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Construction of hydrogen bonding and coordination networks based on ethynylpyridine-appended nucleobases

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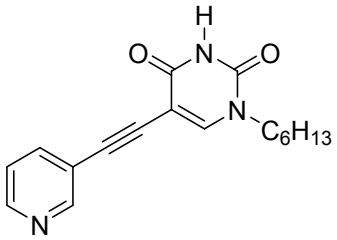


Chemical Formula:
$C_{17}H_{19}N_3O_2$
Exact Mass: 297,15
Molecular Weight: 297,36

Fig. ESI 1. ^{1}H NMR spectrum of **C_6U-3Py** (500 MHz, d_6-DMSO, 298 K). * = water.

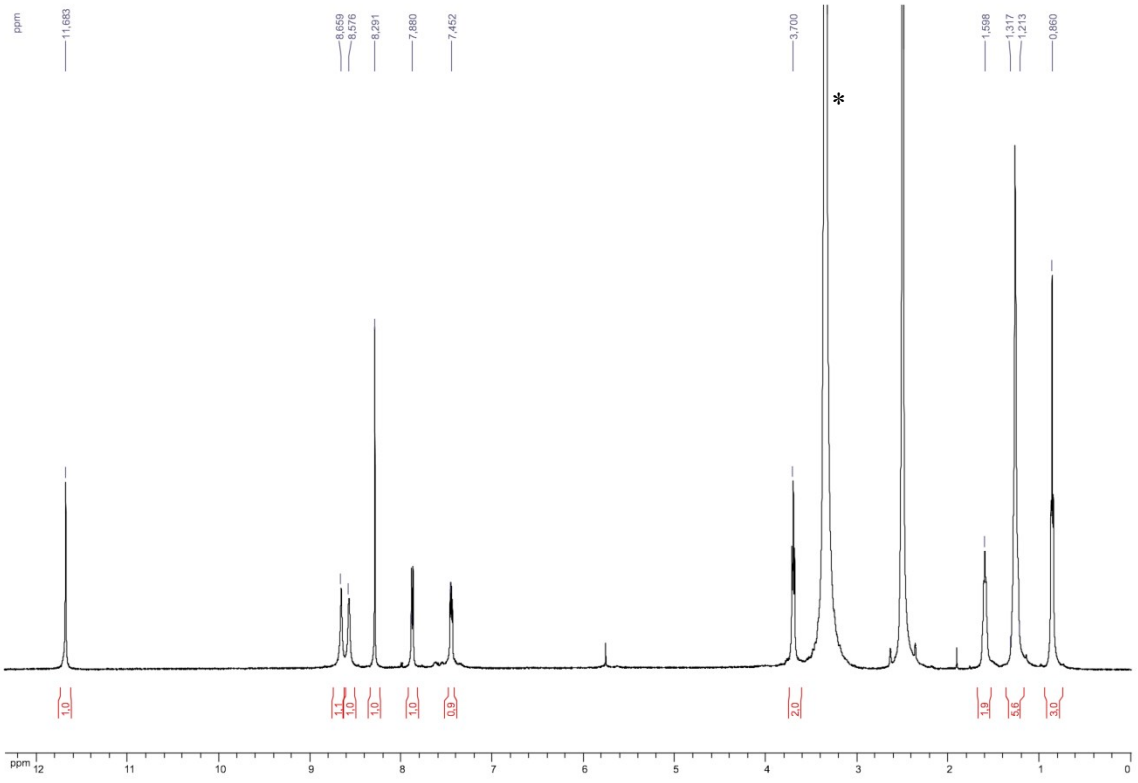


Fig. ESI 2. ^{13}C NMR spectrum of **C_6U-3Py** (125 MHz, d_6-DMSO, 298 K)

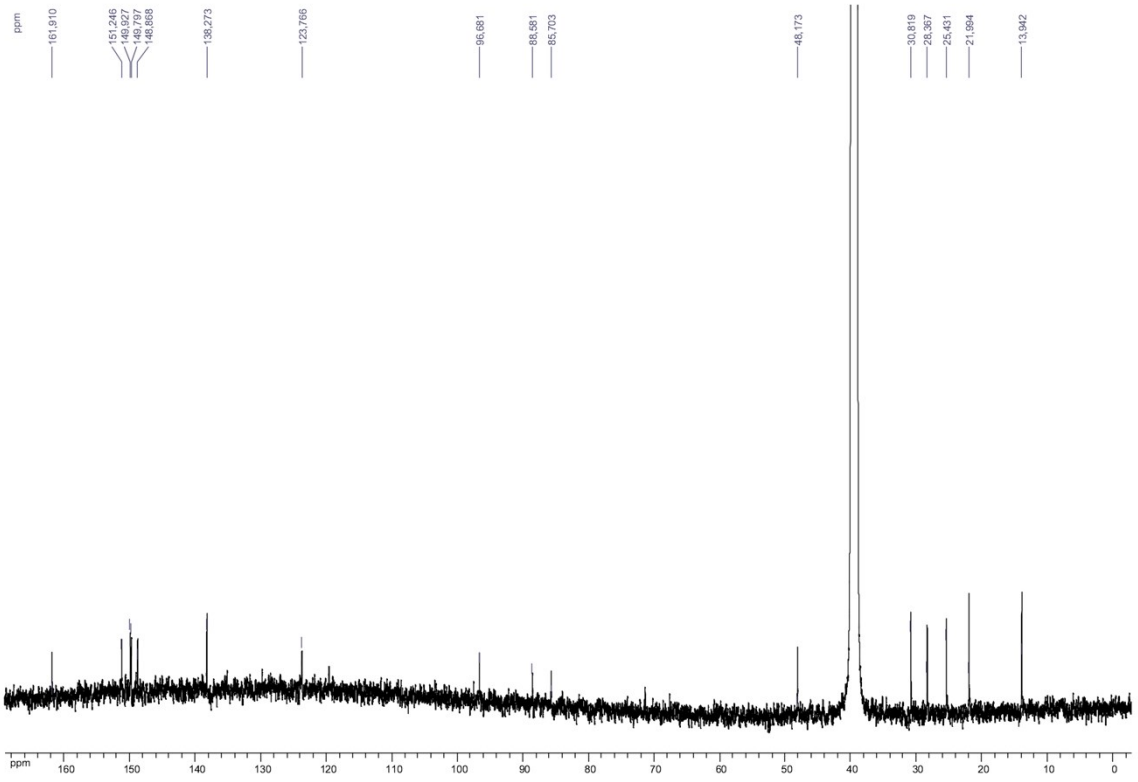


Fig. ESI 3. ^1H-^1H COSY map of **C_6U-3Py** (500 MHz, d_6-DMSO, 298K)

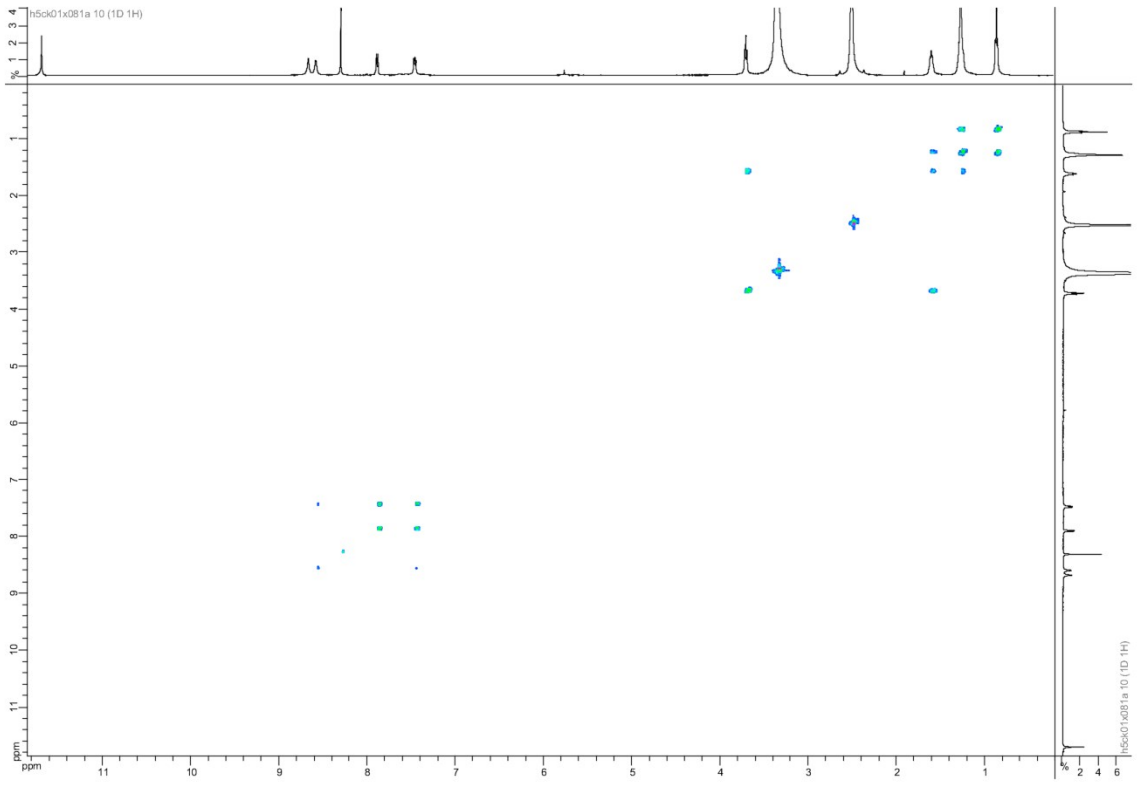


Fig. ESI 4. ^{1}H-^{13}C HMBC (pink) and HSQC (blue) map of **C_6U-3Py** (500 MHz, d_6-DMSO, 298K)

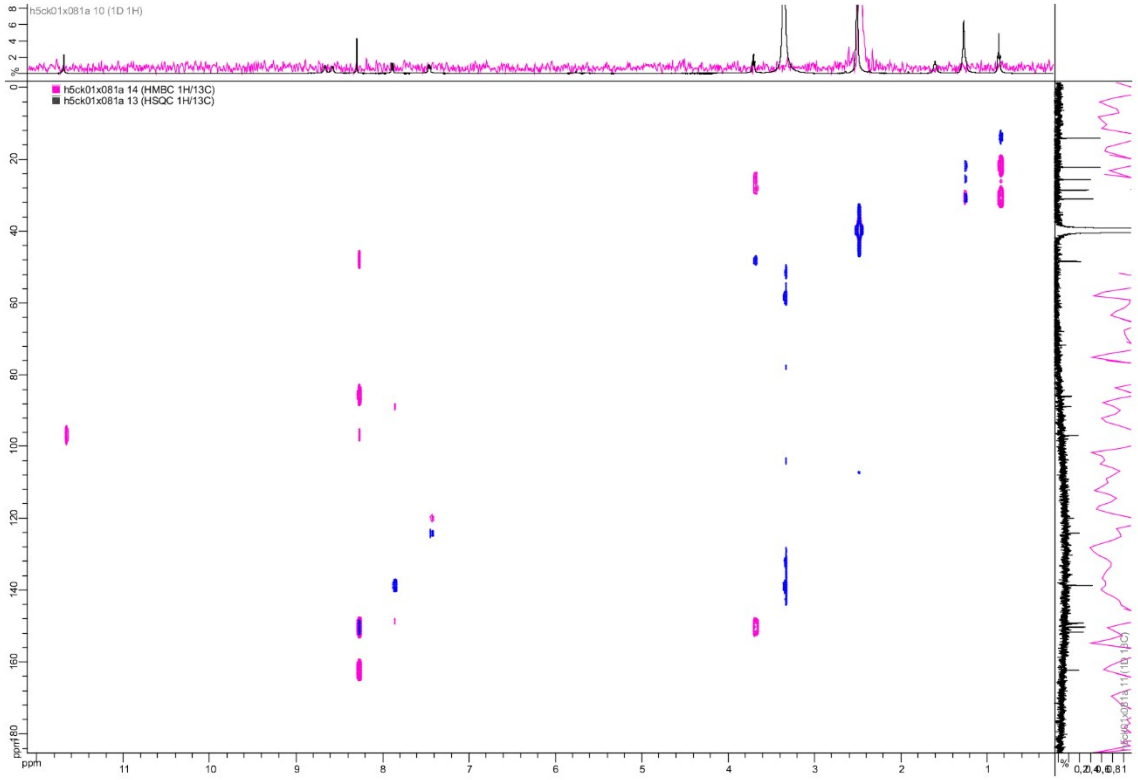
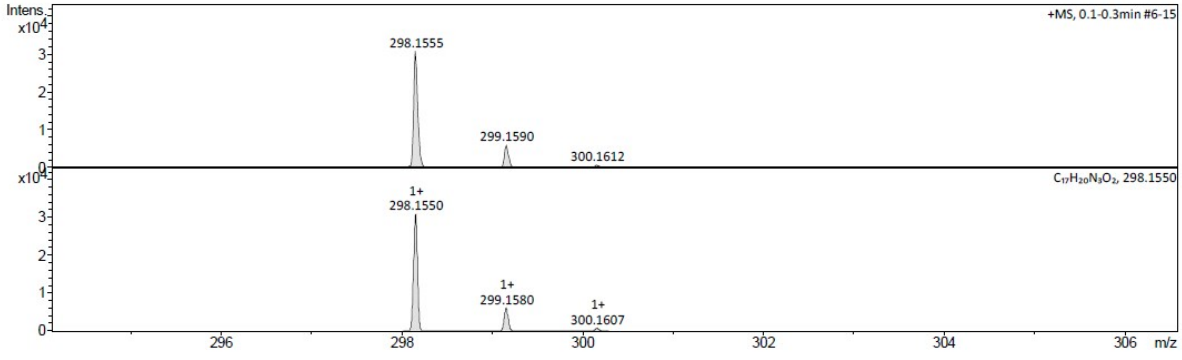
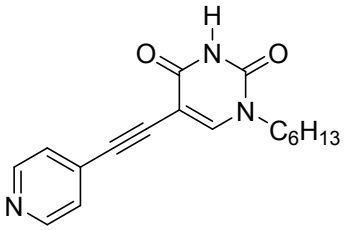


Fig. ESI 5. HRMS calculated for $C_{17}H_{20}N_3O_2$ $[M+H]^+$: 298.1550, found : 298.1555.



Meas. m/z	#	Ion Formula	m/z err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I	VarNorm Std m/z	Diff Std Comb Dev
298.155469	1	C17H20N3O2	298.155003	-1.6	-2.0	9.5	ok	even	2.7	4.1	n.a.	n.a.	n.a.	n.a.



