

# Search for heavy resonances decaying to a pair of Lorentz-boosted Higgs bosons in final states with leptons and a bottom quark pair at $\sqrt{s} = 13$ TeV



## The CMS collaboration

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**ABSTRACT:** A search for new heavy resonances decaying to a pair of Higgs bosons (HH) in proton-proton collisions at a center-of-mass energy of 13 TeV is presented. Data were collected with the CMS detector at the LHC in 2016–2018, corresponding to an integrated luminosity of  $138 \text{ fb}^{-1}$ . Resonances with a mass between 0.8 and 4.5 TeV are considered using events in which one Higgs boson decays into a bottom quark pair and the other into final states with either one or two charged leptons. Specifically, the single-lepton decay channel  $\text{HH} \rightarrow \text{b}\bar{\text{b}}\text{W}\text{W}^* \rightarrow \text{b}\bar{\text{b}}\ell\nu\text{q}\bar{\text{q}}'$  and the dilepton decay channels  $\text{HH} \rightarrow \text{b}\bar{\text{b}}\text{W}\text{W}^* \rightarrow \text{b}\bar{\text{b}}\ell\nu\ell\nu$  and  $\text{HH} \rightarrow \text{b}\bar{\text{b}}\tau\tau \rightarrow \text{b}\bar{\text{b}}\ell\nu\ell\nu$  are examined, where  $\ell$  in the final state corresponds to an electron or muon. The signal is extracted using a two-dimensional maximum likelihood fit of the  $\text{H} \rightarrow \text{b}\bar{\text{b}}$  jet mass and HH invariant mass distributions. No significant excess above the standard model expectation is observed in data. Model-independent exclusion limits are placed on the product of the cross section and branching fraction for narrow spin-0 and spin-2 massive bosons decaying to HH. The results are also interpreted in the context of radion and bulk graviton production in models with a warped extra spatial dimension. The results provide the most stringent limits to date for  $\text{X} \rightarrow \text{HH}$  signatures with final-state leptons and at some masses provide the most sensitive limits of all  $\text{X} \rightarrow \text{HH}$  searches.

**KEYWORDS:** Beyond Standard Model, Hadron-Hadron Scattering, Higgs Physics, Particle and Resonance Production

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## 1 Introduction

The discovery of a Higgs boson (H) at the CERN LHC [1–3] validated the proposed mass generation mechanism within the standard model (SM) [4, 5], the so-called “Brout-Englert-Higgs mechanism.” A number of theoretical difficulties found in the simple model are ameliorated by an extended Higgs sector [6]. Supersymmetry [7–14] requires such an extended Higgs sector that includes additional spin-0 particles. Models with warped extra dimensions, proposed by Randall and Sundrum [15], postulate the existence of a compact fourth spatial dimension with a warped metric. Such compactification creates heavy resonances arising as a tower of Kaluza-Klein excitations, leading to possible spin-0 radions [16–19] or spin-2 bulk gravitons [20–22]. The ATLAS [23–34] and CMS [35–51] Collaborations have conducted a number of searches for these particles, where the new bosons decay into vector bosons and/or SM Higgs bosons (WW, ZZ, WZ, HH, ZH, or WH).

In this paper, we present an expansion of a previous search [52] for heavy resonances (X) decaying to HH. The previous study considered a smaller data set of proton-proton (pp) collisions and searched for a signal in which one Higgs boson decayed to a bottom quark pair ( $b\bar{b}$ ) and the second decayed to a pair of W bosons, with one decaying leptonically and the other hadronically ( $WW^* \rightarrow \ell\nu q\bar{q}'$ ). The data set analyzed in ref. [52] corresponded to collisions at  $\sqrt{s} = 13$  TeV recorded in 2016 with an integrated luminosity of  $36 \text{ fb}^{-1}$ . In this new search, in addition to the  $HH \rightarrow b\bar{b}\ell\nu q\bar{q}'$  decay channel from ref. [52], two other signal decay channels are included by considering dilepton decays of the Higgs boson that does not decay to  $b\bar{b}$ : the  $H \rightarrow WW^* \rightarrow \ell\nu\ell\nu$  and the  $H \rightarrow \tau\tau \rightarrow \ell\nu\ell\nu$  decays. In all three cases, the  $\ell$  denotes an electron or a muon; the analysis is also sensitive to leptonically decaying  $\tau$  leptons in the  $b\bar{b}WW^*$  decays. Events from  $b\bar{b}\tau\tau$  comprise 30–35% of the total expected dilepton signal yield. The analysis is optimized for the three  $X \rightarrow HH$  channels just mentioned, but signal events from  $HH \rightarrow b\bar{b}ZZ^*$  are also included in our acceptance and constitute 1–3% of the total expected signal yield.

This search is performed on a data set of pp collisions at a center-of-mass energy of 13 TeV, collected in 2016–2018 at the CERN LHC, corresponding to an integrated luminosity of  $138 \text{ fb}^{-1}$ , and considers narrow resonances in the mass range  $0.8 < m_X < 4.5$  TeV. The Higgs bosons have a high Lorentz boost because of the large values of  $m_X$  considered, so the decay products of each one are contained in a collimated cone. The degree of collimation is enough such that the hadronically decaying bosons (H and W) are each reconstructed as a single jet that has substructure consistent with a decay to two energetic quarks. The distinguishing characteristic of the signal is a peak in the two-dimensional (2D) plane of the  $H \rightarrow b\bar{b}$  jet mass  $m_{b\bar{b}}$  and the reconstructed HH invariant mass  $m_{HH}$ .

In the single-lepton (SL) channel, the quarks in the  $H \rightarrow WW^* \rightarrow \ell\nu q\bar{q}'$  decay are reconstructed as a single large jet (the  $q\bar{q}'$  jet) with a nearby lepton (e or  $\mu$ ). This jet is required to have substructure consistent with a decay to two energetic quarks. This Higgs boson decay chain is reconstructed as the  $q\bar{q}'$  jet, the lepton, and the missing transverse momentum  $\vec{p}_T^{\text{miss}}$ . In the dilepton (DL) channel, two leptons are reconstructed in close proximity to each other, with  $\vec{p}_T^{\text{miss}}$  nearby, consistent with the expected neutrinos. In all channels considered, the  $H \rightarrow b\bar{b}$  decay is reconstructed as a single large jet (the  $b\bar{b}$  jet) with substructure and high transverse momentum  $p_T$ .

The main SM background in this search arises from top quark pair ( $t\bar{t}$ ) production. This analysis is most sensitive to top quarks that have collimated decay products because of large Lorentz boosts. In the SL channel, the largest background comes from  $t\bar{t}$  decays in which one top quark decays with a charged lepton and a neutrino ( $t \rightarrow Wb \rightarrow \ell\nu b$ ), and the other decays exclusively to quarks ( $t \rightarrow Wb \rightarrow q\bar{q}'b$ ), which can be mistakenly reconstructed as the  $b\bar{b}$  jet candidate. Other significant backgrounds in this channel are the production of W bosons in association with jets with  $W \rightarrow \ell\nu$  (hereafter referred to as W+jets), and multijet events from quantum chromodynamic processes (QCD multijets), with either a lepton originating from heavy flavor decay or a hadron misidentified as a lepton. In the DL channel, the background yield is smaller than that of the SL channel by a factor of  $\approx 60$ . Top quark pair production is the dominant background here too, with approximately equal contributions from  $t\bar{t}$  events with a single lepton in the final state and events in which both top quarks decay leptonically. Single-lepton  $t\bar{t}$  events can fall into the DL channel when some part of the hadronic top quark decay is misidentified as a lepton. The other significant background in this channel is production of  $Z/\gamma^*$  bosons in association with jets ( $Z/\gamma^* + \text{jets}$ ), with  $Z/\gamma^* \rightarrow \ell\ell$ . These backgrounds are distinguished in data using the  $m_{b\bar{b}}$  spectrum. Contributions from backgrounds with an SM Higgs boson (e.g.,  $t\bar{t}H$ ) are considered but found to be negligible in both channels.

The CMS detector and the simulated samples used to build the analysis are described in sections 2 and 3, respectively. Relative to ref. [52], this analysis incorporates new DL signal modes and employs new particle reconstruction and identification techniques in the SL channel. These include more efficient algorithms for identifying electrons and jets with b hadrons (b tagging) as well as an improved reconstruction procedure for the  $H \rightarrow WW^* \rightarrow \ell\nu q\bar{q}'$  decay. The developments are discussed in section 4, which details the event reconstruction and identification, including the final-state particles and the intermediate-state bosons. Section 5 discusses the selection criteria used to discriminate signal from background and the division of all events into 12 exclusive categories by the number of leptons, the lepton flavor, the quality of jet flavor tagging, and the  $H \rightarrow WW^*$  decay kinematics. Section 6 details the model-building process for the signal and the background. The signal and SM background yields are estimated using a simultaneous maximum likelihood fit to the 2D  $m_{b\bar{b}}$  and  $m_{HH}$  mass distributions in all 12 categories. All systematic uncertainties are discussed in section 7, and the post-fit results are presented in section 8. The analysis is summarized in section 9.

Tabulated results are provided in the HEPData record for this analysis [53].

## 2 The CMS detector and global event reconstruction

The central feature of the CMS apparatus is a superconducting solenoid of 6 m internal diameter, providing a magnetic field of 3.8 T. Within the solenoid volume are a silicon pixel and strip tracker, a lead tungstate crystal electromagnetic calorimeter (ECAL), and a brass and scintillator hadron calorimeter (HCAL), each composed of a barrel and two endcap sections. Forward calorimeters extend the pseudorapidity ( $\eta$ ) coverage provided by the barrel and endcap detectors. Muons are measured in gaseous detectors embedded in

the steel flux-return yoke outside the solenoid. A more detailed description of the CMS detector, together with a definition of the coordinate system used and the relevant kinematic variables, can be found in ref. [54].

Events of interest are selected using a two-tiered trigger system. The first level, composed of custom hardware processors, uses information from the calorimeters and muon detectors to select events at a rate of around 100 kHz within a fixed latency of about 4  $\mu$ s [55]. The second level, known as the high-level trigger, consists of a farm of processors running a version of the full event reconstruction software optimized for fast processing and reduces the event rate to around 1 kHz before data storage [56].

Event reconstruction relies on a particle-flow (PF) algorithm [57], which aims to identify each individual particle in an event with an optimized combination of information from the various elements of the CMS detector. The vector  $\vec{p}_T^{\text{miss}}$  is computed as the negative vector  $p_T$  sum of all the PF candidates in an event, and its magnitude is denoted as  $p_T^{\text{miss}}$  [58]. The  $\vec{p}_T^{\text{miss}}$  is modified to account for corrections to the energy scale of the reconstructed jets in the event. In each event, jets are clustered from these PF candidates using the anti- $k_T$  algorithm [59, 60] with a distance parameter of 0.4 (AK4 jets) and of 0.8 (AK8 jets).

The jet momentum is determined as the vectorial sum of all particle momenta in the jet, and is found from simulation to be, on average, within 5–10% of the true momentum over the entire  $p_T$  spectrum and detector acceptance. Additional pp interactions within the same or nearby bunch crossings (pileup) can contribute extra tracks and calorimetric energy depositions, increasing the apparent jet momentum. To mitigate this effect for AK4 jets, tracks identified as originating from pileup vertices are discarded, and an offset correction is applied to correct for residual contributions [57, 60]. For AK8 jets, a different pileup per particle identification algorithm [61, 62] reduces the effect of pileup by considering local shape variables [62] to rescale the momentum of each jet constituent according to its probability to originate from the primary vertex. Jet energy corrections are derived from simulation studies so that the average measured energy of jets becomes identical to that of particle-level jets. In situ measurements of the momentum balance in dijet, photon+jet, Z+jet, and multijet events are used to determine any residual differences between the jet energy scale in data and in simulation, and appropriate corrections are made [63].

### 3 Simulated samples

Signal and background yields are extracted from a fit to the data in the 2D  $m_{b\bar{b}}$  and  $m_{HH}$  mass distribution using templates obtained from samples generated by Monte Carlo (MC) simulation.

The signal processes  $pp \rightarrow X \rightarrow HH \rightarrow b\bar{b}VV^*$  (where  $V = W$  or  $Z$ ) and  $pp \rightarrow X \rightarrow HH \rightarrow b\bar{b}\tau\tau$  are simulated for spin-0 radions and spin-2 gravitons in the bulk scenario of Randall-Sundrum models with warped extra dimensions. Only the  $b\bar{b}WW^*$  and  $b\bar{b}\tau\tau$  events are used to optimize the analysis, but any  $b\bar{b}ZZ^*$  events that pass the full selection are included in the signal acceptance. The simulated X bosons are produced via gluon fusion and with a narrow width (1 MeV) that is small compared to the experimental resolution of roughly 5%. The branching fractions used to normalize the signal correspond to those

expected for SM Higgs boson decays. The signal is generated at leading order (LO) using the MADGRAPH5\_aMC@NLO V5 2.4.2 generator [64] with the MLM merging scheme [65] for  $m_X$  of 0.8–4.5 TeV.

The MADGRAPH5\_aMC@NLO generator is also used to produce the W+jets,  $Z/\gamma^* \rightarrow \ell\ell$ , and QCD multijet background samples at LO. The W+jets and  $Z/\gamma^* \rightarrow \ell\ell$  samples are normalized using next-to-next-to-LO (NNLO) cross sections, calculated with FEWZ v3.1 [66]. Samples of WZ diboson production and of the associated production of  $t\bar{t}$  with either a W or Z boson are also generated with MADGRAPH5\_aMC@NLO but at next-to-LO (NLO) with the FxFx jet merging scheme [67]. The POWHEG v2 generator is used to produce samples for  $t\bar{t}$ , WW, ZZ,  $t\bar{t}H$ , and single top quark production at NLO [68–75]. Furthermore, the  $t\bar{t}$  process is normalized to the NNLO cross section, computed with TOP++ v2.0 [76].

Parton showering and hadronization are simulated in the 2016 samples with PYTHIA v8.226 [77] using the CUETP8M1 [78] tune, except for the  $t\bar{t}$ ,  $t\bar{t}H$ , and  $X \rightarrow HH \rightarrow b\bar{b}V V^*$  signal samples, which are simulated using the CP5 tune. For 2017–2018, PYTHIA v8.230 and the CP5 tune [79] are used to produce the samples. The parton distribution functions (PDFs) used to produce the samples are the NNPDF 3.0 [80] set for the 2016 data set and the NNPDF 3.1 [81] set for the 2017–2018 data sets. The simulation of the CMS detector is performed with the GEANT4 [82] toolkit. The simulated samples are weighted to have the same multiplicity distribution of pileup interactions as observed in data.

