## **Supporting Information**

for

## Ring-opening homo- and co-polymerization of chiral seven-membered lactones mediated by achiral yttrium catalysts: Insights into the catalyst stereocontrol by mass spectrometry

Ali Dhaini,<sup>a</sup> Jérôme Ollivier,<sup>a</sup> Nicolas Le Yondre,<sup>b</sup> Ali Alaaeddine,<sup>c</sup> Sophie M. Guillaume (ORCID: 0000-0003-2917-8657),<sup>a,\*</sup> and Jean-François Carpentier (ORCID: 0000-0002-9160-7662)<sup>a,\*</sup>

<sup>a</sup> Univ. Rennes, CNRS, Institut des Sciences Chimiques de Rennes, UMR 6226, F-35042 Rennes, France.

<sup>b</sup> Univ. Rennes, Centre Régional de Mesures Physiques de l'Ouest, UAR 2025 ScanMAT, F-35042 Rennes, France.

<sup>c</sup> Univ. Libanaise, Campus Universitaire Rafic Hariri Hadath, Faculté des Sciences, Laboratoire de Chimie Médicinale et des Produits Naturels, Beirut, Lebanon.

\* Corresponding authors: E-mail: <u>sophie.guillaume@univ-rennes.fr</u>, jean <u>francois.carpentier@univ-rennes.fr</u>

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Figure S1. <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>, 25 °C) of *rac*-CL<sup>Me</sup>.



Figure S2. JMOD <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (125 MHz, CDCl<sub>3</sub>, 25 °C) of *rac*-CL<sup>Me</sup>.







• First fraction: the first eluted enantiomer with ee > 99 %



RT [min]	Area	Area%
5.71	10723	99.65
6.63	38	0.35
Sum	10761	100.00



• Second fraction: The second eluted enantiomer with ee > 99 %



**Figure S3.** Chiral HPLC traces for *racemic*-CL<sup>Me</sup>, (*S*)-CL<sup>Me</sup> and (*R*)-CL<sup>Me</sup> (see the Experimental section for details)



RT [min]	Area	Area%
5.70	521	50.12
6.83	518	49.88
Sum	1039	100.00



(R)-CL<sup>nBu</sup>

• First fraction: The first eluted enantiomer with ee > 99.5%



RT [min]	Area	Area%
5.69	767	100.00
Sum	767	100.00



• Second fraction: The second eluted enantiomer with ee > 99.5 %



RT [min]	Area	Area%
5.53	2	0.21
6.80	760	99.79
Sum	762	100.00

**Figure S4.** Chiral HPLC traces for *racemic*- $CL^{nBu}$ , (*R*)- $CL^{nBu}$  and (*S*)- $CL^{nBu}$  (see the Experimental section for details)



**Figure S5.** <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>, 25 °C) of a PCL<sup>Me</sup> homopolymer prepared from the ROP of *rac*-CL<sup>Me</sup> (30 equiv) mediated by the **1a**/BnOH (1:1) catalyst system (Table S1, entry 1-105). \* stands for resonances of residual solvent and/or catalyst.



**Figure S6.** JMOD <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (125 MHz, CDCl<sub>3</sub>, 25 °C) of a PCL<sup>Me</sup> homopolymer prepared from the ROP of *rac*-CL<sup>Me</sup> (30 equiv) by the **1a**/BnOH (1:1) catalyst system (Table S1, entry 1-105). \* stands for resonances of residual solvent and/or catalyst.



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**Figure S8.** JMOD <sup>13</sup>C{<sup>1</sup>H} spectrum (500 MHz, CDCl<sub>3</sub>, 25 °C) of a PCL<sup>*n*Bu</sup> homopolymer prepared from the ROP of *rac*-CL<sup>*n*Bu</sup> (30 equiv) mediated by the **1a**/BnOH (1:1) catalyst system (Table S1, entry 1-107). \* stands for resonances of residual solvent and/or catalyst.

	Entry	$\begin{bmatrix} CL^{R} \end{bmatrix}_{0}{}^{b}$ (eq vs. Y)	Catalyst	Time (min)	Conv. [CL <sup>R</sup> ] <sub>0</sub> (%) <sup>c</sup>	$M_{ m n,theo}^{d}$ (g.mol <sup>-1</sup> )	$M_{n,NMR}^{e}$ (g.mol <sup>-1</sup> )	$M_{n,SEC}^{f}$ (g.mol <sup>-1</sup> )	${\mathcal{D}_{\mathrm{M}}}^{f}$	<i>T</i> g <sup><i>g</i></sup> (°C)
	1 /1-105	30	1a/BnOH	180	100	4000	1500	2700	1.38	-45.9
R =	2 / 1-117	30	Zn(BDI)/BnOH	120	100	4000	1800	2650	1.20	-52.6
Me	3 /1-163	60	KOtBu	240	100	7800	$\mathbf{n}\mathbf{d}^i$	$\mathrm{nd}^h$	$\mathrm{nd}^h$	$\mathrm{nd}^h$
	4 / 1-193	60*	Zn(BDI)/BnOH	240	100	7800	4300	$\mathrm{nd}^h$	$\mathrm{nd}^h$	-47.7
	5 / 1-107	30	1a/BnOH	180	100	5200	3700	4700	1.15	-55.4
R = <i>n</i> Bu	6 / 1-114	30	Zn(BDI)/BnOH	120	100	5200	5500	5350	1.17	-55.4
	7 /1-155	60	KO <i>t</i> Bu	300	100	10300	i	$\mathrm{nd}^h$	$\mathrm{nd}^h$	-54.8
	8 /1-164	60*	Zn(BDI)/BnOH	90	100	10300	7600	$\mathrm{nd}^h$	$\mathrm{nd}^h$	-56.0

**Table S1.** ROP of *rac*-CL<sup>*n*Bu</sup> mediated by the **1a**/BnOH, {BDI<sup>DIPP</sup>}Zn(NTMS<sub>2</sub>)/BnOH and KO*t*Bu catalyst systems.<sup>*a*</sup>

<sup>*a*</sup> Reactions performed with  $[CL^{Me}]_0 = 1.0 \text{ M}$  or  $[CL^{nBu}]_0 = 1.0 \text{ M}$  in toluene with  $[\mathbf{1a}]/[BnOH]_0 = 1:1$ . <sup>*b*</sup> Monomer loading. <sup>*c*</sup> Conversion of  $CL^{Me}$  as determined by <sup>1</sup>H NMR analysis of the crude reaction mixture. <sup>*d*</sup> Calculated according to  $M_{n,\text{theo}} = [CL^{Me}]_0/[\mathbf{1a}] \times \text{conv.}(CL^{Me}) \times M(CL^{Me}) + M(BnOH)$ , with  $M(CL^{Me}) = 128 \text{ g.mol}^{-1}$  and  $M(BnOH) = 108 \text{ g.mol}^{-1}$ . <sup>*e*</sup> Determined by <sup>1</sup>H NMR analysis of the isolated polymer, from the resonances of the terminal OBn group (refer to Experimental section). <sup>*f*</sup> Number-average molar mass (uncorrected) and dispersity  $(M_w/M_n)$  determined by SEC analysis in THF at 30 °C vs. polystyrene standards; <sup>*g*</sup> Glass transition temperature as determined by DSC analysis. <sup>*h*</sup> Not determined. <sup>*i*</sup> No chain-ends observed due to formation of cyclic polymer. \* starting from an enantiopure monomer.



**Figure S9.** <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>, 25 °C) of a P(CL<sup>Me</sup>-*co*-CL<sup>*n*Bu</sup>) copolymer prepared from the ROCOP of a 1:1 mixture of (*S*)-CL<sup>Me</sup> and (*R*)-CL<sup>*n*Bu</sup> mediated by the **1b**/BnOH (1:1) catalyst system (Table 1, entry 6). \* stands for resonances of residual solvent and/or catalyst.



**Figure S10.** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (125 MHz, CDCl<sub>3</sub>, 25 °C) of a P(CL<sup>Me</sup>-*co*-CL<sup>*n*Bu</sub>) copolymer prepared from the ROCOP of a 1:1 mixture of (*S*)-CL<sup>Me</sup> and (*R*)-CL<sup>*n*Bu</sup> (1:1) mediated by the **1b**/BnOH (1:1) catalyst system (Table 1, entry 6). \* stands for resonances of residual solvent and/or catalyst.</sup>



**Figure S11.** From bottom to top: <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, 25 °C) spectra of the starting comonomers; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, 25 °C) spectra for the monitoring of the ROCOP of a 1:1 mixture of (*R*)-CL<sup>*n*Bu</sup> and (*S*)-CL<sup>Me</sup> mediated by the **1b**/BnOH (1:1) catalyst system at 20 °C. Reaction time = 1 h: conv(CL<sup>*n*Bu</sup> / CL<sup>Me</sup>) = 58 and 62% respectively; ratio (CL<sup>*n*Bu</sup> / CL<sup>Me</sup>) = 1.14. Reaction time = 2 h: conv(CL<sup>*n*Bu</sup> / CL<sup>Me</sup>) = 71 and 72%, respectively; ratio (CL<sup>*n*Bu</sup> / CL<sup>Me</sup>) = 1.05. Reaction time = 4 h: conv(CL<sup>*n*Bu</sup> / CL<sup>Me</sup>) = 90 and 99%, respectively; ratio (CL<sup>*n*Bu</sup> / CL<sup>Me</sup>) = 10. \* stands for resonances of the copolymer.



**Figure S12.** Fineman –Ross plot for the determination of monomer reactivity ratio of  $CL^{Me}$  and  $CL^{nBu}$  in the copolymerization by the **1a**/BnOH (1:1) system in toluene at 20 °C.



