Yasuda-Shedlovsky Result

Sample name:	**cs000116**	Experiment start time:	**18/08/2011 20:29:18**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-18014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-18014_cs000116_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	3.77	±0.17	36.08	-2398.5415	0.9630	0.191 M	25.2°C
Yasuda-Shedlovsky	9.39	±0.12	-2.11	1039.5350	0.9096	0.191 M	25.2°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1		sK
11H-18014 Points 88 to 138	24.05 %	Up	pH-metric	77.0	43.0 M	0.198 M	25.8°C	✓	3.37	✓	.7
11H-18014 Points 41 to 87	32.25 %	Up	pH-metric	76.7	38.6 M	0.194 M	25.4°C	✓	3.14	✓	.9
11H-18014 Points 3 to 40	45.29 %	Up	pH-metric	75.6	31.6 M	0.180 M	24.5°C	✓	2.86	✓	0.1

Graphs

Sample name:	**cs000116**	Experiment start time:	**18/08/2011 20:29:18**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-18014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-18014_cs000116_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11H-18014 Points 3 to 40 Quality: Good

Sample

cs000116 concentration factor	0.913
Base pKa 1	2.86
Base pKa 2	10.13

Sample graphs

Other graphs

Sample name:	**cs000116**	Experiment start time:	**18/08/2011 20:29:18**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-18014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-18014_cs000116_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11H-18014 Points 41 to 87 Quality: Good

Sample

cs000116 concentration factor	1.013
Base pKa 1	3.14
Base pKa 2	9.91

Sample graphs

Other graphs

Sample name:	**cs000116**	Experiment start time:	**18/08/2011 20:29:18**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-18014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-18014_cs000116_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11H-18014 Points 88 to 138 Quality: Good

Sample

cs000116 concentration factor	0.919
Base pKa 1	3.37
Base pKa 2	9.71

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	cs000116		
Sample by	Weight	18/08/2011 10:41:48	E:\T3 DATA\1108\11H-12015_EX965317449-000_pH-me psKa.t3r
Sample weight	0.000530 g		
Formula weight	351.64 g/mol		
Solubility	Unknown	18/08/2011 10:41:48	E:\T3 DATA\1108\11H-12015_EX965317449-000_pH-me psKa.t3r
Molecular weight	351.64		
Individual pKa ionic environments	No		
Number of pKas	2		
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
pKa 2	10.00		

Sample name:	**cs000116**	Experiment start time:	**18/08/2011 20:29:18**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11H-18014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-18014_cs000116_pH-metric psKa.t3r**		

Assay Model (continued)

Settings	Value	Date/Time changed	Imported from
logP (XH2 2+)	-10.00	18/08/2011 10:41:48	E:\T3 DATA\1108\11H-12015_EX965317449-000_pH-metric psKa.t3r
logp (XH +)	-10.00	18/08/2011 10:41:48	E:\T3 DATA\1108\11H-12015_EX965317449-000_pH-metric psKa.t3r
logP (neutral X)	-10.00		