Chemical Formula:
$C_{17}H_{19}N_3O_2$
Exact Mass: 297,15
Molecular Weight: 297,36

Fig. ESI 6. ^{1}H NMR spectrum of **C_6U-4Py** (500 MHz, $CDCl_3$, 298 K)

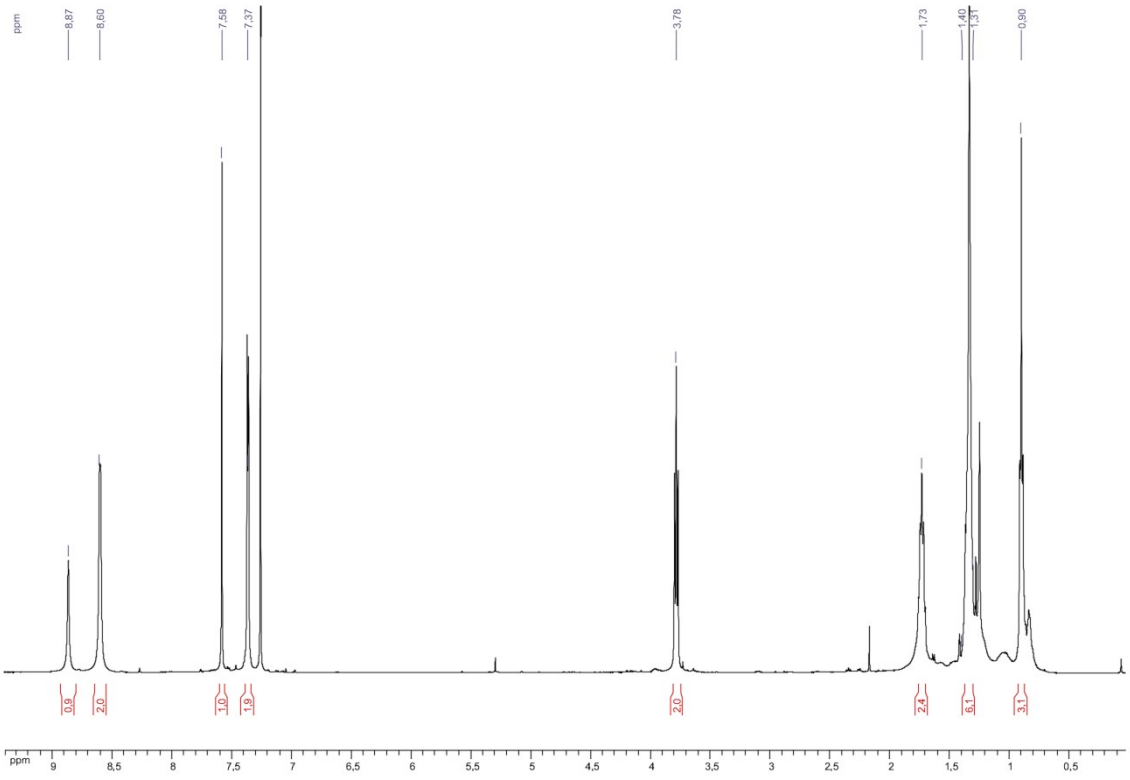


Fig. ESI 7. ^{13}C NMR spectrum of **C_6U-4Py** (125 MHz, $CDCl_3$, 298 K)

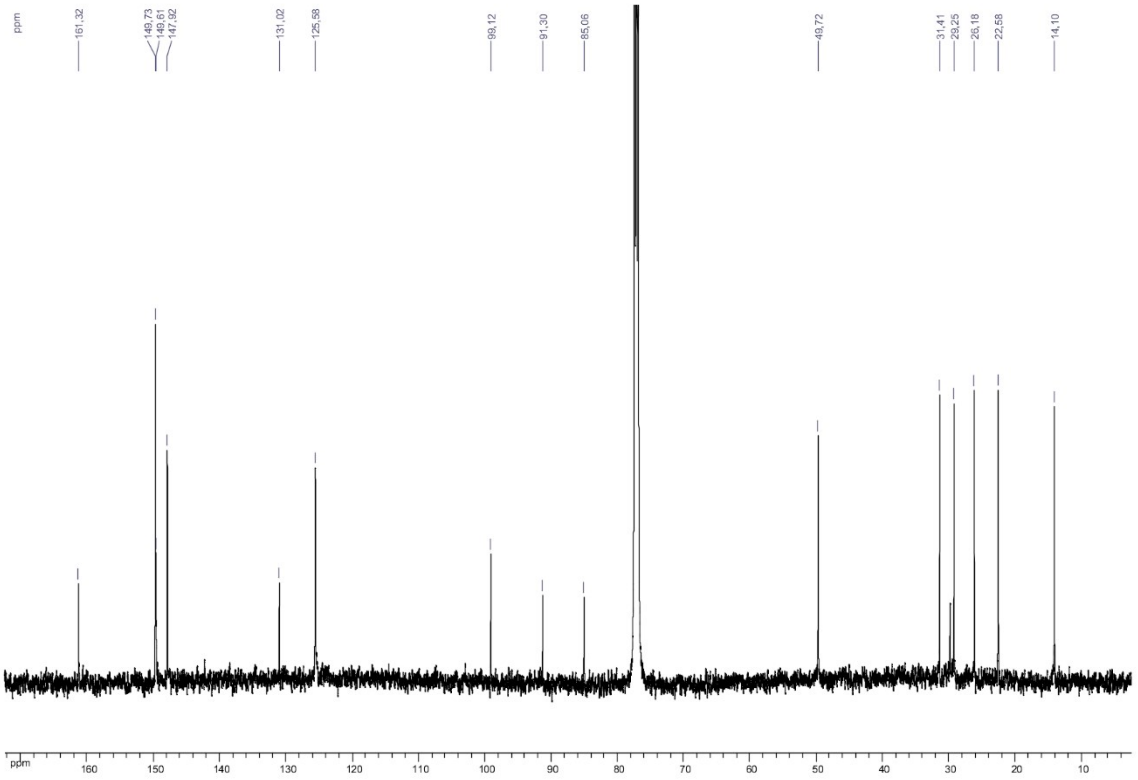


Fig. ESI 8. ^1H-^1H COSY map of **C_6U-4Py** (500 MHz, $CDCl_3$, 298K)

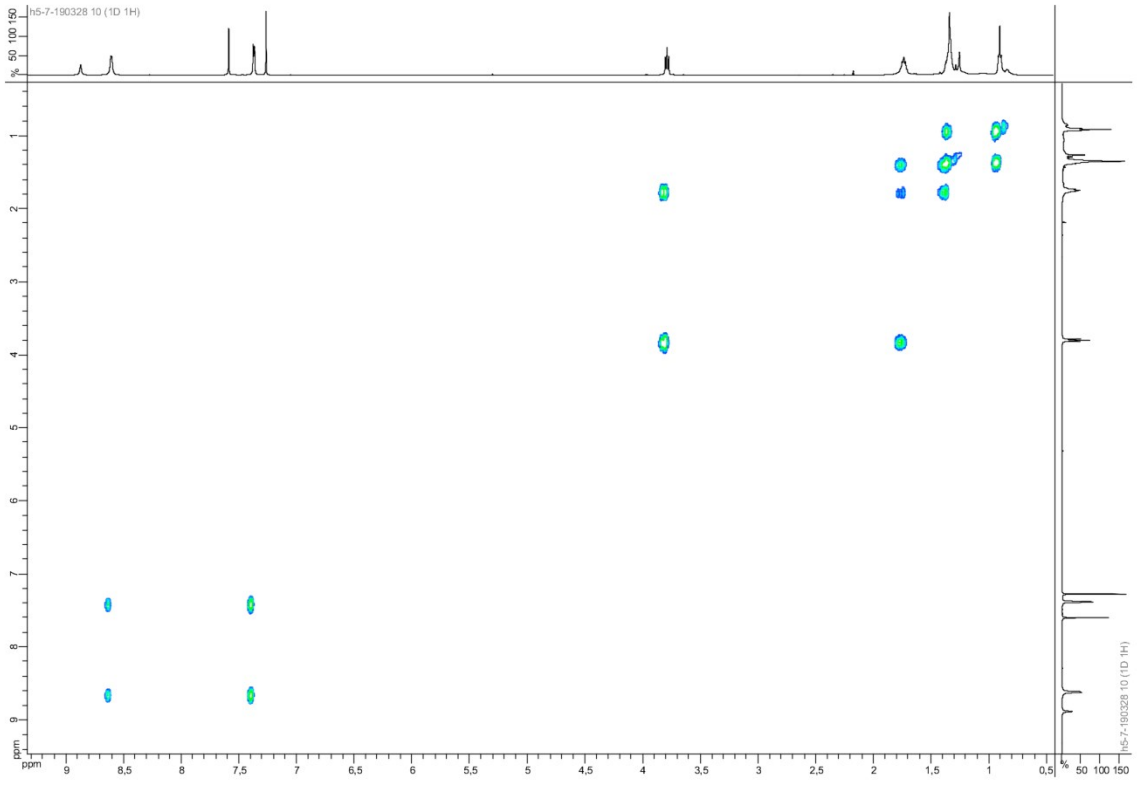


Fig. ESI 9. ^{1}H-^{13}C HMBC (pink) and HSQC (blue) map of **C_6U-4Py** (500 MHz, $CDCl_3$, 298K)

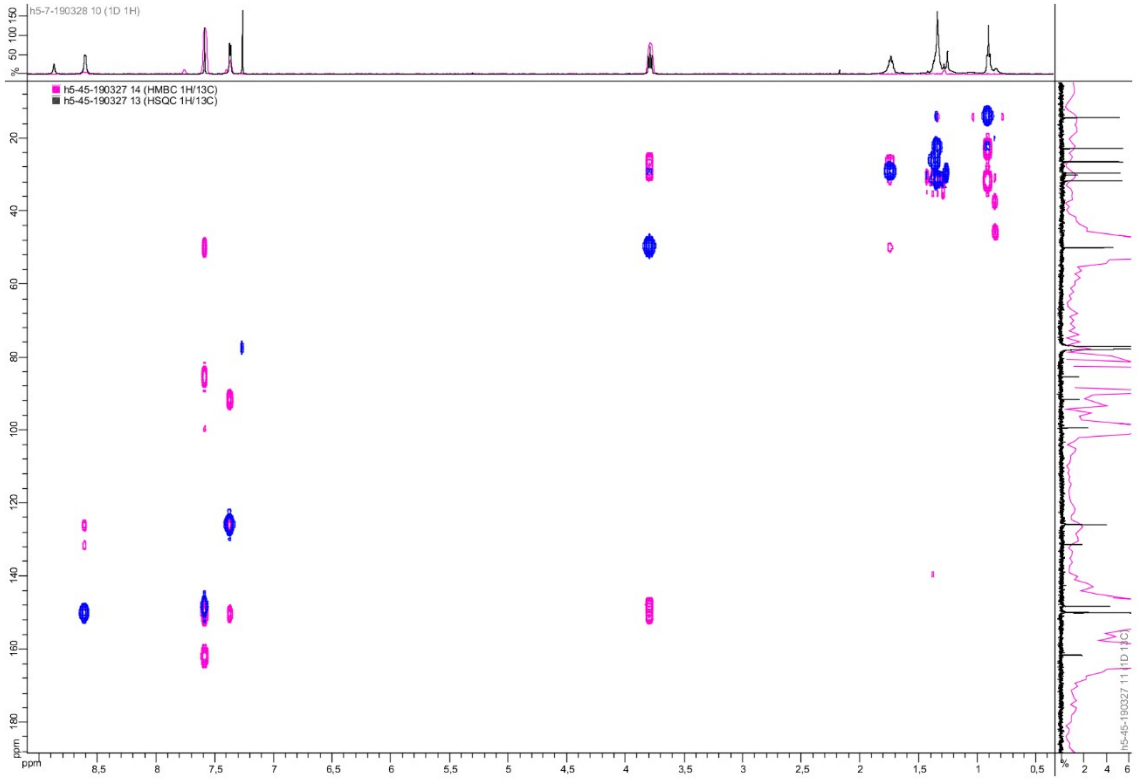
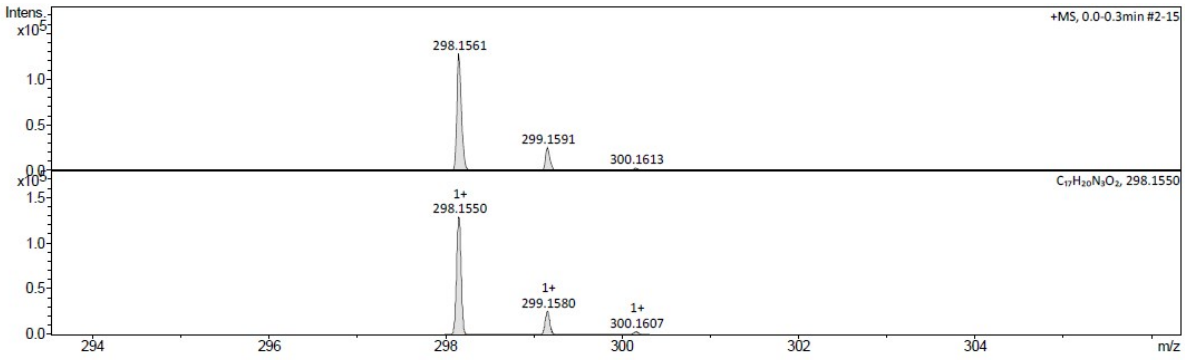
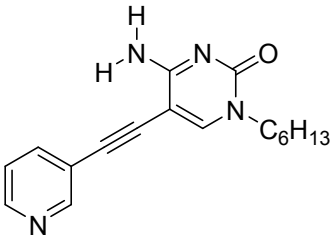


Fig. ESI 10. HRMS calculated for $C_{17}H_{20}N_3O_2$ $[M+H]^+$: 298.1550, found : 298.1561.



Meas. m/z	#	Ion Formula	m/z err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
298.156104	1	C17H20N3O2	298.155003	-3.7	-3.3	9.5	ok	even	0.8	1.2	n.a.	n.a.	n.a.	n.a.



Chemical Formula:
$C_{17}H_{20}N_4O$
Exact Mass: 296,16
Molecular Weight: 296,37

Fig. ESI 11. ^{1}H NMR spectrum of **C_6C-3Py** (500 MHz, d_6-DMSO, 298 K). * = water.

