

Sample name: **CS000243**  
 Assay name: **pH-metric psKa**  
 Assay ID: **11H-31009**  
 Filename: **E:\T3 DATA\1108\11H-31009\_CS000243\_pH-metric psKa.t3r**

Experiment start time: **31/08/2011 15:07:13**  
 Analyst:  
 Instrument ID: **T311042**

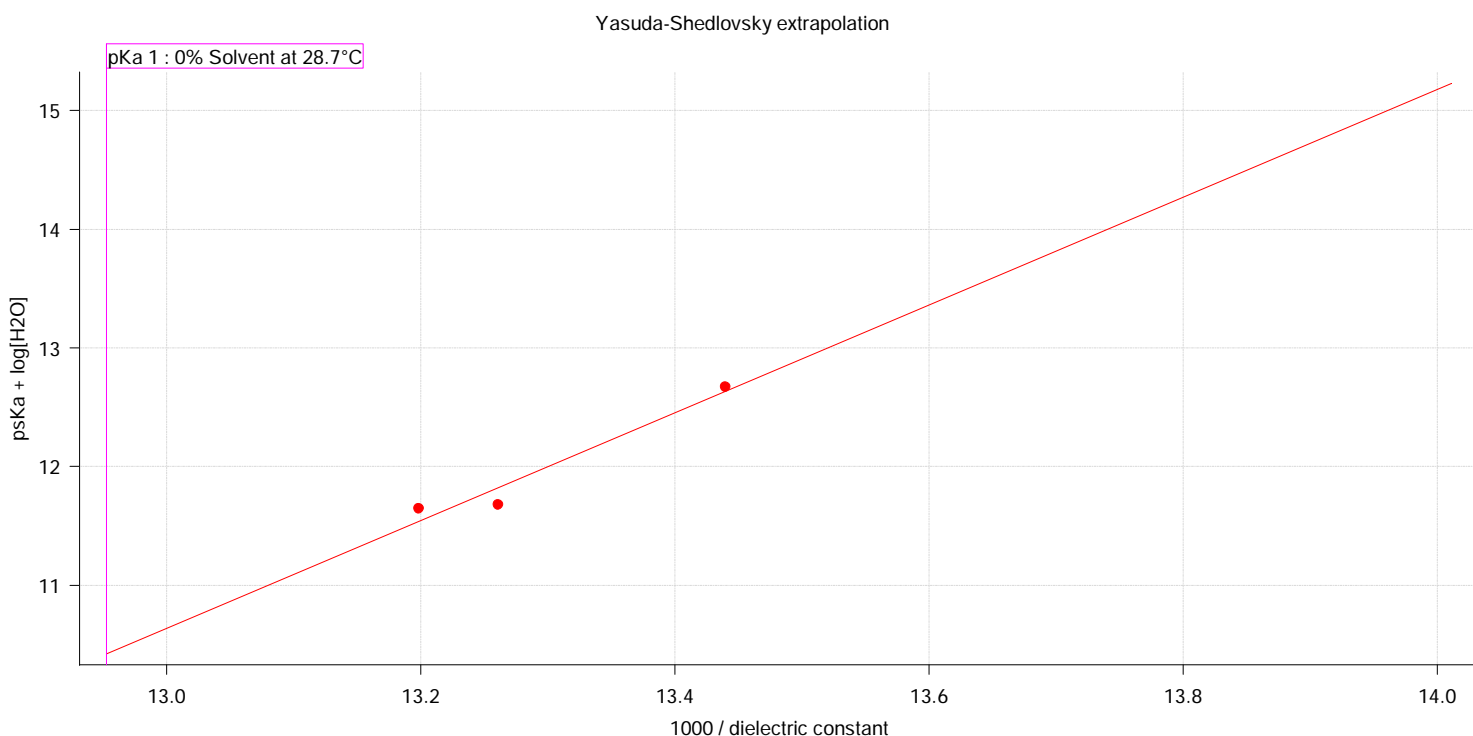
## Yasuda-Shedlovsky result

| Extrapolation type | pKa 0% | SD    | Intercept | Slope     | R <sup>2</sup> | Ionic strength | Temperature |
|--------------------|--------|-------|-----------|-----------|----------------|----------------|-------------|
| Yasuda-Shedlovsky  | 8.68   | ±0.37 | -48.33    | 4536.3700 | 0.9510         | 0.191 M        | 28.7°C      |

