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Synthesis, DFT and Molecular docking study of novel bis 1,2,3-triazole derivatives of 2-hydroxyquinoline-4-carboxylate as antimicrobial agents

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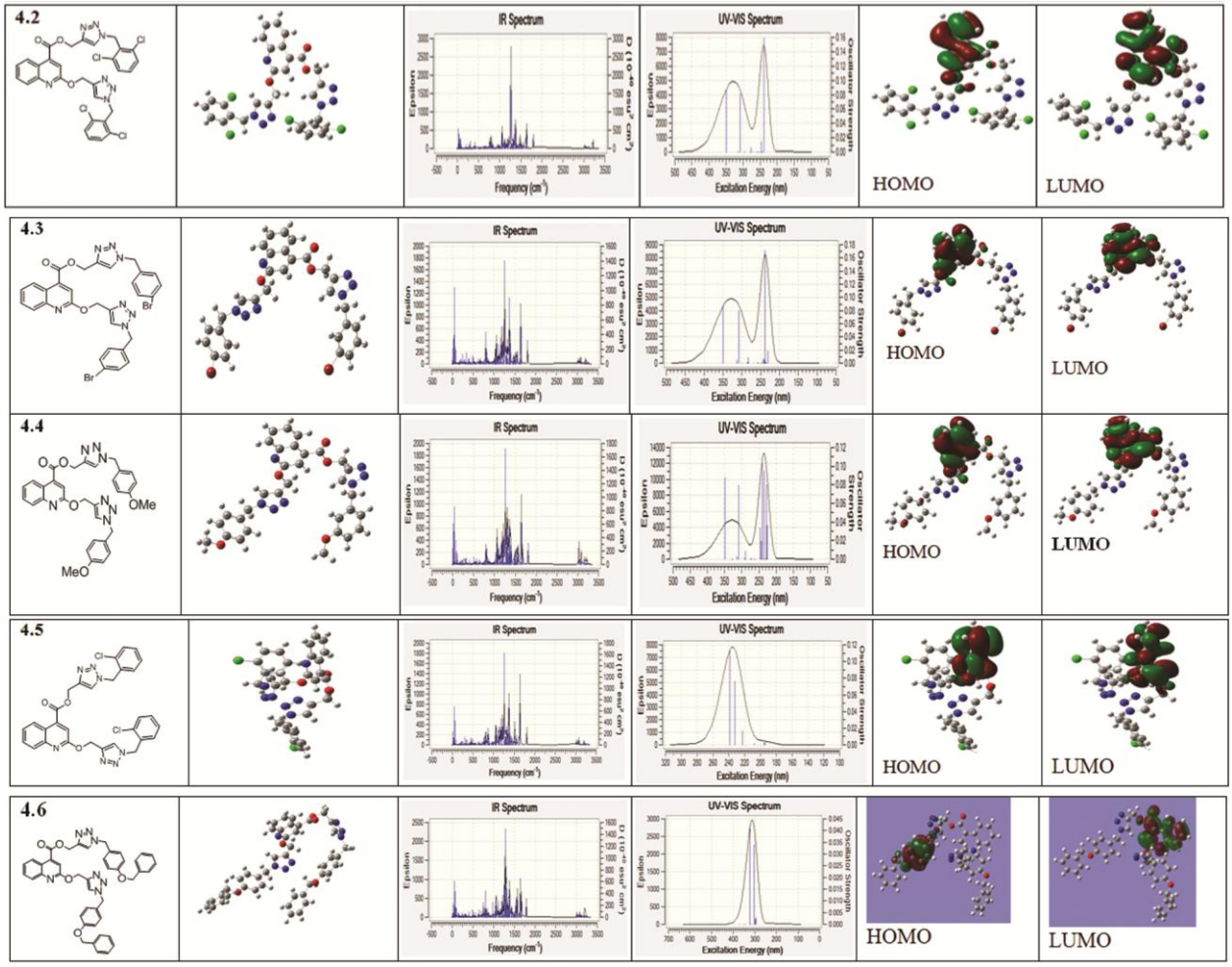
Supplementary Data

