The synthesis and spectroscopic characterization of (+)-demethoxyaspidospermine: DFT calculations of the structural, electronic, nonlinear optic and spectroscopic properties

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Conformational Analysis and Molecular Geometry

Table S1. The relative energies for the five stable conformers of the demethoxyaspidospermine compound at 6-311++G(d,p) basis set

	Gas phase				Chloroform phase			
Conf.	**Tot. energy/ hartree**	**ΔE/ kcalmol^{-1}**	**Free energy/ hartree**	**ΔG/ kcalmol^{-1}**	**Tot, energy/ hartree**	**ΔE/ kcalmol^{-1}**	**Free energy/ hartree**	**ΔG/ kcalmol^{-1}**
				B3LYP/6-311++G(d,p)				
CI	-1001.64535	0.0	-1001.69390	0.0	-1001.65297	0.0	-1001.70115	0.0
CII	-1001.64042	3.1	-1001.68850	3.4	-1001.64792	3.2	-1001.69583	3.3
CIII	-1001.64404	0.8	-1001.69219	1.1	-1001.65134	1.0	-1001.69929	1.2
CIV	-1001.64534	0.0	-1001.69337	0.3	-1001.65282	0.1	-1001.70106	0.1
CV	-1001.64454	0.5	-1001.69243	0.9	-1001.65210	0.5	-1001.70029	0.5
				MO6-2X/6-311++G(d,p)				
CI	-1001.69157	0.2	-1001.27809	0.7	-1001.69938	0.0	-1001.28570	0.5
CII	-1001.68658	3.3	-1001.27196	4.6	-1001.69424	3.2	-1001.27958	3.8
CIII	-1001.69126	0.4	-1001.27767	1.0	-1001.69881	0.4	-1001.28525	0.8
CIV	-1001.69191	0.0	-1001.27927	0.0	-1001.69928	0.1	-1001.28650	0.0
CV	-1001.69091	0.6	-1001.27728	1.2	-1001.69823	0.7	-1001.28431	1.4
				HF/6-311++G(d,p)				
CI	-995.05739	0.6	-995.10435	0.4	-995.06637	0.3	-995.11319	0.2
CII	-995.05112	4.5	-995.09762	4.6	-995.05999	4.3	-995.10653	4.4
CIII	-995.05684	0.9	-995.10329	1.0	-995.06546	0.9	-995.11191	1.0
CIV	-995.05832	0.0	-995.10494	0.0	-995.06691	0.0	-995.11353	0.0
CV	-995.05609	1.4	-995.10295	1.2	-995.06476	1.4	-995.11155	1.2

Table S2. Optimized parameters for the five conformers of the demethoxyaspidospermine compound in the chloroform phase

	B3LYP/ 6-311++G(d,p)						M06-2X/ 6-311++G(d,p)						HF/ 6-311++G(d,p)				
Bond Length (Å)	Exp.	**CI**	**CII**	**CII**	**CIV**	**CV**	**CI**	**CII**	**CII**	**CIV**	**CV**	**CI**	**CII**	**CII**	**CIV**	**CV**
C1-C2	1.39[a]	1.39	1.39	1.39	1.39	1.39	1.39	1.39	1.39	1.39	1.39	1.38	1.38	1.38	1.38	1.38
C1-C6	1.41[a]	1.40	1.40	1.40	1.40	1.41	1.40	1.40	1.40	1.40	1.40	1.39	1.39	1.39	1.39	1.39
C1-N13	1.38[a]	1.42	1.42	1.42	1.42	1.42	1.41	1.41	1.42	1.41	1.41	1.41	1.41	1.41	1.41	1.41
C2-C3	1.37[a]	1.40	1.40	1.40	1.40	1.40	1.40	1.40	1.40	1.40	1.40	1.39	1.39	1.39	1.39	1.39
C2-H12	0.93[a]	1.08	1.08	1.08	1.08	1.08	1.08	1.08	1.08	1.08	1.08	1.07	1.07	1.07	1.07	1.07
C3C-C4	1.39[a]	1.39	1.39	1.39	1.39	1.39	1.39	1.39	1.39	1.39	1.39	1.38	1.38	1.38	1.38	1.38
C4-C5	1.38[a]	1.40	1.40	1.40	1.40	1.40	1.40	1.40	1.40	1.40	1.40	1.39	1.39	1.39	1.39	1.39
C5-C6	1.40[a]	1.39	1.39	1.39	1.39	1.39	1.38	1.38	1.38	1.38	1.38	1.38	1.38	1.38	1.38	1.38
C6-C7	1.44[a]	1.52	1.52	1.52	1.52	1.52	1.52	1.52	1.51	1.51	1.52	1.52	1.52	1.52	1.52	1.52
C7-C14	1.50[a]	1.57	1.57	1.55	1.55	1.57	1.56	1.56	1.54	1.54	1.56	1.56	1.57	1.55	1.55	1.56
C8-N13	1.38[a]	1.49	1.49	1.49	1.49	1.49	1.48	1.48	1.48	1.48	1.48	1.48	1.48	1.48	1.48	1.48
C8-C17	1.50[a]	1.53	1.53	1.54	1.54	1.53	1.52	1.52	1.53	1.53	1.52	1.53	1.52	1.53	1.53	1.52
C14-C15	1.53[a]	1.57	1.58	1.56	1.56	1.56	1.55	1.57	1.54	1.55	1.55	1.56	1.57	1.55	1.55	1.56
C14-N26		1.47	1.47	1.47	1.47	1.47	1.46	1.47	1.46	1.46	1.46	1.46	1.46	1.46	1.46	1.46
C17-H35	0.97[a]	1.09	1.09	1.09	1.09	1.09	1.09	1.09	1.09	1.09	1.09	1.09	1.09	1.09	1.09	1.08
C19-N26		1.47	1.46	1.46	1.46	1.47	1.47	1.45	1.46	1.46	1.47	1.46	1.45	1.45	1.45	1.46
N26-C27		1.46	1.45	1.47	1.47	1.46	1.46	1.45	1.47	1.46	1.46	1.45	1.44	1.46	1.46	1.45
C47-O48		1.23	1.23	1.23	1.23	1.23	1.22	1.22	1.22	1.22	1.22	1.21	1.21	1.21	1.21	1.21
C39-C40		1.53	1.53	1.53	1.53	1.53	1.53	1.53	1.53	1.53	1.53	1.53	1.53	1.53	1.53	1.53
C47-C49		1.52	1.52	1.52	1.52	1.51	1.51	1.51	1.51	1.51	1.51	1.51	1.51	1.51	1.51	1.51
Bond angle (^{0})																
C2-C1-C6	122.40[a]	121.50	121.49	121.40	121.40	120.86	121.61	121.58	121.47	121.50	120.89	121.51	121.51	121.39	121.39	120.98
C2-C1-N13	130.84[b]	129.19	129.27	129.31	129.31	129.96	129.44	129.52	129.59	129.53	130.24	129.27	129.33	129.38	129.37	129.85
C6-C1-N13	107.72[a]	109.31	109.25	109.28	109.29	109.12	108.95	108.90	108.93	108.97	108.80	109.21	109.15	109.22	109.23	109.06
C1-C2-C3	117.60[a]	117.95	117.93	117.91	117.90	118.50	117.63	117.62	117.58	117.59	118.25	117.99	117.98	117.95	117.95	118.51
C1-C2-H12	121.20[a]	120.69	120.71	120.73	120.72	122.05	120.95	120.96	120.98	120.96	122.26	121.15	121.17	121.18	121.18	122.17
C3-C2-H12	121.20[a]	121.36	121.36	121.37	121.37	119.44	121.42	121.42	121.44	121.45	119.48	120.86	120.85	120.87	120.87	119.31
C2-C3-C4	121.20[a]	121.17	121.19	121.25	121.25	121.04	121.38	121.41	121.49	121.46	121.23	121.15	121.16	121.24	121.24	120.97
C2-C3-H11	119.40[a]	119.03	119.02	119.01	119.00	119.01	118.93	118.92	118.90	118.91	118.90	119.03	119.01	119.00	119.00	119.03
C4-C3-H11	119.40[a]	119.80	119.79	119.75	119.75	119.96	119.69	119.68	119.62	119.63	119.87	119.82	119.83	119.76	119.76	119.99
C3-C4-C5	121.70[a]	120.15	120.14	120.13	120.14	119.97	120.21	120.18	120.16	120.17	119.98	120.04	120.03	120.00	120.00	119.89
C3-C4-H10	119.10[a]	120.05	120.05	120.02	120.01	120.10	119.95	119.97	119.93	119.93	120.03	120.11	120.12	120.09	120.08	120.16
C5-C4-H10	119.10[a]	119.81	119.81	119.85	119.85	119.93	119.84	119.85	119.91	119.90	119.98	119.85	119.85	119.91	119.92	119.94
C4-C5-C6	118.90[a]	119.48	119.46	119.39	119.38	119.71	119.17	119.16	119.05	119.08	119.45	119.50	119.51	119.44	119.43	119.75
C4-C5-C9	120.50[a]	119.74	119.76	119.90	119.95	119.66	120.01	120.02	120.25	120.27	119.90	119.51	119.49	119.71	119.76	119.43
C6-C5-H9	120.50[a]	120.78	120.78	120.71	120.68	120.62	120.83	120.82	120.71	120.65	120.65	120.98	121.00	120.86	120.82	120.83
C1-C6-C5		119.75	119.79	119.92	119.93	119.89	120.01	120.05	120.26	120.20	120.15	119.81	119.80	119.98	119.99	119.84
C6-C7-C8	107.04[a]	100.87	100.81	100.90	100.83	101.04	100.85	100.88	101.01	100.92	101.10	100.56	100.53	100.66	100.63	100.67
C6-C7-C14	131.89[a]	115.28	115.82	118.94	118.85	115.12	115.32	115.52	118.63	118.85	114.81	115.72	115.87	119.32	119.21	115.44
C8-C7-C14	121.07[a]	116.62	116.34	114.92	114.88	116.55	116.55	116.38	114.98	114.84	116.63	116.52	116.42	114.81	114.77	116.48
C7-C8-N13	109.84[a]	103.25	103.15	102.70	102.77	103.34	102.76	102.78	102.28	102.46	103.04	103.04	103.07	102.69	102.77	103.12
C7-C8-C17	125.46[a]	113.55	112.68	112.79	112.62	114.46	113.22	111.84	112.25	111.98	114.25	113.57	112.46	112.74	112.56	114.35

N13-C8-C17	124.68[a]	111.36	110.56	110.19	110.30	111.27	111.22	110.27	110.02	110.22	111.05	111.55	110.92	110.43	110.58	111.58
C1-N13-C8	108.88[a]	108.35	108.11	107.96	107.97	108.51	108.44	108.23	108.05	108.11	108.72	108.24	108.09	107.94	107.98	108.34
C7-C14-C15	109.54[a]	118.88	120.56	118.35	118.53	118.72	118.12	120.69	118.05	118.27	118.11	118.55	120.52	118.54	118.72	118.49
C7-C14-N26		104.58	104.02	103.51	103.96	104.62	104.40	103.97	103.66	103.99	104.57	104.27	103.88	103.51	103.93	104.31
C15-C14-N26		111.28	110.77	108.65	108.80	111.24	111.65	110.92	108.26	108.29	111.51	111.60	110.83	108.42	108.56	111.50
C14-C15-C16	108.28[a]	110.75	112.85	108.99	109.14	110.78	110.81	113.20	108.94	109.09	110.76	110.78	113.05	109.03	109.07	110.84
C15-C16-C17	113.30[b]	112.74	115.32	113.93	113.38	112.79	112.01	115.25	113.58	112.62	112.05	112.77	115.33	113.98	113.30	112.78
C17-C16-H37	108.90[b]	108.84	107.79	108.71	108.83	108.87	108.85	107.51	108.54	108.80	108.87	108.56	107.47	108.37	108.54	108.51
H37-C16-H38	107.60[b]	106.08	105.89	106.71	106.35	106.10	106.57	106.23	107.09	106.74	106.60	106.11	105.94	106.59	106.27	106.14
C22-C19-N26		111.28	110.47	110.59	110.21	111.27	111.29	110.15	110.19	109.85	111.26	111.49	110.36	110.46	110.05	111.42
C15-C23-C22	119.29[a]	112.56	114.01	113.41	112.90	112.57	111.61	113.61	112.69	112.20	111.67	112.46	114.17	113.39	112.90	112.51
C22-C23-H25	107.50[a]	108.81	108.41	108.23	108.48	108.85	108.74	108.25	108.13	108.41	108.81	108.45	108.05	107.91	108.26	108.48
C14-N26-C19		113.34	112.79	114.81	114.17	113.34	112.59	111.28	113.17	112.79	112.36	114.19	113.08	114.76	114.12	114.13
C14-N26-C27		106.03	106.20	110.75	111.05	106.18	104.85	105.01	110.20	110.65	105.01	106.18	106.45	111.18	111.44	106.31
C19-N26-C27		113.21	114.44	115.88	116.17	113.32	112.51	114.25	115.96	116.24	112.62	113.21	114.88	116.20	116.53	113.33
N26-C27-C28		103.74	102.43	105.29	105.30	103.75	103.81	101.83	105.18	105.15	103.65	103.88	102.10	105.11	105.12	103.77
N13-C47-O48		121.97	121.98	122.00	122.00	120.26	121.98	122.01	122.00	122.01	120.31	122.19	122.21	122.22	122.22	120.45
O48-C47-C49		120.99	121.05	121.07	121.07	120.67	121.56	121.63	121.67	121.65	121.19	120.38	120.43	120.46	120.45	119.99
Dihedral angle (^{0})																
C6-C1-C2-C3	0.70[a]	0.26	0.23	0.30	0.30	-2.04	0.29	0.17	0.48	0.38	-2.14	-0.18	-0.20	-0.10	-0.09	-2.53
C6-C1-C2-H12		-179.55	-179.58	-179.44	-179.45	176.76	-179.66	-179.76	-179.53	-179.61	176.55	-179.90	-179.92	-179.78	-179.79	176.49
N13-C1-C2-C3	178.90[a]	-179.47	-179.51	-179.17	-179.14	-178.88	-179.24	-179.40	-178.30	-178.58	-178.76	-179.11	-179.17	-178.86	-178.84	-178.56
N13-C1-C2-H12		0.71	0.68	1.10	1.11	-0.07	0.81	0.67	1.69	1.44	-0.07	1.18	1.11	1.46	1.46	0.47
C2-C1-C6-C5	0.70[a]	-0.02	0.09	0.25	0.19	2.19	0.02	0.27	-0.08	0.05	2.37	0.52	0.58	0.68	0.58	2.71
C2-C1-C6-C7	179.03[a]	175.73	175.16	175.11	174.99	179.20	175.53	174.94	175.50	175.14	179.24	176.80	176.20	176.19	176.04	-179.68
N13-C1-C6-C5	179.77[b]	179.76	179.87	179.82	179.73	179.63	179.64	179.92	178.93	179.20	179.64	179.64	179.73	179.66	179.56	179.48
N13-C1-C6-C7	-0.70[a]	-4.49	-5.06	-5.32	-5.47	-3.37	-4.85	-5.41	-5.50	-5.71	-3.49	-4.08	-4.65	-4.83	-4.98	-2.91
C2-C1-N13-C47		-16.03	-15.16	-15.24	-15.17	-22.71	-15.66	-13.58	-15.34	-14.84	-20.31	-20.02	-18.64	-18.86	-18.71	-26.56
C6-C1-N13-C8	0.80[a]	-14.81	-15.00	-15.44	-15.28	-15.39	-15.67	-15.51	-16.13	-15.73	-15.90	-16.13	-15.97	-16.31	-16.04	-16.88
C6-C1-N13-C47		164.21	165.08	165.24	165.34	160.16	164.76	166.80	165.76	166.10	162.76	160.94	162.29	162.27	162.42	157.05
C1-C2-C3-C4	0.30[a]	-0.16	-0.20	-0.32	-0.28	0.67	-0.21	-0.24	-0.27	-0.24	0.65	-0.11	-0.11	-0.24	-0.18	0.83
C2-C3-C4-C5	0.10[a]	-0.18	-0.14	-0.20	-0.23	0.57	-0.19	-0.13	-0.35	-0.31	0.63	0.05	0.04	-0.01	-0.04	0.69
H11-C3-C4-C5		179.97	180.00	179.82	179.84	-178.70	179.96	179.99	179.82	179.86	-178.65	-179.86	-179.87	179.99	-179.99	-178.60
C3-C4-C5-C6	-0.20[a]	0.42	0.46	0.76	0.72	-0.44	0.50	0.57	0.76	0.74	-0.42	0.29	0.33	0.59	0.53	-0.54
C4-C5-C6-C1	-0.20[a]	-0.32	-0.43	-0.78	-0.70	-0.92	-0.42	-0.63	-0.55	-0.61	-1.05	-0.57	-0.64	-0.91	-0.79	-1.13
C4-C5-C6-C7	-178.00[a]	-175.07	-174.31	-174.39	-174.24	-177.24	-174.86	-174.01	-175.04	-174.50	-177.19	-175.96	-175.18	-175.33	-175.15	-178.18
H9-C5-C6-C7		4.65	5.50	5.44	5.75	2.92	4.83	5.92	4.89	5.72	2.91	3.78	4.67	4.49	4.90	1.99
C1-C6-C7-C8		20.44	21.59	22.39	22.45	19.27	21.77	22.64	23.32	23.25	19.89	20.95	21.80	22.37	22.34	19.86
C1-C6-C7-C14		146.97	148.05	149.02	148.92	145.74	148.21	149.03	149.93	149.74	146.33	147.38	148.18	148.91	148.74	146.18
C1-C6-C7-C28		-96.35	-95.57	-95.07	-95.22	-97.68	-94.84	-94.91	-94.26	-94.48	-97.11	-95.57	-95.45	-95.15	-95.40	-96.84
C5-C6-C7-C8	178.20[a]	-164.41	-164.04	-163.48	-163.49	-164.12	-163.34	-163.43	-161.71	-162.33	-163.65	-163.30	-163.22	-162.76	-162.84	-162.85
C5-C6-C7-C14		-37.88	-37.58	-36.85	-37.01	-37.65	-36.89	-37.05	-35.10	-35.84	-37.21	-36.87	-36.84	-36.21	-36.44	-36.54
C5-C6-C7-C28		78.80	78.80	79.06	78.85	78.92	80.05	79.02	80.70	79.94	79.35	80.19	79.54	79.73	79.42	80.44
C6-C7-C8-N13	0.30[a]	-27.72	-28.97	-29.96	-29.93	-26.93	-29.46	-30.26	-31.22	-30.95	-27.79	-28.96	-29.75	-30.46	-30.28	-28.36
C6-C7-C8-C17		93.00	90.28	88.62	88.76	94.23	90.61	88.01	86.66	87.14	92.79	91.86	89.76	88.37	88.69	92.97
C14-C7-C8-N13		-153.36	-155.08	-159.21	-159.00	-152.46	-155.08	-156.07	-160.21	-160.06	-153.02	-154.86	-155.76	-159.95	-159.59	-153.98

