Item No. 1 of 1

ACCESSION NO: 0410078 **SUBFILE:** CRIS
PROJ NO: 1275-32000-001-08R **AGENCY:** ARS 1275
PROJ TYPE: USDA INHOUSE **PROJ STATUS:** TERMINATED
START: 01 JUN 2005 **TERM:** 31 MAY 2009

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VALIDATION OF PHARMOCOPHORE MODELS OF MOSQUITO REPELLENTS

OBJECTIVES: Pharmocophore models and synthesis of new candidates.

APPROACH: Validate new bioassay system, design new synthetic repellents and validate pharmocophore model.

PROGRESS: 2005/06 TO 2009/05
Progress Report Objectives (from AD-416) Pharmocophore models and synthesis of new candidates. Approach (from AD-416) Validate new bioassay system, design new synthetic repellents and validate pharmocophore model. Significant Activities that Support Special Target Populations Computational chemistry and molecular modeling are cutting-age approaches for the identification of new, active chemicals as repellents of arthropod disease vectors. The initial project plan was laid out in the first quarter of 2005. Based on the agreement, we have screened numerous compounds against blood feeding mosquitoes. This fiscal year, we have screened a series of alkyl diol derivatives, which were developed on the basis of pharmacophore models. We evaluated their in vitro efficacy and compared them with computational efficacy against blood-feeding Aedes aegypti females. Based on the result, the pharmacophore model was refined. The next step would be to evaluate a new class of mosquito repellent and repeat the sequence of generating and validating the model. The whole project team, comprised of synthetic/computational chemists, medical entomologists and industrial partners meet on regular basis to discuss progress as well as future directions. Results are presented and/or published for scientific meetings and peer reviewed journals.

PUBLICATIONS (not previously reported): 2005/06 TO 2009/05
No publications reported this period.