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# Search for light long-lived particles in $pp$ collisions at $\sqrt{s} = 13$ TeV using displaced vertices in the ATLAS inner detector

The ATLAS Collaboration

A search for long-lived particles (LLPs) using  $140 \text{ fb}^{-1}$  of  $pp$  collision data with  $\sqrt{s} = 13$  TeV recorded by the ATLAS experiment at the LHC is presented. The search targets LLPs with masses between 5 and 55 GeV that decay hadronically in the ATLAS inner detector. Benchmark models with LLP pair production from exotic decays of the Higgs boson and models featuring long-lived axion-like particles (ALPs) are considered. No significant excess above the expected background is observed. Upper limits are placed on the branching ratio of the Higgs boson to pairs of LLPs, the cross-section for ALPs produced in association with a vector boson, and, for the first time, on the branching ratio of the top quark to an ALP and a  $u/c$  quark.

The majority of experimental searches for dark matter (DM) have concentrated on weakly interacting massive particles (WIMPs) that interact directly with Standard Model (SM) particles with a strength comparable to that of the weak interaction. However, constraints on WIMP-like DM from both direct [1–9] and indirect detection experiments [10] are becoming increasingly stringent. One compelling alternative to the WIMP paradigm is that DM particles belong to a “dark sector” (DS) that is neutral under the SM gauge group and interacts with the SM only via one or more beyond the SM mediator particles [11–15]. If decays of the mediator to DS particles are kinematically forbidden, its decay back into SM particles will be suppressed by the small coupling between the SM and the mediator, giving rise to potentially macroscopic proper decay lengths ( $c\tau \gtrsim 100 \mu\text{m}$ ). These so-called long-lived particles (LLPs) are also predicted in scenarios in which the mediator particle couples to the SM via a higher-dimensional operator, such as in models featuring axion-like particles (ALPs) [16, 17].

This Letter presents a search for neutral LLPs that decay hadronically, giving a distinct signature of one or more hadronic jets originating at a significantly displaced position from the proton–proton ( $pp$ ) collision point, referred to as a displaced vertex (DV). Three benchmark models are explored, motivated by different interactions between the SM and DS states. The first benchmark considers the “Higgs Portal”, in which the SM Higgs boson mediates interactions with the DS through its coupling to a neutral spin-0 boson,  $s$  [18, 19]. This benchmark gives rise to exotic decays of the Higgs boson to a pair of long-lived  $s$  particles that decay back to SM particles with Yukawa-ordered branching ratios. The search targets Higgs boson production in association with a vector boson ( $W/Z$ ) and via the vector boson fusion (VBF) process. The second benchmark considers extending the SM with an ALP,  $a$ , which couples to gluons and  $W/Z$  bosons, while couplings to photons are suppressed [20]. This gives rise to the production of  $a$  in association with a vector boson ( $W/Z$ ) and its subsequent decay exclusively into gluons. The third benchmark considers an ALP,  $a$ , which couples to up-type quarks [21, 22], giving rise to exotic decays of the top quark  $t \rightarrow ac/au$  in  $t\bar{t}$  events. In this model the  $a$  boson decays into charm quark pairs or gluons, with branching ratios of approximately 75% and 25% for  $m_a > 40 \text{ GeV}$ , respectively. Diagrams of the three benchmark processes can be found in Appendix A.

This search is performed with  $140 \text{ fb}^{-1}$  of 13 TeV  $pp$  collision data collected by the ATLAS experiment at the Large Hadron Collider (LHC) [23] from 2015 to 2018. Several previous searches for Higgs boson decays to LLPs have been performed that in combination exclude branching ratios  $\text{BR}(H \rightarrow ss) > 10\%$  for  $s$  masses above 40 GeV and proper decay lengths between  $10^{-3} \text{ m}$  and 10 m [24–32]. However, for masses below 40 GeV, Higgs boson decays to LLPs with proper decay lengths below 100 mm are unconstrained beyond the limit of 12% on the branching ratio of the Higgs boson to undetected states [33]. A limiting factor in probing this region of phase space with the ATLAS experiment has been the reconstruction of displaced tracks in the inner tracking detector (ID). In 2022, an improved version of the track reconstruction pass for large-impact parameter tracks was deployed in ATLAS [34]. This upgrade significantly reduced the rate of reconstructing so-called fake tracks due to random hit combinations, thereby enhancing computational efficiency and enabling the application of this reconstruction to every recorded data event. This Letter reports the first direct application of this new track reconstruction, which significantly expands the reach of this search with respect to previous ATLAS results and allows for sensitivity to previously unexplored phase space. Notably, this is the first search for Higgs boson decays to hadronically decaying LLPs in the ID to probe the VBF topology, and the first search to probe hadronically decaying long-lived ALPs produced in association with a vector boson and via exotic decays of the top quark.

The ATLAS detector [35, 36] is a cylindrical detector with forward–backward symmetry and nearly  $4\pi$  solid-angle coverage.<sup>1</sup> An extensive software suite [37] is used in data simulation, in the reconstruction and

<sup>1</sup> ATLAS uses a right-handed coordinate system with its origin at the nominal interaction point (IP) in the center of the detector

analysis of real and simulated data, in detector operations, and in the trigger and data acquisition systems of the experiment.

