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Letter

Search for heavy neutral Higgs bosons A and H in the $t\bar{t}Z$ channel in proton-proton collisions at 13 TeV

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ABSTRACT

A direct search for new heavy neutral Higgs bosons A and H in the $t\bar{t}Z$ channel is presented, targeting the process $pp \to A \to ZH$ with $H \to t\bar{t}$. For the first time, the channel with decays of the Z boson to muons or electrons in association with all-hadronic decays of the $t\bar{t}$ system is targeted. The analysis uses proton-proton collision data collected at the CERN LHC with the CMS experiment at $\sqrt{s} = 13$ TeV, which correspond to an integrated luminosity of 138 fb^{-1}. No signal is observed. Upper limits on the product of the cross section and branching fractions are derived for narrow resonances A and H with masses up to 2100 and 2000 GeV, respectively, assuming A boson production through gluon fusion. The results are also interpreted within two-Higgs-doublet models, where A and H are *CP*-odd and *CP*-even states, respectively, complementing and substantially extending the reach of previous searches.

1. Introduction

The measured properties of the Higgs boson discovered [1–3] by the ATLAS and CMS Collaborations at the CERN LHC are consistent with the expectations of the standard model (SM) within the current experimental precision [4,5]. However, the particle might be part of an extended Higgs sector, as suggested by several models of physics beyond the SM (BSM), such as supersymmetry [6], models with an axion [7] or dark matter [8], as well as BSM mechanisms of baryogenesis [9].

A common class of extended Higgs models is two-Higgs-doublet models (2HDMs) [10,11], containing one additional Higgs doublet, resulting in the presence of three neutral Higgs bosons, two of which (h and H) are even under charge-parity (*CP*) transformations and one (A) is *CP*-odd, as well as two charged Higgs bosons ($H^{\pm}$). Such models are defined by the following parameters when assuming *CP* conservation: the masses of the five Higgs bosons m_h, m_H, m_A, and $m_{H^{\pm}}$, the ratio of the vacuum expectation values of the two doublets $\tan\beta$, the mixing angle between the two *CP*-even Higgs bosons α, and the soft-breaking term m_{12}^2. Depending on the coupling of the two doublets to the right-handed quarks and the charged leptons, different types of 2HDM are possible. For example, in type-I models the quarks and charged leptons couple to a single Higgs doublet, while in type-II models the down-type quarks and the charged leptons couple to a different Higgs doublet from that coupling to the up-type quarks. When $\cos(\beta - \alpha) \to 0$, referred to as the "alignment limit", the properties of the h boson are expected to be identical to those of a SM Higgs boson with the same mass. In this Letter, h is identified with the observed Higgs boson, which has a mass of approximately 125 GeV.

For sufficiently large mass splittings, $m_A > m_H + m_Z$, the decay $A \to ZH$ becomes kinematically possible and is dominant in a wide range of the 2HDM parameter space [12]. Searches for $A \to ZH$ have been performed in final states targeting H boson decays to $b\bar{b}$, WW, and $\tau^+\tau^-$ [13–15]. Their sensitivity is typically limited to masses of m_H up to approximately 400 GeV, beyond which the $H \to t\bar{t}$ decay becomes kinematically possible and is dominant, in particular for small and moderate values of $\tan\beta$. In models of electroweak baryogenesis that attempt to explain the observed matter-antimatter asymmetry in the universe, a first-order electroweak phase transition becomes possible at these values of masses and $\tan\beta$ [9,16,17]. However, this region of parameter space has not been probed extensively in experimental analyses. Searches for $A/H \to t\bar{t}$ decays provide some sensitivity to the relevant parameter space [18,19], and indirect constraints are obtained, for example, from $t\bar{t}t\bar{t}$ cross section measurements [20,21]. Recently, the ATLAS Collaboration published a direct search for $A \to ZH$ with $H \to t\bar{t}$ in final states corresponding to single-lepton decays of the $t\bar{t}$ system, excluding at 95% confidence level (CL) regions up to approximately $m_A = 1$ TeV for $\tan\beta = 1$ of the type-I 2HDM parameter space. They report an excess in the region around $(m_A, m_H) = (650, 450)$ GeV with a local significance of 2.85 standard deviations (SD) [22].

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In this Letter, a direct search for heavy neutral Higgs bosons A and H is presented, targeting the process $A \to ZH$ with $H \to t\bar{t}$. The final state with decays of the Z boson to muons or electrons in association with all-hadronic decays of the $t\bar{t}$ system is targeted, which has not been studied before. The search is performed with proton-proton (pp) collision data recorded at $\sqrt{s} = 13\,\text{TeV}$ at the LHC during 2016–2018, corresponding to a total integrated luminosity of $138\,\text{fb}^{-1}$ [23–25]. Events are selected by requiring the presence of two same-flavour and oppositely charged leptons ($\ell = \mu, e$) that are compatible with originating from a Z boson decay, as well as at least five jets. Two sensitive observables are reconstructed, following Ref. [12]: Δm, characterizing the mass difference of the A and the H boson candidates, and p_T^Z, characterizing the transverse momentum of the Z boson candidate. The two-dimensional distribution of Δm and p_T^Z, reduced into a one-dimensional histogram, is used as the final discriminating observable in the search. Upper limits on the product of the cross section and branching fractions $\sigma(pp \to A)\mathcal{B}(A \to ZH)\mathcal{B}(H \to t\bar{t})$ are derived as a function of m_A and m_H, assuming gluon fusion production, and narrow *CP*-odd and *CP*-even resonances A and H, respectively. The results are used to constrain the 2HDM parameter space. Tabulated results are provided in the HEPData record for this analysis [26].

2. The CMS detector and event reconstruction

The CMS apparatus [27,28] is a multipurpose, nearly hermetic detector, designed to trigger on [29–31] and identify muons, electrons, photons, and (charged and neutral) hadrons [32–34]. A global "particle-flow" (PF) algorithm [35] aims to reconstruct all individual particles in an event, combining information provided by the all-silicon inner tracker and by the crystal electromagnetic (ECAL) and brass-scintillator hadron calorimeters, operating inside a 3.8 T superconducting solenoid, with data from the gas-ionization muon detectors embedded in the flux-return yoke outside the solenoid. The reconstructed particles are used to build τ leptons, jets, and missing transverse momentum [36–38].

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 μs [29]. 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 [30].

The primary vertex is taken to be the vertex corresponding to the hardest scattering in the event, evaluated using tracking information alone, as described in Section 9.4.1 of Ref. [39].

