

	Value	Error
A	631.77866	288.47674
B	$6.684 \cdot 10^{15}$	$5.166 \cdot 10^{14}$
$ r $	sd(yEr±)	N p
0.991₁₆	569.309	5 9.96.10 ⁻⁴

	Value	Error
A	$3,0517 \cdot 10^{-14}$	$3,2299 \cdot 10^{-14}$
B	$1,1919 \cdot 10^{-17}$	$1,641 \cdot 10^{-18}$
$ r $	sd(yEr±)	N p
0.981₅₇	$5.57 \cdot 10^{-14}$	3 0.99714

	Value	Error
A	$-1.919 \cdot 10^{-15}$	$1.7527 \cdot 10^{-15}$
B	$1.275 \cdot 10^{-17}$	$7.7121 \cdot 10^{-20}$
$ r $	sd(yEr±)	N p
0.999₉₈	$2.466 \cdot 10^{-15}$	3 0.9974

	Value	Error
A	3.29167	2.406
B	$1.88 \cdot 10^{10}$	$3.744 \cdot 10^8$
$ r $	sd(yEr±)	N p
0.999₆	4.147	4 3.95.10 ⁻⁴

$$D_{SD}^{tot} = \sum_i D_{SD}^i = \sum_i 1.3194 \cdot 10^{-17} \times A^i \times \frac{\overline{I_i^2} - (\overline{I_i})^2}{(\overline{I_i} - \overline{I_i})^2} \quad (1)$$

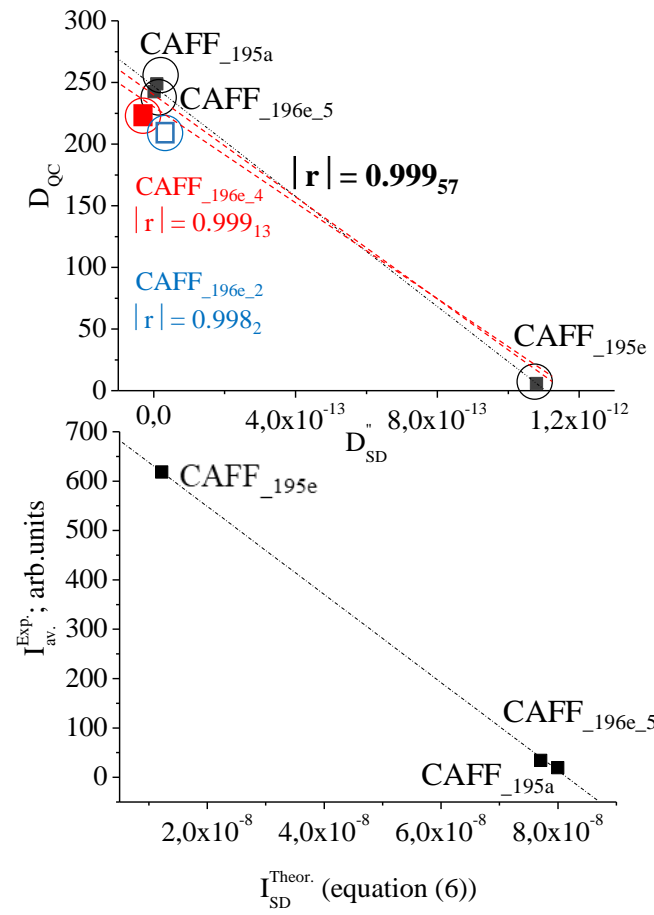
$$D_{SD}^{",tot} = \sum_i D_{SD}^{",i} = \sum_i 2.6388 \cdot 10^{-17} \times (\overline{I_i^2} - (\overline{I_i})^2) \quad (2)$$

$$D_{QC} = \frac{\prod_{i=1}^{3N} \nu_i^0}{\prod_{i=1}^{3N-1} \nu_i^s} \times e^{\frac{\Delta H^\#}{R \times T}} \quad (3)$$

$$D_{SD,l}^{"} + D_{SD,m}^{"} = |r_{l,m}| \times \sqrt{\overline{I_{l,q}^2} - (\overline{I_{l,q}})^2} \times \sqrt{\overline{I_{m,q}^2} - (\overline{I_{m,q}})^2} \quad (4)$$

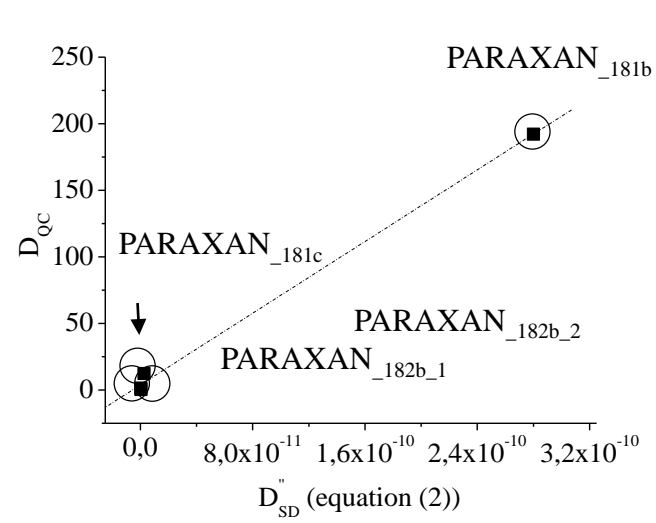
$$D_{SD}^{",q} \approx 2 \times \frac{A_D^q}{A_I^q} \times I_{av}^{TOT,q} \quad (5)$$

$$I_{SD}^{Theor} \sim (2.6388 \cdot 10^{-17} \times D_{QC})^{1/2} \quad (6)$$



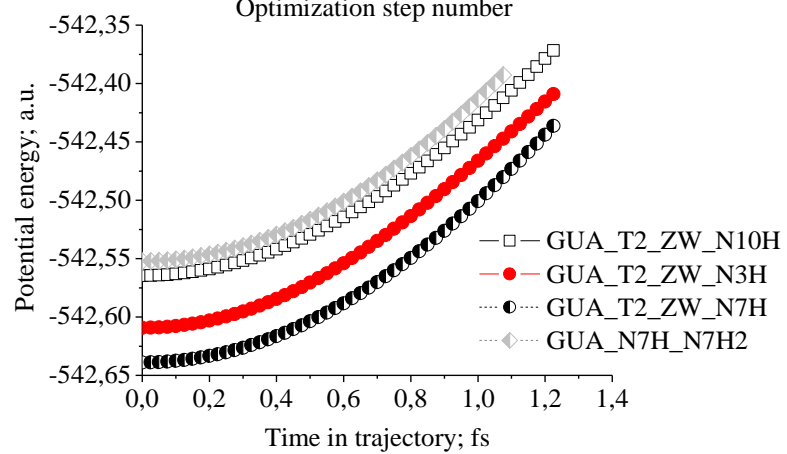
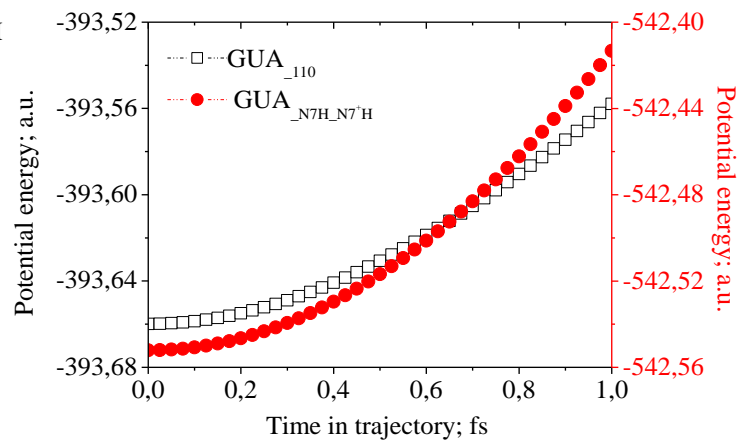
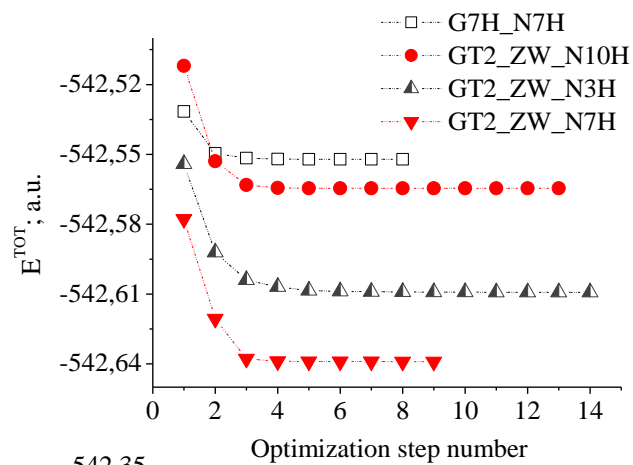
	Value	Error
A	246.84654	4.09054
B	-2.2327.10 ¹⁴	6.56.10 ¹²
r	sd(yEr±)	Np
0.999 ₅₇	5.75624	30.0187

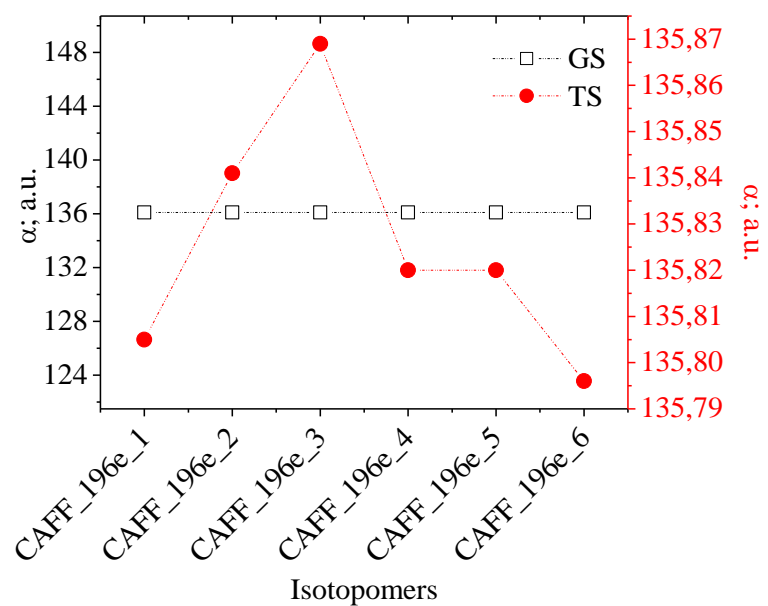
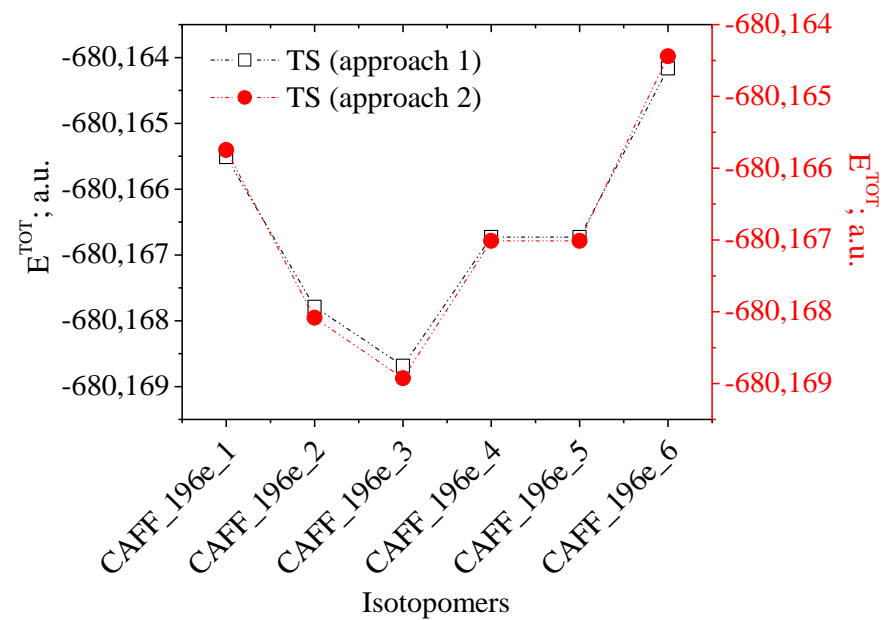
	Value	Error
A	727.02	9.6477
B	-8.915.10 ⁹	1.49.10 ⁸
r	sd(yEr±)	Np
0.999 ₈₆	8.1044	30.0107