A primary charged particle (track) reconstruction pass is used to reconstruct charged-particle trajectories with transverse impact parameter ( $d_0$ ) with respect to the  $pp$  interaction point (IP) of  $|d_0| < 5$  mm. A large-impact parameter pass, using left-over hits from the primary pass, is used to increase tracking acceptance up to  $|d_0| < 300$  mm [34]. The  $pp$  interaction vertex with the highest sum of squared transverse momenta of associated tracks is taken as the primary interaction vertex (PV). Hadronic jets are reconstructed from topological clusters of energy deposits in the calorimeters [38] using the anti- $k_t$  algorithm [39, 40] with a radius parameter of  $R = 0.4$ . The matching of tracks with the calorimeter-based jets is performed via the ghost-association technique [41]. Jets with transverse momentum  $p_T > 20$  GeV are considered in the analysis.

Electron candidates are reconstructed from energy deposits in the calorimeters associated to an ID track, and are required to be within the fiducial region  $|\eta| < 2.47$ , and outside of  $1.37 < |\eta| < 1.52$ . Muons are reconstructed by combining tracks reconstructed in the ID with tracks or track segments found in the muon spectrometer (MS) and are required to have  $|\eta| < 2.5$ . Electrons and muons are required to have  $p_T > 10$  GeV and satisfy the *Medium* identification criterion [42, 43]. To ensure that the selected electrons (muons) originate from the PV, they must satisfy  $|\frac{d_0}{\sigma(d_0)}| < 5$  (3), and  $|(z_0 - z_{PV}) \sin \theta| < 0.5$  mm, where  $z_0$  is the track's longitudinal impact parameter and  $z_{PV}$  is the  $z$  coordinate of the PV. Photon candidates are reconstructed from clustered energy deposits in the electromagnetic calorimeter either without any matching ID track or with a matching photon conversion vertex in the ID material. The *Loose* identification criterion is required [42]. The missing transverse momentum ( $E_T^{\text{miss}}$ ) is defined as the magnitude of the negative vector sum of the transverse momenta of all reconstructed and calibrated electrons, muons, photons, jets, and remaining unclustered energy. The latter is estimated from low- $p_T$  tracks associated with the PV but not assigned to a reconstructed object [44].

Samples of Monte Carlo (MC) simulated events are used to study the three benchmark scenarios. In the Higgs portal benchmark, the decays of the  $s$  particles are simulated assuming a 100% branching ratio to the heaviest quark–antiquark pair that is kinematically allowed. To quantify the dependence of the analysis on the flavor of the final state quarks, additional samples are generated assuming a 100% branching ratio to  $u\bar{u}$ . Signal samples were generated assuming proper decay lengths of the LLP (either  $a$  or  $s$ ) of 1, 10, 100, and 1000 mm, and masses in the range  $5 \leq m_s \leq 55$  GeV and  $40 \leq m_a \leq 55$  GeV for the Higgs portal and ALP benchmarks, respectively. In all samples, the LLP is taken to be a pseudoscalar, although the analysis does not explicitly exploit the  $CP$  properties of the LLPs. Samples of simulated  $t\bar{t}$  and  $V$ +jets background events are used to optimize the event selections and evaluate systematic uncertainties. Details about the event simulation configurations used can be found in Appendix A.

Events are categorized into three search regions, each targeting a different Higgs boson or ALP production mode. The *1-lepton* region is defined by the presence of exactly one lepton ( $e/\mu$ ) with  $p_T > 27$  GeV and  $E_T^{\text{miss}} > 30$  GeV. These criteria target signal processes containing a leptonically decaying  $W$  boson including  $WH$ ,  $Wa$ , and  $t\bar{t}, t \rightarrow ac/au$  production. The *2-lepton* region is defined by the presence of exactly two leptons, with the same flavor and opposite charge. The highest  $p_T$  lepton is required to have  $p_T > 27$  GeV, and the invariant mass of the dilepton system is required to fall between 76 and 106 GeV. These criteria target signal events containing a leptonically decaying  $Z$  boson, including  $ZH$  and  $Za$

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and the  $z$ -axis along the beam pipe. The  $x$ -axis points from the IP to the center of the LHC ring, and the  $y$ -axis points upward. Polar coordinates  $(r, \phi)$  are used in the transverse plane,  $\phi$  being the azimuthal angle around the  $z$ -axis. The pseudorapidity is defined in terms of the polar angle  $\theta$  as  $\eta = -\ln \tan(\theta/2)$ . Angular distance is measured in units of  $\Delta R = \sqrt{\Delta\eta^2 + \Delta\phi^2}$ .

production. Events in the 1- and 2-lepton regions are collected with a combination of single and dilepton triggers [45–47]. In both regions, events are required to have at least two jets with  $|\eta| < 2.5$ . The *VBF enriched* region targets events with the VBF topology. Events are collected with an inclusive VBF trigger enabled during the 2018 data-taking period that is designed to select events with a pair of jets consistent with the VBF process [48]. The data collected with this trigger correspond to a total integrated luminosity of  $37.5 \text{ fb}^{-1}$ . The VBF enriched region is defined by the absence of any lepton, and the presence of a pair of jets with invariant mass  $m_{jj} > 1200 \text{ GeV}$  and angular separation  $|\Delta\eta_{jj}| > 4$  and  $|\Delta\phi_{jj}| < 2$ . The leading (subleading) jet in this pair is required to have transverse momentum  $p_T > 100$  (80) GeV and  $|\eta| < 3.2$  (4.9). These selections ensure that the trigger selection efficiency is approximately 100%. In addition to the pair of jets used to select the VBF topology, events are required to have at least two additional jets with  $|\eta| < 2.5$ .