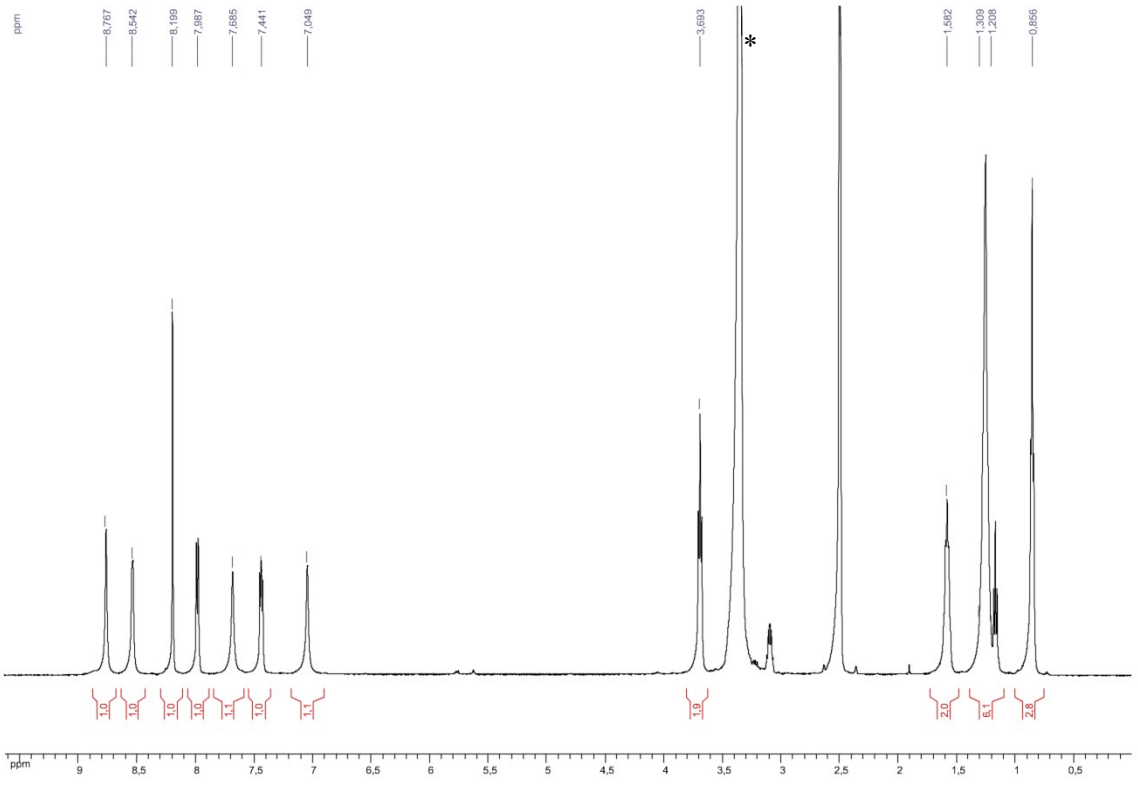


Fig. ESI 12. ^{13}C NMR spectrum of **C_6C-3Py** (125 MHz, d_6-DMSO, 298 K)

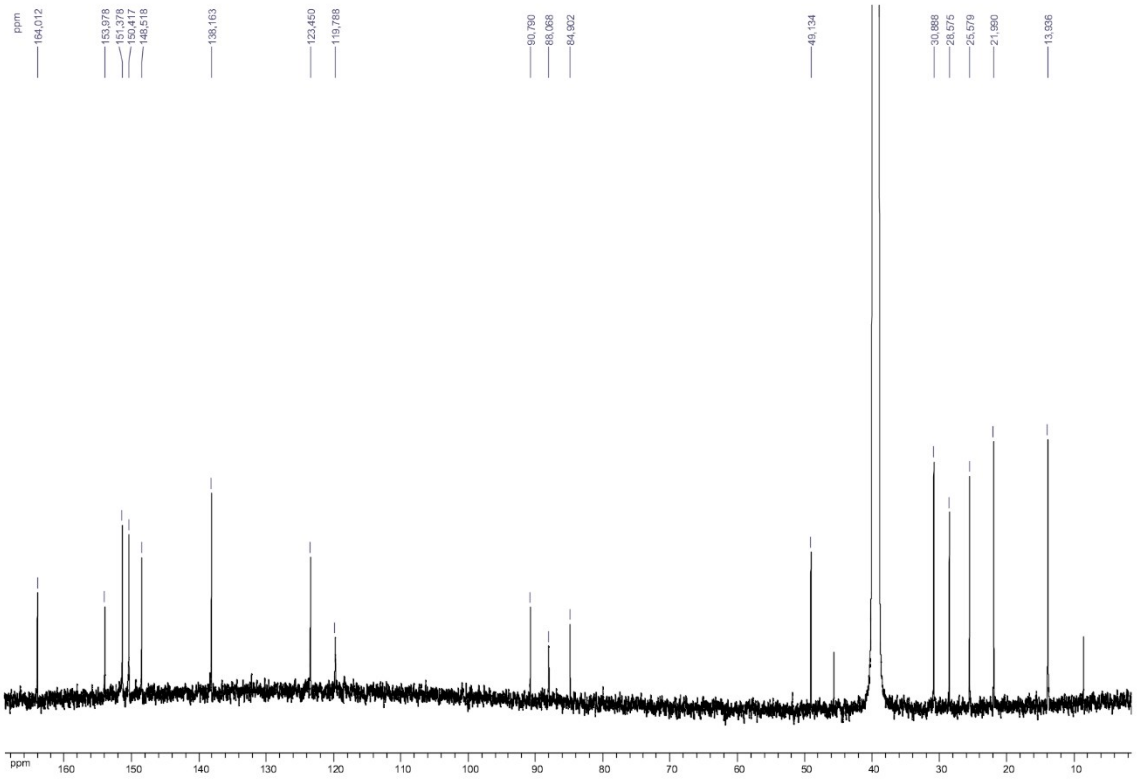


Fig. ESI 13. ^{1}H-^{1}H COSY map of **C_6C-3Py** (500 MHz, d_6-DMSO, 298K)

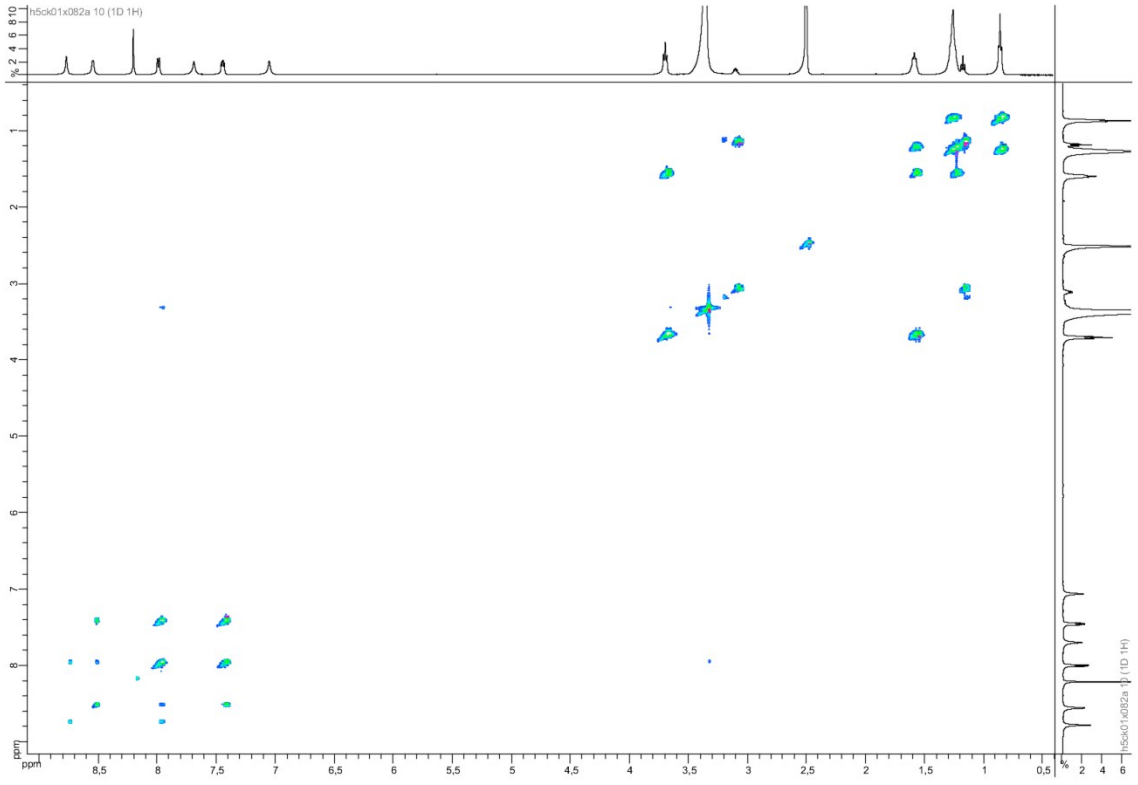


Fig. ESI 14. ^{1}H-^{13}C HMBC (pink) and HSQC (blue) map of **C_6C-3Py** (500 MHz, d_6-DMSO, 298K)

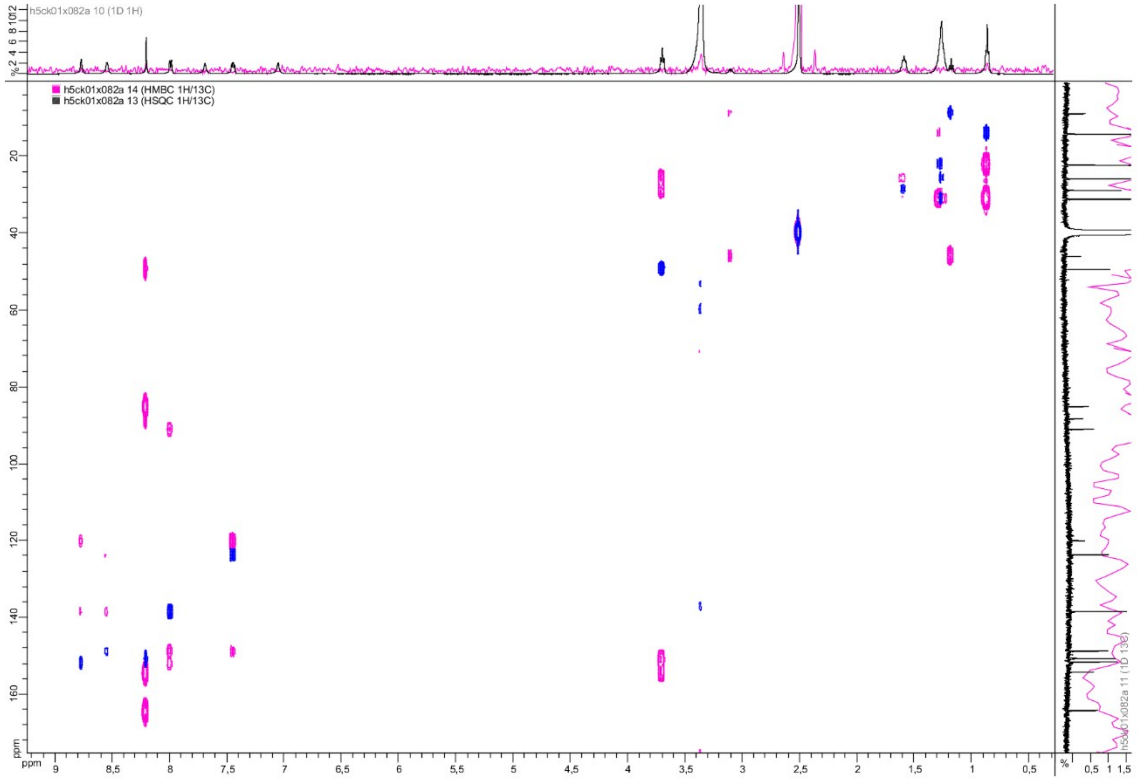
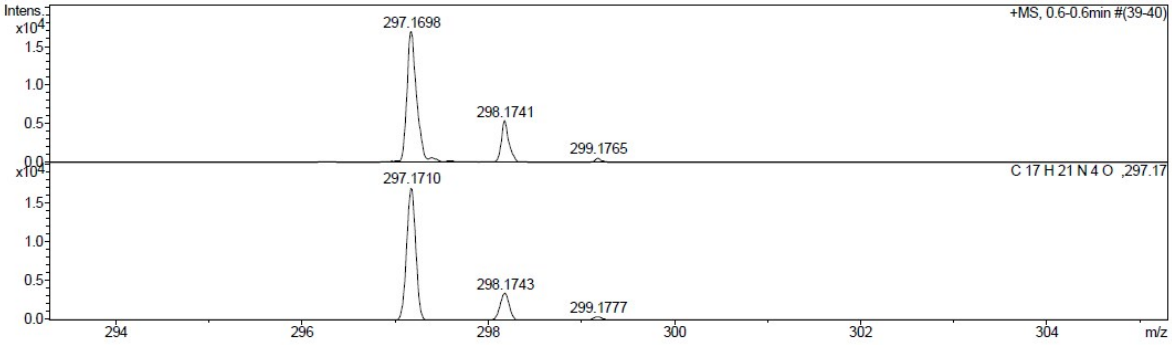
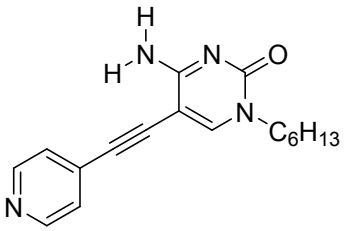


Fig. ESI 15. HRMS calculated for $C_{17}H_{21}N_4O$ $[M+H]^+$: 297.1710, found : 297.1698.



