

RECEIVED: January 29, 2026

REVISED: March 31, 2026

ACCEPTED: July 24, 2026

PUBLISHED: September 4, 2026

Search for $\tau^- \rightarrow \mu^- \mu^+ \mu^-$ decays at the LHCb experiment with Run 2 data



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ABSTRACT: A search for the lepton-flavour-violating decay $\tau^- \rightarrow \mu^- \mu^+ \mu^-$ is carried out using data collected by the LHCb experiment between 2016 and 2018 in proton-proton collisions at the LHC at a centre-of-mass energy of 13 TeV, corresponding to an integrated luminosity of 5.4 fb^{-1} . An upper limit of $1.9 (2.3) \times 10^{-8}$ is set at the 90% (95%) confidence level on the branching fraction of the decay.

KEYWORDS: Beyond Standard Model, Hadron-Hadron Scattering, Rare Decay, Tau Physics

ARXIV EPRINT: [2601.20785](https://arxiv.org/abs/2601.20785)

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1 Introduction

Lepton-flavour-violating decays are forbidden in the Standard Model (SM) under the assumption of massless neutrinos. In a massive-neutrino scenario, lepton-flavour-violating decays are expected to occur at extremely low rates, with branching fractions around 10^{-55} [1], well below the sensitivity of any current or foreseen experimental facilities. Nevertheless, many extensions of the SM including heavy neutrinos [2, 3] or the exchange of an extra neutral gauge boson Z' [4] predict much larger branching fractions at the level of 10^{-10} – 10^{-8} . Therefore, observation of the $\tau^- \rightarrow \mu^- \mu^+ \mu^-$ decay¹ would indicate new physics beyond the SM, while further improving the experimental limit on its branching fraction would provide constraints on SM extensions.

A previous search with the LHCb experiment using the Run 1 (2011–2012) dataset set an upper limit on the branching fraction of the $\tau^- \rightarrow \mu^- \mu^+ \mu^-$ decay of $\mathcal{B}(\tau^- \rightarrow \mu^- \mu^+ \mu^-) < 4.6 \text{ (5.6)} \times 10^{-8}$ at the 90% (95%) confidence level (CL) [5]. The ATLAS collaboration also conducted a search for the $\tau^- \rightarrow \mu^- \mu^+ \mu^-$ decay using data collected in 2012, obtaining an upper limit of 3.8×10^{-7} at 90% CL [6]. A more recent search by the CMS collaboration, based on the full Run 2 dataset, established an upper limit of $2.9 \text{ (3.6)} \times 10^{-8}$ at 90% (95%) CL [7]. The most stringent upper limit from a single experiment was reported by the Belle II collaboration, which obtained 1.9×10^{-8} at 90% CL [8].

In this paper, a search for the lepton-flavour-violating $\tau^- \rightarrow \mu^- \mu^+ \mu^-$ decay is presented, based on data collected by the LHCb experiment in proton-proton (pp) collisions during the years 2016–2018 of Run 2 of the LHC at a centre-of-mass energy of $\sqrt{s} = 13$ TeV, corresponding

¹Charge conjugation is implied throughout the paper.

to an integrated luminosity of 5.4 fb^{-1} . The $\tau^- \rightarrow \mu^- \mu^+ \mu^-$ branching fraction is evaluated relative to the known $D_s^- \rightarrow \phi(1020) \pi^-$ branching fraction, accounting for the fraction of τ^- leptons produced in D_s^- decays.² This normalisation channel, where the intermediate state decays as $\phi \rightarrow \mu^- \mu^+$, is chosen for its similar topology and decay kinematics with respect to the signal. The $\tau^- \rightarrow \mu^- \mu^+ \mu^-$ branching fraction is given by

$$\begin{aligned} \mathcal{B}(\tau^- \rightarrow \mu^- \mu^+ \mu^-) &= \mathcal{B}(D_s^- \rightarrow \phi(\rightarrow \mu^- \mu^+) \pi^-) \times \frac{f_{D_s}^\tau}{\mathcal{B}(D_s^- \rightarrow \tau^- \bar{\nu}_\tau)} \times \frac{\epsilon_{D_s}}{\epsilon_\tau} \times \frac{N_\tau}{N_{D_s}} \\ &= \alpha \times N_\tau, \end{aligned} \quad (1.1)$$

where $\mathcal{B}(D_s^- \rightarrow \phi(\rightarrow \mu^- \mu^+) \pi^-)$ and $\mathcal{B}(D_s^- \rightarrow \tau^- \bar{\nu}_\tau)$ are taken from ref. [9], $f_{D_s}^\tau$ is the fraction of τ^- leptons that are produced by D_s^- decays versus the inclusive production from heavy-hadron decays, ϵ_τ (ϵ_{D_s}) is the efficiency for selecting candidates in the signal (normalisation) channel, and N_τ (N_{D_s}) the number of candidates observed in the signal (normalisation) channel. The total normalisation factor, α , is referred to as the *single-event sensitivity*.