The jets emerging from the decay products of an LLP, referred to as *displaced jets*, exhibit a distinct topology compared to *prompt jets* that originate from a  $pp$  interaction vertex. To distinguish displaced jets from prompt jets, a per-jet boosted decision tree (BDT) is trained using the XGBOOST framework [49]. The output of this classifier is a displaced jet BDT score between zero and one, where a higher score indicates that the jet is more likely to have originated from a displaced decay. This BDT is trained on five jet-level features that discriminate between displaced and prompt jets. The first feature is the fraction of the total jet  $p_T$  carried by tracks with  $|d_0| < 0.5 \text{ mm}$ , which is expected to be smaller for displaced jets than for prompt jets. Similarly, the fraction of the total jet  $p_T$  carried by tracks with  $|d_0| > 0.5 \text{ mm}$  is used, which provides additional information about the contribution from displaced charged particles to the total jet momentum. Third, the fractional value of jet track  $p_T$  originating from tracks with  $|d_0| < 0.5 \text{ mm}$  and  $|(z_0 - z_{\text{vertex}}) \sin \theta| < 0.3 \text{ mm}$  is calculated for each reconstructed  $pp$  interaction vertex, and the maximum value of this set is taken. Finally, the maximum  $|d_0|$  among tracks in the jet, and the median of the logarithmic transverse impact parameter significance of tracks associated to the jet are used. The BDT is trained on a mixed signal sample comprised of  $VH, H \rightarrow ss$  events with  $m_s \in \{16, 55\} \text{ GeV}$  and  $c\tau_s \in \{10, 100\} \text{ mm}$ , and a mixed background sample comprised of  $t\bar{t}, W$ +jets and  $Z$ +jets events in equal parts. Distributions of the BDT score for jets in selected signal samples and in data can be found in the Supplemental Material.

To reconstruct the origin of the hadronic jets produced from the decay of the LLPs, a DV reconstruction algorithm [50] is run on the combined collection of tracks from both the primary and the large-impact parameter tracking passes. Following Ref. [29], selections are placed on the reconstructed vertices to reject DVs from SM processes and random combinations of tracks. DVs are required to have a track multiplicity  $n_{\text{track}} \geq 3$  and vertex goodness of fit  $\chi_{\text{DV}}^2/n_{\text{DoF}} < 5$ . The radial and longitudinal coordinates of the DV position are each required to be less than 300 mm, and a material veto is applied to reject DVs from interactions between high-momentum hadrons and known detector elements [51]. The ratio of the DV invariant mass ( $m_{\text{DV}}$ ) and the maximum angular distance between any two tracks in the DV ( $\Delta R_{\text{max}}$ ) is required to satisfy  $m_{\text{DV}}/\Delta R_{\text{max}} > 4 \text{ GeV}$ , and the scalar sum of the transverse momentum of DV tracks is required to be above 10 GeV. When computing the kinematic properties of the DVs, the track parameters are calculated after extrapolating their trajectory to the DV position. DV tracks must satisfy  $|d_0| > 0.1 \text{ mm}$  and at least one track in the vertex must have  $|d_0| > 3 \text{ mm}$ . To associate DVs to displaced jets, the vectorial sum of the DV track momenta is required to be within  $\Delta R < 0.6$  of a jet with a BDT score greater than 0.5. If multiple DVs are matched to a given jet, only the DV with the smallest  $\Delta R$  to the jet axis is considered.

All events considered in the analysis are required to have at least two jets with a BDT score greater than 0.5. An event-level discriminant ( $\text{BDT}_{j_0} \times \text{BDT}_{j_1}$ ) is computed by taking the product of the BDT scores of the two jets in the event with the largest BDT scores. From each of the three search regions, two signal regions

(SRs) are defined based on the candidate DV multiplicity in the event,  $n_{\text{DV}} = 1$  or  $n_{\text{DV}} \geq 2$ , resulting in a total of six SRs. Events in the  $n_{\text{DV}} = 1$  SRs are required to have  $\text{BDT}_{j_0} \times \text{BDT}_{j_1} > 0.9$ . This condition is relaxed to  $\text{BDT}_{j_0} \times \text{BDT}_{j_1} > 0.7$  in the  $n_{\text{DV}} \geq 2$  SRs. Example distributions of the event-level discriminant can be found in the Supplemental Material.

The dominant sources of background are  $t\bar{t}$  and  $W$ +jets,  $Z$ +jets, and multijet production in the 1-lepton, 2-lepton, and VBF enriched SRs, respectively. The background contribution is estimated using a fully data-driven approach, following the method developed in Ref. [29]. In each of the three search regions, a control region (CR) is defined by requiring  $\text{BDT}_{j_0} \times \text{BDT}_{j_1} < 0.7$ . Assuming a 12% branching ratio of  $H \rightarrow ss$  from Ref [33], the fractional signal contribution in the CRs is expected to be less than 1%. The probability that a jet is matched to a DV is computed separately in each of the three CRs and encoded in a three dimensional map parameterized in jet  $p_{\text{T}}$ , the jet flavor tagging score (DL1r) [52] that separates light and heavy flavor jets, and BDT score. The map is divided evenly in the BDT dimension using a bin width of 0.01 in the 1-lepton region, and 0.025 in the 2-lepton and VBF enriched regions where fewer events are selected. The per-jet probabilities are then used to compute the probability that each event contains exactly one, or greater than one DV based on the  $p_{\text{T}}$ , DL1r, and BDT scores of the jets in the event. The per-event probability weights are applied inclusively to data in the search regions to predict the distributions of  $\text{BDT}_{j_0} \times \text{BDT}_{j_1}$  in events with  $n_{\text{DV}} = 1$  and  $n_{\text{DV}} \geq 2$ .