## 4 Decay chain reconstruction

All signal events, regardless of lepton multiplicity, feature a high- $p_T$  jet that has substructure consistent with two b quark decays. This jet is generally opposite in the transverse plane to a collection of other particles from a boosted Higgs boson decay. In the SL channel, signal events feature a lepton originating from a boosted W boson decay and a nearby jet that has substructure consistent with a  $W \rightarrow q\bar{q}'$  decay. Even at the lowest considered  $m_X$  of 0.8 TeV, the median angular distance  $\Delta R = \sqrt{(\Delta\eta)^2 + (\Delta\phi)^2}$  (where  $\phi$  is the azimuthal angle) between the  $W \rightarrow q\bar{q}'$  decay and the lepton is approximately  $\Delta R = 0.5$ . In the DL channel, there are two high- $p_T$  leptons originating from the decay of either a boosted W boson pair or a boosted  $\tau$  lepton pair, but there is no jet in the vicinity of the leptons, resulting in a cleaner experimental signature.

Events are first selected by the trigger system with small year-to-year differences in the criteria. Events are triggered if they contain one of the following: an isolated muon with  $p_T > 24$  GeV (27 GeV in 2017), an isolated electron with  $p_T > 32$  GeV (27 GeV in 2016), or  $H_T > 1050$  GeV (900 GeV in 2016), where  $H_T$  is the scalar sum of jet  $p_T$  for all trigger-level AK4 jets with  $p_T > 30$  GeV. An inclusive-OR combination of lepton and  $H_T$  triggers is used because the high- $m_X$  SL signal does not have leptons that are sufficiently isolated to pass the online lepton isolation selection, as the decay products  $WW^* \rightarrow \ell\nu q\bar{q}'$  are highly collimated. Additional multiobject triggers that select events with at least one lepton and considerable jet energy supplement these triggers, helping to maintain high trigger efficiency for signal over the entire range of  $m_X$ . In particular, these multiobject triggers fire for events with  $H_T > 450$  GeV (400 GeV in 2016) and a lepton that has  $p_T > 15$  GeV

and looser isolation requirements than for the previously mentioned isolated single-lepton triggers. These multiobject triggers are particularly helpful for the SL signal topology with the lepton close to the jet. The trigger efficiency is measured for  $e\mu t\bar{t}$  events in data for events passing offline selection criteria for  $H_T$  in the SL channel and both  $H_T$  and lepton  $p_T$  in the DL channel. We use  $t\bar{t}$  events because the lepton and jet multiplicities resemble those in signal events. Simulation is corrected such that the trigger efficiency matches that in the data. In the SL channel, the trigger efficiency for signal events is over 96% at  $m_X = 0.8$  TeV and increases to >99% above  $m_X = 1.0$  TeV. In the DL channel, the trigger efficiency is >99% over the full range of  $m_X$ .

#### 4.1 Electron and muon identification

Different selection criteria are required for the SL and DL channels to identify signal-like leptons because of the different decay topologies. First, however, an event in either channel must contain either a muon with  $p_T > 27$  GeV or an electron with  $p_T > 30$  GeV. In the DL channel, the other lepton must have  $p_T > 10$  GeV. All muons are required to have  $|\eta| < 2.4$ . Electrons in the DL channel are required to have  $|\eta| < 2.5$ , but those in the SL channel are restricted to the ECAL barrel region ( $|\eta| < 1.479$ ) to suppress a significant contribution from the QCD multijet background with a small loss in signal acceptance. Leptons must satisfy reconstruction quality and identification requirements that are optimized to maintain high efficiency and low probability for misidentifying hadrons as leptons [83, 84]. Additionally, the impact parameters of lepton tracks with respect to the primary vertex are required to be consistent with those originating from this vertex. Looser constraints on the impact parameter are used in the DL channel because some of the leptons originate from  $H \rightarrow \tau\tau$  decays and thus have significant displacements from the primary vertex. Leptons are required to be isolated with an isolation cone size designed for leptons from boosted decays, in which the cone size becomes smaller with larger  $p_T$  [85]. Because less hadronic energy is expected near the leptons in the DL channel than in the SL channel, the allowed extra transverse energy in the isolation cone is smaller.

In the SL channel, as measured with signal simulation, the electron selection efficiency has a maximum of 70% at  $m_X = 0.8$  TeV and then degrades to 7.5% at  $m_X = 4.5$  TeV. This is caused by a selection imposed at a low-level reconstruction step on the ratio of the energy deposited in the HCAL to that deposited in the ECAL. Electrons in the  $H \rightarrow WW^* \rightarrow e\nu q\bar{q}'$  decay often fail this selection because of nearby energy deposits from the  $q\bar{q}'$  jet, which grow with larger boosts. However, the reconstruction of muons does not rely on such HCAL measurements and so is much more efficient than for electrons, but the isolation of muons is still sensitive to the  $q\bar{q}'$  jet. As a result, the overall selection efficiency for signal muons is better than for electrons but still degrades for larger  $m_X$ ; the muon efficiency ranges from approximately 90% at  $m_X = 0.8$  TeV down to 60% at  $m_X = 4.5$  TeV.

In the DL channel, where there is no  $q\bar{q}'$  jet, the lepton selection efficiency is larger for all  $m_X$  than in the SL channel. Because of the increased boost of the system, the efficiency still drops toward high  $m_X$ . For electrons, the reconstruction efficiency is much larger than in the SL channel, ranging from approximately 82% at  $m_X = 0.8$  TeV down to 71% at  $m_X = 4.5$  TeV. The muon efficiency is also larger, ranging from approximately 96% at

$m_X = 0.8 \text{ TeV}$  down to 91% at  $m_X = 4.5 \text{ TeV}$ . The lepton efficiencies are also measured in simulation and data in a  $Z \rightarrow \ell\ell$  sample, and the simulation is corrected to match the efficiency in data. The systematic uncertainties in these measurements are applied to the normalization of the signal.

## 4.2 Reconstruction and flavor identification of jets

Because of the boost imparted to the Higgs bosons by the decay of the much more massive X boson, the  $H \rightarrow b\bar{b}$  and  $W \rightarrow q\bar{q}'$  decays are each reconstructed as a single, merged AK8 jet with two-prong substructure. In order to prevent the  $q\bar{q}'$  jet from containing the lepton's momentum in the SL channel, the PF candidates associated with the lepton are not included in the clustering of the set of jets from which the  $q\bar{q}'$  jet is selected. Only the PF candidates associated with a lepton that fulfills the analysis requirements are removed, and the same jet energy corrections described in section 2 for AK8 jets are applied to these lepton-subtracted AK8 jets. We ensure the validity of applying these corrections to the lepton-subtracted AK8 jets by comparing the jet energy response in simulation between jets that require lepton subtraction and jets that do not. Jets of both types are required to have  $|\eta| < 2.4$  so that most of the jet particles are within the acceptance of the tracker.

The Higgs bosons have collimated decays and typically are produced back-to-back in the transverse plane, i.e.,  $\Delta\phi(H, H) \approx \pi$ . The  $b\bar{b}$  jet candidate is required to have  $p_T > 200 \text{ GeV}$ . In the SL channel, it is required to have a  $\Delta\phi > 2.0$  separation from the lepton and a  $\Delta R > 1.6$  separation from the  $q\bar{q}'$  jet, while in the DL channel, it is required to have a  $\Delta\phi > 2.0$  separation from the dilepton momentum and to not contain either lepton within the jet cone. The  $q\bar{q}'$  jet in the SL channel is chosen as the closest AK8 jet in  $\Delta R$  to the lepton, provided that it is found within  $\Delta R < 1.2$  of the lepton and has  $p_T > 50 \text{ GeV}$ . Within both the  $b\bar{b}$  and  $q\bar{q}'$  jets, two subjets are reconstructed that must each have  $p_T > 20 \text{ GeV}$ . Constituents of the AK8 jets are first reclustered using the Cambridge-Aachen algorithm [86, 87]. The “modified mass drop tagger” algorithm [88, 89], also known as the “soft drop” (SD) algorithm, with angular exponent  $\beta = 0$ , soft cutoff threshold  $z_{\text{cut}} < 0.1$ , and characteristic radius  $R_0 = 0.8$  [90], is applied to remove soft, wide-angle radiation from the jet. The subjets used are those remaining after the algorithm has removed all recognized soft radiation. The jets in this analysis are required to have exactly two subjets. The SD jet mass is the invariant mass of these two subjets. The SD jet mass of the  $b\bar{b}$  jet is used to obtain the search variable  $m_{b\bar{b}}$ , after applying  $p_T$ -dependent corrections, so that  $m_{b\bar{b}}$  in simulation is on average equal to the Higgs boson mass of 125 GeV.

Identifying the  $H \rightarrow b\bar{b}$  decay in signal events and discriminating against background events relies on tagging jets as likely to have originated from b hadron decays. The AK8 jets are identified as consistent with a  $b\bar{b}$  decay using the DEEPAK8 mass-decorrelated Z/H  $\rightarrow b\bar{b}$  tagger [91], with a discriminator denoted as  $D_{Z/H \rightarrow b\bar{b}}$ , at a working point that has an efficiency of  $\approx 85\%$  for selecting  $b\bar{b}$  jets and a misidentification probability of  $< 1\%$  for pure light-flavor quark and gluon jets. This is a deep neural network based tagger, designed to discriminate high- $p_T$  jets consistent with a  $b\bar{b}$  substructure against light-flavor quark (u, d, s) or gluon jets. Furthermore, by design the tagger does not sculpt the SD jet mass



distributions, thereby enabling the use of the SD jet mass in the background estimation. The b tagging efficiencies are measured in data, and the simulation is corrected for any discrepancies. The uncertainty in this  $b\bar{b}$  tagging efficiency is the dominant systematic uncertainty in the analysis, denoted as “ $b\bar{b}$  jet tagging” in table 7 and discussed later in section 7.2.

In  $t\bar{t}$  events, the most common events misreconstructed as signal, the  $b\bar{b}$  jet candidate is typically reconstructed around the decay of one of the b quarks, while the other b quark decays into the opposite direction in the transverse plane. Identifying a b-tagged AK4 jet that is separated from the  $b\bar{b}$  jet is an effective method of discriminating between such  $t\bar{t}$  events and signal events, in which the  $b\bar{b}$  jet is reconstructed from the two  $H \rightarrow b\bar{b}$  quarks. To be considered a candidate b jet, an AK4 jet must have  $p_T > 30$  GeV and be identified using the DEEPJET tagger [92–94] at a working point that has an efficiency of  $\approx 80\%$  for selecting b jets and a misidentification probability of  $\approx 1\%$  for light-flavor quark and gluon jets.

### 4.3 Reconstructing the HH system mass

Depending on whether the final state has one or two leptons, different strategies are employed to reconstruct the four-momentum of the Higgs boson that does not decay to  $b\bar{b}$ . The mass  $m_{HH}$  is then the invariant mass of this four-momentum and the  $b\bar{b}$  jet four-momentum. The mass of the  $b\bar{b}$  jet used in this calculation is not the SD jet mass  $m_{b\bar{b}}$  but is rather the ungroomed jet mass. In sections 4.3.1 and 4.3.2, respectively, the reconstruction strategies are described for the SL and DL channels.

#### 4.3.1 Single-lepton channel

To reconstruct the Higgs boson four-momentum in the  $H \rightarrow WW^* \rightarrow \ell\nu q\bar{q}'$  decay chain from the visible and invisible decay products, a likelihood-based technique that takes the reconstructed lepton, the  $\vec{p}_T^{\text{miss}}$ , and the  $q\bar{q}'$  jet as input is employed. For each event, values for the following five parameters are extracted by maximizing a likelihood function:

- $\vec{p}_\nu$ : the three components of the neutrino momentum.
- $R_{q\bar{q}'}$ : the jet response correction, a multiplicative scale factor applied to the  $p_T$  of the  $q\bar{q}'$  jet. The jet  $p_T$  is allowed to vary because the uncertainty associated with the estimated  $p_T$  of this jet is large.
- $V_{q\bar{q}'}$ : a boolean indicator of whether the  $q\bar{q}'$  jet favors a larger or smaller mass than the leptonic W boson decay. This is largely a bookkeeping device for the W and  $W^*$  hypotheses.

With these parameters, the  $H \rightarrow WW^*$  four-momentum can be fully determined. This four-momentum is then the sum of the neutrino four-momentum  $p_\nu$ , the  $q\bar{q}'$  jet four-momentum (with  $p_T$  modified by  $R_{q\bar{q}'}$ ), and the four-momentum of the lepton.

The likelihood function is constructed with six probability density functions (pdfs)  $P(x|\vec{y})$  estimated from signal simulation, where  $x$  is the corresponding observable in the pdf. The symbol  $\vec{y}$  represents the set of free parameters associated with that pdf, such as

$V_{q\bar{q}'}$ . These pdfs are represented as one-dimensional (1D) histograms. The full likelihood function is:

$$\mathcal{L} = P(m_{\text{jet}}|V_{q\bar{q}'})P(p_{\text{T}}^{\text{jet}}|R_{q\bar{q}'}, V_{q\bar{q}'})P(m_{\ell\nu q\bar{q}'}|\vec{p}_{\nu}, R_{q\bar{q}'}, V_{q\bar{q}'})P(m_{\ell\nu}|\vec{p}_{\nu}, V_{q\bar{q}'})P(\vec{p}_{\text{T}}^{\text{miss}}|\vec{p}_{\nu}, V_{q\bar{q}'}). \quad (4.1)$$

The observable  $m_{\text{jet}}$  is the SD jet mass of the  $q\bar{q}'$  jet, and its corresponding pdf is coarsely binned to remain insensitive to the precise modeling of the SD algorithm. The observable  $p_{\text{T}}^{\text{jet}}$  is the unmodified  $q\bar{q}'$  jet  $p_{\text{T}}$ , and the pdf  $P(p_{\text{T}}^{\text{jet}}|R_{q\bar{q}'}, V_{q\bar{q}'})$  is the jet  $p_{\text{T}}$  response. Two other observables,  $m_{\ell\nu}$  and  $m_{\ell\nu q\bar{q}'}$ , are masses of the lepton-neutrino pair and the lepton-neutrino- $q\bar{q}'$  jet system.

The last factor in eq. (4.1) represents the product of two pdfs, each corresponding to a single component of  $\vec{p}_{\text{T}}^{\text{miss}}$ :

$$P(\vec{p}_{\text{T}}^{\text{miss}}|\vec{p}_{\nu}, V_{q\bar{q}'}) = P(p_{\text{T},\parallel}^{\text{miss}}|\vec{p}_{\nu}, V_{q\bar{q}'})P(p_{\text{T},\perp}^{\text{miss}}|\vec{p}_{\nu}, V_{q\bar{q}'}). \quad (4.2)$$

The two observables  $p_{\text{T},\parallel}^{\text{miss}}$  and  $p_{\text{T},\perp}^{\text{miss}}$  are defined with respect to the reference frame of the  $H \rightarrow WW^*$  decay, along the direction of  $\vec{p}_{\text{T}}^{\text{reco}}$ :

$$\vec{p}_{\text{T}}^{\text{reco}} = \vec{p}_{\text{T}}^{\text{miss}} + (\vec{p}_{\ell} + \vec{p}_{q\bar{q}' \text{ jet}})_{\text{T}}. \quad (4.3)$$

The two  $\vec{p}_{\text{T}}^{\text{miss}}$  pdf factors are parameterized as the components of the extra  $p_{\text{T}}^{\text{miss}}$  (relative to the neutrino momentum) that are parallel and perpendicular to this vector  $\vec{p}_{\text{T}}^{\text{reco}}$ . The extra  $p_{\text{T}}^{\text{miss}}$  along this direction arises primarily from mismeasurement of the  $b\bar{b}$  jet, while the orthogonal component arises mostly from pileup and the underlying event.

