Supporting Information for

Design of the new closo-dodecarborate-containing gemcitabine analogue for the albumin-based theranostics composition.

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Spectral data for new compounds

4-N-benzoyl-2′-deoxy-2′,2′-difluorocytidine (2)

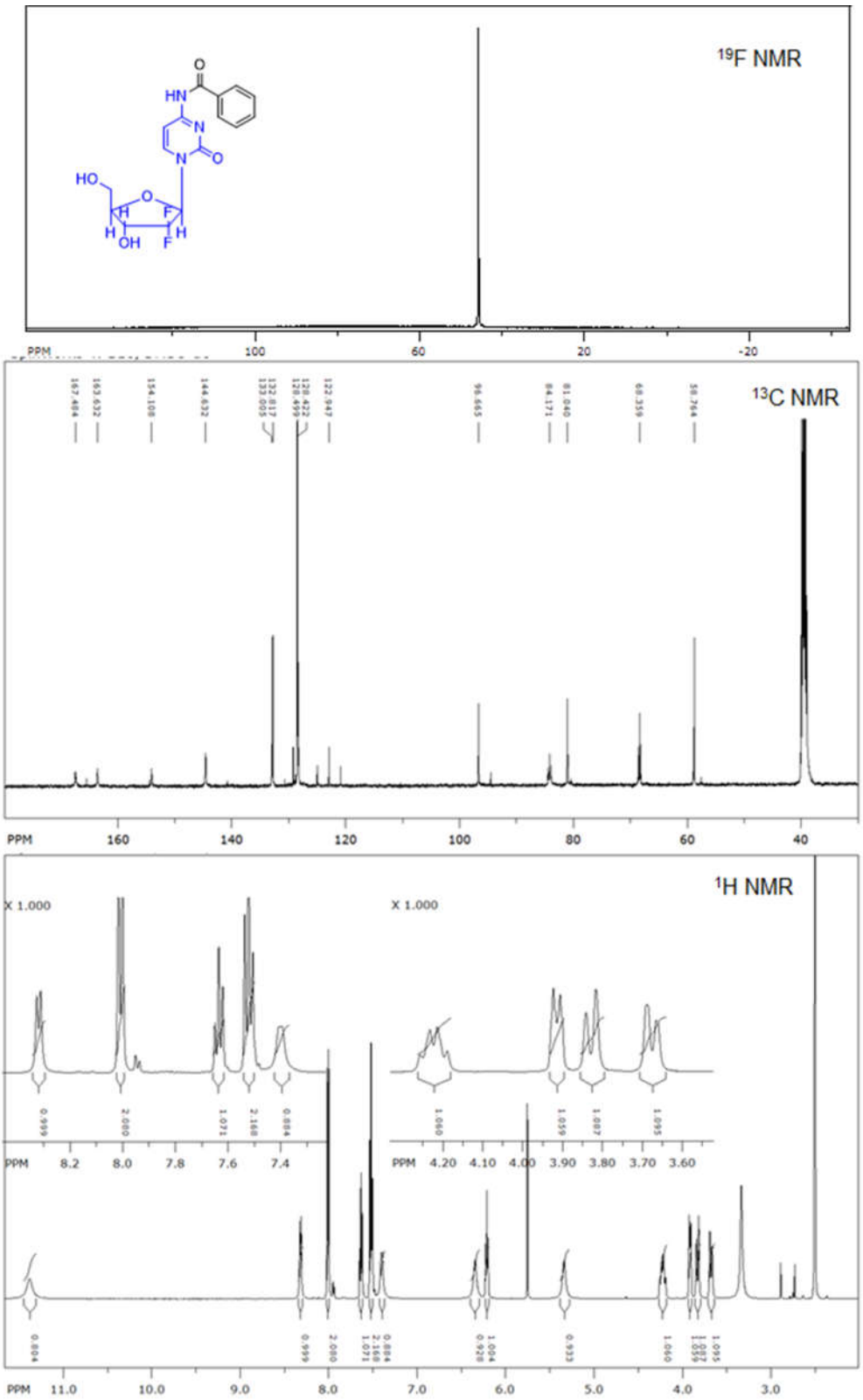

Figure S1. Characterisics of the 4-*N*-benzoyl-2′-deoxy-2′,2′-difluorocytidine.

4-N-(2-dimethylaminoethyl)-2′-deoxy-2′,2′-difluorocytidine (3)

