Supporting Information

Computational Insights into β-Carboline Inhibition of Monoamine Oxidase A

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Table S1. Parameters and atom types for compound 1.

Name	Atom type	Charge	Name	Atom type	Charge
N1	NB	-0.627167	**C10**	CA	-0.258372
C1	CA	0.277849	**C11**	CA	-0.044640
N2	NA	-0.659257	**H1**	HA	0.074191
C2	CA	0.346683	**H2**	HA	0.138254
C3	CA	-0.524251	**H3**	HA	0.155958
C4	C56B	0.314435	**H4**	HA	0.160158
C5	C56B	-0.004619	**H5**	HA	0.181165
C6	C56B	0.433887	**H6**	HA	0.058143
C7	CA	-0.375403	**H7**	HA	0.206540
C8	C56B	-0.165691	**H8**	H	0.421296
C9	CA	-0.109160			

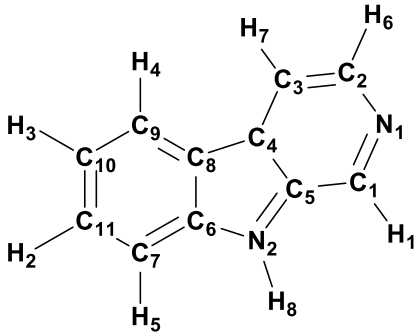


Table S2. Parameters and atom types for compound 2.

Name	Atom type	Charge	Name	Atom type	Charge
C1	CA	-0.124700	**C12**	CT	-0.185016
N1	NAP	0.034460	**H1**	HC	0.154979
C2	CA	-0.070145	**H2**	HC	0.154979
N2	NA	-0.624408	**H3**	HC	0.154979
C3	CA	-0.248609	**H4**	HA	0.181944
C4	C56B	0.146988	**H5**	HA	0.173293
C5	C56B	0.198083	**H6**	HA	0.161804
C6	C56B	0.397271	**H7**	HA	0.200980
C7	CA	-0.355814	**H8**	HA	0.200813
C8	C56B	-0.067840	**H9**	HA	0.215975
C9	CA	-0.148086	**H10**	HA	0.214076
C10	CA	-0.201283	**H11**	H	0.440122
C11	CA	-0.004845			

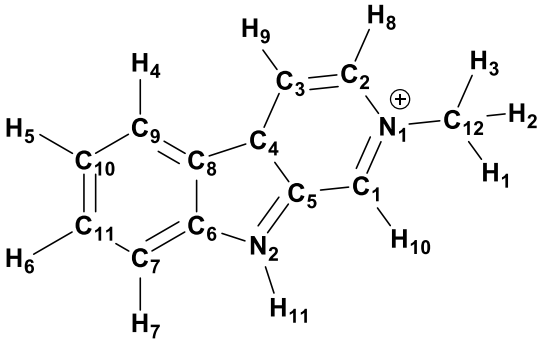


Table S3. Parameters and atom types for compound 3.

Name	Atom type	Charge	Name	Atom type	Charge
C1	CT	-0.523721	**C11**	CA	-0.233281
N1	NB	-0.658430	**C12**	CA	-0.065902
C2	CA	0.595521	**H1**	HA	0.177082
N2	NA	-0.541782	**H2**	HA	0.136823
C3	CA	0.240226	**H3**	HA	0.164965
C4	CA	-0.435624	**H4**	HA	0.174390
C5	C56B	0.176056	**H5**	HA	0.097254
C6	C56B	-0.090646	**H6**	HA	0.179458
C7	C56B	0.373985	**H7**	HC	0.139919
C8	CA	-0.375332	**H8**	HC	0.139919
C9	C56B	-0.029445	**H9**	HC	0.139919
C10	CA	-0.177414	**H10**	H	0.396061

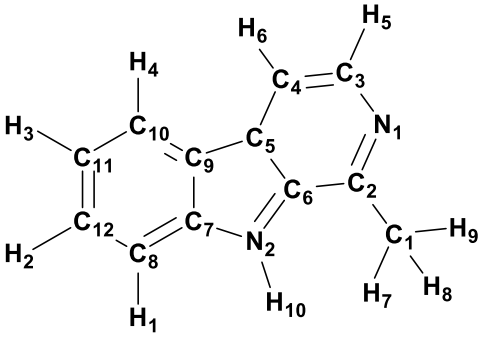


Table S4. Parameters and atom types for compound 4.

Name	Atom type	Charge	Name	Atom type	Charge
C1	CA	0.314960	**C13**	CT	-0.369953
N1	NAP	-0.005213	**H1**	HA	0.190157
C2	CA	-0.130805	**H2**	HA	0.181759
N2	NA	-0.509171	**H3**	HA	0.197921
C3	CA	-0.244798	**H4**	HA	0.159727
C4	C56B	0.078153	**H5**	HC	0.144194
C5	C56B	-0.030148	**H6**	HA	0.211289
C6	C56B	0.360353	**H7**	HA	0.226637
C7	CA	-0.374663	**H8**	HC	0.144194
C8	C56B	0.019461	**H9**	HC	0.144194
C9	CA	-0.190045	**H10**	HC	0.146419
C10	CA	-0.188390	**H11**	HC	0.146419
C11	CA	-0.012521	**H12**	HC	0.146419
C12	CT	-0.164595	**H13**	H	0.408045

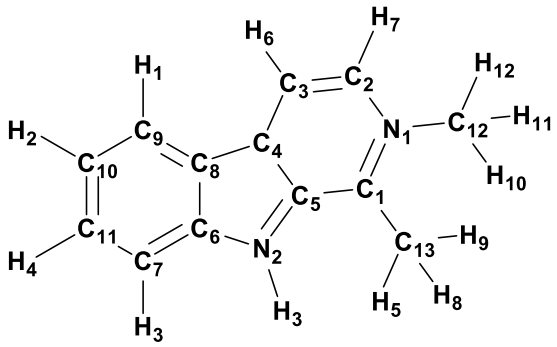


Table S5. Parameters and atom types for compound 5.

Name	Atom type	Charge	Name	Atom type	Charge
C1	CA	0.293121	**H1**	HA	0.166798
N1	NAP	-0.023254	**H2**	HA	0.180803
C2	CA	-0.133842	**H3**	HA	0.158483
N2	NA	-0.056208	**H4**	HA	0.183084
C3	CA	-0.195988	**H5**	HC	0.146197
C4	C56B	0.069653	**H6**	HA	0.214972
C5	C56B	-0.077079	**H7**	HA	0.203382
C6	C56B	0.181622	**H8**	HC	0.120573
C7	CA	-0.291303	**H9**	HC	0.120573
C8	C56B	0.025576	**H10**	HC	0.120573
C9	CA	-0.172491	**H11**	HC	0.146197
C10	CA	-0.179275	**H12**	HC	0.146197
C11	CA	-0.027107	**H13**	HC	0.146986
C12	CT	-0.163345	**H14**	HC	0.146986
C13	CT	-0.195627	**H15**	HC	0.146986
C14	CT	-0.403242			

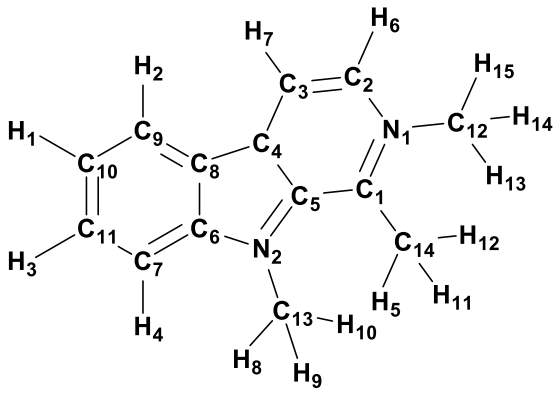


Table S6. Parameters and atom types for compound 6.