**Figure S13.** MALDI-ToF mass spectrum (DCTB matrix, ionized by Na<sup>+</sup>) of a P(CL<sup>Me</sup>-*co*-CL<sup>*n*Bu</sub>) copolymer prepared by ROCOP of (*S*)-CL<sup>Me</sup> and (*R*)-CL<sup>*n*Bu</sup> (1:1) with the **1b**/BnOH catalyst system (Table 1, entry 6).</sup>



**Figure S14.** MALDI-ToF mass spectrum (DCTB matrix, ionized by Na<sup>+</sup>) of a P(CL<sup>Me</sup>-*co*-CL<sup>*n*Bu</sub>) copolymer prepared by ROCOP of (*S*)-CL<sup>Me</sup> and (*R*)-CL<sup>*n*Bu</sup> (1:1) with the **1a**/BnOH catalyst system (Table 1, entry 2).</sup>

🖪, Polymers				×
Polymers Working Files	(In a specific folder, on	ly csv files inside to b	e processed please	ch a folder )
Starting materials	(Formula w/o e	endings with spaces I	like C2 H4 O please	)
monomer A C10 H	18 02	Турі	ically RO-(monomer	s)·R'
v monomer B C7 H12	2 0 2	Initiator (I1) RO	C7 H7 0	
monomer C		Terminal group (T1	I) R'  H	
Length and families       Ax8y/2z w x+y+z <<50	Init 12 13 14 14 15 ✓ Maldi ✓ Na NEG ↓ withdr	T T T T T T T T T T T T T T T T T T T	corresponding t 2 3 4 5 -2Na Minimal C+) Maximal	Range 50 5000
▼ z=1  ⊂ z<=3				
mypolymers.IDNUM.YY.	MM.DD.01.csv			
z <= 3 only with +zH or+	zNa or -zH no mixture		Export calculated	table (CSV)
DataResolutionPPM30	Max. Iso. 6 Threshold 0.1	Compen %	isation 10.0 Si	% mplify

Figure S15. "Polymers" software for automatic generation of theoretical m/z peaks and assignment to experimental m/z mass peaks.



**Figure S16.** ESI-mass spectrum (solvent  $CH_2Cl_2$ ) of a  $P(CL^{Me}-co-CL^{nBu})$  copolymer prepared by ROCOP of a 1:1 mixture of (*S*)-CL<sup>Me</sup> and (*R*)-CL<sup>nBu</sup> with the **1a**/BnOH catalyst system (Table 1, entry 3).



**Figure S17.** Details of the high resolution ESI mass spectra of a P(CL<sup>*n*Bu</sup>-*co*-CL<sup>Me</sup>) copolymer prepared by ROCOP of a 1:1 mixture of (*R*)-CL<sup>*n*Bu</sup> and (*S*)-CL<sup>Me</sup> with the **1a**/BnOH catalyst system (Table 1, entry 3), from top to bottom: (a) experimental spectrum (solvent: CH<sub>2</sub>Cl<sub>2</sub>) for m/z = 1000-1100, (b) zoomed region for m/z = 998-1008, showing resolved peaks for cyclic P[(CL<sup>*n*Bu</sup>)<sub>5</sub>-*co*-(CL<sup>Me</sup>)] ( $m/z_{exp}$ (all <sup>12</sup>C) = 1001.7265) and cyclic P[(CL<sup>*n*Bu</sup>)<sub>2</sub>-*co*-(CL<sup>Me</sup>)<sub>5</sub>] ( $m/z_{exp}$  (all <sup>12</sup>C) = 1003.6694); (c) calculated spectrum (isotopic pattern) for cyclic P[(CL<sup>*n*Bu</sup>)<sub>5</sub>-*co*-(CL<sup>Me</sup>)<sub>5</sub>] ( $m/z_{calcd}$  (all <sup>12</sup>C) = 1001.7263); (d) calculated spectrum (isotopic pattern) for cyclic P[(CL<sup>*n*Bu</sup>)<sub>2</sub>-*co*-(CL<sup>Me</sup>)<sub>5</sub>] ( $m/z_{calcd}$  (all <sup>12</sup>C) = 1003.6692).



**Figure S18.** Details of the high resolution ESI mass spectra of a P(CL<sup>*n*Bu</sup>-*co*-CL<sup>Me</sup>) copolymer prepared by ROCOP of a 1:1 mixture of (*R*)-CL<sup>*n*Bu</sup> and (*S*)-CL<sup>Me</sup> with the **1a**/BnOH catalyst system (Table 1, entry 3), from top to bottom: (a) experimental spectrum (solvent: CH<sub>2</sub>Cl<sub>2</sub>) for m/z = 1000-1100, (b) zoomed region for m/z = 1021-1031, showing resolved peaks for linear P[(CL<sup>*n*Bu</sup>)<sub>3</sub>-*co*-(CL<sup>Me</sup>)<sub>3</sub>]-C<sub>7</sub>H<sub>8</sub>O  $- 2H (m/z_{exp} (all {}^{12}C) = 1023.6748)$  and linear P[(CL<sup>*n*Bu</sup>)<sub>3</sub>-*co*-(CL<sup>Me</sup>)<sub>3</sub>]-C<sub>7</sub>H<sub>8</sub>O ( $m/z_{exp} (all {}^{12}C) =$ 1025.6899); (c) calculated spectrum (isotopic pattern) for cyclic linear P[(CL<sup>*n*Bu</sup>)<sub>3</sub>-*co*-(CL<sup>Me</sup>)<sub>3</sub>]-C<sub>7</sub>H<sub>8</sub>O – 2H ( $m/z_{ealed} (all {}^{12}C) = 1023.6743$ ); (d) calculated spectrum (isotopic pattern) for linear P[(CL<sup>*n*Bu</sup>)<sub>3</sub>-*co*-(CL<sup>Me</sup>)<sub>3</sub>]-C<sub>7</sub>H<sub>8</sub>O ( $m/z_{ealed} (all {}^{12}C) = 1023.6743$ ); (d) calculated spectrum (isotopic pattern) for linear P[(CL<sup>*n*Bu</sup>)<sub>3</sub>-*co*-(CL<sup>Me</sup>)<sub>3</sub>]-C<sub>7</sub>H<sub>8</sub>O ( $m/z_{ealed} (all {}^{12}C) = 1025.6900$ ).



**Figure S19.** Details of the high resolution ESI mass spectra of a P(CL<sup>*n*Bu</sup>-*co*-CL<sup>Me</sup>) copolymer prepared by ROCOP of a 1:1 mixture of (*R*)-CL<sup>*n*Bu</sup> and (*S*)-CL<sup>Me</sup> with the **1a**/BnOH catalyst system (Table 1, entry 3), from top to bottom: (a) experimental spectrum (solvent: CH<sub>2</sub>Cl<sub>2</sub>) for m/z = 1000-1100, (b) zoomed region for m/z = 1041-1051, showing resolved peaks for cyclic P[(CL<sup>*n*Bu</sup>)<sub>6</sub>-*co*-(CL<sup>Me</sup>)<sub>0</sub>] ( $m/z_{exp}$ (all <sup>12</sup>C) = 1043.7739) and cyclic P[(CL<sup>*n*Bu</sup>)<sub>3</sub>-*co*-(CL<sup>Me</sup>)<sub>4</sub>] ( $m/z_{exp}$  (all <sup>12</sup>C) = 1045.7162); (c) calculated spectrum (isotopic pattern) for cyclic P[(CL<sup>*n*Bu</sup>)<sub>6</sub>-*co*-(CL<sup>Me</sup>)<sub>4</sub>] ( $m/z_{calcd}$  (all <sup>12</sup>C) = 1043.7733); (d) calculated spectrum (isotopic pattern) for cyclic P[(CL<sup>*n*Bu</sup>)<sub>3</sub>-*co*-(CL<sup>Me</sup>)<sub>4</sub>] ( $m/z_{calcd}$  (all <sup>12</sup>C) = 1045.7162).



**Figure S20.** Details of the high resolution ESI mass spectra of a P(CL<sup>*n*Bu</sup>-*co*-CL<sup>Me</sup>) copolymer prepared by ROCOP of a 1:1 mixture of (*R*)-CL<sup>*n*Bu</sup> and (*S*)-CL<sup>Me</sup> with the **1a**/BnOH catalyst system (Table 1, entry 3), from top to bottom: (a) experimental spectrum (solvent: CH<sub>2</sub>Cl<sub>2</sub>) for m/z = 1000-1100, (b) zoomed region for m/z = 1063-1073, showing resolved peaks for linear P[(CL<sup>*n*Bu</sup>)<sub>4</sub>-*co*-(CL<sup>Me</sup>)<sub>2</sub>]-C<sub>7</sub>H<sub>8</sub>O  $- 2H (m/z_{exp} (all {}^{12}C) = 1065.7215)$  and linear P[(CL<sup>*n*Bu</sup>)<sub>4</sub>-*co*-(CL<sup>Me</sup>)<sub>2</sub>]-C<sub>7</sub>H<sub>8</sub>O ( $m/z_{exp} (all {}^{12}C) =$ 1067.7373); (c) calculated spectrum (isotopic pattern) for cyclic linear P[(CL<sup>*n*Bu</sup>)<sub>4</sub>-*co*-(CL<sup>Me</sup>)<sub>2</sub>]-C<sub>7</sub>H<sub>8</sub>O – 2H ( $m/z_{calcd} (all {}^{12}C) = 1065.7213$ ); (d) calculated spectrum (isotopic pattern) for linear P[(CL<sup>*n*Bu</sup>)<sub>4</sub>-*co*-(CL<sup>Me</sup>)<sub>2</sub>]-C<sub>7</sub>H<sub>8</sub>O ( $m/z_{calcd} (all {}^{12}C) = 1067.7369$ ).



**Figure S21.** MS/MS fragmentation ESI mass spectrum of the ion m/z = 1622 of a P(CL<sup>Me</sup>-*co*-CL<sup>*n*Bu</sub>) **copolymer** prepared by ROCOP of a 1:1 mixture of (*S*)-CL<sup>Me</sup> and (*R*)-CL<sup>*n*Bu</sup> with the **1a**/BnOH catalyst system (Table 1, entry 3).</sup>

**Table S2.** Comparison of theoretical vs. experimental ESI-MS peaks for a P(CL<sup>nBu</sup>-*co*-CL<sup>Me</sup>) copolymer (Table 1, entry 3) for m/z values in the range 200–1800. A: stands for CL<sup>*n*Bu</sup> and *x* for the number of A units in the polymer chain, B: stands for CL<sup>Me</sup> and *y* for the number of B units in the polymer chain. All non-assigned peaks or beyond the range are excluded from that table.

