# Yasuda-Shedlovsky Result

| | | | |
|---|---|---|---|
| Sample name: | **CS000169** | Experiment start time: | **07/09/2011 17:44:18** |
| Assay name: | **Fast UV psKa** | Analyst: | |
| Assay ID: | **11I-07021** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1109\11I-07021_CS000169_Fast UV psKa.t3r** | | |

## Yasuda-Shedlovsky result

| Extrapolation type | pKa 0% | SD | Intercept | Slope | $R^2$ | Ionic strength | Temperature |
|---|---|---|---|---|---|---|---|

## Component assay results

| Titration | DMSO weight% | Direction | Result type | Dielectric constant | [H2O] | Ionic strength | Temperature |
|---|---|---|---|---|---|---|---|
| 11I-07021 Points 105 to 156 | 19.90 % | Up | UV-metric pKa | 77.2 | 45.1 M | 0.207 M | 25.9°C |
| 11I-07021 Points 53 to 104 | 26.76 % | Up | UV-metric pKa | 77.0 | 41.5 M | 0.204 M | 25.5°C |
| 11I-07021 Points 3 to 52 | 35.83 % | Up | UV-metric pKa | 76.0 | 36.7 M | 0.195 M | 26.5°C |

## Graphs

| | | | |
|---|---|---|---|
| Sample name: | **CS000169** | Experiment start time: | **07/09/2011 17:44:18** |
| Assay name: | **Fast UV psKa** | Analyst: | |
| Assay ID: | **11I-07021** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1109\11I-07021_CS000169_Fast UV psKa.t3r** | | |

# Fast UV psKa Titration 1 of 3 11I-07021 Points 3 to 52

## Graphs

| | | | |
|---|---|---|---|
| Sample name: | **CS000169** | Experiment start time: | **07/09/2011 17:44:18** |
| Assay name: | **Fast UV psKa** | Analyst: | |
| Assay ID: | **11I-07021** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1109\11I-07021_CS000169_Fast UV psKa.t3r** | | |

# Fast UV psKa Titration 2 of 3 11I-07021 Points 53 to 104

## Graphs

| | | | |
|---|---|---|---|
| Sample name: | **CS000169** | Experiment start time: | **07/09/2011 17:44:18** |
| Assay name: | **Fast UV psKa** | Analyst: | |
| Assay ID: | **11I-07021** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1109\11I-07021_CS000169_Fast UV psKa.t3r** | | |

# Fast UV psKa Titration 3 of 3 11I-07021 Points 105 to 156

## Graphs

| | | | |
|---|---|---|---|
| Sample name: | **CS000169** | Experiment start time: | **07/09/2011 17:44:18** |
| Assay name: | **Fast UV psKa** | Analyst: | |
| Assay ID: | **11I-07021** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1109\11I-07021_CS000169_Fast UV psKa.t3r** | | |

## Assay Model

| Settings | Value | Date/Time changed | Imported from |
|---|---|---|---|
| Sample name | CS000169 | | |
| Sample by | Volume | 07/09/2011 14:20:39 | E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r |
| Sample volume | 0.0100 mL | | |
| Solvent | DMSO | | |
| Sample concentration | 0.010000 M | | |
| Solubility | Unknown | 07/09/2011 14:20:39 | E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r |
| Molecular weight | 382.49 | | |
| Individual pKa ionic environments | No | | |
| Number of pKas | 0 | | |
| logP (neutral X) | -10.00 | 07/09/2011 14:20:39 | E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r |