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
297.1698	1	C 17 H 21 N 4 O	297.1710	4.1	3.3	9.5	ok	even	71.60	0.1126	0.0011	0.0442	0.0010	0.8427



Chemical Formula:
$C_{17}H_{20}N_4O$
Exact Mass: 296,16
Molecular Weight: 296,37

Fig. ESI 16. ^{1}H NMR spectrum of **C_6C-4Py** (500 MHz, $CDCl_3$, 298 K)

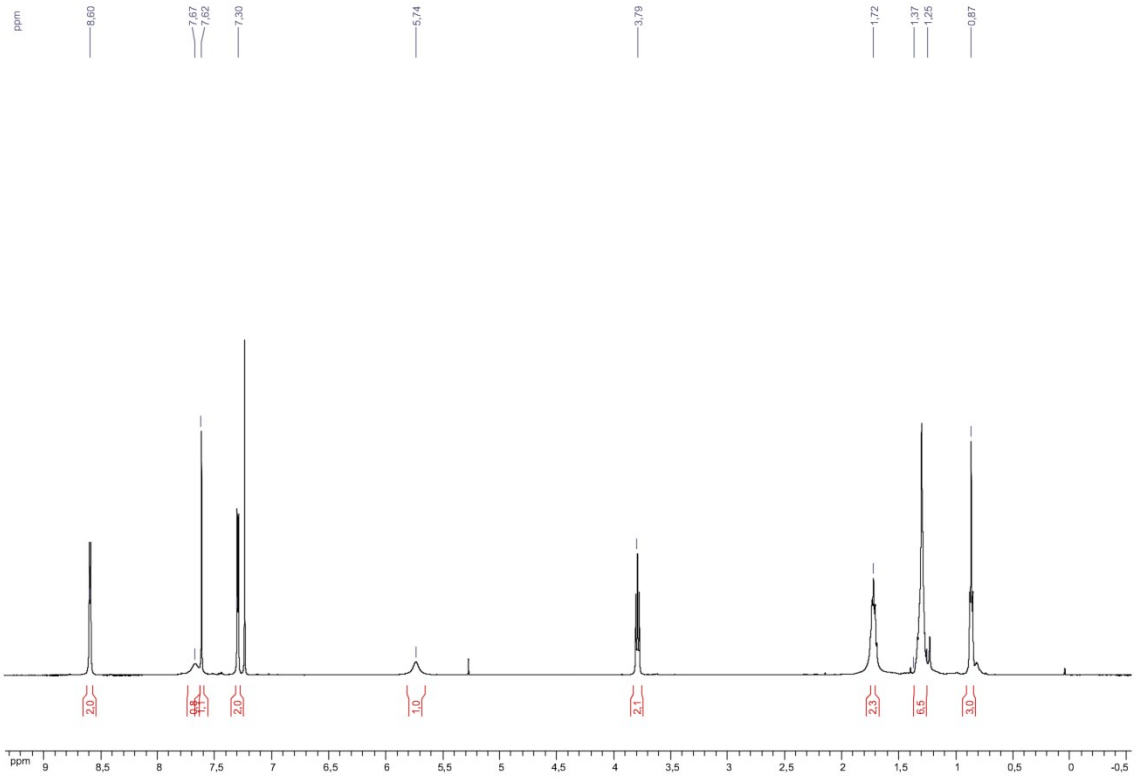


Fig. ESI 17. ^{13}C NMR spectrum of **C_6C-4Py** (125 MHz, $CDCl_3$, 298 K)

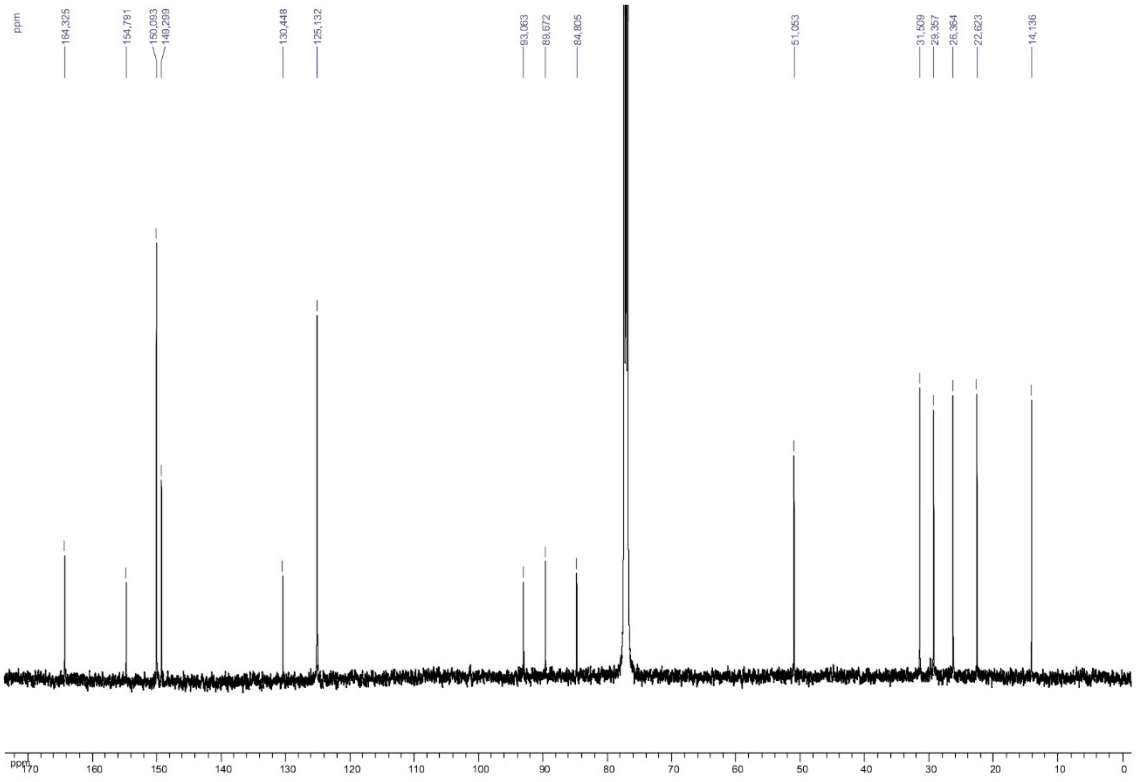


Fig. ESI 18. ^{1}H-^{1}H COSY map of **C_6C-4Py** (500 MHz, $CDCl_3$, 298K)

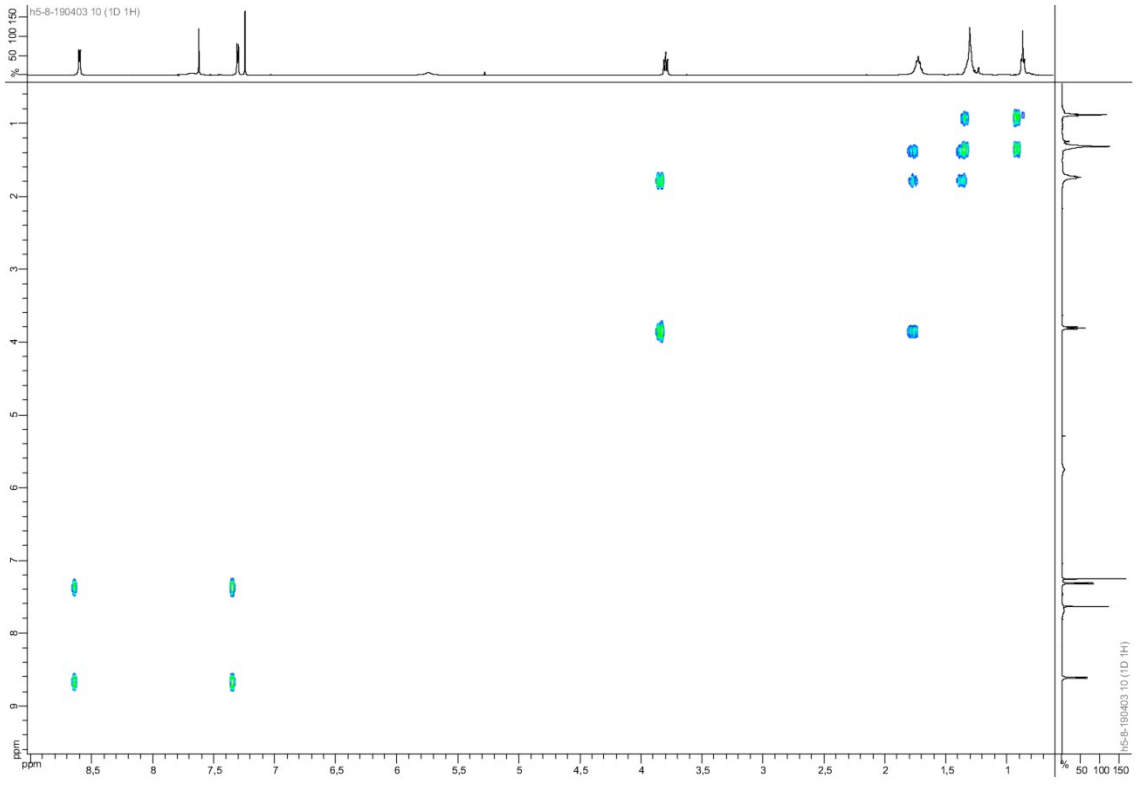


Fig. ESI 19. ^{1}H-^{13}C HMBC (pink) and HSQC (blue) map of **C_6C-4Py** (500 MHz, $CDCl_3$, 298K)

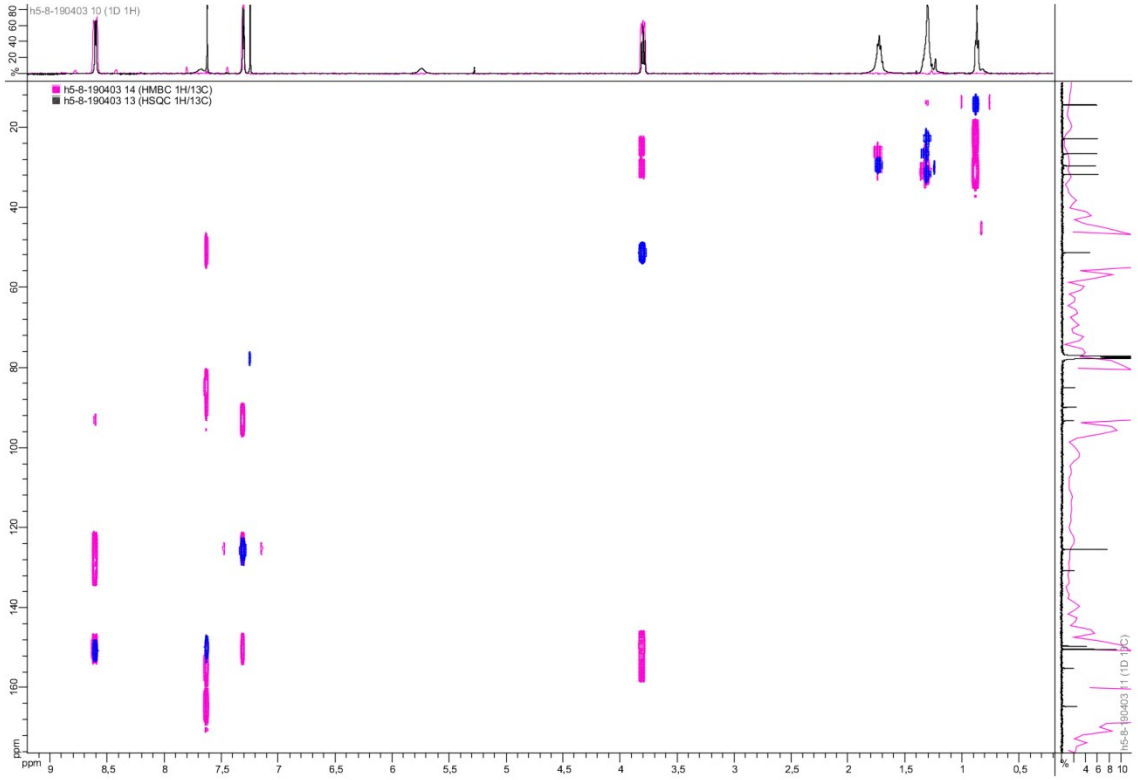
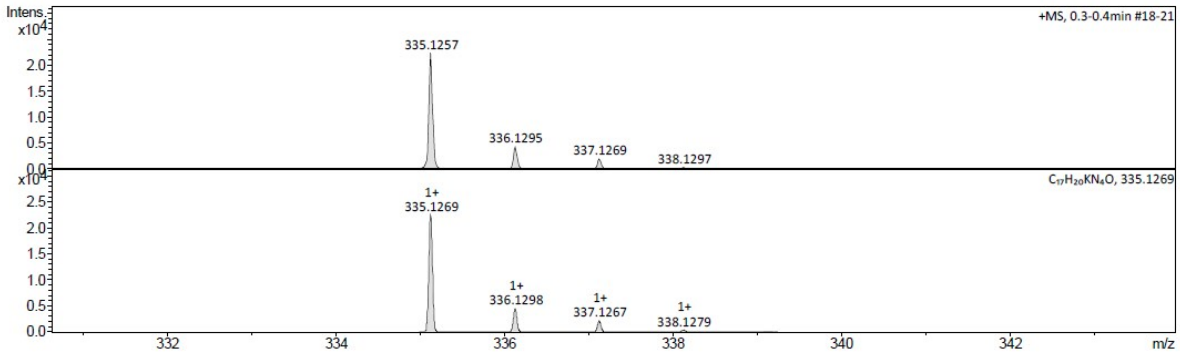
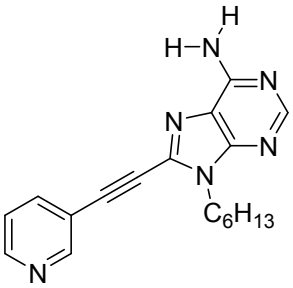


Fig. ESI 20. HRMS calculated for $C_{17}H_{20}N_4OK$ $[M+K]^+$: 335.1269, found : 335.1257.



Meas. m/z	#	Ion Formula	m/z err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I	VarNorm	Std m/z	Diff Std Comb	Dev
335.125733	1	C17H20KN4O	335.126869	3.4	1.1	9.5	ok	even	4.1	7.4	n.a.	n.a.	n.a.	n.a.	n.a.



Chemical Formula: $C_{18}H_{20}N_6$
Exact Mass: 320,17
Molecular Weight: 320,40

Fig. ESI 21. ^{1}H NMR spectrum of **C_6A-3Py** (500 MHz, d_6-DMSO, 298 K). * = water peak.