619.4180         c_AB2         C2440028         Cyrro H         2         2         4         619.4187         1,06         619.40212         4.6328622.5         614.46881         0.63215.5         614.46881         0.632165.5         614.46881         0.632165.5         01731195         02393           664.4650         c_AB1         CDB4000000         CDPO         1         0         4         664.4655         0.77         465723.5         661.466784         7.02249419         3666           055.4266         CLB1500000         CDPO         1         0         4         0.05         0.05         665.43531         1.7722313         7.0224951         0.2224951         0.2224951         0.222         0.2224951         0.2223         0.222         0.2224951         0.2223         0.221         0.22174951         0.7479314         1.789         0.2235         0.72479314         0.79927322         2.159         7.749314         0.7692733         2.2664         0.33         0.2734513         7.7493144         0.7492514         1.67906         0.2335151         7.7493134         0.23055171         2.0644           7.952355         C_AM20         C4447020049         Cyrr0 H         1         5         8.759561         0.1490514         8.159569	m/z theoritical	Interpretation AxBy	Raw Formula	Population	×	y	x+y	m/z experimental HR-ESI T	Erreur (PPM) HR-ESI	Absolute Intensity ESI	m/z experimental MALDI-TOF ज	Erreur (PPM) MALDI	Absolute Intensity MALDI-TOF
14.188         LABB (JNBO)         CPHO (PA)         2         0         3         64.1897         1.46         647.206         64.1464815         1.2013119         2099           653.450         C.AS3         CAMBO         Callestory         Cric         1         3         4         655.4555         0.77         458732.5         665.457831         1.7722334         730           705.115         C.AMBO         Callestory         Cric         1         4         6.5         705.4555         0.664.477         705.11376         0.63133         705.45576         5280110         6.03           705.115         C.AS3         CALL         Callestory         Cric         1         4         7         705.4557         Callestory         707.3133         705.55561         2080733         705.55561         2080733         705.55561         2080733         705.55561         2080733         705.55561         2080733         705.55561         2080733         705.55561         2080733         705.555571         705.55557         705.55557         705.55557         705.55557         705.55557         705.55557         705.55557         705.55557         705.55557         705.555584         705.555584         705.55557         705.555557         705.55557 <td>619,4180</td> <td>c_A2B2</td> <td>C34H60O8Na</td> <td>Cyclic</td> <td>2</td> <td>2</td> <td>4</td> <td>619,4187</td> <td>1,06</td> <td>6306631,5</td> <td>619,4209122</td> <td>4,635268226</td> <td>2638</td>	619,4180	c_A2B2	C34H60O8Na	Cyclic	2	2	4	619,4187	1,06	6306631,5	619,4209122	4,635268226	2638
662,663         c.A33         C.YAB         <	641,4388	I_A3B0_C7H8O	C37H62O7Na	C7H7O_H	3	0	3	641,4397	1,45	485720,6	641,4464819	12,02131196	2099
685.428         I_AD3_CPR0C         C34402         CAM20	661,4650	c_A3B1	C37H66O8Na	Cyclic	3	1	4	661,4655	0,77	4867532,5	661,4697684	7,222499419	3666
T035119         c. A180         Control Control         Cycle         4         T054585         Cold         21556885         T05312306         0.899           T035485         c. A182         Cold	685,4286	I_A1B3_C7H8O	C38H62O9Na	C7H7O_H	1	3	4	685,4289	0,44	496851,2	685,4387311	14,77928334	750
TOD,548         c. A184         C38466010Na         Cyrk         1         4         5         TOD,5455         0.46         219333.3         TOD,5485526         5,28820001         628           727,5756         LAD2, Crillo         CHABCONNA         Cyrk         2         4         727,4756         LOS2         571.3         747,5051         623255         1747,5018         C. 237         727,5756         1747,5018         2,550         1158         1158         1768,5218         1158	703,5119	c_A4B0	C40H72O8Na	Cyclic	4	0	4	703,5117	0,34	2556988,5	703,5125391	0,850132706	3069
122,755         LAB2, CPR00         CH14800Nh         CPU/01         2         2         4         727,7518         0,75         692395,1         727,75019         0,7351202         1155           747,5018         CANB3         CANB3         CANB3         CANB3         747,999384         747,9993847         747,9993847         747,9993847         747,9993847         747,9993847         755,8667         755,86705         755,86705         755,86705         755,86705         755,86705         755,86705         755,86705         755,86705         755,985173         2664           833,5953         C, AB1         CANB1         CANB1         CANB1         CANB1         726,9856         0,13         393,9557,06         833,595860         2,035558842         3,0650033         933         332,5266         CANB1         CANB	705,4548	c_A1B4	C38H66O10Na	Cyclic	1	4	5	705,4545	0,46	2196333,3	705,4585526	5,289620201	628
747.5018         C, A183         CH1220109a         G, wile         2         3         5         747.5016         0.23         257351,3         747.493528         J.227806.141         1478           785.5258         LABL_CH20         C4447780109a         G, wile         3         2         5         785.5487         0, 523         574137         765.52916         811.5596         0,181         3956676         811.55966         2,3259517         2644           835.55957         L, ABL         CH4401019a         G, wile         4         1         5         835.5595         0,141         1460930.4         831,559568         3,24292515.3         2489           855.5595         L, ABL         CH4401019a         Cyclic         5         875,6585         0,44         46840101.6         875,6581         0,468101.6         873,65810         4,2137,2489         925           875,6565         L, ABL         CH4400119a         Cyclic         5         877,6642         0,46         2447610.5         875,58810         4,651201.6         25458410         4,2127,58         393,65126         0,463,8512         2,4683143         1,472           875,6652         L, ABL         CH600 CH4400119a         Cyclic         5         891,6526	727,4756	I_A2B2_C7H8O	C41H68O9Na	C7H7O_H	2	2	4	727,4761	0,75	693295,1	727,4750194	0,730751202	1155
7769.5225         I. ABI. C/HBO         C. ALVID (MID)         C. M. 2         7769.524137         7769.524134         2.1.99265591         1958           785.5487         C. ALVID (MID)         C. M. 1         5         785.5487         2.5567         2.33357172         2.2664           831.5557         C. AMI         CHTMBOUND         C/M. 4         1         5         831.5555         0.211         1.4605.014.8         3.355557         2.6481         3.35557         2.6481         3.35557         2.6481         3.35557         2.6481         3.35557         2.6481         2.3557863         3.35555         5.2.481         COMMON Optic V         2         3         5         855.55881         0.22         4.575.581301         4.213724803         5.3160565         9.24           837.6662         C.AM24         CHMMON Optic V         2         4         6         875.5851         0.46         2.2471.05         875.581801         4.21372480         9.9356532         1.481         CHMON Notic V         1         5         5         5         0.19         CFMAR24         9.937.001         1.412         1.55         917.001572         1.0213724         1.932444         1.25         1.61         1.61         1.65         1.65         9.937.011 <td>747,5018</td> <td>c_A2B3</td> <td>C41H72O10Na</td> <td>Cyclic</td> <td>2</td> <td>3</td> <td>5</td> <td>747,5016</td> <td>0,23</td> <td>2573951,3</td> <td>747,4993582</td> <td>3,227806141</td> <td>1478</td>	747,5018	c_A2B3	C41H72O10Na	Cyclic	2	3	5	747,5016	0,23	2573951,3	747,4993582	3,227806141	1478
788.5487         C, Al82         C, Al42         C, Al42         C, Al42         C, Al42         S         789.5487         0, 18         223708,3         789.548773         25604         235037           831.5957         L, ABD, CHW         CAFHEODMA         Cyrlk         4         1         5         831.5955         0,14         466930,4         831.59588         3,62295153         2489           835.5958         L, ABD, CHW         CAHBHOUNA         Cyrlk         5         875,6852         0,24         453724,1         873,6328051         5,511060355         924           875,5855         C, AL84         CHHWOUNA         Cyrlk         5         875,6851         0,46         24470,10         873,6328051         2,511060355         924           875,6555         C, AL84         CHHWOUNA         Cyrlk         4         2         5         897,6064         0,16         254404,1         897,600732         2,60535417         1472           939,6524         L, AL81         CHWOUNA         Cyrlk         4         2         6         936,6797         0,41         2172,53         938,67021         2,3827262         2,969344         2,0693344         2,0162         3,34         2,0172,33         9,31         2,004,	769,5225	I_A3B1_C7H8O	C44H74O9Na	C7H7O_H	3	1	4	769,5229	0,52	574137	769,5241934	2,199265591	1958
BitL595         L/ABB_C/H80         C/17B00PN         C/H7D_H         4         0         4         81,5957         0.21         145093A         83,5957         2.248           831,5957         C_ABB         C47H800DN         Cyrick         1         3         5         831,5955         0.21         145093A         83,59528         3,24282         3,555588         3,656765         3         933           837,6426         C_ABB         GSH900DNN         Cyrick         5         0         5         875,55588         0,22         45374,1623         875,55818         0,425744,13         4,2157248         925           837,6602         C,ABB         C51H90012NN         Cyrick         3         2         6         875,6551         0,34         579483,4         935,6532         2,06335173         1472           939,6572         C,ABB         C51H90012NN         Cyrick         4         1         6         935,6737         0,31         2045528,5         935,6532         2,0633514         0,003215502         2,399         2,399         2,395         1,466         34,625         0,44         46782,6         935,60372         2,395,67372         2,305,67372         2,385,67372         2,355,68384         2,016 <td< td=""><td>789,5487</td><td>c_A3B2</td><td>C44H78O10Na</td><td>Cyclic</td><td>3</td><td>2</td><td>5</td><td>789,5488</td><td>0,1</td><td>2297048,3</td><td>789,5467073</td><td>2,550451753</td><td>2560</td></td<>	789,5487	c_A3B2	C44H78O10Na	Cyclic	3	2	5	789,5488	0,1	2297048,3	789,5467073	2,550451753	2560
831,5957         c, A491         Cyrlk         4         1         5         831,5955         0.21         1460930,4         831,592368         3,242855538         3,248255538         3,248255538         3,24825553         3,2483           855,5593         C,A380         C,A980         C,A980         C,A980         C,A980         C,A980         C,A980         S,55855         C,A214         C,84840         C,4433741         873,5875         S,55100         3,5127249         925           875,6855         C,A383         C,14800         C,41802         C,4183         S,149001200         C,4783         C,55559         2,551100         2,527249         C,55559         2,551100         2,575535         C,55559         5,551100         2,5727242         2,372783         1538         0,30215502         2,940           935,6734         C,4482         C,4492         C,4493         C,4492         C,4493         C,4492         C,4492         C,4493         C,4493         C,4493         C,4494         C,4493         C,4494         C,4493         C,4493         C,4494         C,4493	811,5695	I_A4B0_C7H8O	C47H80O9Na	C7H7O_H	4	0	4	811,5696	0,18	395667,6	811,5678006	2,033587107	2064
885,5934         (A23,CH80)         C6H80011Na         CH70,H         2         3         5         885,5594         (A)         64378,418         64378,418         64378,418         653,6320         933           873,6426         C.A380         CGH84012Na         Cyclic         2         4         6         875,5851         0.46         2424710,5         873,63780         5511060365         924           875,6821         C,A383         CSH80012Na         Cyclic         3         6         927,6325         0.76440,1         875,6581         0.46         2424710,5         873,66346         0.03215502         2,06338173         1472           939,6532         C,A482         C5H9012Na         Cyclic         4         2         6         935,6797         0.31         204556,5         936,69710         0.31         204556,5         936,97102         2,985,9384         2016           936,701         1.4580,CH800         CSH8012Na         CH70 H         2         4         6         935,6426         0.42         466722,6         938,649702         2,985,9384         2016         103         103         1045,713         1045,7143         104         103         104         103         104         103         1010,7	831,5957	c_A4B1	C47H84O10Na	Cyclic	4	1	5	831,5955	0,21	1460930,4	831,5929689	3,249295153	2489