This article is organised as follows: in section 2, the LHCb detector, data and simulation samples used in the analysis are described; the selection criteria for the signal and normalisation channels are outlined in section 3; the corrections applied to the simulation to improve the description of the data are reported in section 4; the treatment of the different sources of background is discussed in section 5; section 6 reports on the evaluation of the selection efficiencies, the normalisation factors, and the corresponding systematic uncertainties; the procedure to measure the signal yield is discussed in section 7; section 8 reports the strategy adopted for the evaluation of the upper limit and the corresponding results; and finally, conclusions are drawn in section 9.

2 Detector and dataset

The LHCb detector [10, 11] is a single-arm forward spectrometer covering the pseudorapidity range $2 < \eta < 5$, designed for the study of particles containing b or c quarks. The detector used to collect data for this analysis includes a high-precision tracking system consisting of a silicon-strip vertex detector surrounding the pp interaction region [12], a large-area silicon-strip detector located upstream of a dipole magnet with a bending power of about 4 T m, and three stations of silicon-strip detectors and straw drift tubes [13] placed downstream of the magnet. The tracking system provides a measurement of the momentum, p , of charged particles with a relative uncertainty that varies from 0.5% at low momentum to 1.0% at 200 GeV/ c . The minimum distance of a track to a primary pp collision vertex (PV), the impact parameter (IP), is measured with a resolution of $(15 + 29/p_T) \mu\text{m}$, where p_T is the component of the momentum transverse to the beam, in GeV/ c . Different types of charged hadrons are distinguished using information from two ring-imaging Cherenkov detectors [14]. Photons, electrons and hadrons are identified by a calorimeter system consisting of scintillating-pad and preshower detectors, an electromagnetic and a hadronic calorimeter. Muons are identified by a system composed of alternating layers of iron and multiwire proportional chambers [15].

The online event selection is performed by a trigger [16], which consists of a hardware stage, based on information from the calorimeter and muon systems, followed by a software

²In the following, ϕ denotes the $\phi(1020)$ meson.

stage, which applies a full event reconstruction. The hardware trigger selects candidates with either one or two muons with high p_T , while the software trigger adds requirements on the kinematics, track quality and particle-identification (PID) information of the muons. The trigger requirements at the second stage of the software trigger (HLT2) differ between the signal and the normalisation channel, as a dedicated trigger selection for the three-muon final state was available for the signal. In addition, the configuration used to select $D_s^- \rightarrow \phi(\rightarrow \mu^- \mu^+) \pi^-$ candidates in the 2016 data sample differs from that employed in 2017 and 2018 at the HLT2 level, where additional trigger lines were available, resulting in a lower selection efficiency in 2016 compared to the other years. Triggered data further undergo a centralised, offline processing step to deliver physics-analysis-ready data across the entire LHCb physics programme [17].

Simulated samples of $\tau^- \rightarrow \mu^- \mu^+ \mu^-$ and $D_s^- \rightarrow \phi(\rightarrow \mu^- \mu^+) \pi^-$ decays are produced to understand the effects of detector acceptance and the imposed selection requirements. In the simulation, pp collisions are generated using PYTHIA [18] with a specific LHCb configuration [19]. Decays of unstable particles are described by EVTGEN [20], in which final-state radiation is generated using PHOTOS [21]. The interaction of the generated particles with the detector, and its response, are implemented using the GEANT4 toolkit [22] as described in ref. [23] and further corrected to account for known differences between data and simulation in kinematic distributions, detector response, and particle-identification variables of the reconstructed candidates. The $D_s^- \rightarrow \phi(\rightarrow \mu^- \mu^+) \pi^-$ mode is exploited to derive these corrections based on the similarity observed in the distributions of the aforementioned variables with respect to the $\tau^- \rightarrow \mu^- \mu^+ \mu^-$ channel, as described in section 4. Samples are produced accounting for the main sources of τ^- leptons in pp collision. The τ^- production cross-section is dominated by $D_{(s)}^-$ mesons produced either promptly or in b -hadron (secondary) decays, as well as by direct decays of b hadrons. Contributions from Z and W boson decays as well as from the Drell–Yan process are orders of magnitude smaller than that from heavy-hadron production and are therefore neglected [24, 25]. The $\tau^- \rightarrow \mu^- \mu^+ \mu^-$ decay is generated with a uniform phase-space distribution.