Figures



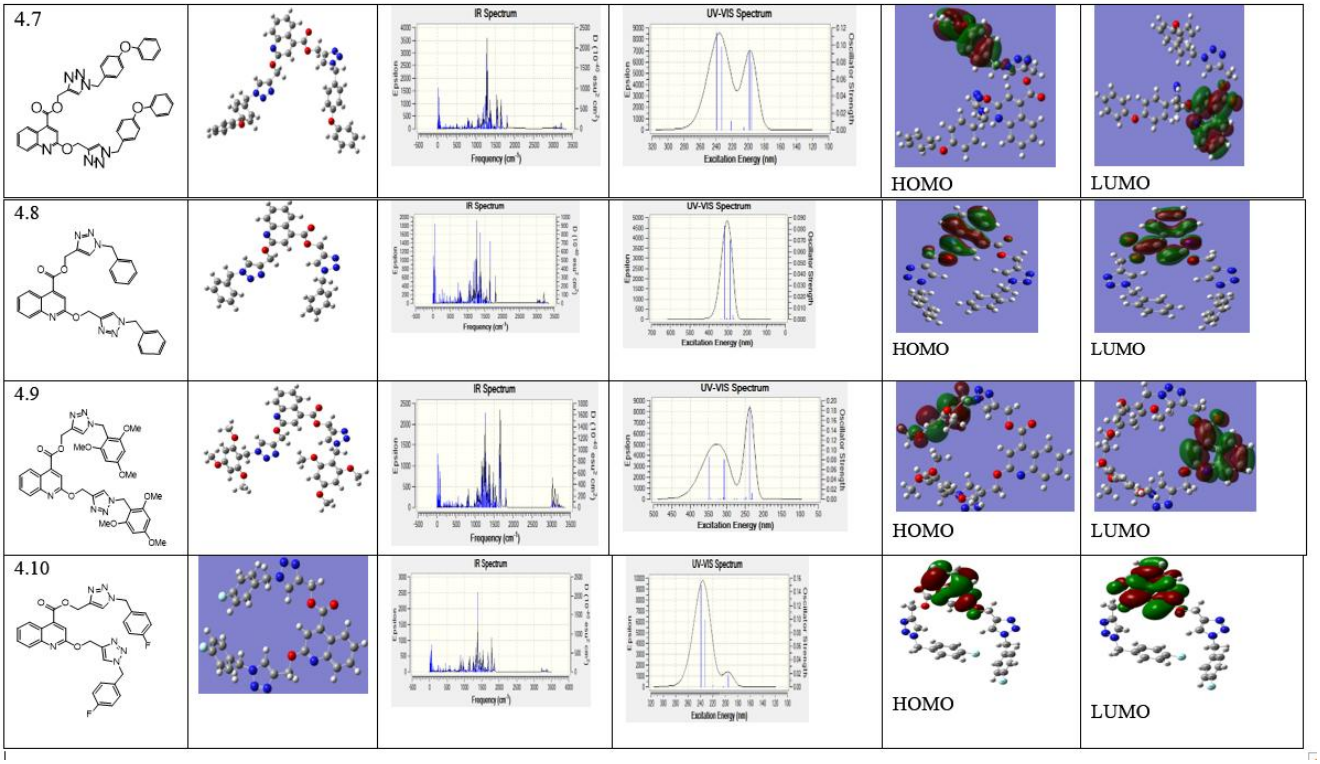


Fig.1 — Display of Chemdraw Structures, Ball and Stick models, UV and IR spectrum and Molecular orbital energy diagrams HOMO and LUMO of Compounds 4.2 to 4.10 using DFT

Molecular Docking Studies:

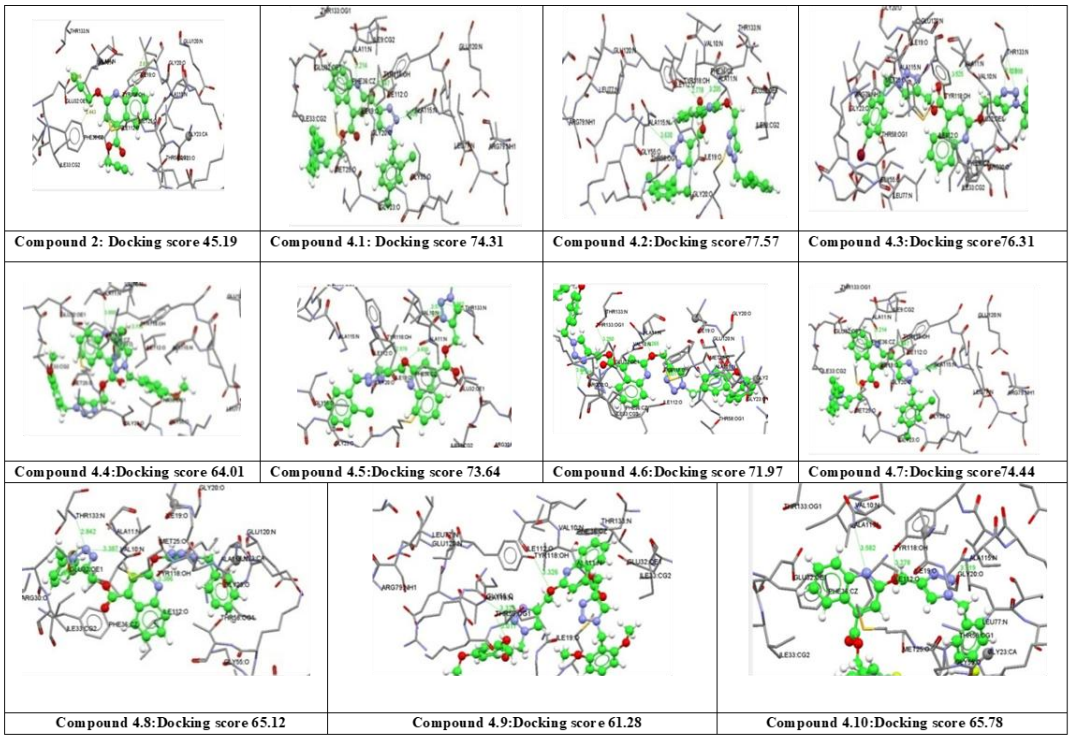


Fig. 2 — Binding orientations of 1,2,3-Triazole derivatives 2, 4.1,4.2 and 4.3 4.4, 4.5, 4.6, 4.7, 4.8,4.9,4.10 in the active site of 1M78