873,6426         c. A380         CSCH490010Na         Cyclk         5         873,6428         0.2         4537,843         873,8478.0         55,5110.06905         924           875,585         c. A381         CGH490012Na         Cyclk         2         4         6875,6851         0.46         875,5851         0.46         875,8851         0.46         875,8851         0.46         875,8851         0.46         875,8851         0.46         875,8851         0.46         875,8851         0.46         875,8851         0.46         877,8622         0.0633144         0.00321502         2940           936,632         I_A481_C7NE0         C54H492011Na         C/H70         4         1         5         939,6535         0.34         27055,65         996,677103         2,39527,852         1066           936,47001         I_A580_C7NE0         C57H490011Na         C/H70         5         0         5         981,6997         0.31         207553.5         983,64037C         2,08639384         2016           936,40307         C,444         21275,3         981,649707C         0.82698.1         1003,5692         7,082,6420         4,24         2,7268,93384         2016           1003,5692         C,4381         C51H49001ANa <t< td=""><td>855,5593</td><td>I_A2B3_C7H8O</td><td>C48H80O11Na</td><td>C7H7O_H</td><td>2</td><td>3</td><td>5</td><td>855,5594</td><td>0,14</td><td>646397,9</td><td>855,5558882</td><td>3,96560253</td><td>933</td></t<>	855,5593	I_A2B3_C7H8O	C48H80O11Na	C7H7O_H	2	3	5	855,5594	0,14	646397,9	855,5558882	3,96560253	933
B75,5855         c. A284         C48H84012Na         Cyclk         2         4         6         B75,5851         0.06         2424710.5         B75,5851.01         4,215372489         925           937,6052         c.A383         C51H90012Na         Cyclk         3         3         6         917,6326         0.19         675449.1         B75,6551         927,630572         2,06338173         1472           939,6532         c.A482         C54H90012Na         Cyclk         4         2         6         939,67974         0.043         295,6532         936,65314         0.00211502         2,9869344         2,0053345         2,995,0797         0.31         2045556,5         993,697102         2,985,7971         0.31         20455763         993,6971023         2,985,7974         2,316         7,971023         2,985,7974         2,317         3,995,7971         0.31         20455763         993,6971023         2,985,9934         2,016,9934         2,016,9934         2,016,9934         2,016,9934         2,016,9934         2,016,9934         2,016,9934         2,016,9934         2,016,9934         2,016,9934         2,916,9936         1,017,9756         1,110,114,11103,1142         1,110,114,11103,1142         1,110,114,11103,1142         1,110,114,1103,1142         1,110,110,1144	873,6426	c_A5B0	C50H90O10Na	Cyclic	5	0	5	873,6428	0,2	453784,1	873,6378063	5,511060365	924
B87.6062         I_AB2_CTH80         CS1H86011Ma         C/H70_H         3         2         5         B97.6027         0.19         678449.1         B97.60278.20         66089594.31         1378           939.6532         I_AM31_CTH80         C54H90011Ma         C/H70_H         4         1         5         939.6533         0.34         579489.4         939.65318         0.00311502         2940           959.6774         C.A482         C54H90011Ma         C/H70_H         5         0         55.9797         0.31         2045526.5         959.67704         2.38.64207         2.38.64207         2.88239849         2.39.52384         2.0102.28521         1666           983.6430         I_A284_CH80         C57H90013Ma         C/H70_H         2         4         6         983.6426         0.44         212725.3         981.6907682         2.682398859         713           1001.7264         C_A285         CS5H90014Ma         Cyric         5         1         6         1001.7265         0.11         860921.4         1001.27785         1.431176302         1.4411           1035.6600         L_A83         CH80013Ma         C/H70_H         3         6         1025.6644         0.6681100.3         1035.76442         1.38.77162	875,5855	c_A2B4	C48H84O12Na	Cyclic	2	4	6	875,5851	0,46	2424710,5	875,5818101	4,215372489	925
917.6225         c.,A83         CS1H90012Na         Cyclic         3         3         6         917.6226         0.16         2548615.5         917.630572         2,06836173         1472           939.6532         LAABL_CHABL         C54H96012Na         Cyclic         4         2         6         959.6797         0.31         2005526.5         959.677032         2,39572852         1696           981,001         LASBL_CHBO         C57H96011Na         CYHO         2         4         6         983.6425         0.42         217275.3         981.697763         2,64228859         713           1001,7264         CASEL         CSFH96011Na         CYHO         2         4         6         983.6425         0.42         466782.6         983.640376         2,64228859         713           1003,6692         CA2ES         CSFH96014Na         CYHC         2         5         1001,7285         0.15         1080275         1001,72785         1.4411         1003,6544         1,4424         1,699239105         1649           1035,7522         CA8B4         CSHH96012Na         CYHC         3         6         1025,6890         0.05         1608703         1035,757245         1641           1033,7733 <td< td=""><td>897,6062</td><td>I A3B2 C7H8O</td><td>C51H86O11Na</td><td>C7H70_H</td><td>3</td><td>2</td><td>5</td><td>897,6064</td><td>0,19</td><td>678449,1</td><td>897,6007829</td><td>6,069565943</td><td>1538</td></td<>	897,6062	I A3B2 C7H8O	C51H86O11Na	C7H70_H	3	2	5	897,6064	0,19	678449,1	897,6007829	6,069565943	1538
999.6532         I.AB3_C7H80         CS4H82011Na         CPUC         4         1         5         993.6734         0.34         939.6535.         936.6534         0.00215502         2940           999.6794         c.AB2         CS4H80012Na         CVIC         4         1         5         993.6790         0.31         204552.5         993.6790         2.20653284         2016           993.6430         I.AB26_C7180         CS7H80011Na         C7H70 H         2         4         6         993.6430         0.44         217275.3         993.67972         2.20859384         2016           1003.6692         c.AS11         CS7H00013Na         CYH70 H         3         4         1001.7265         0.15         10080027.5         1001.72785         1.431179302         1.4211           1005.6600         I.AB2.C7H80         CSH96013Na         CYH70 H         3         3         6         1025.6899         0.06         680370.3         1025.68543         4.04456699         1699           1045.7736         CL1802.07H80         CSH10001ANA         CYH10 H         3         3         6         1025.6899         0.06         680370.3         1025.68544         4.04456699         1699           10457.761         CL	917,6325	c_A3B3	C51H90O12Na	Cyclic	3	3	6	917,6326	0,16	2543615,5	917,6305572	2,063836173	1472
995.0794         C.A482         CS4496012Na         Cyclic         4         2         6         955.6797         0.31         204552.65         959.6771023         2.395272852         1666           981.7001         I.A580         C7880         C55H80011Na         C7870 H         5         0.81.6097         0.42         24572.53         981.60376         2.68228859         713           1001.7264         C.A581         C57H102012Na         Cyclic         5         1         6         1001.7265         0.15         1080027,5         1001.72785         1.431175302         1421           1003.6562         C.A215         C5H490011Na         Cyclic         2         5         7         1005.6694         0.17         882381,1         1003.65847         9.7257624         614           1005,7562         C.A8460         C60H10001Na         Cyclic         6         6         1047,733         0.66         608170,3         1025.6849.4         1045,71404         1.69229105         1098           1005,7562         C.A846         C6H11001Na         CYclic         4         6         107,7373         0.36         558374,4         1045,71404         1.69229105         1098           1007,7383         I.A812,C7H80	939,6532	A4B1_C7H8O	C54H92O11Na	C7H70_H	4	1	5	939,6535	0,34	579489,4	939,653184	0,003215502	2940
981,2001         LASB0_CFM8D         C57H980118a         CHPO_H         5         0         5         981,6937         0.44         217275.3         981,697628         2.206639384         2016           983,6430         L/204_CFM8D         C55H9013Ma         CYHTO_H         2         4         6         983,6430         0.2765         1001,72785         1.431176302         1421           1003,65692         c_A285         C55H96014Ma         Cyclic         5         1         6         1001,7265         0.15         1080027,5         1001,72785         1.431176302         1421           1003,65692         c_A285         C55H96014Ma         Cyclic         2         5         7         1003,65694         0.075         862941,1         1003,56849         9.44445609         1669         1669         1043,77639         0.57         208885,2         1043,76512         6,849451662         298         1045,7162         0.62         944985,9         105,71404         1,99239105         1098         1087,7538         0.66         778343,4         1087,7537         6,107,73330         0.36         558374,5         106,7733404         2,722872025         3041           1078,7581         C,4483         C6H1100031Ma         C/H7O H         3	959,6794	c_A4B2	C54H96O12Na	Cyclic	4	2	6	959,6797	0,31	2045526,5	959,6771023	2,395272852	1696
993.6430         (1.204 C1H80         C55H92013Ma         C/HYD         1         2         4         6         993.6426         0.42         466782.6         993.6426         2,68228859         713           1001,7264         c. A881         C55H90014Ma         Cyclic         5         1         6         1001,7265         0.15         108027.5         1001,727785         1,43176302         1421           1003,6692         c. A883         C55H90014Ma         Cyclic         6         1004,7739         0,57         20889.2         1003,76612         6,849451662         298           10043,7733         c. A680         C65H100013Va         Cyclic         3         4         7         10045,7732         0,57         20889.2         10045,71404         1,699239105         1098           1067,7630         I.A482         C1H0013Na         Cyclic         4         3         7         1087,7338         0,62         788434.4         1087,73604         2,722872025         3041           1087,7631         c. A683         C64H110013Na         Cyclic         5         2         7         1129,8105         0,37         411308,2         1129,80075         6,502269313         1233           1129,8010         c. A683<	981,7001	I A5B0 C7H8O	C57H98O11Na	C7H70_H	5	0	5	981,6997	0,44	217275,3	981,6979628	2,208639384	2016
1001,7264         c.ASB1         CS/H102012Na         Cyclic         5         1         6         1001,7255         0.15         1008027,5         1001,72785         1,431,7302         1421           1003,6692         CA285         CS3H98013Na         C/H70         H         3         3         6         1002,5699         0,66         608170,3         1002,568543         4,404456609         1609           1045,7162         CA884         CSH102014Na         Cyclic         6         0         6         1042,7739         0,57         208886,2         1043,761612         6,84451662         298           1067,7269         LA482         CFHE0         CEHIL04013Na         CYH2         4         2         6         1067,733         0,36         558374,5         1067,734004         2,72287025         3041           1087,7631         LC,A483         CEHIL0013Na         CYH2         4         7         1109,7638         0,62         788434,4         1087,7531         0,62         788434,4         1087,753         1067,734004         2,72287025         3041           1129,8101         C A481         CFH10013Na         CYH2         4         7         1129,8103         0,37         411308,75         1109,7804	983,6430	I_A2B4_C7H8O	C55H92O13Na	С7Н70_Н	2	4	6	983,6426	0,42	466782,6	983,6403726	2,682298859	713
1003.6692         c. A285         C 55H96014Na         Cyclic         2         5         7         1003.6694         0.17         882981.1         1003.65947         9725776245         614           1025.6900         L A383.C7H8O         CS8H99013Na         C7H7O_H         3         3         6         1025.68949         0.066         608170.3         10025.685443         4.404456609         1609           1043.7733         C.A660         C60H108012Na         Cyclic         6         0         6         1043.7739         0.57         208886.9         1045,71404         1.699239105         1098           1067.7369         LAMB2.C/H8O         C6H1100013Na         C/H7O, H         2         6         1067,7373         0.36         558374.5         1067,73637         6.215139708         1579           1097.783         L ASB1.C/H8O         C6H110013Na         C/H7O, H         3         4         7         1158,7737         0.13         351197.5         1087,75637         6.215139708         1579           1171.85707         C A661         C5H110013Na         C/H7O, H         3         4         7         1158,7739         0.18         408366,7         1153,578429         4,560716281         1578           1171.85	1001,7264	c A5B1	C57H102O12Na	Cyclic	5	1	6	1001,7265	0,15	1080027,5	1001,727785	1,431176302	1421