The pdfs  $P$  of the observables are generally independent of  $m_{\text{X}}$ , but there is still some residual dependence. We account for this by producing two sets of pdfs, one at low  $p_{\text{T}}^{\text{reco}}$  ( $<600$  GeV) and one at high  $p_{\text{T}}^{\text{reco}}$  ( $>1400$  GeV). Then, event-by-event, the histogram of the pdf is obtained by interpolating between the two histograms at the two regimes of  $p_{\text{T}}^{\text{reco}}$ . This interpolation is performed linearly as a function of the event  $p_{\text{T}}^{\text{reco}}$ . The  $P$  are all dependent on whether the hadronically decaying W boson is heavier than the leptonically decaying W, so each factor is dependent on the free parameter  $V_{q\bar{q}'}$ . Correlations among the observables in the likelihood were studied and found not to affect the sensitivity significantly.

This method gives an  $m_{\text{HH}}$  resolution for signal events that is very similar to that from a direct calculation using the Higgs boson mass as a constraint (as in [52]), but for background events it typically returns lower values of  $m_{\text{HH}}$  than in the direct calculation. We take advantage of this fact using an alternative likelihood  $\mathcal{L}_{\text{alt}}$ , which is less constrained by the intermediate masses. Instead of fitting for the neutrino  $p_z$ , the masses  $m_{\ell\nu}$  and  $m_{\ell\nu q\bar{q}'}$  are included as free parameters. Both likelihoods are used to construct a discriminating variable between signal and background:

$$D_{\ell\nu q\bar{q}'} = -2 \log \mathcal{L} / \mathcal{L}_{\text{alt}}, \quad (4.4)$$

where  $\mathcal{L}$  is the likelihood described in eq. (4.1). We discuss how  $D_{\ell\nu q\bar{q}'}$  is used in section 5.

### 4.3.2 Dilepton channel

Because of the absence of a  $q\bar{q}'$  jet, the presence of larger  $p_T^{\text{miss}}$ , and much smaller backgrounds, there is no need for a likelihood-based technique to separate signal and background in the DL channel. Instead, we make simple assumptions regarding the decay kinematic distributions in order to reconstruct the full invisible four-momentum  $p_{\text{inv}}$  due to neutrinos. First, the transverse components of  $p_{\text{inv}}$  are taken directly from the  $\vec{p}_T^{\text{miss}}$ . Second, because the decay products of the boosted Higgs boson are collimated, we assume the polar angle  $\theta$  of  $p_{\text{inv}}$  is equal to that of the dilepton momentum:  $\theta_{\text{inv}} = \theta_{\ell\ell}$ . With this constraint, the  $z$ -component of  $p_{\text{inv}}$  is obtained. Lastly, the invisible invariant mass  $m_{\text{inv}}$  due to neutrinos is assumed to be 55 GeV, the mean of the distribution from signal simulation. The corresponding Higgs boson four-momentum is the summed four-momentum of  $p_{\text{inv}}$  and the dilepton four-momentum  $p_{\ell\ell}$ .

## 5 Event selection and categorization

Events are selected in this search if they pass the following criteria indicating that they could include the production and decay of an X boson. They are then divided into 12 distinct categories (eight SL and four DL). A separate set of criteria is applied to define control regions that are used to validate the modeling of background processes.

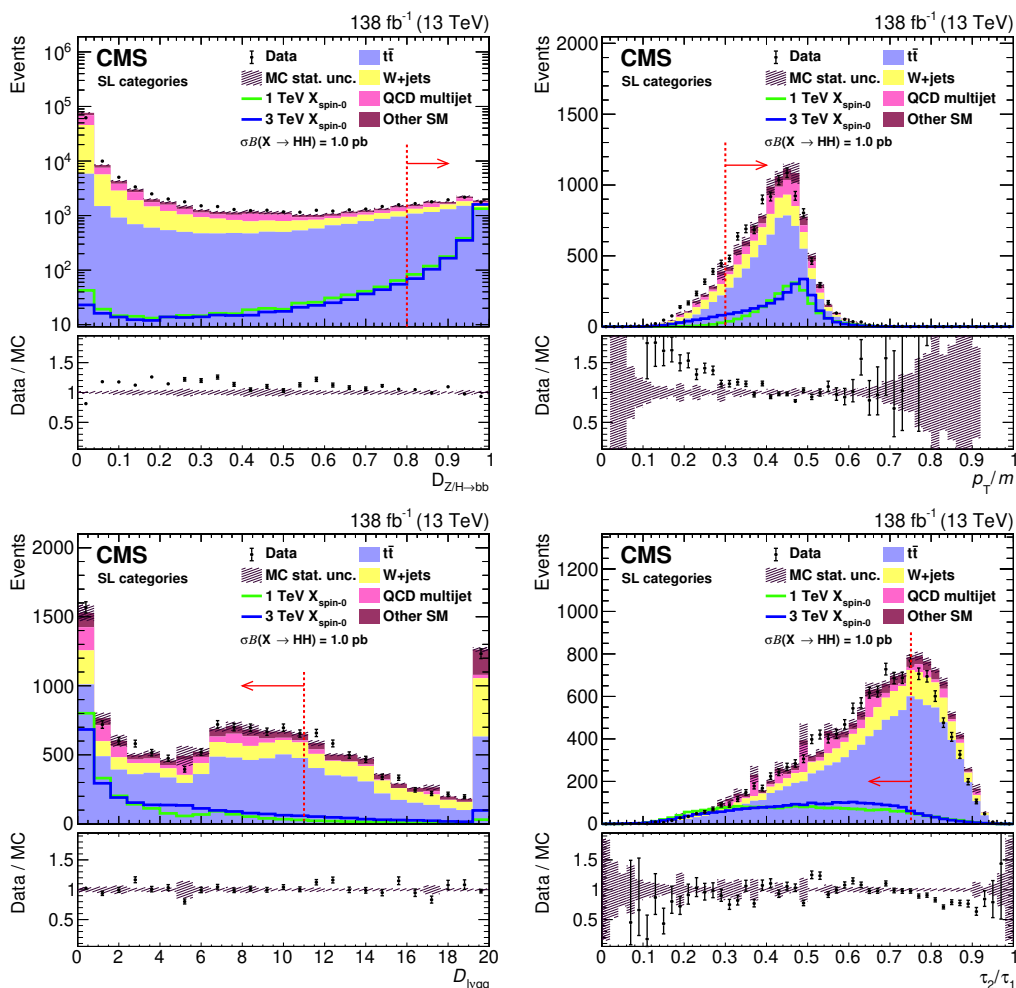
Offline, all events are required to have  $H_T > 400$  GeV, either one electron with  $p_T > 30$  GeV or one muon with  $p_T > 27$  GeV, and a selected  $b\bar{b}$  jet. Background from  $t\bar{t}$  production is reduced by vetoing all events with an AK4 jet that is  $\Delta R > 1.2$  from the  $b\bar{b}$  jet and is identified as a b jet, as described in section 4.2.

We ensure that the sets of events belonging to the SL and DL channels are disjoint. To accomplish this, we first impose that any event with exactly two oppositely charged lepton candidates passing the DL channel lepton selection be assigned as a DL event. Otherwise, if the event has at least one lepton candidate passing the SL channel lepton selection and also has fewer than two lepton candidates passing the DL channel lepton selection, it is classified as an SL event. In this case, the highest- $p_T$  lepton candidate that passes the SL channel lepton selection is selected for Higgs boson reconstruction. If these two criteria cannot be fulfilled by the set of lepton candidates, the event is not used in the analysis.

The following sections review the event selection and categorization of events into the 12 exclusive search regions. Selections that are used only to discriminate signal from background and not to categorize events are detailed in sections 5.1 and 5.2 for the SL and DL channels, respectively. Section 5.3 discusses the discriminating selections that are also used to categorize events.

### 5.1 Single-lepton channel event selection

In the SL channel, the  $q\bar{q}'$  jet is chosen as the closest AK8 jet to the lepton, and it is required to have  $p_T > 50$  GeV and be located within  $\Delta R < 1.2$  of the lepton, where the former requirement is optimized for signal acceptance and the latter for background rejection. Jets in background events tend to be produced at higher  $|\eta|$  than those produced in signal events, which contain jets from the decay of a heavy particle. To exploit this property,



**Figure 1.** Single-lepton channel observables: distributions are shown for data (points), pre-fit simulated SM processes (filled histograms), and simulated signal (solid lines). The statistical uncertainty in the simulated sample is shown as the hatched band. Spin-0 signals for  $m_X$  of 1.0 and 3.0 TeV are displayed. The rightmost bin in the  $D_{\ell\nu q\bar{q}}$  plot contains the overflow events. For both signal models,  $\sigma\mathcal{B}(X \rightarrow HH)$  is set to 1.0 pb. The lower panels of each plot show the ratio of the data to the sum of all background processes. The red dashed line and arrow indicate the selected region of the variable of interest.

the ratio of the  $p_T$  of  $H \rightarrow WW^*$  divided by  $m_{HH}$ , denoted as  $p_T/m$ , is required to be  $>0.3$ . The distribution of  $p_T/m$  is shown in figure 1 (upper right) for the data, expected pre-fit background, and two signal mass hypotheses with a normalization corresponding to a product of the cross section and branching fraction ( $\sigma\mathcal{B}$ ) of 1.0 pb.

## 5.2 Dilepton channel event selection

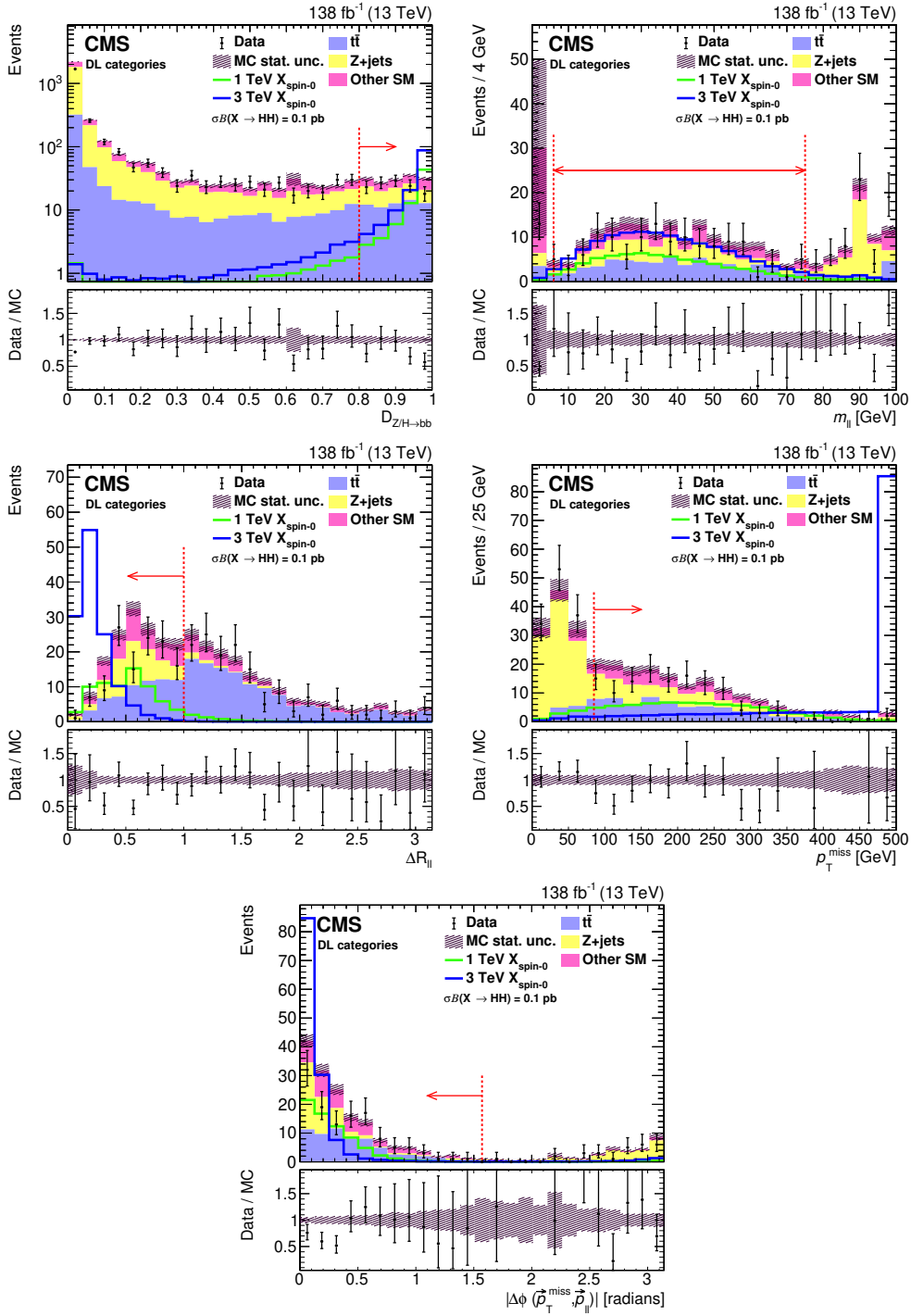
Events in the DL channel must pass additional criteria. In signal events, the invariant mass of the two leptons is kinematically constrained by the mass of the boosted Higgs boson from which they originate, peaking near 30 GeV. Background in the  $m_{\ell\ell}$  spectrum from  $Z/\gamma^*+jets$

populates predominantly lower masses from the continuum and higher masses from the Z boson. Background from  $t\bar{t}$  also populates higher masses since the leptons are typically opposite each other in the transverse plane. Requiring the dilepton invariant mass to satisfy  $6 < m_{\ell\ell} < 75$  GeV reduces these backgrounds while preserving the signal. Requiring that the leptons be close together in  $\eta$ - $\phi$  space with  $\Delta R_{\ell\ell} < 1.0$  further helps to suppress the  $t\bar{t}$  background. In  $Z/\gamma^* + \text{jets}$  the  $\vec{p}_T^{\text{miss}}$  can be in the direction of the  $b\bar{b}$  jet, away from the leptons, due to jet mismeasurements, while in signal the  $\vec{p}_T^{\text{miss}}$  is close to the leptons because of the boosted Higgs boson decay. Thus, we also require that  $|\Delta\phi(\vec{p}_T^{\text{miss}}, \vec{p}_{\ell\ell})| < \pi/2$  to discriminate against  $Z/\gamma^* + \text{jets}$ . Background is further separated from signal by requiring  $p_T^{\text{miss}} > 85$  GeV. Figure 2 shows the distributions of the discriminating variables  $m_{\ell\ell}$  (upper right),  $\Delta R_{\ell\ell}$  (middle left),  $p_T^{\text{miss}}$  (middle right), and  $|\Delta\phi(\vec{p}_T^{\text{miss}}, \vec{p}_{\ell\ell})|$  (lower).