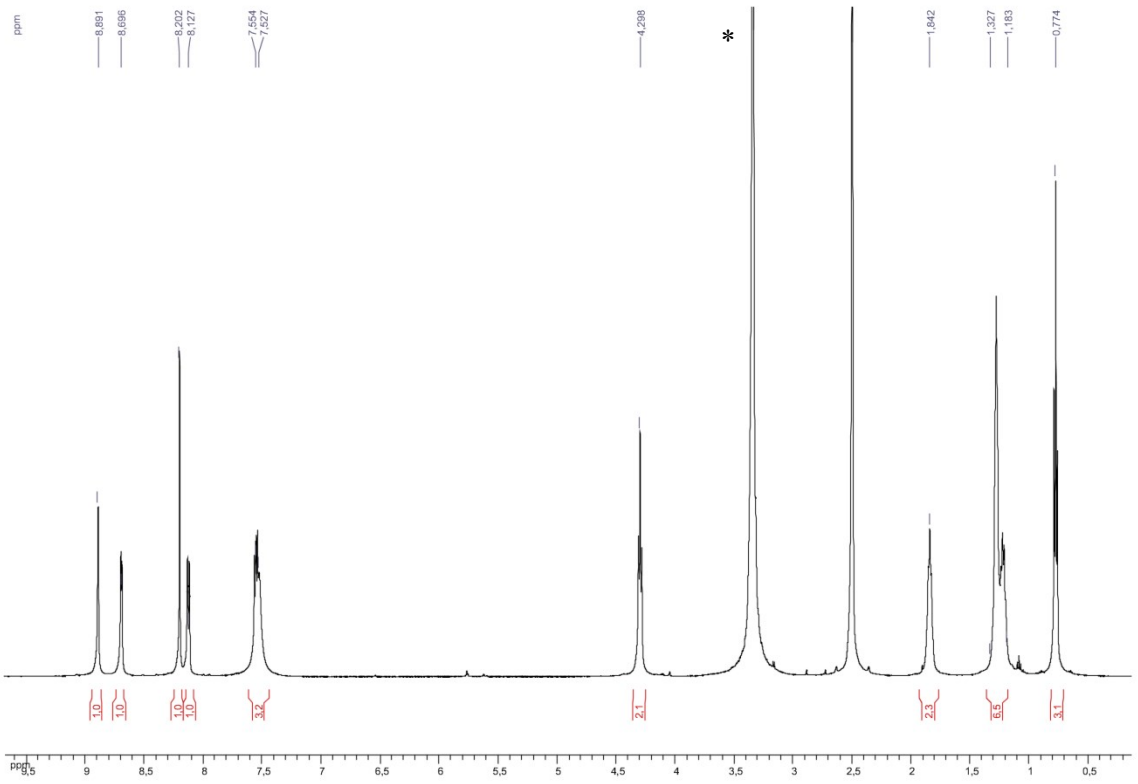


Fig. ESI 22. ^{13}C NMR spectrum of **C_6A-3Py** (125 MHz, d_6-DMSO, 298 K)

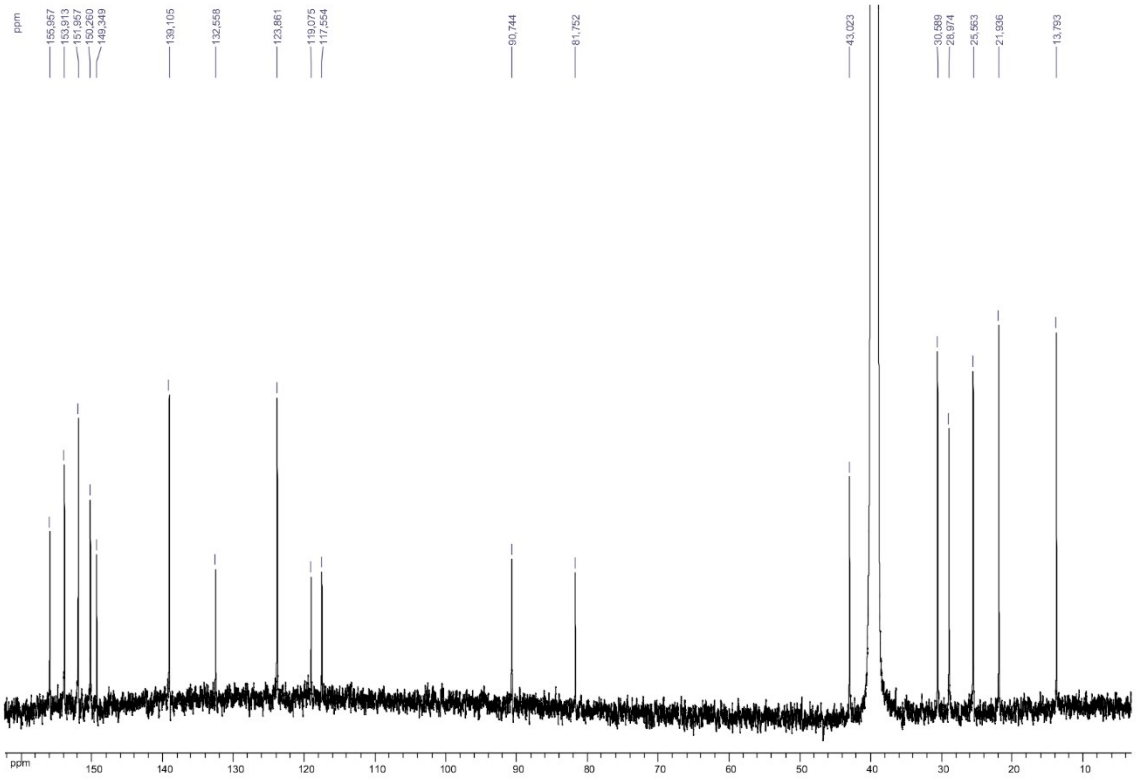


Fig. ESI 23. ^{1}H-^{1}H COSY map of **C_6A-3Py** (500 MHz, d_6-DMSO, 298K)

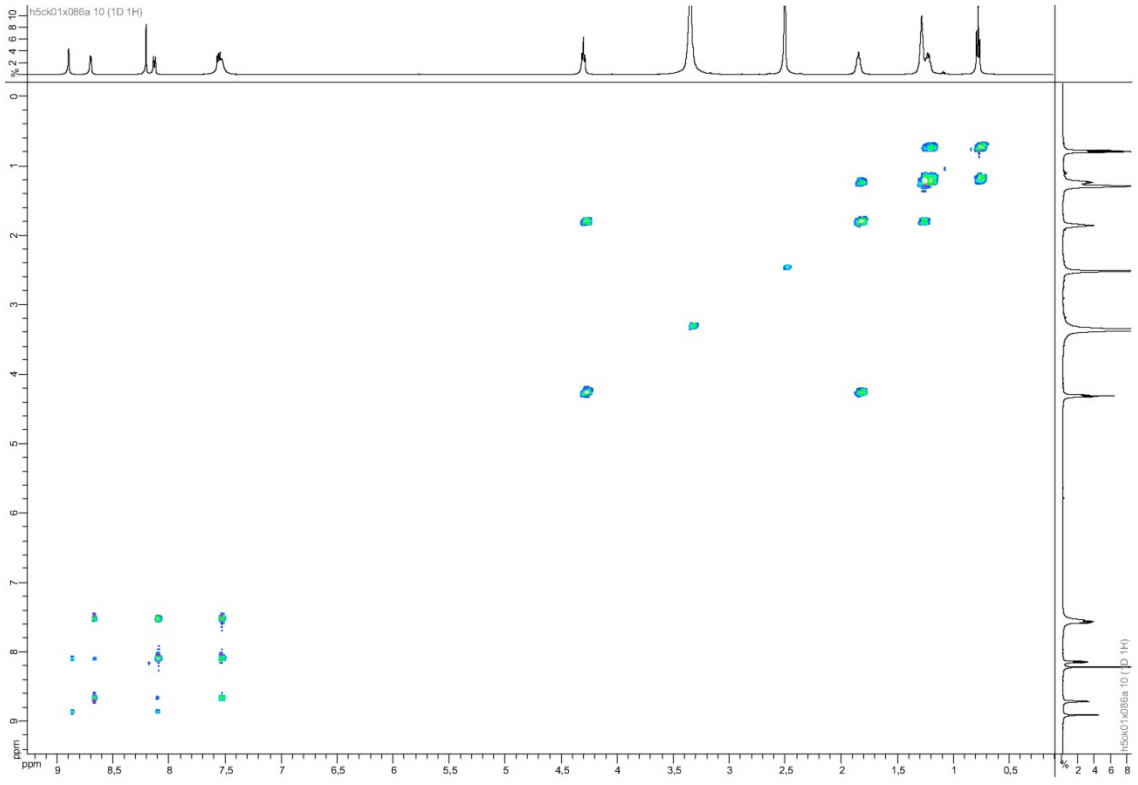


Fig. ESI 24. ^{1}H-^{13}C HMBC (pink) and HSQC (blue) map of **C_6A-3Py** (500 MHz, d_6-DMSO, 298K)

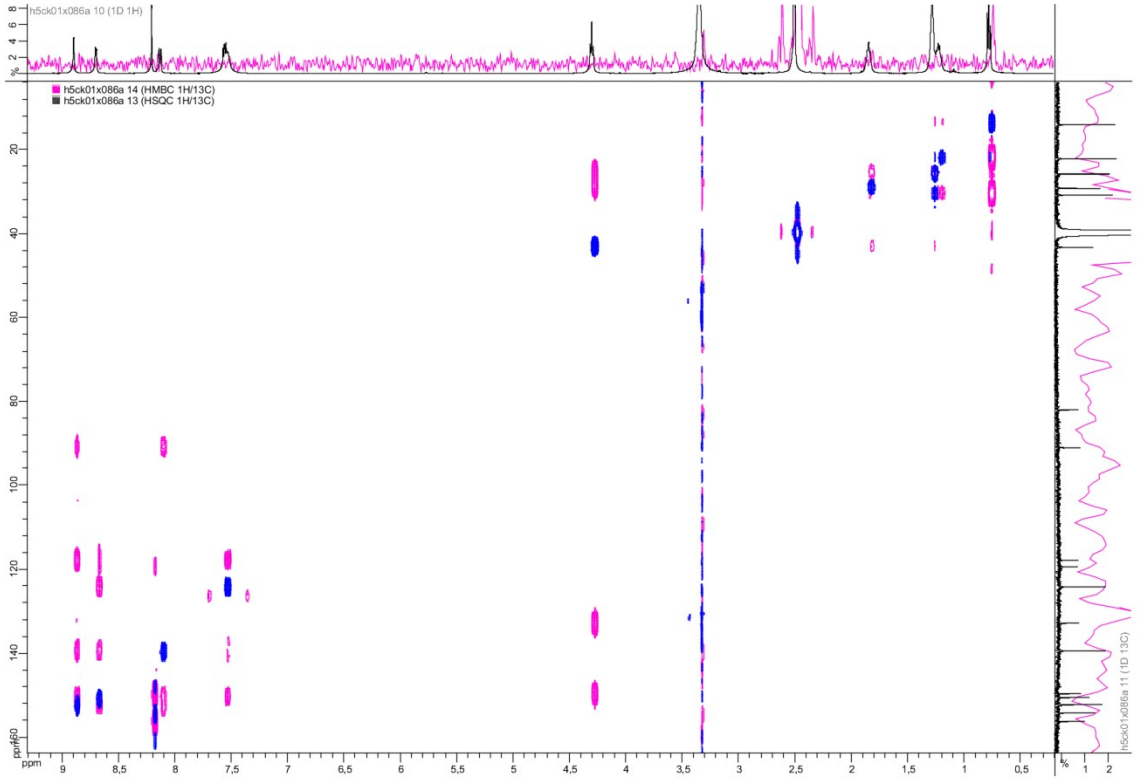
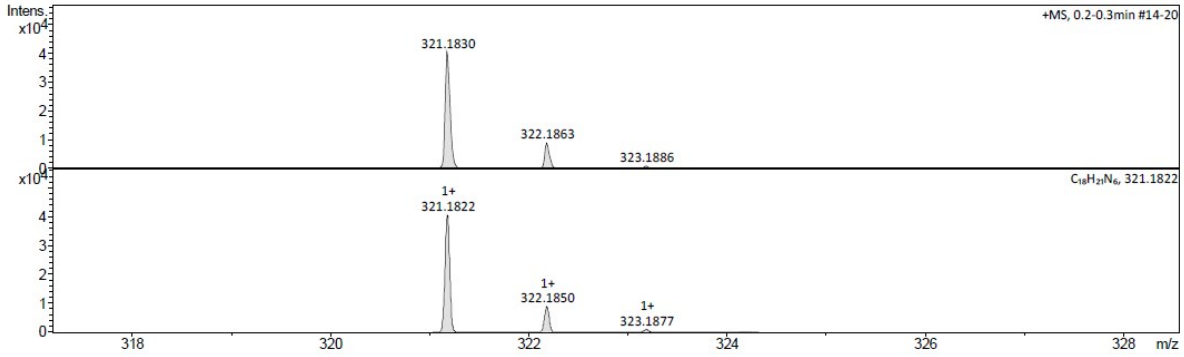
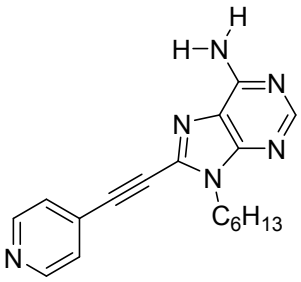


Fig. ESI 25. HRMS calculated for $C_{18}H_{21}N_6$ $[M+H]^+$: 321.1822, found : 321.1830.



Meas. m/z	#	Ion Formula	m/z err [ppm]	Mean err [ppm]	rdb	N-Rule	e¯ Conf	mSigma	Std I	Std Mean m/z	Std I	VarNorm Std m/z	Diff Std Comb	Dev
321.183005	1	C18H21N6	321.182221	-2.4	-2.9	11.5	ok	even	2.0	2.8	n.a.	n.a.	n.a.	n.a.



Chemical Formula: $C_{18}H_{20}N_6$
Exact Mass: 320,17
Molecular Weight: 320,40

Fig. ESI 26. ^{1}H NMR spectrum of **C_6A-4Py** (500 MHz, d_7-DMF, 298 K). * = water.