1025,6900         I_A383_C7H80         C58H96013Na         C7H70 H         3         3         6         1025,6899         0.06         608170.3         1025,6854.3         4.404456609         1609           1043,7733         c_A880         C60H108012Na         Cyclic         6         0         6         1043,7739         0,57         208898,2         1043,76152         6.484451662         298           1067,7360         LAM2_C7H80         C61H10013Na         CYHC         4         2         6         1067,7333         0,36         558374,5         1067,734004         2,722872025         3041           1087,7531         c_A483         C61H10013Na         CYHC         4         3         7         1087,7533         0,62         78834,4         1087,75537         6,5120573         6,5120573         6,5120573         6,5120573         3,733666763         3651           1129,8101         c_A582         C64H11401A4         Cyclic         5         2         7         1129,8105         0,37         411306,2         1123,7642         4,560716281         1578           1171,7599         c_A681         C67H12001Ha         Cyrlic         5         8         1173,8582         1         76813,424         4,560716281	1003,6692	c A2B5	C55H96O14Na	Cyclic	2	5	7	1003,6694	0,17	862981,1	1003,65947	9,725776245	614
1043,7733         c_A680         C60H108012Na         Cyclic         6         1043,7739         0.57         208898,2         1043,76152         6,849451662         299           1045,7162         c_A384         C58H102014Na         Cyclic         3         4         7         1045,7162         0.02         949886,9         1045,716140         1,692393105         1098           1067,7369         I_A82_C7H80         C61H10013Na         C/H70,H         4         2         6         1067,7373         0.36         558374,5         1067,7360         2,72872025         3041           1087,7531         C_A483         C6H110013Na         C/H70,H         4         2         7         1129,810         0,13         351197,715         1109,784         5,20269313         1333           1153,7737         I_A84_C7H80         C6H110015Na         C/H70,H         3         4         7         1173,752         1         408306,7         1153,76829         4,560716281         1578           1171,8570         C_A681         C67H120014Ma         Cyclic         6         1         7         1171,852         1         76918,2         1173,79524         3,8675638         583456594         678           1171,8582         L </td <td>1025,6900</td> <td>I A3B3 C7H8O</td> <td>C58H98O13Na</td> <td>С7Н7О Н</td> <td>3</td> <td>3</td> <td>6</td> <td>1025,6899</td> <td>0,06</td> <td>608170,3</td> <td>1025,685443</td> <td>4,404456609</td> <td>1609</td>	1025,6900	I A3B3 C7H8O	C58H98O13Na	С7Н7О Н	3	3	6	1025,6899	0,06	608170,3	1025,685443	4,404456609	1609
1045,7162         c_A384         CS8H102014Na         Cyclic         3         4         7         1045,7162         0.02         949886,9         1045,71404         1,699339105         1098           1067,7369         I_A482_C7H80         C61H104013Na         CYND_H         4         2         6         1067,733         0,36         S58374,5         1067,73404         2,722872025         3041           1087,7631         c_A483         C61H108013Na         CYND_H         5         1         6         1097,7638         0,62         78843,4         1087,7651         3,79366763         3651           1129,8101         c_A892         C64H110013Na         CYND_H         3         4         7         1129,8105         0,37         411308,2         1129,80273         6,502269313         1233           1123,8101         c_A881         C6H1140015Na         CYHO_H         3         4         7         1153,7739         0,18         408306,7         1153,76842         4,560716281         1578           1173,8579         c_A861         C6H1140015Na         CYHO_H         4         3         7         1198,8211         0,38         459051,6         1155,81586         6218020363         3403           1173,8579 <td>1043,7733</td> <td>c A6B0</td> <td>C60H108O12Na</td> <td>Cyclic</td> <td>6</td> <td>0</td> <td>6</td> <td>1043,7739</td> <td>0,57</td> <td>208898,2</td> <td>1043,766152</td> <td>6,849451662</td> <td>298</td>	1043,7733	c A6B0	C60H108O12Na	Cyclic	6	0	6	1043,7739	0,57	208898,2	1043,766152	6,849451662	298
1067,7369         I_A482_C7480         C61H104013Na         C7H70_H         4         2         6         1067,7333         0.36         558374,5         1067,73004         2,722872025         3041           1087,7631         c_A483         C61H100013Na         C7H70_H         4         3         7         1087,7638         0.62         788434,4         1087,75637         6,215139708         1579           1109,7839         I_A561_C7H80         C64H110013Na         C7H70_H         5         1         6         1109,784         0.13         351197,5         1109,77861         3,793666763         3651           1123,8737         I_A384_C7H80         C64H114014Na         Cyclic         5         2         7         1129,8105         0.37         411308,2         1172,85074         5,53269313         1233           1171,8570         c_A681         C67H120014Na         Cyclic         6         1         7         1173,801         0,93         45302,8         1173,75524         4,81656988         919           1195,8206         I_A484         C68H1120016Na         Cyclic         4         8         1215,8471         0,2         453720,5         1215,839158         6,335628856         1246           1237,8674	1045,7162	c_A3B4	C58H102O14Na	Cyclic	3	4	7	1045,7162	0,02	949886,9	1045,714404	1,699239105	1098
1087,7631         c.A483         C61H108D14Na         Cyclic         4         3         7         1087,7638         0,62         788434,4         1087,75637         6,215139708         1579           1109,7839         I_AS61_C7H80         C64H11001Ma         C/H70_H         5         1         6         1109,784         0,13         351197,5         1109,778651         3,793666763         3651           1129,801737         I_A384_C7H80         C65H110015Na         C/H70_H         3         4         7         1153,7739         0,18         408306,7         1153,768429         4,560716281         1578           1173,7999         c.A385         C65H114016Na         Cyclic         6         1         7         1171,8582         1         76918,2         1173,795823         4,560716281         1578           1173,7999         c.A385         C65H114016Na         Cyclic         4         3         7         1195,8211         0,38         459051,6         1195,813165         6,51802363         3403           1237,8676         L_A582         CH80         C7H70,H         4         8         125,84714         0,22         453720,5         1215,839158         6,35562856         1246           1237,8676 <td< td=""><td>1067,7369</td><td>I A4B2 C7H8O</td><td>C61H104O13Na</td><td>С7Н7О Н</td><td>4</td><td>2</td><td>6</td><td>1067,7373</td><td>0,36</td><td>558374,5</td><td>1067,734004</td><td>2,722872025</td><td>3041</td></td<>	1067,7369	I A4B2 C7H8O	C61H104O13Na	С7Н7О Н	4	2	6	1067,7373	0,36	558374,5	1067,734004	2,722872025	3041
1109,7839         I_ASB1_C7H80         C64H110013Na         C7H70_H         5         1         6         1109,784         0,13         351197,5         1109,779651         3,793666763         3651           1128,8101         c_AS82         C64H11401ANa         Cyclic         5         2         7         1129,8105         0,37         411308,2         1129,80273         6,502269313         1233           1153,7737         L_AB4         C6H112001ANa         Cyclic         6         1         7         1153,7739         0,18         408306,7         1153,78242         4,5535436594         678           1173,7999         c_A681         C65H114016Na         Cyclic         3         8         1173,801         0,93         453022,8         1173,79584         3,481656988         919           1195,8206         L_AM83         C7H80         C68H116015Na         Cyclic         3         7         1195,8211         0,38         453022,8         1173,795824         3,481656988         919           1237,8676         L_AM83         C7H80         G7H70,H         4         3         7         1195,8212         0,32         33771,8         1237,86034         5,66236488         4954           1237,8634         C,AM8	1087,7631	c_A4B3	C61H108O14Na	Cyclic	4	3	7	1087,7638	0,62	788434,4	1087,75637	6,215139708	1579
1129,8101         c         AS82         C64H114014Na         Cyclic         5         2         7         1129,8105         0,37         411308,2         1129,802735         6,502269313         1233           1153,7737         LA384         C7H20         C6AB11         CC57H120014Na         Cyclic         3         4         7         1153,7399         0,18         408306,7         1153,768429         4,560716281         1578           1173,7970         c         AAB5         C65H114016Na         Cyclic         3         5         8         1173,801         0,93         453022,8         1173,795824         3,481656988         919           11215,8469         c         AAB4         C68H110016Na         Cyclic         4         8         1215,8471         0,2         453720,5         1215,83156         6,3562386448         4954           1279,9137         LA582_C7H80         C71H122015Na         C7H70_H         5         2         7         123,8672         0,32         337771,8         1237,860334         5,862396448         4954           1279,9143         LA661         C7H122015Na         C7H70_H         5         8         127,99147         0,12         130301,883         5,17300552         1417,7300552 </td <td>1109,7839</td> <td>I_A5B1_C7H8O</td> <td>C64H110O13Na</td> <td>C7H7O_H</td> <td>5</td> <td>1</td> <td>6</td> <td>1109,784</td> <td>0,13</td> <td>351197,5</td> <td>1109,779651</td> <td>3,793666763</td> <td>3651</td>	1109,7839	I_A5B1_C7H8O	C64H110O13Na	C7H7O_H	5	1	6	1109,784	0,13	351197,5	1109,779651	3,793666763	3651
1153,7737         I_A384_C7H80         C65H110015Na         C/H70_H         3         4         7         1153,7739         0,18         408306,7         1153,768429         4,560716281         1578           1171,8570         c_A661         C67H120014Na         Cyclic         6         1         7         1171,8582         1         76918,2         1171,85044         5,535436594         678           1173,7999         c_A385         C65H1140015Na         Cyclic         4         3         7         1195,8211         0,93         453022,8         1173,795824         3,481655988         919           1195,8206         I_A483_C7H80         C68H116015Na         C/H70_H         4         3         7         1195,8211         0,2         453720,5         1215,83165         6,251802363         3403           1237,8676         I_A582_C7H80         C71H122015Na         C/H70_H         5         2         7         1237,8672         0,32         33771,8         1237,86034         5,862396448         4954           1257,9383         c_A583         C71H122015Na         C/H70_H         6         1         7         127,9147         0,12         130310,8         127,90874         6,771300552         4127 <t< td=""><td>1129,8101</td><td>c A5B2</td><td>C64H114O14Na</td><td>Cyclic</td><td>5</td><td>2</td><td>7</td><td>1129,8105</td><td>0,37</td><td>411308,2</td><td>1129,802735</td><td>6,502269313</td><td>1233</td></t<>	1129,8101	c A5B2	C64H114O14Na	Cyclic	5	2	7	1129,8105	0,37	411308,2	1129,802735	6,502269313	1233
1171,8570         c. A681         C67H120014Na         Cyclic         6         1         7         1171,8582         1         76918,2         1171,850544         5,535436594         678           1173,7999         c.A385         C65H114016Na         Cyclic         3         5         8         1173,801         0,93         453022,8         1173,79524         3,841656988         919           1195,8206         I_A483         C7H400         K         3         7         1195,8211         0,38         459051,6         1195,83156         6,335628856         1246           1237,8676         I_A582         C7H80         C7H1122015Na         C7H70, H         5         2         7         1237,8672         0,32         33771,8         1237,86034         5,862396448         4954           1279,9145         I_A681         C7H80         C7H1126016Na         Cyclic         5         3         8         1257,8944         0,47         253078,7         1257,88203         9,315650105         1442           1279,9145         I_A681         C7H80         C7H126016Na         Cyclic         5         8         128,8567         0,56         244319,7         1281,880635         18,10985424         1905 <t< td=""><td>1153,7737</td><td>A3B4 C7H8O</td><td>C65H110O15Na</td><td>С7Н7О Н</td><td>3</td><td>4</td><td>7</td><td>1153,7739</td><td>0.18</td><td>408306.7</td><td>1153,768429</td><td>4.560716281</td><td>1578</td></t<>	1153,7737	A3B4 C7H8O	C65H110O15Na	С7Н7О Н	3	4	7	1153,7739	0.18	408306.7	1153,768429	4.560716281	1578