Name	Atom type	Charge	Name	Atom type	Charge
C1	CT	-0.357709	**C12**	CA	0.548725
N1	NB	-0.681270	**C13**	CT	0.027979
O1	OS	-0.383457	**H1**	HA	0.080821
C2	CA	0.621389	**H2**	HA	0.204471
N2	NA	-0.455290	**H3**	HA	0.192071
C3	CA	0.294448	**H4**	HA	0.161627
C4	CA	-0.536078	**H5**	HA	0.194987
C5	C56B	0.363125	**H6**	HC	0.093373
C6	C56B	-0.225204	**H7**	HC	0.093373
C7	C56B	0.312346	**H8**	HC	0.093373
C8	CA	-0.498308	**H9**	H	0.372831
C9	C56B	-0.210456	**H10**	HC	0.062240
C10	CA	-0.024785	**H11**	HC	0.062240
C11	CA	-0.469101	**H12**	HC	0.062240

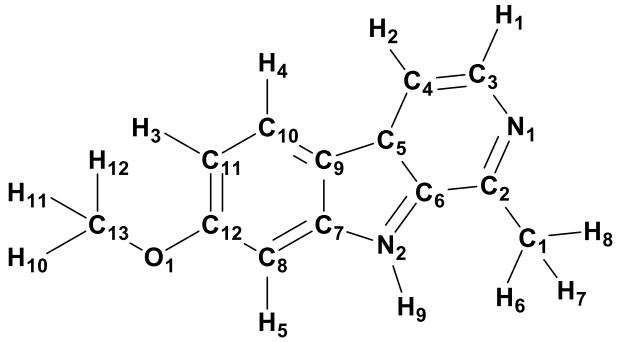


Table S7. Parameters and atom types for compound 7.

Name	Atom type	Charge	Name	Atom type	Charge
C1	CA	0.297264	**H1**	HC	0.144399
N1	NAP	-0.035333	**H2**	HC	0.144399
C2	CA	-0.134899	**H3**	HC	0.144399
N2	NA	-0.508775	**H4**	HC	0.083733
C3	CA	-0.145909	**H5**	HC	0.083733
C4	C56B	0.100178	**H6**	HC	0.083733
C5	C56B	-0.051447	**H7**	HA	0.186213
C6	C56B	0.454071	**H8**	HA	0.199258
C7	CA	-0.646777	**H9**	HA	0.247531
C8	C56B	-0.160466	**H10**	HA	0.218259
C9	CA	-0.131442	**H11**	HA	0.216955
C10	CA	-0.358781	**O1**	OS	-0.369729
C11	CA	0.628524	**H12**	HC	0.151850
C12	CT	-0.181445	**H13**	HC	0.151850
C13	CT	-0.381808	**H14**	HC	0.151850
C14	CT	0.002102	**H15**	H	0.416511

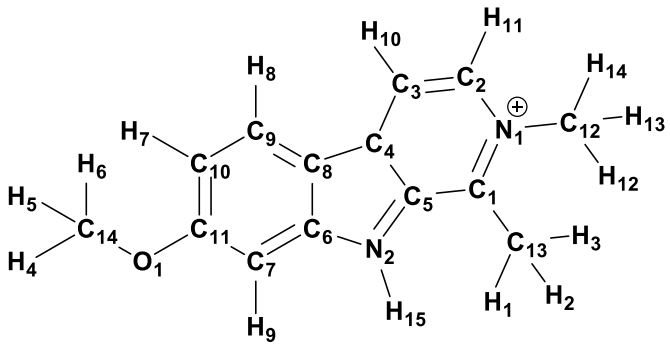


Table S8. Parameters and atom types for compound 8.

Name	Atom type	Charge	Name	Atom type	Charge
C1	CA	0.274315	**H2**	HC	0.035193
N1	NAP	0.091401	**H3**	HC	0.035193
C2	CA	-0.139962	**H4**	HA	0.244872
N2	NA	0.077014	**H5**	HA	0.195140
C3	CA	-0.235150	**H6**	HA	0.217880
C4	C56B	0.115165	**H7**	HA	0.226170
C5	C56B	-0.143271	**H8**	HA	0.203693
C6	C56B	0.186189	**H9**	HC	0.143710
C7	CA	-0.486059	**H10**	HC	0.149475
C8	C56B	-0.032649	**H11**	HC	0.149475
C9	CA	-0.153367	**H12**	HC	0.149475
C10	CA	-0.353112	**H13**	HC	0.143710
C11	CA	0.529660	**H14**	HC	0.143710
C12	CT	-0.286091	**O1**	OS	-0.402910
C13	CT	0.128488	**H15**	HC	0.150805
C14	CT	-0.307855	**H16**	HC	0.150805
C15	CT	-0.387110	**H17**	HC	0.150805
H1	HC	0.035193			

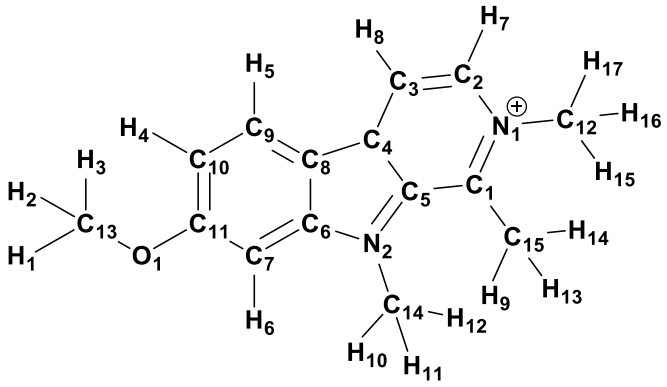


Table S9. Parameters and atom types for compound 9.

Name	Atom type	Charge	Name	Atom type	Charge
C1	CT	-0.474064	**C13**	CT	0.481459
N1	NI	-0.730741	**H1**	HA	0.163041
O1	OS	-0.387008	**H2**	HA	0.190115
C2	CD	0.695351	**H3**	HA	0.197476
N2	NA	-0.442773	**H4**	HA	-0.044034
C3	C5B	0.116397	**H5**	HA	0.090443
C4	C5A	-0.214237	**H6**	HA	0.090443
C5	C56A	0.288777	**H7**	HA	-0.044034
C6	CA	-0.501025	**H8**	HA	0.121525
C7	C56B	-0.153271	**H9**	HA	0.121525
C8	CA	-0.048741	**H10**	HA	0.121525
C9	CA	-0.461798	**H11**	H	0.370836
C10	CA	0.541308	**H12**	HC	0.056286
C11	CT	0.043539	**H13**	HC	0.056286
C12	CT	-0.300895	**H14**	HC	0.056286

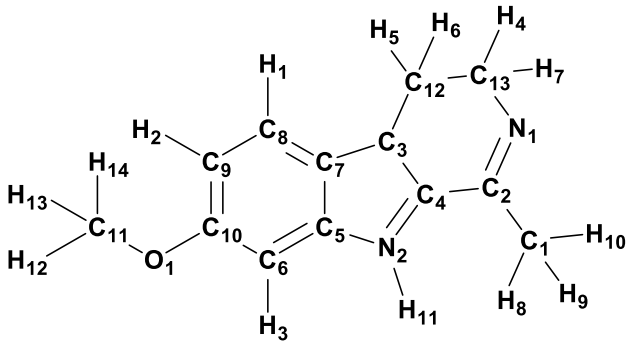


Table S10. Parameters and atom types for compound 10.