### 5.3 Event categorization

Events are categorized by event properties that reflect the signal purity, and the categorization is the same over the full range of  $m_X$ . In the SL channel, electron and muon events are separated because their reconstruction efficiencies for background and signal are different, resulting in different signal purities. The electron and muon categories are labeled “e” and “ $\mu$ ,” respectively, in the figures. Likewise, in the DL channel, events with leptons of the same flavor and of the opposite (different) flavor are separated because the background composition is different between these two cases. These are labeled “SF” and “OF,” respectively, in the figures. We do not separate ee from  $\mu\mu$  in the DL channel because these events have similar ratios of signal to background. For all events, there are two categories for  $b\bar{b}$  jet tagging, constructed from different subsets of the distribution of the DEEPAK8 mass-decorrelated  $Z/H \rightarrow b\bar{b}$  discriminator  $D_{Z/H \rightarrow b\bar{b}}$ , introduced in section 4.2. The distribution of  $D_{Z/H \rightarrow b\bar{b}}$  is shown in the upper left plot of figures 1 and 2 for the SL and DL channels, respectively. The discriminator value ranges from 0 to 1, with larger values indicating that the jet is more consistent with  $b\bar{b}$  substructure. We use two working points that yield a loose category defined by  $0.8 < D_{Z/H \rightarrow b\bar{b}} < 0.97$  (labeled “bL”) and a tight category defined by  $D_{Z/H \rightarrow b\bar{b}} \geq 0.97$  (labeled “bT”). One more criterion for categorization, related to the  $H \rightarrow WW^* \rightarrow \ell\nu q\bar{q}'$  decay, is implemented for the SL channel but not the DL channel. This categorization relies on both the  $\tau_2/\tau_1$   $N$ -subjettiness ratio [95] of the  $q\bar{q}'$  jet (denoted now as  $\tau_2/\tau_1$ ) and the  $H \rightarrow WW^*$  likelihood discriminator  $D_{\ell\nu q\bar{q}'}$  that was first introduced in eq. (4.4). The ratio  $\tau_2/\tau_1$  measures how consistent the jet substructure is with a two-prong decay versus a single-prong decay, with lower values more strongly indicating a two-prong decay. Figure 1 shows the distributions of  $D_{\ell\nu q\bar{q}'}$  (lower left) and  $\tau_2/\tau_1$  (lower right). All events in the SL but not in the DL search region are required to satisfy both  $\tau_2/\tau_1 < 0.75$  and  $D_{\ell\nu q\bar{q}'} < 11.0$ . We construct a low-purity category (labeled “LP”) with events that satisfy either  $0.45 < \tau_2/\tau_1 < 0.75$  or  $2.5 < D_{\ell\nu q\bar{q}'} < 11.0$  and a high-purity category (labeled “HP”) with events that satisfy both  $\tau_2/\tau_1 < 0.45$  and  $D_{\ell\nu q\bar{q}'} < 2.5$ . In 2016 data, the lower working point for  $\tau_2/\tau_1$  is 0.55 instead of 0.45.

The selections just described are combined to produce 12 distinct search categories (eight SL and four DL). When describing a single category, the label is a combination of those listed above. For example, in the SL channel the tightest  $b\bar{b}$  jet tagging category



**Figure 2.** Dilepton channel observables: distributions are shown for data (points), pre-fit simulated SM processes (filled histograms), and simulated signal (solid lines). The statistical uncertainty in the simulated sample is shown as the hatched band. Spin-0 signals for  $m_X$  of 1.0 and 3.0 TeV are displayed. The rightmost bin in the  $m_{\ell\ell}$ ,  $\Delta R_{\ell\ell}$ , and  $p_T^{\text{miss}}$  plots contains the overflow events. For both signal models,  $\sigma\mathcal{B}(X \rightarrow \text{HH}) = 0.1$  pb. The lower panels of each plot show the ratio of the data to the sum of all background processes. The red dashed line and arrow indicate the selected region of the variable of interest.

Categorization type	Selection	Label
Lepton flavor	Electron	e
	Muon	$\mu$
$b\bar{b}$ jet tagging	$0.8 < D_{Z/H \rightarrow b\bar{b}} < 0.97$	bL
	$D_{Z/H \rightarrow b\bar{b}} > 0.97$	bT
$H \rightarrow WW^*$ purity	$0.45(0.55) < \tau_2/\tau_1 < 0.75$ or $2.5 < D_{\ell\nu q\bar{q}'} < 11.0$	LP
	$\tau_2/\tau_1 < 0.45(0.55)$ and $D_{\ell\nu q\bar{q}'} < 2.5$	HP

**Table 1.** The SL channel event categorization and corresponding category labels. All combinations of the two lepton flavors, two  $b\bar{b}$  jet tagging, and two  $H \rightarrow WW^*$  decay purity selections are used to form eight independent event categories. The lower  $\tau_2/\tau_1$  working point is 0.55 (0.45) in 2016 (2017–2018).

Categorization type	Selection	Label
Lepton flavor	Two electrons or two muons	SF
	One electron and one muon	OF
$b\bar{b}$ jet tagging	$0.8 < D_{Z/H \rightarrow b\bar{b}} < 0.97$	bL
	$D_{Z/H \rightarrow b\bar{b}} > 0.97$	bT

**Table 2.** The DL channel event categorization and corresponding category labels. All combinations of the two lepton flavors and two  $b\bar{b}$  jet tagging selections are used to form four independent event categories.

with a low-purity selection on the  $H \rightarrow WW^*$  decay in the electron channel is: “e, bT, LP.” The categories and their corresponding labels are summarized in tables 1 and 2.

The search is performed for  $30 < m_{b\bar{b}} < 210$  GeV and  $700 < m_{HH} < 5050$  GeV. Extending the  $m_{b\bar{b}}$  mass window down to 30 GeV helps to capture the background in the fit, but events below 30 GeV would be relatively difficult to model since these are events for which the SD algorithm removes nearly all of the jet energy. The  $m_{HH}$  lower bound is chosen such that the  $m_{HH}$  distribution is monotonically decreasing for the full background. The upper bound is several hundred GeV above the highest mass event observed in data.

For spin-0 scenarios in the considered HH modes, the total selection efficiency for an SL channel event to pass the criteria of any event category is 9% at  $m_X = 0.8$  TeV. This efficiency includes the branching fraction for  $H \rightarrow b\bar{b}$ . The efficiency increases with  $m_X$  up to 23% at  $m_X = 1.5$  TeV because the Higgs boson decays become more collimated. Above 1.5 TeV, the selection efficiency decreases to a minimum of 14% at  $m_X = 4.5$  TeV for two main reasons: the b tagging efficiency degrades for high- $p_T$  jets and the lepton isolation worsens for extremely collimated Higgs boson decays. For DL channel events, the combined selection efficiency to pass the criteria of any event category is 9% at  $m_X = 0.8$  TeV, increases sharply with  $m_X$  to 30% at  $m_X = 1.5$  TeV, and then increases more slowly to 36% at  $m_X = 4.5$  TeV. The efficiency grows over the full range of  $m_X$  because in the absence of a nearby jet, the leptons become easier to select at high  $p_T$ . Tables 3 and 4 show the efficiencies for each individual selection requirement with the full selection otherwise applied.

SL channel selection	Background	Signal	
		1 TeV	3 TeV
b jet veto	0.31	0.87	0.82
$D_{Z/H \rightarrow b\bar{b}} > 0.8$	0.07	0.81	0.84
$\tau_2/\tau_1 < 0.75$	0.69	0.91	0.92
$D_{\ell\nu q\bar{q}'} < 11.0$	0.63	0.87	0.83
$p_T/m > 0.3$	0.87	0.97	0.86

**Table 3.** Efficiencies of each selection criterion in the SL channel with the rest of the full selection applied. The efficiencies for the total expected SM background and signals at 1.0 and 3.0 TeV are shown.

DL channel selection	Background	Signal	
		1 TeV	3 TeV
b jet veto	0.45	0.86	0.84
$D_{Z/H \rightarrow b\bar{b}} > 0.8$	0.05	0.81	0.83
$p_T^{\text{miss}} > 85 \text{ GeV}$	0.55	0.88	0.97
$6 < m_{\ell\ell} < 75 \text{ GeV}$	0.62	0.95	0.94
$\Delta R_{\ell\ell} < 1.0$	0.51	0.93	0.998
$ \Delta\phi(\vec{p}_T^{\text{miss}}, \vec{p}_{\ell\ell})  < \pi/2$	0.83	0.98	0.97

**Table 4.** Efficiencies of each selection criterion in the DL channel with the rest of the full selection applied. The efficiencies for the total expected SM background and signals at 1.0 and 3.0 TeV are shown.

The Higgs bosons in signal events from a spin-2 X boson are produced at lower values of  $|\eta|$  than those from a spin-0 X, resulting in larger selection efficiencies for spin-2 events. The relative increase in efficiency for spin-2 signal is larger at low mass ( $\approx 40\%$ ) than at high mass ( $\approx 15\%$ ).

### 5.4 Control regions

Two control regions (CRs) are used to validate the SM background estimation and systematic uncertainties. These regions are depleted of signal by construction, and the events within them are not used to search for signal. The first, labeled “top CR,” targets background events with top quarks, particularly  $t\bar{t}$ . Such events are selected by inverting the AK4 jet b tag veto. To increase the statistical power of the sample, the  $p_T/m$  selection is removed for SL channel events, and the  $\Delta R_{\ell\ell}$  selection is altered to  $\Delta R_{\ell\ell} > 0.4$  for DL channel events. Events in this CR are then divided into the 12 categories previously described in section 5.3. The  $m_{b\bar{b}}$  and  $m_{HH}$  distributions in this CR are similar to the distributions in the signal region for backgrounds with top quarks. The top quark  $p_T$  spectrum in  $t\bar{t}$  events has been shown to be mismodeled in simulation [96, 97]. A small  $p_T$ -dependent correction, on the order of a few percent, is measured in an expanded version of this CR and applied to the  $t\bar{t}$  simulation.



While the top CR is an adequate probe of processes that involve top quarks, it is not sensitive to background from  $Z/\gamma^*$ +jets,  $W$ +jets, or QCD multijet processes. Instead, a second CR, labeled “non-top CR,” is used to study the modeling of these processes. The selection of events in this CR is the same as for the signal region, except that the  $b\bar{b}$  jet is required to be inconsistent with having  $b\bar{b}$  substructure, i.e.,  $0.01 < D_{Z/H \rightarrow b\bar{b}} < 0.04$ . We exclude events with  $D_{Z/H \rightarrow b\bar{b}} < 0.01$  because of substantial mismodeling in that region. As a result, events in this CR are not categorized by  $b\bar{b}$  jet tagging, yielding half as many (six) categories here as in the top CR. Because it has fewer categories, the non-top CR cannot in principle test the modeling of the  $b$  tagging of  $q/g$  background jets that contain  $b$  quarks or are misidentified as containing  $b$  quarks. Instead, we rely on the top CR to verify that this modeling is well behaved.

Ultimately, the final values of the normalization and shape of each background component and their corresponding uncertainties are determined in the 2D fit to the data in the search region.

## 6 Background and signal modeling

The search is performed by simultaneously estimating the signal and background yields with a 2D maximum likelihood fit of the data in the 12 event categories. The data are binned in two dimensions,  $m_{b\bar{b}}$  and  $m_{HH}$ , within the ranges  $30 < m_{b\bar{b}} < 210$  GeV and  $700 < m_{HH} < 5050$  GeV. The  $m_{b\bar{b}}$  bin width is 6 GeV, and the  $m_{HH}$  bin width is variable: 25 GeV width at the low end of the mass range, 50 GeV width in the middle of the mass range, and 75 GeV at high mass. These bin widths are smaller than the mass resolutions of the signal in the relevant parts of  $m_{HH}$  space. Signal and background mass distributions are modeled using a number of 2D templates that are created using only simulation, which is smoothed using different strategies described in the rest of this section before the templates are fit to data. Independent templates are used for each event category. Shape and normalization uncertainties that account for possible differences between data and simulation, detailed in section 7, are included while executing the fit. This fitting method was previously presented in ref. [98].

### 6.1 Background component classification

To perform the fit to data, we split the background into components and then generate 2D templates in the  $m_{b\bar{b}}$  and  $m_{HH}$  mass plane for each component independently. The normalization and shape of each component is then allowed to vary in the fit to the data in each search category.