The reconstruction of muons relies on a combination of measurements in the tracker and in the muon detectors [33]. The muons are identified based on the quality of the combined track fit and on the number of hits in the different tracking detectors, with an efficiency of about 95%. The transverse momentum (p_T) resolution in the barrel is better than 1% (7%) for muons with p_T up to 100 GeV (1 TeV) [33]. Electrons are reconstructed by combining the momentum measurement in the tracker with the energy measurement of the corresponding cluster in the ECAL and with the energy sum of all bremsstrahlung photons, obtained from the ECAL, spatially compatible with originating from the electron track [32,40]. The electrons are identified using criteria on the cluster shape in the ECAL, the track quality, and the compatibility between the tracker and ECAL measurements, corresponding to an identification efficiency of approximately 80%, including the isolation requirements described below. The momentum resolution for electrons with $p_T \approx 45\,\text{GeV}$ from $Z \to ee$ decays ranges from 1.6 to 5% [32,40]. Both muons and electrons are required to lie within the acceptance of the tracker, covering pseudorapidity (η) values of $|\eta| < 2.4$, and to have $p_T > 35$ and 20 GeV for the p_T-leading and subleading leptons, respectively. The p_T thresholds were chosen to maximize the expected sensitivity of the search to a potential signal, evaluated using simulation. Electrons reconstructed in the transition region $1.44 < |\eta| < 1.56$ between the barrel and the endcap calorimeters are discarded. Isolation requirements are imposed on the leptons with the aim to suppress leptons originating from decays of heavy hadrons inside jets. The isolation is based on the scalar p_T sum of all PF objects in a cone of radius 0.3 in the η-ϕ plane around the track direction of the lepton, where ϕ denotes the azimuthal angle, and it is corrected by removing contributions arising from additional pp interactions in the same bunch crossing (pileup) [41].

Hadronic jets are clustered from the PF objects using the anti-k_T algorithm [42,43] with a distance parameter of 0.4, omitting charged particles matched to pileup vertices. The jet energy is corrected for the neutral-hadron contribution expected from pileup interactions [44]. Further energy corrections depending on the jet p_T and η are applied, which are derived in simulation such that the average measured energy of the jets becomes identical to that of the particle-level jets. Residual differences between the jet energy scale (JES) in data and in simulation are measured using the momentum balance in dijet, γ+jets, Z+jets, and multijet events, and appropriate corrections are applied. The jet energy resolution (JER) typically amounts to 15–20% at 30 GeV, 10% at 100 GeV, and 5% at 1 TeV. Jets overlapping within a cone of radius 0.4 in the η-ϕ plane with a muon or an electron passing the criteria described above are discarded. Further selection criteria are applied to each jet to remove jets potentially dominated by instrumental effects or reconstruction failures, as well as jets arising from pileup interactions [41]. Only jets within the tracker acceptance of $|\eta| < 2.4$ and with $p_T > 30\,\text{GeV}$ are considered in the analysis. Jets arising from the hadronization of b quarks (b jets) are identified using the DeepJet b tagging algorithm [45–47]. Jets are considered as b tagged if they fulfil a requirement on the DeepJet discriminant that corresponds to a b tagging efficiency of 75–80% and a 1.5–2% (15–17%) misidentification rate for light-flavour quark and gluon (c quark) induced jets.

3. Simulated signal and background event samples

Several Monte Carlo (MC) event generators, interfaced with a detailed detector simulation based on Geant4 v. 9.4 [48], are used to model the signal and background events. The proton structure is described by the parton distribution function (PDF) set NNPDF3.1 [49]. Parton showering (PS) and hadronization are simulated with Pythia v. 8.240 [50], where the parameters for the underlying event description correspond to the CP5 tune [51].

The $pp \to A \to ZH \to Zt\bar{t}$ signal is simulated in the gluon fusion production mode at leading order (LO) precision in QCD using MadGraph5_aMC@NLO v. 2.6.5 [52–54]. Events are generated for different mass configurations of the A and H bosons, modelled as narrow resonances with relative decay widths $\Gamma_{A/H}/m_{A/H} = 3\%$, which is negligible compared to the experimental resolution. Events are additionally generated assuming larger widths for some mass configurations, in order to estimate the effect of the total decay width in the 2HDM interpretation. Interference effects between the signal and SM background from $t\bar{t}$ production in association with a Z boson ($t\bar{t}Z$), which is a minor background in the analysis, are small. They modify the rate and the shape of the Δm and p_T^Z distributions by a few percent at most [12], and are therefore neglected. Other A boson production modes in the 2HDM, for which t and b quark associated production have the largest cross sections, contribute less than 2% of the cross section for $\tan\beta < 2$, which is the parameter region relevant for this analysis, and are therefore neglected.

The final state targeted by this search is dominated by background processes from $t\bar{t}$ production and production of Z/γ^* in association with jets referred to as Z/γ^*+jets. The $t\bar{t}$ background process is simulated at next-to-LO (NLO) precision using powheg v. 2 [55–59], and the inclusive cross section is normalized to a calculation at next-to-NLO (NNLO) in QCD including resummation of next-to-next-to-leading logarithmic

(NNLL) soft-gluon terms [60–66]. The top quark p_T spectrum in simulation has been found to be harder than the one observed in data [67,68], and therefore, the simulated events are corrected as a function of the top quark and antiquark p_T at the parton level, such that the corrected simulation matches the data.

The Z/γ^*+jets background processes are simulated at LO precision with up to four partons at the matrix element (ME) level with the MADGRAPH5_aMC@NLO generator, where the merging of the jets from ME calculations and the PS is done using the MLM [69] prescription. The Z/γ^*+jets events are separated into two mutually exclusive processes, based on the flavour of the jets at the particle-level, where these jets fulfil the acceptance requirements of $p_T > 20$ GeV and of $|\eta| < 2.4$. Events with at least one particle-level jet that contains one or more b- or c-flavoured hadrons are classified as Z/γ^* + heavy-flavour jets (Z/γ^*+HF) events, and all other events are classified as Z/γ^* + light-flavour and gluon jets (Z/γ^*+LF) events. Both Z/γ^*+HF and Z/γ^*+LF events are corrected depending on the vector boson p_T to calculations at NLO precision in electroweak and QCD corrections [70].