1173,7999         c. A385         C65H114016Na         Cyclic         3         5         8         1173,801         0,93         453022,8         1173,795824         3,481656988         919           1195,8206         I_A483_C7H80         C68H116015Na         C/H7O_H         4         3         7         1195,8211         0,38         459051,6         1195,813165         6,251802363         3403           1215,8469         c_A484         C68H120016Na         Cyclic         4         4         8         1215,8471         0,2         453720,5         1215,83165         6,335628856         1226           1237,8676         I_A582_C7H80         C71H12C016Na         Cyclic         5         3         8         127,8934         0,47         253078,7         1257,882093         9,315650105         1442           1279,9145         I_A681_C7H80         C74H128015Na         C/H7O_H         6         1         7         1279,9147         0,12         130310,8         1279,905874         6,73100552         4127           1281,8567         C.24682         C74H128015Na         Cyclic         6         2         8         1229,944         0,59         75080,4         1299,93508         5,573320547         1132	1171,8570	c A6B1	C67H120O14Na	Cyclic	6	1	7	1171,8582	1	76918,2	1171,850544	5,535436594	678
1195,8206         I A483_C7H80         C68H116015Na         C7H70_H         4         3         7         1195,8211         0,38         459051,6         1195,813165         6,251802363         3403           1215,8469         c_A484         C68H120016Na         Cyclic         4         4         8         1215,8471         0,2         453720,5         1215,839158         6,335628856         1246           1237,8676         I_A582_C7H80         C71H12015Na         C/H70_H         5         2         7         1237,8672         0,32         33771,8         1237,8034         5,86239648         4954           1257,8938         c_A583         C71H12015Na         C/H70_H         6         1         7         1279,9147         0,12         130310,8         1279,905874         6,771300552         4127           1281,8574         I_A385_C7H80         C72H122017Na         CH70_H         3         5         8         1289,940         0,59         75080,4         129,930585         5,57320547         1132           1299,9408         c_A662         C74H122018Na         Cyclic         3         6         9         1301,8841         0,35         132025         1301,894979         8,708942305         670	1173,7999	c A3B5	C65H114O16Na	Cyclic	3	5	8	1173,801	0,93	453022,8	1173,795824	3,481656988	919
1215,8469         c_A484         C68H120016Na         Cyclic         4         4         8         1215,8471         0,2         453720,5         1215,839158         6,335628856         1246           1237,8676         I_A582_C7H80         C71H122015Na         C7H70_H         5         2         7         1237,8672         0,32         337771,8         1237,86034         5,662396448         4954           1279,93145         I_A681_C7H80         C7H122015Na         C7H70_H         6         1         7         1279,9147         0,12         130310,8         1279,905874         6,771300552         4127           128,8574         I_A681_C7H80         C74H122017Na         C7H70_H         3         5         8         1281,8567         0,56         244319,7         1281,880633         18,10985424         1905           1299,9408         c_A886         C74H132016Na         Cyclic         6         9         1301,8841         0,35         132025         1301,84979         8,708942305         670           1323,9044         I_A484_C7H80         C75H128017Na         C7H70_H         4         4         8         1323,9037         0,51         344210,51         1323,891908         9,413562936         3681           1343	1195,8206	I A4B3 C7H8O	C68H116O15Na	С7Н7О Н	4	3	7	1195,8211	0,38	459051,6	1195,813165	6,251802363	3403
1237,8676         I_A582_C7H80         C71H122015Na         C7H70_H         5         2         7         1237,8672         0,32         337771,8         1237,86034         5,862396448         4954           1257,8938         c_A583         C71H126016Na         Cyclic         5         3         8         1257,8944         0,47         253078,7         1257,882093         9,315650105         1442           1279,9145         I_A681_C7H80         C74H128015Na         C7H70_H         6         1         7         1279,9147         0,12         130310,8         1279,905874         6,771300552         4127           1281,857         I_A685_C7H80         C72H122017Na         C7H70_H         3         5         8         1281,856         0,56         244319,7         1281,8864         199,93508         5,579320547         1132           1301,8836         c_A682         C74H132018Na         Cyclic         6         2         8         1229,940         0,59         75080,4         1299,93508         5,579320547         1132           1303,8906         c_A485         C75H132018Na         Cyclic         3         6         9         1332,9937         0,51         344210,5         1343,92318         5,514457475         1237	1215,8469	c A4B4	C68H120O16Na	Cyclic	4	4	8	1215,8471	0,2	453720,5	1215,839158	6,335628856	1246
1257,8938         c_ASB3         C71H126016Na         Cyclic         5         3         8         1257,8944         0,47         253078,7         1257,82093         9,315650105         1442           1279,9145         I_A6B1_C7H80         C74H128015Na         C7H70_H         6         1         7         1279,9147         0,12         130310,8         1279,905874         6,771300552         4127           1281,8574         I_A385_C7H80         C72H122017Na         C7H70_H         3         5         8         1289,944         0,59         75080,4         129,933056         5,573320547         1132           1301,8836         c_A682         C74H132016Na         Cyclic         3         6         9         1301,8841         0,35         132025         1301,894979         8,708942305         670           1323,9044         I_A484_C7H80         C75H128017Na         CYH7O_H         4         4         8         1323,9037         0,51         344210,5         1323,891908         9,413562936         3681           1343,9306         c_A485         C75H128017Na         C7H7O_H         4         4         8         1323,9037         0,51         344210,5         1323,891908         9,413562936         3681	1237,8676	I A5B2 C7H8O	C71H122O15Na	С7Н7О Н	5	2	7	1237,8672	0,32	337771,8	1237,860334	5,862396448	4954
1279,9145         I A681_C7H80         C74H128015Na         C7H70_H         6         1         7         1279,9147         0,12         130310,8         1279,905874         6,771300552         4127           1281,8574         I_A385_C7H80         C72H122017Na         C7H70_H         3         5         8         1281,9567         0,56         244319,7         1281,880633         18,10985424         1905           1299,9408         c_A682         C7H12018Na         Cyclic         3         6         9         1301,8841         0,35         132025         1301,894979         8,708942305         670           1323,9044         I_A484_C7H80         C75H128017Na         C7H70_H         4         4         8         1323,9037         0,51         344210,5         1323,891908         9,413562936         3681           1343,9306         c_A485         C75H132018Na         Cyclic         4         5         9         1343,9307         0,08         164776,5         1343,93218         5,514457475         1237           1365,9513         I_A583_C7H80         C78H134017Na         C/H70_H         5         3         8         1365,9508         0,38         348090,8         1365,95138         11,61829447         1518 <tr< td=""><td>1257,8938</td><td>c A5B3</td><td>C71H126O16Na</td><td>Cyclic</td><td>5</td><td>3</td><td>8</td><td>1257,8944</td><td>0,47</td><td>253078,7</td><td>1257,882093</td><td>9,315650105</td><td>1442</td></tr<>	1257,8938	c A5B3	C71H126O16Na	Cyclic	5	3	8	1257,8944	0,47	253078,7	1257,882093	9,315650105	1442
1281,8574         I_A385_C7H80         C72H122017Na         C7H70_H         3         5         8         1281,8567         0.56         244319,7         1281,880635         18,10985424         1905           1299,9408         c_A682         C74H132016Na         Cyclic         6         2         8         1299,940         0,59         75080,4         1299,933508         5,579320547         1132           1301,8836         c_A386         C72H126018Na         Cyclic         3         6         9         1301,8841         0,35         132025         1301,894979         8,708942305         670           1323,9044         I_A484_C7H80         C75H12017Na         C7H7O_H         4         4         8         1323,9037         0,51         344210,5         1323,891908         9,413562936         3681           1343,9306         c_A485         C75H132018Na         Cyclic         4         5         9         1343,9307         0,08         164776,5         1343,92318         5,514457475         1237           1365,9513         I_A583_C7H80         C78H134017Na         C7H7O_H         5         4         9         1385,977         0,39         153601,6         1385,961438         11,77684624         6024	1279,9145	I A6B1 C7H8O	C74H128O15Na	С7Н7О Н	6	1	7	1279,9147	0,12	130310,8	1279,905874	6,771300552	4127
1299,9408         c_A682         C74H132016Na         Cyclic         6         2         8         1299,940         0,59         75080,4         1299,93508         5,579320547         1132           1301,8836         c_A386         C72H126018Na         Cyclic         3         6         9         1301,8841         0,35         132025         1301,894979         8,708942305         670           1323,9044         I_AA84_C7H8O         C75H128017Na         C/H7O_H         4         4         8         1323,9037         0,51         344210,5         1323,891908         9,413562936         3681           1343,9306         c_A485         C75H132018Na         Cyclic         4         5         9         1343,9307         0,08         164776,5         1343,9321         5,514457475         1237           1365,9513         I_A583_C7H8O         C78H134017Na         C/H7O_H         5         3         8         1365,9508         0,38         348090,8         1365,935234         11,7684624         6024           1407,99454         C78H134017Na         C/H7O_H         5         4         9         1385,977         0,39         15361.6         1385,961438         11,61829447         1518           1407,994545         <	1281.8574	A3B5_C7H8O	C72H122O17Na	С7Н7О Н	3	5	8	1281.8567	0.56	244319.7	1281.880635	18.10985424	1905
1301,8836         c_A386         C72H126018Na         Cyclic         3         6         9         1301,8841         0,35         132025         1301,894979         8,708942305         670           1323,9044         I_A484_C7H80         C75H128017Na         C7H70_H         4         4         8         1322,9037         0,51         344210,5         1323,891008         9,413562936         3681           1343,9306         c_A485         C75H123018Na         Cyclic         4         5         9         1343,9307         0,08         164776,5         1343,93108         5,51447475         1237           1365,9513         I_A583_C7H80         C78H134017Na         C7H70_H         5         3         8         1365,9578         0,38         348090,8         1365,95234         11,77684624         6024           1385,9775         c_A584         C78H138018Na         Cyclic         5         4         9         1385,977         0,39         153601,6         1385,96138         11,61829447         1518           1407,9983         I_A682_C7H80         C81H140017Na         C7H70_H         6         2         8         1407,9964         1,33         19770,3         1407,998708         1161           1409,9412         <	1299,9408	c A6B2	C74H132O16Na	Cyclic	6	2	8	1299,94	0,59	75080,4	1299,933508	5,579320547	1132