C14-C7-C8-C17		-32.64	-35.84	-40.63	-40.31	-31.29	-35.01	-37.80	-42.33	-41.97	-32.43	-34.03	-36.25	-41.12	-40.62	-32.65
C28-C7-C8-N13		89.17	86.82	86.29	86.11	90.10	87.33	85.23	85.58	85.28	89.28	87.81	86.03	85.88	85.88	88.62
C28-C7-C8-C17		-150.11	-153.93	-155.13	-155.21	-148.74	-152.60	-156.51	-156.54	-156.63	-150.14	-151.37	-154.46	-155.28	-155.15	-150.05
C6-C7-C14-C15		-97.19	-102.71	-83.38	-84.50	-97.59	-94.31	-102.96	-81.81	-83.59	-95.94	-95.25	-103.67	-83.25	-84.36	-96.32
C6-C7-C14-N26		137.94	132.42	156.40	154.63	137.68	141.00	131.90	158.53	156.33	139.43	139.95	131.51	156.71	154.98	139.01
C8-C7-C14-C15	14.20[b]	20.84	15.47	36.30	34.97	20.50	23.67	15.10	37.82	35.97	22.04	22.63	14.21	36.32	35.03	21.46
C8-C7-C14-N26		-104.03	-109.41	-83.92	-85.90	-104.24	-101.02	-110.04	-81.84	-84.11	-102.59	-102.18	-110.60	-83.72	-85.63	-103.20
C28-C7-C14-C15		142.12	137.69	156.42	155.54	141.79	144.89	138.06	157.71	156.39	143.50	143.70	136.67	156.33	155.49	142.64
C28-C7-C14-N26		17.25	12.82	36.20	34.68	17.05	20.20	12.92	38.05	36.31	18.88	18.90	11.85	36.29	34.83	17.97
C6-C7-C28-C27		-116.17	-110.29	-157.94	-157.06	-115.95	-118.26	-108.29	-160.74	-159.71	-116.29	-118.55	-109.12	-160.37	-159.52	-117.32
C8-C7-C28-C27		133.10	139.29	91.30	92.25	133.06	131.13	141.22	88.16	89.43	132.65	131.12	140.67	89.02	89.88	132.11
C14-C7-C28-C27		7.70	13.68	-31.37	-30.62	7.73	5.76	15.18	-34.40	-33.29	7.11	5.90	14.90	-33.42	-32.74	6.87
C7-C8-N13-C1	-0.70[a]	27.12	28.07	28.86	28.76	26.97	28.77	29.23	30.07	29.69	27.84	28.75	29.22	29.75	29.49	28.83
C7-C8-N13-C47		-151.90	-152.00	-151.83	-151.86	-149.18	-151.67	-153.09	-151.83	-150.99	-152.15	-148.28	-149.03	-148.81	-148.94	-145.86
C17-C8-N13-C1		-95.08	-92.63	-91.54	-91.53	-96.33	-92.68	-90.14	-89.39	-94.91	-89.64	-93.44	-91.34	-90.69	-90.86	-94.37
C17-C8-N13-C47		85.90	87.30	87.78	87.85	87.52	86.89	87.54	88.71	86.26	88.53	89.53	90.41	90.75	90.70	90.95
C7-C8-C17-C16		54.59	58.12	52.73	53.83	53.04	55.88	60.24	53.84	53.84	55.73	54.89	59.21	53.24	54.26	53.92
N13-C8-C17-C16	168.70[a]	170.62	172.96	166.84	168.01	169.72	171.00	173.94	167.03	169.86	169.09	170.80	174.04	167.46	168.57	170.47
C8-N13-C47-O48		-177.39	-177.06	-177.01	-177.07	-5.72	-176.84	-176.13	-176.68	-4.89	-176.64	-179.21	-178.77	-178.79	-178.86	-7.72
C8-N13-C47-C49		4.30	4.62	4.48	4.42	173.22	5.05	5.67	4.94	173.76	4.98	2.27	2.67	2.56	2.47	171.47
C7-C14-C15-C16		-30.19	-16.27	-41.18	-40.35	-30.98	-32.85	-13.78	-42.08	-33.03	-41.10	-31.42	-14.18	-40.70	-40.19	-31.27
C7-C14-C15-C23		-148.84	-134.34	-157.99	-157.82	-149.60	-151.62	-132.28	-158.82	-151.73	-158.49	-150.01	-132.33	-157.43	-157.65	-149.88
C7-C14-C15-C39		92.02	109.10	79.79	82.79	91.27	89.26	110.89	79.03	89.16	81.98	90.98	111.15	80.25	83.12	91.18
N26-C14-C15-C16		91.36	105.38	76.36	78.02	90.47	88.19	108.05	75.14	88.10	76.73	89.73	107.30	76.78	78.08	89.80
N26-C14-C15-C23		-27.29	-12.70	-40.46	-39.46	-28.15	-30.59	-10.44	-41.60	-30.60	-40.65	-28.87	-10.85	-39.95	-39.38	-28.81
N26-C14-C15-C39		-146.43	-129.25	-162.68	-158.85	-147.29	-149.70	-127.28	-163.74	-149.71	-160.19	-147.88	-127.36	-162.27	-158.61	-147.76
C7-C14-N26-C19		-162.46	-162.80	-162.63	-160.92	-162.45	-162.95	-162.40	-160.18	-162.30	-158.98	-164.16	-163.59	-161.43	-159.75	-163.87
C7-C14-N26-C27		-37.68	-36.69	-29.05	-27.23	-37.42	-40.31	-38.30	-28.52	-39.56	-26.84	-38.70	-36.54	-26.98	-25.19	-38.19
C15-C14-N26-C19		67.98	66.27	70.75	71.90	68.19	68.33	66.44	73.68	68.98	74.40	66.72	65.58	71.84	72.98	67.11
C15-C14-N26-C27		-167.24	-167.62	-155.67	-154.41	-166.77	-169.03	-169.46	-154.66	-168.28	-153.46	-167.82	-167.36	-153.71	-152.47	-167.22
C14-C15-C16-C17		53.59	38.98	53.64	53.99	54.37	55.54	36.65	54.23	56.47	55.12	53.87	37.63	53.09	53.83	54.33
C23-C15-C16-C17		172.42	157.59	171.18	171.44	173.18	174.44	155.54	171.38	175.27	172.38	172.71	156.32	170.45	171.08	173.13
C39-C15-C16-C17		-66.09	-85.92	-68.67	-66.62	-65.29	-63.99	-87.30	-67.68	-63.09	-65.42	-65.93	-87.38	-69.58	-67.05	-65.50
C14-C15-C23-C22		-33.58	-45.08	-19.74	-21.93	-32.82	-31.70	-47.32	-20.74	-22.49	-31.79	-31.74	-45.93	-20.61	-22.26	-31.87
C16-C15-C23-C22		-153.82	-166.82	-137.52	-140.01	-153.07	-152.05	-169.57	-138.34	-140.44	-152.03	-151.99	-167.89	-138.34	-140.23	-152.16
C39-C15-C23-C22		83.80	73.78	103.10	96.47	84.49	85.54	70.96	101.47	95.89	85.43	85.59	72.98	102.58	96.19	85.39
C14-C15-C39-C40		-170.95	-67.68	67.53	-171.71	-171.29	-166.68	-68.65	68.27	-167.87	-167.09	-169.75	-69.43	67.54	-170.50	-169.82
C16-C15-C39-C40		-49.32	58.54	-171.76	-50.73	-49.63	-45.09	57.26	-171.13	-46.98	-45.51	-48.01	56.97	-171.60	-49.43	-48.00
C16-C15-C39-H41		-172.05	-64.64	64.44	-173.24	-172.36	-167.60	-65.67	65.72	-169.40	-168.04	-170.54	-65.79	64.63	-171.77	-170.55
C23-C15-C39-C40		70.99	175.12	-53.54	70.13	70.70	75.34	174.25	-52.27	74.05	74.99	72.23	173.38	-53.56	71.50	72.26
C15-C16-C17-C8		-67.29	-61.41	-61.52	-62.90	-66.55	-68.17	-61.31	-62.13	-64.53	-67.71	-66.92	-61.54	-61.45	-63.06	-66.68
N26-C19-C22-C23		-23.79	-4.30	-33.16	-32.62	-24.53	-28.47	-0.13	-32.55	-32.26	-27.53	-27.52	-1.96	-31.96	-31.67	-26.98
C22-C19-N26-C14		-38.90	-56.12	-30.01	-31.66	-38.23	-34.87	-59.82	-32.13	-33.33	-35.92	-34.92	-57.86	-31.76	-33.05	-35.58
C22-C19-N26-C27		-159.70	-177.67	-161.16	-162.90	-159.32	-153.09	-178.51	-160.89	-162.65	-154.26	-156.58	179.67	-163.87	-165.20	-157.46
C14-N26-C27-C28		42.89	45.88	8.89	7.51	42.62	44.28	48.46	6.38	5.41	44.37	42.80	46.54	5.55	4.16	42.94
C19-N26-C27-C28		167.75	170.98	141.93	140.20	167.67	166.97	170.65	136.57	135.76	166.95	168.86	172.52	139.29	137.54	169.09
N26-C27-C28-C7		-30.25	-35.69	14.92	15.29	-30.09	-29.93	-38.27	18.20	18.10	-30.85	-28.92	-36.75	18.26	18.66	-29.61

Table S3. The Second Order Perturbation Theory Analysis Results of the Fock Matrix in NBO Basis for the stable conformers of the demethoxyaspidospermine compound at B3LYP/6-311++G(d,p) level of the theory in chloroform phase

Donor(i)	Hybridization	ED_i/e	Acceptor (j)	Hybridization	ED_j/e	E(2)/ kcalmol^{-1}	E(j)-E(i)/ a.u	F(i.j)/ a.u
CI								
π C1-C2 (2)	$0.7078p_{(C1)}+ 0.7064p_{(C2)}$	1.65012	π^* C3-C4	$p_{(C3)}- p_{(C4)}$	0.33893	20.71	0.29	0.069
			π^* C5-C6	$p_{(C5)}- p_{(C6)}$	0.33243	19.06	0.32	0.070
π C3-C4 (2)	$0.7024p_{(C3)}+ 0.7118p_{(C4)}$	1.68330	π^* C1-C2	$p_{(C1)}- p_{(C2)}$	0.37315	17.73	0.29	0.065
			π^* C5-C6	$p_{(C5)}- p_{(C6)}$	0.33243	17.71	0.32	0.068
π C5-C6 (2)	$0.7103p_{(C5)}+ 0.7039p_{(C6)}$	1.66909	π^* C1-C2	$p_{(C1)}- p_{(C2)}$	0.37315	19.80	0.30	0.070
			π^* C3-C4	$p_{(C3)}- p_{(C4)}$	0.33893	18.14	0.30	0.066
			π^* C5-C6	$p_{(C5)}- p_{(C6)}$	0.33243	1.62	0.33	0.021
σ C7-C14	$0.7169sp^{2.76}_{(C7)}+ 0.6971sp^{2.73}_{(C14)}$	1.96694	π^* C5-C6	$p_{(C5)}- p_{(C6)}$	0.33243	0.61	0.70	0.020
σ C7-C28	$0.7216sp^{3.23}_{(C7)}+ 0.6923sp^{2.76}_{(C28)}$	1.95748	π^* C5-C6	$p_{(C5)}- p_{(C6)}$	0.33243	3.37	0.64	0.045
LP (1) N13	p	1.63808	π^* C1-C2	$p_{(C1)}- p_{(C2)}$	0.37315	32.86	0.29	0.087
π^* C1-C2	$p_{(C1)}- p_{(C2)}$	0.37315	π^* C5-C6	$p_{(C5)}- p_{(C6)}$	0.33243	91.97	0.03	0.085
π^* C3-C4	$p_{(C3)}- p_{(C4)}$	0.33893	π^* C5-C6	$p_{(C5)}- p_{(C6)}$	0.33243	81.00	0.04	0.083
CII								
π C1-C2 (2)	$0.7079p_{(C1)}+ 0.7063p_{(C2)}$	1.65068	π^* C3-C4	$p_{(C3)}- p_{(C4)}$	0.33737	20.67	0.29	0.069
			π^* C5-C6	$p_{(C5)}- p_{(C6)}$	0.33233	19.06	0.32	0.070
π C3-C4 (2)	$0.7025p_{(C3)}+ 0.7117p_{(C4)}$	1.68405	π^* C1-C2	$p_{(C1)}- p_{(C2)}$	0.37179	18.39	0.28	0.065
			π^* C5-C6	$p_{(C5)}- p_{(C6)}$	0.33233	17.83	0.32	0.067
π C5-C6 (2)	$0.7109p_{(C5)}+ 0.7033p_{(C6)}$	1.67092	π^* C1-C2	$p_{(C1)}- p_{(C2)}$	0.37179	22.47	0.27	0.070
			π^* C3-C4	$p_{(C3)}- p_{(C4)}$	0.33737	19.81	0.27	0.065
			π^* C5-C6	$p_{(C5)}- p_{(C6)}$	0.33233	1.93	0.30	0.022
σ C7-C14	$0.7176sp^{2.78}_{(C7)}+ 0.6964sp^{2.70}_{(C14)}$	1.96779	π^* C5-C6	$p_{(C5)}- p_{(C6)}$	0.33233	0.66	0.66	0.020
σ C7-C28	$0.7217sp^{3.22}_{(C7)}+ 0.6922sp^{2.77}_{(C28)}$	1.95674	π^* C5-C6	$p_{(C5)}- p_{(C6)}$	0.33233	3.52	0.64	0.046
π C47-O48	$0.5324p_{(C47)}+ 0.8465p_{(O48)}$	1.98714	π^* C47-O48	$p_{(C47)}- p_{(O48)}$	0.30319	0.97	0.42	0.019
σ C47-C49	$0.7042sp^{1.75}_{(C47)}+ 0.7100sp^{2.67}_{(C49)}$	1.98435	π^* C47-O48	$p_{(C47)}- p_{(O48)}$	0.30319	1.59	0.69	0.032
σ C49-H50	$0.7841sp^{3.08}_{(C49)}+ 0.6206s_{(H50)}$	1.98726	π^* C47-O48	$p_{(C47)}- p_{(O48)}$	0.30319	1.17	0.56	0.025
σ C49-H52	$0.7814sp^{3.20}_{(C49)}+ 0.6240s_{(H52)}$	1.97254	π^* C47-O48	$p_{(C47)}- p_{(O48)}$	0.30319	19.10	0.55	0.099
LP (1) N13	p	1.63806	π^* C1-C2	$p_{(C1)}- p_{(C2)}$	0.37179	33.05	0.29	0.088
			π^* C47-O48	$p_{(C47)}- p_{(O48)}$	0.30319	55.27	0.30	0.117
π^* C1-C2	$p_{(C1)}- p_{(C2)}$	0.37179	π^* C5-C6	$p_{(C5)}- p_{(C6)}$	0.33233	92.71	0.03	0.085
			π^* C47-O48	$p_{(C47)}- p_{(O48)}$	0.30319	1.22	0.01	0.006
π^* C3-C4	$p_{(C3)}- p_{(C4)}$	0.33737	π^* C5-C6	$p_{(C5)}- p_{(C6)}$	0.33233	81.90	0.04	0.083
CIII								
π C1-C2 (2)	$0.7066p_{(C1)}+ 0.7076p_{(C2)}$	1.64715	π^* C3-C4	$p_{(C3)}- p_{(C4)}$	0.33777	21.22	0.28	0.069
			π^* C5-C6	$p_{(C5)}- p_{(C6)}$	0.34231	20.45	0.29	0.069
π C3-C4 (2)	$0.7058p_{(C3)}+ 0.7084p_{(C4)}$	1.67801	π^* C1-C2	$p_{(C1)}- p_{(C2)}$	0.37070	18.33	0.28	0.065
			π^* C5-C6	$p_{(C5)}- p_{(C6)}$	0.34231	19.60	0.29	0.067
π C5-C6 (2)	$0.7031p_{(C5)}+ 0.7111p_{(C6)}$	1.68438	π^* C1-C2	$p_{(C1)}- p_{(C2)}$	0.37070	19.13	0.33	0.072
			π^* C3-C4	$p_{(C3)}- p_{(C4)}$	0.33777	13.13	0.33	0.059
LP (1) N13	p	1.63860	π^* C1-C2	$p_{(C1)}- p_{(C2)}$	0.37070	33.11	0.29	0.088
π^* C3-C4	$p_{(C3)}- p_{(C4)}$	0.33777	π^* C5-C6	$p_{(C5)}- p_{(C6)}$	0.34231	248.74	0.01	0.079
CIV								
π C1-C2 (2)	$0.7079p_{(C1)}+ 0.7063p_{(C2)}$	1.64844	π^* C3-C4	$p_{(C3)}- p_{(C4)}$	0.34033	20.86	0.29	0.069
			π^* C5-C6	$p_{(C5)}- p_{(C6)}$	0.33343	19.17	0.32	0.071
π C3-C4 (2)	$0.7023p_{(C3)}+ 0.7118p_{(C4)}$	1.68130	π^* C1-C2	$p_{(C1)}- p_{(C2)}$	0.37419	18.21	0.28	0.065
			π^* C5-C6	$p_{(C5)}- p_{(C6)}$	0.33343	18.00	0.32	0.068
π C5-C6 (2)	$0.7094p_{(C5)}+ 0.7048p_{(C6)}$	1.66762	π^* C1-C2	$p_{(C1)}- p_{(C2)}$	0.37419	21.19	0.28	0.070
			π^* C3-C4	$p_{(C3)}- p_{(C4)}$	0.34033	18.18	0.28	0.064
			π^* C5-C6	$p_{(C5)}- p_{(C6)}$	0.33343	1.76	0.32	0.021
σC27-C28 (1)	$0.7051sp^{2.52}_{(C27)}+ 0.7091sp^{2.74}_{(C28)}$	1.98194	π^* C5-C6	$p_{(C5)}- p_{(C6)}$	0.33343	3.68	0.64	0.047
LP (1) N13	p	1.63878	π^* C1-C2	$p_{(C1)}- p_{(C2)}$	0.37419	32.54	0.29	0.087
CV								
π C1-C2 (2)	$0.7004p_{(C1)}+ 0.7137p_{(C2)}$	1.66314	π^* C3-C4	$p_{(C3)}- p_{(C4)}$	0.33701	20.75	0.29	0.069
			π^* C5-C6	$p_{(C5)}- p_{(C6)}$	0.32432	18.13	0.33	0.069
π C3-C4 (2)	$0.7021p_{(C3)}+ 0.7121p_{(C4)}$	1.68264	π^* C1-C2	$p_{(C1)}- p_{(C2)}$	0.38538	18.34	0.28	0.065
			π^* C5-C6	$p_{(C5)}- p_{(C6)}$	0.32432	17.91	0.32	0.068
π C5-C6 (2)	$0.7100p_{(C5)}+ 0.7042p_{(C6)}$	1.66498	π^* C1-C2	$p_{(C1)}- p_{(C2)}$	0.38538	23.19	0.26	0.071
			π^* C3-C4	$p_{(C3)}- p_{(C4)}$	0.33701	19.92	0.27	0.065
			π^* C5-C6	$p_{(C5)}- p_{(C6)}$	0.32432	1.92	0.31	0.022
σ C7-C14	$0.7169sp^{2.77}_{(C7)}+ 0.6972sp^{2.73}_{(C14)}$	1.96644	π^* C5-C6	$p_{(C5)}- p_{(C6)}$	0.32432	0.79	0.65	0.022
σ C7-C28	$0.7216sp^{3.24}_{(C7)}+ 0.6923sp^{2.76}_{(C28)}$	1.95687	π^* C5-C6	$p_{(C5)}- p_{(C6)}$	0.32432	3.25	0.63	0.044
σ C47-C49	$0.7053sp^{1.72}_{(C47)}+ 0.7089sp^{2.67}_{(C49)}$	1.98432	π^* C47-O48	$p_{(C47)}- p_{(O48)}$	0.30304	1.41	0.71	0.031
σ C49-H50	$0.7843sp^{3.10}_{(C49)}+ 0.6203s_{(H50)}$	1.98507	π^* C47-O48	$p_{(C47)}- p_{(O48)}$	0.30304	3.84	0.57	0.045
σ C49-H51	$0.7812sp^{3.05}_{(C49)}+ 0.6243s_{(H51)}$	1.97943	π^* C47-O48	$p_{(C47)}- p_{(O48)}$	0.30304	7.88	0.58	0.065
LP (1) N13	p	1.63427	π^* C1-C2	$p_{(C1)}- p_{(C2)}$	0.38538	33.92	0.28	0.088
			π^* C47-O48	$p_{(C47)}- p_{(O48)}$	0.30304	52.79	0.32	0.118
π^* C1-C2	$p_{(C1)}- p_{(C2)}$	0.38538	π^* C5-C6	$p_{(C5)}- p_{(C6)}$	0.32432	77.74	0.04	0.085
			π^* C47-O48	$p_{(C47)}- p_{(O48)}$	0.30304	0.83	0.04	0.009
π^* C3-C4	$p_{(C3)}- p_{(C4)}$	0.33701	π^* C5-C6	$p_{(C5)}- p_{(C6)}$	0.32432	75.50	0.04	0.083