Minor background contributions arise from $t\bar{t}Z$ production and from $t\bar{t}$ production in association with a W boson ($t\bar{t}W$), single top quark production in the t- and s channels and tW production, collectively referred to as single t, as well as from WW, WZ, and ZZ production, collectively referred to as VV. The $t\bar{t}Z$ and $t\bar{t}W$ processes are simulated at NLO precision with MADGRAPH5_aMC@NLO using the FXFX [71] prescription for the ME-PS jet matching, and their inclusive cross sections are scaled to take into account NLO+NNLL QCD and NLO electroweak corrections [72]. The single t processes are simulated at NLO precision, in the t and tW channels with POWHEG [73,74], and in the s channel with MADGRAPH5_aMC@NLO. The inclusive cross sections of the t and s channel processes are normalized to the predictions at NLO precision [75,76] and the tW channel to calculations at approximate NNLO precision [77]. Diboson production is simulated at LO precision using PYTHIA, and the inclusive cross sections are normalized to NNLO precision [78] for the WW process and to NLO precision [79] for the other diboson processes. Contributions from triboson processes, such as WWZ production, are below the per mille level of the total background and are therefore neglected.

For comparison with the observed distributions, the events in the simulated samples are normalized to the same integrated luminosity as the data sample, according to their predicted cross sections. Pileup effects are modelled by adding simulated minimum bias events to all simulated events with a frequency distribution adjusted to match that observed in the data.

4. Event selection and analysis strategy

The data are selected using a combination of triggers. The triggers require the presence of either one or two muon candidates for the $\mu^+\mu^-$ events, and likewise either one or two electron candidates for the e^+e^- events. In addition, to maximize the signal selection efficiency for e^+e^- events, the analysis uses triggers requiring the presence of one or two photon candidates, which at the trigger level can originate from electrons. The selection efficiency with respect to the offline reconstruction achieved for signal events after the event selection described below is above 99% in the $\mu^+\mu^-$ channel in the entire (m_A, m_H) mass plane and above 99 or 97% in the e^+e^- channel for m_H above or below 300 GeV, respectively. The single-object triggers contribute about 6–8% to the signal selection efficiency.

A further offline selection requires events to have exactly two muons or two electrons of opposite charge, and at least five jets. The invariant mass of the selected lepton pair, $m_{\ell\ell}$, is required to be larger than 30 GeV, and p_T^Z to be larger than 15 GeV to suppress events from heavy-flavour resonance decays and low-mass Drell–Yan processes. The selected events are then categorized based on the lepton flavour into two mutually exclusive channels, $\mu^+\mu^-$ and e^+e^-. In each channel, events

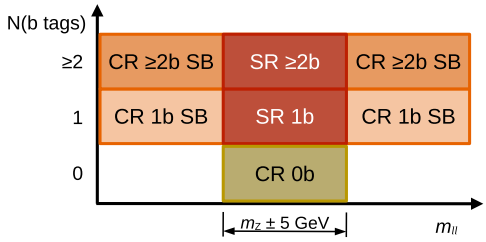


Fig. 1. Definition of the event categories. The five partitions shown apply to each of the classes of jet multiplicity (5j and ≥6j), resulting in 10 categories per lepton flavour channel ($\mu^+\mu^-$ or e^+e^-). A value of 91 GeV is used for the Z boson mass m_Z in the definition of the Z window.

are categorized into events with five jets (5j) and into events with six or more jets (≥6j), and, in each jet multiplicity category, further into events with two or more b-tagged jets (≥2b), one b-tagged jet (1b), and zero b-tagged jets (0b). In each of these six categories in jet and b-tagged jet multiplicity per channel, events are finally separated into one region with $|m_{\ell\ell} - 91\,\text{GeV}| < 5$ GeV (Z window), i.e. close to the Z boson mass, and in one region with $|m_{\ell\ell} - 91\,\text{GeV}| > 5$ GeV (sideband, SB). In the 0b region, only the events with $m_{\ell\ell}$ inside the Z window region are used further in the analysis. This categorization scheme is illustrated in Fig. 1 and leads to ten categories in total per lepton-flavour channel.

The ≥2b and 1b categories inside the Z window are the signal regions (SRs). The overall signal selection efficiency achieved in the four SRs together ranges between 3 and 13%, depending on m_A and m_H. The 5j SRs mainly recover signal events where one jet falls outside the experimental acceptance and, to a lesser extent, signal events where two nearby jets are merged into one single jet, and contribute up to 50% to the total signal selection efficiency at low m_A. Events with fewer than five jets constitute <4% of the signal and therefore are not considered in the analysis.

The normalizations of the overall event yields of the dominant $t\bar{t}$ and Z/γ^*+jets background processes are free parameters of the fit to data described in Section 6, providing flexibility to adjust the predicted yields to those observed in data. The normalizations of the minor background processes are taken from the calculations discussed in Section 3. The SB and the 0b categories are control regions (CRs) that are enriched in $t\bar{t}$ and Z/γ^*+jets events, respectively. Inclusion of the CRs in the fit increases its sensitivity to the normalization parameters and helps to reduce the systematic uncertainties discussed in Section 5.

In each selected event, m_H is reconstructed as the invariant mass of the $t\bar{t}$ system, $m_{t\bar{t}}$, computed as the invariant mass of the reconstructed jets. If there are five or six reconstructed jets in the event, these are used to compute $m_{t\bar{t}}$. If there are more than six reconstructed jets, $m_{t\bar{t}}$ is computed as the invariant mass of the six jets that provide the best compatibility with the $t\bar{t} \to b\bar{b}q\bar{q}q\bar{q}$ decay hypothesis. The six jets are selected by minimizing a χ^2 function, which quantifies the compatibility of the invariant masses of the different two- and three-jet pairings with those of the known masses of the W boson and the t quark from which the jets originate under the $t\bar{t} \to b\bar{b}q\bar{q}q\bar{q}$ decay hypothesis. The χ^2 function takes into account the experimental resolutions in the two- and three-jet invariant masses of 17 GeV and 28 GeV, respectively. The two leptons from the Z boson decay are then included to calculate $m_{t\bar{t}Z}$, the invariant mass of the $t\bar{t}Z$ system.

