

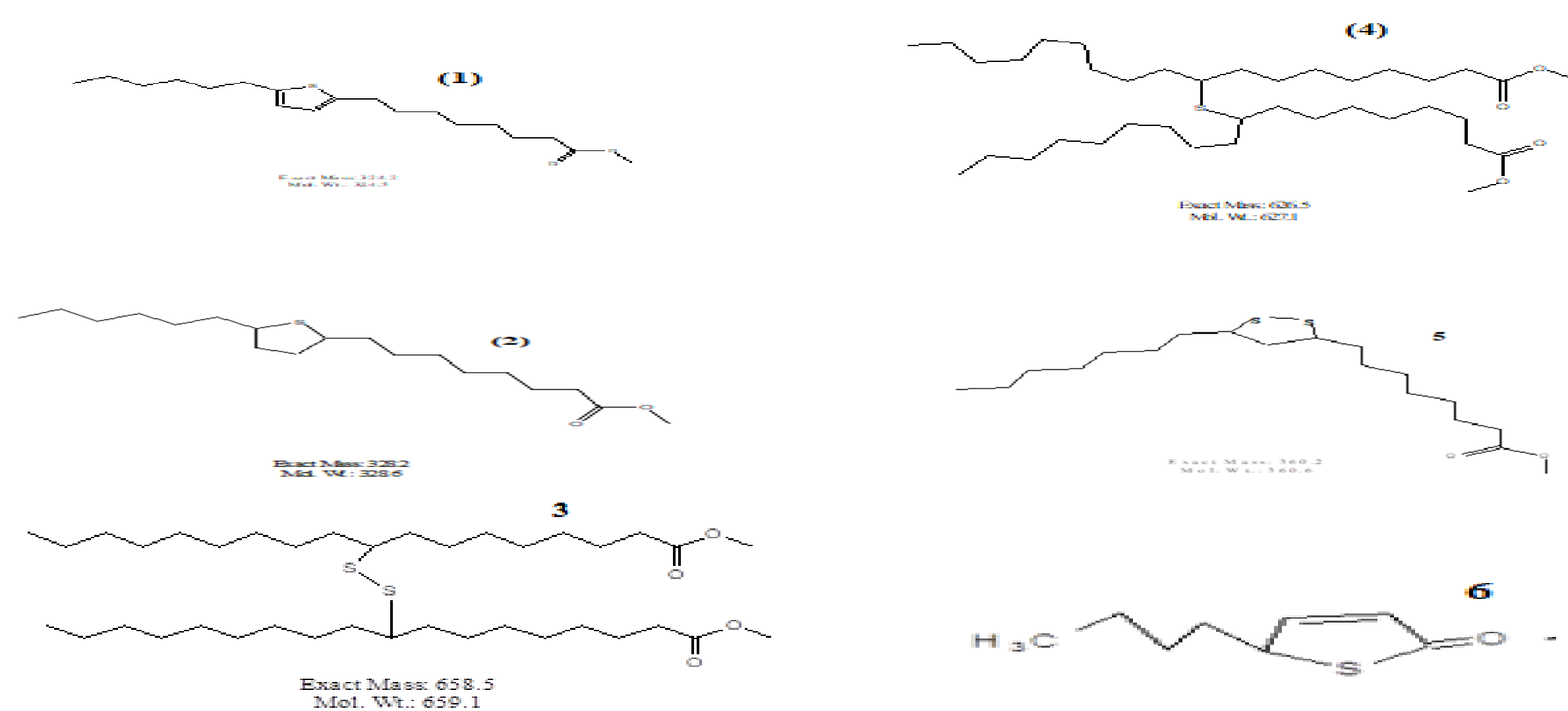
Verification of Sulfonated Compounds Found in Biodiesel Produced from Brown Grease Lipids (BGL)

