Supplemental information of “Homologous series of LC acrylic monomers based on phenyl benzoate core group: synthesis and characterization”

P. Romero-Hasler, D. Arismendi, P. Richter, E.A. Soto-Bustamante\*

Department of Organic and Physical Chemistry, Faculty of Chemical and Pharmaceutical Sciences, University of Chile, Sergio Livingstone 1007, Independencia, Santiago, Chile, email: esoto@ciq.uchile.cl

Department of Inorganic and Analytical Chemistry, Faculty of Chemical and Pharmaceutical Sciences, University of Chile, Sergio Livingstone 1007, Independencia, Santiago, Chile

 

Supplementary figure 1: ATR-FTIR spectra for A6E12.

Supplementary table 1: 1H NMR Chemical shift of the A6En monomers:

|  |
| --- |
|  |
| Compound | H1, dd | H2, dd | H3, dd | H4, t | H5, p | H6, p | H7, p | H8, p | H9, t |
| A6E1 | 5,83 | 6,41 | 6,13 | 4,05 | 1,73 | 1,50 | 1,50 | 1,85 | 4,18 |
| A6E2 | 5,82 | 6,41 | 6,13 | 4,05 | 1,73 | 1,50 | 1,50 | 1,84 | 4,18 |
| A6E3 | 5,82 | 6,41 | 6,13 | 4,05 | 1,73 | 1,50 | 1,50 | 1,82 | 4,18 |
| A6E4 | 5,82 | 6,41 | 6,12 | 4,05 | 1,78 | 1,50 | 1,50 | 1,78 | 4,18 |
| A6E5 | 5,82 | 6,41 | 6,13 | 4,05 | 1,78 | 1,44 | 1,44 | 1,78 | 4,18 |
| A6E6 | 5,82 | 6,41 | 6,12 | 4,05 | 1,78 | 1,48 | 1,48 | 1,78 | 4,18 |
| A6E7 | 5,82 | 6,41 | 6,13 | 4,05 | 1,78 | 1,49 | 1,49 | 1,78 | 4,18 |
| A6E8 | 5,82 | 6,41 | 6,12 | 4,05 | 1,78 | 1,47 | 1,47 | 1,78 | 4,18 |
| A6E9 | 5,82 | 6,41 | 6,13 | 4,05 | 1,78 | 1,50 | 1,50 | 1,78 | 4,18 |
| A6E10 | 5,82 | 6,41 | 6,12 | 4,05 | 1,78 | 1,49 | 1,49 | 1,78 | 4,18 |
| A6E11 | 5,82 | 6,41 | 6,13 | 4,05 | 1,78 | 1,51 | 1,51 | 1,78 | 4,18 |
| A6E12 | 5,82 | 6,41 | 6,13 | 4,05 | 1,78 | 1,51 | 1,51 | 1,78 | 4,18 |
|  |  |  |  |  |  |  |  |  |  |
| Compound | H10, d | H11, d | H12, d | H13, d | H14, t | H15, p | H16, p | H17, m | H18, t |
| A6E1 | 6,95 | 8,13 | 7,12 | 6,93 | - | - | - | - | 3,83\* |
| A6E2 | 6,96 | 8,13 | 7,10 | 6,92 | 4,05 | - | - | - | 1,43 |
| A6E3 | 6,96 | 8,13 | 7,10 | 6,92 | 3,93 | 1,82 | - | - | 1,04 |
| A6E4 | 6,95 | 8,13 | 7,09 | 6,92 | 3,97 | 1,78 | 1,50 | - | 0,98 |
| A6E5 | 6,96 | 8,13 | 7,10 | 6,92 | 3,96 | 1,78 | 1,44 | 1,44 | 0,94 |
| A6E6 | 6,95 | 8,13 | 7,09 | 6,91 | 3,96 | 1,78 | 1,48 | 1,35 | 0,91 |
| A6E7 | 6,96 | 8,13 | 7,09 | 6,92 | 3,95 | 1,78 | 1,49 | 1,32 | 0,90 |
| A6E8 | 6,95 | 8,13 | 7,09 | 6,91 | 3,95 | 1,79 | 1,47 | 1,31 | 0,89 |
| A6E9 | 6,96 | 8,13 | 7,09 | 6,92 | 3,95 | 1,78 | 1,50 | 1,28 | 0,89 |
| A6E10 | 6,95 | 8,13 | 7,09 | 6,91 | 3,95 | 1,79 | 1,49 | 1,28 | 0,88 |
| A6E11 | 6,96 | 8,13 | 7,09 | 6,92 | 3,95 | 1,78 | 1,51 | 1,27 | 0,87 |
| A6E12 | 6,96 | 8,13 | 7,09 | 6,91 | 3,95 | 1,78 | 1,51 | 1,27 | 0,88 |