Finally, two sensitive observables are constructed to discriminate the signal from the background [12]. These exploit kinematic properties of the predominantly on-shell production of the A and H bosons in the $A \to ZH \to Zt\bar{t}$ process. The distributions in $m_{t\bar{t}Z}$ and $m_{t\bar{t}}$ feature Breit–Wigner peaks at approximately m_A and m_H, respectively, and their difference $\Delta m = m_{t\bar{t}Z} - m_{t\bar{t}} \approx m_A - m_H$ is used as an observable of interest. Since the four-momenta of the H and Z bosons are determined by m_A,

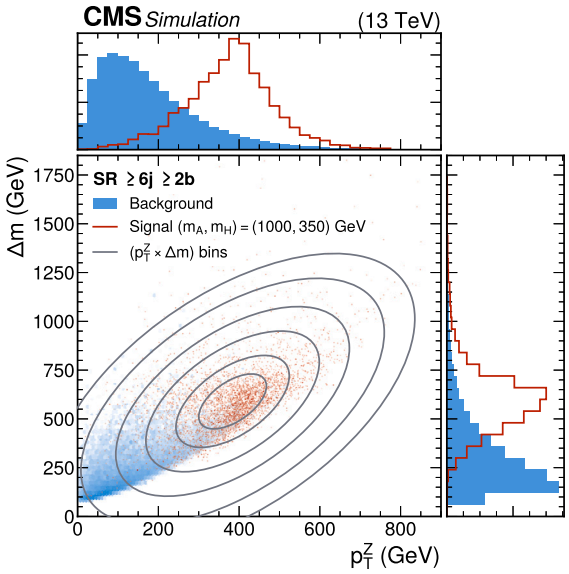


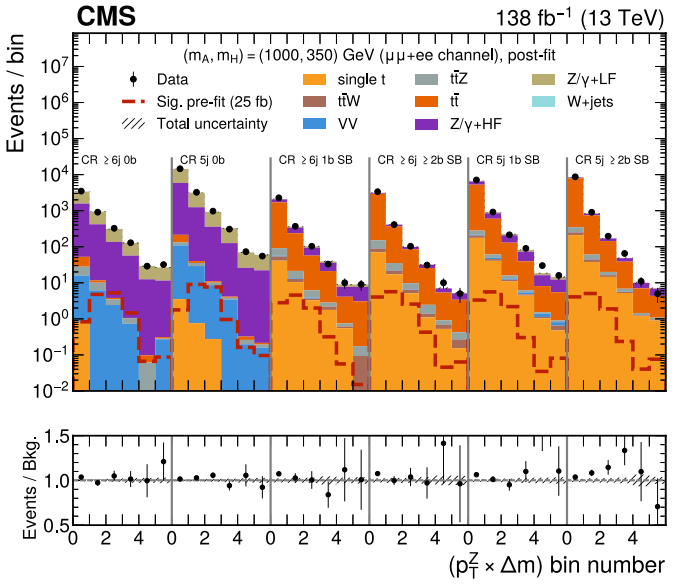
Fig. 2. Expected $(\Delta m, p_{\mathrm{T}}^{\mathrm{Z}})$ distribution for signal events with $m_{\mathrm{A}} = 1000\,\mathrm{GeV}$ and $m_{\mathrm{H}} = 350\,\mathrm{GeV}$ (red) and sum of backgrounds (blue) in the SR ≥6j ≥2b category, and boundaries of the elliptical bins (solid lines) used to construct the final observable.

the $p_{\mathrm{T}}^{\mathrm{Z}}$ spectrum has a characteristic shape with a kinematic edge [12] and is used as the second observable of interest, reconstructed as the p_{T} of the dilepton system. The variables Δm and $p_{\mathrm{T}}^{\mathrm{Z}}$ provide a better experimental resolution than $m_{\mathrm{t\bar{t}Z}}$ and $m_{\mathrm{t\bar{t}}}$ through a reduction of effects from jet mismeasurements. The reconstructed $p_{\mathrm{T}}^{\mathrm{Z}}$ depends only on the excellent lepton momentum resolution and deviations in the reconstructed values of $m_{\mathrm{t\bar{t}Z}}$ and $m_{\mathrm{t\bar{t}}}$ from the true values caused by mismeasurements of jet momenta are correlated and are reduced when using the mass difference Δm.

The two-dimensional distribution in Δm and $p_{\mathrm{T}}^{\mathrm{Z}}$, reduced into a one-dimensional histogram, is used as the final observable to search for the signal. In order to capture the relevant features of the signal distributions with high statistical precision, the information is reduced to a one-dimensional distribution $p_{\mathrm{T}}^{\mathrm{Z}} \times \Delta m$ using concentric elliptical bins in the $(\Delta m, p_{\mathrm{T}}^{\mathrm{Z}})$ plane. The bins are chosen in the CRs based on the background distributions and in the SRs based on the signal distributions for each tested signal hypothesis individually, as follows. The angles and proportions of the major and minor axes of the ellipses are obtained by diagonalizing the covariance matrix of Δm and $p_{\mathrm{T}}^{\mathrm{Z}}$, assuming that Δm and $p_{\mathrm{T}}^{\mathrm{Z}}$ are normally distributed. In the CRs, the ellipses are centred around the mean of the total expected background distribution. In the SRs, the ellipses are centred around the mean of the signal distribution and are chosen specifically for each tested signal hypothesis. Six bins are defined in the SRs (CRs) such that the bin boundaries enclose regions of 34, 68, 82, 95, 97, and 99% of the signal (background) events. An example of how the elliptical bins are constructed and the respective $(\Delta m, p_{\mathrm{T}}^{\mathrm{Z}})$ distributions for the signal test hypothesis with $m_{\mathrm{A}} = 1000\,\mathrm{GeV}$ and $m_{\mathrm{H}} = 350\,\mathrm{GeV}$ are shown in Fig. 2. The $p_{\mathrm{T}}^{\mathrm{Z}} \times \Delta m$ distributions observed in the CRs are shown in Fig. 3, together with the expected background contributions after the fit to data described in Section 6, for two representative mass hypotheses with large and small Δm. The data are well described by the background model within the uncertainties.