Name	Atom type	Charge	Name	Atom type	Charge
C1	CT	-0.456900	**H1**	HA	0.194599
N1	NI	-0.710167	**H2**	HC	0.047052
C2	CD	0.671601	**H3**	HA	0.168913
N2	NA	-0.458449	**H4**	HA	0.181209
C3	CT	0.445969	**H5**	HC	0.047052
C4	CT	-0.294499	**H6**	HC	0.047052
C5	C5B	0.087881	**H7**	HC	0.087832
C6	C5A	-0.156832	**H8**	HC	0.087832
C7	C56A	0.169326	**H9**	HC	-0.034114
C8	CA	-0.186125	**H10**	HC	-0.034114
C9	C56B	-0.042593	**O1**	OS	-0.391438
C10	CA	-0.356187	**H11**	HC	0.118760
C11	CA	0.427084	**H12**	HC	0.118760
C12	CA	-0.338720	**H13**	HC	0.118760
C13	CT	0.070257	**H14**	H	0.370199

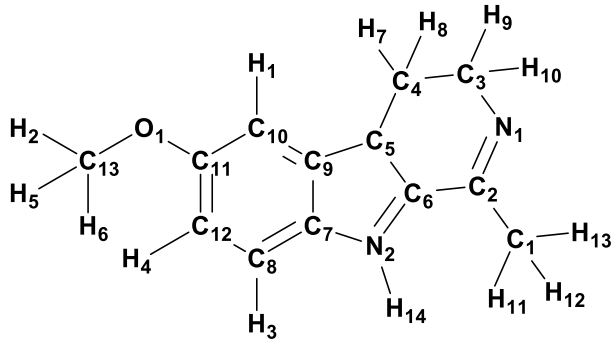


Table S11. Parameters and atom types for compound 11.

Name	Atom type	Charge	Name	Atom type	Charge
C1	CM	0.406343	**H2**	HC	0.072194
N1	NE	-0.183108	**H3**	HC	0.072194
C2	CT	-0.027202	**H4**	HC	0.123986
N2	NIP	-0.431395	**H5**	HC	0.123986
C3	CT	-0.187076	**H6**	HC	0.123986
C4	CM	0.119921	**H7**	HC	0.190101
C5	CM	-0.174237	**H8**	HC	0.191122
C6	CG	0.216533	**H9**	HC	0.188536
C7	CM	-0.230202	**H10**	HC	0.101415
C8	CM	-0.007605	**H11**	HC	0.101415
C9	CM	-0.381159	**H12**	HC	0.124900
C10	CM	0.446756	**H13**	HC	0.124900
C11	CM	-0.218144	**O1**	OS	-0.375086
C12	CT	-0.138609	**H14**	HC	0.136566
C13	CT	0.031355	**H15**	HC	0.136566
C14	CT	-0.281383	**H16**	HC	0.136566
H1	HC	0.072194	**H17**	H	0.393672

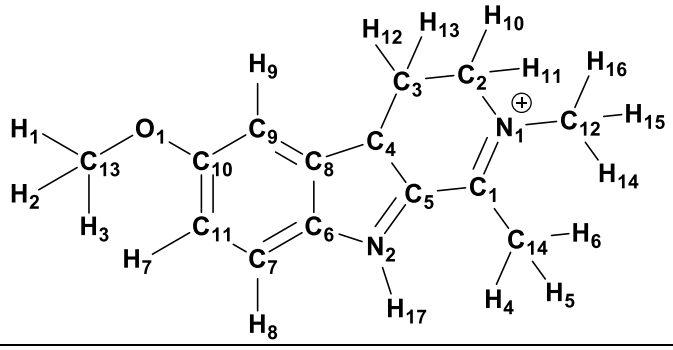


Figure S1. RMSD graph for compound 1.

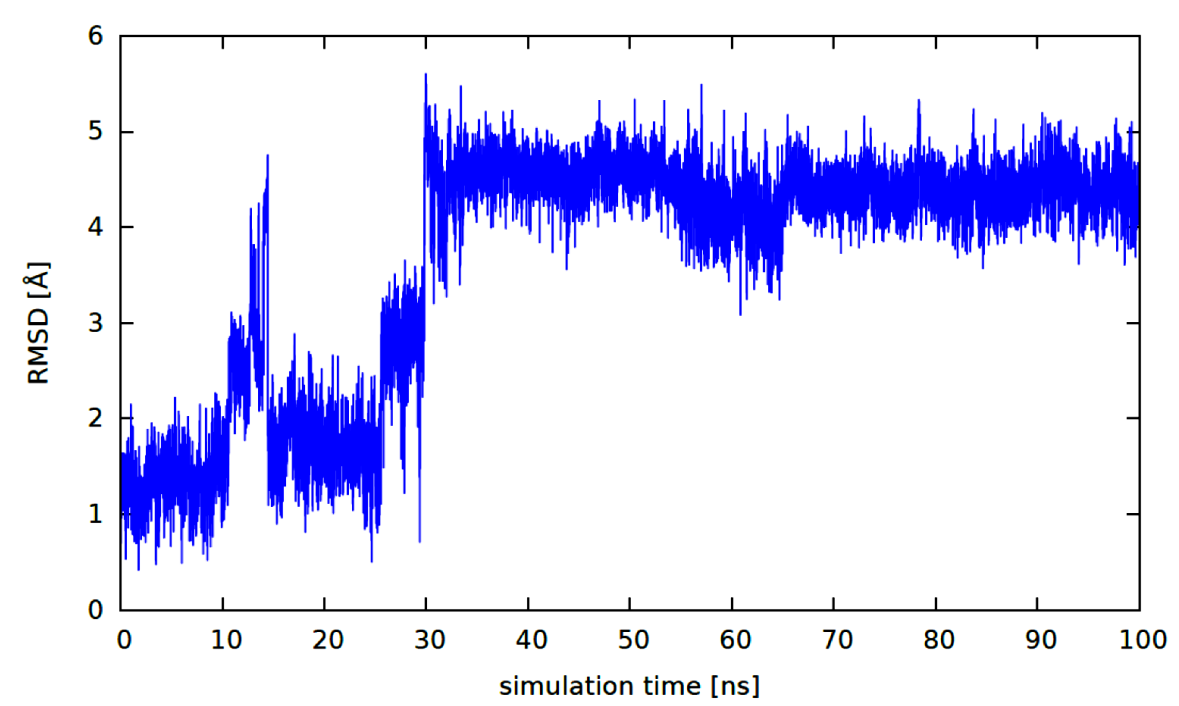


Figure S2. RMSD graph for compound 2.

