Phosphacycloalkyldiones: Synthesis and coordinative behaviour of 6and 7-member cyclic diketophosphanyls

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Figure S1: Molecular structure of MesP(SiMe ₃) ₂	S2
Figure S2: Molecular structure of Compound 5a	S2
Figure S3: Molecular structure of Compound 5d	S 3
Figures S4-S8: NMR Spectra for Compound 2a.	S4
Figures S9-S14: NMR Spectra for Compound 2b.	S6
Figures S15-S18: NMR Spectra for Compound 2c.	S 9
Figures S19-S23: NMR Spectra for Compound 2d.	S11
Figures S24-S29: NMR Spectra for Compound 2e.	S14
Figures S30-S35: NMR Spectra for Compound 3a.	S17
Figures S36-S41: NMR Spectra for Compound 3b.	S20
Figures S42-S46: NMR Spectra for Compound 3c.	S23
Figures S47-S50: NMR Spectra for Compound 3d.	S25
Figures S51-S56: NMR Spectra for Compound 4.	S27
Figures S57-S62: NMR Spectra for Compound 5a.	S30
Figures S63-S68: NMR Spectra for Compound 5b.	S33
Figures S69-S72: NMR Spectra for Compound Sc.	S36
Figures S73-S78: NMR Spectra for Compound 5d.	S38
Figures S79-S87: NMR Spectra for Compound 6.	S41
Figures S88-S92: HRMS-EI for Compounds 2a-2e.	S46
Figures S93-S96: HRMS-EI for Compounds 3a-3d.	S48
Figures S97-S98: LRMS-EI for Compound 6.	S51



Figure S1. Molecular structure of MesP(SiMe₃)₂ with displacement ellipsoids at 50 %. The asymmetric unit contains two independent molecules of comparable geometry. Selected geometric parameters (Å, deg.): P1–Si1 2.2465(5), P1–Si2 2.2529(5), P1–C7 1.8505(13), Si–P–Si 111.04(2), Si1–P1–C7 103.07(5), Si2–P1–C7 114.58(4)



Figure S2. Molecular structure of *5a* with displacement ellipsoids at 50 % and hydrogen atoms omitted for clarity. Selected geometric parameters (Å): W1−P1 2.5065(7), W1−C_{trans} 1.998(3), W1−C_{cis} 2.045(3) – 2.064(4), C−O_{trans} 1.145(4), C−O_{cis} 1.133(5) – 1.143(4), P1−C6 1.815(3), P1−C5 1.881(4), P1−C1 1.880(3), C1−O1 1.202(4) C5−O2 1.206(4).



Figure S3. Molecular structure of 5d with displacement ellipsoids at 50 % and hydrogen atoms omitted for clarity. The asymmetric unit includes a second molecule that is subject to disorder. Selected geometric parameters (Å): W1–P1
2.490(3), W1–C_{trans} 2.009(11), W1–C_{cis} 2.02(1) – 2.05(1), C–O_{trans} 1.14 (2), C–O_{cis} 1.13(1) – 1.17(2), P1–C6 1.818(10), P1–C5
1.889(12), P1–C1 1.882(10), C1–O1 1.212(13) C5–O2 1.205(10).



280 260 240 220 200 180 160 140 120 100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 -260 -280 -30 Figure S4. ³¹P{¹H} NMR Spectrum (CDCl₃, 303 K, 161.72 MHz) for compound **2a**.



Figure S5. ³¹P NMR Spectrum (CDCl₃, 303 K, 161.72 MHz) for compound 2a.



Figure S6. ¹³C{¹H} NMR Spectrum (CDCl₃, 303 K, 100.46 MHz) for compound **2a**.



Figure S7. ¹H NMR Spectrum (C₇D₈, 238 K, 399.49 MHz) for compound **2a**.

30		
20		
10		
0		
- 10		
- 20		ha ar a
- 30		
- 40		MA A A
- 50		
- 60		
- 70		
- 80	M	
13 12 11 10 9	8 7 6 5 f1 (ppm)	4 3 2 1 0 -1

Figure S8. Stacked Variable Temperature ¹H NMR Spectra (C_7D_{8} , 303 K – 193 K, 399.49 MHz) for compound 2a.



280 260 240 220 200 180 160 140 120 100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 -260 -280 -3 f1 (ppm)





Figure S10. ³¹P NMR Spectrum (C₆D₆, 303 K, 161.72 MHz) for compound **2b**.



Figure S11. ¹H NMR Spectrum (C₆D₆, 303 K, 399.49 MHz) for compound 2b.