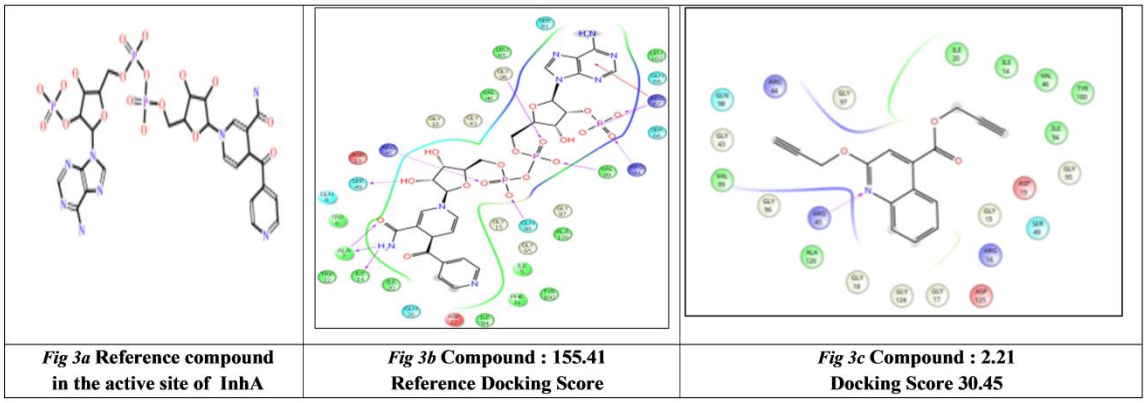


Fig 3a Reference compound in the active site of InhA	*Fig 3b* Compound : 155.41 Reference Docking Score	*Fig 3c* Compound : 2.21 Docking Score 30.45

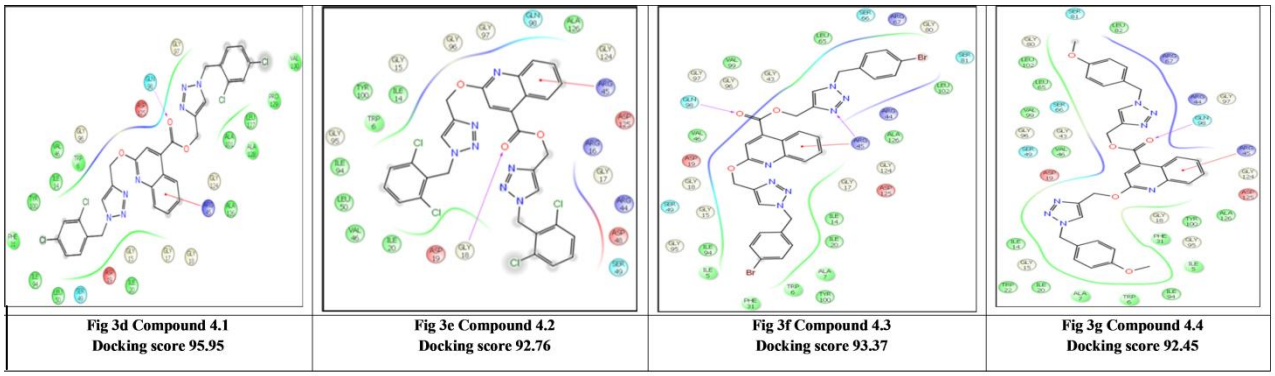


Fig 3d Compound 4.1 Docking score 95.95	Fig 3e Compound 4.2 Docking score 92.76	Fig 3f Compound 4.3 Docking score 93.37	Fig 3g Compound 4.4 Docking score 92.45