3 Selection

The signal $\tau^- \rightarrow \mu^- \mu^+ \mu^-$ decay and the $D_s^- \rightarrow \phi(\rightarrow \mu^- \mu^+) \pi^-$ decay used as the normalisation channel are selected applying criteria that are as similar as possible. The τ^- and D_s^- candidates are reconstructed by combining three tracks with a total charge of -1 . The three tracks are required to be compatible with originating from a common vertex and have significant χ_{IP}^2 with respect to all PVs. Here, χ_{IP}^2 is defined as the difference in the vertex-fit χ^2 of a given PV reconstructed with and without the track under consideration. Loose requirements on the track quality and p_T are placed on all tracks. In case of D_s^- candidates, two oppositely charged tracks should be identified as muons, with the same muon-identification requirement as applied to all three final-state tracks in the τ^- case. Muon identification is based on the track momentum and the pattern of hits in the muon chambers associated with the track [26]. In the selection of D_s^- candidates, the $\mu^- \mu^+ \pi^-$ mass is required to lie within $\pm 50 \text{ MeV}/c^2$ of the known D_s^- mass [9], while the $\mu^- \mu^+$ mass must fall within $\pm 20 \text{ MeV}/c^2$ of the known ϕ -meson mass [9]. Tau candidates are removed if

any of the two $\mu^-\mu^+$ combinations lie within the $\pm 30 \text{ MeV}/c^2$ region around the ϕ mass, and are required to have a mass larger than $450 \text{ MeV}/c^2$ to suppress $D_s^- \rightarrow \eta^{(\prime)}(\rightarrow \mu^-\mu^+\gamma)\mu^-\bar{\nu}_\mu$ decays, as discussed in section 5. The same-sign dimuon mass is instead required to be larger than $250 \text{ MeV}/c^2$ in order to reject candidates containing duplicate tracks reconstructed from hits originated by a single charged particle.

The signal sample is divided based on the three-muon mass $M_{\mu\mu\mu}$ into: a signal region, where the signal selection efficiency, and the signal and background yields are evaluated, defined as $|M_{\mu\mu\mu} - m_\tau| \leq 20 \text{ MeV}/c^2$, with m_τ being the known τ mass [9]; and a sideband region with $|M_{\mu\mu\mu} - m_\tau| > 20 \text{ MeV}/c^2$, which is used to model the background shape and obtain an expectation of the background yield in the signal region. The signal region is masked in data until the end of the analysis, to avoid experimenter's bias.

The main discrimination of $\tau^- \rightarrow \mu^-\mu^+\mu^-$ signal over background is achieved by means of two gradient-boosted decision-tree classifiers, both based on the binary XGBOOST [27] model. The first classifier (C_{AC} , for *anticombinatorial*), based on topological and kinematic information, is designed to suppress the contribution from random combinations of tracks wrongly associated with the same vertex, referred to as combinatorial background. The second classifier (C_{PID}), based on PID and kinematic information, is trained to reduce physics background from hadrons misidentified as muons. The main contribution to this background comes from hadronic $D_{(s)}^-$ decays. Both classifiers are trained using simulated signal candidates as a signal proxy and data candidates in the part of the sideband region close to the signal region ($20 < |M_{\mu\mu\mu} - m_\tau| \leq 30 \text{ MeV}/c^2$) as a background proxy. The use of two separate classifiers improves performance by exploiting different features of the decay. Supervised learning with k -fold ($k = 5$) cross-validation [28] is used to achieve an unbiased classifier response.

The largest discrimination power in the C_{AC} classifier comes from isolation variables that quantify how much the other tracks of the event are likely to originate from the same decay as the signal tracks. The other input variables to the C_{AC} classifier are: the p_T and χ^2_{IP} of each final-state track and of the τ^- particle with respect to their own PV; the τ^- decay time; the track fit χ^2 for the three muons and the fit χ^2 of their vertex, and the displacement of the latter with respect to the PV; the cosine of the angle between the τ^- momentum vector and the vector from the primary to the decay vertex; the number of tracks in a cone built around each final-state track; and the asymmetry between the p_T of the final-state track and the sum of the p_T of all the particles within the cone. Inputs to the C_{PID} classifier are the muon- and kaon-identification probabilities and pseudorapidity of each final-state track. The correlation between the two classifiers is found to be negligible. Selected τ^- candidates are retained if they lie within $C_{AC} > 0.80$ and $C_{PID} > 0.88$, corresponding to a signal efficiency of about 60%. An additional requirement is introduced to remove residual hadronic background as discussed in section 5. No selection based on the C_{AC} or C_{PID} classifiers is applied to the normalisation channel, owing to its already high signal purity.

