Synthesis of Functionalized Ellipticinium and Ellipticine Derivatives via Electrophilic Cyclization

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¹H and ¹³C NMR spectra of 8a





















OSh



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¹H and ¹³C Spectra of **1a**







¹H and ¹³C Spectra of **1b**





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Element Name	Element %	Ret. Time
Nitrogen	4. 51	0. 78
Carbon	54. 85	1. 17
Hydrogen	3. 92	3. 68

Cosh

S25

¹H and ¹³C Spectra of **7b**











¹H and ¹³C Spectra of **8b**









LCMS-2010A DATA REPORT SCHOOL OF CHEMISTRY **UNIVERSITY OF HYDERABAD** User : Admin : KC-11 : 5.000 Sample Inj. Volume Data Name : C:\LCMSsolution\User\Data\KC-11-APCI-POS1.qld Method Name : C:\LCMSsolution\User\Method\esi.qlm LC Chromatogram mAbs Ch1(254.0nm)*1.00 min MS Spectrum Line#:1 R.Time:0.752(Scan#:46) Positive MassPeaks:262 BasePeak:252.20(3776951) RawMode:Single 0.752(46) BG Mode:Peak Start 0.577(35) 10-52 58 96 102 119 128 m/z **OPERATOR** * 5



¹H and ¹³C Spectra of **1c**








S37



Element Name	Element %	Ret. Time	
Nitrogen	3. 89	0. 76	
Carbon	85. 32	1. 11	
Hydrogen	6. 11	3. 83	

ash

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¹H and ¹³C Spectra of **14** -2. 384 -2. 061 -1. 670 -1. 472 -1. 472 -1. 472 -1. 457 -1. 457 -1. 289 -1. 289 -1. 289 -0. 983 888 -0. 885 -0. 885 -0. 885 -0. 2555 -0. 2555 -0. | ||||| | 6 5 3 2 9 8 7 4 1 0 ppm Д 3.371 000 148.893 136.754 135.564 135.131 135.011 133.506 132.694 132.081 130.368 124.505 .539 77.347 77.030 76.712 128. 11



Br

Me

Me

NO₂





¹H and ¹³C Spectra of **15** ____2.812 ____2.577 L7.290 L7.286 L7.245 Me Br Ν Me Ĥ] [1 -1-3 יד 2 10 -1 ppm 9 7 6 4 1 ò 8 5 3.062 139.457 139.151 131.986 124.434 124.154 124.154 124.154 122.487 122.487 122.487 122.487 122.487 122.487 122.487 122.487 122.487 122.487 122.487 122.487 122.487 122.487 122.487 123.487 124.184 124.18 424 106 788 77 . 77 . 76 . N 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ò . ppm



¹H and ¹³C Spectra of **16**





















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Element Name	Element %	Ret. Time
Nitrogen	3 56	0 78
Carbon	65. 41	1. 15
Hydrogen	6. 23	3. 68

OST

S52

¹H and ¹³C Spectra of 1d

4.623 4.605 4.587 8.369 7.654 7.652 7.633 7.620 0.136 0.122 0.048 431 7.285 -1.507Me ,CHO *t*Bu Ph N Et Мe]] ٦ ſ J <u>т</u> 2 1 5 12 و 7 6 4 o 11 10 8 3 ppm 2.159 1.000 3.119 3.345 13.230 3.259 1.089 -131.367 -128.502 -126.524 -126.524 -126.5397 -125.897 -125.897 -123.351 -123.351 (1219.916 (1219.514 (1219.201 -77.380 -77.05 (55.745 -77.380 443 090 225 683 - 39.886 - 34.802 - 31.975 ~17.007 -16.991 ~15.691 143. 140. 135. 41







Element Name	Element %	Ret. Time
Nitrogen	3. 51	0.77
Carbon	85. 32	1. 13
Hydrogen	7. 21	3. 70

OSP

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¹H and ¹³C Spectra of **19**











¹H and ¹³C Spectra of **20**









S62



Element Name	Element %	Ret. Time
Nitrogen	6. 68	0.88
Carbon	87.15	1. 36
Hydrogen	6. 34	4. 75

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¹H and ¹³C Spectra of **21**