Two uncertainties in the background prediction are considered. First, the statistical uncertainty in the background estimate due to the finite number of events in the CR used to derive the maps is computed using ensembles of background estimates from a set of statistically varied per-jet probability maps [29]. The standard deviation of this ensemble of estimates is used to define the up and down statistical variations on the nominal prediction. Second, in the 2-lepton and VBF enriched regions, where a coarser binning is used in the BDT dimension of the per-jet probability map, an uncertainty in the background estimate from the binning choice is quantified. In this regard, the difference between the nominal estimate and an alternate estimate computed from a map with a BDT bin width of 0.01 is taken as a systematic uncertainty. The total uncertainty in the background predictions varies from 10–50%, depending on the signal region.

The background estimate is validated in a subset of the  $n_{\text{DV}} = 1$  events defined by  $0.7 < \text{BDT}_{j_0} \times \text{BDT}_{j_1} < 0.9$  within each of the three search regions, and in a dedicated event selection requiring the presence of a single photon with  $p_{\text{T}} > 160$  GeV and  $|\eta| < 2.47$ , zero leptons, and two jets with  $p_{\text{T}} > 20$  GeV. The distributions of data events are found to be well modeled by the predicted background in all regions, validating the extrapolation of the background estimate from the CR to larger values of  $\text{BDT}_{j_0} \times \text{BDT}_{j_1}$  and to events with  $n_{\text{DV}} \geq 2$ . A more detailed description of the background validation is given in Appendix B.

Instrumental and theoretical uncertainties are assigned on the modeling of the simulated signal samples. The dominant uncertainty is due to the modeling of the BDT score, which is derived as a per-jet uncertainty by comparing the shape of the BDT score between data and the simulated  $Z$ +jets sample in the 2-lepton preselection, and then propagated to the final event yield. The impact of this uncertainty is as large as 15%. Subleading sources of instrumental uncertainty include those on the primary and large-impact parameter track reconstruction efficiencies [34]; lepton trigger, reconstruction, and identification efficiencies [53]; lepton energy scale and resolution [54]; jet energy scale and resolution [38]; modeling of the pileup in simulation [55]; and the total integrated luminosity of the measurement [56, 57]. Theoretical uncertainties are considered to account for variations due to the renormalization and factorization scales, parton distribution functions, and parton showering.

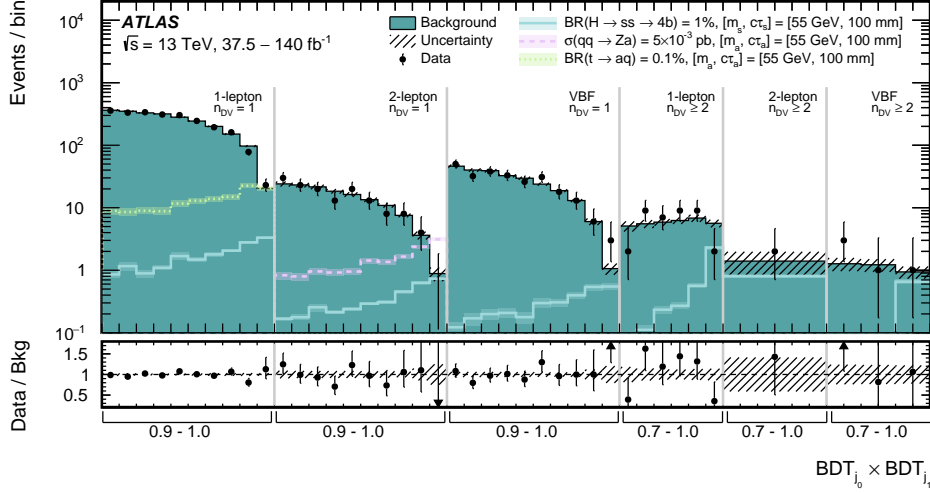


Figure 1: Distributions of  $BDT_{j_0} \times BDT_{j_1}$  for the observed data (black points) and the background prediction (filled histogram) with its uncertainty after the fit to data in the six SRs described in the text. The signal expectation for the Higgs portal model with  $m_s = 55$  GeV and  $c\tau_s = 100$  mm is shown in the solid line, scaled to  $BR(H \rightarrow ss \rightarrow 4b) = 1\%$ . The signal expectation for ALP production in association with a Z boson scaled to  $\sigma(qq \rightarrow Za) = 5 \times 10^{-3}$  pb, and for  $t \rightarrow aq$  scaled to  $BR(t \rightarrow aq) = 0.1\%$  are shown in the dashed and dotted lines, respectively, for  $m_a = 55$  GeV and  $c\tau_a = 100$  mm. The observed data in the 1- and 2-lepton (VBF) regions corresponds to an integrated luminosity of 140 (37.5)  $\text{fb}^{-1}$ . The ratio between the data and predicted background is shown in the bottom panel.

For each signal model considered, a binned maximum-likelihood fit to the  $BDT_{j_0} \times BDT_{j_1}$  distributions in the SRs is performed. For the Higgs portal model, all six SRs are fitted simultaneously, while in the  $Wa$  and  $t \rightarrow aq$  ( $Za$ ) model, only the 1-lepton (2-lepton)  $n_{DV} = 1$  SR is considered. Systematic and MC statistical uncertainties are included as nuisance parameters and are constrained in the fit. Systematic uncertainties on the signal efficiency are correlated across the six signal regions, while the systematic and statistical uncertainties on the background are treated as uncorrelated. In the 1-lepton region where there is no systematic uncertainty on the background prediction, a linear shape uncertainty is included as an additional degree of freedom to the fit to permit the value of the fitted statistical uncertainty to vary.