5. Systematic uncertainties

Several sources of systematic uncertainty alter either the rate or both the rate and the shape of the $p_{\mathrm{T}}^{\mathrm{Z}} \times \Delta m$ distributions for the signal or background processes, and thus affect the measured signal and background yields. Effects from the same uncertainty source are treated as fully correlated across all channels and categories. Theoretical uncertainties are treated as fully correlated among the different data-taking periods, while experimental uncertainties are in most cases treated as uncorrelated between the data recorded in 2016, 2017, and 2018. The latter assumption is motivated by the fact that the experimental uncertainties are mainly of statistical origin related to the limited size of the data and simulation



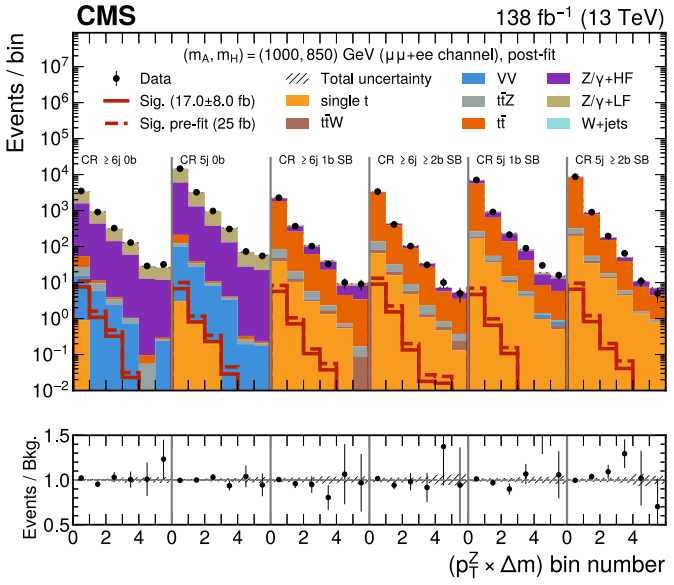


Fig. 3. Distributions of events in the $p_{\mathrm{T}}^{\mathrm{Z}} \times \Delta m$ bins in the CRs after the fit to data described in Section 6 with a signal hypothesis of $m_{\mathrm{A}} = 1000\,\mathrm{GeV}$ and $m_{\mathrm{H}} = 350$ (upper) and $m_{\mathrm{H}} = 850\,\mathrm{GeV}$ (lower). The signal (solid red line) and background (coloured histograms) distributions are shown with their best fit normalizations from the simultaneous fit to the data ("post-fit"), where the sum of the $\mu^+\mu^-$ and e^+e^- channels is shown for illustration purposes. In the upper plot, the post-fit signal cross section is found to be 0.0 ± 0.1 fb. Therefore, the corresponding histogram is not displayed. The signal is also shown for a normalization to 25 fb ("pre-fit") in the dashed red line. The lower panels show the ratio of the observed data to the background events (black points with error bars) and the ratio of the total number of expected signal-plus-background events to the background events (red lines). In both panels, the hatched area represents the total uncertainty.

samples used in auxiliary measurements, which are independent across the data-taking periods.

Since the normalizations of the $t\bar{t}$ and Z/γ^*+jets background processes are free parameters of the fit to data described in Section 6, these are not affected by the theoretical uncertainties of the inclusive cross section predictions. To take into account a possible mismodelling of Z/γ^*+HF production, an additional normalization uncertainty (Z/γ^*+HF norm.) of 40% is assigned to this process. The size of the uncertainty was chosen based on results from Ref. [80], and the results reported in Section 6 have been confirmed to not depend on the chosen size. Furthermore, the flexibility of the background model and its robustness against potential mismodelling of the Z/γ^*+HF component have been verified using pseudo-experiments. A large number of pseudo-experiments have been sampled, both from the nominal and from alternative Z/γ^*+HF predictions with larger cross sections. These tests demonstrated that the strength of an injected signal was extracted without bias when fitting with the nominal background model. Uncertainties in the inclusive cross sections used to predict the rates of the minor background processes arise primarily from variations of the renormalization and factorization scales and the PDFs, and are propagated to the yield estimates. The cross section uncertainties are each separated into their scale and PDF components, and are correlated where appropriate among processes. For example, the PDF uncertainties are taken to be correlated among processes with the same predominant initial state, such that they are correlated among VV and $t\bar{t}W$ production.

Uncertainties in the simulation of the signal and background events are evaluated as follows. Uncertainties arising from missing higher-order terms at the ME level are evaluated by independent variations of the renormalization and factorization scales by factors of 2 and 0.5 with respect to the nominal values. Two independent nuisance parameters per process are assigned in the fit. The uncertainty originating from the PDF set is determined from the PDF variations provided with the NNPDF3.1 set [49], correlating processes for which the same flavour scheme and order in the strong coupling constant α_S are used in the PDF set. The uncertainty in the PYTHIA PS is determined by varying the parameters controlling the amount of initial- and final-state radiation independently by factors of 2 and 0.5 with respect to their nominal value [50]. Uncertainties due to the underlying event tune are found to be negligible. Uncertainties due to the ME-PS matching scheme in the $t\bar{t}$ simulation are evaluated by comparing the reference simulation with samples with varied matching scale parameters. Their effects on the Δm and p_T^Z distributions are found to affect only the rate of the distributions, and separate rate variations are assigned per jet multiplicity category, amounting to 6 and 8% in the 5j and ≥6j categories, respectively. Uncertainties in the corrections applied to the p_T spectrum of the Z boson in the Z/γ^*+jets simulation [70] and of the t quarks in the $t\bar{t}$ simulation [67] are also considered. The former uncertainty ranges from 1 to 10%, depending on the p_T^Z, while the latter ranges up to 7% depending on the p_T of the top quarks.

The variations associated with the theory modelling uncertainties described in the previous paragraph generally affect the overall normalization, the simulated acceptance, and the shapes of the fitted distributions. Since the normalization of the signal as well as the Z/γ^*+jets and $t\bar{t}$ background processes are determined in the fit, the impact of these variations on the overall normalization before any selection is removed. Likewise, for the minor background processes, only the uncertainty in the inclusive cross section prediction is retained to avoid double counting of normalization uncertainties.

Effects of the uncertainty in the distribution of the number of pileup interactions are evaluated by varying the total inelastic cross section used to predict the number of pileup interactions in the simulated events by ±4.6% from its nominal value [41]. The impact of statistical fluctuations in the signal and background prediction due to the limited number of simulated events is accounted for using the Barlow–Beeston-lite approach [81].

The uncertainties in the integrated luminosities are in the 1.2–2.5% range, depending on the year of data taking [23–25], and result in an overall uncertainty of 1.6% for the entire data set, taking into account the correlations. The trigger efficiency is measured in an unbiased sample of events, mostly $t\bar{t}$ leptonic decays, that contain two leptons and fulfil the offline event selection criteria but were collected with triggers based on missing transverse momentum, which feature a negligible correlation with the triggers used in this search. Corrections are derived to match the efficiency in simulation to that observed in data, with uncertainties of 1–6%, dominated by statistical fluctuations in the data samples used in the measurement. Additional corrections are applied for a gradual shift in the timing of the ECAL inputs to the first-level trigger in the region $|\eta| > 2$, which caused a specific trigger inefficiency during the 2016 and 2017 data-taking periods [29], with uncertainties of approximately 0.5%.

