Yasuda-Shedlovsky Result

Sample name:	**CS000041**	Experiment start time:	**26/07/2011 12:26:51**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11G-26011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-26011_CS000041_Fast UV psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	4.04	±0.14	27.54	-1682.2100	0.9121	0.198 M	28.4°C
Yasuda-Shedlovsky	6.71	±0.03	13.71	-407.1290	0.9332	0.198 M	28.4°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11G-26011 Points 101 to 151	20.74 %	Up	UV-metric pKa	76.3	44.6 M	0.205 M	28.3°C	☑	3.90
11G-26011 Points 51 to 100	27.73 %	Up	UV-metric pKa	76.1	41.0 M	0.201 M	27.7°C	☑	3.76
11G-26011 Points 3 to 50	36.34 %	Up	UV-metric pKa	75.1	36.4 M	0.190 M	29.0°C	☑	3.57

Graphs

Sample name:	**CS000041**	Experiment start time:	**26/07/2011 12:26:51**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11G-26011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-26011_CS000041_Fast UV psKa.t3r**		

Fast UV psKa Titration 1 of 3 11G-26011 Points 3 to 50

Graphs

Sample name:	**CS000041**	Experiment start time:	**26/07/2011 12:26:51**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11G-26011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-26011_CS000041_Fast UV psKa.t3r**		

Fast UV psKa Titration 2 of 3 11G-26011 Points 51 to 100

Graphs

Sample name:	**CS000041**	Experiment start time:	**26/07/2011 12:26:51**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11G-26011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-26011_CS000041_Fast UV psKa.t3r**		

Fast UV psKa Titration 3 of 3 11G-26011 Points 101 to 151

Graphs

Sample name:	**CS000041**	Experiment start time:	**26/07/2011 12:26:51**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11G-26011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-26011_CS000041_Fast UV psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000041	26/07/2011 12:26:03	E:\T3 DATA\1107\11G-23004_CS000041_pH-metric psKa.t3r
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	341.39		
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