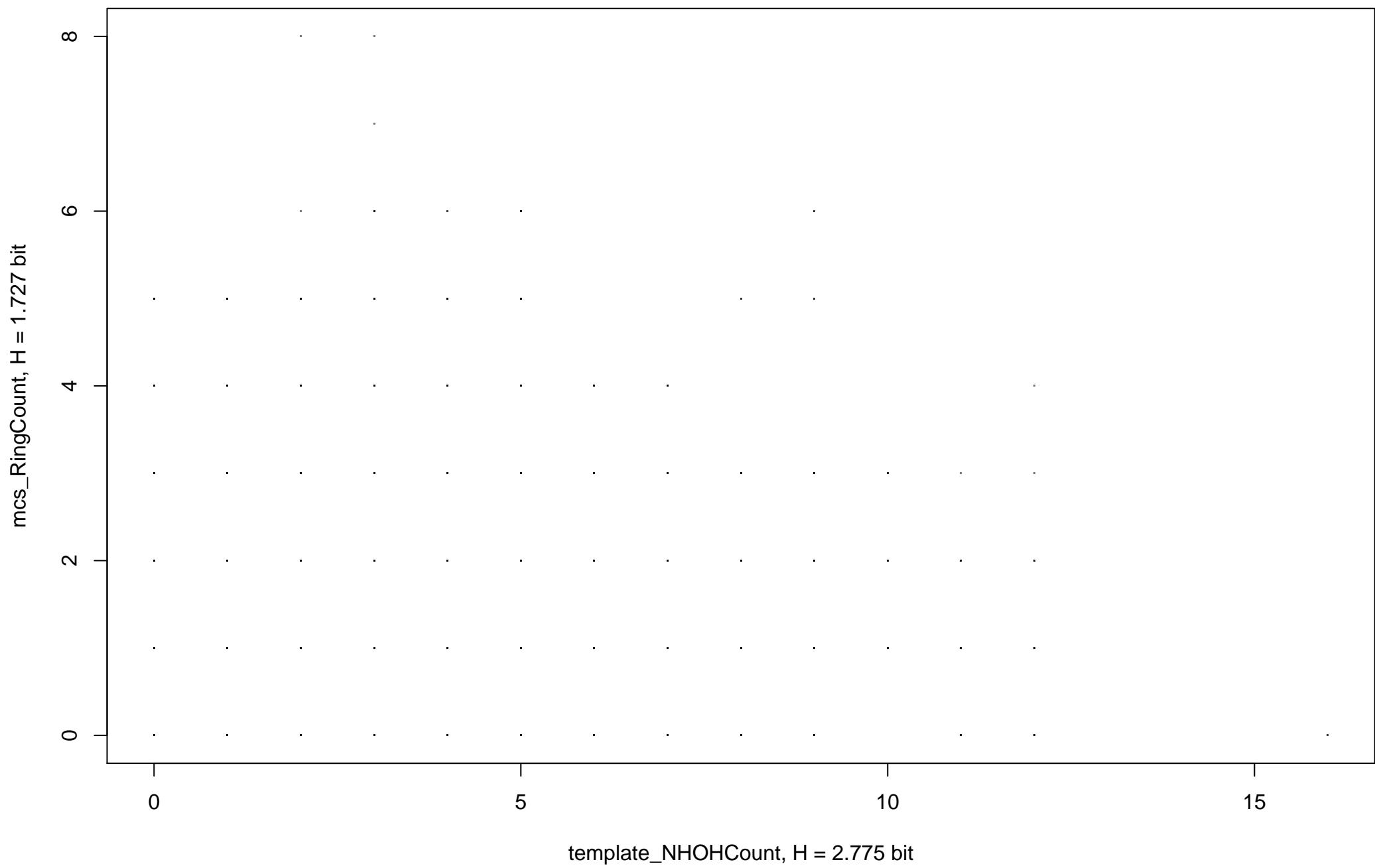
template_NHOHCount-docked_NumRotatableBonds, MI = 0.04789 bit, normMI = 0.01725



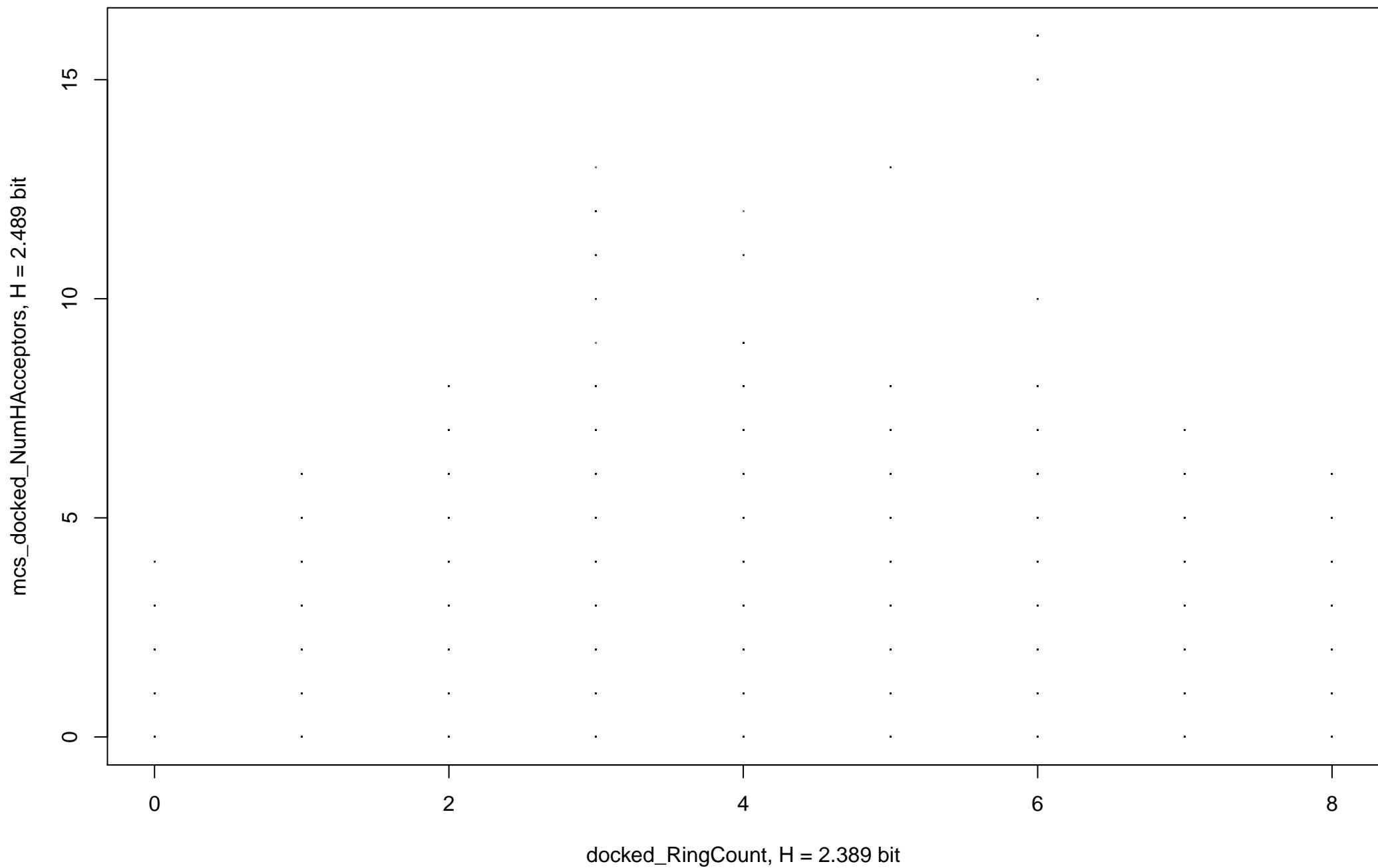
logrmsd-template_NHOHCount, MI = 0.04779 bit, normMI = 0.01722



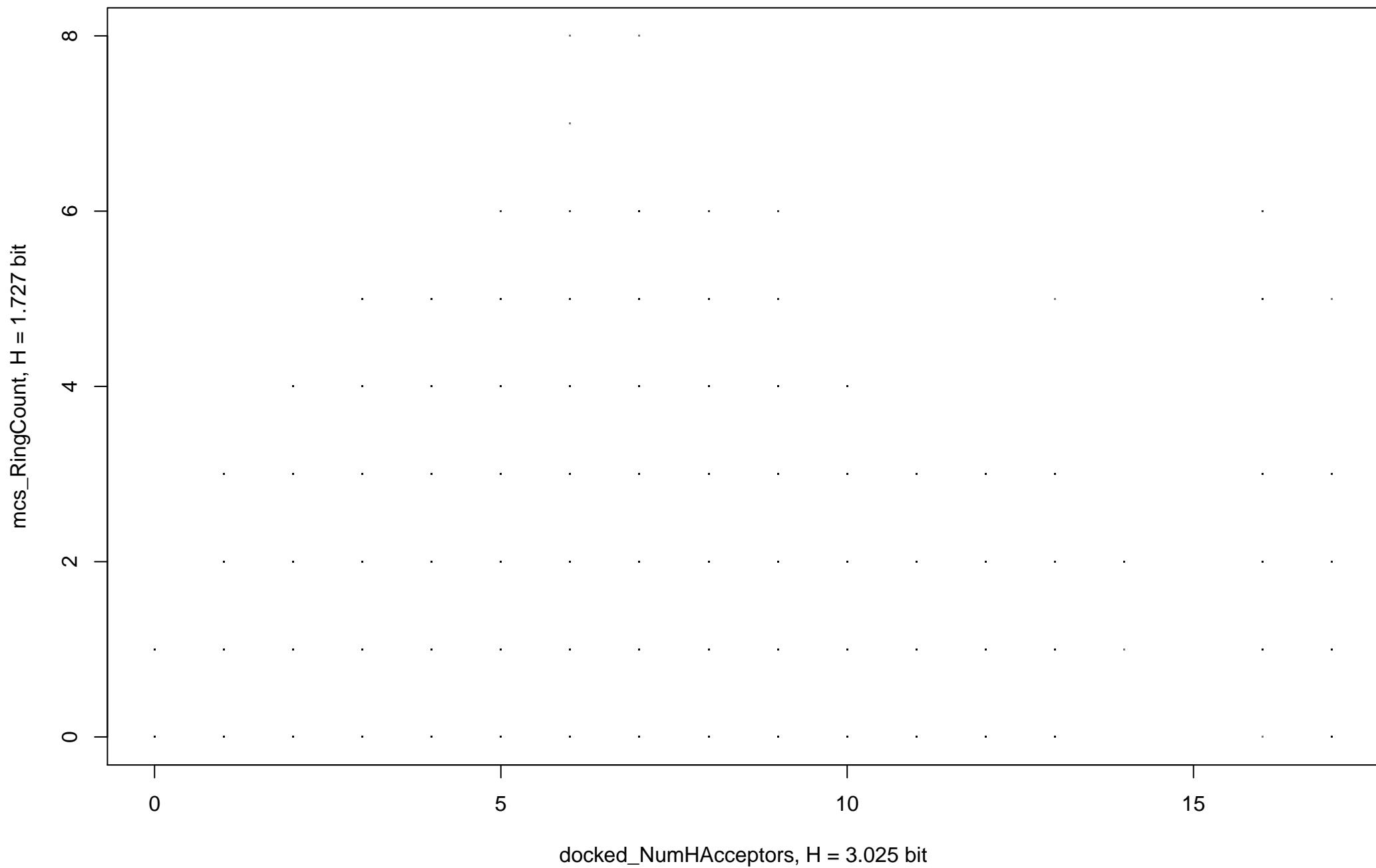
template_NHOHCount-mcs_RingCount, MI = 0.0297 bit, normMI = 0.0172



docked_RingCount-mcs_docked_NumHAcceptors, MI = 0.04105 bit, normMI = 0.01718

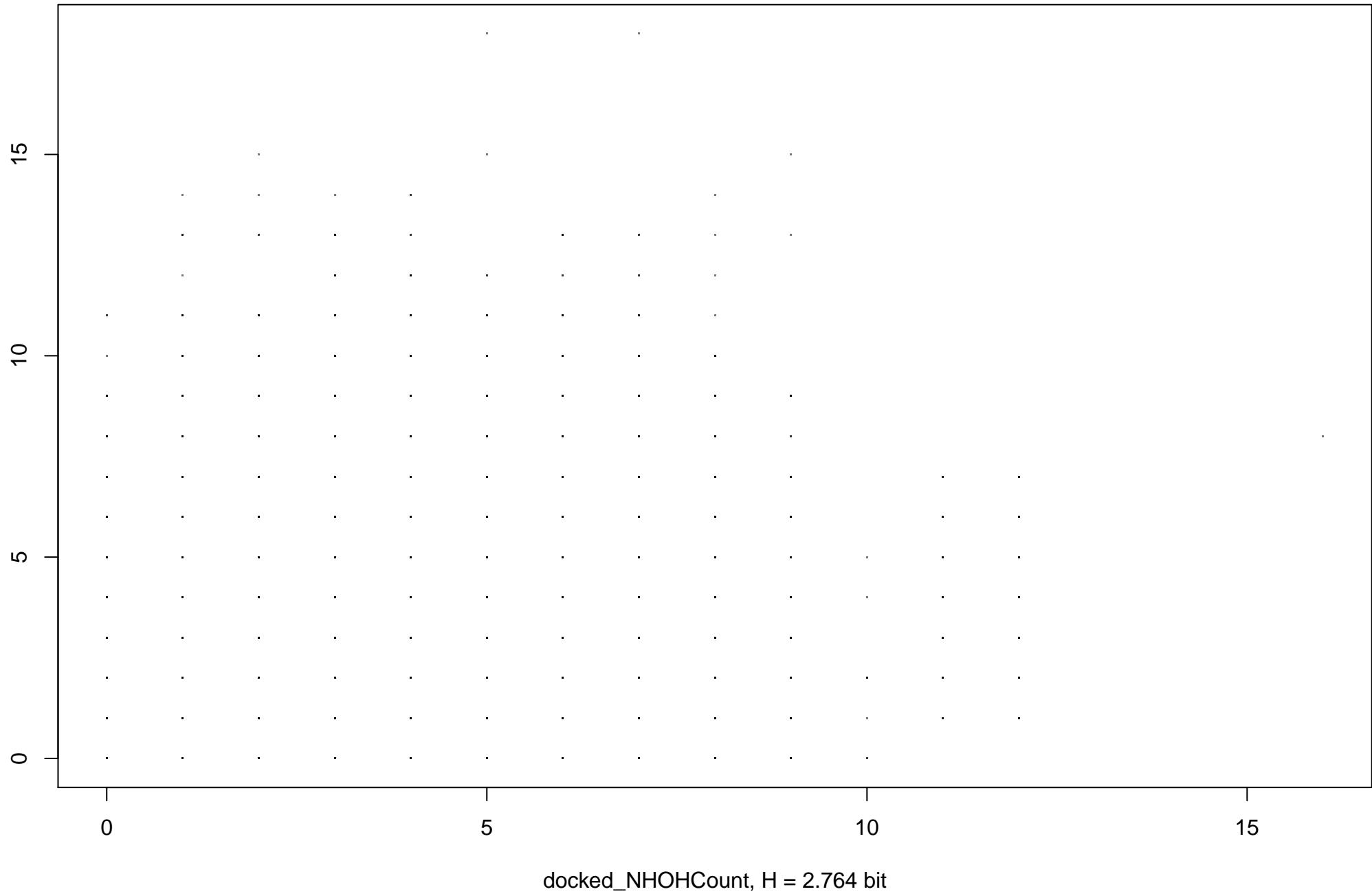


docked_NumHAcceptors-mcs_RingCount, MI = 0.02949 bit, normMI = 0.01707

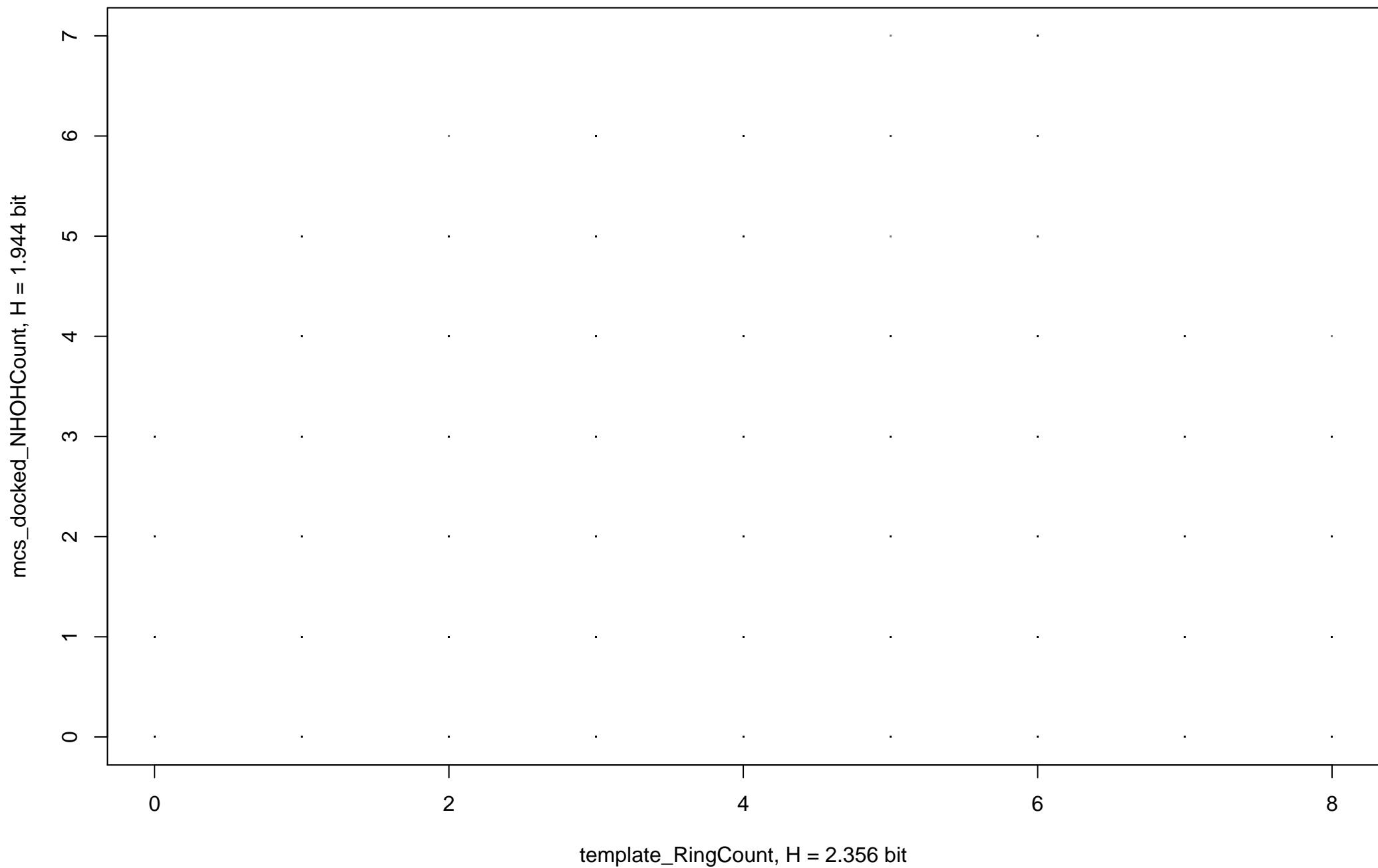


docked_NHOHCount-mcs_template_NumRotatableBonds, MI = 0.04677 bit, normMI = 0.01692

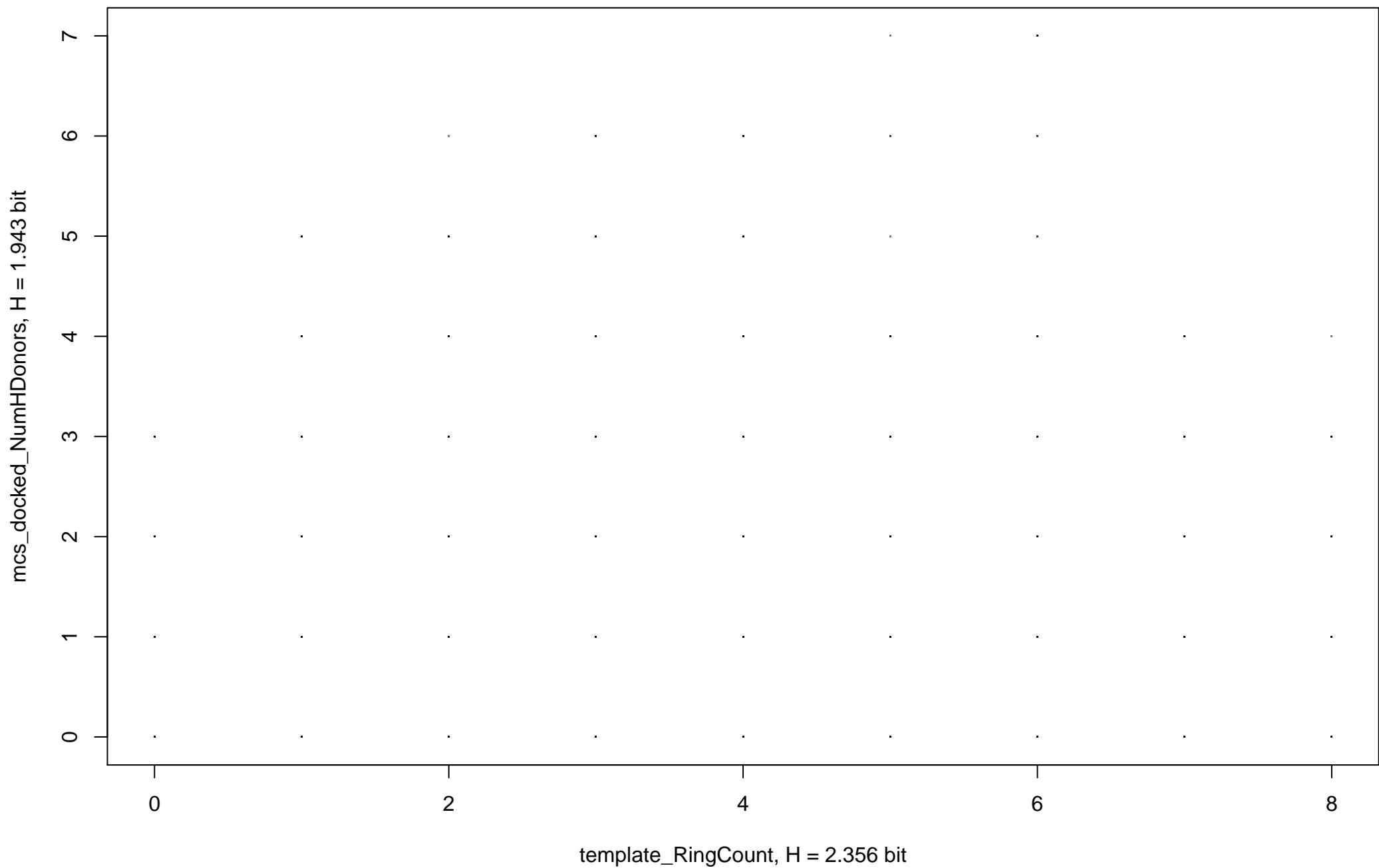
mcs_template_NumRotatableBonds, H = 3.118 bit



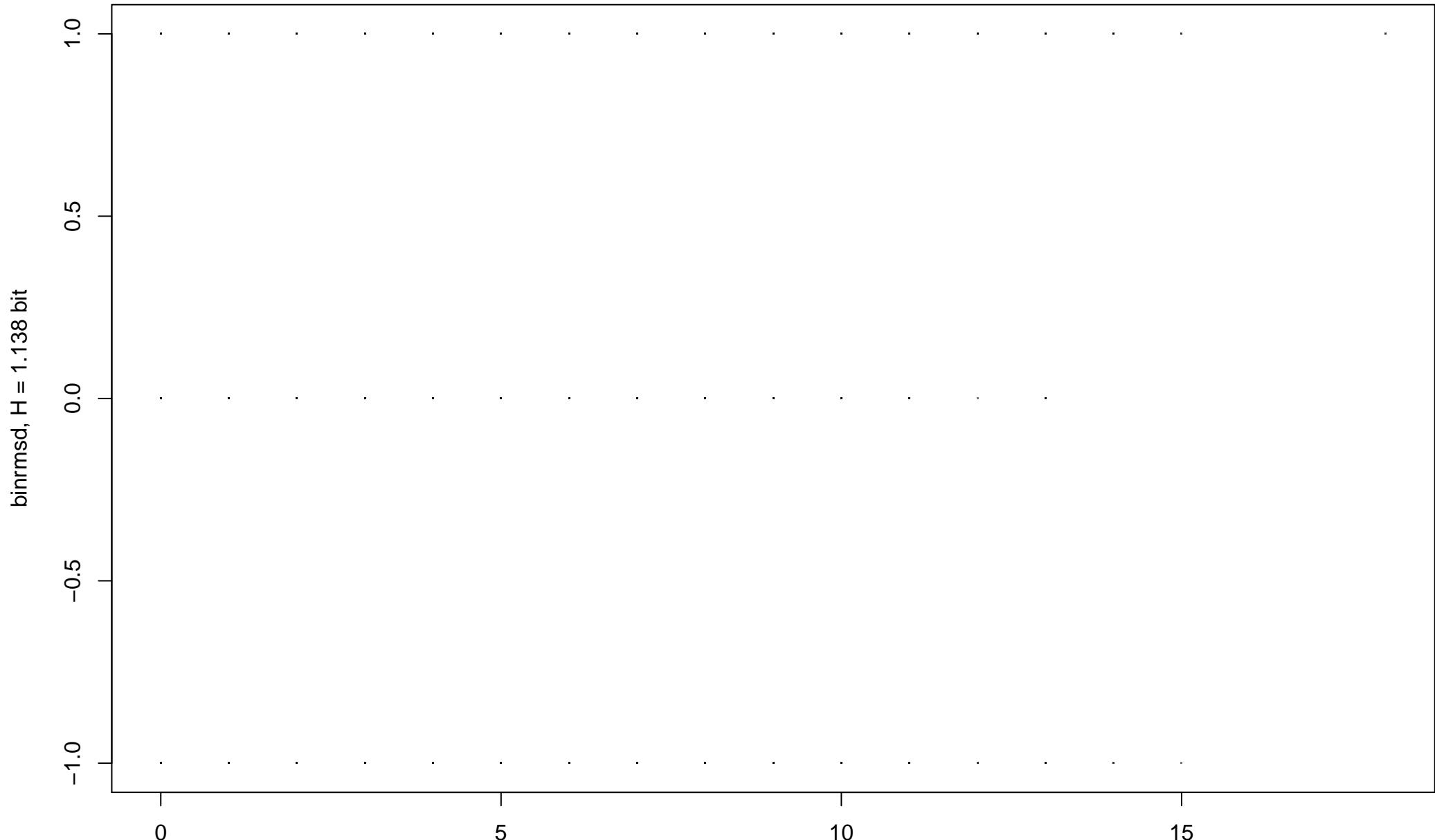
template_RingCount-mcs_docked_NHOHCount, MI = 0.03263 bit, normMI = 0.01679