Figure S12. ¹³C{¹H} NMR Spectrum (C₆D₆, 303 K, 100.46 MHz) for compound **2b**.



Figure S13. ¹*H*-¹³*C HSQC trace* (*C*₆*D*₆*,* 303 *K,* 399.49*,* 100.46 *MHz*) for Compound **2b***.*



Figure S14. ¹H-¹³C HMBC trace (C₆D₆, 303 K, 399.49, 100.46 MHz) for Compound 2b.



Figure S15. ${}^{31}P{}^{1}H{}$ NMR Spectrum (C₆D₆, 303 K, 161.72 MHz) for compound **2c**.

280 260 240 220 200 180 160 140 120 100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 -260 -280 -31 f1 (ppm)



Figure S16. ³¹P NMR Spectrum (C₆D₆, 303 K, 161.72 MHz) for compound **2c**.



Figure S17. ¹H NMR Spectrum (CD₃Cl, 303 K, 399.49 MHz) for compound 2c.



250 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 f1 (ppm)

Figure S18. ¹³C{¹H} NMR Spectrum (C₆D₆, 303 K, 100.46 MHz) for compound 2c.



Figure S19. ³¹P{¹H} NMR Spectrum (CD₂Cl₂, 303 K, 161.72 MHz) for compound **2d**.



Figure S20. ³¹*P* NMR Spectrum (CD₂Cl₂, 303 K, 161.72 MHz) for compound **2d**.



Figure S21. ¹H NMR Spectrum (CD₂Cl₂, 303 K, 399.49 MHz) for compound 2d.



250 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 fl (ppm)

Figure S22. ¹³C{¹H} NMR Spectrum (CD₂Cl₂, 303 K, 100.46 MHz) for compound 2d.



Figure S23. ¹H-¹³C HSQC trace (CD₂Cl₂, 303 K, 399.49, 100.46 MHz) for Compound 2d.



Figure S24. ³¹*P*{¹*H*} *NMR Spectrum (C*₆*D*₆*, 303 K, 161.72 MHz) for compound 2e.*



280 260 240 220 200 180 160 140 120 100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 -260 -280 -3 f1 (ppm)

Figure S25. ³¹*P* NMR Spectrum (C₆D₆, 303 K, 161.72 MHz) for compound **2e**.



250 210 200 190 180 170 160 150 140 130 120 110 100 f1 (ppm) 240 230 20 220 90 80 , 70 60 . 50 40 30 10 ò -10 -20

Figure S27. ¹³*C*{¹*H*} *NMR Spectrum (C*₆*D*₆*, 303 K, 100.46 MHz) for compound 2e.*



Figure S28. ¹H-¹³C HSQC trace (C₆D₆, 303 K, 399.49, 100.46 MHz) for Compound 2e.



Figure S29. ¹*H*-¹³*C HMBC trace* (*C*₆*D*₆*,* 303 *K,* 399.49*,* 100.46 *MHz*) for Compound **2e**.



Figure S30. ³¹*P*{¹*H*} *NMR Spectrum (C*₆*D*₆*, 303 K, 161.72 MHz) for compound* **3***a.*



Figure S31. ³¹P NMR Spectrum (C₆D₆, 303 K, 161.72 MHz) for compound **3a**.



Figure S32. ¹H NMR Spectrum ($C_6D_{6\nu}$, 303 K, 399.49 MHz) for compound **3a**.





Figure S33. ${}^{13}C{}^{1H}$ NMR Spectrum (C₆D₆, 303 K, 100.46 MHz) for compound **3a**.



Figure S35. ¹H-¹³C HMBC trace (C₆D₆, 303 K, 399.49, 100.46 MHz) for Compound **3a**.



280 260 240 220 200 180 160 140 120 100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 -260 -280 -3 f1 (ppm)

Figure S36. ³¹*P*{¹*H*} *NMR Spectrum (C*₆*D*₆*, 303 K, 161.72 MHz) for compound* **3b***.*

Figure S37. ³¹*P* NMR Spectrum (*C*₆*D*₆, 303 K, 161.72 MHz) for compound **3b**.

Figure S38. ¹H NMR Spectrum (C₆D₆, 303 K, 399.49 MHz) for compound **3b**.

Figure S39. ¹³*C*{¹*H*} *NMR Spectrum (C*₆*D*₆*, 303 K, 100.46 MHz) for compound* **3b***.*

Figure S41. ¹H-¹³C HMBC trace (C₆D₆, 303 K, 399.49, 100.46 MHz) for Compound **3b**.