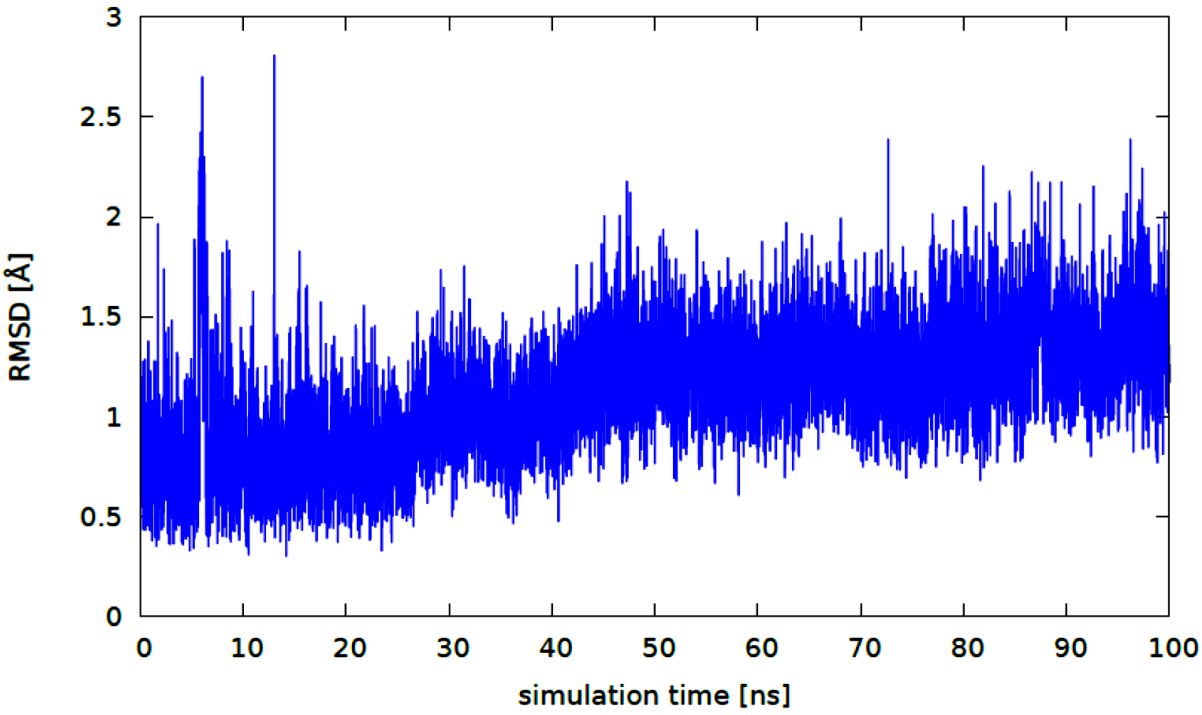


Figure S3. RMSD graph for compound 3.

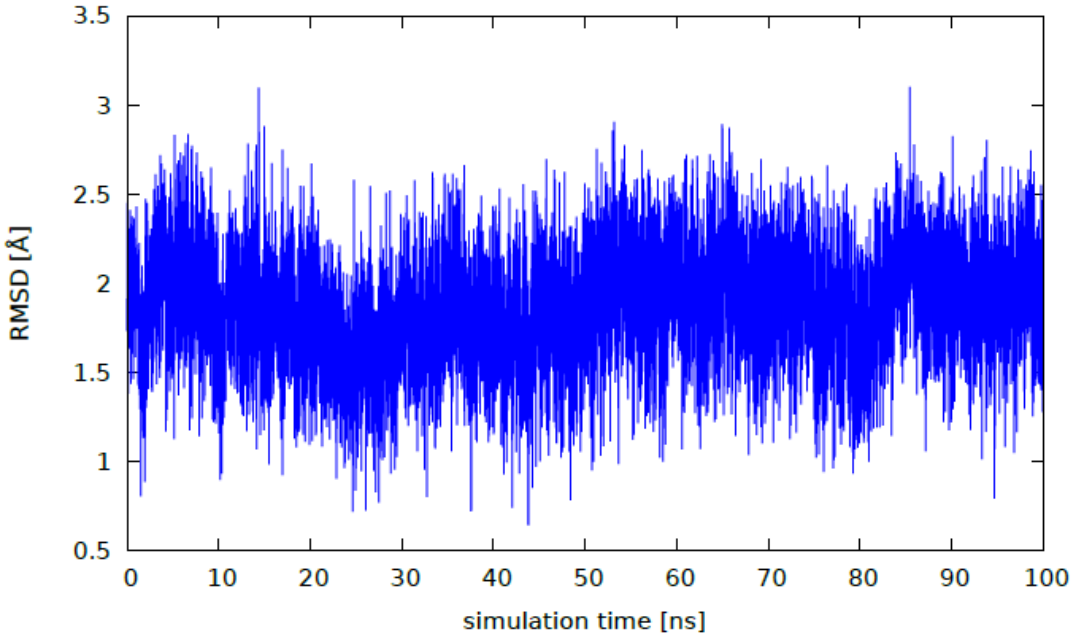


Figure S4. RMSD graph for compound 4.

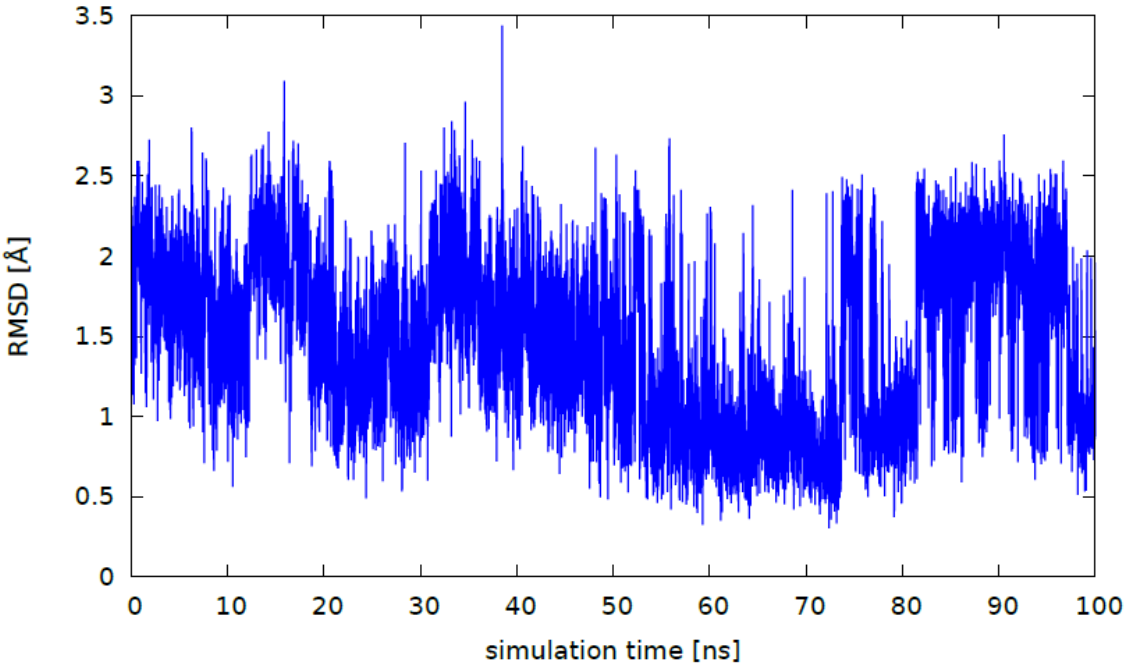


Figure S5. RMSD graph for compound 5.