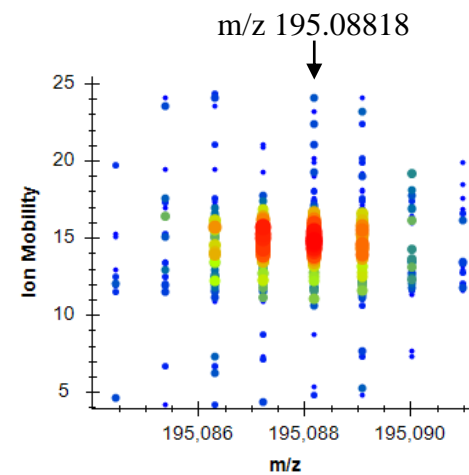
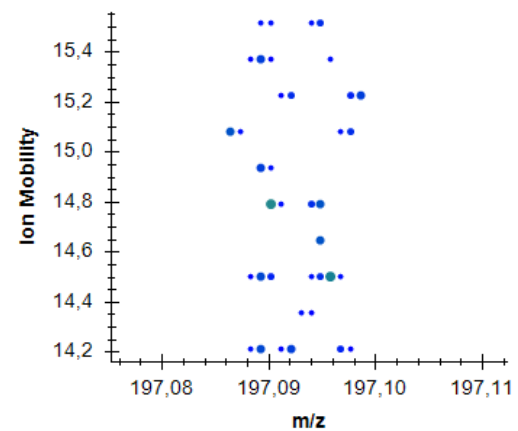
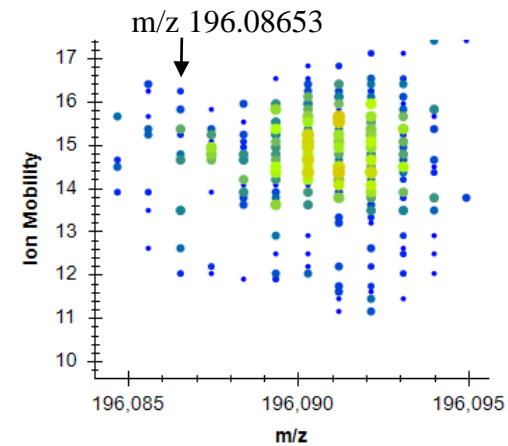
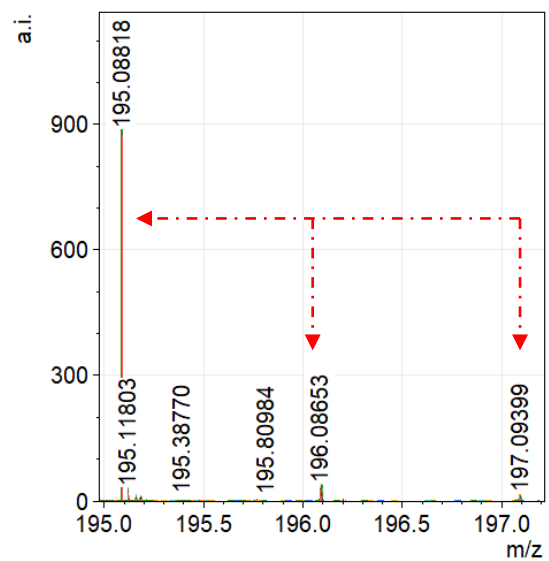
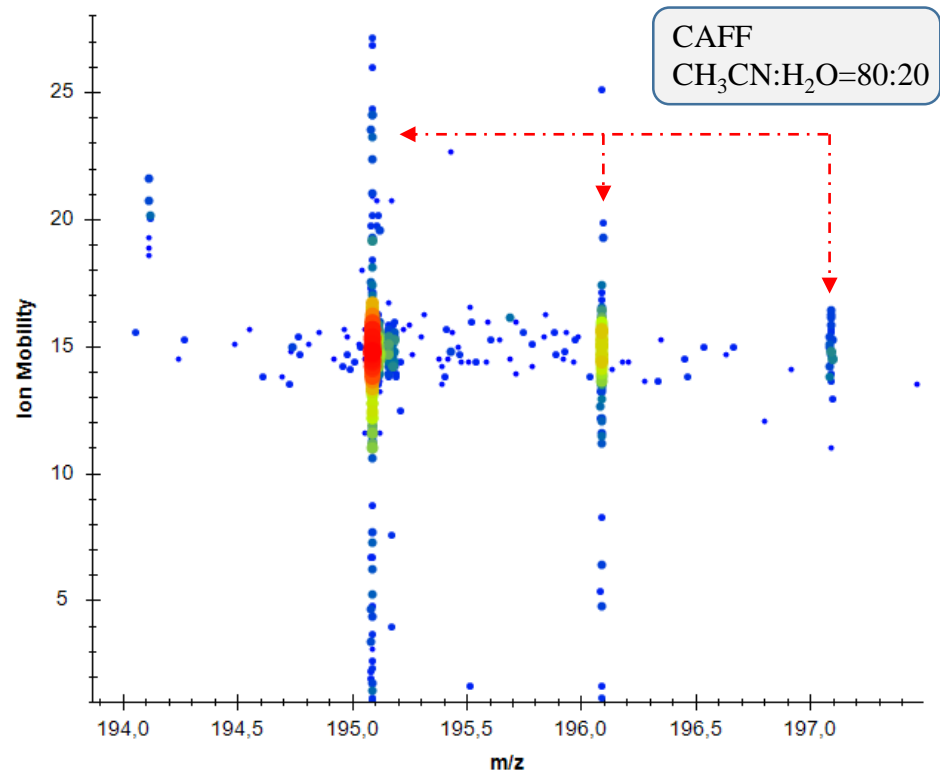


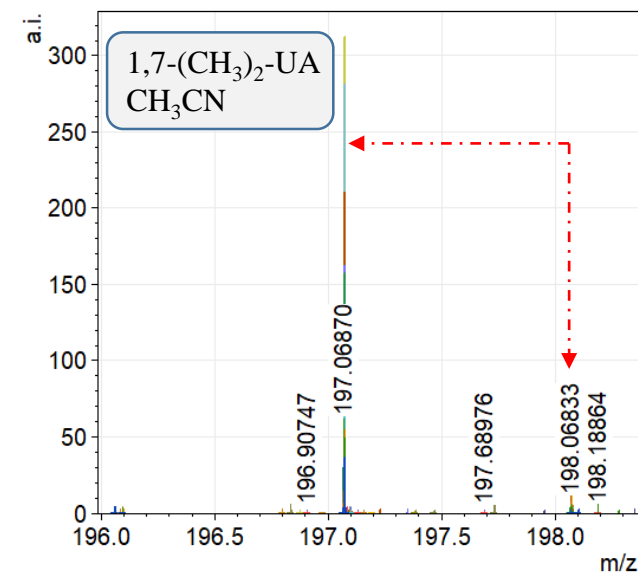
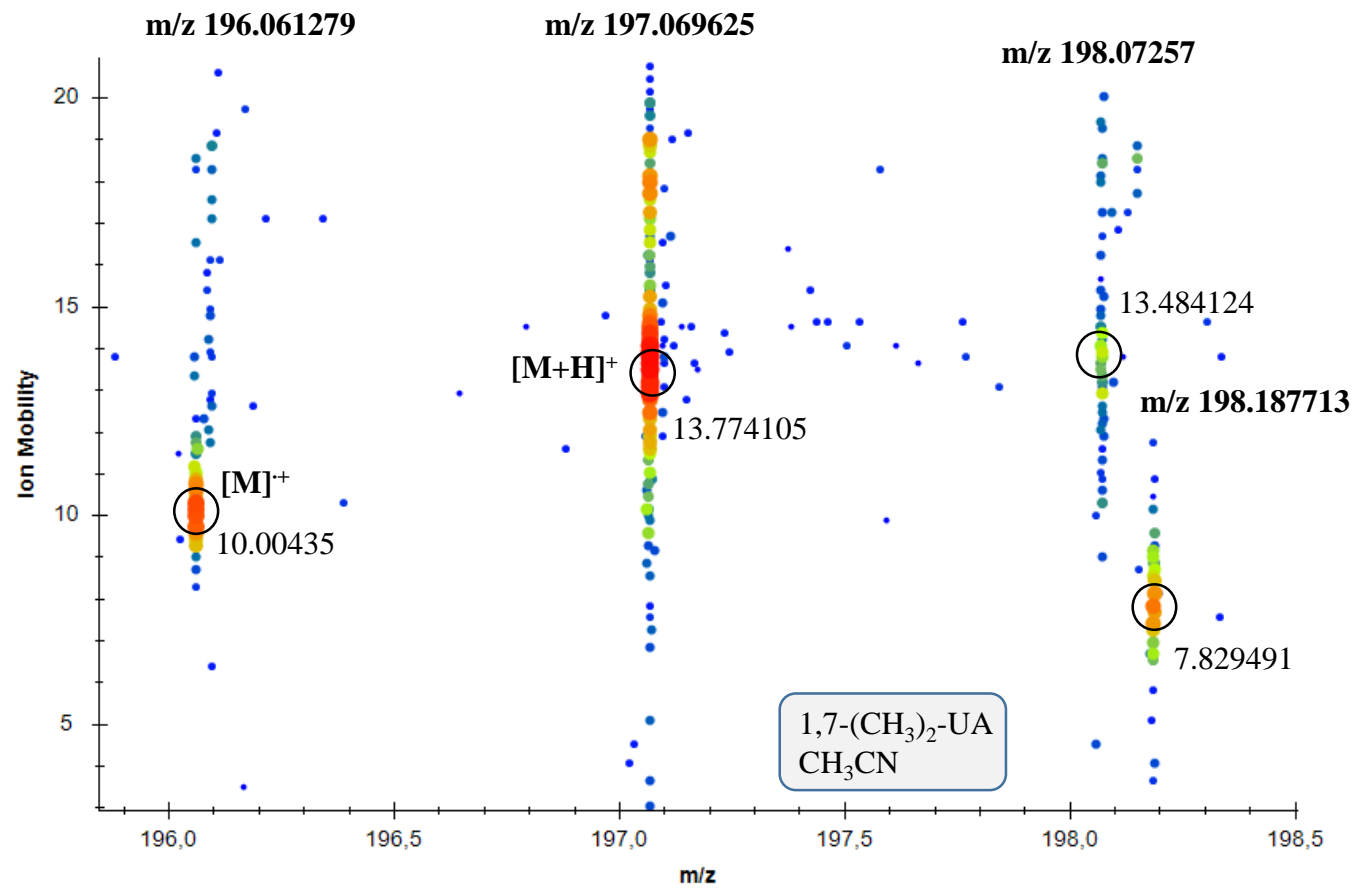
	Value	Error
A	0.50674	0.5405
B	$6.841 \cdot 10^{11}$	$3.3434 \cdot 10^9$
r	sd(yEr±)	Np
0.999 ₉₉	0.76308	30.0031

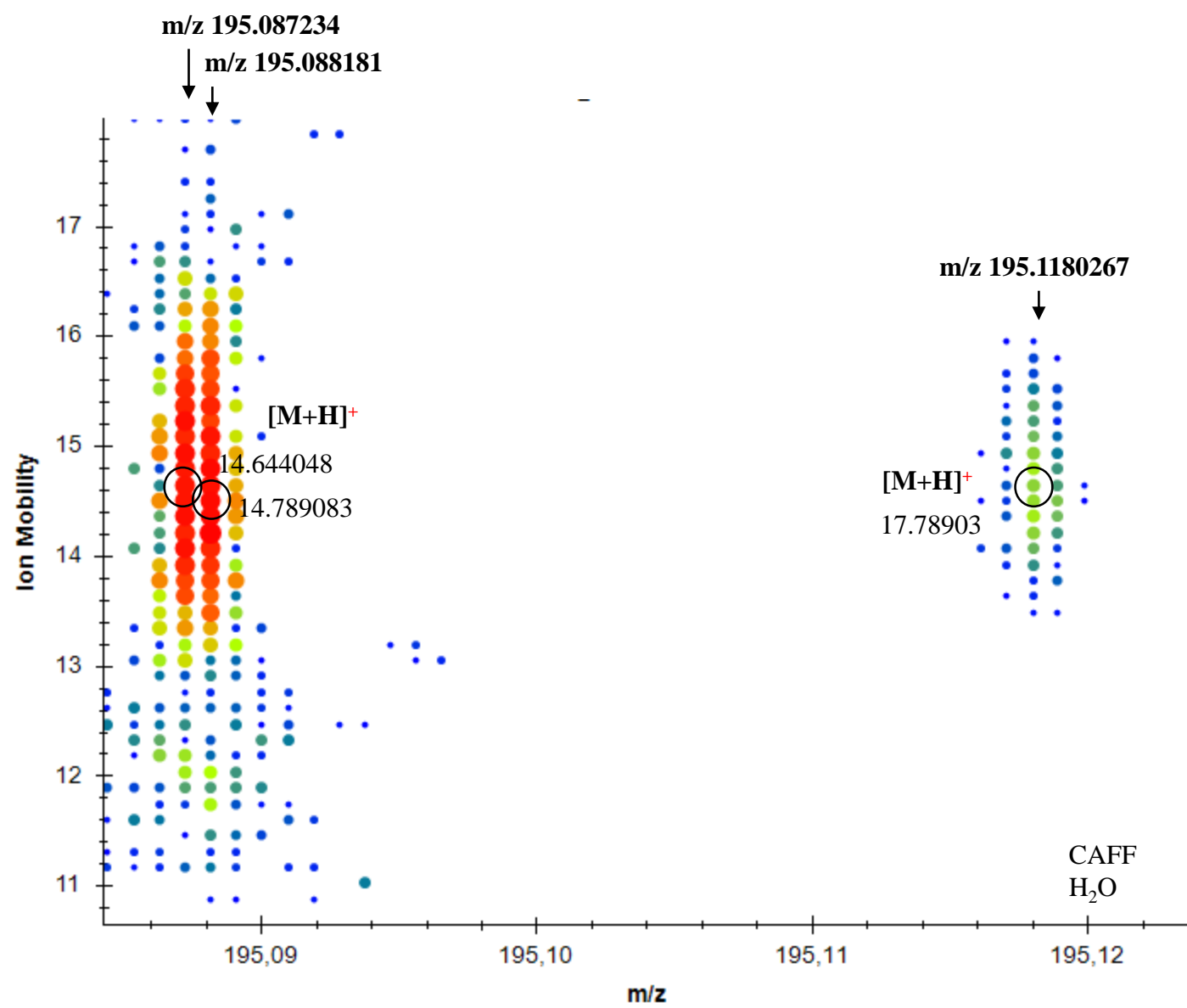
	Value	Error
A	3.87342	3.40751
B	$6.7267 \cdot 10^{11}$	$2.434 \cdot 10^{10}$
r	sd(yEr±)	Np
0.998 ₆₉	5.876	40.0013