Figure S42. ³¹*P*{¹*H*} *NMR Spectrum (CDCl₃, 303 K, 161.72 MHz) for compound 3c.*

Figure S43. ³¹P NMR Spectrum (CDCl₃, 303 K, 161.72 MHz) for compound **3c**.

Figure S44. ¹H NMR Spectrum (CDCl₃, 303 K, 399.49 MHz) for compound **3c**.

Figure S46. ¹*H*-¹³*C HSQC trace* (*CDCl*₃, 303 *K*, 399.49, 100.46 *MHz*) for Compound *3c*.

280 260 240 220 200 180 160 140 120 100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 -260 -280 -31 f1 (ppm)

Figure S47. ³¹*P*{¹*H*} *NMR Spectrum (CDCl*₃*,* 303 *K,* 161.72 *MHz) for compound* **3d***.*

Figure S49. ¹H NMR Spectrum (CDCl₃, 303 K, 399.49 MHz) for compound 3d. * corresponds to H Grease.

Figure S50. ¹³*C*{¹*H*} *NMR Spectrum (CDCl*₃*, 303 K, 100.46 MHz) for compound 3d.*

Figure S51. ³¹P{¹H} NMR Spectrum (CD₂Cl₂, 303 K, 161.72 MHz, D1 = 30 s) for compound 4.

Figure S52. ³¹P NMR Spectrum (CD₂Cl₂, 303 K, 161.72 MHz, D1 = 30 s) for compound 4.

Figure S53. ¹H NMR Spectrum (CD₂Cl₂, 303 K, 399.49 MHz) for compound **4**.

Figure S55. ¹H-¹³C HSQC trace (CD₂Cl₂, 303 K, 399.49, 100.46 MHz) for Compound 4.

Figure S56. ¹⁹⁵Pt{¹H} NMR Spectrum (CD₂Cl₂, 303 K, 85.49 MHz) for Compound 4.

280 260 240 220 200 180 160 140 120 100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 -260 -280 -3 f1 (ppm)

Figure S57. ³¹*P*{¹*H*} *NMR Spectrum (C*₆*D*₆, 303 *K*, 161.72 *MHz) for compound 5a*.

Figure S58. ³¹P NMR Spectrum (C₆D₆, 303 K, 161.72 MHz) for compound 5a.

Figure S59. ¹*H NMR Spectrum (C*₆*D*₆*, 303 K, 399.49 MHz) for compound 5a*.

Figure S60. ¹³C{¹H} NMR Spectrum (C₆D₆, 303 K, 100.46 MHz) for compound **5a**.

Figure S61. ¹H-¹³C HSQC trace (C₆D₆, 303 K, 399.49, 100.46 MHz) for Compound 5a.

-20

Figure S62. ¹H-¹³C HMBC trace (C₆D₆, 303 K, 399.49, 100.46 MHz) for Compound 5a.

280 260 240 220 200 180 160 140 120 100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 -260 -280 -31 f1 (ppm)

Figure S63. ${}^{31}P{}^{1}H$ NMR Spectrum (C₆D₆, 303 K, 161.72 MHz) for compound **5b**.

Figure S64. ³¹P NMR Spectrum (C₆D₆, 303 K, 161.72 MHz) for compound **5b**.

Figure S65. ¹H NMR Spectrum (C₆D₆, 303 K, 399.49 MHz) for compound **5b**. * corresponds to H Grease, which was later traced back to impurities in the NMR solvent.

190 180 170 160 150 140 130 120 110 f1 (ppm) 250 240 230 -10 -20

Figure S66. ¹³C{¹H} NMR Spectrum (C₆D₆, 303 K, 100.46 MHz) for compound 5b.

Figure S67. ¹H-¹³C HSQC trace (C₆D₆, 303 K, 399.49, 100.46 MHz) for Compound 5b.

Figure S68. ¹H-¹³C HMBC trace (C₆D₆, 303 K, 399.49, 100.46 MHz) for Compound 5b.

Figure S69. ${}^{31}P{}^{1}H$ NMR Spectrum (C₆D₆, 303 K, 161.72 MHz) for compound Sc.

Figure S70. ³¹P NMR Spectrum (C₆D₆, 303 K, 161.72 MHz) for compound 5c.

Figure S71. ¹*H* NMR Spectrum (*C*₆*D*₆, 303 K, 399.49 MHz) for compound *5c*.

Figure S72. ¹³C{¹H} NMR Spectrum (C₆D₆, 303 K, 100.46 MHz) for compound **5c**.