template_RingCount-mcs_docked_NumHDonors, MI = 0.03262 bit, normMI = 0.01678

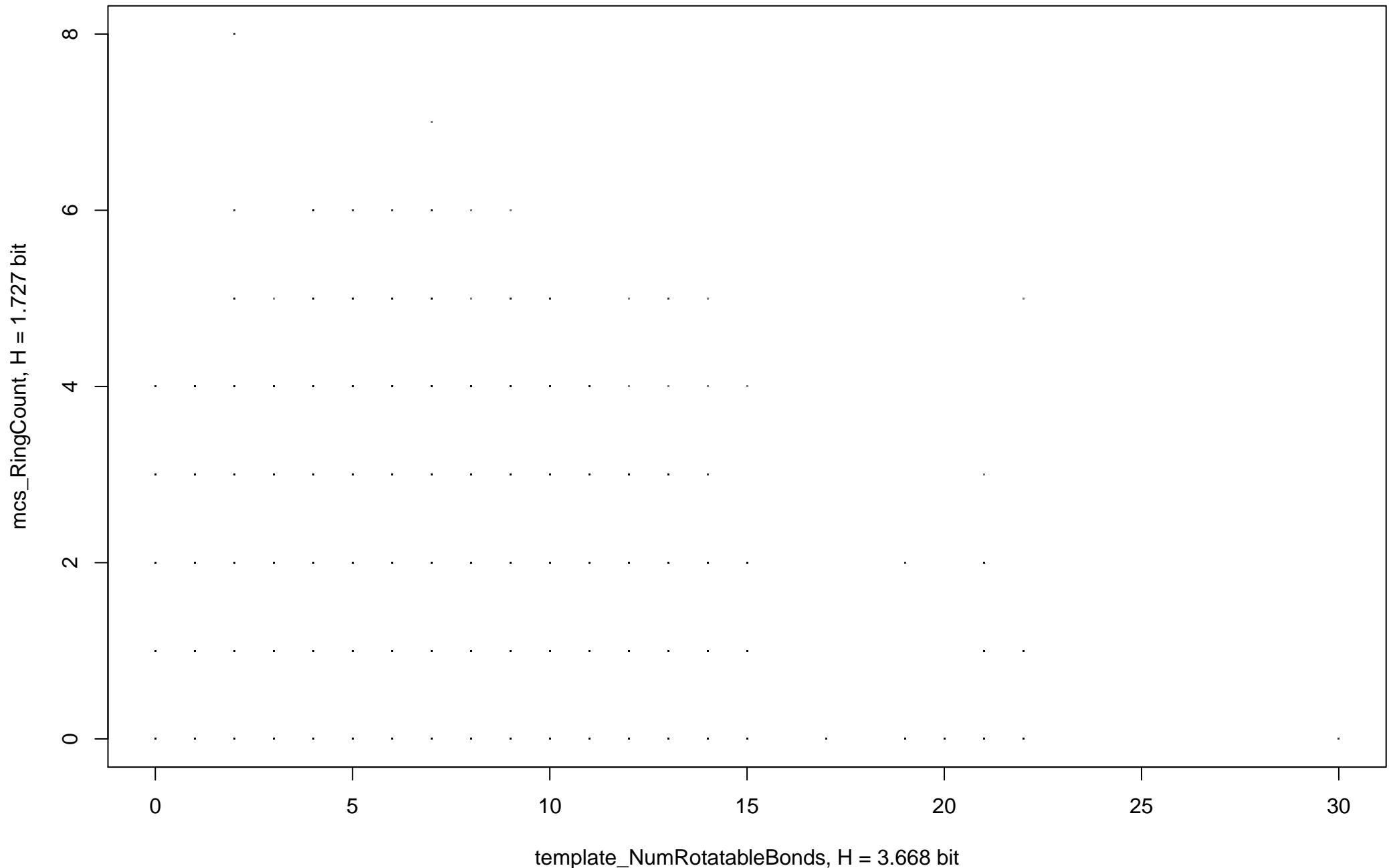


mcs_docked_NumRotatableBonds–binrmsd, MI = 0.01909 bit, normMI = 0.01677

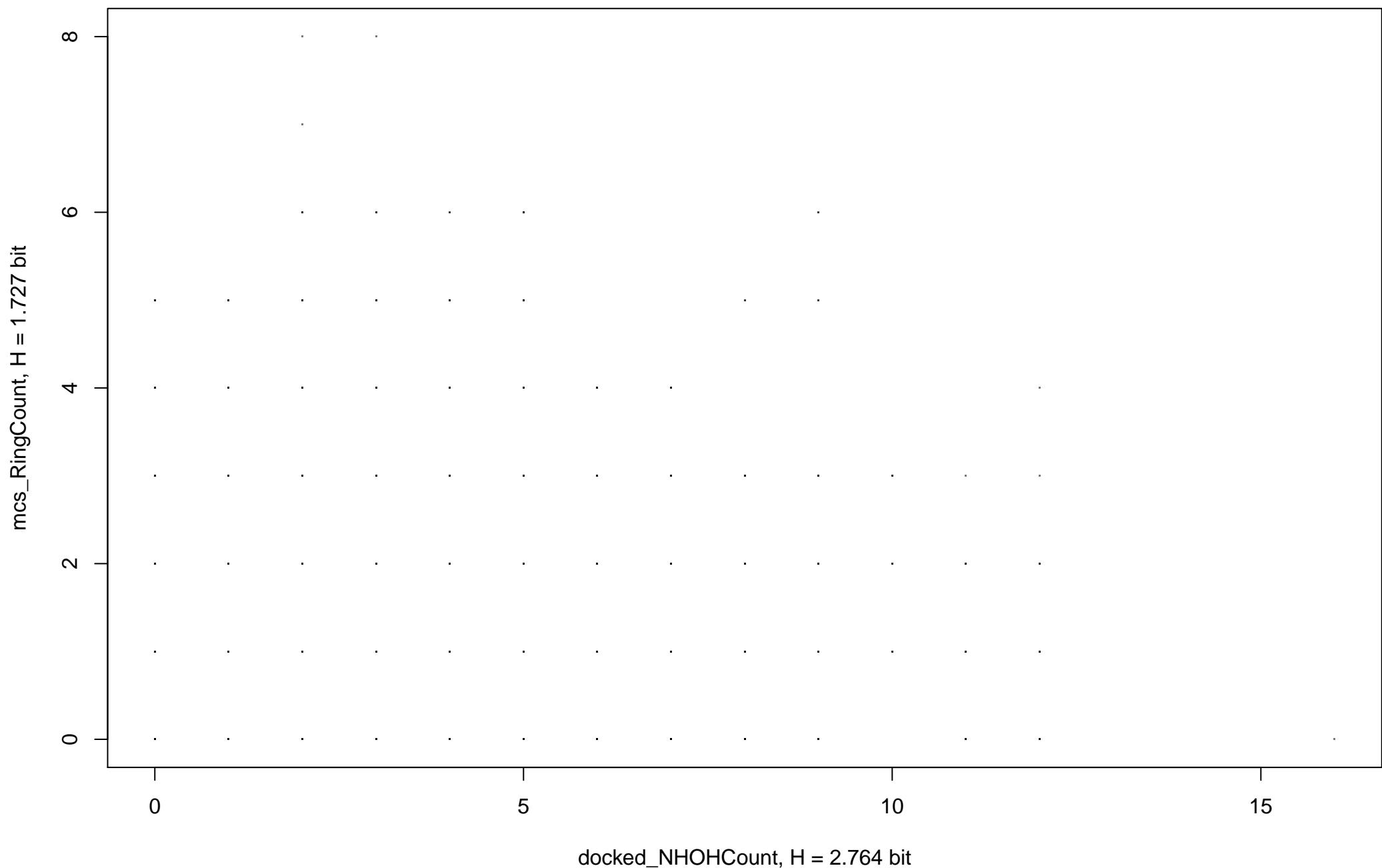


mcs_docked_NumRotatableBonds, H = 3.117 bit

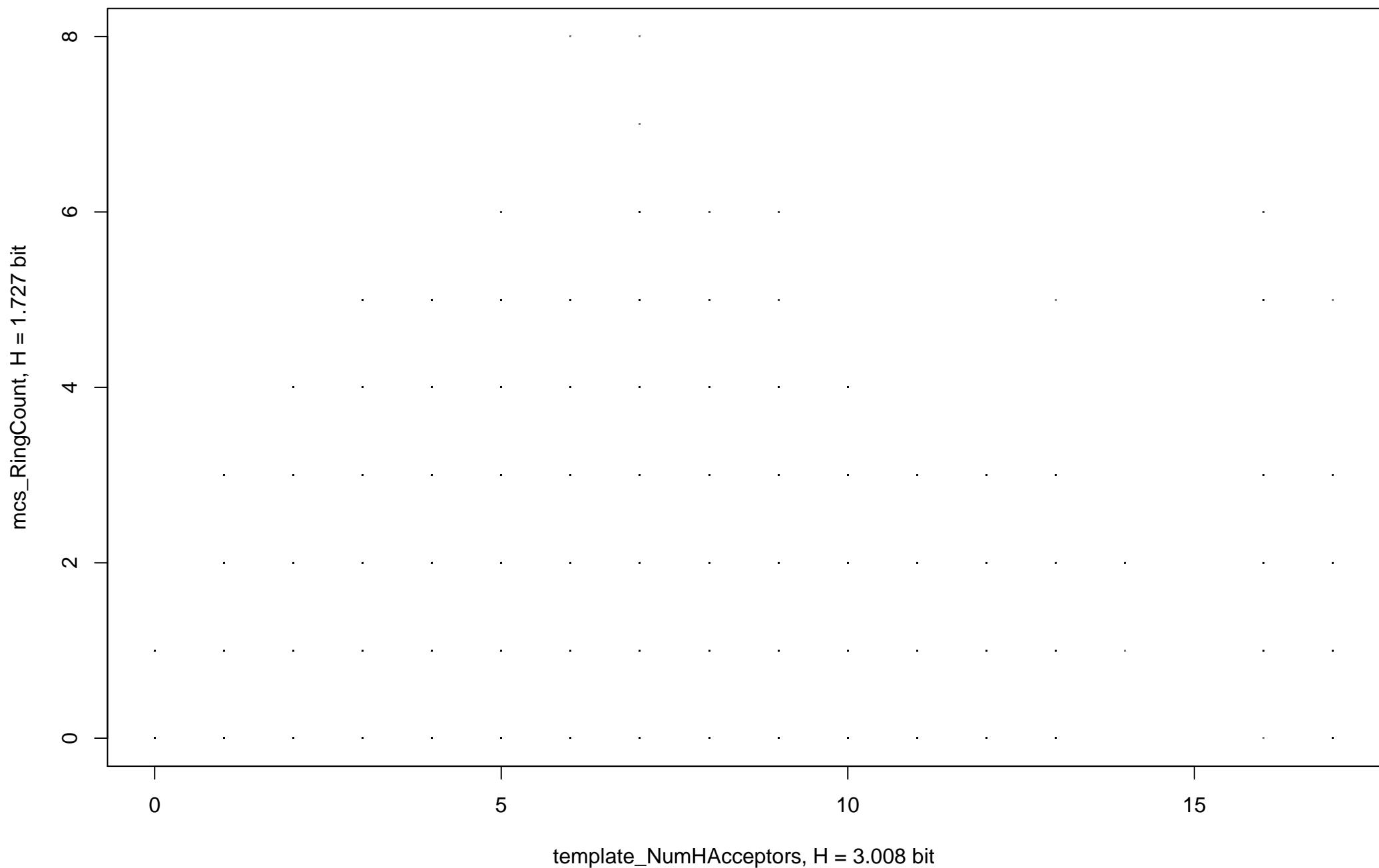
template_NumRotatableBonds-mcs_RingCount, MI = 0.02862 bit, normMI = 0.01657



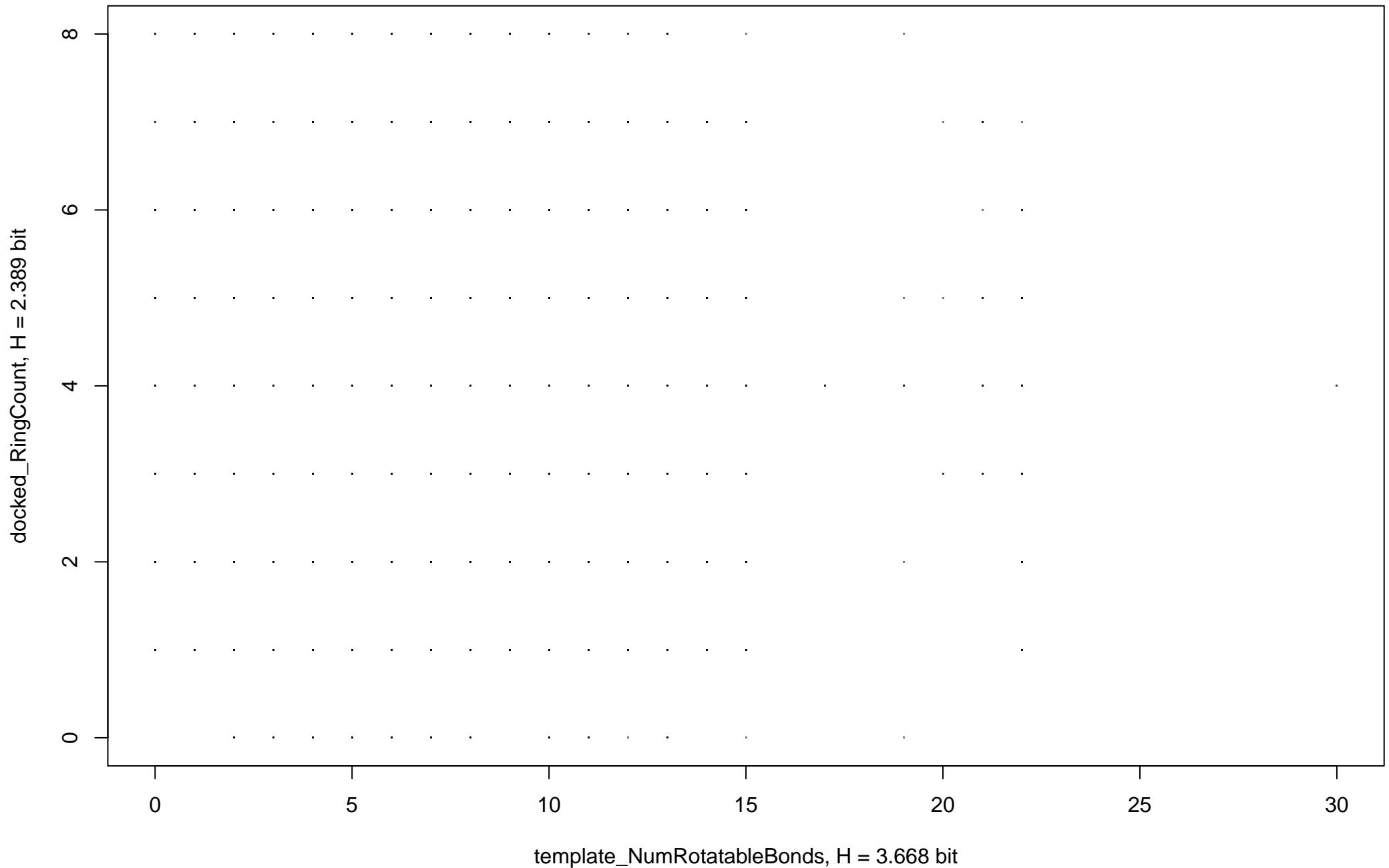
docked_NHOHCount-mcs_RingCount, MI = 0.02847 bit, normMI = 0.01648



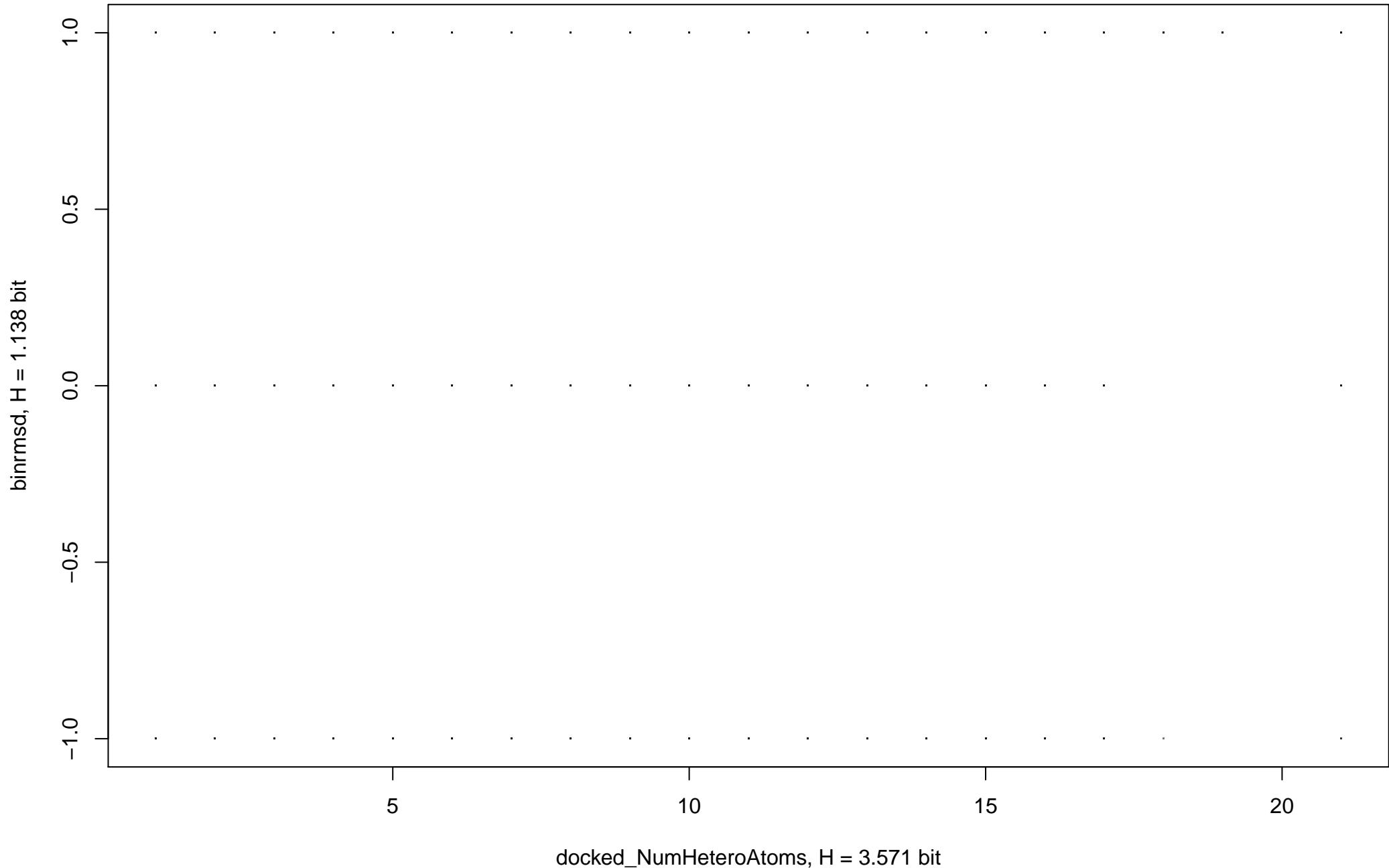
template_NumHAcceptors-mcs_RingCount, MI = 0.02843 bit, normMI = 0.01646



template_NumRotatableBonds-docked_RingCount, MI = 0.03899 bit, normMI = 0.01632

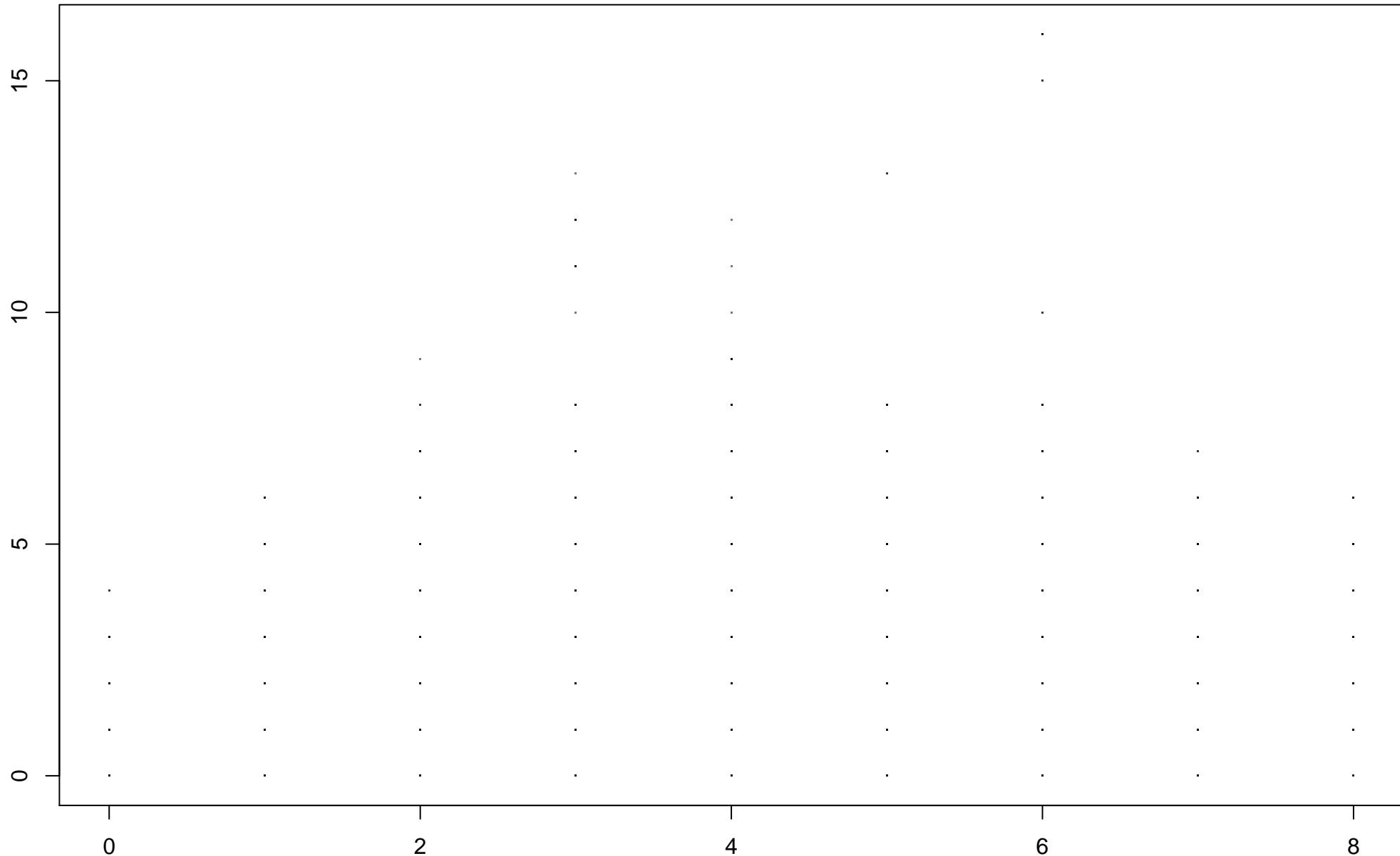


docked_NumHeteroAtoms-binrmsd, MI = 0.01846 bit, normMI = 0.01622



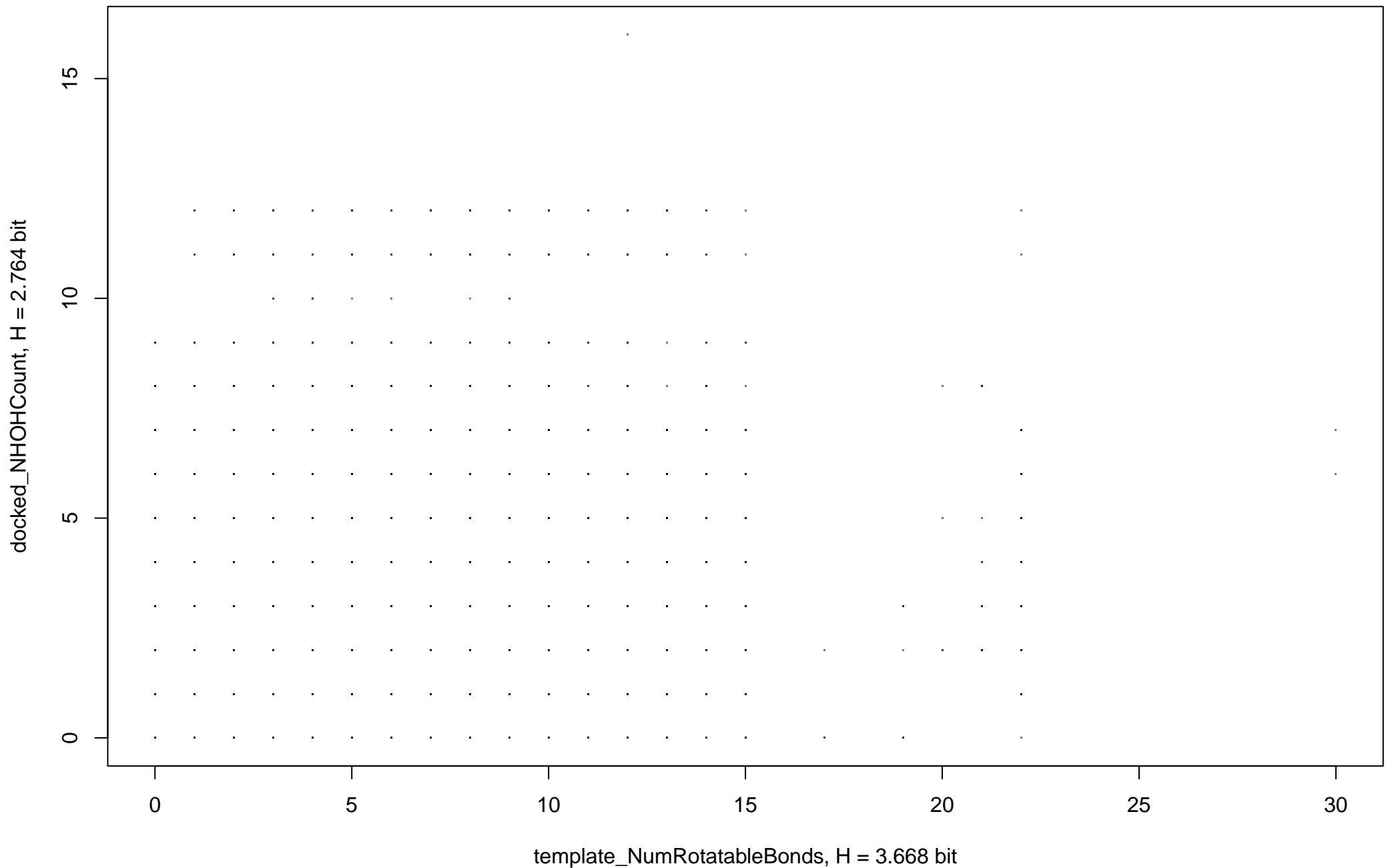
docked_RingCount-mcs_template_NumHAcceptors, MI = 0.03864 bit, normMI = 0.01617

mcs_template_NumHAcceptors, H = 2.488 bit

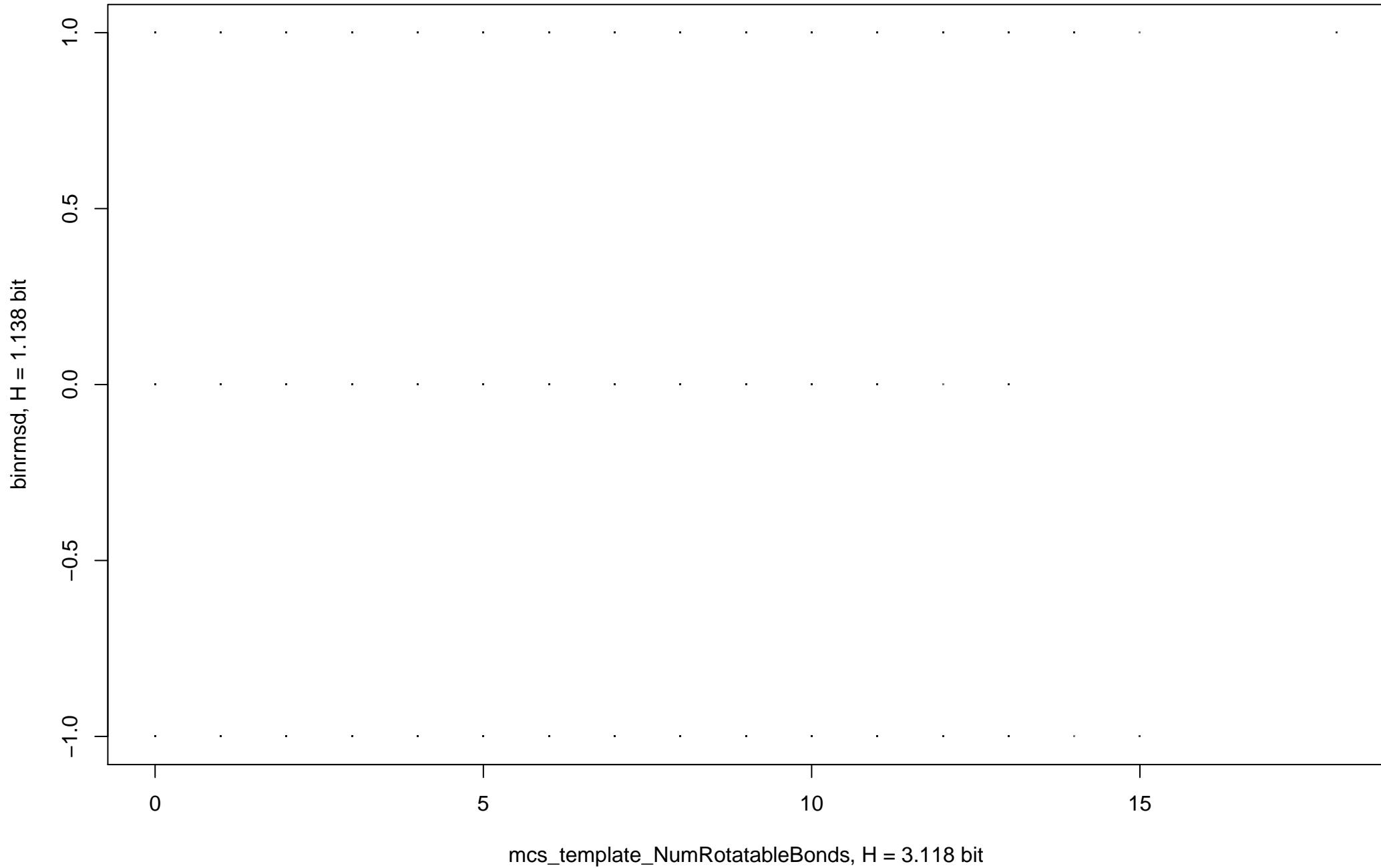


docked_RingCount, H = 2.389 bit

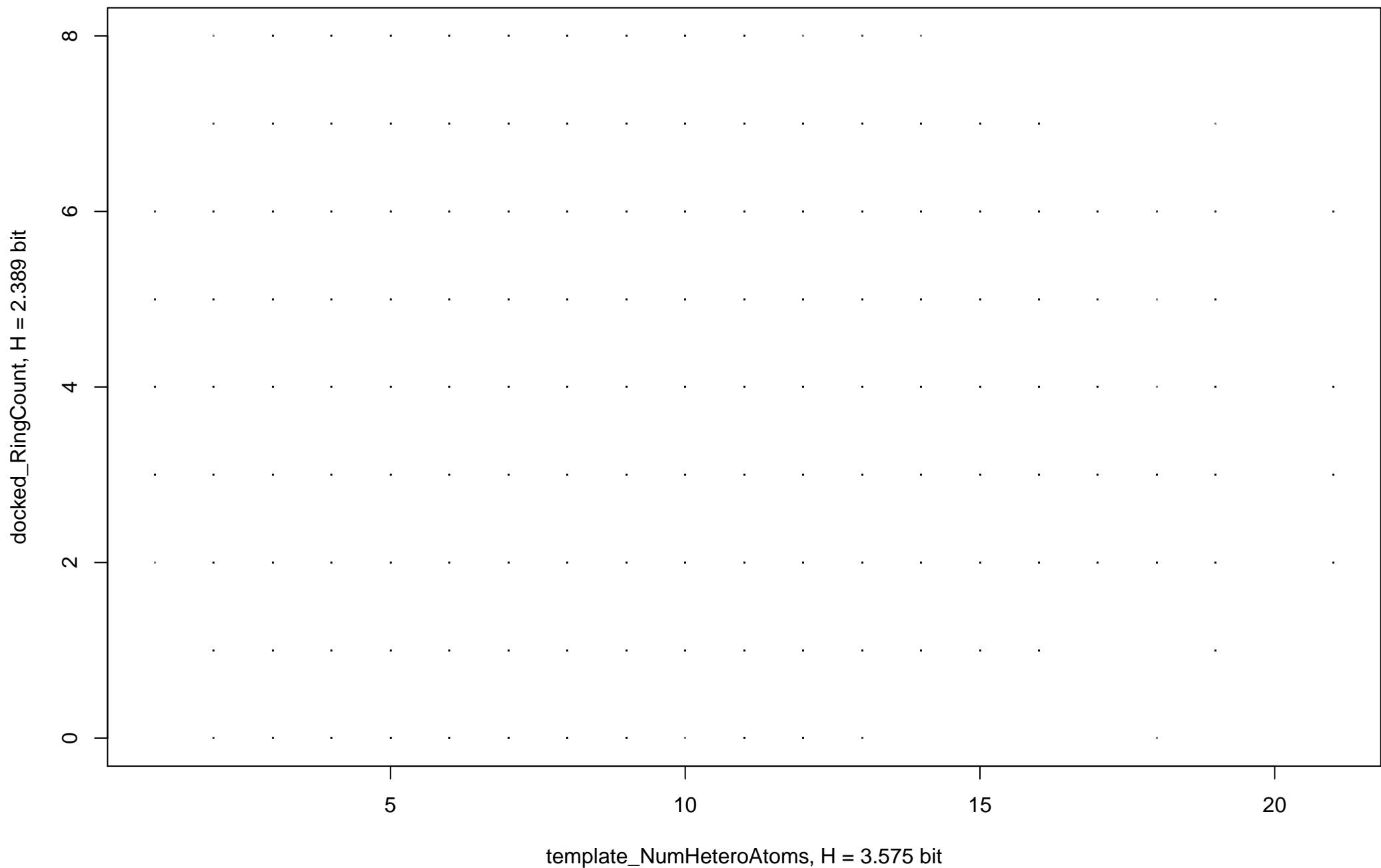
template_NumRotatableBonds-docked_NHOHCount, MI = 0.04428 bit, normMI = 0.01602



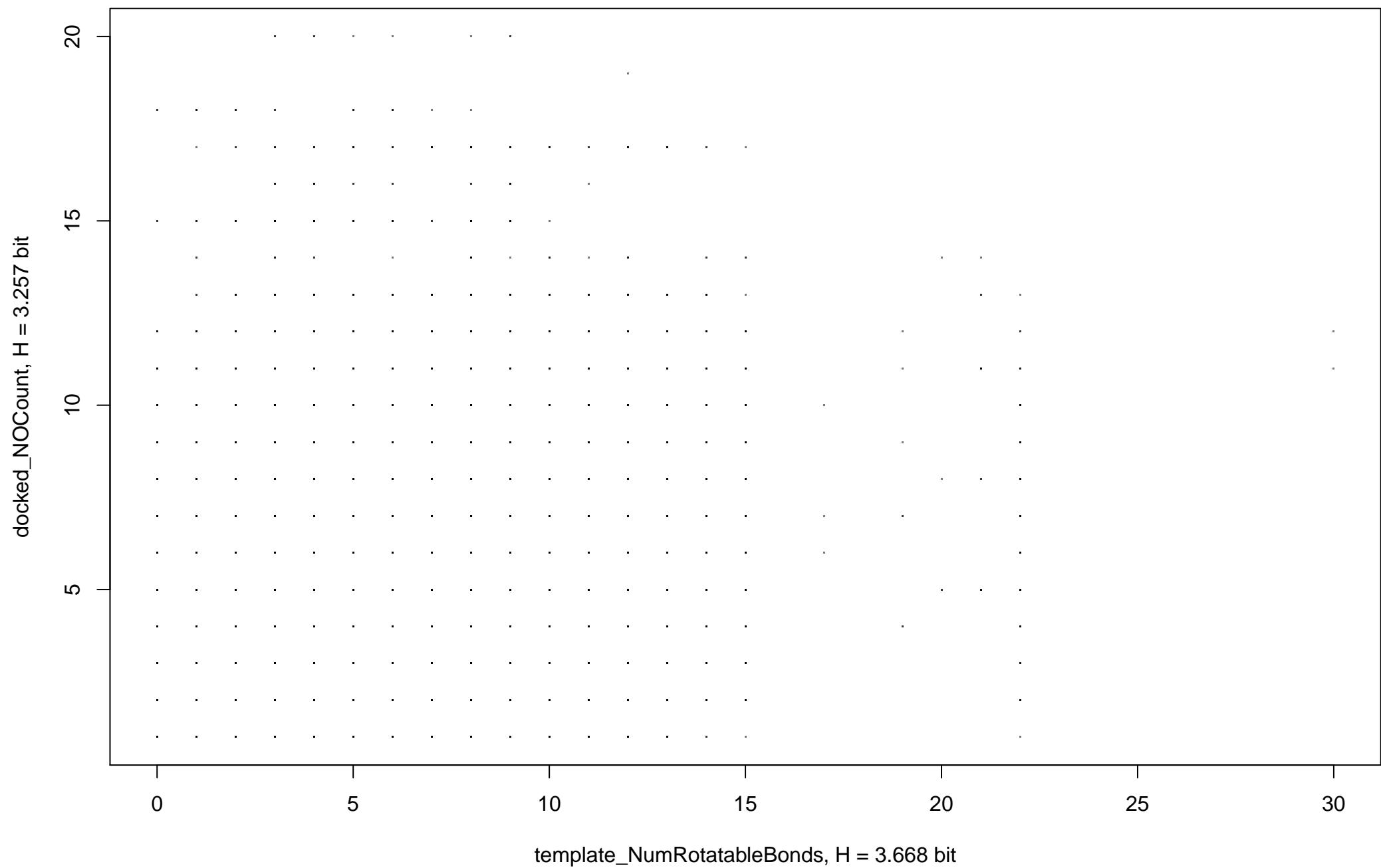
mcs_template_NumRotatableBonds–binrmsd, MI = 0.01819 bit, normMI = 0.01598



