Yasuda-Shedlovsky Result

Sample name:	**CS00055**	Experiment start time:	**02/08/2011 18:34:18**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-02011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-02011_CS00055_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R^2	Ionic strength	Temperature
Yasuda-Shedlovsky	6.09	±0.83	-71.02	6141.0400	0.8537	0.186 M	26.9°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-02011 Points 100 to 148	24.33 %	Up	pH-metric	76.7	42.8 M	0.194 M	26.8°C	☑	7.64
11H-02011 Points 55 to 99	31.75 %	Up	pH-metric	76.1	38.9 M	0.189 M	27.0°C	☑	7.73
11H-02011 Points 3 to 54	41.22 %	Up	pH-metric	75.3	33.8 M	0.176 M	26.8°C	☑	9.12

Graphs

Sample name:	**CS00055**	Experiment start time:	**02/08/2011 18:34:18**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-02011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-02011_CS00055_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11H-02011 Points 3 to 54

Sample

- CS00055 concentration factor 0.351
- Base pKa 1 9.12

Sample graphs

Other graphs

Sample name:	**CS00055**	Experiment start time:	**02/08/2011 18:34:18**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-02011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-02011_CS00055_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11H-02011 Points 55 to 99

Sample

- CS00055 concentration factor 0.514
- Base pKa 1 7.73

Sample graphs

Other graphs

Sample name:	**CS00055**	Experiment start time:	**02/08/2011 18:34:18**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-02011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-02011_CS00055_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11H-02011 Points 100 to 148

Sample

- CS00055 concentration factor 0.576
- Base pKa 1 7.64

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS00055		
Sample by	Weight		
Sample weight	0.001050 g		
Formula weight	303.32 g/mol		
Solubility	Unknown		
Molecular weight	303.32		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base		
pKa 1	10.00		
logp (XH +)	-10.00		
logP (neutral X)	-10.00		