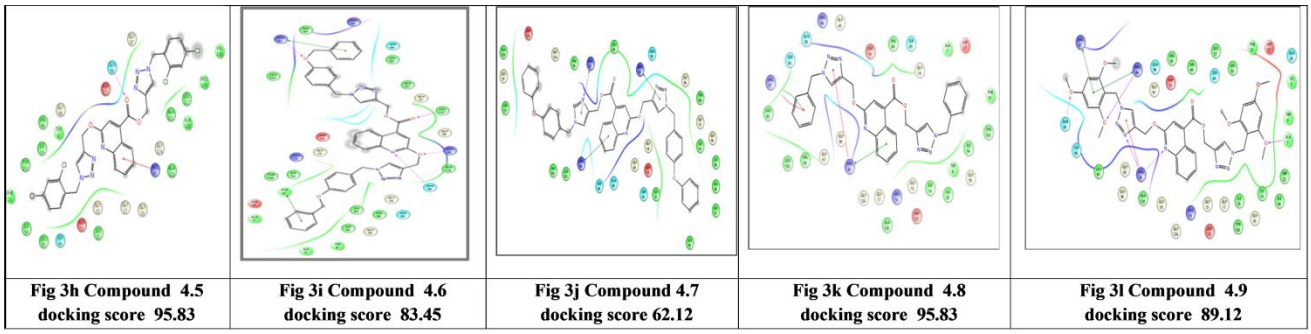
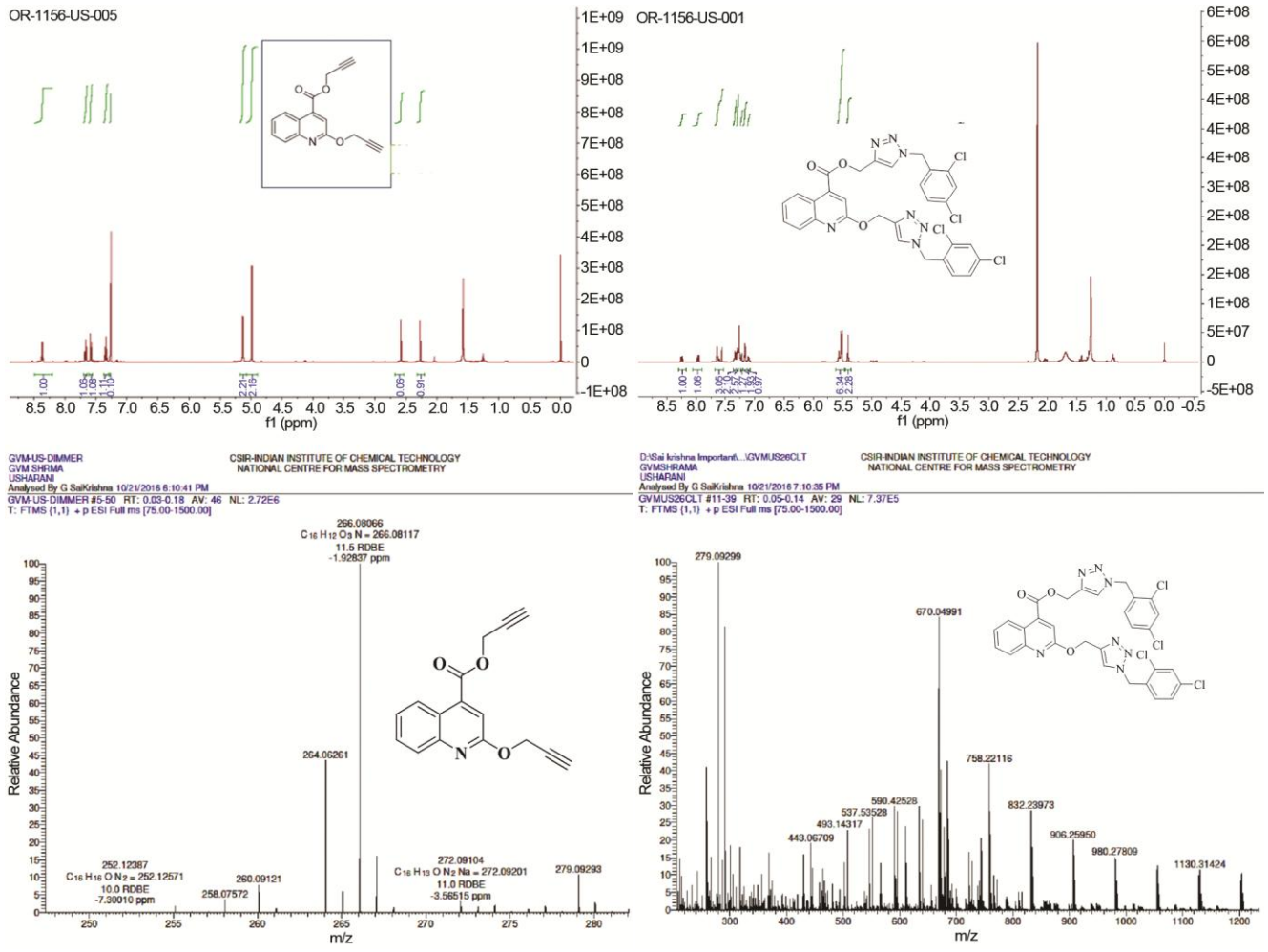
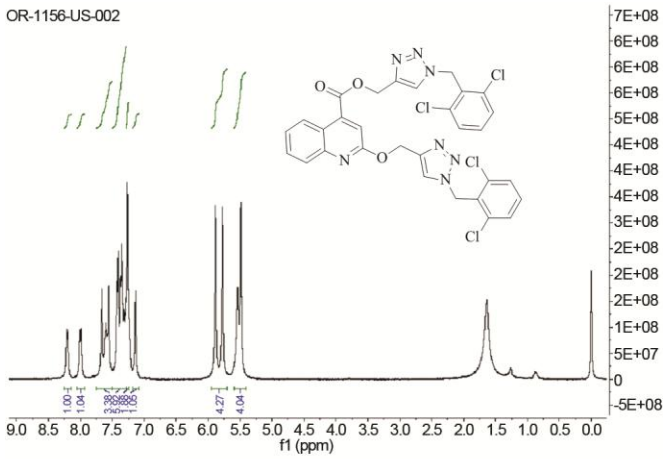