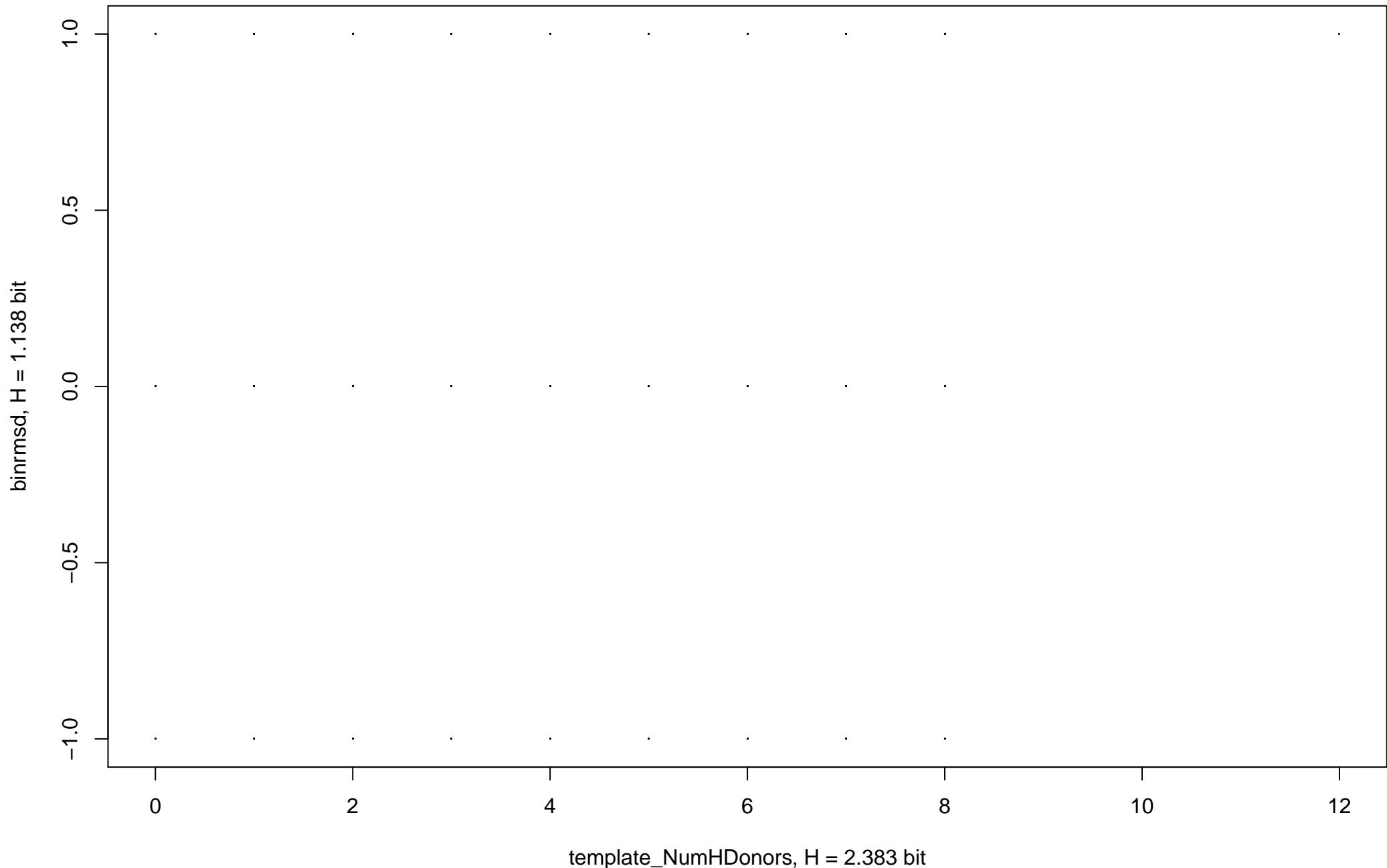
template_NumHeteroAtoms-docked_RingCount, MI = 0.03803 bit, normMI = 0.01592



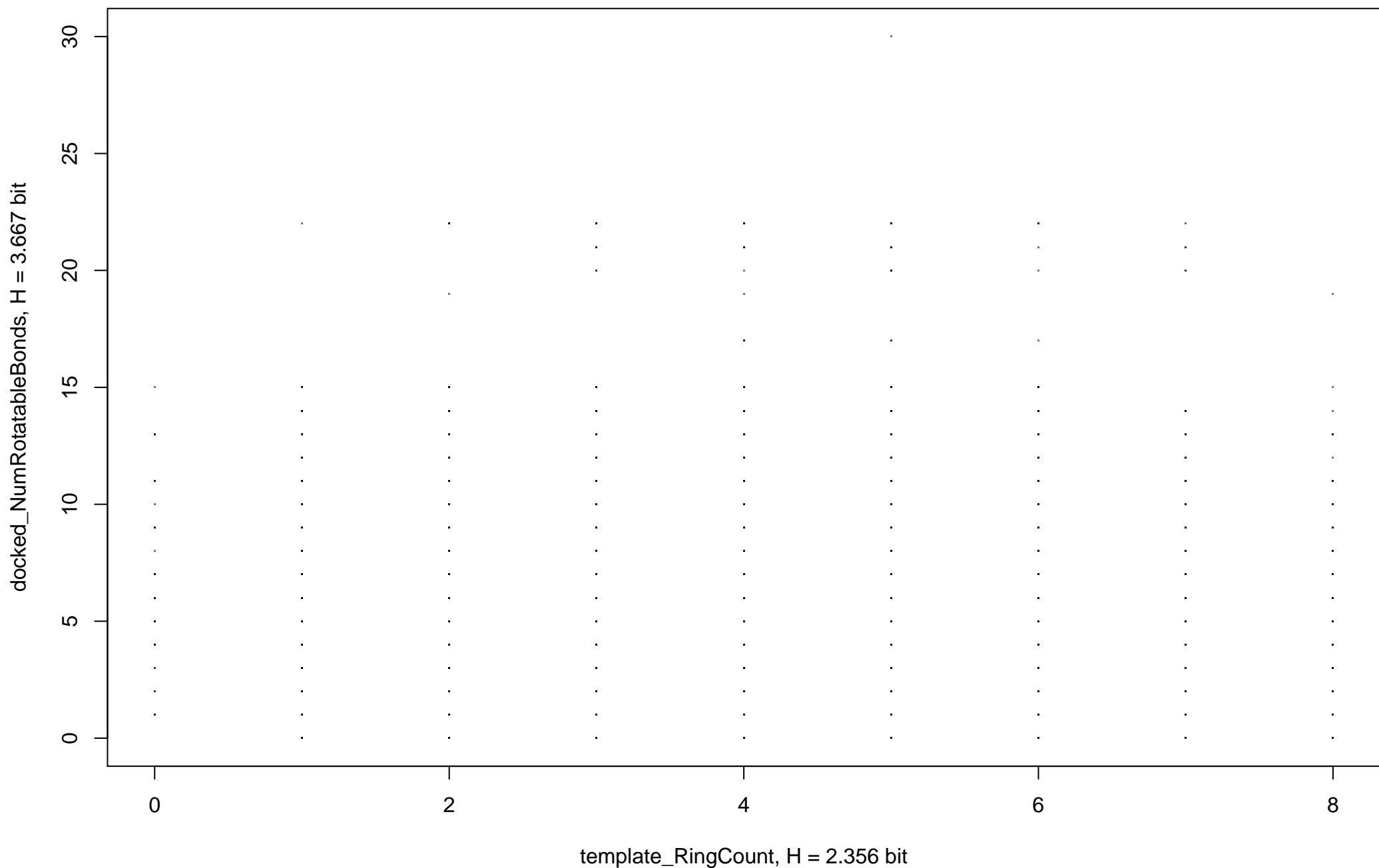
template_NumRotatableBonds-docked_NOCount, MI = 0.05183 bit, normMI = 0.01592



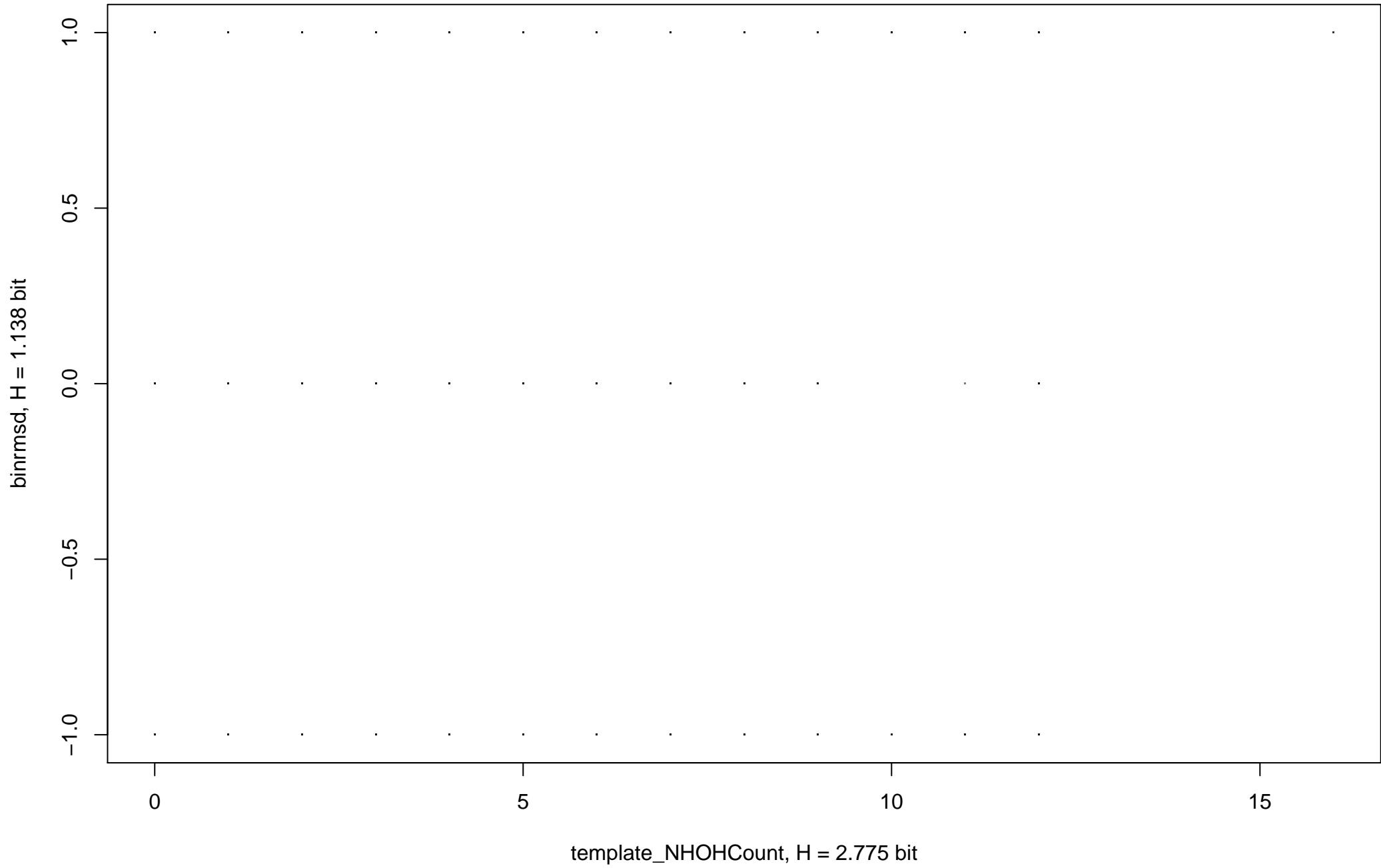
template_NuHDonors-binrmsd, MI = 0.01811 bit, normMI = 0.01591



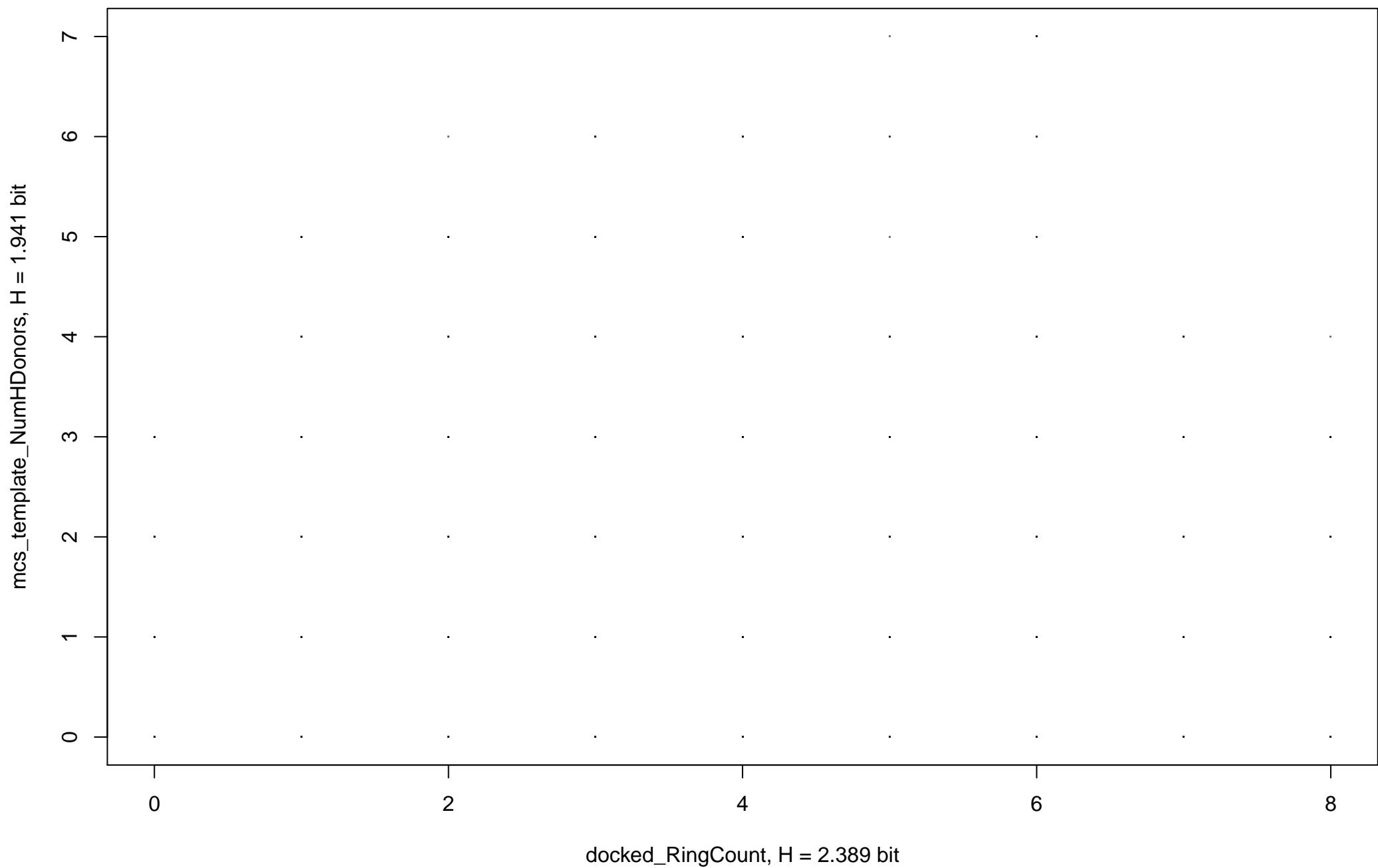
template_RingCount-docked_NumRotatableBonds, MI = 0.03745 bit, normMI = 0.0159



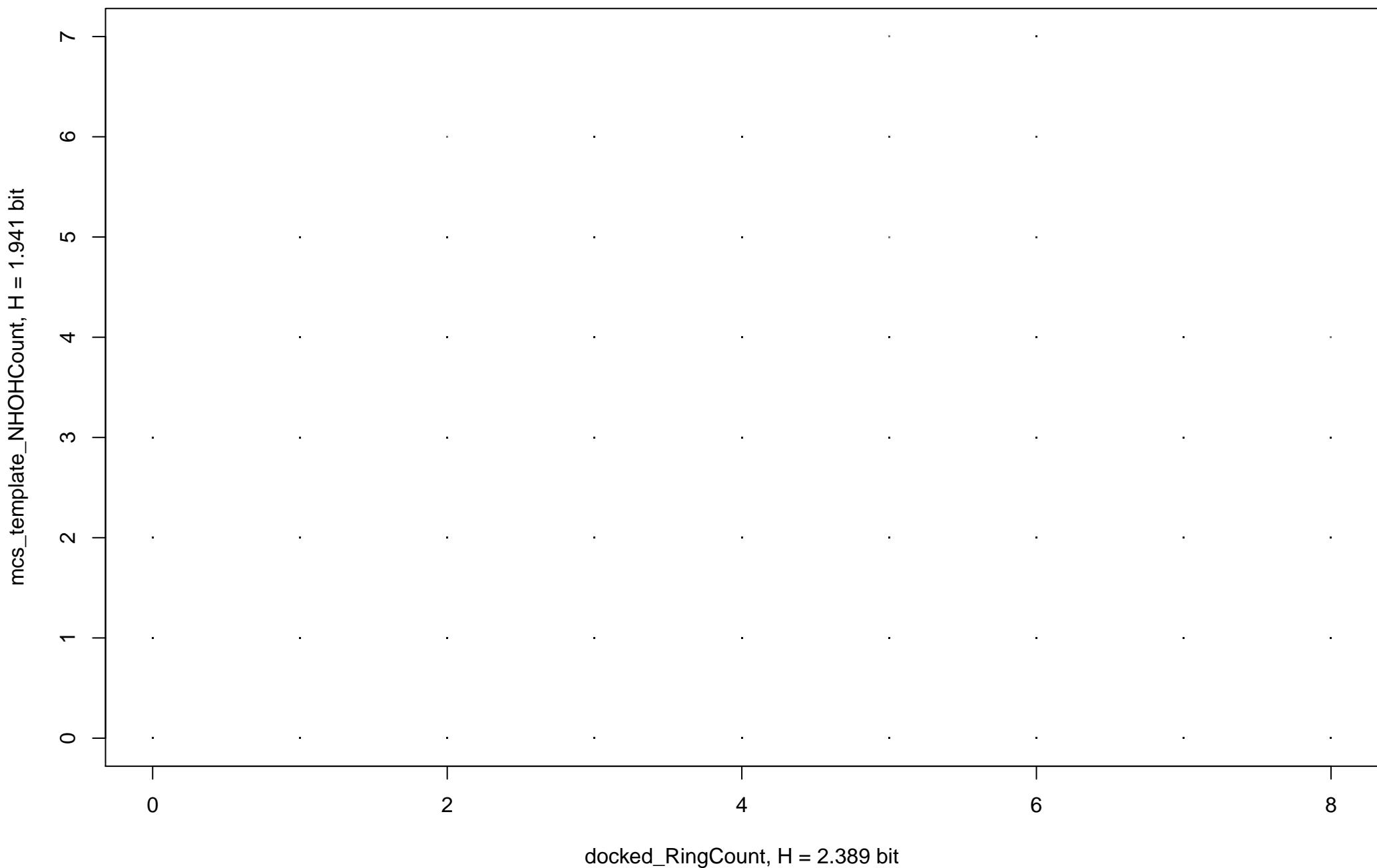
template_NHOHCount-binrmsd, MI = 0.01764 bit, normMI = 0.0155



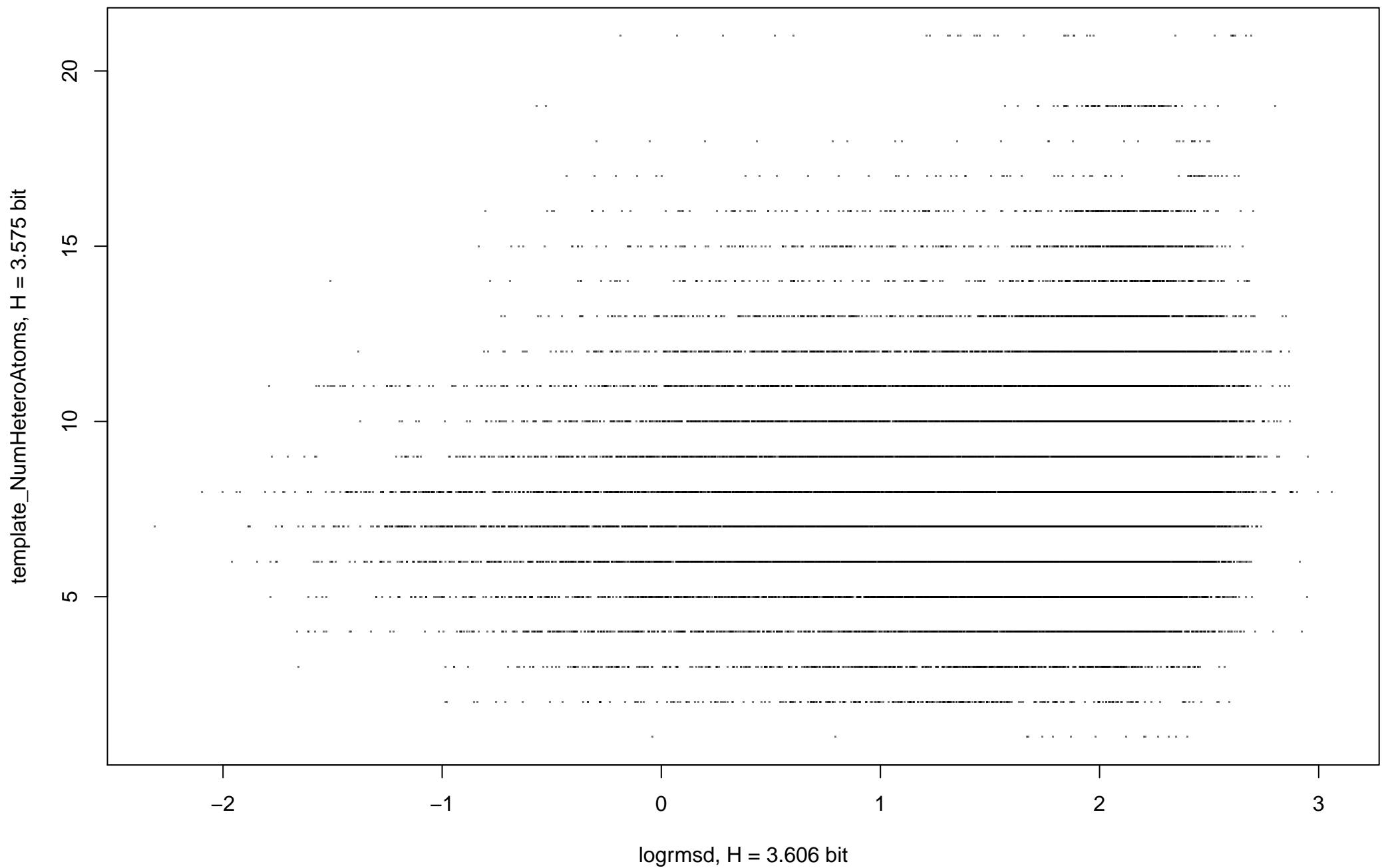
docked_RingCount-mcs_template_NumHDonors, MI = 0.02989 bit, normMI = 0.0154



docked_RingCount-mcs_template_NHOHCount, MI = 0.02988 bit, normMI = 0.01539

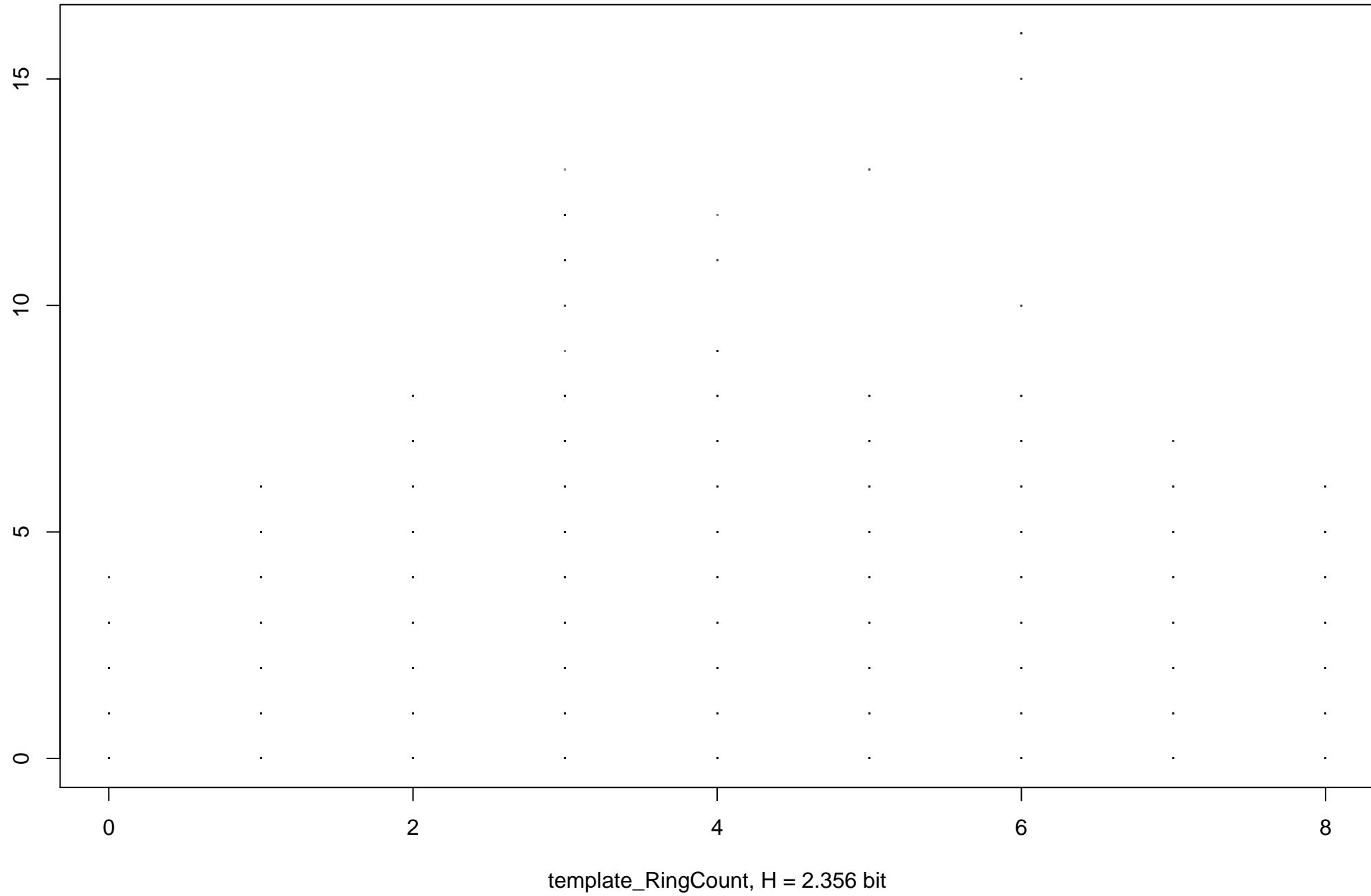


logrmsd-template_NumHeteroAtoms, MI = 0.05493 bit, normMI = 0.01537

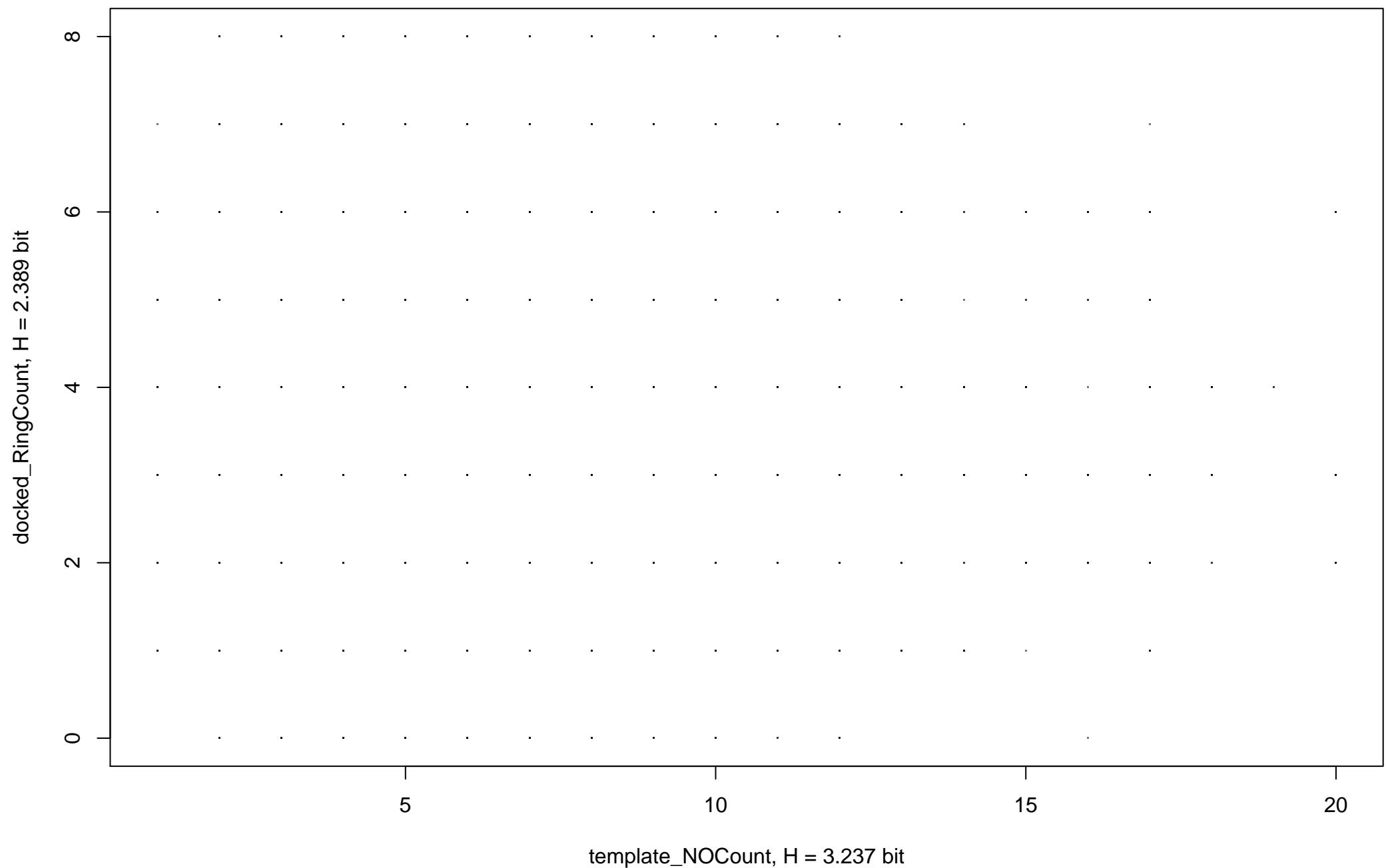


template_RingCount-mcs_template_NumHAcceptors, MI = 0.0357 bit, normMI = 0.01515

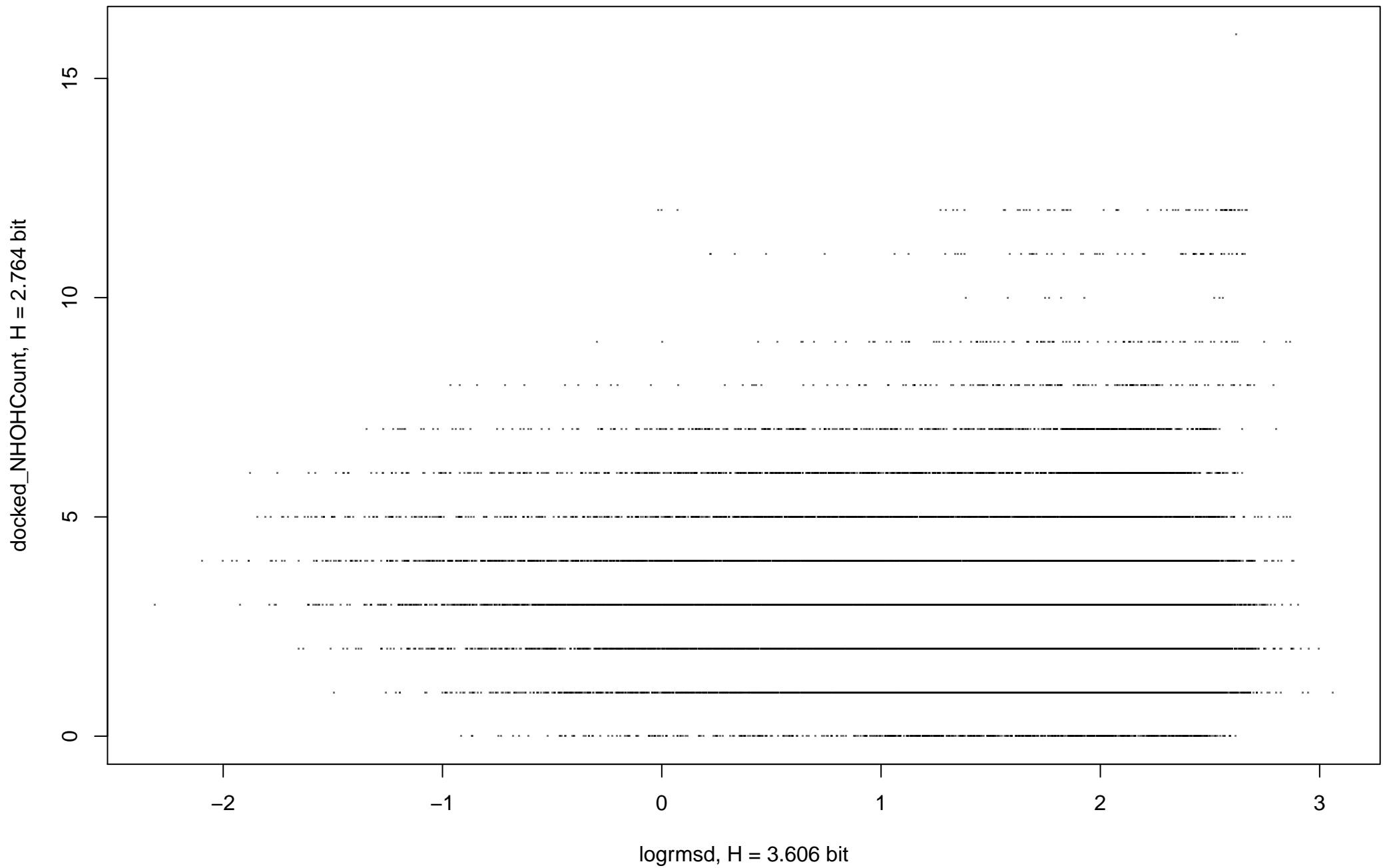
mcs_template_NumHAcceptors, H = 2.488 bit