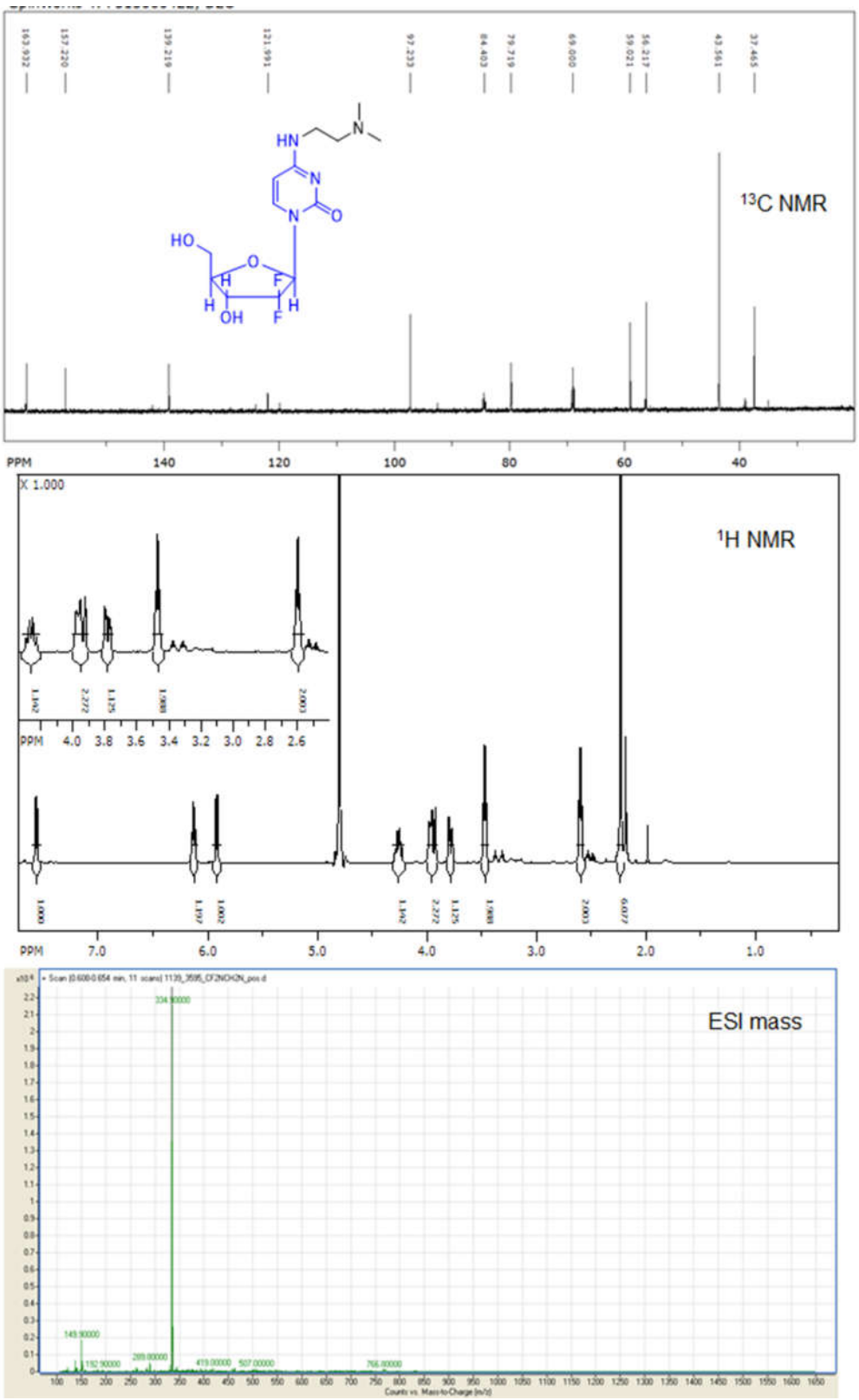

Figure S2. Characterisics of the 4-*N*-(2-dimethylaminoethyl)-2′-deoxy-2′,2′-difluorocytidine