* E(2) means the energy of hyper conjugative interaction (stabilization energy).

NLO (Non-Linear Optical) Analysis

Table S4. The electric dipole moment(μ), the mean polarizability (α_0), the anisotropy of the polarizability (Δα) and the first order hyperpolarizability (β) of the four stable conformers for the demethoxyaspidospermine compound in the gas phase

	B3LYP/6-311++G(d,p)					M06-2X/6-311++G(d,p)					HF/6-311++G(d,p)				
	CI	**CII**	**CII**	**CIV**	**CV**	**CI**	**CII**	**CII**	**CIV**	**CV**	**CI**	**CII**	**CII**	**CIV**	**CV**
μ (Debye)															
μ_x	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
μ_y	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
μ_z	4.437	4.401	4.365	4.363	3.371	4.401	4.320	4.307	4.317	0.346	4.539	4.486	4.469	4.456	3.652
μ	4.437	4.401	4.365	4.363	3.371	4.401	4.320	4.307	4.317	0.346	4.539	4.486	4.469	4.456	3.652
α_{xx}	38.691	39.020	39.231	38.492	41.635	37.000	37.468	37.810	37.024	40.573	34.354	34.682	35.039	34.370	37.883
α_{xy}	-0.258	-0.402	-1.595	-1.208	2.566	-0.357	-0.251	-1.462	-1.104	2.073	-0.432	-0.380	-1.426	-1.115	1.937
α_{yy}	31.410	30.632	30.455	31.569	32.137	30.594	29.706	29.344	30.532	31.008	29.160	28.496	28.086	29.056	29.579
α_{zx}	0.660	0.451	0.399	0.116	0.955	0.412	0.292	0.314	-0.010	0.727	0.254	0.119	0.088	-0.128	0.196
α_{zy}	0.770	0.819	0.630	0.511	-0.291	0.722	0.798	0.308	0.188	-0.070	0.727	0.892	0.417	0.297	0.122
α_{zz}	42.491	42.843	42.855	42.685	39.162	41.294	41.658	41.559	41.381	37.629	38.586	38.850	38.832	38.702	34.812
α_0	37.531	37.498	37.513	37.582	37.645	36.296	36.278	36.238	36.312	36.403	34.033	34.010	33.986	34.043	34.091
$\Delta\alpha$	9.920	10.961	11.456	9.987	9.777	9.457	10.615	11.156	9.653	9.300	8.319	9.180	9.785	8.606	8.019
β_{xxx}	1.598	1.473	0.593	0.918	-0.746	1.344	1.229	0.763	0.958	-0.394	1.138	1.056	0.690	0.858	-0.190
β_{xxy}	0.732	0.400	0.603	0.784	-0.394	0.449	0.148	0.344	0.493	-0.206	0.300	0.108	0.302	0.380	-0.117
β_{yxy}	0.825	0.728	0.796	0.911	-0.154	0.607	0.524	0.472	0.568	-0.062	0.555	0.500	0.555	0.607	-0.185
β_{yyy}	0.386	0.027	1.367	1.462	-0.750	0.232	-0.055	0.727	0.809	-0.284	-0.053	-0.155	0.203	0.264	-0.101
β_{xxz}	-1.402	-1.344	-1.275	-1.285	0.711	-1.268	-1.293	-1.245	-1.242	0.356	-1.119	-1.103	-1.070	-1.071	0.155
β_{yxz}	0.313	0.211	0.675	0.715	-0.273	0.275	0.161	0.410	0.464	-0.286	0.135	0.088	0.271	0.283	-0.256
β_{yyz}	0.198	0.253	0.709	0.623	1.056	0.241	0.224	0.498	0.424	0.686	0.065	0.100	0.157	0.145	0.587
β_{zxz}	-0.248	-0.122	-0.501	-0.464	-1.737	-0.478	-0.327	-0.571	-0.552	-1.637	-0.309	-0.201	-0.359	-0.376	-1.254
β_{zyz}	0.246	-0.032	0.483	0.609	-1.515	0.194	-0.016	0.275	0.405	-1.037	0.148	0.043	0.164	0.219	-0.825
β_{zzz}	0.395	0.464	1.084	0.873	2.546	0.332	0.278	0.602	0.483	1.989	0.284	0.195	0.478	0.388	1.829
β_x	2.175	2.079	0.888	1.365	-2.636	1.473	1.427	0.663	0.974	-2.094	1.384	1.355	0.886	1.089	-1.629
β_y	1.364	0.394	2.454	2.855	-2.659	0.874	0.077	1.346	1.706	-1.527	0.395	-0.004	0.669	0.863	-1.043
β_z	-0.810	-0.626	0.519	0.212	4.313	-0.696	-0.791	-0.145	-0.335	3.031	-0.769	-0.808	-0.434	-0.539	2.571
β	2.692	2.207	2.661	3.172	5.712	1.849	1.633	1.507	1.993	3.988	1.632	1.578	1.192	1.490	3.217

Table S5. The calculated quantum chemical and physicochemical parameters of the five stable conformers for the demethoxyaspidospermine compound in the gas phase

	CI	**CII**	**CIII**	**CIV**	**CV**
			B3LYP/6-311++G(d,p)		
HOMO (-I)	-0.2184	-0.2187	-0.2127	-0.2131	-0.2199
LUMO (-A)	-0.0230	-0.0230	-0.0226	-0.0227	-0.0292
ΔE (Energy Gap)	5.3166	5.3264	5.1748	5.1813	5.1906
χ	-3.2836	-3.2885	-3.2016	-3.2089	-3.3888
η	2.6583	2.6632	2.5874	2.5907	2.5953
ω	2.0280	2.0303	1.9807	1.9873	2.2124
ΔN_{max}	1.2352	1.2348	1.2374	1.2386	1.3057
			M06-2X/6-311++G(d,p)		
HOMO (-I)	-0.2642	-0.2643	-0.2648	-0.2647	-0.2665
LUMO (-A)	-0.0099	-0.0096	-0.0102	-0.0105	-0.0083
ΔE (Energy Gap)	6.9207	6.9295	6.9297	6.9169	7.0254
χ	-3.7289	-3.7262	-3.7413	-3.7436	-3.7394
η	3.4603	3.4647	3.4648	3.4584	3.5127
ω	2.0092	2.0037	2.0199	2.0261	1.9903
ΔN_{max}	1.0776	1.0755	1.0798	1.0825	1.0645
			HF/6-311++G(d,p)		
HOMO (-I)	-0.2978	-0.2980	-0.2984	-0.2984	-0.3032
LUMO (-A)	-0.0347	-0.0348	-0.0346	-0.0344	-0.0349
ΔE (Energy Gap)	7.1590	7.1637	7.1773	7.1838	7.3016
χ	-4.5232	-4.5282	-4.5302	-4.5269	-4.6002
η	3.5795	3.5818	3.5886	3.5919	3.6508
ω	2.8578	2.8624	2.8593	2.8526	2.8983
ΔN_{max}	1.2636	1.2642	1.2624	1.2603	1.2601

*ΔE (Energy Gap), χ, η, ω and $\Delta Nmax$ are in eV; HOMO and LUMO energies are in au.

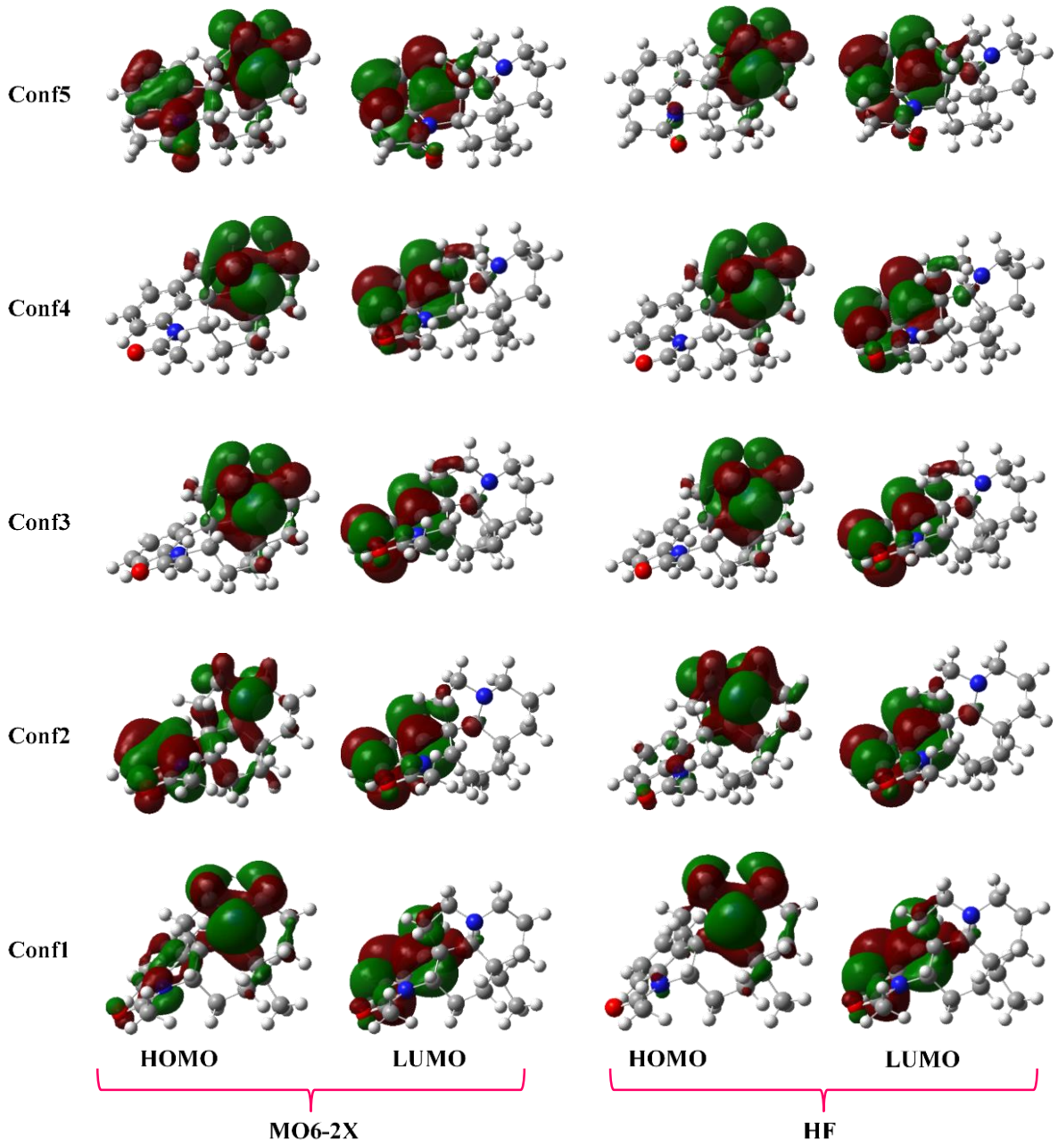


Fig. S1a. HOMO and LUMO amplitudes of the four stable conformers for the demethoxyaspidospermine compound for both methods by using the 6-311++G(d,p) basis set in the chloroform phase (isoval:0.02)

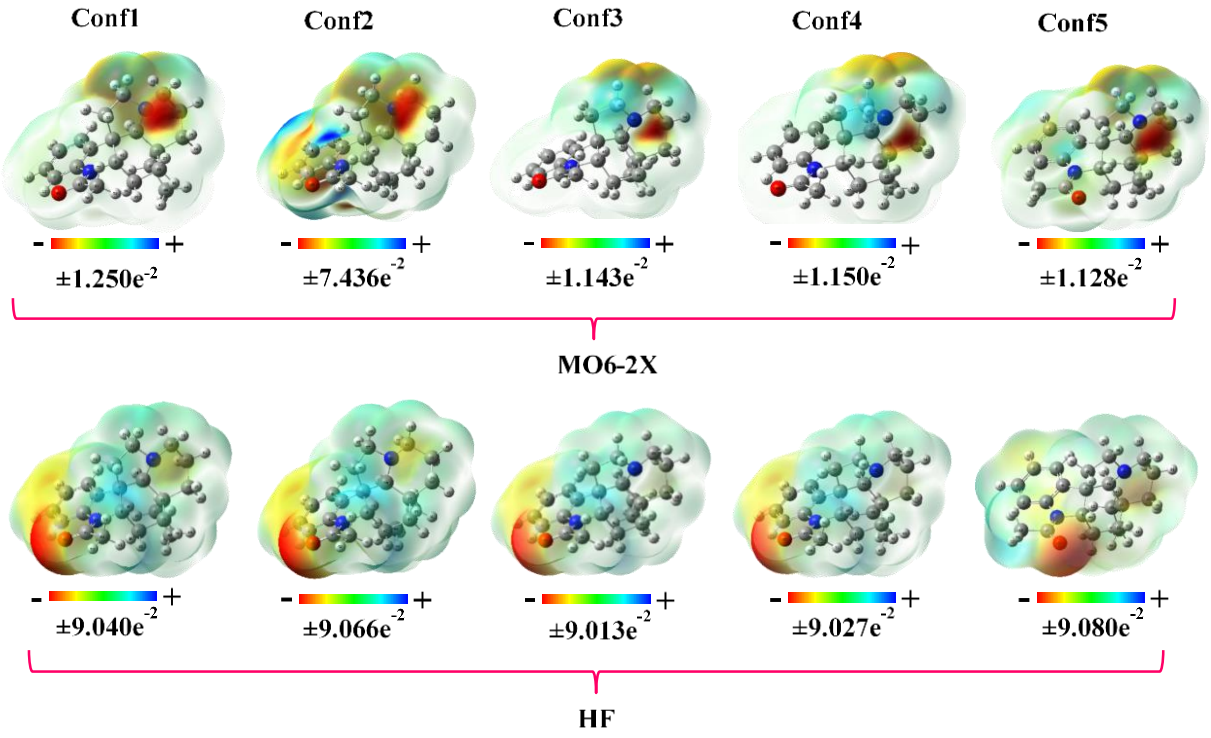


Fig. S1b. The electron density surface from total SCF mapped with ESP for the four stable conformers for the demethoxyaspidospermine compound for both methods by using the 6-311++G(d,p) basis set in the chloroform phase (Iso value:0.0004)