Instead of splitting by SM process, we distinguish four components by particle-level information, such that they each have distinct  $m_{b\bar{b}}$  distribution shapes. The background is divided by counting in simulation the number of generator-level quarks from the immediate decay of a top quark or vector boson within  $\Delta R < 0.8$  of the  $b\bar{b}$  jet axis. The first component is the “ $m_t$  background,” in which all three quarks from a single top quark decay fulfill this criterion. The second component is the “ $m_W$  background,” identified as the events that do not fulfill the  $m_t$  background criterion but in which both quarks from

Bkg. category	Dominant SM processes	Resonant in $m_{b\bar{b}}$	Num. of particle-level quarks
$m_t$	$t\bar{t}$	top quark mass	3 from top quark
$m_W$	$t\bar{t}$	W boson mass	2 from W boson
lost-t/W	$t\bar{t}$	No	1 or 2
q/g	V+jets and QCD multijet	No	0

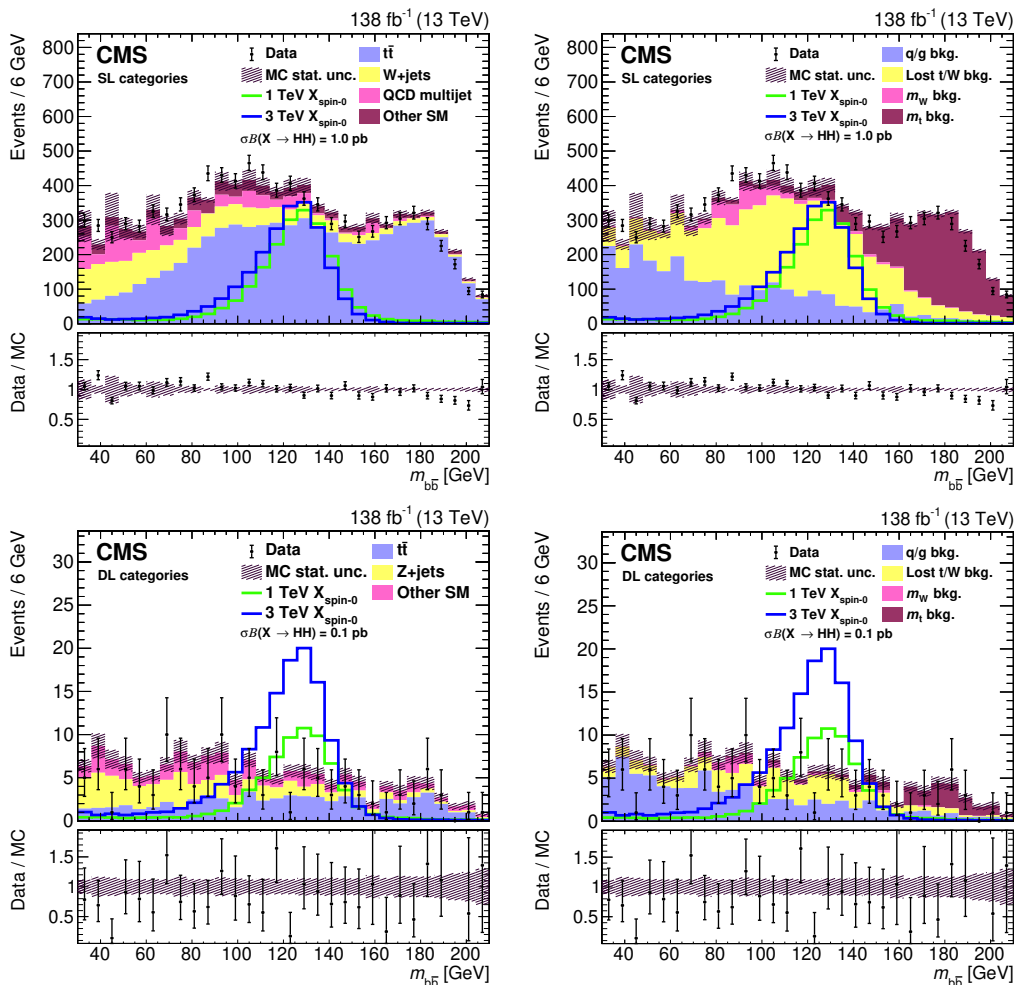
**Table 5.** The four background components with their kinematical properties and defining number of generator-level quarks within  $\Delta R < 0.8$  of the  $b\bar{b}$  jet axis.

either a Z or W boson fall within the jet cone. Both of these backgrounds contain resonant peaks in the  $m_{b\bar{b}}$  shape corresponding to either the top quark or W boson mass. The “lost-t/W background” contains events in which at least one quark is contained within the  $b\bar{b}$  jet cone, but not the full set needed to satisfy one of the previous two requirements. Finally, all other events are designated by the “q/g background”. The first three categories are primarily composed of  $t\bar{t}$  events, while the q/g background is composed mostly of W+jets and QCD multijet processes in the SL channel and of  $Z/\gamma^*$ +jets in the DL channel. The background classification is summarized in table 5. Figure 3 shows the pre-fit  $m_{b\bar{b}}$  spectrum separately for the SL and DL channels. The background components are shown either as SM processes or with the background classification just described.

## 6.2 Template construction strategy

For each of the four background components, a unique template in the  $m_{b\bar{b}}$  and  $m_{HH}$  mass plane is produced for each of the 12 event categories. First, we produce a small set of inclusive templates that have more statistical power than the set of events in each individual search category. These inclusive templates are made by combining events in multiple categories and by relaxing selections, provided that the inclusive shape remains consistent with the shape for the full selection. Then, for each of the 12 event categories, the inclusive templates are fit to the simulated mass distributions to produce templates with their own individual shapes. This fit is performed in a similar manner and with a similar parameterization of the template shape as is done for the fit to data. The background templates and associated systematic uncertainties are ultimately validated by fitting to data in dedicated CRs, a procedure described in section 6.5.

In the SL channel, a modified approach is used when building templates that reduces fluctuations due to the limited size of the QCD multijet simulated event sample. The  $b\bar{b}$  jet reconstruction in the QCD multijet simulation is similar to that in W+jets, and the W+jets simulation has much more statistical power. Both processes contribute significantly to the q/g background, with light-flavored quark or gluon AK8 jets that are misidentified as b jets, yielding very similar falling shapes in the  $m_{b\bar{b}}$  spectrum and similar  $b\bar{b}$  jet tagging distributions. Instead of using the QCD simulation directly in the q/g background modeling, a combined distribution is created by measuring the ratio of QCD to W+jets event yields as a function of  $m_{HH}$  and then using these corrections to scale up the W+jets simulation. Corrections and distributions are obtained for each lepton flavor and  $H \rightarrow WW^*$  purity



**Figure 3.** The pre-fit  $m_{b\bar{b}}$  distributions for the SL (upper row) and DL (lower row) channels. The data are shown as the points with error bars. In each plot, the pre-fit background (filled histograms) is shown broken down either according to the SM process (left) or according to the background classification of section 6.1 (right). The total simulated background is the same in each case. The statistical uncertainty in the simulated sample is shown as the hatched band. Spin-0 signals for  $m_X$  of 1.0 and 3.0 TeV are also shown (solid lines). The product  $\sigma\mathcal{B}(X \rightarrow \text{HH})$  is set to 1.0 pb for the SL channel and 0.1 pb for the DL channel. The lower panels of each plot show the ratio of the data to the sum of all background processes.

category, since the  $b\bar{b}$  jet tagging between  $W$ +jets and QCD is equivalent. This distribution is then used as input to the  $q/g$  background modeling to account for both processes.

### 6.3 Background modeling

The background templates are modeled using conditional probabilities of  $m_{b\bar{b}}$  as a function of  $m_{\text{HH}}$  so that the templates include the correlation of these two variables, fully described in ref. [52]. The full 2D template is defined as:

$$P_{\text{bkg}}(m_{b\bar{b}}, m_{\text{HH}}) = P_{b\bar{b}}(m_{b\bar{b}} | m_{\text{HH}}, \theta_1) P_{\text{HH}}(m_{\text{HH}} | \theta_2), \quad (6.1)$$

where  $P_{b\bar{b}}$  is a 2D conditional probability distribution,  $P_{HH}$  is a 1D probability distribution, and  $\theta_1$  and  $\theta_2$  are sets of nuisance parameters used to account for background shape uncertainties. The sets  $\theta_1$  and  $\theta_2$  do not share any common nuisance parameters.

The  $P_{HH}$  templates are produced by smoothing 1D  $m_{HH}$  histograms with kernel density estimation (KDE) [99–101]. To produce these templates, we use Gaussian kernels with adaptive bandwidths, which are parameters of the KDE that control the smoothing and are dependent on the local event density. We do this to apply less smoothing to regions of the distribution with many events and more smoothing to regions with few events. For  $m_{HH} \gtrsim 2$  TeV, where there are very few events in simulation or in data, the  $m_{HH}$  tail is further smoothed by fitting with an exponential function.

The 2D templates  $P_{b\bar{b}}$  are obtained with different methods for the resonant and nonresonant background components. For each of the resonant backgrounds ( $m_t$  and  $m_W$ ), we fit the  $m_{b\bar{b}}$  distributions with a double Crystal Ball function [102, 103] centered around  $m_t$  and  $m_W$ , respectively. This function has a Gaussian core, which is used to model the bulk of the  $m_{b\bar{b}}$  resonance, and power-law tails, which account for the effects of jet misreconstruction. The fits are performed for events binned in  $m_{HH}$  to capture the dependence of the  $m_{b\bar{b}}$  shape on  $m_{HH}$ . For the nonresonant backgrounds (lost-t/W and q/g), the  $P_{b\bar{b}}$  are estimated from 2D histograms using 2D KDE. Independent KDE parameters are used for each dimension and each background when building the  $P_{b\bar{b}}$  templates. As done for the  $P_{HH}$  tail modeling, the high-mass  $m_{HH}$  distribution tail here is exponentially smoothed. The normalizations from simulation are used as the initial values for the background normalizations in the fit to data.

## 6.4 Signal modeling

The signal templates are also defined following ref. [52] using conditional probabilities:

$$P_{\text{signal}}(m_{b\bar{b}}, m_{HH} | m_X) = P_{HH}(m_{HH} | m_{b\bar{b}}, m_X, \theta'_1) P_{b\bar{b}}(m_{b\bar{b}} | m_X, \theta'_2). \quad (6.2)$$

The sets  $\theta'_1$  and  $\theta'_2$  do not share any common nuisance parameters. However,  $\theta'_2$  and  $\theta_1$  from eq. (6.1) do share two nuisance parameters corresponding to the mass scale and resolution uncertainties of SD jets in the  $m_{b\bar{b}}$  dimension. This is discussed in more detail in section 7.1.2.

The  $P_{\text{signal}}$  distributions are first obtained for discrete  $m_X$  values by fitting histograms of the signal mass distributions. The mass shapes for spin-0 and spin-2 signals are very similar, and so the modeling is performed on the combined set of events and applied to both spin hypotheses. Models continuous in  $m_X$  are then produced by interpolating the fit parameters. The 1D  $P_{b\bar{b}}$  templates are created by fitting the  $m_{b\bar{b}}$  spectra with a double Crystal Ball function, and the mass resolution is slightly larger than 10%, with the largest resolution at low mass. The modeling of events in the bL category also contains an exponential component to model the small fraction of signal events with no resonant peak in the distribution.

The 2D  $P_{HH}$  templates are designed to account for correlations between  $m_{HH}$  and  $m_{b\bar{b}}$ . These  $m_{HH}$  distributions are also modeled with a double Crystal Ball function, but with an additional linear dependence on  $m_{b\bar{b}}$ , parameterized by  $\Delta_{b\bar{b}} = (m_{b\bar{b}} - \mu_{b\bar{b}})/\sigma_{b\bar{b}}$ . Here,  $\mu_{b\bar{b}}$

and  $\sigma_{b\bar{b}}$  are the mean and width parameters, respectively, in the fit to the  $m_{b\bar{b}}$  spectra. To accomplish this, the mean parameter  $\mu_{\text{HH}}$  in the Crystal Ball function fit is then taken to be

$$\mu_{\text{HH}} = \mu_0(1 + \mu_1\Delta_{b\bar{b}}), \tag{6.3}$$

where  $\mu_0$  and  $\mu_1$  are fit parameters. With this approach, we can account for mismeasurements of the  $b\bar{b}$  jet that result in mismeasurements of  $m_{\text{HH}}$ . The resolution of the  $m_{\text{HH}}$  resonance, denoted as  $\sigma_{\text{HH}}$ , is also dependent on  $m_{b\bar{b}}$  such that

$$\sigma_{\text{HH}} = \begin{cases} \sigma_0(1 + \sigma_1|\Delta_{b\bar{b}}|), & \Delta_{b\bar{b}} < 0 \\ \sigma_0, & \Delta_{b\bar{b}} > 0 \end{cases} \tag{6.4}$$

where  $\sigma_0$  and  $\sigma_1$  are fit parameters. In the case that the SD algorithm produces an undermeasurement of  $m_{b\bar{b}}$  by removing too much energy from the Higgs boson decay, the correlation increases, and the  $m_{\text{HH}}$  resolution grows wider. For  $|\Delta_{b\bar{b}}| > 2.5$ , we use the value at the boundary, since the correlation does not hold for severe mismeasurements. The  $m_{\text{HH}}$  resolution is  $\approx 5\%$ .

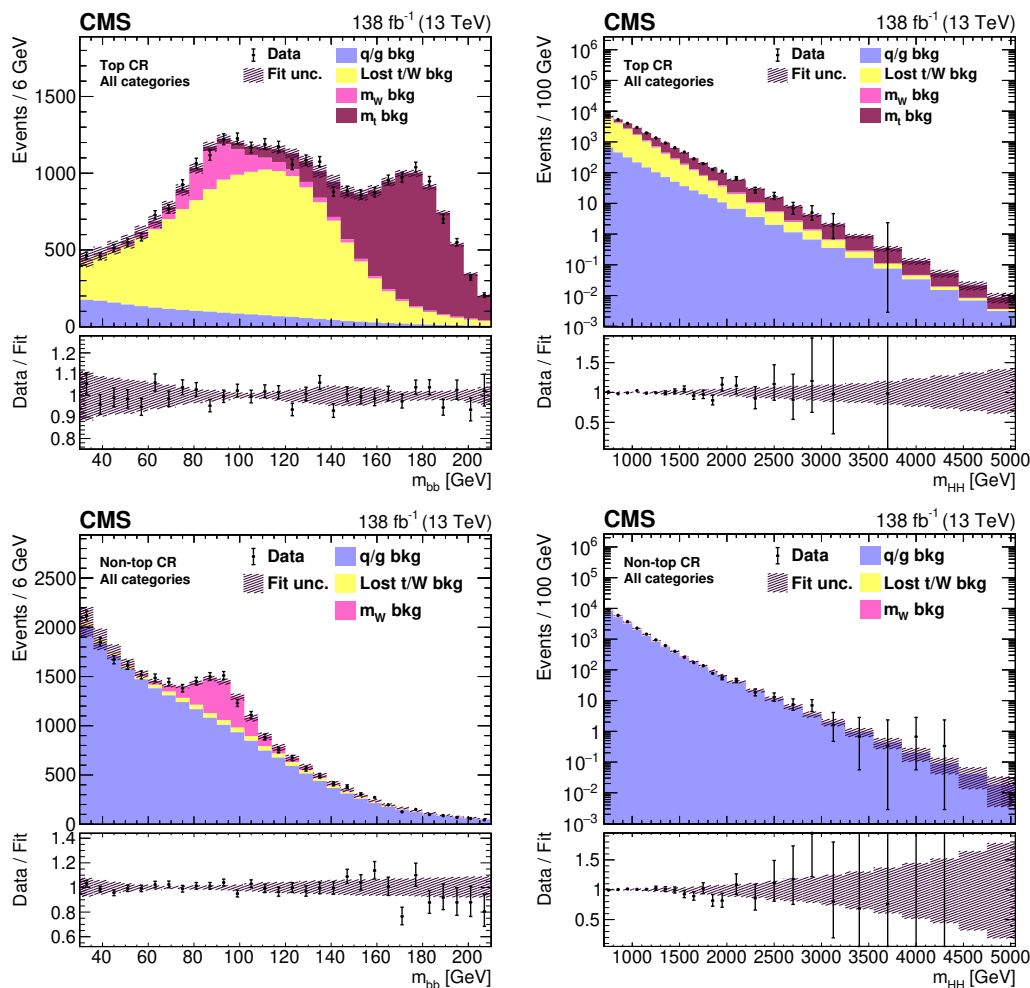
The product of the acceptance and efficiency for  $X \rightarrow \text{HH}$  events to fall into any of the individual search categories is taken from simulation. As done for the signal shape parameters, the efficiency is interpolated along  $m_X$ . Uncertainties in the relative acceptances and in the integrated luminosity of the sample are included in the 2D maximum likelihood fit that is used to obtain confidence intervals for the  $X \rightarrow \text{HH}$  process. The signal modeling is tested using pseudo-experiments in which we fit the templates to pseudodata that contain a fixed amount of signal; no significant bias in the fitted signal yield is found.