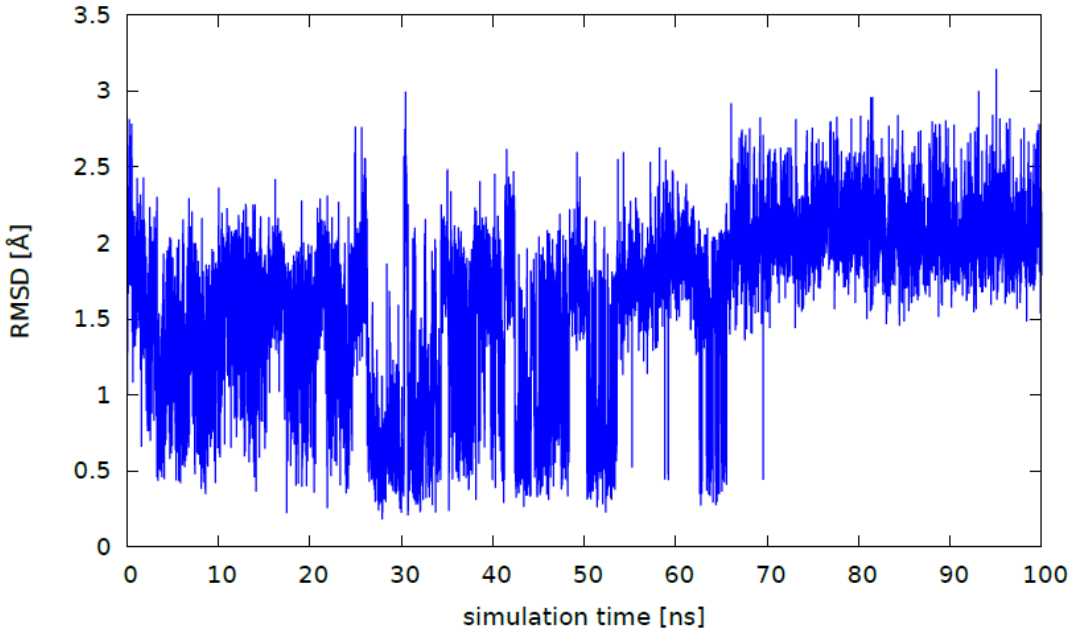


Figure S6. RMSD graph for compound 6.

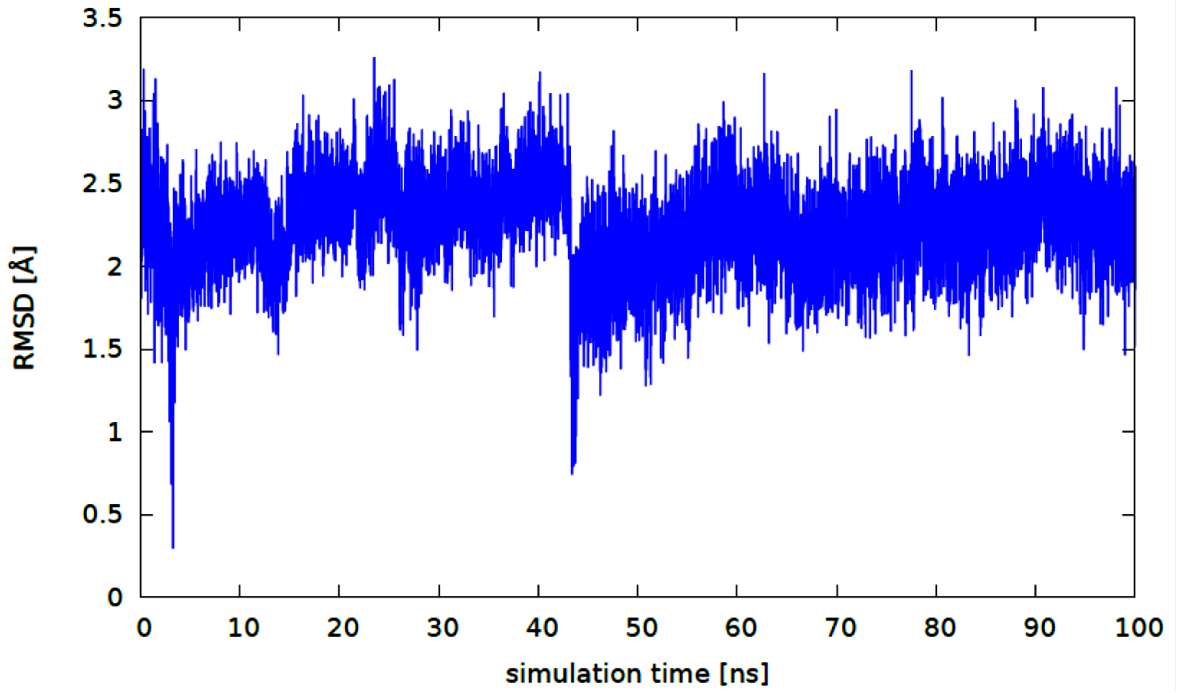


Figure S7. RMSD graph for compound 7.

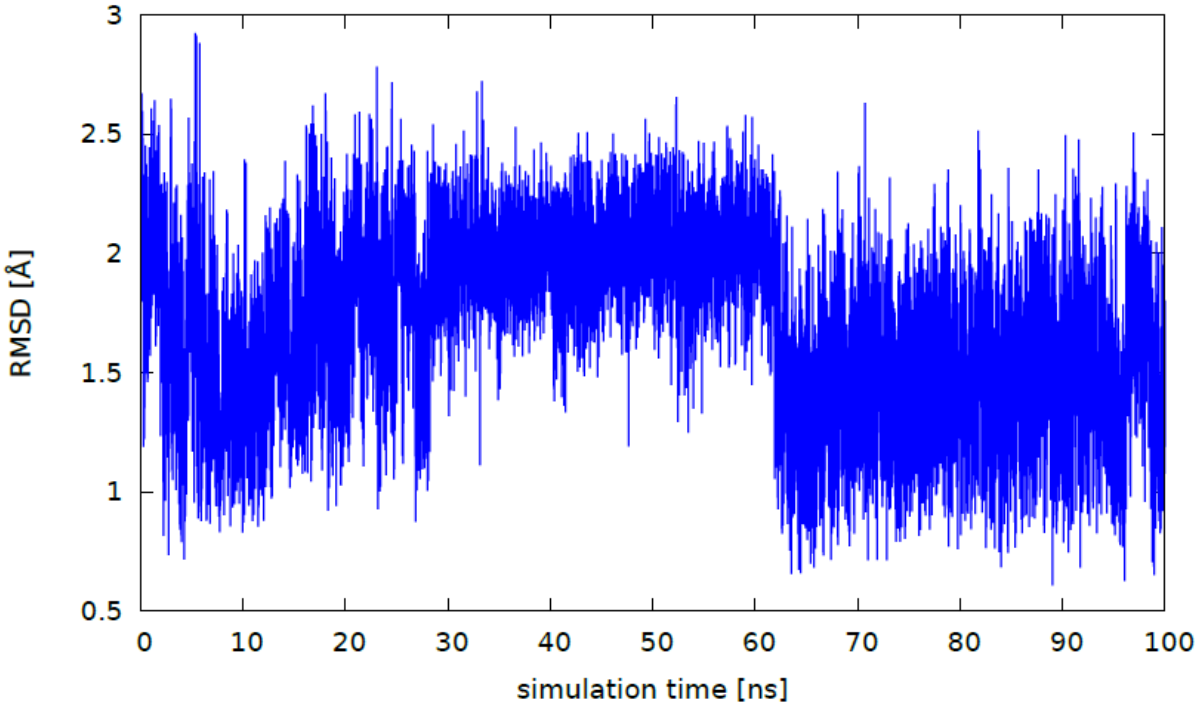


Figure S8. RMSD graph for compound 8.