The distributions of  $BDT_{j_0} \times BDT_{j_1}$  for the observed data and the background prediction after the fit to data in the six SRs are shown in Figure 1. No significant deviation from the SM expectation is observed. The absence of a data excess is translated into exclusion limits at 95% confidence level (CL) on  $BR(H \rightarrow ss \rightarrow 4b)$ ,  $\sigma(qq \rightarrow Va)$ , and  $BR(t \rightarrow aq)$ . The CLs prescription [58] is used to compute the limits using asymptotic formulae for the profile likelihood ratio [59]. The expected and observed exclusion limits are shown in Figure 2. For the Higgs portal benchmark, the limits set by this search are considerably stronger than previous ATLAS results [29] using the same dataset, with improvements by as much as a factor of 20 for  $m_s = 55$  GeV and  $c\tau_s < 10$  mm. These improvements are driven by the updated large-impact parameter track reconstruction, the addition of the 1-lepton and VBF search regions, and the inclusion of  $n_{DV} = 1$  signal regions. In particular, the VBF enriched region contributes a similar level of sensitivity as the other two search regions despite having a considerably smaller integrated luminosity.

In summary, this Letter reports the results of a search for LLPs with masses between 5 and 55 GeV that decay hadronically in the ATLAS inner detector. No significant excess beyond the SM prediction is observed. The reported constraints on the Higgs boson branching ratio are the most stringent to date for

$m_s < 40$  GeV and  $1 < c\tau_s < 100$  mm. For  $H \rightarrow ss \rightarrow 4b$ , branching ratios greater than 1% are excluded for  $m_s = 55$  GeV and  $6 < c\tau_s < 68$  mm. The exclusion limits are stronger for light-quark final states, with  $4 < c\tau_s < 107$  mm excluded for  $H \rightarrow ss \rightarrow 4u$  and  $m_s = 55$  GeV. For the first time at the LHC, branching ratios beyond the limit of 12% imposed on Higgs boson decays to undetected states are probed for  $m_s < 16$  GeV and  $c\tau_s < 100$  mm, with  $\text{BR}(H \rightarrow ss \rightarrow 4c) > 10\%$  excluded for  $m_s = 5$  GeV and  $3 < c\tau_s < 20$  mm. The first limits on long-lived ALP models with suppressed coupling to photons are set, excluding cross-sections for  $qq \rightarrow Va$  greater than 0.1 pb for  $m_a > 40$  GeV and  $1.2 < c\tau_a < 192$  mm. Long-lived ALPs produced via  $t \rightarrow aq$  are probed for the first time, excluding  $t \rightarrow aq$  branching ratios greater than 0.1% between  $4 < c\tau_a < 36$  mm for  $m_a > 40$  GeV.

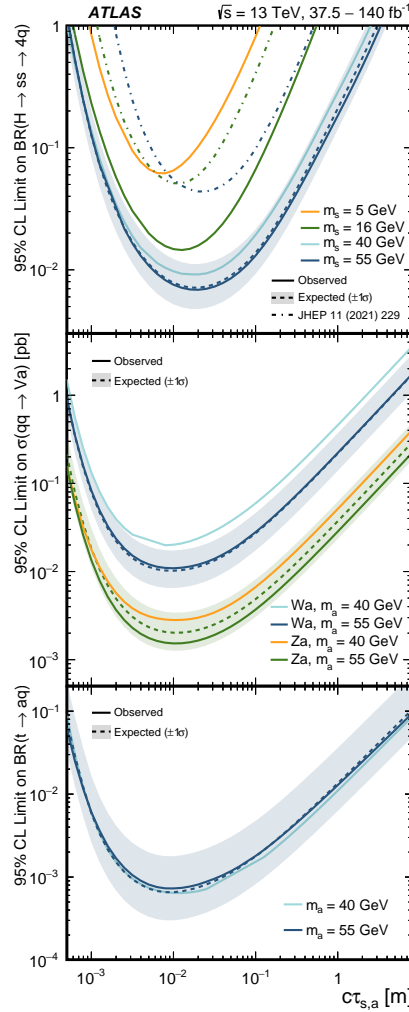


Figure 2: The 95% confidence level limits on (upper) the Higgs boson branching ratio  $H \rightarrow ss \rightarrow 4q$ , (middle)  $q\bar{q} \rightarrow Va$  cross-section where  $V = W$  or  $Z$ , and (lower)  $t \rightarrow aq$  branching ratio shown as a function of the mean proper decay length  $c\tau$  of the long-lived particle. In the upper plot, the limits shown are on the Higgs boson branching ratio  $H \rightarrow ss \rightarrow 4b$  for  $m_s = 16, 40, 55$  GeV, and  $H \rightarrow ss \rightarrow 4c$  for  $m_s = 5$  GeV. The observed limits are shown with a solid line and the expected limit and  $\pm 1\sigma$  uncertainty bands on this expectation are shown with dashed lines and shaded bands, respectively. In the upper plot, the observed limits for the Higgs Portal model from the previous ATLAS search [29] are shown with the dotted lines.

## Acknowledgments

We thank CERN for the very successful operation of the LHC and its injectors, as well as the support staff at CERN and at our institutions worldwide without whom ATLAS could not be operated efficiently.