H⁺[Conjugate 5]⁻

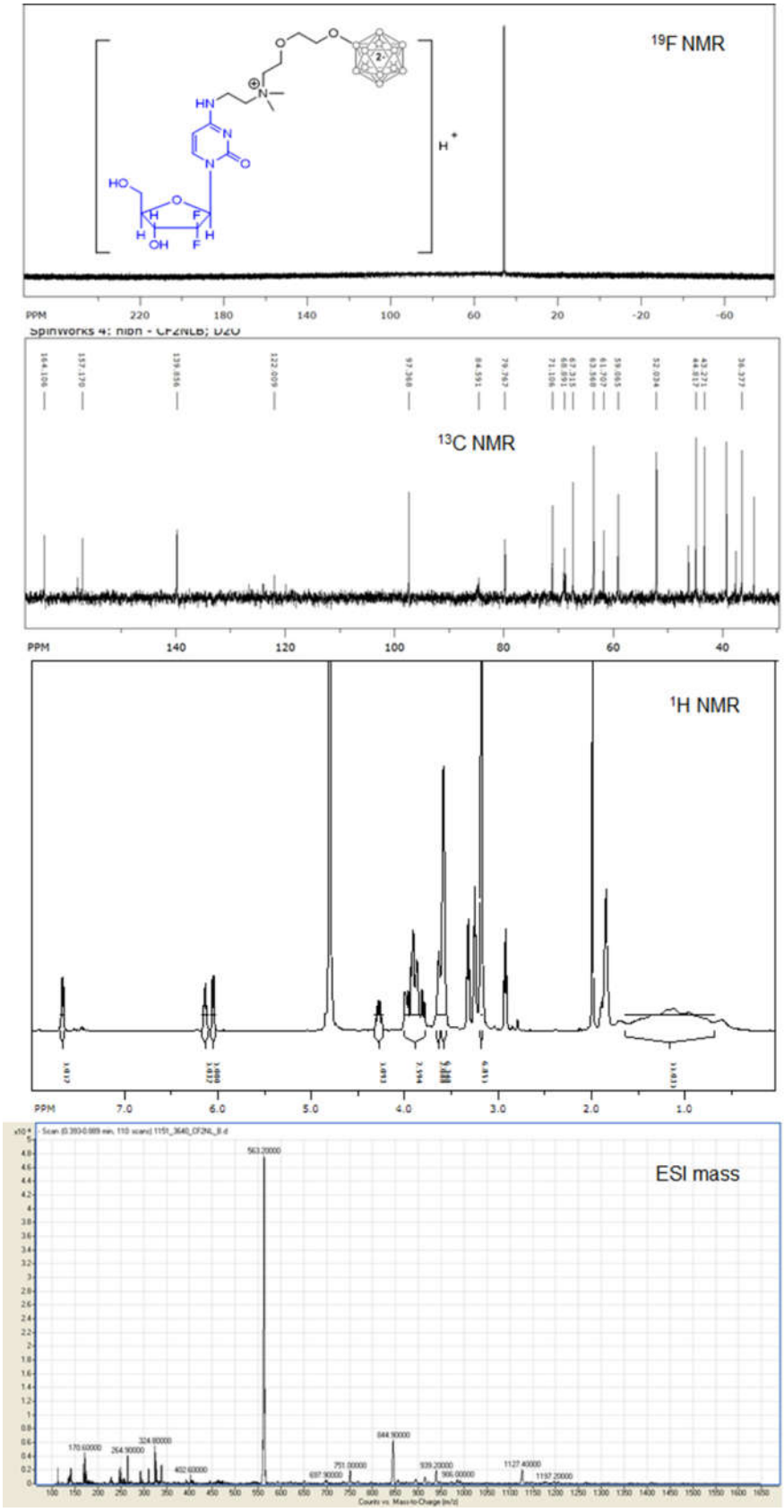

Figure S3. Characterisics of the H⁺[Compound 5]⁻.

[Compound 6](TEA)$_3$

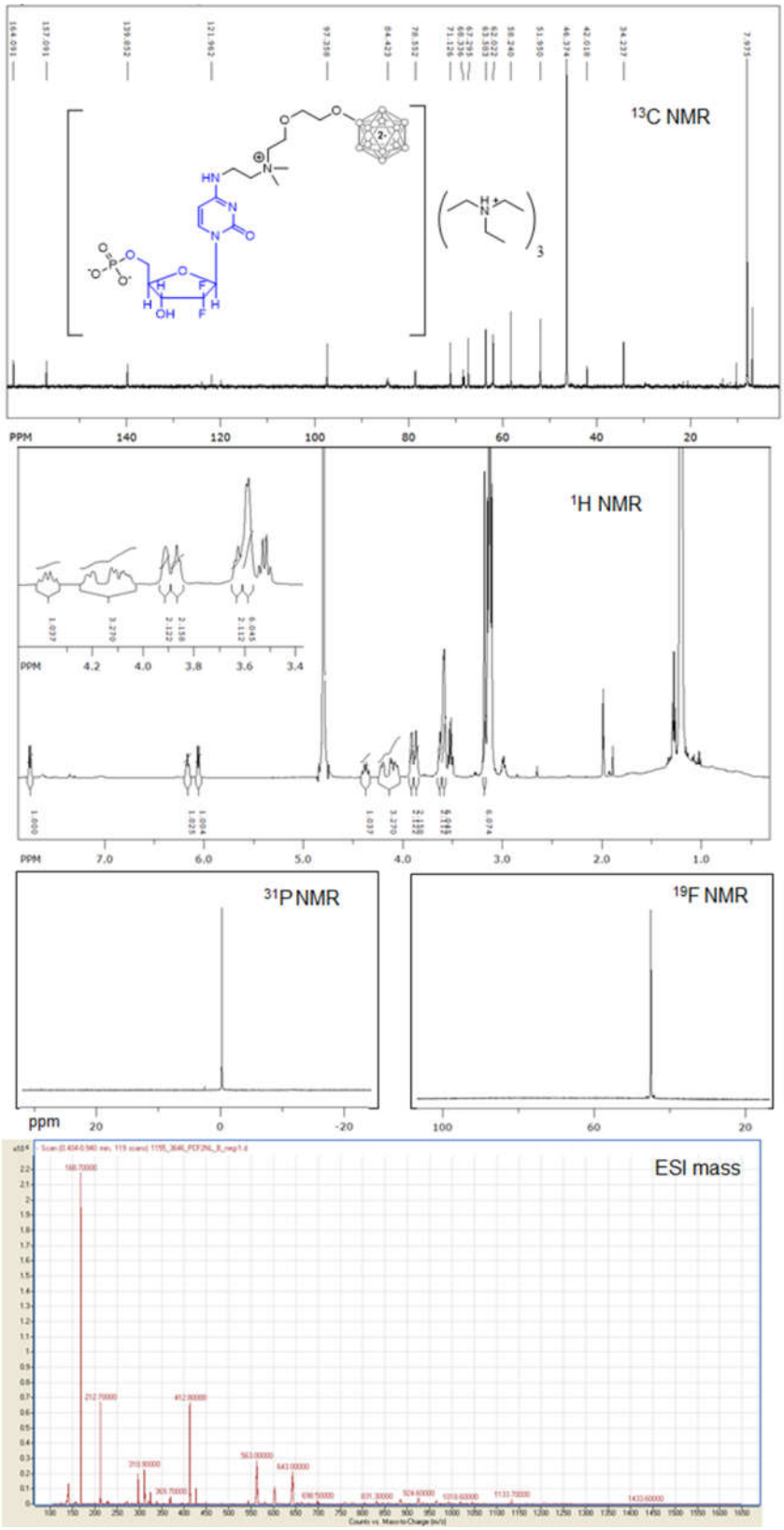

Figure S4. Characterisics of the [Compound 6](TEA)$_3$.