### 6.5 Validation of background models with control region data

The background models are validated in the top CR and non-top CR data samples. For both CRs, background templates are constructed in the same way as for the search region, except using the CR selection. The background templates are then fit to the CR data with the same nuisance parameters that are used in the standard 2D maximum likelihood fit. In the non-top CR, the  $m_t$  background is negligible and not included in the modeling. The result of the simultaneous fit is shown in figure 4 for both CRs. To improve visualization, the displayed binning in these and subsequent histograms is coarser than the binning used in the maximum likelihood fit. The projections in both mass dimensions are shown for the combination of all event categories. In both CRs, the fit results model the data well in all categories, indicating that the shape uncertainties can account sufficiently for potential differences between data and simulation.

## 7 Systematic uncertainties

Systematic uncertainties that affect the normalization and shape of the signal and background are modeled with nuisance parameters in the 2D maximum likelihood fit to data. Nuisance parameters for shape uncertainties have Gaussian constraints, while normalization uncertainties have log-normal constraints. In certain cases a single nuisance parameter may



**Figure 4.** The post-fit model compared to data in the top CR (upper plots) and non-top CR (lower plots), projected into  $m_{b\bar{b}}$  (left) and  $m_{HH}$  (right). Events from all categories are combined. The fit result is the filled histogram, with the different colors indicating different background components. The background shape uncertainty is shown as the hatched band. The lower panels of each plot show the ratio of the data to the fit result.

affect both the normalization and the shape of a resonance, in which case the nuisance parameter constraint is Gaussian. Detailed methods of parameterizing the background and signal uncertainties are described in sections 7.1 and 7.2, respectively.

To implement nonresonant mass shape uncertainties, templates are first generated with modified event weights that include multiplicative parameters proportional to  $m_{b\bar{b}}$ ,  $m_{HH}$ ,  $1/m_{b\bar{b}}$ , and  $1/m_{HH}$ . Each of these four modifications produces two alternative templates that represent an upward and downward shift from the nominal model. The 2D fit then interpolates between these two alternative templates to constrain the magnitudes of these parameters. Resonant mass shape uncertainties are implemented as uncertainties in the mean and width parameters of a double Crystal Ball function. In most cases, different nuisance parameters are used for the background shape uncertainties from those used for the signal uncertainties.

All background and signal uncertainties are listed in tables 6 and 7, respectively, with their initial sizes. A single uncertainty type can be applied to multiple event categories with independent nuisance parameters for each category. The background model contains 104 total nuisance parameters, while the signal model contains 27, with two parameters shared between signal and background. The descriptions of all uncertainties and their correlations are also described in the rest of this section.

## 7.1 Background uncertainties

Background uncertainty parameters are chosen by considering possible discrepancies between data and simulation, such as in the relative background composition or in the jet energy scale. Studies of the two CRs are used to verify that the chosen uncertainties cover such differences. The fitted values and the sensitivity to signal do not depend strongly on the sizes of the pre-fit uncertainties because they serve as loose constraints on the fit. We verify this by inflating all pre-fit background uncertainties by a factor of two and observing that the final result does not change. Therefore, the pre-fit uncertainties are sufficiently large to account for discrepancies between data and simulation in the CRs. More complex background models, such as those with more nuisance parameters or higher-order shape distortions, were studied following the same approach as in ref. [52] and not found to be necessary.

In the following subsections, we detail the parameterization of the different uncertainties for the background.

### 7.1.1 Background normalization uncertainties

The  $m_W$ ,  $m_t$ , and lost-t/W backgrounds all primarily arise from  $t\bar{t}$  production. Consequently, some uncertainties are applied by treating these three backgrounds together, referred to collectively as the  $t\bar{t}$  background in table 6. We account for differences between data and simulation in the  $t\bar{t}$  normalization by including independent nuisance parameters for each category that allow the normalizations of these backgrounds to vary in a correlated manner (“ $t\bar{t}$  normalization”). However, the three  $t\bar{t}$ -dominated background components exhibit differences in the b tagging efficiency and the  $b\bar{b}$  jet  $p_T$  spectrum, so we include additional nuisance parameters (“ $t\bar{t}$  relative normalization”) that allow the relative normalizations of each of these to vary within the absolute normalization, which itself also varies. Separate nuisance parameters are used to control the q/g background normalization, as this is the only background component to arise primarily from non- $t\bar{t}$  processes.

### 7.1.2 Background shape uncertainties

The shape uncertainties for the backgrounds are modeled differently depending on whether or not the shape is resonant in the  $m_{b\bar{b}}$  dimension. All backgrounds are nonresonant in the  $m_{HH}$  dimension, and mismodeling of the background  $p_T$  spectrum can manifest as an incorrect  $m_{HH}$  scale. To account for this, the  $m_{HH}$  shape uncertainties are implemented with alternative background templates built with parameters proportional to  $m_{HH}$  (“scale”) and  $1/m_{HH}$  (“inverse scale”), as described in the beginning of section 7. For the q/g background, a pair of these nuisance parameters is included for each category in the SL channel and for each b tagging category in the DL channel. For the  $t\bar{t}$ -dominated backgrounds, we include

Uncertainty type	Processes	$N_p$	$\sigma_I$	$\sigma_C/\sigma_I$
SD jet $m_{b\bar{b}}$ scale	$m_W, m_t, \text{signal}$	2	0.54%, 2.0% ( $m_t$ )	98%, 19% ( $m_t$ )
SD jet $m_{b\bar{b}}$ resolution	$m_W, m_t, \text{signal}$	2	8.6%, 17.2% ( $m_t$ )	95%, 25% ( $m_t$ )
q/g normalization	q/g	12	50% (1 $\ell$ ), 100% (2 $\ell$ )	37–78%
q/g $m_{HH}$ scale	q/g	10	$\pm 0.5 m_{HH}/\text{TeV}$	78–99%
q/g $m_{HH}$ inverse scale	q/g	10	$\pm 1.4 \text{TeV}/m_{HH}$	64–99%
q/g $m_{b\bar{b}}$ scale	q/g	4	$\pm 0.00375 m_{b\bar{b}}/\text{GeV}$	81–99%
q/g $m_{b\bar{b}}$ inverse scale	q/g	4	$\pm 15 \text{GeV}/m_{b\bar{b}}$	77–99%
Lost-t/W $m_{b\bar{b}}$ scale	lost-t/W	4	$\pm 0.003 m_{b\bar{b}}/\text{GeV}$	71–99%
Lost-t/W $m_{b\bar{b}}$ inverse scale	lost-t/W	4	$\pm 18 \text{GeV}/m_{b\bar{b}}$	88–99%
$t\bar{t}$ normalization	lost-t/W, $m_W, m_t$	12	35% (1 $\ell$ ), 70% (2 $\ell$ )	19–68%
$t\bar{t}$ relative normalization	lost-t/W, $m_W, m_t$	8	35% (1 $\ell$ ), 70% (2 $\ell$ )	9–96%
$t\bar{t}$ $m_{HH}$ scale	lost-t/W, $m_W, m_t$	12	$\pm 0.25 m_{HH}/\text{TeV}$	84–99%
$t\bar{t}$ $m_{HH}$ relative scale	lost-t/W, $m_W, m_t$	8	$\pm 0.25 m_{HH}/\text{TeV}$	74–99%
$t\bar{t}$ $m_{HH}$ inverse scale	lost-t/W, $m_W, m_t$	12	$\pm 0.7 \text{TeV}/m_{HH}$	61–99%

**Table 6.** Background systematic uncertainties included in the maximum likelihood fit. The uncertainty types with “normalization” correspond to uncertainties in the background yield, while all others are uncertainties in the background shape. The  $N_p$  column indicates the number of nuisance parameters used to model the uncertainty. In the last two columns,  $\sigma_I$  refers to the initial estimate of the uncertainty, and  $\sigma_C$  refers to the constrained uncertainty obtained post-fit. For the q/g,  $t\bar{t}$ , and lost-t/W shape uncertainties, “scale” uncertainties are those implemented with alternative templates with multiplicative parameters proportional to mass  $m$ , and “inverse scale” uncertainties are those implemented with parameters proportional to  $1/m$ .

a pair of these nuisance parameters for each search category. Furthermore, to allow the  $t\bar{t}$ -dominated backgrounds to be anticorrelated, we include nuisance parameters for the relative  $m_{HH}$  scale (alternative templates built with factors proportional to  $m_{HH}$ ) for each b tagging category, separately for the SL and DL channels.

The q/g and lost-t/W backgrounds are nonresonant in  $m_{b\bar{b}}$ , and thus alternative templates are also used to encode the shape uncertainties for the  $m_{b\bar{b}}$  dimension with factors proportional to  $m_{b\bar{b}}$  or  $1/m_{b\bar{b}}$ . The uncertainties account for mismodeling in the simulated jet energy scale and resolution. For both of these nonresonant backgrounds, the  $m_{b\bar{b}}$  shape does not depend on the lepton flavor or the  $H \rightarrow WW^*$  purity, and so there is a pair of nuisance parameters for each background and each  $b\bar{b}$  jet tagging category, separately for the SL and DL channels.

For the  $m_W$  and  $m_t$  backgrounds in the  $m_{b\bar{b}}$  dimension, where resonances are constructed using AK8 SD jets, the jet mass uncertainties are dependent on the jet substructure. Because of this, the jet mass uncertainties for the signal and the  $m_W$  background, respectively from the two-prong decays  $H \rightarrow b\bar{b}$  and  $W \rightarrow q\bar{q}'$ , are correlated. This is the only such instance where signal and background are correlated, sharing nuisance parameters.



Uncertainty type	$N_p$	Uncertainty values
SD jet $m_{b\bar{b}}$ scale	1	$S(m_{b\bar{b}})$ : 0.54%
SD jet $m_{b\bar{b}}$ resolution	1	$R(m_{b\bar{b}})$ : 8.6%
Integrated luminosity	1	1.6%
PDFs+scales	1	spin-0: 2.0%, spin-2: 2.5%
Trigger	6	1 $l$ : 2.0%, 2 $l$ : 3.0%
Pileup	1	1 $l$ : 1.0%, 2 $l$ : 0.6%
Electron reconstruction	1	1 $l$ : 0.5%, 2 $l$ : <0.8%
Electron identification	2	1 $l$ : 4.2%, 2 $l$ : <2.6%
Muon identification	2	1 $l$ : 2.3%, 2 $l$ : <2.3%
Electron isolation	1	1 $l$ : 6%, 2 $l$ : 3% for each electron
Muon isolation	1	1 $l$ : 6%, 2 $l$ : 2% for each muon
Jet energy scale	1	$Y$ : 2%, $S(m_{HH})$ : 0.8%, $R(m_{HH})$ : 3%
Jet energy resolution	1	$Y$ : 0.5%, $S(m_{HH})$ : 0.3%, $R(m_{HH})$ : 4%
Unclustered energy	1	$Y$ : 0.5%, $S(m_{HH})$ : 0.1%, $R(m_{HH})$ : 1.5%
Other detector effects	2	$Y$ : 0.6%, $R(m_{HH})$ : 1.0%
AK4 b tag efficiency	1	<4.0%
AK4 b tag misidentification rate	1	<2.5%
$b\bar{b}$ jet tagging	1	bL: 8.5%, bT: 11.5%
$q\bar{q}'$ jet $\tau_2/\tau_1$ efficiency	1	LP: 26% HP: 6.7%

**Table 7.** Signal systematic uncertainties included in the maximum likelihood fit. The  $N_p$  column indicates the number of nuisance parameters used to model the uncertainty. In the ‘‘Uncertainty values’’ column, some uncertainties are noted as affecting both the yield ( $Y$ ) and  $m_{HH}$  shape ( $S$  for scale,  $R$  for resolution) of the signal. All other uncertainties, except the SD jet mass uncertainties, are uncertainties in the signal yield alone.

Uncertainties that have been measured in data for W boson decays into merged jets in  $t\bar{t}$  events are found to cover discrepancies between our simulation and data for the  $m_W$  background but not for the  $m_t$  background. We do not expect these uncertainties to cover discrepancies in the  $m_t$  background because the SD algorithm behaves differently for the three-prong top quark jets ( $t \rightarrow bq\bar{q}'$ ) in this background. Thus, these uncertainties are larger than for two-prong jets and are not correlated with the  $m_W$  jet mass shape uncertainties, as seen in the upper two rows of table 6.

## 7.2 Signal uncertainties

As shown in table 7, uncertainties are applied to the normalization of the signal to account for mismeasurements in the total integrated luminosity [104–106], the pileup profile, the trigger efficiency, the lepton selection efficiencies, and other detector effects. Signal acceptance uncertainties from the choices of the PDFs and also the factorization and renormalization

scales are also applied. The scale uncertainties are obtained following refs. [107, 108], and the PDF uncertainty is evaluated using the NNPDF 3.1 PDF set [81].

The signal acceptance and the  $m_{\text{HH}}$  resonance scale and resolution all have uncertainties due to the jet energy scale and resolution, the unclustered energy resolution, and other detector effects. The same  $m_{\text{b}\bar{\text{b}}}$  resonance scale and resolution uncertainties that are applied for the  $m_{\text{W}}$  background are applied to the signal because they are both SD jets with two-prong substructure.

The  $\text{q}\bar{\text{q}}'$  jet  $\tau_2/\tau_1$  selection efficiency is measured in a  $\text{t}\bar{\text{t}}$  data sample enriched with hadronically decaying W bosons. The uncertainties in this measurement are included as normalization uncertainties in the  $\text{H} \rightarrow \text{WW}^*$  decay purity categories, and the LP and HP uncertainties are anticorrelated. Normalization uncertainties are also applied to account for the efficiency and misidentification rate of AK4 jet b tagging used to identify and reject jets from  $\text{t}\bar{\text{t}}$  production. The uncertainty in the  $\text{b}\bar{\text{b}}$  jet tagging efficiency is included as a single nuisance parameter that varies the signal normalization and is dependent on both the  $\text{b}\bar{\text{b}}$  jet tagging category and  $m_{\text{X}}$ . These  $\text{b}\bar{\text{b}}$  jet tagging uncertainties are the dominant systematic uncertainties associated with the signal normalization, followed by the uncertainties in the  $\tau_2/\tau_1$  efficiencies.