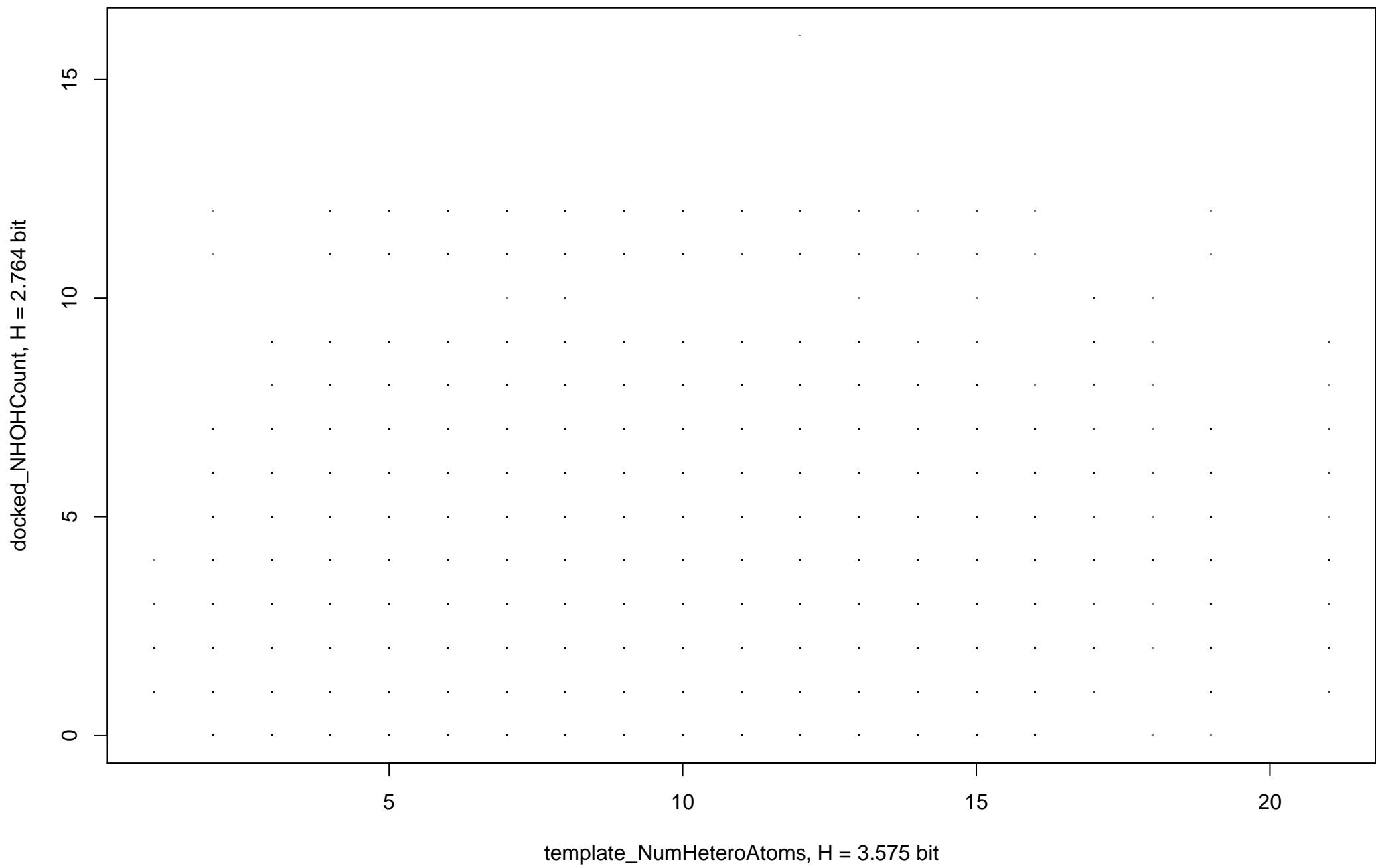
template_NOCount-docked_RingCount, MI = 0.03594 bit, normMI = 0.01504



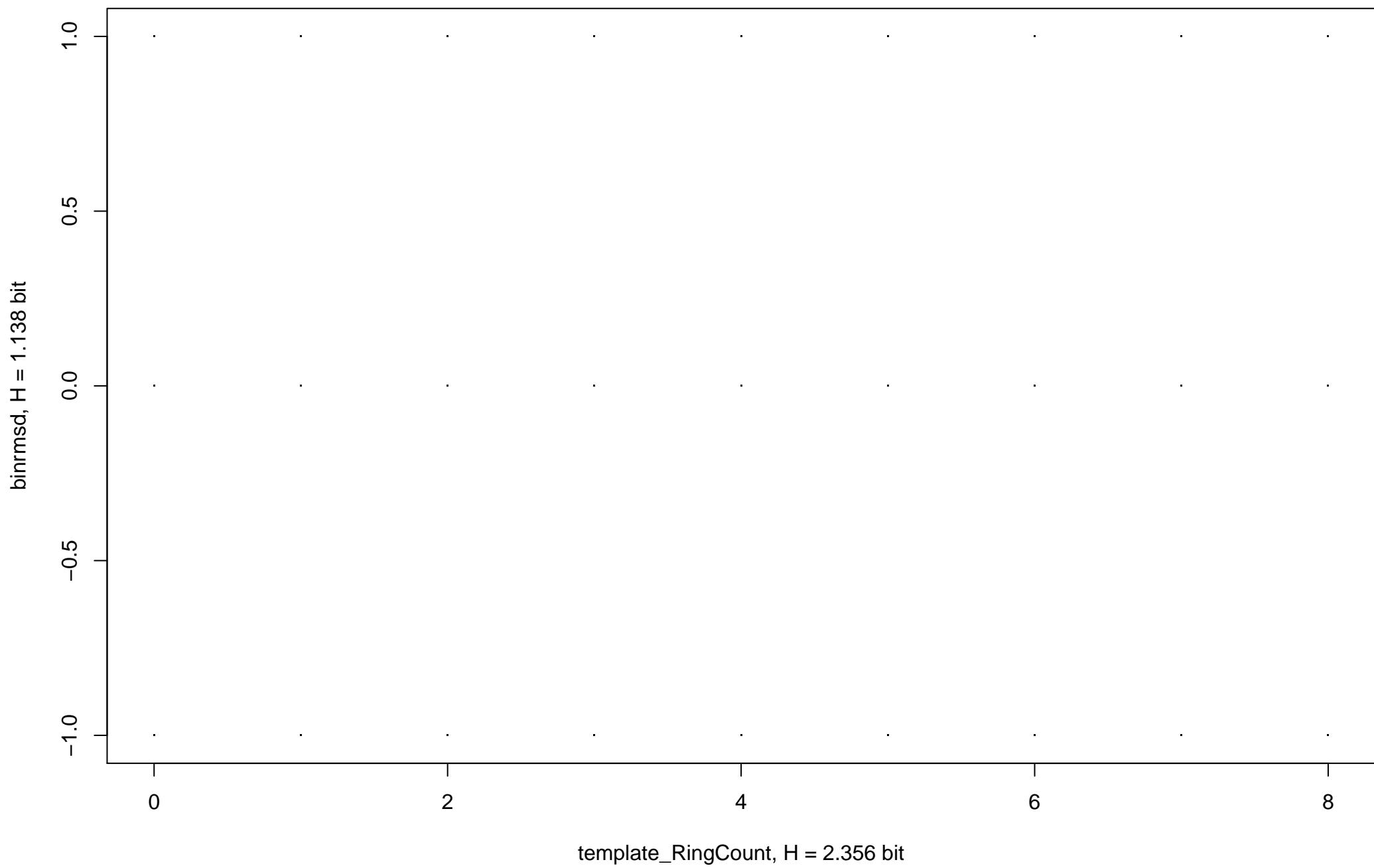
logrmsd-docked_NHOHCount, MI = 0.0411 bit, normMI = 0.01487



template_NumHeteroAtoms-docked_NHOHCount, MI = 0.04107 bit, normMI = 0.01486

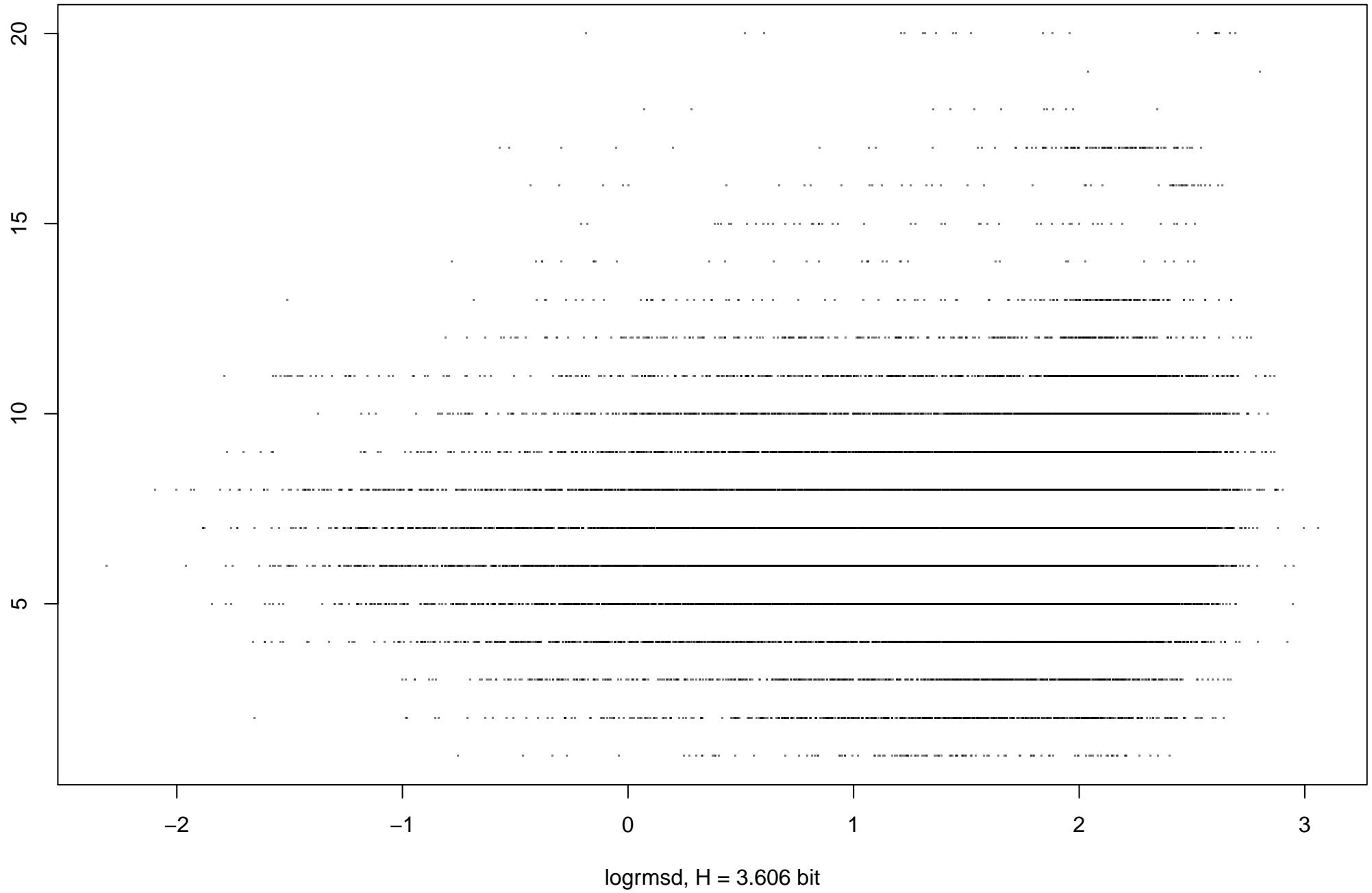


template_RingCount-binrmsd, MI = 0.0168 bit, normMI = 0.01476

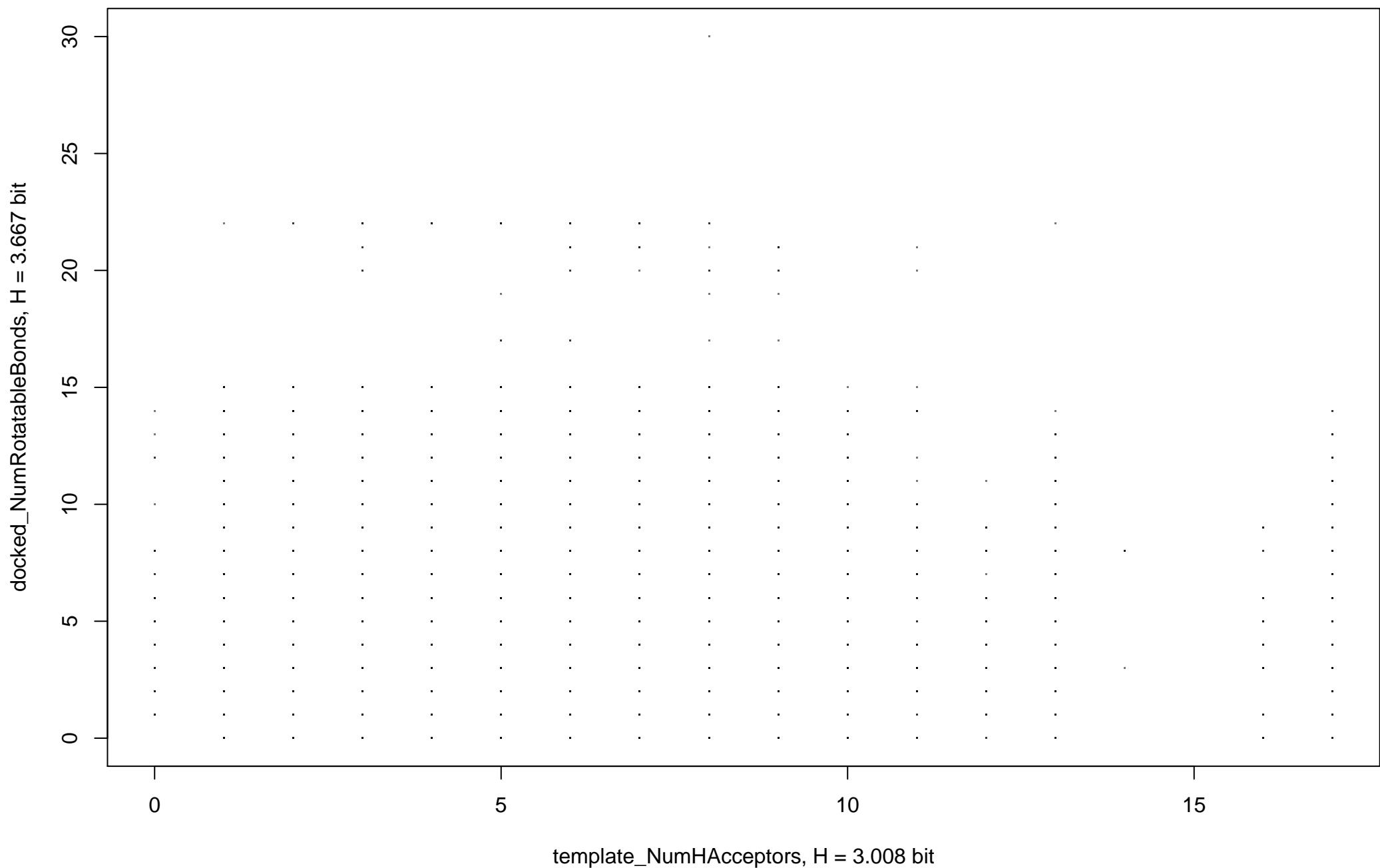


logrmsd-template_NOCount, MI = 0.04728 bit, normMI = 0.01461

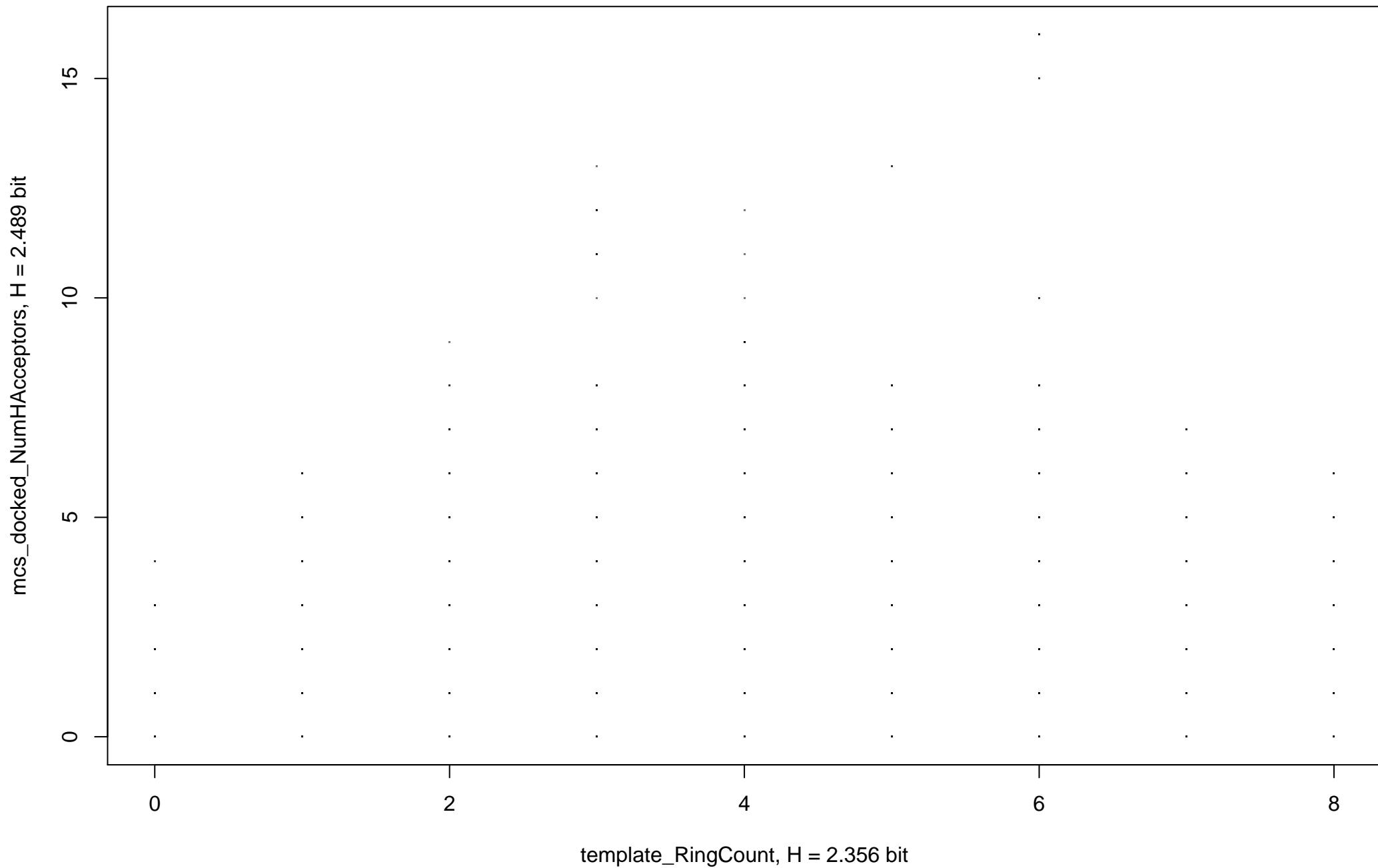
template_NOCount, $H = 3.237$ bit



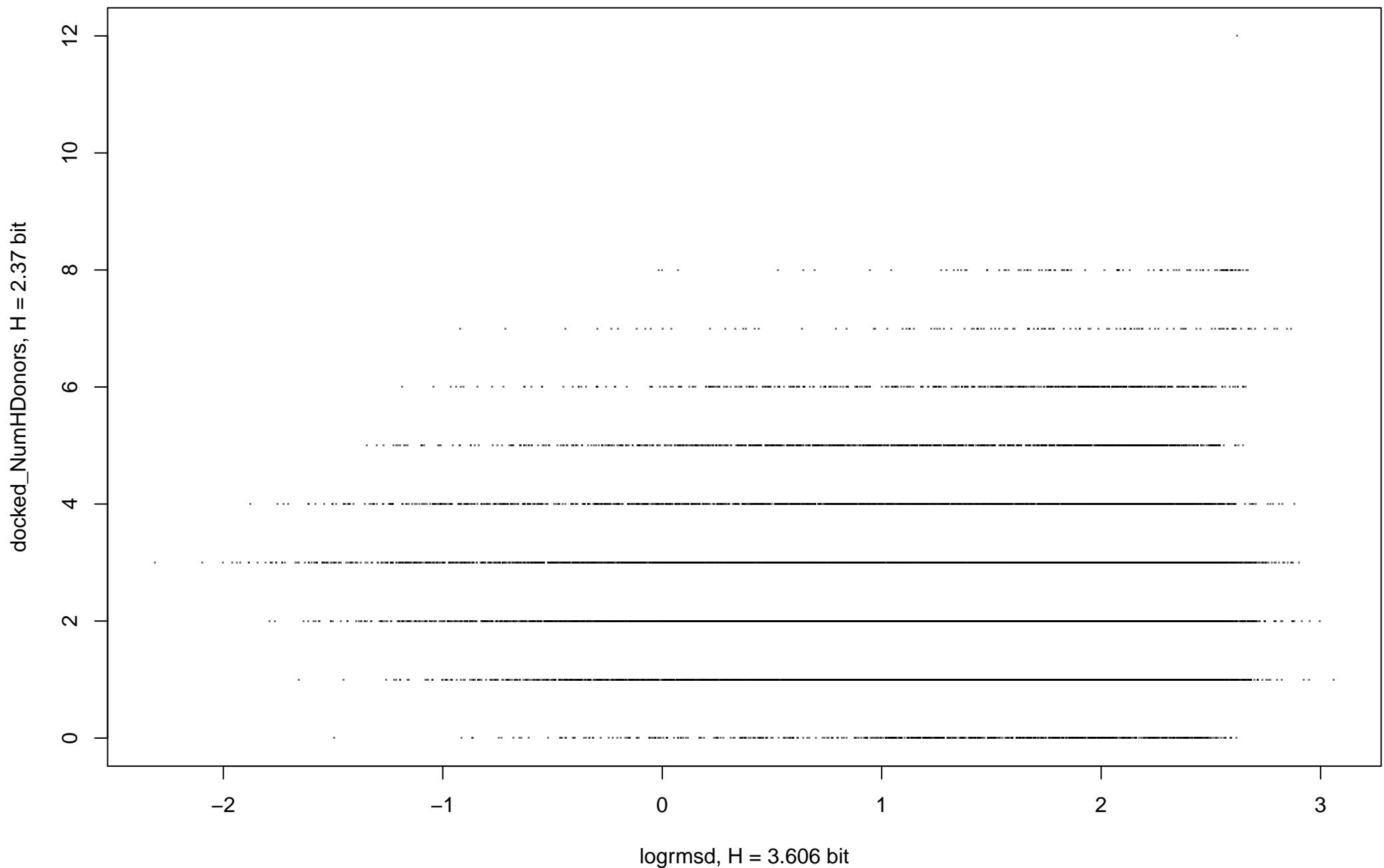
template_NumHAcceptors-docked_NumRotatableBonds, MI = 0.04391 bit, normMI = 0.0146



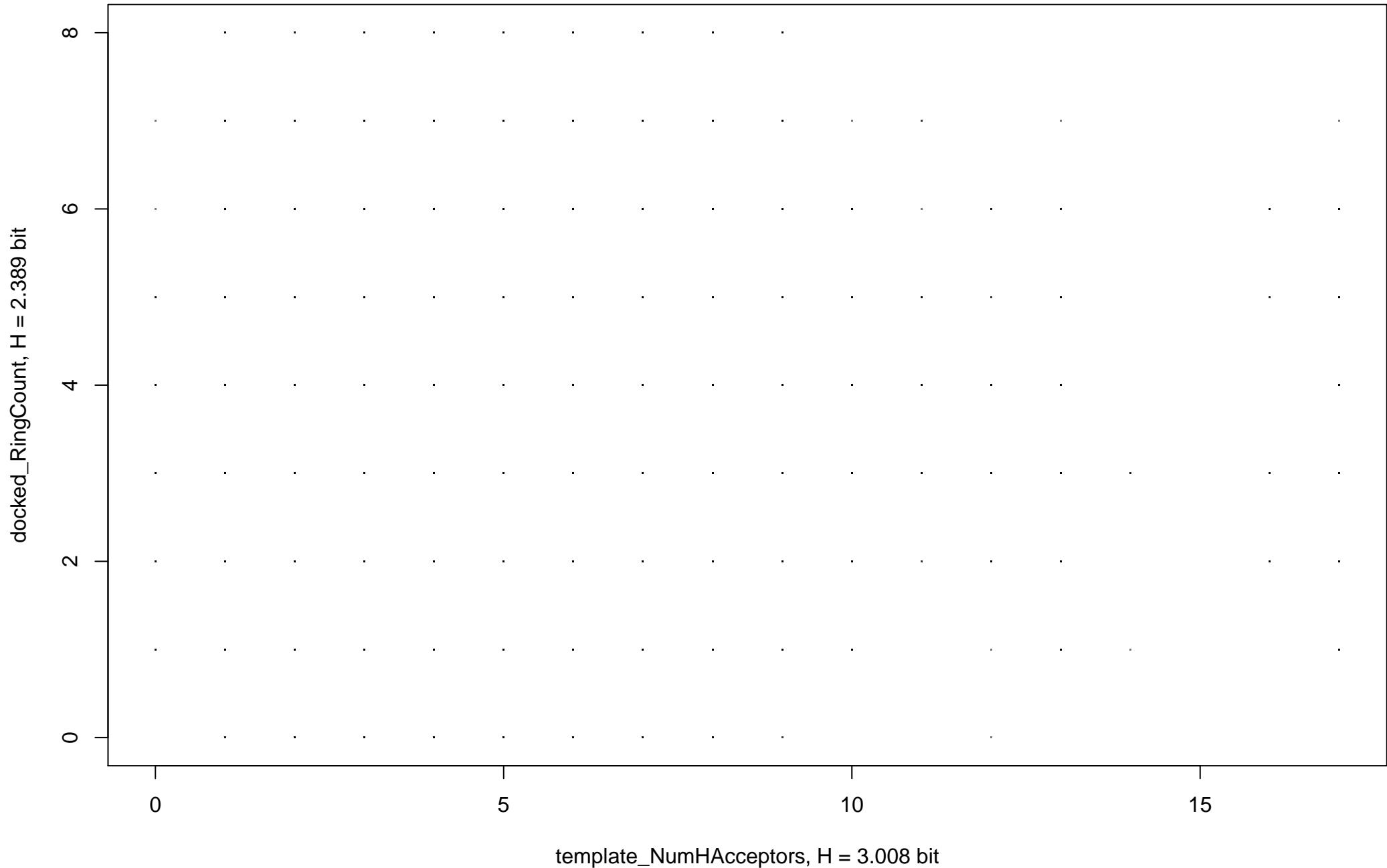
template_RingCount-mcs_docked_NumHAcceptors, MI = 0.03439 bit, normMI = 0.0146