Isah, S. ¹, Cairncross, R. ², Jones, K. ³, Ozbay G. ¹ and Wyatt V. ^{T3}

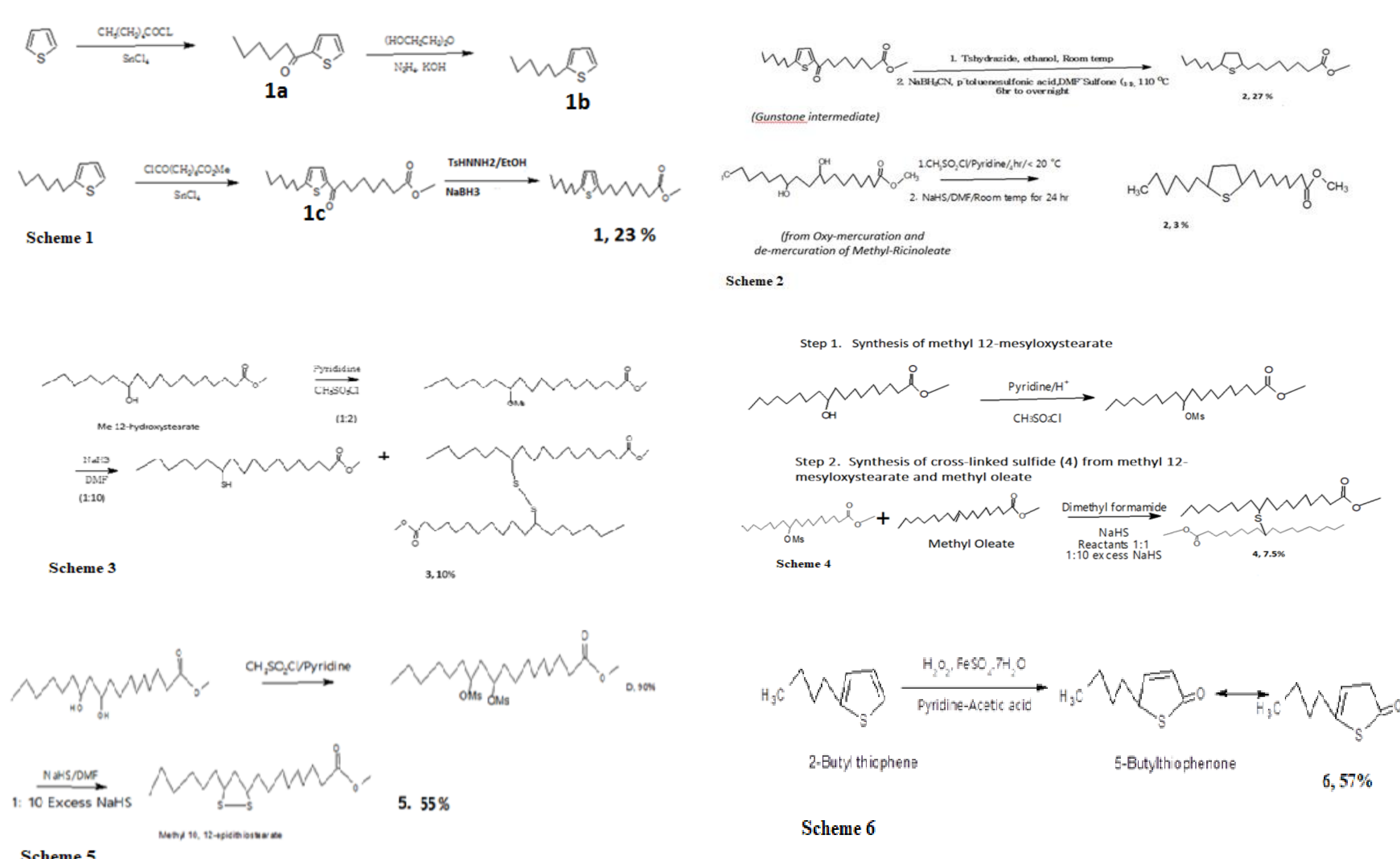
Abstract

Methyl 8-(2'5'-hexylthienyl) octanoate (**1**, 23%), epithiostearate (**2**, 27%), cross-linked disulfide (bis-methyl[9,9-dithiol] stearate) (**3**, 10%), crosslinked sulfide (bis-methyl[9-thiol] stearate) (**4**, 7.5%) epidithiostearate (**5**, 55%) and 5-butyl-dihydrothiophene (**6**, 52%) have been synthesized and characterized by GC-MS, GC-PFPD and NMR techniques. Previous research suggests that these molecules are among the sulfur (S)-bearing impurities found in biodiesel produced from brown grease lipids (BGL). These compounds do not exist in the MS library; therefore, a small degree of uncertainty surrounds their identification. In this project, the S-bearing compounds of interest were synthesized in quantities sufficient to characterize them by analytical methods such as GC-MS, GC-PFPD and NMR. The identification of S-bearing compounds in BGL-derived biodiesel is necessary to devise effective desulfurization protocols needed to reduce the concentration of S-bearing impurities in biodiesel to < 15 ppm, as specified by ASTM.

