Supplementary Material (ESI) for Chemical Communications

Supplementary material for the determination of %GC yield:

Firstly response factor needs to be determined.
Let the response factor be F for the olefins with respect to internal standard.
Now, area of olefin signal / moles of olefin = F × area of standard signal / moles of standard.
That is, $a_o / m_o = F \times a_s / m_s$.
Therefore, $F = a_o \times m_s / a_s \times m_o$…………..(1) where m_o and m_s are the moles of olefin and that of standard respectively. a_o and a_s are the area of olefin and that of standard respectively at zero time of the mixing.
This equation presumes a linear response of the detector to both olefin and the standard.
Constancy of F has been checked by varying randomly the moles of olefins and recording the chromatogram at zero time.
Similarly, a known quantity of epoxide is mixed with the same quantity of the standard as in equation (1) and is chromatographed to find the response factor of this system.
Therefore, $F' = a_e \times m_s / a_s' \times m_e$……………(2) where a_e and a_s' are the area of epoxide and standard, and m_e and m_s are the moles of epoxide and standard, respectively. The F' = response factor for the epoxides with respect to standard.
Constancy of F' has been checked by varying randomly the moles of olefins. The constancy of both F and F' having been checked, varying moles of standard randomly without changing the moles of olefin and epoxide respectively, it can be concluded that equation (1) and (2) should always be valid.

In case of olefin after reaction is over,

$$a_o' / m_o' = F \times a_s'' / m_s'$$

Therefore, $m_o' = a_o' \times m_s' / a_s'' \times F$……………(3), where a_o' and a_s'' are the area of olefin and standard respectively. m_o' is the unknown moles of olefin and m_s' is the moles of standard.
From this equation m_o' can be determined by applying known values of a_o', a_s'' and m_s'.

In the case of epoxide after the reaction is over,

$$a_e'' / m_e'' = F' \times a_s''' / m_s''$$

Therefore, $m_e'' = a_e'' \times m_s'' / a_s''' \times F'$………… (4), where a_e'' and a_s''' are the area of epoxide and standard respectively. m_s'' is the moles of standard and m_e'' is the unknown moles of epoxide.
Thus, from the equation (4) m_e'' has been calculated as all other terms are known.

Therefore, % GC yield= [moles of epoxide (m_e'') / {moles of olefin (m_o') + moles of epoxide (m_e'')}]×100.