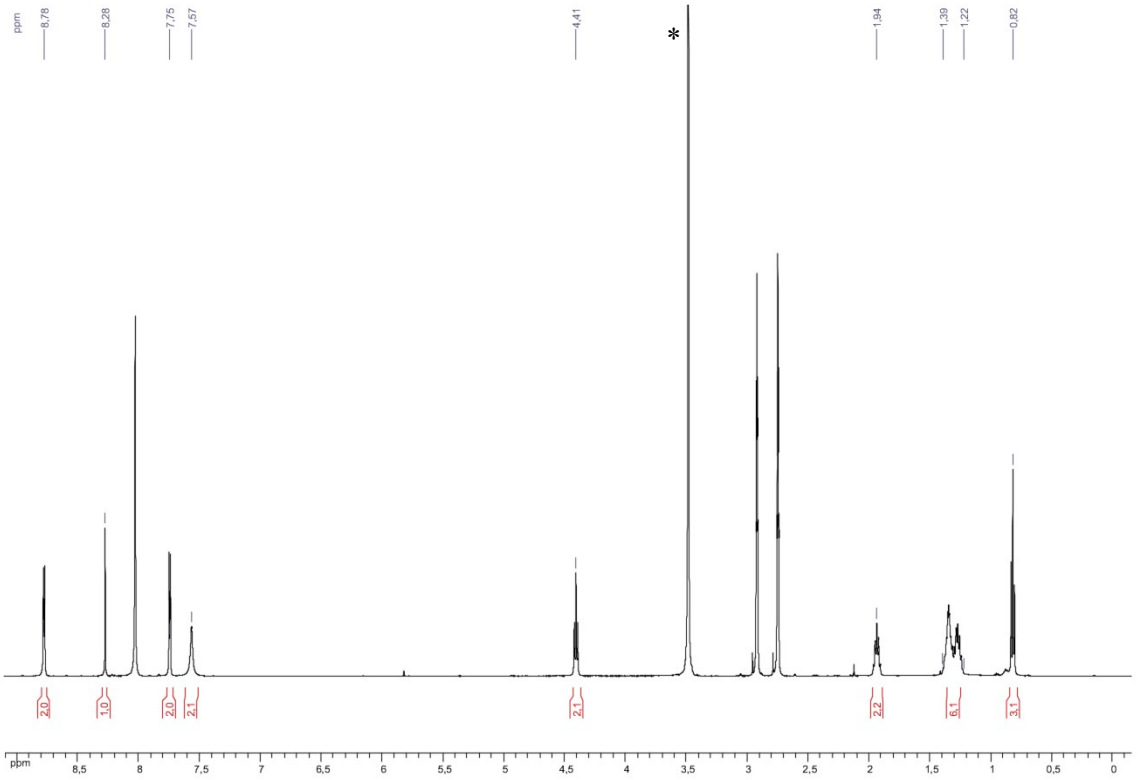


Fig. ESI 27. ^{13}C NMR spectrum of **C_6A-4Py** (125 MHz, d_7-DMF, 298 K)

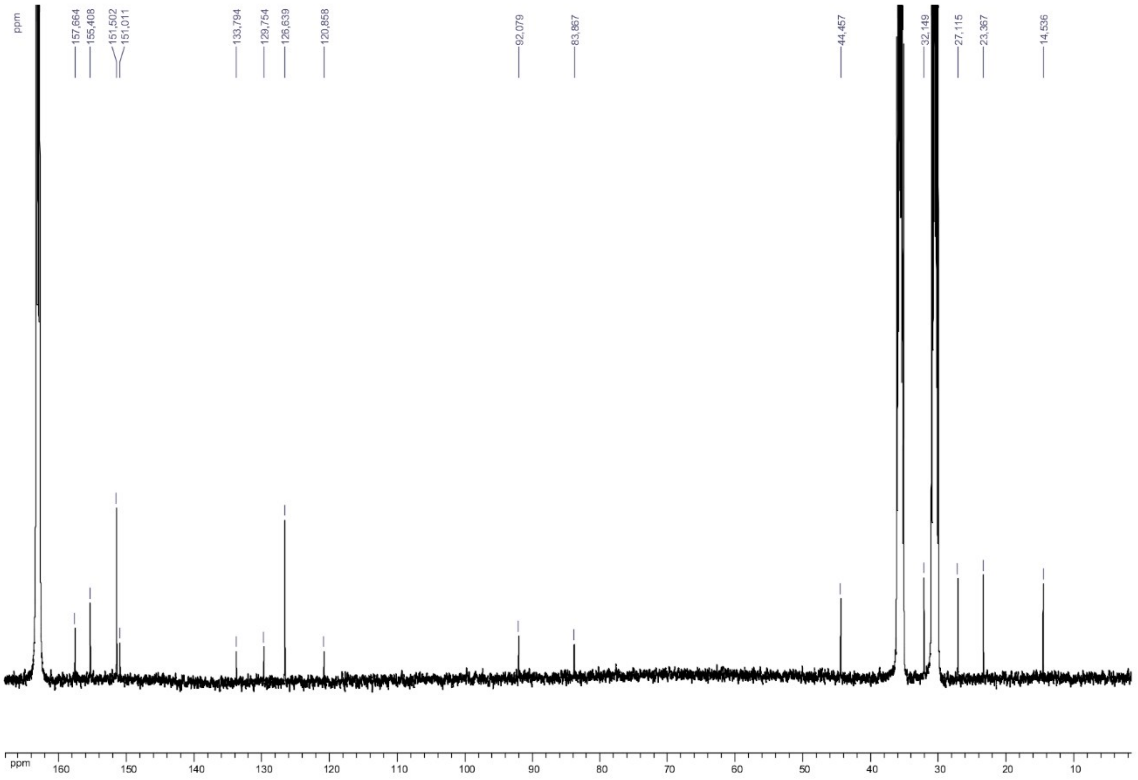


Fig. ESI 28. ^{1}H-^{1}H COSY map of **C_6A-4Py** (500 MHz, d_7-DMF, 298K)

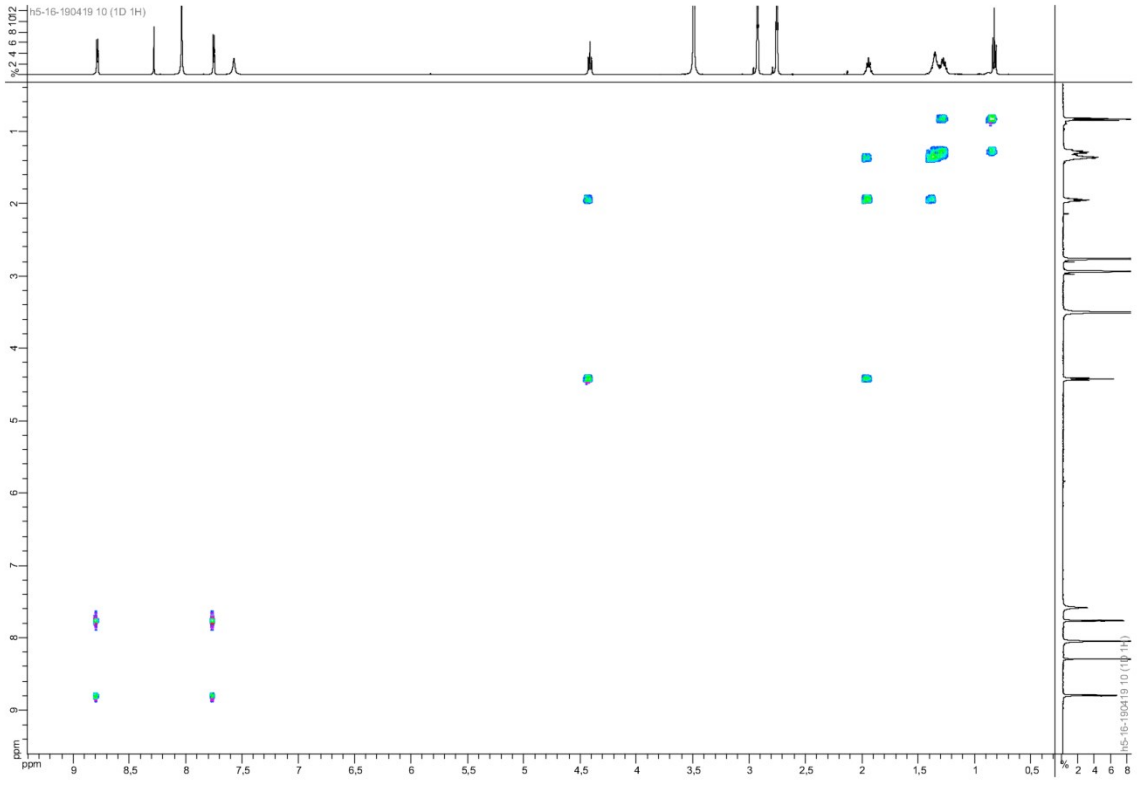


Fig. ESI 29. ^{1}H-^{13}C HMBC (pink) and HSQC (blue) map of **C_6A-4Py** (500 MHz, d_7-DMF, 298K)

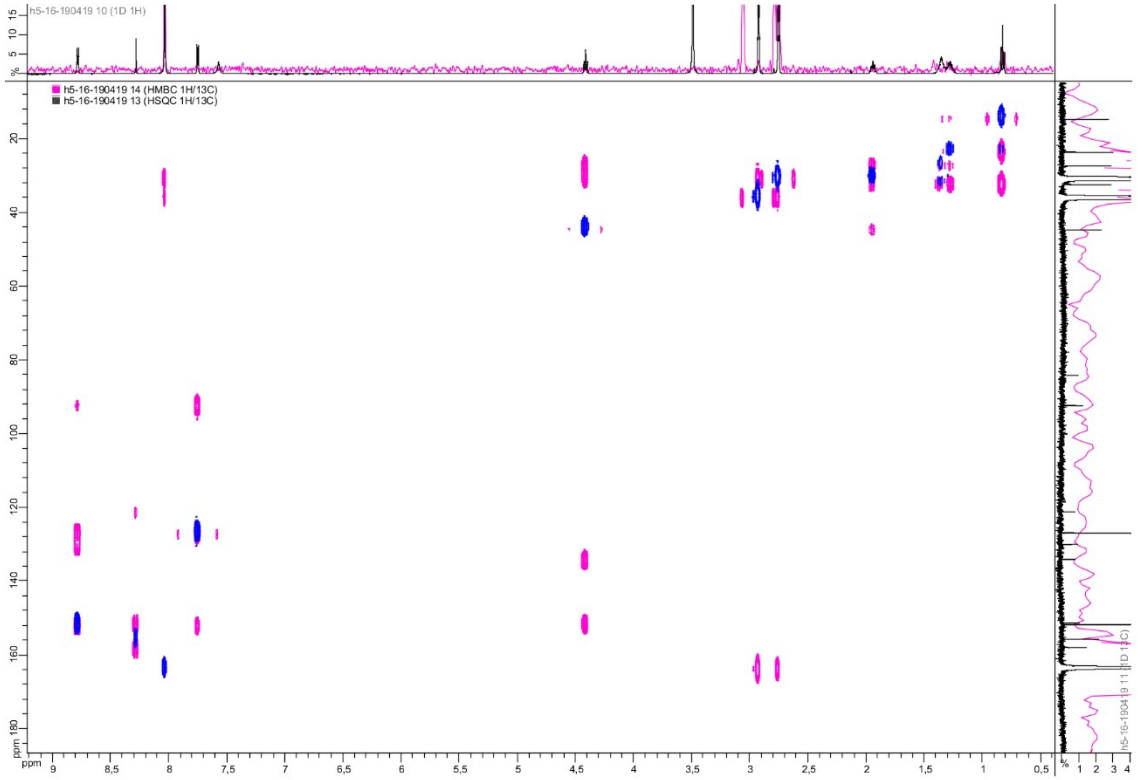
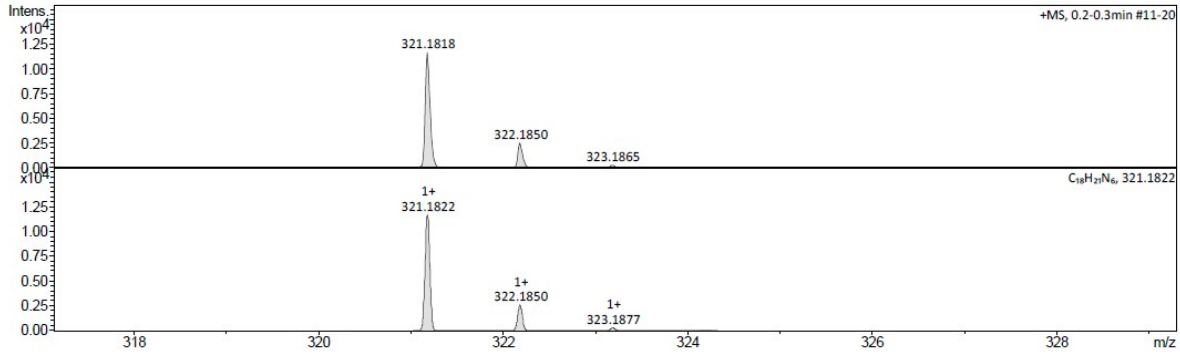
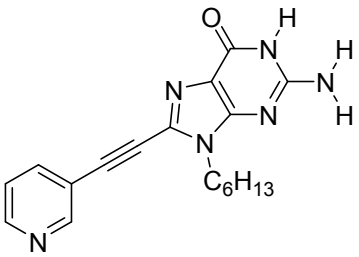


Fig. ESI 30. HRMS calculated for $C_{18}H_{21}N_6$ $[M+H]^+$: 321.1822, found : 321.1818.



Meas. m/z	#	Ion Formula	m/z err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
321.181849	1	C18H21N6	321.182221	1.2	1.4	11.5	ok	even	3.7	5.1	n.a.	n.a.	n.a.	n.a.



Chemical Formula:
$C_{18}H_{20}N_6O$
Exact Mass: 336,17
Molecular Weight: 336,40

Fig. ESI 31. ^{1}H NMR spectrum of **C_6G-3Py** (500 MHz, d_6-DMSO, 298 K). * = water.