It is also possible to reconstruct decays in which one of the muons falls outside the acceptance of the muon system or has insufficient momentum to penetrate it, by considering candidates for which only two tracks satisfy the muon-identification requirements of the analysis. However, the larger background contamination, together with the limitations of the

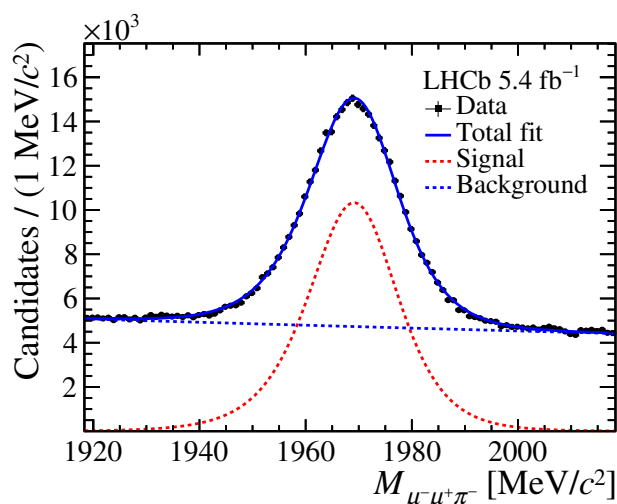


Figure 1. Mass distribution of selected $\mu^-\mu^+\pi^-$ candidates together with the fit result.

hardware trigger, which primarily selects tracks with high p_T , make the sensitivity to the $\tau^- \rightarrow \mu^-\mu^+\mu^-$ channel significantly worse than in the case where all tracks are identified as muons. The contribution of this category to the upper limit is found to be negligible and is therefore excluded from the final result presented in this paper.

4 Simulation calibration

Simulation samples produced for the relevant sources of τ^- leptons are combined with relative fractions determined using the $b\bar{b}$ and $c\bar{c}$ cross-sections as measured by the LHCb experiment in pp collisions at $\sqrt{s} = 13$ TeV [29, 30] and the inclusive $b \rightarrow D_{(s)}^-$, $c \rightarrow D_{(s)}^-$, $b \rightarrow \tau^-$ and $D_{(s)}^- \rightarrow \tau^-$ branching fractions from ref. [9]. The ratio between prompt and secondary charm production is then adjusted to data using the $D_s^- \rightarrow \phi(\rightarrow \mu^-\mu^+)\pi^-$ channel by comparing the distributions of the logarithm of χ^2_{IP} of the D_s^- meson in simulation and background-subtracted data. The background-subtracted distribution is obtained from a maximum-likelihood fit to the $\mu^-\mu^+\pi^-$ mass distribution of selected D_s^- candidates, using the *sPlot* technique [31]. The signal probability density function (PDF) is parametrised by a Johnson’s S_U function [32] and the background by an exponential function. The tail parameters of the Johnson’s S_U function are fixed from a fit to simulation, while the peak position and width, as well as the slope of the exponential component, are free to vary. The fit result is shown in figure 1 for the combined 2016–2018 dataset.

A weighting algorithm from the `hep_ml` package [33] based on decision trees is used to correct for global differences in kinematics and detector response. The input features are topological and kinematic variables of the D_s^- and the total number of tracks in the event. Corrections to the muon-identification variables are evaluated from the ratio of the distributions in data and simulation in different regions of total number of tracks, momentum and pseudorapidity of the muon with the lowest muon-identification probability. Small residual disagreements between data and simulation are observed in the output of the C_{AC} and C_{PID} classifiers when applied to the $D_s^- \rightarrow \phi(\rightarrow \mu^-\mu^+)\pi^-$ channel. The ratios of

the corresponding one-dimensional distributions in data and simulation are used to derive correction factors that account for these differences. The ratio of the signal- to normalisation-channel efficiencies is further corrected to account for differences between data and simulation arising from track reconstruction and trigger selections in the two channels. The tracking efficiency is calibrated through a sample of prompt $J/\psi \rightarrow \mu^+\mu^-$ decays [34], by comparing the performance of the track-finding algorithm obtained excluding at least one subdetector with that obtained including all subdetectors. This calibration is determined as a function of the event multiplicity, track p and η by computing the overall correction as the product of the single-track efficiency for each final-state particle. The trigger efficiency corrections are derived from a sample of $D_s^- \rightarrow \phi(\rightarrow \mu^-\mu^+)\pi^-$ candidates triggered independently of the signal decay chain and comparing the performance of the signal trigger lines in data and simulation in bins of the p_T and χ_{IP}^2 of the final-state track with the highest p_T [16]. The correction factors are evaluated independently for each year of data taking and are of the order (0.1–3.0)%.