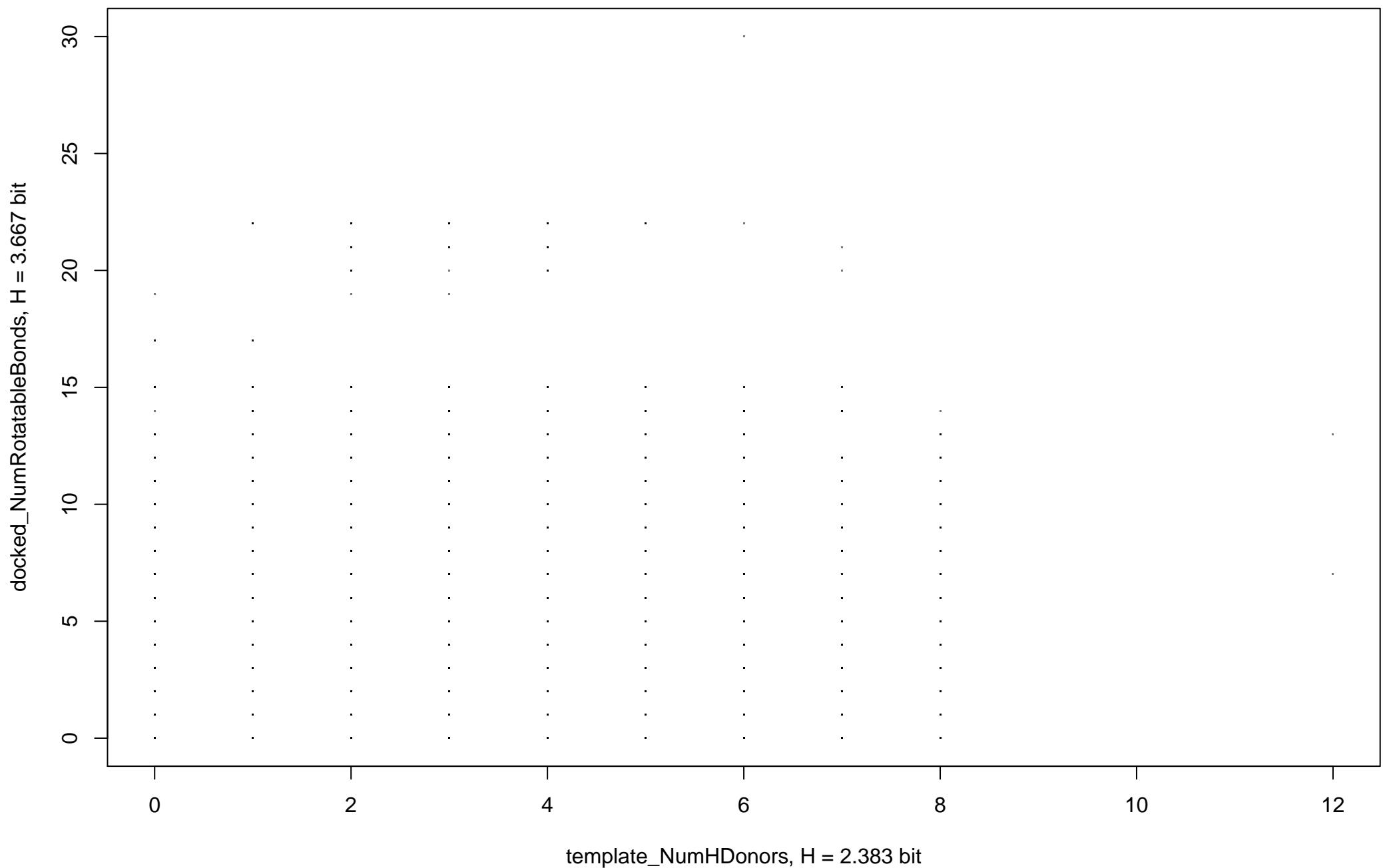
logrmsd-docked_NumHDonors, MI = 0.03417 bit, normMI = 0.01441



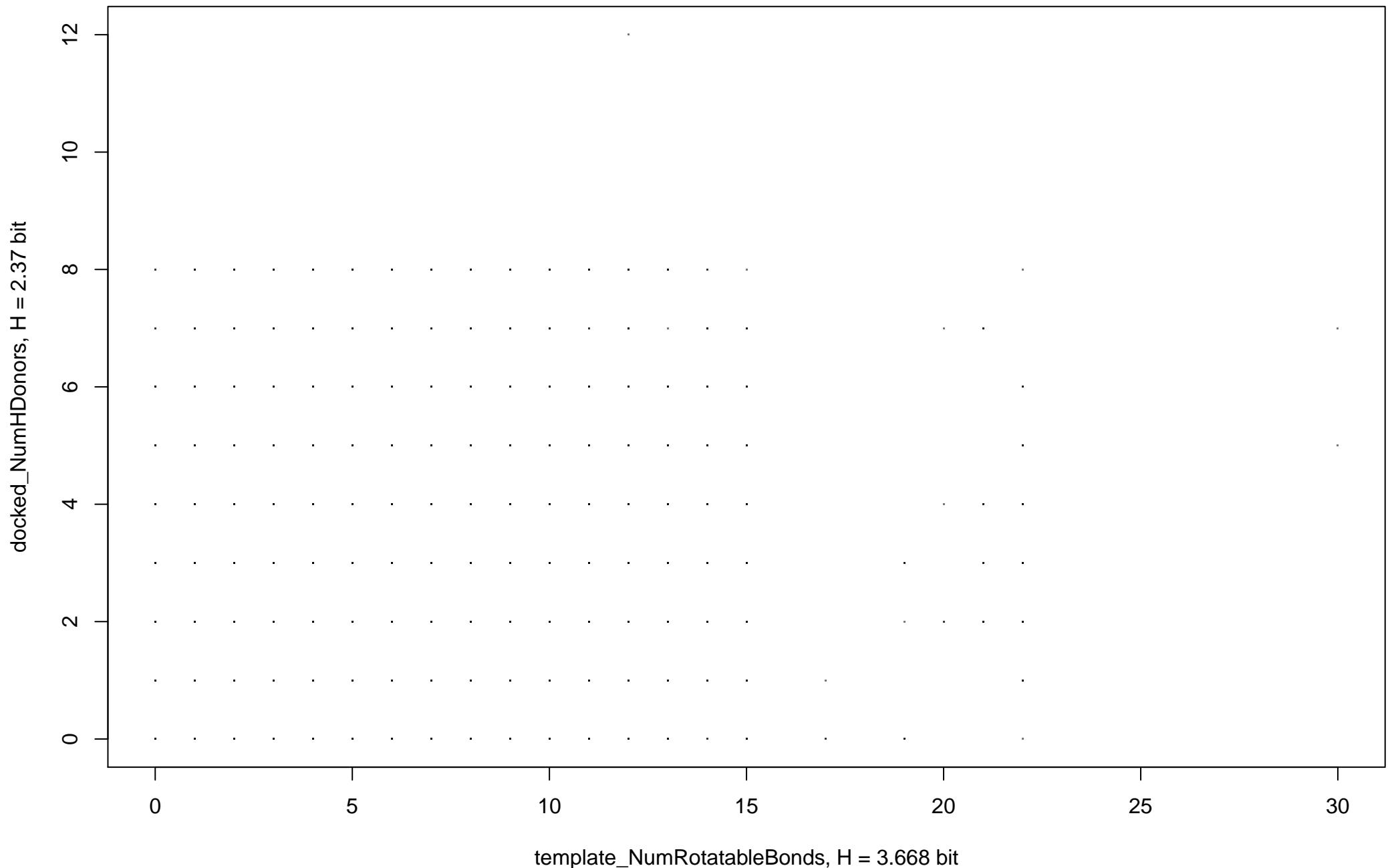
template_NumHAcceptors-docked_RingCount, MI = 0.03402 bit, normMI = 0.01424



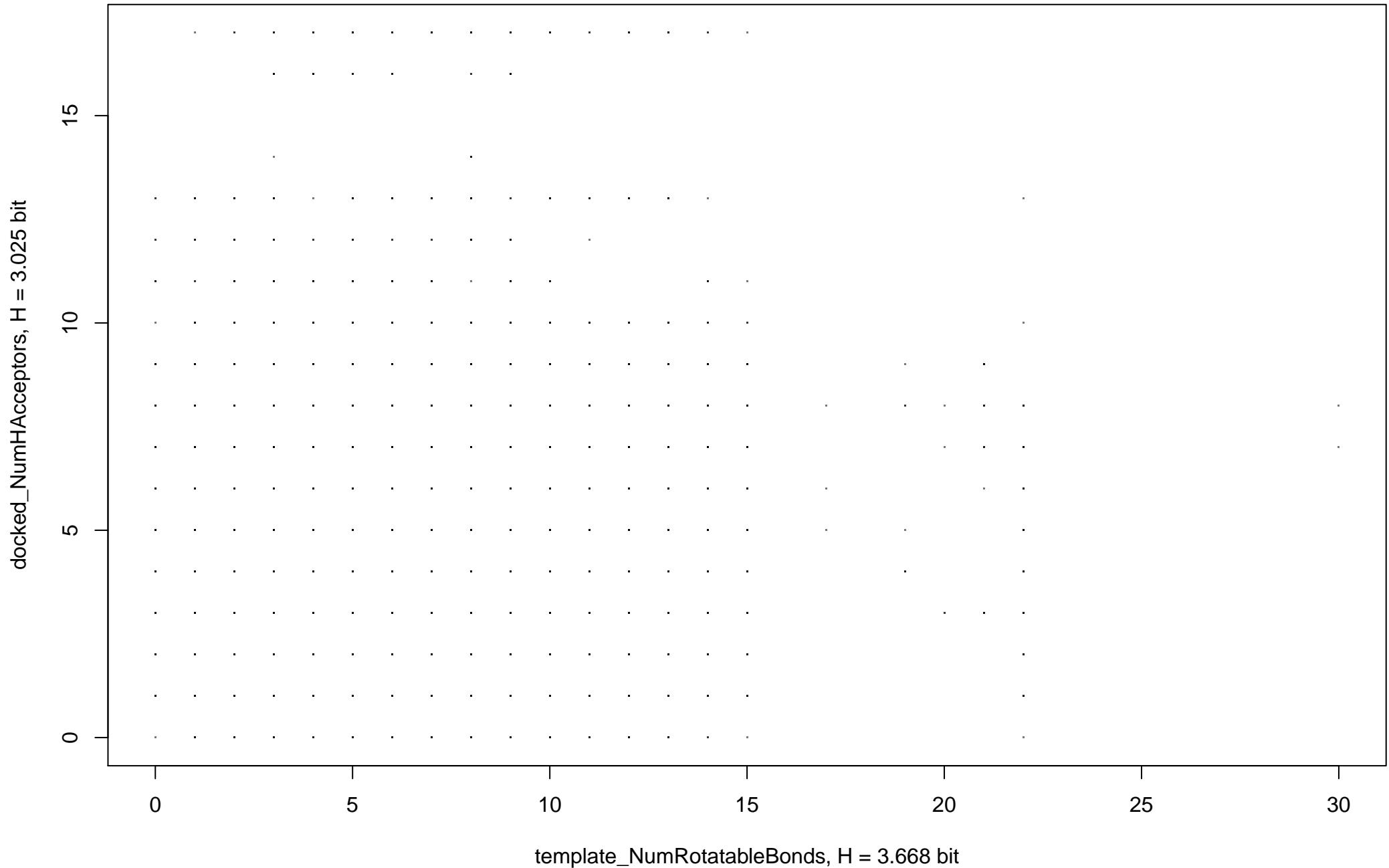
template_NumHDonors-docked_NumRotatableBonds, MI = 0.03379 bit, normMI = 0.01418



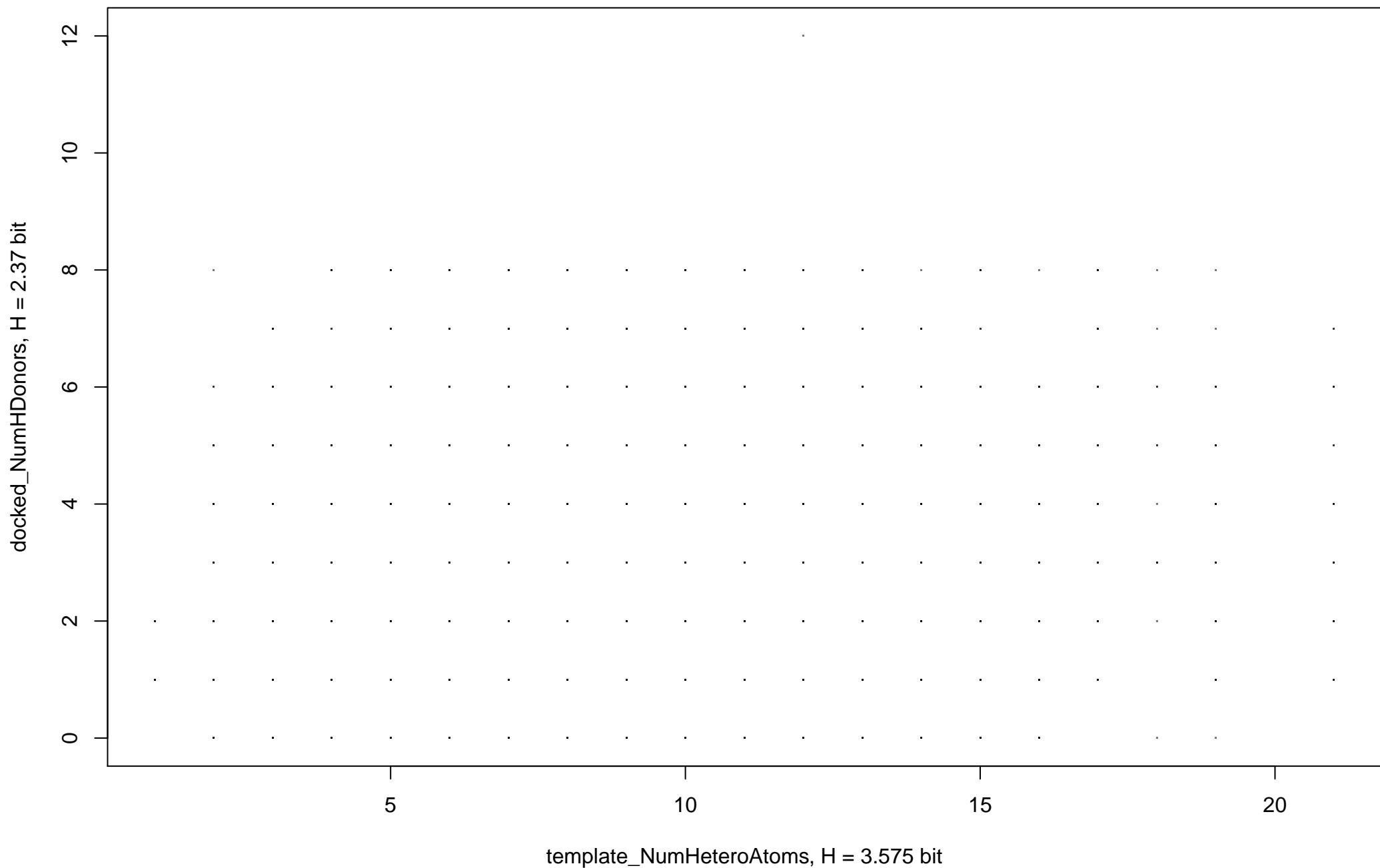
template_NumRotatableBonds-docked_NumHDonors, MI = 0.03316 bit, normMI = 0.01399



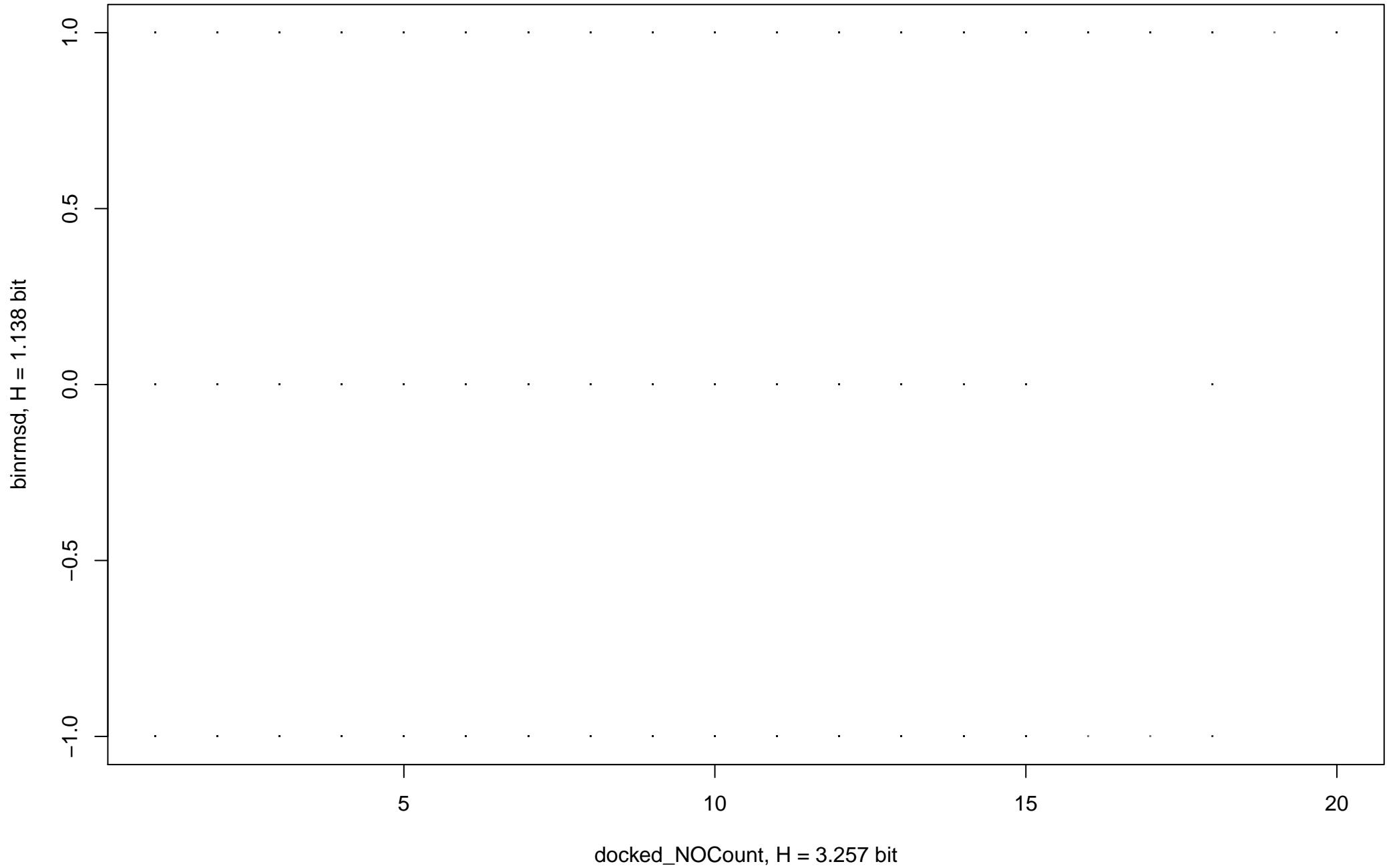
template_NumRotatableBonds-docked_NumHAcceptors, MI = 0.04213 bit, normMI = 0.01392



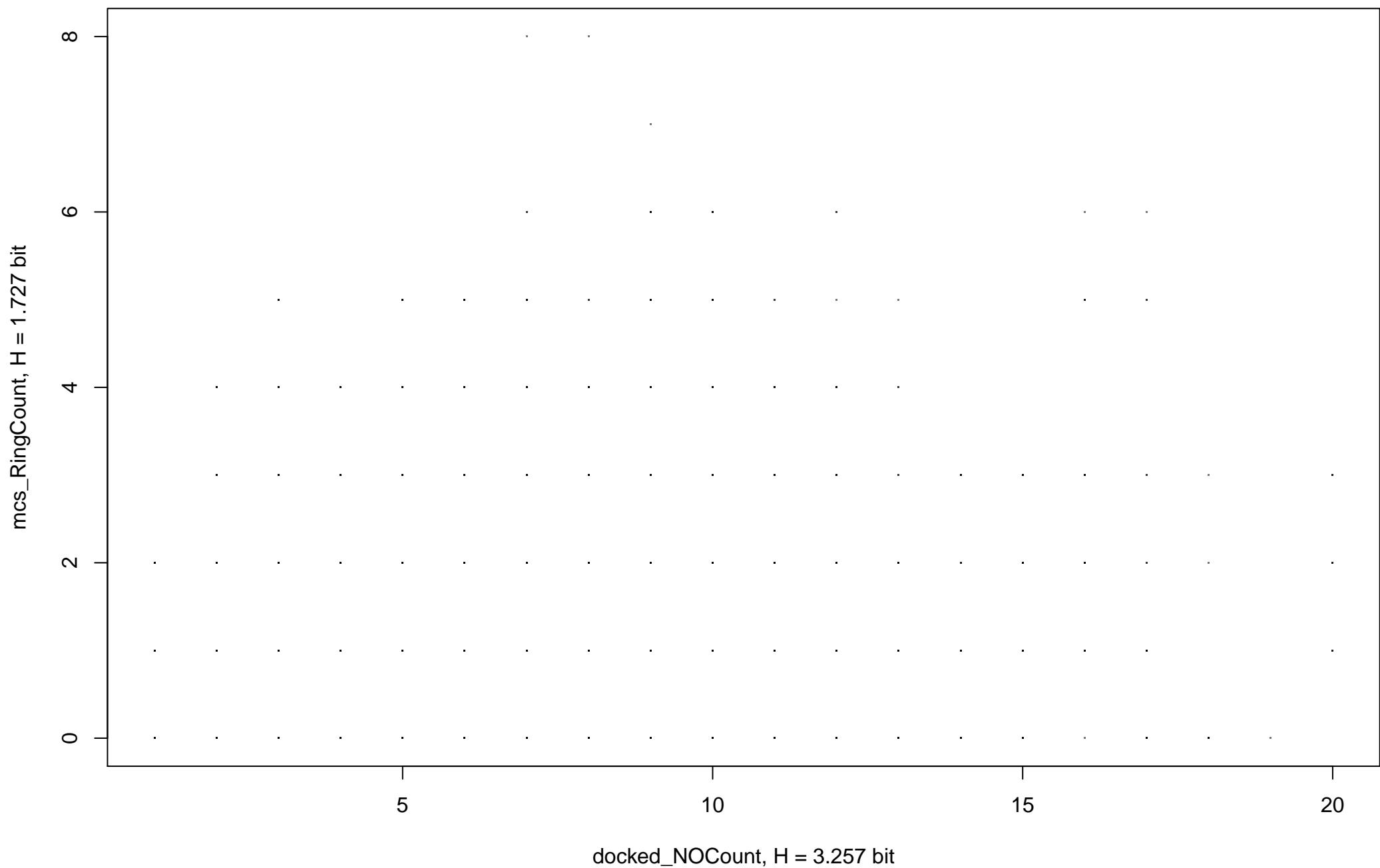
template_NumHeteroAtoms-docked_NumHDonors, MI = 0.033 bit, normMI = 0.01392



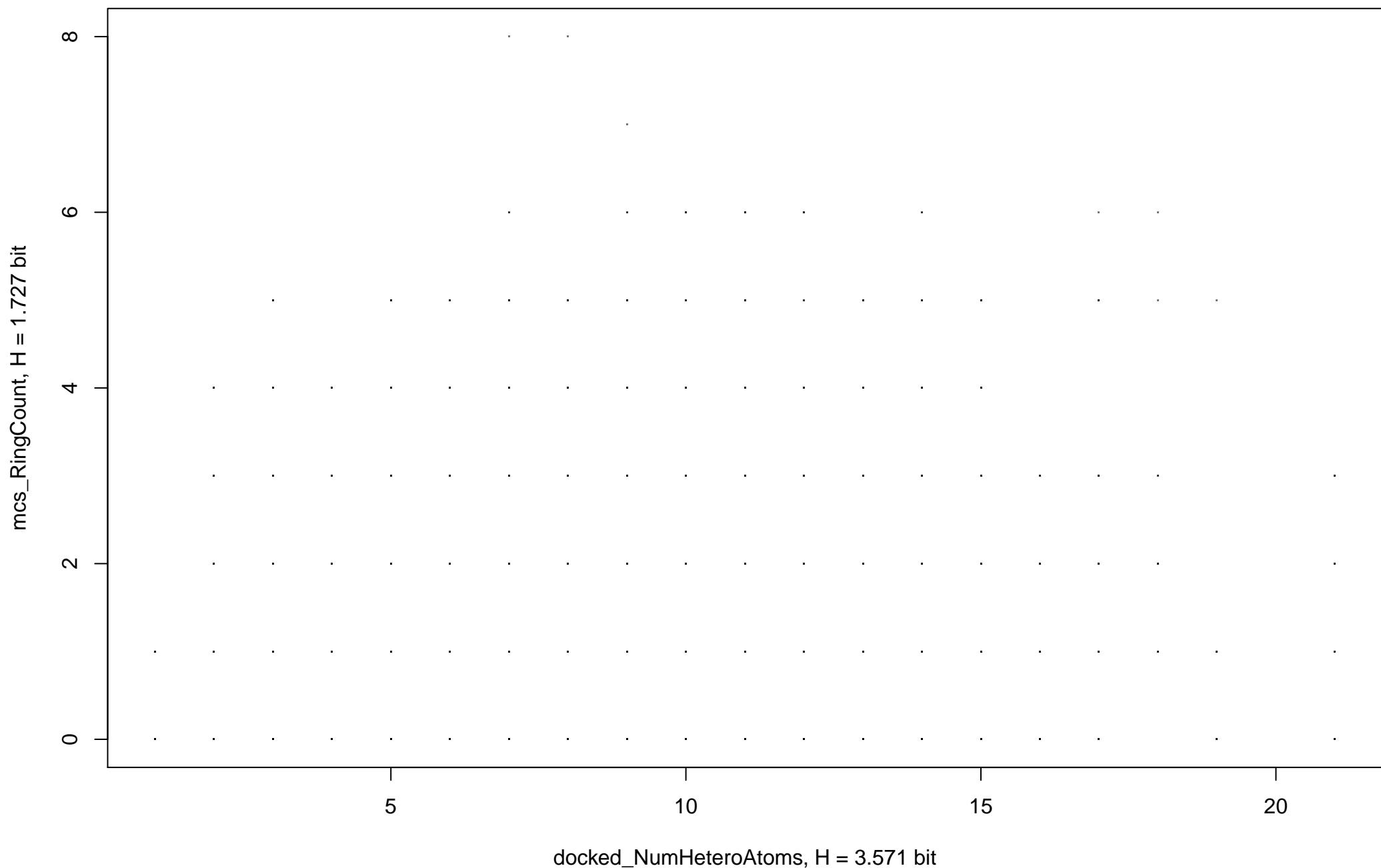
docked_NOCOUNT-binrmsd, MI = 0.01584 bit, normMI = 0.01391



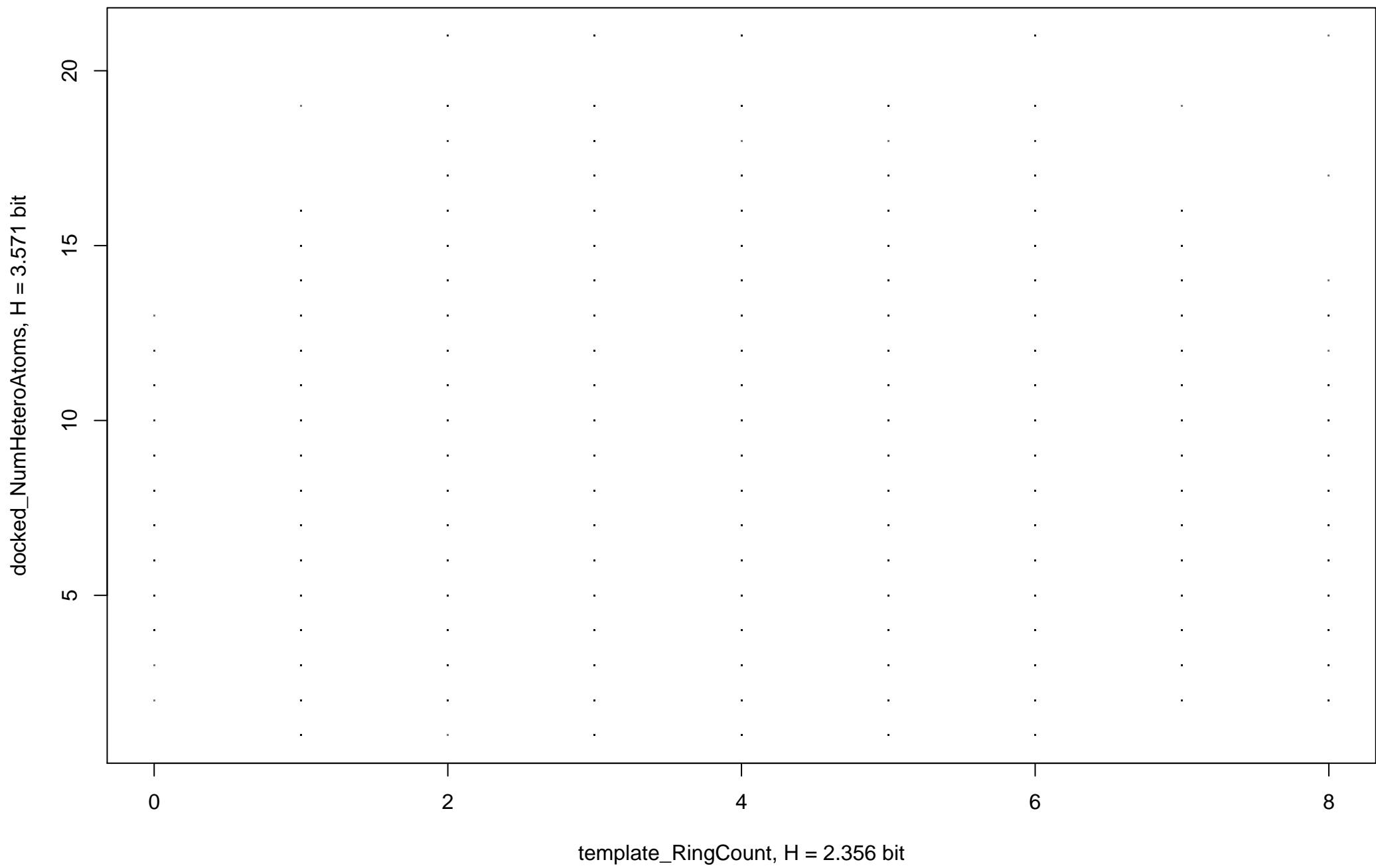
docked_NOCOUNT-mcs_RingCount, MI = 0.02385 bit, normMI = 0.01381



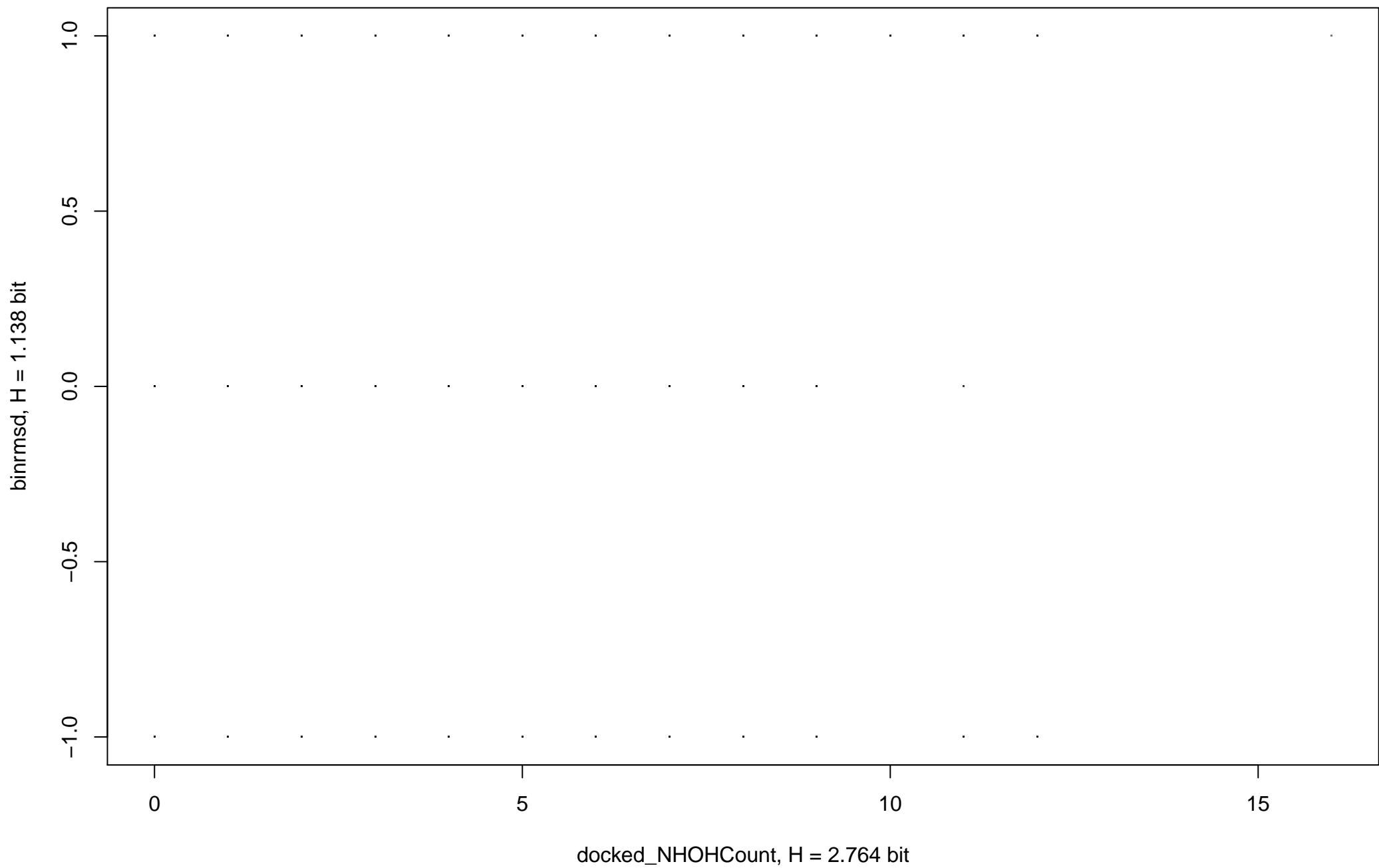
docked_NumHeteroAtoms-mcs_RingCount, MI = 0.02369 bit, normMI = 0.01372



