Yasuda-Shedlovsky Result

Sample name:	**cs000105**	Experiment start time:	**18/08/2011 15:11:55**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-18009**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-18009_cs000105_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R^2	Ionic strength	Temperature
Yasuda-Shedlovsky	4.18	±0.03	32.46	-2073.9626	0.9972	0.194 M	26.1°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-18009 Points 81 to 122	23.25 %	Up	pH-metric	76.8	43.4 M	0.200 M	26.7°C	☑	3.82
11H-18009 Points 39 to 80	30.99 %	Up	pH-metric	76.4	39.3 M	0.196 M	26.2°C	☑	3.73
11H-18009 Points 3 to 38	41.66 %	Up	pH-metric	75.7	33.5 M	0.186 M	25.4°C	☑	3.55

Graphs

Sample name:	**cs000105**	Experiment start time:	**18/08/2011 15:11:55**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-18009**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-18009_cs000105_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11H-18009 Points 3 to 38 Quality: Good

Sample

cs000105 concentration factor	0.800
Base pKa 1	3.55

Sample graphs

Other graphs

Sample name:	**cs000105**	Experiment start time:	**18/08/2011 15:11:55**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-18009**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-18009_cs000105_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11H-18009 Points 39 to 80 Quality: Good

Sample

cs000105 concentration factor	0.852
Base pKa 1	3.73

Sample graphs

Other graphs

Sample name:	**cs000105**	Experiment start time:	**18/08/2011 15:11:55**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-18009**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-18009_cs000105_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11H-18009 Points 81 to 122 Quality: Good

Sample

cs000105 concentration factor	0.927
Base pKa 1	3.82

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	cs000105		
Sample by	Weight	18/08/2011 10:41:48	E:\T3 DATA\1108\11H-12015_EX965317449-000_pH-me psKa.t3r
Sample weight	0.000890 g		
Formula weight	290.39 g/mol		
Solubility	Unknown	18/08/2011 10:41:48	E:\T3 DATA\1108\11H-12015_EX965317449-000_pH-me psKa.t3r
Molecular weight	290.39		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base	18/08/2011 10:41:48	E:\T3 DATA\1108\11H-12015_EX965317449-000_pH-me psKa.t3r
pKa 1	4.00	18/08/2011 10:41:48	E:\T3 DATA\1108\11H-12015_EX965317449-000_pH-me psKa.t3r
logp (XH +)	-10.00	18/08/2011 10:41:48	E:\T3 DATA\1108\11H-12015_EX965317449-000_pH-me psKa.t3r

Sample name:	**cs000105**	Experiment start time:	**18/08/2011 15:11:55**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-18009**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-18009_cs000105_pH-metric psKa.t3r**		

Assay Model (continued)

Settings	Value	Date/Time changed	Imported from
logP (neutral X)	-10.00	18/08/2011 10:41:48	E:\T3 DATA\1108\11H-12015_EX965317449-000_pH-metric psKa.t3r