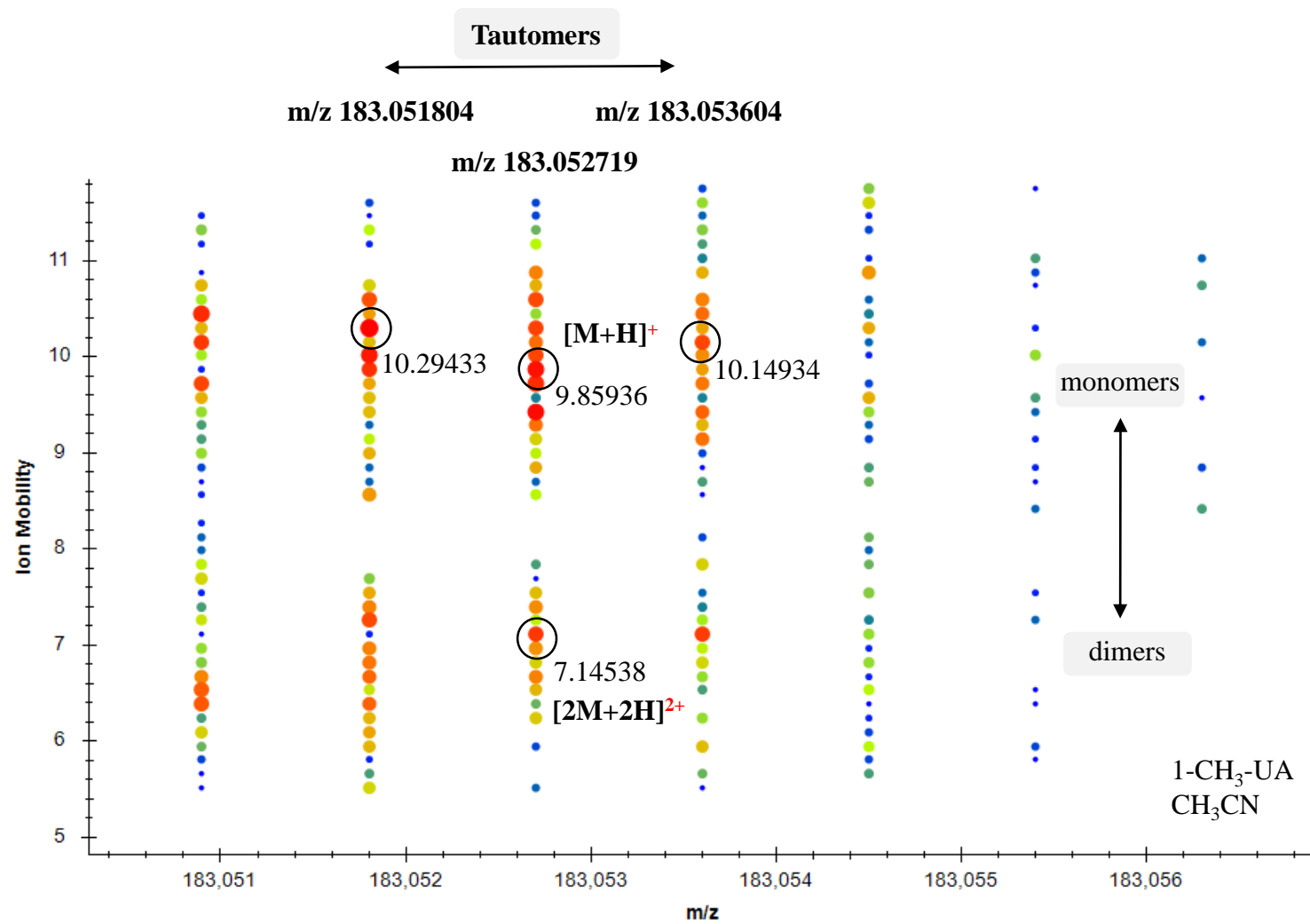


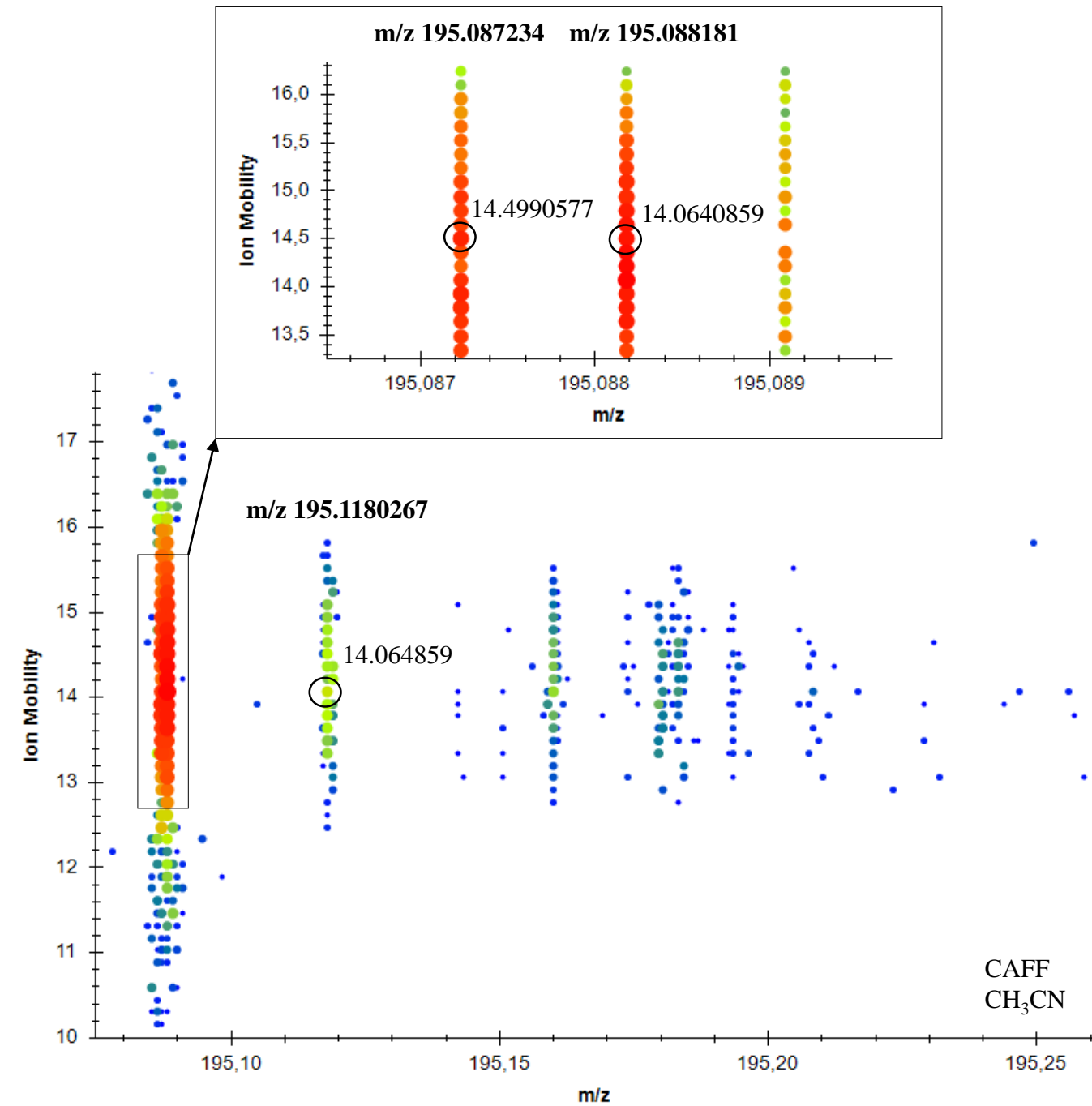




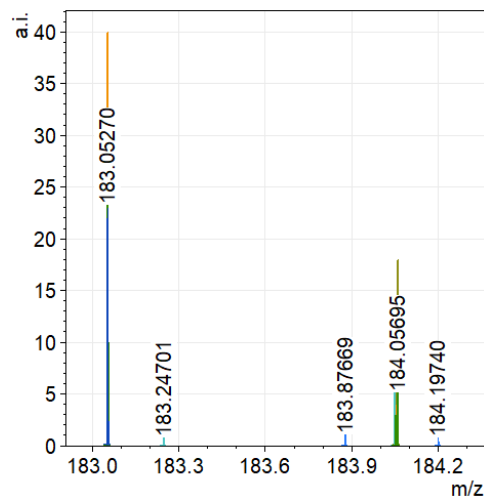
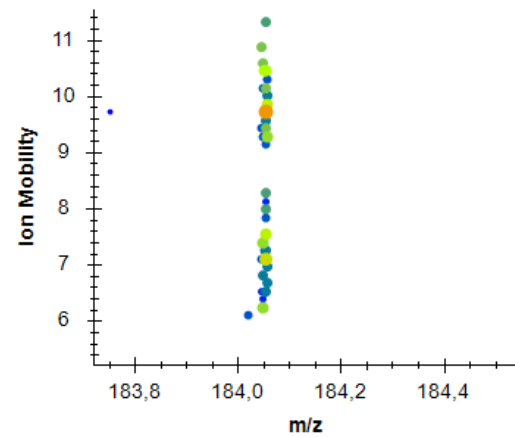
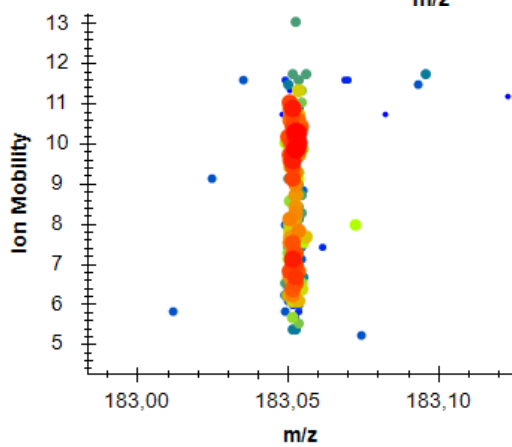
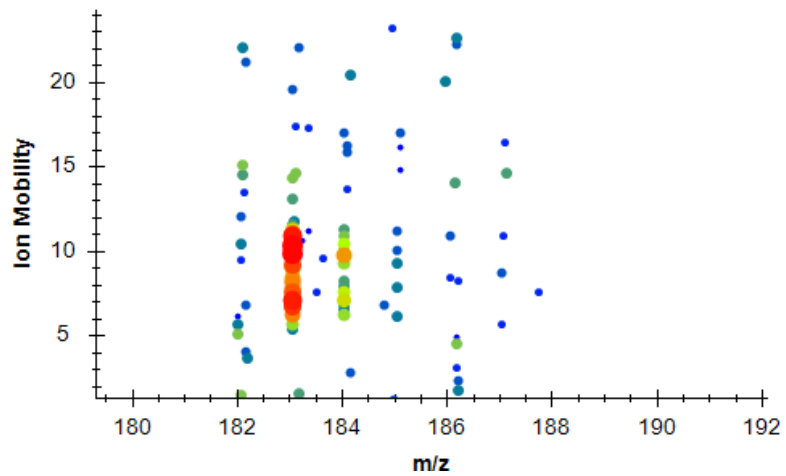