## Component assay results

| Titration                  | DMSO weight% | Direction | Result type | Dielectric constant | [H <sub>2</sub> O] | Ionic strength | Temperature | psKa 1  |
|----------------------------|--------------|-----------|-------------|---------------------|--------------------|----------------|-------------|---------|
| 11H-31009 Points 90 to 140 | 24.88 %      | Up        | pH-metric   | 75.8                | 42.5 M             | 0.199 M        | 29.3°C      | ✓ 10.02 |
| 11H-31009 Points 45 to 89  | 33.28 %      | Up        | pH-metric   | 75.4                | 38.0 M             | 0.194 M        | 28.8°C      | ✓ 10.10 |
| 11H-31009 Points 3 to 44   | 44.76 %      | Up        | pH-metric   | 74.4                | 31.8 M             | 0.181 M        | 28.2°C      | ✓ 11.17 |

## Graphs



Sample name: **CS000243**  
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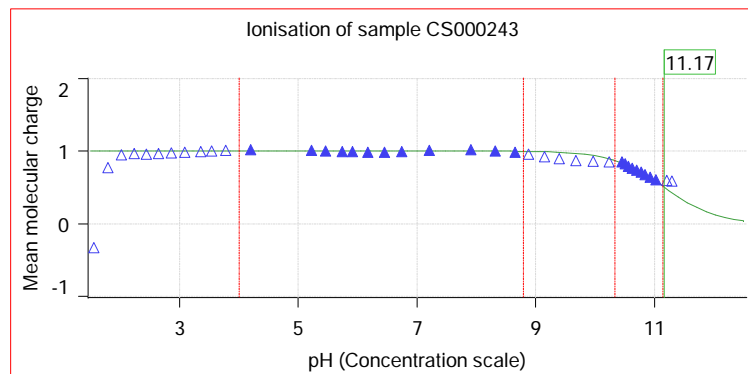
Experiment start time: **31/08/2011 15:07:13**  
 Analyst:  
 Instrument ID: **T311042**

## pH-metric psKa Titration 1 of 3 11H-31009 Points 3 to 44

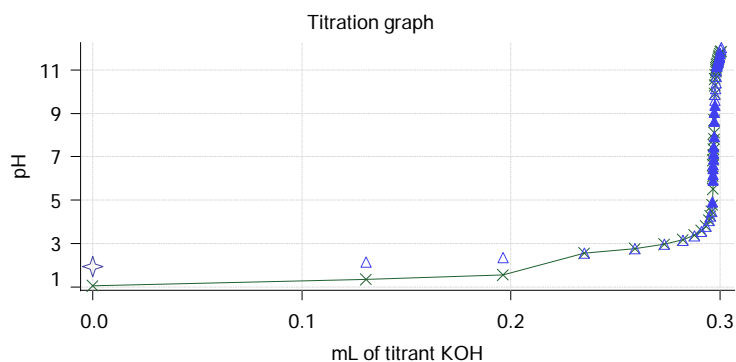
### Sample

CS000243 concentration factor 1.000  
 Base pKa 1 11.17

### Sample graphs



### Other graphs



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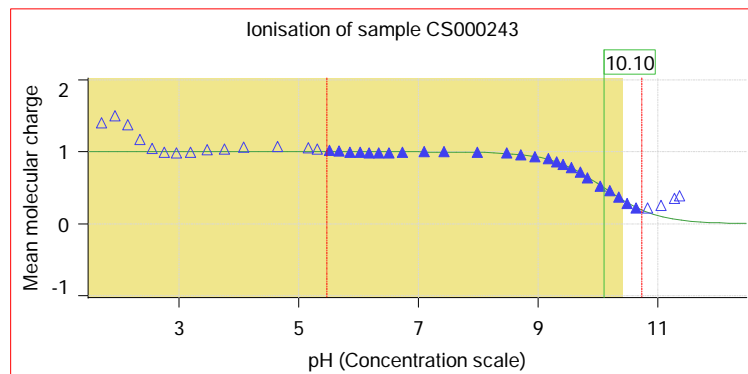
Experiment start time: **31/08/2011 15:07:13**  
 Analyst:  
 Instrument ID: **T311042**