1323,9044         I_A484_C7H80         C75H128017Na         C7H70_H         4         4         8         1323,9037         0,51         344210,5         1323,891908         9,413562936         3681           1343,9306         c_A485         C75H132018Na         Cyclic         4         5         9         1343,9307         0,08         164776,5         1343,9218         5,514457475         1237           1365,9513         I_A583_C7H80         C78H134017Na         C7H70_H         5         3         8         1365,9508         0,38         348090,8         1365,95234         11,77684624         6024           1385,977         c_A584         C78H134017Na         C7H70_H         5         3         8         1365,9508         0,38         348090,8         1365,95234         11,77684624         6024           1385,977         c_A584         C78H134017Na         C7H70_H         6         2         8         1407,9964         1,33         197370,3         1407,984568         9,731936579         6712           1409,9412         L_A386_C7H80         C8H144018Na         Cyclic         6         9         1409,9409         0,18         98665,2         1409,971772         21,71790733         2661           1450,0472 <td>1301,8836</td> <td>c_A3B6</td> <td>C72H126O18Na</td> <td>Cyclic</td> <td>3</td> <td>6</td> <td>9</td> <td>1301,8841</td> <td>0,35</td> <td>132025</td> <td>1301,894979</td> <td>8,708942305</td> <td>670</td>	1301,8836	c_A3B6	C72H126O18Na	Cyclic	3	6	9	1301,8841	0,35	132025	1301,894979	8,708942305	670
1343,9306         c_A85         C75H132018Na         Cyclic         4         5         9         1343,9307         0,08         164776,5         1343,92318         5,514457475         1237           1365,9513         I_A583         C7N80         C78H134017Na         C7H70,H         5         3         8         1365,9508         0,38         348090,8         1365,95124         1,77684624         6024           1385,9775         c_A584         C78H138018Na         Cyclic         5         4         9         1385,977         0,39         153601,6         1385,961438         11,61829447         1518           1407,9983         I_A682         C7H80         C81H140017Na         C7H70,H         6         2         8         1407,9946         1,33         197370,3         1407,984568         9,731936579         6712           1409,9412         I_A386_C7H80         C79H134017Na         C7H70,H         3         6         9         1409,9409         0,18         98665,2         1409,971772         21,71790733         2641           1428,0245         c_A683         C81H144018Na         Cyclic         6         3         9         1428,0234         0,76         53733,2         1428,03104         9419649708         11	1323,9044	I A4B4 C7H8O	C75H128O17Na	С7Н7О Н	4	4	8	1323,9037	0,51	344210,5	1323,891908	9,413562936	3681
1365,9513         I A583_C7H80         C78H134017Na         C7H70_H         5         3         8         1365,9508         0,38         348090,8         1365,935234         11,77684624         6024           1385,9775         c_A584         C78H138018Na         Cyciic         5         4         9         1385,977         0,39         153601,6         1385,96138         11,77684624         6024           1407,9983         I A682_C7H80         C81H140017Na         CYCIC         5         4         9         1385,977         0,39         153601,6         1385,96138         11,61829447         1518           1409,9412         I A682_C7H80         C81H140017Na         C7H7O_H         6         2         8         1407,9964         1,33         197370,3         1407,984568         9,731936579         6712           1409,9412         I A682_C7H80         C78H134019Na         CYH7O_H         3         6         9         1429,9234         0,76         53733,2         1428,01104         9,419649708         1161           1450,0452         I A781_C7H80         C84H146017Na         CYH7O_H         7         1         8         1450,0472         1,36         42270,5         1450,030103         10,42602319         3382	1343,9306	c A4B5	C75H132O18Na	Cyclic	4	5	9	1343,9307	0.08	164776.5	1343.92318	5.514457475	1237
1385,9775         C_A584         C78H138018Na         Cyclic         5         4         9         1385,977         0,39         153601,6         1385,961438         11,61829447         1518           1407,9983         I_A682_C7H80         C81H140017Na         C7H70_H         6         2         8         1407,9964         1,33         197370,3         1407,984568         9,731936579         6712           1409,9412         I_A385_C7H80         C81H140017Na         C7H70_H         3         6         9         1409,9409         0,18         98665,2         1409,91772         21,71790733         2641           1428,0245         c_A683         C81H140017Na         Cyclic         6         3         9         1428,0234         0,76         53733,2         1428,0104         9,419649708         1161           1450,0452         I_A781_C7H80         C84H146017Na         C7H70_H         7         1         8         1450,0472         1,36         42270,5         1450,030103         10,42602319         3382           1451,9881         I_A485_C7H80         C82H140019Na         C7H70_H         4         5         9         1451,9868         0,9         216783,5         1451,990387         1,57442404         3552	1365,9513	I A5B3 C7H8O	C78H134O17Na	С7Н7О Н	5	3	8	1365,9508	0,38	348090,8	1365,935234	11,77684624	6024
1407,9983         I         A662         C7H80         C81H140017Na         C7H70 H         6         2         8         1407,9964         1,33         197370,3         1407,984568         9,731936579         6712           1409,9412         I         A366         C7H80         C7H70 H         3         6         9         1409,9409         0,18         98665,2         1409,971772         21,71790733         2641           1428,0245         c         A6B3         C81H144018Na         Cyclic         6         3         9         1428,0234         0,76         53733,2         1428,0104         9,19649708         1161           1450,0452         I         A7B1 C7H80         C84H146017Na         C7H70 H         7         1         8         1450,0472         1,36         42270,5         1450,0301         0,42602319         3382           1451,9881         I         A485         C7H80         C82H146017Na         C7H70 H         4         5         9         1451,9868         0,9         216783,5         1451,90387         1,57442404         3552           1494,0351         I         A584         C7H80         C85H146019Na         C7H70 H         5         4         9         1494,0331	1385,9775	c A5B4	C78H138O18Na	Cyclic	5	4	9	1385,977	0,39	153601,6	1385,961438	11,61829447	1518
1409,9412         I_A386_C7H80         C79H134019Na         C7H70_H         3         6         9         1409,9402         0.76         53733,2         1409,91772         21,71790733         2641           1428,0245         c_A683         C81H144018Na         Cyclic         6         3         9         1428,0234         0,76         53733,2         1428,01104         9,419649708         1161           1450,0452         I_A781_C7H80         C84H146017Na         C7H70_H         7         1         8         1450,0472         1,36         42270,5         1450,00103         10,42602319         3382           1451,9881         I_A485_C7H80         C82H140019Na         C7H70_H         5         9         1451,9868         0,9         216783,5         1451,990387         1,57424404         3552           1494,0351         I_A584_C7H80         C85H146019Na         C7H70_H         5         4         9         1494,0331         1,31         286080         1494,014932         13,46639192         6146           1540,0831         c_A585         C85H15020Na         Cyclic         5         5         10         1514,05956         1,1         47504         1514,042471         12,1678008         1049           1536,0821 <td>1407,9983</td> <td>I A6B2 C7H8O</td> <td>C81H140O17Na</td> <td>С7Н7О Н</td> <td>6</td> <td>2</td> <td>8</td> <td>1407.9964</td> <td>1,33</td> <td>197370.3</td> <td>1407.984568</td> <td>9,731936579</td> <td>6712</td>	1407,9983	I A6B2 C7H8O	C81H140O17Na	С7Н7О Н	6	2	8	1407.9964	1,33	197370.3	1407.984568	9,731936579	6712
1428,0245         c. A683         C81H144018Na         Cyclic         6         3         9         1428,024         0,76         53733,2         1428,0110         9,419649708         1161           1450,0452         I A781_C7H80         C84H146017Na         C7H70_H         7         1         8         1450,0472         1,36         42270,5         1428,0103         10,42602319         3382           1451,9881         I_A855_C7H80         C82H140019Na         C7H70_H         4         5         9         1451,9868         0,9         216783,5         1451,990387         1,57442404         3552           1494,0351         I_A584_C7H80         C85H146019Na         C7H70_H         5         4         9         1494,0331         1,31         286080         1494,014932         13,46639192         6146           1514,0613         c_A585         C85H150020Na         Cyclic         5         5         10         1514,0596         1,1         47504         1514,042471         12,41678008         1049           1536,0820         I_A685_C7H80         C88H152019Na         C/H70 H         6         3         9         1536,0811         0.59         246633,4         1536,08751         15,154,058751         15,154,058751         1	1409,9412	L A3B6 C7H80	C79H134O19Na	С7Н7О Н	3	6	9	1409,9409	0.18	98665.2	1409.971772	21.71790733	2641
1450,0452         I A781_C7H80         C84H146017Na         C7H70_H         7         1         8         1450,0472         1,36         42270,5         1450,00103         0,10,2602319         3382           1451,9881         I A485_C7H80         C82H140019Na         C7H70_H         4         5         9         1451,9868         0,9         216783,5         1451,990387         1,57442404         3552           1494,0351         I A584_C7H80         C82H146019Na         C7H70_H         5         4         9         1494,0331         1,31         286080         1494,014932         13,46639192         6146           1514,0613         c_A585         C85H150020Na         Cyclic         5         5         10         1514,0596         1,1         47504         1514,042471         12,41678008         1049           1536,0820         I A685         C7H80         C88H150020Na         Cyclic         5         5         10         1514,0596         1,1         47504         1514,042471         12,41678008         1049           1536,0820         I A685         C7H80         C88H150020Na         Cyclic         5         5         10         1514,0596         1,1         47504         1514,042471         12,416780088	1428.0245	c A6B3	C81H144O18Na	Cvclic	6	3	9	1428.0234	0.76	53733.2	1428.01104	9,419649708	1161
1451,9881         I_A485_C7H80         C82H140019Na         C7H70_H         4         5         9         1451,9868         0,9         216783,5         1451,99038         1,57442404         3552           1494,0351         I_A584_C7H80         C85H146019Na         C7H70_H         5         4         9         1494,0331         1,31         286080         1494,014932         13,46639192         6146           1514,0613         c_A585         C85H150020Na         Cyclic         5         5         10         1514,0596         1,1         47504         1514,042471         12,41678008         1049           1536,0820         I_A685_C7H80         C88H150020Na         Cyclic         5         5         10         1514,0596         1,1         47504         1514,042471         12,41678008         1049           1536,0820         I_A685_C7H80         C88H15020Na         Cyclic         5         5         10         1514,0596         1,1         47504         1514,042471         12,41678008         1049           1536,0821         I_A683,27H80         C88H152019Na         C7H70 H         6         3         9         1536,0811         0.59         24663,4         1536,08317         1536,08317,15,15,15,15,15,15,15,15,15,15,15,15,15,	1450.0452	A7B1 C7H8O	C84H146O17Na	С7Н7О Н	7	1	8	1450.0472	1.36	42270.5	1450.030103	10.42602319	3382
1494,0351         I_ASB4_C7H8O         C85H146019Na         C7H7O_H         5         4         9         1494,0331         1,31         286080         1494,01392         13,46639192         6146           1514,0613         c_ASB5         C85H150020Na         Cyclic         5         5         10         1514,0596         1,1         47504         1514,04271         12,41678008         1049           1536,0820         I_A6B3         C7H8O         C88H152019Na         C7H7O H         6         3         9         1536,0811         0.59         246633,4         1536,08751         15,153,588187         7607	1451,9881	L A4B5_C7H8O	C82H140O19Na	С7Н7О Н	4	5	9	1451,9868	0.9	216783.5	1451,990387	1.574424404	3552
1514,0613         c_ASB5         C85H150020Na         CVclic         5         5         10         1514,0596         1,1         47504         1514,042471         12,41678008         1049           1536,0820         I_A6B3         C7H80         C88H152019Na         C/CH7D         6         3         9         1536,0811         0.59         246633.4         1536,08751         15,13588187         7607	1494.0351	L A5B4_C7H8O	C85H146O19Na	С7Н7О Н	5	4	9	1494.0331	1.31	286080	1494.014932	13.46639192	6146
1536.0820   A6B3 C7H80 C88H152019Na C7H70 H 6 3 9 1536.0811 0.59 246633.4 1536.08751 15.1358.8187 7607	1514.0613	c A585	C85H150O20Na	Cyclic	5	5	10	1514.0596	1.1	47504	1514.042471	12,41678008	1049
	1536,0820	L A6B3 C7H8O	C88H152O19Na	C7H70 H	6	3	9	1536.0811	0.59	246633.4	1536.058751	15.13588187	7607