5 Background

Background contamination to the $\tau^- \rightarrow \mu^-\mu^+\mu^-$ decay mainly arises from random combinations of muons or misidentified hadrons from decays of heavy or light hadrons, forming a three-track vertex displaced from the PV, with a mass close to that of the τ^- lepton. The dominant background processes are charm meson decays into three charged hadrons, all misidentified as muons. These decays are strongly suppressed by the selection based on the C_{AC} and C_{PID} classifiers. However, when the pion and kaon mass hypotheses are assigned to the three final-state tracks in all possible combinations within the selected data sample, peaking structures are observed in the mass distributions corresponding to the $\pi^-K^+\pi^-$ and $\pi^-\pi^+\pi^-$ mass hypotheses. These structures are consistent with contributions from $D^- \rightarrow \pi^-K^+\pi^-$ and $D_{(s)}^- \rightarrow \pi^-\pi^+\pi^-$ decays, characterised by branching fractions at the permille to percent level [9]. To further suppress the $D^- \rightarrow \pi^-K^+\pi^-$ contribution, a tight kaon-identification requirement is imposed on the final-state track with charge opposite to that of the parent particle. This requirement is applied when the $\pi^-K^+\pi^-$ mass hypothesis has a combined mass below $1900 \text{ MeV}/c^2$ and rejects more than 99.9% of the D^- candidates according to simulation. The expected remaining contribution is found to be negligible and is therefore ignored in the fit to the $\mu^-\mu^+\mu^-$ mass distribution. In contrast, contaminations from $D_{(s)}^- \rightarrow \pi^-\pi^+\pi^-$ decays are not significantly reduced by the application of tighter particle-identification requirements and are therefore modelled in the final fit. The expected contamination is estimated by fitting the three-track mass distribution in the sidebands and extrapolating the yields of the two sources into the signal region. The fit is performed twice, once with the C_{AC} cut only and once with the C_{AC} cut and a reversed C_{PID} cut. The difference between the results of the two fits is taken as the estimate of the yield of remaining hadronic decays in the signal region. Contributions from $D_{(s)}^- \rightarrow V(\rightarrow \mu^-\mu^+)\pi^-$ decays with $V = \eta, \rho/\omega, \eta'$ are assumed to be subdominant with respect to $D_{(s)}^- \rightarrow \pi^-\pi^+\pi^-$ decays and are therefore ignored in the analysis.

Another source of background comes from decays into three genuine muons, with $D_s^- \rightarrow \eta^{(\prime)}(\rightarrow \mu^-\mu^+\gamma)\mu^-\bar{\nu}_\mu$ providing the main contribution. Although these decays are largely suppressed by the selection on the minimum dimuon mass, a residual contribution remains

in the low-mass sideband, where it exhibits a continuous, decreasing distribution. This contribution is explicitly taken into account in the fit to the $\mu^-\mu^+\mu^-$ mass distribution in data to correctly estimate the shape of the background in the signal region.

6 Normalisation and systematic uncertainties

The $\tau^- \rightarrow \mu^-\mu^+\mu^-$ yield, extracted as described in section 7, is converted into a branching fraction through normalising to the yield of $D_s^- \rightarrow \phi(\rightarrow \mu^-\mu^+)\pi^-$ decays according to eq. (1.1). The fraction of τ^- leptons produced via D_s^- decays, $f_{D_s}^\tau$, is given by the ratio between the production cross-section of τ^- leptons from D_s^- decays and the inclusive production cross-section from heavy-hadron decays. It is calculated using the $b\bar{b}$ and $c\bar{c}$ cross-sections and the inclusive $b \rightarrow D_{(s)}^-$, $c \rightarrow D_{(s)}^-$, $b \rightarrow \tau^-$ and $D_{(s)}^- \rightarrow \tau^-$ branching fractions as defined in section 4. The efficiency for selecting signal and $D_s^- \rightarrow \phi(\rightarrow \mu^-\mu^+)\pi^-$ candidates includes the detector acceptance, reconstruction, particle identification, trigger, and selection effects. It is calculated from simulation after correcting for differences with respect to data, as described in section 4.