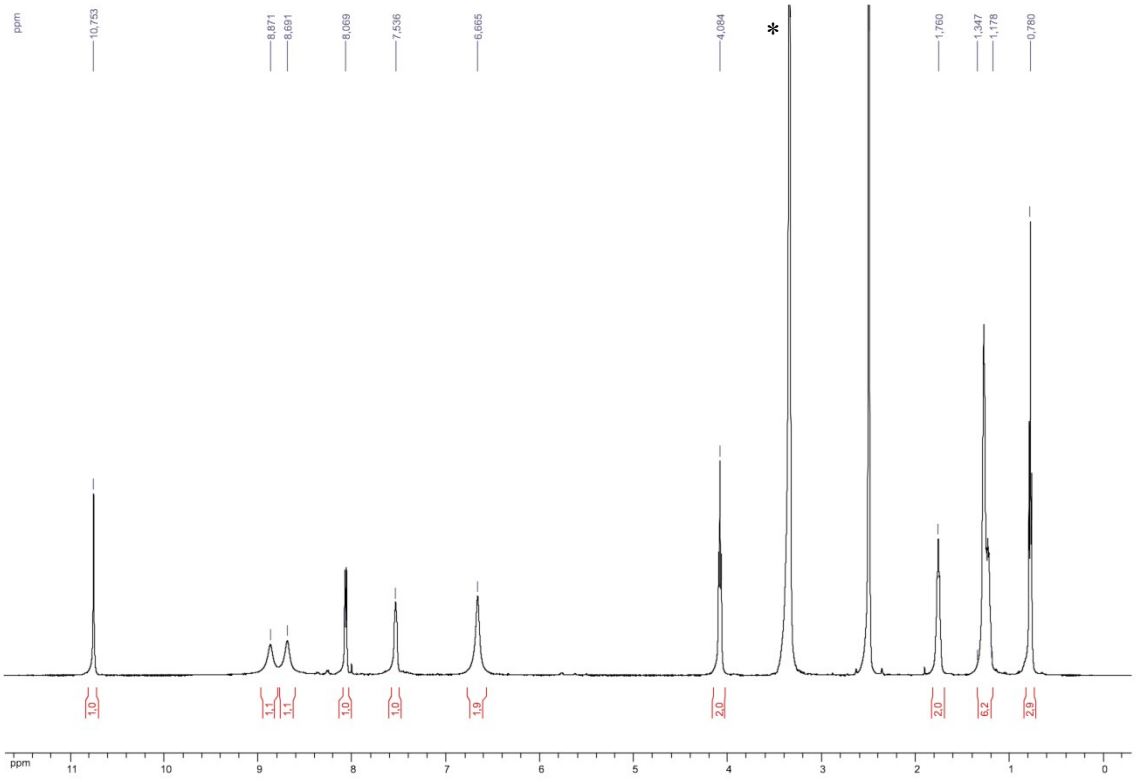


Fig. ESI 32. ^{13}C NMR spectrum of **C_6G-3Py** (125 MHz, d_6-DMSO, 298 K)

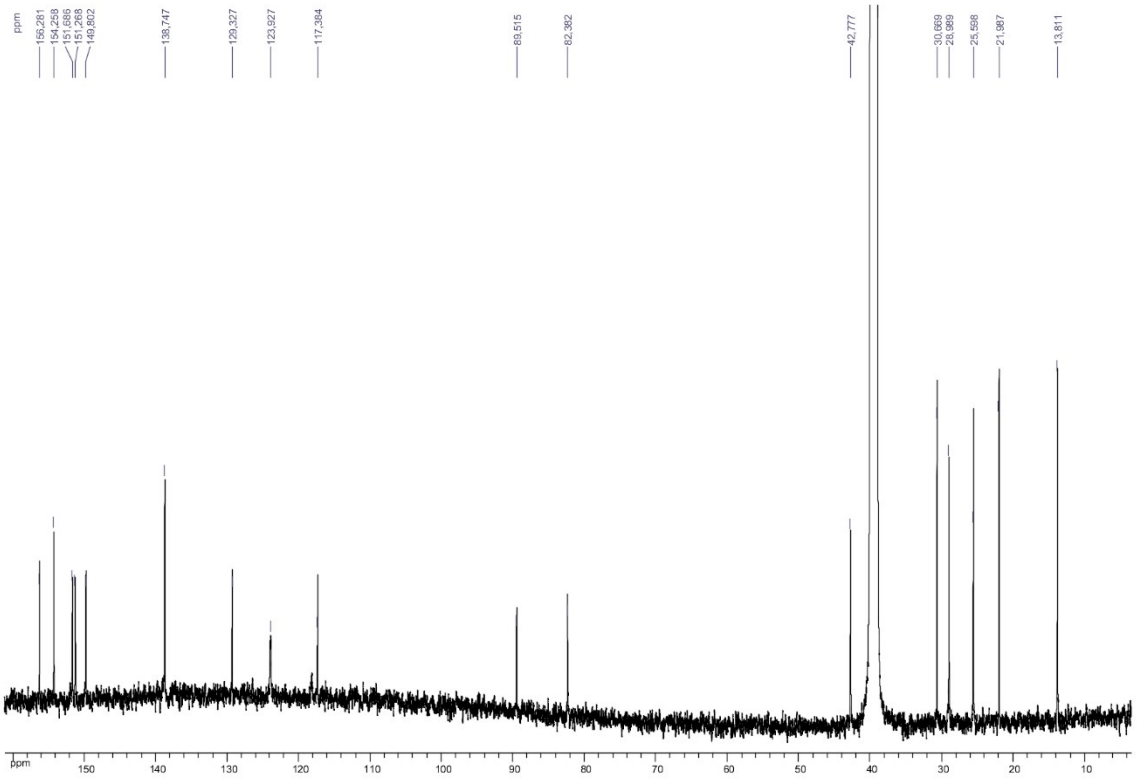


Fig. ESI 33. ^{1}H-^{1}H COSY map of **C_6G-3Py** (500 MHz, d_6-DMSO, 298K)

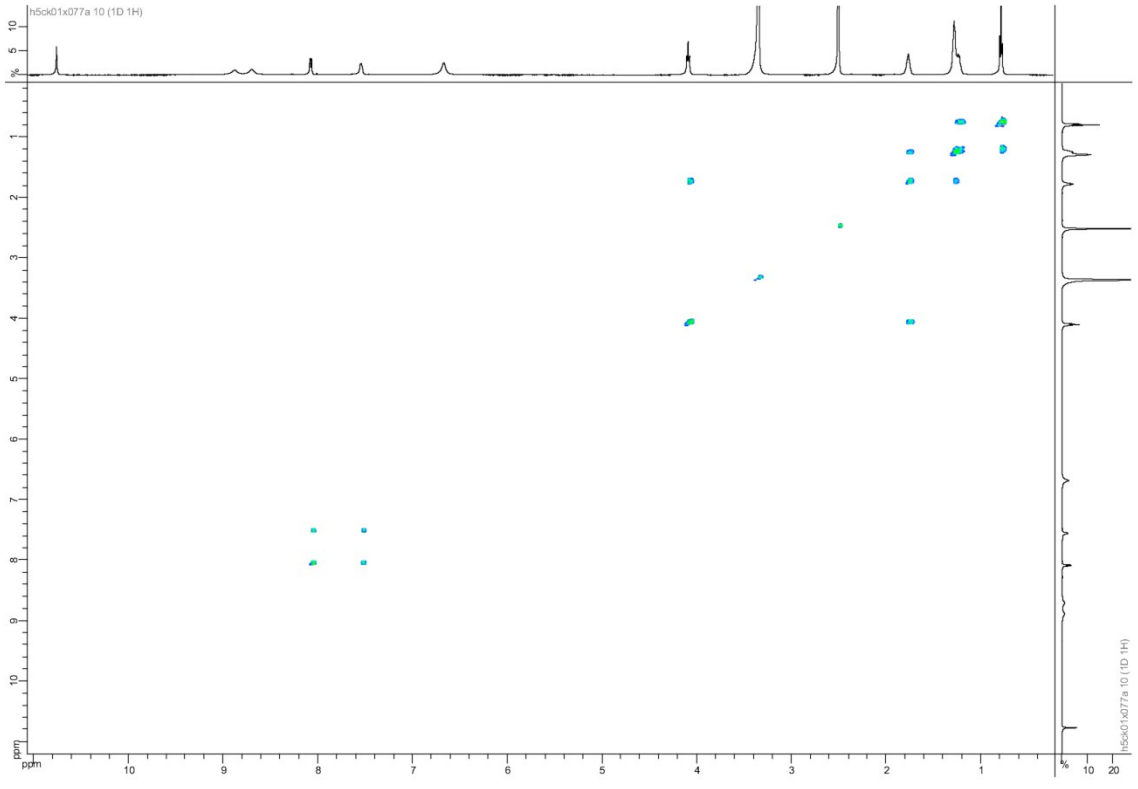


Fig. ESI 34. ^{1}H-^{13}C HMBC (pink) and HSQC (blue) map of **C_6G-3Py** (500 MHz, d_6-DMSO, 298K)

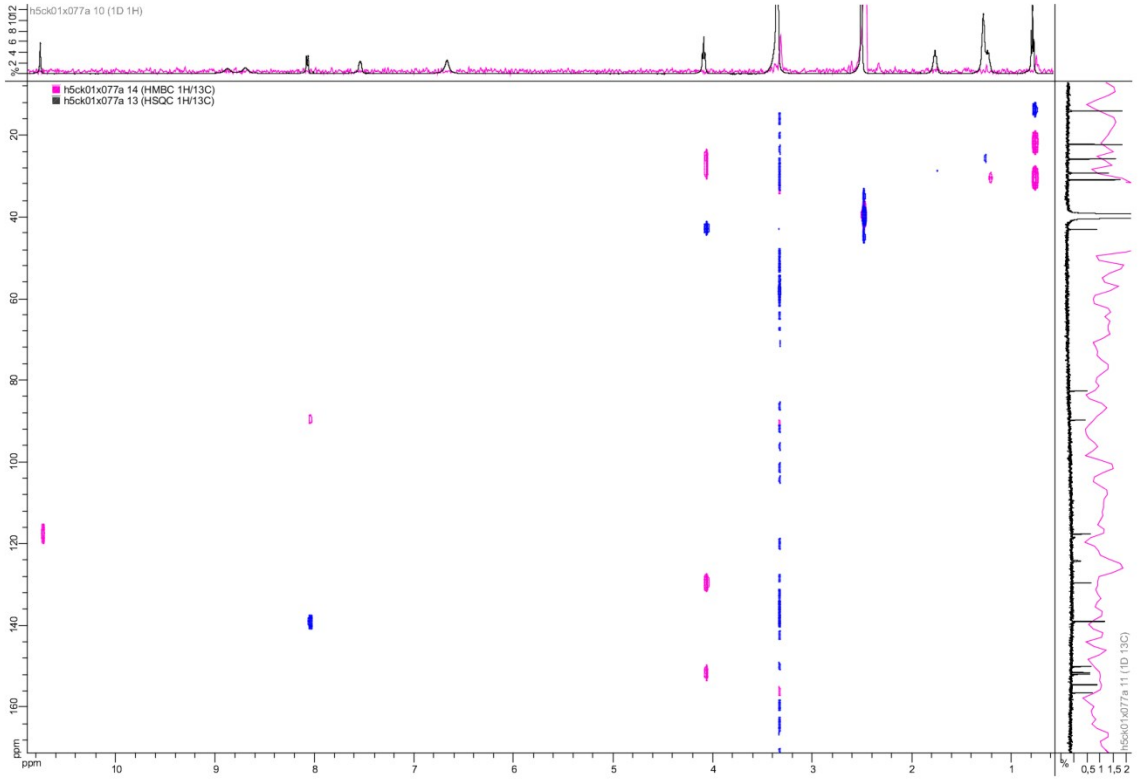
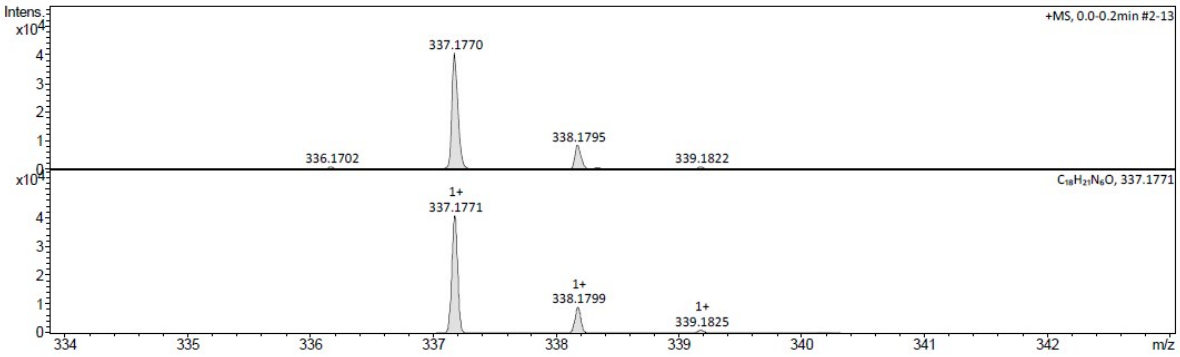
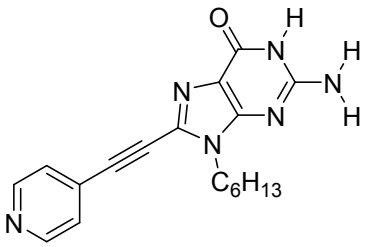


Fig. ESI 35. HRMS calculated for $C_{18}H_{21}N_6O$ $[M+H]^+$: 337.1771, found : 337.1770.



Meas. m/z	#	Ion Formula	m/z err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I	VarNorm	Std m/z	Diff Std Comb	Dev
337.177016	1	C18H21N6O	337.177136	0.4	0.7	11.5	ok	even	5.9	9.8	n.a.		n.a.		n.a.



Chemical Formula:
$C_{18}H_{20}N_6O$
Exact Mass: 336,17
Molecular Weight: 336,40

Fig. ESI 36. ^{1}H NMR spectrum of **C_6G-4Py** (500 MHz, d_6-DMSO, 298 K). * = water.