Fig 3h Compound 4.5 docking score 95.83	Fig 3i Compound 4.6 docking score 83.45	Fig 3j Compound 4.7 docking score 62.12	Fig 3k Compound 4.8 docking score 95.83	Fig 3l Compound 4.9 docking score 89.12

Fig 3a-c — Binding orientations of Reference compound and compound 2 in the active site of InhA; and
3d-l — Binding orientations of 1,2,3-Triazole derivatives 4.1, 4.2, 4.3, 4.4, 4.5,4.6,4.7,4.8,4.9,4.10 in the active site of InhA

^{1}H NMR and Mass Spectral Data

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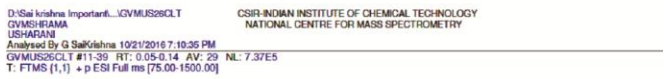
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USHARANI
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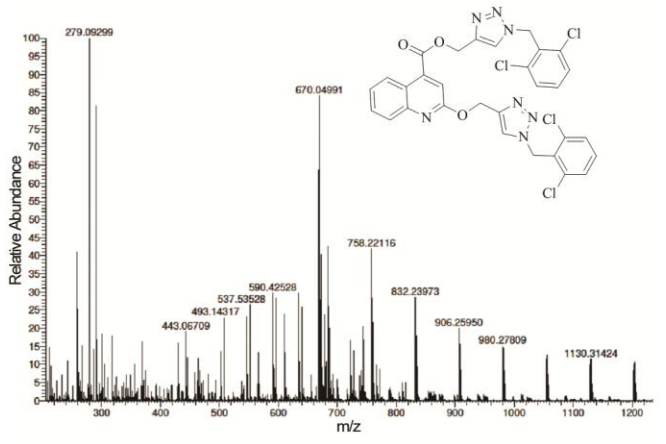
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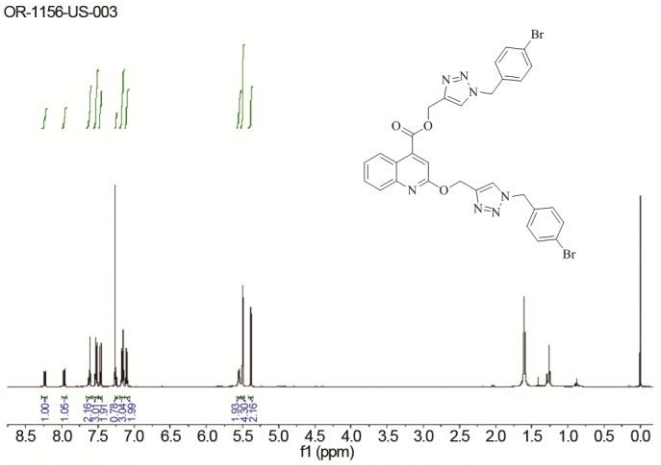
758.22116
590.42528
537.53528
493.14317
443.06709
832.23973
906.25950
980.27809
1130.31424
Relative Abundance