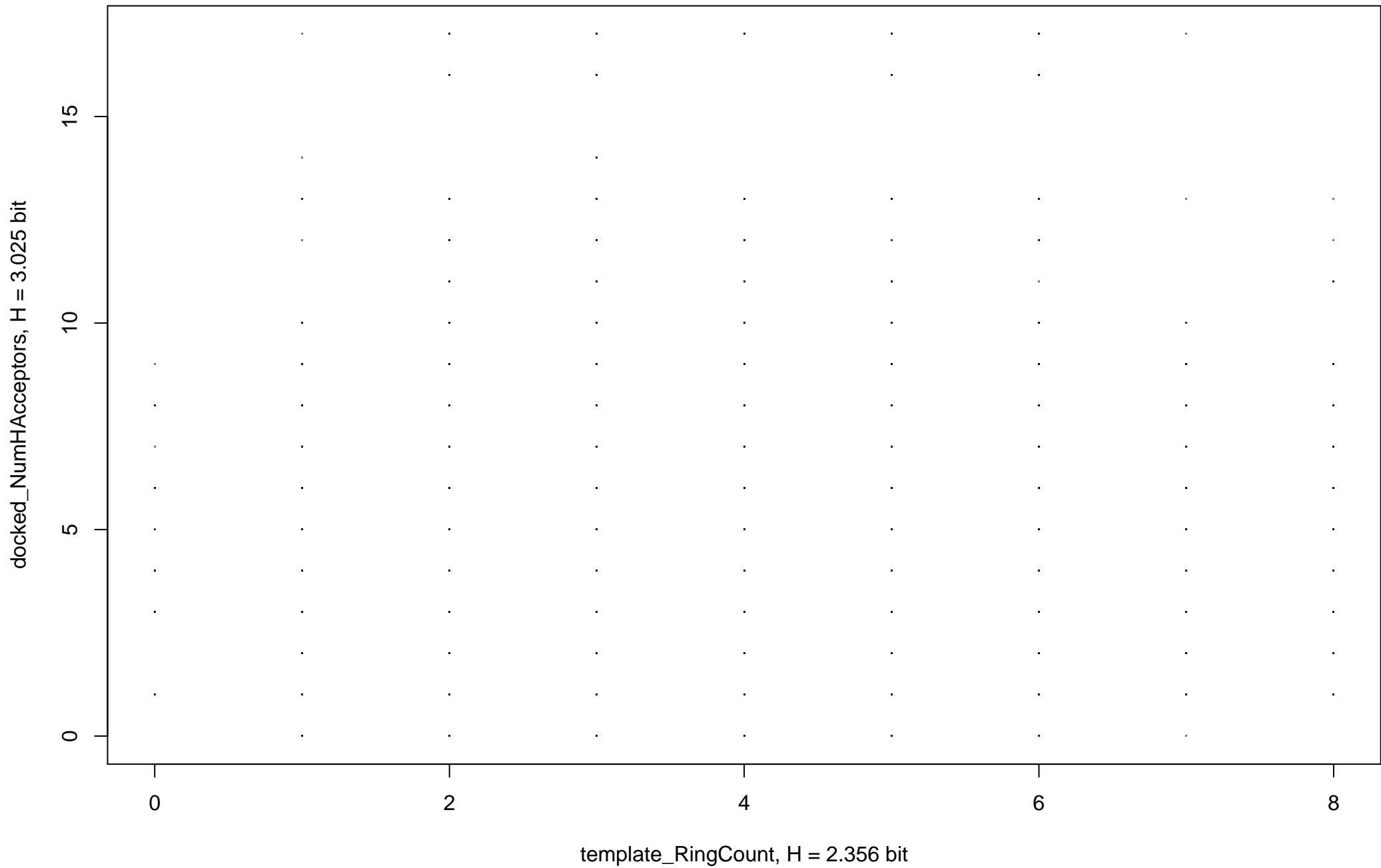
template_RingCount-docked_NumHeteroAtoms, MI = 0.03201 bit, normMI = 0.01359



docked_NHOHCount–binrmsd, MI = 0.01509 bit, normMI = 0.01326

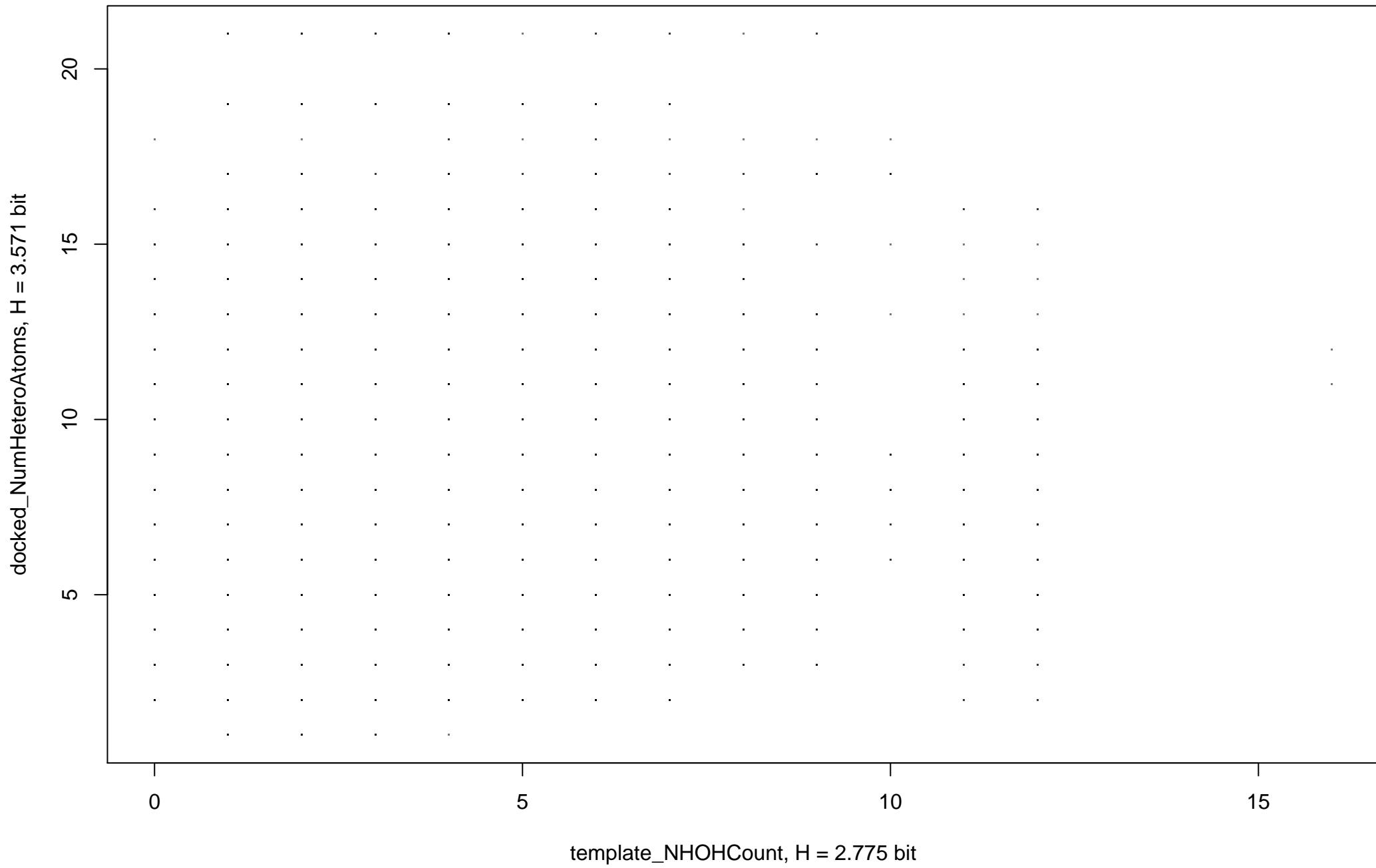


template_RingCount-docked_NumHAcceptors, MI = 0.03116 bit, normMI = 0.01323



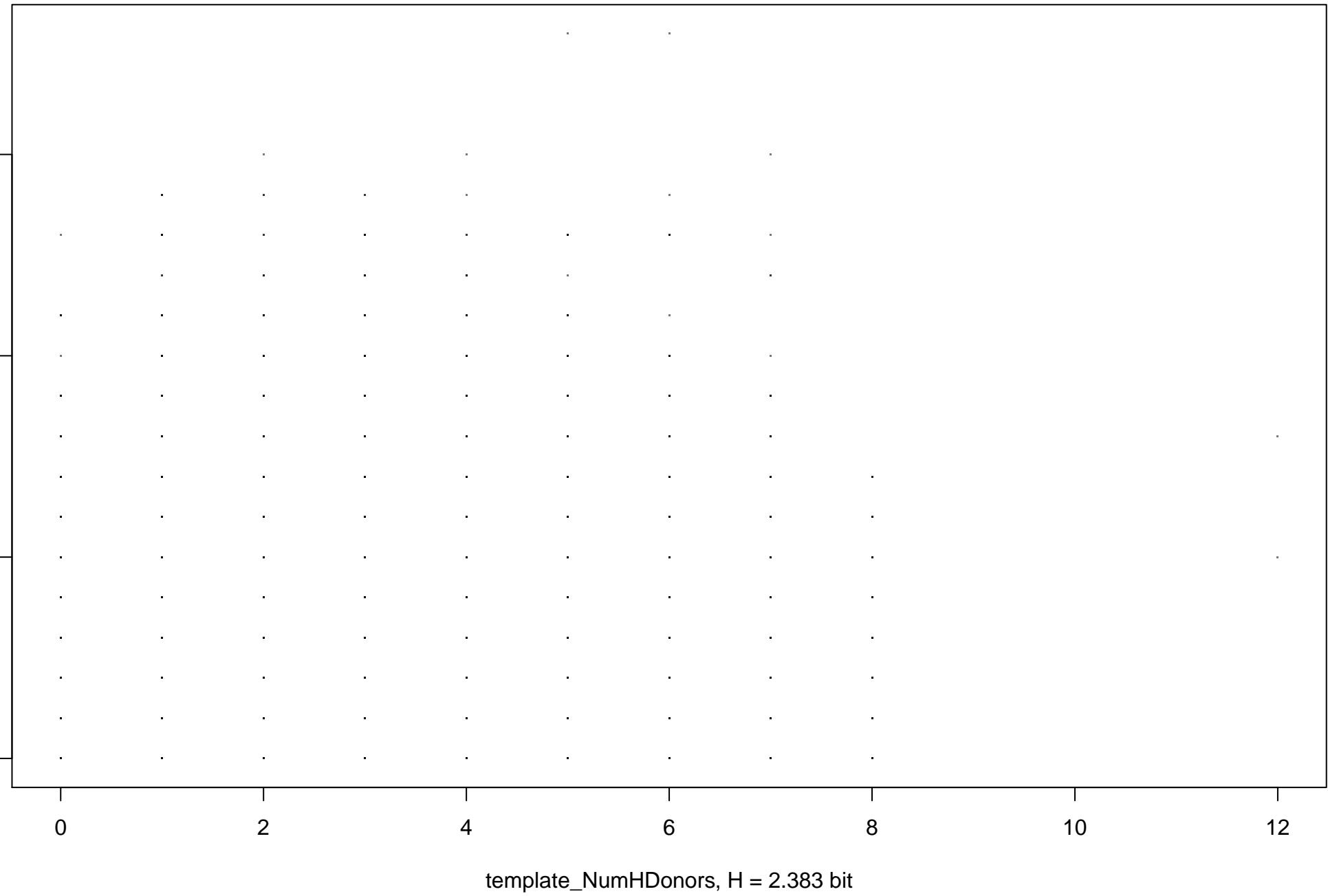
template_RingCount, H = 2.356 bit

template_NHOHCount-docked_NumHeteroAtoms, MI = 0.03671 bit, normMI = 0.01323

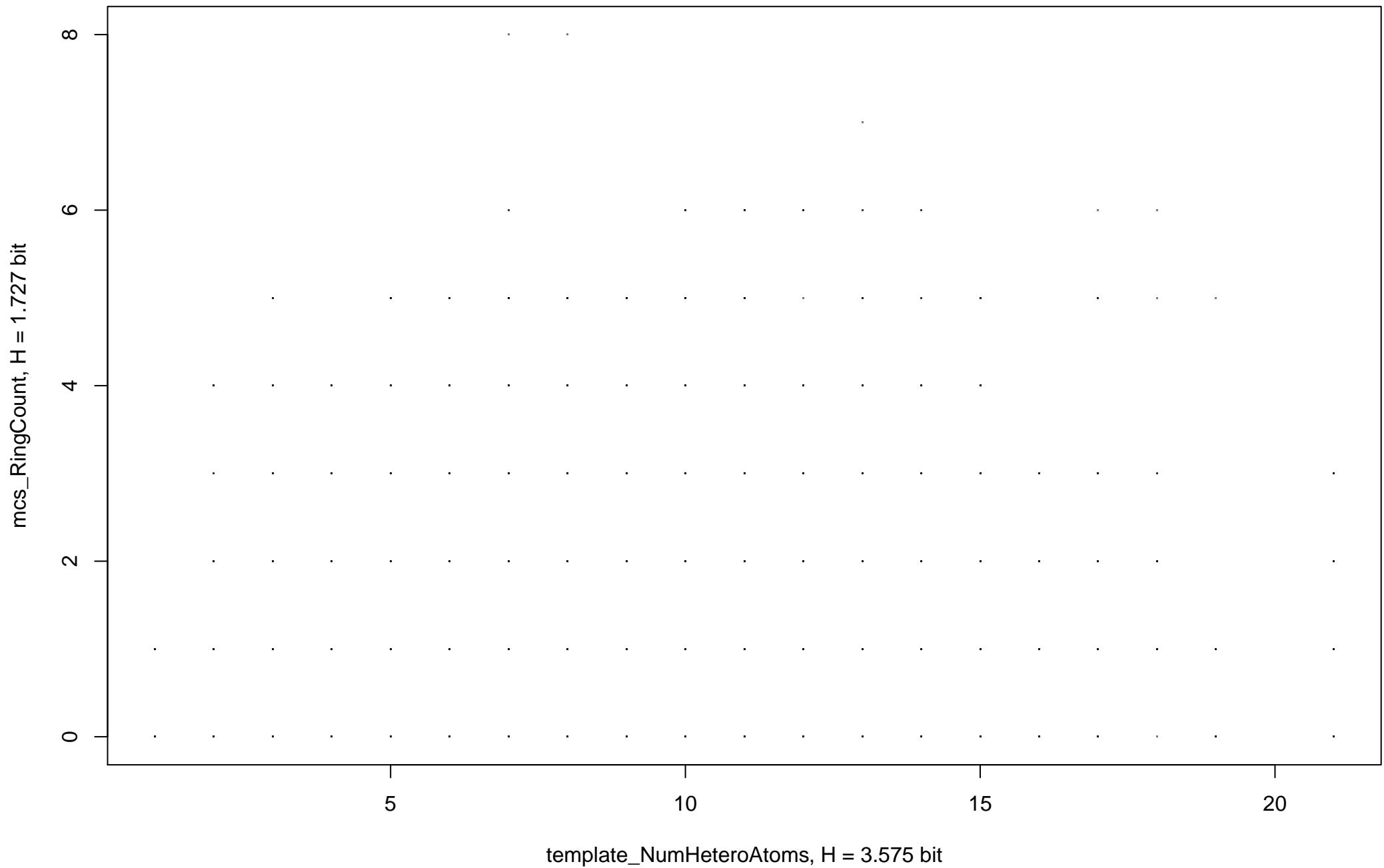


template_NumHDonors-mcs_docked_NumRotatableBonds, MI = 0.03112 bit, normMI = 0.01306

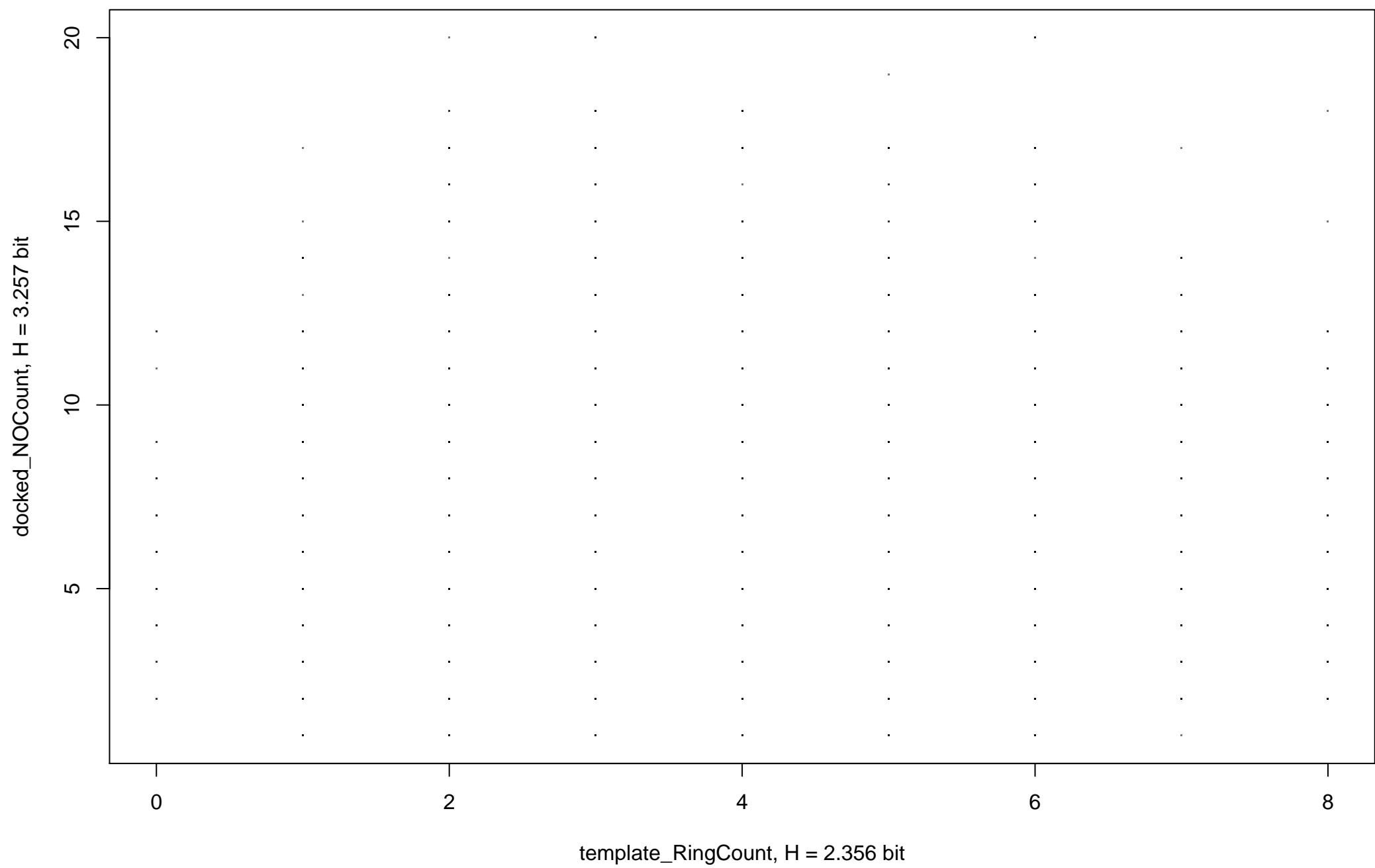
mcs_docked_NumRotatableBonds, H = 3.117 bit



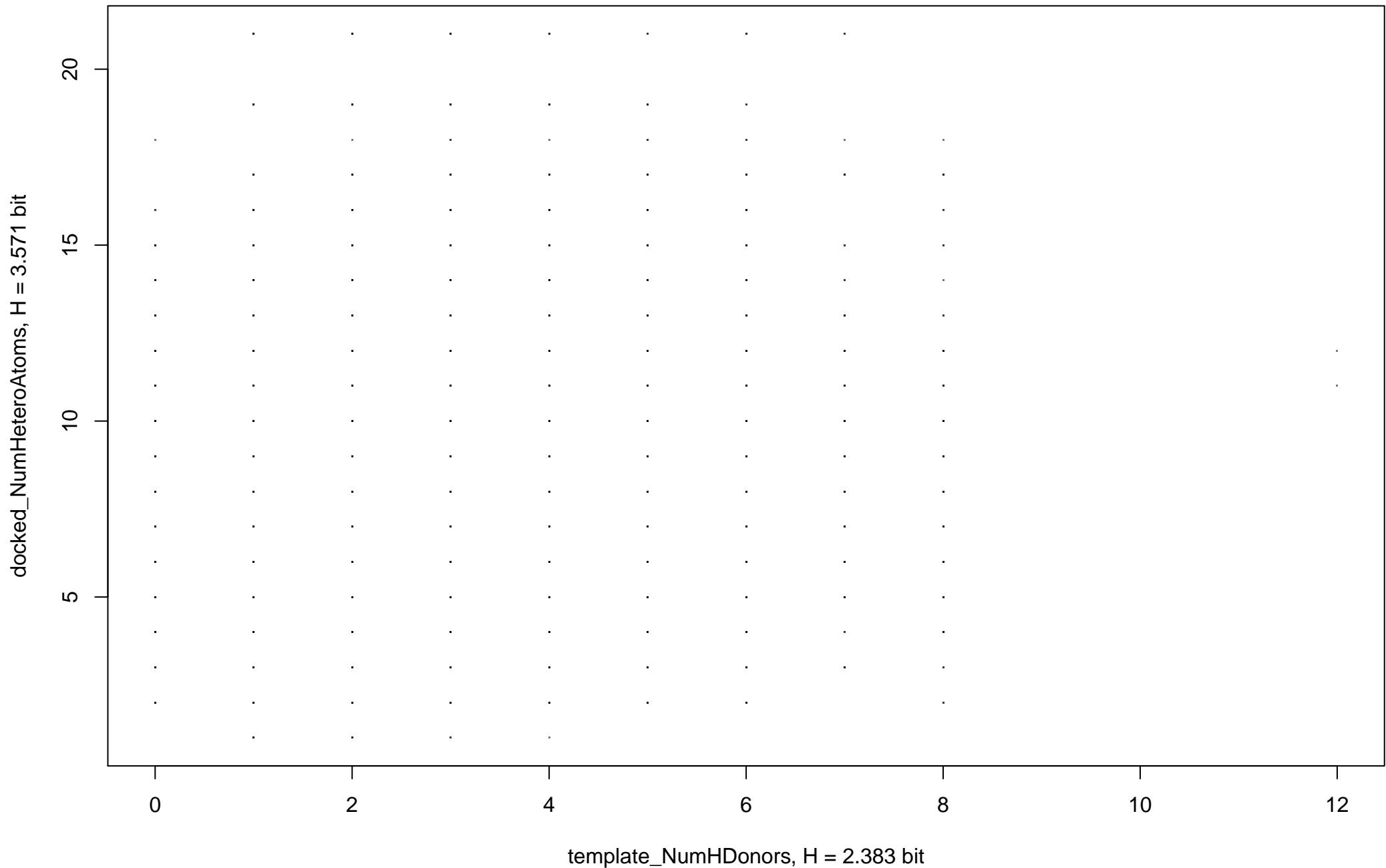
template_NumHeteroAtoms-mcs_RingCount, MI = 0.02211 bit, normMI = 0.0128



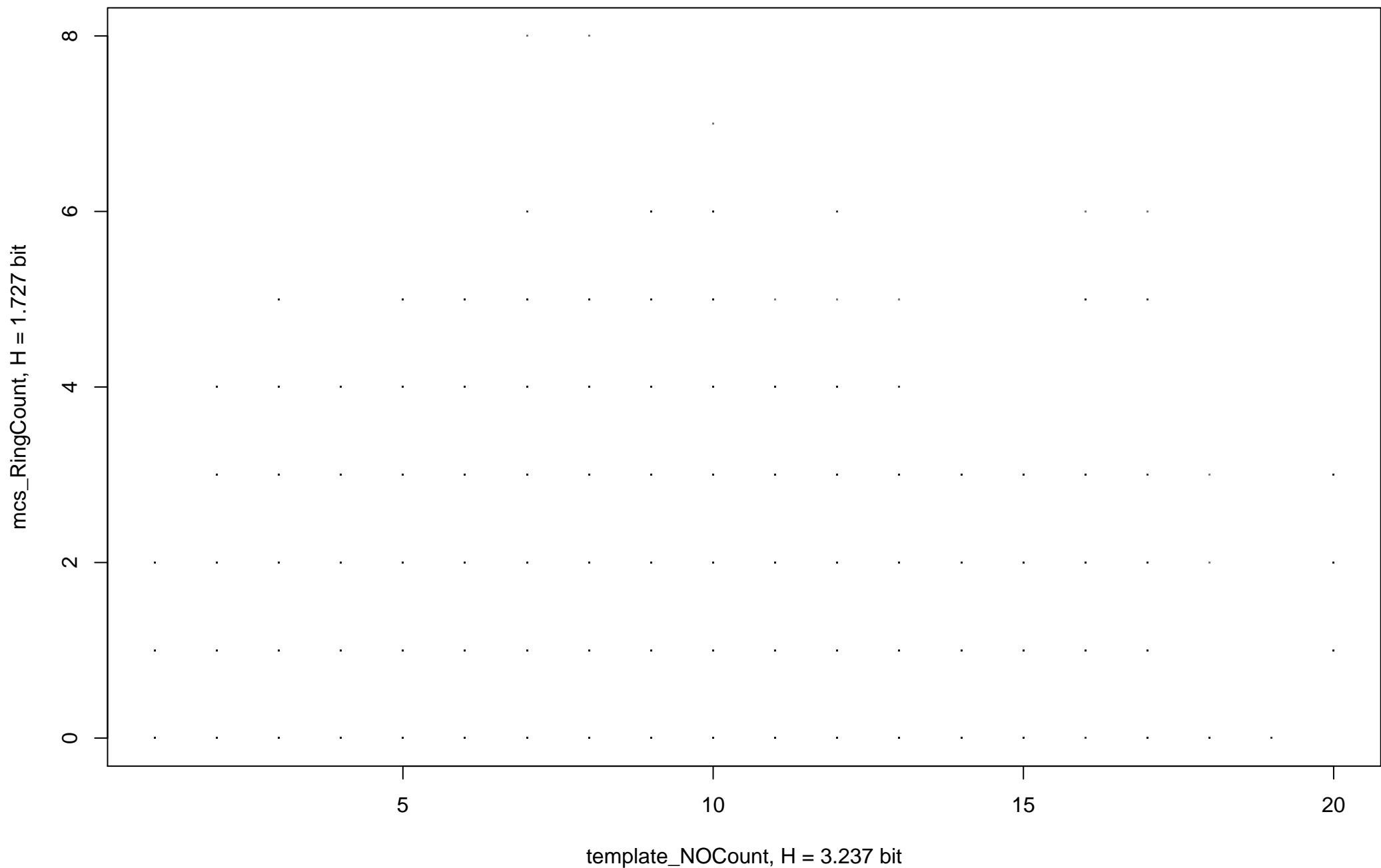
template_RingCount-docked_NOCount, MI = 0.02955 bit, normMI = 0.01254



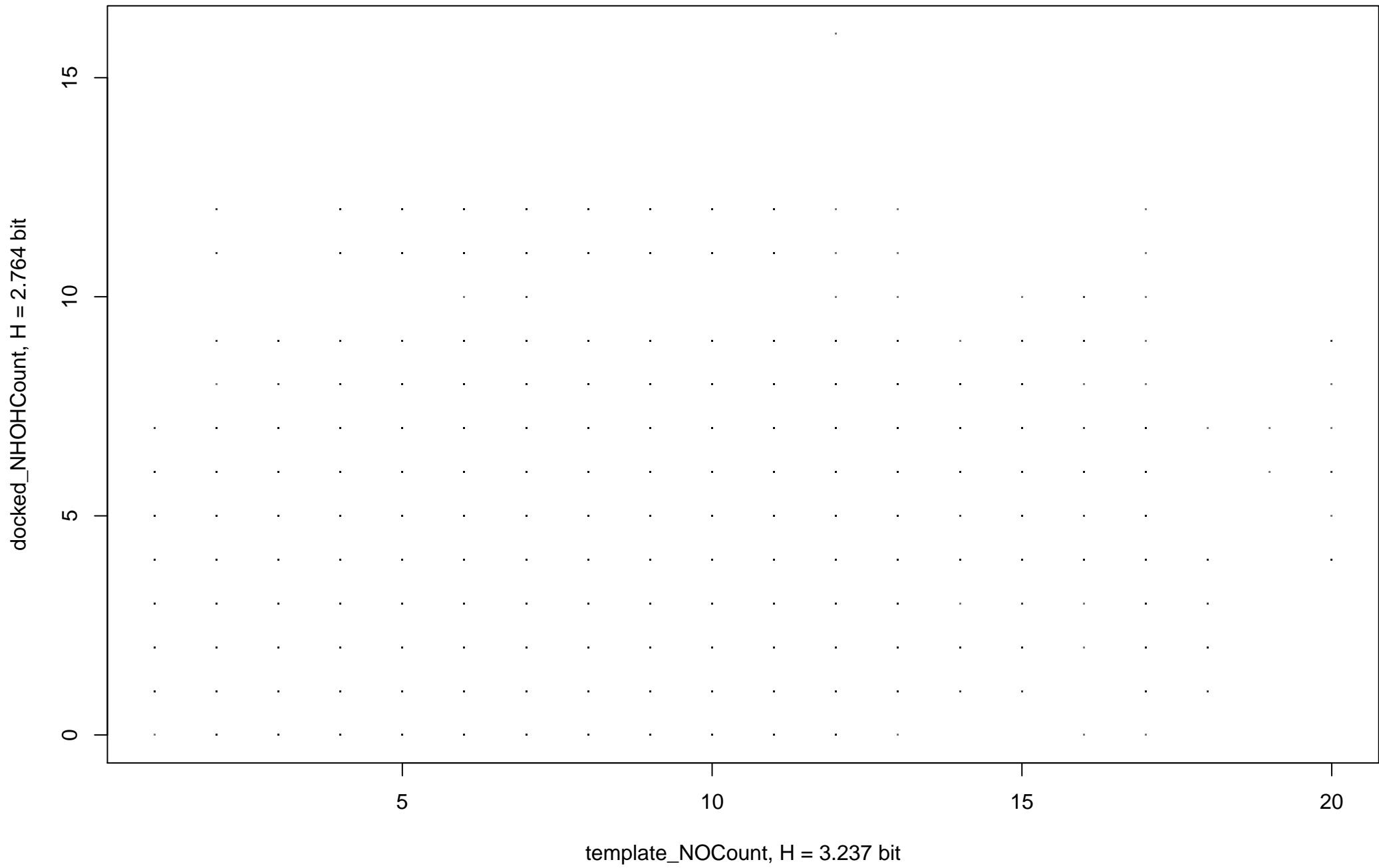
template_NumHDonors-docked_NumHeteroAtoms, MI = 0.02886 bit, normMI = 0.01211