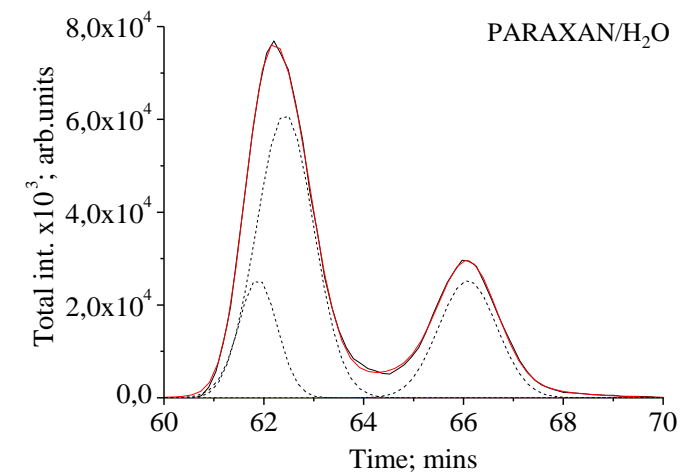
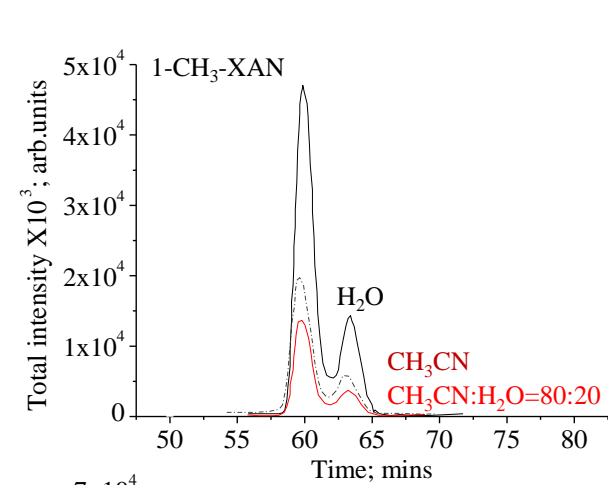
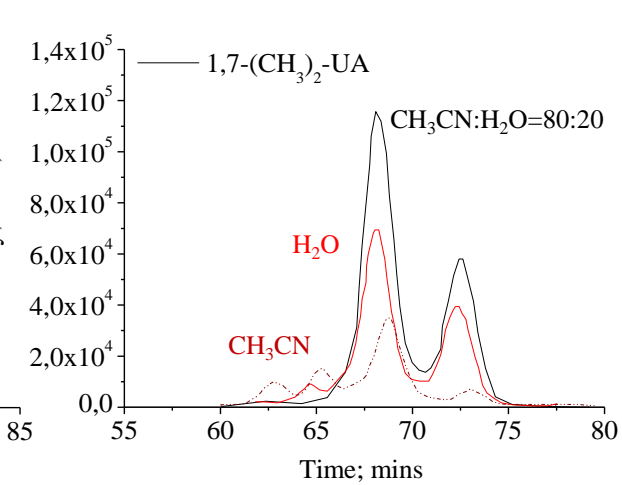
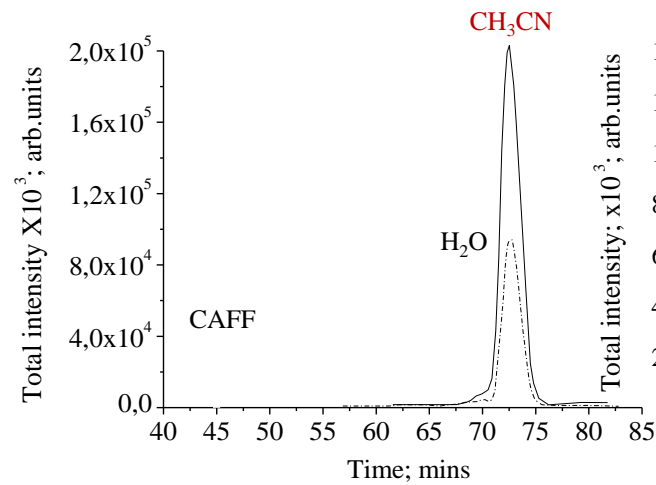
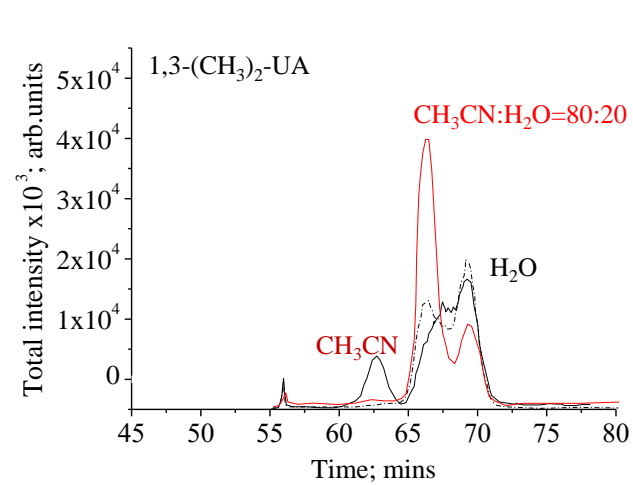




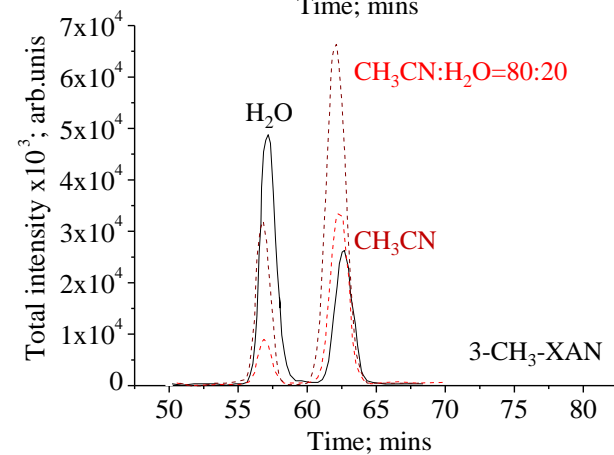
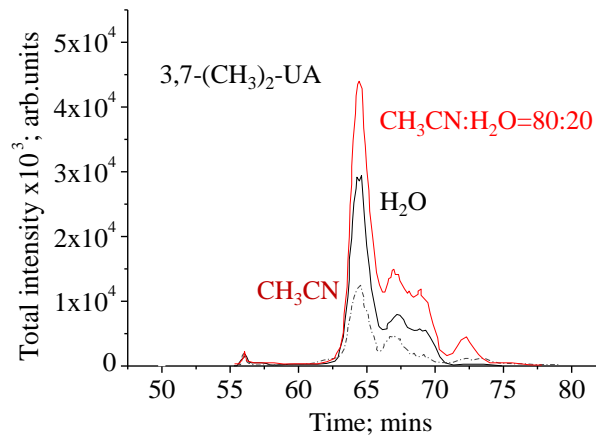


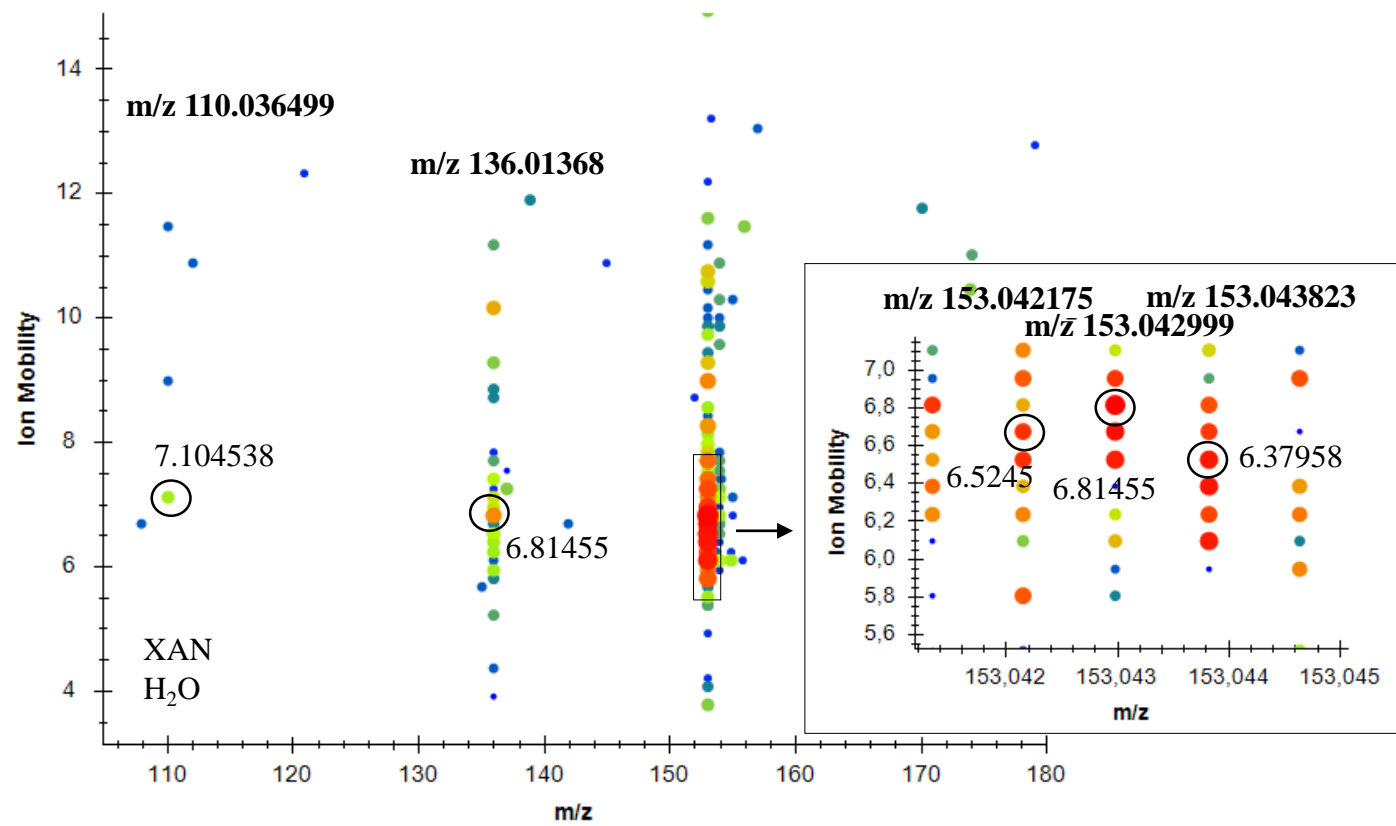
1-CH₃-UA/CH₃CN

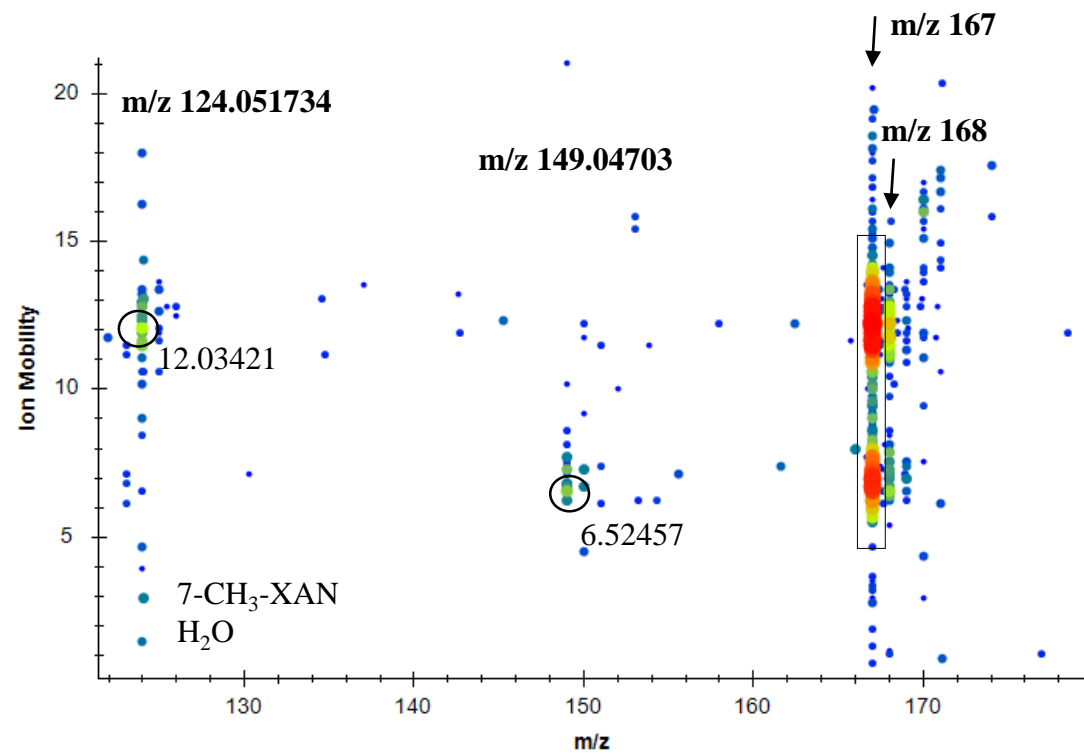


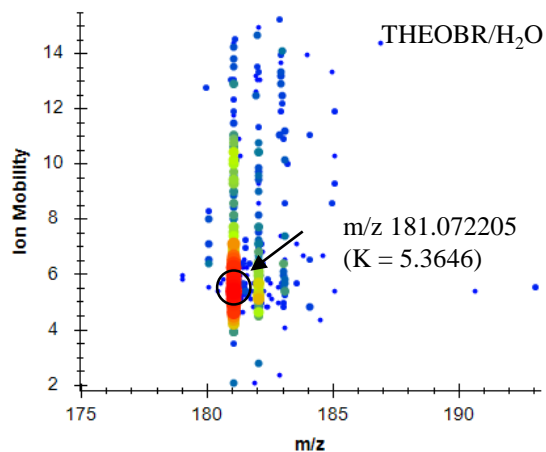


χ^2/DoF	248970.287	
r^2	0.9995₄	
xc1	61.878	± 0.023
A1	24915.96	± 14208.73
xc2	62.426	± 0.08636
A2	87374.26	± 16126.594
xc4	66.0863	± 0.0077
A4	36903.776	± 1663.342

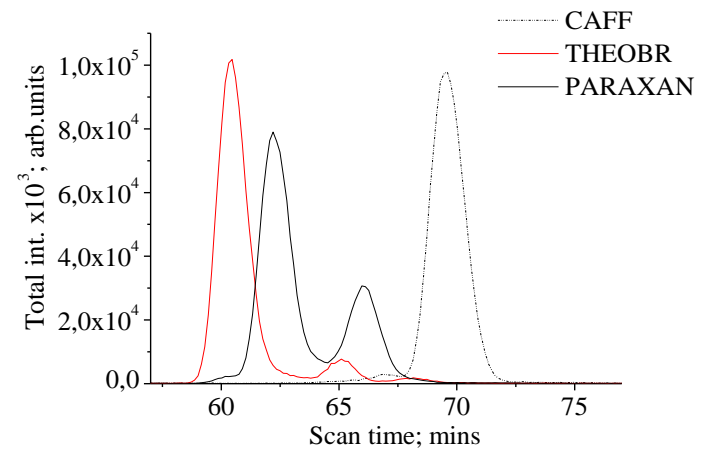
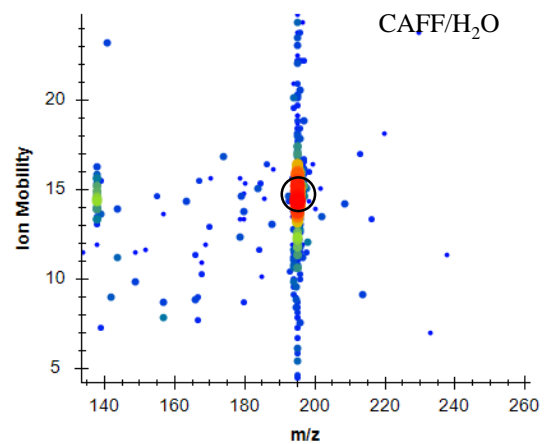


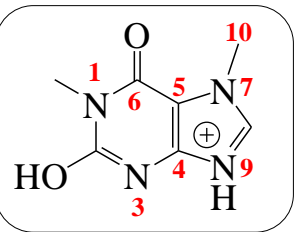




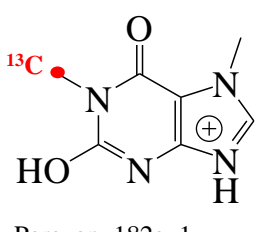


Ion mobility spectrometric data on THEOBR, and CAFF in solvent water; selected protomers, having mass spectrometric measurand m/z 181 of $[M+H]^+$ parent cation.

