# Yasuda-Shedlovsky Result

| | | | |
|---|---|---|---|
| Sample name: | **CS000109** | Experiment start time: | **25/08/2011 18:18:33** |
| Assay name: | **Fast UV psKa** | Analyst: | |
| Assay ID: | **11H-25020** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1108\11H-25020_CS000109_Fast UV psKa.t3r** | | |

## Yasuda-Shedlovsky result

| Extrapolation type | pKa 0% | SD | Intercept | Slope | R² | Ionic strength | Temperature |
|---|---|---|---|---|---|---|---|
| Yasuda-Shedlovsky | 3.44 | ±0.07 | 32.07 | -2091.7879 | 0.9849 | 0.205 M | 27.1°C |

## Component assay results

| Titration | DMSO weight% | Direction | Result type | Dielectric constant | [H2O] | Ionic strength | Temperature | | psKa 1 |
|---|---|---|---|---|---|---|---|---|---|
| 11H-25020 Points 104 to 155 | 20.88 % | Up | UV-metric pKa | 76.7 | 44.6 M | 0.210 M | 27.2°C | ☑ | 3.18 |
| 11H-25020 Points 53 to 103 | 27.44 % | Up | UV-metric pKa | 76.5 | 41.2 M | 0.206 M | 26.9°C | ☑ | 3.07 |
| 11H-25020 Points 3 to 52 | 37.63 % | Up | UV-metric pKa | 75.5 | 35.7 M | 0.199 M | 27.3°C | ☑ | 2.83 |

## Graphs

| | | | |
|---|---|---|---|
| Sample name: | **CS000109** | Experiment start time: | **25/08/2011 18:18:33** |
| Assay name: | **Fast UV psKa** | Analyst: | |
| Assay ID: | **11H-25020** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1108\11H-25020_CS000109_Fast UV psKa.t3r** | | |

# Fast UV psKa Titration 1 of 3 11H-25020 Points 3 to 52

## Graphs

| | | | |
|---|---|---|---|
| Sample name: | **CS000109** | Experiment start time: | **25/08/2011 18:18:33** |
| Assay name: | **Fast UV psKa** | Analyst: | |
| Assay ID: | **11H-25020** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1108\11H-25020_CS000109_Fast UV psKa.t3r** | | |

# Fast UV psKa Titration 2 of 3 11H-25020 Points 53 to 103

## Graphs

| | | | |
|---|---|---|---|
| Sample name: | **CS000109** | Experiment start time: | **25/08/2011 18:18:33** |
| Assay name: | **Fast UV psKa** | Analyst: | |
| Assay ID: | **11H-25020** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1108\11H-25020_CS000109_Fast UV psKa.t3r** | | |

# Fast UV psKa Titration 3 of 3 11H-25020 Points 104 to 155

## Graphs

| | | | |
|---|---|---|---|
| Sample name: | **CS000109** | Experiment start time: | **25/08/2011 18:18:33** |
| Assay name: | **Fast UV psKa** | Analyst: | |
| Assay ID: | **11H-25020** | Instrument ID: | **T311042** |
| Filename: | **E:\T3 DATA\1108\11H-25020_CS000109_Fast UV psKa.t3r** | | |

## Assay Model

| Settings | Value | Date/Time changed | Imported from |
|---|---|---|---|
| Sample name | CS000109 | | |
| Sample by | Volume | | |
| Sample volume | 0.0100 mL | | |
| Solvent | DMSO | | |
| Sample concentration | 0.010000 M | | |
| Solubility | Unknown | 25/08/2011 14:45:10 | E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r |
| Molecular weight | 481.96 | | |
| Individual pKa ionic environments | No | | |
| Number of pKas | 1 | | |
| Sample is a | Base | 25/08/2011 14:45:10 | E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r |
| pKa 1 | 4.00 | 25/08/2011 14:45:10 | E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r |
| logp (XH +) | -10.00 | 25/08/2011 14:45:10 | E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r |
| logP (neutral X) | -10.00 | 25/08/2011 14:45:10 | E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r |