## pH-metric psKa Titration 2 of 3 11H-31009 Points 45 to 89

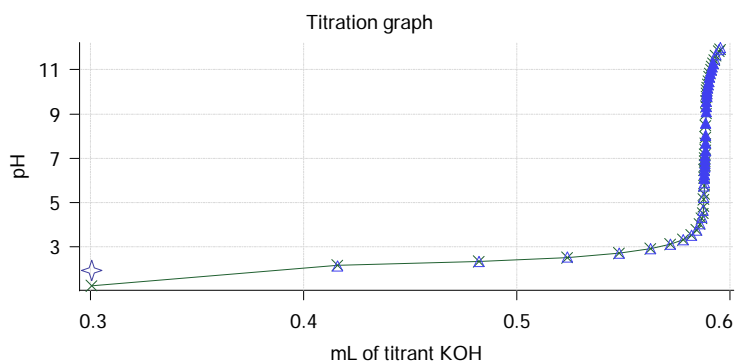
### Sample

CS000243 concentration factor 0.565  
 Base pKa 1 10.10

### Sample graphs



### Other graphs



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 Assay ID: **11H-31009**  
 Filename: **E:\T3 DATA\1108\11H-31009\_CS000243\_pH-metric psKa.t3r**

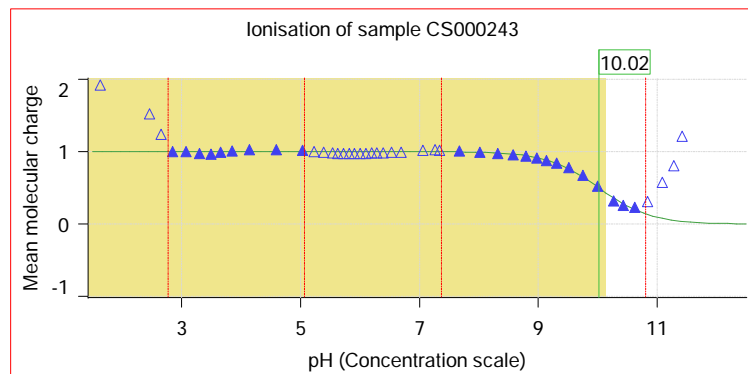
Experiment start time: **31/08/2011 15:07:13**  
 Analyst:  
 Instrument ID: **T311042**

## pH-metric psKa Titration 3 of 3 11H-31009 Points 90 to 140

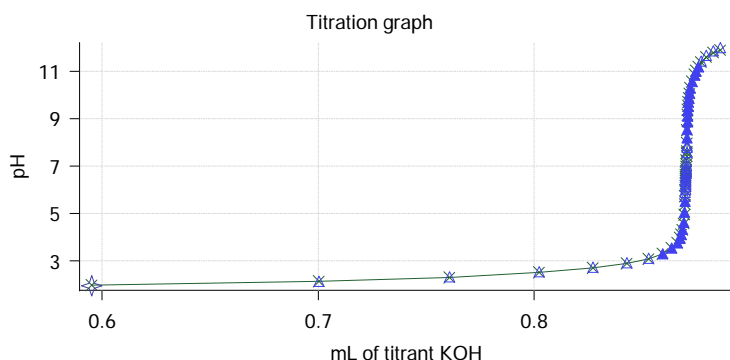
### Sample

CS000243 concentration factor 0.565  
 Base pKa 1 10.02

### Sample graphs



### Other graphs



### Assay Model

| Settings                          | Value        | Date/Time changed   | Imported from  |
|-----------------------------------|--------------|---------------------|--|
| Sample name                       | CS000243     |                     |  |
| Sample by                         | Weight       | 31/08/2011 10:24:46 | E:\T3<br>DATA\1108\11H-01005_CS00080_pH-metric<br>psKa.t3r |
| Sample weight                     | 0.000850 g   |                     |  |
| Formula weight                    | 371.39 g/mol |                     |  |
| Solubility                        | Unknown      | 31/08/2011 10:24:46 | E:\T3<br>DATA\1108\11H-01005_CS00080_pH-metric<br>psKa.t3r |
| Molecular weight                  | 371.39       |                     |  |
| Individual pKa ionic environments | No           |                     |  |
| Number of pKas                    | 1            |                     |  |
| Sample is a                       | Base         | 31/08/2011 10:24:46 | E:\T3<br>DATA\1108\11H-01005_CS00080_pH-metric<br>psKa.t3r |
| pKa 1                             | 8.00         |                     |  |
| logp (XH +)                       | -10.00       | 31/08/2011 10:24:46 | E:\T3<br>DATA\1108\11H-01005_CS00080_pH-metric<br>psKa.t3r |
| logP (neutral X)                  | -10.00       |                     |  |