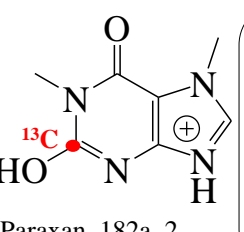




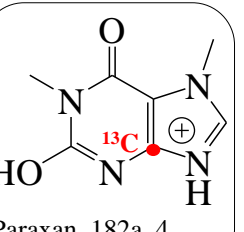
PARAXAN_181_a



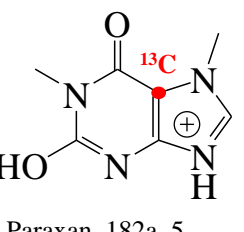
Paraxan_182a_1



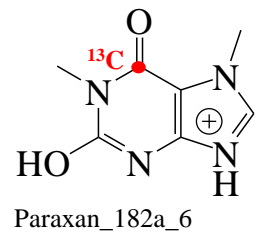
Paraxan_182a_2



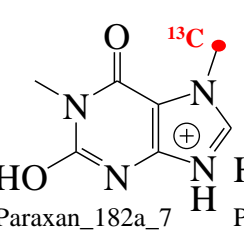
Paraxan_182a_4



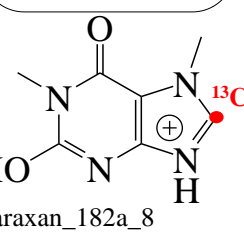
Paraxan_182a_5



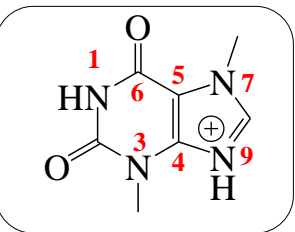
Paraxan_182a_6



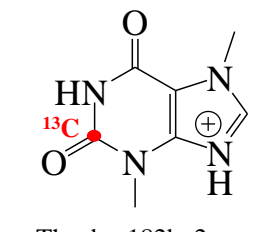
Paraxan_182a_7



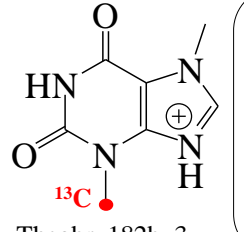
Paraxan_182a_8



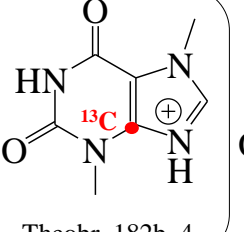
THEOBR_181_b



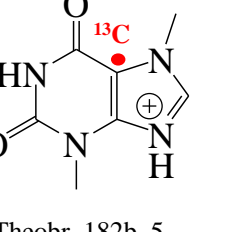
Theobr_182b_2



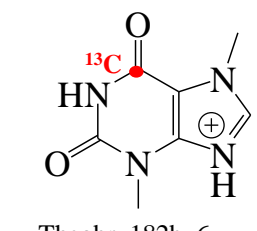
Theobr_182b_3



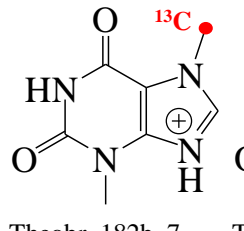
Theobr_182b_4



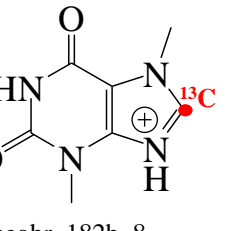
Theobr_182b_5



Theobr_182b_6

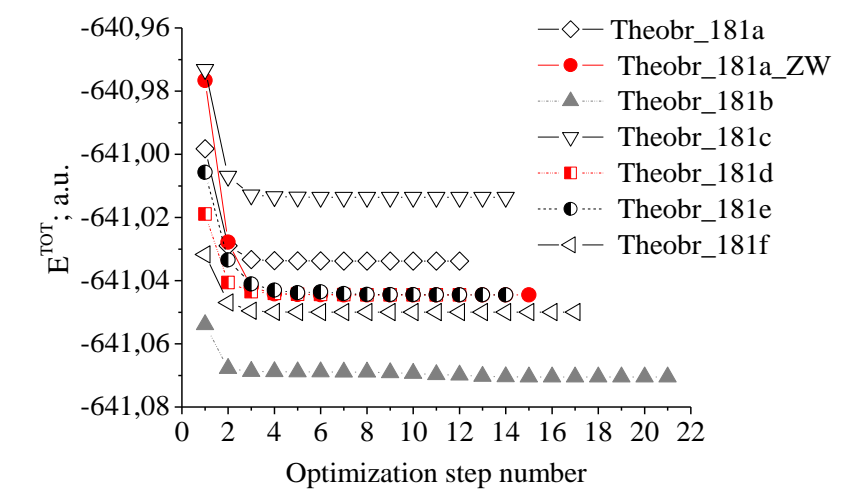
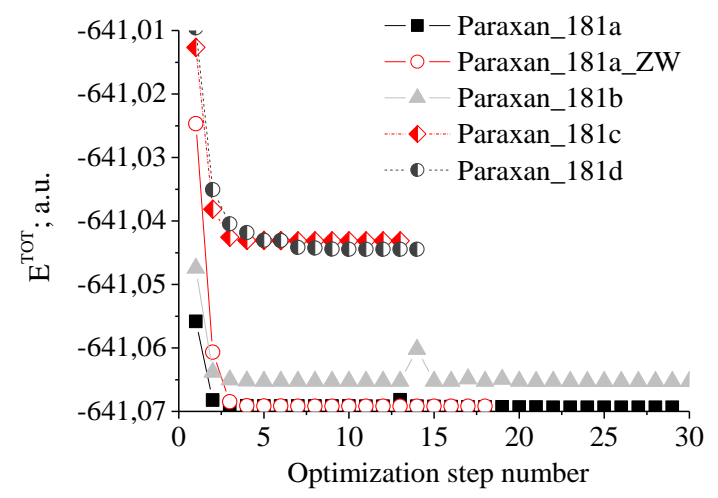


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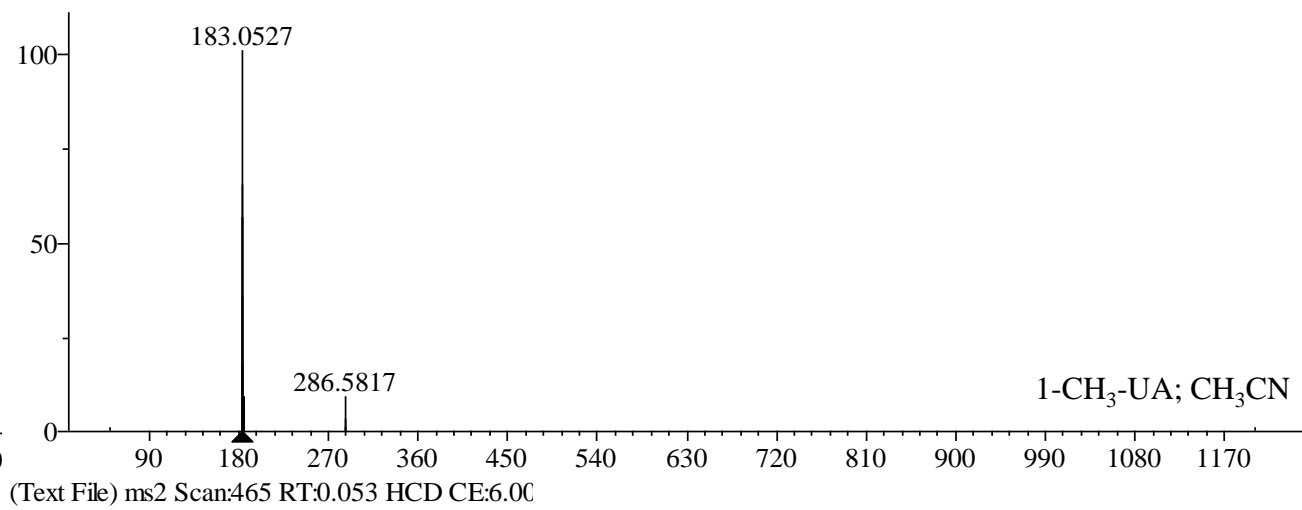
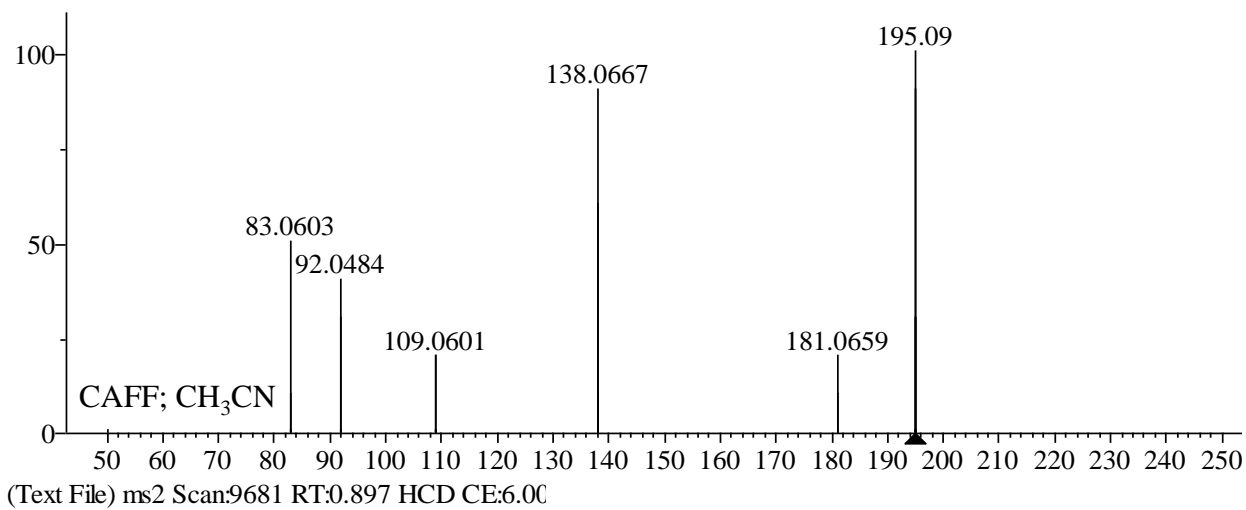
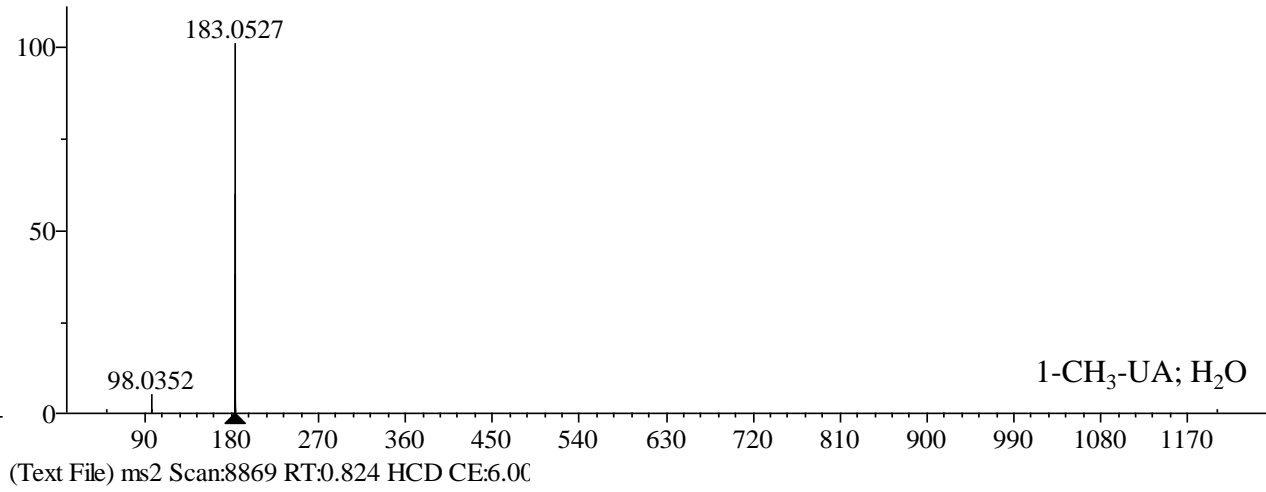
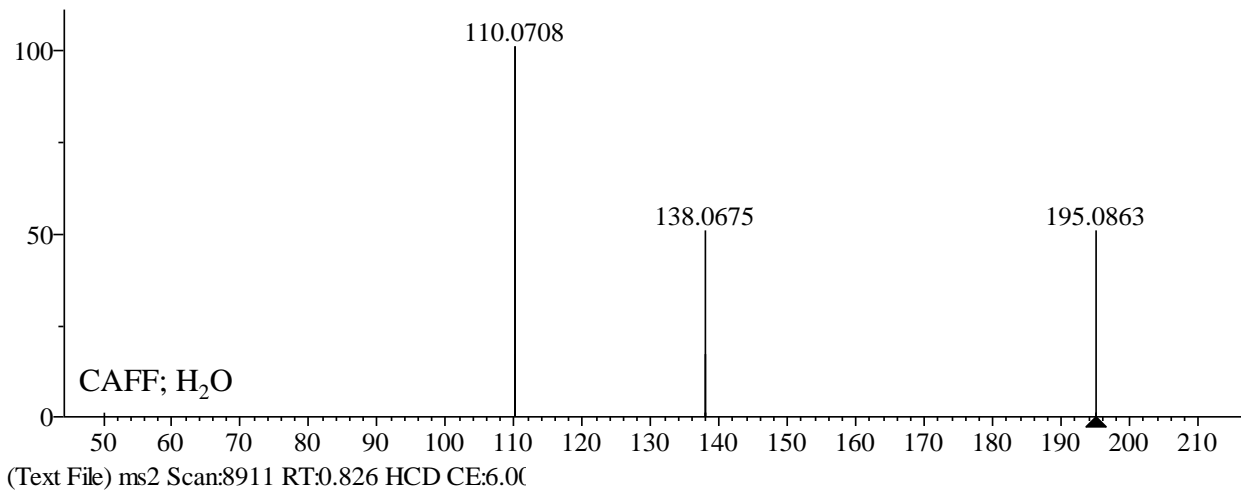