The statistical uncertainty on the corrections is considered as a systematic uncertainty in the upper-limit evaluation. Systematic uncertainties on the track reconstruction and trigger efficiency corrections discussed in section 4 take into account variations in the binning scheme, defined in the relevant kinematic variables for each correction, and, for the track reconstruction efficiency, differences in the hadronic interaction of pions and muons in the detector material. A correction of $(1.8 \pm 0.9)\%$ is applied to the normalisation channel to account for the truncated ϕ mass window present in simulation.

The yields of $D_s^- \rightarrow \phi(\rightarrow \mu^-\mu^+)\pi^-$ candidates in data are determined from fits to the reconstructed $\mu^-\mu^+\pi^-$ mass distributions, as described in section 4, performed separately on each data-taking year. To assign a systematic uncertainty on the normalisation yield, the fit to data is repeated using two alternative signal models: a two-sided Crystal Ball function [35] and a two-sided version of the Hypatia function [36]. In both cases, the peak position and resolution parameters of the PDFs are free to vary, while the other parameters are fixed from a fit to simulation. The greatest variation obtained on the normalisation yield is taken as its systematic uncertainty.

Input values to the normalisation factor are reported in table 1, together with the resulting single-event sensitivity α obtained for each data-taking year. The dominant contributions to the systematic uncertainties on α come from external inputs, i.e. from the knowledge of the D_s^- decay branching fractions and production fraction $f_{D_s}^\tau$, whereas the leading source of statistical uncertainty on α comes from the determination of the ratio of efficiencies. The $D_s^- \rightarrow \phi(\rightarrow \mu^-\mu^+)\pi^-$ yield N_{D_s} and the efficiency ratio $\epsilon_{D_s}/\epsilon_\tau$ are lower in the 2016 data sample with respect to the other years due to the less efficient trigger selection described in section 2. In the evaluation of the upper limit, the statistical and systematic uncertainties on α are summed in quadrature and treated as a single uncertainty.

7 Fit strategy

In order to increase the sensitivity to the signal decay, the upper limit on the branching fraction is evaluated in bins of the output of the two classifiers C_{AC} and C_{PID} . The optimal

	External inputs		
$\mathcal{B}(D_s^- \rightarrow \phi(\rightarrow \mu^- \mu^+) \pi^-)$	$(1.289 \pm 0.094) \times 10^{-5}$		
$f_{D_s}^\tau$	$(78.4 \pm 3.7) \times 10^{-2}$		
$\mathcal{B}(D_s^- \rightarrow \tau^- \bar{\nu}_\tau)$	$(5.32 \pm 0.11) \times 10^{-2}$		
	2016	2017	2018
N_{D_s}	$(43.1 \pm 0.6) \times 10^3$	$(88.5 \pm 1.2) \times 10^3$	$(103.8 \pm 1.1) \times 10^3$
$\epsilon_{D_s}/\epsilon_\tau$	0.322 ± 0.022	0.562 ± 0.034	0.575 ± 0.036
α	$(1.42 \pm 0.16) \times 10^{-9}$	$(1.21 \pm 0.13) \times 10^{-9}$	$(1.05 \pm 0.11) \times 10^{-9}$

Table 1. Terms entering the normalisation factor and resulting single-event sensitivity α . For each term, the statistical and systematic uncertainties are combined and quoted as a single uncertainty which is considered systematic. Branching fractions are taken from ref. [9]. The individual integrated luminosities are 1.6, 1.7, and 2.1 fb⁻¹ for 2016, 2017, and 2018, respectively.

binning scheme is chosen to maximise the signal-to-background separation quantified by the difference between the median expected likelihood ratios under the signal-plus-background and background-only hypotheses following the procedure of refs. [37, 38]. In the optimisation, the signal yield in the full sample is assumed to be unity, and the efficiency in each bin is determined from simulation, while the expected background yield is estimated by fitting the data sidebands with an exponential function and extrapolating the yield into the signal region. The binning is further constrained to keep the total number of bins commensurate with the size of the available data sample and results in a 4×4 scheme.