FT-IR Spectral Analysis

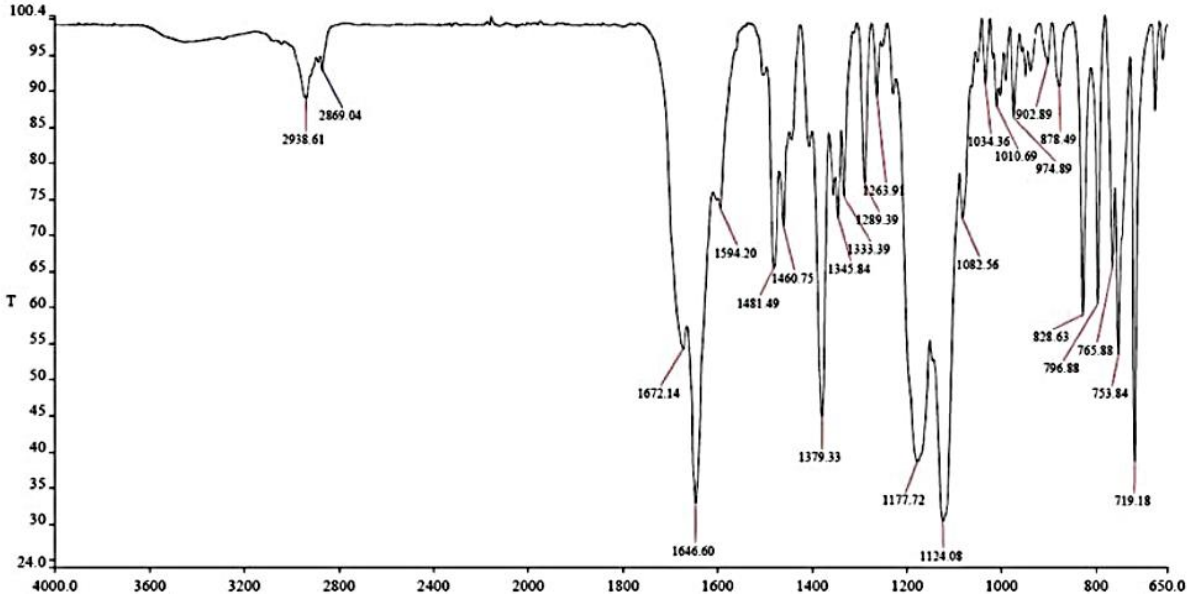


Figure S2a. The recorded *FT-IR* spectrum of the demethoxyaspidospermine

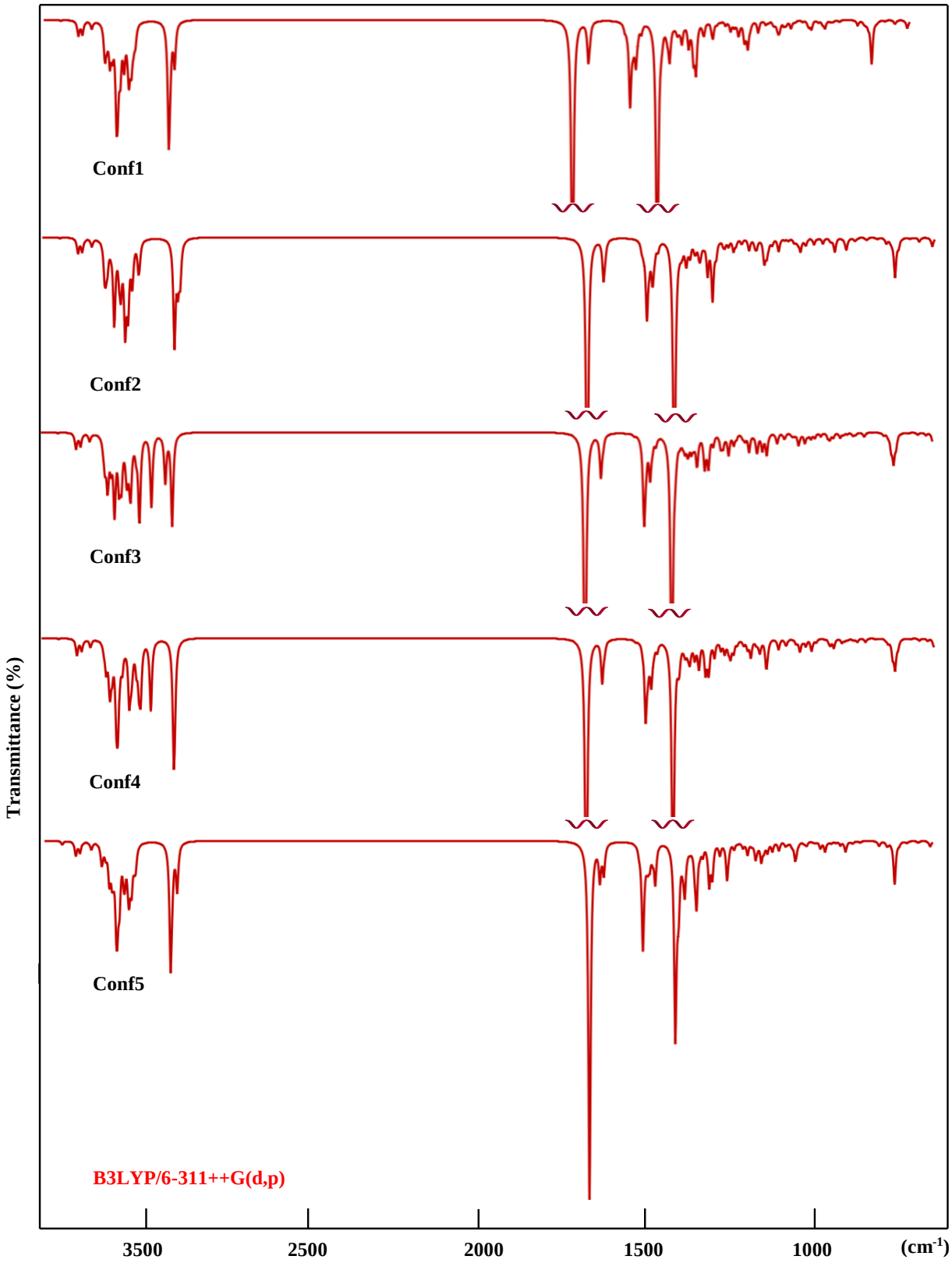


Figure S2b. The simulated *FT-IR* spectrum of the stable conformers of the demethoxyaspidospermine at B3LYP level

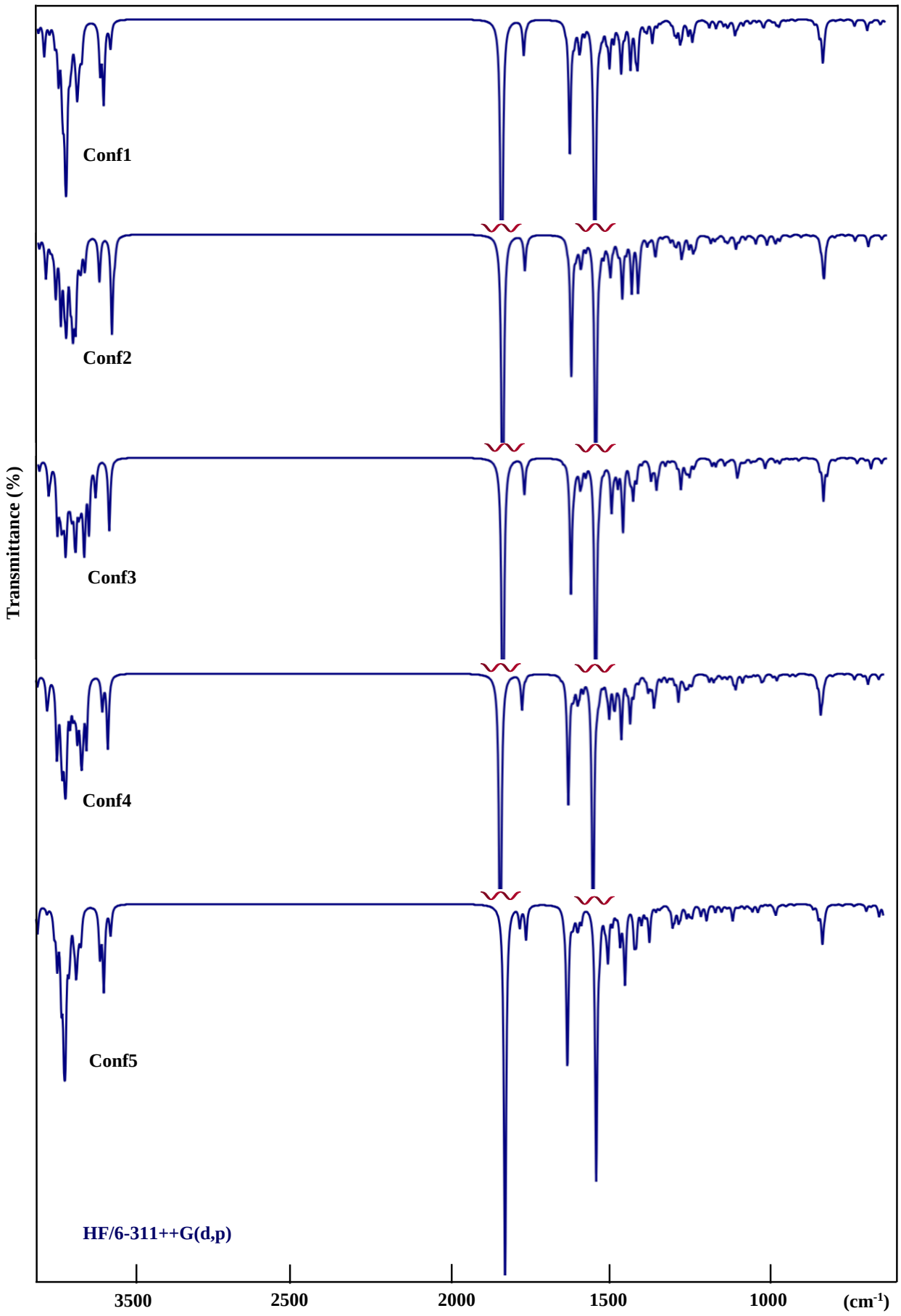


Figure S2c. The simulated *FT-IR* spectrum of the stable conformers of the demethoxyaspidospermine at HF method

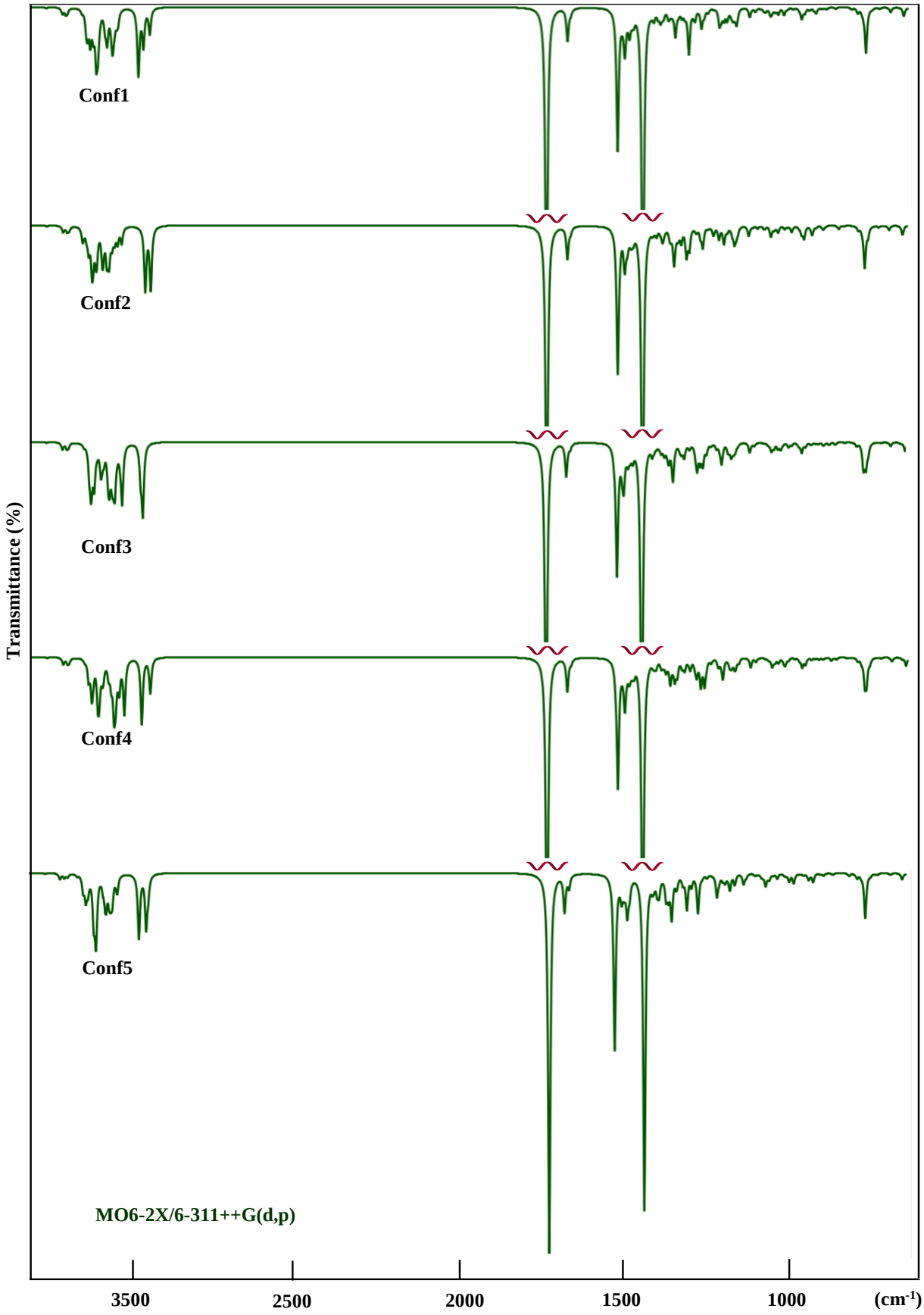


Figure S2d. The simulated *FT-IR* spectrum of the stable conformers of the demethoxyaspidospermine at M06-2X level

Table S6. The observed and calculated vibrational frequencies (in cm^{-1}) of the demethoxyaspidospermine (**CI**) in chloroform phase