m/z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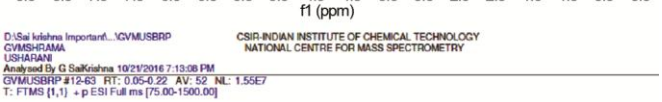
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USHARANI
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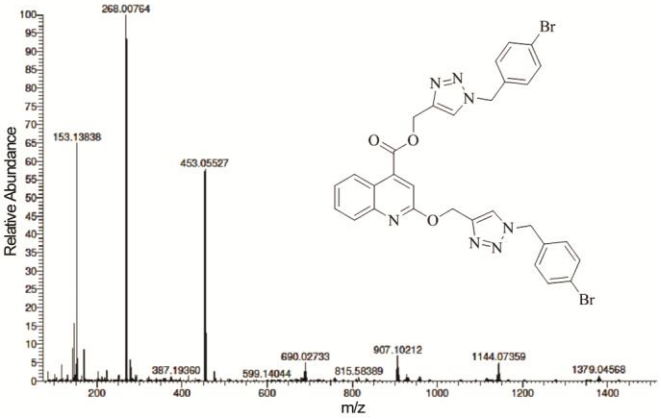
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153.13838
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907.10212
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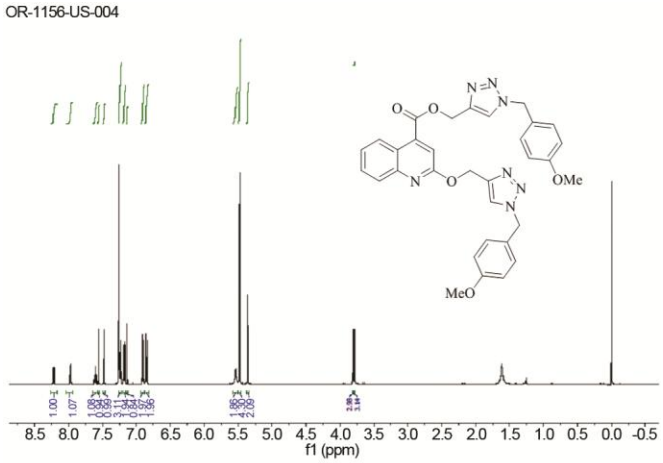
Relative Abundance
m/z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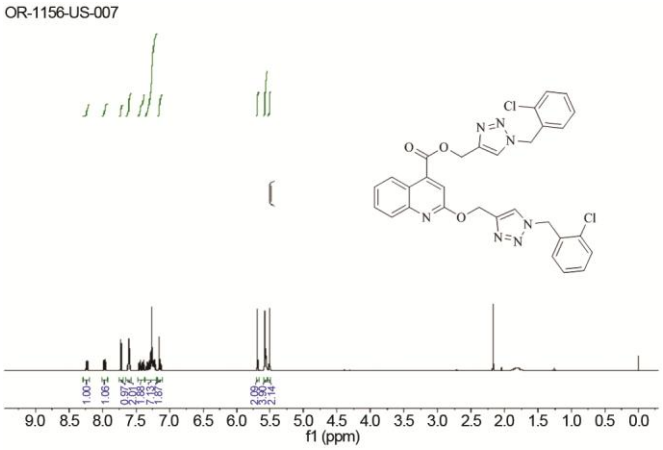
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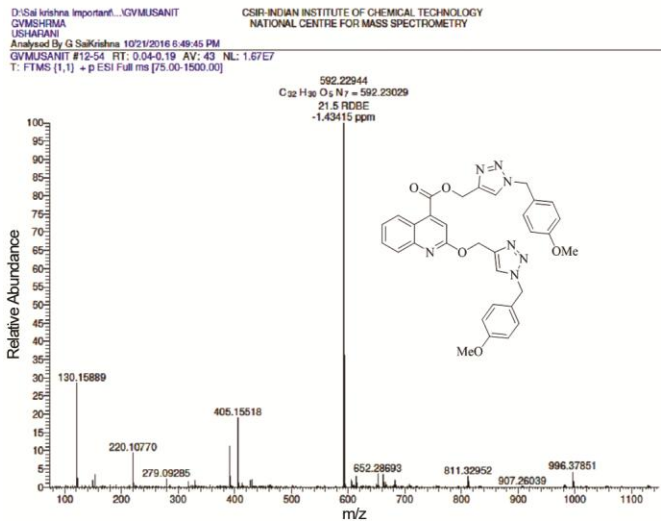
CSIR-INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
NATIONAL CENTRE FOR MASS SPECTROMETRY
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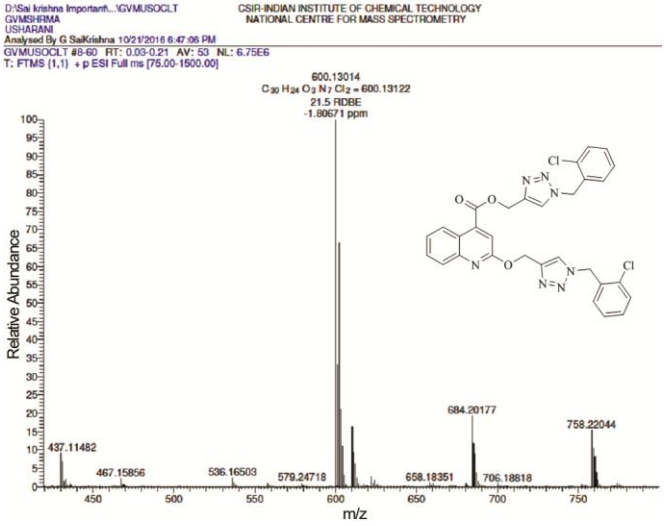
-1.43415 ppm
Relative Abundance
m/z


