

## Center for Pharmacometrics and Molecular Discovery (PharMD)

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Submitted by: \_\_\_\_\_ Date: \_\_\_\_\_

E-mail: \_\_\_\_\_ Phone: \_\_\_\_\_

(results will be sent via email)

Address: \_\_\_\_\_

PO#: \_\_\_\_\_

Sample Name: \_\_\_\_\_ Molecular weight: \_\_\_\_\_

Sample is in or is soluble in (MeOH/H<sub>2</sub>O/ACN): \_\_\_\_\_

Estimated quantity (conc or mg): \_\_\_\_\_ Known Hazards: \_\_\_\_\_

**Additional comments:**

### Services Requested:

\_\_\_\_\_ LC-MS (ESI)—low resolution mass (\$20 per sample)—separation not required

\_\_\_\_\_ LC-MS (ESI)—low resolution mass (\$100 per hour/method)—separation required

\_\_\_\_\_ NMR (\$50 per hour for academic or non-profit orgs: \$100 per hour for corporate)\*

\_\_\_\_\_ <sup>1</sup>H NMR

\_\_\_\_\_ <sup>13</sup>C NMR

\_\_\_\_\_ DEPT135 (90 or 45)

\_\_\_\_\_ COSY (proton correlation)

\_\_\_\_\_ HSQC (proton:DEPT135 correlation)

\_\_\_\_\_ HMBC (long range coupling)

\_\_\_\_\_ NOESY (through-space proton correlations)

\_\_\_\_\_ ROESY (through-space proton correlations, small molecules)

\_\_\_\_\_ <sup>19</sup>F

\_\_\_\_\_ Variable temperature NMR (additional \$50 per hour)

\_\_\_\_\_ other \_\_\_\_\_

\_\_\_\_\_ FTIR (neat)--\$10 per sample

### Instrumentation

Waters H-Class UPLC with single quad MS and PDA—(ESI) for routine analysis of small molecules in positive or negative mode

Bruker Avance III Nanobay 400 MHz NMR with BBFO probe

PerkinElmer Spectrum 65 FTIR with UATR

\*Minimum 1 hour