90 80 70 60 50 40 30 20 10 0 -10 -20

170 160 150 140 130 120 110 100 f1 (ppm)

250

240 230

220

210 200

190 180

280 260 240 220 200 180 160 140 120 100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 -260 -280 -3 f1 (ppm)

Figure S74. ³¹*P* NMR Spectrum (C₆D₆, 303 K, 161.72 MHz) for compound *5d*.

Figure S75. ¹*H* NMR Spectrum (*C*₆*D*₆, 303 K, 399.49 MHz) for compound *5d*.

180 170 160 150 140 130 120 110 100 f1 (ppm) -10 -20 . 240 . 70

Figure S76. ¹³*C*{¹*H*} *NMR Spectrum (C*₆*D*₆*, 303 K, 100.46 MHz) for compound 5d*.

Figure S77. ¹*H*-¹³*C HSQC trace* (*C*₆*D*₆*, 303 K, 399.49, 100.46 MHz*) *for Compound 5d.*

Figure S78. ¹*H*-¹³*C HMBC trace* (*C*₆*D*₆, 303 *K*, 399.49, 100.46 *MHz*) for Compound *5d*.

Figure S79. ³¹P{¹H} NMR Spectrum (C_6D_6 , 303 K, 161.72 MHz) for compound **6**.

Figure S80. ³¹P NMR Spectrum (C₆D₆, 303 K, 161.72 MHz) for compound **6**.

Figure S81. ¹*H* NMR Spectrum (*C*₆*D*₆, 303 K, 399.49 MHz) for compound **6**.

250 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 f1 (ppm)

-20

Figure S84. ¹H-¹³C HSQC trace (C₆D₆, 303 K, 399.49, 100.46 MHz) for Compound **6**, W(CO)₆ present.

Figure S85. ¹*H*-¹³*C HSQC trace* (*C*₆*D*₆, 303 K, 399.49, 100.46 MHz) for Compound **6**, *W*(*CO*)₆ *removed*.

Figure S86. ¹*H*-¹³*C HMBC* trace (C₆D₆, 303 K, 399.49, 100.46 MHz) for Compound 6, W(CO)₆ present.

Figure S87. ¹*H*-¹³*C HMBC trace* (*C*₆*D*₆*, 303 K, 399.49, 100.46 MHz*) *for Compound 6, W*(*CO*)₆ *removed.*

Single Mass Analysis

Tolerance = 70.0 PPM / DBE: min = -1.5, max = 50.0 Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions 12 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) Elements Used: C: 0-10 H: 0-1000 O: 0-2 P: 0-1 KGP-160 KYLE10885A 100 (7.174) Cm (94:106) 100-144.0337 Magnet EI+ 420 100-% 145.0342 0 - m/z 144.00 144.20 144.40 144.60 144.80 145.00 Minimum: -1.5 50.0 Maximum: 5.0 70.0 Mass Calc. Mass mDa PPM DBE i-FIT Formula 144.0340 144.0337

2773013.8 C6 H9 O2

Ρ

3.0

-2.1

Elemental Composition Report

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0 Selected filters: None

-0.3

Monoisotopic Mass, Odd and Even Electron Ions 7 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) Elements Used: C: 0-9 H: 0-1000 O: 0-2 P: 0-1 KGP-199 KYLE10883 24 (1.723) Magnet EI+ 186.0818 5.93 100-% 0 - m/z 185.900 186.050 185.950 186.000 186.100 186.150 186.200 186.250 Minimum: -1.5 50.0 Maximum: 5.0 50.0 Mass Calc. Mass mDa PPM DBE i-FIT Formula 186.0818 186.0810 5546025.5 C9 H15 O2 P 0.8 4.3 3.0

Figure S89. HRMS-EI for Compound 2b.

Single Mass Analysis Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0 Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions 7 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) Elements Used: C: 0-9 H: 0-1000 O: 0-2 P: 0-1 KGP-181 KYLE10884 105 (7.540) Cm (101:105) Magnet EI+ 186.0795 43 100-% ¬ m/z 0-186.250 186.050 186.100 186,150 186,200 185.900 185.950 186.000 Minimum: -1.5 50.0 5.0 50.0 Maximum: DBE Mass Calc. Mass mDa PPM i-FIT Formula 186.0810 5546029.5 C9 H15 O2 P 186.0795 -1.5 -8.1 3.0

Figure S90. HRMS-EI for Compound 2c.