		B3LYP				M06-2X				HF			
Exp.		***Unscaled***	***Scaled***	I_{IR}	*PED %*[a]	***Unscaled***	***Scaled***	I_{IR}	*PED %*[a]	***Unscaled***	***Scaled***	I_{IR}	***PED %***[a]
	150	3242	3112	2	νCH R**A** (98)	3254	3088	2	νCH R**A** (89)	3412	3088	1	νCH R**A** (96)
	149	3188	3060	28	νCH R**A** (96)	3205	3041	12	νCH R**A** (92)	3349	3031	29	νCH R**A** (89)
	148	3176	3049	25	ν_{as}CH R**A** (98)	3194	3031	12	ν_{as}CH R**A** (92)	3336	3019	33	ν_{as}CH R**A** (88)
	147	3166	3039	0	ν_{as}CH R**A** (96)	3190	3027	7	$\nu_{as}C_{49}H2$ (87)	3321	3006	2	ν_{as}CH R**A** (91)
	146	3148	3022	14	$\nu_{as}C_{49}H$ (89)	3184	3021	0	ν_{as}CH R**A** (93)	3297	2984	21	$\nu_{as}C_{49}H2$ (91)
	145	3109	2985	28	ν_{as} $C_{49}H2$+ νC_8H (86)	3146	2985	6	ν_{as} $C_{49}H2$ (90)	3279	2968	67	νC_8H (92)
	144	3106	2982	40	ν_{as}CH2 R**E**+ νC_8H (75)+ νCH2 R**E** (11)	3133	2973	29	$\nu_{as}C_{40}H2$ (90)	3263	2953	18	$\nu_{as}C_{49}H2$ (92)
	143	3101	2977	24	νC_8H+ νCH2 R**E** (81)	3129	2969	36	ν_{as}CH2 R**E** (78)+ νC_8H+ $\nu_{as}C_{40}H2$ (10)	3246	2937	36	ν_{as}CH2 R**E** (85)
	142	3092	2968	66	$\nu_{as}C_{40}H2$ (81)	3121	2962	14	ν_{as}CH2 R**C**+ $\nu_{as}C_{40}H2$ (70)	3234	2927	102	$\nu_{as}C_{40}H2$ (62)+ νCH R**C**+ $\nu_{as}C_{39}H2$ (10)
	141	3085	2962	45	$\nu_{as}C_{40}H2$ (86)	3121	2961	45	νC_8H+ $\nu_{as}C_{40}H2$ (79)	3223	2917	59	νCH R**CD**+ $\nu C_{40}H2$ (82)
	140	3072	2949	99	ν_{as}CH2 R**CD** (85)	3112	2953	43	ν_{as}CH2 R**E** (94)	3220	2914	106	νCH R**C**+ $\nu_{as}C_{40}H2$ (71)
	139	3071	2948	30	ν_{as}CH2 R**CD** (86)	3103	2944	60	ν_{as}CH2 R**D** (75)	3213	2908	151	ν_{as}CH R**CD**+ $\nu_{as}C_{40}H2$ (81)
2939	138	3069	2946	101	νCH2 R**CD** (76)	3102	2944	26	νCH2 R**CD** (78)	3211	2906	63	ν_{as}CH R**CD**+ $\nu_{as}C_{40}H2$ (66)
	137	3066	2943	12	ν_{as}CH2 R**CD** (82)	3098	2939	66	ν_{as}CH2 R**CD** (83)	3210	2905	66	νCH R**DE** (63)+ ν_{as}CH2 R**D** (10)
	136	3060	2938	81	νCH2 R**E** (82)+ ν_{as}CH2 R**E** + νC_8H (12)	3093	2935	10	ν_{as}CH2 R**C** (78)	3209	2904	102	ν_{as}CH2 R**D**+ νCH2 R**E** (76)
	135	3049	2927	43	$\nu_{as}C_{39}H2$ (78)	3076	2919	30	$\nu_{as}C_{39}H2$ (91)	3199	2895	61	$\nu_{as}C_{39}H2$ (67)+ $\nu_{as}C_{40}H2$ (10)
	134	3048	2926	28	νCH2 R**E** (90)	3070	2913	15	$\nu C_{49}H3$+ νCH2 R**E** (89)	3194	2890	35	νCH R**E** (90)
	133	3045	2923	4	$\nu C_{49}H3$ (85)	3070	2913	15	$\nu C_{49}H3$+ νCH2 R**E** (84)	3191	2888	4	$\nu C_{49}H3$ (92)
	132	3039	2917	15	νCH2 R**C** (84)	3069	2912	28	νCH2 R**D** (80)	3184	2882	16	νCH R**C** (72)
	131	3035	2914	59	νCH2 R**D** (77)	3057	2901	18	νCH2 R**C** (77)	3180	2878	33	νCH R**CD** (78)
	130	3033	2912	37	νCH2 R**D** (78)	3054	2897	58	νCH2 R**CD**+ $\nu C_{40}H3$ (65)	3176	2874	103	νCH2 R**D** (76)
	129	3028	2907	12	$\nu C_{40}H3$+ $\nu C_{19}H$ (83)	3050	2895	19	νCH2 R**D**+ $\nu C_{40}H3$ (77)	3172	2871	40	νCH R**D** (69)
	128	3026	2905	61	νCH R**D** + ν($C_{40}H3$) (84)	3047	2891	19	νCH2 R**CD** (77)	3167	2866	26	νCH R**D**+ ν($C_{39}H$+ $C_{40}H2$) (64)
	127	3020	2899	28	$\nu C_{39}H2$ (79)	3040	2885	18	νCH2 R**D**+ $\nu C_{39}H$ (85)	3163	2862	19	νCH R**C** (71)
	126	3014	2893	31	νCH R**C** (82)	3036	2881	20	νCH2 R**C** (79)	3161	2861	42	ν($C_{39}H2$+ $C_{40}H3$) (74)
2809	125	2912	2796	216	νCH R**D+** $\nu C_{14}H$ (92)	2975	2823	127	νCH R**D** (93)	3104	2809	93	$\nu C_{14}H$ (93)
	124	2908	2792	51	νCH2 R**D**+ ν_{as}CH2 R**D+** $\nu C_{14}H$ (98)	2960	2809	71	νCH R**E** (93)	3093	2799	155	νCH R**D** (88)
	123	2894	2778	78	νCH R**E** (93)	2941	2790	49	$\nu C_{14}H$ (94)	3072	2780	52	νCH R**E** (91)
1672	122	1679	1612	578	**ν(C=O) (72)**	1742	1653	643	**ν(C=O) (80)**	1848	1672	686	**ν(C=O) (75)**
1647	121	1631	1566	71	νCC R**A** (62)	1678	1592	61	νCC R**A** (45)	1779	1610	68	νCC R**A** (60)
1594	120	1626	1561	18	νCC R**A** (66)	1668	1583	9	νCC R**A** (73)	1769	1601	6	νCC R**A** (66)
1482	119	1519	1458	12	σCH2 R**DE** (76)	1527	1449	267	ipb HCC R**A** (30)+ νCC R**A** (22)	1649	1492	9	σCH2 R**DE** (74)
	118	1513	1452	7	σCH2 (R**CDE**+ $C_{39}H2$+ $C_{40}H2$) (71)	1523	1445	2	σCH2 R**DE** (76)	1638	1482	6	σCH2 R**DE** (56)+ ipb HCC R**A** (11)
	117	1509	1449	2	σCH2 R**DE** (78)	1514	1436	11	σ(CH2 R**C+** $C_{39}H2$+ $C_{40}H2$) (54)	1635	1480	140	νCC R**A+** σ(CH2 R**CDE+** $C_{39}H2$) (48)
	116	1505	1445	4	σ(CH2 R**C**+ $C_{39}H2$+ $C_{40}H2$) (61)	1509	1432	4	σCH2 R**DE** (71)	1635	1479	111	σ(CH2 R**CDE+** $C_{39}H2$) (45)
1461	115	1503	1443	143	ipb HCC R**A** (28)+ νCC R**A+** $\nu N_{13}C$ (12)	1506	1429	16	σ(CH2 R**E+** $C_{39}H2$+ $C_{40}H2$+ $C_{49}H3$ (44)	1626	1471	12	σ(CH2 R**C**+ $C_{39}H2$+ $C_{40}H2$) (51)
	114	1498	1438	14	σCH2 (R**CD**+ $C_{40}H2$) (73)	1504	1428	62	σ($C_{39}H2$+ $C_{40}H2$)+ ipb HCC R**A** (31)+ α R**A** (18)	1621	1467	7	σCH2 R**CDE** (46)
	113	1496	1436	1	σCH2 (R**D**+ $C_{40}H2$) (79)	1500	1423	5	σ(CH2 R**C**+ $C_{39}H2$+$C_{40}H3$) (69)	1621	1467	20	σ(CH2 R**CD**+ $C_{39}H2$+ $C_{40}H2$) (59)
	112	1494	1434	19	σCH2 R**CD** (73)	1495	1419	4	σCH2 R**D** (76)	1616	1463	4	σCH2 R**E** (69)
	111	1492	1432	11	σCH2 R**E** (75)	1491	1415	30	σ(CH2 R**CD+** $C_{49}H2$) (63)	1615	1461	1	σ(CH2 R**CD**+ $C_{39}H2$+ $C_{40}H2$) (61)
	110	1487	1428	8	σ(CH2 R**CD** + $C_{39}H2$+ $C_{49}H2$) (64)	1489	1413	11	σCH2 R**CD** (67)	1609	1456	3	σ($C_{39}H2$+ $C_{40}H2$) (54)
	109	1485	1426	64	ipb HCC R**A** (50)+ νCC R**A** (13)	1486	1410	4	σCH2 R**E** (74)	1605	1453	36	ipb HCC R**A** (63)+ νCC R**A** (22)
	108	1480	1421	9	σ(CH2 R**CD**+ $C_{49}H2$) (70)	1483	1407	10	σ(CH2 R**CD**+ $C_{39}H2$) (63)	1604	1452	5	σ($C_{39}H2$+ $C_{40}H2$+ $C_{49}H2$) (44)
	107	1478	1419	4	σ(CH2 R**CD**+ $C_{49}H2$) (75)	1478	1403	15	σ$C_{49}H2$ (61)	1601	1449	26	σ$C_{49}H2$ (67)+ σ($C_{39}H2$+ $C_{40}H2$) (12)
	106	1469	1410	17	σ$C_{49}H2$ (79)	1476	1400	2	σ(CH2 R**CD**+ $C_{39}H2$)) (60)	1589	1438	19	σ$C_{49}H2$ (78)
1379	105	1420	1363	542	$\nu N_{13}C$ (34)+ sb$C_{49}H3$ (18)	1450	1376	676	$\nu N_{13}C$ (39)+ ipb HCC R**A** (10)+ sb$C_{49}H3$	1556	1409	587	$\nu N_{13}C$ (29)
	104	1417	1360	6	sb$C_{40}H3$ (60)+ ωCH2 R**DE+** ipb HCN_{26} (19)	1425	1352	3	ωCH2 R**DE+** sb$C_{40}H3$ (22)	1550	1403	11	ωCH2 R**DE** (51)
	103	1409	1353	15	ω R**DE+** sb$C_{40}H3$+ ipb HCN_{26} (41)	1417	1345	15	sb$C_{40}H3$ (55)	1541	1395	12	ω(CH2 R**CDE+** $C_{39}H2$) (39)
	102	1405	1349	13	ωCH2 R**DE+** χ$HCN_{26}C$ (43)	1416	1343	3	ωCH2 R**DE+** sb$C_{40}H3$ (10)+ χ$HCN_{26}C$ (35)	1538	1392	9	sb$C_{40}H3$ (68)

1346	101	1392	1336	6	ipb HCC RC**D** (31)+ sbC_{49}H3 (11)	1404	1333	12	ipb (HCN_{26}+ HCC R**C**) (43)	1532	1387	15	ωCH2 R**C** (38)
	100	1389	1333	15	sbC_{49}H3+ ipb HCC R**CD** (47)	1397	1326	20	ωCH2 R**DE+** χHCN_{26}C (16)	1521	1376	18	ω(CH2 R**CD)**+ ipb $H_{18}CN_{26}$ (54)
	99	1386	1331	4	sbC_{49}H3+ ωCH2 R**CD** (40)+ ωCH2 R**E** (18)	1393	1322	6	ipb HCC R**CD**+ ω(CH2 R**C+** C_{39}H2) (31)	1518	1374	11	ipb HCC R**CD** (39)
1333	98	1382	1327	64	sbC_{49}H3+ ωCH2 R**CD** (20)	1388	1317	12	sbC_{49}H3 (57)	1511	1367	81	sbC_{49}H3 (62)
	97	1376	1321	4	ωC_{39}H2 (28)+ τC_{39}H2 (12)	1385	1314	2	ωC_{39}H2 (19)	1508	1365	1	ωC_{39}H2+ sbC_{40}H3 (38)
	96	1369	1314	4	ipb HCC R**CD**+ ωCH2 R**C** (38)+ τCH2 R**CD** (12)	1373	1303	16	ωCH2 R**CDE** (15)	1497	1355	33	ω(CH2 R**CDE+** C_{39}H2) (35)+ τCH2 R**CD** (10)
	95	1363	1308	4	ωCH2 R**DE** (34)+ χHCN_{26}C (13)	1369	1299	7	νCC R**A** (27)+ ipb HCC R**C** (14)	1487	1345	7	ω(CH2 R**CDE+** C_{39}H2) (37)
	94	1358	1304	18	ωCH2 R**CE** (35)+ νCC R**A** (12)	1363	1294	6	ipb HCC R**C**+ ωCH2 R**C**	1482	1341	8	ω(CH2 R**CD)** (26)+ τCH2 R**DE** (13)
	93	1352	1298	8	ωCH2 R**E** (27)	1359	1290	4	ωCH2 R**CDE** (24)	1474	1334	96	ωCH2 R**C** (39)+ sbC_{49}H3 (27)
	92	1345	1291	37	νCC R**A** (35)+ ωCH2 R**E** (16)	1352	1283	51	ipb HCC R**C** (27)+ ωCH2 R**DE+** χHCN_{26}C (18)	1463	1324	21	ωCH2 R**E**+ χ$HCCN_{26}$ (45)
	91	1336	1283	3	ωCH2 R**E** (35)	1342	1274	9	ωCH2 R**E** + χ$HCCN_{26}$ (49)	1445	1308	90	ipb HCN_{13} (34)+ ωCH2 R**C** (10)+ νN_{13}C (14)
1289	90	1324	1271	44	ipb (HCN_{13}+ HCC R**A**) (38)	1332	1264	15	ipb (HCC R**A**+ HN_{13}C) (38)	1429	1293	49	τCH2 R**DE** (18)+ τCH2 R**DE** (10)
	89	1317	1264	5	τC_{39}H2 (44)	1323	1256	13	ipb HCN_{26} (32)	1424	1289	14	τC_{39}H2 (48)
1264	88	1309	1257	63	τCH2 R**CDE**+ ipb HCC R**A** (25)	1313	1246	5	τC_{39}H2 (40)	1422	1287	69	τC_{39}H2+ τCH2 R**D** (19)
	87	1302	1250	88	τCH2 R**D**+ ipb HCC R**A** (36)+ νCC R**A** (10)	1311	1244	82	τCH2 R**D+** ipb HCC R**A** (43)+ ipb HCN_{26} (10)	1401	1268	14	τCH2 R**CE (11)**
	86	1281	1230	8	τCH2 R**CD**+ ipb HCN_{26} (35)+ ωC_{28}H2 (14)	1297	1231	7	τCH2 R**CDE** (13)	1394	1261	19	τCH2 R**DE** (21)+ ω(CH2 R**CD)** (12)
	85	1277	1226	21	τCH2 R**DE** (34)	1293	1227	19	τCH2 R**DE** (19)	1377	1246	43	τCH2 R**DE** (11)
	84	1254	1204	10	τCH2 R**CDE** (17)	1273	1208	37	τCH2 R**DE** (22)	1362	1232	12	τCH2 R**CDE** (33)
	83	1250	1200	28	τCH2 R**E**+ ipb HCN_{26} (17)	1265	1200	14	τCH2 R**CD+** ωC_{39}H2 (10)	1351	1222	5	τCH2 R**CDE** (11)
	82	1238	1188	6	τCH2 R**CDE** (15)	1253	1189	9	τCH2 R**CDE**	1343	1215	2	τCH2 R**DE** (22)
	81	1227	1178	2	τCH2 R**E**+ ipb HCN_{26} (33)	1236	1173	2	τCH2 R**DE** (38)	1318	1193	6	ipb HCC R**A**+ τ CH2 R**CDE** (16)+ νCC R**A** (29
1178	80	1212	1164	9	τCH2 R**CD+** ipb HCN_{26} (36)	1219	1156	31	τCH2 R**CD** (14)+ νN_{26}C (11)	1308	1183	20	ipb HCC R**A**+ τ CH2 R**CDE** (14)
	79	1196	1148	19	νN_{26}C+ ipb HCC R**A** (18)	1213	1151	16	νN_{26}C (23)+ τCH2 R**CD** (13)	1301	1177	25	ν(N_{26}C+N_{13}C) (21)
	78	1186	1139	10	νN_{13}C+ νN_{26}C+ νCC R**A** (24)	1205	1143	20	ipb HCC R**A**+ τ CH2 R**DE**	1290	1167	37	ν(N_{26}C+N_{13}C+ CC R**BCE**) (26)
	77	1180	1133	2	ipb HCC R**A** (54)+ νCC R**A** (10)	1196	1134	22	τ CH2 R**CDE**	1284	1162	22	τCH2 R**DE**
1124	76	1172	1125	23	νCC R**C**+ νN_{26}C+ ipb HCC R**A** (25)	1185	1125	4	ν(N_{13}C+ N_{26}C) (31)	1271	1151	2	τCH2 R**CDE**
	75	1169	1122	6	τ CH2 R**CE**	1182	1121	8	τCH2 R**C+** ρC_{39}H2 (11)+ σ(CH2 R**C+** C_{39}H2+ C_{40}H2) (13)	1264	1144	26	ν(N_{26}C+N_{13}C) (26)
1124	74	1154	1108	35	νN_{26}C+ ipb HCC R**A** (34)	1178	1118	15	νN_{26}C+ ipb HCC R**A** (15)	1256	1137	0	ωCH2 R**CE+** ν(N_{26}C+N_{13}C)
	73	1148	1102	8	χ HCN_{26}C (15)+ ρCH2 R**DE** (10)	1172	1112	10	ipb HCC R**A** (45)+ ν(N_{13}C+ N_{26}C) (18)	1251	1133	38	ν(N_{26}C+N_{13}C) (16)
	72	1143	1097	46	νN_{13}C+ νCC R**A** (30)+ α RA+ ipb (CCN_{13}+N_{13}C=O) (12)	1167	1107	27	τ CH2 R**E** (11)	1246	1127	11	νN_{26}C+ τ CH2 R**E** (35)
	71	1136	1091	9	νN_{26}C+ νCC R**C** (30)	1163	1104	5	χ (CCCC) R**CDE**	1210	1095	3	νCC R**A**+ ipb HCC R**A** (38)
1083	70	1112	1068	22	νCC R**A** (20)+ ipb HCC R**A** (26)	1127	1070	18	α R**A+** ipb HCC R**A** (44)	1198	1085	15	ipb HCC R**A** (34)
	69	1089	1045	8	νCC R**B** (32)	1110	1053	8	α R**C+** ipb HCC R**C** (11)	1177	1065	16	νCC R**ACD** (17)+ α R**C** (12)
	68	1081	1038	4	χ HCN_{26}C (10)	1094	1038	2	νN_{26}C+ νCC R**CD** (22)	1173	1062	1	νCC R**CD** (26)
1034	67	1067	1024	3	(τ+ω)C_{40}H2 (23)	1085	1030	5	νN_{26}C+ νCC R**C** (32)**+** χ HCCC (12)	1154	1044	4	τC_{40}H2 (16)
	66	1063	1020	8	ν(CC R**CD**+ $C_{39}C_{40}$) (27)+ χ HCN_{26}C(11)	1080	1025	8	νN_{26}C+ νCC R**CD** (25)	1153	1044	7	τC_{49}H2+ χ OCNC (68)
	65	1054	1012	8	ρCH2 R**DE** (10)	1067	1012	6	νCC R**E** (21)+ νCC R**D** (13)	1146	1037	0	τC_{40}H2+ ωCH2 R**D+** ρCH2 R**E**
	64	1050	1008	14	νCC R**A+** νC_7C_{28} (28)+ ipb HCC R**A** (10)	1063	1009	10	νCC R**A** (23)+ ρCH2 R**E** (21)	1142	1033	12	τC_{49}H2 (14)+ σC_{49}H2 (13)+ νCC R**A** (11)
	63	1047	1005	5	χOCNC+ τC_{49}H2 (70)	1060	1006	5	ρCH2 R**E** (11)+ ρCH2 R**D** (14)	1137	1029	5	ρCH2 R**E** (11)+ α R**A +** ipb CCN_{26} (10)
1011	62	1046	1004	8	νCC R**A** (32)	1052	999	4	χOCNC+ ωC_{49}H2 (65)	1118	1012	28	τC_{49}H2 (14)+ σC_{49}H2 (14)
	61	1033	992	9	ν($C_{39}C_{40}$+ CC R**CE**) (39)	1049	995	5	νCC R**D+** ν$C_{39}C_{40}$ (26)	1111	1005	11	νCC R**A** (52)
	60	1026	985	8	νCC R**C** (18)	1041	987	12	νCC R**CE** (13)+ νCC R**D** (20)	1107	1002	0	opb HCC R**A** (85)
975	59	1011	971	15	ωC_{49}H2 (13)+ νCC R**C** (11)+ ν($C_{39}C_{40}$+ CC R**CE**) (19)	1023	971	14	τC_{49}H2 (22)+ νCC R**CE** (15)	1106	1001	4	νCC R**C+** ν$C_{39}C_{40}$ (31)
	58	999	959	3	νCC R**E** (58)	1015	963	0	opb HCC R**A** (90)	1092	988	11	ωCH2 R**C+** ν$C_{39}C_{40}$
	57	996	956	0	opb HCC R**A** (86)	1013	961	3	νCC R**E** (48)	1071	970	6	opb HCC R**A** (41)+ νCC R**A** (25)
	56	976	937	3	νCC R**CD** (28)	995	944	3	νN_{26}C+ νCC R**CD+** τC_{39}H2 (37)	1067	966	4	opb HCC R**A** (35)+ νCC R**A** (26)
	55	961	923	3	opb HCC R**A** (73)	978	928	4	opb HCC R**A** (79)	1050	950	5	νCC R**CD+** τC_{39}H2 (35)
	54	957	919	11	τC_{40}H2	970	920	21	ν($C_{47}C_{49}$+ N_{13}C)+ α R**A**	1031	933	8	ν$C_{39}C_{40}$
903	53	949	911	16	νCC R**CD**+ν($C_{47}C_{49}$+ N_{13}C) (28)	961	912	10	ρCH2 R**C**+ τC_{49}H2 (12)	1027	930	12	ρCH2 R**CD**
	52	927	890	4	τR**CDE** (11)	946	898	5	νCC R**C+** νN_{26}C+ ν$C_{39}C_{40}$ (55)	1001	906	5	τCH2 **RE**

