Yasuda-Shedlovsky Result

Sample name:	**CS000166**	Experiment start time:	**06/09/2011 15:01:21**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11I-06014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-06014_CS000166_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	8.03	±0.43	7.71	161.9185	0.8270	0.171 M	24.8°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11I-06014 Points 87 to 137	40.53 %	Up	pH-metric	60.8	29.7 M	0.176 M	24.9°C	☑	8.99
11I-06014 Points 37 to 86	53.47 %	Up	pH-metric	54.8	22.5 M	0.173 M	24.9°C	☑	9.15
11I-06014 Points 3 to 36	65.03 %	Up	pH-metric	49.3	16.5 M	0.164 M	24.7°C	☑	9.85

Graphs

Sample name:	**CS000166**	Experiment start time:	**06/09/2011 15:01:21**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11I-06014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-06014_CS000166_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11I-06014 Points 3 to 36

Sample

CS000166 concentration factor	0.962
Base pKa 1	9.85

Sample graphs

Other graphs

Sample name:	**CS000166**	Experiment start time:	**06/09/2011 15:01:21**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11I-06014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-06014_CS000166_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11I-06014 Points 37 to 86

Sample

- CS000166 concentration factor 0.467
- Base pKa 1 9.15

Sample graphs

Other graphs

Sample name:	**CS000166**	Experiment start time:	**06/09/2011 15:01:21**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11I-06014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-06014_CS000166_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11I-06014 Points 87 to 137

Sample

CS000166 concentration factor	0.412
Base pKa 1	8.99

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000166		
Sample by	Weight		
Sample weight	0.001110 g		
Formula weight	446.49 g/mol		
Solubility	Unknown	06/09/2011 11:28:31	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
Molecular weight	446.49		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base	06/09/2011 11:28:31	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
pKa 1	9.65		
logp (XH +)	-10.00	06/09/2011 11:28:31	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
logP (neutral X)	-10.00	06/09/2011 11:28:31	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r