CSIR-INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
NATIONAL CENTRE FOR MASS SPECTROMETRY
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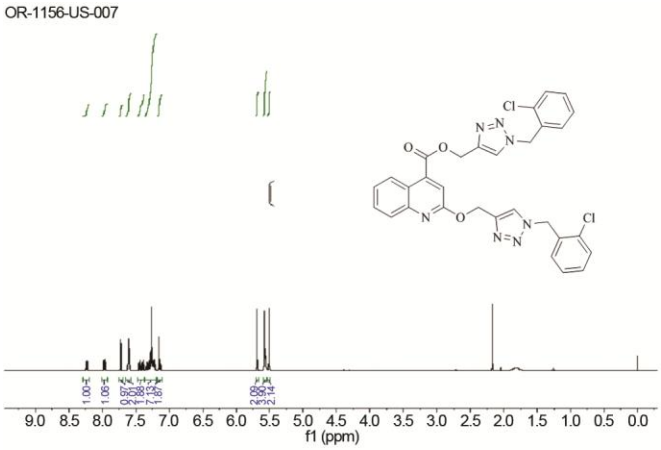
-1.80671 ppm
Relative Abundance
m/z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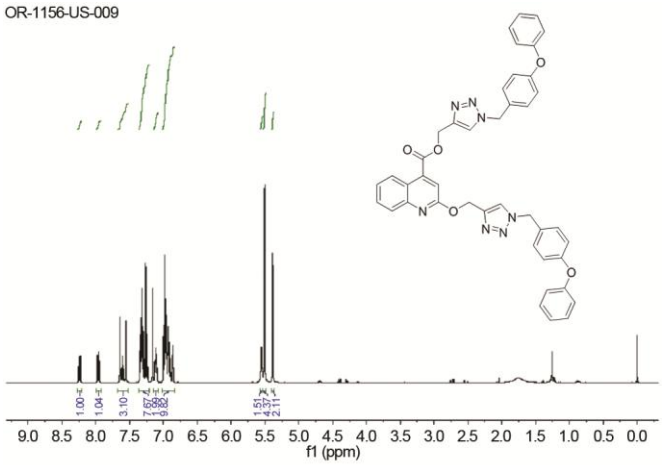
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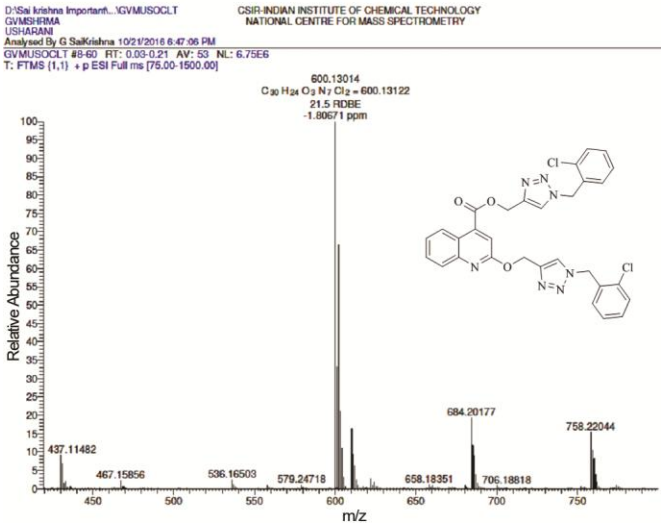
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NATIONAL CENTRE FOR MASS SPECTROMETRY
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21.5 RDBE
-1.80671 ppm
Relative Abundance
m/z
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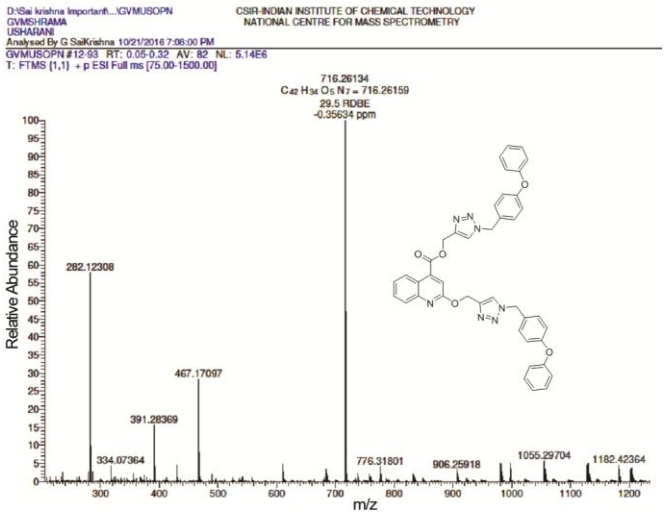
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NATIONAL CENTRE FOR MASS SPECTROMETRY
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-0.35634 ppm
Relative Abundance
m/z