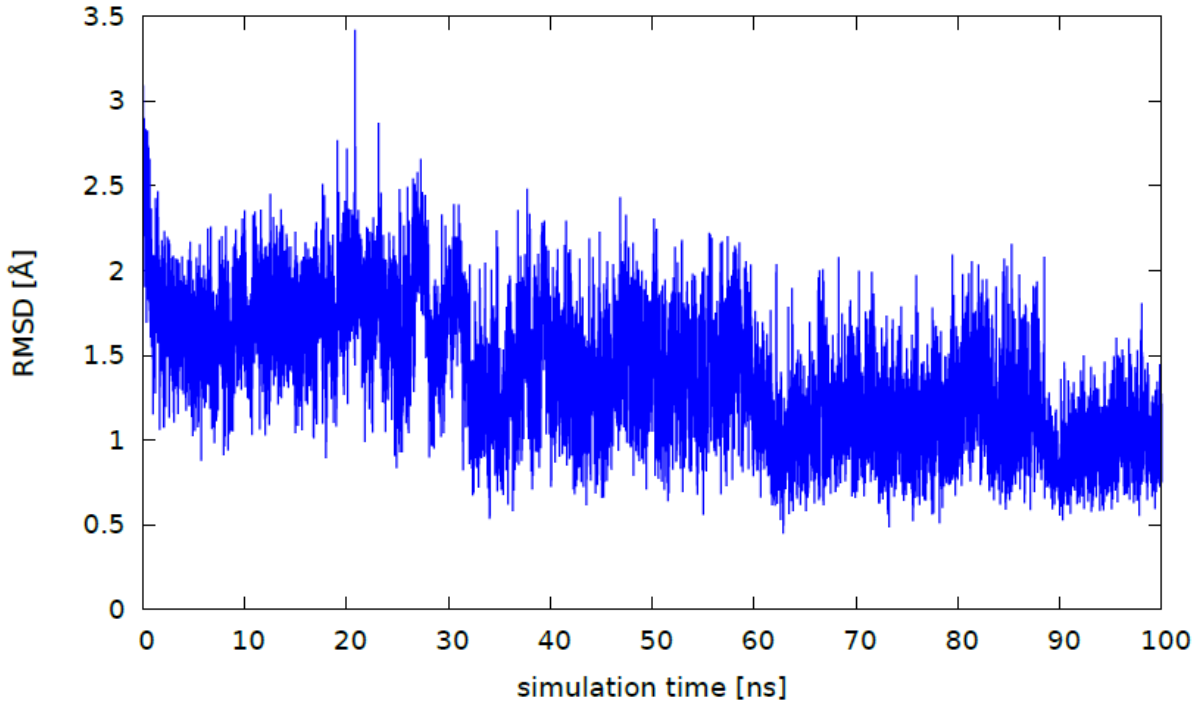


Figure S9. RMSD graph for compound 9.

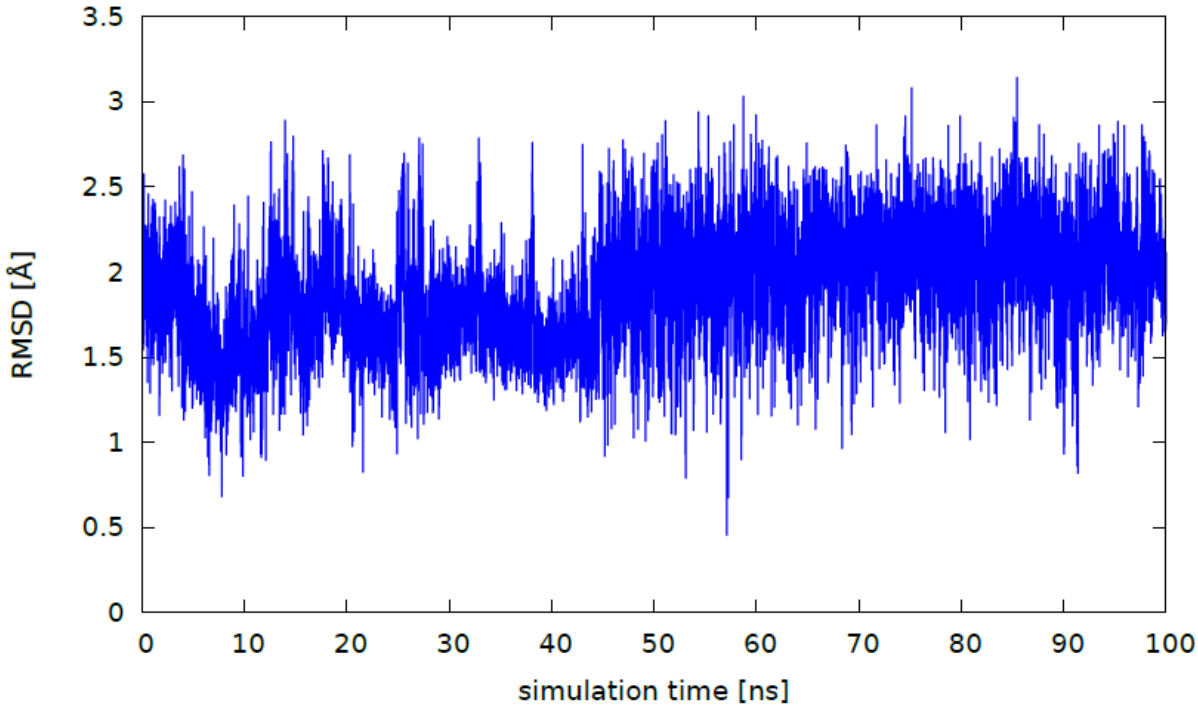


Figure S10. RMSD graph for compound 10.