Residual differences between the lepton reconstruction, identification, and isolation efficiencies in data and simulation are corrected based on efficiency measurements using a "tag-and-probe" method in data samples of $Z \to \ell\ell$ events [32,33]. The uncertainties are smaller than 1 and 2% for the muon and electron correction factors, respectively.

The uncertainties in the JES and JER are obtained by varying the corrections applied to all jets in the signal and background simulations within their uncertainty. These uncertainties are divided into nine independent sources, which include uncertainties due to different jet flavour compositions in the simulated samples used in the derivation of the corrections. While most of the sources are dominated by statistical fluctuations in auxiliary measurements, some sources are related to theoretical predictions in the MC simulation and are thus treated as correlated among the data-taking periods. The b jet (mis)identification probabilities in simulated events are corrected to match the efficiencies measured in data [45]. The uncertainties in these corrections, which can arise from the contamination of background processes in the data samples used for their derivation, are considered separately for light jets and b/c jets, and vary between 5 and 30% depending on the jet type and p_T [47].

6. Results

A simultaneous binned profile likelihood fit of the signal and background templates to the observed $p_T^Z \times \Delta m$ distribution in all channels and categories is performed, using the COMBINE program [82]. Separate fits are conducted for each (m_A, m_H) hypothesis considered, where the binning of the $p_T^Z \times \Delta m$ distributions in the SRs has been optimized for each hypothesis, as described in Section 4. The mass hypotheses probed range from 430 to 2100 GeV in m_A, and 330 to 2000 GeV in m_H, with steps of 50 GeV at low masses and 100 GeV at higher masses. The spacing has been chosen based on the expected sensitivity to a potential signal, evaluated using simulation, and taking into account the experimental resolution. The exact mass values are provided in the HEPData record for this analysis [26]. The rates of the $t\bar{t}$ and Z/γ^*+jets backgrounds are free parameters in the fit, and the systematic uncertainties described in Section 5 are taken into account via nuisance parameters in the likelihood function. Log-normal distributions are used to model the effects of nuisance parameters on the overall rate, while nuisance parameters that affect the shape of the distributions are parametrized using an interpolation between alternative templates [81,82]. Representative $p_T^Z \times \Delta m$ distributions for (m_A, m_H) hypotheses with large and small mass splittings in the SRs are shown in Fig. 4.

The post-fit values of the background normalization parameters are consistent for all tested mass hypotheses. The values range between 0.82 and 0.94 with uncertainties of approximately 10% for $t\bar{t}$, and between 0.81 and 0.97 with uncertainties of approximately 14% for Z/γ^*+jets, relative to the nominal predictions. The observed yield of the Z/γ^*+HF background component is approximately 40% larger than the pre-fit

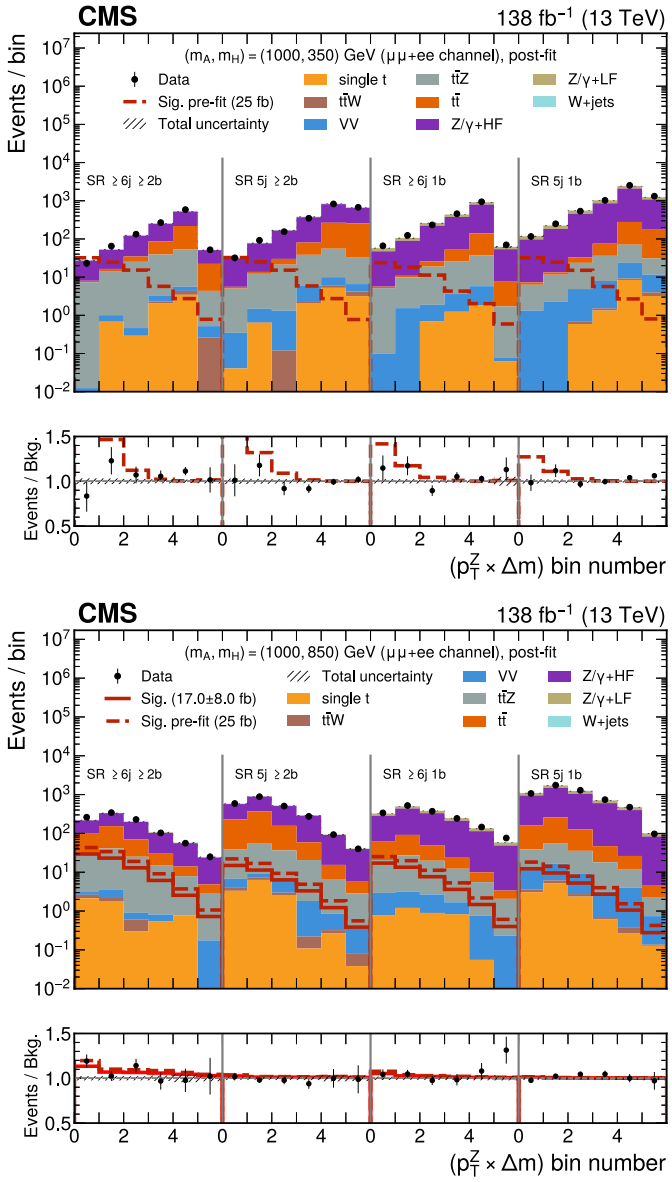


Fig. 4. Distributions of $p_T^Z \times \Delta m$ in the SRs after the fit to data with a signal hypothesis of $m_A = 1000\,\text{GeV}$ and $m_H = 350$ (upper) and $m_H = 850\,\text{GeV}$ (lower). The signal (solid red line) and background (coloured histograms) distributions are shown with their best fit normalizations from the simultaneous fit to the data ("post-fit"), where the sum of the $\mu^+\mu^-$ and e^+e^- channels is shown for illustration purposes. In the upper plot, the post-fit signal cross section is found to be 0.0 ± 0.1 fb. Therefore, the corresponding histogram is not displayed. The signal is also shown for a normalization to 25 fb ("pre-fit") in the dashed red line. The lower panels show the ratio of the observed data to the background events (black points with error bars) and the ratio of the total number of expected signal-plus-background events to the background events (red lines). In both panels, the hatched area represents the total uncertainty.

expectation, driven by the combined effect of the Z/γ^*+jets normalization parameter together with variations of the nuisance parameters associated with the Z/γ^*+HF norm. and the renormalization scale uncertainties. It has been verified that the observed yield of the Z/γ^*+HF component does not depend on the size of the Z/γ^*+HF norm. uncertainty, for example by increasing the Z/γ^*+HF norm. uncertainty from 40% to 100%. The post-fit values of the other nuisance parameters are consistent for the different fits and are generally well within 1 SD of their prior uncertainties.