template_NOCount-mcs_RingCount, MI = 0.02086 bit, normMI = 0.01208

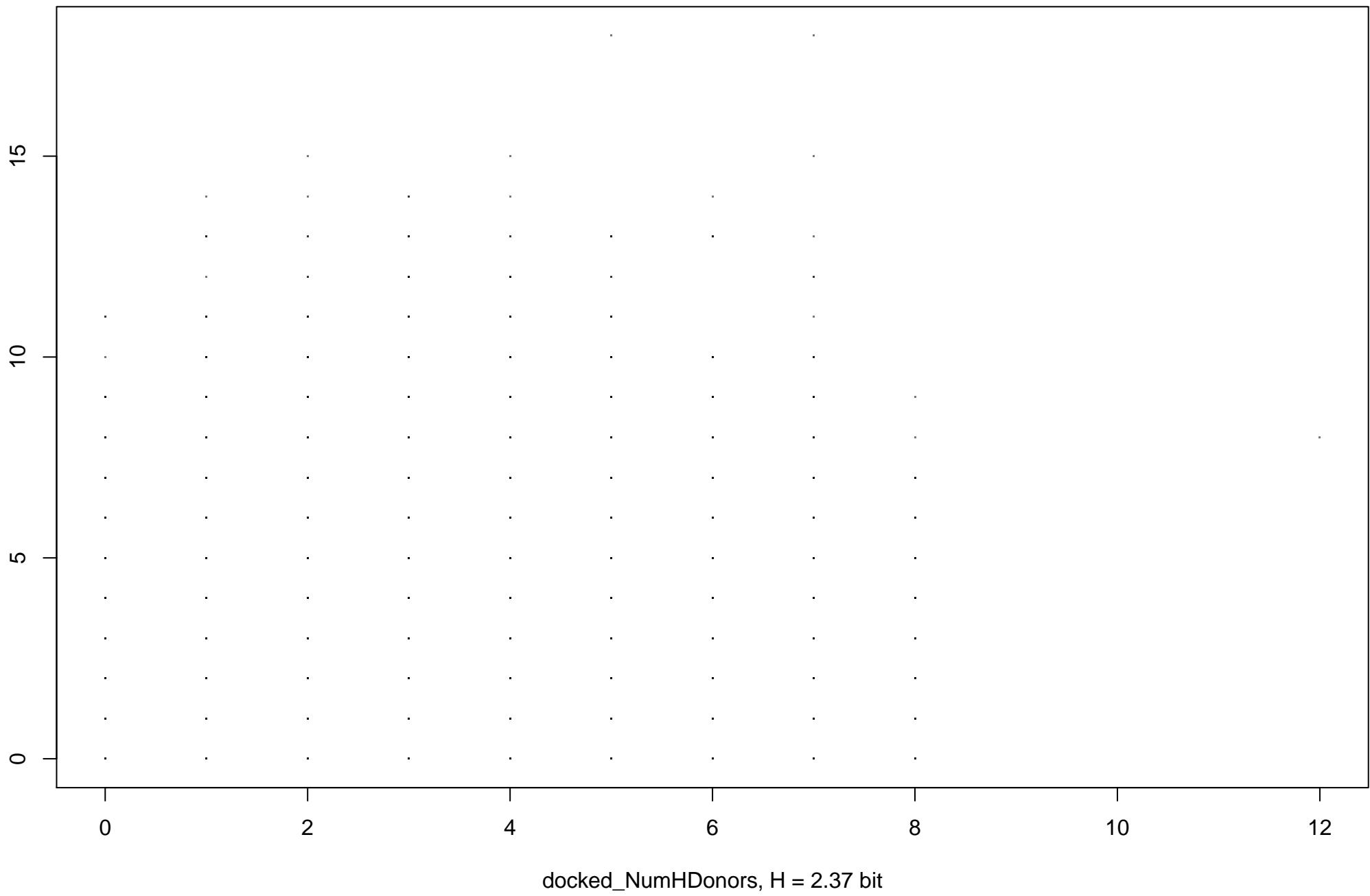


template_NOCount–docked_NHOHCount, MI = 0.03278 bit, normMI = 0.01186



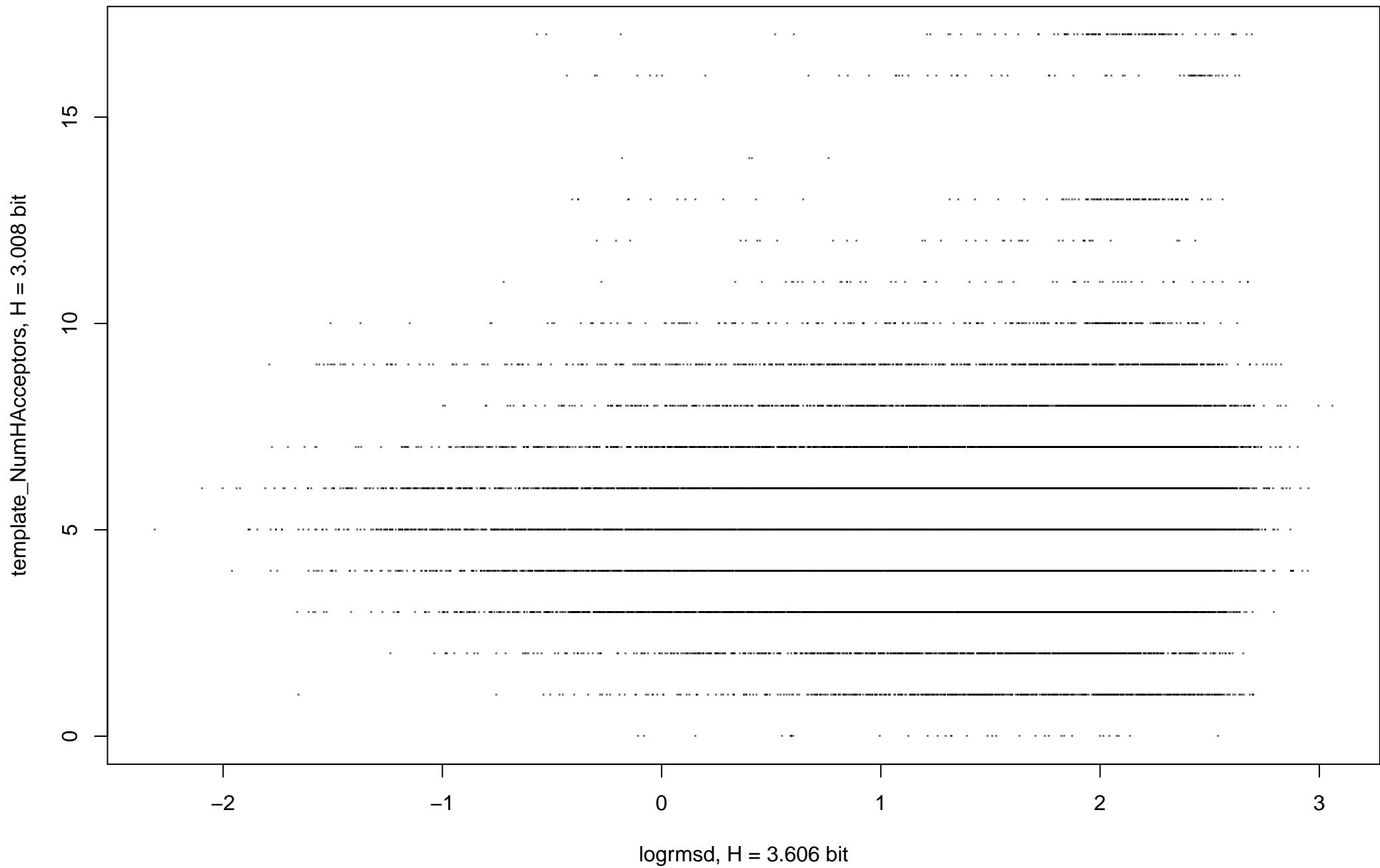
docked_NumHDonors-mcs_template_NumRotatableBonds, MI = 0.0281 bit, normMI = 0.01185

mcs_template_NumRotatableBonds, H = 3.118 bit

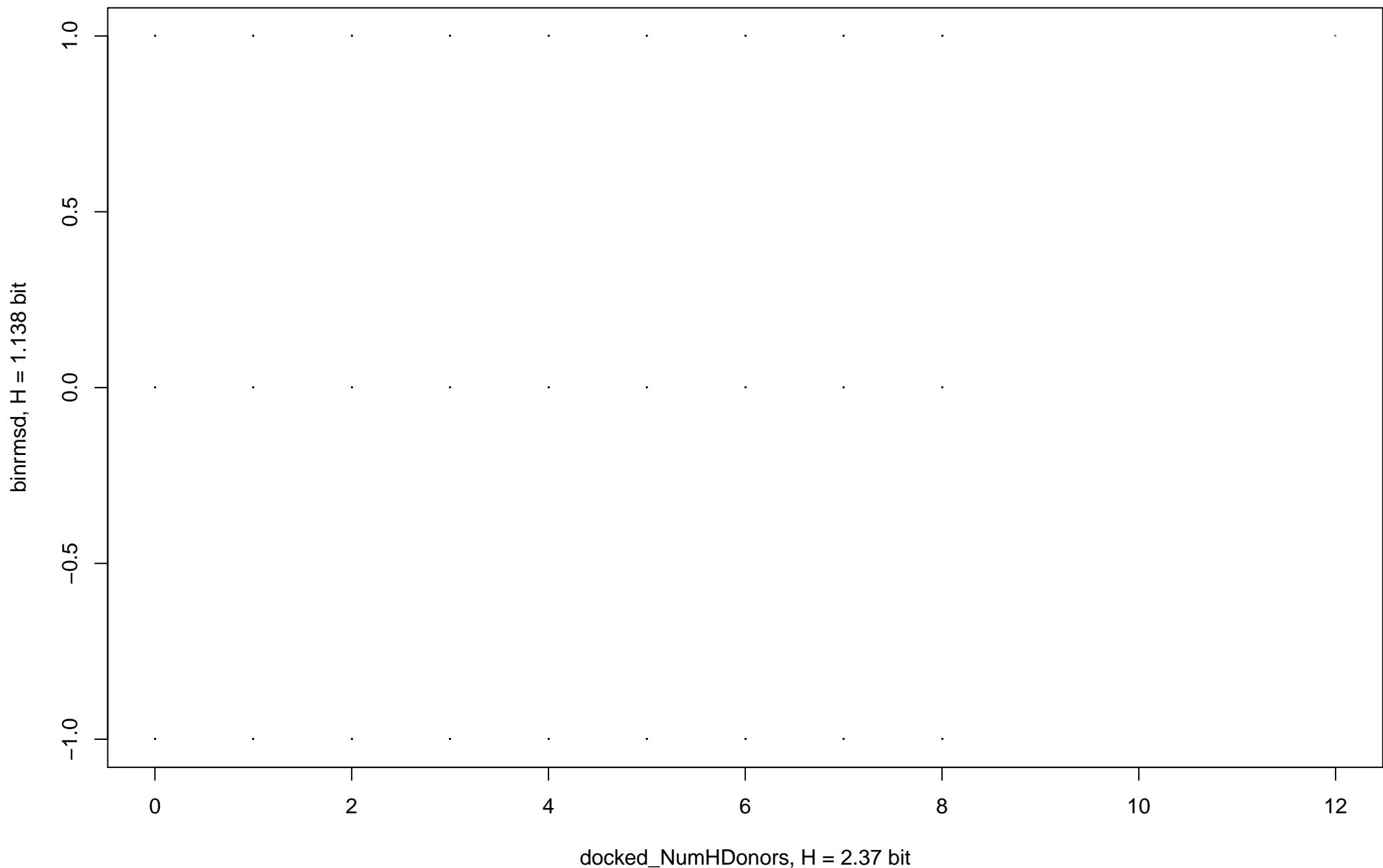


docked_NumHDonors, H = 2.37 bit

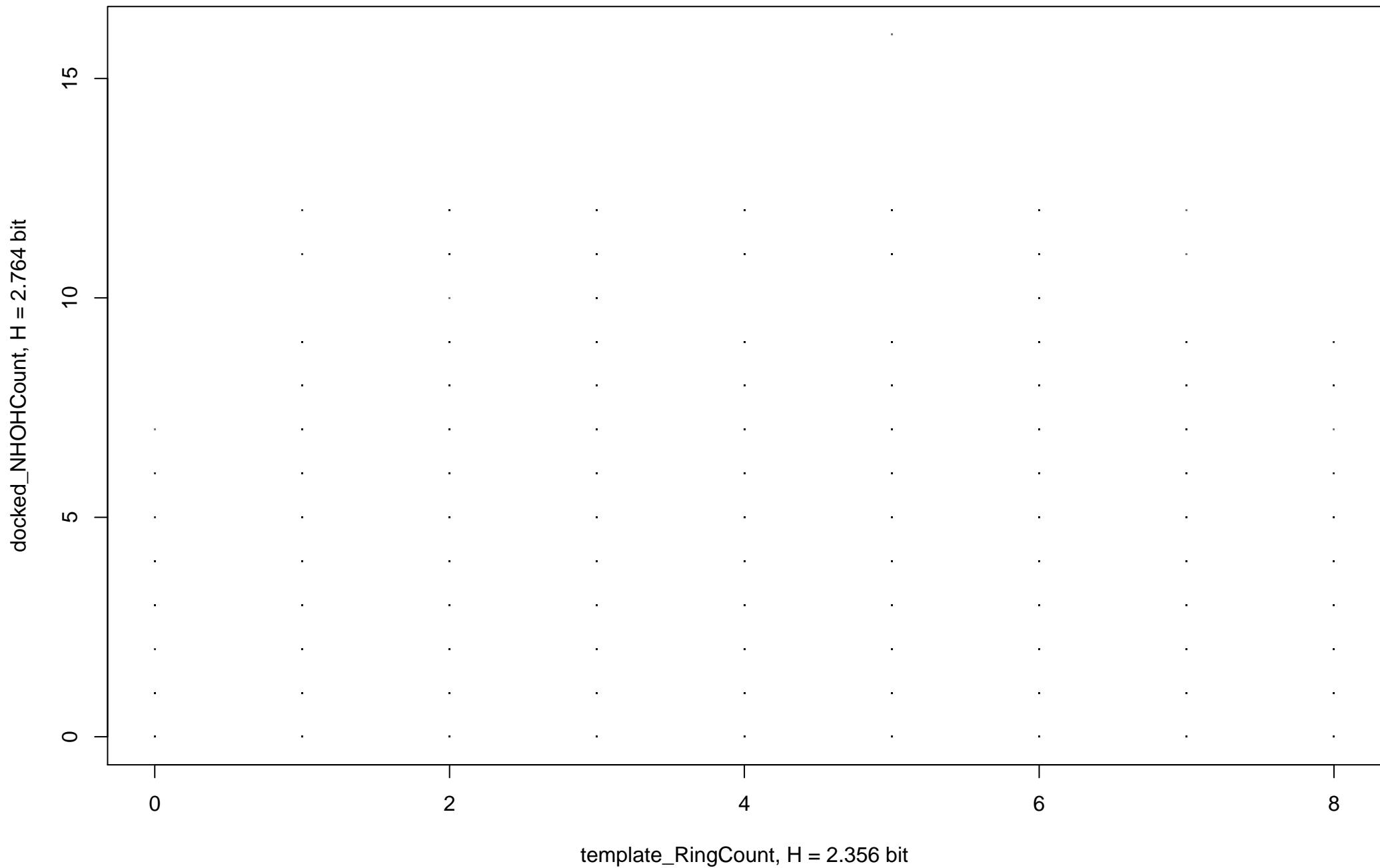
logrmsd-template_NumHAcceptors, MI = 0.0348 bit, normMI = 0.01157



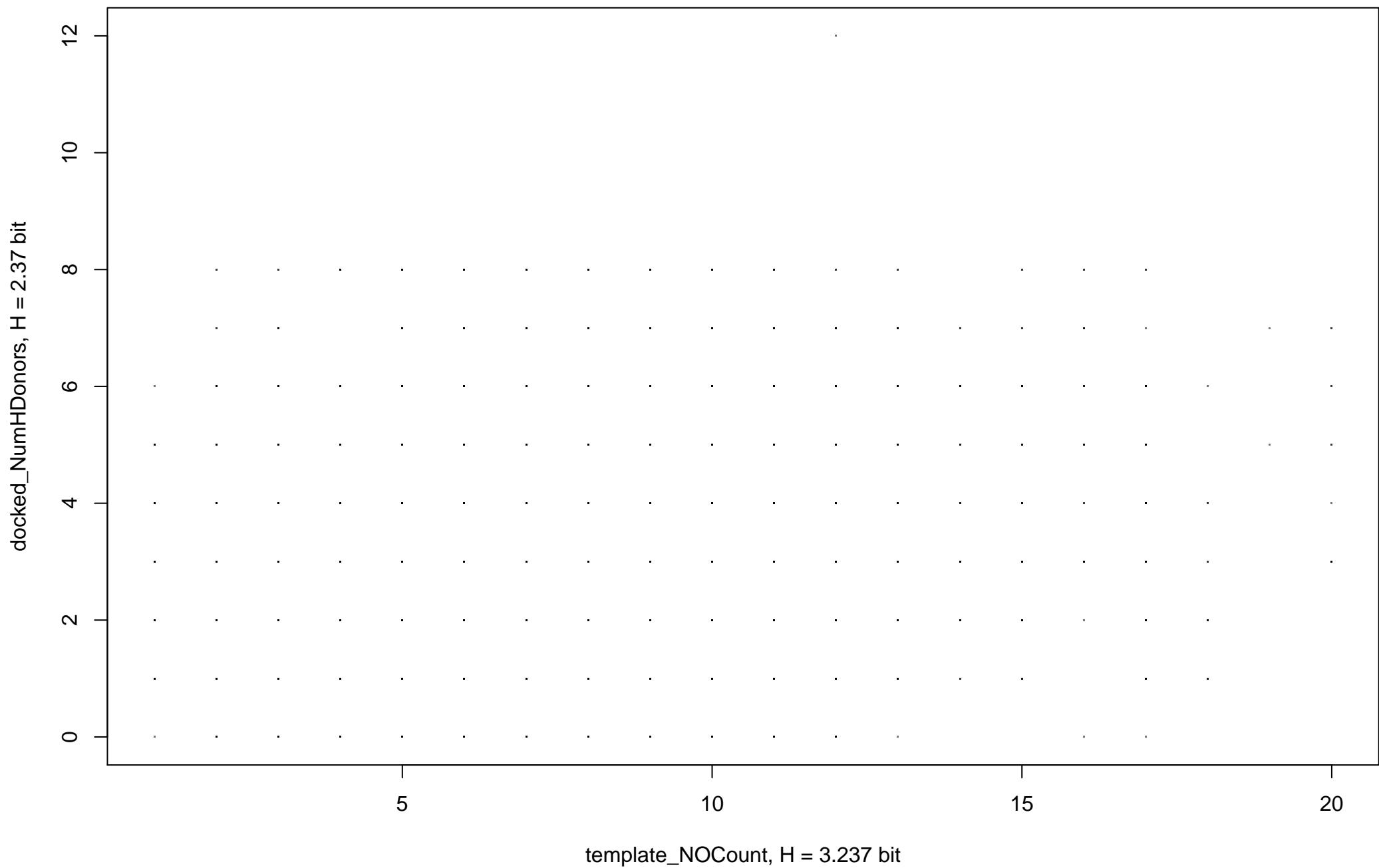
docked_NumHDonors–binrmsd, MI = 0.01281 bit, normMI = 0.01126



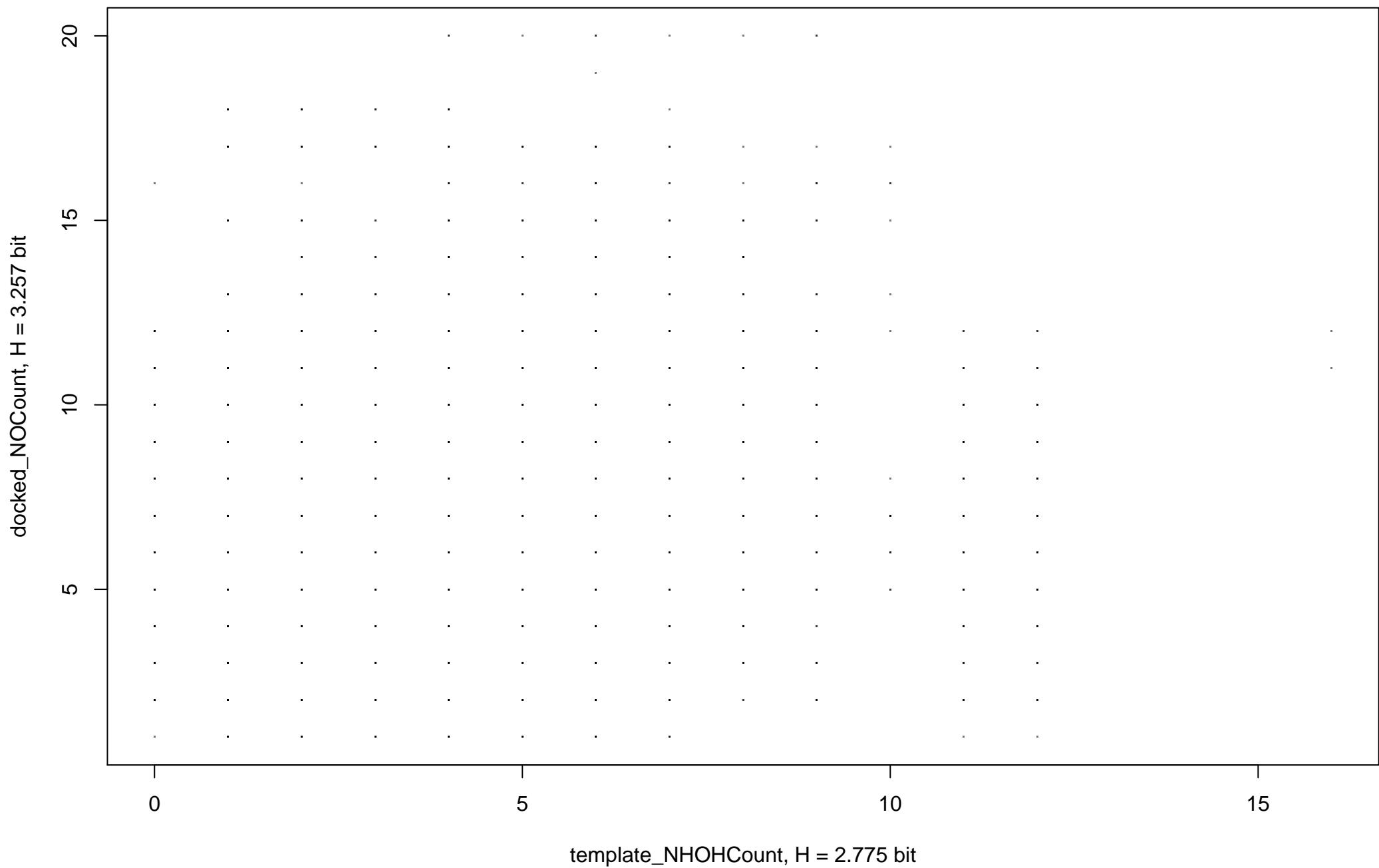
template_RingCount–docked_NHOHCount, MI = 0.02632 bit, normMI = 0.01117



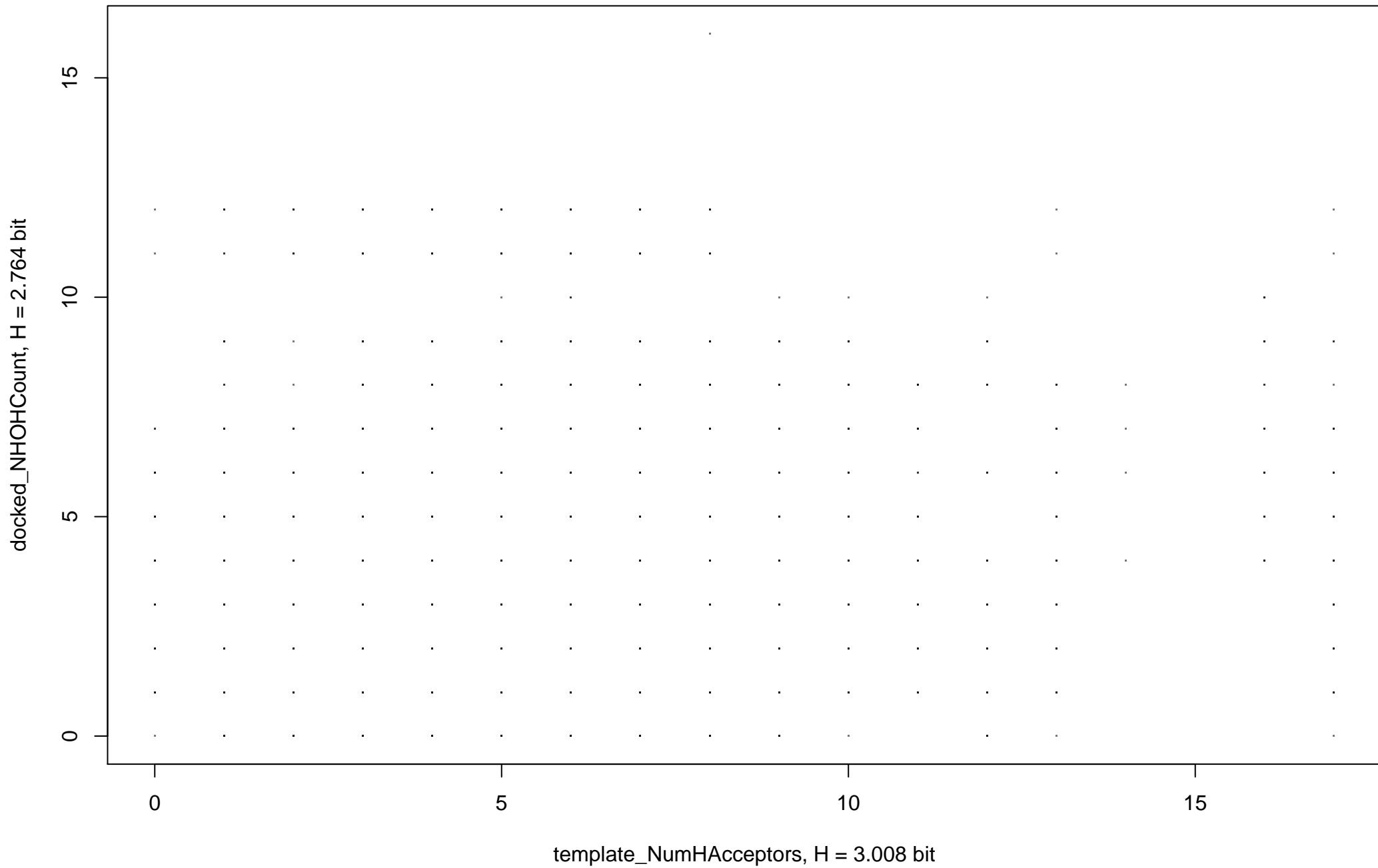
template_NOCount-docked_NumHDonors, MI = 0.02587 bit, normMI = 0.01092



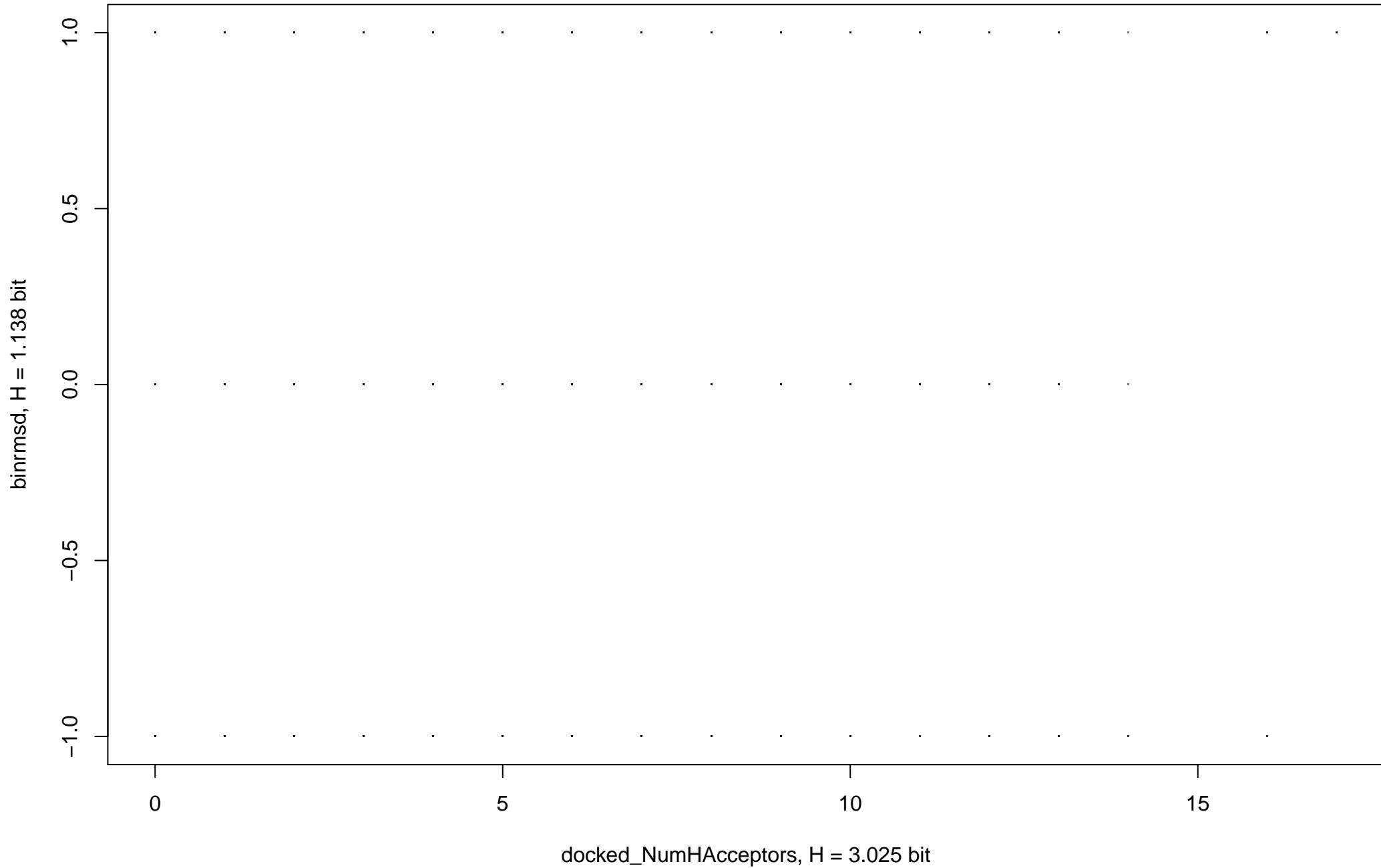
template_NHOHCount–docked_NOCount, MI = 0.02973 bit, normMI = 0.01071



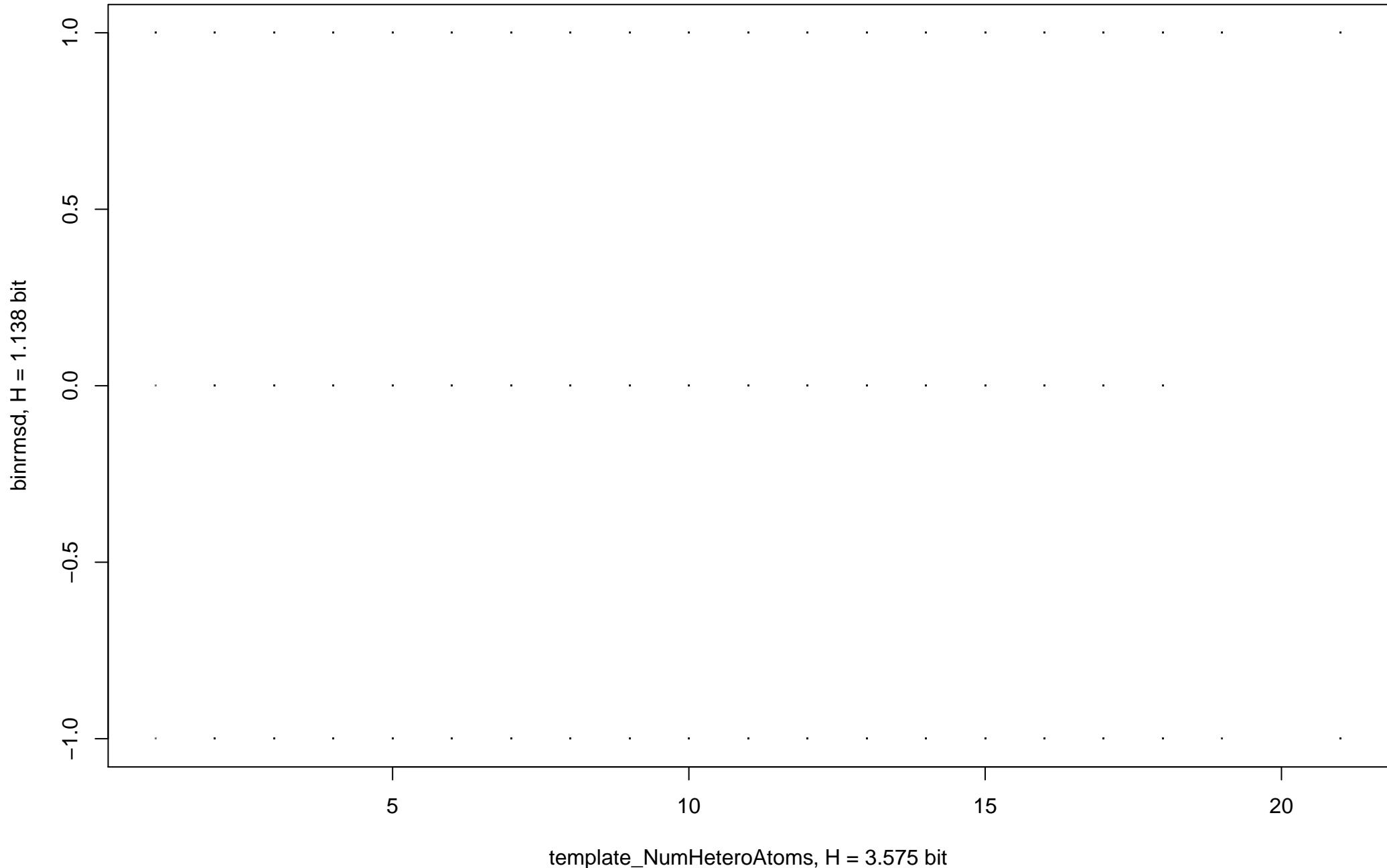
template_NumHAcceptors-docked_NHOHCount, MI = 0.02935 bit, normMI = 0.01062