The crucial computing support from all WLCG partners is acknowledged gratefully, in particular from CERN, the ATLAS Tier-1 facilities at TRIUMF/SFU (Canada), NDGF (Denmark, Norway, Sweden), CC-IN2P3 (France), KIT/GridKA (Germany), INFN-CNAF (Italy), NL-T1 (Netherlands), PIC (Spain), RAL (UK) and BNL (USA), the Tier-2 facilities worldwide and large non-WLCG resource providers. Major contributors of computing resources are listed in Ref. [60].

We gratefully acknowledge the support of ANPCyT, Argentina; YerPhI, Armenia; ARC, Australia; BMWFW and FWF, Austria; ANAS, Azerbaijan; CNPq and FAPESP, Brazil; NSERC, NRC and CFI, Canada; CERN; ANID, Chile; CAS, MOST and NSFC, China; Minciencias, Colombia; MEYS CR, Czech Republic; DNRF and DNSRC, Denmark; IN2P3-CNRS and CEA-DRF/IRFU, France; SRNSFG, Georgia; BMBF, HGF and MPG, Germany; GSRI, Greece; RGC and Hong Kong SAR, China; ISF and Benoziyo Center, Israel; INFN, Italy; MEXT and JSPS, Japan; CNRST, Morocco; NWO, Netherlands; RCN, Norway; MEiN, Poland; FCT, Portugal; MNE/IFA, Romania; MESTD, Serbia; MSSR, Slovakia; ARRS and MIZŠ, Slovenia; DSI/NRF, South Africa; MICINN, Spain; SRC and Wallenberg Foundation, Sweden; SERI, SNSF and Cantons of Bern and Geneva, Switzerland; MOST, Taipei; TENMAK, Türkiye; STFC, United Kingdom; DOE and NSF, United States of America.

Individual groups and members have received support from BCKDF, CANARIE, CRC and DRAC, Canada; PRIMUS 21/SCI/017, Czech Republic; COST, ERC, ERDF, Horizon 2020, ICSC-NextGenerationEU and Marie Skłodowska-Curie Actions, European Union; Investissements d’Avenir Labex, Investissements d’Avenir IDEX and ANR, France; DFG and AvH Foundation, Germany; Herakleitos, Thales and Aristeia programmes co-financed by EU-ESF and the Greek NSRF, Greece; BSF-NSF and MINERVA, Israel; Norwegian Financial Mechanism 2014-2021, Norway; NCN and NAWA, Poland; La Caixa Banking Foundation, CERCA Programme Generalitat de Catalunya and PROMETEO and GenT Programmes Generalitat Valenciana, Spain; Göran Gustafssons Stiftelse, Sweden; The Royal Society and Leverhulme Trust, United Kingdom.

In addition, individual members wish to acknowledge support from CERN: European Organization for Nuclear Research (CERN P.J.A.S.); Chile: Agencia Nacional de Investigación y Desarrollo (FONDECYT 1190886, FONDECYT 1210400, FONDECYT 1230987); China: National Natural Science Foundation of China (NSFC - 12175119, NSFC 12275265); Czech Republic: Ministry of Education Youth and Sports (FORTE CZ.02.01.01/00/22\_008/0004632); European Union: European Research Council (ERC - 948254, ERC 101089007), Horizon 2020 Framework Programme (MUCCA - CHIST-ERA-19-XAI-00), Italian Center for High Performance Computing, Big Data and Quantum Computing (ICSC, NextGenerationEU); France: Agence Nationale de la Recherche (ANR-20-CE31-0013, ANR-21-CE31-0022), Investissements d’Avenir Labex (ANR-11-LABX-0012); Germany: Baden-Württemberg Stiftung (BW Stiftung-Postdoc Eliteprogramme), Deutsche Forschungsgemeinschaft (DFG - 469666862, DFG - CR 312/5-2); Italy: Istituto Nazionale di Fisica Nucleare (ICSC, NextGenerationEU); Japan: Japan Society for the Promotion of Science (JSPS KAKENHI 22H01227, JSPS KAKENHI 22KK0227, JSPS KAKENHI JP21H05085, JSPS KAKENHI JP22H04944); Netherlands: Netherlands Organisation for Scientific Research (NWO Veni 2020 - VI.Veni.202.179); Norway: Research Council of Norway (RCN-314472); Poland: Polish National Agency for Academic Exchange (PPN/PPO/2020/1/00002/U/00001), Polish National Science Centre (NCN 2021/42/E/ST2/00350, NCN OPUS nr 2022/47/B/ST2/03059, NCN UMO-2019/34/E/ST2/00393,



UMO-2020/37/B/ST2/01043, UMO-2021/40/C/ST2/00187, UMO-2022/47/O/ST2/00148); Slovenia: Slovenian Research Agency (ARIS grant J1-3010); Spain: Generalitat Valenciana (Artemisa, FEDER, IDIFEDER/2018/048), Ministry of Science and Innovation (RYC2019-028510-I, RYC2020-030254-I), PROMETEO and GenT Programmes Generalitat Valenciana (CIDEAGENT/2019/023, CIDEAGENT/2019/027); Sweden: Swedish Research Council (VR 2022-03845, VR 2023-03403), Knut and Alice Wallenberg Foundation (KAW 2022.0358); Switzerland: Swiss National Science Foundation (SNSF - PCEFP2\_194658); United Kingdom: Leverhulme Trust (Leverhulme Trust RPG-2020-004); United States of America: Neubauer Family Foundation.