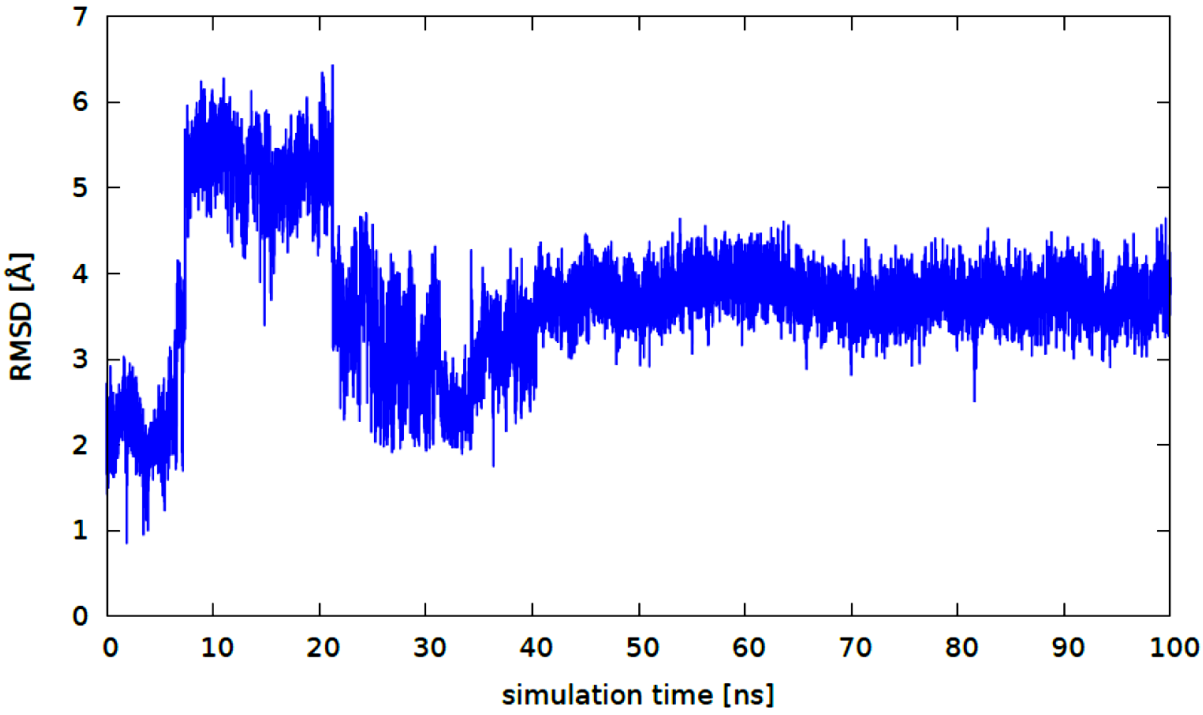


Figure S11. RMSD graph for compound 11.

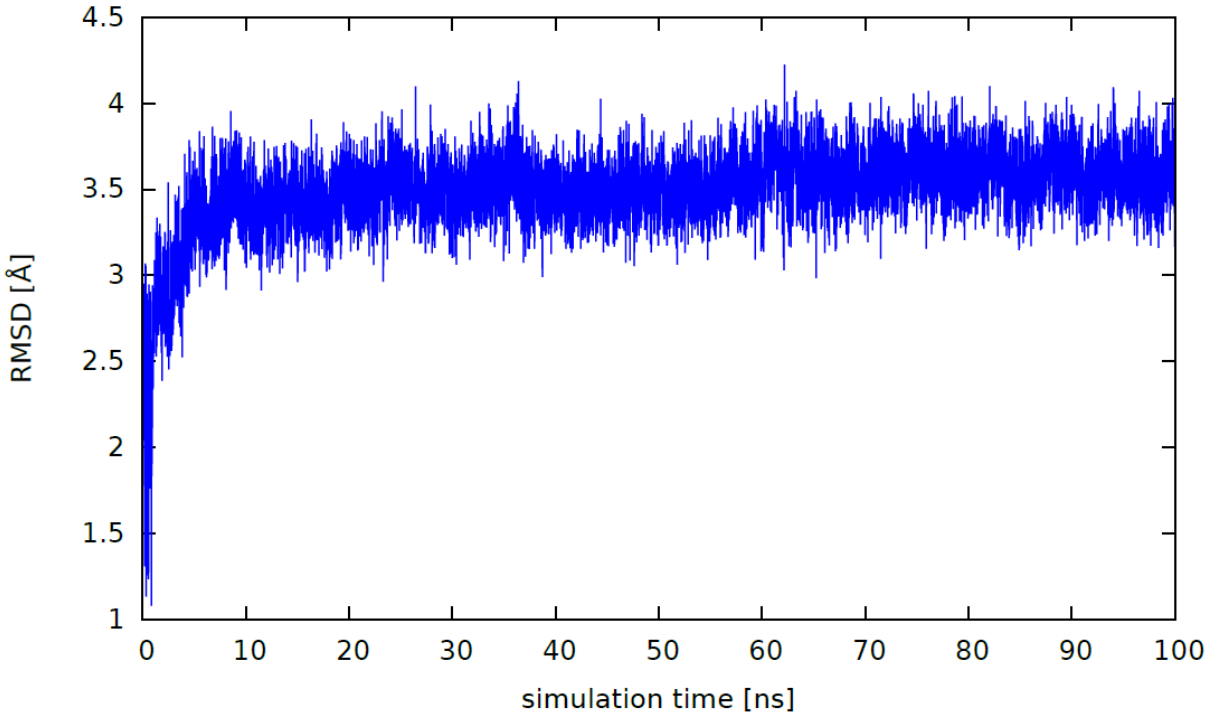


Figure S12. Overview of the interaction pattern obtained with dynophore analysis for compounds 2-5. Calculated percentage of the occurrence of a dynamic pharmacophore element on the basis of all frames broken into element-interacting amino acids pairs.

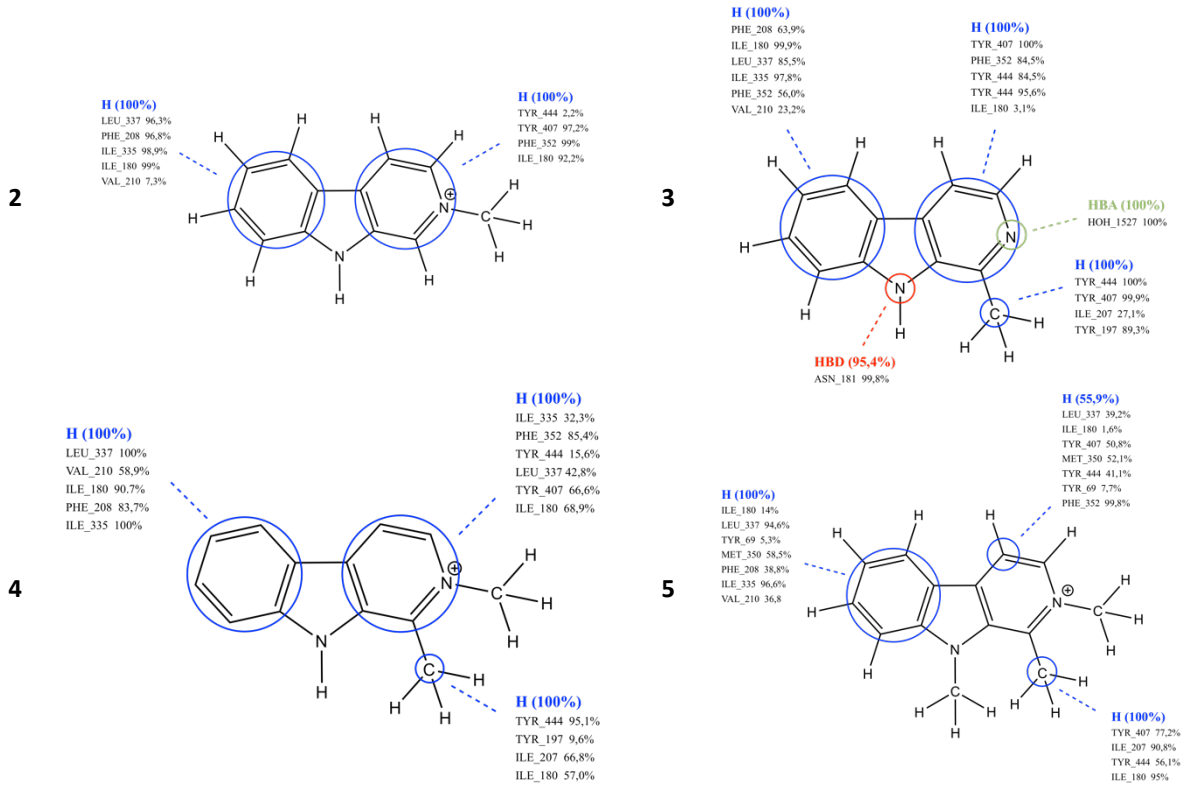


Figure S13. Overview of the interaction pattern obtained with dynophore analysis for compounds 7-9. Calculated percentage of the occurrence of a dynamic pharmacophore element on the basis of all frames broken into element-interacting amino acids pairs.