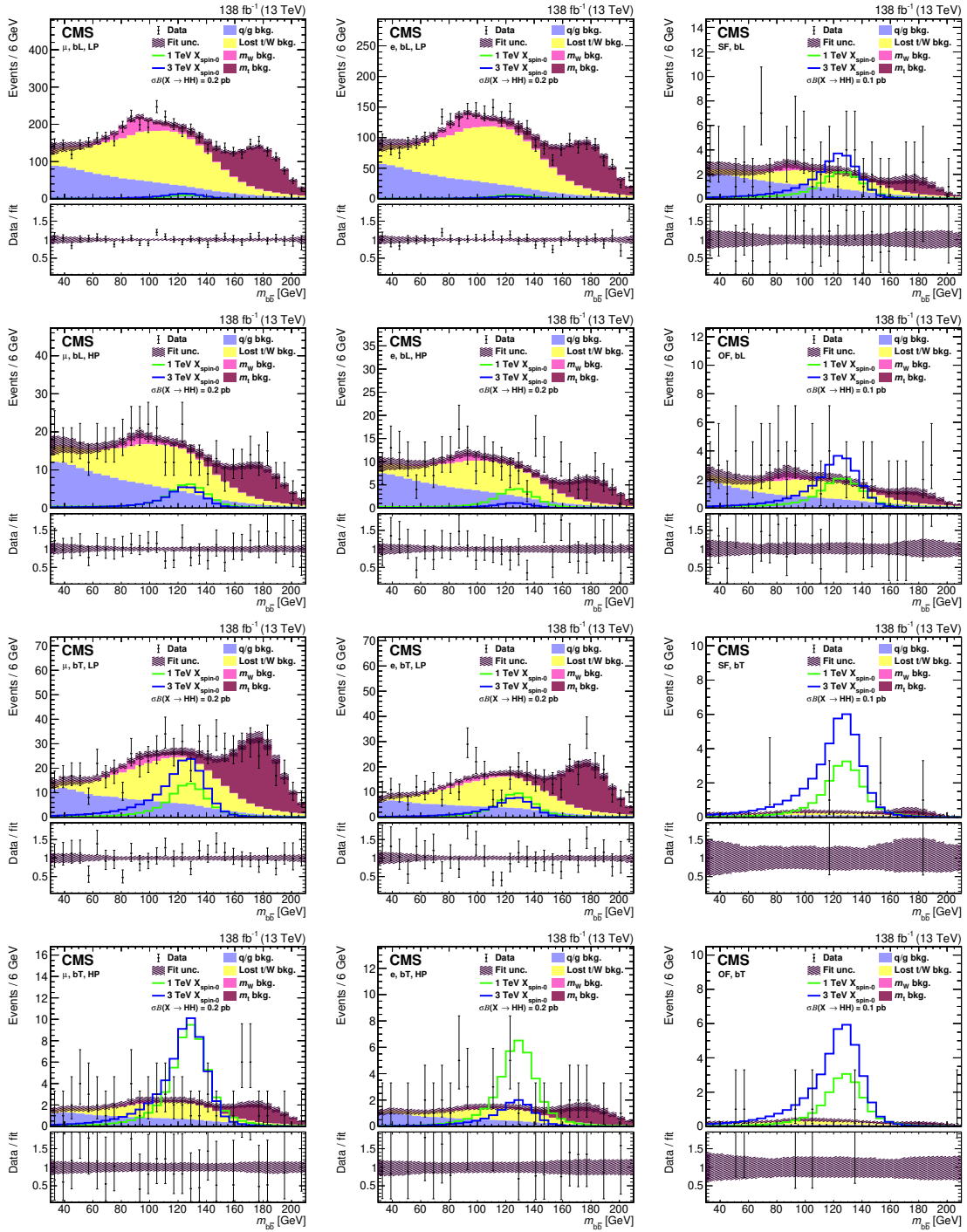
## 8 Results

The data are interpreted by performing a maximum likelihood fit in the 2D  $(m_{\text{b}\bar{\text{b}}}, m_{\text{HH}})$  mass plane using one model containing only background processes and using one containing both background and signal processes. We find that the background-only model fits the data well. We interpret the results as upper limits at 95% confidence level (CL) on  $\sigma\mathcal{B}(\text{X} \rightarrow \text{HH})$ .

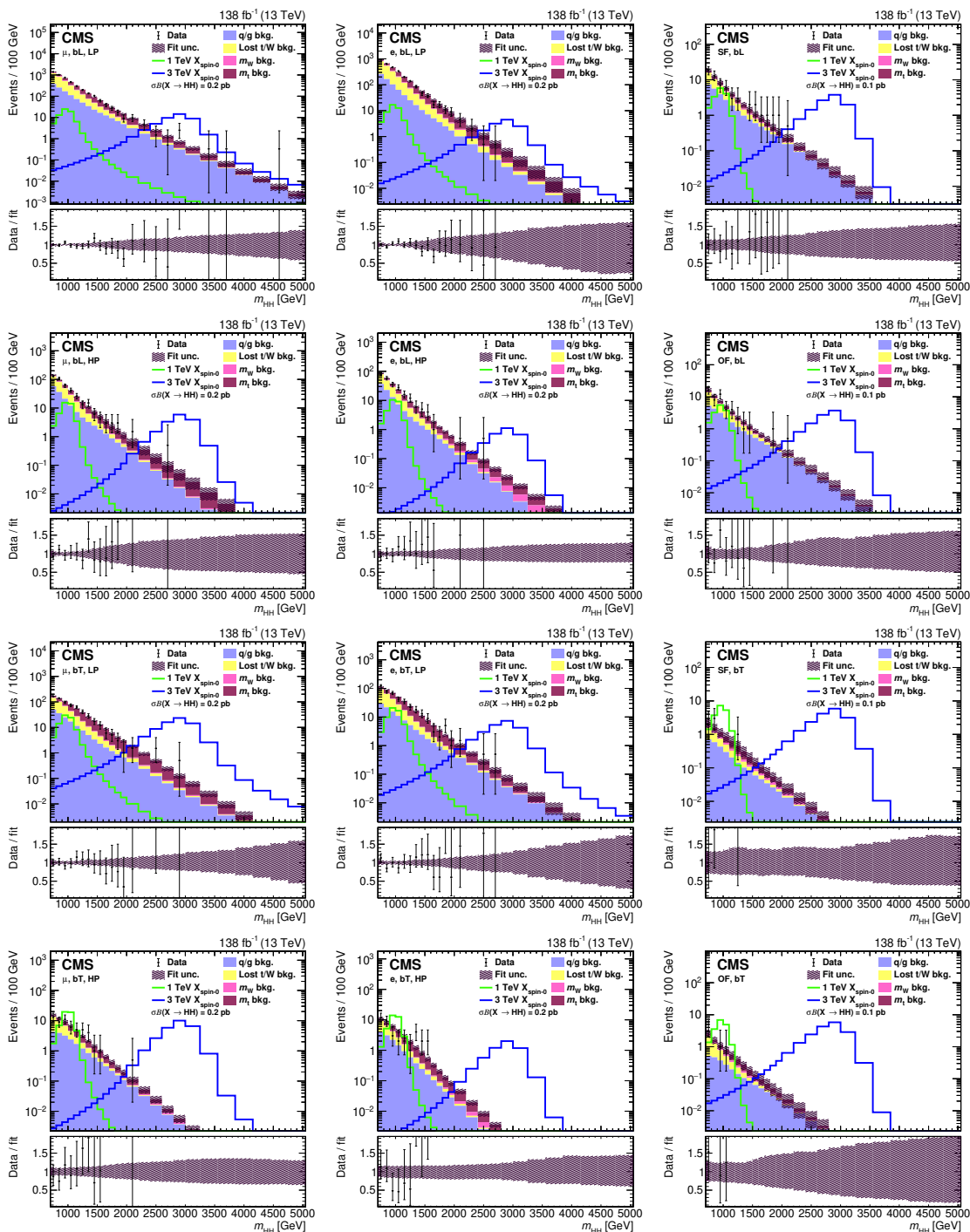
The quality of the fit is quantified with a likelihood ratio goodness-of-fit test using the saturated model [109]. The probability distribution function of the test statistic is obtained with pseudo-experiments, and the observed value is within the central 68% interval of expected results. The best-fit values of the nuisance parameters are consistent with the initial 1 standard deviation range of uncertainty.

The fit result and the data are projected in  $m_{\text{b}\bar{\text{b}}}$  for each event category in figure 5. The  $m_{\text{b}\bar{\text{b}}}$  shape is modeled well by the background-only model, and each background component is important in at least some subspace of the mass range. Particularly, the resonant peaks corresponding to the W boson and top quark are correctly modeled by the fit. Similarly, the  $m_{\text{HH}}$  projections of the fit are shown in figure 6. There is good agreement for the full  $m_{\text{HH}}$  mass range in these figures as well.

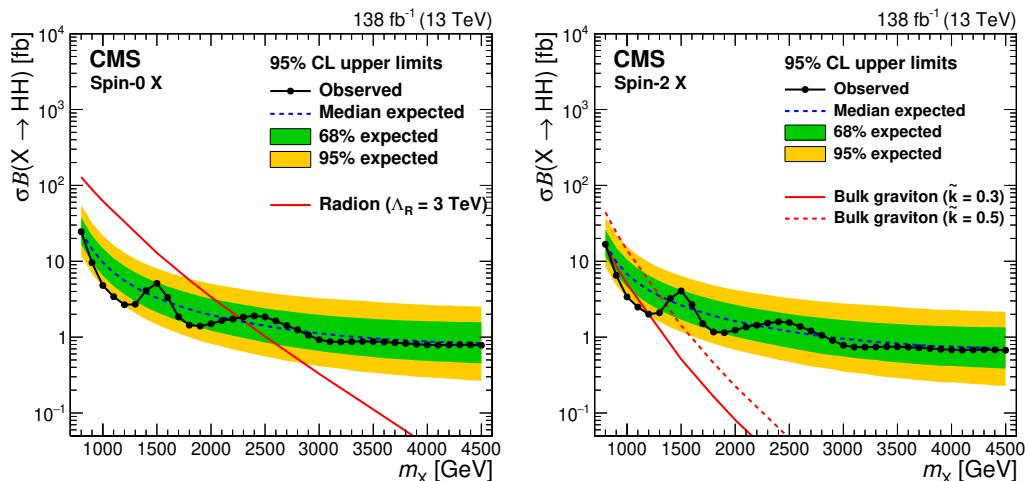
Upper limits are shown at 95% CL in figure 7 for both the spin-0 and spin-2 boson scenarios. The limits are evaluated using the asymptotic approximation [110] of the  $\text{CL}_s$  method [111, 112], and the validity of this approximation was confirmed by calculating limits with pseudo-experiments. The difference in the limits calculated with pseudo-experiments versus the asymptotic approximation is significantly smaller than 1 standard deviation in the expected limit. The observed exclusion limits are consistent with the expected limits. A spin-0 signal at  $m_{\text{X}} = 0.8$  TeV is excluded for  $\sigma\mathcal{B} > 24.5$  fb, and the exclusion limits strengthen over the full mass range to  $\sigma\mathcal{B} > 0.78$  fb at  $m_{\text{X}} = 4.5$  TeV. Spin-2 signals have



**Figure 5.** The background-only 2D fit result compared to data projected onto the  $m_{b\bar{b}}$  axis for both the SL and DL channels. The label for each search category is in the upper left of each plot. The fit result is the filled histogram, with the different colors indicating different background components. The background shape uncertainty from the fit is shown as the hatched band. Example spin-0 signal distributions for  $m_X = 1.0$  and  $3.0$  TeV are shown as solid lines, with  $\sigma\mathcal{B}(X \rightarrow HH)$  set to 0.2 and 0.1 pb for the SL and DL channels, respectively. The lower panels show the ratio of the data to the fit result. Only nonzero data entries are shown in the interest of clarity.



**Figure 6.** The background-only 2D fit result compared to data projected onto the  $m_{\text{HH}}$  axis for both the SL and DL channels. The label for each search category is in the upper left of each plot. The fit result is the filled histogram, with the different colors indicating different background components. The background shape uncertainty from the fit is shown as the hatched band. Example spin-0 signal distributions for  $m_X = 1.0$  and  $3.0$  TeV are shown as solid lines, with  $\sigma\mathcal{B}(X \rightarrow \text{HH})$  set to 0.2 and 0.1 pb for the SL and DL channels, respectively. The lower panels of each plot show the ratio of the data to the fit result. Only nonzero data entries are shown in the interest of clarity.



**Figure 7.** Observed and expected 95% CL upper limits on the product of the cross section and branching fraction to HH for a generic spin-0 (left) and spin-2 (right) boson X, as functions of mass. Example radion and bulk graviton predictions are also shown. The HH branching fraction is assumed to be 25% for radions and 10% for bulk gravitons.

larger acceptance, and so the exclusion limits on these signals are stronger: at  $m_X = 0.8 \text{ TeV}$ , we exclude  $\sigma\mathcal{B} > 16.7 \text{ fb}$ , and at  $m_X = 4.5 \text{ TeV}$  we exclude  $\sigma\mathcal{B} > 0.67 \text{ fb}$ .

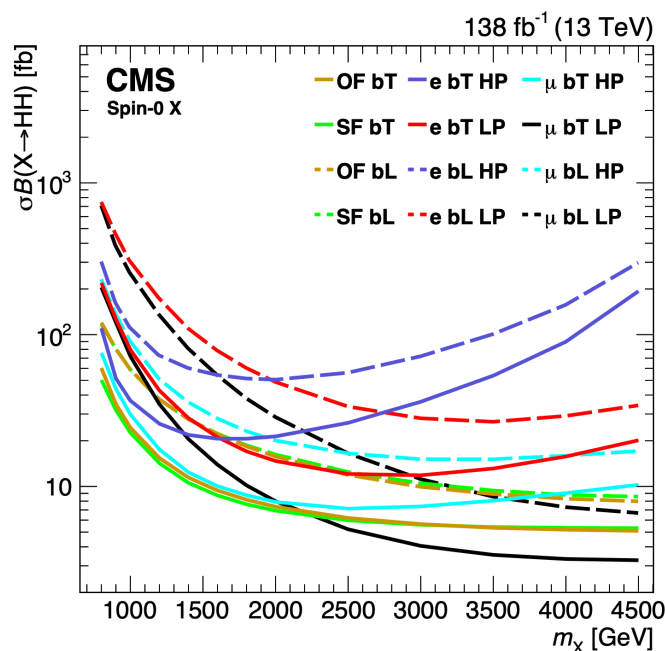
Table 8 shows the event yields for each search category that are observed in data and are expected before and after a background-only fit, along with the associated post-fit uncertainty in the total background yield in each category. Figure 8 shows the expected exclusion limit at 95% CL for each search category alone. In general, the tight (bT)  $b\bar{b}$  jet tagging categories are the most sensitive over the full range of  $m_X$ , since these contain the most signal and the least background. The DL categories are generally more sensitive than most SL categories since the background yields are much lower in the DL channel. A notable exception to this trend is the  $\mu$  bT LP category, which is the most sensitive above approximately 2.5 TeV. At high  $m_X$ , the electron categories in the SL channel are the least sensitive because the electron reconstruction efficiency is degraded.