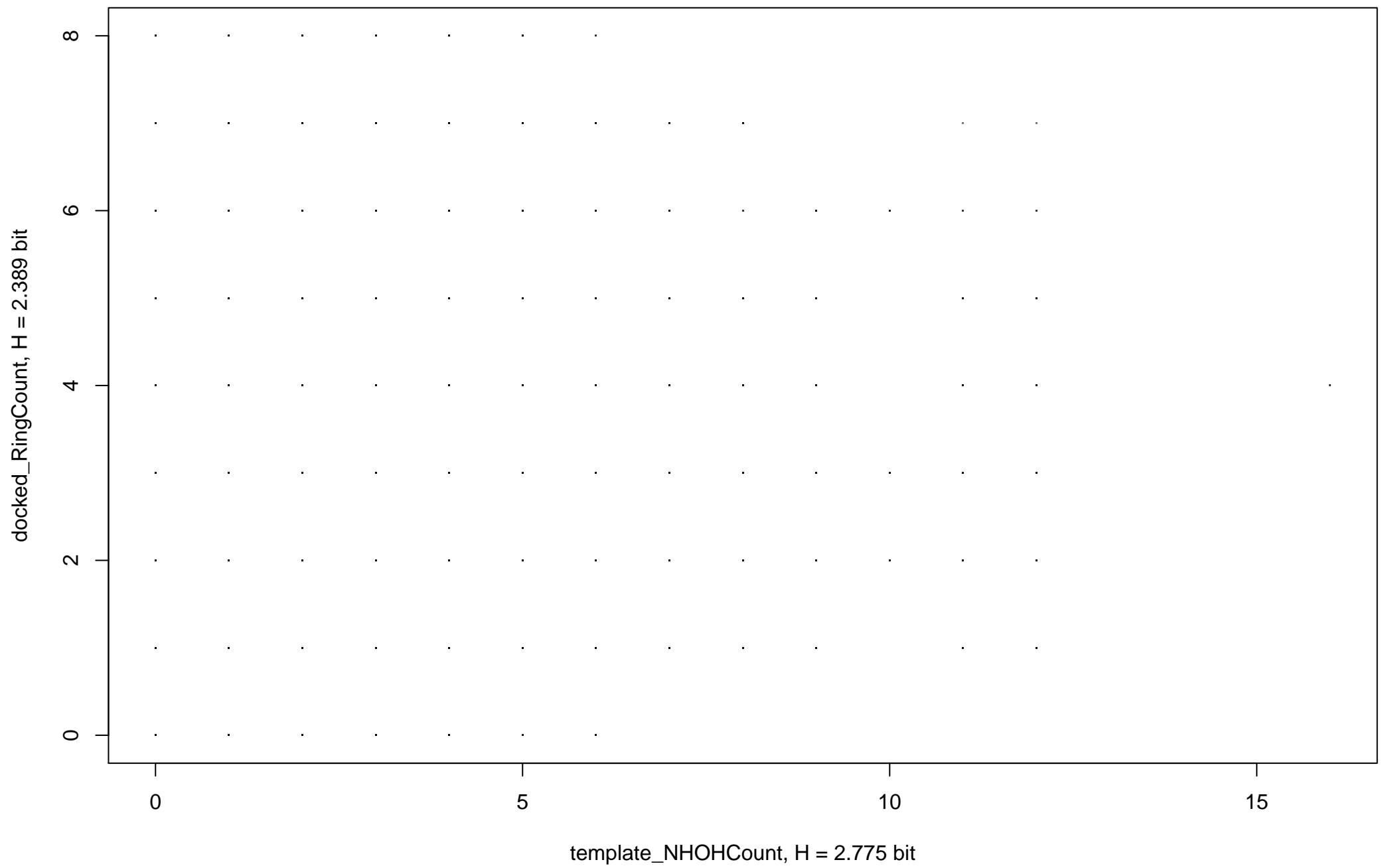
docked_NumHAcceptors–binrmsd, MI = 0.01149 bit, normMI = 0.01009



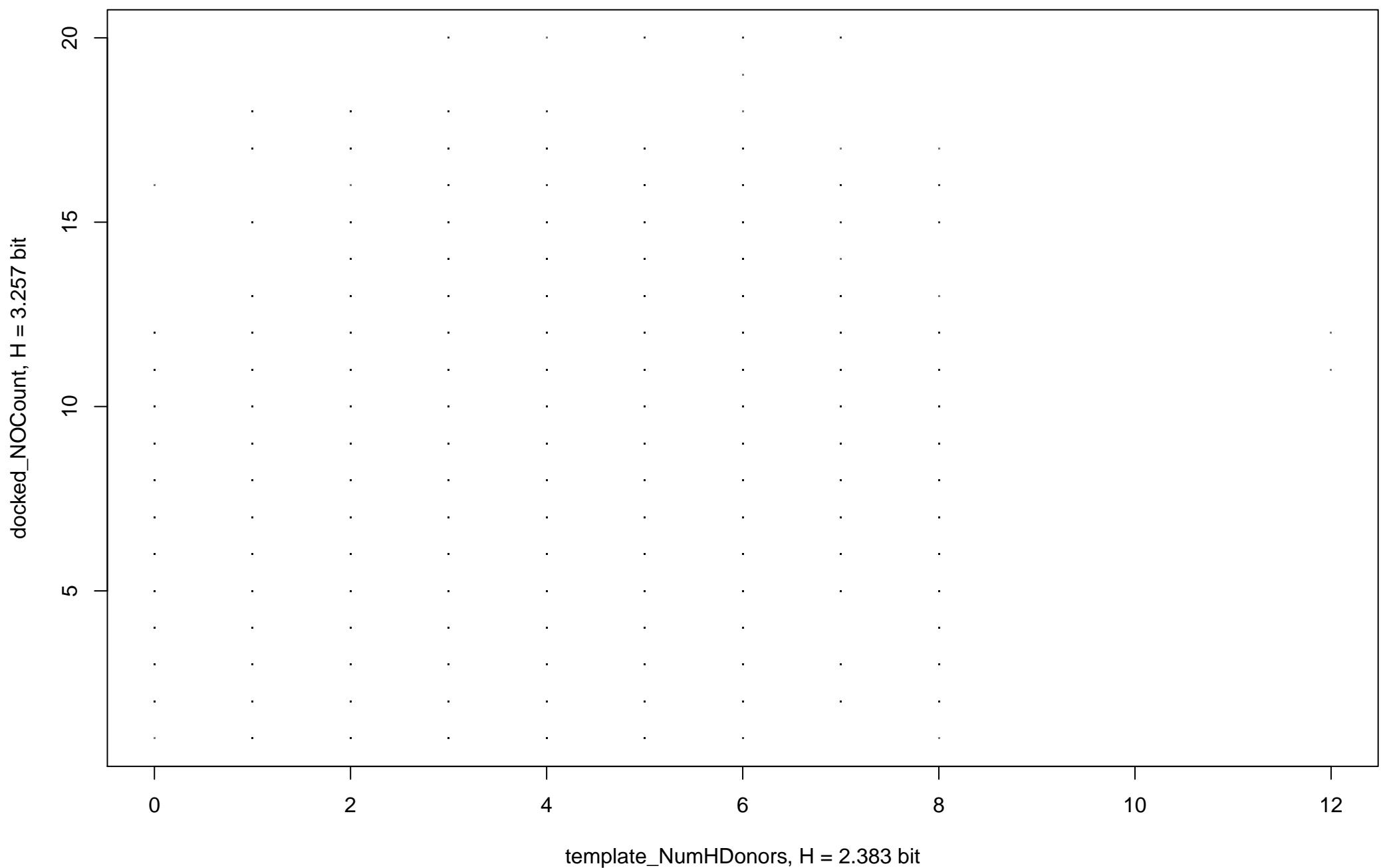
template_NumHeteroAtoms-binrmsd, MI = 0.01133 bit, normMI = 0.009959



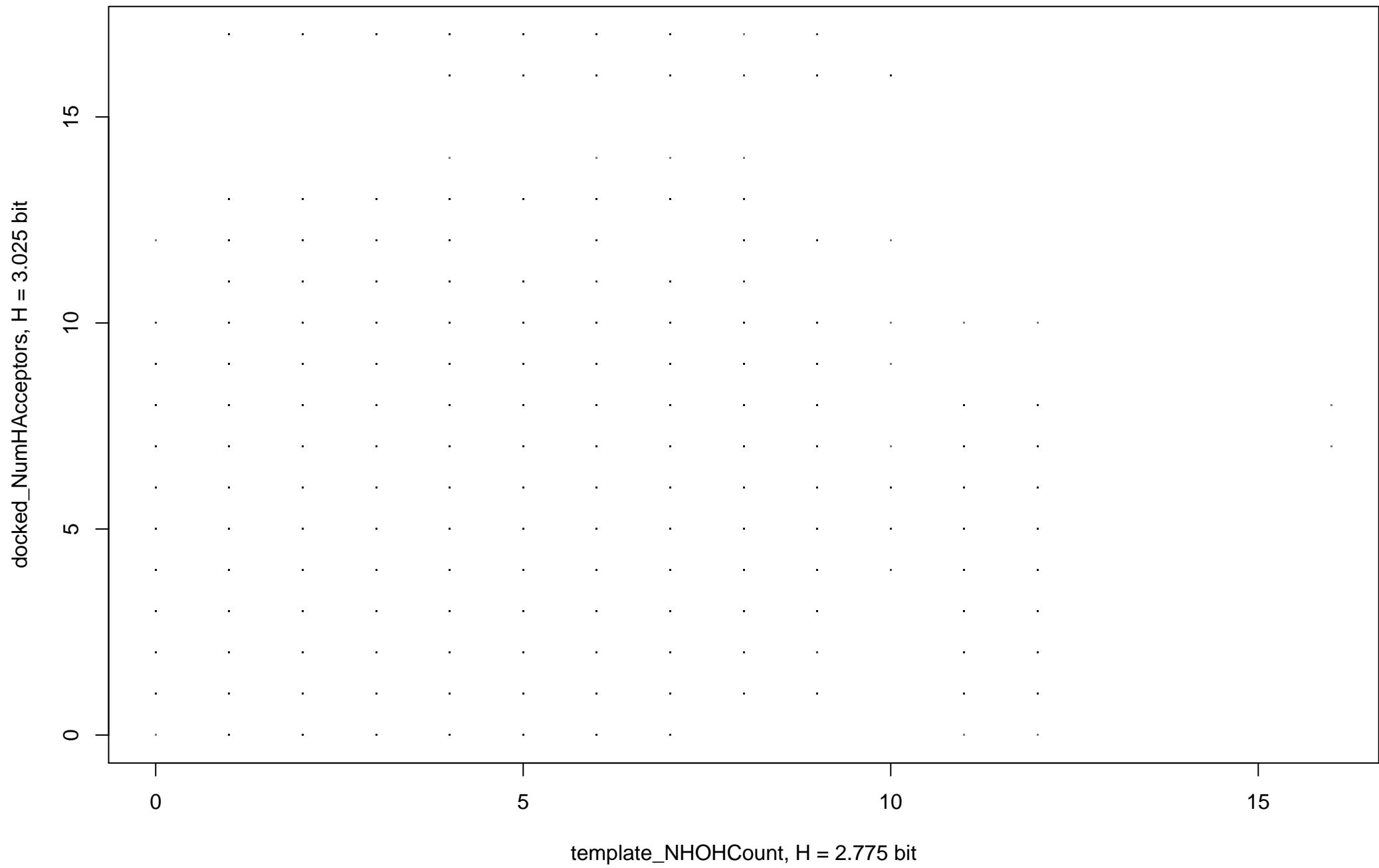
template_NHOHCount-docked_RingCount, MI = 0.02363 bit, normMI = 0.009892



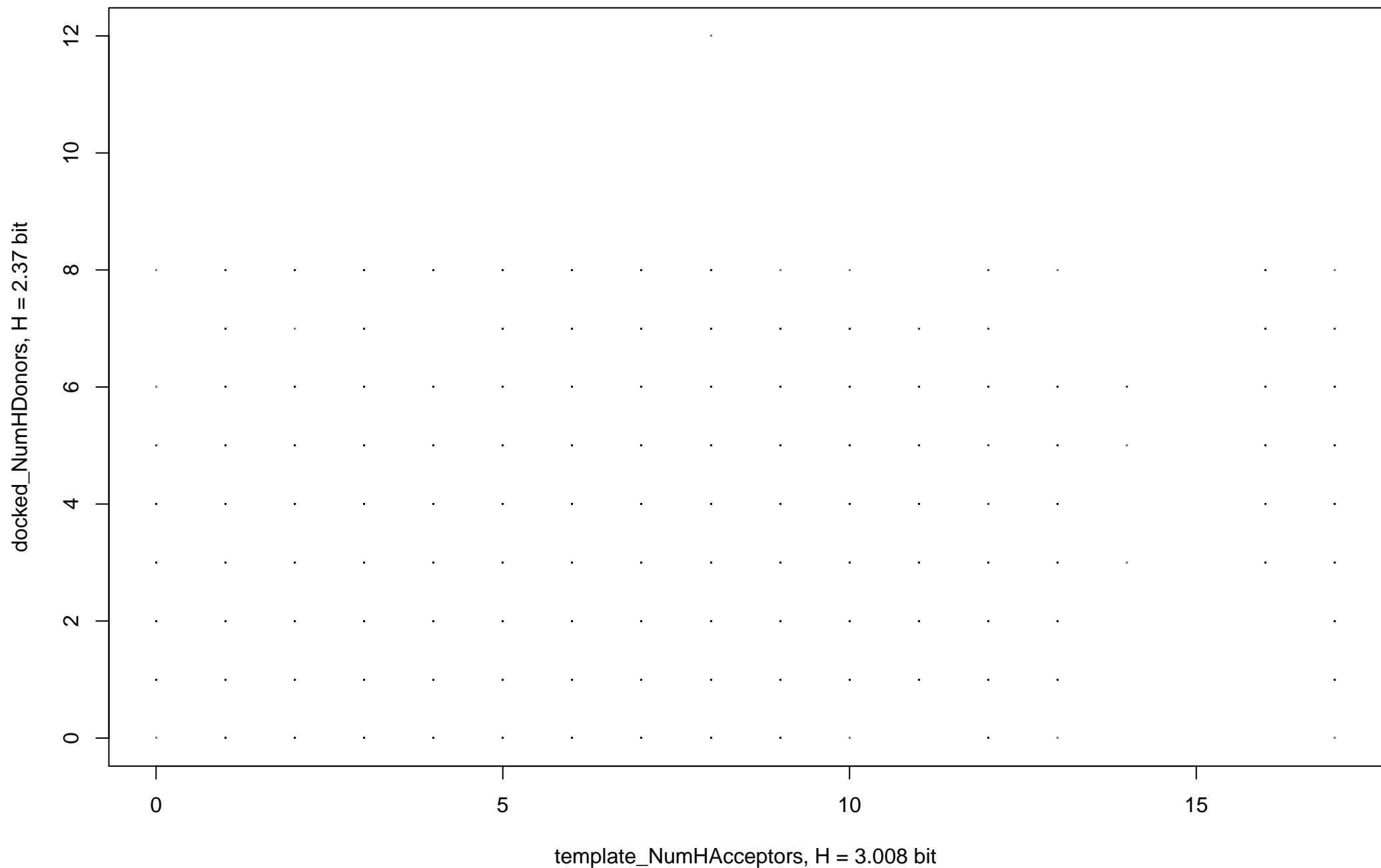
template_NumHDonors-docked_NOCount, MI = 0.02287 bit, normMI = 0.009595



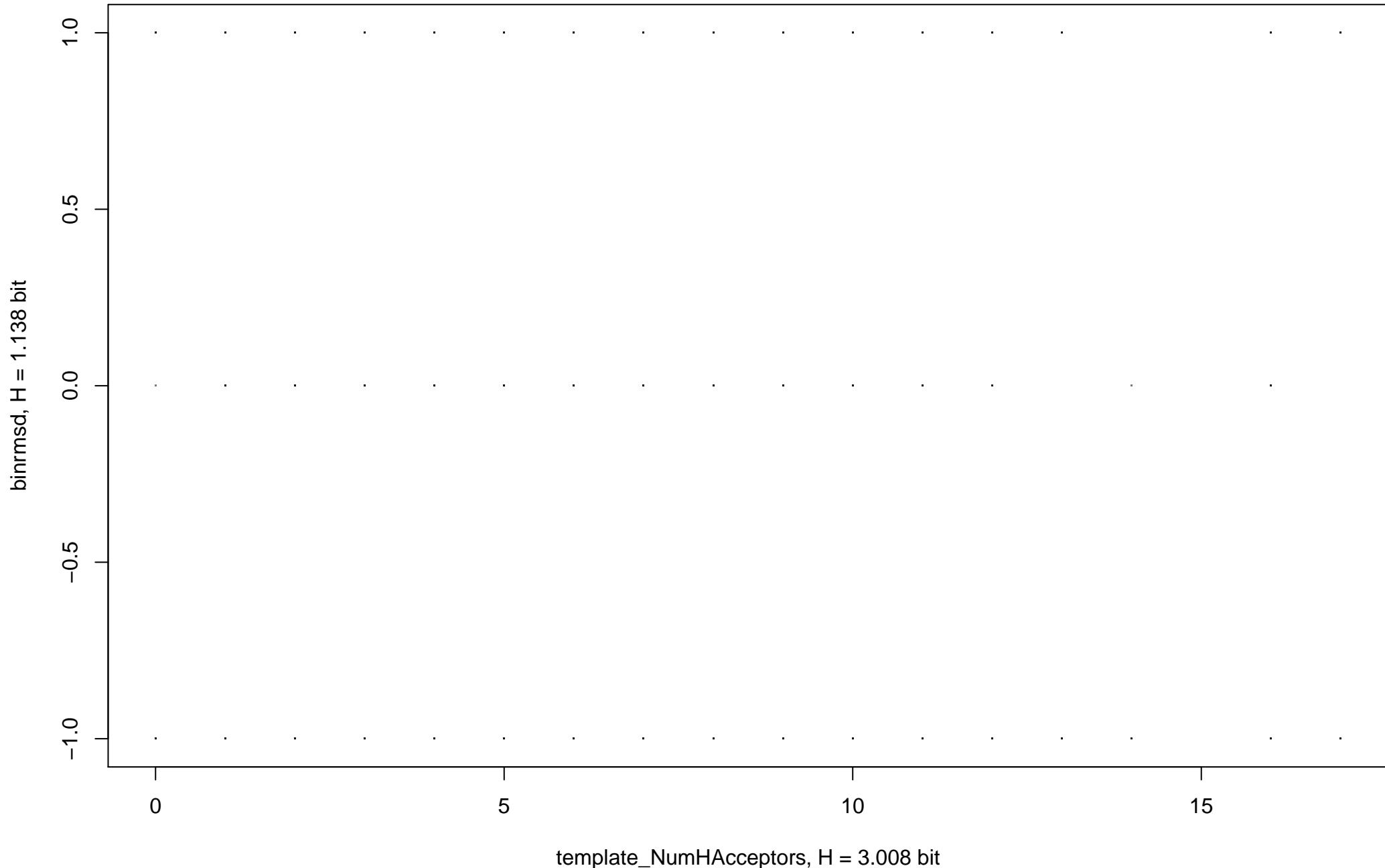
template_NHOHCount-docked_NumHAcceptors, MI = 0.02453 bit, normMI = 0.008838



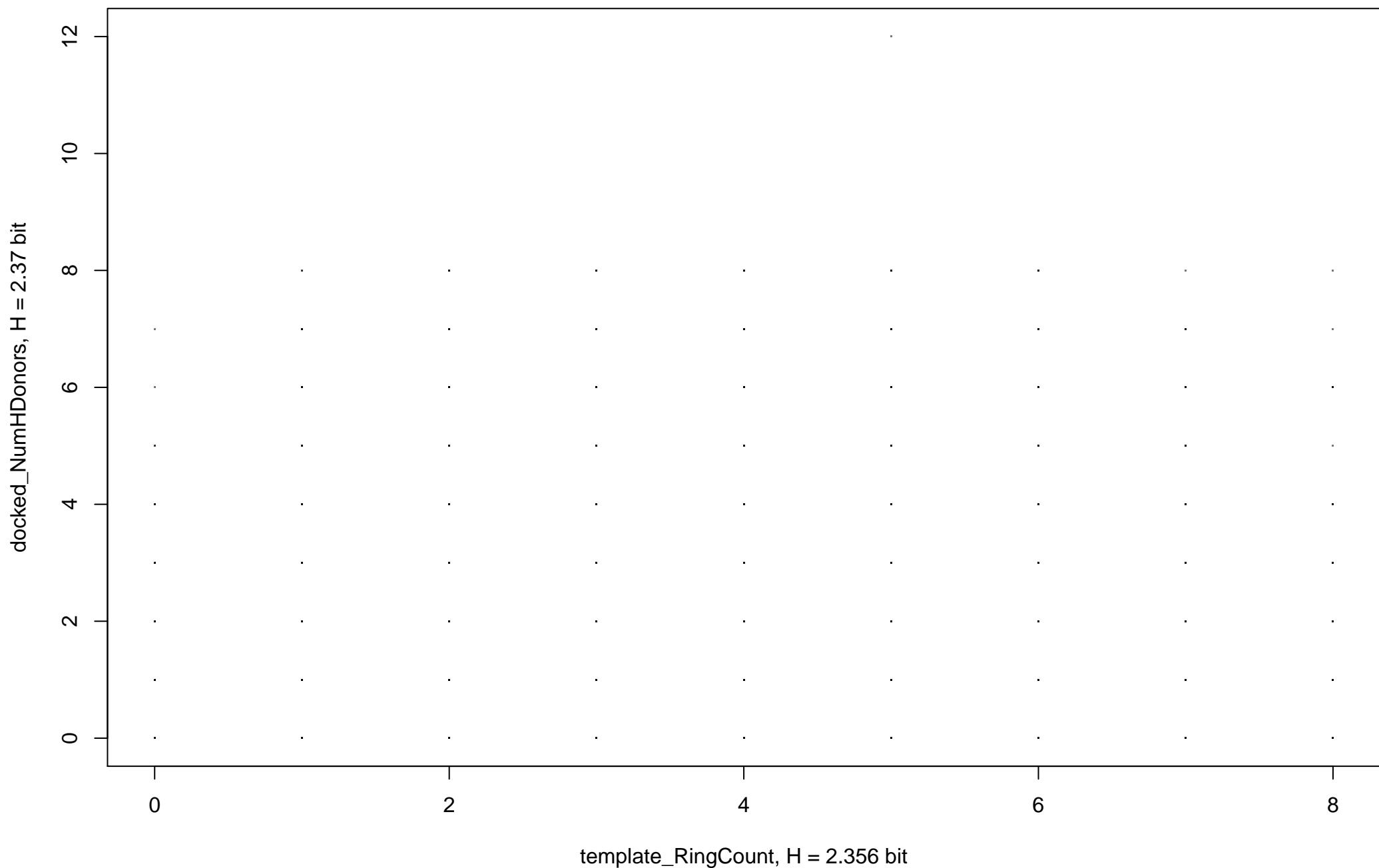
template_NumHAcceptors–docked_NumHDonors, MI = 0.02012 bit, normMI = 0.008486



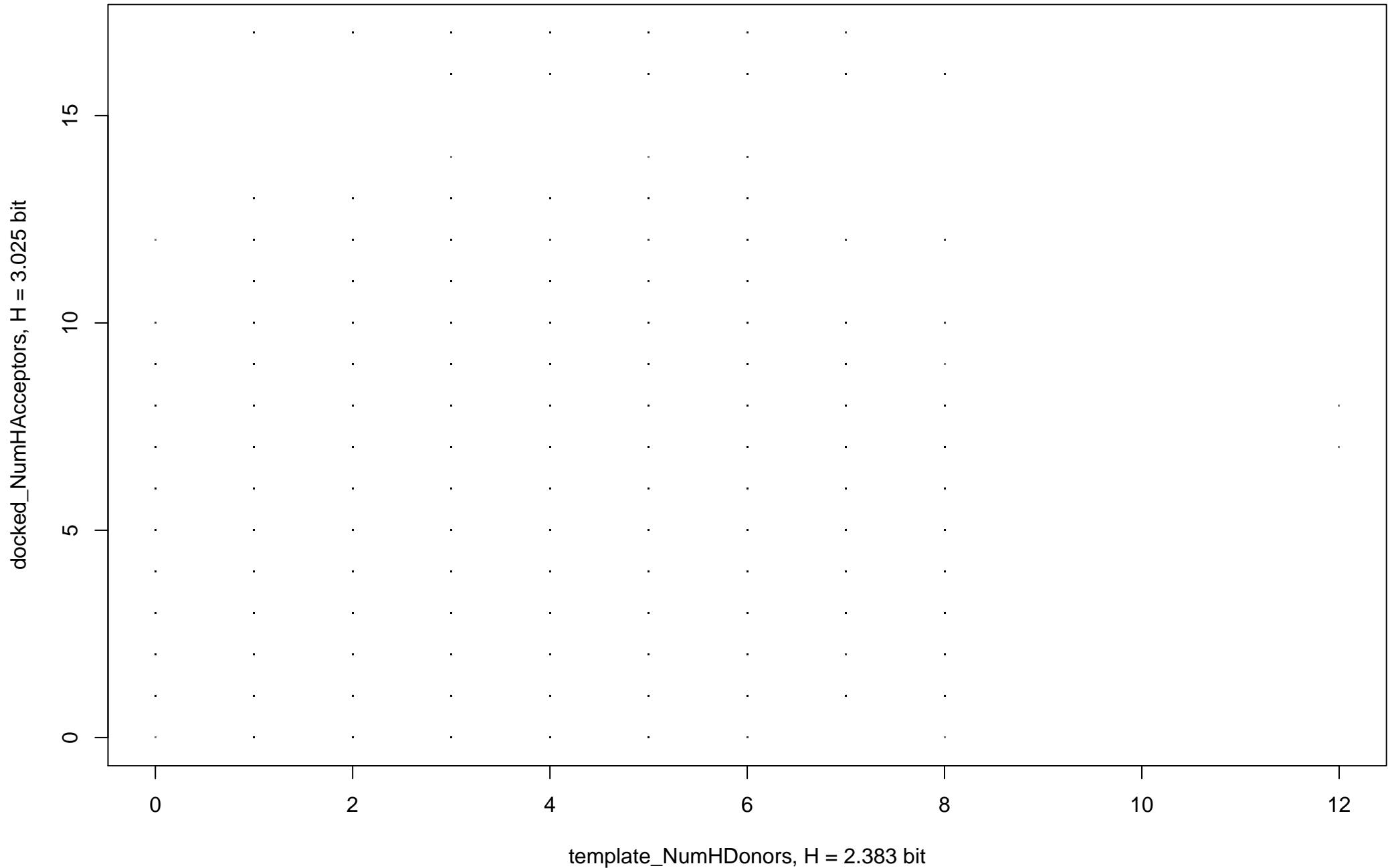
template_NumHAcceptors–binrmsd, MI = 0.008438 bit, normMI = 0.007414



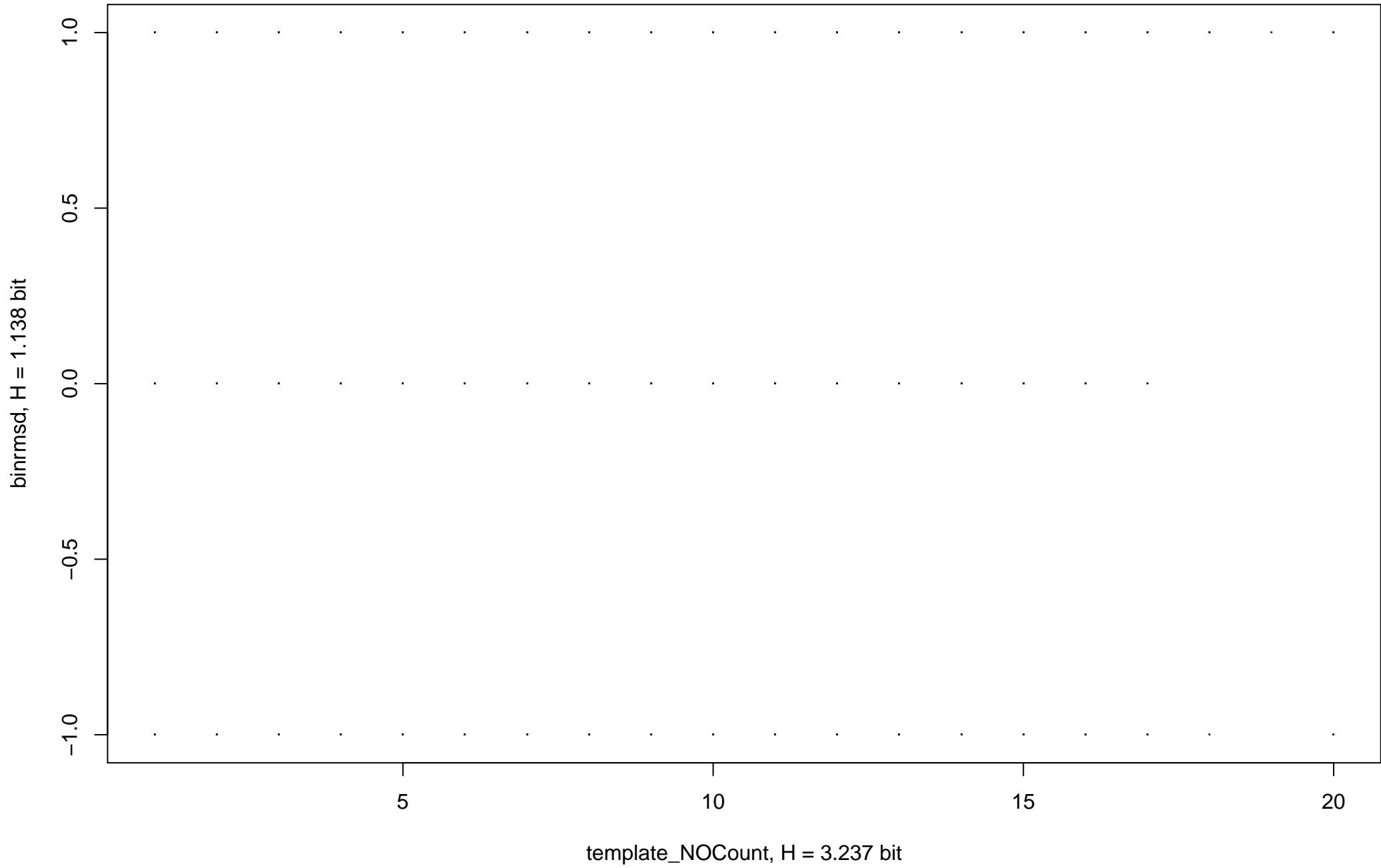
template_RingCount-docked_NumHDonors, MI = 0.01701 bit, normMI = 0.007222



template_NumHDonors–docked_NumHAcceptors, MI = 0.01647 bit, normMI = 0.006913



template_NOCount-binrmsd, MI = 0.007229 bit, normMI = 0.006352



template_NumHDonors-docked_RingCount, MI = 0.01444 bit, normMI = 0.006057