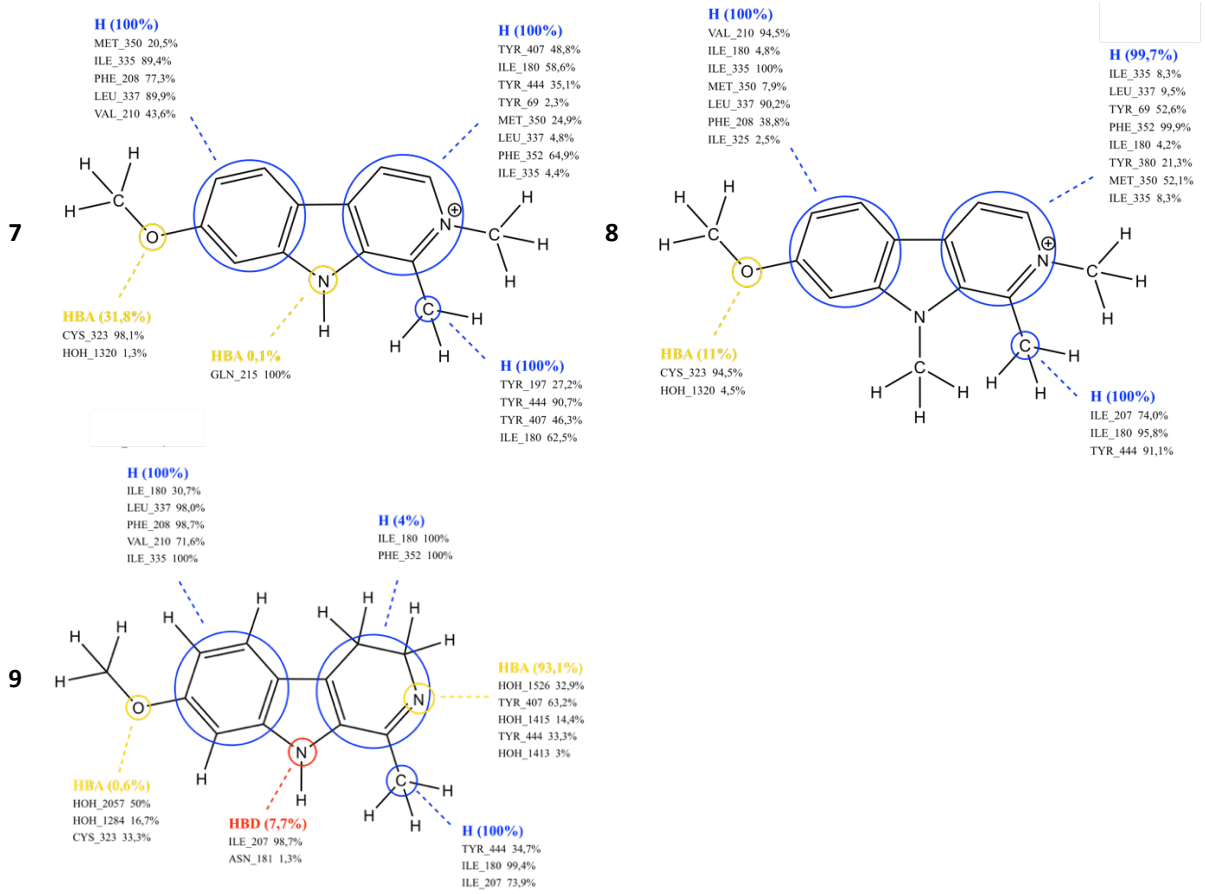


Figure S14. Comparison between X-ray binding pose of harmine (compound 6, in silver) with the determined binding modes using scoring functions ChemScore (in green), GoldScore (in violet) and ChemPLP (in red).

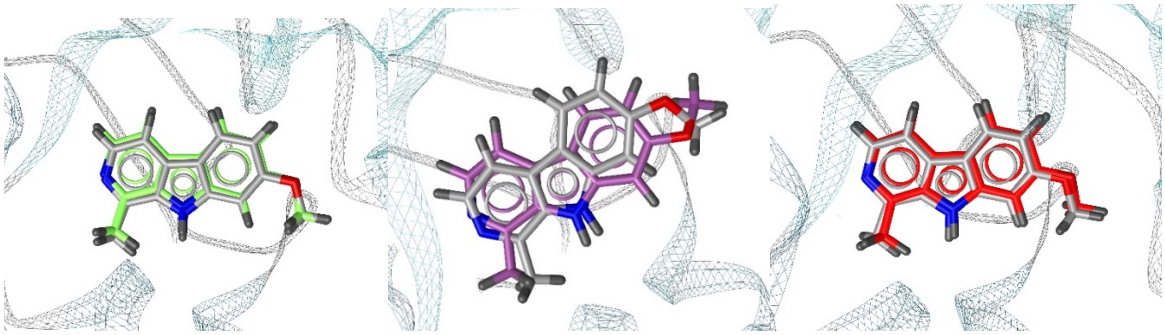
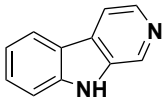
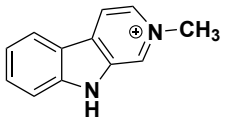
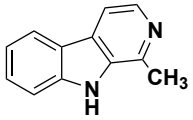
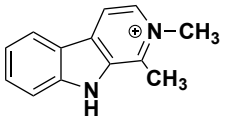
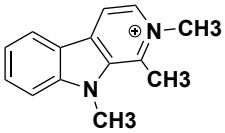
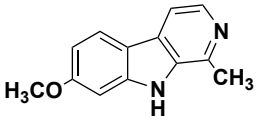
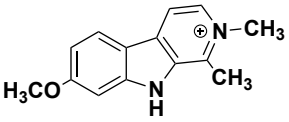
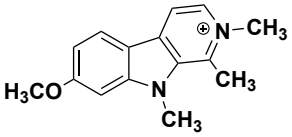
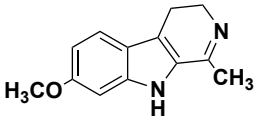
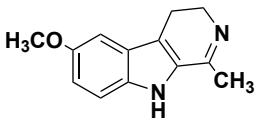
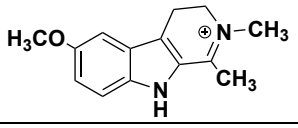


Table S12. The average number of water molecules present in the MAO-A active site (i.e., within 5 Å of the pertinent compound) during the molecular dynamics simulation, with standard deviations also provided.

Compound	Structure	Average num. of water molecules	ST. DEV.
1		6.1	2.1
2		7.4	1.1
3		4.3	0.9
4		3.4	1.0
5		4.9	0.9
6		4.9	0.9
7		6.2	1.1
8		4.3	0.9
9		2.5	0.6
10		6.1	1.3
11		5.2	1.6