## APPENDIX A: SIMULATED DATA SAMPLES

Samples of MC simulated events are used to study the three benchmark scenarios. Higgs boson production in association with a vector boson and via vector-boson fusion (VBF) was simulated using POWHEG Box v2 [61–64] and interfaced with PYTHIA 8.2 [65] to simulate the  $H \rightarrow ss$  decay and the subsequent decay of the  $s$ . PYTHIA 8.2 is also used for simulating parton shower and non-perturbative effects, with parameters set according to the AZNLO tune [66]. The POWHEG Box prediction is accurate to next-to-leading-order (NLO) for  $VH$  boson plus one-jet production. The loop-induced  $gg \rightarrow ZH$  process was generated separately at leading-order (LO). Samples of  $qq \rightarrow Va$  and  $gg \rightarrow t\bar{t}$  with  $t \rightarrow ac/au$  were simulated using MADGRAPH [67] v2.9.9 and interfaced with PYTHIA 8.307. The effect of multiple  $pp$  interactions in the same or neighboring bunches (pileup) was modeled by overlaying the hard-scatter process with simulated inelastic  $pp$  scattering events. Feynman diagrams of the simulated signal processes are shown in Figure 3.

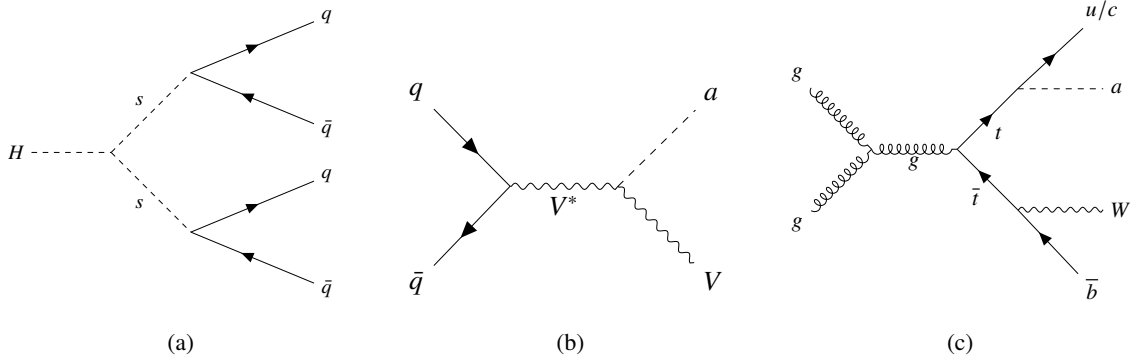


Figure 3: Feynman diagrams for (a) the exotic Higgs boson decay mode  $H \rightarrow ss \rightarrow 4q$ , (b) the  $q\bar{q} \rightarrow Va$  ALP production mode, where the ALP decays exclusively into gluons, and (c) the ALP production via the exotic top-quark decay  $t \rightarrow qa$  in  $t\bar{t}$  events, where the  $a$  can decay into either  $gg$  or  $c\bar{c}$ , and the  $W$  boson decays into  $lv$ .

The production of  $t\bar{t}$  events was modeled using the POWHEG Box v2 generator at NLO and interfaced with PYTHIA 8.230 with parameters set according to the A14 tune [68]. The production of  $V$ +jets was simulated with the SHERPA 2.2.1 [69] generator using NLO matrix elements for up to two partons, and LO matrix elements for up to four partons calculated with the Comix [70] and OPENLOOPS [71–73] libraries. They were matched with the SHERPA parton shower [74] using the MEPS@NLO prescription [75–78]. The samples were normalized to a next-to-next-to-leading-order prediction [79].

## APPENDIX B: VALIDATION OF BACKGROUND ESTIMATE

The method of estimating the distributions of events with  $n_{\text{DV}} = 1$  from the per-jet probabilities is validated by performing closure tests in the CRs. The weighted distributions of  $\text{BDT}_{j_0} \times \text{BDT}_{j_1}$  in the three CRs are found to reproduce the observed distributions of events with  $n_{\text{DV}} = 1$  within uncertainties. The distributions of the leading and subleading jet  $p_{\text{T}}$ ,  $\text{DL}1r$ , and BDT scores are also found to be well modeled by the estimate in CR events with  $n_{\text{DV}} = 1$ .

The extrapolation of the background estimate from the CR to larger values of  $\text{BDT}_{j_0} \times \text{BDT}_{j_1}$  is validated in a subset of the  $n_{\text{DV}} = 1$  events defined by  $0.7 < \text{BDT}_{j_0} \times \text{BDT}_{j_1} < 0.9$ , within the 1-lepton, 2-lepton and VBF enriched search regions. The observed data in these three validation regions (VRs) are found to agree with the predicted background within uncertainties, as shown in Figure 4.

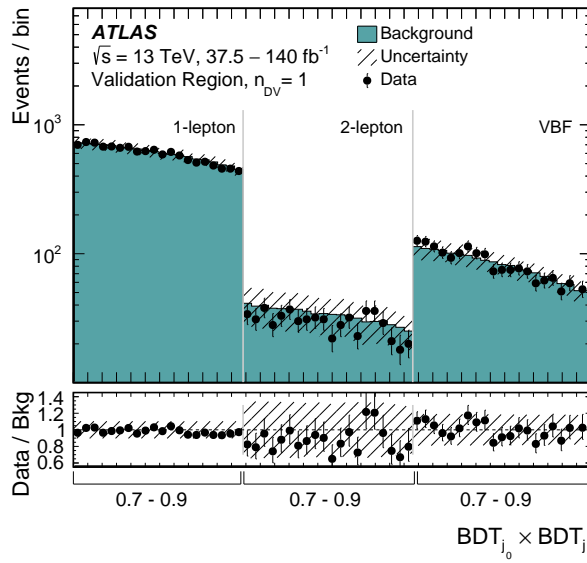


Figure 4: Distributions of  $\text{BDT}_{j_0} \times \text{BDT}_{j_1}$  for the observed data (black points) and the background prediction (teal filled histogram) with its uncertainty in the three  $n_{\text{DV}} = 1$  validation regions with  $0.7 < \text{BDT}_{j_0} \times \text{BDT}_{j_1} < 0.9$ . The ratio between the data and predicted background is shown in the bottom panel. The background estimates are computed using events in the three CRs with  $\text{BDT}_{j_0} \times \text{BDT}_{j_1} < 0.7$ .