	51	915	878	7	νCC R**CD**+νC$_{47}$C$_{49}$ (38)	933	886	5	νCC R**D** (16)	989	895	10	opb HCC R**A** (43)+ νN$_{26}$C (20)
878	50	908	872	15	νN$_{26}$C (27)	926	879	11	νC$_{47}$C$_{49+}$ νCC R**B** (22)+ ρCH2 R**E** (10)	982	888	4	νC$_{47}$C$_{49}$ (14)+ opb HCC R**A** (25)
	49	892	856	2	χHCCC+ opb HCC R**A** (14)	909	863	2	νCC R**D** (19)	980	887	9	νN$_{26}$C (10)+ opb HCC R**A** (14)+ ρCH2 R**DE** (1
	48	885	850	3	opb HCC R**A** (40)+ χHCCC (13)	902	856	2	opb HCC R**A** (82)	959	868	2	νCC R**CD** (28)
	47	881	846	2	opb HCC R**A** (31)	895	849	4	ρCH2 R**CE** (15)	950	860	2	ρCH2 R**CE** (19)
829	46	864	829	4	ρCH2 R**DE** (42)	867	823	3	ρCH2 R**D** (15)+ χ HCN$_{26}$C (29)	930	841	3	ρCH2 R**CDE** (26)
797	45	808	776	10	ρCH2 R**CDE** (22)	819	777	3	νCC R**C+** νN$_{26}$C (31)	869	786	7	ρCH2 R**DE** (16)
766	44	789	757	4	ipb (CN$_{13}$C+ C$_{15}$C$_{39}$C$_{40}$+ R**CD**)	801	760	10	ρCH2 R**CDE**	854	773	29	opb HCC R**A**+ χ N$_{13}$CCC (40)
	43	784	753	6	ρC$_{39}$H2+ τC$_{40}$H2 (52)+ νCC R**CD** (11)	788	748	4	ρC$_{39}$H2+ τC$_{40}$H2 (48)	843	763	64	opb HCC R**A** (70)
	42	775	744	9	β R**A+** opb HCC R**A** (61)	783	743	9	β R**A+** opb HCC R**A** (55)	842	762	13	opb HCC R**A** (15)+ χCCCC (22)
754	41	765	734	81	opb HCC R**A** (78)	776	736	85	β R**A+** opb HCC R**A** (76)	838	759	17	νCC R**CD (12)+** ρC$_{39}$H2+ τC$_{40}$H2 (29)
719	40	750	720	3	β R**A**+ ipb CCN$_{13}$ (11)+ νC$_{15}$C$_{49+}$ νCC R**B** (20)	758	719	3	χ CCN$_{26}$C	803	726	3	ν(N$_{13}$C+CC R**A**) (12)+ β R**A** (15)
	39	724	695	2	ρCH2 R**CD**+ νCC R**CD** (38)	735	697	3	νCC R**C** (29)+ α R**A** (11)+ ρCH2 R**C** (13)	777	703	2	νC$_{15}$C (32)+ (α+ β) R**A** (11)
	38	694	666	7	α R**A** (30)	701	665	9	ν (CC R**B+** C$_{47}$C$_{49}$) (24)	744	673	13	ν(N$_{13}$C+C$_{47}$C$_{49}$) (22)+ α R**A** (29)
	37	656	630	15	ipb CCN$_{13}$+ opb N$_{13}$C=O (39)	662	628	17	β R**AB** (27)	704	637	21	(α+ β) R**A** (28)
	36	643	617	4	ipb CCN$_{26}$+ (α+β) R**CD** (40)	641	609	4	β R**E+** ipb CCN$_{26}$ (42)	690	624	5	α R**A +** ipb CCN$_{26}$ (41)
	35	609	585	7	χ (CHCH+ CN$_{13}$C=O) (38)+ β R**CD**+ ipb CN$_{13}$C (19)	611	580	7	χ (CHCH+ CN$_{13}$C=O)+ ρCH2 R**DE** (30)	663	600	10	χCN$_{13}$CO+ τC$_{49}$H2 (54)
	34	603	579	2	β R**CD**+ ipb CN$_{13}$C (13)	607	576	1	χ (CHCH+ CN$_{13}$C=O)+ ρCH2 R**DE** (24)	647	586	5	β R**CD** (10)
	33	574	551	11	α R**A +** ipb CC=O (41)	578	549	12	β R**A +** opb CC=O (31)+ β R**DE** (11)	617	558	13	β R**A+** ipb CC=O (46)
	32	569	546	1	β R**A**+ opb CCN$_{13}$+ opb HCC R**A** (36)	573	544	1	β R**A** (36)+ opb HCC R**A** (39)	615	557	0	β R**A+** opb HCC R**A** (50)
	31	552	530	3	χ (R**ACD+** CCCN$_{13}$)	555	526	2	β R**DE** (11)	590	534	3	α R**A**+ β R**CD+** opb CC$_{39}$C$_{40}$ (31)
	30	543	521	3	α R**C+** opb (HCC RA+ CCN$_{13}$) (21)	549	521	3	β R**A+** opb HCC R**A** (13)	586	530	5	(α+ β) R**CD**+ ρCH2 R**C** (20)
	29	517	496	1	(α+β) R**DE+** ipb CCN$_{13}$ (28)+ α R**B**+ ipb (CN$_{26}$C+ CC=O) (20)	517	491	1	(α+β) R**D** (26)	551	499	1	(α+ β) R**CD** (29)
	28	504	484	1	χCCCN$_{13}$ (15)+ α R**B**+ ipb (CN$_{26}$C+ CC=O) (10)	513	486	1	χ (CCCC**+** CCCN$_{13}$) (12)+ χ CCN$_{13}$C (18)	543	492	2	ipb (CN$_{26}$C+C$_{16}$C$_{15}$C$_{23}$) (15)
	27	459	441	6	β R**BC+** (opb CC=O**+** CCN$_{13}$) (15)+ χ CCCC (48)	466	442	5	α R**B**+ opb NC=O (16)	500	452	8	χC$_{14}$C$_6$C$_8$C$_7$+ opb HCC R**A**
	26	454	436	3	α R**B**+ ipb (CN$_{26}$C+ CC=O) (26)	461	437	3	β R**A+** χ (CCCC+ CCCN$_{13}$) (11)	489	443	2	(α+ β) R**CD** (15)
	25	441	423	3	β R**D**+ ipb CN$_{26}$C (29)	449	426	5	χ CCCC (11)	473	428	3	β R**CD**+ opb C$_{23}$C$_{15}$N$_{39}$ (22)
	24	422	405	2	β R**ABC**+ ipb CN$_{26}$C+ opb CC=O) (27)	430	408	3	α R**B**+ opb NC=O (21)	455	412	3	β R**BCD** (34)
	23	386	371	2	α R**B**+ ipb (CN$_{26}$C+ CC=O) (13)	398	377	3	ipb C$_{23}$C$_{15}$C$_{39}$+ ipb CN$_{26}$C (42)	415	376	2	ipb CN$_{26}$C+ β **RD** (30)
	22	376	361	6	ipb CCN$_{13}$ (41)	384	364	5	ipb CCN$_{13}$ (42)	402	364	7	ipb CCN$_{13}$ (33)
	21	349	335	1	β R**CD** (13)	362	343	0	α R**C**+ opb C$_{15}$C$_{39}$C$_{40}$ (36)+ (α+β) R**BCDE** (10)	373	337	0	χCCCC (22)
	20	335	322	1	β R**BCD**+ ipb (CN$_{13}$C+ C$_{15}$C$_{39}$C$_{40}$) (32)	348	330	1	ipb (C$_{23}$C$_{15}$C$_{39}$+CN$_{26}$C) (22)	363	329	1	ipb C$_6$C$_7$C$_{28}$ (12)
	19	333	320	1	β R**CD**+ χ CCCC (24)	343	325	0	β R**BCDE** (28)	358	324	1	χ (CCCC+ CCCN$_{26}$) (26)
	18	330	317	1	χ CCCC (40)	332	315	1	χ CCCC (38)	354	321	1	χ (CCCN$_{26}$+ CCCN$_{13}$) (29)
	17	305	293	5	χ (CCCC+ CCCN$_{26}$) (31)	319	303	4	χ (CCCC+ CCCN$_{26}$) (41)+ χN$_{13}$CCC (13)	332	300	5	(α+β) R**BCE** (39)
	16	283	272	0	ipb C$_{15}$C$_{39}$C$_{40}$ (30)+ β R**CD** (14)	291	276	0	(α+β) R**BCDE** (22)	305	276	0	α R**CD**+ ipb C$_{15}$C$_{39}$C$_{40}$ (20)+ χ CCCC (14)
	15	261	251	3	opb HC$_{39}$C$_{40}$+ β R**BDE** (13)	264	250	4	ipb C$_{16}$C$_{15}$C$_{39}$ (29)	280	253	3	χCCCC
	14	245	235	1	ρC$_{40}$H3 (20)+ β R**CD** (10)	253	240	0	ρC$_{40}$H3 (49)+ ρC$_{49}$H3 (12)	262	237	1	ρC$_{40}$H3 (29)+ χ (CCCC+ CCCN$_{26}$) (12)
	13	236	227	0	χ CCCC (39)	242	230	0	χ CCCC (17)+ χ C$_{39}$CCC (16)	252	228	0	χCCCC (42)
	12	207	199	1	ρC$_{40}$H3 (13)	212	201	0	ρC$_{49}$H3 (42)	221	200	1	ρC$_{40}$H3 (22)
	11	172	165	5	ipb CN$_{13}$C (45)	211	200	1	ρC$_{49}$H3 (46)	185	167	6	ipb CN$_{13}$C (46)
	10	170	163	1	χ (CCCC+ CCCN$_{26}$) (34)	182	172	4	ipb CN$_{13}$C (40)	178	161	2	χCCCC (22)
	9	151	145	0	χ (CCCC+ CCCN$_{26}$) (50)	171	162	2	χ (CN$_{26}$CC+ CCCN$_{26}$) (48)	156	141	0	χ CCCN$_{26}$ (45)+ χCCCC (14)
	8	134	129	1	ρC$_{49}$H3+ χ CCCC (24)+ χ (CN$_{13}$CC+ CCCN$_{13}$) (10)	154	146	0	χ (CCCC+ CCCN$_{26}$) (17)+ χ N$_{13}$CCC (11)	151	137	0	ρC$_{49}$H3+χ CCCO (86)
	7	126	121	0	ρC$_{49}$H3 (88)	143	136	1	χ (CCCC+ CCC$_{39}$C$_{40}$) (57)+ ipb CN$_{13}$C (12)	143	129	1	χCCCC (25)+ opb HCC R**A** (16)
	6	116	111	0	ρ(C$_{39}$H2+ C$_{49}$H3) (51)	134	127	1	χ CCCC (46)	128	116	0	χ CCCC+ ρ(C$_{39}$H2+ C$_{40}$H2) (58)+ χCN$_{13}$CC **(10**
	5	94	90	4	χ CN$_{13}$CC (68)	100	95	4	χ (CN$_{13}$CC+ CCCN$_{26}$) (66)	98	89	3	χ (CCCC+N$_{13}$CCC) (51)
	4	86	83	1	χ CCCC (48)+ χ (CN$_{13}$CC+ CCCN$_{13}$) (26)	93	88	1	χ(CCCC+ N$_{13}$CCC) (32)	94	86	4	χ CN$_{13}$CC (56)+ χCCCC (10)
	3	74	71	3	χ (CN$_{13}$CC+ CCCN$_{13}$) (46)+ χ (CN$_{26}$CC+ CCCN$_{26}$) (13)	74	71	2	χ CCN$_{13}$C (39)+ χCCCC (16)	74	67	2	χ (CCN$_{26}$C+ CCN$_{13}$C) (26)
	2	48	46	2	χCCCC (40)	56	53	3	χCCCC (12)	55	50	3	χCCCC (29)
	1	34	33	1	χ (CN$_{26}$CC+ CCCN$_{26}$) (37)	31	30	0	χ (CN$_{26}$CC+ CCCN$_{26}$) (53)+ χCCCC (16)	38	35	0	χ (CCCN$_{13}$C+ CCCN$_{26}$) (53)

^{13}C and ^{1}H NMR spectral analysis

Table S7a. The observed and calculated NMR isotropic chemical shifts (with respect to TMS, all values in ppm) for the demethoxyaspidospermine molecule at B3LYP/6-311++G(d,p)

		B3LYP/6-311++G(d,p)									
		Gas					Chloroform				
^{13}C	Exp.	**CI**	**CII**	**CIII**	**CIV**	**CV**	**CI**	**CII**	**CIII**	**CIV**	**CV**
1C	142.0	149.2	149.3	150.1	150.2	148.5	149.4	149.6	150.3	150.4	148.8
2C	119.1	125.0	125.1	125.2	125.1	119.6	124.5	124.7	124.6	124.6	121.4
3C	128.8	134.5	134.5	134.6	134.5	133.4	134.4	134.4	134.5	134.4	134.0
4C	125.1	129.1	129.0	129.3	129.4	128.3	130.1	130.0	130.4	130.4	129.6
5C	123.4	127.4	127.8	126.8	127.5	129.7	129.1	129.5	128.6	129.4	130.5
6C	138.2	147.7	147.6	144.5	144.7	151.9	150.2	150.1	147.2	147.5	152.9
7C	53.5	59.8	61.4	60.4	60.4	57.7	60.1	61.7	60.8	60.9	58.4
8C	71.0	79.9	78.3	71.3	71.4	79.3	80.4	78.9	72.2	72.5	79.9
14C	67.0	76.8	76.6	63.5	70.4	77.3	77.3	77.2	64.1	71.2	77.5
15C	36.6	43.6	43.5	43.7	45.1	43.4	44.0	43.9	44.1	45.5	43.9
16C	30.5	33.1	39.7	40.6	32.7	32.6	33.3	39.8	40.9	33.0	33.0
17C	23.7	28.4	31.8	29.4	29.2	26.4	28.4	31.9	29.5	29.2	27.1
19C	52.3	55.9	53.3	56.4	56.9	56.0	56.3	53.9	57.0	57.4	56.5
22C	21.2	22.8	22.9	26.2	24.2	22.8	23.0	23.1	26.5	24.4	23.0
23C	33.9	34.3	42.2	40.6	37.6	34.3	34.6	42.6	40.9	37.8	34.7
27C	53.1	59.2	56.9	55.9	55.7	59.2	59.5	57.3	56.5	56.2	59.6
28C	39.1	51.4	51.0	44.6	44.9	51.4	51.5	51.0	45.0	45.2	51.5
39C	26.1	30.2	42.3	35.1	29.8	30.3	30.7	42.4	35.6	30.2	30.7
40C	7.2	9.4	13.2	11.3	9.4	9.4	9.7	13.5	11.5	9.6	9.6
47C	169.2	171.9	171.9	172.2	172.3	172.0	175.9	175.8	176.2	176.2	175.7
49C	23.0	25.5	25.6	25.5	25.5	26.3	26.4	26.4	26.4	26.4	26.9
^{1}H											
9H	7.15	7.37	7.40	7.36	7.29	7.47	7.54	7.57	7.54	7.47	7.59
10H	6.97	7.19	7.20	7.19	7.18	7.15	7.31	7.32	7.31	7.30	7.29
11H	7.15	7.44	7.44	7.42	7.42	7.36	7.51	7.50	7.49	7.48	7.48
12H	8.51	8.67	8.68	8.64	8.64	7.08	8.47	8.47	8.43	8.43	7.25
18H	2.24	2.50	2.34	3.71	3.31	2.43	2.54	2.37	3.75	3.33	2.50
20H	3.03	3.22	3.14	3.16	3.19	3.23	3.23	3.17	3.16	3.18	3.24
21H	2.23	2.38	2.30	2.76	2.76	2.37	2.41	2.29	2.75	2.76	2.40
24H	1.40	1.54	1.13	1.56	1.63	1.52	1.58	1.18	1.58	1.66	1.57
25H	1.08	1.26	1.87	1.21	0.99	1.27	1.22	1.82	1.21	0.99	1.21
29H	2.19	2.21	2.23	2.52	2.50	2.20	2.24	2.23	2.54	2.54	2.24
30H	2.99	3.05	2.84	3.40	3.39	3.05	3.08	2.89	3.41	3.40	3.09
31H	1.93	1.81	1.81	1.74	1.75	1.75	1.78	1.76	1.77	1.77	1.77
32H	2.02	2.11	2.07	2.01	2.01	2.20	2.19	2.16	2.05	2.05	2.20
33H	1.60	1.73	1.70	1.92	1.88	1.70	1.76	1.73	1.93	1.89	1.74
34H	1.51	1.56	1.77	1.59	1.50	1.55	1.59	1.79	1.62	1.53	1.57
35H	1.54	1.66	1.72	1.70	1.69	2.14	1.75	1.80	1.79	1.77	1.98
36H	1.17	1.28	1.56	1.48	1.31	0.96	1.26	1.49	1.43	1.27	1.03
37H	1.40	1.34	1.39	1.95	1.62	1.41	1.33	1.43	1.92	1.59	1.38
38H	1.54	1.57	1.65	1.13	1.48	1.50	1.61	1.69	1.17	1.52	1.54
41H	0.86	1.23	1.04	1.59	1.07	1.18	1.28	1.08	1.51	1.13	1.22
42H	0.80	1.17	1.82	0.77	1.41	1.07	1.08	1.85	0.81	1.30	1.02
43H	0.57	0.69	0.73	0.86	0.69	0.64	0.67	0.72	0.84	0.66	0.63
44H	0.57	0.74	0.71	1.18	0.76	0.74	0.76	0.72	1.20	0.78	0.76
45H	0.57	0.55	0.55	1.00	0.55	0.57	0.56	0.44	1.03	0.56	0.55
46H	3.80	3.75	3.65	3.79	3.79	4.54	3.91	3.81	3.94	3.94	4.52
50H	1.93	1.98	1.98	1.99	1.99	2.17	1.93	1.92	1.93	1.93	2.11
51H	2.19	2.17	2.13	2.17	2.18	2.32	2.33	2.29	2.33	2.33	2.42
52H	2.19	2.28	2.29	2.29	2.29	2.26	2.45	2.46	2.47	2.47	2.45