[Compound 7](TEA)$_2$

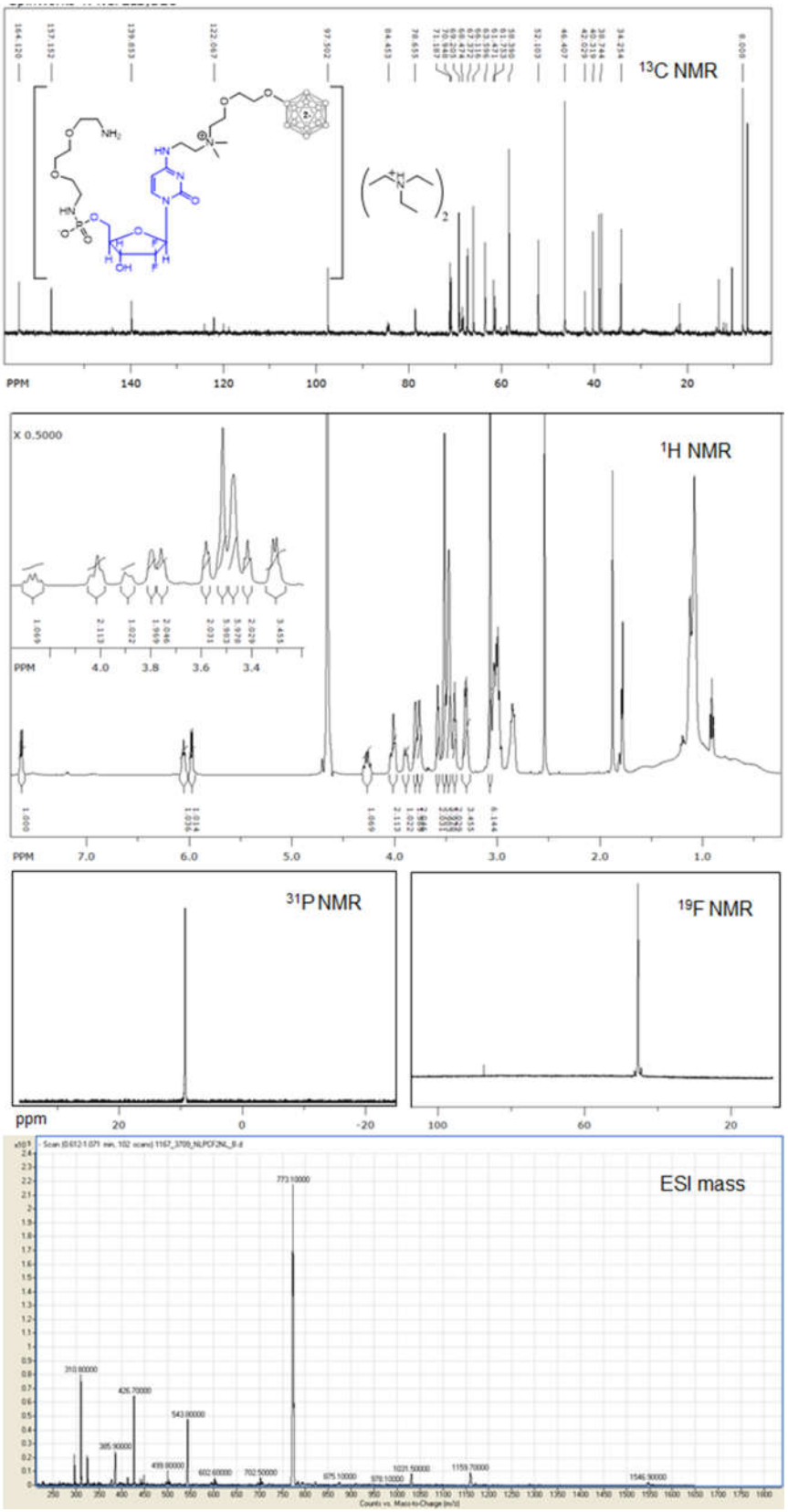

Figure S5. Characterisics of the [Compound 7](TEA)$_2$.