To validate the extrapolation to higher values of  $\text{BDT}_{j_0} \times \text{BDT}_{j_1}$  and to events with  $n_{\text{DV}} \geq 2$ , a dedicated *photon VR* is used defined by the presence of a single photon with  $p_{\text{T}} > 160 \text{ GeV}$  and  $|\eta| < 2.47$ , zero leptons, and two jets with  $p_{\text{T}} > 20 \text{ GeV}$ . This selection effectively rejects events from all signal models considered and provides an independent set of data events on which to test the background estimation method. The same background estimation strategy is applied to this region as in the three search regions, using a dedicated map computed from events in the photon VR with  $\text{BDT}_{j_0} \times \text{BDT}_{j_1} < 0.7$ . The distributions of data events with  $n_{\text{DV}} = 1$  and  $\text{BDT}_{j_0} \times \text{BDT}_{j_1} > 0.7$  and data events with  $n_{\text{DV}} \geq 2$  are found to be well modeled by the predicted background, as shown in Figure 5.

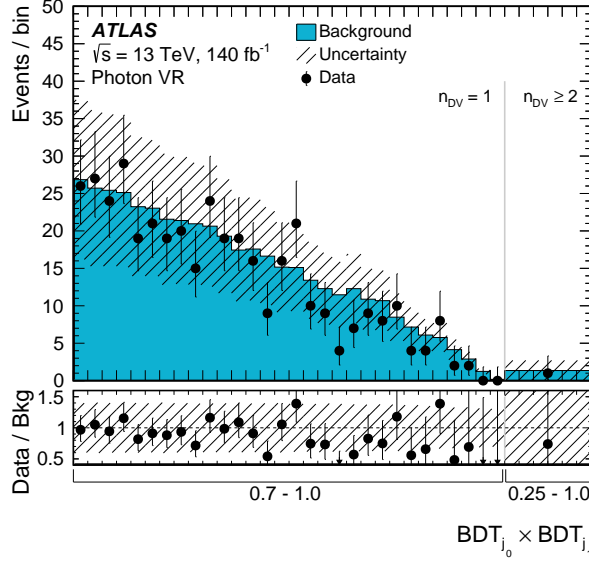


Figure 5: Distributions of  $BDT_{j_0} \times BDT_{j_1}$  for the observed data (black points) and the background prediction (blue) with its uncertainty in the photon validation region (VR) for events with  $n_{DV} = 1$  and  $n_{DV} \geq 2$ . The ratio between the data and predicted background is shown in the bottom panel. The background estimate is computed using events in the photon VR with  $BDT_{j_0} \times BDT_{j_1} < 0.7$ .

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## Supplemental Material

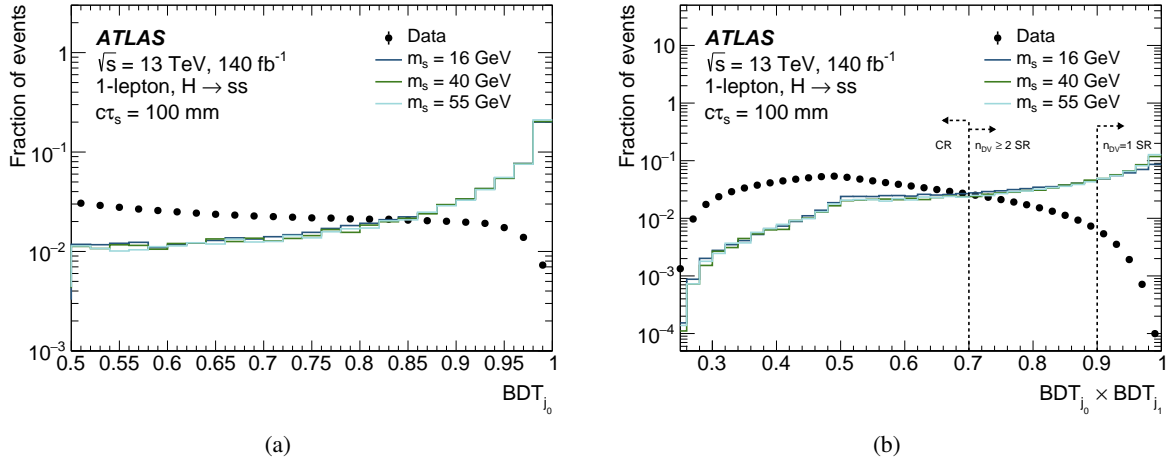


Figure 6: The distribution of (a) the BDT score of the jet with the highest BDT score in the event ( $BDT_{j_0}$ ) and (b) the product of the BDT scores of the two jets in the event with the largest BDT scores ( $BDT_{j_0} \times BDT_{j_1}$ ), in simulated signal samples (solid lines) and a background-enriched data sample (black points) for events in the 1-lepton search region described in the text, with the additional requirement that the events contain at least two jets with BDT scores greater than 0.5. The distributions are normalized to unit area.

## The ATLAS Collaboration

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