Elemental Composition Report

Single Mass Analysis Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0 Selected filters: None

Monoisotopic Mass, Odd and Even Electron lons 9 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) Elements Used: C: 0-12 H: 0-1000 O: 0-2 P: 0-1 KGP-198 KYLE10368 16 (1.253) Magnet EI+ 344 206.0486 100-% 207.0569 205.0583 207.25 0 206.50 206.75 207.00 205.75 206.00 206 25 205.25 205.50 205.00 -1.5 Minimum: 50.0 5.0 Maximum: i-FIT Formula mDa PPM DBE Calc. Mass Mass 2773016.5 C11 H11 O2 P -5.3 7.0 206.0497 -1.1 206.0486

Figure S91. HRMS-EI for Compound 2d.

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0 Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions 7 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) Elements Used: C: 0-14 H: 0-1000 O: 0-2 P: 0-1 Vs013 KYLE10886 37 (2.657) Magnet EI+ 248.0960 68.7 100 % 241.1449 249.0995 ---- m/z 0-245.00 241.00 242.00 243.00 244.00 246.00 247.00 248.00 249.00 Minimum: -1.5 50.0 5.0 10.0 Maximum: Mass Calc. Mass mDa PPM DBE i-FIT Formula 248.0966 7.0 2773013.5 C14 H17 O2 Ρ 248.0960 -0.6 -2.4

Figure S92. HRMS-EI for Compound 2e.

Elemental Composition Report

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0 Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions 12 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) Elements Used: C: 0-10 H: 0-1000 O: 0-2 P: 0-1 KGP-217 KYLE10890A 35 (2.511) Cm (35:38) 100- 158.0495 Magnet EI+ 185 100-% 159.0526 0 m/z 158.00 158.20 158.40 158.60 158.80 159.00 159.20 Minimum: -1.5 50.0 Maximum: 5.0 50.0 Mass Calc. Mass mDa PPM DBE i-FTT Formula 158.0495 158.0497 -0.2 -1.3 3.0 2773014.3 C7 H11 O2 P

Single Mass Analysis

Tolerance = 10000.0 PPM / DBE: min = -1.5, max = 50.0 Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions 7 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) Elements Used: C: 0-10 H: 0-1000 O: 0-2 P: 0-1 KGP-360 KYLE_11052 12 (0.862) Magnet EI+ 200.0980 15.2 100-% 0 ----- m/z 199.900 199.950 200.000 200.050 200.100 200.150 200.200 200.250 Minimum: -1.5 Maximum: 5.0 10000.0 50.0 mDa Mass Calc. Mass PPM DBE i-FIT Formula 200.0966 200.0980 7.0 3.0 5310.1 C10 H17 O2 P 1.4

Figure S94. HRMS-EI for Compound 3b.

Elemental Composition Report

Single Mass Analysis

Tolerance = 10000.0 PPM / DBE: min = -1.5, max = 50.0 Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions 7 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) Elements Used: C: 0-10 H: 0-1000 O: 0-2 P: 0-1 KGP-359 KYLE_11051A 17 (1.221) Cm (2:41) Magnet EI+ 200.0863 100-% ----- m/z 0 199.900 199.950 200.000 200.050 200.100 200.150 200.200 200.250 Minimum: -1.5 50.0 10000.0 5.0 Maximum: DBE Mass Calc. Mass mDa PPM i-FIT Formula 200.0863 200.0966 -10.3 -51.5 3.0 353.6 C10 H17 O2 P

Figure S95. HRMS-EI for Compound 3c (very volatile, gave only one scan out of 3 samples, leading to higher error).

S49

Page 1

Single Ma Tolerance Selected f	ass Analysi = 10.0 PPN filters: None	i s M / DBE:	min = -1.	5, max =	50.0				4 8
Monoisotopi 7 formula(e) Elements U C: 0-12 H:	ic Mass, Odd a evaluated wit sed: 0-1000 O: (and Even Ele h 1 results w 0-2 P: 0-1	ctron lons ithin limits (a	all results (u	up to 1000) for (each mass)			
KYLE_11050 3	39 (2.800) Cm (33	3:39)							Magnet EI+
100				220.065	50				16
-									
-				5 m					· * * .
				-					
0/0				1					
-									
-									
-									
0									
219.850	219,900	219,950	220.000	220,050	220,100	220,150	220,200	220,250	m/z
Minimum:		E O	10 0	-1.5					
Maximum;		5.0	10.0	50.0					
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula			
220.0650	220.0653	-0.3	-1.4	7.0	5546026.0	C12 H13	02 P		

Figure S96. HRMS-EI for Compound 3d.

Figure S97. LRMS-EI Theoretical Isotope Distribution for Compound 6.

Figure S98. LRMS-EI for Compound 6.