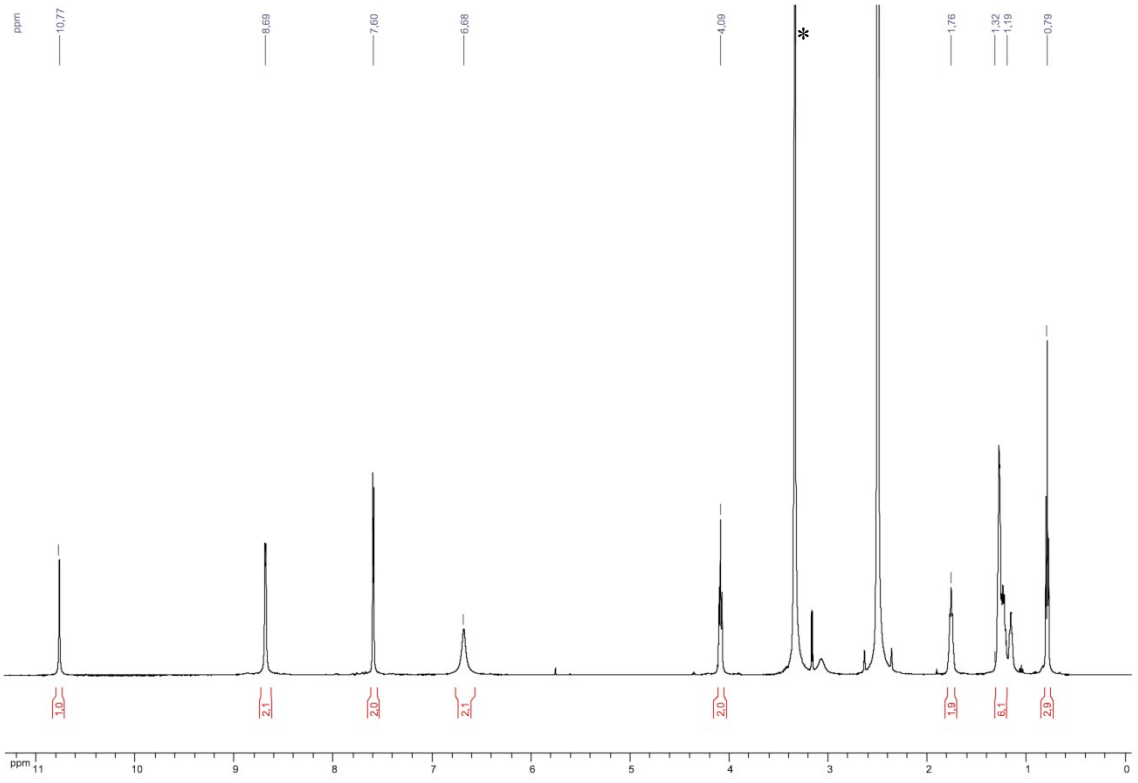


Fig. ESI 37. ^{13}C NMR spectrum of **C_6G-4Py** (125 MHz, d_6-DMSO, 298 K)

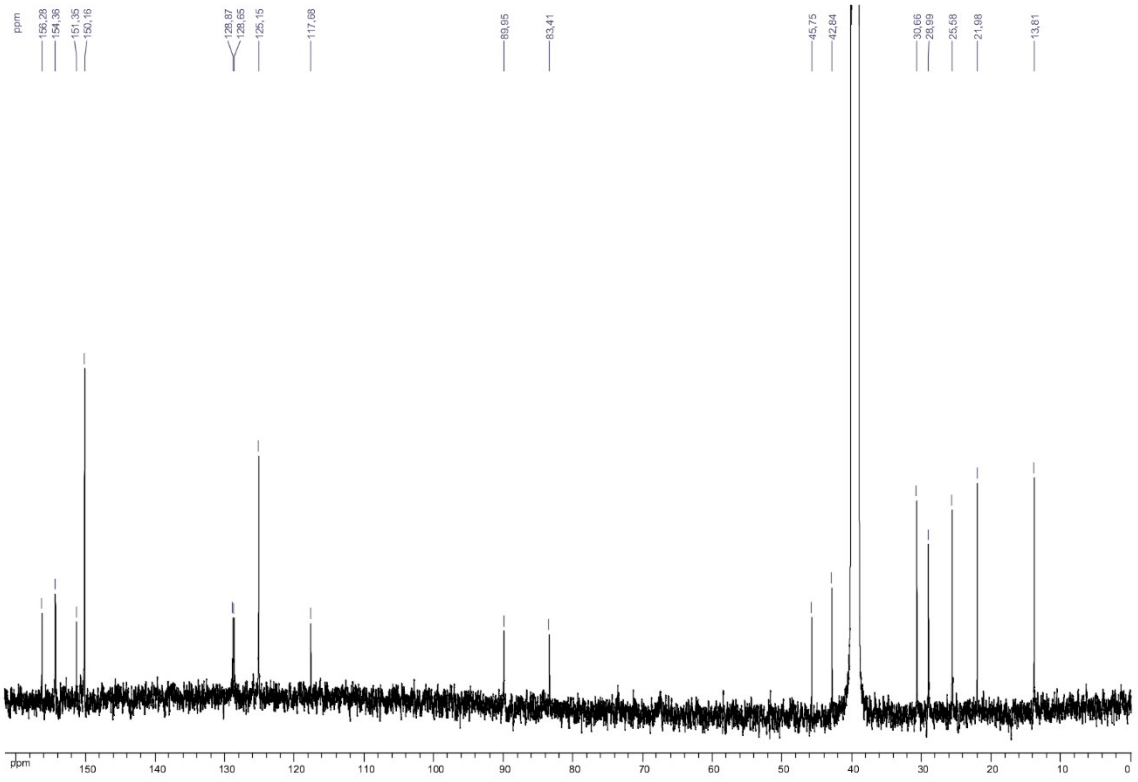


Fig. ESI 38. ^1H-^1H COSY map of **C_6G-4Py** (500 MHz, d_6-DMSO, 298K)

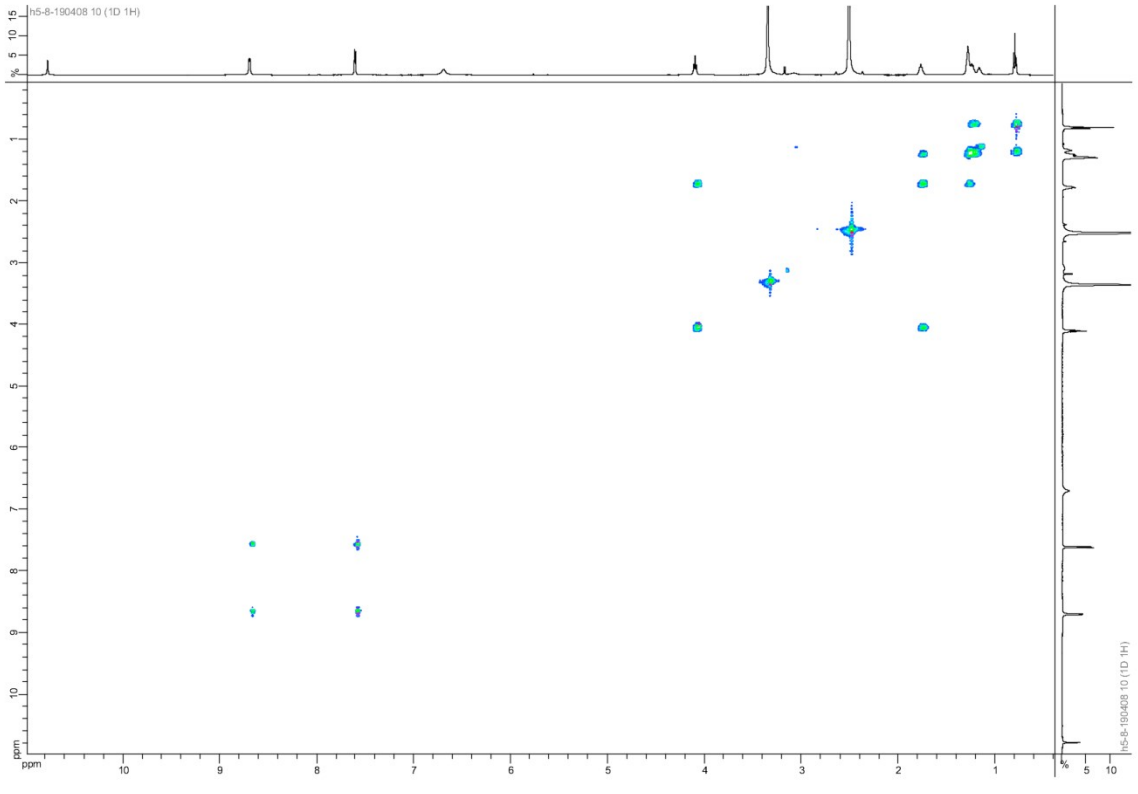


Fig. ESI 39. ^{1}H-^{13}C HMBC (pink) and HSQC (blue) map of **C_6G-4Py** (500 MHz, d_6-DMSO, 298K)

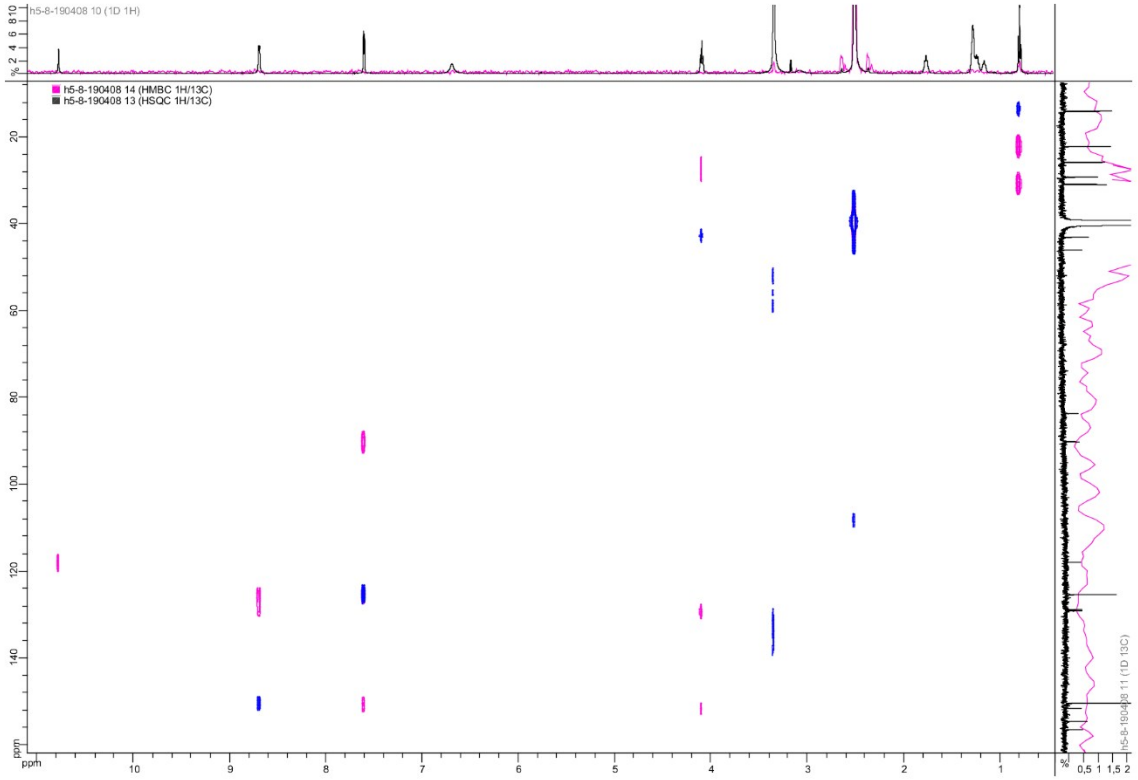
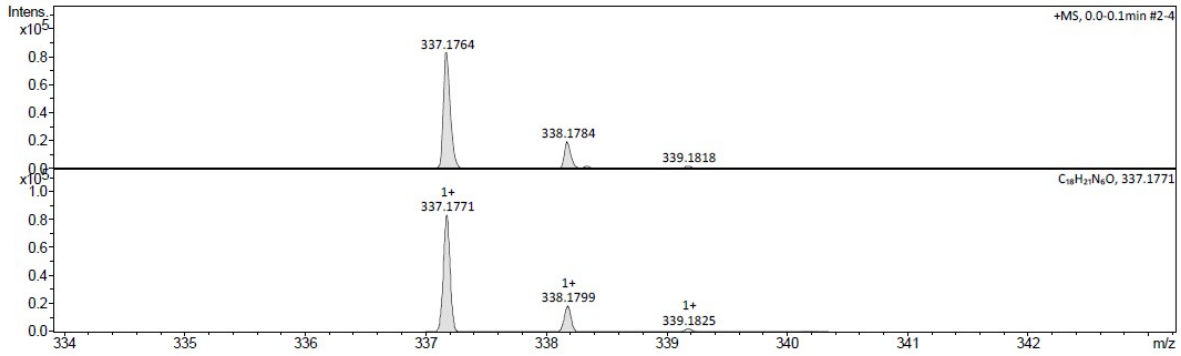


Fig. ESI 40. HRMS calculated for $C_{18}H_{21}N_6O$ $[M+H]^+$: 337.1771, found : 337.1764.



Meas. m/z	#	Ion Formula	m/z err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I	VarNorm Std m/z	Diff Std Comb	Dev
337.176438	1	C18H21N6O	337.177136	2.1	2.7	11.5	ok	even	8.4	14.0	n.a.	n.a.	n.a.	n.a.

Fig. ESI 41. Simulated (red) and experimental (black) PRXD pattern for **C_6G-4Py•C_6C-4Py**.

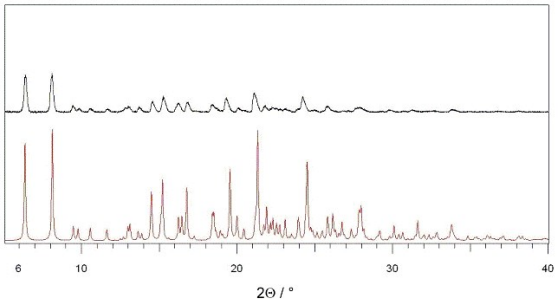


Fig. ESI 42. Simulated (red) and experimental (black) PRXD pattern for [(**C_6C-3Py**)$_2$(Cu(OAc)$_2$)$_2$](H$_2$O)$_2$.

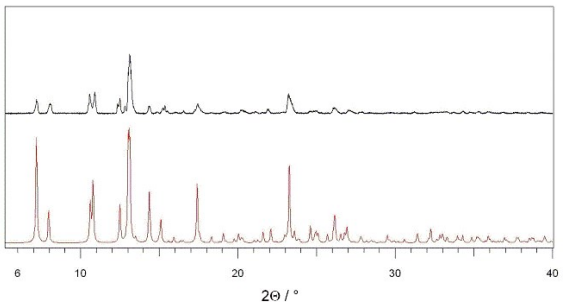


Fig. ESI 43. Simulated (red) and experimental (black) PRXD pattern for [(**C_6A-3Py**)Cu(hfac)$_2$](H$_2$O). Difference in intensity arise from preferential orientation.

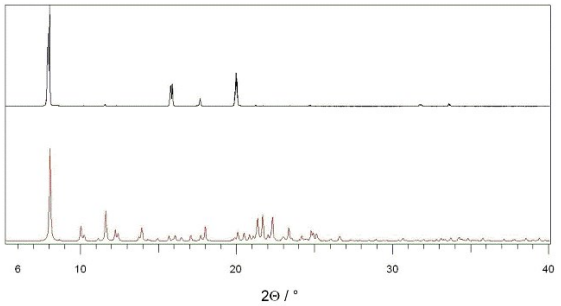


Fig. ESI 44. Simulated (red) and experimental (black) PRXD pattern for [(**C_6A-4Py**)(Cd(NO$_3$)$_2$(H$_2$O))](1,2-DCE). Broadening of the peaks indicates solvent loss.