[Compound 1](TEA)$_2$

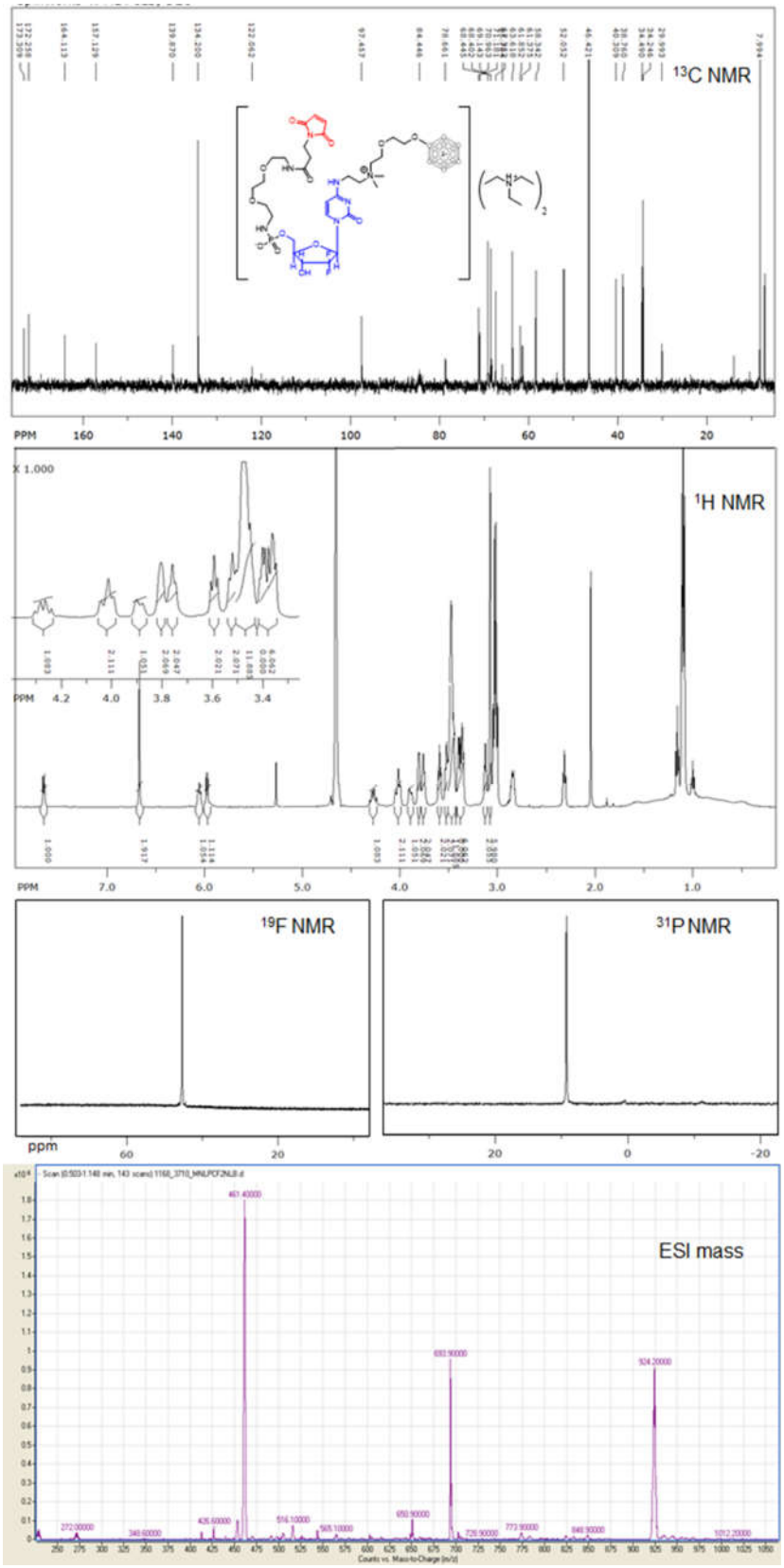

Figure S6. Characterisics of the [Compound 1](TEA)$_2$.

