# Yasuda-Shedlovsky Result

| | | | |
|---|---|---|---|
| Sample name: | **CS000196** | Experiment start time: | **08/09/2011 11:51:57** |
| Assay name: | **Fast UV psKa** | Analyst: | |
| Assay ID: | **11I-08009** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1109\11I-08009_CS000196_Fast UV psKa.t3r** | | |

## Yasuda-Shedlovsky result

| Extrapolation type | pKa 0% | SD | Intercept | Slope | R² | Ionic strength | Temperature |
|---|---|---|---|---|---|---|---|
| Yasuda-Shedlovsky | 6.50 | ±0.05 | 22.14 | -1079.8441 | 0.9705 | 0.207 M | 27.4°C |
| Yasuda-Shedlovsky | 8.70 | ±0.02 | 14.93 | -348.8518 | 0.9615 | 0.207 M | 27.4°C |

## Component assay results

| Titration | DMSO weight% | Direction | Result type | Dielectric constant | [H2O] | Ionic strength | Temperature | | psKa 1 | |
|---|---|---|---|---|---|---|---|---|---|---|
| 11I-08009 Points 105 to 156 | 20.61 % | Up | UV-metric pKa | 76.6 | 44.7 M | 0.210 M | 27.7°C | ☑ | 6.41 | ☑ |
| 11I-08009 Points 53 to 104 | 27.99 % | Up | UV-metric pKa | 76.4 | 40.9 M | 0.209 M | 27.0°C | ☑ | 6.37 | ☑ |
| 11I-08009 Points 3 to 52 | 38.03 % | Up | UV-metric pKa | 75.5 | 35.5 M | 0.202 M | 27.4°C | ☑ | 6.29 | ☑ |

## Graphs

| | | | |
|---|---|---|---|
| Sample name: | **CS000196** | Experiment start time: | **08/09/2011 11:51:57** |
| Assay name: | **Fast UV psKa** | Analyst: | |
| Assay ID: | **11I-08009** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1109\11I-08009_CS000196_Fast UV psKa.t3r** | | |

# Fast UV psKa Titration 1 of 3 11I-08009 Points 3 to 52

## Graphs

| | | | |
|---|---|---|---|
| Sample name: | **CS000196** | Experiment start time: | **08/09/2011 11:51:57** |
| Assay name: | **Fast UV psKa** | Analyst: | |
| Assay ID: | **11I-08009** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1109\11I-08009_CS000196_Fast UV psKa.t3r** | | |

# Fast UV psKa Titration 2 of 3 11I-08009 Points 53 to 104

## Graphs

| | | | |
|---|---|---|---|
| Sample name: | **CS000196** | Experiment start time: | **08/09/2011 11:51:57** |
| Assay name: | **Fast UV psKa** | Analyst: | |
| Assay ID: | **11I-08009** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1109\11I-08009_CS000196_Fast UV psKa.t3r** | | |

# Fast UV psKa Titration 3 of 3 11I-08009 Points 105 to 156

## Graphs

| | | | |
|---|---|---|---|
| Sample name: | **CS000196** | Experiment start time: | **08/09/2011 11:51:57** |
| Assay name: | **Fast UV psKa** | Analyst: | |
| Assay ID: | **11I-08009** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1109\11I-08009_CS000196_Fast UV psKa.t3r** | | |

## Assay Model

| Settings | Value | Date/Time changed | Imported from |
|---|---|---|---|
| Sample name | CS000196 | | |
| Sample by | Volume | | |
| Sample volume | 0.0100 mL | | |
| Solvent | DMSO | | |
| Sample concentration | 0.010000 M | | |
| Solubility | Unknown | | |
| Molecular weight | 458.52 | | |
| Individual pKa ionic environments | No | | |
| Number of pKas | 2 | | |
| Sample is a | Base | | |
| pKa 1 | 6.50 | | |
| pKa 2 | 8.90 | | |
| logP (XH2 2+) | -10.00 | | |
| logp (XH +) | -10.00 | | |
| logP (neutral X) | -10.00 | | |