Table S7b. The observed and calculated ^{1}H and ^{13}C NMR isotropic chemical shifts (concerning TMS, all values in ppm) for the demethoxyaspidospermine molecule at MO62X/6-311++G(d,p) level of the theory

		MO62X/6-311++G(d,p) basis									
		Gas					Chloroform				
^{13}C	Exp.	**CI**	**CII**	**CIII**	**CIV**	**CV**	**CI**	**CII**	**CIII**	**CIV**	**CV**
1C	142.0	162.9	163.0	163.8	163.9	162.1	163.1	163.3	164.0	164.1	162.4
2C	119.1	139.4	139.4	139.6	139.4	133.3	139.0	139.0	139.2	139.0	135.5
3C	128.8	150.5	150.6	150.6	150.5	149.0	150.6	150.7	150.7	150.5	149.9
4C	125.1	144.4	144.0	144.4	144.4	143.4	145.7	145.4	145.8	145.7	145.2
5C	123.4	142.4	143.3	141.9	143.0	145.2	144.4	145.2	143.9	145.1	146.2
6C	138.2	163.1	163.5	159.6	159.8	167.7	166.1	166.2	162.7	162.8	168.9
7C	53.5	58.8	61.0	59.5	59.8	56.4	59.1	61.2	60.1	60.5	57.2
8C	71.0	80.2	78.4	71.2	71.3	80.3	81.1	79.0	72.2	72.5	80.9
14C	67.0	75.9	78.7	63.7	70.6	77.6	77.1	79.3	64.2	71.4	78.2
15C	36.6	40.4	40.2	40.4	42.2	40.2	40.7	40.5	40.8	42.6	40.5
16C	30.5	32.5	39.3	39.9	32.1	32.1	32.8	39.3	40.4	32.5	32.4
17C	23.7	27.8	31.3	28.2	28.2	25.4	27.9	31.5	28.4	28.4	26.1
19C	52.3	56.2	53.4	56.4	56.6	56.2	56.6	53.9	57.0	57.2	56.7
22C	21.2	21.2	20.8	24.8	22.5	21.2	21.4	21.0	25.1	22.7	21.4
23C	33.9	34.7	41.1	40.2	37.8	34.3	34.8	41.6	40.5	38.0	34.7
27C	53.1	60.8	57.5	55.2	54.8	60.7	61.1	58.0	55.8	55.3	61.2
28C	39.1	51.2	51.4	45.2	45.6	51.7	51.6	51.7	45.6	45.9	52.1
39C	26.1	29.4	42.3	33.7	28.7	29.5	30.0	42.6	34.3	29.1	30.0
40C	7.2	8.8	12.8	10.8	9.0	8.8	9.1	13.2	11.0	9.2	9.0
47C	169.2	184.1	184.2	184.5	184.5	184.2	188.6	188.6	188.9	188.9	188.5
49C	23.0	27.2	27.3	27.2	27.2	28.3	28.0	28.1	28.1	28.1	28.9
^{1}H											
9H	7.15	8.03	8.09	8.06	7.96	8.16	8.23	8.27	8.25	8.15	8.29
10H	6.97	7.80	7.81	7.80	7.79	7.77	7.94	7.94	7.94	7.93	7.93
11H	7.15	8.06	8.07	8.05	8.03	7.98	8.15	8.15	8.13	8.11	8.11
12H	8.51	9.20	9.22	9.18	9.18	7.70	9.00	9.02	8.96	8.96	7.89
18H	2.24	2.55	2.07	3.63	3.22	2.42	2.56	2.12	3.67	3.26	2.47
20H	3.03	3.22	3.14	3.11	3.14	3.22	3.23	3.18	3.12	3.14	3.23
21H	2.23	2.31	2.10	2.70	2.71	2.28	2.35	2.12	2.70	2.72	2.32
24H	1.40	1.46	1.08	1.48	1.48	1.42	1.49	1.14	1.51	1.51	1.46
25H	1.08	1.11	1.82	1.16	0.95	1.16	1.11	1.75	1.14	0.93	1.11
29H	2.19	2.14	2.08	2.47	2.45	2.10	2.15	2.09	2.51	2.50	2.14
30H	2.99	3.11	2.78	3.35	3.33	3.09	3.13	2.84	3.36	3.34	3.12
31H	1.93	1.71	1.72	1.71	1.71	1.68	1.68	1.67	1.73	1.74	1.70
32H	2.02	2.12	2.03	2.00	2.01	2.17	2.17	2.10	2.02	2.04	2.16
33H	1.60	1.71	1.64	1.91	1.83	1.66	1.74	1.67	1.93	1.85	1.70
34H	1.51	1.42	1.75	1.52	1.44	1.43	1.47	1.77	1.55	1.47	1.47
35H	1.54	1.58	1.61	1.61	1.60	2.16	1.69	1.72	1.72	1.69	1.98
36H	1.17	1.22	1.54	1.41	1.25	0.85	1.18	1.45	1.35	1.20	0.92
37H	1.40	1.39	1.32	1.93	1.60	1.41	1.33	1.36	1.89	1.56	1.37
38H	1.54	1.47	1.60	1.10	1.43	1.42	1.53	1.65	1.15	1.47	1.46
41H	0.86	1.12	0.96	1.58	1.00	1.08	1.19	1.00	1.47	1.06	1.13
42H	0.80	1.15	1.69	0.67	1.42	1.00	1.02	1.72	0.71	1.29	0.91
43H	0.57	0.63	0.70	0.87	0.64	0.57	0.62	0.70	0.85	0.62	0.57
44H	0.57	0.65	0.68	1.23	0.67	0.66	0.68	0.69	1.26	0.70	0.68
45H	0.57	0.49	0.56	1.02	0.52	0.52	0.50	0.42	1.05	0.51	0.50
46H	3.80	3.83	3.71	3.91	3.90	4.50	3.98	3.88	4.06	4.04	4.50
50H	1.93	2.07	2.07	2.08	2.09	2.28	2.03	2.03	2.05	2.05	2.23
51H	2.19	2.16	2.14	2.19	2.19	2.38	2.33	2.30	2.34	2.34	2.48
52H	2.19	2.27	2.29	2.28	2.28	2.28	2.45	2.47	2.46	2.46	2.47

Table S7c. The observed and calculated ^{1}H and ^{13}C NMR isotropic chemical shifts (concerning TMS, all values in ppm) for the demethoxyaspidospermine molecule at HF/6-311++G(d,p) level of the theory

		HF/6-311++G(d,p) basis									
		Gas					Chlo				
^{13}C	Exp.	**CI**	**CII**	**CIII**	**CIV**	**CV**	**CI**	**CII**	**CIII**	**CIV**	**CV**
1C	142.0	149.9	150.1	150.8	150.8	150.1	150.0	150.1	150.8	150.8	149.7
2C	119.1	126.0	125.9	125.9	125.9	120.0	125.2	125.2	125.2	125.2	121.7
3C	128.8	135.9	136.0	136.2	136.1	135.1	135.5	135.6	135.8	135.7	135.3
4C	125.1	129.2	129.0	129.1	129.2	128.5	130.0	129.8	129.9	129.9	129.7
5C	123.4	129.4	129.9	129.3	130.0	132.3	131.0	131.5	130.9	131.6	132.7
6C	138.2	146.3	146.5	142.9	143.1	150.3	148.7	148.8	145.3	145.6	151.1
7C	53.5	47.9	49.4	48.9	49.0	46.3	48.1	49.5	49.1	49.2	46.7
8C	71.0	66.9	65.5	59.1	59.3	67.4	67.4	66.0	59.8	60.0	67.7
14C	67.0	62.2	63.1	52.8	58.7	63.1	62.6	63.3	53.2	59.0	63.1
15C	36.6	33.3	33.3	33.6	34.6	33.3	33.5	33.4	33.8	34.8	33.5
16C	30.5	28.3	33.9	34.9	27.8	28.0	28.4	33.7	35.0	27.9	28.2
17C	23.7	24.8	27.1	25.3	25.2	22.9	24.7	27.1	25.2	25.1	23.3
19C	52.3	47.3	44.7	47.8	48.0	47.2	47.5	44.9	48.0	48.4	47.5
22C	21.2	19.3	19.1	21.9	20.4	19.3	19.3	19.1	21.9	20.4	19.3
23C	33.9	29.8	36.5	34.4	32.1	29.6	29.9	36.7	34.5	32.1	29.8
27C	53.1	50.8	48.6	47.0	46.8	50.8	50.9	48.8	47.2	47.0	51.0
28C	39.1	44.0	44.2	38.9	39.1	44.2	44.0	44.1	39.0	39.3	44.1
39C	26.1	26.0	36.6	29.9	25.5	26.2	26.3	36.6	30.2	25.7	26.3
40C	7.2	10.0	12.4	11.3	10.0	10.0	10.0	12.5	11.3	10.0	10.0
47C	169.2	173.6	173.5	173.8	173.8	174.0	177.8	177.8	178.0	178.0	178.2
49C	23.0	24.9	25.0	24.9	25.0	25.5	25.4	25.5	25.5	25.4	25.8
^{1}H											
9H	7.15	7.49	7.50	7.50	7.46	7.62	7.68	7.68	7.68	7.65	7.74
10H	6.97	7.32	7.32	7.32	7.31	7.30	7.44	7.44	7.43	7.42	7.44
11H	7.15	7.62	7.63	7.61	7.60	7.55	7.68	7.68	7.67	7.66	7.66
12H	8.51	8.63	8.63	8.61	8.61	7.15	8.40	8.40	8.37	8.37	7.34
18H	2.24	2.09	1.88	2.99	2.66	1.97	2.12	1.91	3.03	2.70	2.04
20H	3.03	2.83	2.74	2.74	2.75	2.83	2.82	2.76	2.72	2.73	2.82
21H	2.23	2.10	2.00	2.39	2.41	2.08	2.12	2.01	2.39	2.41	2.10
24H	1.40	1.29	0.94	1.27	1.30	1.24	1.30	0.96	1.27	1.30	1.27
25H	1.08	0.97	1.53	0.97	0.80	1.02	0.93	1.45	0.95	0.77	0.95
29H	2.19	1.93	1.92	2.20	2.19	1.89	1.95	1.93	2.22	2.22	1.93
30H	2.99	2.75	2.52	2.90	2.90	2.74	2.76	2.55	2.90	2.89	2.75
31H	1.93	1.50	1.48	1.48	1.49	1.43	1.44	1.42	1.49	1.49	1.43
32H	2.02	1.82	1.76	1.73	1.72	1.93	1.88	1.82	1.73	1.74	1.91
33H	1.60	1.47	1.43	1.60	1.58	1.44	1.49	1.44	1.60	1.59	1.46
34H	1.51	1.31	1.57	1.36	1.31	1.32	1.33	1.56	1.37	1.31	1.33
35H	1.54	1.32	1.32	1.36	1.35	1.85	1.41	1.43	1.46	1.45	1.67
36H	1.17	1.07	1.25	1.22	1.09	0.75	1.02	1.17	1.14	1.02	0.79
37H	1.40	1.11	1.08	1.55	1.30	1.19	1.08	1.11	1.50	1.25	1.13
38H	1.54	1.27	1.34	0.96	1.21	1.23	1.29	1.37	0.99	1.23	1.24
41H	0.86	0.95	0.81	1.15	0.84	0.90	0.98	0.82	1.03	0.88	0.94
42H	0.80	0.84	1.43	0.54	1.02	0.69	0.71	1.45	0.55	0.88	0.61
43H	0.57	0.67	0.68	0.84	0.66	0.61	0.62	0.65	0.78	0.62	0.58
44H	0.57	0.69	0.59	1.05	0.71	0.69	0.70	0.59	1.06	0.71	0.69
45H	0.57	0.51	0.39	0.96	0.52	0.54	0.50	0.24	0.96	0.51	0.50
46H	3.80	3.29	3.22	3.34	3.34	4.12	3.44	3.39	3.48	3.48	4.06
50H	1.93	2.08	2.08	2.09	2.10	2.20	2.00	2.00	2.02	2.02	2.13
51H	2.19	1.97	1.95	1.99	2.00	2.18	2.14	2.12	2.15	2.15	2.28
52H	2.19	2.12	2.14	2.13	2.13	2.25	2.31	2.32	2.31	2.31	2.43

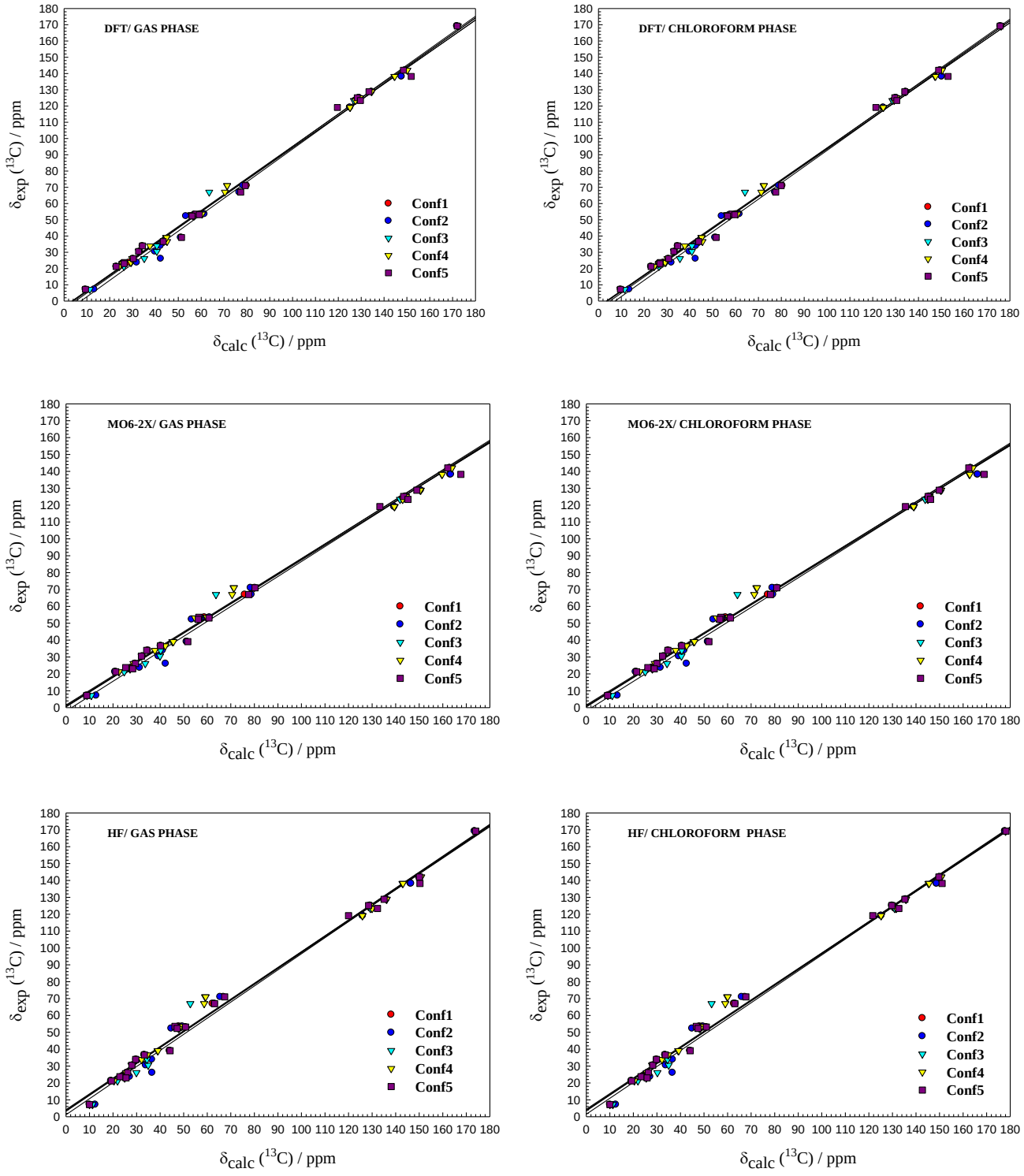


Figure S3a. The comparison of the experimental and calculated *13C* NMR isotropic chemical shifts (with respect to TMS) for the most stable conformers of the demethoxyaspidospermine