Compound 9

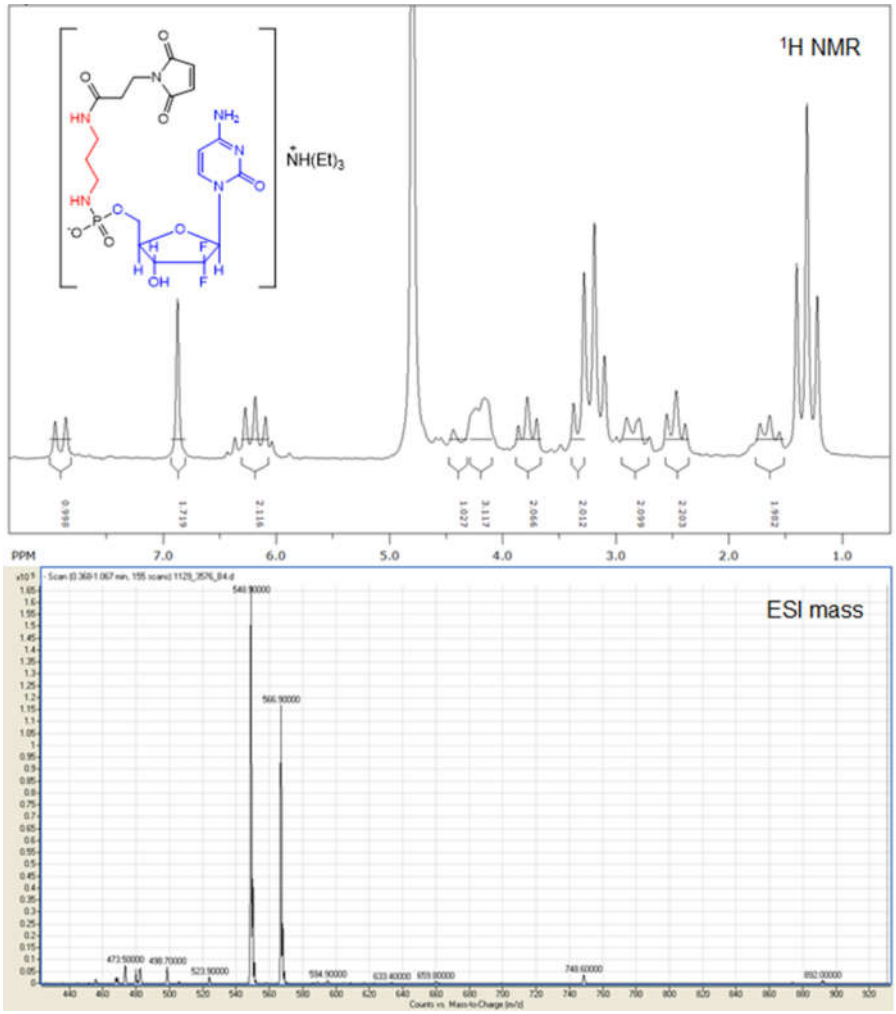

Figure S7. Characterisics of the [Compound 9](TEA).

^{1}H NMR (D_2O): 7.91 (1H, d, *J* 7.6, H6), 6.88 (2H, s, CH=CH), 6.31-6.07 (2H, m, H1', H5), 4.47-4.31 (1H, m, H3'), 4.30-4.09 (3H, m, H4', H5'), 3.78 (2H, t, *J* 6.5, CH2N), 3.39-3.28 (2H, m, CH_2NHCO), 2.95-2.71 (2H, m, CH_2CO), 2.46 (2H, t, *J* 6.5, CH_2NHP), 1.64 (2H, t, *J* 6.8, CH_2). $[M-H]^-$ calcd. for $C_{19}H_{24}F_2N_6O_9P^-$ 549.13; found 548.90.

*Compound 9**

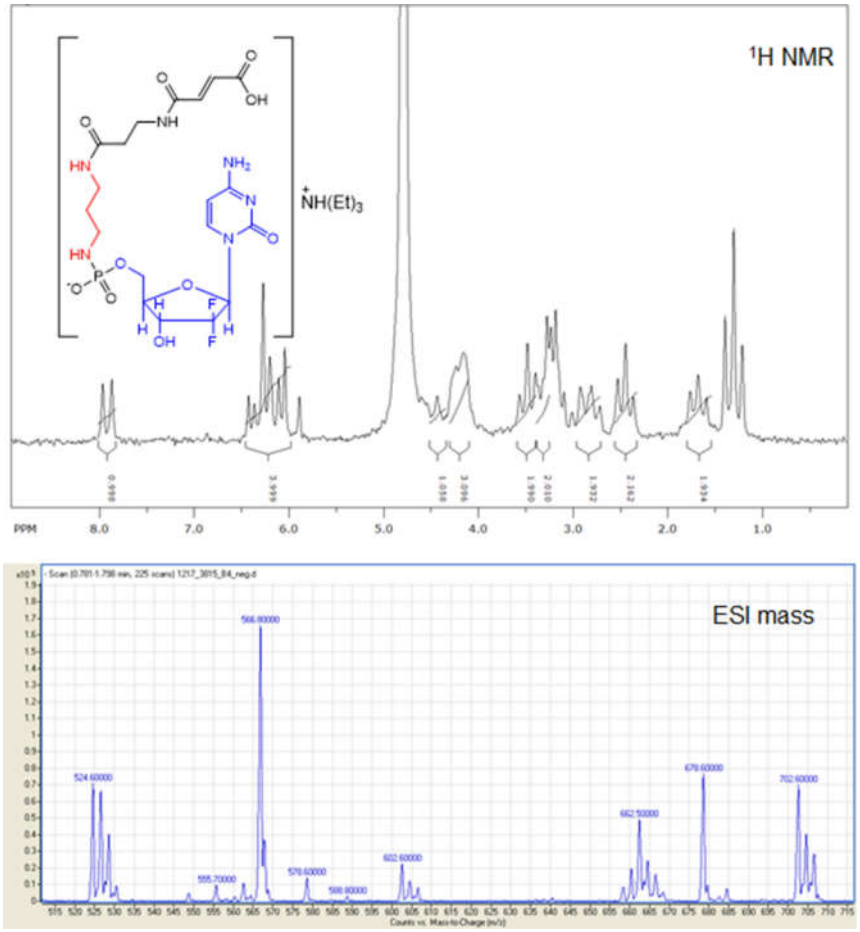

Figure S8. Characterisics of the [Compound 9*](TEA).

^{1}H NMR (D_2O): 7.92 (1H, d, *J* 7.6, H6), 6.46-5.98 (4H, m, CH=CH, H5, H1′), 4.52-4.34 (1H, m, H3′), 4.30-4.10 (3H, m, H4′, H5′), 3.48 (2H, t, *J* 6.7, CH_2NH), 3.38-3.25 (2H, m, CH_2NHCO), 2.96-2.71 (2H, m, CH_2CO), 2.45 (2H, t, *J* 6.7, CH_2NHP), 1.68 (2H, t, *J* 6.8, CH_2). $[M-H]^-$ calcd. for $C_{19}H_{26}F_2N_6O_{10}P^-$ 567.14; found 566.90.