None of the fits show any significant signal excess with respect to the background-only hypothesis. The largest fluctuation is observed for $m_A = 1000\,\text{GeV}$ and $m_H = 850\,\text{GeV}$, corresponding to a local significance of 2.1 SD. This is visible, for example, in the SR ≥6j ≥2b category in the lower plot of Fig. 4. Upper limits on the product of cross section and branching fractions, $\sigma(pp \to A)\mathcal{B}(A \to ZH)\mathcal{B}(H \to t\bar{t})$, of Higgs-like narrow resonances A and H are derived. The limits are determined using the CL_s criterion [83,84], assuming asymptotic distributions [85] of the profile likelihood ratio test statistics defined in Ref. [82]. The observed and expected upper limits at 95% CL are presented in Fig. 5 in the (m_A, m_H) plane and cover the region up to $m_A = 2100\,\text{GeV}$ and $m_H = 2000\,\text{GeV}$. It has been confirmed using signal injection tests that the search is sensitive to a potential signal at mass configurations between the tested hypotheses, with negligible loss in sensitivity, owing to the finite experimental resolution and the density of the tested points in the (m_A, m_H) plane. Therefore, the limits are interpolated in Fig. 5 to cover the whole (m_A, m_H) plane. The excess of events reported by the ATLAS Collaboration in the region around $(m_A, m_H) = (650, 450)\,\text{GeV}$ with a local significance of 2.85 SD [22] is not observed in the search presented here, which has a similar expected sensitivity. The local significance of the deviation from the background at this point amounts to 0.4 SD, and a $A \to ZH \to Zt\bar{t}$ signal with a cross section larger than 0.25 pb is excluded at 95% CL.

The upper limits on $\sigma(pp \to A)\mathcal{B}(A \to ZH)\mathcal{B}(H \to t\bar{t})$ are also interpreted in the context of type-II 2HDMs. Cross section predictions in the 2HDM are computed with the program SusHi v. 1.7.0 [86] and the branching fractions with 2HDMC v. 1.8.0 [87]. The calculations are performed following Ref. [88] for different values of m_A, m_H, and $\tan\beta$, with m_{12}^2 set to $m_H^2 \sin(\beta)\cos(\beta)$ to ensure vacuum stability over the entire (m_A, m_H) plane. If not specified otherwise, $\cos(\beta - \alpha)$ is set to 0, i.e. corresponding to the alignment limit.

The excluded regions of the 2HDM parameter space are shown in Fig. 6 as a function of m_A and m_H for different values of $\tan\beta$, assuming narrow resonances. The results exclude parts of the parameter space relevant for models of electroweak baryogenesis [9]. In Fig. 7, the excluded regions are shown as a function of $\tan\beta$ and m_A for $m_H = 400\,\text{GeV}$, and as a function of $\tan\beta$ and $\cos(\beta - \alpha)$ for $m_A = 600\,\text{GeV}$ and $m_H = 400\,\text{GeV}$, probing the parameter space away from the alignment limit.

The total decay width Γ_A of the A boson in the 2HDM depends on m_A and $\tan\beta$, as shown by the dotted lines in Figs. 6 and 7. The width can become sizeable compared to the experimental resolution, especially for large values of m_A beyond 1 TeV and small values of $\tan\beta$, reducing the sensitivity of the analysis compared to the case of narrow resonances of the same mass. The effect has been evaluated using signal events simulated with different values of Γ_A. For larger signal widths, we verified that the signal significance is reduced by at most 10% compared to a narrow-resonance signal. This includes all Γ_A values in the 2HDM parameter space considered in this analysis. Thus the narrow-resonance search would be sensitive to a 2HDM signal and the observed absence of a significant excess also constrains this class of models. For $\tan\beta = 1$, the expected limit on $\sigma(pp \to A)\mathcal{B}(A \to ZH)\mathcal{B}(H \to t\bar{t})$ is 20% larger compared to the limit obtained for narrow resonances at $(m_A, m_H) = (750, 330)\,\text{GeV}$, corresponding to $\Gamma_A/m_A = 15\%$, and 47% larger at $(1000, 400)\,\text{GeV}$, corresponding to $\Gamma_A/m_A = 25\%$. The reduction in sensitivity at a given mass point depends on $\tan\beta$: it is larger for $\tan\beta = 0.5$ than for $\tan\beta = 1$ because Γ_A is larger, and smaller for $\tan\beta = 1.5$ because Γ_A is smaller.

7. Summary

A direct search for heavy neutral Higgs bosons A and H in the $t\bar{t}Z$ channel has been conducted, using proton-proton collision data collected by the CMS experiment at $\sqrt{s} = 13\,\text{TeV}$, corresponding to an integrated luminosity of $138\,\text{fb}^{-1}$. The search targets the process

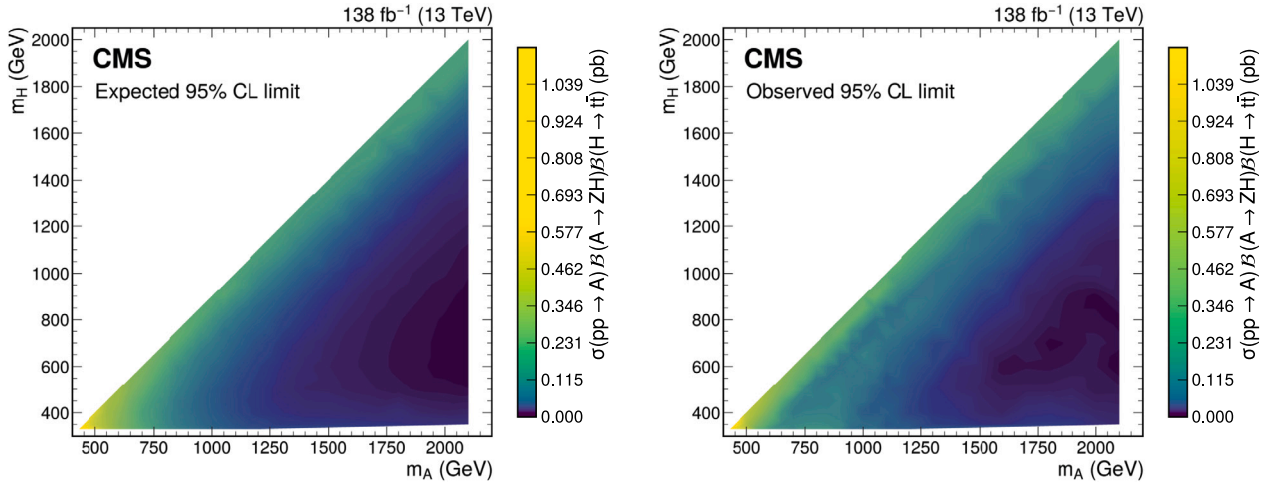


Fig. 5. Expected (left) and observed (right) 95% CL upper limits on the product of production cross section and branching fractions of the $A \to ZH \to Zt\bar{t}$ process in the (m_A, m_H) plane.