Molecular structures of identified S-bearing impurities



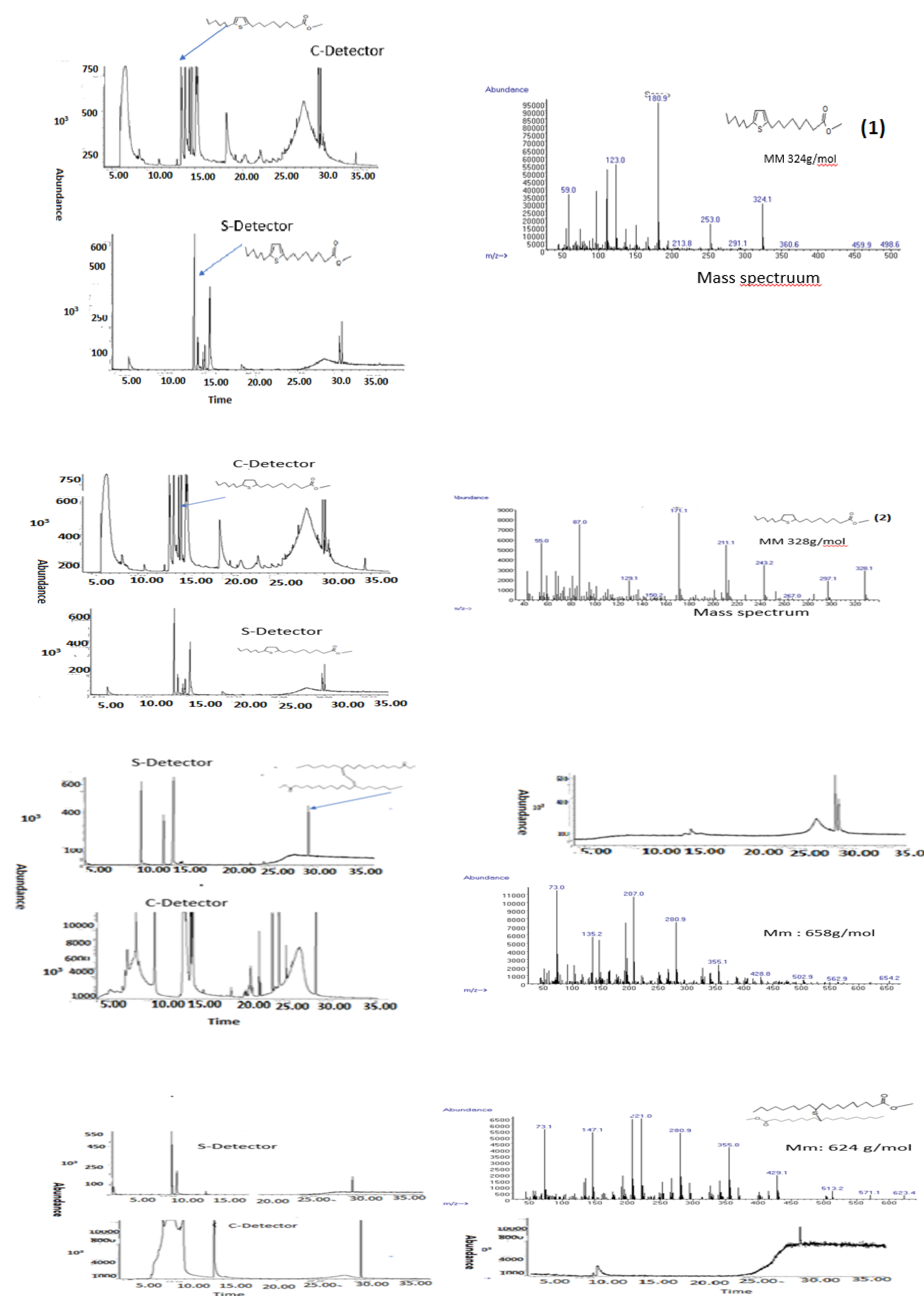
Experimental Schemes



Experimental

Reaction progress and products were monitored and characterized using GC-MS (Agilent technology 7890 GC) and GC-pulsed flame photometric detector (GC-PFPD) (S-detector)