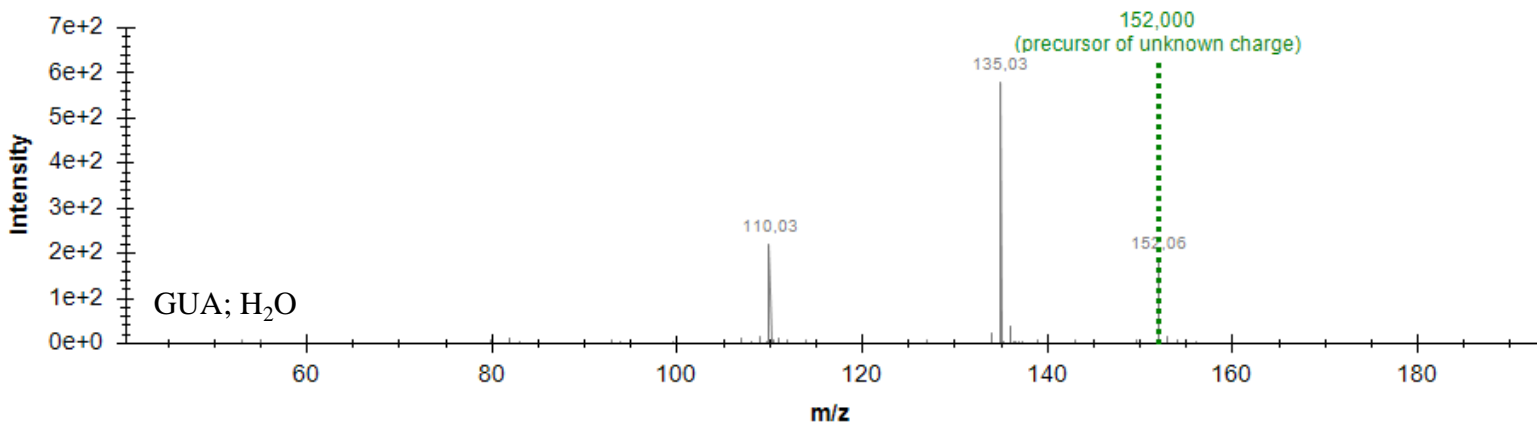
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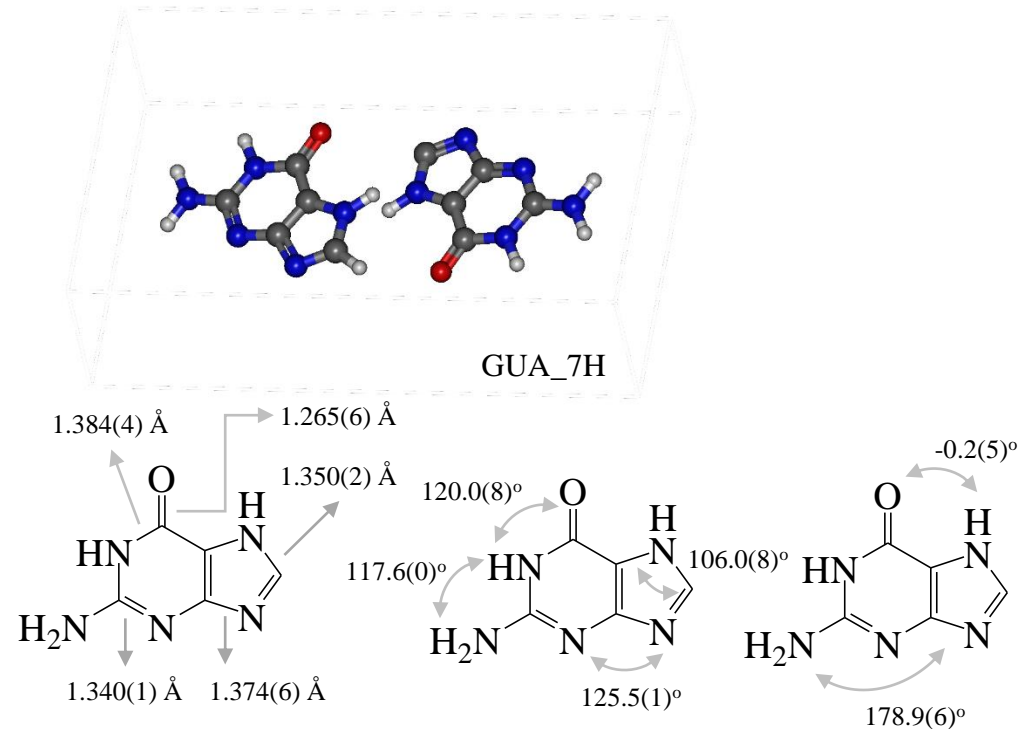
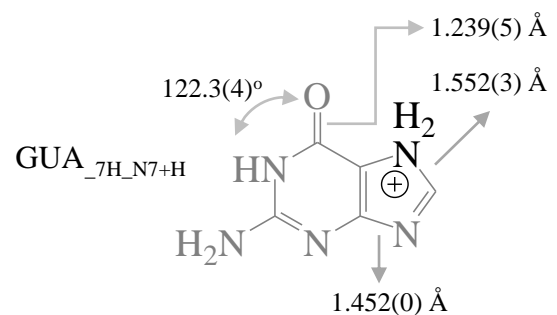
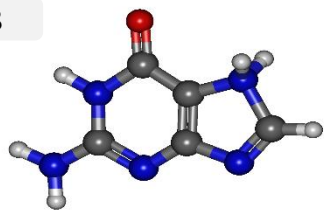
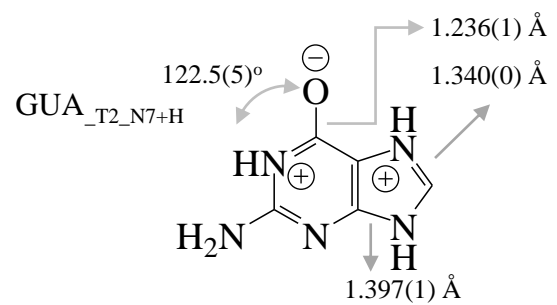
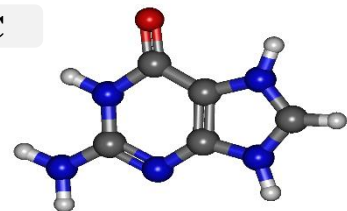
Protomers of $[M+H]^+$ ion of PARAXAN and THEOBR; most stable species are highlighted.