1H-NMR at 300 MHZ. s, singlet; d, duplet; dd, double duplet; t, triplet; q, quartet; p, pentuplet; m, multiplet.

Supplementary table 2: List of ESI-MS masses observed for A6En. For each compound, the rows are [M-Na+], [M-K+] and [2M-Na+] respectively.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Monomers | Formula | Adduct | Theoretical (Da) | Experimental (Da) | Error (ppm) |
| A6E1 | C23H26O6 | [M+Na]+ | 421,1622 | 421,1691 | -16 |
| [M+K]+ | 437,1361 | 437,1429 | -16 |
| [2M+Na]+ | 819,3351 | 819,3455 | -13 |
| A6E2 | C24H28O6 | [M+Na]+ | 435,1778 | 435,1821 | -10 |
| [M+K]+ | 451,1518 | 451,1584 | -15 |
| [2M+Na]+ | 847,3664 | 847,3720 | -7 |
| A6E3 | C25H30O6 | [M+Na]+ | 449,1935 | 449,2016 | -18 |
| [M+K]+ | 465,1674 | 465,1758 | -18 |
| [2M+Na]+ | 875,3977 | 875,4111 | -15 |
| A6E4 | C26H32O6 | [M+Na]+ | 463,2091 | 463,2185 | -20 |
| [M+K]+ | 479,1830 | 479,1917 | -18 |
| [2M+Na]+ | 903,4290 | 903,4470 | -20 |
| A6E5 | C27H34O6 | [M+Na]+ | 477,2248 | 477,2280 | -7 |
| [M+K]+ | 493,1987 | 493,2004 | -3 |
| [2M+Na]+ | 931,4603 | 931,4660 | -6 |
| A6E6 | C28H36O6 | [M+Na]+ | 491,2404 | 491,2499 | -19 |
| [M+K]+ | 507,2143 | 507,2226 | -16 |
| [2M+Na]+ | 959,4916 | 959,5083 | -17 |
| A6E7 | C29H38O6 | [M+Na]+ | 505,2561 | 505,2585 | -5 |
| [M+K]+ | 521,2299 | 521,2318 | -4 |
| [2M+Na]+ | 987,5229 | 987,5266 | -4 |
| A6E8 | C30H40O6 | [M+Na]+ | 519,2717 | 519,2789 | -14 |
| [M+K]+ | 535,2456 | 535,2521 | -12 |
| [2M+Na]+ | 1015,5542 | 1015,5719 | -17 |
| A6E9 | C31H42O6 | [M+Na]+ | 533,2874 | 533,2949 | -14 |
| [M+K]+ | 549,2613 | 549,2687 | -13 |
| [2M+Na]+ | 1043,5855 | 1043,5994 | -13 |
| A6E10 | C32H44O6 | [M+Na]+ | 547,3030 | 547,3116 | -16 |
| [M+K]+ | 563,2769 | 563,2871 | -18 |
| [2M+Na]+ | 1071,6168 | 1071,6360 | -18 |
| A6E11 | C33H46O6 | [M+Na]+ | 561,3187 | 561,3267 | -14 |
| [M+K]+ | 577,2926 | 577,2995 | -12 |
| [2M+Na]+ | 1099,6481 | 1099,6655 | -16 |
| A6E12 | C34H48O6 | [M+Na]+ | 575,3343 | 575,3448 | -18 |
| [M+K]+ | 591,3082 | 591,3174 | -16 |
| [2M+Na]+ | 1127,6794 | 1127,7002 | -18 |