Yasuda-Shedlovsky Result

Sample name:	**cs000104**	Experiment start time:	**19/08/2011 14:17:22**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-19012**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-19012_cs000104_UV-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R^2	Ionic strength	Temperature
Yasuda-Shedlovsky	3.74	±0.06	39.44	-2632.8237	0.9947	0.182 M	27.8°C
Yasuda-Shedlovsky	9.28	±0.02	0.50	816.0709	0.9963	0.182 M	27.8°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1	
11H-19012 Points 92 to 140	23.27 %	Up	UV-metric pKa	76.3	43.3 M	0.189 M	28.1°C	☑	3.27	☑
11H-19012 Points 45 to 90	30.99 %	Up	UV-metric pKa	75.8	39.2 M	0.185 M	28.1°C	☑	3.13	☑
11H-19012 Points 4 to 43	40.96 %	Up	UV-metric pKa	75.2	33.9 M	0.173 M	27.2°C	☑	2.89	☑

Graphs

Sample name:	**cs000104**	Experiment start time:	**19/08/2011 14:17:22**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-19012**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-19012_cs000104_UV-metric psKa.t3r**		

UV-metric psKa Titration 1 of 3 11H-19012 Points 4 to 43

Graphs

Sample name:	**cs000104**	Experiment start time:	**19/08/2011 14:17:22**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-19012**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-19012_cs000104_UV-metric psKa.t3r**		

UV-metric psKa Titration 2 of 3 11H-19012 Points 45 to 90

Graphs

Sample name:	**cs000104**	Experiment start time:	**19/08/2011 14:17:22**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-19012**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-19012_cs000104_UV-metric psKa.t3r**		

UV-metric psKa Titration 3 of 3 11H-19012 Points 92 to 140

Graphs

Sample name:	**cs000104**	Experiment start time:	**19/08/2011 14:17:22**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-19012**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-19012_cs000104_UV-metric psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	cs000104		
Sample by	Volume		
Sample volume	0.0050 mL		
Solvent	DMSO		
Sample concentration	0.010000 M		
Solubility	Unknown	19/08/2011 11:40:08	E:\T3 DATA\1108\11H-15007-1_EX965325003-001_pH-m psKa.t3r
Molecular weight	351.64		
Individual pKa ionic environments	No		
Number of pKas	2	19/08/2011 11:40:08	E:\T3 DATA\1108\11H-15007-1_EX965325003-001_pH-m psKa.t3r
Sample is a	Base		
pKa 1	3.20		
pKa 2	9.50		
logP (XH2 2+)	-10.00	19/08/2011 11:40:08	E:\T3 DATA\1108\11H-15007-1_EX965325003-001_pH-m psKa.t3r
logp (XH +)	-10.00	19/08/2011 11:40:08	E:\T3 DATA\1108\11H-15007-1_EX965325003-001_pH-m psKa.t3r
logP (neutral X)	-10.00	19/08/2011 11:40:08	E:\T3 DATA\1108\11H-15007-1_EX965325003-001_pH-m psKa.t3r