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776.31801
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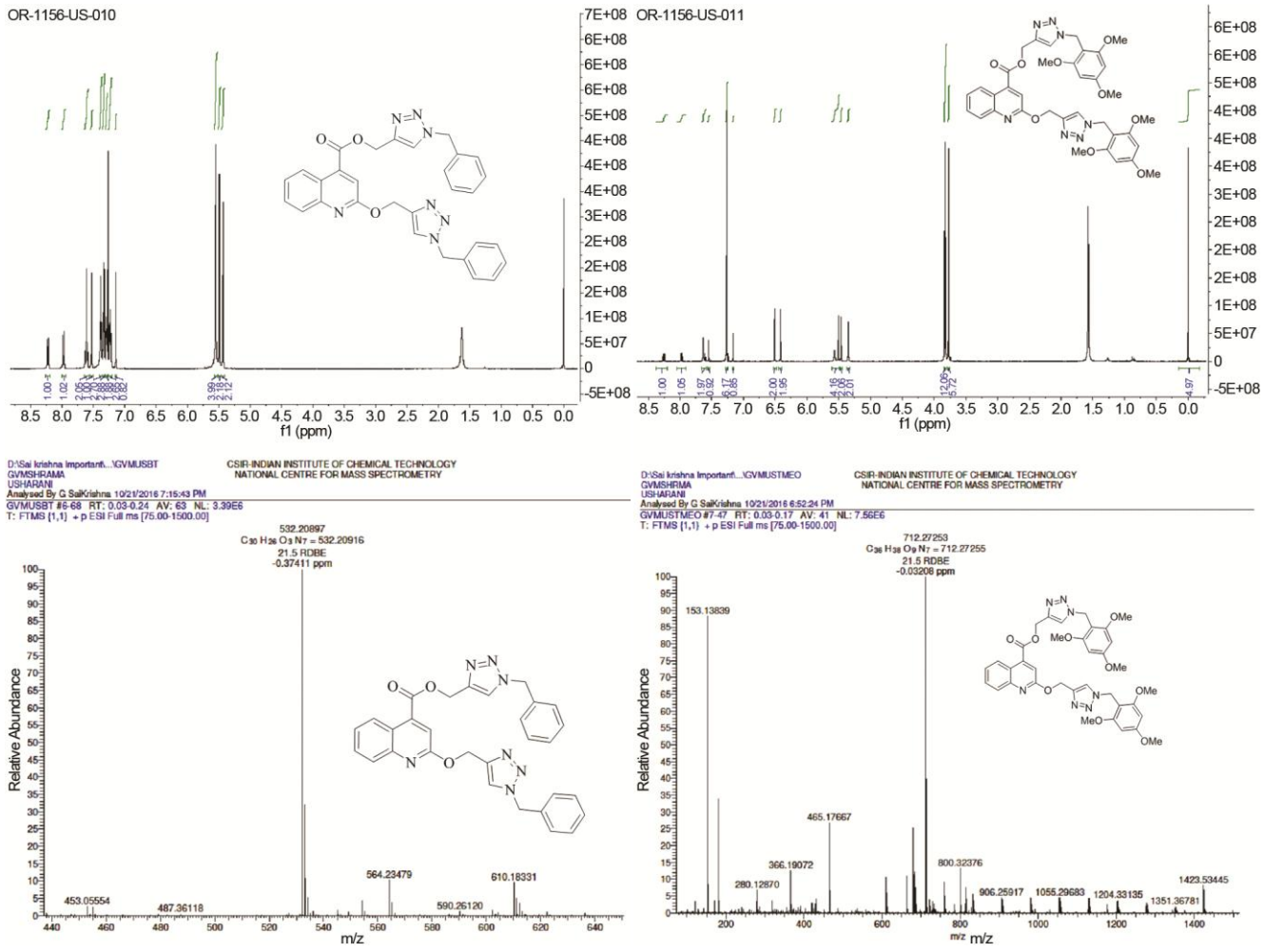
1182.42364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f1 (ppm)
OR-1156-US-011
f1 (ppm)
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-0.37411 ppm
Relative Abundance
m/z
453.05554
487.36118
564.23479
590.26120
610.18331
CSIR-INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY
NATIONAL CENTRE FOR MASS SPECTROMETRY
GVMUSTMEO #7-47 RT: 0.03-0.17 AV: 41 NL: 7.56E6
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-0.03208 ppm
Relative Abundance
m/z
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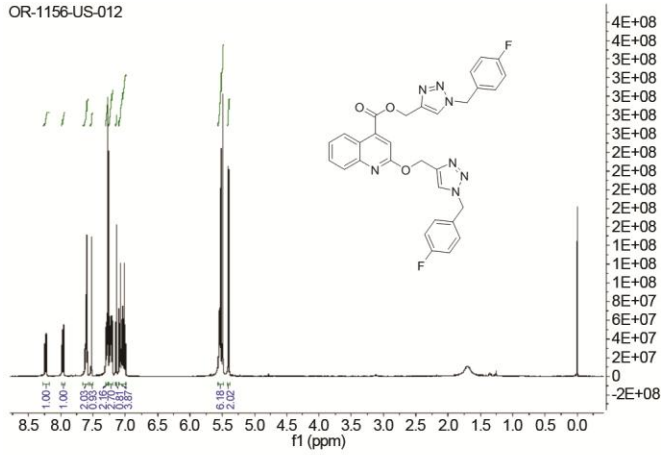
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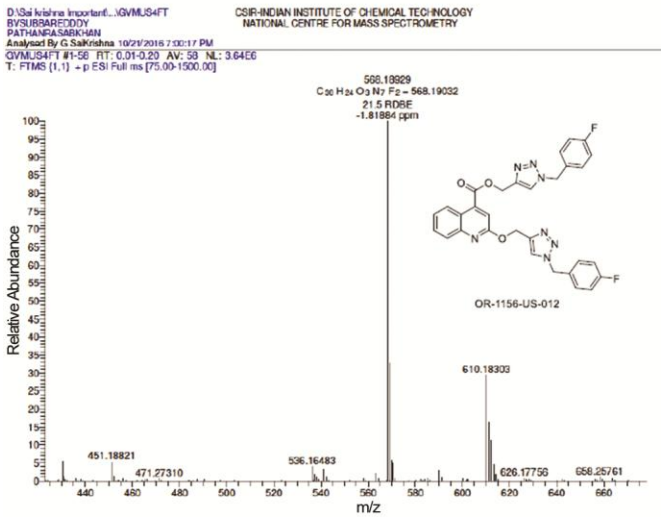
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626.17756
658.25761
Relative Abundance
m/z