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			- '				
43.21	1.18		1				
_34.24			ł				
25.26							
(mVolt)					•		
16.29	0.77						
-	0.76						
7.31	0.76	3.74	+				
-1.66	0.76	3.74	+				-
7.31-	2.4	3.74	4.8 (m	in) 7.2		9.6	12.0
7.31-	2.4	3.74	4.8 (m	in) 7.2		9.6	12.0
7.31-	2.4	3.74	4.8 (m	in) 7.2		9.6	12.0
7.31-	Element Name Nitrogen	3.74	4.8 (m Element % 6. 75	in) 7.2	Ret. Time 0. 76	9.6	12.0
7.31-	Element Name Nitrogen Carbon Hydrogen	3.74	4.8 (m Element % 6. 75 85. 23 7. 76	in) 7.2	Ret. Time 0. 76 1. 18 3. 74	9.6	12.0
7.31-	Element Name Nitrogen Carbon Hydrogen	3.74	4.8 (m Element % 6. 75 85. 23 7. 76	in) 7.2	Ret. Time 0. 76 1. 18 3. 74	9.6	12.0
7.31	Element Name Nitrogen Carbon Hydrogen	3.74	4.8 (m Element % 6. 75 85. 23 7. 76	in) 7.2	Ret. Time 0. 76 1. 18 3. 74	9.6	12.0
7.31-	Element Name Nitrogen Carbon Hydrogen	3.72	4.8 (m Element % 6. 75 85. 23 7. 76	in) 7.2	Ret. Time 0. 76 1. 18 3. 74	2.6	12.0

¹H and ¹³C Spectra of **22**







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S72
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Element Name	Element %	Ret. Time
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Nitrogen	6. 45	0.89
Carbon	87. 12	1. 36
Hydrogen	6. 59	4.99

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S73

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¹H and ¹³C Spectra of **24**





FLASH EA 1112 SERIES CHN REPORT SCHOOL OF CHEMISTRY UNIVERSITY OF HYDERABAD

Method filename: I:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_exa KC-E4 (# 81) Sample ID: Analysis type: Chromatogram filename: Sample weight: UnkNown UNK-20122010-11.dat .988 46.92 1.18 37.62 28.32 (mVolt) 19.01 0.77 9.71 3.76 0.41 -0.0 2.4 4.8 7.2 9.6 (min) 12.0

Element Name	Element %	Ret. Time
Nitrogen	6. 32	0. 77
Carbon	83. 85	1. 18
Hydrogen	6. 41	3. 76

ash

S76

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S77



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Nitrogen 6. 53 0. 77 Carbon 83. 39 1. 15 Hydrogen 6. 28 3. 71	Element Name	Element %	Ret. Time
Nitrogen 6. 53 0. 77 Carbon 83. 39 1. 15 Hydrogen 6. 28 3. 71			
	Nitrogen Carbon Hydrogen	6. 53 83. 39 6. 28	0. 77 1. 15 3. 71

OSh

S79



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Liement Name	Element %	Ret. Time
Nitrogen Carbon Hydrogen	6. 12 80. 45 5. 71	0. 77 1. 17 3. 77

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S82



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Ph





Method filename: Sample ID: Analysis type: Chromatogram filename: Sample weight: I:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_exa KC-E7 (# 82) UnkNown UNK-20122010-12.dat 1.117



Element Name	Element %	Ret. Time
Nitrogen	7.07	0, 89
Carbon	85. 76	1.39
Hydrogen	6. 91	4, 72

ash

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¹H and ¹³C Spectra of **28**

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Element Name	Element %	Ret. Time
Nitrogen	5. 45	0. 77
Carbon	81. 32	1. 18
Hydrogen	6. 57	3.80

Bh

S88







Element Name	Element %	Ret. Time
Nitrogen	5. 71	0. 88
Carbon	86. 73	1. 37
Hydrogen	7. 55	4.96

ash

S91

¹H and ¹³C Spectra of **30**





FLASH EA 1112 SERIES CHN REPORT SCHOOL OF CHEMISTRY UNIVERSITY OF HYDERABAD

Method filename:I:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_exaSample ID:KC-E1 (# 80)Analysis type:UnkNownChromatogram filename:UNK-20122010-10.datSample weight:1.129



Element Name	Element %	Ret. Time
Nitrogen	5. 56	0. 89
Carbon	84.07	1, 39
Hydrogen	7. 31	4 72

Osh

S94

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¹H and ¹³C Spectra of **3a**















Element Name	Element %	Ret. Time
Nitrogen	8 61	0 78
Carbon	85. 49	1. 16
Hydrogen	5. 71	3. 74

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ORTEP diagram of 2-(4-chlorophenyl)-6-ethyl-9-methyl-3-phenyl-6H-pyrido[4,3-b]carbazol-2-ium triflate: Hydrogen atoms are omitted for clarity.



S105

ORTEP diagram of 6-ethyl-7,9-dimethyl-3-phenyl-2-p-tolyl-6H-pyrido[4,3-b]carbazol-2-ium triflate: Hydrogen atoms are omitted for clarity.