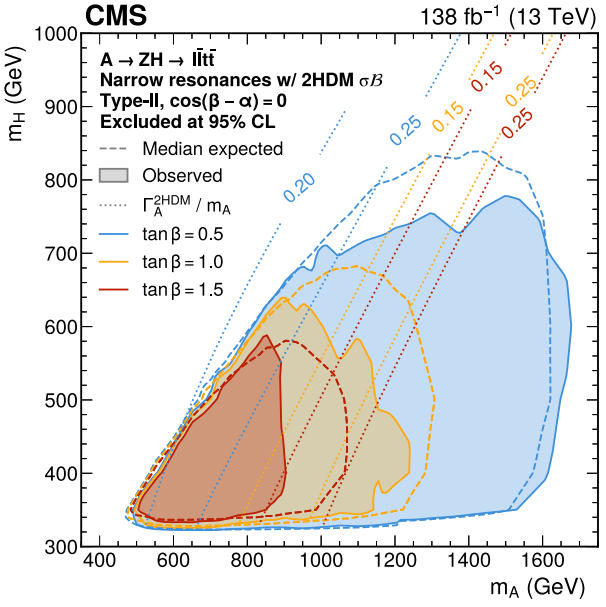


Fig. 6. Median expected (dashed lines) and observed (filled contours) 95% CL exclusion regions in the (m_H, m_A) parameter space of the type-II 2HDM for $\tan\beta = 0.5$ (blue), 1 (orange), and 1.5 (red), derived assuming narrow resonances. The enclosed regions are excluded. The dotted lines indicate points of constant total decay width Γ_A of the A boson relative to its mass in the 2HDM, for the $\tan\beta$ value of the corresponding colour.

$pp \to A \to ZH$ with $H \to t\bar{t}$. For the first time, the final state with decays of the Z boson to muons or electrons in association with all-hadronic decays of the $t\bar{t}$ system is considered.

No evidence for a signal is observed. Stringent upper limits are set on the product of the cross section and branching fractions for A and H boson masses up to $m_A = 2100$ GeV and $m_H = 2000$ GeV, respectively, assuming narrow resonances. The results are further used to constrain the parameter space of two-Higgs-doublet models as a function of the $\tan\beta$ and $\cos(\beta - \alpha)$ parameters. The excess of events reported by the ATLAS Collaboration in the region around $(m_A, m_H) = (650, 450)$ GeV with a local significance of 2.85 standard deviations [22] is not observed in the search presented here, which has similar expected sensitivity. The results complement and substantially extend the reach of previous searches, constraining parameter regions relevant for models explaining baryogenesis.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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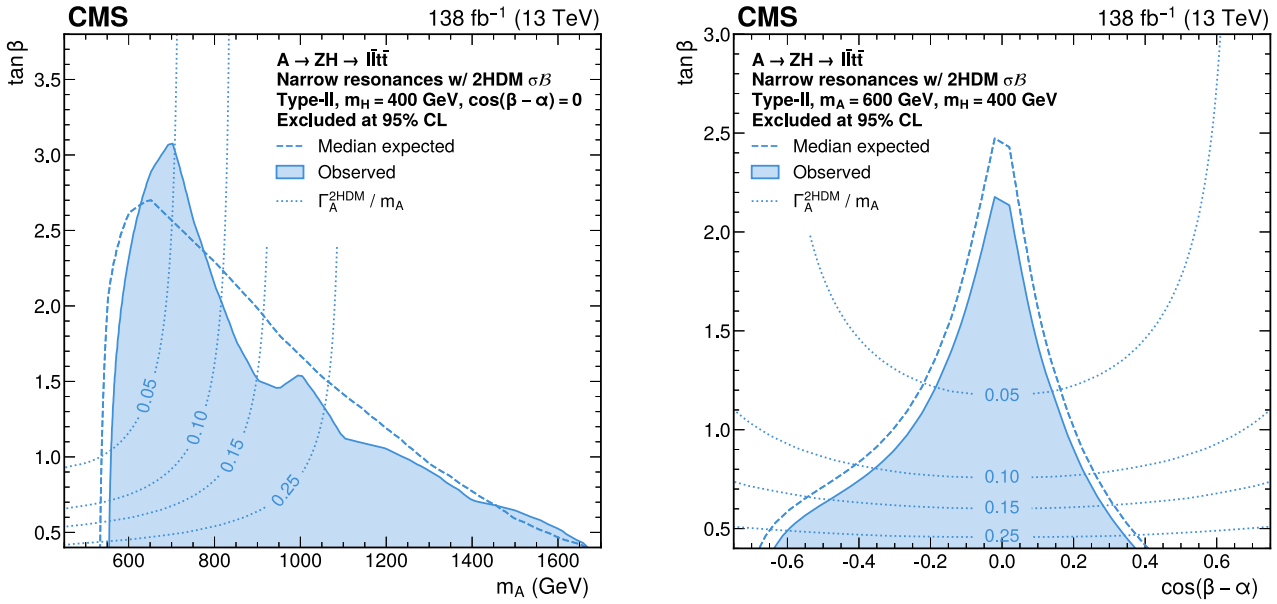


Fig. 7. Median expected (dashed lines) and observed (filled contours) 95% CL exclusion regions in the type-II 2HDM $(\tan\beta, m_A)$ parameter space at $m_H = 400\,\text{GeV}$ (left) and in the $(\tan\beta, \cos(\beta-\alpha))$ parameter space at $m_A = 600\,\text{GeV}$ and $m_H = 400\,\text{GeV}$ (right), derived assuming narrow resonances. The enclosed regions are excluded. The dotted lines indicate points of constant total decay width Γ_A of the A boson relative to its mass in the 2HDM.

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Data availability

Release and preservation of data used by the CMS Collaboration as the basis for publications is guided by the CMS data preservation, re-use and open access policy.

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