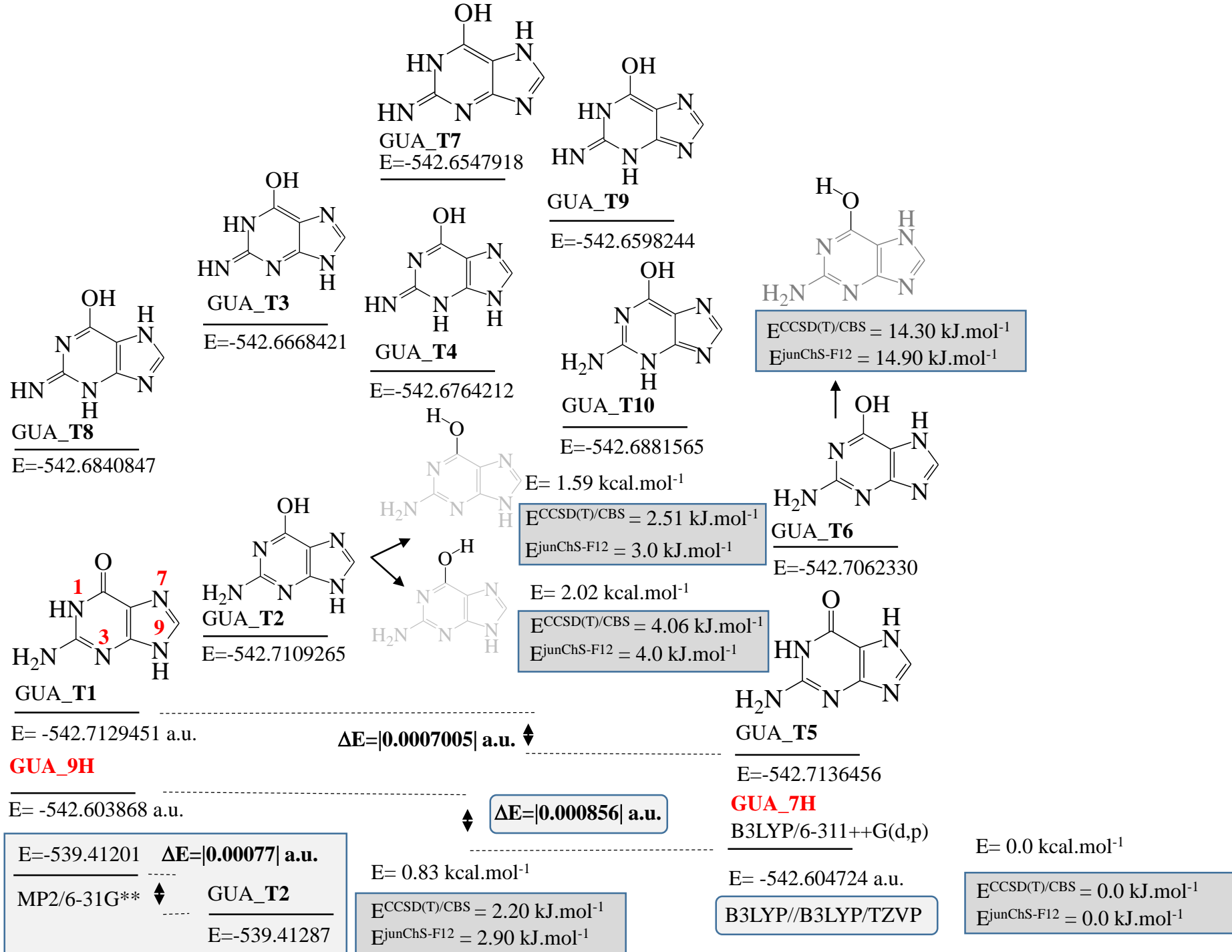


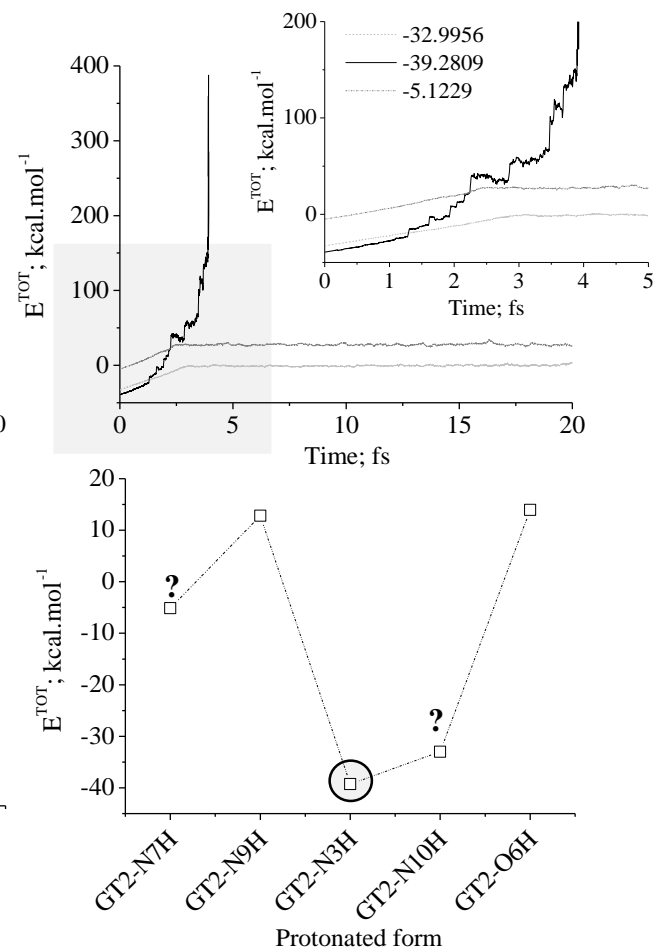
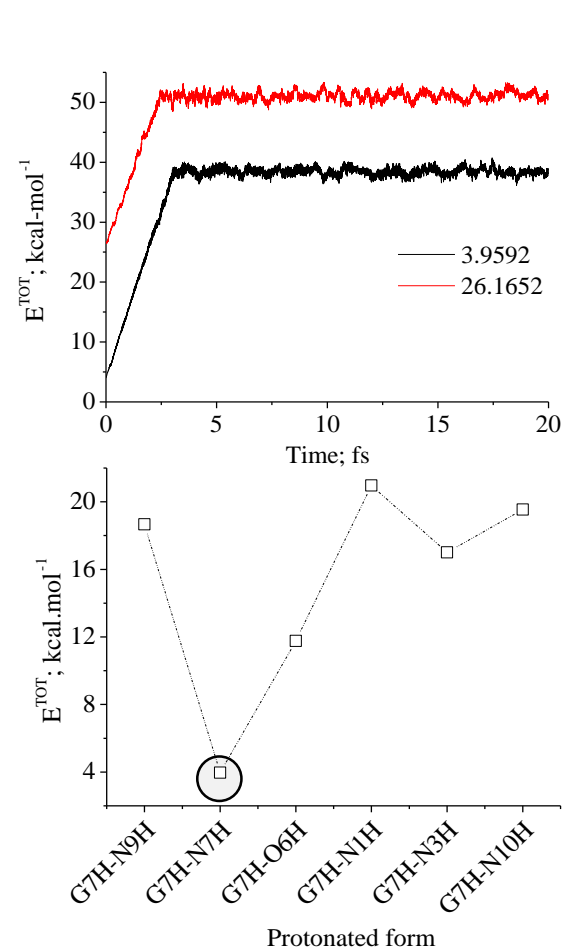
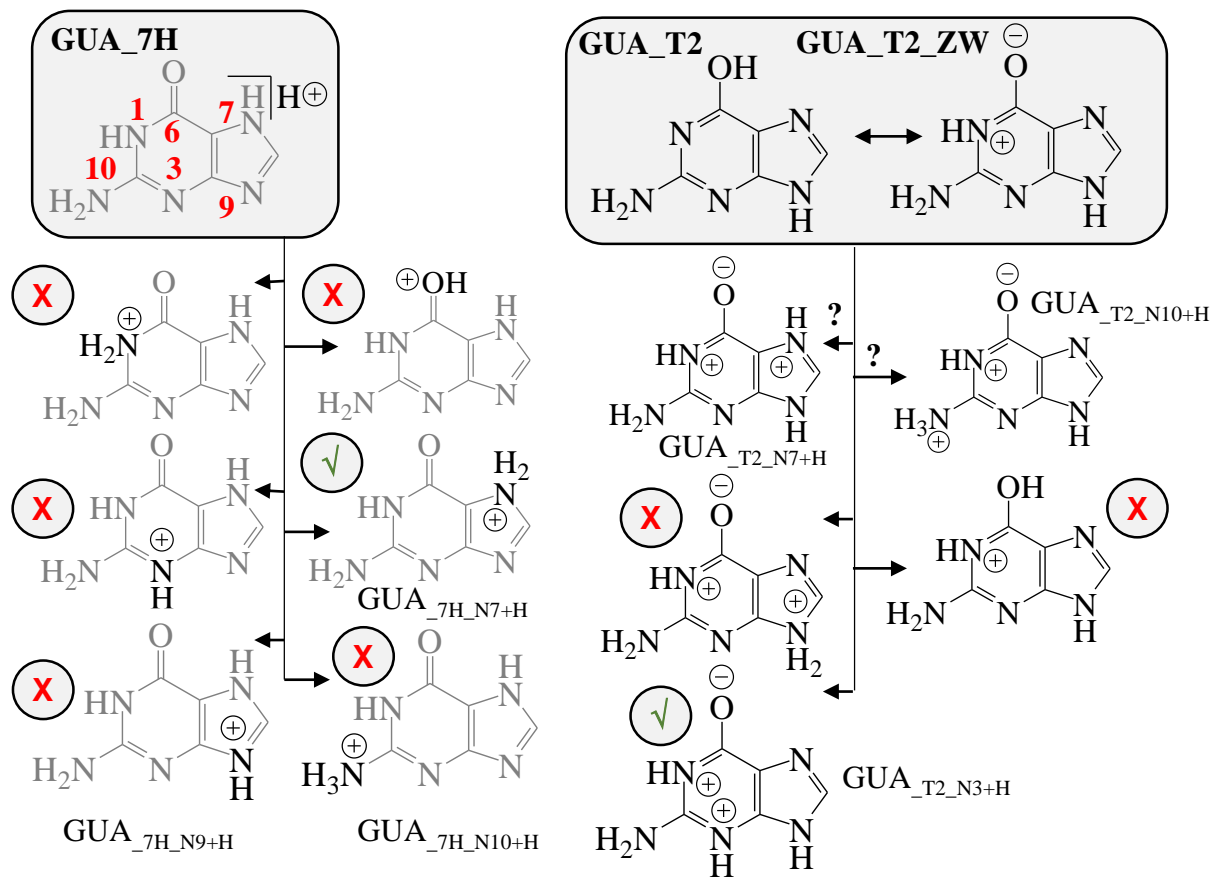
M062X/SDD optimization of protomers of $[M+H]^+$ ion of PARAXAN and THEOBR.

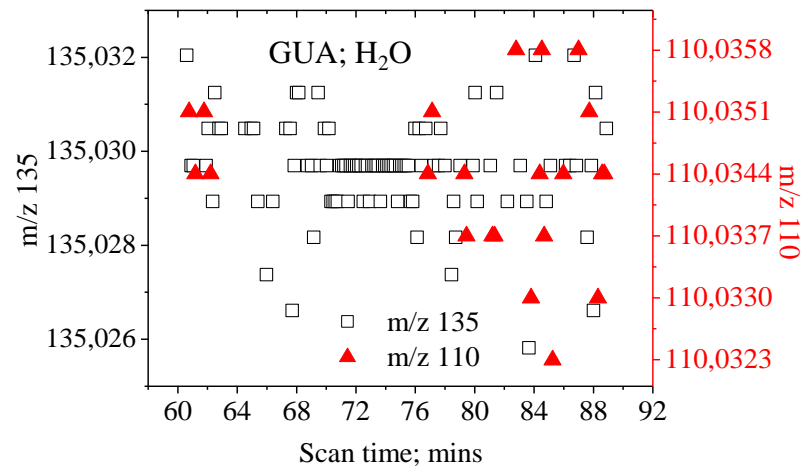




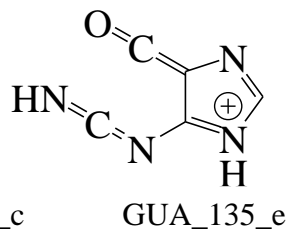
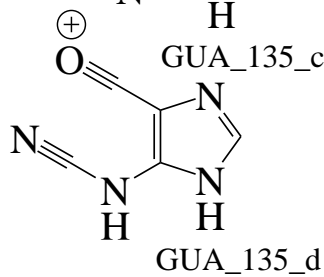
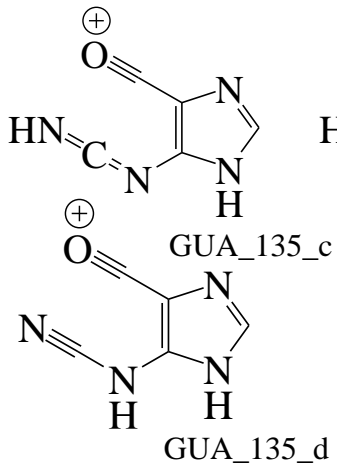
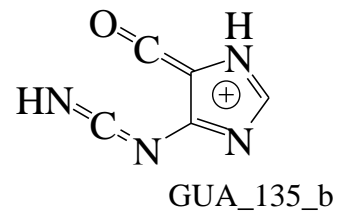
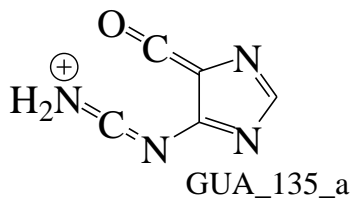
A**B****C**

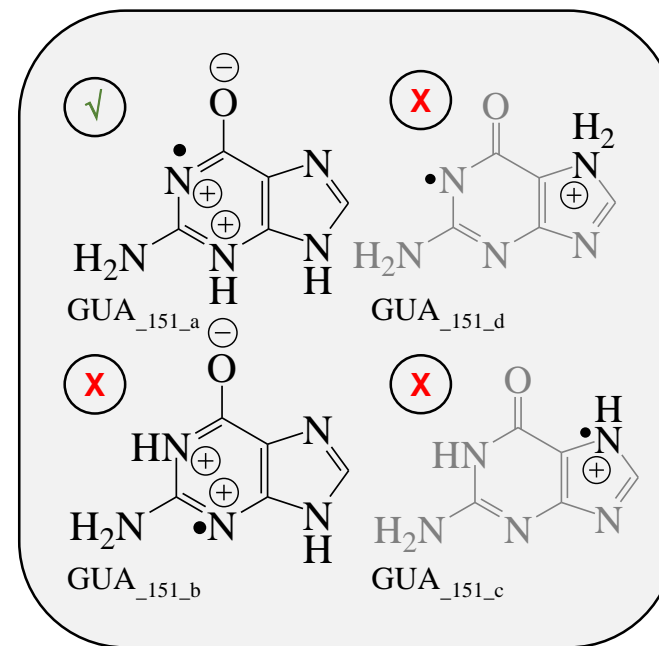
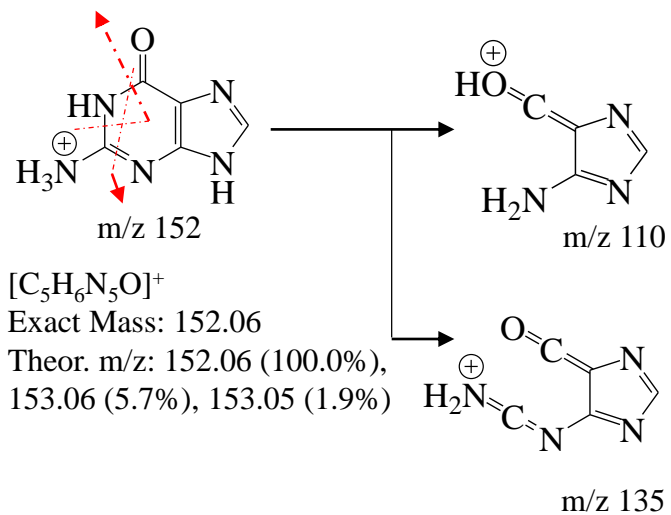
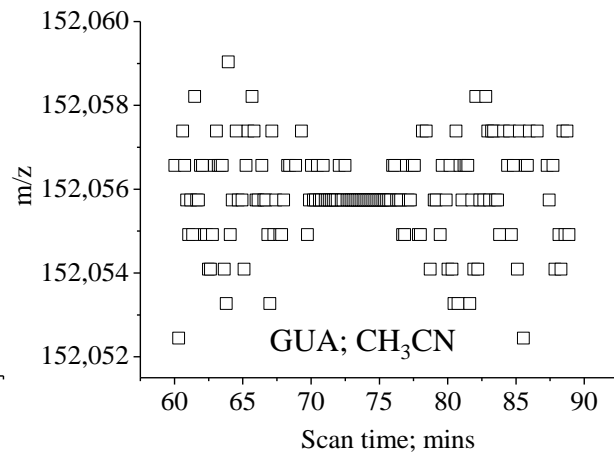
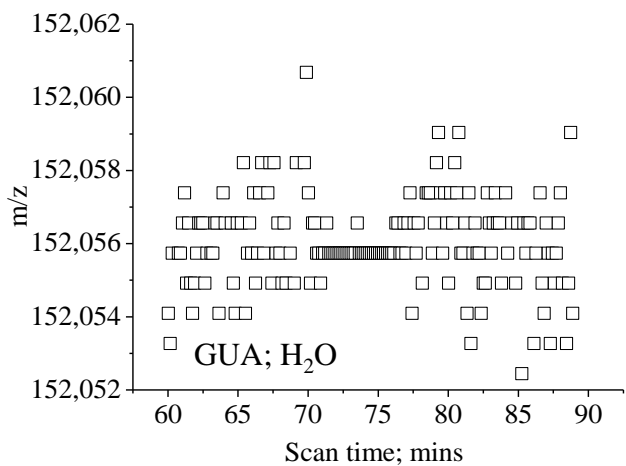