Results



Results

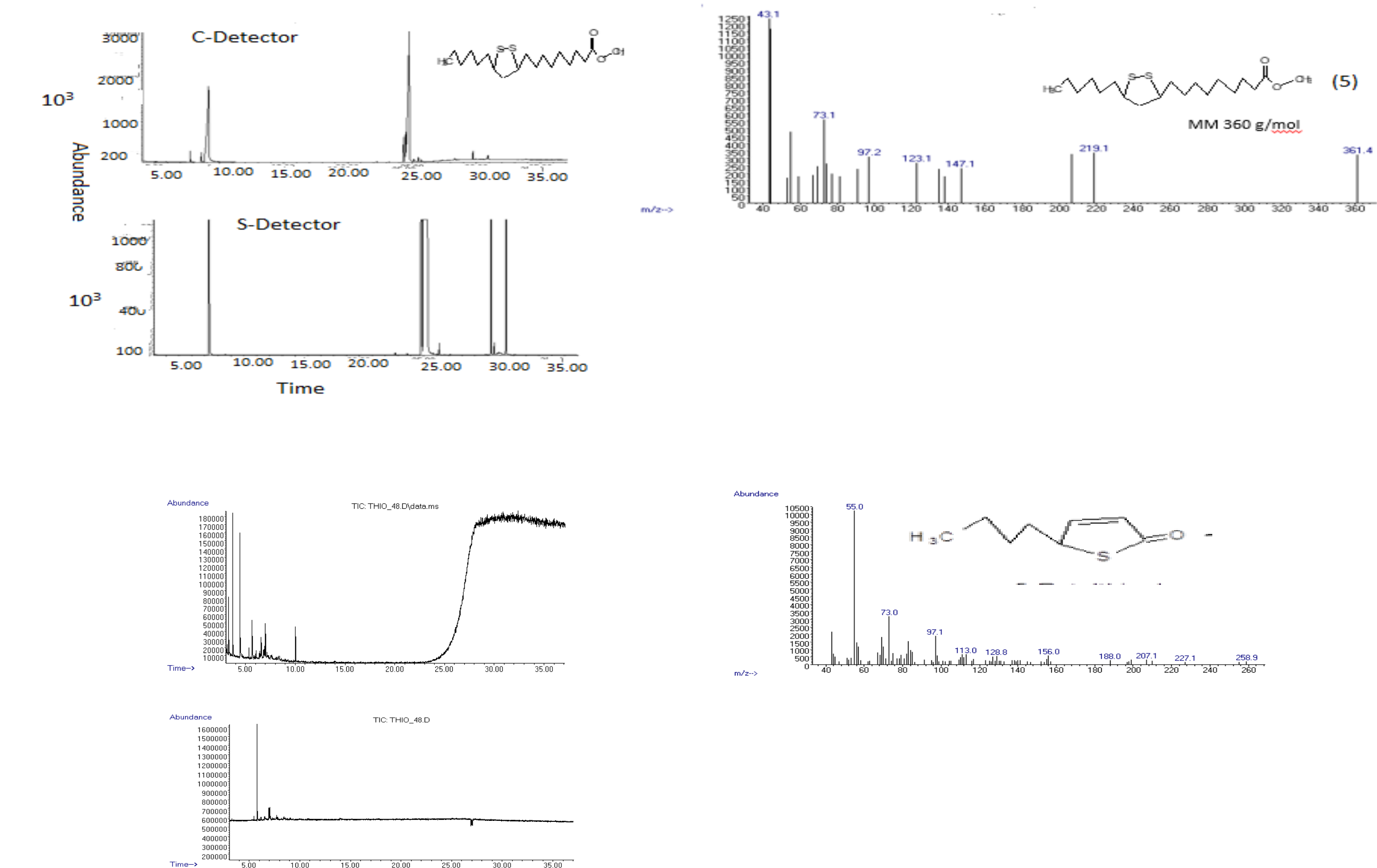


Fig. 1 GC total ion chromatograms (TIC), GC-PFPD and mass spectra of products **1, 2, 3, 4, 5** and **6**

Discussions

The GC-MS and GC-PFPD retention times of these S-bearing impurities were 13, 14, 31, 29, 22 and 6 mins for products **1, 2, 3, 4, 5** and **6** respectively. These compared well with the literature values identified by Hughes et al. (2017). Products were also identified by their molecular ion peaks m/z (324, 328, 659, 626, 360 and 156) for products 1 – 6.

References

- The preparation and properties of methyl monomercaptostearates, some related thiols and some methyl epithiostearates. *Chem and phys. of lipids.* **13**, 71-91
- Hughes, M., Jones, K.C., Hums, M.E., Cairncross, R.A and Wyatt, V.T. (2018). Identification unstone, F.D., Hussain, M.G., and Smith, D.M. (1974). Fatty acids, part 42. of Sulfur-containing impurities in biodiesel produced from brown grease. *J. Am Oil Chem Soc.* **95**, 407-420

Acknowledgement

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