Yasuda-Shedlovsky Result

Sample name:	**CS000115**	Experiment start time:	**26/08/2011 19:04:58**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-26014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-26014_CS000115_UV-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R^2	Ionic strength	Temperature
Yasuda-Shedlovsky	3.11	±0.01	26.20	-1661.6800	0.9998	0.186 M	27.0°C
Yasuda-Shedlovsky	9.39	±0.02	0.64	816.7442	0.9957	0.186 M	27.0°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1	
11H-26014 Points 89 to 134	25.76 %	Up	UV-metric pKa	76.3	42.0 M	0.192 M	27.6°C	☑	2.81	☑
11H-26014 Points 45 to 87	33.90 %	Up	UV-metric pKa	75.9	37.7 M	0.188 M	27.3°C	☑	2.72	☑
11H-26014 Points 4 to 43	44.68 %	Up	UV-metric pKa	75.1	31.9 M	0.177 M	26.2°C	☑	2.57	☑

Graphs

Sample name:	**CS000115**	Experiment start time:	**26/08/2011 19:04:58**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-26014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-26014_CS000115_UV-metric psKa.t3r**		

UV-metric psKa Titration 1 of 3 11H-26014 Points 4 to 43

Graphs

Sample name:	**CS000115**	Experiment start time:	**26/08/2011 19:04:58**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-26014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-26014_CS000115_UV-metric psKa.t3r**		

UV-metric psKa Titration 2 of 3 11H-26014 Points 45 to 87

Graphs

Sample name:	**CS000115**	Experiment start time:	**26/08/2011 19:04:58**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-26014**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-26014_CS000115_UV-metric psKa.t3r**		

UV-metric psKa Titration 3 of 3 11H-26014 Points 89 to 134

Graphs

Sample name: **CS000115**
Assay name: **UV-metric psKa**
Assay ID: **11H-26014**
Filename: **E:\T3 DATA\1108\11H-26014_CS000115_UV-metric psKa.t3r**

Experiment start time: **26/08/2011 19:04:58**
Analyst:
Instrument ID: **T311042**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000115	26/08/2011 19:04:28	E:\T3 DATA\1108\11H-25023_CS000115_Fast UV psKa.t3r
Sample by	Volume	26/08/2011 19:04:28	E:\T3 DATA\1108\11H-25023_CS000115_Fast UV psKa.t3r
Sample volume	0.0050 mL		
Solvent	DMSO		
Sample concentration	0.010000 M		
Solubility	Unknown	26/08/2011 19:04:28	E:\T3 DATA\1108\11H-25023_CS000115_Fast UV psKa.t3r
Molecular weight	297.32		
Individual pKa ionic environments	No		
Number of pKas	2	26/08/2011 19:04:28	E:\T3 DATA\1108\11H-25023_CS000115_Fast UV psKa.t3r
Sample is a	Base	26/08/2011 19:04:28	E:\T3 DATA\1108\11H-25023_CS000115_Fast UV psKa.t3r
pKa 1	4.00	26/08/2011 19:04:28	E:\T3 DATA\1108\11H-25023_CS000115_Fast UV psKa.t3r
pKa 2	9.20	26/08/2011 19:04:28	E:\T3 DATA\1108\11H-25023_CS000115_Fast UV psKa.t3r
logP (XH2 2+)	-10.00	26/08/2011 19:04:28	E:\T3 DATA\1108\11H-25023_CS000115_Fast UV psKa.t3r
logp (XH +)	-10.00	26/08/2011 19:04:28	E:\T3 DATA\1108\11H-25023_CS000115_Fast UV psKa.t3r
logP (neutral X)	-10.00	26/08/2011 19:04:28	E:\T3 DATA\1108\11H-25023_CS000115_Fast UV psKa.t3r