The total uncertainty in the signal sensitivity is dominated by the statistical uncertainty of the data in the analysis. As mentioned in section 7.2, the dominant systematic uncertainty for all  $m_X$  comes from the  $b\bar{b}$  jet tagging efficiency for the signal. Most of the background systematic uncertainties do not have an impact on the signal sensitivity. For high  $m_X$  signals, none of the background systematic uncertainties have a significant impact, and only the signal systematic uncertainties have an effect. For low  $m_X$  signals, however, the background normalization uncertainties in the most sensitive categories (those with the least background) have an impact.

Relative to the  $X \rightarrow b\bar{b}lvq\bar{q}'$  search in ref. [52], this analysis ranges from 6 times more sensitive at low  $m_X$  to 14 times more sensitive at high  $m_X$ . The improvements in sensitivity arise primarily from three developments. First, an improvement in the expected upper limits by a factor of  $\approx 3.5$  is achieved because of the larger integrated luminosity alone. This

Search category	Observed	Expected (pre-fit)	Expected (post-fit)	Post-fit uncertainty
$\mu$ bL LP	4542	4362.2	4540.9	1.5%
$\mu$ bL HP	417	402.4	416.1	4.8%
$\mu$ bT LP	657	731.8	658.5	4.2%
$\mu$ bT HP	56	67.0	57.3	10.0%
e bL LP	2945	2973.7	2945.4	1.9%
e bL HP	248	246.1	247.7	5.7%
e bT LP	423	443.0	423.9	4.2%
e bT HP	37	41.0	37.7	14.6%
SF bL	59	70.2	59.6	14.2%
OF bL	50	61.1	50.8	13.5%
SF bT	6	11.3	7.9	31.6%
OF bT	6	11.6	8.1	25.8%

**Table 8.** Event yields broken down by search category. For each category, shown are the event yields observed in data, expected before and after a fit of the background-only model, and the corresponding relative uncertainty.



**Figure 8.** Median expected upper limits at 95% confidence level for each of the 12 search categories individually.

level of improvement is expected because the number of background events is much smaller than the number of signal events under a typical signal peak, even at low  $m_X$ . Second, because of improved techniques in the SL channel alone, we achieve similar sensitivity at  $m_X = 0.8$  TeV and up to a  $\approx 2$  times improvement at  $m_X = 4.5$  TeV. Finally, the addition of the DL channel provides significant improvement in sensitivity. At low  $m_X$ , the DL channel is  $\approx 70\%$  more sensitive than the SL channel, largely because the background level is over an order of magnitude smaller. At high  $m_X$ , where there is virtually no background in any channel, the DL channel has similar sensitivity to the SL channel. This occurs because the dilepton signal efficiency is largest at high mass, and in the SL channel, despite the larger branching fraction, the lepton efficiency (particularly for electrons) degrades at high mass because of the nearby  $q\bar{q}'$  jet.

This search yields the most sensitive upper limits for  $X \rightarrow HH$  production with leptons in the final state. The only  $X \rightarrow HH$  searches that are more sensitive in any subspace of the considered  $m_X$  and for any spin hypothesis are those in the  $b\bar{b}b\bar{b}$  final state from ATLAS and CMS, each of which extend only up to 3.0 TeV. From 0.8 to 3.0 TeV, the sensitivity of this search is mostly comparable to and in some places stronger than the  $b\bar{b}b\bar{b}$  searches.

Predicted radion and bulk graviton cross sections [113] are also shown in figure 7 in the context of Randall-Sundrum models that allow the SM fields to propagate through an extra dimension. Typical model parameters are chosen as proposed in ref. [114]. A branching fraction of 25% to HH and an ultraviolet cutoff  $\Lambda_R = 3$  TeV are assumed for the radion, which is excluded for  $m_X < 2.25$  TeV. A 10% branching fraction is assumed for the bulk graviton, which occurs in scenarios that include significant coupling between the bulk graviton and top quarks. Bulk graviton production cross sections depend on the dimensionless quantity  $\tilde{k} = \sqrt{8\pi}k/M_{\text{Pl}}$ , where  $k$  is the curvature of the extra dimension and  $M_{\text{Pl}}$  is the Planck mass. For this interpretation, we choose  $\tilde{k} = 0.3$  and 0.5. The bulk gravitons with  $\tilde{k} = 0.3$  and 0.5 are excluded for  $m_X < 1.20$  and 1.35 TeV, respectively. For these particular signal parameters, the radion and bulk graviton decay widths are larger than the 1 MeV width chosen for signal sample generation but much smaller than the detector resolution.

## 9 Summary

A search has been performed for new bosons (narrow resonances) decaying to a pair of Higgs bosons (HH) where one decays into a bottom quark pair ( $b\bar{b}$ ) and the other via one of three different modes into final states with leptons. The large Lorentz boost of the Higgs bosons produces a distinct experimental signature with one jet that has substructure consistent with the decay  $H \rightarrow b\bar{b}$ . For the Higgs boson that does not decay to  $b\bar{b}$ , the single-lepton decay  $H \rightarrow WW^* \rightarrow \ell\nu q\bar{q}'$  and the dilepton decays  $H \rightarrow WW^* \rightarrow \ell\nu\ell\nu$  and  $H \rightarrow \tau\tau \rightarrow \ell\nu\nu\ell\nu$  are considered. In the single-lepton channel, the experimental signature is characterized by a second large jet with a nearby lepton, which is consistent with the decay of  $H \rightarrow WW^*$ . In the dilepton channel, the experimental signature contains two leptons and significant missing transverse momentum. This search uses a sample of proton-proton collisions at  $\sqrt{s} = 13$  TeV, corresponding to an integrated luminosity of  $138 \text{ fb}^{-1}$ , collected by the CMS

detector at the LHC. The primary standard model backgrounds — production of top quark pairs and of vector bosons in association with jets — are suppressed by reconstructing the HH decay chain and applying selections to discriminate signal from background. The signal and background yields are estimated by a two-dimensional template fit in the plane of the  $b\bar{b}$  jet mass and the HH resonance mass. The templates are validated in a variety of data control regions and are shown to model the data well. The data are consistent with the expected standard model background. Upper limits are set on the product of the cross section and branching fraction for new bosons decaying to HH. The observed limit at 95% confidence level for a spin-0 (spin-2) boson ranges from 24.5 (16.7) fb at 0.8 TeV to 0.78 (0.67) fb at 4.5 TeV. The results of this search provide the most stringent exclusion limits to date for  $X \rightarrow HH$  signatures with leptons in the final state and are among the most stringent of all  $X \rightarrow HH$  searches, at certain mass points the most sensitive.

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








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





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


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




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



















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
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









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S. Czellar, D. Fasanella , F. Fienga , J. Karancki<sup>28</sup> , J. Molnar, Z. Szillasi, D. Teyssier

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






















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






















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


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



















A. Benaglia<sup>a</sup> , G. Boldrini , F. Brivio<sup>a,b</sup>, F. Cetorelli<sup>a,b</sup>, F. De Guio<sup>a,b</sup> , M.E. Dinardo<sup>a,b</sup> , P. Dini<sup>a</sup> , S. Gennai<sup>a</sup> , A. Ghezzi<sup>a,b</sup> , P. Govoni<sup>a,b</sup> , L. Guzzi<sup>a,b</sup> 

M.T. Lucchini<sup>a,b</sup> , M. Malberti<sup>a</sup>, S. Malvezzi<sup>a</sup> , A. Massironi<sup>a</sup> , D. Menasce<sup>a</sup> ,  
L. Moroni<sup>a</sup> , M. Paganoni<sup>a,b</sup> , D. Pedrini<sup>a</sup> , B.S. Pinolini, S. Ragazzi<sup>a,b</sup> ,  
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A.O.M. Iorio<sup>a,b</sup> , L. Lista<sup>a,b,47</sup> , S. Meola<sup>a,d,20</sup> , P. Paolucci<sup>a,20</sup> , B. Rossi<sup>a</sup> ,  
C. Sciacca<sup>a,b</sup> 













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U. Gasparini<sup>a,b</sup> , G. Grosso, S.Y. Hoh<sup>a,b</sup> , L. Layer<sup>a,48</sup>, E. Lusiani , M. Margoni<sup>a,b</sup> ,  
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G. Strong<sup>a</sup> , M. Tosi<sup>a,b</sup> , H. Yarar<sup>a,b</sup>, M. Zanetti<sup>a,b</sup> , P. Zotto<sup>a,b</sup> , A. Zucchetta<sup>a,b</sup> ,  
G. Zumerle<sup>a,b</sup> 




























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V. Re<sup>a</sup> , C. Riccardi<sup>a,b</sup> , P. Salvini<sup>a</sup> , I. Vai<sup>a</sup> , P. Vitulo<sup>a,b</sup> 














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






















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

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




























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











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
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



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





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





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






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J. Alison , S. An , M.B. Andrews, P. Bryant , T. Ferguson , A. Harilal, C. Liu, T. Mudholkar , M. Paulini , A. Sanchez, W. Terrill











































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

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









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E. Adams, A. Baden, O. Baron, A. Belloni , S.C. Eno , N.J. Hadley , S. Jabeen , R.G. Kellogg, T. Koeth, Y. Lai, S. Lascio, A.C. Mignerey, S. Nabili, C. Palmer , M. Seidel , A. Skuja , L. Wang, K. Wong 

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D. Abercrombie, G. Andreassi, R. Bi, W. Busza , I.A. Cali, Y. Chen , M. D'Alfonso , J. Eysermans, C. Freer , G. Gomez Ceballos, M. Goncharov, P. Harris, M. Hu, M. Klute , D. Kovalskyi , J. Krupa, Y.-J. Lee , C. Mironov , C. Paus , D. Rankin , C. Roland , G. Roland, Z. Shi , G.S.F. Stephans , J. Wang, Z. Wang , B. Wyslouch 











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R.M. Chatterjee, A. Evans , J. Hiltbrand, Sh. Jain , M. Krohn, Y. Kubota, J. Mans ,  
M. Revering, R. Rusack , R. Saradhy, N. Schroeder , N. Strobbe , M.A. Wadud










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




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J. Mariano, N. Marinelli, I. Mcalister, T. McCauley , C. Mcgrady, K. Mohrman, C. Moore,  
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- 46: Also at Centro Siciliano di Fisica Nucleare e di Struttura Della Materia, Catania, Italy
- 47: Also at Scuola Superiore Meridionale, Università di Napoli Federico II, Napoli, Italy
- 48: Also at Università di Napoli ‘Federico II’, Napoli, Italy
- 49: Also at Consiglio Nazionale delle Ricerche — Istituto Officina dei Materiali, Perugia, Italy
- 50: Also at Riga Technical University, Riga, Latvia
- 51: Also at Consejo Nacional de Ciencia y Tecnología, Mexico City, Mexico
- 52: Also at IRFU, CEA, Université Paris-Saclay, Gif-sur-Yvette, France
- 53: Also at Institute for Nuclear Research, Moscow, Russia
- 54: Now at National Research Nuclear University ‘Moscow Engineering Physics Institute’ (MEPhI), Moscow, Russia
- 55: Also at Institute of Nuclear Physics of the Uzbekistan Academy of Sciences, Tashkent, Uzbekistan
- 56: Also at St. Petersburg Polytechnic University, St. Petersburg, Russia
- 57: Also at University of Florida, Gainesville, Florida, U.S.A.
- 58: Also at Imperial College, London, United Kingdom
- 59: Also at P.N. Lebedev Physical Institute, Moscow, Russia
- 60: Also at California Institute of Technology, Pasadena, California, U.S.A.
- 61: Also at Budker Institute of Nuclear Physics, Novosibirsk, Russia
- 62: Also at Faculty of Physics, University of Belgrade, Belgrade, Serbia
- 63: Also at Trincomalee Campus, Eastern University, Sri Lanka, Nilaveli, Sri Lanka
- 64: Also at INFN Sezione di Pavia, Università di Pavia, Pavia, Italy
- 65: Also at National and Kapodistrian University of Athens, Athens, Greece
- 66: Also at Ecole Polytechnique Fédérale Lausanne, Lausanne, Switzerland
- 67: Also at Universität Zürich, Zurich, Switzerland
- 68: Also at Stefan Meyer Institute for Subatomic Physics, Vienna, Austria
- 69: Also at Laboratoire d’Annecy-le-Vieux de Physique des Particules, IN2P3-CNRS, Annecy-le-Vieux, France
- 70: Also at Şirnak University, Şirnak, Turkey
- 71: Also at Near East University, Research Center of Experimental Health Science, Nicosia, Turkey
- 72: Also at Konya Technical University, Konya, Turkey
- 73: Also at Piri Reis University, Istanbul, Turkey
- 74: Also at Adiyaman University, Adiyaman, Turkey
- 75: Also at Necmettin Erbakan University, Konya, Turkey
- 76: Also at Bozok Universiteleri Rektörlüğü, Yozgat, Turkey
- 77: Also at Marmara University, Istanbul, Turkey
- 78: Also at Milli Savunma University, Istanbul, Turkey
- 79: Also at Kafkas University, Kars, Turkey
- 80: Also at Istanbul Bilgi University, Istanbul, Turkey
- 81: Also at Hacettepe University, Ankara, Turkey
- 82: Also at Istanbul University — Cerrahpasa, Faculty of Engineering, Istanbul, Turkey
- 83: Also at Ozyegin University, Istanbul, Turkey
- 84: Also at Vrije Universiteit Brussel, Brussel, Belgium
- 85: Also at School of Physics and Astronomy, University of Southampton, Southampton, United Kingdom
- 86: Also at Rutherford Appleton Laboratory, Didcot, United Kingdom
- 87: Also at IPPP Durham University, Durham, United Kingdom

- 88: Also at Monash University, Faculty of Science, Clayton, Australia
- 89: Also at Università di Torino, Torino, Italy
- 90: Also at Bethel University, St. Paul, Minnesota, U.S.A.
- 91: Also at Karamanoğlu Mehmetbey University, Karaman, Turkey
- 92: Also at United States Naval Academy, Annapolis, N/A, U.S.A.
- 93: Also at Ain Shams University, Cairo, Egypt
- 94: Also at Bingol University, Bingol, Turkey
- 95: Also at Georgian Technical University, Tbilisi, Georgia
- 96: Also at Sinop University, Sinop, Turkey
- 97: Also at Erciyes University, Kayseri, Turkey
- 98: Also at Institute of Modern Physics and Key Laboratory of Nuclear Physics and Ion-beam Application (MOE) — Fudan University, Shanghai, China
- 99: Also at Texas A&M University at Qatar, Doha, Qatar
- 100: Also at Kyungpook National University, Daegu, Korea