Figure S22. Contour-plots generated by the COCONUT software<sup>i</sup> from MALDI-ToF MS data of a  $P(CL^{nBu})_x$ -co- $(CL^{Me})_y$  copolymer (Left: linear population; Right: cyclic population) (Table 1, entry 3).



**Figure S23.** Contour-plots generated by the COCONUT<sup>i</sup> software from MALDI-ToF MS data of a  $P(CL^{nBu})_x$ -*co*-( $CL^{Me})_v$  copolymer (Left: linear population; Right: cyclic population) (Table 1, entry 1).

<sup>&</sup>lt;sup>i</sup> M. S. Engler, S. Crotty, M. J. Barthel, C. Pietsch, K. Knop, U. S. Schubert, S. Böcker, COCONUT-An efficient tool for estimating copolymer compositions from mass spectra. *Anal. Chem.*, **2015**, *87*, 5223-5231.



**Figure S24.** Contour-plots generated by the COCONUT software<sup>i</sup> from MALDI-ToF MS data of a  $P(CL^{nBu})_x$ -*co*-( $CL^{Me})_v$  copolymer (Left: linear population; Right: cyclic population) (Table 1, entry 6).



**Figure S25.** Contour-plots generated by the COCONUT software<sup>i</sup> from MALDI-ToF MS data of a  $P(CL^{nBu})_x$ -*co*-( $CL^{Me})_v$  copolymer (Left: linear population; Right: cyclic population) (Table 1, entry 2).



**Figure S26.** Representative SEC traces of homopolymers prepared from the ROP of *rac*-CL<sup>Me</sup> and *rac*-CL<sup>nBu</sup> with yttrium catalyst systems **1a-b**/BnOH (see Table S1, entries 1/(1-015); 2/(1-117); 5/(1-107); 6/(1-114)). \* stands for signal from residual ligand catalyst.



**Figure S27.** Representative SEC traces of copolymers prepared from the ROP of equimolar mixtures of (*S*)-CL<sup>Me</sup> and (*R*)-CL<sup>*n*Bu</sup> with yttrium catalyst systems **1a-b**/BnOH (see Table 1, entries 1-7). \* stands for signal from residual ligand catalyst



**Figure S28.** DSC thermogram (heating rate of 10 °C min<sup>-1</sup>, second heating cycle, from -80 to +200 °C) of a PCL<sup>Me</sup> homopolymer prepared from the ROP of *rac*-CL<sup>Me</sup> with the **1a**/BnOH catalyst system (Table S1, entry 1 /1-105).



**Figure S29.** DSC thermogram (heating rate of 10 °C min<sup>-1</sup>, second heating cycle, from -80 to +200 °C) of a PCL<sup>Me</sup> homopolymer prepared from the ROP of *rac*-CL<sup>Me</sup> with the Zn(BDI)/BnOH catalyst system (Table S1, entry 2 / 1-117).



**Figure S30.** DSC thermogram (heating rate of 10 °C min<sup>-1</sup>, second heating cycle, from -80 to +200 °C) of a PCL<sup>Me</sup> homopolymer prepared from the ROP of (*S*)-CL<sup>Me</sup> with the Zn(BDI)/BnOH catalyst system (Table S1, entry 4 / 1-193).



**Figure S31.** DSC thermogram (heating rate of 10 °C min<sup>-1</sup>, second heating cycle, from -80 to +200 °C) of a PCL<sup>*n*Bu</sup> homopolymer prepared from the ROP of *rac*-CL<sup>*n*Bu</sup> with the **1a**/BnOH catalyst system (Table S1, entry 5 / 1-107).



**Figure S32.** DSC thermogram (heating rate of 10 °C min<sup>-1</sup>, second heating cycle, from -80 to +200 °C) of a PCL<sup>*n*Bu</sup> homopolymer prepared from the ROP of *rac*-CL<sup>*n*Bu</sup> with the Zn(BDI)/BnOH catalyst system (Table S1, entry 6 / 1-114).



**Figure S33.** DSC thermogram (heating rate of 10 °C min<sup>-1</sup>, second heating cycle, from -80 to +200 °C) of a PCL<sup>*n*Bu</sup> homopolymer prepared from the ROP of *rac*-CL<sup>*n*Bu</sup> with the Zn(BDI)/BnOH catalyst system (Table S1, entry 8 / 1-164).



**Figure S34.** DSC thermogram (heating rate of 10 °C min<sup>-1</sup>, second heating cycle, from -80 to +200 °C) of a P(CL<sup>Me</sup>-*co*-CL<sup>*n*Bu</sup>) copolymer prepared from the ROCOP of a 1:1 mixture of (*S*)-CL<sup>Me</sup> and (*R*)-CL<sup>*n*Bu</sup> mediated by the **1a**/BnOH (1:1) catalyst system (Table 1, entry 1).



**Figure S35.** DSC thermogram (heating rate of 10 °C min<sup>-1</sup>, second heating cycle, from -80 to +200 °C) of a P(CL<sup>Me</sup>-*co*-CL<sup>*n*Bu</sup>) copolymer prepared from the ROCOP of a 1:1 mixture of (*S*)-CL<sup>Me</sup> and (*R*)-CL<sup>*n*Bu</sup> mediated by the **1b**/BnOH (1:1) catalyst system (Table 1, entry 6).



**Figure S36.** DSC thermogram (heating rate of 10 °C min<sup>-1</sup>, second heating cycle, from -80 to +200 °C) of a P(CL<sup>Me</sup>-*co*-CL<sup>*n*Bu</sup>) copolymer prepared from the ROCOP of a 1:1 mixture of (*S*)-CL<sup>Me</sup> and (*R*)-CL<sup>*n*Bu</sup> mediated by the **1b**/BnOH (1:1) catalyst system (Table 1, entry 7).