Compound 10

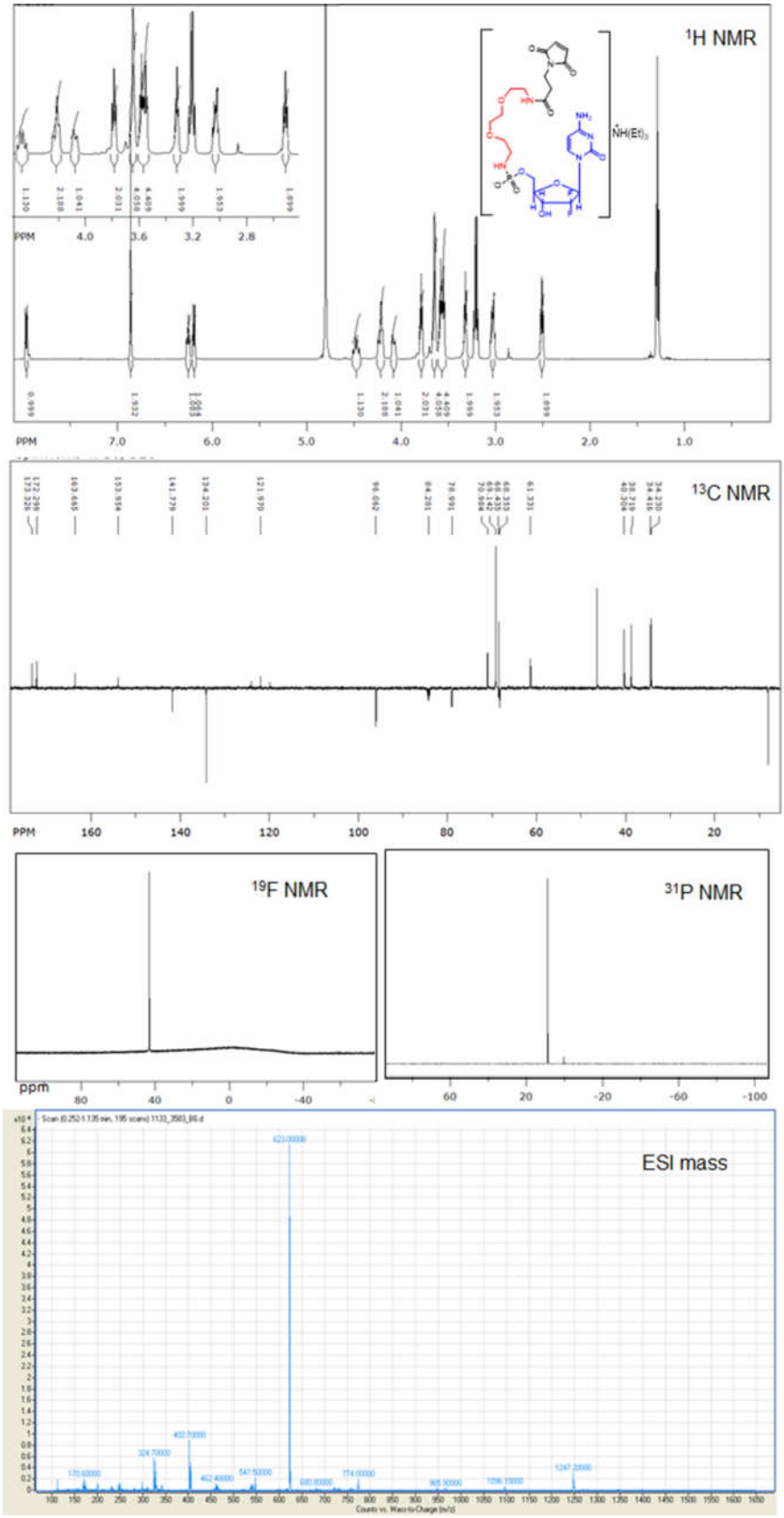

Figure S9. Characterisics of the [Compound 10](TEA).

^{1}H NMR (D_2O): 7.97 (1H, d, *J* 7.7, H6), 6.86 (2H, s, CH=CH), 6.26 (1H, t, *J* 7.1, H1'), 6.20 (1H, d, *J* 7.7, H5), 4.52-4.43 (1H, m, H3'), 4.26-4.18 (2H, m, H5'), 4.11-4.05 (1H, m, H4'), 3.79 (2H, t, *J* 6.3, CH_2N), 3.67-3.62 (4H, m, CH_2O), 3.58 (2H, t, *J* 5.5, O$\underline{CH_2}CH_2O$), 3.55 (2H, t, *J* 5.5, $OCH_2\underline{CH_2}O$), 3.32 (2H, br t, *J* 5.3, $\underline{CH_2}NHCO$), 3.05-3.01 (2H, m, $\underline{CH_2}NHP$), 2.51 (2H, t, *J* 6.4, $\underline{CH_2}CONH$). ^{13}C NMR (D_2O): 173.33, 172.30, 163.67, 153.95, 141.78, 134.20, 121.97 (t, J_{CF} 259), 96.06, 84.28 (t, J_{CF} 23), 78.99, 70.98, 69.14, 68.44, 68.35 (t, J_{CF} 23), 61.33, 40.30, 38.72, 34.42, 34.23. ^{19}F NMR (D_2O): 43.14 (br s, CF_2). ^{31}P NMR: 8.67 (s). $[M-H]^-$ calcd. for $C_{22}H_{30}F_2N_6O_{11}P^-$ 623.17; found 623.00.