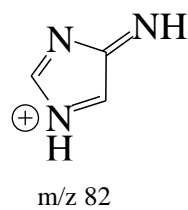
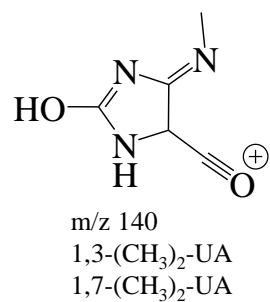
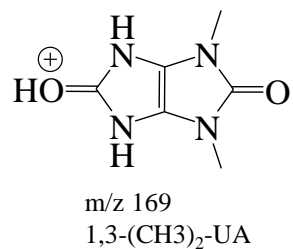
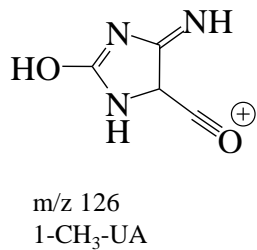
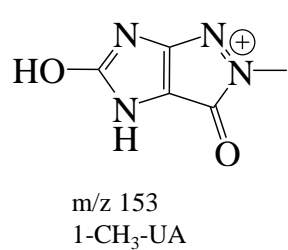
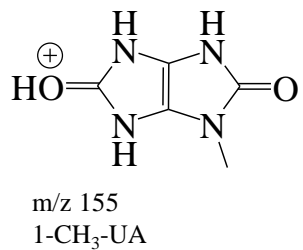
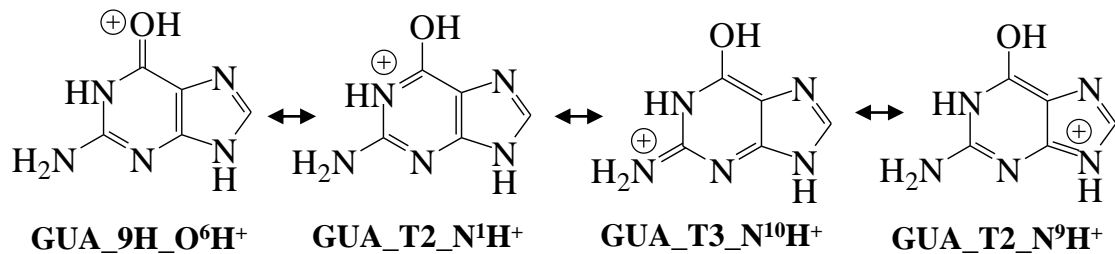
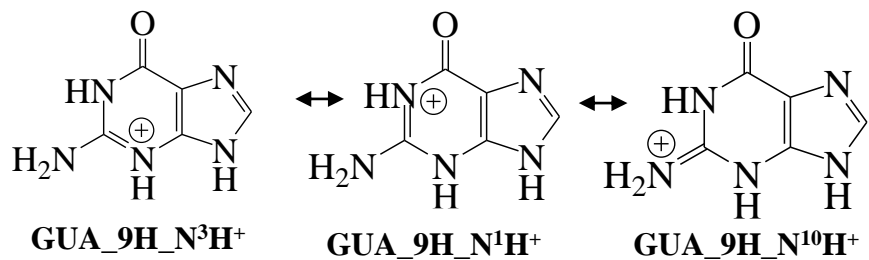
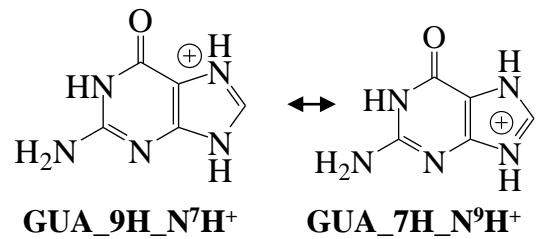


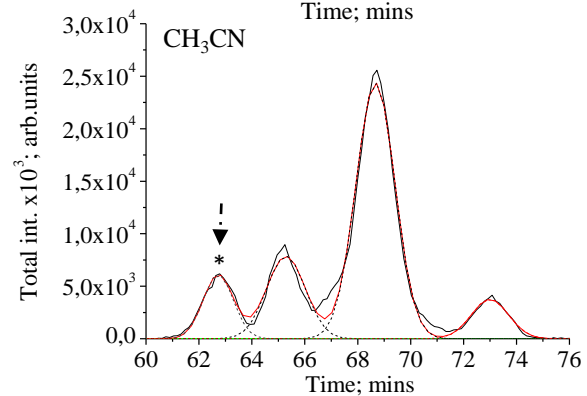
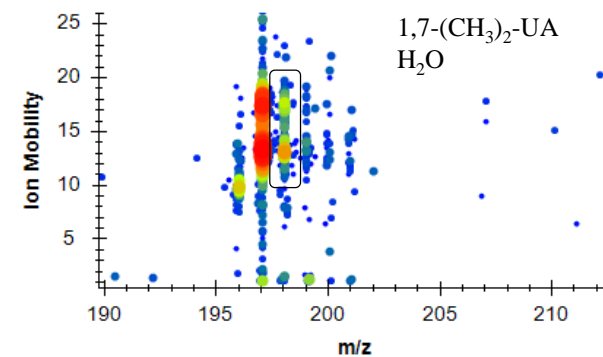
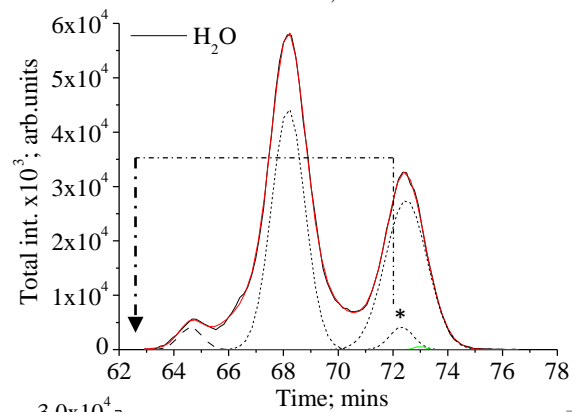
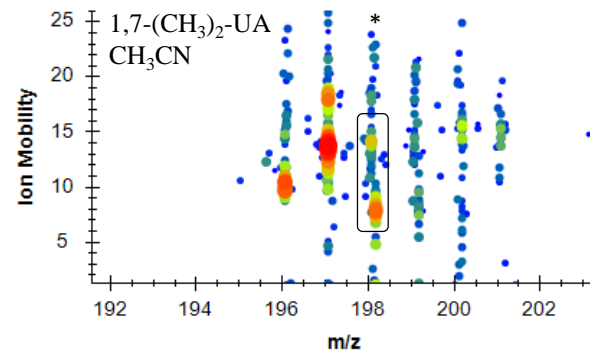
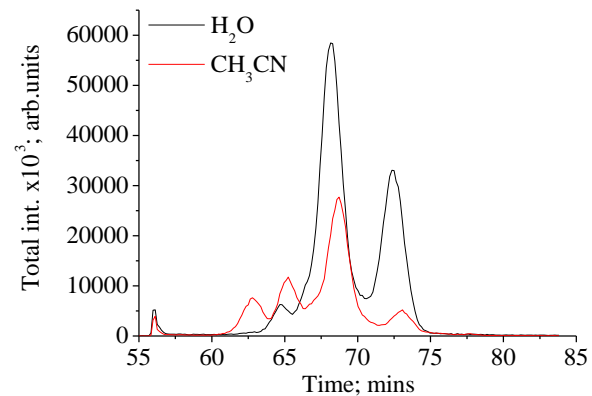


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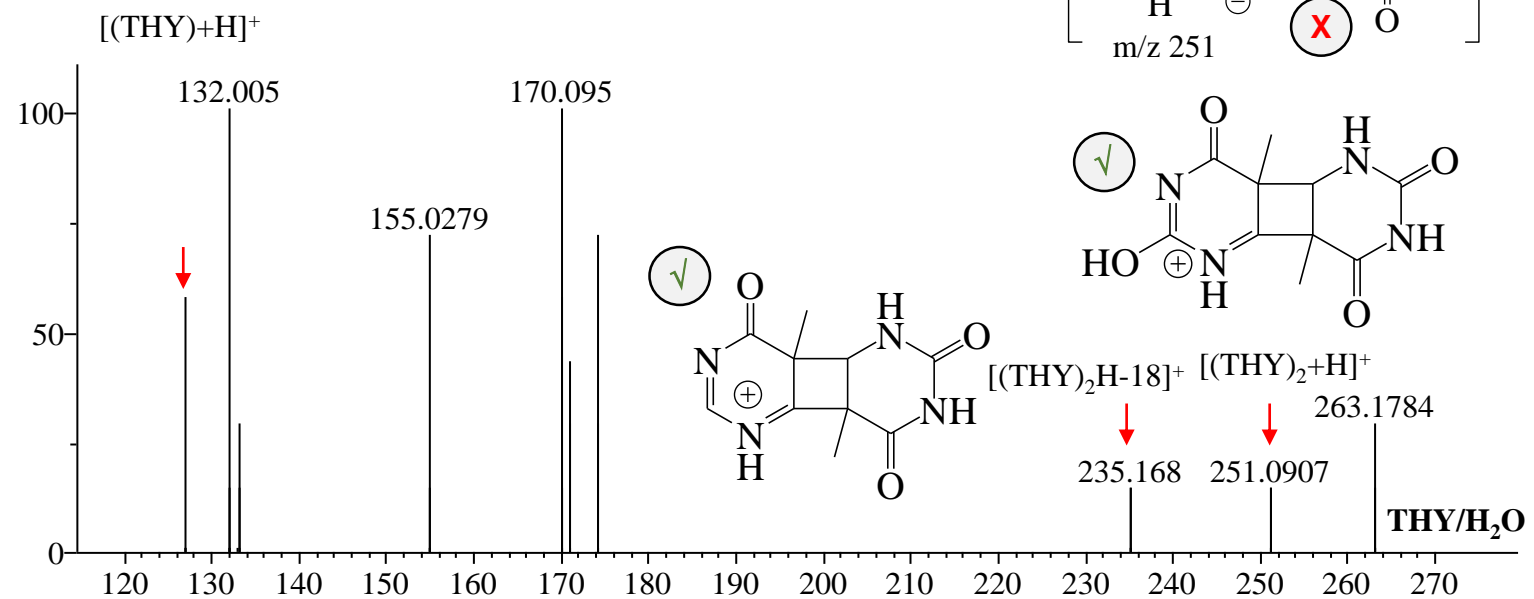
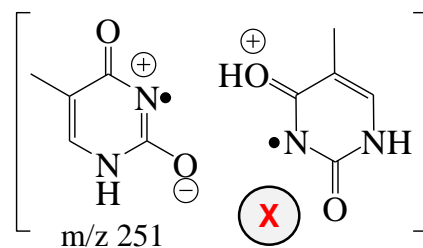
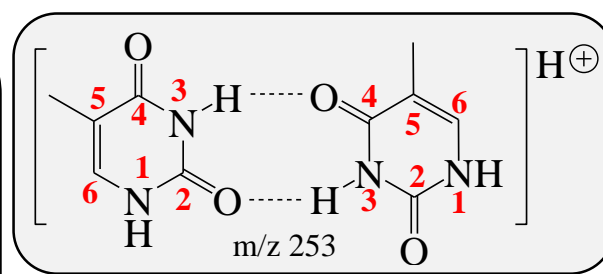
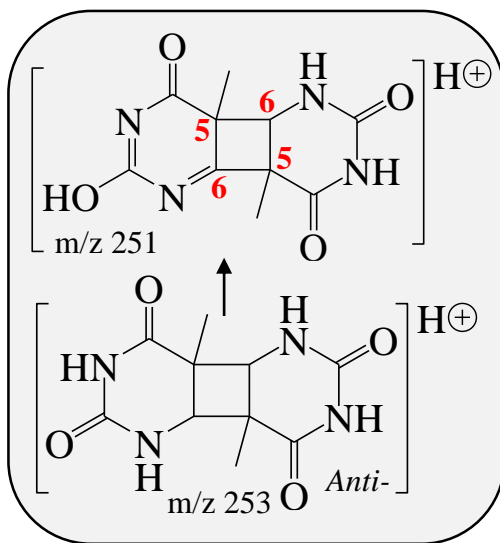
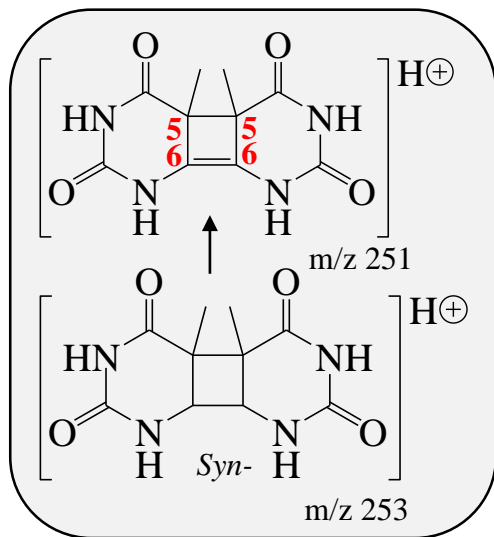








χ^2/DoF		173641.12		
r^2	0.9994₈		r^2	0.9881₈
xc1	64.613	± 0.0349	xc1	62.72 ± 0.04
A1	4362.87	± 724.995	A1	8671.7 ± 482.5
xc2	68.711	± 1.56	xc3	65.287 ± 0.031
A2	27983.5	± 54845.18	A3	14417.2 ± 551.2
xc4	68.1779	± 0.0063	xc4	72.994 ± 0.061
A4	67240.2	± 3055.65	A4	6627.6 ± 497.5
xc5	68.0012	± 0.3666		
A5	33056.9	± 55921.89		
xc6	72.4812	± 0.03055		
A6	52512.6	± 5006.04		
xc7	72.314	± 0.104		
A7	4480.77	± 5865.482		



(Text File) ms2 Scan:92 RT:68.145 HCL