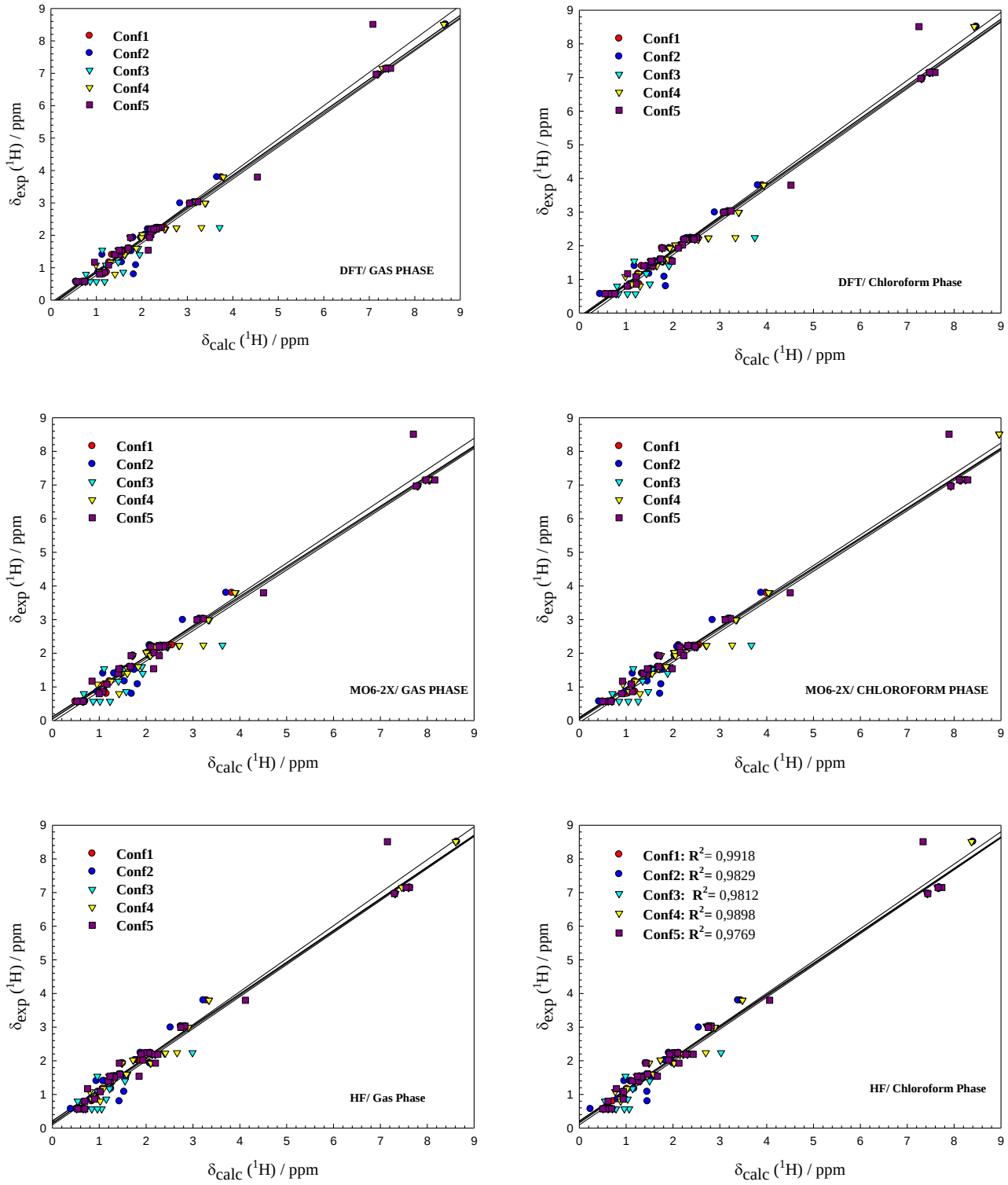


Figure S3b. The comparison of the experimental and calculated ^{1}H isotropic chemical shifts (with respect to TMS) for the most stable conformers of the demethoxyaspidospermine

Table S8. The correlation equations between observed and calculated *^{1}H* and *^{13}C* NMR shifts of the most stable conformers of the demethoxyaspidospermine compound.

Method/ phase	Conformer	*^{13}C*	*^{1}H*
B3LYP/ gas	**CI**	δ_{exp}= 0.9834 δ_{calc} -4.0318 (R^2= 0.9966, S= 3.0059)	δ_{exp}= 0.9853 δ_{calc} -0.0796 (R^2= 0.9971, S= 0.1193)
	CII	δ_{exp}= 1.0099 δ_{calc} -7.4294 (R^2= 0.9949, S= 3.6632)	δ_{exp}= 0.9888 δ_{calc} -0.1132 (R^2= 0.9858, S= 0.2656)
	CII	δ_{exp}= 1.0015 δ_{calc} -5.0253 (R^2= 0.9964, S= 3.0848)	δ_{exp}= 0.9896 δ_{calc} -0.2196 (R^2= 0.9757, S= 0.3477)
	CIV	δ_{exp}= 0.9863 δ_{calc} -3.3951 (R^2= 0.9984, S= 2.0264)	δ_{exp}= 0.9844 δ_{calc} -0.1411 (R^2= 0.9874, S= 0.2506)
	CV	δ_{exp}= 0.9799 δ_{calc} -3.5189 (R^2= 0.9951, S= 3.5845)	δ_{exp}= 1.0288 δ_{calc} -0.1723 (R^2= 0.9742, S= 0.3580)
B3LYP/ chloroform	**CI**	δ_{exp}= 0.9730 δ_{calc} -3.8782 (R^2= 0.9968, S= 2.8907)	δ_{exp}= 0.9813 δ_{calc} -0.1012 (R^2= 0.9961, S= 0.1365)
	CII	δ_{exp}= 0.9986 δ_{calc} -7.2149 (R^2= 0.9949, S= 3.5674)	δ_{exp}= 0.9848 δ_{calc} -0.1317 (R^2= 0.9853, S= 0.2652)
	CII	δ_{exp}= 0.9910 δ_{calc} -4.9719 (R^2= 0.9965, S= 2.9653)	δ_{exp}= 0.9871 δ_{calc} -0.2410 (R^2= 0.9758, S= 0.3406)
	CIV	δ_{exp}= 0.9759 δ_{calc} -3.3271 (R^2= 0.9986, S= 1.8499)	δ_{exp}= 0.9814 δ_{calc} -0.1591 (R^2= 0.9872, S= 0.2476)
	CV	δ_{exp}= 0.9707 δ_{calc} -3.5401 (R^2= 0.9956, S= 3.3185)	δ_{exp}= 1.0103 δ_{calc} -0.1576 (R^2= 0.9768, S= 0.3337)
HF/ gas	**CI**	δ_{exp}= 0.9379 δ_{calc} +3.4128 (R^2= 0.9953, S= 3.4991)	δ_{exp}= 0.9435 δ_{calc} +0.2150 (R^2= 0.9926, S= 0.1913)
	CII	δ_{exp}= 0.9540 δ_{calc} +1.1462 (R^2= 0.9911, S= 4.8365)	δ_{exp}= 0.9432 δ_{calc} +0.2116 (R^2= 0.9828, S= 0.2925)
	CII	δ_{exp}= 0.9449 δ_{calc} +3.2298 (R^2= 0.9883, S= 5.5411)	δ_{exp}= 0.9521 δ_{calc} +0.0972 (R^2= 0.9812, S= 0.3055)
	CIV	δ_{exp}= 0.9364 δ_{calc} +4.2108 (R^2= 0.9927, S= 4.3888)	δ_{exp}= 0.9475 δ_{calc} +0.1594 (R^2= 0.9904, S= 0.2182)
	CV	δ_{exp}= 0.9335 δ_{calc} +3.8056 (R^2= 0.9942, S= 3.8861)	δ_{exp}= 0.9799 δ_{calc} +0.1357 (R^2= 0.9742, S= 0.3582)
HF/ chloroform	**CI**	δ_{exp}= 0.9276 δ_{calc} +3.6938 (R^2= 0.9955, S= 3.4321)	δ_{exp}= 0.9385 δ_{calc} +0.2098 (R^2= 0.9918, S= 0.2022)
	CII	δ_{exp}= 0.9433 δ_{calc} +1.4903 (R^2= 0.9913, S= 4.7793)	δ_{exp}= 0.9380 δ_{calc} +0.2069 (R^2= 0.9830, S= 0.2907)
	CII	δ_{exp}= 0.9350 δ_{calc} +3.4486 (R^2= 0.9882, S= 5.4249)	δ_{exp}= 0.9475 δ_{calc} +0.0952 (R^2= 0.9805, S= 0.3058)
	CIV	δ_{exp}= 0.9264 δ_{calc} +4.4399 (R^2= 0.9927, S= 4.2544)	δ_{exp}= 0.9422 δ_{calc} +0.1593 (R^2= 0.9894, S= 0.2253)
	CV	δ_{exp}= 0.9245 δ_{calc} +3.9765 (R^2= 0.9944, S= 3.7389)	δ_{exp}= 0.9599 δ_{calc} +0.1674 (R^2= 0.9761, S= 0.3386)
M06-2X/ gas	**CI**	δ_{exp}= 0.8685 δ_{calc} +0.6982 (R^2= 0.9965, S= 3.0502)	δ_{exp}= 0.8933 δ_{calc} +0.1162 (R^2= 0.9956, S= 0.1486)
	CII	δ_{exp}= 0.8866 δ_{calc} - 2.0940 (R^2= 0.9933, S= 4.2064)	δ_{exp}= 0.8951 δ_{calc} +0.1020 (R^2= 0.9836, S= 0.2860)
	CII	δ_{exp}= 0.8782 δ_{calc} +0.3810 (R^2= 0.9929, S= 4.3119)	δ_{exp}= 0.9023 δ_{calc} -0.0375 (R^2= 0.9781, S= 0.3299)
	CIV	δ_{exp}= 0.8683 δ_{calc} +1.5374 (R^2= 0.9958, S= 3.3326)	δ_{exp}= 0.8971 δ_{calc} +0.0471 (R^2= 0.9897, S= 0.2262)
	CV	δ_{exp}= 0.8657 δ_{calc} +1.0923 (R^2= 0.9949, S= 3.6476)	δ_{exp}= 0.9268 δ_{calc} +0.0466 (R^2= 0.9766, S= 0.3410)
M06-2X/ chloroform	**CI**	δ_{exp}= 0.8590 δ_{calc} +0.7635 (R^2= 0.9970, S= 2.7957)	δ_{exp}= 0.8881 δ_{calc} +0.1008 (R^2= 0.9945, S= 0.1656)
	CII	δ_{exp}= 0.8769 δ_{calc} - 1.9631 (R^2= 0.9939, S= 4.0120)	δ_{exp}= 0.8904 δ_{calc} +0.0847 (R^2= 0.9837, S= 0.2845)
	CII	δ_{exp}= 0.8693 δ_{calc} +3.3643 (R^2= 0.9936, S= 4.0928)	δ_{exp}= 0.8989 δ_{calc} - 0.0559 (R^2= 0.9784, S= 0.3280)
	CIV	δ_{exp}= 0.8593 δ_{calc} +1.5363 (R^2= 0.9966, S= 2.9858)	δ_{exp}= 0.8928 δ_{calc} +0.0324 (R^2= 0.9894, S= 0.2293)
	CV	δ_{exp}= 0.8568 δ_{calc} +1.0661 (R^2= 0.9958, S= 3.3210)	δ_{exp}= 0.9093 δ_{calc} +0.0620 (R^2= 0.9797, S= 0.3179)

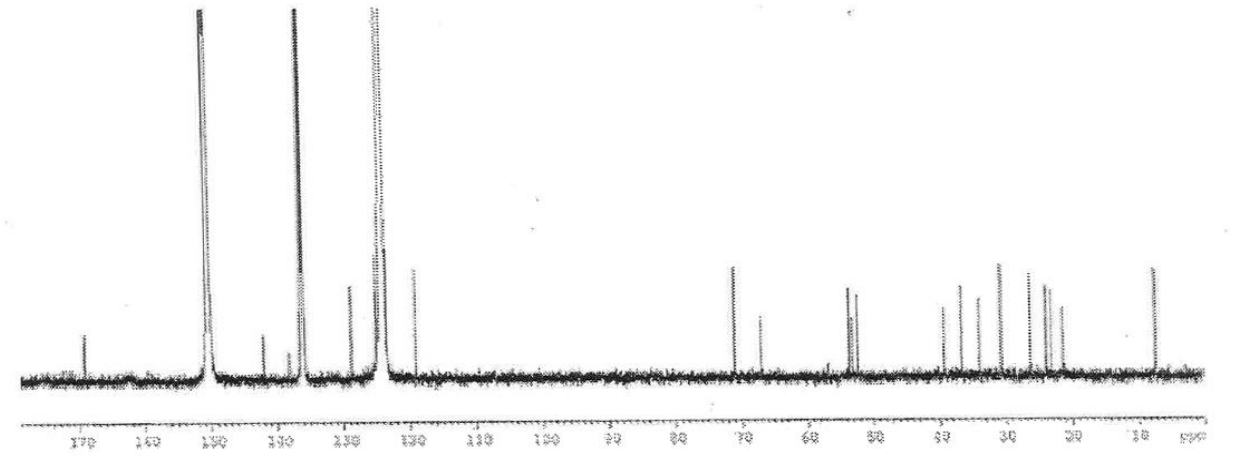


Figure S4a. The recorded *^{13}C NMR* spectrum of the demethoxyaspidospermine

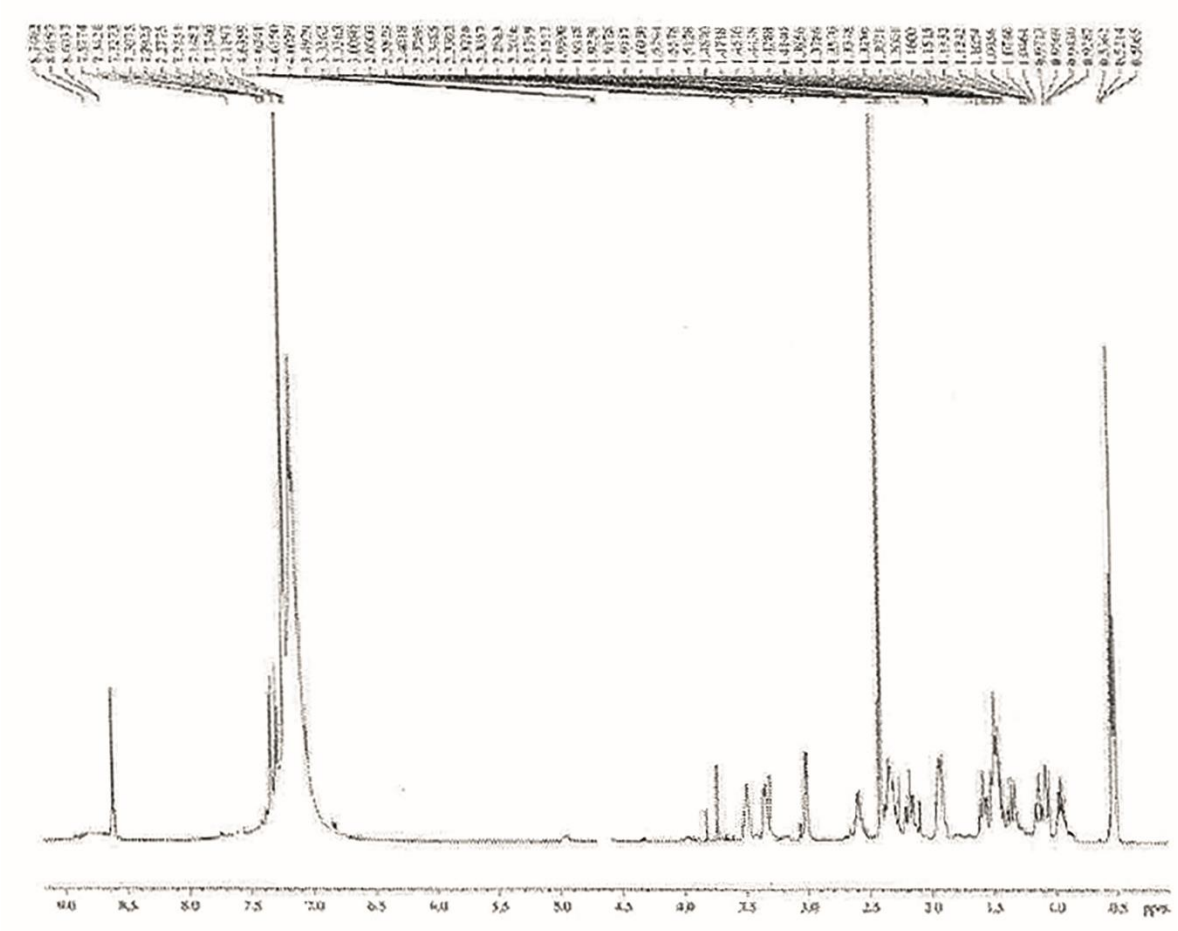


Figure S4b. The recorded *^{1}H NMR* spectrum of the demethoxyaspidospermine compound