In the final fit to the data, the signal PDF is modelled with a Johnson’s S_U function, where the peak position and width parameters are extracted from simulation and calibrated using the normalisation channel, exploiting the similarity of the mass distributions. The background PDF is the sum of three contributions representing the combinatorial, the three-muon and the three-hadron components. The combinatorial background component is modelled by an exponential function, with both the slope and yield parameters free to vary independently in each bin. For the other two background contributions, the mass shapes are assumed to be identical across all bins, as no significant variations are observed in simulated candidates passing the signal selection criteria. The total yields are constrained with a Gaussian prior to the values obtained from a fit to the full data sample. The shape and per-bin fractions of the $D_s^- \rightarrow \eta^{(\prime)}(\rightarrow \mu^- \mu^+ \gamma) \mu^- \bar{\nu}_\mu$ component are determined from simulation, with the latter constrained in the fit with a Gaussian prior. The charm background is composed of residual $D^- \rightarrow \pi^- \pi^+ \pi^-$ and $D_s^- \rightarrow \pi^- \pi^+ \pi^-$ decays. It is modelled with two Johnson’s S_U functions, where the peak positions and widths are fixed to the values determined from a fit to the full data sample, while the tail parameters are allowed to vary with a Gaussian constraint with mean and width determined from simulation. The per-bin fractions are extracted from dedicated fits to data in bins of C_{AC} or C_{PID} and Gaussian-constrained in the fit. The relative yield of the D^- meson with respect to the D_s^- component is fixed according to the value derived from the known branching fractions [9], production rates [29] and the corresponding selection efficiencies. The fit stability is found to improve when rejecting

C_{AC} bin	C_{PID} bin	Expected	Observed
[0.800, 0.930]	[0.951, 0.978]	288.3 ± 7.3	284
	[0.978, 0.991]	187.3 ± 5.8	174
	[0.991, 1.000]	111.2 ± 4.6	110
[0.930, 0.974]	[0.880, 0.959]	194.5 ± 6.4	203
	[0.959, 0.982]	110.3 ± 4.7	121
	[0.982, 0.992]	79.1 ± 3.7	67
	[0.992, 1.000]	56.5 ± 3.3	41
[0.974, 0.990]	[0.880, 0.966]	129.9 ± 4.9	133
	[0.966, 0.985]	63.1 ± 3.5	62
	[0.985, 0.993]	40.8 ± 2.9	50
	[0.993, 1.000]	31.3 ± 2.5	42
[0.990, 1.000]	[0.880, 0.970]	64.6 ± 3.8	79
	[0.970, 0.987]	34.0 ± 2.9	33
	[0.987, 0.994]	33.3 ± 2.8	29
	[0.994, 1.000]	20.3 ± 2.3	23
Total		1444 ± 17	1451

Table 2. Number of expected background and observed candidates in the signal region in the 15 C_{AC} and C_{PID} bins for the whole dataset integrated over the three data-taking years. The least sensitive bin is excluded from the limit evaluation.

the least sensitive bin, i.e. that corresponding to the lowest values of the C_{AC} and C_{PID} outputs, where more background is present.

For each bin, the expected background yield for the combined 2016–2018 dataset is reported in table 2. It is estimated by fitting the data sidebands with the background-only PDF and extrapolating the resulting yield into the signal region.

Systematic uncertainties are incorporated into the upper-limit evaluation by treating the single-event sensitivities, the bin-by-bin efficiencies, and the parameters describing the signal and background shapes as nuisance parameters, constrained by Gaussian functions with widths set to their estimated uncertainties.

8 Results

The evaluation of the upper limit on the branching fraction is based on the CL_s method [39] and implemented using the ROOSTATS toolkit [40]. The expected upper limit for the 2016–2018 dataset is found to be $2.0\ (2.5) \times 10^{-8}$ at 90% (95%) CL. The impact of the systematic uncertainties is of order a few percent.

The number of candidates observed in each bin in the signal region is reported in the last column of table 2 for the combined dataset. An unbinned extended maximum-likelihood fit to the mass spectrum of the three muons is performed simultaneously in the 15 C_{AC} and C_{PID} bins for each data-taking year. The total fit PDF is a combination of the background

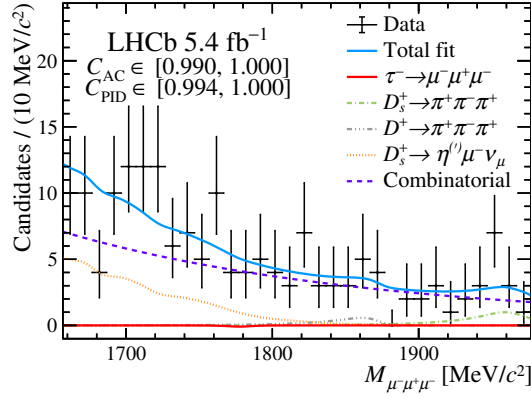


Figure 2. Result of the fit to the mass spectrum of the three muons in the most sensitive bin for the combined dataset.

