Yasuda-Shedlovsky Result

Sample name:	**CS000140**	Experiment start time:	**01/09/2011 12:42:01**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-01013**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-01013_CS000140_Fast UV psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	3.49	±0.11	28.51	-1811.0023	0.9504	0.202 M	27.1°C
Yasuda-Shedlovsky	10.41	±0.01	14.33	-169.3286	0.8975	0.202 M	27.1°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1	
11I-01013 Points 108 to 161	20.03 %	Up	UV-metric pKa	76.8	45.0 M	0.208 M	27.0°C	☑	3.33	☑
11I-01013 Points 55 to 107	26.63 %	Up	UV-metric pKa	76.6	41.6 M	0.205 M	26.5°C	☑	3.21	☑
11I-01013 Points 3 to 54	35.25 %	Up	UV-metric pKa	75.6	37.0 M	0.194 M	27.7°C	☑	3.00	☑

Graphs

Sample name:	**CS000140**	Experiment start time:	**01/09/2011 12:42:01**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-01013**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-01013_CS000140_Fast UV psKa.t3r**		

Fast UV psKa Titration 1 of 3 11I-01013 Points 3 to 54

Graphs

Sample name:	**CS000140**	Experiment start time:	**01/09/2011 12:42:01**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-01013**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-01013_CS000140_Fast UV psKa.t3r**		

Fast UV psKa Titration 2 of 3 11I-01013 Points 55 to 107

Graphs

Sample name:	**CS000140**	Experiment start time:	**01/09/2011 12:42:01**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-01013**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-01013_CS000140_Fast UV psKa.t3r**		

Fast UV psKa Titration 3 of 3 11I-01013 Points 108 to 161

Graphs

Sample name:	**CS000140**	Experiment start time:	**01/09/2011 12:42:01**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-01013**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-01013_CS000140_Fast UV psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000140		
Sample by	Volume		
Sample volume	0.0100 mL		
Solvent	DMSO		
Sample concentration	0.010000 M		
Solubility	Unknown	01/09/2011 10:40:23	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Molecular weight	376.46		
Individual pKa ionic environments	No		
Number of pKas	2		
Sample is a	Base	01/09/2011 10:40:23	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
pKa 1	4.00	01/09/2011 10:40:23	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
pKa 2	8.50		
logP (XH2 2+)	-10.00	01/09/2011 10:40:23	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logp (XH +)	-10.00	01/09/2011 10:40:23	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logP (neutral X)	-10.00		