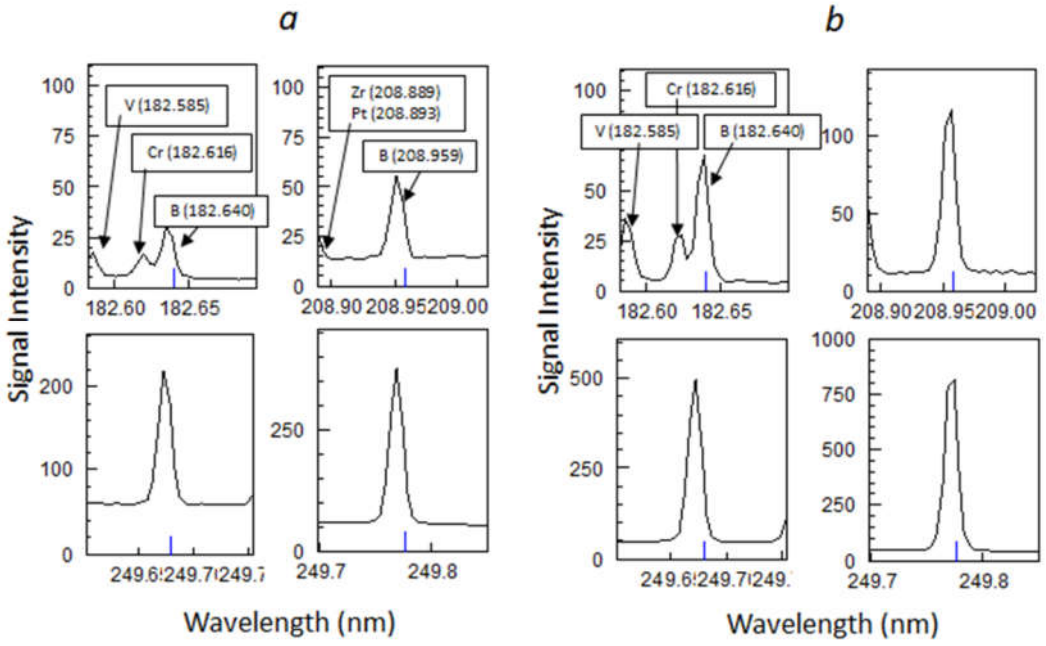

Figure S10. Inductively coupled plasma atomic emission spectrometry (ICP AES) for HSA-Cy5-HcyTFAc-GC$B_{12}H_{11}$ (*a*) and HSA-Cy7-HcyTFAc-GC$B_{12}H_{11}$ (*b*). Boron spectral lines 182.640, 208.959, 249.678 and 249.773 nm.

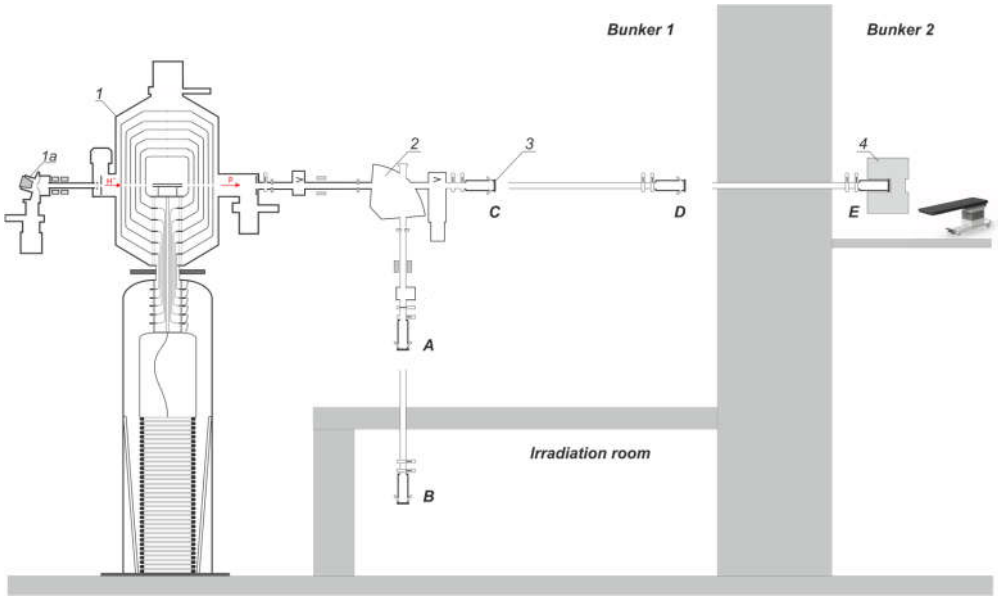

Figure S11. Layout of the experimental facility: *1* – vacuum insulated tandem accelerator, *2* – bending magnet, *3* – lithium target, *4* – beam shaping assembly. *A*, *B*, *C*, *D*, *E* – lithium target placement positions.