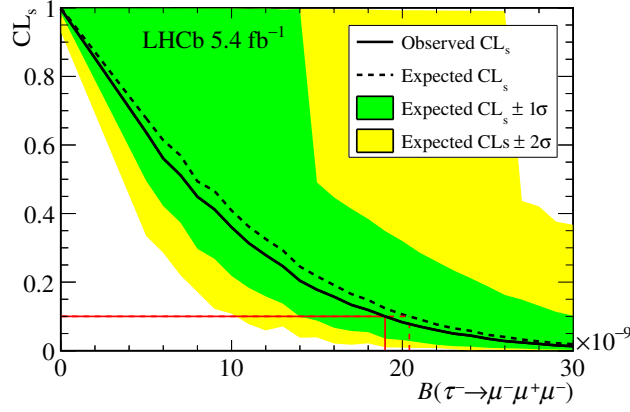


Figure 3. CL_s distribution as a function of the assumed branching fraction for $\tau^- \rightarrow \mu^- \mu^+ \mu^-$ decays, for both the observed data (solid line) and background-only expectation (dashed line) together with its intervals of one and two standard deviations (σ). The red line corresponds to the 90% confidence level.

PDF and the signal PDF, discussed in section 7. The result of the fit in the bin with the largest score in C_{AC} and C_{PID} output is shown in figure 2 for the combined dataset.

The central value of the signal branching fraction extracted from the fit is $(-0.1 \pm 1.1) \times 10^{-8}$, where the uncertainty includes both statistical and systematic sources, leading to an observed upper limit on the branching fraction of

$$\mathcal{B}(\tau^- \rightarrow \mu^- \mu^+ \mu^-) < 1.9 (2.3) \times 10^{-8} \text{ at } 90\% (95\%) \text{ CL.}$$

The expected and observed CL_s distributions are shown in figure 3 as a function of the assumed branching-fraction values. This result supersedes the LHCb Run 1 limit of $4.6 (5.6) \times 10^{-8}$ at 90% (95%) CL [5].

9 Conclusion

A search for the $\tau^- \rightarrow \mu^- \mu^+ \mu^-$ decay is carried out on data collected by the LHCb experiment between 2016 and 2018, corresponding to a total integrated luminosity of 5.4 fb^{-1} . No significant excess of signal is found and an upper limit of $1.9 (2.3) \times 10^{-8}$ at 90% (95%) CL is set on the branching fraction of the decay. This result provides a complementary constraint on SM extensions in the context of existing searches, with a sensitivity comparable to that achieved by the Belle II experiment [8]. Future analyses with the upgraded LHCb detector will benefit from higher luminosity and trigger efficiencies, leading to improved sensitivity to the signal decay.

Acknowledgments

We express our gratitude to our colleagues in the CERN accelerator departments for the excellent performance of the LHC. We thank the technical and administrative staff at the LHCb institutes. We acknowledge support from CERN and from the national agencies: ARC (Australia); CAPES, CNPq, FAPERJ and FINEP (Brazil); MOST and NSFC (China); CNRS/IN2P3 (France); BMFTR, DFG and MPG (Germany); INFN (Italy); NWO (Netherlands); MNiSW and NCN (Poland); MCID/IFA (Romania); MICIU and AEI (Spain); SNSF and SER (Switzerland); NASU (Ukraine); STFC (United Kingdom); DOE NP and NSF (U.S.A.). We acknowledge the computing resources that are provided by ARDC (Australia), CBPF (Brazil), CERN, IHEP and LZU (China), IN2P3 (France), KIT and DESY (Germany), INFN (Italy), SURF (Netherlands), Polish WLCG (Poland), IFIN-HH (Romania), PIC (Spain), CSCS (Switzerland), and GridPP (United Kingdom). We are indebted to the communities behind the multiple open-source software packages on which we depend. Individual groups or members have received support from Key Research Program of Frontier Sciences of CAS, CAS PIFI, CAS CCEPP, Minciencias (Colombia); EPLANET, Marie Skłodowska-Curie Actions, ERC and NextGenerationEU (European Union); A*MIDEX, ANR, IPhU and Labex P2IO, and Région Auvergne-Rhône-Alpes (France); Alexander-von-Humboldt Foundation (Germany); ICSC (Italy); Severo Ochoa and María de Maeztu Units of Excellence, GVA, XuntaGal, GENCAT, InTalent-Inditex and Prog. Atracción Talento CM (Spain); SRC (Sweden); the Leverhulme Trust, the Royal Society and UKRI (United Kingdom).

Data Availability Statement. This article has no associated data or the data will not be deposited.

Code Availability Statement. This article has no associated code or the code will not be deposited.

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