Yasuda-Shedlovsky Result

Sample name:	**CS000100**	Experiment start time:	**26/07/2011 17:16:53**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11G-26023**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-26023_CS000100_Fast UV psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R^2	Ionic strength	Temperature
Yasuda-Shedlovsky	4.45	±0.10	26.89	-1596.9200	0.9666	0.207 M	28.8°C
Yasuda-Shedlovsky	7.02	±0.05	-0.67	727.7120	0.9585	0.207 M	28.8°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11G-26023 Points 119 to 177	24.15 %	Up	UV-metric pKa	76.0	42.9 M	0.213 M	28.8°C	☑	4.28
11G-26023 Points 60 to 118	32.12 %	Up	UV-metric pKa	75.6	38.6 M	0.209 M	28.4°C	☑	4.13
11G-26023 Points 3 to 59	42.90 %	Up	UV-metric pKa	74.3	32.8 M	0.198 M	29.3°C	☑	3.88

Graphs

Sample name:	**CS000100**	Experiment start time:	**26/07/2011 17:16:53**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11G-26023**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-26023_CS000100_Fast UV psKa.t3r**		

Fast UV psKa Titration 1 of 3 11G-26023 Points 3 to 59

Graphs

Sample name:	**CS000100**	Experiment start time:	**26/07/2011 17:16:53**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11G-26023**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-26023_CS000100_Fast UV psKa.t3r**		

Fast UV psKa Titration 2 of 3 11G-26023 Points 60 to 118

Graphs

Sample name:	**CS000100**	Experiment start time:	**26/07/2011 17:16:53**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11G-26023**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-26023_CS000100_Fast UV psKa.t3r**		

Fast UV psKa Titration 3 of 3 11G-26023 Points 119 to 177

Graphs

Sample name:	**CS000100**	Experiment start time:	**26/07/2011 17:16:53**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11G-26023**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-26023_CS000100_Fast UV psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000100		
Sample by	Volume		
Sample volume	0.0200 mL		
Solvent	DMSO		
Sample concentration	0.010000 M		
Solubility	Unknown	26/07/2011 12:26:03	E:\T3 DATA\1107\11G-23004_CS000041_pH-metric psKa.t3r
Molecular weight	473.30		
Individual pKa ionic environments	No		
Number of pKas	2	26/07/2011 12:26:03	E:\T3 DATA\1107\11G-23004_CS000041_pH-metric psKa.t3r
Sample is a	Base	26/07/2011 12:26:03	E:\T3 DATA\1107\11G-23004_CS000041_pH-metric psKa.t3r
pKa 1	4.00	26/07/2011 12:26:03	E:\T3 DATA\1107\11G-23004_CS000041_pH-metric psKa.t3r
pKa 2	10.00	26/07/2011 12:26:03	E:\T3 DATA\1107\11G-23004_CS000041_pH-metric psKa.t3r
logP (XH2 2+)	-10.00	26/07/2011 12:26:03	E:\T3 DATA\1107\11G-23004_CS000041_pH-metric psKa.t3r
logp (XH +)	-10.00	26/07/2011 12:26:03	E:\T3 DATA\1107\11G-23004_CS000041_pH-metric psKa.t3r
logP (neutral X)	-10.00	26/07/2011 12:26:03	E:\T3 DATA\1107\11G-23004_CS000041_pH-metric psKa.t3r